



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2021 – 12:49 PM EDT

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

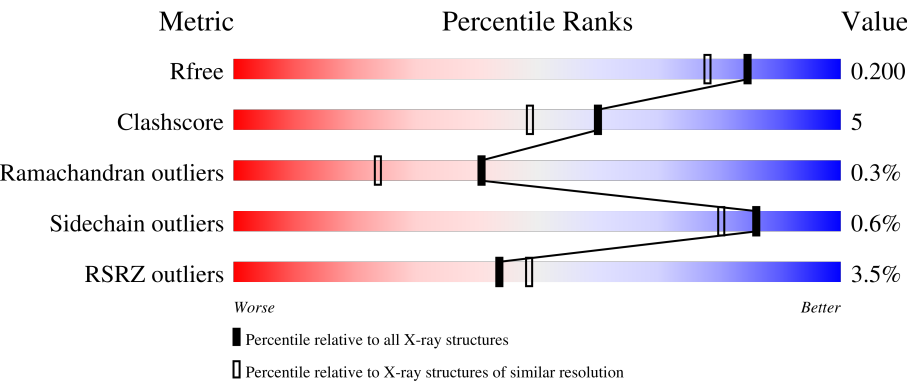
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.19  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.19

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div><div>3%</div><div><div></div><div>89%</div><div>9%</div><div>.</div></div></div>
1	B	1025	<div><div>4%</div><div><div></div><div>90%</div><div>8%</div><div>..</div></div></div>
1	C	1025	<div><div>3%</div><div><div></div><div>88%</div><div>9%</div><div>.</div></div></div>
1	D	1025	<div><div>4%</div><div><div></div><div>90%</div><div>9%</div><div>.</div></div></div>

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

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

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

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 35847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

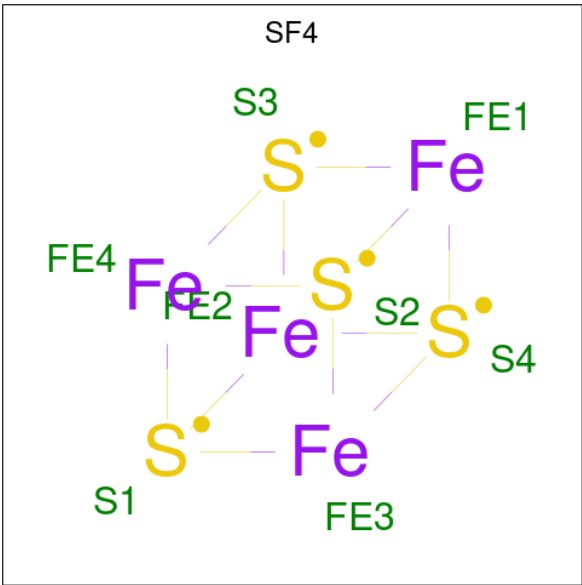
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	42	4	0
			7705	4886	1306	1459	54			
1	B	1011	Total	C	N	O	S	34	3	0
			7734	4905	1309	1466	54			
1	C	1007	Total	C	N	O	S	0	2	0
			7671	4869	1297	1452	53			
1	D	1017	Total	C	N	O	S	43	1	0
			7740	4910	1313	1462	55			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).





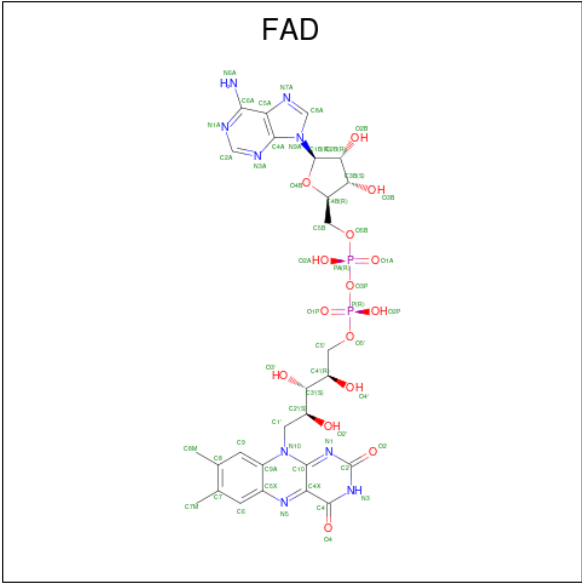
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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

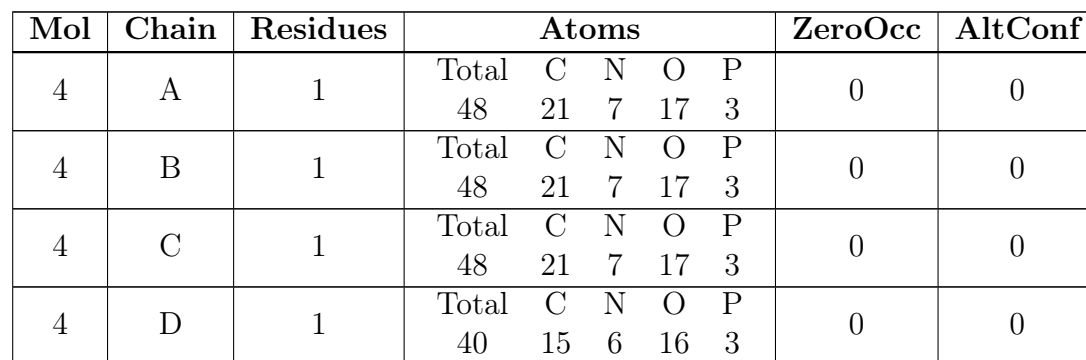
Continued on next page...

Continued from previous page...

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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

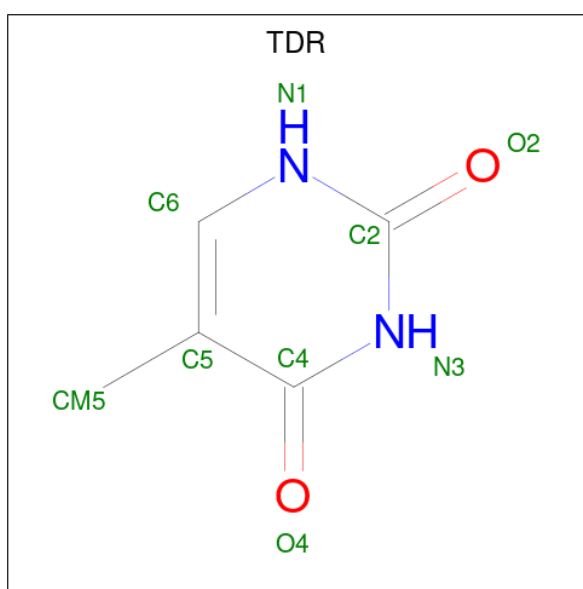




- 
- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms, N1 and N5, and two carbonyl groups, C2=O2 and C4=O4). The ring is substituted with a ribitol chain at the C10 position (labeled C1' in the diagram). The ribitol chain is a five-carbon chain (C1' to C5') with hydroxyl groups at C1' (labeled OH, O2'), C2' (labeled OH, O3'), C3' (labeled OH, O4'), and C4' (labeled OH, O5'). The C5' carbon is attached to a phosphate group (O1P, O2P, O3P, O4P, O5P). The ribitol chain is shown in a specific conformation with wedged and dashed bonds indicating stereochemistry.

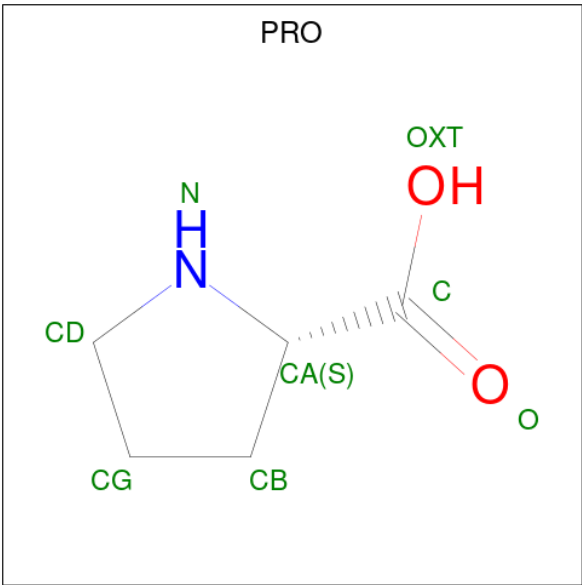
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



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

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



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

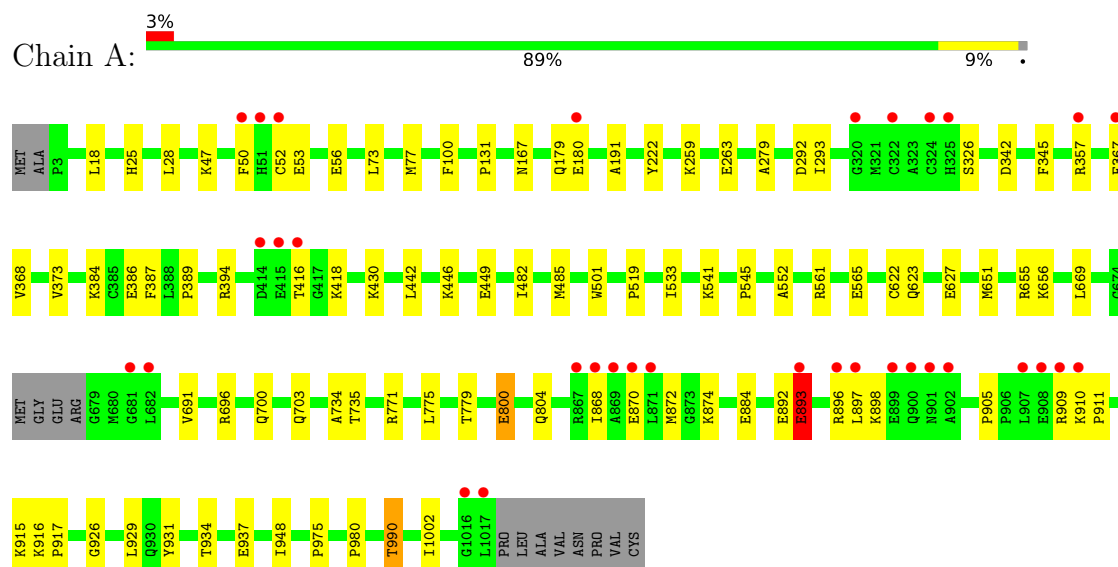
- Molecule 8 is water.

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

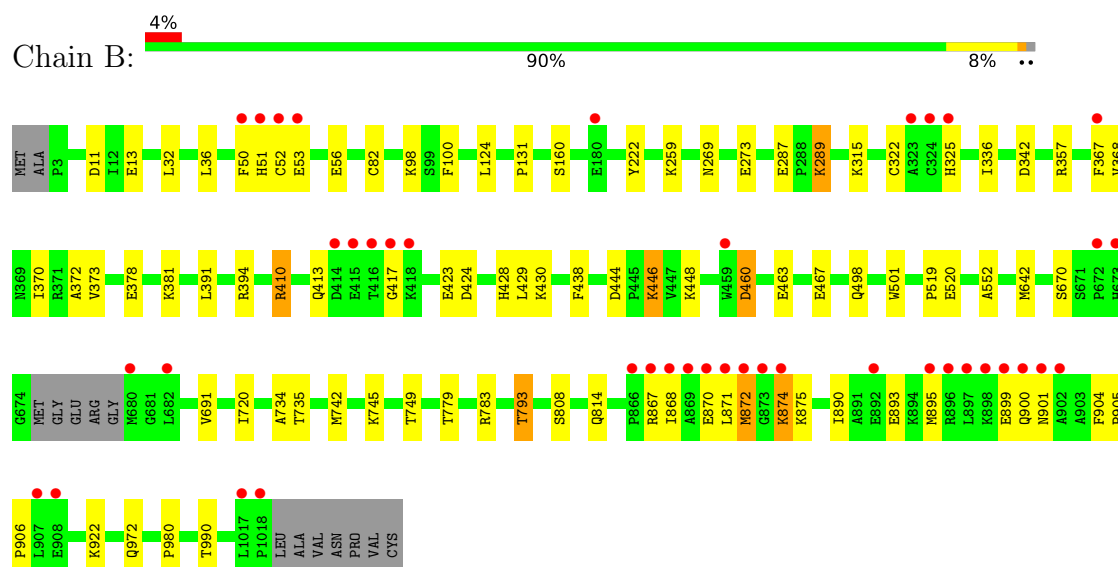
### 3 Residue-property plots

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.

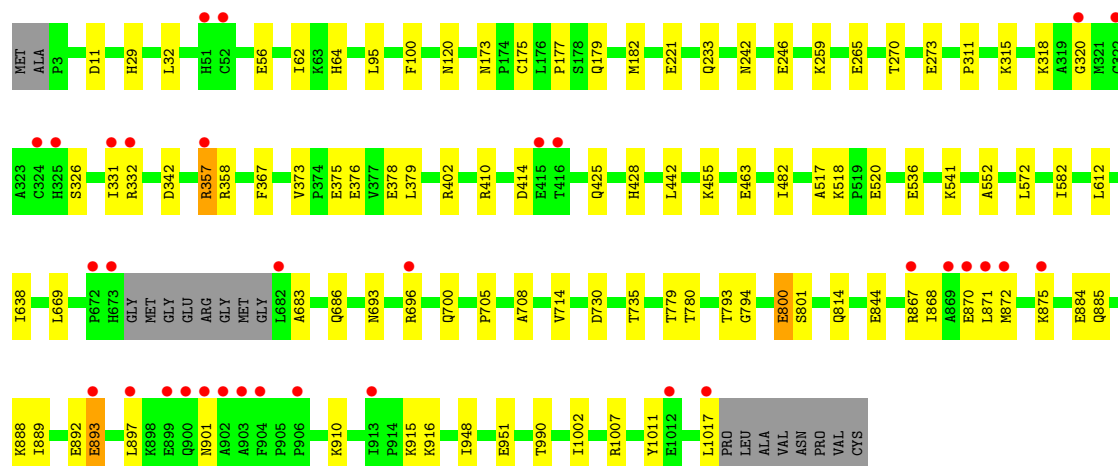
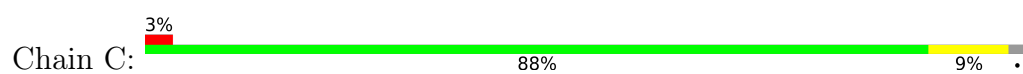
- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



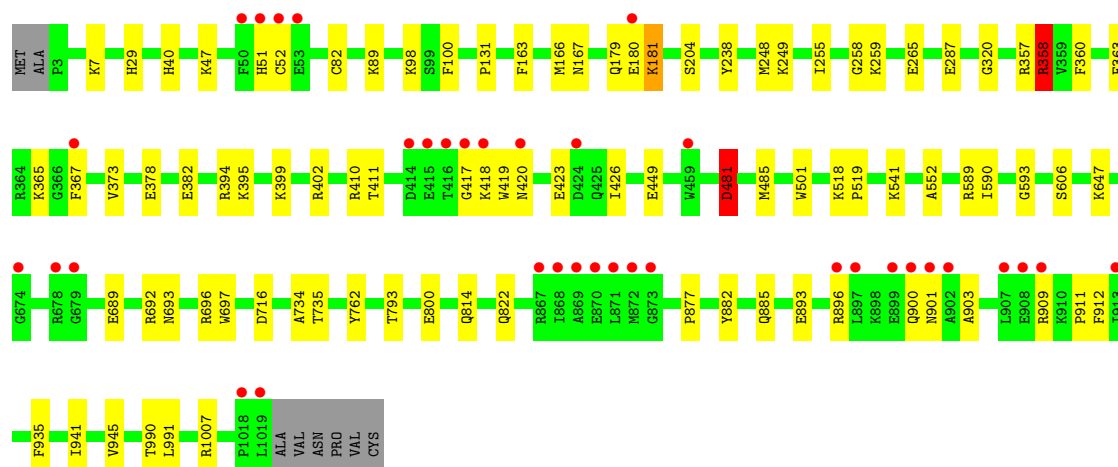
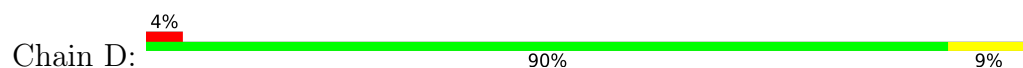
- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



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



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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SF4, TDR, NAP, FAD, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/7865	0.57	2/10665 (0.0%)
1	B	0.32	0/7895	0.57	1/10701 (0.0%)
1	C	0.32	0/7829	0.86	7/10616 (0.1%)
1	D	0.31	0/7902	0.63	8/10714 (0.1%)
All	All	0.31	0/31491	0.67	18/42696 (0.0%)

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

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	520	GLU	OE1-CD-OE2	-39.23	76.22	123.30
1	C	893	GLU	OE1-CD-OE2	-34.84	81.49	123.30
1	C	893	GLU	CG-CD-OE1	21.13	160.56	118.30
1	C	520	GLU	CG-CD-OE1	19.86	158.01	118.30
1	C	893	GLU	CG-CD-OE2	-19.35	79.60	118.30
1	C	520	GLU	CG-CD-OE2	-18.00	82.30	118.30
1	D	481	ASP	CB-CG-OD2	-14.33	105.40	118.30
1	D	481	ASP	CB-CG-OD1	12.55	129.59	118.30
1	D	358	ARG	CG-CD-NE	7.79	128.16	111.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	481	ASP	OD1-CG-OD2	-6.42	111.09	123.30
1	D	991	LEU	CB-CG-CD2	-6.12	100.60	111.00
1	D	363	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	D	363	PHE	CB-CG-CD2	5.71	124.80	120.80
1	A	893	GLU	CA-CB-CG	5.61	125.74	113.40
1	B	460	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	800	GLU	CA-CB-CG	5.30	125.05	113.40
1	D	7	LYS	CA-CB-CG	5.29	125.04	113.40
1	C	779	THR	CA-CB-CG2	5.06	119.49	112.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7705	0	7690	72	0
1	B	7734	0	7754	79	1
1	C	7671	0	7668	71	0
1	D	7740	0	7746	71	1
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
3	C	53	0	31	1	0
3	D	53	0	31	0	0
4	A	48	0	25	5	0
4	B	48	0	25	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	48	0	25	4	0
4	D	40	0	19	1	0
5	A	31	0	19	1	0
5	B	31	0	19	1	0
5	C	31	0	19	1	0
5	D	31	0	19	1	0
6	A	9	0	6	0	0
6	B	9	0	6	0	0
6	C	9	0	6	0	0
6	D	9	0	6	0	0
7	C	7	0	7	0	0
8	A	1072	0	0	27	2
8	B	1004	0	0	24	4
8	C	1103	0	0	23	6
8	D	1127	0	0	25	6
All	All	35847	0	31183	285	11

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:MET:SD	8:D:2247:HOH:O	2.19	1.01
1:A:884:GLU:OE1	8:A:1201:HOH:O	1.83	0.96
1:B:315:LYS:NZ	8:B:1204:HOH:O	1.97	0.95
1:A:541:LYS:NZ	8:A:1207:HOH:O	2.02	0.93
1:B:793[B]:THR:HG22	1:B:814:GLN:HB2	1.49	0.93
1:B:467:GLU:OE1	8:B:1201:HOH:O	1.90	0.90
1:B:325:HIS:ND1	8:B:1207:HOH:O	2.05	0.90
1:B:287:GLU:OE2	8:B:1202:HOH:O	1.90	0.89
1:C:318:LYS:O	8:C:1201:HOH:O	1.92	0.87
1:A:893:GLU:HB3	8:A:2079:HOH:O	1.74	0.87
1:C:901:ASN:ND2	8:C:1204:HOH:O	2.06	0.86
1:C:175:CYS:SG	8:C:1213:HOH:O	2.36	0.83
1:A:179:GLN:NE2	8:A:1211:HOH:O	2.12	0.82
1:D:420:ASN:OD1	8:D:1202:HOH:O	1.99	0.81
1:B:52:CYS:O	8:B:1205:HOH:O	1.98	0.81
1:D:320:GLY:O	8:D:1203:HOH:O	1.99	0.81
1:D:716:ASP:OD2	8:D:1201:HOH:O	1.97	0.81
1:A:700:GLN:NE2	8:A:1213:HOH:O	2.14	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:NZ	8:A:1202:HOH:O	1.92	0.80
1:C:700:GLN:OE1	8:C:1202:HOH:O	2.00	0.79
1:A:416:THR:HG23	1:A:418:LYS:HB3	1.65	0.79
1:C:793:THR:HG22	1:C:814:GLN:HB2	1.63	0.79
1:C:358:ARG:NE	8:C:1209:HOH:O	2.16	0.78
1:D:287:GLU:OE1	8:D:1204:HOH:O	2.00	0.78
1:A:179:GLN:OE1	8:A:1205:HOH:O	2.00	0.77
1:A:656:LYS:NZ	8:A:1214:HOH:O	2.16	0.77
1:B:222:TYR:OH	8:B:1206:HOH:O	2.02	0.77
1:B:444:ASP:OD1	1:B:446:LYS:HE3	1.86	0.76
1:C:885:GLN:HG2	8:C:2130:HOH:O	1.85	0.75
1:A:52:CYS:HB3	1:A:384:LYS:HB2	1.69	0.75
1:A:909:ARG:NH1	8:A:1206:HOH:O	2.00	0.74
1:C:871:LEU:O	8:C:1203:HOH:O	2.05	0.73
1:A:541:LYS:HD2	8:A:1983:HOH:O	1.88	0.73
1:D:893:GLU:OE1	1:D:896:ARG:NH1	2.21	0.73
1:C:951:GLU:OE2	8:C:1203:HOH:O	2.06	0.72
1:C:696:ARG:O	1:C:700:GLN:HG3	1.89	0.72
1:D:259:LYS:NZ	8:D:1210:HOH:O	2.21	0.72
1:A:263:GLU:O	8:A:1208:HOH:O	2.07	0.72
1:D:418:LYS:HG2	1:D:419:TRP:H	1.52	0.71
1:A:222:TYR:OH	8:A:1204:HOH:O	1.97	0.71
1:D:800:GLU:OE1	8:D:1205:HOH:O	2.10	0.69
4:A:1106:NAP:O7N	8:A:1210:HOH:O	2.10	0.69
1:D:167:ASN:OD1	8:D:1206:HOH:O	2.11	0.69
1:B:342:ASP:HB3	4:B:1106:NAP:C4N	2.23	0.68
1:C:11:ASP:OD1	8:C:1205:HOH:O	2.11	0.68
1:A:292:ASP:OD1	8:A:1209:HOH:O	2.10	0.68
4:B:1106:NAP:O3D	8:B:1209:HOH:O	2.10	0.68
1:D:793:THR:HG22	1:D:814:GLN:HB2	1.75	0.67
1:A:167:ASN:ND2	8:A:1217:HOH:O	2.27	0.67
1:A:342:ASP:HB3	4:A:1106:NAP:C4N	2.26	0.66
1:C:246:GLU:OE2	8:C:1207:HOH:O	2.11	0.66
1:D:357:ARG:HH12	1:D:358:ARG:HH11	1.44	0.66
1:B:51:HIS:O	8:B:1210:HOH:O	2.13	0.65
1:D:40:HIS:ND1	8:D:1215:HOH:O	2.29	0.65
1:B:53:GLU:HG3	8:B:1295:HOH:O	1.95	0.65
1:D:395:LYS:NZ	8:D:1214:HOH:O	2.28	0.65
1:D:265:GLU:OE1	8:D:1208:HOH:O	2.14	0.65
1:D:449:GLU:OE1	8:D:1207:HOH:O	2.13	0.64
1:B:342:ASP:OD2	1:B:372:ALA:HA	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ARG:HD3	1:D:360:PHE:CE2	2.35	0.62
1:C:884:GLU:OE1	8:C:1208:HOH:O	2.16	0.61
1:D:358:ARG:HD3	1:D:360:PHE:CZ	2.35	0.61
1:D:180:GLU:HG2	1:D:181:LYS:HD2	1.82	0.61
1:D:518:LYS:NZ	1:D:518:LYS:HB3	2.15	0.61
1:C:552:ALA:HB2	5:C:1109:FMN:HM73	1.82	0.61
1:B:448:LYS:NZ	1:B:460:ASP:OD1	2.31	0.61
1:C:536:GLU:OE2	1:C:541:LYS:HG2	2.01	0.61
1:C:735:THR:O	1:C:793:THR:OG1	2.18	0.61
1:B:871:LEU:CA	1:B:874:LYS:HZ1	2.14	0.60
1:C:270:THR:HA	1:C:273:GLU:HG2	1.82	0.60
1:D:647:LYS:HG3	1:D:697:TRP:CD1	2.36	0.60
1:D:179:GLN:NE2	8:D:1219:HOH:O	2.34	0.60
1:B:871:LEU:HA	1:B:874:LYS:HZ1	1.65	0.60
1:A:893:GLU:HA	1:A:896:ARG:HG2	1.83	0.59
1:C:265:GLU:OE2	8:C:1210:HOH:O	2.17	0.59
1:B:131:PRO:HB2	1:B:373:VAL:HG11	1.85	0.58
1:B:875:LYS:HE3	8:B:2032:HOH:O	2.04	0.58
1:C:376:GLU:OE2	4:C:1107:NAP:H4N	2.02	0.58
1:C:867:ARG:HD2	1:C:872:MET:HE3	1.85	0.58
1:A:25:HIS:ND1	1:B:520:GLU:OE2	2.37	0.58
1:D:735:THR:O	1:D:793:THR:OG1	2.22	0.57
1:D:410:ARG:HG2	1:D:411:THR:N	2.19	0.57
1:D:900:GLN:CD	1:D:901:ASN:H	2.08	0.57
1:A:910:LYS:HG2	1:A:911:PRO:HD2	1.86	0.57
1:B:463:GLU:HG3	8:B:1614:HOH:O	2.05	0.57
1:D:418:LYS:HG2	1:D:419:TRP:N	2.18	0.57
1:B:745:LYS:HE2	1:B:749:THR:OG1	2.05	0.56
1:C:893:GLU:OE1	8:C:1211:HOH:O	2.18	0.56
1:A:131:PRO:HB2	1:A:373:VAL:HG11	1.85	0.56
1:B:82:CYS:O	1:B:98:LYS:HD2	2.05	0.56
1:D:52:CYS:N	8:D:1217:HOH:O	2.33	0.56
1:C:844:GLU:HG3	1:C:915:LYS:HD2	1.86	0.56
1:D:249:LYS:HE3	1:D:255:ILE:HD12	1.86	0.56
1:B:871:LEU:HD11	1:B:890:ILE:HG13	1.89	0.55
1:D:896:ARG:NH2	8:D:1223:HOH:O	2.39	0.55
1:B:269:ASN:O	1:B:273:GLU:HG3	2.07	0.55
1:A:367:PHE:CZ	1:B:367:PHE:CE2	2.94	0.55
1:A:926:GLY:HA3	1:D:941:ILE:HD13	1.88	0.55
1:D:395:LYS:HE3	8:D:1884:HOH:O	2.07	0.55
1:B:394:ARG:NH2	1:B:423:GLU:OE1	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:PRO:HB2	1:D:373:VAL:HG11	1.88	0.55
1:D:552:ALA:HB2	5:D:1108:FMN:HM73	1.89	0.54
1:C:95:LEU:HD11	1:C:120:ASN:HB2	1.89	0.54
1:D:167:ASN:HB3	1:D:911:PRO:HA	1.89	0.54
1:B:259:LYS:NZ	8:B:1225:HOH:O	2.39	0.54
1:C:62:ILE:HD12	1:C:379:LEU:HD22	1.90	0.54
1:A:696:ARG:O	1:A:700:GLN:HG3	2.09	0.53
1:C:867:ARG:HD2	1:C:872:MET:CE	2.38	0.53
1:A:552:ALA:HB2	5:A:1107:FMN:HM73	1.90	0.53
1:A:56:GLU:OE2	1:A:898:LYS:NZ	2.41	0.53
1:D:394:ARG:NH2	1:D:423:GLU:OE2	2.41	0.53
1:D:163:PHE:O	1:D:166:MET:HB2	2.08	0.53
1:A:73:LEU:O	1:A:77:MET:HG3	2.09	0.52
8:A:1880:HOH:O	1:D:941:ILE:HD12	2.08	0.52
1:C:367:PHE:CZ	1:D:367:PHE:CZ	2.98	0.52
1:C:582:ILE:HA	8:C:1259:HOH:O	2.09	0.52
1:D:689:GLU:CD	1:D:692:ARG:HH12	2.13	0.52
1:C:259:LYS:NZ	8:C:1216:HOH:O	2.25	0.52
1:D:89:LYS:NZ	8:D:1218:HOH:O	2.33	0.52
1:C:221:GLU:OE1	8:C:1212:HOH:O	2.19	0.52
1:B:742:MET:O	1:B:742:MET:HG3	2.09	0.51
1:A:259:LYS:HB3	8:A:1333:HOH:O	2.10	0.51
1:C:242:ASN:O	1:C:246:GLU:HG3	2.10	0.51
1:D:885:GLN:NE2	8:D:1236:HOH:O	2.43	0.51
1:D:258:GLY:O	1:D:259:LYS:HE2	2.10	0.51
1:C:693:ASN:OD1	1:C:696:ARG:NH1	2.44	0.51
1:C:910:LYS:HE2	1:C:910:LYS:HA	1.93	0.51
1:B:899:GLU:O	1:B:901:ASN:N	2.44	0.51
1:C:331:ILE:HG22	1:C:331:ILE:O	2.11	0.51
1:A:703:GLN:NE2	8:A:1215:HOH:O	2.18	0.50
1:D:394:ARG:HH21	1:D:423:GLU:CD	2.14	0.50
1:B:552:ALA:HB2	5:B:1108:FMN:HM73	1.93	0.50
1:A:622:CYS:SG	1:A:656:LYS:HG2	2.51	0.50
1:B:315:LYS:HG2	1:B:322:CYS:SG	2.52	0.50
1:A:386:GLU:OE2	1:B:368:VAL:HG22	2.12	0.49
1:B:870:GLU:OE1	1:B:870:GLU:N	2.45	0.49
1:D:647:LYS:HG3	1:D:697:TRP:CG	2.47	0.49
1:C:1017:LEU:HD22	8:C:1771:HOH:O	2.11	0.49
1:B:13:GLU:OE2	8:B:1211:HOH:O	2.20	0.49
1:B:895:MET:HE2	1:B:895:MET:HA	1.94	0.49
1:C:916:LYS:HD3	8:C:2135:HOH:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:LYS:HE3	8:D:1441:HOH:O	2.12	0.49
1:C:428:HIS:O	1:D:410:ARG:NH1	2.39	0.49
1:A:446:LYS:NZ	8:A:1239:HOH:O	2.44	0.49
1:A:53:GLU:N	8:A:1244:HOH:O	2.46	0.49
1:A:416:THR:CG2	1:A:418:LYS:HB3	2.40	0.49
1:B:325:HIS:CE1	8:B:1207:HOH:O	2.57	0.48
1:B:868:ILE:O	1:B:872:MET:HG3	2.12	0.48
1:C:455:LYS:HE3	1:C:463:GLU:OE2	2.13	0.48
1:C:893:GLU:OE2	1:C:897:LEU:HD11	2.12	0.48
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.95	0.48
1:B:870:GLU:C	1:B:874:LYS:HZ1	2.16	0.48
1:B:867:ARG:HG3	1:B:872:MET:HE1	1.96	0.48
1:C:179:GLN:NE2	8:C:1238:HOH:O	2.45	0.48
1:A:180:GLU:H	1:A:180:GLU:CD	2.16	0.48
1:A:293:ILE:HD13	1:A:394:ARG:HA	1.96	0.48
1:D:204:SER:OG	1:D:248:MET:HG3	2.12	0.48
1:B:336:ILE:HD11	1:B:429:LEU:HG	1.95	0.48
1:A:357:ARG:NH2	8:A:1203:HOH:O	1.94	0.48
1:A:326:SER:HB3	8:A:1549:HOH:O	2.14	0.47
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.96	0.47
1:D:238:TYR:OH	8:D:1209:HOH:O	2.19	0.47
1:C:342:ASP:HB2	4:C:1107:NAP:C5N	2.44	0.47
1:C:233:GLN:OE1	1:C:318:LYS:HG2	2.14	0.47
1:A:800:GLU:O	1:A:804:GLN:HG3	2.15	0.47
4:A:1106:NAP:H2N	8:A:1210:HOH:O	2.14	0.47
1:B:289:LYS:HD2	1:B:438:PHE:O	2.13	0.47
1:B:871:LEU:C	1:B:874:LYS:NZ	2.68	0.47
1:C:686:GLN:HG2	1:C:714:VAL:HG12	1.97	0.47
1:B:325:HIS:CE1	8:B:1242:HOH:O	2.67	0.47
1:D:167:ASN:CG	8:D:1206:HOH:O	2.49	0.47
1:C:173:ASN:OD1	8:C:1213:HOH:O	2.21	0.46
1:B:871:LEU:C	1:B:872:MET:HG2	2.35	0.46
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.96	0.46
1:B:779:THR:HG22	1:B:808:SER:HB3	1.98	0.46
1:B:871:LEU:C	1:B:874:LYS:HZ2	2.17	0.46
1:A:367:PHE:HE1	1:A:389:PRO:HG3	1.80	0.46
1:A:501:TRP:CZ2	1:A:519:PRO:HA	2.50	0.46
1:A:870:GLU:O	1:A:874:LYS:HG3	2.16	0.46
3:B:1105:FAD:C6	4:B:1106:NAP:C5N	2.94	0.46
1:A:368:VAL:O	1:B:50:PHE:HD1	1.98	0.46
1:A:929:LEU:HD12	1:D:941:ILE:HG21	1.96	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:HIS:CE1	8:B:1237:HOH:O	2.69	0.46
1:A:430:LYS:HE2	8:A:1782:HOH:O	2.15	0.45
1:C:425:GLN:HG2	1:D:426:ILE:HD12	1.99	0.45
8:C:1445:HOH:O	1:D:29:HIS:HB2	2.16	0.45
1:A:734:ALA:HA	1:A:735:THR:HA	1.74	0.45
1:C:669:LEU:HD11	1:C:708:ALA:HB1	1.99	0.45
3:C:1106:FAD:C5X	4:C:1107:NAP:C5N	2.94	0.45
1:B:342:ASP:HB2	4:B:1106:NAP:C6N	2.46	0.45
1:C:373:VAL:HG23	1:C:375:GLU:HG2	1.98	0.45
1:D:734:ALA:HA	1:D:735:THR:HA	1.72	0.45
1:B:691:VAL:HG21	1:B:720:ILE:HG23	1.99	0.45
1:C:64:HIS:CE1	1:C:378:GLU:OE2	2.70	0.45
1:A:18:LEU:HD11	1:A:975:PRO:HA	1.98	0.45
1:A:916:LYS:HB2	1:A:917:PRO:HD2	1.99	0.45
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.98	0.45
1:B:342:ASP:HB3	4:B:1106:NAP:C3N	2.46	0.45
1:B:391:LEU:CD2	1:B:410:ARG:HD2	2.47	0.45
1:B:783:ARG:NE	8:B:1219:HOH:O	2.32	0.45
1:B:370:ILE:HG22	1:B:372:ALA:H	1.82	0.44
1:B:867:ARG:HG3	1:B:872:MET:CE	2.47	0.44
1:C:572:LEU:HD13	1:C:638:ILE:HB	1.98	0.44
1:A:893:GLU:OE1	1:A:897:LEU:HD13	2.17	0.44
1:C:32:LEU:HB2	1:D:485:MET:HE1	1.98	0.44
1:C:357:ARG:HA	1:C:357:ARG:HD3	1.63	0.44
1:A:623:GLN:O	1:A:627:GLU:HG3	2.18	0.44
1:C:29:HIS:HB2	8:D:1256:HOH:O	2.17	0.44
1:B:378:GLU:OE2	1:B:381:LYS:HE3	2.18	0.44
1:C:311:PRO:O	1:C:315:LYS:HG3	2.18	0.44
1:B:448:LYS:NZ	8:B:1208:HOH:O	2.10	0.44
1:D:82:CYS:O	1:D:98:LYS:HD2	2.17	0.44
1:A:561:ARG:O	1:A:565:GLU:HG3	2.18	0.44
1:B:868:ILE:HD13	1:B:893:GLU:HG2	2.00	0.44
1:B:990:THR:HG22	1:B:990:THR:O	2.18	0.44
1:A:28:LEU:HD11	1:B:498:GLN:HA	1.99	0.44
1:B:32:LEU:O	1:B:36:LEU:HG	2.18	0.44
1:B:222:TYR:OH	8:B:1203:HOH:O	1.95	0.43
1:B:922:LYS:NZ	8:B:1245:HOH:O	2.50	0.43
1:C:888:LYS:O	1:C:892:GLU:HG3	2.18	0.43
1:C:320:GLY:O	8:C:1214:HOH:O	2.21	0.43
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	1.99	0.43
3:A:1105:FAD:C5X	4:A:1106:NAP:C4N	2.96	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:NH2	8:B:1222:HOH:O	2.34	0.43
1:C:56:GLU:CD	1:C:332:ARG:HH21	2.21	0.43
1:C:517:ALA:C	1:C:518:LYS:HD2	2.39	0.43
1:B:501:TRP:CZ2	1:B:519:PRO:HA	2.53	0.43
1:B:871:LEU:CA	1:B:874:LYS:NZ	2.81	0.43
1:D:693:ASN:OD1	1:D:696:ARG:NH1	2.51	0.43
1:C:990:THR:O	1:C:990:THR:HG22	2.18	0.43
1:A:948:ILE:HD13	1:A:980:PRO:HG2	2.00	0.43
1:D:877:PRO:HD2	1:D:882:TYR:CG	2.54	0.43
1:B:56:GLU:HG2	1:B:895:MET:HE1	2.01	0.43
1:D:909:ARG:HB2	8:D:1845:HOH:O	2.18	0.43
1:A:191:ALA:O	1:A:279:ALA:HA	2.19	0.42
1:C:410:ARG:HG3	1:C:425:GLN:HB3	2.01	0.42
1:A:775:LEU:O	1:A:779[B]:THR:HG23	2.19	0.42
1:B:124:LEU:HD13	1:B:160:SER:HB2	2.01	0.42
1:D:689:GLU:OE2	1:D:692:ARG:NH1	2.51	0.42
1:D:399:LYS:NZ	8:D:1263:HOH:O	2.52	0.42
1:A:345:PHE:HE1	1:A:387:PHE:HE2	1.67	0.42
1:B:871:LEU:HD11	1:B:890:ILE:CG1	2.49	0.42
1:A:651:MET:O	1:A:655:ARG:HG3	2.20	0.42
1:C:342:ASP:HB3	4:C:1107:NAP:C4N	2.50	0.42
1:C:875:LYS:NZ	8:C:1253:HOH:O	2.50	0.42
1:C:612:LEU:HD11	1:D:935:PHE:CE1	2.55	0.42
1:C:870:GLU:HG3	1:C:889:ILE:HD13	2.02	0.42
1:D:378:GLU:O	1:D:382:GLU:HG2	2.19	0.42
1:A:892:GLU:HG3	8:A:1938:HOH:O	2.19	0.42
1:B:895:MET:HA	1:B:895:MET:CE	2.50	0.42
1:C:780:THR:HG22	1:D:762:TYR:CZ	2.55	0.42
1:A:263:GLU:HG3	1:A:449:GLU:CD	2.41	0.41
1:A:915:LYS:HG2	8:A:1296:HOH:O	2.20	0.41
1:A:771:ARG:HD2	8:B:1379:HOH:O	2.20	0.41
1:A:934:THR:OG1	1:A:937:GLU:HG3	2.19	0.41
1:D:501:TRP:CZ2	1:D:519:PRO:HA	2.55	0.41
1:D:945:VAL:HG13	1:D:1007:ARG:HG2	2.02	0.41
1:B:430:LYS:NZ	8:B:1237:HOH:O	2.46	0.41
1:B:872:MET:N	1:B:874:LYS:HZ2	2.19	0.41
1:D:365:LYS:HE2	4:D:1106:NAP:O1X	2.20	0.41
1:D:990:THR:HG22	1:D:990:THR:O	2.20	0.41
1:B:424:ASP:OD1	1:B:424:ASP:N	2.49	0.41
1:C:518:LYS:HD2	1:C:518:LYS:N	2.35	0.41
1:A:342:ASP:HB3	4:A:1106:NAP:C3N	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:MET:HE1	8:A:1397:HOH:O	2.19	0.41
1:A:990:THR:HG22	1:A:990:THR:O	2.21	0.41
1:B:325:HIS:CD2	8:B:1242:HOH:O	2.73	0.41
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.20	0.41
1:C:868:ILE:O	1:C:872:MET:HG2	2.21	0.41
1:D:593:GLY:HA3	1:D:606:SER:OG	2.21	0.41
1:A:263:GLU:HG3	1:A:449:GLU:OE1	2.21	0.40
1:A:533:ILE:O	1:A:545:PRO:HD3	2.20	0.40
1:A:868:ILE:O	1:A:872:MET:HG2	2.21	0.40
1:B:413:GLN:NE2	1:B:417:GLY:O	2.43	0.40
1:B:734:ALA:HA	1:B:735:THR:HA	1.72	0.40
1:B:868:ILE:HG22	1:B:870:GLU:H	1.87	0.40
1:A:931:TYR:CZ	1:B:749:THR:HG22	2.56	0.40
1:B:642:MET:CE	1:B:670:SER:HB2	2.51	0.40
1:D:167:ASN:HB2	1:D:912:PHE:CD2	2.56	0.40
1:A:669:LEU:HD13	1:A:691:VAL:HG22	2.02	0.40
1:B:972:GLN:O	1:B:980:PRO:HA	2.22	0.40
1:C:177:PRO:HG2	1:C:182:MET:SD	2.62	0.40
1:C:800:GLU:CG	1:C:801:SER:N	2.82	0.40
1:D:358:ARG:HA	8:D:1626:HOH:O	2.21	0.40
1:D:589:ARG:HG3	1:D:590:ILE:HG13	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1986:HOH:O	8:D:2013:HOH:O[2_646]	1.61	0.59
8:B:2039:HOH:O	8:C:2227:HOH:O[2_645]	1.85	0.35
8:A:2018:HOH:O	8:C:2268:HOH:O[1_556]	1.95	0.25
8:C:1931:HOH:O	8:D:1724:HOH:O[2_555]	1.97	0.23
1:B:460:ASP:OD2	1:D:395:LYS:NZ[1_656]	1.98	0.22
8:B:1527:HOH:O	8:D:2007:HOH:O[1_656]	1.98	0.22
8:C:2135:HOH:O	8:D:2295:HOH:O[2_555]	1.98	0.22
8:A:2265:HOH:O	8:C:2270:HOH:O[2_645]	2.00	0.20
8:C:1440:HOH:O	8:D:2072:HOH:O[2_555]	2.01	0.19
8:B:2032:HOH:O	8:B:2183:HOH:O[1_455]	2.06	0.14
8:D:1668:HOH:O	8:D:1938:HOH:O[1_455]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

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

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	905	PRO
1	B	900	GLN
1	B	905	PRO
1	C	326	SER
1	C	683	ALA
1	C	414	ASP
1	D	903	ALA
1	D	417	GLY
1	A	990	THR
1	B	904	PHE
1	D	822	GLN
1	B	906	PRO
1	C	794	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

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

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PHE
1	A	893	GLU
1	B	11[A]	ASP
1	B	11[B]	ASP
1	B	100	PHE
1	B	289	LYS
1	B	410	ARG
1	B	446	LYS
1	B	793[A]	THR
1	B	793[B]	THR
1	B	872	MET
1	B	874	LYS
1	C	100	PHE
1	C	357	ARG
1	C	800	GLU
1	D	47	LYS
1	D	51	HIS
1	D	100	PHE
1	D	181	LYS
1	D	402	ARG
1	D	481	ASP
1	D	541	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	700	GLN
1	A	930	GLN
1	B	487	ASN
1	B	885	GLN
1	C	64	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	179	GLN
1	C	885	GLN
1	D	847	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SF4	D	1104	1	0,12,12	0.00	-	-		
2	SF4	A	1103	1	0,12,12	0.00	-	-		
2	SF4	C	1105	1	0,12,12	0.00	-	-		
3	FAD	B	1105	-	51,58,58	1.22	6 (11%)	60,89,89	2.21	7 (11%)
2	SF4	A	1104	1	0,12,12	0.00	-	-		
7	PRO	C	1101	-	5,7,8	0.51	0	7,8,10	1.27	0
2	SF4	A	1101	1	0,12,12	0.00	-	-		
4	NAP	D	1106	-	36,43,52	2.35	6 (16%)	44,67,80	1.72	10 (22%)
5	FMN	B	1108	-	31,33,33	4.00	14 (45%)	40,50,50	1.70	9 (22%)
2	SF4	A	1102	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	C	1106	-	51,58,58	1.22	5 (9%)	60,89,89	2.19	7 (11%)
2	SF4	B	1104	1	0,12,12	0.00	-	-		
2	SF4	C	1104	1	0,12,12	0.00	-	-		
3	FAD	D	1105	-	51,58,58	1.20	5 (9%)	60,89,89	2.19	7 (11%)
5	FMN	D	1108	-	31,33,33	3.97	13 (41%)	40,50,50	1.74	10 (25%)
4	NAP	B	1106	-	45,52,52	2.75	13 (28%)	56,80,80	1.93	13 (23%)
2	SF4	D	1101	1	0,12,12	0.00	-	-		
6	TDR	C	1108	-	8,9,9	4.14	7 (87%)	6,12,12	5.75	4 (66%)
4	NAP	A	1106	-	45,52,52	2.79	11 (24%)	56,80,80	1.96	14 (25%)
6	TDR	A	1108	-	8,9,9	4.20	7 (87%)	6,12,12	5.66	4 (66%)
2	SF4	B	1103	1	0,12,12	0.00	-	-		
2	SF4	C	1103	1	0,12,12	0.00	-	-		
6	TDR	B	1107	-	8,9,9	4.10	7 (87%)	6,12,12	5.53	4 (66%)
6	TDR	D	1107	-	8,9,9	4.05	7 (87%)	6,12,12	5.64	4 (66%)
4	NAP	C	1107	-	45,52,52	2.59	12 (26%)	56,80,80	1.90	14 (25%)
3	FAD	A	1105	-	51,58,58	1.23	5 (9%)	60,89,89	2.18	7 (11%)
2	SF4	C	1102	1	0,12,12	0.00	-	-		
5	FMN	C	1109	-	31,33,33	3.98	12 (38%)	40,50,50	1.85	9 (22%)
2	SF4	D	1103	1	0,12,12	0.00	-	-		
2	SF4	B	1102	1	0,12,12	0.00	-	-		
2	SF4	D	1102	1	0,12,12	0.00	-	-		
5	FMN	A	1107	-	31,33,33	4.00	13 (41%)	40,50,50	1.84	10 (25%)
2	SF4	B	1101	1	0,12,12	0.00	-	-		

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	D	1104	1	-	-	0/6/5/5
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	C	1105	1	-	-	0/6/5/5
3	FAD	B	1105	-	-	2/30/50/50	0/6/6/6
2	SF4	A	1104	1	-	-	0/6/5/5
7	PRO	C	1101	-	-	0/0/9/11	0/1/1/1
2	SF4	A	1101	1	-	-	0/6/5/5
4	NAP	D	1106	-	-	6/23/59/67	0/4/4/5
5	FMN	B	1108	-	-	1/18/18/18	0/3/3/3

Continued on next page...

*Continued from previous page...*

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

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	NAP	P2B-O2B	12.69	1.83	1.59
4	B	1106	NAP	P2B-O2B	12.14	1.82	1.59
4	C	1107	NAP	P2B-O2B	11.92	1.81	1.59
4	D	1106	NAP	P2B-O2B	11.65	1.81	1.59
5	D	1108	FMN	C10-N1	11.37	1.47	1.33
5	B	1108	FMN	C10-N1	11.30	1.47	1.33
5	A	1107	FMN	C10-N1	11.19	1.47	1.33
5	C	1109	FMN	C10-N1	10.99	1.47	1.33
6	A	1108	TDR	C6-N1	6.99	1.49	1.34
6	B	1107	TDR	C6-N1	6.91	1.49	1.34
6	D	1107	TDR	C6-N1	6.83	1.48	1.34
6	C	1108	TDR	C6-N1	6.78	1.48	1.34
4	B	1106	NAP	C4N-C3N	6.73	1.50	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1109	FMN	C4-C4A	6.67	1.52	1.41
5	D	1108	FMN	C9A-N10	6.64	1.47	1.38
5	B	1108	FMN	C4-C4A	6.62	1.52	1.41
5	A	1107	FMN	C4-C4A	6.57	1.52	1.41
5	B	1108	FMN	C4A-N5	6.54	1.42	1.33
4	A	1106	NAP	C4N-C3N	6.49	1.50	1.39
5	A	1107	FMN	C4A-N5	6.44	1.42	1.33
5	C	1109	FMN	C9A-N10	6.43	1.47	1.38
5	C	1109	FMN	C4A-N5	6.42	1.42	1.33
5	A	1107	FMN	C9A-N10	6.41	1.47	1.38
5	D	1108	FMN	C4A-N5	6.32	1.42	1.33
5	B	1108	FMN	O4-C4	6.31	1.40	1.24
5	B	1108	FMN	C9A-N10	6.30	1.47	1.38
5	D	1108	FMN	C4-C4A	6.29	1.52	1.41
5	D	1108	FMN	O4-C4	6.18	1.40	1.24
5	A	1107	FMN	O4-C4	6.18	1.40	1.24
5	A	1107	FMN	C5A-N5	6.07	1.45	1.35
5	C	1109	FMN	O4-C4	6.00	1.39	1.24
5	C	1109	FMN	C5A-N5	6.00	1.45	1.35
4	B	1106	NAP	C5N-C4N	5.90	1.51	1.38
5	D	1108	FMN	C5A-N5	5.86	1.45	1.35
5	B	1108	FMN	C5A-N5	5.77	1.44	1.35
5	A	1107	FMN	C9A-C5A	-5.75	1.31	1.42
5	C	1109	FMN	C9A-C5A	-5.68	1.31	1.42
5	B	1108	FMN	C9A-C5A	-5.54	1.31	1.42
4	A	1106	NAP	C5N-C4N	5.53	1.50	1.38
3	A	1105	FAD	C4X-C10	5.49	1.44	1.38
4	C	1107	NAP	C5N-C4N	5.47	1.50	1.38
3	B	1105	FAD	C4X-C10	5.47	1.44	1.38
6	A	1108	TDR	C4-C5	5.46	1.53	1.41
5	D	1108	FMN	C9A-C5A	-5.45	1.31	1.42
6	C	1108	TDR	C4-N3	5.44	1.42	1.33
6	A	1108	TDR	C4-N3	5.44	1.42	1.33
5	C	1109	FMN	C4A-C10	-5.43	1.33	1.38
3	C	1106	FAD	C4X-C10	5.36	1.44	1.38
3	D	1105	FAD	C4X-C10	5.34	1.44	1.38
5	D	1108	FMN	C6-C5A	5.31	1.50	1.41
5	A	1107	FMN	C6-C5A	5.28	1.50	1.41
4	C	1107	NAP	C4N-C3N	5.24	1.48	1.39
6	B	1107	TDR	C4-C5	5.24	1.52	1.41
6	D	1107	TDR	C4-C5	5.23	1.52	1.41
6	B	1107	TDR	C4-N3	5.21	1.42	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1109	FMN	C6-C5A	5.20	1.49	1.41
6	C	1108	TDR	C4-C5	5.16	1.52	1.41
5	B	1108	FMN	C6-C5A	5.16	1.49	1.41
6	D	1107	TDR	C4-N3	5.06	1.41	1.33
5	B	1108	FMN	C4A-C10	-5.00	1.33	1.38
5	D	1108	FMN	C4A-C10	-4.97	1.33	1.38
5	A	1107	FMN	C9-C9A	4.95	1.50	1.40
5	B	1108	FMN	C9-C9A	4.94	1.50	1.40
5	C	1109	FMN	C9-C9A	4.90	1.50	1.40
5	D	1108	FMN	C9-C9A	4.89	1.50	1.40
5	A	1107	FMN	C4A-C10	-4.87	1.34	1.38
5	B	1108	FMN	C4-N3	4.86	1.41	1.33
5	A	1107	FMN	C4-N3	4.76	1.41	1.33
5	D	1108	FMN	C4-N3	4.56	1.41	1.33
5	C	1109	FMN	C4-N3	4.48	1.40	1.33
4	A	1106	NAP	PN-O5D	4.24	1.76	1.59
4	B	1106	NAP	PN-O5D	3.96	1.75	1.59
6	C	1108	TDR	C2-N1	3.94	1.46	1.38
4	A	1106	NAP	C2N-N1N	3.88	1.39	1.35
4	C	1107	NAP	PN-O5D	3.88	1.75	1.59
6	B	1107	TDR	C2-N1	3.81	1.45	1.38
4	B	1106	NAP	C2N-N1N	3.77	1.39	1.35
6	A	1108	TDR	C2-N1	3.74	1.45	1.38
6	D	1107	TDR	C2-N1	3.72	1.45	1.38
3	D	1105	FAD	C4-N3	3.41	1.39	1.33
5	A	1107	FMN	C2-N1	3.41	1.44	1.38
4	A	1106	NAP	C7N-N7N	3.38	1.39	1.33
4	C	1107	NAP	C3N-C7N	-3.36	1.45	1.50
3	C	1106	FAD	C4-N3	3.35	1.38	1.33
3	A	1105	FAD	C4-N3	3.20	1.38	1.33
4	B	1106	NAP	C3N-C7N	-3.17	1.45	1.50
5	C	1109	FMN	C2-N1	3.16	1.44	1.38
4	D	1106	NAP	O2B-C2B	-3.14	1.32	1.44
5	B	1108	FMN	C2-N1	3.05	1.44	1.38
4	B	1106	NAP	O2B-C2B	-3.04	1.33	1.44
3	B	1105	FAD	C4-N3	3.01	1.38	1.33
4	A	1106	NAP	O2B-C2B	-2.99	1.33	1.44
4	C	1107	NAP	C7N-N7N	2.93	1.38	1.33
4	B	1106	NAP	C7N-N7N	2.91	1.38	1.33
5	D	1108	FMN	C2-N1	2.91	1.43	1.38
4	C	1107	NAP	O2B-C2B	-2.87	1.33	1.44
6	C	1108	TDR	C6-C5	-2.80	1.34	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1106	NAP	PN-O5D	2.78	1.70	1.59
6	A	1108	TDR	C6-C5	-2.69	1.35	1.39
6	D	1107	TDR	C6-C5	-2.68	1.35	1.39
4	A	1106	NAP	C3N-C7N	-2.65	1.46	1.50
3	C	1106	FAD	C5X-N5	2.64	1.39	1.35
3	A	1105	FAD	C5X-N5	2.59	1.39	1.35
6	B	1107	TDR	C6-C5	-2.58	1.35	1.39
3	A	1105	FAD	C4-C4X	2.40	1.45	1.41
3	C	1106	FAD	C4-C4X	2.39	1.45	1.41
3	D	1105	FAD	C5X-N5	2.36	1.39	1.35
6	B	1107	TDR	C2-N3	2.36	1.42	1.38
4	D	1106	NAP	C2A-N1A	2.35	1.38	1.33
4	B	1106	NAP	C2A-N1A	2.34	1.38	1.33
3	D	1105	FAD	C4-C4X	2.33	1.45	1.41
4	D	1106	NAP	O2D-C2D	-2.32	1.37	1.43
4	C	1107	NAP	C6N-C5N	-2.31	1.33	1.38
4	C	1107	NAP	C2N-C3N	-2.31	1.35	1.39
6	C	1108	TDR	O4-C4	-2.30	1.18	1.24
3	B	1105	FAD	C4-C4X	2.29	1.45	1.41
6	C	1108	TDR	C2-N3	2.28	1.42	1.38
4	A	1106	NAP	C6N-C5N	-2.26	1.33	1.38
4	B	1106	NAP	C6N-N1N	2.26	1.40	1.35
6	A	1108	TDR	C2-N3	2.25	1.42	1.38
6	D	1107	TDR	O4-C4	-2.24	1.18	1.24
6	A	1108	TDR	O4-C4	-2.22	1.19	1.24
4	B	1106	NAP	C6N-C5N	-2.21	1.33	1.38
4	A	1106	NAP	C6N-N1N	2.19	1.40	1.35
5	D	1108	FMN	P-O3P	-2.19	1.46	1.54
3	B	1105	FAD	C5X-N5	2.18	1.38	1.35
4	A	1106	NAP	C2A-N1A	2.17	1.37	1.33
3	A	1105	FAD	C9A-N10	2.15	1.41	1.38
5	B	1108	FMN	P-O2P	-2.15	1.46	1.54
4	B	1106	NAP	O5D-C5D	-2.15	1.36	1.44
4	C	1107	NAP	C2A-N1A	2.14	1.37	1.33
4	B	1106	NAP	C4A-N3A	2.13	1.38	1.35
4	C	1107	NAP	C6N-N1N	2.12	1.40	1.35
6	B	1107	TDR	O4-C4	-2.11	1.19	1.24
3	D	1105	FAD	C9A-N10	2.08	1.41	1.38
5	B	1108	FMN	P-O3P	-2.08	1.46	1.54
3	B	1105	FAD	C9A-N10	2.08	1.41	1.38
4	D	1106	NAP	C4A-N3A	2.04	1.38	1.35
6	D	1107	TDR	C2-N3	2.04	1.42	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1107	NAP	C2N-N1N	2.01	1.37	1.35
5	A	1107	FMN	P-O2P	-2.01	1.47	1.54
3	C	1106	FAD	C9A-N10	2.01	1.41	1.38
3	B	1105	FAD	C4X-N5	-2.00	1.30	1.33

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1105	FAD	C4-N3-C2	13.03	126.15	115.14
3	C	1106	FAD	C4-N3-C2	12.87	126.01	115.14
3	D	1105	FAD	C4-N3-C2	12.85	125.99	115.14
3	A	1105	FAD	C4-N3-C2	12.81	125.96	115.14
6	C	1108	TDR	N1-C2-N3	-11.44	119.33	128.43
6	D	1107	TDR	N1-C2-N3	-10.96	119.72	128.43
6	A	1108	TDR	N1-C2-N3	-10.94	119.73	128.43
6	B	1107	TDR	N1-C2-N3	-10.78	119.86	128.43
3	C	1106	FAD	C4X-C4-N3	-7.09	113.73	123.43
3	D	1105	FAD	C4X-C4-N3	-7.05	113.79	123.43
4	B	1106	NAP	C5N-C4N-C3N	-6.99	112.07	120.34
3	A	1105	FAD	C4X-C4-N3	-6.98	113.89	123.43
3	B	1105	FAD	C4X-C4-N3	-6.95	113.93	123.43
4	C	1107	NAP	C5N-C4N-C3N	-6.74	112.37	120.34
4	A	1106	NAP	C5N-C4N-C3N	-6.68	112.44	120.34
6	D	1107	TDR	C4-N3-C2	6.59	120.70	115.14
6	C	1108	TDR	C4-N3-C2	6.14	120.33	115.14
6	B	1107	TDR	C4-N3-C2	6.03	120.23	115.14
6	A	1108	TDR	C4-N3-C2	5.90	120.12	115.14
4	A	1106	NAP	PN-O3-PA	-5.75	113.10	132.83
5	A	1107	FMN	C4-N3-C2	5.67	119.93	115.14
5	C	1109	FMN	C1'-N10-C9A	5.58	122.68	118.29
4	B	1106	NAP	PN-O3-PA	-5.57	113.72	132.83
5	D	1108	FMN	C4-N3-C2	5.39	119.69	115.14
4	C	1107	NAP	PN-O3-PA	-5.36	114.42	132.83
5	B	1108	FMN	C4-N3-C2	5.32	119.64	115.14
6	A	1108	TDR	C5-C6-N1	-5.25	119.81	125.16
4	D	1106	NAP	PN-O3-PA	-5.19	115.01	132.83
5	A	1107	FMN	C1'-N10-C9A	5.09	122.30	118.29
5	C	1109	FMN	C4-N3-C2	5.07	119.42	115.14
6	B	1107	TDR	C5-C6-N1	-4.75	120.33	125.16
3	B	1105	FAD	C10-C4X-N5	4.66	124.48	121.26
4	A	1106	NAP	O7N-C7N-C3N	4.65	125.20	119.63
6	C	1108	TDR	C5-C6-N1	-4.61	120.47	125.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1105	FAD	C10-C4X-N5	4.59	124.43	121.26
3	A	1105	FAD	C10-C4X-N5	4.58	124.42	121.26
3	C	1106	FAD	C10-C4X-N5	4.49	124.36	121.26
6	D	1107	TDR	C5-C6-N1	-4.48	120.60	125.16
4	D	1106	NAP	O2B-P2B-O1X	-4.00	93.95	109.39
3	C	1106	FAD	C4-C4X-C10	-3.82	117.42	119.95
3	D	1105	FAD	C4-C4X-C10	-3.73	117.48	119.95
5	B	1108	FMN	C1'-N10-C9A	3.72	121.22	118.29
3	A	1105	FAD	C4-C4X-C10	-3.72	117.49	119.95
4	D	1106	NAP	PN-O5D-C5D	-3.68	100.12	121.68
3	B	1105	FAD	C4-C4X-C10	-3.63	117.55	119.95
3	B	1105	FAD	C4X-C10-N10	-3.62	116.59	120.30
4	B	1106	NAP	O7N-C7N-C3N	3.59	123.93	119.63
4	C	1107	NAP	O7N-C7N-C3N	3.52	123.85	119.63
5	D	1108	FMN	C5A-C9A-N10	3.51	120.26	117.72
5	A	1107	FMN	C9A-N10-C10	-3.49	117.34	121.91
4	B	1106	NAP	C2N-C3N-C4N	3.47	122.19	118.26
4	C	1107	NAP	C2N-C3N-C4N	3.46	122.18	118.26
5	A	1107	FMN	C5A-C9A-N10	3.46	120.22	117.72
3	A	1105	FAD	C4X-C10-N10	-3.44	116.77	120.30
5	D	1108	FMN	C9A-N10-C10	-3.44	117.41	121.91
3	D	1105	FAD	C4X-C10-N10	-3.39	116.81	120.30
3	C	1106	FAD	C4X-C10-N10	-3.39	116.82	120.30
5	C	1109	FMN	C9A-N10-C10	-3.33	117.55	121.91
4	A	1106	NAP	C2N-C3N-C4N	3.31	122.01	118.26
5	B	1108	FMN	C5A-C9A-N10	3.31	120.11	117.72
4	B	1106	NAP	O2B-P2B-O1X	-3.25	96.86	109.39
5	C	1109	FMN	C5A-C9A-N10	3.23	120.06	117.72
4	C	1107	NAP	O2B-P2B-O1X	-3.13	97.33	109.39
5	B	1108	FMN	C9A-N10-C10	-3.12	117.82	121.91
3	C	1106	FAD	C1'-N10-C9A	3.12	120.75	118.29
5	D	1108	FMN	C1'-N10-C9A	3.11	120.74	118.29
5	C	1109	FMN	O5'-P-O1P	3.09	115.13	106.47
4	D	1106	NAP	O5D-PN-O1N	-3.07	97.08	109.07
3	D	1105	FAD	C1'-N10-C9A	3.06	120.70	118.29
6	A	1108	TDR	C6-N1-C2	3.06	120.40	115.36
5	D	1108	FMN	C4A-C4-N3	-2.99	119.35	123.43
3	A	1105	FAD	C1'-N10-C9A	2.98	120.64	118.29
5	B	1108	FMN	C4A-C4-N3	-2.97	119.37	123.43
6	C	1108	TDR	C6-N1-C2	2.92	120.18	115.36
3	B	1105	FAD	C1'-N10-C9A	2.91	120.58	118.29
5	D	1108	FMN	O5'-P-O1P	2.90	114.61	106.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	FMN	C4A-C4-N3	-2.88	119.49	123.43
5	B	1108	FMN	O3P-P-O5'	2.88	114.39	106.73
5	C	1109	FMN	C4A-C4-N3	-2.84	119.54	123.43
4	A	1106	NAP	O7N-C7N-N7N	-2.83	118.55	122.58
5	A	1107	FMN	O2P-P-O5'	2.82	114.25	106.73
4	A	1106	NAP	O2B-P2B-O1X	-2.76	98.73	109.39
4	B	1106	NAP	O7N-C7N-N7N	-2.74	118.69	122.58
5	C	1109	FMN	O3P-P-O5'	2.72	113.98	106.73
5	D	1108	FMN	O3P-P-O5'	2.71	113.95	106.73
6	B	1107	TDR	C6-N1-C2	2.70	119.81	115.36
5	A	1107	FMN	O3P-P-O5'	2.68	113.87	106.73
4	B	1106	NAP	PA-O5B-C5B	-2.62	106.30	121.68
6	D	1107	TDR	C6-N1-C2	2.61	119.66	115.36
4	C	1107	NAP	C3B-C2B-C1B	-2.60	98.01	102.89
4	D	1106	NAP	O3X-P2B-O2X	2.57	117.45	107.64
4	A	1106	NAP	C3B-C2B-C1B	-2.56	98.09	102.89
5	B	1108	FMN	O5'-P-O1P	2.55	113.63	106.47
4	D	1106	NAP	C3B-C2B-C1B	-2.53	98.13	102.89
4	C	1107	NAP	O7N-C7N-N7N	-2.51	119.02	122.58
4	D	1106	NAP	PA-O5B-C5B	-2.50	107.05	121.68
4	A	1106	NAP	PA-O5B-C5B	-2.49	107.08	121.68
4	A	1106	NAP	O3X-P2B-O2X	2.49	117.13	107.64
4	C	1107	NAP	O3X-P2B-O2X	2.47	117.09	107.64
4	B	1106	NAP	O4B-C4B-C3B	2.47	110.00	105.11
4	B	1106	NAP	O3X-P2B-O2X	2.46	117.05	107.64
4	C	1107	NAP	PN-O5D-C5D	-2.40	107.61	121.68
4	C	1107	NAP	PA-O5B-C5B	-2.40	107.63	121.68
5	C	1109	FMN	O2P-P-O5'	2.39	113.09	106.73
5	B	1108	FMN	C4A-N5-C5A	2.38	119.15	116.77
5	D	1108	FMN	C4A-N5-C5A	2.37	119.14	116.77
4	A	1106	NAP	C2A-N1A-C6A	-2.36	114.72	118.75
5	D	1108	FMN	O2P-P-O5'	2.34	112.96	106.73
3	B	1105	FAD	C5A-C6A-N6A	2.32	123.88	120.35
4	B	1106	NAP	C2A-N1A-C6A	-2.31	114.80	118.75
3	C	1106	FAD	C5A-C6A-N6A	2.30	123.85	120.35
5	C	1109	FMN	C4A-N5-C5A	2.30	119.07	116.77
3	A	1105	FAD	C5A-C6A-N6A	2.29	123.83	120.35
4	D	1106	NAP	C2A-N1A-C6A	-2.24	114.92	118.75
3	D	1105	FAD	C5A-C6A-N6A	2.23	123.75	120.35
5	A	1107	FMN	O5'-P-O1P	2.23	112.72	106.47
5	D	1108	FMN	C1'-N10-C10	2.20	120.38	118.41
4	A	1106	NAP	O4B-C4B-C3B	2.19	109.45	105.11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	FMN	C4A-N5-C5A	2.18	118.95	116.77
5	B	1108	FMN	O2P-P-O5'	2.16	112.49	106.73
4	C	1107	NAP	O5D-PN-O1N	-2.15	100.66	109.07
4	A	1106	NAP	PN-O5D-C5D	-2.15	109.08	121.68
4	A	1106	NAP	O5D-PN-O1N	-2.14	100.69	109.07
5	A	1107	FMN	C10-C4A-N5	-2.14	119.78	121.26
4	C	1107	NAP	C6N-C5N-C4N	2.13	122.54	119.44
4	B	1106	NAP	C5B-C4B-C3B	-2.10	107.31	115.18
4	D	1106	NAP	O4B-C4B-C3B	2.06	109.18	105.11
4	A	1106	NAP	C6N-C5N-C4N	2.05	122.41	119.44
4	D	1106	NAP	O2N-PN-O1N	2.04	122.34	112.24
4	B	1106	NAP	C6N-C5N-C4N	2.04	122.41	119.44
4	C	1107	NAP	O4B-C4B-C3B	2.03	109.14	105.11
4	B	1106	NAP	C5D-C4D-C3D	-2.03	107.57	115.18
4	C	1107	NAP	C2A-N1A-C6A	-2.01	115.31	118.75

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1105	FAD	PA-O3P-P-O5'
4	A	1106	NAP	C2B-O2B-P2B-O3X
4	D	1106	NAP	O4D-C4D-C5D-O5D
4	D	1106	NAP	C3D-C4D-C5D-O5D
5	B	1108	FMN	C4'-C5'-O5'-P
5	C	1109	FMN	C4'-C5'-O5'-P
5	D	1108	FMN	C4'-C5'-O5'-P
3	A	1105	FAD	PA-O3P-P-O5'
3	B	1105	FAD	PA-O3P-P-O5'
3	C	1106	FAD	PA-O3P-P-O5'
5	A	1107	FMN	C4'-C5'-O5'-P
4	D	1106	NAP	C2B-O2B-P2B-O2X
4	D	1106	NAP	C5D-O5D-PN-O3
4	B	1106	NAP	O4B-C4B-C5B-O5B
4	D	1106	NAP	O4B-C4B-C5B-O5B
4	A	1106	NAP	O4B-C4B-C5B-O5B
3	A	1105	FAD	O4B-C4B-C5B-O5B
3	D	1105	FAD	O4B-C4B-C5B-O5B
4	C	1107	NAP	O4B-C4B-C5B-O5B
3	B	1105	FAD	O4B-C4B-C5B-O5B
3	C	1106	FAD	O4B-C4B-C5B-O5B
4	B	1106	NAP	C5D-O5D-PN-O1N

*Continued on next page...*

*Continued from previous page...*

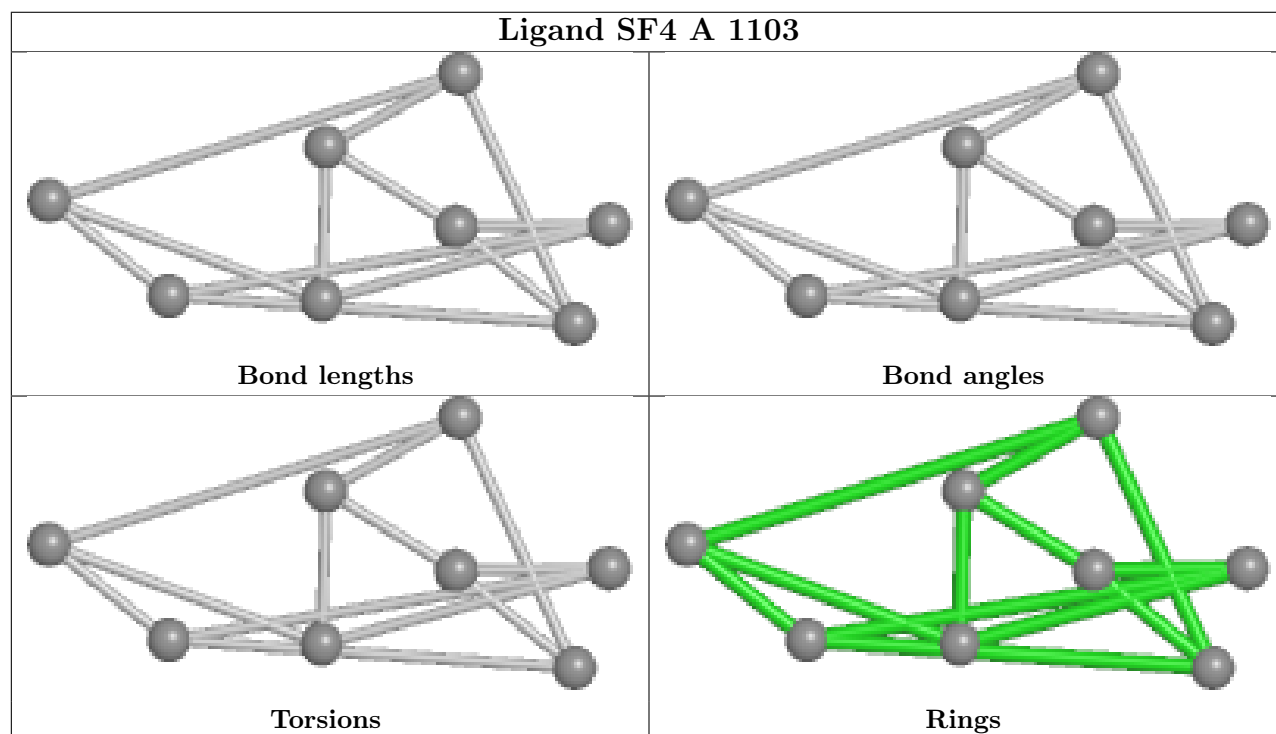
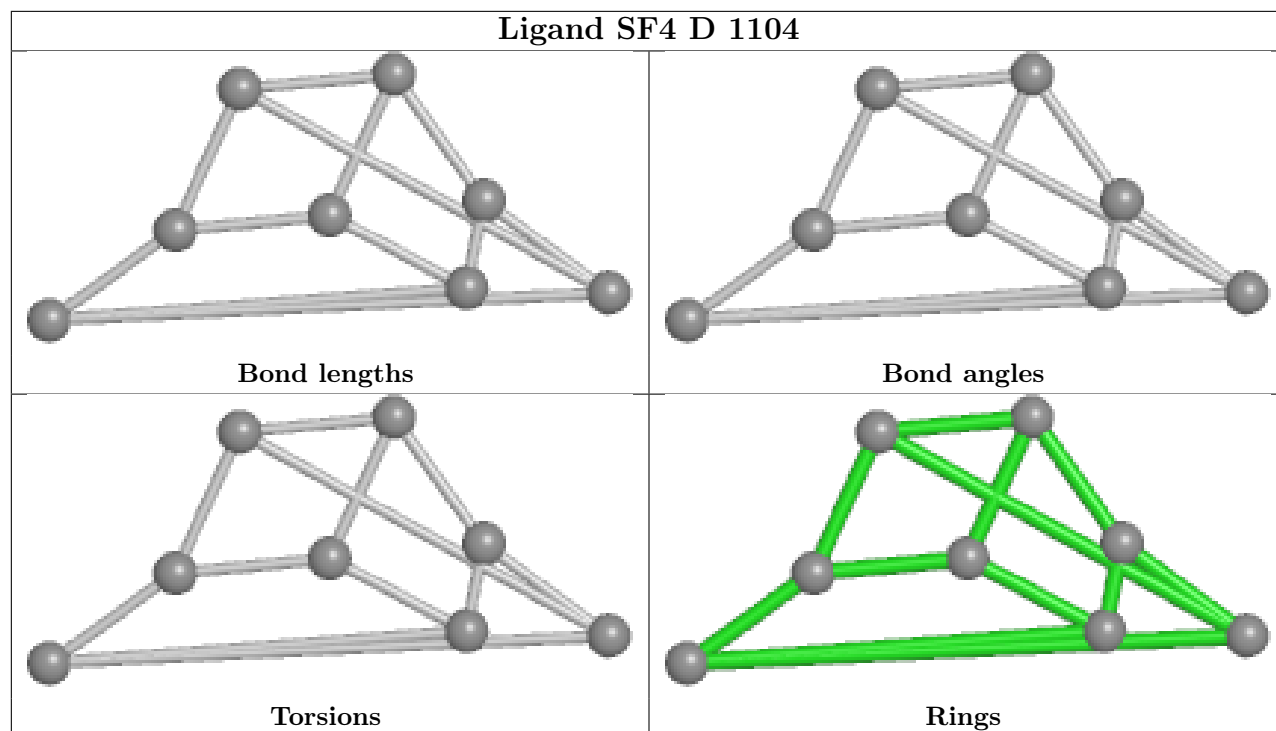
Mol	Chain	Res	Type	Atoms
4	D	1106	NAP	C5D-O5D-PN-O1N

There are no ring outliers.

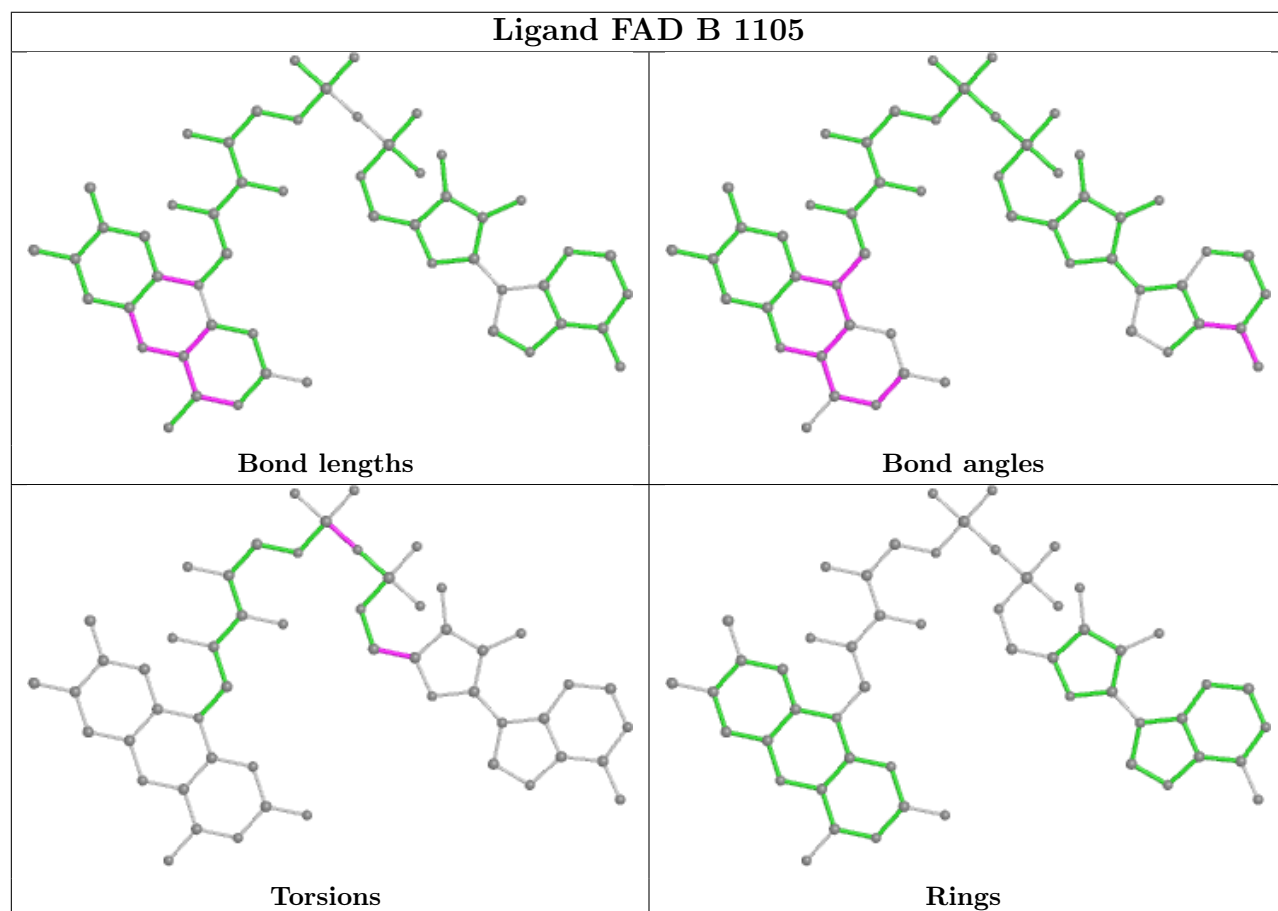
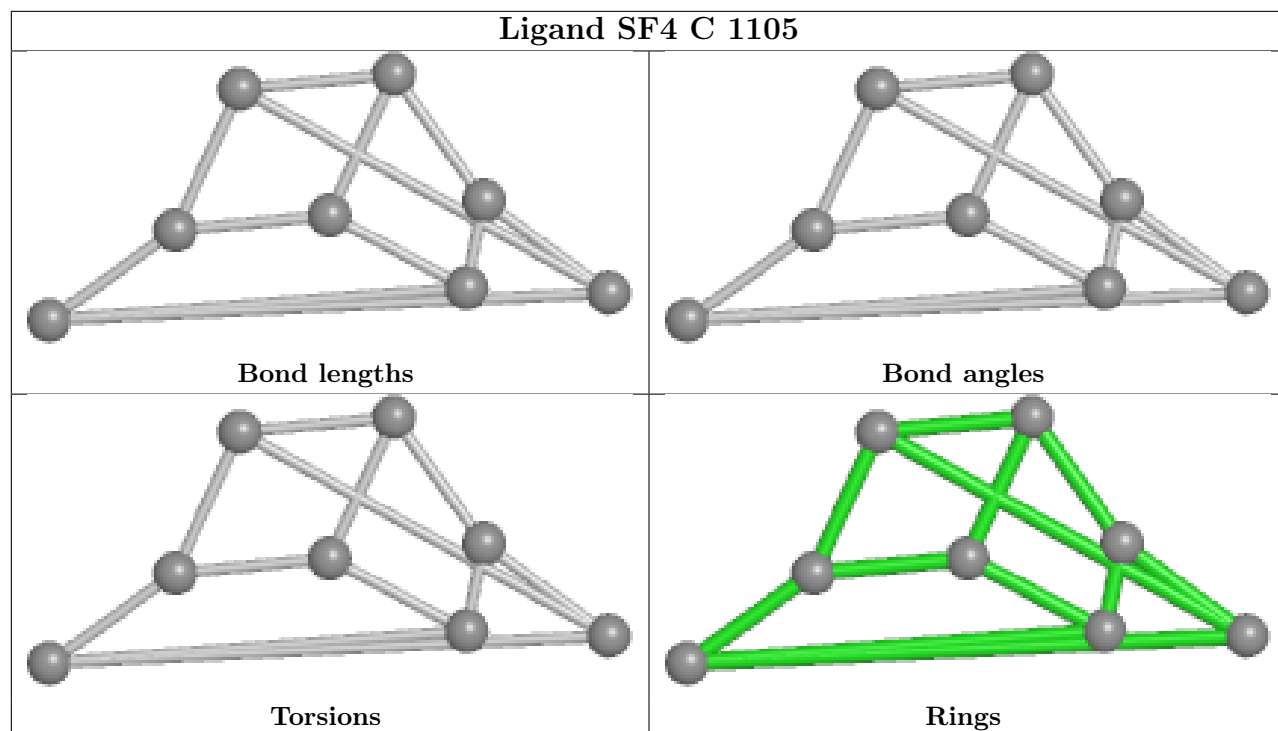
11 monomers are involved in 19 short contacts:

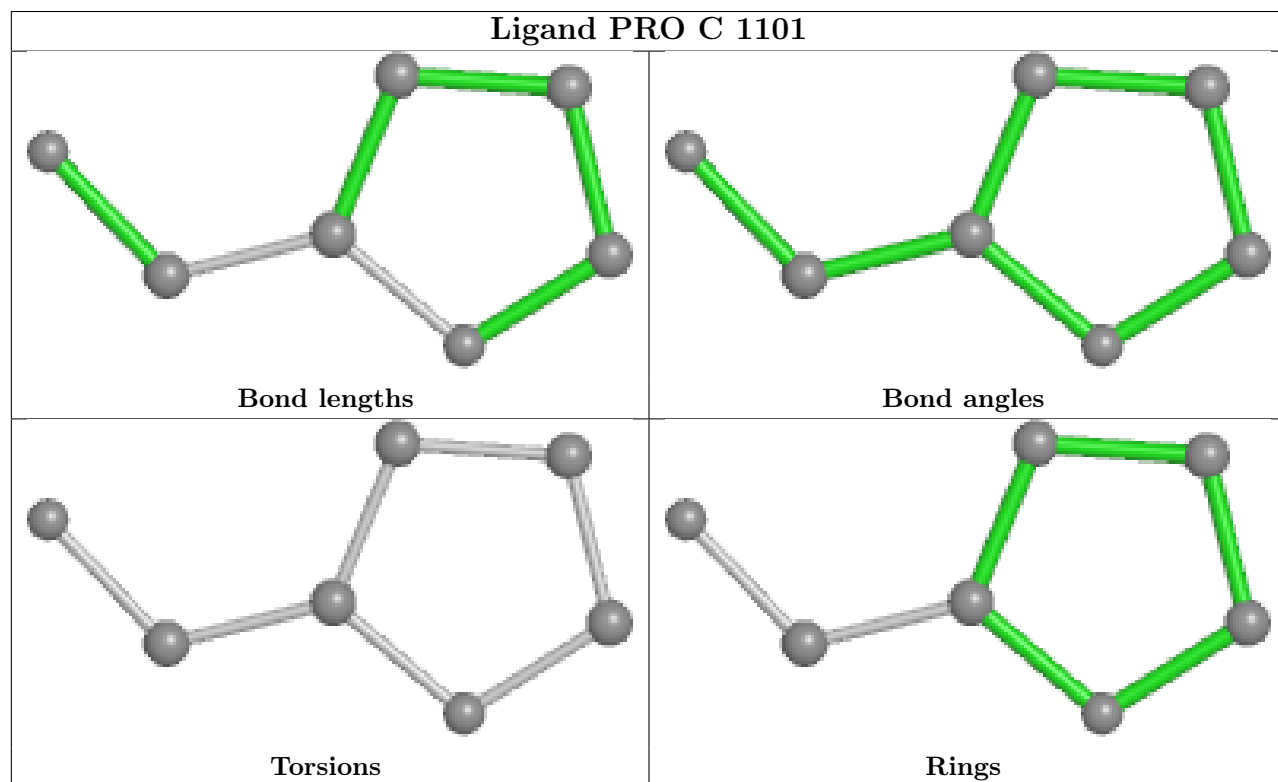
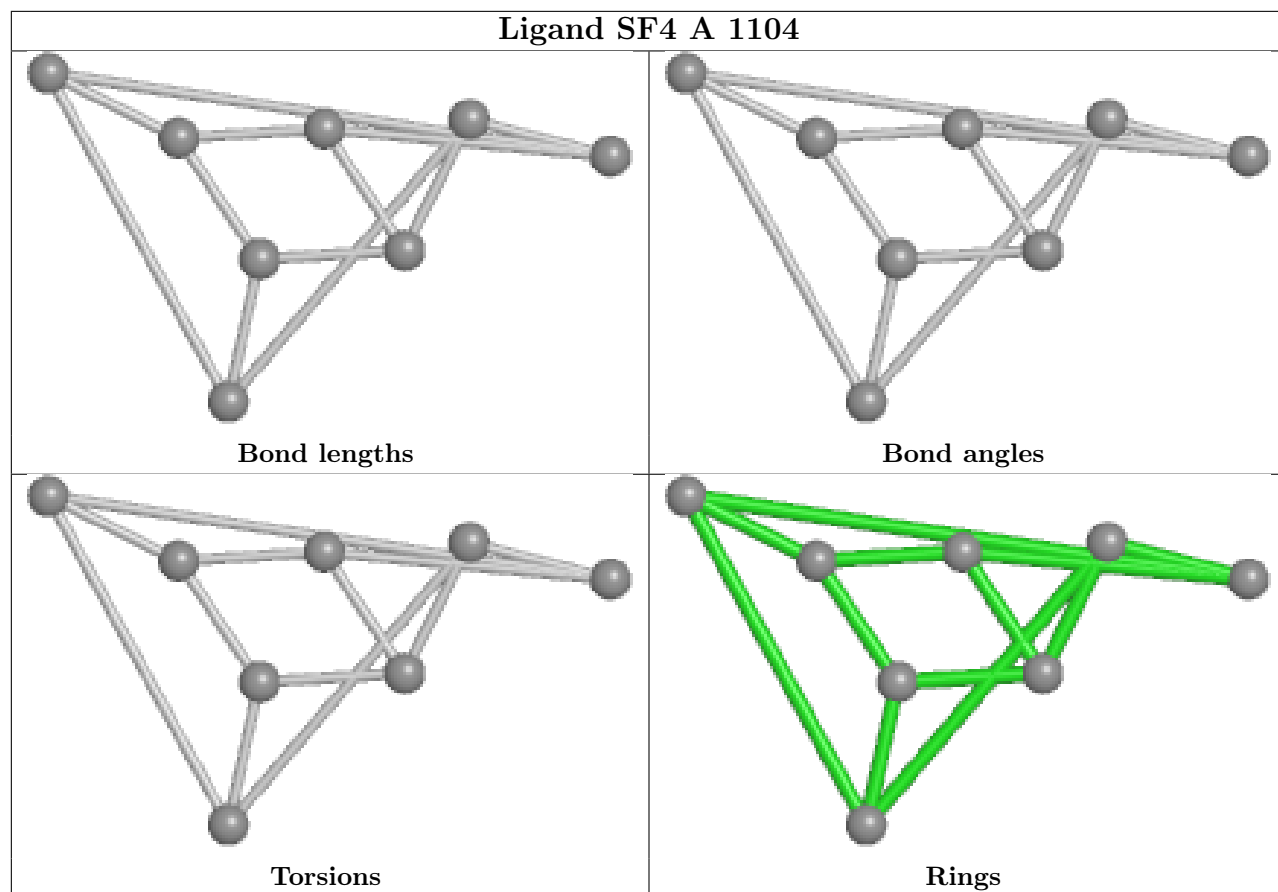
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1105	FAD	1	0
4	D	1106	NAP	1	0
5	B	1108	FMN	1	0
3	C	1106	FAD	1	0
5	D	1108	FMN	1	0
4	B	1106	NAP	5	0
4	A	1106	NAP	5	0
4	C	1107	NAP	4	0
3	A	1105	FAD	1	0
5	C	1109	FMN	1	0
5	A	1107	FMN	1	0

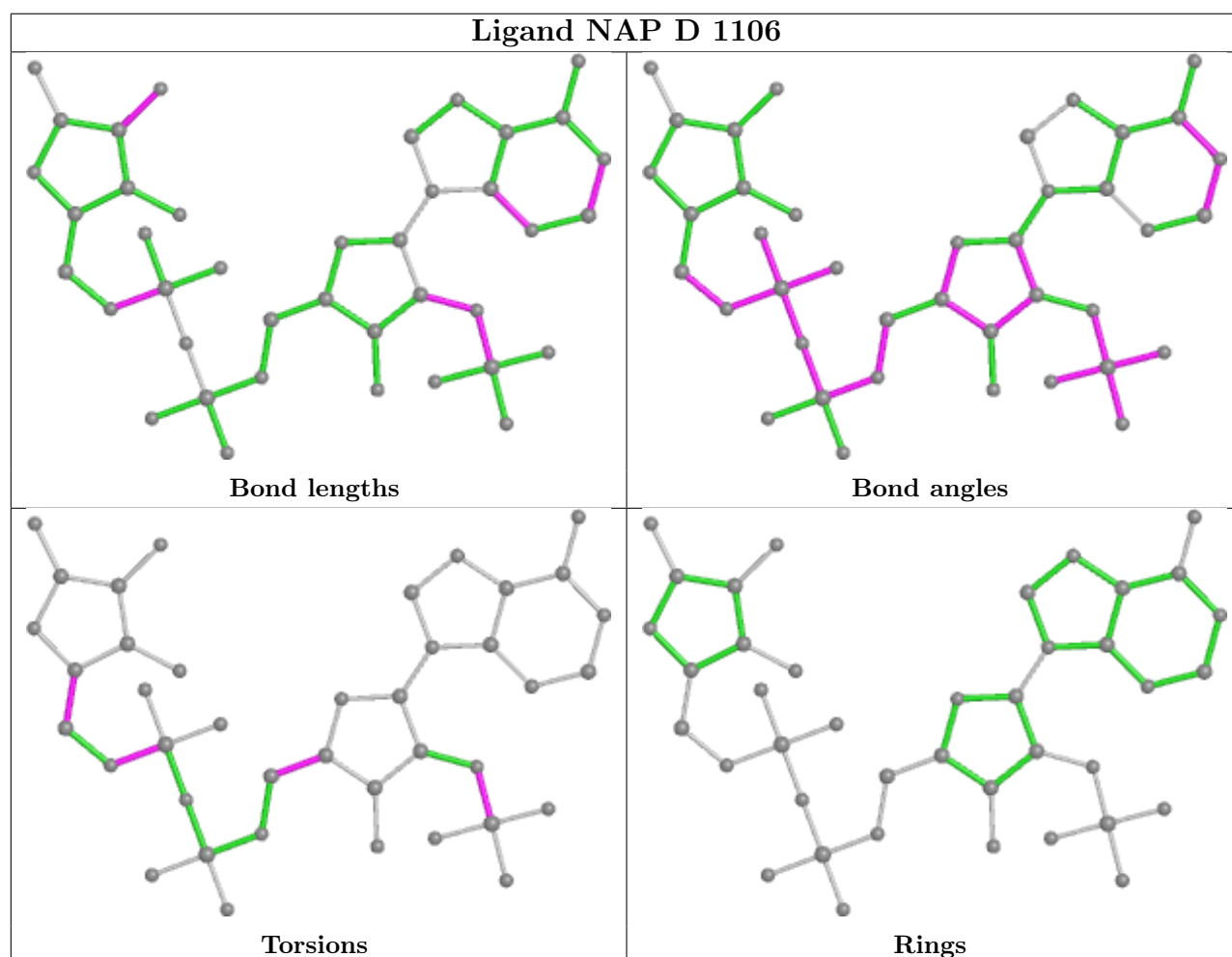
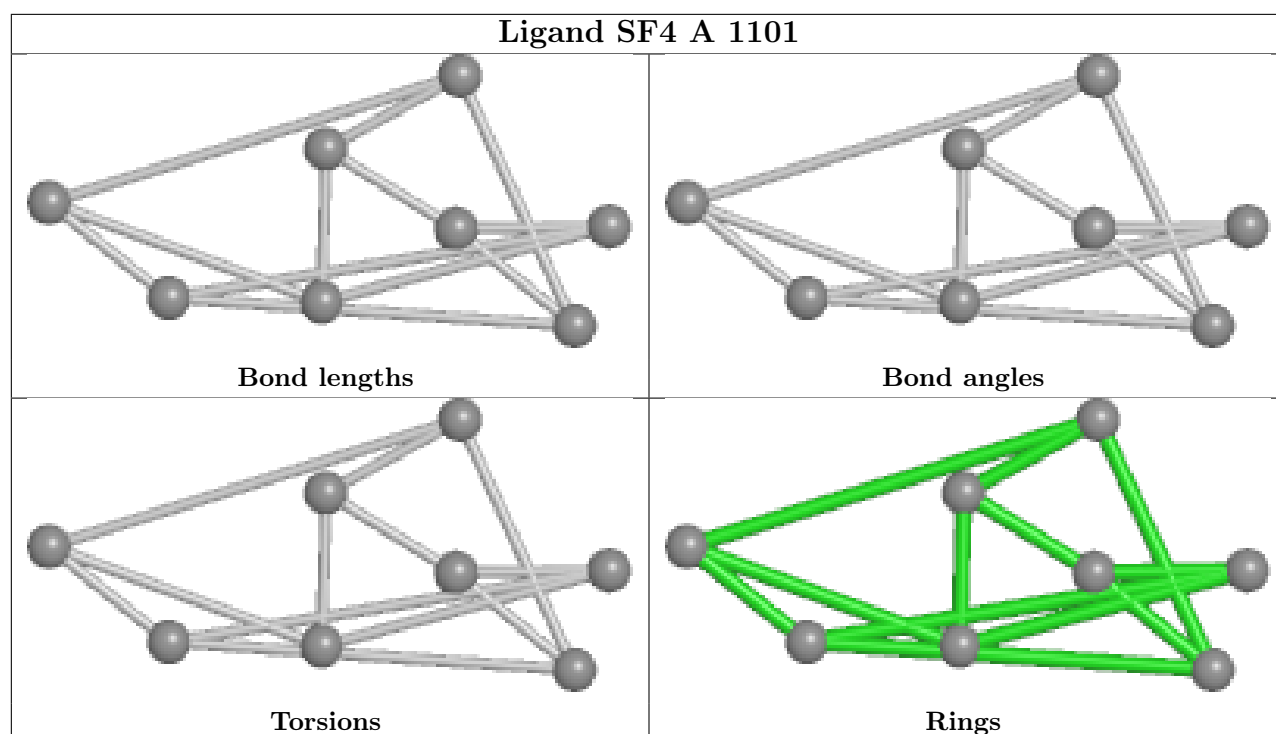
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



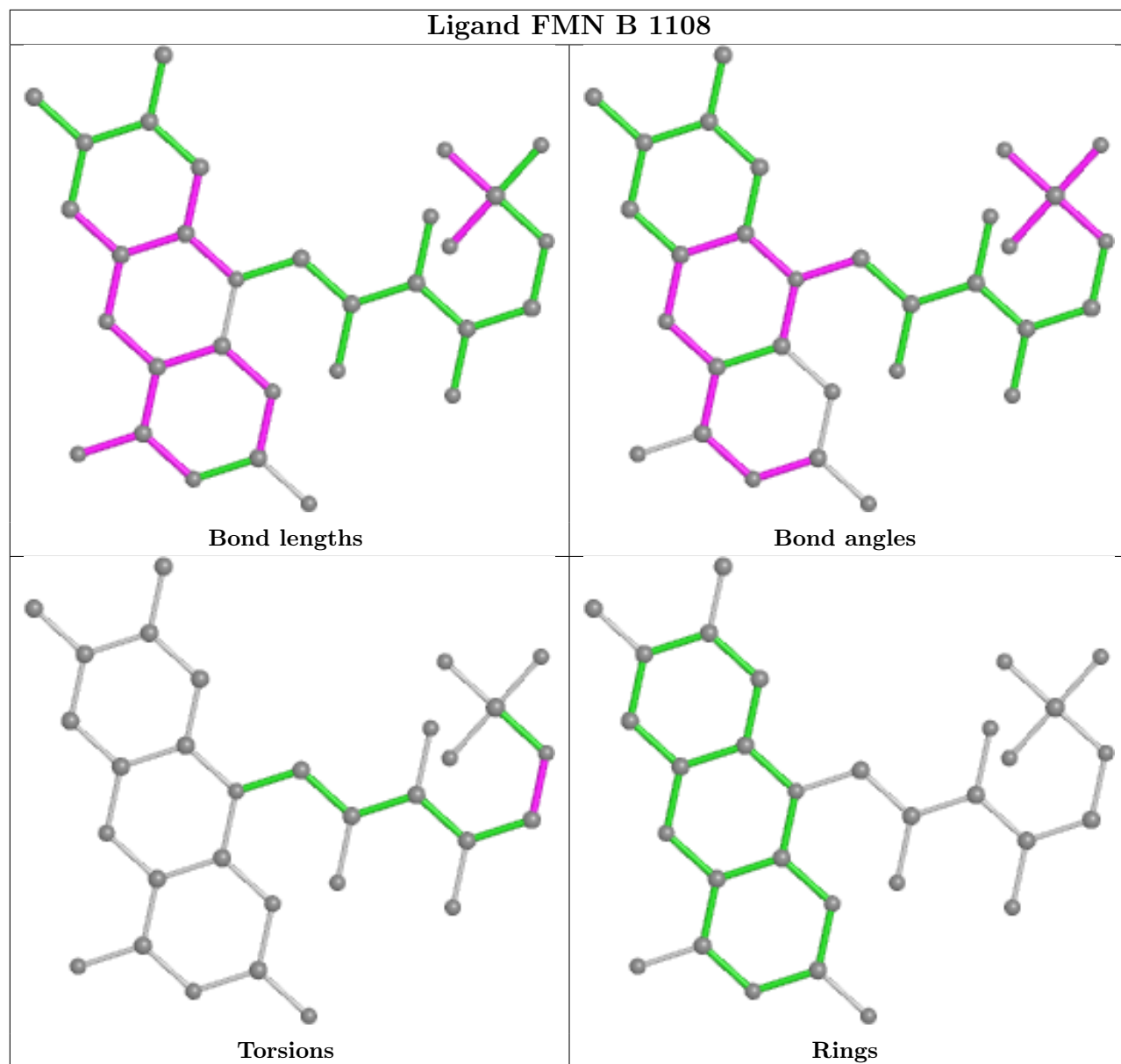


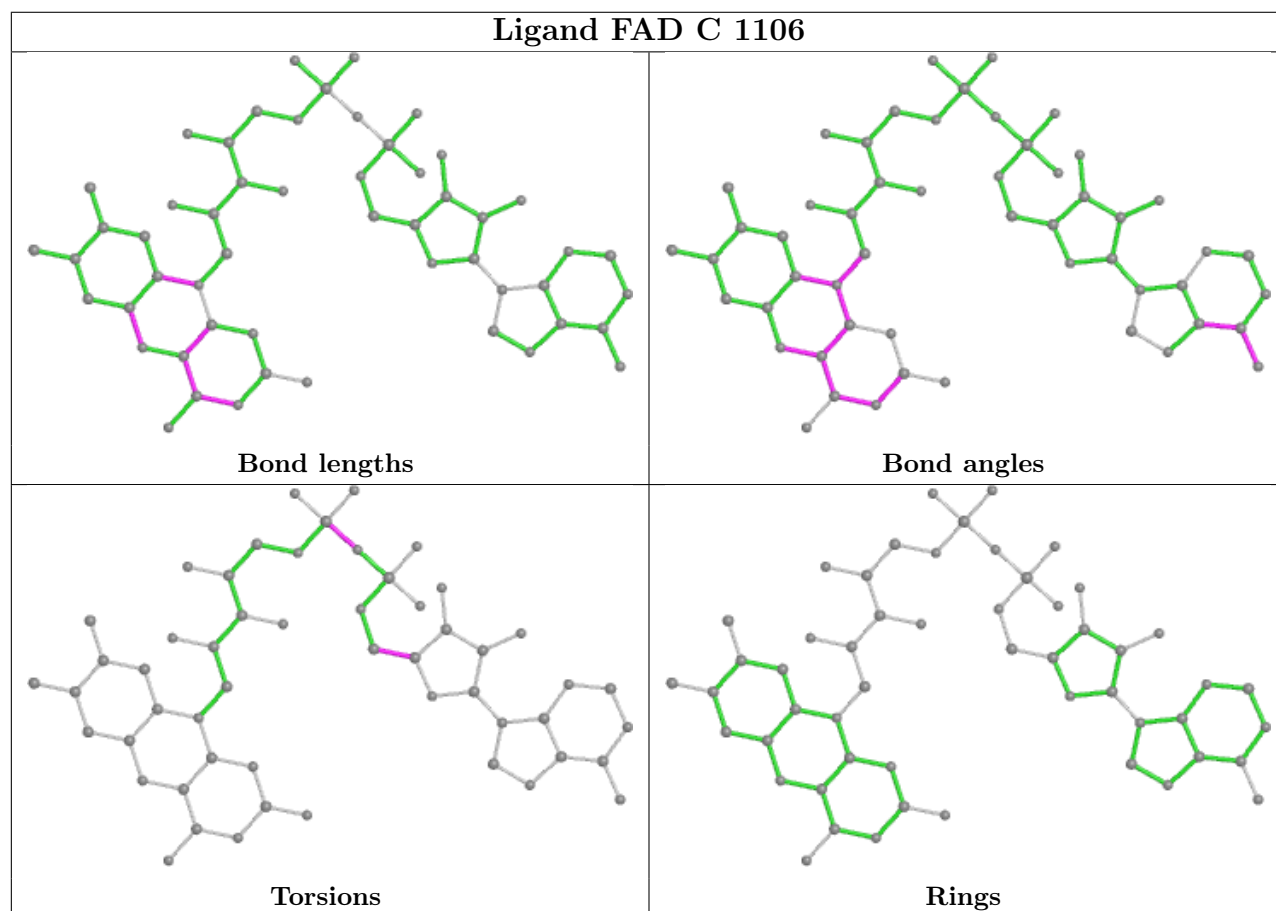
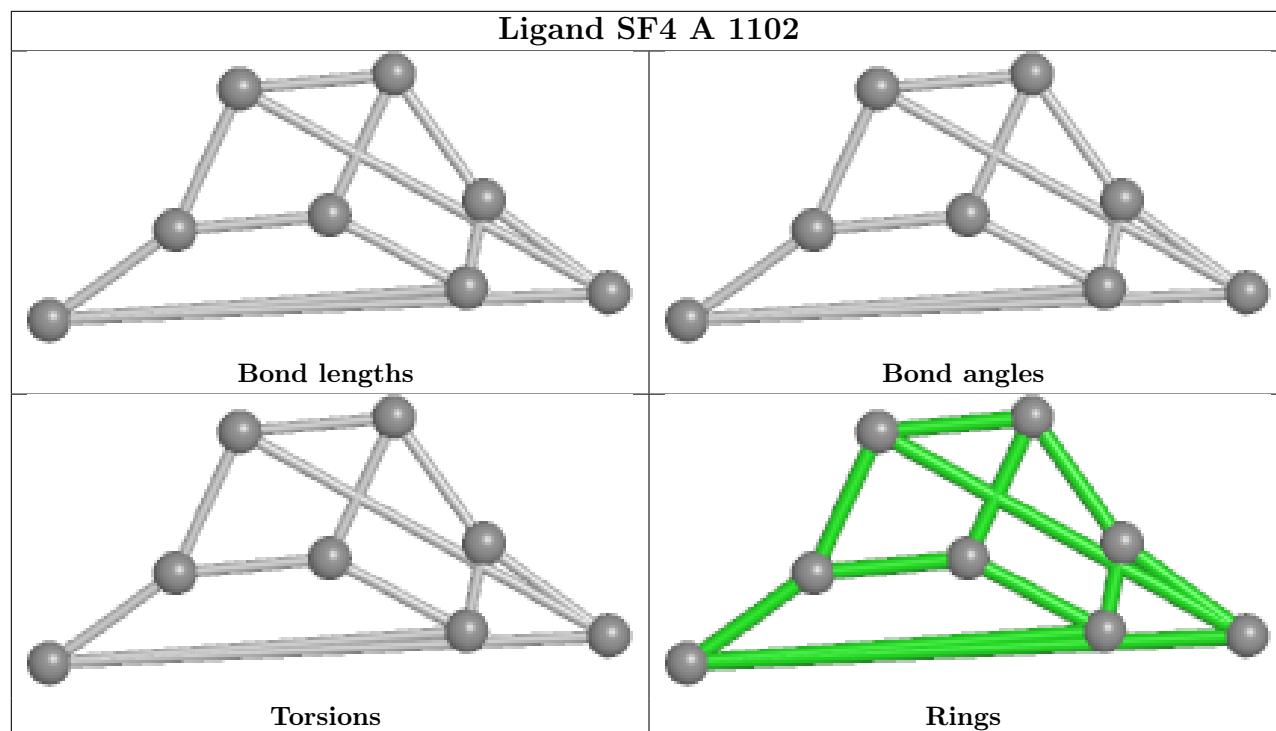


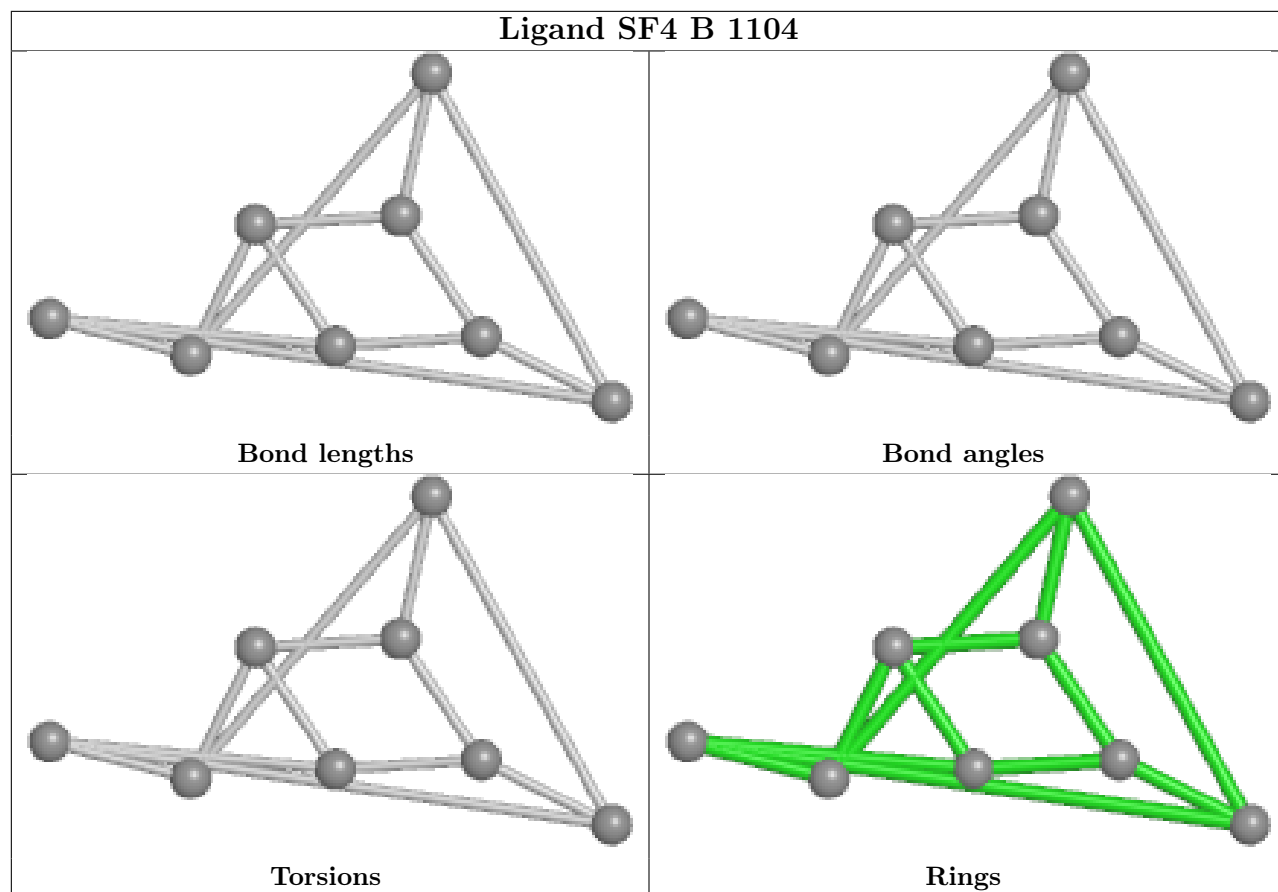


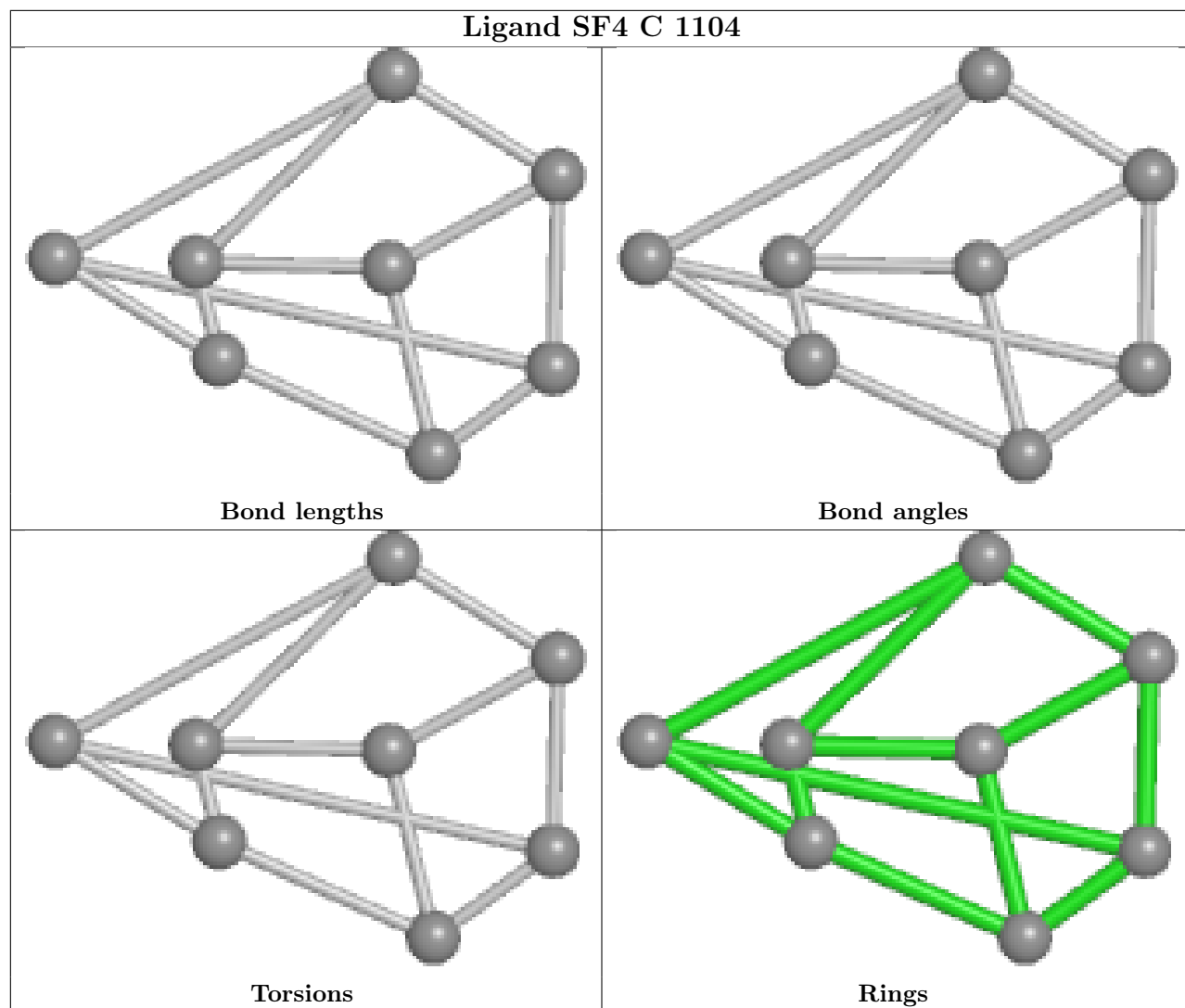


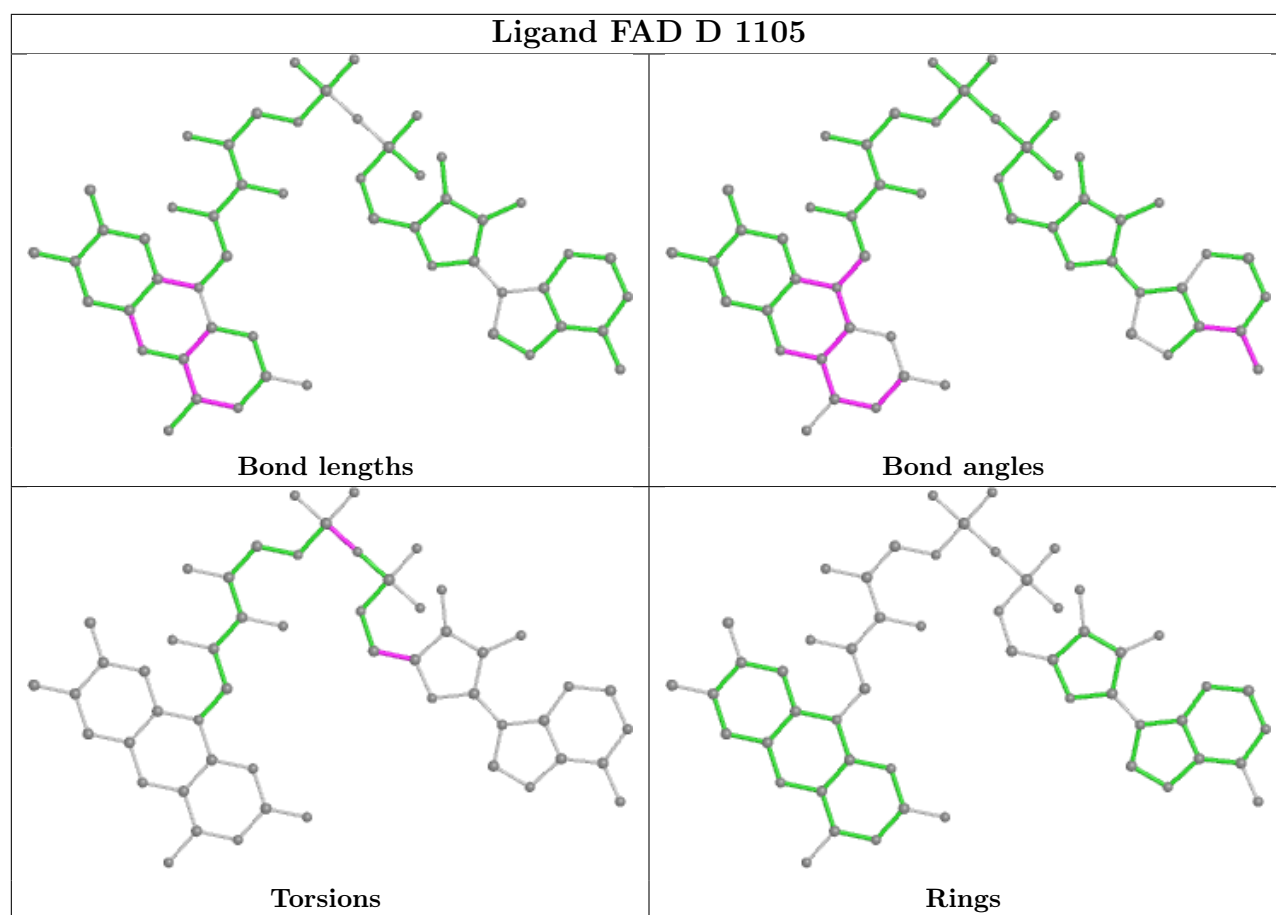
## Ligand FMN B 1108





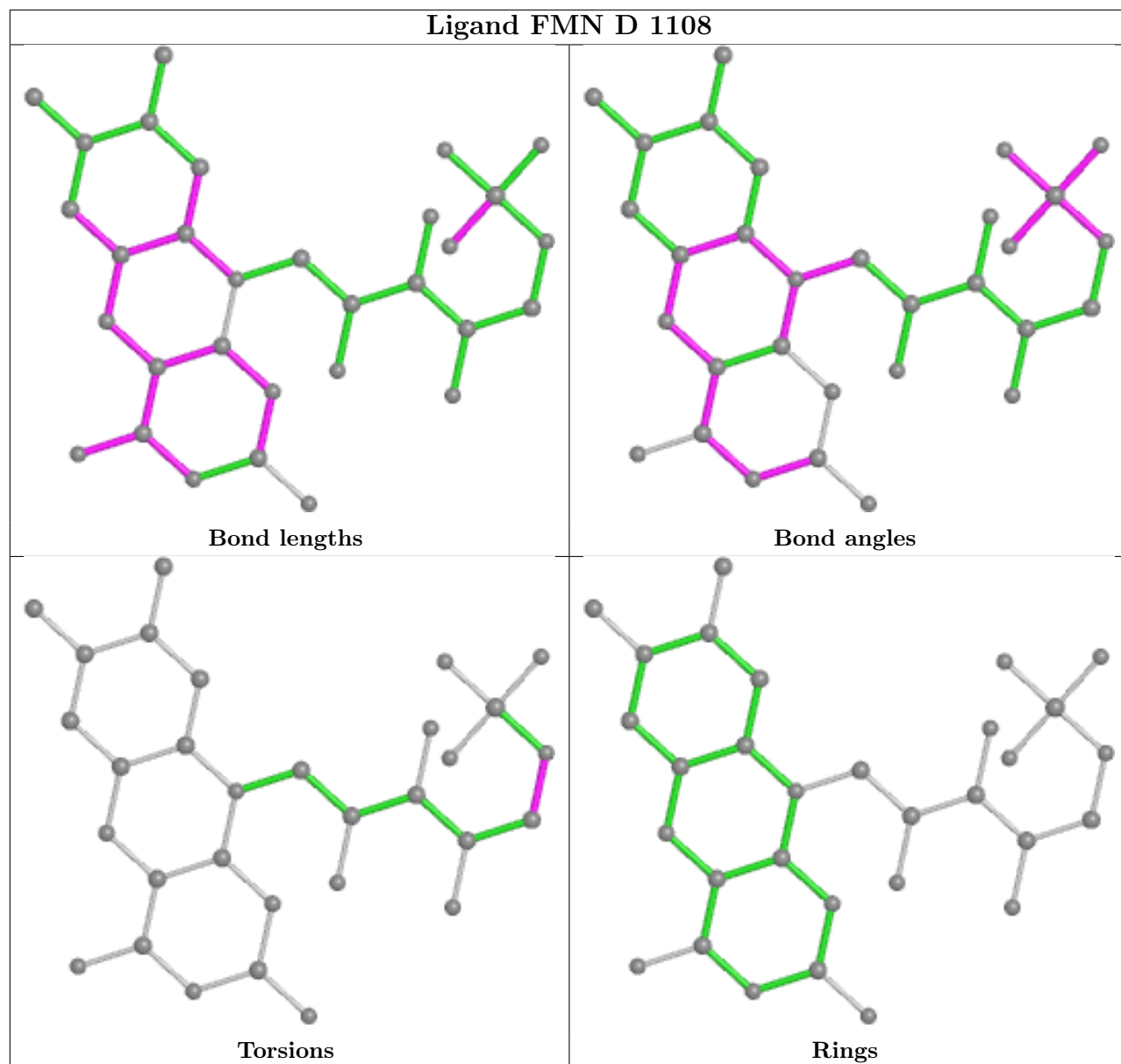




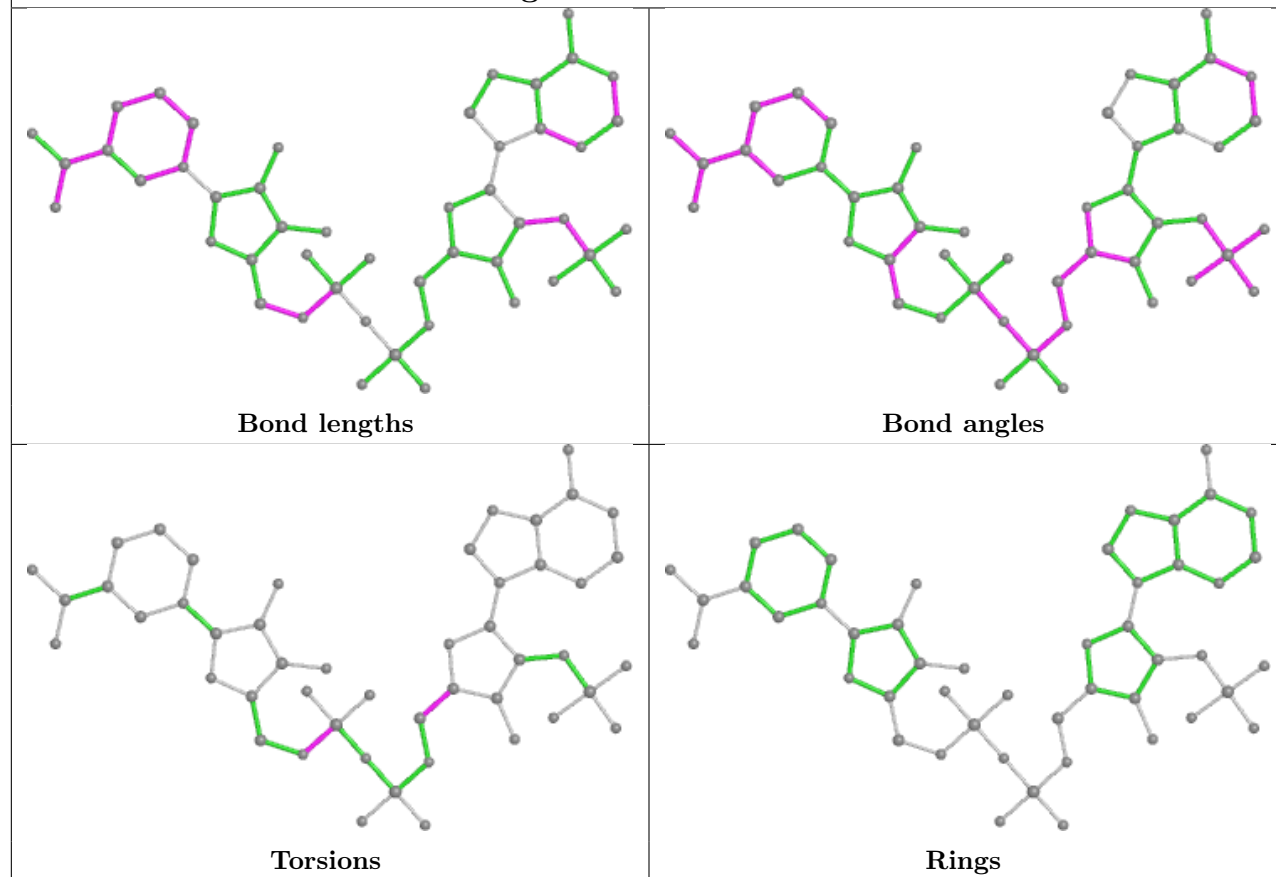




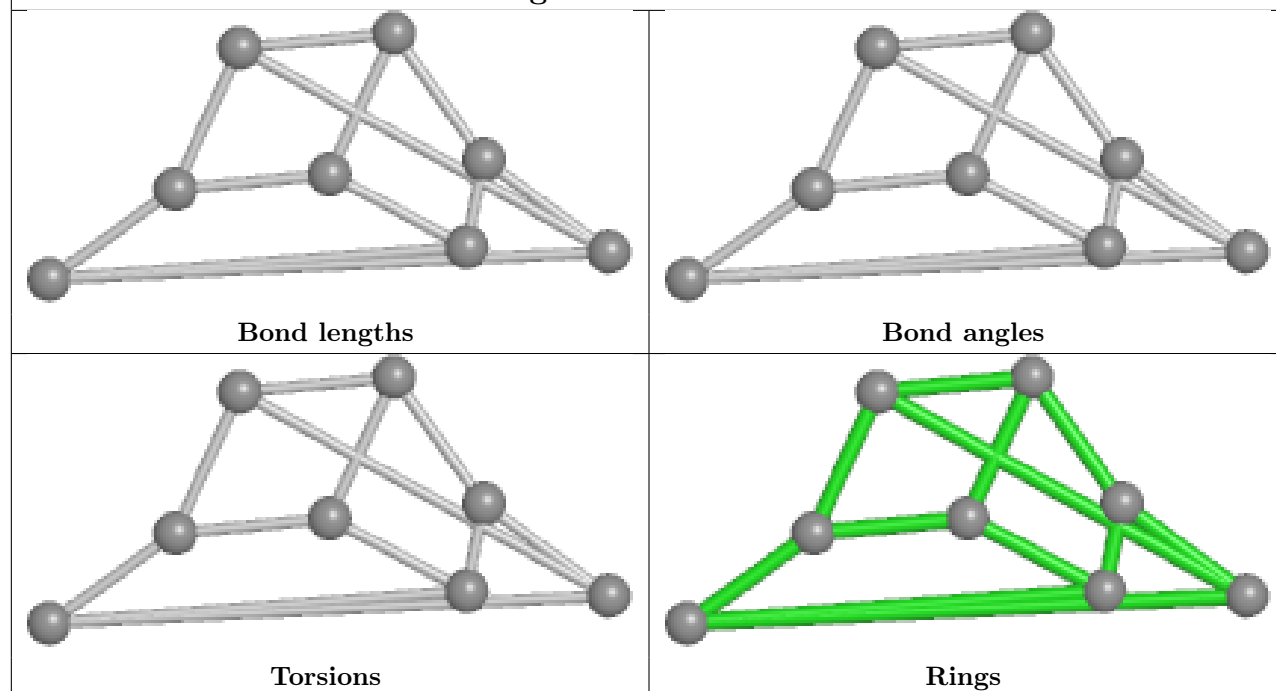
## Ligand FMN D 1108

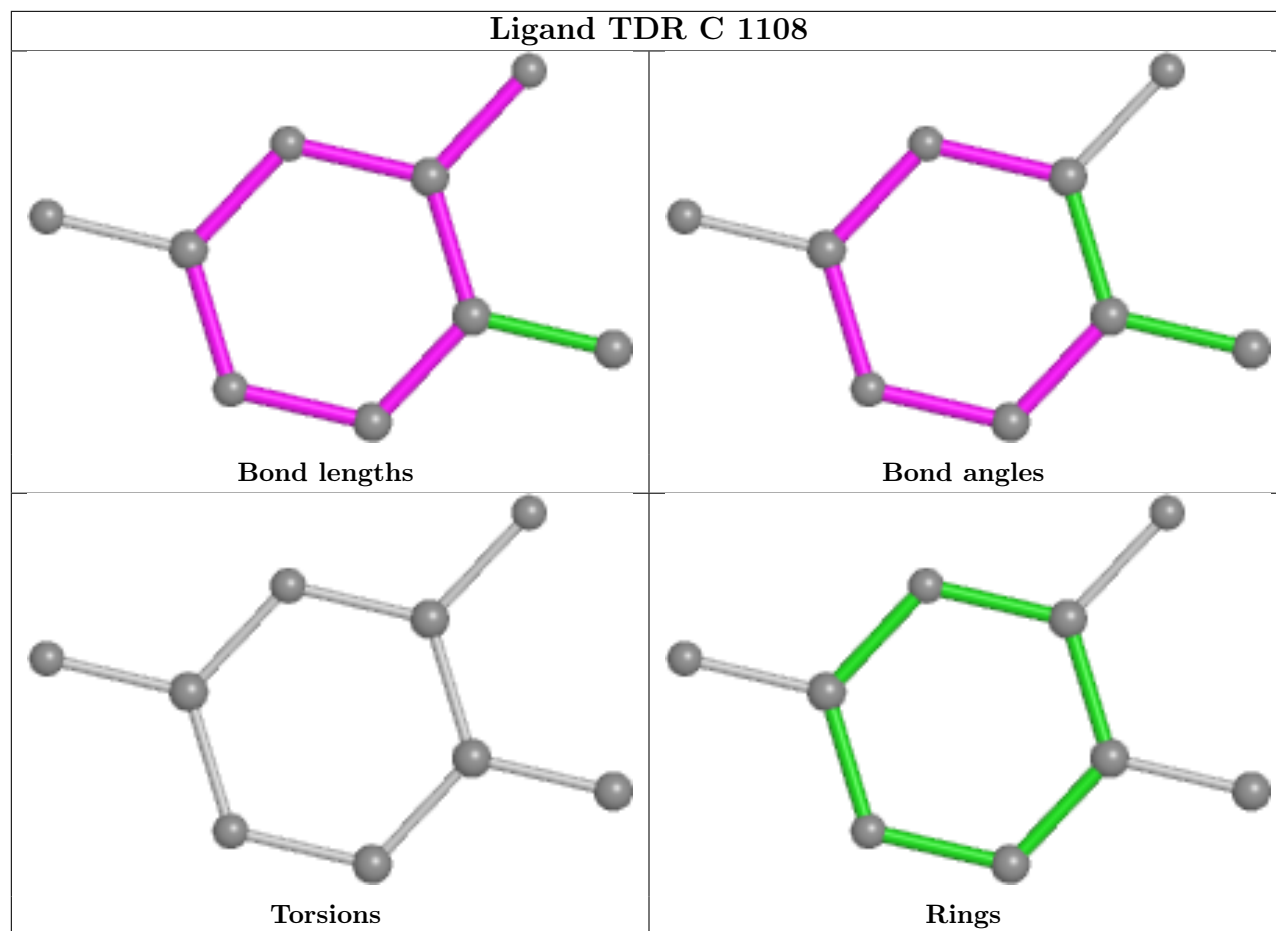


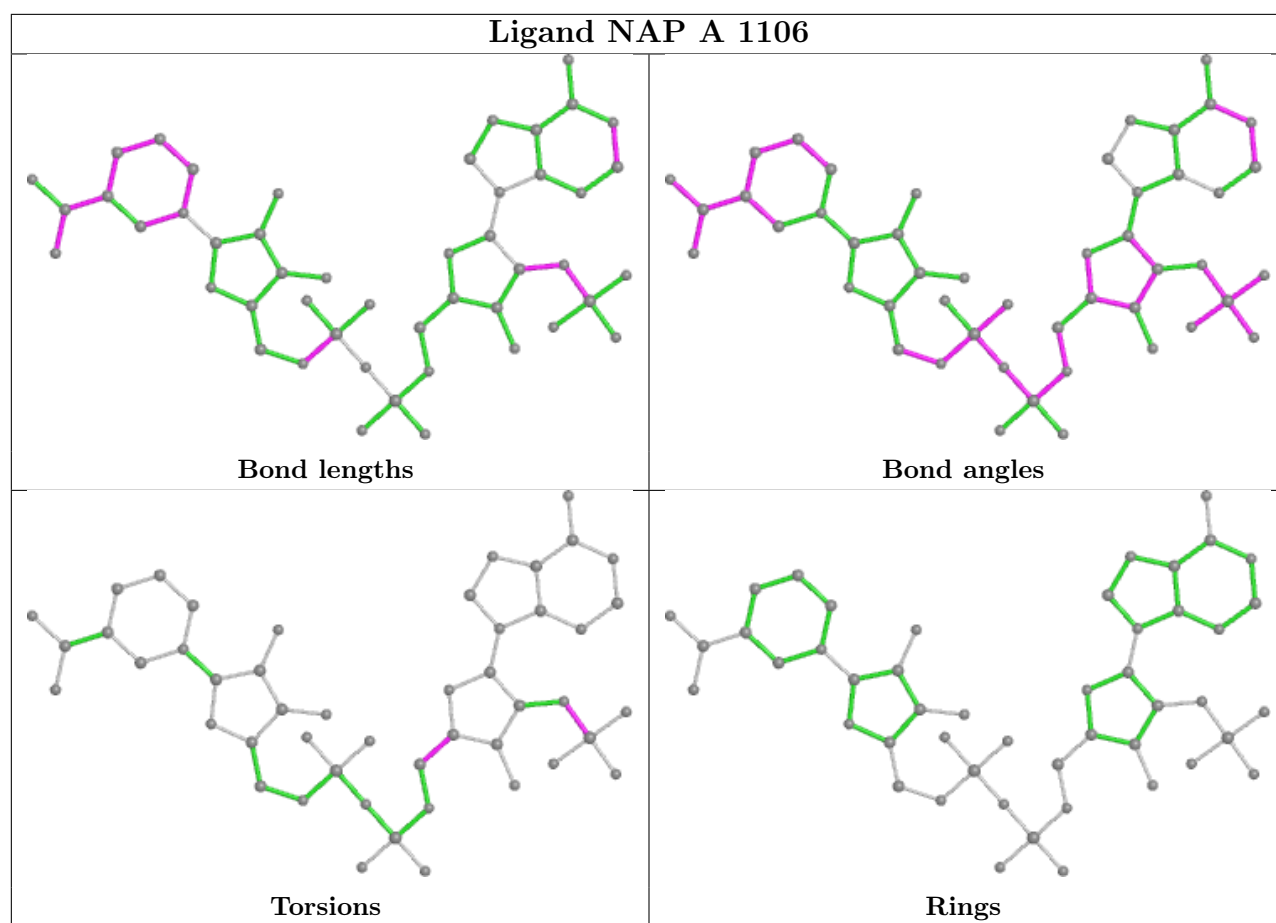
## Ligand NAP B 1106



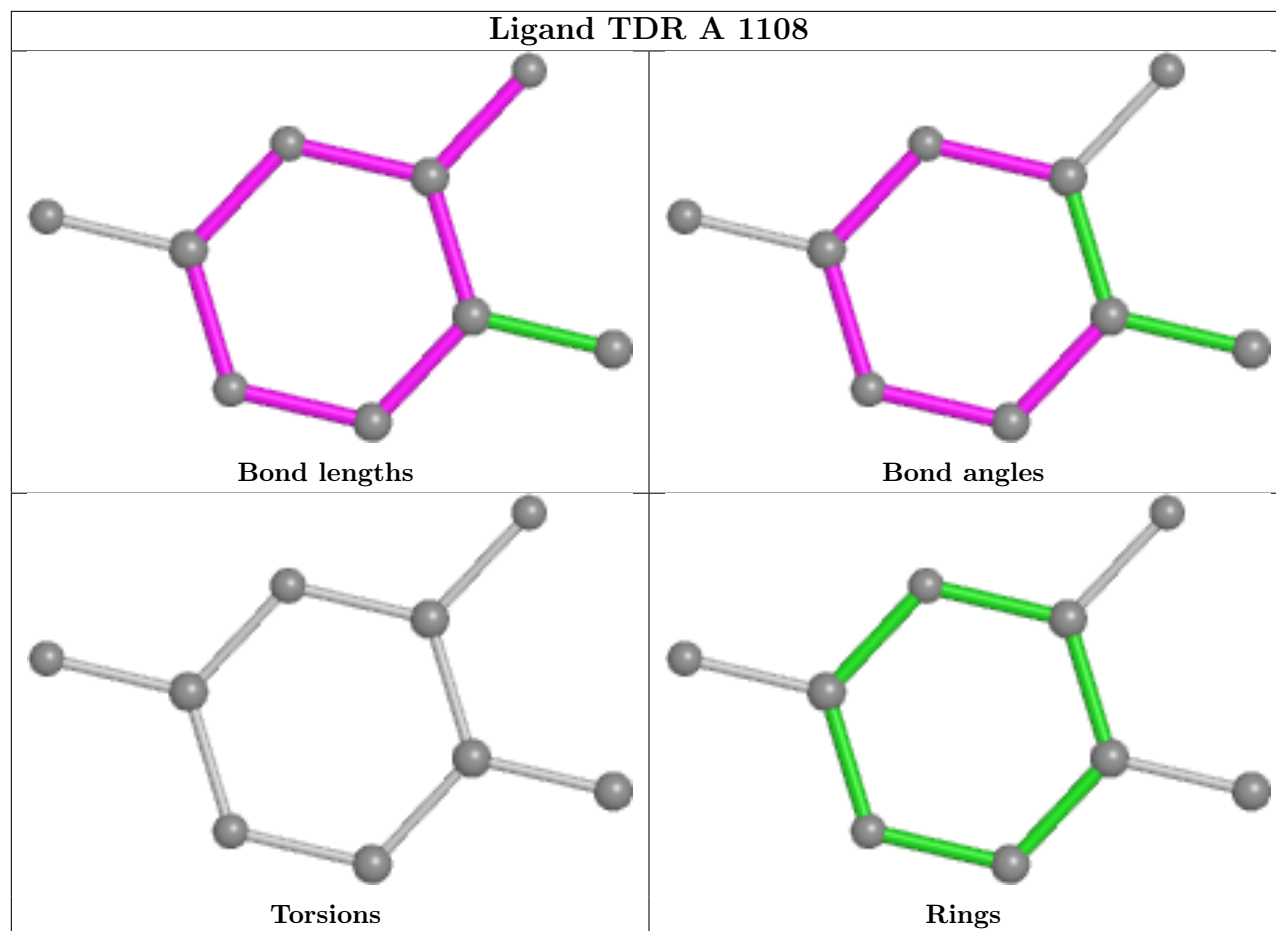
## Ligand SF4 D 1101



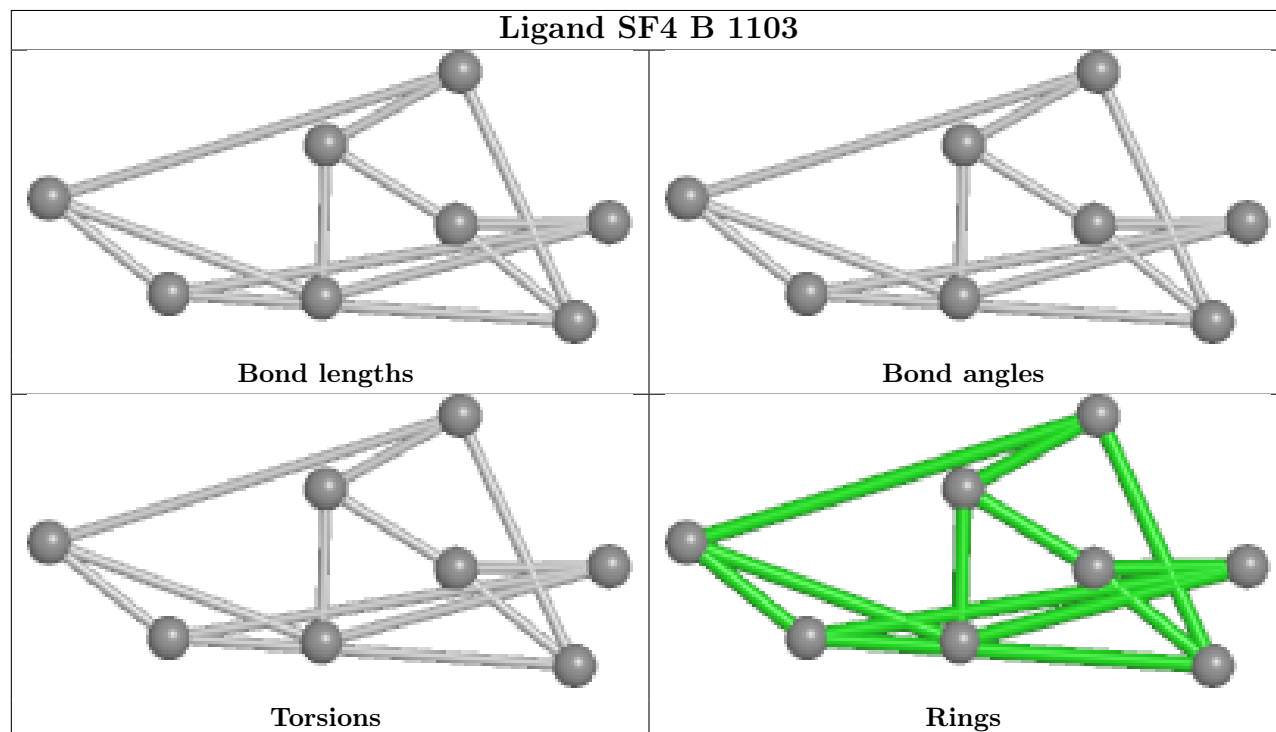


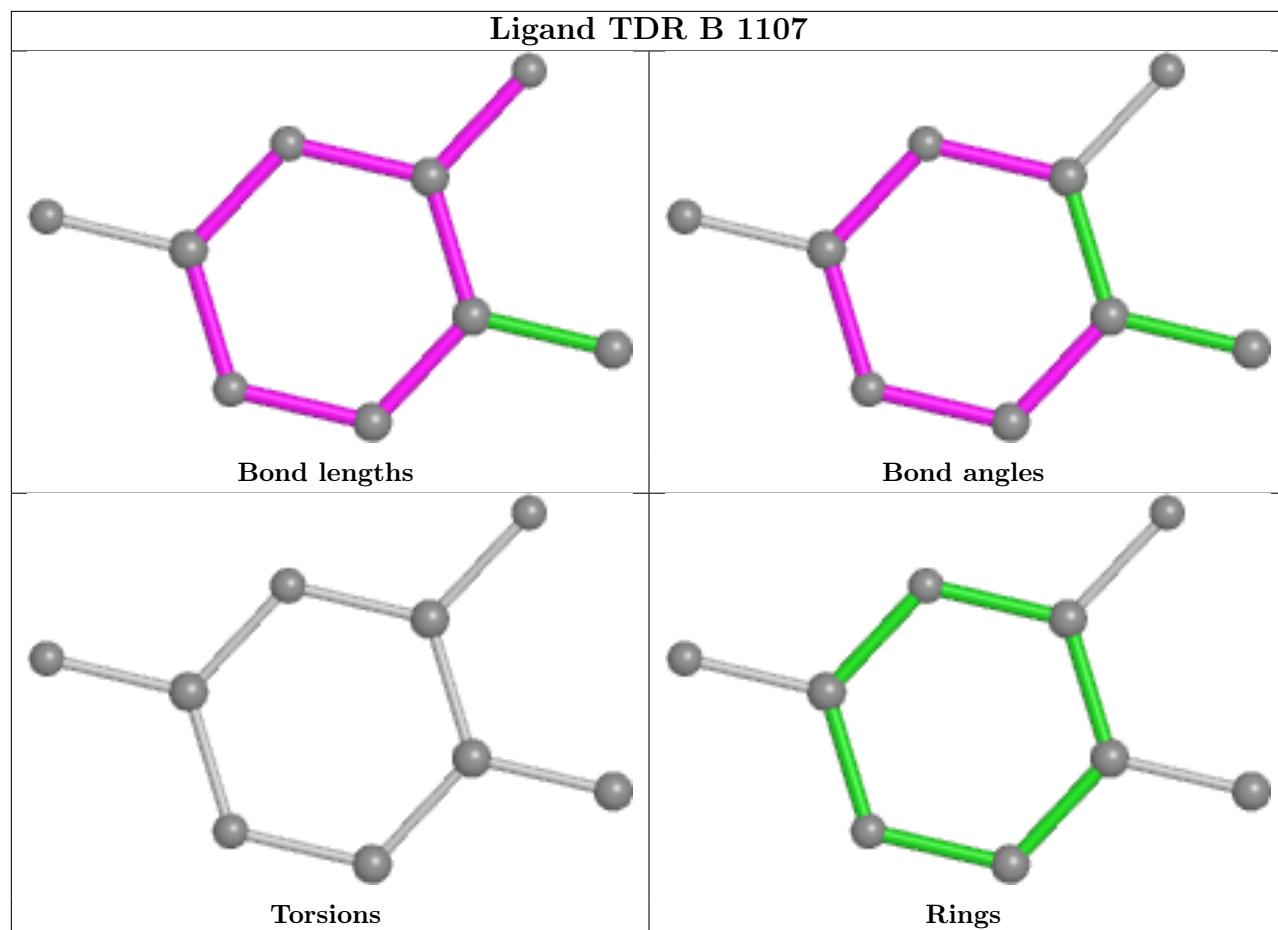
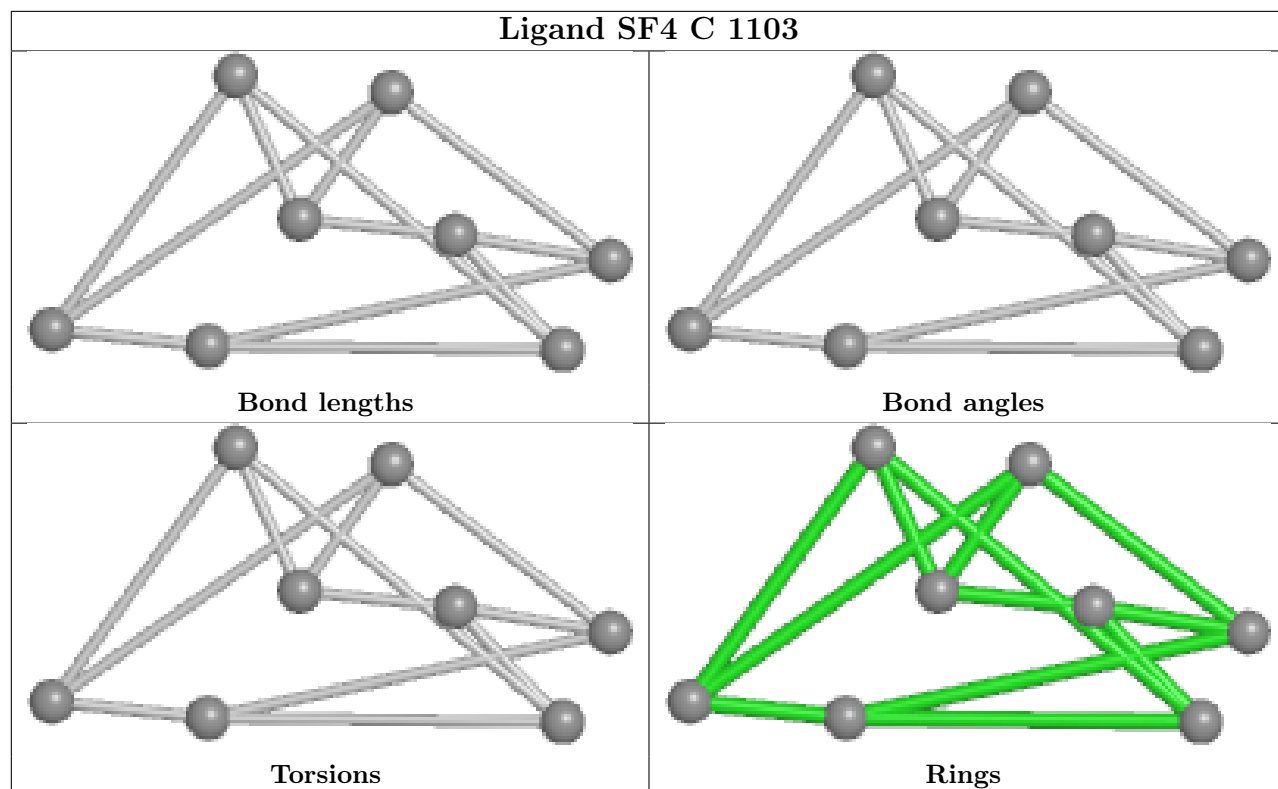


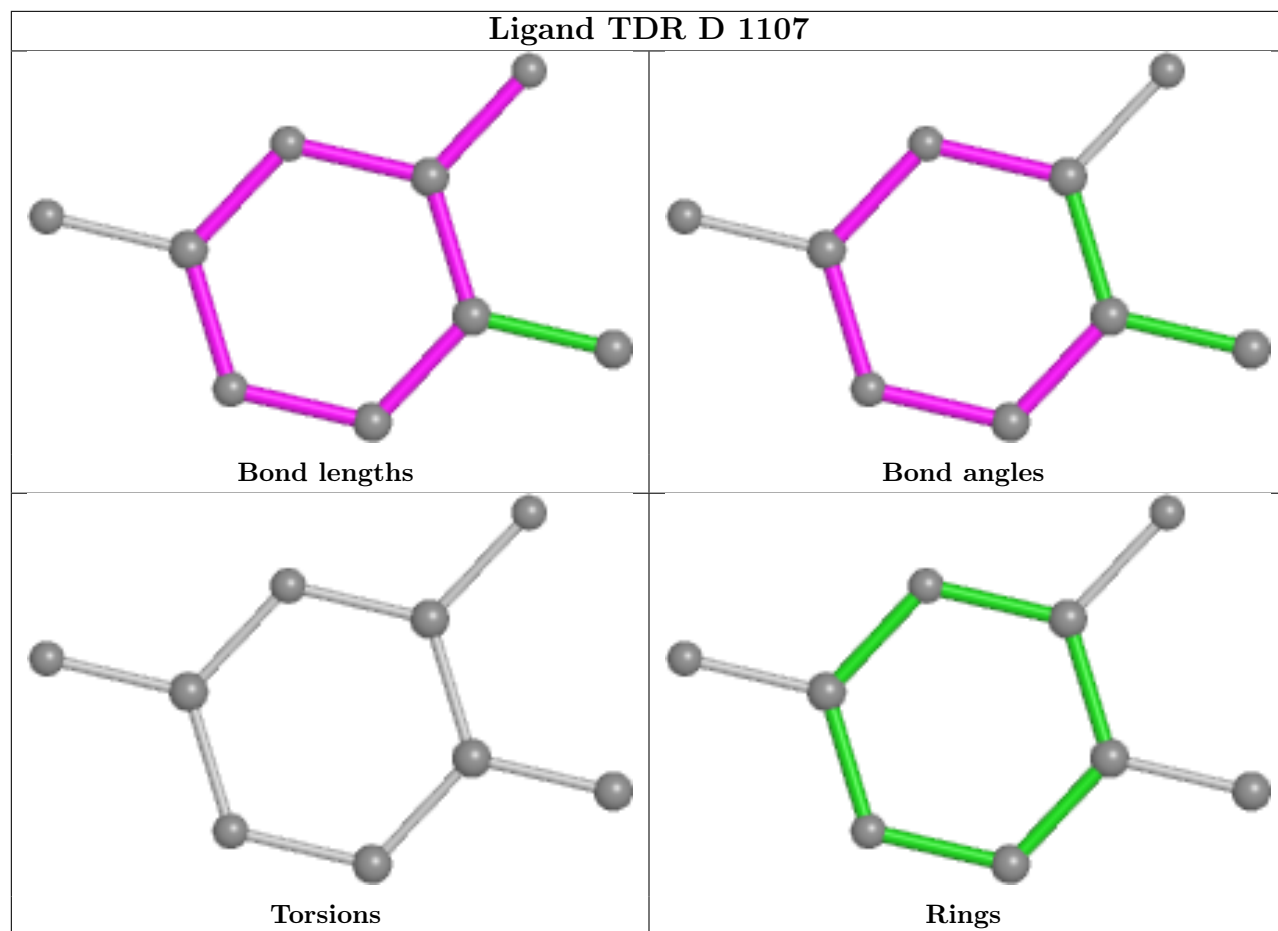
## Ligand TDR A 1108

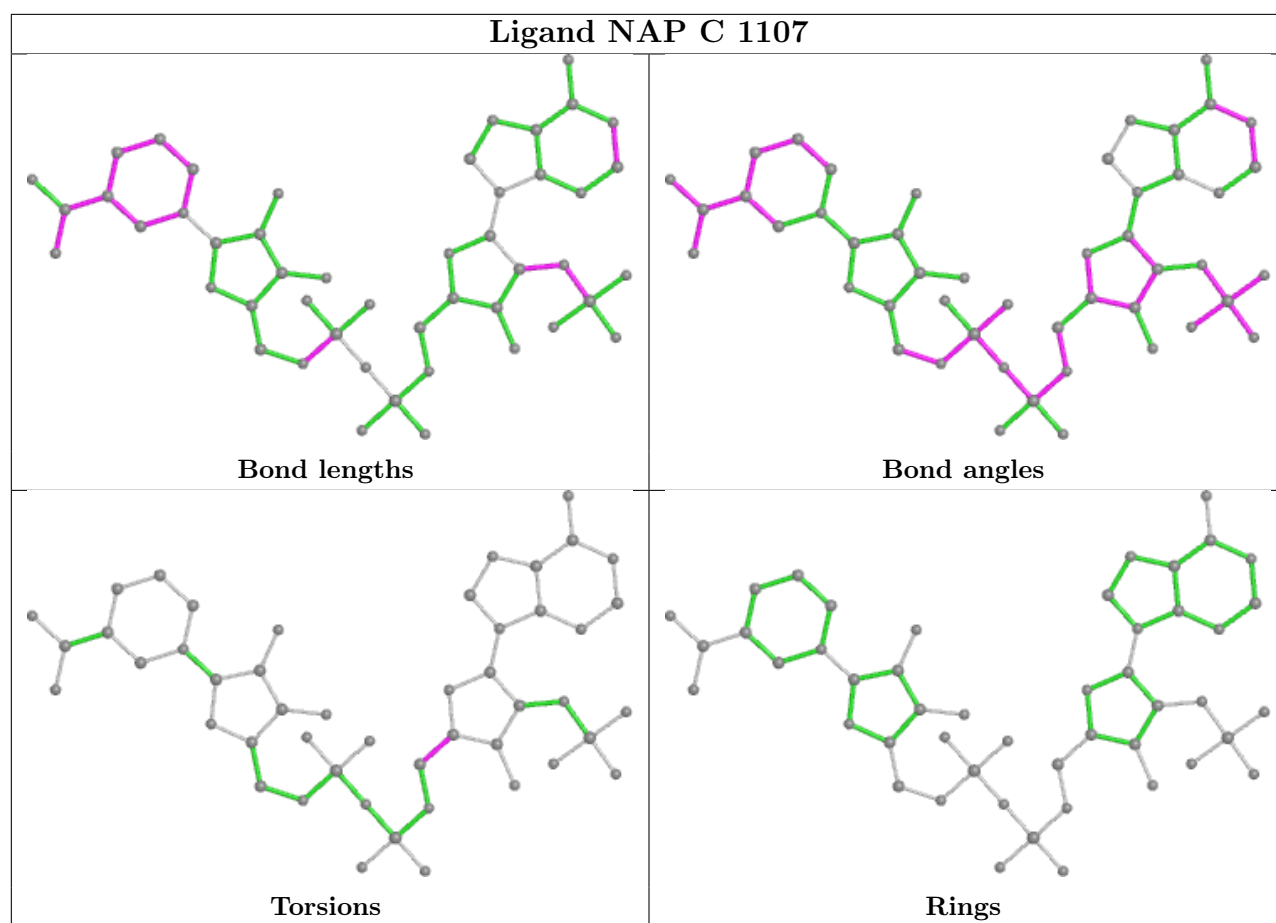


## Ligand SF4 B 1103

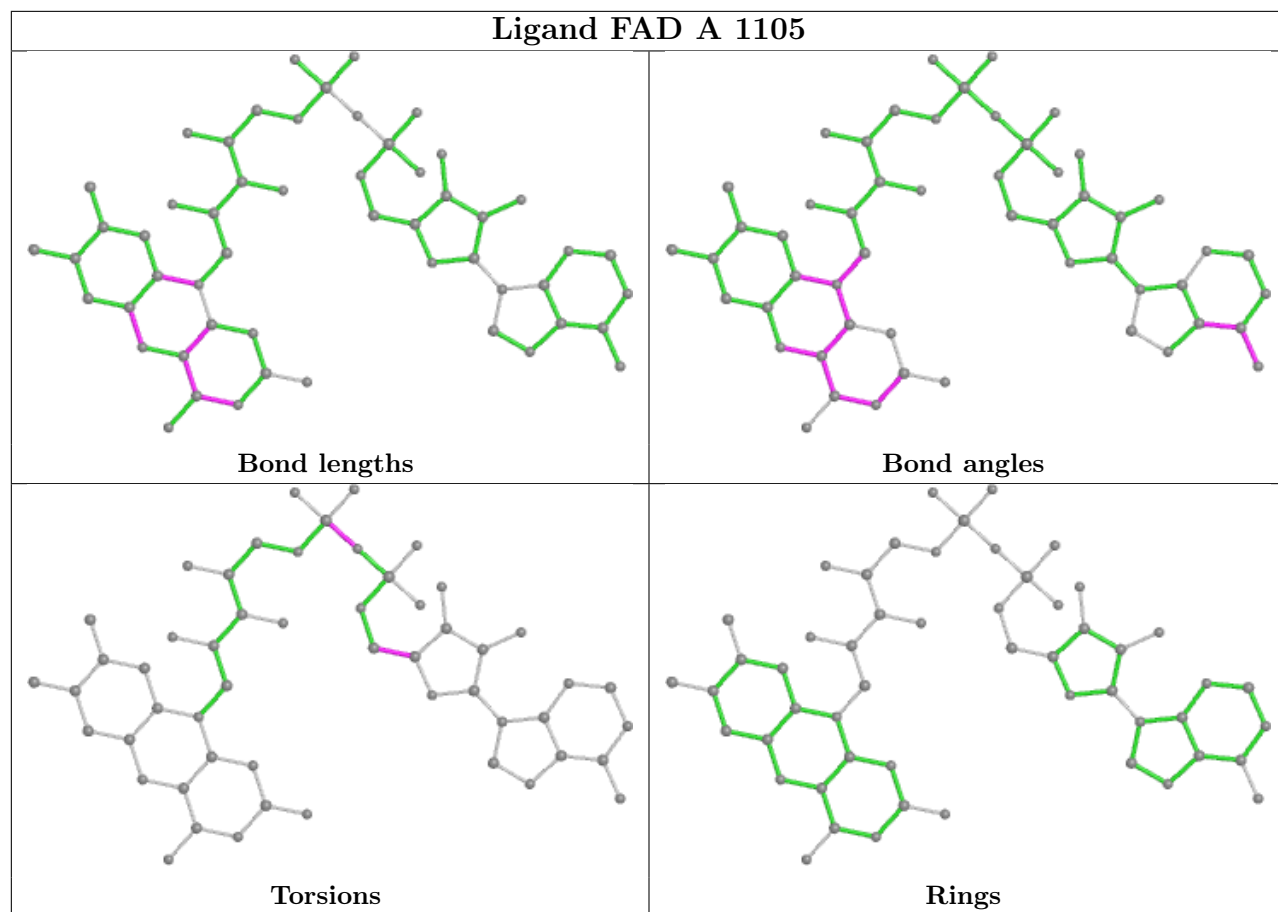


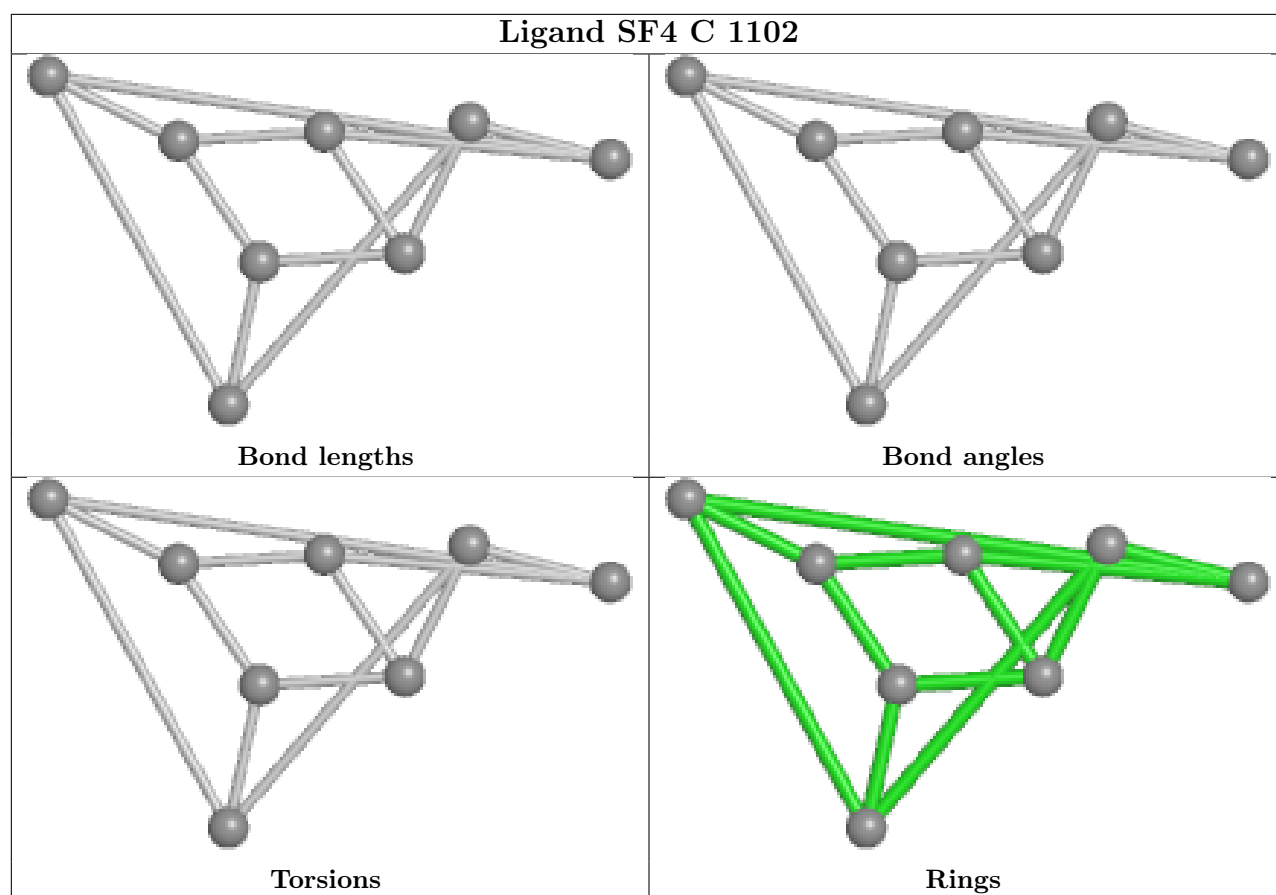




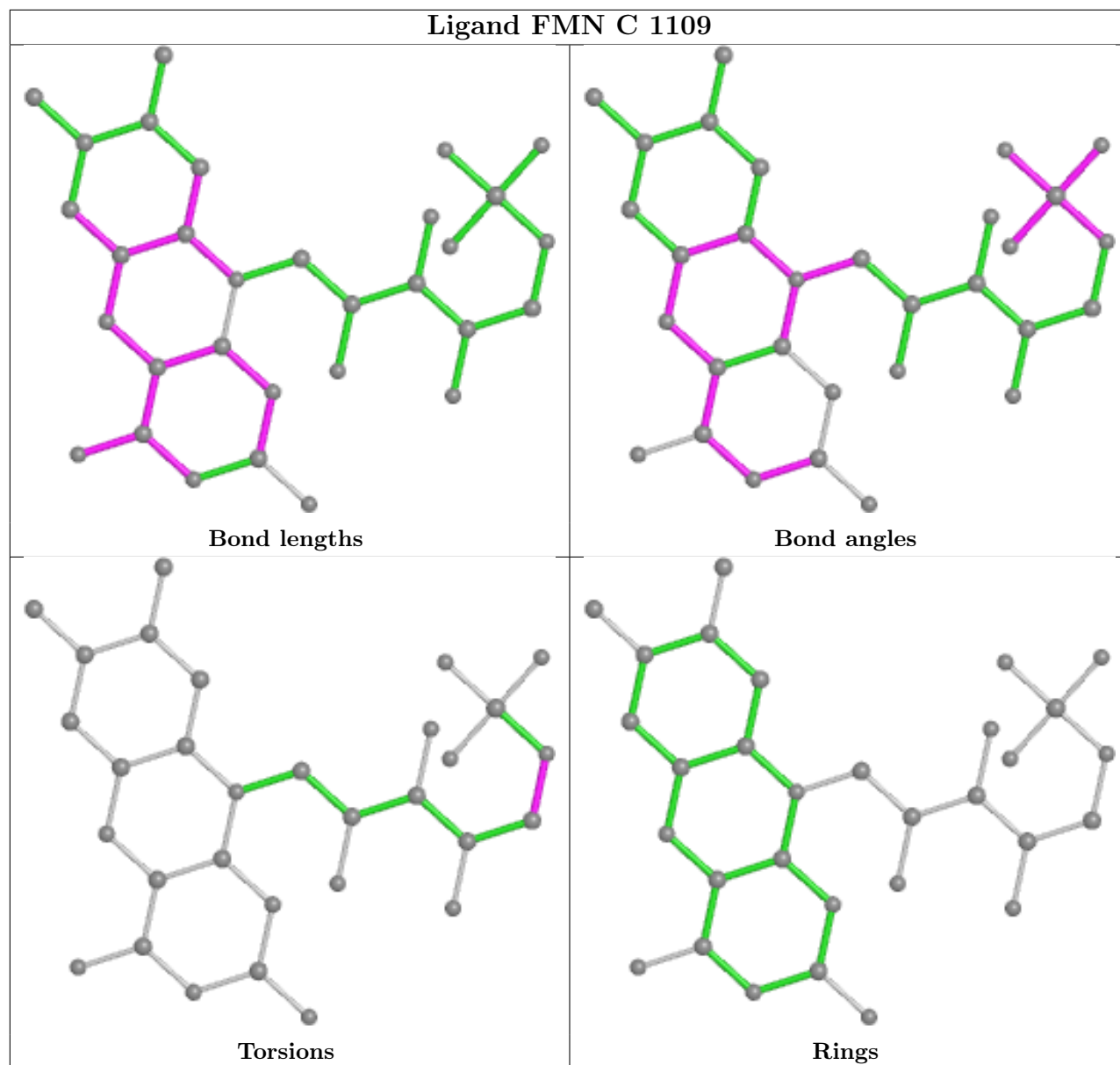


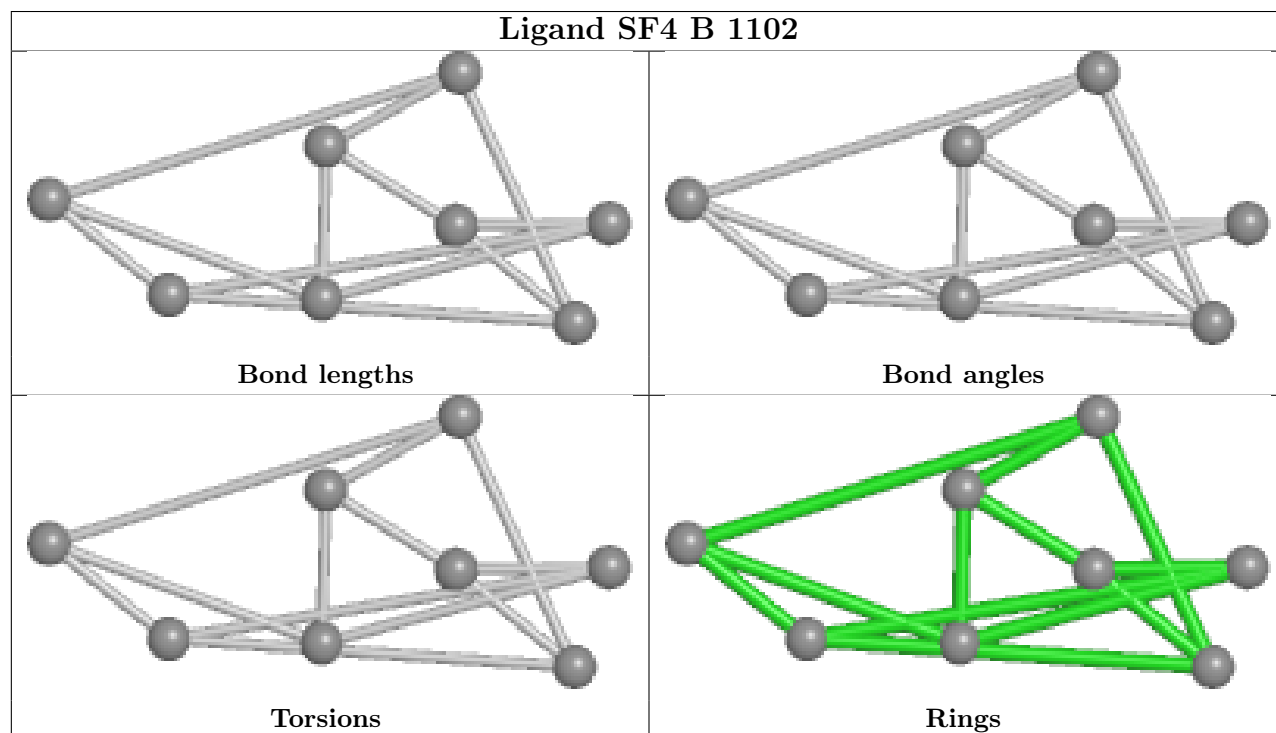
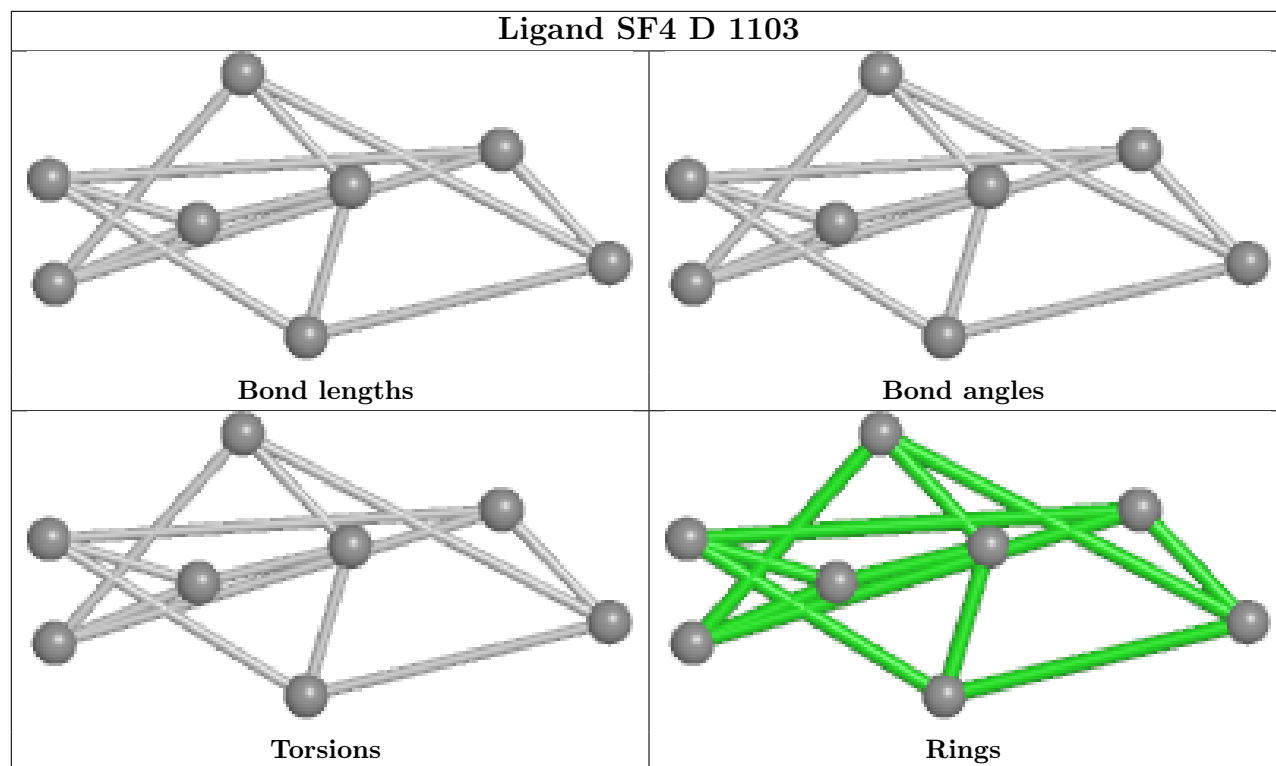


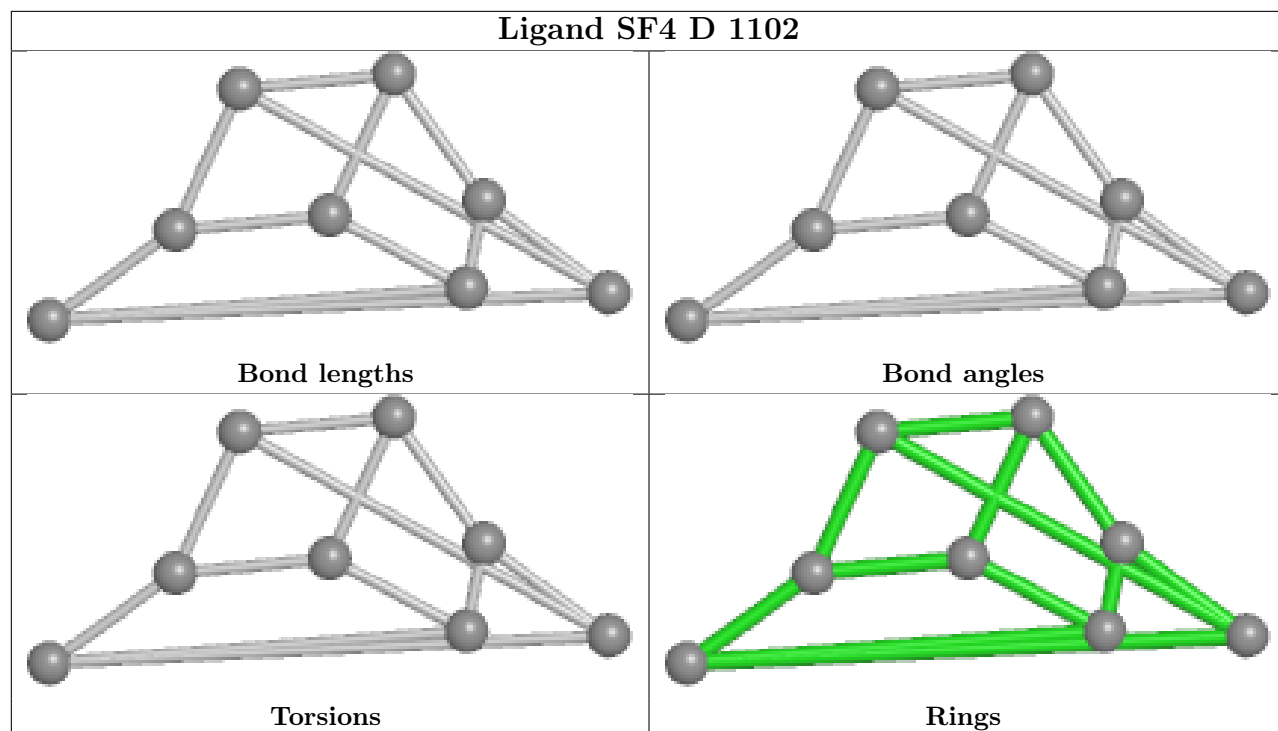




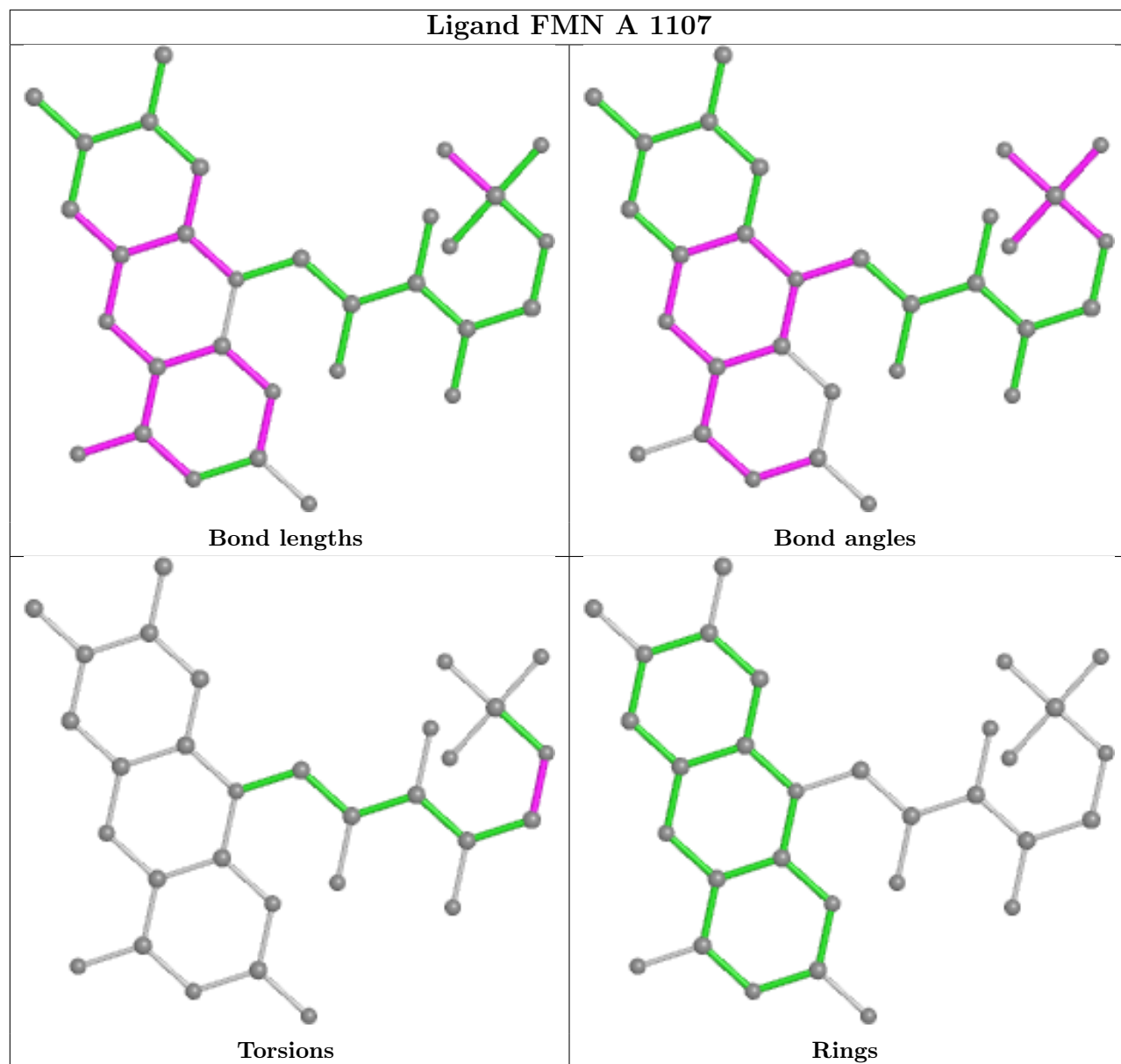
## Ligand FMN C 1109

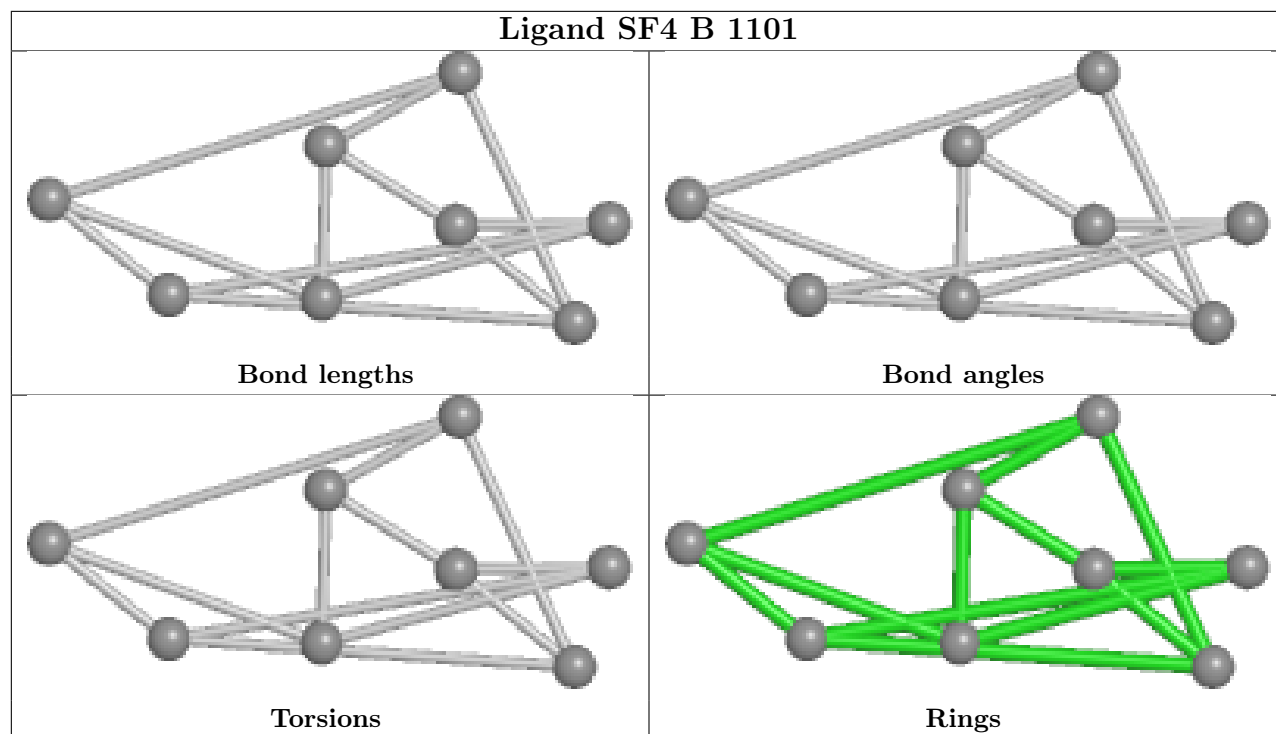






## Ligand FMN A 1107





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1005/1025 (98%)	-0.02	33 (3%) 46 51	15, 22, 45, 85	0
1	B	1006/1025 (98%)	-0.01	41 (4%) 37 41	16, 23, 48, 84	0
1	C	1007/1025 (98%)	-0.10	33 (3%) 46 51	12, 21, 45, 73	0
1	D	1011/1025 (98%)	-0.06	36 (3%) 42 47	13, 21, 46, 81	0
All	All	4029/4100 (98%)	-0.05	143 (3%) 44 49	12, 22, 47, 85	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	907	LEU	19.8
1	B	897	LEU	9.3
1	B	907	LEU	8.6
1	B	902	ALA	7.5
1	D	907	LEU	7.3
1	A	324	CYS	7.2
1	A	50	PHE	7.1
1	B	899	GLU	7.1
1	B	901	ASN	6.8
1	A	52	CYS	6.6
1	D	52	CYS	6.4
1	D	415	GLU	6.4
1	B	52	CYS	6.4
1	D	51	HIS	6.2
1	A	901	ASN	6.2
1	A	899	GLU	6.2
1	D	897	LEU	6.1
1	B	870	GLU	6.1
1	B	900	GLN	6.0
1	D	900	GLN	5.9
1	C	325	HIS	5.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	901	ASN	5.5
1	D	902	ALA	5.5
1	A	51	HIS	5.5
1	D	416	THR	5.3
1	B	869	ALA	5.2
1	D	869	ALA	5.2
1	A	908	GLU	5.1
1	B	417	GLY	5.1
1	B	867	ARG	5.1
1	D	899	GLU	5.1
1	A	415	GLU	5.1
1	D	913	ILE	5.0
1	A	902	ALA	5.0
1	C	872	MET	4.9
1	C	415	GLU	4.9
1	B	871	LEU	4.9
1	A	900	GLN	4.8
1	C	416	THR	4.8
1	B	680	MET	4.4
1	A	897	LEU	4.4
1	D	414	ASP	4.4
1	A	416	THR	4.4
1	C	52	CYS	4.4
1	A	1017	LEU	4.4
1	C	902	ALA	4.3
1	D	873	GLY	4.2
1	B	324	CYS	4.2
1	A	870	GLU	4.1
1	C	904	PHE	4.0
1	B	415	GLU	3.9
1	B	872	MET	3.9
1	B	908	GLU	3.9
1	C	357	ARG	3.8
1	B	51	HIS	3.8
1	C	901	ASN	3.8
1	C	900	GLN	3.8
1	B	459	TRP	3.7
1	D	868	ILE	3.7
1	B	896	ARG	3.7
1	D	459	TRP	3.7
1	B	898	LYS	3.6
1	D	867	ARG	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	324	CYS	3.5
1	A	868	ILE	3.5
1	D	870	GLU	3.5
1	B	673	HIS	3.5
1	B	416	THR	3.4
1	A	896	ARG	3.4
1	C	870	GLU	3.3
1	A	867	ARG	3.3
1	C	331	ILE	3.3
1	B	323	ALA	3.2
1	B	325	HIS	3.1
1	C	867	ARG	3.1
1	D	872	MET	3.1
1	C	320	GLY	3.1
1	C	682	LEU	3.1
1	C	897	LEU	3.1
1	D	909	ARG	3.0
1	D	367	PHE	3.0
1	C	332	ARG	3.0
1	C	871	LEU	3.0
1	A	869	ALA	3.0
1	C	322	CYS	2.9
1	A	909	ARG	2.8
1	C	903	ALA	2.8
1	B	874	LYS	2.8
1	B	1017	LEU	2.8
1	B	682	LEU	2.8
1	B	672	PRO	2.8
1	C	51	HIS	2.7
1	B	895	MET	2.7
1	D	418	LYS	2.7
1	B	367	PHE	2.7
1	D	908	GLU	2.7
1	B	892	GLU	2.6
1	C	913	ILE	2.6
1	A	322	CYS	2.6
1	D	871	LEU	2.6
1	B	1018	PRO	2.6
1	B	873	GLY	2.6
1	D	1019	LEU	2.6
1	C	673	HIS	2.6
1	C	672	PRO	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	414	ASP	2.5
1	D	674	GLY	2.5
1	A	367	PHE	2.5
1	B	53	GLU	2.5
1	D	53	GLU	2.5
1	D	679	GLY	2.5
1	D	1018	PRO	2.4
1	C	899	GLU	2.4
1	D	420	ASN	2.4
1	A	871	LEU	2.4
1	A	325	HIS	2.4
1	A	414	ASP	2.3
1	D	678	ARG	2.3
1	A	681	GLY	2.3
1	B	868	ILE	2.3
1	A	893	GLU	2.3
1	A	682	LEU	2.3
1	C	869	ALA	2.3
1	C	906	PRO	2.3
1	C	1012	GLU	2.3
1	C	1017	LEU	2.2
1	A	320	GLY	2.2
1	B	866	PRO	2.2
1	A	910	LYS	2.2
1	C	875	LYS	2.2
1	C	696	ARG	2.2
1	B	418	LYS	2.2
1	A	180	GLU	2.2
1	B	50	PHE	2.1
1	A	1016	GLY	2.1
1	B	180	GLU	2.1
1	D	50	PHE	2.1
1	D	180	GLU	2.1
1	A	357	ARG	2.1
1	D	424	ASP	2.1
1	D	896	ARG	2.1
1	D	417	GLY	2.1
1	C	893	GLU	2.0

## 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<sup>th</sup> 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.

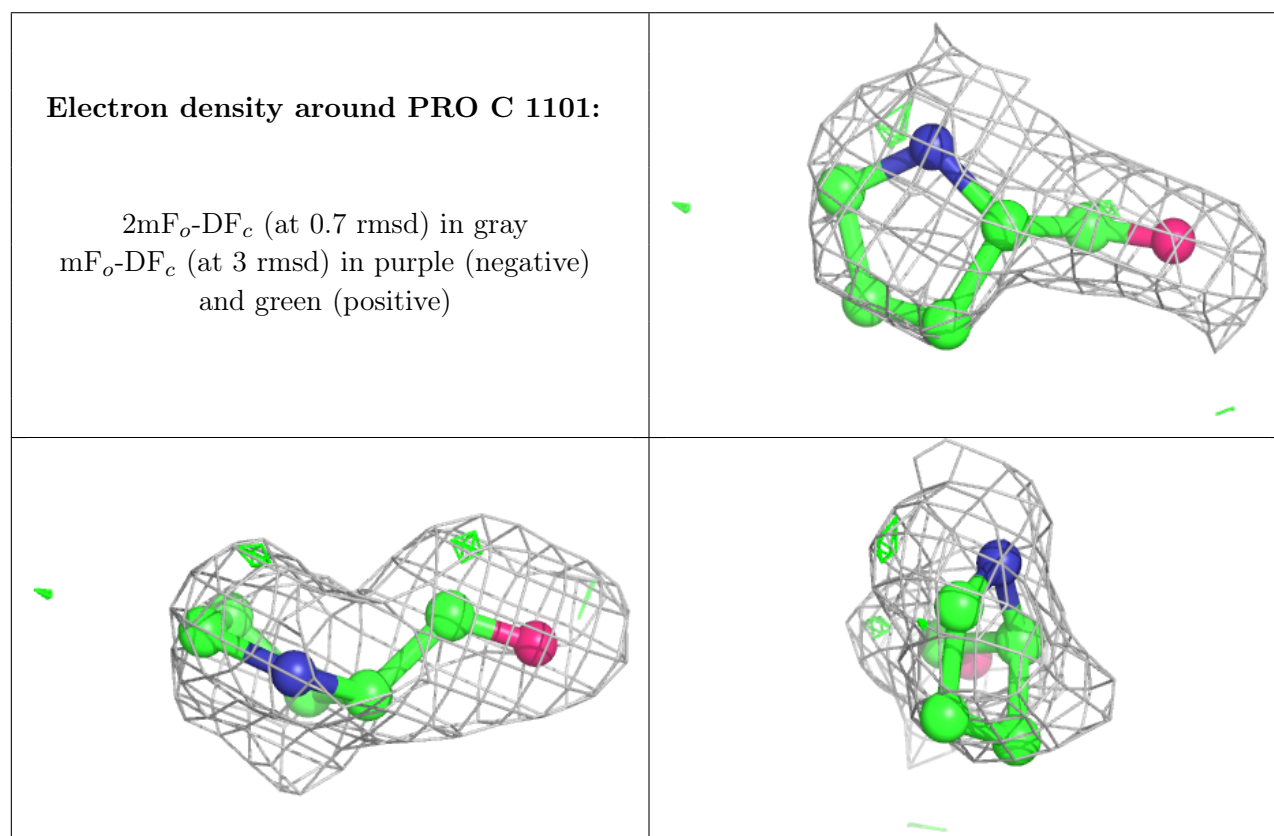
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PRO	C	1101	7/8	0.68	0.17	53,55,57,59	0
4	NAP	B	1106	48/48	0.95	0.12	19,27,42,47	0
3	FAD	B	1105	53/53	0.96	0.08	16,20,26,28	0
4	NAP	D	1106	40/48	0.96	0.10	19,25,48,66	0
5	FMN	A	1107	31/31	0.96	0.11	14,18,23,28	0
4	NAP	A	1106	48/48	0.96	0.11	18,26,38,41	0
3	FAD	A	1105	53/53	0.97	0.08	15,19,23,27	0
3	FAD	C	1106	53/53	0.97	0.07	16,20,25,29	0
5	FMN	B	1108	31/31	0.97	0.08	14,19,22,30	0
5	FMN	C	1109	31/31	0.97	0.09	12,16,18,20	0
5	FMN	D	1108	31/31	0.97	0.10	13,16,20,27	0
6	TDR	C	1108	9/9	0.97	0.08	15,16,17,18	0
6	TDR	D	1107	9/9	0.97	0.08	14,15,17,20	0
4	NAP	C	1107	48/48	0.97	0.09	17,26,36,38	0
6	TDR	A	1108	9/9	0.98	0.09	16,18,20,22	0
3	FAD	D	1105	53/53	0.98	0.07	14,18,21,24	0
2	SF4	C	1103	8/8	0.99	0.05	15,16,16,16	0
2	SF4	C	1104	8/8	0.99	0.06	14,15,15,16	0
2	SF4	D	1103	8/8	0.99	0.07	15,15,15,15	0
2	SF4	D	1104	8/8	0.99	0.06	16,16,17,17	0
2	SF4	A	1103	8/8	0.99	0.05	17,18,18,19	0
2	SF4	B	1101	8/8	0.99	0.06	16,16,17,17	0
2	SF4	B	1102	8/8	0.99	0.07	17,18,18,18	0
6	TDR	B	1107	9/9	0.99	0.07	17,19,20,20	0
2	SF4	B	1103	8/8	0.99	0.05	18,18,19,19	0
2	SF4	B	1104	8/8	0.99	0.05	17,17,18,18	0
2	SF4	C	1102	8/8	0.99	0.05	15,16,16,16	0
2	SF4	A	1104	8/8	1.00	0.04	17,18,18,19	0
2	SF4	A	1102	8/8	1.00	0.06	16,16,17,17	0
2	SF4	C	1105	8/8	1.00	0.07	17,18,18,18	0
2	SF4	D	1101	8/8	1.00	0.04	16,16,17,17	0
2	SF4	D	1102	8/8	1.00	0.04	16,16,17,17	0

*Continued on next page...*

*Continued from previous page...*

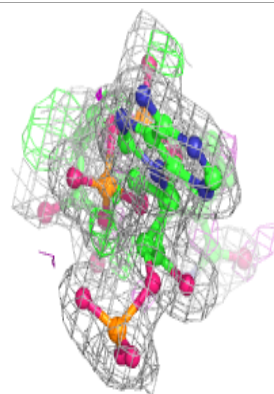
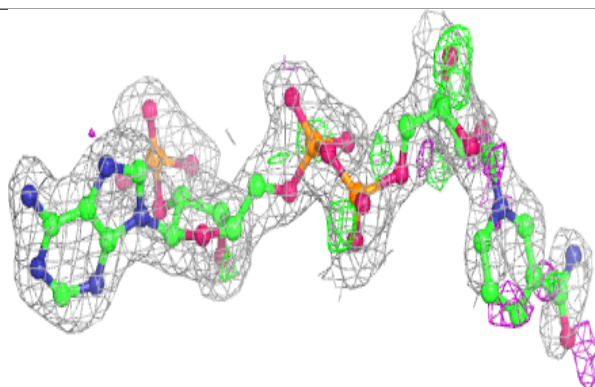
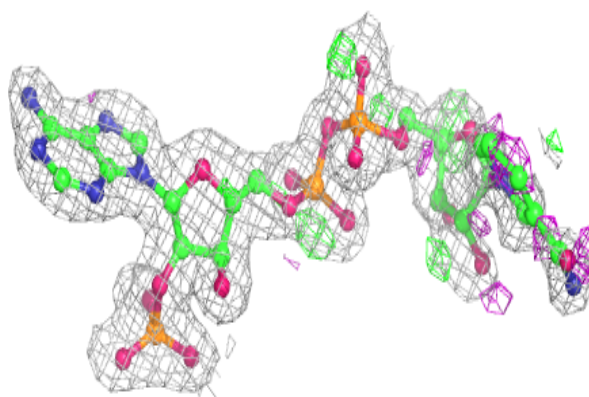
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SF4	A	1101	8/8	1.00	0.06	17,17,18,18	0

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

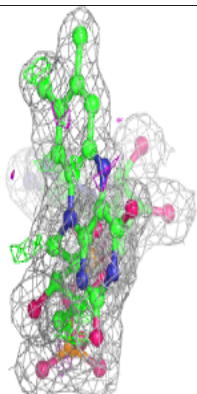
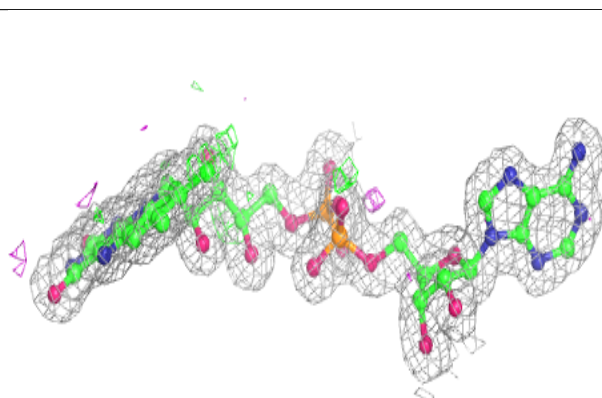
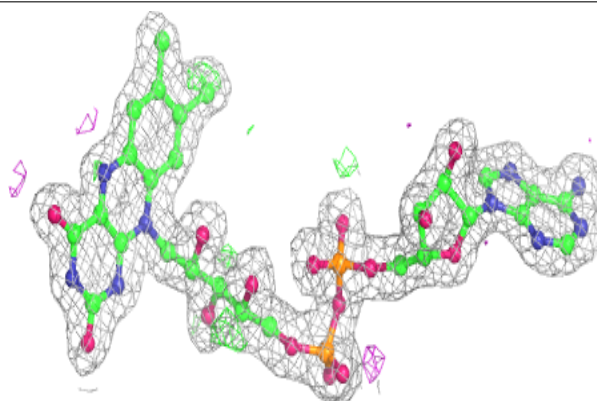


**Electron density around NAP B 1106:**

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

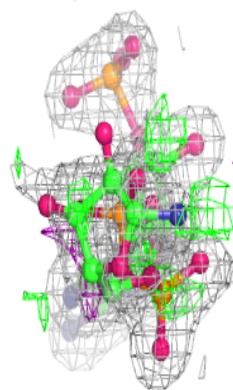
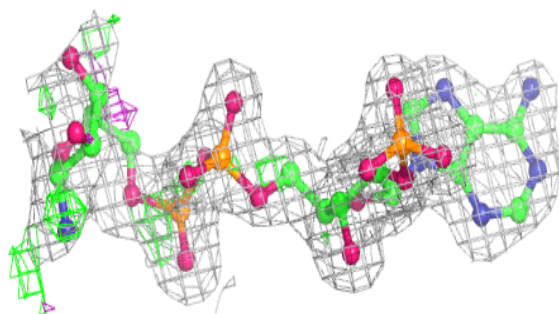
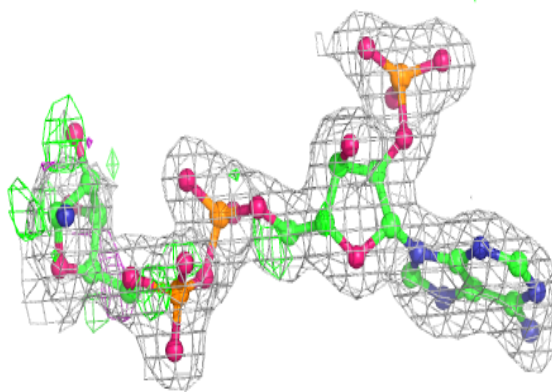
**Electron density around FAD B 1105:**

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



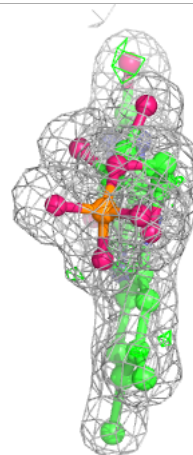
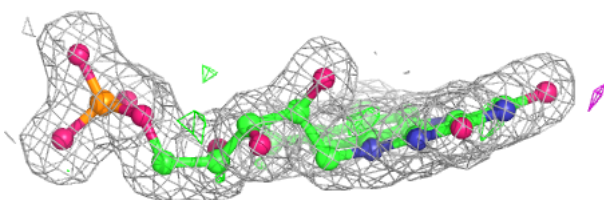
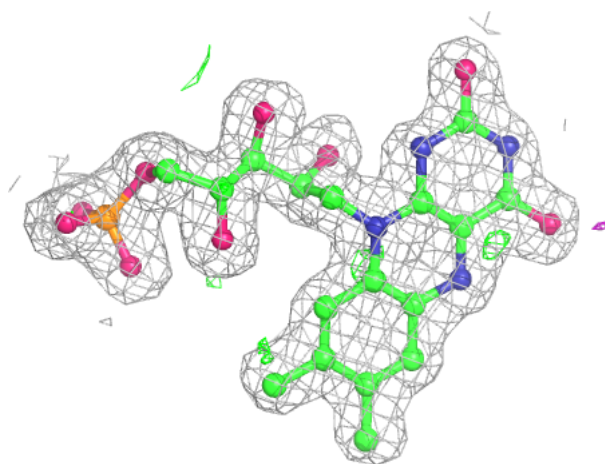
**Electron density around NAP D 1106:**

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



**Electron density around FMN A 1107:**

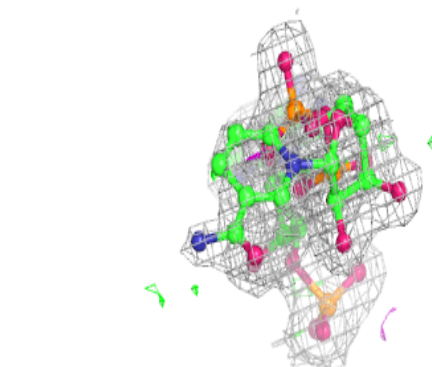
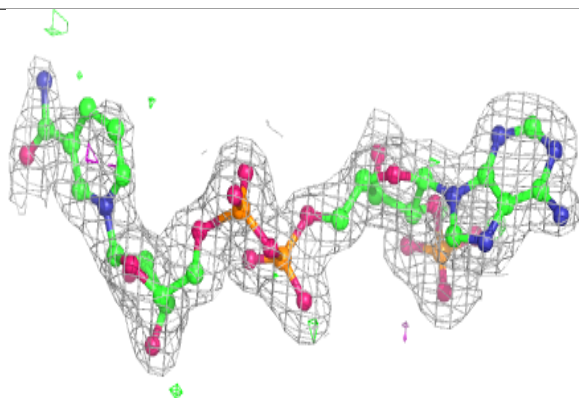
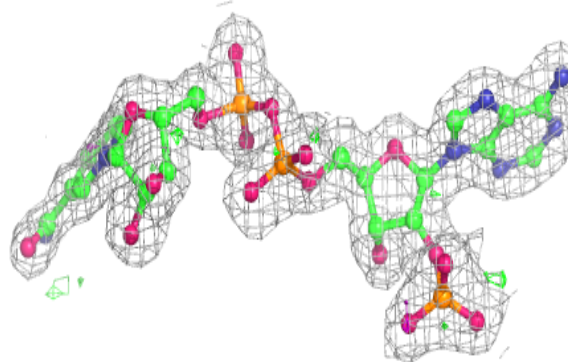
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



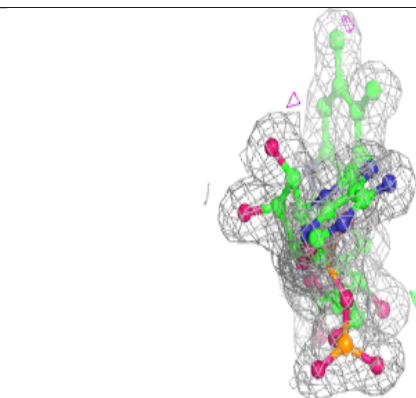
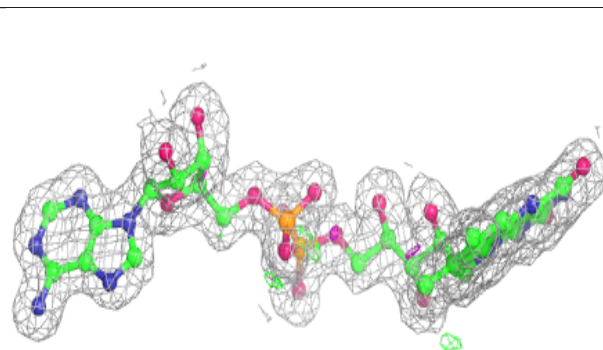
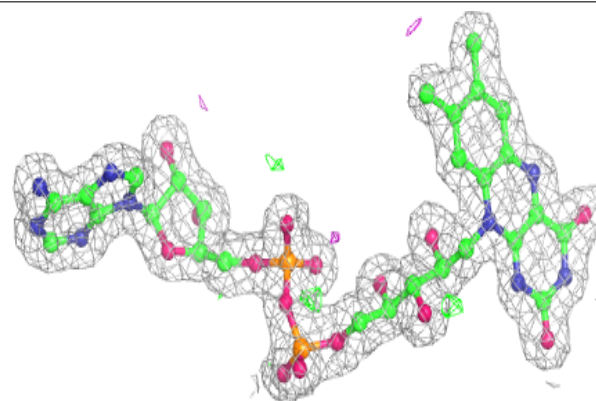


**Electron density around NAP A 1106:**

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

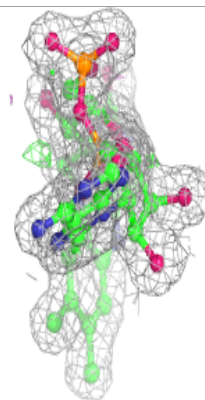
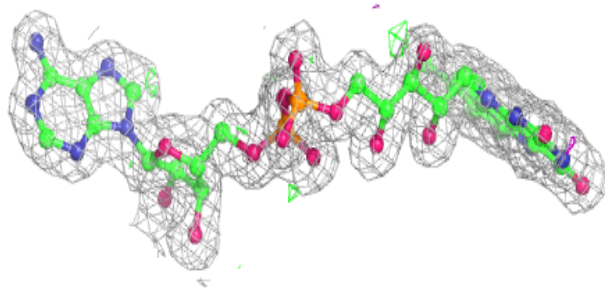
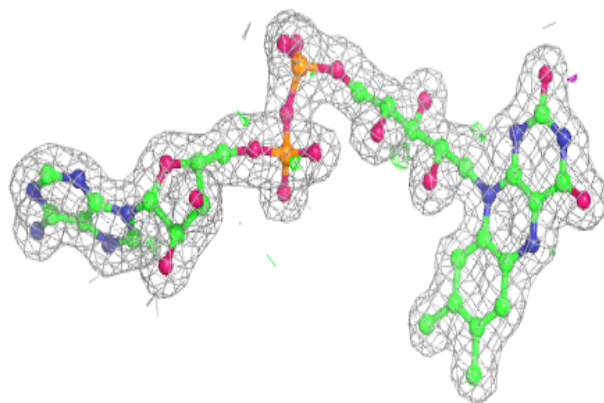
**Electron density around FAD A 1105:**

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



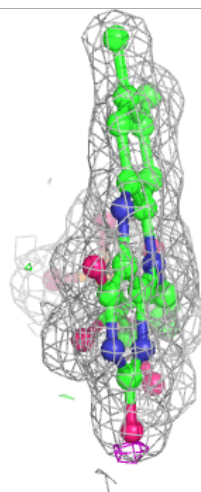
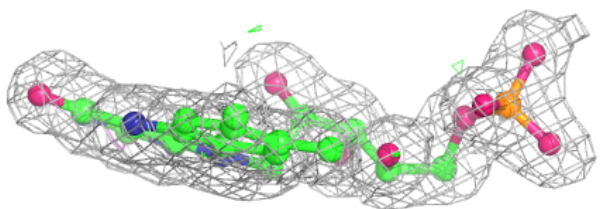
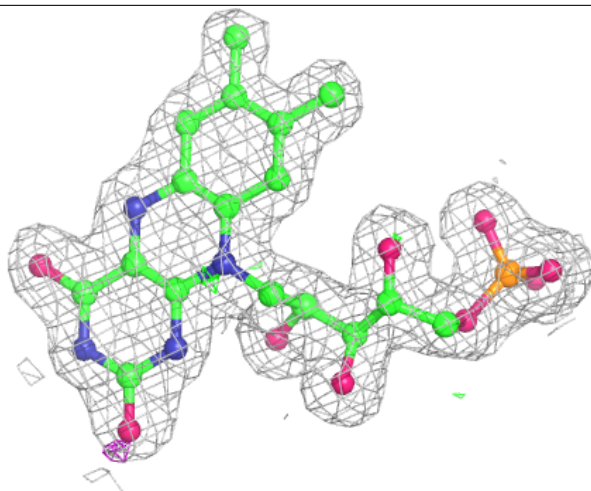
**Electron density around FAD C 1106:**

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



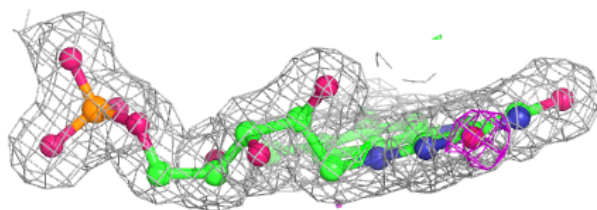
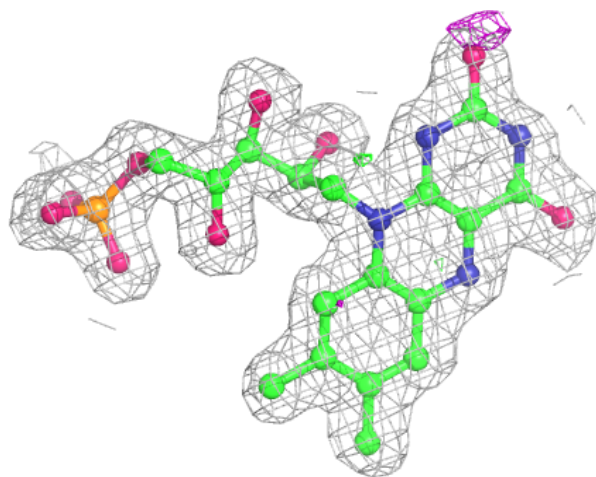
**Electron density around FMN B 1108:**

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



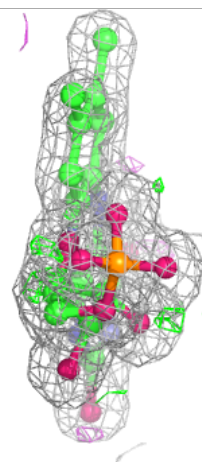
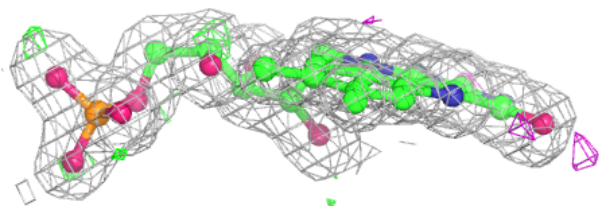
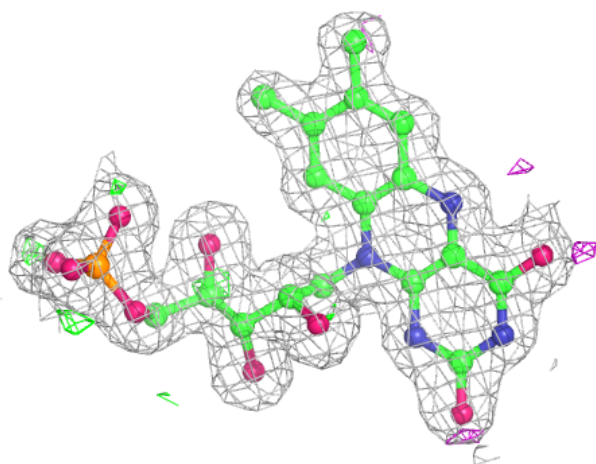
**Electron density around FMN C 1109:**

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



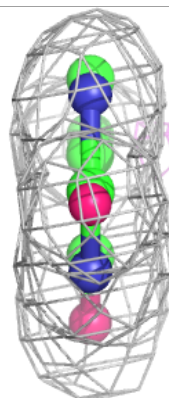
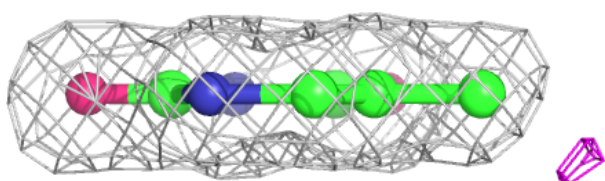
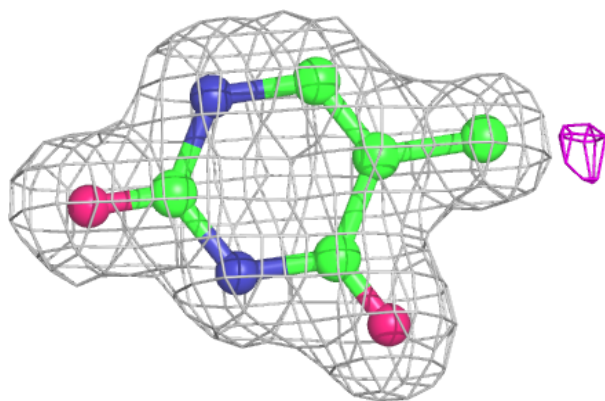
**Electron density around FMN D 1108:**

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

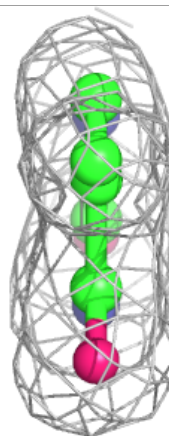
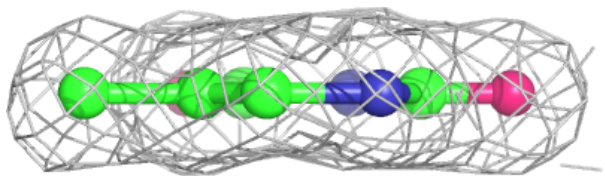
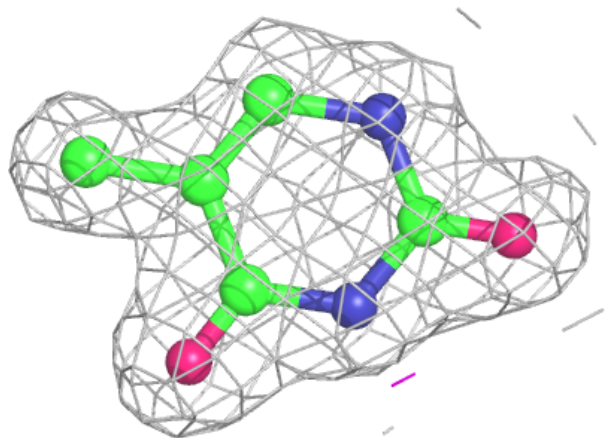


**Electron density around TDR C 1108:**

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

**Electron density around TDR D 1107:**

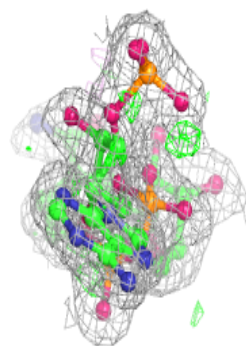
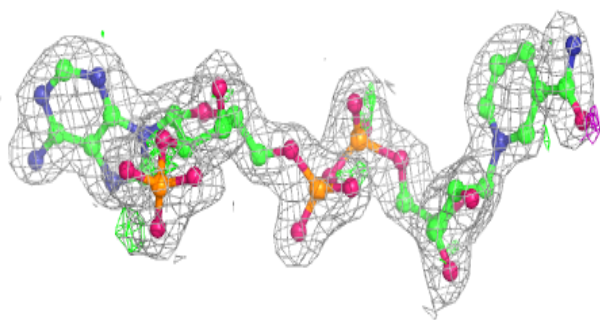
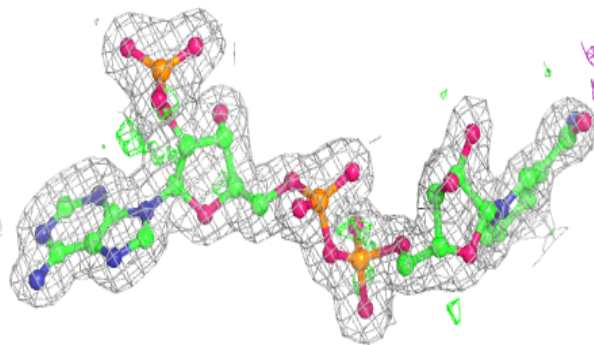
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





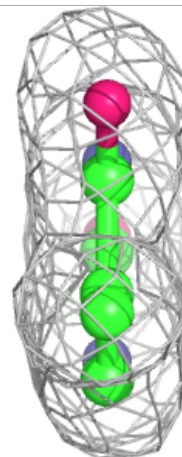
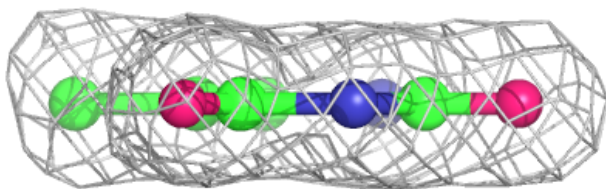
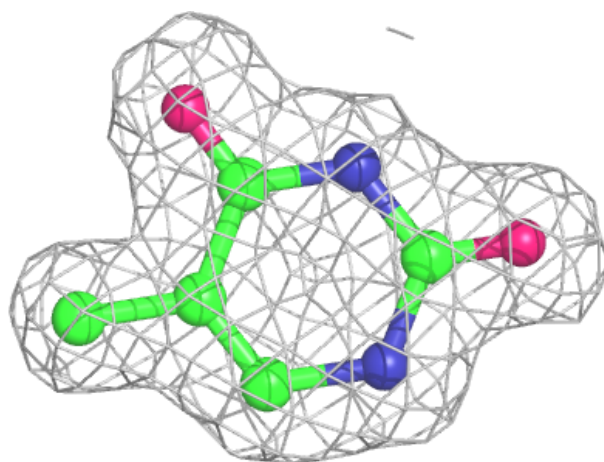
**Electron density around NAP C 1107:**

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



**Electron density around TDR A 1108:**

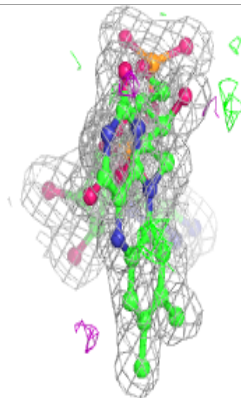
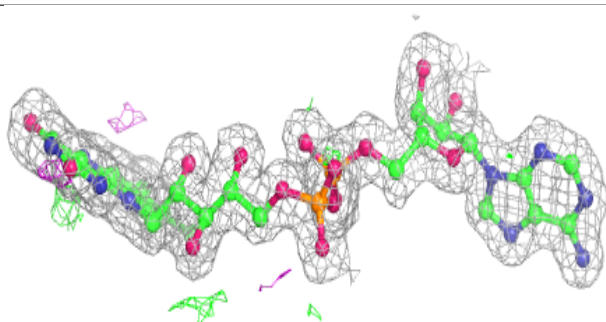
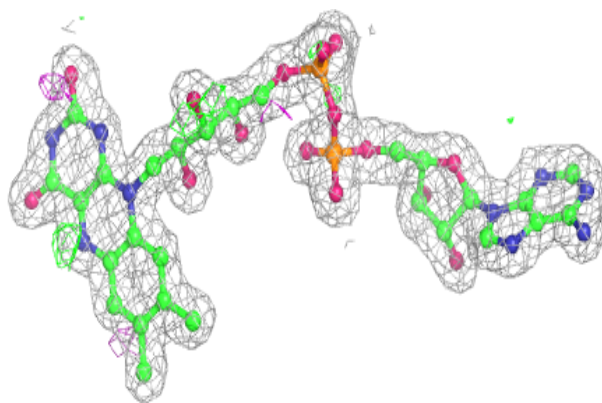
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





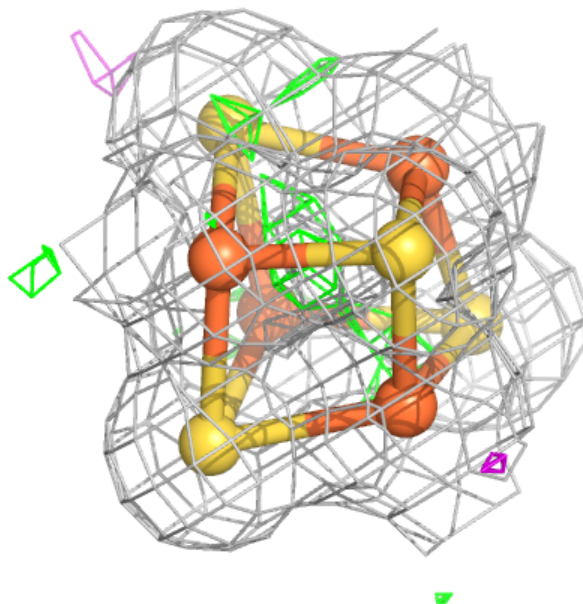
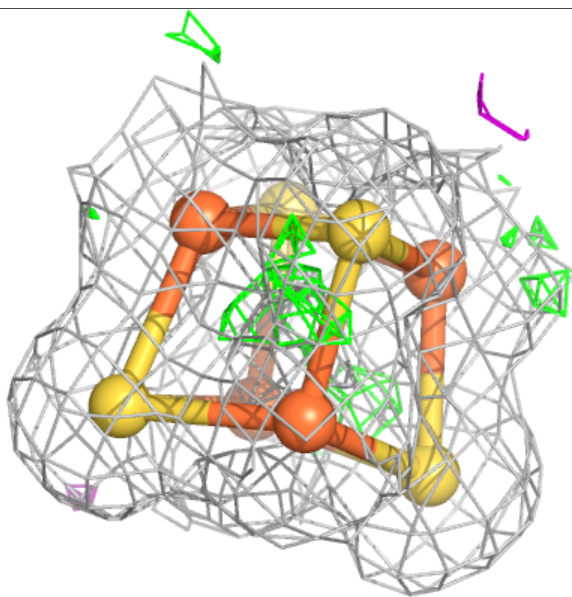
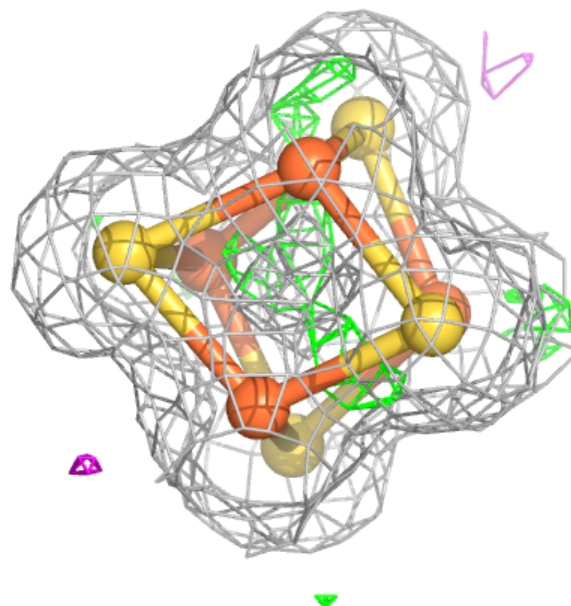
**Electron density around FAD D 1105:**

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



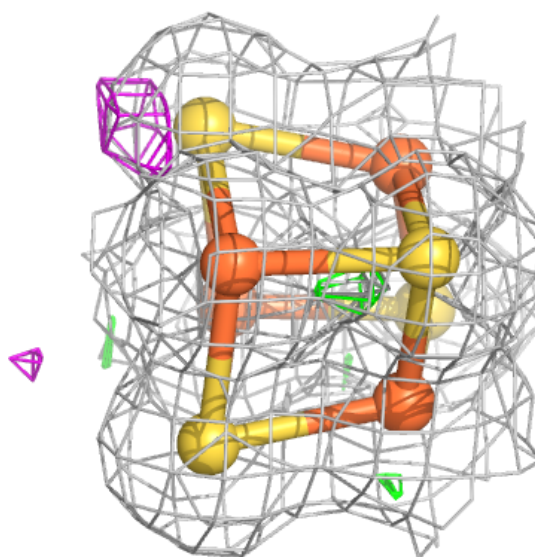
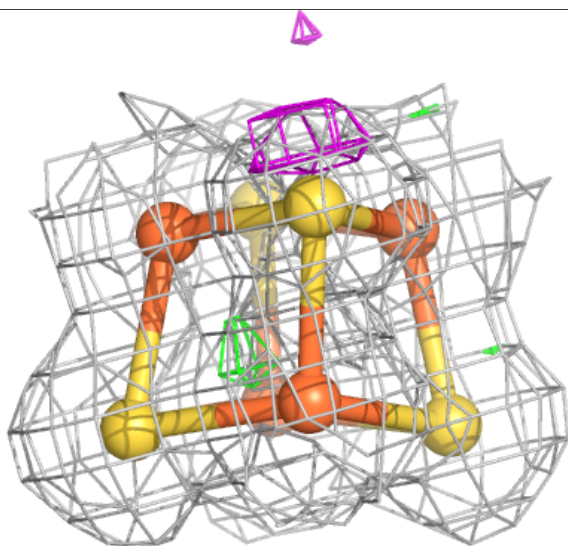
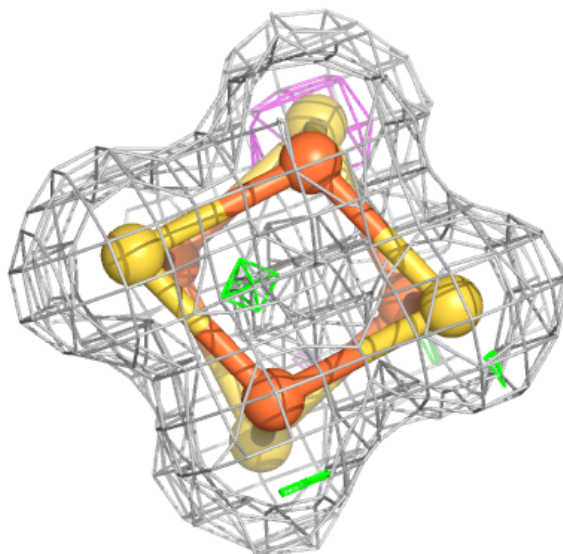
**Electron density around SF4 C 1103:**

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



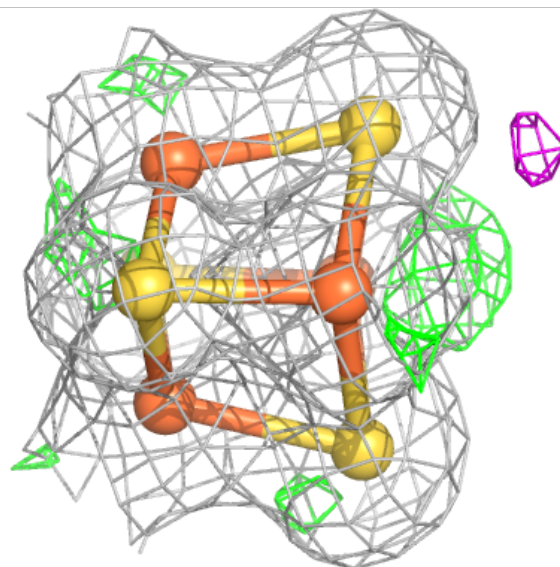
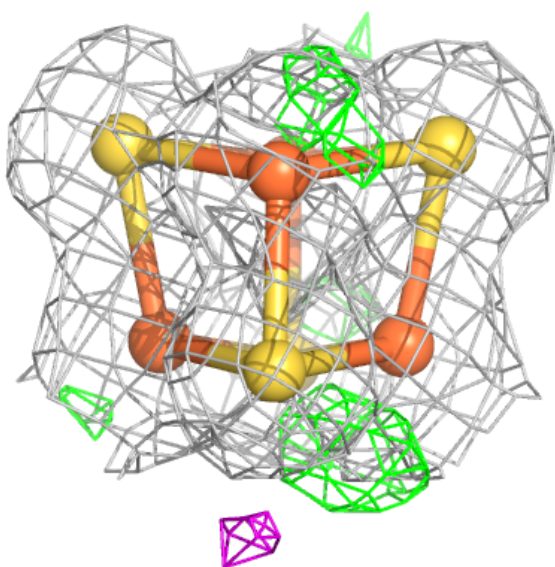
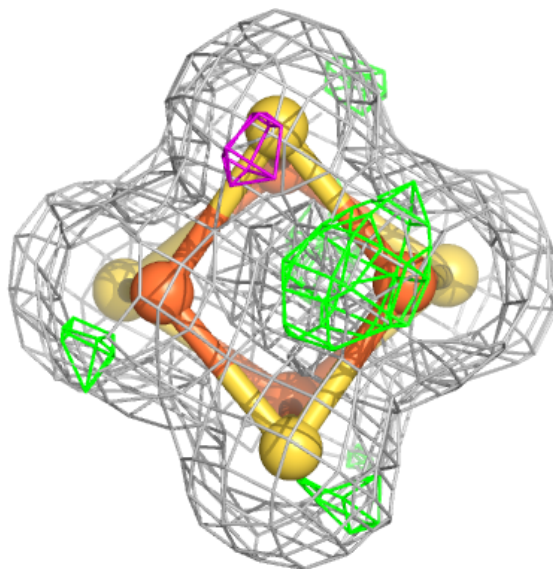
**Electron density around SF4 C 1104:**

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



**Electron density around SF4 D 1103:**

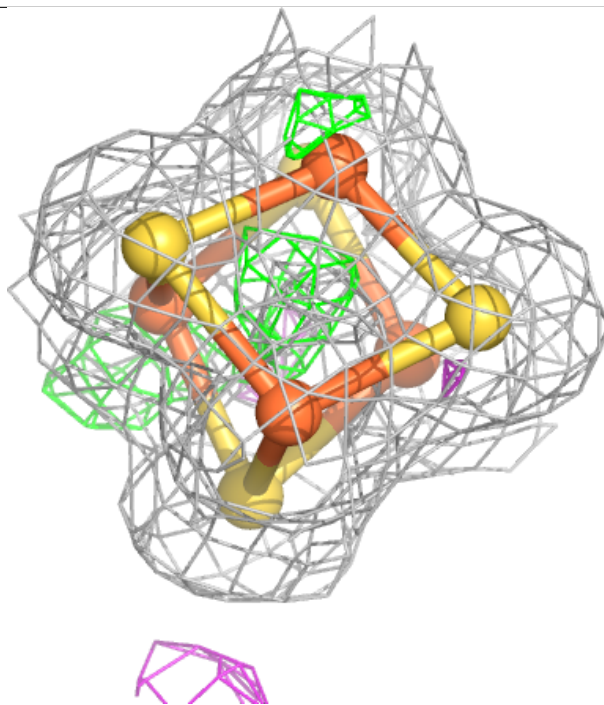
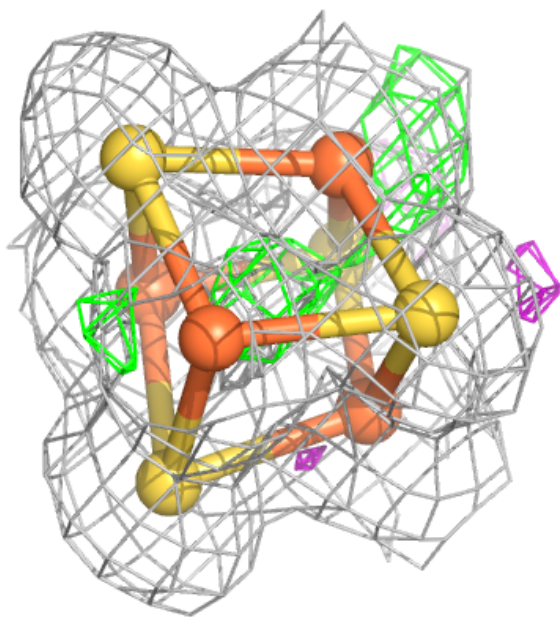
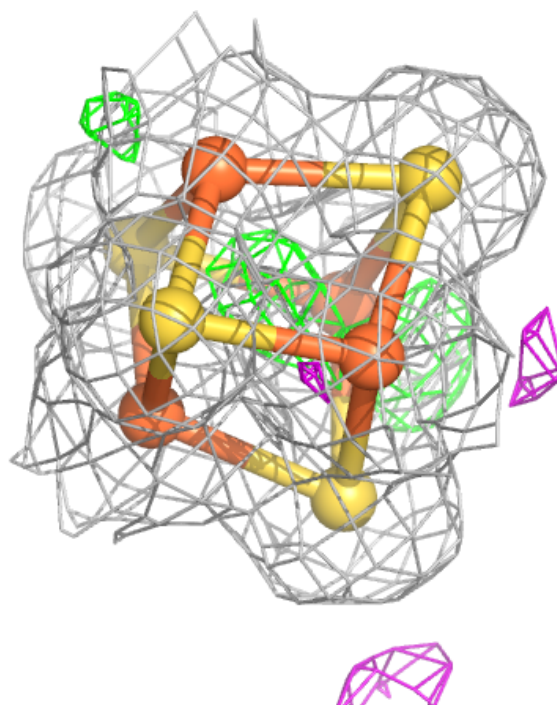
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





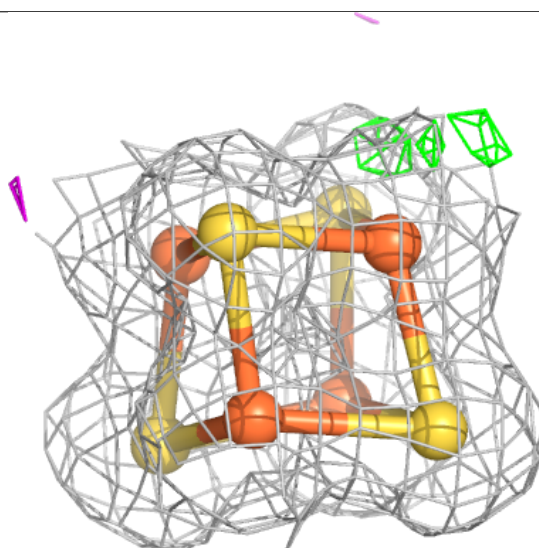
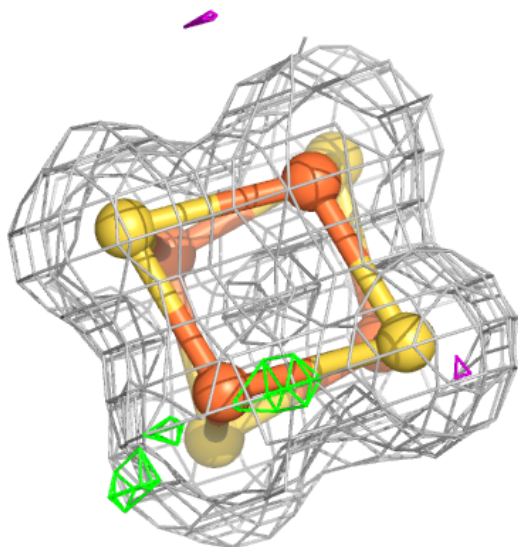
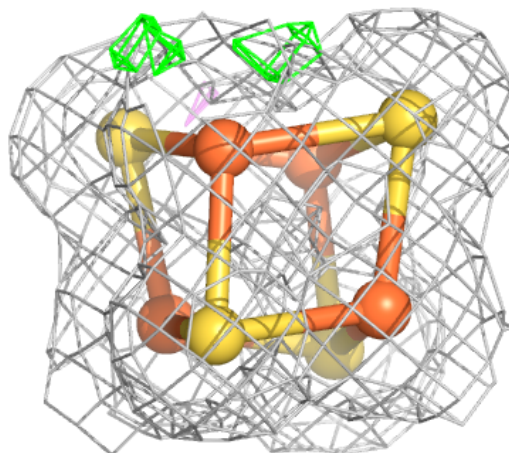
**Electron density around SF4 D 1104:**

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



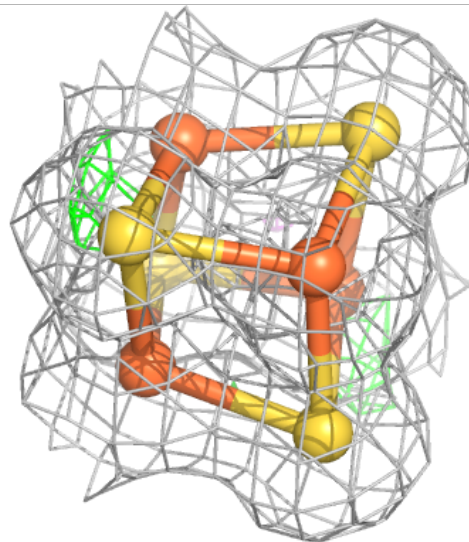
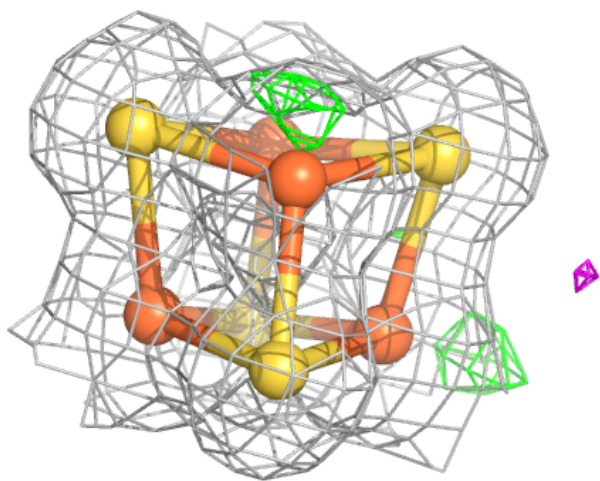
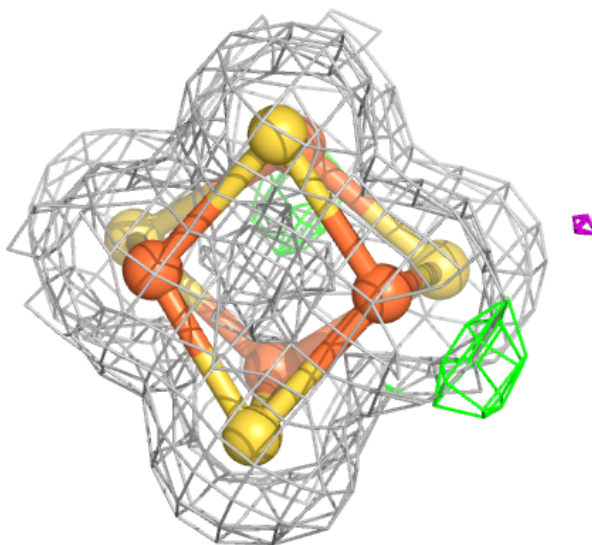
**Electron density around SF4 A 1103:**

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



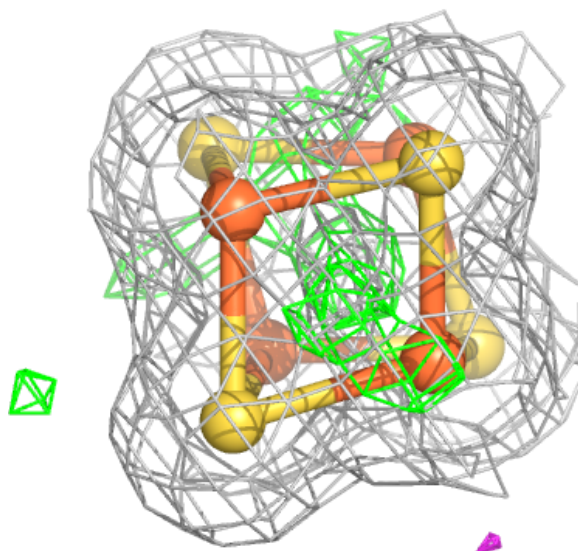
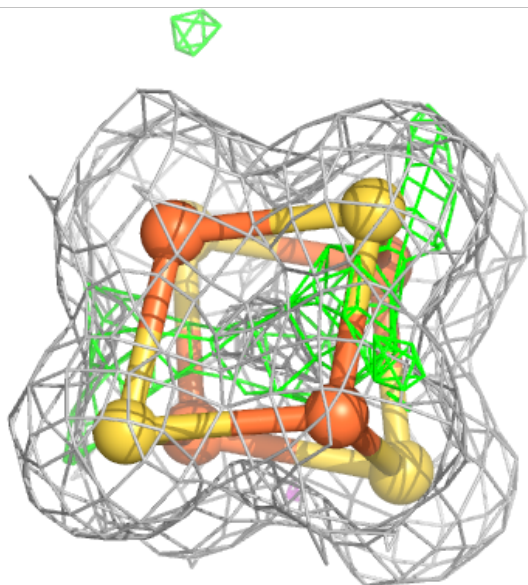
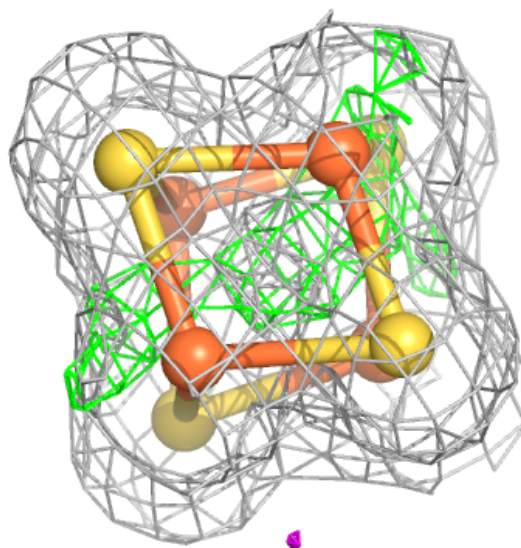
**Electron density around SF4 B 1101:**

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



**Electron density around SF4 B 1102:**

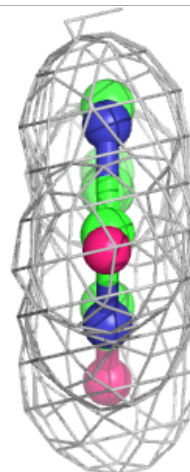
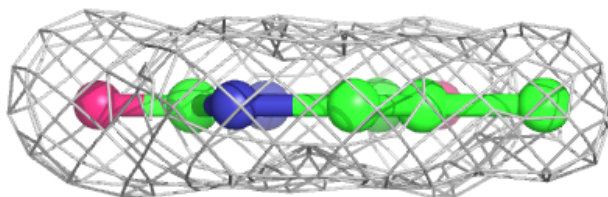
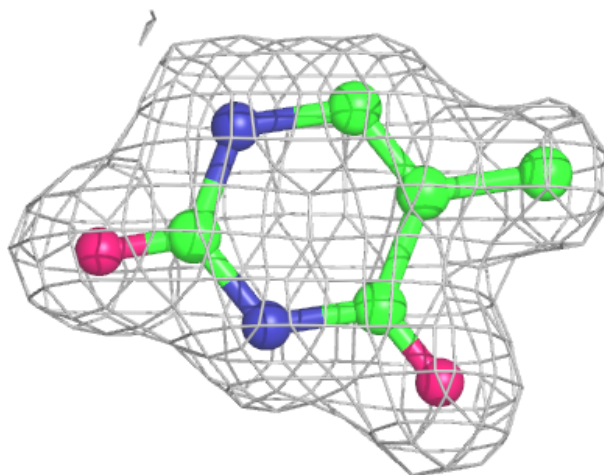
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





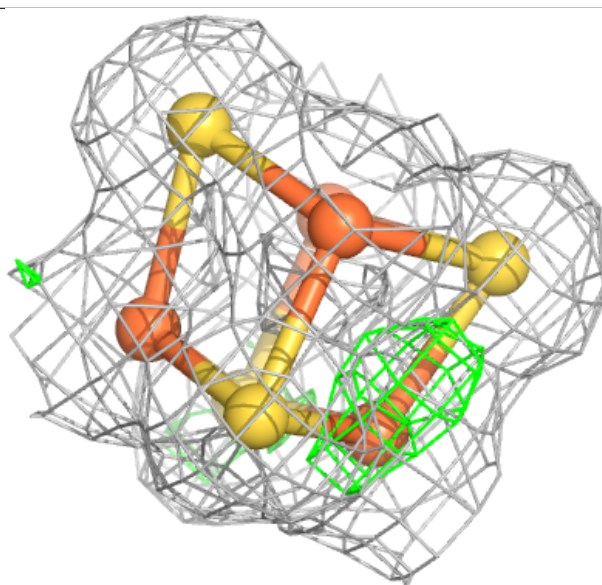
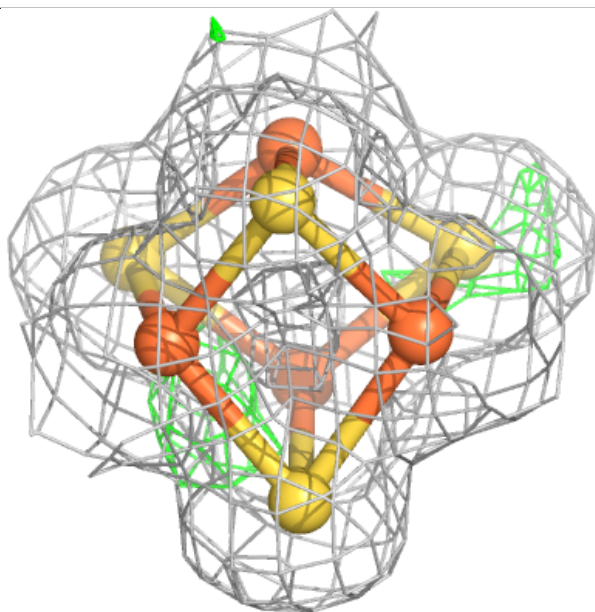
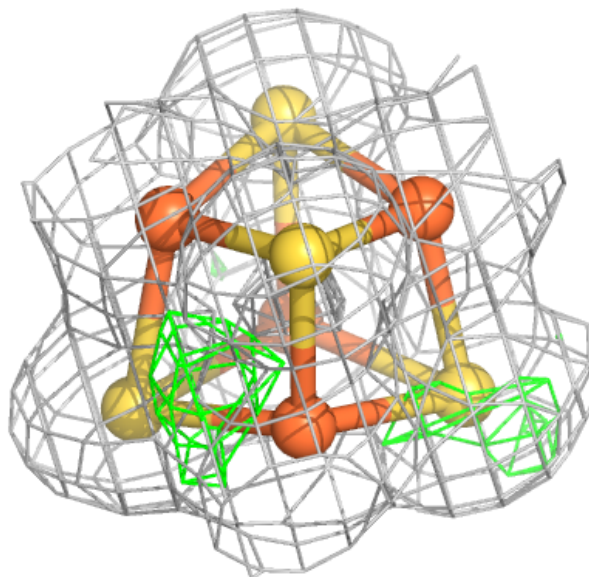
**Electron density around TDR B 1107:**

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



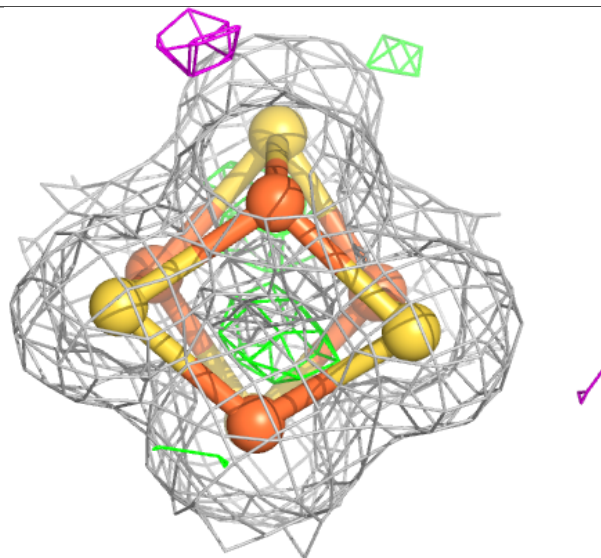
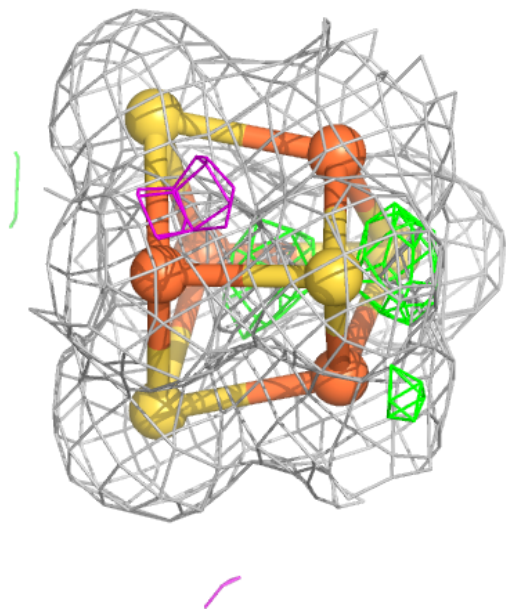
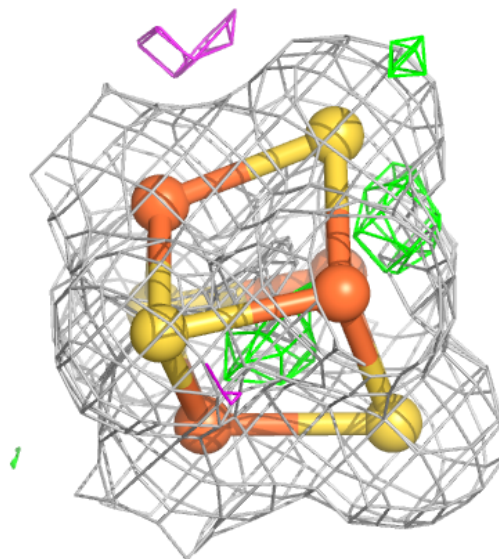
**Electron density around SF4 B 1103:**

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



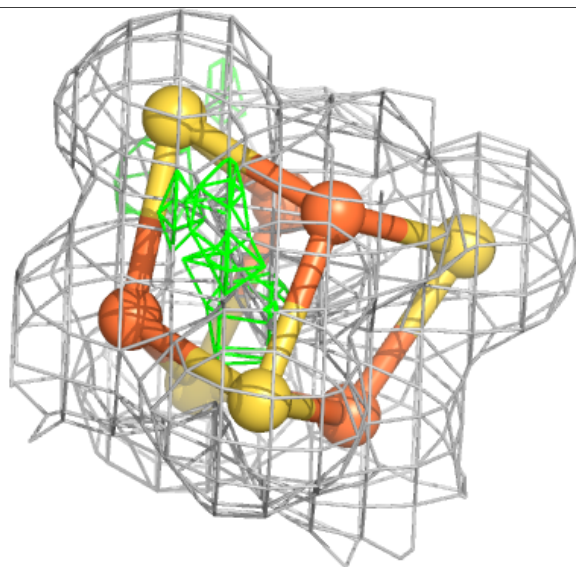
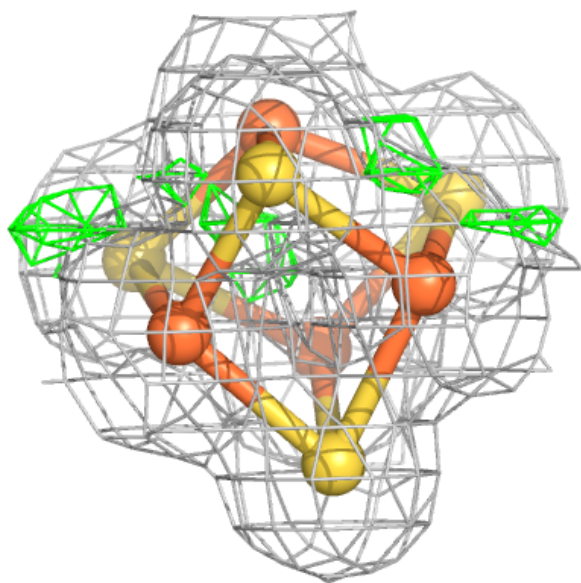
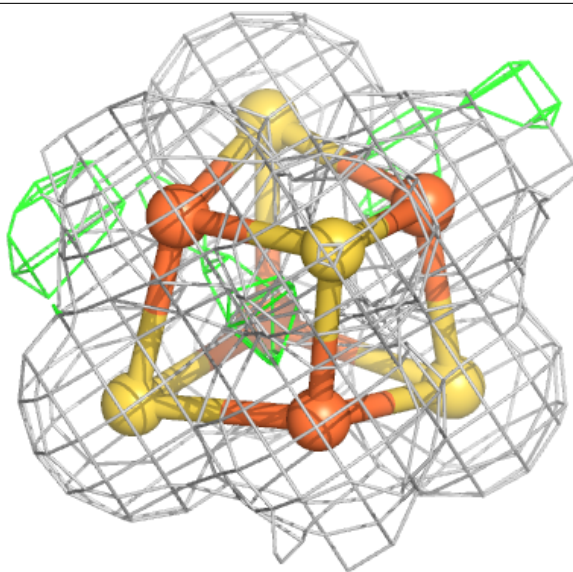
**Electron density around SF4 B 1104:**

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



**Electron density around SF4 C 1102:**

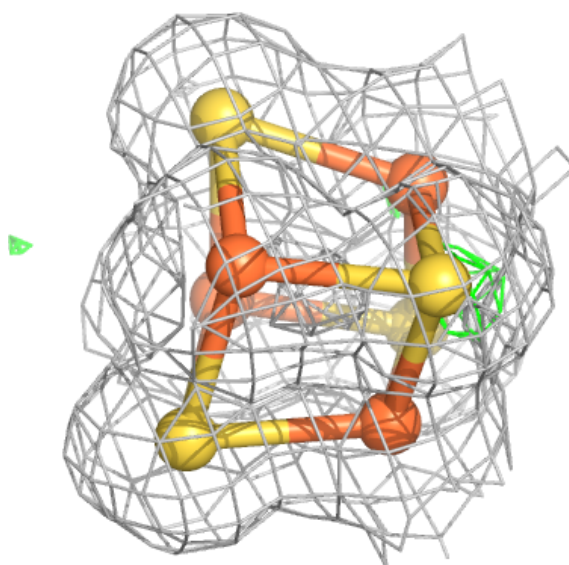
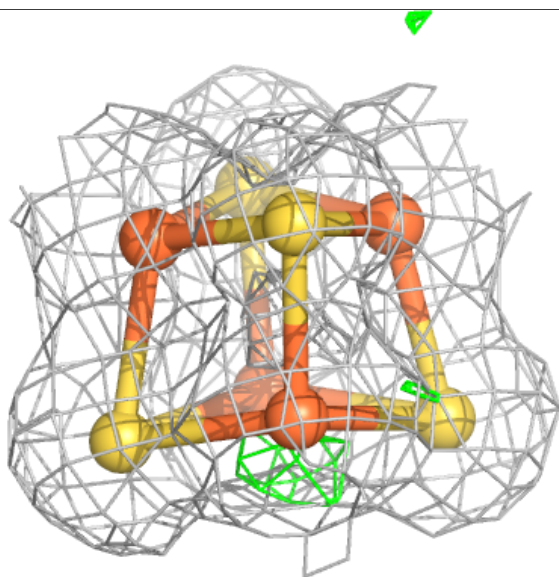
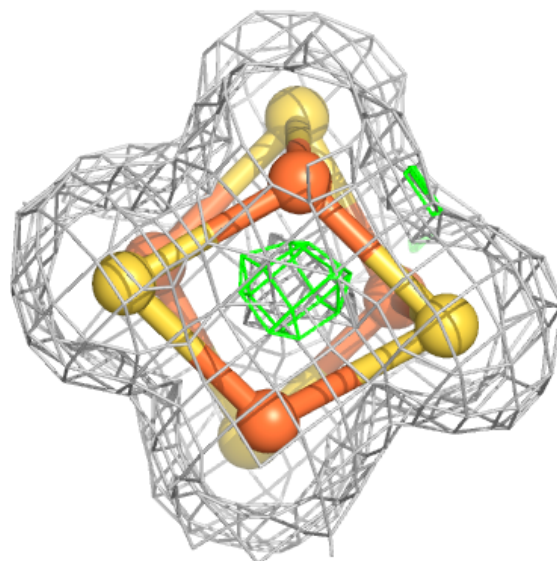
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





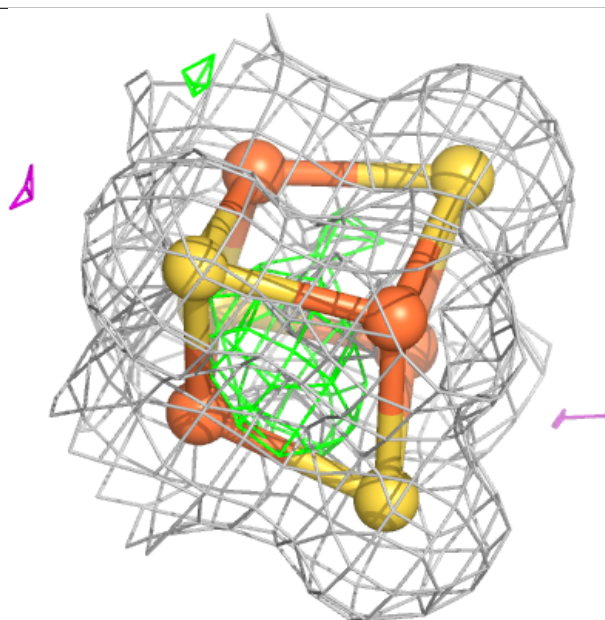
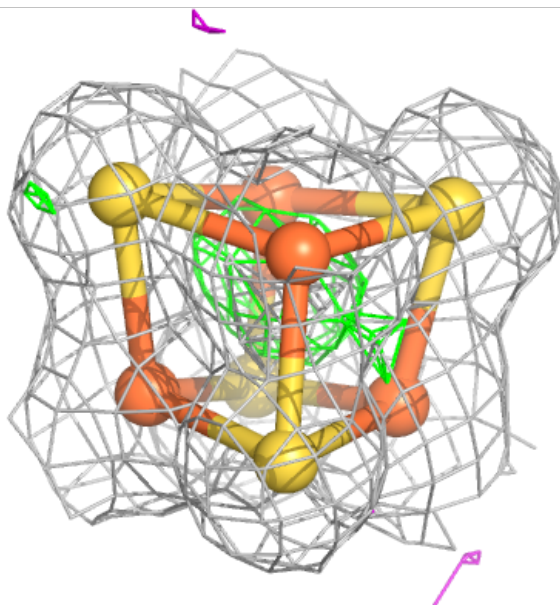
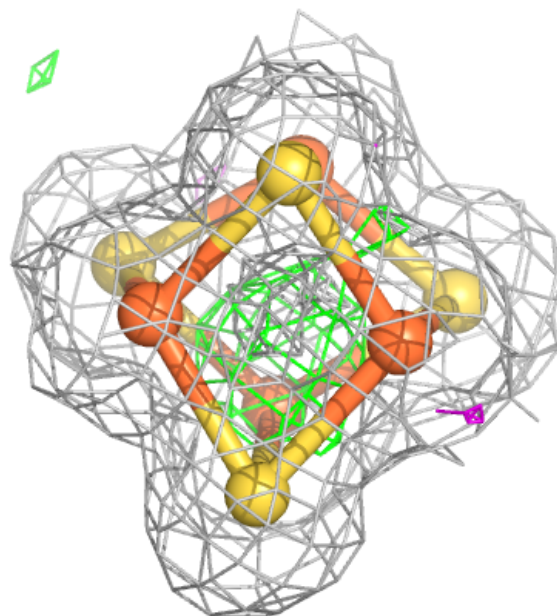
**Electron density around SF4 A 1104:**

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



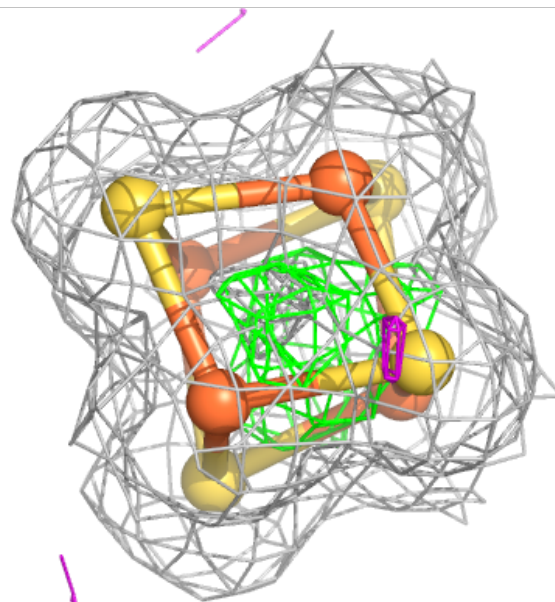
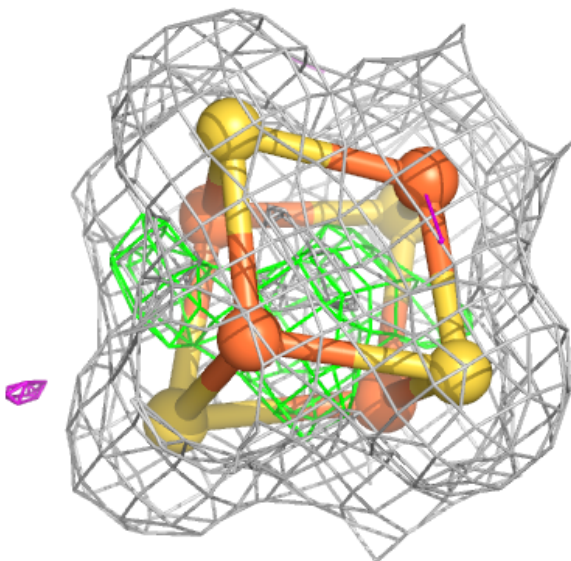
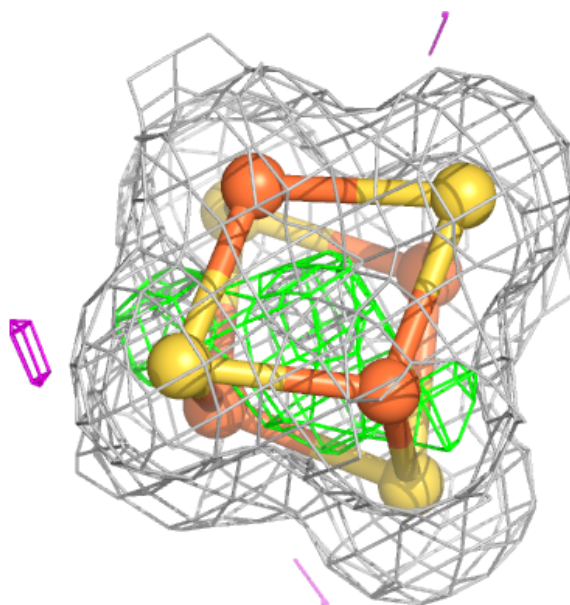
**Electron density around SF4 A 1102:**

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



**Electron density around SF4 C 1105:**

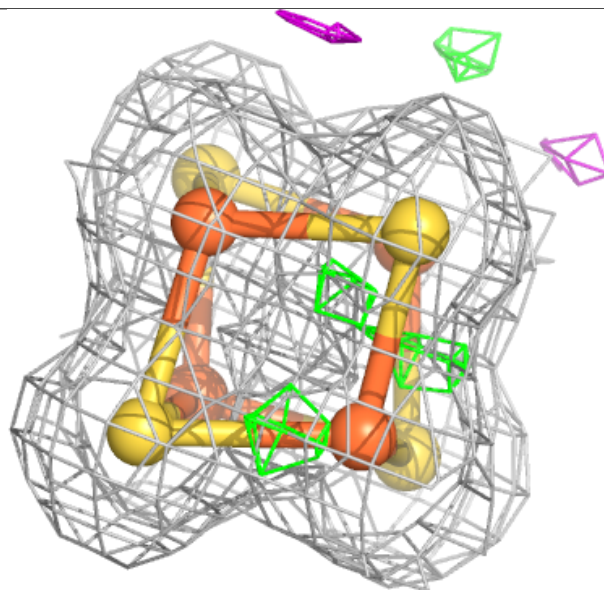
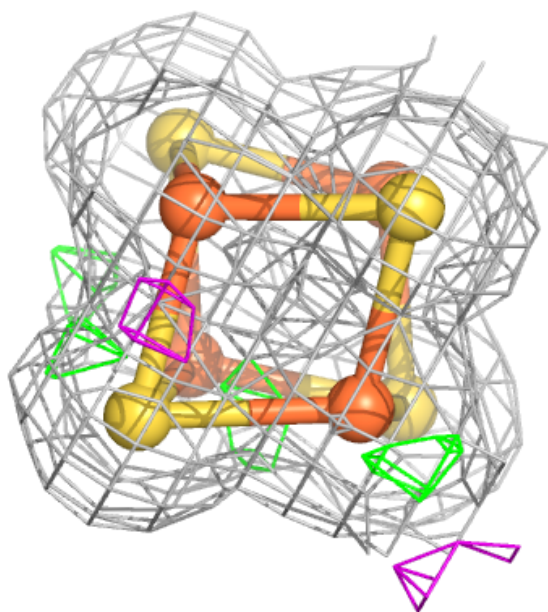
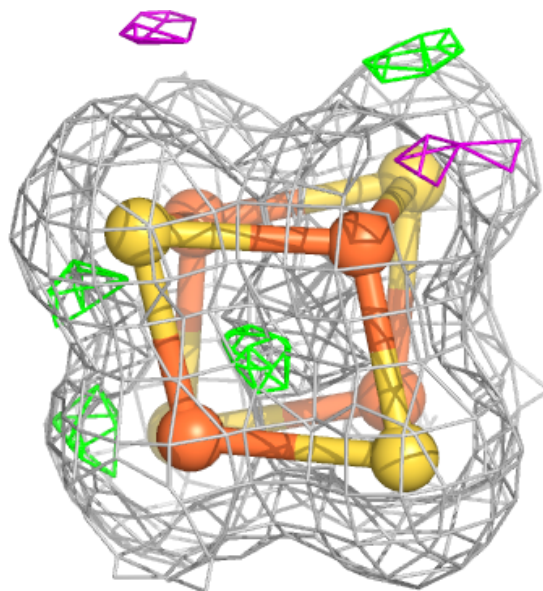
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SF4 D 1101:**

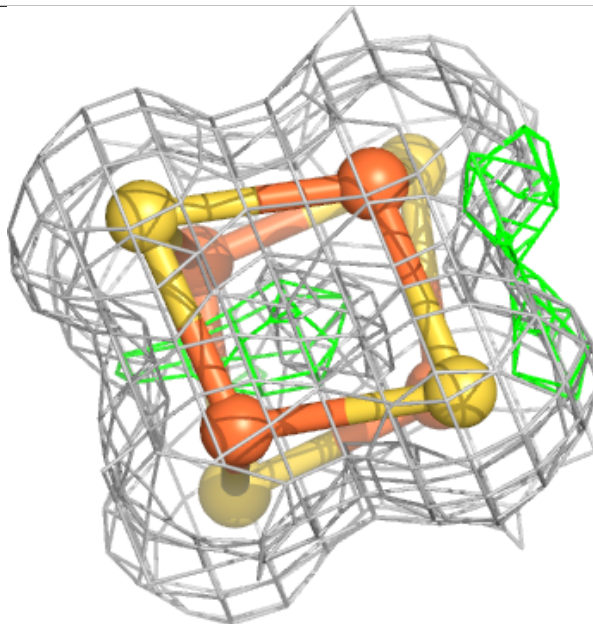
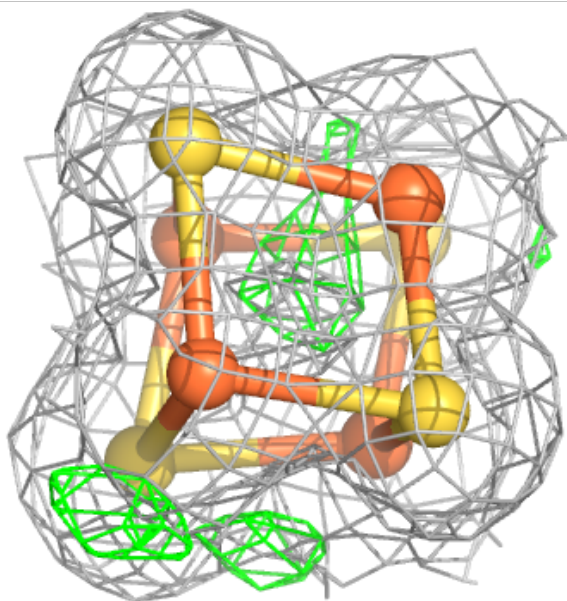
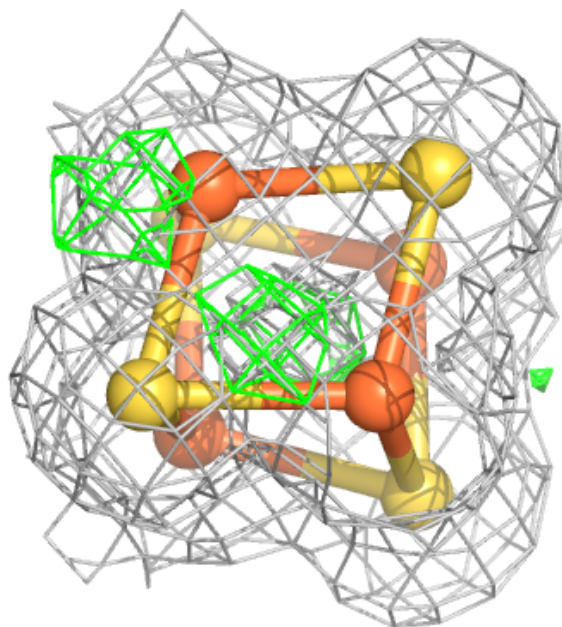
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





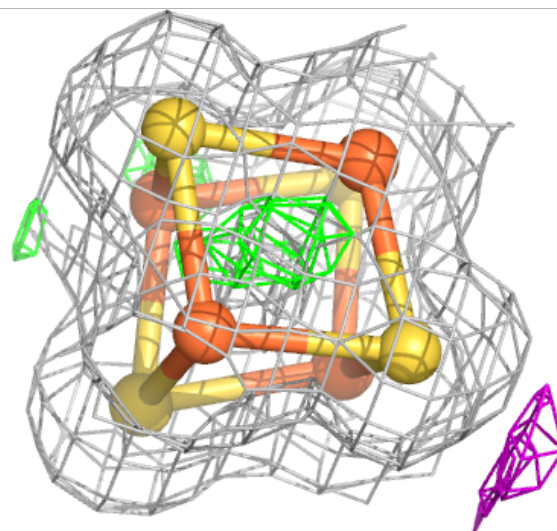
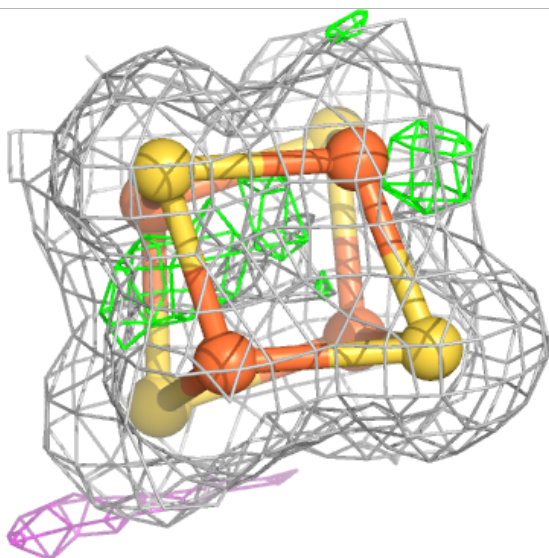
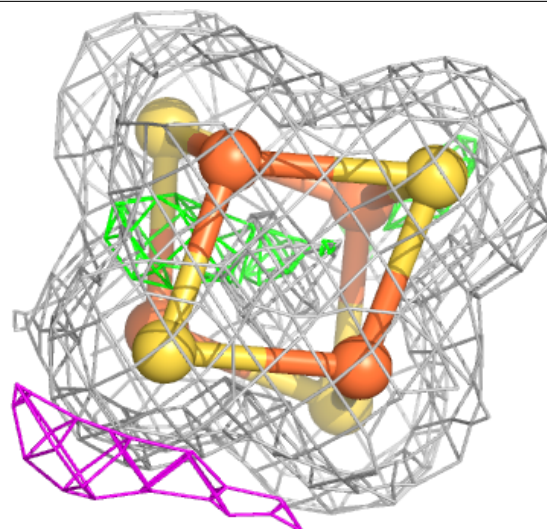
**Electron density around SF4 D 1102:**

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



**Electron density around SF4 A 1101:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.