



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 10:27 PM JST

PDB ID : 7CZ9
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

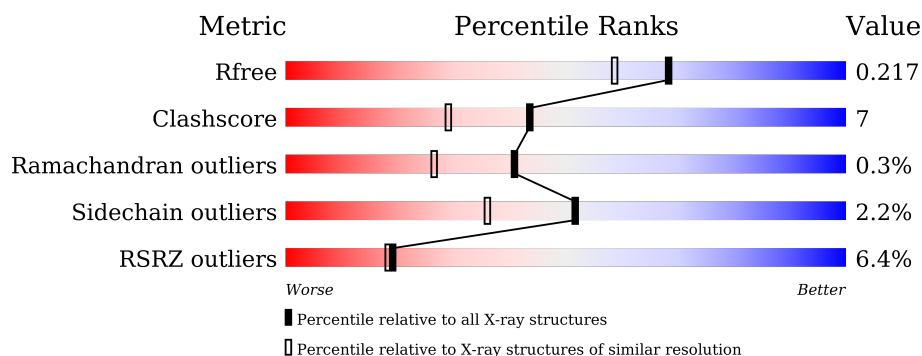
1 Overall quality at a glance

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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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	<div> <div>5%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	B	1042	<div> <div>8%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	1042	<div> <div>5%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	D	1042	<div> <div>10%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	E	1042	<div> <div>5%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	F	1042	<div> <div>5%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	D	1109	-	-	-	X
4	GOL	A	1113	-	X	-	-
4	GOL	A	1116	-	X	-	-
4	GOL	A	1120	-	X	-	-
4	GOL	E	1116	-	X	X	-
4	GOL	E	1119	-	X	-	-
4	GOL	E	1123	-	X	-	-

2 Entry composition [i](#)

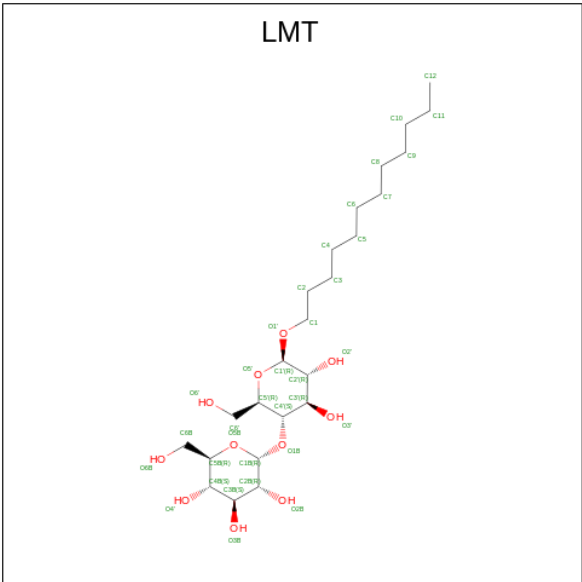
There are 5 unique types of molecules in this entry. The entry contains 53422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-MALTOSE (three-letter code: 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

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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

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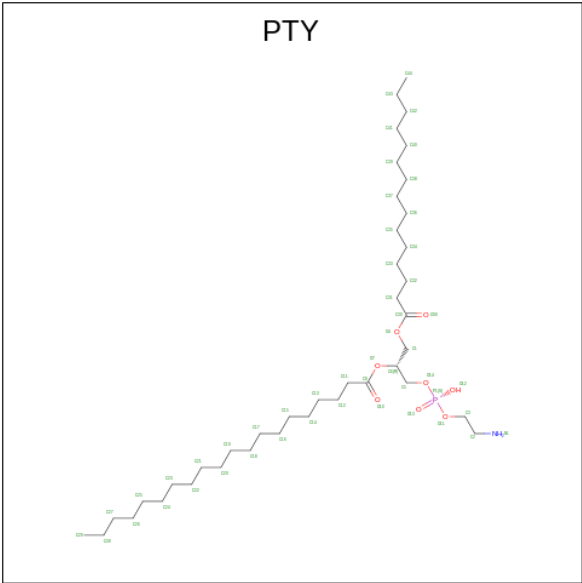
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0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

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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 (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).



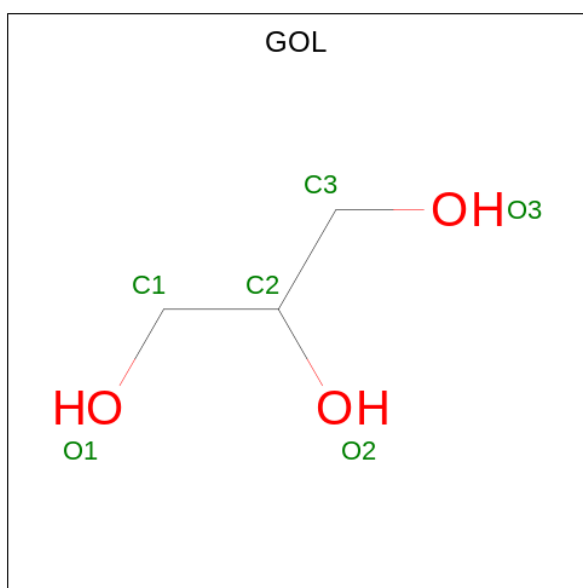
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
3	C	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

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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 (three-letter code: 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		

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

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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		

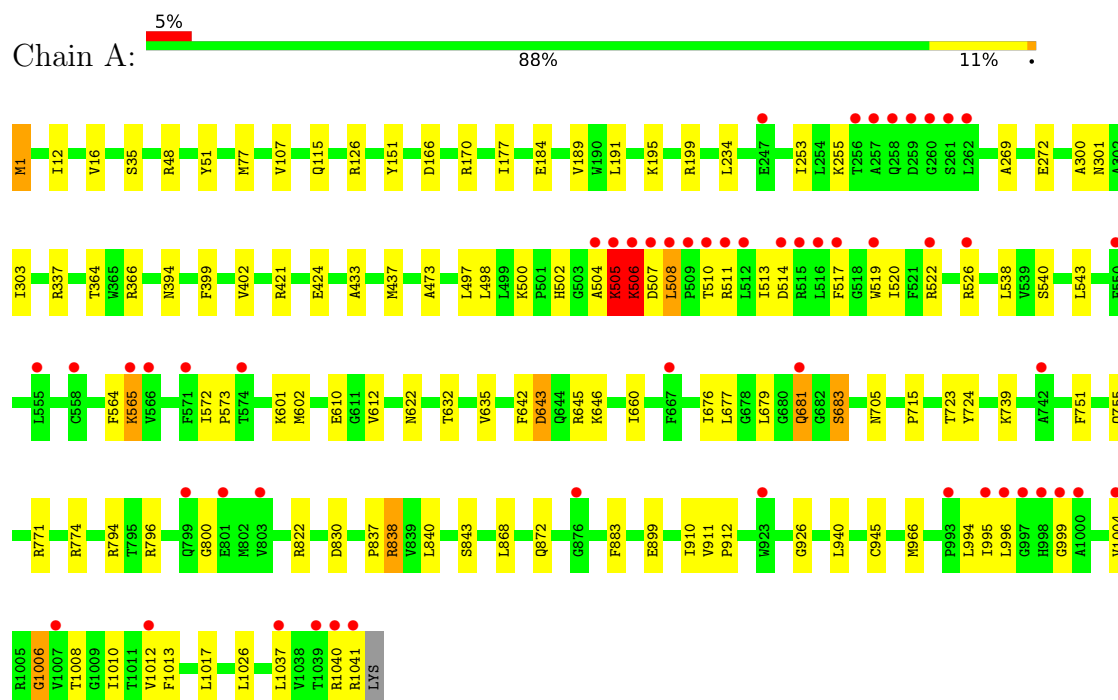
- Molecule 5 is water.

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		

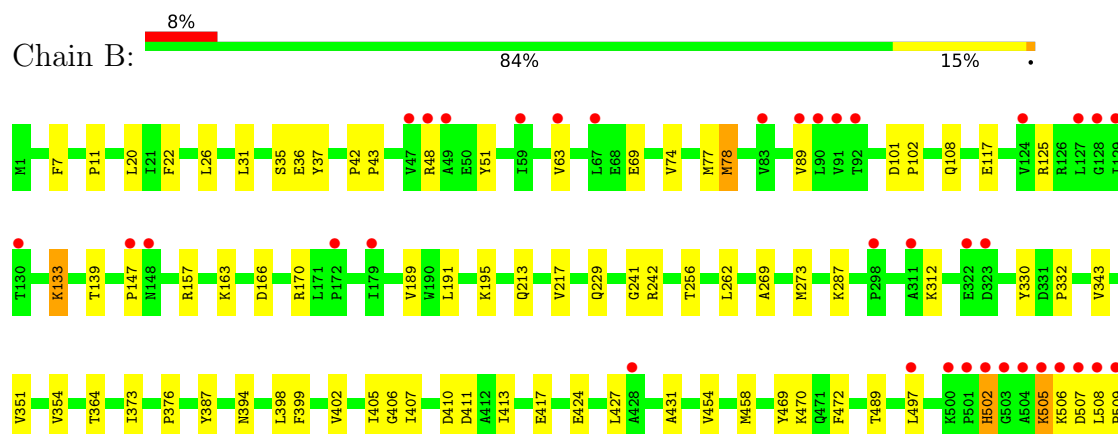
3 Residue-property plots [i](#)

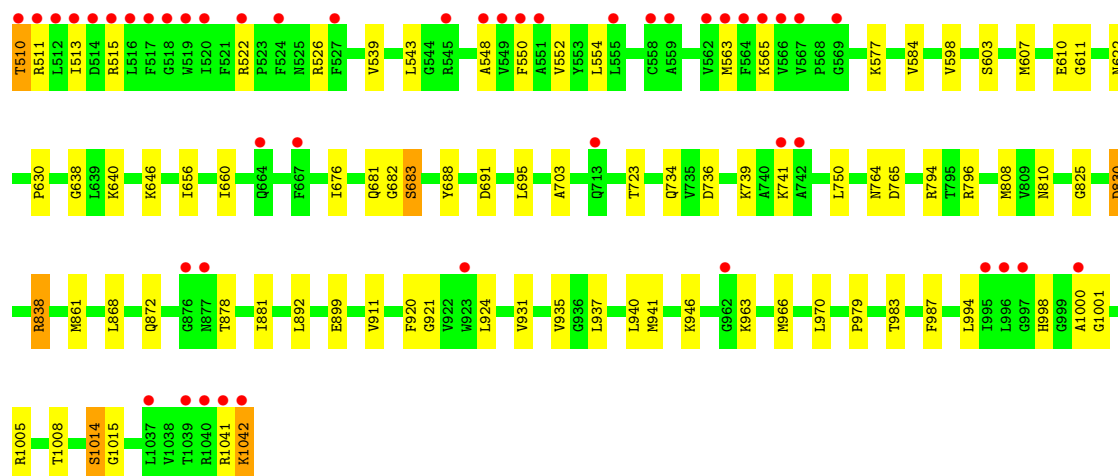
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

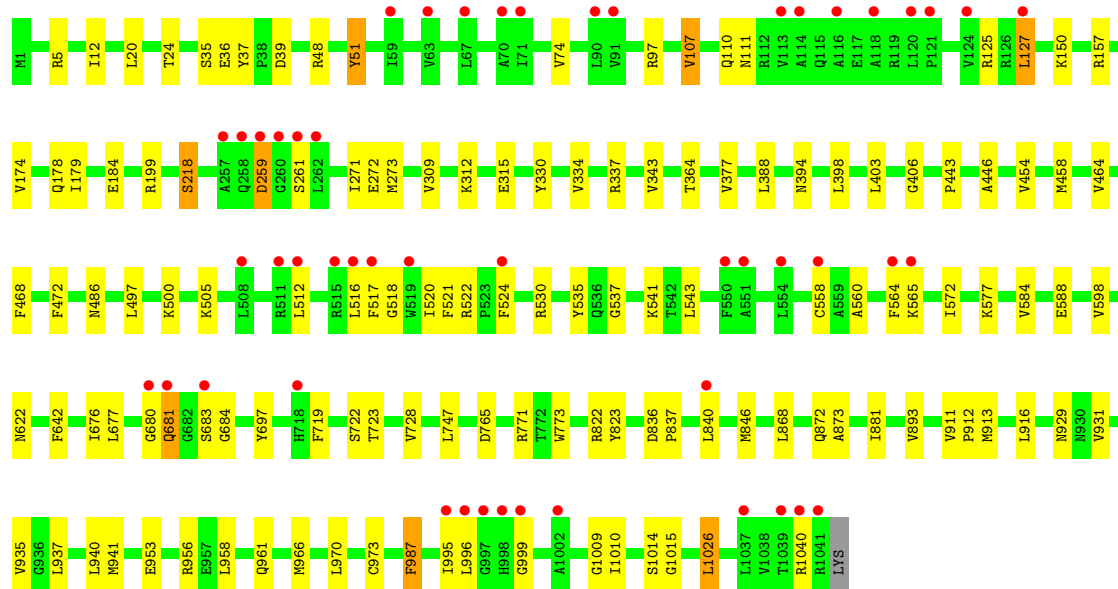
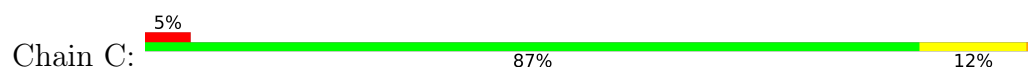


• Molecule 1: Efflux pump membrane transporter

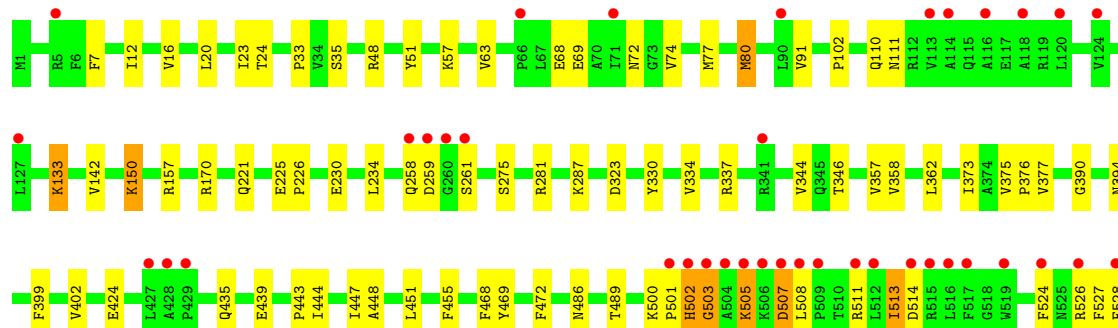
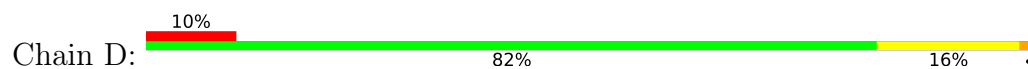


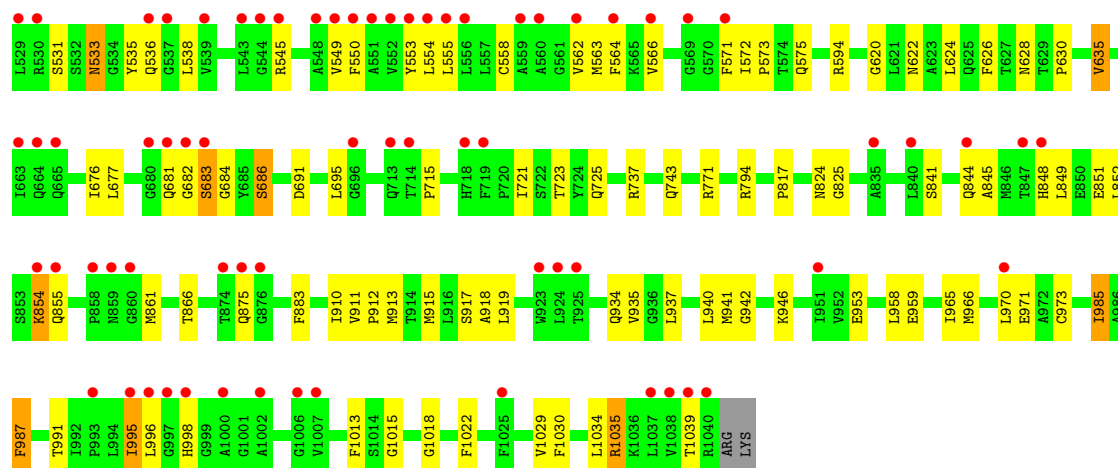


• Molecule 1: Efflux pump membrane transporter

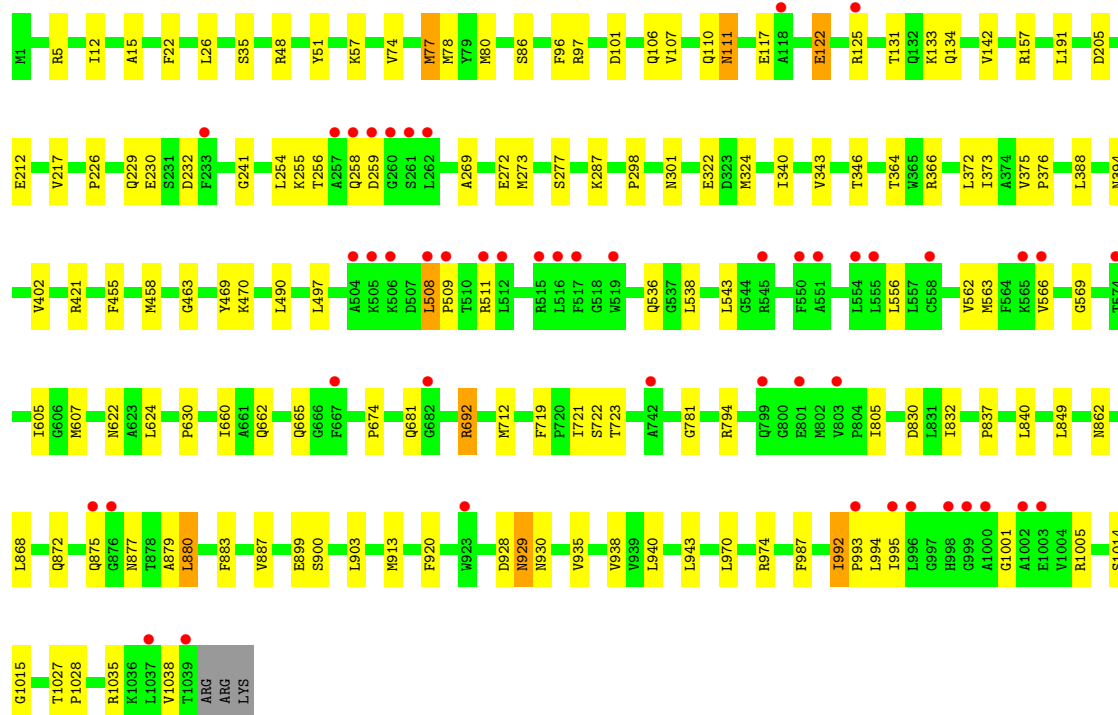
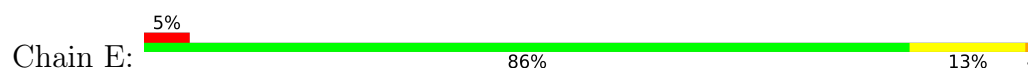


• Molecule 1: Efflux pump membrane transporter

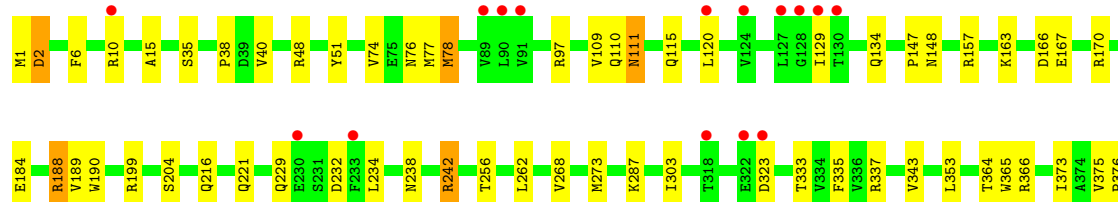
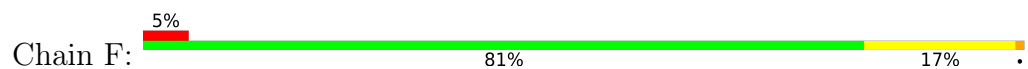


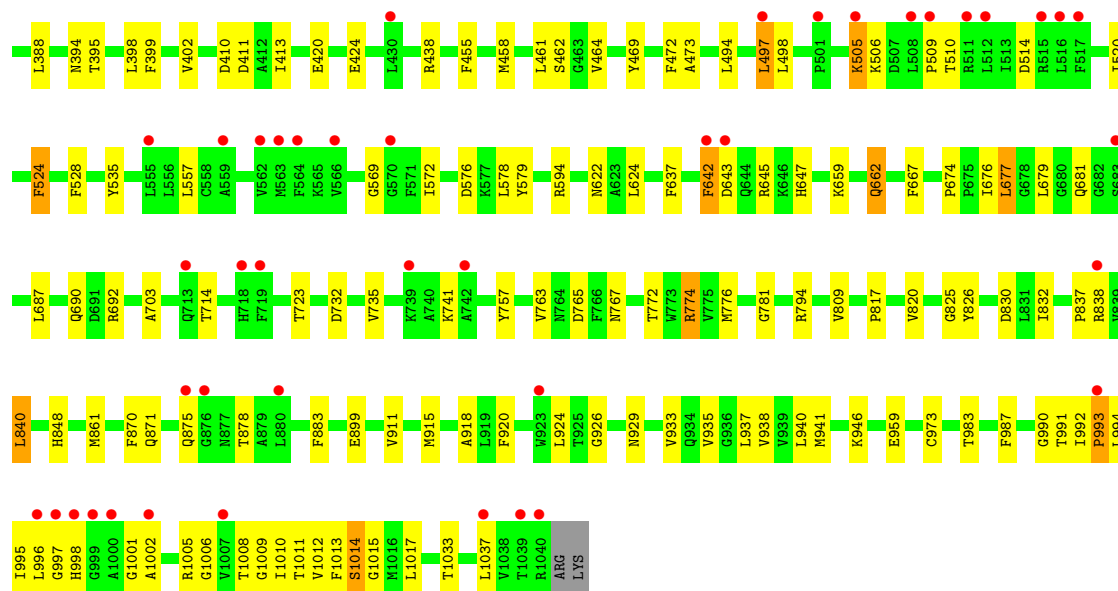


• Molecule 1: Efflux pump membrane transporter



• 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 48.45 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.28-1.85) 96.8 (48.45-1.85)	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 0.180 , 0.217	Depositor DCC
R_{free} test set	35735 reflections (5.04%)	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)	0.36 , 57.9	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: GOL, LMT, PTY

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	0.87	7/8111 (0.1%)	0.83	9/11042 (0.1%)
1	B	0.71	4/8089 (0.0%)	0.76	10/11013 (0.1%)
1	C	0.86	7/8080 (0.1%)	0.83	9/11002 (0.1%)
1	D	0.76	6/8069 (0.1%)	0.78	8/10988 (0.1%)
1	E	0.84	5/8100 (0.1%)	0.84	11/11027 (0.1%)
1	F	0.81	8/8078 (0.1%)	0.80	11/11000 (0.1%)
All	All	0.81	37/48527 (0.1%)	0.81	58/66072 (0.1%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	757	TYR	CD1-CE1	8.51	1.52	1.39
1	A	151	TYR	CD2-CE2	7.43	1.50	1.39
1	F	111	ASN	CB-CG	6.93	1.67	1.51
1	D	142	VAL	CB-CG2	6.76	1.67	1.52
1	A	189	VAL	CB-CG1	6.72	1.67	1.52
1	C	107	VAL	CB-CG2	6.70	1.67	1.52
1	F	189	VAL	CB-CG1	6.57	1.66	1.52
1	E	212	GLU	CG-CD	6.36	1.61	1.51
1	B	189	VAL	CB-CG1	6.23	1.66	1.52
1	F	109	VAL	CB-CG1	6.21	1.65	1.52
1	A	635	VAL	CB-CG2	6.16	1.65	1.52
1	F	268	VAL	CB-CG2	6.06	1.65	1.52
1	E	122	GLU	CB-CG	5.99	1.63	1.52
1	B	89	VAL	CB-CG1	5.87	1.65	1.52
1	B	63	VAL	CB-CG2	5.76	1.65	1.52
1	D	91	VAL	CB-CG1	5.70	1.64	1.52
1	A	945	CYS	CB-SG	-5.46	1.73	1.81
1	C	823	TYR	CD1-CE1	5.43	1.47	1.39
1	E	96	PHE	CD2-CE2	5.42	1.50	1.39
1	F	188	ARG	CG-CD	5.35	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	VAL	CB-CG1	5.34	1.64	1.52
1	F	763	VAL	CB-CG2	5.22	1.63	1.52
1	C	309	VAL	CB-CG1	5.22	1.63	1.52
1	D	635	VAL	CB-CG2	5.21	1.63	1.52
1	C	74	VAL	CB-CG2	-5.20	1.42	1.52
1	D	375	VAL	CB-CG2	5.20	1.63	1.52
1	A	421	ARG	CZ-NH1	5.16	1.39	1.33
1	B	69	GLU	CG-CD	5.14	1.59	1.51
1	A	724	TYR	CD2-CE2	5.12	1.47	1.39
1	A	612	VAL	CB-CG1	5.12	1.63	1.52
1	E	142	VAL	CB-CG2	5.10	1.63	1.52
1	E	111	ASN	CB-CG	5.07	1.62	1.51
1	F	190	TRP	CB-CG	5.07	1.59	1.50
1	C	51	TYR	CD1-CE1	5.07	1.47	1.39
1	C	773	TRP	CE3-CZ3	5.06	1.47	1.38
1	D	275	SER	CB-OG	5.06	1.48	1.42
1	D	63	VAL	CB-CG2	5.04	1.63	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	D	771	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	F	774	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	E	692	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	E	692	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	F	188	ARG	NE-CZ-NH2	-9.91	115.35	120.30
1	E	421	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	F	774	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	C	771	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	E	830	ASP	CB-CG-OD1	8.12	125.60	118.30
1	B	242	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	421	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	77	MET	CG-SD-CE	-7.94	87.50	100.20
1	E	421	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	B	794	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	B	796	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	D	48	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	F	794	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	B	830	ASP	CB-CG-OD1	6.67	124.30	118.30
1	D	771	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	822	ARG	NE-CZ-NH2	-6.50	117.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	508	LEU	CA-CB-CG	6.50	130.24	115.30
1	F	776	MET	CG-SD-CE	6.40	110.44	100.20
1	D	794	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	F	794	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	126	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	F	78	MET	CG-SD-CE	6.15	110.04	100.20
1	B	794	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	796	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	78	MET	CG-SD-CE	6.01	109.82	100.20
1	A	830	ASP	CB-CG-OD1	5.95	123.66	118.30
1	E	101	ASP	CB-CG-OD1	5.87	123.58	118.30
1	F	2	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	C	199	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	765	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	5	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	D	737	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	497	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	107	VAL	CG1-CB-CG2	-5.56	102.00	110.90
1	E	607	MET	CG-SD-CE	-5.56	91.31	100.20
1	E	205	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	127	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	C	48	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	822	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	715	PRO	C-N-CA	-5.39	110.99	122.30
1	F	765	ASP	CB-CG-OD1	5.36	123.12	118.30
1	E	794	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	D	281	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	B	101	ASP	CB-CG-OD1	5.32	123.09	118.30
1	F	242	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	D	80	MET	CG-SD-CE	-5.22	91.85	100.20
1	E	5	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	765	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	794	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	199	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	F	48	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	C	5	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	743	GLN	CB-CA-C	-5.08	100.25	110.40

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	88	0
1	B	7932	0	8140	103	0
1	C	7923	0	8127	83	0
1	D	7912	0	8114	128	0
1	E	7931	0	8153	119	0
1	F	7918	0	8120	148	0
2	A	374	0	480	18	0
2	B	308	0	413	12	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
4	F	30	0	39	2	0
5	A	553	0	0	5	0
5	B	439	0	0	4	0
5	C	564	0	0	11	0
5	D	415	0	0	6	0
5	E	528	0	0	7	0
5	F	441	0	0	12	0
All	All	53422	0	52729	691	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 (691) 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: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:C:956:ARG:HG2	4:C:1116:GOL:H2	1.59	0.84
1:E:74:VAL:HG12	1:E:77:MET:HE2	1.59	0.83
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:E:712:MET:HE2	1:E:719:PHE:HB2	1.66	0.76
1:D:825:GLY:HA3	2:D:1109:LMT:H102	1.70	0.74
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:F:1:MET:N	5:F:1204:HOH:O	2.21	0.72
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:F:97:ARG:HG2	2:F:1110:LMT:H6'2	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:110:GLN:NE2	1:E:111:ASN:HB2	2.10	0.67
1:E:556:LEU:HD13	1:E:913:MET:HE2	1.75	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: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: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: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: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:E:258:GLN:CD	1:E:258:GLN:H	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:411:ASP:OD1	1:F:946:LYS:NZ	2.23	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: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: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
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:994:LEU:HB3	1:F:1009:GLY:HA3	1.84	0.59
1:A:1:MET:N	1:A:1:MET:SD	2.70	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:36:GLU:OE2	1:C:577:LYS:NZ	2.36	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
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: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:B:1005:ARG:HG3	2:B:1103:LMT:H11	1.88	0.56
1:E:674:PRO:HB3	1:E:681:GLN:HA	1.87	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:74:VAL:HG12	1:E:77:MET:CE	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:PHE:HD2	1:A:999:GLY:HA2	1.72	0.55
1:C:271:ILE:HD12	4:C:1115:GOL:H31	1.87	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: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:D:915:MET:O	1:D:918:ALA:N	2.37	0.54
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:D:258:GLN:H	1:D:258:GLN:CD	2.10	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:B:411:ASP:OD1	1:B:946:LYS:NZ	2.28	0.54
1:D:941:MET:HE1	2:D:1112:LMT:H102	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:259:ASP:OD2	1:C:261:SER:OG	2.22	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
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: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:57:LYS:NZ	5:E:1207:HOH:O	2.28	0.51
1:F:256:THR:HG22	1:F:262:LEU:HD23	1.92	0.51
1:A:645:ARG:C	1:A:646:LYS:HE2	2.30	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:B:911:VAL:HG12	1:B:941:MET:CE	2.40	0.51
1:D:500:LYS:HE2	1:D:501:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:846:MET:HE1	1:C:873:ALA:HB2	1.92	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:F:703:ALA:HB2	1:F:861:MET:HE1	1.91	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: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: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:D:695:LEU:HD12	1:D:861:MET:HG3	1.94	0.50
1:E:563:MET:HE1	1:E:920:PHE:HA	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: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: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: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:E:74:VAL:CG1	1:E:77:MET:HE2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:ASN:OD1	1:F:97:ARG:NH1	2.46	0.49
1:F:458:MET:HE2	1:F:883:PHE:HE1	1.77	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
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: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: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:E:22:PHE:CE2	1:E:26:LEU:HD11	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:TYR:OH	1:F:973:CYS:HB3	2.14	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: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:458:MET:HE2	1:F:883:PHE:CE1	2.50	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
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: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
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:F:679:LEU:HA	1:F:679:LEU:HD23	1.59	0.46
1:F:996:LEU:O	1:F:1002:ALA:HB1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:563:MET:CE	1:E:920:PHE:HA	2.46	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:F:992:ILE:C	1:F:994:LEU:H	2.20	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:1005:ARG:HG3	2:E:1103:LMT:H1'	1.98	0.46
1:F:74:VAL:CG2	1:F:77:MET:HE2	2.46	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:B:703:ALA:CB	1:B:861:MET:HE1	2.46	0.45
1:A:739:LYS:HE2	1:A:739:LYS:HB2	1.74	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
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:E:80:MET:HE2	1:E:80:MET:HB2	1.82	0.45
1:F:579:TYR:HA	1:F:637:PHE:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:502:HIS:C	1:A:504:ALA:H	2.20	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: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:A:643:ASP:OD1	1:A:643:ASP:N	2.44	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
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:C:995:ILE:HD11	1:C:1009:GLY:C	2.38	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:C:454:VAL:HG22	2:C:1101:LMT:H102	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:911:VAL:HG12	1:B:941:MET:HE2	2.00	0.43
1:C:677:LEU:HD11	2:C:1107:LMT:H41	1.99	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:E:324:MET:HE3	1:E:324:MET:HB3	1.78	0.43
1:F:157:ARG:HH22	2:F:1105:LMT:C4B	2.31	0.43
1:B:470:LYS:NZ	2:B:1109:LMT:O5'	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:750:LEU:HD12	1:B:808:MET:HE1	2.00	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
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
1:D:226:PRO:O	1:E:781:GLY:HA3	2.20	0.42
1:D:824:ASN:C	2:D:1109:LMT:H81	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:915:MET:HG3	1:F:941:MET:HE2	2.02	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: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:549:VAL:HG11	1:D:1029:VAL:HG11	2.01	0.42
1:E:48[A]:ARG:NH1	2:E:1105:LMT:H4'	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:687:LEU:C	1:F:687:LEU:HD12	2.40	0.41
1:B:163:LYS:HE3	5:C:1638:HOH:O	2.20	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: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
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: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
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:B:750:LEU:HD12	1:B:808:MET:HE2	2.01	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: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:990:GLY:C	1:F:993:PRO:HD2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:272:GLU:O	1:E:272:GLU:HG3	2.21	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: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:255:LYS:HZ1	4:A:1121:GOL:H31	1.85	0.41
1:A:433:ALA:O	1:A:437:MET:HG2	2.21	0.41
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
2:A:1105:LMT:H2O1	2:A:1105:LMT:H3O2	1.56	0.40
1:B:217:VAL:HG23	1:B:241:GLY:HA3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1105:LMT:H2O1	2:E:1105:LMT:H3O2	1.61	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:417:GLU:CD	1:B:979:PRO:HD3	2.40	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
1:D:995:ILE:HG13	1:D:996:LEU:HG	2.04	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1042/1042 (100%)	1010 (97%)	28 (3%)	4 (0%)	34	19
1	B	1040/1042 (100%)	1021 (98%)	15 (1%)	4 (0%)	34	19
1	C	1039/1042 (100%)	1020 (98%)	18 (2%)	1 (0%)	51	36
1	D	1038/1042 (100%)	1005 (97%)	27 (3%)	6 (1%)	25	12
1	E	1041/1042 (100%)	1021 (98%)	20 (2%)	0	100	100
1	F	1039/1042 (100%)	1015 (98%)	23 (2%)	1 (0%)	51	36
All	All	6239/6252 (100%)	6092 (98%)	131 (2%)	16 (0%)	41	26

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
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 ⓘ

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%)	839 (98%)	14 (2%)	62	49
1	B	851/851 (100%)	830 (98%)	21 (2%)	47	31
1	C	850/851 (100%)	831 (98%)	19 (2%)	52	36
1	D	849/851 (100%)	823 (97%)	26 (3%)	40	23
1	E	852/851 (100%)	836 (98%)	16 (2%)	57	43
1	F	850/851 (100%)	832 (98%)	18 (2%)	53	38
All	All	5105/5106 (100%)	4991 (98%)	114 (2%)	52	36

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	51	TYR
1	A	364	THR
1	A	505	LYS
1	A	506	LYS
1	A	508	LEU
1	A	540	SER
1	A	565	LYS
1	A	643	ASP
1	A	683	SER
1	A	838	ARG
1	A	843	SER
1	A	1040	ARG
1	A	1041	ARG
1	B	20	LEU
1	B	51	TYR
1	B	77	MET
1	B	133	LYS
1	B	157	ARG
1	B	273	MET
1	B	364	THR
1	B	497	LEU

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Mol	Chain	Res	Type
1	B	502	HIS
1	B	505	LYS
1	B	508	LEU
1	B	510	THR
1	B	515	ARG
1	B	550	PHE
1	B	565	LYS
1	B	646	LYS
1	B	838	ARG
1	B	878	THR
1	B	966	MET
1	B	1014	SER
1	B	1042	LYS
1	C	51	TYR
1	C	150	LYS
1	C	157	ARG
1	C	218	SER
1	C	259	ASP
1	C	273	MET
1	C	312	LYS
1	C	364	THR
1	C	512	LEU
1	C	522	ARG
1	C	558	CYS
1	C	564	PHE
1	C	681	GLN
1	C	683	SER
1	C	929	ASN
1	C	987	PHE
1	C	1014	SER
1	C	1026	LEU
1	C	1040	ARG
1	D	23	ILE
1	D	51	TYR
1	D	74	VAL
1	D	77	MET
1	D	133	LYS
1	D	150	LYS
1	D	157	ARG
1	D	505	LYS
1	D	507	ASP
1	D	508	LEU

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Mol	Chain	Res	Type
1	D	513	ILE
1	D	526	ARG
1	D	533	ASN
1	D	538	LEU
1	D	635	VAL
1	D	683	SER
1	D	686	SER
1	D	854	LYS
1	D	910	ILE
1	D	966	MET
1	D	985	ILE
1	D	987	PHE
1	D	995	ILE
1	D	998	HIS
1	D	1035	ARG
1	D	1039	THR
1	E	51	TYR
1	E	77	MET
1	E	133	LYS
1	E	229	GLN
1	E	259	ASP
1	E	273	MET
1	E	364	THR
1	E	372	LEU
1	E	805	ILE
1	E	849	LEU
1	E	880	LEU
1	E	929	ASN
1	E	943	LEU
1	E	992	ILE
1	E	995	ILE
1	E	1014	SER
1	F	51	TYR
1	F	163	LYS
1	F	199	ARG
1	F	216	GLN
1	F	221	GLN
1	F	273	MET
1	F	364	THR
1	F	497	LEU
1	F	505	LYS
1	F	524	PHE

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Mol	Chain	Res	Type
1	F	642	PHE
1	F	643	ASP
1	F	645	ARG
1	F	662	GLN
1	F	677	LEU
1	F	732	ASP
1	F	840	LEU
1	F	1014	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	575	GLN
1	B	178	GLN
1	B	734	GLN
1	B	872	GLN
1	C	872	GLN
1	D	533	ASN
1	D	844	GLN
1	D	872	GLN
1	E	110	GLN
1	E	872	GLN
1	F	111	ASN
1	F	115	GLN
1	F	132	GLN
1	F	134	GLN
1	F	743	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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
2	LMT	B	1109	-	36,36,36	0.99	2 (5%)	47,47,47	1.06	3 (6%)
2	LMT	F	1101	-	36,36,36	1.10	3 (8%)	47,47,47	1.08	2 (4%)
4	GOL	C	1117	-	5,5,5	0.71	0	5,5,5	0.81	0
2	LMT	F	1107	-	36,36,36	1.13	3 (8%)	47,47,47	1.06	3 (6%)
2	LMT	A	1110	-	25,25,36	0.99	1 (4%)	30,30,47	1.09	2 (6%)
2	LMT	E	1106	-	36,36,36	1.12	5 (13%)	47,47,47	1.39	7 (14%)
3	PTY	D	1113	-	47,47,49	0.96	2 (4%)	50,52,54	1.09	2 (4%)
2	LMT	C	1111	-	36,36,36	1.12	3 (8%)	47,47,47	1.07	2 (4%)
3	PTY	F	1115	-	47,47,49	0.97	3 (6%)	50,52,54	1.09	2 (4%)
2	LMT	E	1103	-	36,36,36	1.11	3 (8%)	47,47,47	1.20	7 (14%)
2	LMT	C	1110	-	36,36,36	1.05	1 (2%)	47,47,47	1.51	9 (19%)
2	LMT	E	1102	-	36,36,36	1.21	3 (8%)	47,47,47	1.24	6 (12%)
2	LMT	B	1105	-	36,36,36	1.14	4 (11%)	47,47,47	1.22	5 (10%)
2	LMT	B	1106	-	36,36,36	1.06	2 (5%)	47,47,47	1.07	4 (8%)
2	LMT	E	1107	-	36,36,36	1.09	1 (2%)	47,47,47	1.07	3 (6%)
2	LMT	B	1101	-	36,36,36	1.02	1 (2%)	47,47,47	1.10	5 (10%)
4	GOL	E	1116	-	5,5,5	1.64	2 (40%)	5,5,5	1.22	0
4	GOL	E	1122	-	5,5,5	3.13	3 (60%)	5,5,5	1.98	1 (20%)
2	LMT	C	1103	-	36,36,36	1.08	2 (5%)	47,47,47	1.22	6 (12%)
2	LMT	F	1110	-	36,36,36	1.11	3 (8%)	47,47,47	1.34	6 (12%)
2	LMT	C	1101	-	36,36,36	1.14	1 (2%)	47,47,47	1.04	3 (6%)
2	LMT	C	1108	-	36,36,36	1.16	4 (11%)	47,47,47	1.51	6 (12%)
2	LMT	D	1106	-	36,36,36	1.05	3 (8%)	47,47,47	1.23	6 (12%)
2	LMT	F	1104	-	36,36,36	1.12	2 (5%)	47,47,47	1.42	5 (10%)
4	GOL	D	1117	-	5,5,5	1.12	0	5,5,5	0.99	0
4	GOL	A	1116	-	5,5,5	1.86	2 (40%)	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	C	1118	-	5,5,5	2.43	1 (20%)	5,5,5	0.68	0
3	PTY	B	1111	-	45,45,49	0.94	3 (6%)	48,50,54	0.98	2 (4%)
4	GOL	F	1117	-	5,5,5	1.53	2 (40%)	5,5,5	1.69	1 (20%)
4	GOL	A	1113	-	5,5,5	1.27	0	5,5,5	1.64	2 (40%)
4	GOL	E	1121	-	5,5,5	1.61	2 (40%)	5,5,5	1.27	0
2	LMT	C	1102	-	36,36,36	1.12	2 (5%)	47,47,47	1.05	3 (6%)
4	GOL	D	1116	-	5,5,5	1.18	1 (20%)	5,5,5	0.78	0
2	LMT	D	1108	-	36,36,36	1.07	3 (8%)	47,47,47	0.94	1 (2%)
2	LMT	C	1107	-	36,36,36	1.15	3 (8%)	47,47,47	1.21	4 (8%)
4	GOL	A	1114	-	5,5,5	1.57	1 (20%)	5,5,5	0.81	0
2	LMT	F	1113	-	36,36,36	1.02	3 (8%)	47,47,47	0.96	3 (6%)
4	GOL	E	1120	-	5,5,5	0.71	0	5,5,5	1.34	1 (20%)
4	GOL	B	1113	-	5,5,5	1.11	0	5,5,5	0.81	0
2	LMT	A	1111	-	36,36,36	1.23	6 (16%)	47,47,47	1.20	5 (10%)
2	LMT	C	1104	-	36,36,36	1.10	4 (11%)	47,47,47	1.12	3 (6%)
2	LMT	A	1104	-	36,36,36	1.28	3 (8%)	47,47,47	1.15	3 (6%)
2	LMT	B	1102	-	36,36,36	1.19	3 (8%)	47,47,47	1.29	2 (4%)
2	LMT	C	1106	-	36,36,36	1.08	4 (11%)	47,47,47	1.07	3 (6%)
4	GOL	A	1121	-	5,5,5	1.04	0	5,5,5	1.07	1 (20%)
2	LMT	F	1109	-	36,36,36	1.02	1 (2%)	47,47,47	1.10	3 (6%)
4	GOL	D	1115	-	5,5,5	1.54	1 (20%)	5,5,5	1.13	0
2	LMT	B	1104	-	36,36,36	1.09	4 (11%)	47,47,47	1.16	2 (4%)
4	GOL	F	1119	-	5,5,5	1.31	0	5,5,5	1.44	1 (20%)
2	LMT	B	1110	-	36,36,36	1.13	4 (11%)	47,47,47	1.02	3 (6%)
3	PTY	A	1112	-	45,45,49	0.92	3 (6%)	48,50,54	1.02	2 (4%)
2	LMT	E	1109	-	36,36,36	1.09	2 (5%)	47,47,47	1.09	4 (8%)
3	PTY	B	1112	-	47,47,49	0.92	3 (6%)	50,52,54	1.06	2 (4%)
2	LMT	D	1112	-	36,36,36	1.13	3 (8%)	47,47,47	1.28	5 (10%)
2	LMT	D	1110	-	9,9,36	0.34	0	8,8,47	0.81	0
2	LMT	E	1101	-	36,36,36	1.14	5 (13%)	47,47,47	1.12	4 (8%)
4	GOL	F	1118	-	5,5,5	1.28	0	5,5,5	0.82	0
2	LMT	F	1108	-	12,12,36	0.29	0	11,11,47	0.91	0
2	LMT	A	1101	-	36,36,36	1.18	4 (11%)	47,47,47	1.15	5 (10%)
2	LMT	D	1111	-	36,36,36	1.09	4 (11%)	47,47,47	1.15	3 (6%)
2	LMT	B	1103	-	36,36,36	0.94	2 (5%)	47,47,47	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMT	C	1109	-	36,36,36	1.08	3 (8%)	47,47,47	1.08	3 (6%)
2	LMT	A	1103	-	36,36,36	1.01	3 (8%)	47,47,47	1.18	4 (8%)
2	LMT	A	1109	-	36,36,36	1.07	2 (5%)	47,47,47	0.83	0
4	GOL	A	1119	-	5,5,5	1.91	2 (40%)	5,5,5	1.09	0
2	LMT	E	1111	-	11,11,36	0.17	0	10,10,47	0.72	0
2	LMT	E	1108	-	36,36,36	1.22	5 (13%)	47,47,47	1.09	2 (4%)
2	LMT	D	1103	-	36,36,36	1.19	4 (11%)	47,47,47	1.20	3 (6%)
2	LMT	D	1101	-	36,36,36	1.13	3 (8%)	47,47,47	1.03	2 (4%)
2	LMT	E	1112	-	36,36,36	1.07	3 (8%)	47,47,47	1.22	5 (10%)
2	LMT	D	1102	-	36,36,36	1.05	2 (5%)	47,47,47	1.10	2 (4%)
2	LMT	A	1108	-	35,35,36	1.14	4 (11%)	46,46,47	1.12	3 (6%)
2	LMT	E	1110	-	36,36,36	1.02	1 (2%)	47,47,47	0.90	1 (2%)
4	GOL	C	1114	-	5,5,5	1.32	1 (20%)	5,5,5	1.20	0
2	LMT	F	1106	-	36,36,36	1.07	2 (5%)	47,47,47	1.37	7 (14%)
4	GOL	A	1120	-	5,5,5	0.86	0	5,5,5	1.98	2 (40%)
2	LMT	A	1105	-	36,36,36	1.18	2 (5%)	47,47,47	1.19	5 (10%)
4	GOL	C	1116	-	5,5,5	1.09	0	5,5,5	1.33	0
4	GOL	C	1120	-	5,5,5	0.94	0	5,5,5	0.89	0
3	PTY	C	1113	-	47,47,49	0.98	3 (6%)	50,52,54	1.15	4 (8%)
2	LMT	F	1102	-	36,36,36	1.07	3 (8%)	47,47,47	1.01	3 (6%)
2	LMT	A	1107	-	36,36,36	1.04	2 (5%)	47,47,47	1.11	2 (4%)
4	GOL	F	1116	-	5,5,5	1.84	1 (20%)	5,5,5	1.14	0
3	PTY	F	1114	-	36,36,49	0.88	2 (5%)	37,37,54	1.05	2 (5%)
2	LMT	E	1104	-	36,36,36	1.11	2 (5%)	47,47,47	1.00	2 (4%)
4	GOL	A	1118	-	5,5,5	1.49	1 (20%)	5,5,5	1.22	0
2	LMT	D	1107	-	36,36,36	1.14	4 (11%)	47,47,47	1.26	4 (8%)
4	GOL	D	1114	-	5,5,5	1.07	1 (20%)	5,5,5	1.35	1 (20%)
2	LMT	D	1109	-	36,36,36	1.11	3 (8%)	47,47,47	1.15	5 (10%)
2	LMT	E	1113	-	9,9,36	0.25	0	8,8,47	0.73	0
2	LMT	D	1104	-	36,36,36	1.25	3 (8%)	47,47,47	1.19	5 (10%)
2	LMT	F	1112	-	5,5,36	0.22	0	4,4,47	0.66	0
4	GOL	A	1117	-	5,5,5	0.92	0	5,5,5	0.98	0
2	LMT	C	1112	-	36,36,36	1.16	5 (13%)	47,47,47	1.34	6 (12%)
2	LMT	F	1111	-	16,16,36	0.52	0	15,15,47	0.67	0
2	LMT	C	1105	-	36,36,36	0.92	1 (2%)	47,47,47	1.30	6 (12%)
2	LMT	D	1105	-	36,36,36	1.16	6 (16%)	47,47,47	1.17	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	E	1123	-	5,5,5	1.56	2 (40%)	5,5,5	0.95	0
4	GOL	C	1119	-	5,5,5	1.02	0	5,5,5	1.17	0
4	GOL	C	1115	-	5,5,5	1.46	0	5,5,5	1.39	1 (20%)
2	LMT	A	1106	-	36,36,36	1.14	4 (11%)	47,47,47	1.35	6 (12%)
3	PTY	E	1115	-	47,47,49	0.97	3 (6%)	50,52,54	0.96	2 (4%)
4	GOL	F	1120	-	5,5,5	0.59	0	5,5,5	1.43	1 (20%)
2	LMT	B	1108	-	11,11,36	0.21	0	10,10,47	0.73	0
2	LMT	F	1105	-	36,36,36	1.12	3 (8%)	47,47,47	1.24	6 (12%)
4	GOL	E	1119	-	5,5,5	1.20	1 (20%)	5,5,5	1.72	1 (20%)
2	LMT	B	1107	-	15,15,36	0.44	0	14,14,47	0.72	0
2	LMT	A	1102	-	36,36,36	0.94	1 (2%)	47,47,47	1.07	2 (4%)
3	PTY	E	1114	-	45,45,49	0.93	3 (6%)	48,50,54	1.06	2 (4%)
4	GOL	B	1115	-	5,5,5	0.88	0	5,5,5	1.63	2 (40%)
4	GOL	E	1118	-	5,5,5	1.51	1 (20%)	5,5,5	0.72	0
4	GOL	A	1115	-	5,5,5	1.66	2 (40%)	5,5,5	0.90	0
2	LMT	E	1105	-	36,36,36	1.03	1 (2%)	47,47,47	1.08	4 (8%)
4	GOL	B	1114	-	5,5,5	0.89	0	5,5,5	0.96	0
4	GOL	E	1117	-	5,5,5	1.12	0	5,5,5	0.76	0
2	LMT	F	1103	-	36,36,36	1.22	3 (8%)	47,47,47	1.24	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	B	1109	-	-	12/21/61/61	0/2/2/2
2	LMT	F	1101	-	-	7/21/61/61	0/2/2/2
4	GOL	C	1117	-	-	2/4/4/4	-
2	LMT	F	1107	-	-	13/21/61/61	0/2/2/2
2	LMT	A	1110	-	-	11/17/37/61	0/1/1/2
2	LMT	E	1106	-	-	7/21/61/61	0/2/2/2
3	PTY	D	1113	-	-	23/51/51/53	-
2	LMT	C	1111	-	-	14/21/61/61	0/2/2/2
3	PTY	F	1115	-	-	21/51/51/53	-
2	LMT	E	1103	-	-	7/21/61/61	0/2/2/2
2	LMT	C	1110	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	E	1102	-	-	14/21/61/61	0/2/2/2
2	LMT	B	1105	-	-	10/21/61/61	0/2/2/2
2	LMT	B	1106	-	-	10/21/61/61	0/2/2/2
2	LMT	E	1107	-	-	8/21/61/61	0/2/2/2
2	LMT	B	1101	-	-	11/21/61/61	0/2/2/2
4	GOL	E	1116	-	-	4/4/4/4	-
4	GOL	E	1122	-	-	0/4/4/4	-
2	LMT	C	1103	-	-	12/21/61/61	0/2/2/2
2	LMT	F	1110	-	-	12/21/61/61	0/2/2/2
2	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	C	1108	-	-	13/21/61/61	0/2/2/2
2	LMT	D	1106	-	-	10/21/61/61	0/2/2/2
2	LMT	F	1104	-	-	6/21/61/61	0/2/2/2
4	GOL	D	1117	-	-	2/4/4/4	-
4	GOL	A	1116	-	-	4/4/4/4	-
4	GOL	C	1118	-	-	2/4/4/4	-
3	PTY	B	1111	-	-	24/49/49/53	-
4	GOL	F	1117	-	-	1/4/4/4	-
4	GOL	A	1113	-	-	4/4/4/4	-
4	GOL	E	1121	-	-	2/4/4/4	-
2	LMT	C	1102	-	-	6/21/61/61	0/2/2/2
4	GOL	D	1116	-	-	2/4/4/4	-
2	LMT	D	1108	-	-	10/21/61/61	0/2/2/2
2	LMT	C	1107	-	-	3/21/61/61	0/2/2/2
4	GOL	A	1114	-	-	3/4/4/4	-
2	LMT	F	1113	-	-	9/21/61/61	0/2/2/2
4	GOL	E	1120	-	-	0/4/4/4	-
4	GOL	B	1113	-	-	1/4/4/4	-
2	LMT	A	1111	-	-	9/21/61/61	0/2/2/2
2	LMT	C	1104	-	-	7/21/61/61	0/2/2/2
2	LMT	A	1104	-	-	4/21/61/61	0/2/2/2
2	LMT	B	1102	-	-	13/21/61/61	0/2/2/2
2	LMT	C	1106	-	-	11/21/61/61	0/2/2/2
4	GOL	A	1121	-	-	2/4/4/4	-
2	LMT	F	1109	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	1115	-	-	4/4/4/4	-
2	LMT	B	1104	-	-	8/21/61/61	0/2/2/2
4	GOL	F	1119	-	-	4/4/4/4	-
2	LMT	B	1110	-	-	8/21/61/61	0/2/2/2
3	PTY	A	1112	-	-	22/49/49/53	-
2	LMT	E	1109	-	-	6/21/61/61	0/2/2/2
3	PTY	B	1112	-	-	33/51/51/53	-
2	LMT	D	1112	-	-	13/21/61/61	0/2/2/2
2	LMT	D	1110	-	-	2/7/7/61	-
2	LMT	E	1101	-	-	4/21/61/61	0/2/2/2
4	GOL	F	1118	-	-	4/4/4/4	-
2	LMT	F	1108	-	-	5/10/10/61	-
2	LMT	A	1101	-	-	9/21/61/61	0/2/2/2
2	LMT	D	1111	-	-	12/21/61/61	0/2/2/2
2	LMT	B	1103	-	-	10/21/61/61	0/2/2/2
2	LMT	C	1109	-	-	7/21/61/61	0/2/2/2
2	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
2	LMT	A	1109	-	-	9/21/61/61	0/2/2/2
4	GOL	A	1119	-	-	1/4/4/4	-
2	LMT	E	1111	-	-	8/9/9/61	-
2	LMT	E	1108	-	-	16/21/61/61	0/2/2/2
2	LMT	D	1103	-	-	6/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	E	1112	-	-	9/21/61/61	0/2/2/2
2	LMT	D	1102	-	-	2/21/61/61	0/2/2/2
2	LMT	A	1108	-	-	7/20/60/61	0/2/2/2
2	LMT	E	1110	-	-	10/21/61/61	0/2/2/2
4	GOL	C	1114	-	-	1/4/4/4	-
2	LMT	F	1106	-	-	12/21/61/61	0/2/2/2
4	GOL	A	1120	-	-	4/4/4/4	-
2	LMT	A	1105	-	-	12/21/61/61	0/2/2/2
4	GOL	C	1116	-	-	4/4/4/4	-
4	GOL	C	1120	-	-	2/4/4/4	-
3	PTY	C	1113	-	-	23/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	F	1102	-	-	6/21/61/61	0/2/2/2
2	LMT	A	1107	-	-	13/21/61/61	0/2/2/2
4	GOL	F	1116	-	-	2/4/4/4	-
3	PTY	F	1114	-	-	17/36/36/53	-
2	LMT	E	1104	-	-	7/21/61/61	0/2/2/2
4	GOL	A	1118	-	-	2/4/4/4	-
2	LMT	D	1107	-	-	11/21/61/61	0/2/2/2
4	GOL	D	1114	-	-	1/4/4/4	-
2	LMT	D	1109	-	-	13/21/61/61	0/2/2/2
2	LMT	E	1113	-	-	2/7/7/61	-
2	LMT	D	1104	-	-	10/21/61/61	0/2/2/2
2	LMT	F	1112	-	-	2/3/3/61	-
4	GOL	A	1117	-	-	1/4/4/4	-
2	LMT	C	1112	-	-	13/21/61/61	0/2/2/2
2	LMT	F	1111	-	-	8/14/14/61	-
2	LMT	C	1105	-	-	7/21/61/61	0/2/2/2
2	LMT	D	1105	-	-	11/21/61/61	0/2/2/2
4	GOL	E	1123	-	-	4/4/4/4	-
4	GOL	C	1119	-	-	4/4/4/4	-
4	GOL	C	1115	-	-	2/4/4/4	-
2	LMT	A	1106	-	-	12/21/61/61	0/2/2/2
3	PTY	E	1115	-	-	24/51/51/53	-
4	GOL	F	1120	-	-	1/4/4/4	-
2	LMT	B	1108	-	-	3/9/9/61	-
2	LMT	F	1105	-	-	14/21/61/61	0/2/2/2
4	GOL	E	1119	-	-	4/4/4/4	-
2	LMT	B	1107	-	-	9/13/13/61	-
2	LMT	A	1102	-	-	3/21/61/61	0/2/2/2
3	PTY	E	1114	-	-	28/49/49/53	-
4	GOL	B	1115	-	-	2/4/4/4	-
4	GOL	E	1118	-	-	1/4/4/4	-
4	GOL	A	1115	-	-	2/4/4/4	-
2	LMT	E	1105	-	-	13/21/61/61	0/2/2/2
4	GOL	B	1114	-	-	4/4/4/4	-
4	GOL	E	1117	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	F	1103	-	-	10/21/61/61	0/2/2/2

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1118	GOL	O2-C2	-5.13	1.28	1.43
4	E	1122	GOL	O1-C1	4.53	1.61	1.42
2	A	1104	LMT	O3'-C3'	-4.14	1.33	1.43
4	E	1122	GOL	C1-C2	3.66	1.66	1.51
2	D	1102	LMT	O3'-C3'	-3.64	1.34	1.43
4	E	1122	GOL	C3-C2	3.62	1.66	1.51
2	A	1105	LMT	O4'-C4B	-3.49	1.34	1.43
2	F	1103	LMT	O2B-C2B	-3.46	1.34	1.43
2	A	1104	LMT	C4B-C3B	3.42	1.61	1.52
2	A	1106	LMT	O3'-C3'	-3.41	1.34	1.43
2	F	1104	LMT	C4B-C3B	3.38	1.60	1.52
2	B	1102	LMT	C4B-C3B	3.34	1.60	1.52
2	C	1107	LMT	C4B-C3B	3.33	1.60	1.52
4	A	1116	GOL	C3-C2	3.28	1.65	1.51
2	E	1102	LMT	O3'-C3'	-3.19	1.35	1.43
4	F	1116	GOL	C1-C2	3.18	1.64	1.51
2	C	1101	LMT	O3'-C3'	-3.11	1.35	1.43
2	B	1102	LMT	O3'-C3'	-3.11	1.35	1.43
2	D	1103	LMT	C4B-C3B	3.09	1.60	1.52
2	C	1103	LMT	O3'-C3'	-3.04	1.35	1.43
3	D	1113	PTY	O7-C8	3.03	1.42	1.34
2	F	1103	LMT	O3'-C3'	-3.01	1.35	1.43
2	B	1105	LMT	C4B-C3B	3.00	1.60	1.52
3	C	1113	PTY	O4-C30	2.99	1.42	1.33
2	B	1106	LMT	O3'-C3'	-2.96	1.36	1.43
3	E	1115	PTY	O4-C30	2.90	1.41	1.33
2	E	1105	LMT	O4'-C4B	-2.88	1.36	1.43
2	E	1107	LMT	O3'-C3'	-2.87	1.36	1.43
2	C	1102	LMT	O3'-C3'	-2.86	1.36	1.43
3	D	1113	PTY	O4-C30	2.85	1.41	1.33
2	C	1107	LMT	C3B-C2B	2.83	1.59	1.52
2	C	1108	LMT	O2'-C2'	-2.81	1.36	1.43
2	D	1104	LMT	O2'-C2'	-2.81	1.36	1.43
2	E	1103	LMT	O3'-C3'	-2.80	1.36	1.43
3	B	1112	PTY	O4-C30	2.79	1.41	1.33
3	B	1111	PTY	O4-C30	2.76	1.41	1.33
2	A	1111	LMT	O3'-C3'	-2.75	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1106	LMT	O3'-C3'	-2.73	1.36	1.43
2	E	1104	LMT	O3'-C3'	-2.73	1.36	1.43
2	A	1111	LMT	O2'-C2'	-2.72	1.36	1.43
2	A	1104	LMT	O5B-C5B	-2.72	1.37	1.44
4	A	1119	GOL	C3-C2	2.71	1.62	1.51
2	A	1108	LMT	O3B-C3B	-2.71	1.36	1.43
3	F	1114	PTY	O7-C8	2.70	1.41	1.33
4	A	1119	GOL	C1-C2	2.69	1.62	1.51
2	A	1101	LMT	O3'-C3'	-2.66	1.36	1.43
2	A	1108	LMT	O2B-C2B	-2.66	1.36	1.43
2	D	1101	LMT	O2'-C2'	-2.64	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	2.62	1.41	1.34
3	E	1115	PTY	O7-C8	2.62	1.41	1.34
2	E	1104	LMT	C4B-C3B	2.61	1.59	1.52
2	F	1107	LMT	O3'-C3'	-2.61	1.36	1.43
2	D	1101	LMT	O3B-C3B	-2.61	1.36	1.43
2	F	1101	LMT	O3'-C3'	-2.61	1.36	1.43
2	F	1102	LMT	O3B-C3B	-2.60	1.36	1.43
2	D	1104	LMT	O3'-C3'	-2.58	1.36	1.43
3	E	1114	PTY	O4-C30	2.57	1.40	1.33
2	D	1107	LMT	O3'-C3'	-2.57	1.36	1.43
3	C	1113	PTY	O7-C8	2.57	1.41	1.34
2	A	1110	LMT	O3'-C3'	-2.56	1.36	1.43
2	D	1103	LMT	O3'-C3'	-2.54	1.37	1.43
2	E	1108	LMT	O4'-C4B	-2.51	1.37	1.43
2	F	1105	LMT	O2'-C2'	-2.51	1.37	1.43
3	B	1112	PTY	O7-C8	2.51	1.41	1.34
2	F	1109	LMT	O3'-C3'	-2.51	1.37	1.43
2	E	1101	LMT	O1'-C1'	-2.50	1.35	1.40
2	C	1112	LMT	O3'-C3'	-2.50	1.37	1.43
2	D	1103	LMT	O5B-C5B	-2.50	1.38	1.44
2	D	1105	LMT	O2B-C2B	-2.49	1.37	1.43
3	A	1112	PTY	O7-C8	2.49	1.41	1.34
2	C	1104	LMT	O3B-C3B	-2.49	1.37	1.43
2	B	1105	LMT	C4B-C5B	2.48	1.58	1.53
2	B	1101	LMT	O3'-C3'	-2.48	1.37	1.43
2	A	1111	LMT	C4'-C5'	2.48	1.59	1.52
2	E	1101	LMT	O3'-C3'	-2.47	1.37	1.43
2	D	1112	LMT	O3'-C3'	-2.47	1.37	1.43
4	A	1114	GOL	O1-C1	2.47	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1105	LMT	O3'-C3'	-2.47	1.37	1.43
2	C	1112	LMT	C3'-C2'	2.46	1.58	1.52
2	E	1101	LMT	O3B-C3B	-2.46	1.37	1.43
2	B	1105	LMT	O2'-C2'	-2.46	1.37	1.43
2	E	1112	LMT	O3'-C3'	-2.45	1.37	1.43
2	E	1112	LMT	O2'-C2'	-2.45	1.37	1.43
2	F	1110	LMT	C1'-C2'	2.45	1.59	1.52
2	F	1110	LMT	C3'-C2'	2.44	1.58	1.52
2	E	1108	LMT	O2B-C2B	-2.44	1.37	1.43
3	A	1112	PTY	O4-C30	2.44	1.40	1.33
2	A	1108	LMT	O3'-C3'	-2.43	1.37	1.43
2	E	1108	LMT	O3'-C3'	-2.43	1.37	1.43
2	C	1112	LMT	O2B-C2B	-2.43	1.37	1.43
2	B	1110	LMT	O3B-C3B	-2.42	1.37	1.43
3	E	1114	PTY	O7-C8	2.42	1.41	1.34
2	A	1111	LMT	O3B-C3B	-2.42	1.37	1.43
3	B	1111	PTY	O7-C8	2.42	1.41	1.34
2	B	1110	LMT	O3'-C3'	-2.40	1.37	1.43
2	E	1106	LMT	O3'-C3'	-2.39	1.37	1.43
4	A	1115	GOL	C3-C2	2.39	1.61	1.51
2	B	1104	LMT	O4'-C4B	-2.38	1.37	1.43
2	E	1109	LMT	O3'-C3'	-2.38	1.37	1.43
4	E	1121	GOL	C3-C2	2.38	1.61	1.51
2	D	1109	LMT	O2B-C2B	-2.37	1.37	1.43
2	F	1103	LMT	O2'-C2'	-2.37	1.37	1.43
3	C	1113	PTY	O7-C6	-2.36	1.40	1.46
2	C	1108	LMT	C4B-C5B	2.36	1.58	1.53
2	D	1111	LMT	O3'-C3'	-2.35	1.37	1.43
2	E	1109	LMT	O2'-C2'	-2.35	1.37	1.43
2	E	1101	LMT	O2'-C2'	-2.35	1.37	1.43
2	D	1106	LMT	O3'-C3'	-2.34	1.37	1.43
2	D	1108	LMT	O3'-C3'	-2.34	1.37	1.43
2	D	1111	LMT	O3B-C3B	-2.33	1.37	1.43
2	D	1102	LMT	O3B-C3B	-2.33	1.37	1.43
4	A	1116	GOL	O3-C3	2.31	1.52	1.42
2	C	1106	LMT	C3B-C2B	2.31	1.58	1.52
2	C	1107	LMT	O3'-C3'	-2.30	1.37	1.43
2	A	1108	LMT	O2'-C2'	-2.30	1.37	1.43
2	D	1111	LMT	O2'-C2'	-2.30	1.37	1.43
2	A	1109	LMT	O3'-C3'	-2.30	1.37	1.43
4	E	1121	GOL	O3-C3	2.30	1.52	1.42
2	E	1103	LMT	C4'-C5'	2.28	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1104	LMT	O3'-C3'	-2.28	1.37	1.43
2	E	1108	LMT	O3B-C3B	-2.28	1.37	1.43
4	F	1117	GOL	C3-C2	2.27	1.61	1.51
3	E	1114	PTY	O7-C6	-2.27	1.40	1.46
2	A	1103	LMT	O3B-C3B	-2.26	1.37	1.43
2	A	1106	LMT	O1B-C4'	-2.26	1.38	1.43
4	E	1123	GOL	C1-C2	2.26	1.61	1.51
2	C	1109	LMT	O3'-C3'	-2.26	1.37	1.43
2	E	1110	LMT	O3'-C3'	-2.25	1.37	1.43
2	B	1103	LMT	O3'-C3'	-2.25	1.37	1.43
3	A	1112	PTY	O7-C6	-2.24	1.41	1.46
2	C	1111	LMT	O3B-C3B	-2.24	1.37	1.43
2	E	1101	LMT	O4'-C4B	-2.24	1.37	1.43
4	D	1116	GOL	C3-C2	2.24	1.60	1.51
4	A	1118	GOL	C3-C2	2.24	1.60	1.51
4	E	1119	GOL	O2-C2	2.24	1.50	1.43
2	F	1101	LMT	O4'-C4B	-2.23	1.37	1.43
4	E	1116	GOL	O1-C1	2.23	1.51	1.42
2	B	1109	LMT	O3'-C3'	-2.23	1.37	1.43
2	C	1109	LMT	C3'-C2'	2.23	1.58	1.52
2	F	1102	LMT	O3'-C3'	-2.22	1.37	1.43
4	E	1118	GOL	C1-C2	2.22	1.60	1.51
2	D	1111	LMT	O4'-C4B	-2.22	1.37	1.43
2	F	1105	LMT	C4B-C3B	2.22	1.58	1.52
2	C	1103	LMT	O4'-C4B	-2.21	1.37	1.43
2	D	1112	LMT	O4'-C4B	-2.21	1.37	1.43
2	B	1105	LMT	O3'-C3'	-2.20	1.37	1.43
2	C	1104	LMT	O4'-C4B	-2.20	1.37	1.43
2	B	1110	LMT	O2B-C2B	-2.20	1.37	1.43
2	F	1101	LMT	O3B-C3B	-2.20	1.37	1.43
2	B	1106	LMT	O3B-C3B	-2.20	1.37	1.43
3	F	1115	PTY	O7-C6	-2.20	1.41	1.46
2	D	1109	LMT	O3'-C3'	-2.20	1.37	1.43
2	D	1105	LMT	O3B-C3B	-2.19	1.37	1.43
2	A	1101	LMT	O3B-C3B	-2.19	1.37	1.43
2	E	1102	LMT	O1'-C1'	-2.19	1.36	1.40
2	A	1106	LMT	O4'-C4B	-2.19	1.37	1.43
2	D	1107	LMT	O3B-C3B	-2.19	1.37	1.43
2	C	1110	LMT	O3'-C3'	-2.19	1.37	1.43
2	C	1111	LMT	O3'-C3'	-2.18	1.37	1.43
2	D	1105	LMT	O5'-C5'	-2.18	1.39	1.44
2	B	1102	LMT	C3B-C2B	2.18	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1106	LMT	O2'-C2'	-2.18	1.37	1.43
2	A	1107	LMT	O2'-C2'	-2.17	1.37	1.43
2	D	1101	LMT	O3'-C3'	-2.17	1.37	1.43
2	D	1106	LMT	O3B-C3B	-2.17	1.37	1.43
2	E	1108	LMT	O2'-C2'	-2.17	1.37	1.43
2	A	1106	LMT	O2'-C2'	-2.17	1.37	1.43
2	F	1113	LMT	O3B-C3B	-2.16	1.37	1.43
2	D	1104	LMT	C4B-C3B	2.16	1.57	1.52
2	D	1112	LMT	O3B-C3B	-2.16	1.37	1.43
2	C	1106	LMT	C4B-C3B	2.15	1.57	1.52
2	C	1105	LMT	O1'-C1'	-2.15	1.36	1.40
2	E	1102	LMT	O3B-C3B	-2.15	1.37	1.43
2	F	1113	LMT	O2B-C2B	-2.15	1.37	1.43
2	C	1102	LMT	O2B-C2B	-2.15	1.37	1.43
2	D	1105	LMT	C4B-C5B	2.14	1.57	1.53
2	A	1102	LMT	O3'-C3'	-2.14	1.37	1.43
2	A	1107	LMT	O3'-C3'	-2.14	1.37	1.43
4	E	1116	GOL	C3-C2	2.14	1.60	1.51
2	D	1107	LMT	O2B-C2B	-2.13	1.38	1.43
2	C	1112	LMT	O5'-C5'	-2.12	1.39	1.44
2	E	1106	LMT	C1B-C2B	2.11	1.58	1.52
2	A	1111	LMT	C3B-C2B	2.11	1.57	1.52
2	E	1103	LMT	O2'-C2'	-2.11	1.38	1.43
2	F	1104	LMT	C3'-C2'	2.11	1.57	1.52
3	B	1111	PTY	O7-C6	-2.11	1.41	1.46
2	A	1105	LMT	O2'-C2'	-2.11	1.38	1.43
2	C	1106	LMT	O2'-C2'	-2.10	1.38	1.43
4	E	1123	GOL	O2-C2	-2.10	1.37	1.43
2	C	1112	LMT	O3B-C3B	-2.10	1.38	1.43
4	A	1115	GOL	O2-C2	-2.09	1.37	1.43
2	F	1102	LMT	O2'-C2'	-2.09	1.38	1.43
4	F	1117	GOL	C1-C2	2.09	1.60	1.51
2	A	1103	LMT	O2'-C2'	-2.08	1.38	1.43
2	D	1106	LMT	C3'-C2'	2.08	1.57	1.52
2	B	1104	LMT	O3B-C3B	-2.08	1.38	1.43
2	A	1109	LMT	C4B-C3B	2.08	1.57	1.52
2	F	1113	LMT	C3'-C2'	2.08	1.57	1.52
2	B	1103	LMT	O1'-C1'	-2.07	1.36	1.40
2	A	1101	LMT	C3'-C2'	2.07	1.57	1.52
2	D	1103	LMT	C3B-C2B	2.06	1.57	1.52
2	D	1108	LMT	O2'-C2'	-2.06	1.38	1.43
2	F	1110	LMT	O3B-C3B	-2.06	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1112	PTY	O7-C6	-2.06	1.41	1.46
2	C	1109	LMT	C3B-C2B	2.06	1.57	1.52
2	A	1103	LMT	O3'-C3'	-2.06	1.38	1.43
2	C	1108	LMT	C3'-C2'	2.06	1.57	1.52
2	B	1104	LMT	O3'-C3'	-2.06	1.38	1.43
2	A	1111	LMT	C1B-C2B	2.05	1.58	1.52
2	C	1104	LMT	O1'-C1'	-2.05	1.36	1.40
4	D	1115	GOL	C1-C2	2.05	1.60	1.51
3	E	1115	PTY	O7-C6	-2.05	1.41	1.46
2	D	1109	LMT	O3B-C3B	-2.05	1.38	1.43
4	C	1114	GOL	C3-C2	2.05	1.60	1.51
2	D	1107	LMT	O4'-C4B	-2.04	1.38	1.43
2	D	1105	LMT	O1'-C1'	-2.04	1.36	1.40
2	B	1104	LMT	O2B-C2B	-2.04	1.38	1.43
2	C	1106	LMT	O3'-C3'	-2.04	1.38	1.43
2	F	1107	LMT	O3B-C3B	-2.04	1.38	1.43
2	E	1106	LMT	C3B-C2B	2.03	1.57	1.52
4	D	1114	GOL	C1-C2	2.02	1.60	1.51
2	D	1108	LMT	O2B-C2B	-2.02	1.38	1.43
2	B	1109	LMT	O3B-C3B	-2.02	1.38	1.43
2	B	1110	LMT	O2'-C2'	-2.02	1.38	1.43
2	A	1101	LMT	O4'-C4B	-2.01	1.38	1.43
2	C	1108	LMT	C4B-C3B	2.01	1.57	1.52
2	D	1105	LMT	O3'-C3'	-2.01	1.38	1.43
2	E	1106	LMT	C4'-C5'	2.01	1.58	1.52
2	E	1106	LMT	C3'-C2'	2.01	1.57	1.52
2	E	1112	LMT	O2B-C2B	-2.01	1.38	1.43
2	C	1111	LMT	O2B-C2B	-2.00	1.38	1.43
2	F	1107	LMT	O2'-C2'	-2.00	1.38	1.43

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1108	LMT	O1'-C1'-C2'	5.54	116.96	108.30
3	F	1115	PTY	O7-C8-C11	4.69	121.61	111.50
2	C	1112	LMT	C1'-O5'-C5'	-4.66	104.55	113.69
2	B	1104	LMT	O1'-C1'-C2'	4.30	115.01	108.30
2	B	1102	LMT	O1'-C1'-C2'	4.23	114.91	108.30
2	A	1106	LMT	O5B-C5B-C4B	4.06	117.07	109.69
2	D	1107	LMT	C3'-C4'-C5'	-4.04	101.67	110.93
2	A	1103	LMT	O1'-C1'-C2'	3.99	114.53	108.30
3	D	1113	PTY	O7-C8-C11	3.93	119.98	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1105	LMT	C1-O1'-C1'	-3.90	107.38	113.84
2	C	1108	LMT	O5B-C5B-C4B	3.84	116.67	109.69
3	C	1113	PTY	O7-C8-C11	3.83	119.75	111.50
3	E	1114	PTY	O7-C8-C11	3.79	119.66	111.50
2	B	1102	LMT	C4B-C3B-C2B	3.78	117.42	110.82
2	C	1107	LMT	C4B-C3B-C2B	3.74	117.36	110.82
3	E	1115	PTY	O7-C8-C11	3.72	119.51	111.50
2	D	1112	LMT	O1'-C1'-C2'	3.70	114.09	108.30
2	F	1110	LMT	C1'-C2'-C3'	3.68	117.65	110.00
2	D	1105	LMT	C1'-O5'-C5'	-3.66	106.51	113.69
3	B	1111	PTY	O7-C8-C11	3.66	119.39	111.50
2	D	1103	LMT	C4B-C3B-C2B	3.66	117.21	110.82
4	E	1122	GOL	O1-C1-C2	3.64	127.66	110.20
2	C	1103	LMT	O5B-C5B-C4B	3.63	116.28	109.69
2	D	1112	LMT	C1'-O5'-C5'	-3.58	106.67	113.69
3	B	1112	PTY	O7-C8-C11	3.54	119.13	111.50
2	C	1112	LMT	C2'-C3'-C4'	3.49	117.66	109.68
2	B	1105	LMT	O3B-C3B-C4B	3.48	118.41	110.35
2	C	1110	LMT	O5B-C5B-C4B	3.48	116.02	109.69
2	E	1106	LMT	C3'-C4'-C5'	-3.39	103.14	110.93
2	E	1112	LMT	O5B-C5B-C6B	3.38	114.83	106.44
2	C	1108	LMT	C1B-O5B-C5B	3.34	120.25	113.69
2	C	1110	LMT	O1'-C1'-C2'	3.31	113.47	108.30
3	A	1112	PTY	O7-C8-C11	3.31	118.63	111.50
2	A	1108	LMT	O5B-C5B-C4B	3.28	115.65	109.69
2	F	1104	LMT	C4B-C3B-C2B	3.25	116.50	110.82
2	C	1106	LMT	C4B-C3B-C2B	3.25	116.49	110.82
2	F	1106	LMT	C1'-O5'-C5'	-3.25	107.32	113.69
2	C	1111	LMT	C1'-O5'-C5'	-3.24	107.33	113.69
2	D	1107	LMT	O5'-C1'-C2'	3.21	117.15	110.35
2	F	1106	LMT	C3B-C4B-C5B	-3.21	104.51	110.24
2	A	1106	LMT	C1'-C2'-C3'	-3.16	103.41	110.00
2	E	1106	LMT	O5B-C1B-C2B	3.13	116.98	110.35
2	E	1112	LMT	O5B-C1B-C2B	3.12	116.95	110.35
2	D	1109	LMT	O5'-C5'-C4'	3.12	116.32	109.75
2	F	1104	LMT	C6B-C5B-C4B	-3.11	105.71	113.00
2	D	1111	LMT	O1B-C4'-C3'	3.11	115.55	107.28
2	C	1105	LMT	O1'-C1'-C2'	3.11	113.15	108.30
2	E	1106	LMT	C3B-C4B-C5B	-3.10	104.71	110.24
2	F	1104	LMT	O1'-C1'-C2'	3.09	113.13	108.30
2	E	1102	LMT	O1B-C4'-C3'	3.08	115.47	107.28
2	E	1109	LMT	C3'-C4'-C5'	-3.05	103.93	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1109	LMT	C1'-O5'-C5'	-3.05	107.71	113.69
2	C	1107	LMT	O1'-C1'-C2'	3.04	113.05	108.30
2	C	1110	LMT	C1'-C2'-C3'	-3.02	103.71	110.00
2	C	1110	LMT	C1'-O5'-C5'	-3.01	107.78	113.69
2	A	1111	LMT	O4'-C4B-C5B	2.96	116.65	109.30
2	A	1111	LMT	C3B-C4B-C5B	-2.96	104.96	110.24
2	D	1106	LMT	C3B-C4B-C5B	-2.93	105.01	110.24
2	D	1105	LMT	O5B-C5B-C4B	2.93	115.02	109.69
2	A	1104	LMT	O1'-C1'-C2'	2.90	112.83	108.30
2	D	1111	LMT	C3'-C4'-C5'	-2.86	104.37	110.93
2	F	1107	LMT	O1'-C1'-C2'	2.85	112.75	108.30
2	D	1101	LMT	O5B-C5B-C4B	2.82	114.82	109.69
2	F	1105	LMT	O5B-C5B-C4B	2.82	114.82	109.69
2	F	1103	LMT	O1B-C1B-C2B	2.81	115.39	108.10
4	C	1115	GOL	C3-C2-C1	-2.80	100.81	111.70
2	B	1106	LMT	C1-O1'-C1'	2.79	118.47	113.84
2	C	1105	LMT	O5'-C1'-O1'	-2.79	103.37	109.97
2	E	1105	LMT	C1-O1'-C1'	2.78	118.46	113.84
2	B	1104	LMT	C1'-O5'-C5'	-2.77	108.25	113.69
2	E	1103	LMT	O5'-C5'-C4'	2.77	115.59	109.75
2	A	1107	LMT	O5B-C5B-C4B	2.76	114.71	109.69
3	E	1114	PTY	O4-C30-C31	2.75	120.54	111.91
2	D	1109	LMT	O5'-C1'-C2'	-2.74	104.55	110.35
2	A	1106	LMT	C1B-O5B-C5B	2.74	119.07	113.69
2	D	1104	LMT	C3'-C4'-C5'	-2.74	104.65	110.93
2	A	1103	LMT	O5B-C5B-C4B	2.73	114.65	109.69
2	F	1106	LMT	O1'-C1'-C2'	2.72	112.55	108.30
4	F	1120	GOL	C3-C2-C1	-2.71	101.17	111.70
2	E	1107	LMT	O5B-C5B-C4B	2.69	114.58	109.69
2	E	1102	LMT	C3'-C4'-C5'	-2.69	104.76	110.93
4	E	1119	GOL	O2-C2-C3	2.69	120.95	109.12
3	E	1115	PTY	O4-C30-C31	2.68	120.32	111.91
2	E	1108	LMT	C3B-C4B-C5B	-2.66	105.49	110.24
3	F	1114	PTY	O7-C8-C11	2.66	120.26	111.91
2	E	1107	LMT	C3'-C4'-C5'	-2.66	104.83	110.93
2	A	1108	LMT	C1'-O5'-C5'	-2.66	108.47	113.69
4	A	1113	GOL	O2-C2-C3	2.65	120.82	109.12
4	A	1120	GOL	O2-C2-C1	2.65	120.81	109.12
2	F	1101	LMT	O5B-C5B-C4B	2.65	114.51	109.69
2	F	1106	LMT	O5B-C1B-C2B	2.65	115.96	110.35
2	F	1110	LMT	O5'-C1'-C2'	2.64	115.95	110.35
2	E	1107	LMT	O1'-C1'-C2'	2.64	112.43	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1114	PTY	O4-C30-C31	2.64	120.20	111.91
2	E	1109	LMT	O1'-C1'-C2'	2.63	112.41	108.30
2	E	1112	LMT	C3'-C4'-C5'	-2.63	104.90	110.93
2	A	1101	LMT	C1'-C2'-C3'	2.63	115.47	110.00
2	F	1105	LMT	C4B-C3B-C2B	2.62	115.41	110.82
2	D	1106	LMT	C1'-C2'-C3'	-2.62	104.54	110.00
2	F	1110	LMT	C3'-C4'-C5'	-2.62	104.92	110.93
2	E	1106	LMT	O1B-C4'-C5'	2.61	116.60	109.45
2	C	1102	LMT	C4B-C3B-C2B	2.61	115.38	110.82
2	F	1110	LMT	O5B-C1B-C2B	2.60	115.86	110.35
3	B	1112	PTY	O4-C30-C31	2.60	120.08	111.91
3	C	1113	PTY	O4-C30-C31	2.60	120.07	111.91
3	A	1112	PTY	O4-C30-C31	2.59	120.02	111.91
2	D	1103	LMT	O1'-C1'-C2'	2.58	112.33	108.30
2	A	1102	LMT	O5B-C5B-C6B	2.58	112.84	106.44
3	D	1113	PTY	O4-C30-C31	2.56	119.95	111.91
2	C	1104	LMT	O1'-C1'-C2'	2.55	112.29	108.30
2	B	1101	LMT	O1B-C4'-C3'	2.55	114.06	107.28
2	C	1110	LMT	C1B-O5B-C5B	2.55	118.69	113.69
2	B	1105	LMT	O5B-C5B-C4B	2.53	114.29	109.69
2	F	1104	LMT	O3B-C3B-C2B	-2.53	104.50	110.35
2	D	1104	LMT	O5B-C5B-C6B	2.53	112.72	106.44
2	C	1108	LMT	O5B-C1B-C2B	2.52	115.68	110.35
2	C	1112	LMT	O5B-C5B-C4B	2.52	114.26	109.69
2	E	1103	LMT	O1'-C1'-C2'	2.51	112.21	108.30
4	F	1117	GOL	O2-C2-C1	2.50	120.15	109.12
2	D	1106	LMT	O1'-C1'-C2'	2.50	112.20	108.30
2	A	1107	LMT	C3'-C4'-C5'	-2.49	105.21	110.93
2	A	1111	LMT	O1'-C1'-C2'	2.49	112.19	108.30
2	C	1109	LMT	O1'-C1'-C2'	2.49	112.19	108.30
2	D	1106	LMT	O5'-C5'-C6'	2.49	112.62	106.44
2	F	1109	LMT	C3B-C4B-C5B	-2.48	105.81	110.24
2	D	1111	LMT	O5B-C5B-C4B	2.48	114.20	109.69
2	C	1105	LMT	C1B-O5B-C5B	2.48	118.55	113.69
2	A	1101	LMT	C3'-C4'-C5'	-2.47	105.27	110.93
2	B	1105	LMT	O5'-C5'-C6'	2.46	112.56	106.44
3	C	1113	PTY	O4-C1-C6	2.46	115.60	108.43
2	F	1105	LMT	C6B-C5B-C4B	-2.45	107.26	113.00
2	E	1105	LMT	O5B-C5B-C6B	2.45	112.53	106.44
2	B	1106	LMT	O5'-C1'-O1'	-2.45	104.17	109.97
2	B	1101	LMT	C1-O1'-C1'	2.45	117.91	113.84
2	D	1105	LMT	O1'-C1'-C2'	2.45	112.13	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1108	LMT	O3B-C3B-C4B	2.45	116.01	110.35
2	B	1101	LMT	O5B-C5B-C4B	2.44	114.13	109.69
2	E	1112	LMT	C1B-O5B-C5B	2.44	118.48	113.69
2	B	1110	LMT	O1'-C1'-C2'	2.44	112.11	108.30
4	A	1120	GOL	O2-C2-C3	2.44	119.86	109.12
2	F	1106	LMT	C1B-C2B-C3B	2.43	115.06	110.00
2	B	1109	LMT	C1'-O5'-C5'	-2.43	108.92	113.69
2	F	1107	LMT	C1'-O5'-C5'	-2.43	108.92	113.69
4	F	1119	GOL	C3-C2-C1	-2.43	102.27	111.70
2	F	1113	LMT	O5B-C5B-C6B	2.43	112.47	106.44
2	C	1109	LMT	C1'-O5'-C5'	-2.42	108.93	113.69
2	D	1109	LMT	O1'-C1'-C2'	2.41	112.07	108.30
2	E	1102	LMT	C1'-O5'-C5'	-2.41	108.96	113.69
2	D	1101	LMT	O5B-C5B-C6B	2.41	112.42	106.44
2	F	1110	LMT	C1-O1'-C1'	2.41	117.83	113.84
2	F	1102	LMT	C1-O1'-C1'	2.40	117.82	113.84
2	F	1109	LMT	C3'-C4'-C5'	-2.39	105.44	110.93
2	E	1101	LMT	O5B-C5B-C4B	2.38	114.02	109.69
2	E	1109	LMT	O5B-C5B-C6B	2.38	112.36	106.44
2	D	1112	LMT	C1-O1'-C1'	2.38	117.79	113.84
2	F	1103	LMT	O5B-C5B-C4B	2.38	114.02	109.69
2	F	1107	LMT	C3'-C4'-C5'	-2.36	105.51	110.93
2	D	1109	LMT	O5B-C5B-C4B	2.36	113.98	109.69
2	C	1108	LMT	O5'-C1'-O1'	-2.36	104.39	109.97
2	A	1105	LMT	O1B-C1B-C2B	2.36	114.20	108.10
2	A	1110	LMT	O1'-C1'-C2'	2.35	111.97	108.30
3	F	1115	PTY	O4-C30-C31	2.35	119.28	111.91
2	F	1105	LMT	O5B-C5B-C6B	2.35	112.27	106.44
2	E	1101	LMT	O5B-C5B-C6B	2.33	112.23	106.44
2	D	1112	LMT	O5B-C5B-C4B	2.33	113.93	109.69
2	C	1110	LMT	O5'-C5'-C6'	2.33	112.22	106.44
2	A	1104	LMT	O5B-C5B-C4B	2.33	113.92	109.69
2	F	1103	LMT	C2'-C3'-C4'	2.32	114.99	109.68
2	B	1101	LMT	O1'-C1'-C2'	2.29	111.88	108.30
2	E	1103	LMT	O1B-C1B-C2B	2.29	114.04	108.10
2	F	1104	LMT	C1B-C2B-C3B	2.29	114.77	110.00
2	C	1106	LMT	O5'-C1'-O1'	-2.29	104.55	109.97
2	E	1103	LMT	O5B-C5B-C4B	2.29	113.85	109.69
2	A	1105	LMT	C1-O1'-C1'	2.28	117.61	113.84
2	C	1110	LMT	O5B-C5B-C6B	2.27	112.07	106.44
2	B	1106	LMT	C3'-C4'-C5'	-2.26	105.74	110.93
2	F	1110	LMT	C1B-C2B-C3B	2.26	114.70	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1103	LMT	C1-O1'-C1'	2.26	117.58	113.84
2	D	1104	LMT	O6'-C6'-C5'	-2.25	103.56	111.29
2	E	1103	LMT	O4'-C4B-C5B	2.25	114.89	109.30
2	E	1110	LMT	C4B-C3B-C2B	2.25	114.75	110.82
2	E	1106	LMT	O5B-C5B-C6B	2.25	112.02	106.44
2	A	1105	LMT	C1B-O5B-C5B	-2.24	109.28	113.69
2	F	1106	LMT	C1-O1'-C1'	2.24	117.56	113.84
2	F	1102	LMT	O1'-C1-C2	-2.24	101.71	109.56
2	A	1105	LMT	O5B-C5B-C6B	2.24	112.01	106.44
2	B	1105	LMT	C3'-C4'-C5'	-2.24	105.80	110.93
2	E	1101	LMT	O1'-C1'-C2'	2.24	111.80	108.30
2	D	1106	LMT	O5B-C5B-C6B	2.23	111.99	106.44
2	F	1109	LMT	C1-O1'-C1'	2.23	117.54	113.84
2	F	1103	LMT	O5B-C5B-C6B	2.23	111.98	106.44
2	F	1103	LMT	O5'-C1'-C2'	-2.23	105.63	110.35
2	D	1102	LMT	O6'-C6'-C5'	-2.23	103.64	111.29
2	C	1107	LMT	C6B-C5B-C4B	-2.23	107.79	113.00
2	C	1103	LMT	O5B-C5B-C6B	2.23	111.97	106.44
2	F	1102	LMT	C3'-C4'-C5'	-2.22	105.83	110.93
4	B	1115	GOL	O1-C1-C2	-2.22	99.57	110.20
2	C	1111	LMT	C3B-C4B-C5B	-2.22	106.29	110.24
2	E	1102	LMT	C4B-C3B-C2B	2.21	114.68	110.82
2	D	1112	LMT	C3'-C4'-C5'	-2.21	105.86	110.93
2	C	1103	LMT	O1'-C1'-C2'	2.20	111.74	108.30
2	E	1103	LMT	C1B-O5B-C5B	2.20	118.01	113.69
2	A	1111	LMT	C3'-C4'-C5'	-2.20	105.89	110.93
2	D	1102	LMT	C1B-O5B-C5B	2.18	117.98	113.69
2	C	1109	LMT	O5B-C5B-C4B	2.18	113.66	109.69
2	B	1109	LMT	O5B-C5B-C4B	2.18	113.65	109.69
2	D	1109	LMT	C2'-C3'-C4'	2.18	114.66	109.68
2	B	1109	LMT	C3'-C4'-C5'	-2.17	105.94	110.93
2	D	1104	LMT	O5B-C5B-C4B	2.17	113.64	109.69
4	D	1114	GOL	C3-C2-C1	-2.17	103.25	111.70
2	E	1106	LMT	C6'-C5'-C4'	2.17	119.64	113.33
2	A	1111	LMT	O5'-C5'-C4'	2.17	114.32	109.75
2	B	1101	LMT	C3'-C4'-C5'	-2.16	105.97	110.93
2	C	1102	LMT	C1B-C2B-C3B	2.16	114.49	110.00
3	B	1111	PTY	O4-C30-C31	2.16	118.68	111.91
2	A	1101	LMT	C2'-C3'-C4'	2.16	114.61	109.68
2	A	1101	LMT	O5'-C1'-C2'	2.15	114.91	110.35
2	C	1103	LMT	O3B-C3B-C4B	2.15	115.31	110.35
2	C	1110	LMT	O1'-C1-C2	-2.14	102.07	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1106	LMT	O1B-C4'-C3'	-2.14	101.59	107.28
2	E	1101	LMT	C1'-O5'-C5'	-2.14	109.49	113.69
2	C	1101	LMT	O5'-C5'-C6'	2.14	111.75	106.44
3	C	1113	PTY	C33-C32-C31	-2.14	105.51	113.19
2	A	1110	LMT	O5'-C1'-O1'	-2.13	104.92	109.97
2	D	1106	LMT	C1'-O5'-C5'	-2.13	109.50	113.69
2	B	1106	LMT	C3B-C4B-C5B	-2.13	106.44	110.24
2	C	1101	LMT	C3'-C4'-C5'	-2.13	106.04	110.93
2	A	1101	LMT	C3B-C4B-C5B	-2.13	106.44	110.24
2	A	1103	LMT	C1'-O5'-C5'	-2.13	109.51	113.69
2	E	1103	LMT	C3B-C4B-C5B	-2.13	106.44	110.24
2	A	1108	LMT	O5'-C5'-C6'	2.13	111.72	106.44
2	C	1103	LMT	O1B-C1B-C2B	2.13	113.61	108.10
2	A	1106	LMT	O5B-C5B-C6B	2.12	111.71	106.44
2	A	1105	LMT	O5'-C1'-O1'	-2.12	104.95	109.97
2	D	1107	LMT	C1'-C2'-C3'	2.12	114.41	110.00
2	A	1106	LMT	O5B-C1B-C2B	2.12	114.83	110.35
2	D	1107	LMT	C3B-C4B-C5B	-2.11	106.48	110.24
2	C	1105	LMT	C3B-C4B-C5B	-2.11	106.48	110.24
4	A	1113	GOL	O2-C2-C1	2.11	118.39	109.12
2	C	1104	LMT	C1'-O5'-C5'	-2.10	109.56	113.69
2	B	1110	LMT	O5'-C5'-C4'	2.10	114.18	109.75
2	A	1102	LMT	C6B-C5B-C4B	-2.09	108.10	113.00
4	A	1121	GOL	C3-C2-C1	-2.08	103.61	111.70
2	E	1108	LMT	C1'-O5'-C5'	-2.08	109.61	113.69
2	F	1113	LMT	O5B-C5B-C4B	2.08	113.47	109.69
2	E	1104	LMT	O1'-C1'-C2'	2.07	111.54	108.30
2	F	1103	LMT	C1'-O5'-C5'	-2.07	109.62	113.69
2	F	1113	LMT	O5'-C5'-C4'	2.07	114.12	109.75
2	B	1110	LMT	C3B-C4B-C5B	-2.07	106.55	110.24
2	E	1105	LMT	O1B-C1B-C2B	2.07	113.45	108.10
2	C	1110	LMT	C4-C3-C2	-2.06	103.94	114.42
2	E	1106	LMT	C1B-O1B-C4'	2.06	123.07	117.96
2	F	1105	LMT	C1'-O5'-C5'	-2.05	109.66	113.69
4	E	1120	GOL	O1-C1-C2	-2.05	100.37	110.20
2	F	1103	LMT	O3B-C3B-C4B	2.05	115.08	110.35
2	C	1112	LMT	O1B-C4'-C5'	-2.04	103.85	109.45
2	F	1101	LMT	O1'-C1'-C2'	2.04	111.49	108.30
2	C	1112	LMT	O1'-C1'-C2'	2.04	111.49	108.30
2	D	1108	LMT	O5B-C5B-C6B	2.04	111.51	106.44
2	C	1112	LMT	O5B-C5B-C6B	2.04	111.51	106.44
2	A	1103	LMT	C1-O1'-C1'	2.04	117.22	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1112	LMT	C1B-C2B-C3B	2.03	114.23	110.00
2	F	1103	LMT	O1'-C1'-C2'	2.03	111.48	108.30
2	C	1105	LMT	O4'-C4B-C5B	2.03	114.34	109.30
2	D	1103	LMT	C1B-C2B-C3B	2.03	114.22	110.00
2	E	1104	LMT	O5B-C5B-C4B	2.03	113.38	109.69
2	F	1106	LMT	C2'-C3'-C4'	2.03	114.31	109.68
2	C	1101	LMT	C4B-C3B-C2B	2.03	114.36	110.82
2	C	1102	LMT	C3'-C4'-C5'	-2.02	106.28	110.93
2	D	1104	LMT	C1'-O5'-C5'	-2.02	109.72	113.69
2	E	1102	LMT	O5B-C5B-C6B	2.02	111.45	106.44
2	C	1104	LMT	C1-O1'-C1'	-2.02	110.50	113.84
2	E	1105	LMT	C6B-C5B-C4B	-2.02	108.28	113.00
2	C	1107	LMT	C1B-C2B-C3B	2.02	114.19	110.00
2	A	1104	LMT	C4B-C3B-C2B	2.01	114.33	110.82
2	B	1105	LMT	O4'-C4B-C3B	2.01	115.00	110.35
4	B	1115	GOL	O2-C2-C3	2.01	117.97	109.12
2	C	1106	LMT	O5B-C5B-C6B	2.01	111.43	106.44
2	F	1105	LMT	C1-O1'-C1'	2.01	117.17	113.84
2	E	1102	LMT	C4-C3-C2	-2.00	104.26	114.42

There are no chirality outliers.

All (944) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	LMT	O5'-C1'-O1'-C1
2	A	1103	LMT	C2-C1-O1'-C1'
2	A	1105	LMT	C2-C1-O1'-C1'
2	A	1106	LMT	C2'-C1'-O1'-C1
2	A	1106	LMT	O5'-C1'-O1'-C1
2	A	1106	LMT	C2-C1-O1'-C1'
2	A	1107	LMT	C2'-C1'-O1'-C1
2	A	1107	LMT	O5'-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	1102	LMT	C2'-C1'-O1'-C1
2	B	1102	LMT	O5'-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'

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Mol	Chain	Res	Type	Atoms
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	1104	LMT	C2-C1-O1'-C1'
2	C	1111	LMT	C2'-C1'-O1'-C1
2	C	1111	LMT	O5'-C1'-O1'-C1
2	C	1111	LMT	C2-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	1111	LMT	C2-C1-O1'-C1'
2	D	1112	LMT	C2-C1-O1'-C1'
2	E	1102	LMT	C2'-C1'-O1'-C1
2	E	1102	LMT	O5'-C1'-O1'-C1
2	E	1103	LMT	C2-C1-O1'-C1'
2	E	1105	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	E	1112	LMT	C2-C1-O1'-C1'
2	F	1104	LMT	C2'-C1'-O1'-C1
2	F	1104	LMT	O5'-C1'-O1'-C1
2	F	1106	LMT	C2'-C1'-O1'-C1
2	F	1106	LMT	O5'-C1'-O1'-C1
2	F	1106	LMT	C2-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
3	B	1111	PTY	C11-C8-O7-C6
3	B	1111	PTY	C3-O11-P1-O13

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Mol	Chain	Res	Type	Atoms
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	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-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-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	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	C5-O14-P1-O11
3	E	1115	PTY	C5-O14-P1-O13
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
4	A	1113	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
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	1117	GOL	O1-C1-C2-C3
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
3	B	1112	PTY	O30-C30-O4-C1
3	F	1114	PTY	O30-C30-O4-C1
2	D	1111	LMT	C3'-C4'-O1B-C1B
2	F	1110	LMT	C3'-C4'-O1B-C1B
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

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

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Mol	Chain	Res	Type	Atoms
2	F	1107	LMT	O5B-C5B-C6B-O6B
2	C	1111	LMT	C4B-C5B-C6B-O6B
2	D	1101	LMT	C4B-C5B-C6B-O6B
2	D	1108	LMT	C4B-C5B-C6B-O6B
2	D	1108	LMT	C4'-C5'-C6'-O6'
2	E	1110	LMT	C4B-C5B-C6B-O6B
2	F	1110	LMT	C4'-C5'-C6'-O6'
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	B	1106	LMT	O5'-C5'-C6'-O6'
2	E	1112	LMT	O5B-C5B-C6B-O6B
2	A	1103	LMT	C4B-C5B-C6B-O6B
2	C	1110	LMT	C4B-C5B-C6B-O6B
2	A	1107	LMT	O5B-C5B-C6B-O6B
2	B	1101	LMT	O5'-C5'-C6'-O6'
2	D	1112	LMT	O5'-C5'-C6'-O6'
2	E	1109	LMT	O5'-C5'-C6'-O6'
2	F	1106	LMT	O5'-C5'-C6'-O6'
2	E	1105	LMT	C4B-C5B-C6B-O6B
2	E	1105	LMT	C3-C4-C5-C6
2	B	1104	LMT	O5'-C5'-C6'-O6'
2	E	1110	LMT	O5'-C5'-C6'-O6'
2	F	1113	LMT	O5'-C5'-C6'-O6'
2	C	1101	LMT	C4'-C5'-C6'-O6'
2	A	1103	LMT	O5'-C1'-O1'-C1
2	A	1105	LMT	O5'-C1'-O1'-C1
2	A	1108	LMT	O5'-C1'-O1'-C1
2	D	1103	LMT	O5'-C1'-O1'-C1
2	D	1108	LMT	O5'-C1'-O1'-C1
2	F	1103	LMT	O5'-C1'-O1'-C1
2	F	1105	LMT	O5'-C1'-O1'-C1
2	E	1110	LMT	C11-C10-C9-C8
2	A	1106	LMT	O5B-C5B-C6B-O6B
2	D	1106	LMT	O5'-C5'-C6'-O6'
2	D	1111	LMT	C7-C8-C9-C10
2	B	1105	LMT	C4'-C5'-C6'-O6'
2	F	1105	LMT	C4B-C5B-C6B-O6B
3	E	1114	PTY	C16-C17-C18-C19
2	C	1111	LMT	C4'-C5'-C6'-O6'
2	E	1102	LMT	C4B-C5B-C6B-O6B
2	E	1109	LMT	C4'-C5'-C6'-O6'
2	A	1110	LMT	C3'-C4'-O1B-C1B
2	F	1103	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
2	A	1110	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	C4'-C5'-C6'-O6'
2	F	1109	LMT	C4'-C5'-C6'-O6'
2	F	1110	LMT	C4B-C5B-C6B-O6B
2	C	1111	LMT	C3-C4-C5-C6
2	C	1111	LMT	O5'-C5'-C6'-O6'
3	F	1114	PTY	O4-C1-C6-O7
2	A	1109	LMT	C4B-C5B-C6B-O6B
2	D	1111	LMT	C4B-C5B-C6B-O6B
2	A	1103	LMT	C2'-C1'-O1'-C1
2	A	1110	LMT	C2'-C1'-O1'-C1
2	C	1103	LMT	C2'-C1'-O1'-C1
2	E	1108	LMT	C2'-C1'-O1'-C1
2	F	1110	LMT	C2'-C1'-O1'-C1
2	F	1113	LMT	C4'-C5'-C6'-O6'
2	D	1109	LMT	C5'-C4'-O1B-C1B
2	D	1104	LMT	C3-C4-C5-C6
2	A	1107	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	D	1106	LMT	C4'-C5'-C6'-O6'
2	E	1106	LMT	C3'-C4'-O1B-C1B
2	D	1111	LMT	O5'-C5'-C6'-O6'
2	F	1107	LMT	C4B-C5B-C6B-O6B
3	F	1114	PTY	C8-C11-C12-C13
2	E	1108	LMT	O5'-C5'-C6'-O6'
4	D	1115	GOL	O2-C2-C3-O3
4	D	1116	GOL	O2-C2-C3-O3
3	A	1112	PTY	C30-C31-C32-C33
3	C	1113	PTY	C30-C31-C32-C33
2	B	1105	LMT	O5B-C5B-C6B-O6B
2	D	1104	LMT	O5'-C5'-C6'-O6'
2	E	1108	LMT	C4'-C5'-C6'-O6'
2	E	1110	LMT	C4'-C5'-C6'-O6'
2	D	1107	LMT	O1'-C1-C2-C3
2	E	1102	LMT	O5'-C5'-C6'-O6'
2	C	1111	LMT	C5-C6-C7-C8
2	F	1107	LMT	O1'-C1-C2-C3
3	B	1112	PTY	C8-C11-C12-C13
2	D	1109	LMT	C3'-C4'-O1B-C1B
2	D	1104	LMT	O1'-C1-C2-C3
2	E	1105	LMT	O5B-C5B-C6B-O6B
2	C	1102	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	1105	LMT	C4B-C5B-C6B-O6B
2	A	1102	LMT	O1'-C1-C2-C3
2	A	1103	LMT	O1'-C1-C2-C3
2	F	1106	LMT	O1'-C1-C2-C3
2	A	1108	LMT	C4'-C5'-C6'-O6'
2	C	1103	LMT	C4B-C5B-C6B-O6B
2	C	1108	LMT	C4'-C5'-C6'-O6'
2	B	1103	LMT	O5'-C1'-O1'-C1
2	E	1104	LMT	O5'-C1'-O1'-C1
2	A	1110	LMT	O1'-C1-C2-C3
2	C	1103	LMT	O1'-C1-C2-C3
2	C	1104	LMT	O1'-C1-C2-C3
2	D	1107	LMT	O5'-C5'-C6'-O6'
2	A	1103	LMT	O5B-C5B-C6B-O6B
2	D	1101	LMT	O5B-C5B-C6B-O6B
2	B	1110	LMT	C4'-C5'-C6'-O6'
2	C	1106	LMT	C4'-C5'-C6'-O6'
2	D	1105	LMT	C4'-C5'-C6'-O6'
3	A	1112	PTY	C11-C8-O7-C6
2	C	1110	LMT	C3-C4-C5-C6
3	B	1112	PTY	C3-O11-P1-O14
3	C	1113	PTY	C5-O14-P1-O11
3	D	1113	PTY	C5-O14-P1-O11
3	E	1114	PTY	C3-O11-P1-O14
3	E	1115	PTY	C3-O11-P1-O14
3	F	1115	PTY	C3-O11-P1-O14
3	F	1115	PTY	C5-O14-P1-O11
2	E	1105	LMT	O1'-C1-C2-C3
2	B	1106	LMT	C4'-C5'-C6'-O6'
2	B	1104	LMT	O1'-C1-C2-C3
3	A	1112	PTY	O10-C8-O7-C6
2	C	1110	LMT	C4'-C5'-C6'-O6'
2	B	1110	LMT	O5B-C5B-C6B-O6B
2	E	1108	LMT	C4B-C5B-C6B-O6B
2	D	1101	LMT	O1'-C1-C2-C3
2	B	1104	LMT	C4'-C5'-C6'-O6'
2	F	1113	LMT	C4B-C5B-C6B-O6B
2	D	1101	LMT	O5B-C1B-O1B-C4'
2	D	1111	LMT	C11-C10-C9-C8
2	E	1112	LMT	C4-C5-C6-C7
2	A	1108	LMT	O5'-C5'-C6'-O6'
2	A	1105	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	1107	LMT	C5'-C4'-O1B-C1B
2	C	1105	LMT	C3-C4-C5-C6
2	D	1104	LMT	C4-C5-C6-C7
2	E	1110	LMT	C6-C7-C8-C9
3	A	1112	PTY	C39-C40-C41-C42
3	D	1113	PTY	C22-C23-C24-C25
2	A	1105	LMT	C7-C8-C9-C10
2	A	1107	LMT	C2-C3-C4-C5
2	B	1107	LMT	C5-C6-C7-C8
2	D	1112	LMT	C5-C6-C7-C8
2	E	1102	LMT	C3-C4-C5-C6
3	F	1115	PTY	C19-C20-C21-C22
2	C	1111	LMT	C2-C3-C4-C5
2	C	1112	LMT	C3-C4-C5-C6
2	E	1111	LMT	C6-C7-C8-C9
3	B	1112	PTY	C11-C12-C13-C14
2	E	1111	LMT	C4-C5-C6-C7
2	F	1101	LMT	C5-C6-C7-C8
2	F	1111	LMT	C11-C10-C9-C8
2	B	1104	LMT	C6-C7-C8-C9
2	B	1109	LMT	C6-C7-C8-C9
2	D	1105	LMT	O1'-C1-C2-C3
2	E	1109	LMT	C5-C6-C7-C8
2	F	1105	LMT	C6-C7-C8-C9
2	F	1110	LMT	C11-C10-C9-C8
2	F	1113	LMT	C3-C4-C5-C6
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	B	1103	LMT	C7-C8-C9-C10
2	B	1105	LMT	C2-C3-C4-C5
2	C	1110	LMT	C7-C8-C9-C10
2	E	1108	LMT	C5-C6-C7-C8
3	B	1111	PTY	C14-C15-C16-C17
3	B	1112	PTY	C33-C34-C35-C36
3	E	1115	PTY	C18-C19-C20-C21
2	A	1105	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	C	1108	LMT	O1'-C1-C2-C3
2	D	1102	LMT	C6-C7-C8-C9
2	D	1104	LMT	C7-C8-C9-C10
2	E	1101	LMT	C2-C3-C4-C5
2	E	1111	LMT	C11-C10-C9-C8
2	F	1106	LMT	C2-C3-C4-C5
2	F	1112	LMT	C3-C4-C5-C6
3	F	1115	PTY	C21-C22-C23-C24
3	B	1111	PTY	C8-C11-C12-C13
2	B	1109	LMT	C3-C4-C5-C6
3	B	1111	PTY	C12-C13-C14-C15
3	B	1112	PTY	C14-C15-C16-C17
2	C	1108	LMT	C4-C5-C6-C7
2	E	1105	LMT	C7-C8-C9-C10
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	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	B	1110	LMT	C1-C2-C3-C4
2	C	1112	LMT	C5-C6-C7-C8
2	E	1102	LMT	C5-C6-C7-C8
2	E	1107	LMT	C3-C4-C5-C6
3	C	1113	PTY	C18-C19-C20-C21
3	F	1114	PTY	C21-C22-C23-C24
2	A	1103	LMT	C2-C3-C4-C5
2	A	1103	LMT	C3-C4-C5-C6
2	A	1103	LMT	C11-C10-C9-C8
2	B	1104	LMT	C3-C4-C5-C6
2	C	1103	LMT	C4-C5-C6-C7
2	C	1112	LMT	C7-C8-C9-C10
2	D	1104	LMT	C5-C6-C7-C8
2	D	1105	LMT	C4-C5-C6-C7
2	F	1106	LMT	C3-C4-C5-C6
3	E	1114	PTY	C39-C40-C41-C42
2	A	1104	LMT	O5'-C1'-O1'-C1
2	A	1109	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
2	A	1111	LMT	O5'-C1'-O1'-C1
2	C	1107	LMT	O5'-C1'-O1'-C1
2	C	1111	LMT	C7-C8-C9-C10
2	D	1108	LMT	O1'-C1-C2-C3
2	F	1106	LMT	C7-C8-C9-C10
3	B	1112	PTY	C21-C22-C23-C24
2	F	1107	LMT	C1-C2-C3-C4
2	B	1107	LMT	C11-C10-C9-C8
3	E	1114	PTY	C37-C38-C39-C40
3	F	1114	PTY	C31-C32-C33-C34
2	D	1112	LMT	C6-C7-C8-C9
3	F	1115	PTY	C36-C37-C38-C39
2	E	1105	LMT	C1-C2-C3-C4
2	D	1111	LMT	O1'-C1-C2-C3
2	B	1109	LMT	C2-C1-O1'-C1'
2	C	1102	LMT	C2-C1-O1'-C1'
2	C	1112	LMT	C2-C1-O1'-C1'
2	D	1106	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'
2	A	1102	LMT	C4-C5-C6-C7
2	B	1107	LMT	C4-C5-C6-C7
2	D	1101	LMT	C2-C3-C4-C5
2	E	1105	LMT	C4-C5-C6-C7
2	F	1110	LMT	O1'-C1-C2-C3
3	E	1114	PTY	C31-C32-C33-C34
3	F	1114	PTY	C33-C34-C35-C36
2	F	1108	LMT	C1-C2-C3-C4
2	B	1103	LMT	C6-C7-C8-C9
2	C	1112	LMT	C2-C3-C4-C5
3	B	1112	PTY	C20-C21-C22-C23
2	C	1108	LMT	C5-C6-C7-C8
2	E	1108	LMT	O1'-C1-C2-C3
3	C	1113	PTY	C11-C12-C13-C14
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

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Mol	Chain	Res	Type	Atoms
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	1107	LMT	C3-C4-C5-C6
2	E	1108	LMT	C3-C4-C5-C6
3	E	1115	PTY	C34-C35-C36-C37
3	E	1114	PTY	C20-C21-C22-C23
2	D	1104	LMT	C1-C2-C3-C4
2	F	1105	LMT	O5'-C5'-C6'-O6'
2	C	1102	LMT	C1-C2-C3-C4
2	C	1111	LMT	C1-C2-C3-C4
2	D	1107	LMT	C1-C2-C3-C4
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	A	1109	LMT	C4'-C5'-C6'-O6'
2	E	1101	LMT	O1'-C1-C2-C3
2	F	1101	LMT	C3-C4-C5-C6
2	D	1109	LMT	O5B-C1B-O1B-C4'
2	C	1109	LMT	C11-C10-C9-C8
3	D	1113	PTY	C18-C19-C20-C21
3	F	1114	PTY	C35-C36-C37-C38
2	B	1107	LMT	C1-C2-C3-C4
2	C	1106	LMT	C1-C2-C3-C4
2	F	1106	LMT	C4B-C5B-C6B-O6B
3	E	1114	PTY	C36-C37-C38-C39
2	A	1107	LMT	C1-C2-C3-C4
2	E	1103	LMT	C1-C2-C3-C4
2	E	1104	LMT	C4B-C5B-C6B-O6B
2	D	1111	LMT	C2-C3-C4-C5
2	F	1105	LMT	C4-C5-C6-C7
2	F	1105	LMT	C2B-C1B-O1B-C4'
2	F	1102	LMT	C3-C4-C5-C6
3	A	1112	PTY	C40-C41-C42-C43
2	C	1104	LMT	C1-C2-C3-C4
2	B	1108	LMT	C3-C4-C5-C6
2	C	1108	LMT	C2-C3-C4-C5
2	E	1106	LMT	C5'-C4'-O1B-C1B
2	A	1105	LMT	C6-C7-C8-C9
2	A	1107	LMT	C6-C7-C8-C9
2	B	1109	LMT	C5-C6-C7-C8
2	D	1108	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	1106	LMT	C5-C6-C7-C8
2	C	1106	LMT	O1'-C1-C2-C3
2	F	1105	LMT	C7-C8-C9-C10
3	A	1112	PTY	C15-C16-C17-C18
3	E	1115	PTY	C8-C11-C12-C13
2	A	1107	LMT	C5-C6-C7-C8
2	E	1111	LMT	C3-C4-C5-C6
2	B	1105	LMT	C11-C10-C9-C8
2	F	1108	LMT	C2-C3-C4-C5
3	F	1115	PTY	C32-C33-C34-C35
2	C	1103	LMT	O5B-C1B-O1B-C4'
2	B	1107	LMT	C3-C4-C5-C6
2	C	1110	LMT	C11-C10-C9-C8
2	E	1110	LMT	C4-C5-C6-C7
2	F	1102	LMT	C5-C6-C7-C8
2	B	1103	LMT	C1-C2-C3-C4
2	E	1105	LMT	C2B-C1B-O1B-C4'
2	A	1108	LMT	C7-C8-C9-C10
2	D	1101	LMT	O5'-C1'-O1'-C1
2	F	1113	LMT	O5'-C1'-O1'-C1
2	A	1102	LMT	C3-C4-C5-C6
2	B	1103	LMT	C11-C10-C9-C8
2	A	1111	LMT	C6-C7-C8-C9
3	C	1113	PTY	C22-C23-C24-C25
2	D	1106	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	C2'-C1'-O1'-C1
2	C	1108	LMT	O5B-C5B-C6B-O6B
2	D	1101	LMT	C7-C8-C9-C10
2	E	1108	LMT	C6-C7-C8-C9
3	C	1113	PTY	C23-C24-C25-C26
3	F	1115	PTY	C18-C19-C20-C21
2	B	1101	LMT	C2B-C1B-O1B-C4'
2	B	1102	LMT	C3-C4-C5-C6
2	B	1104	LMT	C11-C10-C9-C8
3	B	1112	PTY	C39-C40-C41-C42
2	F	1103	LMT	O5B-C5B-C6B-O6B
3	C	1113	PTY	C38-C39-C40-C41
2	B	1102	LMT	C1-C2-C3-C4
2	F	1107	LMT	C11-C10-C9-C8
2	B	1109	LMT	C7-C8-C9-C10
2	C	1112	LMT	C6-C7-C8-C9
2	D	1109	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	E	1108	LMT	C11-C10-C9-C8
2	F	1110	LMT	C6-C7-C8-C9
2	A	1106	LMT	C1-C2-C3-C4
2	A	1109	LMT	C1-C2-C3-C4
2	F	1106	LMT	C1-C2-C3-C4
2	C	1112	LMT	O5B-C5B-C6B-O6B
2	C	1105	LMT	C4-C5-C6-C7
3	E	1115	PTY	C14-C15-C16-C17
3	D	1113	PTY	C30-C31-C32-C33
2	F	1105	LMT	C1-C2-C3-C4
2	F	1110	LMT	C1-C2-C3-C4
2	D	1101	LMT	C5-C6-C7-C8
2	C	1112	LMT	C11-C10-C9-C8
3	C	1113	PTY	C12-C13-C14-C15
2	C	1103	LMT	C1-C2-C3-C4
3	D	1113	PTY	C40-C41-C42-C43
2	D	1109	LMT	C6-C7-C8-C9
2	D	1111	LMT	C4'-C5'-C6'-O6'
2	C	1112	LMT	C4-C5-C6-C7
2	E	1101	LMT	C7-C8-C9-C10
2	E	1105	LMT	C6-C7-C8-C9
3	A	1112	PTY	C20-C21-C22-C23
2	B	1109	LMT	C4-C5-C6-C7
2	C	1101	LMT	C5-C6-C7-C8
2	D	1105	LMT	C5-C6-C7-C8
2	F	1107	LMT	C7-C8-C9-C10
2	E	1105	LMT	O5'-C5'-C6'-O6'
2	D	1109	LMT	O5B-C5B-C6B-O6B
2	C	1110	LMT	C9-C10-C11-C12
2	D	1106	LMT	C6-C7-C8-C9
2	E	1102	LMT	C6-C7-C8-C9
2	B	1108	LMT	C9-C10-C11-C12
2	E	1107	LMT	C7-C8-C9-C10
2	E	1111	LMT	C2-C3-C4-C5
2	C	1109	LMT	C9-C10-C11-C12
2	C	1103	LMT	C9-C10-C11-C12
2	C	1111	LMT	O1'-C1-C2-C3
2	F	1112	LMT	C4-C5-C6-C7
3	D	1113	PTY	C41-C42-C43-C44
3	F	1114	PTY	C20-C21-C22-C23
4	A	1116	GOL	O1-C1-C2-O2
4	A	1118	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
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
3	B	1112	PTY	C23-C24-C25-C26
2	B	1109	LMT	C4'-C5'-C6'-O6'
2	F	1102	LMT	C4B-C5B-C6B-O6B
2	A	1105	LMT	C2B-C1B-O1B-C4'
2	A	1105	LMT	O5'-C5'-C6'-O6'
2	C	1112	LMT	C9-C10-C11-C12
3	B	1111	PTY	C31-C32-C33-C34
2	E	1103	LMT	C9-C10-C11-C12
2	E	1102	LMT	C2-C3-C4-C5
3	A	1112	PTY	C13-C14-C15-C16
2	A	1105	LMT	O5B-C1B-O1B-C4'
2	A	1111	LMT	C5-C6-C7-C8
2	D	1106	LMT	C7-C8-C9-C10
2	E	1102	LMT	C5'-C4'-O1B-C1B
3	F	1115	PTY	C38-C39-C40-C41
2	A	1105	LMT	C1-C2-C3-C4
2	E	1103	LMT	C4'-C5'-C6'-O6'
2	E	1113	LMT	C7-C8-C9-C10
3	F	1115	PTY	C17-C18-C19-C20
2	C	1102	LMT	C2-C3-C4-C5
2	B	1102	LMT	C9-C10-C11-C12
2	E	1105	LMT	C5-C6-C7-C8
2	E	1101	LMT	C2'-C1'-O1'-C1
2	E	1109	LMT	C7-C8-C9-C10
2	B	1101	LMT	C1-C2-C3-C4
2	A	1107	LMT	C3'-C4'-O1B-C1B
2	E	1104	LMT	C5-C6-C7-C8
2	C	1108	LMT	O5'-C5'-C6'-O6'
2	C	1106	LMT	C3-C4-C5-C6
2	C	1108	LMT	C4B-C5B-C6B-O6B
3	A	1112	PTY	C41-C42-C43-C44
3	B	1112	PTY	C15-C16-C17-C18
2	B	1106	LMT	C9-C10-C11-C12
2	E	1107	LMT	C1-C2-C3-C4
2	A	1111	LMT	C4-C5-C6-C7
2	C	1109	LMT	C5'-C4'-O1B-C1B
2	D	1105	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	E	1114	PTY	C18-C19-C20-C21
2	A	1109	LMT	O1'-C1-C2-C3
3	B	1111	PTY	C13-C14-C15-C16
2	A	1107	LMT	C4-C5-C6-C7
3	A	1112	PTY	C14-C15-C16-C17
3	F	1114	PTY	C32-C33-C34-C35
2	E	1109	LMT	C3-C4-C5-C6
2	D	1108	LMT	C11-C10-C9-C8
2	F	1111	LMT	C1'-C2'-C3'-O3'
3	D	1113	PTY	C34-C35-C36-C37
2	B	1102	LMT	C4B-C5B-C6B-O6B
2	E	1111	LMT	C9-C10-C11-C12
2	D	1107	LMT	C6-C7-C8-C9
2	F	1105	LMT	C5-C6-C7-C8
2	D	1105	LMT	C2-C3-C4-C5
2	F	1107	LMT	C4-C5-C6-C7
3	C	1113	PTY	C31-C30-O4-C1
3	A	1112	PTY	C8-C11-C12-C13
2	D	1103	LMT	C1-C2-C3-C4
2	A	1104	LMT	C2-C1-O1'-C1'
2	A	1107	LMT	C2-C1-O1'-C1'
2	B	1102	LMT	C2-C1-O1'-C1'
2	C	1107	LMT	C2-C1-O1'-C1'
2	D	1101	LMT	C2-C1-O1'-C1'
2	D	1103	LMT	C2-C1-O1'-C1'
2	D	1107	LMT	C2-C1-O1'-C1'
2	D	1109	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	C	1106	LMT	C7-C8-C9-C10
3	E	1115	PTY	C21-C22-C23-C24
2	C	1101	LMT	C3-C4-C5-C6
2	D	1107	LMT	C7-C8-C9-C10
3	E	1115	PTY	C22-C23-C24-C25
2	C	1103	LMT	C3-C4-C5-C6
2	D	1112	LMT	O5B-C5B-C6B-O6B
3	B	1111	PTY	O4-C1-C6-C5
3	D	1113	PTY	O4-C1-C6-C5
3	E	1114	PTY	O4-C1-C6-C5
3	E	1115	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
3	D	1113	PTY	C11-C12-C13-C14
2	B	1102	LMT	C6-C7-C8-C9
2	D	1105	LMT	C1-C2-C3-C4
2	F	1113	LMT	C4-C5-C6-C7
2	E	1110	LMT	C7-C8-C9-C10
3	C	1113	PTY	C20-C21-C22-C23
3	B	1111	PTY	C34-C35-C36-C37
2	A	1103	LMT	O5B-C1B-O1B-C4'
3	E	1115	PTY	C12-C13-C14-C15
2	D	1109	LMT	C9-C10-C11-C12
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
2	F	1111	LMT	O1'-C1-C2-C3
2	E	1112	LMT	C1-C2-C3-C4
2	F	1109	LMT	C1-C2-C3-C4
2	B	1103	LMT	C2-C3-C4-C5
2	D	1101	LMT	C3-C4-C5-C6
2	F	1107	LMT	C9-C10-C11-C12
2	F	1111	LMT	C5-C6-C7-C8
2	F	1113	LMT	C9-C10-C11-C12
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	C	1108	LMT	C3-C4-C5-C6
3	E	1114	PTY	C33-C34-C35-C36
2	B	1107	LMT	C6-C7-C8-C9
3	A	1112	PTY	C11-C12-C13-C14
2	E	1112	LMT	C9-C10-C11-C12
2	B	1108	LMT	C4-C5-C6-C7
2	A	1106	LMT	C3-C4-C5-C6
3	D	1113	PTY	C19-C20-C21-C22
2	B	1101	LMT	O1'-C1-C2-C3
2	A	1111	LMT	C11-C10-C9-C8
2	B	1101	LMT	O5B-C1B-O1B-C4'
2	C	1111	LMT	C6-C7-C8-C9
2	D	1108	LMT	C1-C2-C3-C4
2	A	1107	LMT	O1'-C1-C2-C3
2	F	1108	LMT	C7-C8-C9-C10
2	E	1110	LMT	C1-C2-C3-C4
2	F	1102	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
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	D	1105	LMT	C3-C4-C5-C6
2	A	1110	LMT	C5'-C4'-O1B-C1B
2	B	1104	LMT	C1-C2-C3-C4
2	F	1102	LMT	C1-C2-C3-C4
2	F	1111	LMT	C2-C3-C4-C5
3	B	1112	PTY	C31-C32-C33-C34
3	F	1115	PTY	C12-C13-C14-C15
2	B	1102	LMT	O5B-C5B-C6B-O6B
2	A	1105	LMT	O1'-C1-C2-C3
2	C	1105	LMT	C2-C3-C4-C5
3	F	1114	PTY	C38-C39-C40-C41
2	B	1104	LMT	C7-C8-C9-C10
2	E	1111	LMT	C7-C8-C9-C10
2	B	1103	LMT	C4B-C5B-C6B-O6B
2	B	1101	LMT	C9-C10-C11-C12
3	E	1114	PTY	C32-C33-C34-C35
3	F	1114	PTY	C40-C41-C42-C43
2	C	1103	LMT	C2-C3-C4-C5
3	B	1112	PTY	C37-C38-C39-C40
2	C	1108	LMT	C1-C2-C3-C4
3	B	1111	PTY	C18-C19-C20-C21
2	D	1109	LMT	O5'-C1'-O1'-C1
2	F	1107	LMT	O5'-C1'-O1'-C1
3	B	1112	PTY	C34-C35-C36-C37
3	B	1112	PTY	O14-C5-C6-O7
2	D	1109	LMT	C4'-C5'-C6'-O6'
2	F	1103	LMT	C4-C5-C6-C7
3	F	1115	PTY	C20-C21-C22-C23
3	B	1112	PTY	O4-C1-C6-O7
3	A	1112	PTY	C16-C17-C18-C19
4	A	1119	GOL	O1-C1-C2-O2
4	B	1114	GOL	O1-C1-C2-O2
4	E	1121	GOL	O1-C1-C2-O2
3	C	1113	PTY	O30-C30-O4-C1
2	E	1105	LMT	O5B-C1B-O1B-C4'
2	C	1109	LMT	C1-C2-C3-C4
2	A	1101	LMT	C11-C10-C9-C8
2	A	1111	LMT	C7-C8-C9-C10
2	E	1108	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	F	1107	LMT	C5-C6-C7-C8
2	B	1103	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	C6-C7-C8-C9
2	E	1108	LMT	C9-C10-C11-C12
4	E	1119	GOL	O1-C1-C2-C3
2	F	1104	LMT	C5-C6-C7-C8
2	C	1105	LMT	C1-C2-C3-C4
2	A	1110	LMT	C3-C4-C5-C6
3	F	1114	PTY	C11-C12-C13-C14
2	E	1102	LMT	C9-C10-C11-C12
2	C	1105	LMT	O1'-C1-C2-C3
2	B	1109	LMT	C2B-C1B-O1B-C4'
3	B	1112	PTY	C16-C17-C18-C19
2	B	1107	LMT	C2'-C1'-O1'-C1
3	A	1112	PTY	C5-O14-P1-O13
3	E	1115	PTY	C5-O14-P1-O12
3	F	1115	PTY	C5-O14-P1-O13
2	D	1112	LMT	C1-C2-C3-C4
3	B	1111	PTY	O14-C5-C6-C1
2	A	1101	LMT	C4-C5-C6-C7
2	B	1110	LMT	C9-C10-C11-C12
2	E	1111	LMT	C5-C6-C7-C8
2	A	1101	LMT	C7-C8-C9-C10
2	C	1101	LMT	C9-C10-C11-C12
3	C	1113	PTY	C15-C16-C17-C18
2	E	1107	LMT	C2-C3-C4-C5
2	D	1103	LMT	C4'-C5'-C6'-O6'
2	F	1102	LMT	C2-C3-C4-C5
2	E	1108	LMT	C1-C2-C3-C4
2	C	1104	LMT	C4-C5-C6-C7
2	D	1110	LMT	C6-C7-C8-C9
2	F	1105	LMT	C2-C3-C4-C5
3	C	1113	PTY	O14-C5-C6-O7
2	F	1101	LMT	C1-C2-C3-C4
2	C	1109	LMT	C6-C7-C8-C9
2	F	1107	LMT	C2-C1-O1'-C1'
2	A	1108	LMT	C11-C10-C9-C8
2	C	1102	LMT	C11-C10-C9-C8
2	E	1112	LMT	O5B-C1B-O1B-C4'
3	E	1115	PTY	C20-C21-C22-C23
3	E	1115	PTY	C32-C33-C34-C35
2	B	1107	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
2	B	1106	LMT	C4-C5-C6-C7
2	C	1105	LMT	C4B-C5B-C6B-O6B
2	F	1103	LMT	O1'-C1-C2-C3
2	F	1113	LMT	C7-C8-C9-C10
3	E	1114	PTY	C22-C23-C24-C25
2	E	1112	LMT	O1'-C1-C2-C3
2	D	1112	LMT	O5'-C1'-O1'-C1
2	D	1111	LMT	C5-C6-C7-C8
2	D	1101	LMT	O5'-C5'-C6'-O6'
2	F	1108	LMT	C9-C10-C11-C12
2	F	1111	LMT	C9-C10-C11-C12
2	E	1104	LMT	O5B-C5B-C6B-O6B
2	B	1109	LMT	O5B-C5B-C6B-O6B
2	D	1109	LMT	C2-C3-C4-C5
2	F	1106	LMT	O5B-C5B-C6B-O6B
2	C	1104	LMT	C3-C4-C5-C6
2	D	1112	LMT	C9-C10-C11-C12
2	F	1111	LMT	O1'-C1'-C2'-C3'
2	A	1103	LMT	C2B-C1B-O1B-C4'
2	B	1102	LMT	C2-C3-C4-C5
3	E	1115	PTY	O4-C30-C31-C32
2	D	1104	LMT	C6-C7-C8-C9
2	A	1110	LMT	C9-C10-C11-C12
2	C	1106	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	C11-C10-C9-C8
2	F	1105	LMT	O1'-C1-C2-C3
3	F	1115	PTY	O30-C30-O4-C1
2	A	1106	LMT	C2-C3-C4-C5
2	A	1111	LMT	O1'-C1-C2-C3
2	A	1106	LMT	O5'-C5'-C6'-O6'
2	C	1109	LMT	O5'-C1'-O1'-C1
2	D	1106	LMT	C2'-C1'-O1'-C1
2	F	1107	LMT	C2'-C1'-O1'-C1
2	A	1108	LMT	O5B-C5B-C6B-O6B
2	A	1106	LMT	C4B-C5B-C6B-O6B
2	E	1102	LMT	C4'-C5'-C6'-O6'
2	B	1110	LMT	C7-C8-C9-C10
2	F	1105	LMT	O5B-C1B-O1B-C4'
2	F	1109	LMT	C2-C3-C4-C5
2	D	1109	LMT	O1'-C1-C2-C3
3	C	1113	PTY	C21-C22-C23-C24
2	D	1109	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
2	E	1112	LMT	C4B-C5B-C6B-O6B
3	E	1114	PTY	C34-C35-C36-C37
2	D	1107	LMT	O5B-C1B-O1B-C4'
3	A	1112	PTY	C22-C23-C24-C25
4	F	1119	GOL	C1-C2-C3-O3
3	D	1113	PTY	C6-C5-O14-P1
2	C	1102	LMT	C9-C10-C11-C12
2	C	1112	LMT	C5'-C4'-O1B-C1B
2	F	1101	LMT	C6-C7-C8-C9
3	E	1115	PTY	C37-C38-C39-C40
4	C	1117	GOL	O1-C1-C2-O2
4	C	1118	GOL	O1-C1-C2-O2
3	F	1115	PTY	C31-C30-O4-C1
2	C	1105	LMT	C6-C7-C8-C9
2	C	1106	LMT	O5'-C1'-O1'-C1
3	F	1114	PTY	C39-C40-C41-C42
3	D	1113	PTY	N1-C2-C3-O11
2	D	1112	LMT	C11-C10-C9-C8
2	B	1103	LMT	C5-C6-C7-C8
2	A	1109	LMT	C11-C10-C9-C8
2	D	1107	LMT	C9-C10-C11-C12
2	C	1106	LMT	C5'-C4'-O1B-C1B
2	B	1102	LMT	C4-C5-C6-C7
3	E	1115	PTY	C6-C5-O14-P1
2	F	1101	LMT	O5'-C5'-C6'-O6'
2	F	1107	LMT	C3-C4-C5-C6
2	D	1107	LMT	C4'-C5'-C6'-O6'
2	E	1106	LMT	C7-C8-C9-C10
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	1105	LMT	O5'-C1'-O1'-C1
2	B	1109	LMT	O5'-C1'-O1'-C1
2	D	1106	LMT	O5'-C1'-O1'-C1
2	B	1106	LMT	C2-C3-C4-C5
2	D	1103	LMT	C4-C5-C6-C7
2	A	1106	LMT	C7-C8-C9-C10
2	D	1106	LMT	O5B-C5B-C6B-O6B
2	E	1107	LMT	C6-C7-C8-C9
2	E	1103	LMT	C4B-C5B-C6B-O6B
2	F	1108	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	B	1112	PTY	C36-C37-C38-C39
2	A	1106	LMT	C9-C10-C11-C12
2	F	1103	LMT	C11-C10-C9-C8
2	F	1109	LMT	C6-C7-C8-C9
2	B	1105	LMT	C4-C5-C6-C7
2	B	1110	LMT	C6-C7-C8-C9
2	E	1103	LMT	C4-C5-C6-C7
4	B	1113	GOL	C1-C2-C3-O3
4	C	1117	GOL	O1-C1-C2-C3
2	A	1110	LMT	C7-C8-C9-C10
2	D	1110	LMT	C5-C6-C7-C8
2	C	1110	LMT	C6-C7-C8-C9
3	E	1115	PTY	C12-C11-C8-O7
2	A	1103	LMT	C9-C10-C11-C12
2	B	1106	LMT	C7-C8-C9-C10
3	B	1112	PTY	C12-C13-C14-C15
4	C	1116	GOL	O2-C2-C3-O3
4	F	1119	GOL	O2-C2-C3-O3
2	D	1112	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	C6-C7-C8-C9
2	A	1111	LMT	C4B-C5B-C6B-O6B
2	E	1108	LMT	O5B-C1B-O1B-C4'
2	D	1102	LMT	C9-C10-C11-C12
2	F	1101	LMT	C11-C10-C9-C8
3	B	1111	PTY	C40-C41-C42-C43
2	C	1108	LMT	C3'-C4'-O1B-C1B
2	B	1109	LMT	O5B-C1B-O1B-C4'
2	E	1113	LMT	C5-C6-C7-C8
2	E	1110	LMT	C9-C10-C11-C12
3	C	1113	PTY	C40-C41-C42-C43
3	E	1114	PTY	O4-C30-C31-C32
2	C	1108	LMT	C6-C7-C8-C9
2	F	1101	LMT	C7-C8-C9-C10
3	B	1111	PTY	C12-C11-C8-O7
2	C	1106	LMT	C4-C5-C6-C7
3	F	1115	PTY	O4-C1-C6-O7
2	A	1105	LMT	C9-C10-C11-C12
2	F	1111	LMT	C2-C1-O1'-C1'
2	B	1101	LMT	C11-C10-C9-C8
4	E	1117	GOL	O2-C2-C3-O3
2	C	1106	LMT	C3'-C4'-O1B-C1B
2	F	1109	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
2	E	1109	LMT	O5B-C5B-C6B-O6B
2	B	1102	LMT	C5-C6-C7-C8
2	C	1108	LMT	O5'-C1'-O1'-C1
2	A	1104	LMT	C5-C6-C7-C8
3	E	1114	PTY	C38-C39-C40-C41
4	A	1114	GOL	O1-C1-C2-C3
4	B	1114	GOL	O1-C1-C2-C3
4	E	1118	GOL	C1-C2-C3-O3
3	D	1113	PTY	C31-C30-O4-C1
3	D	1113	PTY	O30-C30-O4-C1
2	B	1106	LMT	C5'-C4'-O1B-C1B
2	C	1101	LMT	C2-C3-C4-C5
2	C	1103	LMT	C2B-C1B-O1B-C4'
3	B	1112	PTY	O4-C1-C6-C5
3	E	1114	PTY	O30-C30-C31-C32
2	D	1104	LMT	O5B-C5B-C6B-O6B
3	D	1113	PTY	O4-C1-C6-O7
3	E	1114	PTY	N1-C2-C3-O11
3	B	1112	PTY	C41-C42-C43-C44
2	D	1107	LMT	C2B-C1B-O1B-C4'
2	F	1109	LMT	C3-C4-C5-C6
2	D	1106	LMT	C2-C3-C4-C5
3	B	1111	PTY	C2-C3-O11-P1
3	B	1112	PTY	C2-C3-O11-P1
3	E	1114	PTY	C2-C3-O11-P1
2	F	1104	LMT	C4-C5-C6-C7
2	E	1106	LMT	C9-C10-C11-C12
4	C	1116	GOL	O1-C1-C2-O2
4	D	1114	GOL	O2-C2-C3-O3
2	C	1112	LMT	C3'-C4'-O1B-C1B
2	B	1102	LMT	C11-C10-C9-C8
3	D	1113	PTY	C24-C25-C26-C27
2	C	1110	LMT	O1'-C1-C2-C3
2	B	1105	LMT	C6-C7-C8-C9
2	D	1105	LMT	C5'-C4'-O1B-C1B
3	B	1111	PTY	C12-C11-C8-O10
3	E	1114	PTY	C6-C5-O14-P1
2	B	1107	LMT	O1'-C1-C2-C3
2	C	1103	LMT	C2-C1-O1'-C1'
3	B	1112	PTY	O4-C30-C31-C32
2	D	1111	LMT	C9-C10-C11-C12
2	F	1106	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
2	A	1110	LMT	C1-C2-C3-C4
3	B	1112	PTY	C12-C11-C8-O7

There are no ring outliers.

80 monomers are involved in 202 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1109	LMT	1	0
4	C	1117	GOL	1	0
2	F	1107	LMT	1	0
2	A	1110	LMT	5	0
2	E	1106	LMT	1	0
3	D	1113	PTY	1	0
2	C	1111	LMT	3	0
3	F	1115	PTY	1	0
2	E	1103	LMT	7	0
2	E	1102	LMT	1	0
2	E	1107	LMT	5	0
2	B	1101	LMT	3	0
4	E	1116	GOL	5	0
4	E	1122	GOL	1	0
2	C	1103	LMT	3	0
2	F	1110	LMT	4	0
2	C	1101	LMT	2	0
2	C	1108	LMT	2	0
2	D	1106	LMT	1	0
2	F	1104	LMT	1	0
4	A	1116	GOL	1	0
4	C	1118	GOL	3	0
3	B	1111	PTY	1	0
4	F	1117	GOL	1	0
4	E	1121	GOL	2	0
2	C	1102	LMT	2	0
2	D	1108	LMT	1	0
2	C	1107	LMT	3	0
4	A	1114	GOL	2	0
2	F	1113	LMT	1	0
2	A	1111	LMT	4	0
2	C	1104	LMT	1	0
2	A	1104	LMT	1	0
2	B	1102	LMT	3	0
4	A	1121	GOL	2	0

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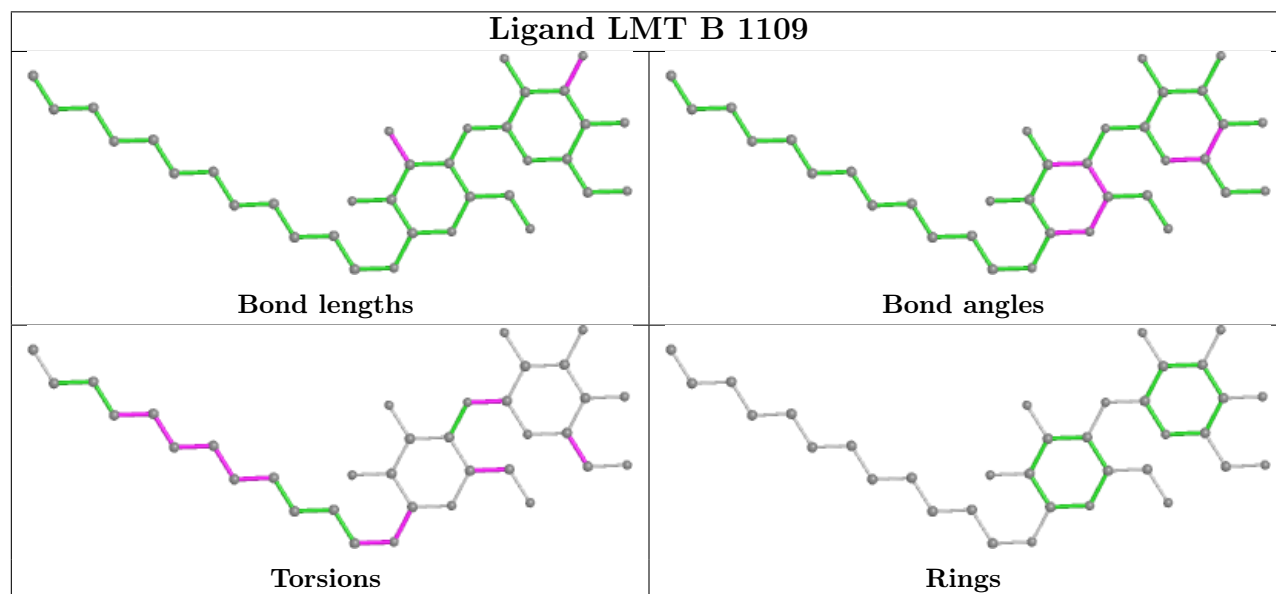
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1109	LMT	1	0
3	A	1112	PTY	4	0
2	E	1109	LMT	3	0
3	B	1112	PTY	2	0
2	D	1112	LMT	4	0
2	E	1101	LMT	2	0
2	F	1108	LMT	2	0
2	B	1103	LMT	2	0
2	A	1103	LMT	1	0
4	A	1119	GOL	1	0
2	E	1108	LMT	11	0
2	D	1103	LMT	5	0
2	D	1101	LMT	4	0
2	E	1112	LMT	2	0
2	D	1102	LMT	1	0
2	A	1108	LMT	2	0
2	E	1110	LMT	2	0
4	C	1114	GOL	1	0
2	A	1105	LMT	3	0
4	C	1116	GOL	2	0
3	C	1113	PTY	1	0
2	F	1102	LMT	3	0
2	A	1107	LMT	1	0
4	F	1116	GOL	1	0
3	F	1114	PTY	2	0
2	D	1107	LMT	8	0
2	D	1109	LMT	9	0
2	E	1113	LMT	1	0
2	D	1104	LMT	5	0
4	A	1117	GOL	2	0
2	C	1112	LMT	4	0
2	F	1111	LMT	3	0
2	D	1105	LMT	2	0
4	C	1115	GOL	2	0
2	A	1106	LMT	1	0
3	E	1115	PTY	2	0
2	B	1108	LMT	2	0
2	F	1105	LMT	3	0
4	E	1119	GOL	1	0
2	B	1107	LMT	1	0
3	E	1114	PTY	3	0
4	A	1115	GOL	2	0

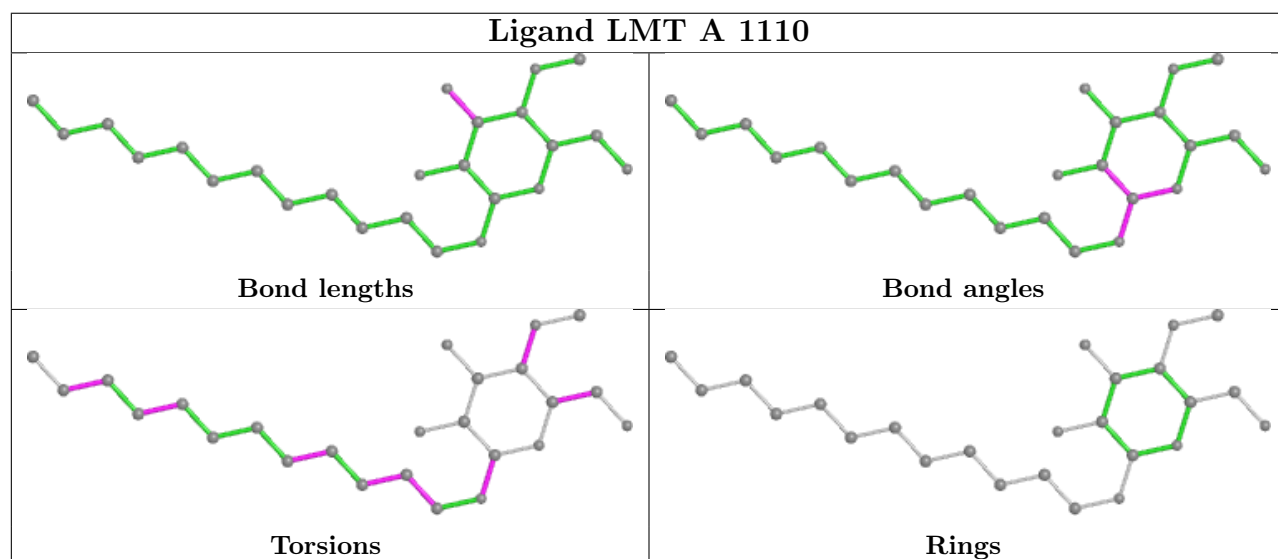
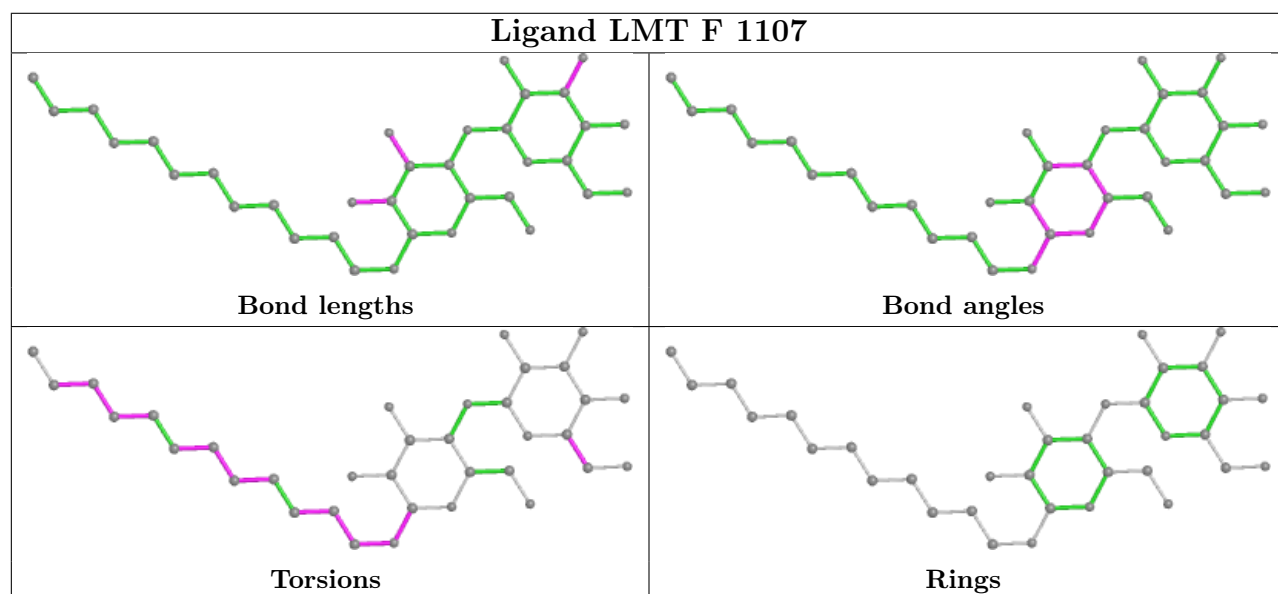
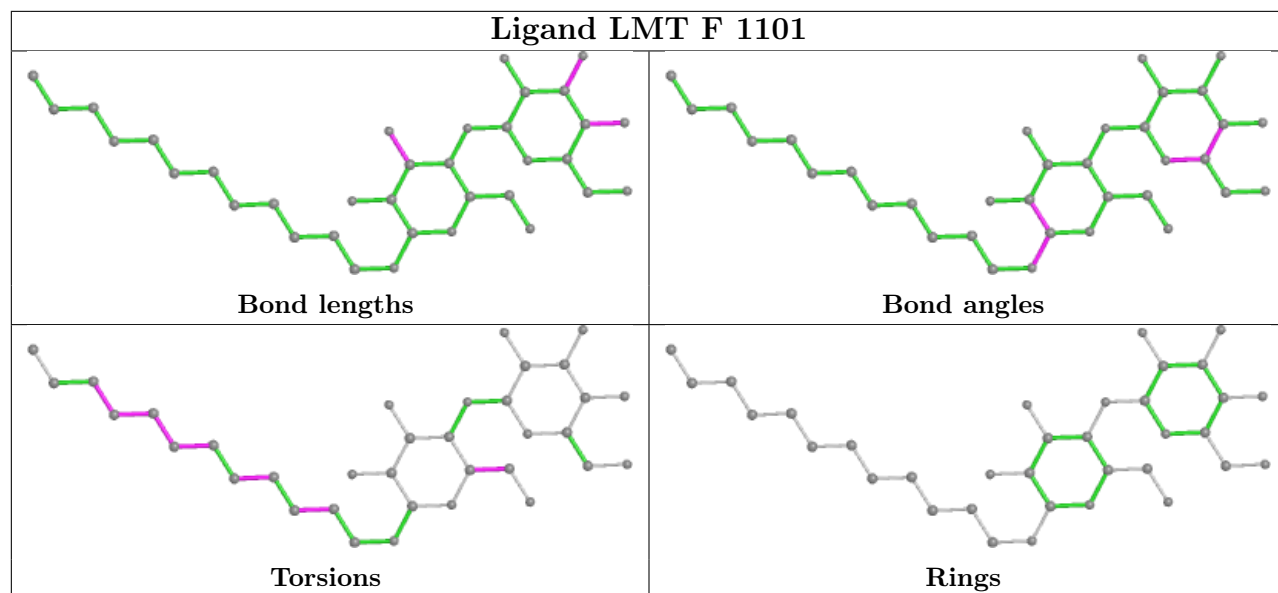
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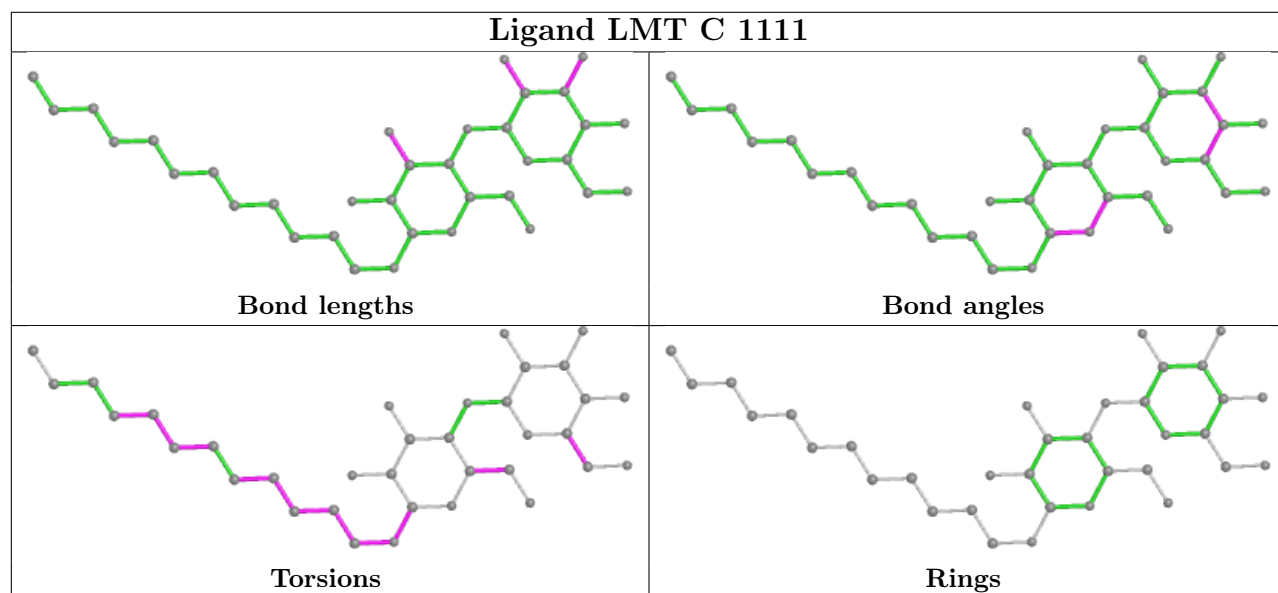
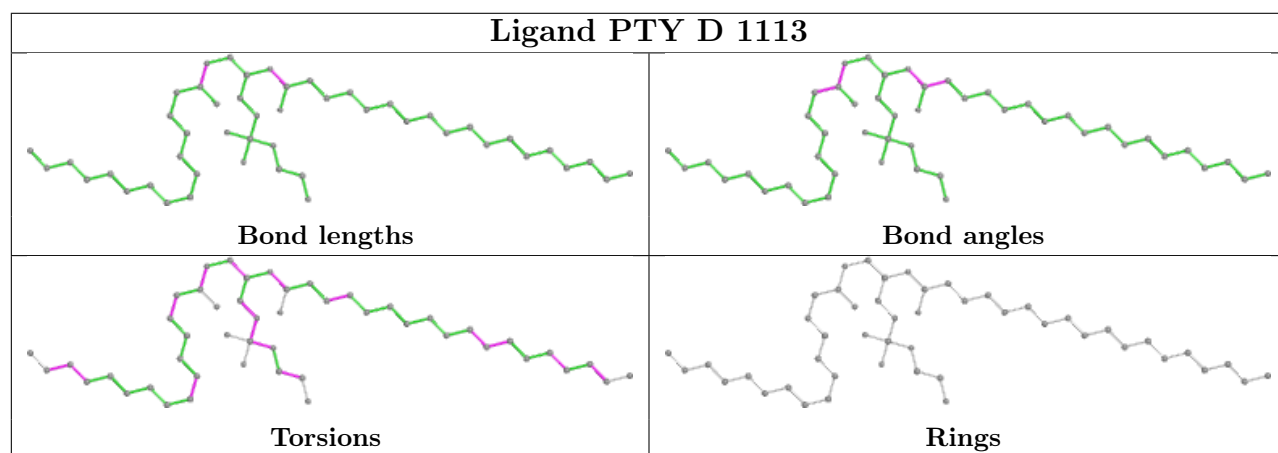
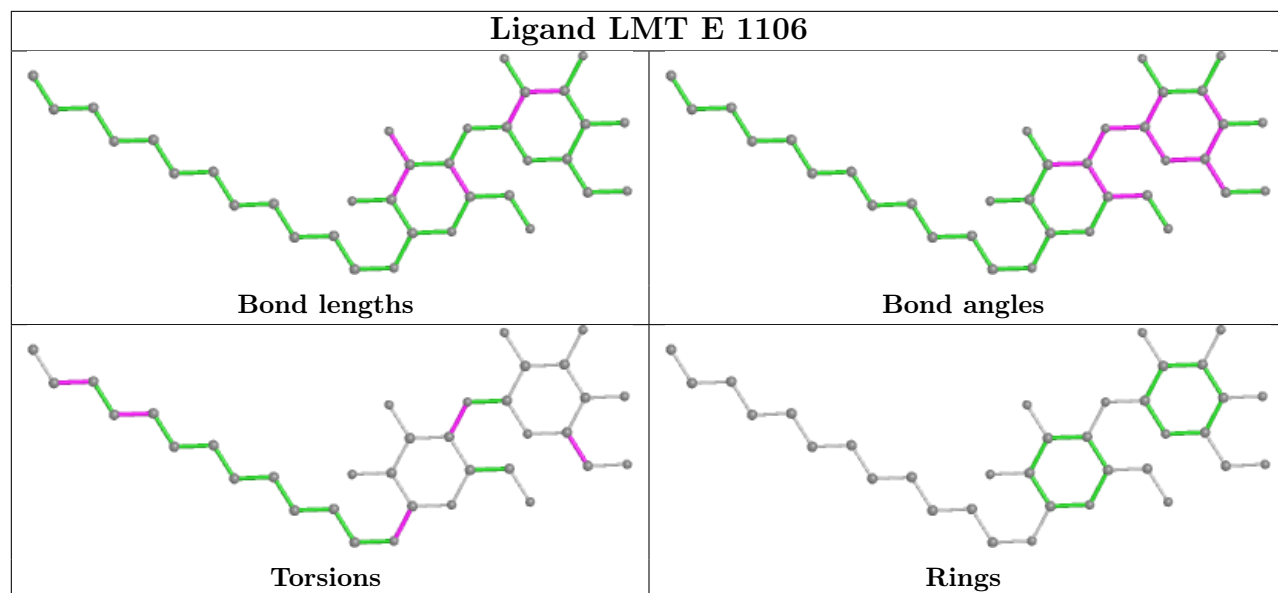
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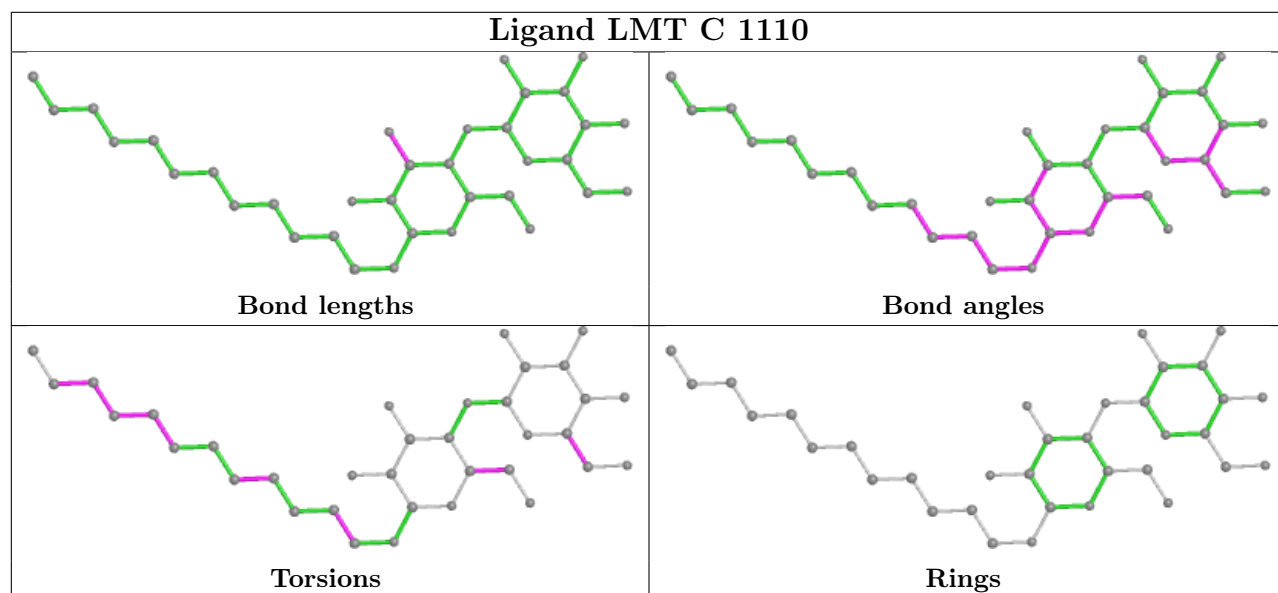
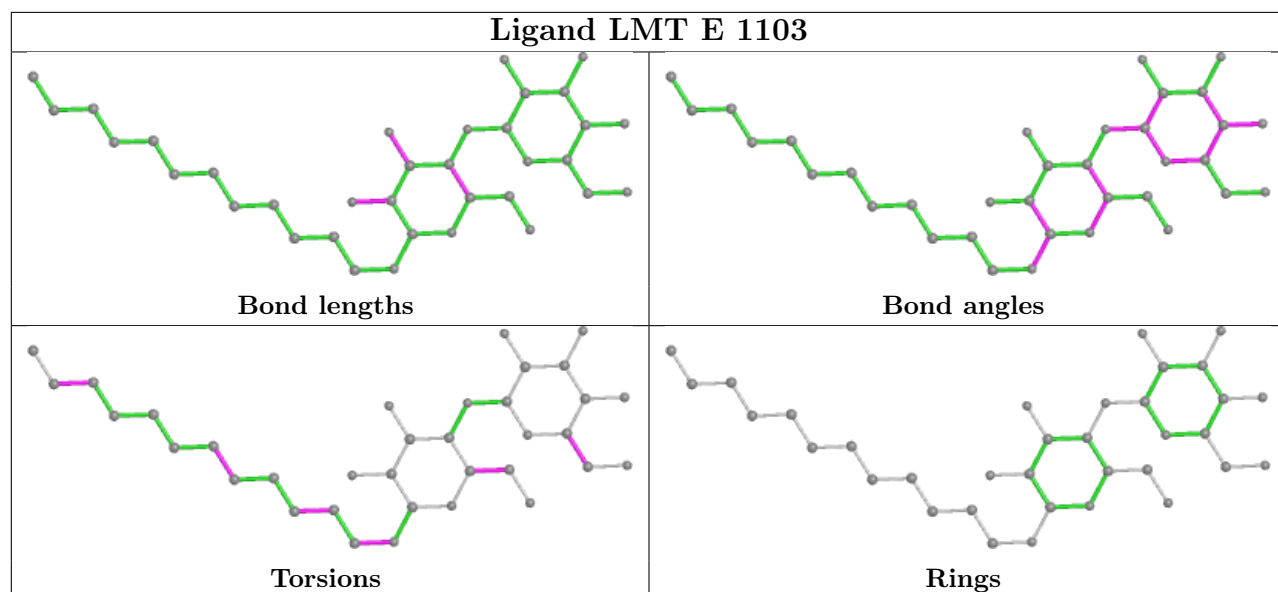
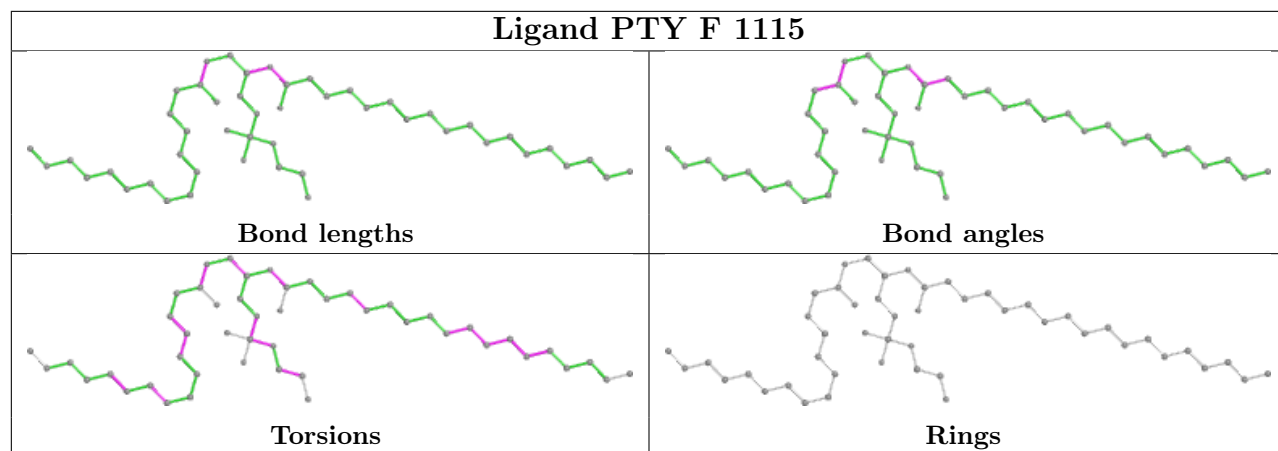
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1105	LMT	9	0
4	B	1114	GOL	1	0
2	F	1103	LMT	7	0

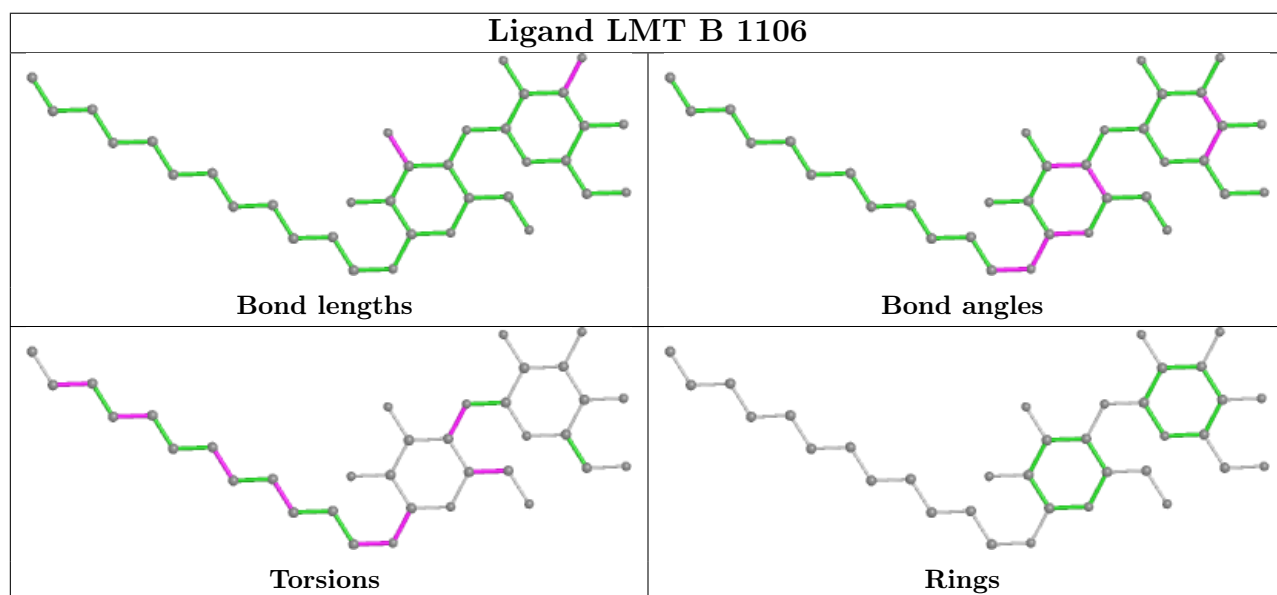
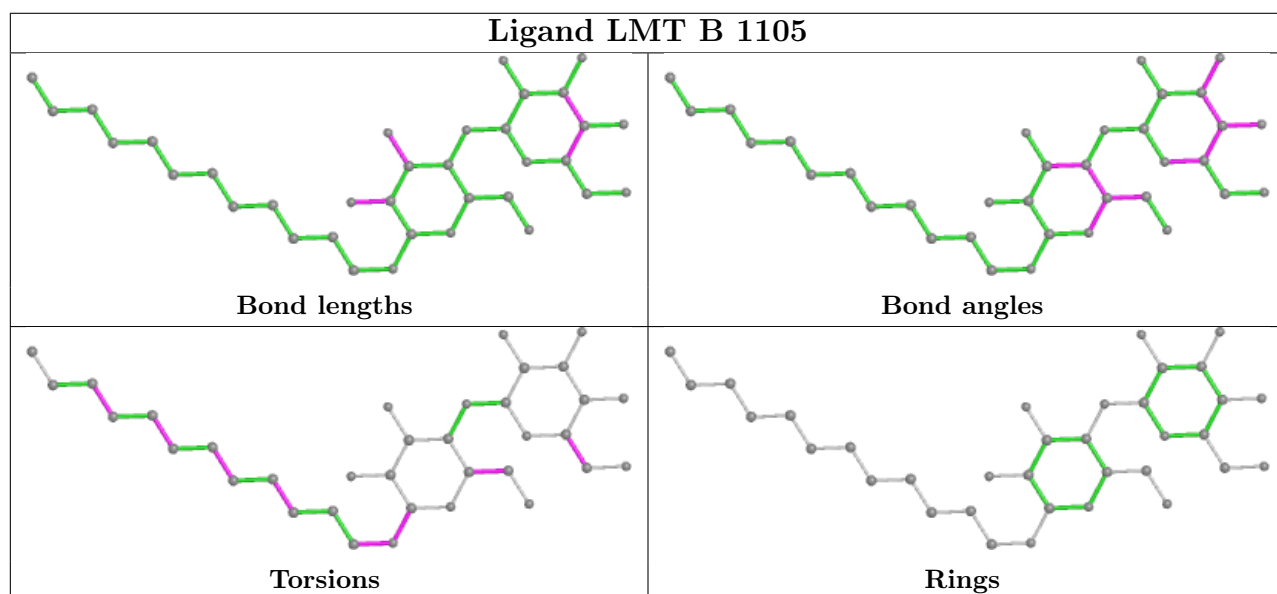
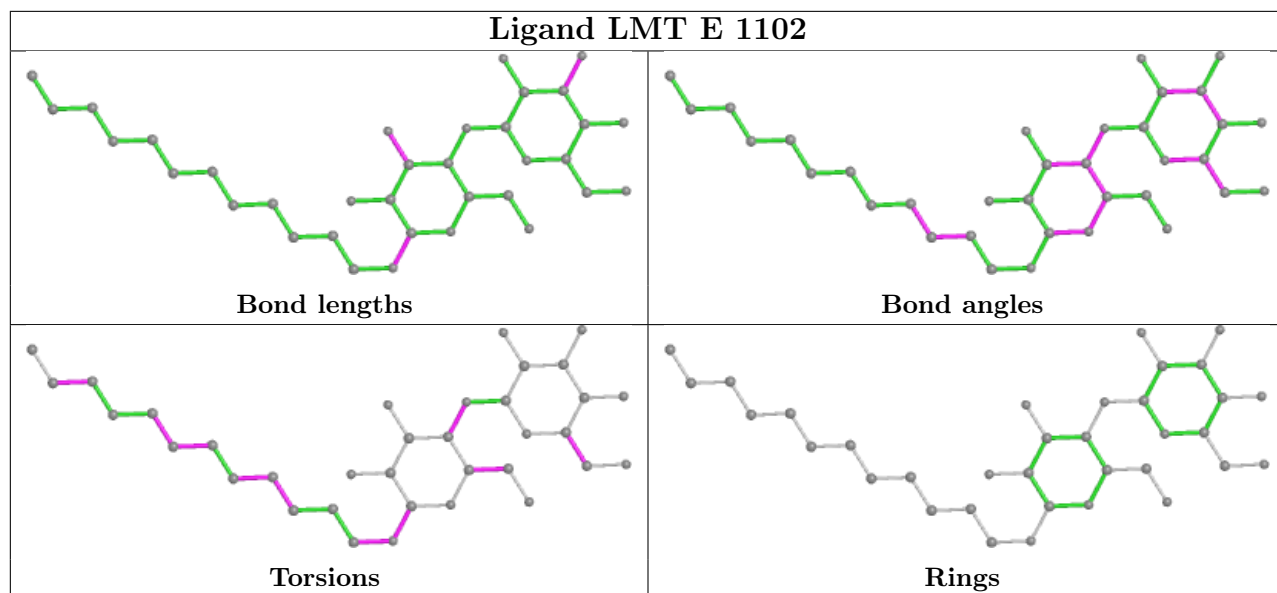
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

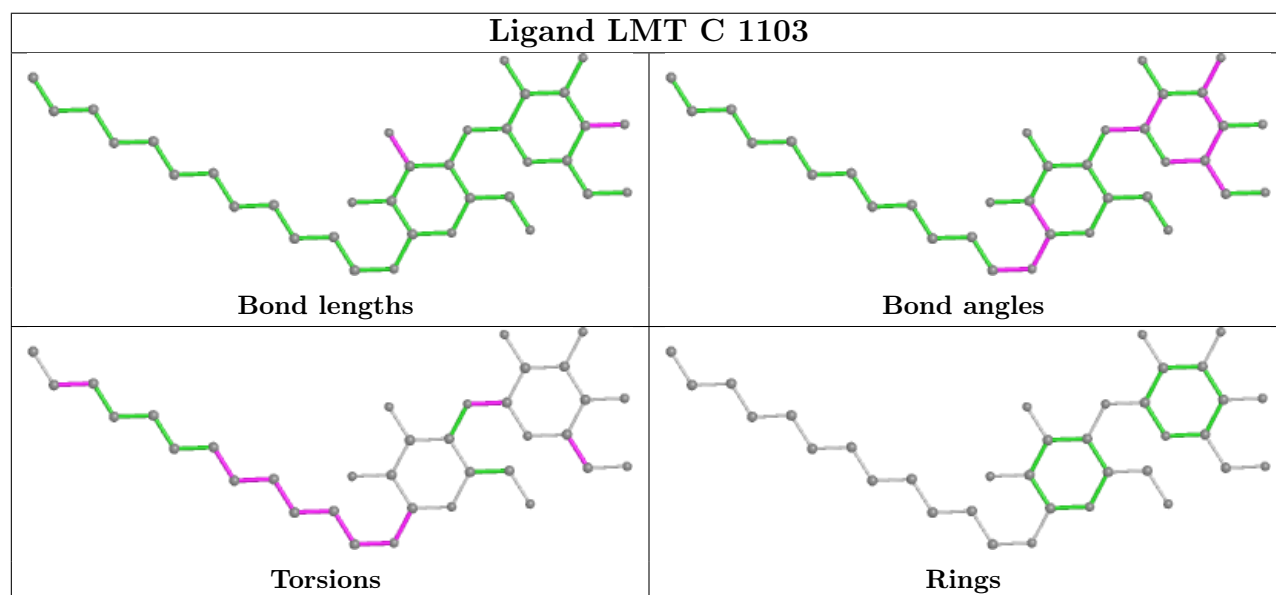
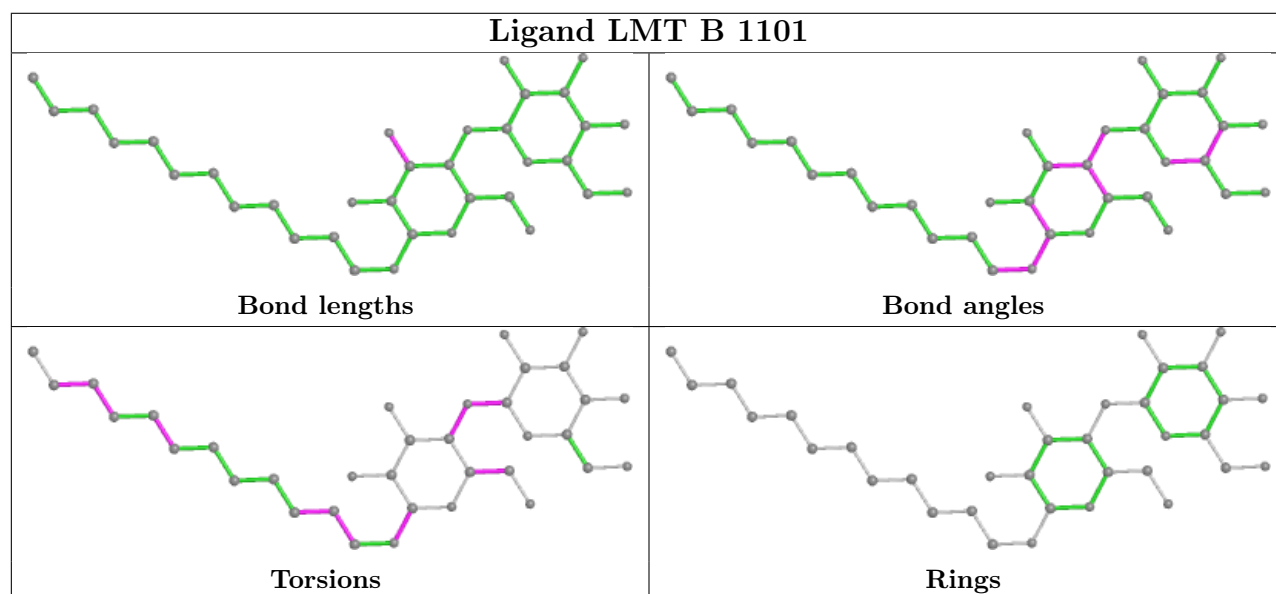
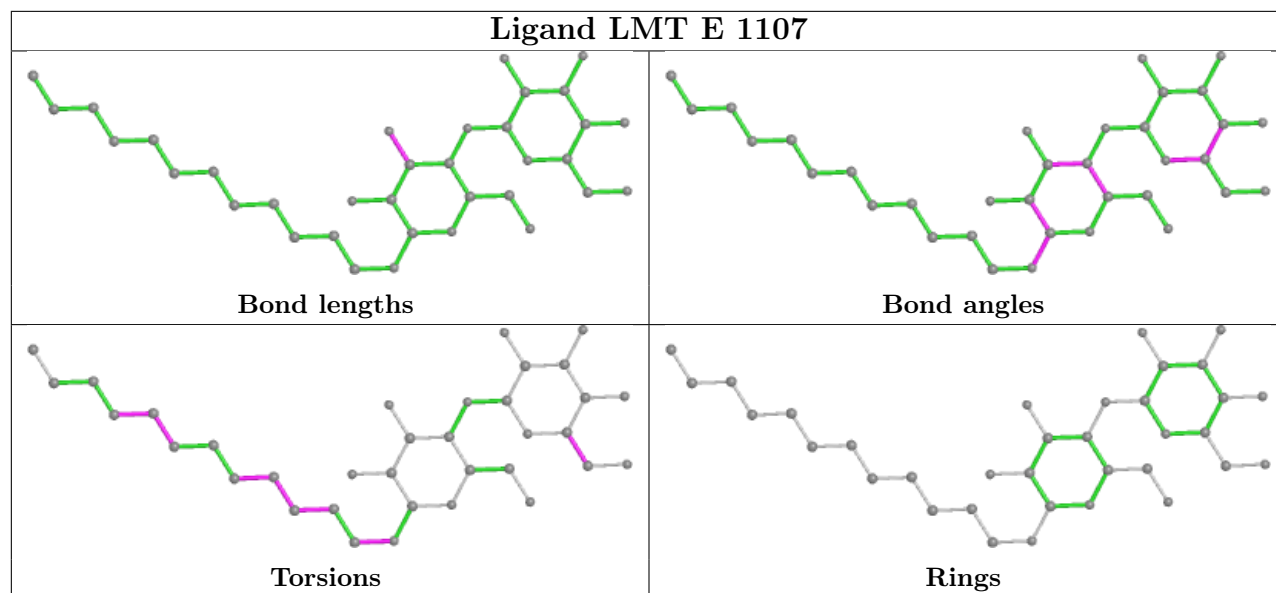


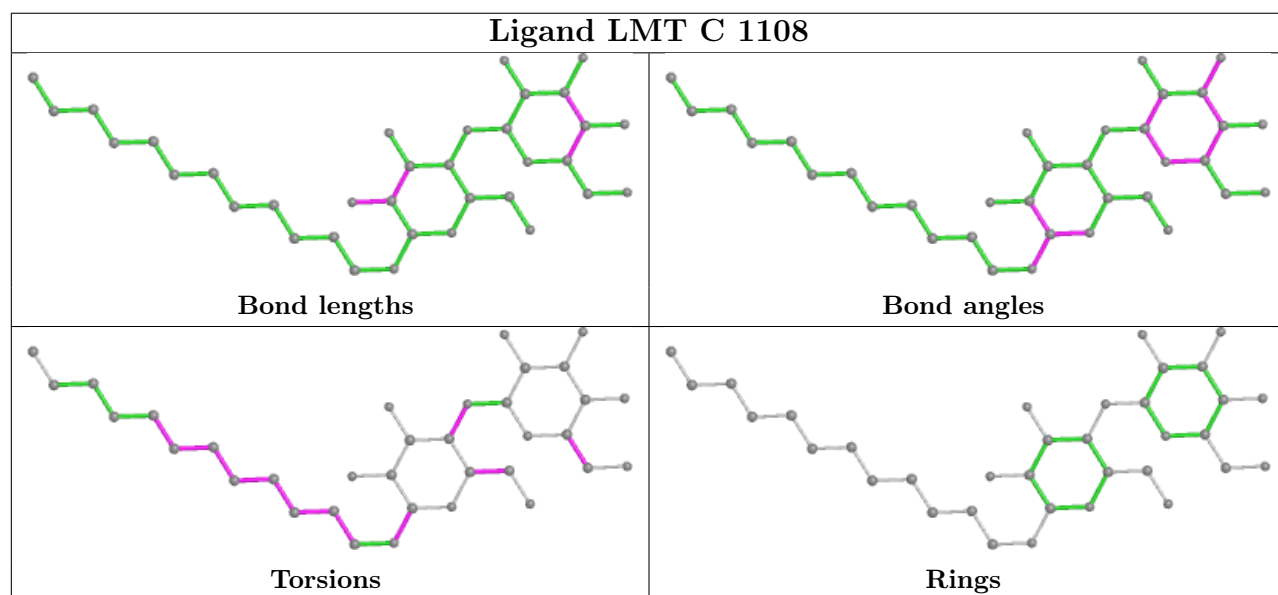
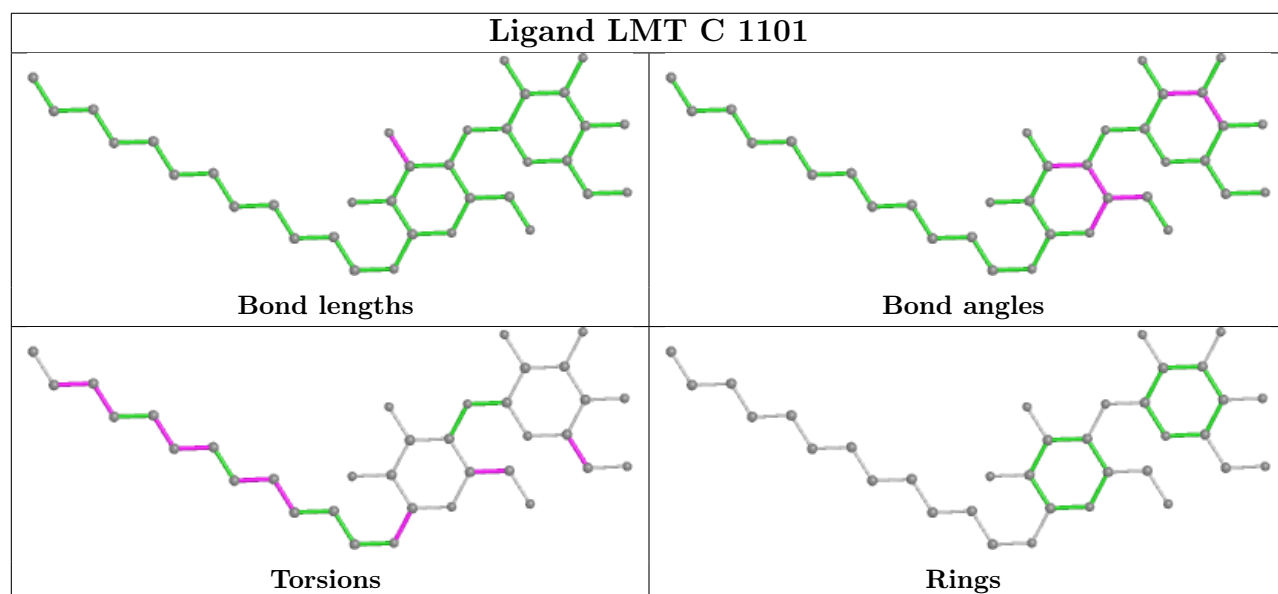
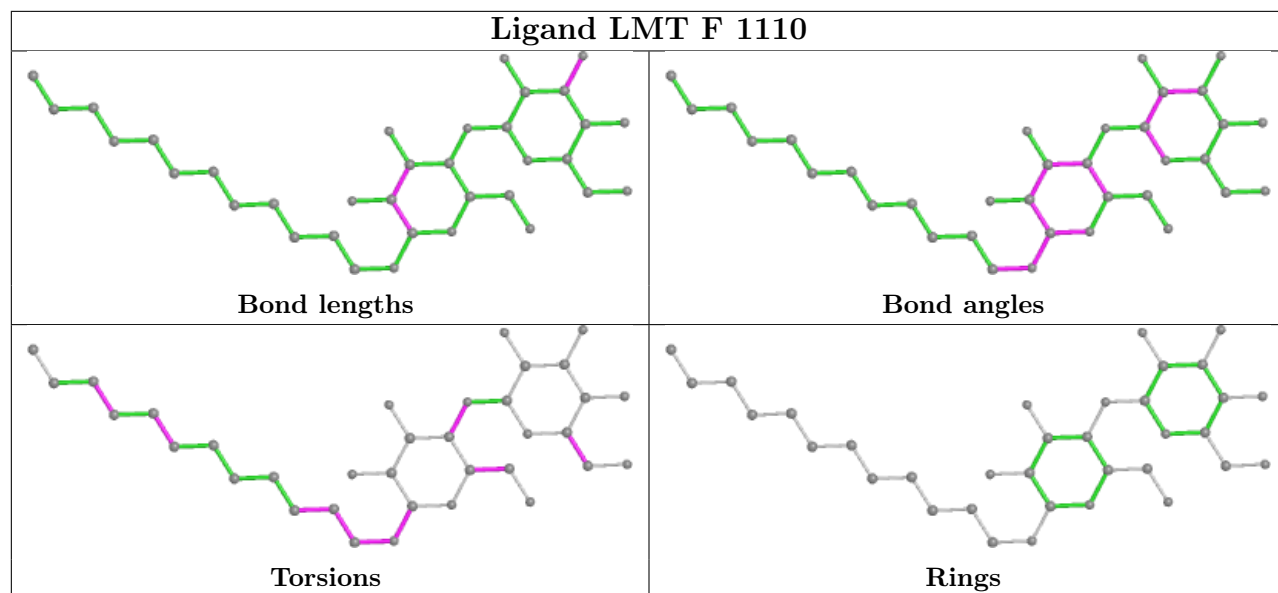


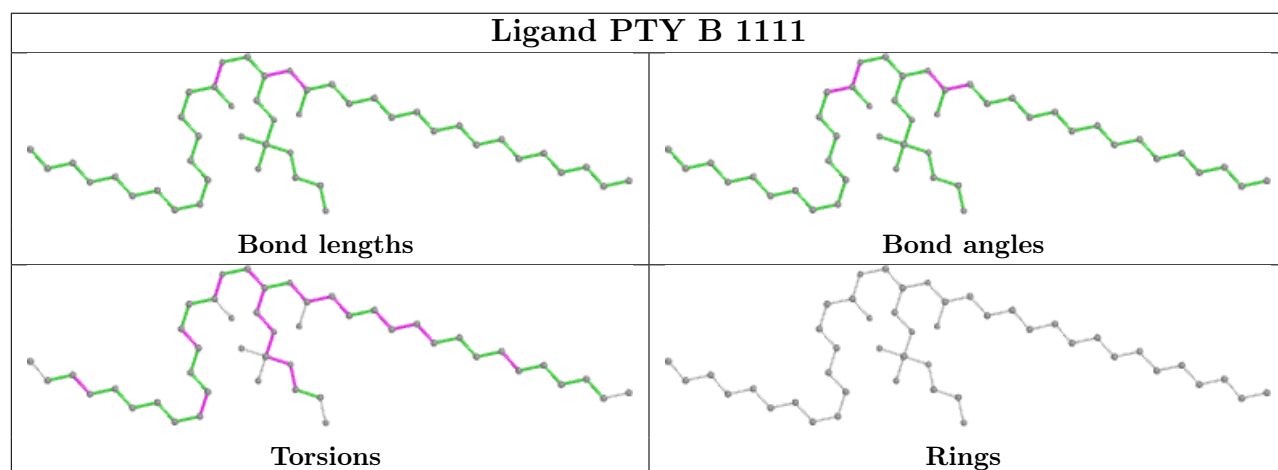
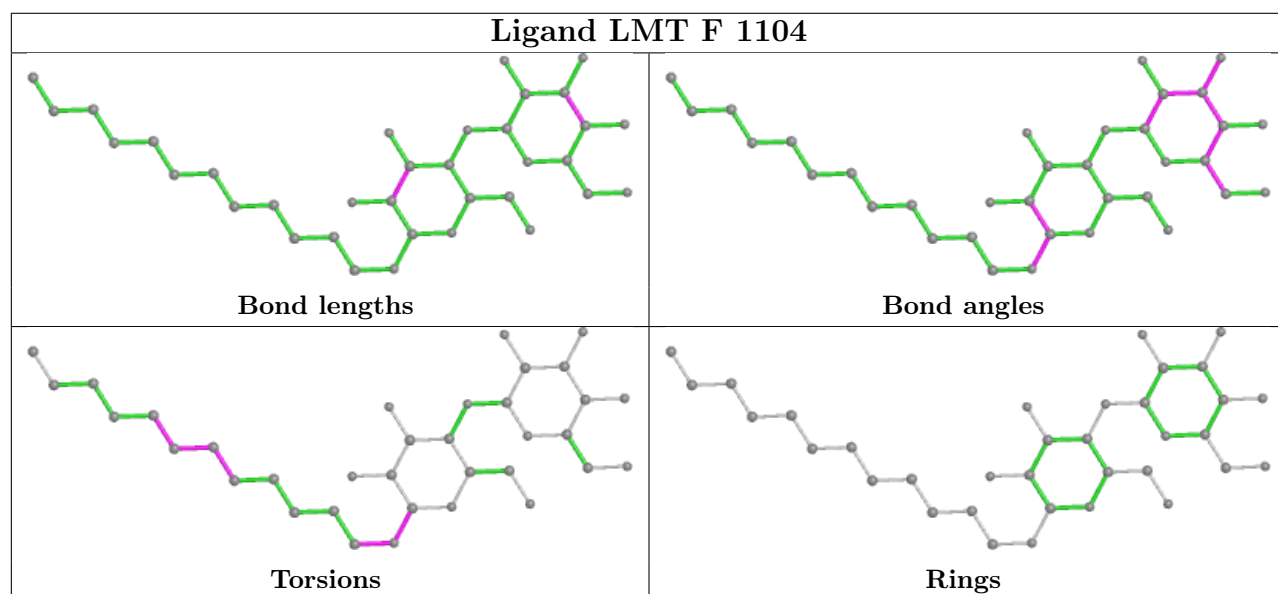
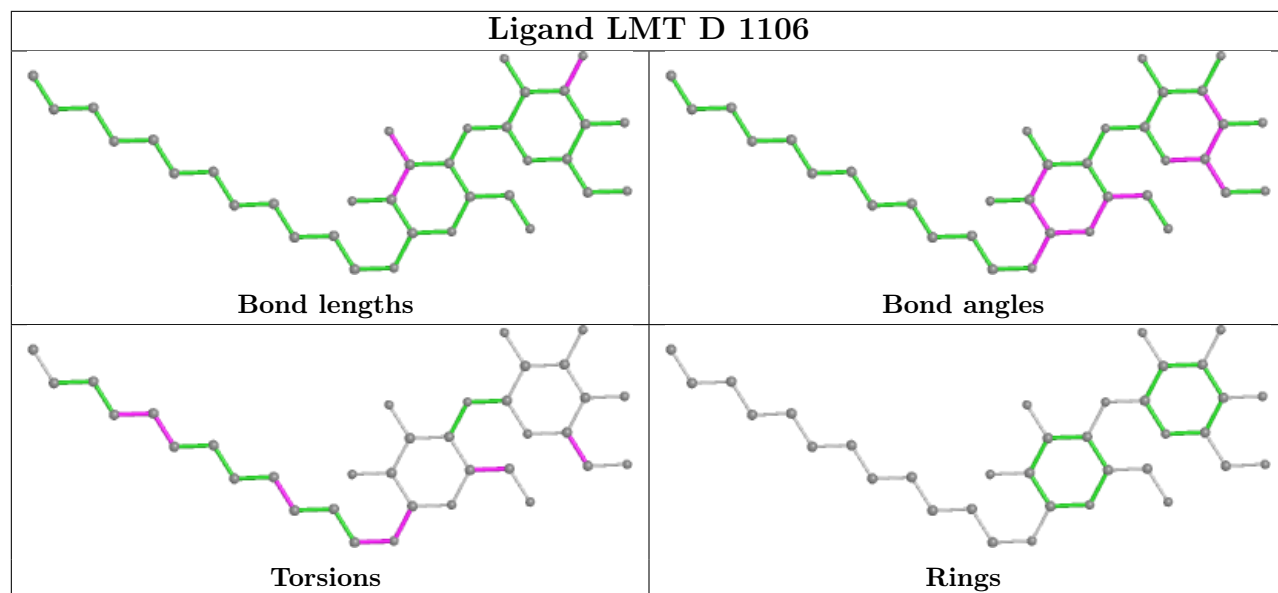


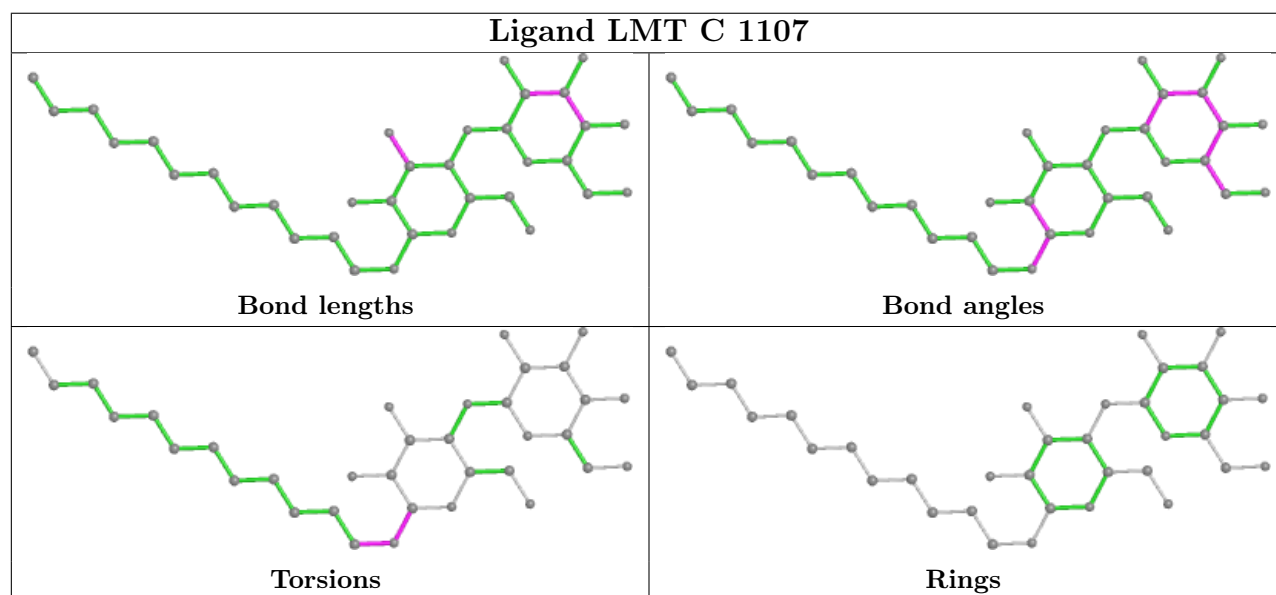
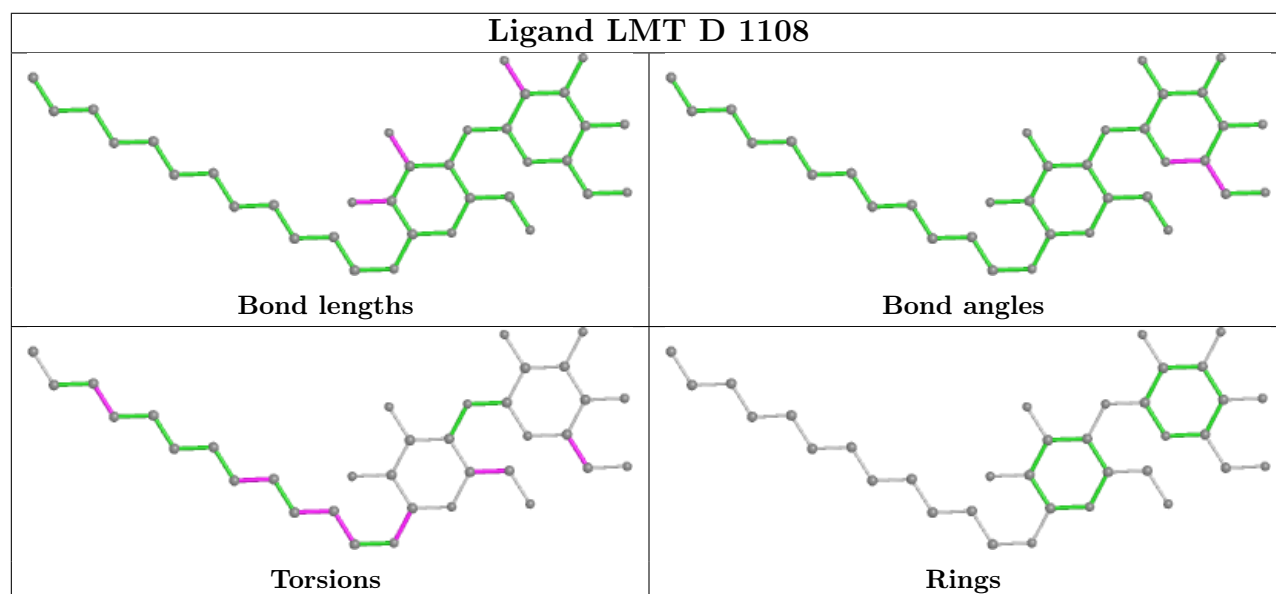
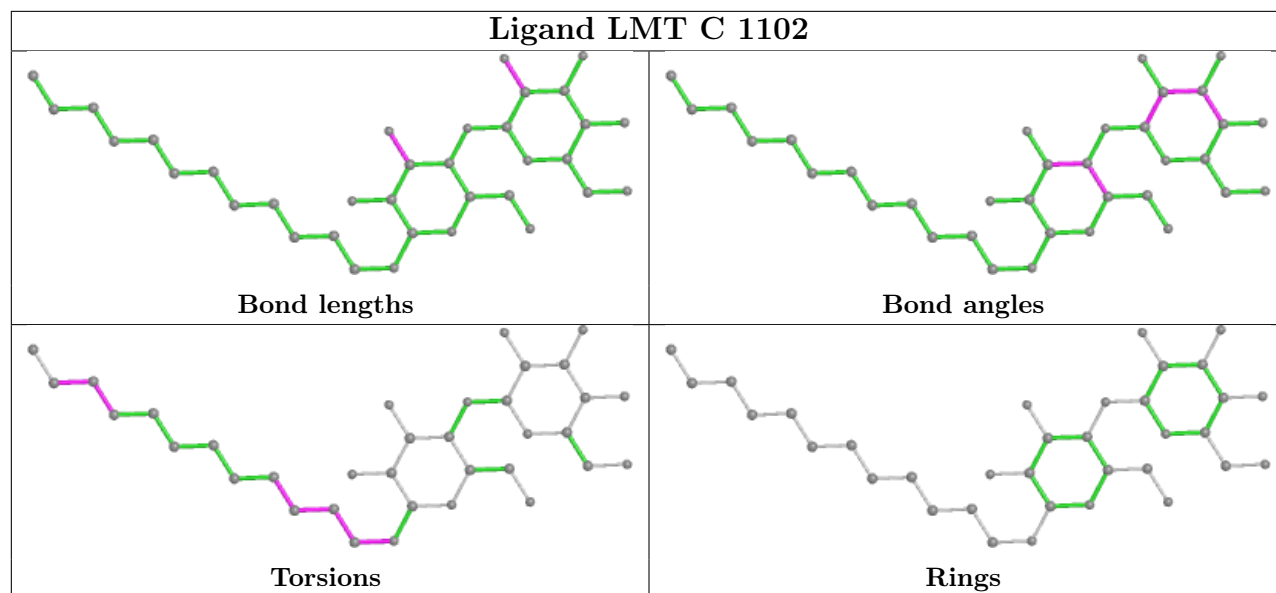


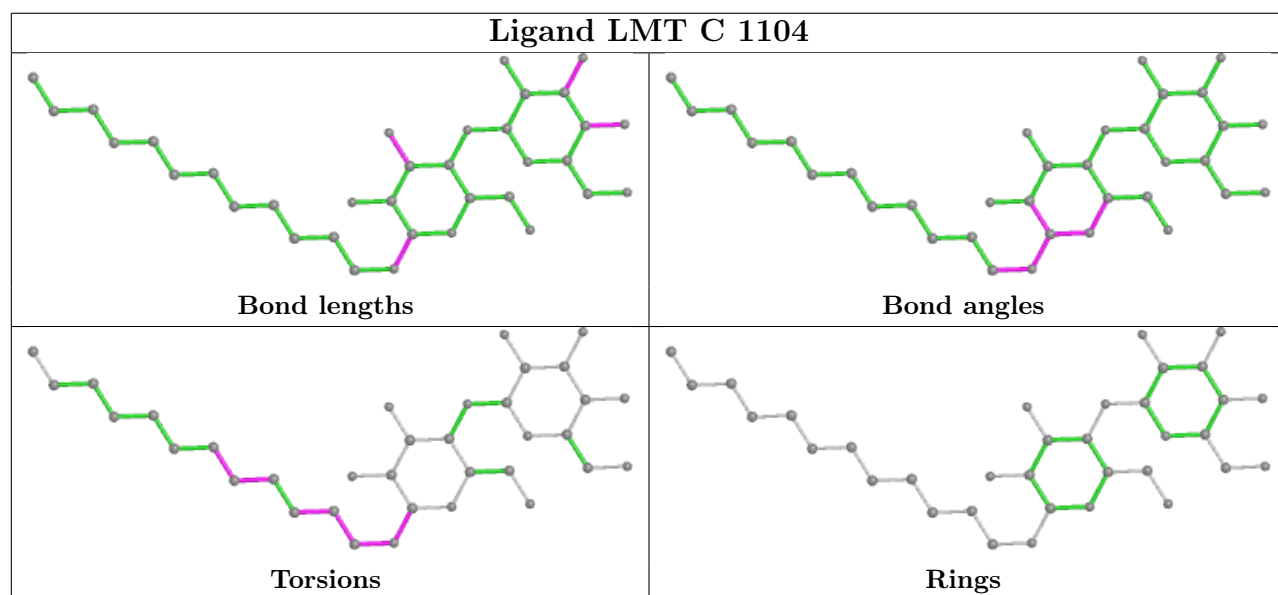
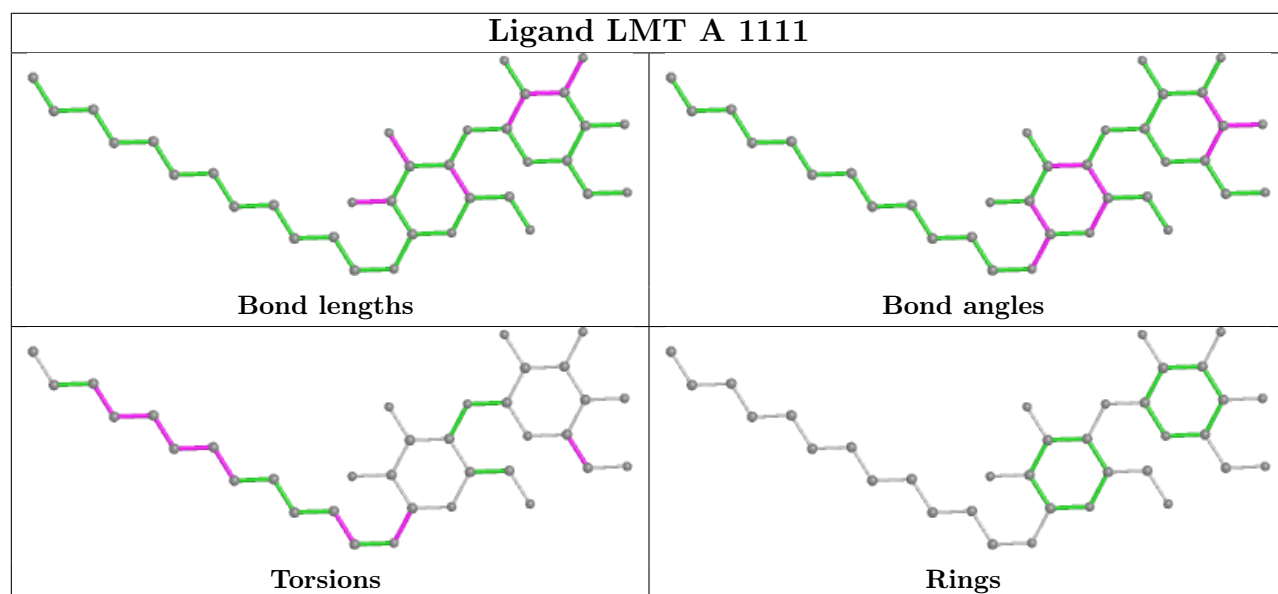
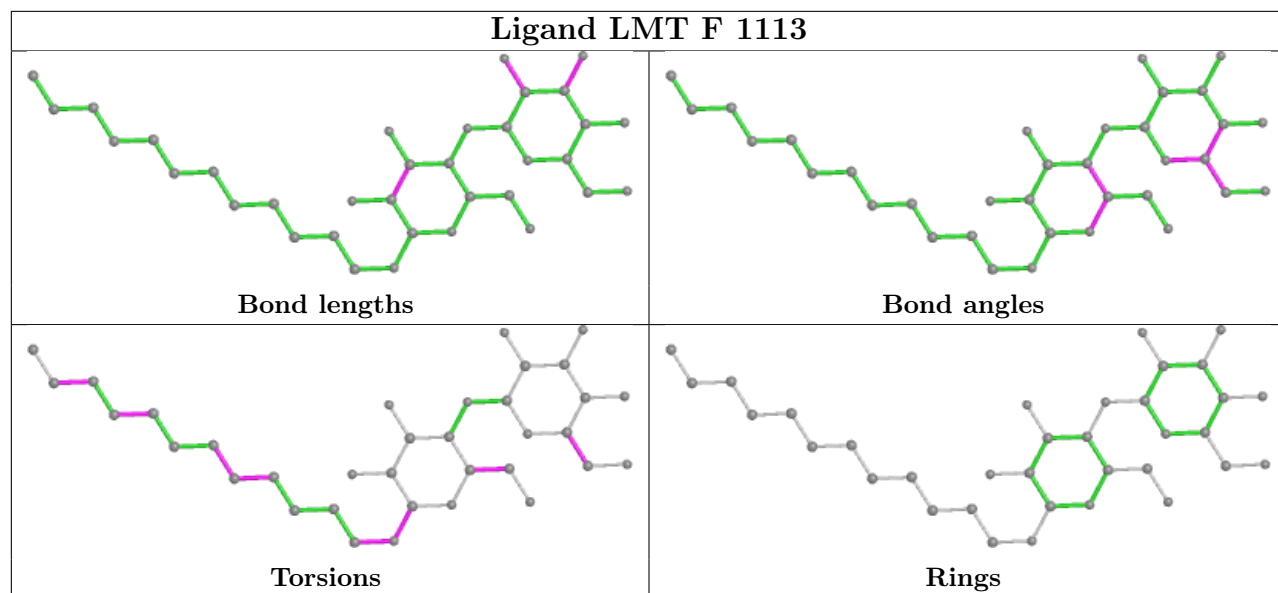


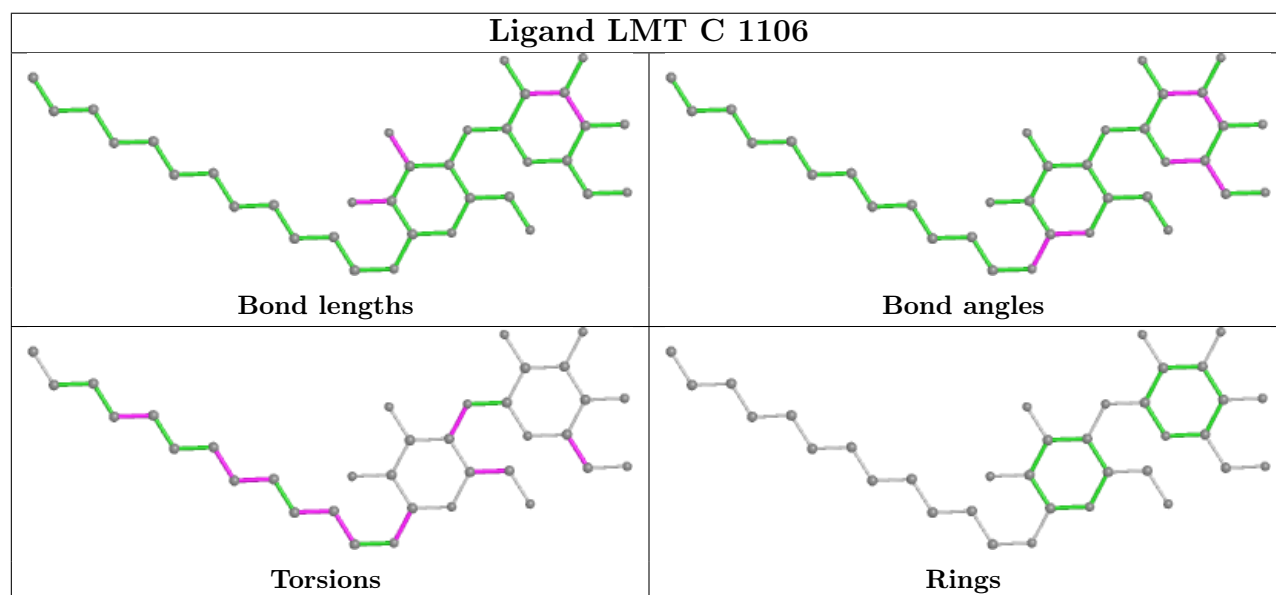
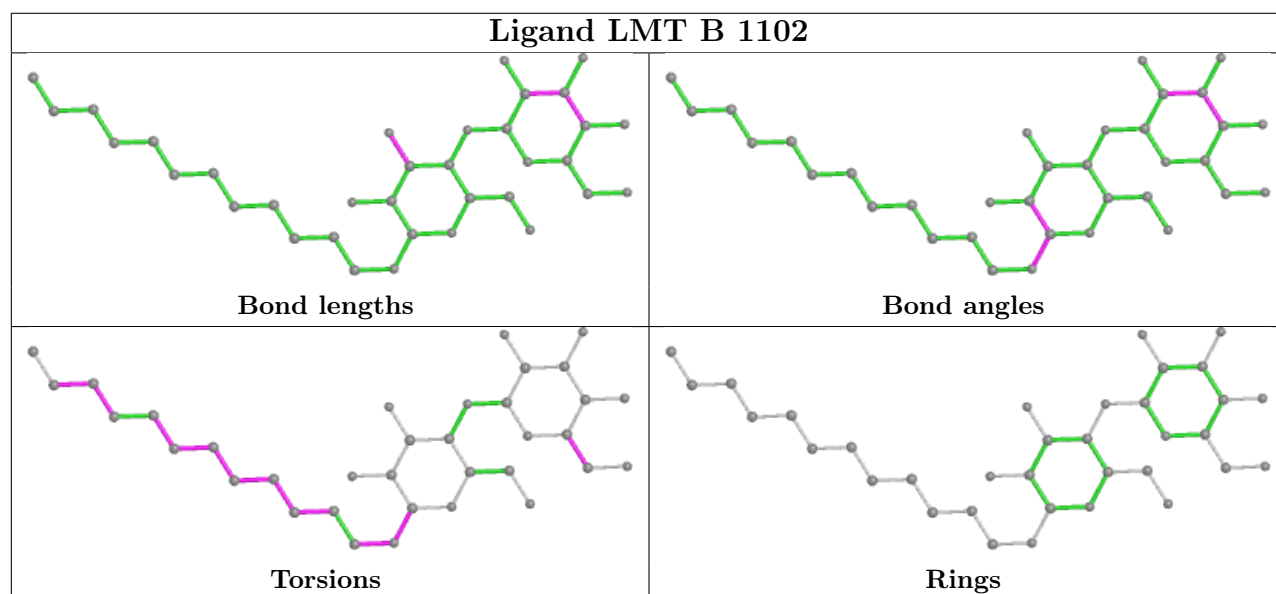
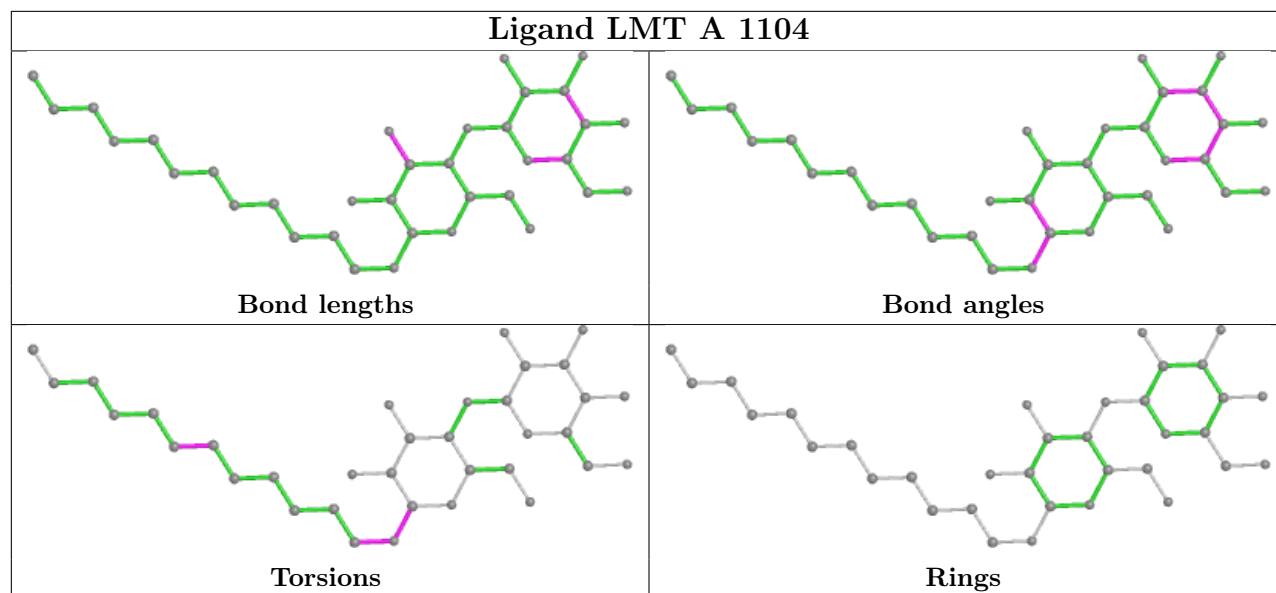


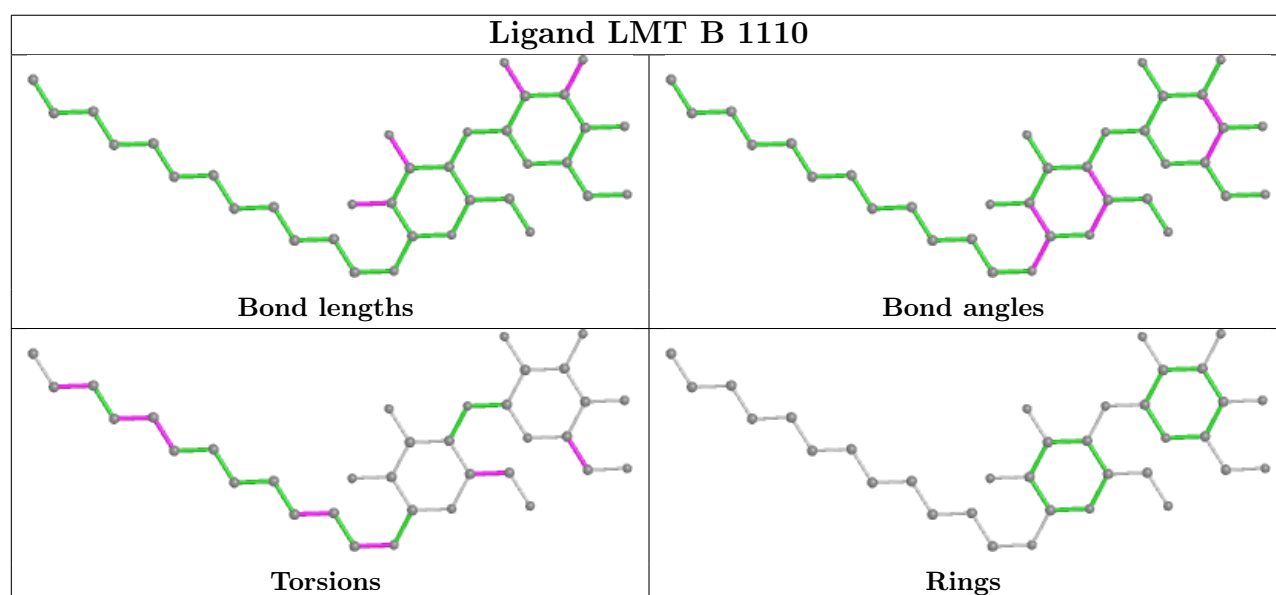
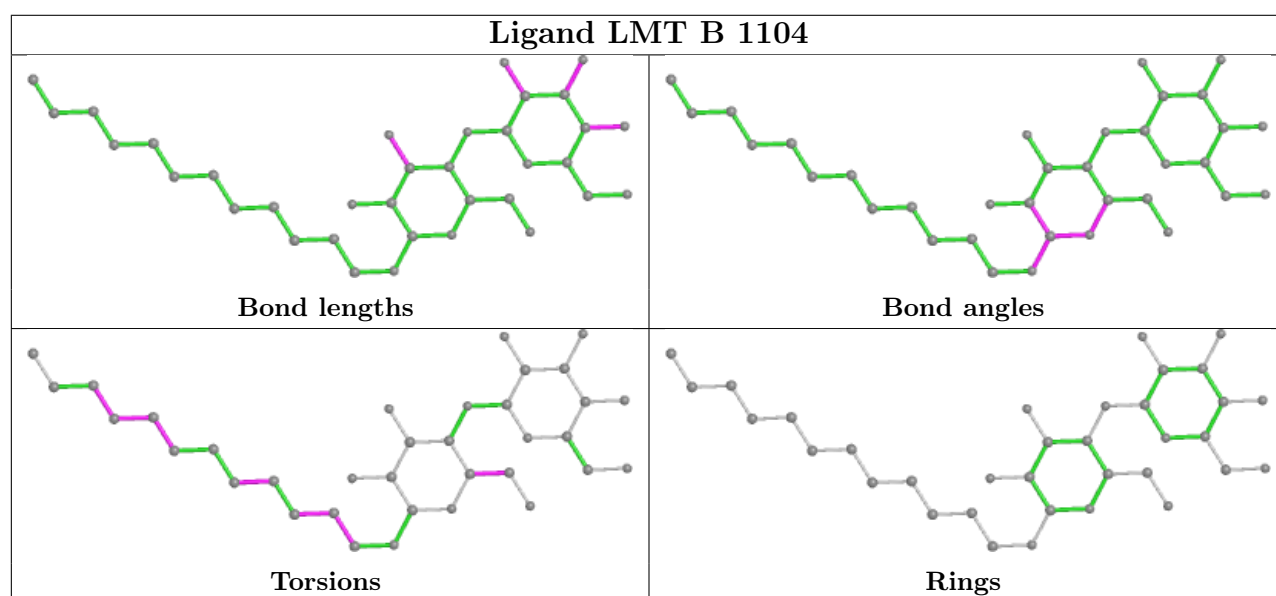
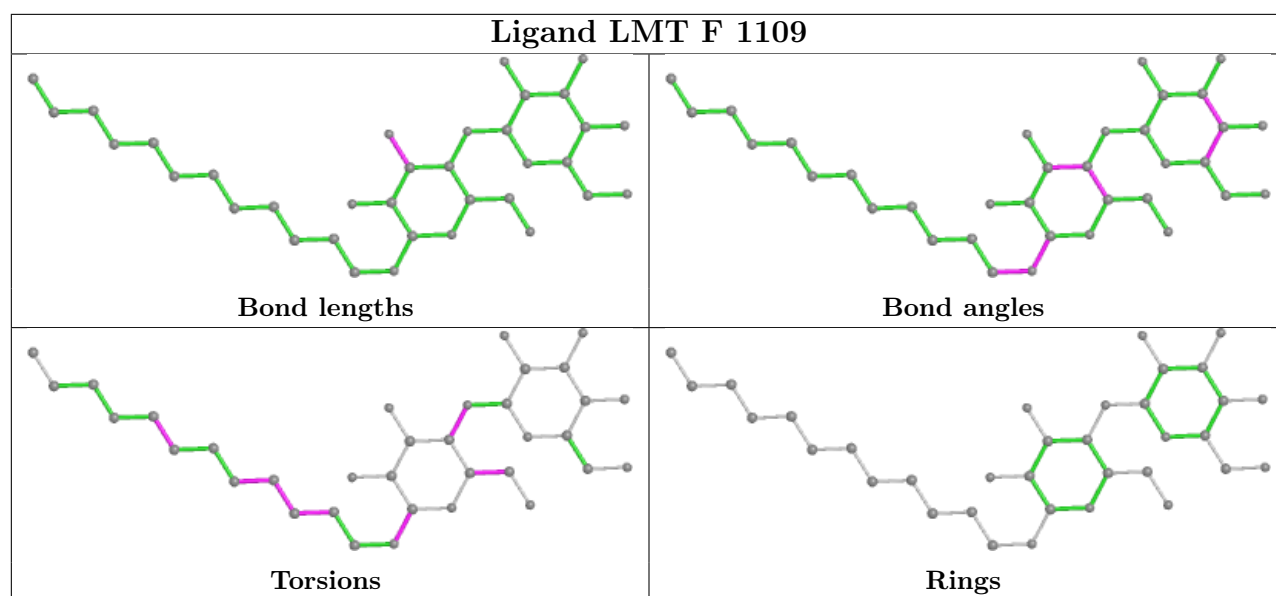




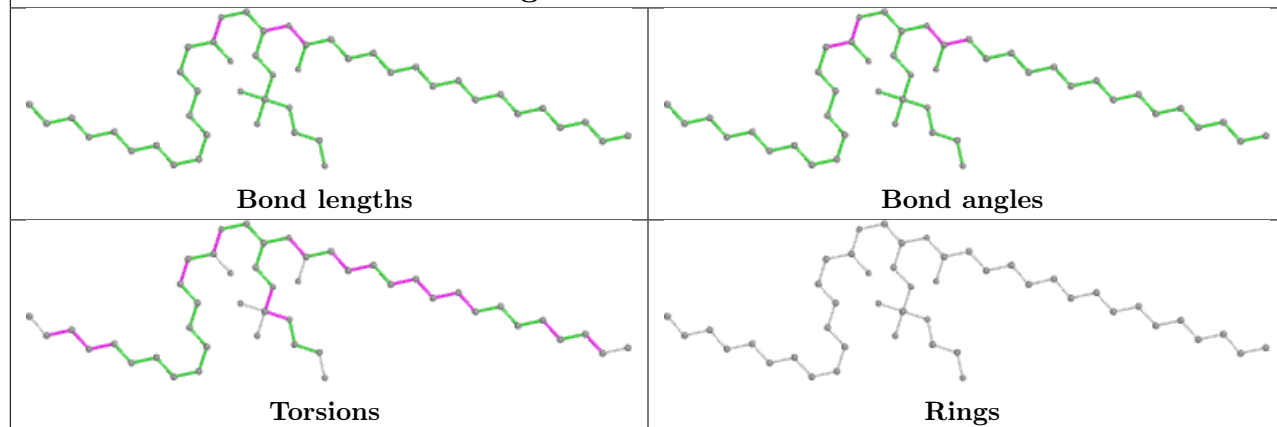




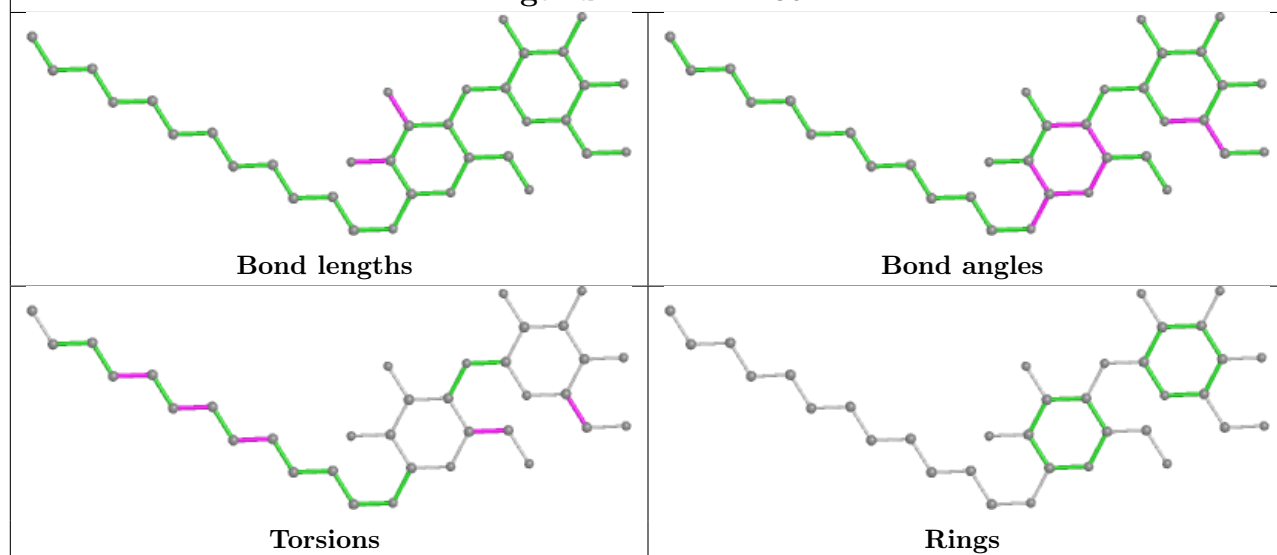




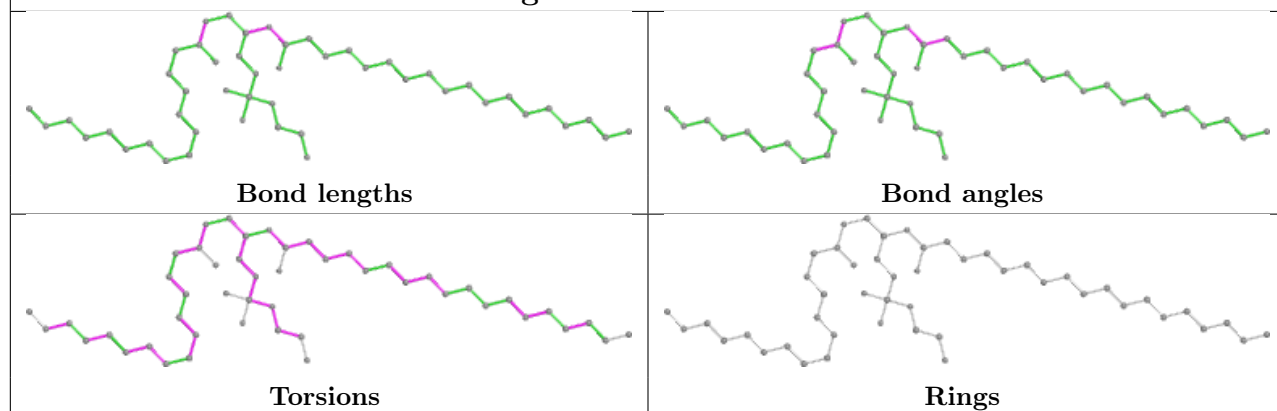
Ligand PTY A 1112

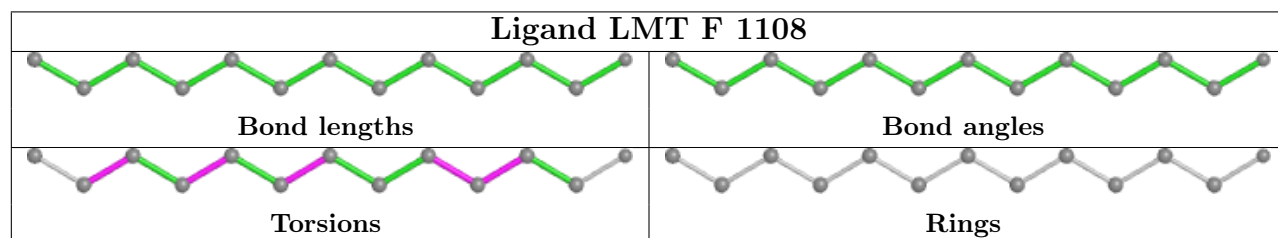
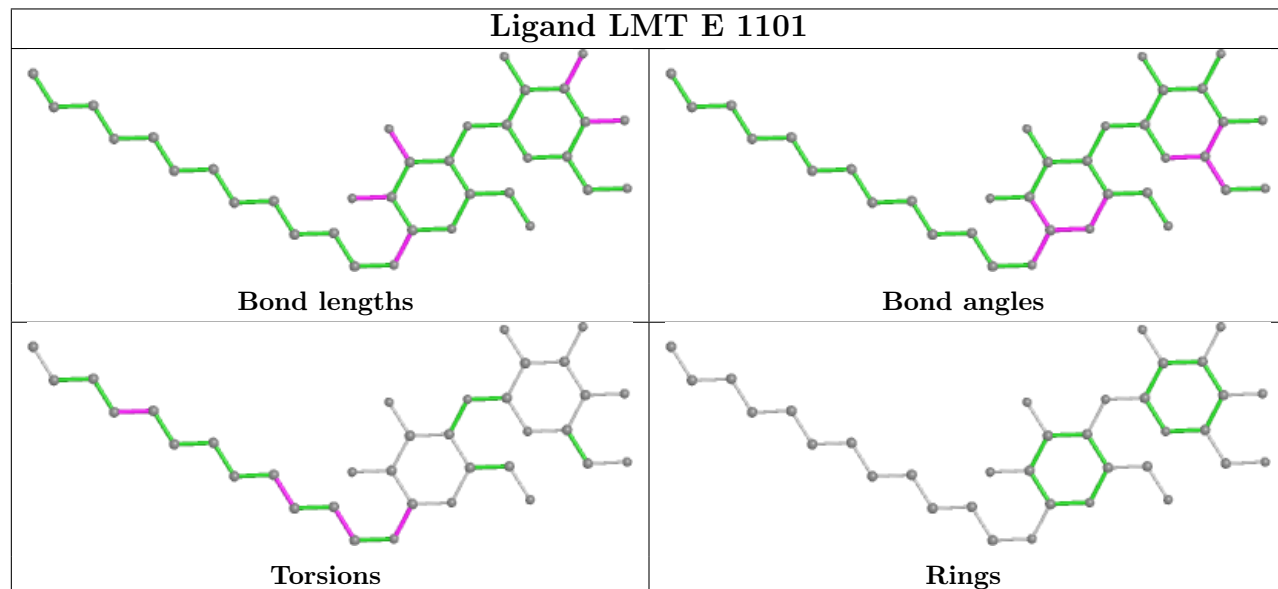
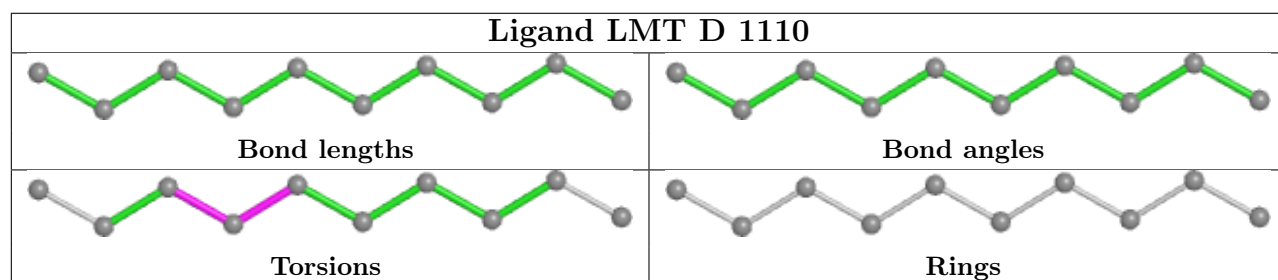
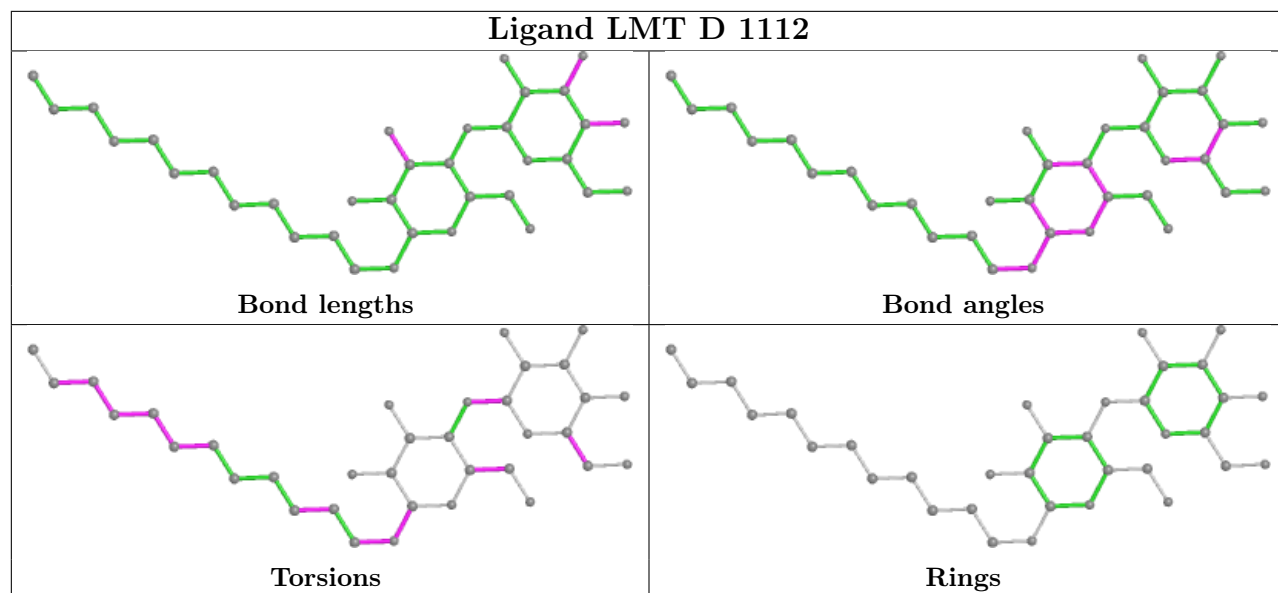


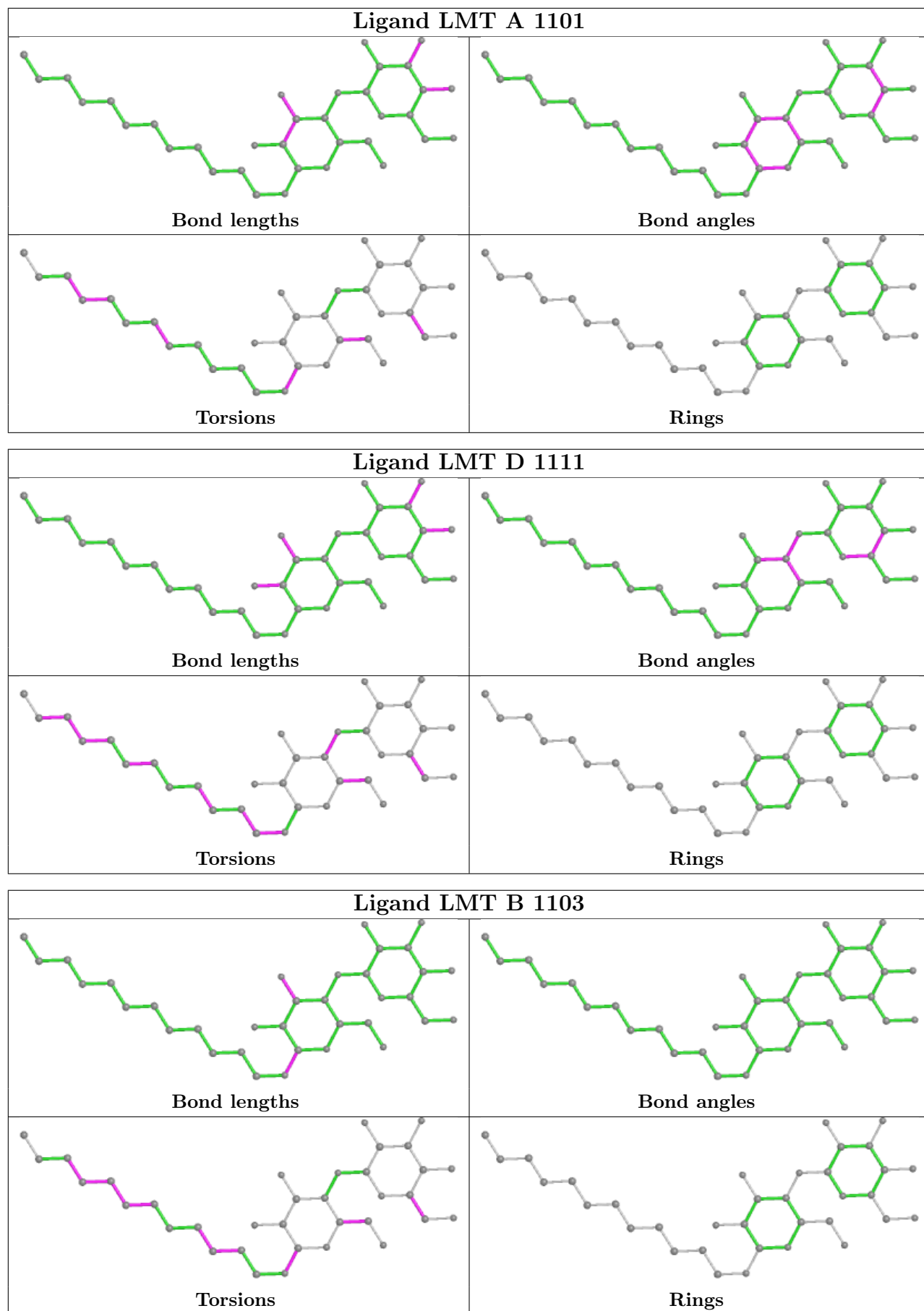
Ligand LMT E 1109

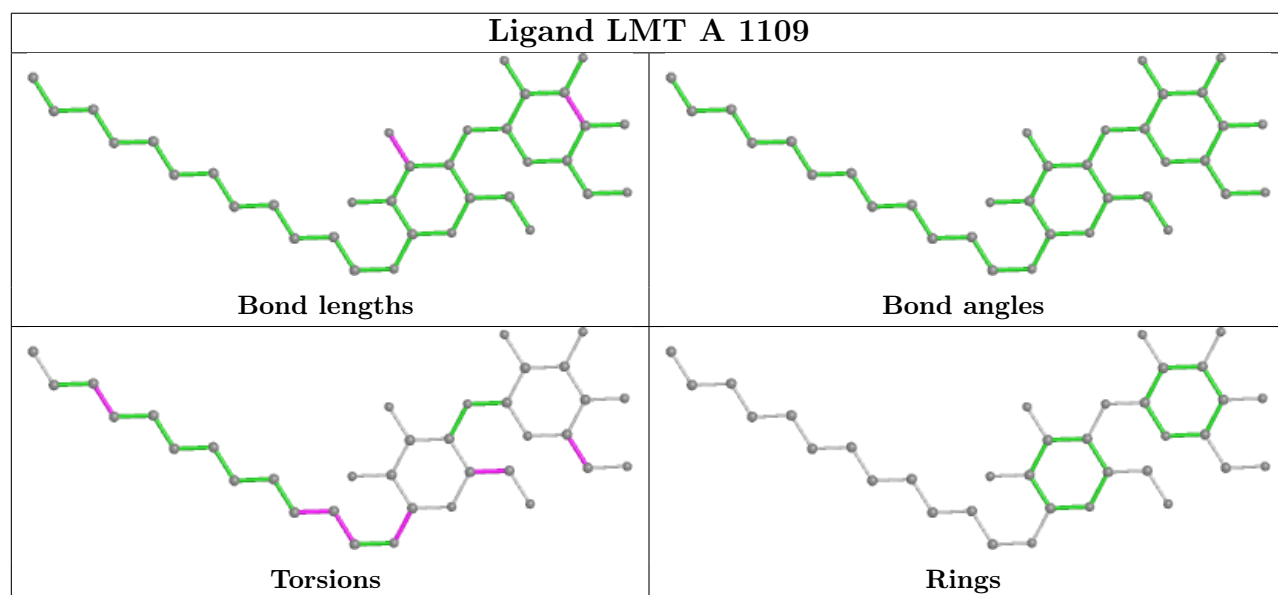
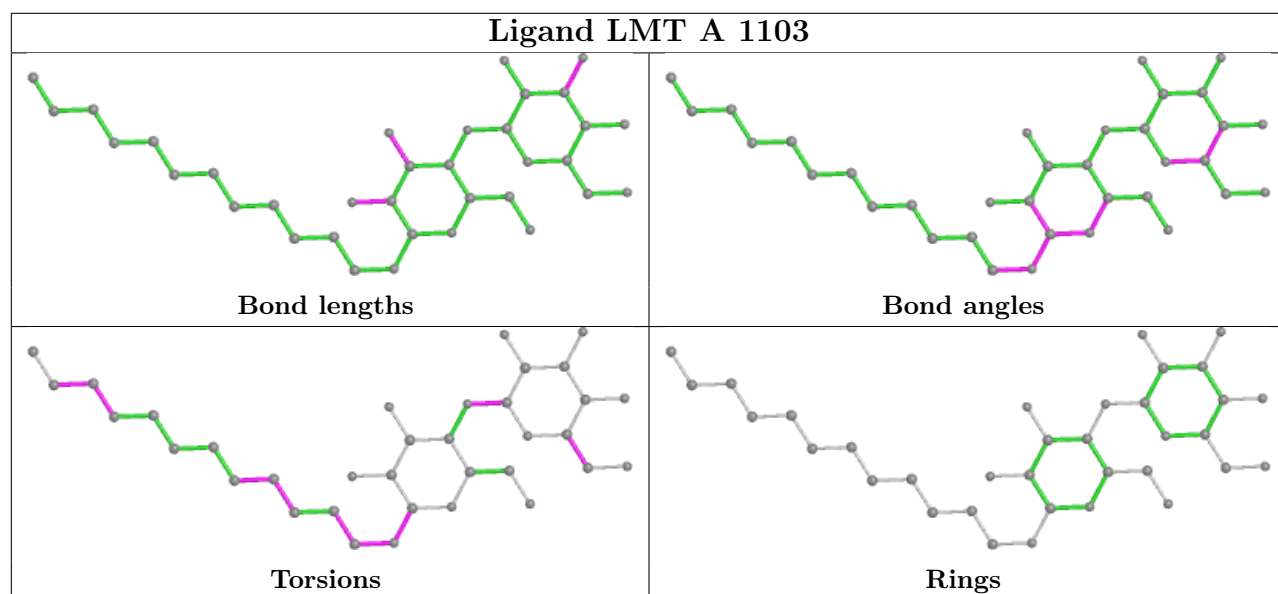
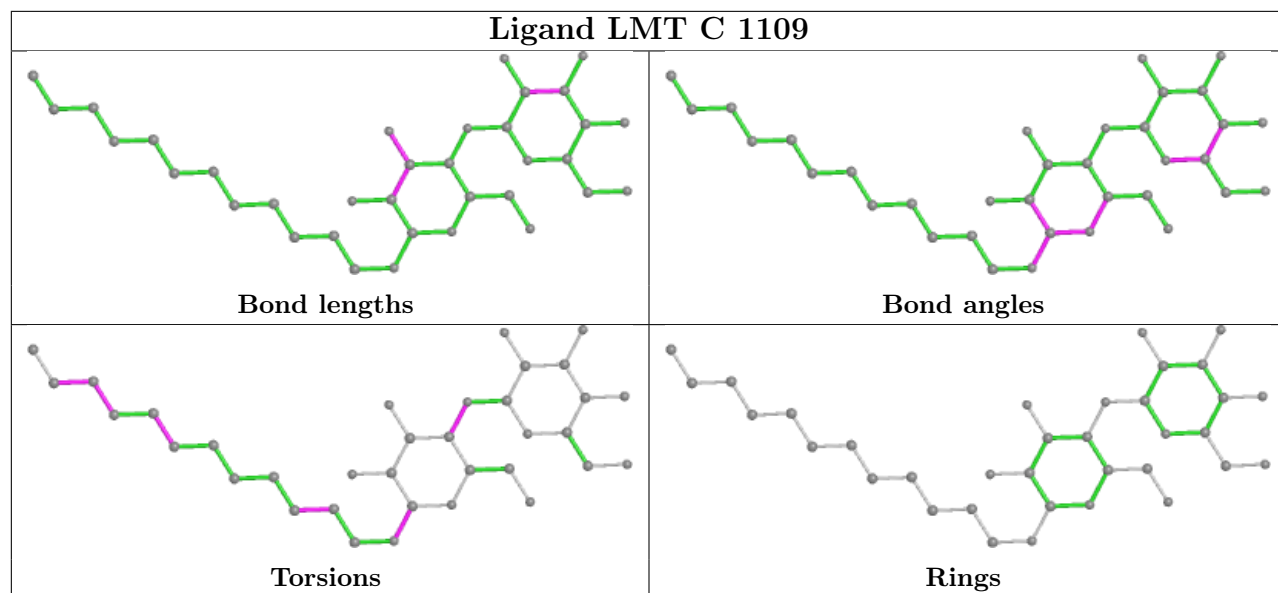


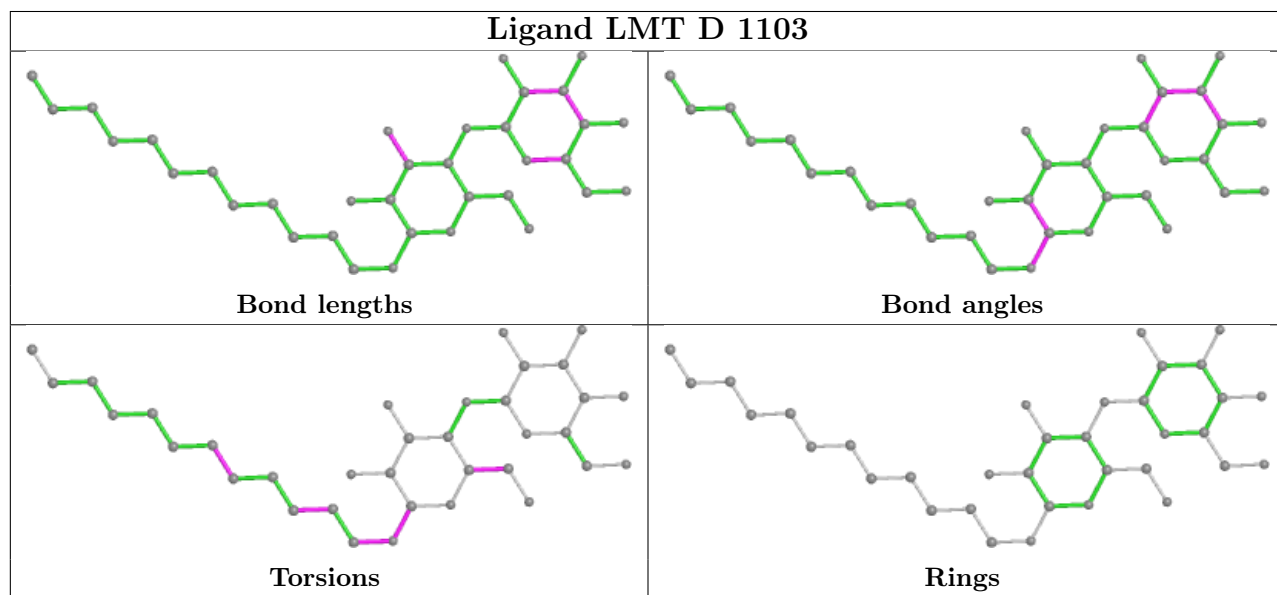
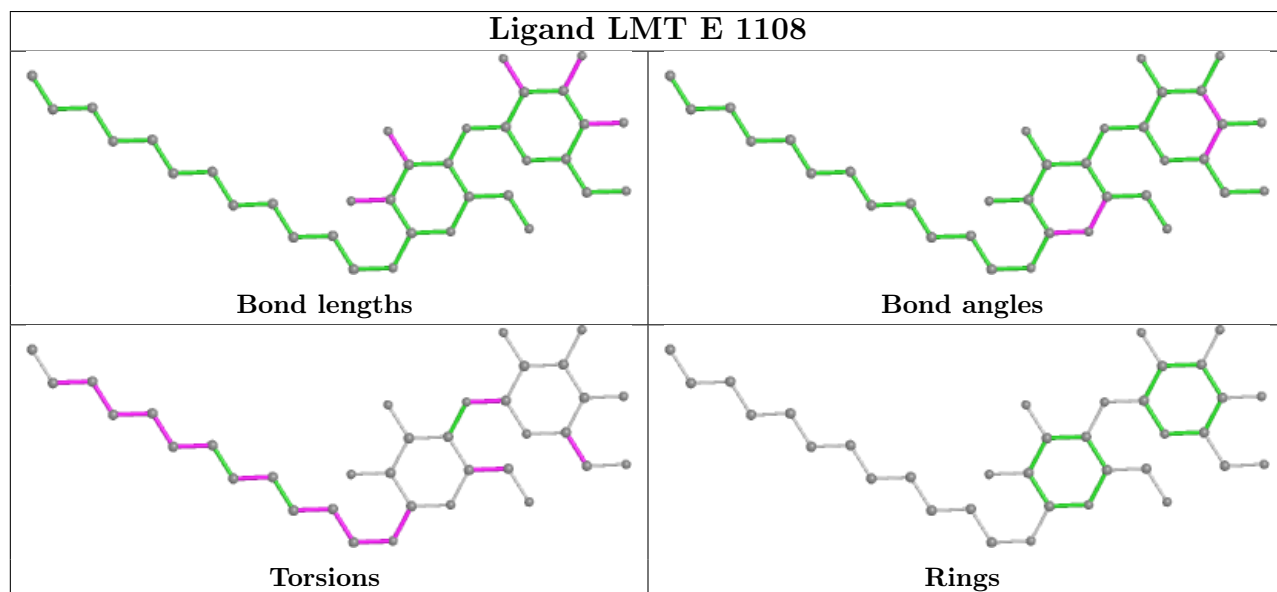
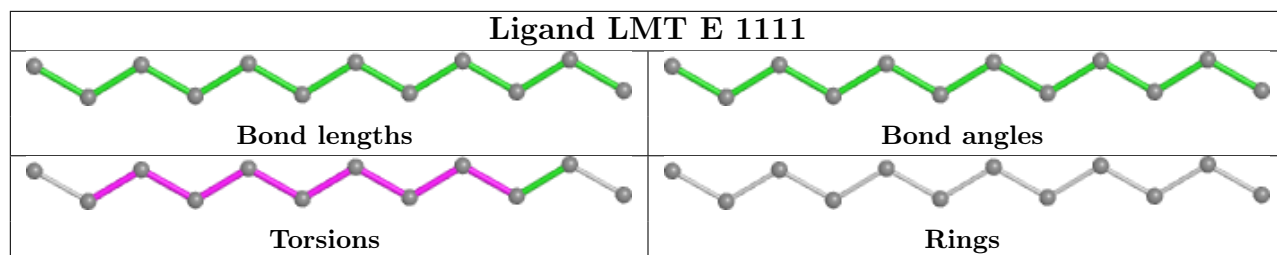
Ligand PTY B 1112

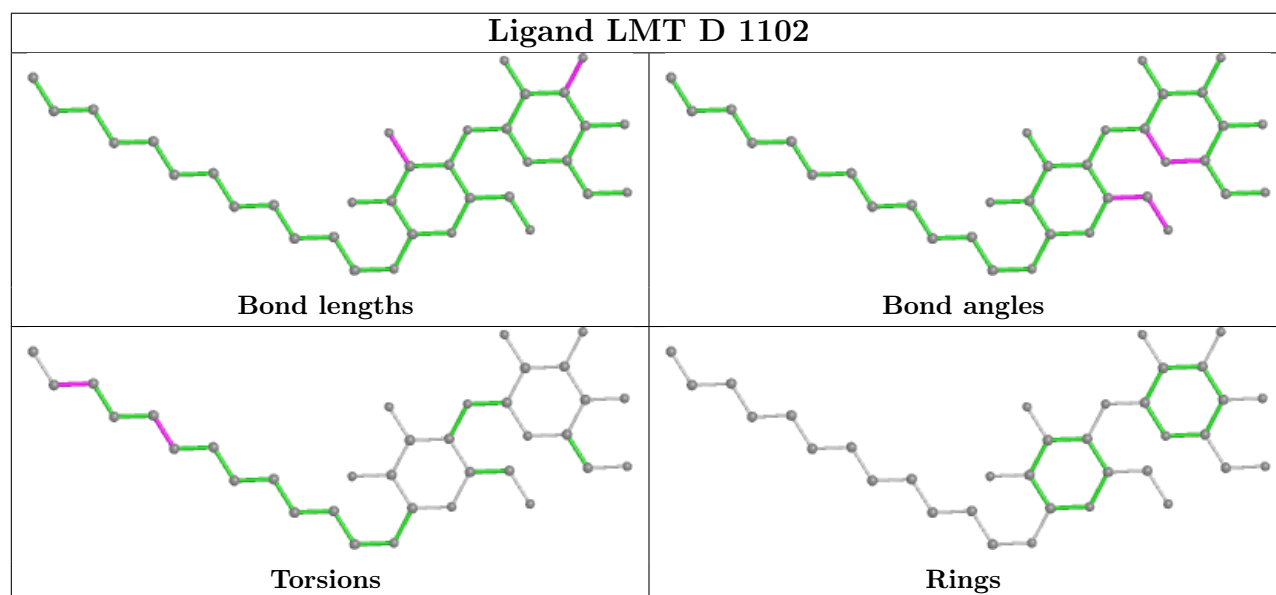
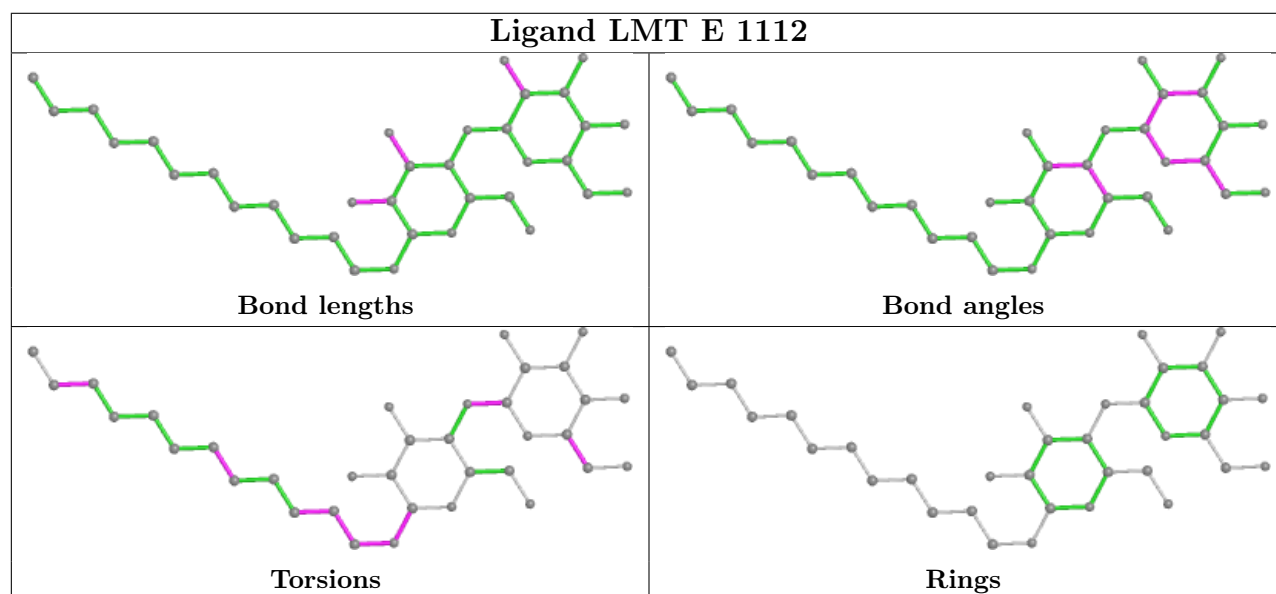
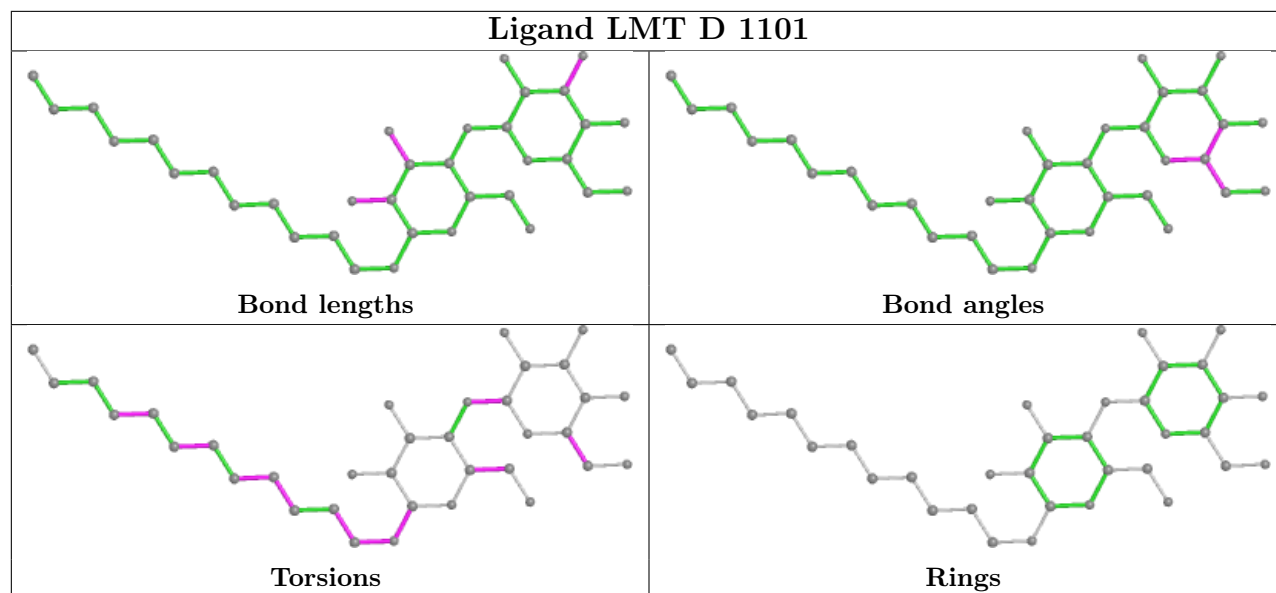


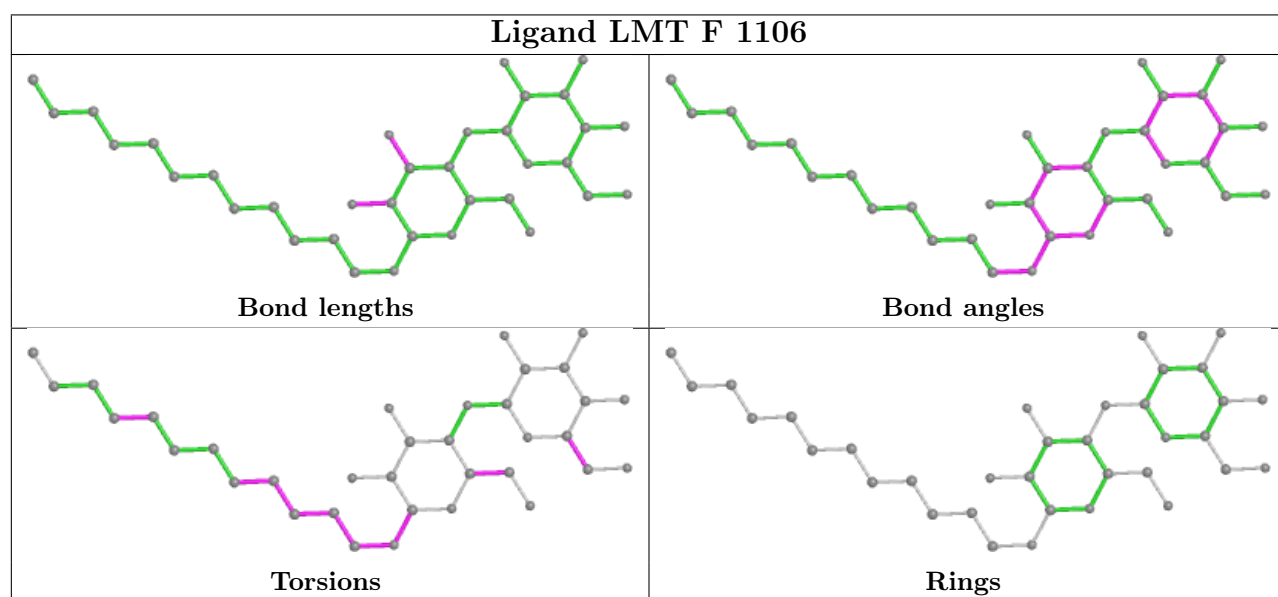
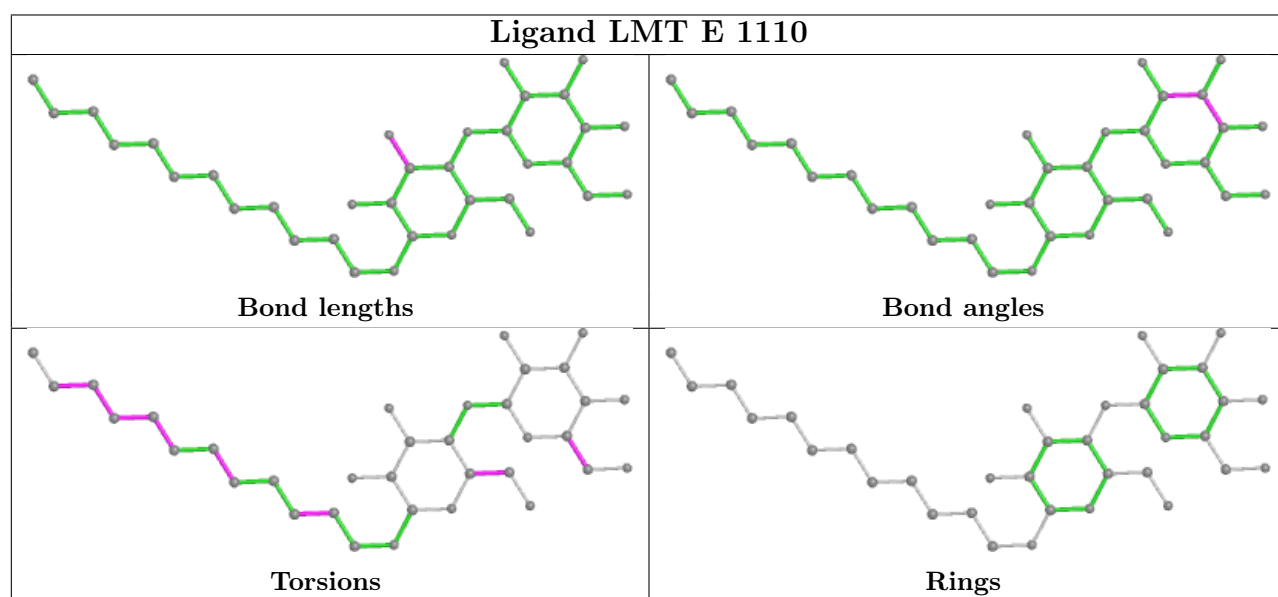
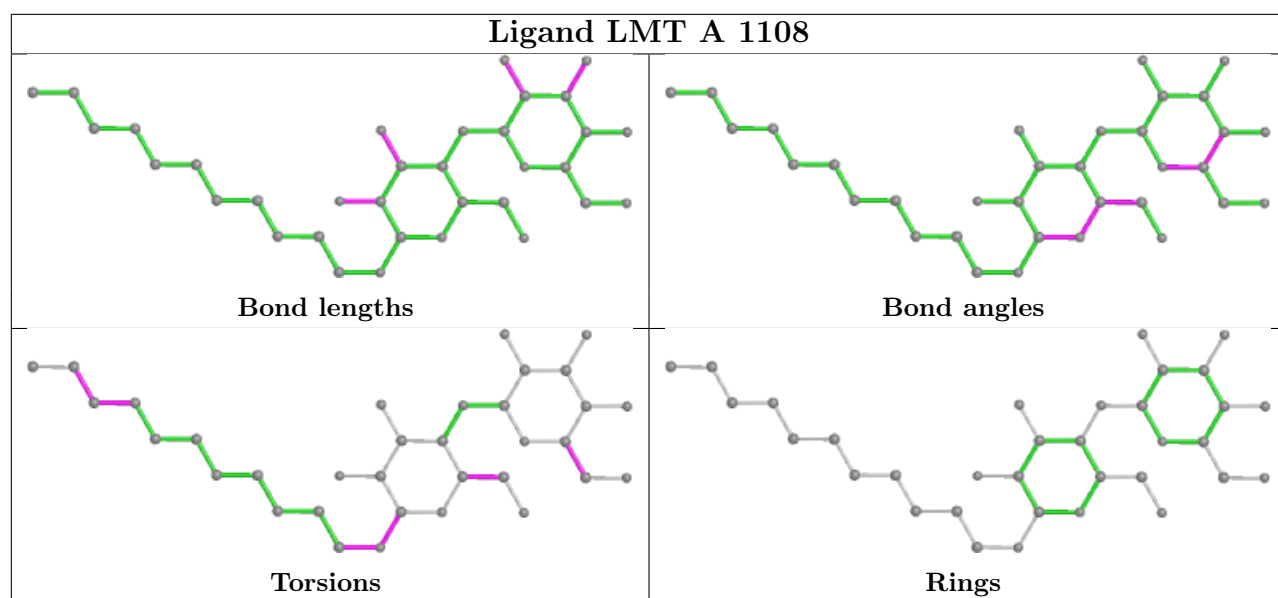




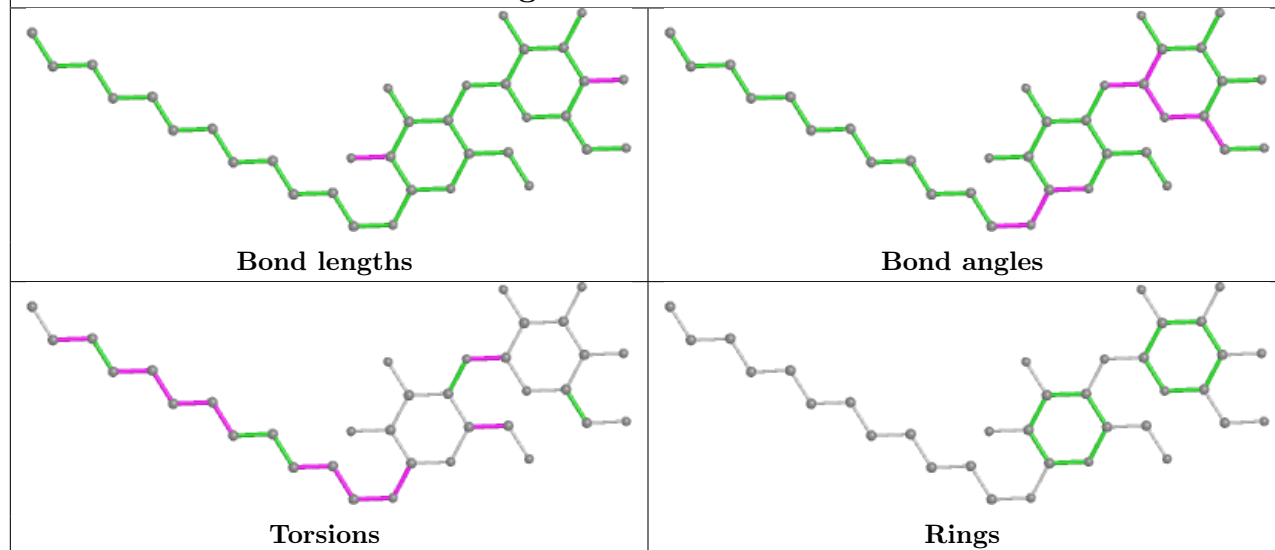




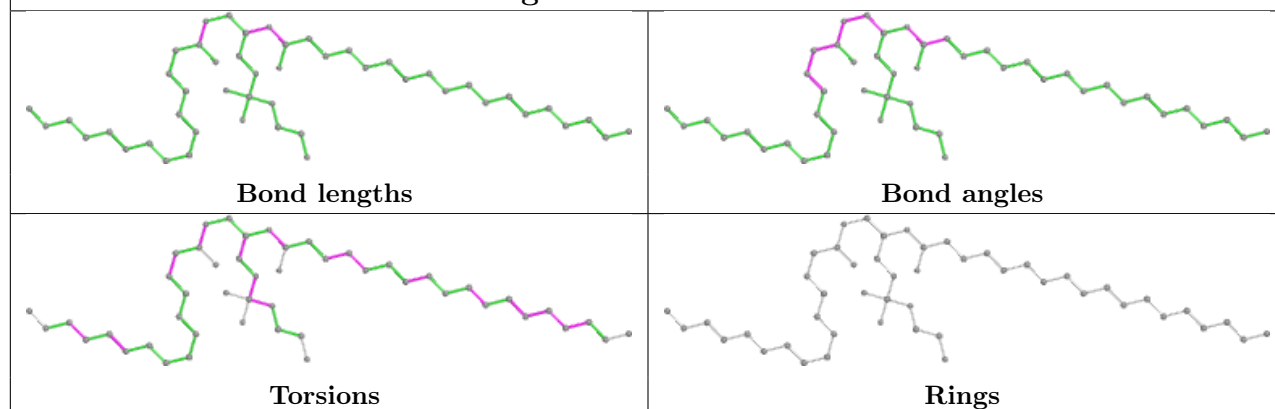




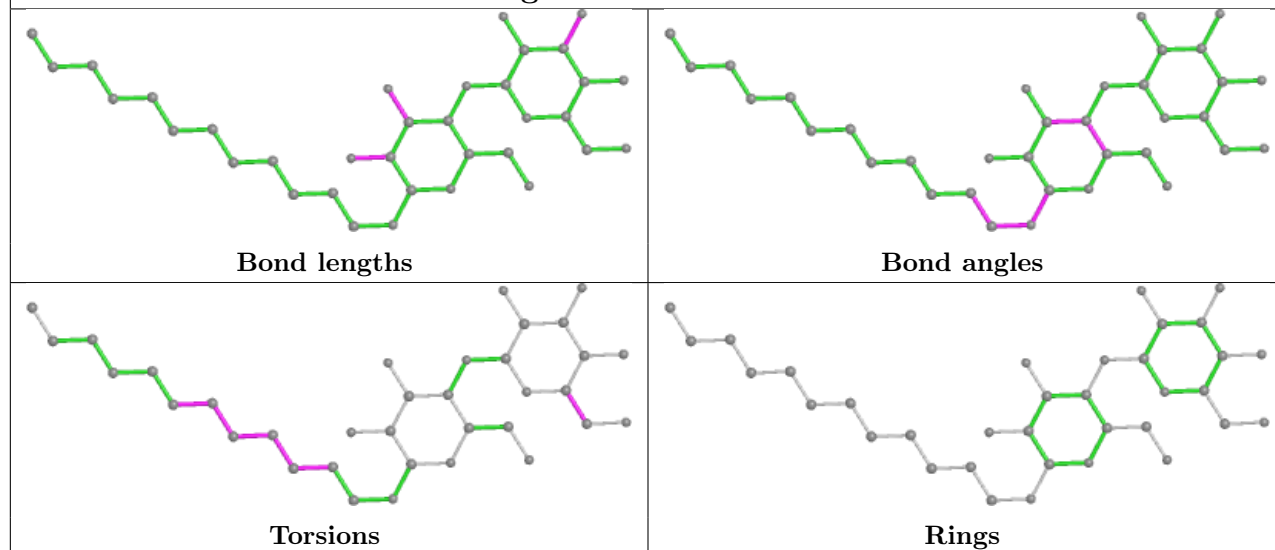
Ligand LMT A 1105

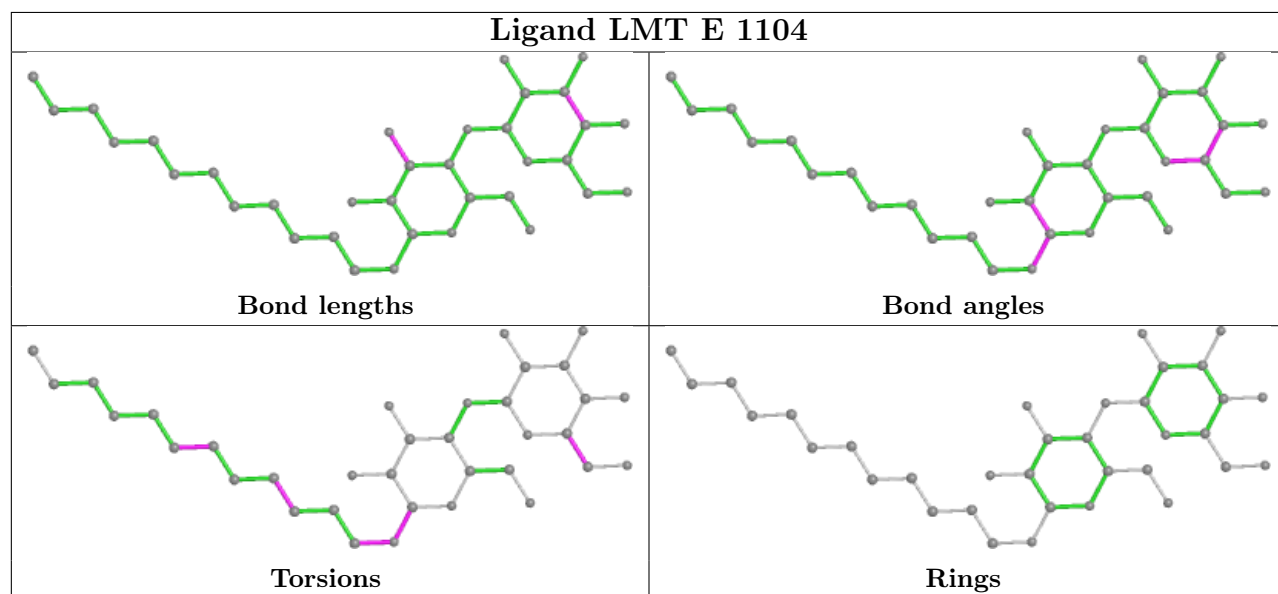
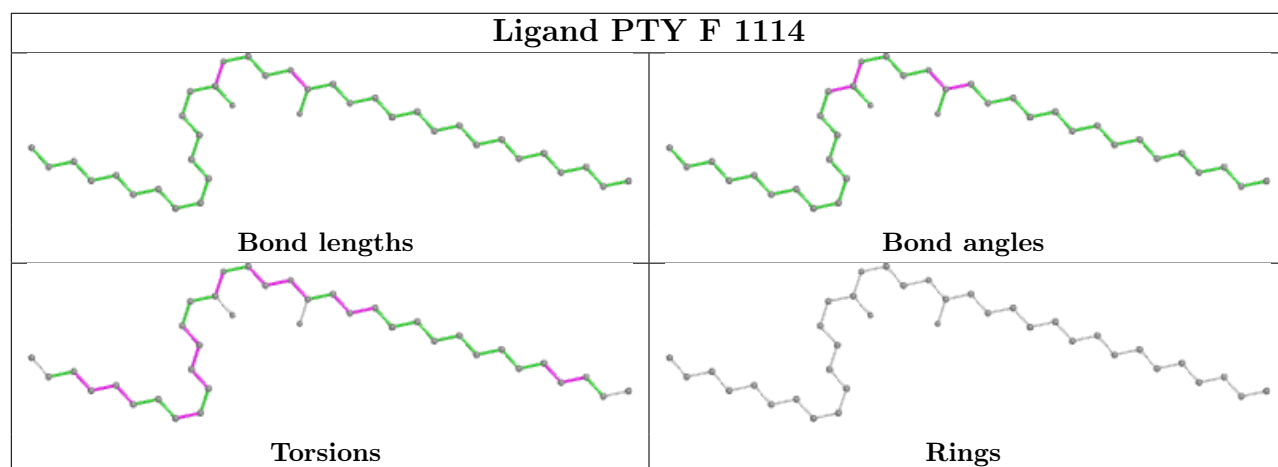
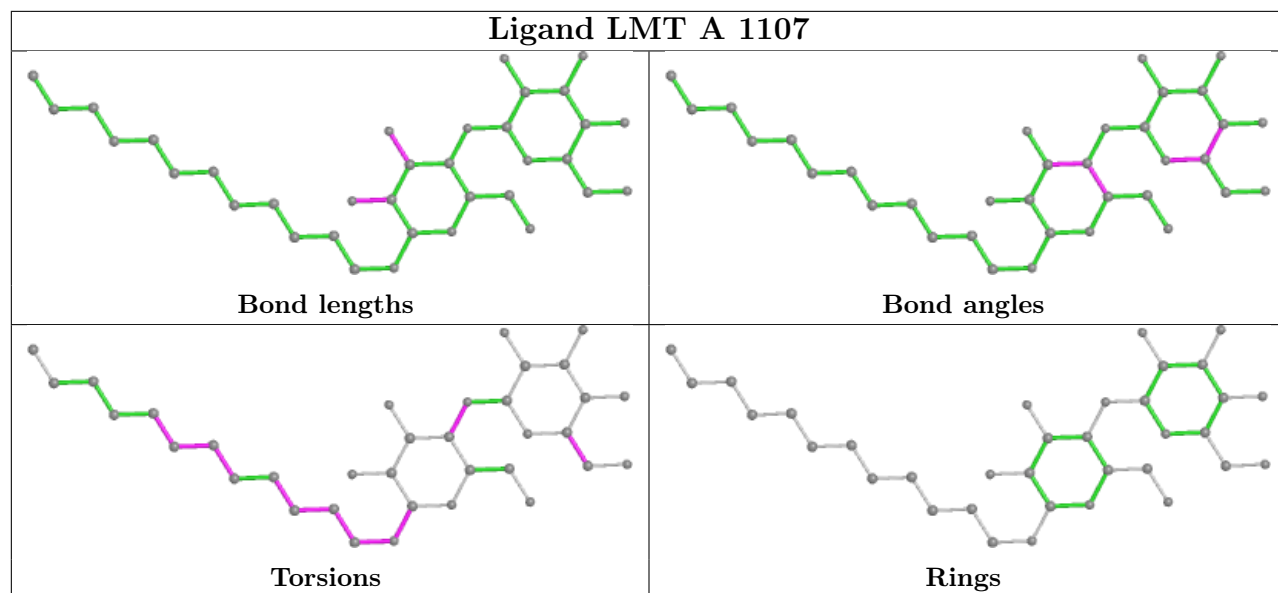


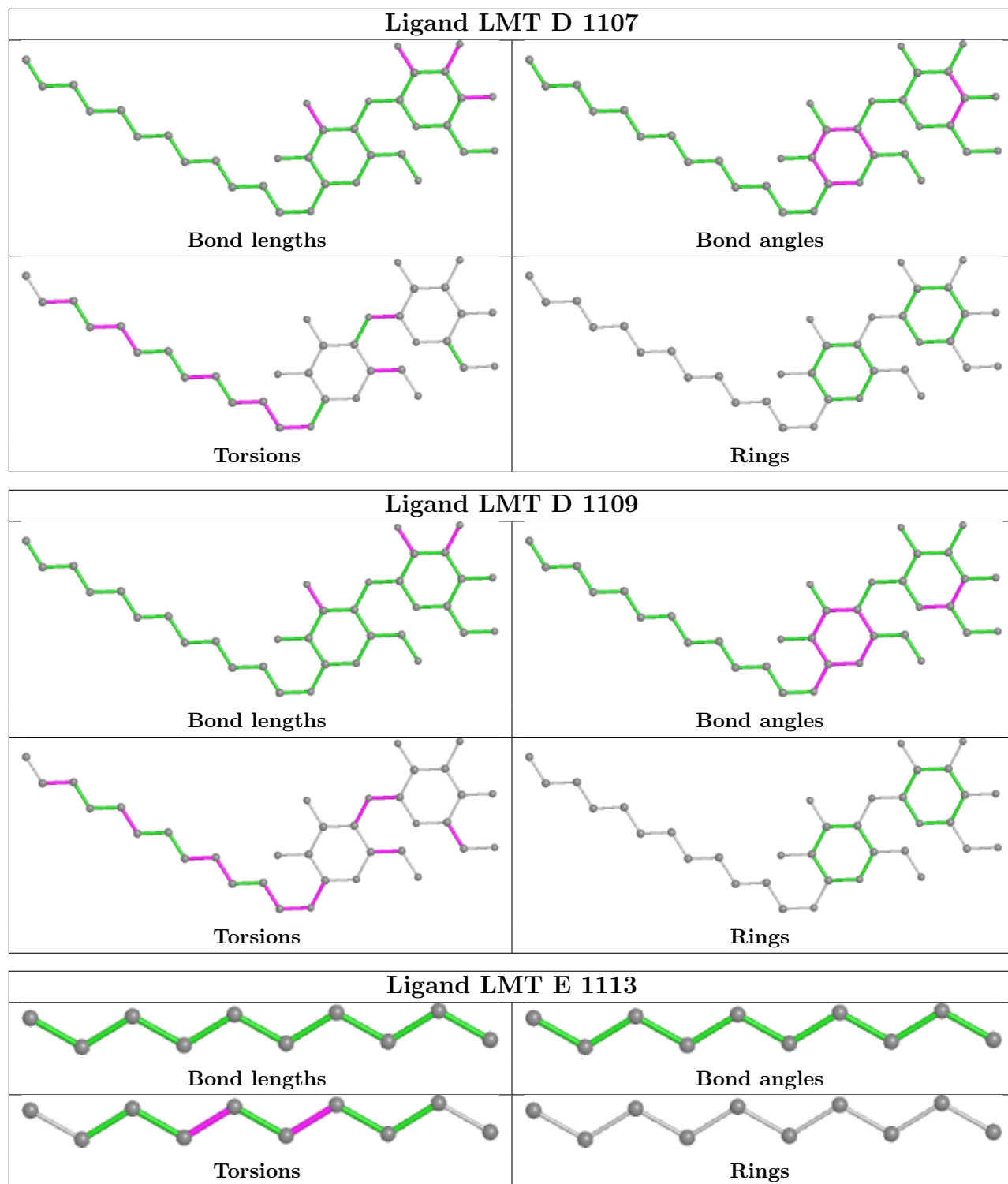
Ligand PTY C 1113

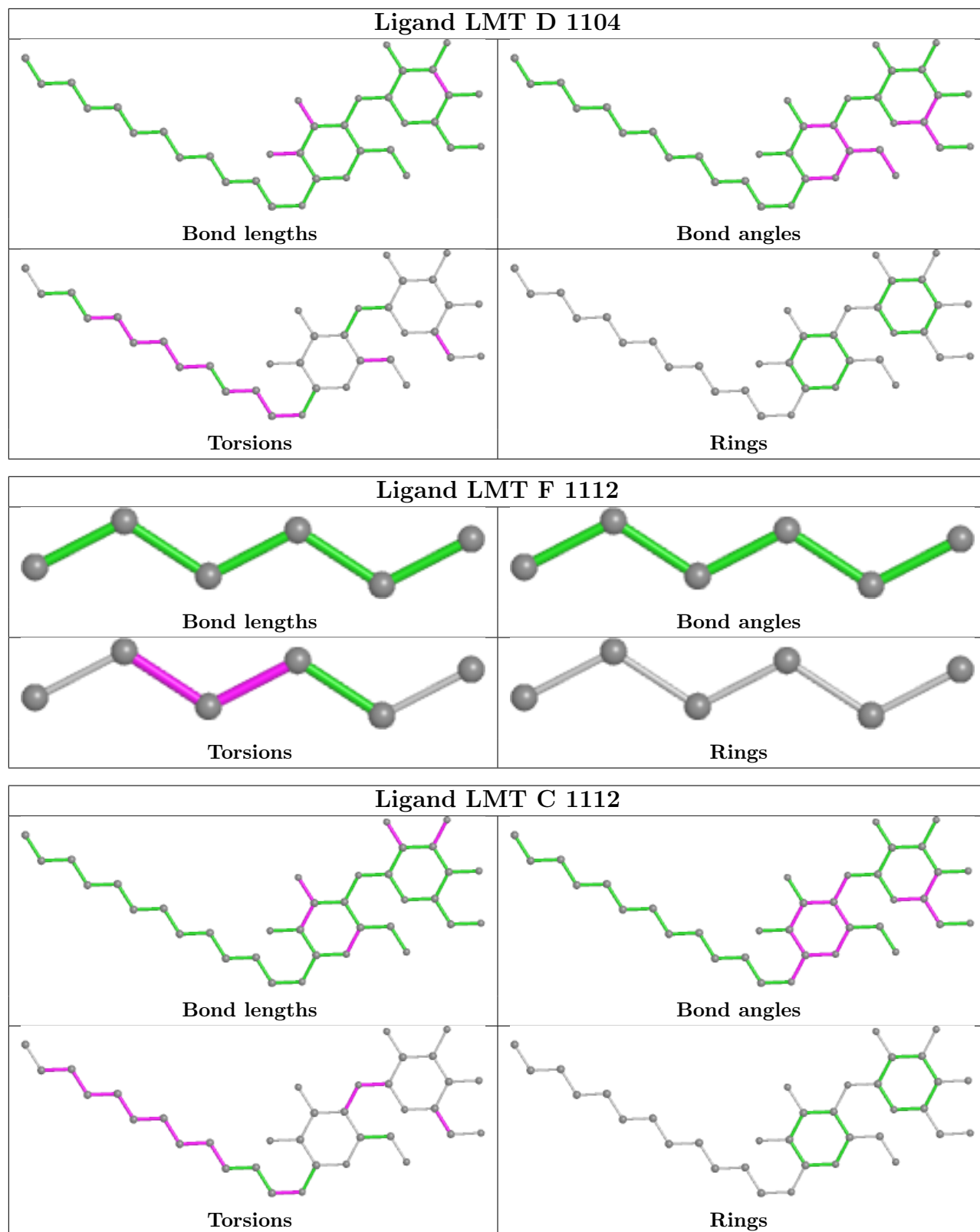


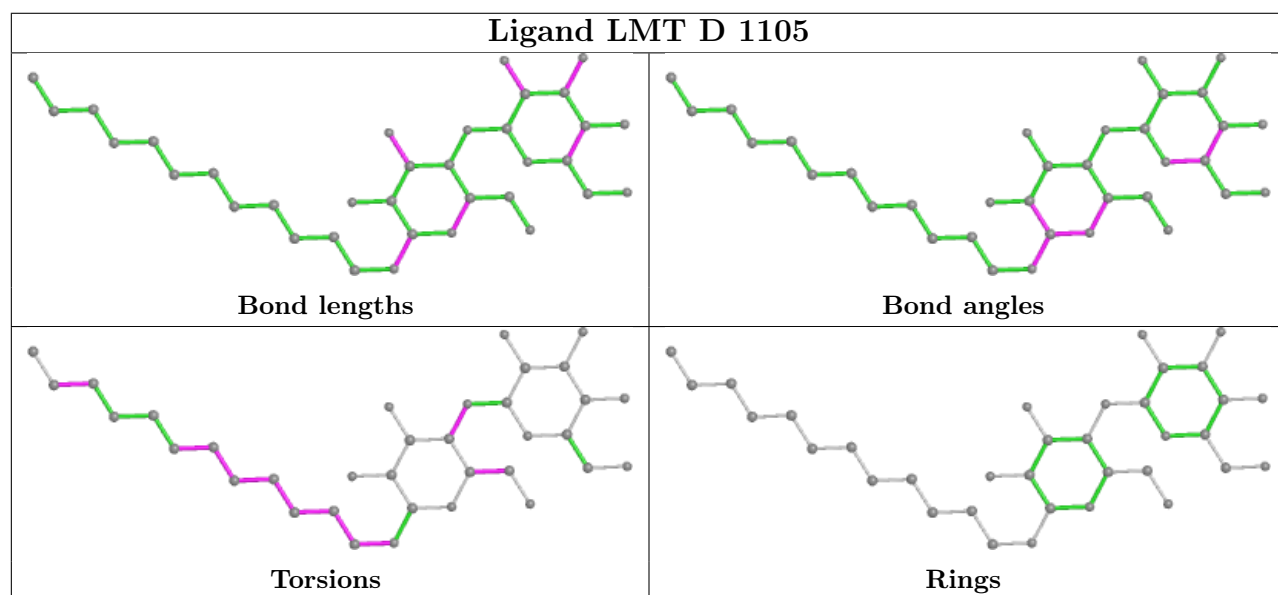
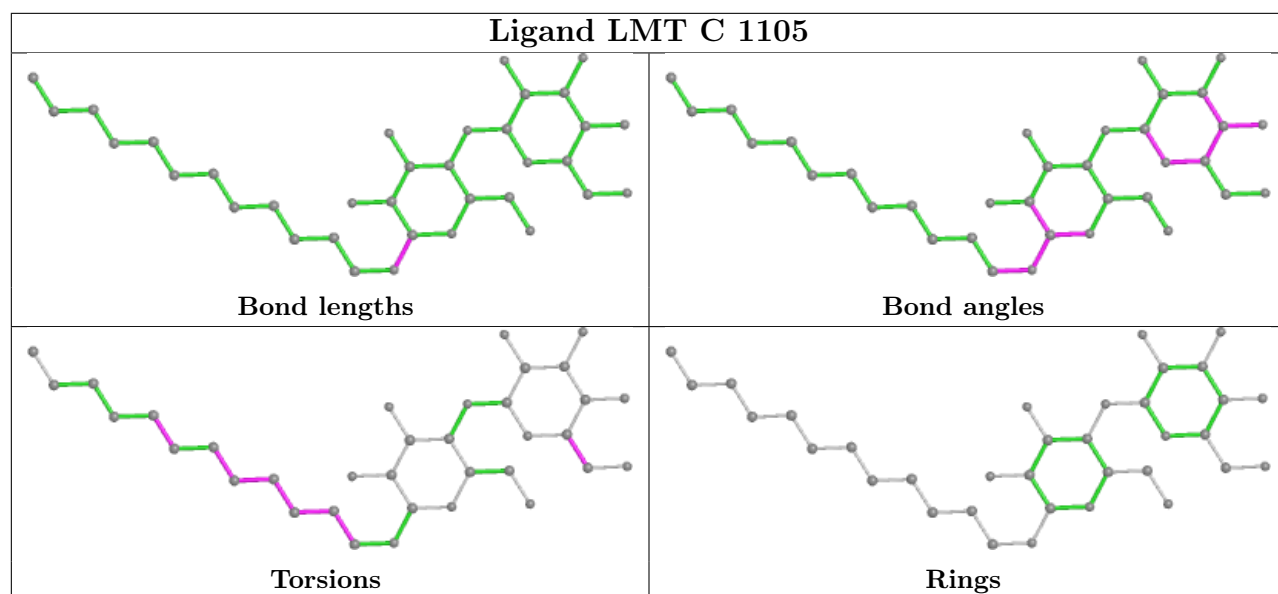
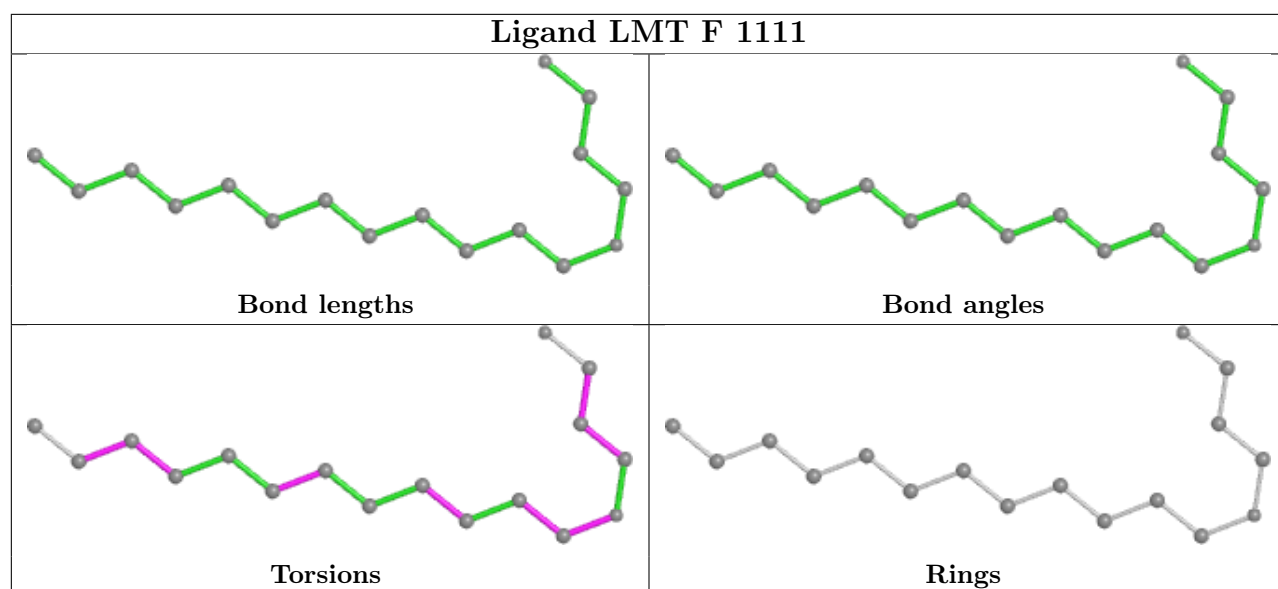
Ligand LMT F 1102

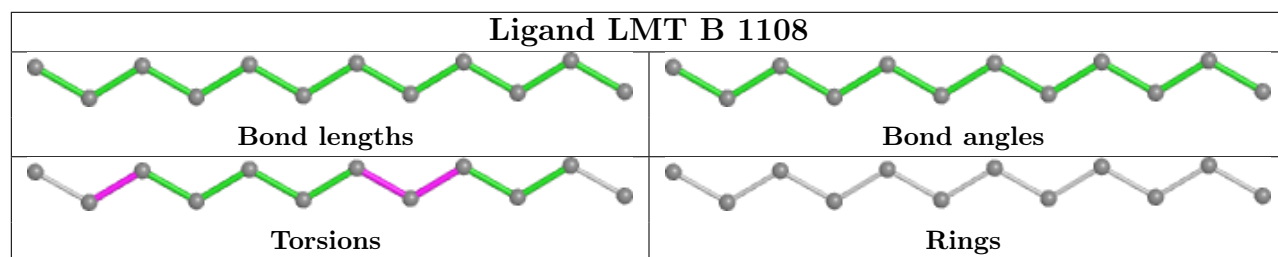
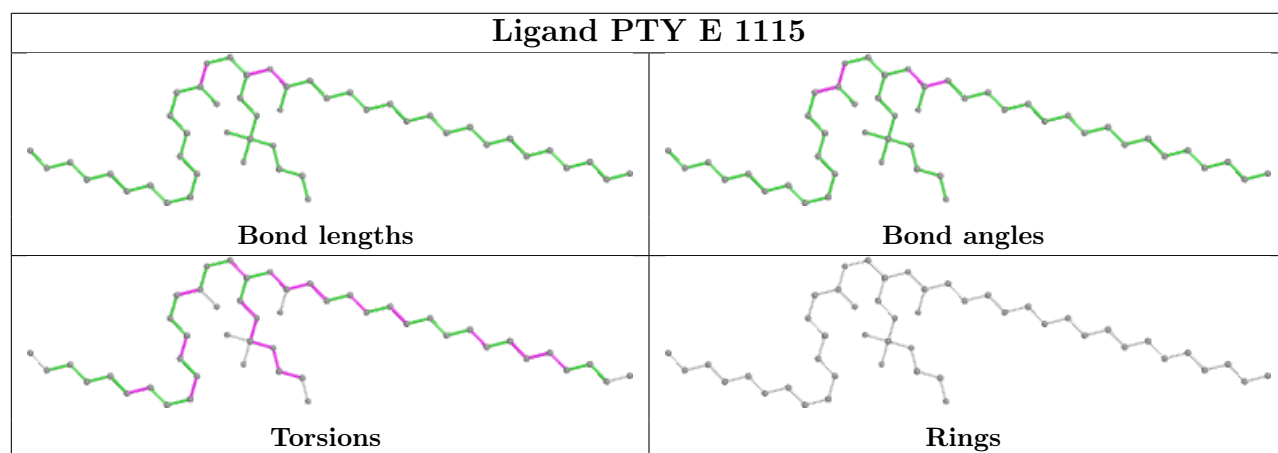
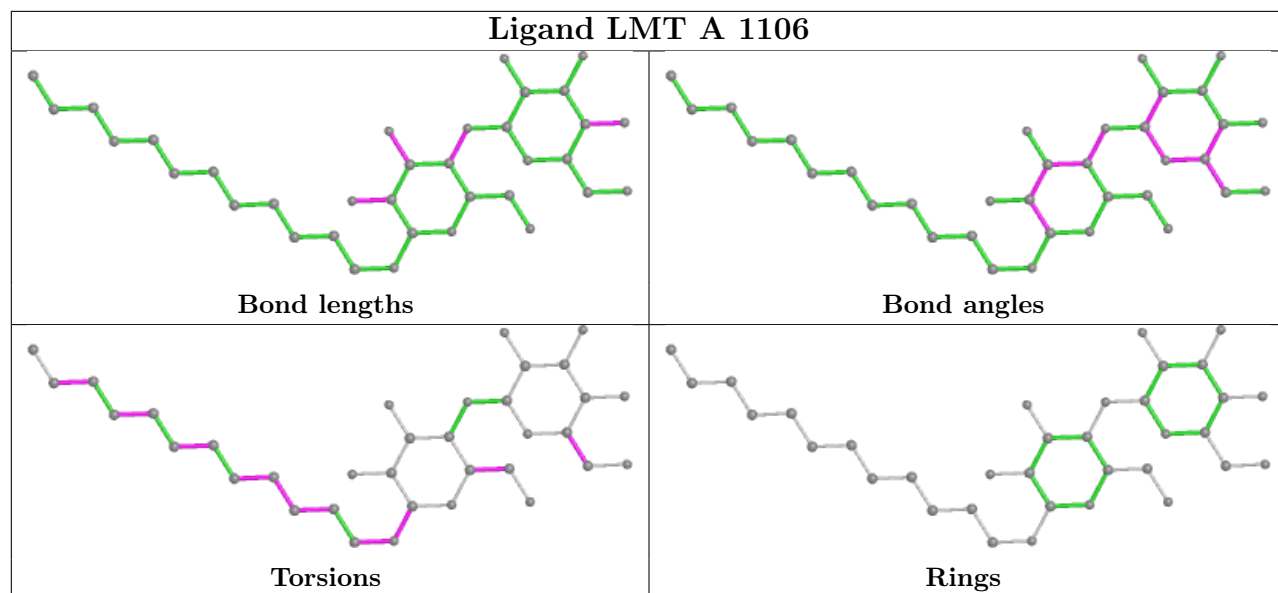


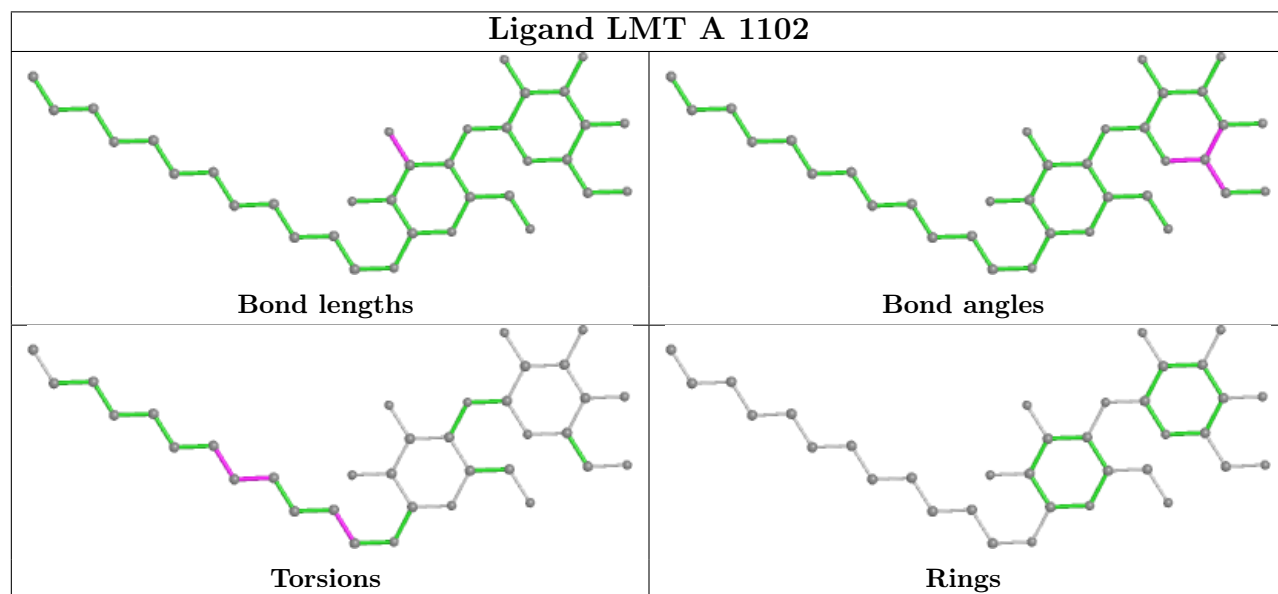
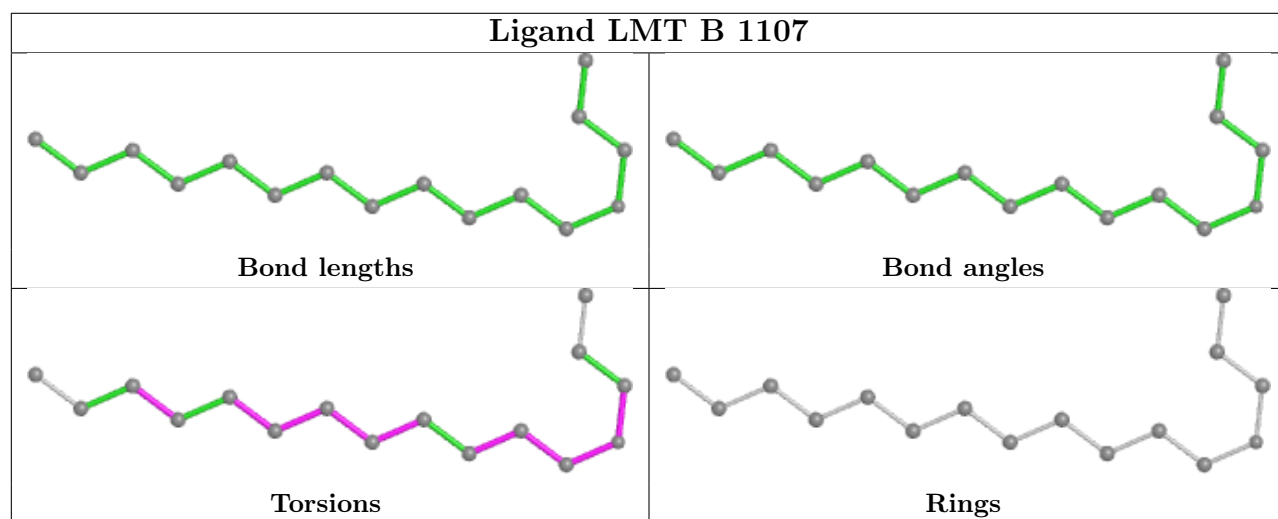
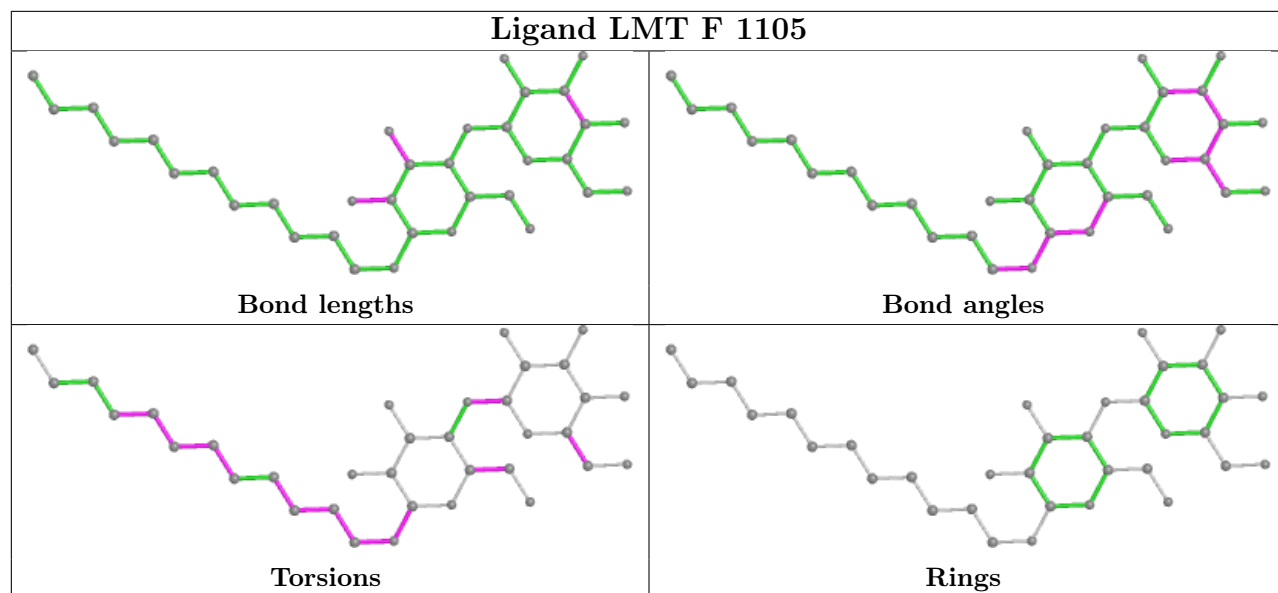


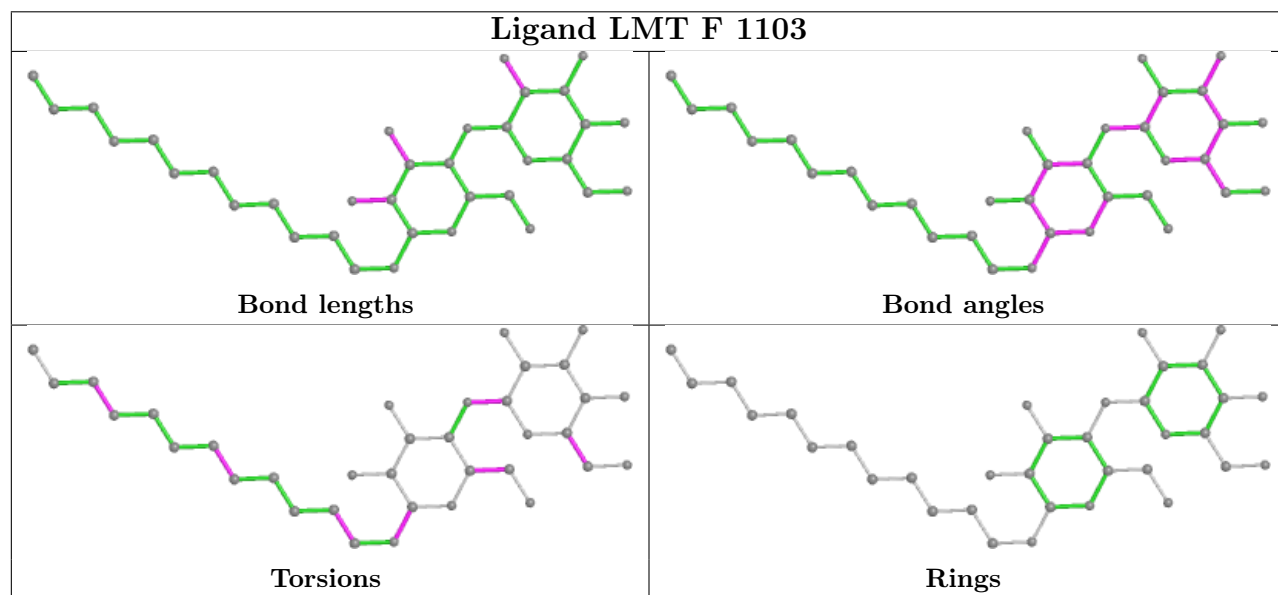
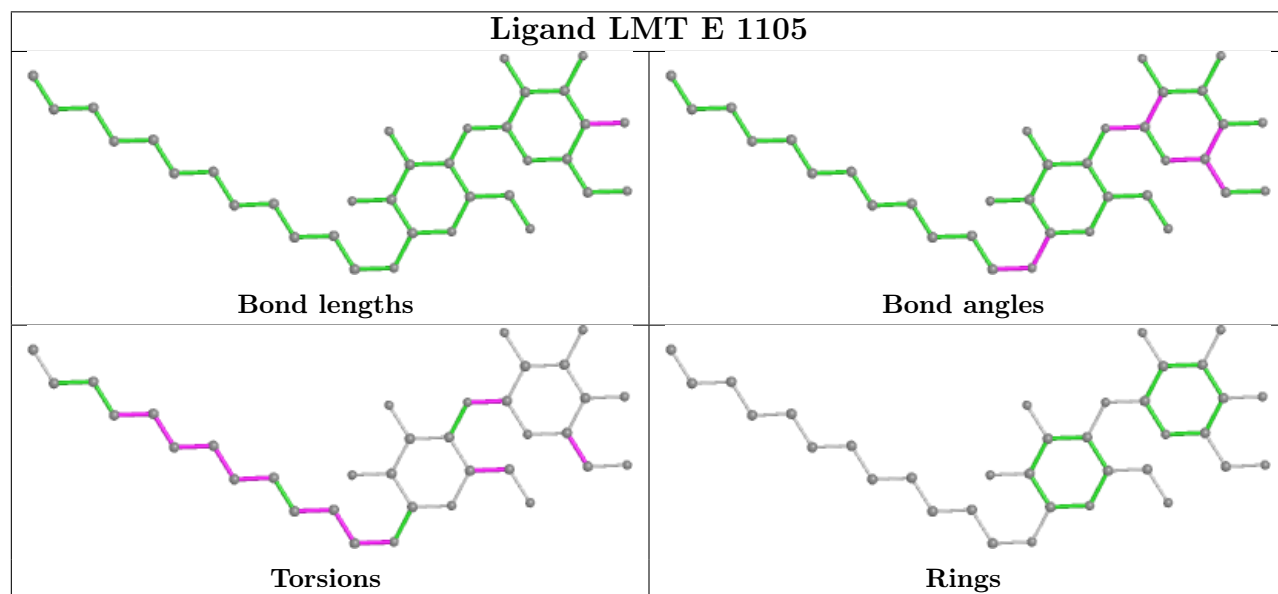
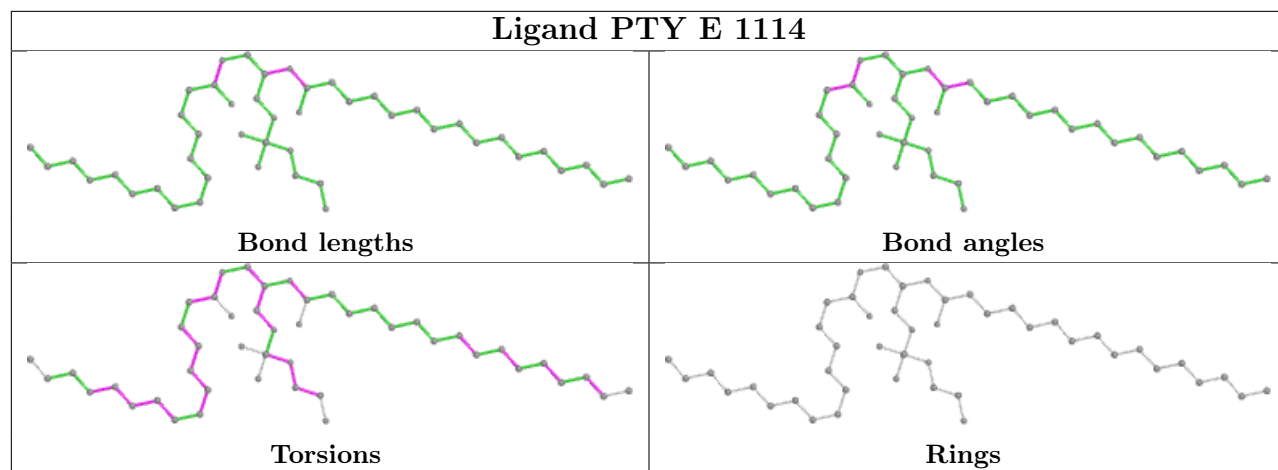












5.7 Other polymers [i](#)

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(Å²)	Q<0.9
1	A	1041/1042 (99%)	0.07	53 (5%)	28	26	25, 41, 70, 133	0
1	B	1042/1042 (100%)	0.22	83 (7%)	12	12	28, 49, 79, 162	0
1	C	1041/1042 (99%)	-0.04	50 (4%)	30	29	26, 41, 64, 127	0
1	D	1040/1042 (99%)	0.29	106 (10%)	6	6	28, 47, 90, 140	0
1	E	1039/1042 (99%)	0.05	48 (4%)	32	31	27, 41, 69, 148	0
1	F	1040/1042 (99%)	0.10	57 (5%)	25	24	27, 45, 71, 138	0
All	All	6243/6252 (99%)	0.12	397 (6%)	19	18	25, 44, 78, 162	0

All (397) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	504	ALA	10.8
1	B	517	PHE	10.0
1	A	999	GLY	9.8
1	B	1041	ARG	9.8
1	F	643	ASP	9.6
1	B	511	ARG	9.4
1	A	1041	ARG	9.1
1	E	508	LEU	8.9
1	B	997	GLY	8.7
1	B	508	LEU	8.5
1	A	1040	ARG	8.1
1	B	516	LEU	8.0
1	D	997	GLY	7.3
1	C	1041	ARG	7.3
1	B	515	ARG	7.3
1	F	999	GLY	7.2
1	F	998	HIS	7.2
1	B	519	TRP	7.0
1	A	508	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	555	LEU	6.7
1	A	512	LEU	6.6
1	D	552	VAL	6.4
1	B	505	LYS	6.3
1	B	512	LEU	6.1
1	C	998	HIS	6.1
1	C	1040	ARG	6.1
1	B	503	GLY	6.1
1	D	511	ARG	6.1
1	F	508	LEU	6.0
1	B	1042	LYS	5.8
1	A	997	GLY	5.8
1	D	1040	ARG	5.7
1	D	516	LEU	5.7
1	D	508	LEU	5.5
1	E	555	LEU	5.5
1	E	515	ARG	5.5
1	B	513	ILE	5.5
1	A	505	LYS	5.4
1	D	505	LYS	5.4
1	B	564	PHE	5.4
1	D	548	ALA	5.4
1	F	512	LEU	5.2
1	E	993	PRO	5.1
1	A	511	ARG	5.1
1	D	1039	THR	5.0
1	B	566	VAL	4.9
1	B	504	ALA	4.8
1	A	515	ARG	4.8
1	C	995	ILE	4.7
1	B	127	LEU	4.7
1	D	996	LEU	4.7
1	A	258	GLN	4.7
1	A	257	ALA	4.6
1	D	998	HIS	4.6
1	B	502	HIS	4.6
1	D	507	ASP	4.5
1	F	511	ARG	4.5
1	D	544	GLY	4.5
1	B	514	ASP	4.5
1	F	742	ALA	4.5
1	D	512	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	510	THR	4.5
1	D	995	ILE	4.5
1	D	543	LEU	4.5
1	F	127	LEU	4.4
1	C	554	LEU	4.4
1	F	1000	ALA	4.3
1	B	148	ASN	4.3
1	A	519	TRP	4.3
1	C	258	GLN	4.3
1	D	529	LEU	4.2
1	A	516	LEU	4.2
1	C	550	PHE	4.2
1	E	803	VAL	4.2
1	F	1037	LEU	4.1
1	B	876	GLY	4.1
1	E	995	ILE	4.1
1	C	1037	LEU	4.0
1	F	564	PHE	4.0
1	C	515	ARG	4.0
1	A	260	GLY	4.0
1	A	998	HIS	4.0
1	F	1039	THR	4.0
1	F	1002	ALA	4.0
1	D	550	PHE	4.0
1	D	114	ALA	4.0
1	D	844	GLN	3.9
1	E	996	LEU	3.9
1	F	91	VAL	3.9
1	A	517	PHE	3.8
1	C	997	GLY	3.8
1	D	970	LEU	3.8
1	A	993	PRO	3.8
1	E	511	ARG	3.8
1	E	504	ALA	3.8
1	A	555	LEU	3.8
1	F	10	ARG	3.8
1	B	562	VAL	3.8
1	D	116	ALA	3.8
1	B	1040	ARG	3.8
1	B	527	PHE	3.8
1	B	548	ALA	3.8
1	F	515	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	512	LEU	3.7
1	D	258	GLN	3.7
1	D	1037	LEU	3.7
1	D	566	VAL	3.7
1	D	564	PHE	3.7
1	D	713	GLN	3.7
1	C	257	ALA	3.7
1	C	519	TRP	3.7
1	E	512	LEU	3.7
1	E	517	PHE	3.7
1	B	996	LEU	3.6
1	F	517	PHE	3.6
1	D	923	TRP	3.6
1	F	642	PHE	3.6
1	B	565	LYS	3.6
1	C	517	PHE	3.6
1	D	517	PHE	3.6
1	E	519	TRP	3.6
1	D	680	GLY	3.6
1	C	116	ALA	3.6
1	D	501	PRO	3.6
1	D	524	PHE	3.6
1	D	428	ALA	3.6
1	F	505	LYS	3.6
1	D	559	ALA	3.5
1	D	562	VAL	3.5
1	F	1040	ARG	3.5
1	E	999	GLY	3.5
1	C	120	LEU	3.5
1	F	497	LEU	3.5
1	E	506	LYS	3.5
1	D	551	ALA	3.5
1	B	1039	THR	3.5
1	D	519	TRP	3.5
1	D	515	ARG	3.5
1	E	505	LYS	3.5
1	C	683	SER	3.5
1	C	999	GLY	3.4
1	A	1000	ALA	3.4
1	B	91	VAL	3.4
1	C	508	LEU	3.4
1	F	555	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	524	PHE	3.4
1	F	876	GLY	3.4
1	F	683	SER	3.4
1	F	516	LEU	3.4
1	B	322	GLU	3.4
1	D	124	VAL	3.4
1	D	924	LEU	3.4
1	D	854	LYS	3.4
1	C	511	ARG	3.4
1	B	90	LEU	3.4
1	D	120	LEU	3.3
1	A	514	ASP	3.3
1	C	118	ALA	3.3
1	C	681	GLN	3.3
1	C	516	LEU	3.3
1	E	262	LEU	3.3
1	D	683	SER	3.3
1	F	570	GLY	3.3
1	E	516	LEU	3.3
1	E	258	GLN	3.3
1	B	507	ASP	3.2
1	D	502	HIS	3.2
1	B	129	ILE	3.2
1	B	742	ALA	3.2
1	D	118	ALA	3.2
1	C	680	GLY	3.2
1	D	876	GLY	3.2
1	D	260	GLY	3.2
1	D	526	ARG	3.2
1	B	923	TRP	3.2
1	A	506	LYS	3.2
1	E	998	HIS	3.2
1	E	667	PHE	3.2
1	A	995	ILE	3.2
1	B	509	PRO	3.1
1	D	859	ASN	3.1
1	D	682	GLY	3.1
1	E	565	LYS	3.1
1	E	259	ASP	3.1
1	F	318	THR	3.1
1	B	563	MET	3.1
1	D	860	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	1007	VAL	3.1
1	B	522	ARG	3.1
1	D	259	ASP	3.0
1	D	549	VAL	3.0
1	D	127	LEU	3.0
1	F	996	LEU	3.0
1	C	114	ALA	3.0
1	D	554	LEU	3.0
1	F	129	ILE	3.0
1	A	565	LYS	3.0
1	E	801	GLU	3.0
1	B	47	VAL	3.0
1	A	1037	LEU	3.0
1	F	430	LEU	3.0
1	A	522	ARG	3.0
1	B	664	GLN	3.0
1	C	127	LEU	3.0
1	C	996	LEU	3.0
1	B	147	PRO	3.0
1	D	506	LYS	3.0
1	E	257	ALA	3.0
1	A	259	ASP	3.0
1	B	179	ILE	2.9
1	B	569	GLY	2.9
1	F	997	GLY	2.9
1	E	1039	THR	2.9
1	D	719	PHE	2.9
1	E	558	CYS	2.9
1	D	530	ARG	2.9
1	B	49	ALA	2.9
1	B	555	LEU	2.9
1	B	520	ILE	2.9
1	E	554	LEU	2.9
1	E	260	GLY	2.9
1	B	551	ALA	2.9
1	D	848	HIS	2.8
1	E	876	GLY	2.8
1	F	322	GLU	2.8
1	A	923	TRP	2.8
1	A	742	ALA	2.8
1	E	1002	ALA	2.8
1	B	172	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	858	PRO	2.8
1	D	539	VAL	2.8
1	D	427	LEU	2.8
1	B	501	PRO	2.8
1	A	558	CYS	2.8
1	B	124	VAL	2.8
1	A	799	GLN	2.8
1	A	510	THR	2.8
1	D	835	ALA	2.8
1	F	128	GLY	2.8
1	E	261	SER	2.8
1	D	5	ARG	2.7
1	F	323	ASP	2.7
1	B	128	GLY	2.7
1	A	803	VAL	2.7
1	F	90	LEU	2.7
1	F	718	HIS	2.7
1	C	113	VAL	2.7
1	A	801	GLU	2.7
1	B	298	PRO	2.7
1	C	524	PHE	2.7
1	A	681	GLN	2.7
1	C	63	VAL	2.7
1	D	1000	ALA	2.6
1	F	124	VAL	2.6
1	D	556	LEU	2.6
1	D	681	GLN	2.6
1	B	713	GLN	2.6
1	F	993	PRO	2.6
1	C	67	LEU	2.6
1	C	70	ALA	2.6
1	A	509	PRO	2.6
1	A	526	ARG	2.6
1	D	503	GLY	2.6
1	D	113	VAL	2.6
1	F	233	PHE	2.6
1	F	566	VAL	2.6
1	E	923	TRP	2.6
1	C	71	ILE	2.6
1	A	1012	VAL	2.6
1	A	262	LEU	2.5
1	E	799	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	951	ILE	2.5
1	D	528	PHE	2.5
1	E	551	ALA	2.5
1	C	121	PRO	2.5
1	D	718	HIS	2.5
1	D	925	THR	2.5
1	C	124	VAL	2.5
1	D	537	GLY	2.5
1	A	566	VAL	2.5
1	F	559	ALA	2.5
1	D	553	TYR	2.5
1	D	665	GLN	2.5
1	D	569	GLY	2.5
1	A	571	PHE	2.5
1	A	996	LEU	2.5
1	B	130	THR	2.5
1	F	89	VAL	2.4
1	D	714	THR	2.4
1	B	1037	LEU	2.4
1	C	1002	ALA	2.4
1	D	545	ARG	2.4
1	B	500	LYS	2.4
1	D	90	LEU	2.4
1	B	558	CYS	2.4
1	C	1039	THR	2.4
1	E	574	THR	2.4
1	A	1007	VAL	2.4
1	F	509	PRO	2.4
1	D	840	LEU	2.4
1	B	667	PHE	2.4
1	C	261	SER	2.4
1	A	507	ASP	2.4
1	D	874	THR	2.4
1	B	506	LYS	2.4
1	F	875	GLN	2.4
1	B	428	ALA	2.3
1	B	559	ALA	2.3
1	F	719	PHE	2.3
1	A	256	THR	2.3
1	B	89	VAL	2.3
1	F	120	LEU	2.3
1	C	564	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	565	LYS	2.3
1	E	545	ARG	2.3
1	B	549	VAL	2.3
1	B	1000	ALA	2.3
1	C	90	LEU	2.3
1	C	260	GLY	2.3
1	E	1037	LEU	2.3
1	D	664	GLN	2.3
1	F	923	TRP	2.3
1	D	847	THR	2.3
1	B	497	LEU	2.2
1	C	551	ALA	2.2
1	D	71	ILE	2.2
1	D	536	GLN	2.2
1	D	855	GLN	2.2
1	E	1003	GLU	2.2
1	F	713	GLN	2.2
1	E	125[A]	ARG	2.2
1	B	741	LYS	2.2
1	B	995	ILE	2.2
1	C	59	ILE	2.2
1	A	261	SER	2.2
1	A	667	PHE	2.2
1	D	1002	ALA	2.2
1	E	742	ALA	2.2
1	A	876	GLY	2.2
1	C	91	VAL	2.2
1	E	566	VAL	2.2
1	D	66	PRO	2.2
1	D	261	SER	2.2
1	F	739	LYS	2.2
1	D	875	GLN	2.2
1	F	563	MET	2.2
1	A	574	THR	2.2
1	B	48	ARG	2.2
1	B	311	ALA	2.2
1	D	1006	GLY	2.2
1	A	550	PHE	2.2
1	D	514	ASP	2.2
1	D	571	PHE	2.2
1	B	567	VAL	2.2
1	D	1038	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	962	GLY	2.1
1	E	1000	ALA	2.1
1	D	1025	PHE	2.1
1	E	550	PHE	2.1
1	D	993	PRO	2.1
1	B	545	ARG	2.1
1	A	1039	THR	2.1
1	B	877	ASN	2.1
1	C	259	ASP	2.1
1	E	682	GLY	2.1
1	B	550	PHE	2.1
1	B	323	ASP	2.1
1	B	518	GLY	2.1
1	F	230	GLU	2.1
1	A	504	ALA	2.1
1	C	262	LEU	2.1
1	F	880	LEU	2.1
1	B	59	ILE	2.1
1	E	118	ALA	2.1
1	A	247	GLU	2.1
1	D	509	PRO	2.1
1	F	130	THR	2.1
1	E	233	PHE	2.1
1	F	562	VAL	2.1
1	E	875	GLN	2.1
1	D	663	ILE	2.1
1	E	509	PRO	2.1
1	F	501	PRO	2.1
1	D	696	GLY	2.1
1	B	92	THR	2.0
1	B	63	VAL	2.0
1	B	83	VAL	2.0
1	D	1007	VAL	2.0
1	D	341	ARG	2.0
1	F	838	ARG	2.0
1	C	840	LEU	2.0
1	A	1004	VAL	2.0
1	D	429	PRO	2.0
1	D	560	ALA	2.0
1	B	67	LEU	2.0
1	C	718	HIS	2.0
1	C	558	CYS	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 monosaccharides 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(\AA^2)	Q<0.9
2	LMT	D	1109	35/35	0.42	0.46	44,115,139,147	0
2	LMT	B	1110	35/35	0.50	0.27	62,113,136,137	0
3	PTY	E	1114	46/50	0.52	0.30	55,97,189,204	0
3	PTY	E	1115	48/50	0.53	0.22	54,74,118,138	0
2	LMT	D	1112	35/35	0.56	0.28	79,121,148,149	0
2	LMT	E	1112	35/35	0.56	0.34	66,112,138,141	0
2	LMT	E	1106	35/35	0.57	0.24	68,111,129,133	0
2	LMT	F	1111	17/35	0.57	0.28	72,80,94,95	0
2	LMT	A	1107	35/35	0.58	0.27	60,99,140,143	0
3	PTY	D	1113	48/50	0.59	0.26	48,76,120,141	0
2	LMT	D	1107	35/35	0.59	0.36	59,120,136,144	0
2	LMT	E	1110	35/35	0.59	0.24	48,86,109,114	0
3	PTY	B	1111	46/50	0.60	0.21	60,99,142,152	0
2	LMT	B	1109	35/35	0.60	0.22	54,105,138,139	0
2	LMT	D	1104	35/35	0.61	0.21	47,79,92,97	0
2	LMT	D	1105	35/35	0.61	0.25	76,103,126,126	0
2	LMT	F	1109	35/35	0.61	0.33	63,86,108,114	0
2	LMT	A	1101	35/35	0.61	0.30	91,113,132,139	0
3	PTY	F	1115	48/50	0.61	0.23	59,81,130,148	0
2	LMT	F	1110	35/35	0.62	0.26	43,94,127,131	0
2	LMT	C	1112	35/35	0.63	0.27	40,83,119,121	0
4	GOL	A	1119	6/6	0.65	0.23	51,60,65,67	0
2	LMT	A	1109	35/35	0.66	0.22	51,90,113,119	0
4	GOL	D	1117	6/6	0.66	0.29	64,68,75,80	0
4	GOL	E	1121	6/6	0.67	0.24	46,54,62,66	0
2	LMT	D	1108	35/35	0.68	0.19	53,96,120,122	0
2	LMT	F	1103	35/35	0.68	0.22	53,78,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PTY	C	1113	48/50	0.68	0.22	51,73,124,141	0
3	PTY	F	1114	37/50	0.68	0.26	71,94,129,133	0
2	LMT	C	1110	35/35	0.69	0.28	56,85,114,116	0
2	LMT	E	1109	35/35	0.69	0.19	62,93,134,135	0
2	LMT	F	1106	35/35	0.69	0.17	57,91,116,118	0
2	LMT	C	1108	35/35	0.69	0.19	46,66,86,89	0
2	LMT	B	1107	16/35	0.70	0.29	69,81,88,89	0
2	LMT	E	1108	35/35	0.70	0.28	53,94,113,116	0
2	LMT	A	1110	25/35	0.70	0.22	48,77,121,134	0
2	LMT	D	1103	35/35	0.70	0.21	37,76,101,113	0
3	PTY	B	1112	48/50	0.71	0.21	59,81,120,130	0
4	GOL	E	1116	6/6	0.71	0.17	53,58,64,65	0
3	PTY	A	1112	46/50	0.71	0.32	58,88,154,171	0
2	LMT	D	1106	35/35	0.72	0.30	55,85,115,117	0
2	LMT	B	1101	35/35	0.72	0.28	80,104,131,137	0
2	LMT	C	1111	35/35	0.72	0.21	47,90,103,106	0
4	GOL	A	1113	6/6	0.72	0.29	55,60,69,73	0
4	GOL	E	1123	6/6	0.72	0.18	57,64,71,72	0
2	LMT	A	1108	34/35	0.73	0.25	46,85,98,103	0
2	LMT	E	1105	35/35	0.74	0.18	55,72,82,98	0
2	LMT	B	1105	35/35	0.74	0.19	53,70,80,87	0
2	LMT	C	1109	35/35	0.75	0.16	65,95,111,112	0
2	LMT	C	1101	35/35	0.75	0.24	55,96,143,149	0
2	LMT	F	1107	35/35	0.75	0.18	66,105,157,159	0
2	LMT	C	1107	35/35	0.76	0.21	34,63,80,82	0
2	LMT	A	1105	35/35	0.76	0.19	52,71,83,104	0
2	LMT	E	1104	35/35	0.76	0.20	32,64,79,84	0
4	GOL	A	1114	6/6	0.77	0.23	52,54,63,78	0
2	LMT	E	1113	10/35	0.78	0.18	71,76,79,80	0
4	GOL	B	1114	6/6	0.78	0.11	78,82,86,91	0
4	GOL	E	1119	6/6	0.78	0.36	49,50,59,67	0
4	GOL	C	1115	6/6	0.78	0.23	45,63,66,67	0
4	GOL	D	1115	6/6	0.78	0.16	59,63,67,76	0
2	LMT	E	1102	35/35	0.79	0.21	54,77,104,114	0
2	LMT	E	1111	12/35	0.79	0.23	62,72,75,75	0
2	LMT	A	1106	35/35	0.79	0.24	61,82,112,119	0
4	GOL	F	1116	6/6	0.79	0.17	47,55,68,75	0
2	LMT	B	1106	35/35	0.80	0.19	65,94,134,136	0
4	GOL	A	1116	6/6	0.80	0.16	55,69,72,72	0
2	LMT	E	1107	35/35	0.80	0.24	54,86,114,115	0
2	LMT	B	1102	35/35	0.80	0.16	40,67,83,89	0
2	LMT	C	1106	35/35	0.81	0.16	43,83,104,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LMT	A	1111	35/35	0.81	0.21	40,63,77,82	0
4	GOL	F	1117	6/6	0.81	0.24	49,58,67,67	0
4	GOL	A	1115	6/6	0.82	0.22	49,55,61,65	0
2	LMT	D	1111	35/35	0.82	0.17	59,86,115,125	0
4	GOL	E	1118	6/6	0.82	0.18	51,66,72,80	0
2	LMT	A	1102	35/35	0.82	0.17	45,58,75,79	0
4	GOL	C	1119	6/6	0.83	0.13	50,56,59,68	0
2	LMT	D	1101	35/35	0.83	0.18	59,82,96,101	0
2	LMT	D	1102	35/35	0.83	0.25	55,65,77,84	0
2	LMT	F	1105	35/35	0.83	0.18	53,70,90,94	0
2	LMT	A	1104	35/35	0.83	0.16	32,58,66,67	0
4	GOL	E	1122	6/6	0.84	0.15	44,49,53,60	0
4	GOL	A	1117	6/6	0.84	0.10	62,69,71,72	0
4	GOL	C	1120	6/6	0.85	0.12	50,57,65,67	0
2	LMT	A	1103	35/35	0.85	0.16	54,65,82,86	0
2	LMT	F	1113	35/35	0.85	0.20	51,83,101,103	0
2	LMT	E	1103	35/35	0.85	0.18	44,64,79,83	0
4	GOL	E	1117	6/6	0.85	0.14	69,78,84,90	0
2	LMT	F	1102	35/35	0.85	0.20	58,82,95,99	0
2	LMT	F	1104	35/35	0.86	0.14	40,57,69,72	0
2	LMT	C	1102	35/35	0.86	0.14	53,68,83,89	0
4	GOL	C	1116	6/6	0.87	0.39	52,70,71,74	0
2	LMT	E	1101	35/35	0.87	0.16	44,59,68,78	0
2	LMT	F	1112	6/35	0.87	0.15	62,66,68,71	0
4	GOL	A	1118	6/6	0.87	0.17	33,49,59,62	0
2	LMT	F	1108	13/35	0.87	0.23	52,58,86,89	0
2	LMT	B	1103	35/35	0.87	0.18	50,71,81,85	0
2	LMT	B	1108	12/35	0.87	0.18	59,68,84,84	0
4	GOL	F	1120	6/6	0.87	0.11	49,57,62,74	0
4	GOL	F	1118	6/6	0.88	0.41	63,67,75,79	0
2	LMT	B	1104	35/35	0.89	0.15	52,75,91,97	0
4	GOL	B	1113	6/6	0.89	0.14	81,87,87,92	0
4	GOL	E	1120	6/6	0.90	0.16	49,55,58,60	0
4	GOL	F	1119	6/6	0.90	0.17	37,52,53,66	0
2	LMT	F	1101	35/35	0.90	0.13	47,68,86,98	0
4	GOL	D	1116	6/6	0.91	0.07	54,59,62,63	0
2	LMT	C	1104	35/35	0.91	0.17	45,56,66,70	0
2	LMT	C	1103	35/35	0.91	0.16	55,69,78,87	0
2	LMT	C	1105	35/35	0.92	0.15	43,52,69,76	0
4	GOL	C	1117	6/6	0.92	0.18	43,54,60,75	0
4	GOL	A	1120	6/6	0.92	0.14	40,50,52,53	0
4	GOL	A	1121	6/6	0.92	0.26	61,66,75,77	0

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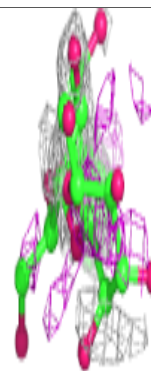
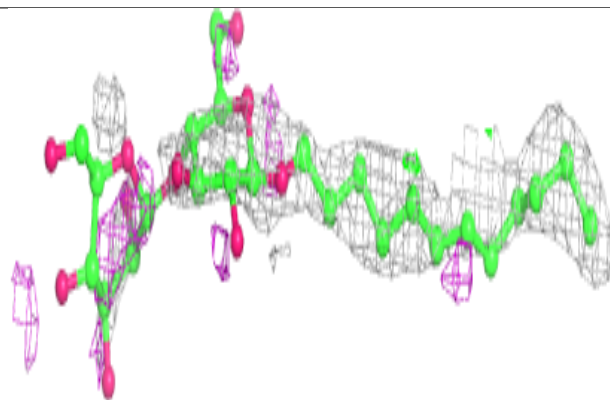
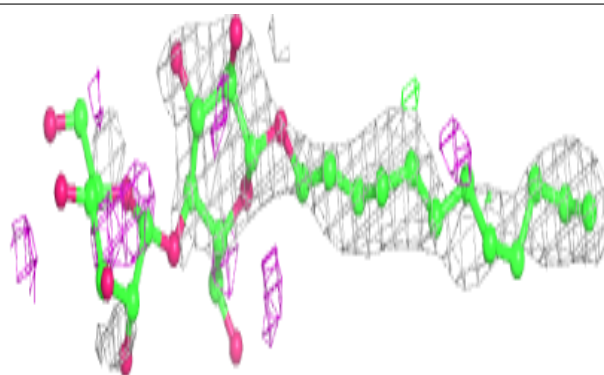
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	1115	6/6	0.93	0.13	44,48,58,60	0
2	LMT	D	1110	10/35	0.94	0.12	51,56,67,78	0
4	GOL	C	1118	6/6	0.94	0.26	45,58,62,69	0
4	GOL	C	1114	6/6	0.96	0.11	36,45,46,55	0
4	GOL	D	1114	6/6	0.96	0.10	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.

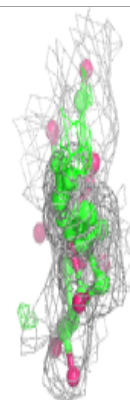
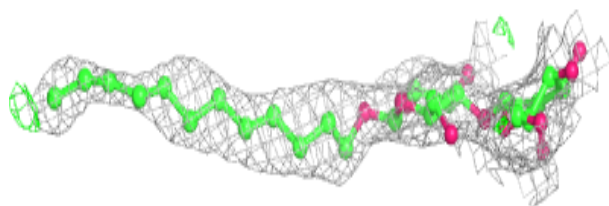
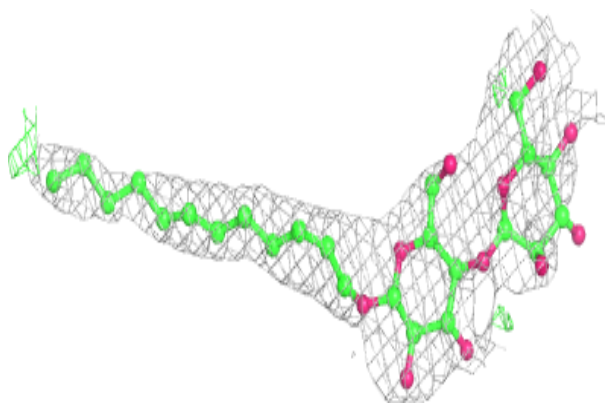
Electron density around LMT D 1109:

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

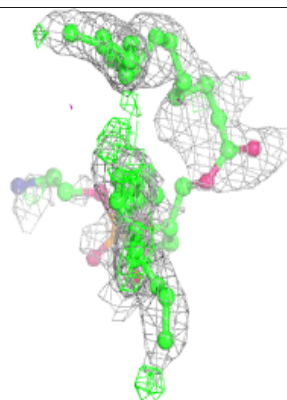
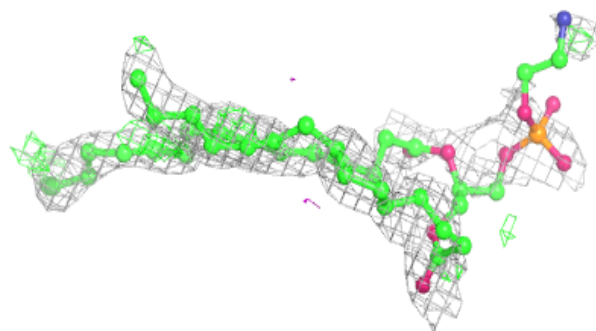
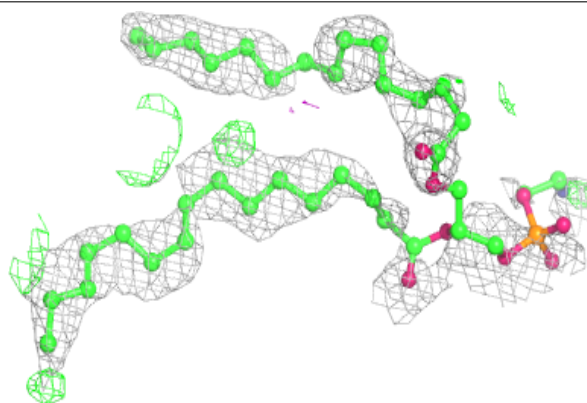


Electron density around LMT B 1110:

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

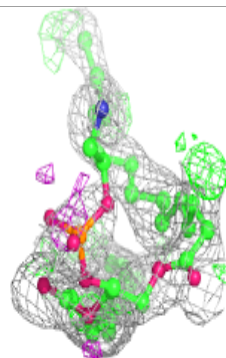
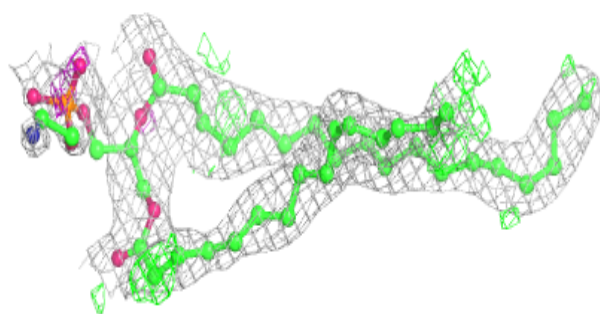
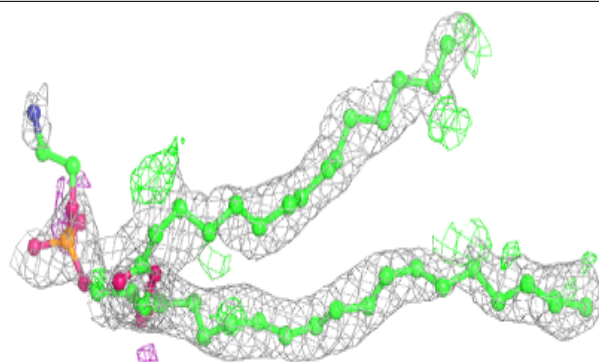
**Electron density around PTY E 1114:**

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

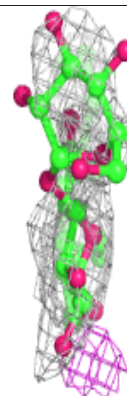
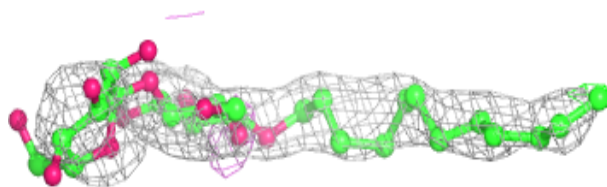
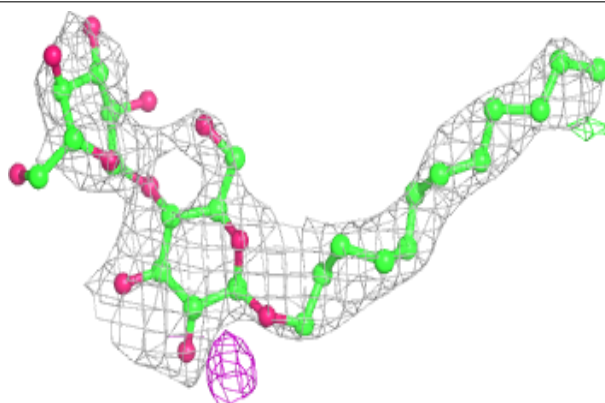


Electron density around PTY E 1115:

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

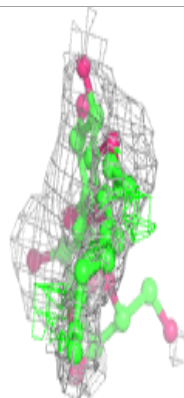
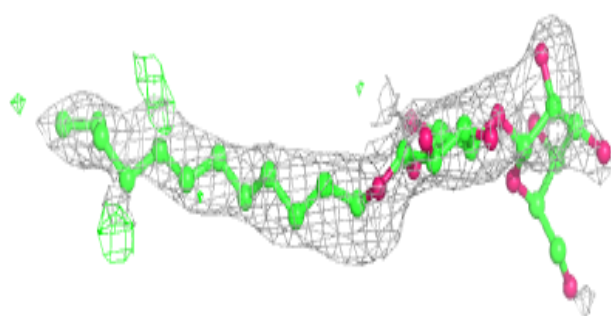
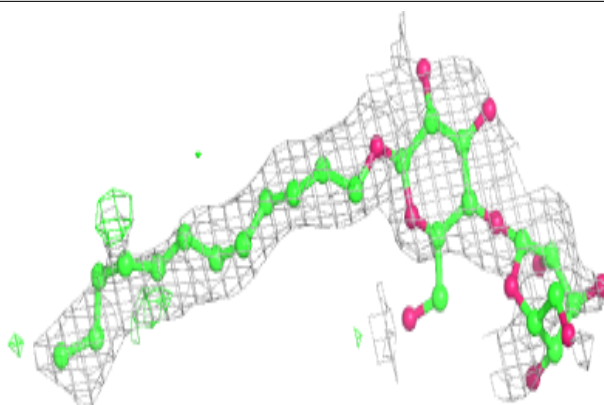
**Electron density around LMT D 1112:**

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

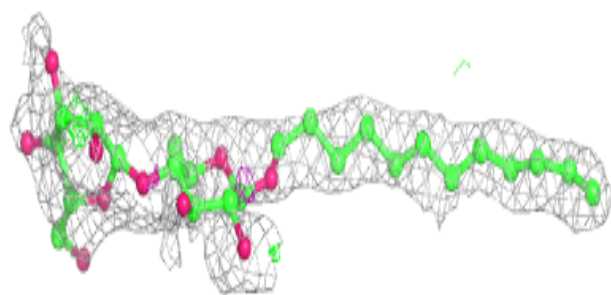
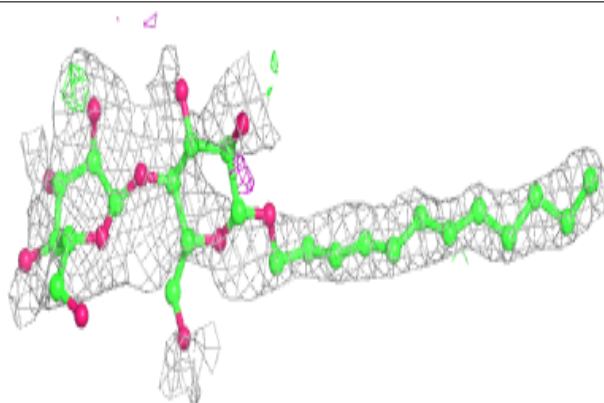


Electron density around LMT E 1112:

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

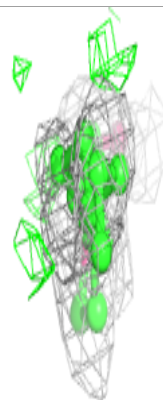
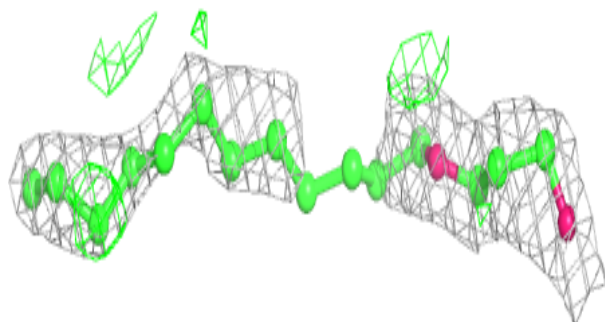
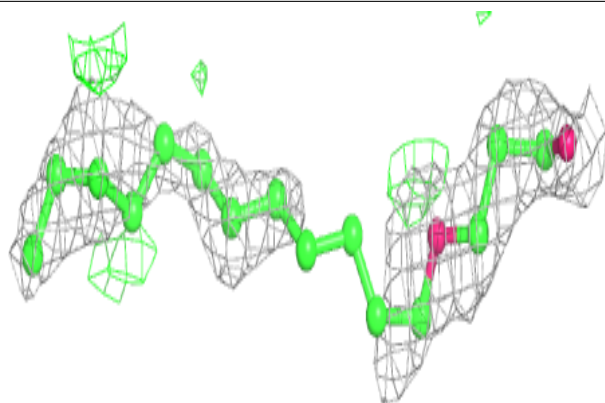
**Electron density around LMT E 1106:**

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

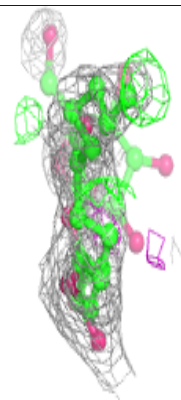
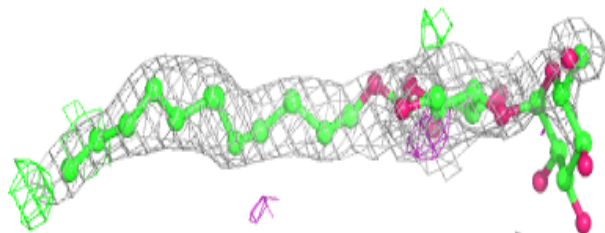
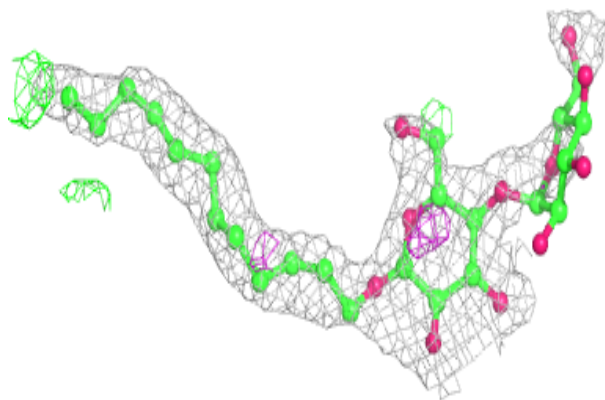


Electron density around LMT F 1111:

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

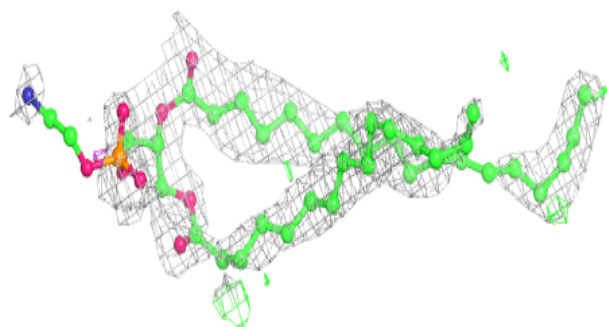
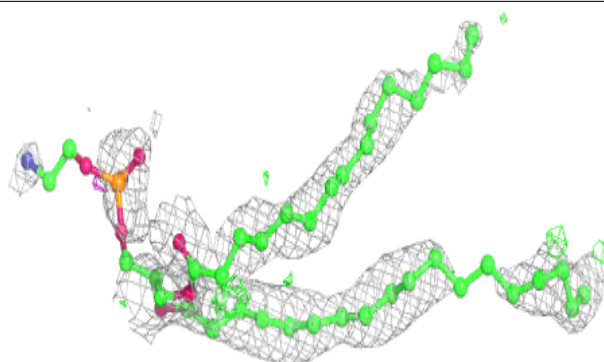
**Electron density around LMT A 1107:**

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

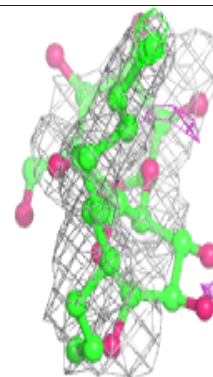
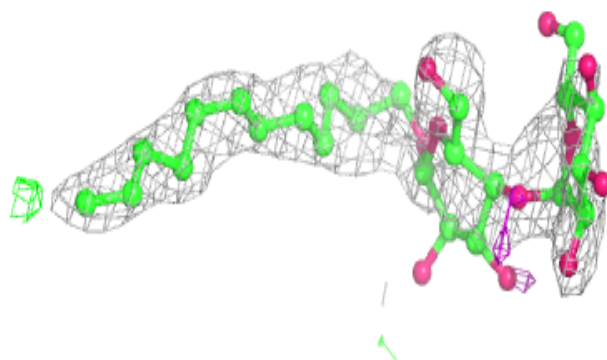
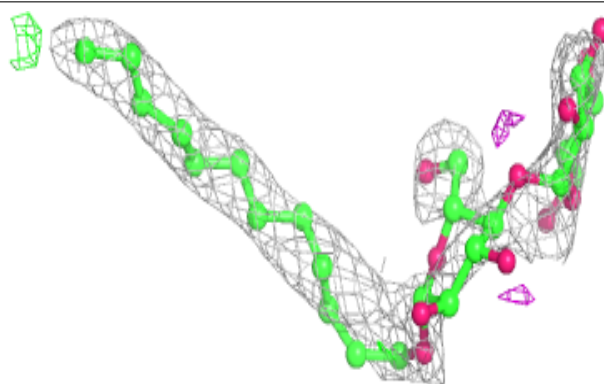


Electron density around PTY D 1113:

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

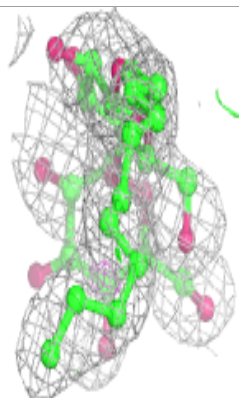
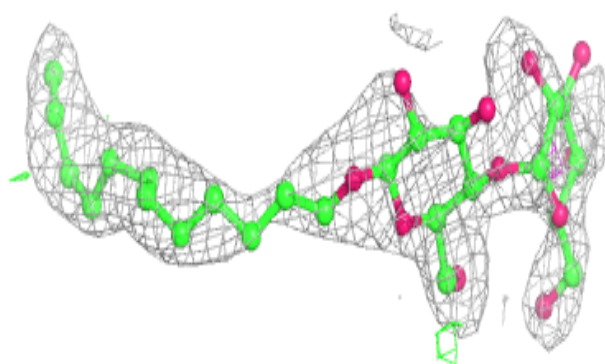
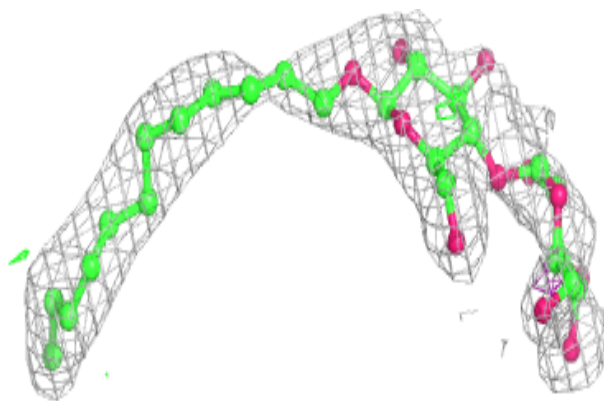
**Electron density around LMT D 1107:**

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

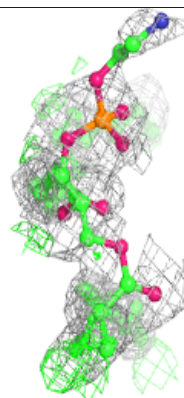
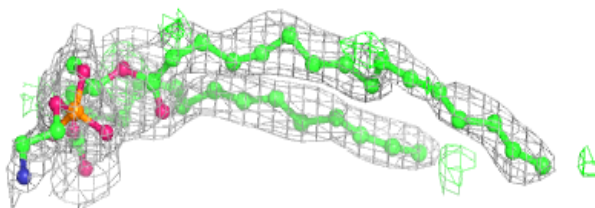
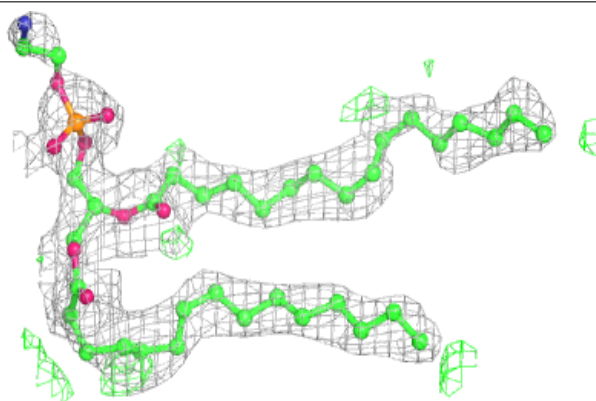


Electron density around LMT E 1110:

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

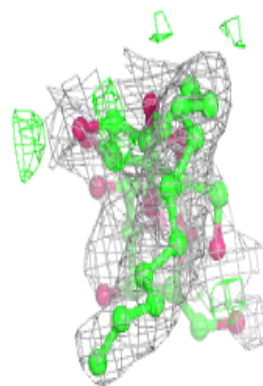
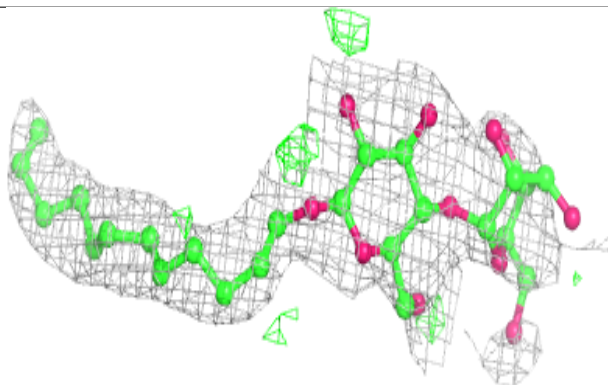
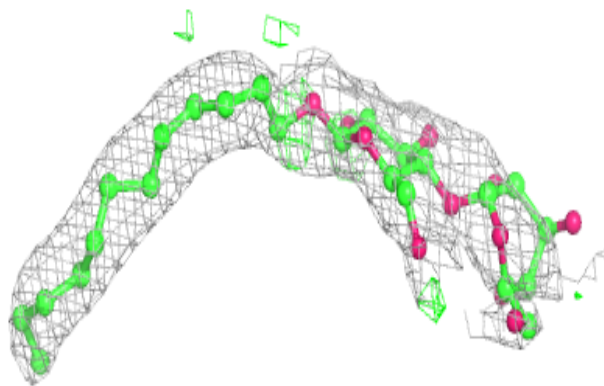
**Electron density around PTY B 1111:**

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



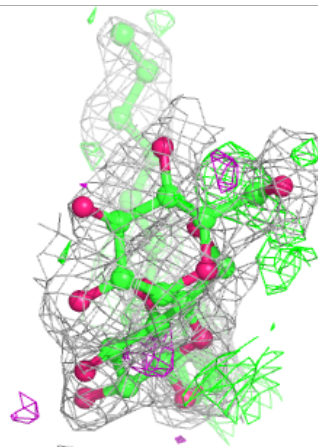
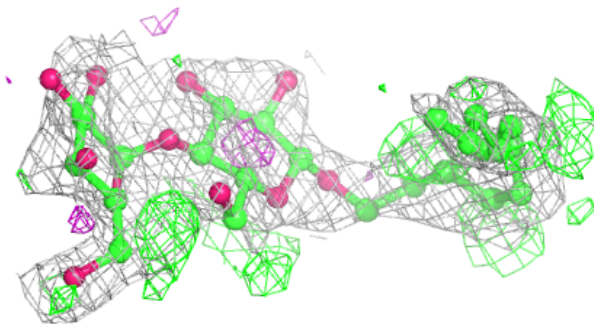
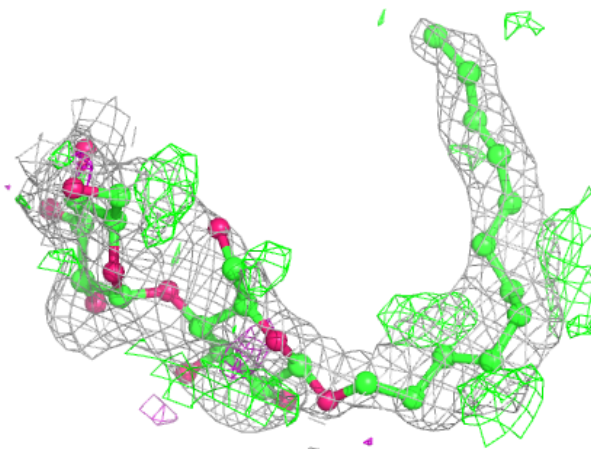
Electron density around LMT B 1109:

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



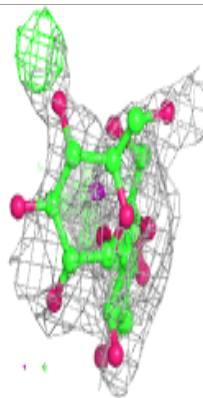
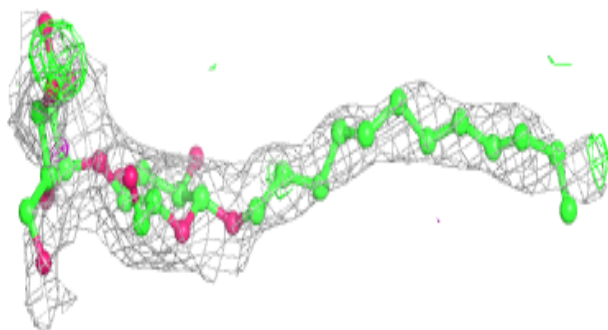
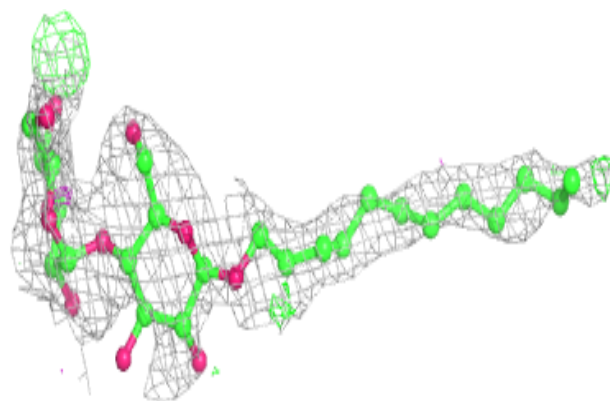
Electron density around LMT D 1104:

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

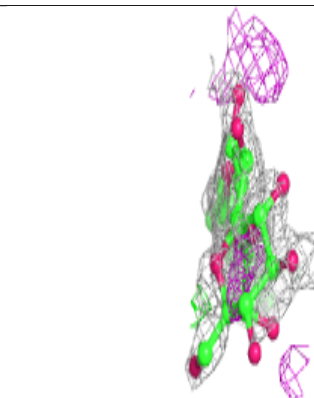
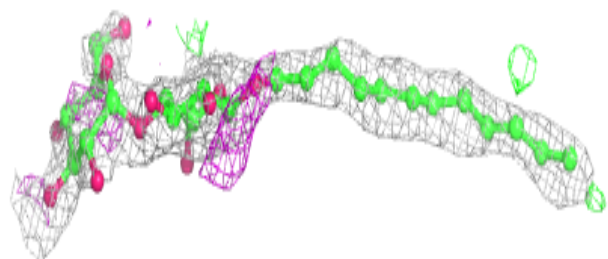
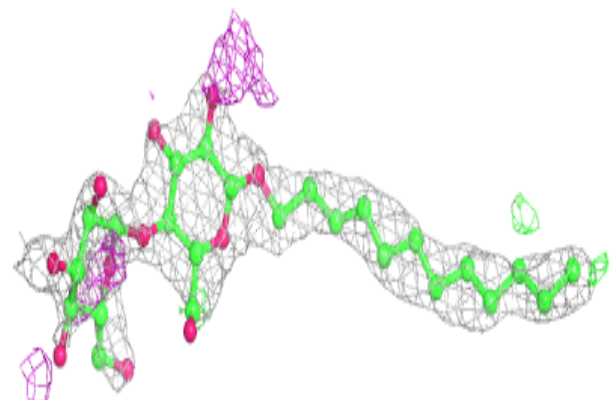


Electron density around LMT D 1105:

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

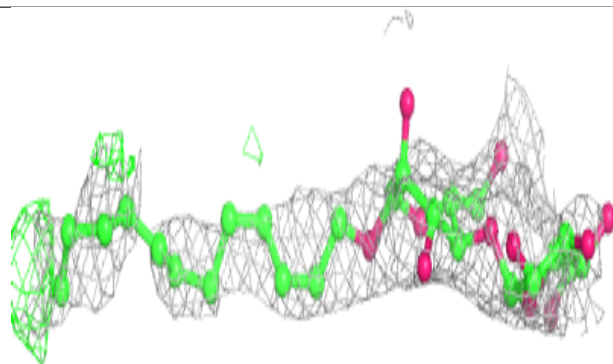
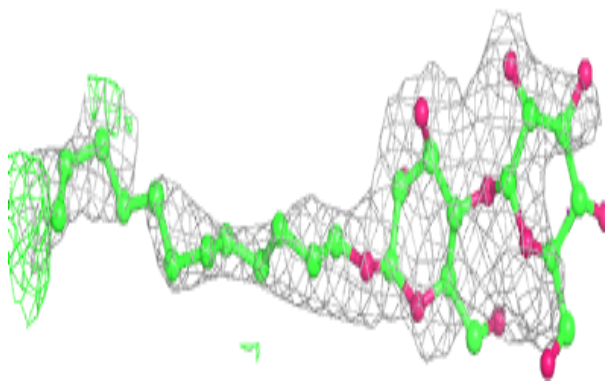
**Electron density around LMT F 1109:**

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

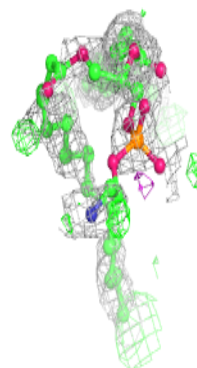
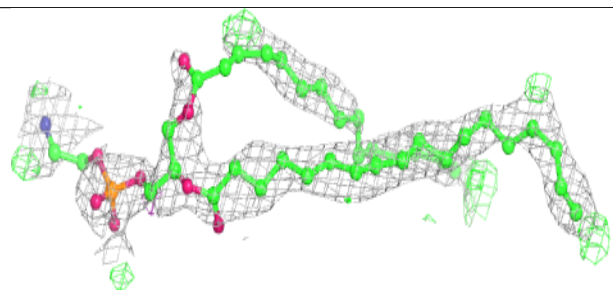
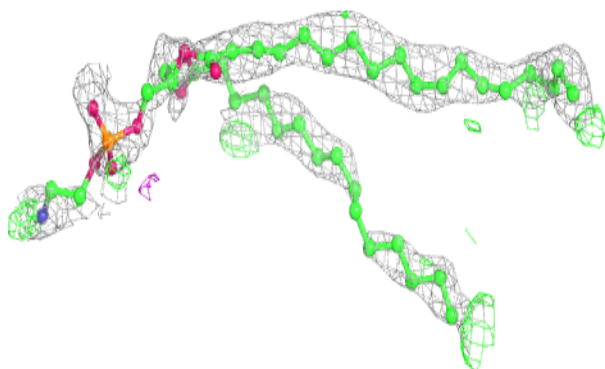


Electron density around LMT A 1101:

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

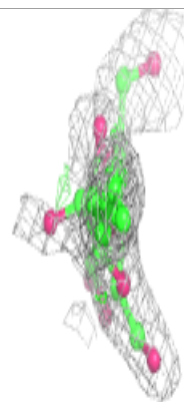
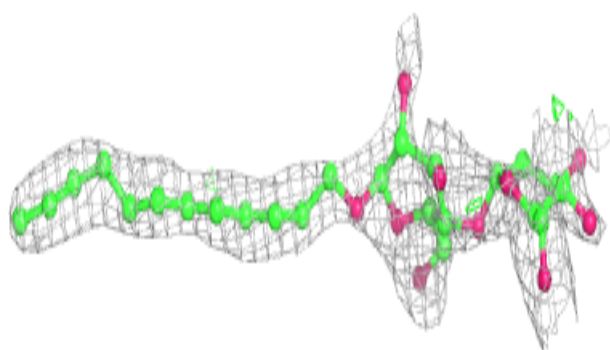
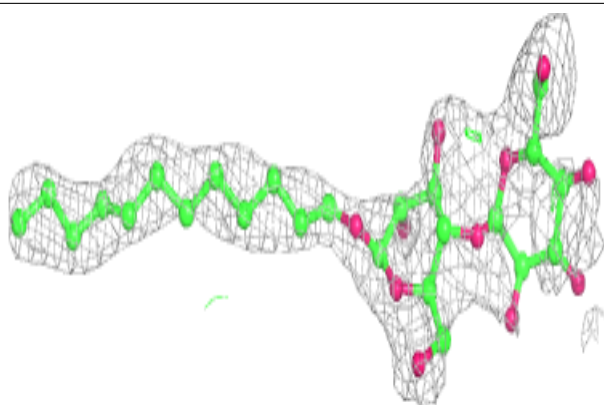
**Electron density around PTY F 1115:**

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

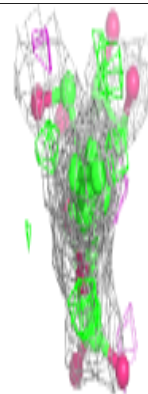
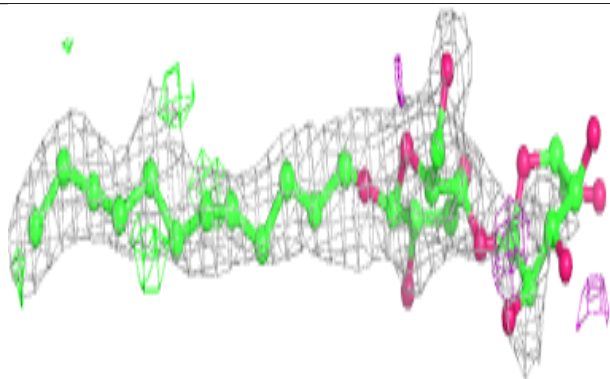
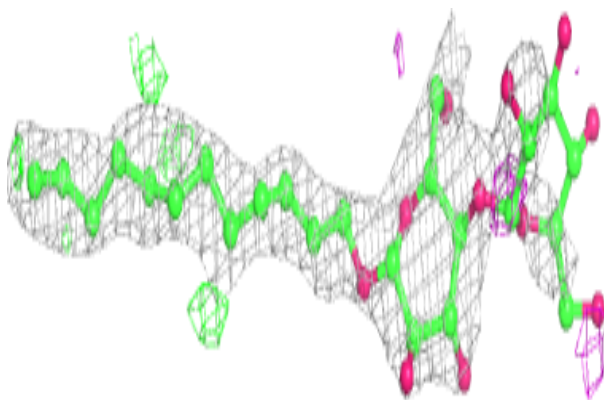


Electron density around LMT F 1110:

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

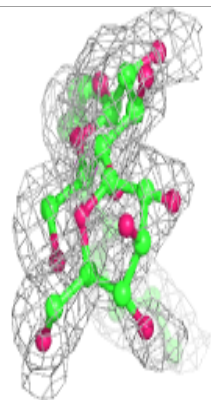
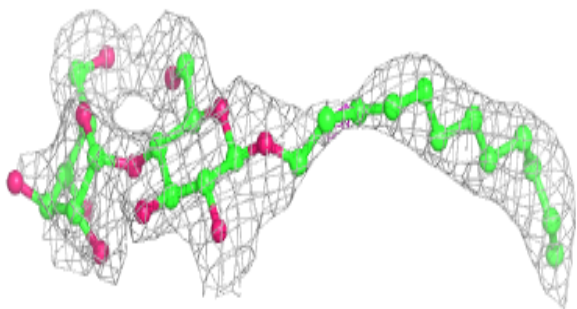
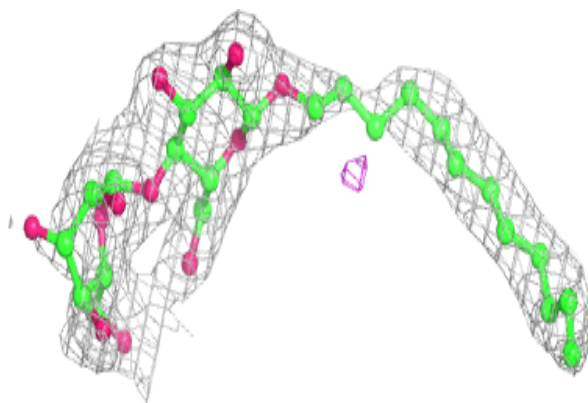
**Electron density around LMT C 1112:**

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

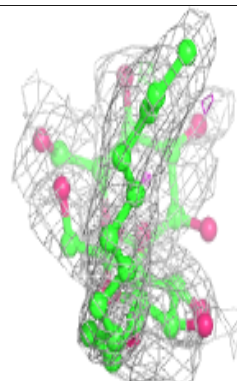
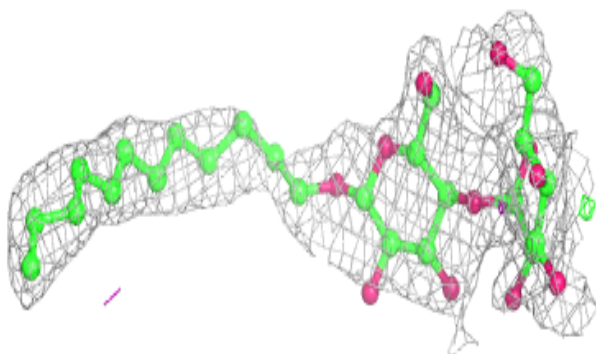
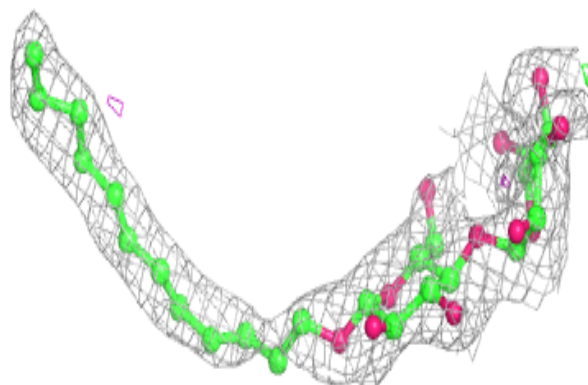


Electron density around LMT A 1109:

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

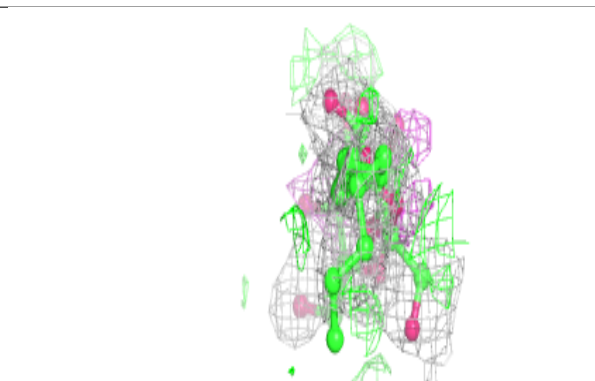
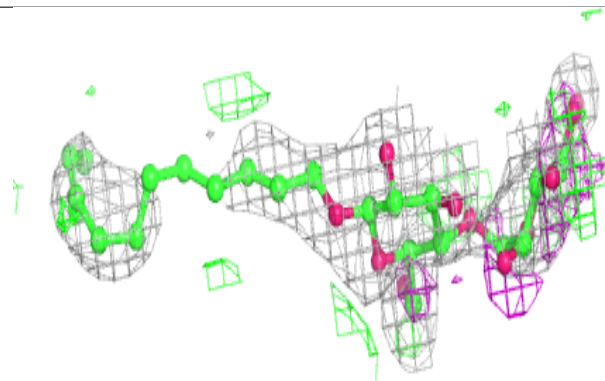
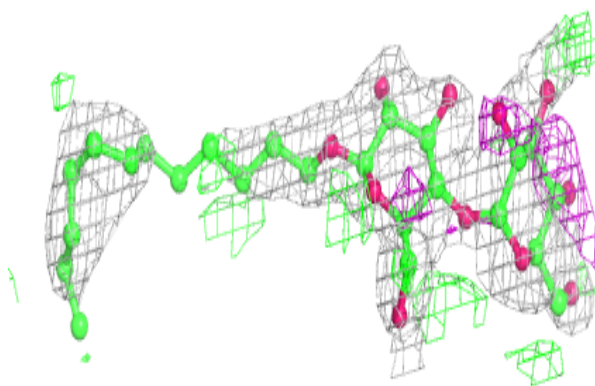
**Electron density around LMT D 1108:**

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

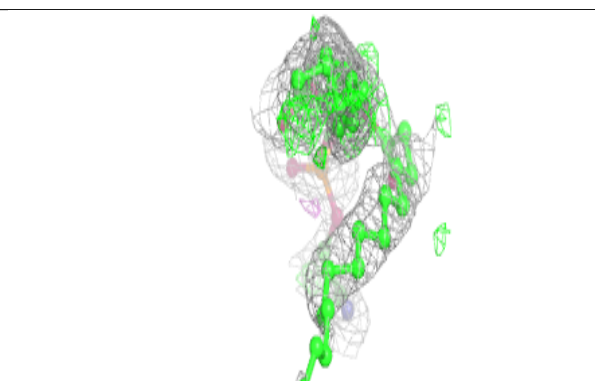
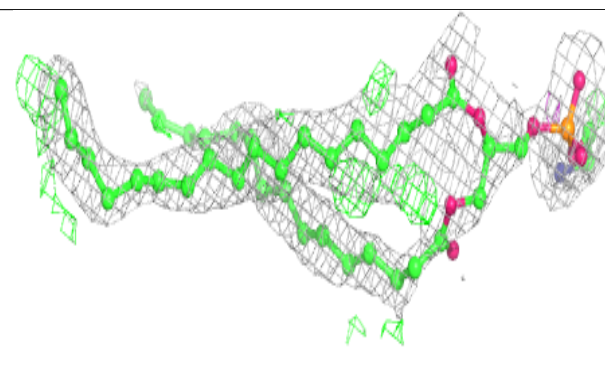
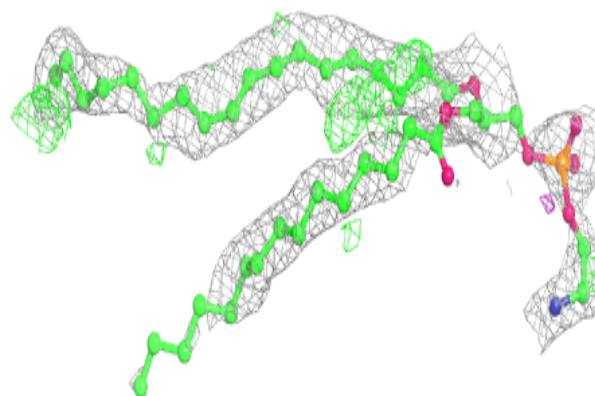


Electron density around LMT F 1103:

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

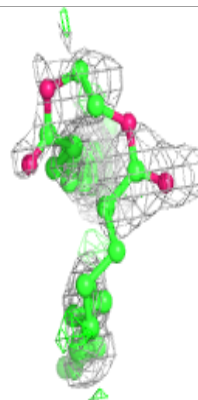
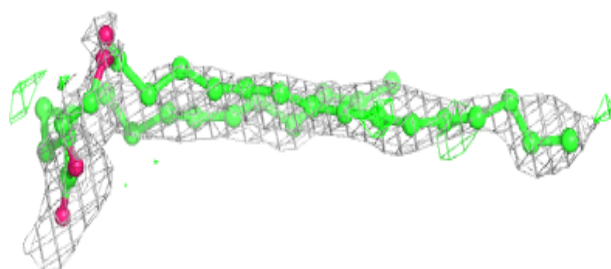
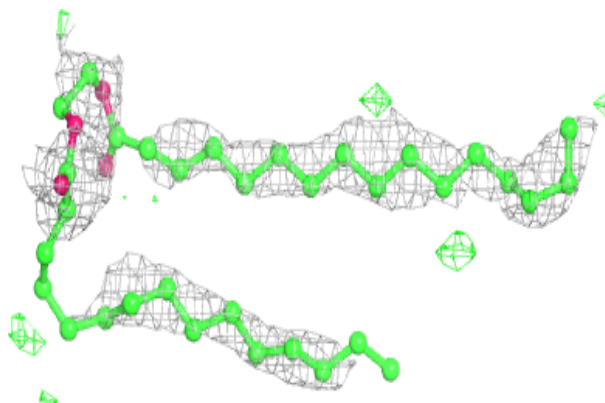
**Electron density around PTY C 1113:**

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

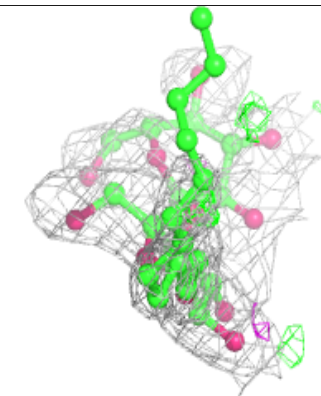
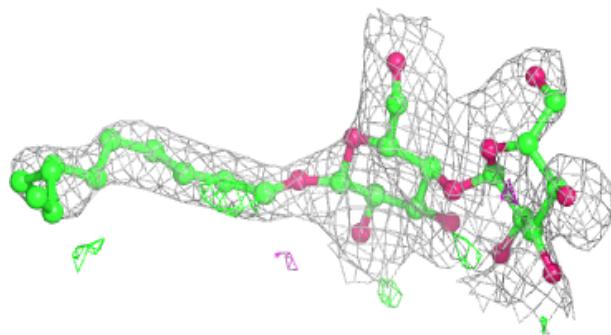
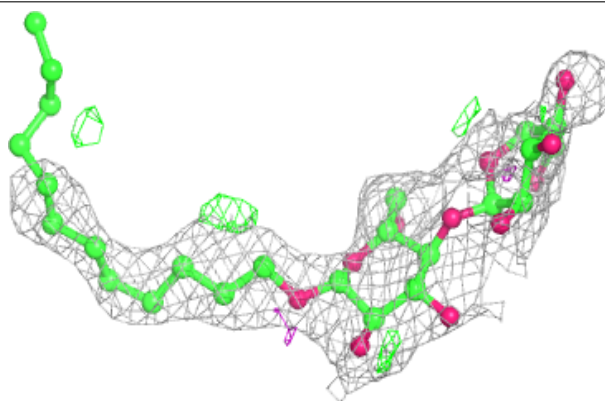


Electron density around PTY F 1114:

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

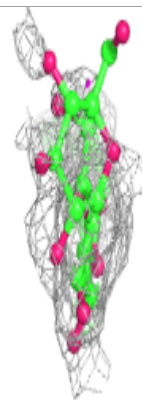
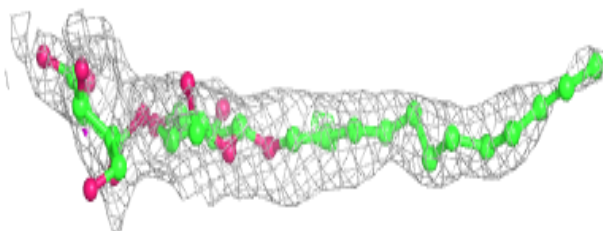
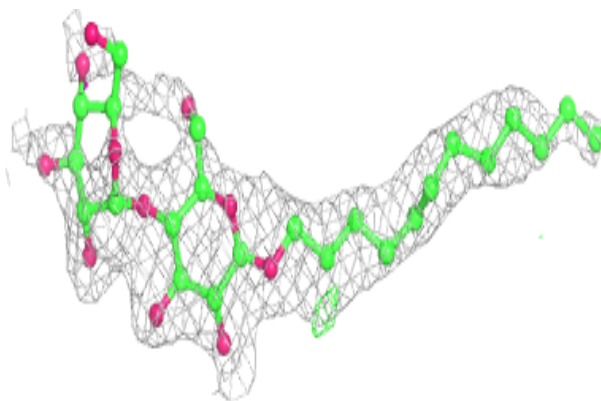
**Electron density around LMT C 1110:**

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

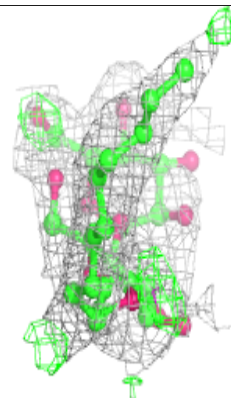
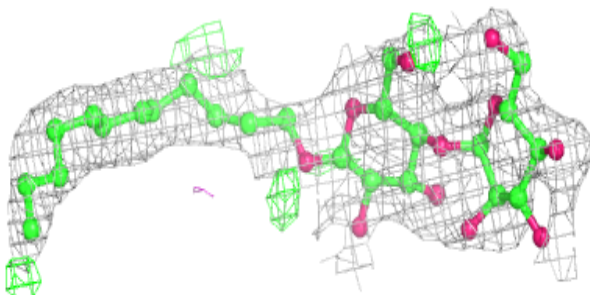
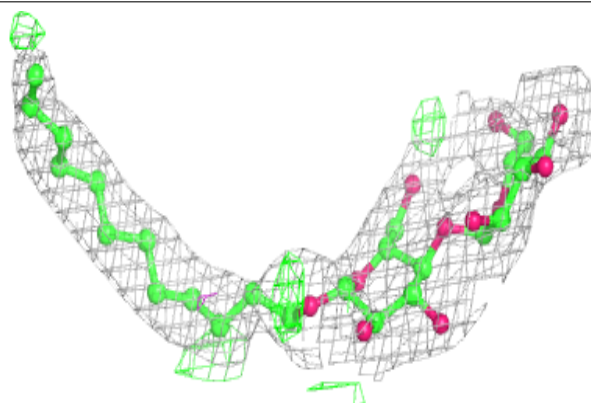


Electron density around LMT E 1109:

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

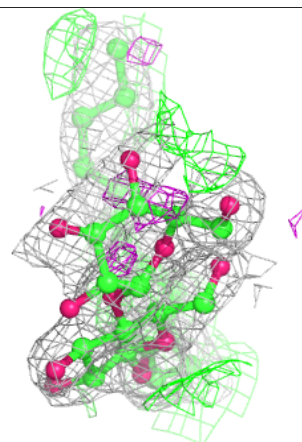
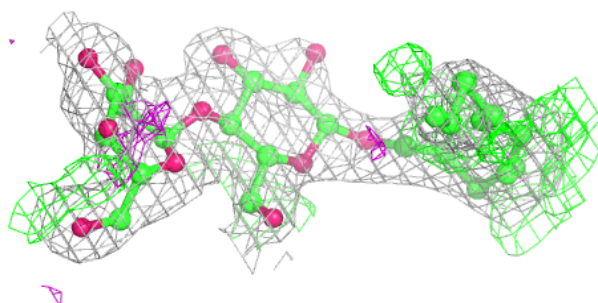
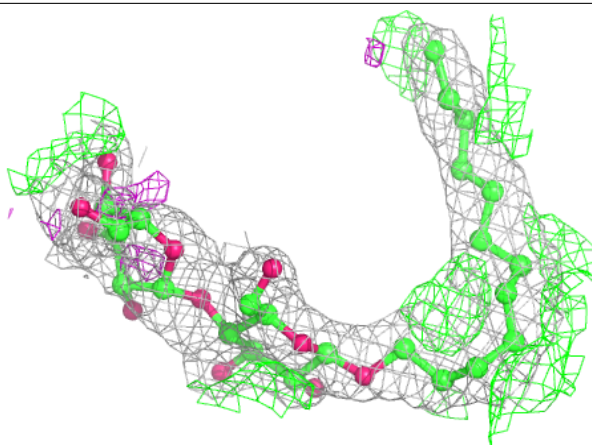
**Electron density around LMT F 1106:**

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

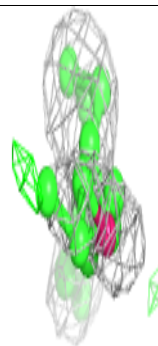
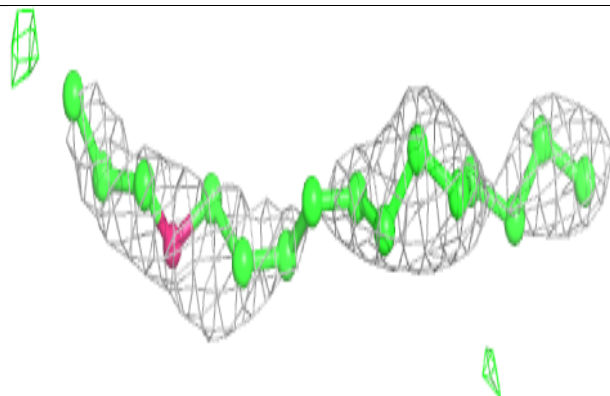
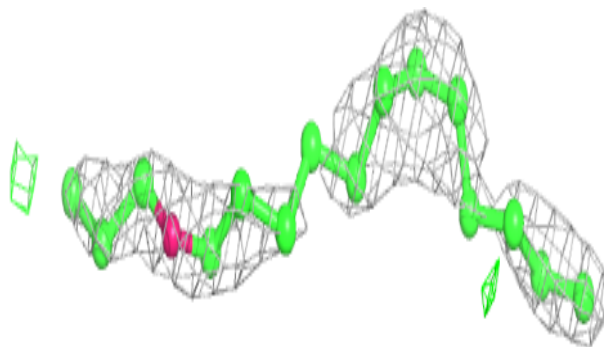


Electron density around LMT C 1108:

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

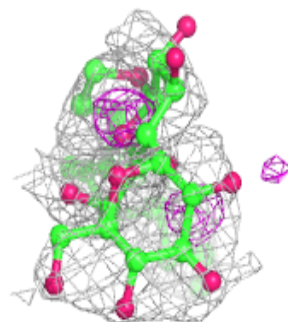
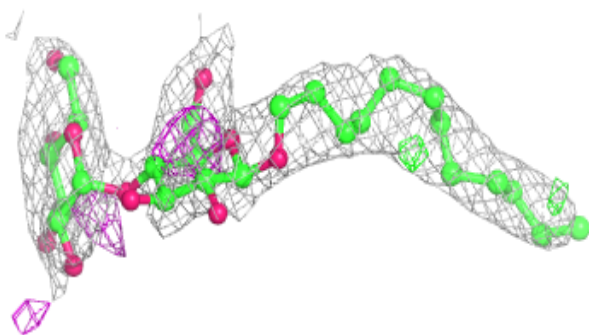
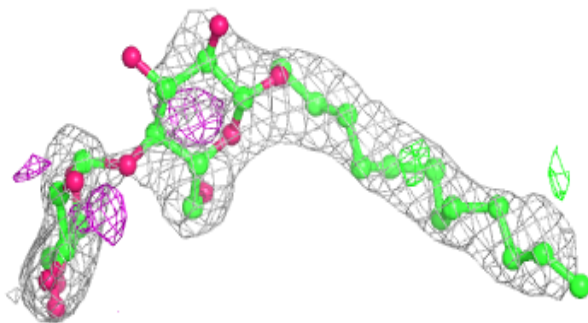
**Electron density around LMT B 1107:**

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

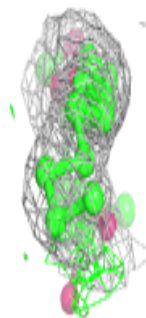
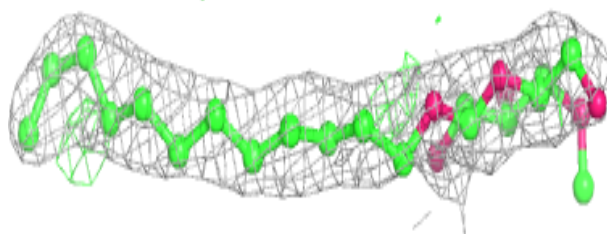
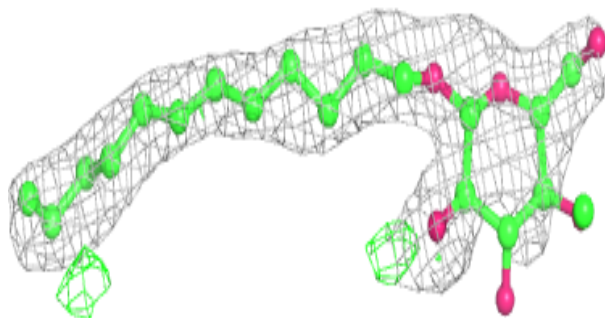


Electron density around LMT E 1108:

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

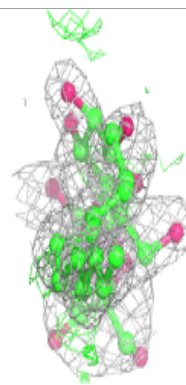
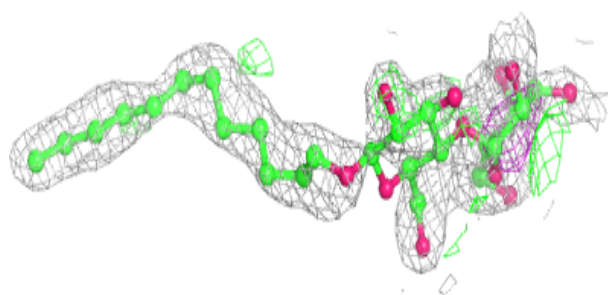
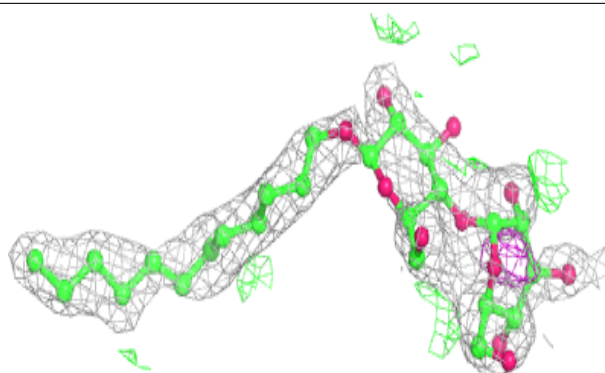
**Electron density around LMT A 1110:**

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

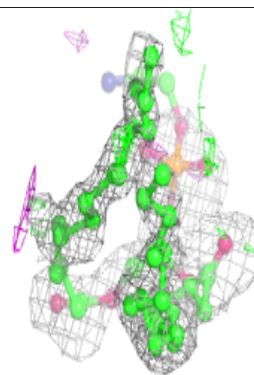
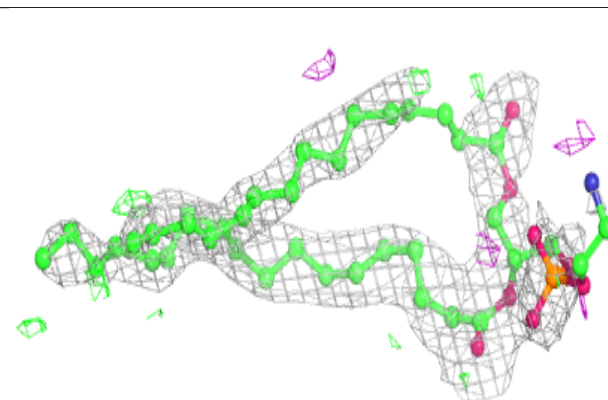
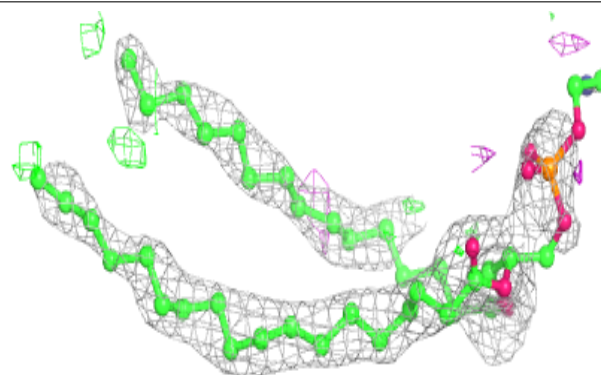


Electron density around LMT D 1103:

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

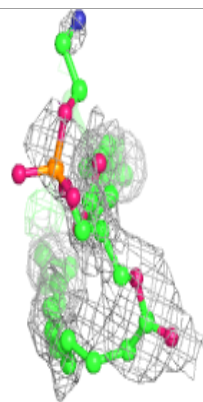
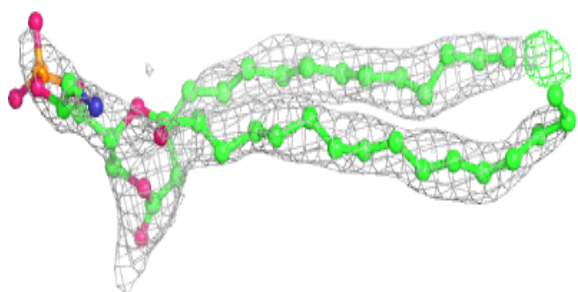
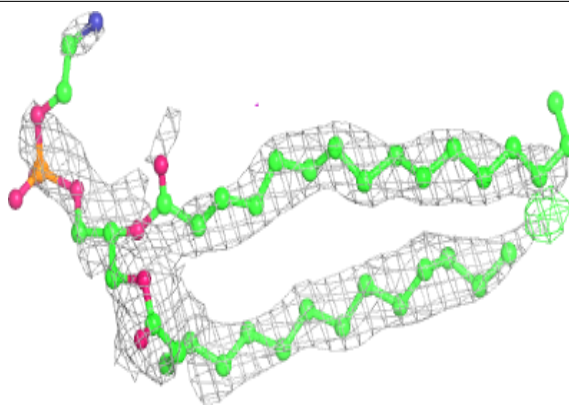
**Electron density around PTY B 1112:**

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

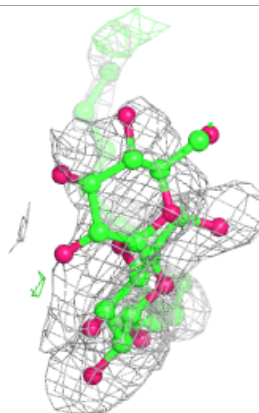
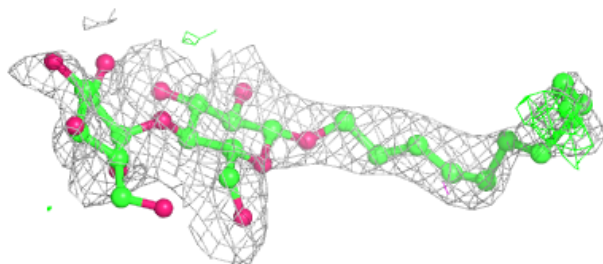
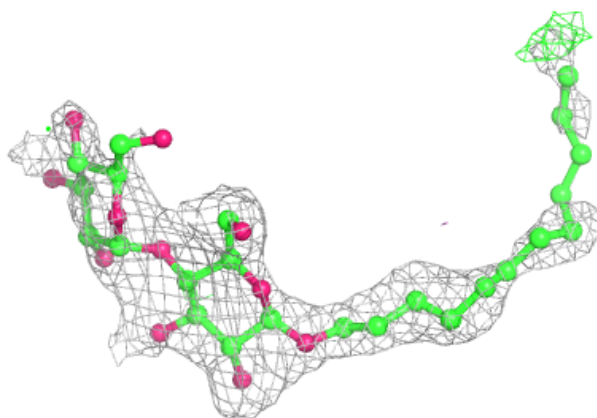


Electron density around PTY A 1112:

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

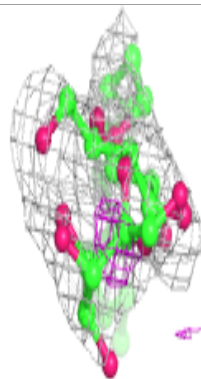
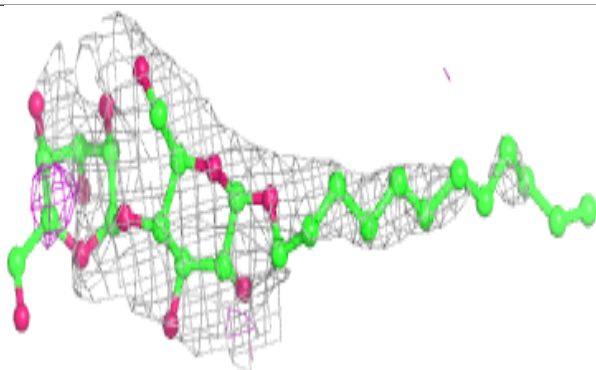
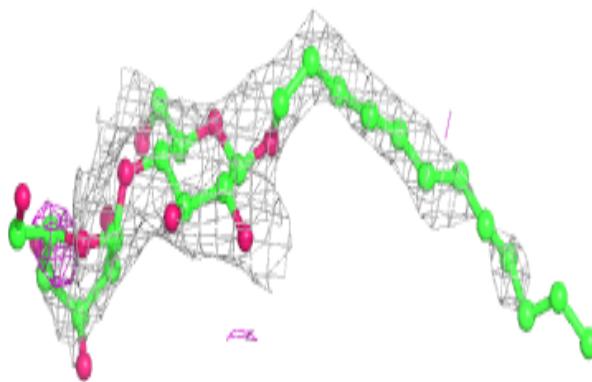
**Electron density around LMT D 1106:**

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

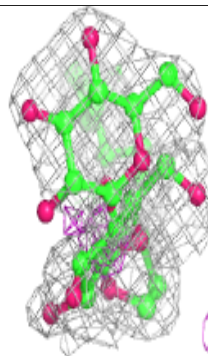
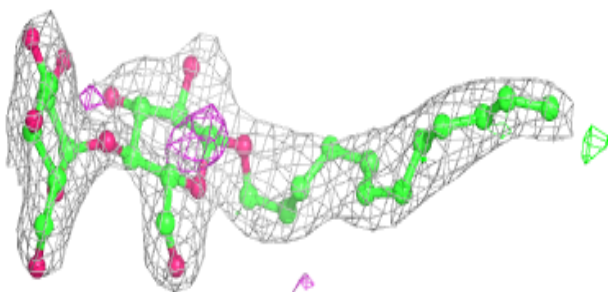
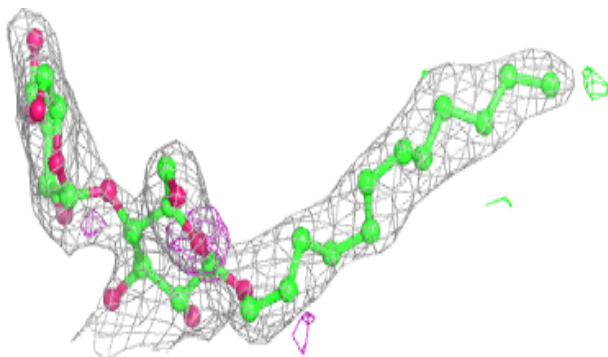


Electron density around LMT B 1101:

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

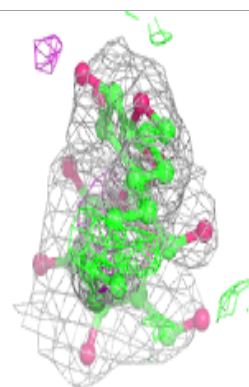
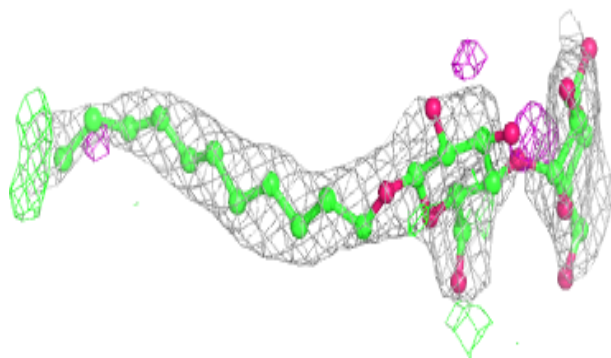
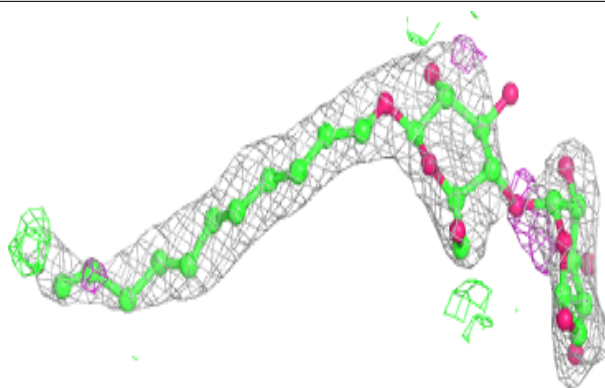
**Electron density around LMT C 1111:**

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



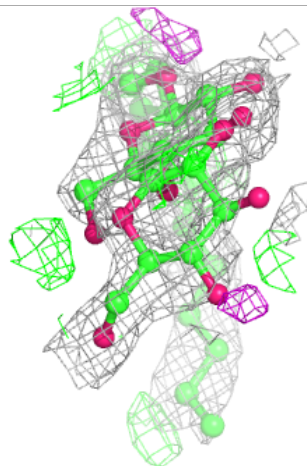
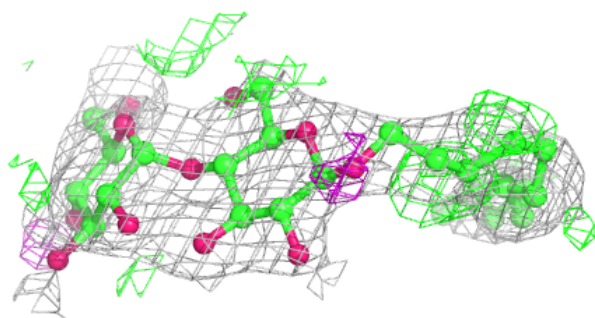
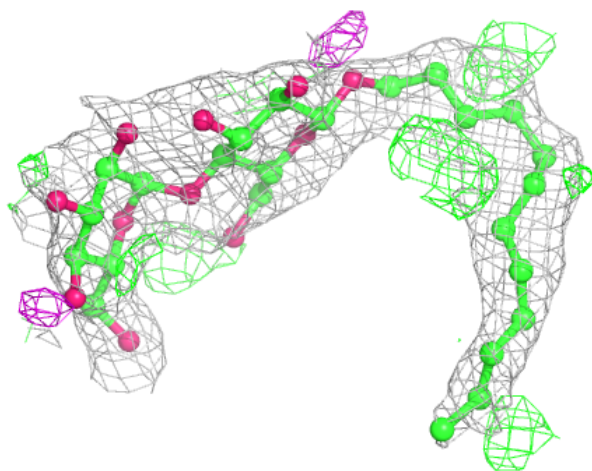
Electron density around LMT A 1108:

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



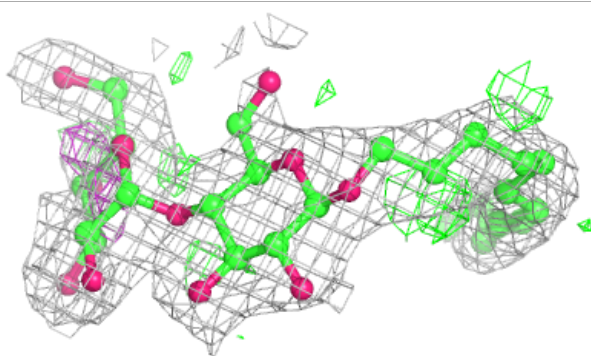
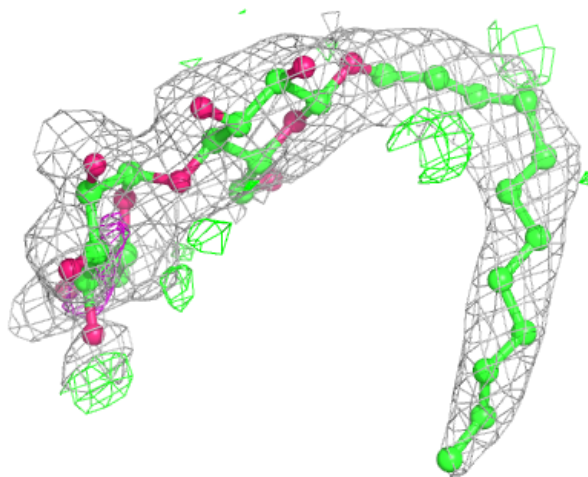
Electron density around LMT E 1105:

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



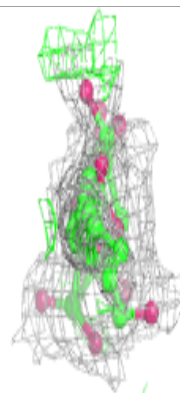
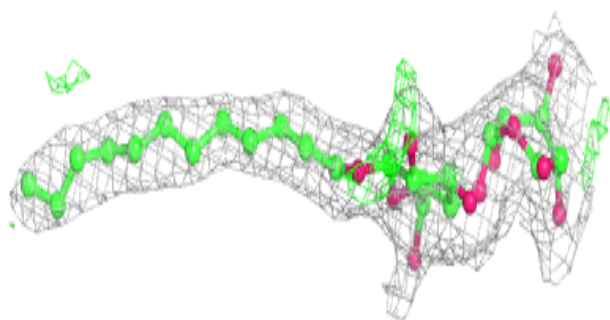
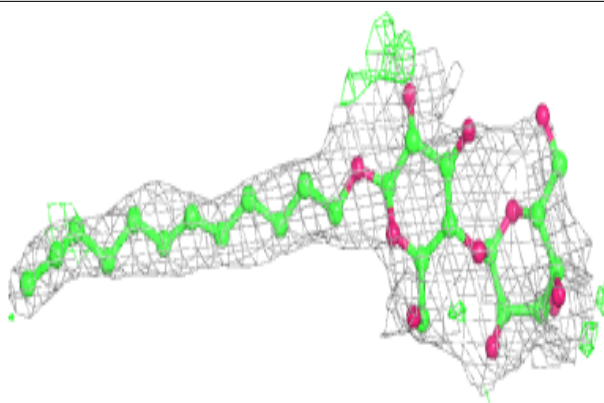
Electron density around LMT B 1105:

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

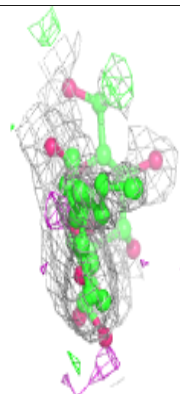
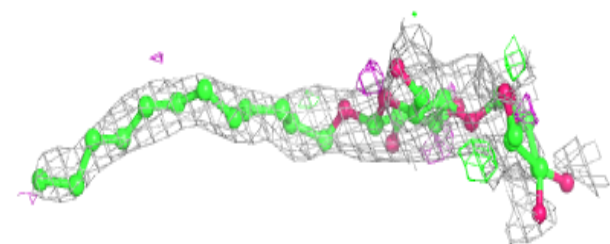
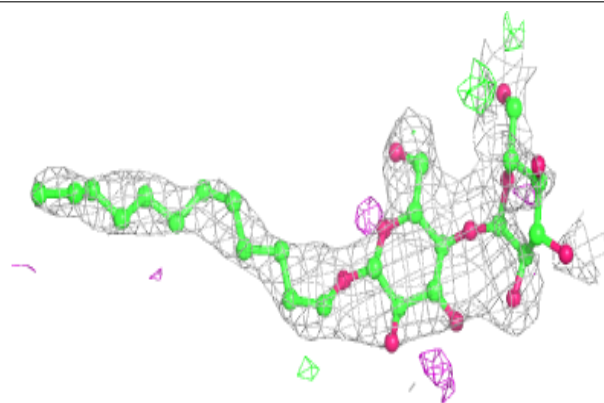


Electron density around LMT C 1109:

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

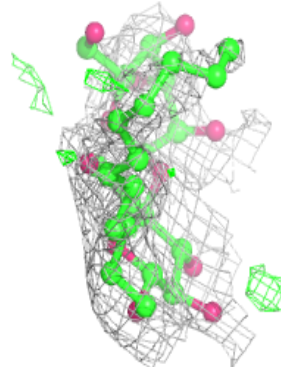
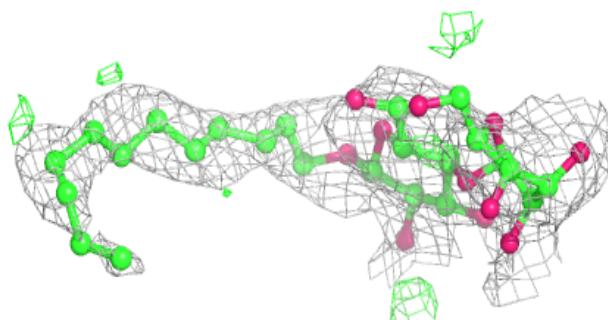
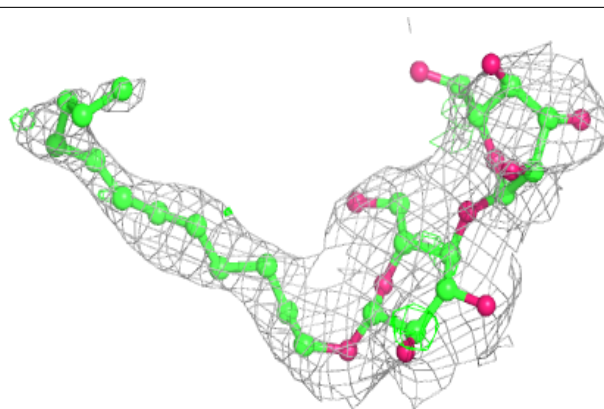
**Electron density around LMT C 1101:**

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

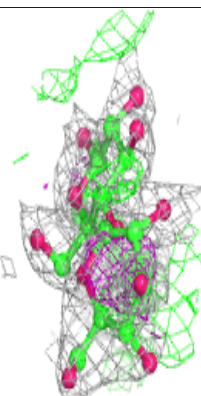
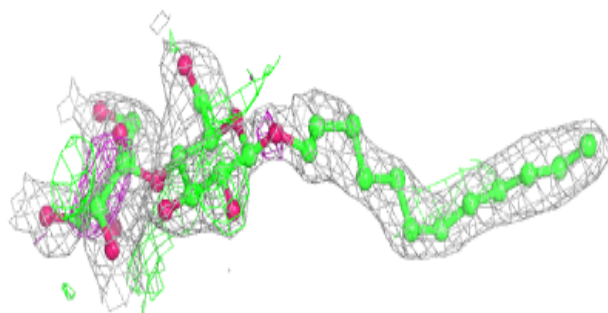
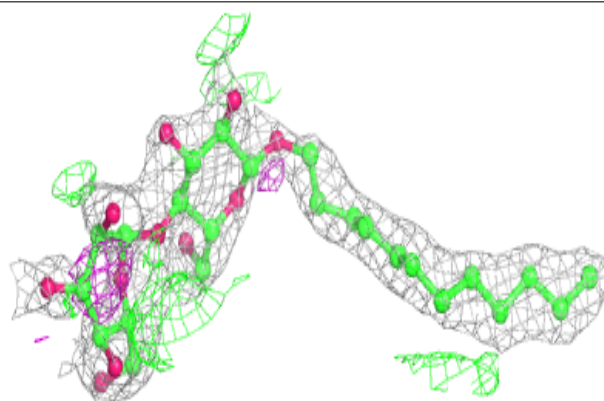


Electron density around LMT F 1107:

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

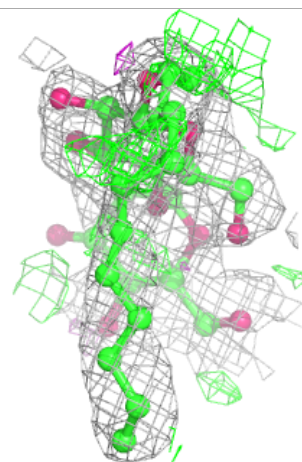
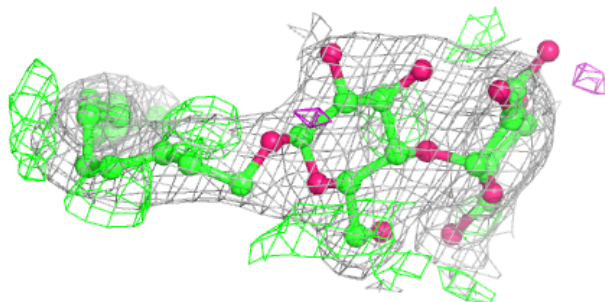
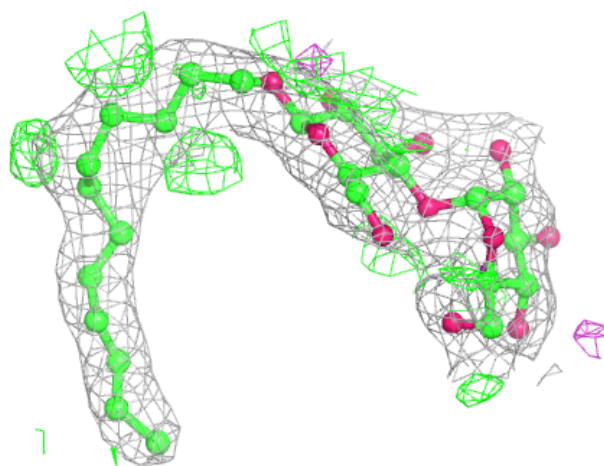
**Electron density around LMT C 1107:**

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



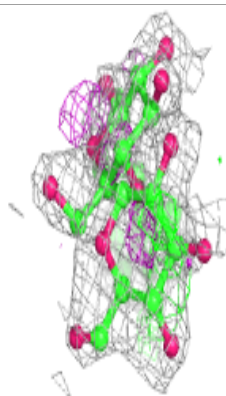
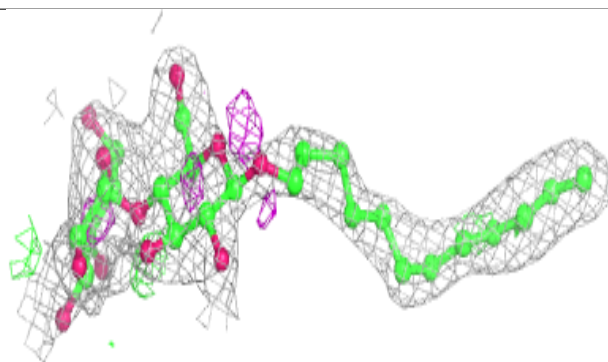
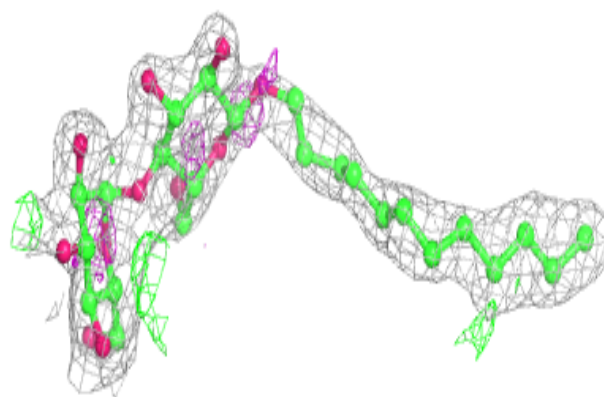
Electron density around LMT A 1105:

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

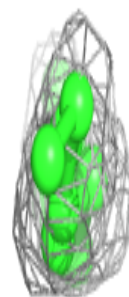
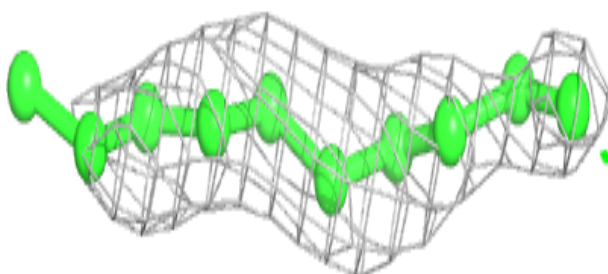
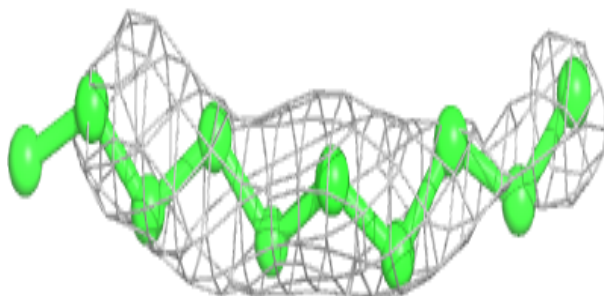


Electron density around LMT E 1104:

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

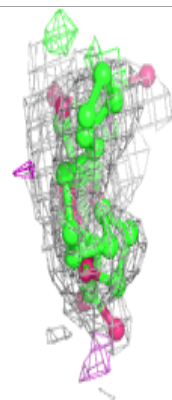
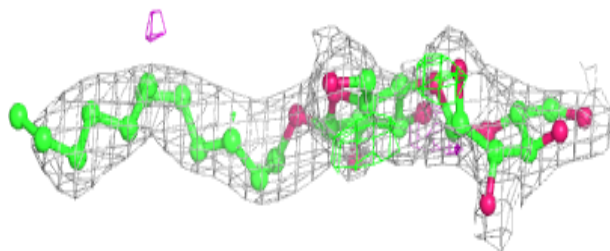
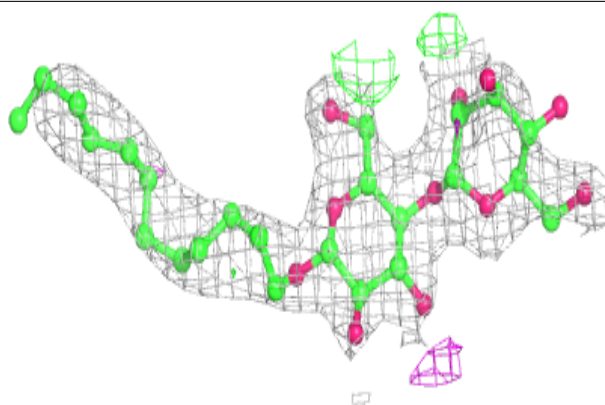
**Electron density around LMT E 1113:**

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

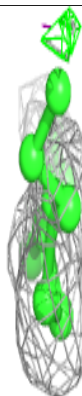
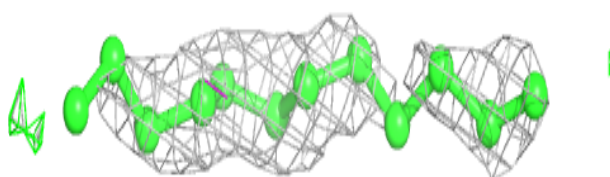
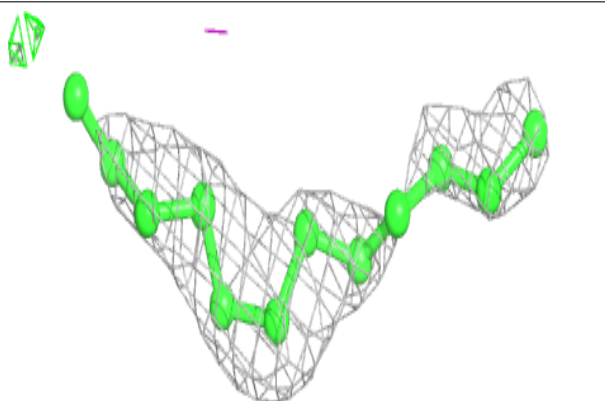


Electron density around LMT E 1102:

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

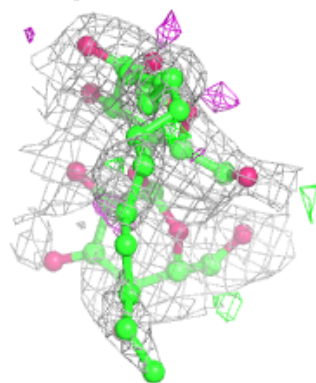
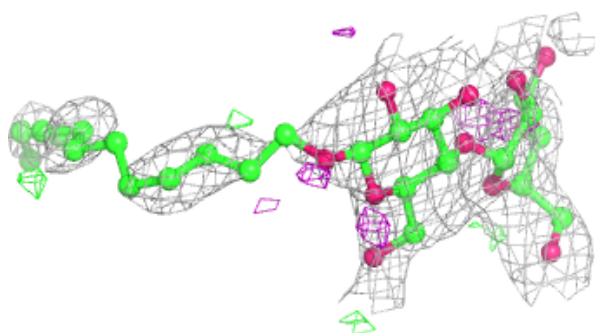
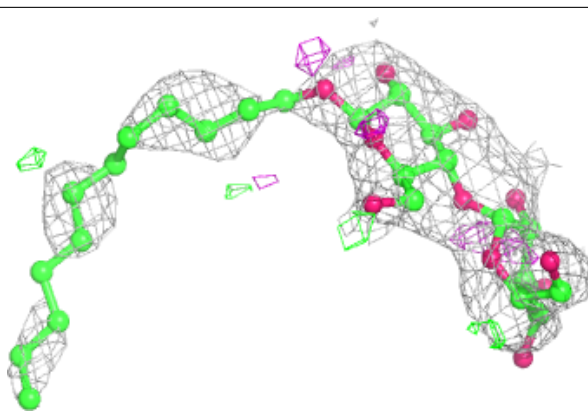
**Electron density around LMT E 1111:**

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

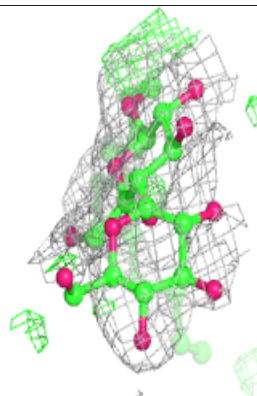
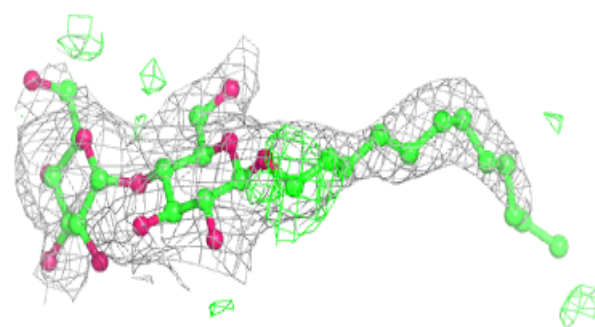
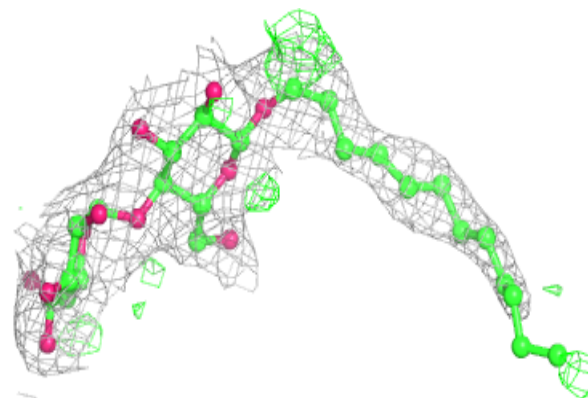


Electron density around LMT A 1106:

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

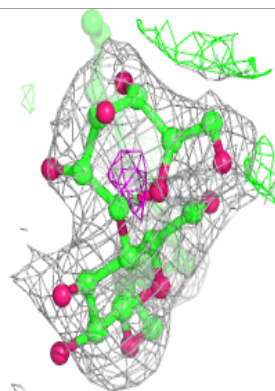
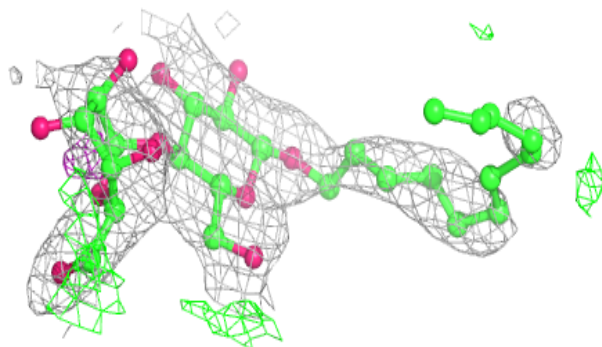
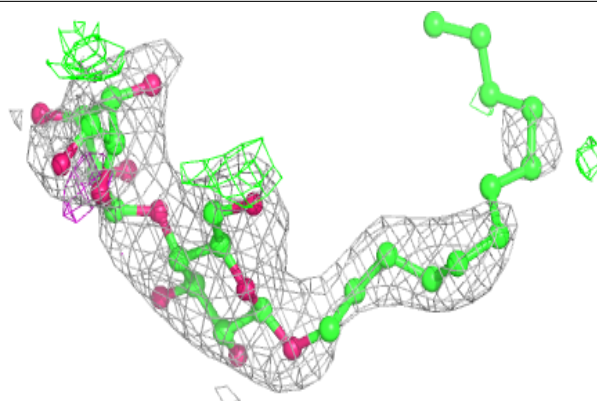
**Electron density around LMT B 1106:**

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

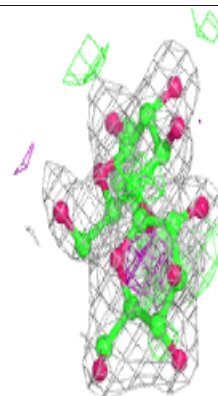
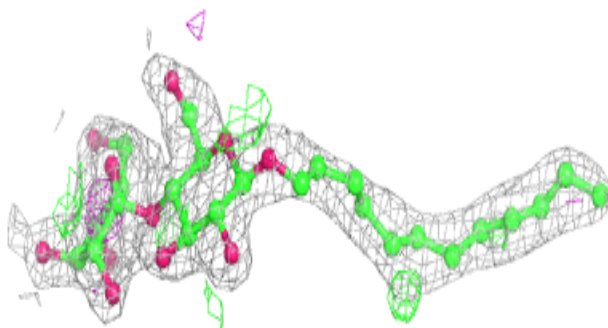
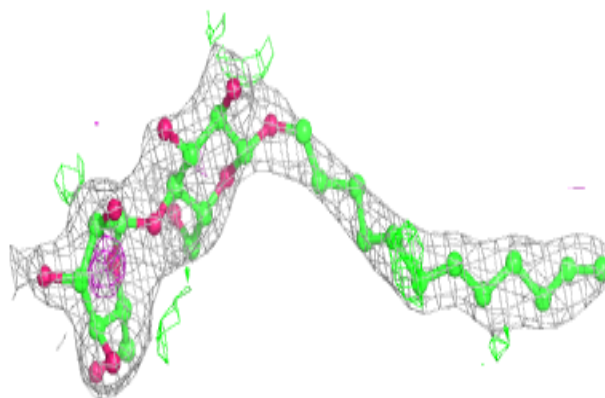


Electron density around LMT E 1107:

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

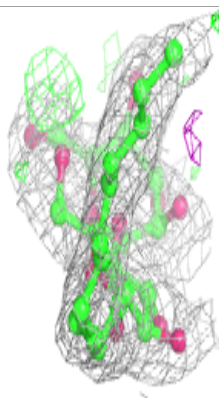
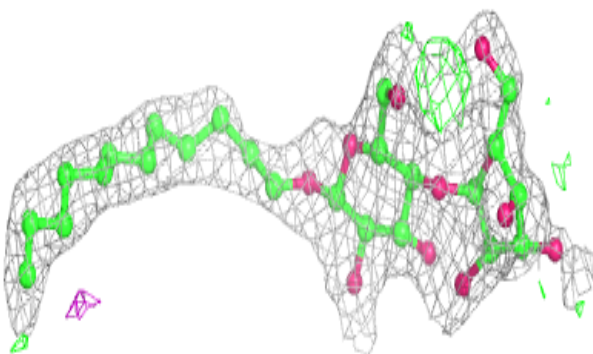
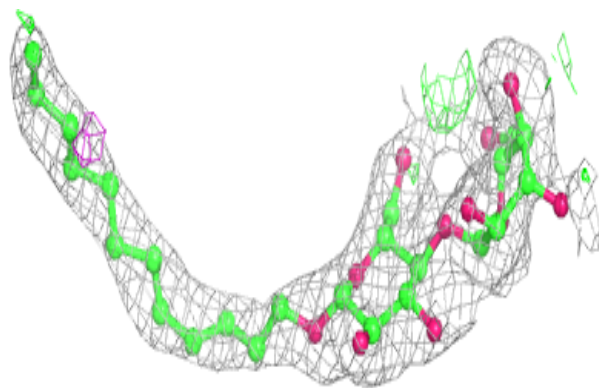
**Electron density around LMT B 1102:**

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

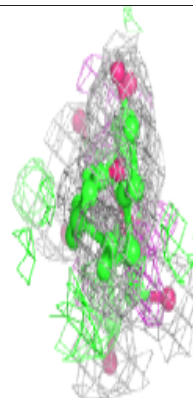
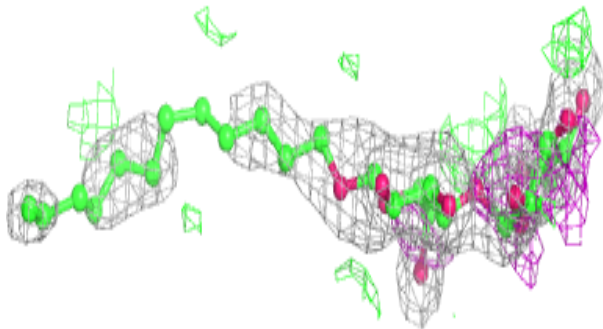
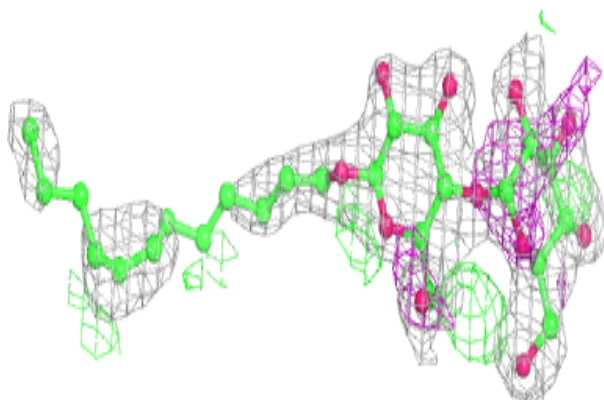


Electron density around LMT C 1106:

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

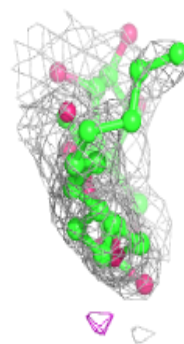
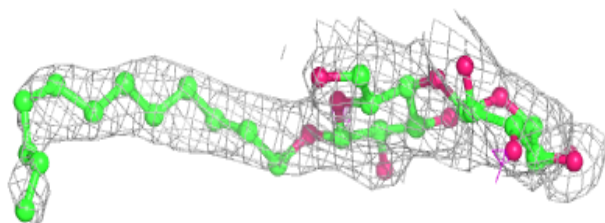
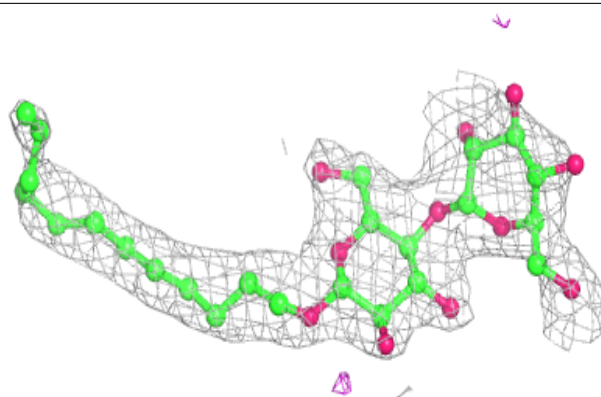
**Electron density around LMT A 1111:**

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

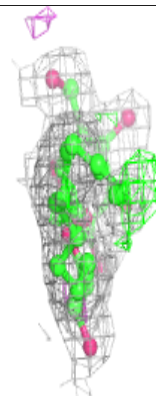
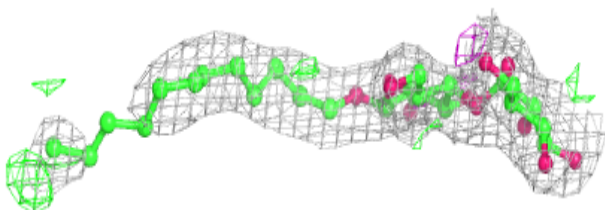
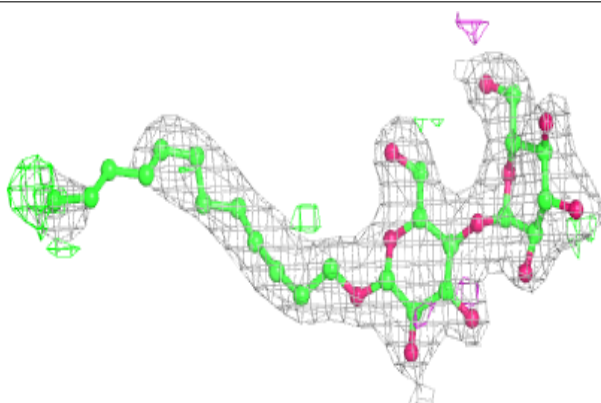


Electron density around LMT D 1111:

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

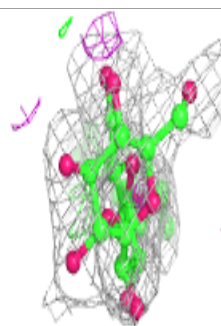
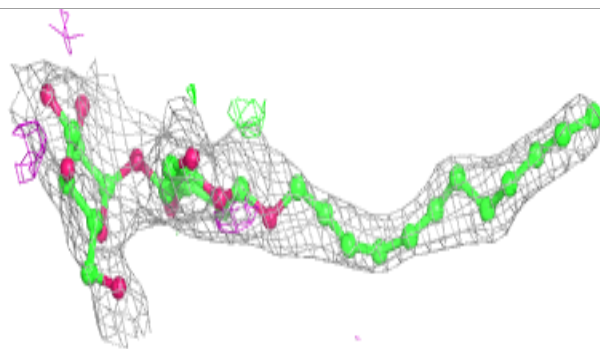
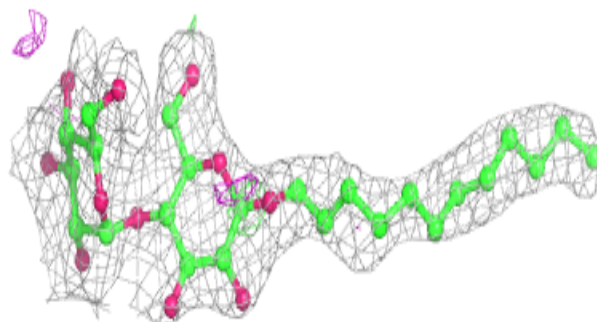
**Electron density around LMT A 1102:**

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

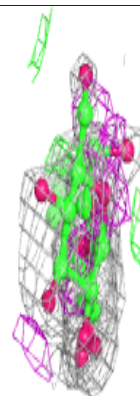
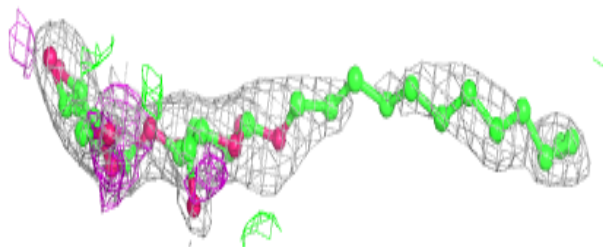
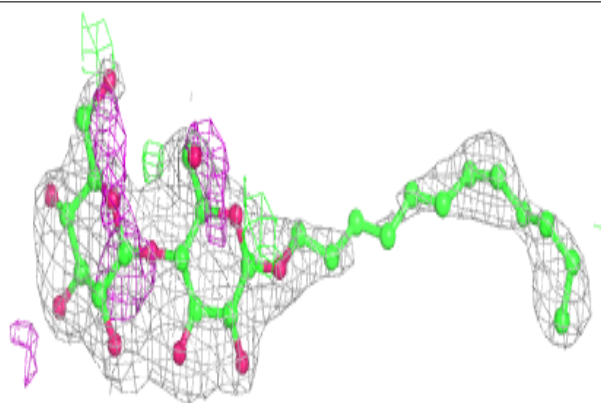


Electron density around LMT D 1101:

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

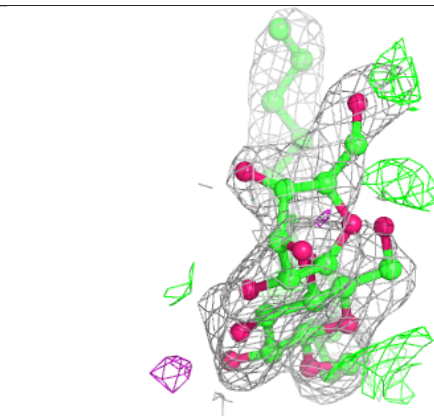
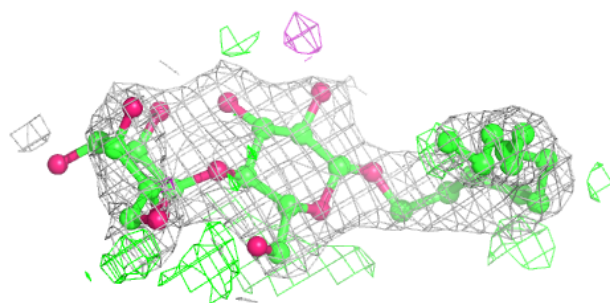
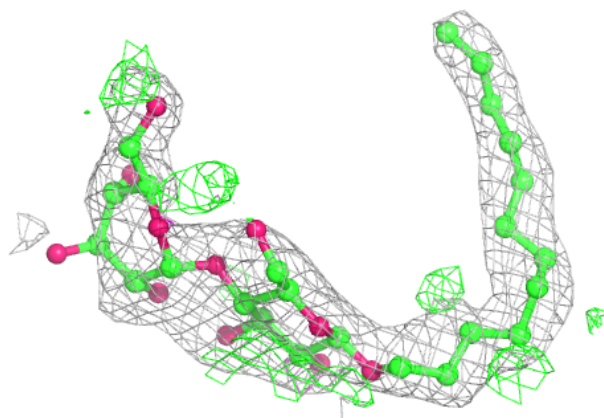
**Electron density around LMT D 1102:**

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

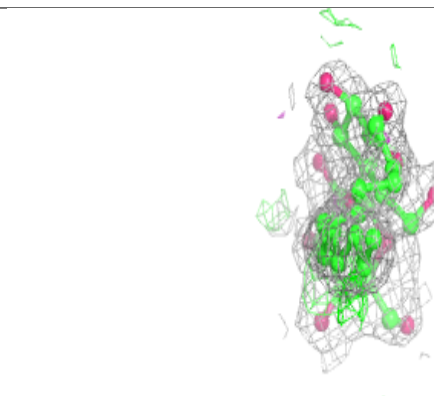
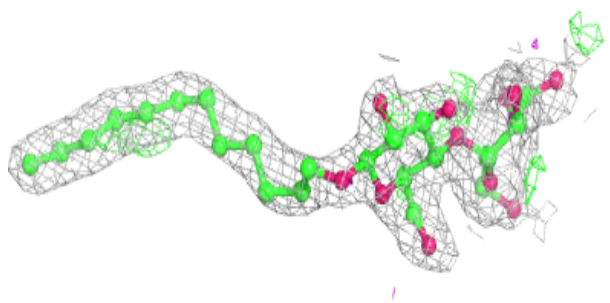
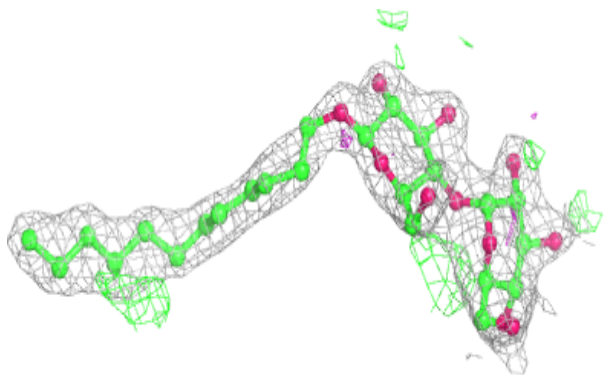


Electron density around LMT F 1105:

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

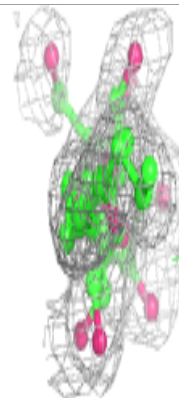
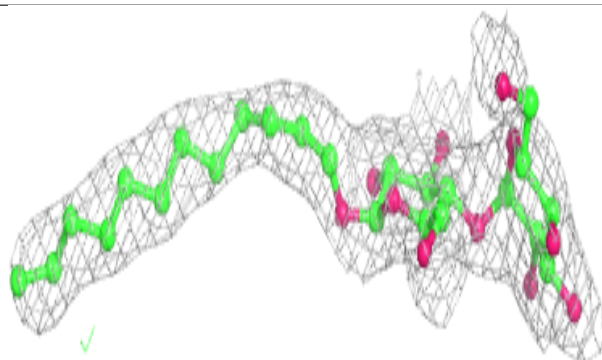
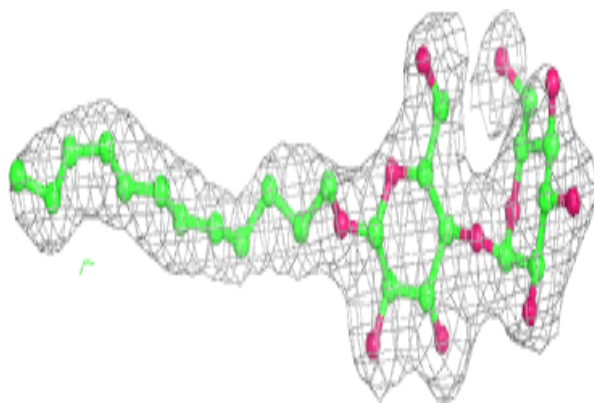
**Electron density around LMT A 1104:**

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

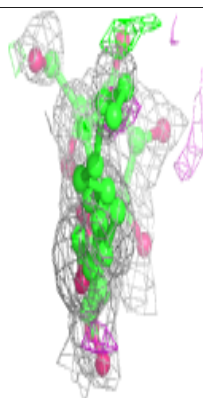
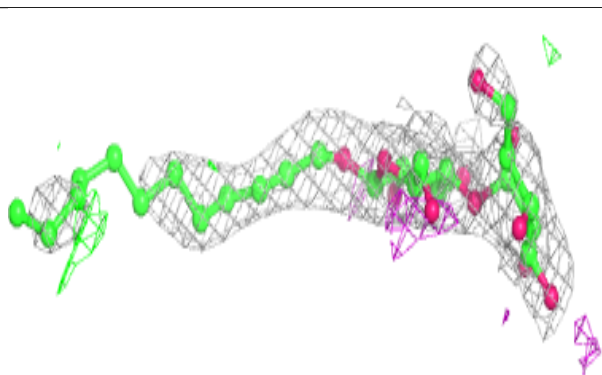
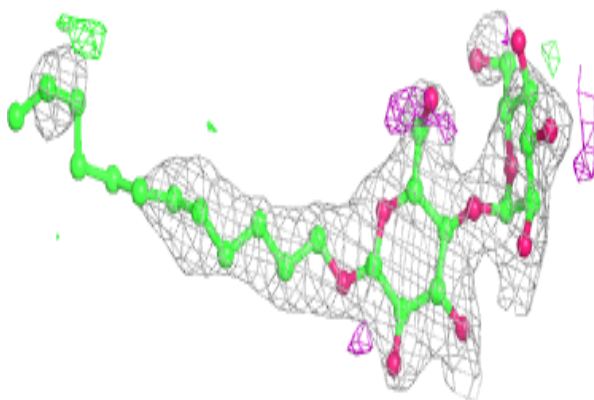


Electron density around LMT A 1103:

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

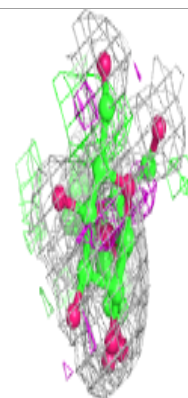
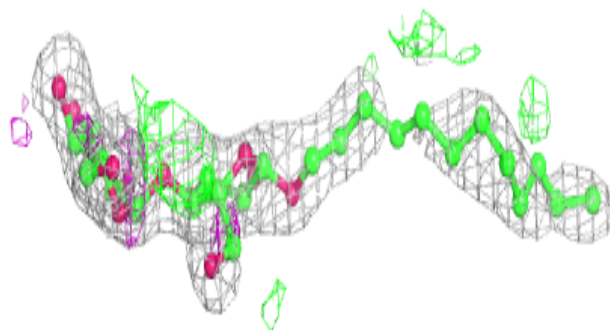
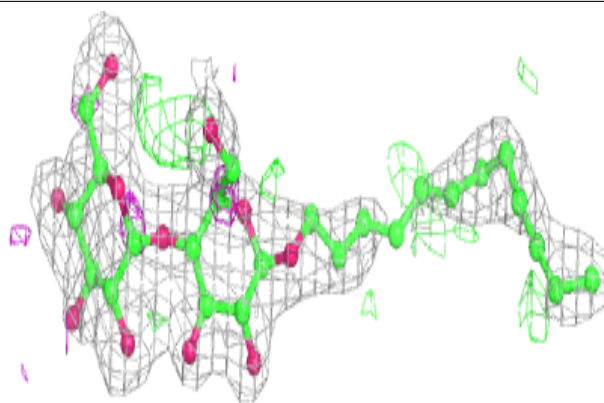
**Electron density around LMT F 1113:**

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

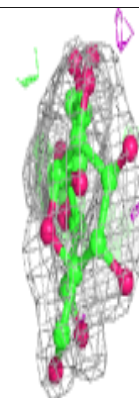
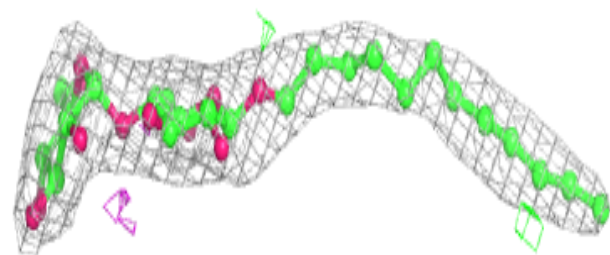
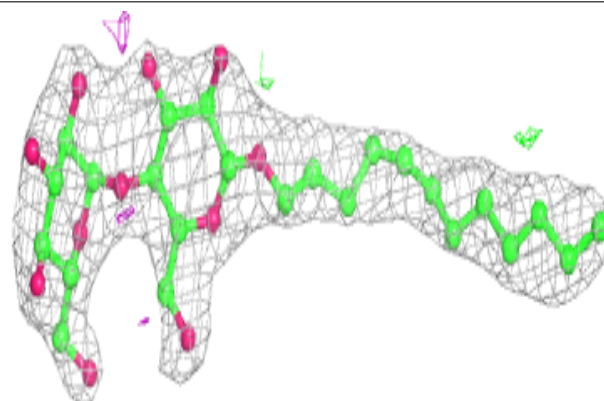


Electron density around LMT E 1103:

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

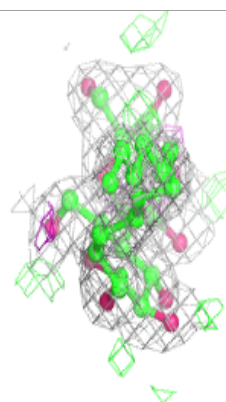
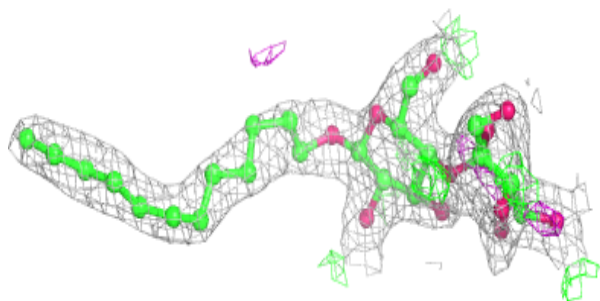
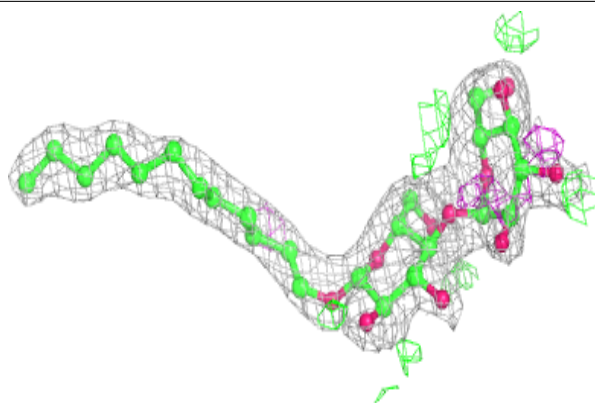
**Electron density around LMT F 1102:**

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

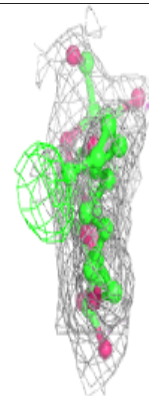
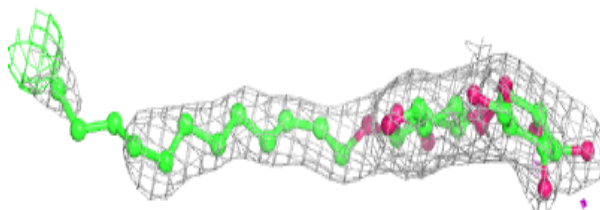
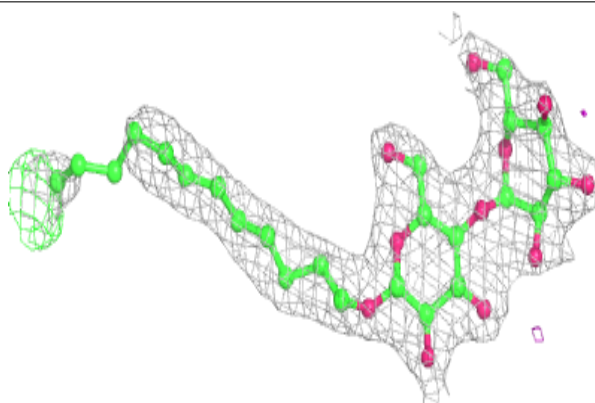


Electron density around LMT F 1104:

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

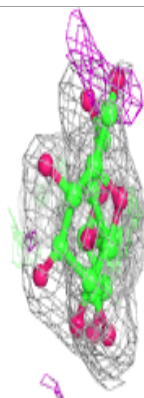
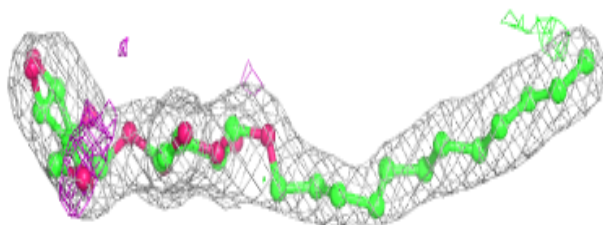
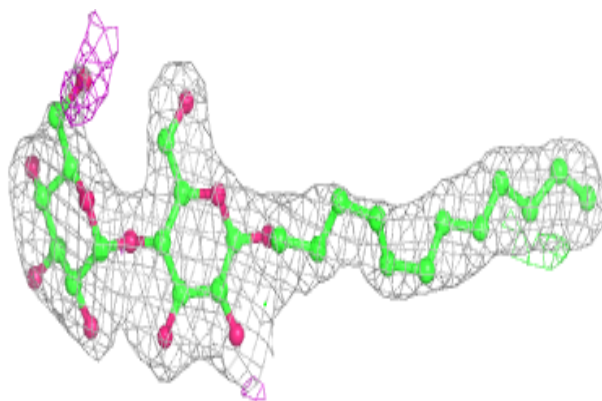
**Electron density around LMT C 1102:**

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

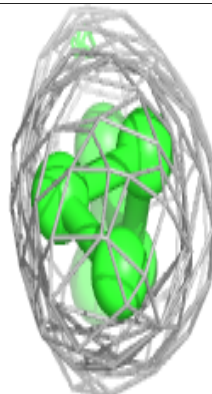
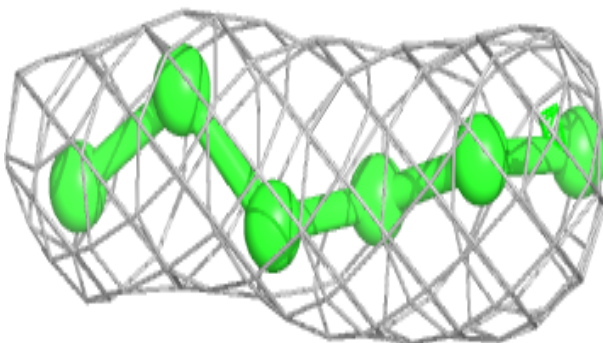
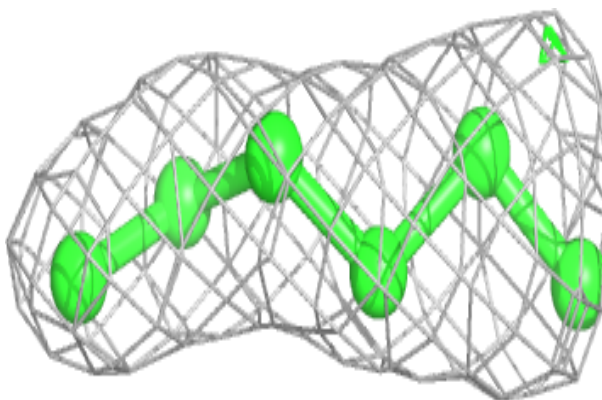


Electron density around LMT E 1101:

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

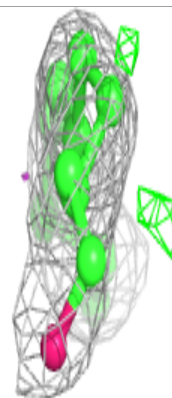
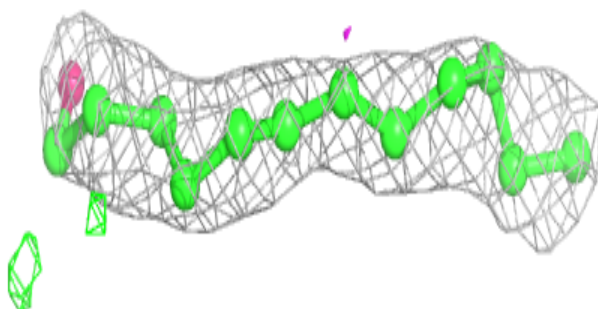
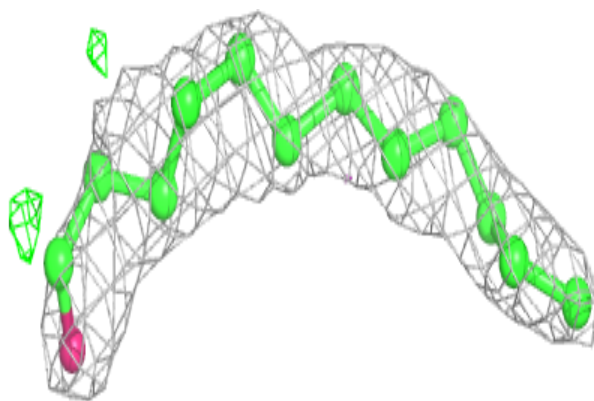
**Electron density around LMT F 1112:**

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

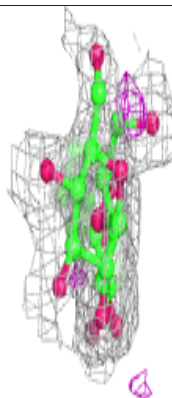
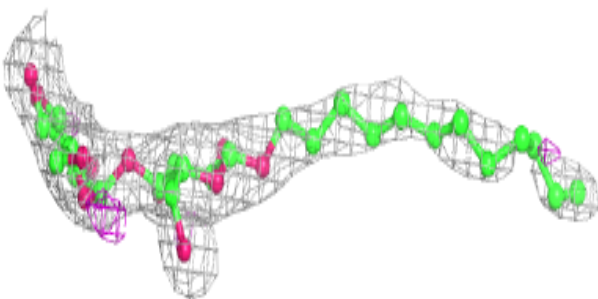
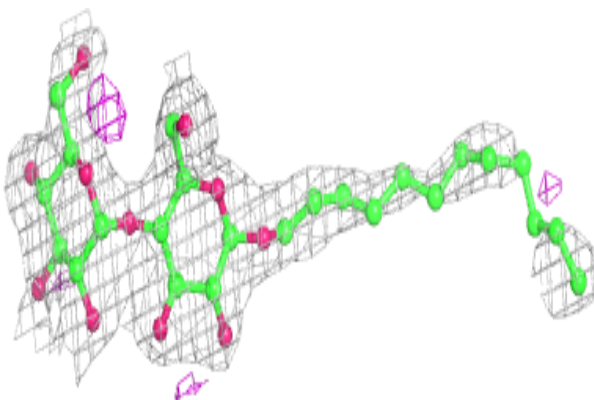


Electron density around LMT F 1108:

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

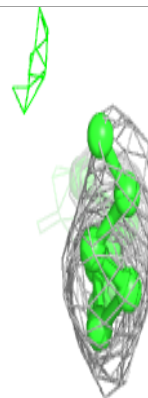
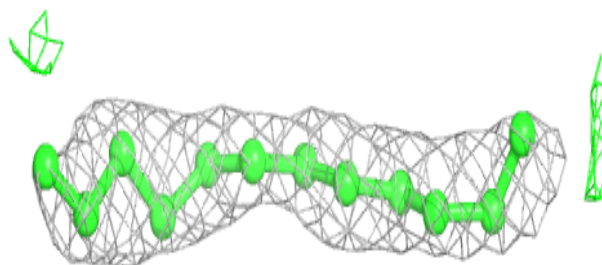
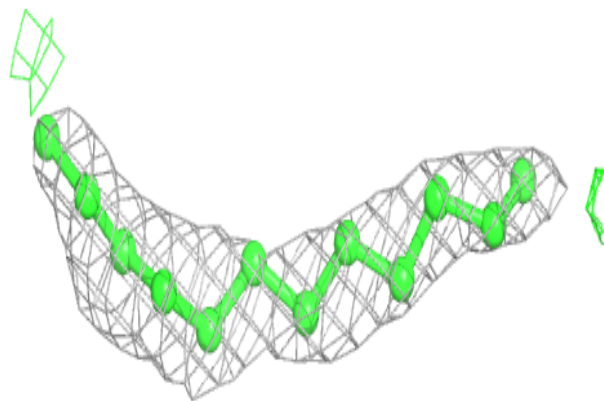
**Electron density around LMT B 1103:**

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

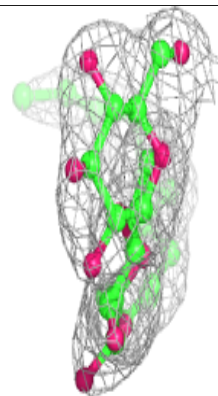
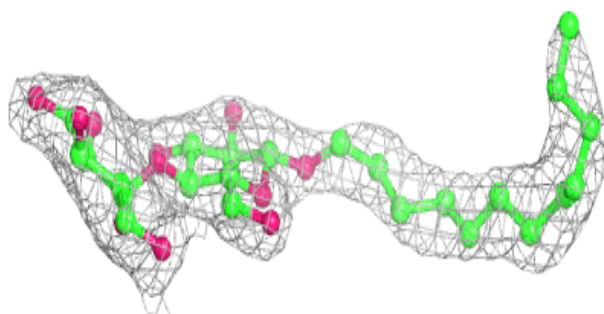
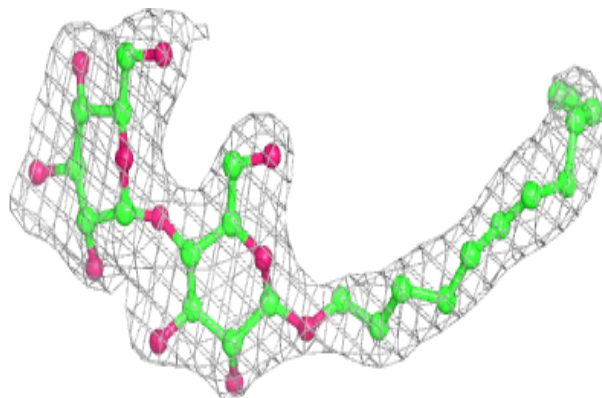


Electron density around LMT B 1108:

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

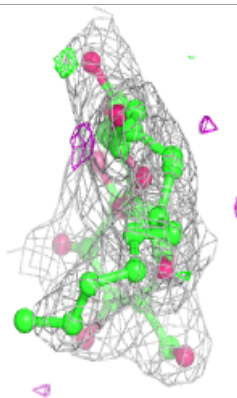
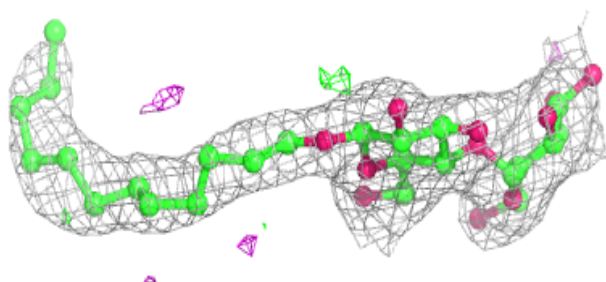
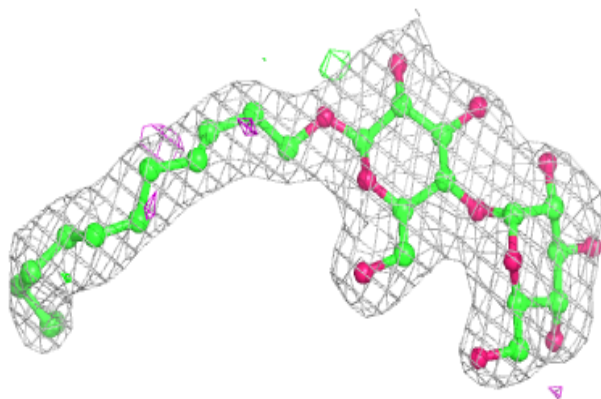
**Electron density around LMT B 1104:**

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

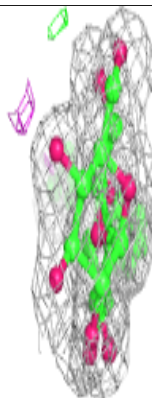
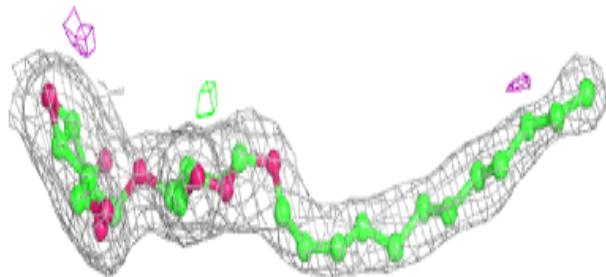
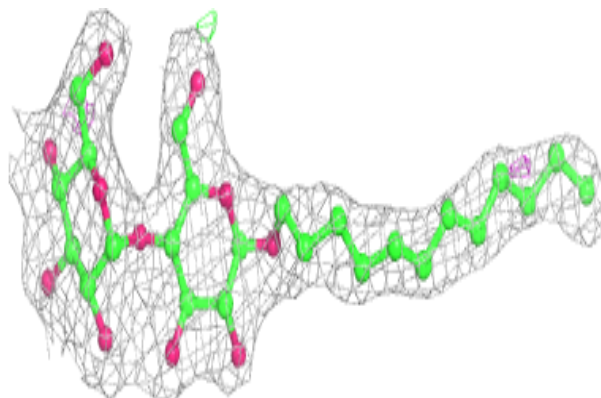


Electron density around LMT F 1101:

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

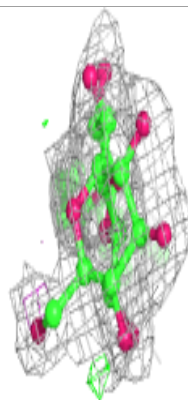
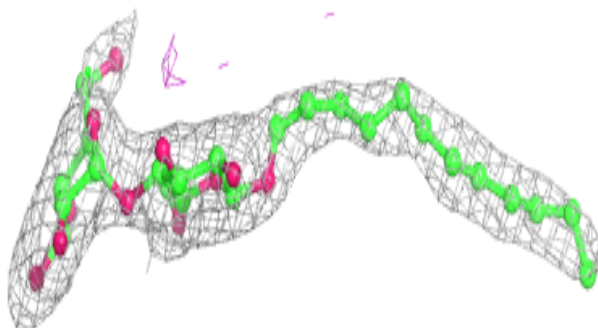
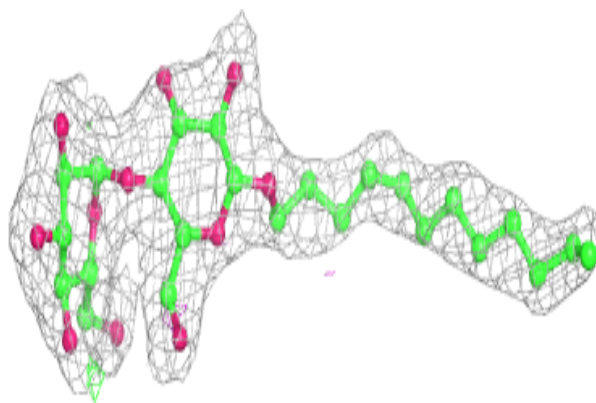
**Electron density around LMT C 1104:**

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

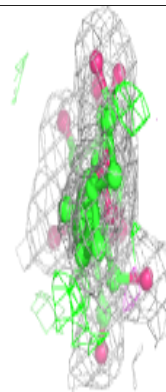
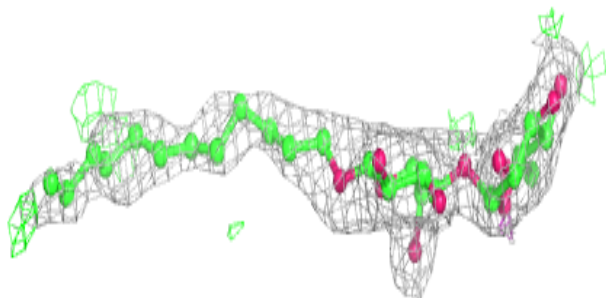
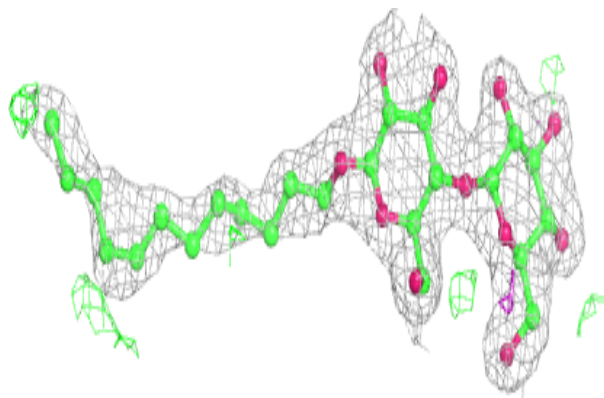


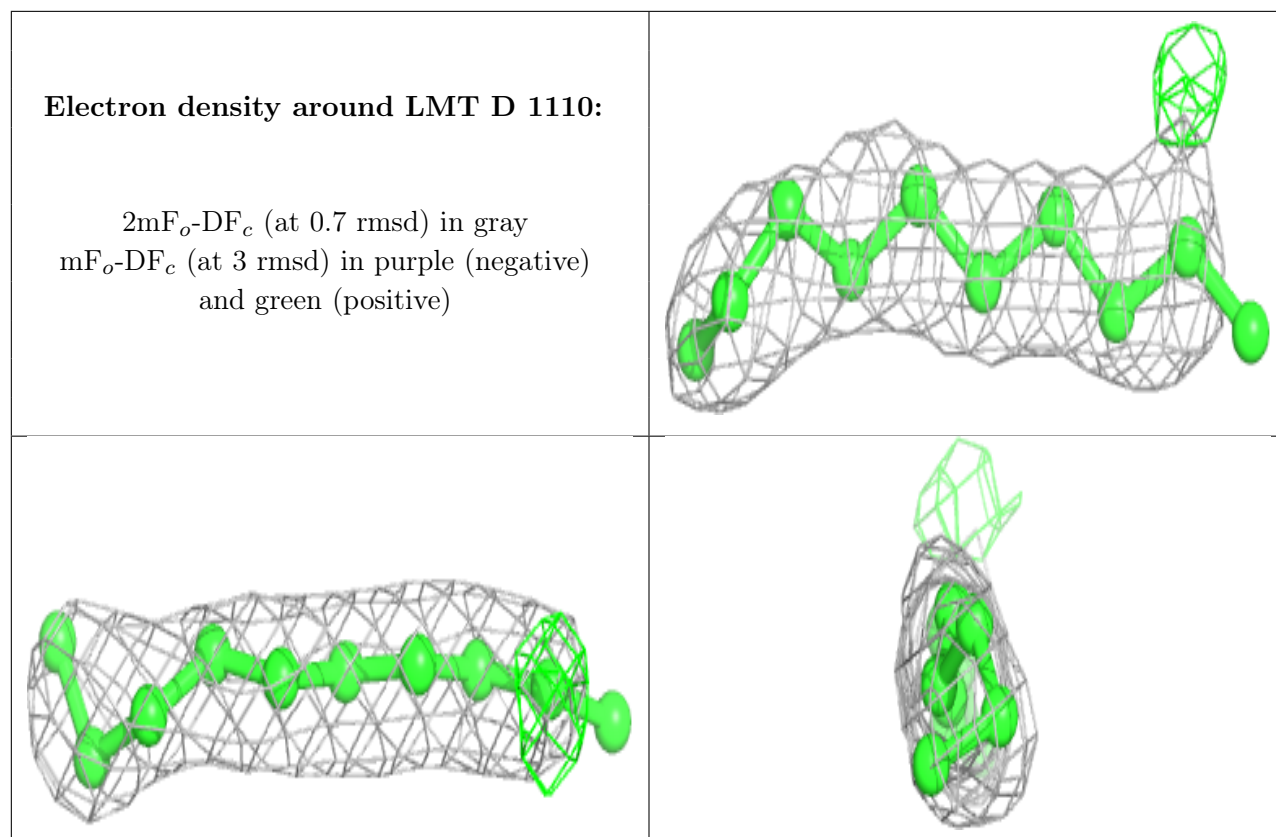
Electron density around LMT C 1103:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.