



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:37 PM UTC

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

This is a 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

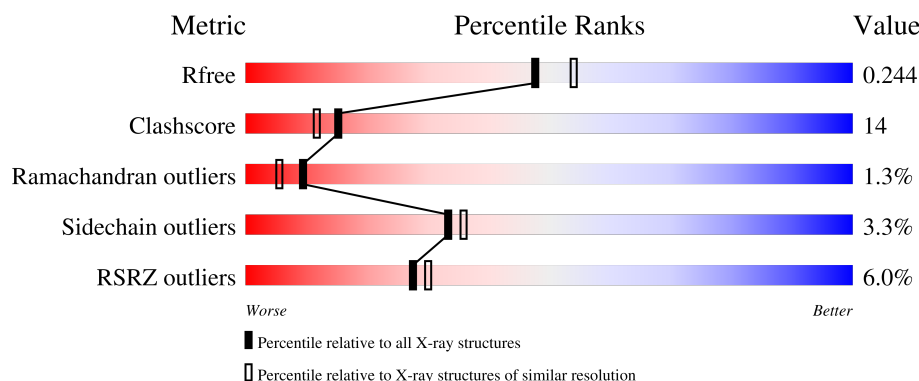
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1025	5% 65% 29% • •
1	B	1025	6% 66% 27% • •
1	C	1025	5% 66% 28% • •
1	D	1025	7% 65% 29% • • •

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

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

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

2 Entry composition

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

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

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

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

There are 36 discrepancies between the modelled and reference sequences:

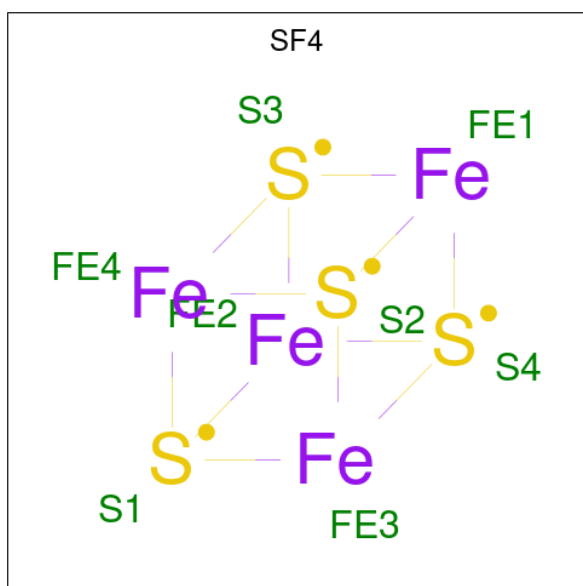
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
A	671	SER	CYS	engineered mutation	UNP Q28943
A	1019	LEU	-	expression tag	UNP Q28943
A	1020	ALA	-	expression tag	UNP Q28943
A	1021	VAL	-	expression tag	UNP Q28943
A	1022	ASN	-	expression tag	UNP Q28943
A	1023	PRO	-	expression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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



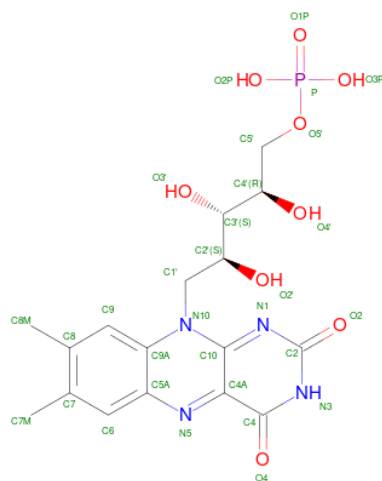
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0

Continued on next page...

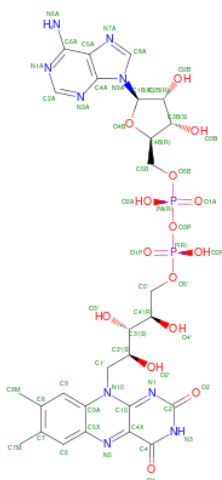
Continued from previous page...

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

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

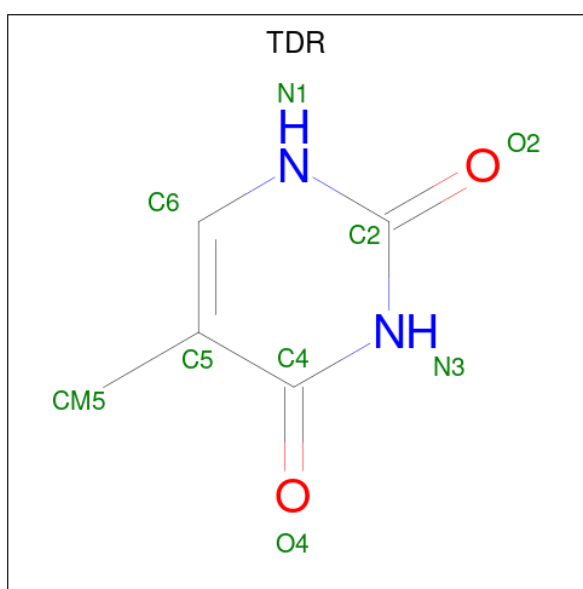


- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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



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

- Molecule 6 is water.

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

Continued on next page...

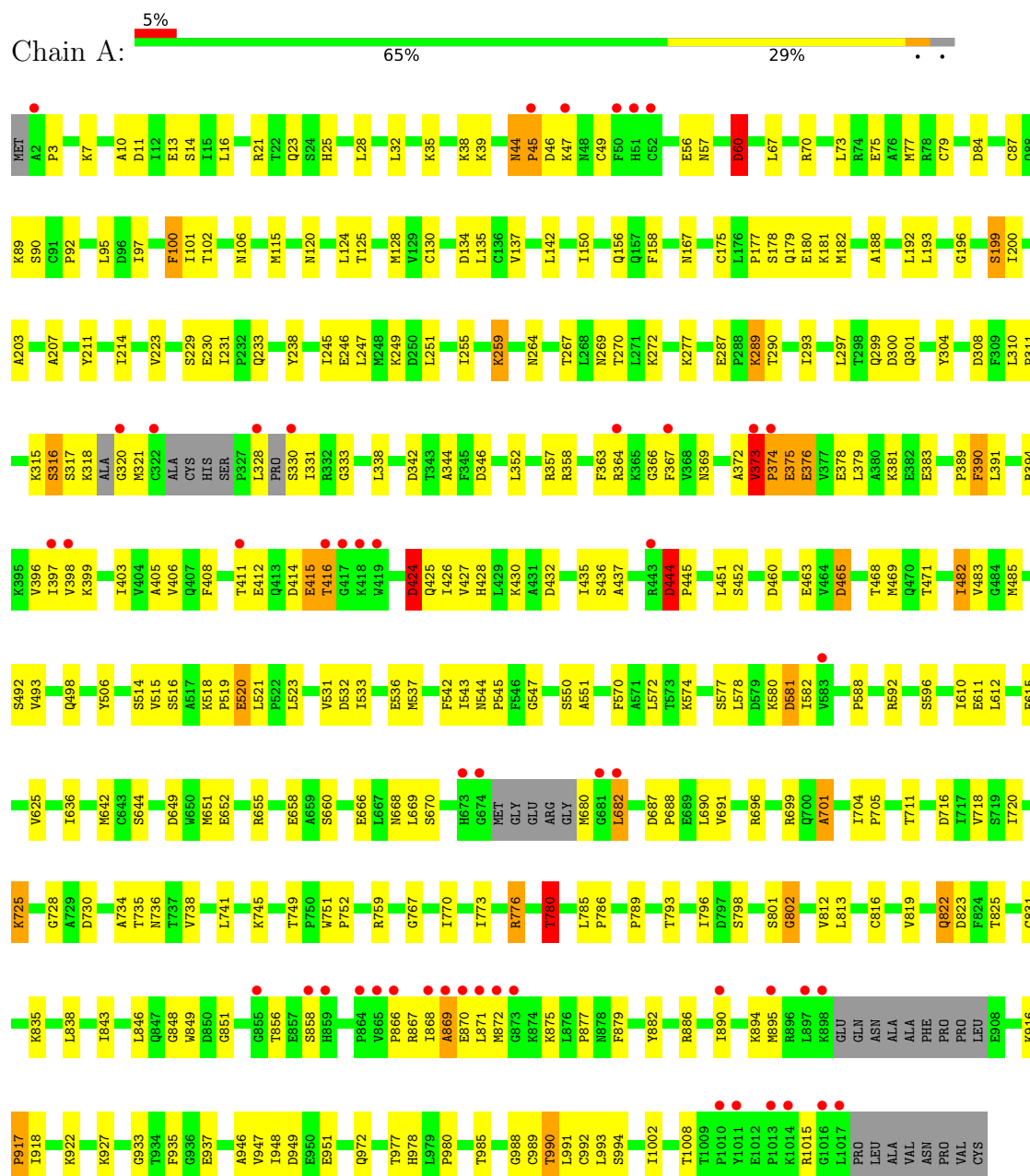
Continued from previous page...

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

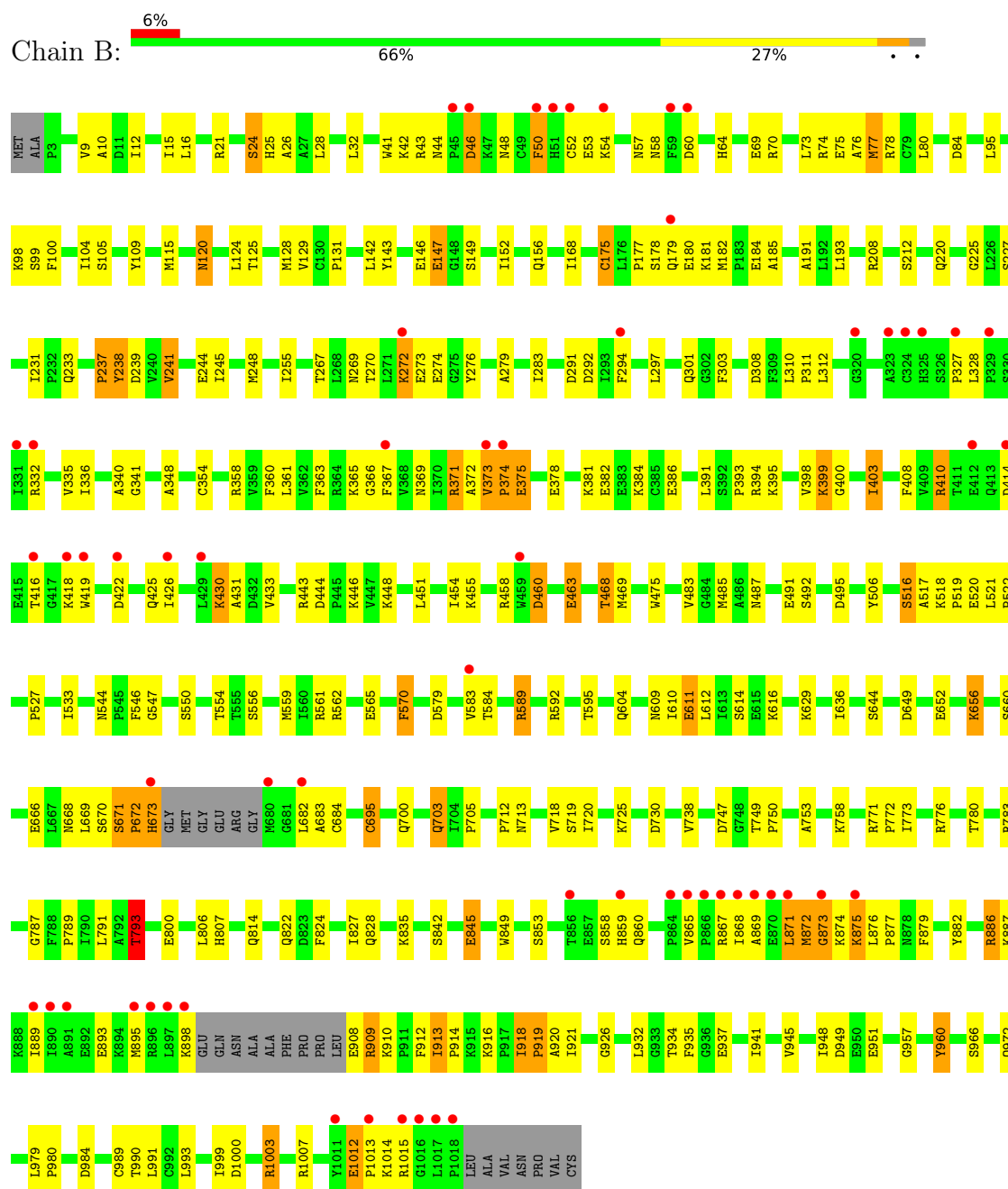
3 Residue-property plots

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

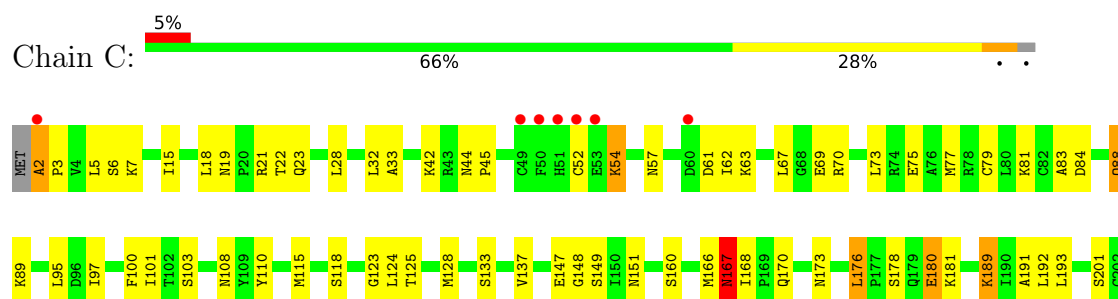
- Molecule 1: Dihydropyrimidine dehydrogenase [NAD(+)]

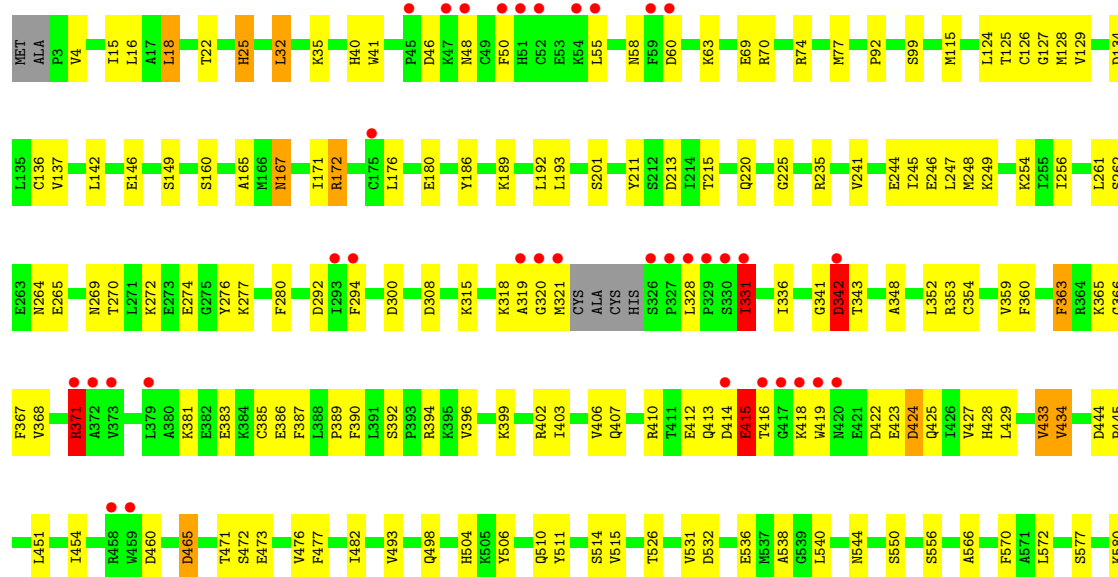


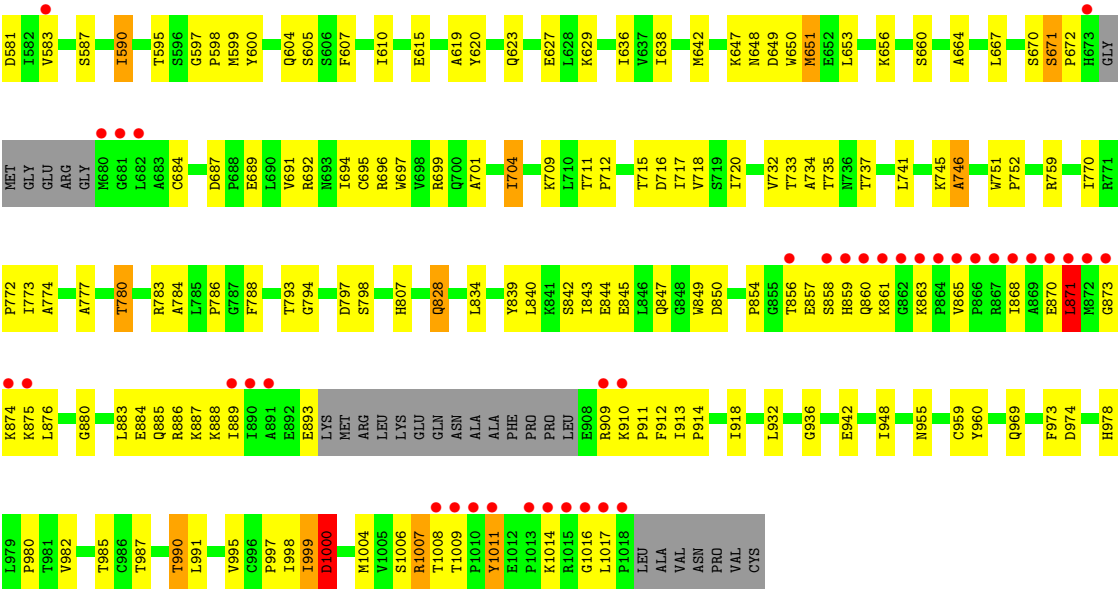
- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



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

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

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

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

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	671	SER	C-N	-31.50	0.96	1.33
1	B	671	SER	C-N	-9.55	1.11	1.33
1	A	652	GLU	CG-CD	8.38	1.73	1.52
1	D	828	GLN	CG-CD	7.96	1.72	1.52
1	B	175	CYS	CB-SG	7.67	2.06	1.81
1	A	666	GLU	CD-OE1	7.21	1.39	1.25
1	D	671	SER	C-N	-7.18	1.25	1.33
1	A	259	LYS	CE-NZ	6.97	1.70	1.49
1	B	695	CYS	CB-SG	6.90	2.04	1.81
1	B	60	ASP	CB-CG	6.88	1.69	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	GLU	CG-CD	6.78	1.69	1.52
1	D	342	ASP	CG-OD2	6.75	1.38	1.25
1	C	908	GLU	CB-CG	6.69	1.72	1.52
1	C	666	GLU	CD-OE2	6.58	1.37	1.25
1	A	106	ASN	CG-OD1	6.56	1.36	1.23
1	D	460	ASP	CB-CG	6.53	1.68	1.52
1	A	536	GLU	CG-CD	6.53	1.68	1.52
1	B	828	GLN	CG-CD	6.46	1.68	1.52
1	B	381	LYS	CB-CG	6.41	1.71	1.52
1	B	918	ILE	CG1-CD1	-6.36	1.26	1.51
1	D	371	ARG	CG-CD	6.36	1.71	1.52
1	B	16	LEU	CA-C	6.35	1.63	1.52
1	C	88	GLN	CD-NE2	6.30	1.46	1.33
1	B	609	ASN	CB-CG	6.26	1.67	1.52
1	B	104	ILE	CB-CG2	-6.23	1.31	1.52
1	A	60	ASP	CB-CG	6.20	1.67	1.52
1	A	373	VAL	C-N	6.19	1.48	1.33
1	D	264	ASN	CB-CG	6.18	1.67	1.52
1	A	725	LYS	CD-CE	6.16	1.71	1.52
1	B	984	ASP	CB-CG	6.12	1.67	1.52
1	C	517	ALA	C-N	6.09	1.46	1.33
1	B	152	ILE	C-N	6.05	1.42	1.33
1	C	2	ALA	CA-C	6.03	1.65	1.52
1	B	468	THR	CB-CG2	-6.01	1.32	1.52
1	A	246	GLU	CG-CD	6.01	1.67	1.52
1	A	838	LEU	CG-CD1	6.01	1.72	1.52
1	C	758	LYS	CG-CD	6.00	1.70	1.52
1	C	487	ASN	CB-CG	5.97	1.67	1.52
1	D	712	PRO	CG-CD	5.94	1.71	1.50
1	C	845	GLU	CG-CD	5.93	1.66	1.52
1	D	828	GLN	CB-CG	5.93	1.70	1.52
1	A	819	VAL	CB-CG1	5.89	1.72	1.52
1	B	793	THR	CA-CB	5.88	1.65	1.53
1	C	525	TYR	CZ-OH	5.87	1.50	1.38
1	B	554	THR	CB-CG2	-5.85	1.33	1.52
1	C	758	LYS	CD-CE	5.84	1.70	1.52
1	C	167	ASN	CB-CG	-5.84	1.37	1.52
1	B	147	GLU	CD-OE2	5.82	1.36	1.25
1	C	803	LEU	CG-CD2	5.74	1.71	1.52
1	B	913	ILE	C-N	5.73	1.40	1.33
1	B	570	PHE	C-O	5.71	1.30	1.23
1	B	75	GLU	CD-OE1	5.71	1.36	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	920	ALA	C-O	5.70	1.31	1.23
1	A	922	LYS	CE-NZ	5.68	1.66	1.49
1	D	969	GLN	CD-NE2	5.64	1.45	1.33
1	D	134	ASP	CG-OD1	5.63	1.36	1.25
1	C	625	VAL	CB-CG2	-5.63	1.33	1.52
1	B	960	TYR	CZ-OH	5.62	1.49	1.38
1	A	156	GLN	CD-OE1	5.62	1.34	1.23
1	C	583	VAL	CB-CG2	5.59	1.71	1.52
1	B	147	GLU	CG-CD	5.58	1.66	1.52
1	D	371	ARG	CZ-NH2	5.58	1.40	1.33
1	C	272	LYS	CD-CE	5.55	1.69	1.52
1	B	670	SER	C-N	-5.53	1.03	1.34
1	A	848	GLY	CA-C	5.53	1.59	1.51
1	A	77	MET	SD-CE	5.51	1.93	1.79
1	D	597	GLY	C-N	5.51	1.46	1.33
1	D	424	ASP	CB-CG	5.50	1.65	1.52
1	A	84	ASP	CG-OD1	5.50	1.35	1.25
1	B	495	ASP	CB-CG	5.45	1.65	1.52
1	D	498	GLN	CD-OE1	5.44	1.33	1.23
1	A	444	ASP	CG-OD1	5.44	1.35	1.25
1	A	725	LYS	CE-NZ	5.38	1.65	1.49
1	C	960	TYR	CZ-OH	5.38	1.49	1.38
1	D	715	THR	CB-CG2	-5.38	1.34	1.52
1	A	736	ASN	CG-ND2	5.38	1.44	1.33
1	B	835	LYS	CD-CE	-5.37	1.36	1.52
1	B	381	LYS	CG-CD	5.33	1.68	1.52
1	B	544	ASN	CG-OD1	5.33	1.33	1.23
1	C	203	ALA	C-O	5.33	1.30	1.24
1	A	532	ASP	CB-CG	5.33	1.65	1.52
1	B	546	PHE	C-N	5.33	1.40	1.33
1	D	745	LYS	CE-NZ	5.32	1.65	1.49
1	B	120	ASN	CG-OD1	5.31	1.33	1.23
1	D	704	ILE	CG1-CD1	5.29	1.72	1.51
1	D	746	ALA	C-N	5.28	1.42	1.33
1	B	77	MET	CB-CG	-5.27	1.36	1.52
1	A	776	ARG	CG-CD	-5.20	1.36	1.52
1	C	825	THR	CA-C	5.19	1.59	1.52
1	D	1000	ASP	CB-CG	-5.18	1.39	1.52
1	C	730	ASP	CB-CG	5.16	1.65	1.52
1	B	181	LYS	CG-CD	5.13	1.67	1.52
1	D	60	ASP	CB-CG	5.12	1.64	1.52
1	A	381	LYS	CB-CG	-5.08	1.37	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	793	THR	CA-CB	5.08	1.64	1.54
1	B	272	LYS	CG-CD	5.08	1.67	1.52
1	C	245[A]	ILE	C-N	5.08	1.41	1.34
1	C	245[B]	ILE	C-N	5.08	1.41	1.34
1	B	824	PHE	CD1-CE1	5.07	1.53	1.38
1	C	950	GLU	CD-OE2	5.07	1.34	1.25
1	D	695	CYS	CB-SG	5.07	1.98	1.81
1	C	260	SER	CA-CB	-5.06	1.44	1.53
1	A	120	ASN	CB-CG	-5.06	1.39	1.52
1	B	824	PHE	CD2-CE2	5.06	1.53	1.38
1	D	280	PHE	CD2-CE2	5.06	1.53	1.38
1	B	527	PRO	CG-CD	5.05	1.68	1.50
1	A	16	LEU	CG-CD1	5.04	1.69	1.52
1	C	2	ALA	C-N	5.03	1.45	1.33
1	D	995	VAL	CB-CG1	5.02	1.69	1.52
1	D	171	ILE	CB-CG2	-5.02	1.35	1.52
1	B	656	LYS	CD-CE	5.01	1.67	1.52
1	D	544	ASN	CG-OD1	5.01	1.33	1.23
1	C	908	GLU	CG-CD	5.01	1.64	1.52
1	A	531	VAL	C-N	5.01	1.40	1.33

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	670	SER	O-C-N	-23.24	93.76	122.35
1	D	167[A]	ASN	CA-C-N	11.34	132.72	122.85
1	D	167[A]	ASN	C-N-CA	11.34	132.72	122.85
1	D	167[B]	ASN	CA-C-N	11.34	132.72	122.85
1	D	167[B]	ASN	C-N-CA	11.34	132.72	122.85
1	B	670	SER	O-C-N	-10.94	104.80	122.42
1	D	186	TYR	CA-C-N	-8.74	109.50	122.86
1	D	186	TYR	C-N-CA	-8.74	109.50	122.86
1	B	283	ILE	N-CA-C	-8.73	104.19	112.83
1	C	681	GLY	N-CA-C	8.70	123.01	112.48
1	D	32	LEU	CB-CG-CD1	-8.30	85.79	110.70
1	C	758	LYS	CG-CD-CE	8.26	130.29	111.30
1	D	15	ILE	CG1-CB-CG2	-8.11	86.39	110.70
1	C	21	ARG	CG-CD-NE	-8.04	94.32	112.00
1	C	168	ILE	N-CA-C	7.87	115.40	108.63
1	C	669	LEU	CD1-CG-CD2	-7.84	93.54	110.80
1	A	463	GLU	CA-C-N	-7.68	110.55	122.68
1	A	463	GLU	C-N-CA	-7.68	110.55	122.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	SER	CA-CB-OG	-7.56	95.98	111.10
1	A	544	ASN	CA-C-N	-7.52	112.37	120.94
1	A	544	ASN	C-N-CA	-7.52	112.37	120.94
1	C	118	SER	CA-C-N	-7.45	109.38	122.26
1	C	118	SER	C-N-CA	-7.45	109.38	122.26
1	C	766	SER	CA-CB-OG	-7.41	96.28	111.10
1	B	212	SER	CA-C-N	-7.36	111.91	123.24
1	B	212	SER	C-N-CA	-7.36	111.91	123.24
1	B	463	GLU	CA-C-N	-7.35	113.03	123.03
1	B	463	GLU	C-N-CA	-7.35	113.03	123.03
1	D	1006	SER	CA-C-N	-7.21	109.87	120.75
1	D	1006	SER	C-N-CA	-7.21	109.87	120.75
1	D	684	CYS	CA-CB-SG	-7.11	98.04	114.40
1	A	780	THR	OG1-CB-CG2	-7.11	95.09	109.30
1	D	99	SER	CA-C-N	-7.10	108.61	120.68
1	D	99	SER	C-N-CA	-7.10	108.61	120.68
1	B	24	SER	CA-CB-OG	-7.07	96.97	111.10
1	C	720	ILE	CG1-CB-CG2	-6.96	89.81	110.70
1	A	130	CYS	CA-CB-SG	6.92	130.31	114.40
1	D	595	THR	CA-C-N	-6.89	112.95	122.87
1	D	595	THR	C-N-CA	-6.89	112.95	122.87
1	A	317	SER	CA-C-N	-6.88	111.79	122.59
1	A	317	SER	C-N-CA	-6.88	111.79	122.59
1	A	574	LYS	CG-CD-CE	-6.86	95.51	111.30
1	A	444	ASP	N-CA-C	6.82	124.88	109.81
1	C	950	GLU	CA-CB-CG	6.81	127.73	114.10
1	D	1000	ASP	CB-CA-C	-6.80	97.38	110.65
1	C	916	LYS	N-CA-C	-6.75	99.77	110.10
1	C	845	GLU	CB-CG-CD	6.68	123.96	112.60
1	A	90	SER	CA-CB-OG	-6.65	97.80	111.10
1	A	142	LEU	O-C-N	-6.64	111.78	122.41
1	C	23	GLN	CA-C-N	-6.62	108.90	121.15
1	C	23	GLN	C-N-CA	-6.62	108.90	121.15
1	D	850	ASP	CA-C-N	-6.61	108.72	121.01
1	D	850	ASP	C-N-CA	-6.61	108.72	121.01
1	B	371	ARG	CA-CB-CG	6.60	127.30	114.10
1	C	308	ASP	CB-CA-C	-6.55	99.78	110.79
1	A	851	GLY	CA-C-N	-6.54	111.31	122.56
1	A	851	GLY	C-N-CA	-6.54	111.31	122.56
1	B	403	ILE	CA-C-N	-6.51	110.25	121.97
1	B	403	ILE	C-N-CA	-6.51	110.25	121.97
1	D	1008	THR	CA-C-N	6.46	140.75	122.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1008	THR	C-N-CA	6.46	140.75	122.21
1	A	259	LYS	CG-CD-CE	6.46	126.15	111.30
1	B	614	SER	CA-C-N	-6.46	111.88	122.54
1	B	614	SER	C-N-CA	-6.46	111.88	122.54
1	B	584	THR	CA-C-N	-6.45	109.07	122.03
1	B	584	THR	C-N-CA	-6.45	109.07	122.03
1	A	780	THR	CA-CB-OG1	-6.42	99.97	109.60
1	C	211	TYR	CA-CB-CG	-6.36	102.45	113.90
1	B	241	VAL	CA-C-N	-6.26	111.26	120.28
1	B	241	VAL	C-N-CA	-6.26	111.26	120.28
1	B	700	GLN	CA-CB-CG	6.22	126.54	114.10
1	C	263	GLU	CB-CG-CD	6.15	123.05	112.60
1	B	671	SER	CA-C-N	6.12	127.49	119.84
1	B	671	SER	C-N-CA	6.12	127.49	119.84
1	A	128	MET	CA-CB-CG	-6.09	101.91	114.10
1	B	25	HIS	CB-CA-C	6.08	121.73	109.38
1	B	393	PRO	CA-C-N	6.07	131.83	122.42
1	B	393	PRO	C-N-CA	6.07	131.83	122.42
1	B	595	THR	CA-C-N	-6.06	111.68	123.13
1	B	595	THR	C-N-CA	-6.06	111.68	123.13
1	D	598	PRO	CA-C-N	6.05	130.47	122.42
1	D	598	PRO	C-N-CA	6.05	130.47	122.42
1	A	736	ASN	N-CA-C	-6.03	100.74	109.31
1	C	103	SER	CA-CB-OG	-6.02	99.06	111.10
1	C	274	GLU	CA-C-N	-5.99	113.17	122.69
1	C	274	GLU	C-N-CA	-5.99	113.17	122.69
1	A	994	SER	N-CA-C	5.99	119.41	111.75
1	A	199	SER	CA-C-N	-5.97	112.28	120.46
1	A	199	SER	C-N-CA	-5.97	112.28	120.46
1	B	128	MET	CA-CB-CG	-5.97	102.16	114.10
1	A	701	ALA	CA-C-N	-5.95	114.35	122.92
1	A	701	ALA	C-N-CA	-5.95	114.35	122.92
1	C	189	LYS	CD-CE-NZ	5.90	130.78	111.90
1	B	562	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	C	246	GLU	CB-CG-CD	5.88	122.60	112.60
1	B	824	PHE	CA-C-N	-5.88	110.17	121.94
1	B	824	PHE	C-N-CA	-5.88	110.17	121.94
1	C	847	GLN	CA-CB-CG	-5.88	102.34	114.10
1	C	500	SER	CA-C-N	-5.88	112.80	120.44
1	C	500	SER	C-N-CA	-5.88	112.80	120.44
1	C	685	GLY	CA-C-N	-5.88	112.45	122.56
1	C	685	GLY	C-N-CA	-5.88	112.45	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	780	THR	OG1-CB-CG2	-5.87	97.56	109.30
1	B	238	TYR	CA-C-N	-5.85	109.59	121.18
1	B	238	TYR	C-N-CA	-5.85	109.59	121.18
1	B	872	MET	CG-SD-CE	-5.84	88.05	100.90
1	B	99	SER	CA-C-N	-5.81	111.47	120.31
1	B	99	SER	C-N-CA	-5.81	111.47	120.31
1	C	961	MET	CA-CB-CG	-5.81	102.48	114.10
1	A	798	SER	CA-CB-OG	-5.79	99.53	111.10
1	D	445	PRO	CA-N-CD	-5.77	103.92	112.00
1	D	587	SER	CA-CB-OG	5.75	122.61	111.10
1	A	625	VAL	CA-CB-CG2	-5.73	100.65	110.40
1	B	175	CYS	CA-CB-SG	5.73	127.58	114.40
1	D	433	VAL	CA-C-N	-5.72	114.98	122.94
1	D	433	VAL	C-N-CA	-5.72	114.98	122.94
1	D	660	SER	CA-C-N	-5.72	114.73	122.63
1	D	660	SER	C-N-CA	-5.72	114.73	122.63
1	A	831	CYS	CA-CB-SG	-5.71	101.26	114.40
1	D	220	GLN	CA-CB-CG	-5.71	102.67	114.10
1	D	69	GLU	CB-CG-CD	5.71	122.30	112.60
1	B	984	ASP	CA-C-N	-5.69	112.77	122.56
1	B	984	ASP	C-N-CA	-5.69	112.77	122.56
1	C	404	VAL	CA-C-N	-5.69	112.07	121.80
1	C	404	VAL	C-N-CA	-5.69	112.07	121.80
1	B	147	GLU	CA-CB-CG	5.67	125.44	114.10
1	B	381	LYS	CB-CG-CD	5.67	124.34	111.30
1	B	354	CYS	CA-CB-SG	-5.66	101.38	114.40
1	A	642	MET	CG-SD-CE	-5.64	88.48	100.90
1	B	16	LEU	CA-C-O	-5.64	109.88	118.91
1	B	15	ILE	CG1-CB-CG2	-5.64	93.79	110.70
1	D	556	SER	CA-CB-OG	-5.63	99.84	111.10
1	B	583	VAL	N-CA-CB	-5.61	105.37	112.60
1	A	363	PHE	CA-C-N	5.58	132.20	121.54
1	A	363	PHE	C-N-CA	5.58	132.20	121.54
1	C	950	GLU	CB-CG-CD	5.58	122.08	112.60
1	B	948	ILE	N-CA-C	5.56	115.95	108.17
1	D	590	ILE	CG1-CB-CG2	-5.55	94.03	110.70
1	A	520	GLU	CB-CG-CD	5.53	122.00	112.60
1	D	1016	GLY	CA-C-N	5.52	133.63	122.70
1	D	1016	GLY	C-N-CA	5.52	133.63	122.70
1	C	707	PHE	CA-C-N	-5.52	114.41	122.19
1	C	707	PHE	C-N-CA	-5.52	114.41	122.19
1	C	750	PRO	CA-C-N	-5.52	111.47	122.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	750	PRO	C-N-CA	-5.52	111.47	122.40
1	A	316	SER	CA-C-N	-5.51	113.84	122.49
1	A	316	SER	C-N-CA	-5.51	113.84	122.49
1	A	471	THR	CA-CB-OG1	-5.51	101.34	109.60
1	C	593	GLY	N-CA-C	-5.50	104.28	113.02
1	D	798	SER	CA-CB-OG	-5.48	100.13	111.10
1	D	444	ASP	N-CA-C	5.47	117.48	109.71
1	B	793	THR	OG1-CB-CG2	-5.43	98.44	109.30
1	D	514	SER	CA-CB-OG	-5.42	100.26	111.10
1	C	932	LEU	CB-CG-CD2	-5.41	94.47	110.70
1	D	25	HIS	CA-C-N	-5.41	114.59	122.65
1	D	25	HIS	C-N-CA	-5.41	114.59	122.65
1	D	1007	ARG	N-CA-C	-5.37	103.05	110.35
1	D	959	CYS	CA-C-N	5.36	127.41	120.44
1	D	959	CYS	C-N-CA	5.36	127.41	120.44
1	B	272	LYS	CG-CD-CE	5.36	123.62	111.30
1	A	403	ILE	CA-C-N	-5.35	114.04	121.53
1	A	403	ILE	C-N-CA	-5.35	114.04	121.53
1	D	653	LEU	CB-CG-CD2	-5.34	94.69	110.70
1	C	719	SER	CA-C-N	-5.34	112.84	120.42
1	C	719	SER	C-N-CA	-5.34	112.84	120.42
1	D	656	LYS	CA-C-N	-5.31	111.75	121.52
1	D	656	LYS	C-N-CA	-5.31	111.75	121.52
1	A	523	LEU	CB-CG-CD1	-5.29	94.82	110.70
1	A	73	LEU	CD1-CG-CD2	-5.29	99.16	110.80
1	B	611	GLU	CA-CB-CG	-5.29	103.52	114.10
1	C	61	ASP	CA-C-N	-5.28	114.82	122.69
1	C	61	ASP	C-N-CA	-5.28	114.82	122.69
1	D	590	ILE	CA-CB-CG2	5.28	119.48	110.50
1	C	927	LYS	CA-CB-CG	-5.28	103.55	114.10
1	A	802	GLY	N-CA-C	-5.27	106.40	112.83
1	C	201	SER	CA-CB-OG	-5.27	100.56	111.10
1	B	276	TYR	CA-CB-CG	-5.25	104.44	113.90
1	D	264	ASN	CA-CB-CG	5.25	117.85	112.60
1	D	651	MET	CG-SD-CE	-5.25	89.34	100.90
1	C	402	ARG	CG-CD-NE	5.23	123.50	112.00
1	D	991	LEU	CA-CB-CG	-5.22	98.03	116.30
1	C	1000	ASP	CB-CA-C	-5.21	104.19	111.80
1	A	660	SER	CA-CB-OG	-5.21	100.68	111.10
1	A	115	MET	CG-SD-CE	-5.21	89.44	100.90
1	C	482	ILE	CG1-CB-CG2	-5.19	95.13	110.70
1	B	611	GLU	CB-CG-CD	5.16	121.38	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	GLU	CA-CB-CG	-5.15	103.79	114.10
1	B	610	ILE	CB-CG1-CD1	5.14	124.60	113.80
1	D	35	LYS	CA-C-N	-5.13	111.95	120.68
1	D	35	LYS	C-N-CA	-5.13	111.95	120.68
1	A	917	PRO	CA-C-N	-5.13	111.51	120.59
1	A	917	PRO	C-N-CA	-5.13	111.51	120.59
1	C	770	ILE	CA-CB-CG2	5.12	119.21	110.50
1	B	237	PRO	N-CA-C	-5.12	103.25	111.38
1	C	968	TYR	CA-CB-CG	-5.12	104.69	113.90
1	B	104	ILE	CA-CB-CG2	-5.11	101.81	110.50
1	C	233	GLN	CA-C-N	-5.11	111.62	121.58
1	C	233	GLN	C-N-CA	-5.11	111.62	121.58
1	D	422	ASP	CA-C-N	5.10	128.84	120.63
1	D	422	ASP	C-N-CA	5.10	128.84	120.63
1	A	158	PHE	CA-C-N	-5.08	113.47	120.28
1	A	158	PHE	C-N-CA	-5.08	113.47	120.28
1	A	424	ASP	N-CA-CB	-5.08	101.50	110.39
1	A	14	SER	N-CA-CB	-5.07	102.64	110.20
1	D	172	ARG	CB-CG-CD	-5.06	99.66	111.30
1	D	371	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	581	ASP	CA-CB-CG	5.05	117.66	112.60
1	D	249	LYS	CG-CD-CE	5.05	122.92	111.30
1	B	533	ILE	CG1-CB-CG2	-5.05	95.56	110.70
1	A	230	GLU	CA-C-N	-5.04	112.80	122.13
1	A	230	GLU	C-N-CA	-5.04	112.80	122.13
1	D	716	ASP	N-CA-C	5.04	118.24	107.70
1	C	583	VAL	CG1-CB-CG2	5.03	121.86	110.80
1	C	178	SER	CA-CB-OG	-5.02	101.05	111.10
1	A	688	PRO	CA-C-N	-5.02	112.68	120.31
1	A	688	PRO	C-N-CA	-5.02	112.68	120.31
1	A	985	THR	CA-CB-CG2	5.01	119.02	110.50
1	A	596	SER	CA-CB-OG	-5.01	101.09	111.10
1	C	703	GLN	CA-CB-CG	-5.00	104.10	114.10

There are no chirality outliers.

All (31) planarity outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	696	ARG	Sidechain
1	A	70	ARG	Sidechain
1	A	759	ARG	Sidechain
1	A	886	ARG	Sidechain
1	B	1003	ARG	Sidechain
1	B	21	ARG	Sidechain
1	B	372	ALA	Peptide
1	B	373	VAL	Peptide
1	B	410[A]	ARG	Sidechain
1	B	410[B]	ARG	Sidechain
1	B	443	ARG	Sidechain
1	B	589	ARG	Sidechain
1	B	776	ARG	Sidechain
1	B	871	LEU	Peptide
1	B	886	ARG	Sidechain
1	B	919	PRO	Peptide
1	C	1003	ARG	Sidechain
1	C	319	ALA	Peptide
1	C	333	GLY	Peptide
1	C	422	ASP	Peptide
1	D	318	LYS	Peptide
1	D	371	ARG	Sidechain
1	D	696	ARG	Sidechain
1	D	70	ARG	Sidechain
1	D	74	ARG	Sidechain
1	D	783	ARG	Sidechain
1	D	871	LEU	Peptide

5.2 Too-close contacts

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	32	0	0	3	0
2	D	32	0	0	1	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
3	C	31	0	19	1	0
3	D	31	0	19	1	0
4	A	53	0	31	1	0
4	B	53	0	31	2	0
4	C	53	0	31	1	0
4	D	53	0	31	2	0
5	A	9	0	6	1	0
5	B	9	0	6	0	0
5	C	9	0	6	0	0
5	D	9	0	6	0	0
6	A	149	0	0	24	0
6	B	141	0	0	23	0
6	C	159	0	0	18	0
6	D	144	0	0	10	0
All	All	31607	0	30861	841	0

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

All (841) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:NZ	1:A:259:LYS:CE	1.70	1.53
1:B:695:CYS:CB	1:B:695:CYS:SG	2.04	1.46
1:B:175:CYS:SG	1:B:175:CYS:CB	2.06	1.42
1:B:414:ASP:HB3	1:B:416:THR:HG22	1.32	1.09
1:B:115:MET:SD	6:B:1334:HOH:O	2.08	1.08
1:B:394:ARG:NH1	6:B:1201:HOH:O	1.90	1.02
1:B:399:LYS:NZ	6:B:1202:HOH:O	1.94	0.99
1:C:410:ARG:NH2	6:C:1202:HOH:O	1.85	0.97
1:B:341:GLY:HA2	1:B:371:ARG:HB3	1.49	0.93
1:C:381:LYS:HE2	1:D:381:LYS:HE2	1.50	0.93
1:C:246:GLU:OE2	6:C:1201:HOH:O	1.84	0.93
1:D:1011:TYR:OH	6:D:1201:HOH:O	1.85	0.92
1:A:32:LEU:HD13	1:B:485:MET:HE1	1.53	0.89
1:A:373:VAL:O	1:A:376:GLU:N	2.06	0.88
1:C:886:ARG:HA	1:C:889:ILE:HD12	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:LYS:HD2	1:A:917:PRO:HD2	1.55	0.87
1:B:783:ARG:NH2	6:B:1207:HOH:O	2.07	0.86
1:C:220:GLN:NE2	6:C:1203:HOH:O	1.88	0.85
1:D:604:GLN:OE1	6:D:1202:HOH:O	1.93	0.84
1:A:728:GLY:O	6:A:1202:HOH:O	1.94	0.83
1:C:613:ILE:HG21	1:C:642:MET:HE2	1.61	0.83
1:B:373:VAL:O	1:B:375:GLU:N	2.11	0.82
1:B:233:GLN:HE22	1:B:238:TYR:H	1.27	0.82
1:A:46:ASP:HB3	1:A:49:CYS:HB3	1.60	0.82
1:C:850:ASP:OD1	6:C:1204:HOH:O	2.00	0.80
1:A:776:ARG:HD3	6:A:1214:HOH:O	1.80	0.80
1:B:518:LYS:NZ	6:B:1209:HOH:O	2.12	0.80
1:B:416:THR:HG23	1:B:418:LYS:H	1.45	0.80
1:B:332:ARG:NH2	6:B:1211:HOH:O	2.14	0.79
1:A:651:MET:O	1:A:655:ARG:HG3	1.83	0.79
1:C:448:LYS:HE2	1:C:460:ASP:OD1	1.83	0.78
1:B:592:ARG:O	6:B:1204:HOH:O	2.00	0.78
1:B:46:ASP:OD2	1:B:48:ASN:HB2	1.84	0.77
1:B:875:LYS:O	1:B:876:LEU:HD23	1.83	0.77
1:D:570:PHE:HB2	1:D:636:ILE:HB	1.65	0.77
1:B:73:LEU:O	1:B:77:MET:HG3	1.86	0.76
1:D:193:LEU:HD12	1:D:261:LEU:HB2	1.67	0.76
1:A:872:MET:O	6:A:1204:HOH:O	2.03	0.76
1:A:651:MET:HG2	1:A:701:ALA:HB2	1.66	0.75
1:D:246:GLU:HG3	1:D:909:ARG:HG2	1.67	0.75
1:B:358:ARG:NH1	6:B:1203:HOH:O	1.96	0.75
1:C:124:LEU:HD13	1:C:160:SER:HB2	1.68	0.75
1:B:703:GLN:NE2	6:B:1213:HOH:O	2.18	0.75
1:B:42:LYS:HE3	1:B:44:ASN:OD1	1.86	0.74
1:B:604:GLN:OE1	6:B:1205:HOH:O	2.06	0.74
1:C:718:VAL:HG23	1:C:780:THR:HG23	1.69	0.73
1:C:592:ARG:O	6:C:1207:HOH:O	2.07	0.73
1:A:658:GLU:O	6:A:1205:HOH:O	2.07	0.73
1:B:966:SER:O	6:B:1206:HOH:O	2.06	0.73
1:D:844:GLU:O	1:D:847:GLN:HG2	1.88	0.73
1:B:893:GLU:N	6:B:1215:HOH:O	2.22	0.73
1:B:556:SER:HB2	1:B:559:MET:HE3	1.71	0.72
1:B:1000:ASP:HB3	1:B:1003:ARG:HH21	1.54	0.72
1:D:396:VAL:HG13	1:D:406:VAL:HG22	1.69	0.72
1:A:615:GLU:OE2	1:B:1013:PRO:HB2	1.88	0.72
1:B:990:THR:HG22	1:B:990:THR:O	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:GLN:HB2	1:C:419:TRP:CZ3	2.23	0.72
1:C:583:VAL:HA	6:C:1210:HOH:O	1.90	0.72
1:C:870:GLU:OE1	1:C:874:LYS:HD3	1.89	0.72
1:C:976:GLU:OE2	6:C:1205:HOH:O	2.06	0.72
1:B:125:THR:O	1:B:129:VAL:HG22	1.90	0.72
1:C:54:LYS:HG2	1:C:895:MET:HE1	1.72	0.71
1:C:220:GLN:HG3	1:C:222:TYR:CE2	2.25	0.71
1:B:267:THR:OG1	1:B:270:THR:HG23	1.91	0.71
1:C:584:THR:N	6:C:1210:HOH:O	2.23	0.71
1:B:233:GLN:HA	1:B:233:GLN:HE21	1.55	0.71
1:C:583:VAL:CA	6:C:1210:HOH:O	2.38	0.70
1:B:291:ASP:OD1	1:B:292:ASP:N	2.24	0.69
1:B:867:ARG:C	1:B:872:MET:HE1	2.18	0.69
1:D:581:ASP:OD2	6:D:1203:HOH:O	2.09	0.69
1:D:415:GLU:CD	1:D:416:THR:H	2.00	0.69
2:C:1102:SF4:FE3	2:C:1102:SF4:S2	1.84	0.69
1:A:60:ASP:OD2	1:A:894:LYS:NZ	2.26	0.69
1:C:416:THR:OG1	1:C:418:LYS:HE2	1.93	0.68
1:B:589:ARG:HD2	1:B:611:GLU:HG3	1.75	0.68
1:C:413:GLN:HG2	1:C:417:GLY:HA2	1.76	0.68
1:A:299:GLN:NE2	1:A:308:ASP:HB3	2.08	0.68
1:B:666:GLU:OE1	6:B:1208:HOH:O	2.12	0.68
1:A:35:LYS:O	1:A:39:LYS:NZ	2.27	0.68
2:A:1103:SF4:FE2	2:A:1103:SF4:S3	1.87	0.67
1:C:537:MET:HE1	1:C:791:LEU:HD21	1.76	0.67
1:B:394:ARG:HB3	1:B:395:LYS:HD2	1.76	0.67
1:D:860:GLN:OE1	6:D:1204:HOH:O	2.12	0.67
1:C:173:ASN:HB3	1:C:176:LEU:HD12	1.75	0.67
1:D:580:LYS:NZ	1:D:649:ASP:OD2	2.28	0.67
1:D:870:GLU:C	1:D:874:LYS:HG3	2.20	0.67
1:C:306:SER:OG	6:C:1208:HOH:O	2.13	0.66
1:C:364:ARG:H	1:C:364:ARG:HD3	1.60	0.66
1:A:47:LYS:HE2	1:B:374:PRO:HD3	1.78	0.66
1:B:1014:LYS:O	6:B:1210:HOH:O	2.12	0.65
2:B:1101:SF4:FE1	2:B:1101:SF4:S2	1.87	0.65
1:D:550:SER:HB2	1:D:572:LEU:HB3	1.77	0.65
1:C:291:ASP:OD1	1:C:293:ILE:HG23	1.96	0.65
1:A:682:LEU:H	1:A:682:LEU:HD23	1.62	0.64
2:D:1101:SF4:FE2	2:D:1101:SF4:S1	1.89	0.64
1:B:9:VAL:CG2	1:B:12:ILE:HG12	2.28	0.64
1:C:535:VAL:HG22	1:C:536:GLU:N	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:999:ILE:O	1:D:1000:ASP:HB2	1.97	0.64
1:C:220:GLN:HG3	1:C:222:TYR:CZ	2.32	0.64
1:C:593:GLY:HA2	1:C:742:MET:SD	2.37	0.64
2:B:1103:SF4:FE4	2:B:1103:SF4:S1	1.89	0.64
1:A:398:VAL:O	1:A:399:LYS:HG3	1.97	0.63
2:A:1102:SF4:FE2	2:A:1102:SF4:S4	1.90	0.63
2:A:1103:SF4:FE3	2:A:1103:SF4:S4	1.90	0.63
1:B:652:GLU:OE2	6:B:1212:HOH:O	2.15	0.63
1:B:793:THR:HB	1:B:814:GLN:HB2	1.80	0.63
1:A:424:ASP:OD2	1:A:425:GLN:NE2	2.31	0.63
1:B:868:ILE:HG22	1:B:869:ALA:H	1.64	0.63
1:B:451:LEU:HD13	1:B:454:ILE:HD11	1.80	0.63
1:A:7:LYS:NZ	6:A:1213:HOH:O	2.30	0.63
1:A:669:LEU:HD13	1:A:691:VAL:HG22	1.80	0.63
1:A:846:LEU:HD22	1:A:849:TRP:CE2	2.34	0.63
1:B:867:ARG:HA	1:B:872:MET:CE	2.28	0.63
1:B:868:ILE:N	1:B:872:MET:HE1	2.14	0.63
1:B:873:GLY:C	1:B:874:LYS:HD3	2.24	0.62
1:A:427:VAL:HG13	1:B:410[A]:ARG:HD2	1.80	0.62
1:D:845:GLU:OE1	1:D:845:GLU:N	2.33	0.62
1:A:367:PHE:HB2	1:B:386:GLU:OE1	1.99	0.62
1:A:776:ARG:NH1	6:A:1214:HOH:O	2.32	0.62
1:A:867:ARG:HH12	1:A:951:GLU:HG3	1.63	0.62
1:A:318:LYS:O	1:A:320:GLY:N	2.33	0.62
1:A:389:PRO:HB2	1:A:390:PHE:CD2	2.35	0.62
1:A:993:LEU:C	1:A:993:LEU:HD23	2.25	0.62
1:A:376:GLU:OE1	1:A:376:GLU:HA	2.00	0.61
1:A:543:ILE:N	6:A:1201:HOH:O	1.86	0.61
1:B:378:GLU:O	1:B:382:GLU:HG2	2.00	0.61
1:D:842:SER:OG	1:D:914:PRO:HB3	2.00	0.61
1:C:373:VAL:O	1:C:375:GLU:N	2.33	0.61
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.83	0.61
2:C:1102:SF4:FE1	2:C:1102:SF4:S4	1.91	0.61
1:B:272:LYS:NZ	6:B:1220:HOH:O	2.32	0.61
1:C:647:LYS:O	1:C:651:MET:HG3	2.01	0.61
1:D:577[A]:SER:OG	1:D:642:MET:O	2.16	0.60
1:C:88:GLN:HG3	1:C:95:LEU:O	2.02	0.60
1:C:189:LYS:HE2	1:C:213:ASP:OD2	2.01	0.60
1:D:570:PHE:CB	1:D:636:ILE:HB	2.31	0.60
1:D:860:GLN:HG2	6:D:1204:HOH:O	2.01	0.60
1:B:629:LYS:HE2	1:B:629:LYS:HA	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:THR:OG1	1:C:270:THR:HG23	2.02	0.60
1:B:74:ARG:HD2	6:B:1249:HOH:O	2.00	0.60
1:B:989:CYS:O	1:B:990:THR:HB	2.02	0.60
1:B:845:GLU:HG3	1:B:912:PHE:CD1	2.37	0.60
1:B:867:ARG:CA	1:B:872:MET:HE1	2.31	0.60
1:A:378:GLU:OE2	1:A:378:GLU:HA	2.02	0.60
1:B:787:GLY:O	1:B:789:PRO:HD3	2.02	0.59
1:A:786:PRO:HB2	1:D:942:GLU:HG2	1.83	0.59
1:B:867:ARG:HA	1:B:872:MET:HE1	1.84	0.59
1:C:962[A]:THR:HG21	1:C:991:LEU:HB3	1.83	0.59
1:A:373:VAL:O	1:A:375:GLU:N	2.35	0.59
1:A:927:LYS:NZ	1:D:936:GLY:O	2.31	0.59
1:C:57:ASN:HD22	1:C:898:LYS:HD2	1.67	0.59
1:A:611:GLU:O	5:A:1107:TDR:H6	2.02	0.59
1:B:747:ASP:OD1	1:B:749:THR:HG23	2.02	0.59
1:C:791:LEU:HD12	1:C:791:LEU:N	2.18	0.59
1:B:556:SER:CB	1:B:559:MET:HE3	2.33	0.59
1:C:533:ILE:O	1:C:545:PRO:HD3	2.03	0.59
1:C:948:ILE:HD13	1:C:980:PRO:HG2	1.86	0.58
1:A:223:VAL:HG23	1:A:245[A]:ILE:HD13	1.85	0.58
1:A:267:THR:OG1	1:A:270:THR:HG23	2.03	0.58
1:A:948:ILE:HD13	1:A:980:PRO:HG2	1.84	0.58
1:C:285:LEU:HB3	1:C:440:SER:HB3	1.84	0.58
1:C:949:ASP:HB2	1:C:1003:ARG:HH21	1.67	0.58
1:D:262:SER:HB3	1:D:265:GLU:H	1.67	0.58
1:C:191:ALA:O	1:C:279:ALA:HA	2.04	0.58
1:A:28:LEU:HD22	1:B:519:PRO:HB3	1.85	0.58
1:A:483:VAL:HG12	1:A:485:MET:HG3	1.86	0.58
1:A:741:LEU:O	1:B:772:PRO:HA	2.04	0.57
1:A:786:PRO:HB2	1:D:942:GLU:CG	2.34	0.57
1:C:205:PHE:CD1	1:C:521:LEU:HD13	2.39	0.57
1:C:272:LYS:NZ	6:C:1209:HOH:O	2.14	0.57
1:B:341:GLY:CA	1:B:371:ARG:HB3	2.31	0.57
1:B:934:THR:HG23	1:B:937:GLU:OE1	2.05	0.57
1:C:413:GLN:CG	1:C:417:GLY:HA2	2.34	0.57
1:A:428:HIS:HB2	1:B:425:GLN:NE2	2.18	0.57
1:D:269:ASN:O	1:D:270:THR:C	2.47	0.57
1:A:316:SER:OG	1:A:328:LEU:HD23	2.04	0.57
1:C:783:ARG:HG3	1:C:929:LEU:HD22	1.86	0.57
1:D:394:ARG:HB3	1:D:407:GLN:O	2.05	0.57
1:A:180:GLU:HG2	1:A:181:LYS:HD3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.05	0.57
1:D:651:MET:HE3	1:D:701:ALA:HB2	1.85	0.57
1:A:822:GLN:O	1:A:823:ASP:HB3	2.05	0.57
1:B:233:GLN:HE22	1:B:238:TYR:N	1.98	0.57
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.86	0.57
1:A:379:LEU:O	1:A:383:GLU:HG3	2.04	0.57
1:D:360:PHE:CD1	1:D:386:GLU:HB3	2.41	0.56
1:D:506:TYR:O	1:D:510:GLN:HG2	2.06	0.56
1:D:985:THR:O	1:D:1014:LYS:NZ	2.37	0.56
1:B:673:HIS:NE2	1:B:682:LEU:O	2.37	0.56
1:C:411:THR:HA	1:C:420:ASN:O	2.05	0.56
1:A:188:ALA:HB1	1:A:277:LYS:HG3	1.86	0.56
1:A:518:LYS:HD2	1:A:518:LYS:C	2.30	0.56
1:C:386:GLU:OE1	1:D:368:VAL:HG23	2.04	0.56
1:C:482:ILE:HG12	1:C:482:ILE:O	2.04	0.56
1:D:390:PHE:HB2	1:D:410[B]:ARG:NH1	2.21	0.56
1:B:70:ARG:HB2	1:B:999:ILE:HG13	1.87	0.56
1:A:498:GLN:HA	1:B:28:LEU:HD11	1.87	0.56
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.87	0.56
1:C:776:ARG:NH1	6:C:1218:HOH:O	2.37	0.56
1:A:100:PHE:CD1	1:A:100:PHE:C	2.84	0.56
1:A:315:LYS:CG	1:A:321:MET:HE2	2.36	0.56
1:C:54:LYS:HB3	1:C:891:ALA:HB1	1.87	0.56
1:B:336:ILE:HD12	1:B:431:ALA:CB	2.34	0.56
1:B:233:GLN:HE21	1:B:233:GLN:CA	2.14	0.56
1:C:844:GLU:O	1:C:847:GLN:HG2	2.06	0.56
1:A:373:VAL:HG23	1:A:376:GLU:HB2	1.88	0.55
1:C:170:GLN:OE1	1:C:251:LEU:HD11	2.06	0.55
1:D:115:MET:HE2	6:D:1221:HOH:O	2.05	0.55
1:A:424:ASP:OD1	1:A:424:ASP:N	2.27	0.55
1:C:749:THR:HG21	1:C:758:LYS:HD2	1.89	0.55
1:D:870:GLU:O	1:D:871:LEU:HB2	2.06	0.55
1:B:177:PRO:HD2	1:B:182:MET:SD	2.46	0.55
1:C:110:TYR:CD1	1:C:110:TYR:C	2.85	0.55
1:D:193:LEU:CD1	1:D:261:LEU:HB2	2.36	0.55
1:D:506:TYR:CD1	1:D:506:TYR:C	2.84	0.55
1:A:333:GLY:HA3	1:A:432:ASP:OD2	2.07	0.55
1:C:223:VAL:HG23	1:C:245[A]:ILE:HD13	1.87	0.55
1:D:353:ARG:NH1	1:D:383:GLU:OE2	2.40	0.55
1:A:776:ARG:HG2	1:A:776:ARG:O	2.07	0.55
1:D:241:VAL:O	1:D:245:ILE:HG12	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:GLN:HG3	1:D:419:TRP:CE2	2.41	0.55
1:A:580:LYS:HB3	6:A:1203:HOH:O	2.06	0.55
1:D:331:ILE:HD12	1:D:433:VAL:HG21	1.89	0.55
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.07	0.54
1:B:561:ARG:O	1:B:565:GLU:HG3	2.06	0.54
1:C:856:THR:HG22	1:C:857:GLU:O	2.08	0.54
1:A:428:HIS:H	1:B:425:GLN:NE2	2.05	0.54
1:A:338:LEU:O	1:A:437:ALA:HB3	2.06	0.54
1:C:193:LEU:HD13	1:C:217:PHE:HB2	1.90	0.54
1:D:638:ILE:HG12	1:D:664:ALA:HB3	1.88	0.54
1:A:612:LEU:HD11	1:B:935:PHE:CE1	2.43	0.54
1:A:427:VAL:HG11	1:B:410[B]:ARG:HD2	1.90	0.54
1:A:427:VAL:CG1	1:B:410[A]:ARG:HD2	2.37	0.54
1:C:689:GLU:HA	1:C:692:ARG:HH12	1.73	0.54
1:D:718:VAL:CG2	1:D:780:THR:HG22	2.38	0.54
1:A:56:GLU:OE2	1:A:895:MET:SD	2.66	0.54
1:A:877:PRO:HD2	1:A:882:TYR:CG	2.43	0.54
1:B:239:ASP:HB2	1:B:909:ARG:HH22	1.73	0.54
1:A:44:ASN:HB2	1:A:45:PRO:HD2	1.90	0.53
1:A:38:LYS:NZ	6:A:1207:HOH:O	2.17	0.53
1:A:990:THR:HG22	1:A:990:THR:O	2.07	0.53
1:B:340:ALA:HB2	1:B:363:PHE:CD1	2.44	0.53
1:C:654:SER:HB2	1:C:665:LEU:HD11	1.89	0.53
1:D:999:ILE:O	1:D:999:ILE:HG22	2.09	0.53
1:A:843:ILE:HG21	1:A:846:LEU:HD12	1.89	0.53
1:C:949:ASP:HB2	1:C:1003:ARG:NH2	2.23	0.53
1:D:165:ALA:O	1:D:167[A]:ASN:ND2	2.41	0.53
1:A:580:LYS:NZ	1:A:649:ASP:OD1	2.36	0.53
6:C:1229:HOH:O	1:D:807:HIS:HD2	1.91	0.53
1:D:55:LEU:O	1:D:58:ASN:HB2	2.08	0.53
1:A:75:GLU:OE2	1:A:150:ILE:HA	2.09	0.53
1:A:328:LEU:C	1:A:330:SER:N	2.67	0.53
1:A:396:VAL:HG22	1:A:406:VAL:HG22	1.91	0.53
1:B:9:VAL:HG23	1:B:12:ILE:HG12	1.91	0.53
1:A:28:LEU:HD22	1:B:519:PRO:CB	2.38	0.53
1:A:297:LEU:HA	1:A:301:GLN:OE1	2.08	0.53
1:A:871:LEU:C	1:A:872:MET:HE3	2.34	0.53
1:C:97:ILE:HA	1:C:100:PHE:CD2	2.44	0.53
1:C:331:ILE:HD12	1:C:433:VAL:HG21	1.89	0.53
1:D:849:TRP:N	1:D:849:TRP:CD1	2.75	0.53
1:B:98:LYS:HE2	1:B:822:GLN:NE2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:HD11	1:C:975:PRO:HA	1.91	0.53
1:C:32:LEU:O	1:C:33:ALA:C	2.52	0.53
1:D:642:MET:CE	1:D:670:SER:HB2	2.39	0.53
1:A:193:LEU:HD22	1:A:193:LEU:N	2.24	0.53
1:B:373:VAL:C	1:B:375:GLU:H	2.11	0.52
1:D:532:ASP:OD1	1:D:532:ASP:C	2.51	0.52
1:A:935:PHE:CE1	1:B:612:LEU:HD11	2.44	0.52
1:B:233:GLN:HA	1:B:233:GLN:NE2	2.22	0.52
1:A:408:PHE:O	1:A:426:ILE:HA	2.09	0.52
1:B:10:ALA:N	6:B:1225:HOH:O	2.41	0.52
1:C:414:ASP:O	1:C:416:THR:N	2.40	0.52
1:B:871:LEU:HD11	1:B:886:ARG:HG2	1.91	0.52
1:C:410:ARG:NH1	1:C:425:GLN:OE1	2.41	0.52
1:D:213:ASP:OD1	1:D:254:LYS:NZ	2.24	0.52
1:A:373:VAL:CG2	1:A:376:GLU:HB2	2.40	0.52
1:B:241:VAL:O	1:B:245:ILE:HG12	2.09	0.52
1:D:180:GLU:CD	1:D:180:GLU:N	2.68	0.52
1:D:583:VAL:O	1:D:615:GLU:HG2	2.10	0.52
1:D:691:VAL:HG21	1:D:720:ILE:HG23	1.91	0.52
1:B:695:CYS:SG	1:B:695:CYS:CA	2.93	0.52
1:B:868:ILE:O	1:B:872:MET:HE2	2.10	0.52
1:A:357:ARG:HH22	1:A:430:LYS:HD3	1.75	0.52
1:A:468:THR:O	1:A:469:MET:HB2	2.09	0.52
1:D:415:GLU:OE2	1:D:415:GLU:N	2.43	0.51
1:C:375:GLU:O	1:C:378:GLU:HB3	2.09	0.51
1:D:341:GLY:HA2	1:D:371:ARG:HB3	1.92	0.51
1:D:651:MET:HG2	1:D:701:ALA:HB2	1.92	0.51
1:A:414:ASP:O	1:A:416:THR:N	2.42	0.51
1:B:718:VAL:HG23	1:B:780:THR:CG2	2.40	0.51
1:C:89:LYS:HD3	1:D:41:TRP:CZ2	2.45	0.51
1:D:124:LEU:HD13	1:D:160:SER:HB2	1.92	0.51
1:A:238:TYR:O	1:A:238:TYR:CD1	2.63	0.51
1:A:427:VAL:CG1	1:B:410[B]:ARG:HD2	2.40	0.51
1:B:791:LEU:N	1:B:791:LEU:HD12	2.26	0.51
1:C:180:GLU:OE2	1:C:180:GLU:N	2.27	0.51
1:A:92:PRO:HD3	1:A:135:LEU:HD22	1.91	0.51
1:B:69:GLU:OE2	1:B:853:SER:HB3	2.11	0.51
1:D:137:VAL:HG13	1:D:149:SER:HB3	1.93	0.51
1:D:415:GLU:CD	1:D:416:THR:N	2.67	0.51
1:A:518:LYS:HD2	1:A:518:LYS:O	2.10	0.51
1:A:592:ARG:NH1	6:A:1217:HOH:O	2.35	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ALA:HB1	1:B:105:SER:HB3	1.92	0.51
1:B:233:GLN:NE2	1:B:237:PRO:HA	2.26	0.51
1:B:859:HIS:O	1:B:860:GLN:HG2	2.10	0.51
1:D:328:LEU:HD21	1:D:354:CYS:HA	1.92	0.51
1:C:367:PHE:HB3	1:D:386:GLU:OE1	2.10	0.50
1:C:373:VAL:HG23	1:C:376:GLU:HB2	1.93	0.50
1:A:7:LYS:HG2	1:B:561:ARG:NE	2.26	0.50
1:A:687:ASP:HB3	1:A:690:LEU:HD12	1.92	0.50
1:B:12:ILE:HD13	1:B:12:ILE:N	2.27	0.50
1:B:57:ASN:HB2	1:B:898:LYS:NZ	2.25	0.50
1:A:978:HIS:NE2	1:B:84:ASP:OD2	2.33	0.50
1:C:22:THR:HB	1:D:828:GLN:HG3	1.92	0.50
1:B:842:SER:HA	1:B:916:LYS:HG2	1.93	0.50
1:C:856:THR:HG21	1:C:859:HIS:HD2	1.76	0.50
1:D:40:HIS:O	1:D:880:GLY:HA3	2.10	0.50
1:D:759:ARG:HG2	1:D:759:ARG:HH11	1.76	0.50
1:C:793:THR:HG22	1:C:814:GLN:HB2	1.93	0.50
1:C:959:CYS:O	1:C:962[B]:THR:HG22	2.12	0.50
1:D:960:TYR:CD1	1:D:973:PHE:HB2	2.47	0.50
1:B:57:ASN:OD1	1:B:328:LEU:HD22	2.11	0.50
1:A:211:TYR:HB2	1:A:214:ILE:HD11	1.93	0.50
1:B:308:ASP:O	1:B:312:LEU:HD12	2.10	0.50
1:B:913:ILE:HG22	1:B:914:PRO:O	2.11	0.50
1:B:1013:PRO:HG2	1:B:1015:ARG:HH21	1.76	0.50
1:C:856:THR:HG22	1:C:857:GLU:N	2.26	0.50
1:D:885:GLN:O	1:D:889:ILE:HG13	2.11	0.50
1:A:46:ASP:HB3	1:A:49:CYS:CB	2.38	0.50
1:A:223:VAL:HG11	1:A:255:ILE:HG21	1.94	0.50
1:C:652:GLU:O	1:C:656:LYS:HG2	2.11	0.50
1:D:225:GLY:HA2	4:D:1106:FAD:H3B	1.94	0.50
1:C:42:LYS:NZ	1:C:44:ASN:OD1	2.43	0.49
1:C:535:VAL:CG2	1:C:536:GLU:N	2.75	0.49
1:A:23:GLN:O	6:A:1208:HOH:O	2.18	0.49
1:B:42:LYS:HE2	1:B:46:ASP:HB2	1.94	0.49
1:B:180:GLU:CD	1:B:180:GLU:H	2.20	0.49
1:B:468:THR:O	1:B:469:MET:HB2	2.12	0.49
1:B:269:ASN:HB3	1:B:273:GLU:OE2	2.11	0.49
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.94	0.49
1:C:79:CYS:CB	1:C:101:ILE:HG21	2.42	0.49
1:A:872:MET:HE3	1:A:872:MET:N	2.28	0.49
1:B:989:CYS:SG	1:B:990:THR:N	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ASN:O	1:D:272:LYS:N	2.45	0.49
1:B:178:SER:OG	1:B:179:GLN:N	2.46	0.49
1:B:845:GLU:HG3	1:B:912:PHE:CG	2.48	0.49
1:C:62:ILE:C	1:C:62:ILE:HD12	2.37	0.49
1:C:263:GLU:O	1:C:264:ASN:HB2	2.13	0.49
1:C:613:ILE:HG21	1:C:642:MET:CE	2.38	0.49
1:A:580:LYS:N	6:A:1203:HOH:O	2.02	0.49
1:B:455:LYS:HE2	1:B:463:GLU:OE1	2.12	0.49
1:C:63:LYS:HE3	1:C:128:MET:HG2	1.94	0.49
1:D:277:LYS:HD2	1:D:511:TYR:CE1	2.47	0.49
1:A:315:LYS:HG2	1:A:321:MET:HE2	1.93	0.49
1:B:875:LYS:C	1:B:876:LEU:HD23	2.38	0.49
1:C:490:VAL:HG12	6:C:1206:HOH:O	2.13	0.49
1:C:692:ARG:HB3	1:C:692:ARG:NH1	2.27	0.49
1:D:911:PRO:O	1:D:913:ILE:HG13	2.12	0.49
1:A:357:ARG:O	1:A:358:ARG:HG3	2.13	0.49
1:C:166:MET:HE2	1:C:840:LEU:HD11	1.94	0.49
1:C:362:VAL:HG13	1:C:391:LEU:HB2	1.94	0.49
1:A:801:SER:O	1:A:802:GLY:C	2.54	0.48
1:B:753:ALA:HB1	1:B:758:LYS:HB3	1.95	0.48
1:B:877:PRO:HD2	1:B:882:TYR:CG	2.47	0.48
1:C:804:GLN:O	1:C:808:SER:OG	2.30	0.48
2:C:1102:SF4:S2	2:C:1102:SF4:S4	3.11	0.48
1:D:277:LYS:HD2	1:D:511:TYR:HE1	1.77	0.48
1:B:358:ARG:HD3	6:B:1203:HOH:O	2.14	0.48
1:D:22:THR:OG1	6:D:1206:HOH:O	2.20	0.48
1:D:664:ALA:HA	1:D:704:ILE:HD12	1.95	0.48
1:A:867:ARG:HA	1:A:872:MET:SD	2.54	0.48
1:C:5:LEU:HD13	1:D:620:TYR:CD2	2.48	0.48
1:C:428:HIS:O	1:D:410[A]:ARG:NH1	2.46	0.48
1:A:67:LEU:HD23	1:B:146:GLU:HG2	1.96	0.48
1:A:482:ILE:HG12	1:A:482:ILE:O	2.13	0.48
1:A:543:ILE:HG23	6:A:1201:HOH:O	2.12	0.48
1:C:772:PRO:HA	1:D:741:LEU:O	2.13	0.48
1:D:292:ASP:O	1:D:294:PHE:N	2.46	0.48
1:A:259:LYS:NZ	6:A:1220:HOH:O	2.40	0.48
1:C:346:ASP:OD2	4:C:1106:FAD:H6	2.12	0.48
1:C:509:ALA:O	1:C:510:GLN:C	2.56	0.48
1:C:669:LEU:HD13	1:C:669:LEU:HA	1.49	0.48
1:A:550:SER:HB2	1:A:572:LEU:HB3	1.96	0.48
1:B:335:VAL:HG22	1:B:433:VAL:HB	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:TYR:C	1:A:506:TYR:CD2	2.91	0.48
1:B:270:THR:O	1:B:274:GLU:HB2	2.13	0.48
1:B:719:SER:OG	1:B:720:ILE:N	2.46	0.48
1:C:83:ALA:O	1:C:84:ASP:C	2.57	0.48
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.79	0.48
1:C:281:ILE:HD13	1:C:281:ILE:N	2.28	0.48
1:B:448:LYS:NZ	1:B:460:ASP:OD1	2.45	0.48
1:B:749:THR:OG1	6:B:1214:HOH:O	2.20	0.48
1:C:379:LEU:HA	1:C:382:GLU:HG2	1.94	0.48
1:C:807:HIS:HB3	1:C:928:ALA:HB2	1.96	0.48
1:D:454:ILE:HG22	1:D:473:GLU:HG2	1.96	0.48
1:A:372:ALA:O	1:A:374:PRO:HD3	2.14	0.48
1:A:375:GLU:O	1:A:379:LEU:HD22	2.13	0.48
1:A:1015:ARG:O	1:B:616:LYS:HA	2.12	0.48
1:A:868:ILE:O	1:A:870:GLU:N	2.46	0.47
1:C:230:GLU:HG2	1:C:310:LEU:HB2	1.96	0.47
1:A:725:LYS:NZ	6:A:1229:HOH:O	2.48	0.47
1:B:227:SER:HA	1:B:231:ILE:HD12	1.95	0.47
1:B:673:HIS:CD2	1:B:673:HIS:N	2.83	0.47
1:C:413:GLN:HB2	1:C:419:TRP:CH2	2.49	0.47
1:C:464:VAL:CG1	1:C:478:ALA:HB3	2.44	0.47
1:C:568:TRP:CE2	1:C:827:ILE:HB	2.48	0.47
1:B:58:ASN:C	1:B:58:ASN:OD1	2.57	0.47
1:C:999:ILE:HD11	1:D:600:TYR:CE2	2.49	0.47
1:D:477:PHE:N	1:D:477:PHE:CD1	2.83	0.47
1:A:249:LYS:NZ	6:A:1224:HOH:O	2.43	0.47
1:A:796:ILE:HD13	1:A:796:ILE:HG21	1.65	0.47
1:B:43:ARG:HD3	1:B:879:PHE:HB3	1.97	0.47
1:C:173:ASN:HB3	1:C:176:LEU:CD1	2.43	0.47
1:D:536:GLU:HG3	1:D:540:LEU:O	2.14	0.47
1:A:428:HIS:CB	1:B:425:GLN:HE22	2.27	0.47
1:A:451:LEU:O	1:A:452:SER:C	2.58	0.47
1:C:651:MET:O	1:C:655:ARG:HB2	2.14	0.47
1:D:248:MET:HE2	1:D:248:MET:HB3	1.81	0.47
1:A:711:THR:HG23	1:A:711:THR:O	2.15	0.47
1:A:949:ASP:C	1:A:949:ASP:OD1	2.57	0.47
1:B:336:ILE:HD12	1:B:431:ALA:HB2	1.97	0.47
1:B:845:GLU:CD	1:B:845:GLU:H	2.20	0.47
1:C:776:ARG:O	1:C:780:THR:HB	2.14	0.47
1:D:352:LEU:HA	1:D:352:LEU:HD23	1.37	0.47
1:A:668:ASN:OD1	1:A:670:SER:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:ILE:HD12	1:B:871:LEU:HD22	1.96	0.47
1:B:972:GLN:O	1:B:980:PRO:HA	2.15	0.47
1:C:373:VAL:O	1:C:376:GLU:N	2.45	0.47
1:A:199:SER:O	1:A:200:ILE:C	2.56	0.46
1:A:304:TYR:O	1:A:435:ILE:HA	2.14	0.46
1:A:346:ASP:OD2	4:A:1106:FAD:H6	2.15	0.46
1:A:582:ILE:HA	1:A:582:ILE:HD12	1.62	0.46
1:B:301:GLN:O	1:B:403:ILE:HG12	2.14	0.46
1:D:471:THR:HG23	1:D:476:VAL:O	2.15	0.46
1:A:588:PRO:HB3	1:B:990:THR:OG1	2.15	0.46
1:B:806:LEU:HD13	1:B:921:ILE:HG23	1.97	0.46
1:C:647:LYS:HE3	1:C:697:TRP:CD1	2.50	0.46
1:C:859:HIS:CE1	1:C:998:ILE:HG23	2.51	0.46
1:D:201:SER:HB2	1:D:493:VAL:HG13	1.97	0.46
1:B:858:SER:O	1:B:865:VAL:HG23	2.15	0.46
1:C:465:ASP:C	1:C:465:ASP:OD1	2.59	0.46
1:C:572:LEU:HD13	1:C:638:ILE:HB	1.98	0.46
1:C:837:LEU:HD23	1:C:837:LEU:HA	1.71	0.46
1:A:101:ILE:O	1:A:102:THR:C	2.58	0.46
1:A:315:LYS:HG3	1:A:321:MET:HE2	1.97	0.46
1:B:895:MET:HE3	1:B:898:LYS:HE3	1.96	0.46
1:B:990:THR:O	1:B:990:THR:CG2	2.63	0.46
1:D:883:LEU:HG	1:D:887:LYS:HE3	1.96	0.46
1:B:649:ASP:OD1	1:B:649:ASP:N	2.45	0.46
1:C:115:MET:HE2	1:C:115:MET:HB2	1.71	0.46
1:D:849:TRP:N	1:D:849:TRP:HD1	2.14	0.46
1:B:475:TRP:HB3	1:B:506:TYR:CZ	2.51	0.46
1:A:367:PHE:CZ	1:B:367:PHE:CZ	3.03	0.46
1:A:390:PHE:O	1:A:391:LEU:HD23	2.15	0.46
1:B:78:ARG:NH1	1:B:147:GLU:HG2	2.30	0.46
1:B:225:GLY:HA2	4:B:1106:FAD:H3B	1.98	0.46
1:B:444:ASP:OD1	1:B:446:LYS:HB2	2.16	0.46
1:C:57:ASN:HD22	1:C:898:LYS:CD	2.27	0.46
1:C:741:LEU:O	1:D:772:PRO:HA	2.15	0.46
1:D:465:ASP:OD1	1:D:465:ASP:C	2.58	0.46
1:D:860:GLN:CG	6:D:1204:HOH:O	2.62	0.46
1:D:868:ILE:HG12	1:D:893:GLU:HG2	1.98	0.46
1:D:974:ASP:OD1	1:D:974:ASP:C	2.58	0.46
1:D:990:THR:OG1	1:D:1004:MET:HE2	2.16	0.46
1:A:680:MET:N	6:A:1228:HOH:O	2.47	0.46
1:A:767:GLY:O	1:A:770:ILE:HG12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:PHE:O	1:B:384:LYS:HD2	2.16	0.46
1:B:69:GLU:OE1	1:B:109:TYR:OH	2.24	0.46
1:B:993:LEU:C	1:B:993:LEU:HD23	2.40	0.46
1:C:941:ILE:HD12	1:C:941:ILE:HG23	1.76	0.46
1:A:10:ALA:HA	1:A:13:GLU:HB2	1.98	0.46
1:B:989:CYS:O	1:B:990:THR:CB	2.64	0.46
1:C:167:ASN:HB3	1:C:912:PHE:CD2	2.51	0.46
1:C:285:LEU:CB	1:C:440:SER:HB3	2.45	0.46
1:C:410:ARG:NH1	1:D:428:HIS:O	2.49	0.46
1:D:451:LEU:O	1:D:454:ILE:HG13	2.16	0.46
1:A:465:ASP:C	1:A:465:ASP:OD1	2.59	0.46
1:A:610:ILE:O	1:A:610:ILE:HG13	2.15	0.46
1:A:682:LEU:HD23	1:A:682:LEU:N	2.30	0.46
1:C:2:ALA:HB1	1:D:623:GLN:OE1	2.16	0.46
1:C:269:ASN:HD22	1:C:269:ASN:H	1.64	0.46
1:C:791:LEU:HD12	1:C:791:LEU:H	1.80	0.46
1:D:717:ILE:HD13	1:D:717:ILE:HG21	1.61	0.46
1:B:656:LYS:HD2	6:B:1219:HOH:O	2.16	0.45
1:B:993:LEU:HD23	1:B:993:LEU:O	2.16	0.45
1:C:416:THR:OG1	1:C:418:LYS:CE	2.64	0.45
1:A:816:CYS:HB3	3:A:1105:FMN:O1P	2.16	0.45
1:B:191:ALA:O	1:B:279:ALA:HA	2.16	0.45
1:B:589:ARG:CD	1:B:611:GLU:HG3	2.44	0.45
1:C:386:GLU:OE2	1:D:367:PHE:HB2	2.16	0.45
1:C:428:HIS:H	1:D:425:GLN:HE21	1.64	0.45
1:A:177:PRO:HG2	1:A:182:MET:SD	2.56	0.45
1:C:461:LEU:HD23	1:C:461:LEU:HA	1.61	0.45
1:C:601:GLY:HA3	1:D:997:PRO:HB3	1.98	0.45
1:C:941:ILE:HD13	1:C:941:ILE:HA	1.35	0.45
1:D:16:LEU:HD23	1:D:16:LEU:HA	1.71	0.45
1:D:860:GLN:HB2	1:D:865:VAL:CG2	2.46	0.45
1:A:45:PRO:HD2	1:B:143:TYR:OH	2.16	0.45
1:A:776:ARG:O	1:A:780:THR:HG22	2.16	0.45
1:B:10:ALA:HB3	6:B:1225:HOH:O	2.15	0.45
1:B:492:SER:OG	4:B:1106:FAD:H5'2	2.17	0.45
1:B:957:GLY:O	1:B:960:TYR:HB3	2.16	0.45
1:C:948:ILE:HD13	1:C:980:PRO:CG	2.46	0.45
1:A:342:ASP:OD1	1:A:373:VAL:HG13	2.16	0.45
1:C:547:GLY:HA3	1:C:570:PHE:CE1	2.52	0.45
1:D:845:GLU:HG3	1:D:912:PHE:CE1	2.51	0.45
1:A:785:LEU:HA	1:A:785:LEU:HD23	1.67	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:PHE:CD1	1:B:303:PHE:CE1	3.05	0.45
1:D:416:THR:HG23	1:D:418:LYS:HB2	1.98	0.45
1:A:287:GLU:OE2	1:A:444:ASP:HB2	2.16	0.45
1:A:428:HIS:CB	1:B:425:GLN:NE2	2.79	0.45
1:C:256:ILE:HG22	1:C:259:LYS:HG3	1.98	0.45
1:D:126:CYS:O	1:D:127:GLY:C	2.60	0.45
1:D:396:VAL:HG11	1:D:403:ILE:HD13	1.98	0.45
1:D:948:ILE:HG21	1:D:980:PRO:HG2	1.99	0.45
1:A:289:LYS:NZ	6:A:1209:HOH:O	2.21	0.45
1:B:398:VAL:HG22	1:B:403:ILE:HD13	1.99	0.45
1:B:738:VAL:HG21	1:B:773:ILE:CD1	2.47	0.45
1:C:289:LYS:HG3	1:C:441:VAL:HG13	1.98	0.45
1:A:518:LYS:NZ	1:A:520:GLU:HB3	2.32	0.45
1:A:868:ILE:C	1:A:870:GLU:H	2.25	0.45
1:D:300:ASP:N	1:D:300:ASP:OD1	2.49	0.45
1:D:341:GLY:O	1:D:342:ASP:C	2.59	0.45
1:B:475:TRP:HB3	1:B:506:TYR:OH	2.17	0.45
1:B:771:ARG:O	1:B:772:PRO:C	2.56	0.45
1:C:470:GLN:HG3	1:C:477:PHE:CE2	2.52	0.45
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.64	0.45
1:A:264:ASN:HB2	6:A:1212:HOH:O	2.17	0.44
1:A:866:PRO:CG	1:A:890:ILE:HD11	2.47	0.44
1:A:877:PRO:HB2	1:A:879:PHE:CE2	2.52	0.44
1:B:124:LEU:O	1:B:125:THR:C	2.60	0.44
1:B:945:VAL:HG13	1:B:1007:ARG:HG2	1.98	0.44
1:C:741:LEU:HD12	1:C:741:LEU:HA	1.63	0.44
1:D:572:LEU:N	1:D:572:LEU:CD2	2.80	0.44
1:A:716:ASP:OD1	1:A:718:VAL:HB	2.17	0.44
1:C:267:THR:O	1:C:268:LEU:C	2.57	0.44
1:D:402:ARG:HB3	1:D:402:ARG:NH1	2.33	0.44
1:A:344:ALA:HA	1:A:437:ALA:HB1	1.97	0.44
1:A:547:GLY:HA3	1:A:570:PHE:CE1	2.52	0.44
1:B:636:ILE:HD13	1:B:636:ILE:HA	1.55	0.44
1:C:720:ILE:HD12	1:C:720:ILE:HG23	1.42	0.44
1:A:56:GLU:HG2	1:A:57:ASN:N	2.32	0.44
1:A:192:LEU:HD12	1:A:192:LEU:N	2.32	0.44
1:A:397:ILE:HD12	1:A:405:ALA:HB3	1.99	0.44
1:C:413:GLN:NE2	6:C:1226:HOH:O	2.45	0.44
1:D:124:LEU:HB3	1:D:244:GLU:OE2	2.17	0.44
1:A:578:LEU:HD23	1:A:578:LEU:HA	1.65	0.44
1:B:872:MET:SD	1:B:872:MET:N	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:ILE:O	1:B:889:ILE:HG22	2.17	0.44
1:D:363:PHE:HZ	1:D:387:PHE:HB3	1.82	0.44
1:B:52:CYS:HB2	1:B:384:LYS:HG3	1.99	0.44
1:B:365:LYS:HB3	1:B:366:GLY:H	1.61	0.44
1:B:669:LEU:HD23	1:B:669:LEU:HA	1.81	0.44
1:B:725:LYS:NZ	6:B:1227:HOH:O	2.42	0.44
1:C:19:ASN:OD1	1:C:964:ASN:ND2	2.48	0.44
1:C:292:ASP:O	1:C:295:GLN:HB2	2.18	0.44
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.72	0.44
1:C:410:ARG:HG3	1:C:411:THR:N	2.32	0.44
1:C:654:SER:HB2	1:C:665:LEU:CD1	2.47	0.44
1:D:366:GLY:HA2	1:D:390:PHE:CZ	2.53	0.44
1:D:687:ASP:OD1	1:D:687:ASP:C	2.61	0.44
1:A:615:GLU:O	1:B:1015:ARG:HD3	2.17	0.44
1:B:849:TRP:N	1:B:849:TRP:CD1	2.85	0.44
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.47	0.44
1:C:147:GLU:HG2	1:C:148:GLY:N	2.33	0.44
1:C:958:LYS:HB3	1:C:958:LYS:HE3	1.73	0.44
1:D:406:VAL:HG21	1:D:434:VAL:HG11	1.99	0.44
1:B:750:PRO:O	1:B:753:ALA:HB2	2.17	0.44
1:C:568:TRP:NE1	1:C:827:ILE:HB	2.32	0.44
1:C:583:VAL:CB	6:C:1210:HOH:O	2.64	0.44
1:A:366:GLY:HA3	1:A:390:PHE:CZ	2.52	0.43
1:C:73:LEU:O	1:C:77:MET:HG3	2.18	0.43
1:B:53:GLU:HG2	1:B:54:LYS:H	1.83	0.43
1:C:75:GLU:OE1	1:C:75:GLU:HA	2.18	0.43
1:D:63:LYS:HE3	1:D:128:MET:HG2	2.00	0.43
1:D:246:GLU:OE2	6:D:1207:HOH:O	2.21	0.43
1:D:607:PHE:N	1:D:607:PHE:CD1	2.86	0.43
1:D:651:MET:CE	1:D:701:ALA:HB2	2.48	0.43
1:B:579:ASP:N	1:B:579:ASP:OD1	2.50	0.43
1:C:470:GLN:HG3	1:C:477:PHE:CZ	2.53	0.43
1:D:248:MET:O	1:D:248:MET:HG2	2.15	0.43
1:B:239:ASP:O	1:B:909:ARG:NH2	2.52	0.43
1:B:547:GLY:HA3	1:B:570:PHE:CE1	2.54	0.43
1:C:800:GLU:HB2	6:C:1291:HOH:O	2.19	0.43
1:D:315:LYS:HD3	1:D:321:MET:HG2	2.00	0.43
1:D:737:THR:HG23	3:D:1105:FMN:H1'2	2.00	0.43
1:D:982:VAL:O	6:D:1208:HOH:O	2.21	0.43
1:A:203:ALA:HB1	1:A:214:ILE:HG21	1.99	0.43
1:A:485:MET:HB3	1:A:485:MET:HE2	1.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:HB3	1:B:522:PRO:HG2	1.99	0.43
1:B:979:LEU:HD23	1:B:979:LEU:HA	1.80	0.43
1:C:151:ASN:OD1	1:C:151:ASN:C	2.60	0.43
1:D:167[B]:ASN:ND2	1:D:911:PRO:HA	2.34	0.43
1:D:352:LEU:HD21	1:D:359:VAL:CG2	2.48	0.43
1:D:454:ILE:HG22	1:D:473:GLU:CG	2.48	0.43
1:D:699:ARG:NE	1:D:699:ARG:HA	2.34	0.43
1:A:537:MET:HG3	1:A:789:PRO:HB3	2.00	0.43
1:B:100:PHE:CZ	1:B:156:GLN:HB2	2.54	0.43
1:B:297:LEU:HD21	1:B:398:VAL:HG21	2.01	0.43
1:B:365:LYS:HG2	1:B:419:TRP:CZ2	2.53	0.43
1:C:62:ILE:HD13	1:C:379:LEU:HD22	2.01	0.43
1:C:89:LYS:HD3	1:D:41:TRP:CE2	2.53	0.43
1:C:124:LEU:HD23	1:C:240:VAL:HG13	2.01	0.43
1:C:586:VAL:O	1:C:589:ARG:HD3	2.18	0.43
1:C:734:ALA:HA	1:C:735:THR:HA	1.67	0.43
1:D:25:HIS:N	1:D:25:HIS:ND1	2.67	0.43
1:A:25:HIS:ND1	1:A:25:HIS:N	2.67	0.43
1:B:336:ILE:CD1	1:B:431:ALA:HB2	2.48	0.43
1:B:521:LEU:HA	1:B:522:PRO:HD3	1.73	0.43
1:B:999:ILE:HG21	1:B:999:ILE:HD13	1.45	0.43
1:C:6:SER:N	1:D:627:GLU:OE1	2.51	0.43
1:C:69:GLU:O	1:C:70:ARG:C	2.60	0.43
1:C:193:LEU:N	1:C:193:LEU:HD22	2.33	0.43
1:C:297:LEU:HA	1:C:301:GLN:OE1	2.18	0.43
1:C:547:GLY:O	1:C:814:GLN:HA	2.19	0.43
1:C:620:TYR:CA	1:D:1017:LEU:HD12	2.48	0.43
1:D:840:LEU:HD23	1:D:840:LEU:HA	1.81	0.43
1:B:949:ASP:OD1	1:B:951:GLU:HB2	2.19	0.43
1:C:692:ARG:CB	1:C:692:ARG:CZ	2.97	0.43
1:D:294:PHE:CD1	1:D:396:VAL:HG21	2.54	0.43
1:A:196:GLY:N	6:A:1227:HOH:O	2.47	0.43
1:A:207:ALA:HB1	1:A:251:LEU:HB3	2.00	0.43
1:A:933:GLY:HA3	1:A:937:GLU:OE1	2.19	0.43
1:B:80:LEU:HD11	1:B:142:LEU:HD21	2.00	0.43
1:B:668:ASN:OD1	1:B:668:ASN:C	2.61	0.43
1:B:671:SER:HA	1:B:672:PRO:HD3	1.56	0.43
1:C:242:ASN:O	1:C:246:GLU:HG2	2.18	0.43
1:C:537:MET:CG	1:C:789:PRO:HB3	2.49	0.43
1:C:858:SER:OG	1:C:867:ARG:NH2	2.49	0.43
1:D:629:LYS:HE3	1:D:629:LYS:HB3	1.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:OD1	1:A:269:ASN:N	2.52	0.43
1:A:533:ILE:HD13	1:A:835:LYS:HG3	2.01	0.43
1:B:131:PRO:HB3	1:B:373:VAL:HG21	2.01	0.43
1:C:124:LEU:O	1:C:125:THR:C	2.58	0.43
1:C:137:VAL:HG13	1:C:149:SER:HB3	2.00	0.43
1:C:581:ASP:O	1:C:583:VAL:HG13	2.19	0.43
1:C:885:GLN:OE1	1:C:889:ILE:HD11	2.18	0.43
1:C:1017:LEU:HA	1:C:1017:LEU:HD23	1.59	0.43
1:D:888:LYS:O	1:D:888:LYS:HG2	2.19	0.43
1:A:542:PHE:HA	6:A:1201:HOH:O	2.18	0.42
1:A:991:LEU:HD23	1:A:991:LEU:HA	1.88	0.42
1:C:360:PHE:CD1	1:C:386:GLU:HB3	2.54	0.42
1:D:849:TRP:CG	1:D:854:PRO:HA	2.54	0.42
1:A:300:ASP:OD1	1:A:300:ASP:N	2.52	0.42
1:A:369:ASN:OD1	1:A:369:ASN:N	2.51	0.42
1:A:992:CYS:O	1:A:993:LEU:C	2.62	0.42
1:B:367:PHE:C	1:B:369:ASN:H	2.26	0.42
1:C:108:ASN:HA	1:C:852:GLN:NE2	2.34	0.42
1:C:653:LEU:HD12	1:C:653:LEU:HA	1.60	0.42
1:C:671:SER:HA	1:C:672:PRO:HD3	1.46	0.42
1:C:776:ARG:HD3	6:C:1218:HOH:O	2.18	0.42
1:D:270:THR:O	1:D:274:GLU:HG3	2.18	0.42
1:D:774:ALA:O	1:D:777:ALA:HB3	2.19	0.42
1:A:518:LYS:HZ1	1:A:520:GLU:HB3	1.85	0.42
1:A:972:GLN:O	1:A:980:PRO:HA	2.19	0.42
1:B:908:GLU:O	1:B:910:LYS:N	2.52	0.42
1:A:871:LEU:HB2	1:A:872:MET:CE	2.49	0.42
1:C:364:ARG:H	1:C:364:ARG:CD	2.28	0.42
1:C:455:LYS:HG3	1:C:472:SER:CB	2.49	0.42
1:C:779:THR:HG21	1:C:932:LEU:HG	2.00	0.42
1:D:172:ARG:NH1	1:D:176:LEU:HB2	2.34	0.42
1:D:394:ARG:HA	1:D:394:ARG:HD3	1.75	0.42
1:D:751:TRP:HA	1:D:752:PRO:C	2.44	0.42
1:A:231:ILE:HD13	1:A:231:ILE:HG21	1.76	0.42
1:A:444:ASP:C	1:A:444:ASP:OD1	2.61	0.42
1:A:612:LEU:HA	1:A:612:LEU:HD23	1.65	0.42
1:B:516:SER:OG	1:B:517:ALA:N	2.53	0.42
1:C:379:LEU:H	1:C:379:LEU:HG	1.53	0.42
1:D:348:ALA:HB1	1:D:385:CYS:SG	2.60	0.42
1:D:671:SER:HA	1:D:672:PRO:HD3	1.81	0.42
1:A:87:CYS:HB2	1:A:97:ILE:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:VAL:HG21	1:A:720:ILE:HG23	2.02	0.42
1:B:941:ILE:HA	1:B:941:ILE:HD13	1.75	0.42
1:C:193:LEU:CD1	1:C:217:PHE:HB2	2.50	0.42
1:C:268:LEU:HD23	1:C:268:LEU:HA	1.58	0.42
1:C:620:TYR:CD1	1:C:620:TYR:C	2.98	0.42
1:C:856:THR:HG22	1:C:857:GLU:H	1.85	0.42
1:D:336:ILE:HD13	1:D:429:LEU:HD23	2.00	0.42
1:D:402:ARG:HB3	1:D:402:ARG:HH11	1.84	0.42
1:A:35:LYS:NZ	1:B:491:GLU:OE2	2.46	0.42
1:A:578:LEU:O	1:A:581:ASP:HB2	2.20	0.42
1:A:751:TRP:HA	1:A:752:PRO:C	2.45	0.42
1:B:193:LEU:HD13	1:B:193:LEU:HA	1.87	0.42
1:B:941:ILE:HD12	1:B:941:ILE:HG23	1.73	0.42
1:C:22:THR:HG21	1:D:566:ALA:O	2.19	0.42
1:C:77:MET:SD	1:D:599:MET:HE3	2.60	0.42
1:C:304:TYR:HB3	1:C:308:ASP:HB2	2.01	0.42
1:C:629:LYS:HD2	1:C:629:LYS:HA	1.89	0.42
1:D:647:LYS:HA	1:D:697:TRP:CE3	2.54	0.42
1:D:694:ILE:HG21	1:D:694:ILE:HD13	1.79	0.42
1:D:732:VAL:HG13	1:D:788:PHE:CE2	2.55	0.42
1:A:866:PRO:HG3	1:A:890:ILE:CD1	2.50	0.42
1:A:989:CYS:O	1:A:990:THR:HB	2.19	0.42
1:C:79:CYS:O	1:C:81:LYS:NZ	2.53	0.42
1:C:500:SER:O	1:C:501:TRP:C	2.57	0.42
1:C:598:PRO:HD2	1:D:77:MET:SD	2.59	0.42
1:D:610:ILE:HG13	1:D:610:ILE:O	2.20	0.42
1:D:998:ILE:HD12	1:D:998:ILE:HG23	1.78	0.42
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.54	0.42
1:A:570:PHE:HB2	1:A:636:ILE:HB	2.01	0.42
1:B:403:ILE:HD12	1:B:403:ILE:HG23	1.75	0.42
1:B:426:ILE:HD13	1:B:426:ILE:HG21	1.72	0.42
1:B:550:SER:O	3:B:1105:FMN:C10	2.68	0.42
1:B:867:ARG:HA	1:B:872:MET:HE3	1.98	0.42
1:C:167:ASN:OD1	1:C:911:PRO:HA	2.20	0.42
1:C:412:GLU:O	1:C:412:GLU:HG2	2.19	0.42
1:A:124:LEU:O	1:A:125:THR:C	2.63	0.42
1:A:533:ILE:O	1:A:545:PRO:HD3	2.20	0.42
1:C:414:ASP:C	1:C:416:THR:H	2.27	0.42
1:C:485:MET:HE2	1:C:485:MET:HB3	1.79	0.42
1:D:125:THR:O	1:D:126:CYS:C	2.58	0.42
1:D:784:ALA:O	1:D:786:PRO:HD3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1007:ARG:NE	1:D:1011:TYR:HB3	2.35	0.42
1:A:704:ILE:HB	1:A:705:PRO:HD2	2.02	0.41
1:C:455:LYS:HG3	1:C:472:SER:OG	2.20	0.41
1:C:672:PRO:HA	1:C:682:LEU:O	2.20	0.41
1:C:841:LYS:NZ	1:D:746:ALA:O	2.53	0.41
1:D:142:LEU:HD23	1:D:142:LEU:HA	1.86	0.41
1:D:211:TYR:OH	1:D:504:HIS:ND1	2.47	0.41
1:D:689:GLU:HA	1:D:692:ARG:NH1	2.35	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.82	0.41
1:A:492:SER:O	1:A:493:VAL:C	2.61	0.41
1:A:745:LYS:HE2	1:A:749:THR:OG1	2.20	0.41
1:A:869:ALA:C	6:A:1204:HOH:O	2.62	0.41
1:B:220:GLN:NE2	1:B:220:GLN:HA	2.34	0.41
1:C:230:GLU:HG2	1:C:310:LEU:CB	2.50	0.41
1:C:428:HIS:H	1:D:425:GLN:NE2	2.18	0.41
1:C:1017:LEU:HD12	1:D:619:ALA:HB1	2.02	0.41
1:A:738:VAL:HG21	1:A:773:ILE:HD13	2.02	0.41
1:B:408:PHE:O	1:B:426:ILE:HA	2.20	0.41
1:C:883:LEU:HD12	1:C:883:LEU:HA	1.71	0.41
1:D:650:TRP:HZ3	1:D:667:LEU:HD22	1.85	0.41
1:D:770:ILE:HG21	1:D:770:ILE:HD13	1.75	0.41
1:D:797:ASP:N	1:D:797:ASP:OD1	2.51	0.41
1:D:834:LEU:HD12	1:D:834:LEU:HA	1.78	0.41
1:A:518:LYS:HD2	1:A:519:PRO:O	2.21	0.41
1:B:64:HIS:HE1	1:B:382:GLU:OE2	2.03	0.41
1:B:908:GLU:O	1:B:909:ARG:C	2.62	0.41
1:D:331:ILE:HD13	1:D:331:ILE:HA	1.64	0.41
1:D:861:LYS:HE2	1:D:863:LYS:HE3	2.01	0.41
1:B:310:LEU:N	1:B:311:PRO:CD	2.84	0.41
1:B:348:ALA:HB2	1:B:361:LEU:HD21	2.03	0.41
1:B:518:LYS:O	1:B:520:GLU:HG2	2.21	0.41
1:B:877:PRO:HD2	1:B:882:TYR:CB	2.50	0.41
1:C:550:SER:O	3:C:1105:FMN:C10	2.69	0.41
1:D:189:LYS:HB3	1:D:276:TYR:CD1	2.55	0.41
1:D:843:ILE:HD13	1:D:843:ILE:HA	1.84	0.41
1:D:875:LYS:C	1:D:876:LEU:HD23	2.46	0.41
1:A:233:GLN:O	1:A:233:GLN:HG3	2.20	0.41
1:B:120:ASN:OD1	1:B:120:ASN:C	2.62	0.41
1:C:247:LEU:O	1:C:248:MET:C	2.62	0.41
1:D:410[A]:ARG:CZ	1:D:412:GLU:OE1	2.69	0.41
1:A:444:ASP:HA	1:A:445:PRO:HD3	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LEU:HB2	1:B:26:ALA:HB3	2.01	0.41
1:B:475:TRP:H	1:B:475:TRP:CD1	2.39	0.41
1:B:683:ALA:O	1:B:684:CYS:C	2.62	0.41
1:C:211:TYR:HB2	1:C:214:ILE:HD11	2.02	0.41
1:C:620:TYR:HA	1:D:1017:LEU:HD12	2.02	0.41
1:D:389:PRO:HB2	1:D:390:PHE:CD2	2.56	0.41
1:D:1007:ARG:CZ	1:D:1011:TYR:HB3	2.50	0.41
1:A:193:LEU:HD13	1:A:193:LEU:HA	1.93	0.41
1:A:877:PRO:HG2	1:A:882:TYR:CD2	2.56	0.41
1:A:977:THR:O	1:A:978:HIS:HB2	2.20	0.41
1:B:391:LEU:HD23	1:B:391:LEU:HA	1.94	0.41
1:B:1012:GLU:OE2	1:B:1014:LYS:HE3	2.21	0.41
1:C:345:PHE:HB3	1:C:376:GLU:HG3	2.03	0.41
1:C:681:GLY:HA3	1:C:686:GLN:HB2	2.03	0.41
1:D:46:ASP:HB3	1:D:48:ASN:O	2.21	0.41
1:D:414:ASP:HB3	1:D:415:GLU:OE2	2.20	0.41
1:D:987:THR:HG22	1:D:1014:LYS:HZ2	1.85	0.41
1:A:223:VAL:CG2	1:A:245[A]:ILE:HD13	2.49	0.41
1:A:229:SER:O	1:A:311:PRO:HA	2.21	0.41
1:A:255:ILE:HG21	1:A:255:ILE:HD13	1.69	0.41
1:A:515:VAL:O	1:A:516:SER:C	2.64	0.41
1:A:734:ALA:HA	1:A:735:THR:HA	1.75	0.41
1:A:812:VAL:C	1:A:813:LEU:HG	2.46	0.41
1:A:823:ASP:OD1	1:A:825:THR:OG1	2.31	0.41
1:A:866:PRO:HG3	1:A:890:ILE:HD11	2.02	0.41
1:B:32:LEU:HA	1:B:32:LEU:HD12	1.93	0.41
1:B:125:THR:OG1	1:B:244:GLU:OE2	2.33	0.41
1:B:184:GLU:O	1:B:185:ALA:C	2.64	0.41
1:B:248:MET:HE1	1:B:255:ILE:HD11	2.03	0.41
1:B:827:ILE:HA	1:B:827:ILE:HD12	1.79	0.41
1:C:192:LEU:HD12	1:C:192:LEU:N	2.35	0.41
1:C:408:PHE:CE1	1:C:429:LEU:HD23	2.56	0.41
1:C:515:VAL:O	1:C:516:SER:C	2.63	0.41
1:C:535:VAL:HG22	1:C:536:GLU:H	1.85	0.41
1:C:949:ASP:OD1	1:C:949:ASP:C	2.64	0.41
1:D:773:ILE:HG21	1:D:773:ILE:HD13	1.93	0.41
1:D:857:GLU:O	1:D:859:HIS:N	2.54	0.41
1:D:871:LEU:HD21	1:D:886:ARG:NH1	2.36	0.41
1:A:394:ARG:HG3	1:A:394:ARG:NH1	2.35	0.41
1:C:193:LEU:HD13	1:C:193:LEU:HA	1.85	0.41
1:C:281:ILE:HG23	1:C:281:ILE:HD12	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:SER:HB2	1:C:766:SER:O	2.19	0.41
1:C:840:LEU:HD23	1:C:840:LEU:HA	1.64	0.41
1:C:889:ILE:O	1:C:889:ILE:HG22	2.21	0.41
1:D:407:GLN:HA	1:D:427:VAL:O	2.21	0.41
1:A:412:GLU:OE1	1:B:430:LYS:NZ	2.47	0.40
1:A:946:ALA:HB1	1:A:1002:ILE:CG2	2.51	0.40
1:C:837:LEU:O	1:C:841:LYS:HG3	2.21	0.40
1:D:454:ILE:HA	1:D:472:SER:OG	2.21	0.40
1:D:734:ALA:HA	1:D:735:THR:HA	1.80	0.40
1:B:168:ILE:HD13	1:B:168:ILE:HG21	1.78	0.40
1:B:358:ARG:NE	1:B:360:PHE:CZ	2.89	0.40
1:B:867:ARG:C	1:B:872:MET:CE	2.91	0.40
1:C:543:ILE:HD11	1:C:569:GLY:HA2	2.03	0.40
1:D:235:ARG:NH1	4:D:1106:FAD:O4	2.38	0.40
1:D:454:ILE:HG22	1:D:473:GLU:HB2	2.02	0.40
1:D:531:VAL:HG21	1:D:839:TYR:HB2	2.02	0.40
1:D:590:ILE:HG21	1:D:590:ILE:HD13	1.78	0.40
1:D:709:LYS:HG3	1:D:733:THR:HB	2.03	0.40
1:A:331:ILE:O	1:A:331:ILE:HG22	2.21	0.40
1:A:577:SER:O	1:A:578:LEU:C	2.63	0.40
1:A:868:ILE:C	1:A:870:GLU:N	2.80	0.40
1:B:483:VAL:O	1:B:483:VAL:CG1	2.69	0.40
1:B:991:LEU:HA	1:B:991:LEU:HD23	1.90	0.40
1:C:328:LEU:HD23	1:C:328:LEU:HA	1.88	0.40
1:C:466:PRO:HB2	1:D:32:LEU:HD13	2.03	0.40
1:C:876:LEU:O	1:C:886:ARG:NH1	2.48	0.40
1:D:4:VAL:H	1:D:4:VAL:HG23	1.63	0.40
1:D:246:GLU:O	1:D:247:LEU:C	2.59	0.40
1:A:178:SER:HB3	1:A:181:LYS:HG2	2.04	0.40
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.73	0.40
1:A:988:GLY:O	1:A:989:CYS:C	2.63	0.40
1:D:192:LEU:C	1:D:193:LEU:HD22	2.46	0.40
1:A:89:LYS:HD2	1:B:41:TRP:CE2	2.56	0.40
1:A:134:ASP:HA	1:B:42:LYS:NZ	2.36	0.40
1:A:196:GLY:CA	6:A:1227:HOH:O	2.69	0.40
1:A:699:ARG:NH1	6:A:1202:HOH:O	2.46	0.40
1:A:858:SER:OG	1:A:867:ARG:NH2	2.55	0.40
1:B:807:HIS:O	1:B:926:GLY:HA2	2.22	0.40
1:B:918:ILE:O	1:B:919:PRO:C	2.63	0.40
1:C:2:ALA:HB1	1:D:623:GLN:HE22	1.87	0.40
1:C:410:ARG:O	1:C:421:GLU:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:VAL:CG2	1:C:780:THR:HG23	2.46	0.40
1:D:861:LYS:HB3	1:D:863:LYS:HE3	2.04	0.40
1:D:910:LYS:O	1:D:910:LYS:HG3	2.21	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	988/1025 (96%)	895 (91%)	80 (8%)	13 (1%)	9	5
1	B	1000/1025 (98%)	904 (90%)	83 (8%)	13 (1%)	9	5
1	C	998/1025 (97%)	913 (92%)	70 (7%)	15 (2%)	8	4
1	D	989/1025 (96%)	892 (90%)	85 (9%)	12 (1%)	10	6
All	All	3975/4100 (97%)	3604 (91%)	318 (8%)	53 (1%)	9	5

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	A	415	GLU
1	B	875	LYS
1	C	52	CYS
1	C	176	LEU
1	D	319	ALA
1	D	871	LEU
1	A	869	ALA
1	B	327	PRO
1	B	400	GLY
1	B	422	ASP
1	B	713	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	873	GLY
1	B	909	ARG
1	C	580	LYS
1	C	645	TYR
1	C	871	LEU
1	C	875	LYS
1	D	50	PHE
1	D	342	ASP
1	A	3	PRO
1	A	289	LYS
1	A	374	PRO
1	A	822	GLN
1	B	672	PRO
1	C	321	MET
1	C	415	GLU
1	D	320	GLY
1	D	538	ALA
1	D	858	SER
1	A	551	ALA
1	A	875	LYS
1	B	50	PHE
1	B	516	SER
1	C	54	LYS
1	C	990	THR
1	D	794	GLY
1	D	873	GLY
1	A	373	VAL
1	A	390	PHE
1	A	444	ASP
1	B	458	ARG
1	C	374	PRO
1	D	415	GLU
1	D	990	THR
1	A	990	THR
1	B	149	SER
1	C	3	PRO
1	D	331	ILE
1	B	374	PRO
1	C	865	VAL
1	C	123	GLY
1	C	482	ILE

5.3.2 Protein sidechains ⓘ

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

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

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

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	60	ASP
1	A	79	CYS
1	A	95	LEU
1	A	100	PHE
1	A	137	VAL
1	A	167	ASN
1	A	175	CYS
1	A	179	GLN
1	A	272	LYS
1	A	290	THR
1	A	293	ILE
1	A	375	GLU
1	A	376	GLU
1	A	411	THR
1	A	416	THR
1	A	424	ASP
1	A	436	SER
1	A	460	ASP
1	A	465	ASP
1	A	482	ILE
1	A	514	SER
1	A	644	SER
1	A	682	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	780	THR
1	A	793	THR
1	A	856	THR
1	A	918	ILE
1	A	947[A]	VAL
1	A	947[B]	VAL
1	A	1008	THR
1	B	24	SER
1	B	46	ASP
1	B	95	LEU
1	B	375	GLU
1	B	399	LYS
1	B	430	LYS
1	B	460	ASP
1	B	487	ASN
1	B	644	SER
1	B	660	SER
1	B	673	HIS
1	B	703	GLN
1	B	712	PRO
1	B	793	THR
1	B	800	GLU
1	B	845	GLU
1	B	887	LYS
1	B	932[A]	LEU
1	B	932[B]	LEU
1	B	1012	GLU
1	C	7	LYS
1	C	15	ILE
1	C	28	LEU
1	C	133	SER
1	C	167	ASN
1	C	180	GLU
1	C	181	LYS
1	C	293	ILE
1	C	306	SER
1	C	322	CYS
1	C	357	ARG
1	C	364	ARG
1	C	412	GLU
1	C	440	SER
1	C	483	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	487	ASN
1	C	514	SER
1	C	543	ILE
1	C	711	THR
1	C	745	LYS
1	C	780	THR
1	C	793	THR
1	C	808	SER
1	C	857	GLU
1	C	868	ILE
1	C	896	ARG
1	C	927	LYS
1	C	985	THR
1	D	18	LEU
1	D	92	PRO
1	D	129	VAL
1	D	136	CYS
1	D	215	THR
1	D	256	ILE
1	D	308	ASP
1	D	331	ILE
1	D	343	THR
1	D	363	PHE
1	D	365	LYS
1	D	392	SER
1	D	399	LYS
1	D	415	GLU
1	D	423	GLU
1	D	424	ASP
1	D	434	VAL
1	D	465	ASP
1	D	482	ILE
1	D	515	VAL
1	D	526	THR
1	D	605	SER
1	D	648	ASN
1	D	711	THR
1	D	793	THR
1	D	856	THR
1	D	884	GLU
1	D	918	ILE
1	D	932[A]	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	932[B]	LEU
1	D	999	ILE
1	D	1000	ASP
1	D	1009	THR
1	D	1011	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	299	GLN
1	A	413	GLN
1	A	494	ASN
1	A	822	GLN
1	A	828	GLN
1	B	23	GLN
1	B	25	HIS
1	B	64	HIS
1	B	170	GLN
1	B	220	GLN
1	B	233	GLN
1	B	242	ASN
1	B	413	GLN
1	B	425	GLN
1	B	457	ASN
1	B	494	ASN
1	B	498	GLN
1	B	828	GLN
1	B	878	ASN
1	C	57	ASN
1	C	88	GLN
1	C	264	ASN
1	C	269	ASN
1	C	407	GLN
1	C	413	GLN
1	C	508	GLN
1	C	623	GLN
1	C	804	GLN
1	C	859	HIS
1	D	23	GLN
1	D	57	ASN
1	D	88	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	179	GLN
1	D	220	GLN
1	D	264	ASN
1	D	407	GLN
1	D	498	GLN
1	D	820	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	TDR	D	1107	-	9,9,9	2.64	5 (55%)	12,12,12	1.74	2 (16%)
2	SF4	D	1103	1	0,12,12	-	-	-		
2	SF4	A	1102	1	0,12,12	-	-	-		
2	SF4	A	1104	1	0,12,12	-	-	-		
2	SF4	C	1104	1	0,12,12	-	-	-		
2	SF4	B	1101	1	0,12,12	-	-	-		
4	FAD	D	1106	-	58,58,58	0.95	2 (3%)	85,89,89	0.84	4 (4%)
2	SF4	D	1104	1	0,12,12	-	-	-		
4	FAD	A	1106	-	58,58,58	0.86	3 (5%)	85,89,89	1.12	8 (9%)
2	SF4	B	1102	1	0,12,12	-	-	-		
2	SF4	A	1101	1	0,12,12	-	-	-		
3	FMN	A	1105	-	33,33,33	1.87	7 (21%)	48,50,50	2.41	20 (41%)
4	FAD	C	1106	-	58,58,58	1.29	2 (3%)	85,89,89	0.66	0
5	TDR	B	1107	-	9,9,9	1.54	2 (22%)	12,12,12	1.53	2 (16%)
2	SF4	B	1103	1	0,12,12	-	-	-		
2	SF4	C	1102	1	0,12,12	-	-	-		
2	SF4	D	1102	1	0,12,12	-	-	-		
2	SF4	D	1101	1	0,12,12	-	-	-		
3	FMN	D	1105	-	33,33,33	1.99	11 (33%)	48,50,50	2.29	17 (35%)
3	FMN	B	1105	-	33,33,33	1.48	5 (15%)	48,50,50	2.40	22 (45%)
5	TDR	C	1107	-	9,9,9	1.40	1 (11%)	12,12,12	2.74	5 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	C	1101	1	-	-	0/6/5/5
3	FMN	C	1105	-	-	2/18/18/18	0/3/3/3
5	TDR	A	1107	-	-	-	0/1/1/1
2	SF4	B	1104	1	-	-	0/6/5/5
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
4	FAD	B	1106	-	-	1/34/50/50	0/6/6/6
5	TDR	D	1107	-	-	-	0/1/1/1
2	SF4	D	1103	1	-	-	0/6/5/5
2	SF4	A	1102	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
2	SF4	B	1101	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	C	1104	1	-	-	0/6/5/5
4	FAD	D	1106	-	-	2/34/50/50	0/6/6/6
4	FAD	A	1106	-	-	5/34/50/50	0/6/6/6
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
3	FMN	A	1105	-	-	1/18/18/18	0/3/3/3
4	FAD	C	1106	-	-	2/34/50/50	0/6/6/6
5	TDR	B	1107	-	-	-	0/1/1/1
2	SF4	B	1103	1	-	-	0/6/5/5
2	SF4	C	1102	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	D	1101	1	-	-	0/6/5/5
3	FMN	D	1105	-	-	5/18/18/18	0/3/3/3
3	FMN	B	1105	-	-	2/18/18/18	0/3/3/3
5	TDR	C	1107	-	-	-	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1106	FAD	C10-N1	-5.86	1.21	1.33
4	C	1106	FAD	P-O3P	-5.73	1.53	1.59
3	A	1105	FMN	C4A-N5	5.39	1.42	1.30
5	D	1107	TDR	C2-N1	4.83	1.43	1.36
3	C	1105	FMN	C4A-N5	4.73	1.41	1.30
3	D	1105	FMN	C5'-C4'	4.37	1.57	1.51
4	D	1106	FAD	P-O3P	4.05	1.63	1.59
4	B	1106	FAD	C10-N1	3.90	1.41	1.33
3	C	1105	FMN	C6-C5A	3.84	1.45	1.40
5	D	1107	TDR	C4-C5	3.80	1.51	1.44
3	D	1105	FMN	O4-C4	3.73	1.30	1.23
3	D	1105	FMN	C10-N10	3.70	1.45	1.37
3	A	1105	FMN	C5A-N5	3.61	1.46	1.39
3	A	1105	FMN	C10-N1	3.58	1.40	1.33
4	D	1106	FAD	PA-O5B	-3.54	1.45	1.59
3	B	1105	FMN	C4A-C10	-3.46	1.34	1.44
3	A	1105	FMN	C6-C7	-3.46	1.34	1.39
4	B	1106	FAD	C4-N3	3.44	1.45	1.38
5	B	1107	TDR	C2-N1	3.41	1.41	1.36
3	D	1105	FMN	C4'-C3'	-3.26	1.47	1.53
3	C	1105	FMN	C10-N1	3.21	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1105	FMN	C4A-N5	3.07	1.37	1.30
3	D	1105	FMN	C9-C9A	2.95	1.44	1.39
3	A	1105	FMN	C4'-C3'	2.95	1.58	1.53
5	D	1107	TDR	C6-N1	2.90	1.41	1.36
4	A	1106	FAD	C4-N3	2.85	1.44	1.38
3	C	1105	FMN	P-O1P	2.84	1.59	1.50
3	B	1105	FMN	O4'-C4'	-2.75	1.37	1.43
5	D	1107	TDR	C6-C5	2.74	1.38	1.34
3	B	1105	FMN	C9-C8	2.70	1.43	1.39
3	C	1105	FMN	C5'-C4'	2.62	1.55	1.51
5	A	1107	TDR	C2-N1	2.62	1.40	1.36
3	D	1105	FMN	C10-N1	2.61	1.38	1.33
5	C	1107	TDR	C6-N1	2.58	1.40	1.36
3	C	1105	FMN	O4-C4	2.53	1.28	1.23
3	D	1105	FMN	P-O1P	2.42	1.58	1.50
5	B	1107	TDR	C6-N1	2.41	1.40	1.36
3	B	1105	FMN	C8M-C8	2.34	1.55	1.51
3	A	1105	FMN	P-O1P	2.34	1.57	1.50
3	D	1105	FMN	O2-C2	-2.32	1.19	1.24
3	B	1105	FMN	C10-N1	2.32	1.37	1.33
3	D	1105	FMN	C5A-N5	-2.32	1.35	1.39
5	D	1107	TDR	CM5-C5	2.29	1.56	1.50
3	A	1105	FMN	C9-C9A	2.25	1.43	1.39
3	D	1105	FMN	C1'-C2'	2.19	1.55	1.52
4	A	1106	FAD	C10-N1	2.18	1.37	1.33
4	B	1106	FAD	P-O3P	2.10	1.61	1.59
4	A	1106	FAD	PA-O5B	-2.08	1.51	1.59

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1107	TDR	CM5-C5-C4	-6.70	111.63	118.78
3	C	1105	FMN	C4A-C10-N10	5.85	124.85	116.48
3	C	1105	FMN	C4'-C3'-C2'	-5.84	103.86	113.57
3	D	1105	FMN	C4A-C10-N10	5.69	124.62	116.48
3	A	1105	FMN	C4-N3-C2	-5.40	116.05	125.64
4	B	1106	FAD	O3'-C3'-C2'	5.34	121.05	108.93
3	D	1105	FMN	C10-C4A-N5	-5.27	114.04	124.81
3	C	1105	FMN	C5A-C9A-N10	5.19	122.66	117.97
3	D	1105	FMN	C4-C4A-C10	5.04	125.58	116.93
3	A	1105	FMN	C10-N1-C2	4.95	127.56	116.85
3	A	1105	FMN	C4A-C4-N3	4.86	125.63	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1105	FMN	C4-N3-C2	-4.81	117.09	125.64
3	B	1105	FMN	C9A-C5A-N5	-4.76	117.40	122.45
3	B	1105	FMN	C4A-C10-N10	4.63	123.12	116.48
3	D	1105	FMN	C4A-C10-N1	-4.51	113.53	124.59
4	B	1106	FAD	O2B-C2B-C1B	-4.50	94.60	110.10
3	A	1105	FMN	C4A-C10-N10	4.32	122.66	116.48
5	C	1107	TDR	CM5-C5-C6	4.30	127.65	123.23
4	B	1106	FAD	O4'-C4'-C5'	-4.27	100.57	109.99
5	A	1107	TDR	C6-N1-C2	-4.26	118.74	122.69
4	A	1106	FAD	O2'-C2'-C3'	-4.20	99.42	109.25
3	A	1105	FMN	C8M-C8-C9	4.19	126.95	119.57
3	A	1105	FMN	C4A-C10-N1	-4.18	114.33	124.59
3	C	1105	FMN	C1'-N10-C9A	4.13	128.65	120.63
5	D	1107	TDR	C5-C4-N3	4.10	118.89	115.32
3	B	1105	FMN	C4A-C10-N1	-4.06	114.63	124.59
3	A	1105	FMN	C4-C4A-N5	4.02	123.77	118.21
3	B	1105	FMN	C5A-N5-C4A	4.01	124.58	118.09
3	B	1105	FMN	O4'-C4'-C5'	-3.82	101.56	109.99
3	B	1105	FMN	C6-C5A-C9A	3.82	124.29	119.05
3	A	1105	FMN	O3P-P-O2P	-3.78	93.62	107.80
4	A	1106	FAD	O2P-P-O1P	3.73	129.80	112.44
3	B	1105	FMN	C10-C4A-N5	-3.65	117.35	124.81
3	A	1105	FMN	O4-C4-C4A	-3.64	116.92	126.53
3	C	1105	FMN	C9A-N10-C10	-3.61	115.24	120.75
3	C	1105	FMN	C9A-C9-C8	3.56	126.38	119.22
3	B	1105	FMN	C10-N1-C2	3.56	124.55	116.85
3	D	1105	FMN	C5A-N5-C4A	3.55	123.83	118.09
5	B	1107	TDR	O2-C2-N1	3.51	126.41	122.79
3	D	1105	FMN	C4-N3-C2	-3.47	119.47	125.64
3	B	1105	FMN	C4-C4A-C10	3.45	122.85	116.93
3	C	1105	FMN	C4-N3-C2	-3.41	119.59	125.64
3	B	1105	FMN	C4A-C4-N3	3.37	121.82	113.25
3	C	1105	FMN	C10-C4A-N5	-3.36	117.94	124.81
5	C	1107	TDR	O4-C4-C5	-3.30	121.14	124.92
3	A	1105	FMN	C10-C4A-N5	-3.29	118.10	124.81
3	D	1105	FMN	C9-C9A-N10	3.26	126.23	121.85
4	D	1106	FAD	O2'-C2'-C3'	-3.19	101.78	109.25
3	B	1105	FMN	O2'-C2'-C3'	3.18	116.69	109.25
3	C	1105	FMN	C9-C9A-C5A	-3.17	114.42	120.03
3	B	1105	FMN	C9-C8-C7	3.13	124.29	119.69
4	B	1106	FAD	O2'-C2'-C3'	-3.09	102.02	109.25
3	D	1105	FMN	C10-N1-C2	3.04	123.43	116.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1105	FMN	C9-C9A-C5A	-3.03	114.67	120.03
5	A	1107	TDR	C5-C6-N1	3.01	125.65	122.42
3	D	1105	FMN	C9A-N10-C10	-3.00	116.18	120.75
4	A	1106	FAD	O2A-PA-O5B	-3.00	93.98	107.57
3	C	1105	FMN	C9A-C5A-N5	-2.97	119.30	122.45
3	D	1105	FMN	O4-C4-N3	-2.96	114.54	120.11
3	A	1105	FMN	C5A-C6-C7	2.91	126.21	120.83
4	A	1106	FAD	O3'-C3'-C2'	-2.89	102.37	108.93
3	C	1105	FMN	C4A-C10-N1	-2.89	117.51	124.59
3	C	1105	FMN	O3'-C3'-C2'	2.89	115.49	108.93
3	A	1105	FMN	O3'-C3'-C2'	-2.87	102.40	108.93
3	B	1105	FMN	O3P-P-O1P	2.84	121.90	110.83
3	B	1105	FMN	O4-C4-C4A	-2.82	119.08	126.53
5	C	1107	TDR	C5-C6-N1	-2.81	119.40	122.42
3	C	1105	FMN	C4-C4A-C10	2.79	121.72	116.93
3	A	1105	FMN	C9-C9A-N10	2.73	125.53	121.85
3	A	1105	FMN	C6-C5A-C9A	-2.72	115.31	119.05
4	D	1106	FAD	O3'-C3'-C2'	-2.67	102.85	108.93
3	A	1105	FMN	O5'-P-O1P	2.66	113.64	106.44
3	B	1105	FMN	C4'-C3'-C2'	-2.62	109.22	113.57
4	A	1106	FAD	C4'-C3'-C2'	2.61	117.91	113.57
3	B	1105	FMN	O3P-P-O5'	-2.59	99.92	106.67
3	B	1105	FMN	O2P-P-O1P	-2.57	100.83	110.83
3	A	1105	FMN	C8M-C8-C7	-2.52	115.61	120.76
3	D	1105	FMN	C8M-C8-C9	2.51	124.00	119.57
3	D	1105	FMN	C8M-C8-C7	-2.51	115.64	120.76
3	D	1105	FMN	O5'-C5'-C4'	-2.49	102.71	109.36
4	B	1106	FAD	O3B-C3B-C4B	-2.46	104.02	111.08
3	D	1105	FMN	O4'-C4'-C3'	-2.44	103.53	109.25
4	A	1106	FAD	O5B-PA-O1A	2.44	118.59	108.94
5	D	1107	TDR	C5-C6-N1	-2.37	119.86	122.42
3	A	1105	FMN	O2P-P-O1P	2.28	119.73	110.83
3	C	1105	FMN	O5'-P-O1P	2.28	112.60	106.44
3	D	1105	FMN	O3'-C3'-C4'	-2.27	103.77	108.93
4	B	1106	FAD	O2'-C2'-C1'	-2.26	100.90	110.20
3	C	1105	FMN	C6-C5A-C9A	2.25	122.14	119.05
3	C	1105	FMN	C9-C8-C7	-2.21	116.44	119.69
4	A	1106	FAD	O3P-P-O1P	-2.19	104.11	110.70
3	A	1105	FMN	C5A-C9A-N10	-2.19	115.99	117.97
3	B	1105	FMN	O2-C2-N3	2.18	122.76	118.58
3	B	1105	FMN	O3P-P-O2P	2.17	115.95	107.80
4	D	1106	FAD	O2A-PA-O1A	2.17	122.55	112.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1105	FMN	O3P-P-O2P	-2.16	99.69	107.80
5	C	1107	TDR	C6-C5-C4	2.14	120.66	117.73
5	B	1107	TDR	C6-N1-C2	-2.12	120.72	122.69
3	B	1105	FMN	O2-C2-N1	-2.07	118.37	121.80
4	A	1106	FAD	O5B-C5B-C4B	2.06	116.00	108.99
4	D	1106	FAD	O2P-P-O1P	2.05	122.00	112.44
3	A	1105	FMN	O2-C2-N3	2.05	122.51	118.58
3	A	1105	FMN	O2P-P-O5'	2.01	111.90	106.67
3	B	1105	FMN	O3'-C3'-C4'	-2.00	104.38	108.93

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1105	FMN	C5'-O5'-P-O3P
3	C	1105	FMN	C2'-C3'-C4'-O4'
4	A	1106	FAD	P-O3P-PA-O5B
4	A	1106	FAD	C5B-O5B-PA-O3P
3	A	1105	FMN	C4'-C5'-O5'-P
3	D	1105	FMN	C5'-O5'-P-O1P
4	A	1106	FAD	C2B-C1B-N9A-C8A
3	C	1105	FMN	C4'-C5'-O5'-P
3	B	1105	FMN	O3'-C3'-C4'-C5'
4	C	1106	FAD	O4B-C4B-C5B-O5B
3	B	1105	FMN	C4'-C5'-O5'-P
3	D	1105	FMN	O3'-C3'-C4'-C5'
3	D	1105	FMN	C4'-C5'-O5'-P
4	C	1106	FAD	C2B-C1B-N9A-C8A
4	B	1106	FAD	O4B-C4B-C5B-O5B
4	D	1106	FAD	C2B-C1B-N9A-C4A
3	D	1105	FMN	O3'-C3'-C4'-O4'
4	A	1106	FAD	O4B-C4B-C5B-O5B
4	A	1106	FAD	O4B-C1B-N9A-C8A
4	D	1106	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

15 monomers are involved in 20 short contacts:

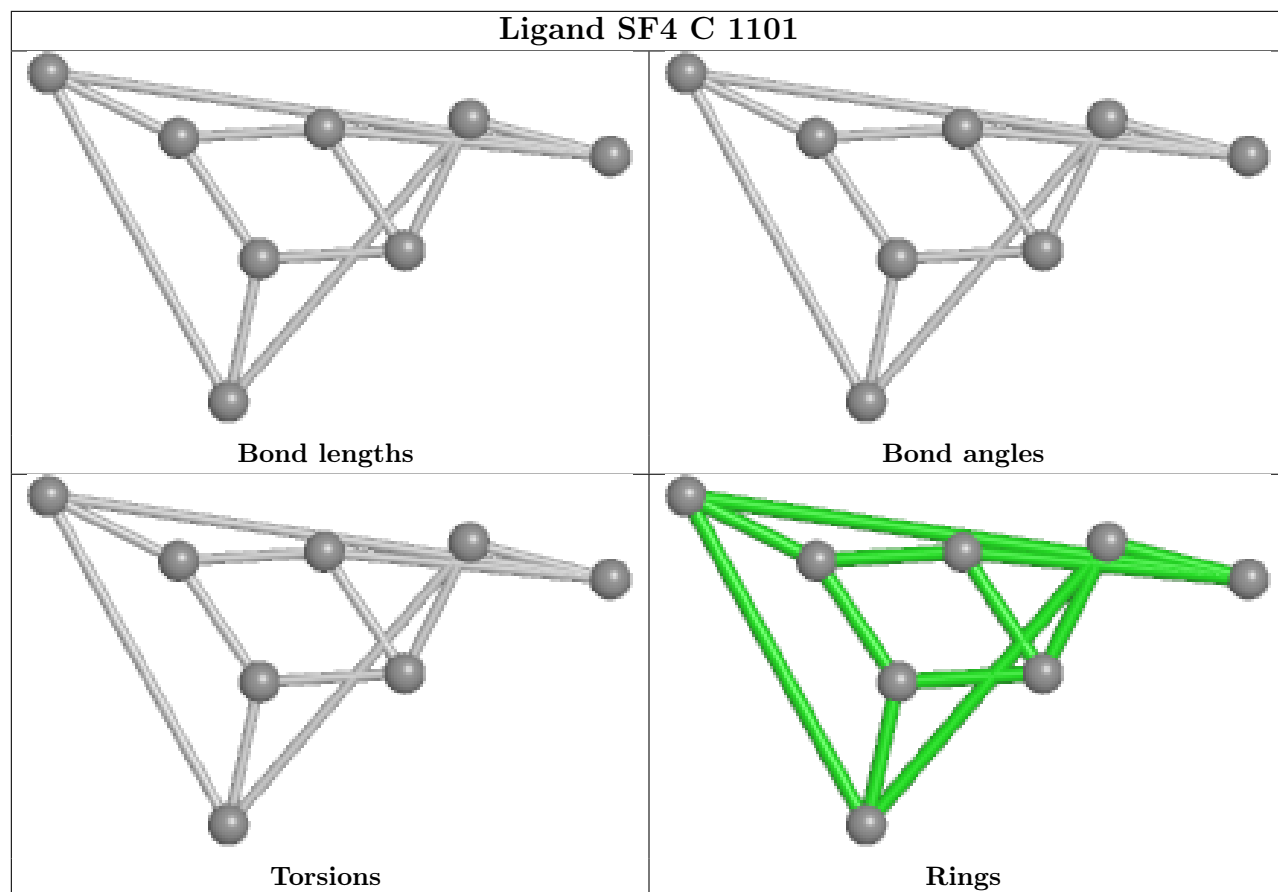
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1105	FMN	1	0
5	A	1107	TDR	1	0

Continued on next page...

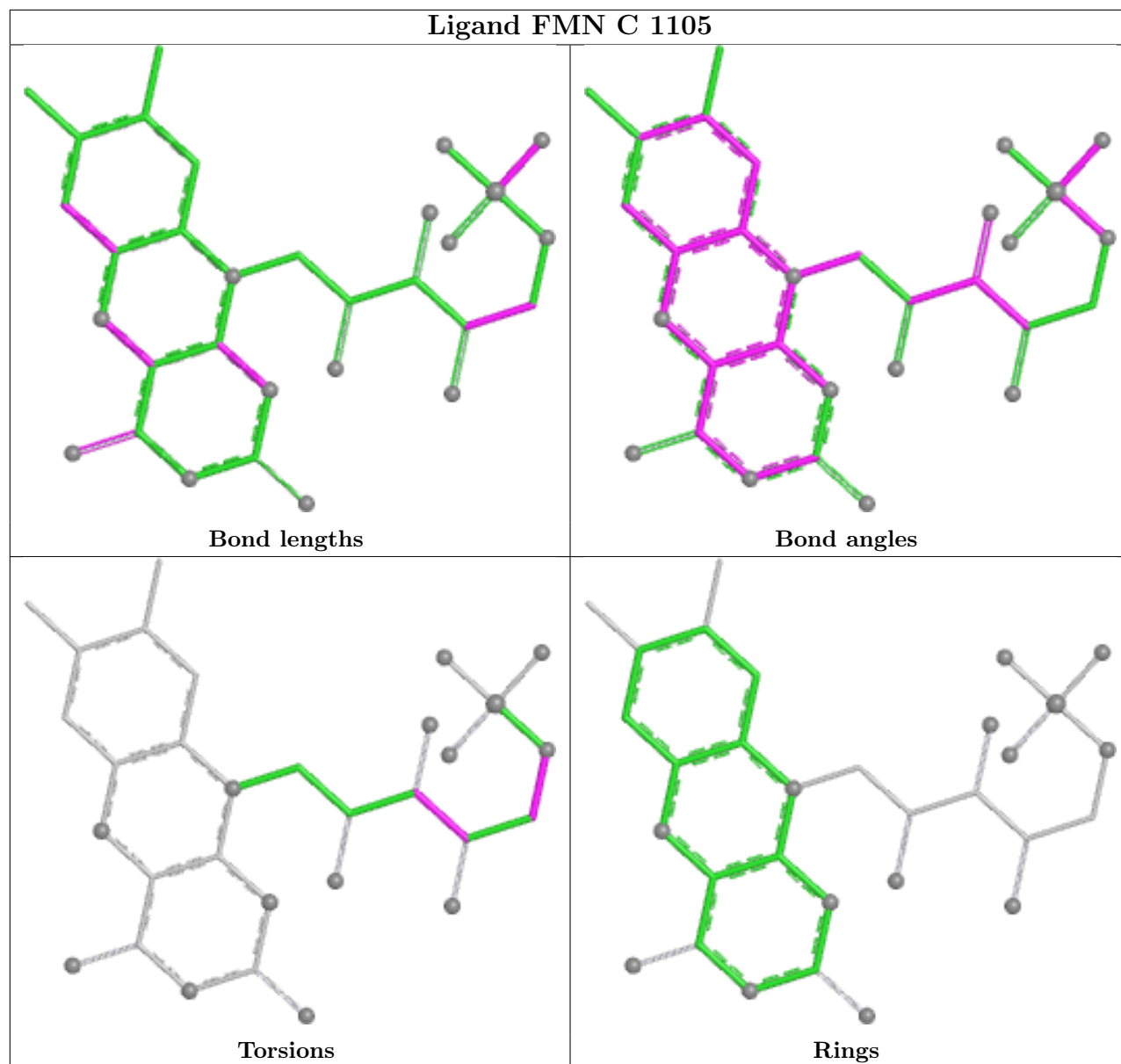
Continued from previous page...

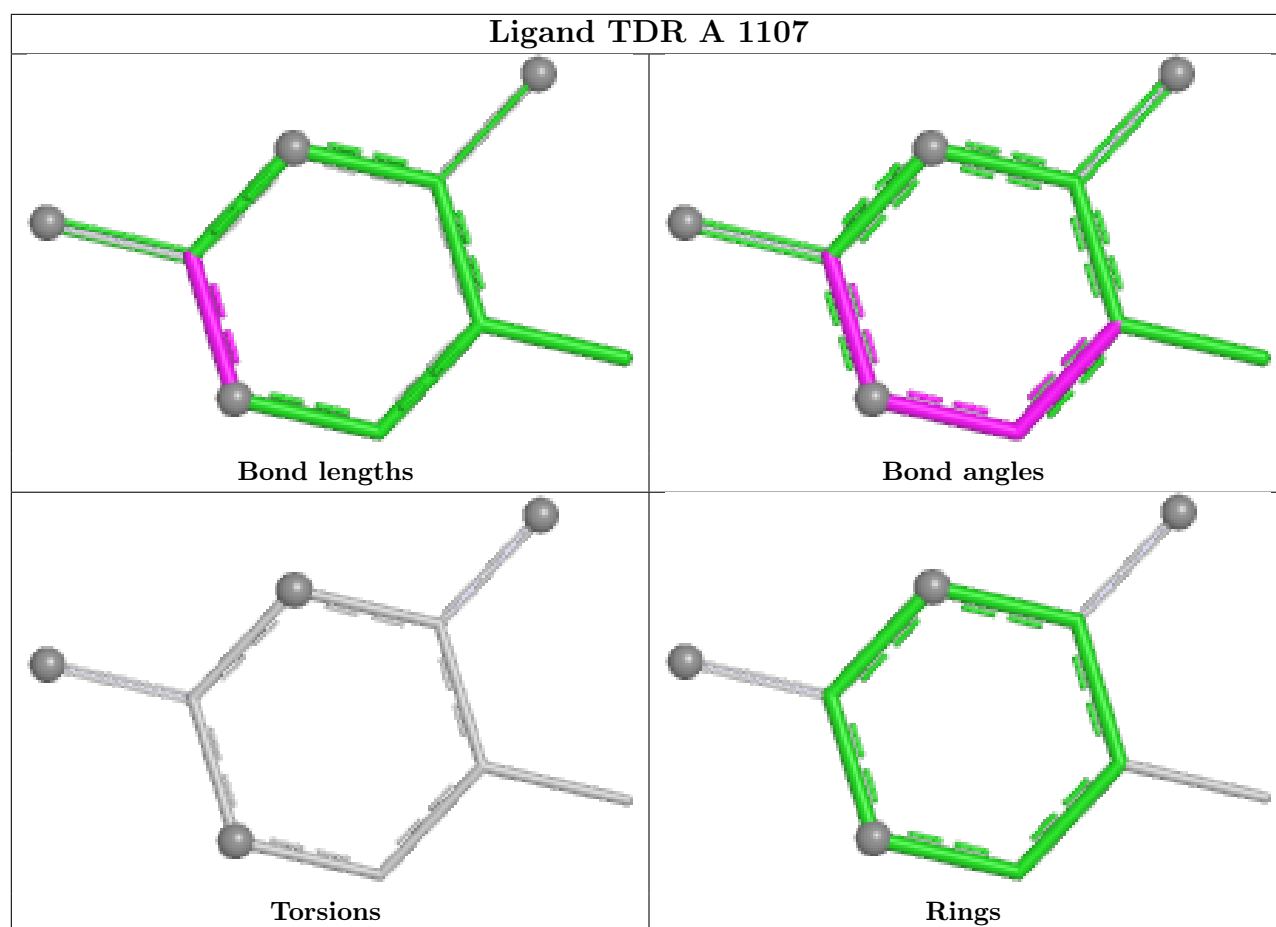
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1103	SF4	2	0
4	B	1106	FAD	2	0
2	A	1102	SF4	1	0
2	B	1101	SF4	1	0
4	D	1106	FAD	2	0
4	A	1106	FAD	1	0
3	A	1105	FMN	1	0
4	C	1106	FAD	1	0
2	B	1103	SF4	1	0
2	C	1102	SF4	3	0
2	D	1101	SF4	1	0
3	D	1105	FMN	1	0
3	B	1105	FMN	1	0

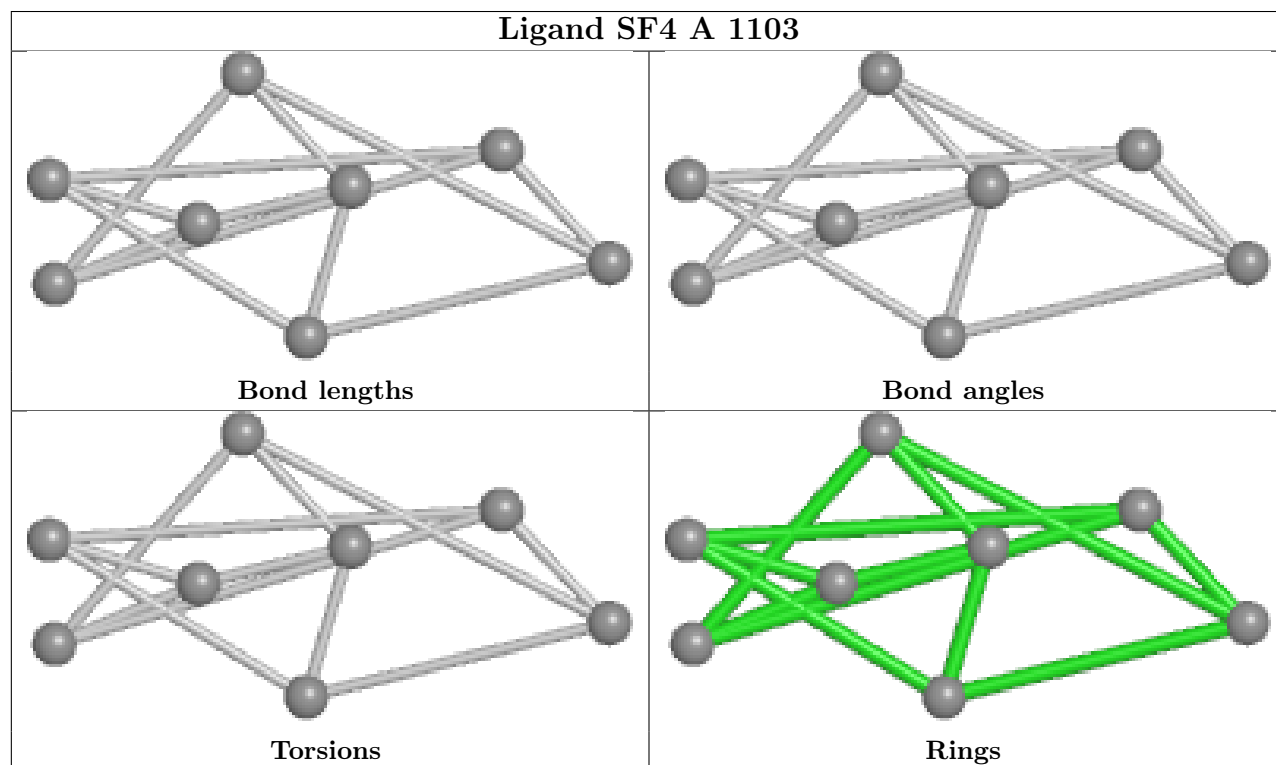
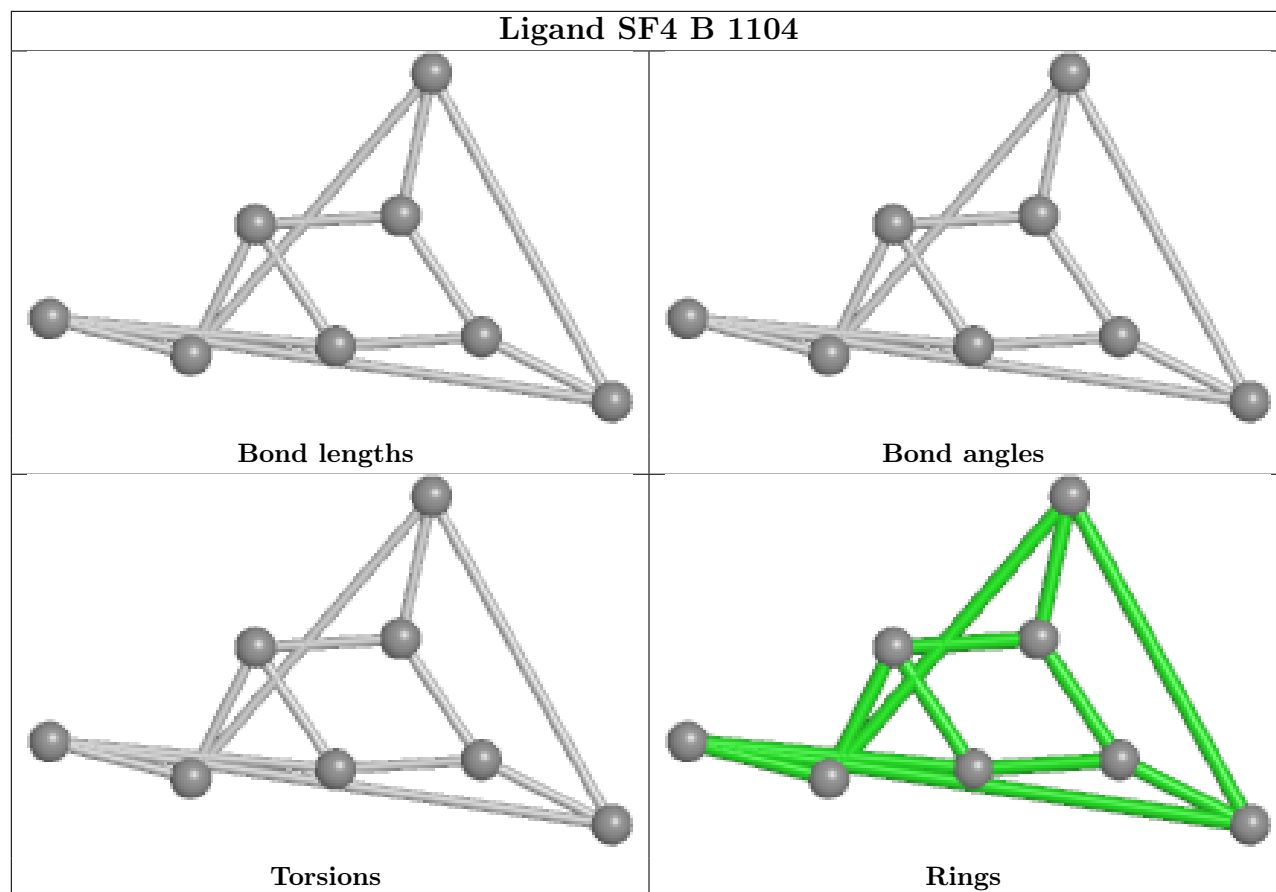
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

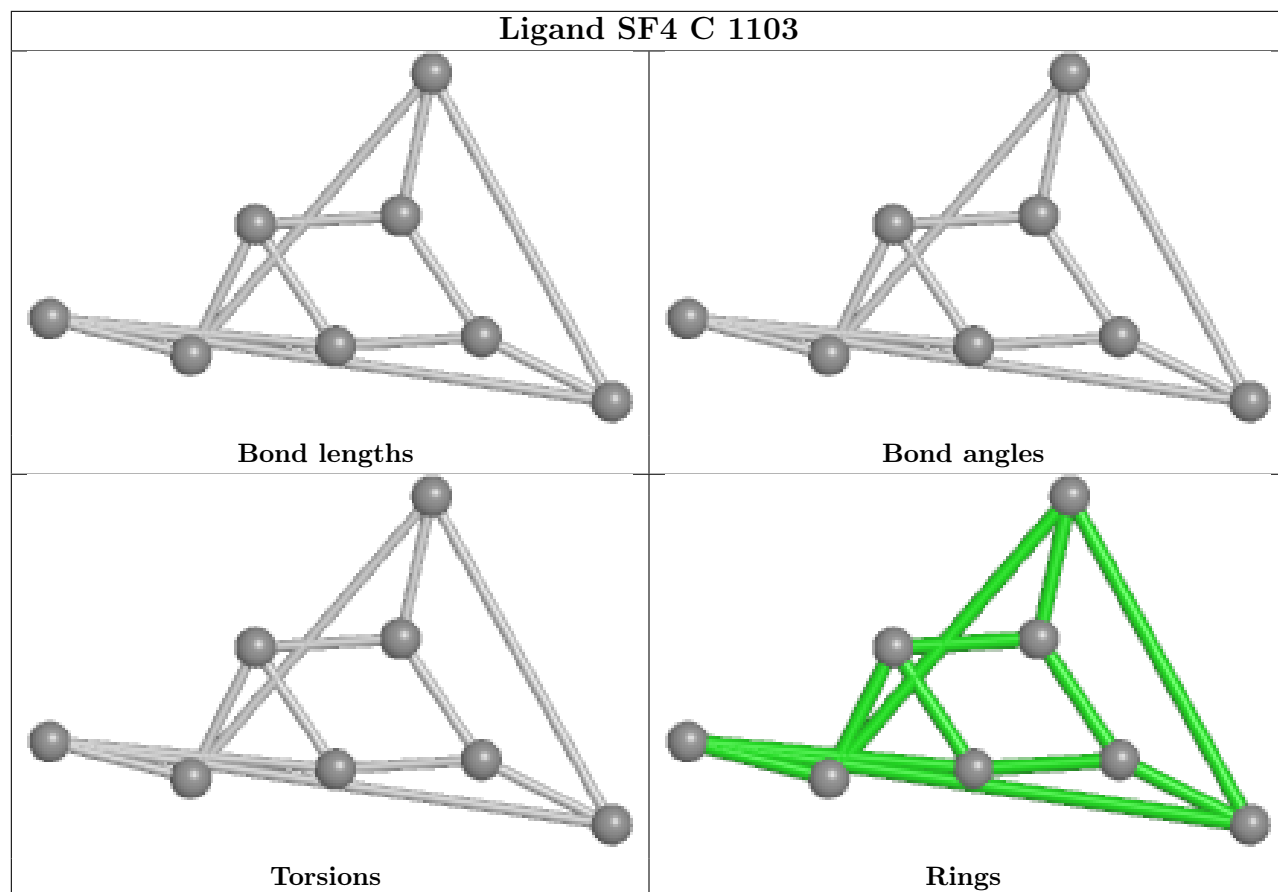


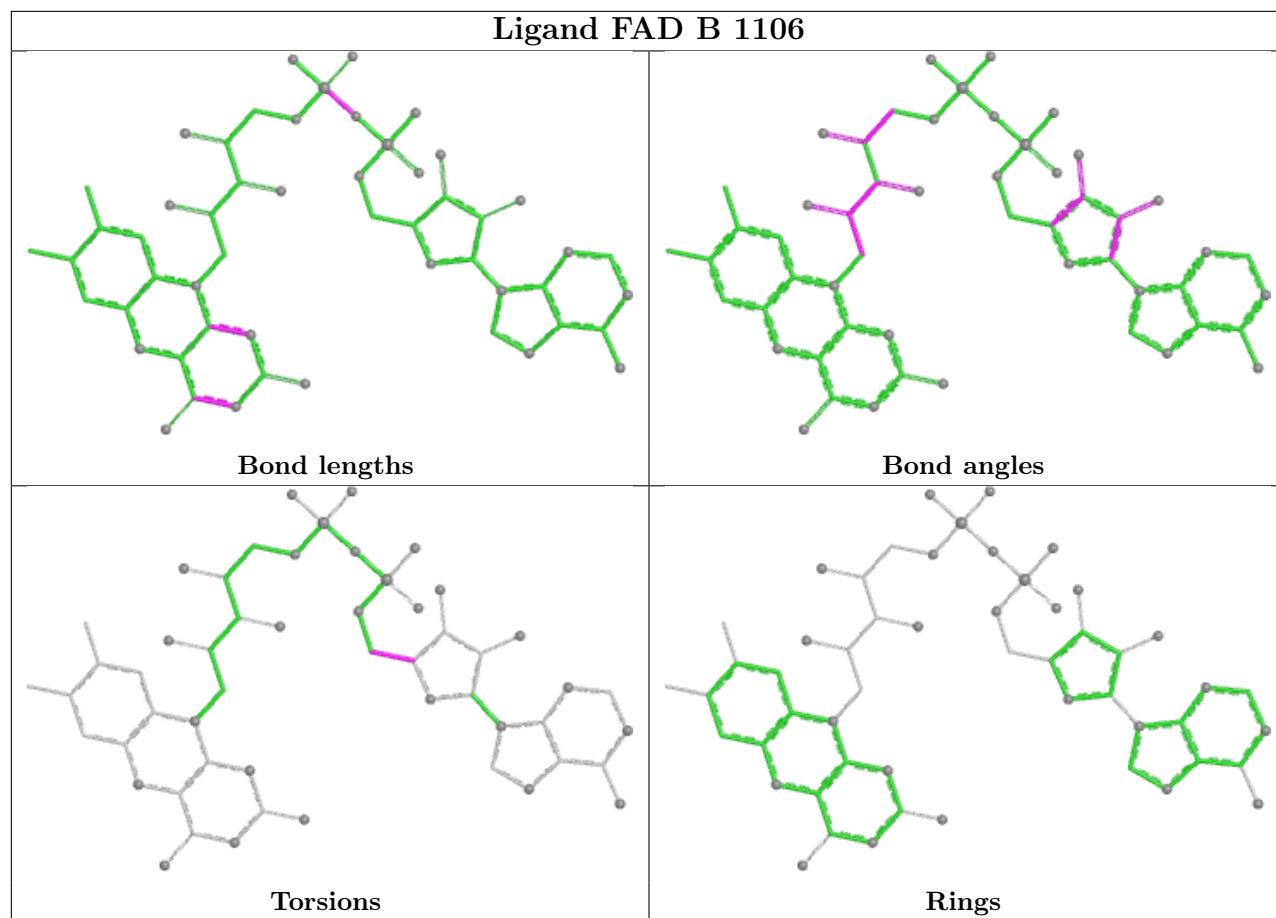
Ligand FMN C 1105

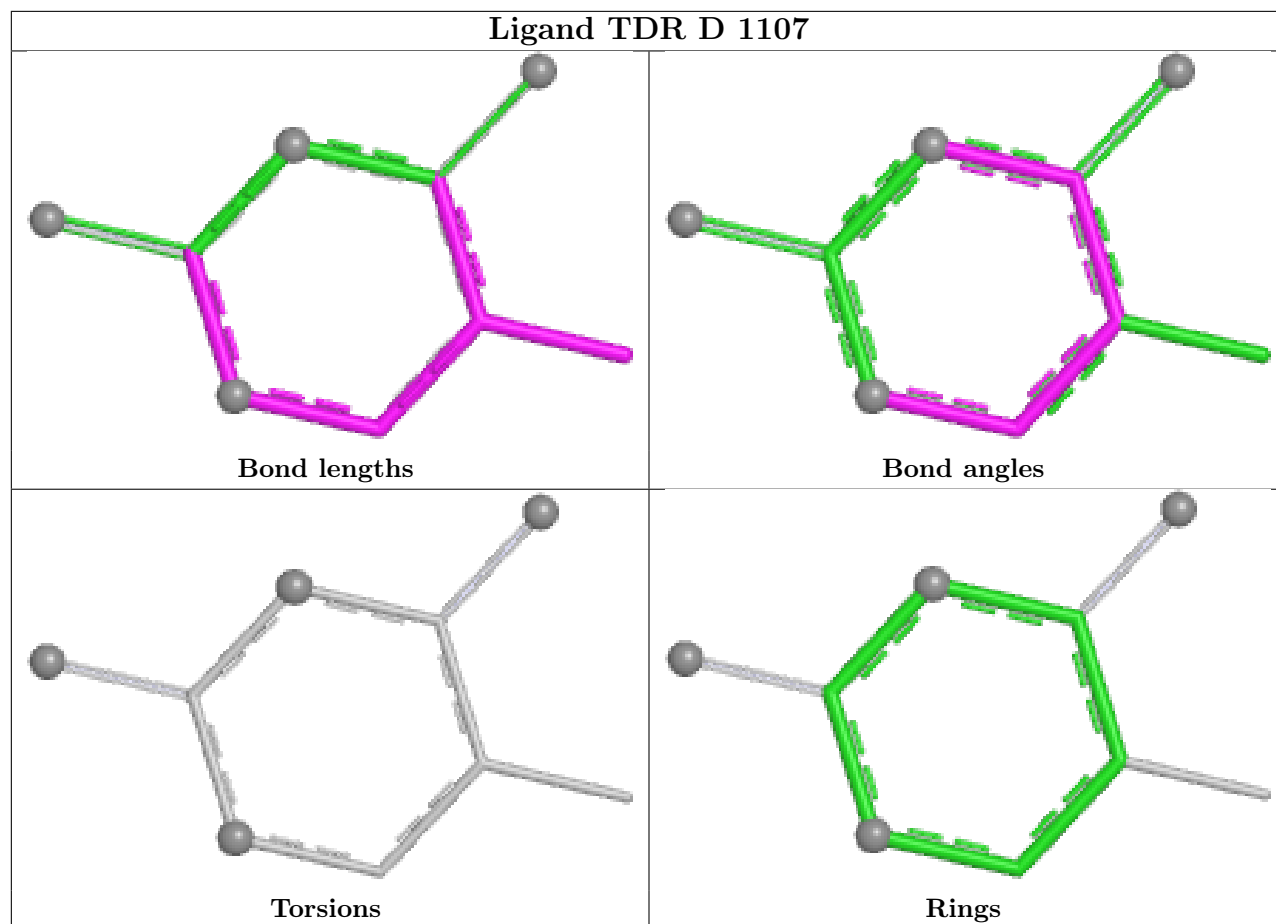


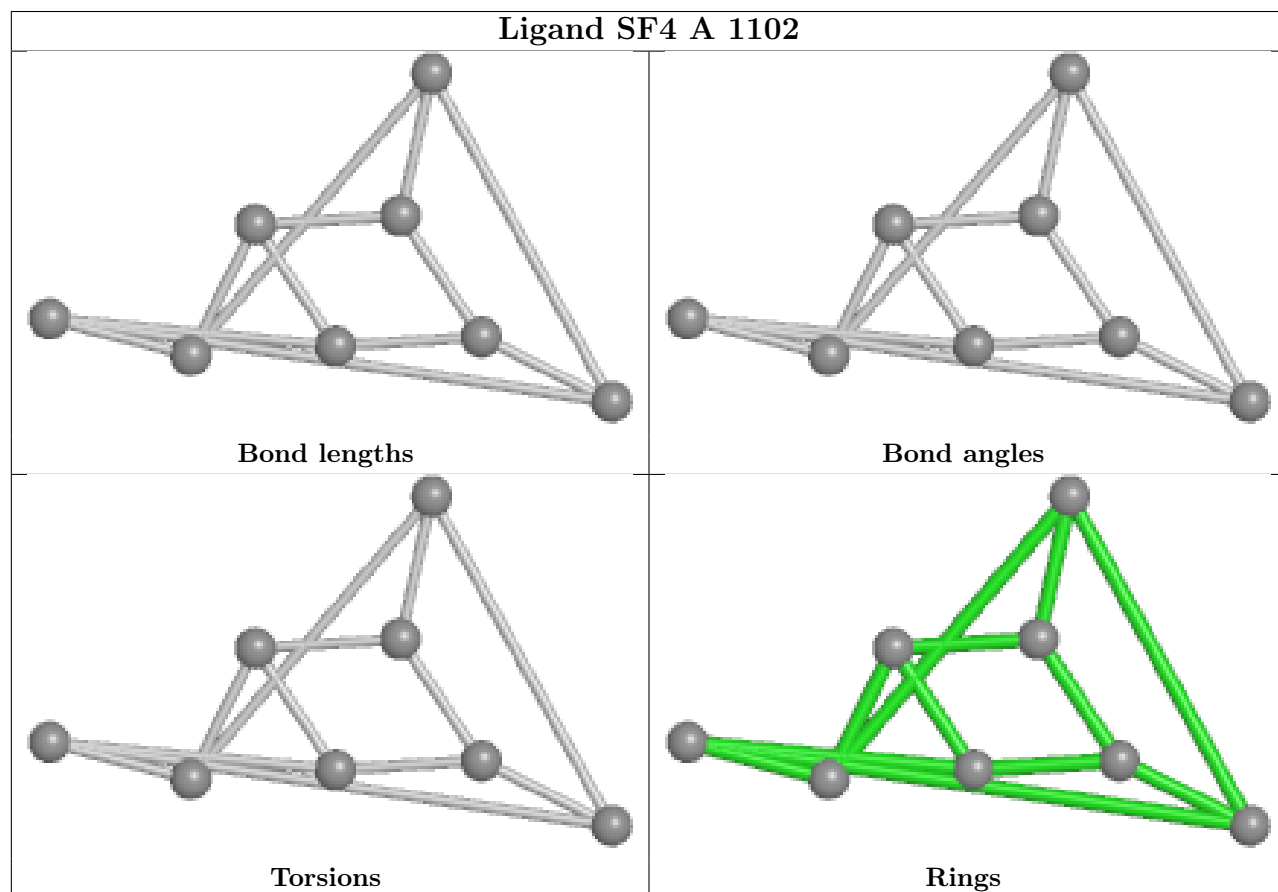
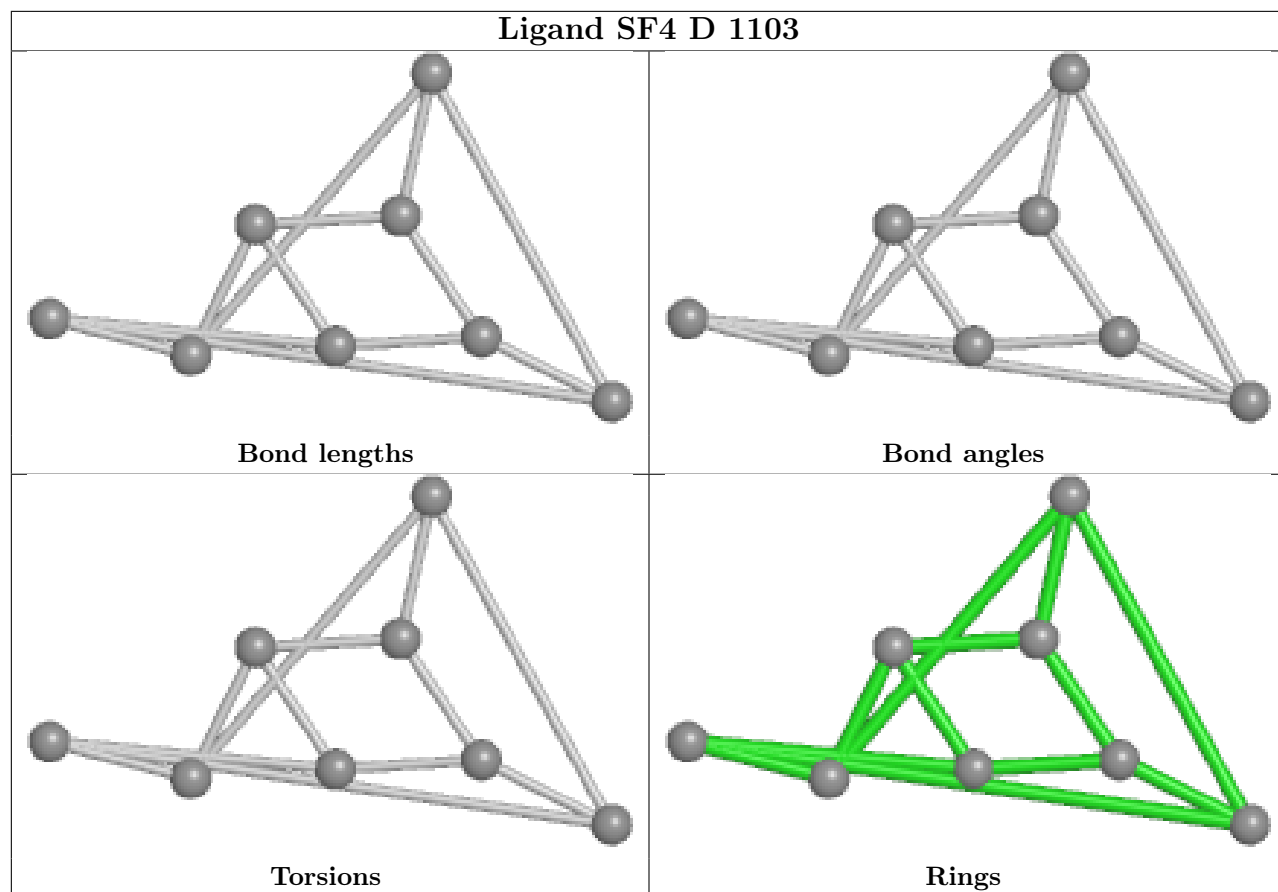


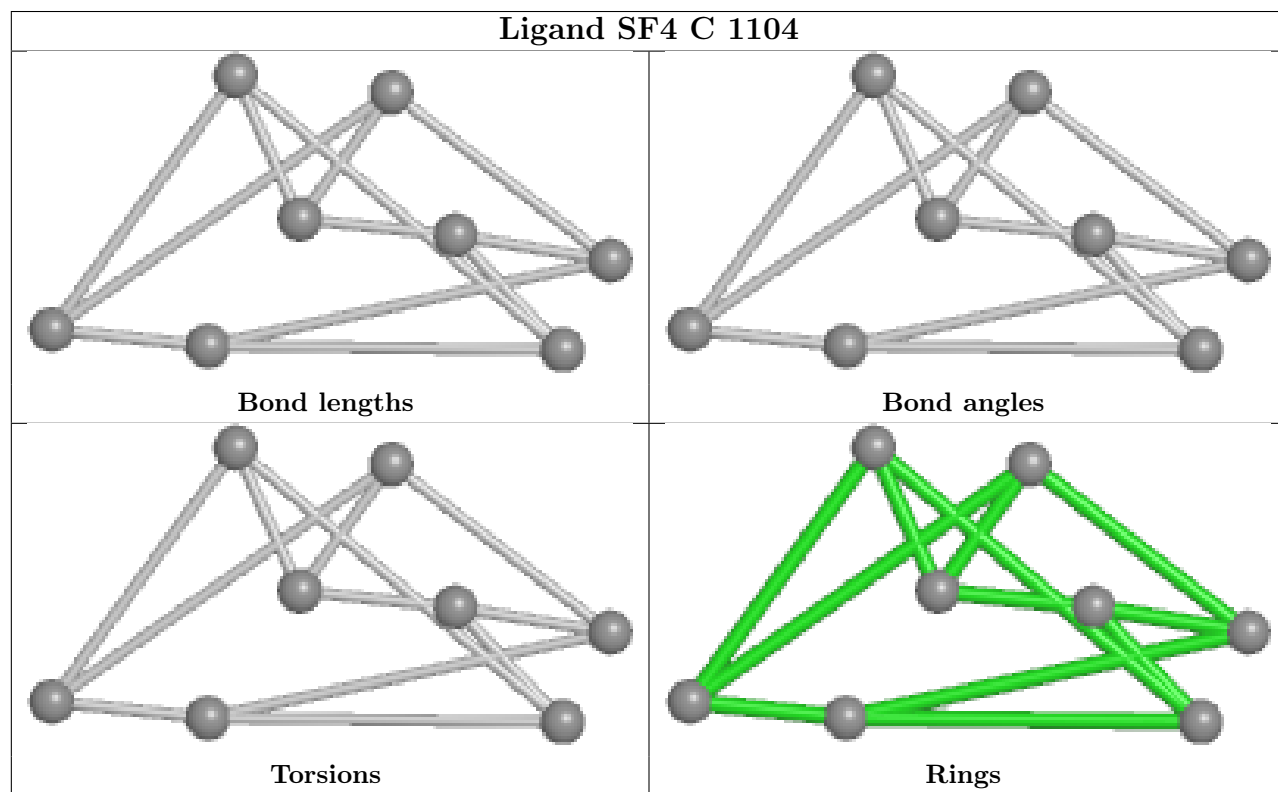
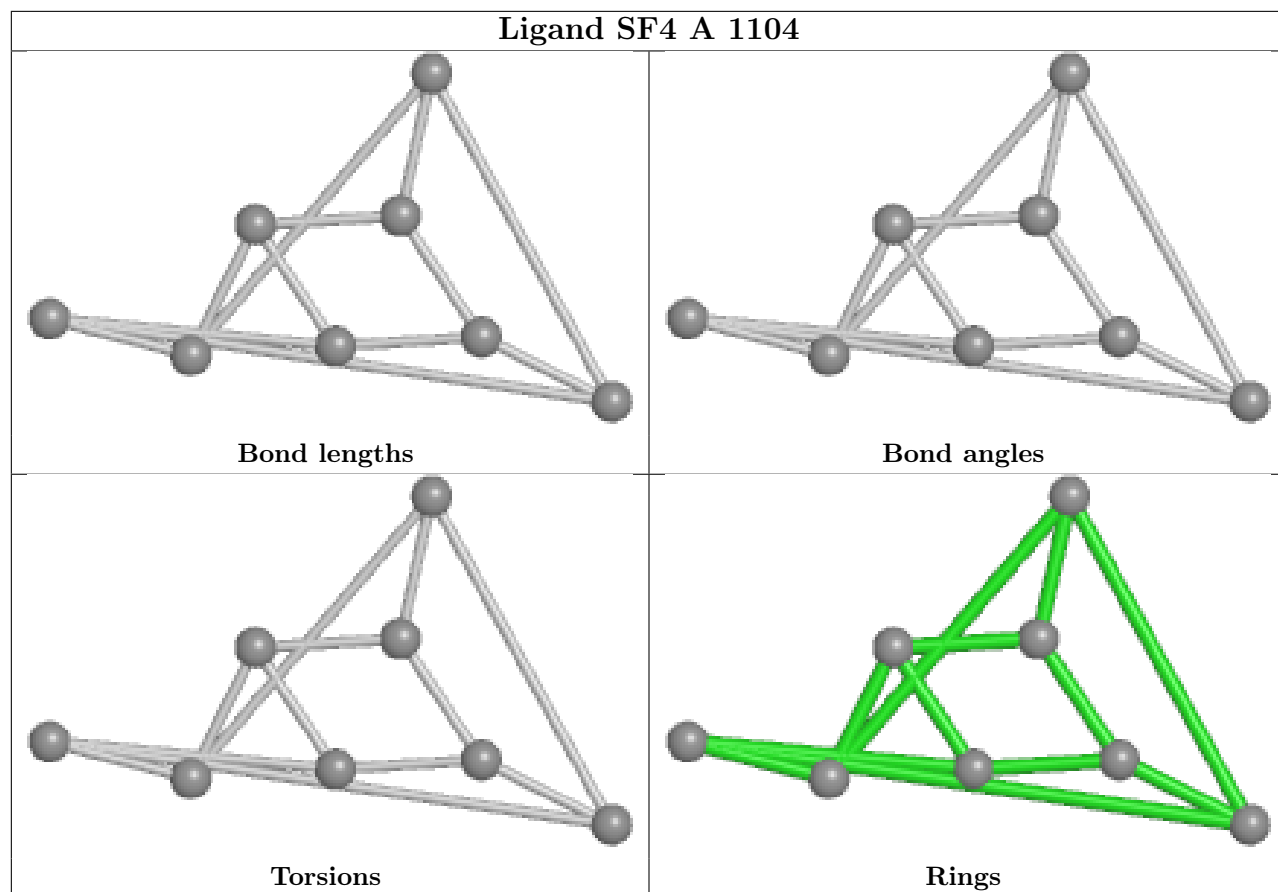


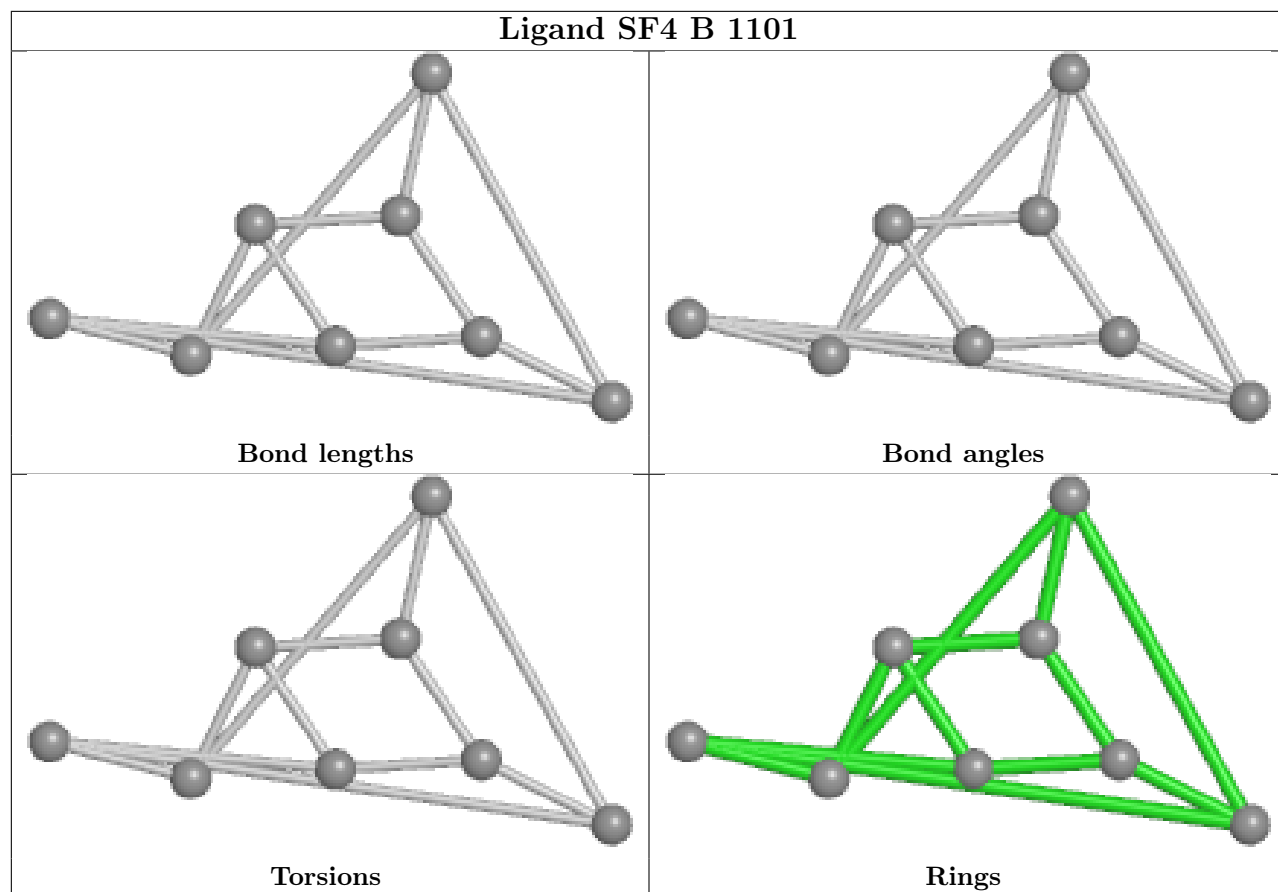


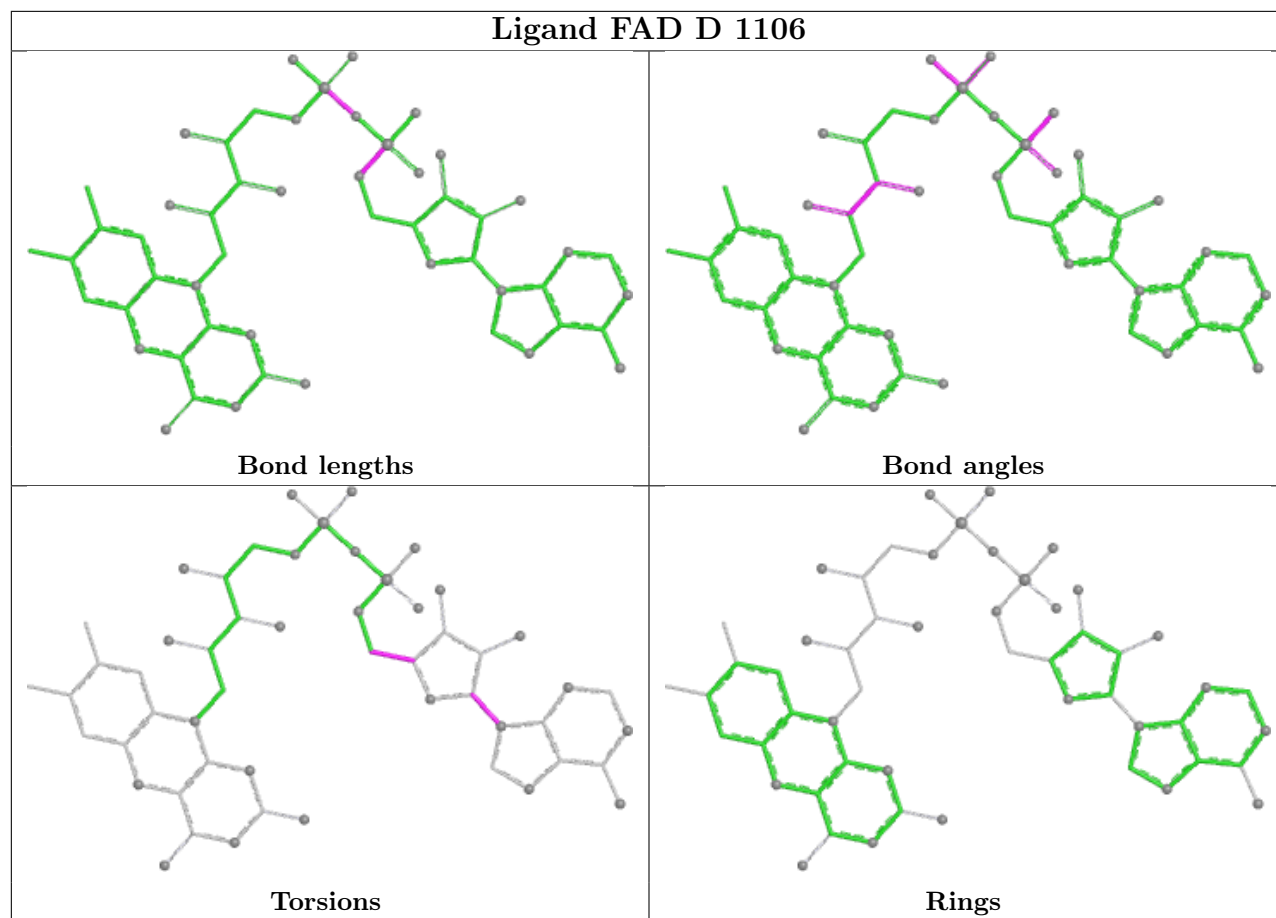


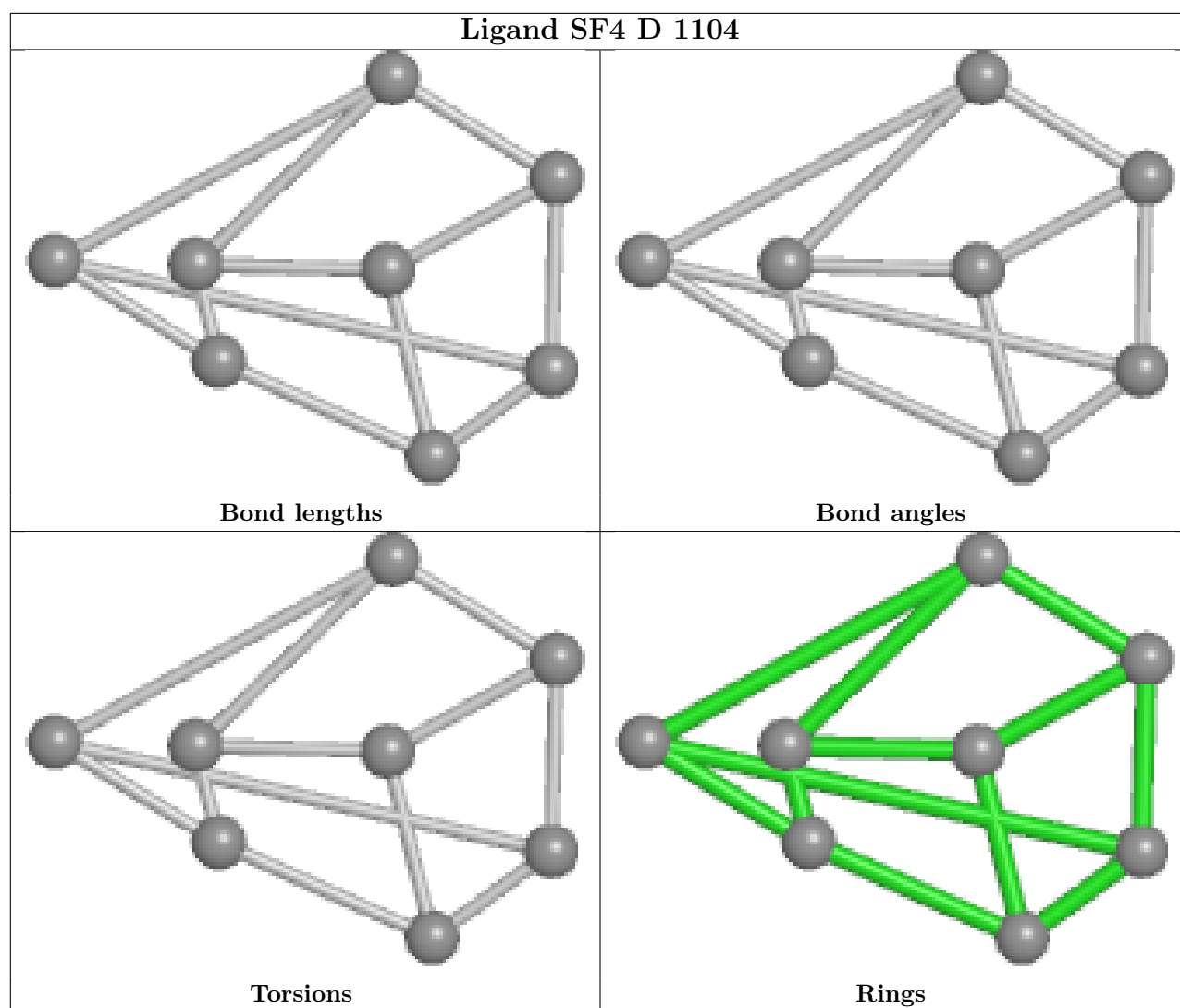


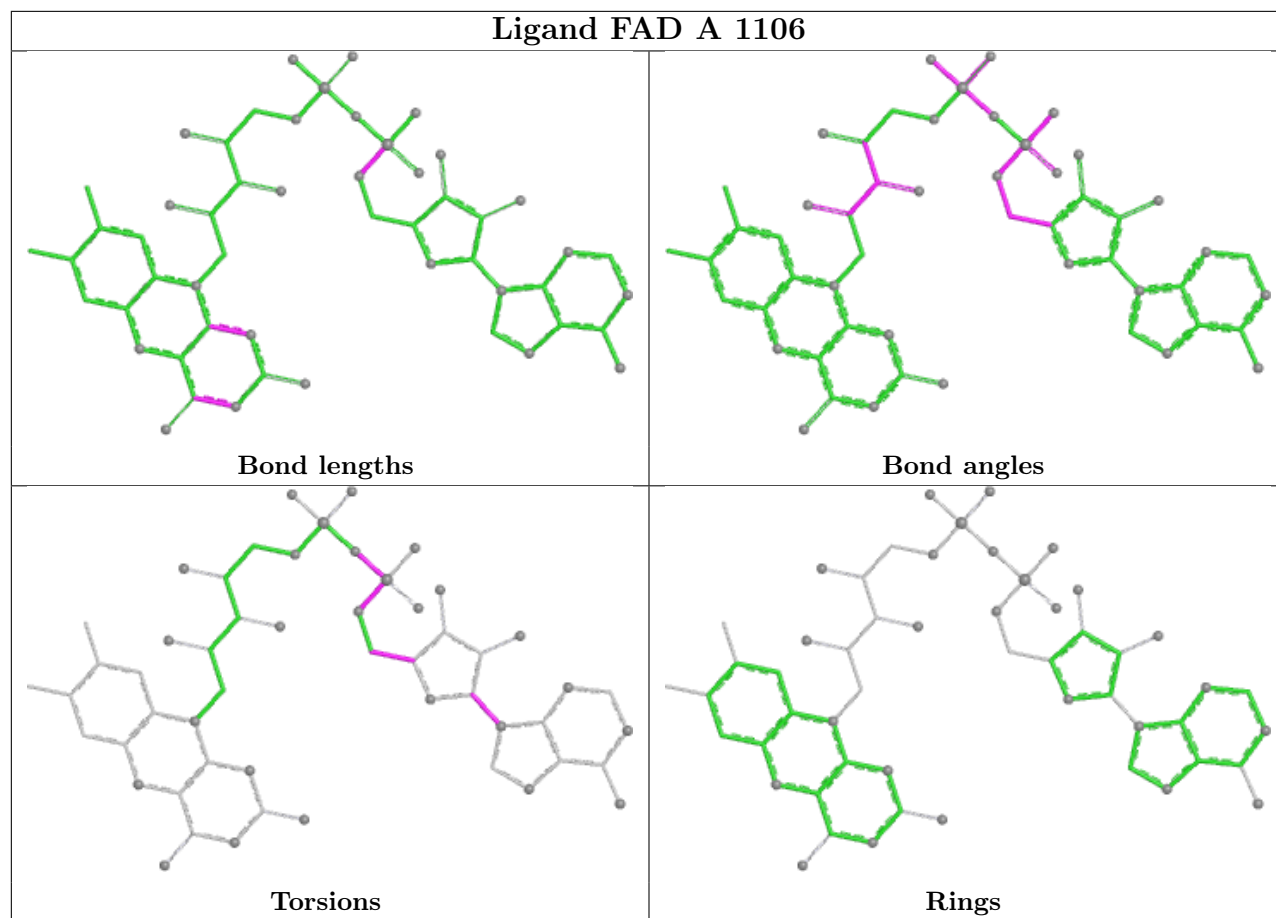


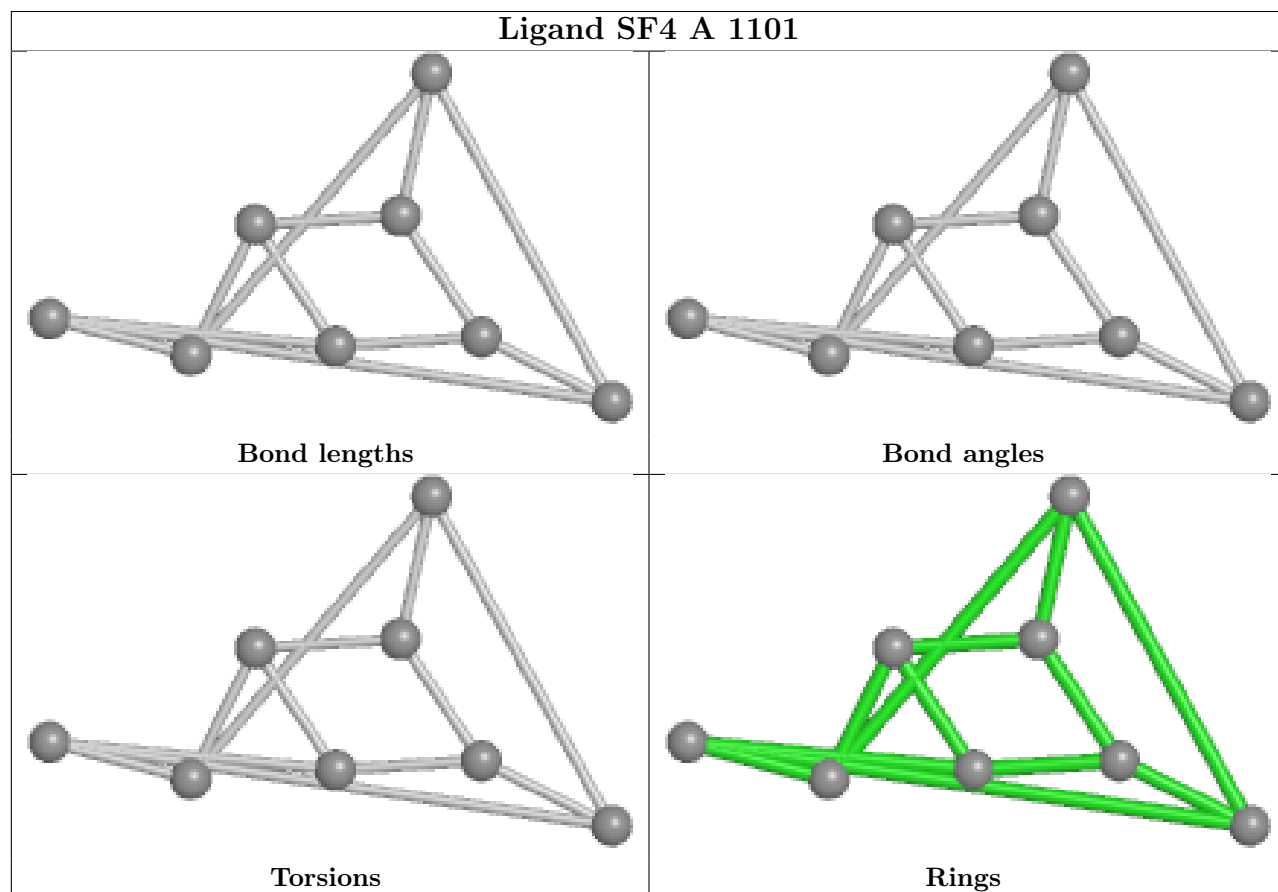
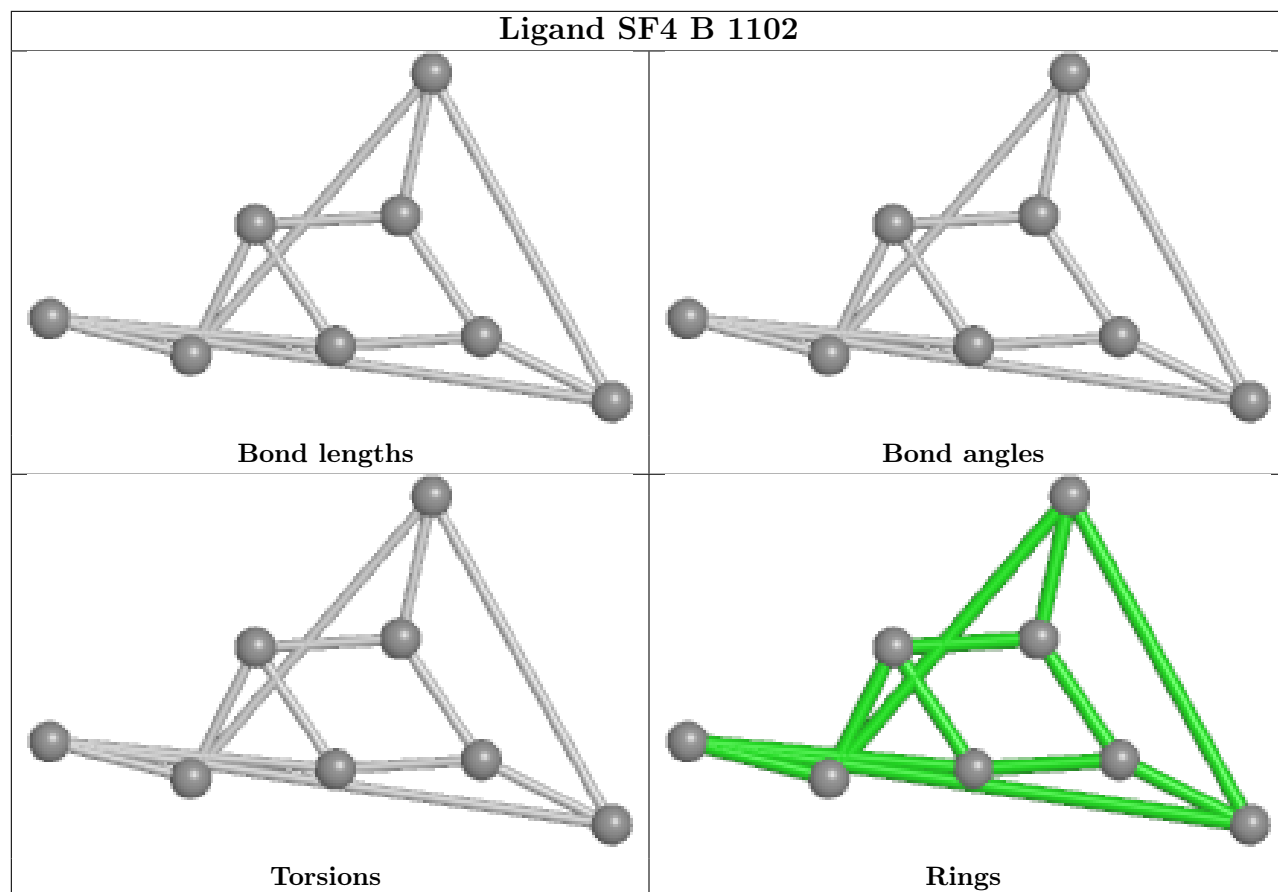




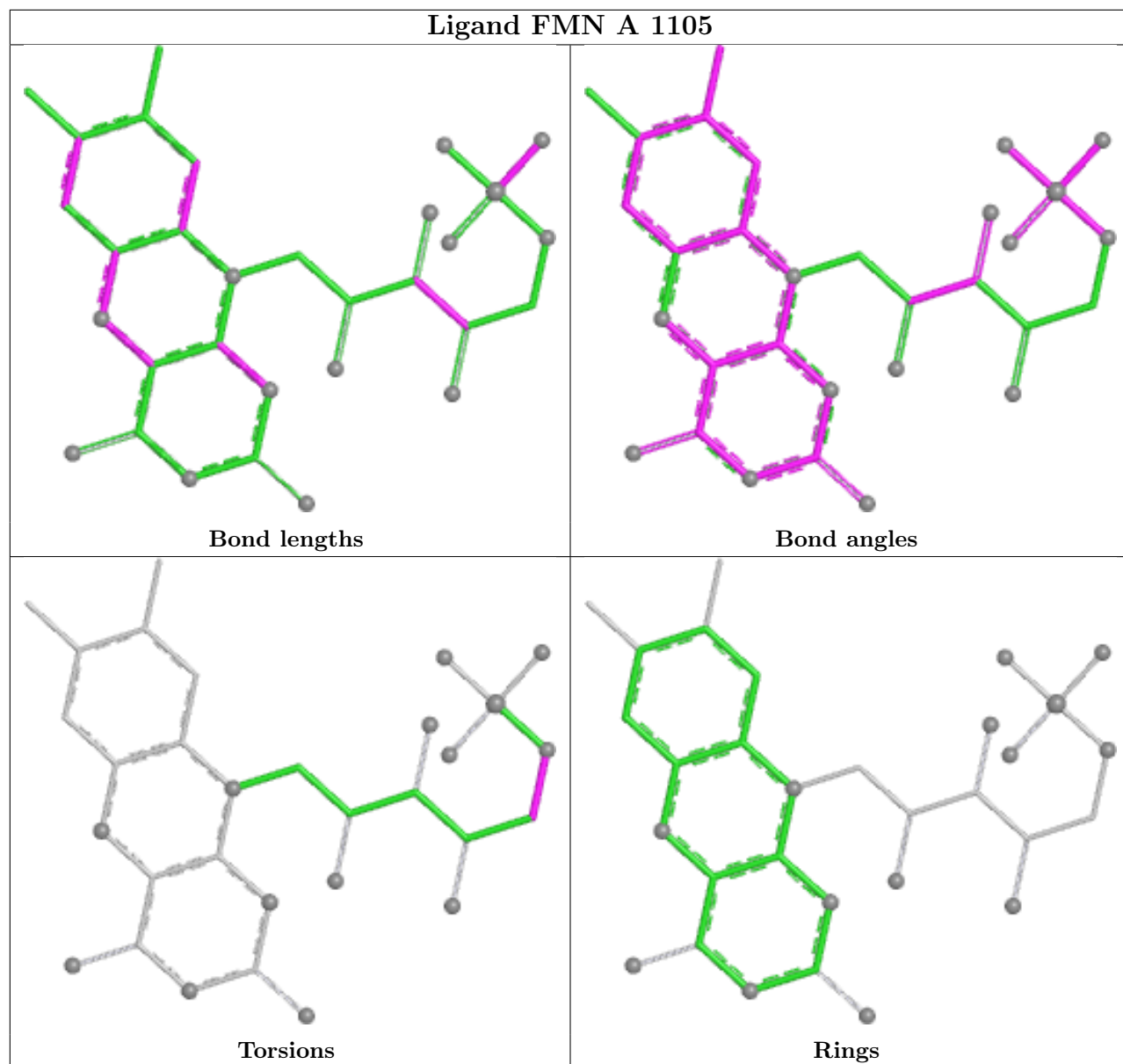


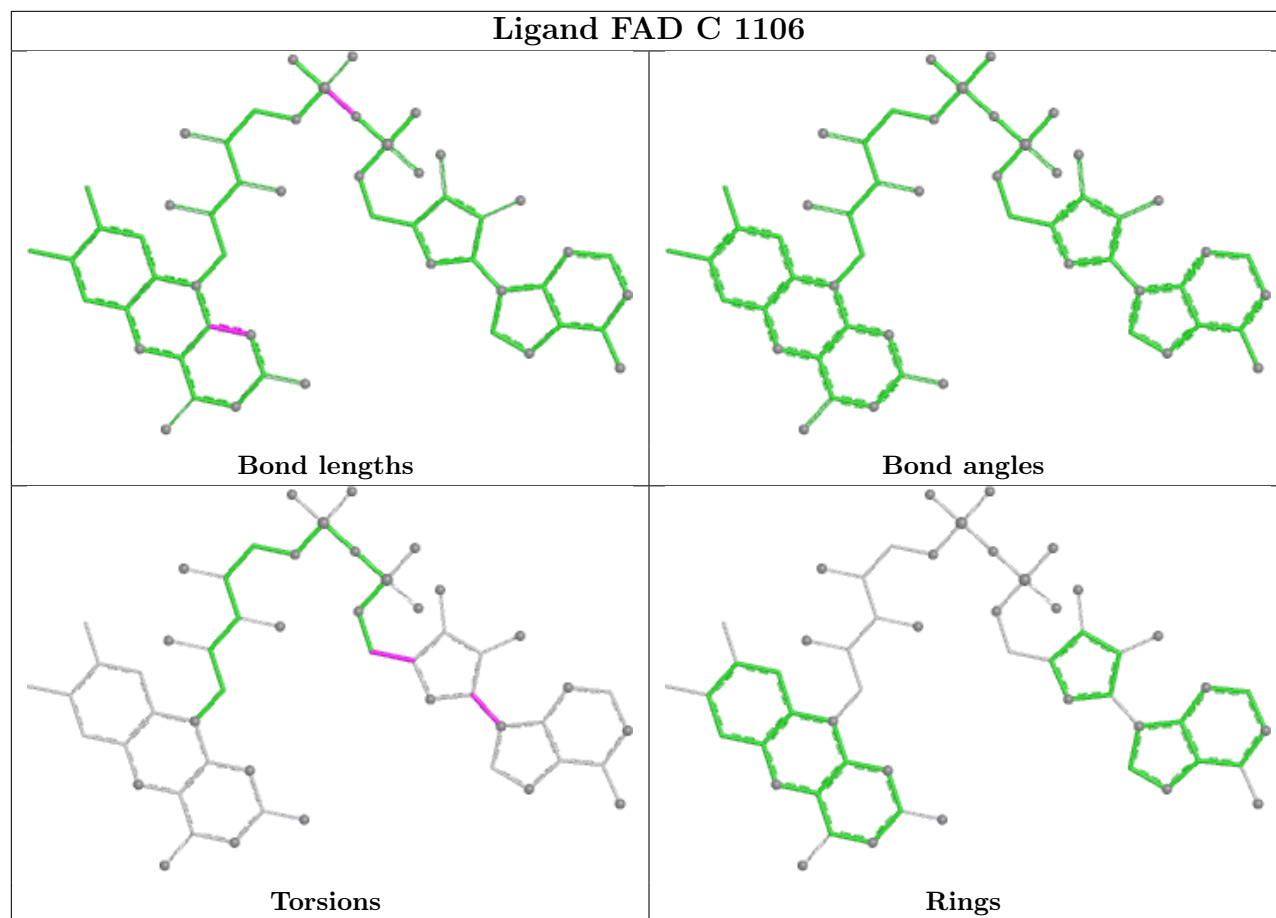




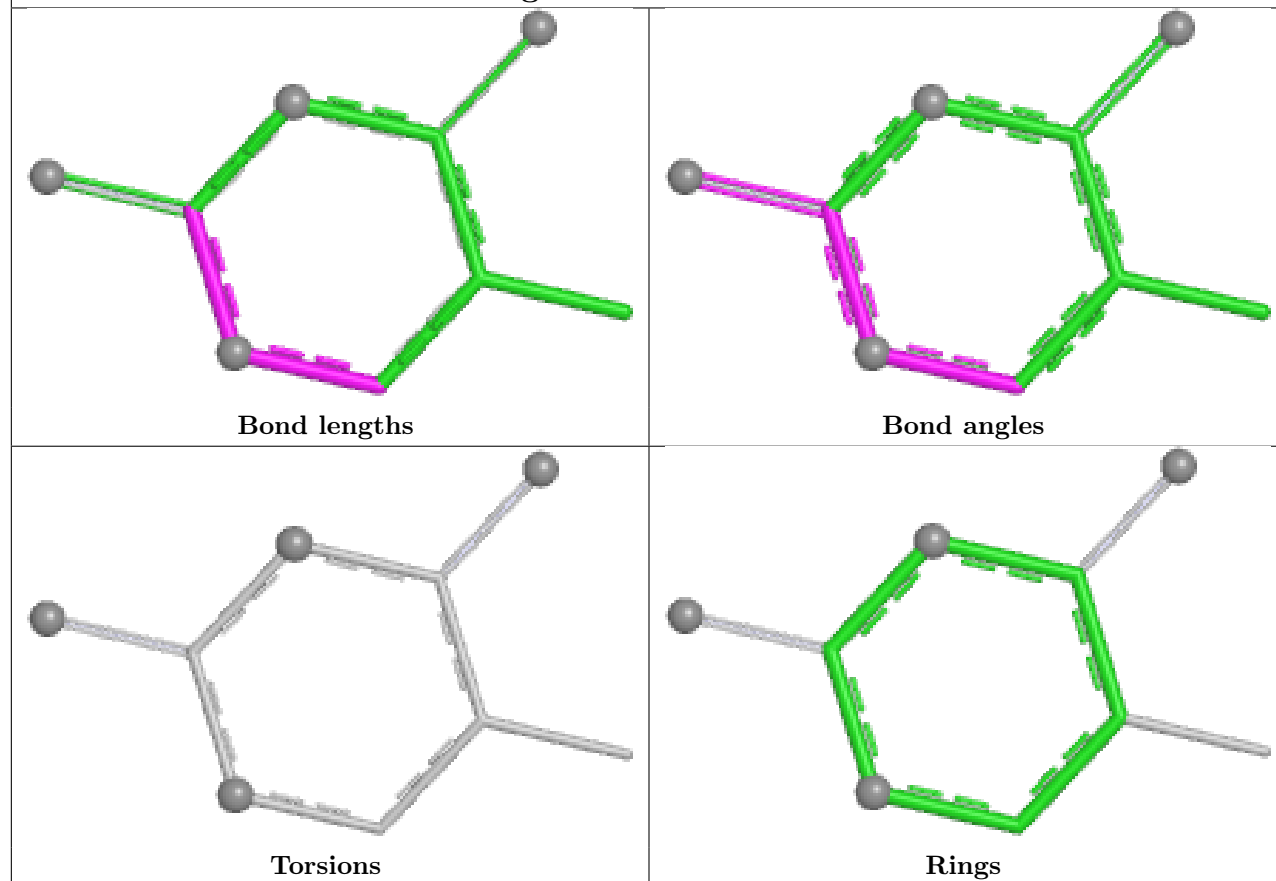


Ligand FMN A 1105

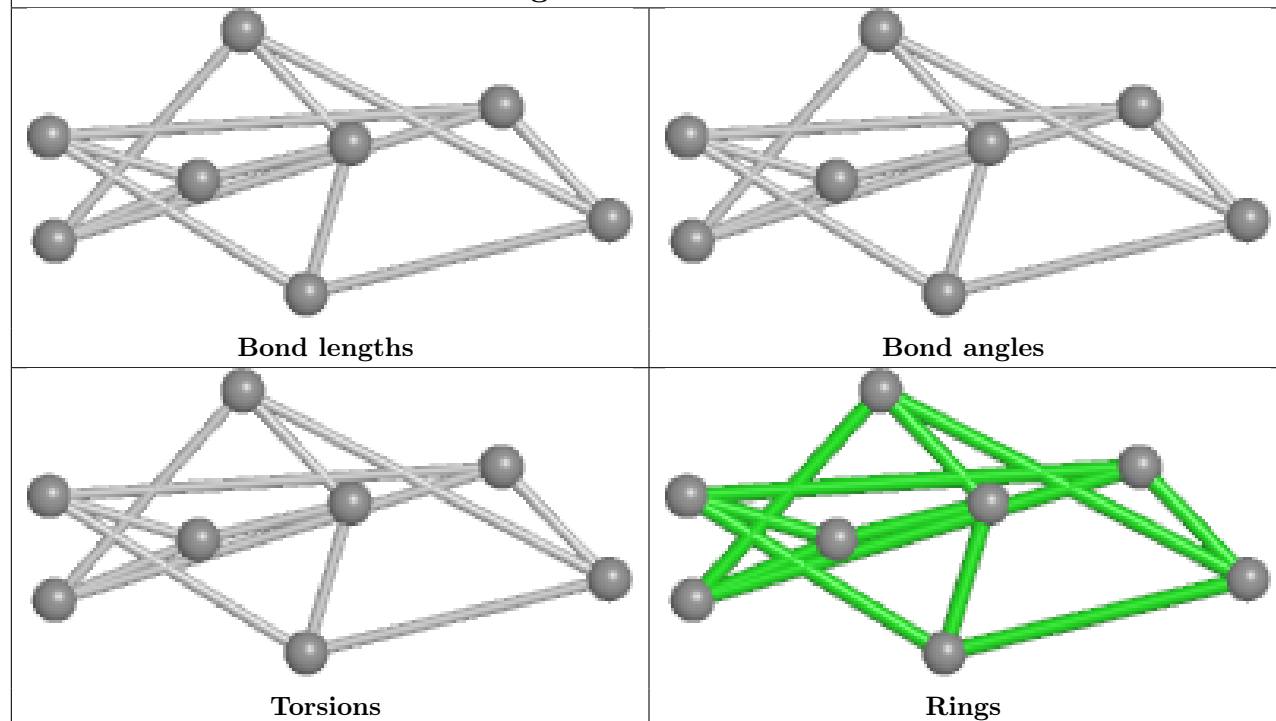


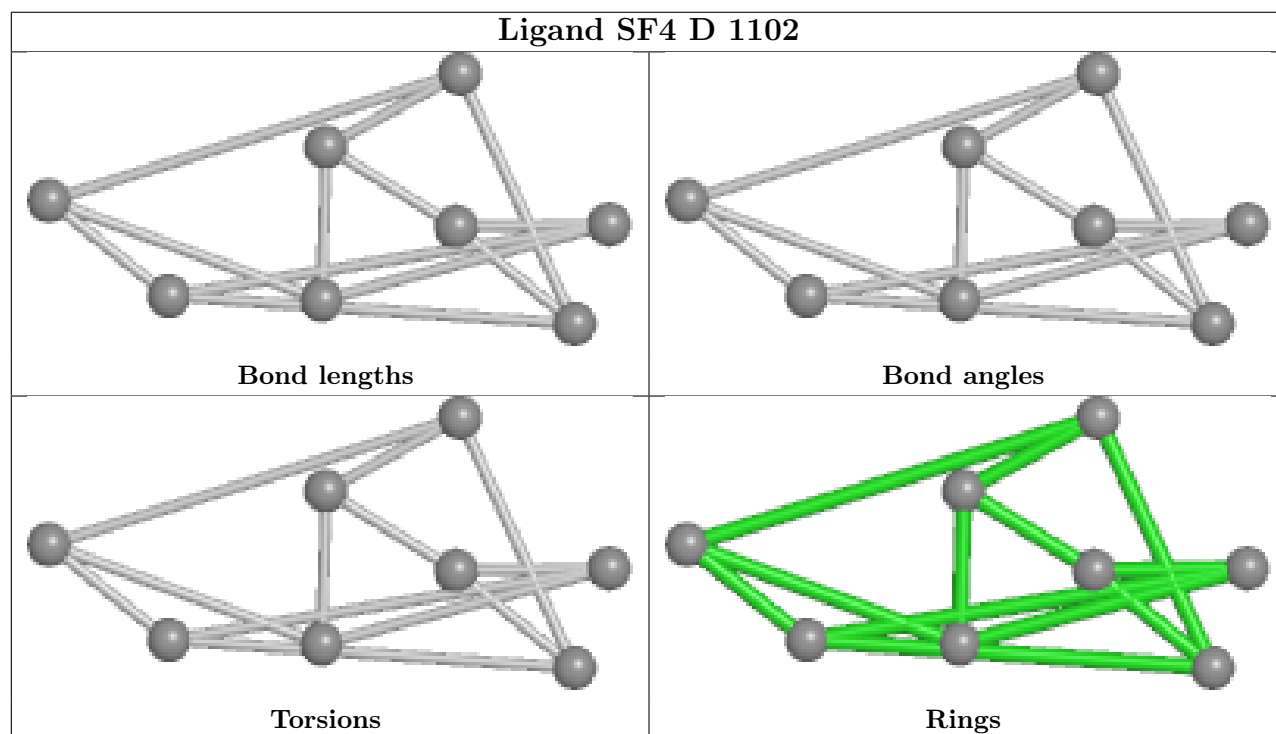
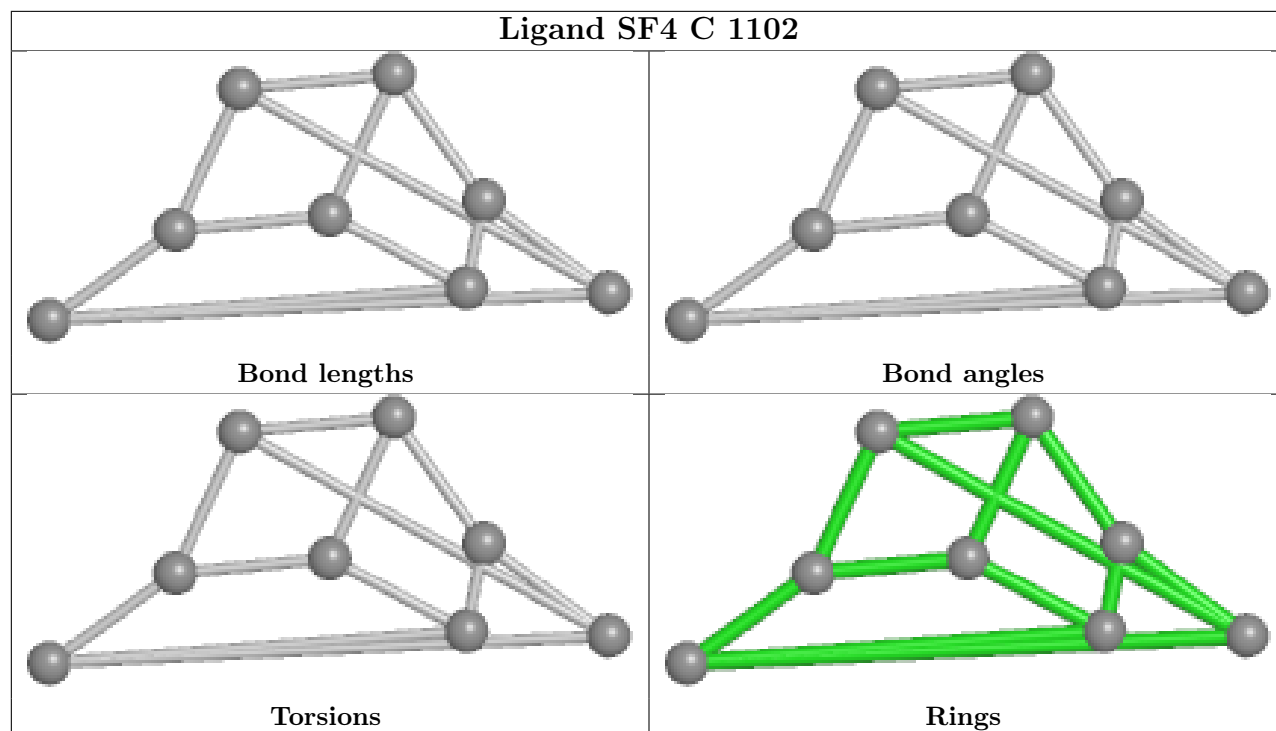


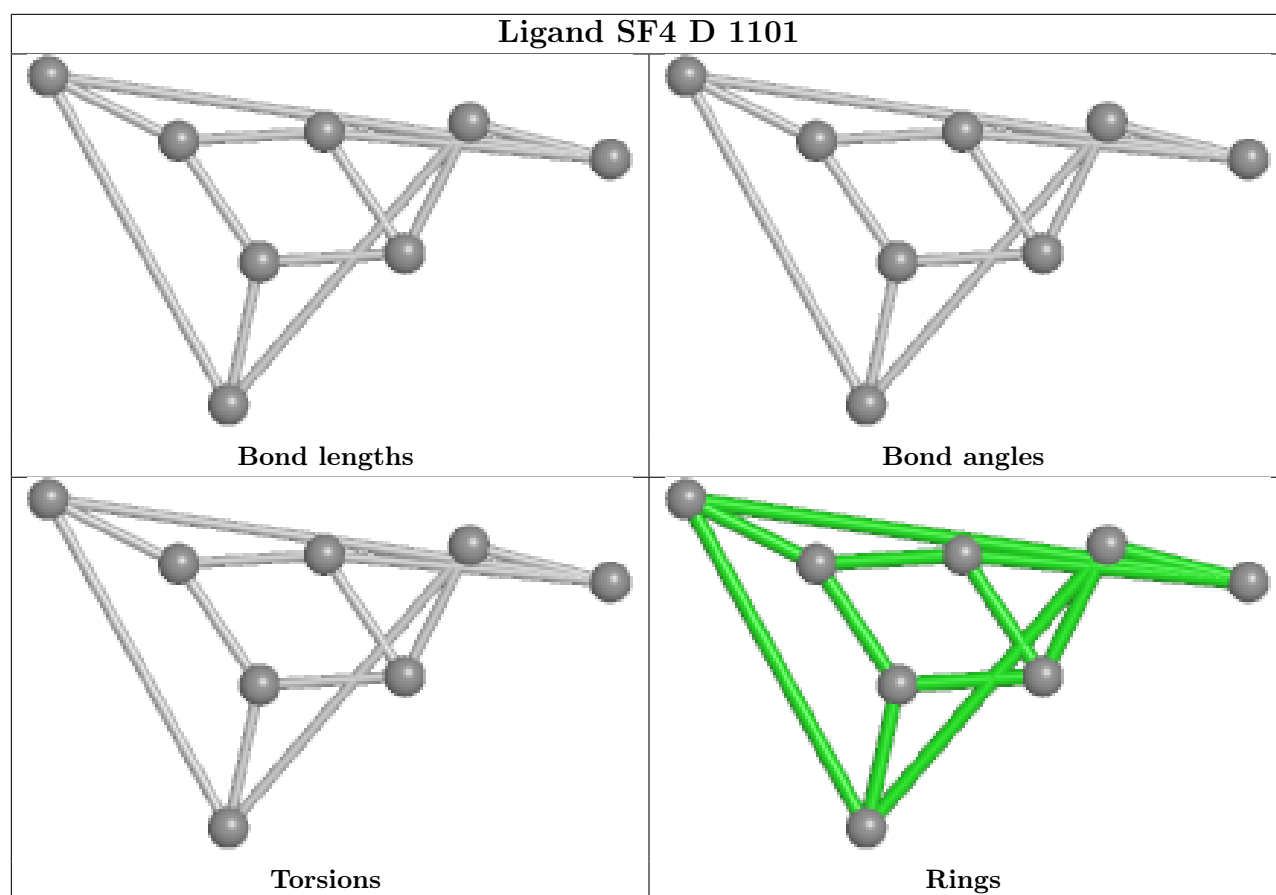
Ligand TDR B 1107



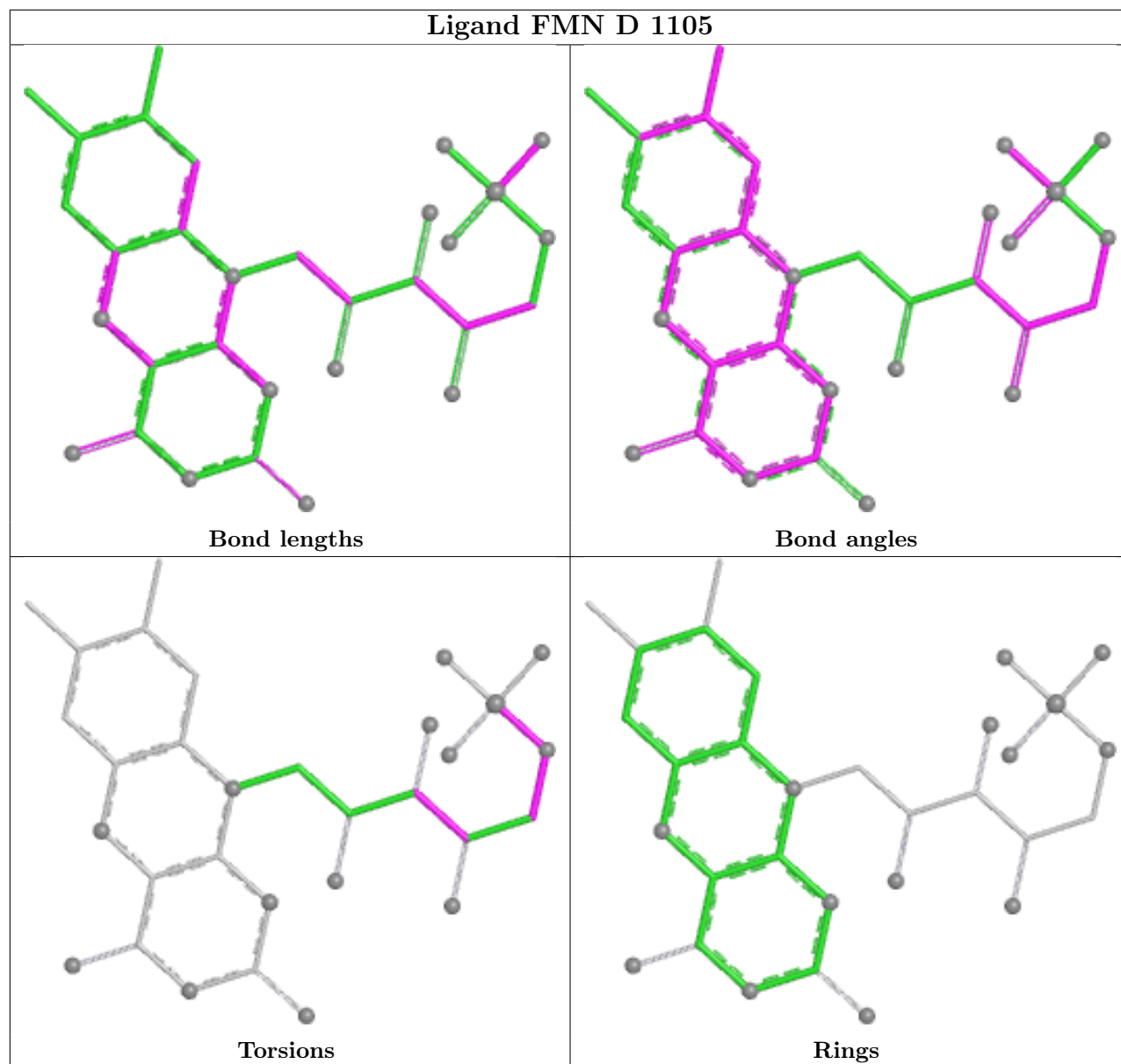
Ligand SF4 B 1103



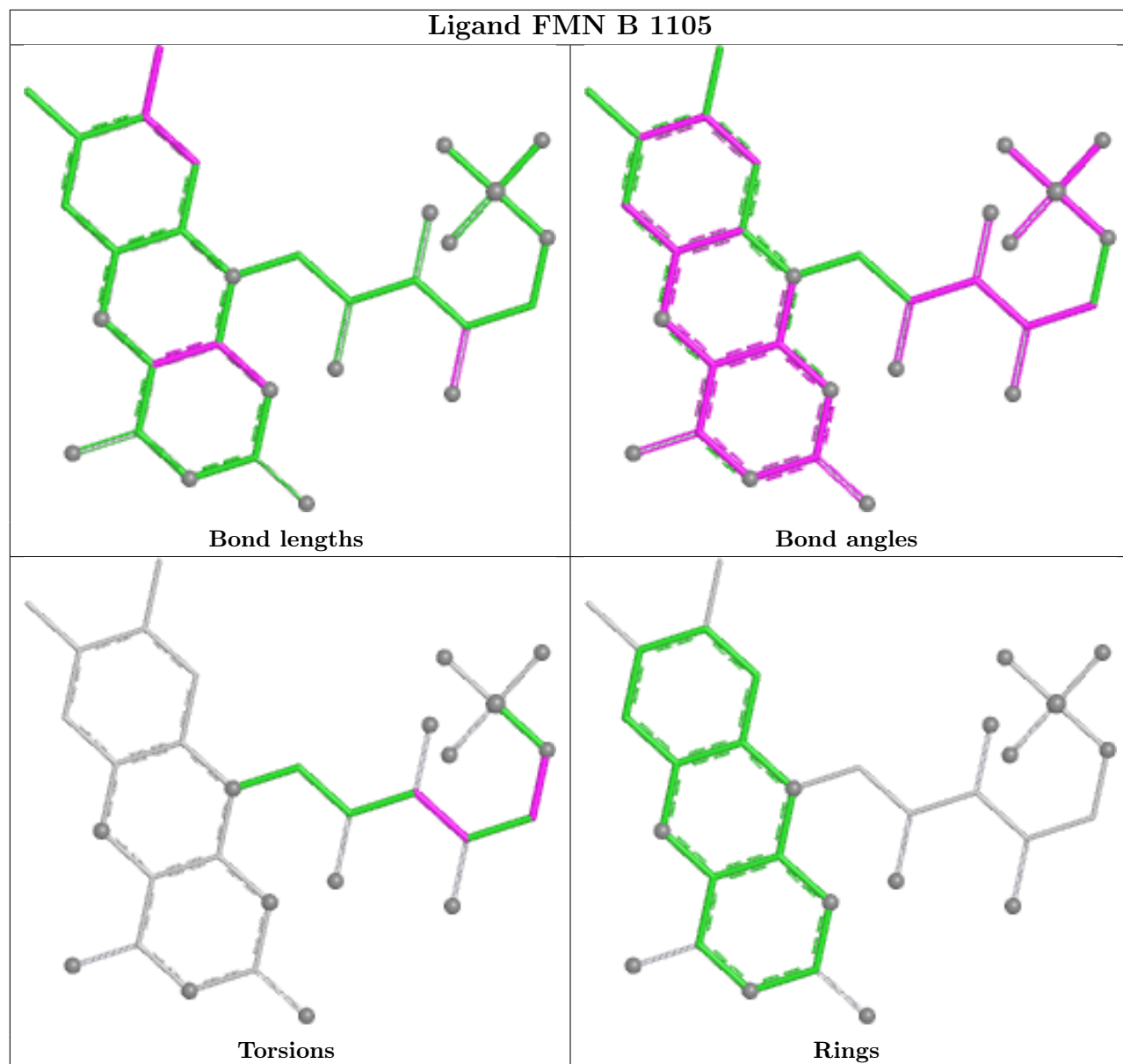


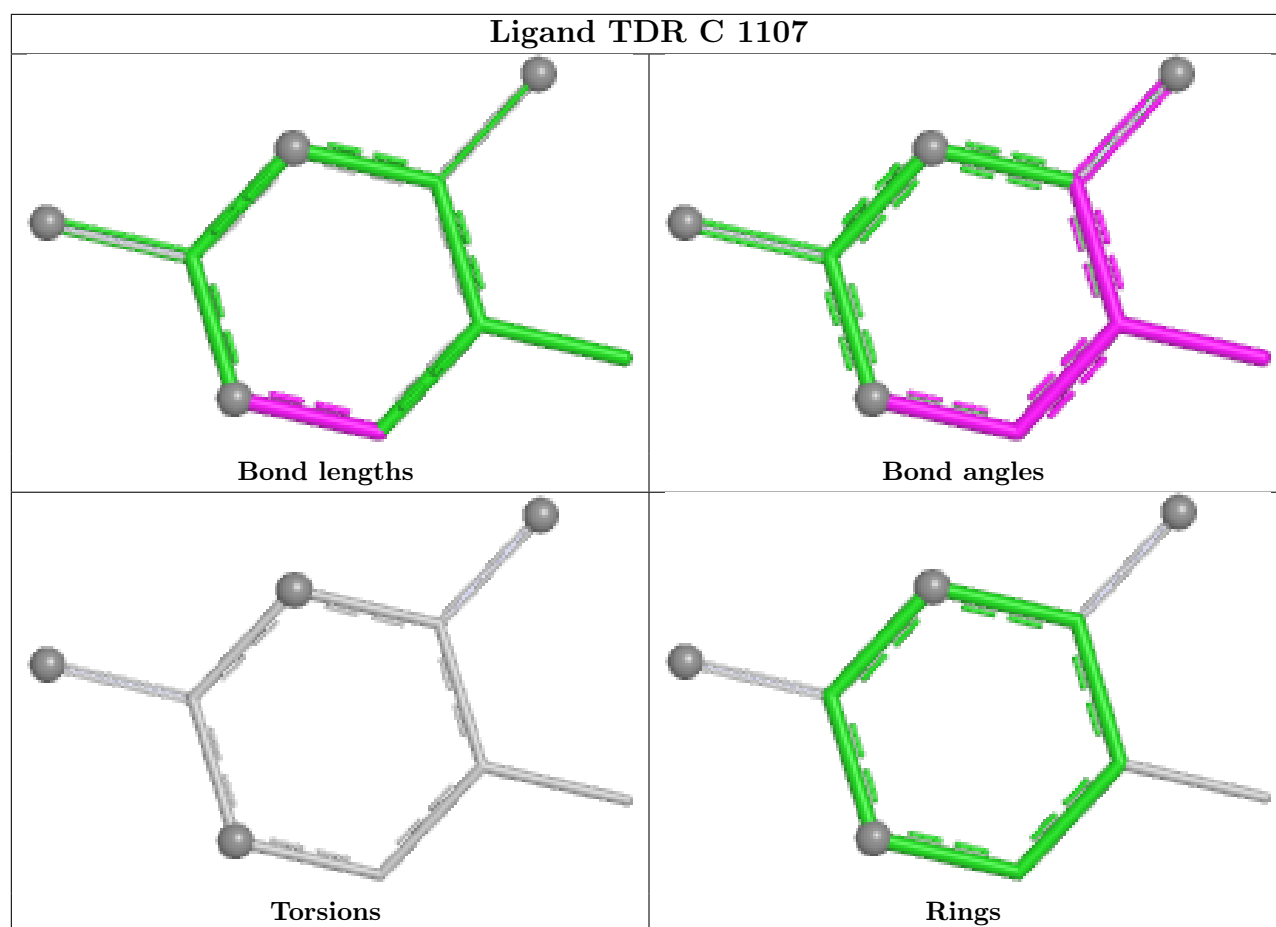


Ligand FMN D 1105



Ligand FMN B 1105





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

Continued on next page...

Continued from previous page...

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

6 Fit of model and data

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

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	868	ILE	7.7
1	A	2	ALA	7.2
1	A	868	ILE	6.6
1	A	1017	LEU	6.2
1	D	868	ILE	6.0
1	D	869	ALA	5.8
1	D	327	PRO	5.8
1	C	868	ILE	5.7
1	B	897	LEU	5.6
1	D	866	PRO	5.4
1	C	866	PRO	5.4
1	D	865	VAL	5.3
1	D	1008	THR	5.2
1	D	859	HIS	5.1
1	B	866	PRO	5.1
1	D	328	LEU	5.1
1	C	680	MET	5.1
1	B	373	VAL	5.0
1	D	50	PHE	5.0
1	A	864	PRO	4.9
1	D	864	PRO	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	859	HIS	4.8
1	B	869	ALA	4.8
1	B	871	LEU	4.8
1	C	1013	PRO	4.7
1	C	1011	TYR	4.7
1	A	859	HIS	4.7
1	B	50	PHE	4.7
1	C	864	PRO	4.7
1	A	1013	PRO	4.6
1	D	326	SER	4.5
1	A	417	GLY	4.5
1	D	1009	THR	4.4
1	B	865	VAL	4.4
1	B	891	ALA	4.4
1	C	865	VAL	4.4
1	B	890	ILE	4.4
1	B	323	ALA	4.4
1	C	869	ALA	4.3
1	C	374	PRO	4.3
1	C	1010	PRO	4.3
1	D	52	CYS	4.3
1	C	52	CYS	4.2
1	D	45	PRO	4.2
1	D	680	MET	4.1
1	A	1011	TYR	4.1
1	D	1017	LEU	4.1
1	A	865	VAL	4.1
1	C	859	HIS	4.1
1	C	2	ALA	4.0
1	C	323	ALA	4.0
1	C	871	LEU	4.0
1	C	897	LEU	4.0
1	D	1018	PRO	4.0
1	D	331	ILE	4.0
1	D	372	ALA	4.0
1	D	329	PRO	3.9
1	B	459	TRP	3.9
1	D	1013	PRO	3.9
1	C	50	PHE	3.8
1	D	681	GLY	3.8
1	D	319	ALA	3.8
1	D	861	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	890	ILE	3.7
1	C	322	CYS	3.7
1	A	890	ILE	3.6
1	A	869	ALA	3.6
1	A	897	LEU	3.6
1	C	320	GLY	3.6
1	D	1016	GLY	3.5
1	D	863	LYS	3.5
1	C	367	PHE	3.5
1	C	672	PRO	3.5
1	B	1016	GLY	3.5
1	D	673	HIS	3.5
1	B	331	ILE	3.4
1	C	583	VAL	3.4
1	D	862	GLY	3.4
1	D	320	GLY	3.4
1	D	891	ALA	3.4
1	B	52	CYS	3.4
1	D	373	VAL	3.4
1	A	419	TRP	3.3
1	C	321	MET	3.3
1	C	1014	LYS	3.3
1	A	373	VAL	3.3
1	C	873	GLY	3.3
1	D	330	SER	3.3
1	D	889	ILE	3.3
1	D	60	ASP	3.3
1	B	51	HIS	3.3
1	C	895	MET	3.3
1	A	866	PRO	3.3
1	C	373	VAL	3.3
1	B	895	MET	3.3
1	D	871	LEU	3.2
1	D	459	TRP	3.2
1	B	898	LYS	3.2
1	D	1011	TYR	3.1
1	A	47	LYS	3.1
1	D	1015	ARG	3.1
1	D	682	LEU	3.1
1	B	680	MET	3.1
1	D	418	LYS	3.1
1	B	1017	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	51	HIS	3.0
1	B	673	HIS	3.0
1	A	895	MET	3.0
1	D	583	VAL	3.0
1	D	54	LYS	3.0
1	D	858	SER	3.0
1	B	864	PRO	3.0
1	C	327	PRO	3.0
1	A	1014	LYS	3.0
1	A	50	PHE	3.0
1	D	294	PHE	3.0
1	D	909	ARG	2.9
1	A	322	CYS	2.9
1	B	320	GLY	2.9
1	C	681	GLY	2.9
1	B	374	PRO	2.9
1	B	867	ARG	2.9
1	A	873	GLY	2.9
1	D	175	CYS	2.9
1	D	870	GLU	2.9
1	C	910	LYS	2.9
1	B	889	ILE	2.8
1	B	1011	TYR	2.8
1	B	422	ASP	2.8
1	A	681	GLY	2.8
1	A	411	THR	2.8
1	D	416	THR	2.8
1	B	327	PRO	2.7
1	D	1010	PRO	2.7
1	A	330	SER	2.7
1	C	891	ALA	2.7
1	A	374	PRO	2.7
1	D	51	HIS	2.7
1	C	858	SER	2.7
1	D	910	LYS	2.7
1	C	1008	THR	2.7
1	C	51	HIS	2.7
1	B	46	ASP	2.7
1	A	364	ARG	2.7
1	D	379	LEU	2.6
1	D	321	MET	2.6
1	A	416	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	890	ILE	2.6
1	D	293	ILE	2.6
1	D	856	THR	2.6
1	B	367	PHE	2.6
1	B	332	ARG	2.6
1	D	371	ARG	2.6
1	B	1015	ARG	2.5
1	D	55	LEU	2.5
1	D	873	GLY	2.5
1	C	364	ARG	2.5
1	A	871	LEU	2.5
1	B	429	LEU	2.5
1	A	1016	GLY	2.5
1	B	418	LYS	2.5
1	C	418	LYS	2.5
1	C	674	GLY	2.5
1	B	329	PRO	2.5
1	D	874	LYS	2.5
1	A	52	CYS	2.4
1	B	870	GLU	2.4
1	D	860	GLN	2.4
1	B	414	ASP	2.4
1	B	426	ILE	2.4
1	A	858	SER	2.4
1	B	60	ASP	2.4
1	B	419	TRP	2.4
1	B	896	ARG	2.4
1	C	49	CYS	2.4
1	C	898	LYS	2.4
1	D	875	LYS	2.4
1	D	1014	LYS	2.4
1	C	862	GLY	2.4
1	D	48	ASN	2.4
1	A	398	VAL	2.4
1	A	583	VAL	2.4
1	A	872	MET	2.4
1	D	419	TRP	2.4
1	C	1017	LEU	2.3
1	A	898	LYS	2.3
1	B	583	VAL	2.3
1	B	856	THR	2.3
1	D	420	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	367	PHE	2.3
1	B	294	PHE	2.3
1	A	397	ILE	2.3
1	B	325	HIS	2.3
1	C	856	THR	2.3
1	A	674	GLY	2.3
1	C	415	GLU	2.3
1	D	59	PHE	2.3
1	A	45	PRO	2.3
1	A	870	GLU	2.2
1	C	1012	GLU	2.2
1	B	875	LYS	2.2
1	D	414	ASP	2.2
1	D	867	ARG	2.2
1	A	1010	PRO	2.2
1	C	424	ASP	2.2
1	D	872	MET	2.2
1	B	682	LEU	2.2
1	B	54	LYS	2.2
1	D	342	ASP	2.2
1	A	320	GLY	2.2
1	A	328	LEU	2.2
1	B	416	THR	2.2
1	B	412	GLU	2.1
1	C	908	GLU	2.1
1	B	1013	PRO	2.1
1	B	179	GLN	2.1
1	A	682	LEU	2.1
1	C	874	LYS	2.1
1	D	47	LYS	2.1
1	A	418	LYS	2.1
1	C	487	ASN	2.1
1	B	272	LYS	2.1
1	B	59	PHE	2.1
1	C	419	TRP	2.1
1	A	443	ARG	2.0
1	D	458	ARG	2.0
1	B	873	GLY	2.0
1	C	53	GLU	2.0
1	C	872	MET	2.0
1	C	60	ASP	2.0
1	C	332	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	324	CYS	2.0
1	A	673	HIS	2.0
1	C	861	LYS	2.0
1	B	45	PRO	2.0
1	B	1018	PRO	2.0
1	A	855	GLY	2.0
1	D	417	GLY	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(Å ²)	Q<0.9
2	SF4	C	1104	8/8	0.95	0.06	21,22,23,23	0
2	SF4	D	1103	8/8	0.95	0.06	17,22,24,25	0
2	SF4	B	1102	8/8	0.96	0.06	20,21,23,23	0
2	SF4	B	1103	8/8	0.96	0.05	18,19,21,21	0
2	SF4	B	1104	8/8	0.96	0.06	19,21,23,23	0
2	SF4	C	1101	8/8	0.96	0.06	19,21,22,23	0
2	SF4	C	1103	8/8	0.96	0.05	17,20,21,21	0
2	SF4	A	1101	8/8	0.96	0.05	18,21,22,23	0
2	SF4	D	1101	8/8	0.96	0.06	22,24,27,27	0
2	SF4	A	1104	8/8	0.96	0.06	20,23,24,24	0
5	TDR	D	1107	9/9	0.96	0.06	22,25,27,27	0
2	SF4	B	1101	8/8	0.97	0.05	19,21,21,22	0
2	SF4	A	1103	8/8	0.97	0.05	19,22,24,24	0
2	SF4	D	1102	8/8	0.97	0.05	19,20,21,21	0
2	SF4	C	1102	8/8	0.97	0.05	21,22,23,24	0
2	SF4	D	1104	8/8	0.97	0.06	21,23,25,25	0

Continued on next page...

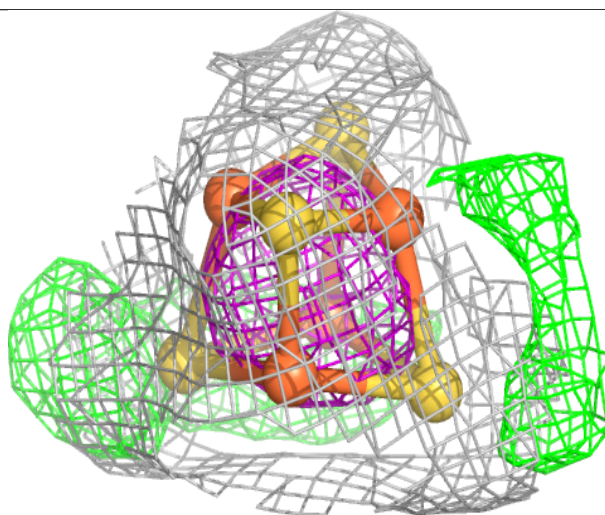
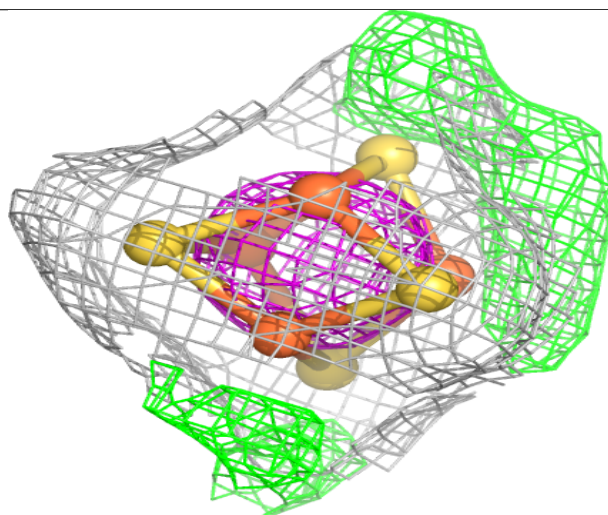
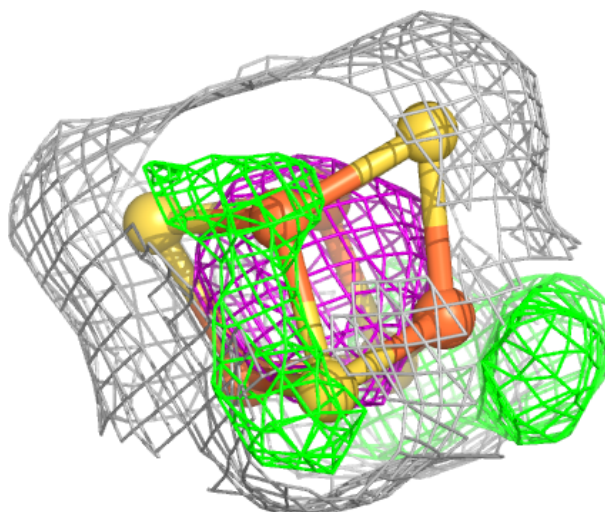
Continued from previous page...

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

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

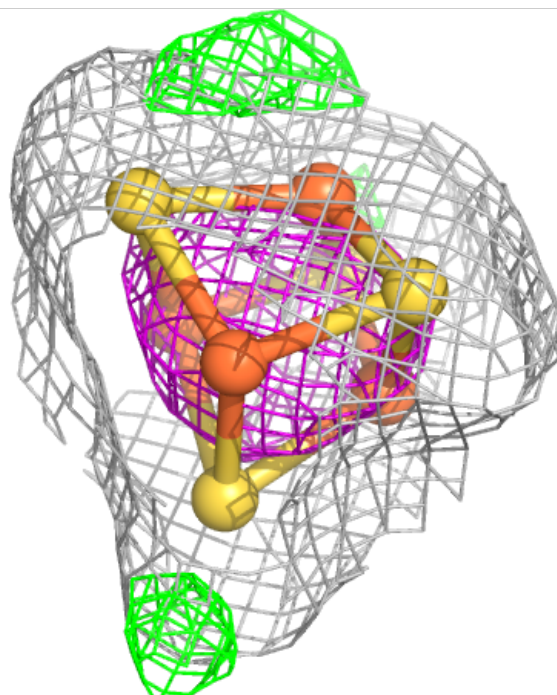
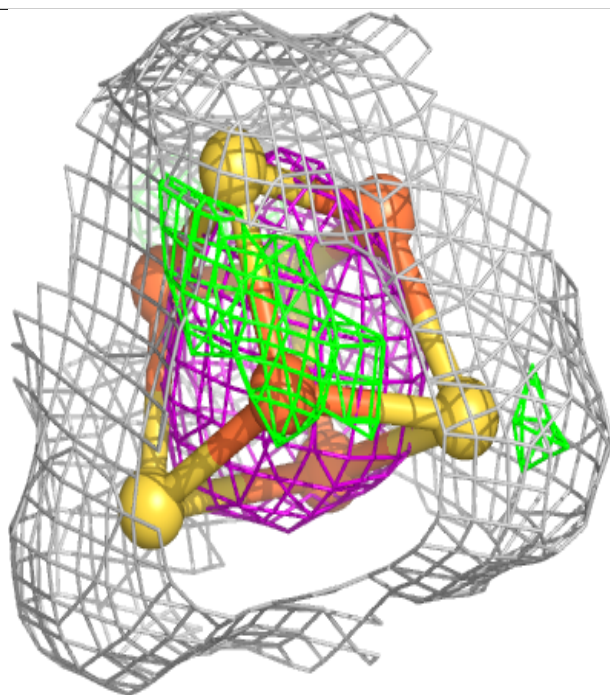
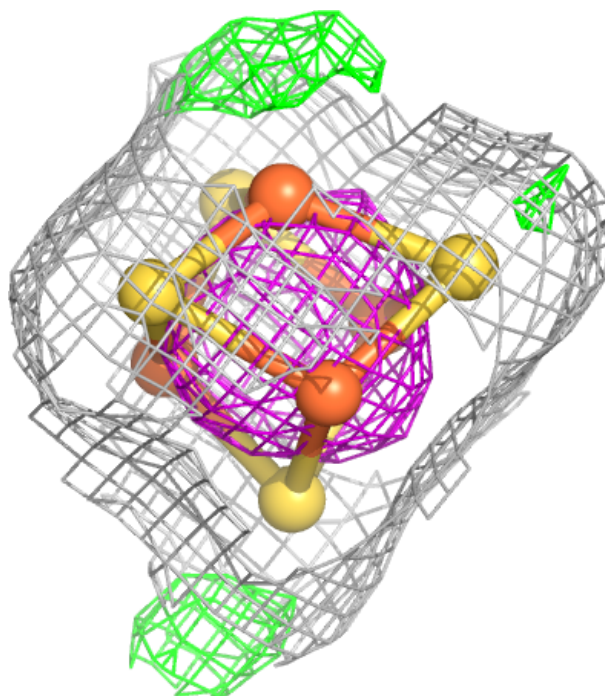
Electron density around SF4 C 1104:

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



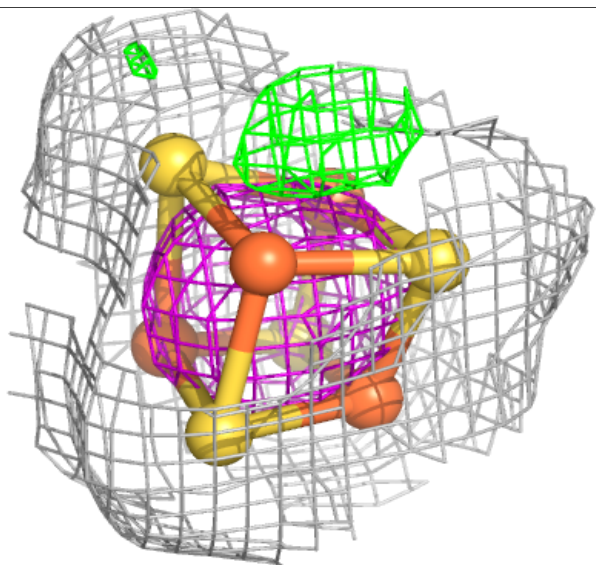
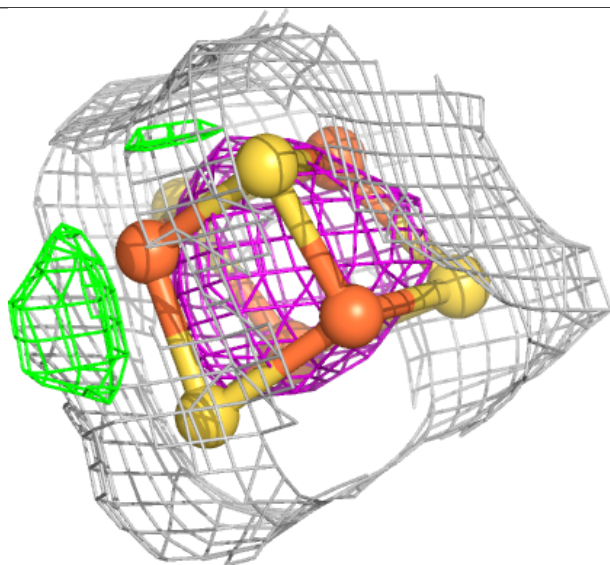
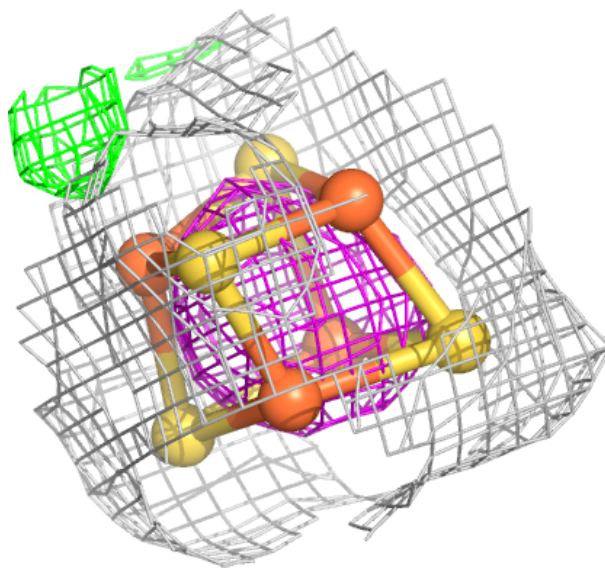
Electron density around SF4 D 1103:

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



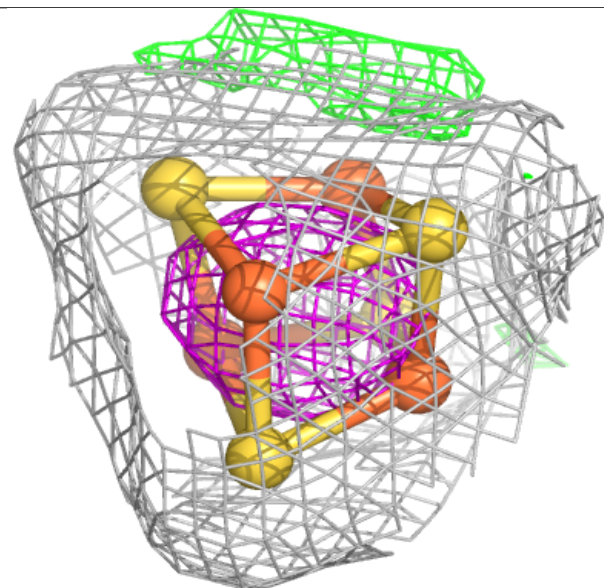
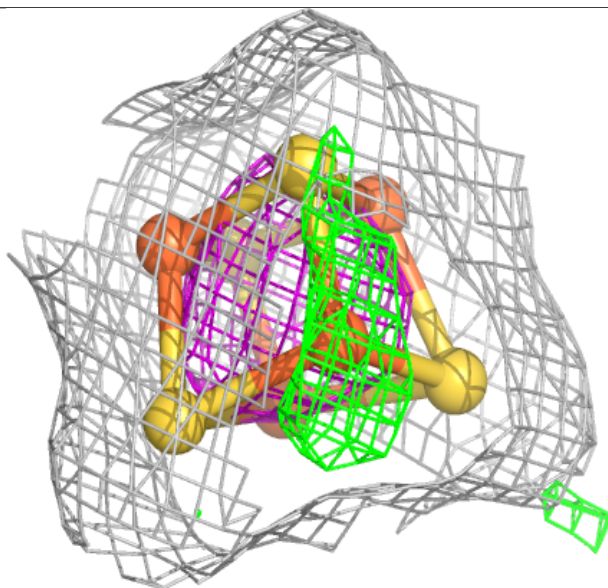
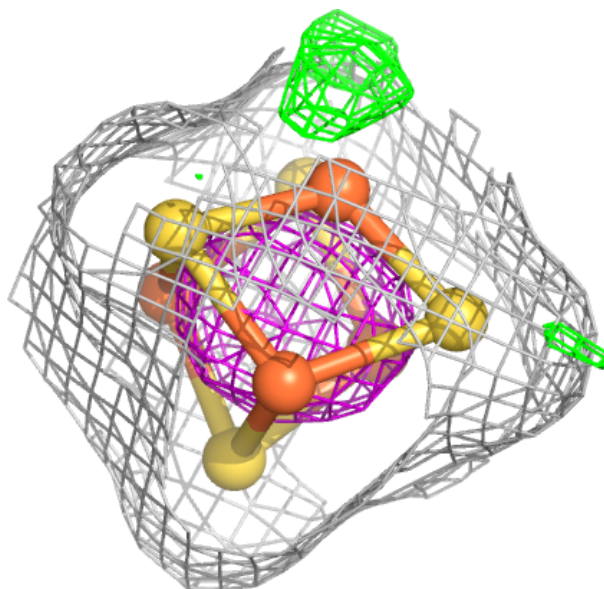
Electron density around SF4 B 1102:

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



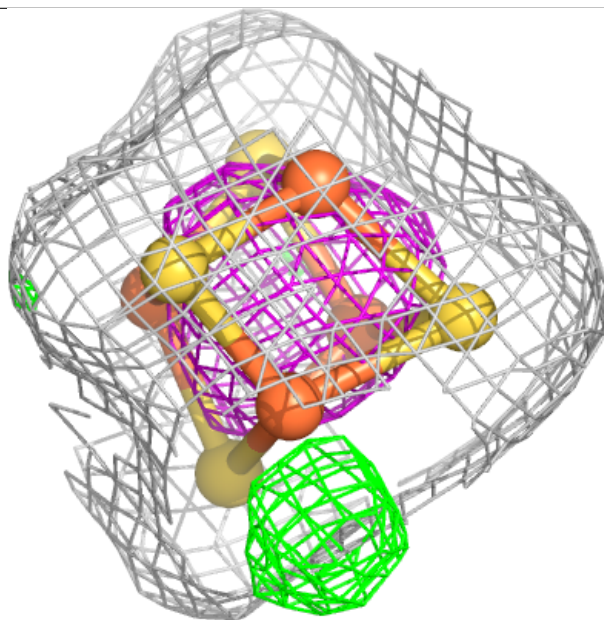
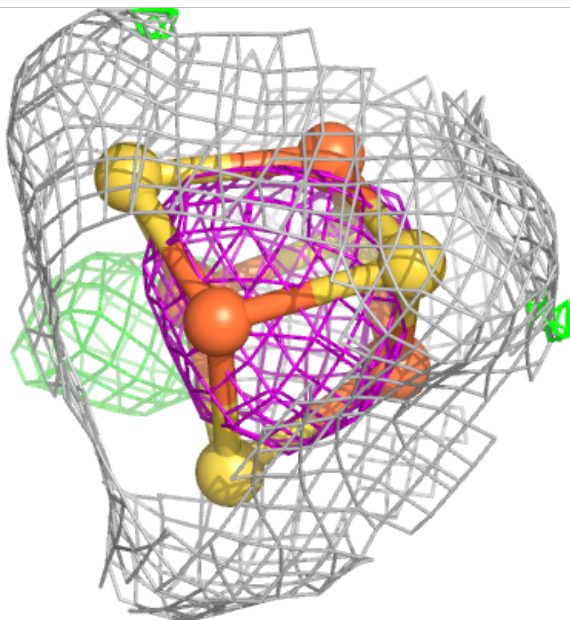
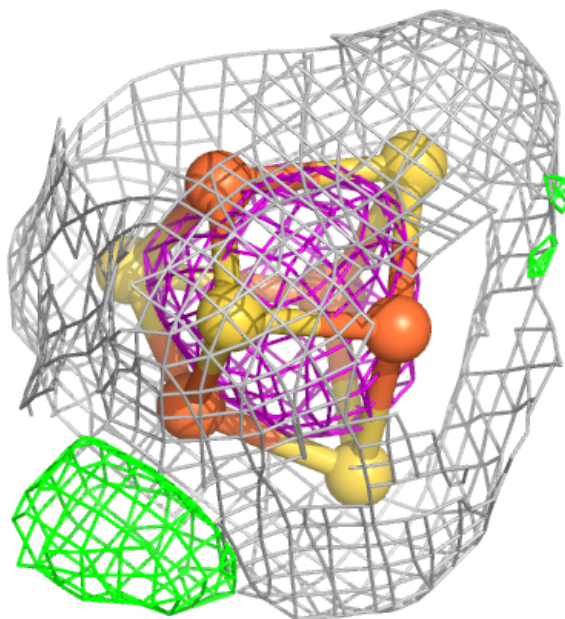
Electron density around SF4 B 1103:

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



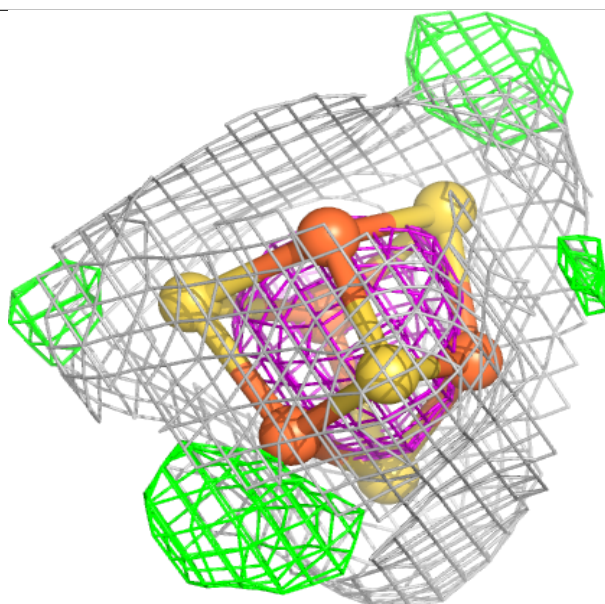
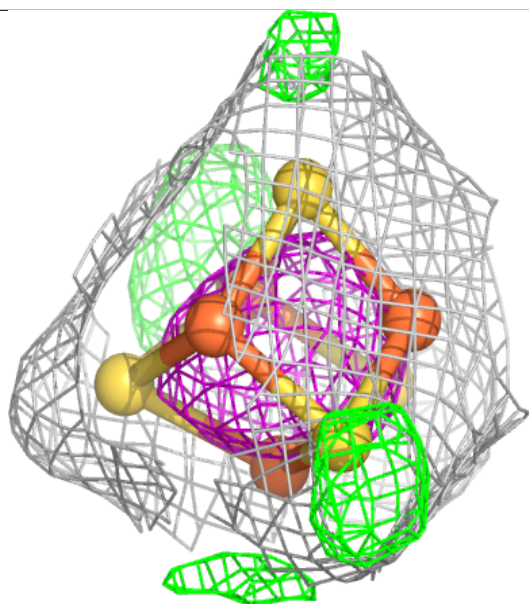
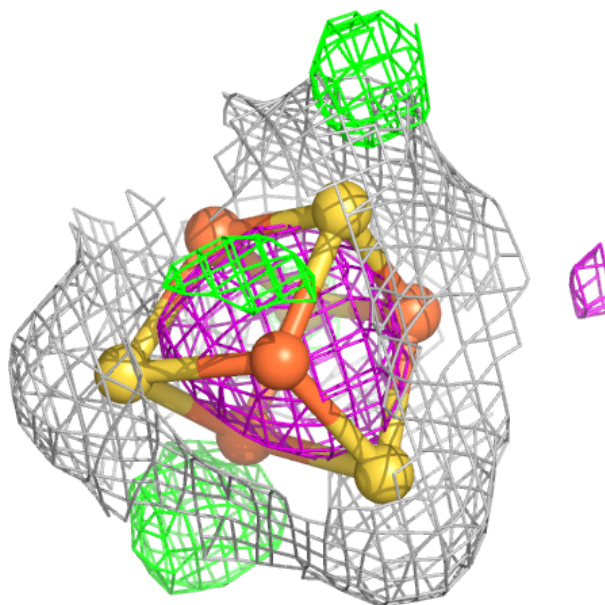
Electron density around SF4 B 1104:

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



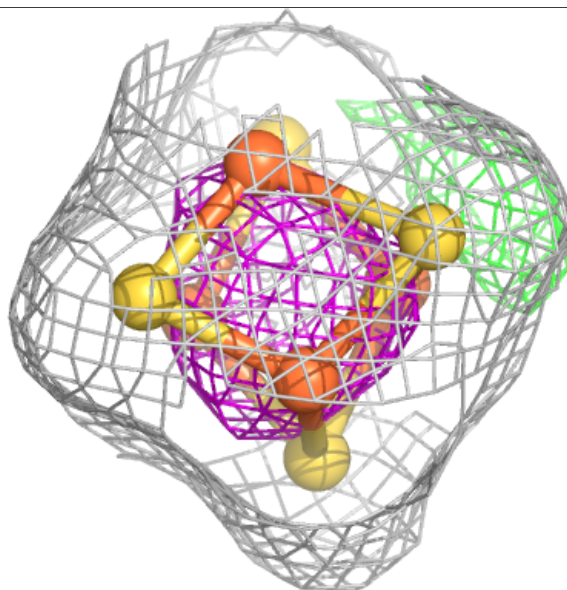
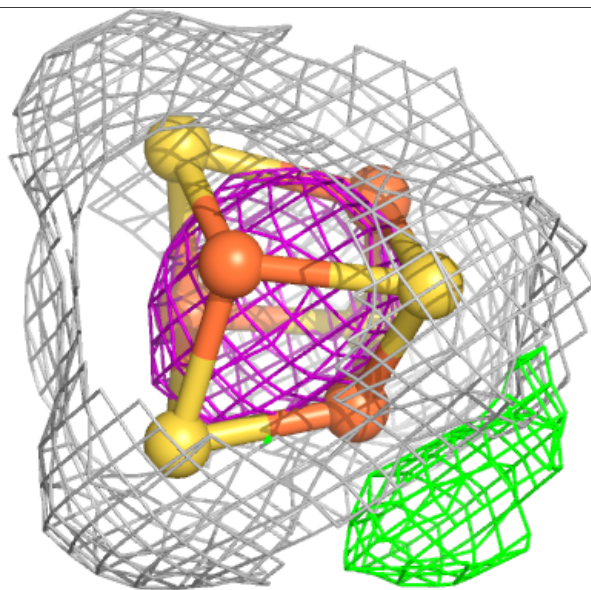
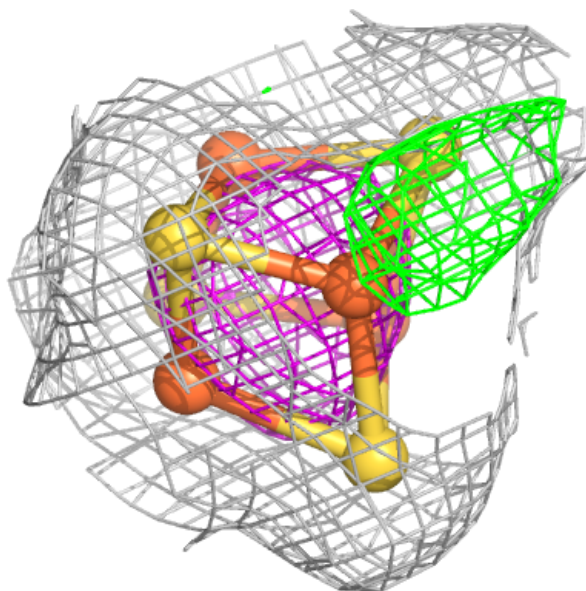
Electron density around SF4 C 1101:

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



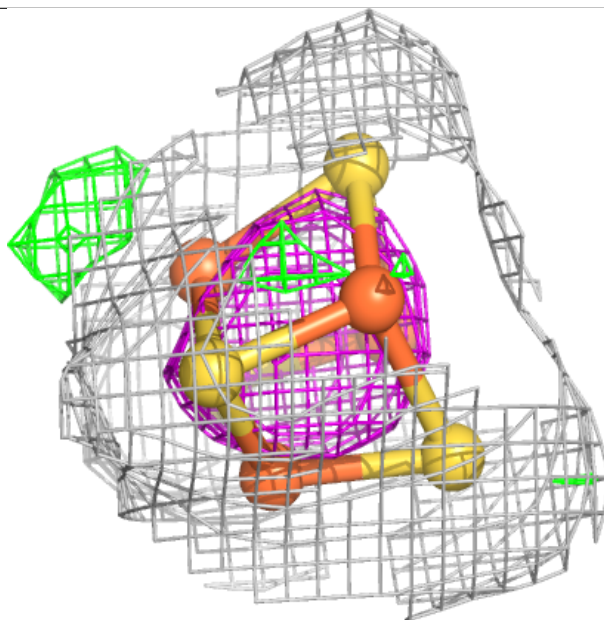
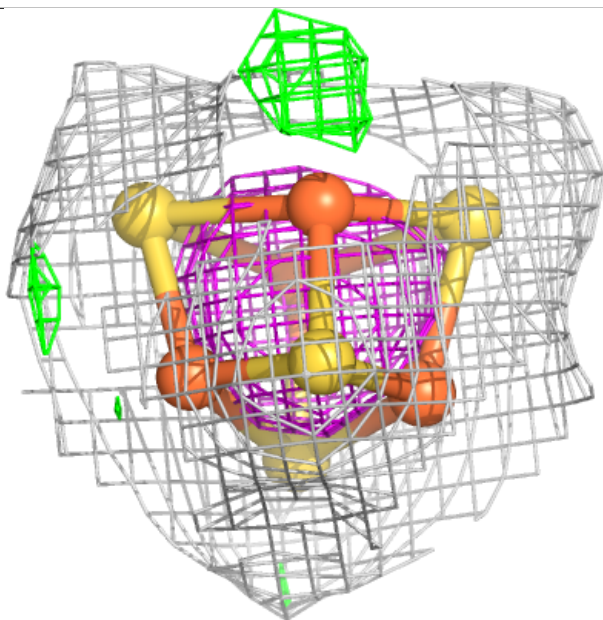
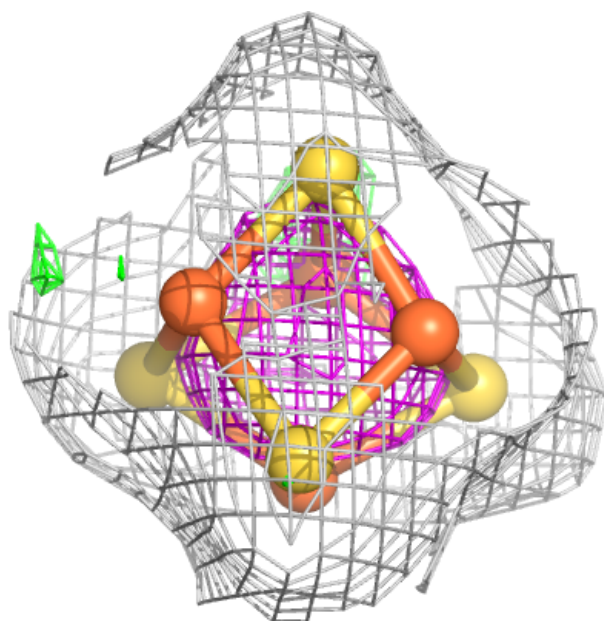
Electron density around SF4 C 1103:

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



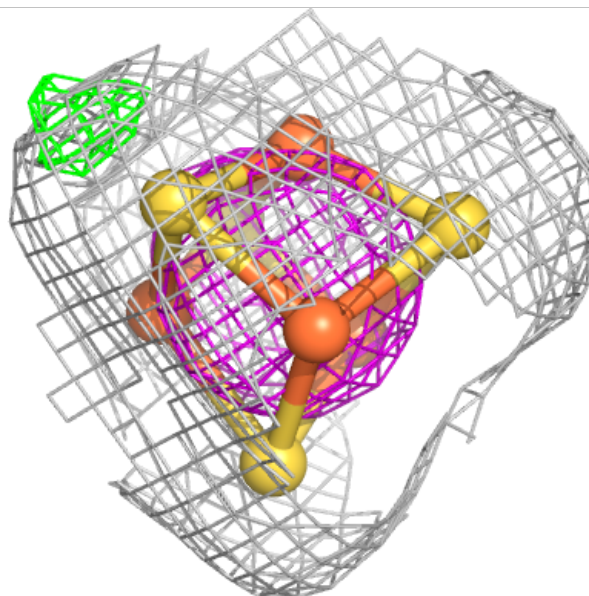
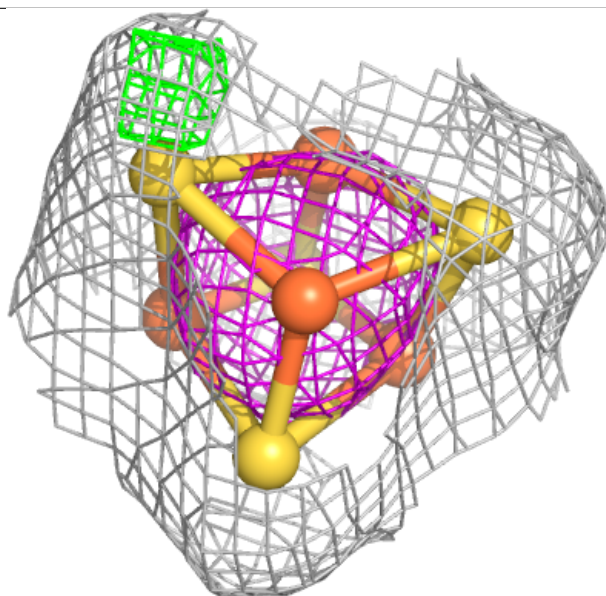
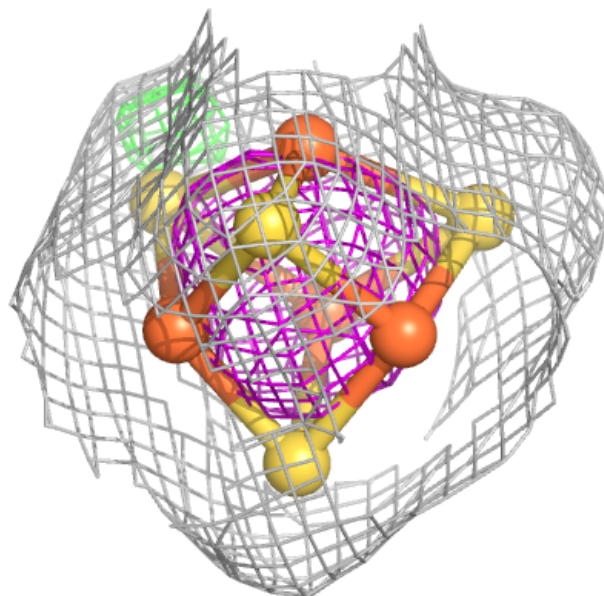
Electron density around SF4 A 1101:

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



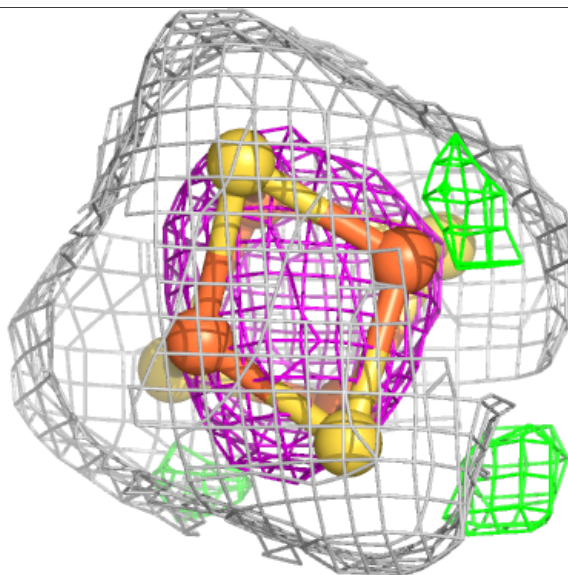
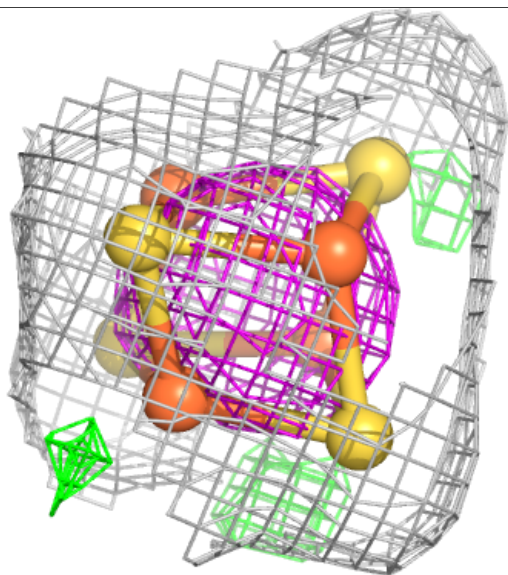
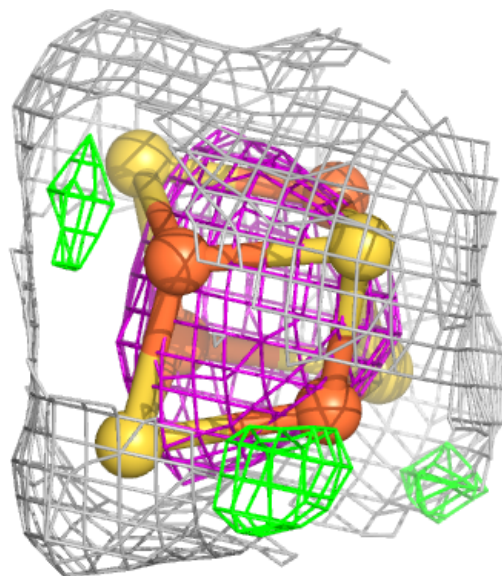
Electron density around SF4 D 1101:

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



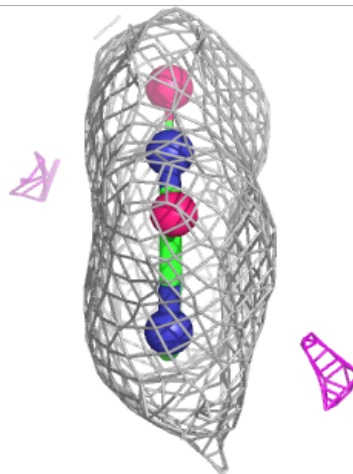
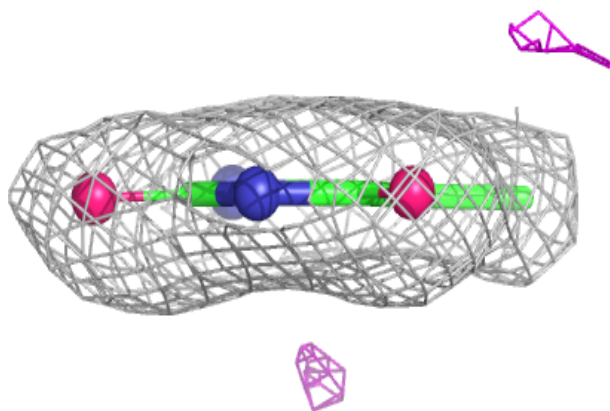
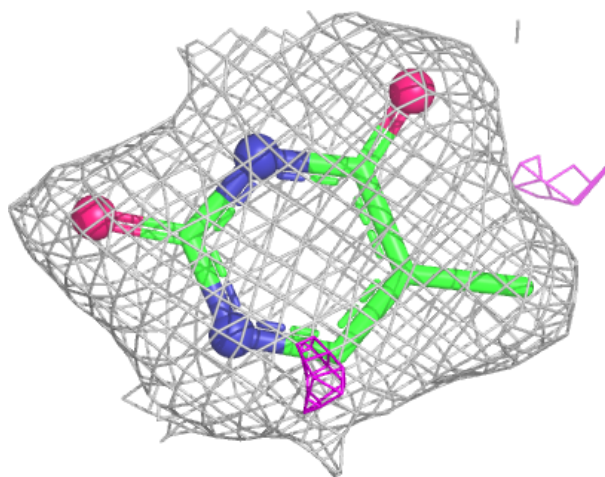
Electron density around SF4 A 1104:

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



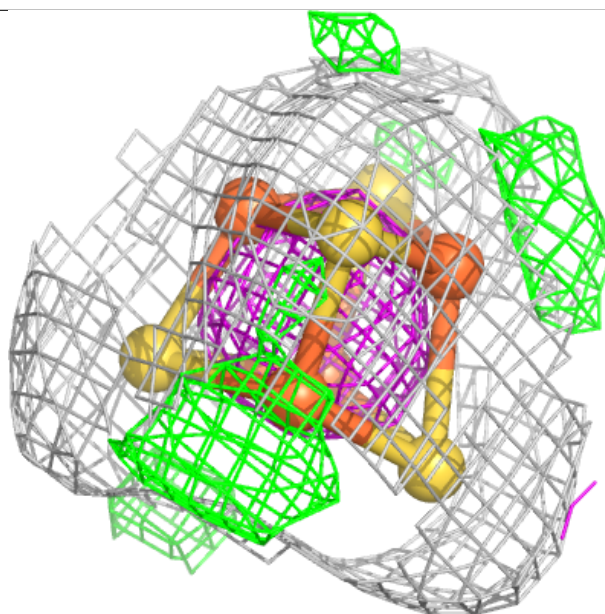
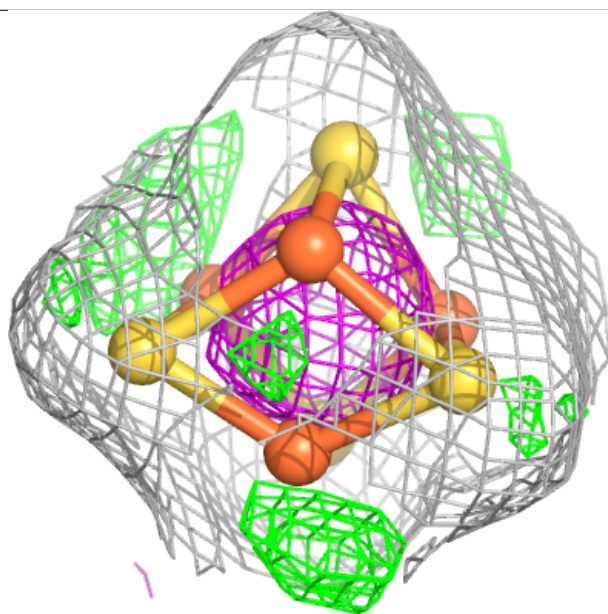
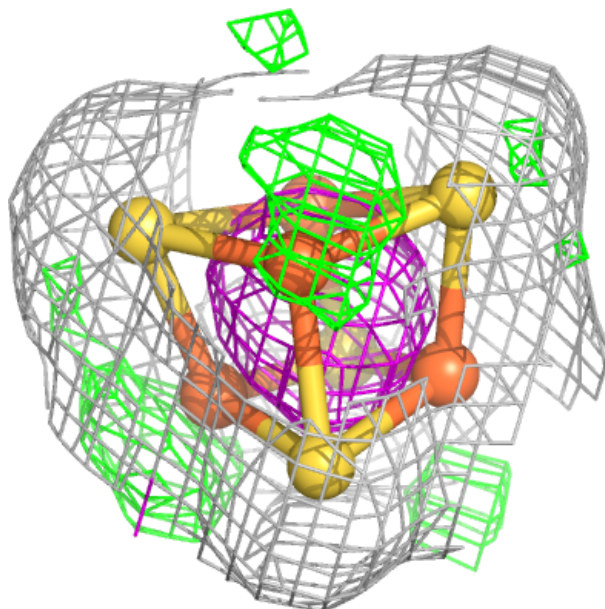
Electron density around TDR D 1107:

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



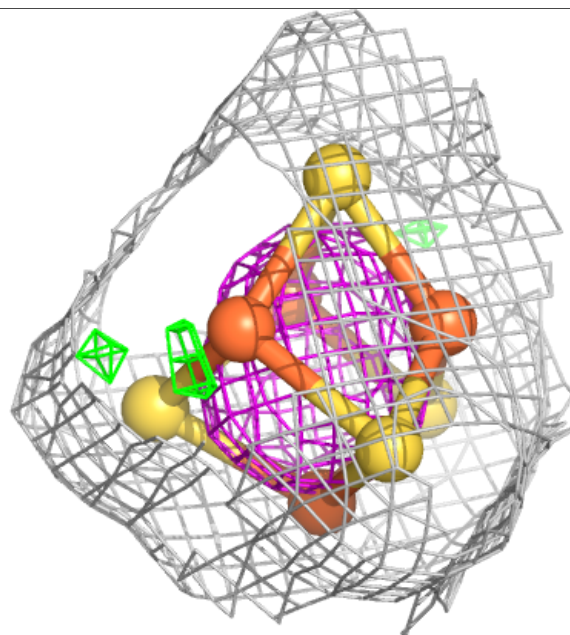
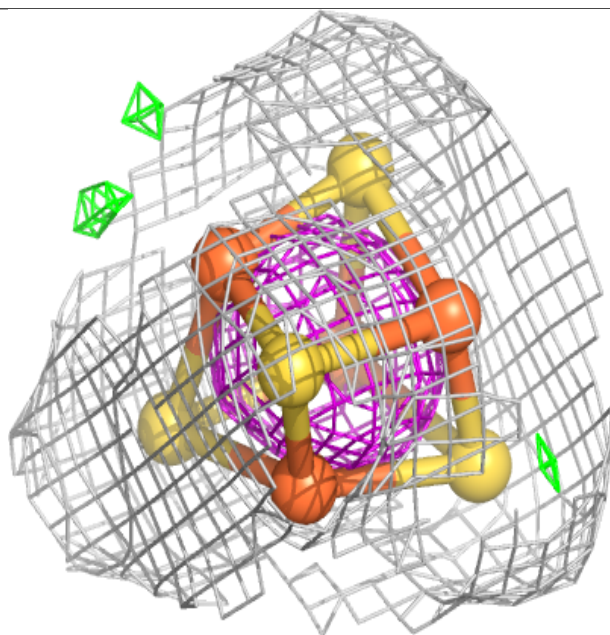
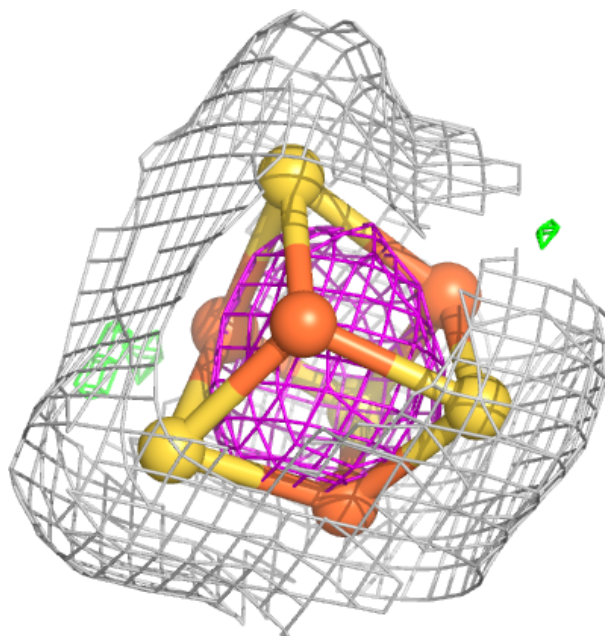
Electron density around SF4 B 1101:

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



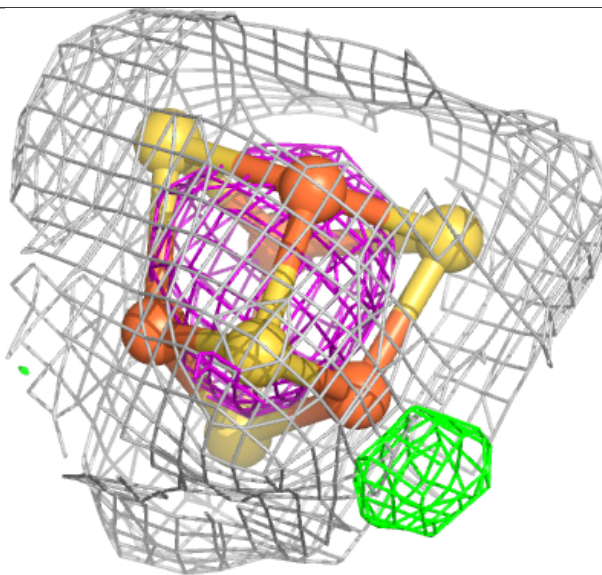
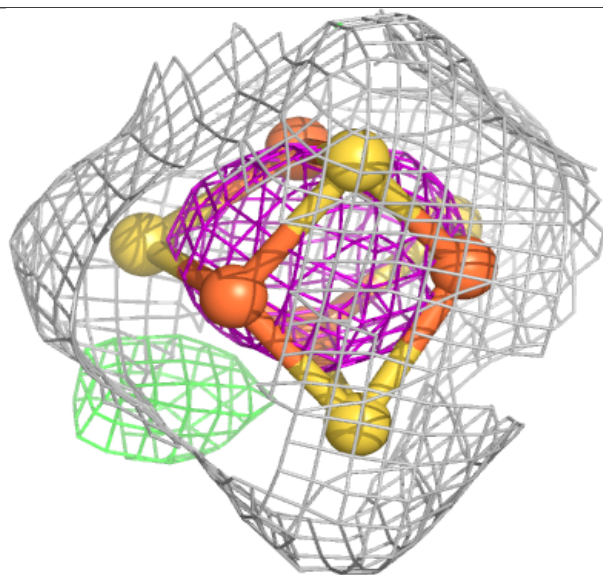
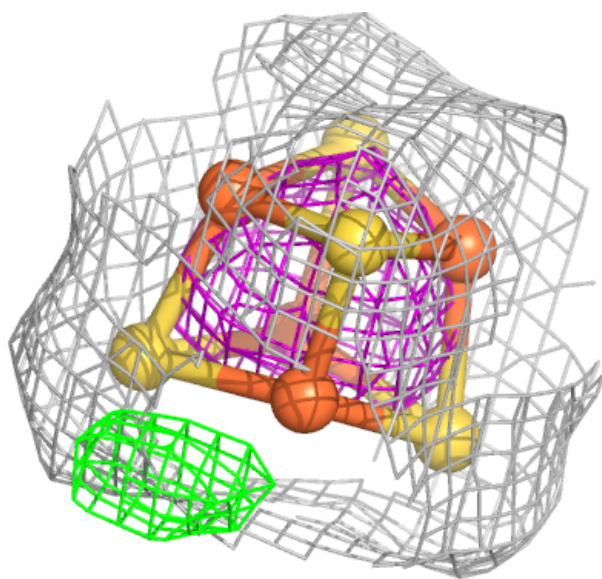
Electron density around SF4 A 1103:

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



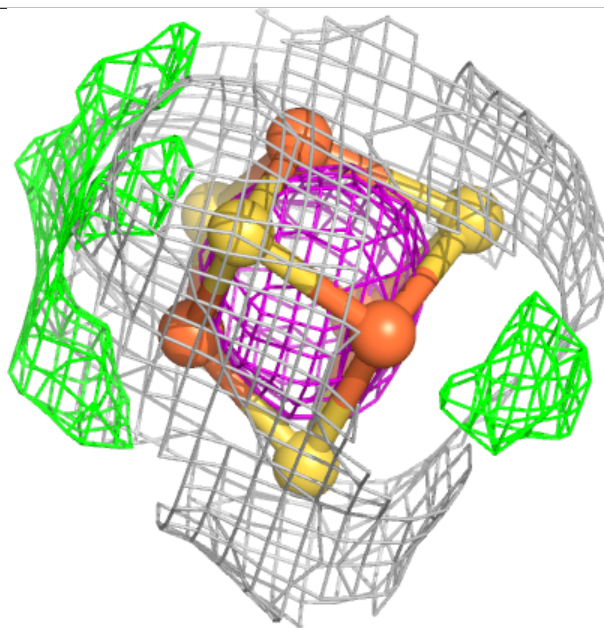
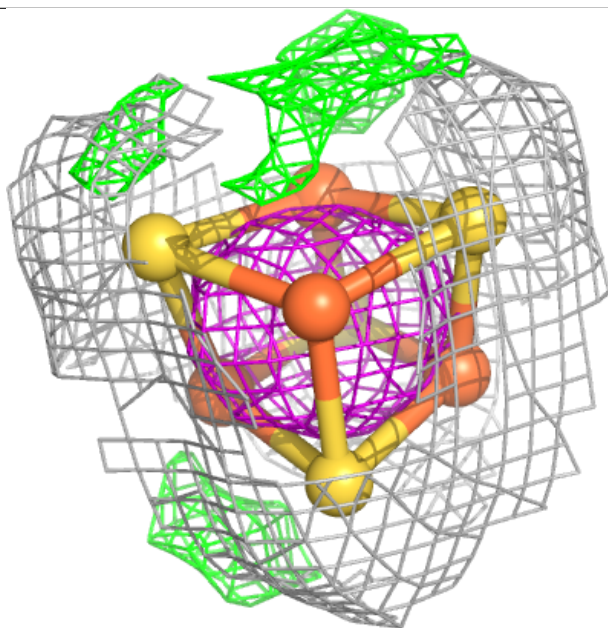
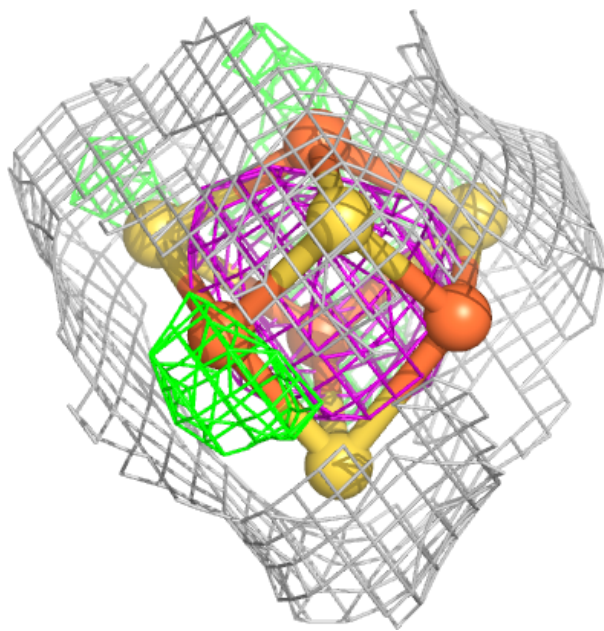
Electron density around SF4 D 1102:

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



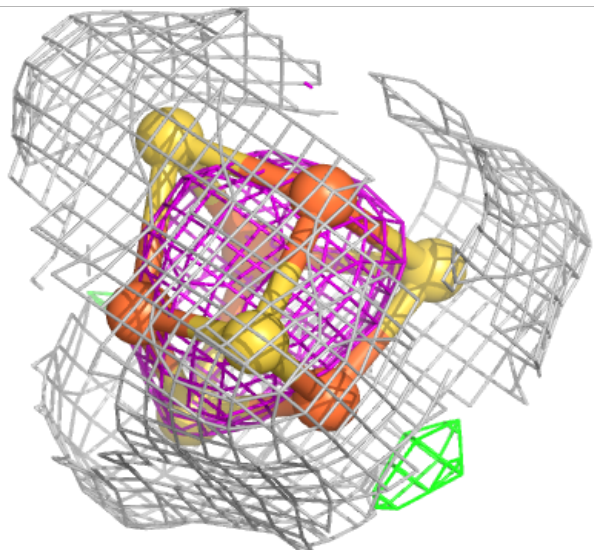
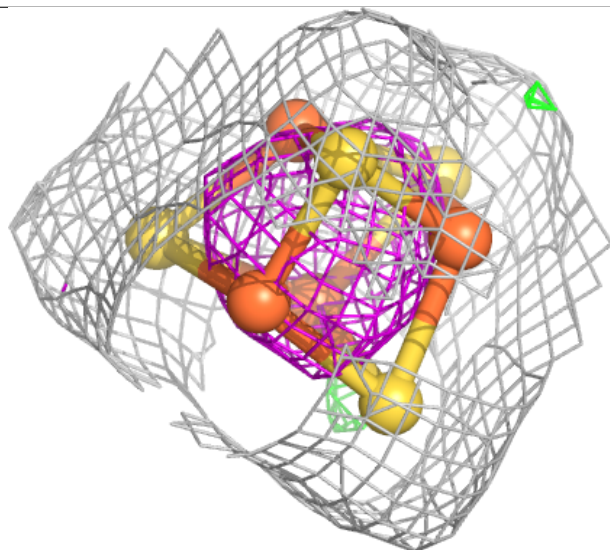
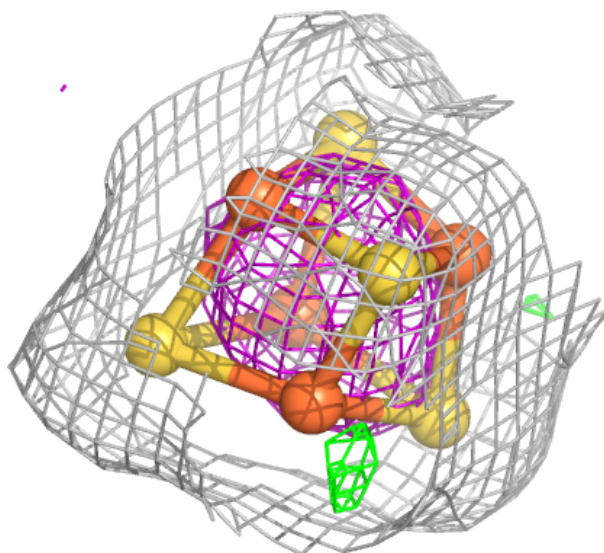
Electron density around SF4 C 1102:

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



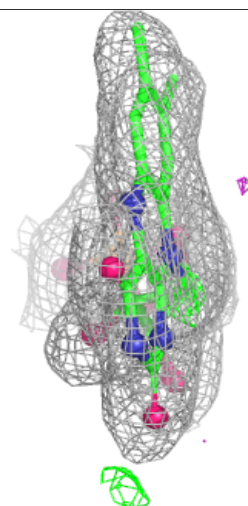
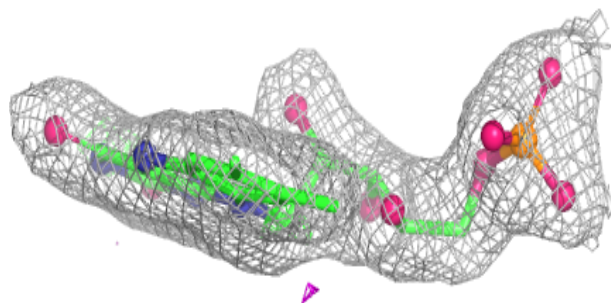
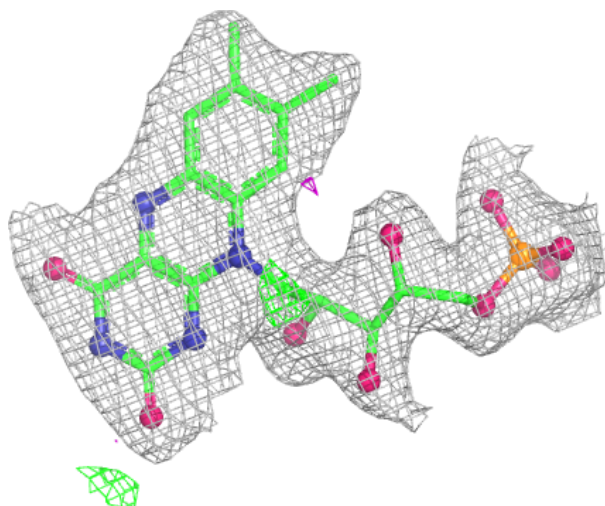
Electron density around SF4 D 1104:

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



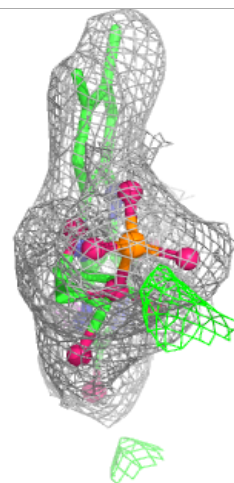
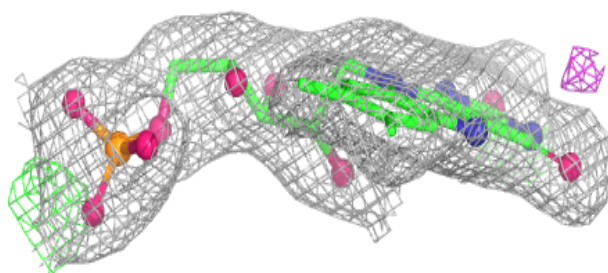
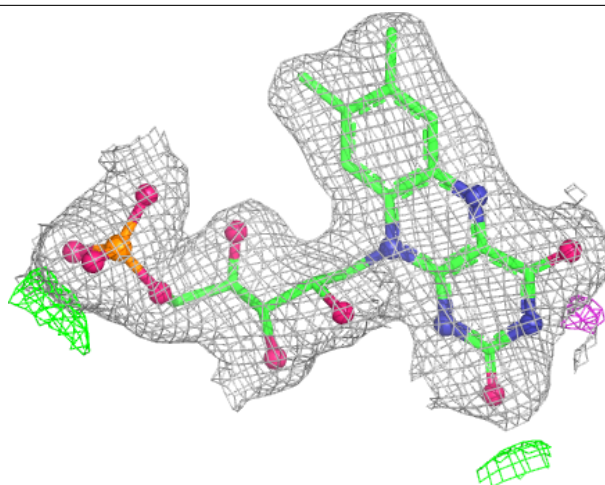
Electron density around FMN C 1105:

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



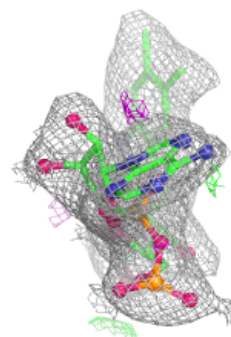
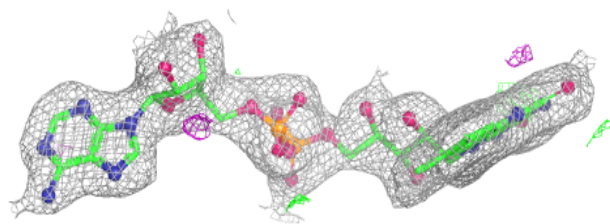
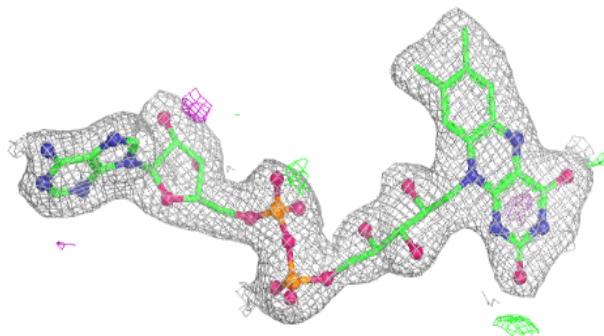
Electron density around FMN D 1105:

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

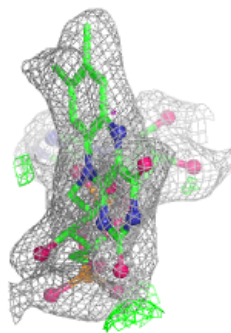
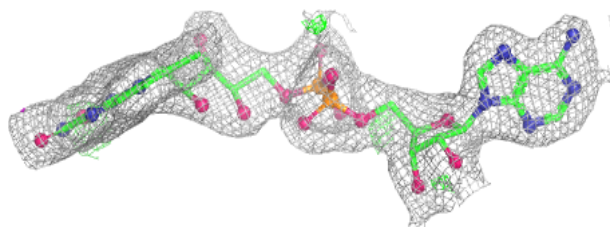
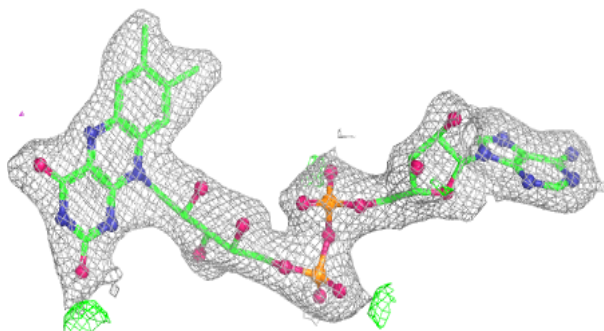


Electron density around FAD A 1106:

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

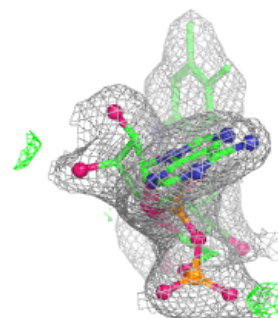
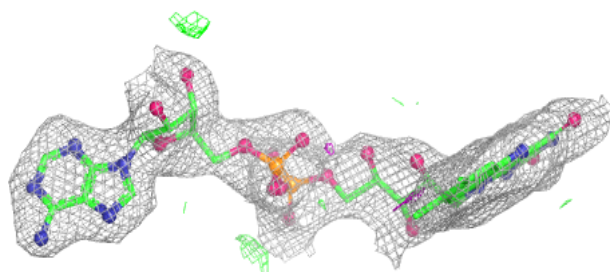
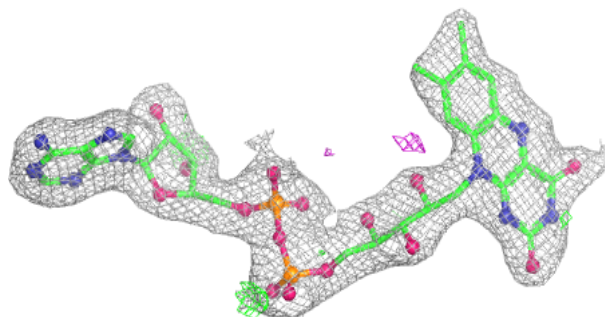
**Electron density around FAD B 1106:**

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

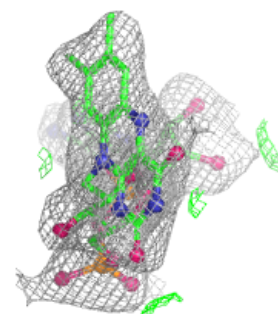
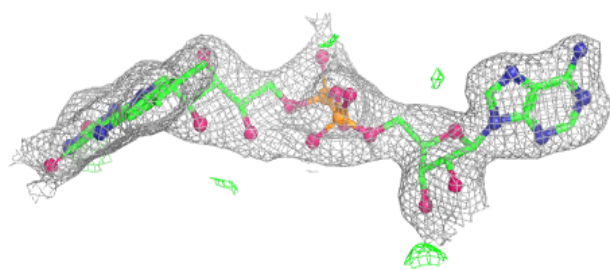
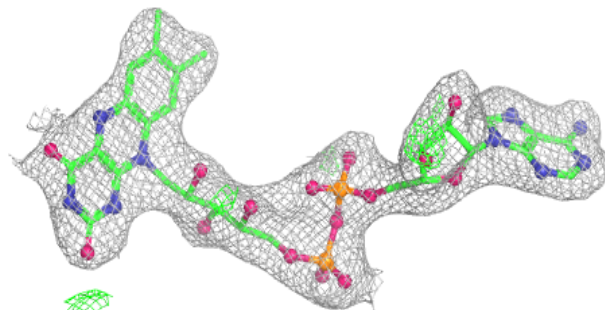


Electron density around FAD C 1106:

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

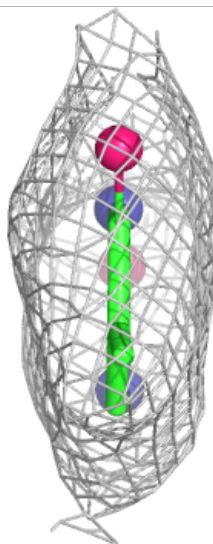
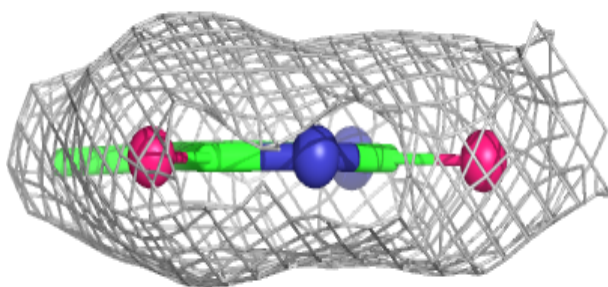
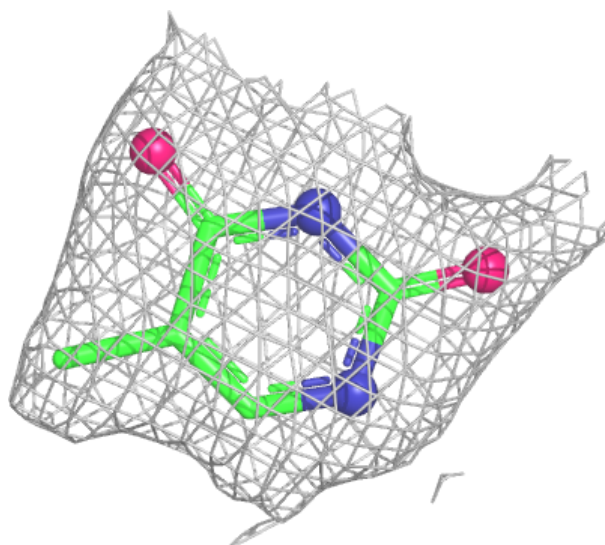
**Electron density around FAD D 1106:**

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



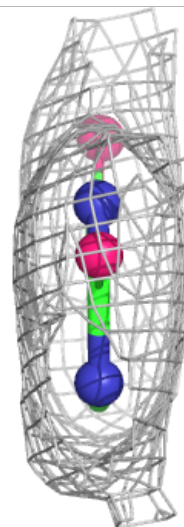
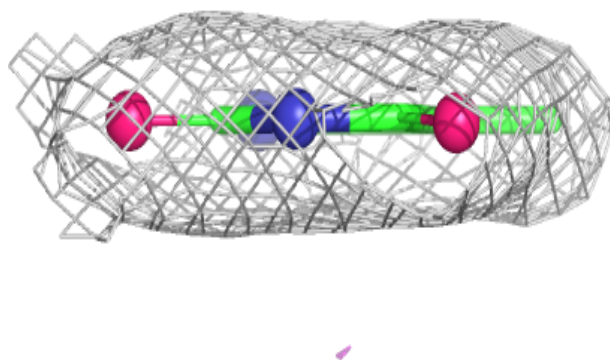
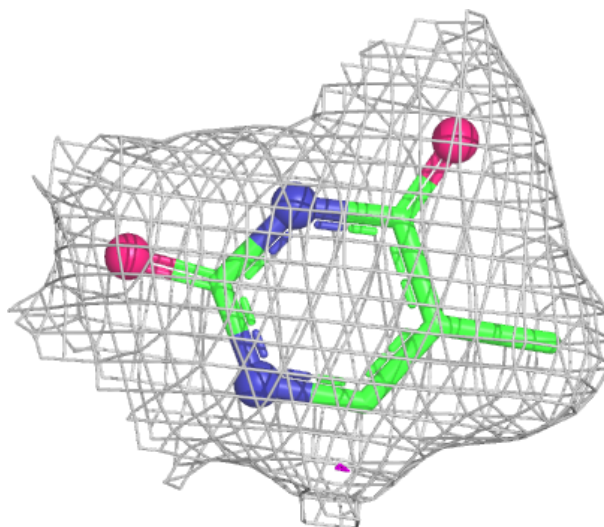
Electron density around TDR A 1107:

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



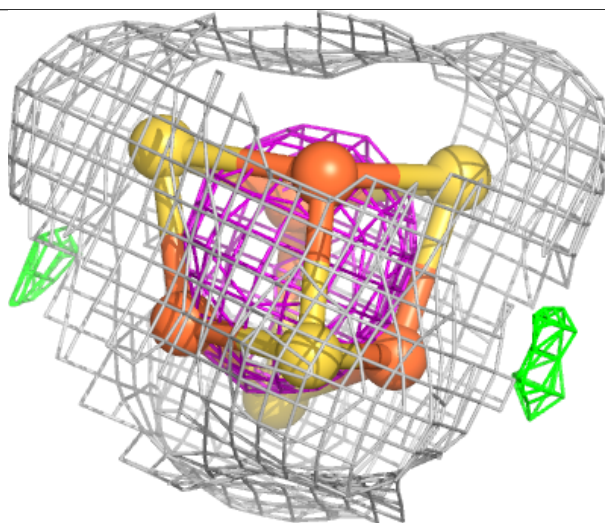
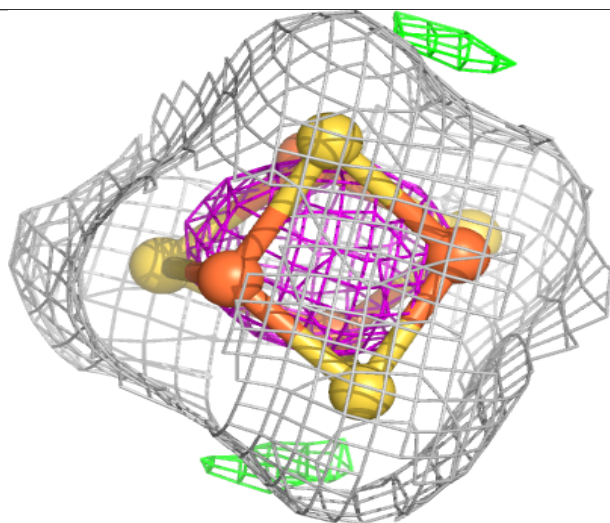
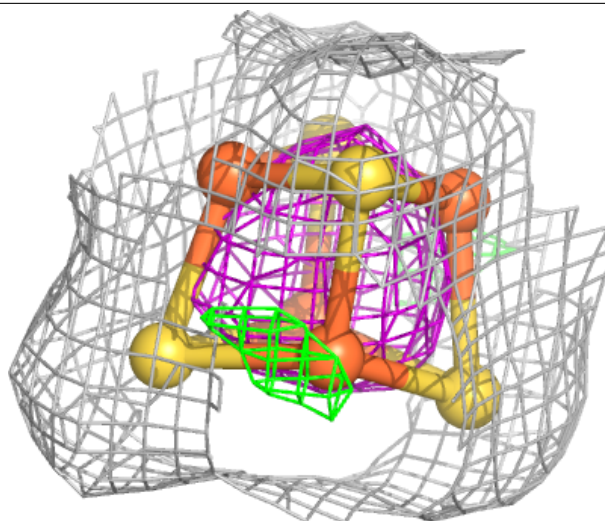
Electron density around TDR B 1107:

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



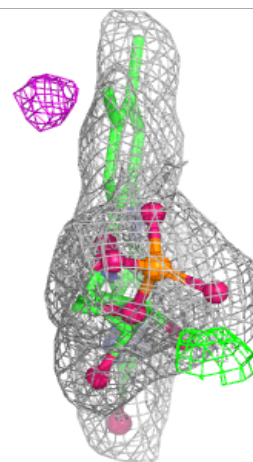
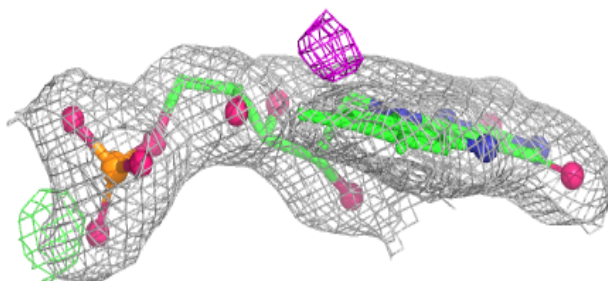
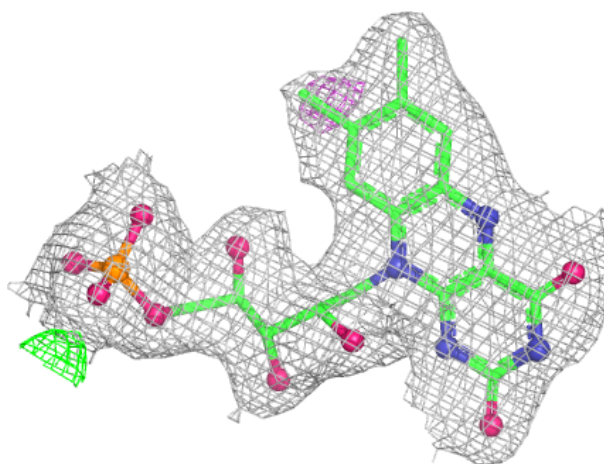
Electron density around SF4 A 1102:

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



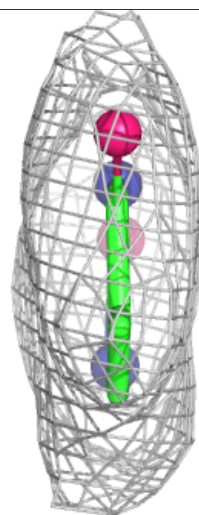
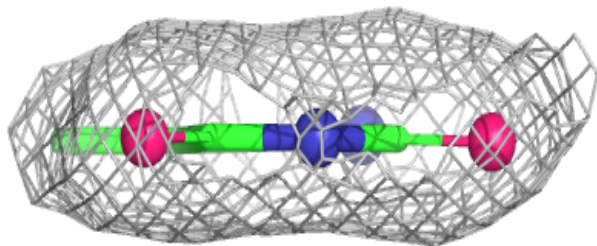
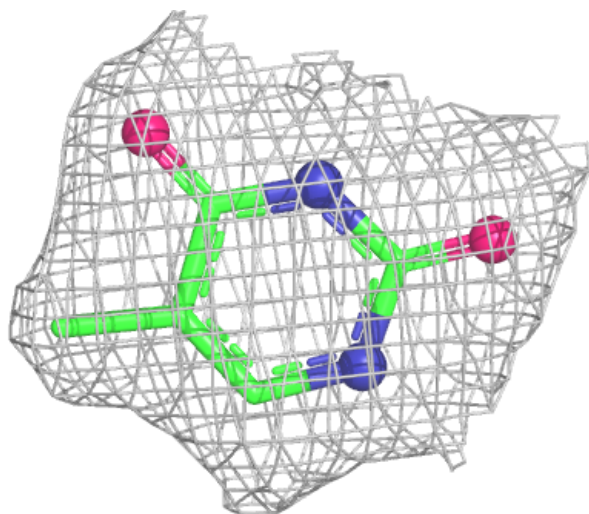
Electron density around FMN B 1105:

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



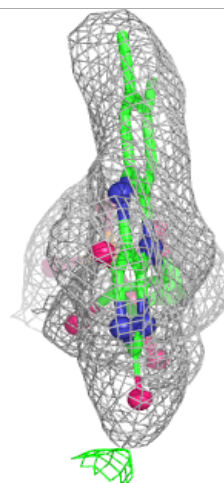
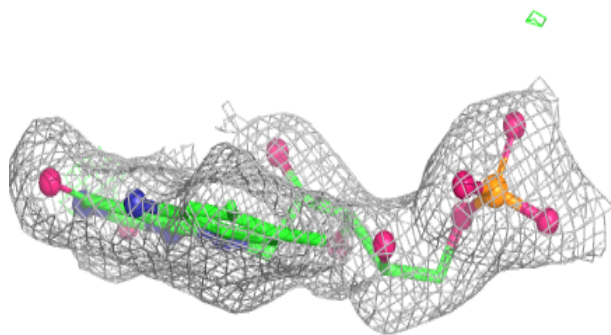
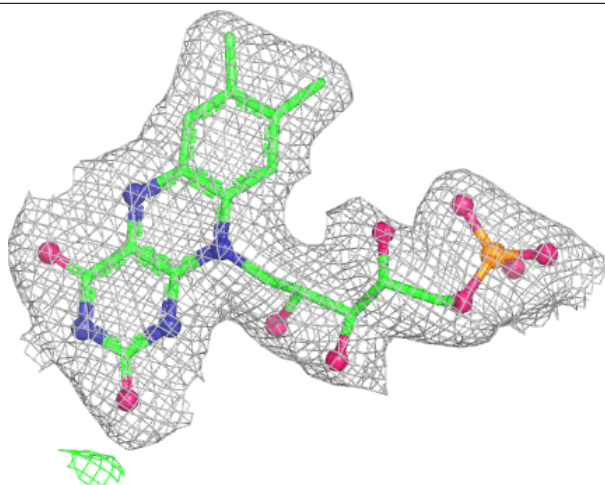
Electron density around TDR C 1107:

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



Electron density around FMN A 1105:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.