



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 06:23 AM EDT

PDB ID : 8F5W / pdb_00008f5w
Title : Dihydropyrimidine Dehydrogenase (DPD) C671S Mutant Soaked with Dihydrothymine and NADPH Quasi-Anaerobically
Authors : Kaley, N.; Smith, M.; Forouzesh, D.; Liu, D.; Moran, G.
Deposited on : 2022-11-15
Resolution : 1.97 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

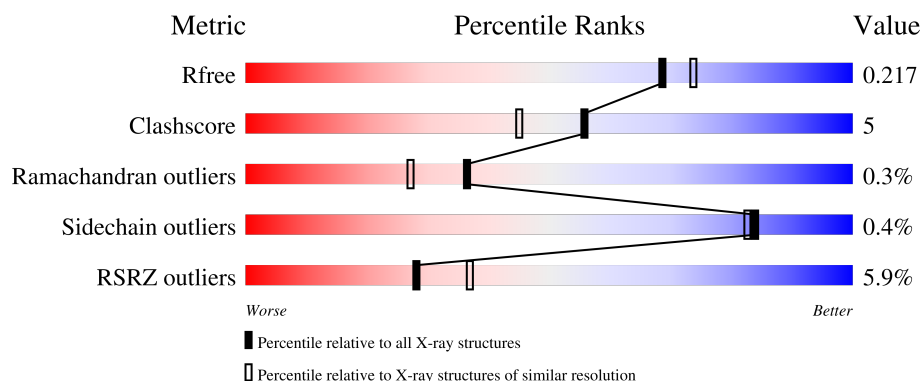
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

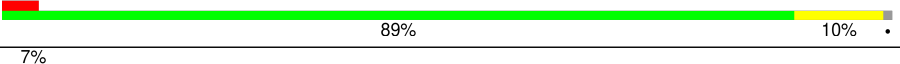
The reported resolution of this entry is 1.97 Å.

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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	
1	B	1025	
1	C	1025	
1	D	1025	

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

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

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32519 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.

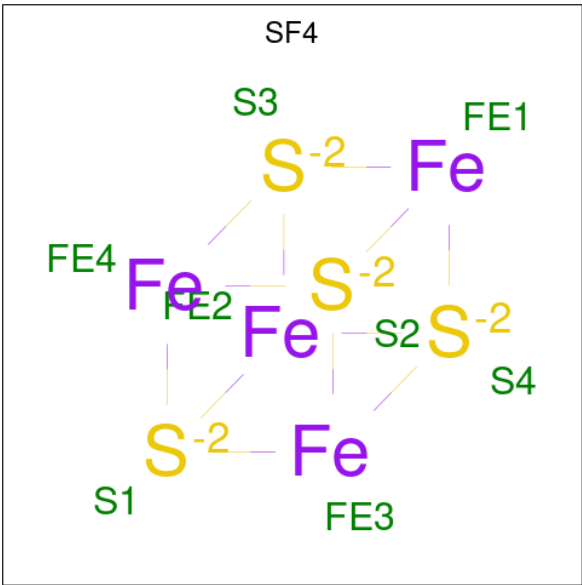
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1010	Total	C	N	O	S	0	0	0
			7702	4889	1303	1458	52			
1	B	1012	Total	C	N	O	S	30	0	0
			7713	4896	1306	1458	53			
1	C	1018	Total	C	N	O	S	0	0	0
			7735	4909	1311	1462	53			
1	D	1010	Total	C	N	O	S	30	0	0
			7700	4887	1302	1458	53			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
A	671	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).



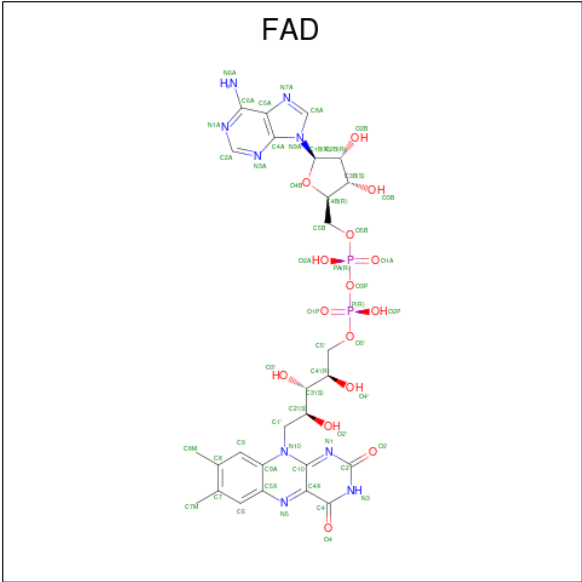
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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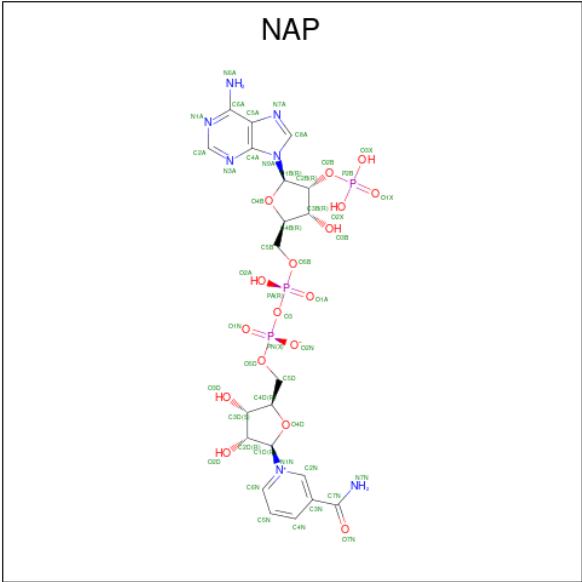
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	D	1	8	4	4	0	0
2	D	1	8	4	4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



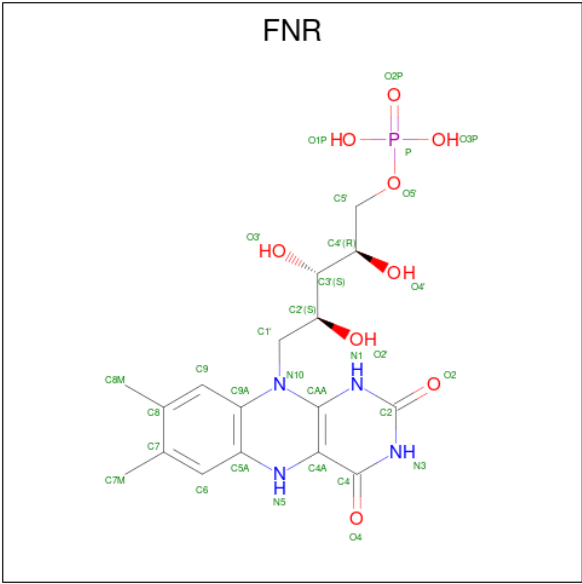
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



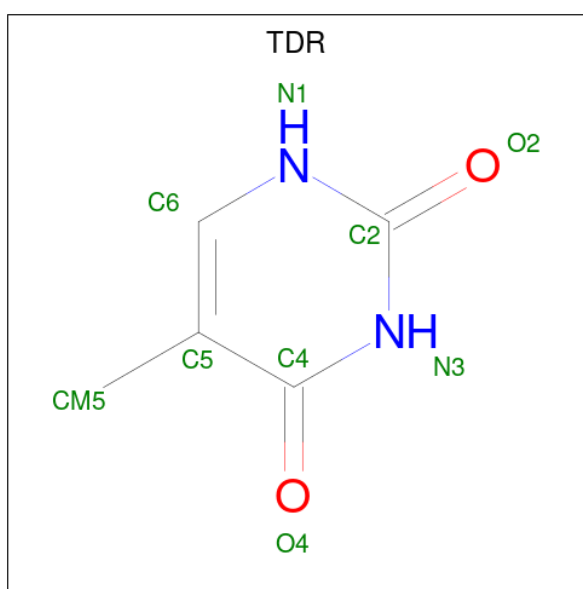
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]PT ERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (CCD ID: FNR) (formula: C₁₇H₂₃N₄O₉P) (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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	248	Total	O	0	0
			248	248		

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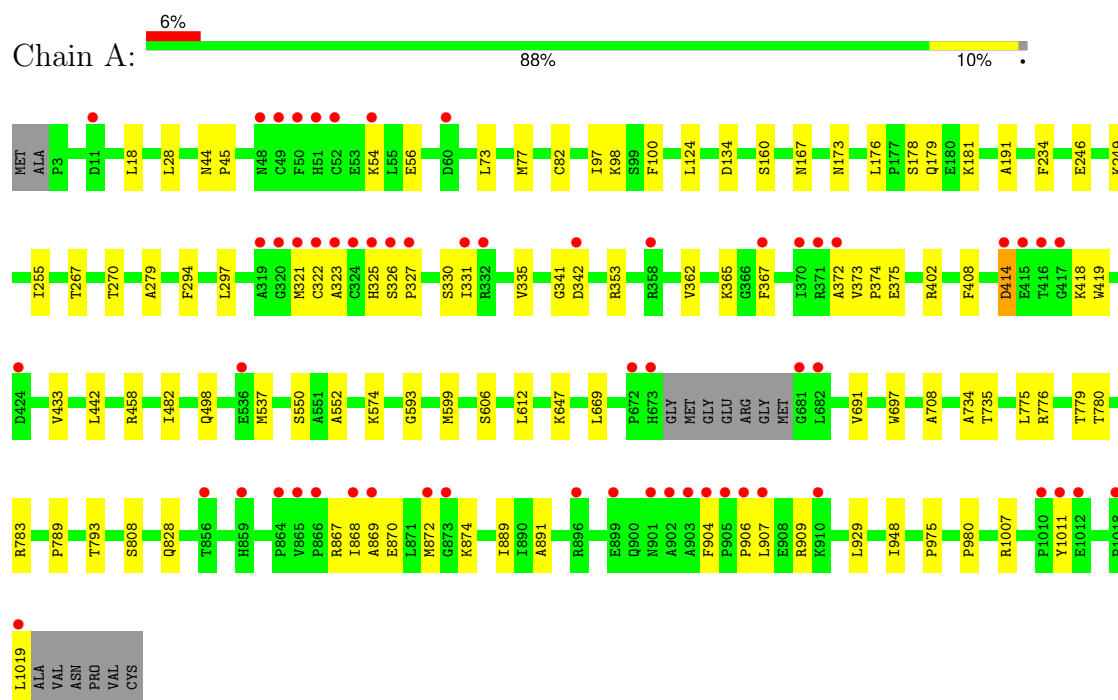
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	229	Total 229	O 229	0	0
7	C	266	Total 266	O 266	0	0
7	D	234	Total 234	O 234	0	0

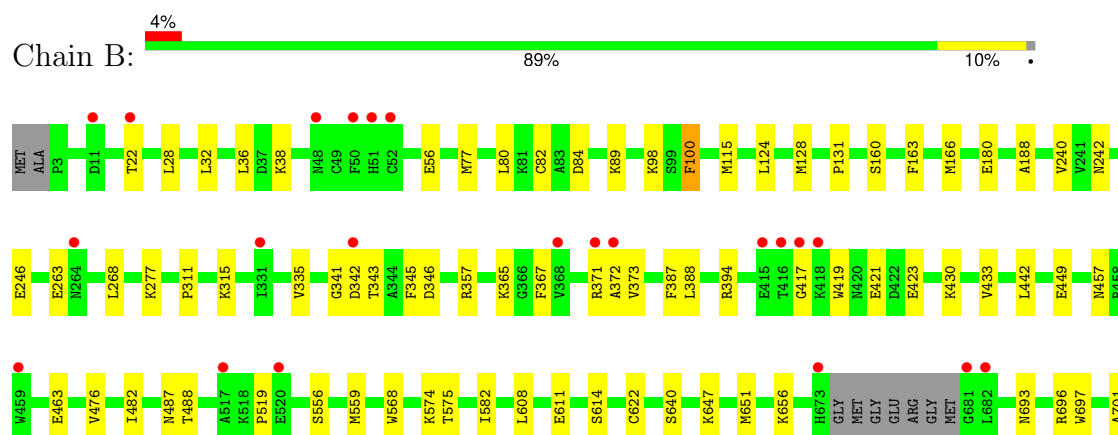
3 Residue-property plots [i](#)

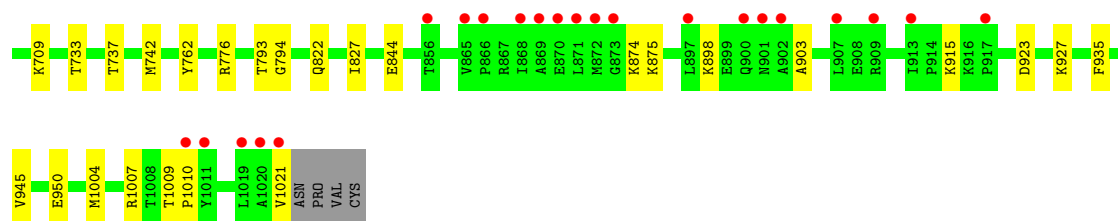
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

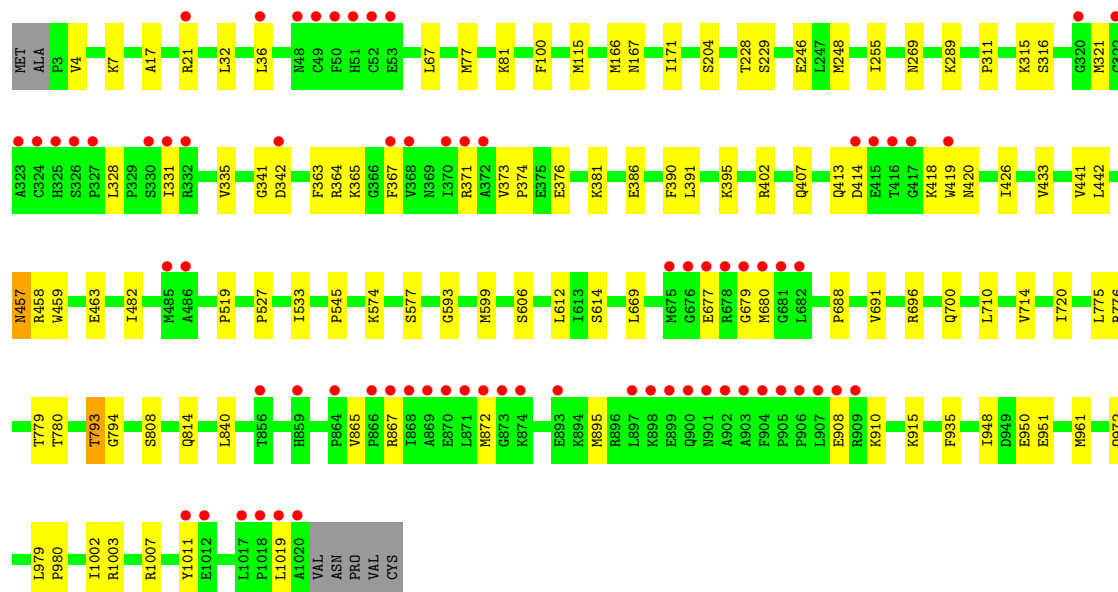
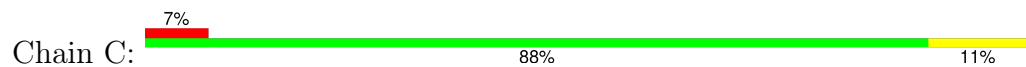


- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

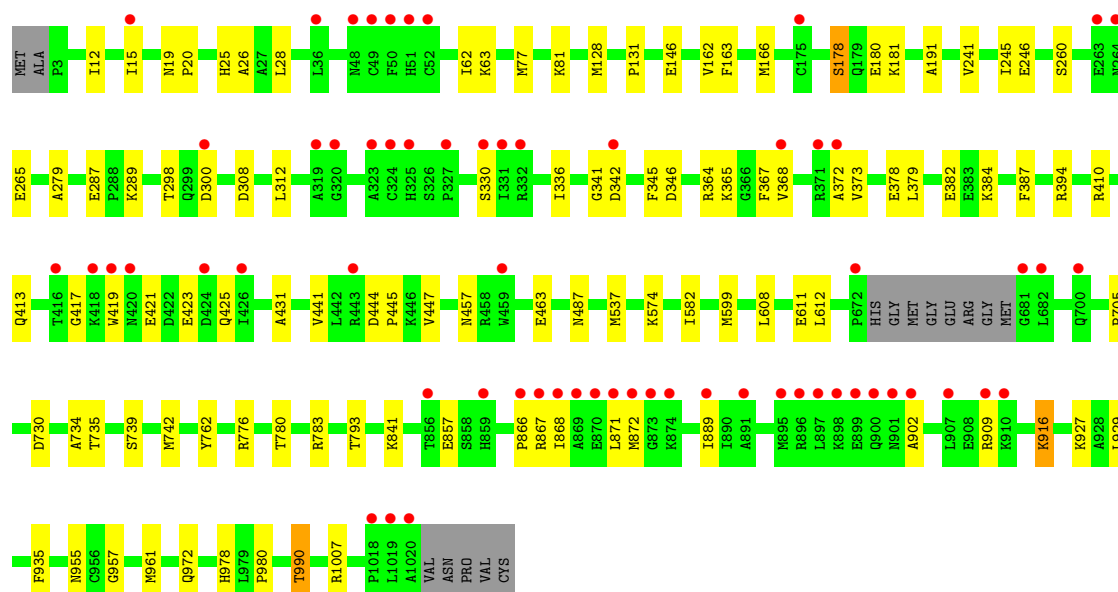
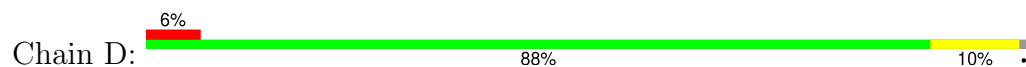




• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



• 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	81.73Å 158.00Å 162.40Å 90.00° 96.06° 90.00°	Depositor
Resolution (Å)	47.23 – 1.97 47.23 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.23-1.97) 98.5 (47.23-1.97)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.179 , 0.217 0.179 , 0.217	Depositor DCC
R_{free} test set	14080 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32519	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.35	0/7862	0.57	0/10658
1	B	0.34	0/7874	0.57	0/10676
1	C	0.35	0/7896	0.60	2/10705 (0.0%)
1	D	0.36	2/7860 (0.0%)	0.63	5/10656 (0.0%)
All	All	0.35	2/31492 (0.0%)	0.59	7/42695 (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
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	PRO	CB-CG	-8.50	1.07	1.49
1	D	445	PRO	CG-CD	-8.18	1.23	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	445	PRO	N-CD-CG	-18.70	75.14	103.20
1	D	445	PRO	CA-CB-CG	-17.81	70.67	104.50
1	D	445	PRO	CA-N-CD	-7.53	101.46	112.00
1	C	457	ASN	CA-C-N	6.98	129.94	120.38
1	C	457	ASN	C-N-CA	6.98	129.94	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	445	PRO	N-CA-CB	-6.24	96.66	103.39
1	D	445	PRO	CB-CG-CD	5.37	123.27	106.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	HIS	Peptide
1	C	1003	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7702	0	7728	74	0
1	B	7713	0	7738	73	0
1	C	7735	0	7754	81	0
1	D	7700	0	7726	77	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	53	0	31	4	0
3	B	53	0	31	3	0
3	C	53	0	31	2	0
3	D	53	0	31	2	0
4	A	48	0	17	8	0
4	B	48	0	17	9	0
4	C	48	0	17	11	0
4	D	48	0	17	7	0
5	A	31	0	22	6	0
5	B	31	0	22	5	0
5	C	31	0	22	2	0
5	D	31	0	22	3	0
6	A	9	0	6	0	0
6	B	9	0	6	1	0
6	C	9	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	9	0	6	0	0
7	A	248	0	0	2	0
7	B	229	0	0	2	0
7	C	266	0	0	5	0
7	D	234	0	0	1	0
All	All	32519	0	31250	294	0

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

All (294) 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:C:342:ASP:HB2	4:C:1106:NAP:C5N	1.97	0.94
1:A:179:GLN:NE2	7:A:1201:HOH:O	2.04	0.91
1:B:875:LYS:HE3	1:B:875:LYS:HA	1.58	0.83
1:B:342:ASP:HB2	4:B:1106:NAP:C4N	2.12	0.80
1:B:342:ASP:HB2	4:B:1106:NAP:C5N	2.13	0.79
1:A:342:ASP:HB2	4:A:1106:NAP:C6N	2.14	0.78
1:D:298:THR:OG1	1:D:300:ASP:OD1	2.01	0.77
1:D:574:LYS:NZ	5:D:1107:FNR:H5	1.82	0.77
1:C:776:ARG:NH2	7:C:1202:HOH:O	2.19	0.75
1:D:342:ASP:HB2	4:D:1106:NAP:C5N	2.16	0.75
1:B:131:PRO:HB2	1:B:373:VAL:HG11	1.70	0.73
1:A:178:SER:HB3	1:A:181:LYS:HE2	1.70	0.73
1:D:342:ASP:HB2	4:D:1106:NAP:C4N	2.18	0.72
1:C:342:ASP:HB2	4:C:1106:NAP:C6N	2.19	0.72
1:D:574:LYS:HZ2	5:D:1107:FNR:H5	1.35	0.72
1:C:269:ASN:OD1	7:C:1201:HOH:O	2.07	0.71
1:C:341:GLY:H	4:C:1106:NAP:H52A	1.56	0.71
1:C:599:MET:HG2	1:D:77:MET:HE1	1.72	0.71
1:D:131:PRO:HB2	1:D:373:VAL:HG11	1.74	0.70
1:B:394:ARG:NH1	1:B:423:GLU:OE1	2.23	0.69
1:C:402:ARG:HG3	1:C:402:ARG:HH11	1.59	0.68
1:C:775:LEU:O	1:C:779:THR:HG23	1.95	0.68
1:A:775:LEU:O	1:A:779:THR:HG23	1.94	0.67
1:C:680:MET:HE3	1:C:688:PRO:HD2	1.76	0.67
1:A:779:THR:HG22	1:A:808:SER:HB3	1.77	0.66
1:A:179:GLN:OE1	7:A:1202:HOH:O	2.13	0.66
1:A:341:GLY:H	4:A:1106:NAP:H52A	1.61	0.65
1:C:246:GLU:OE1	1:C:908:GLU:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:ARG:HD3	1:A:1011:TYR:HB2	1.79	0.65
1:A:870:GLU:HG3	1:A:889:ILE:HD13	1.80	0.64
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.79	0.63
1:A:321:MET:HG2	1:A:322:CYS:N	2.12	0.63
1:C:335:VAL:HG22	1:C:433:VAL:HB	1.81	0.63
1:C:342:ASP:HB2	4:C:1106:NAP:C4N	2.28	0.63
1:A:867:ARG:HD2	1:A:872:MET:HE2	1.80	0.62
1:D:289:LYS:HG3	1:D:441:VAL:HG13	1.81	0.62
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.80	0.62
1:A:783:ARG:HG3	1:A:929:LEU:HD22	1.82	0.62
1:A:342:ASP:HB2	4:A:1106:NAP:C5N	2.30	0.61
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.84	0.60
1:C:779:THR:HG22	1:C:808:SER:HB3	1.82	0.60
1:D:783:ARG:HH11	1:D:783:ARG:HG2	1.67	0.60
1:B:776:ARG:NH1	7:B:1201:HOH:O	2.24	0.60
1:B:874:LYS:HE2	1:B:874:LYS:N	2.17	0.60
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	1.84	0.60
3:A:1105:FAD:C5X	4:A:1106:NAP:C5N	2.80	0.59
1:C:371:ARG:NH1	4:C:1106:NAP:O1A	2.37	0.58
1:A:599:MET:HG2	1:B:77:MET:HE1	1.84	0.58
1:B:844:GLU:HG3	1:B:915:LYS:HD3	1.86	0.58
1:C:167:ASN:ND2	1:C:910:LYS:O	2.31	0.57
1:D:162:VAL:HG12	1:D:166:MET:HE3	1.87	0.57
5:B:1108:FNR:H9	5:B:1108:FNR:C2'	2.33	0.57
1:A:365:LYS:HG2	1:A:419:TRP:CZ2	2.39	0.57
1:B:693:ASN:OD1	1:B:696:ARG:NH2	2.38	0.56
1:B:342:ASP:OD2	1:B:372:ALA:HA	2.05	0.56
1:C:17:ALA:O	1:C:21:ARG:NH2	2.39	0.56
1:C:395:LYS:HE2	1:C:407:GLN:OE1	2.05	0.56
1:D:308:ASP:O	1:D:312:LEU:HG	2.06	0.56
1:B:487:ASN:O	4:B:1106:NAP:H2N	2.05	0.56
1:A:647:LYS:HG3	1:A:697:TRP:CD1	2.40	0.56
1:C:228:THR:HG23	1:C:321:MET:HG3	1.87	0.55
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.88	0.55
1:D:12:ILE:HA	1:D:15:ILE:HG22	1.89	0.55
3:C:1105:FAD:C5X	4:C:1106:NAP:C5N	2.85	0.55
1:B:345:PHE:HE1	1:B:387:PHE:HE2	1.55	0.55
1:D:246:GLU:OE1	1:D:909:ARG:HB2	2.06	0.55
1:B:488:THR:HG22	4:B:1106:NAP:N7N	2.22	0.54
1:C:32:LEU:O	1:C:36:LEU:HD22	2.08	0.54
1:A:73:LEU:O	1:A:77:MET:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:GLN:HG3	1:B:22:THR:HG23	1.89	0.54
1:D:487:ASN:O	4:D:1106:NAP:H2N	2.07	0.54
1:A:362:VAL:HG11	1:A:408:PHE:CE2	2.42	0.54
1:B:32:LEU:O	1:B:36:LEU:HD13	2.08	0.53
1:D:342:ASP:OD1	1:D:372:ALA:HA	2.08	0.53
1:A:249:LYS:HE3	1:A:255:ILE:HD12	1.90	0.53
1:B:180:GLU:CD	1:B:180:GLU:H	2.17	0.53
1:D:163:PHE:O	1:D:166:MET:HB2	2.08	0.53
1:D:857:GLU:OE1	1:D:867:ARG:NH2	2.41	0.53
1:B:574:LYS:NZ	5:B:1108:FNR:H5	2.07	0.53
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.91	0.53
1:D:287:GLU:OE2	7:D:1201:HOH:O	2.19	0.53
1:A:246:GLU:OE2	1:A:909:ARG:N	2.39	0.53
1:D:783:ARG:HG2	1:D:783:ARG:NH1	2.23	0.53
1:A:780:THR:HG22	1:B:762:TYR:CZ	2.44	0.52
1:B:263:GLU:OE1	1:B:449:GLU:HG2	2.10	0.52
1:D:410:ARG:HD3	1:D:425:GLN:OE1	2.09	0.52
1:A:178:SER:H	1:A:181:LYS:CE	2.23	0.52
1:B:574:LYS:HZ3	5:B:1108:FNR:H5	1.57	0.52
1:C:402:ARG:HG3	1:C:402:ARG:NH1	2.25	0.52
1:C:311:PRO:O	1:C:315:LYS:HD2	2.10	0.52
1:C:1019:LEU:HD11	1:D:582:ILE:HG12	1.92	0.52
1:C:950:GLU:HG2	1:C:979:LEU:HD22	1.91	0.51
1:D:444:ASP:OD2	1:D:447:VAL:HG23	2.10	0.51
1:A:342:ASP:CB	4:A:1106:NAP:C5N	2.88	0.51
1:C:342:ASP:HB3	1:C:376:GLU:HG2	1.92	0.51
1:A:498:GLN:HA	1:B:28:LEU:HD11	1.92	0.51
1:A:948:ILE:HD13	1:A:980:PRO:HG2	1.93	0.51
1:B:188:ALA:HB1	1:B:277:LYS:HG3	1.92	0.51
1:C:386:GLU:OE2	1:D:368:VAL:HG22	2.11	0.51
1:D:972:GLN:O	1:D:980:PRO:HA	2.11	0.51
1:B:574:LYS:HB3	1:B:614:SER:HB2	1.93	0.51
1:B:371:ARG:NH1	4:B:1106:NAP:O1X	2.44	0.50
1:B:556:SER:O	1:B:559:MET:HB2	2.11	0.50
1:A:574:LYS:NZ	5:A:1107:FNR:H5	2.09	0.50
1:C:364:ARG:HD3	4:C:1106:NAP:N3A	2.26	0.50
1:C:77:MET:HE1	1:D:599:MET:HG2	1.92	0.50
1:B:242:ASN:O	1:B:246:GLU:HG2	2.12	0.50
1:C:780:THR:HG22	1:D:762:TYR:CZ	2.46	0.50
1:D:25:HIS:HD2	1:D:26:ALA:O	1.95	0.50
1:B:608:LEU:HB2	1:B:742:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:CYS:O	1:A:98:LYS:HD2	2.13	0.49
1:C:364:ARG:HD3	4:C:1106:NAP:C2A	2.43	0.49
1:D:868:ILE:O	1:D:872:MET:HG3	2.12	0.49
1:A:1019:LEU:HD21	1:B:582:ILE:HD13	1.94	0.49
1:B:647:LYS:HG3	1:B:697:TRP:CD1	2.47	0.49
1:C:574:LYS:NZ	5:C:1107:FNR:H5	2.11	0.49
1:D:866:PRO:O	1:D:872:MET:HE3	2.12	0.49
1:C:457:ASN:HB3	1:C:463:GLU:HG2	1.94	0.49
1:D:62:ILE:HD13	1:D:379:LEU:HD22	1.94	0.49
1:C:4:VAL:HG11	1:C:7:LYS:HD2	1.94	0.49
1:A:173:ASN:HB3	1:A:176:LEU:HG	1.94	0.49
1:D:341:GLY:H	4:D:1106:NAP:H52A	1.78	0.49
1:C:166:MET:HE2	1:C:840:LEU:HD11	1.95	0.48
1:B:341:GLY:H	4:B:1106:NAP:H52A	1.78	0.48
1:B:311:PRO:O	1:B:315:LYS:HG3	2.12	0.48
1:C:948:ILE:HD13	1:C:980:PRO:HG2	1.95	0.48
1:A:54:LYS:HD2	1:A:56:GLU:H	1.77	0.48
1:A:867:ARG:C	1:A:868:ILE:HD13	2.39	0.48
1:A:54:LYS:HG2	1:A:891:ALA:HB1	1.96	0.48
1:A:874:LYS:HD3	1:A:874:LYS:N	2.28	0.48
1:D:365:LYS:HG2	1:D:419:TRP:CZ2	2.49	0.48
1:A:167:ASN:HD21	1:A:909:ARG:HD3	1.78	0.47
1:B:737:THR:HG23	5:B:1108:FNR:H1'2	1.96	0.47
1:B:82:CYS:O	1:B:98:LYS:HD2	2.14	0.47
1:A:54:LYS:CG	1:A:891:ALA:HB1	2.44	0.47
1:A:342:ASP:OD1	1:A:372:ALA:HA	2.14	0.47
1:D:457:ASN:HB3	1:D:463:GLU:HG2	1.96	0.47
1:D:537:MET:HE2	1:D:537:MET:HB3	1.88	0.47
1:B:56:GLU:OE2	1:B:898:LYS:NZ	2.48	0.47
1:B:575:THR:HG1	1:B:640:SER:HG	1.60	0.47
1:D:12:ILE:O	1:D:15:ILE:HG22	2.15	0.47
1:D:260:SER:O	1:D:265:GLU:HG2	2.15	0.47
1:A:776:ARG:O	1:A:780:THR:HG23	2.15	0.46
1:D:19:ASN:OD1	1:D:20:PRO:HD2	2.16	0.46
1:C:577:SER:HB2	7:C:1257:HOH:O	2.15	0.46
1:D:574:LYS:NZ	1:D:611:GLU:OE2	2.47	0.46
3:C:1105:FAD:N5	4:C:1106:NAP:C4N	2.78	0.46
1:A:1007:ARG:CD	1:A:1011:TYR:HB2	2.45	0.46
1:B:394:ARG:NH2	1:B:421:GLU:OE1	2.49	0.46
1:A:574:LYS:HZ3	5:A:1107:FNR:H5	1.63	0.46
1:B:709:LYS:HA	1:B:733:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:SER:O	5:A:1107:FNR:CAA	2.64	0.46
1:B:346:ASP:OD2	3:B:1105:FAD:H6	2.16	0.46
3:B:1105:FAD:C5X	4:B:1106:NAP:C5N	2.94	0.46
5:A:1107:FNR:H1'2	5:A:1107:FNR:H9	1.83	0.46
1:B:100:PHE:CD1	1:B:100:PHE:C	2.94	0.46
1:B:915:LYS:HD2	7:B:1203:HOH:O	2.16	0.46
1:A:331:ILE:HG22	1:A:331:ILE:O	2.16	0.45
1:C:81:LYS:O	1:D:961:MET:HE1	2.17	0.45
1:B:124:LEU:HD13	1:B:160:SER:HB2	1.99	0.45
1:B:365:LYS:HE2	4:B:1106:NAP:O2X	2.17	0.45
1:C:915:LYS:HG2	7:C:1227:HOH:O	2.16	0.45
1:B:115:MET:HE2	1:B:115:MET:HB2	1.94	0.45
1:D:63:LYS:HE3	1:D:128:MET:HB3	1.98	0.45
1:C:413:GLN:HG3	1:C:419:TRP:CE2	2.52	0.45
1:D:776:ARG:O	1:D:780:THR:HG23	2.17	0.44
1:D:957:GLY:O	1:D:961:MET:HG3	2.17	0.44
1:C:418:LYS:HE3	1:C:420:ASN:OD1	2.17	0.44
1:A:373:VAL:HG13	1:A:375:GLU:HG2	1.99	0.44
1:C:696:ARG:O	1:C:700:GLN:HG3	2.18	0.44
1:D:178:SER:HB3	1:D:180:GLU:OE2	2.18	0.44
1:A:669:LEU:HD11	1:A:708:ALA:HB1	2.00	0.44
1:A:868:ILE:HG22	1:A:870:GLU:H	1.83	0.44
1:C:865:VAL:HG11	1:C:951:GLU:OE1	2.17	0.44
1:A:537:MET:HG3	1:A:789:PRO:HB3	2.00	0.44
1:A:869:ALA:O	1:A:874:LYS:HE3	2.18	0.44
1:C:289:LYS:HG3	1:C:441:VAL:HG13	1.99	0.44
1:D:608:LEU:HB2	1:D:742:MET:HE2	2.00	0.44
1:A:267:THR:OG1	1:A:270:THR:HG23	2.18	0.44
1:B:1009:THR:HB	1:B:1010:PRO:HD2	1.98	0.44
1:C:331:ILE:HG22	1:C:331:ILE:O	2.16	0.44
1:C:935:PHE:CE1	1:D:612:LEU:HD11	2.53	0.44
1:A:18:LEU:HD21	1:A:975:PRO:HA	1.99	0.43
1:A:191:ALA:O	1:A:279:ALA:HA	2.17	0.43
1:B:611:GLU:O	6:B:1107:TDR:H6	2.18	0.43
1:C:229:SER:HA	1:C:321:MET:HE3	1.98	0.43
1:A:402:ARG:HD2	1:A:402:ARG:HA	1.86	0.43
1:C:533:ILE:O	1:C:545:PRO:HD3	2.18	0.43
1:C:612:LEU:HD11	1:D:935:PHE:CE1	2.53	0.43
1:C:867:ARG:HD2	1:C:872:MET:HE3	2.01	0.43
1:D:394:ARG:NH1	1:D:421:GLU:OE1	2.49	0.43
1:A:669:LEU:HD13	1:A:691:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ARG:HD2	1:C:459:TRP:CZ2	2.54	0.43
1:A:134:ASP:O	1:B:38:LYS:HD2	2.19	0.43
1:B:84:ASP:OD1	1:B:89:LYS:NZ	2.48	0.43
1:C:972:GLN:O	1:C:980:PRO:HA	2.19	0.43
1:B:80:LEU:HB2	1:B:82:CYS:SG	2.58	0.43
1:D:345:PHE:HE2	1:D:387:PHE:HE2	1.64	0.43
1:A:552:ALA:HB2	5:A:1107:FNR:H7M3	2.00	0.43
1:C:248:MET:HE1	1:C:255:ILE:HD11	2.00	0.43
1:A:294:PHE:HA	1:A:297:LEU:HD12	2.01	0.43
1:B:128:MET:HE3	1:B:240:VAL:HG21	2.01	0.43
1:C:574:LYS:HB3	1:C:614:SER:HB2	2.01	0.43
1:C:793:THR:HG22	1:C:814:GLN:HB2	2.01	0.43
1:D:241:VAL:O	1:D:245:ILE:HG12	2.18	0.43
1:D:413:GLN:HG3	1:D:419:TRP:CE2	2.54	0.43
1:A:330:SER:O	1:A:330:SER:OG	2.36	0.42
1:B:651:MET:HG2	1:B:701:ALA:HB2	2.01	0.42
1:B:1004:MET:HE3	1:B:1004:MET:HB3	1.83	0.42
1:C:367:PHE:CZ	1:D:367:PHE:CZ	3.08	0.42
1:C:593:GLY:HA3	1:C:606:SER:OG	2.19	0.42
1:D:384:LYS:HA	1:D:384:LYS:HD3	1.83	0.42
1:A:367:PHE:CZ	1:B:367:PHE:CE2	3.06	0.42
1:A:414:ASP:OD2	1:A:418:LYS:HB3	2.19	0.42
1:D:364:ARG:HD3	4:D:1106:NAP:C2A	2.49	0.42
1:D:394:ARG:HH21	1:D:423:GLU:CD	2.26	0.42
1:B:343:THR:HA	3:B:1105:FAD:HM72	2.01	0.42
1:B:430:LYS:HB2	1:B:430:LYS:HE2	1.90	0.42
1:C:342:ASP:CB	4:C:1106:NAP:C4N	2.96	0.42
1:A:28:LEU:HD22	1:B:519:PRO:HB3	2.02	0.42
1:A:365:LYS:HG2	1:A:419:TRP:CE2	2.54	0.42
5:B:1108:FNR:C2'	5:B:1108:FNR:C9	2.96	0.42
1:D:871:LEU:HG	1:D:889:ILE:HG21	2.02	0.42
1:D:990:THR:HG22	1:D:990:THR:O	2.19	0.42
3:A:1105:FAD:N5	4:A:1106:NAP:C5N	2.83	0.42
1:C:342:ASP:CB	4:C:1106:NAP:C5N	2.85	0.42
1:C:669:LEU:HD13	1:C:691:VAL:HG22	2.01	0.42
1:D:178:SER:HB2	1:D:181:LYS:HG3	2.02	0.42
1:A:234:PHE:CE2	1:A:353:ARG:HD3	2.55	0.42
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.20	0.42
1:A:44:ASN:HB2	1:A:45:PRO:HD2	2.01	0.42
1:A:373:VAL:HG22	1:A:374:PRO:HD2	2.01	0.42
1:B:357:ARG:HG2	1:B:357:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:PHE:CZ	1:D:367:PHE:CE2	3.08	0.42
1:D:394:ARG:NH2	1:D:421:GLU:OE1	2.52	0.42
3:A:1105:FAD:N5	4:A:1106:NAP:C4N	2.82	0.41
1:C:519:PRO:HB3	1:D:28:LEU:HD22	2.01	0.41
1:D:342:ASP:CB	4:D:1106:NAP:C4N	2.93	0.41
1:A:335:VAL:HG22	1:A:433:VAL:HB	2.02	0.41
1:A:612:LEU:HD11	1:B:935:PHE:CE1	2.56	0.41
1:C:228:THR:CG2	1:C:321:MET:HG3	2.50	0.41
1:C:248:MET:HE2	1:C:248:MET:HB3	1.93	0.41
1:D:178:SER:HB3	1:D:180:GLU:CD	2.45	0.41
1:A:323:ALA:HB2	1:A:904:PHE:HE2	1.84	0.41
1:A:326:SER:OG	1:A:327:PRO:HD2	2.19	0.41
1:A:734:ALA:HA	1:A:735:THR:HA	1.86	0.41
1:B:163:PHE:HA	1:B:166:MET:HG3	2.02	0.41
1:C:21:ARG:NH1	7:C:1215:HOH:O	2.50	0.41
1:C:776:ARG:HE	1:D:739:SER:HB3	1.85	0.41
1:C:316:SER:HB2	1:C:328:LEU:HD23	2.03	0.41
5:C:1107:FNR:H1'2	5:C:1107:FNR:H9	1.67	0.41
1:B:268:LEU:HD13	1:B:476:VAL:HG21	2.02	0.41
1:C:390:PHE:O	1:C:391:LEU:HD23	2.20	0.41
1:C:710:LEU:HD22	1:C:720:ILE:HG22	2.02	0.41
1:C:171:ILE:HG23	1:C:527:PRO:HD3	2.03	0.41
1:C:365:LYS:NZ	1:C:419:TRP:NE1	2.68	0.41
1:D:378:GLU:O	1:D:382:GLU:HG2	2.20	0.41
3:D:1105:FAD:C5X	4:D:1106:NAP:C5N	2.99	0.41
1:A:1019:LEU:HD11	1:B:582:ILE:HD13	2.03	0.41
1:C:373:VAL:HG22	1:C:374:PRO:HD2	2.03	0.41
1:D:734:ALA:HA	1:D:735:THR:HA	1.79	0.41
1:B:875:LYS:HZ3	1:B:950:GLU:HG3	1.85	0.41
1:B:945:VAL:HG13	1:B:1007:ARG:HG2	2.03	0.41
1:D:330:SER:O	1:D:330:SER:OG	2.39	0.41
1:A:906:PRO:O	1:A:907:LEU:C	2.64	0.41
1:B:488:THR:HG22	4:B:1106:NAP:H72N	1.83	0.41
1:B:568:TRP:CE2	1:B:827:ILE:HB	2.56	0.41
1:B:622:CYS:SG	1:B:656:LYS:HD3	2.61	0.41
1:C:680:MET:CE	1:C:688:PRO:HD2	2.46	0.41
1:D:783:ARG:HG3	1:D:929:LEU:HD22	2.02	0.41
1:D:191:ALA:O	1:D:279:ALA:HA	2.21	0.41
1:D:574:LYS:HZ1	5:D:1107:FNR:H5	1.66	0.41
3:A:1105:FAD:C4X	4:A:1106:NAP:C4N	3.00	0.40
1:B:875:LYS:HE3	1:B:875:LYS:CA	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:MET:HE1	1:D:81:LYS:O	2.21	0.40
1:D:955:ASN:HB3	1:D:978:HIS:HB3	2.01	0.40
1:A:593:GLY:HA3	1:A:606:SER:OG	2.20	0.40
5:A:1107:FNR:HN1	5:A:1107:FNR:HI'1	1.64	0.40
1:B:335:VAL:HG22	1:B:433:VAL:HB	2.04	0.40
1:C:204:SER:OG	1:C:248:MET:HG3	2.20	0.40
1:C:895:MET:HE3	1:C:895:MET:HA	2.02	0.40
1:D:336:ILE:HD12	1:D:431:ALA:HB2	2.03	0.40
1:B:387:PHE:O	1:B:388:LEU:HD23	2.22	0.40
1:C:115:MET:HB2	1:C:115:MET:HE2	1.54	0.40
1:D:841:LYS:O	1:D:916:LYS:HE2	2.22	0.40
1:A:124:LEU:HD13	1:A:160:SER:HB2	2.02	0.40
1:B:365:LYS:HD3	1:B:419:TRP:CE2	2.56	0.40
1:B:457:ASN:HB3	1:B:463:GLU:HG3	2.03	0.40
1:B:923:ASP:O	1:B:927:LYS:HE3	2.21	0.40
1:C:381:LYS:HE3	1:C:381:LYS:HB2	1.81	0.40
1:C:714:VAL:HG11	1:C:720:ILE:HD13	2.04	0.40
1:D:346:ASP:OD2	3:D:1105:FAD:H6	2.20	0.40
1:D:927:LYS:HD2	1:D:927:LYS:HA	1.72	0.40
1:A:97:ILE:HA	1:A:100:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1006/1025 (98%)	971 (96%)	33 (3%)	2 (0%)	43	35
1	B	1008/1025 (98%)	965 (96%)	39 (4%)	4 (0%)	30	20
1	C	1016/1025 (99%)	975 (96%)	37 (4%)	4 (0%)	30	20
1	D	1006/1025 (98%)	965 (96%)	38 (4%)	3 (0%)	36	27
All	All	4036/4100 (98%)	3876 (96%)	147 (4%)	13 (0%)	36	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	677	GLU
1	D	902	ALA
1	B	417	GLY
1	C	414	ASP
1	A	414	ASP
1	A	458	ARG
1	B	903	ALA
1	D	990	THR
1	B	822	GLN
1	D	417	GLY
1	B	794	GLY
1	C	679	GLY
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	841/854 (98%)	840 (100%)	1 (0%)	88	89
1	B	842/854 (99%)	839 (100%)	3 (0%)	84	82
1	C	840/854 (98%)	836 (100%)	4 (0%)	81	79
1	D	841/854 (98%)	837 (100%)	4 (0%)	81	79
All	All	3364/3416 (98%)	3352 (100%)	12 (0%)	84	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	793	THR
1	B	100	PHE
1	B	793	THR
1	B	1021	VAL
1	C	100	PHE
1	C	363	PHE
1	C	426	ILE

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Mol	Chain	Res	Type
1	C	793	THR
1	D	178	SER
1	D	793	THR
1	D	916	LYS
1	D	1007	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	51	HIS
1	A	167	ASN
1	A	828	GLN
1	A	847	GLN
1	A	900	GLN
1	B	420	ASN
1	B	828	GLN
1	C	23	GLN
1	C	25	HIS
1	C	51	HIS
1	C	900	GLN
1	D	25	HIS
1	D	167	ASN
1	D	179	GLN
1	D	494	ASN
1	D	693	ASN
1	D	828	GLN
1	D	859	HIS

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

32 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	B	1101	1	0,12,12	-	-	-		
2	SF4	D	1102	1	0,12,12	-	-	-		
2	SF4	A	1104	1	0,12,12	-	-	-		
3	FAD	D	1105	-	58,58,58	0.39	0	85,89,89	0.43	0
2	SF4	D	1103	1	0,12,12	-	-	-		
5	FNR	A	1107	-	32,33,33	5.84	17 (53%)	41,50,50	7.92	28 (68%)
4	NAP	A	1106	1	50,52,52	3.07	20 (40%)	71,80,80	2.99	27 (38%)
4	NAP	C	1106	-	50,52,52	3.00	18 (36%)	71,80,80	3.01	25 (35%)
6	TDR	C	1108	-	9,9,9	0.49	0	12,12,12	0.65	0
2	SF4	D	1101	1	0,12,12	-	-	-		
2	SF4	C	1102	1	0,12,12	-	-	-		
2	SF4	C	1104	1	0,12,12	-	-	-		
6	TDR	A	1108	-	9,9,9	0.43	0	12,12,12	0.61	0
4	NAP	B	1106	-	50,52,52	3.42	18 (36%)	71,80,80	3.09	29 (40%)
3	FAD	A	1105	-	58,58,58	0.38	0	85,89,89	0.39	0
5	FNR	C	1107	-	32,33,33	5.75	15 (46%)	41,50,50	8.08	22 (53%)
6	TDR	B	1107	-	9,9,9	0.61	0	12,12,12	0.73	0
2	SF4	D	1104	1	0,12,12	-	-	-		
2	SF4	B	1102	1	0,12,12	-	-	-		
6	TDR	D	1108	-	9,9,9	0.61	0	12,12,12	0.90	0
3	FAD	B	1105	-	58,58,58	0.33	0	85,89,89	0.43	0
2	SF4	B	1104	1	0,12,12	-	-	-		
4	NAP	D	1106	-	50,52,52	3.28	18 (36%)	71,80,80	3.11	28 (39%)
2	SF4	A	1101	1	0,12,12	-	-	-		
2	SF4	C	1101	1	0,12,12	-	-	-		
2	SF4	A	1103	1	0,12,12	-	-	-		
2	SF4	C	1103	1	0,12,12	-	-	-		
2	SF4	A	1102	1	0,12,12	-	-	-		
5	FNR	D	1107	-	32,33,33	5.74	16 (50%)	41,50,50	8.01	27 (65%)
2	SF4	B	1103	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FNR	B	1108	-	32,33,33	5.80	17 (53%)	41,50,50	8.09	27 (65%)
3	FAD	C	1105	-	58,58,58	0.37	0	85,89,89	0.43	0

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	B	1101	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
3	FAD	D	1105	-	-	3/34/50/50	0/6/6/6
2	SF4	D	1103	1	-	-	0/6/5/5
5	FNR	A	1107	-	-	10/18/18/18	0/3/3/3
4	NAP	C	1106	-	8/8/12/12	10/35/67/67	0/5/5/5
4	NAP	A	1106	1	8/8/12/12	12/35/67/67	0/5/5/5
6	TDR	C	1108	-	-	-	0/1/1/1
2	SF4	D	1101	1	-	-	0/6/5/5
2	SF4	C	1102	1	-	-	0/6/5/5
2	SF4	C	1104	1	-	-	0/6/5/5
6	TDR	A	1108	-	-	-	0/1/1/1
4	NAP	B	1106	-	8/8/12/12	13/35/67/67	0/5/5/5
3	FAD	A	1105	-	-	3/34/50/50	0/6/6/6
5	FNR	C	1107	-	-	8/18/18/18	0/3/3/3
6	TDR	B	1107	-	-	-	0/1/1/1
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
6	TDR	D	1108	-	-	-	0/1/1/1
3	FAD	B	1105	-	-	2/34/50/50	0/6/6/6
2	SF4	B	1104	1	-	-	0/6/5/5
4	NAP	D	1106	-	8/8/12/12	13/35/67/67	0/5/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
2	SF4	C	1101	1	-	-	0/6/5/5
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
2	SF4	A	1102	1	-	-	0/6/5/5
5	FNR	D	1107	-	-	4/18/18/18	0/3/3/3
2	SF4	B	1103	1	-	-	0/6/5/5
5	FNR	B	1108	-	-	9/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	1105	-	-	2/34/50/50	0/6/6/6

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1108	FNR	C5A-C9A	-13.20	1.26	1.40
5	D	1107	FNR	C5A-C9A	-12.52	1.26	1.40
5	A	1107	FNR	C5A-C9A	-12.27	1.27	1.40
5	C	1107	FNR	C5A-C9A	-12.10	1.27	1.40
5	B	1108	FNR	C9-C9A	-11.98	1.20	1.39
4	B	1106	NAP	O4D-C1D	-11.78	1.25	1.40
5	A	1107	FNR	C4A-N5	11.59	1.58	1.35
5	A	1107	FNR	C5A-N5	11.58	1.59	1.39
5	B	1108	FNR	C6-C5A	-11.58	1.21	1.39
5	A	1107	FNR	C9-C9A	-11.38	1.21	1.39
5	C	1107	FNR	C5A-N5	11.35	1.59	1.39
5	B	1108	FNR	C4A-N5	11.21	1.57	1.35
5	C	1107	FNR	C4A-N5	11.16	1.57	1.35
5	D	1107	FNR	C4A-N5	11.07	1.57	1.35
5	D	1107	FNR	C9-C9A	-10.91	1.22	1.39
5	D	1107	FNR	C6-C5A	-10.89	1.22	1.39
5	C	1107	FNR	C9-C9A	-10.86	1.22	1.39
5	D	1107	FNR	C9A-N10	10.81	1.59	1.41
4	D	1106	NAP	O4D-C1D	-10.78	1.26	1.40
5	C	1107	FNR	C9A-N10	10.77	1.59	1.41
5	C	1107	FNR	C6-C5A	-10.76	1.22	1.39
5	D	1107	FNR	C5A-N5	10.75	1.58	1.39
5	B	1108	FNR	C5A-N5	10.50	1.57	1.39
5	A	1107	FNR	C6-C5A	-10.24	1.23	1.39
5	A	1107	FNR	C9A-N10	10.16	1.58	1.41
5	B	1108	FNR	C9A-N10	9.52	1.57	1.41
5	D	1107	FNR	CAA-N10	9.04	1.54	1.38
5	A	1107	FNR	CAA-N10	8.60	1.53	1.38
5	C	1107	FNR	CAA-N10	8.37	1.52	1.38
4	A	1106	NAP	O4D-C1D	-8.24	1.30	1.40
5	B	1108	FNR	CAA-N10	8.17	1.52	1.38
4	C	1106	NAP	O4D-C1D	-7.94	1.30	1.40
5	A	1107	FNR	C2-N3	7.80	1.50	1.37
5	C	1107	FNR	C2-N1	7.70	1.50	1.37
5	C	1107	FNR	C2-N3	7.63	1.50	1.37
4	B	1106	NAP	O4D-C4D	-7.61	1.28	1.45
5	A	1107	FNR	C2-N1	7.40	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1106	NAP	O4D-C4D	-7.21	1.29	1.45
5	D	1107	FNR	C2-N1	7.19	1.49	1.37
5	B	1108	FNR	C2-N3	7.10	1.49	1.37
5	D	1107	FNR	C2-N3	7.07	1.49	1.37
4	B	1106	NAP	PA-O3	6.98	1.67	1.59
4	A	1106	NAP	PA-O3	6.95	1.67	1.59
5	B	1108	FNR	C2-N1	6.69	1.48	1.37
4	D	1106	NAP	O4B-C4B	-6.64	1.30	1.45
4	D	1106	NAP	C7N-N7N	6.61	1.45	1.33
4	C	1106	NAP	C7N-N7N	6.48	1.44	1.33
4	B	1106	NAP	O4B-C4B	-6.32	1.30	1.45
4	A	1106	NAP	O4D-C4D	-6.22	1.31	1.45
4	B	1106	NAP	C7N-N7N	6.22	1.44	1.33
4	D	1106	NAP	PA-O3	6.16	1.66	1.59
4	A	1106	NAP	C7N-N7N	6.10	1.44	1.33
4	C	1106	NAP	O4D-C4D	-6.05	1.31	1.45
4	A	1106	NAP	O4B-C4B	-6.02	1.31	1.45
5	D	1107	FNR	CAA-N1	5.81	1.47	1.37
4	C	1106	NAP	C3B-C4B	-5.77	1.38	1.53
4	C	1106	NAP	O4B-C4B	-5.75	1.32	1.45
4	B	1106	NAP	C3N-C7N	5.75	1.59	1.50
4	B	1106	NAP	C3D-C4D	-5.72	1.38	1.53
5	B	1108	FNR	CAA-N1	5.70	1.47	1.37
4	C	1106	NAP	PA-O3	5.67	1.65	1.59
4	D	1106	NAP	C3B-C4B	-5.62	1.38	1.53
4	D	1106	NAP	C3D-C4D	-5.55	1.38	1.53
4	B	1106	NAP	PN-O3	5.37	1.65	1.59
5	A	1107	FNR	CAA-N1	5.35	1.46	1.37
5	C	1107	FNR	CAA-N1	5.34	1.46	1.37
4	B	1106	NAP	C3B-C4B	-5.33	1.39	1.53
4	A	1106	NAP	C3B-C4B	-5.29	1.39	1.53
4	D	1106	NAP	C3N-C7N	5.20	1.58	1.50
5	C	1107	FNR	C4-N3	5.12	1.48	1.38
4	C	1106	NAP	C3D-C4D	-5.04	1.40	1.53
5	A	1107	FNR	C4-N3	4.91	1.48	1.38
4	A	1106	NAP	C3D-C4D	-4.90	1.40	1.53
4	D	1106	NAP	C2B-C1B	-4.84	1.41	1.53
4	A	1106	NAP	C2B-C1B	-4.82	1.41	1.53
4	D	1106	NAP	O4B-C1B	-4.79	1.30	1.42
4	C	1106	NAP	C3N-C7N	4.71	1.57	1.50
4	B	1106	NAP	O4B-C1B	-4.63	1.31	1.42
4	A	1106	NAP	PN-O3	4.59	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	NAP	C3N-C7N	4.56	1.57	1.50
4	C	1106	NAP	O4B-C1B	-4.55	1.31	1.42
4	A	1106	NAP	O4B-C1B	-4.55	1.31	1.42
4	C	1106	NAP	PN-O3	4.50	1.64	1.59
4	C	1106	NAP	C6A-N6A	4.48	1.45	1.34
4	D	1106	NAP	C6A-N6A	4.41	1.45	1.34
4	A	1106	NAP	C6A-N6A	4.40	1.45	1.34
5	A	1107	FNR	C7M-C7	4.36	1.59	1.51
5	B	1108	FNR	C4-N3	4.35	1.47	1.38
5	C	1107	FNR	C7M-C7	4.33	1.59	1.51
4	C	1106	NAP	C3B-C2B	-4.30	1.43	1.53
4	B	1106	NAP	C2B-C1B	-4.30	1.42	1.53
5	D	1107	FNR	C4-N3	4.25	1.46	1.38
4	D	1106	NAP	C3B-C2B	-4.18	1.43	1.53
5	A	1107	FNR	C4A-C4	4.17	1.54	1.41
4	B	1106	NAP	C6A-N6A	4.16	1.44	1.34
4	C	1106	NAP	C2B-C1B	-4.16	1.42	1.53
5	B	1108	FNR	C4'-C3'	-4.09	1.46	1.53
4	B	1106	NAP	C3B-C2B	-4.08	1.44	1.53
4	A	1106	NAP	C3B-C2B	-3.95	1.44	1.53
5	A	1107	FNR	C4'-C3'	-3.93	1.46	1.53
5	D	1107	FNR	C7M-C7	3.84	1.58	1.51
5	B	1108	FNR	C8M-C8	3.79	1.58	1.51
5	A	1107	FNR	C5'-C4'	3.78	1.57	1.51
5	B	1108	FNR	C5'-C4'	3.70	1.56	1.51
5	D	1107	FNR	C8M-C8	3.61	1.57	1.51
5	B	1108	FNR	C7M-C7	3.57	1.57	1.51
5	C	1107	FNR	C4A-C4	3.56	1.52	1.41
4	D	1106	NAP	PN-O3	3.47	1.63	1.59
5	A	1107	FNR	C8M-C8	3.37	1.57	1.51
5	C	1107	FNR	C8M-C8	3.33	1.57	1.51
4	A	1106	NAP	PA-O5B	3.30	1.72	1.59
5	D	1107	FNR	C4A-C4	3.27	1.51	1.41
4	C	1106	NAP	PA-O5B	3.12	1.71	1.59
5	B	1108	FNR	C4A-C4	3.04	1.51	1.41
4	D	1106	NAP	PA-O5B	2.95	1.70	1.59
4	B	1106	NAP	P2B-O2B	2.92	1.64	1.59
4	B	1106	NAP	PA-O5B	2.90	1.70	1.59
4	A	1106	NAP	PN-O5D	2.88	1.70	1.59
4	A	1106	NAP	C5A-N7A	-2.88	1.33	1.39
4	A	1106	NAP	C2D-C3D	-2.87	1.45	1.53
4	B	1106	NAP	C5A-N7A	-2.84	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1106	NAP	C5A-N7A	-2.80	1.34	1.39
4	C	1106	NAP	C5A-N7A	-2.77	1.34	1.39
4	C	1106	NAP	P2B-O2B	2.70	1.64	1.59
5	D	1107	FNR	O5'-C5'	-2.67	1.34	1.44
4	C	1106	NAP	C2D-C3D	-2.67	1.46	1.53
4	D	1106	NAP	C8A-N9A	-2.65	1.33	1.37
4	D	1106	NAP	P2B-O2B	2.60	1.64	1.59
5	C	1107	FNR	O5'-C5'	-2.57	1.34	1.44
4	C	1106	NAP	PN-O5D	2.56	1.69	1.59
4	B	1106	NAP	C2D-C3D	-2.48	1.46	1.53
4	D	1106	NAP	C2D-C3D	-2.38	1.46	1.53
4	A	1106	NAP	P2B-O2B	2.32	1.63	1.59
5	B	1108	FNR	O4-C4	-2.19	1.19	1.23
4	B	1106	NAP	C8A-N9A	-2.19	1.33	1.37
5	A	1107	FNR	O4-C4	-2.19	1.19	1.23
4	A	1106	NAP	C8A-N9A	-2.18	1.33	1.37
5	D	1107	FNR	O2'-C2'	-2.08	1.39	1.43
4	A	1106	NAP	O2B-C2B	-2.04	1.37	1.44

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	FNR	C9-C9A-N10	-25.87	87.06	121.85
5	C	1107	FNR	C9-C9A-N10	-25.36	87.75	121.85
5	B	1108	FNR	C9-C9A-N10	-25.06	88.16	121.85
5	D	1107	FNR	C9-C9A-N10	-24.76	88.56	121.85
5	D	1107	FNR	C6-C5A-N5	-20.07	84.92	119.76
5	B	1108	FNR	C6-C5A-N5	-19.78	85.42	119.76
5	C	1107	FNR	C6-C5A-N5	-19.45	86.00	119.76
5	A	1107	FNR	C6-C5A-N5	-18.78	87.16	119.76
5	D	1107	FNR	C6-C5A-C9A	16.93	138.32	119.80
5	C	1107	FNR	C6-C5A-C9A	16.07	137.38	119.80
5	B	1108	FNR	C6-C5A-C9A	15.92	137.22	119.80
5	C	1107	FNR	C5'-C4'-C3'	-15.33	83.30	112.22
5	A	1107	FNR	C6-C5A-C9A	14.79	135.98	119.80
5	C	1107	FNR	C9A-C9-C8	-14.69	89.69	119.22
5	A	1107	FNR	C9A-C9-C8	-14.50	90.07	119.22
5	B	1108	FNR	C9A-C9-C8	-14.25	90.57	119.22
5	D	1107	FNR	C9A-C9-C8	-14.11	90.84	119.22
5	B	1108	FNR	C5A-C6-C7	-13.46	91.23	119.92
5	A	1107	FNR	C5A-C6-C7	-13.27	91.65	119.92
5	C	1107	FNR	C5A-C6-C7	-13.22	91.75	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1107	FNR	C5A-C6-C7	-13.13	91.95	119.92
5	C	1107	FNR	C9-C9A-C5A	12.93	138.00	119.95
5	B	1108	FNR	C9-C9A-C5A	12.89	137.95	119.95
5	D	1107	FNR	C5'-C4'-C3'	-12.69	88.28	112.22
5	D	1107	FNR	C9-C9A-C5A	12.44	137.32	119.95
5	A	1107	FNR	C9-C9A-C5A	11.81	136.44	119.95
5	C	1107	FNR	C7M-C7-C6	-10.13	101.72	119.57
5	B	1108	FNR	C7M-C7-C6	-10.10	101.78	119.57
4	C	1106	NAP	C2B-C1B-N9A	10.08	130.34	113.75
5	D	1107	FNR	C9A-C5A-N5	10.04	131.61	119.37
5	D	1107	FNR	C7M-C7-C6	-9.99	101.97	119.57
5	D	1107	FNR	C5A-C9A-N10	9.74	129.03	118.01
4	B	1106	NAP	C2B-C1B-N9A	9.46	129.32	113.75
5	C	1107	FNR	C9A-C5A-N5	9.43	130.87	119.37
5	B	1108	FNR	C9A-C5A-N5	9.32	130.74	119.37
5	A	1107	FNR	C7M-C7-C6	-9.29	103.21	119.57
4	D	1106	NAP	C2B-C1B-N9A	9.01	128.57	113.75
5	A	1107	FNR	C5'-C4'-C3'	-8.86	95.51	112.22
4	A	1106	NAP	C2B-C1B-N9A	8.85	128.32	113.75
5	C	1107	FNR	C5A-C9A-N10	8.65	127.79	118.01
5	D	1107	FNR	C5A-N5-C4A	-8.64	101.11	121.08
5	A	1107	FNR	C1'-N10-C9A	8.39	136.94	120.63
5	B	1108	FNR	C1'-N10-C9A	8.21	136.58	120.63
5	C	1107	FNR	C5A-N5-C4A	-8.19	102.16	121.08
5	B	1108	FNR	C5'-C4'-C3'	-8.17	96.80	112.22
5	B	1108	FNR	C5A-N5-C4A	-8.03	102.53	121.08
4	A	1106	NAP	O4B-C1B-N9A	7.93	123.33	108.09
5	B	1108	FNR	C1'-C2'-C3'	-7.90	88.24	109.66
5	A	1107	FNR	C1'-C2'-C3'	-7.81	88.47	109.66
5	B	1108	FNR	C5A-C9A-N10	7.77	126.80	118.01
5	B	1108	FNR	C4'-C3'-C2'	-7.77	100.64	113.57
5	A	1107	FNR	C9A-C5A-N5	7.68	128.74	119.37
4	C	1106	NAP	O4B-C1B-N9A	7.52	122.53	108.09
5	A	1107	FNR	C5A-C9A-N10	7.50	126.49	118.01
4	D	1106	NAP	O4B-C1B-N9A	7.39	122.28	108.09
5	C	1107	FNR	C1'-N10-C9A	7.39	134.99	120.63
5	A	1107	FNR	C5A-N5-C4A	-7.38	104.02	121.08
4	B	1106	NAP	O4B-C1B-N9A	7.24	121.99	108.09
5	C	1107	FNR	C9-C8-C7	7.23	130.31	119.69
5	A	1107	FNR	O2'-C2'-C3'	7.20	126.09	109.25
5	B	1108	FNR	O4'-C4'-C5'	6.98	125.37	109.99
5	D	1107	FNR	C1'-N10-C9A	6.90	134.03	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1107	FNR	C9-C8-C7	6.82	129.71	119.69
5	A	1107	FNR	C9-C8-C7	6.75	129.60	119.69
4	C	1106	NAP	O2B-C2B-C1B	6.65	133.42	110.05
4	A	1106	NAP	O3D-C3D-C4D	6.54	129.87	111.08
4	A	1106	NAP	C5A-C4A-N3A	-6.46	117.83	126.72
5	B	1108	FNR	O2'-C2'-C3'	6.36	124.13	109.25
5	B	1108	FNR	C9-C8-C7	6.31	128.95	119.69
4	B	1106	NAP	O5D-C5D-C4D	-6.28	87.61	108.99
4	D	1106	NAP	O3B-C3B-C2B	6.17	128.46	111.19
4	C	1106	NAP	C5A-C4A-N3A	-6.08	118.34	126.72
4	B	1106	NAP	O2B-C2B-C1B	6.08	131.44	110.05
4	A	1106	NAP	O3B-C3B-C2B	5.97	127.89	111.19
4	B	1106	NAP	O3B-C3B-C2B	5.95	127.85	111.19
4	C	1106	NAP	O4B-C4B-C5B	5.95	128.40	109.33
5	A	1107	FNR	O4'-C4'-C5'	5.94	123.09	109.99
4	B	1106	NAP	C5D-C4D-C3D	5.85	136.28	115.21
4	C	1106	NAP	O3D-C3D-C4D	5.84	127.87	111.08
4	C	1106	NAP	O3B-C3B-C2B	5.82	127.48	111.19
4	B	1106	NAP	O3D-C3D-C4D	5.75	127.61	111.08
4	B	1106	NAP	O3B-C3B-C4B	5.74	127.58	111.08
4	D	1106	NAP	O2B-C2B-C1B	5.74	130.22	110.05
4	D	1106	NAP	O3D-C3D-C4D	5.73	127.53	111.08
4	C	1106	NAP	O3B-C3B-C4B	5.71	127.48	111.08
5	C	1107	FNR	C7M-C7-C8	5.70	132.40	120.76
4	B	1106	NAP	O3D-C3D-C2D	5.69	130.07	111.82
4	A	1106	NAP	O4B-C4B-C5B	5.64	127.39	109.33
4	A	1106	NAP	O3B-C3B-C4B	5.63	127.25	111.08
4	D	1106	NAP	O5D-C5D-C4D	-5.62	89.85	108.99
4	D	1106	NAP	O3D-C3D-C2D	5.61	129.79	111.82
4	D	1106	NAP	O4B-C4B-C5B	5.59	127.24	109.33
4	D	1106	NAP	C5D-C4D-C3D	5.58	135.31	115.21
4	B	1106	NAP	O4B-C4B-C5B	5.56	127.15	109.33
5	D	1107	FNR	C7M-C7-C8	5.54	132.07	120.76
4	A	1106	NAP	N3A-C4A-N9A	5.52	136.55	127.17
4	A	1106	NAP	O2B-C2B-C1B	5.52	129.45	110.05
5	B	1108	FNR	C7M-C7-C8	5.48	131.96	120.76
4	D	1106	NAP	C5A-C4A-N3A	-5.45	119.21	126.72
4	D	1106	NAP	O3B-C3B-C4B	5.45	126.74	111.08
4	B	1106	NAP	C5A-C4A-N3A	-5.41	119.27	126.72
5	C	1107	FNR	C8M-C8-C9	-5.26	110.30	119.57
4	C	1106	NAP	N3A-C4A-N9A	5.14	135.91	127.17
4	C	1106	NAP	O2D-C2D-C3D	5.13	128.25	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1106	NAP	N3A-C2A-N1A	-5.05	120.94	128.58
5	A	1107	FNR	C4'-C3'-C2'	-5.02	105.21	113.57
5	B	1108	FNR	C8M-C8-C9	-4.99	110.78	119.57
4	C	1106	NAP	O3D-C3D-C2D	4.98	127.80	111.82
5	A	1107	FNR	C7M-C7-C8	4.92	130.80	120.76
5	A	1107	FNR	O3'-C3'-C2'	4.88	120.02	108.93
5	A	1107	FNR	C8M-C8-C9	-4.86	111.01	119.57
4	B	1106	NAP	N3A-C2A-N1A	-4.79	121.33	128.58
4	C	1106	NAP	N3A-C2A-N1A	-4.77	121.36	128.58
4	A	1106	NAP	O2D-C2D-C3D	4.75	127.04	111.82
4	D	1106	NAP	C6N-N1N-C1D	-4.67	110.57	119.73
4	D	1106	NAP	N3A-C4A-N9A	4.66	135.10	127.17
5	A	1107	FNR	O4'-C4'-C3'	-4.55	98.60	109.25
5	B	1108	FNR	C6-C7-C8	4.48	126.27	119.69
5	D	1107	FNR	C8M-C8-C9	-4.43	111.77	119.57
5	D	1107	FNR	O1P-P-O5'	-4.39	95.23	106.67
4	A	1106	NAP	O3D-C3D-C2D	4.39	125.88	111.82
5	C	1107	FNR	O3P-P-O5'	-4.38	95.24	106.67
4	A	1106	NAP	N3A-C2A-N1A	-4.32	122.05	128.58
5	B	1108	FNR	O4'-C4'-C3'	-4.30	99.20	109.25
5	A	1107	FNR	C6-C7-C8	4.29	125.98	119.69
5	D	1107	FNR	C6-C7-C8	4.27	125.95	119.69
5	C	1107	FNR	C6-C7-C8	4.22	125.88	119.69
4	B	1106	NAP	N3A-C4A-N9A	4.20	134.32	127.17
4	A	1106	NAP	P2B-O2B-C2B	-4.15	112.36	123.43
4	C	1106	NAP	O4D-C4D-C5D	4.10	122.47	109.33
4	A	1106	NAP	C5D-C4D-C3D	4.05	129.79	115.21
4	B	1106	NAP	C6N-N1N-C1D	-4.02	111.84	119.73
4	B	1106	NAP	O2D-C2D-C3D	4.02	124.69	111.82
4	D	1106	NAP	O2D-C2D-C3D	3.99	124.62	111.82
4	D	1106	NAP	O5B-C5B-C4B	-3.93	95.61	108.99
4	C	1106	NAP	P2B-O2B-C2B	-3.93	112.94	123.43
5	B	1108	FNR	O3'-C3'-C2'	3.90	117.79	108.93
4	C	1106	NAP	C2A-N3A-C4A	3.82	121.16	111.83
4	D	1106	NAP	C2N-N1N-C1D	3.76	127.44	119.13
4	D	1106	NAP	O2B-C2B-C3B	3.75	125.12	111.68
4	D	1106	NAP	C2A-N3A-C4A	3.75	120.98	111.83
4	A	1106	NAP	C2A-N3A-C4A	3.74	120.97	111.83
4	B	1106	NAP	C2A-N3A-C4A	3.73	120.95	111.83
4	A	1106	NAP	O2B-C2B-C3B	3.72	125.02	111.68
5	A	1107	FNR	C4A-C4-N3	3.59	121.99	112.13
5	C	1107	FNR	C4A-C4-N3	3.58	121.97	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1106	NAP	C1B-N9A-C8A	-3.57	119.18	127.09
4	A	1106	NAP	O4D-C4D-C5D	3.50	120.53	109.33
5	A	1107	FNR	C4-N3-C2	-3.48	121.58	126.37
5	A	1107	FNR	O5'-C5'-C4'	-3.45	100.14	109.36
4	B	1106	NAP	O4D-C4D-C3D	3.44	111.98	105.15
4	C	1106	NAP	C5D-C4D-C3D	3.39	127.42	115.21
5	D	1107	FNR	C4-N3-C2	-3.37	121.72	126.37
4	B	1106	NAP	O5B-C5B-C4B	-3.37	97.52	108.99
4	D	1106	NAP	C4D-O4D-C1D	3.37	113.01	109.92
5	B	1108	FNR	C4A-C4-N3	3.36	121.35	112.13
4	D	1106	NAP	C4A-N9A-C8A	3.35	109.26	105.74
5	D	1107	FNR	C4A-C4-N3	3.31	121.22	112.13
4	B	1106	NAP	O2B-C2B-C3B	3.30	123.53	111.68
5	C	1107	FNR	O4'-C4'-C3'	3.21	116.76	109.25
4	D	1106	NAP	N9A-C8A-N7A	-3.17	109.44	113.94
4	D	1106	NAP	O4D-C4D-C3D	3.11	111.33	105.15
4	B	1106	NAP	N9A-C8A-N7A	-3.09	109.55	113.94
5	D	1107	FNR	O4'-C4'-C3'	3.06	116.42	109.25
4	C	1106	NAP	C5N-C4N-C3N	-3.03	117.39	120.36
5	C	1107	FNR	C4-N3-C2	-3.00	122.24	126.37
5	C	1107	FNR	O4-C4-C4A	-3.00	120.03	127.26
4	A	1106	NAP	C5N-C4N-C3N	-2.99	117.43	120.36
4	B	1106	NAP	C4D-O4D-C1D	2.98	112.65	109.92
4	B	1106	NAP	C5A-N7A-C8A	2.97	108.12	103.45
5	B	1108	FNR	O4-C4-C4A	-2.94	120.16	127.26
5	D	1107	FNR	O3P-P-O5'	2.93	114.31	106.67
5	D	1107	FNR	O4-C4-C4A	-2.91	120.24	127.26
5	D	1107	FNR	O5'-C5'-C4'	-2.88	101.66	109.36
4	C	1106	NAP	C1B-N9A-C8A	-2.87	120.73	127.09
5	B	1108	FNR	C4-N3-C2	-2.83	122.47	126.37
4	B	1106	NAP	O4B-C4B-C3B	2.78	110.68	105.15
4	B	1106	NAP	C4A-C5A-N7A	-2.78	107.40	110.58
4	D	1106	NAP	C5A-N7A-C8A	2.77	107.81	103.45
4	D	1106	NAP	O4B-C4B-C3B	2.71	110.54	105.15
4	A	1106	NAP	C4A-N9A-C1B	2.69	132.92	126.63
4	B	1106	NAP	C2N-N1N-C1D	2.65	124.99	119.13
4	B	1106	NAP	C4A-N9A-C8A	2.65	108.52	105.74
5	A	1107	FNR	O3P-P-O5'	2.62	113.51	106.67
4	D	1106	NAP	O2A-PA-O3	2.58	114.25	107.27
4	C	1106	NAP	O2B-C2B-C3B	2.48	120.59	111.68
4	C	1106	NAP	O4D-C4D-C3D	2.47	110.05	105.15
5	B	1108	FNR	O5'-C5'-C4'	-2.46	102.81	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1107	FNR	O5'-P-O2P	2.44	113.03	106.44
4	D	1106	NAP	C4A-C5A-N7A	-2.43	107.80	110.58
4	A	1106	NAP	C5A-N7A-C8A	2.41	107.23	103.45
4	B	1106	NAP	O7N-C7N-N7N	-2.39	119.16	122.62
4	C	1106	NAP	C6N-N1N-C1D	-2.35	115.11	119.73
5	A	1107	FNR	O4-C4-C4A	-2.34	121.61	127.26
4	C	1106	NAP	O4B-C4B-C3B	2.31	109.74	105.15
5	D	1107	FNR	O4'-C4'-C5'	-2.30	104.91	109.99
5	A	1107	FNR	C4-C4A-N5	2.27	122.18	116.37
5	D	1107	FNR	N3-C2-N1	2.24	119.26	115.74
4	A	1106	NAP	O4D-C4D-C3D	2.24	109.60	105.15
4	A	1106	NAP	C4D-O4D-C1D	2.22	111.96	109.92
5	D	1107	FNR	C1'-C2'-C3'	-2.21	103.67	109.66
4	A	1106	NAP	O4B-C4B-C3B	2.19	109.51	105.15
4	C	1106	NAP	C4A-N9A-C1B	2.18	131.72	126.63
4	A	1106	NAP	C5B-C4B-C3B	2.17	123.02	115.21
4	D	1106	NAP	O3X-P2B-O2B	2.12	114.13	105.85
4	C	1106	NAP	C5A-N7A-C8A	2.12	106.79	103.45
4	B	1106	NAP	P2B-O2B-C2B	-2.11	117.81	123.43
4	A	1106	NAP	N9A-C8A-N7A	-2.10	110.96	113.94
4	B	1106	NAP	O2A-PA-O3	2.06	112.84	107.27
5	D	1107	FNR	C4'-C3'-C2'	-2.06	110.15	113.57
5	B	1108	FNR	C2'-C1'-N10	-2.04	100.54	110.20
4	A	1106	NAP	C4A-N9A-C8A	2.04	107.88	105.74
4	C	1106	NAP	O5D-C5D-C4D	-2.02	102.11	108.99

All (32) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1106	NAP	C2B
4	A	1106	NAP	C4B
4	A	1106	NAP	C4D
4	A	1106	NAP	C3D
4	A	1106	NAP	C1D
4	A	1106	NAP	C1B
4	A	1106	NAP	C2D
4	A	1106	NAP	C3B
4	B	1106	NAP	C2B
4	B	1106	NAP	C4B
4	B	1106	NAP	C4D
4	B	1106	NAP	C3D
4	B	1106	NAP	C1D

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Mol	Chain	Res	Type	Atom
4	B	1106	NAP	C1B
4	B	1106	NAP	C2D
4	B	1106	NAP	C3B
4	C	1106	NAP	C2B
4	C	1106	NAP	C4B
4	C	1106	NAP	C4D
4	C	1106	NAP	C3D
4	C	1106	NAP	C1D
4	C	1106	NAP	C1B
4	C	1106	NAP	C2D
4	C	1106	NAP	C3B
4	D	1106	NAP	C2B
4	D	1106	NAP	C4B
4	D	1106	NAP	C4D
4	D	1106	NAP	C3D
4	D	1106	NAP	C1D
4	D	1106	NAP	C1B
4	D	1106	NAP	C2D
4	D	1106	NAP	C3B

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1105	FAD	PA-O3P-P-O5'
3	C	1105	FAD	PA-O3P-P-O5'
4	A	1106	NAP	C5B-O5B-PA-O2A
4	A	1106	NAP	O4B-C4B-C5B-O5B
4	A	1106	NAP	PA-O3-PN-O5D
4	A	1106	NAP	C4D-C5D-O5D-PN
4	A	1106	NAP	C2D-C1D-N1N-C2N
4	A	1106	NAP	C2D-C1D-N1N-C6N
4	B	1106	NAP	C5B-O5B-PA-O1A
4	B	1106	NAP	C5B-O5B-PA-O2A
4	B	1106	NAP	C5B-O5B-PA-O3
4	B	1106	NAP	O4D-C4D-C5D-O5D
4	B	1106	NAP	O4D-C1D-N1N-C2N
4	B	1106	NAP	O4D-C1D-N1N-C6N
4	C	1106	NAP	C5B-O5B-PA-O1A
4	C	1106	NAP	C5B-O5B-PA-O2A
4	C	1106	NAP	O4B-C4B-C5B-O5B
4	C	1106	NAP	C4D-C5D-O5D-PN
4	C	1106	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	C	1106	NAP	C2D-C1D-N1N-C6N
4	D	1106	NAP	C5B-O5B-PA-O1A
4	D	1106	NAP	C5B-O5B-PA-O2A
4	D	1106	NAP	C5B-O5B-PA-O3
4	D	1106	NAP	O4D-C4D-C5D-O5D
4	D	1106	NAP	O4D-C1D-N1N-C2N
4	D	1106	NAP	O4D-C1D-N1N-C6N
5	A	1107	FNR	N10-C1'-C2'-O2'
5	A	1107	FNR	N10-C1'-C2'-C3'
5	A	1107	FNR	C1'-C2'-C3'-O3'
5	A	1107	FNR	C1'-C2'-C3'-C4'
5	A	1107	FNR	O2'-C2'-C3'-C4'
5	A	1107	FNR	C3'-C4'-C5'-O5'
5	A	1107	FNR	O4'-C4'-C5'-O5'
5	B	1108	FNR	N10-C1'-C2'-O2'
5	B	1108	FNR	N10-C1'-C2'-C3'
5	B	1108	FNR	C1'-C2'-C3'-O3'
5	B	1108	FNR	C1'-C2'-C3'-C4'
5	B	1108	FNR	O2'-C2'-C3'-O3'
5	B	1108	FNR	O2'-C2'-C3'-C4'
5	B	1108	FNR	C3'-C4'-C5'-O5'
5	B	1108	FNR	O4'-C4'-C5'-O5'
5	C	1107	FNR	C2'-C3'-C4'-O4'
5	C	1107	FNR	O3'-C3'-C4'-O4'
5	C	1107	FNR	C5'-O5'-P-O2P
5	C	1107	FNR	C5'-O5'-P-O3P
5	D	1107	FNR	C2'-C3'-C4'-O4'
5	D	1107	FNR	C2'-C3'-C4'-C5'
5	D	1107	FNR	O3'-C3'-C4'-O4'
5	C	1107	FNR	O3'-C3'-C4'-C5'
5	D	1107	FNR	O3'-C3'-C4'-C5'
5	C	1107	FNR	C2'-C3'-C4'-C5'
4	C	1106	NAP	C3B-C2B-O2B-P2B
5	A	1107	FNR	O2'-C2'-C3'-O3'
4	B	1106	NAP	O4B-C4B-C5B-O5B
4	D	1106	NAP	O4B-C4B-C5B-O5B
4	A	1106	NAP	C3B-C2B-O2B-P2B
4	B	1106	NAP	C3B-C2B-O2B-P2B
4	D	1106	NAP	C3B-C2B-O2B-P2B
4	B	1106	NAP	C3D-C4D-C5D-O5D
4	C	1106	NAP	O4D-C4D-C5D-O5D
4	A	1106	NAP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
5	A	1107	FNR	O3'-C3'-C4'-C5'
3	B	1105	FAD	PA-O3P-P-O5'
3	D	1105	FAD	PA-O3P-P-O5'
4	B	1106	NAP	PA-O3-PN-O5D
4	D	1106	NAP	PA-O3-PN-O5D
4	D	1106	NAP	C3D-C4D-C5D-O5D
3	D	1105	FAD	C2B-C1B-N9A-C8A
4	B	1106	NAP	PN-O3-PA-O2A
4	D	1106	NAP	PN-O3-PA-O2A
5	C	1107	FNR	O4'-C4'-C5'-O5'
4	A	1106	NAP	C5B-O5B-PA-O1A
4	A	1106	NAP	C5B-O5B-PA-O3
4	C	1106	NAP	C5B-O5B-PA-O3
4	A	1106	NAP	C2B-O2B-P2B-O2X
5	C	1107	FNR	C4'-C5'-O5'-P
4	B	1106	NAP	C4D-C5D-O5D-PN
4	D	1106	NAP	C4D-C5D-O5D-PN
3	C	1105	FAD	C2B-C1B-N9A-C8A
4	A	1106	NAP	C3D-C4D-C5D-O5D
3	B	1105	FAD	C2B-C1B-N9A-C8A
4	B	1106	NAP	PN-O3-PA-O1A
5	A	1107	FNR	O3'-C3'-C4'-O4'
4	C	1106	NAP	C2B-O2B-P2B-O3X
3	A	1105	FAD	C2B-C1B-N9A-C8A
3	D	1105	FAD	C2B-C1B-N9A-C4A
5	B	1108	FNR	O3'-C3'-C4'-C5'
4	D	1106	NAP	PN-O3-PA-O1A
3	A	1105	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

13 monomers are involved in 55 short contacts:

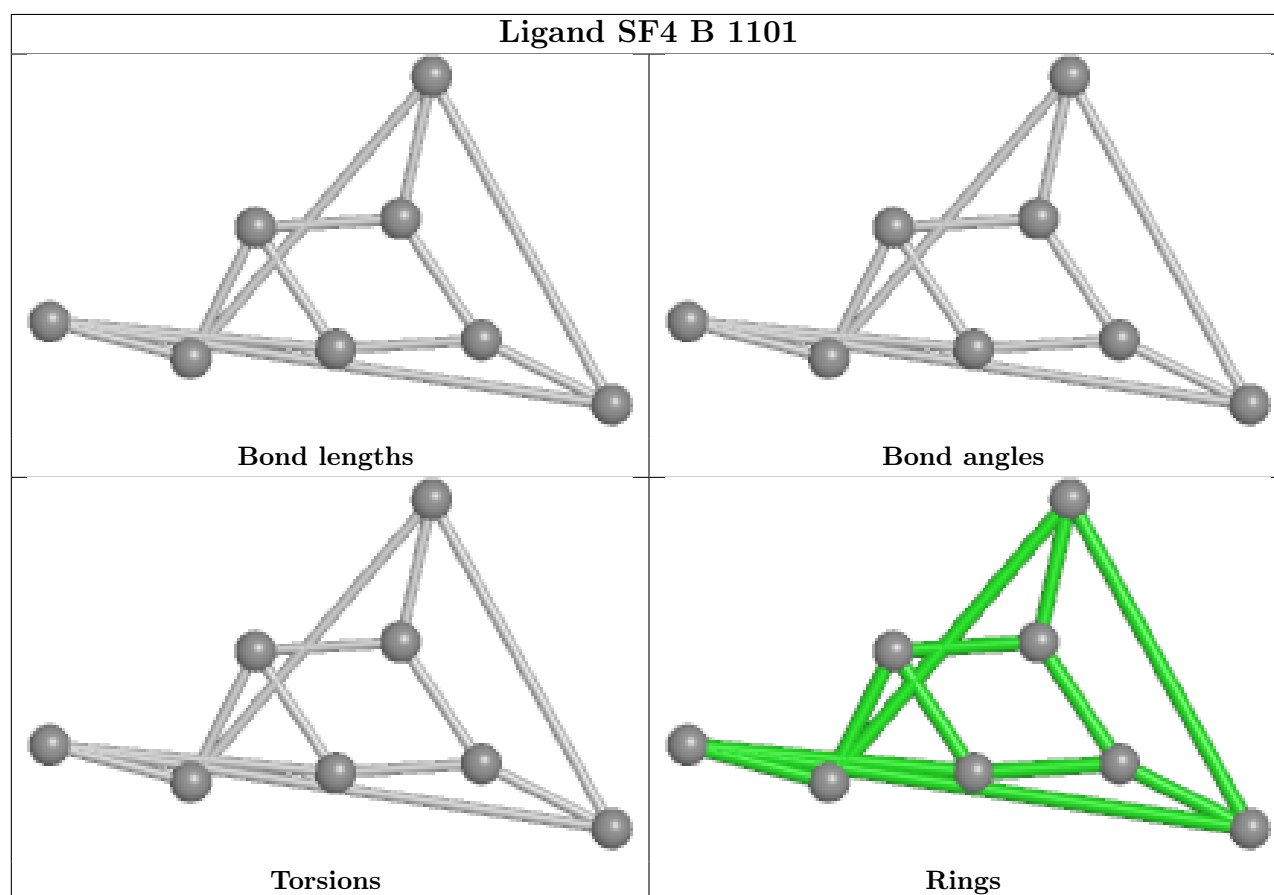
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1105	FAD	2	0
5	A	1107	FNR	6	0
4	A	1106	NAP	8	0
4	C	1106	NAP	11	0
4	B	1106	NAP	9	0
3	A	1105	FAD	4	0
5	C	1107	FNR	2	0
6	B	1107	TDR	1	0
3	B	1105	FAD	3	0

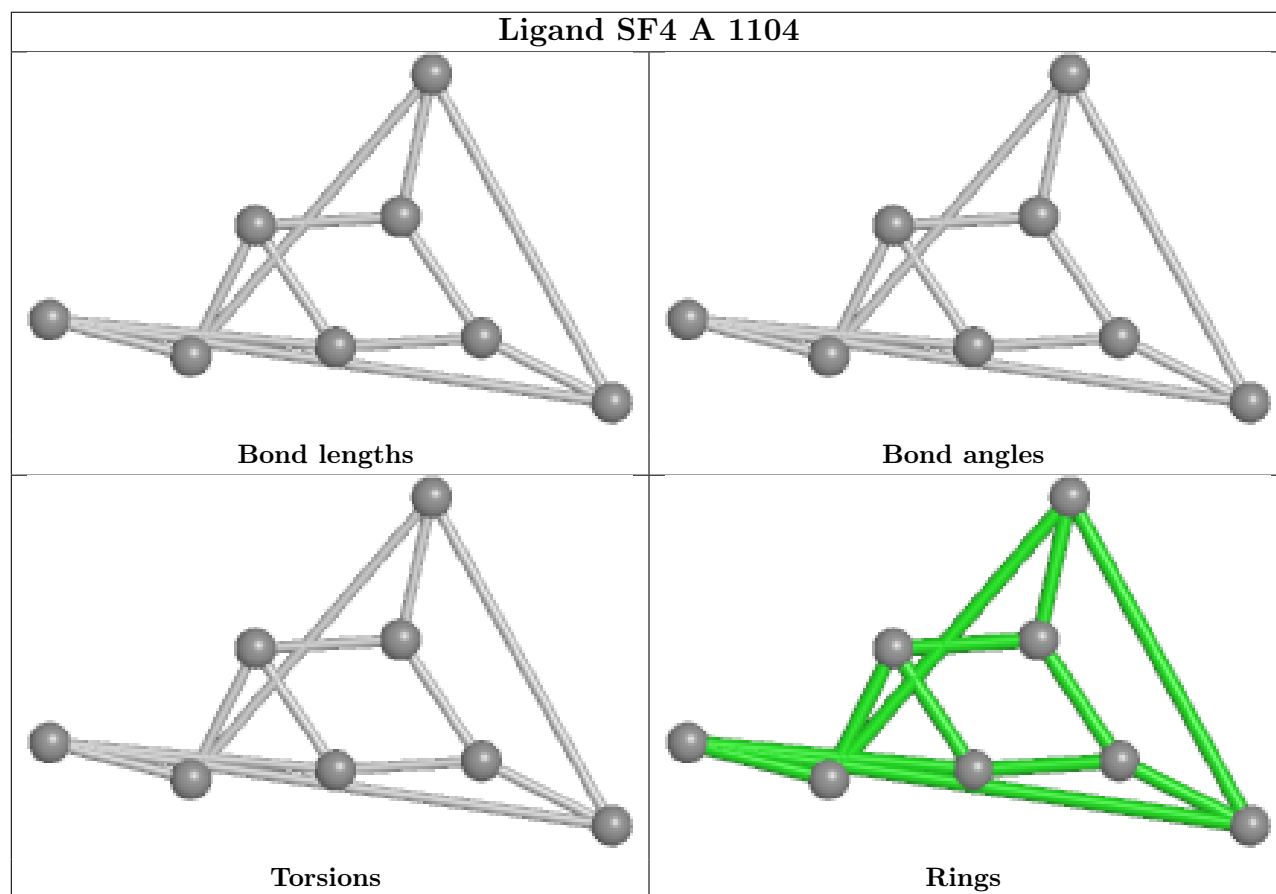
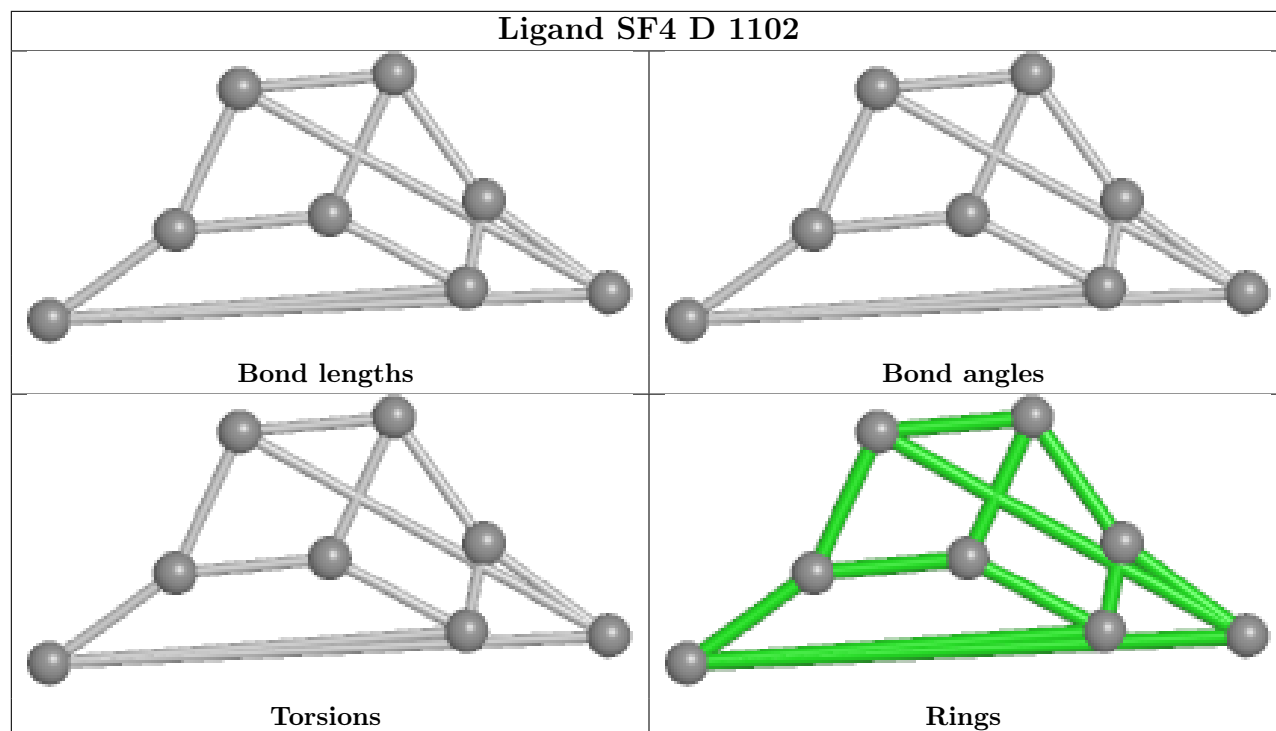
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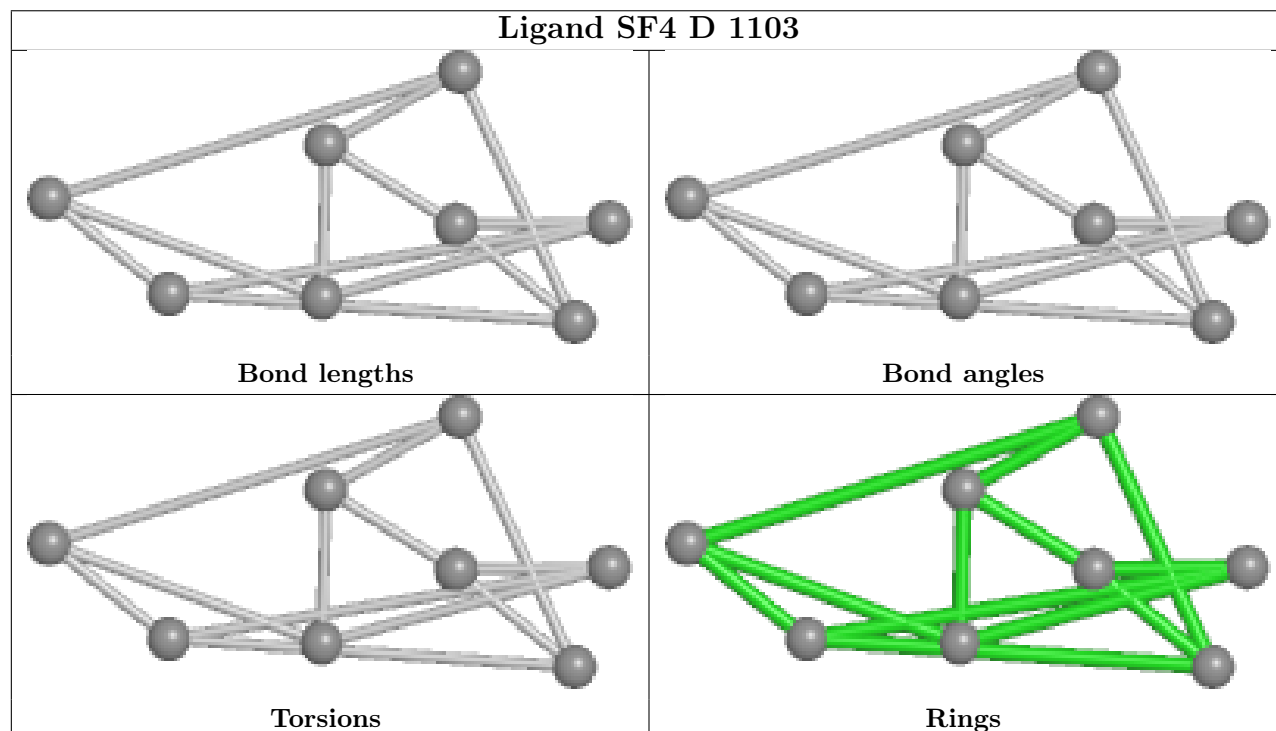
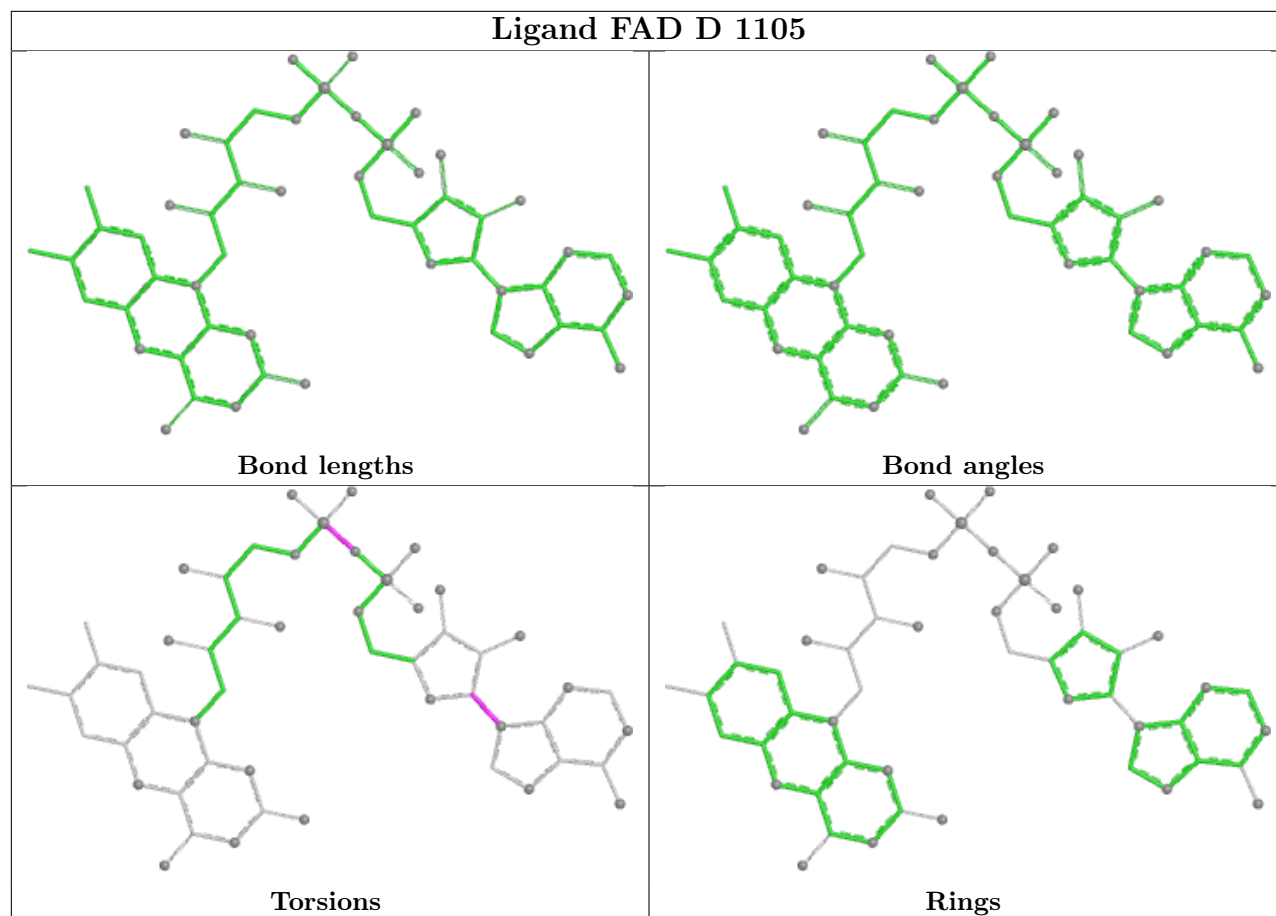
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1106	NAP	7	0
5	D	1107	FNR	3	0
5	B	1108	FNR	5	0
3	C	1105	FAD	2	0

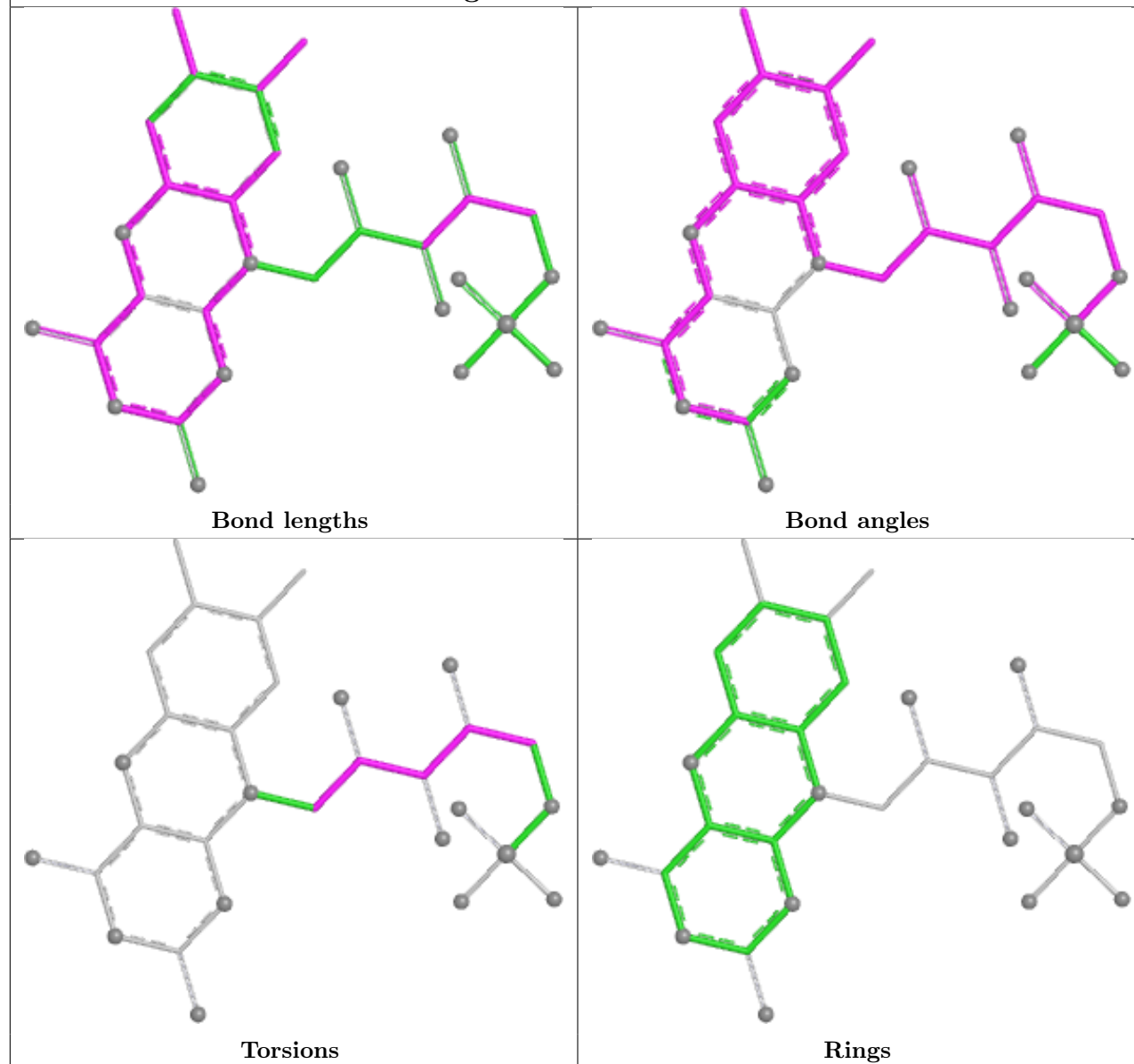
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

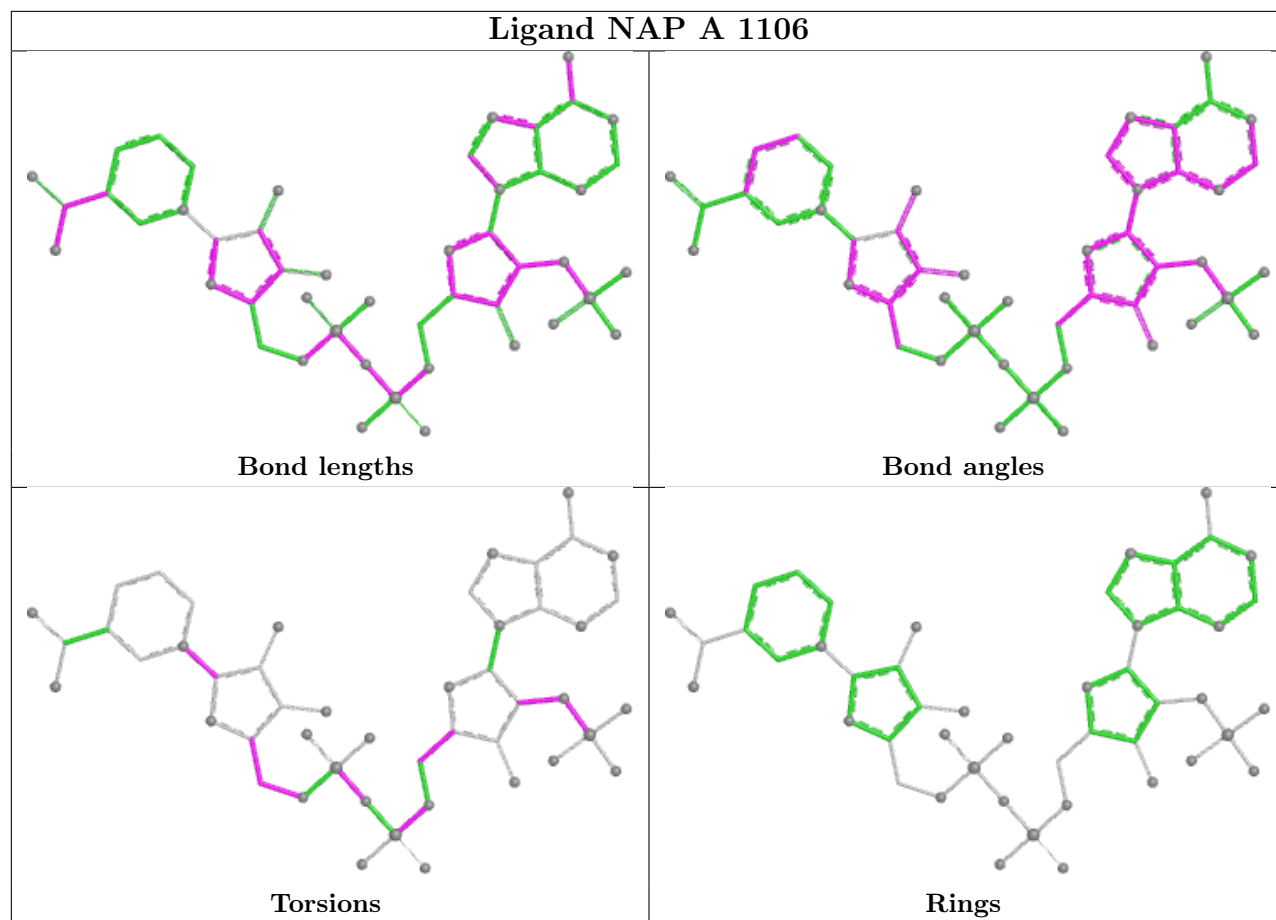


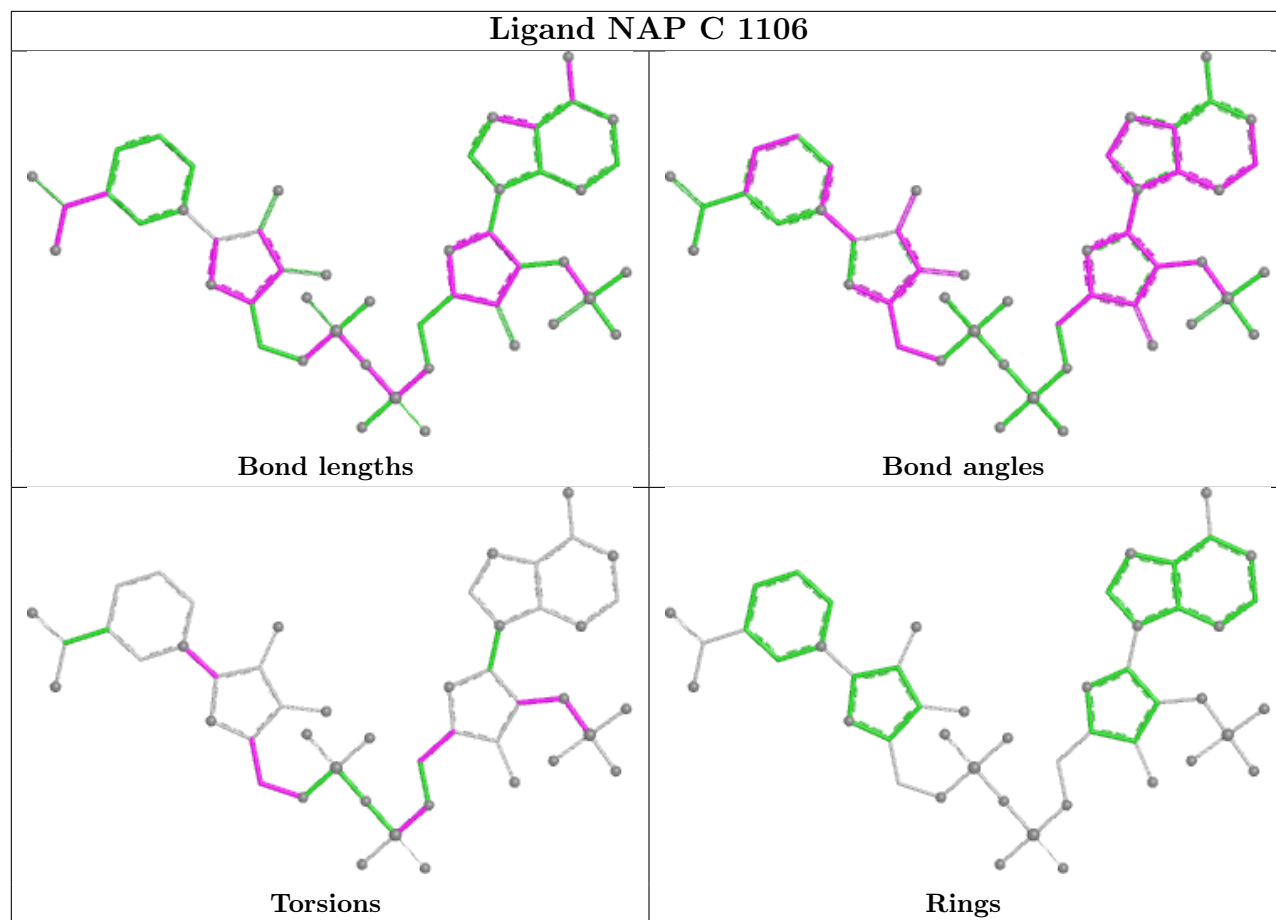




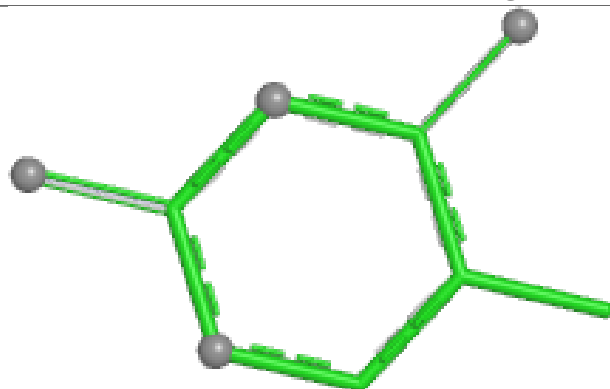
Ligand FNR A 1107



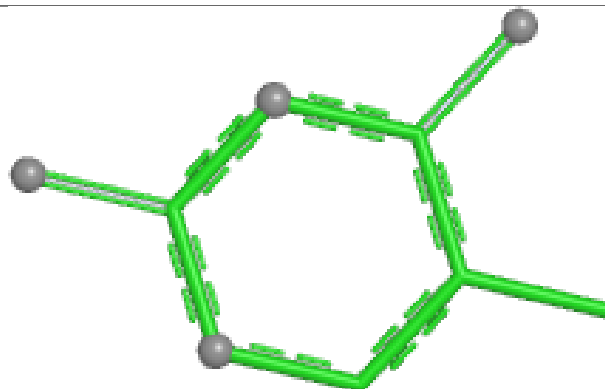




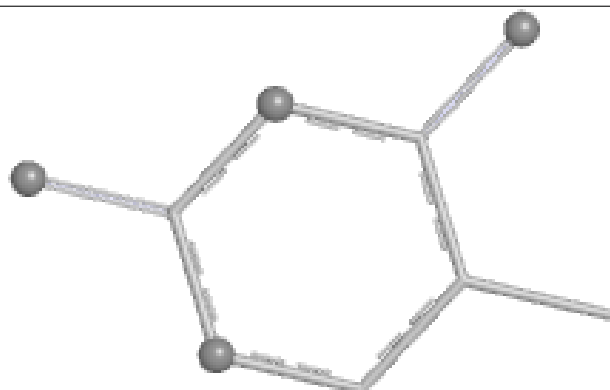
Ligand TDR C 1108



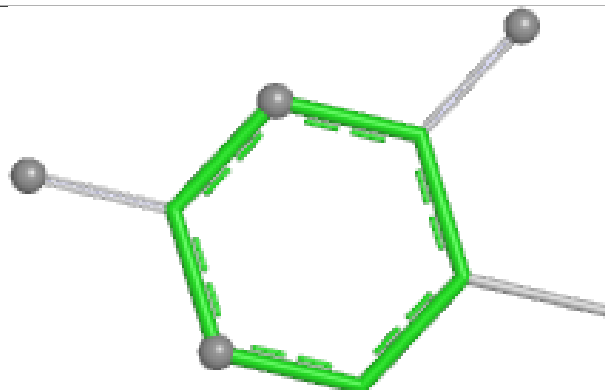
Bond lengths



Bond angles

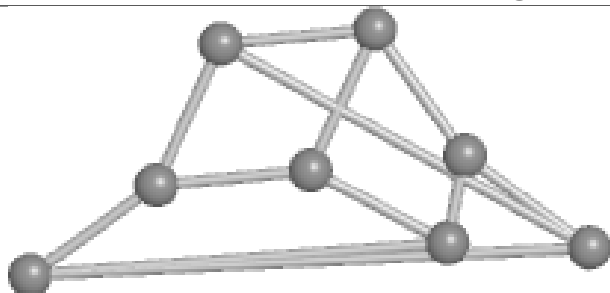


Torsions

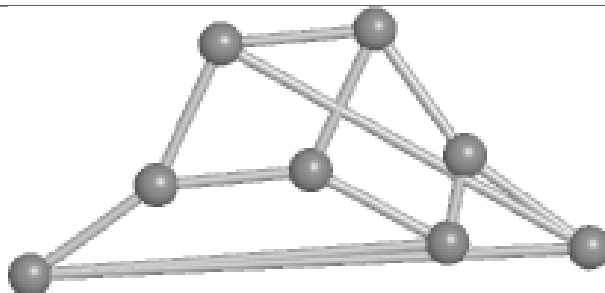


Rings

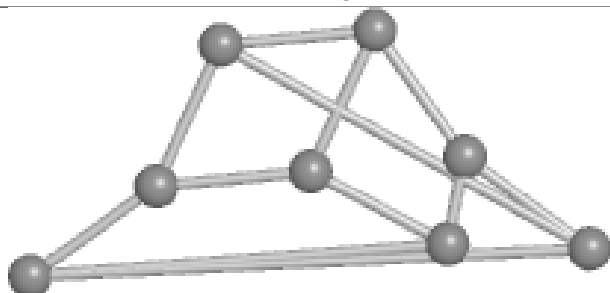
Ligand SF4 D 1101



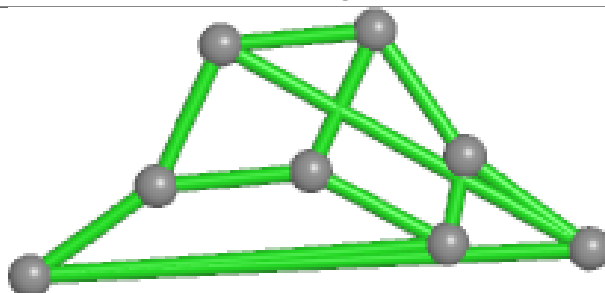
Bond lengths



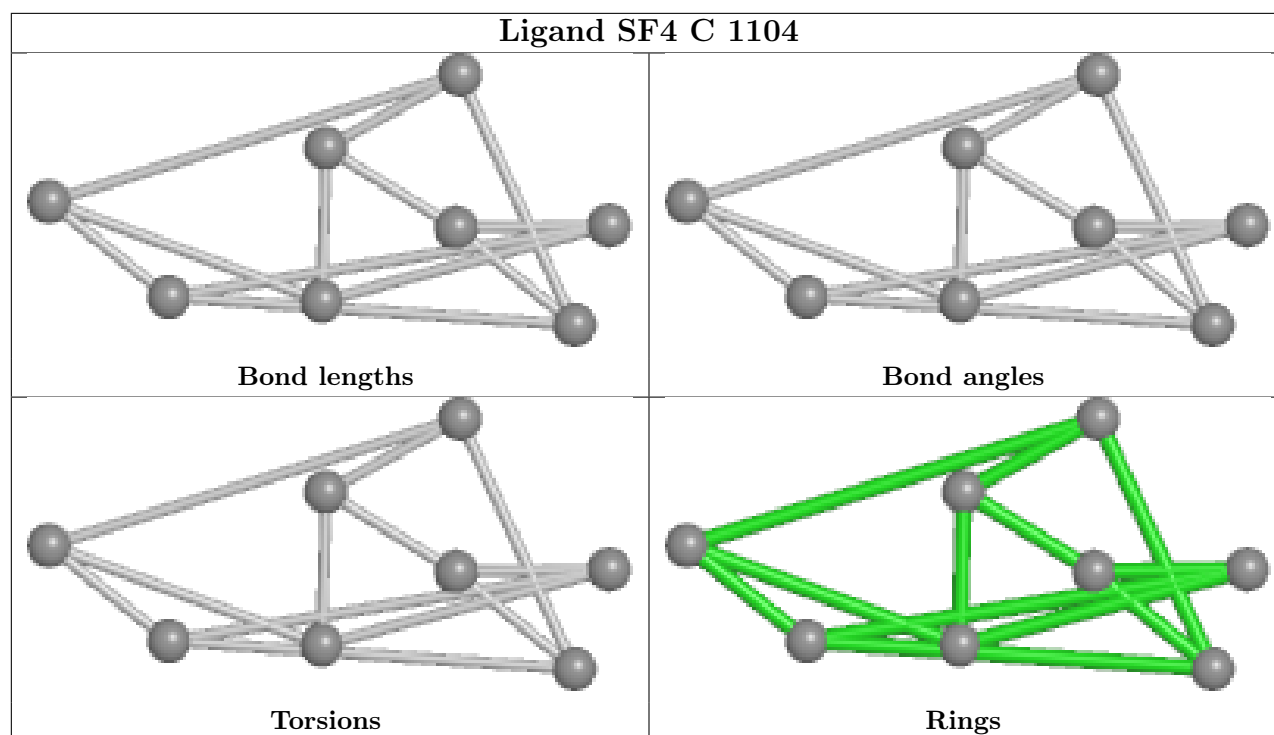
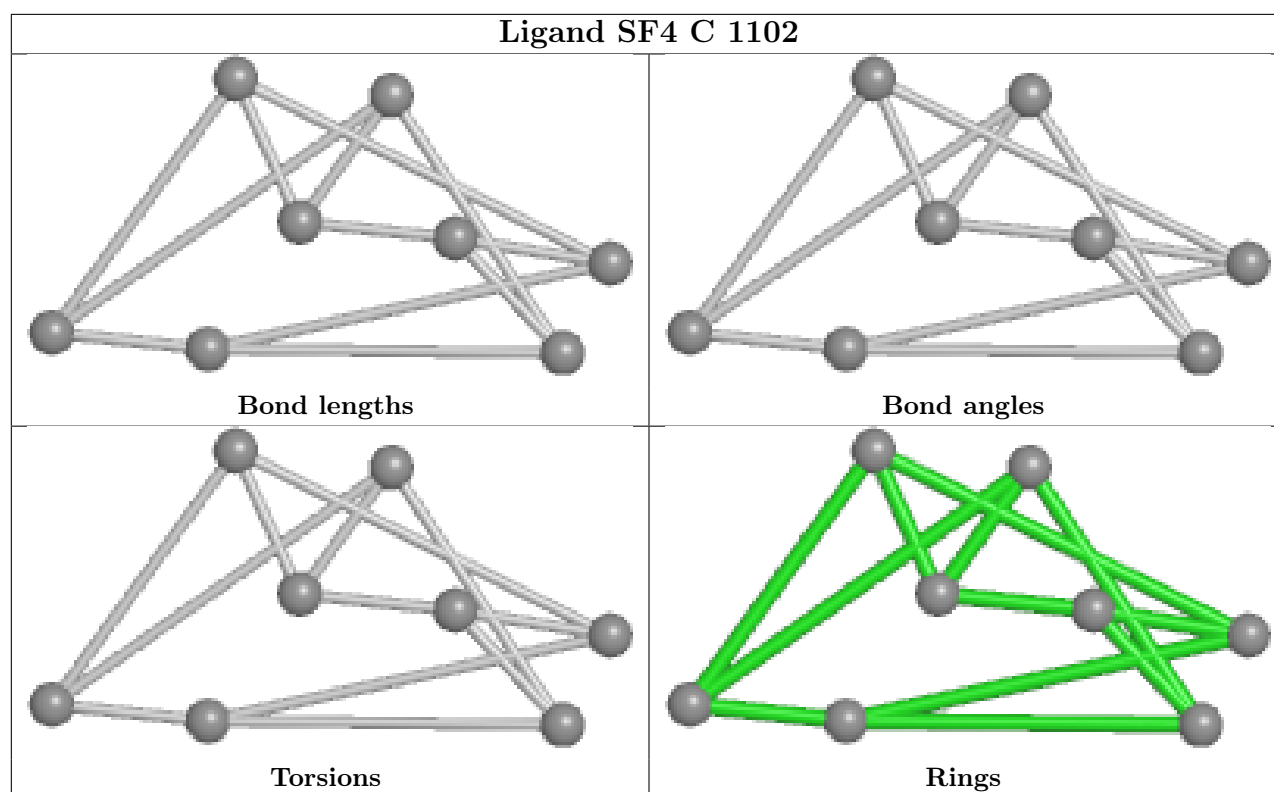
Bond angles

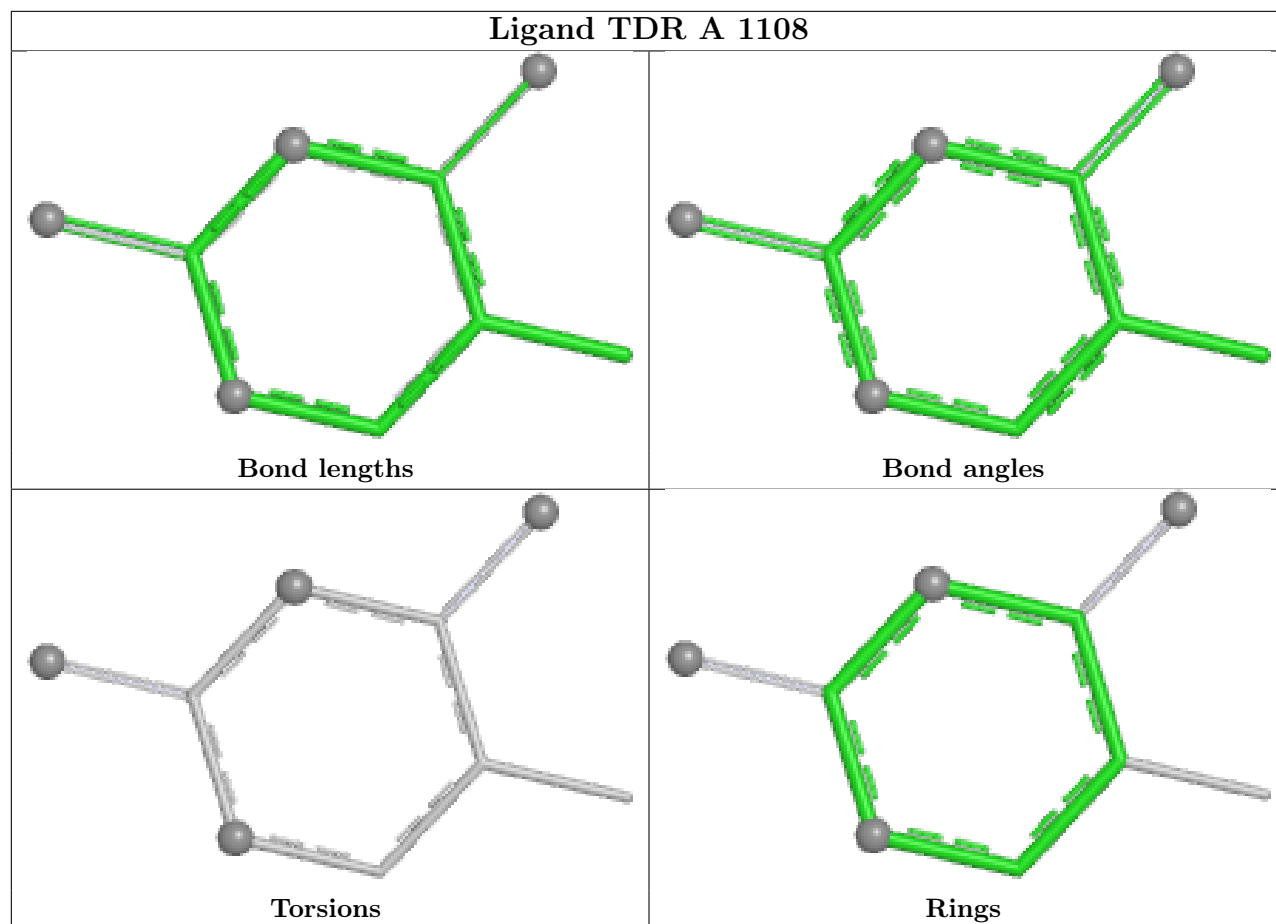


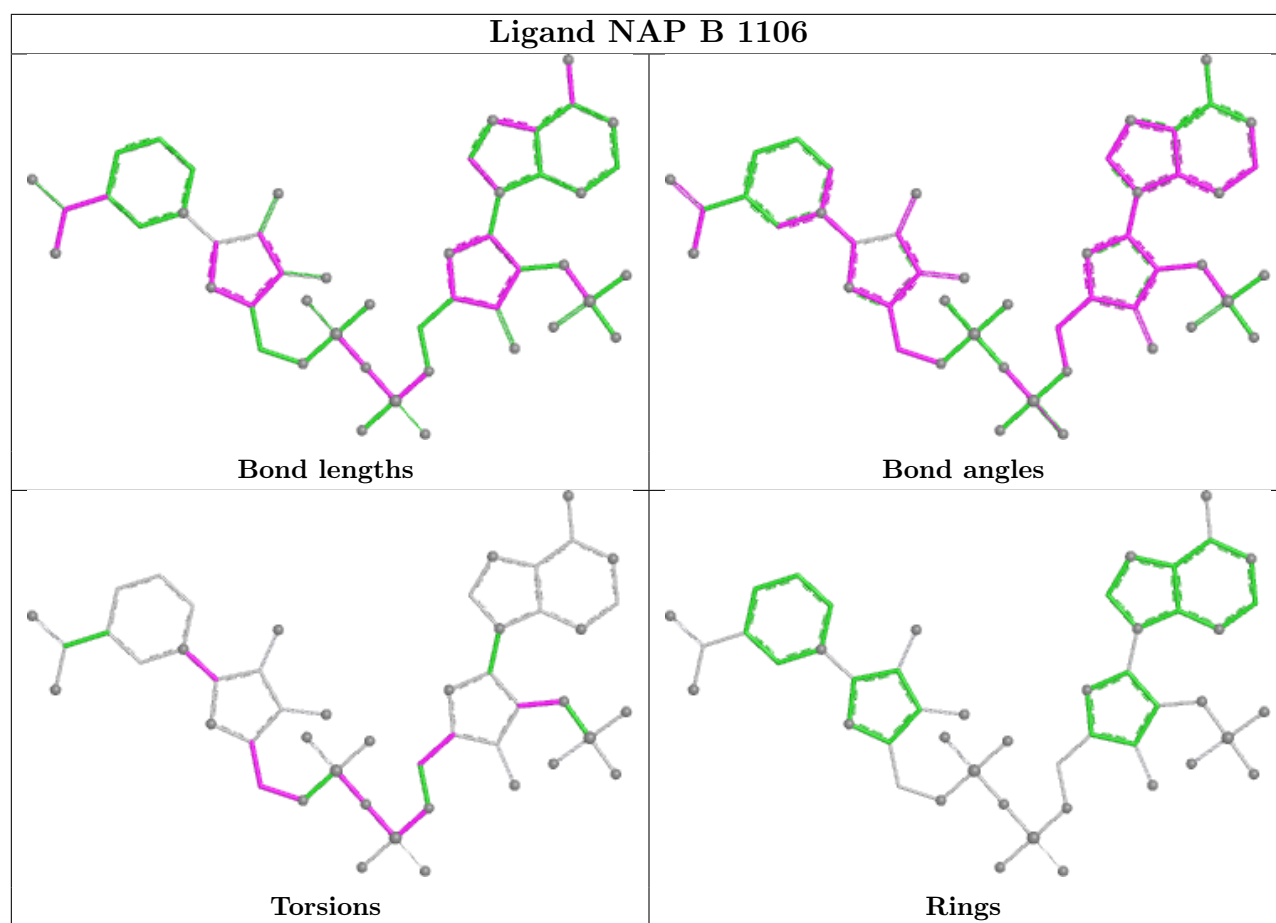
Torsions

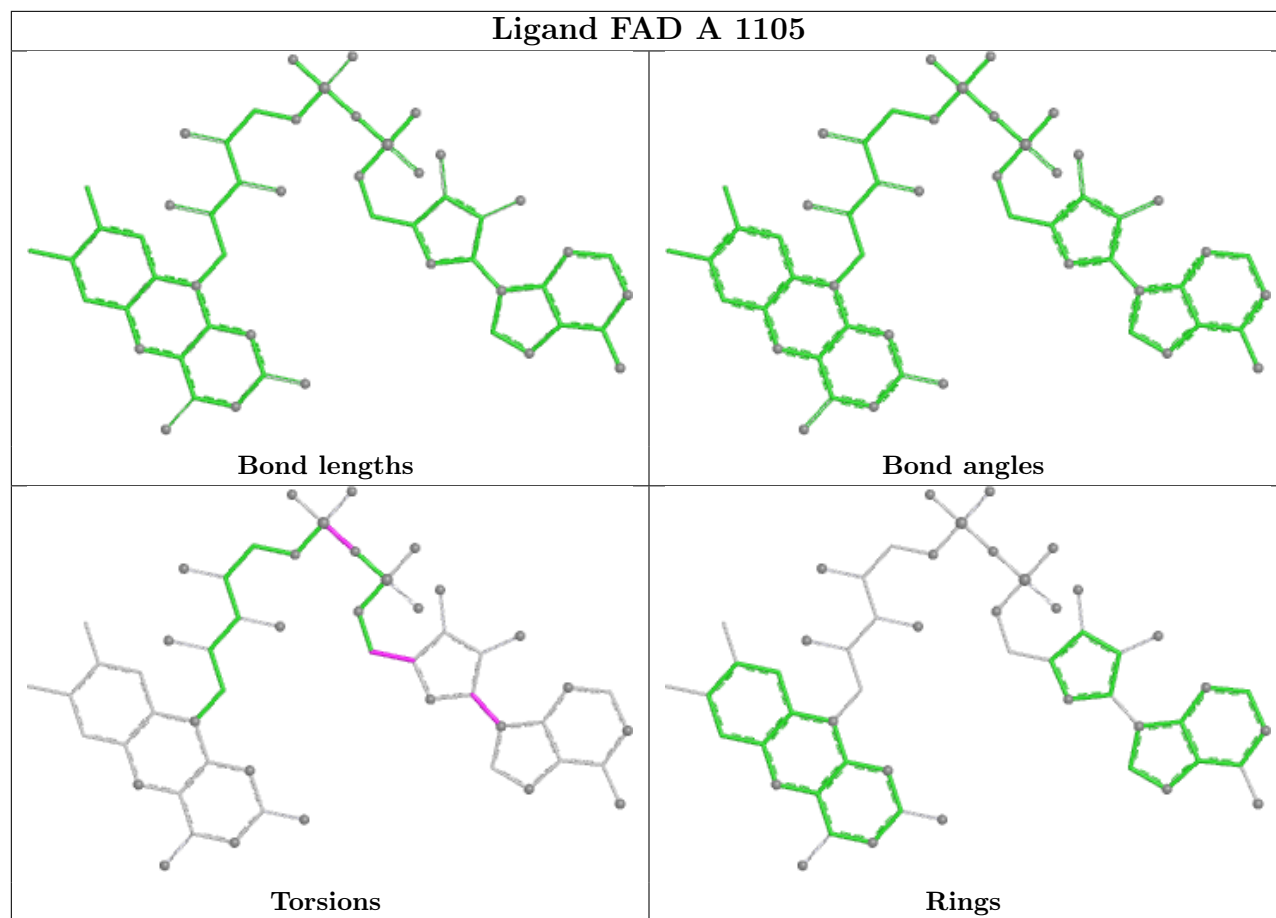


Rings

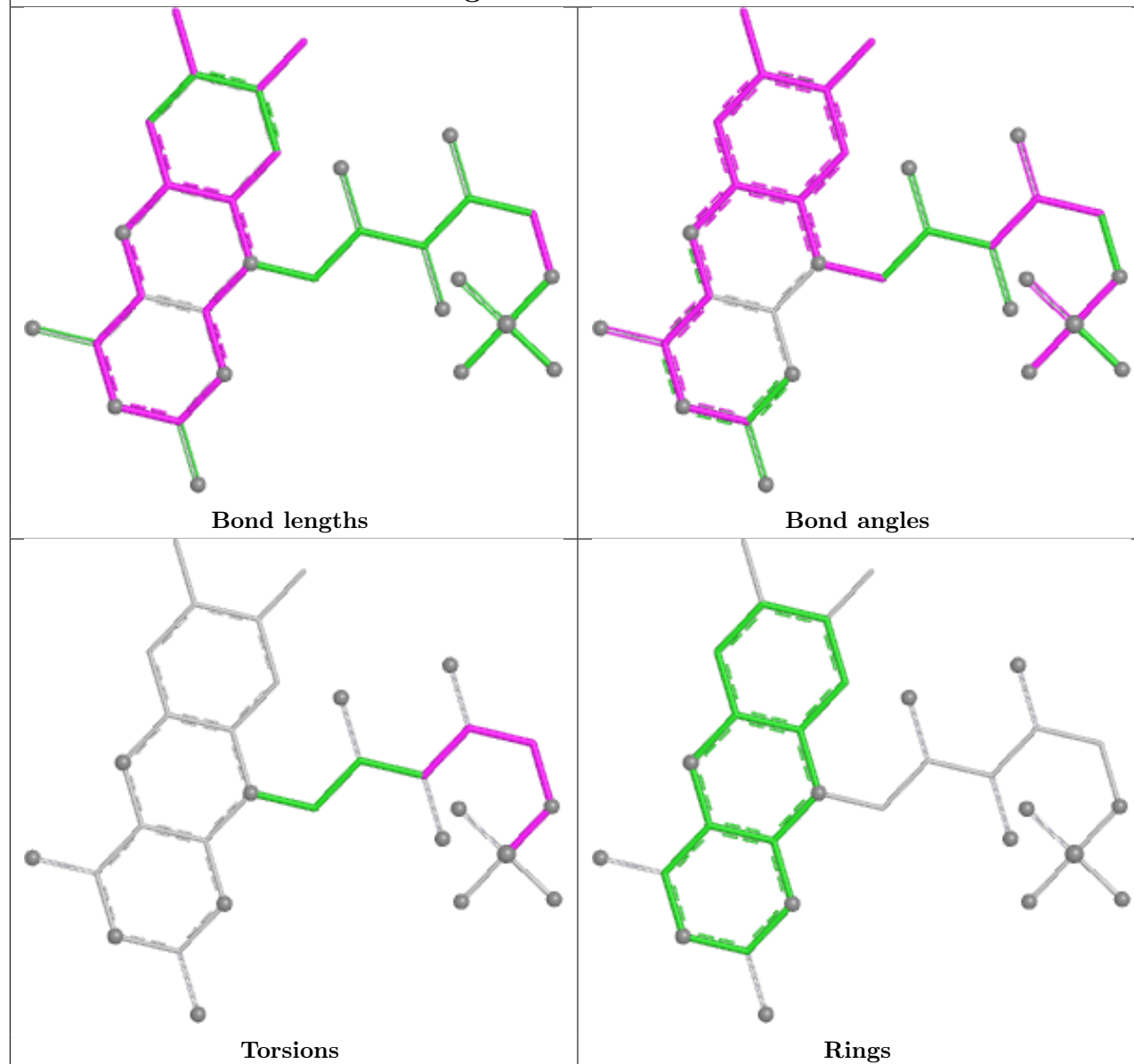




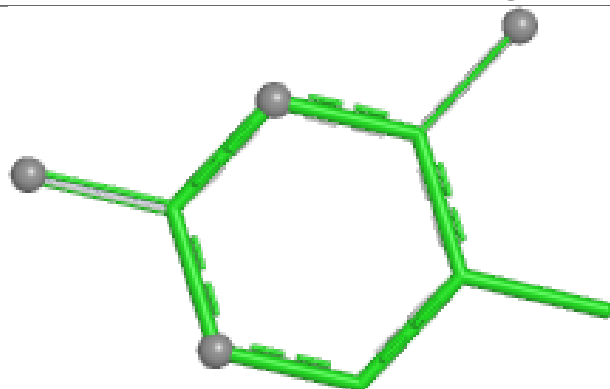




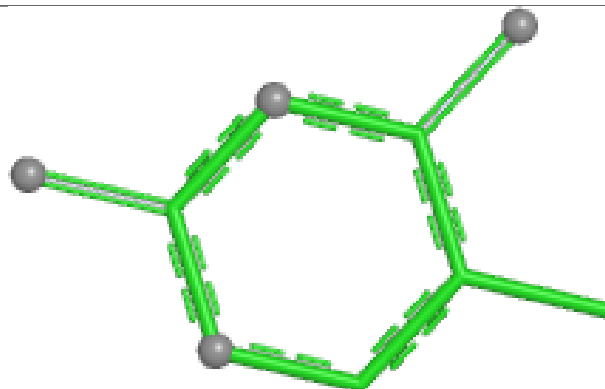
Ligand FNR C 1107



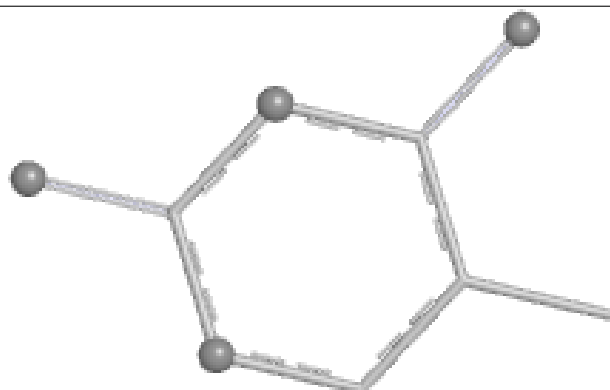
Ligand TDR B 1107



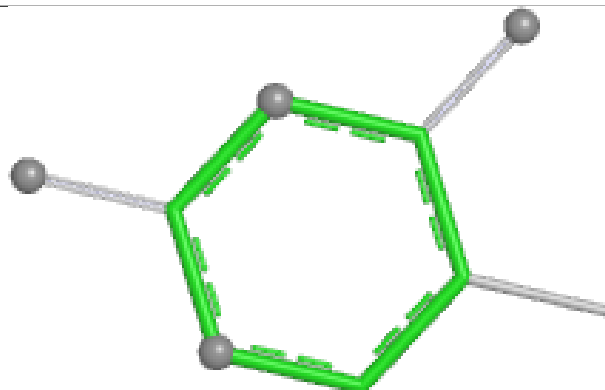
Bond lengths



Bond angles

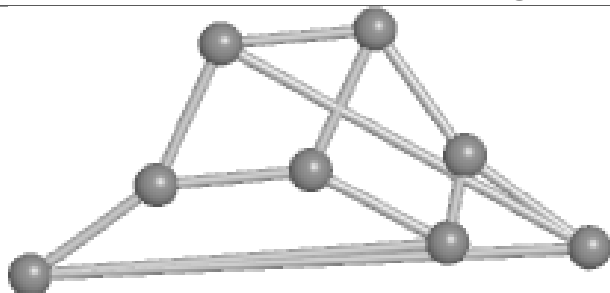


Torsions

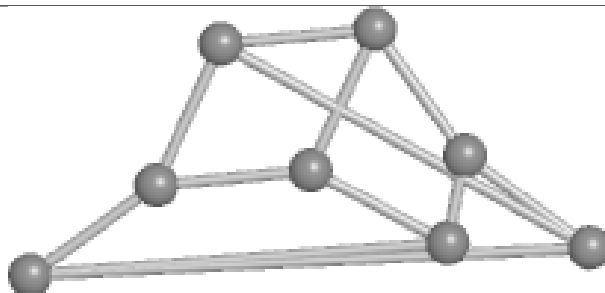


Rings

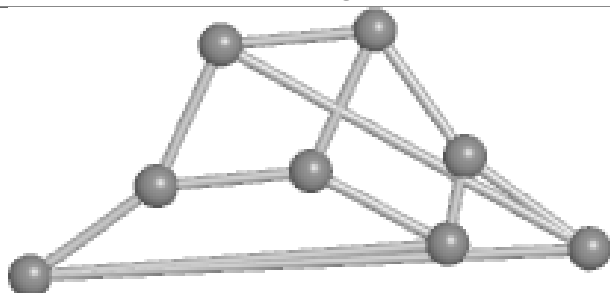
Ligand SF4 D 1104



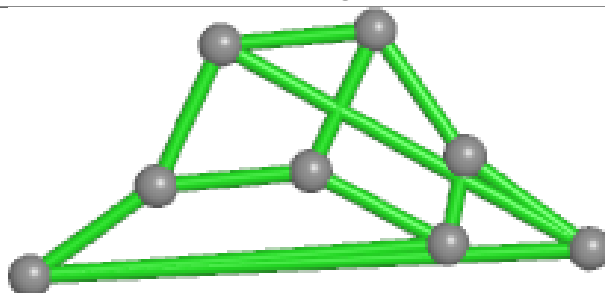
Bond lengths



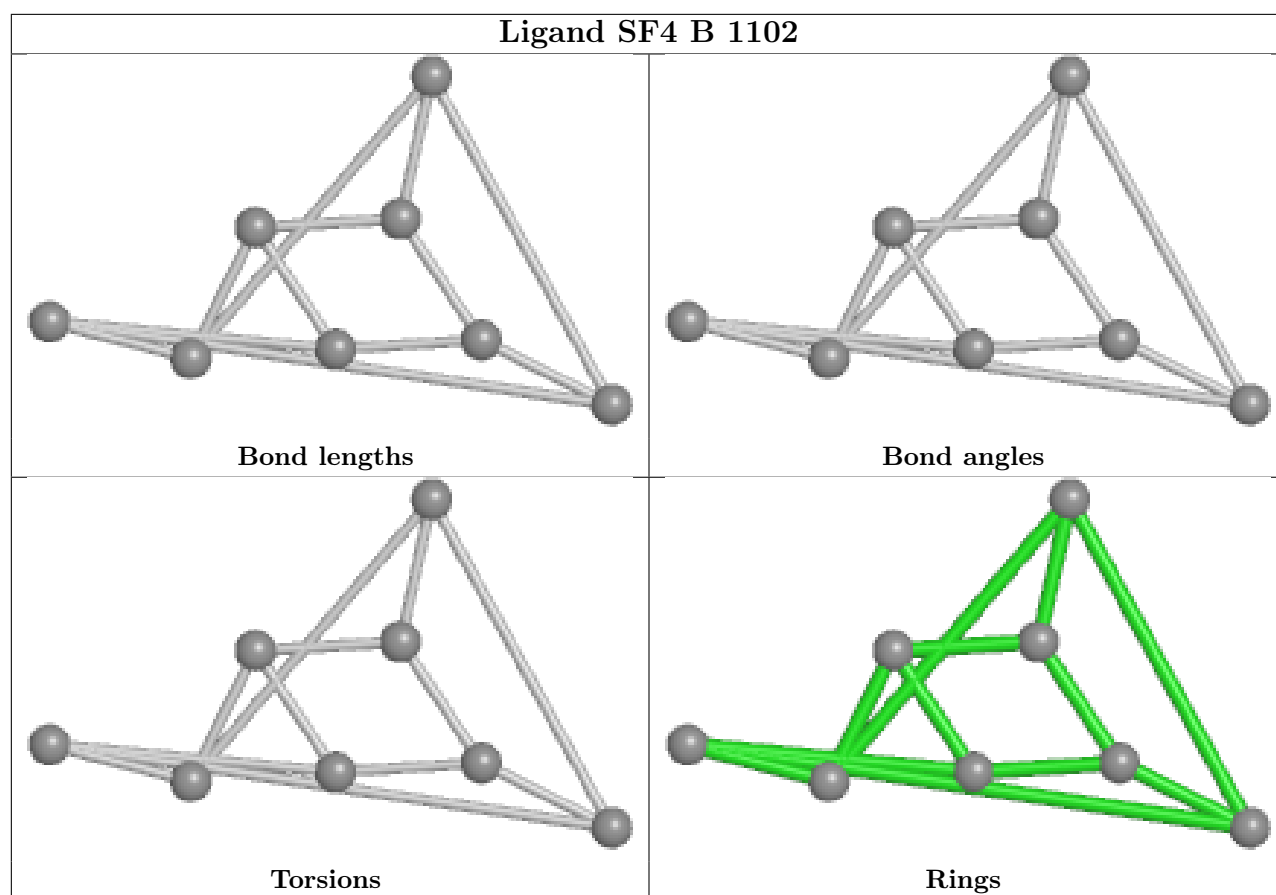
Bond angles

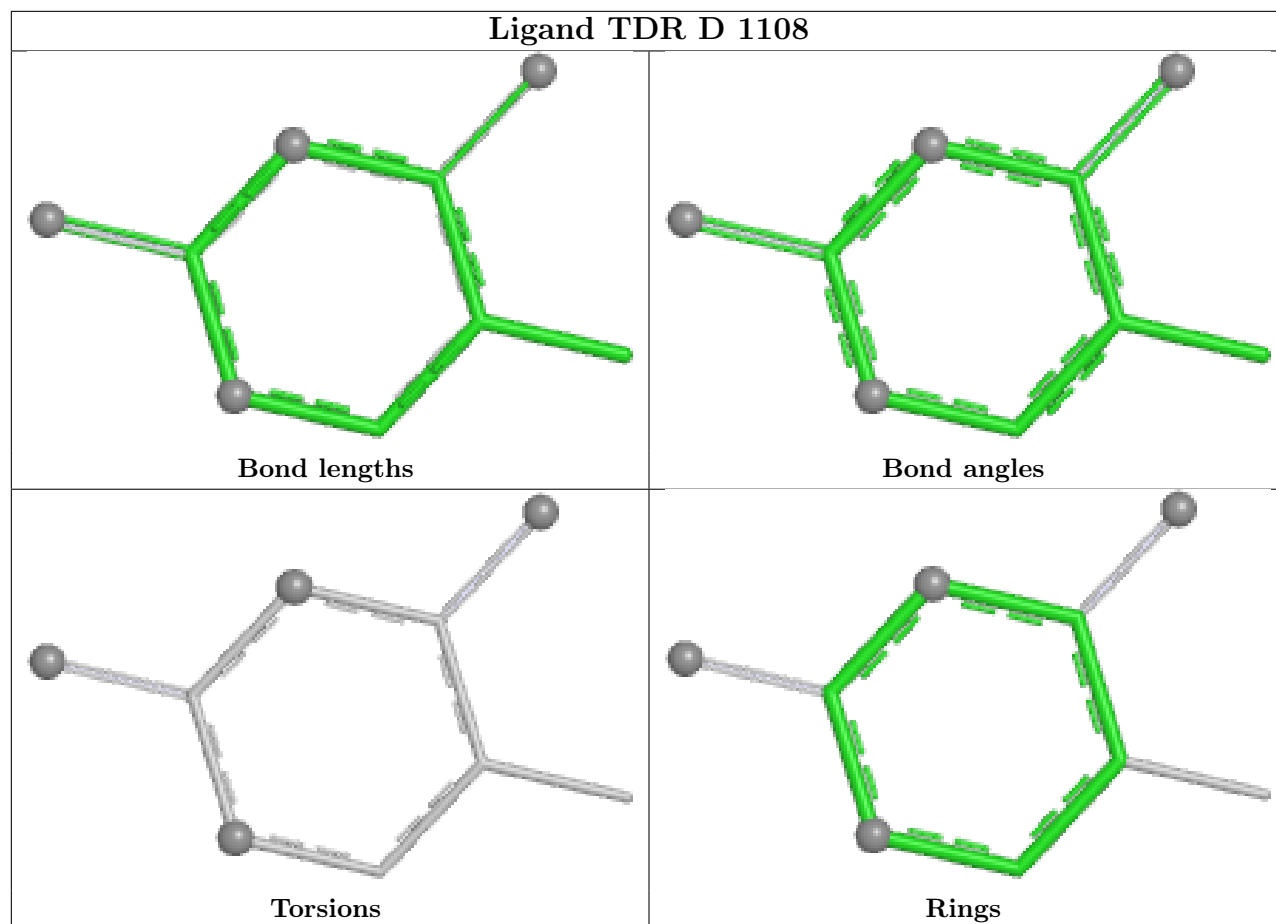


Torsions

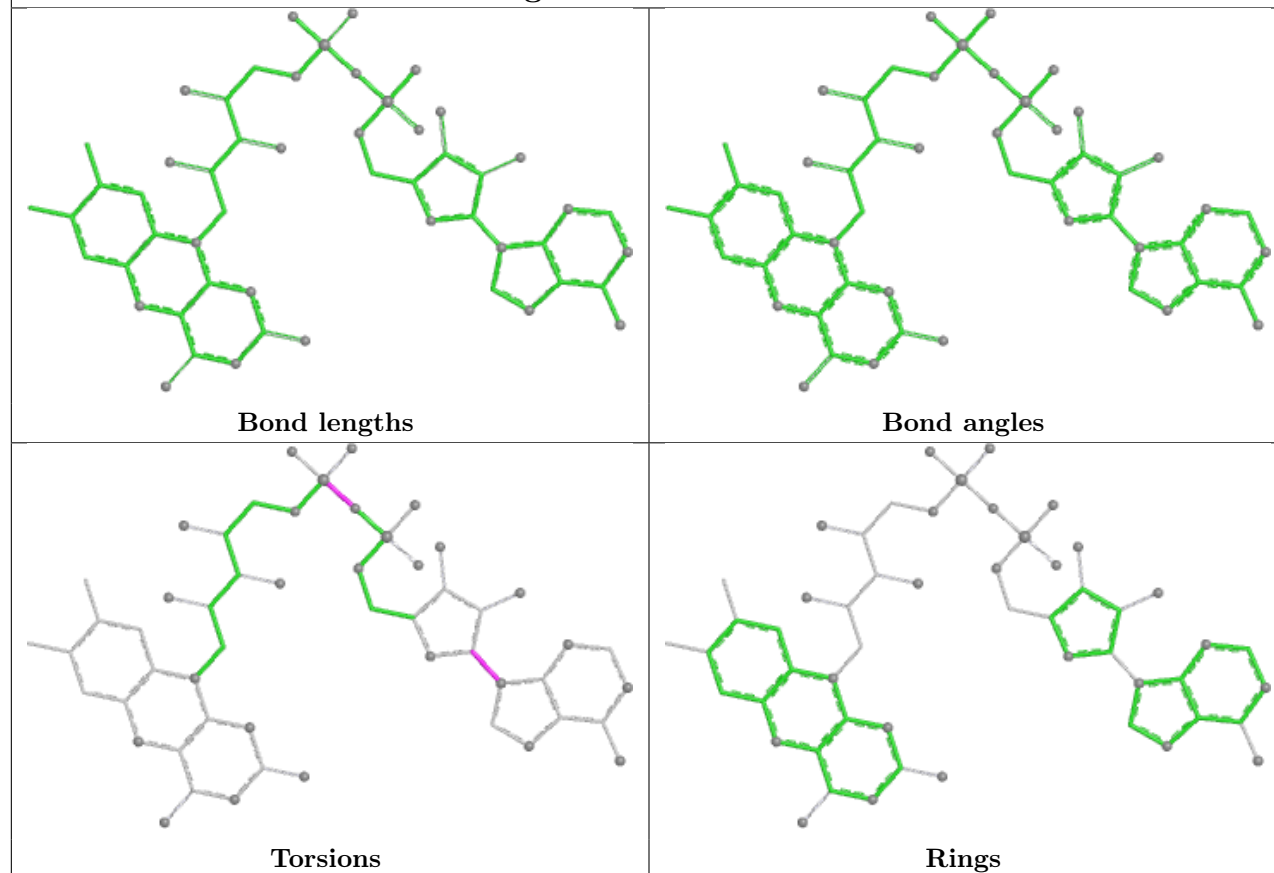


Rings

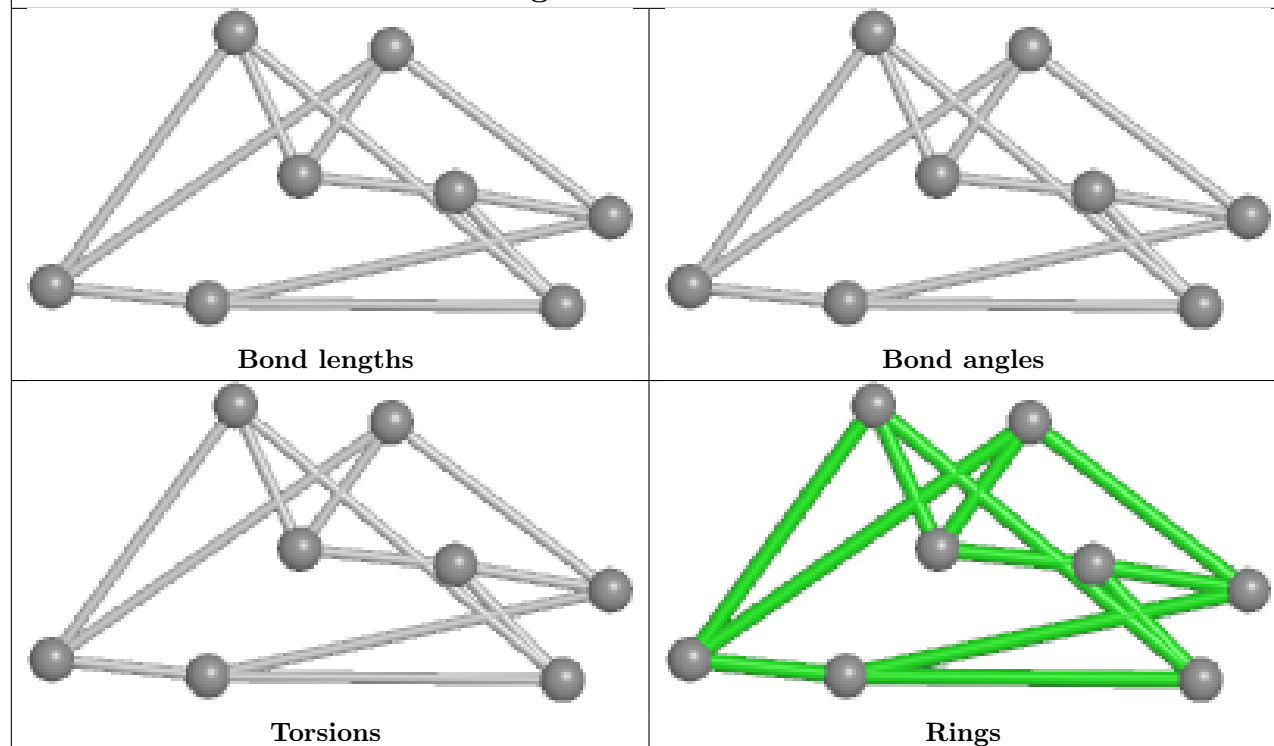


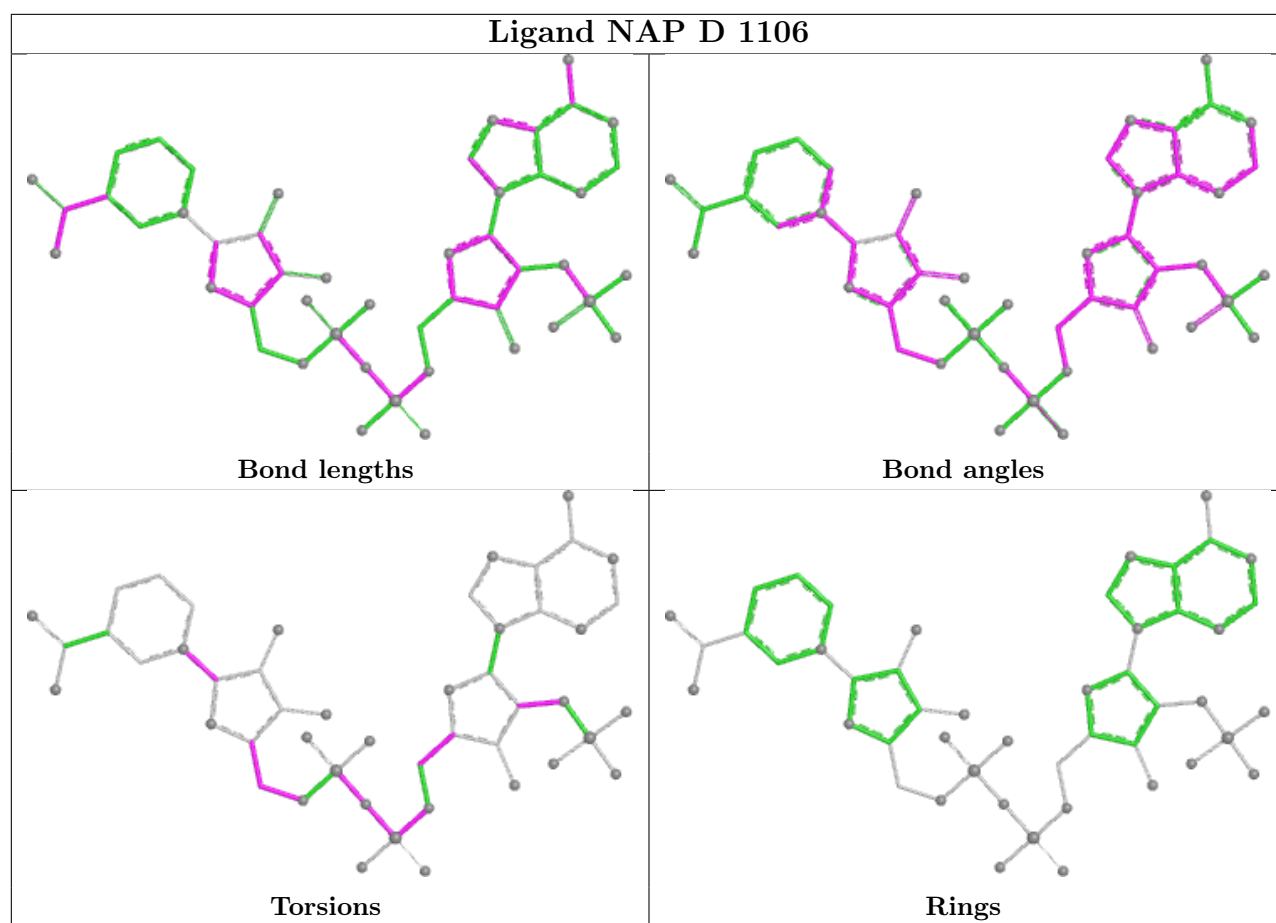


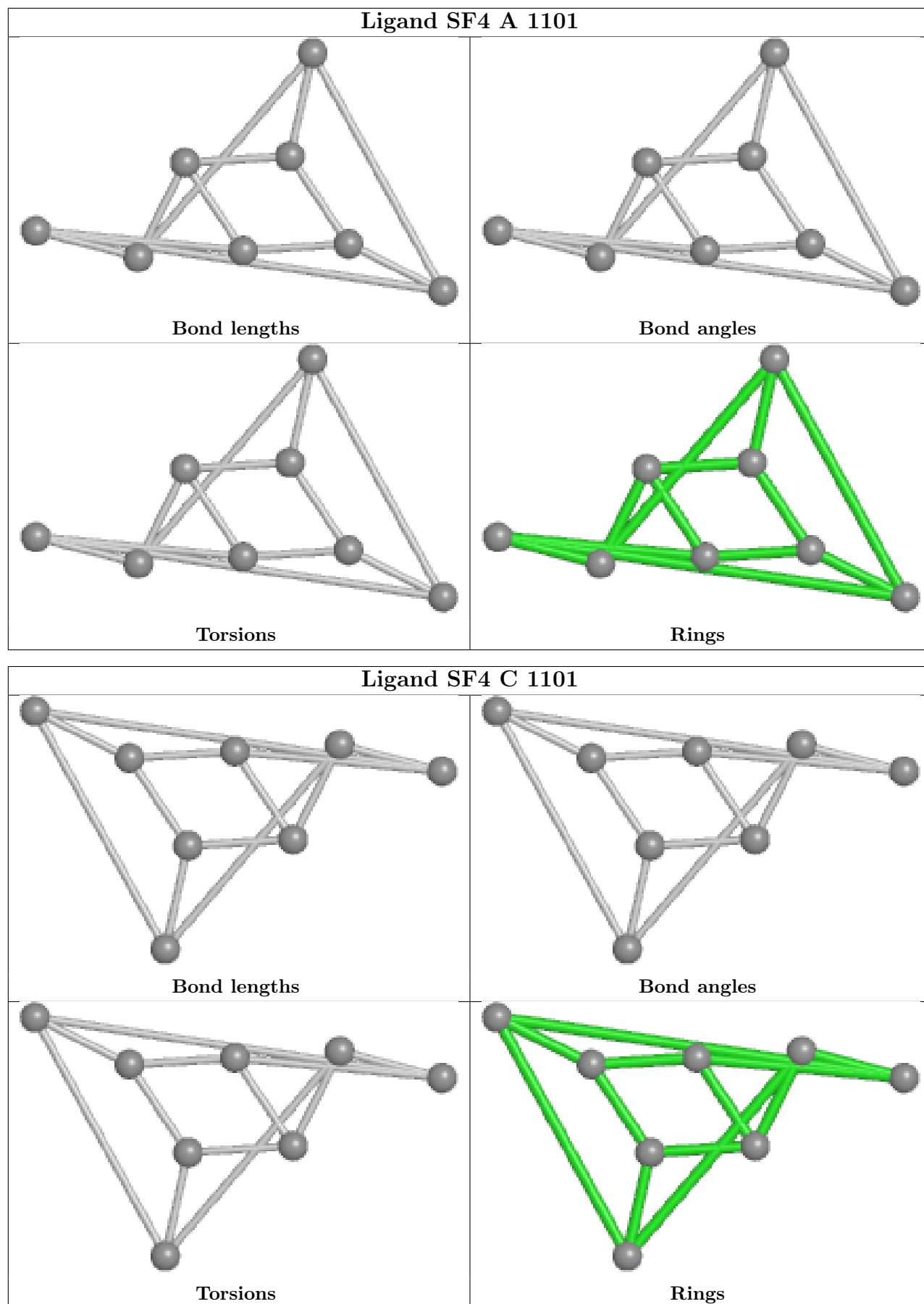
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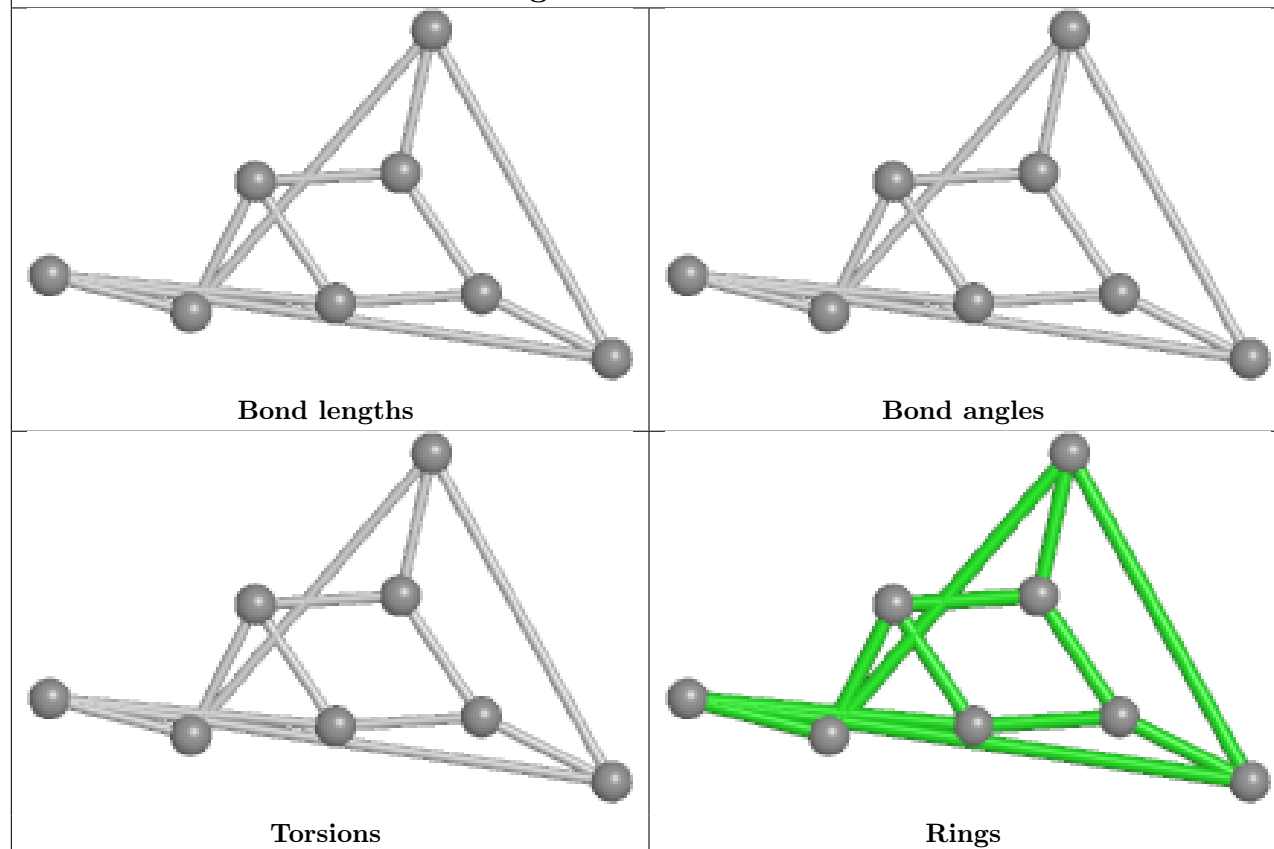
Ligand SF4 B 1104



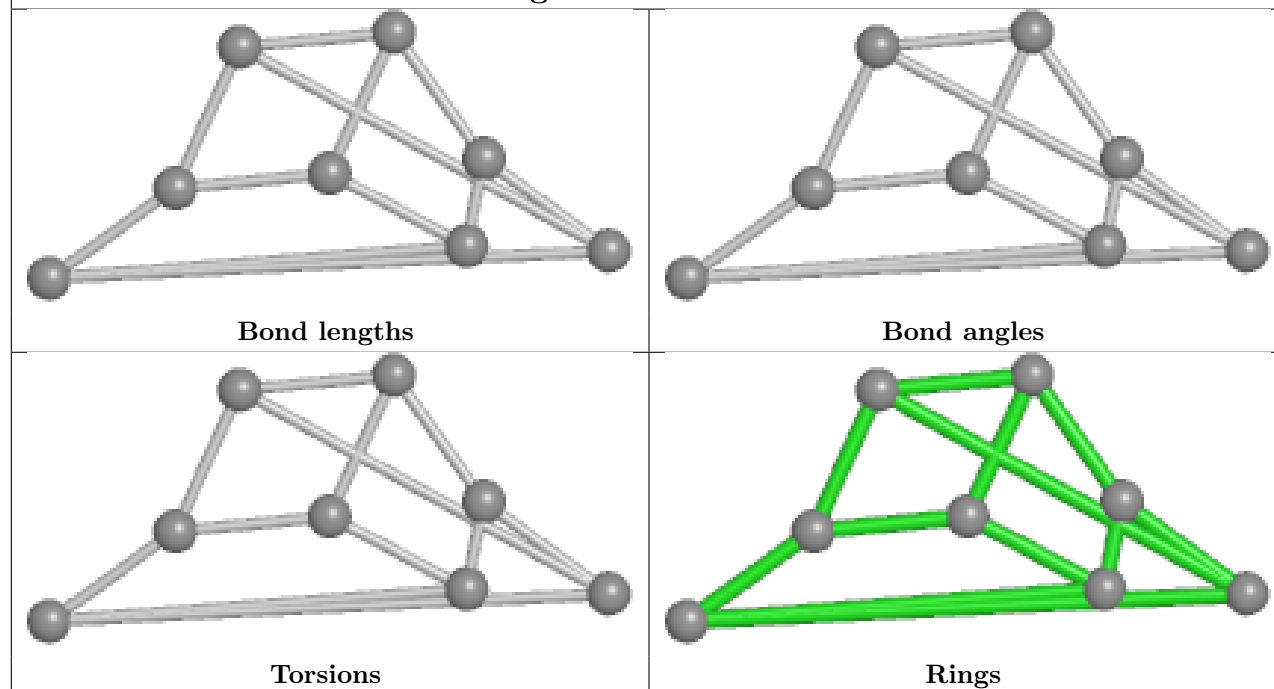


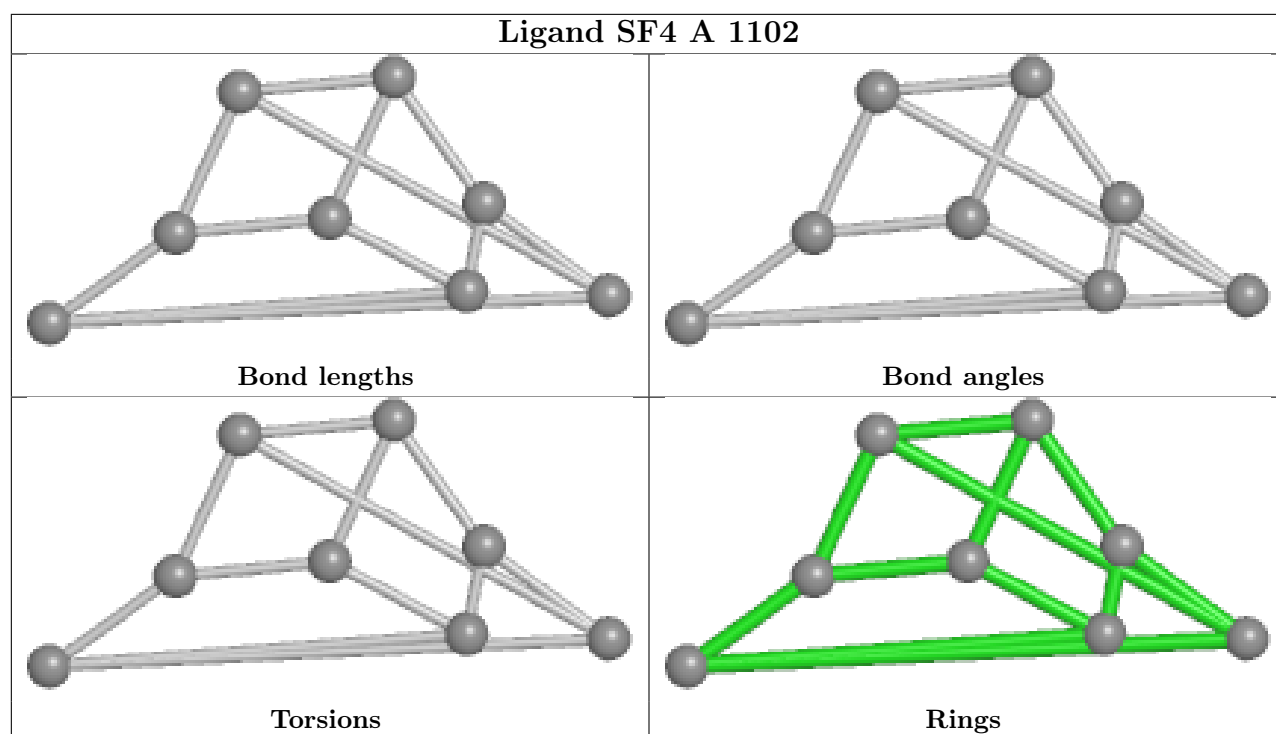


Ligand SF4 A 1103

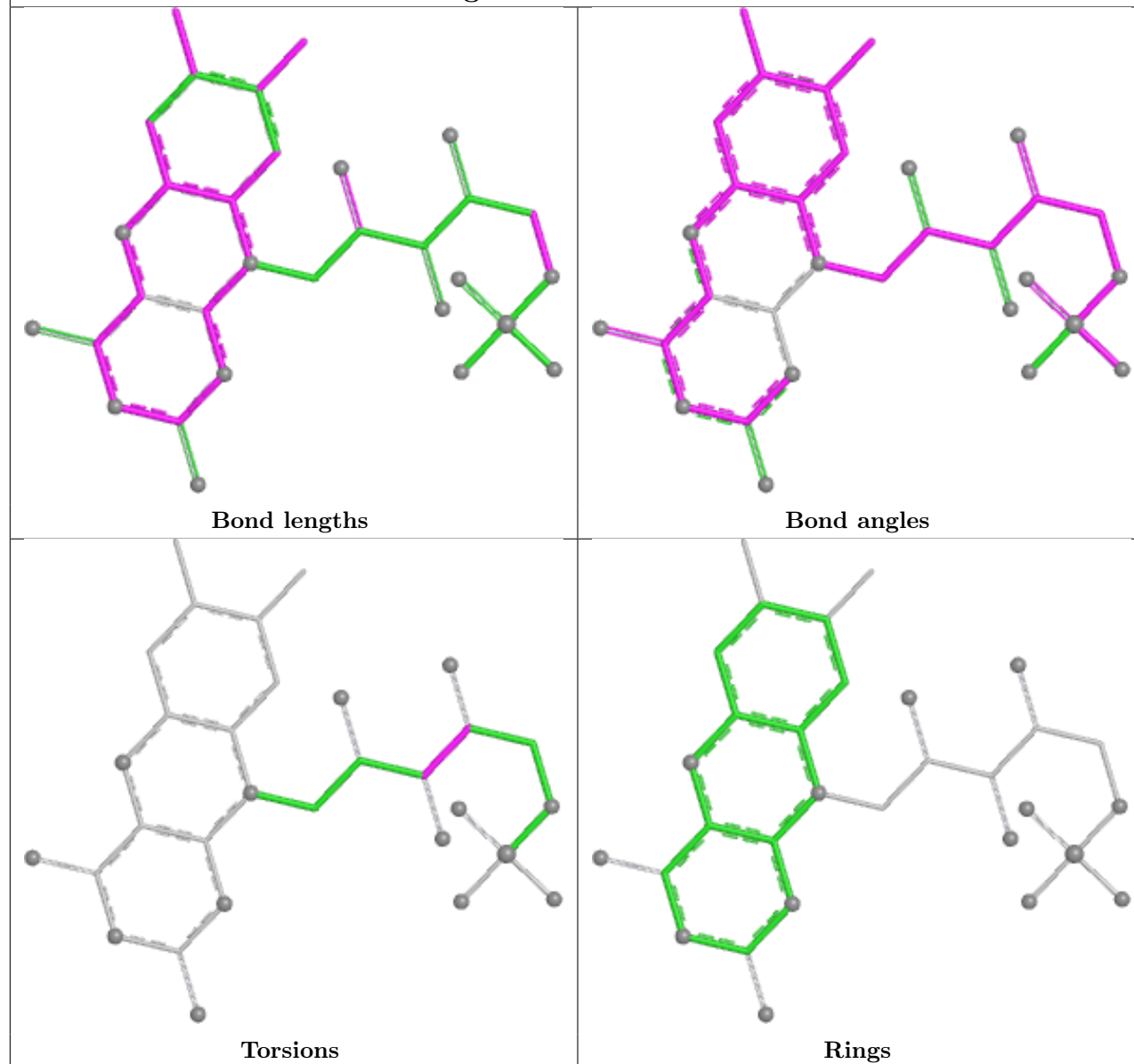


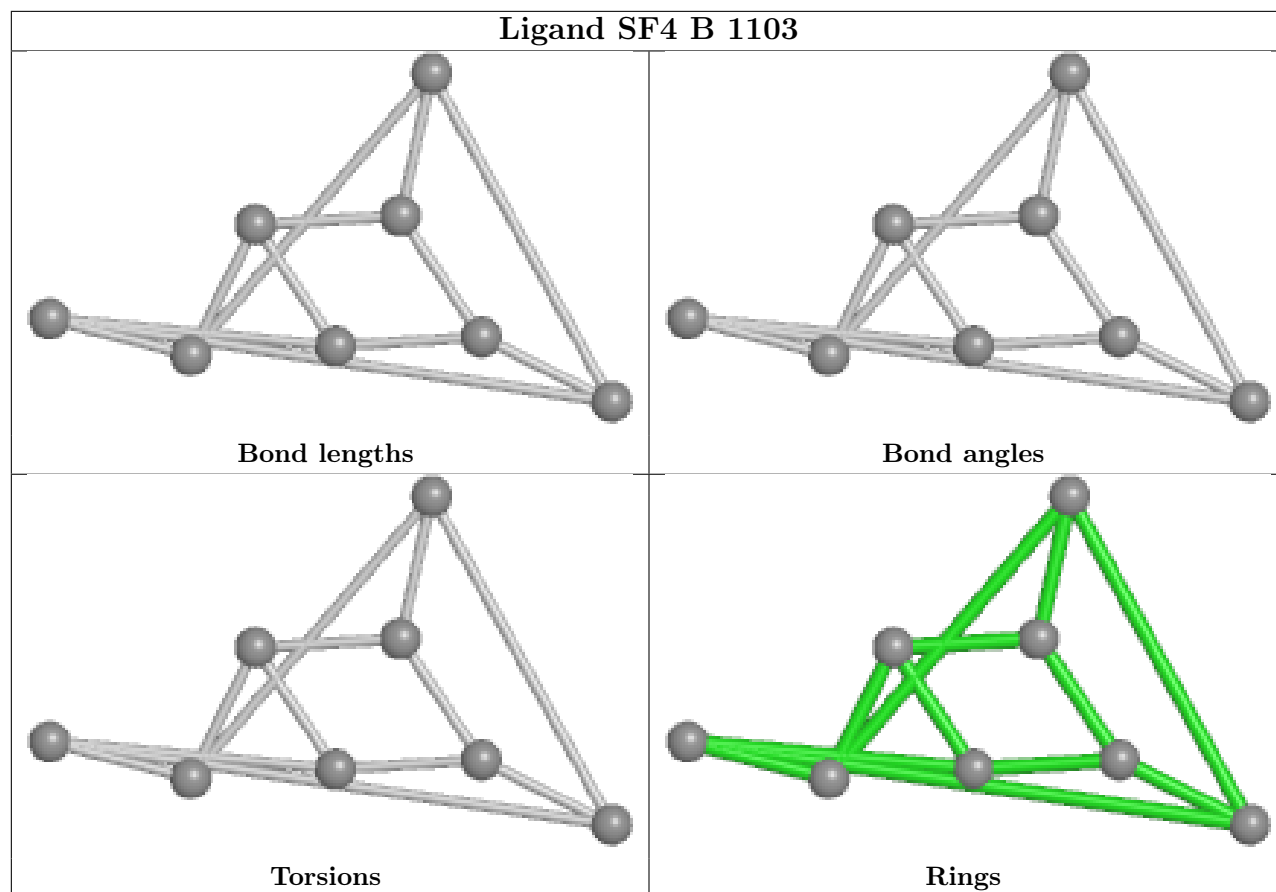
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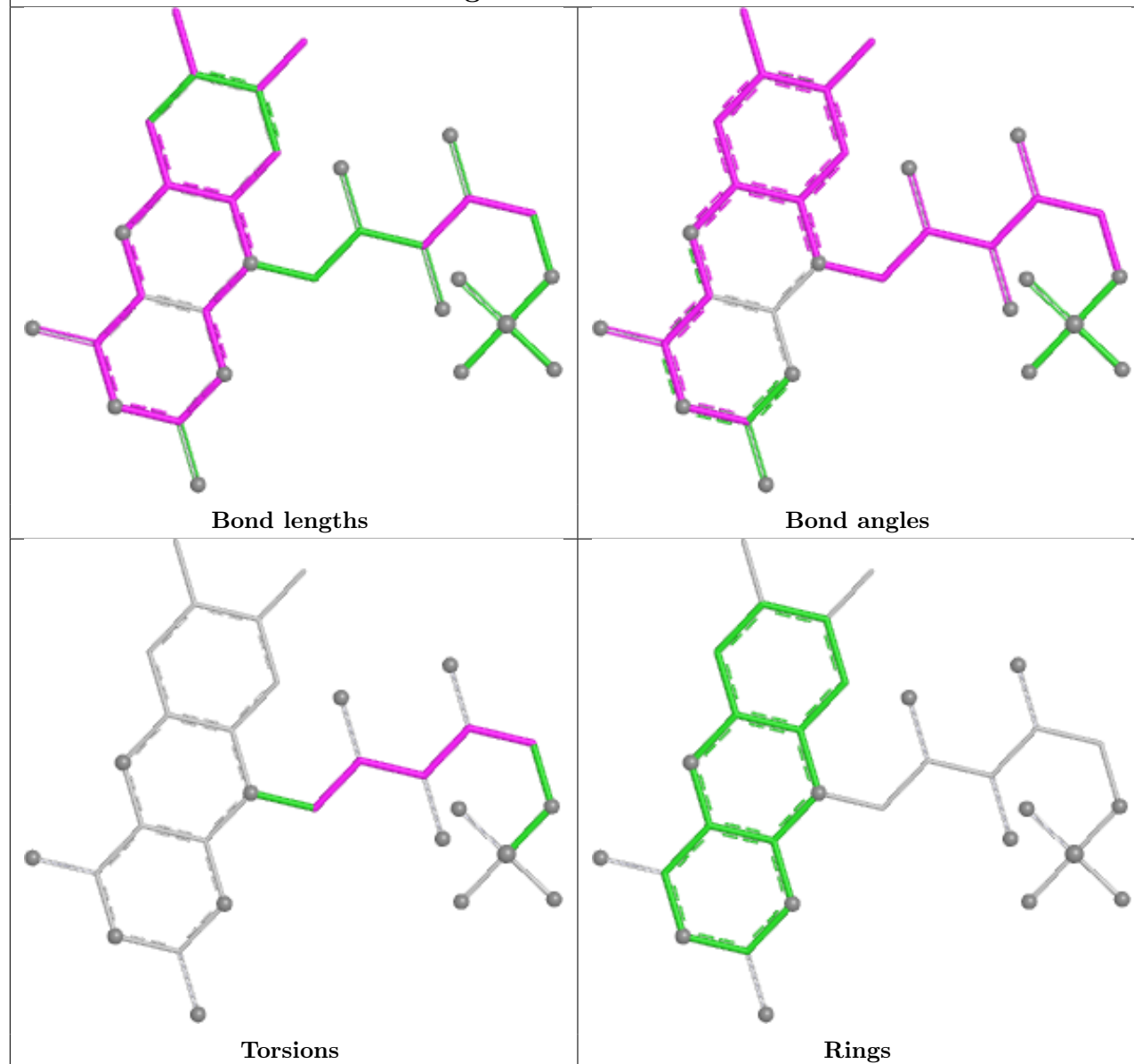


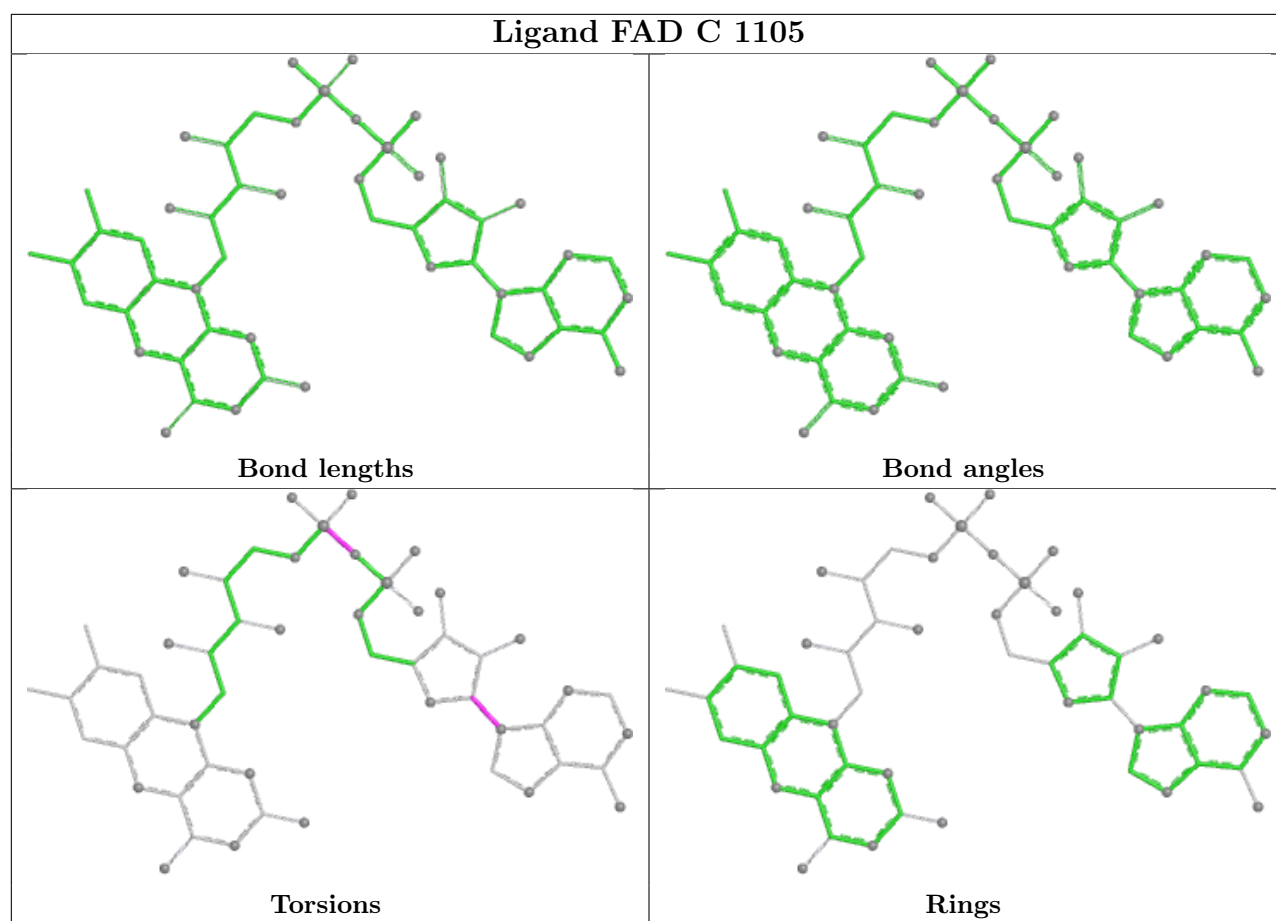
Ligand FNR D 1107





Ligand FNR B 1108





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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1010/1025 (98%)	0.20	59 (5%)	29 37	19, 28, 53, 83	0
1	B	1008/1025 (98%)	0.18	44 (4%)	39 49	20, 29, 52, 88	0
1	C	1018/1025 (99%)	0.24	71 (6%)	22 30	20, 28, 59, 101	0
1	D	1006/1025 (98%)	0.23	63 (6%)	26 34	19, 30, 55, 99	0
All	All	4042/4100 (98%)	0.21	237 (5%)	28 37	19, 29, 55, 101	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	CYS	8.2
1	A	319	ALA	8.1
1	C	323	ALA	7.9
1	D	902	ALA	7.9
1	C	907	LEU	7.5
1	D	897	LEU	7.3
1	C	322	CYS	6.7
1	C	324	CYS	6.6
1	B	902	ALA	6.3
1	A	907	LEU	6.0
1	C	902	ALA	5.8
1	C	326	SER	5.6
1	C	904	PHE	5.5
1	A	323	ALA	5.4
1	D	907	LEU	5.3
1	B	1020	ALA	5.3
1	C	903	ALA	5.1
1	B	459	TRP	5.1
1	C	906	PRO	5.0
1	B	1021	VAL	5.0
1	B	907	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	322	CYS	5.0
1	A	325	HIS	4.9
1	A	904	PHE	4.8
1	C	50	PHE	4.8
1	C	679	GLY	4.7
1	A	903	ALA	4.7
1	A	320	GLY	4.5
1	B	52	CYS	4.5
1	A	906	PRO	4.5
1	A	866	PRO	4.4
1	C	681	GLY	4.4
1	C	52	CYS	4.3
1	C	905	PRO	4.3
1	C	1019	LEU	4.2
1	D	324	CYS	4.1
1	A	681	GLY	4.1
1	C	868	ILE	4.1
1	D	899	GLU	4.1
1	D	901	ASN	4.1
1	B	1010	PRO	4.1
1	A	326	SER	4.1
1	D	51	HIS	4.0
1	C	342	ASP	4.0
1	A	372	ALA	4.0
1	D	869	ALA	4.0
1	A	49	CYS	3.9
1	C	1018	PRO	3.9
1	A	52	CYS	3.9
1	B	50	PHE	3.9
1	C	678	ARG	3.9
1	A	1010	PRO	3.9
1	D	50	PHE	3.8
1	C	325	HIS	3.8
1	C	370	ILE	3.8
1	B	342	ASP	3.7
1	D	459	TRP	3.7
1	C	909	ARG	3.7
1	A	331	ILE	3.7
1	D	323	ALA	3.7
1	C	677	GLU	3.7
1	D	52	CYS	3.7
1	A	50	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	372	ALA	3.6
1	C	680	MET	3.6
1	D	325	HIS	3.6
1	C	49	CYS	3.6
1	B	51	HIS	3.6
1	B	866	PRO	3.6
1	A	371	ARG	3.5
1	B	22	THR	3.5
1	C	676	GLY	3.5
1	D	681	GLY	3.5
1	D	1020	ALA	3.4
1	B	871	LEU	3.4
1	D	682	LEU	3.4
1	A	673	HIS	3.4
1	A	417	GLY	3.4
1	C	330	SER	3.4
1	B	897	LEU	3.4
1	C	371	ARG	3.4
1	D	371	ARG	3.3
1	D	416	THR	3.3
1	D	871	LEU	3.3
1	A	902	ALA	3.3
1	C	1020	ALA	3.2
1	D	856	THR	3.2
1	C	872	MET	3.2
1	A	1011	TYR	3.2
1	A	905	PRO	3.2
1	A	342	ASP	3.2
1	D	331	ILE	3.2
1	B	682	LEU	3.2
1	C	873	GLY	3.1
1	B	856	THR	3.1
1	B	869	ALA	3.1
1	B	1011	TYR	3.1
1	A	367	PHE	3.1
1	C	416	THR	3.1
1	A	672	PRO	3.1
1	C	320	GLY	3.1
1	C	870	GLU	3.0
1	B	868	ILE	3.0
1	C	682	LEU	3.0
1	A	856	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	417	GLY	3.0
1	C	866	PRO	3.0
1	D	868	ILE	3.0
1	A	51	HIS	3.0
1	D	900	GLN	3.0
1	B	909	ARG	3.0
1	B	900	GLN	2.9
1	C	867	ARG	2.9
1	C	367	PHE	2.9
1	C	53	GLU	2.9
1	B	673	HIS	2.9
1	A	370	ILE	2.9
1	C	414	ASP	2.9
1	C	368	VAL	2.9
1	A	872	MET	2.9
1	A	1018	PRO	2.9
1	C	900	GLN	2.9
1	C	897	LEU	2.9
1	A	1019	LEU	2.9
1	C	871	LEU	2.9
1	A	868	ILE	2.8
1	D	327	PRO	2.8
1	A	415	GLU	2.8
1	A	416	THR	2.8
1	D	48	ASN	2.8
1	C	856	THR	2.8
1	C	864	PRO	2.8
1	A	48	ASN	2.7
1	C	486	ALA	2.7
1	C	51	HIS	2.7
1	D	320	GLY	2.7
1	A	682	LEU	2.7
1	C	327	PRO	2.7
1	B	368	VAL	2.7
1	D	419	TRP	2.7
1	C	908	GLU	2.7
1	B	681	GLY	2.7
1	B	416	THR	2.7
1	A	60	ASP	2.7
1	C	415	GLU	2.7
1	C	1012	GLU	2.7
1	B	872	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	263	GLU	2.6
1	D	898	LYS	2.6
1	C	859	HIS	2.6
1	D	264	ASN	2.6
1	A	873	GLY	2.6
1	A	865	VAL	2.6
1	B	1019	LEU	2.6
1	D	332	ARG	2.6
1	B	873	GLY	2.6
1	C	874	LYS	2.6
1	D	874	LYS	2.6
1	C	869	ALA	2.6
1	C	331	ILE	2.5
1	C	675	MET	2.5
1	B	264	ASN	2.5
1	B	901	ASN	2.5
1	D	867	ARG	2.5
1	D	889	ILE	2.5
1	A	899	GLU	2.5
1	A	869	ALA	2.5
1	B	372	ALA	2.5
1	D	1018	PRO	2.5
1	D	49	CYS	2.4
1	D	896	ARG	2.4
1	D	672	PRO	2.4
1	A	414	ASP	2.4
1	D	300	ASP	2.4
1	C	48	ASN	2.4
1	B	415	GLU	2.4
1	B	917	PRO	2.4
1	D	872	MET	2.4
1	D	175	CYS	2.4
1	B	11	ASP	2.3
1	D	424	ASP	2.3
1	D	319	ALA	2.3
1	A	327	PRO	2.3
1	A	859	HIS	2.3
1	B	520	GLU	2.3
1	A	321	MET	2.3
1	A	910	LYS	2.3
1	C	332	ARG	2.3
1	C	893	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	485	MET	2.3
1	D	418	LYS	2.3
1	D	866	PRO	2.3
1	A	332	ARG	2.3
1	A	901	ASN	2.3
1	C	901	ASN	2.3
1	A	54	LYS	2.3
1	B	418	LYS	2.3
1	C	1017	LEU	2.3
1	C	417	GLY	2.2
1	D	891	ALA	2.2
1	D	700	GLN	2.2
1	B	865	VAL	2.2
1	B	48	ASN	2.2
1	D	859	HIS	2.2
1	C	36	LEU	2.2
1	C	899	GLU	2.2
1	C	898	LYS	2.2
1	A	896	ARG	2.2
1	B	870	GLU	2.2
1	D	342	ASP	2.2
1	B	517	ALA	2.2
1	D	15	ILE	2.2
1	D	895	MET	2.2
1	D	368	VAL	2.2
1	A	424	ASP	2.2
1	A	358	ARG	2.2
1	B	371	ARG	2.2
1	D	909	ARG	2.2
1	A	536	GLU	2.1
1	B	331	ILE	2.1
1	D	426	ILE	2.1
1	C	21	ARG	2.1
1	D	372	ALA	2.1
1	B	913	ILE	2.1
1	D	873	GLY	2.1
1	D	910	LYS	2.1
1	A	1012	GLU	2.1
1	A	864	PRO	2.1
1	C	1011	TYR	2.1
1	D	870	GLU	2.1
1	C	419	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	420	ASN	2.1
1	D	1019	LEU	2.1
1	D	36	LEU	2.0
1	A	11	ASP	2.0
1	D	443	ARG	2.0
1	D	330	SER	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
4	NAP	C	1106	48/48	0.76	0.16	44,55,63,66	0
4	NAP	A	1106	48/48	0.81	0.14	41,55,60,67	0
4	NAP	D	1106	48/48	0.82	0.15	38,49,56,58	0
4	NAP	B	1106	48/48	0.84	0.14	39,48,54,55	0
5	FNR	B	1108	31/31	0.93	0.10	19,23,26,29	0
5	FNR	A	1107	31/31	0.94	0.09	19,22,26,30	0
5	FNR	C	1107	31/31	0.94	0.08	18,22,26,32	0
5	FNR	D	1107	31/31	0.94	0.09	21,23,28,30	0
6	TDR	B	1107	9/9	0.95	0.07	22,24,27,29	0
6	TDR	C	1108	9/9	0.95	0.07	20,22,25,25	0
6	TDR	D	1108	9/9	0.95	0.06	25,26,28,31	0
6	TDR	A	1108	9/9	0.96	0.06	21,22,24,25	0
3	FAD	A	1105	53/53	0.97	0.06	21,25,34,36	0
3	FAD	B	1105	53/53	0.97	0.06	22,27,32,32	0
3	FAD	C	1105	53/53	0.97	0.06	21,26,33,35	0
3	FAD	D	1105	53/53	0.97	0.06	24,29,33,34	0
2	SF4	A	1102	8/8	0.99	0.03	20,22,23,23	0

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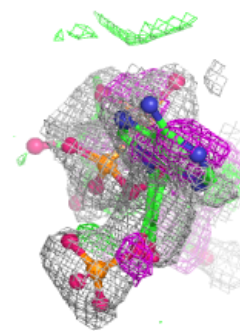
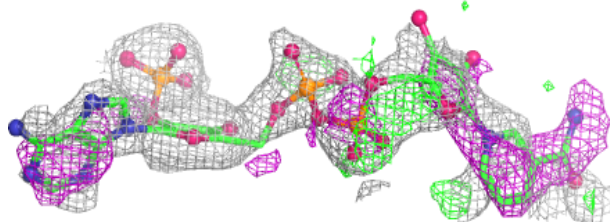
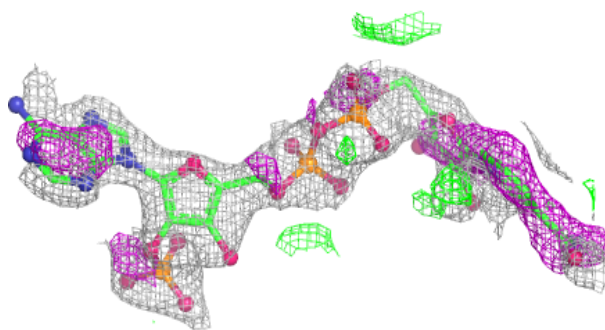
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	A	1103	8/8	0.99	0.03	19,20,22,22	0
2	SF4	A	1104	8/8	0.99	0.02	22,23,24,24	0
2	SF4	B	1101	8/8	0.99	0.02	20,23,24,25	0
2	SF4	B	1102	8/8	0.99	0.02	21,22,23,24	0
2	SF4	B	1103	8/8	0.99	0.02	18,21,21,21	0
2	SF4	B	1104	8/8	0.99	0.03	22,22,23,24	0
2	SF4	C	1101	8/8	0.99	0.03	19,22,24,24	0
2	SF4	C	1102	8/8	0.99	0.03	23,23,25,26	0
2	SF4	C	1103	8/8	0.99	0.03	20,21,22,24	0
2	SF4	C	1104	8/8	0.99	0.02	21,22,23,23	0
2	SF4	D	1101	8/8	0.99	0.03	22,23,24,25	0
2	SF4	D	1102	8/8	0.99	0.02	19,22,23,23	0
2	SF4	D	1104	8/8	0.99	0.03	22,22,24,25	0
2	SF4	A	1101	8/8	0.99	0.02	20,21,22,23	0
2	SF4	D	1103	8/8	1.00	0.02	19,21,22,24	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.

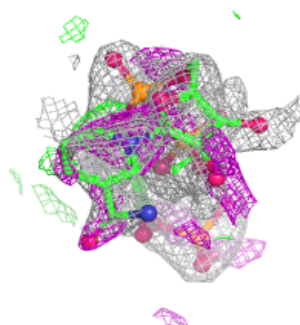
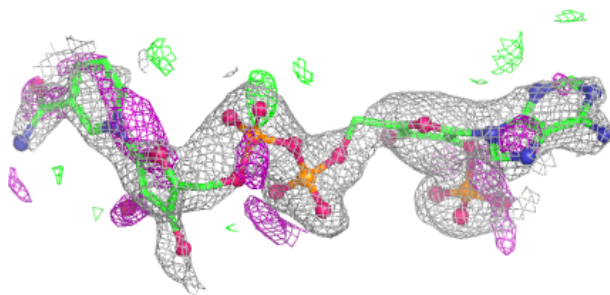
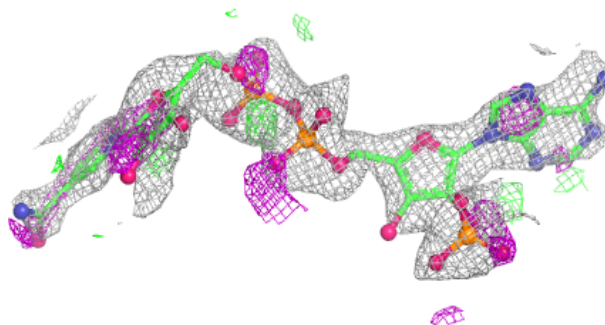
Electron density around NAP C 1106:

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

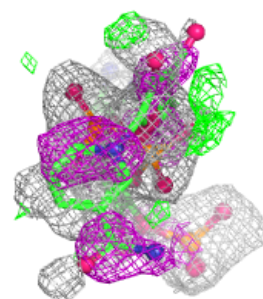
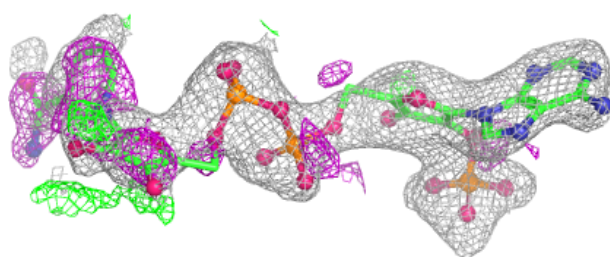
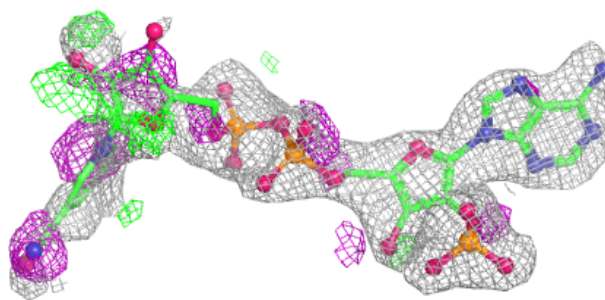


Electron density around NAP A 1106:

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

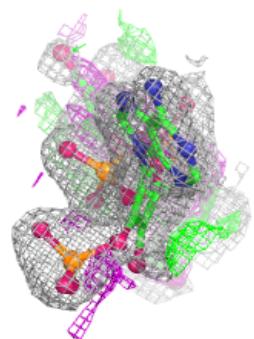
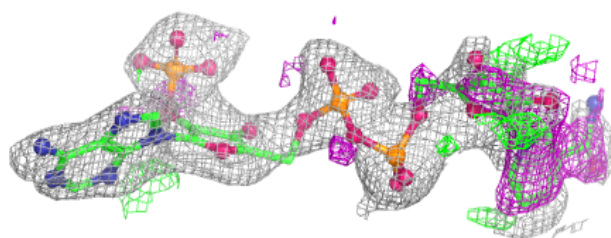
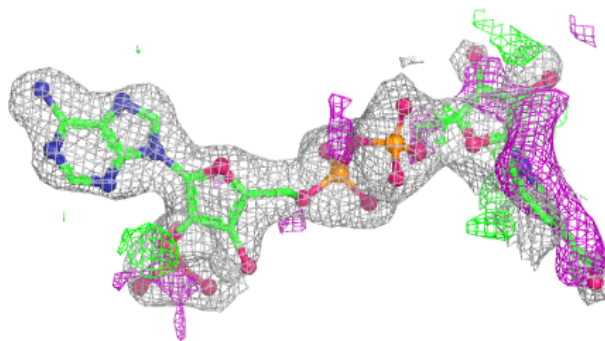
**Electron density around NAP D 1106:**

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



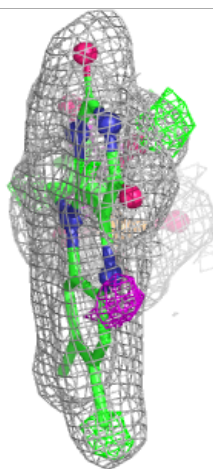
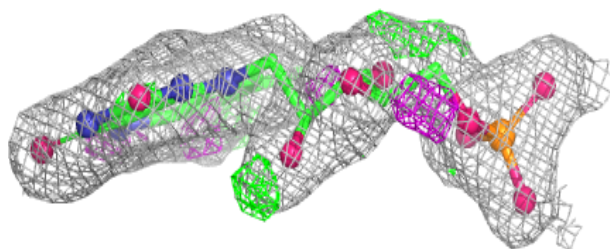
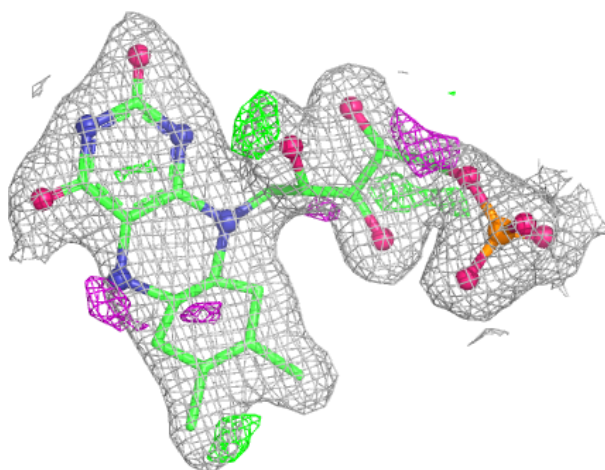
Electron density around NAP B 1106:

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



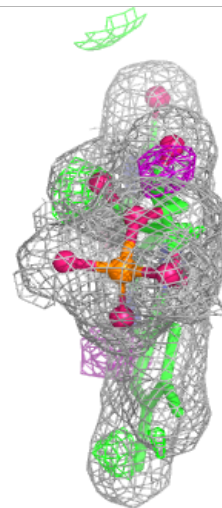
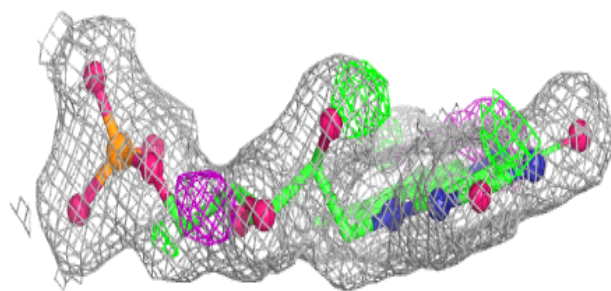
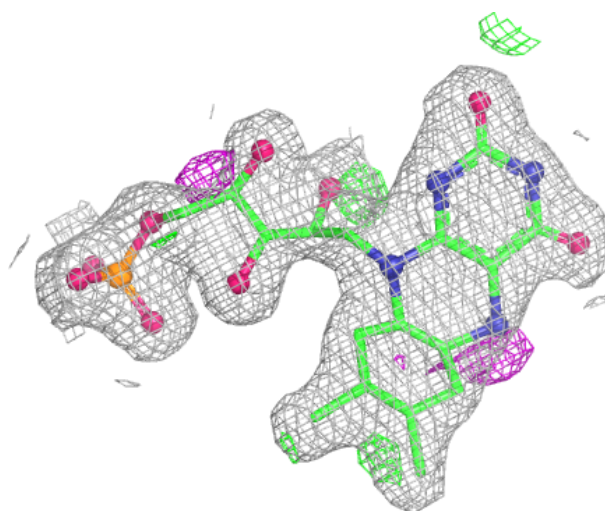
Electron density around FNR B 1108:

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



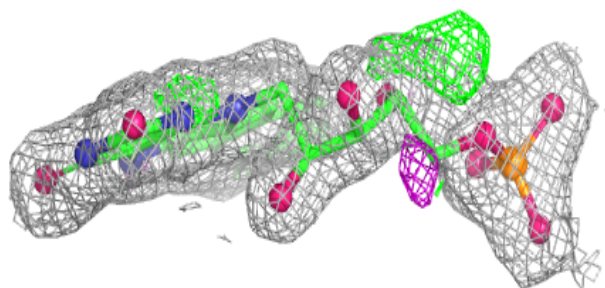
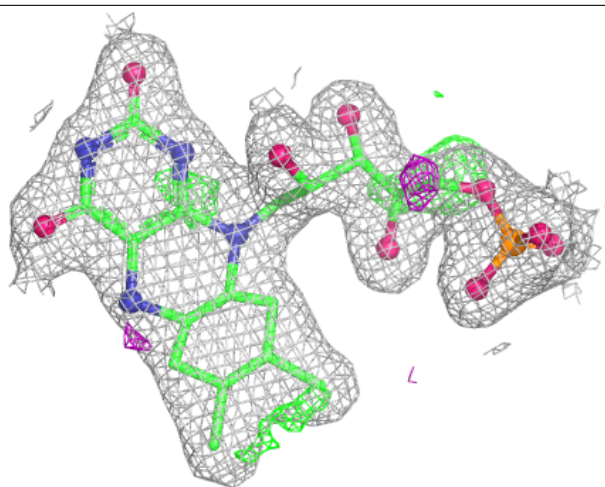
Electron density around FNR A 1107:

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



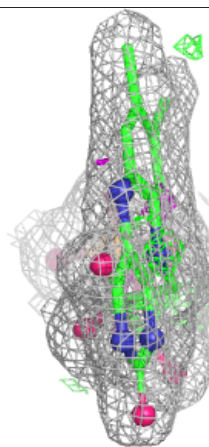
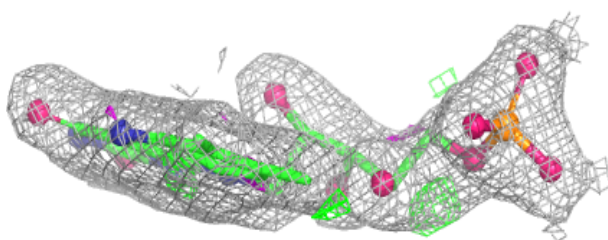
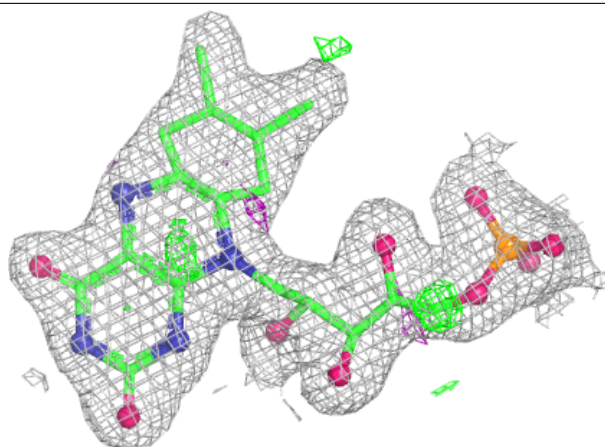
Electron density around FNR C 1107:

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



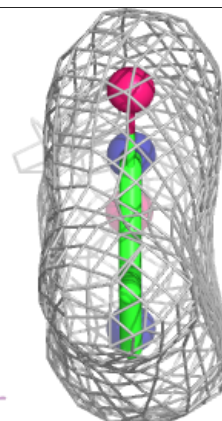
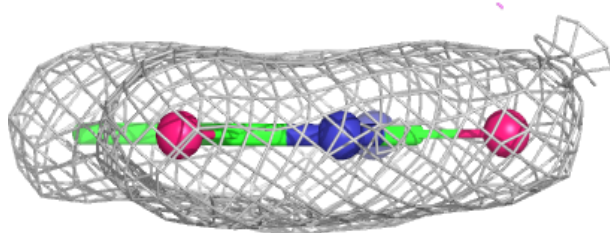
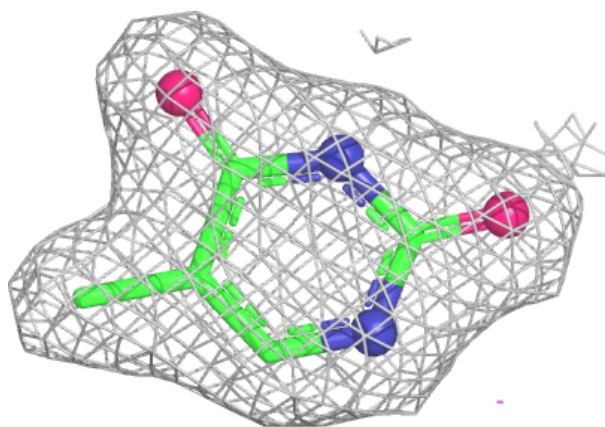
Electron density around FNR D 1107:

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



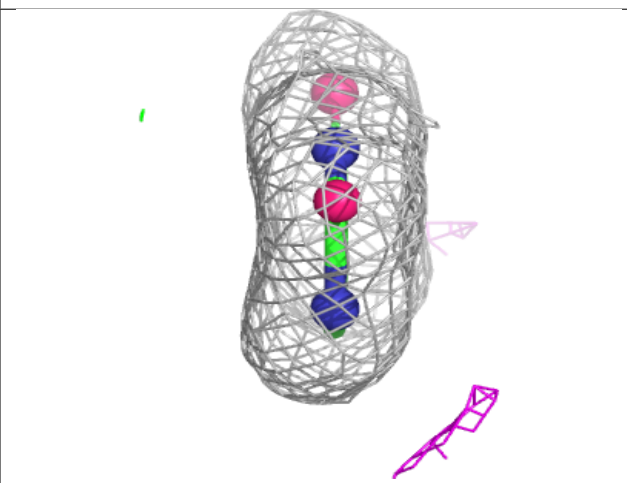
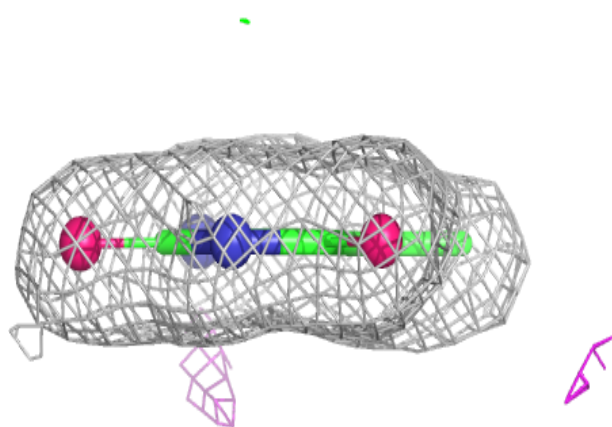
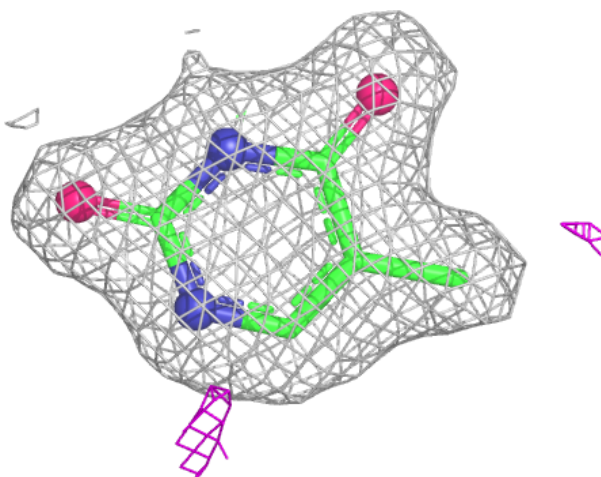
Electron density around TDR B 1107:

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



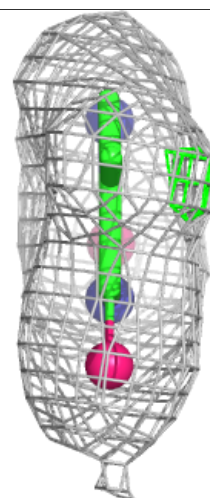
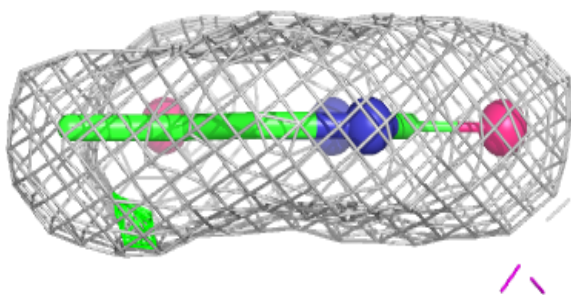
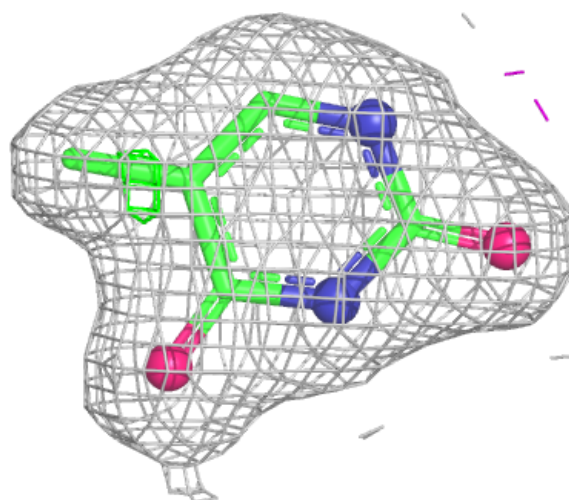
Electron density around TDR C 1108:

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



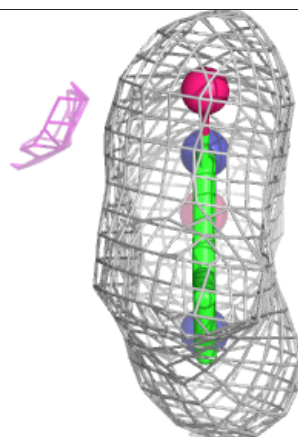
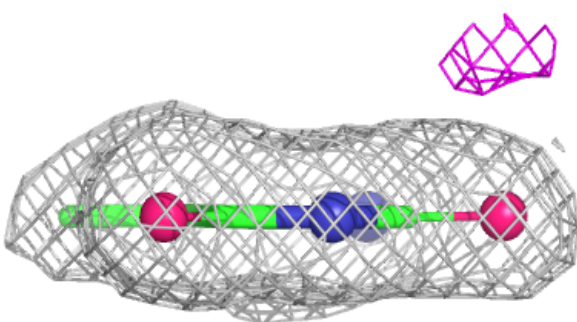
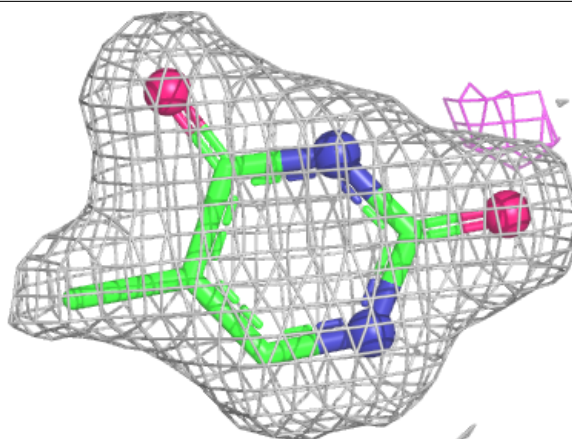
Electron density around TDR D 1108:

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

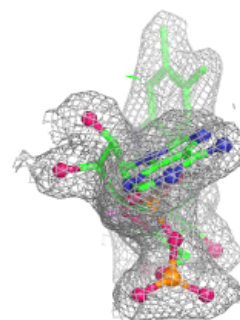
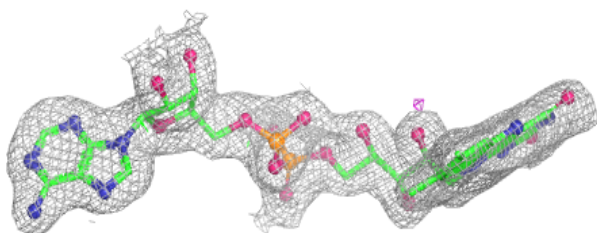
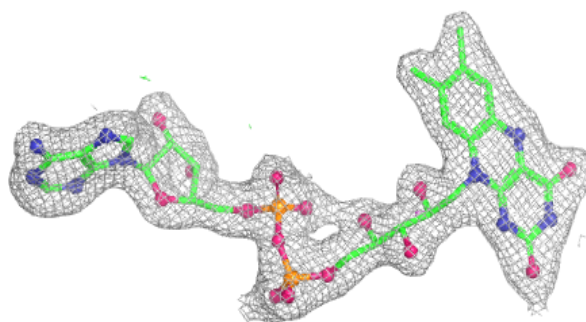


Electron density around TDR A 1108:

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

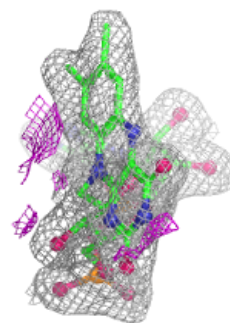
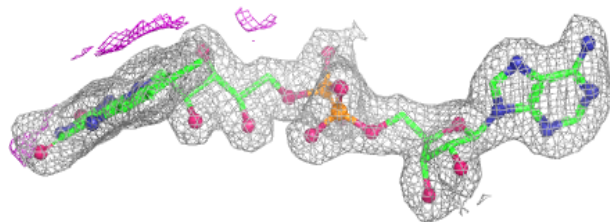
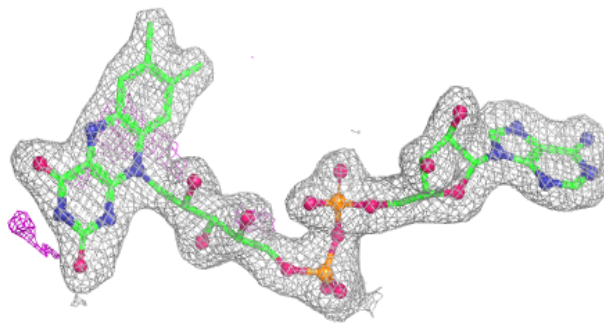
**Electron density around FAD A 1105:**

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

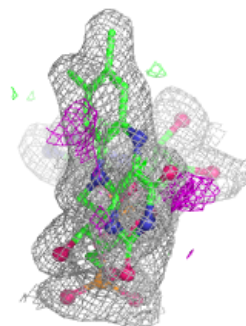
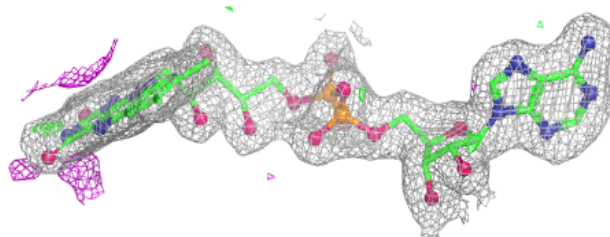
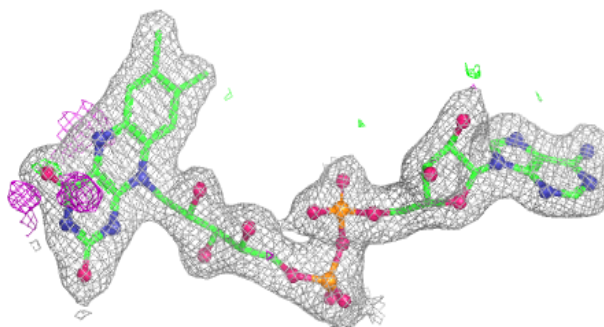


Electron density around FAD B 1105:

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

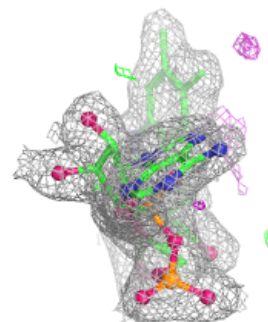
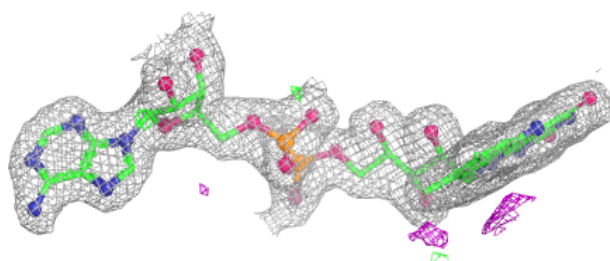
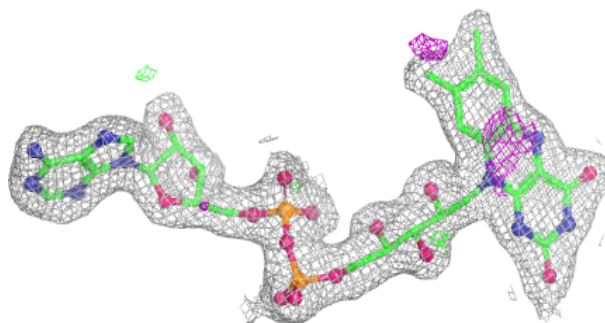
**Electron density around FAD C 1105:**

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



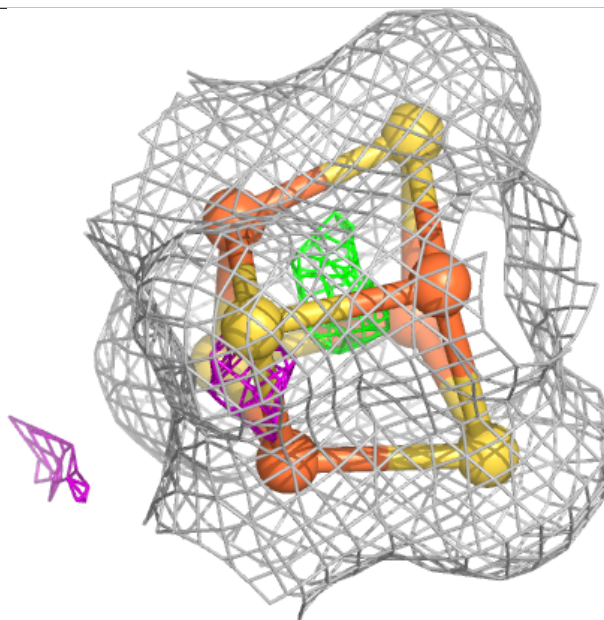
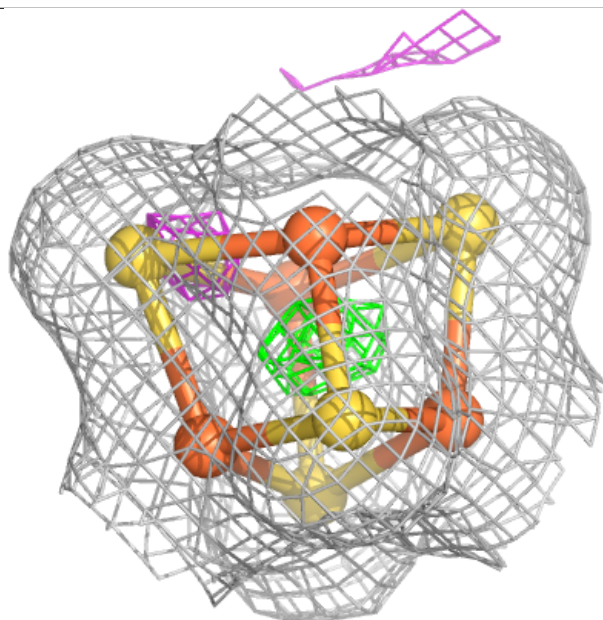
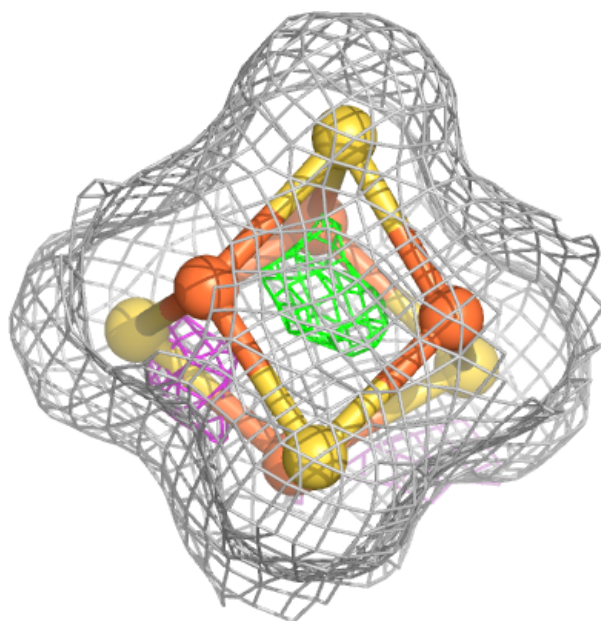
Electron density around FAD D 1105:

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



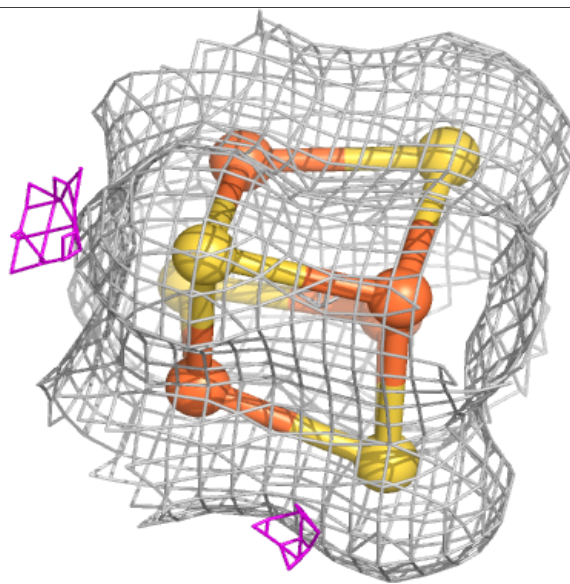
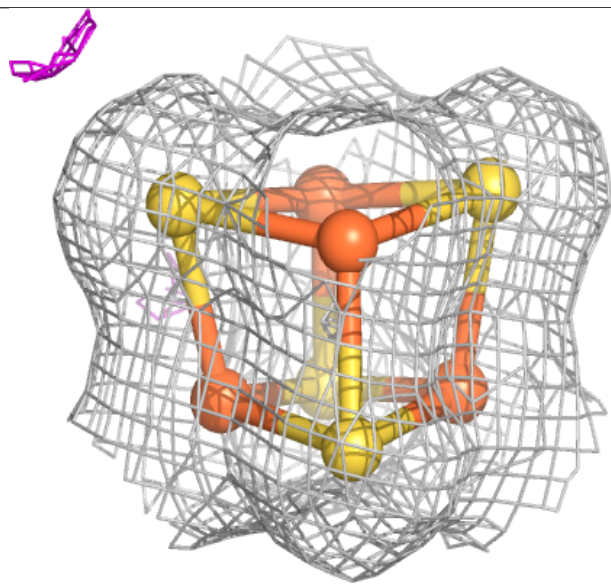
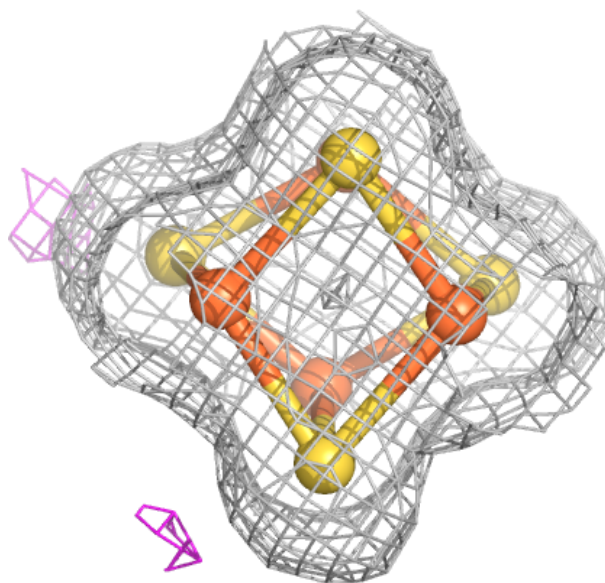
Electron density around SF4 A 1102:

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



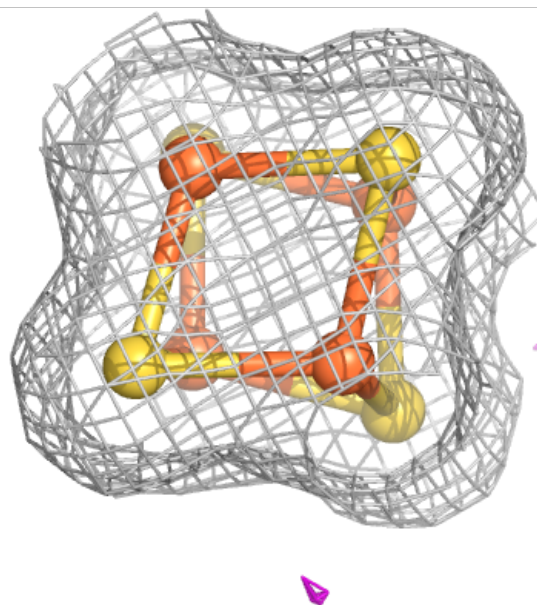
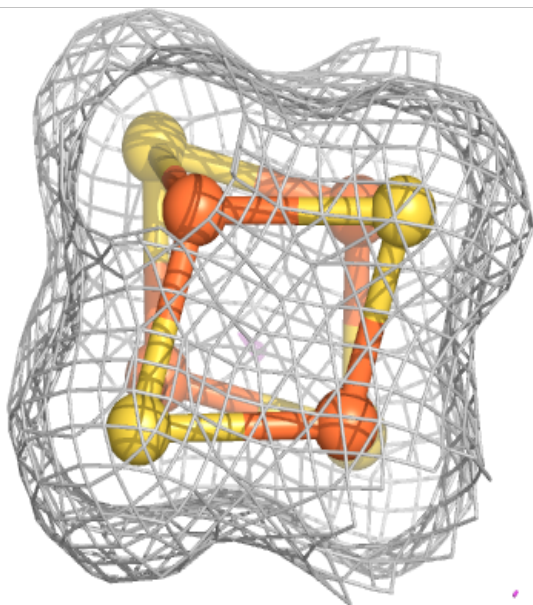
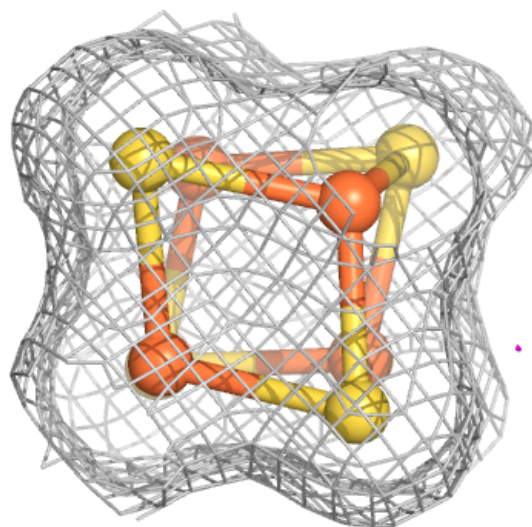
Electron density around SF4 A 1103:

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



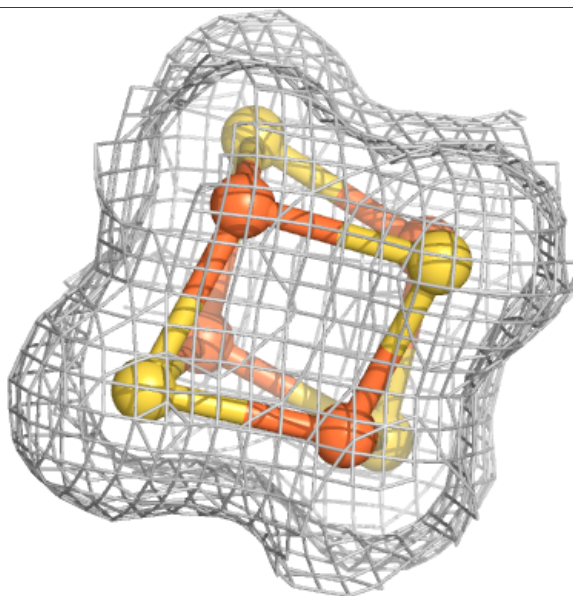
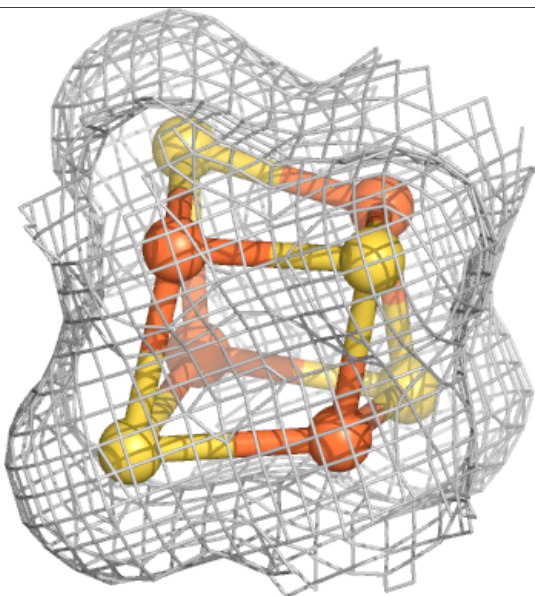
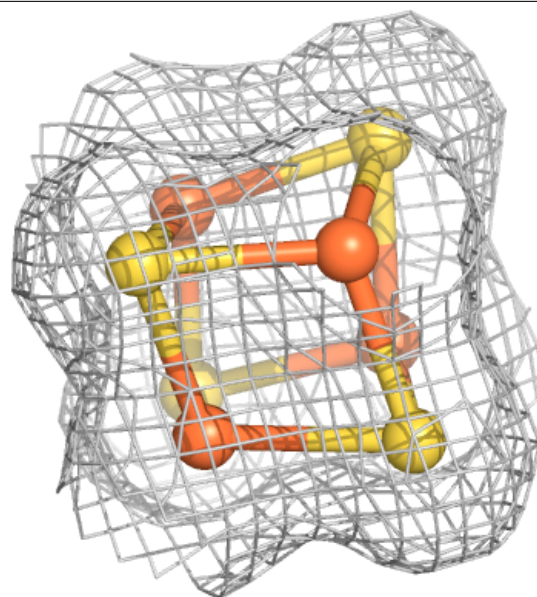
Electron density around SF4 A 1104:

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



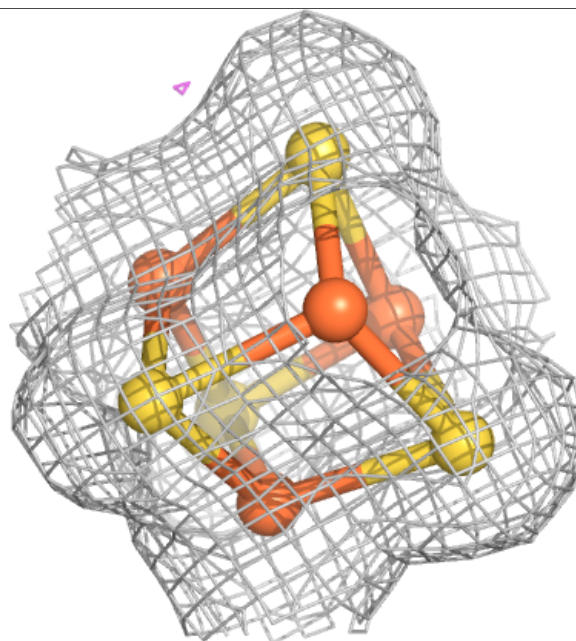
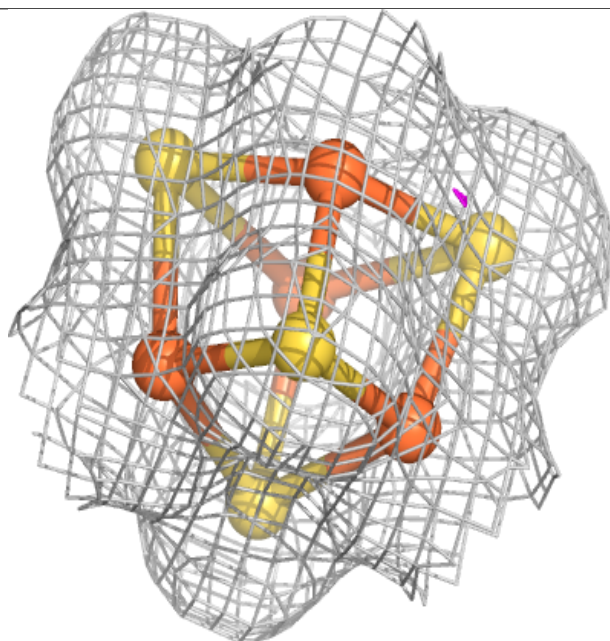
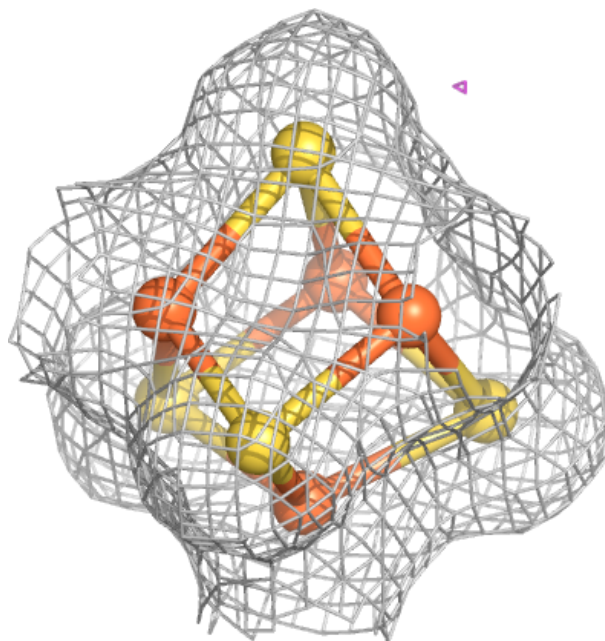
Electron density around SF4 B 1101:

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



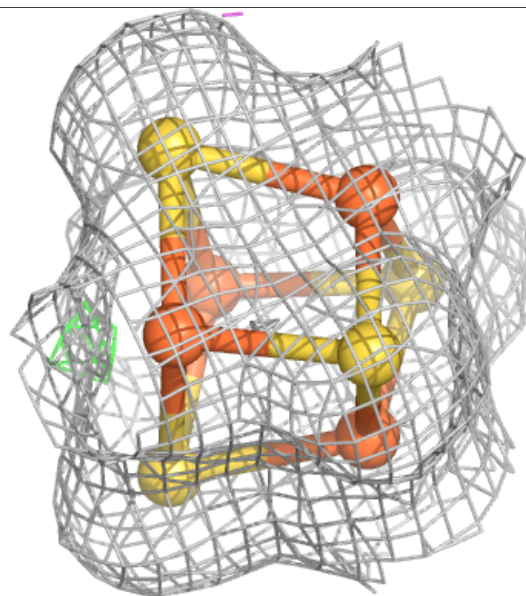
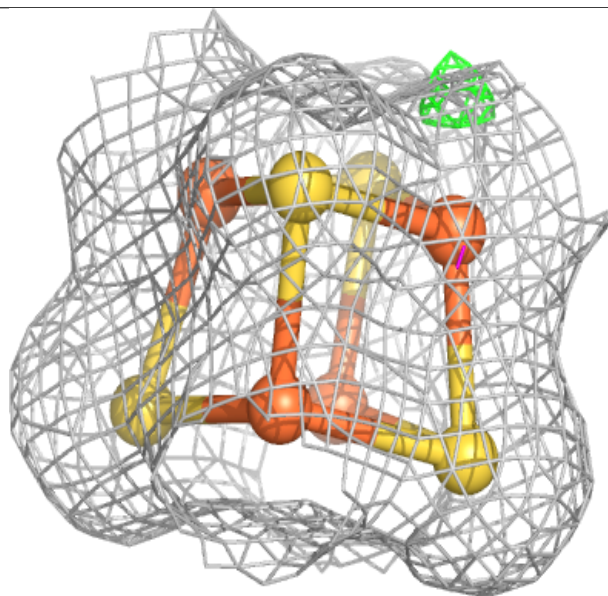
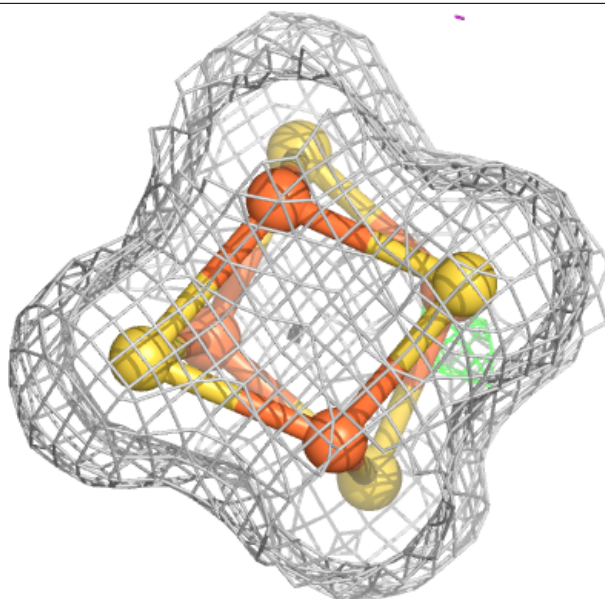
Electron density around SF4 B 1102:

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



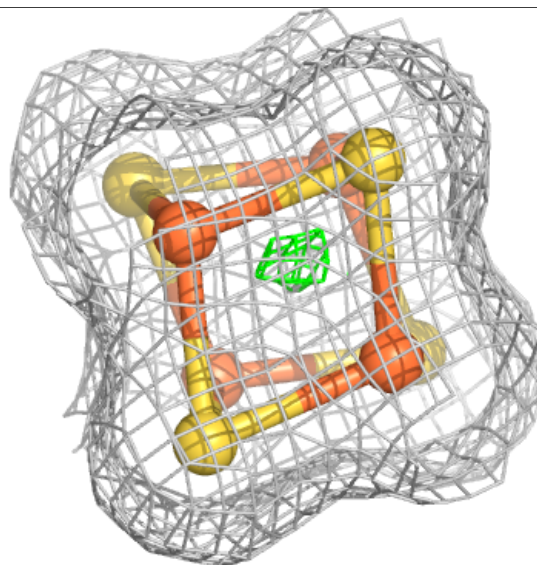
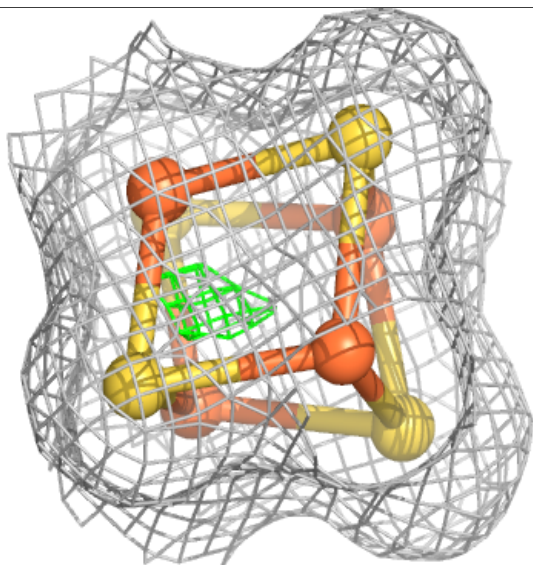
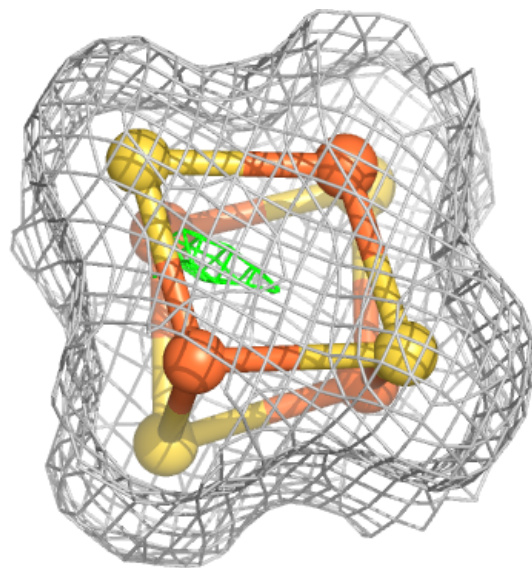
Electron density around SF4 B 1103:

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



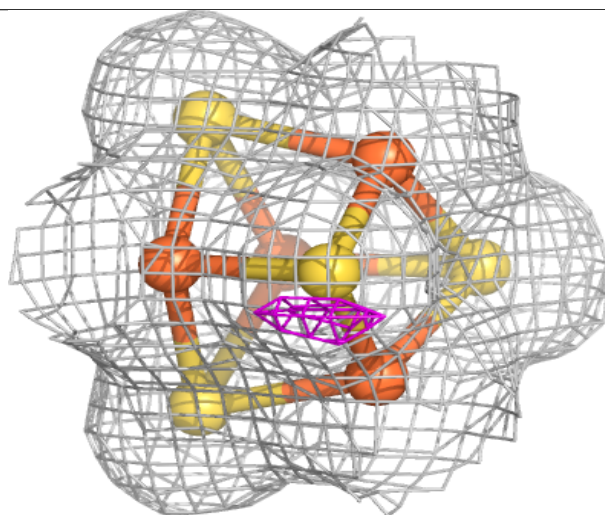
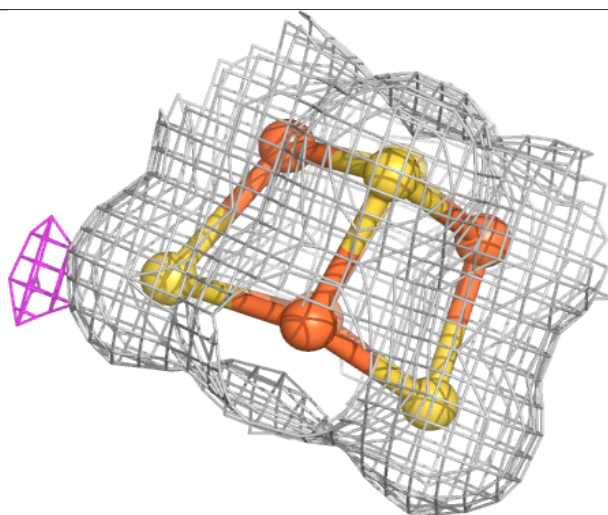
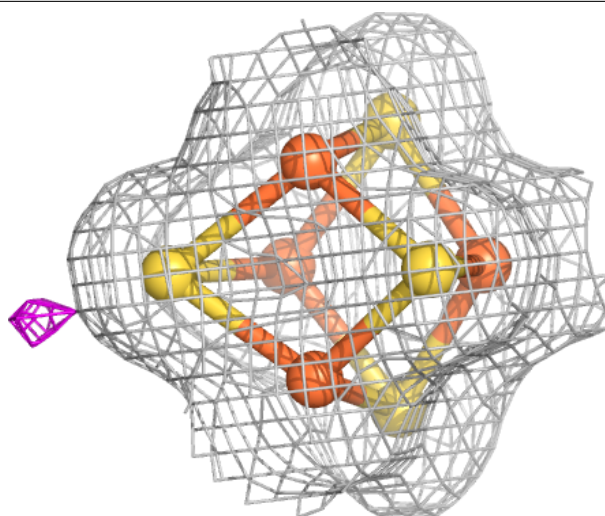
Electron density around SF4 B 1104:

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



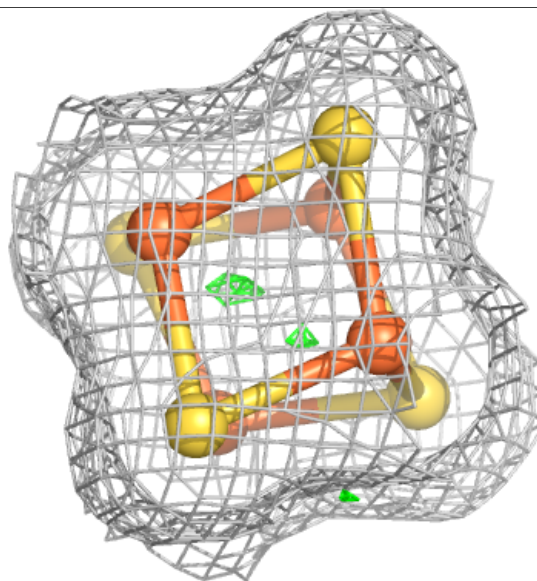
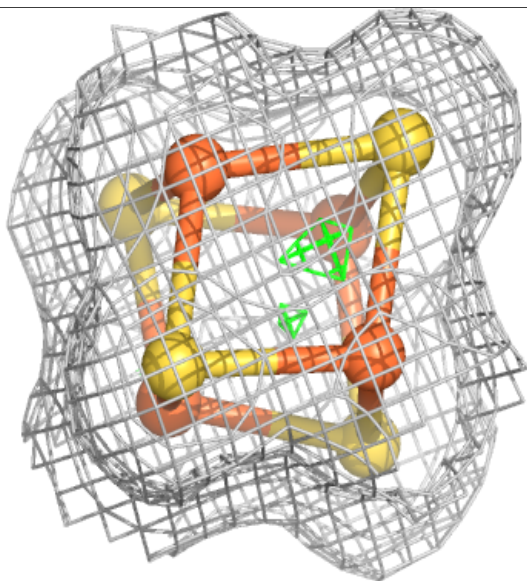
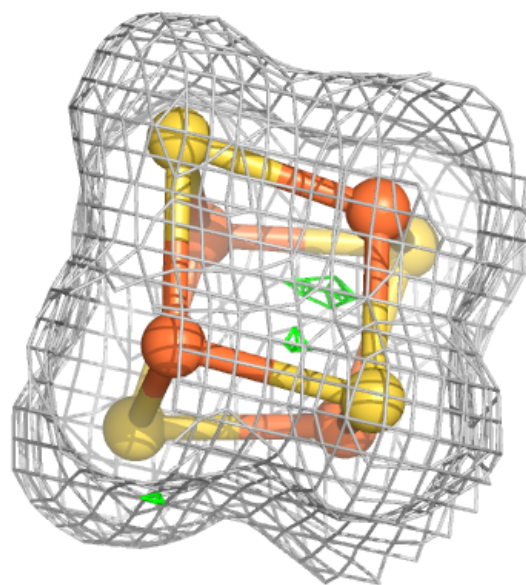
Electron density around SF4 C 1101:

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



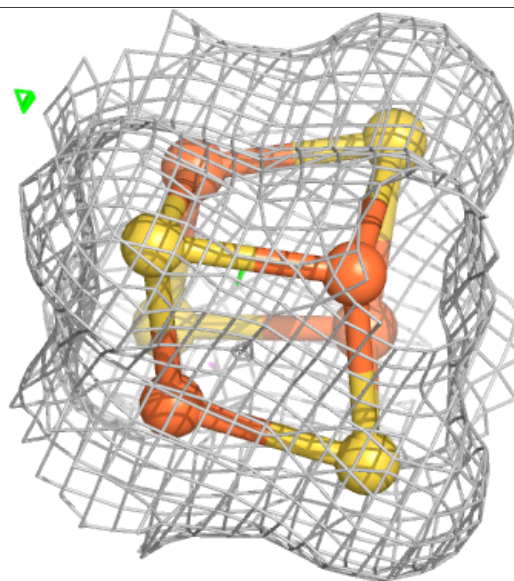
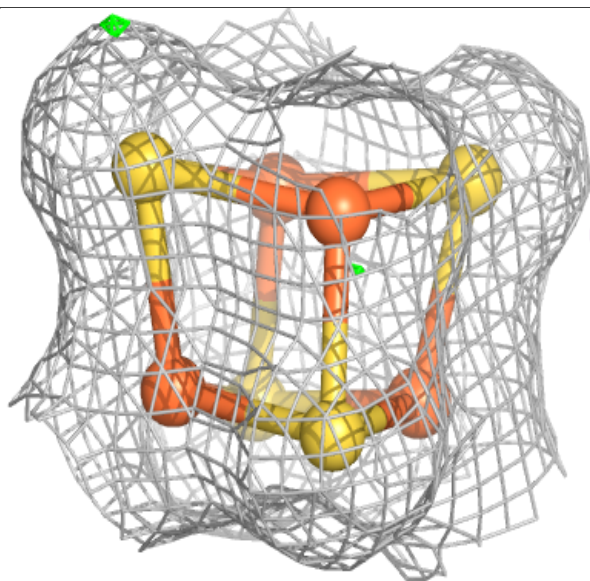
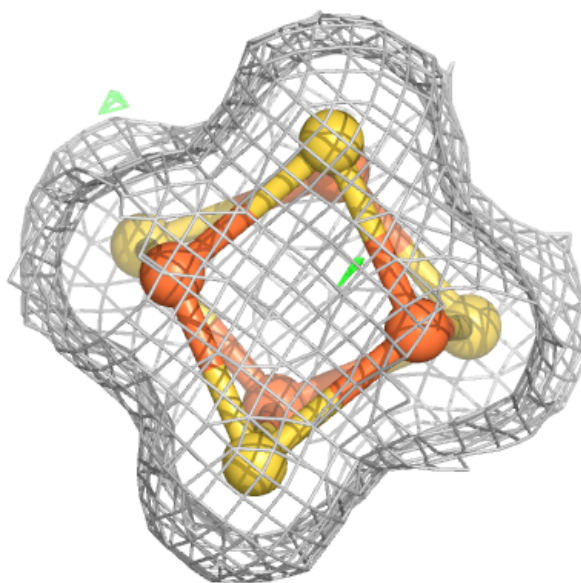
Electron density around SF4 C 1102:

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



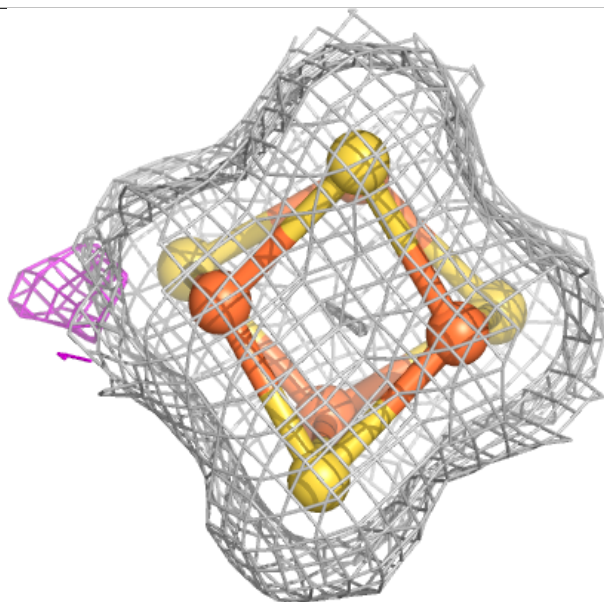
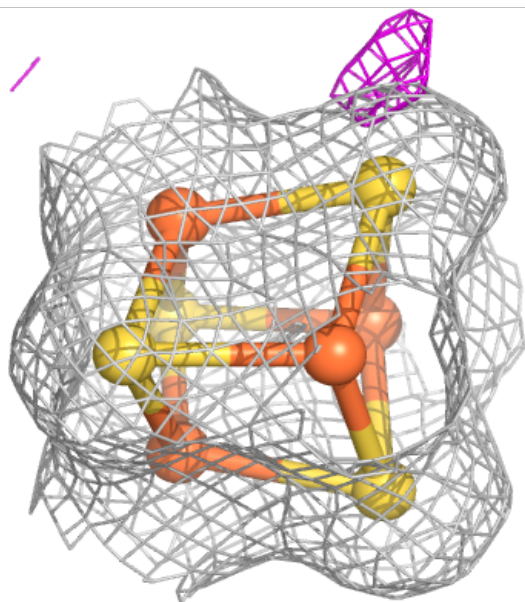
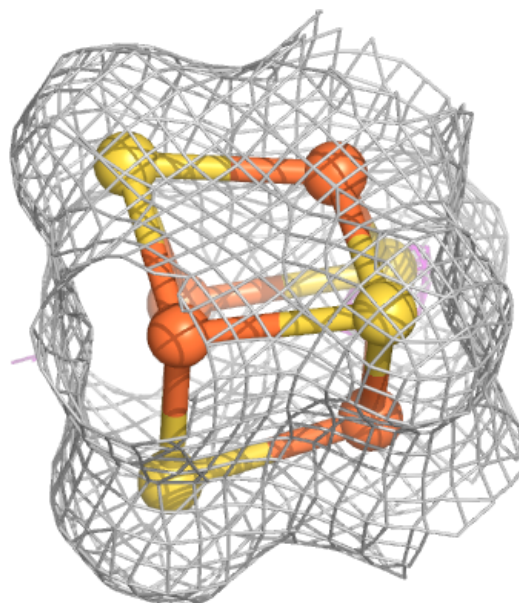
Electron density around SF4 C 1103:

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



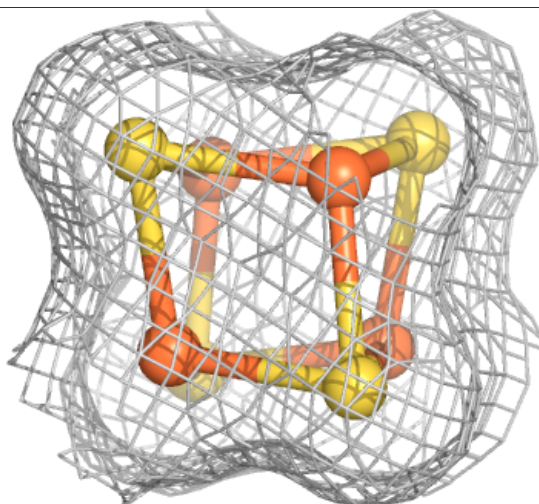
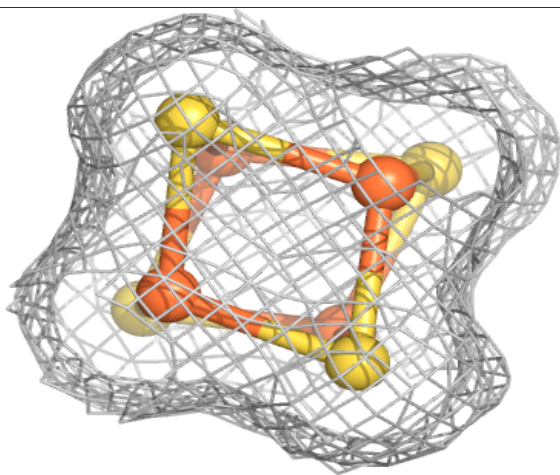
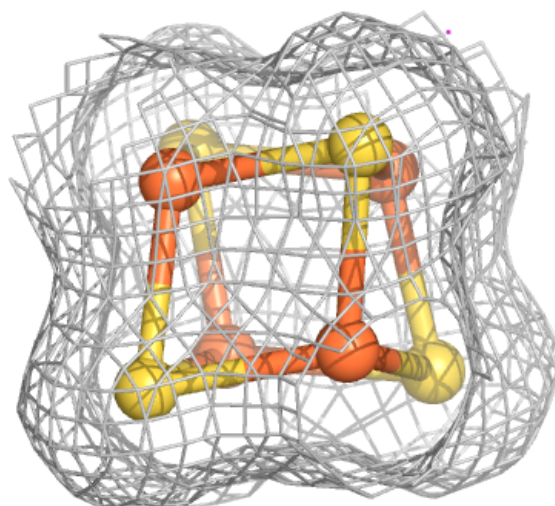
Electron density around SF4 C 1104:

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



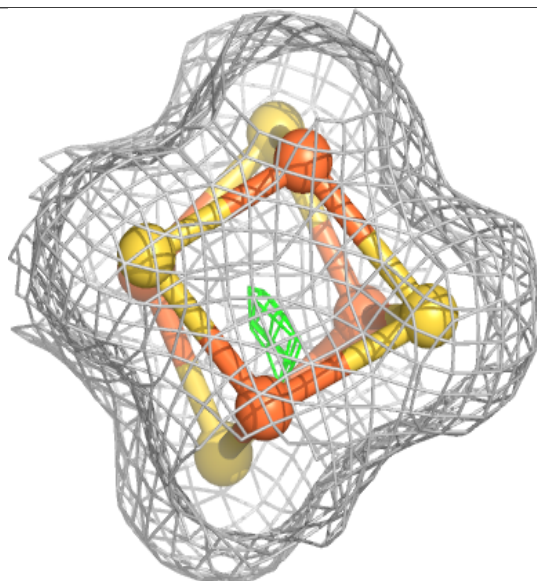
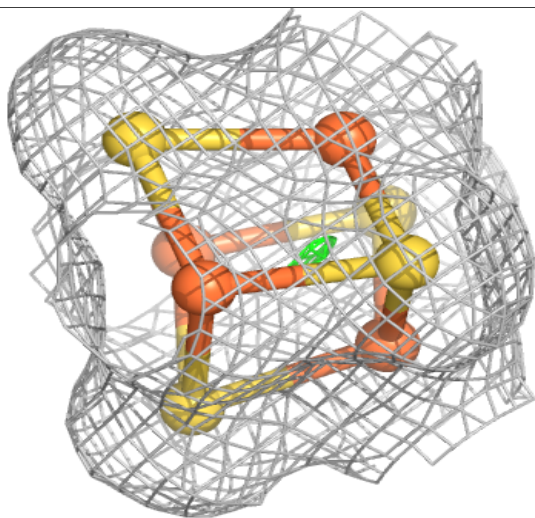
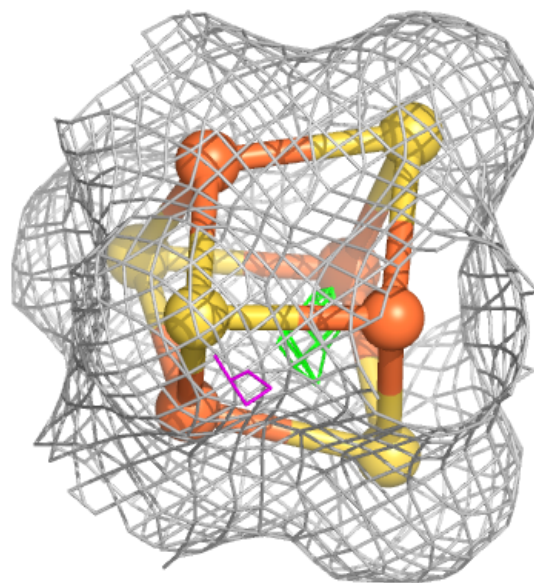
Electron density around SF4 D 1101:

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



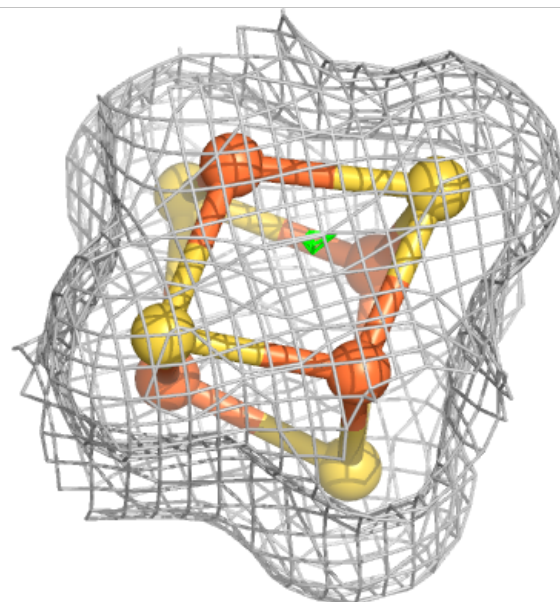
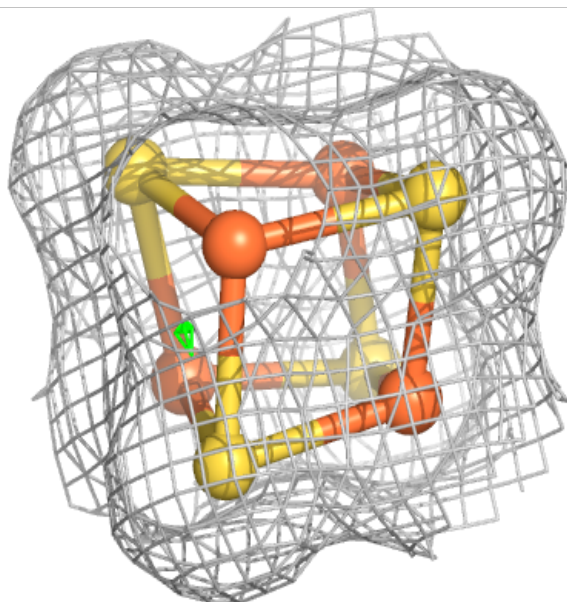
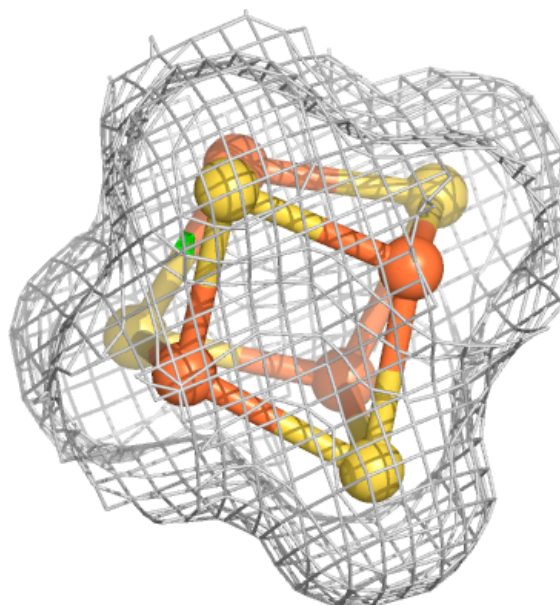
Electron density around SF4 D 1102:

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



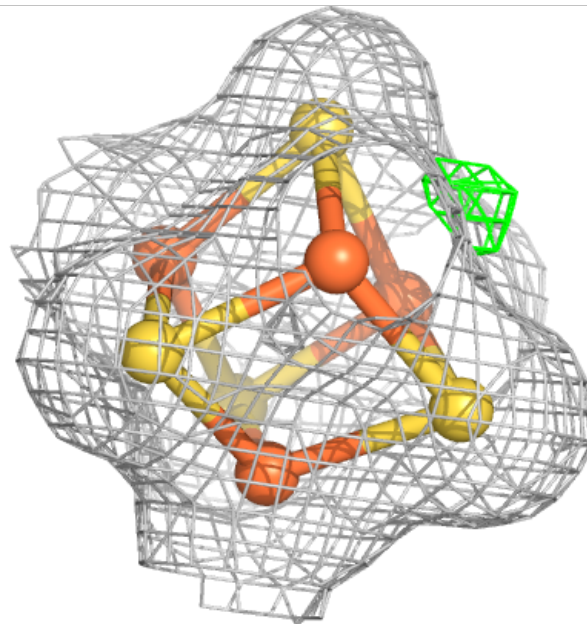
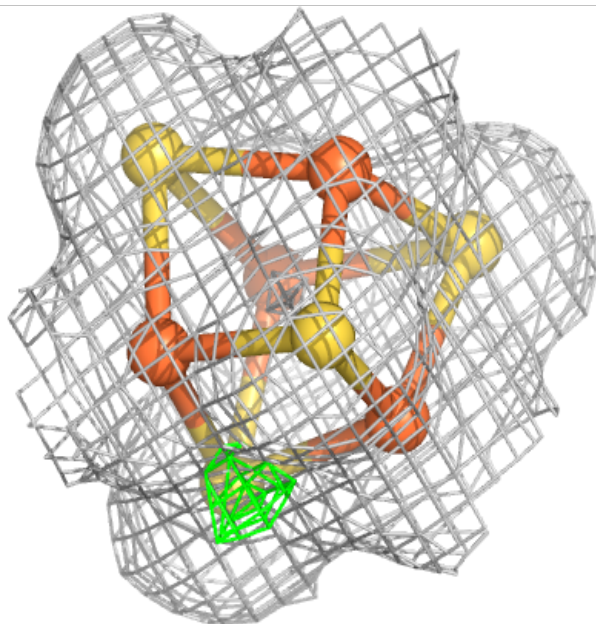
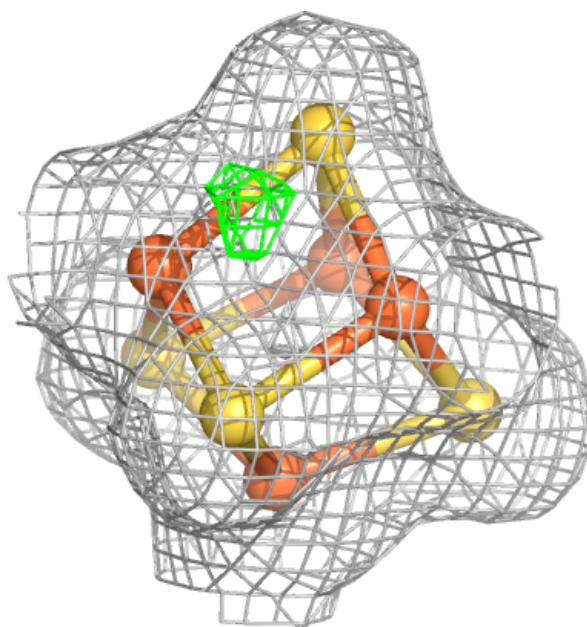
Electron density around SF4 D 1104:

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



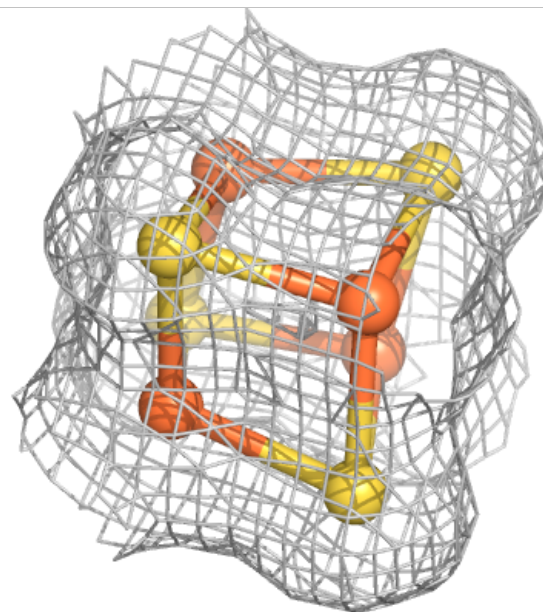
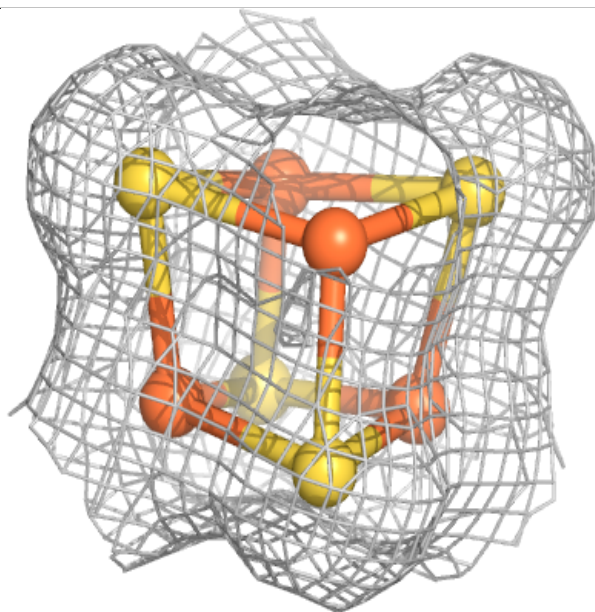
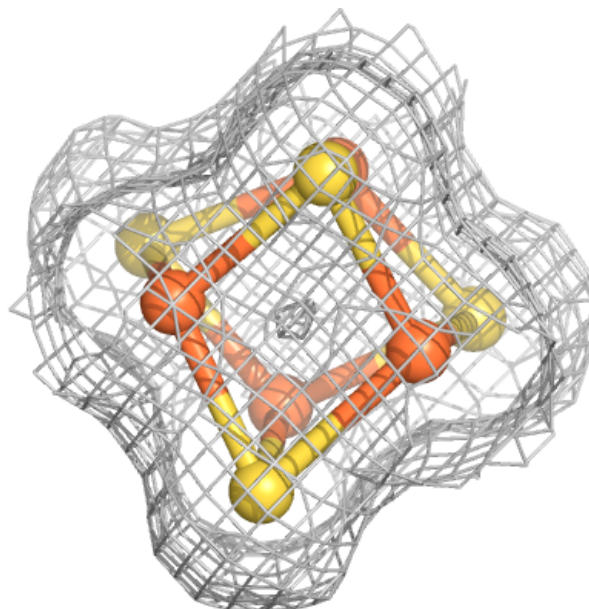
Electron density around SF4 A 1101:

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



Electron density around SF4 D 1103:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.