



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:58 AM UTC

PDB ID : 7M31 / pdb_00007m31
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

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

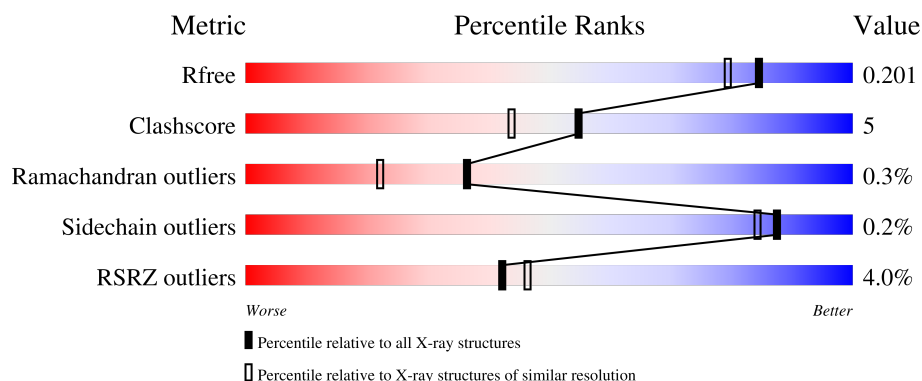
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 ≥ 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	4% 89% 9%
1	B	1025	4% 89% 9%
1	C	1025	4% 88% 10%
1	D	1025	4% 90% 9%

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.

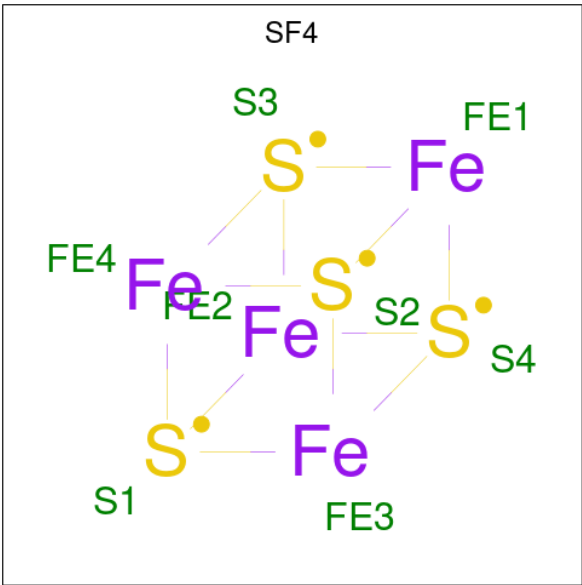
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

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 (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



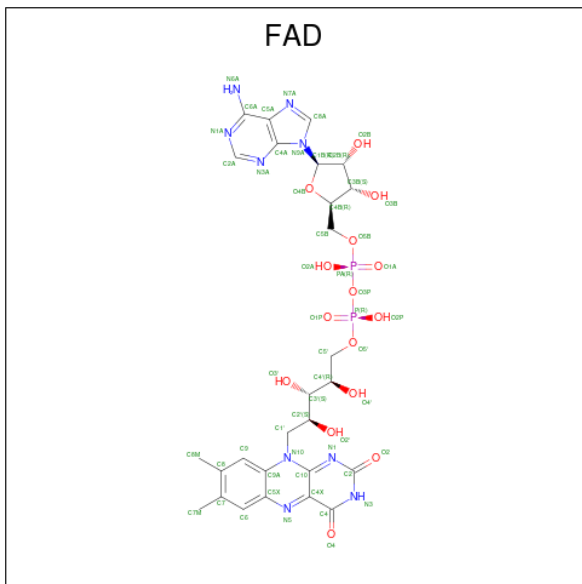
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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

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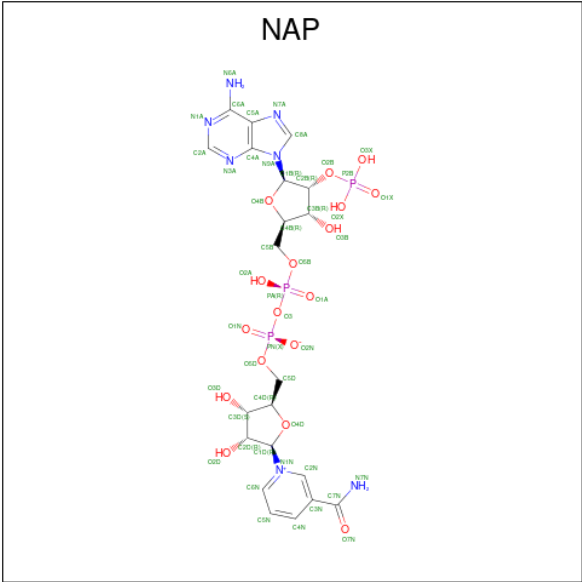
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



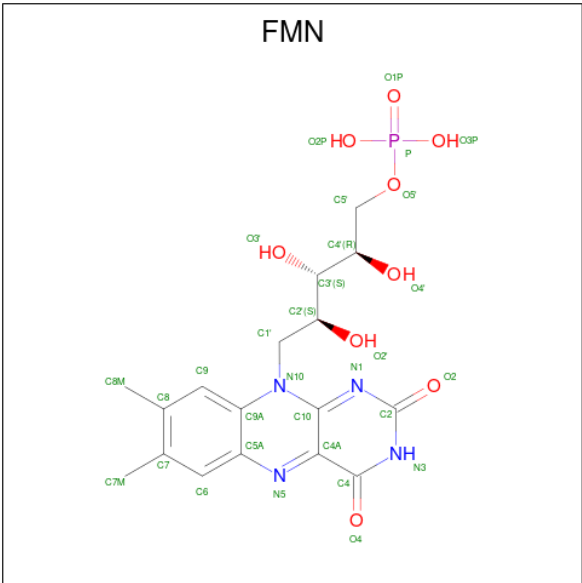
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



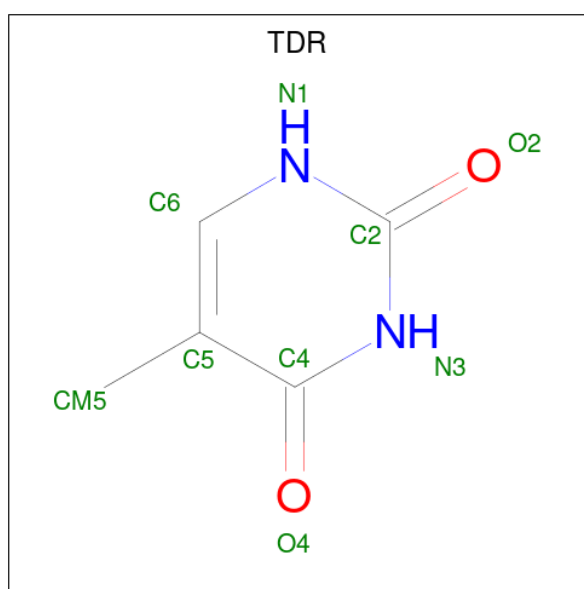
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

- Molecule 5 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



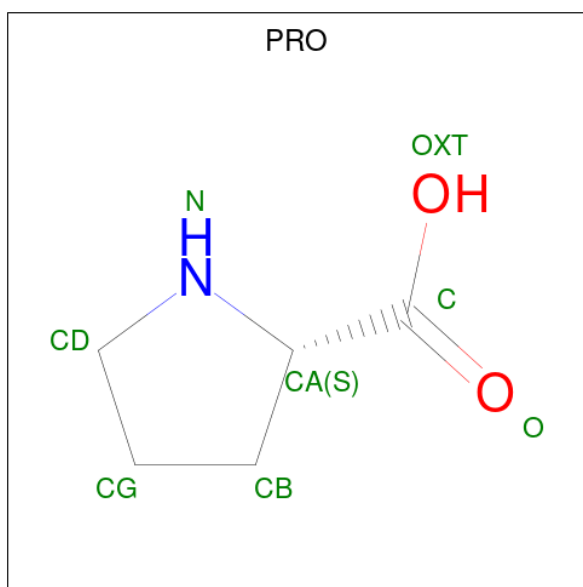
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 6 is THYMINE (CCD ID: 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 (CCD ID: 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		

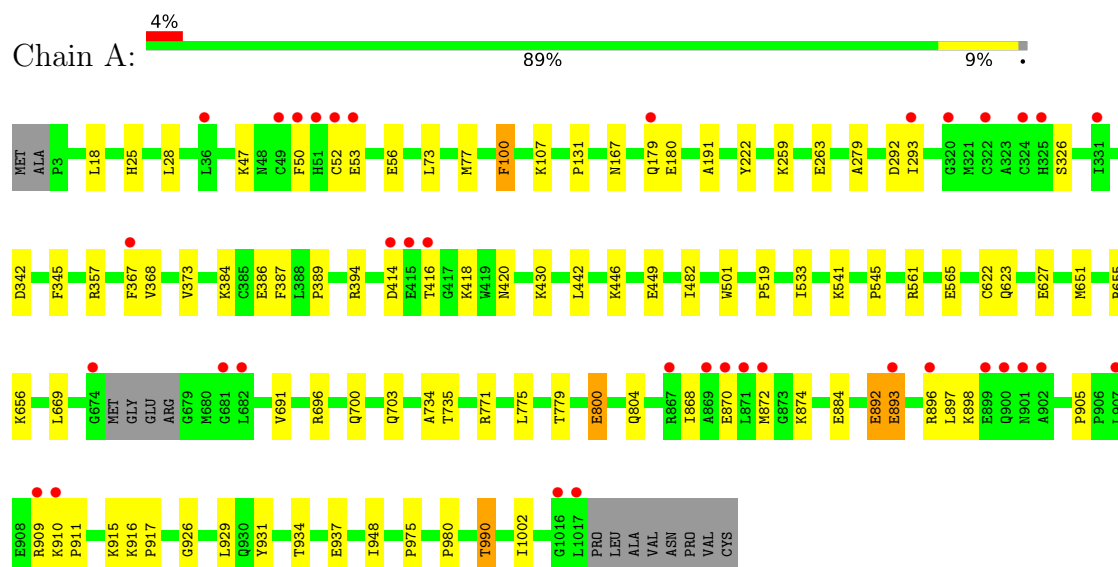
- Molecule 8 is water.

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		

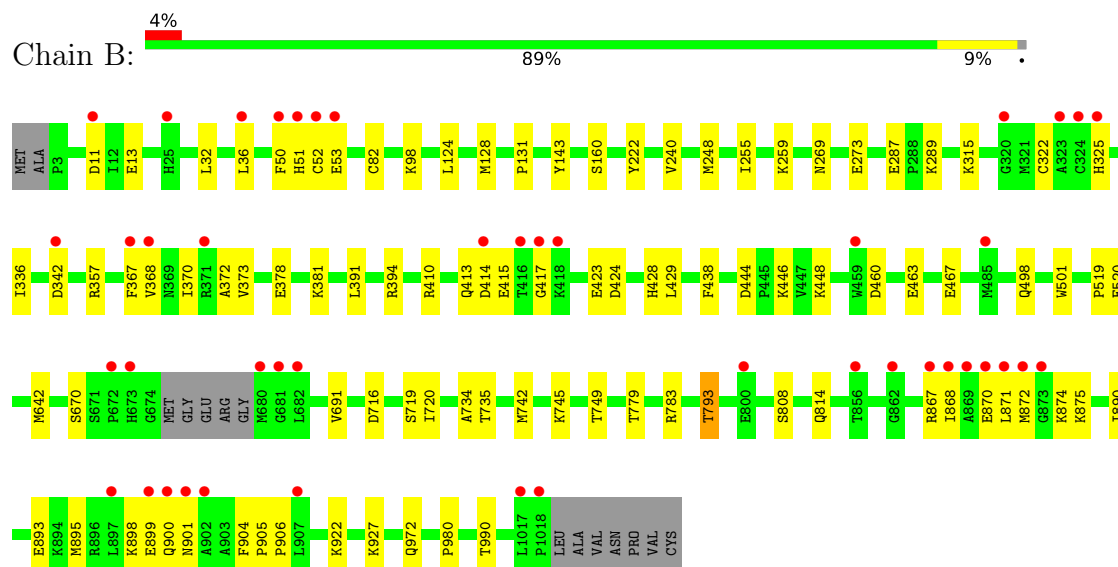
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

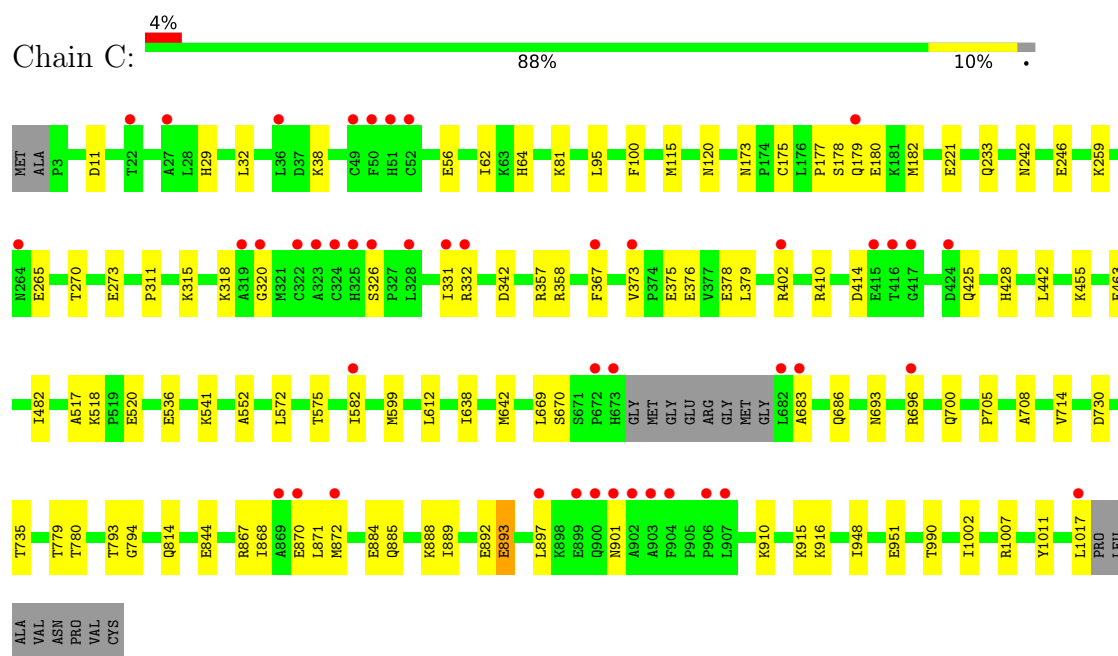
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



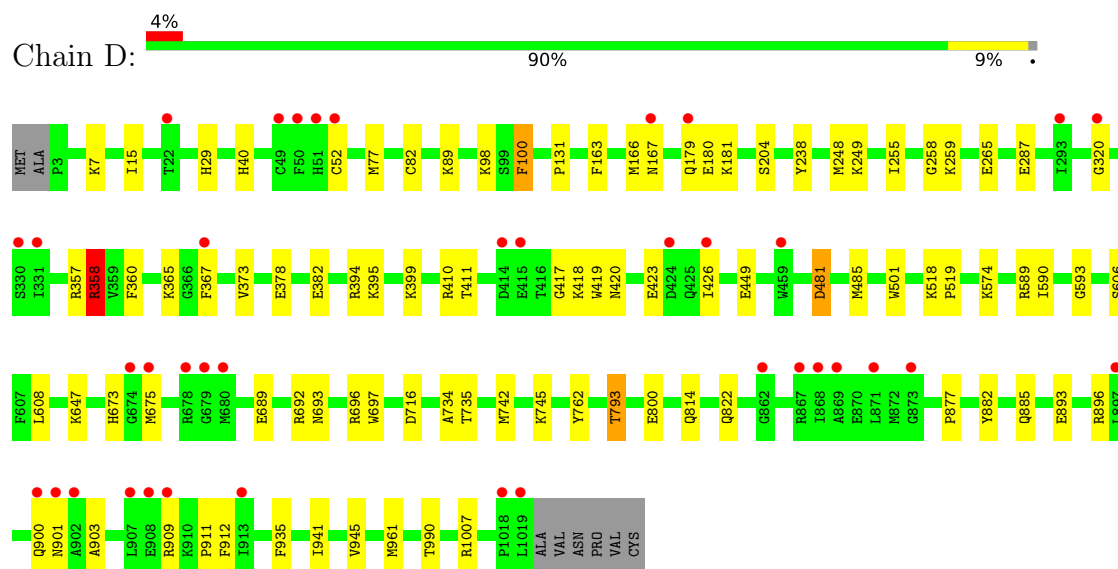
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



• 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, α , β , γ	82.04Å 159.56Å 162.95Å 90.00° 95.75° 90.00°	Depositor
Resolution (Å)	36.15 – 1.69 36.15 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.15-1.69) 99.0 (36.15-1.69)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.177 , 0.200 0.177 , 0.201	Depositor DCC
R_{free} test set	22721 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, FMN, FAD, SF4, TDR

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	0.20	0/7865	0.49	4/10665 (0.0%)
1	B	0.22	0/7895	0.49	0/10701
1	C	0.22	0/7829	0.65	7/10616 (0.1%)
1	D	0.22	0/7902	0.51	3/10714 (0.0%)
All	All	0.22	0/31491	0.54	14/42696 (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 (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	520	GLU	OE1-CD-OE2	-19.45	76.22	122.90
1	C	893	GLU	CG-CD-OE1	18.33	160.56	118.40
1	C	893	GLU	OE1-CD-OE2	-17.25	81.49	122.90
1	C	520	GLU	CG-CD-OE1	17.22	158.01	118.40
1	C	893	GLU	CG-CD-OE2	-16.87	79.60	118.40
1	C	520	GLU	CG-CD-OE2	-15.70	82.30	118.40
1	D	358	ARG	CG-CD-NE	7.35	128.16	112.00
1	A	893	GLU	CA-CB-CG	5.82	125.74	114.10
1	D	481	ASP	CB-CG-OD2	-5.65	105.40	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	GLU	CA-CB-CG	5.48	125.05	114.10
1	D	7	LYS	CA-CB-CG	5.47	125.04	114.10
1	A	892	GLU	CA-C-N	-5.44	113.57	122.54
1	A	892	GLU	C-N-CA	-5.44	113.57	122.54
1	C	779	THR	CA-CB-CG2	5.29	119.49	110.50

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	73	0
1	B	7734	0	7754	82	1
1	C	7671	0	7668	78	0
1	D	7740	0	7746	77	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
4	C	48	0	25	4	0
4	D	40	0	19	1	0
5	A	31	0	19	0	0
5	B	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	31	0	19	2	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	25	4
8	C	1103	0	0	24	6
8	D	1127	0	0	26	6
All	All	35847	0	31183	300	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 (300) 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: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:B:315:LYS:NZ	8:B:1204:HOH:O	1.97	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:B:222:TYR:OH	8:B:1203:HOH:O	1.95	0.84
1:C:175:CYS:SG	8:C:1213:HOH:O	2.36	0.83
1:A:222:TYR:OH	8:A:1204:HOH:O	1.97	0.82
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:263:GLU:O	8:A:1208:HOH:O	2.07	0.72
1:B:895:MET:HE2	1:B:895:MET:HA	1.71	0.71
1:D:418:LYS:HG2	1:D:419:TRP:H	1.52	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: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
1:D:358:ARG:HD3	1:D:360:PHE:CE2	2.35	0.62
1:B:871:LEU:CA	1:B:874:LYS:HZ1	2.12	0.62
1:D:900:GLN:CD	1:D:901:ASN:H	2.08	0.62
1:C:884:GLU:OE1	8:C:1208:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:89:LYS:NZ	8:D:1218:HOH:O	2.33	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: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: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:C:38:LYS:NZ	8:C:1226:HOH:O	2.37	0.57
1:D:689:GLU:CD	1:D:692:ARG:HH12	2.13	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:D:418:LYS:HG2	1:D:419:TRP:N	2.18	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:B:870:GLU:C	1:B:874:LYS:HZ1	2.14	0.55
1:D:394:ARG:HH21	1:D:423:GLU:CD	2.14	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
1:D:131:PRO:HB2	1:D:373:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:867:ARG:HA	1:C:872:MET:HE2	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:395:LYS:NZ	8:D:1214:HOH:O	2.28	0.53
1:A:180:GLU:H	1:A:180:GLU:CD	2.16	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:C:259:LYS:NZ	8:C:1216:HOH:O	2.25	0.52
1:C:221:GLU:OE1	8:C:1212:HOH:O	2.19	0.52
1:D:745:LYS:NZ	8:D:1231:HOH:O	2.40	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:B:871:LEU:C	1:B:872:MET:HG2	2.35	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:167:ASN:CG	8:D:1206:HOH:O	2.49	0.51
1:B:128:MET:HE3	1:B:240:VAL:HG21	1.92	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:B:871:LEU:C	1:B:874:LYS:NZ	2.68	0.50
1:A:703:GLN:NE2	8:A:1215:HOH:O	2.18	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:C:916:LYS:HD3	8:C:2135:HOH:O	2.12	0.49
1:D:259:LYS:HE3	8:D:1441:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:871:LEU:C	1:B:874:LYS:HZ2	2.20	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:107:LYS:NZ	8:A:1223:HOH:O	2.36	0.48
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.95	0.48
1:B:248:MET:HE1	1:B:255:ILE:HD11	1.95	0.48
1:C:179:GLN:NE2	8:C:1238:HOH:O	2.45	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:C:56:GLU:CD	1:C:332:ARG:HH21	2.21	0.48
1:A:357:ARG:NH2	8:A:1203:HOH:O	1.94	0.48
1:C:517:ALA:C	1:C:518:LYS:HD2	2.39	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:599:MET:HG2	1:D:77:MET:HE1	1.97	0.47
1:C:32:LEU:HB2	1:D:485:MET:HE1	1.96	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: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:B:143:TYR:OH	8:B:1212:HOH:O	2.20	0.46
1:C:173:ASN:OD1	8:C:1213:HOH:O	2.21	0.46
1:A:263:GLU:HG3	1:A:449:GLU:CD	2.41	0.46
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.96	0.46
1:D:608:LEU:HB2	1:D:742:MET:HE2	1.97	0.46
1:B:779:THR:HG22	1:B:808:SER:HB3	1.98	0.46
1:C:642:MET:HE1	1:C:670:SER:HB2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:428:HIS:CE1	8:B:1237:HOH:O	2.69	0.46
1:D:574:LYS:NZ	5:D:1108:FMN:O4	2.43	0.45
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:895:MET:HE1	1:B:898:LYS:HE3	1.99	0.44
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: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:259:LYS:NZ	8:B:1225:HOH:O	2.39	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:922:LYS:NZ	8:B:1245:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:357:ARG:NH2	8:B:1222:HOH:O	2.34	0.43
1:B:642:MET:HE1	1:B:670:SER:HB2	2.00	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: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:A:414:ASP:CG	1:A:420:ASN:HD21	2.27	0.42
1:C:410:ARG:HG3	1:C:425:GLN:HB3	2.01	0.42
1:D:673:HIS:HB2	1:D:675:MET:HE3	2.00	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:C:115:MET:HE2	1:C:115:MET:HB2	1.91	0.42
1:D:689:GLU:OE2	1:D:692:ARG:NH1	2.51	0.42
1:C:867:ARG:HD2	1:C:872:MET:HE1	2.01	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:C:81:LYS:O	1:D:961:MET:HE1	2.20	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: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:B:716:ASP:OD2	1:B:719:SER:OG	2.37	0.42
1:A:892:GLU:HG3	8:A:1938:HOH:O	2.19	0.42
1:C:178:SER:HG	1:C:180:GLU:CD	2.28	0.42
1:C:780:THR:HG22	1:D:762:TYR:CZ	2.55	0.42
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:414:ASP:CG	1:B:415:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:LYS:NZ	8:B:1248:HOH:O	2.51	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:A:100:PHE:CD1	1:A:100:PHE:C	2.98	0.41
1:B:867:ARG:HG3	1:B:872:MET:HE1	2.03	0.41
1:C:552:ALA:HB2	5:C:1109:FMN:HM73	2.01	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:D:259:LYS:NZ	8:D:1210:HOH:O	2.21	0.41
1:A:342:ASP:HB3	4:A:1106:NAP:C3N	2.51	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:575:THR:HG1	5:C:1109:FMN:HN3	1.67	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:D:100:PHE:CD1	1:D:100:PHE:C	2.99	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:C:320:GLY:C	8:C:1214:HOH:O	2.65	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1011/1025 (99%)	970 (96%)	39 (4%)	2 (0%)	43	28
1	B	1010/1025 (98%)	970 (96%)	36 (4%)	4 (0%)	30	16
1	C	1005/1025 (98%)	971 (97%)	30 (3%)	4 (0%)	30	16
1	D	1016/1025 (99%)	976 (96%)	37 (4%)	3 (0%)	36	22
All	All	4042/4100 (99%)	3887 (96%)	142 (4%)	13 (0%)	36	22

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

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Mol	Chain	Res	Type
1	B	904	PHE
1	D	822	GLN
1	B	906	PRO
1	C	794	GLY

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	836/854 (98%)	835 (100%)	1 (0%)	88	85
1	B	846/854 (99%)	842 (100%)	4 (0%)	81	76
1	C	832/854 (97%)	831 (100%)	1 (0%)	88	85
1	D	841/854 (98%)	837 (100%)	4 (0%)	81	76
All	All	3355/3416 (98%)	3345 (100%)	10 (0%)	87	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PHE
1	B	11[A]	ASP
1	B	11[B]	ASP
1	B	793[A]	THR
1	B	793[B]	THR
1	C	100	PHE
1	D	15[A]	ILE
1	D	15[B]	ILE
1	D	100	PHE
1	D	793	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	494	ASN

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Mol	Chain	Res	Type
1	A	700	GLN
1	A	878	ASN
1	A	930	GLN
1	B	167	ASN
1	B	242	ASN
1	B	487	ASN
1	B	700	GLN
1	B	885	GLN
1	C	23	GLN
1	C	25	HIS
1	C	64	HIS
1	C	179	GLN
1	C	295	GLN
1	C	413	GLN
1	C	885	GLN
1	C	900	GLN
1	D	623	GLN
1	D	700	GLN
1	D	828	GLN
1	D	847	GLN
1	D	885	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 ⓘ

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
6	TDR	B	1107	-	9,9,9	4.16	5 (55%)	12,12,12	3.08	7 (58%)
6	TDR	A	1108	-	9,9,9	4.20	5 (55%)	12,12,12	3.06	8 (66%)
2	SF4	C	1103	1	0,12,12	-	-	-		
2	SF4	A	1101	1	0,12,12	-	-	-		
2	SF4	D	1103	1	0,12,12	-	-	-		
4	NAP	D	1106	-	42,43,52	2.61	9 (21%)	62,67,80	1.64	14 (22%)
4	NAP	B	1106	-	50,52,52	3.02	16 (32%)	71,80,80	1.91	18 (25%)
4	NAP	C	1107	-	50,52,52	2.79	15 (30%)	71,80,80	1.84	19 (26%)
3	FAD	D	1105	-	58,58,58	0.34	0	85,89,89	0.38	0
2	SF4	C	1104	1	0,12,12	-	-	-		
5	FMN	B	1108	-	33,33,33	3.60	15 (45%)	48,50,50	1.45	9 (18%)
5	FMN	A	1107	-	33,33,33	3.62	14 (42%)	48,50,50	1.46	10 (20%)
2	SF4	C	1102	1	0,12,12	-	-	-		
7	PRO	C	1101	-	6,7,8	0.60	0	7,8,10	1.28	1 (14%)
2	SF4	D	1104	1	0,12,12	-	-	-		
2	SF4	A	1103	1	0,12,12	-	-	-		
2	SF4	D	1102	1	0,12,12	-	-	-		
2	SF4	B	1102	1	0,12,12	-	-	-		
3	FAD	A	1105	-	58,58,58	0.29	0	85,89,89	0.31	0
2	SF4	B	1101	1	0,12,12	-	-	-		
2	SF4	B	1104	1	0,12,12	-	-	-		
6	TDR	C	1108	-	9,9,9	4.15	5 (55%)	12,12,12	3.04	7 (58%)
5	FMN	C	1109	-	33,33,33	3.55	14 (42%)	48,50,50	1.53	11 (22%)
5	FMN	D	1108	-	33,33,33	3.59	14 (42%)	48,50,50	1.48	11 (22%)
2	SF4	B	1103	1	0,12,12	-	-	-		
3	FAD	C	1106	-	58,58,58	0.31	0	85,89,89	0.32	0
6	TDR	D	1107	-	9,9,9	4.09	6 (66%)	12,12,12	2.97	7 (58%)
2	SF4	C	1105	1	0,12,12	-	-	-		
2	SF4	A	1104	1	0,12,12	-	-	-		
2	SF4	D	1101	1	0,12,12	-	-	-		
3	FAD	B	1105	-	58,58,58	0.32	0	85,89,89	0.32	0
4	NAP	A	1106	-	50,52,52	3.00	15 (30%)	71,80,80	1.84	17 (23%)
2	SF4	A	1102	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TDR	B	1107	-	-	-	0/1/1/1
6	TDR	A	1108	-	-	-	0/1/1/1
2	SF4	C	1103	1	-	-	0/6/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
2	SF4	D	1103	1	-	-	0/6/5/5
4	NAP	D	1106	-	-	7/27/59/67	0/4/4/5
4	NAP	B	1106	-	-	2/35/67/67	0/5/5/5
4	NAP	C	1107	-	-	1/35/67/67	0/5/5/5
3	FAD	D	1105	-	-	3/34/50/50	0/6/6/6
2	SF4	C	1104	1	-	-	0/6/5/5
5	FMN	B	1108	-	-	1/18/18/18	0/3/3/3
5	FMN	A	1107	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1102	1	-	-	0/6/5/5
7	PRO	C	1101	-	-	0/0/9/11	0/1/1/1
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
3	FAD	A	1105	-	-	3/34/50/50	0/6/6/6
2	SF4	B	1101	1	-	-	0/6/5/5
2	SF4	B	1104	1	-	-	0/6/5/5
6	TDR	C	1108	-	-	-	0/1/1/1
5	FMN	C	1109	-	-	1/18/18/18	0/3/3/3
5	FMN	D	1108	-	-	1/18/18/18	0/3/3/3
3	FAD	C	1106	-	-	2/34/50/50	0/6/6/6
2	SF4	B	1103	1	-	-	0/6/5/5
6	TDR	D	1107	-	-	-	0/1/1/1
2	SF4	C	1105	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
2	SF4	D	1101	1	-	-	0/6/5/5
3	FAD	B	1105	-	-	3/34/50/50	0/6/6/6
4	NAP	A	1106	-	-	2/35/67/67	0/5/5/5
2	SF4	A	1102	1	-	-	0/6/5/5

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	NAP	P2B-O2B	13.55	1.83	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1106	NAP	P2B-O2B	12.96	1.82	1.59
4	C	1107	NAP	P2B-O2B	12.72	1.81	1.59
4	D	1106	NAP	P2B-O2B	12.43	1.81	1.59
5	B	1108	FMN	O4-C4	8.88	1.40	1.23
5	D	1108	FMN	O4-C4	8.71	1.40	1.23
5	A	1107	FMN	O4-C4	8.71	1.40	1.23
5	C	1109	FMN	O4-C4	8.48	1.39	1.23
6	A	1108	TDR	C6-N1	7.87	1.49	1.36
6	B	1107	TDR	C6-N1	7.76	1.49	1.36
6	D	1107	TDR	C6-N1	7.67	1.48	1.36
6	C	1108	TDR	C6-N1	7.59	1.48	1.36
4	B	1106	NAP	C4N-C3N	7.53	1.50	1.39
5	A	1107	FMN	O2-C2	7.48	1.39	1.24
5	D	1108	FMN	O2-C2	7.38	1.39	1.24
5	B	1108	FMN	O2-C2	7.34	1.38	1.24
4	B	1106	NAP	C5N-C4N	7.28	1.51	1.38
4	A	1106	NAP	C4N-C3N	7.25	1.50	1.39
5	D	1108	FMN	C10-N1	7.21	1.47	1.33
4	D	1106	NAP	PA-O3	7.18	1.67	1.59
5	B	1108	FMN	C10-N1	7.17	1.47	1.33
6	C	1108	TDR	C2-N1	7.15	1.46	1.36
5	C	1109	FMN	O2-C2	7.11	1.38	1.24
5	A	1107	FMN	C10-N1	7.10	1.47	1.33
5	C	1109	FMN	C10-N1	6.97	1.47	1.33
6	B	1107	TDR	C2-N1	6.94	1.45	1.36
6	A	1108	TDR	C2-N1	6.84	1.45	1.36
4	A	1106	NAP	C5N-C4N	6.82	1.50	1.38
6	D	1107	TDR	C2-N1	6.81	1.45	1.36
5	A	1107	FMN	C9-C9A	6.80	1.50	1.39
5	B	1108	FMN	C9-C9A	6.79	1.50	1.39
4	C	1107	NAP	C5N-C4N	6.74	1.50	1.38
5	C	1109	FMN	C9-C9A	6.74	1.50	1.39
5	D	1108	FMN	C9-C9A	6.72	1.50	1.39
5	D	1108	FMN	C6-C5A	6.66	1.50	1.40
4	B	1106	NAP	PA-O3	6.66	1.66	1.59
5	A	1107	FMN	C6-C5A	6.63	1.50	1.40
5	C	1109	FMN	C6-C5A	6.54	1.49	1.40
5	B	1108	FMN	C6-C5A	6.50	1.49	1.40
5	A	1107	FMN	C9A-C5A	-6.37	1.31	1.41
5	C	1109	FMN	C9A-C5A	-6.28	1.31	1.41
5	B	1108	FMN	C9A-C5A	-6.10	1.31	1.41
5	D	1108	FMN	C9A-C5A	-5.99	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1107	NAP	C4N-C3N	5.85	1.48	1.39
5	B	1108	FMN	C4A-N5	5.52	1.42	1.30
5	A	1107	FMN	C4A-N5	5.46	1.42	1.30
5	C	1109	FMN	C4A-N5	5.44	1.42	1.30
5	D	1108	FMN	C4A-N5	5.38	1.42	1.30
4	C	1107	NAP	PA-O3	5.36	1.65	1.59
4	A	1106	NAP	PA-O3	5.14	1.65	1.59
6	A	1108	TDR	C4-C5	5.12	1.53	1.44
6	B	1107	TDR	C4-C5	4.82	1.52	1.44
6	D	1107	TDR	C4-C5	4.82	1.52	1.44
6	C	1108	TDR	C4-C5	4.73	1.52	1.44
4	A	1106	NAP	PN-O5D	4.36	1.76	1.59
4	A	1106	NAP	C2N-N1N	4.28	1.39	1.35
4	B	1106	NAP	C2N-N1N	4.15	1.39	1.35
4	B	1106	NAP	PN-O5D	4.07	1.75	1.59
4	C	1107	NAP	PN-O5D	3.99	1.75	1.59
5	C	1109	FMN	C4A-C10	-3.67	1.33	1.44
5	A	1107	FMN	C2-N1	3.66	1.44	1.36
5	D	1108	FMN	C9A-N10	3.66	1.47	1.41
5	B	1108	FMN	C4A-C10	-3.52	1.33	1.44
5	D	1108	FMN	C4A-C10	-3.51	1.33	1.44
4	A	1106	NAP	C7N-N7N	3.51	1.39	1.33
5	C	1109	FMN	C9A-N10	3.49	1.47	1.41
5	A	1107	FMN	C9A-N10	3.48	1.47	1.41
5	A	1107	FMN	C4A-C10	-3.48	1.34	1.44
5	C	1109	FMN	C2-N1	3.44	1.44	1.36
4	C	1107	NAP	C3N-C7N	-3.40	1.45	1.50
5	B	1108	FMN	C9A-N10	3.39	1.47	1.41
5	D	1108	FMN	C10-N10	3.36	1.44	1.37
5	B	1108	FMN	C2-N1	3.34	1.44	1.36
4	D	1106	NAP	O2B-C2B	-3.34	1.32	1.44
6	B	1107	TDR	C2-N3	3.26	1.42	1.37
5	A	1107	FMN	C5A-N5	3.24	1.45	1.39
4	B	1106	NAP	O2B-C2B	-3.24	1.33	1.44
5	D	1108	FMN	C2-N1	3.22	1.43	1.36
4	B	1106	NAP	C3N-C7N	-3.21	1.45	1.50
4	A	1106	NAP	O2B-C2B	-3.19	1.33	1.44
5	C	1109	FMN	C5A-N5	3.18	1.45	1.39
6	C	1108	TDR	C2-N3	3.17	1.42	1.37
6	A	1108	TDR	C2-N3	3.12	1.42	1.37
5	A	1107	FMN	C10-N10	3.09	1.44	1.37
4	C	1107	NAP	O2B-C2B	-3.06	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1108	FMN	C5A-N5	3.05	1.45	1.39
4	C	1107	NAP	C7N-N7N	3.04	1.38	1.33
5	C	1109	FMN	C10-N10	3.04	1.43	1.37
4	B	1106	NAP	C7N-N7N	3.02	1.38	1.33
5	B	1108	FMN	C10-N10	3.02	1.43	1.37
5	B	1108	FMN	C5A-N5	2.97	1.44	1.39
6	D	1107	TDR	C2-N3	2.87	1.42	1.37
4	D	1106	NAP	PN-O5D	2.85	1.70	1.59
4	A	1106	NAP	C3N-C7N	-2.69	1.46	1.50
4	D	1106	NAP	C5A-C4A	2.55	1.43	1.39
6	C	1108	TDR	O4-C4	-2.53	1.18	1.23
4	C	1107	NAP	C6N-C5N	-2.47	1.33	1.38
4	B	1106	NAP	C6N-N1N	2.46	1.40	1.35
6	D	1107	TDR	O4-C4	-2.45	1.18	1.23
4	D	1106	NAP	C2A-N1A	2.44	1.38	1.33
4	A	1106	NAP	C5A-C4A	2.44	1.43	1.39
4	B	1106	NAP	C2A-N1A	2.43	1.38	1.33
6	A	1108	TDR	O4-C4	-2.43	1.19	1.23
4	A	1106	NAP	C6N-C5N	-2.42	1.33	1.38
4	A	1106	NAP	C6N-N1N	2.38	1.40	1.35
4	B	1106	NAP	C6N-C5N	-2.37	1.33	1.38
4	B	1106	NAP	C5A-C4A	2.35	1.43	1.39
4	C	1107	NAP	C5A-C4A	2.33	1.43	1.39
4	C	1107	NAP	C6N-N1N	2.31	1.40	1.35
6	B	1107	TDR	O4-C4	-2.28	1.19	1.23
4	A	1106	NAP	C8A-N9A	2.27	1.41	1.37
5	D	1108	FMN	P-O3P	-2.26	1.46	1.54
5	C	1109	FMN	C4A-C4	2.26	1.52	1.44
4	C	1107	NAP	C2N-C3N	-2.26	1.35	1.39
4	A	1106	NAP	C2A-N1A	2.25	1.37	1.33
5	B	1108	FMN	C4A-C4	2.24	1.52	1.44
4	B	1106	NAP	C4A-N3A	2.23	1.38	1.34
4	C	1107	NAP	C2A-N1A	2.22	1.37	1.33
5	B	1108	FMN	P-O2P	-2.22	1.46	1.54
5	A	1107	FMN	C4A-C4	2.21	1.52	1.44
4	C	1107	NAP	C2N-N1N	2.21	1.37	1.35
4	D	1106	NAP	O2D-C2D	-2.20	1.37	1.43
4	D	1106	NAP	C4A-N3A	2.16	1.38	1.34
5	B	1108	FMN	P-O3P	-2.15	1.46	1.54
4	B	1106	NAP	O5D-C5D	-2.14	1.36	1.44
4	A	1106	NAP	C4A-N3A	2.11	1.38	1.34
5	D	1108	FMN	C4A-C4	2.08	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1107	FMN	P-O2P	-2.07	1.47	1.54
4	D	1106	NAP	C8A-N9A	2.07	1.41	1.37
6	D	1107	TDR	O2-C2	-2.05	1.19	1.23
4	C	1107	NAP	C8A-N9A	2.04	1.41	1.37
4	B	1106	NAP	C8A-N9A	2.03	1.41	1.37
5	C	1109	FMN	P-O2P	-2.03	1.47	1.54

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1106	NAP	C5N-C4N-C3N	-8.44	112.07	120.36
4	C	1107	NAP	C5N-C4N-C3N	-8.13	112.37	120.36
4	A	1106	NAP	C5N-C4N-C3N	-8.06	112.44	120.36
6	C	1108	TDR	C5-C4-N3	5.25	119.88	115.32
6	B	1107	TDR	C5-C4-N3	5.08	119.74	115.32
6	A	1108	TDR	C5-C4-N3	5.05	119.71	115.32
6	D	1107	TDR	C5-C4-N3	4.81	119.51	115.32
4	A	1106	NAP	O7N-C7N-C3N	4.58	125.20	119.60
6	A	1108	TDR	C4-N3-C2	-4.54	120.12	126.37
6	B	1107	TDR	C4-N3-C2	-4.46	120.23	126.37
6	B	1107	TDR	N1-C2-N3	4.45	119.86	115.17
6	C	1108	TDR	C4-N3-C2	-4.39	120.33	126.37
6	A	1108	TDR	N1-C2-N3	4.33	119.73	115.17
6	D	1107	TDR	N1-C2-N3	4.32	119.72	115.17
4	D	1106	NAP	O2B-P2B-O1X	-4.31	93.95	109.33
4	D	1106	NAP	O2N-PN-O3	4.14	118.46	107.27
4	C	1107	NAP	O3-PA-O1A	-4.12	98.31	110.70
4	D	1106	NAP	O3-PA-O1A	-4.11	98.33	110.70
6	D	1107	TDR	C4-N3-C2	-4.11	120.70	126.37
6	B	1107	TDR	O4-C4-C5	-4.03	120.30	124.92
4	B	1106	NAP	O3-PA-O1A	-3.96	98.79	110.70
6	C	1108	TDR	N1-C2-N3	3.95	119.33	115.17
4	A	1106	NAP	O3-PA-O1A	-3.85	99.12	110.70
6	C	1108	TDR	O4-C4-C5	-3.72	120.67	124.92
4	D	1106	NAP	PN-O5D-C5D	-3.70	100.12	121.35
4	B	1106	NAP	O7N-C7N-C3N	3.54	123.93	119.60
5	C	1109	FMN	C4A-C10-N10	3.53	121.54	116.48
5	A	1107	FMN	C4A-C10-N10	3.52	121.52	116.48
5	C	1109	FMN	C4-N3-C2	-3.50	119.42	125.64
4	B	1106	NAP	O2B-P2B-O1X	-3.50	96.86	109.33
6	C	1108	TDR	CM5-C5-C6	-3.50	119.63	123.23
4	C	1107	NAP	O7N-C7N-C3N	3.48	123.85	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1107	TDR	O4-C4-C5	-3.46	120.96	124.92
6	A	1108	TDR	O4-C4-C5	-3.43	120.99	124.92
6	A	1108	TDR	CM5-C5-C6	-3.40	119.73	123.23
5	B	1108	FMN	C4-N3-C2	-3.38	119.64	125.64
4	B	1106	NAP	C2N-C3N-C4N	3.38	122.19	118.26
4	C	1107	NAP	C2N-C3N-C4N	3.37	122.18	118.26
4	C	1107	NAP	O2B-P2B-O1X	-3.37	97.33	109.33
5	D	1108	FMN	C4-N3-C2	-3.35	119.69	125.64
4	B	1106	NAP	P2B-O2B-C2B	-3.34	114.50	123.43
4	B	1106	NAP	O2N-PN-O3	3.28	116.14	107.27
4	C	1107	NAP	P2B-O2B-C2B	-3.28	114.67	123.43
5	D	1108	FMN	C4A-C10-N10	3.27	121.16	116.48
6	D	1107	TDR	C6-N1-C2	-3.26	119.66	122.69
5	B	1108	FMN	C4A-C10-N10	3.26	121.15	116.48
4	A	1106	NAP	C2N-C3N-C4N	3.23	122.01	118.26
5	A	1107	FMN	C4-N3-C2	-3.22	119.93	125.64
5	C	1109	FMN	O5'-P-O1P	3.21	115.13	106.44
6	D	1107	TDR	CM5-C5-C6	-3.21	119.93	123.23
6	B	1107	TDR	C6-N1-C2	-3.11	119.81	122.69
5	D	1108	FMN	O5'-P-O1P	3.02	114.61	106.44
4	D	1106	NAP	O5D-PN-O1N	-2.99	97.08	108.94
4	A	1106	NAP	O2B-P2B-O1X	-2.97	98.73	109.33
5	B	1108	FMN	O3P-P-O5'	2.96	114.39	106.67
5	A	1107	FMN	O2P-P-O5'	2.91	114.25	106.67
6	B	1107	TDR	CM5-C5-C6	-2.83	120.32	123.23
4	A	1106	NAP	O7N-C7N-N7N	-2.81	118.55	122.62
5	C	1109	FMN	O3P-P-O5'	2.81	113.98	106.67
5	D	1108	FMN	O3P-P-O5'	2.79	113.95	106.67
5	A	1107	FMN	O3P-P-O5'	2.76	113.87	106.67
4	B	1106	NAP	O7N-C7N-N7N	-2.72	118.69	122.62
6	C	1108	TDR	C6-N1-C2	-2.71	120.18	122.69
5	B	1108	FMN	O5'-P-O1P	2.66	113.63	106.44
4	B	1106	NAP	PA-O5B-C5B	-2.63	106.30	121.35
4	D	1106	NAP	P2B-O2B-C2B	-2.59	116.52	123.43
6	A	1108	TDR	O2-C2-N1	-2.59	120.12	122.79
4	D	1106	NAP	O3X-P2B-O2X	2.57	117.45	107.80
5	D	1108	FMN	C5A-C9A-N10	2.54	120.26	117.97
4	C	1107	NAP	C3B-C2B-C1B	-2.51	98.01	102.81
5	D	1108	FMN	O4-C4-C4A	-2.50	119.94	126.53
6	C	1108	TDR	O2-C2-N1	-2.50	120.21	122.79
4	D	1106	NAP	PA-O5B-C5B	-2.50	107.05	121.35
6	B	1107	TDR	O2-C2-N1	-2.49	120.22	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	FMN	C5A-C9A-N10	2.49	120.22	117.97
4	C	1107	NAP	O7N-C7N-N7N	-2.49	119.02	122.62
4	A	1106	NAP	PA-O5B-C5B	-2.49	107.08	121.35
4	A	1106	NAP	O3X-P2B-O2X	2.49	117.13	107.80
4	C	1107	NAP	O3X-P2B-O2X	2.48	117.09	107.80
5	C	1109	FMN	C4A-C4-N3	2.47	119.54	113.25
4	B	1106	NAP	O3X-P2B-O2X	2.47	117.05	107.80
4	A	1106	NAP	C3B-C2B-C1B	-2.47	98.09	102.81
6	A	1108	TDR	C6-N1-C2	-2.46	120.40	122.69
5	A	1107	FMN	C10-C4A-N5	-2.46	119.78	124.81
5	C	1109	FMN	O2P-P-O5'	2.46	113.09	106.67
5	A	1107	FMN	C4A-C4-N3	2.45	119.49	113.25
4	A	1106	NAP	C2A-N1A-C6A	-2.44	114.72	118.73
5	C	1109	FMN	O4-C4-C4A	-2.44	120.08	126.53
4	D	1106	NAP	C3B-C2B-C1B	-2.44	98.13	102.81
5	B	1108	FMN	O4-C4-C4A	-2.44	120.09	126.53
4	B	1106	NAP	O4B-C4B-C3B	2.44	110.00	105.15
6	A	1108	TDR	C5-C6-N1	-2.42	119.81	122.42
6	D	1107	TDR	O2-C2-N1	-2.42	120.29	122.79
5	D	1108	FMN	O2P-P-O5'	2.41	112.96	106.67
5	C	1109	FMN	C10-C4A-N5	-2.41	119.90	124.81
5	B	1108	FMN	C4A-C4-N3	2.40	119.37	113.25
4	C	1107	NAP	PN-O5D-C5D	-2.40	107.61	121.35
5	C	1109	FMN	O2-C2-N1	-2.40	117.82	121.80
4	C	1107	NAP	PA-O5B-C5B	-2.40	107.63	121.35
5	D	1108	FMN	C4A-C4-N3	2.39	119.35	113.25
4	B	1106	NAP	C2A-N1A-C6A	-2.39	114.80	118.73
5	B	1108	FMN	C10-C4A-N5	-2.38	119.96	124.81
5	B	1108	FMN	C5A-C9A-N10	2.37	120.11	117.97
5	A	1107	FMN	O4-C4-C4A	-2.35	120.33	126.53
4	D	1106	NAP	N3A-C4A-N9A	2.33	131.13	127.17
5	A	1107	FMN	O5'-P-O1P	2.33	112.72	106.44
4	D	1106	NAP	C2A-N1A-C6A	-2.32	114.92	118.73
5	C	1109	FMN	C5A-C9A-N10	2.31	120.06	117.97
4	B	1106	NAP	N3A-C4A-N9A	2.31	131.09	127.17
4	A	1106	NAP	N3A-C4A-N9A	2.26	131.01	127.17
4	B	1106	NAP	O3X-P2B-O2B	-2.25	97.07	105.85
5	A	1107	FMN	C9A-N10-C10	-2.24	117.34	120.75
5	B	1108	FMN	O2P-P-O5'	2.23	112.49	106.67
5	D	1108	FMN	C10-C4A-N5	-2.22	120.27	124.81
4	C	1107	NAP	O3X-P2B-O2B	-2.21	97.24	105.85
4	A	1106	NAP	P2B-O2B-C2B	-2.21	117.54	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1106	NAP	C5B-C4B-C3B	-2.20	107.31	115.21
5	D	1108	FMN	C9A-N10-C10	-2.19	117.41	120.75
4	A	1106	NAP	O4B-C4B-C3B	2.17	109.45	105.15
4	A	1106	NAP	C5A-C4A-N3A	-2.16	123.74	126.72
4	C	1107	NAP	C4D-O4D-C1D	-2.15	107.95	109.92
5	D	1108	FMN	C4-C4A-C10	2.15	120.62	116.93
4	C	1107	NAP	C6N-C5N-C4N	2.14	122.54	119.45
4	A	1106	NAP	PN-O5D-C5D	-2.14	109.08	121.35
4	B	1106	NAP	C5A-C4A-N3A	-2.13	123.78	126.72
4	D	1106	NAP	O2N-PN-O1N	2.13	122.34	112.44
4	B	1106	NAP	C5D-C4D-C3D	-2.12	107.57	115.21
4	D	1106	NAP	C5A-C4A-N3A	-2.10	123.83	126.72
5	C	1109	FMN	C9A-N10-C10	-2.10	117.55	120.75
4	C	1107	NAP	N3A-C4A-N9A	2.09	130.72	127.17
4	C	1107	NAP	O5D-PN-O1N	-2.09	100.66	108.94
4	C	1107	NAP	C2A-N1A-C6A	-2.08	115.31	118.73
4	A	1106	NAP	O5D-PN-O1N	-2.08	100.69	108.94
4	A	1106	NAP	C6N-C5N-C4N	2.06	122.41	119.45
4	B	1106	NAP	C6N-C5N-C4N	2.05	122.41	119.45
4	D	1106	NAP	O4B-C4B-C3B	2.03	109.18	105.15
7	C	1101	PRO	O-C-CA	-2.02	119.58	124.77
4	C	1107	NAP	O4B-C4B-C3B	2.01	109.14	105.15
4	C	1107	NAP	O2N-PN-O1N	2.00	121.75	112.44

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1105	FAD	PA-O3P-P-O5'
4	D	1106	NAP	O4D-C4D-C5D-O5D
4	D	1106	NAP	C3D-C4D-C5D-O5D
3	A	1105	FAD	PA-O3P-P-O5'
3	B	1105	FAD	PA-O3P-P-O5'
3	C	1106	FAD	PA-O3P-P-O5'
4	B	1106	NAP	C5D-O5D-PN-O1N
4	D	1106	NAP	C5D-O5D-PN-O3
4	D	1106	NAP	C5D-O5D-PN-O1N
5	B	1108	FMN	C4'-C5'-O5'-P
5	C	1109	FMN	C4'-C5'-O5'-P
5	D	1108	FMN	C4'-C5'-O5'-P
5	A	1107	FMN	C4'-C5'-O5'-P
3	C	1106	FAD	C2B-C1B-N9A-C8A

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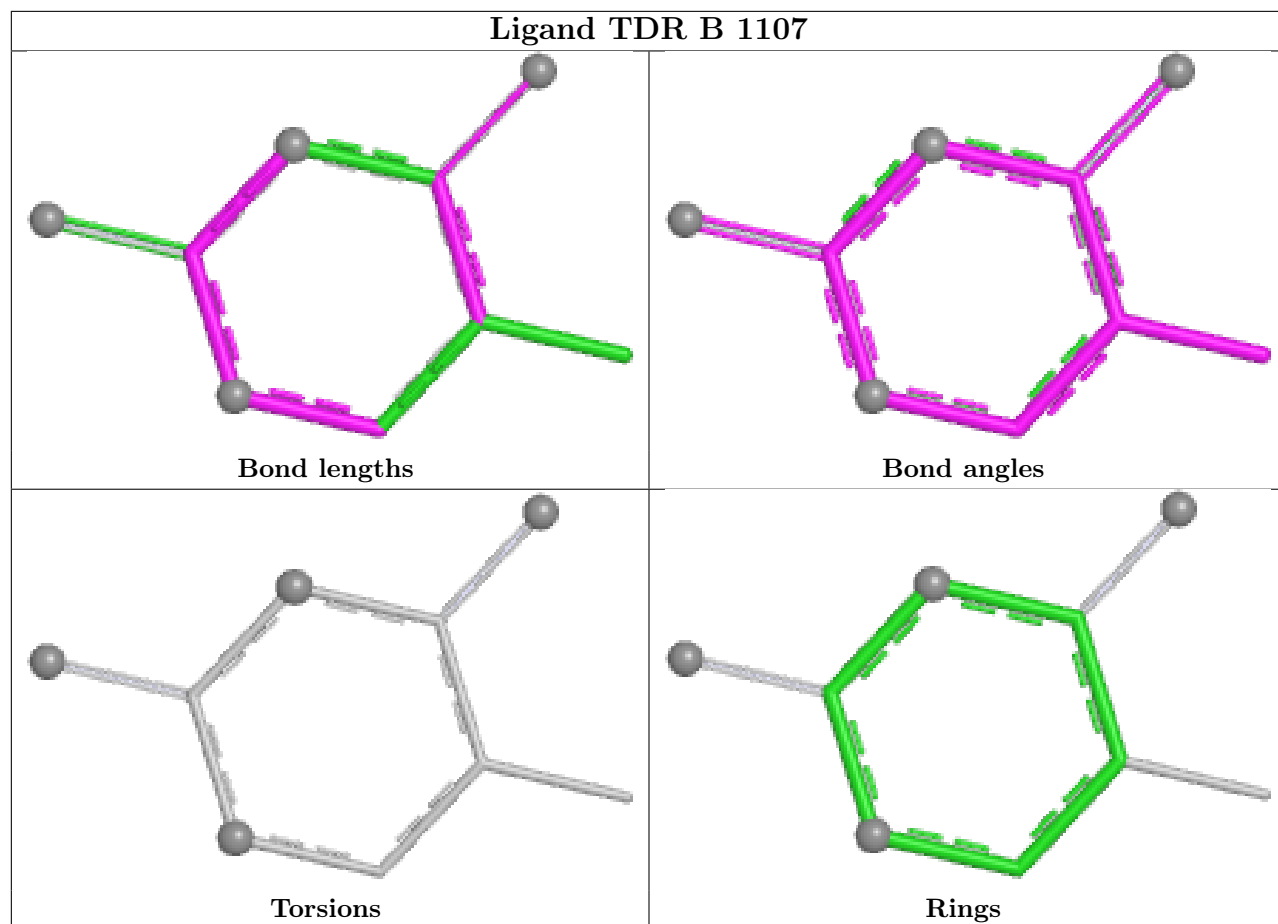
Mol	Chain	Res	Type	Atoms
4	A	1106	NAP	C2B-O2B-P2B-O3X
3	B	1105	FAD	C2B-C1B-N9A-C8A
3	A	1105	FAD	C2B-C1B-N9A-C8A
4	B	1106	NAP	O4B-C4B-C5B-O5B
4	D	1106	NAP	O4B-C4B-C5B-O5B
3	D	1105	FAD	C2B-C1B-N9A-C8A
4	D	1106	NAP	C2B-O2B-P2B-O2X
3	A	1105	FAD	O4B-C4B-C5B-O5B
3	D	1105	FAD	O4B-C4B-C5B-O5B
4	A	1106	NAP	O4B-C4B-C5B-O5B
4	D	1106	NAP	C1B-C2B-O2B-P2B
3	B	1105	FAD	O4B-C4B-C5B-O5B
4	C	1107	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

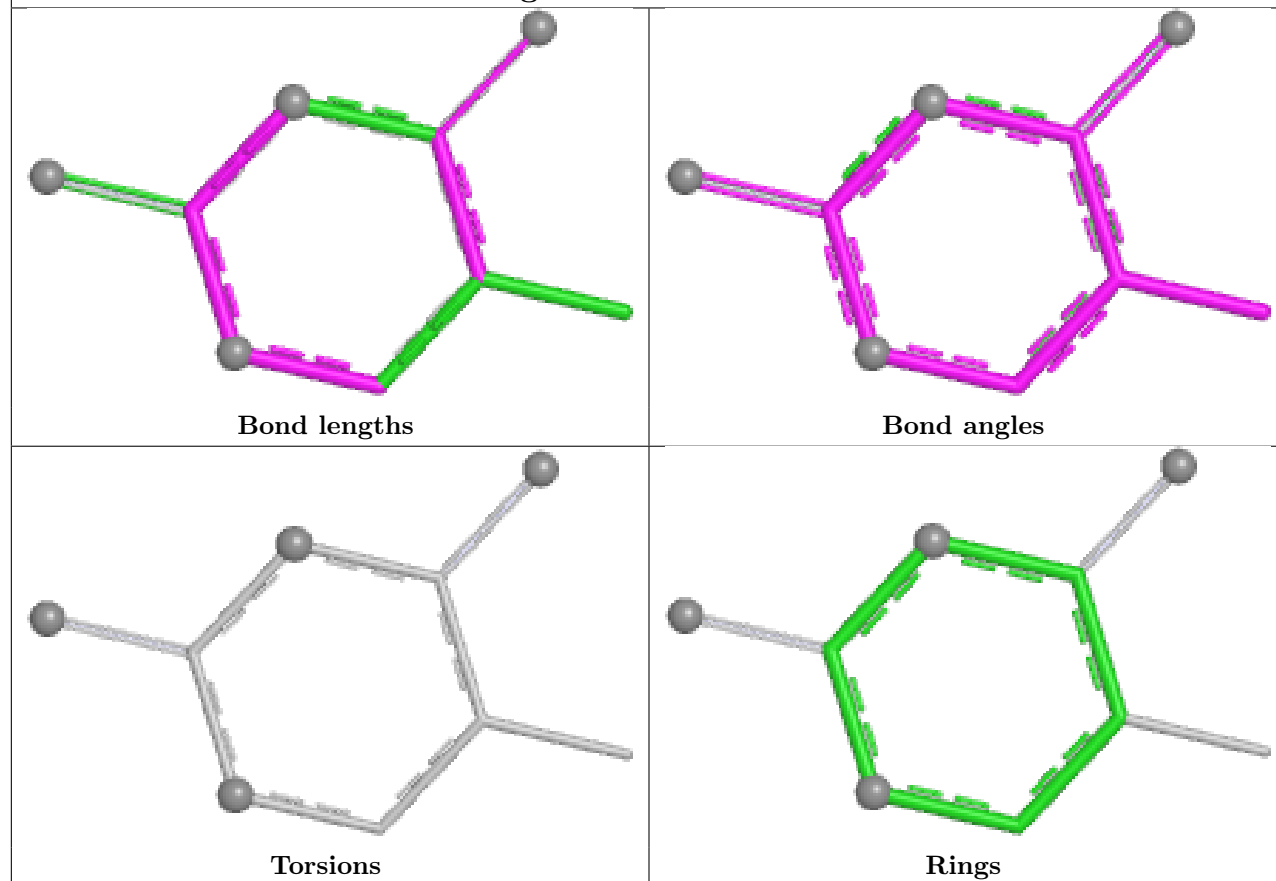
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1106	NAP	1	0
4	B	1106	NAP	5	0
4	C	1107	NAP	4	0
3	A	1105	FAD	1	0
5	C	1109	FMN	2	0
5	D	1108	FMN	1	0
3	C	1106	FAD	1	0
3	B	1105	FAD	1	0
4	A	1106	NAP	5	0

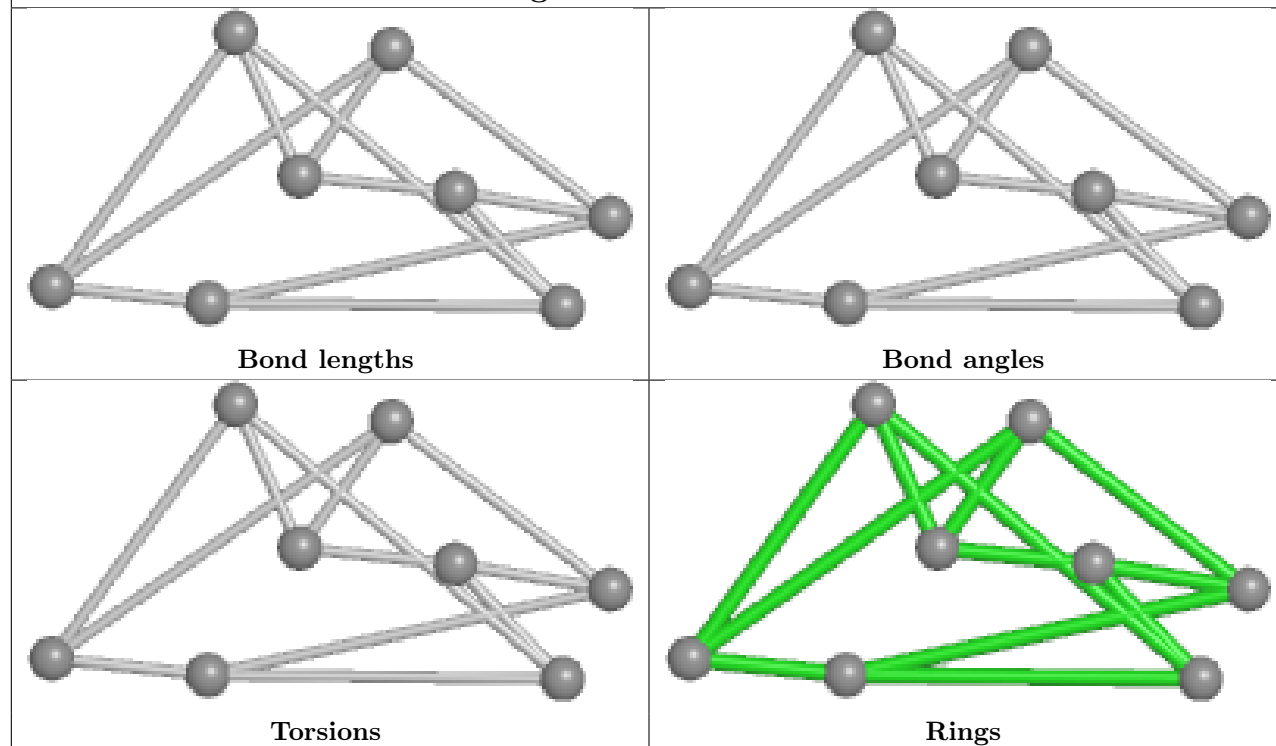
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

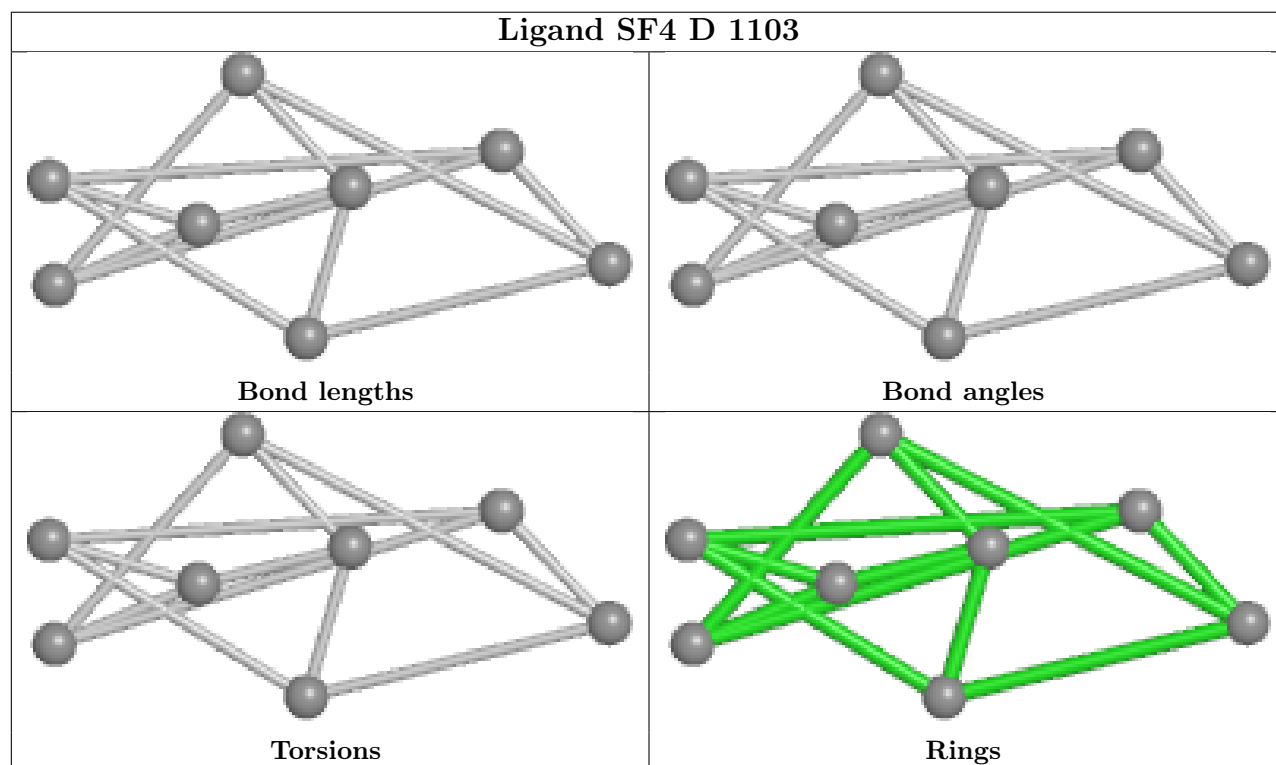
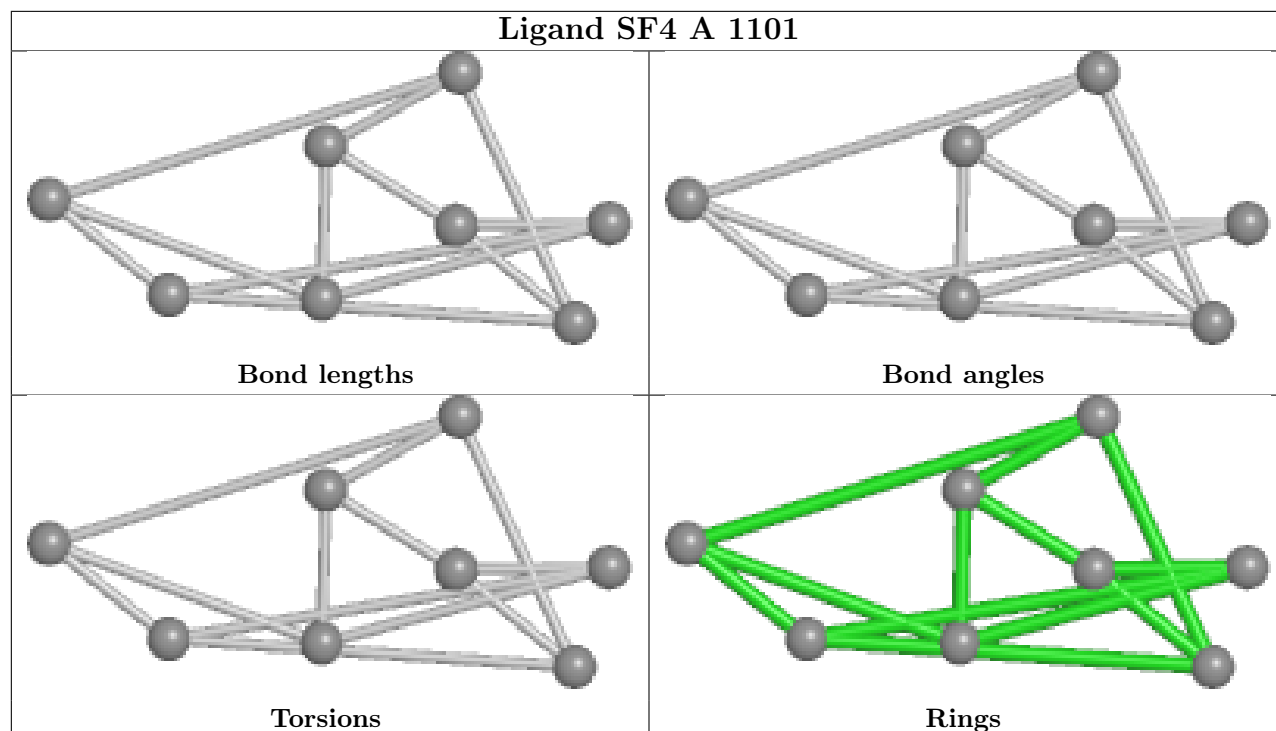


Ligand TDR A 1108

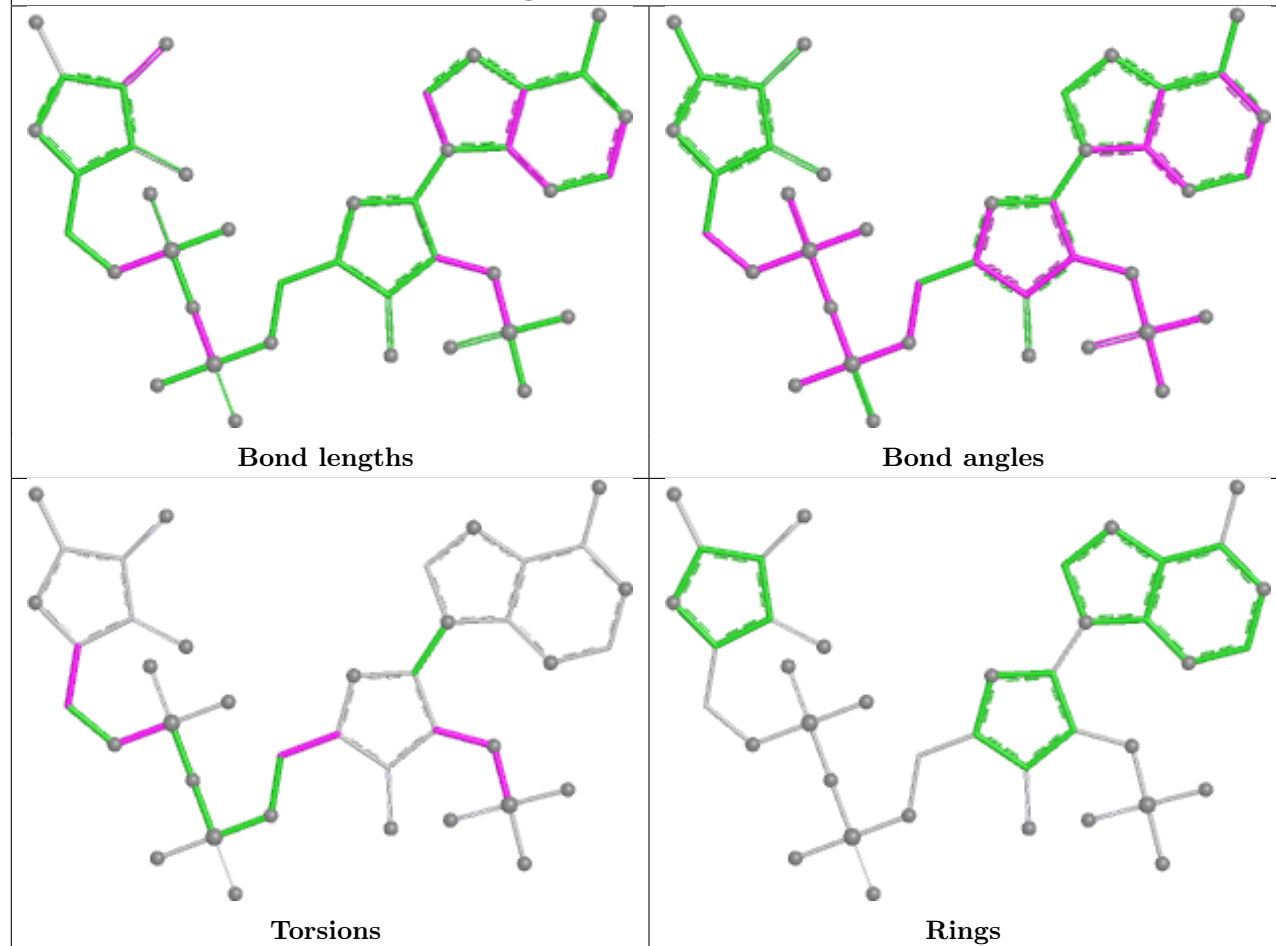


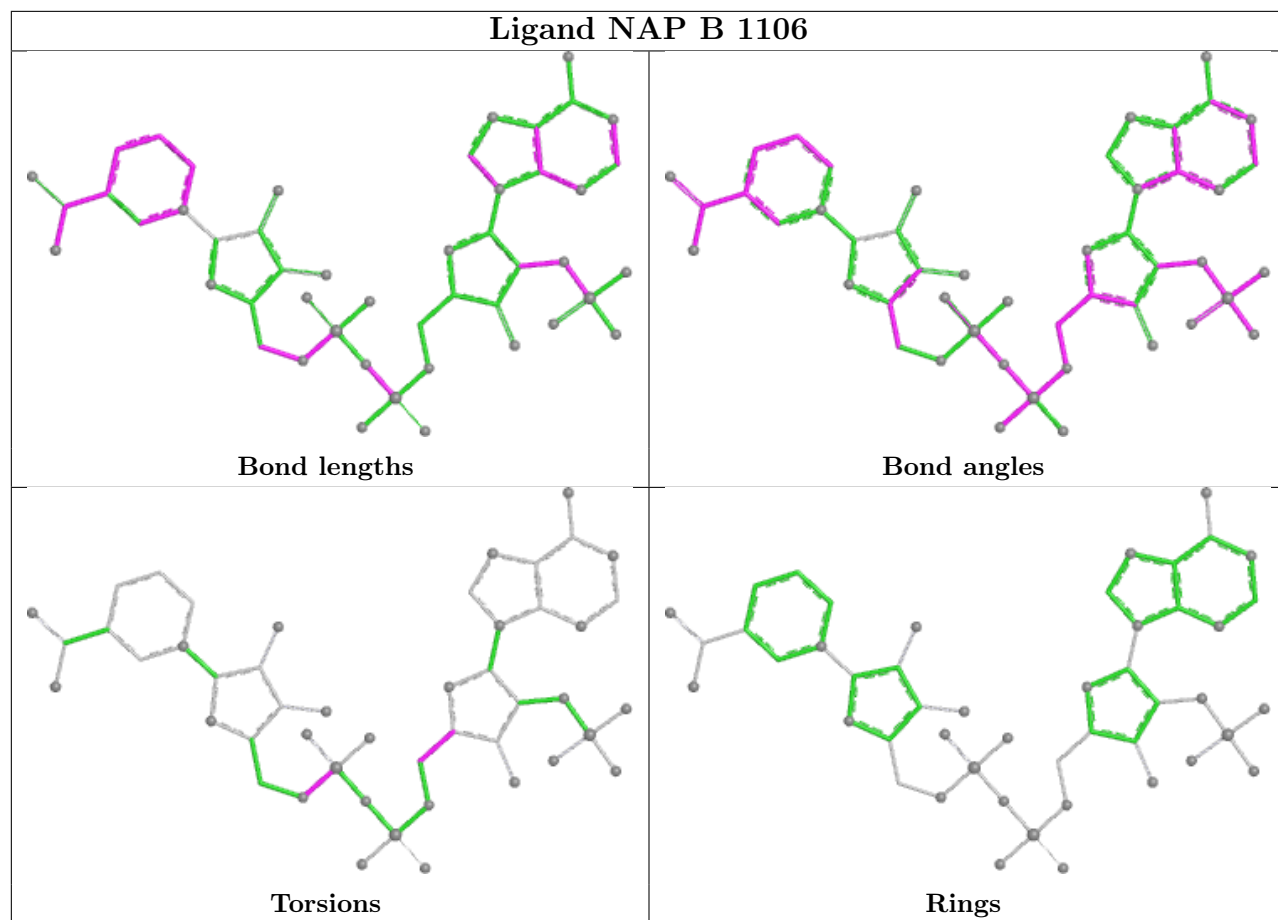
Ligand SF4 C 1103

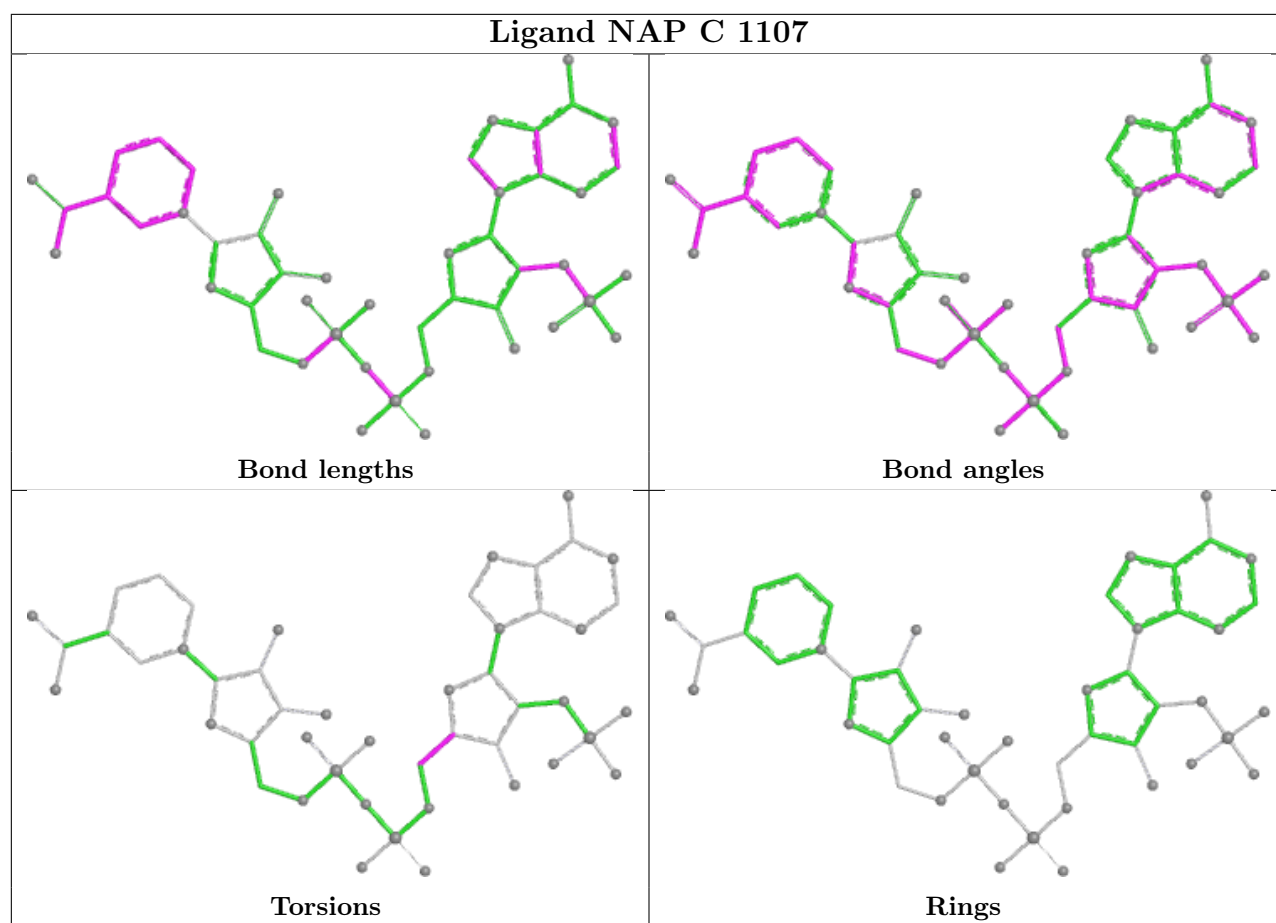


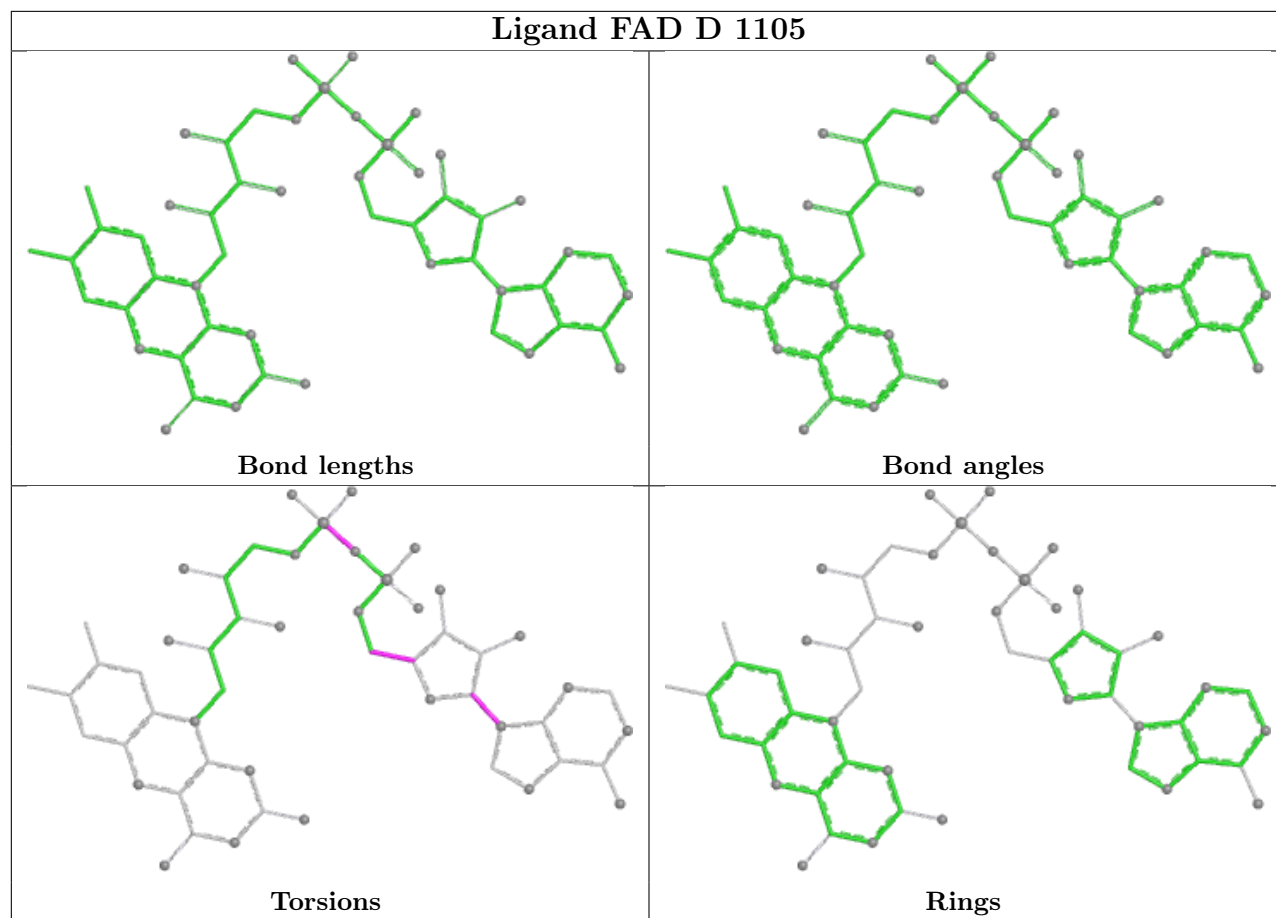


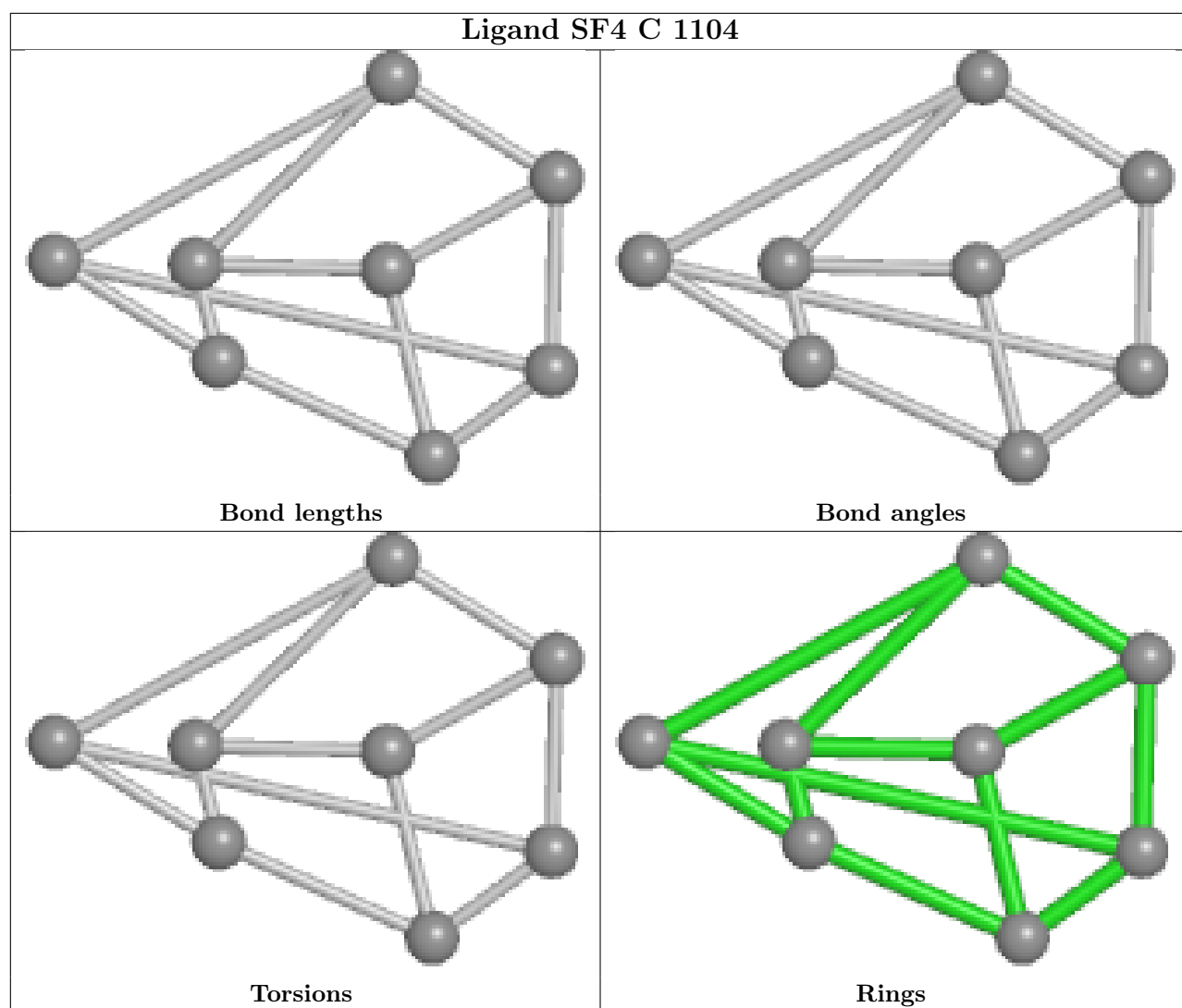
Ligand NAP D 1106



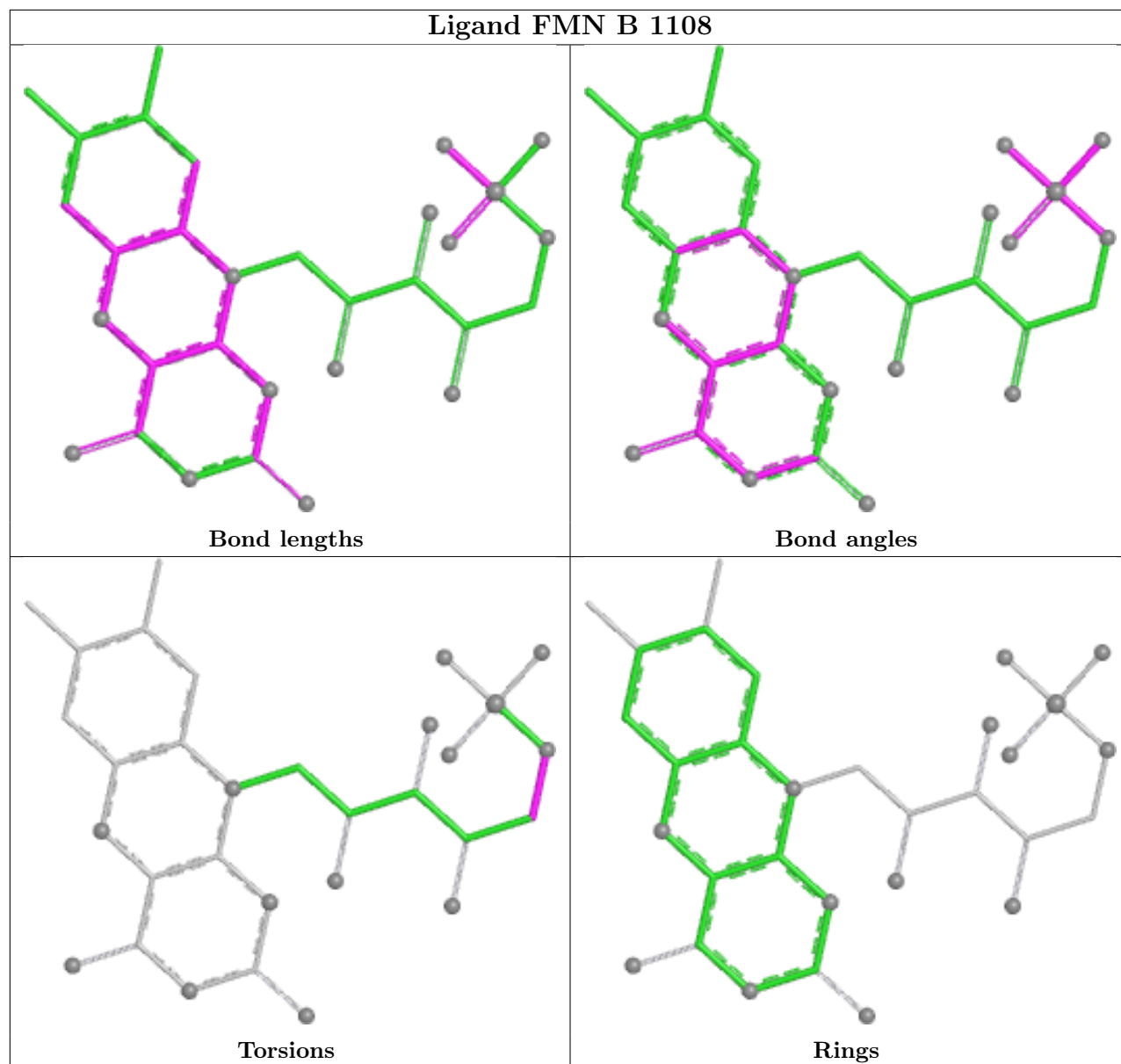




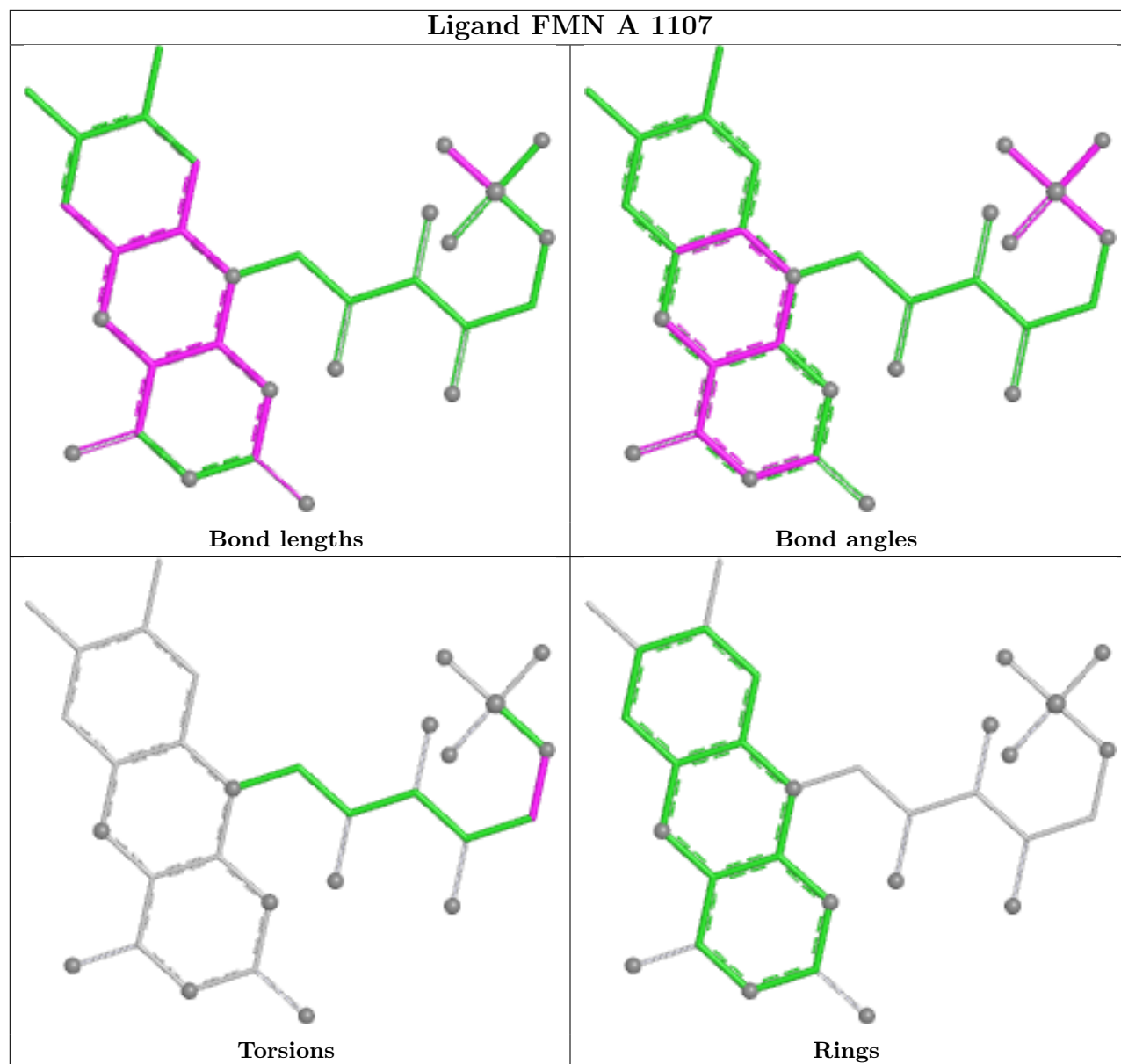


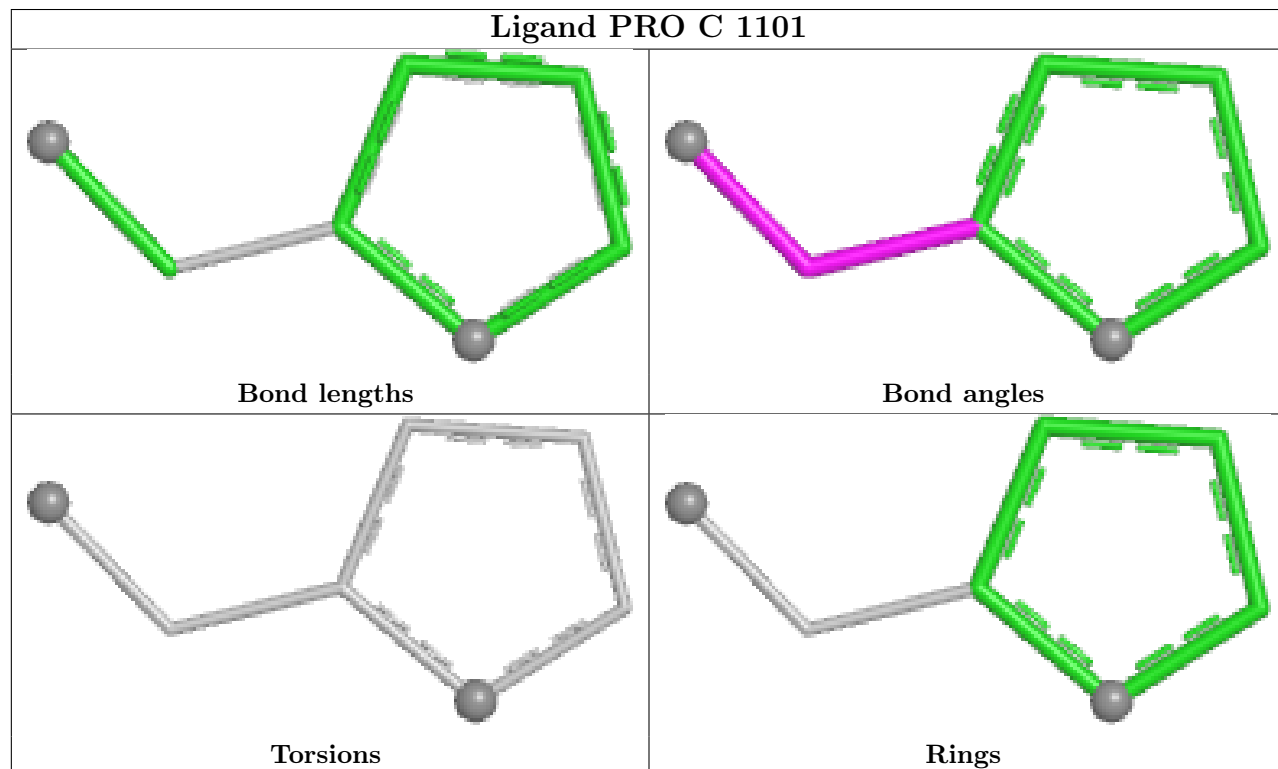
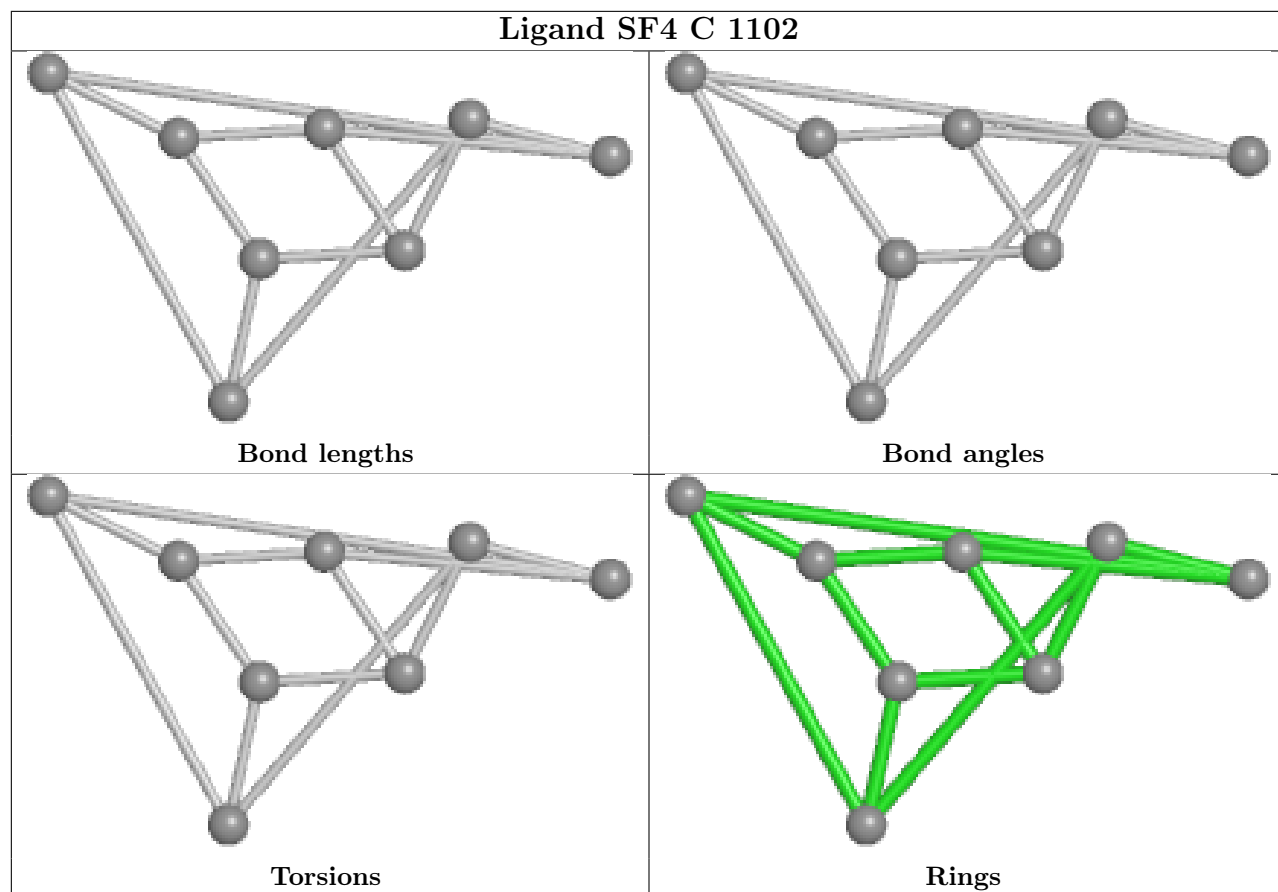


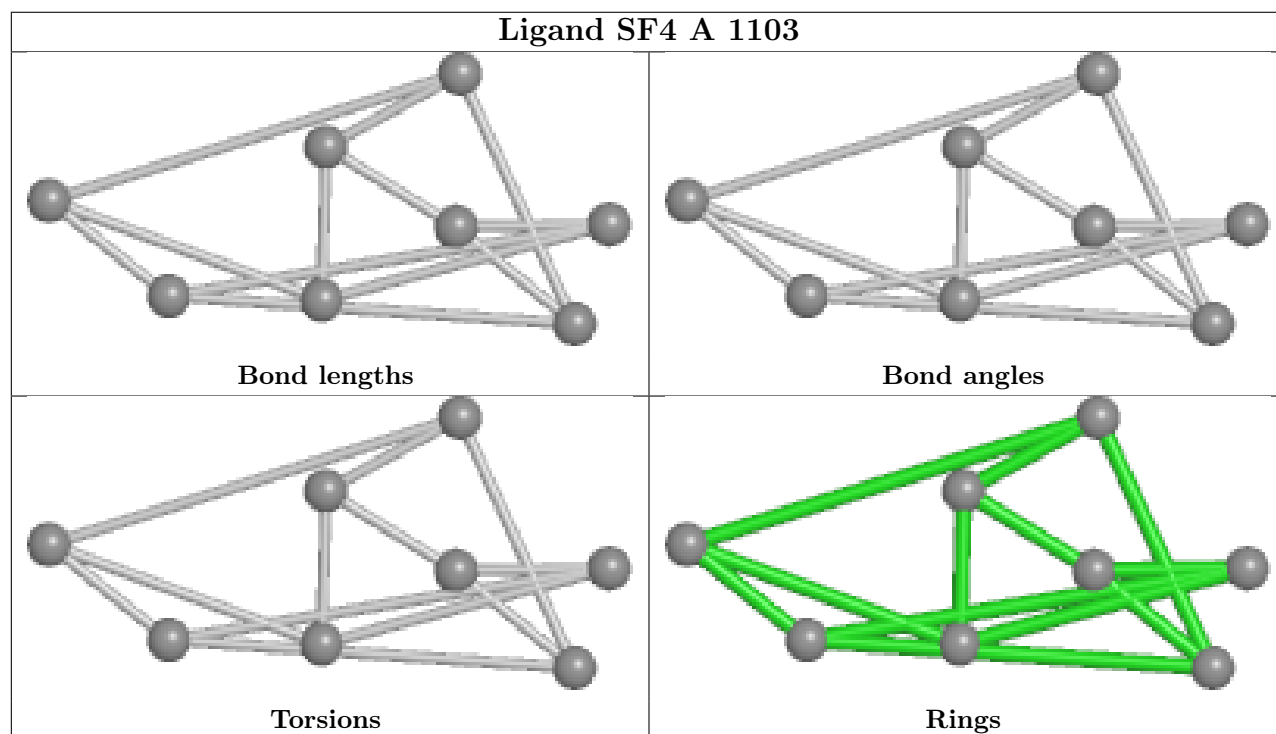
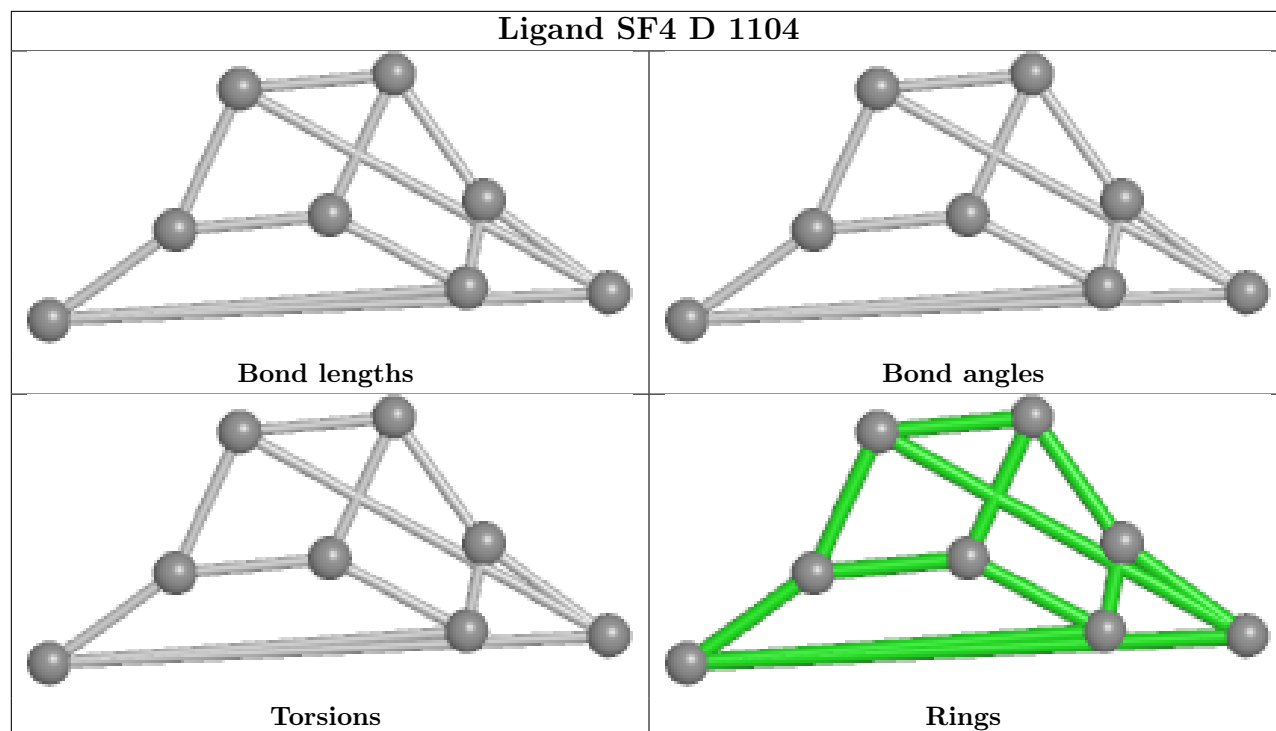
Ligand FMN B 1108

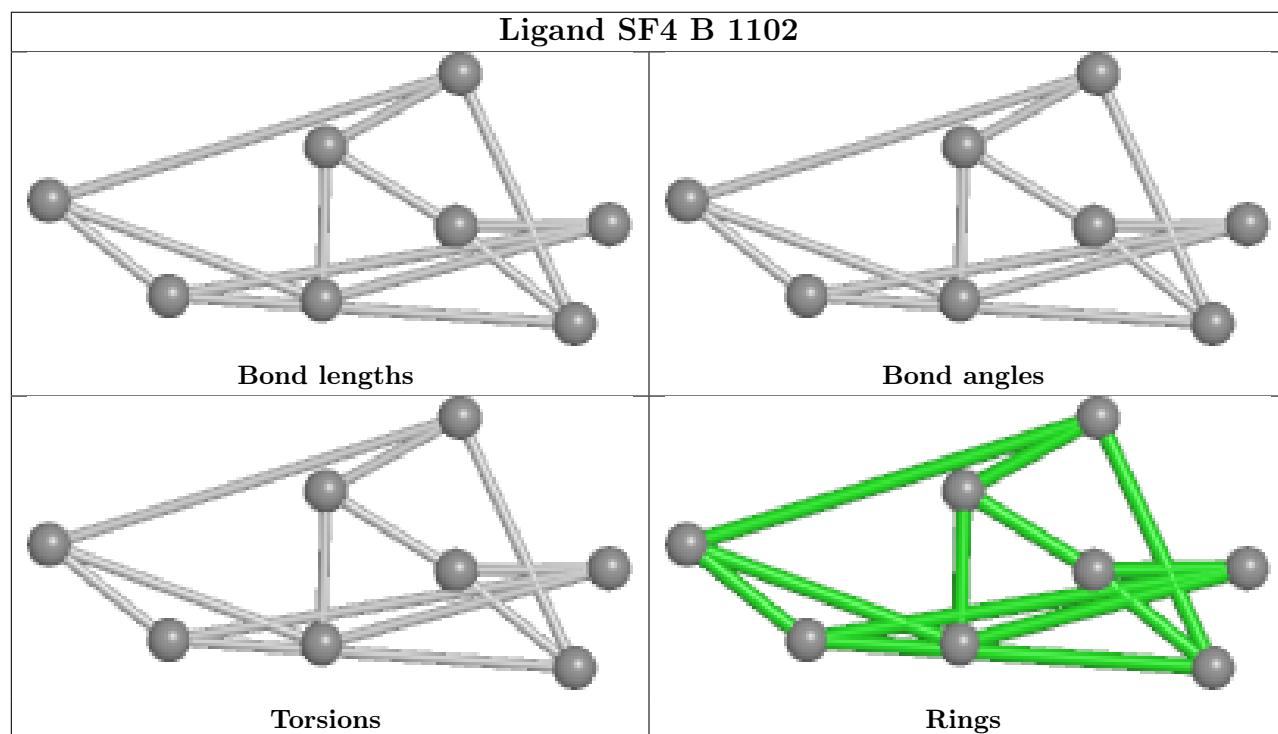
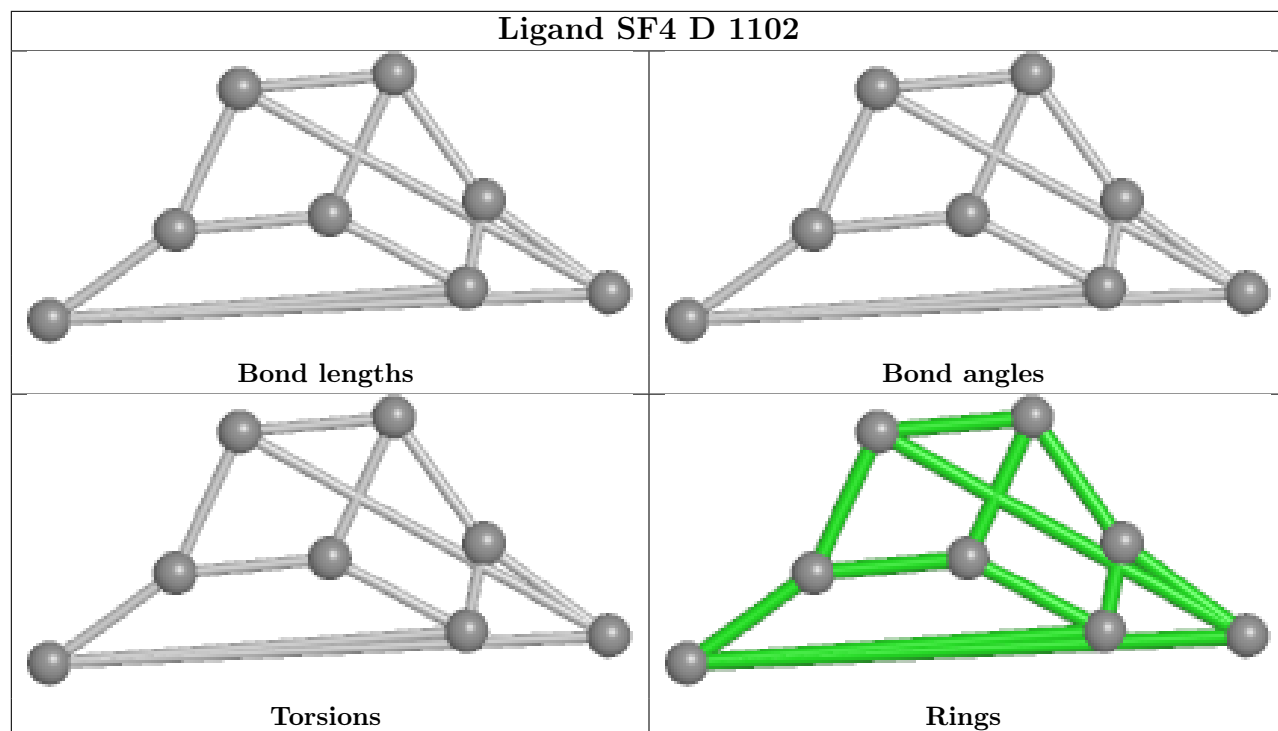


Ligand FMN A 1107

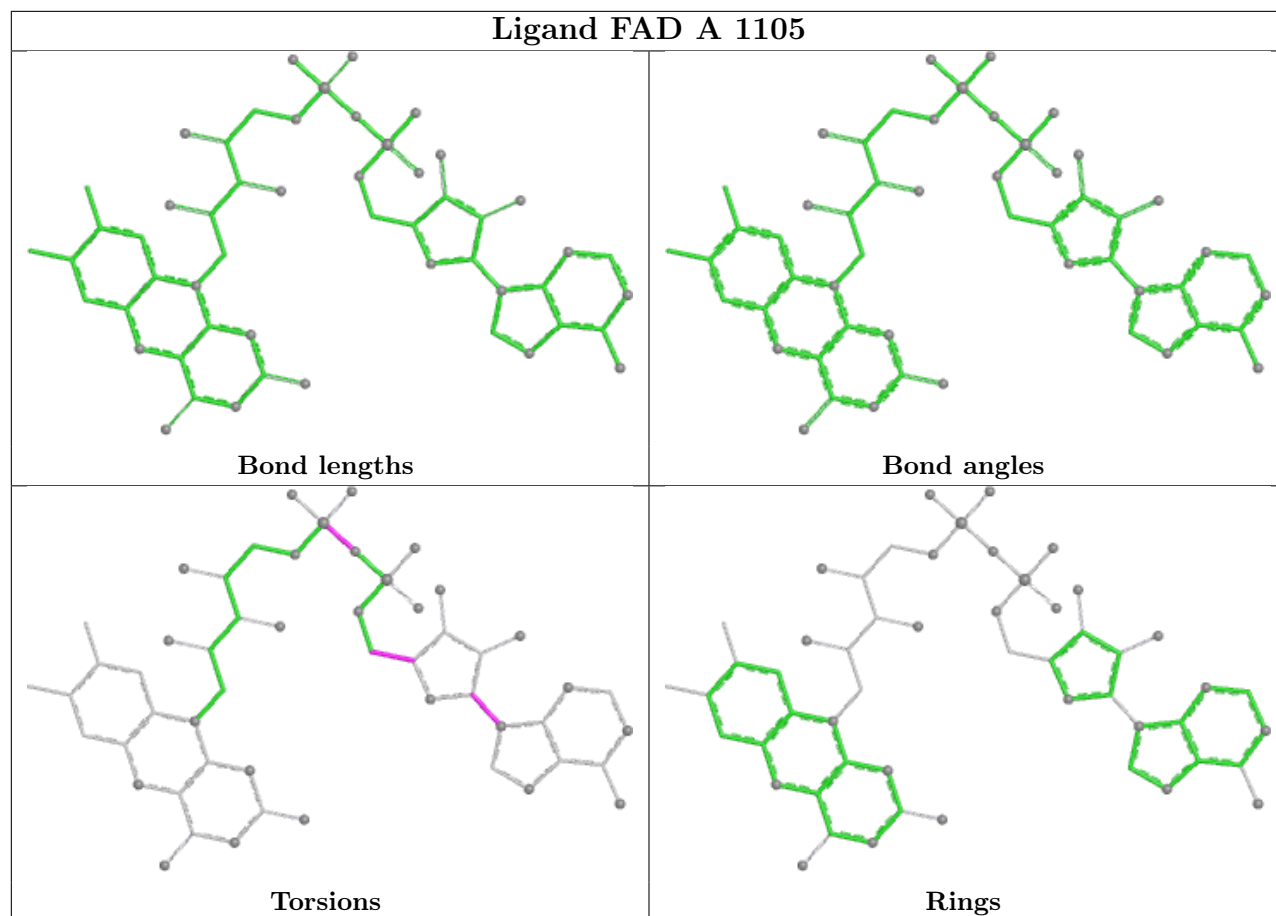




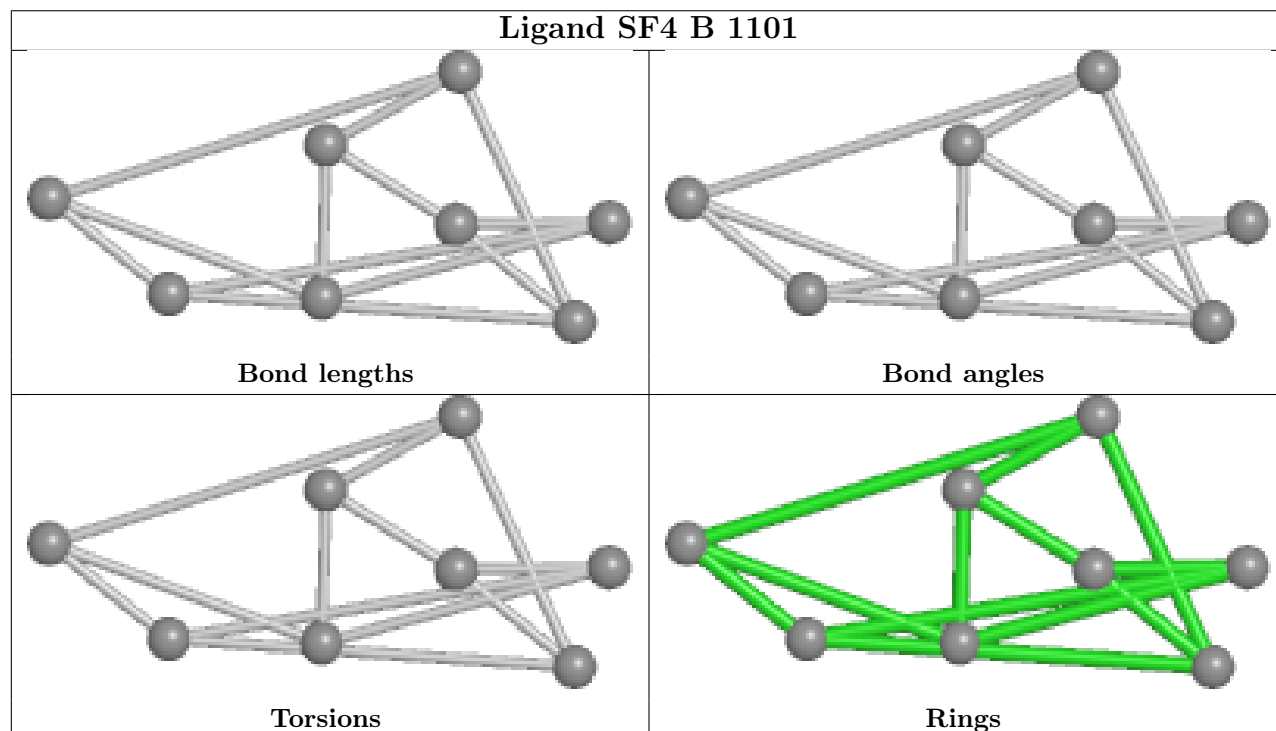


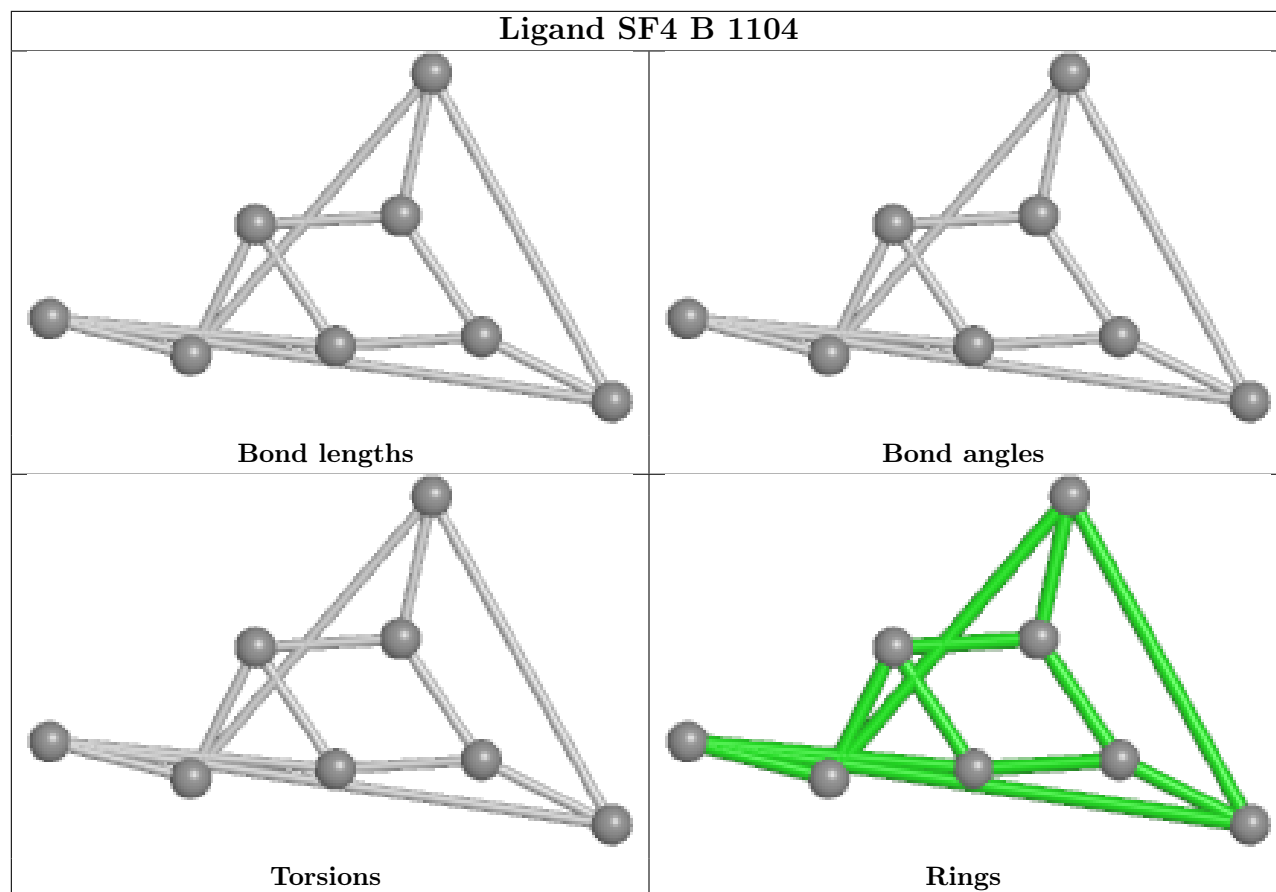


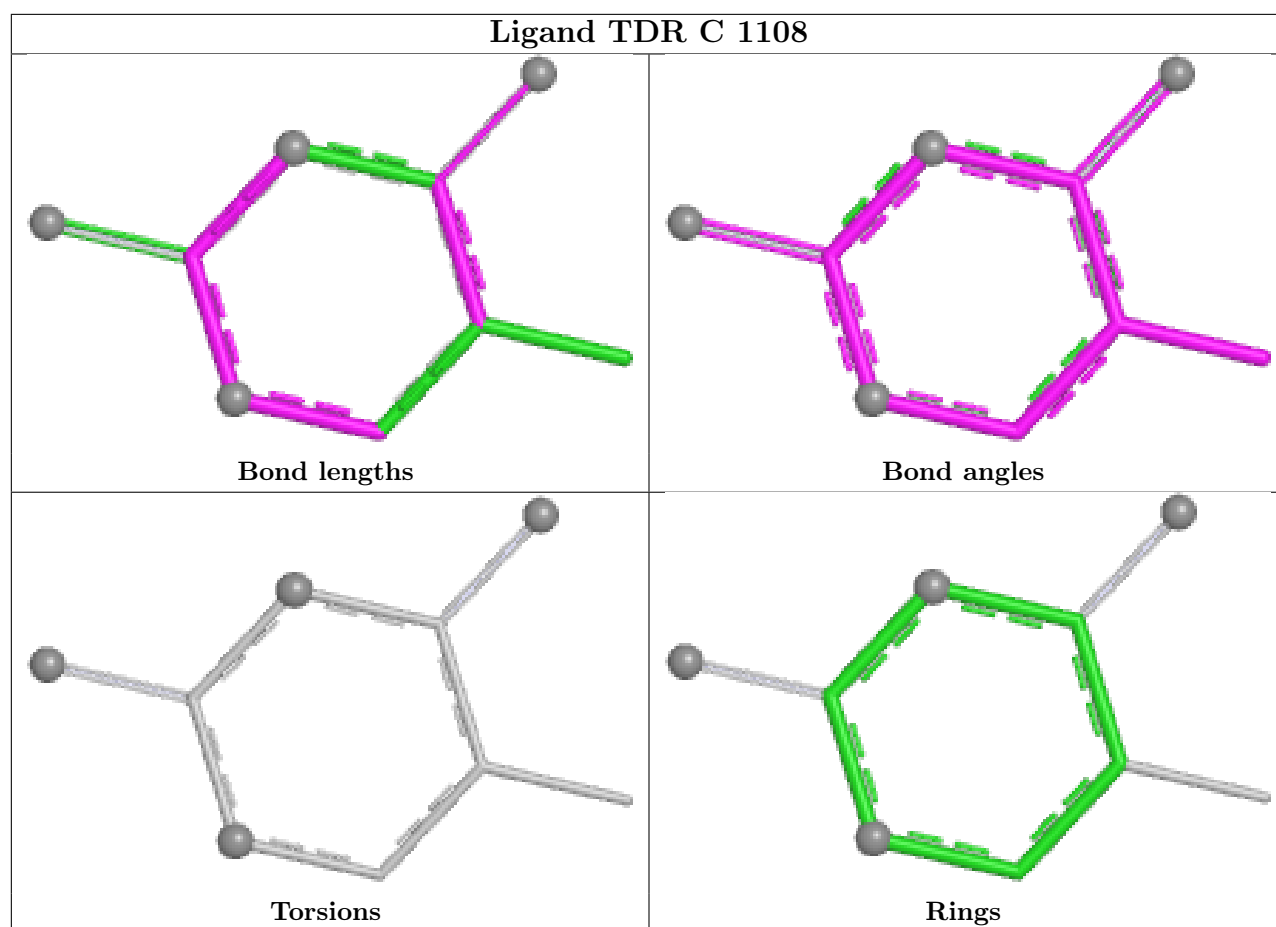
Ligand FAD A 1105

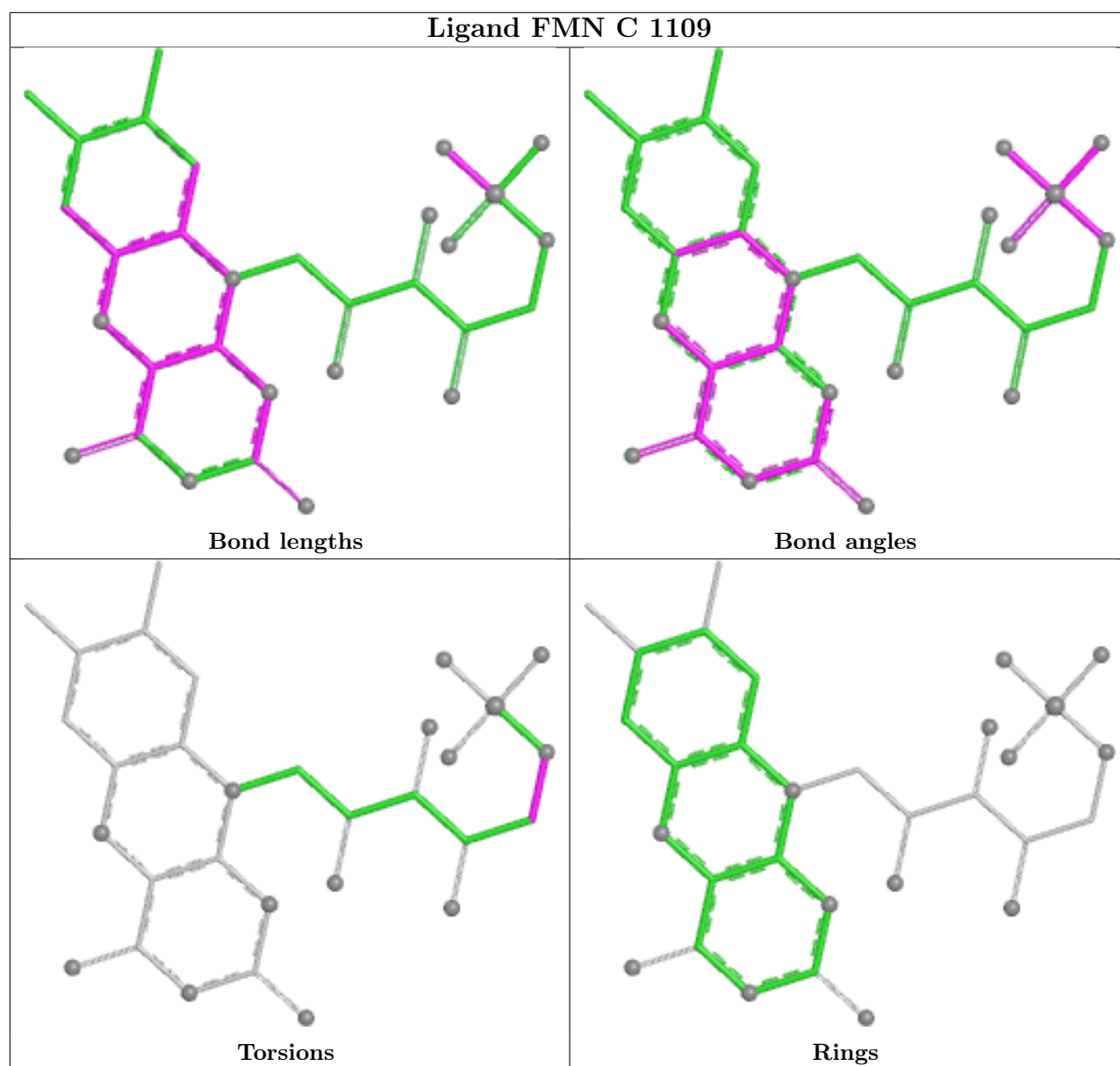


Ligand SF4 B 1101

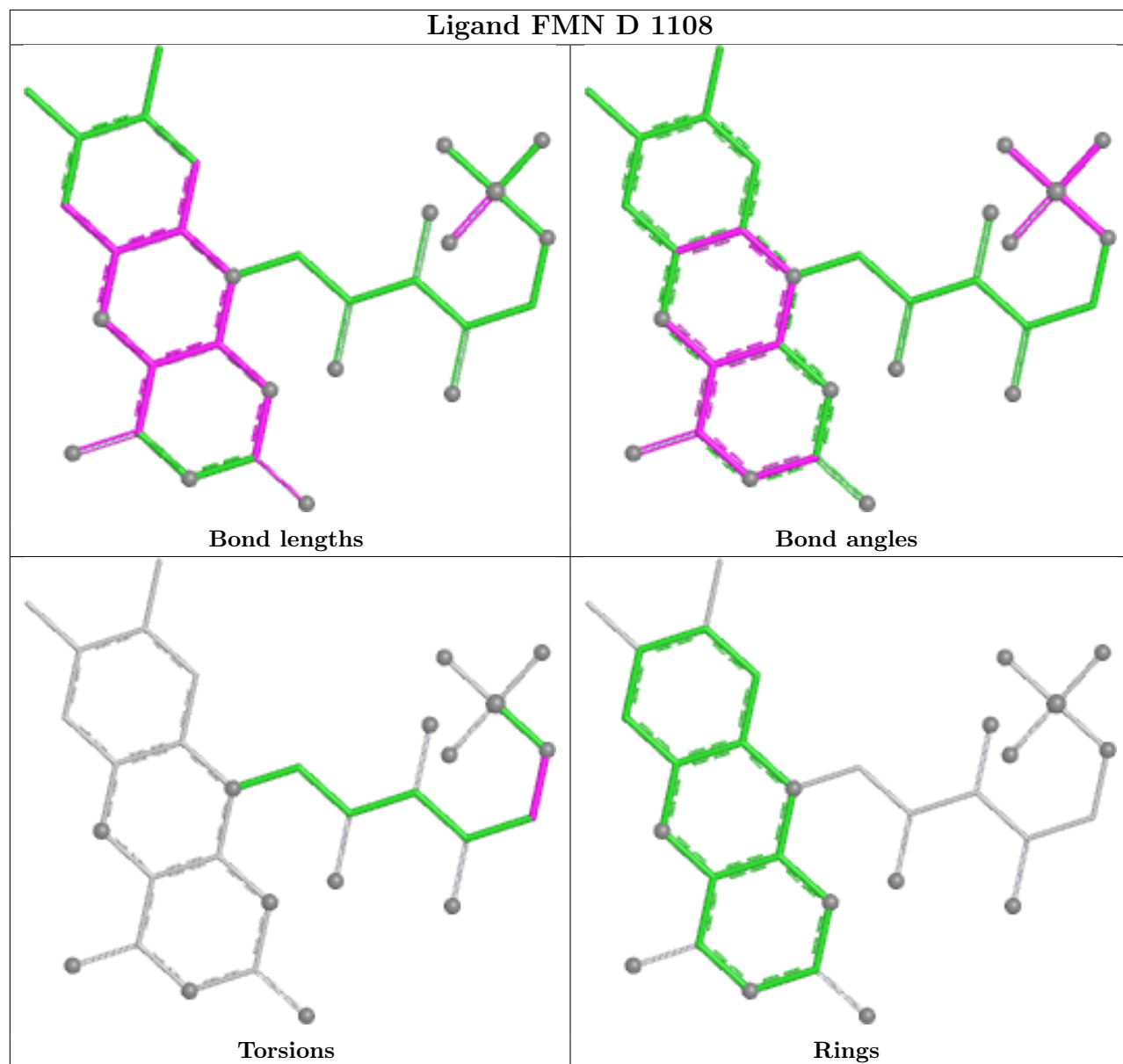


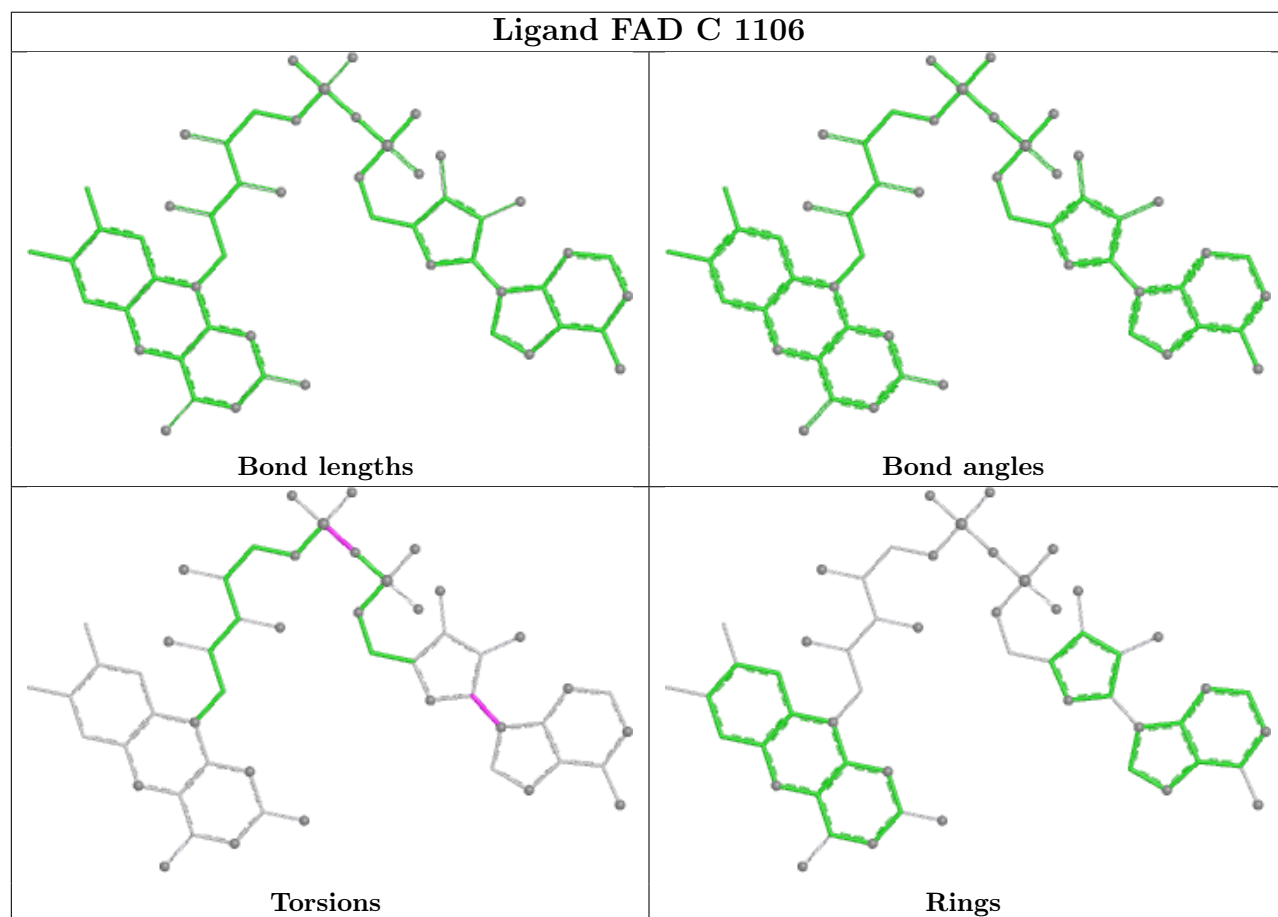
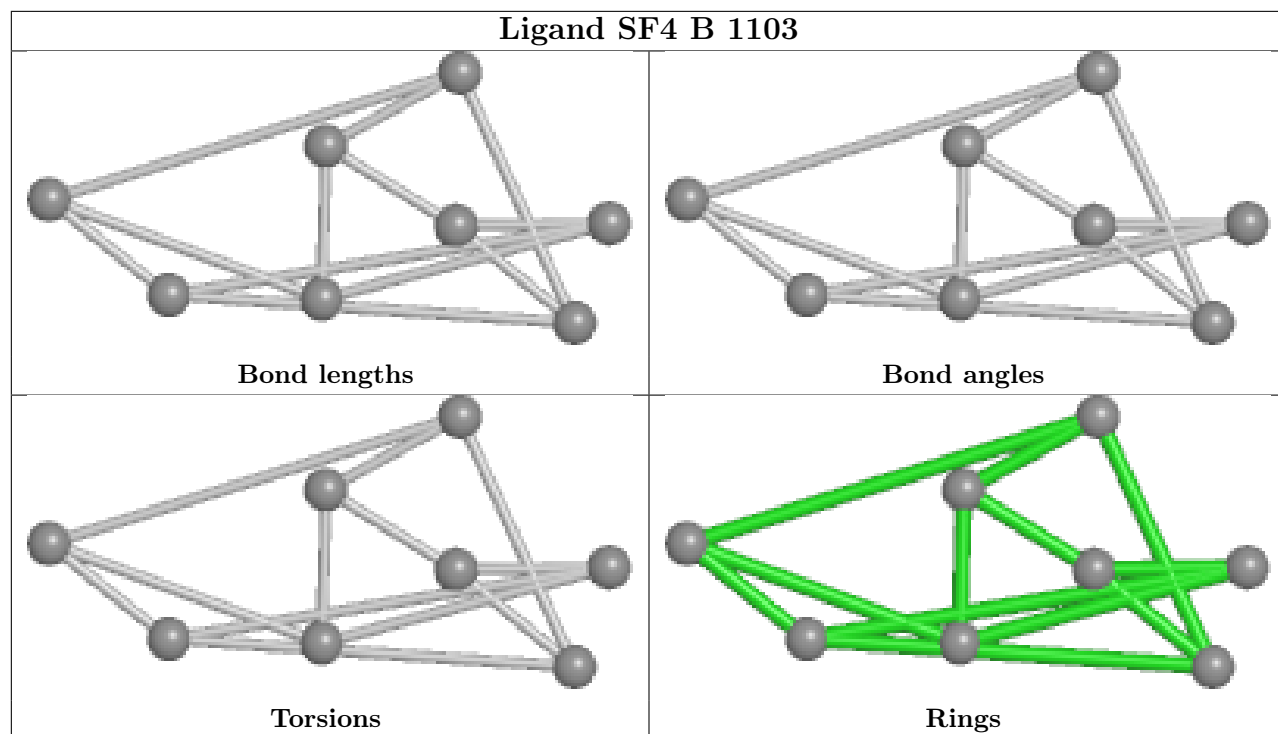




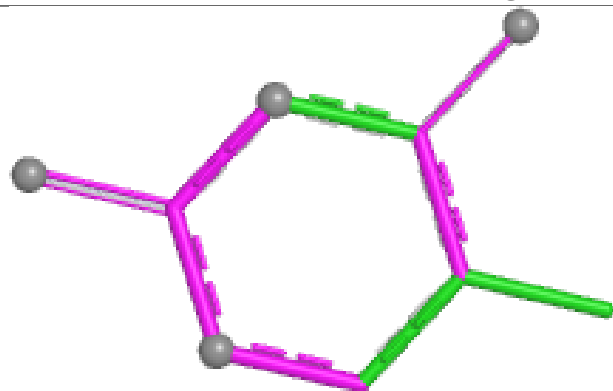


Ligand FMN D 1108

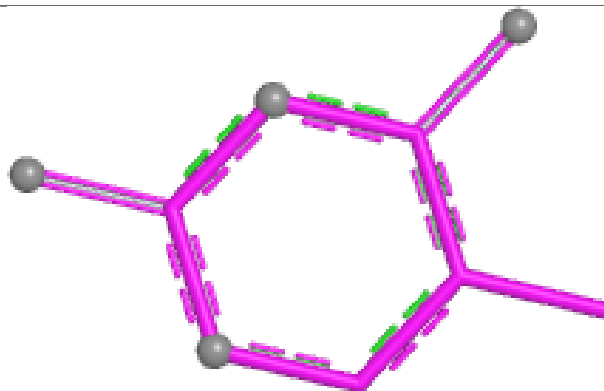




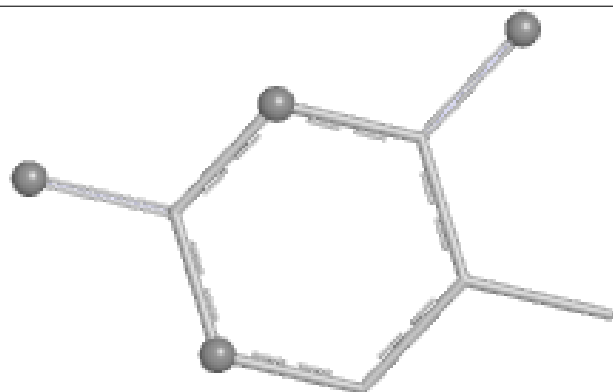
Ligand TDR D 1107



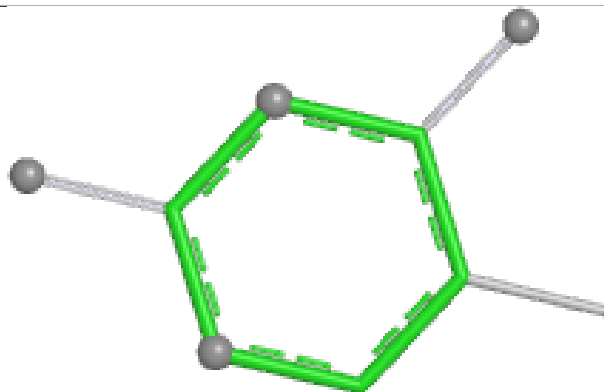
Bond lengths



Bond angles

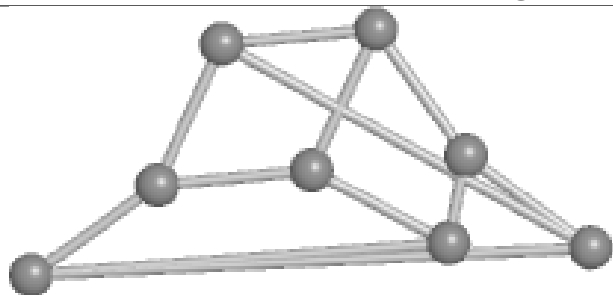


Torsions

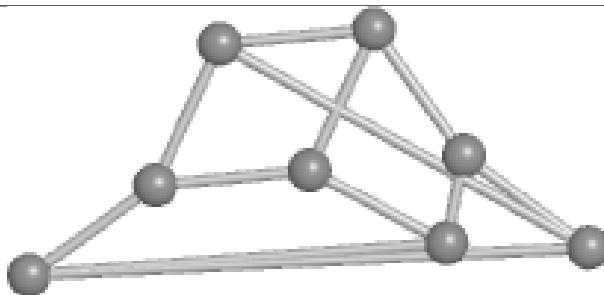


Rings

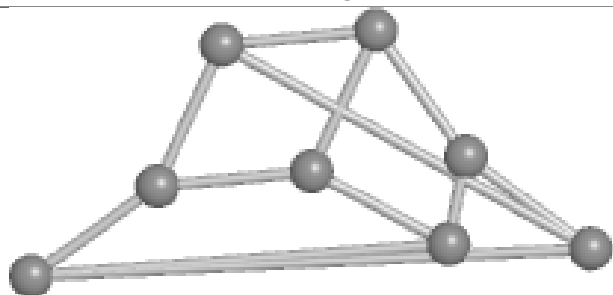
Ligand SF4 C 1105



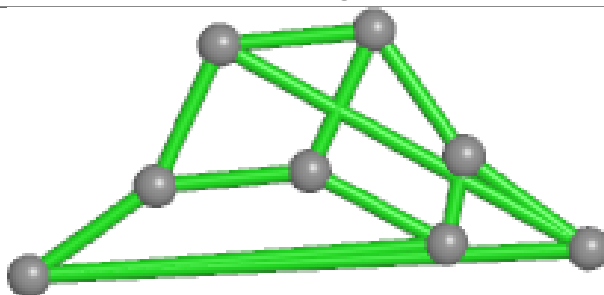
Bond lengths



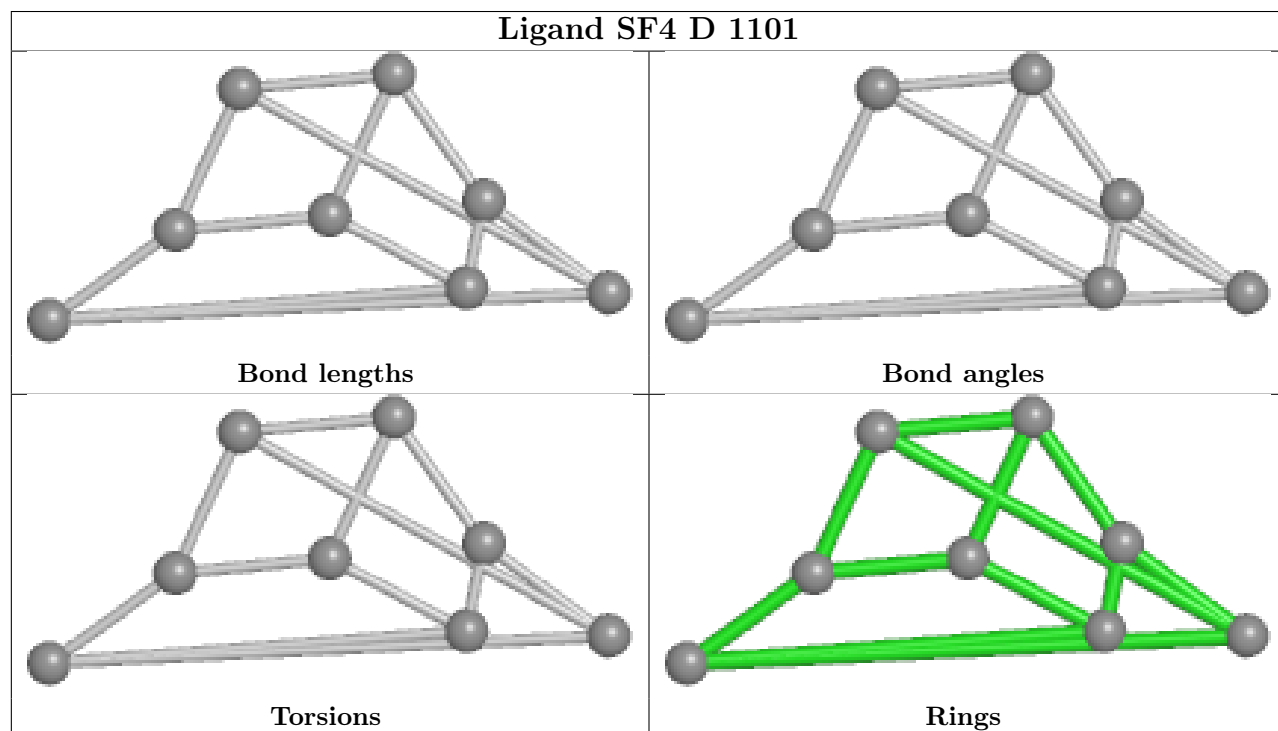
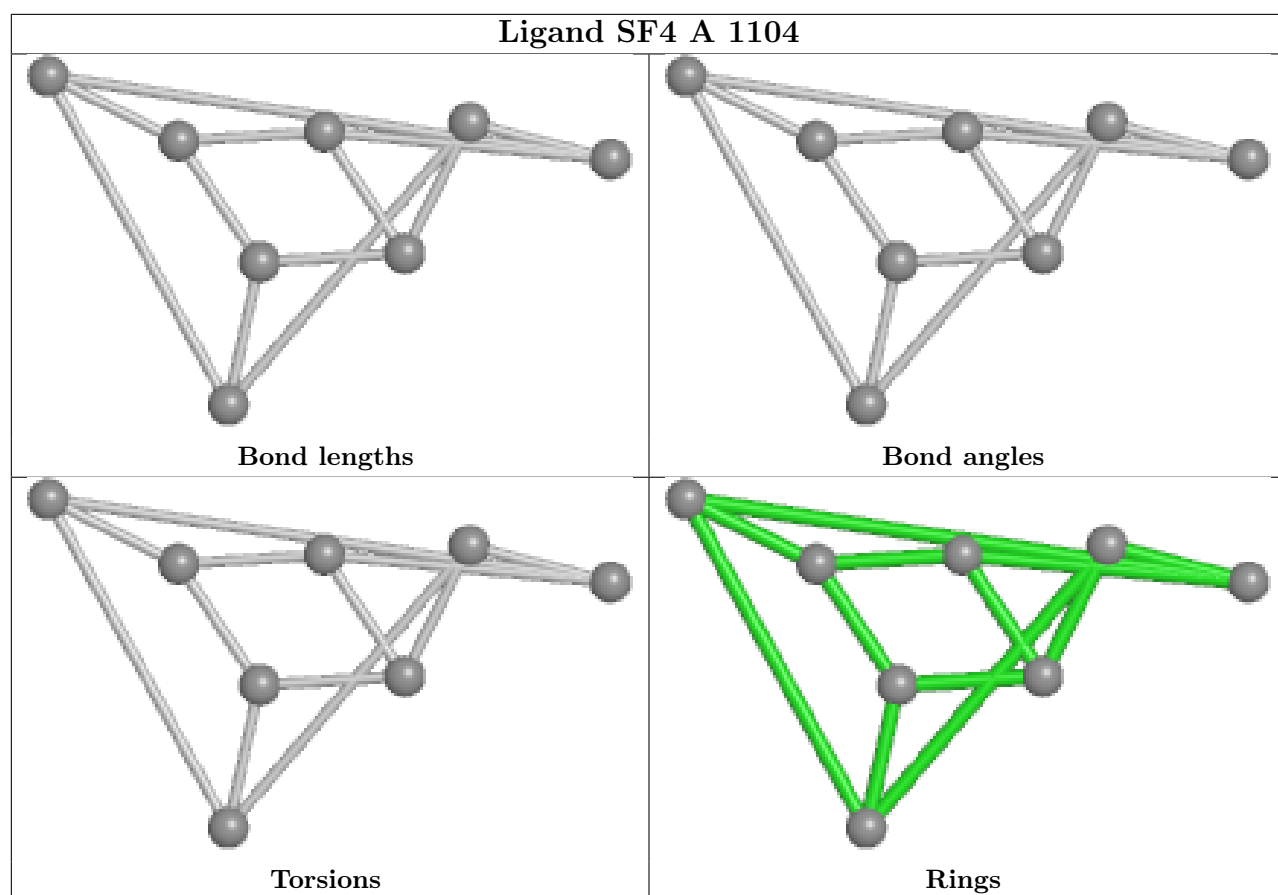
Bond angles

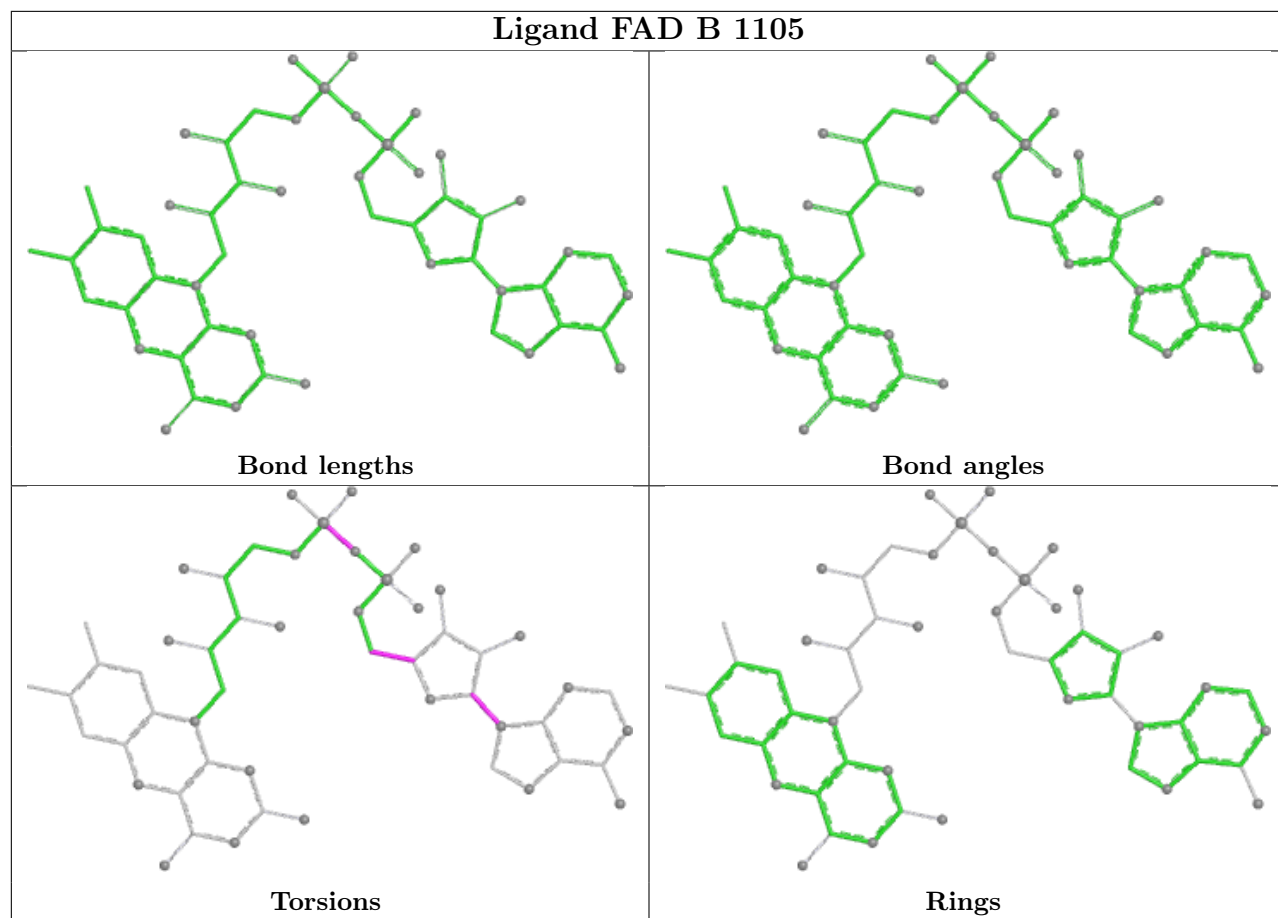


Torsions

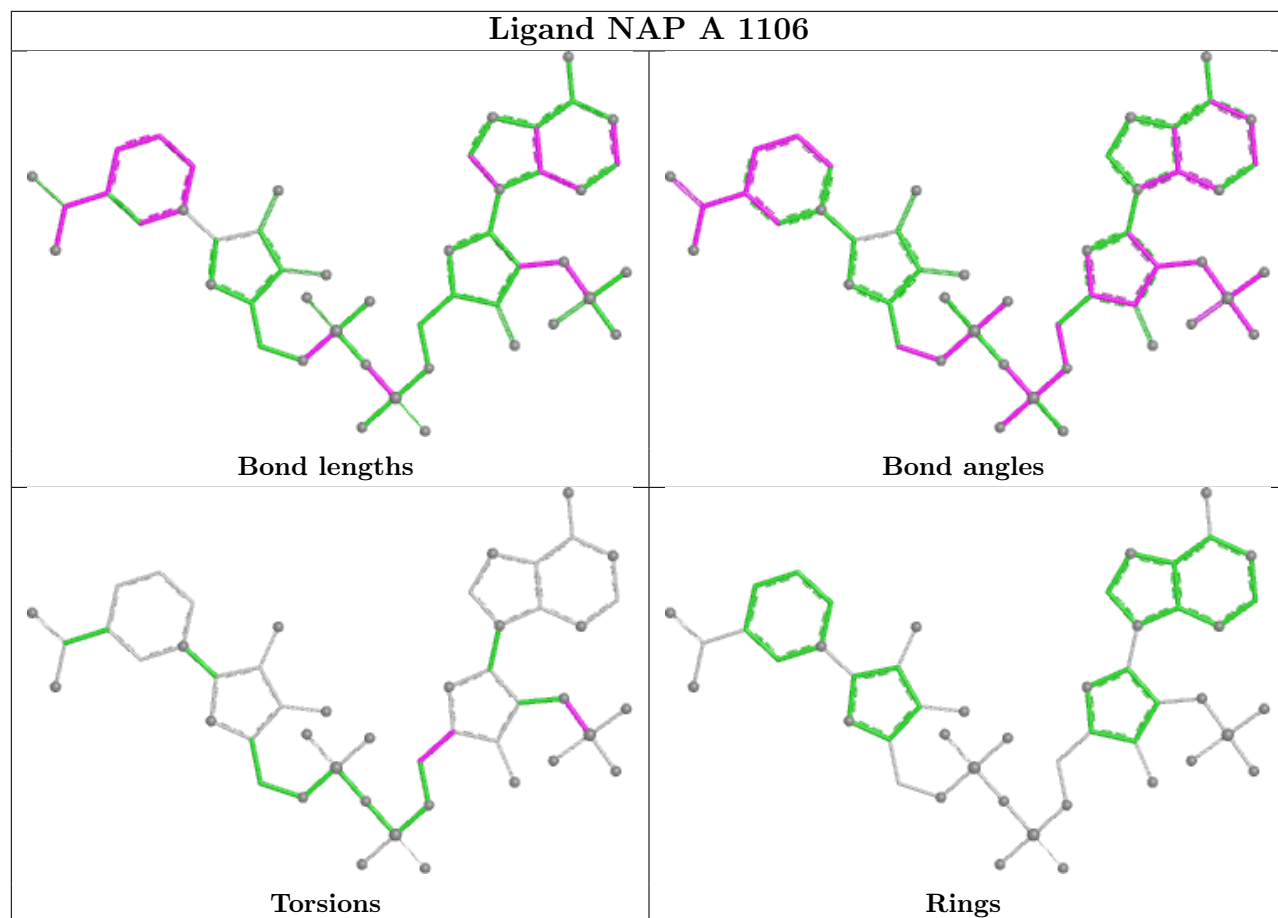


Rings

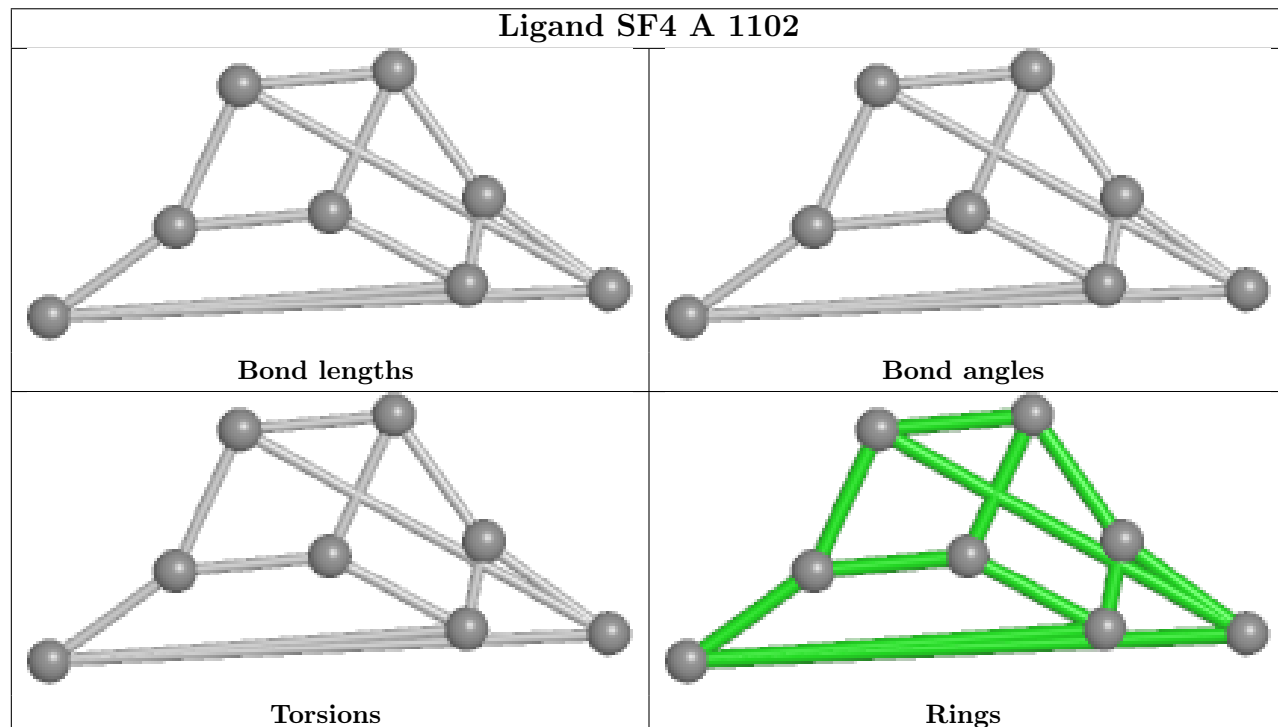




Ligand NAP A 1106



Ligand SF4 A 1102



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1005/1025 (98%)	0.06	36 (3%)	46	50	10, 22, 45, 85	4 (0%)
1	B	1006/1025 (98%)	0.10	44 (4%)	39	42	12, 23, 48, 84	3 (0%)
1	C	1007/1025 (98%)	-0.00	45 (4%)	38	42	9, 21, 45, 73	2 (0%)
1	D	1011/1025 (98%)	0.03	38 (3%)	44	48	12, 21, 46, 81	1 (0%)
All	All	4029/4100 (98%)	0.05	163 (4%)	42	46	9, 22, 47, 85	10 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	902	ALA	5.9
1	A	50	PHE	5.8
1	A	907	LEU	5.4
1	D	902	ALA	4.8
1	C	324	CYS	4.8
1	C	325	HIS	4.5
1	D	907	LEU	4.4
1	B	899	GLU	4.3
1	A	902	ALA	4.2
1	C	904	PHE	4.2
1	B	897	LEU	4.1
1	B	367	PHE	4.0
1	D	52	CYS	3.9
1	C	331	ILE	3.9
1	D	51	HIS	3.9
1	C	1017	LEU	3.9
1	A	52	CYS	3.8
1	C	326	SER	3.8
1	C	901	ASN	3.8
1	D	862	GLY	3.8
1	D	50	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	682	LEU	3.7
1	B	907	LEU	3.7
1	D	367	PHE	3.6
1	C	320	GLY	3.6
1	D	913	ILE	3.6
1	D	459	TRP	3.5
1	A	324	CYS	3.5
1	A	899	GLU	3.5
1	B	51	HIS	3.5
1	B	459	TRP	3.5
1	A	51	HIS	3.5
1	A	367	PHE	3.4
1	C	682	LEU	3.4
1	D	873	GLY	3.4
1	C	902	ALA	3.4
1	A	1017	LEU	3.4
1	A	414	ASP	3.3
1	A	331	ILE	3.3
1	B	50	PHE	3.3
1	D	679	GLY	3.3
1	B	1017	LEU	3.3
1	C	416	THR	3.3
1	B	52	CYS	3.2
1	C	319	ALA	3.2
1	C	903	ALA	3.2
1	B	416	THR	3.2
1	B	871	LEU	3.1
1	C	907	LEU	3.1
1	A	416	THR	3.1
1	D	1019	LEU	3.0
1	C	322	CYS	3.0
1	D	674	GLY	3.0
1	B	36	LEU	3.0
1	D	897	LEU	2.9
1	B	417	GLY	2.9
1	D	167	ASN	2.9
1	D	900	GLN	2.8
1	A	320	GLY	2.8
1	B	673	HIS	2.8
1	A	909	ARG	2.8
1	D	320	GLY	2.8
1	C	52	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	320	GLY	2.8
1	D	1018	PRO	2.7
1	B	680	MET	2.7
1	D	680	MET	2.7
1	A	322	CYS	2.7
1	D	331	ILE	2.7
1	B	870	GLU	2.7
1	C	373	VAL	2.7
1	C	328	LEU	2.7
1	B	672	PRO	2.7
1	B	325	HIS	2.7
1	B	901	ASN	2.6
1	A	681	GLY	2.6
1	D	871	LEU	2.6
1	B	872	MET	2.6
1	D	901	ASN	2.6
1	C	179	GLN	2.6
1	C	897	LEU	2.6
1	D	293	ILE	2.6
1	B	867	ARG	2.6
1	B	414	ASP	2.5
1	D	22	THR	2.5
1	C	50	PHE	2.5
1	B	324	CYS	2.5
1	C	402	ARG	2.5
1	C	415	GLU	2.5
1	B	682	LEU	2.5
1	C	36	LEU	2.5
1	B	323	ALA	2.5
1	C	673	HIS	2.5
1	B	869	ALA	2.5
1	D	426	ILE	2.5
1	A	870	GLU	2.5
1	B	856	THR	2.5
1	A	893	GLU	2.4
1	A	36	LEU	2.4
1	A	1016	GLY	2.4
1	B	681	GLY	2.4
1	B	873	GLY	2.4
1	D	908	GLU	2.4
1	B	900	GLN	2.4
1	B	1018	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	906	PRO	2.4
1	C	367	PHE	2.4
1	A	415	GLU	2.4
1	A	901	ASN	2.3
1	A	49	CYS	2.3
1	C	696	ARG	2.3
1	C	51	HIS	2.3
1	D	868	ILE	2.3
1	A	179	GLN	2.3
1	D	414	ASP	2.3
1	B	418	LYS	2.3
1	C	683	ALA	2.3
1	B	25	HIS	2.3
1	C	22	THR	2.3
1	C	323	ALA	2.3
1	B	53	GLU	2.3
1	C	900	GLN	2.2
1	D	869	ALA	2.2
1	C	332	ARG	2.2
1	D	330	SER	2.2
1	A	872	MET	2.2
1	D	675	MET	2.2
1	B	368	VAL	2.2
1	B	485	MET	2.2
1	B	800	GLU	2.2
1	D	909	ARG	2.2
1	C	872	MET	2.2
1	C	49	CYS	2.2
1	A	871	LEU	2.2
1	C	417	GLY	2.2
1	B	342	ASP	2.1
1	D	415	GLU	2.1
1	B	371	ARG	2.1
1	D	49	CYS	2.1
1	B	862	GLY	2.1
1	B	11[A]	ASP	2.1
1	C	27	ALA	2.1
1	A	900	GLN	2.1
1	C	424	ASP	2.1
1	C	899	GLU	2.1
1	D	179	GLN	2.1
1	A	896	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	867	ARG	2.1
1	A	293	ILE	2.1
1	B	868	ILE	2.1
1	C	582	ILE	2.1
1	A	325	HIS	2.1
1	A	869	ALA	2.1
1	A	867	ARG	2.1
1	D	678	ARG	2.1
1	A	53	GLU	2.0
1	C	869	ALA	2.0
1	D	424	ASP	2.0
1	A	910	LYS	2.0
1	C	672	PRO	2.0
1	C	870	GLU	2.0
1	A	674	GLY	2.0
1	C	264	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
7	PRO	C	1101	7/8	0.75	0.17	53,55,57,59	0
4	NAP	B	1106	48/48	0.94	0.11	19,27,42,47	0
4	NAP	C	1107	48/48	0.96	0.09	17,26,36,38	0
4	NAP	D	1106	40/48	0.96	0.09	19,25,48,66	0
6	TDR	C	1108	9/9	0.96	0.05	15,16,17,18	0
6	TDR	D	1107	9/9	0.96	0.06	14,15,17,20	0
4	NAP	A	1106	48/48	0.96	0.09	18,26,38,41	0

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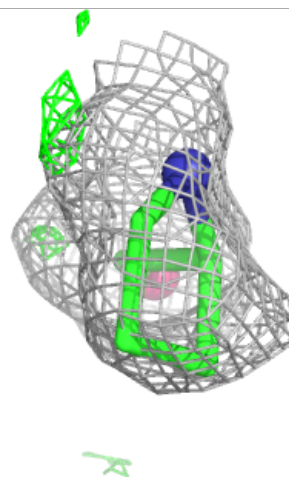
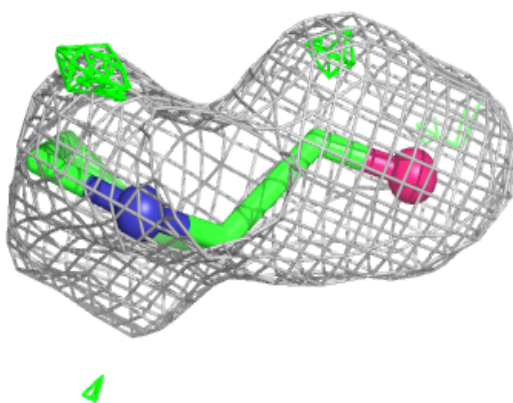
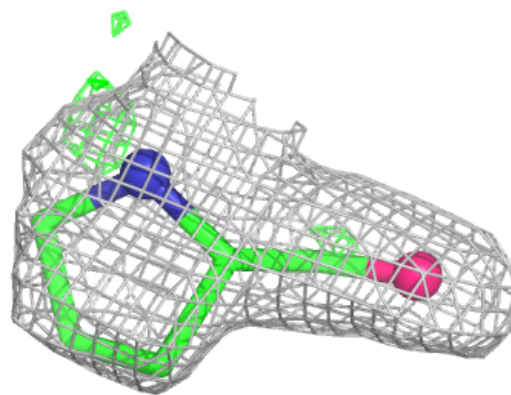
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	D	1105	53/53	0.97	0.05	14,18,21,24	0
5	FMN	A	1107	31/31	0.97	0.06	14,18,23,28	0
5	FMN	B	1108	31/31	0.97	0.06	14,19,22,30	0
5	FMN	C	1109	31/31	0.97	0.06	12,16,18,20	0
5	FMN	D	1108	31/31	0.97	0.06	13,16,20,27	0
6	TDR	A	1108	9/9	0.97	0.05	16,18,20,22	0
3	FAD	A	1105	53/53	0.97	0.06	15,19,23,27	0
3	FAD	B	1105	53/53	0.97	0.06	16,20,26,28	0
3	FAD	C	1106	53/53	0.97	0.06	16,20,25,29	0
6	TDR	B	1107	9/9	0.98	0.04	17,19,20,20	0
2	SF4	D	1104	8/8	0.99	0.02	16,16,17,17	0
2	SF4	A	1102	8/8	0.99	0.02	16,16,17,17	0
2	SF4	B	1103	8/8	0.99	0.02	18,18,19,19	0
2	SF4	B	1104	8/8	1.00	0.02	17,17,18,18	0
2	SF4	C	1102	8/8	1.00	0.02	15,16,16,16	0
2	SF4	C	1103	8/8	1.00	0.02	15,16,16,16	0
2	SF4	C	1104	8/8	1.00	0.02	14,15,15,16	0
2	SF4	C	1105	8/8	1.00	0.03	17,18,18,18	0
2	SF4	D	1101	8/8	1.00	0.02	16,16,17,17	0
2	SF4	D	1102	8/8	1.00	0.01	16,16,17,17	0
2	SF4	D	1103	8/8	1.00	0.02	15,15,15,15	0
2	SF4	A	1103	8/8	1.00	0.02	17,18,18,19	0
2	SF4	A	1104	8/8	1.00	0.02	17,18,18,19	0
2	SF4	B	1101	8/8	1.00	0.02	16,16,17,17	0
2	SF4	B	1102	8/8	1.00	0.02	17,18,18,18	0
2	SF4	A	1101	8/8	1.00	0.02	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.

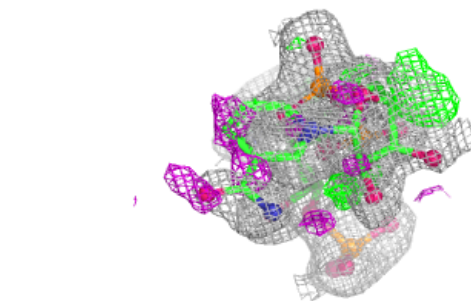
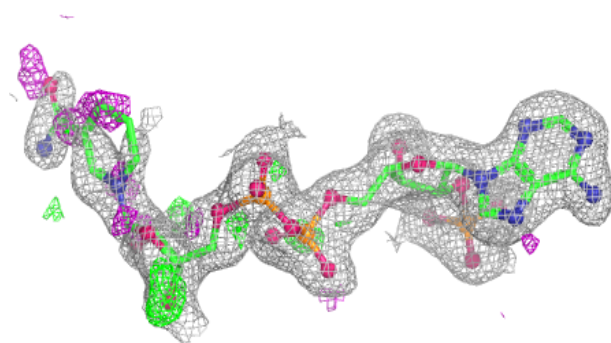
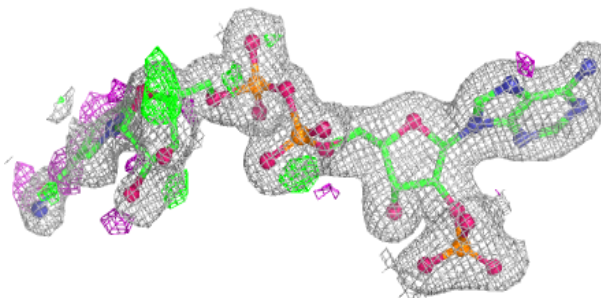
Electron density around PRO C 1101:

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

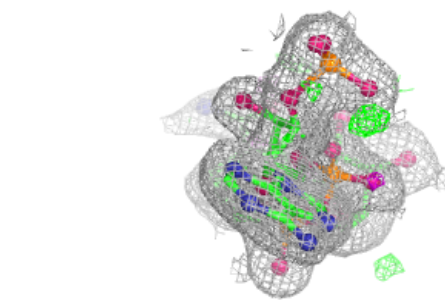
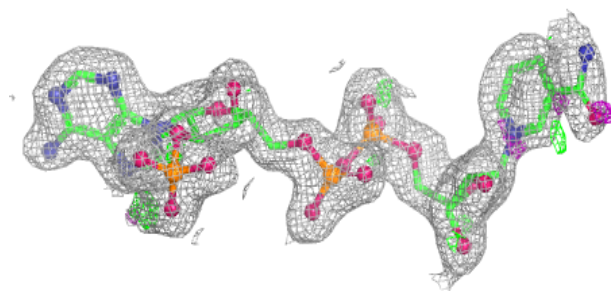
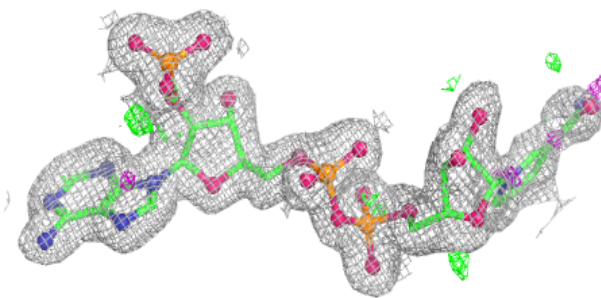


Electron density around NAP B 1106:

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

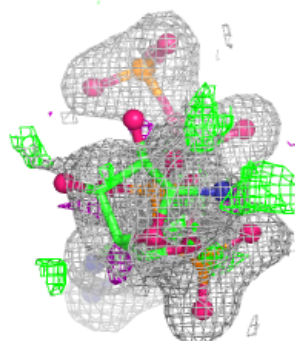
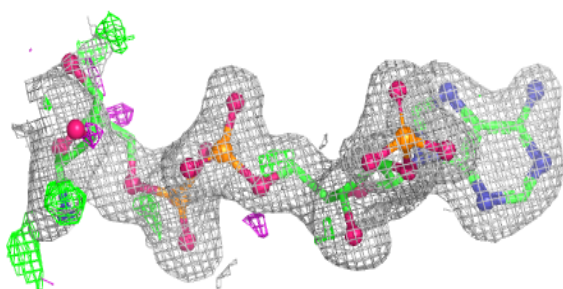
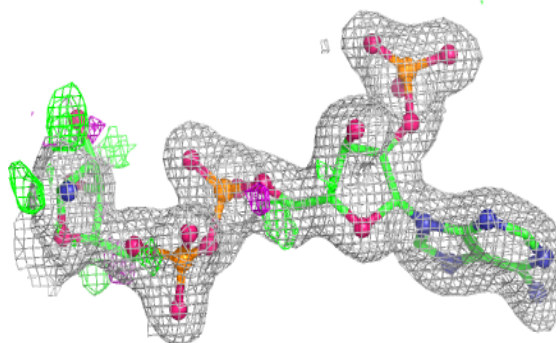
**Electron density around NAP C 1107:**

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

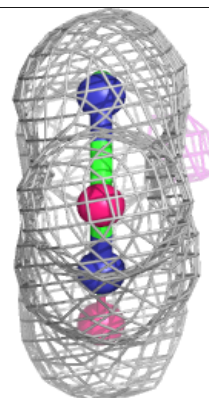
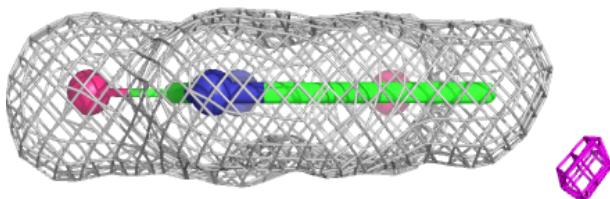
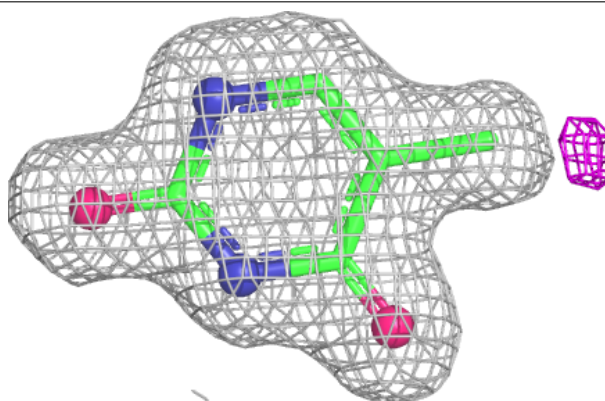


Electron density around NAP D 1106:

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

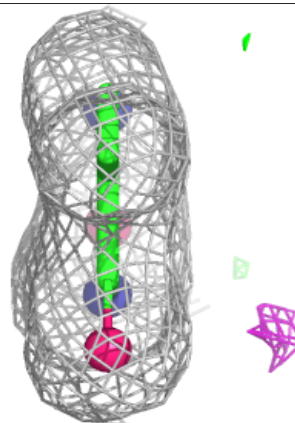
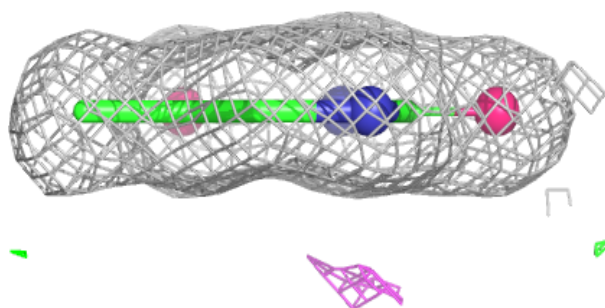
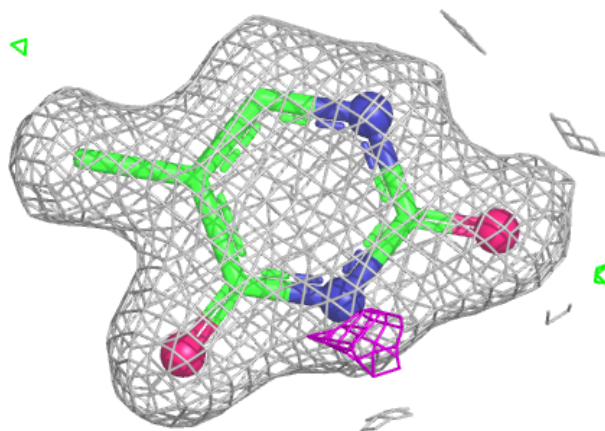
**Electron density around TDR C 1108:**

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

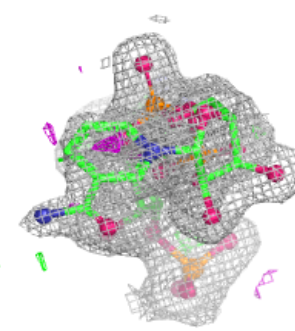
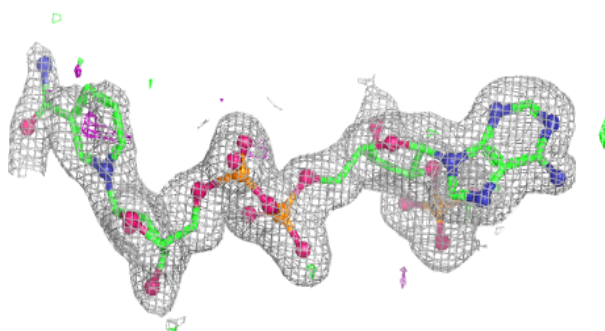
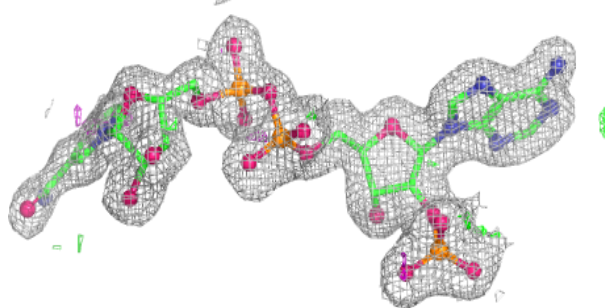


Electron density around TDR D 1107:

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

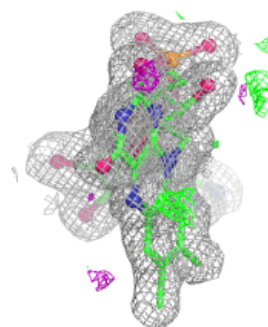
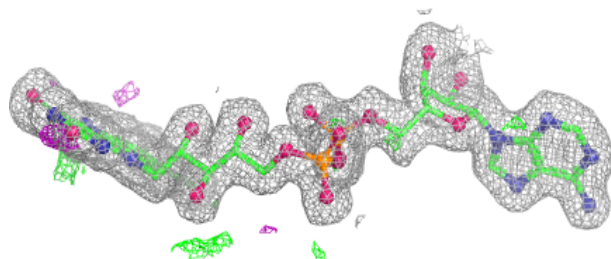
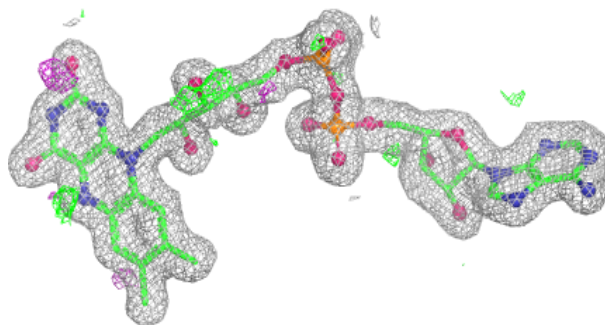
**Electron density around NAP A 1106:**

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



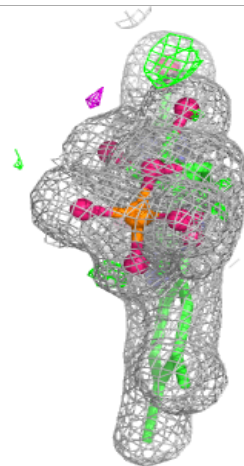
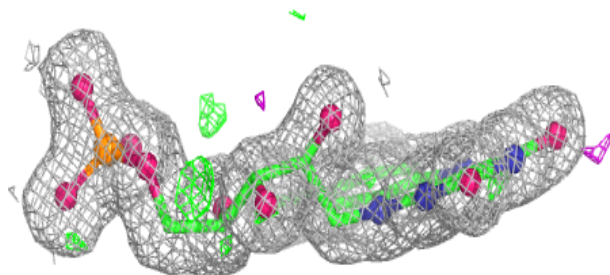
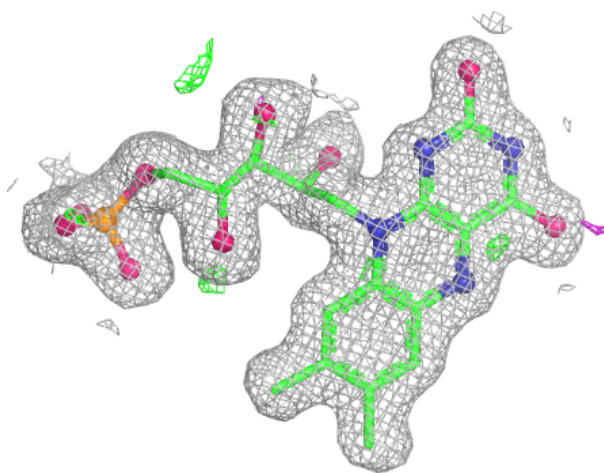
Electron density around FAD D 1105:

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



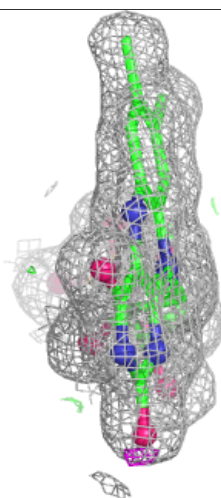
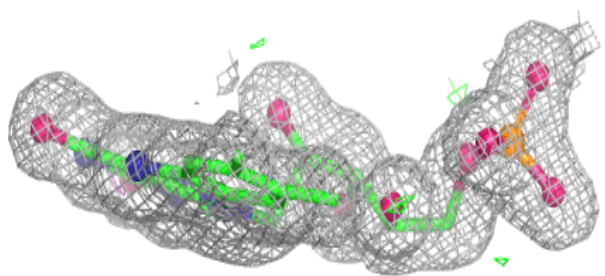
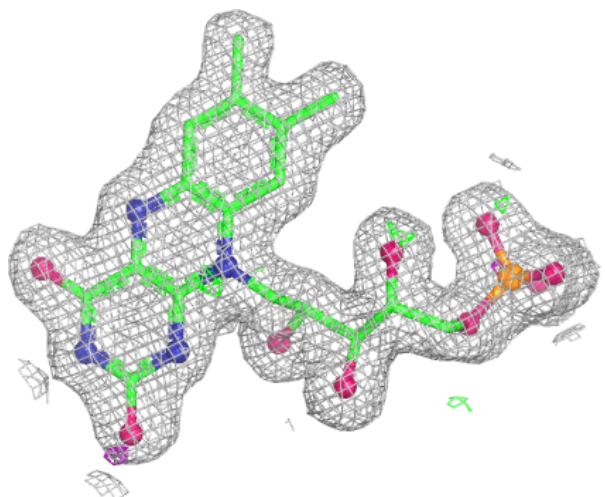
Electron density around FMN A 1107:

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



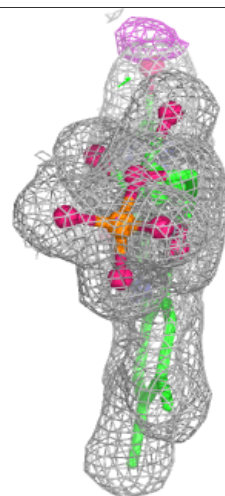
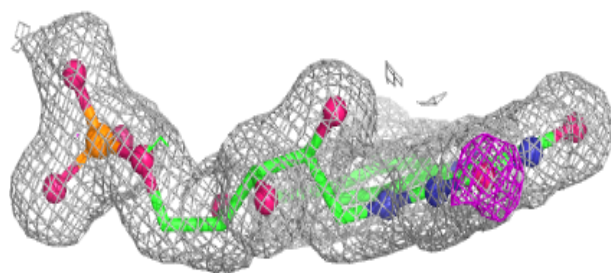
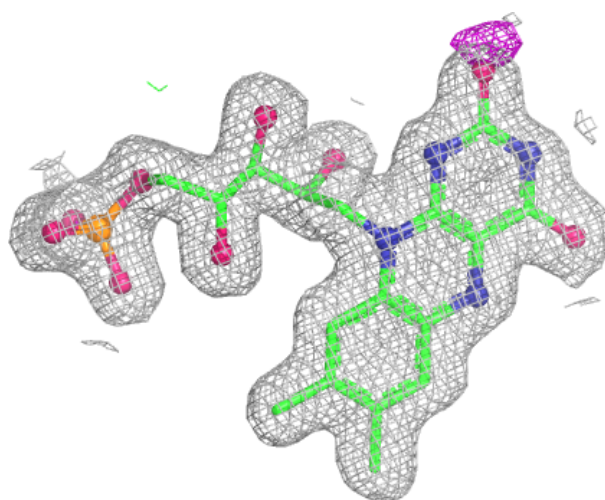
Electron density around FMN B 1108:

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



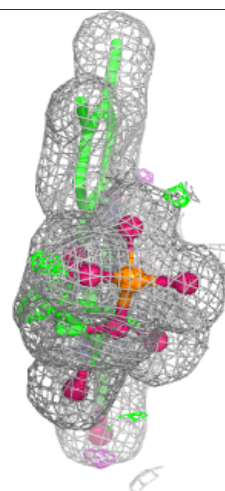
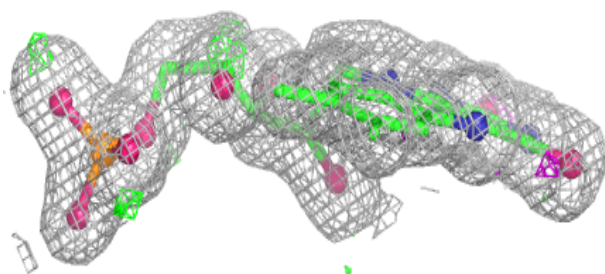
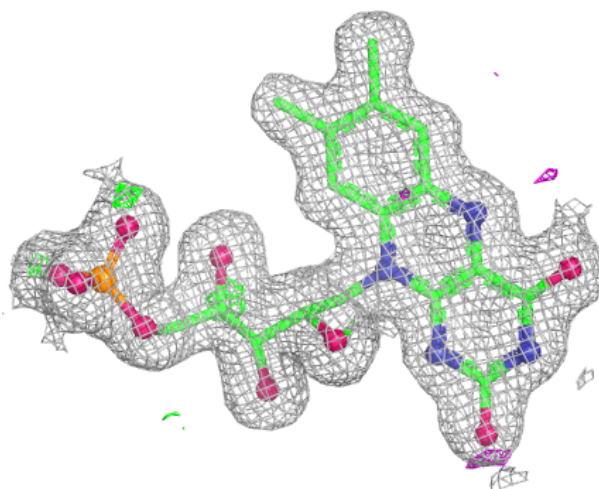
Electron density around FMN C 1109:

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



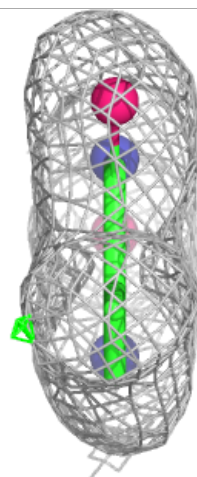
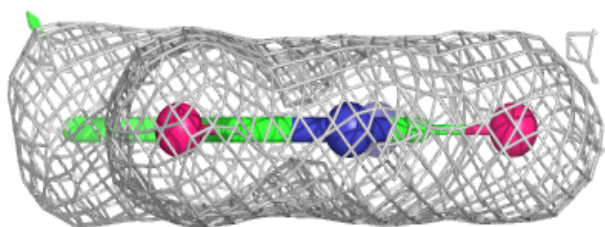
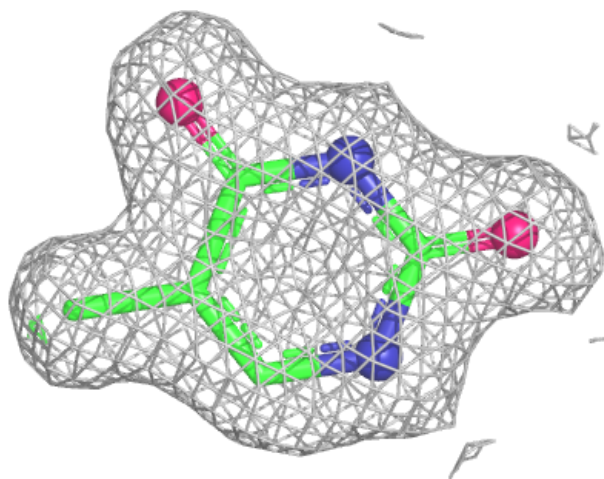
Electron density around FMN D 1108:

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



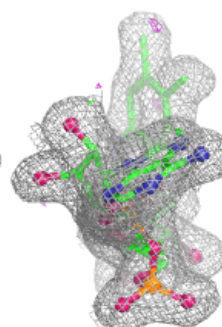
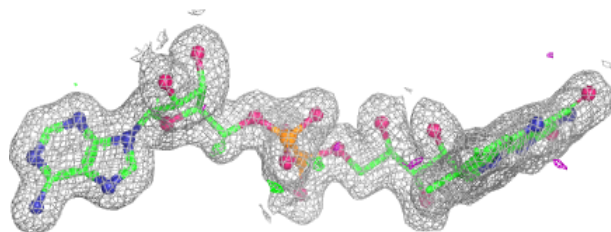
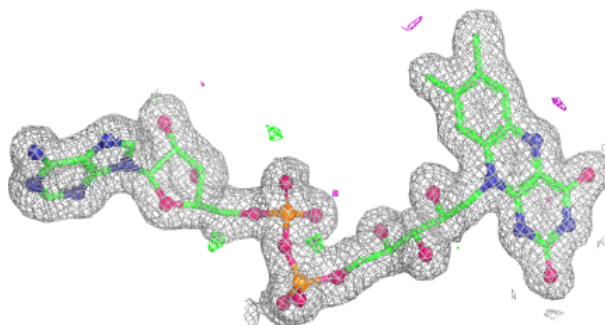
Electron density around TDR A 1108:

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

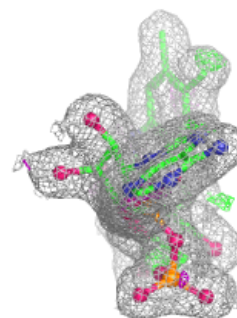
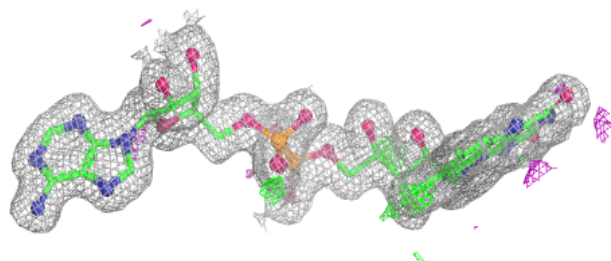
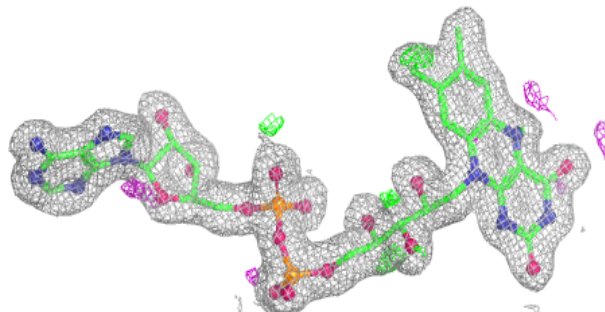


Electron density around FAD A 1105:

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

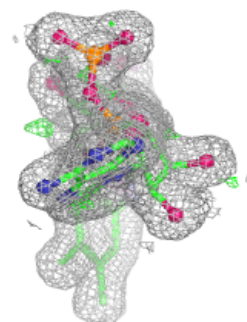
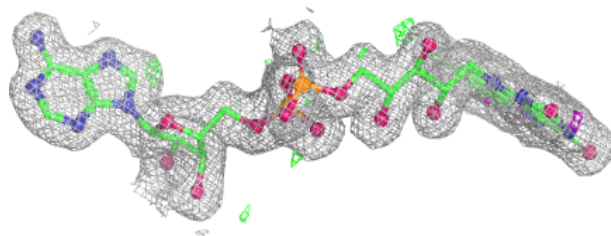
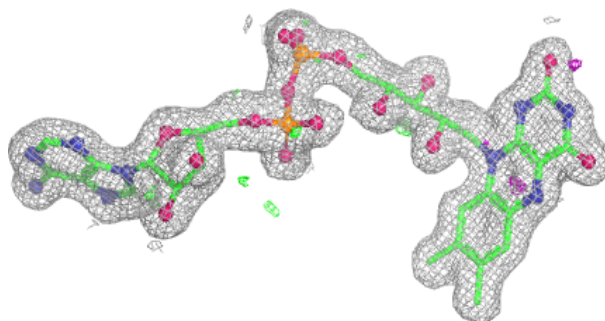
**Electron density around FAD B 1105:**

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



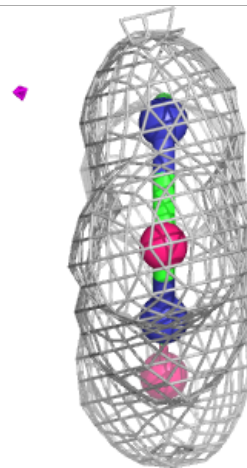
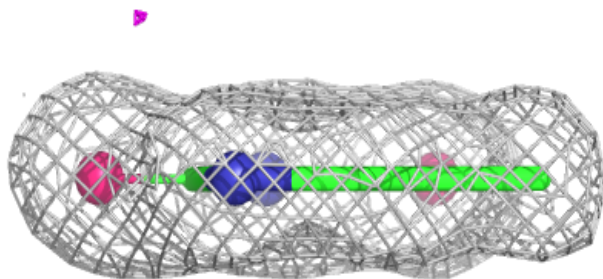
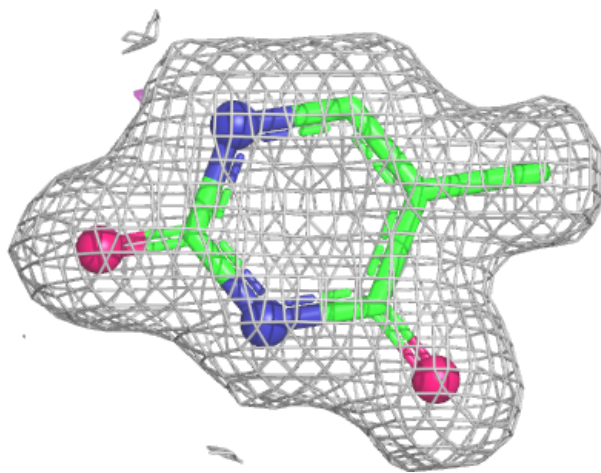
Electron density around FAD C 1106:

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



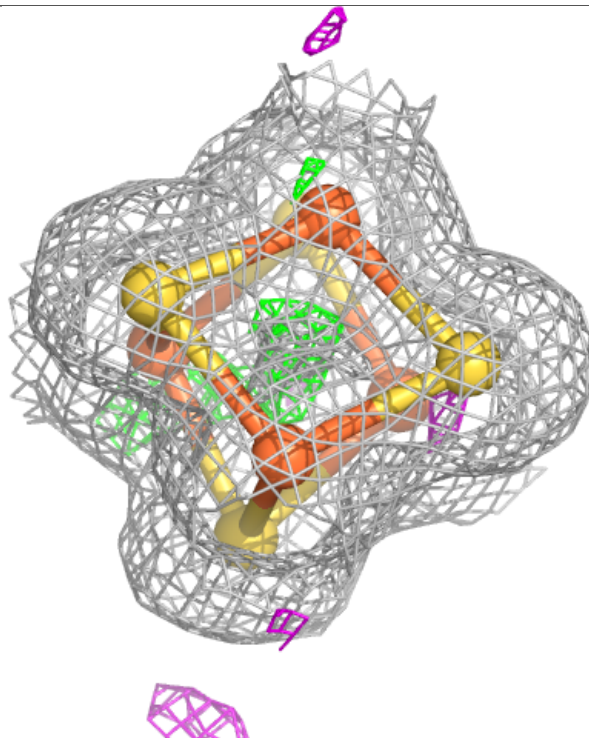
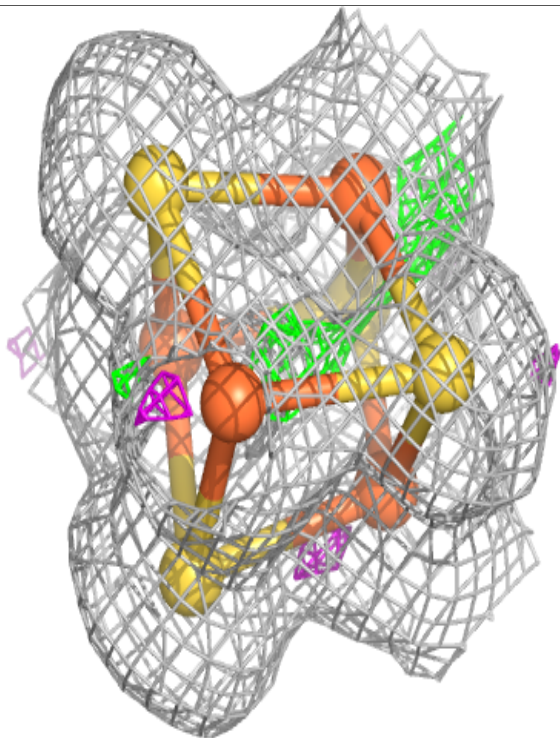
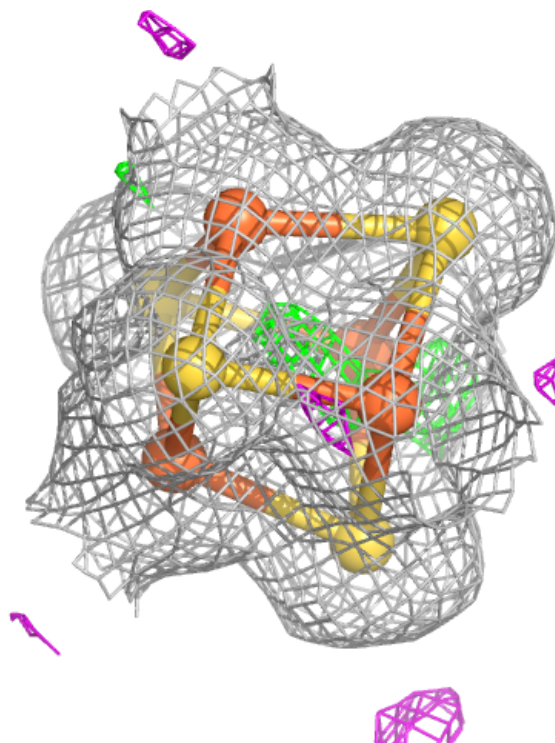
Electron density around TDR B 1107:

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



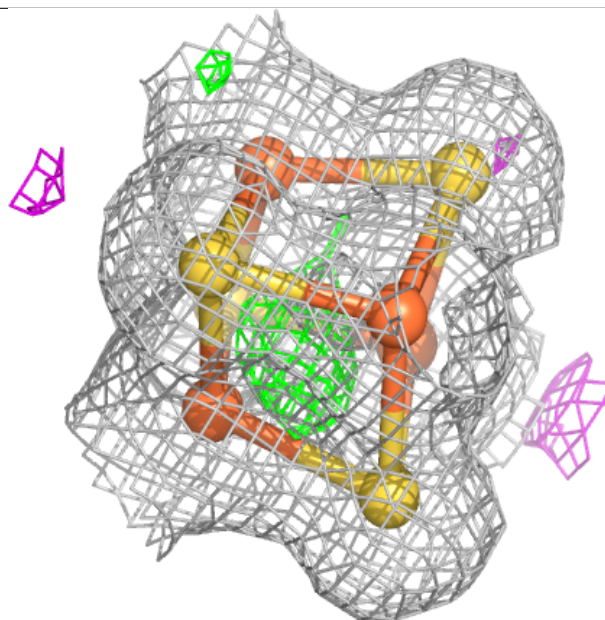
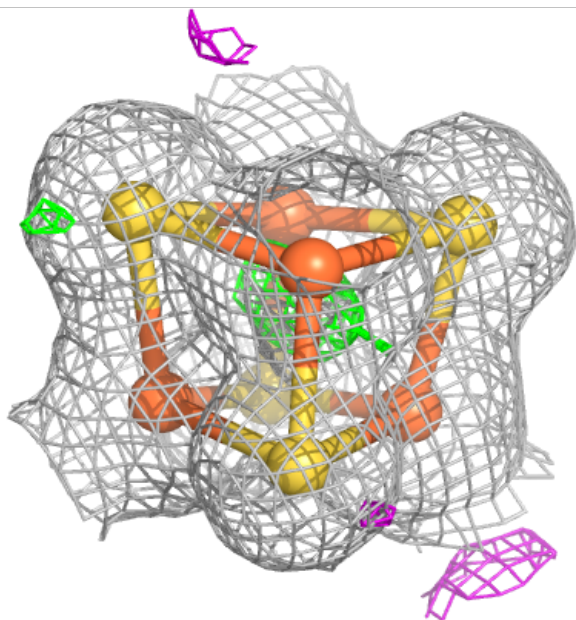
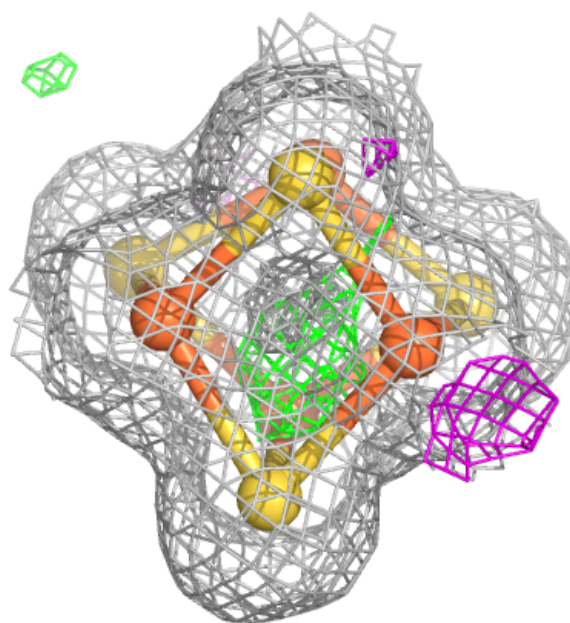
Electron density around SF4 D 1104:

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



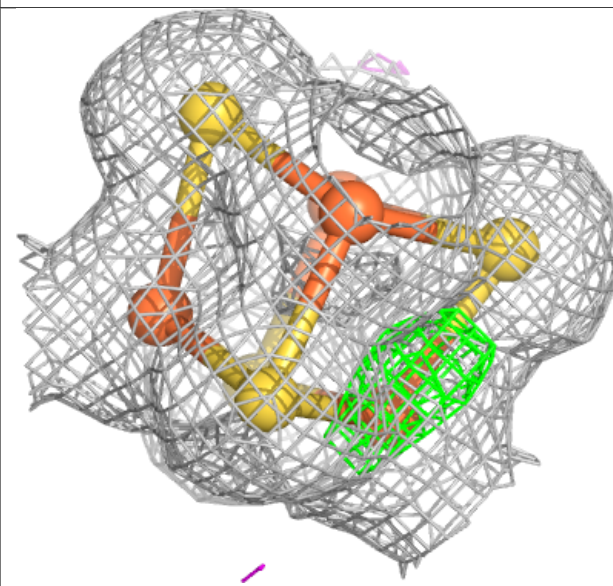
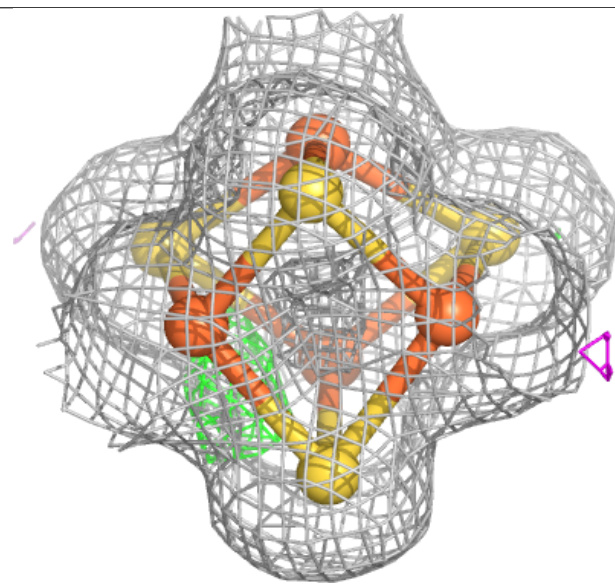
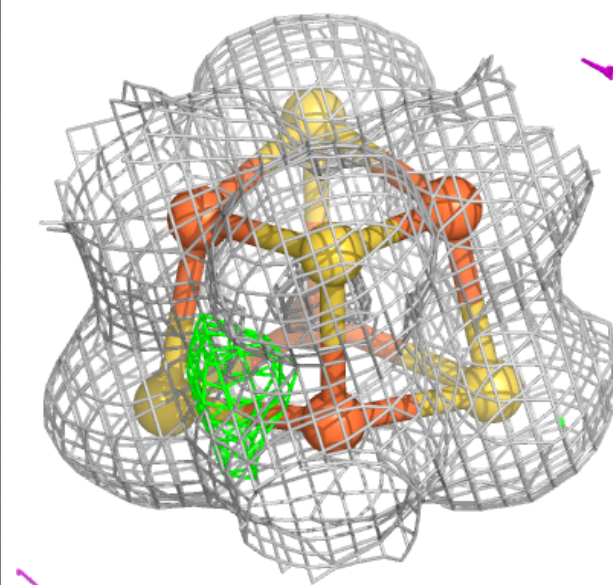
Electron density around SF4 A 1102:

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



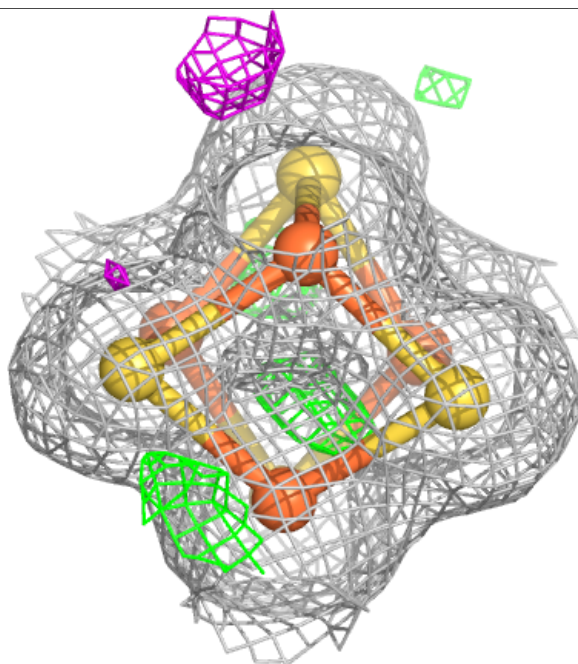
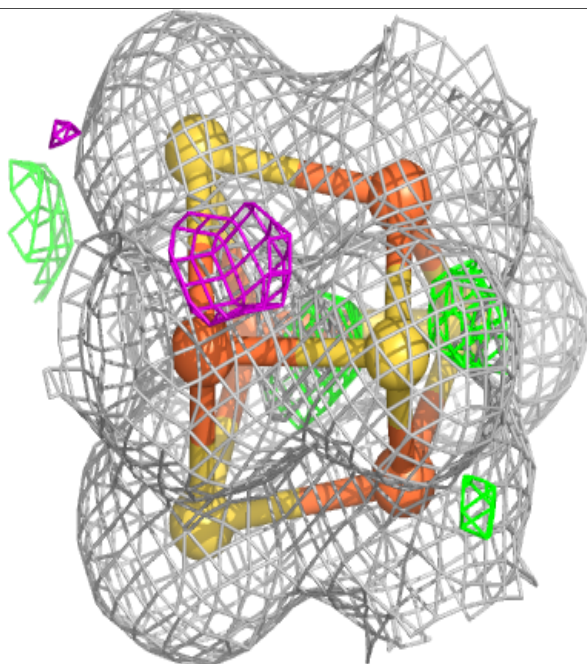
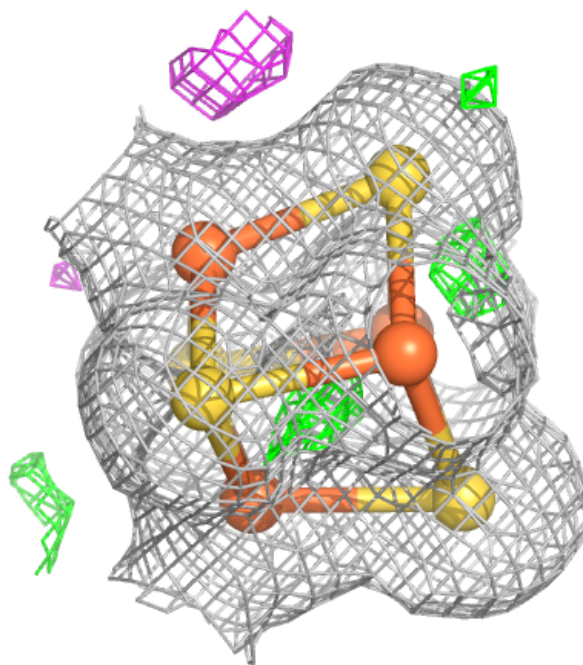
Electron density around SF4 B 1103:

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



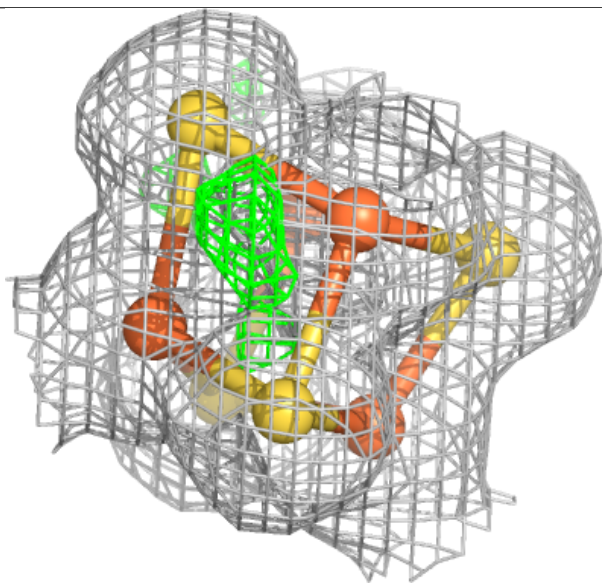
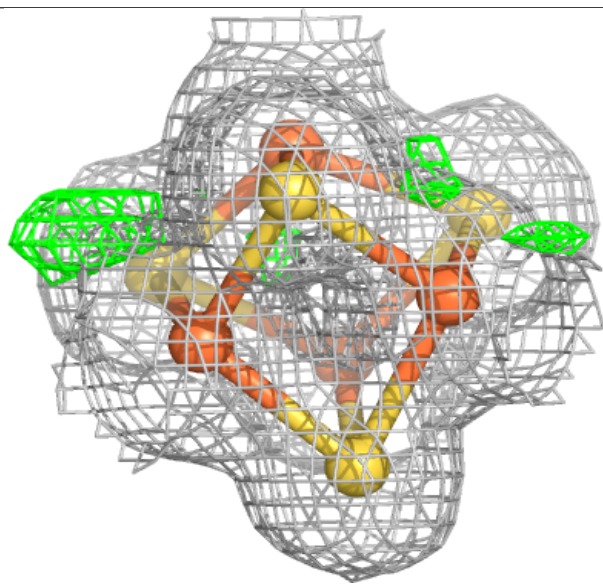
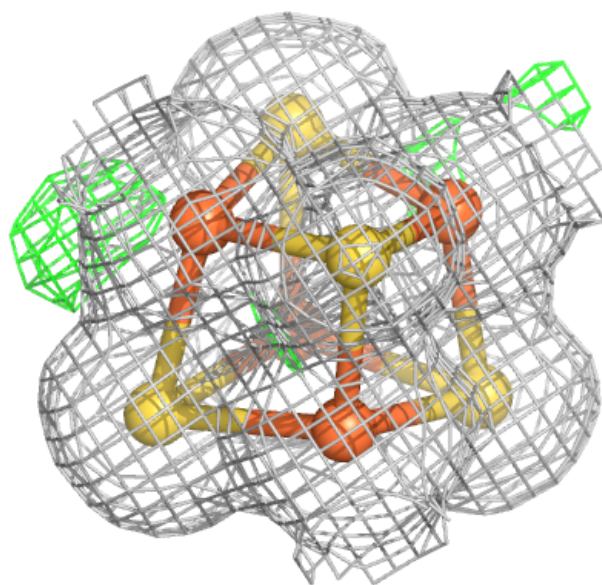
Electron density around SF4 B 1104:

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



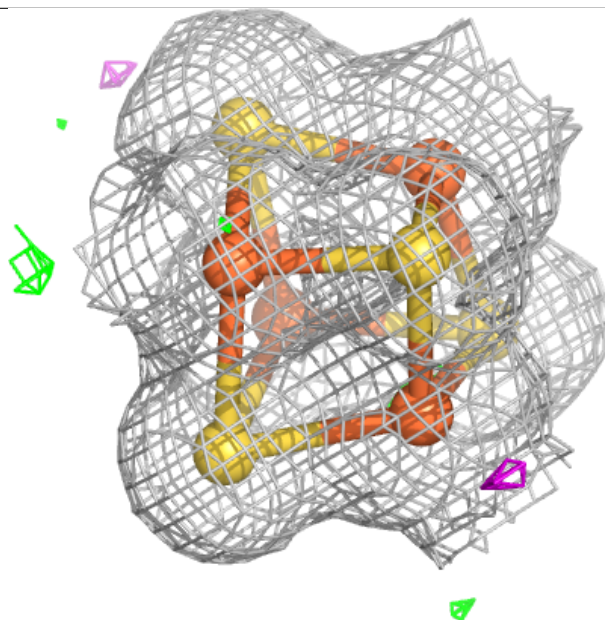
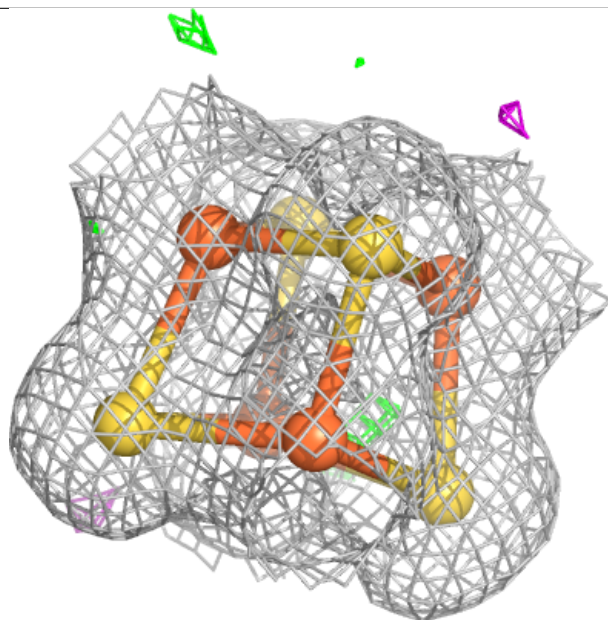
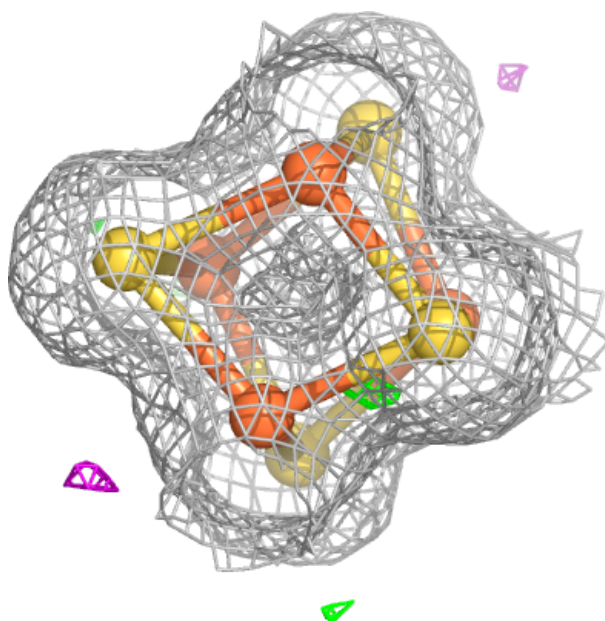
Electron density around SF4 C 1102:

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



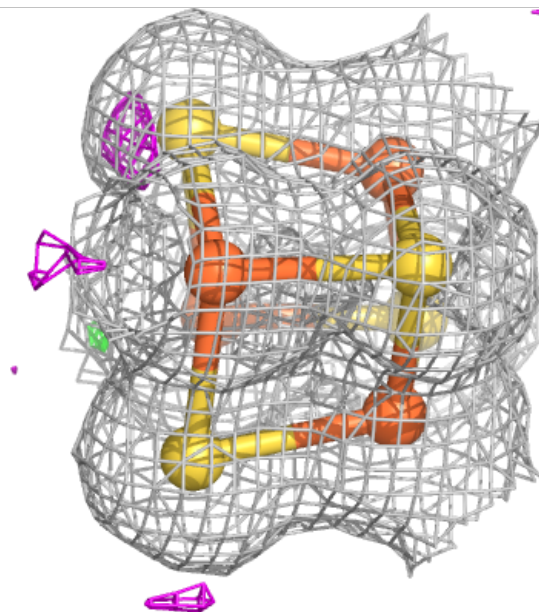
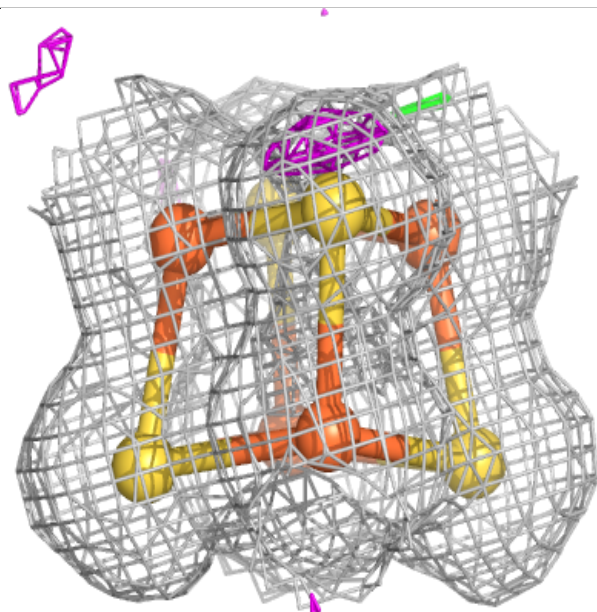
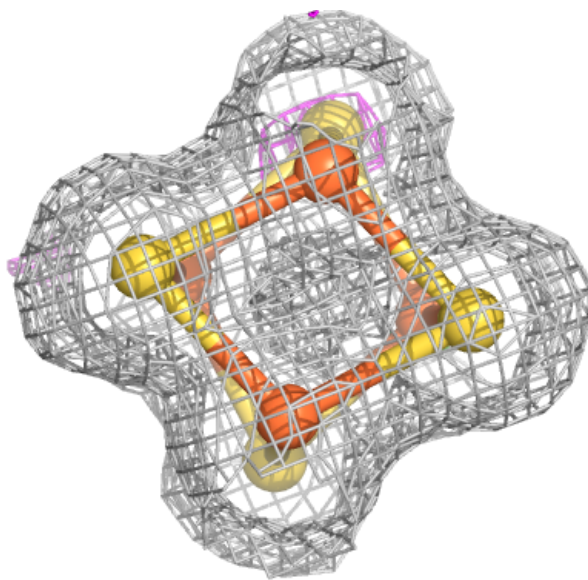
Electron density around SF4 C 1103:

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



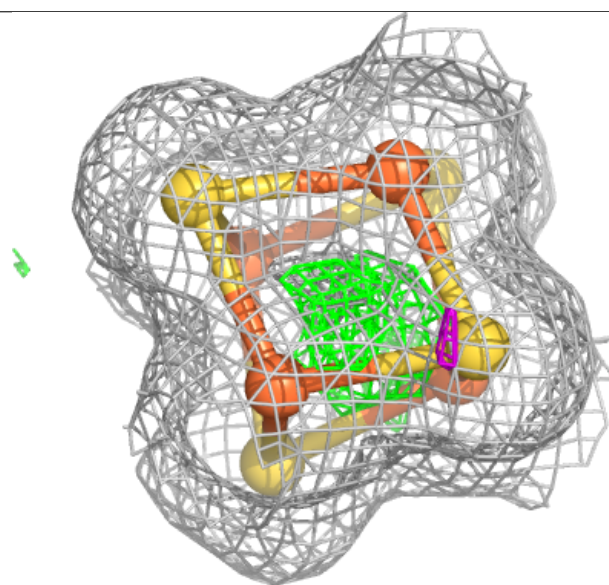
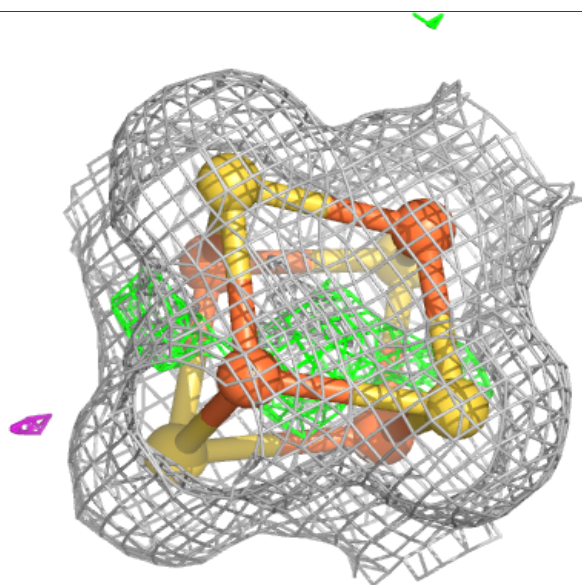
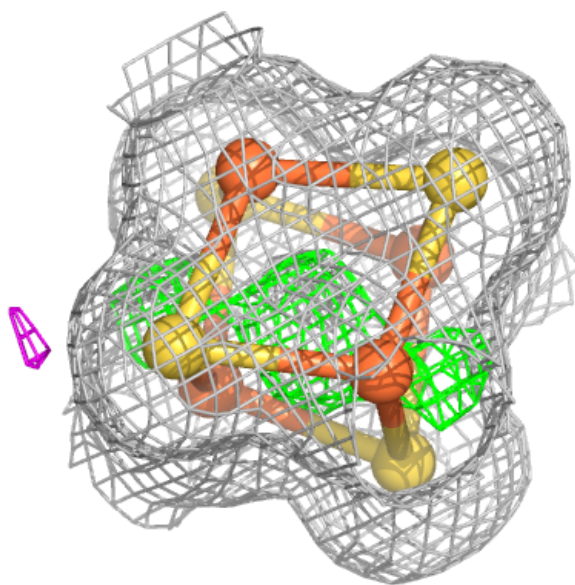
Electron density around SF4 C 1104:

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



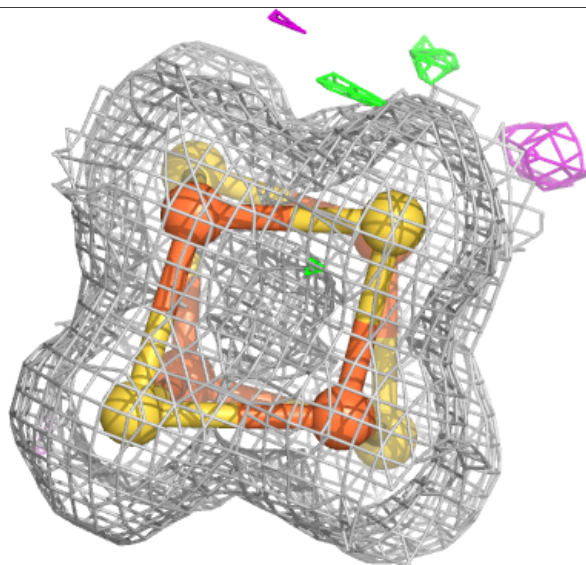
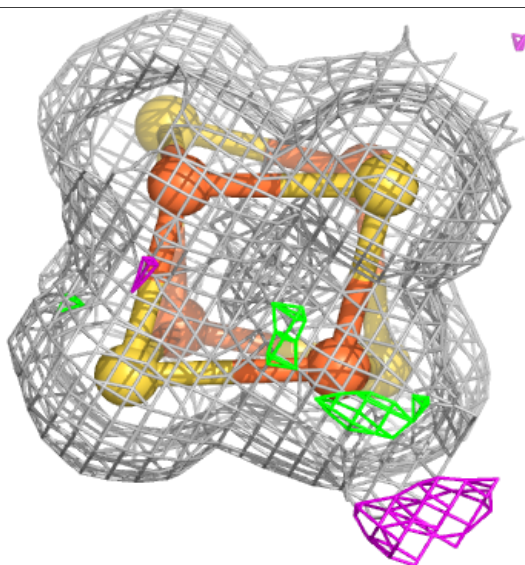
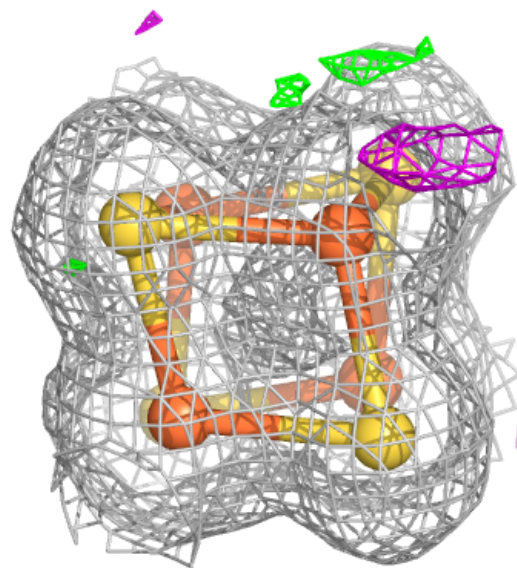
Electron density around SF4 C 1105:

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



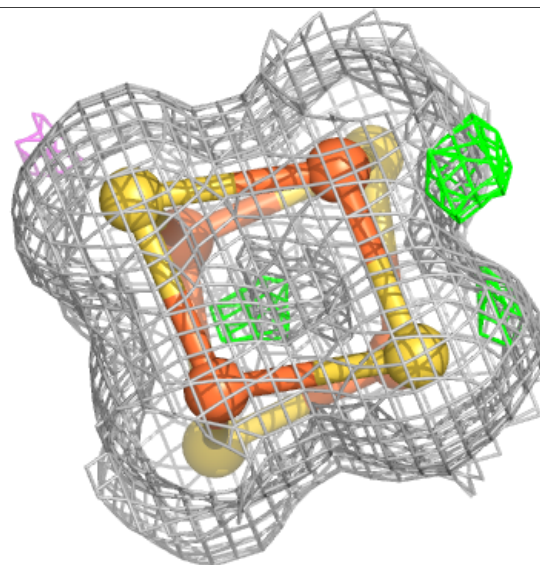
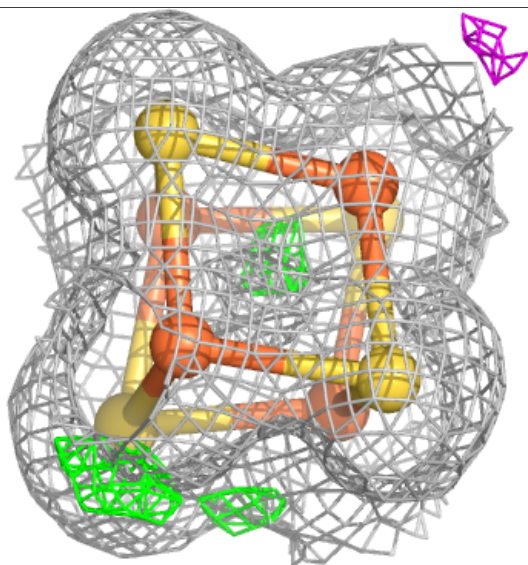
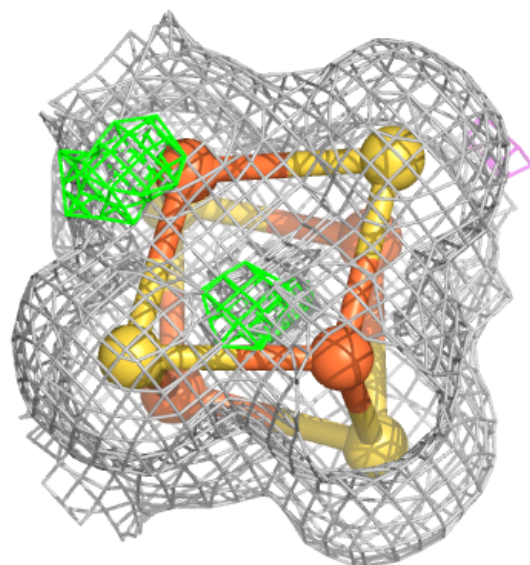
Electron density around SF4 D 1101:

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



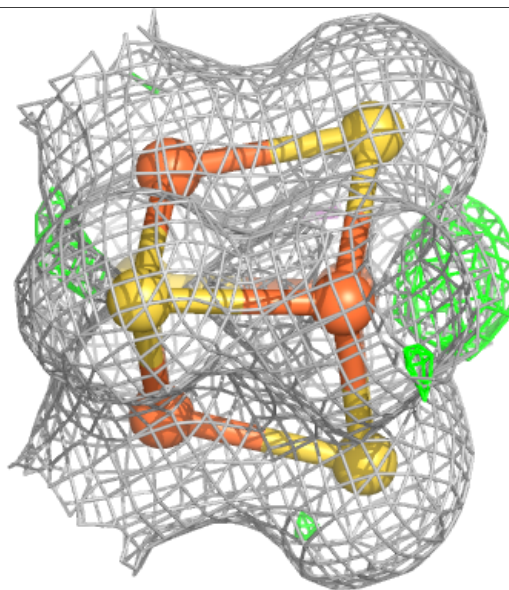
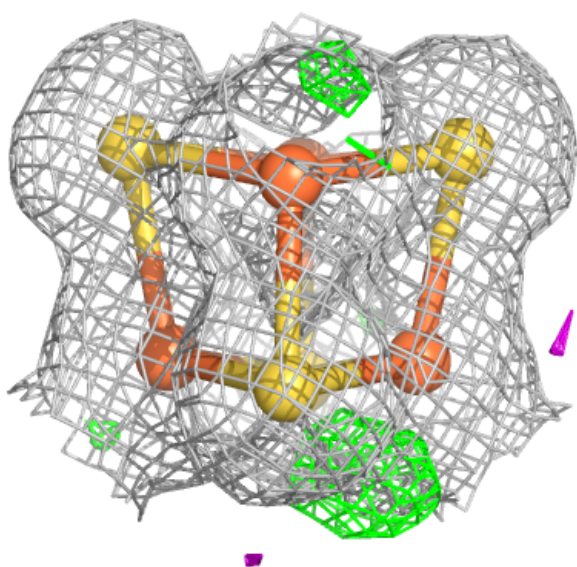
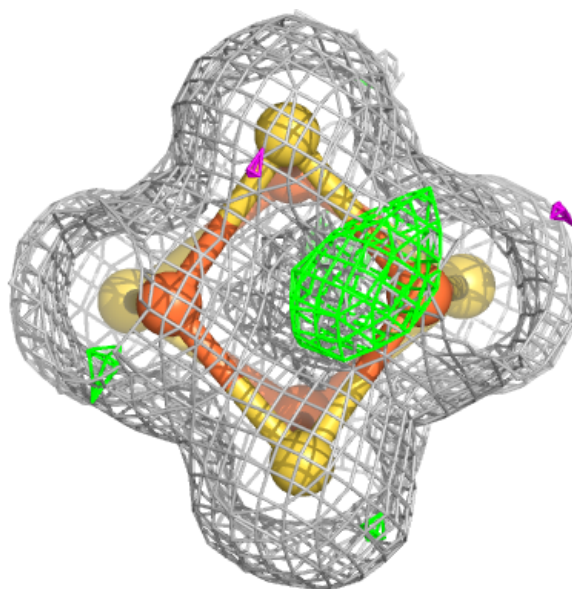
Electron density around SF4 D 1102:

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



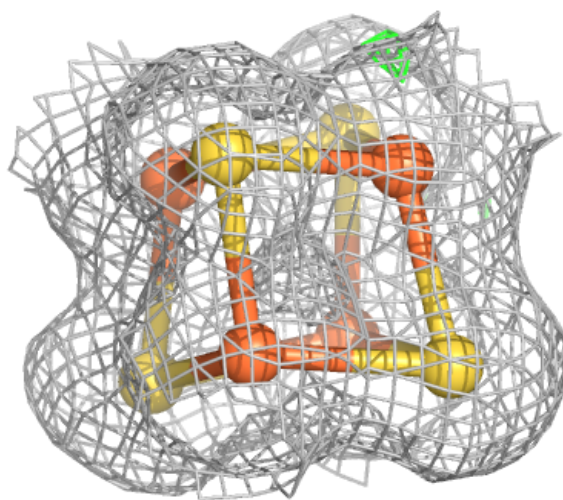
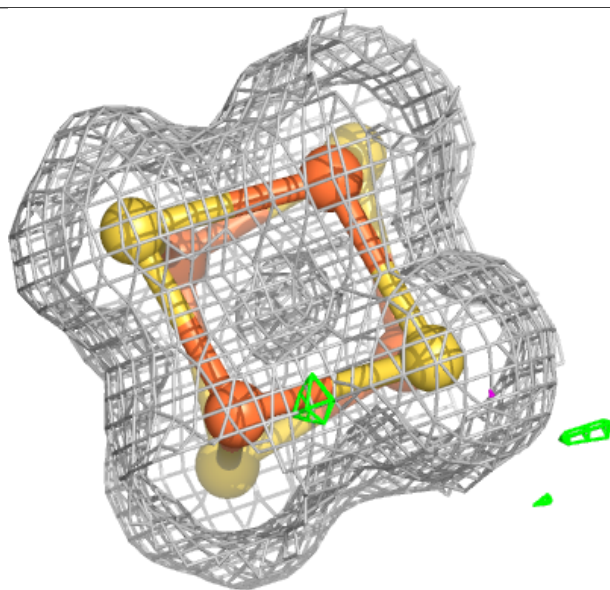
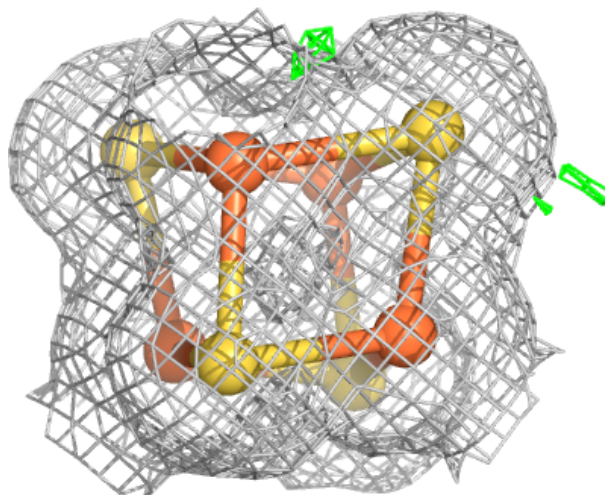
Electron density around SF4 D 1103:

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



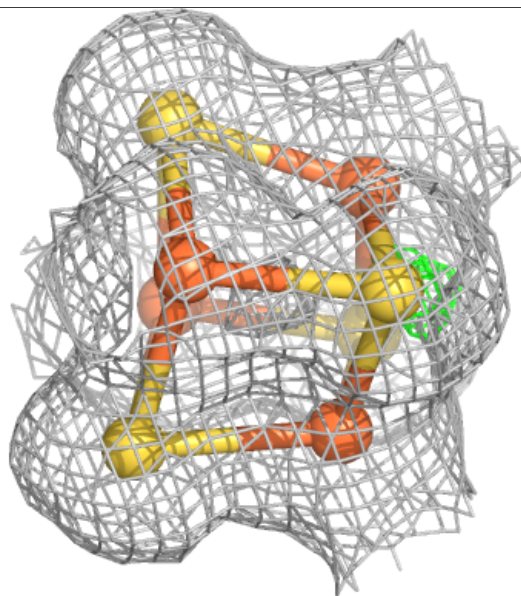
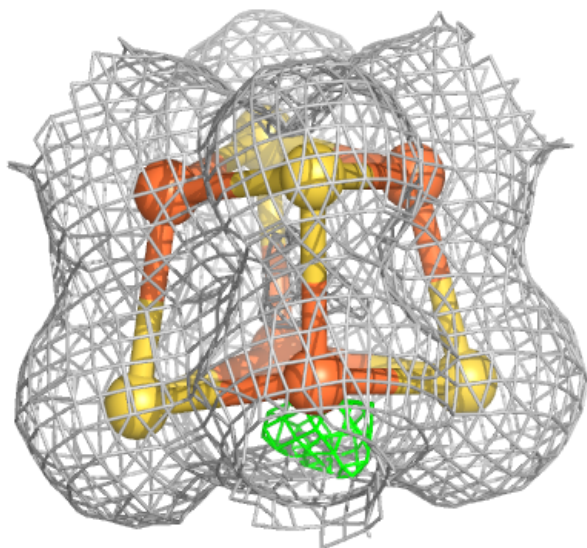
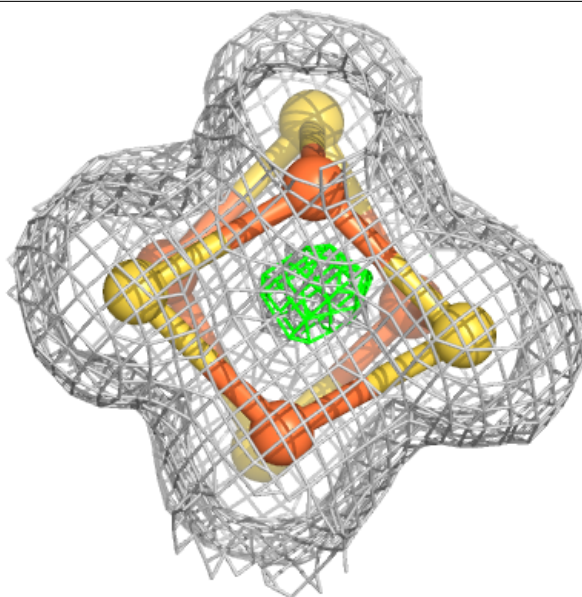
Electron density around SF4 A 1103:

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



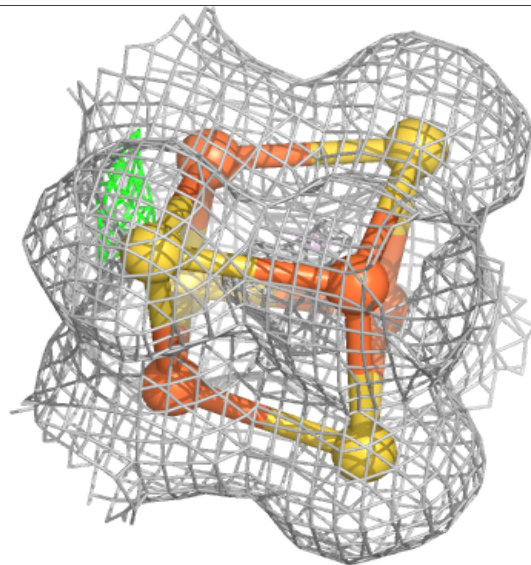
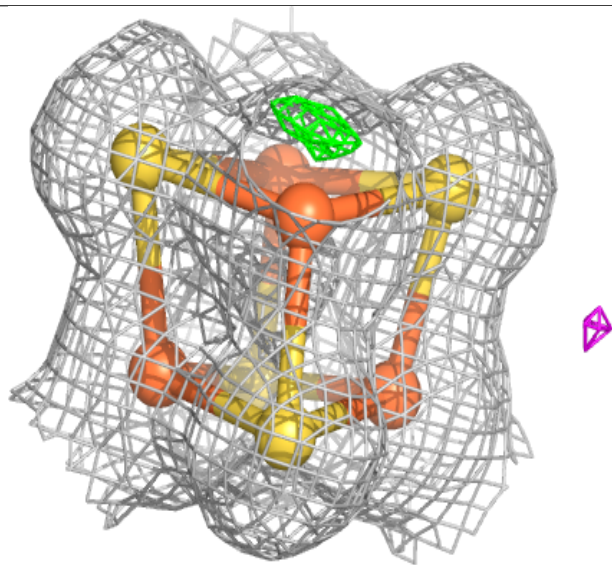
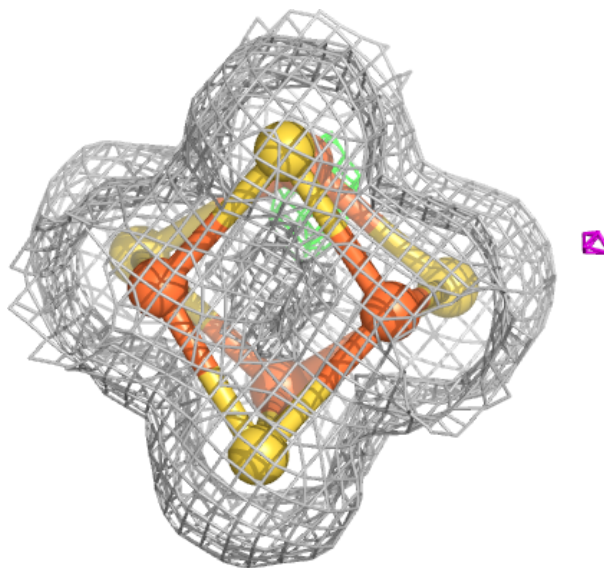
Electron density around SF4 A 1104:

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



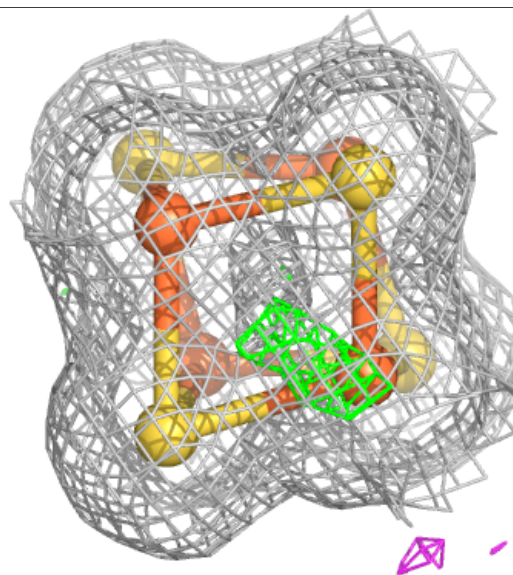
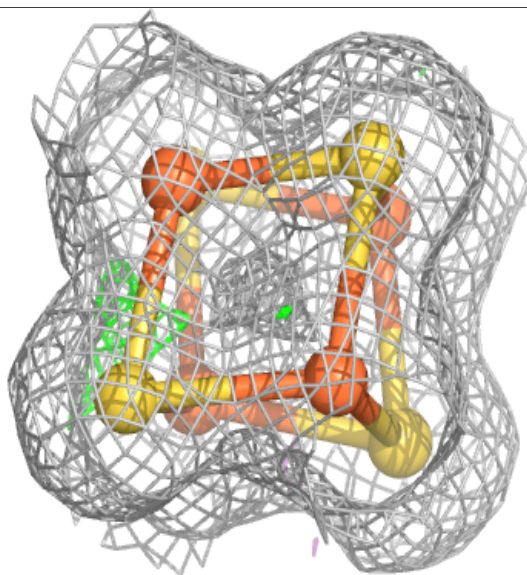
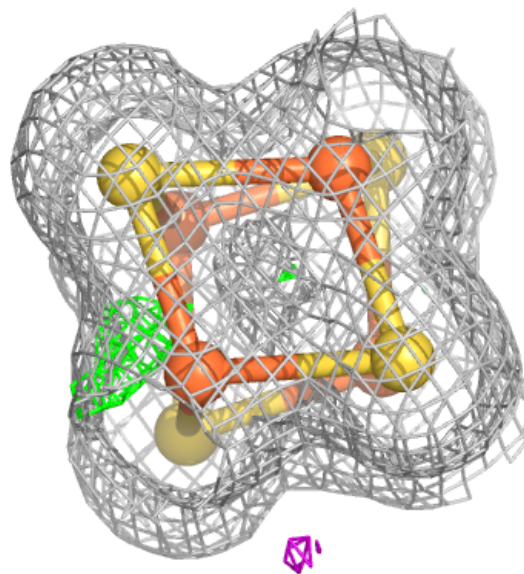
Electron density around SF4 B 1101:

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



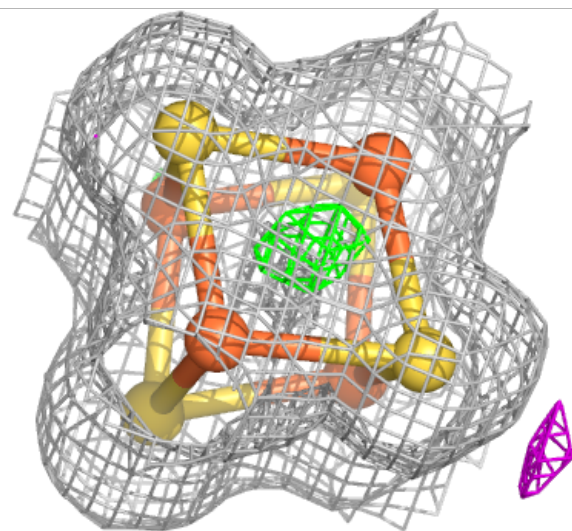
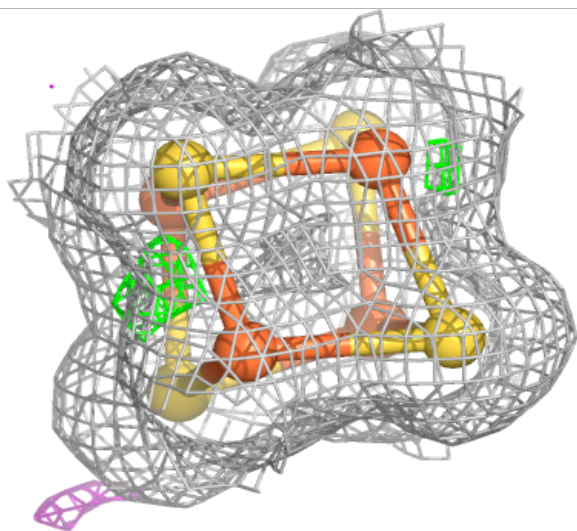
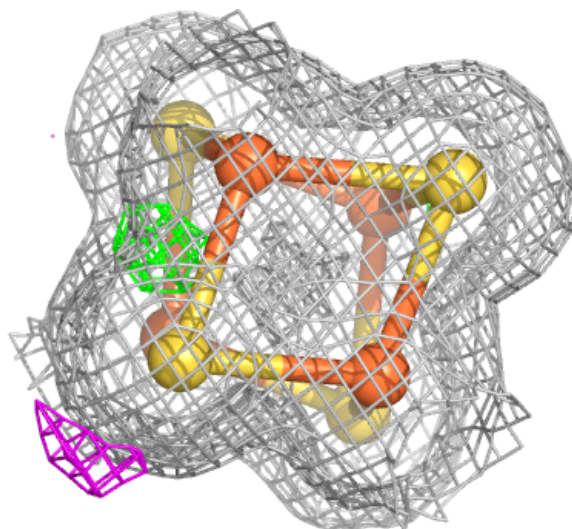
Electron density around SF4 B 1102:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.