



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:09 AM UTC

PDB ID : 7CZ9 / pdb_00007cz9
Title : Crystal structure of multidrug efflux transporter OqxB from *Klebsiella pneumoniae*
Authors : Murakami, S.; Okada, U.; Yamashita, E.
Deposited on : 2020-09-07
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

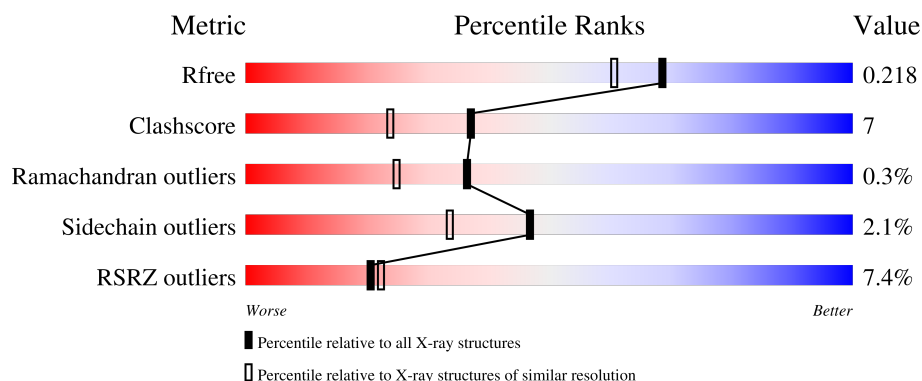
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	1042	6% 88% 11%
1	B	1042	7% 84% 15%
1	C	1042	5% 88% 11%
1	D	1042	13% 83% 15%
1	E	1042	6% 87% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1042	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1113	-	X	-	-
4	GOL	A	1116	-	X	-	-
4	GOL	A	1120	-	X	-	-
4	GOL	D	1115	-	X	-	-
4	GOL	E	1116	-	X	X	-
4	GOL	E	1119	-	X	-	-
4	GOL	E	1123	-	X	-	-
4	GOL	F	1119	-	X	-	-

2 Entry composition ⓘ

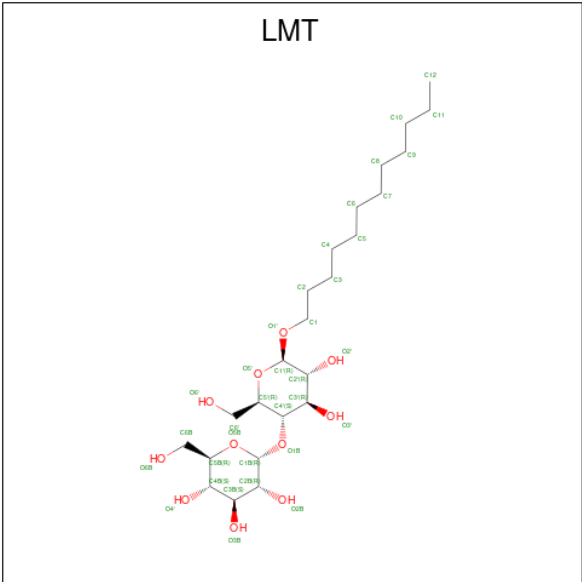
There are 5 unique types of molecules in this entry. The entry contains 53422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1041	Total	C	N	O	S	0	3	0
			7945	5118	1345	1448	34			
1	B	1042	Total	C	N	O	S	0	0	0
			7932	5110	1340	1448	34			
1	C	1041	Total	C	N	O	S	0	0	0
			7923	5104	1338	1447	34			
1	D	1040	Total	C	N	O	S	0	0	0
			7912	5098	1334	1446	34			
1	E	1039	Total	C	N	O	S	0	4	0
			7931	5112	1340	1445	34			
1	F	1040	Total	C	N	O	S	0	1	0
			7918	5102	1334	1448	34			

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 34 23 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 25 19 6	0	0
2	A	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 16 15 1	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C 10 10	0	0

Continued on next page...

Continued from previous page...

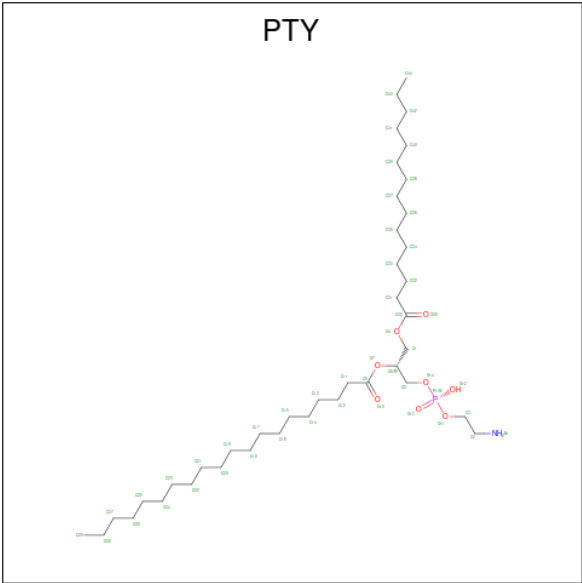
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C 12 12	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C 10 10	0	0
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			13	12	1		
2	F	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			17	15	2		
2	F	1	Total	C		0	0
			6	6			
2	F	1	Total	C	O	0	0
			35	24	11		

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



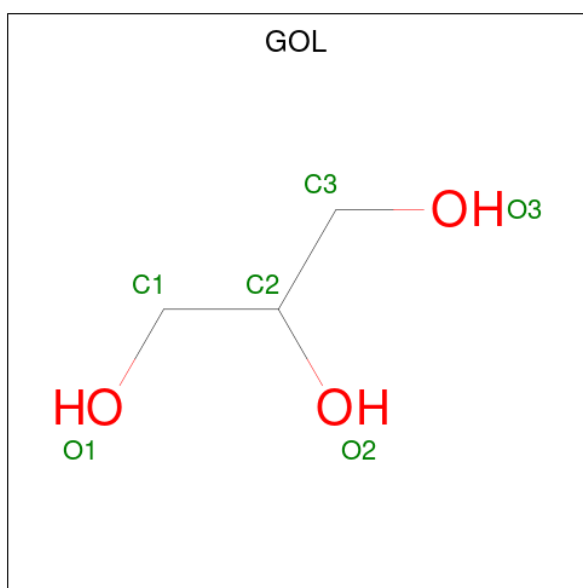
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
3	C	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
3	E	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
3	E	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
3	F	1	Total	C	O			0	0
			37	33	4				
3	F	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

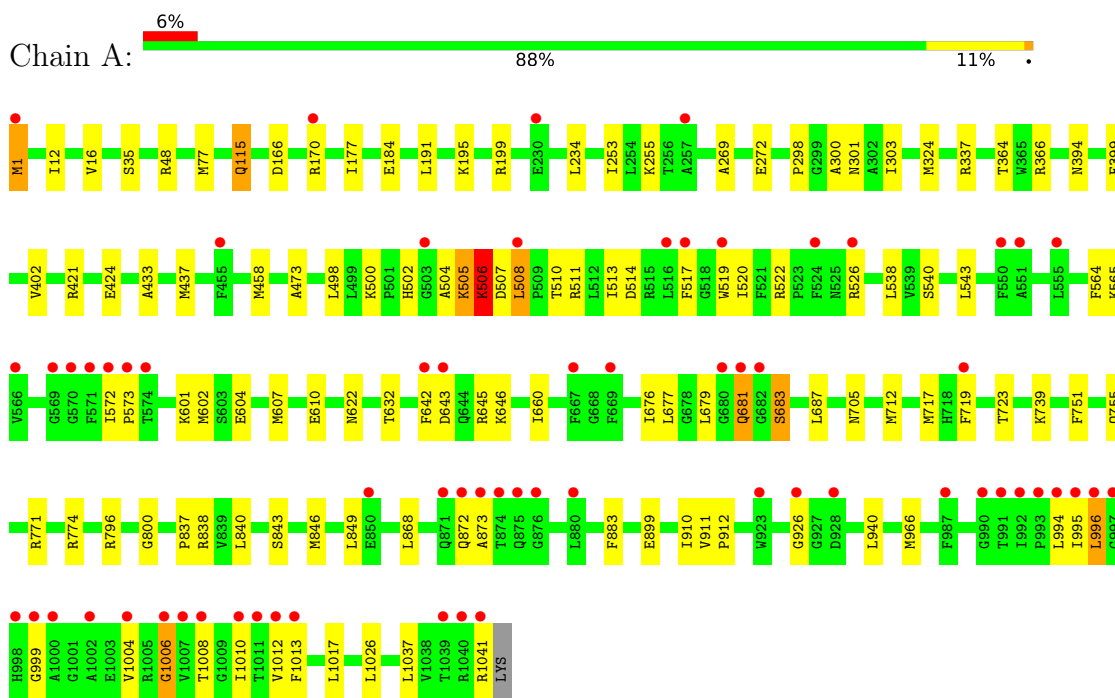
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	553	Total	O	0	0
			553	553		
5	B	439	Total	O	0	0
			439	439		
5	C	564	Total	O	0	0
			564	564		
5	D	415	Total	O	0	0
			415	415		
5	E	528	Total	O	0	0
			528	528		
5	F	441	Total	O	0	0
			441	441		

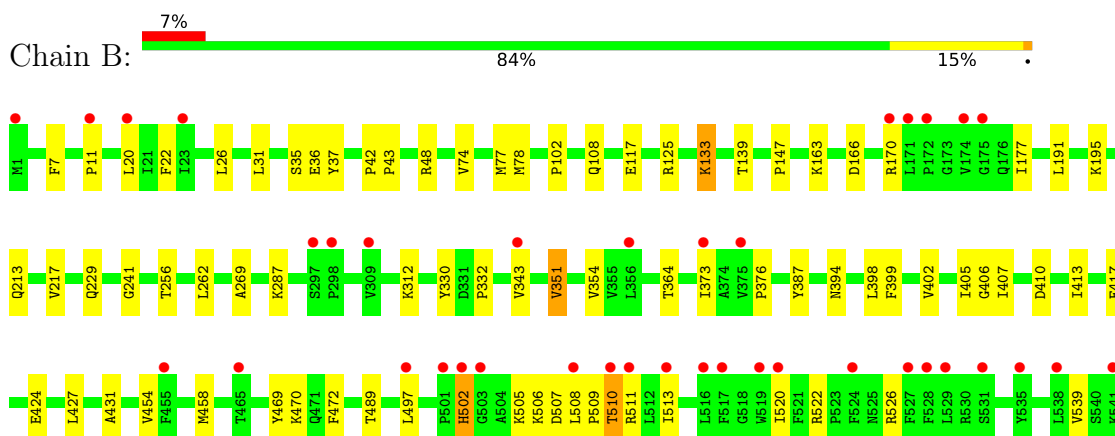
3 Residue-property plots [i](#)

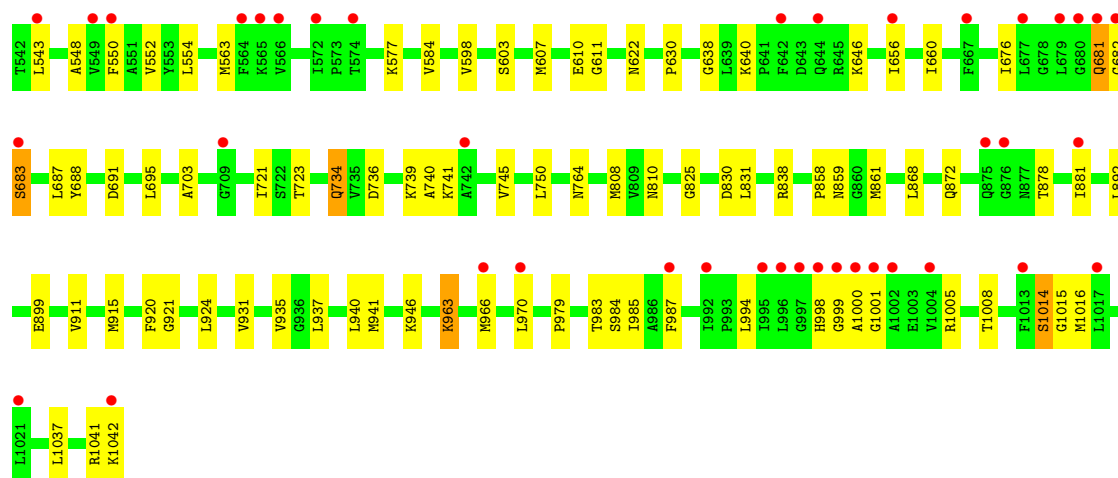
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Efflux pump membrane transporter

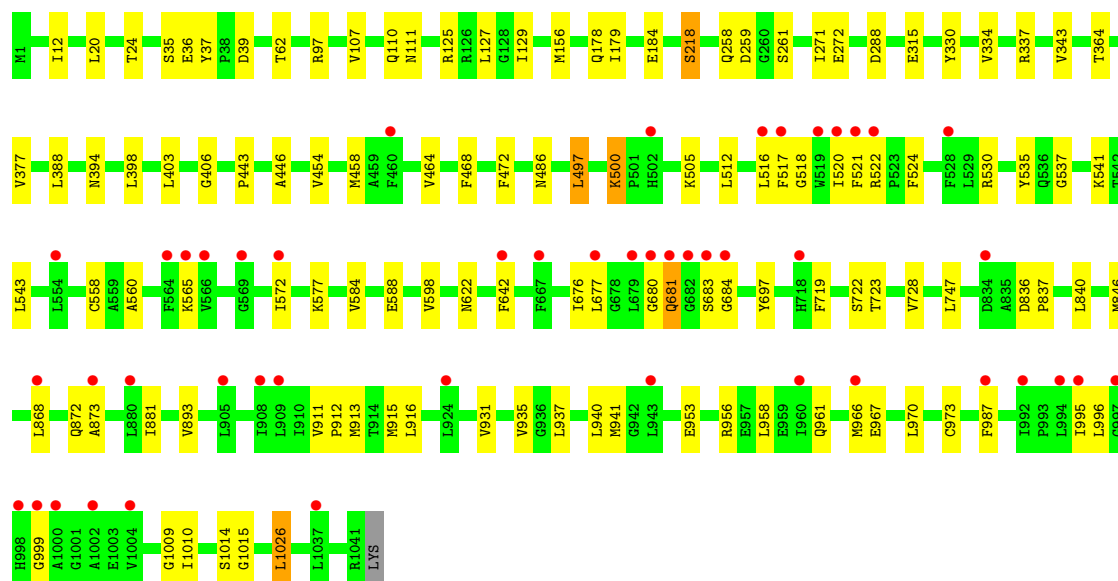
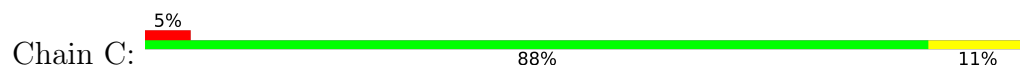


- Molecule 1: Efflux pump membrane transporter

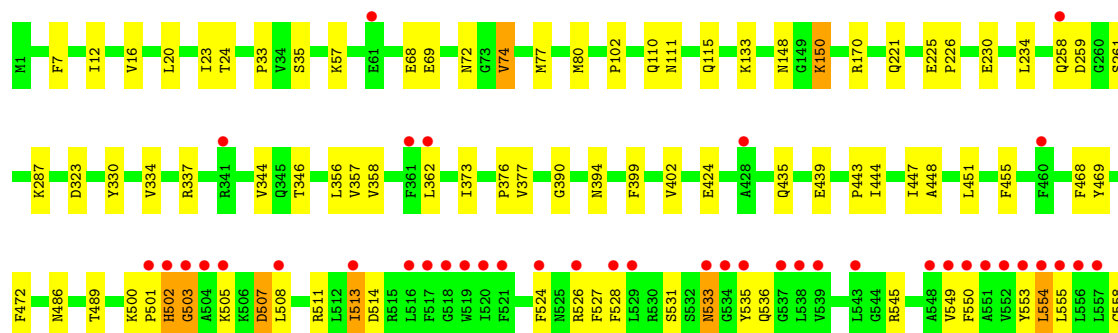
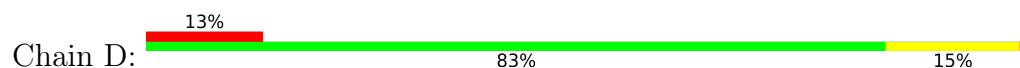


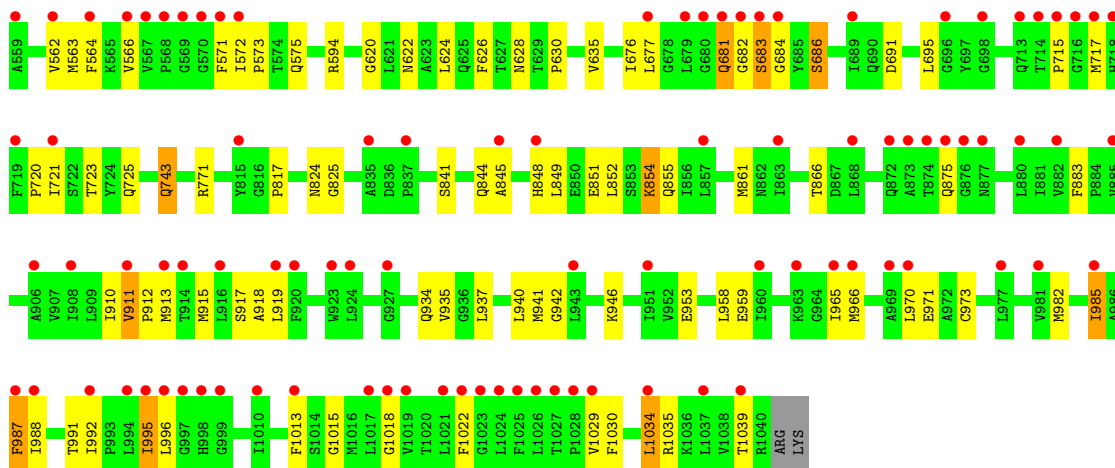


• Molecule 1: Efflux pump membrane transporter

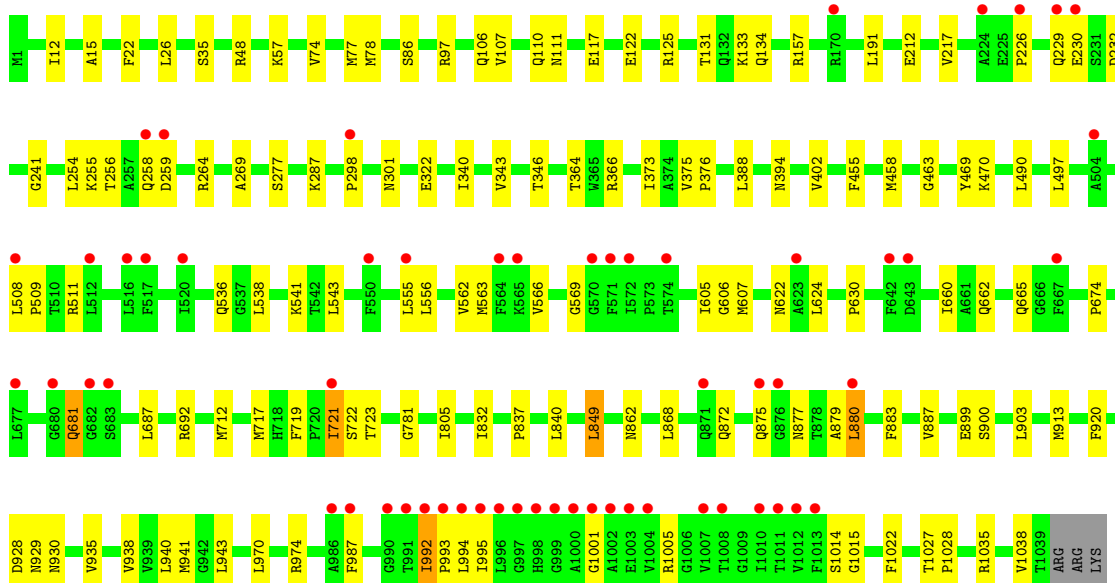
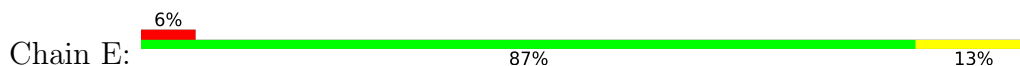


• Molecule 1: Efflux pump membrane transporter

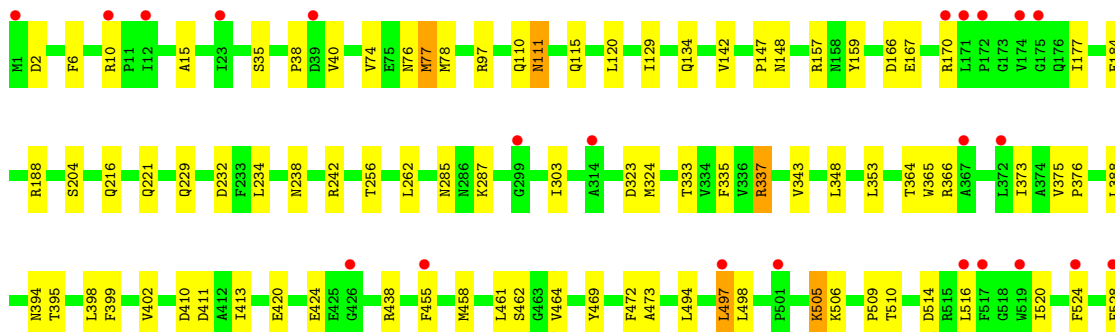
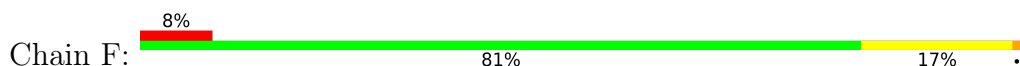


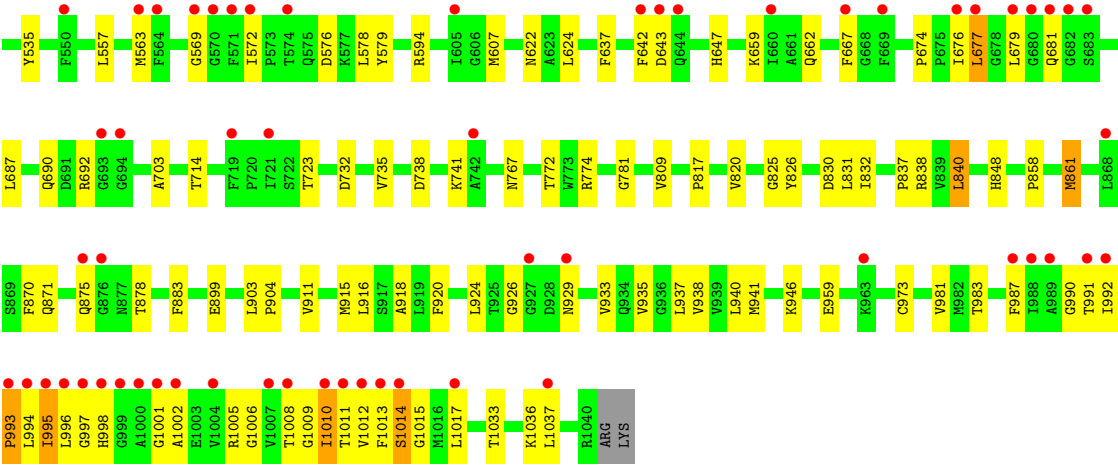


- Molecule 1: Efflux pump membrane transporter



- Molecule 1: Efflux pump membrane transporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	128.95Å 128.78Å 137.26Å 91.28° 90.01° 103.57°	Depositor
Resolution (Å)	43.28 – 1.85 43.28 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.28-1.85) 96.8 (43.28-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.18_3845: ???)	Depositor
R, R_{free}	0.180 , 0.217 0.181 , 0.218	Depositor DCC
R_{free} test set	35735 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l 0.007 for k,h,-l 0.004 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53422	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: LMT, PTY, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.83	1/8111 (0.0%)	0.84	4/11042 (0.0%)
1	B	0.69	0/8089	0.76	3/11013 (0.0%)
1	C	0.84	0/8080	0.84	2/11002 (0.0%)
1	D	0.73	0/8069	0.77	5/10988 (0.0%)
1	E	0.82	1/8100 (0.0%)	0.83	2/11027 (0.0%)
1	F	0.78	3/8078 (0.0%)	0.80	0/11000
All	All	0.78	5/48527 (0.0%)	0.81	16/66072 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	77	MET	SD-CE	-7.36	1.61	1.79
1	F	861	MET	SD-CE	-7.25	1.61	1.79
1	F	111	ASN	CB-CG	5.98	1.67	1.52
1	E	607	MET	SD-CE	-5.55	1.65	1.79
1	A	421	ARG	CZ-NH1	5.01	1.39	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	MET	CG-SD-CE	-6.09	87.50	100.90
1	B	681	GLN	CA-C-N	5.97	132.44	121.70
1	B	681	GLN	C-N-CA	5.97	132.44	121.70
1	A	298	PRO	CA-C-N	-5.83	112.34	122.83
1	A	298	PRO	C-N-CA	-5.83	112.34	122.83
1	B	999	GLY	N-CA-C	5.79	115.47	110.21
1	D	681	GLN	CA-C-N	5.63	131.83	121.70
1	D	681	GLN	C-N-CA	5.63	131.83	121.70
1	C	62	THR	CA-C-N	-5.62	117.20	123.16
1	C	62	THR	C-N-CA	-5.62	117.20	123.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	GLN	CA-CB-CG	-5.56	102.99	114.10
1	D	743	GLN	CB-CA-C	-5.19	100.25	110.11
1	D	771	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	E	606	GLY	CA-C-N	-5.13	111.02	121.18
1	E	606	GLY	C-N-CA	-5.13	111.02	121.18
1	D	115	GLN	CA-CB-CG	-5.05	104.00	114.10

There are no chirality outliers.

There are no planarity outliers.

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	7945	0	8161	96	0
1	B	7932	0	8140	113	0
1	C	7923	0	8127	87	0
1	D	7912	0	8114	134	0
1	E	7931	0	8153	127	0
1	F	7918	0	8120	154	0
2	A	374	0	480	18	0
2	B	308	0	413	13	0
2	C	420	0	545	19	0
2	D	395	0	516	39	0
2	E	407	0	541	42	0
2	F	386	0	513	26	0
3	A	46	0	68	4	0
3	B	94	0	140	3	0
3	C	48	0	72	1	0
3	D	48	0	72	1	0
3	E	94	0	140	5	0
3	F	85	0	131	3	0
4	A	54	0	70	10	0
4	B	18	0	23	1	0
4	C	42	0	55	9	0
4	D	24	0	32	0	0
4	E	48	0	64	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	30	0	39	2	0
5	A	553	0	0	7	0
5	B	439	0	0	5	0
5	C	564	0	0	11	0
5	D	415	0	0	7	0
5	E	528	0	0	7	0
5	F	441	0	0	11	0
All	All	53422	0	52729	729	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 7.

All (729) 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)
2:C:1103:LMT:H5B	2:C:1103:LMT:H6E	1.39	1.03
1:E:74:VAL:HG12	1:E:77:MET:HE2	1.44	0.97
1:E:277:SER:OG	4:E:1122:GOL:H12	1.76	0.86
1:F:303:ILE:HG23	1:F:337:ARG:HH11	1.38	0.86
1:B:74:VAL:HG12	1:B:77:MET:HE2	1.58	0.85
1:C:956:ARG:HG2	4:C:1116:GOL:H2	1.59	0.84
1:B:911:VAL:HG12	1:B:941:MET:HE2	1.59	0.84
1:E:903:LEU:HG	4:E:1116:GOL:H31	1.59	0.82
1:A:505:LYS:HG3	1:A:506:LYS:H	1.45	0.81
1:A:170:ARG:HD2	2:A:1110:LMT:H2'	1.62	0.81
1:C:681:GLN:HG3	1:C:684:GLY:H	1.43	0.80
1:C:893:VAL:HG22	2:C:1102:LMT:H101	1.63	0.80
1:F:229:GLN:NE2	5:F:1202:HOH:O	2.09	0.79
1:A:253:ILE:HG21	1:B:741:LYS:HG3	1.66	0.78
1:C:468:PHE:HE2	1:C:572:ILE:HD11	1.48	0.78
1:F:505:LYS:H	1:F:505:LYS:HD2	1.46	0.78
1:A:622:ASN:HD21	1:A:723:THR:HG23	1.49	0.77
1:C:697:TYR:H	4:C:1117:GOL:H2	1.49	0.77
2:B:1101:LMT:H6'	2:B:1101:LMT:H2O1	1.25	0.77
2:E:1105:LMT:O6B	5:E:1201:HOH:O	2.03	0.77
1:F:204:SER:HB3	4:F:1116:GOL:H11	1.67	0.77
3:A:1112:PTY:H231	3:A:1112:PTY:H442	1.67	0.77
1:C:468:PHE:CE2	1:C:572:ILE:HD11	2.20	0.77
1:A:751:PHE:O	1:A:755[B]:GLN:HG3	1.85	0.76
1:D:717:MET:HE1	1:D:849:LEU:HD21	1.68	0.75
1:D:825:GLY:HA3	2:D:1109:LMT:H102	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:PHE:CD2	1:C:935:VAL:HG11	2.22	0.74
1:A:507:ASP:OD1	1:A:510:THR:HG22	1.90	0.72
1:E:563:MET:HE3	1:E:920:PHE:HA	1.71	0.71
1:E:935:VAL:HG23	2:E:1108:LMT:H121	1.70	0.71
1:C:107:VAL:HA	1:C:110:GLN:HG2	1.73	0.71
1:F:167:GLU:OE2	5:F:1201:HOH:O	2.08	0.71
1:D:991:THR:HG21	1:D:1013:PHE:HB2	1.73	0.71
1:C:622:ASN:ND2	1:C:723:THR:HG23	2.06	0.71
1:E:301:ASN:HD21	2:E:1107:LMT:H2'	1.55	0.71
1:E:497:LEU:HD21	2:E:1112:LMT:H5'	1.72	0.69
1:D:841:SER:H	1:D:844:GLN:HE21	1.38	0.69
1:A:622:ASN:ND2	1:A:723:THR:HG23	2.08	0.69
2:A:1110:LMT:H12	1:B:78:MET:O	1.93	0.69
1:E:928:ASP:OD1	5:E:1202:HOH:O	2.10	0.68
1:D:362:LEU:HD21	1:D:982:MET:HE1	1.76	0.68
1:F:97:ARG:HG2	2:F:1110:LMT:H6'2	1.75	0.68
1:B:740:ALA:CB	1:B:808:MET:HE3	2.24	0.68
1:A:300:ALA:HA	4:A:1114:GOL:H31	1.76	0.67
1:C:719:PHE:CE2	4:C:1118:GOL:H11	2.28	0.67
2:C:1108:LMT:H6'1	5:C:1629:HOH:O	1.93	0.67
1:F:528:PHE:HB3	2:F:1113:LMT:H11	1.75	0.67
1:D:1030:PHE:O	1:D:1034:LEU:HD23	1.94	0.67
1:E:258:GLN:CD	1:E:258:GLN:H	1.99	0.67
1:D:110:GLN:NE2	1:E:111:ASN:HB2	2.10	0.67
2:E:1108:LMT:H5B	2:E:1108:LMT:H6D	1.78	0.66
1:A:755[B]:GLN:HG2	1:C:218:SER:O	1.96	0.66
1:E:712:MET:HE3	1:E:719:PHE:CD1	2.31	0.66
1:D:287:LYS:NZ	5:D:1206:HOH:O	2.28	0.66
1:A:564:PHE:HE1	2:A:1107:LMT:H12	1.60	0.65
1:B:229:GLN:HG2	5:B:1566:HOH:O	1.96	0.65
1:D:12:ILE:HG21	1:E:899:GLU:HA	1.77	0.65
2:D:1104:LMT:O4'	5:D:1202:HOH:O	2.13	0.65
2:D:1107:LMT:H42	2:D:1107:LMT:H1'	1.77	0.65
1:E:883:PHE:HZ	2:E:1108:LMT:H31	1.61	0.65
1:E:57:LYS:NZ	5:E:1207:HOH:O	2.28	0.65
1:F:994:LEU:HD21	2:F:1103:LMT:H31	1.77	0.65
1:D:69:GLU:OE1	1:F:772:THR:HG23	1.97	0.65
1:A:705:ASN:HB2	4:A:1115:GOL:H2	1.79	0.65
1:A:868:LEU:O	1:A:872:GLN:HG3	1.96	0.65
1:D:563:MET:HA	1:D:566:VAL:HG22	1.79	0.65
1:B:750:LEU:HD12	1:B:808:MET:HE2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1041:ARG:HG2	1:B:1042:LYS:HD3	1.79	0.64
1:F:774:ARG:HD3	5:F:1597:HOH:O	1.98	0.64
1:C:935:VAL:HG12	2:C:1111:LMT:H92	1.79	0.64
1:D:550:PHE:O	1:D:554:LEU:HD22	1.97	0.64
1:E:366:ARG:HH12	2:E:1112:LMT:H3B	1.63	0.64
1:D:630:PRO:HG3	1:F:234:LEU:HD23	1.80	0.64
2:D:1101:LMT:H5B	2:D:1101:LMT:H6D	1.80	0.64
1:C:622:ASN:HD21	1:C:723:THR:HG23	1.63	0.63
1:B:963:LYS:NZ	4:B:1114:GOL:O2	2.23	0.63
2:F:1105:LMT:H6'2	5:F:1471:HOH:O	1.98	0.63
1:A:1:MET:N	1:A:1:MET:SD	2.70	0.63
1:D:935:VAL:HG22	2:D:1107:LMT:H112	1.80	0.63
1:E:256:THR:OG1	1:F:741:LYS:NZ	2.32	0.63
1:E:402:VAL:HG11	2:E:1103:LMT:H41	1.81	0.63
1:B:413:ILE:HD12	1:B:983:THR:HG22	1.80	0.62
1:E:569:GLY:HA3	1:E:929:ASN:HB3	1.79	0.62
1:F:569:GLY:HA3	1:F:929:ASN:HB3	1.81	0.62
1:B:36:GLU:OE1	1:B:577:LYS:NZ	2.32	0.62
1:B:750:LEU:HD12	1:B:808:MET:CE	2.30	0.62
1:F:420:GLU:O	1:F:424:GLU:HG3	1.99	0.62
1:B:406:GLY:HA3	1:B:987:PHE:CZ	2.34	0.62
1:E:131:THR:H	1:F:115:GLN:HE22	1.47	0.62
1:B:603:SER:O	1:B:607:MET:HG2	2.00	0.62
1:E:1035:ARG:HH11	4:E:1116:GOL:H11	1.64	0.62
1:E:624:LEU:HD11	1:E:721:ILE:HG13	1.82	0.61
1:D:913:MET:HB3	1:D:1022:PHE:CD2	2.34	0.61
1:E:622:ASN:ND2	1:E:723:THR:HG23	2.15	0.61
1:D:677:LEU:CD2	2:D:1103:LMT:H41	2.30	0.61
1:F:647:HIS:HD2	5:F:1226:HOH:O	1.83	0.61
2:D:1107:LMT:H6D	2:D:1107:LMT:H5B	1.82	0.61
1:D:937:LEU:O	1:D:941:MET:HG3	2.00	0.60
1:E:913:MET:HE2	1:E:1022:PHE:CE1	2.36	0.60
1:A:48[B]:ARG:NH2	2:A:1105:LMT:H4'	2.15	0.60
1:F:667:PHE:HZ	2:F:1111:LMT:H52	1.66	0.60
2:A:1103:LMT:H5B	2:A:1103:LMT:H6E	1.82	0.60
1:F:413:ILE:HD12	1:F:983:THR:HG22	1.83	0.60
1:B:915:MET:HE1	2:B:1107:LMT:H32	1.83	0.60
1:F:303:ILE:HG23	1:F:337:ARG:NH1	2.13	0.60
1:F:838:ARG:NH2	1:F:926:GLY:O	2.35	0.60
1:A:676:ILE:HD12	1:A:679:LEU:HD12	1.82	0.60
1:B:505:LYS:HE2	1:B:505:LYS:HA	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:994:LEU:HD22	1:B:1005:ARG:HG2	1.83	0.60
1:D:444:ILE:O	1:D:447:ILE:HG13	2.02	0.60
1:A:255:LYS:NZ	4:A:1121:GOL:H31	2.17	0.60
1:A:838:ARG:NH2	1:A:926:GLY:O	2.35	0.60
1:E:340:ILE:HG23	2:E:1107:LMT:H51	1.84	0.60
1:F:832:ILE:HD11	4:F:1117:GOL:H32	1.83	0.60
1:E:879:ALA:HB1	1:E:883:PHE:CE2	2.37	0.59
1:F:285:ASN:HB3	1:F:607:MET:HE3	1.83	0.59
1:F:994:LEU:HB3	1:F:1009:GLY:HA3	1.84	0.59
1:E:122:GLU:OE1	1:E:125[B]:ARG:NH2	2.31	0.59
1:F:1001:GLY:CA	2:F:1103:LMT:H3B	2.33	0.59
1:E:868:LEU:O	1:E:872:GLN:HG3	2.02	0.59
1:E:157:ARG:NH2	2:E:1105:LMT:O4'	2.36	0.59
1:F:78:MET:HG3	1:F:97:ARG:HG3	1.84	0.59
3:A:1112:PTY:H331	3:A:1112:PTY:H112	1.84	0.59
1:D:258:GLN:H	1:D:258:GLN:CD	2.10	0.59
1:F:410:ASP:OD1	1:F:983:THR:HG21	2.03	0.58
1:E:106:GLN:HE21	1:E:110:GLN:HE21	1.50	0.58
1:E:508:LEU:HD12	1:E:509:PRO:HD3	1.86	0.58
1:C:388:LEU:HD11	3:C:1113:PTY:H421	1.83	0.58
1:E:469:TYR:CD1	2:E:1108:LMT:H82	2.38	0.58
1:A:184:GLU:HG2	4:A:1119:GOL:H2	1.85	0.58
1:D:20:LEU:O	1:D:24:THR:HG23	2.04	0.58
1:A:506:LYS:HE2	1:A:514:ASP:OD2	2.03	0.58
1:C:330:TYR:HB2	2:C:1107:LMT:H111	1.85	0.58
1:F:335:PHE:CD1	2:F:1103:LMT:H4B	2.38	0.58
1:D:472:PHE:CD2	1:D:935:VAL:HG21	2.39	0.57
1:A:402:VAL:HG11	2:A:1111:LMT:H41	1.86	0.57
1:B:166:ASP:O	1:B:170:ARG:HG3	2.05	0.57
1:B:691:ASP:HA	1:B:861:MET:HG2	1.87	0.57
1:A:681:GLN:HG3	1:A:683:SER:N	2.20	0.57
1:C:377:VAL:HG12	1:C:486:ASN:HD21	1.69	0.57
1:B:688:TYR:CE2	1:B:830:ASP:HB3	2.40	0.57
1:B:937:LEU:O	1:B:941:MET:HG3	2.04	0.57
1:D:234:LEU:HD23	1:E:630:PRO:HG3	1.85	0.57
1:D:527:PHE:O	1:D:531:SER:OG	2.20	0.57
1:F:817:PRO:HG2	1:F:820:VAL:HG22	1.86	0.57
1:C:520:ILE:HG23	1:C:524:PHE:CD2	2.40	0.57
1:E:721:ILE:HD12	5:E:1436:HOH:O	2.03	0.57
1:E:508:LEU:HB3	1:E:511:ARG:HH21	1.70	0.57
1:A:994:LEU:HD11	2:A:1111:LMT:H42	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48[B]:ARG:CZ	2:A:1105:LMT:H1B	2.35	0.56
1:A:681:GLN:HG3	1:A:683:SER:H	1.70	0.56
4:C:1115:GOL:H32	5:C:1598:HOH:O	2.05	0.56
1:E:940:LEU:HD13	1:E:1015:GLY:HA3	1.87	0.56
2:E:1105:LMT:O3'	2:E:1105:LMT:O2B	2.17	0.56
1:F:940:LEU:HD11	1:F:1012:VAL:HA	1.87	0.56
1:A:543:LEU:HD13	1:A:966:MET:SD	2.45	0.56
1:B:915:MET:HE3	1:B:941:MET:SD	2.45	0.56
1:C:184:GLU:HG2	5:C:1212:HOH:O	2.04	0.56
1:E:883:PHE:CZ	2:E:1108:LMT:H31	2.40	0.56
1:D:883:PHE:HZ	2:D:1107:LMT:H61	1.71	0.56
1:F:677:LEU:HD21	2:F:1104:LMT:H41	1.87	0.56
1:F:1006:GLY:O	1:F:1010:ILE:HG13	2.06	0.56
1:A:645:ARG:C	1:A:646:LYS:HE2	2.30	0.56
1:B:1005:ARG:HG3	2:B:1103:LMT:H11	1.88	0.56
1:D:941:MET:HE1	2:D:1112:LMT:H102	1.87	0.56
1:E:674:PRO:HB3	1:E:681:GLN:HA	1.87	0.56
1:D:74:VAL:CG2	1:D:77:MET:HE2	2.36	0.56
1:E:624:LEU:HD22	1:E:832:ILE:HD12	1.88	0.56
1:D:959:GLU:OE2	1:D:1035:ARG:HD3	2.05	0.56
1:A:899:GLU:HA	1:C:12:ILE:HG21	1.87	0.55
1:F:959:GLU:HG3	5:F:1228:HOH:O	2.05	0.55
1:E:662:GLN:OE1	5:E:1203:HOH:O	2.18	0.55
1:A:1004:VAL:O	1:A:1008:THR:HG23	2.07	0.55
1:C:178:GLN:NE2	5:C:1214:HOH:O	2.38	0.55
1:E:131:THR:H	1:F:115:GLN:NE2	2.02	0.55
1:E:470:LYS:HE3	2:E:1110:LMT:H12	1.89	0.55
1:A:642:PHE:HD2	1:A:999:GLY:HA2	1.72	0.55
1:F:858:PRO:HD2	1:F:861:MET:HE2	1.89	0.55
1:C:271:ILE:HD12	4:C:1115:GOL:H31	1.87	0.55
1:E:712:MET:HE3	1:E:719:PHE:HD1	1.70	0.55
1:F:937:LEU:O	1:F:941:MET:HG3	2.06	0.55
1:D:919:LEU:HD12	1:D:919:LEU:H	1.72	0.55
1:E:994:LEU:HD21	2:E:1103:LMT:H51	1.88	0.55
1:F:576:ASP:HB3	1:F:642:PHE:HE2	1.72	0.55
1:E:556:LEU:HB3	1:E:913:MET:HE1	1.88	0.55
1:B:563:MET:HE3	1:B:920:PHE:HA	1.89	0.55
1:C:97:ARG:HG2	2:C:1112:LMT:C6'	2.37	0.55
1:D:535:TYR:OH	1:D:973:CYS:HB3	2.07	0.54
1:B:750:LEU:CD1	1:B:808:MET:HE2	2.37	0.54
1:D:915:MET:O	1:D:918:ALA:N	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:674:PRO:HB3	1:F:681:GLN:HG2	1.89	0.54
1:C:464:VAL:HG11	1:C:868:LEU:HD21	1.88	0.54
1:B:638:GLY:HA3	2:B:1102:LMT:H123	1.90	0.54
1:E:900:SER:HB2	4:E:1116:GOL:H32	1.89	0.54
1:F:825:GLY:HA3	2:F:1110:LMT:H82	1.89	0.54
1:F:399:PHE:HZ	1:F:1008:THR:HG21	1.72	0.54
1:F:469:TYR:CD1	2:F:1108:LMT:H101	2.43	0.54
1:E:343:VAL:HG22	1:E:402:VAL:HG23	1.89	0.54
1:A:995:ILE:HG13	1:A:996:LEU:H	1.73	0.54
1:D:549:VAL:HG11	1:D:1029:VAL:HG21	1.90	0.54
1:E:887:VAL:HG22	2:E:1109:LMT:H111	1.89	0.54
1:A:473:ALA:HA	2:A:1108:LMT:H102	1.89	0.54
1:F:462:SER:N	1:F:878:THR:HG21	2.23	0.54
1:B:736:ASP:OD2	1:B:739:LYS:HE3	2.08	0.53
1:C:956:ARG:CG	4:C:1116:GOL:H2	2.35	0.53
1:D:377:VAL:HG12	1:D:486:ASN:HD21	1.72	0.53
1:D:681:GLN:HB3	1:D:682:GLY:HA2	1.90	0.53
1:E:117:GLU:O	1:E:125[B]:ARG:HD3	2.07	0.53
1:A:1013:PHE:CE1	1:A:1017:LEU:HD11	2.44	0.53
1:B:147:PRO:O	1:B:287:LYS:HE3	2.08	0.53
1:B:920:PHE:CE2	1:B:924:LEU:HD11	2.43	0.53
1:E:78:MET:HG2	1:E:97:ARG:HG2	1.90	0.53
1:B:399:PHE:CZ	1:B:1008:THR:HG21	2.43	0.53
1:C:543:LEU:HD12	1:C:970:LEU:HD21	1.90	0.53
1:D:230:GLU:HA	5:D:1554:HOH:O	2.09	0.53
1:F:667:PHE:CZ	2:F:1111:LMT:H52	2.44	0.53
1:F:1001:GLY:HA3	2:F:1103:LMT:H3B	1.90	0.53
1:B:563:MET:CE	1:B:920:PHE:HA	2.38	0.53
1:D:677:LEU:HD21	2:D:1103:LMT:H41	1.89	0.53
1:E:106:GLN:HE21	1:E:110:GLN:NE2	2.06	0.53
1:F:994:LEU:HG	1:F:1005:ARG:HG2	1.90	0.53
1:C:97:ARG:HD2	2:C:1112:LMT:O6'	2.08	0.53
1:C:995:ILE:HG22	1:C:996:LEU:HD23	1.91	0.53
1:D:424:GLU:HG2	1:D:502:HIS:CE1	2.44	0.53
1:E:373:ILE:HG22	1:E:490:LEU:HD21	1.91	0.53
1:F:157:ARG:HH22	2:F:1105:LMT:H4B	1.73	0.53
1:A:602:MET:HG2	1:A:660:ILE:HD12	1.91	0.53
1:C:97:ARG:HG2	2:C:1112:LMT:H6D	1.91	0.53
1:D:74:VAL:HG22	1:D:77:MET:HE2	1.91	0.53
1:D:111:ASN:HB2	1:F:110:GLN:NE2	2.24	0.53
1:F:674:PRO:HB3	1:F:681:GLN:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:918:ALA:HA	1:F:1014:SER:HB2	1.90	0.53
1:A:399:PHE:CZ	1:A:1008:THR:HG21	2.43	0.52
1:C:537:GLY:O	1:C:541:LYS:HG2	2.10	0.52
1:E:12:ILE:HG21	1:F:899:GLU:HA	1.91	0.52
1:B:695:LEU:HD12	1:B:861:MET:HG3	1.92	0.52
1:D:524:PHE:O	1:D:528:PHE:N	2.40	0.52
1:E:665:GLN:N	1:E:665:GLN:OE1	2.40	0.52
1:B:507:ASP:OD1	1:B:510:THR:HG22	2.10	0.52
1:B:734:GLN:NE2	1:B:810:ASN:HD22	2.08	0.52
3:A:1112:PTY:H391	3:A:1112:PTY:H171	1.92	0.52
1:D:940:LEU:HD13	1:D:1015:GLY:HA3	1.91	0.52
1:E:1035:ARG:HD2	4:E:1116:GOL:C1	2.39	0.52
1:F:462:SER:H	1:F:878:THR:HG21	1.75	0.52
1:E:74:VAL:CG1	1:E:77:MET:HE2	2.29	0.52
1:E:388:LEU:HD11	3:E:1115:PTY:H421	1.92	0.52
1:E:1035:ARG:HD2	4:E:1116:GOL:H12	1.91	0.52
1:D:170:ARG:NH2	5:D:1201:HOH:O	2.13	0.52
1:A:35:SER:O	1:A:394:ASN:HA	2.09	0.51
1:E:157:ARG:HH22	2:E:1105:LMT:H6'1	1.76	0.51
1:A:771:ARG:HH11	4:A:1117:GOL:H2	1.75	0.51
1:E:941:MET:HE1	2:E:1109:LMT:H51	1.93	0.51
1:F:256:THR:HG22	1:F:262:LEU:HD23	1.92	0.51
1:B:682:GLY:HA2	1:B:683:SER:OG	2.11	0.51
1:D:362:LEU:N	1:D:362:LEU:HD22	2.26	0.51
1:E:928:ASP:OD2	1:E:930:ASN:ND2	2.42	0.51
1:A:519:TRP:CE2	1:A:520:ILE:HD11	2.46	0.51
1:D:500:LYS:HE2	1:D:501:PRO:HD3	1.93	0.51
1:E:226:PRO:O	1:F:781:GLY:HA3	2.11	0.51
1:E:721:ILE:HD12	1:E:722:SER:H	1.75	0.51
1:A:572:ILE:HD11	1:A:676:ILE:HD11	1.92	0.51
1:D:571:PHE:CD2	1:D:572:ILE:HG12	2.46	0.51
2:D:1104:LMT:O6'	2:D:1104:LMT:H5B	2.10	0.51
1:C:931:VAL:O	1:C:935:VAL:HG13	2.11	0.51
1:E:232:ASP:O	1:F:594:ARG:HD3	2.11	0.51
1:A:705:ASN:CB	4:A:1115:GOL:H2	2.40	0.51
1:D:987:PHE:HA	2:D:1102:LMT:H111	1.91	0.51
1:F:159:TYR:CD1	1:F:324:MET:HE1	2.46	0.51
1:F:411:ASP:OD1	1:F:946:LYS:NZ	2.23	0.50
1:F:992:ILE:C	1:F:994:LEU:H	2.20	0.50
1:A:717:MET:HE1	1:A:849:LEU:HD11	1.93	0.50
1:F:703:ALA:CB	1:F:861:MET:HE1	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:915:MET:HG3	1:F:941:MET:HE2	1.93	0.50
1:A:458:MET:HE1	2:A:1107:LMT:H72	1.93	0.50
1:D:435:GLN:O	1:D:439:GLU:HG3	2.11	0.50
1:E:134:GLN:NE2	2:E:1105:LMT:O2'	2.38	0.50
1:A:255:LYS:HZ3	4:A:1121:GOL:H31	1.75	0.50
1:A:846:MET:HE1	1:A:873:ALA:HB2	1.92	0.50
1:B:37:TYR:CE2	1:B:676:ILE:HG12	2.46	0.50
1:B:506:LYS:HD3	1:B:511:ARG:NH2	2.26	0.50
1:D:958:LEU:HD13	1:D:971:GLU:HB3	1.92	0.50
1:E:543:LEU:HD12	1:E:970:LEU:HD21	1.92	0.50
2:E:1107:LMT:H5B	2:E:1107:LMT:H6E	1.93	0.50
1:F:667:PHE:CE2	2:F:1111:LMT:H32	2.47	0.50
1:F:996:LEU:HD12	1:F:1006:GLY:HA3	1.94	0.50
1:B:402:VAL:HA	1:B:405:ILE:HD12	1.93	0.50
1:D:1018:GLY:O	1:D:1022:PHE:HB2	2.11	0.50
1:E:107:VAL:HA	1:E:110:GLN:HG2	1.92	0.50
1:A:632:THR:HB	4:A:1116:GOL:H32	1.92	0.50
1:C:36:GLU:OE2	1:C:577:LYS:NZ	2.36	0.50
1:C:846:MET:HE1	1:C:873:ALA:HB2	1.93	0.50
1:D:695:LEU:HD12	1:D:861:MET:HG3	1.94	0.50
1:B:102:PRO:HB2	1:B:133:LYS:HD2	1.94	0.50
1:E:935:VAL:HG23	2:E:1108:LMT:C12	2.41	0.50
1:D:555:LEU:O	1:D:558:CYS:HB3	2.12	0.50
1:C:722:SER:HB3	4:C:1118:GOL:H2	1.92	0.50
4:C:1114:GOL:O1	1:E:287[A]:LYS:NZ	2.45	0.49
1:F:366:ARG:HD3	1:F:498:LEU:O	2.12	0.49
1:A:502:HIS:C	1:A:504:ALA:H	2.20	0.49
1:B:458:MET:HG2	2:B:1108:LMT:H101	1.94	0.49
1:D:443:PRO:HG3	1:D:953:GLU:HG2	1.95	0.49
1:F:1001:GLY:O	1:F:1005:ARG:HB2	2.12	0.49
1:F:458:MET:HE2	1:F:883:PHE:CE1	2.48	0.49
1:C:958:LEU:HA	1:C:961:GLN:HG2	1.94	0.49
1:D:469:TYR:CZ	2:D:1107:LMT:H51	2.48	0.49
1:C:995:ILE:HD11	1:C:1009:GLY:C	2.38	0.49
1:F:714:THR:HG21	1:F:848:HIS:CD2	2.48	0.49
3:A:1112:PTY:H412	3:A:1112:PTY:H191	1.95	0.49
2:D:1101:LMT:H5B	2:D:1101:LMT:C6'	2.41	0.49
1:F:76:ASN:OD1	1:F:97:ARG:NH1	2.46	0.49
1:A:994:LEU:HD11	2:A:1111:LMT:C4	2.42	0.49
1:C:20:LEU:O	1:C:24:THR:HG23	2.13	0.49
1:E:463:GLY:HA3	1:E:875:GLN:OE1	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:ARG:NH2	5:F:1209:HOH:O	2.30	0.49
1:F:461:LEU:HA	1:F:878:THR:HG21	1.93	0.49
1:F:147:PRO:HA	1:F:287:LYS:HD2	1.94	0.48
1:F:388:LEU:HD11	3:F:1115:PTY:H421	1.95	0.48
1:F:458:MET:HE2	1:F:883:PHE:HE1	1.77	0.48
1:C:913:MET:HG3	1:C:1026:LEU:HD12	1.95	0.48
1:D:934:GLN:HG2	2:D:1112:LMT:H11	1.95	0.48
1:F:572:ILE:H	1:F:572:ILE:HD12	1.77	0.48
1:E:15:ALA:HB2	2:E:1101:LMT:H31	1.94	0.48
1:E:110:GLN:OE1	1:F:111:ASN:HB2	2.14	0.48
1:B:1001:GLY:HA3	2:B:1103:LMT:H3'	1.96	0.48
1:D:624:LEU:HD11	1:D:721:ILE:HG22	1.96	0.48
1:F:1013:PHE:CE2	1:F:1017:LEU:HD11	2.49	0.48
1:C:458:MET:HG3	2:C:1111:LMT:H102	1.96	0.48
1:D:848:HIS:O	1:D:852:LEU:HG	2.13	0.48
1:D:965:ILE:HD13	1:D:1035:ARG:HB3	1.95	0.48
1:F:996:LEU:HA	1:F:1006:GLY:HA3	1.95	0.48
1:A:1:MET:N	5:A:1217:HOH:O	2.44	0.48
1:B:213:GLN:HG2	1:C:747:LEU:HD12	1.95	0.48
1:D:259:ASP:OD1	1:D:261:SER:OG	2.28	0.48
1:A:12:ILE:HG21	1:B:899:GLU:HA	1.95	0.48
1:A:646:LYS:HE2	1:A:646:LYS:N	2.28	0.48
1:B:611:GLY:HA2	1:B:640:LYS:HD3	1.95	0.48
1:C:111:ASN:ND2	5:C:1207:HOH:O	2.28	0.48
1:D:68:GLU:HB3	2:D:1109:LMT:H91	1.95	0.48
1:D:681:GLN:CB	1:D:682:GLY:HA2	2.44	0.48
1:B:117:GLU:OE1	1:B:125:ARG:NH2	2.47	0.48
1:C:530:ARG:NH2	5:C:1202:HOH:O	2.21	0.48
1:D:917:SER:OG	1:D:1018:GLY:HA3	2.13	0.48
1:E:78:MET:CG	1:E:97:ARG:HG2	2.43	0.48
1:E:622:ASN:HD21	1:E:723:THR:HG23	1.79	0.48
1:A:170:ARG:HD3	2:A:1110:LMT:H22	1.96	0.48
1:D:221:GLN:NE2	1:E:86:SER:O	2.47	0.48
1:A:646:LYS:NZ	5:A:1224:HOH:O	2.47	0.47
1:B:470:LYS:NZ	2:B:1109:LMT:O5'	2.45	0.47
1:B:745:VAL:HG11	1:B:808:MET:HE1	1.96	0.47
1:E:556:LEU:CB	1:E:913:MET:HE1	2.43	0.47
1:E:22:PHE:CE2	1:E:26:LEU:HD11	2.48	0.47
1:E:556:LEU:HD13	1:E:913:MET:HE1	1.95	0.47
1:B:191:LEU:HD23	1:B:269:ALA:HB2	1.96	0.47
1:D:848:HIS:CE1	1:D:852:LEU:HD21	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:SER:HB3	4:E:1121:GOL:H2	1.97	0.47
1:F:458:MET:SD	2:F:1108:LMT:H111	2.54	0.47
1:F:535:TYR:OH	1:F:973:CYS:HB3	2.14	0.47
1:D:824:ASN:C	2:D:1109:LMT:H81	2.40	0.47
1:B:931:VAL:O	1:B:935:VAL:HG23	2.14	0.47
1:C:937:LEU:O	1:C:941:MET:HG3	2.13	0.47
1:D:469:TYR:OH	2:D:1107:LMT:H51	2.13	0.47
1:E:230:GLU:HG2	5:F:1551:HOH:O	2.13	0.47
1:E:712:MET:HE2	1:E:719:PHE:HB2	1.96	0.47
1:A:910:ILE:HD13	1:A:1026:LEU:HD23	1.97	0.47
2:E:1108:LMT:H11	2:E:1109:LMT:H6D	1.97	0.47
1:F:35:SER:O	1:F:394:ASN:HA	2.15	0.47
1:A:500:LYS:HA	1:A:500:LYS:HD3	1.69	0.47
1:C:37:TYR:CE2	1:C:676:ILE:HG12	2.50	0.47
1:C:995:ILE:HD11	1:C:1010:ILE:N	2.29	0.47
1:D:845:ALA:O	1:D:849:LEU:HG	2.15	0.47
1:E:605:ILE:HD13	1:E:660:ILE:HD13	1.96	0.47
1:F:134:GLN:HG3	5:F:1339:HOH:O	2.15	0.47
1:F:506:LYS:NZ	1:F:514:ASP:OD2	2.34	0.47
2:F:1102:LMT:H51	3:F:1114:PTY:H162	1.97	0.47
1:E:877:ASN:HB3	1:E:880:LEU:HD22	1.96	0.47
1:F:148:ASN:HB2	1:F:323:ASP:OD2	2.15	0.47
1:F:365:TRP:CD1	1:F:509:PRO:HB2	2.50	0.47
1:F:497:LEU:HD13	5:F:1266:HOH:O	2.14	0.47
1:F:506:LYS:HG2	1:F:510:THR:HG21	1.97	0.47
1:A:508:LEU:HD13	1:A:511:ARG:HH21	1.79	0.47
1:D:72:ASN:OD1	2:D:1109:LMT:H71	2.14	0.47
1:D:468:PHE:HZ	1:D:676:ILE:HD11	1.79	0.47
1:D:686:SER:HB3	1:D:866:THR:HG22	1.97	0.47
1:A:604:GLU:HA	1:A:607:MET:HE3	1.97	0.47
2:E:1106:LMT:H6E	2:E:1106:LMT:H1B	1.97	0.47
1:B:195:LYS:NZ	5:B:1220:HOH:O	2.47	0.46
1:B:584:VAL:HG21	1:B:598:VAL:HG11	1.98	0.46
1:B:868:LEU:O	1:B:872:GLN:HG3	2.15	0.46
1:C:406:GLY:HA3	1:C:987:PHE:CZ	2.50	0.46
1:D:942:GLY:O	1:D:946:LYS:HG3	2.14	0.46
1:A:995:ILE:HG13	1:A:996:LEU:N	2.29	0.46
1:C:259:ASP:OD2	1:C:261:SER:OG	2.22	0.46
1:C:535:TYR:OH	1:C:973:CYS:HB3	2.16	0.46
1:D:681:GLN:HG3	1:D:682:GLY:HA2	1.97	0.46
1:D:854:LYS:HA	1:D:854:LYS:HD2	1.62	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:871:GLN:O	1:F:875:GLN:HG3	2.15	0.46
1:F:1033:THR:O	1:F:1037:LEU:HD12	2.15	0.46
1:A:366:ARG:HD3	1:A:498:LEU:O	2.15	0.46
1:C:966:MET:HB2	1:C:966:MET:HE2	1.69	0.46
1:F:679:LEU:HA	1:F:679:LEU:HD23	1.59	0.46
1:F:687:LEU:C	1:F:687:LEU:HD12	2.40	0.46
1:F:996:LEU:O	1:F:1002:ALA:HB1	2.14	0.46
2:F:1110:LMT:H3'	2:F:1110:LMT:H1B	1.50	0.46
3:B:1111:PTY:HC12	3:B:1111:PTY:H311	1.67	0.46
2:C:1101:LMT:O5'	2:C:1111:LMT:H21	2.16	0.46
1:E:1001:GLY:HA3	2:E:1103:LMT:H3'	1.98	0.46
1:B:469:TYR:CE2	2:B:1108:LMT:H62	2.50	0.46
1:D:825:GLY:N	2:D:1109:LMT:H81	2.31	0.46
1:D:110:GLN:HE22	1:E:111:ASN:HB2	1.80	0.46
1:D:469:TYR:CD1	2:D:1107:LMT:H92	2.51	0.46
1:F:2:ASP:H	1:F:438:ARG:HA	1.79	0.46
1:F:494:LEU:HD21	2:F:1102:LMT:H61	1.96	0.46
1:A:166:ASP:O	1:A:170:ARG:HG3	2.15	0.46
1:D:564:PHE:HE1	2:D:1112:LMT:H12	1.81	0.46
1:B:410:ASP:OD1	1:B:983:THR:HG21	2.15	0.46
1:F:395:THR:O	2:F:1103:LMT:O6'	2.34	0.46
1:A:1008:THR:O	1:A:1012:VAL:HG22	2.16	0.46
1:F:455:PHE:CZ	1:F:938:VAL:HG12	2.50	0.46
1:B:427:LEU:HD22	1:B:431:ALA:HB1	1.98	0.46
2:D:1112:LMT:H52	2:D:1112:LMT:H21	1.70	0.46
1:E:563:MET:HE3	1:E:920:PHE:CA	2.44	0.46
1:E:1005:ARG:HG3	2:E:1103:LMT:H1'	1.98	0.46
1:F:659:LYS:O	1:F:662:GLN:HG3	2.16	0.46
1:C:543:LEU:HD13	1:C:966:MET:SD	2.56	0.45
1:C:565:LYS:HA	1:C:565:LYS:HD2	1.59	0.45
1:A:234:LEU:HD23	1:B:630:PRO:HG3	1.98	0.45
1:A:301:ASN:H	4:A:1114:GOL:H31	1.80	0.45
1:A:402:VAL:CG1	2:A:1111:LMT:H41	2.46	0.45
1:B:548:ALA:O	1:B:552:VAL:HG23	2.15	0.45
1:A:739:LYS:HE2	1:A:739:LYS:HB2	1.74	0.45
1:B:984:SER:HA	1:B:1016:MET:HE2	1.98	0.45
1:C:156:MET:HE1	1:C:288:ASP:O	2.17	0.45
1:C:520:ILE:HG23	1:C:524:PHE:CE2	2.52	0.45
1:E:48[A]:ARG:NH2	5:E:1223:HOH:O	2.46	0.45
1:B:622:ASN:ND2	1:B:723:THR:HG23	2.31	0.45
1:C:125:ARG:NH1	5:C:1229:HOH:O	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:PRO:HD2	2:C:1103:LMT:H6D	1.98	0.45
1:C:836:ASP:O	1:C:840:LEU:HD23	2.16	0.45
1:F:74:VAL:CG2	1:F:77:MET:HE2	2.47	0.45
1:F:579:TYR:HA	1:F:637:PHE:O	2.16	0.45
1:B:417:GLU:CD	1:B:979:PRO:HD3	2.40	0.45
1:C:272:GLU:O	1:C:272:GLU:HG3	2.16	0.45
1:D:468:PHE:CE2	1:D:572:ILE:HD11	2.51	0.45
1:B:399:PHE:CE1	1:B:1008:THR:HG21	2.52	0.45
1:C:179:ILE:O	2:C:1108:LMT:H3B	2.17	0.45
1:D:57:LYS:HE3	1:F:238:ASN:OD1	2.16	0.45
1:D:824:ASN:HA	2:D:1109:LMT:H61	1.98	0.45
1:D:875:GLN:OE1	2:D:1107:LMT:O3'	2.27	0.45
1:E:35:SER:O	1:E:394:ASN:HA	2.17	0.45
1:E:879:ALA:HB1	1:E:883:PHE:CD2	2.52	0.45
1:C:681:GLN:HG3	1:C:684:GLY:N	2.22	0.45
1:D:344:VAL:HG22	2:D:1106:LMT:H71	1.99	0.45
1:D:524:PHE:HA	1:D:527:PHE:HB3	1.99	0.45
1:D:536:GLN:HG2	1:D:970:LEU:HD12	1.99	0.45
1:D:1035:ARG:NH1	5:D:1229:HOH:O	2.50	0.45
1:E:538:LEU:HD23	1:E:538:LEU:HA	1.78	0.45
1:F:6:PHE:CE1	1:F:10:ARG:HD2	2.52	0.45
1:A:883:PHE:HZ	2:A:1108:LMT:H21	1.82	0.45
1:C:719:PHE:HE2	4:C:1118:GOL:H11	1.78	0.45
1:D:911:VAL:HG22	1:D:912:PRO:HD3	1.99	0.45
1:F:399:PHE:O	1:F:402:VAL:HG22	2.17	0.45
1:B:7:PHE:CD2	1:B:489:THR:HG22	2.51	0.45
1:C:403:LEU:HA	1:C:403:LEU:HD23	1.78	0.45
1:F:870:PHE:HZ	2:F:1110:LMT:H4'	1.82	0.45
1:F:987:PHE:N	1:F:987:PHE:CD1	2.83	0.45
1:F:987:PHE:O	1:F:991:THR:HG23	2.17	0.45
1:F:990:GLY:C	1:F:993:PRO:HD2	2.41	0.45
1:A:508:LEU:HD13	1:A:508:LEU:HA	1.84	0.44
1:B:424:GLU:HG2	1:B:502:HIS:NE2	2.31	0.44
1:B:838:ARG:HH11	1:B:838:ARG:HB3	1.81	0.44
2:A:1106:LMT:H2B	5:A:1337:HOH:O	2.17	0.44
1:C:881:ILE:HD12	1:C:881:ILE:N	2.32	0.44
1:F:837:PRO:HA	1:F:840:LEU:O	2.17	0.44
1:F:1008:THR:O	1:F:1012:VAL:HG22	2.17	0.44
1:B:35:SER:O	1:B:394:ASN:HA	2.18	0.44
1:B:351:VAL:HA	1:B:354:VAL:HG12	1.99	0.44
1:D:16:VAL:O	1:D:20:LEU:HG	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:ASN:HD22	1:D:533:ASN:HA	1.65	0.44
1:A:771:ARG:NH1	4:A:1117:GOL:H2	2.32	0.44
1:D:346:THR:HG21	1:D:402:VAL:CG2	2.47	0.44
1:A:115:GLN:NE2	5:A:1201:HOH:O	2.21	0.44
1:A:687:LEU:C	1:A:687:LEU:HD12	2.43	0.44
1:C:454:VAL:HG22	2:C:1101:LMT:H102	2.00	0.44
1:E:340:ILE:HD13	2:E:1107:LMT:H11	1.99	0.44
1:F:578:LEU:HD21	1:F:642:PHE:CE1	2.52	0.44
1:A:677:LEU:HD21	2:A:1104:LMT:H41	2.00	0.44
1:B:195:LYS:NZ	5:B:1227:HOH:O	2.50	0.44
1:B:506:LYS:HD3	1:B:511:ARG:HH21	1.82	0.44
1:A:1037:LEU:HD12	1:A:1037:LEU:O	2.17	0.44
1:D:511:ARG:HA	1:D:514:ASP:OD1	2.18	0.44
1:E:1038:VAL:HG12	3:E:1114:PTY:HC6	1.99	0.44
1:A:911:VAL:HG22	1:A:912:PRO:HD3	1.99	0.44
1:B:703:ALA:CB	1:B:861:MET:HE1	2.47	0.44
1:F:997:GLY:HA3	1:F:998:HIS:HA	1.55	0.44
1:B:343:VAL:HG21	1:B:398:LEU:HD22	1.99	0.44
1:B:740:ALA:HA	1:B:808:MET:HE3	2.00	0.44
1:C:315:GLU:HA	1:E:322:GLU:HG2	2.00	0.44
1:C:518:GLY:HA2	1:C:521:PHE:CD2	2.52	0.44
1:F:373:ILE:HD11	3:F:1114:PTY:H422	2.00	0.44
1:A:940:LEU:HD11	1:A:1012:VAL:HA	1.98	0.43
1:C:677:LEU:HD11	2:C:1107:LMT:H41	1.99	0.43
1:C:915:MET:HB2	1:C:941:MET:HE2	2.00	0.43
1:D:7:PHE:CD2	1:D:489:THR:HG22	2.53	0.43
1:D:12:ILE:HG22	2:D:1101:LMT:O6'	2.18	0.43
1:D:33:PRO:HD3	2:D:1105:LMT:O3B	2.18	0.43
1:D:851:GLU:O	1:D:855:GLN:HG3	2.17	0.43
1:E:48[A]:ARG:CZ	2:E:1105:LMT:H1B	2.47	0.43
1:F:157:ARG:HH22	2:F:1105:LMT:C4B	2.31	0.43
1:F:563:MET:HE2	1:F:916:LEU:HD12	2.00	0.43
1:C:500:LYS:HE2	1:C:500:LYS:HA	2.00	0.43
1:D:323:ASP:HA	5:D:1219:HOH:O	2.18	0.43
1:B:522:ARG:O	1:B:526:ARG:HG2	2.17	0.43
1:B:656:ILE:O	1:B:660:ILE:HG12	2.18	0.43
2:C:1103:LMT:H5B	2:C:1103:LMT:C6'	2.29	0.43
2:C:1107:LMT:O3B	5:C:1201:HOH:O	2.21	0.43
1:E:217:VAL:HG23	1:E:241:GLY:HA3	2.00	0.43
1:F:353:LEU:HD23	1:F:353:LEU:HA	1.91	0.43
1:F:676:ILE:HG23	1:F:679:LEU:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD23	1:A:269:ALA:HB2	1.99	0.43
1:A:505:LYS:HG3	1:A:506:LYS:N	2.24	0.43
1:A:522:ARG:HB3	1:A:526:ARG:NH2	2.33	0.43
1:B:539:VAL:HG13	1:B:543:LEU:HD23	2.00	0.43
1:C:505:LYS:HG3	5:C:1366:HOH:O	2.19	0.43
1:D:330:TYR:HB2	2:D:1103:LMT:H111	2.01	0.43
2:E:1101:LMT:H2'	2:E:1101:LMT:H12	1.84	0.43
1:B:48:ARG:NE	5:B:1202:HOH:O	2.29	0.43
1:C:642:PHE:CD2	1:C:999:GLY:HA2	2.54	0.43
1:D:102:PRO:HB2	1:D:133:LYS:HD2	2.01	0.43
1:D:507:ASP:OD1	1:D:507:ASP:N	2.40	0.43
1:F:242:ARG:NH1	1:F:767:ASN:OD1	2.49	0.43
1:B:74:VAL:HG23	1:B:108:GLN:HB3	1.99	0.43
1:B:312:LYS:HA	1:B:312:LYS:HD3	1.75	0.43
1:C:97:ARG:NH2	2:C:1112:LMT:O4'	2.51	0.43
1:D:357:VAL:HG22	1:D:985:ILE:HD13	2.00	0.43
2:D:1109:LMT:H32	1:F:170:ARG:HG2	2.01	0.43
1:F:933:VAL:HG13	1:F:1011:THR:OG1	2.18	0.43
1:A:565:LYS:HB2	1:A:565:LYS:HE2	1.87	0.43
1:A:572:ILE:HG22	1:A:573:PRO:O	2.18	0.43
1:A:774[A]:ARG:HD2	5:A:1204:HOH:O	2.18	0.43
1:D:545:ARG:HA	1:D:545:ARG:NE	2.33	0.43
2:D:1104:LMT:H31	2:D:1104:LMT:H62	1.75	0.43
2:D:1105:LMT:H101	3:D:1113:PTY:H242	2.01	0.43
1:B:330:TYR:HB2	2:B:1102:LMT:H101	2.00	0.43
1:D:35:SER:O	1:D:394:ASN:HA	2.17	0.43
1:D:513:ILE:HA	1:D:513:ILE:HD13	1.67	0.43
1:E:254:LEU:O	1:E:255:LYS:HB3	2.19	0.43
1:A:16:VAL:HG13	1:B:892:LEU:HB3	1.99	0.43
1:C:967:GLU:CD	1:C:967:GLU:H	2.26	0.43
3:E:1115:PTY:HC12	3:E:1115:PTY:H122	2.00	0.43
1:F:120:LEU:HD13	1:F:129:ILE:HD11	2.01	0.43
1:A:601:LYS:NZ	5:A:1240:HOH:O	2.51	0.43
1:B:554:LEU:HD23	1:B:554:LEU:HA	1.78	0.43
1:C:911:VAL:HG22	1:C:912:PRO:HD3	2.00	0.43
1:D:373:ILE:O	1:D:376:PRO:HD2	2.19	0.43
1:E:107:VAL:O	1:E:110:GLN:HG2	2.18	0.43
1:F:166:ASP:O	1:F:170:ARG:HG3	2.19	0.43
1:F:692:ARG:HG2	1:F:826:TYR:CE1	2.54	0.43
1:C:443:PRO:HG3	1:C:953:GLU:HG2	2.01	0.42
1:D:80:MET:SD	2:D:1109:LMT:H82	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:PRO:O	1:E:781:GLY:HA3	2.20	0.42
2:D:1101:LMT:H6E	1:E:899:GLU:HB3	2.01	0.42
1:E:562:VAL:O	1:E:566:VAL:HG22	2.19	0.42
1:F:157:ARG:NH2	1:F:184:GLU:OE2	2.50	0.42
1:F:946:LYS:HB3	1:F:946:LYS:HE2	1.89	0.42
1:A:324:MET:HE3	1:A:324:MET:HB3	1.92	0.42
1:D:622:ASN:HD21	1:D:723:THR:HG23	1.83	0.42
2:E:1102:LMT:H21	2:E:1113:LMT:H52	2.00	0.42
1:B:638:GLY:CA	2:B:1102:LMT:H123	2.48	0.42
1:D:358:VAL:HG13	1:D:362:LEU:HD23	2.01	0.42
1:D:500:LYS:HA	1:D:500:LYS:CE	2.49	0.42
1:D:501:PRO:O	1:D:503:GLY:N	2.45	0.42
1:D:691:ASP:HA	1:D:861:MET:HG2	2.00	0.42
1:F:557:LEU:HD23	1:F:557:LEU:HA	1.84	0.42
1:B:858:PRO:O	1:B:859:ASN:C	2.62	0.42
1:C:516:LEU:HG	1:C:517:PHE:CD2	2.54	0.42
1:E:536:GLN:OE1	1:E:974:ARG:HD3	2.19	0.42
1:F:929:ASN:HD22	2:F:1109:LMT:C2'	2.30	0.42
1:E:346:THR:HG21	1:E:402:VAL:HG13	2.00	0.42
1:E:375:VAL:HB	1:E:376:PRO:HD3	2.01	0.42
1:A:712:MET:HE3	1:A:719:PHE:HB2	2.02	0.42
1:B:921:GLY:HA3	1:B:1014:SER:OG	2.20	0.42
1:D:225:GLU:HB3	1:D:226:PRO:HA	2.01	0.42
1:D:721:ILE:HD13	1:D:721:ILE:N	2.35	0.42
1:F:920:PHE:CE2	1:F:924:LEU:HD11	2.55	0.42
1:A:303:ILE:HG23	1:A:337:ARG:CZ	2.49	0.42
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.68	0.42
1:A:1006:GLY:O	1:A:1010:ILE:HD12	2.20	0.42
1:C:560:ALA:HA	1:C:916:LEU:HD13	2.01	0.42
1:D:148:ASN:CG	5:D:1219:HOH:O	2.63	0.42
1:D:549:VAL:HG11	1:D:1029:VAL:HG11	2.01	0.42
1:D:720:PRO:C	1:D:721:ILE:HD13	2.44	0.42
1:E:48[A]:ARG:NH1	2:E:1105:LMT:H4'	2.35	0.42
1:E:563:MET:CE	1:E:920:PHE:HA	2.46	0.42
1:F:830:ASP:OD1	1:F:830:ASP:N	2.53	0.42
1:A:837:PRO:HA	1:A:840:LEU:O	2.19	0.42
1:B:387:TYR:CE1	2:B:1101:LMT:H2B	2.54	0.42
1:C:107:VAL:HA	1:C:110:GLN:CG	2.47	0.42
1:D:550:PHE:O	1:D:553:TYR:HB3	2.19	0.42
2:E:1108:LMT:O6B	2:E:1108:LMT:O4'	2.30	0.42
1:F:911:VAL:HG13	1:F:941:MET:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD21	3:B:1112:PTY:H121	2.02	0.42
1:B:1000:ALA:HB1	5:B:1213:HOH:O	2.20	0.42
1:D:447:ILE:HD12	1:D:448:ALA:N	2.35	0.42
1:D:472:PHE:CG	1:D:935:VAL:HG21	2.55	0.42
1:A:170:ARG:NH1	2:A:1110:LMT:H31	2.35	0.41
1:B:454:VAL:HG22	2:B:1107:LMT:H101	2.01	0.41
1:C:334:VAL:HA	1:C:337:ARG:HD2	2.01	0.41
1:C:837:PRO:HA	1:C:840:LEU:O	2.20	0.41
1:D:562:VAL:O	1:D:566:VAL:HG13	2.20	0.41
1:D:991:THR:O	1:D:991:THR:HG22	2.19	0.41
2:D:1103:LMT:H72	2:D:1104:LMT:H92	2.02	0.41
1:E:508:LEU:HB3	1:E:511:ARG:NH2	2.34	0.41
1:F:159:TYR:CE1	1:F:324:MET:HE1	2.55	0.41
1:F:333:THR:OG1	1:F:337:ARG:NH2	2.53	0.41
1:F:622:ASN:ND2	1:F:723:THR:HG23	2.34	0.41
1:B:163:LYS:HE3	5:C:1638:HOH:O	2.20	0.41
1:B:687:LEU:C	1:B:687:LEU:HD12	2.45	0.41
1:B:881:ILE:N	1:B:881:ILE:HD12	2.34	0.41
3:B:1112:PTY:H122	3:B:1112:PTY:H152	1.74	0.41
1:C:35:SER:O	1:C:394:ASN:HA	2.20	0.41
1:D:549:VAL:CG1	1:D:1029:VAL:HG11	2.50	0.41
1:E:938:VAL:HG22	2:E:1109:LMT:H62	2.02	0.41
1:B:373:ILE:O	1:B:376:PRO:HD2	2.20	0.41
1:B:505:LYS:HD3	1:B:506:LYS:N	2.36	0.41
1:B:610:GLU:HA	1:B:610:GLU:OE1	2.21	0.41
1:B:911:VAL:HG12	1:B:941:MET:CE	2.40	0.41
1:C:588:GLU:HB3	1:C:728:VAL:HA	2.02	0.41
4:E:1119:GOL:H2	5:E:1212:HOH:O	2.20	0.41
1:C:868:LEU:O	1:C:872:GLN:HG3	2.20	0.41
1:E:687:LEU:HD12	1:E:687:LEU:C	2.45	0.41
2:A:1110:LMT:H91	1:B:825:GLY:HA3	2.03	0.41
1:B:399:PHE:O	1:B:402:VAL:HG22	2.20	0.41
1:B:406:GLY:HA3	1:B:987:PHE:HZ	1.81	0.41
1:D:626:PHE:CD1	2:D:1103:LMT:H6E	2.55	0.41
1:E:191:LEU:HD23	1:E:269:ALA:HB2	2.01	0.41
1:E:402:VAL:CG1	2:E:1103:LMT:H41	2.50	0.41
1:E:455:PHE:O	1:E:458:MET:HB2	2.21	0.41
1:E:692:ARG:CD	1:E:862:ASN:OD1	2.68	0.41
1:E:717:MET:HE1	1:E:849:LEU:HD21	2.03	0.41
1:E:837:PRO:HA	1:E:840:LEU:O	2.20	0.41
3:E:1114:PTY:H371	3:E:1114:PTY:H342	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:TRP:NE1	1:F:509:PRO:HB2	2.36	0.41
1:F:399:PHE:CZ	1:F:1008:THR:HG21	2.54	0.41
2:F:1103:LMT:H71	2:F:1103:LMT:H101	1.93	0.41
1:A:195:LYS:O	1:A:199:ARG:HG2	2.19	0.41
1:C:343:VAL:HG21	1:C:398:LEU:HD22	2.02	0.41
1:C:584:VAL:HG21	1:C:598:VAL:HG11	2.03	0.41
1:E:110:GLN:CD	1:F:111:ASN:HB2	2.46	0.41
1:F:624:LEU:HD22	1:F:832:ILE:HD12	2.02	0.41
1:A:424:GLU:HG2	1:A:502:HIS:HE1	1.85	0.41
1:C:446:ALA:HB2	2:C:1102:LMT:H31	2.03	0.41
1:D:451:LEU:HB3	1:D:455:PHE:CE2	2.56	0.41
1:F:343:VAL:HG21	1:F:398:LEU:HD22	2.01	0.41
1:F:987:PHE:O	1:F:991:THR:N	2.54	0.41
1:F:993:PRO:O	1:F:994:LEU:HD12	2.21	0.41
2:F:1107:LMT:H11	5:F:1344:HOH:O	2.20	0.41
1:A:610:GLU:HB3	5:A:1231:HOH:O	2.20	0.41
1:B:256:THR:HG22	1:B:262:LEU:HD23	2.03	0.41
1:B:343:VAL:HG22	1:B:402:VAL:CG1	2.51	0.41
1:B:472:PHE:CD2	1:B:935:VAL:HG21	2.54	0.41
1:D:399:PHE:O	1:D:402:VAL:HG12	2.21	0.41
1:D:573:PRO:O	1:D:575:GLN:HG3	2.20	0.41
1:E:992:ILE:N	1:E:993:PRO:HD2	2.36	0.41
1:E:1027:THR:N	1:E:1028:PRO:HD2	2.35	0.41
1:F:375:VAL:HB	1:F:376:PRO:HD3	2.02	0.41
1:F:987:PHE:N	1:F:987:PHE:HD1	2.19	0.41
1:A:177:ILE:HG21	1:A:177:ILE:HD13	1.85	0.41
1:A:796:ARG:HD3	1:A:800:GLY:HA2	2.03	0.41
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.56	0.41
1:B:139:THR:O	1:B:332:PRO:HD2	2.21	0.41
1:B:970:LEU:HD23	1:B:970:LEU:HA	1.92	0.41
1:D:150:LYS:HE3	1:D:150:LYS:HB2	1.70	0.41
1:D:468:PHE:HZ	1:D:676:ILE:CD1	2.33	0.41
1:E:298:PRO:O	4:E:1121:GOL:H11	2.21	0.41
1:E:458:MET:HG3	2:E:1108:LMT:H92	2.03	0.41
1:E:556:LEU:HD13	1:E:913:MET:CE	2.50	0.41
1:F:74:VAL:HG22	1:F:77:MET:CE	2.51	0.41
1:F:147:PRO:HD2	1:F:323:ASP:OD1	2.21	0.41
1:F:461:LEU:HD23	1:F:878:THR:HG23	2.03	0.41
1:F:572:ILE:HD12	1:F:572:ILE:N	2.36	0.41
1:F:735:VAL:HG22	1:F:809:VAL:HG12	2.03	0.41
1:A:433:ALA:O	1:A:437:MET:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ASP:OD1	5:C:1203:HOH:O	2.22	0.41
1:D:725:GLN:O	1:D:817:PRO:HA	2.20	0.41
1:E:994:LEU:HD21	2:E:1103:LMT:H42	2.03	0.41
2:E:1107:LMT:H1'	2:E:1107:LMT:H22	1.89	0.41
1:F:335:PHE:HD1	2:F:1103:LMT:H4B	1.83	0.41
1:A:272:GLU:O	1:A:272:GLU:HG3	2.21	0.40
1:A:513:ILE:O	1:A:517:PHE:N	2.51	0.40
1:B:217:VAL:HG23	1:B:241:GLY:HA3	2.03	0.40
1:B:745:VAL:CG1	1:B:808:MET:HE1	2.51	0.40
2:B:1101:LMT:H3'	2:B:1101:LMT:H1B	1.86	0.40
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.92	0.40
1:C:940:LEU:HD13	1:C:1015:GLY:HA3	2.03	0.40
1:D:626:PHE:CE2	2:D:1104:LMT:H72	2.56	0.40
1:E:935:VAL:CG2	2:E:1108:LMT:H121	2.46	0.40
2:E:1110:LMT:H82	2:E:1110:LMT:H112	1.65	0.40
1:F:455:PHE:O	1:F:473:ALA:HB1	2.22	0.40
1:F:472:PHE:HB3	1:F:935:VAL:HG21	2.01	0.40
1:F:692:ARG:HG2	1:F:826:TYR:CD1	2.55	0.40
1:F:995:ILE:HG13	1:F:996:LEU:H	1.86	0.40
1:B:343:VAL:HG22	1:B:402:VAL:HG13	2.02	0.40
1:B:511:ARG:CZ	1:B:511:ARG:HA	2.51	0.40
1:E:1038:VAL:HA	3:E:1114:PTY:HC51	2.03	0.40
1:F:15:ALA:HB2	2:F:1102:LMT:H31	2.04	0.40
1:B:1041:ARG:HA	1:B:1042:LYS:HA	1.78	0.40
1:D:72:ASN:OD1	2:D:1109:LMT:C7	2.69	0.40
1:D:334:VAL:HA	1:D:337:ARG:HD2	2.03	0.40
1:E:994:LEU:HD21	2:E:1103:LMT:C4	2.50	0.40
1:F:940:LEU:HD13	1:F:1015:GLY:HA3	2.03	0.40
1:B:42:PRO:HA	1:B:43:PRO:HD3	1.94	0.40
1:B:407:ILE:HG23	1:B:946:LYS:HE3	2.03	0.40
1:D:620:GLY:O	1:D:628:ASN:HA	2.20	0.40
1:D:849:LEU:N	1:D:849:LEU:HD23	2.37	0.40
1:E:458:MET:HG3	2:E:1108:LMT:H111	2.02	0.40
1:F:520:ILE:O	1:F:524:PHE:HB2	2.22	0.40
1:F:690:GLN:OE1	1:F:692:ARG:NH2	2.53	0.40
1:A:519:TRP:HA	1:A:522:ARG:NH2	2.36	0.40
1:B:509:PRO:O	1:B:513:ILE:HG12	2.22	0.40
1:B:940:LEU:HD13	1:B:1015:GLY:HA3	2.04	0.40
1:C:497:LEU:HD21	2:C:1104:LMT:H21	2.04	0.40
1:D:390:GLY:O	2:D:1108:LMT:H3B	2.21	0.40
1:D:594:ARG:HD3	1:F:232:ASP:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:995:ILE:HG13	1:D:996:LEU:HG	2.04	0.40
1:E:264:ARG:HH22	1:F:738:ASP:CG	2.29	0.40
1:E:987:PHE:N	1:E:987:PHE:HD1	2.19	0.40
2:E:1105:LMT:H2O1	2:E:1105:LMT:C3'	2.30	0.40
1:F:38:PRO:HG2	1:F:40:VAL:HG13	2.03	0.40
1:F:464:VAL:HG11	1:F:679:LEU:HD11	2.04	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	1042/1042 (100%)	1010 (97%)	28 (3%)	4 (0%)	30	17
1	B	1040/1042 (100%)	1021 (98%)	15 (1%)	4 (0%)	30	17
1	C	1039/1042 (100%)	1020 (98%)	18 (2%)	1 (0%)	48	35
1	D	1038/1042 (100%)	1005 (97%)	27 (3%)	6 (1%)	21	10
1	E	1041/1042 (100%)	1021 (98%)	20 (2%)	0	100	100
1	F	1039/1042 (100%)	1015 (98%)	23 (2%)	1 (0%)	48	35
All	All	6239/6252 (100%)	6092 (98%)	131 (2%)	16 (0%)	36	25

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	683	SER
1	A	506	LYS
1	A	1006	GLY
1	D	502	HIS
1	D	684	GLY
1	A	681	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	681	GLN
1	D	683	SER
1	D	715	PRO
1	C	680	GLY
1	A	505	LYS
1	B	764	ASN
1	B	998	HIS
1	D	505	LYS
1	D	503	GLY
1	F	993	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	853/851 (100%)	843 (99%)	10 (1%)	63	55
1	B	851/851 (100%)	830 (98%)	21 (2%)	42	27
1	C	850/851 (100%)	837 (98%)	13 (2%)	57	47
1	D	849/851 (100%)	824 (97%)	25 (3%)	37	22
1	E	852/851 (100%)	836 (98%)	16 (2%)	50	38
1	F	850/851 (100%)	828 (97%)	22 (3%)	40	25
All	All	5105/5106 (100%)	4998 (98%)	107 (2%)	47	33

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	364	THR
1	A	506	LYS
1	A	508	LEU
1	A	540	SER
1	A	643	ASP
1	A	683	SER
1	A	843	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	996	LEU
1	A	1041	ARG
1	B	20	LEU
1	B	133	LYS
1	B	177	ILE
1	B	351	VAL
1	B	364	THR
1	B	497	LEU
1	B	502	HIS
1	B	508	LEU
1	B	510	THR
1	B	520	ILE
1	B	550	PHE
1	B	646	LYS
1	B	721	ILE
1	B	734	GLN
1	B	831	LEU
1	B	878	THR
1	B	963	LYS
1	B	966	MET
1	B	985	ILE
1	B	1014	SER
1	B	1037	LEU
1	C	129	ILE
1	C	218	SER
1	C	258	GLN
1	C	364	THR
1	C	497	LEU
1	C	500	LYS
1	C	512	LEU
1	C	522	ARG
1	C	558	CYS
1	C	681	GLN
1	C	683	SER
1	C	1014	SER
1	C	1026	LEU
1	D	23	ILE
1	D	74	VAL
1	D	150	LYS
1	D	356	LEU
1	D	507	ASP
1	D	508	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	513	ILE
1	D	526	ARG
1	D	533	ASN
1	D	554	LEU
1	D	635	VAL
1	D	683	SER
1	D	686	SER
1	D	743	GLN
1	D	854	LYS
1	D	910	ILE
1	D	911	VAL
1	D	966	MET
1	D	985	ILE
1	D	987	PHE
1	D	988	ILE
1	D	992	ILE
1	D	995	ILE
1	D	1034	LEU
1	D	1039	THR
1	E	133	LYS
1	E	212	GLU
1	E	229	GLN
1	E	259	ASP
1	E	364	THR
1	E	541	LYS
1	E	555	LEU
1	E	681	GLN
1	E	721	ILE
1	E	805	ILE
1	E	849	LEU
1	E	880	LEU
1	E	943	LEU
1	E	992	ILE
1	E	995	ILE
1	E	1014	SER
1	F	142	VAL
1	F	177	ILE
1	F	216	GLN
1	F	221	GLN
1	F	337	ARG
1	F	348	LEU
1	F	364	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	497	LEU
1	F	505	LYS
1	F	516	LEU
1	F	643	ASP
1	F	677	LEU
1	F	732	ASP
1	F	831	LEU
1	F	840	LEU
1	F	903	LEU
1	F	904	PRO
1	F	981	VAL
1	F	995	ILE
1	F	1010	ILE
1	F	1014	SER
1	F	1036	LYS

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	178	GLN
1	A	363	GLN
1	A	467	GLN
1	A	525	ASN
1	A	575	GLN
1	A	929	ASN
1	B	178	GLN
1	B	307	ASN
1	B	622	ASN
1	B	681	GLN
1	B	810	ASN
1	C	104	GLN
1	C	108	GLN
1	C	111	ASN
1	C	486	ASN
1	C	875	GLN
1	D	486	ASN
1	D	533	ASN
1	D	628	ASN
1	D	767	ASN
1	D	844	GLN
1	D	872	GLN
1	D	961	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	106	GLN
1	E	662	GLN
1	E	681	GLN
1	E	743	GLN
1	E	872	GLN
1	E	961	GLN
1	F	115	GLN
1	F	132	GLN
1	F	134	GLN
1	F	216	GLN
1	F	244	HIS
1	F	533	ASN
1	F	743	GLN
1	F	799	GLN
1	F	859	ASN
1	F	872	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](#)

116 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
3	PTY	A	1112	-	45,45,49	0.93	3 (6%)	48,50,54	1.03	2 (4%)
4	GOL	A	1116	-	5,5,5	1.96	2 (40%)	5,5,5	0.99	0
4	GOL	F	1119	-	5,5,5	1.39	1 (20%)	5,5,5	1.54	1 (20%)
2	LMT	A	1106	-	36,36,36	1.11	4 (11%)	47,47,47	1.37	7 (14%)
4	GOL	E	1119	-	5,5,5	1.23	1 (20%)	5,5,5	1.83	1 (20%)
2	LMT	C	1101	-	36,36,36	1.12	1 (2%)	47,47,47	1.05	3 (6%)
2	LMT	E	1108	-	36,36,36	1.21	6 (16%)	47,47,47	1.09	2 (4%)
2	LMT	E	1110	-	36,36,36	1.00	1 (2%)	47,47,47	0.91	1 (2%)
3	PTY	D	1113	-	47,47,49	0.97	3 (6%)	50,52,54	1.09	2 (4%)
4	GOL	E	1122	-	5,5,5	3.26	3 (60%)	5,5,5	2.09	2 (40%)
4	GOL	C	1115	-	5,5,5	1.54	1 (20%)	5,5,5	1.48	1 (20%)
4	GOL	C	1120	-	5,5,5	0.99	0	5,5,5	0.95	0
3	PTY	E	1114	-	45,45,49	0.95	3 (6%)	48,50,54	1.07	2 (4%)
4	GOL	B	1114	-	5,5,5	0.94	0	5,5,5	1.03	0
2	LMT	D	1106	-	36,36,36	1.03	3 (8%)	47,47,47	1.23	7 (14%)
2	LMT	D	1111	-	36,36,36	1.07	4 (11%)	47,47,47	1.17	4 (8%)
2	LMT	B	1104	-	36,36,36	1.06	1 (2%)	47,47,47	1.18	2 (4%)
2	LMT	A	1103	-	36,36,36	0.99	1 (2%)	47,47,47	1.20	4 (8%)
2	LMT	F	1108	-	12,12,36	0.35	0	11,11,47	0.91	0
2	LMT	D	1108	-	36,36,36	1.05	1 (2%)	47,47,47	0.95	1 (2%)
4	GOL	F	1120	-	5,5,5	0.60	0	5,5,5	1.53	1 (20%)
4	GOL	C	1119	-	5,5,5	1.05	0	5,5,5	1.25	0
2	LMT	C	1105	-	36,36,36	0.91	1 (2%)	47,47,47	1.30	6 (12%)
2	LMT	E	1101	-	36,36,36	1.12	5 (13%)	47,47,47	1.13	4 (8%)
2	LMT	C	1107	-	36,36,36	1.12	3 (8%)	47,47,47	1.22	3 (6%)
2	LMT	B	1102	-	36,36,36	1.17	3 (8%)	47,47,47	1.31	2 (4%)
2	LMT	C	1110	-	36,36,36	1.03	1 (2%)	47,47,47	1.52	9 (19%)
2	LMT	A	1107	-	36,36,36	1.01	2 (5%)	47,47,47	1.12	2 (4%)
2	LMT	D	1110	-	9,9,36	0.41	0	8,8,47	0.83	0
2	LMT	E	1113	-	9,9,36	0.30	0	8,8,47	0.73	0
2	LMT	A	1110	-	25,25,36	1.00	1 (4%)	30,30,47	1.12	2 (6%)
2	LMT	C	1111	-	36,36,36	1.11	2 (5%)	47,47,47	1.08	2 (4%)
2	LMT	F	1102	-	36,36,36	1.04	2 (5%)	47,47,47	1.01	3 (6%)
2	LMT	B	1105	-	36,36,36	1.12	4 (11%)	47,47,47	1.22	4 (8%)
4	GOL	A	1121	-	5,5,5	1.07	0	5,5,5	1.15	1 (20%)
2	LMT	B	1108	-	11,11,36	0.25	0	10,10,47	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMT	B	1107	-	15,15,36	0.47	0	14,14,47	0.71	0
2	LMT	F	1113	-	36,36,36	0.99	3 (8%)	47,47,47	0.97	4 (8%)
4	GOL	A	1113	-	5,5,5	1.34	0	5,5,5	1.74	2 (40%)
2	LMT	E	1112	-	36,36,36	1.04	2 (5%)	47,47,47	1.23	5 (10%)
4	GOL	F	1116	-	5,5,5	1.94	1 (20%)	5,5,5	1.23	0
4	GOL	D	1115	-	5,5,5	1.62	2 (40%)	5,5,5	1.20	0
2	LMT	A	1104	-	36,36,36	1.25	3 (8%)	47,47,47	1.16	2 (4%)
2	LMT	E	1111	-	11,11,36	0.21	0	10,10,47	0.73	0
2	LMT	B	1101	-	36,36,36	1.00	1 (2%)	47,47,47	1.12	5 (10%)
4	GOL	C	1116	-	5,5,5	1.13	0	5,5,5	1.42	1 (20%)
4	GOL	A	1114	-	5,5,5	1.62	1 (20%)	5,5,5	0.86	0
4	GOL	C	1117	-	5,5,5	0.73	0	5,5,5	0.87	0
2	LMT	C	1102	-	36,36,36	1.09	2 (5%)	47,47,47	1.06	3 (6%)
2	LMT	B	1109	-	36,36,36	0.97	1 (2%)	47,47,47	1.06	3 (6%)
2	LMT	D	1103	-	36,36,36	1.17	4 (11%)	47,47,47	1.21	3 (6%)
4	GOL	A	1117	-	5,5,5	0.96	0	5,5,5	1.06	0
2	LMT	A	1102	-	36,36,36	0.93	2 (5%)	47,47,47	1.08	2 (4%)
4	GOL	D	1116	-	5,5,5	1.25	1 (20%)	5,5,5	0.85	0
4	GOL	D	1117	-	5,5,5	1.19	1 (20%)	5,5,5	1.06	0
2	LMT	C	1104	-	36,36,36	1.09	4 (11%)	47,47,47	1.12	2 (4%)
4	GOL	A	1120	-	5,5,5	0.89	0	5,5,5	2.11	3 (60%)
2	LMT	D	1107	-	36,36,36	1.12	3 (8%)	47,47,47	1.27	4 (8%)
2	LMT	B	1110	-	36,36,36	1.11	3 (8%)	47,47,47	1.03	3 (6%)
2	LMT	C	1108	-	36,36,36	1.14	3 (8%)	47,47,47	1.53	6 (12%)
2	LMT	A	1109	-	36,36,36	1.05	2 (5%)	47,47,47	0.83	0
2	LMT	B	1106	-	36,36,36	1.04	2 (5%)	47,47,47	1.07	4 (8%)
2	LMT	A	1105	-	36,36,36	1.16	1 (2%)	47,47,47	1.21	6 (12%)
2	LMT	F	1104	-	36,36,36	1.11	2 (5%)	47,47,47	1.43	6 (12%)
2	LMT	C	1103	-	36,36,36	1.05	2 (5%)	47,47,47	1.23	6 (12%)
2	LMT	F	1106	-	36,36,36	1.04	2 (5%)	47,47,47	1.38	7 (14%)
2	LMT	D	1104	-	36,36,36	1.22	3 (8%)	47,47,47	1.20	6 (12%)
4	GOL	A	1118	-	5,5,5	1.56	1 (20%)	5,5,5	1.30	0
2	LMT	E	1102	-	36,36,36	1.20	3 (8%)	47,47,47	1.26	5 (10%)
4	GOL	B	1115	-	5,5,5	0.91	0	5,5,5	1.74	2 (40%)
2	LMT	E	1105	-	36,36,36	1.00	1 (2%)	47,47,47	1.09	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	E	1116	-	5,5,5	1.71	2 (40%)	5,5,5	1.29	0
4	GOL	E	1117	-	5,5,5	1.19	1 (20%)	5,5,5	0.82	0
2	LMT	E	1103	-	36,36,36	1.09	2 (5%)	47,47,47	1.21	7 (14%)
3	PTY	E	1115	-	47,47,49	0.99	3 (6%)	50,52,54	0.97	2 (4%)
4	GOL	D	1114	-	5,5,5	1.13	1 (20%)	5,5,5	1.45	1 (20%)
4	GOL	A	1119	-	5,5,5	2.03	2 (40%)	5,5,5	1.17	0
2	LMT	F	1112	-	5,5,36	0.26	0	4,4,47	0.72	0
2	LMT	F	1105	-	36,36,36	1.09	3 (8%)	47,47,47	1.24	6 (12%)
2	LMT	E	1104	-	36,36,36	1.09	2 (5%)	47,47,47	1.00	2 (4%)
2	LMT	C	1112	-	36,36,36	1.13	4 (11%)	47,47,47	1.35	6 (12%)
2	LMT	D	1102	-	36,36,36	1.02	3 (8%)	47,47,47	1.10	2 (4%)
3	PTY	F	1115	-	47,47,49	0.98	3 (6%)	50,52,54	1.10	2 (4%)
2	LMT	F	1103	-	36,36,36	1.18	3 (8%)	47,47,47	1.25	7 (14%)
2	LMT	F	1107	-	36,36,36	1.10	1 (2%)	47,47,47	1.08	3 (6%)
2	LMT	C	1109	-	36,36,36	1.06	3 (8%)	47,47,47	1.09	3 (6%)
2	LMT	F	1101	-	36,36,36	1.07	3 (8%)	47,47,47	1.09	2 (4%)
2	LMT	F	1110	-	36,36,36	1.09	2 (5%)	47,47,47	1.35	8 (17%)
2	LMT	D	1112	-	36,36,36	1.10	3 (8%)	47,47,47	1.30	5 (10%)
4	GOL	F	1118	-	5,5,5	1.35	1 (20%)	5,5,5	0.88	0
2	LMT	A	1111	-	36,36,36	1.19	6 (16%)	47,47,47	1.21	6 (12%)
2	LMT	E	1107	-	36,36,36	1.06	1 (2%)	47,47,47	1.09	3 (6%)
2	LMT	D	1109	-	36,36,36	1.07	2 (5%)	47,47,47	1.17	5 (10%)
3	PTY	F	1114	-	36,36,49	0.88	2 (5%)	37,37,54	1.06	2 (5%)
2	LMT	F	1111	-	16,16,36	0.53	0	15,15,47	0.66	0
2	LMT	B	1103	-	36,36,36	0.93	2 (5%)	47,47,47	0.94	0
4	GOL	E	1118	-	5,5,5	1.59	2 (40%)	5,5,5	0.79	0
2	LMT	F	1109	-	36,36,36	1.00	1 (2%)	47,47,47	1.11	3 (6%)
3	PTY	B	1112	-	47,47,49	0.93	3 (6%)	50,52,54	1.06	2 (4%)
2	LMT	A	1101	-	36,36,36	1.16	4 (11%)	47,47,47	1.16	5 (10%)
4	GOL	B	1113	-	5,5,5	1.15	0	5,5,5	0.88	0
4	GOL	A	1115	-	5,5,5	1.73	2 (40%)	5,5,5	0.97	0
2	LMT	A	1108	-	35,35,36	1.11	4 (11%)	46,46,47	1.12	3 (6%)
4	GOL	C	1114	-	5,5,5	1.39	1 (20%)	5,5,5	1.28	0
4	GOL	E	1120	-	5,5,5	0.73	0	5,5,5	1.45	1 (20%)
4	GOL	E	1123	-	5,5,5	1.63	2 (40%)	5,5,5	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	F	1117	-	5,5,5	1.63	2 (40%)	5,5,5	1.80	1 (20%)
2	LMT	E	1106	-	36,36,36	1.10	2 (5%)	47,47,47	1.42	7 (14%)
2	LMT	E	1109	-	36,36,36	1.06	2 (5%)	47,47,47	1.10	4 (8%)
3	PTY	C	1113	-	47,47,49	1.00	4 (8%)	50,52,54	1.16	4 (8%)
3	PTY	B	1111	-	45,45,49	0.96	3 (6%)	48,50,54	0.99	2 (4%)
4	GOL	C	1118	-	5,5,5	2.51	1 (20%)	5,5,5	0.73	0
2	LMT	D	1101	-	36,36,36	1.11	3 (8%)	47,47,47	1.03	2 (4%)
2	LMT	C	1106	-	36,36,36	1.06	2 (5%)	47,47,47	1.07	3 (6%)
4	GOL	E	1121	-	5,5,5	1.67	2 (40%)	5,5,5	1.35	0
2	LMT	D	1105	-	36,36,36	1.14	5 (13%)	47,47,47	1.18	3 (6%)

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
3	PTY	A	1112	-	-	22/49/49/53	-
4	GOL	A	1116	-	-	4/4/4/4	-
4	GOL	F	1119	-	-	4/4/4/4	-
2	LMT	A	1106	-	-	12/21/61/61	0/2/2/2
4	GOL	E	1119	-	-	4/4/4/4	-
2	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	E	1108	-	-	16/21/61/61	0/2/2/2
2	LMT	E	1110	-	-	10/21/61/61	0/2/2/2
3	PTY	D	1113	-	-	23/51/51/53	-
4	GOL	E	1122	-	-	0/4/4/4	-
4	GOL	C	1115	-	-	2/4/4/4	-
4	GOL	C	1120	-	-	2/4/4/4	-
3	PTY	E	1114	-	-	26/49/49/53	-
4	GOL	B	1114	-	-	3/4/4/4	-
2	LMT	D	1106	-	-	10/21/61/61	0/2/2/2
2	LMT	D	1111	-	-	12/21/61/61	0/2/2/2
2	LMT	B	1104	-	-	8/21/61/61	0/2/2/2
2	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
2	LMT	F	1108	-	-	5/10/10/61	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	D	1108	-	-	10/21/61/61	0/2/2/2
4	GOL	F	1120	-	-	1/4/4/4	-
4	GOL	C	1119	-	-	4/4/4/4	-
2	LMT	C	1105	-	-	7/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	4/21/61/61	0/2/2/2
2	LMT	C	1107	-	-	3/21/61/61	0/2/2/2
2	LMT	B	1102	-	-	13/21/61/61	0/2/2/2
2	LMT	C	1110	-	-	9/21/61/61	0/2/2/2
2	LMT	A	1107	-	-	13/21/61/61	0/2/2/2
2	LMT	D	1110	-	-	2/7/7/61	-
2	LMT	E	1113	-	-	2/7/7/61	-
2	LMT	A	1110	-	-	10/17/37/61	0/1/1/2
2	LMT	C	1111	-	-	14/21/61/61	0/2/2/2
2	LMT	F	1102	-	-	6/21/61/61	0/2/2/2
2	LMT	B	1105	-	-	10/21/61/61	0/2/2/2
4	GOL	A	1121	-	-	2/4/4/4	-
2	LMT	B	1108	-	-	3/9/9/61	-
2	LMT	B	1107	-	-	9/13/13/61	-
2	LMT	F	1113	-	-	9/21/61/61	0/2/2/2
4	GOL	A	1113	-	-	4/4/4/4	-
2	LMT	E	1112	-	-	9/21/61/61	0/2/2/2
4	GOL	F	1116	-	-	2/4/4/4	-
4	GOL	D	1115	-	-	4/4/4/4	-
2	LMT	A	1104	-	-	4/21/61/61	0/2/2/2
2	LMT	E	1111	-	-	8/9/9/61	-
2	LMT	B	1101	-	-	11/21/61/61	0/2/2/2
4	GOL	C	1116	-	-	4/4/4/4	-
4	GOL	A	1114	-	-	2/4/4/4	-
4	GOL	C	1117	-	-	1/4/4/4	-
2	LMT	C	1102	-	-	6/21/61/61	0/2/2/2
2	LMT	B	1109	-	-	12/21/61/61	0/2/2/2
2	LMT	D	1103	-	-	6/21/61/61	0/2/2/2
4	GOL	A	1117	-	-	1/4/4/4	-
2	LMT	A	1102	-	-	3/21/61/61	0/2/2/2
4	GOL	D	1116	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	1117	-	-	2/4/4/4	-
2	LMT	C	1104	-	-	7/21/61/61	0/2/2/2
4	GOL	A	1120	-	-	4/4/4/4	-
2	LMT	D	1107	-	-	11/21/61/61	0/2/2/2
2	LMT	B	1110	-	-	8/21/61/61	0/2/2/2
2	LMT	C	1108	-	-	12/21/61/61	0/2/2/2
2	LMT	A	1109	-	-	9/21/61/61	0/2/2/2
2	LMT	B	1106	-	-	10/21/61/61	0/2/2/2
2	LMT	A	1105	-	-	12/21/61/61	0/2/2/2
2	LMT	F	1104	-	-	6/21/61/61	0/2/2/2
2	LMT	C	1103	-	-	11/21/61/61	0/2/2/2
2	LMT	F	1106	-	-	12/21/61/61	0/2/2/2
2	LMT	D	1104	-	-	10/21/61/61	0/2/2/2
4	GOL	A	1118	-	-	2/4/4/4	-
2	LMT	E	1102	-	-	14/21/61/61	0/2/2/2
4	GOL	B	1115	-	-	2/4/4/4	-
2	LMT	E	1105	-	-	13/21/61/61	0/2/2/2
4	GOL	E	1116	-	-	4/4/4/4	-
4	GOL	E	1117	-	-	2/4/4/4	-
2	LMT	E	1103	-	-	7/21/61/61	0/2/2/2
3	PTY	E	1115	-	-	24/51/51/53	-
4	GOL	D	1114	-	-	1/4/4/4	-
4	GOL	A	1119	-	-	1/4/4/4	-
2	LMT	F	1112	-	-	2/3/3/61	-
2	LMT	F	1105	-	-	14/21/61/61	0/2/2/2
2	LMT	E	1104	-	-	7/21/61/61	0/2/2/2
2	LMT	C	1112	-	-	13/21/61/61	0/2/2/2
2	LMT	D	1102	-	-	2/21/61/61	0/2/2/2
3	PTY	F	1115	-	-	21/51/51/53	-
2	LMT	F	1103	-	-	10/21/61/61	0/2/2/2
2	LMT	F	1107	-	-	13/21/61/61	0/2/2/2
2	LMT	C	1109	-	-	7/21/61/61	0/2/2/2
2	LMT	F	1101	-	-	7/21/61/61	0/2/2/2
2	LMT	F	1110	-	-	12/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	D	1112	-	-	12/21/61/61	0/2/2/2
4	GOL	F	1118	-	-	4/4/4/4	-
2	LMT	A	1111	-	-	9/21/61/61	0/2/2/2
2	LMT	E	1107	-	-	8/21/61/61	0/2/2/2
2	LMT	D	1109	-	-	13/21/61/61	0/2/2/2
3	PTY	F	1114	-	-	17/36/36/53	-
2	LMT	F	1111	-	-	8/14/14/61	-
2	LMT	B	1103	-	-	10/21/61/61	0/2/2/2
4	GOL	E	1118	-	-	0/4/4/4	-
2	LMT	F	1109	-	-	8/21/61/61	0/2/2/2
3	PTY	B	1112	-	-	31/51/51/53	-
2	LMT	A	1101	-	-	9/21/61/61	0/2/2/2
4	GOL	B	1113	-	-	1/4/4/4	-
4	GOL	A	1115	-	-	2/4/4/4	-
2	LMT	A	1108	-	-	7/20/60/61	0/2/2/2
4	GOL	C	1114	-	-	1/4/4/4	-
4	GOL	E	1120	-	-	0/4/4/4	-
4	GOL	E	1123	-	-	4/4/4/4	-
4	GOL	F	1117	-	-	1/4/4/4	-
2	LMT	E	1106	-	-	7/21/61/61	0/2/2/2
2	LMT	E	1109	-	-	6/21/61/61	0/2/2/2
3	PTY	C	1113	-	-	23/51/51/53	-
3	PTY	B	1111	-	-	23/49/49/53	-
4	GOL	C	1118	-	-	2/4/4/4	-
2	LMT	D	1101	-	-	13/21/61/61	0/2/2/2
2	LMT	C	1106	-	-	11/21/61/61	0/2/2/2
4	GOL	E	1121	-	-	2/4/4/4	-
2	LMT	D	1105	-	-	11/21/61/61	0/2/2/2

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1118	GOL	O2-C2	-5.26	1.28	1.43
4	E	1122	GOL	O1-C1	4.55	1.61	1.42
4	E	1122	GOL	C1-C2	3.94	1.66	1.51
2	A	1104	LMT	O3'-C3'	-3.93	1.33	1.43
4	E	1122	GOL	C3-C2	3.90	1.66	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1116	GOL	C3-C2	3.52	1.65	1.51
2	D	1102	LMT	O3'-C3'	-3.45	1.34	1.43
4	F	1116	GOL	C1-C2	3.41	1.64	1.51
2	A	1104	LMT	C4B-C3B	3.35	1.61	1.52
2	F	1104	LMT	C4B-C3B	3.31	1.60	1.52
2	A	1105	LMT	O4'-C4B	-3.31	1.34	1.43
2	F	1103	LMT	O2B-C2B	-3.29	1.34	1.43
2	B	1102	LMT	C4B-C3B	3.27	1.60	1.52
2	C	1107	LMT	C4B-C3B	3.26	1.60	1.52
2	A	1106	LMT	O3'-C3'	-3.23	1.34	1.43
3	D	1113	PTY	O7-C8	3.03	1.42	1.34
2	E	1102	LMT	O3'-C3'	-3.03	1.35	1.43
2	D	1103	LMT	C4B-C3B	3.03	1.60	1.52
3	C	1113	PTY	O4-C30	3.00	1.42	1.33
2	C	1101	LMT	O3'-C3'	-2.95	1.35	1.43
2	B	1102	LMT	O3'-C3'	-2.95	1.35	1.43
2	B	1105	LMT	C4B-C3B	2.94	1.60	1.52
4	A	1119	GOL	C3-C2	2.91	1.62	1.51
3	E	1115	PTY	O4-C30	2.90	1.41	1.33
4	A	1119	GOL	C1-C2	2.89	1.62	1.51
2	C	1103	LMT	O3'-C3'	-2.88	1.35	1.43
2	F	1103	LMT	O3'-C3'	-2.85	1.35	1.43
3	D	1113	PTY	O4-C30	2.85	1.41	1.33
2	B	1106	LMT	O3'-C3'	-2.81	1.36	1.43
3	B	1112	PTY	O4-C30	2.79	1.41	1.33
2	C	1107	LMT	C3B-C2B	2.77	1.59	1.52
3	B	1111	PTY	O4-C30	2.76	1.41	1.33
2	E	1105	LMT	O4'-C4B	-2.73	1.36	1.43
2	E	1107	LMT	O3'-C3'	-2.72	1.36	1.43
2	C	1102	LMT	O3'-C3'	-2.71	1.36	1.43
2	A	1104	LMT	O5B-C5B	-2.71	1.37	1.44
3	F	1114	PTY	O7-C8	2.70	1.41	1.33
2	C	1108	LMT	O2'-C2'	-2.66	1.36	1.43
2	D	1104	LMT	O2'-C2'	-2.66	1.36	1.43
2	E	1103	LMT	O3'-C3'	-2.66	1.36	1.43
3	F	1115	PTY	O4-C30	2.63	1.41	1.33
3	F	1114	PTY	O4-C30	2.63	1.41	1.33
3	F	1115	PTY	O7-C8	2.63	1.41	1.34
3	E	1115	PTY	O7-C8	2.63	1.41	1.34
2	A	1111	LMT	O3'-C3'	-2.61	1.36	1.43
2	F	1106	LMT	O3'-C3'	-2.59	1.36	1.43
2	E	1104	LMT	O3'-C3'	-2.59	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O1'-C1'	-2.59	1.35	1.40
2	A	1111	LMT	O2'-C2'	-2.58	1.36	1.43
3	C	1113	PTY	O7-C8	2.57	1.41	1.34
3	E	1114	PTY	O4-C30	2.57	1.40	1.33
2	A	1108	LMT	O3B-C3B	-2.57	1.36	1.43
2	E	1104	LMT	C4B-C3B	2.56	1.59	1.52
4	A	1115	GOL	C3-C2	2.56	1.61	1.51
4	E	1121	GOL	C3-C2	2.55	1.61	1.51
2	A	1101	LMT	O3'-C3'	-2.52	1.36	1.43
2	A	1108	LMT	O2B-C2B	-2.52	1.36	1.43
3	B	1112	PTY	O7-C8	2.52	1.41	1.34
3	C	1113	PTY	O7-C6	-2.51	1.40	1.46
2	D	1101	LMT	O2'-C2'	-2.51	1.36	1.43
3	A	1112	PTY	O7-C8	2.50	1.41	1.34
2	D	1103	LMT	O5B-C5B	-2.49	1.38	1.44
4	A	1114	GOL	O1-C1	2.48	1.52	1.42
2	F	1107	LMT	O3'-C3'	-2.48	1.36	1.43
2	D	1101	LMT	O3B-C3B	-2.47	1.36	1.43
2	F	1101	LMT	O3'-C3'	-2.47	1.36	1.43
2	F	1102	LMT	O3B-C3B	-2.46	1.36	1.43
2	B	1105	LMT	C4B-C5B	2.46	1.58	1.53
2	D	1104	LMT	O3'-C3'	-2.45	1.36	1.43
4	F	1117	GOL	C3-C2	2.44	1.61	1.51
2	D	1107	LMT	O3'-C3'	-2.44	1.36	1.43
3	A	1112	PTY	O4-C30	2.44	1.40	1.33
3	E	1114	PTY	O7-C8	2.43	1.41	1.34
2	A	1111	LMT	C4'-C5'	2.43	1.59	1.52
3	B	1111	PTY	O7-C8	2.43	1.41	1.34
2	A	1110	LMT	O3'-C3'	-2.43	1.36	1.43
4	E	1123	GOL	C1-C2	2.42	1.61	1.51
2	C	1112	LMT	C3'-C2'	2.41	1.58	1.52
3	E	1114	PTY	O7-C6	-2.41	1.40	1.46
2	D	1103	LMT	O3'-C3'	-2.41	1.37	1.43
4	D	1116	GOL	C3-C2	2.40	1.60	1.51
4	A	1118	GOL	C3-C2	2.40	1.60	1.51
2	F	1110	LMT	C1'-C2'	2.39	1.59	1.52
2	F	1110	LMT	C3'-C2'	2.39	1.58	1.52
3	A	1112	PTY	O7-C6	-2.39	1.41	1.46
2	E	1108	LMT	O4'-C4B	-2.38	1.37	1.43
2	F	1105	LMT	O2'-C2'	-2.38	1.37	1.43
4	E	1118	GOL	C1-C2	2.38	1.60	1.51
2	F	1109	LMT	O3'-C3'	-2.38	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1112	LMT	O3'-C3'	-2.37	1.37	1.43
2	D	1105	LMT	O2B-C2B	-2.36	1.37	1.43
2	C	1104	LMT	O3B-C3B	-2.36	1.37	1.43
2	B	1101	LMT	O3'-C3'	-2.35	1.37	1.43
2	E	1101	LMT	O3'-C3'	-2.34	1.37	1.43
2	D	1112	LMT	O3'-C3'	-2.34	1.37	1.43
3	F	1115	PTY	O7-C6	-2.34	1.41	1.46
2	F	1105	LMT	O3'-C3'	-2.34	1.37	1.43
2	E	1101	LMT	O3B-C3B	-2.33	1.37	1.43
2	C	1108	LMT	C4B-C5B	2.33	1.58	1.53
2	B	1105	LMT	O2'-C2'	-2.33	1.37	1.43
2	E	1112	LMT	O3'-C3'	-2.32	1.37	1.43
2	E	1112	LMT	O2'-C2'	-2.32	1.37	1.43
4	A	1116	GOL	O3-C3	2.32	1.52	1.42
2	E	1108	LMT	O2B-C2B	-2.31	1.37	1.43
2	A	1106	LMT	O1B-C4'	-2.31	1.38	1.43
4	E	1119	GOL	O2-C2	2.31	1.50	1.43
2	A	1108	LMT	O3'-C3'	-2.31	1.37	1.43
4	E	1121	GOL	O3-C3	2.31	1.52	1.42
2	E	1108	LMT	O3'-C3'	-2.30	1.37	1.43
2	C	1112	LMT	O2B-C2B	-2.30	1.37	1.43
2	B	1110	LMT	O3B-C3B	-2.30	1.37	1.43
4	E	1116	GOL	C3-C2	2.29	1.60	1.51
2	A	1111	LMT	O3B-C3B	-2.29	1.37	1.43
2	B	1110	LMT	O3'-C3'	-2.27	1.37	1.43
2	E	1106	LMT	O3'-C3'	-2.27	1.37	1.43
2	E	1102	LMT	O1'-C1'	-2.26	1.36	1.40
2	C	1106	LMT	C3B-C2B	2.26	1.58	1.52
2	B	1104	LMT	O4'-C4B	-2.26	1.37	1.43
2	E	1109	LMT	O3'-C3'	-2.25	1.37	1.43
2	D	1109	LMT	O2B-C2B	-2.25	1.37	1.43
3	B	1111	PTY	O7-C6	-2.24	1.41	1.46
4	E	1116	GOL	O1-C1	2.24	1.51	1.42
2	F	1103	LMT	O2'-C2'	-2.24	1.37	1.43
2	E	1103	LMT	C4'-C5'	2.24	1.59	1.52
4	F	1117	GOL	C1-C2	2.23	1.60	1.51
2	C	1105	LMT	O1'-C1'	-2.23	1.36	1.40
2	D	1111	LMT	O3'-C3'	-2.23	1.37	1.43
2	E	1109	LMT	O2'-C2'	-2.23	1.37	1.43
2	E	1101	LMT	O2'-C2'	-2.22	1.37	1.43
2	D	1106	LMT	O3'-C3'	-2.22	1.37	1.43
2	D	1108	LMT	O3'-C3'	-2.22	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1111	LMT	O3B-C3B	-2.21	1.37	1.43
2	D	1102	LMT	O3B-C3B	-2.20	1.37	1.43
4	D	1115	GOL	C1-C2	2.20	1.60	1.51
3	B	1112	PTY	O7-C6	-2.20	1.41	1.46
4	C	1114	GOL	C3-C2	2.19	1.60	1.51
2	C	1109	LMT	C3'-C2'	2.18	1.58	1.52
2	C	1107	LMT	O3'-C3'	-2.18	1.37	1.43
3	E	1115	PTY	O7-C6	-2.18	1.41	1.46
2	A	1108	LMT	O2'-C2'	-2.18	1.37	1.43
2	D	1111	LMT	O2'-C2'	-2.18	1.37	1.43
2	D	1105	LMT	O5'-C5'	-2.18	1.39	1.44
2	A	1109	LMT	O3'-C3'	-2.18	1.37	1.43
2	F	1105	LMT	C4B-C3B	2.17	1.58	1.52
4	D	1114	GOL	C1-C2	2.17	1.60	1.51
2	C	1104	LMT	O3'-C3'	-2.16	1.37	1.43
2	E	1108	LMT	O3B-C3B	-2.16	1.37	1.43
4	E	1123	GOL	O2-C2	-2.15	1.37	1.43
2	A	1103	LMT	O3B-C3B	-2.15	1.37	1.43
2	B	1103	LMT	O1'-C1'	-2.14	1.36	1.40
4	E	1117	GOL	C3-C2	2.14	1.59	1.51
4	A	1115	GOL	O2-C2	-2.14	1.37	1.43
2	C	1109	LMT	O3'-C3'	-2.14	1.37	1.43
2	E	1110	LMT	O3'-C3'	-2.13	1.37	1.43
2	B	1103	LMT	O3'-C3'	-2.13	1.37	1.43
2	B	1102	LMT	C3B-C2B	2.13	1.57	1.52
2	C	1104	LMT	O1'-C1'	-2.13	1.36	1.40
2	C	1111	LMT	O3B-C3B	-2.12	1.37	1.43
2	D	1105	LMT	C4B-C5B	2.12	1.57	1.53
2	E	1101	LMT	O4'-C4B	-2.12	1.37	1.43
2	F	1101	LMT	O4'-C4B	-2.12	1.37	1.43
2	C	1112	LMT	O5'-C5'	-2.12	1.39	1.44
2	B	1109	LMT	O3'-C3'	-2.11	1.37	1.43
2	D	1104	LMT	C4B-C3B	2.11	1.57	1.52
2	D	1105	LMT	O1'-C1'	-2.11	1.36	1.40
2	C	1106	LMT	C4B-C3B	2.11	1.57	1.52
2	F	1102	LMT	O3'-C3'	-2.11	1.37	1.43
4	F	1118	GOL	C1-C2	2.10	1.59	1.51
2	D	1111	LMT	O4'-C4B	-2.10	1.37	1.43
4	C	1115	GOL	C3-C2	2.10	1.59	1.51
2	C	1103	LMT	O4'-C4B	-2.09	1.37	1.43
2	D	1112	LMT	O4'-C4B	-2.09	1.37	1.43
2	B	1105	LMT	O3'-C3'	-2.09	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1104	LMT	O4'-C4B	-2.09	1.37	1.43
2	B	1110	LMT	O2B-C2B	-2.09	1.37	1.43
2	F	1101	LMT	O3B-C3B	-2.08	1.37	1.43
2	B	1106	LMT	O3B-C3B	-2.08	1.37	1.43
2	D	1109	LMT	O3'-C3'	-2.08	1.37	1.43
2	D	1105	LMT	O3B-C3B	-2.08	1.37	1.43
2	A	1101	LMT	O3B-C3B	-2.08	1.37	1.43
2	A	1106	LMT	O4'-C4B	-2.07	1.37	1.43
2	D	1107	LMT	O3B-C3B	-2.07	1.37	1.43
2	C	1110	LMT	O3'-C3'	-2.07	1.37	1.43
2	C	1111	LMT	O3'-C3'	-2.07	1.37	1.43
2	A	1111	LMT	C3B-C2B	2.07	1.57	1.52
2	E	1106	LMT	C1B-C2B	2.07	1.58	1.52
2	F	1104	LMT	C3'-C2'	2.07	1.57	1.52
3	D	1113	PTY	O7-C6	-2.07	1.41	1.46
2	F	1106	LMT	O2'-C2'	-2.06	1.37	1.43
2	A	1107	LMT	O2'-C2'	-2.06	1.37	1.43
2	D	1101	LMT	O3'-C3'	-2.06	1.37	1.43
2	D	1106	LMT	O3B-C3B	-2.05	1.37	1.43
2	E	1108	LMT	O2'-C2'	-2.05	1.37	1.43
2	A	1106	LMT	O2'-C2'	-2.05	1.37	1.43
2	F	1113	LMT	O3B-C3B	-2.05	1.37	1.43
2	D	1112	LMT	O3B-C3B	-2.04	1.37	1.43
2	A	1102	LMT	O1'-C1'	-2.04	1.36	1.40
4	D	1115	GOL	C3-C2	2.04	1.59	1.51
2	D	1106	LMT	C3'-C2'	2.04	1.57	1.52
2	E	1102	LMT	O3B-C3B	-2.04	1.37	1.43
2	F	1113	LMT	O2B-C2B	-2.04	1.37	1.43
4	D	1117	GOL	C1-C2	2.04	1.59	1.51
2	A	1109	LMT	C4B-C3B	2.04	1.57	1.52
2	C	1102	LMT	O2B-C2B	-2.03	1.37	1.43
2	F	1113	LMT	C3'-C2'	2.03	1.57	1.52
2	A	1102	LMT	O3'-C3'	-2.03	1.37	1.43
2	A	1107	LMT	O3'-C3'	-2.03	1.37	1.43
2	A	1101	LMT	C3'-C2'	2.03	1.57	1.52
4	E	1118	GOL	O2-C2	-2.02	1.37	1.43
2	D	1103	LMT	C3B-C2B	2.02	1.57	1.52
2	C	1109	LMT	C3B-C2B	2.02	1.57	1.52
2	C	1108	LMT	C3'-C2'	2.02	1.57	1.52
2	D	1107	LMT	O2B-C2B	-2.01	1.38	1.43
2	E	1108	LMT	O1'-C1'	-2.01	1.36	1.40
2	A	1111	LMT	C1B-C2B	2.01	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1102	LMT	O1'-C1'	-2.01	1.36	1.40
2	A	1101	LMT	O1'-C1'	-2.01	1.36	1.40
3	C	1113	PTY	P1-O14	2.01	1.67	1.59
4	F	1119	GOL	C3-C2	2.00	1.59	1.51

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1108	LMT	O1'-C1'-C2'	5.72	116.96	108.27
2	C	1112	LMT	C1'-O5'-C5'	-4.70	104.55	113.72
3	F	1115	PTY	O7-C8-C11	4.68	121.61	111.48
2	B	1104	LMT	O1'-C1'-C2'	4.44	115.01	108.27
2	B	1102	LMT	O1'-C1'-C2'	4.37	114.91	108.27
2	D	1107	LMT	C3'-C4'-C5'	-4.18	101.67	110.93
2	A	1103	LMT	O1'-C1'-C2'	4.12	114.53	108.27
2	A	1106	LMT	O5B-C5B-C4B	4.09	117.07	109.70
3	D	1113	PTY	O7-C8-C11	3.93	119.98	111.48
2	C	1108	LMT	O5B-C5B-C4B	3.87	116.67	109.70
4	E	1122	GOL	O1-C1-C2	3.84	127.66	110.38
2	D	1112	LMT	O1'-C1'-C2'	3.83	114.09	108.27
3	C	1113	PTY	O7-C8-C11	3.82	119.75	111.48
3	E	1114	PTY	O7-C8-C11	3.78	119.66	111.48
2	B	1102	LMT	C4B-C3B-C2B	3.76	117.42	110.83
2	C	1107	LMT	C4B-C3B-C2B	3.72	117.36	110.83
3	E	1115	PTY	O7-C8-C11	3.71	119.51	111.48
2	D	1105	LMT	C1'-O5'-C5'	-3.69	106.51	113.72
2	C	1105	LMT	C1-O1'-C1'	-3.69	107.38	113.68
3	B	1111	PTY	O7-C8-C11	3.65	119.39	111.48
2	C	1103	LMT	O5B-C5B-C4B	3.65	116.28	109.70
2	F	1110	LMT	C1'-C2'-C3'	3.63	117.65	110.01
2	D	1103	LMT	C4B-C3B-C2B	3.63	117.21	110.83
2	D	1112	LMT	C1'-O5'-C5'	-3.61	106.67	113.72
3	B	1112	PTY	O7-C8-C11	3.54	119.13	111.48
2	C	1112	LMT	C2'-C3'-C4'	3.52	117.66	109.68
2	E	1106	LMT	C3'-C4'-C5'	-3.51	103.14	110.93
2	C	1110	LMT	O5B-C5B-C4B	3.51	116.02	109.70
2	C	1110	LMT	O1'-C1'-C2'	3.42	113.47	108.27
2	B	1105	LMT	O3B-C3B-C4B	3.41	118.41	110.38
2	E	1112	LMT	O5B-C5B-C6B	3.39	114.83	106.44
2	C	1108	LMT	C1B-O5B-C5B	3.34	120.25	113.72
3	A	1112	PTY	O7-C8-C11	3.31	118.63	111.48
2	A	1108	LMT	O5B-C5B-C4B	3.30	115.65	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1107	LMT	O5'-C1'-C2'	3.30	117.15	110.37
2	F	1106	LMT	C1'-O5'-C5'	-3.28	107.32	113.72
2	D	1111	LMT	O1B-C4'-C3'	3.27	115.55	107.23
2	C	1111	LMT	C1'-O5'-C5'	-3.27	107.33	113.72
2	E	1102	LMT	O1B-C4'-C3'	3.24	115.47	107.23
2	F	1104	LMT	C4B-C3B-C2B	3.23	116.50	110.83
2	C	1106	LMT	C4B-C3B-C2B	3.22	116.49	110.83
2	E	1106	LMT	O5B-C1B-C2B	3.22	116.98	110.37
2	C	1105	LMT	O1'-C1'-C2'	3.21	113.15	108.27
2	E	1112	LMT	O5B-C1B-C2B	3.20	116.95	110.37
2	F	1104	LMT	O1'-C1'-C2'	3.20	113.13	108.27
2	D	1109	LMT	O5'-C5'-C4'	3.19	116.32	109.72
2	E	1109	LMT	C3'-C4'-C5'	-3.16	103.93	110.93
2	F	1106	LMT	C3B-C4B-C5B	-3.16	104.51	110.23
2	C	1107	LMT	O1'-C1'-C2'	3.14	113.05	108.27
2	A	1106	LMT	C1'-C2'-C3'	-3.14	103.41	110.01
2	E	1109	LMT	C1'-O5'-C5'	-3.08	107.71	113.72
2	E	1106	LMT	C3B-C4B-C5B	-3.05	104.71	110.23
2	C	1110	LMT	C1'-O5'-C5'	-3.04	107.78	113.72
2	A	1104	LMT	O1'-C1'-C2'	3.00	112.83	108.27
2	C	1110	LMT	C1'-C2'-C3'	-3.00	103.71	110.01
4	C	1115	GOL	C3-C2-C1	-2.99	100.81	111.80
2	A	1111	LMT	O4'-C4B-C5B	2.98	116.65	109.32
2	F	1104	LMT	C6B-C5B-C4B	-2.98	105.71	113.02
2	F	1103	LMT	O1B-C1B-C2B	2.97	115.39	108.09
2	D	1111	LMT	C3'-C4'-C5'	-2.96	104.37	110.93
2	D	1105	LMT	O5B-C5B-C4B	2.95	115.02	109.70
2	F	1107	LMT	O1'-C1'-C2'	2.95	112.75	108.27
2	A	1111	LMT	C3B-C4B-C5B	-2.91	104.96	110.23
4	F	1120	GOL	C3-C2-C1	-2.90	101.17	111.80
2	D	1106	LMT	C3B-C4B-C5B	-2.88	105.01	110.23
3	E	1114	PTY	O4-C30-C31	2.85	120.54	111.83
2	D	1101	LMT	O5B-C5B-C4B	2.84	114.82	109.70
4	E	1119	GOL	O2-C2-C3	2.84	120.95	109.18
2	F	1105	LMT	O5B-C5B-C4B	2.84	114.82	109.70
2	E	1103	LMT	O5'-C5'-C4'	2.84	115.59	109.72
2	D	1109	LMT	O5'-C1'-C2'	-2.84	104.55	110.37
2	D	1104	LMT	C3'-C4'-C5'	-2.83	104.65	110.93
2	C	1105	LMT	O5'-C1'-O1'	-2.82	103.37	110.04
2	F	1106	LMT	O1'-C1'-C2'	2.82	112.55	108.27
4	A	1113	GOL	O2-C2-C3	2.81	120.82	109.18
4	A	1120	GOL	O2-C2-C1	2.81	120.81	109.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1106	LMT	C1-O1'-C1'	2.81	118.47	113.68
2	B	1104	LMT	C1'-O5'-C5'	-2.80	108.25	113.72
2	E	1105	LMT	C1-O1'-C1'	2.80	118.46	113.68
2	E	1102	LMT	C3'-C4'-C5'	-2.78	104.76	110.93
3	E	1115	PTY	O4-C30-C31	2.78	120.32	111.83
2	A	1107	LMT	O5B-C5B-C4B	2.78	114.71	109.70
3	F	1114	PTY	O7-C8-C11	2.76	120.26	111.83
2	E	1107	LMT	C3'-C4'-C5'	-2.75	104.83	110.93
2	A	1103	LMT	O5B-C5B-C4B	2.75	114.65	109.70
3	F	1114	PTY	O4-C30-C31	2.74	120.20	111.83
2	A	1106	LMT	C1B-O5B-C5B	2.74	119.07	113.72
2	E	1107	LMT	O1'-C1'-C2'	2.74	112.43	108.27
2	F	1106	LMT	O5B-C1B-C2B	2.72	115.96	110.37
2	E	1109	LMT	O1'-C1'-C2'	2.72	112.41	108.27
2	E	1112	LMT	C3'-C4'-C5'	-2.72	104.90	110.93
2	E	1106	LMT	O1B-C4'-C5'	2.72	116.60	109.48
2	F	1110	LMT	O5'-C1'-C2'	2.71	115.95	110.37
2	F	1110	LMT	C3'-C4'-C5'	-2.71	104.92	110.93
2	E	1107	LMT	O5B-C5B-C4B	2.71	114.58	109.70
3	B	1112	PTY	O4-C30-C31	2.70	120.08	111.83
3	C	1113	PTY	O4-C30-C31	2.70	120.07	111.83
2	A	1108	LMT	C1'-O5'-C5'	-2.69	108.47	113.72
2	B	1101	LMT	O1B-C4'-C3'	2.69	114.06	107.23
3	A	1112	PTY	O4-C30-C31	2.68	120.02	111.83
2	F	1110	LMT	O5B-C1B-C2B	2.67	115.86	110.37
2	D	1103	LMT	O1'-C1'-C2'	2.67	112.33	108.27
2	F	1101	LMT	O5B-C5B-C4B	2.67	114.51	109.70
3	D	1113	PTY	O4-C30-C31	2.66	119.95	111.83
4	F	1117	GOL	O2-C2-C1	2.65	120.15	109.18
2	C	1104	LMT	O1'-C1'-C2'	2.65	112.29	108.27
2	E	1108	LMT	C3B-C4B-C5B	-2.62	105.49	110.23
2	F	1105	LMT	C4B-C3B-C2B	2.61	115.41	110.83
2	D	1106	LMT	C1'-C2'-C3'	-2.60	104.54	110.01
4	F	1119	GOL	C3-C2-C1	-2.60	102.27	111.80
2	E	1103	LMT	O1'-C1'-C2'	2.60	112.21	108.27
2	A	1101	LMT	C1'-C2'-C3'	2.59	115.47	110.01
2	C	1102	LMT	C4B-C3B-C2B	2.59	115.38	110.83
2	D	1106	LMT	O1'-C1'-C2'	2.59	112.20	108.27
2	C	1108	LMT	O5B-C1B-C2B	2.59	115.68	110.37
2	A	1102	LMT	O5B-C5B-C6B	2.58	112.84	106.44
2	A	1111	LMT	O1'-C1'-C2'	2.58	112.19	108.27
2	A	1107	LMT	C3'-C4'-C5'	-2.58	105.21	110.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1109	LMT	O1'-C1'-C2'	2.58	112.19	108.27
4	A	1120	GOL	O2-C2-C3	2.58	119.86	109.18
2	A	1101	LMT	C3'-C4'-C5'	-2.55	105.27	110.93
2	B	1105	LMT	O5B-C5B-C4B	2.55	114.29	109.70
2	C	1110	LMT	C1B-O5B-C5B	2.54	118.69	113.72
2	D	1105	LMT	O1'-C1'-C2'	2.54	112.13	108.27
2	D	1104	LMT	O5B-C5B-C6B	2.53	112.72	106.44
2	C	1112	LMT	O5B-C5B-C4B	2.53	114.26	109.70
2	B	1110	LMT	O1'-C1'-C2'	2.53	112.11	108.27
2	D	1111	LMT	O5B-C5B-C4B	2.50	114.20	109.70
2	D	1109	LMT	O1'-C1'-C2'	2.50	112.07	108.27
3	C	1113	PTY	O4-C1-C6	2.50	115.60	108.40
2	D	1106	LMT	O5'-C5'-C6'	2.49	112.62	106.44
2	F	1104	LMT	O3B-C3B-C2B	-2.49	104.50	110.38
2	B	1106	LMT	O5'-C1'-O1'	-2.49	104.17	110.04
2	A	1105	LMT	O1B-C1B-C2B	2.48	114.20	108.09
2	F	1109	LMT	C3'-C4'-C5'	-2.47	105.44	110.93
2	B	1101	LMT	C1-O1'-C1'	2.47	117.91	113.68
2	C	1105	LMT	C1B-O5B-C5B	2.47	118.55	113.72
2	B	1105	LMT	O5'-C5'-C6'	2.47	112.56	106.44
2	E	1105	LMT	O5B-C5B-C6B	2.46	112.53	106.44
2	B	1101	LMT	O5B-C5B-C4B	2.46	114.13	109.70
2	B	1109	LMT	C1'-O5'-C5'	-2.46	108.92	113.72
2	F	1107	LMT	C1'-O5'-C5'	-2.46	108.92	113.72
2	C	1109	LMT	C1'-O5'-C5'	-2.45	108.93	113.72
2	F	1107	LMT	C3'-C4'-C5'	-2.45	105.51	110.93
3	F	1115	PTY	O4-C30-C31	2.44	119.28	111.83
2	F	1109	LMT	C3B-C4B-C5B	-2.44	105.81	110.23
2	E	1102	LMT	C1'-O5'-C5'	-2.44	108.96	113.72
2	E	1112	LMT	C1B-O5B-C5B	2.44	118.48	113.72
2	A	1110	LMT	O1'-C1'-C2'	2.44	111.97	108.27
2	F	1113	LMT	O5B-C5B-C6B	2.43	112.47	106.44
2	F	1110	LMT	C1-O1'-C1'	2.43	117.83	113.68
2	F	1102	LMT	C1-O1'-C1'	2.42	117.82	113.68
2	E	1103	LMT	O1B-C1B-C2B	2.42	114.04	108.09
2	D	1101	LMT	O5B-C5B-C6B	2.41	112.42	106.44
2	D	1112	LMT	C1-O1'-C1'	2.41	117.79	113.68
4	B	1115	GOL	O1-C1-C2	-2.40	99.57	110.38
2	E	1101	LMT	O5B-C5B-C4B	2.40	114.02	109.70
2	F	1106	LMT	C1B-C2B-C3B	2.40	115.06	110.01
2	F	1103	LMT	O5B-C5B-C4B	2.40	114.02	109.70
2	C	1108	LMT	O5'-C1'-O1'	-2.39	104.39	110.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1108	LMT	O3B-C3B-C4B	2.39	116.01	110.38
2	E	1109	LMT	O5B-C5B-C6B	2.39	112.36	106.44
2	B	1101	LMT	O1'-C1'-C2'	2.38	111.88	108.27
2	D	1109	LMT	O5B-C5B-C4B	2.38	113.98	109.70
2	F	1105	LMT	O5B-C5B-C6B	2.35	112.27	106.44
2	F	1105	LMT	C6B-C5B-C4B	-2.35	107.26	113.02
2	D	1112	LMT	O5B-C5B-C4B	2.35	113.93	109.70
2	B	1106	LMT	C3'-C4'-C5'	-2.34	105.74	110.93
2	A	1104	LMT	O5B-C5B-C4B	2.34	113.92	109.70
2	F	1103	LMT	C2'-C3'-C4'	2.34	114.99	109.68
2	E	1101	LMT	O5B-C5B-C6B	2.34	112.23	106.44
2	C	1110	LMT	O5'-C5'-C6'	2.33	112.22	106.44
4	D	1114	GOL	C3-C2-C1	-2.33	103.25	111.80
2	C	1106	LMT	O5'-C1'-O1'	-2.32	104.55	110.04
2	E	1101	LMT	O1'-C1'-C2'	2.32	111.80	108.27
2	B	1105	LMT	C3'-C4'-C5'	-2.32	105.80	110.93
2	F	1103	LMT	O5'-C1'-C2'	-2.31	105.63	110.37
2	A	1105	LMT	C1-O1'-C1'	2.30	117.61	113.68
2	E	1103	LMT	O5B-C5B-C4B	2.30	113.85	109.70
2	F	1102	LMT	C3'-C4'-C5'	-2.30	105.83	110.93
2	D	1112	LMT	C3'-C4'-C5'	-2.29	105.86	110.93
2	C	1103	LMT	C1-O1'-C1'	2.29	117.58	113.68
2	C	1103	LMT	O1'-C1'-C2'	2.28	111.74	108.27
2	D	1104	LMT	O6'-C6'-C5'	-2.28	103.56	111.33
2	A	1111	LMT	C3'-C4'-C5'	-2.27	105.89	110.93
2	A	1105	LMT	C1B-O5B-C5B	-2.27	109.28	113.72
2	C	1110	LMT	O5B-C5B-C6B	2.27	112.07	106.44
2	F	1106	LMT	C1-O1'-C1'	2.27	117.56	113.68
2	E	1103	LMT	O4'-C4B-C5B	2.26	114.89	109.32
2	F	1109	LMT	C1-O1'-C1'	2.26	117.54	113.68
2	F	1104	LMT	C1B-C2B-C3B	2.26	114.77	110.01
2	D	1102	LMT	O6'-C6'-C5'	-2.26	103.64	111.33
2	F	1102	LMT	O1'-C1-C2	-2.26	101.71	109.37
2	E	1106	LMT	O5B-C5B-C6B	2.25	112.02	106.44
2	B	1109	LMT	C3'-C4'-C5'	-2.25	105.94	110.93
2	A	1105	LMT	O5B-C5B-C6B	2.25	112.01	106.44
3	B	1111	PTY	O4-C30-C31	2.25	118.68	111.83
2	C	1103	LMT	O1B-C1B-C2B	2.24	113.61	108.09
2	B	1101	LMT	C3'-C4'-C5'	-2.24	105.97	110.93
2	D	1106	LMT	O5B-C5B-C6B	2.24	111.99	106.44
2	F	1103	LMT	O5B-C5B-C6B	2.24	111.98	106.44
2	E	1110	LMT	C4B-C3B-C2B	2.23	114.75	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1121	GOL	C3-C2-C1	-2.23	103.61	111.80
2	C	1103	LMT	O5B-C5B-C6B	2.23	111.97	106.44
2	F	1110	LMT	C1B-C2B-C3B	2.23	114.70	110.01
4	A	1113	GOL	O2-C2-C1	2.23	118.39	109.18
2	E	1106	LMT	C6'-C5'-C4'	2.22	119.64	113.38
4	E	1120	GOL	O1-C1-C2	-2.22	100.37	110.38
2	A	1111	LMT	O5'-C5'-C4'	2.22	114.32	109.72
2	A	1106	LMT	O1B-C4'-C3'	-2.22	101.59	107.23
2	A	1101	LMT	O5'-C1'-C2'	2.21	114.91	110.37
2	C	1101	LMT	C3'-C4'-C5'	-2.21	106.04	110.93
2	C	1109	LMT	O5B-C5B-C4B	2.20	113.66	109.70
2	E	1103	LMT	C1B-O5B-C5B	2.20	118.01	113.72
2	E	1102	LMT	C4B-C3B-C2B	2.20	114.68	110.83
2	B	1109	LMT	O5B-C5B-C4B	2.19	113.65	109.70
2	D	1109	LMT	C2'-C3'-C4'	2.19	114.66	109.68
2	D	1104	LMT	O5B-C5B-C4B	2.19	113.64	109.70
2	E	1105	LMT	O1B-C1B-C2B	2.18	113.45	108.09
2	D	1102	LMT	C1B-O5B-C5B	2.18	117.98	113.72
2	C	1111	LMT	C3B-C4B-C5B	-2.18	106.29	110.23
2	A	1101	LMT	C2'-C3'-C4'	2.17	114.61	109.68
2	A	1106	LMT	O5B-C1B-C2B	2.17	114.83	110.37
2	A	1110	LMT	O5'-C1'-O1'	-2.17	104.92	110.04
2	E	1101	LMT	C1'-O5'-C5'	-2.17	109.49	113.72
2	D	1106	LMT	C1'-O5'-C5'	-2.16	109.50	113.72
2	A	1103	LMT	C1'-O5'-C5'	-2.16	109.51	113.72
2	A	1105	LMT	O5'-C1'-O1'	-2.16	104.95	110.04
2	B	1110	LMT	O5'-C5'-C4'	2.15	114.18	109.72
2	E	1104	LMT	O1'-C1'-C2'	2.15	111.54	108.27
2	C	1110	LMT	O1'-C1-C2	-2.15	102.07	109.37
2	E	1106	LMT	C1B-O1B-C4'	2.15	123.07	117.98
2	C	1112	LMT	O1B-C4'-C5'	-2.15	103.85	109.48
2	C	1101	LMT	O5'-C5'-C6'	2.14	111.75	106.44
2	C	1102	LMT	C1B-C2B-C3B	2.13	114.49	110.01
2	C	1107	LMT	C6B-C5B-C4B	-2.13	107.79	113.02
2	A	1108	LMT	O5'-C5'-C6'	2.13	111.72	106.44
2	C	1104	LMT	C1'-O5'-C5'	-2.13	109.56	113.72
2	A	1106	LMT	O5B-C5B-C6B	2.13	111.71	106.44
2	F	1113	LMT	O5'-C5'-C4'	2.12	114.12	109.72
4	B	1115	GOL	O2-C2-C3	2.12	117.97	109.18
2	F	1101	LMT	O1'-C1'-C2'	2.12	111.49	108.27
2	C	1112	LMT	O1'-C1'-C2'	2.12	111.49	108.27
4	A	1120	GOL	C3-C2-C1	-2.11	104.05	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1103	LMT	O1'-C1'-C2'	2.11	111.48	108.27
2	E	1108	LMT	C1'-O5'-C5'	-2.11	109.61	113.72
2	F	1103	LMT	C1'-O5'-C5'	-2.10	109.62	113.72
2	C	1102	LMT	C3'-C4'-C5'	-2.10	106.28	110.93
2	C	1103	LMT	O3B-C3B-C4B	2.09	115.31	110.38
2	B	1106	LMT	C3B-C4B-C5B	-2.09	106.44	110.23
2	A	1101	LMT	C3B-C4B-C5B	-2.09	106.44	110.23
2	F	1113	LMT	O5B-C5B-C4B	2.09	113.47	109.70
2	D	1107	LMT	C1'-C2'-C3'	2.09	114.41	110.01
4	C	1116	GOL	O2-C2-C3	2.09	117.83	109.18
2	E	1103	LMT	C3B-C4B-C5B	-2.09	106.44	110.23
4	E	1122	GOL	O2-C2-C1	2.08	117.80	109.18
2	F	1105	LMT	C1'-O5'-C5'	-2.08	109.66	113.72
3	C	1113	PTY	C33-C32-C31	-2.07	105.51	113.13
2	D	1107	LMT	C3B-C4B-C5B	-2.07	106.48	110.23
2	A	1103	LMT	C1-O1'-C1'	2.07	117.22	113.68
2	C	1105	LMT	C3B-C4B-C5B	-2.07	106.48	110.23
2	C	1110	LMT	C4-C3-C2	-2.06	103.94	114.37
2	D	1104	LMT	C1'-O5'-C5'	-2.05	109.72	113.72
2	D	1108	LMT	O5B-C5B-C6B	2.05	111.51	106.44
2	C	1112	LMT	O5B-C5B-C6B	2.04	111.51	106.44
2	A	1106	LMT	O1B-C4'-C5'	-2.04	104.12	109.48
2	E	1104	LMT	O5B-C5B-C4B	2.04	113.38	109.70
2	F	1106	LMT	C2'-C3'-C4'	2.04	114.31	109.68
2	F	1105	LMT	C1-O1'-C1'	2.04	117.17	113.68
2	C	1105	LMT	O4'-C4B-C5B	2.04	114.34	109.32
2	F	1104	LMT	C1B-O1B-C4'	-2.03	113.16	117.98
2	F	1110	LMT	O1'-C1'-C2'	2.03	111.36	108.27
2	B	1110	LMT	C3B-C4B-C5B	-2.03	106.55	110.23
2	A	1105	LMT	O1'-C1'-C2'	2.03	111.35	108.27
2	E	1102	LMT	O5B-C5B-C6B	2.02	111.45	106.44
2	D	1104	LMT	O5'-C1'-O1'	-2.02	105.27	110.04
2	F	1113	LMT	O2B-C2B-C1B	-2.01	105.28	110.08
2	C	1106	LMT	O5B-C5B-C6B	2.01	111.43	106.44
2	A	1111	LMT	O1B-C1B-C2B	2.01	113.04	108.09
2	F	1110	LMT	O5'-C1'-O1'	-2.01	105.29	110.04
2	C	1101	LMT	C4B-C3B-C2B	2.01	114.36	110.83
2	D	1106	LMT	O5B-C1B-C2B	2.01	114.50	110.37
2	E	1112	LMT	C1B-C2B-C3B	2.01	114.23	110.01
2	D	1111	LMT	O5B-C5B-C6B	2.00	111.40	106.44
2	A	1102	LMT	C6B-C5B-C4B	-2.00	108.10	113.02
2	D	1103	LMT	C1B-C2B-C3B	2.00	114.22	110.01

There are no chirality outliers.

All (932) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	LMT	O5'-C1'-O1'-C1
2	A	1106	LMT	C2'-C1'-O1'-C1
2	A	1106	LMT	C2-C1-O1'-C1'
2	A	1108	LMT	C2-C1-O1'-C1'
2	A	1110	LMT	O5'-C1'-O1'-C1
2	B	1101	LMT	C2'-C1'-O1'-C1
2	B	1105	LMT	C2-C1-O1'-C1'
2	B	1106	LMT	C2'-C1'-O1'-C1
2	B	1106	LMT	O5'-C1'-O1'-C1
2	B	1106	LMT	C2-C1-O1'-C1'
2	B	1110	LMT	C2-C1-O1'-C1'
2	C	1101	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	O5'-C1'-O1'-C1
2	C	1103	LMT	O5'-C1'-O1'-C1
2	C	1104	LMT	C2'-C1'-O1'-C1
2	C	1104	LMT	O5'-C1'-O1'-C1
2	C	1111	LMT	C2'-C1'-O1'-C1
2	C	1111	LMT	O5'-C1'-O1'-C1
2	D	1103	LMT	C2'-C1'-O1'-C1
2	D	1104	LMT	C2-C1-O1'-C1'
2	D	1105	LMT	C2-C1-O1'-C1'
2	D	1108	LMT	C2'-C1'-O1'-C1
2	D	1112	LMT	C2-C1-O1'-C1'
2	E	1103	LMT	C2-C1-O1'-C1'
2	E	1106	LMT	O5'-C1'-O1'-C1
2	E	1108	LMT	O5'-C1'-O1'-C1
2	E	1108	LMT	C2-C1-O1'-C1'
2	E	1112	LMT	O5'-C1'-O1'-C1
2	F	1106	LMT	O5'-C1'-O1'-C1
2	F	1109	LMT	O5'-C1'-O1'-C1
2	F	1110	LMT	O5'-C1'-O1'-C1
3	A	1112	PTY	C3-O11-P1-O12
3	A	1112	PTY	C3-O11-P1-O13
3	A	1112	PTY	C3-O11-P1-O14
3	A	1112	PTY	C5-O14-P1-O11
3	A	1112	PTY	C5-O14-P1-O12
3	B	1111	PTY	C31-C30-O4-C1
3	B	1111	PTY	O30-C30-O4-C1
3	B	1111	PTY	C6-C5-O14-P1
3	B	1111	PTY	O10-C8-O7-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1111	PTY	C11-C8-O7-C6
3	B	1111	PTY	C3-O11-P1-O13
3	B	1111	PTY	C3-O11-P1-O14
3	B	1111	PTY	C5-O14-P1-O11
3	B	1111	PTY	C5-O14-P1-O12
3	B	1111	PTY	C5-O14-P1-O13
3	B	1112	PTY	N1-C2-C3-O11
3	B	1112	PTY	C6-C5-O14-P1
3	B	1112	PTY	C11-C8-O7-C6
3	B	1112	PTY	C3-O11-P1-O12
3	B	1112	PTY	C3-O11-P1-O13
3	B	1112	PTY	C3-O11-P1-O14
3	B	1112	PTY	C5-O14-P1-O11
3	C	1113	PTY	C11-C8-O7-C6
3	C	1113	PTY	C3-O11-P1-O12
3	C	1113	PTY	C3-O11-P1-O13
3	C	1113	PTY	C3-O11-P1-O14
3	C	1113	PTY	C5-O14-P1-O11
3	C	1113	PTY	C5-O14-P1-O12
3	C	1113	PTY	C5-O14-P1-O13
3	D	1113	PTY	O10-C8-O7-C6
3	D	1113	PTY	C11-C8-O7-C6
3	D	1113	PTY	C3-O11-P1-O12
3	D	1113	PTY	C3-O11-P1-O13
3	D	1113	PTY	C3-O11-P1-O14
3	D	1113	PTY	C5-O14-P1-O11
3	D	1113	PTY	C5-O14-P1-O12
3	D	1113	PTY	C5-O14-P1-O13
3	E	1114	PTY	C31-C30-O4-C1
3	E	1114	PTY	O30-C30-O4-C1
3	E	1114	PTY	O14-C5-C6-O7
3	E	1114	PTY	C11-C8-O7-C6
3	E	1114	PTY	C3-O11-P1-O12
3	E	1114	PTY	C3-O11-P1-O13
3	E	1114	PTY	C3-O11-P1-O14
3	E	1115	PTY	N1-C2-C3-O11
3	E	1115	PTY	C2-C3-O11-P1
3	E	1115	PTY	C11-C8-O7-C6
3	E	1115	PTY	C3-O11-P1-O13
3	E	1115	PTY	C3-O11-P1-O14
3	E	1115	PTY	C5-O14-P1-O11
3	E	1115	PTY	C5-O14-P1-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	1114	PTY	C31-C30-O4-C1
3	F	1114	PTY	C1-C6-O7-C8
3	F	1115	PTY	N1-C2-C3-O11
3	F	1115	PTY	C11-C8-O7-C6
3	F	1115	PTY	C3-O11-P1-O12
3	F	1115	PTY	C3-O11-P1-O13
3	F	1115	PTY	C3-O11-P1-O14
3	F	1115	PTY	C5-O14-P1-O11
4	A	1113	GOL	O1-C1-C2-O2
4	A	1114	GOL	C1-C2-C3-O3
4	A	1115	GOL	O1-C1-C2-O2
4	A	1116	GOL	O1-C1-C2-C3
4	A	1116	GOL	C1-C2-C3-O3
4	A	1118	GOL	C1-C2-C3-O3
4	A	1120	GOL	O1-C1-C2-C3
4	A	1120	GOL	C1-C2-C3-O3
4	A	1120	GOL	O2-C2-C3-O3
4	B	1114	GOL	C1-C2-C3-O3
4	B	1115	GOL	C1-C2-C3-O3
4	C	1115	GOL	O1-C1-C2-C3
4	C	1116	GOL	O1-C1-C2-C3
4	C	1116	GOL	C1-C2-C3-O3
4	C	1119	GOL	C1-C2-C3-O3
4	C	1119	GOL	O2-C2-C3-O3
4	C	1120	GOL	O1-C1-C2-C3
4	D	1115	GOL	C1-C2-C3-O3
4	D	1116	GOL	C1-C2-C3-O3
4	D	1117	GOL	C1-C2-C3-O3
4	D	1117	GOL	O2-C2-C3-O3
4	E	1116	GOL	O1-C1-C2-C3
4	E	1119	GOL	C1-C2-C3-O3
4	E	1119	GOL	O2-C2-C3-O3
4	E	1121	GOL	O1-C1-C2-C3
4	E	1123	GOL	O1-C1-C2-O2
4	E	1123	GOL	O1-C1-C2-C3
4	E	1123	GOL	C1-C2-C3-O3
4	F	1118	GOL	O1-C1-C2-O2
4	F	1118	GOL	O1-C1-C2-C3
4	F	1118	GOL	C1-C2-C3-O3
4	F	1119	GOL	O1-C1-C2-C3
2	B	1101	LMT	C3'-C4'-O1B-C1B
2	D	1111	LMT	C3'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	1110	LMT	C3'-C4'-O1B-C1B
3	B	1112	PTY	O30-C30-O4-C1
3	F	1114	PTY	O30-C30-O4-C1
2	C	1112	LMT	O5B-C1B-O1B-C4'
2	D	1112	LMT	O5B-C1B-O1B-C4'
2	F	1103	LMT	O5B-C1B-O1B-C4'
3	B	1112	PTY	C31-C30-O4-C1
3	F	1114	PTY	O10-C8-O7-C6
2	F	1103	LMT	C2B-C1B-O1B-C4'
3	B	1112	PTY	O10-C8-O7-C6
3	C	1113	PTY	O10-C8-O7-C6
3	E	1114	PTY	O10-C8-O7-C6
3	E	1115	PTY	O10-C8-O7-C6
3	F	1115	PTY	O10-C8-O7-C6
2	F	1110	LMT	O5'-C5'-C6'-O6'
3	F	1114	PTY	C11-C8-O7-C6
2	E	1106	LMT	O5B-C5B-C6B-O6B
2	E	1107	LMT	O5B-C5B-C6B-O6B
2	C	1109	LMT	C3'-C4'-O1B-C1B
2	C	1110	LMT	O5B-C5B-C6B-O6B
2	C	1111	LMT	O5B-C5B-C6B-O6B
2	A	1109	LMT	O5B-C5B-C6B-O6B
3	A	1112	PTY	C31-C30-O4-C1
2	D	1111	LMT	O5B-C5B-C6B-O6B
2	D	1108	LMT	O5'-C5'-C6'-O6'
2	E	1110	LMT	O5B-C5B-C6B-O6B
2	F	1105	LMT	O5B-C5B-C6B-O6B
2	D	1112	LMT	C4'-C5'-C6'-O6'
2	E	1102	LMT	C3'-C4'-O1B-C1B
2	A	1101	LMT	O5B-C5B-C6B-O6B
2	B	1105	LMT	O5'-C5'-C6'-O6'
2	C	1101	LMT	O5'-C5'-C6'-O6'
2	E	1103	LMT	O5'-C5'-C6'-O6'
3	A	1112	PTY	O30-C30-O4-C1
2	E	1106	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	C4B-C5B-C6B-O6B
2	F	1103	LMT	C4'-C5'-C6'-O6'
2	A	1109	LMT	O5'-C5'-C6'-O6'
2	B	1110	LMT	O5'-C5'-C6'-O6'
2	C	1101	LMT	O5B-C5B-C6B-O6B
2	D	1108	LMT	O5B-C5B-C6B-O6B
2	E	1102	LMT	O5B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	1109	LMT	O5'-C5'-C6'-O6'
2	D	1108	LMT	C4B-C5B-C6B-O6B
2	E	1107	LMT	C4B-C5B-C6B-O6B
2	F	1110	LMT	C4'-C5'-C6'-O6'
2	A	1110	LMT	O5'-C5'-C6'-O6'
2	C	1106	LMT	O5'-C5'-C6'-O6'
2	D	1105	LMT	O5'-C5'-C6'-O6'
2	D	1101	LMT	C4B-C5B-C6B-O6B
2	D	1108	LMT	C4'-C5'-C6'-O6'
2	E	1110	LMT	C4B-C5B-C6B-O6B
2	B	1106	LMT	O5'-C5'-C6'-O6'
2	B	1109	LMT	O5'-C5'-C6'-O6'
2	F	1110	LMT	O5B-C5B-C6B-O6B
2	C	1111	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	E	1108	LMT	O5B-C5B-C6B-O6B
2	F	1107	LMT	O5B-C5B-C6B-O6B
2	A	1103	LMT	C4B-C5B-C6B-O6B
2	C	1110	LMT	C4B-C5B-C6B-O6B
2	A	1105	LMT	O5'-C1'-O1'-C1
2	A	1106	LMT	O5'-C1'-O1'-C1
2	A	1107	LMT	O5'-C1'-O1'-C1
2	A	1108	LMT	O5'-C1'-O1'-C1
2	B	1102	LMT	O5'-C1'-O1'-C1
2	D	1108	LMT	O5'-C1'-O1'-C1
2	E	1102	LMT	O5'-C1'-O1'-C1
2	F	1103	LMT	O5'-C1'-O1'-C1
2	F	1104	LMT	O5'-C1'-O1'-C1
2	F	1105	LMT	O5'-C1'-O1'-C1
2	B	1104	LMT	O5'-C5'-C6'-O6'
2	C	1101	LMT	C4'-C5'-C6'-O6'
2	E	1105	LMT	C4B-C5B-C6B-O6B
2	A	1106	LMT	O5B-C5B-C6B-O6B
2	A	1107	LMT	O5B-C5B-C6B-O6B
2	B	1101	LMT	O5'-C5'-C6'-O6'
2	D	1106	LMT	O5'-C5'-C6'-O6'
2	D	1112	LMT	O5'-C5'-C6'-O6'
2	E	1109	LMT	O5'-C5'-C6'-O6'
2	E	1112	LMT	O5B-C5B-C6B-O6B
2	E	1110	LMT	O5'-C5'-C6'-O6'
2	F	1106	LMT	O5'-C5'-C6'-O6'
2	F	1113	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	1105	LMT	C4B-C5B-C6B-O6B
2	C	1111	LMT	C4'-C5'-C6'-O6'
2	E	1109	LMT	C4'-C5'-C6'-O6'
2	F	1103	LMT	O5'-C5'-C6'-O6'
2	A	1109	LMT	C4B-C5B-C6B-O6B
2	A	1110	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	C4'-C5'-C6'-O6'
2	B	1105	LMT	C4'-C5'-C6'-O6'
2	D	1111	LMT	C4B-C5B-C6B-O6B
2	F	1109	LMT	C4'-C5'-C6'-O6'
2	F	1110	LMT	C4B-C5B-C6B-O6B
2	A	1107	LMT	C2'-C1'-O1'-C1
2	A	1110	LMT	C2'-C1'-O1'-C1
2	B	1102	LMT	C2'-C1'-O1'-C1
2	C	1103	LMT	C2'-C1'-O1'-C1
2	E	1102	LMT	C2'-C1'-O1'-C1
2	E	1108	LMT	C2'-C1'-O1'-C1
2	F	1104	LMT	C2'-C1'-O1'-C1
2	F	1106	LMT	C2'-C1'-O1'-C1
2	E	1105	LMT	C3-C4-C5-C6
2	E	1110	LMT	C11-C10-C9-C8
2	C	1111	LMT	O5'-C5'-C6'-O6'
2	E	1102	LMT	C4B-C5B-C6B-O6B
2	F	1113	LMT	C4'-C5'-C6'-O6'
2	D	1109	LMT	C5'-C4'-O1B-C1B
2	A	1107	LMT	C4B-C5B-C6B-O6B
2	D	1106	LMT	C4'-C5'-C6'-O6'
2	D	1111	LMT	C7-C8-C9-C10
2	E	1106	LMT	C3'-C4'-O1B-C1B
2	F	1107	LMT	C4B-C5B-C6B-O6B
3	F	1114	PTY	O4-C1-C6-O7
2	D	1111	LMT	O5'-C5'-C6'-O6'
3	E	1114	PTY	C16-C17-C18-C19
2	D	1109	LMT	C3'-C4'-O1B-C1B
4	D	1115	GOL	O2-C2-C3-O3
4	D	1116	GOL	O2-C2-C3-O3
2	E	1108	LMT	C4'-C5'-C6'-O6'
2	E	1110	LMT	C4'-C5'-C6'-O6'
2	A	1110	LMT	C3'-C4'-O1B-C1B
2	B	1105	LMT	O5B-C5B-C6B-O6B
2	F	1107	LMT	O1'-C1-C2-C3
2	E	1108	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1111	LMT	C3-C4-C5-C6
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	D	1104	LMT	O1'-C1-C2-C3
2	D	1107	LMT	O1'-C1-C2-C3
2	D	1104	LMT	O5'-C5'-C6'-O6'
2	E	1102	LMT	O5'-C5'-C6'-O6'
2	E	1105	LMT	O5B-C5B-C6B-O6B
3	A	1112	PTY	C30-C31-C32-C33
3	C	1113	PTY	C30-C31-C32-C33
3	F	1114	PTY	C8-C11-C12-C13
2	A	1108	LMT	C4'-C5'-C6'-O6'
2	C	1102	LMT	O1'-C1-C2-C3
2	A	1103	LMT	O5'-C1'-O1'-C1
2	B	1103	LMT	O5'-C1'-O1'-C1
2	D	1103	LMT	O5'-C1'-O1'-C1
2	E	1104	LMT	O5'-C1'-O1'-C1
2	D	1104	LMT	C3-C4-C5-C6
2	A	1102	LMT	O1'-C1-C2-C3
2	C	1103	LMT	O1'-C1-C2-C3
2	C	1104	LMT	O1'-C1-C2-C3
2	F	1106	LMT	O1'-C1-C2-C3
3	B	1112	PTY	C8-C11-C12-C13
2	A	1103	LMT	O1'-C1-C2-C3
2	A	1110	LMT	O1'-C1-C2-C3
2	B	1110	LMT	C4'-C5'-C6'-O6'
2	C	1106	LMT	C4'-C5'-C6'-O6'
2	D	1105	LMT	C4'-C5'-C6'-O6'
2	A	1103	LMT	O5B-C5B-C6B-O6B
2	D	1101	LMT	O5B-C5B-C6B-O6B
2	D	1107	LMT	O5'-C5'-C6'-O6'
3	A	1112	PTY	C11-C8-O7-C6
2	C	1110	LMT	C4'-C5'-C6'-O6'
2	E	1105	LMT	O1'-C1-C2-C3
3	A	1112	PTY	O10-C8-O7-C6
2	B	1105	LMT	C4B-C5B-C6B-O6B
2	C	1111	LMT	C5-C6-C7-C8
2	B	1104	LMT	O1'-C1-C2-C3
2	C	1103	LMT	C4B-C5B-C6B-O6B
2	C	1108	LMT	C4'-C5'-C6'-O6'
2	D	1101	LMT	O5B-C1B-O1B-C4'
2	A	1107	LMT	C5'-C4'-O1B-C1B
2	B	1110	LMT	O5B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1103	LMT	C2'-C1'-O1'-C1
2	A	1104	LMT	C2'-C1'-O1'-C1
2	A	1109	LMT	C2'-C1'-O1'-C1
2	A	1111	LMT	C2'-C1'-O1'-C1
2	B	1103	LMT	C2'-C1'-O1'-C1
2	C	1107	LMT	C2'-C1'-O1'-C1
2	D	1101	LMT	C2'-C1'-O1'-C1
2	E	1104	LMT	C2'-C1'-O1'-C1
2	F	1103	LMT	C2'-C1'-O1'-C1
2	F	1110	LMT	C2'-C1'-O1'-C1
2	D	1101	LMT	O1'-C1-C2-C3
2	B	1106	LMT	C4'-C5'-C6'-O6'
4	A	1113	GOL	O1-C1-C2-C3
4	A	1113	GOL	C1-C2-C3-O3
4	A	1115	GOL	O1-C1-C2-C3
4	A	1117	GOL	O1-C1-C2-C3
4	A	1121	GOL	C1-C2-C3-O3
4	C	1118	GOL	O1-C1-C2-C3
4	C	1119	GOL	O1-C1-C2-C3
4	D	1115	GOL	O1-C1-C2-C3
4	E	1116	GOL	C1-C2-C3-O3
4	E	1117	GOL	C1-C2-C3-O3
4	F	1116	GOL	O1-C1-C2-C3
2	E	1108	LMT	C4B-C5B-C6B-O6B
2	C	1110	LMT	C3-C4-C5-C6
2	B	1110	LMT	C1-C2-C3-C4
2	D	1105	LMT	O1'-C1-C2-C3
2	A	1108	LMT	O5'-C5'-C6'-O6'
2	A	1104	LMT	O5'-C1'-O1'-C1
2	A	1109	LMT	O5'-C1'-O1'-C1
2	A	1111	LMT	O5'-C1'-O1'-C1
2	C	1107	LMT	O5'-C1'-O1'-C1
2	B	1104	LMT	C4'-C5'-C6'-O6'
2	F	1113	LMT	C4B-C5B-C6B-O6B
2	C	1108	LMT	O1'-C1-C2-C3
2	E	1105	LMT	C1-C2-C3-C4
2	F	1107	LMT	C1-C2-C3-C4
2	D	1108	LMT	O1'-C1-C2-C3
2	C	1105	LMT	C3-C4-C5-C6
2	D	1104	LMT	C4-C5-C6-C7
2	F	1108	LMT	C1-C2-C3-C4
2	D	1111	LMT	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1112	PTY	C39-C40-C41-C42
2	B	1107	LMT	C5-C6-C7-C8
2	E	1112	LMT	C4-C5-C6-C7
2	A	1105	LMT	C4-C5-C6-C7
2	A	1107	LMT	C2-C3-C4-C5
2	C	1112	LMT	C3-C4-C5-C6
2	E	1110	LMT	C6-C7-C8-C9
2	F	1101	LMT	C5-C6-C7-C8
3	D	1113	PTY	C22-C23-C24-C25
3	F	1115	PTY	C19-C20-C21-C22
2	A	1103	LMT	C2-C1-O1'-C1'
2	A	1105	LMT	C2-C1-O1'-C1'
2	C	1104	LMT	C2-C1-O1'-C1'
2	C	1111	LMT	C2-C1-O1'-C1'
2	E	1105	LMT	C2-C1-O1'-C1'
2	E	1112	LMT	C2-C1-O1'-C1'
2	F	1106	LMT	C2-C1-O1'-C1'
4	A	1113	GOL	O2-C2-C3-O3
4	A	1114	GOL	O2-C2-C3-O3
4	A	1116	GOL	O2-C2-C3-O3
4	A	1120	GOL	O1-C1-C2-O2
4	B	1115	GOL	O2-C2-C3-O3
4	C	1115	GOL	O1-C1-C2-O2
4	C	1119	GOL	O1-C1-C2-O2
4	D	1115	GOL	O1-C1-C2-O2
4	E	1116	GOL	O2-C2-C3-O3
4	E	1119	GOL	O1-C1-C2-O2
4	F	1118	GOL	O2-C2-C3-O3
4	F	1119	GOL	O1-C1-C2-O2
2	D	1112	LMT	C5-C6-C7-C8
2	E	1109	LMT	C5-C6-C7-C8
2	F	1110	LMT	C11-C10-C9-C8
2	F	1113	LMT	C3-C4-C5-C6
3	B	1112	PTY	C11-C12-C13-C14
3	B	1111	PTY	C8-C11-C12-C13
3	E	1115	PTY	C18-C19-C20-C21
2	A	1105	LMT	C7-C8-C9-C10
2	E	1102	LMT	C3-C4-C5-C6
2	D	1104	LMT	C1-C2-C3-C4
2	B	1109	LMT	C6-C7-C8-C9
3	B	1111	PTY	C14-C15-C16-C17
2	F	1110	LMT	O1'-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1110	LMT	C7-C8-C9-C10
2	C	1102	LMT	C1-C2-C3-C4
2	C	1111	LMT	C2-C3-C4-C5
2	D	1102	LMT	C6-C7-C8-C9
2	E	1111	LMT	C6-C7-C8-C9
2	F	1111	LMT	C11-C10-C9-C8
2	D	1111	LMT	O1'-C1-C2-C3
2	B	1103	LMT	C7-C8-C9-C10
2	E	1111	LMT	C4-C5-C6-C7
2	E	1106	LMT	C5'-C4'-O1B-C1B
2	E	1108	LMT	O1'-C1-C2-C3
2	B	1107	LMT	C1-C2-C3-C4
2	C	1106	LMT	C1-C2-C3-C4
2	C	1111	LMT	C1-C2-C3-C4
2	D	1107	LMT	C1-C2-C3-C4
2	E	1103	LMT	C1-C2-C3-C4
2	C	1103	LMT	C4-C5-C6-C7
2	D	1105	LMT	C4-C5-C6-C7
2	B	1104	LMT	C6-C7-C8-C9
2	F	1105	LMT	C6-C7-C8-C9
3	C	1113	PTY	C18-C19-C20-C21
2	A	1107	LMT	C1-C2-C3-C4
2	D	1109	LMT	O5B-C1B-O1B-C4'
2	B	1105	LMT	C2-C3-C4-C5
2	D	1104	LMT	C7-C8-C9-C10
2	E	1108	LMT	C5-C6-C7-C8
2	E	1111	LMT	C11-C10-C9-C8
2	F	1106	LMT	C2-C3-C4-C5
2	F	1106	LMT	C7-C8-C9-C10
3	F	1115	PTY	C21-C22-C23-C24
2	A	1103	LMT	C11-C10-C9-C8
2	A	1105	LMT	C5-C6-C7-C8
2	E	1101	LMT	C2-C3-C4-C5
3	B	1112	PTY	C21-C22-C23-C24
3	B	1112	PTY	C33-C34-C35-C36
2	C	1104	LMT	C1-C2-C3-C4
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	A	1109	LMT	C4'-C5'-C6'-O6'
3	B	1112	PTY	C14-C15-C16-C17
3	F	1114	PTY	C31-C32-C33-C34
2	E	1105	LMT	C4-C5-C6-C7
2	F	1112	LMT	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	1114	PTY	C33-C34-C35-C36
2	F	1105	LMT	O5'-C5'-C6'-O6'
3	B	1111	PTY	C12-C13-C14-C15
3	B	1112	PTY	C20-C21-C22-C23
2	E	1104	LMT	C4B-C5B-C6B-O6B
2	E	1101	LMT	O1'-C1-C2-C3
2	C	1112	LMT	C5-C6-C7-C8
2	E	1102	LMT	C5-C6-C7-C8
2	B	1109	LMT	C3-C4-C5-C6
2	C	1108	LMT	C4-C5-C6-C7
2	E	1107	LMT	C3-C4-C5-C6
3	C	1113	PTY	C11-C12-C13-C14
3	F	1114	PTY	C21-C22-C23-C24
2	D	1107	LMT	C3-C4-C5-C6
2	E	1105	LMT	C7-C8-C9-C10
2	E	1108	LMT	C3-C4-C5-C6
2	C	1106	LMT	O1'-C1-C2-C3
2	A	1103	LMT	C2-C3-C4-C5
2	F	1101	LMT	C3-C4-C5-C6
2	F	1106	LMT	C3-C4-C5-C6
2	D	1101	LMT	O5'-C1'-O1'-C1
2	A	1103	LMT	C3-C4-C5-C6
2	C	1112	LMT	C7-C8-C9-C10
2	C	1103	LMT	O5B-C1B-O1B-C4'
2	C	1111	LMT	C7-C8-C9-C10
2	B	1103	LMT	C1-C2-C3-C4
2	B	1104	LMT	C3-C4-C5-C6
2	D	1104	LMT	C5-C6-C7-C8
3	D	1113	PTY	C18-C19-C20-C21
3	E	1114	PTY	C39-C40-C41-C42
2	F	1106	LMT	C4B-C5B-C6B-O6B
3	E	1114	PTY	C20-C21-C22-C23
3	F	1114	PTY	C35-C36-C37-C38
2	D	1111	LMT	C2-C3-C4-C5
3	E	1114	PTY	C36-C37-C38-C39
2	F	1105	LMT	C4-C5-C6-C7
2	D	1112	LMT	C6-C7-C8-C9
2	F	1102	LMT	C3-C4-C5-C6
3	A	1112	PTY	C40-C41-C42-C43
3	E	1114	PTY	C37-C38-C39-C40
2	A	1106	LMT	C1-C2-C3-C4
2	B	1107	LMT	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1108	LMT	C3-C4-C5-C6
3	F	1115	PTY	C36-C37-C38-C39
2	A	1109	LMT	C1-C2-C3-C4
2	B	1102	LMT	C1-C2-C3-C4
2	F	1106	LMT	C1-C2-C3-C4
2	C	1108	LMT	C2-C3-C4-C5
3	E	1115	PTY	C8-C11-C12-C13
2	F	1103	LMT	O5B-C5B-C6B-O6B
2	A	1107	LMT	C5-C6-C7-C8
2	F	1105	LMT	C1-C2-C3-C4
2	B	1107	LMT	C4-C5-C6-C7
2	A	1102	LMT	C4-C5-C6-C7
2	D	1101	LMT	C2-C3-C4-C5
2	E	1110	LMT	C4-C5-C6-C7
2	F	1102	LMT	C5-C6-C7-C8
2	C	1103	LMT	C1-C2-C3-C4
2	F	1110	LMT	C1-C2-C3-C4
2	C	1110	LMT	C11-C10-C9-C8
3	E	1114	PTY	C31-C32-C33-C34
2	B	1103	LMT	C6-C7-C8-C9
3	E	1115	PTY	C34-C35-C36-C37
2	C	1108	LMT	O5B-C5B-C6B-O6B
2	D	1106	LMT	C4B-C5B-C6B-O6B
2	C	1108	LMT	C5-C6-C7-C8
2	C	1112	LMT	C2-C3-C4-C5
2	C	1112	LMT	O5B-C5B-C6B-O6B
2	B	1103	LMT	C11-C10-C9-C8
2	C	1109	LMT	C11-C10-C9-C8
3	C	1113	PTY	C22-C23-C24-C25
3	C	1113	PTY	C23-C24-C25-C26
3	F	1115	PTY	C18-C19-C20-C21
2	B	1104	LMT	C11-C10-C9-C8
4	A	1116	GOL	O1-C1-C2-O2
4	A	1118	GOL	O2-C2-C3-O3
4	A	1121	GOL	O2-C2-C3-O3
4	B	1114	GOL	O2-C2-C3-O3
4	E	1116	GOL	O1-C1-C2-O2
4	E	1123	GOL	O2-C2-C3-O3
4	F	1117	GOL	O1-C1-C2-O2
2	D	1101	LMT	C7-C8-C9-C10
2	E	1108	LMT	C6-C7-C8-C9
3	C	1113	PTY	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1109	LMT	C5-C6-C7-C8
2	D	1108	LMT	C3-C4-C5-C6
2	A	1105	LMT	C6-C7-C8-C9
2	A	1106	LMT	C5-C6-C7-C8
2	A	1107	LMT	C6-C7-C8-C9
2	F	1107	LMT	C11-C10-C9-C8
2	E	1102	LMT	C5'-C4'-O1B-C1B
3	A	1112	PTY	C15-C16-C17-C18
2	E	1111	LMT	C3-C4-C5-C6
2	F	1105	LMT	C7-C8-C9-C10
2	F	1105	LMT	C2B-C1B-O1B-C4'
2	F	1108	LMT	C2-C3-C4-C5
2	E	1105	LMT	O5'-C5'-C6'-O6'
2	B	1107	LMT	C3-C4-C5-C6
2	B	1105	LMT	C11-C10-C9-C8
3	F	1115	PTY	C32-C33-C34-C35
2	D	1101	LMT	C5-C6-C7-C8
2	B	1109	LMT	C4'-C5'-C6'-O6'
2	D	1109	LMT	O5B-C5B-C6B-O6B
2	E	1101	LMT	C2'-C1'-O1'-C1
2	D	1111	LMT	C4'-C5'-C6'-O6'
2	A	1108	LMT	C7-C8-C9-C10
2	F	1111	LMT	C1'-C2'-C3'-O3'
2	A	1105	LMT	O5'-C5'-C6'-O6'
2	C	1111	LMT	O1'-C1-C2-C3
2	A	1102	LMT	C3-C4-C5-C6
2	F	1107	LMT	C7-C8-C9-C10
2	A	1105	LMT	C1-C2-C3-C4
2	A	1107	LMT	C3'-C4'-O1B-C1B
2	A	1111	LMT	C6-C7-C8-C9
2	D	1106	LMT	C6-C7-C8-C9
2	E	1102	LMT	C6-C7-C8-C9
2	E	1105	LMT	C2B-C1B-O1B-C4'
3	B	1112	PTY	C39-C40-C41-C42
2	B	1102	LMT	C3-C4-C5-C6
2	E	1103	LMT	C4'-C5'-C6'-O6'
3	F	1114	PTY	C20-C21-C22-C23
3	D	1113	PTY	C30-C31-C32-C33
2	C	1109	LMT	C5'-C4'-O1B-C1B
2	C	1112	LMT	C6-C7-C8-C9
2	D	1109	LMT	C3-C4-C5-C6
2	E	1108	LMT	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1109	LMT	C7-C8-C9-C10
2	C	1105	LMT	C4-C5-C6-C7
2	F	1110	LMT	C6-C7-C8-C9
3	E	1115	PTY	C14-C15-C16-C17
2	F	1102	LMT	C4B-C5B-C6B-O6B
2	B	1101	LMT	C2B-C1B-O1B-C4'
2	F	1113	LMT	O5'-C1'-O1'-C1
2	E	1107	LMT	C7-C8-C9-C10
3	B	1111	PTY	C31-C32-C33-C34
2	C	1112	LMT	C11-C10-C9-C8
2	D	1109	LMT	C6-C7-C8-C9
3	C	1113	PTY	C12-C13-C14-C15
3	D	1113	PTY	C40-C41-C42-C43
2	C	1112	LMT	C9-C10-C11-C12
2	E	1101	LMT	C7-C8-C9-C10
2	C	1101	LMT	C5-C6-C7-C8
2	D	1106	LMT	C7-C8-C9-C10
3	A	1112	PTY	C20-C21-C22-C23
3	F	1115	PTY	C38-C39-C40-C41
2	C	1110	LMT	C9-C10-C11-C12
2	B	1109	LMT	C4-C5-C6-C7
2	C	1112	LMT	C4-C5-C6-C7
2	D	1105	LMT	C5-C6-C7-C8
2	E	1105	LMT	C6-C7-C8-C9
2	C	1109	LMT	C9-C10-C11-C12
2	E	1111	LMT	C2-C3-C4-C5
2	E	1103	LMT	C9-C10-C11-C12
2	B	1108	LMT	C9-C10-C11-C12
3	C	1113	PTY	C31-C30-O4-C1
2	C	1108	LMT	O5'-C5'-C6'-O6'
2	F	1112	LMT	C4-C5-C6-C7
2	B	1101	LMT	C1-C2-C3-C4
3	B	1112	PTY	C23-C24-C25-C26
3	D	1113	PTY	C41-C42-C43-C44
2	C	1103	LMT	C9-C10-C11-C12
2	C	1108	LMT	C4B-C5B-C6B-O6B
2	E	1104	LMT	C5-C6-C7-C8
2	A	1109	LMT	O1'-C1-C2-C3
2	C	1106	LMT	C3-C4-C5-C6
2	E	1102	LMT	C2-C3-C4-C5
3	A	1112	PTY	C13-C14-C15-C16
2	A	1104	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1102	LMT	C2-C1-O1'-C1'
2	B	1109	LMT	C2-C1-O1'-C1'
2	C	1107	LMT	C2-C1-O1'-C1'
2	C	1112	LMT	C2-C1-O1'-C1'
2	D	1103	LMT	C2-C1-O1'-C1'
2	D	1106	LMT	C2-C1-O1'-C1'
2	D	1107	LMT	C2-C1-O1'-C1'
2	D	1111	LMT	C2-C1-O1'-C1'
2	E	1102	LMT	C2-C1-O1'-C1'
2	E	1104	LMT	C2-C1-O1'-C1'
2	E	1107	LMT	C2-C1-O1'-C1'
2	F	1104	LMT	C2-C1-O1'-C1'
2	F	1105	LMT	C2-C1-O1'-C1'
2	F	1110	LMT	C2-C1-O1'-C1'
2	F	1113	LMT	C2-C1-O1'-C1'
4	C	1114	GOL	O2-C2-C3-O3
4	C	1120	GOL	O1-C1-C2-O2
4	F	1116	GOL	O1-C1-C2-O2
4	F	1120	GOL	O2-C2-C3-O3
3	F	1115	PTY	C17-C18-C19-C20
2	A	1111	LMT	C5-C6-C7-C8
2	E	1113	LMT	C7-C8-C9-C10
2	A	1103	LMT	O5B-C1B-O1B-C4'
2	B	1102	LMT	C9-C10-C11-C12
2	E	1107	LMT	C1-C2-C3-C4
2	A	1101	LMT	C2'-C1'-O1'-C1
2	A	1111	LMT	C4-C5-C6-C7
2	C	1102	LMT	C2-C3-C4-C5
2	E	1105	LMT	C5-C6-C7-C8
2	E	1109	LMT	C7-C8-C9-C10
2	D	1105	LMT	C9-C10-C11-C12
3	A	1112	PTY	C41-C42-C43-C44
3	B	1111	PTY	C13-C14-C15-C16
2	B	1106	LMT	C9-C10-C11-C12
2	E	1109	LMT	C3-C4-C5-C6
3	F	1114	PTY	C32-C33-C34-C35
3	B	1112	PTY	C15-C16-C17-C18
3	E	1114	PTY	C18-C19-C20-C21
2	B	1102	LMT	C4B-C5B-C6B-O6B
2	D	1112	LMT	O5B-C5B-C6B-O6B
2	D	1103	LMT	C1-C2-C3-C4
2	D	1105	LMT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1107	LMT	C6-C7-C8-C9
2	A	1105	LMT	C2B-C1B-O1B-C4'
2	A	1107	LMT	C4-C5-C6-C7
3	B	1111	PTY	O4-C1-C6-C5
3	E	1114	PTY	O4-C1-C6-C5
3	E	1115	PTY	O4-C1-C6-C5
3	A	1112	PTY	C14-C15-C16-C17
3	D	1113	PTY	C34-C35-C36-C37
2	D	1108	LMT	C11-C10-C9-C8
2	F	1111	LMT	O1'-C1-C2-C3
2	E	1111	LMT	C9-C10-C11-C12
2	F	1105	LMT	C5-C6-C7-C8
2	E	1112	LMT	C1-C2-C3-C4
2	F	1109	LMT	C1-C2-C3-C4
2	F	1113	LMT	C9-C10-C11-C12
2	D	1105	LMT	C2-C3-C4-C5
2	C	1103	LMT	C3-C4-C5-C6
2	F	1107	LMT	C4-C5-C6-C7
2	D	1109	LMT	C9-C10-C11-C12
2	C	1101	LMT	C3-C4-C5-C6
2	C	1106	LMT	C7-C8-C9-C10
3	E	1115	PTY	C21-C22-C23-C24
3	B	1111	PTY	O4-C1-C6-O7
3	E	1114	PTY	O4-C1-C6-O7
3	E	1115	PTY	O4-C1-C6-O7
2	D	1107	LMT	C7-C8-C9-C10
3	D	1113	PTY	C11-C12-C13-C14
3	E	1115	PTY	C22-C23-C24-C25
2	A	1105	LMT	O5B-C1B-O1B-C4'
2	B	1101	LMT	O1'-C1-C2-C3
2	F	1113	LMT	C4-C5-C6-C7
2	B	1102	LMT	C6-C7-C8-C9
2	E	1110	LMT	C7-C8-C9-C10
3	B	1111	PTY	C34-C35-C36-C37
3	C	1113	PTY	C20-C21-C22-C23
3	A	1112	PTY	C8-C11-C12-C13
3	E	1115	PTY	C12-C13-C14-C15
2	D	1108	LMT	C1-C2-C3-C4
2	B	1103	LMT	C2-C3-C4-C5
2	D	1101	LMT	C3-C4-C5-C6
2	A	1110	LMT	C5'-C4'-O1B-C1B
2	E	1110	LMT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1107	LMT	C6-C7-C8-C9
2	F	1111	LMT	C5-C6-C7-C8
2	F	1107	LMT	C9-C10-C11-C12
4	A	1119	GOL	O1-C1-C2-O2
4	B	1114	GOL	O1-C1-C2-O2
4	E	1121	GOL	O1-C1-C2-O2
2	B	1102	LMT	O5B-C5B-C6B-O6B
3	A	1112	PTY	C11-C12-C13-C14
3	E	1114	PTY	C33-C34-C35-C36
2	C	1108	LMT	C3-C4-C5-C6
2	A	1107	LMT	O1'-C1-C2-C3
2	A	1106	LMT	C3-C4-C5-C6
2	B	1108	LMT	C4-C5-C6-C7
3	D	1113	PTY	C19-C20-C21-C22
3	B	1112	PTY	O14-C5-C6-C1
3	C	1113	PTY	O14-C5-C6-C1
3	E	1114	PTY	O14-C5-C6-C1
2	B	1104	LMT	C1-C2-C3-C4
2	A	1111	LMT	C11-C10-C9-C8
2	E	1112	LMT	C9-C10-C11-C12
2	F	1102	LMT	C1-C2-C3-C4
2	C	1111	LMT	C6-C7-C8-C9
2	F	1108	LMT	C7-C8-C9-C10
2	B	1103	LMT	C4B-C5B-C6B-O6B
2	F	1102	LMT	C4-C5-C6-C7
3	C	1113	PTY	O30-C30-O4-C1
2	A	1105	LMT	O1'-C1-C2-C3
2	C	1105	LMT	C2-C3-C4-C5
3	B	1112	PTY	O14-C5-C6-O7
2	D	1105	LMT	C3-C4-C5-C6
2	F	1111	LMT	C2-C3-C4-C5
3	F	1115	PTY	C12-C13-C14-C15
2	F	1107	LMT	O5'-C1'-O1'-C1
3	D	1113	PTY	O4-C1-C6-C5
3	B	1112	PTY	C31-C32-C33-C34
3	E	1114	PTY	C32-C33-C34-C35
2	C	1108	LMT	C1-C2-C3-C4
3	B	1112	PTY	O4-C1-C6-O7
3	F	1114	PTY	C38-C39-C40-C41
2	B	1103	LMT	C4'-C5'-C6'-O6'
2	B	1104	LMT	C7-C8-C9-C10
2	E	1111	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1103	LMT	C2-C3-C4-C5
2	D	1109	LMT	C4'-C5'-C6'-O6'
3	B	1112	PTY	C34-C35-C36-C37
3	B	1112	PTY	C37-C38-C39-C40
3	B	1111	PTY	C18-C19-C20-C21
3	F	1114	PTY	C40-C41-C42-C43
2	B	1101	LMT	C9-C10-C11-C12
2	E	1112	LMT	O5B-C1B-O1B-C4'
3	A	1112	PTY	C16-C17-C18-C19
2	C	1109	LMT	C1-C2-C3-C4
2	F	1103	LMT	C4-C5-C6-C7
3	F	1115	PTY	C20-C21-C22-C23
2	C	1105	LMT	O1'-C1-C2-C3
2	B	1107	LMT	C2'-C1'-O1'-C1
2	C	1102	LMT	C2-C1-O1'-C1'
2	F	1107	LMT	C2-C1-O1'-C1'
2	E	1102	LMT	C9-C10-C11-C12
2	A	1101	LMT	C11-C10-C9-C8
2	E	1108	LMT	C7-C8-C9-C10
2	F	1107	LMT	C5-C6-C7-C8
2	A	1111	LMT	C7-C8-C9-C10
2	D	1103	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	C6-C7-C8-C9
2	C	1105	LMT	C1-C2-C3-C4
3	F	1114	PTY	C11-C12-C13-C14
2	A	1110	LMT	C3-C4-C5-C6
2	F	1104	LMT	C5-C6-C7-C8
3	B	1112	PTY	C16-C17-C18-C19
2	B	1101	LMT	O5B-C1B-O1B-C4'
2	A	1101	LMT	C4-C5-C6-C7
2	E	1108	LMT	C9-C10-C11-C12
3	C	1113	PTY	O14-C5-C6-O7
2	E	1111	LMT	C5-C6-C7-C8
2	A	1103	LMT	C2B-C1B-O1B-C4'
2	D	1112	LMT	C1-C2-C3-C4
2	A	1101	LMT	C7-C8-C9-C10
3	C	1113	PTY	C15-C16-C17-C18
2	E	1107	LMT	C2-C3-C4-C5
2	F	1103	LMT	O1'-C1-C2-C3
2	F	1102	LMT	C2-C3-C4-C5
2	F	1105	LMT	C2-C3-C4-C5
2	E	1108	LMT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1104	LMT	C4-C5-C6-C7
2	D	1110	LMT	C6-C7-C8-C9
2	B	1110	LMT	C9-C10-C11-C12
2	C	1105	LMT	C4B-C5B-C6B-O6B
2	D	1109	LMT	O5'-C1'-O1'-C1
2	C	1109	LMT	C6-C7-C8-C9
2	E	1112	LMT	O1'-C1-C2-C3
2	C	1101	LMT	C9-C10-C11-C12
2	C	1102	LMT	C11-C10-C9-C8
2	F	1101	LMT	C1-C2-C3-C4
3	A	1112	PTY	C5-O14-P1-O13
3	D	1113	PTY	N1-C2-C3-O11
3	E	1115	PTY	C5-O14-P1-O12
3	F	1115	PTY	C5-O14-P1-O13
3	E	1115	PTY	C20-C21-C22-C23
2	F	1113	LMT	C7-C8-C9-C10
3	E	1115	PTY	C32-C33-C34-C35
2	F	1111	LMT	O1'-C1'-C2'-C3'
2	B	1106	LMT	C4-C5-C6-C7
2	D	1101	LMT	O5'-C5'-C6'-O6'
2	A	1108	LMT	C11-C10-C9-C8
2	E	1104	LMT	O5B-C5B-C6B-O6B
2	F	1106	LMT	O5B-C5B-C6B-O6B
2	D	1107	LMT	O5B-C1B-O1B-C4'
4	C	1117	GOL	O1-C1-C2-O2
4	C	1118	GOL	O1-C1-C2-O2
2	D	1109	LMT	C2B-C1B-O1B-C4'
2	B	1109	LMT	O5B-C5B-C6B-O6B
4	F	1119	GOL	C1-C2-C3-O3
2	E	1105	LMT	O5B-C1B-O1B-C4'
3	E	1114	PTY	C22-C23-C24-C25
2	C	1106	LMT	C4B-C5B-C6B-O6B
2	D	1111	LMT	C5-C6-C7-C8
2	F	1111	LMT	C9-C10-C11-C12
2	B	1107	LMT	C2-C1-O1'-C1'
3	B	1111	PTY	O14-C5-C6-C1
2	F	1108	LMT	C9-C10-C11-C12
2	C	1112	LMT	C5'-C4'-O1B-C1B
2	B	1109	LMT	C2B-C1B-O1B-C4'
2	A	1111	LMT	O1'-C1-C2-C3
2	F	1107	LMT	C2'-C1'-O1'-C1
2	D	1112	LMT	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1106	LMT	C4B-C5B-C6B-O6B
2	E	1102	LMT	C4'-C5'-C6'-O6'
2	A	1110	LMT	C9-C10-C11-C12
3	F	1115	PTY	O30-C30-O4-C1
2	F	1105	LMT	O1'-C1-C2-C3
2	D	1109	LMT	C2-C3-C4-C5
2	C	1104	LMT	C3-C4-C5-C6
2	A	1106	LMT	O5'-C5'-C6'-O6'
2	B	1102	LMT	C2-C3-C4-C5
2	D	1104	LMT	C6-C7-C8-C9
2	A	1108	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	C11-C10-C9-C8
3	E	1115	PTY	O4-C30-C31-C32
2	E	1112	LMT	C4B-C5B-C6B-O6B
2	C	1106	LMT	C5'-C4'-O1B-C1B
2	A	1106	LMT	C2-C3-C4-C5
2	D	1112	LMT	O5'-C1'-O1'-C1
2	D	1109	LMT	O1'-C1-C2-C3
2	A	1107	LMT	C2-C1-O1'-C1'
2	B	1110	LMT	C7-C8-C9-C10
3	E	1114	PTY	C34-C35-C36-C37
2	F	1109	LMT	C2-C3-C4-C5
3	F	1115	PTY	C31-C30-O4-C1
3	A	1112	PTY	C22-C23-C24-C25
2	C	1102	LMT	C9-C10-C11-C12
3	C	1113	PTY	C21-C22-C23-C24
2	D	1107	LMT	C4'-C5'-C6'-O6'
2	F	1101	LMT	C6-C7-C8-C9
3	E	1115	PTY	C37-C38-C39-C40
2	C	1105	LMT	C6-C7-C8-C9
2	A	1109	LMT	C11-C10-C9-C8
3	F	1114	PTY	C39-C40-C41-C42
2	F	1101	LMT	O5'-C5'-C6'-O6'
2	D	1112	LMT	C11-C10-C9-C8
4	B	1113	GOL	C1-C2-C3-O3
4	E	1119	GOL	O1-C1-C2-C3
2	F	1105	LMT	O5B-C1B-O1B-C4'
2	B	1103	LMT	C5-C6-C7-C8
2	D	1107	LMT	C9-C10-C11-C12
2	B	1102	LMT	C4-C5-C6-C7
2	F	1107	LMT	C3-C4-C5-C6
4	C	1116	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	F	1119	GOL	O2-C2-C3-O3
2	E	1106	LMT	C7-C8-C9-C10
2	E	1103	LMT	C4B-C5B-C6B-O6B
2	D	1106	LMT	O5B-C5B-C6B-O6B
3	F	1115	PTY	C31-C32-C33-C34
2	E	1104	LMT	C2-C3-C4-C5
2	F	1104	LMT	C6-C7-C8-C9
2	D	1112	LMT	C7-C8-C9-C10
2	B	1106	LMT	C2-C3-C4-C5
2	E	1108	LMT	O5B-C1B-O1B-C4'
2	D	1103	LMT	C4-C5-C6-C7
2	A	1106	LMT	C7-C8-C9-C10
2	C	1109	LMT	O5'-C1'-O1'-C1
3	D	1113	PTY	C6-C5-O14-P1
2	E	1107	LMT	C6-C7-C8-C9
2	C	1108	LMT	C3'-C4'-O1B-C1B
2	D	1106	LMT	C2'-C1'-O1'-C1
2	F	1108	LMT	C5-C6-C7-C8
2	A	1106	LMT	C9-C10-C11-C12
3	B	1112	PTY	C36-C37-C38-C39
2	F	1103	LMT	C11-C10-C9-C8
2	D	1109	LMT	C2-C1-O1'-C1'
4	E	1117	GOL	O2-C2-C3-O3
2	F	1109	LMT	C6-C7-C8-C9
2	B	1105	LMT	C4-C5-C6-C7
3	E	1115	PTY	C12-C11-C8-O7
2	B	1110	LMT	C6-C7-C8-C9
2	E	1103	LMT	C4-C5-C6-C7
3	E	1115	PTY	C6-C5-O14-P1
3	B	1112	PTY	C12-C13-C14-C15
2	A	1110	LMT	C7-C8-C9-C10
2	A	1111	LMT	C4B-C5B-C6B-O6B
2	D	1110	LMT	C5-C6-C7-C8
2	C	1110	LMT	C6-C7-C8-C9
2	F	1109	LMT	C5'-C4'-O1B-C1B
2	A	1103	LMT	C9-C10-C11-C12
2	B	1106	LMT	C7-C8-C9-C10
2	C	1106	LMT	C3'-C4'-O1B-C1B
2	C	1101	LMT	C6-C7-C8-C9
2	C	1103	LMT	C2B-C1B-O1B-C4'
2	B	1105	LMT	O5'-C1'-O1'-C1
2	C	1106	LMT	O5'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	1101	LMT	C11-C10-C9-C8
2	B	1106	LMT	C5'-C4'-O1B-C1B
3	B	1111	PTY	C40-C41-C42-C43
4	D	1114	GOL	O2-C2-C3-O3
2	F	1111	LMT	C2-C1-O1'-C1'
2	D	1102	LMT	C9-C10-C11-C12
2	E	1113	LMT	C5-C6-C7-C8
3	C	1113	PTY	C40-C41-C42-C43
2	D	1107	LMT	C2B-C1B-O1B-C4'
2	E	1110	LMT	C9-C10-C11-C12
2	E	1109	LMT	O5B-C5B-C6B-O6B
2	F	1101	LMT	C7-C8-C9-C10
2	C	1108	LMT	C6-C7-C8-C9
2	C	1112	LMT	C3'-C4'-O1B-C1B
2	D	1105	LMT	C5'-C4'-O1B-C1B
2	C	1106	LMT	C4-C5-C6-C7
2	B	1101	LMT	C11-C10-C9-C8
2	A	1105	LMT	C9-C10-C11-C12
2	D	1104	LMT	O5B-C5B-C6B-O6B
2	A	1104	LMT	C5-C6-C7-C8
2	B	1102	LMT	C5-C6-C7-C8
3	E	1114	PTY	O4-C30-C31-C32
2	D	1101	LMT	C2-C1-O1'-C1'
4	C	1116	GOL	O1-C1-C2-O2
3	B	1112	PTY	O4-C1-C6-C5
3	E	1114	PTY	C38-C39-C40-C41
2	B	1109	LMT	O5'-C1'-O1'-C1
2	D	1106	LMT	O5'-C1'-O1'-C1
3	B	1111	PTY	C12-C11-C8-O7
3	D	1113	PTY	O4-C1-C6-O7
3	F	1115	PTY	O4-C1-C6-O7
3	D	1113	PTY	O30-C30-O4-C1
2	B	1109	LMT	O5B-C1B-O1B-C4'
2	C	1101	LMT	C2-C3-C4-C5
3	D	1113	PTY	C31-C30-O4-C1
3	B	1112	PTY	C41-C42-C43-C44
2	C	1110	LMT	O1'-C1-C2-C3
2	F	1109	LMT	C3-C4-C5-C6
2	F	1106	LMT	C4'-C5'-C6'-O6'
2	D	1106	LMT	C2-C3-C4-C5
2	E	1106	LMT	C9-C10-C11-C12
2	F	1104	LMT	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1113	PTY	C24-C25-C26-C27
2	B	1107	LMT	O1'-C1-C2-C3
3	E	1114	PTY	O30-C30-C31-C32
2	D	1101	LMT	C2B-C1B-O1B-C4'
2	B	1102	LMT	C11-C10-C9-C8
3	E	1114	PTY	C6-C5-O14-P1
2	D	1111	LMT	C9-C10-C11-C12
2	B	1105	LMT	C6-C7-C8-C9
3	B	1112	PTY	C19-C20-C21-C22
3	B	1111	PTY	C12-C11-C8-O10

There are no ring outliers.

80 monomers are involved in 203 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1112	PTY	4	0
4	A	1116	GOL	1	0
2	A	1106	LMT	1	0
4	E	1119	GOL	1	0
2	C	1101	LMT	2	0
2	E	1108	LMT	11	0
2	E	1110	LMT	2	0
3	D	1113	PTY	1	0
4	E	1122	GOL	1	0
4	C	1115	GOL	2	0
3	E	1114	PTY	3	0
4	B	1114	GOL	1	0
2	D	1106	LMT	1	0
2	A	1103	LMT	1	0
2	F	1108	LMT	2	0
2	D	1108	LMT	1	0
2	E	1101	LMT	2	0
2	C	1107	LMT	3	0
2	B	1102	LMT	3	0
2	A	1107	LMT	2	0
2	E	1113	LMT	1	0
2	A	1110	LMT	5	0
2	C	1111	LMT	3	0
2	F	1102	LMT	3	0
4	A	1121	GOL	2	0
2	B	1108	LMT	2	0
2	B	1107	LMT	2	0

Continued on next page...

Continued from previous page...

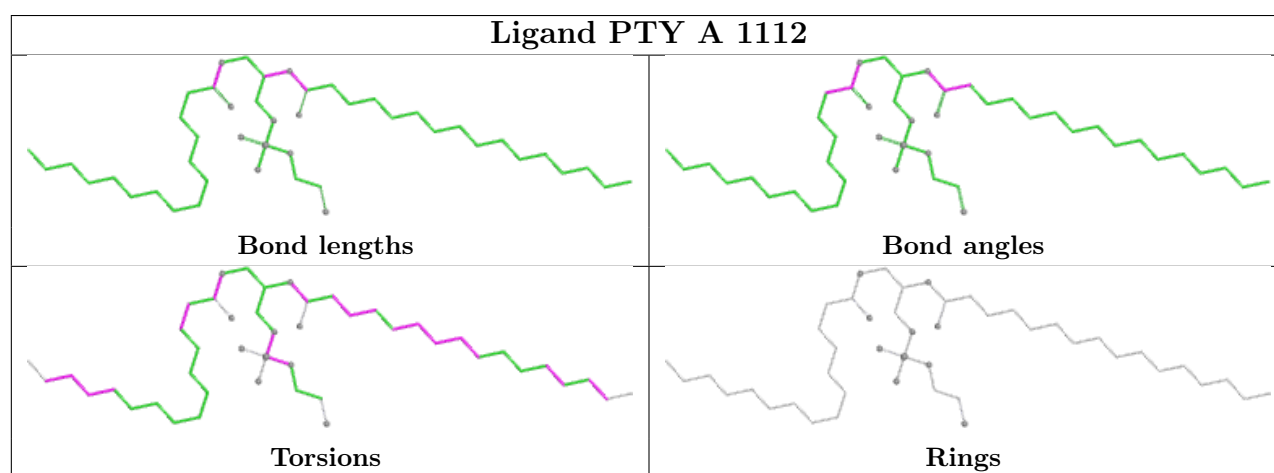
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1113	LMT	1	0
2	E	1112	LMT	2	0
4	F	1116	GOL	1	0
2	A	1104	LMT	1	0
2	B	1101	LMT	3	0
4	C	1116	GOL	2	0
4	A	1114	GOL	2	0
4	C	1117	GOL	1	0
2	C	1102	LMT	2	0
2	B	1109	LMT	1	0
2	D	1103	LMT	5	0
4	A	1117	GOL	2	0
2	C	1104	LMT	1	0
2	D	1107	LMT	8	0
2	C	1108	LMT	2	0
2	A	1105	LMT	2	0
2	F	1104	LMT	1	0
2	C	1103	LMT	3	0
2	D	1104	LMT	5	0
2	E	1102	LMT	1	0
2	E	1105	LMT	8	0
4	E	1116	GOL	5	0
2	E	1103	LMT	7	0
3	E	1115	PTY	2	0
4	A	1119	GOL	1	0
2	F	1105	LMT	3	0
2	C	1112	LMT	4	0
2	D	1102	LMT	1	0
3	F	1115	PTY	1	0
2	F	1103	LMT	7	0
2	F	1107	LMT	1	0
2	F	1110	LMT	4	0
2	D	1112	LMT	4	0
2	A	1111	LMT	4	0
2	E	1107	LMT	5	0
2	D	1109	LMT	9	0
3	F	1114	PTY	2	0
2	F	1111	LMT	3	0
2	B	1103	LMT	2	0
2	F	1109	LMT	1	0
3	B	1112	PTY	2	0
4	A	1115	GOL	2	0

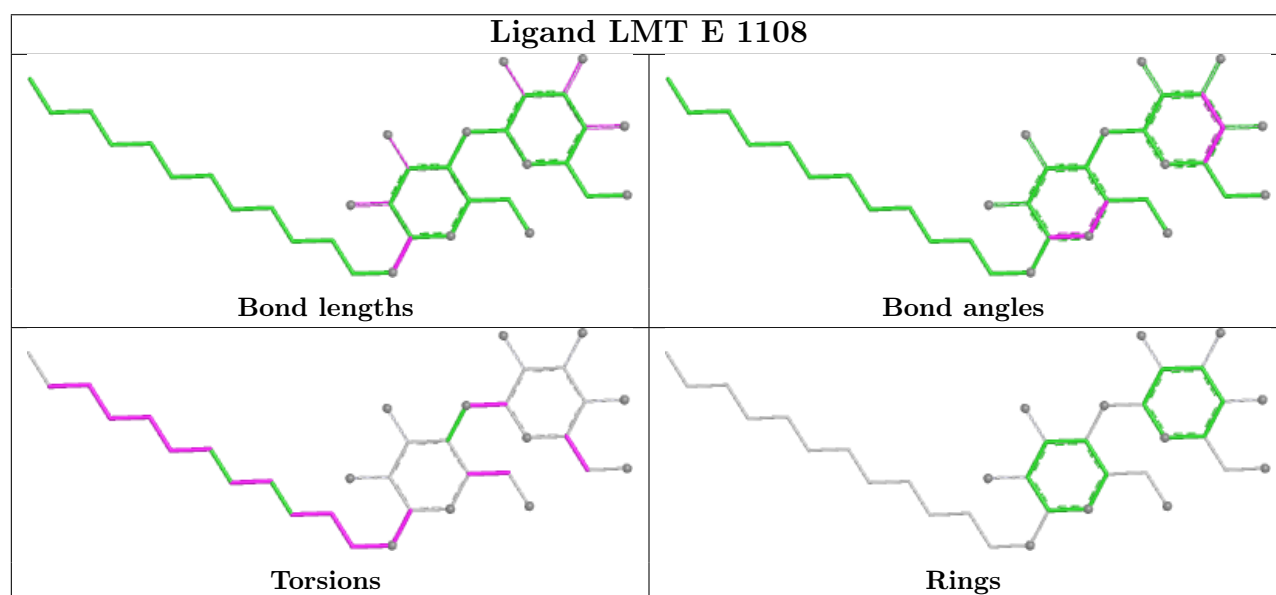
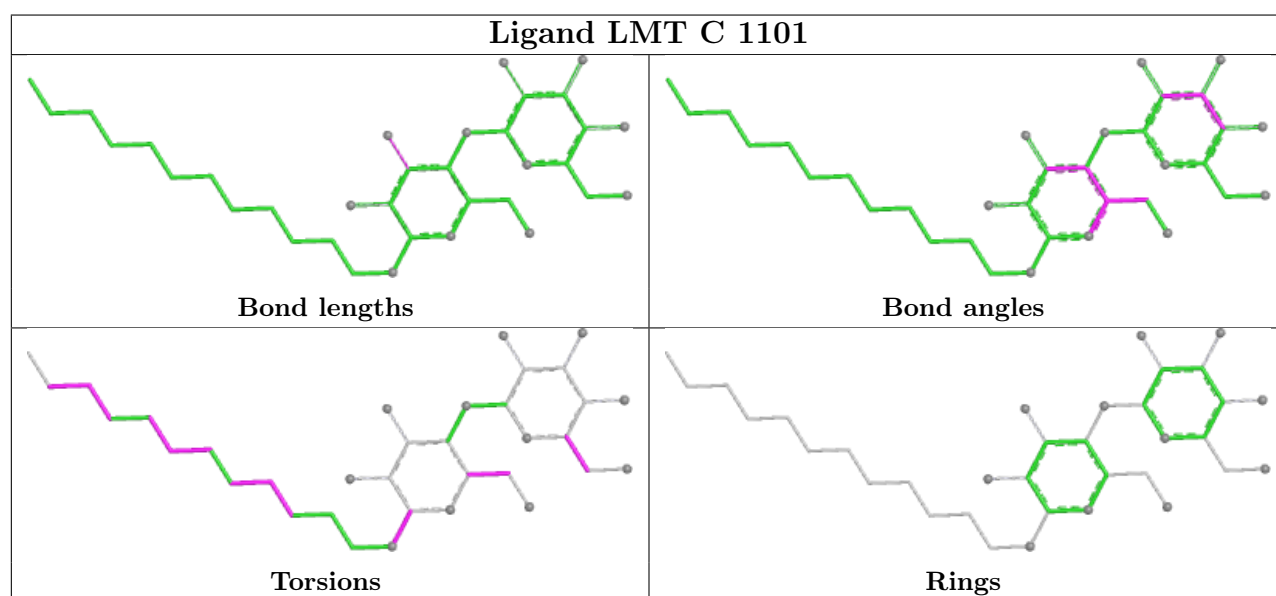
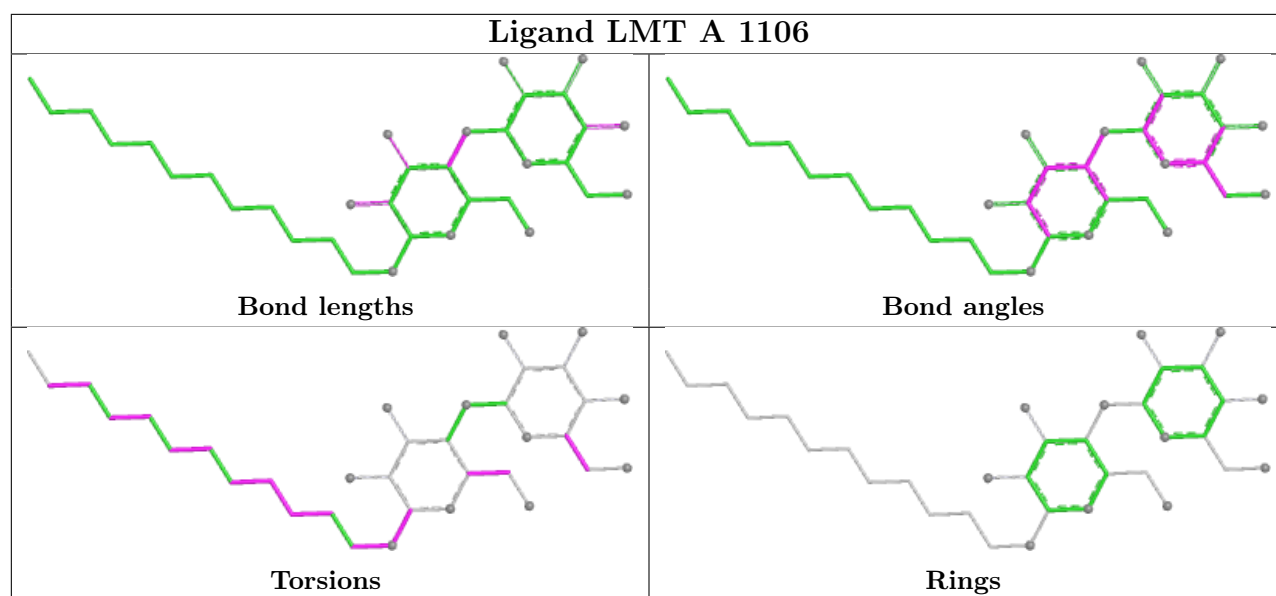
Continued on next page...

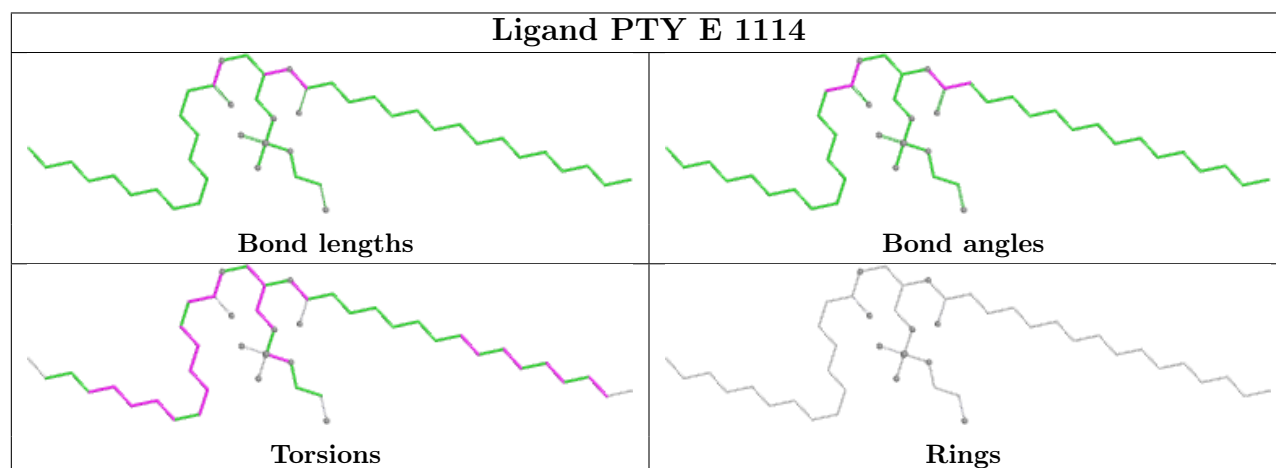
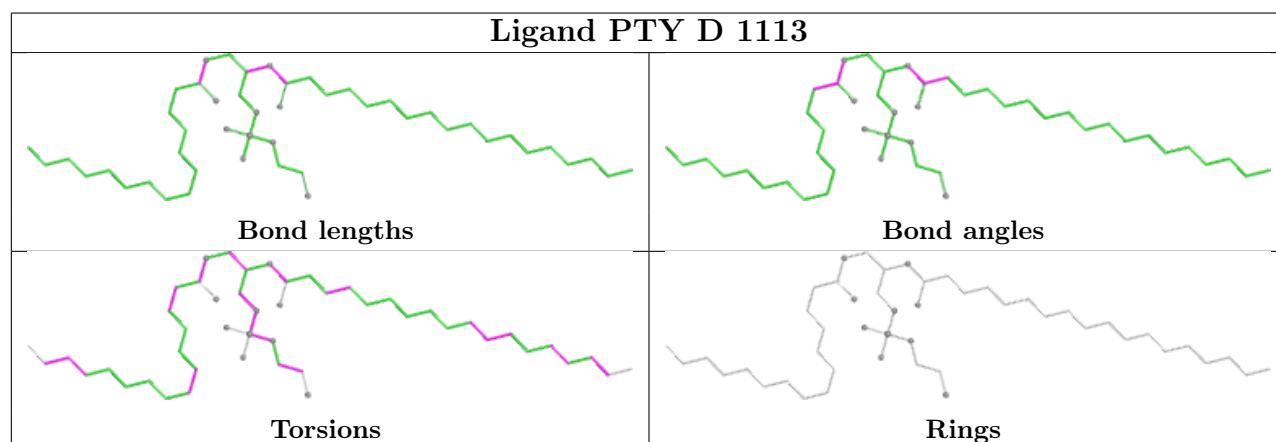
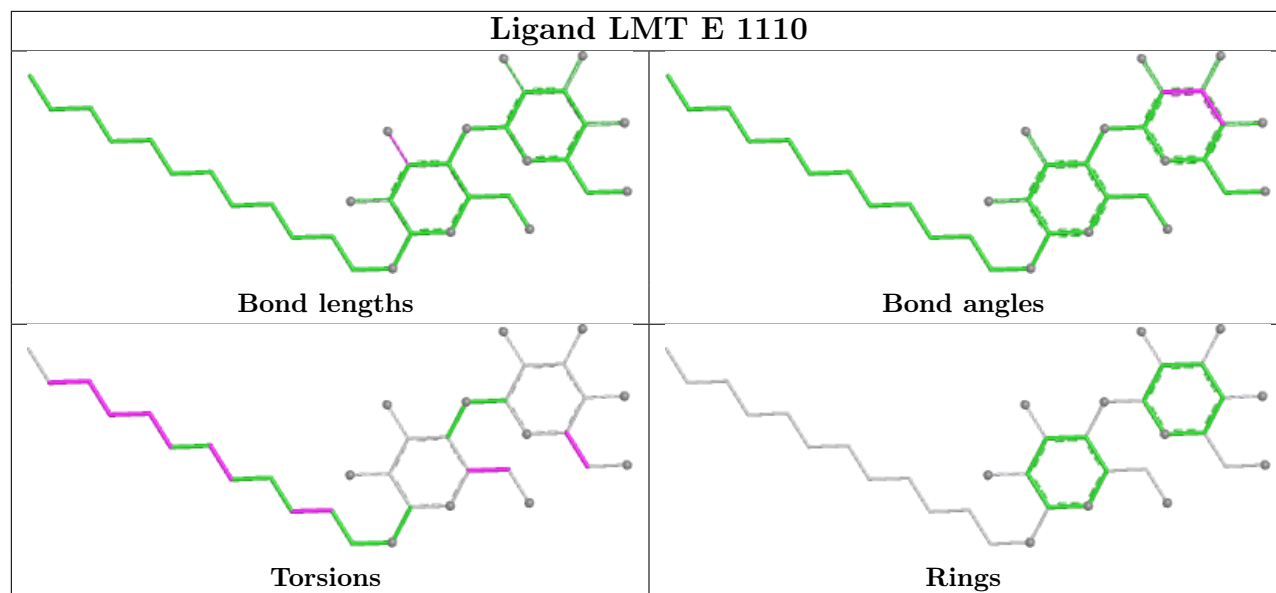
Continued from previous page...

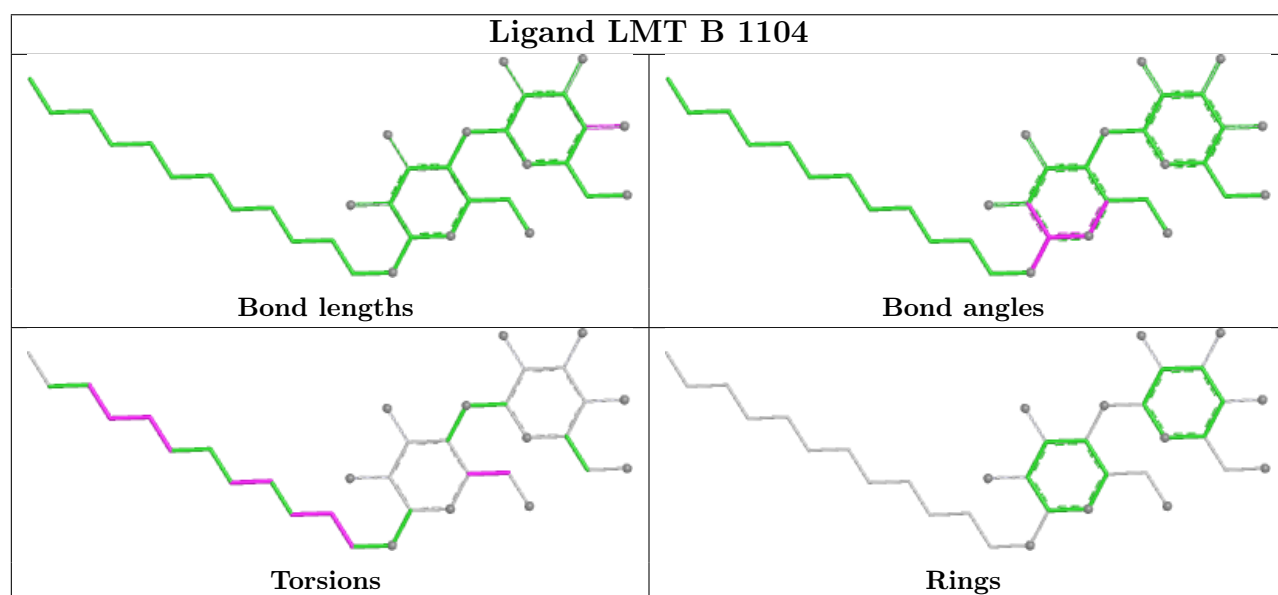
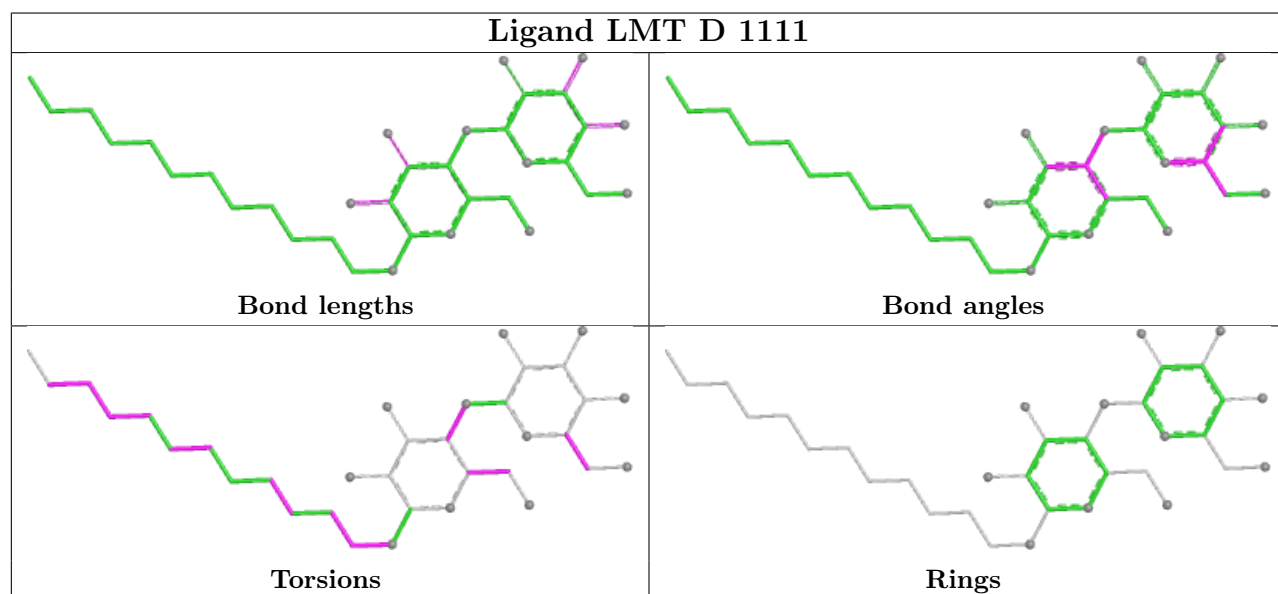
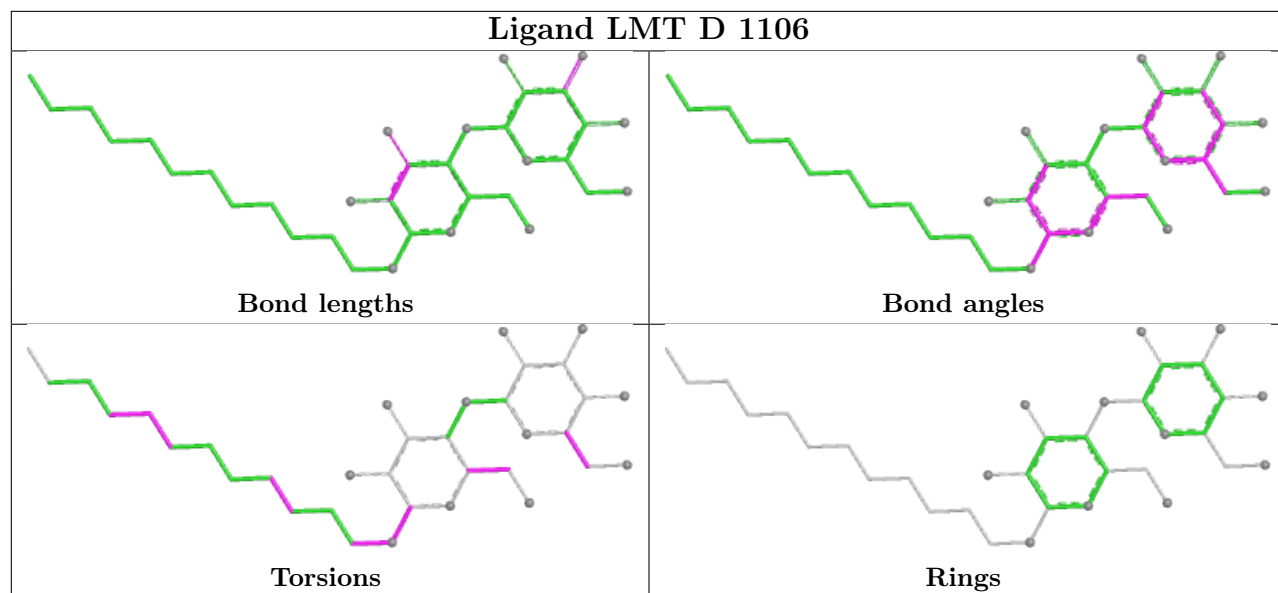
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1108	LMT	2	0
4	C	1114	GOL	1	0
4	F	1117	GOL	1	0
2	E	1106	LMT	1	0
2	E	1109	LMT	4	0
3	C	1113	PTY	1	0
3	B	1111	PTY	1	0
4	C	1118	GOL	3	0
2	D	1101	LMT	4	0
4	E	1121	GOL	2	0
2	D	1105	LMT	2	0

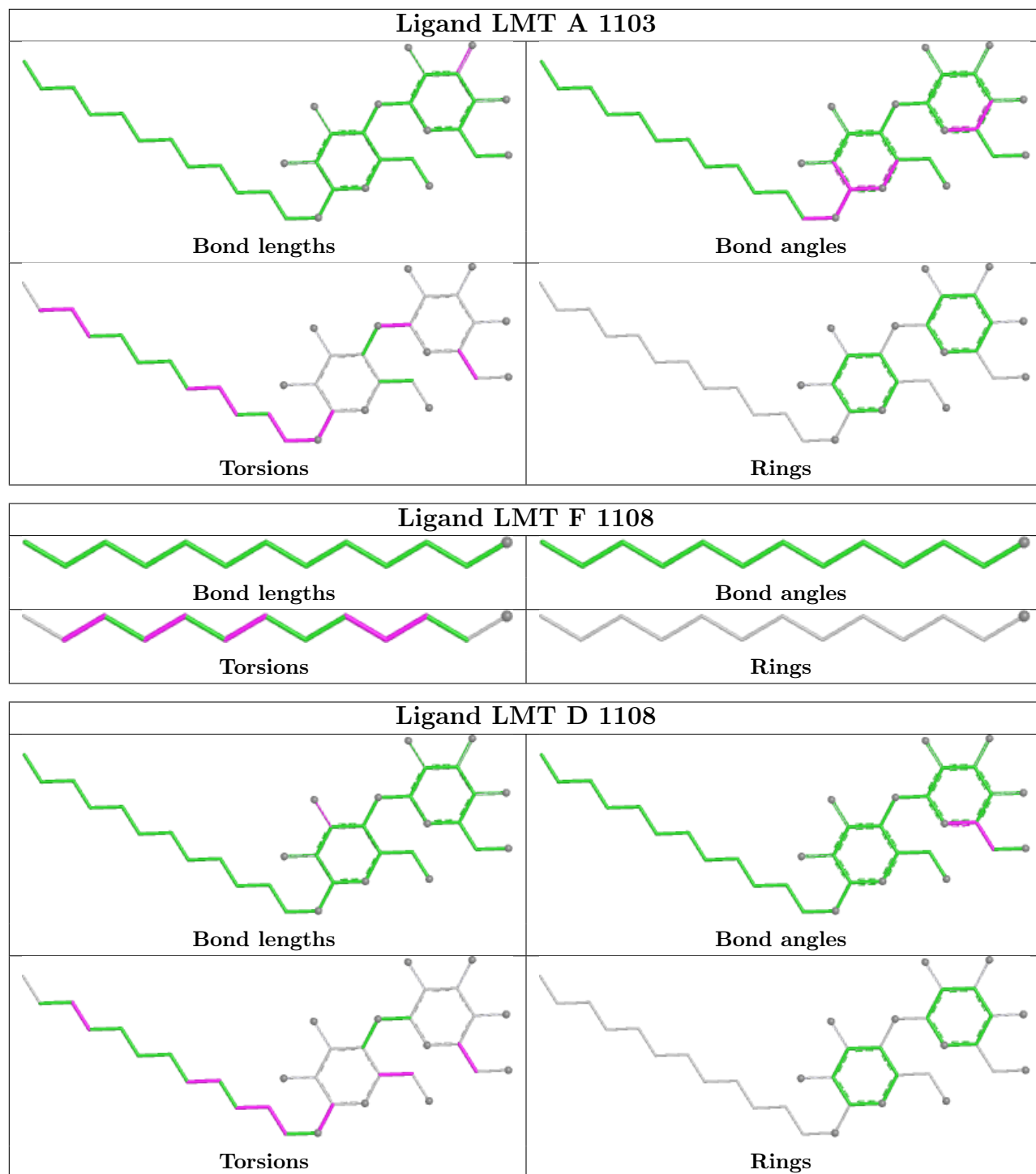
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

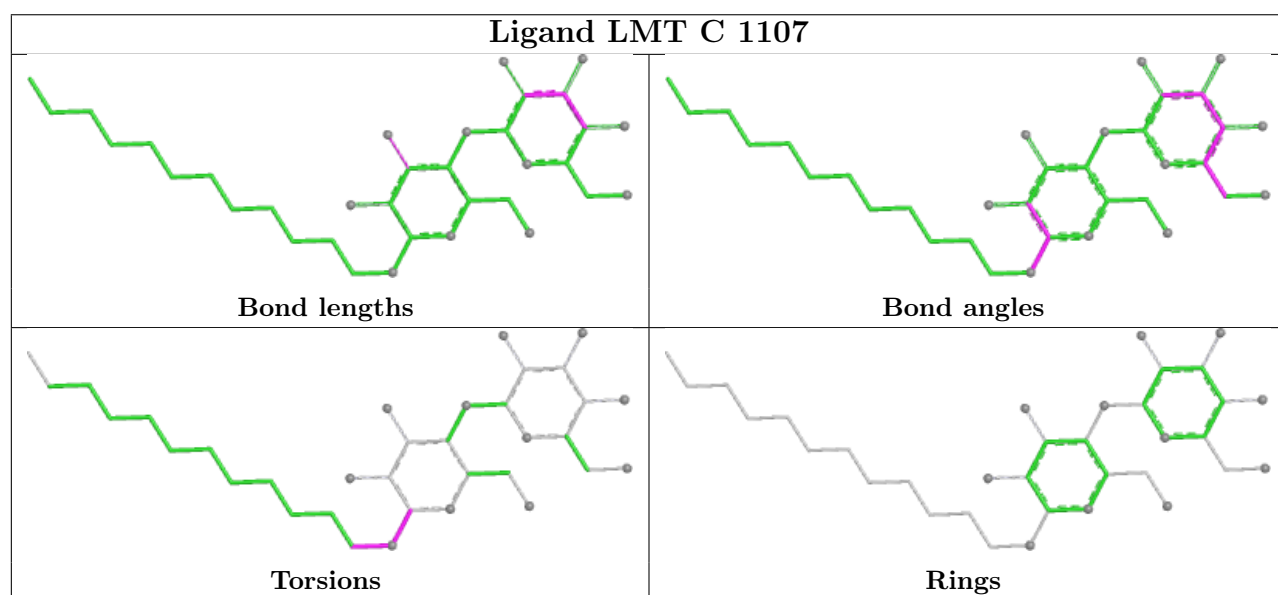
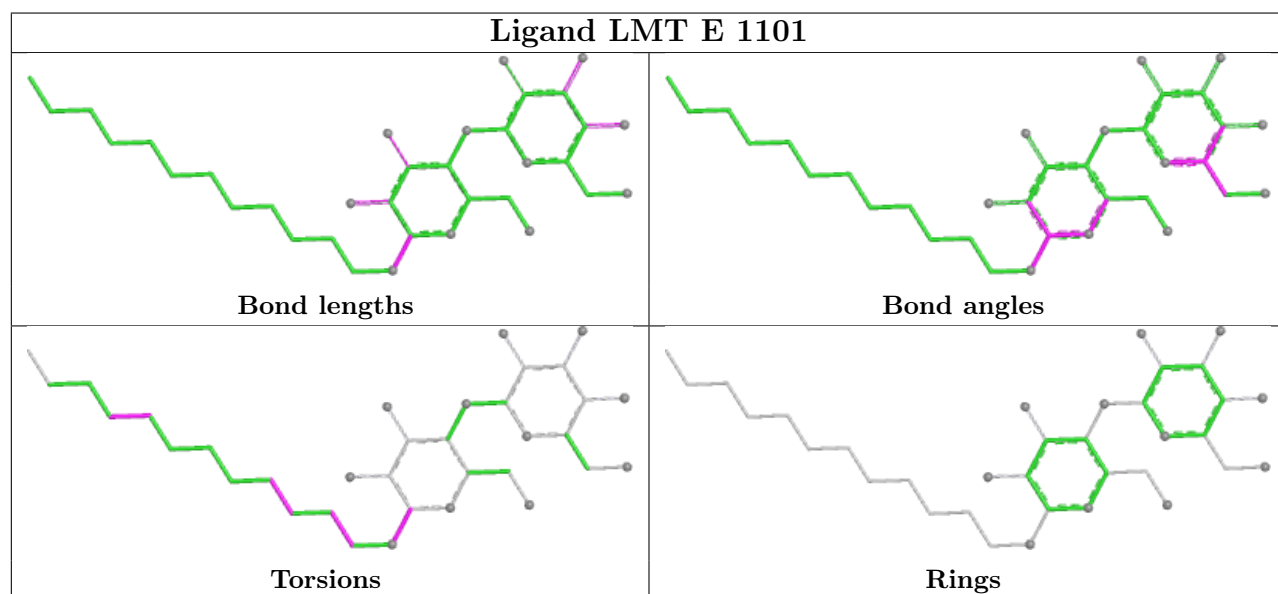
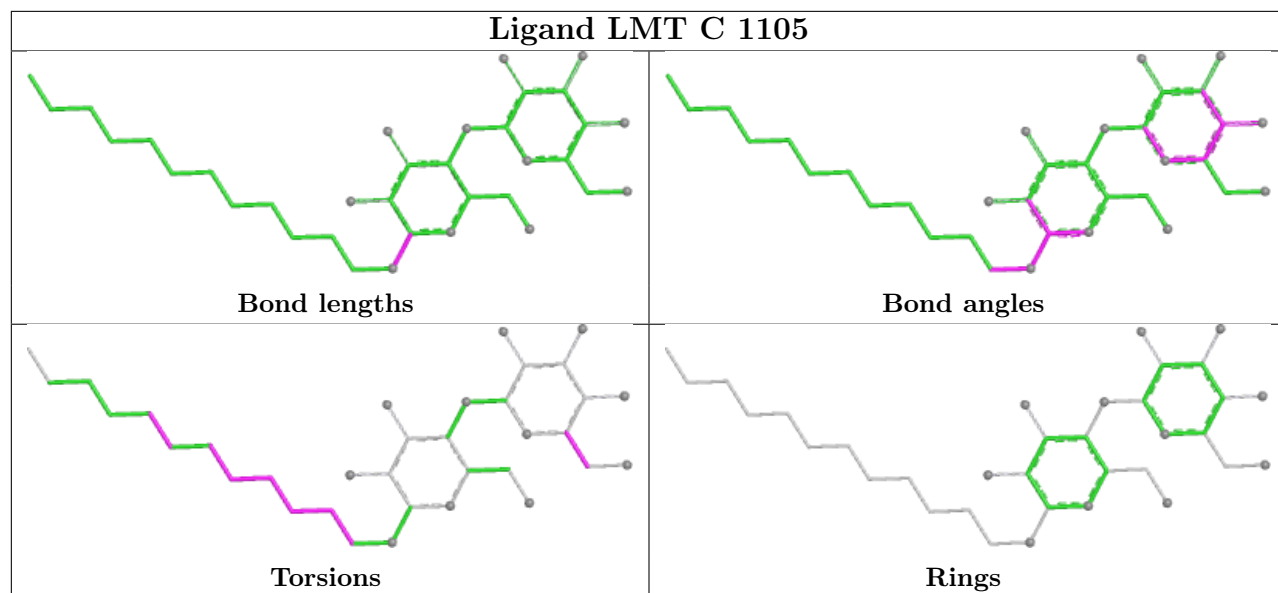


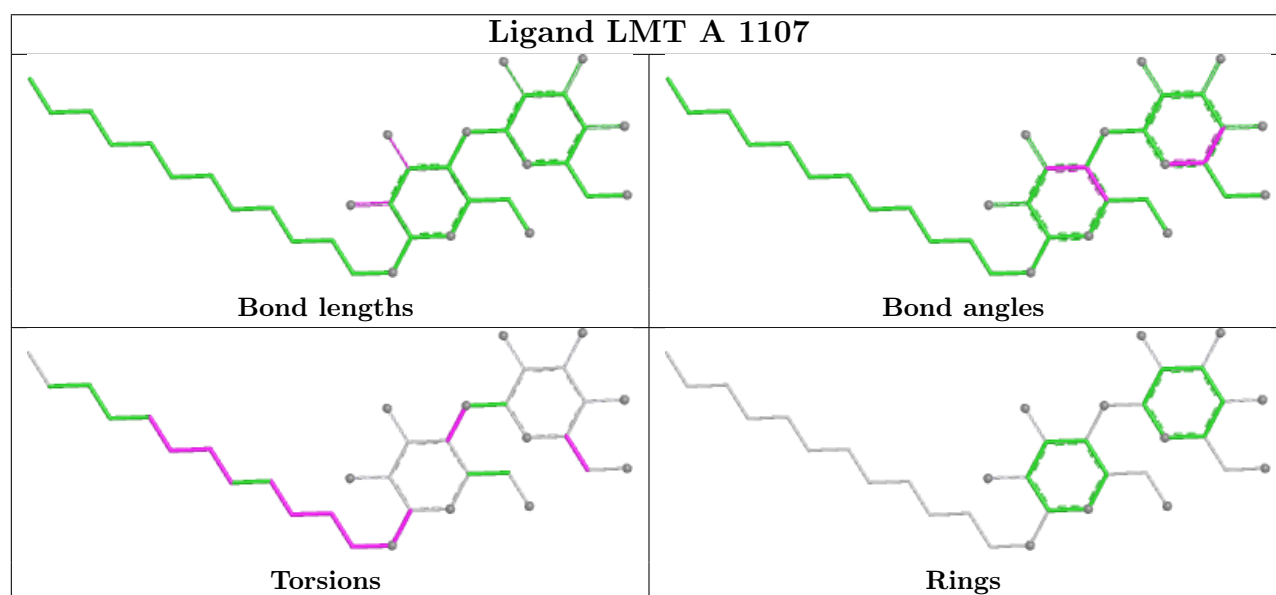
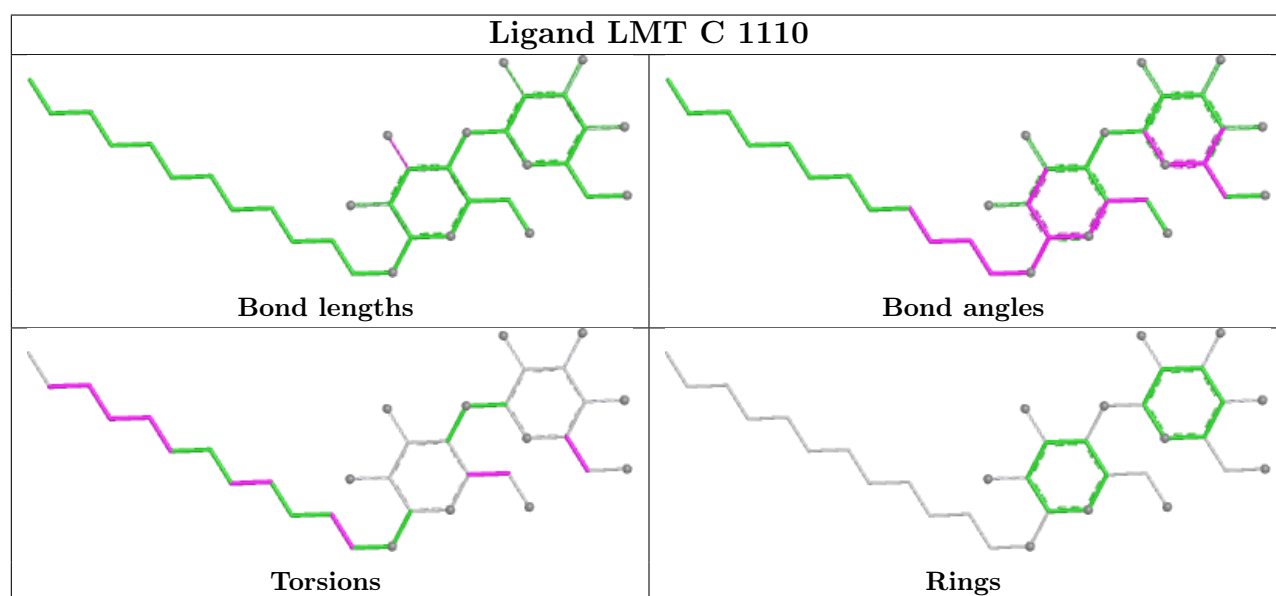
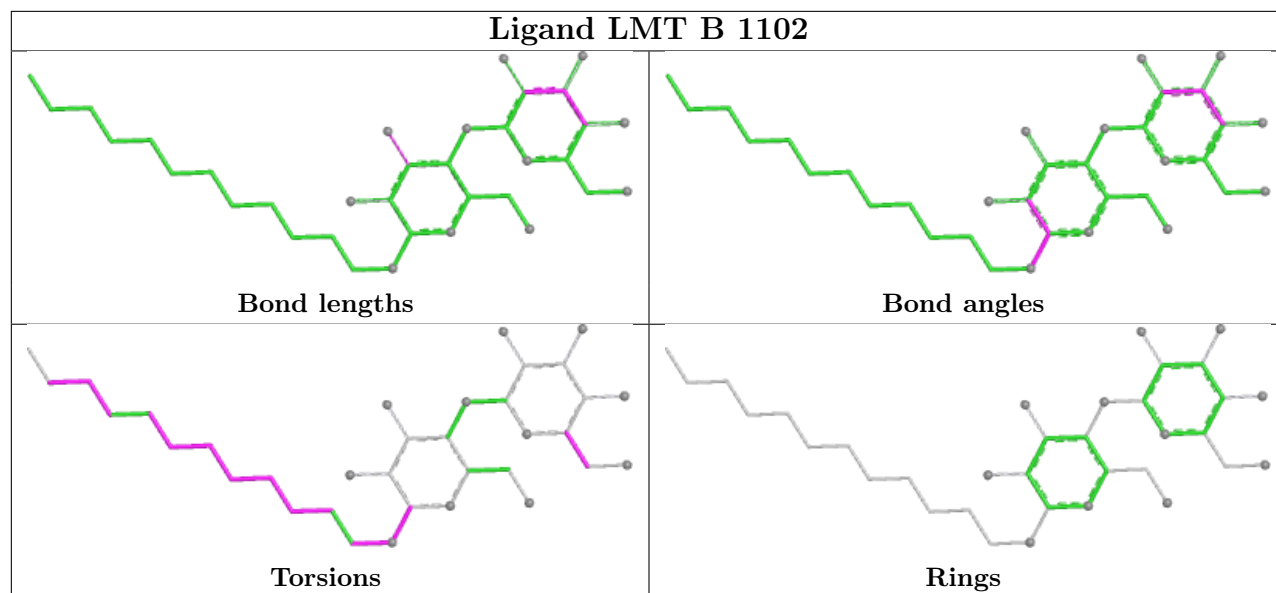


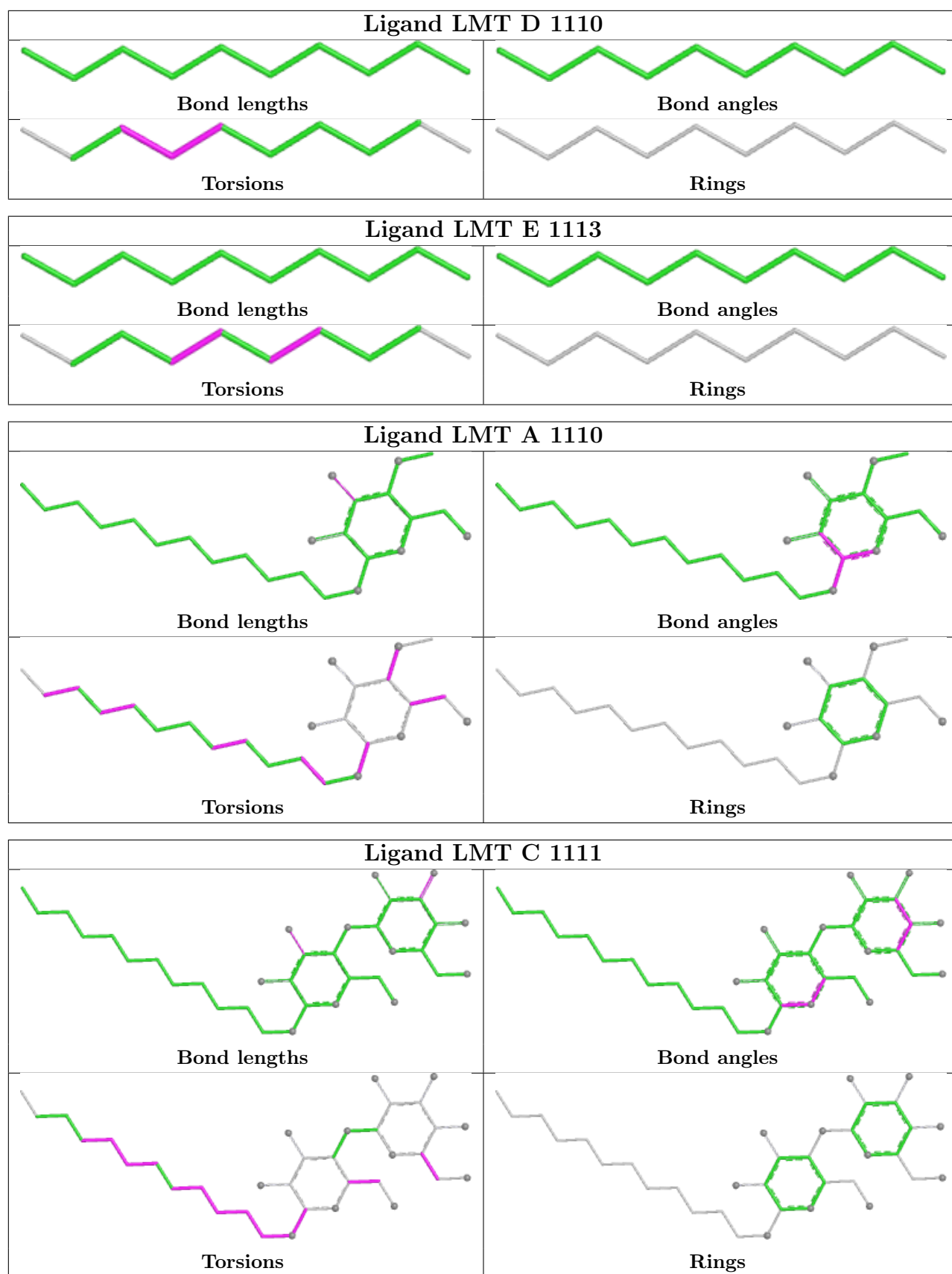


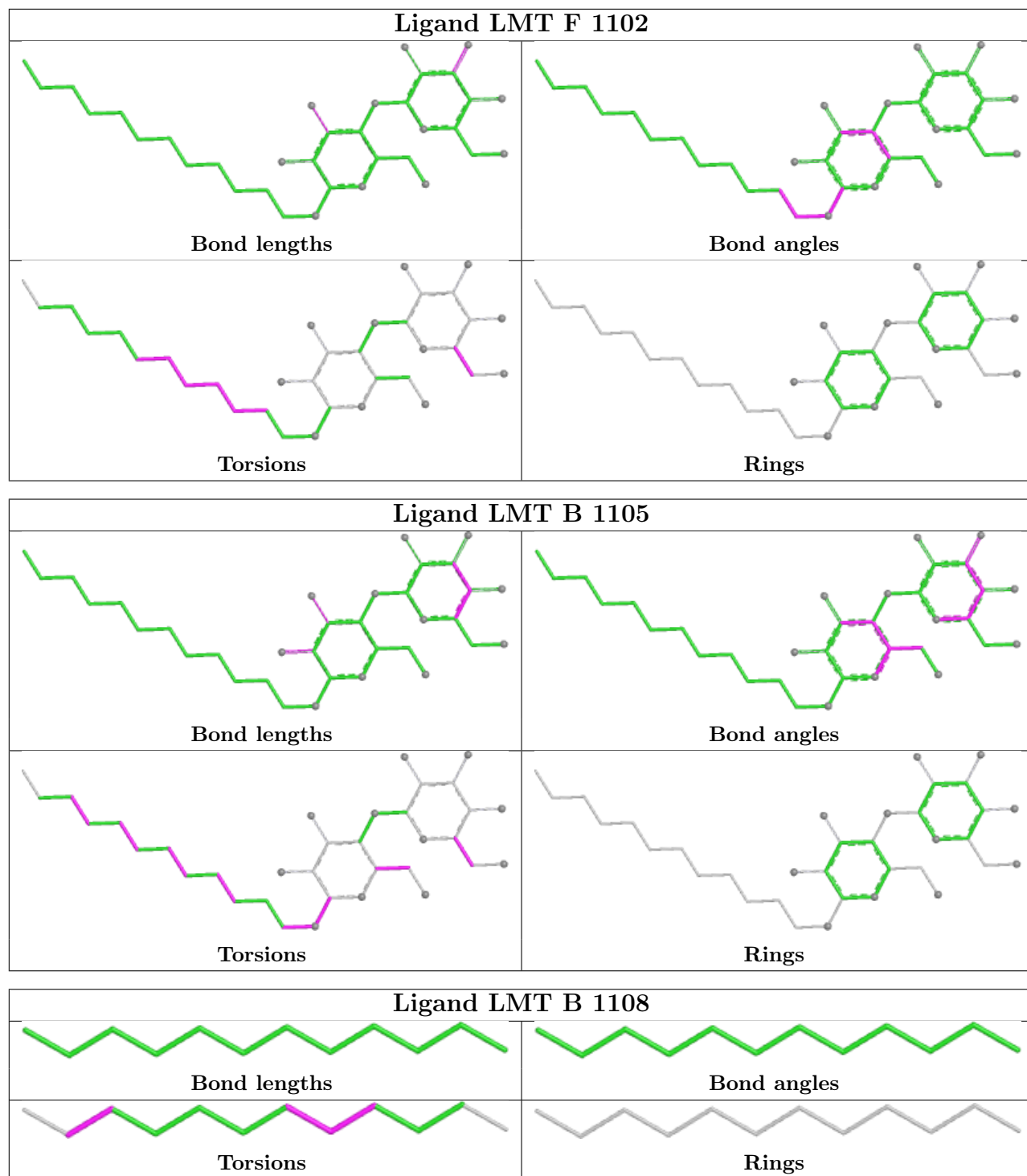


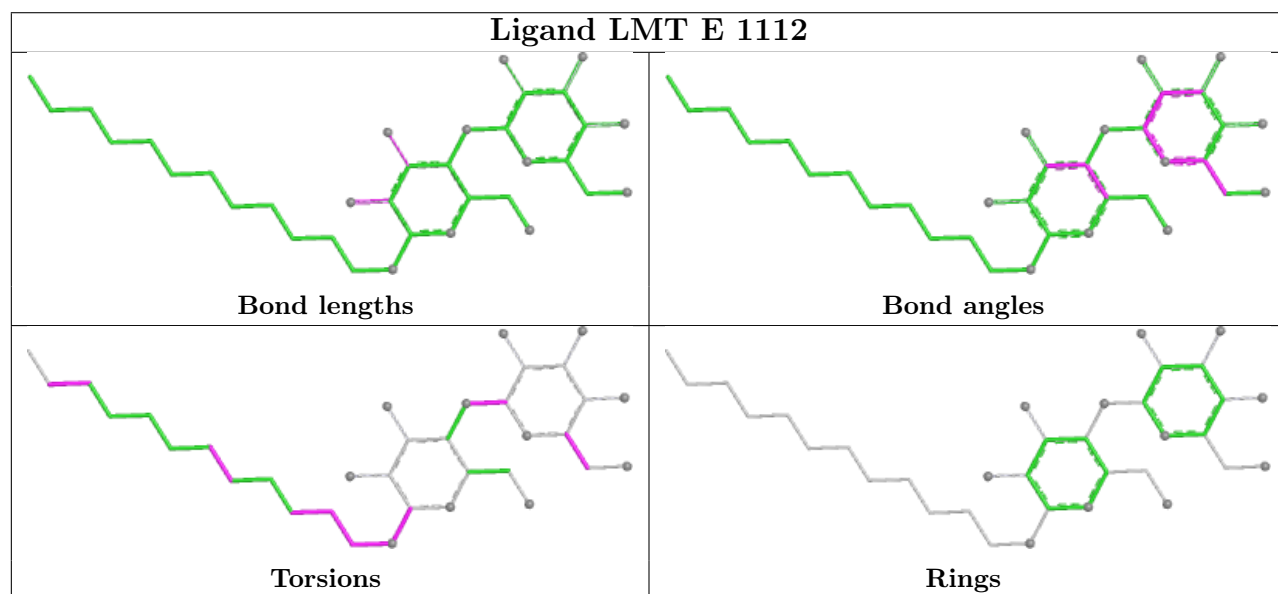
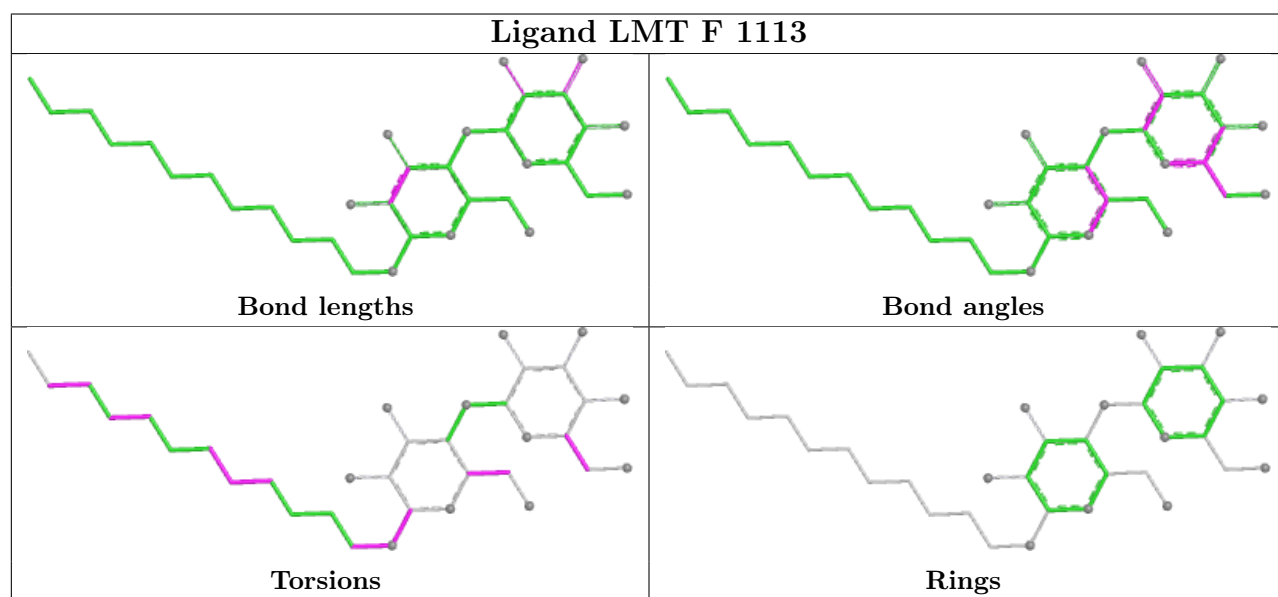
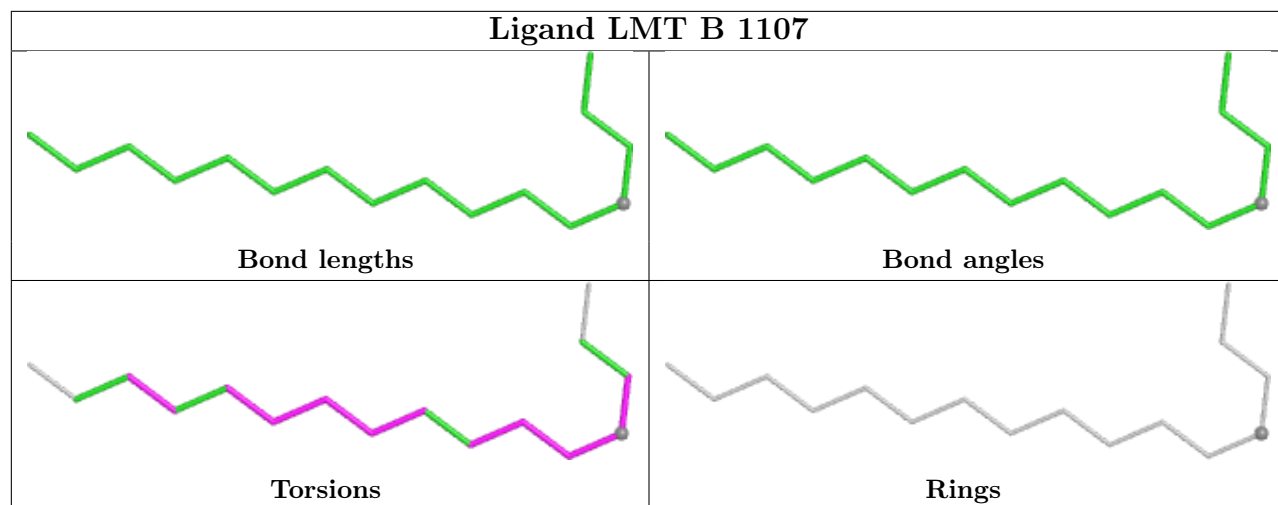


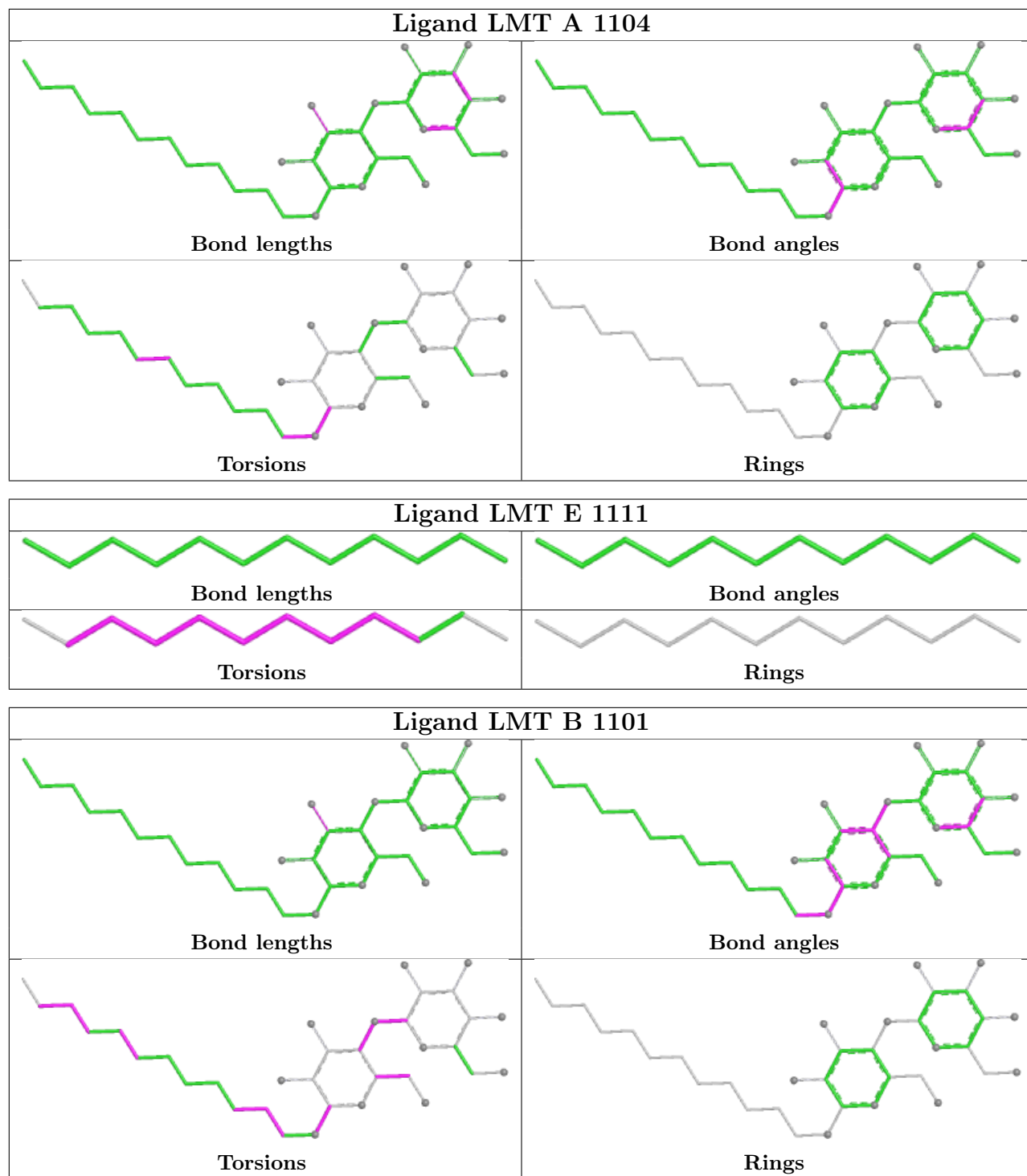


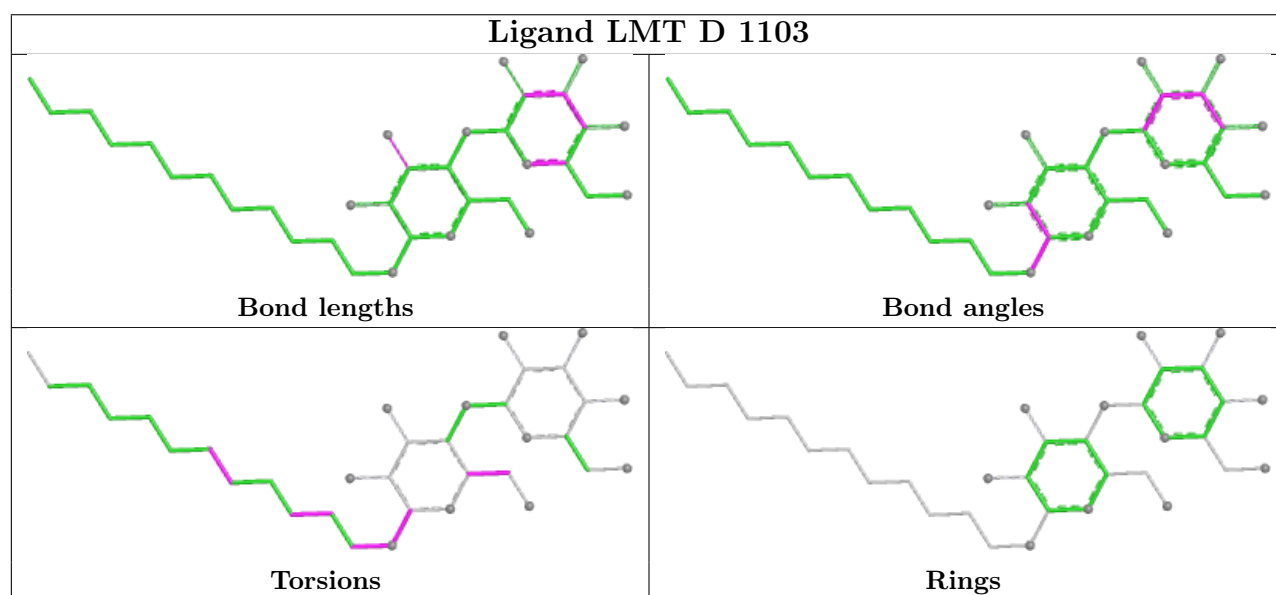
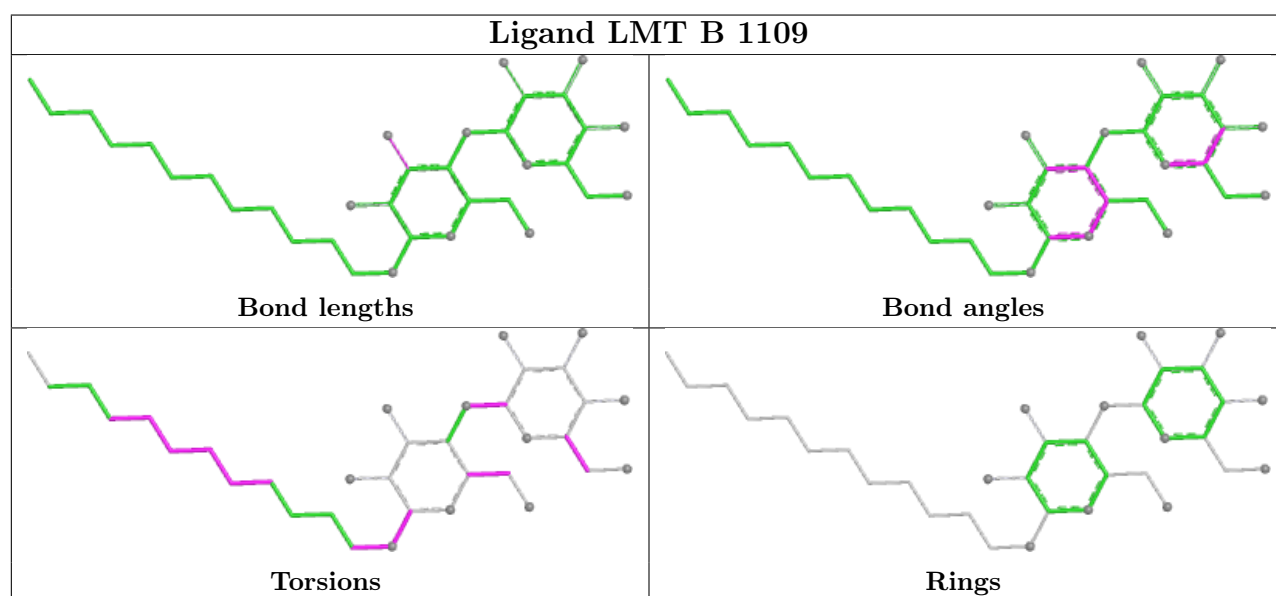
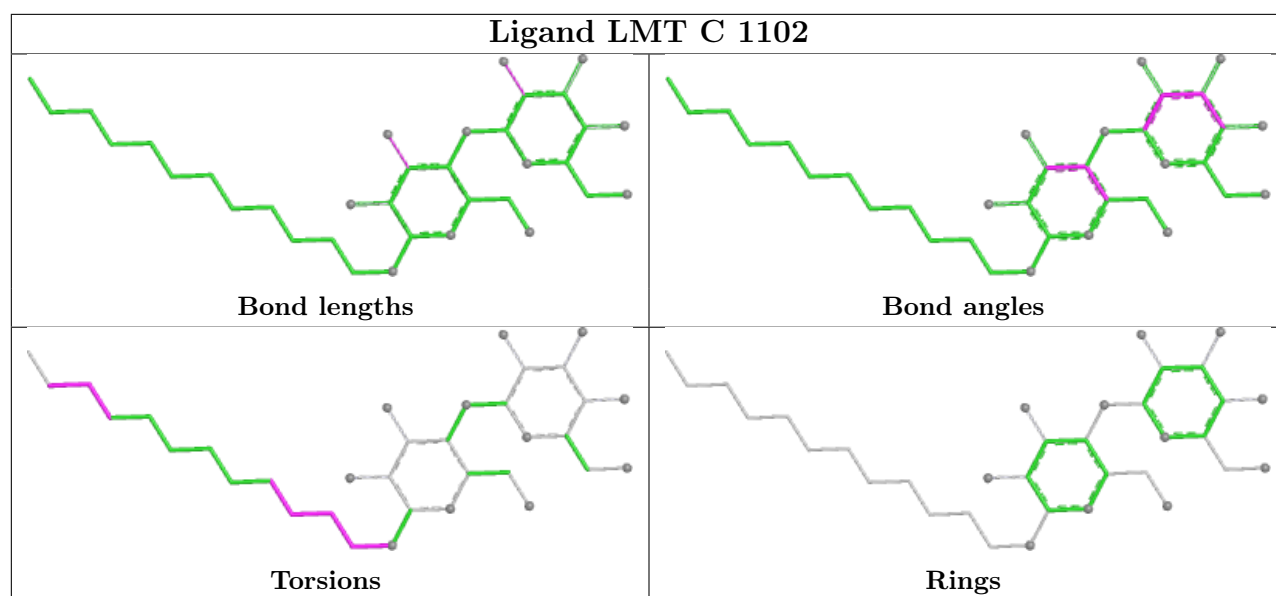


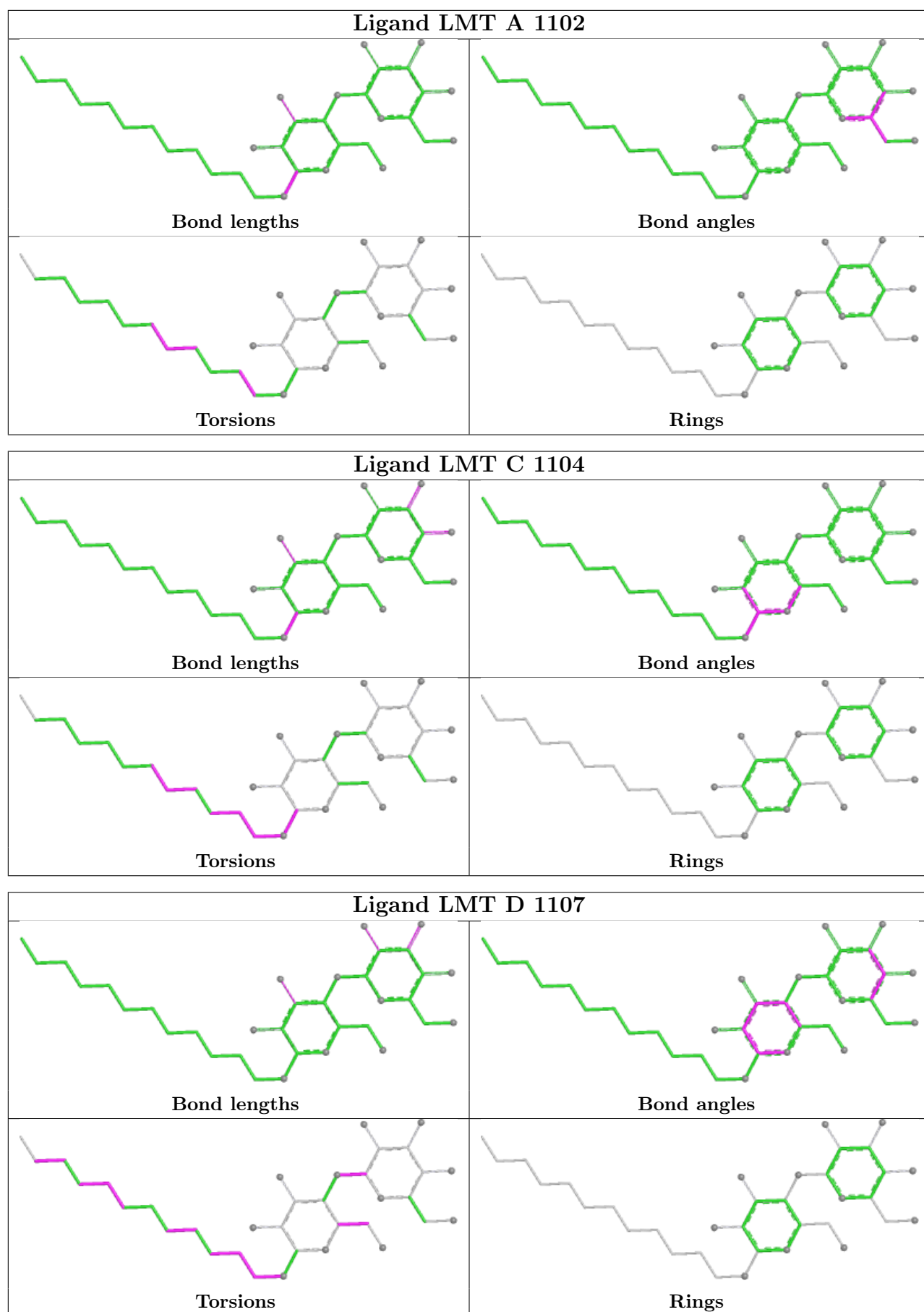


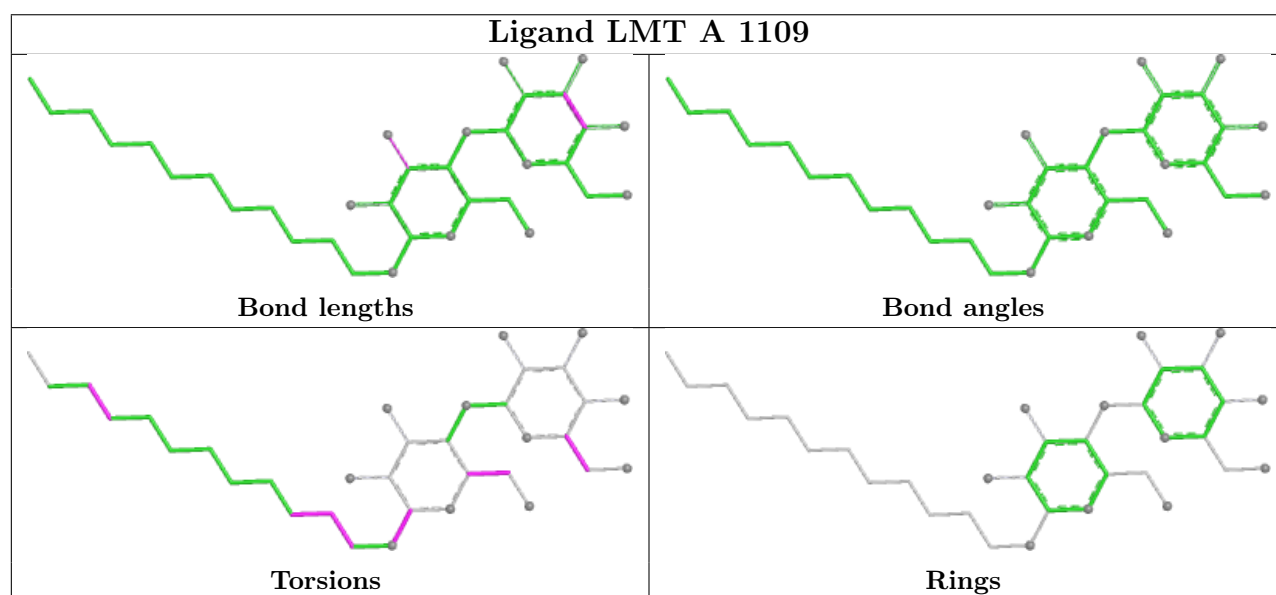
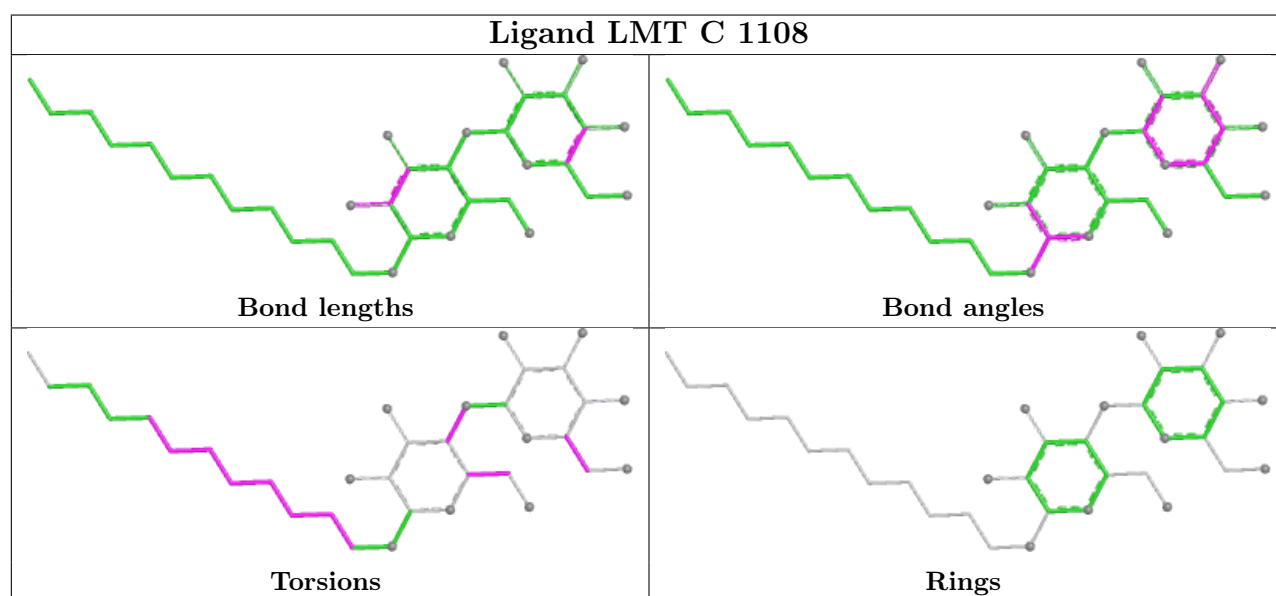
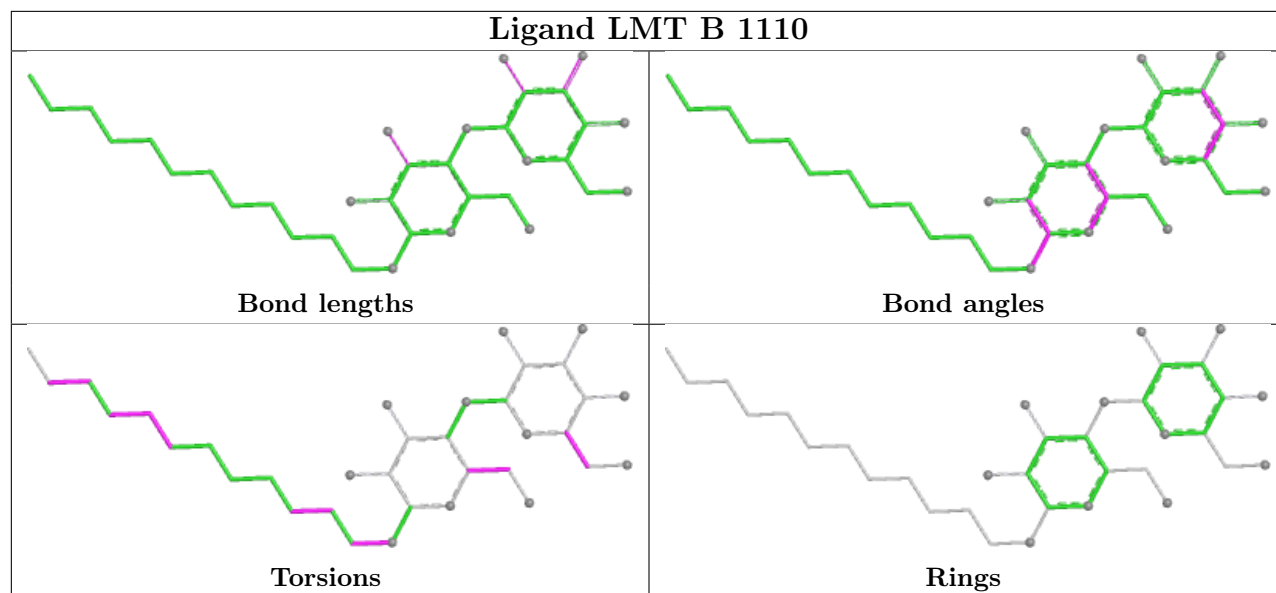


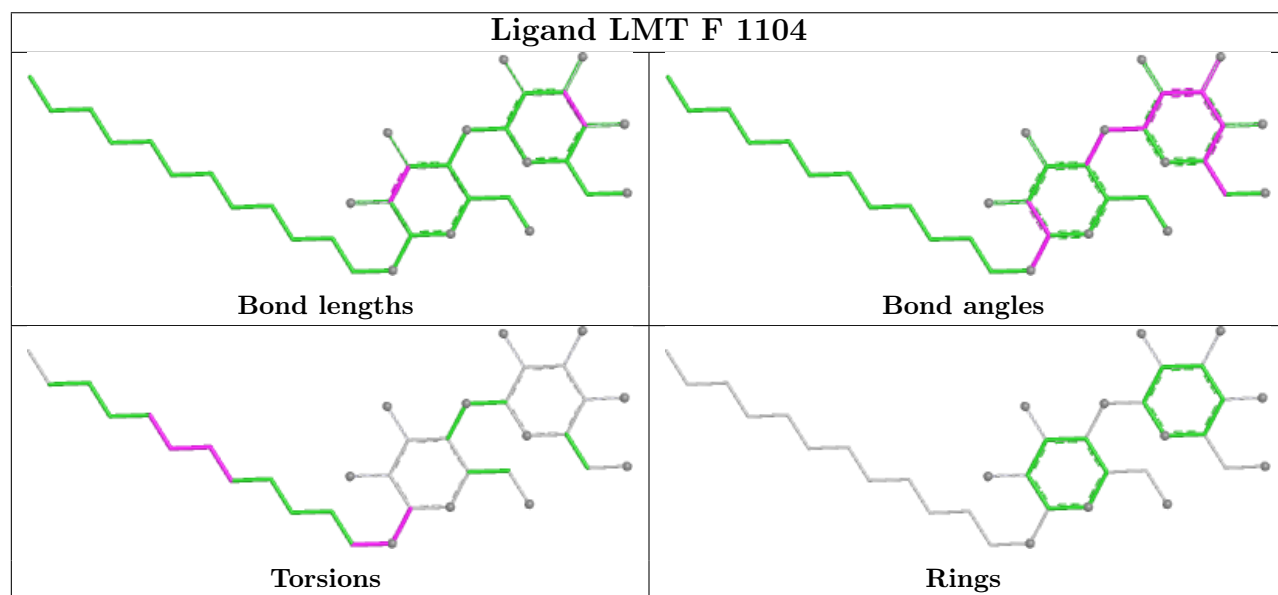
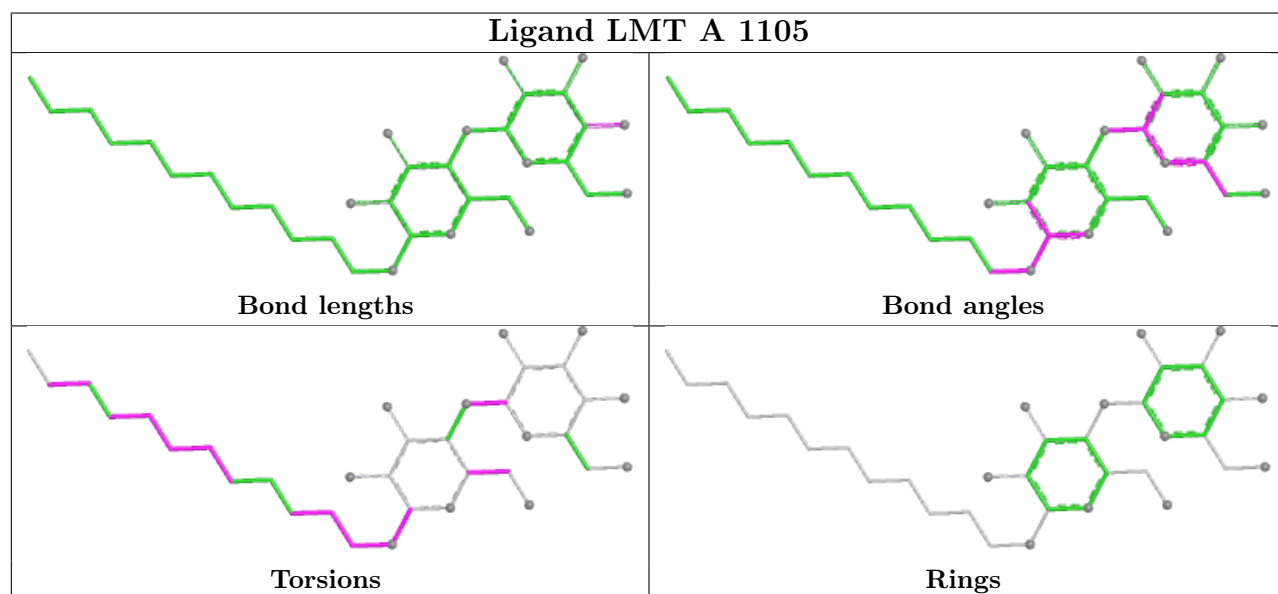
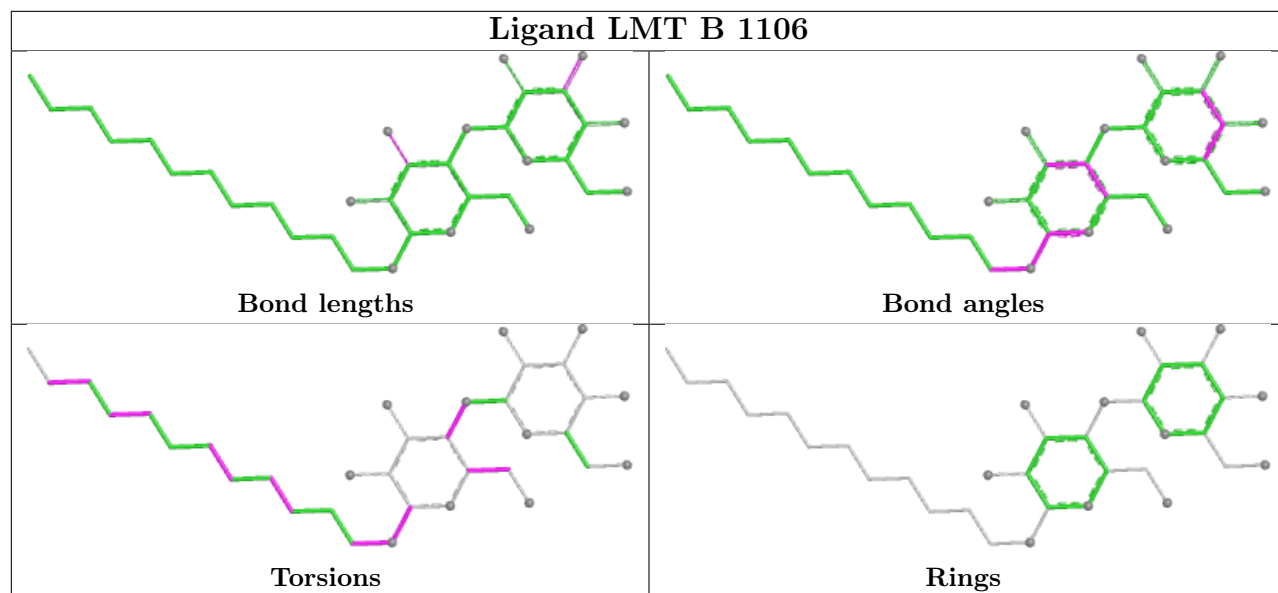


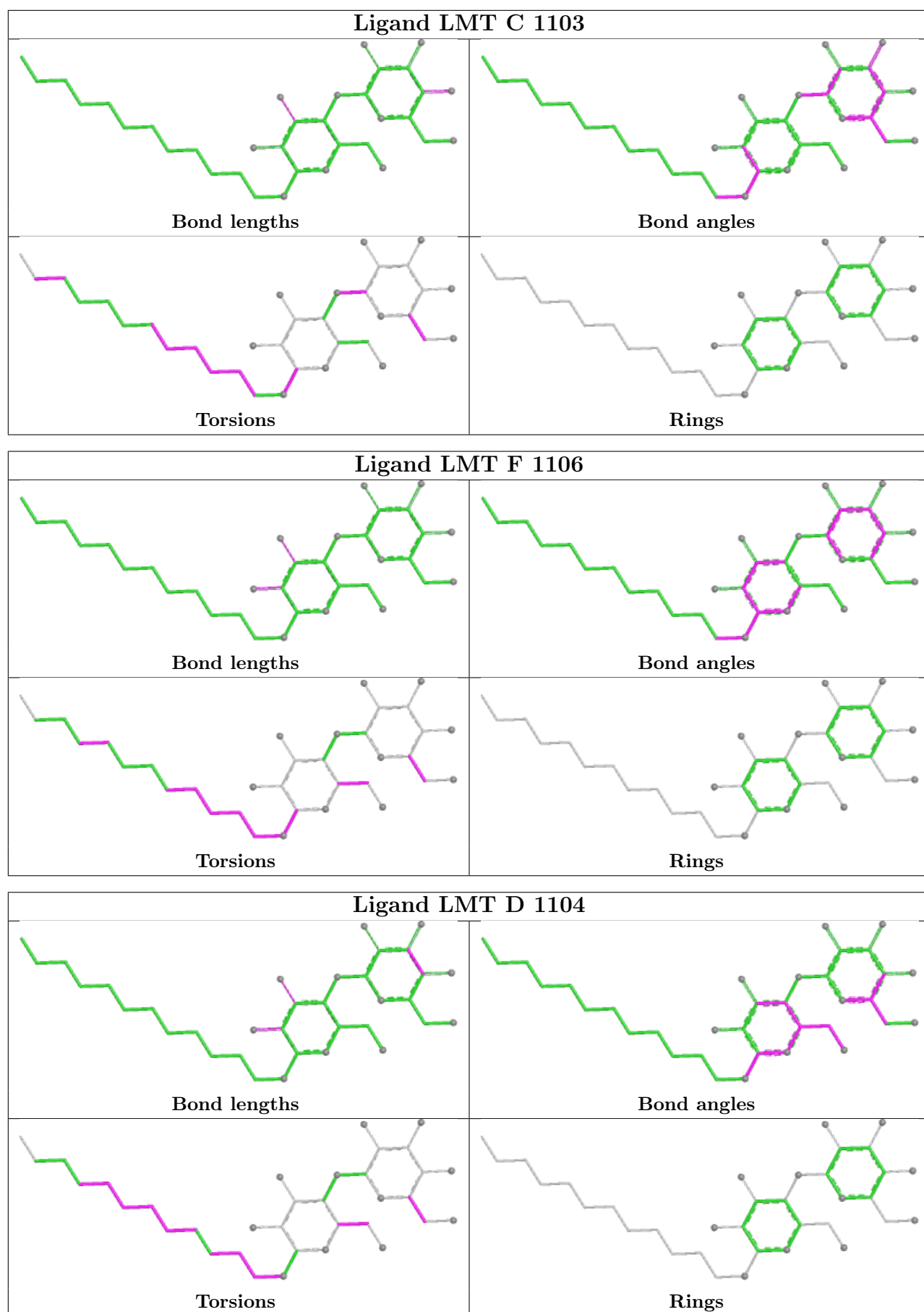


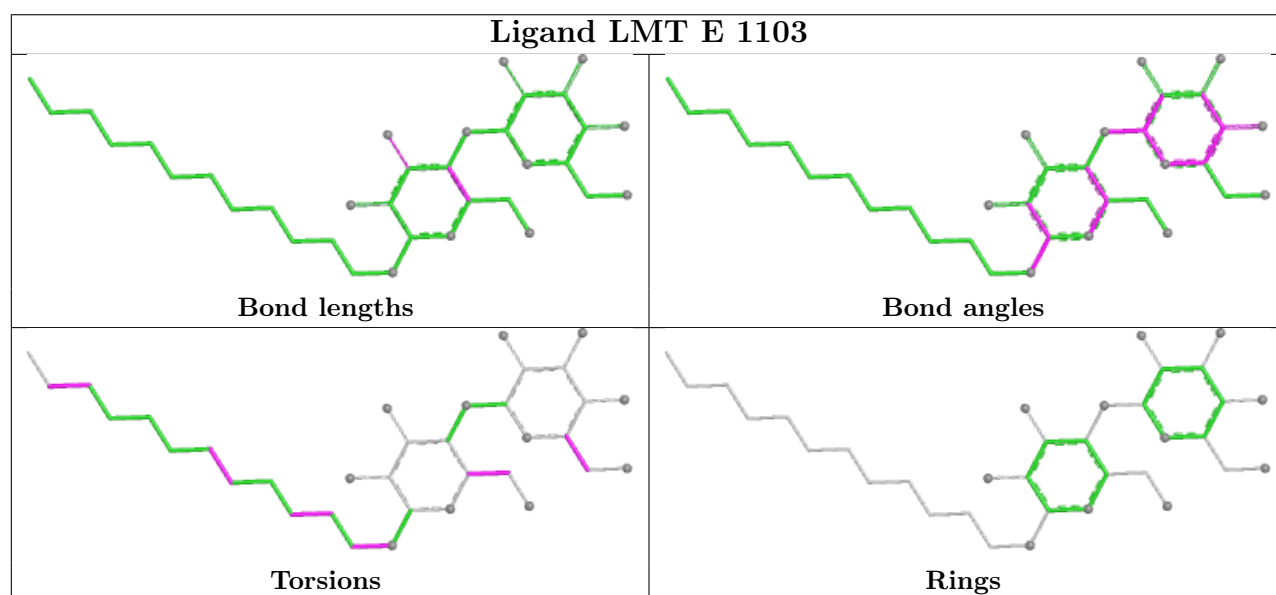
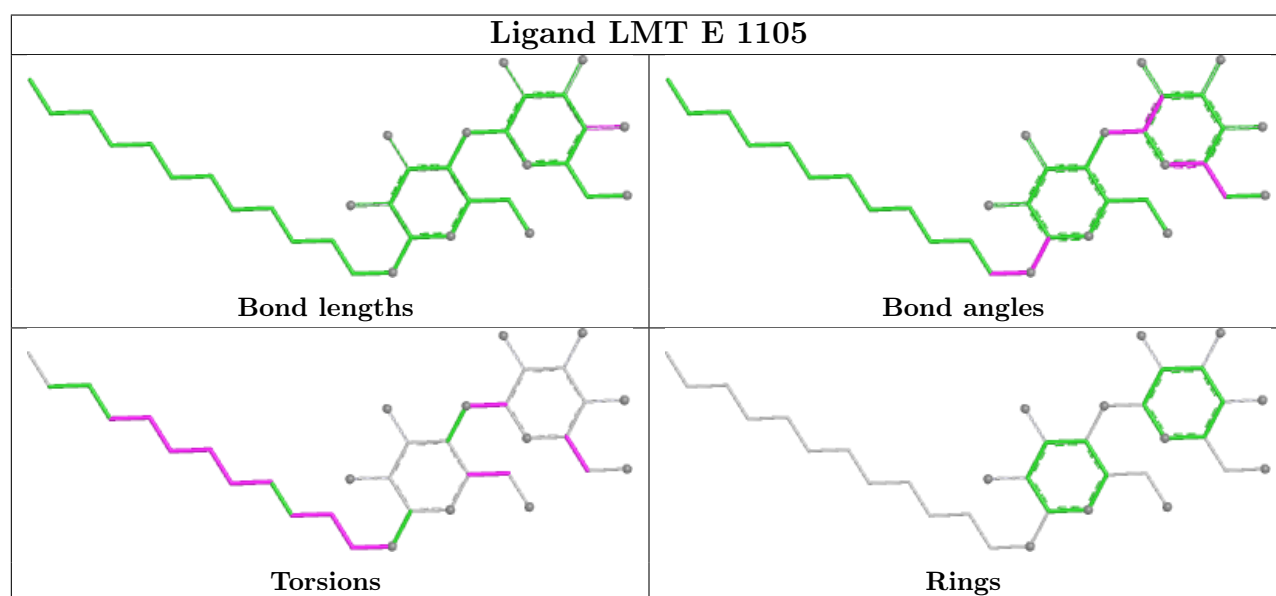
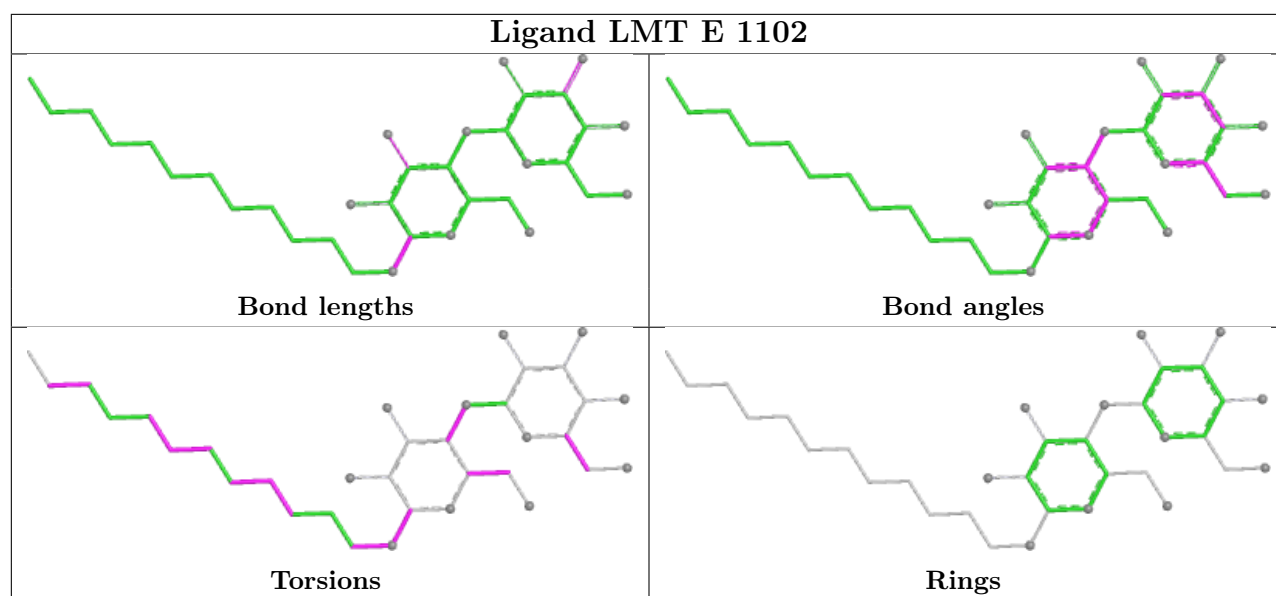


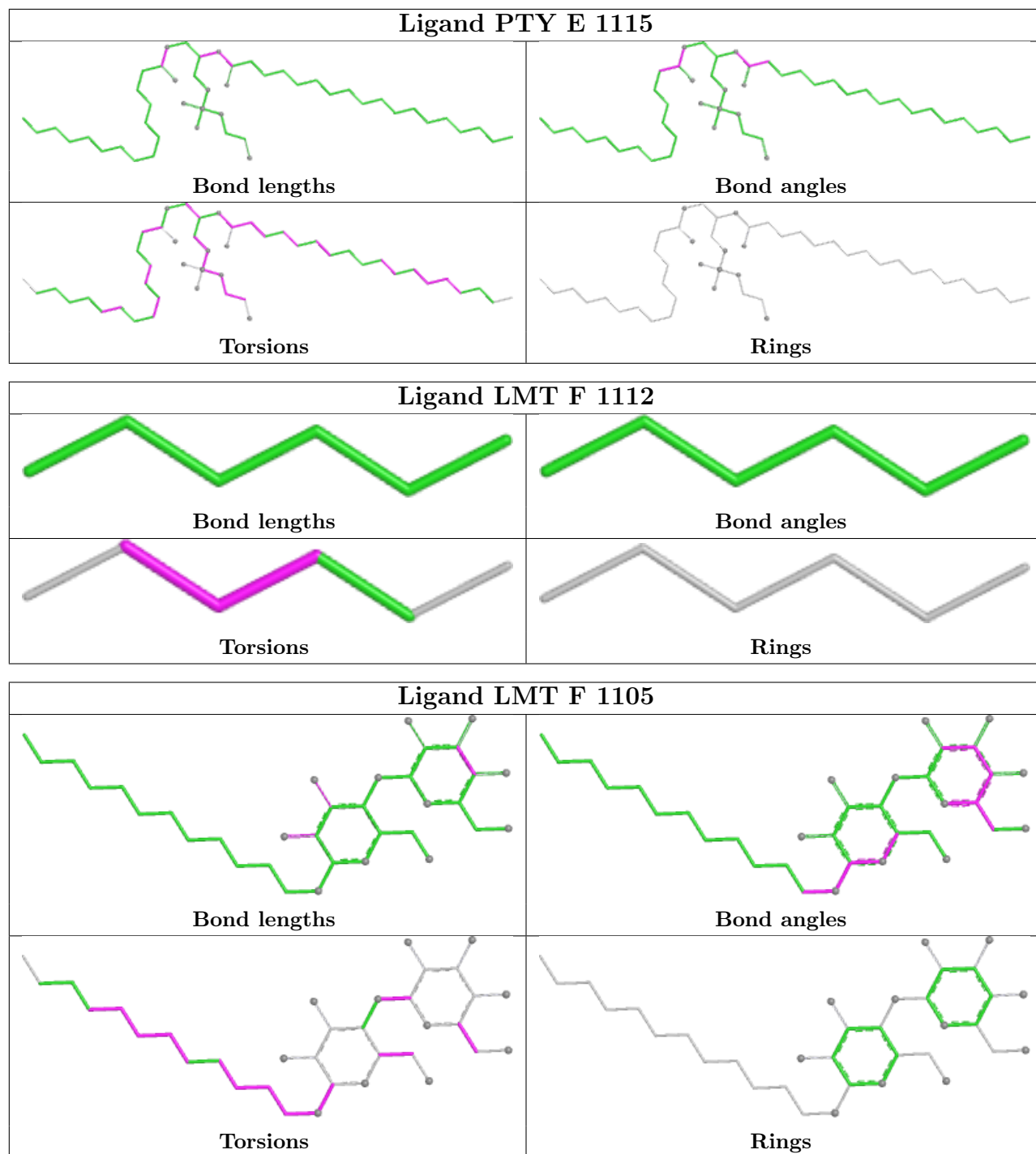


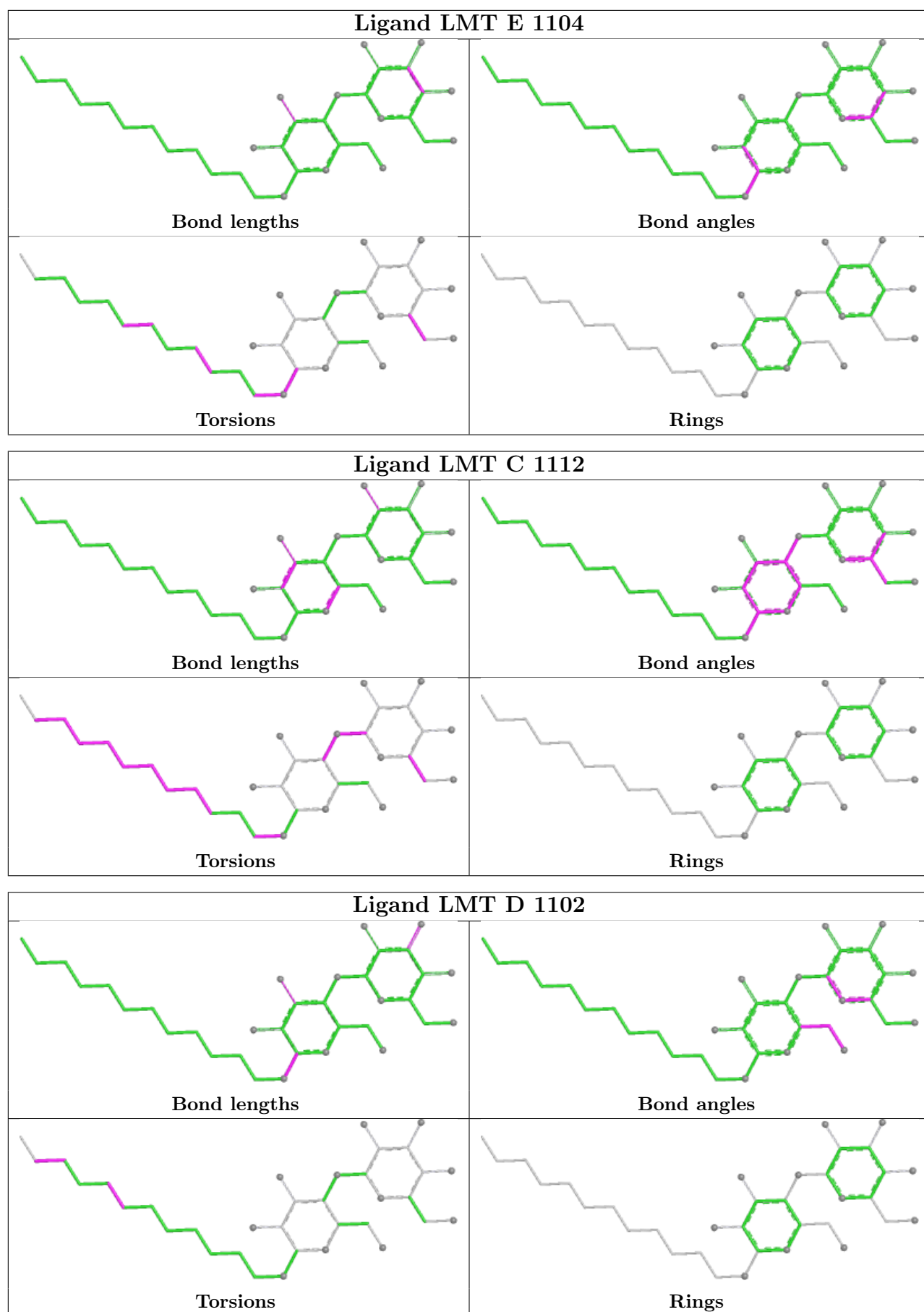


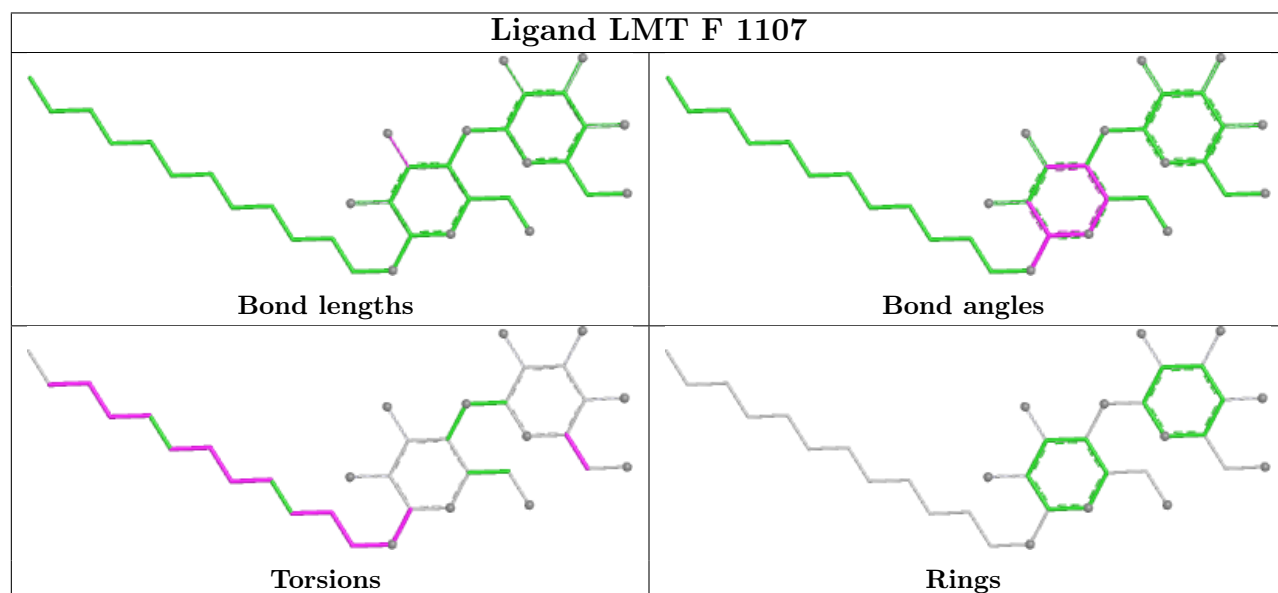
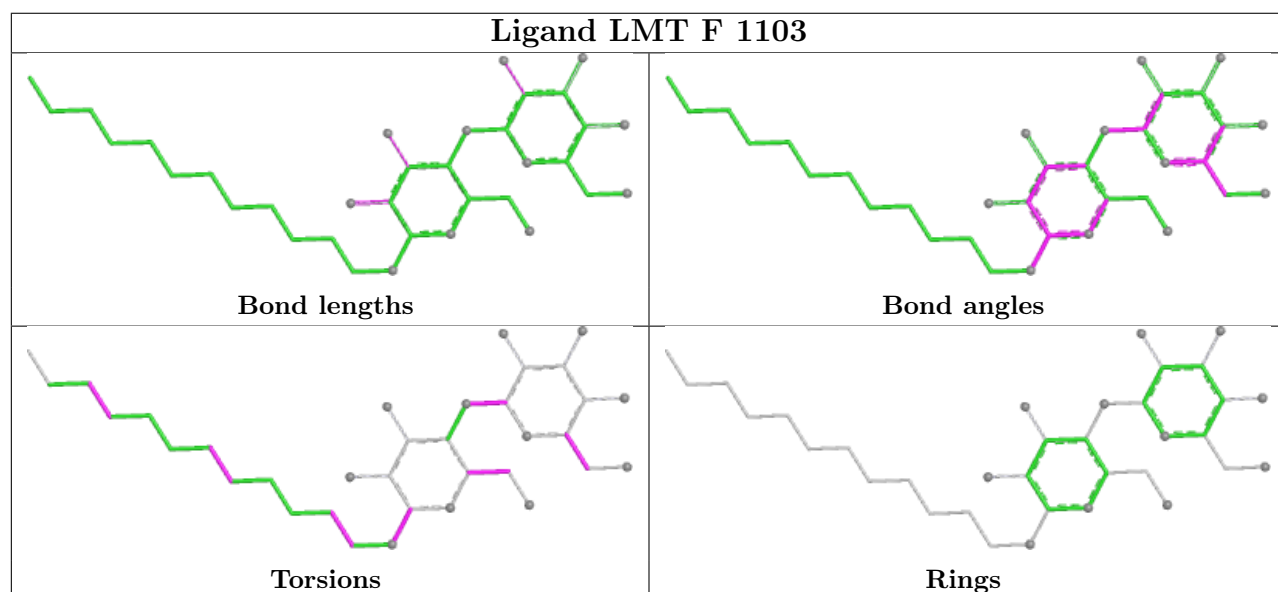
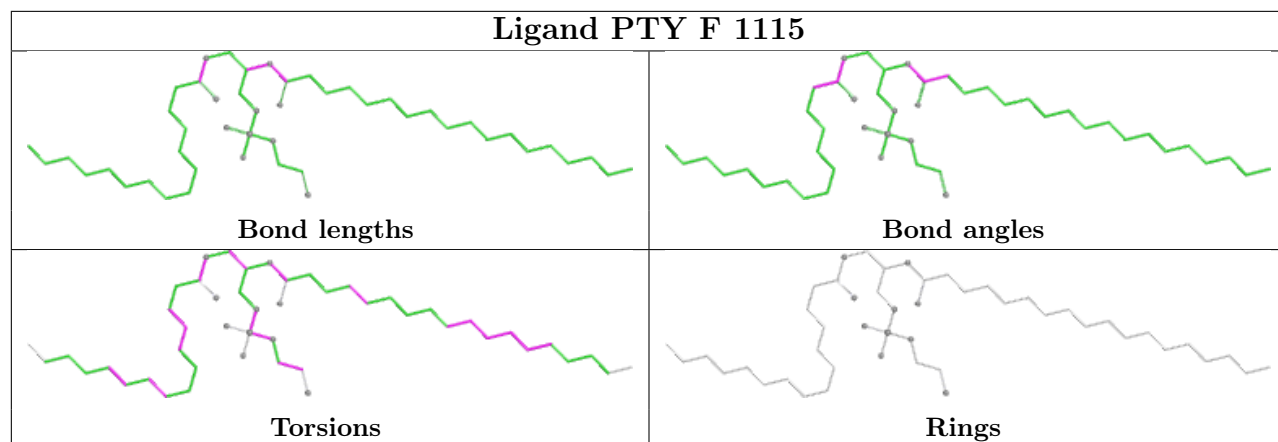


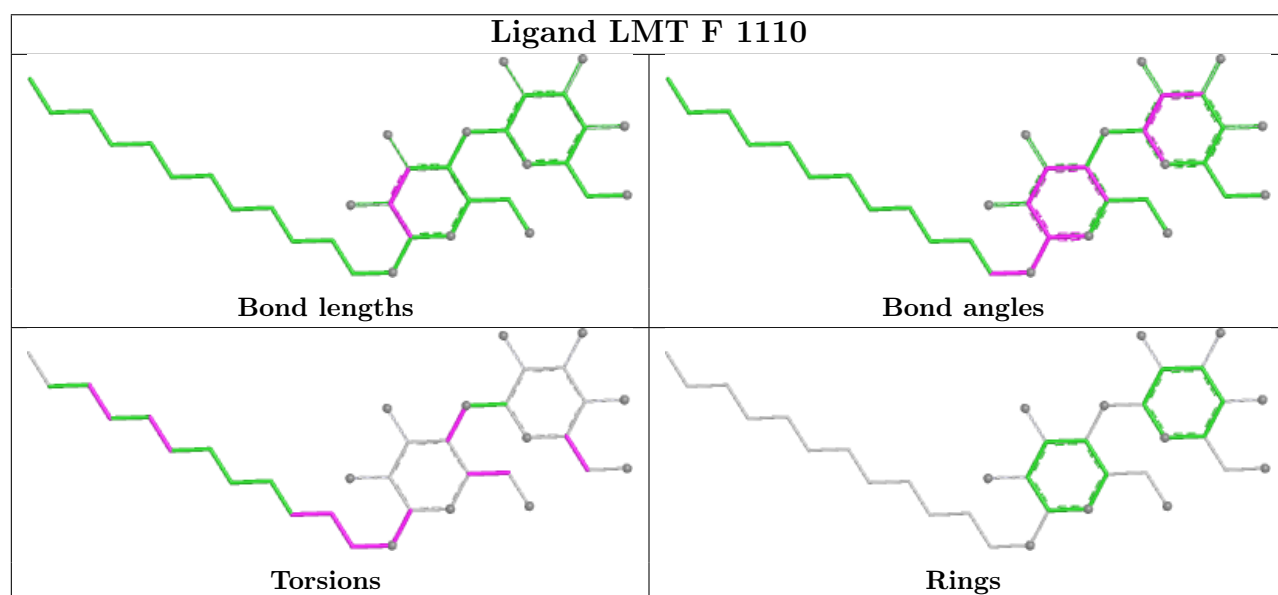
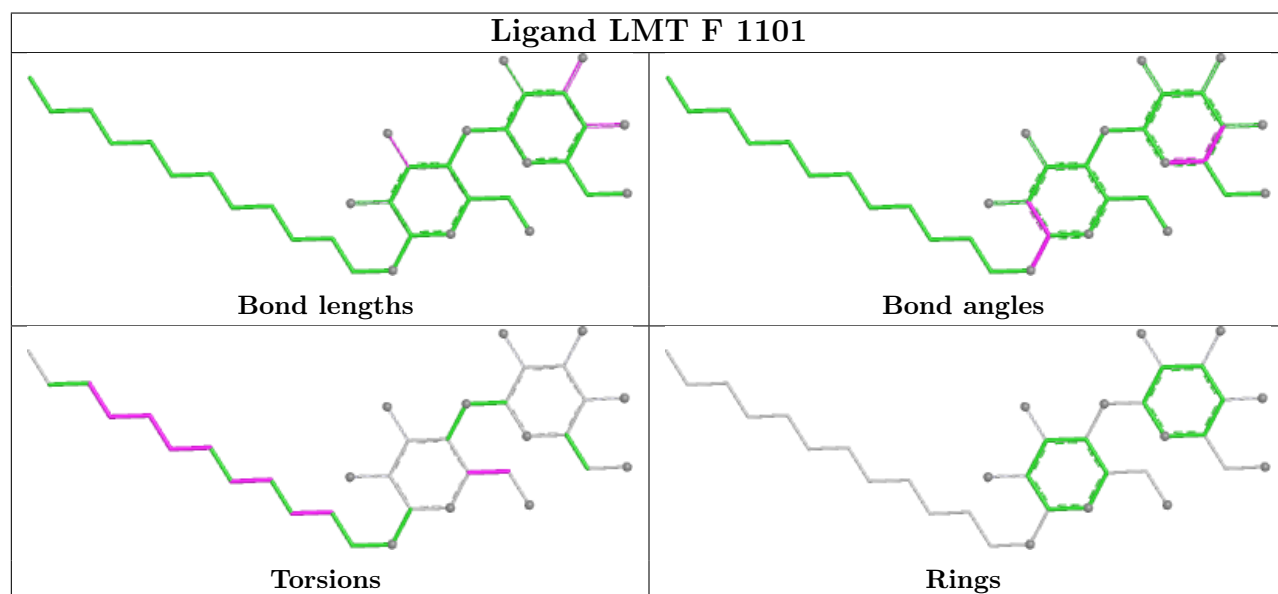
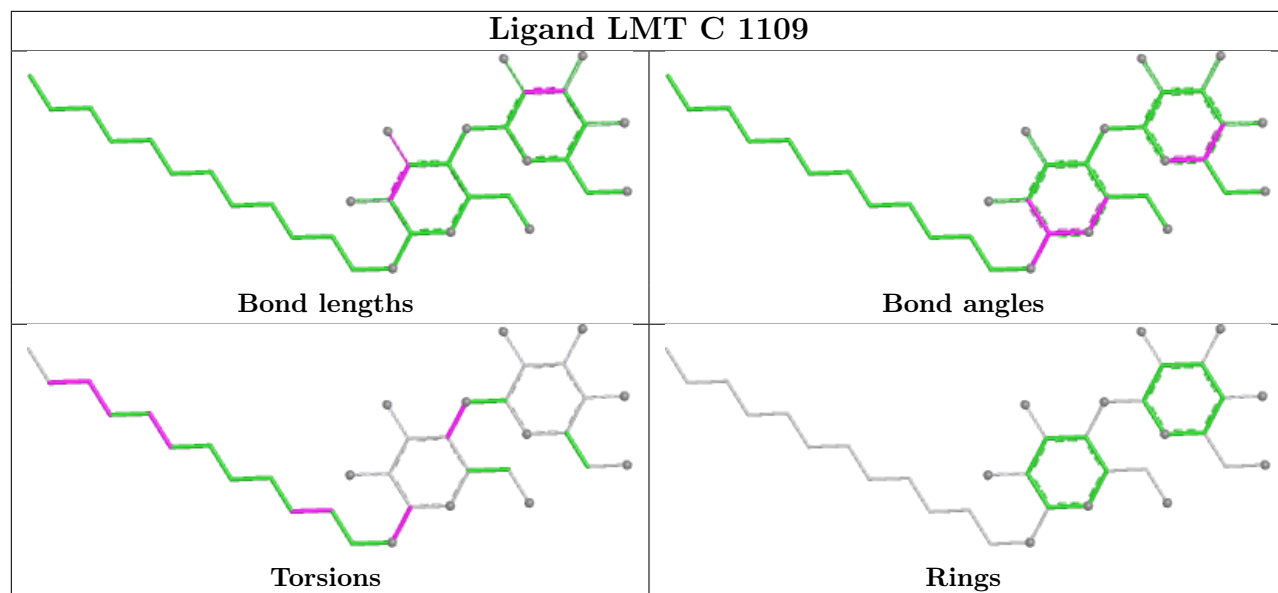


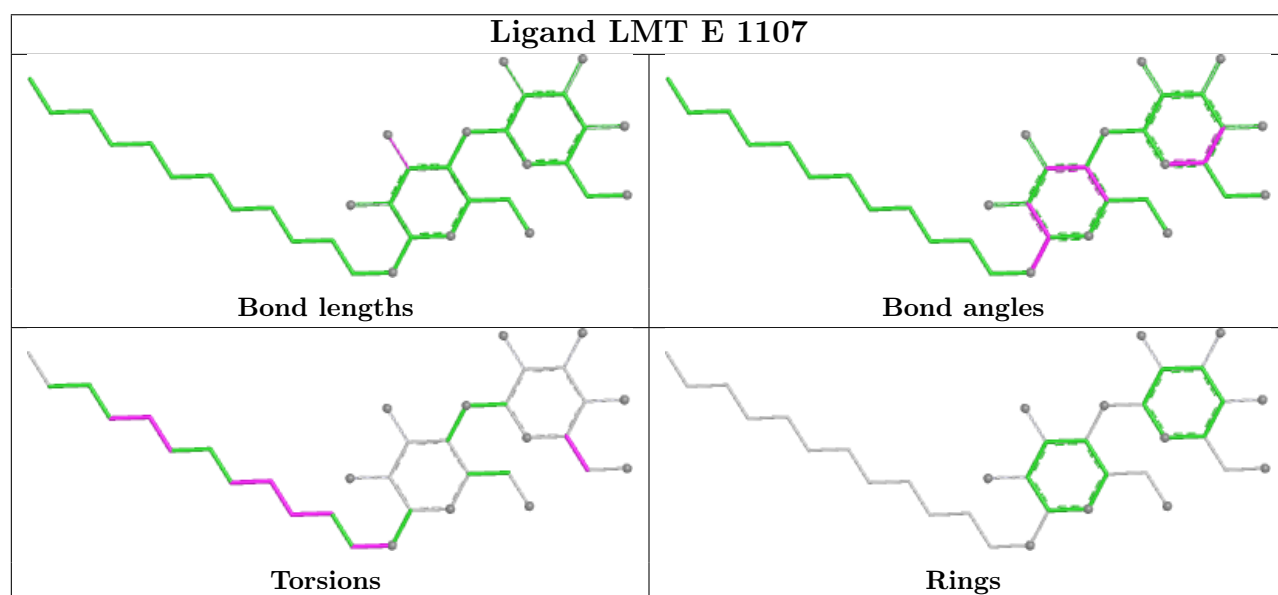
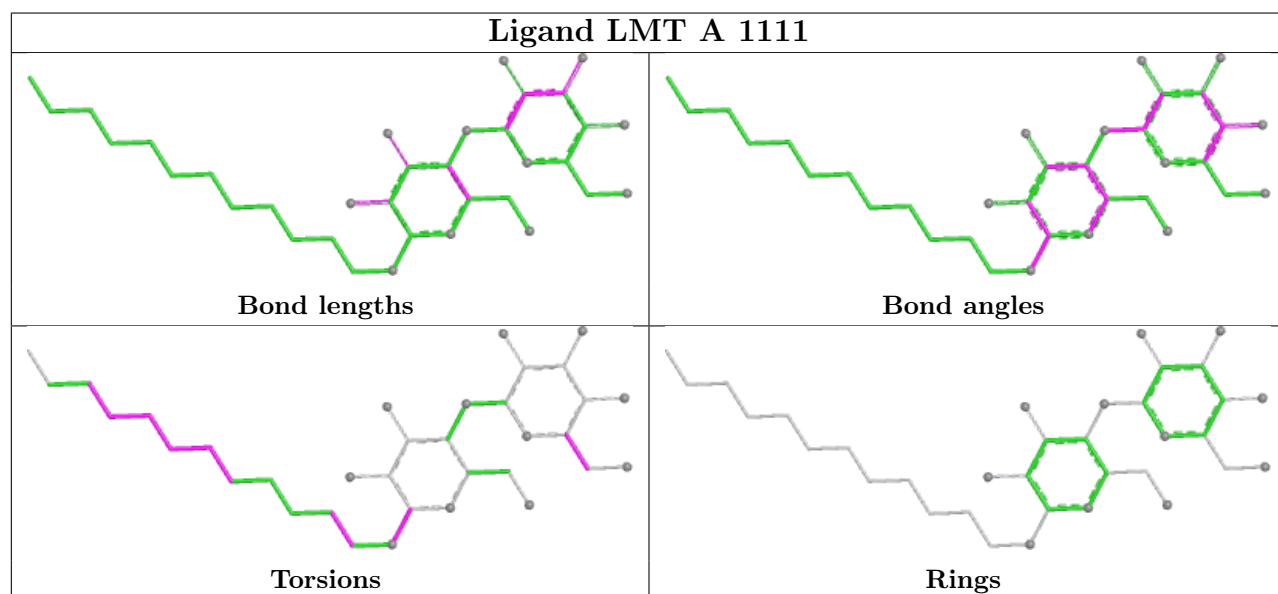
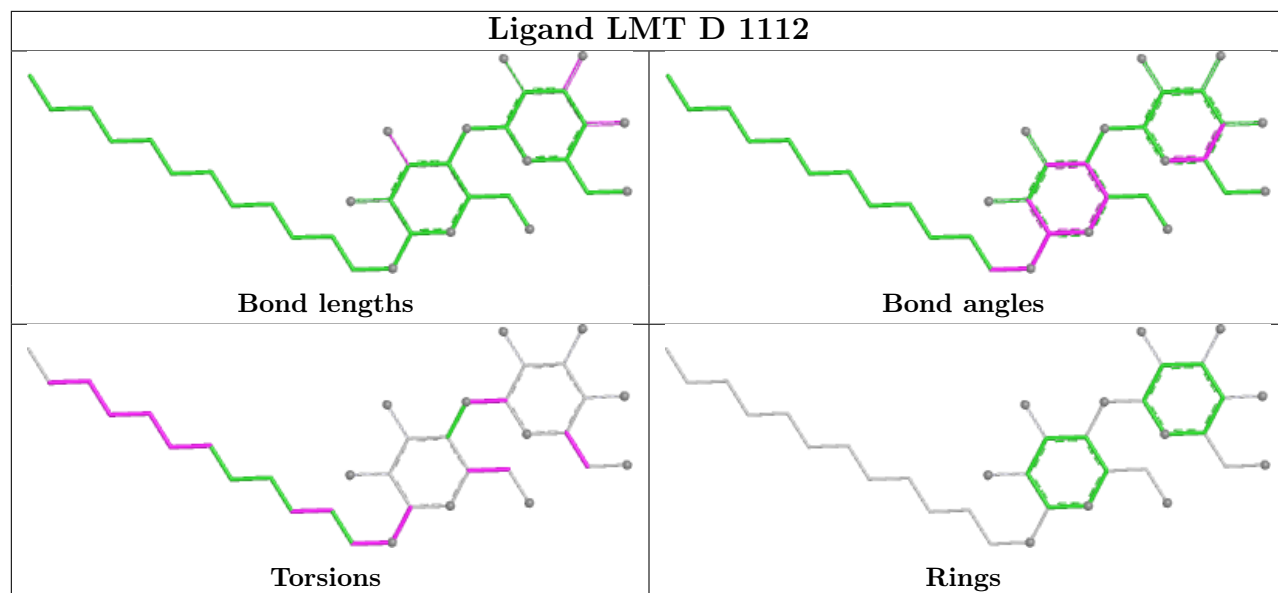


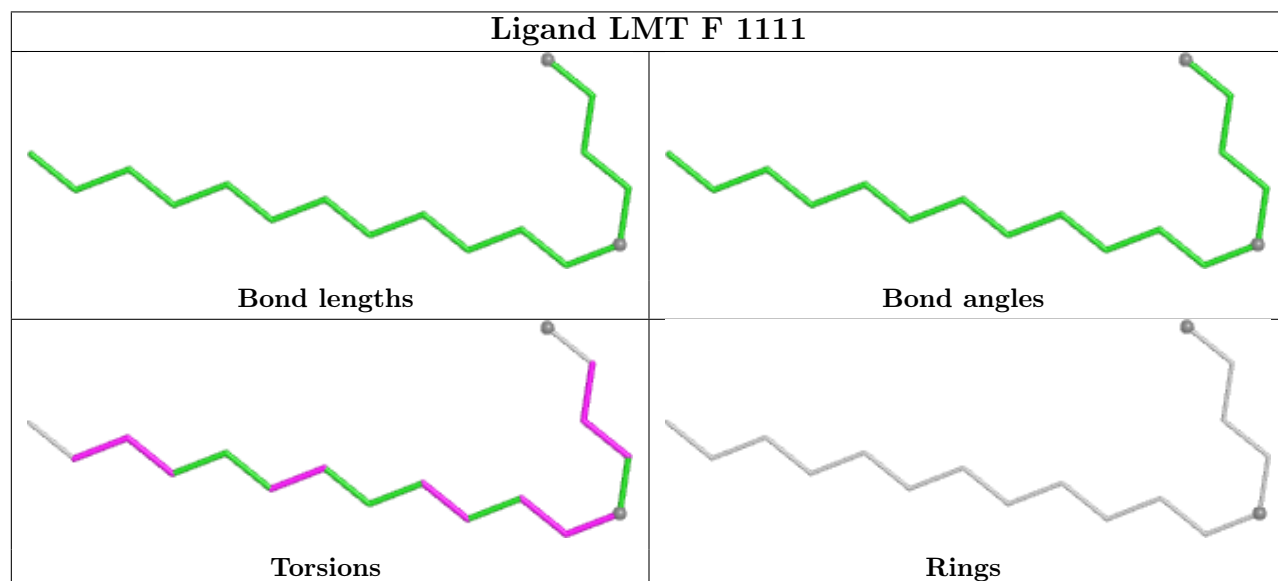
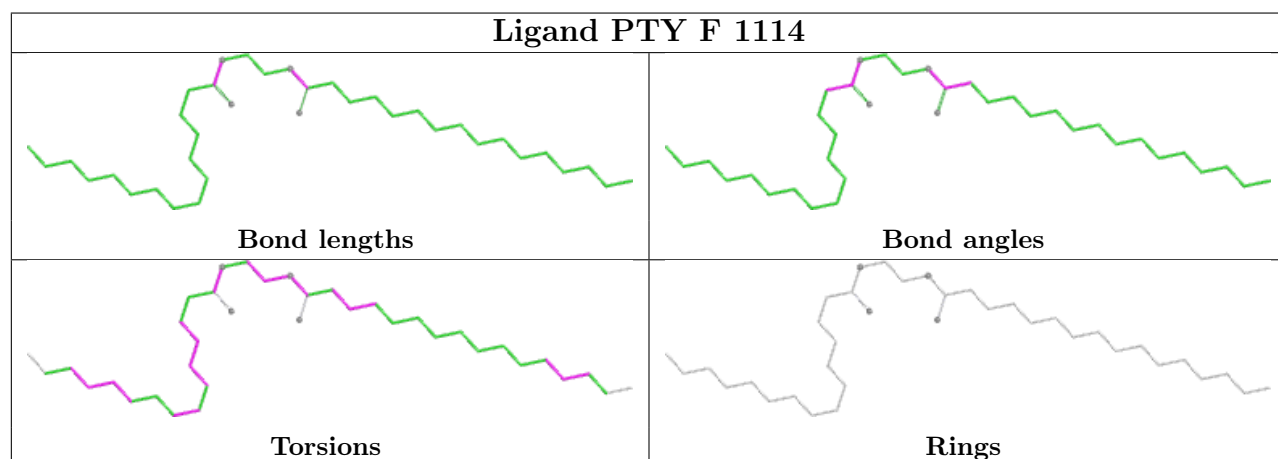
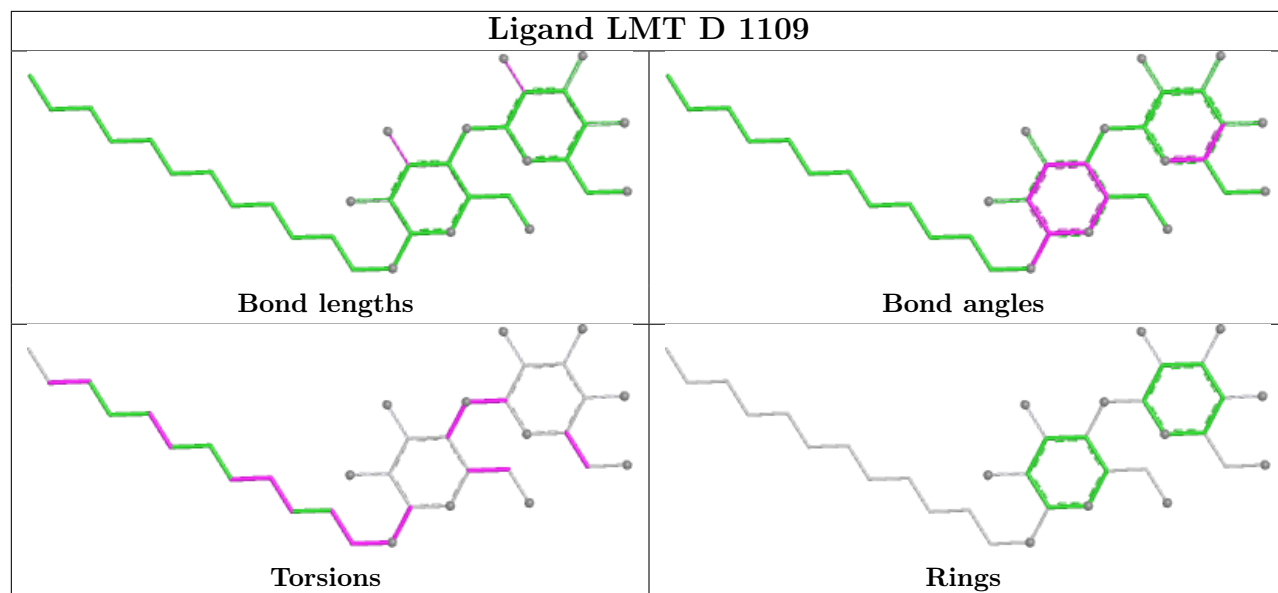


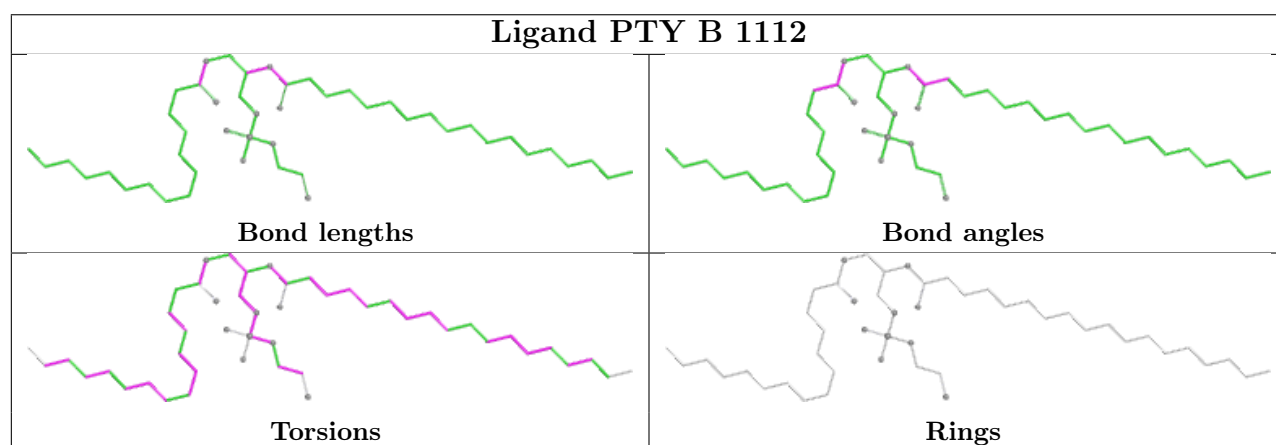
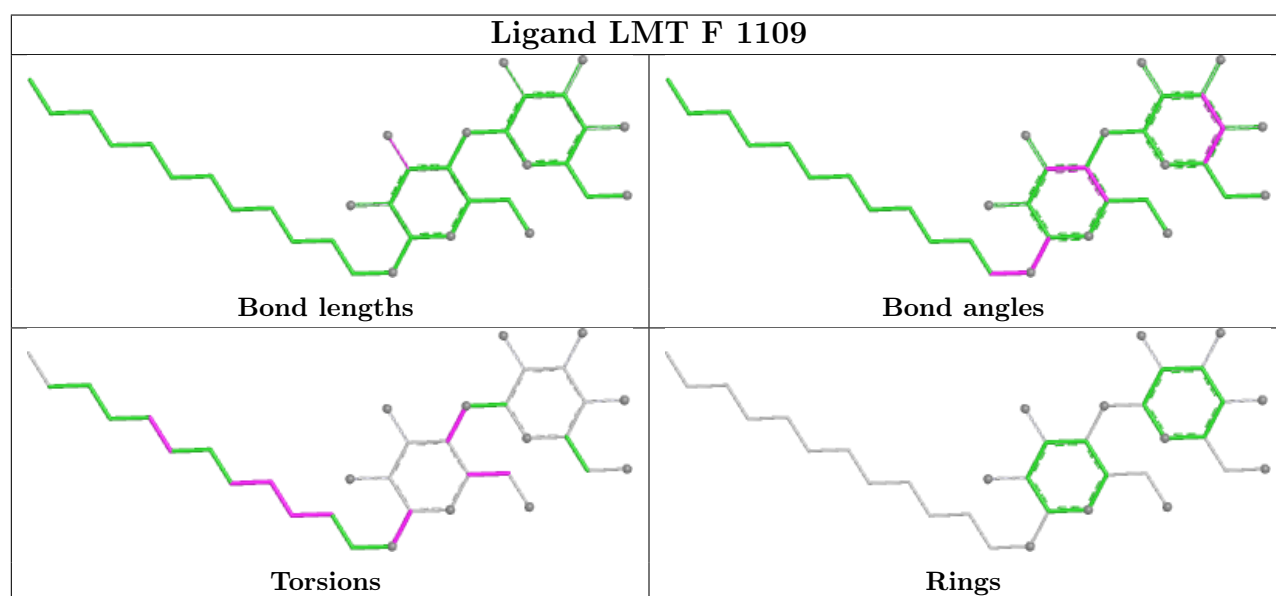
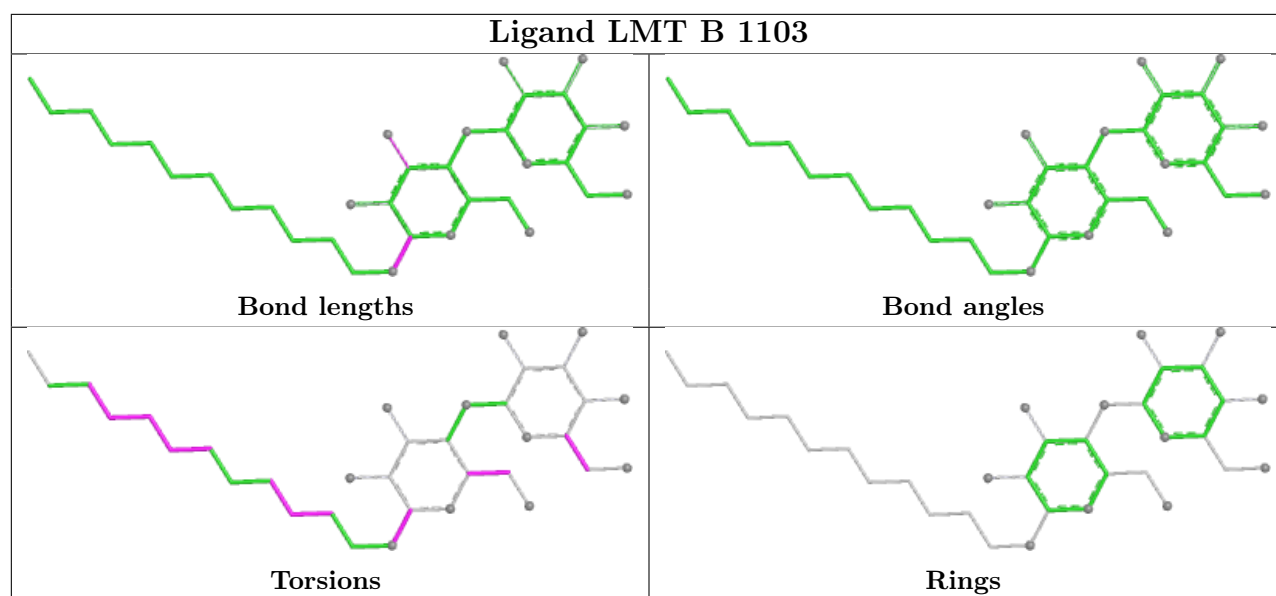


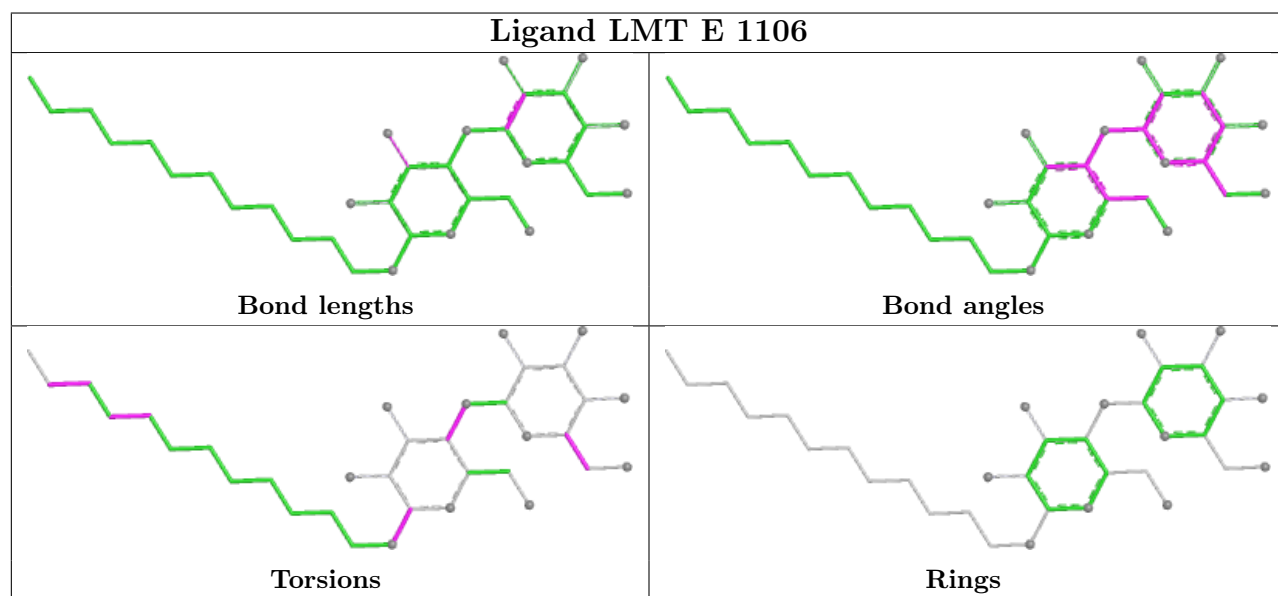
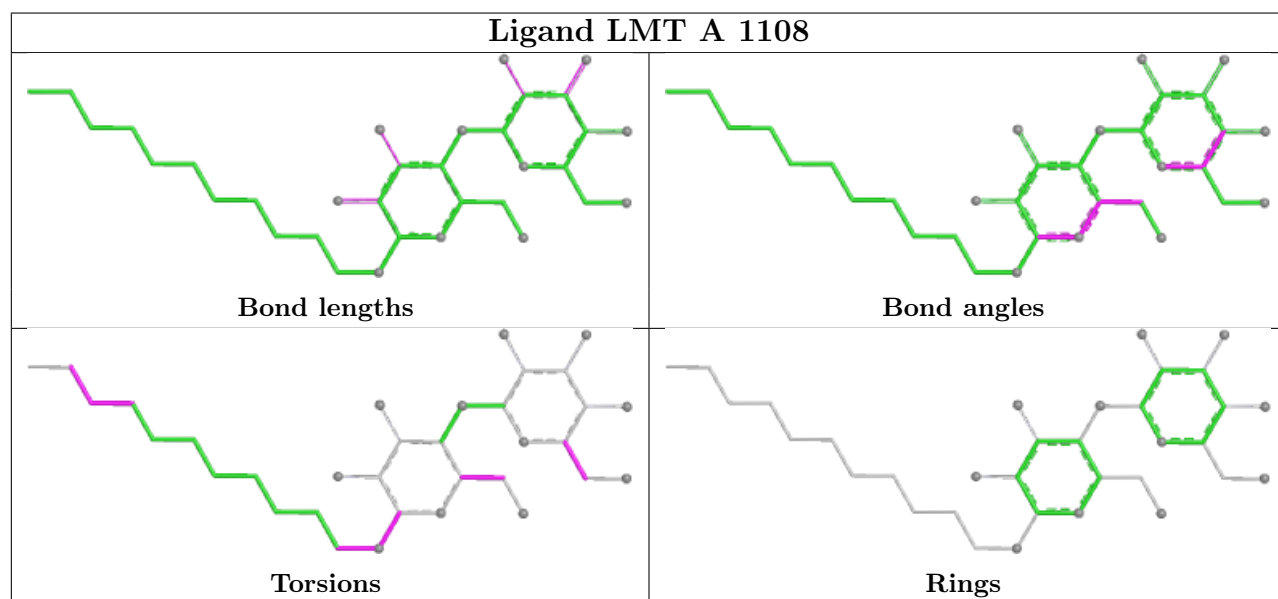
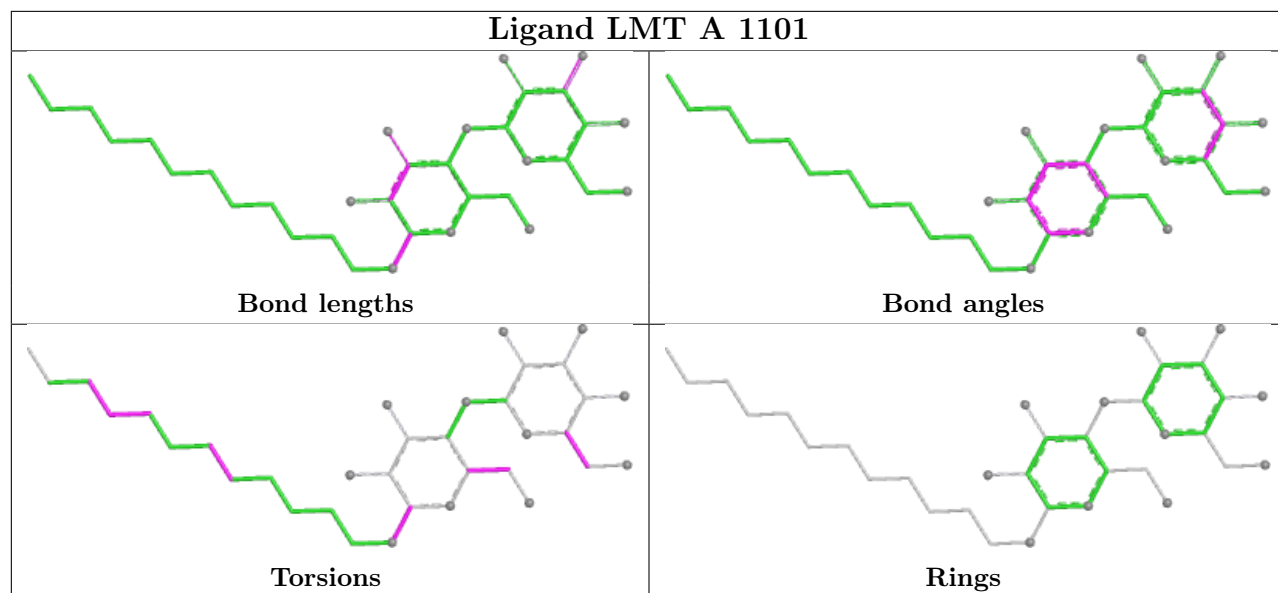


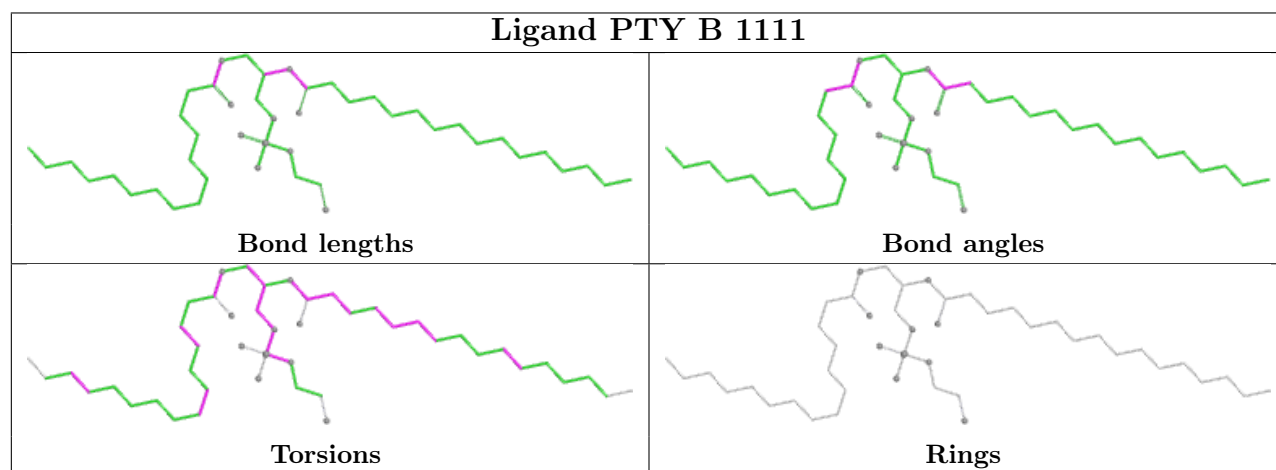
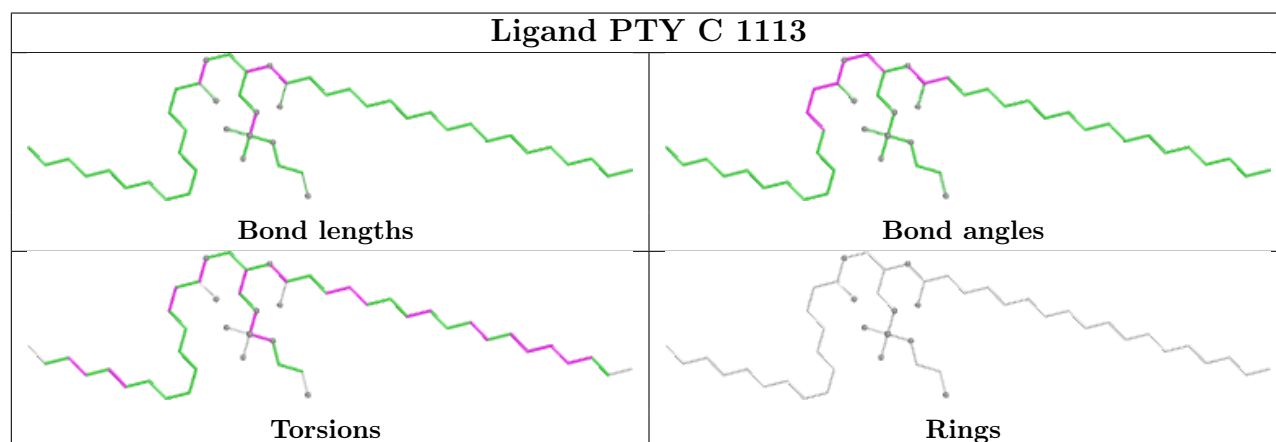
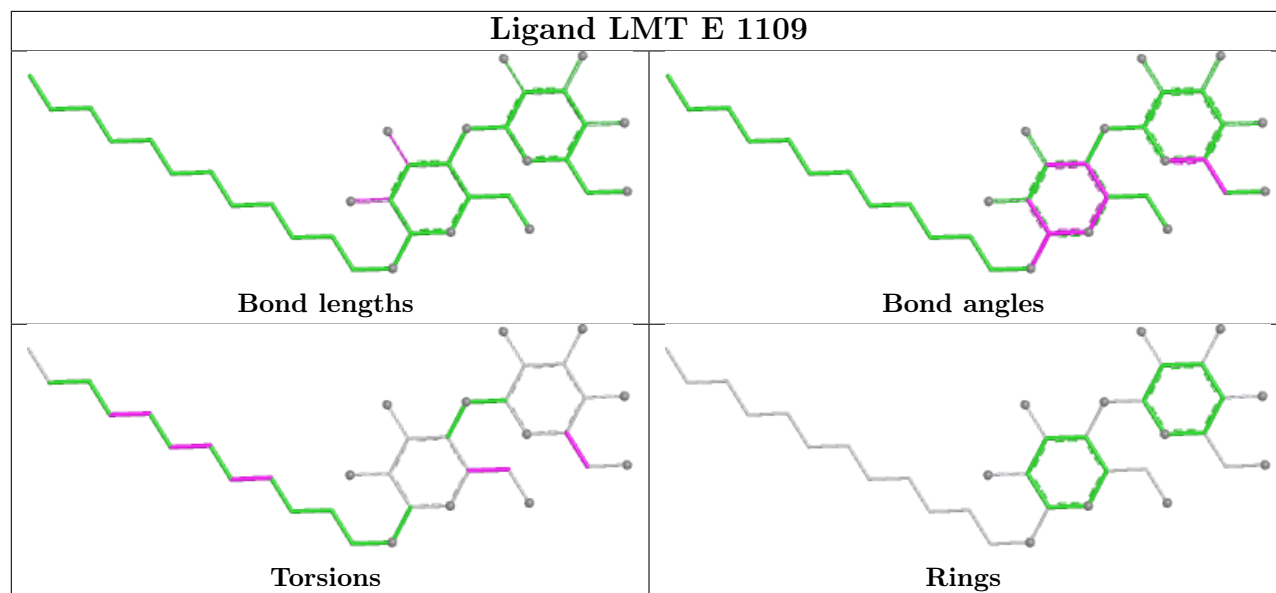


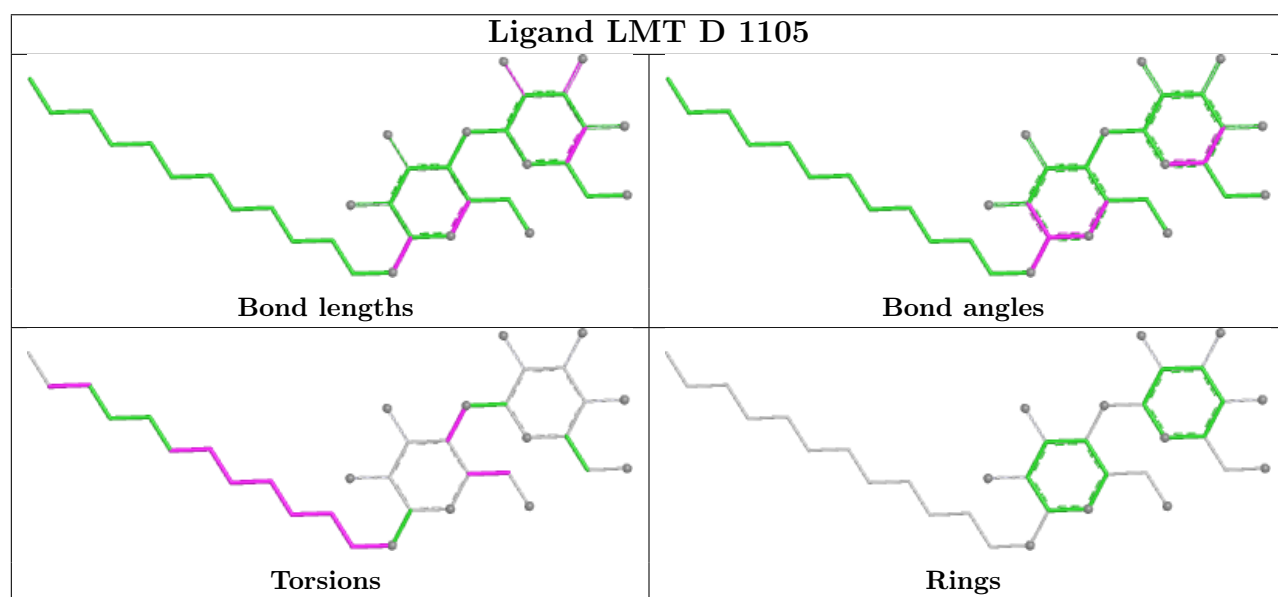
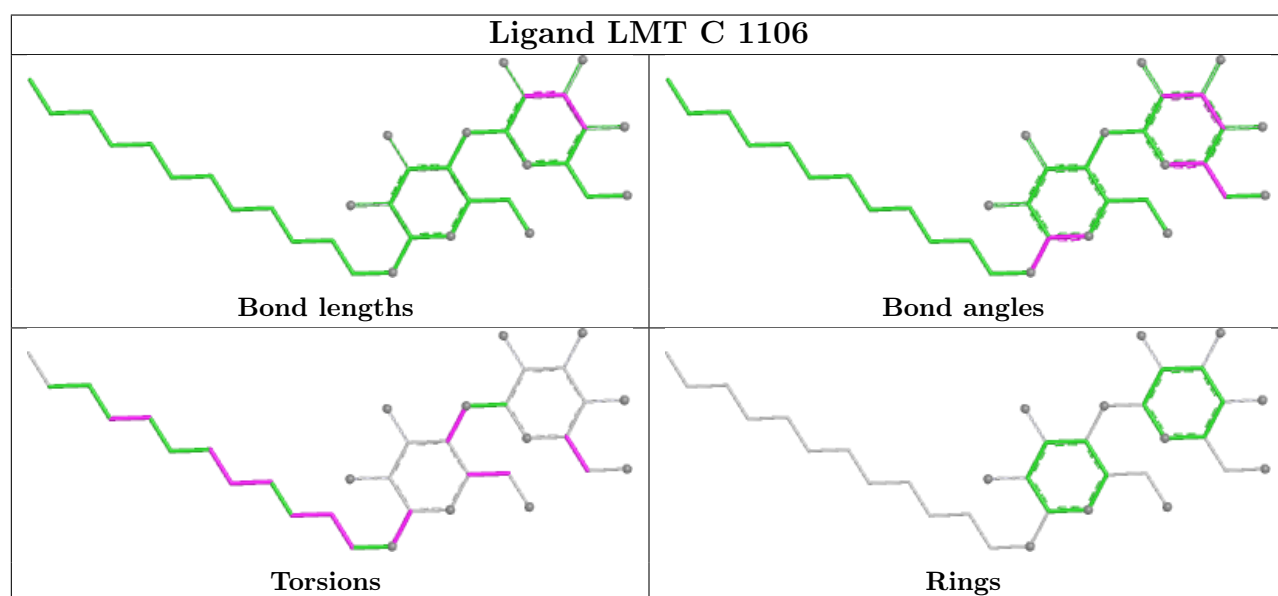
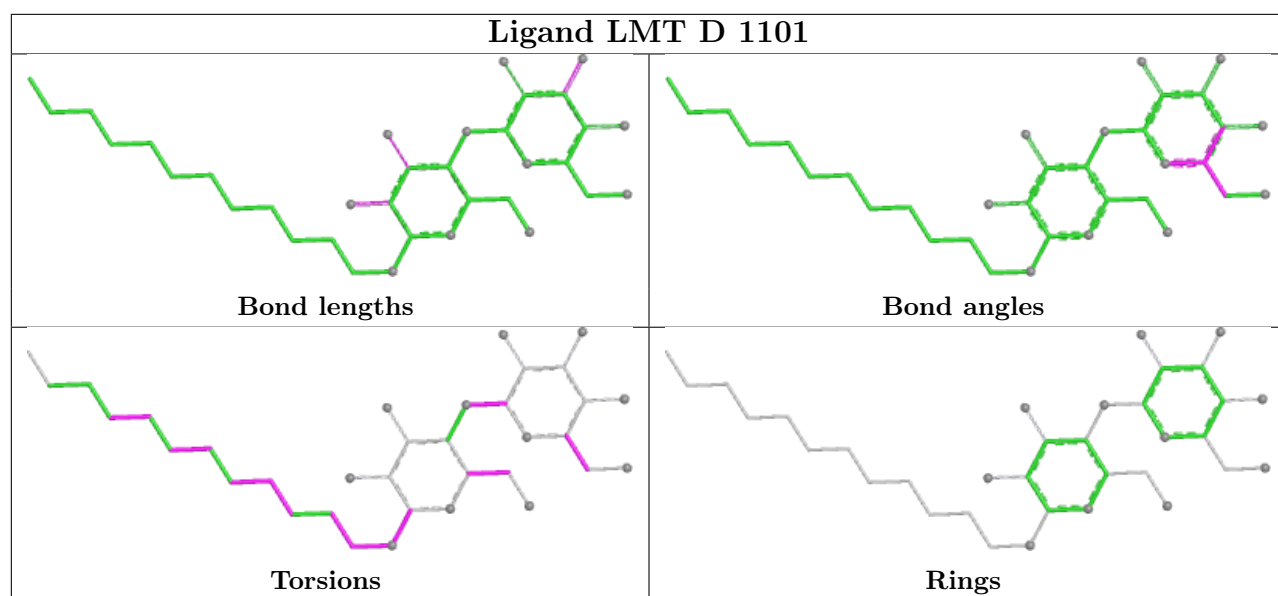












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1041/1042 (99%)	0.32	65 (6%)	26	29	18, 41, 70, 133	3 (0%)
1	B	1042/1042 (100%)	0.57	78 (7%)	20	22	28, 49, 79, 162	0
1	C	1041/1042 (99%)	0.30	47 (4%)	38	41	26, 41, 64, 127	0
1	D	1040/1042 (99%)	0.71	134 (12%)	7	7	28, 47, 90, 140	0
1	E	1039/1042 (99%)	0.37	58 (5%)	30	33	20, 41, 69, 148	4 (0%)
1	F	1040/1042 (99%)	0.59	81 (7%)	19	20	27, 45, 71, 138	1 (0%)
All	All	6243/6252 (99%)	0.48	463 (7%)	20	22	18, 44, 78, 162	8 (0%)

All (463) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	680	GLY	6.5
1	F	996	LEU	6.3
1	A	996	LEU	6.1
1	F	995	ILE	5.9
1	D	680	GLY	5.4
1	B	564	PHE	5.3
1	D	683	SER	5.3
1	E	995	ILE	5.2
1	D	555	LEU	5.2
1	C	999	GLY	5.1
1	A	995	ILE	5.0
1	D	529	LEU	4.9
1	D	504	ALA	4.9
1	F	680	GLY	4.8
1	F	992	ILE	4.7
1	A	574	THR	4.7
1	B	171	LEU	4.7
1	A	680	GLY	4.6
1	F	642	PHE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	1002	ALA	4.5
1	F	572	ILE	4.5
1	E	1008	THR	4.4
1	E	996	LEU	4.4
1	D	1021	LEU	4.3
1	A	1007	VAL	4.3
1	F	497	LEU	4.3
1	F	1037	LEU	4.3
1	B	528	PHE	4.2
1	E	1002	ALA	4.2
1	A	1012	VAL	4.2
1	F	643	ASP	4.2
1	D	524	PHE	4.2
1	F	1004	VAL	4.2
1	A	999	GLY	4.2
1	B	683	SER	4.2
1	F	172	PRO	4.2
1	B	517	PHE	4.1
1	D	966	MET	4.1
1	D	1017	LEU	4.1
1	B	987	PHE	4.1
1	A	1004	VAL	4.1
1	F	742	ALA	4.0
1	E	987	PHE	4.0
1	A	681	GLN	4.0
1	A	992	ILE	4.0
1	D	951	ILE	4.0
1	C	677	LEU	4.0
1	D	508	LEU	4.0
1	D	562	VAL	3.9
1	B	516	LEU	3.9
1	A	1002	ALA	3.9
1	B	876	GLY	3.9
1	F	682	GLY	3.9
1	D	981	VAL	3.9
1	E	572	ILE	3.9
1	C	528	PHE	3.9
1	F	683	SER	3.8
1	F	998	HIS	3.8
1	C	520	ILE	3.8
1	D	987	PHE	3.8
1	D	513	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	992	ILE	3.7
1	E	667	PHE	3.7
1	F	997	GLY	3.7
1	D	543	LEU	3.7
1	F	1017	LEU	3.7
1	E	571	PHE	3.7
1	B	966	MET	3.6
1	D	995	ILE	3.6
1	F	1012	VAL	3.6
1	D	876	GLY	3.6
1	D	552	VAL	3.6
1	D	682	GLY	3.6
1	A	873	ALA	3.5
1	B	681	GLN	3.5
1	D	537	GLY	3.5
1	F	1001	GLY	3.5
1	E	574	THR	3.5
1	C	987	PHE	3.5
1	B	497	LEU	3.5
1	D	501	PRO	3.5
1	D	549	VAL	3.5
1	F	524	PHE	3.5
1	C	1037	LEU	3.5
1	D	970	LEU	3.5
1	A	990	GLY	3.5
1	B	682	GLY	3.5
1	D	696	GLY	3.5
1	E	565	LYS	3.5
1	F	1000	ALA	3.5
1	B	175	GLY	3.5
1	D	569	GLY	3.5
1	A	1008	THR	3.4
1	D	835	ALA	3.4
1	E	682	GLY	3.4
1	D	539	VAL	3.4
1	C	683	SER	3.4
1	A	571	PHE	3.4
1	A	994	LEU	3.4
1	D	679	LEU	3.4
1	D	880	LEU	3.4
1	D	535	TYR	3.3
1	B	538	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	994	LEU	3.3
1	D	362	LEU	3.3
1	D	517	PHE	3.3
1	E	998	HIS	3.3
1	A	503	GLY	3.3
1	A	682	GLY	3.3
1	F	1010	ILE	3.3
1	D	548	ALA	3.2
1	A	928	ASP	3.2
1	A	555	LEU	3.2
1	D	538	LEU	3.2
1	E	993	PRO	3.2
1	D	1022	PHE	3.2
1	C	682	GLY	3.2
1	D	519	TRP	3.2
1	B	172	PRO	3.2
1	A	516	LEU	3.2
1	D	848	HIS	3.2
1	A	1011	THR	3.2
1	D	566	VAL	3.2
1	D	677	LEU	3.2
1	F	987	PHE	3.2
1	A	1	MET	3.1
1	D	924	LEU	3.1
1	D	997	GLY	3.1
1	F	994	LEU	3.1
1	D	998	HIS	3.1
1	E	517	PHE	3.1
1	B	529	LEU	3.1
1	F	171	LEU	3.1
1	A	987	PHE	3.1
1	B	527	PHE	3.1
1	D	528	PHE	3.1
1	C	681	GLN	3.1
1	F	170	ARG	3.1
1	C	998	HIS	3.1
1	C	992	ILE	3.1
1	D	556	LEU	3.1
1	D	550	PHE	3.1
1	D	1025	PHE	3.1
1	D	992	ILE	3.0
1	F	660	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	516	LEU	3.0
1	D	1037	LEU	3.0
1	B	550	PHE	3.0
1	C	502	HIS	3.0
1	D	715	PRO	3.0
1	A	643	ASP	3.0
1	B	572	ILE	3.0
1	E	721	ILE	3.0
1	B	1017	LEU	3.0
1	B	519	TRP	3.0
1	B	524	PHE	3.0
1	D	1013	PHE	3.0
1	F	1013	PHE	3.0
1	E	991	THR	3.0
1	A	570	GLY	3.0
1	A	993	PRO	3.0
1	D	837	PRO	3.0
1	B	531	SER	3.0
1	C	642	PHE	3.0
1	F	571	PHE	3.0
1	F	570	GLY	3.0
1	D	428	ALA	3.0
1	E	1003	GLU	3.0
1	B	23	ILE	3.0
1	D	520	ILE	3.0
1	B	20	LEU	2.9
1	F	516	LEU	2.9
1	A	874	THR	2.9
1	E	999	GLY	2.9
1	D	568	PRO	2.9
1	B	11	PRO	2.9
1	A	1000	ALA	2.9
1	B	1002	ALA	2.9
1	D	868	LEU	2.9
1	E	677	LEU	2.9
1	D	503	GLY	2.9
1	D	716	GLY	2.9
1	E	1012	VAL	2.9
1	D	553	TYR	2.9
1	D	914	THR	2.9
1	B	502	HIS	2.9
1	B	1	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	996	LEU	2.9
1	F	669	PHE	2.8
1	B	970	LEU	2.8
1	D	977	LEU	2.8
1	D	874	THR	2.8
1	C	1000	ALA	2.8
1	E	258	GLN	2.8
1	C	522	ARG	2.8
1	F	1007	VAL	2.8
1	F	989	ALA	2.8
1	E	550	PHE	2.8
1	A	569	GLY	2.8
1	A	876	GLY	2.8
1	F	693	GLY	2.8
1	A	991	THR	2.8
1	F	1	MET	2.8
1	F	517	PHE	2.7
1	A	1039	THR	2.7
1	B	510	THR	2.7
1	F	991	THR	2.7
1	C	554	LEU	2.7
1	C	924	LEU	2.7
1	F	868	LEU	2.7
1	D	533	ASN	2.7
1	E	230	GLU	2.7
1	D	502	HIS	2.7
1	A	1006	GLY	2.7
1	B	999	GLY	2.7
1	E	259	ASP	2.7
1	F	1011	THR	2.7
1	D	554	LEU	2.7
1	F	372	LEU	2.7
1	E	226	PRO	2.7
1	F	501	PRO	2.7
1	B	465	THR	2.7
1	E	508	LEU	2.7
1	E	683	SER	2.7
1	E	1007	VAL	2.7
1	A	257	ALA	2.6
1	C	997	GLY	2.6
1	E	680	GLY	2.6
1	F	999	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	923	TRP	2.6
1	A	526	ARG	2.6
1	D	361	PHE	2.6
1	A	508	LEU	2.6
1	F	679	LEU	2.6
1	E	1004	VAL	2.6
1	B	644	GLN	2.6
1	D	681	GLN	2.6
1	B	541	LYS	2.6
1	F	564	PHE	2.6
1	F	667	PHE	2.6
1	B	997	GLY	2.6
1	E	570	GLY	2.6
1	F	927	GLY	2.6
1	D	559	ALA	2.6
1	D	1019	VAL	2.6
1	E	1011	THR	2.6
1	D	521	PHE	2.6
1	E	555	LEU	2.6
1	D	872	GLN	2.6
1	D	1018	GLY	2.6
1	D	1023	GLY	2.6
1	E	990	GLY	2.6
1	B	1004	VAL	2.6
1	B	170	ARG	2.5
1	B	298	PRO	2.5
1	A	550	PHE	2.5
1	D	719	PHE	2.5
1	F	681	GLN	2.5
1	D	965	ILE	2.5
1	E	1001	GLY	2.5
1	D	906	ALA	2.5
1	B	875	GLN	2.5
1	D	1024	LEU	2.5
1	D	1026	LEU	2.5
1	B	709	GLY	2.5
1	E	997	GLY	2.5
1	F	175	GLY	2.5
1	C	908	ILE	2.5
1	B	998	HIS	2.5
1	E	170	ARG	2.5
1	A	875	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	911	VAL	2.5
1	D	1028	PRO	2.5
1	F	39	ASP	2.5
1	A	997	GLY	2.5
1	B	503	GLY	2.5
1	B	508	LEU	2.5
1	B	667	PHE	2.5
1	C	868	LEU	2.5
1	F	694	GLY	2.5
1	A	1041	ARG	2.5
1	D	721	ILE	2.5
1	F	644	GLN	2.5
1	D	567	VAL	2.5
1	B	680	GLY	2.4
1	D	534	GLY	2.4
1	E	876	GLY	2.4
1	A	517	PHE	2.4
1	A	667	PHE	2.4
1	F	528	PHE	2.4
1	F	1014	SER	2.4
1	B	995	ILE	2.4
1	D	882	VAL	2.4
1	B	511	ARG	2.4
1	A	926	GLY	2.4
1	D	518	GLY	2.4
1	B	543	LEU	2.4
1	D	919	LEU	2.4
1	E	516	LEU	2.4
1	A	572	ILE	2.4
1	B	881	ILE	2.4
1	D	908	ILE	2.4
1	C	1002	ALA	2.4
1	F	993	PRO	2.4
1	D	923	TRP	2.4
1	A	872	GLN	2.4
1	D	994	LEU	2.4
1	F	963	LYS	2.4
1	E	1013	PHE	2.4
1	F	574	THR	2.4
1	F	676	ILE	2.4
1	B	174	VAL	2.4
1	F	426	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	996	LEU	2.3
1	E	512	LEU	2.3
1	A	1013	PHE	2.3
1	B	455	PHE	2.3
1	D	564	PHE	2.3
1	D	714	THR	2.3
1	D	713	GLN	2.3
1	D	1010	ILE	2.3
1	E	1010	ILE	2.3
1	F	12	ILE	2.3
1	F	367	ALA	2.3
1	A	573	PRO	2.3
1	D	698	GLY	2.3
1	C	1004	VAL	2.3
1	D	341	ARG	2.3
1	F	10	ARG	2.3
1	F	875	GLN	2.3
1	D	920	PHE	2.3
1	E	564	PHE	2.3
1	D	845	ALA	2.3
1	F	721	ILE	2.3
1	B	565	LYS	2.3
1	A	566	VAL	2.3
1	C	834	ASP	2.3
1	E	643	ASP	2.3
1	E	875	GLN	2.3
1	C	679	LEU	2.3
1	D	877	ASN	2.3
1	F	929	ASN	2.3
1	A	455	PHE	2.3
1	A	524	PHE	2.3
1	C	517	PHE	2.3
1	C	521	PHE	2.3
1	C	564	PHE	2.3
1	B	742	ALA	2.3
1	F	605	ILE	2.3
1	D	875	GLN	2.3
1	A	880	LEU	2.3
1	B	574	THR	2.3
1	D	717	MET	2.3
1	D	943	LEU	2.3
1	D	1027	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1034	LEU	2.3
1	D	1039	THR	2.3
1	A	230	GLU	2.2
1	D	815	TYR	2.2
1	F	550	PHE	2.2
1	A	1010	ILE	2.2
1	D	863	ILE	2.2
1	F	988	ILE	2.2
1	B	309	VAL	2.2
1	D	1029	VAL	2.2
1	B	1042	LYS	2.2
1	A	170	ARG	2.2
1	A	1040	ARG	2.2
1	D	857	LEU	2.2
1	A	871	GLN	2.2
1	D	684	GLY	2.2
1	F	876	GLY	2.2
1	F	314	ALA	2.2
1	B	642	PHE	2.2
1	B	1013	PHE	2.2
1	D	460	PHE	2.2
1	B	520	ILE	2.2
1	B	566	VAL	2.2
1	C	566	VAL	2.2
1	F	1008	THR	2.2
1	D	999	GLY	2.2
1	A	551	ALA	2.2
1	D	969	ALA	2.2
1	E	1000	ALA	2.2
1	F	455	PHE	2.2
1	B	656	ILE	2.2
1	D	985	ILE	2.2
1	C	966	MET	2.2
1	D	913	MET	2.2
1	B	679	LEU	2.2
1	D	916	LEU	2.2
1	E	880	LEU	2.2
1	B	1000	ALA	2.2
1	D	551	ALA	2.2
1	D	873	ALA	2.2
1	E	623	ALA	2.2
1	E	986	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	718	HIS	2.1
1	C	460	PHE	2.1
1	D	61	GLU	2.1
1	C	960	ILE	2.1
1	E	520	ILE	2.1
1	E	871	GLN	2.1
1	D	885	VAL	2.1
1	F	299	GLY	2.1
1	B	356	LEU	2.1
1	B	501	PRO	2.1
1	B	1021	LEU	2.1
1	C	905	LEU	2.1
1	C	565	LYS	2.1
1	D	526	ARG	2.1
1	D	557	LEU	2.1
1	F	563	MET	2.1
1	A	719	PHE	2.1
1	D	258	GLN	2.1
1	B	992	ILE	2.1
1	C	572	ILE	2.1
1	C	995	ILE	2.1
1	A	519	TRP	2.1
1	B	375	VAL	2.1
1	A	998	HIS	2.1
1	E	298	PRO	2.1
1	F	677	LEU	2.1
1	E	229	GLN	2.1
1	E	504	ALA	2.1
1	A	669	PHE	2.1
1	A	850	GLU	2.1
1	B	1001	GLY	2.1
1	C	569	GLY	2.1
1	F	569	GLY	2.1
1	C	519	TRP	2.1
1	F	174	VAL	2.1
1	B	677	LEU	2.1
1	C	516	LEU	2.1
1	C	880	LEU	2.1
1	C	873	ALA	2.1
1	C	667	PHE	2.0
1	D	988	ILE	2.0
1	E	642	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	719	PHE	2.0
1	B	535	TYR	2.0
1	C	684	GLY	2.0
1	D	570	GLY	2.0
1	D	927	GLY	2.0
1	B	549	VAL	2.0
1	C	909	LEU	2.0
1	C	943	LEU	2.0
1	C	994	LEU	2.0
1	F	519	TRP	2.0
1	E	224	ALA	2.0
1	D	505	LYS	2.0
1	D	963	LYS	2.0
1	B	297	SER	2.0
1	A	642	PHE	2.0
1	B	373	ILE	2.0
1	B	513	ILE	2.0
1	C	718	HIS	2.0
1	D	571	PHE	2.0
1	D	572	ILE	2.0
1	D	689	ILE	2.0
1	D	960	ILE	2.0
1	F	23	ILE	2.0
1	B	343	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LMT	D	1104	35/35	0.66	0.23	47,79,92,97	0
2	LMT	E	1112	35/35	0.68	0.16	66,112,138,141	0
3	PTY	E	1114	46/50	0.69	0.20	55,97,189,204	0
2	LMT	A	1101	35/35	0.70	0.18	91,113,132,139	0
2	LMT	F	1111	17/35	0.72	0.28	72,80,94,95	0
2	LMT	B	1101	35/35	0.72	0.18	80,104,131,137	0
3	PTY	F	1115	48/50	0.72	0.20	59,81,130,148	0
2	LMT	D	1107	35/35	0.73	0.18	59,120,136,144	0
4	GOL	B	1113	6/6	0.73	0.19	81,87,87,92	0
2	LMT	C	1108	35/35	0.74	0.18	46,66,86,89	0
2	LMT	F	1109	35/35	0.74	0.17	63,86,108,114	0
2	LMT	B	1110	35/35	0.75	0.17	62,113,136,137	0
2	LMT	A	1107	35/35	0.75	0.16	60,99,140,143	0
2	LMT	F	1103	35/35	0.75	0.20	53,78,86,87	0
4	GOL	A	1119	6/6	0.75	0.24	51,60,65,67	0
2	LMT	B	1109	35/35	0.75	0.18	54,105,138,139	0
3	PTY	B	1111	46/50	0.76	0.18	60,99,142,152	0
2	LMT	D	1105	35/35	0.76	0.16	76,103,126,126	0
2	LMT	E	1105	35/35	0.76	0.19	55,72,82,98	0
4	GOL	A	1115	6/6	0.76	0.16	49,55,61,65	0
2	LMT	F	1113	35/35	0.76	0.20	51,83,101,103	0
3	PTY	A	1112	46/50	0.76	0.17	58,88,154,171	0
4	GOL	D	1117	6/6	0.76	0.15	64,68,75,80	0
2	LMT	D	1109	35/35	0.77	0.21	44,115,139,147	0
4	GOL	C	1115	6/6	0.77	0.17	45,63,66,67	0
3	PTY	C	1113	48/50	0.77	0.20	51,73,124,141	0
4	GOL	E	1118	6/6	0.77	0.24	51,66,72,80	0
4	GOL	F	1116	6/6	0.77	0.17	47,55,68,75	0
2	LMT	C	1101	35/35	0.78	0.19	55,96,143,149	0
4	GOL	A	1118	6/6	0.78	0.17	33,49,59,62	0
2	LMT	A	1108	34/35	0.78	0.16	46,85,98,103	0
2	LMT	C	1112	35/35	0.78	0.17	40,83,119,121	0
3	PTY	D	1113	48/50	0.78	0.20	48,76,120,141	0
2	LMT	D	1112	35/35	0.78	0.15	79,121,148,149	0
4	GOL	E	1117	6/6	0.78	0.16	69,78,84,90	0
2	LMT	A	1105	35/35	0.78	0.18	52,71,83,104	0
4	GOL	E	1121	6/6	0.78	0.17	46,54,62,66	0
4	GOL	E	1123	6/6	0.78	0.21	57,64,71,72	0
4	GOL	A	1113	6/6	0.78	0.18	55,60,69,73	0
4	GOL	F	1117	6/6	0.78	0.21	49,58,67,67	0
2	LMT	F	1106	35/35	0.79	0.17	57,91,116,118	0
2	LMT	D	1106	35/35	0.79	0.16	55,85,115,117	0
2	LMT	C	1110	35/35	0.79	0.17	56,85,114,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LMT	E	1107	35/35	0.79	0.17	54,86,114,115	0
2	LMT	E	1111	12/35	0.79	0.19	62,72,75,75	0
2	LMT	D	1108	35/35	0.79	0.15	53,96,120,122	0
3	PTY	B	1112	48/50	0.79	0.19	59,81,120,130	0
2	LMT	B	1106	35/35	0.79	0.16	65,94,134,136	0
4	GOL	E	1116	6/6	0.80	0.17	53,58,64,65	0
2	LMT	C	1106	35/35	0.80	0.14	43,83,104,106	0
2	LMT	E	1106	35/35	0.80	0.16	68,111,129,133	0
2	LMT	D	1103	35/35	0.80	0.17	37,76,101,113	0
3	PTY	E	1115	48/50	0.80	0.20	54,74,118,138	0
2	LMT	F	1107	35/35	0.80	0.17	66,105,157,159	0
2	LMT	C	1107	35/35	0.80	0.16	34,63,80,82	0
4	GOL	B	1114	6/6	0.81	0.18	78,82,86,91	0
2	LMT	A	1111	35/35	0.81	0.17	40,63,77,82	0
4	GOL	E	1119	6/6	0.81	0.18	49,50,59,67	0
4	GOL	C	1116	6/6	0.81	0.18	52,70,71,74	0
4	GOL	D	1115	6/6	0.81	0.21	59,63,67,76	0
2	LMT	E	1108	35/35	0.81	0.16	53,94,113,116	0
2	LMT	E	1110	35/35	0.81	0.16	48,86,109,114	0
3	PTY	F	1114	37/50	0.82	0.18	71,94,129,133	0
2	LMT	F	1105	35/35	0.82	0.15	53,70,90,94	0
2	LMT	F	1108	13/35	0.82	0.21	52,58,86,89	0
2	LMT	B	1105	35/35	0.82	0.17	53,70,80,87	0
2	LMT	C	1111	35/35	0.83	0.15	47,90,103,106	0
2	LMT	A	1109	35/35	0.83	0.15	51,90,113,119	0
2	LMT	E	1102	35/35	0.83	0.16	54,77,104,114	0
2	LMT	E	1104	35/35	0.83	0.15	32,64,79,84	0
2	LMT	B	1107	16/35	0.83	0.22	69,81,88,89	0
2	LMT	F	1110	35/35	0.83	0.17	43,94,127,131	0
2	LMT	A	1106	35/35	0.83	0.17	61,82,112,119	0
4	GOL	F	1118	6/6	0.83	0.15	63,67,75,79	0
4	GOL	E	1120	6/6	0.84	0.16	49,55,58,60	0
2	LMT	B	1102	35/35	0.84	0.15	40,67,83,89	0
2	LMT	C	1102	35/35	0.84	0.12	53,68,83,89	0
2	LMT	D	1101	35/35	0.84	0.14	59,82,96,101	0
2	LMT	B	1108	12/35	0.84	0.23	59,68,84,84	0
2	LMT	E	1103	35/35	0.84	0.16	44,64,79,83	0
2	LMT	E	1113	10/35	0.85	0.18	71,76,79,80	0
2	LMT	F	1102	35/35	0.85	0.13	58,82,95,99	0
2	LMT	A	1110	25/35	0.85	0.18	48,77,121,134	0
2	LMT	D	1111	35/35	0.85	0.14	59,86,115,125	0
2	LMT	E	1109	35/35	0.85	0.15	62,93,134,135	0

Continued on next page...

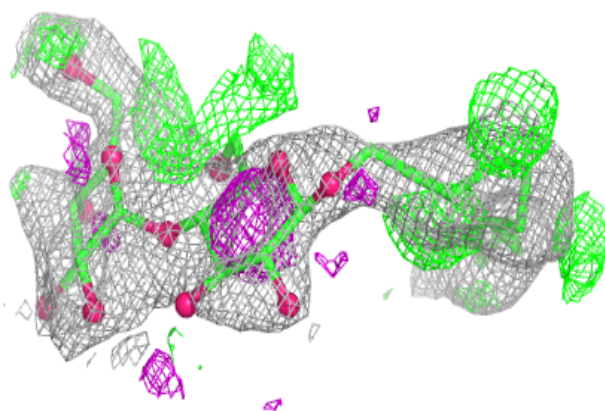
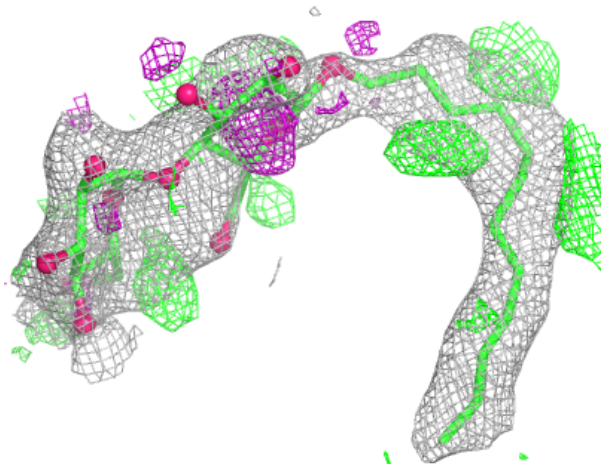
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	1117	6/6	0.86	0.15	62,69,71,72	0
4	GOL	C	1117	6/6	0.86	0.13	43,54,60,75	0
2	LMT	F	1104	35/35	0.86	0.12	40,57,69,72	0
4	GOL	E	1122	6/6	0.86	0.14	44,49,53,60	0
2	LMT	D	1102	35/35	0.86	0.17	55,65,77,84	0
2	LMT	A	1104	35/35	0.86	0.13	32,58,66,67	0
2	LMT	C	1109	35/35	0.86	0.14	65,95,111,112	0
2	LMT	B	1103	35/35	0.86	0.14	50,71,81,85	0
2	LMT	A	1102	35/35	0.87	0.14	45,58,75,79	0
4	GOL	A	1114	6/6	0.87	0.14	52,54,63,78	0
2	LMT	C	1103	35/35	0.87	0.12	55,69,78,87	0
4	GOL	D	1116	6/6	0.87	0.14	54,59,62,63	0
4	GOL	F	1120	6/6	0.87	0.14	49,57,62,74	0
4	GOL	F	1119	6/6	0.88	0.14	37,52,53,66	0
4	GOL	A	1121	6/6	0.88	0.12	61,66,75,77	0
2	LMT	C	1105	35/35	0.89	0.14	43,52,69,76	0
2	LMT	E	1101	35/35	0.89	0.12	44,59,68,78	0
2	LMT	F	1101	35/35	0.89	0.11	47,68,86,98	0
4	GOL	C	1119	6/6	0.89	0.12	50,56,59,68	0
2	LMT	C	1104	35/35	0.89	0.11	45,56,66,70	0
4	GOL	C	1118	6/6	0.90	0.11	45,58,62,69	0
4	GOL	B	1115	6/6	0.90	0.12	44,48,58,60	0
2	LMT	A	1103	35/35	0.90	0.11	54,65,82,86	0
2	LMT	B	1104	35/35	0.91	0.11	52,75,91,97	0
4	GOL	A	1116	6/6	0.91	0.14	55,69,72,72	0
4	GOL	A	1120	6/6	0.91	0.12	40,50,52,53	0
2	LMT	D	1110	10/35	0.91	0.15	51,56,67,78	0
2	LMT	F	1112	6/35	0.92	0.18	62,66,68,71	0
4	GOL	C	1114	6/6	0.93	0.09	36,45,46,55	0
4	GOL	C	1120	6/6	0.95	0.10	50,57,65,67	0
4	GOL	D	1114	6/6	0.97	0.07	34,37,45,46	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.

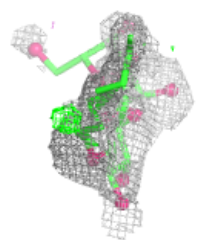
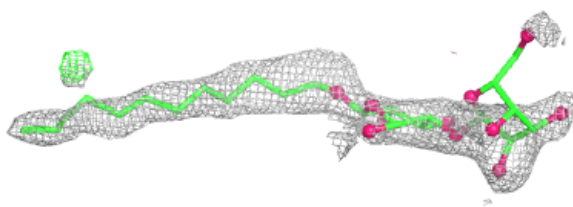
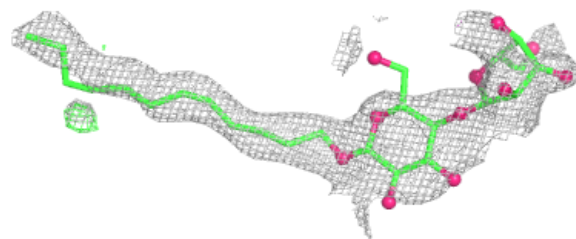
Electron density around LMT D 1104:

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

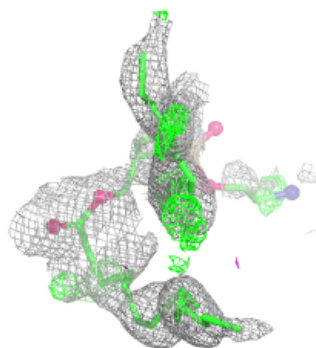
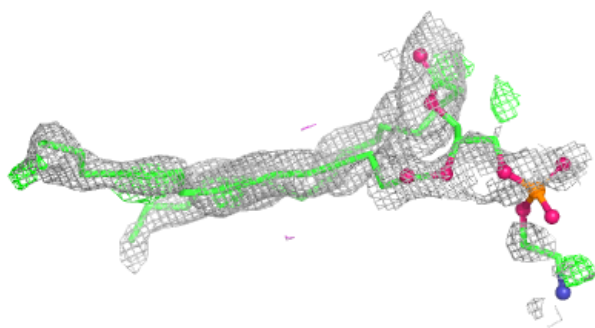
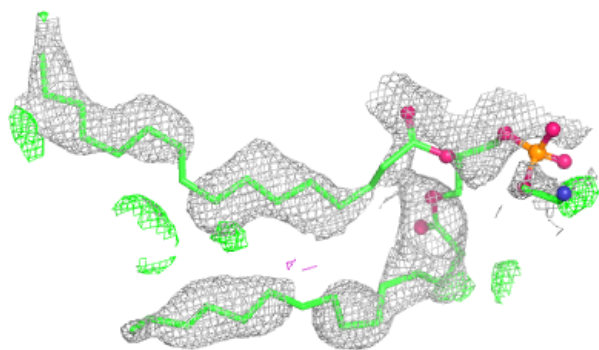


Electron density around LMT E 1112:

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

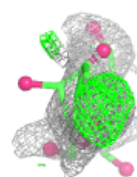
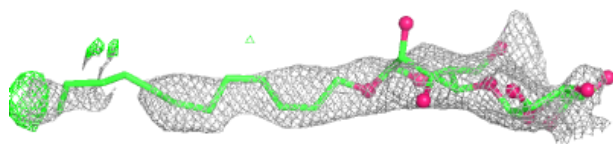
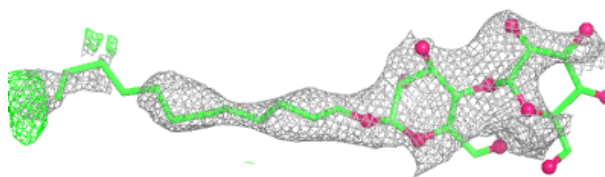
**Electron density around PTY E 1114:**

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

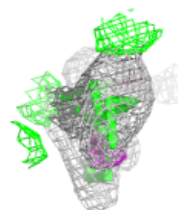
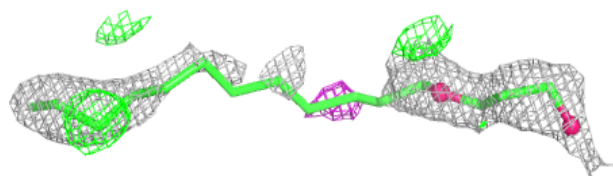
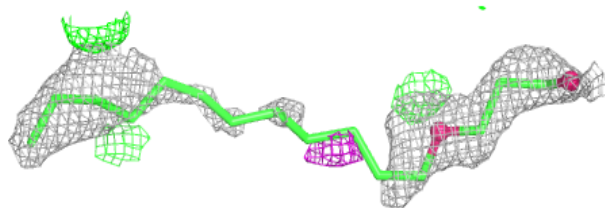


Electron density around LMT A 1101:

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

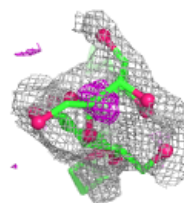
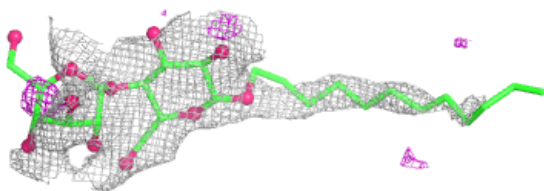
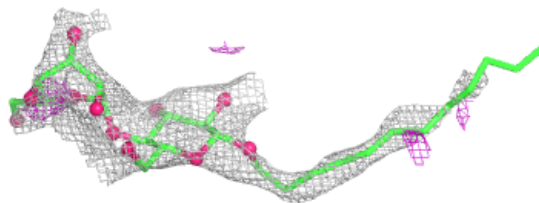
**Electron density around LMT F 1111:**

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

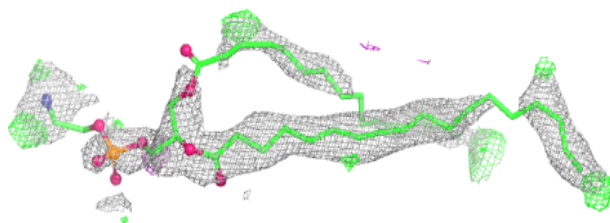
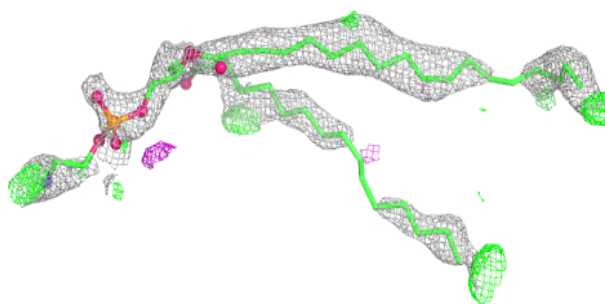


Electron density around LMT B 1101:

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

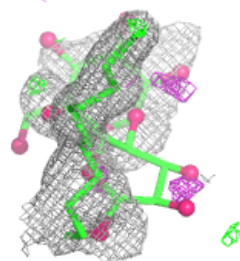
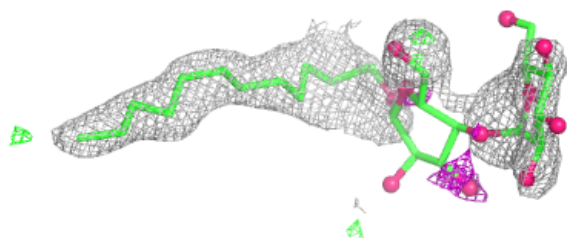
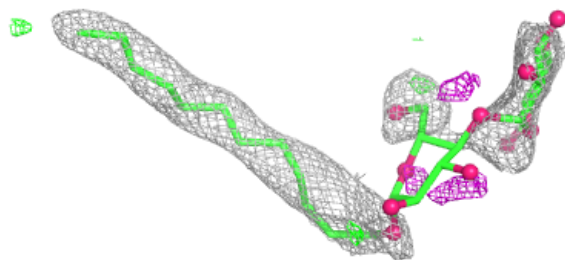
**Electron density around PTY F 1115:**

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



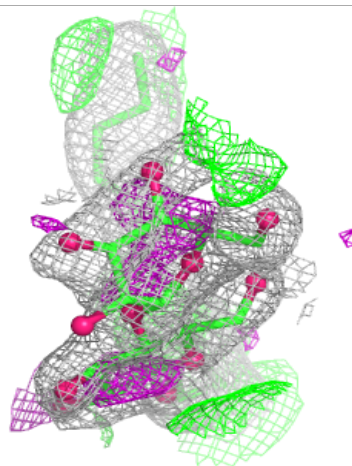
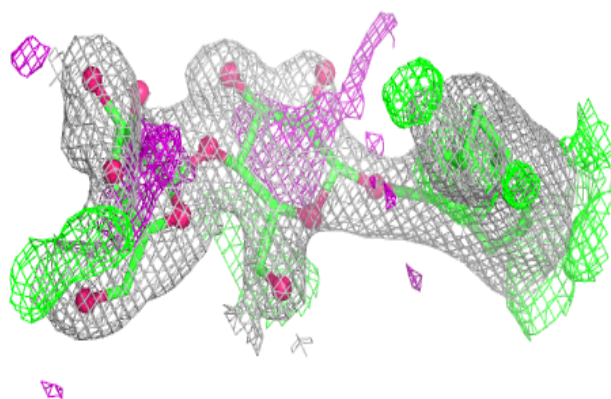
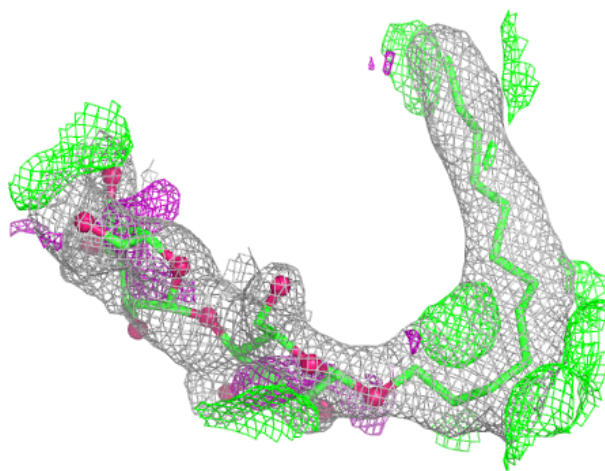
Electron density around LMT D 1107:

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



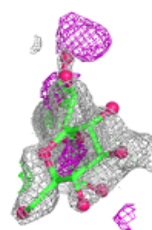
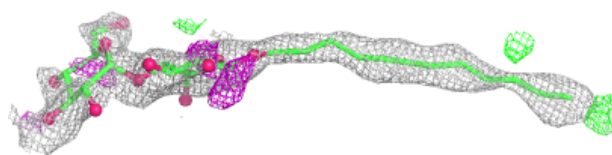
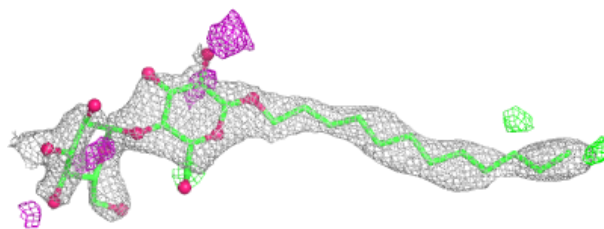
Electron density around LMT C 1108:

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

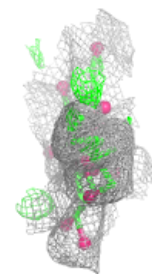
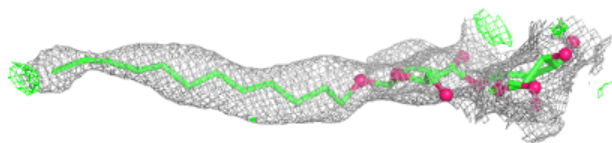
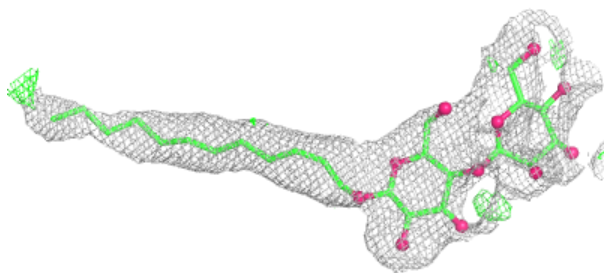


Electron density around LMT F 1109:

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

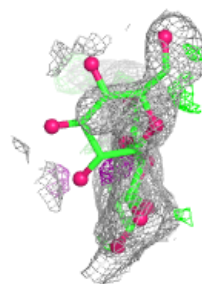
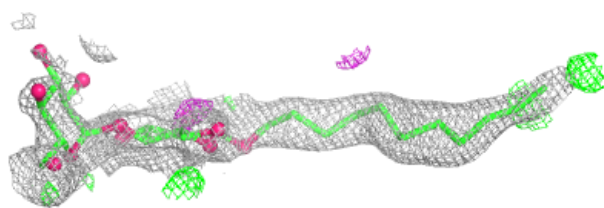
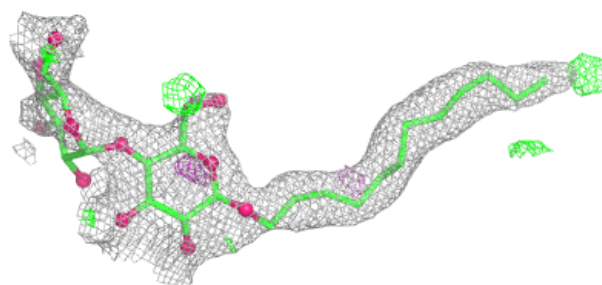
**Electron density around LMT B 1110:**

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

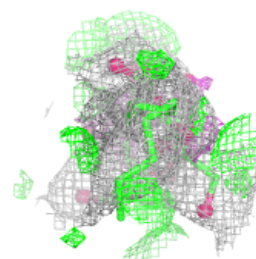
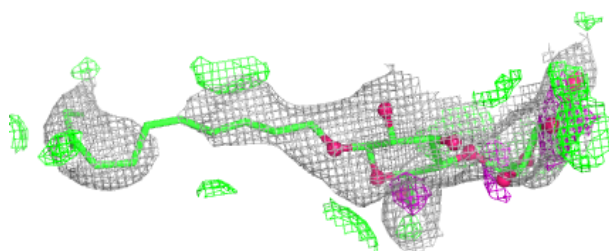
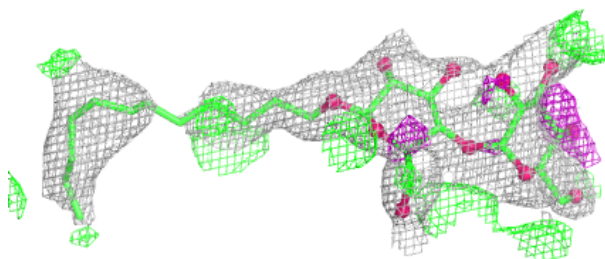


Electron density around LMT A 1107:

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

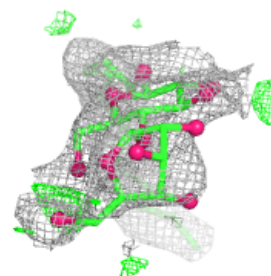
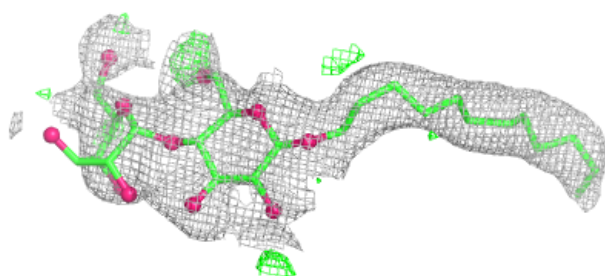
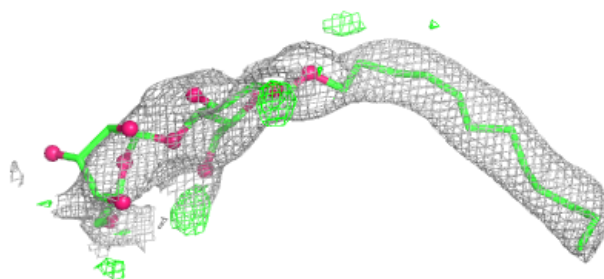
**Electron density around LMT F 1103:**

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

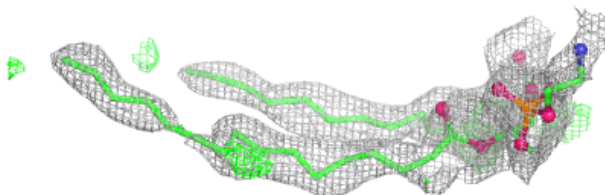
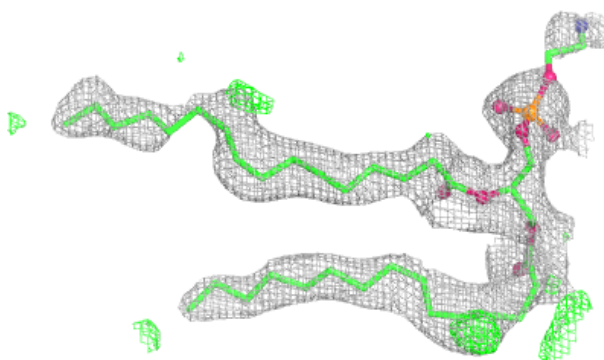


Electron density around LMT B 1109:

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

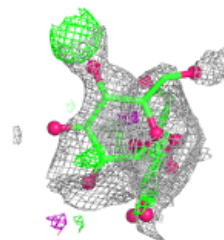
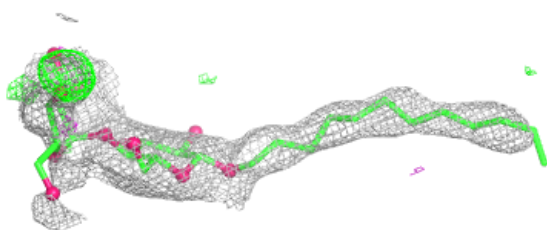
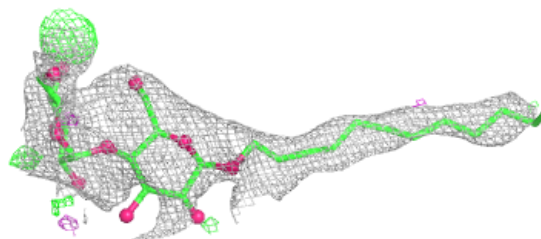
**Electron density around PTY B 1111:**

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



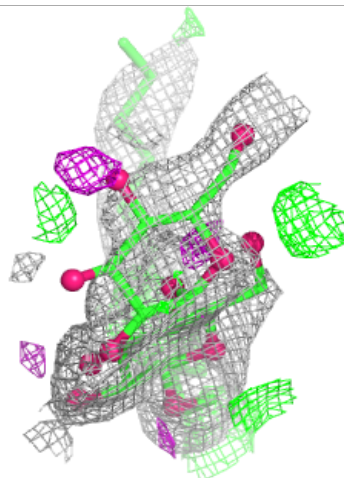
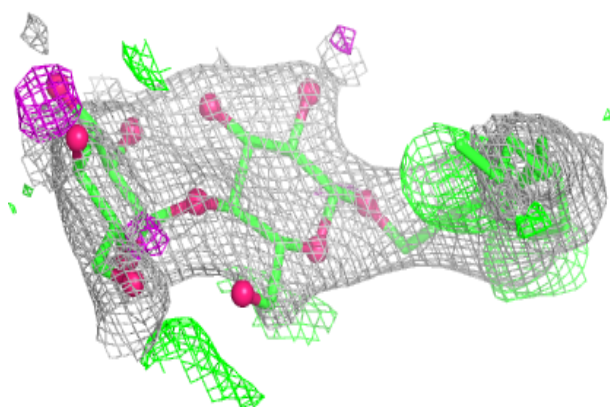
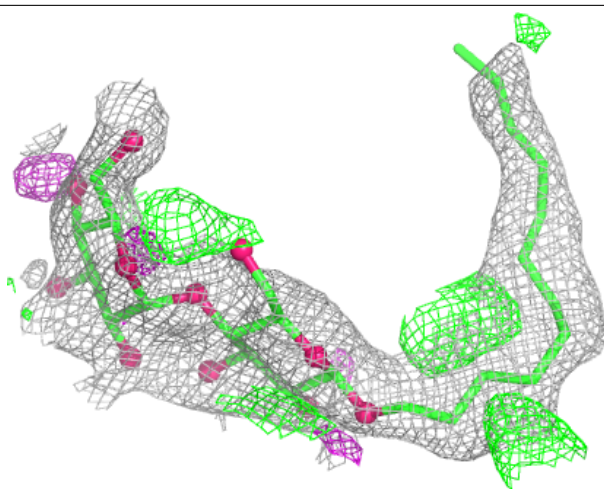
Electron density around LMT D 1105:

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



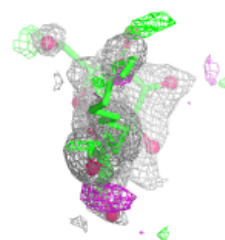
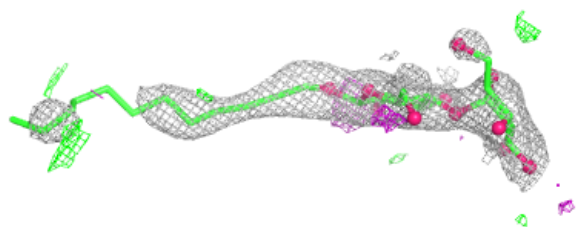
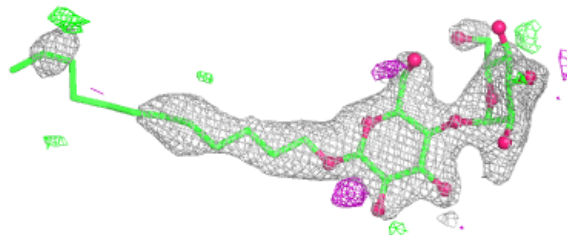
Electron density around LMT E 1105:

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

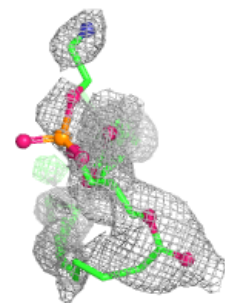
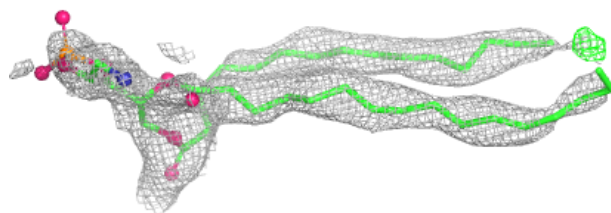
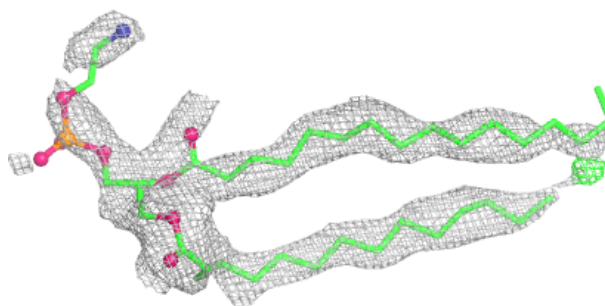


Electron density around LMT F 1113:

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

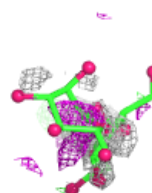
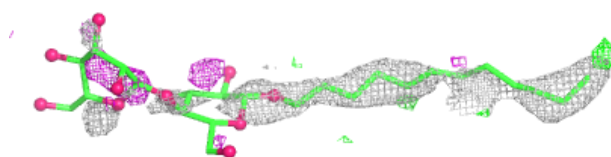
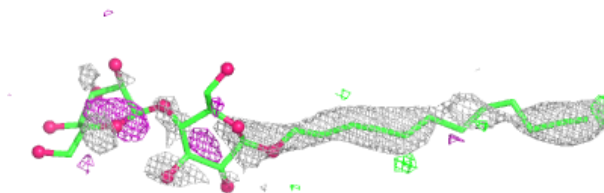
**Electron density around PTY A 1112:**

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

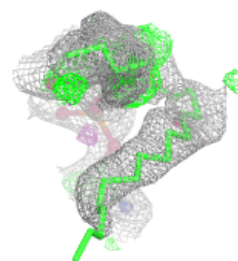
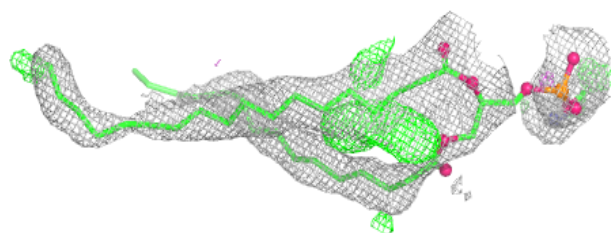
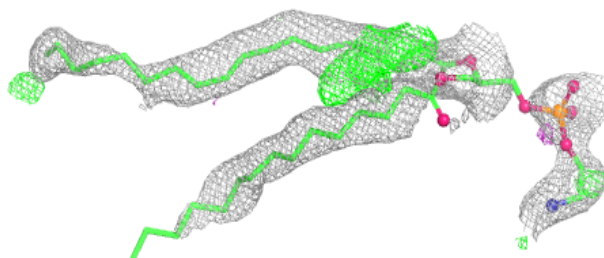


Electron density around LMT D 1109:

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

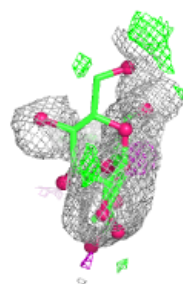
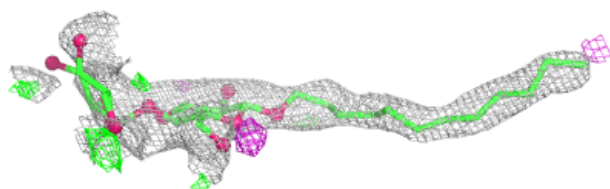
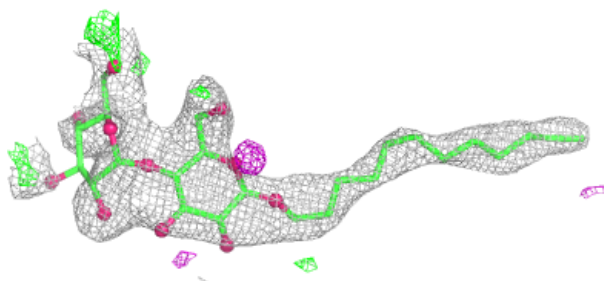
**Electron density around PTY C 1113:**

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

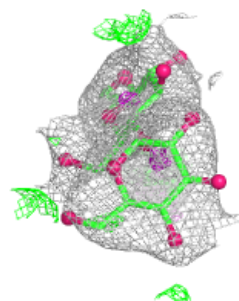
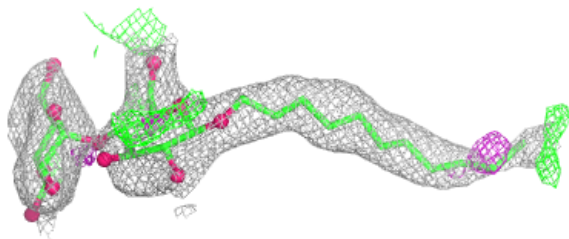
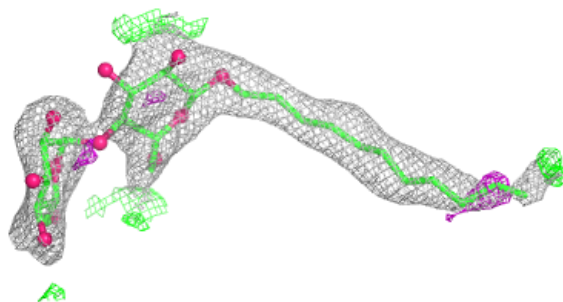


Electron density around LMT C 1101:

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

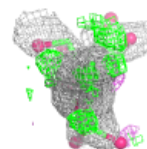
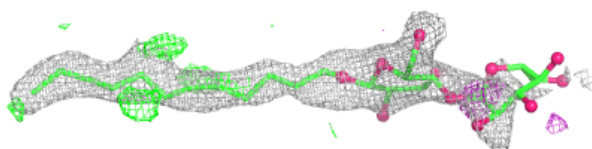
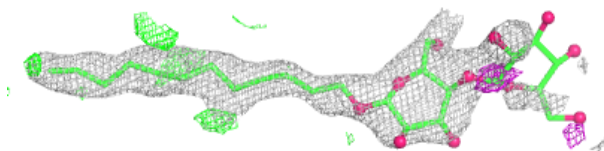
**Electron density around LMT A 1108:**

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

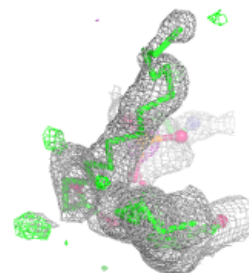
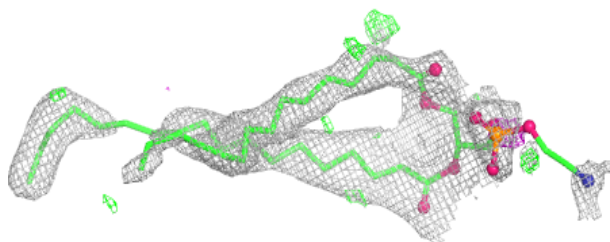
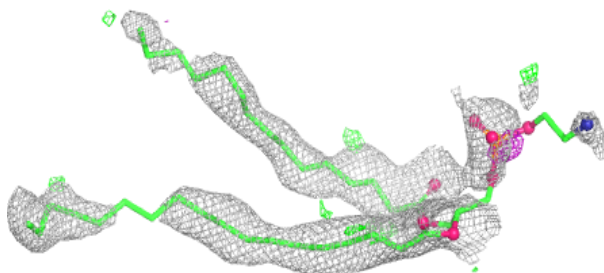


Electron density around LMT C 1112:

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

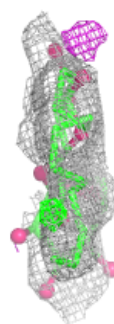
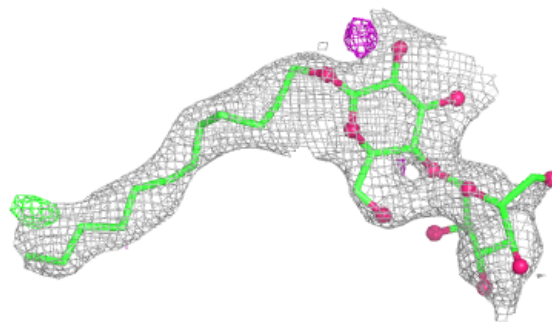
**Electron density around PTY D 1113:**

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



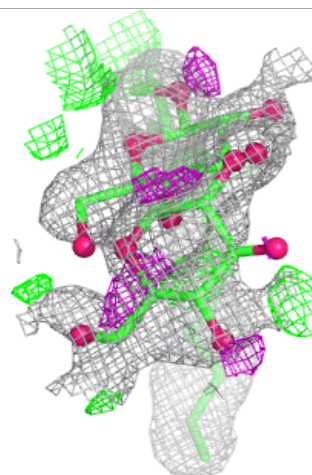
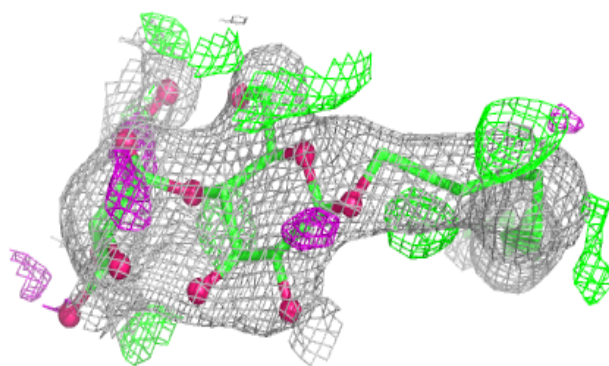
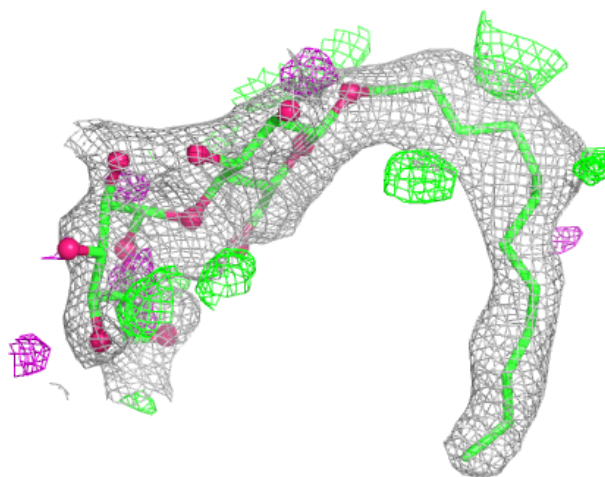
Electron density around LMT D 1112:

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



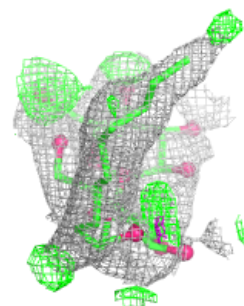
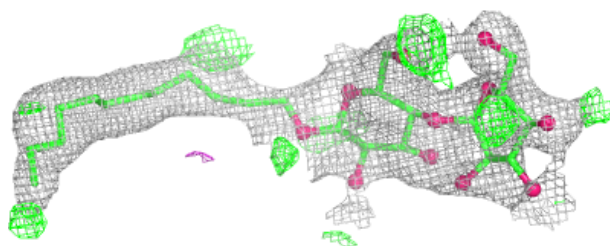
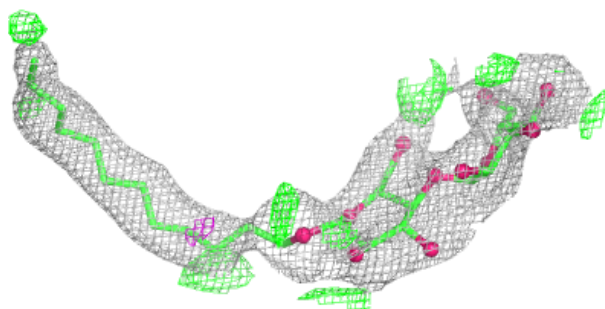
Electron density around LMT A 1105:

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

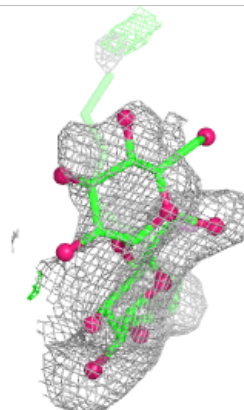
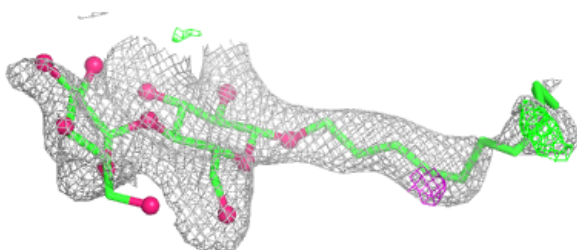
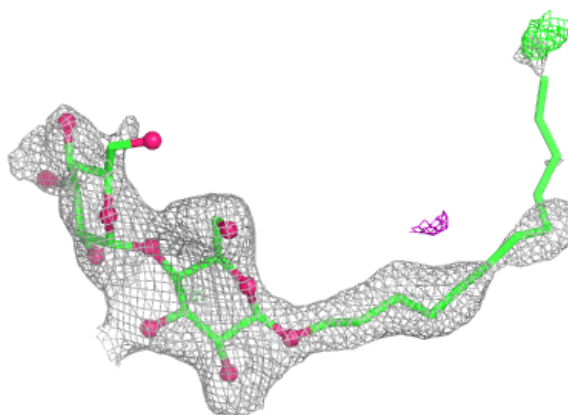


Electron density around LMT F 1106:

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

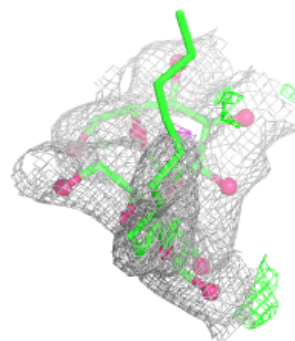
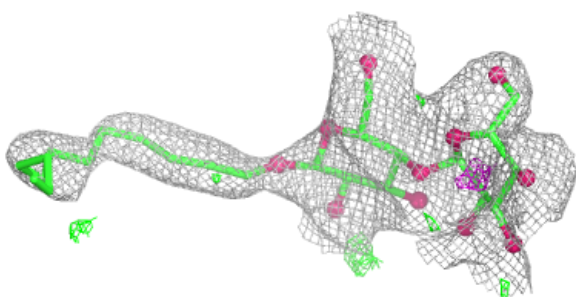
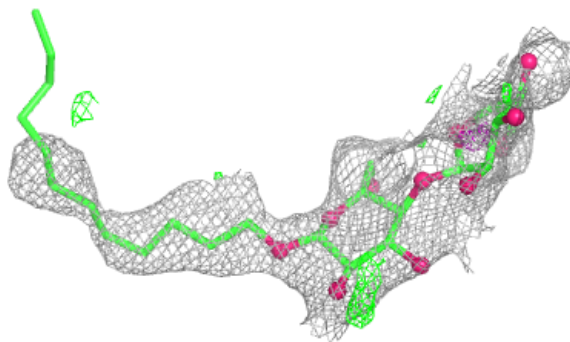
**Electron density around LMT D 1106:**

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

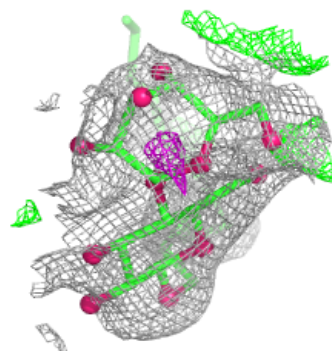
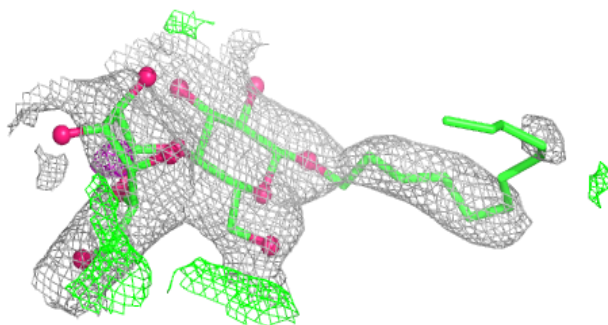
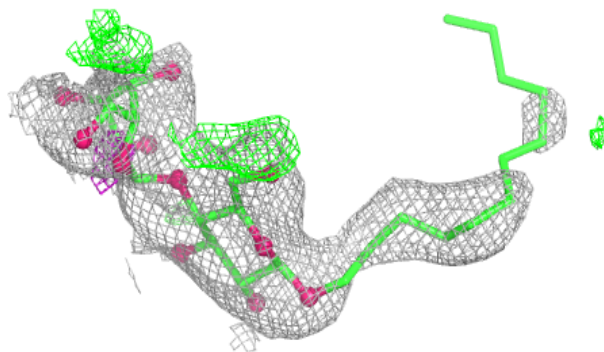


Electron density around LMT C 1110:

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

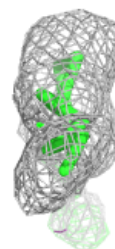
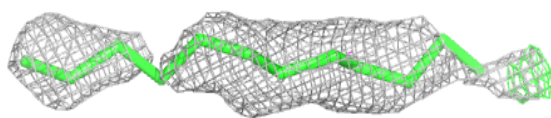
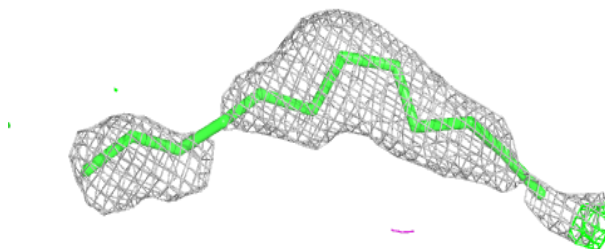
**Electron density around LMT E 1107:**

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

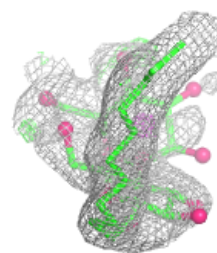
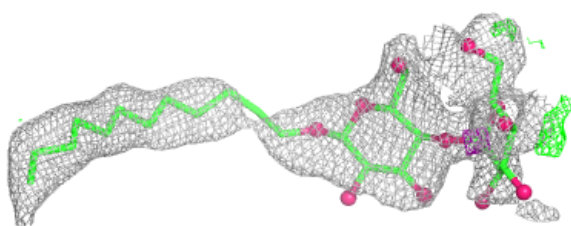
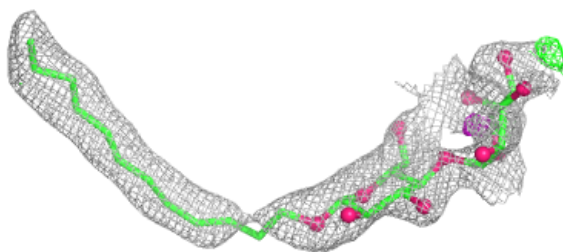


Electron density around LMT E 1111:

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

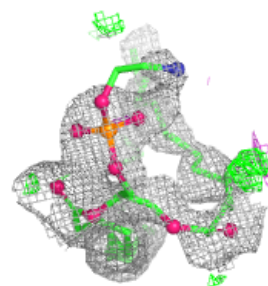
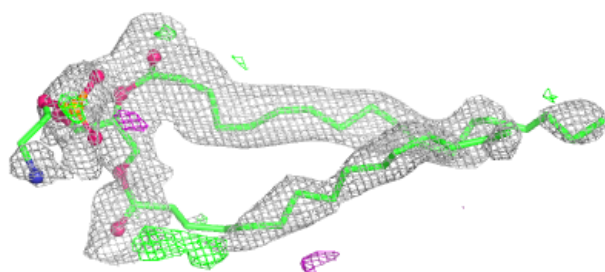
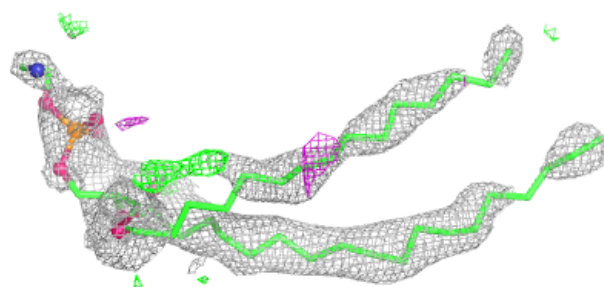
**Electron density around LMT D 1108:**

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

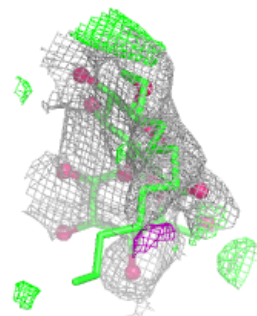
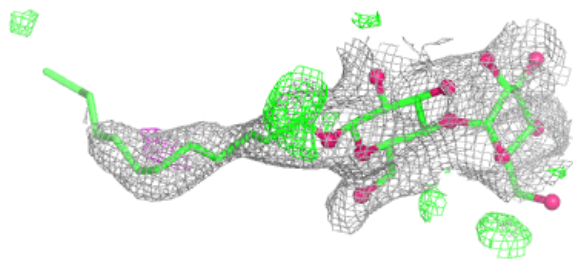
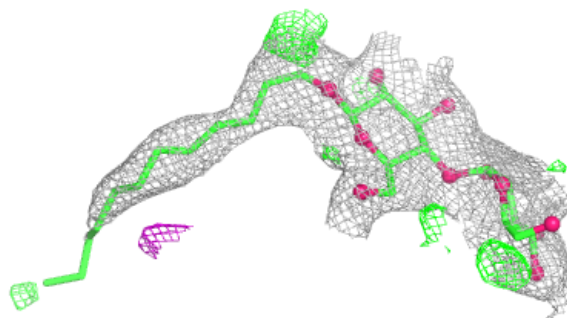


Electron density around PTY B 1112:

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

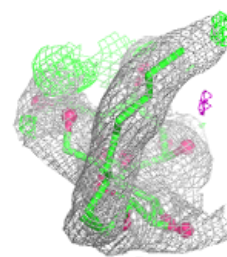
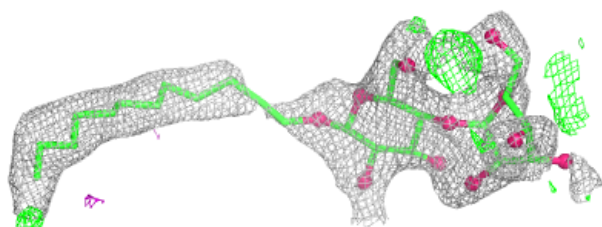
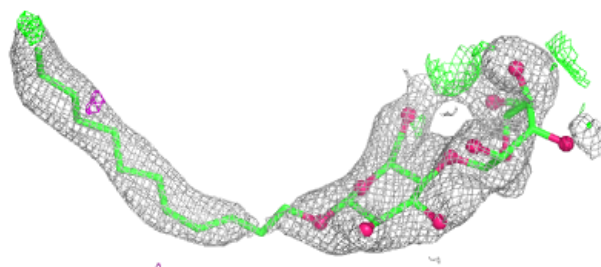
**Electron density around LMT B 1106:**

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

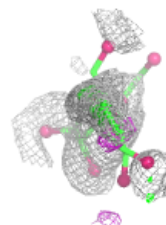
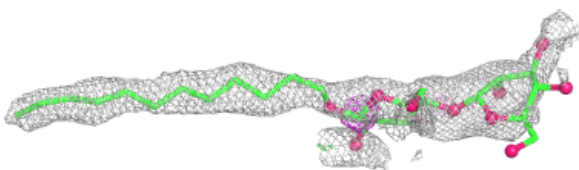
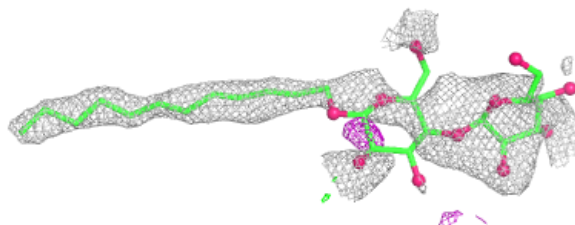


Electron density around LMT C 1106:

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

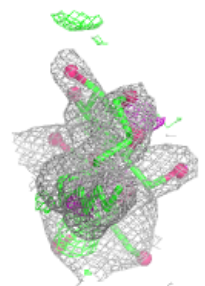
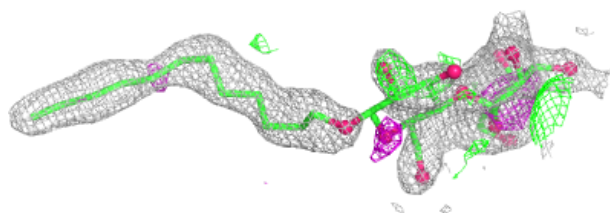
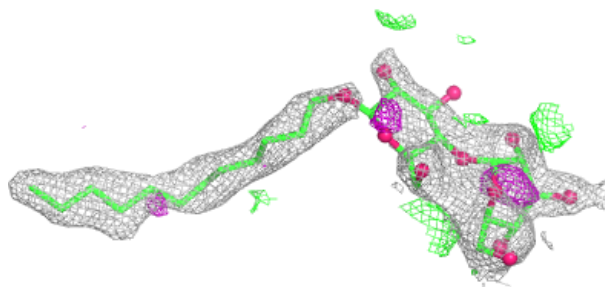
**Electron density around LMT E 1106:**

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

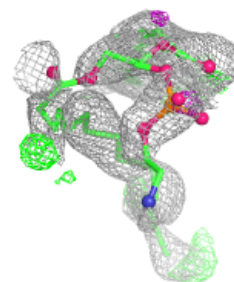
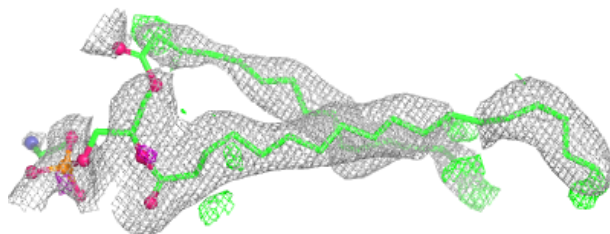
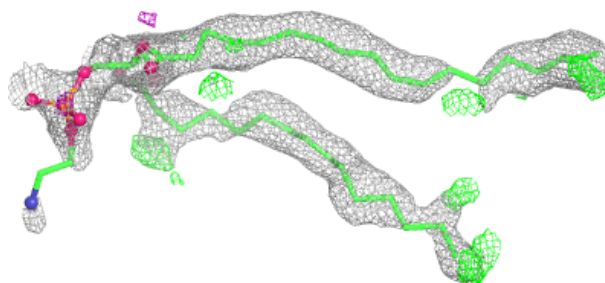


Electron density around LMT D 1103:

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

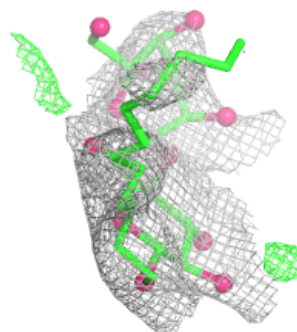
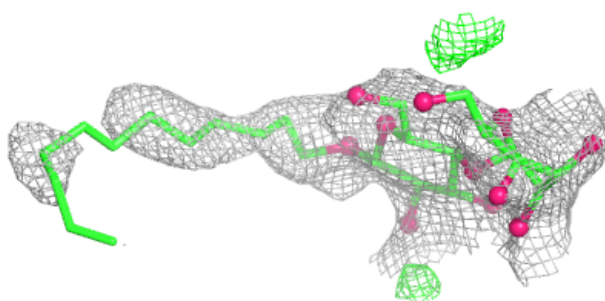
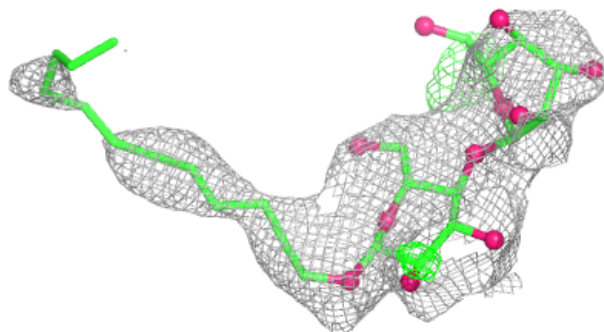
**Electron density around PTY E 1115:**

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

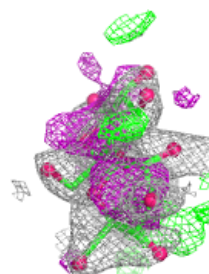
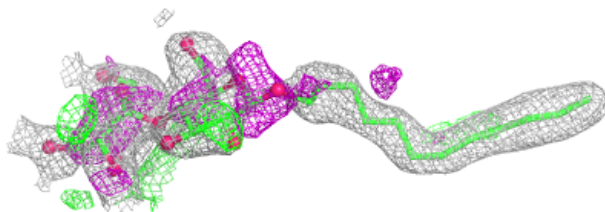
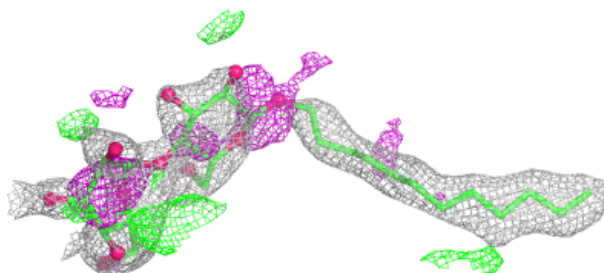


Electron density around LMT F 1107:

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

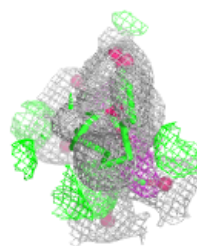
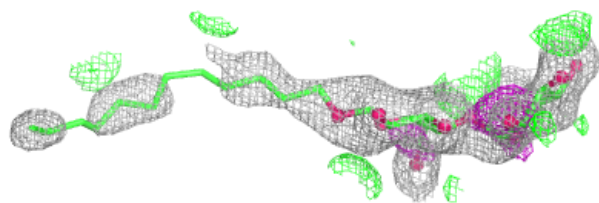
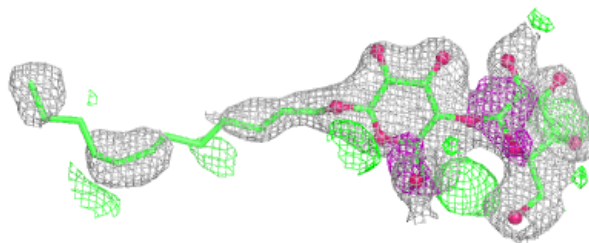
**Electron density around LMT C 1107:**

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

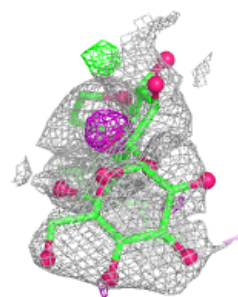
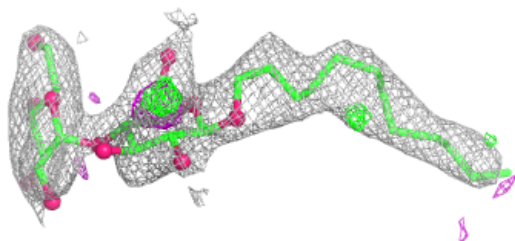
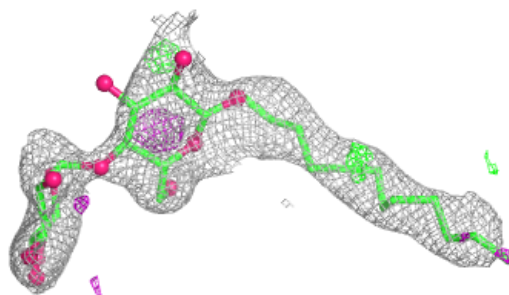


Electron density around LMT A 1111:

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

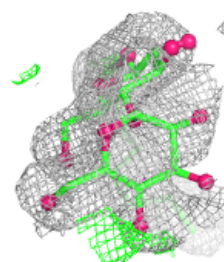
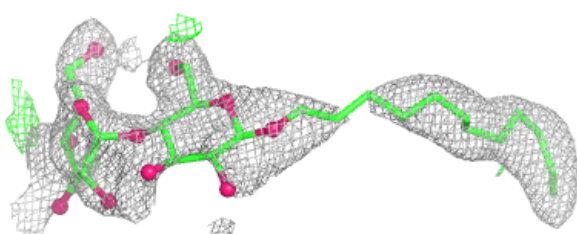
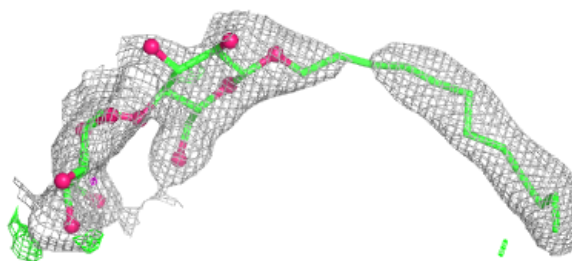
**Electron density around LMT E 1108:**

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

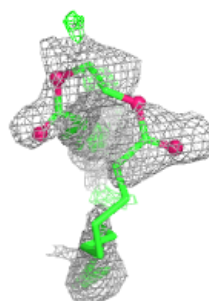
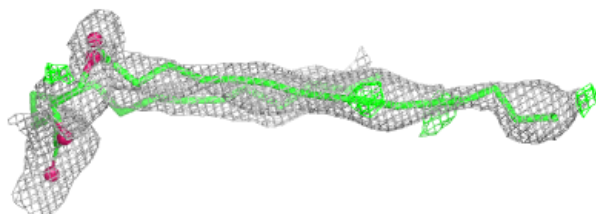
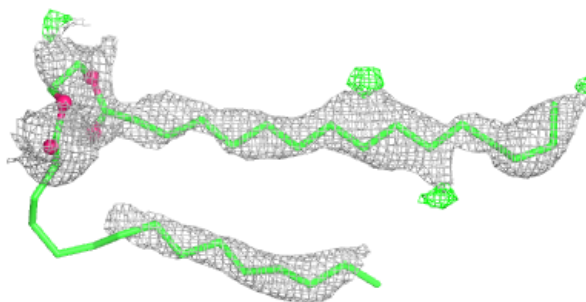


Electron density around LMT E 1110:

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

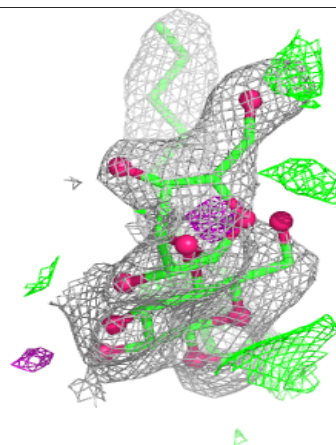
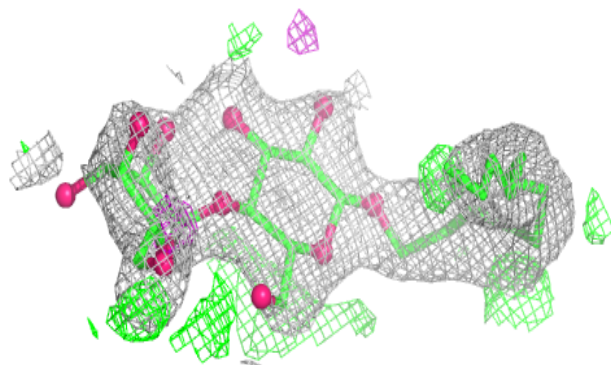
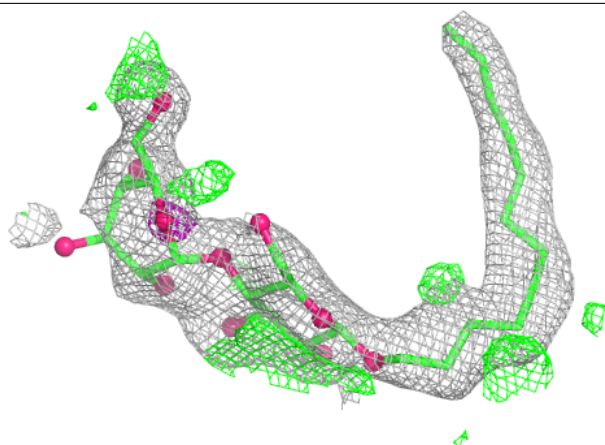
**Electron density around PTY F 1114:**

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

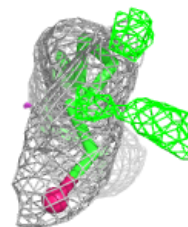
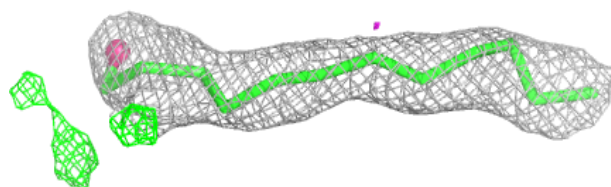
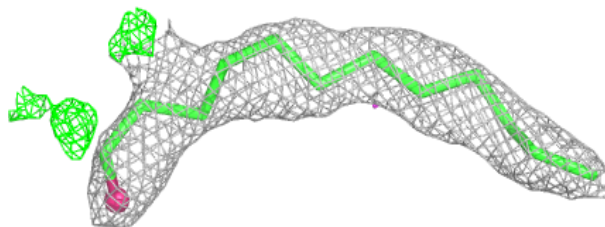


Electron density around LMT F 1105:

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

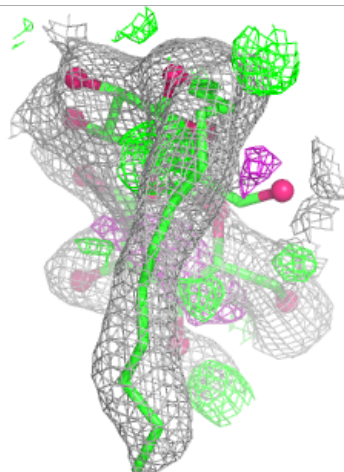
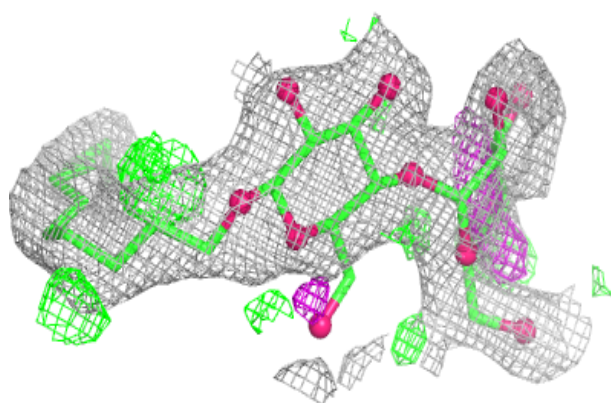
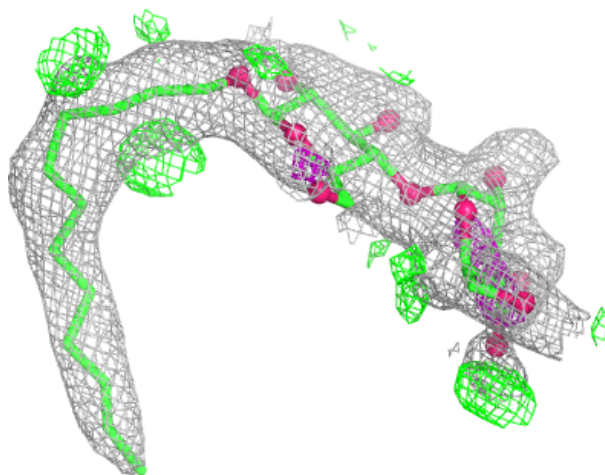
**Electron density around LMT F 1108:**

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



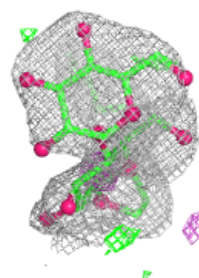
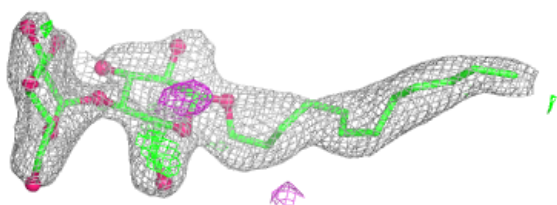
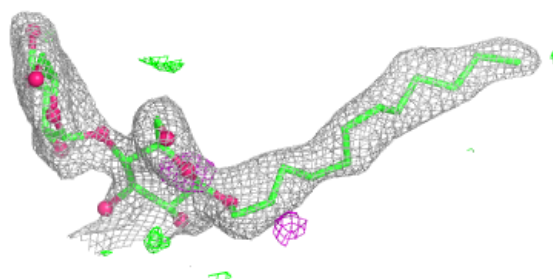
Electron density around LMT B 1105:

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

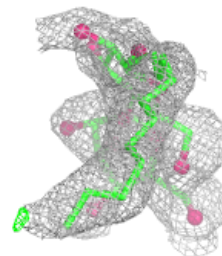
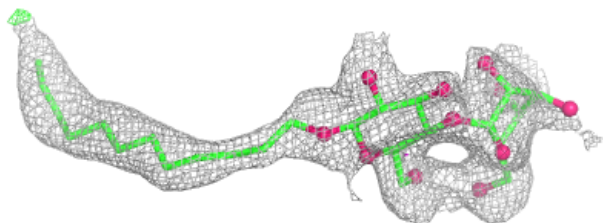
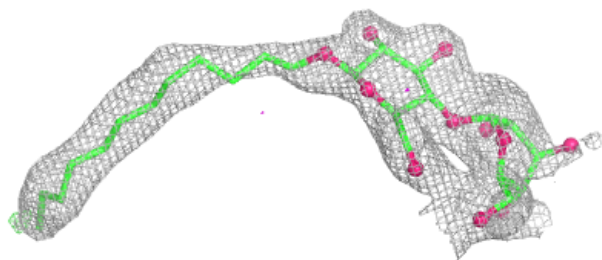


Electron density around LMT C 1111:

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

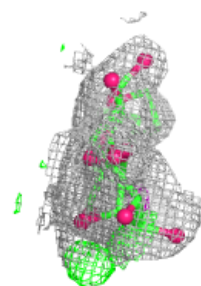
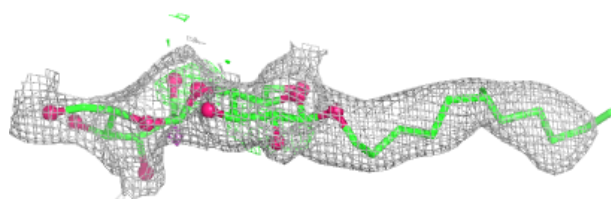
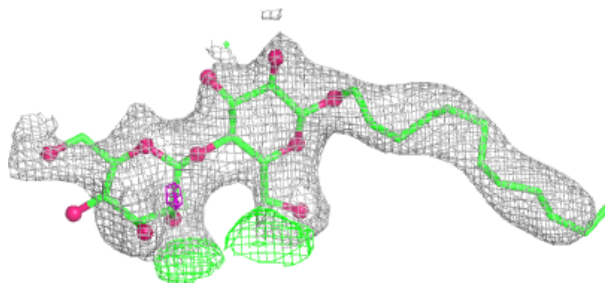
**Electron density around LMT A 1109:**

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

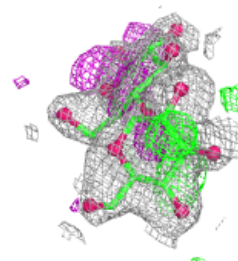
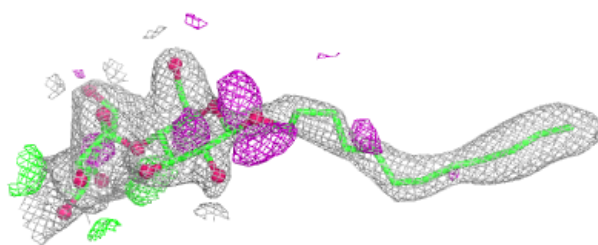
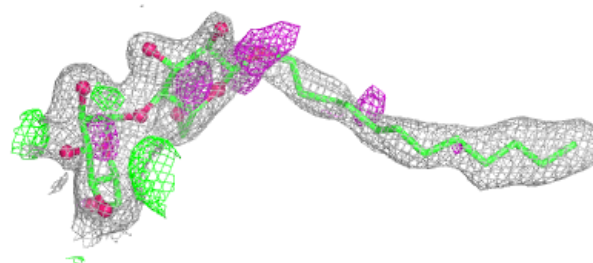


Electron density around LMT E 1102:

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

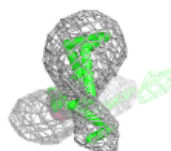
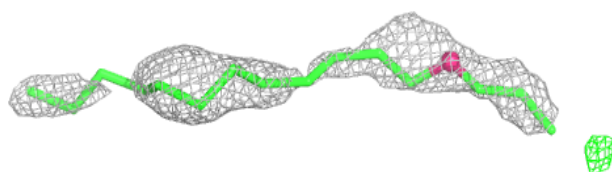
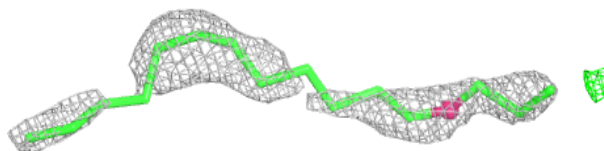
**Electron density around LMT E 1104:**

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

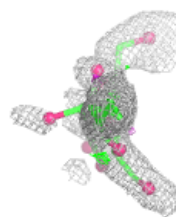
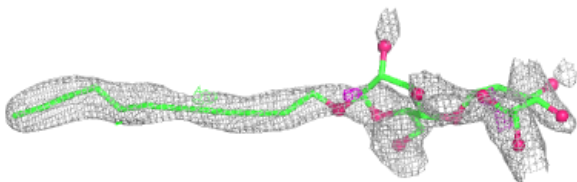
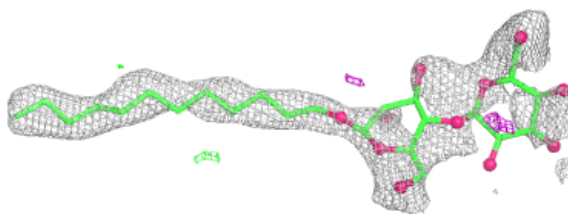


Electron density around LMT B 1107:

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

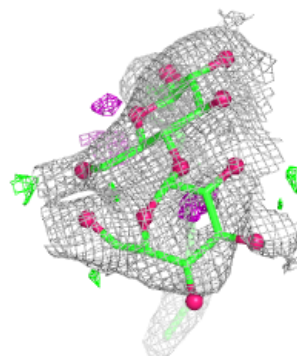
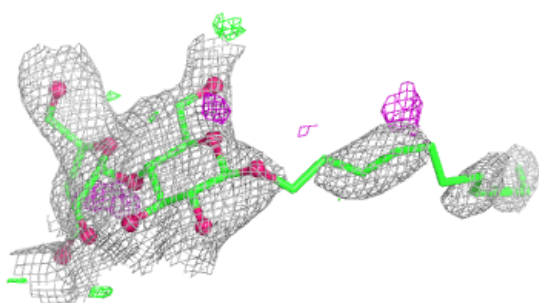
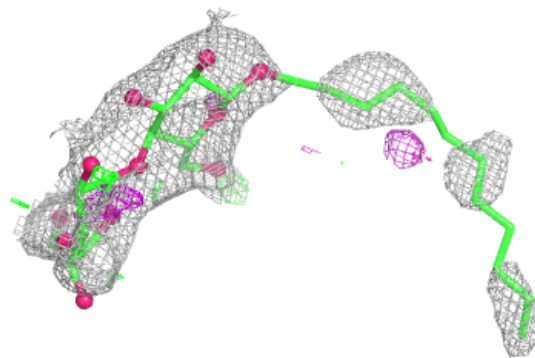
**Electron density around LMT F 1110:**

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

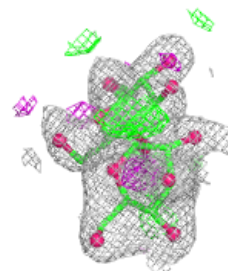
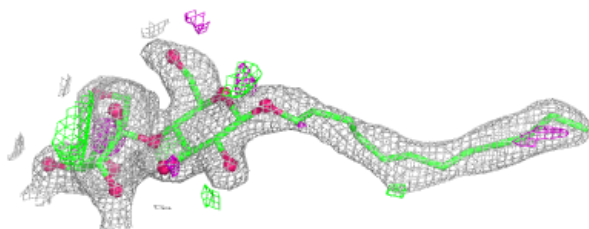
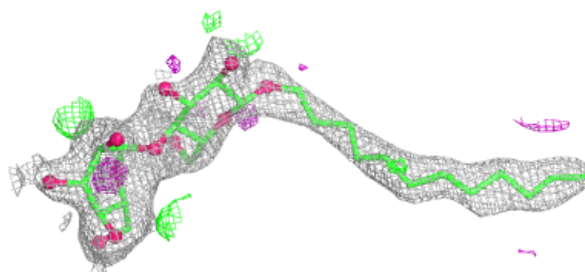


Electron density around LMT A 1106:

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

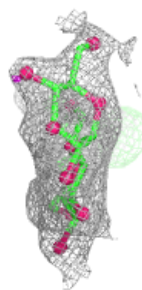
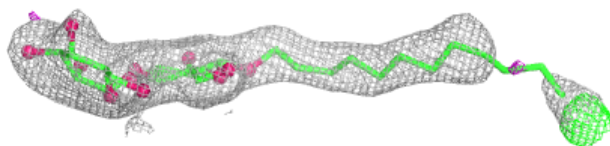
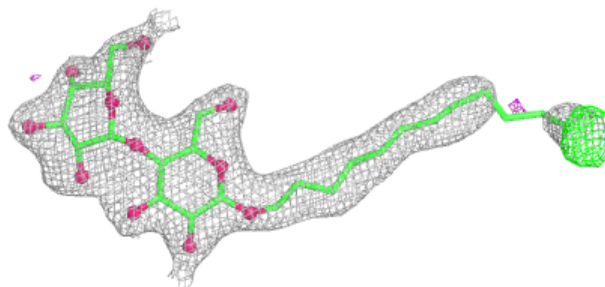
**Electron density around LMT B 1102:**

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

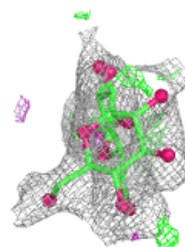
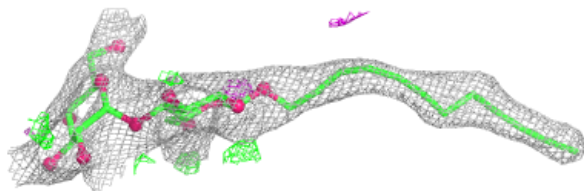
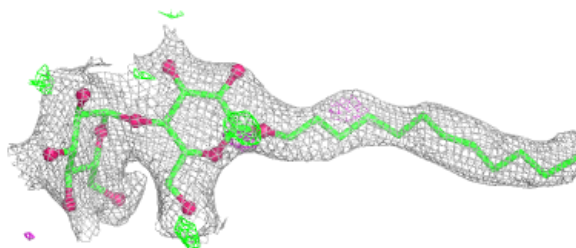


Electron density around LMT C 1102:

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

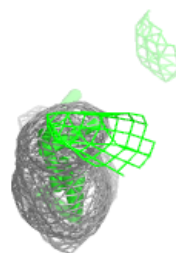
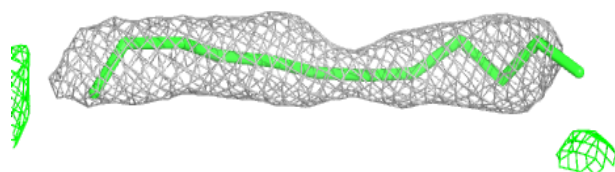
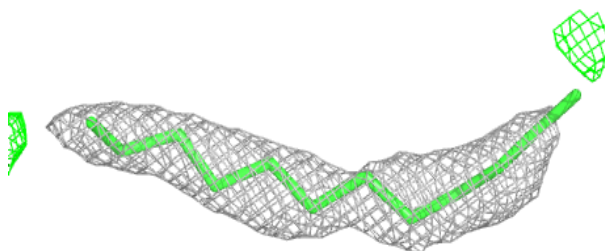
**Electron density around LMT D 1101:**

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

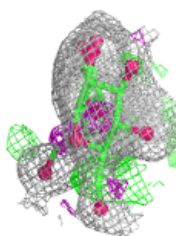
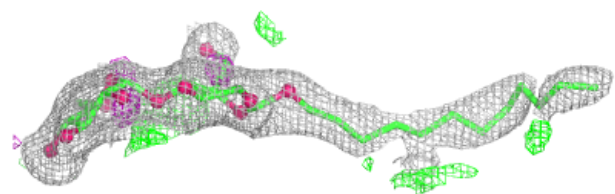
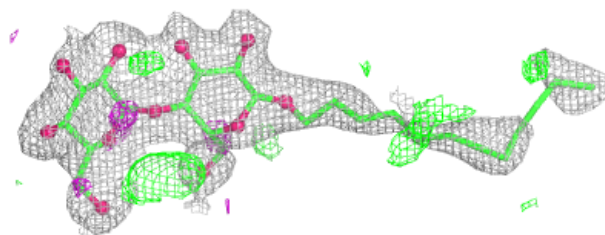


Electron density around LMT B 1108:

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

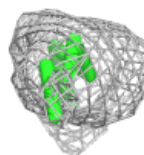
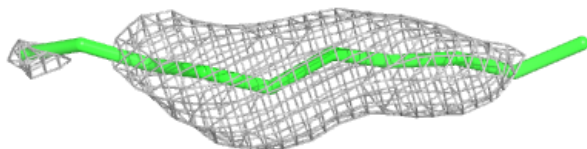
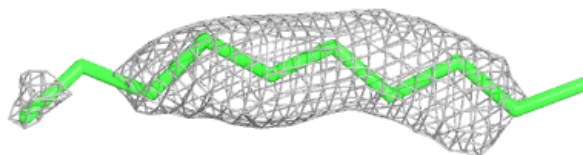
**Electron density around LMT E 1103:**

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

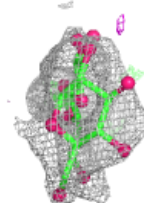
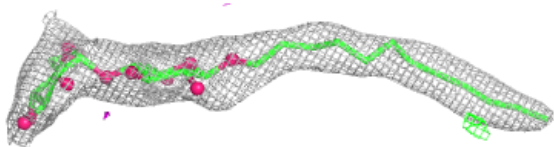
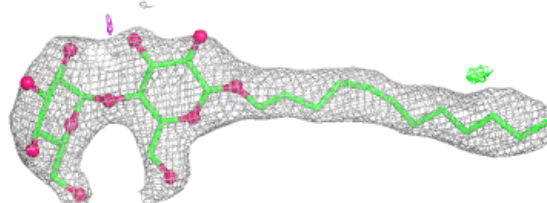


Electron density around LMT E 1113:

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

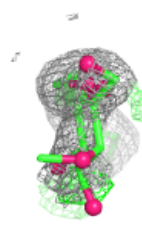
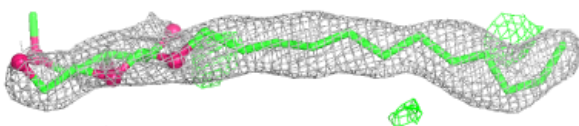
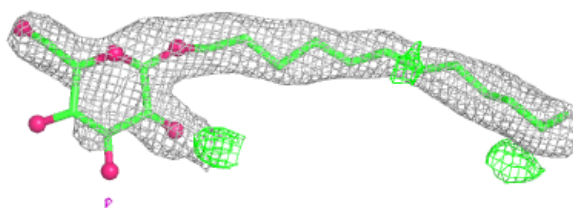
**Electron density around LMT F 1102:**

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

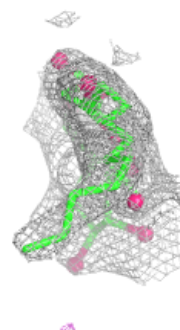
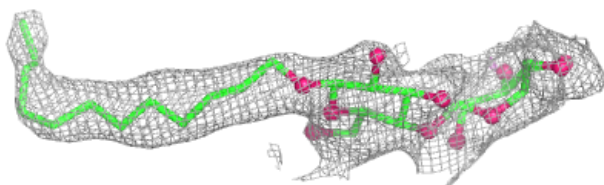
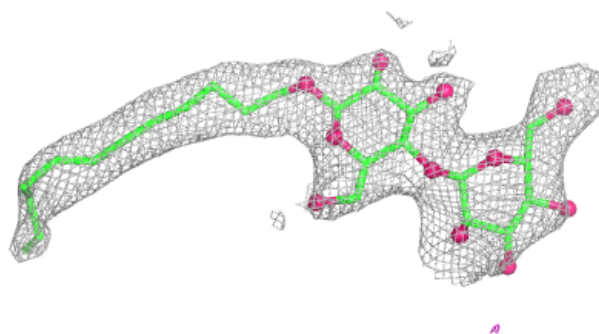


Electron density around LMT A 1110:

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

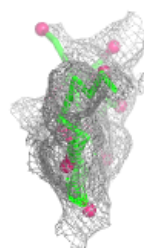
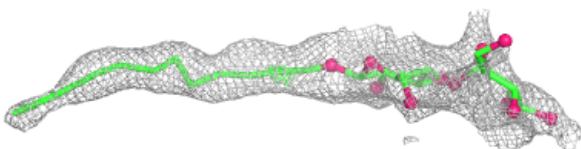
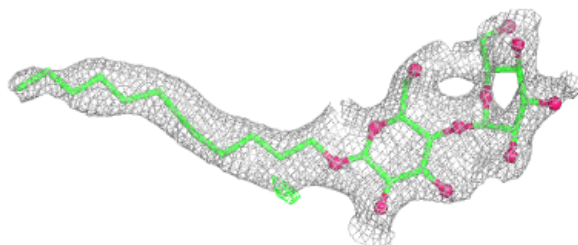
**Electron density around LMT D 1111:**

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

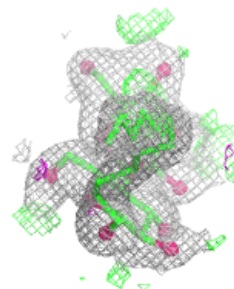
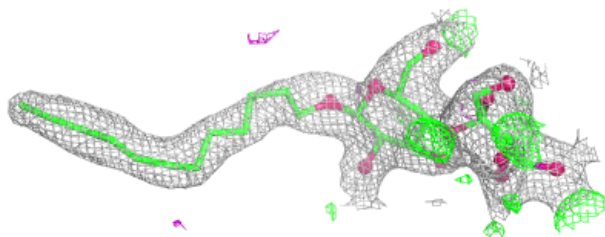
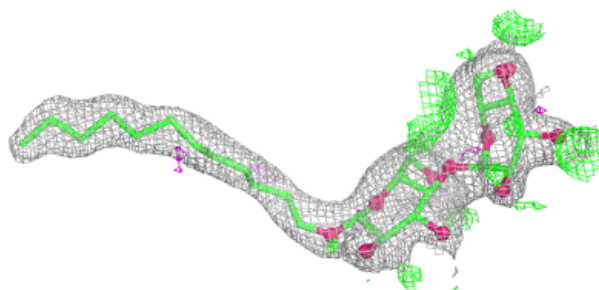


Electron density around LMT E 1109:

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

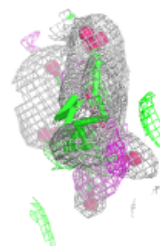
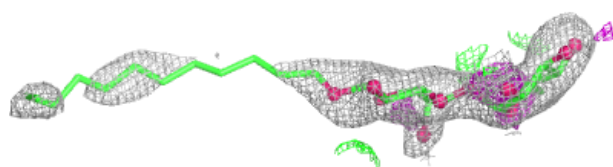
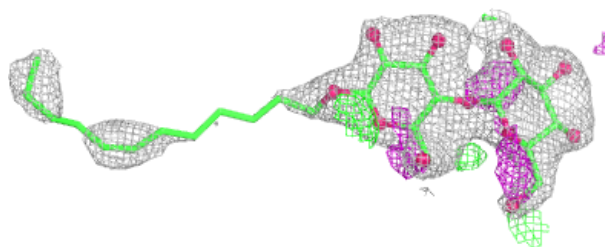
**Electron density around LMT F 1104:**

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

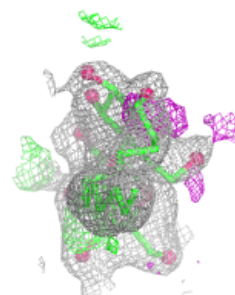
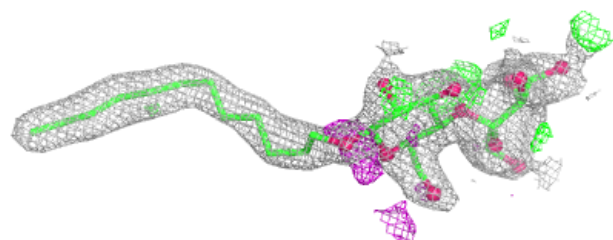
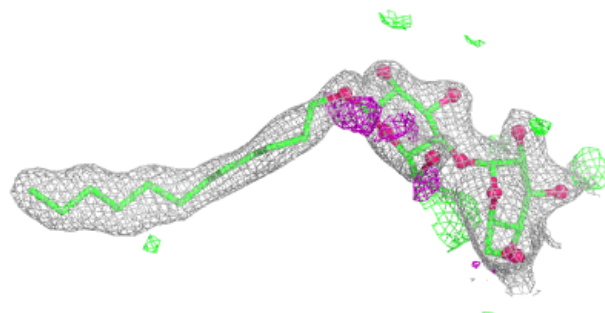


Electron density around LMT D 1102:

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

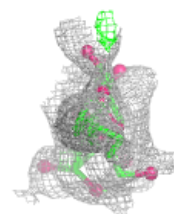
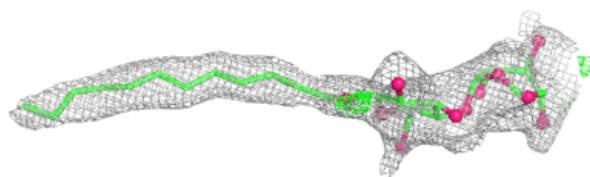
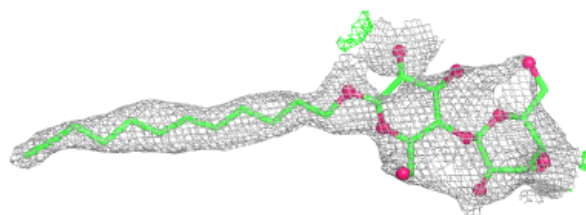
**Electron density around LMT A 1104:**

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

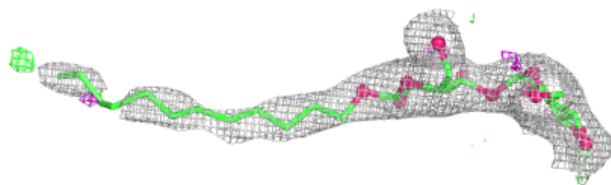
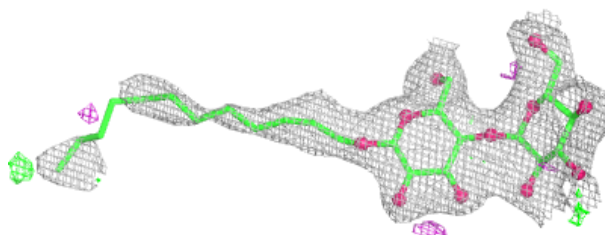


Electron density around LMT C 1109:

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

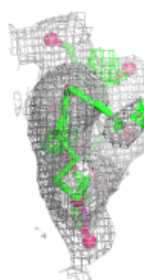
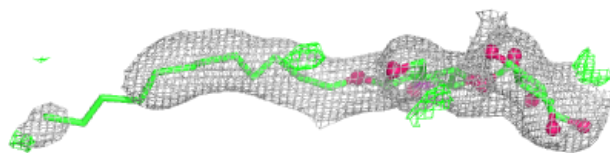
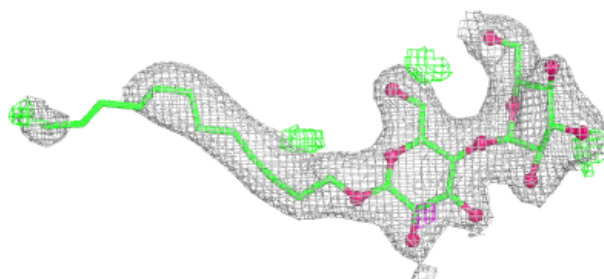
**Electron density around LMT B 1103:**

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

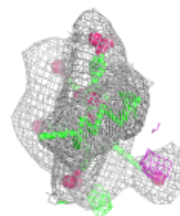
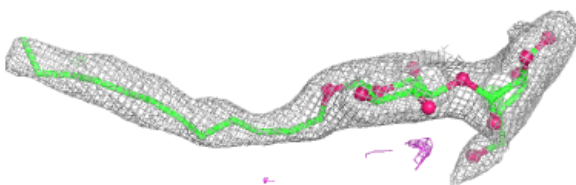
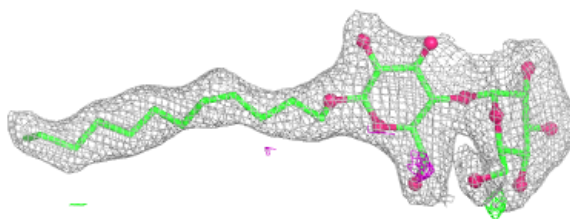


Electron density around LMT A 1102:

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

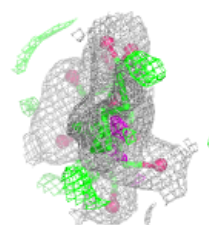
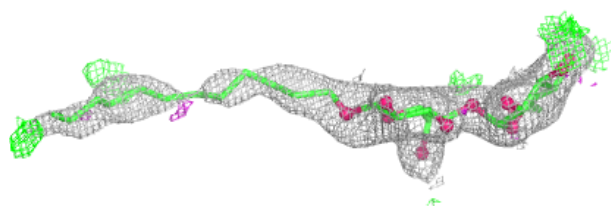
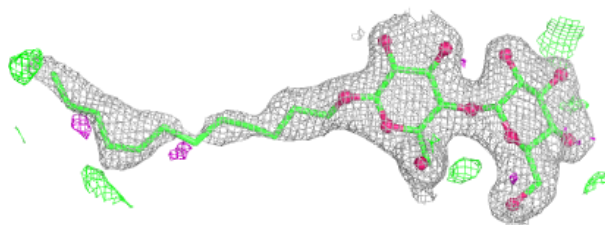
**Electron density around LMT C 1103:**

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

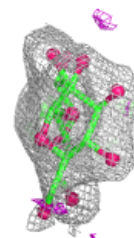
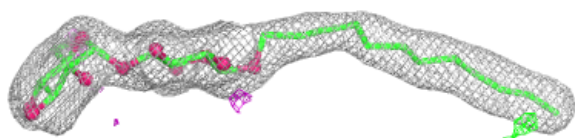
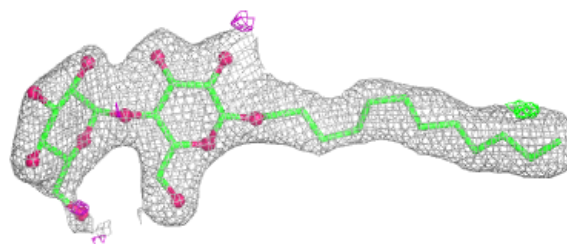


Electron density around LMT C 1105:

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

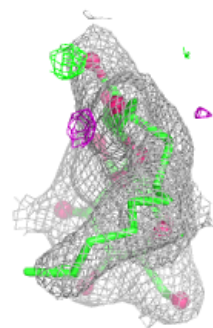
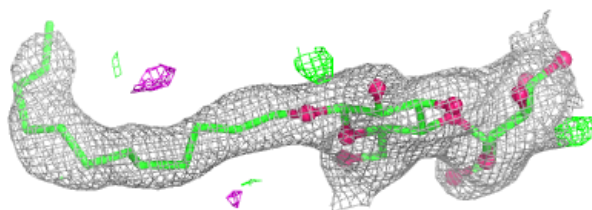
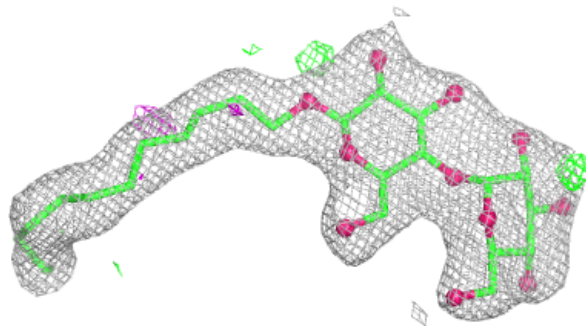
**Electron density around LMT E 1101:**

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

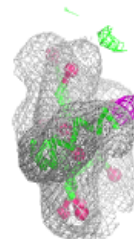
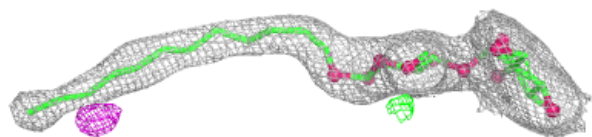
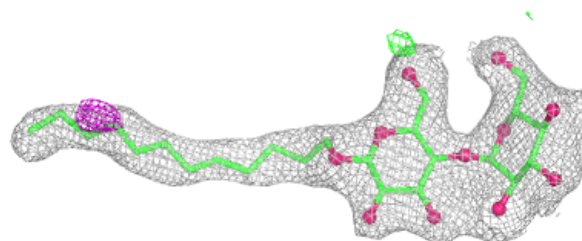


Electron density around LMT F 1101:

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

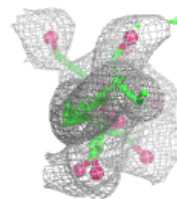
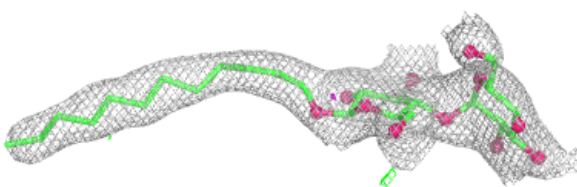
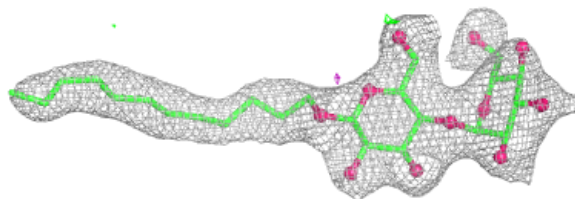
**Electron density around LMT C 1104:**

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

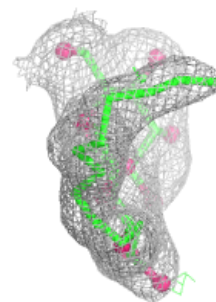
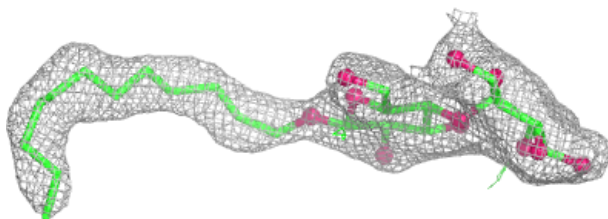
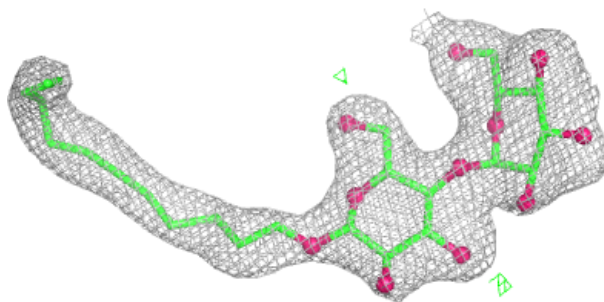


Electron density around LMT A 1103:

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

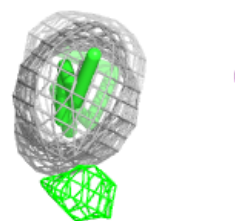
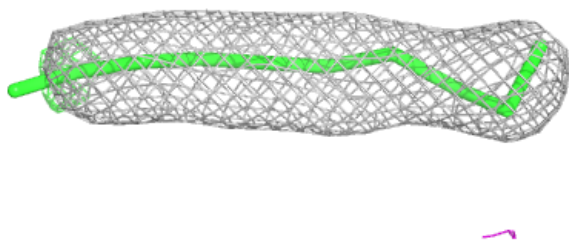
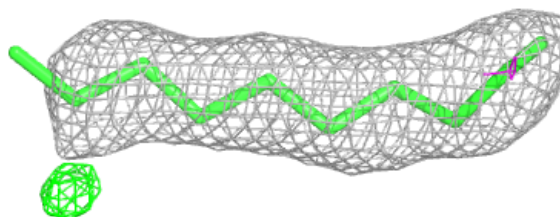
**Electron density around LMT B 1104:**

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

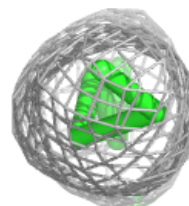
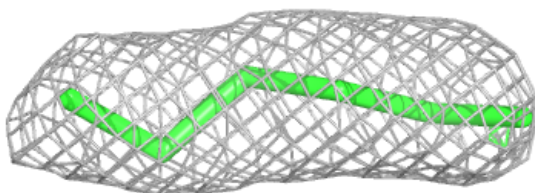
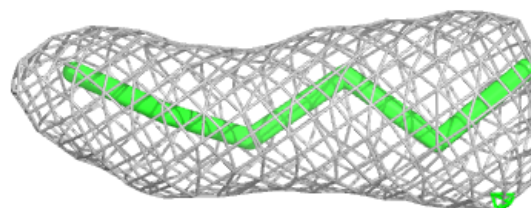


Electron density around LMT D 1110:

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

**Electron density around LMT F 1112:**

$2mF_o-DF_c$ (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.