wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 05:44 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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

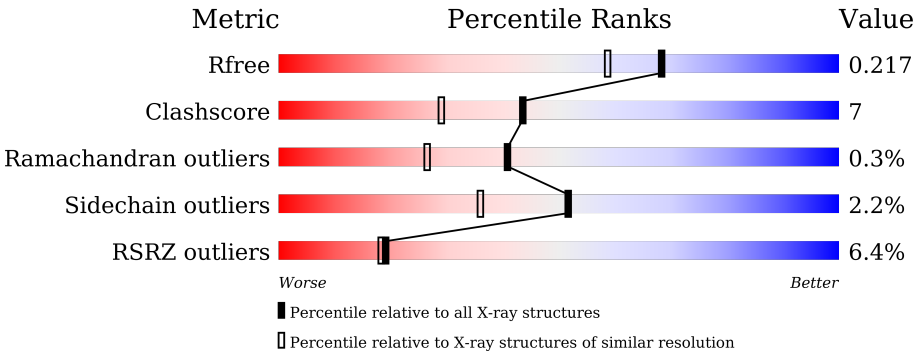
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 <=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	5% 88% 11%
1	B	1042	8% 84% 15%
1	C	1042	5% 87% 12%
1	D	1042	10% 82% 16%
1	E	1042	5% 86% 13%
1	F	1042	5% 81% 17%

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)

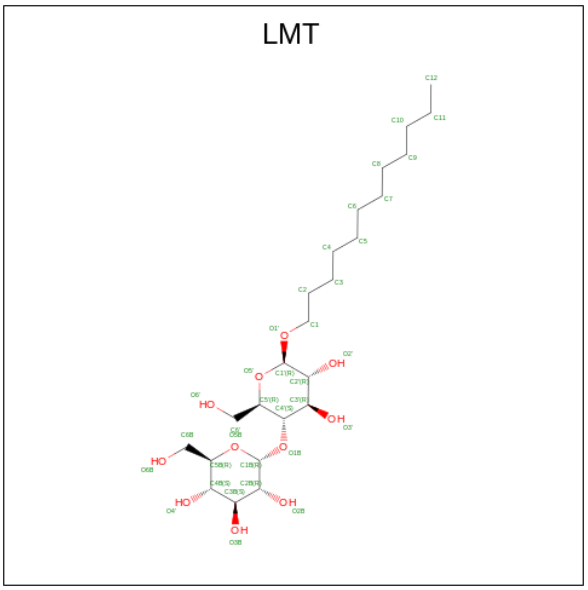
There are 5 unique types of molecules in this entry. The entry contains 53422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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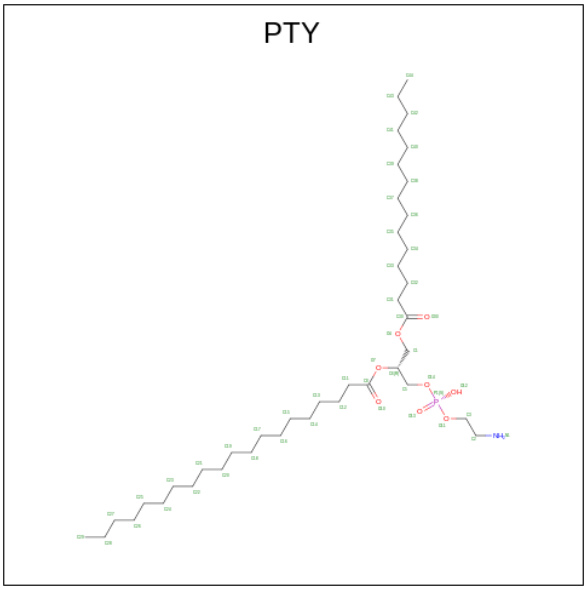
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 13 12 1	0	0
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 35 24 11	0	0
2	F	1	Total C O 17 15 2	0	0
2	F	1	Total C 6 6	0	0
2	F	1	Total C O 35 24 11	0	0

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

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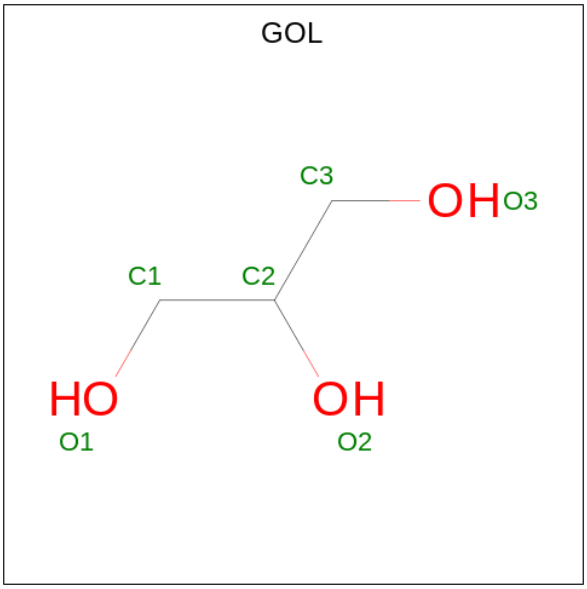
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C N O P 48 38 1 8 1	0	0
3	E	1	Total C N O P 46 36 1 8 1	0	0
3	E	1	Total C N O P 48 38 1 8 1	0	0
3	F	1	Total C O 37 33 4	0	0
3	F	1	Total C N O P 48 38 1 8 1	0	0

- 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 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

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

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

- Molecule 5 is water.

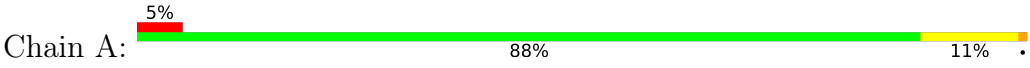
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	553	Total O 553 553	0	0
5	B	439	Total O 439 439	0	0
5	C	564	Total O 564 564	0	0
5	D	415	Total O 415 415	0	0
5	E	528	Total O 528 528	0	0
5	F	441	Total O 441 441	0	0

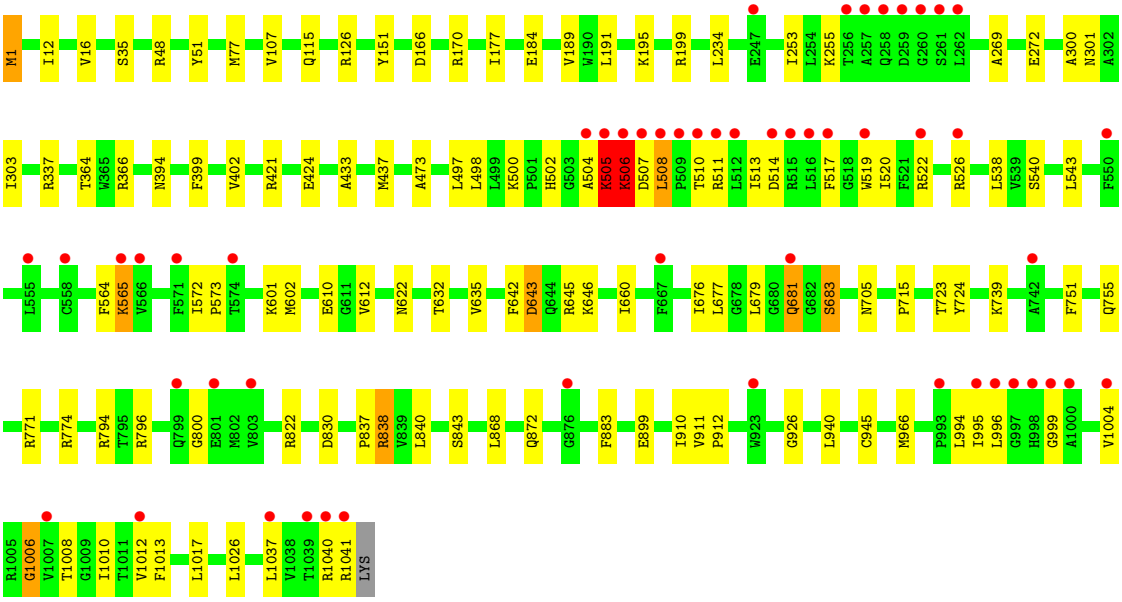
3 Residue-property plots (i)

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

• Molecule 1: Efflux pump membrane transporter

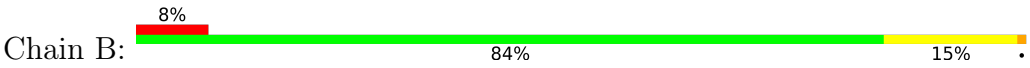
Chain A:

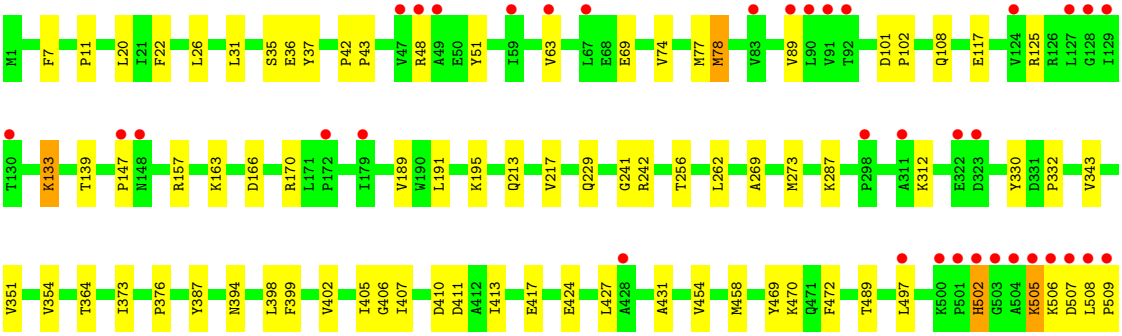


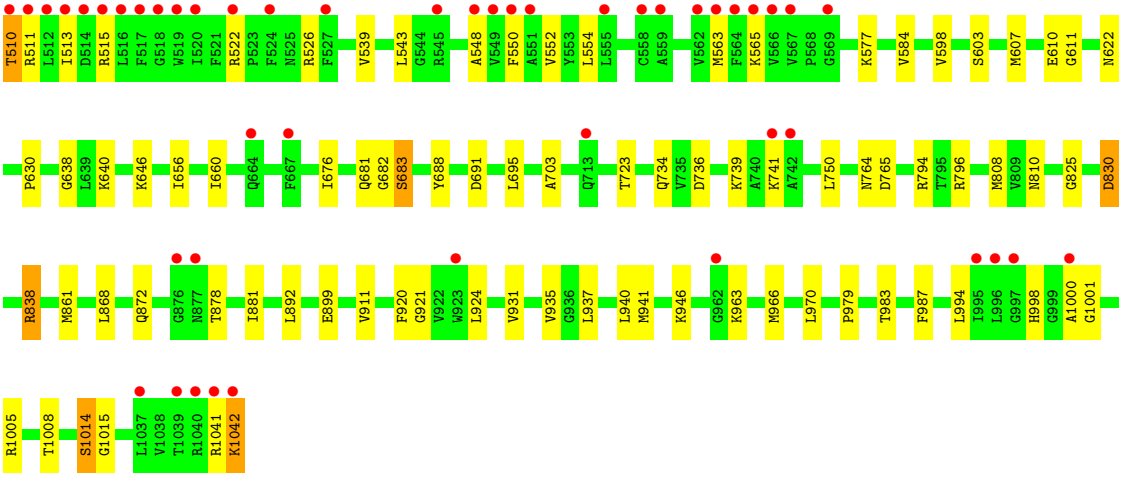


• Molecule 1: Efflux pump membrane transporter

Chain B:

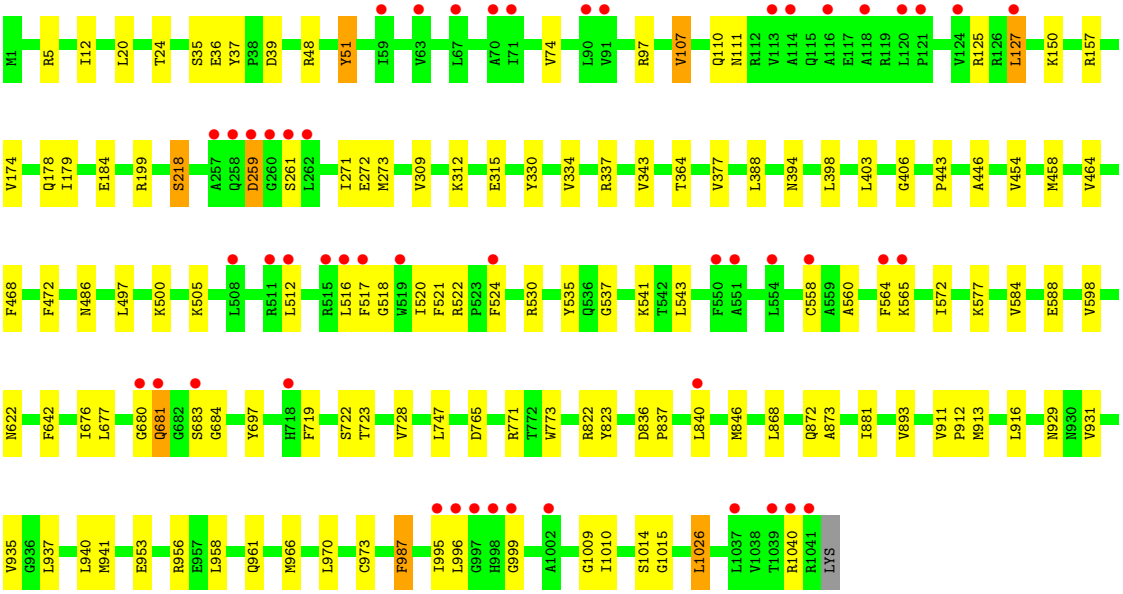






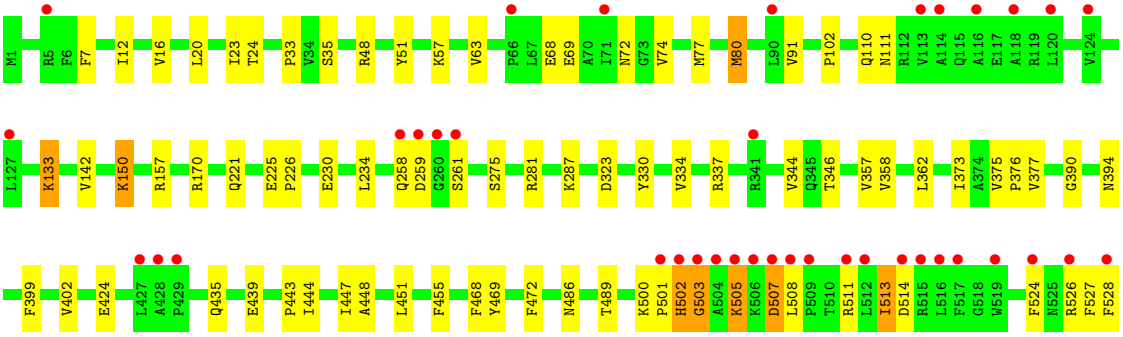
• Molecule 1: Efflux pump membrane transporter

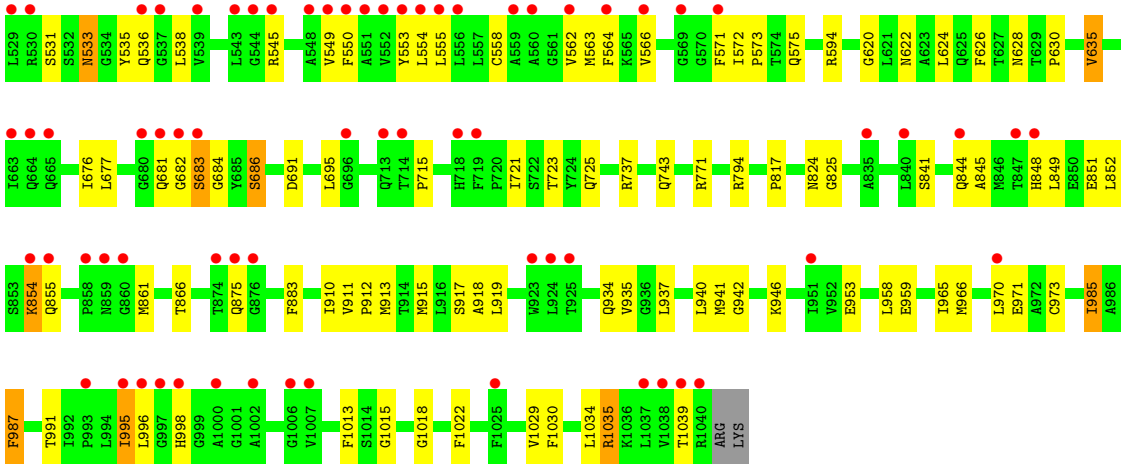
Chain C:



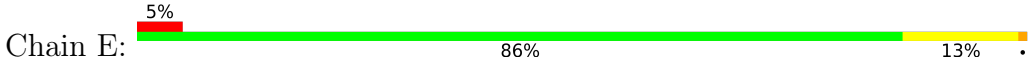
• Molecule 1: Efflux pump membrane transporter

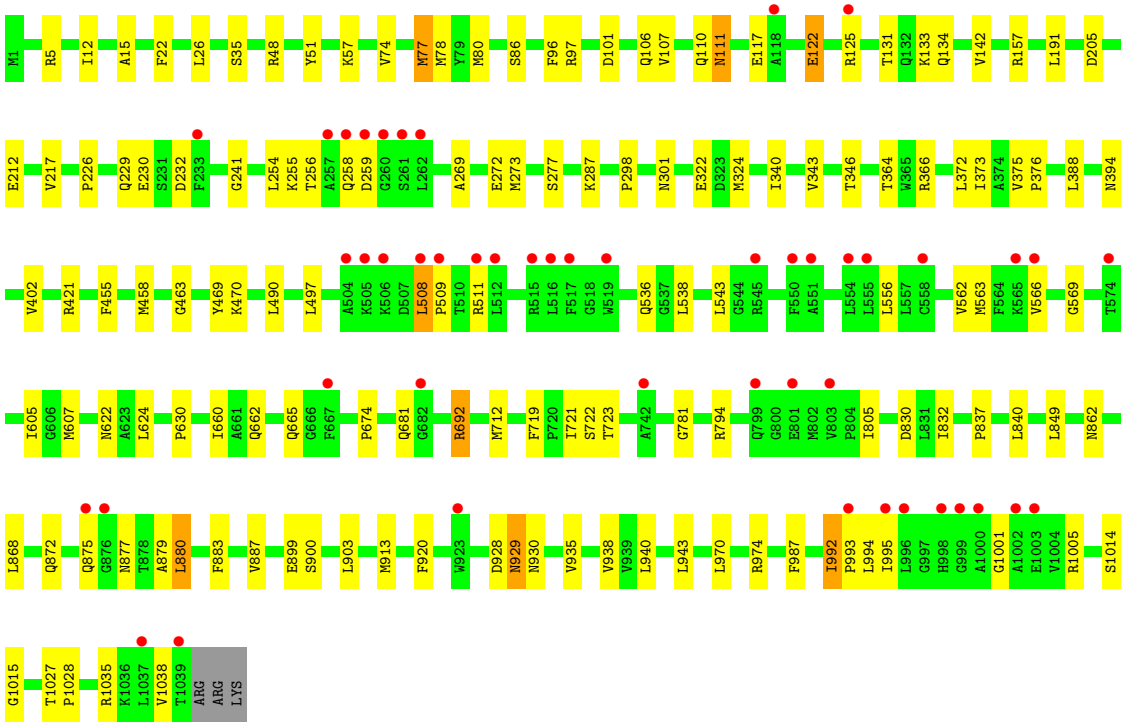
Chain D:



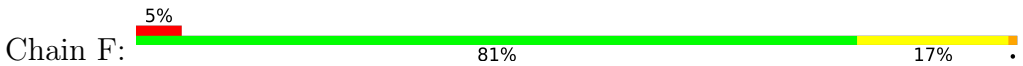


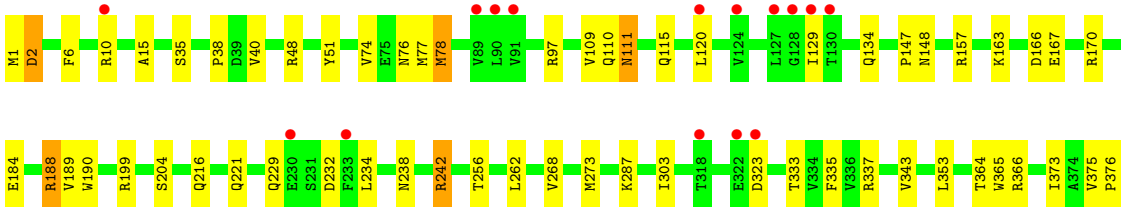
• Molecule 1: Efflux pump membrane transporter

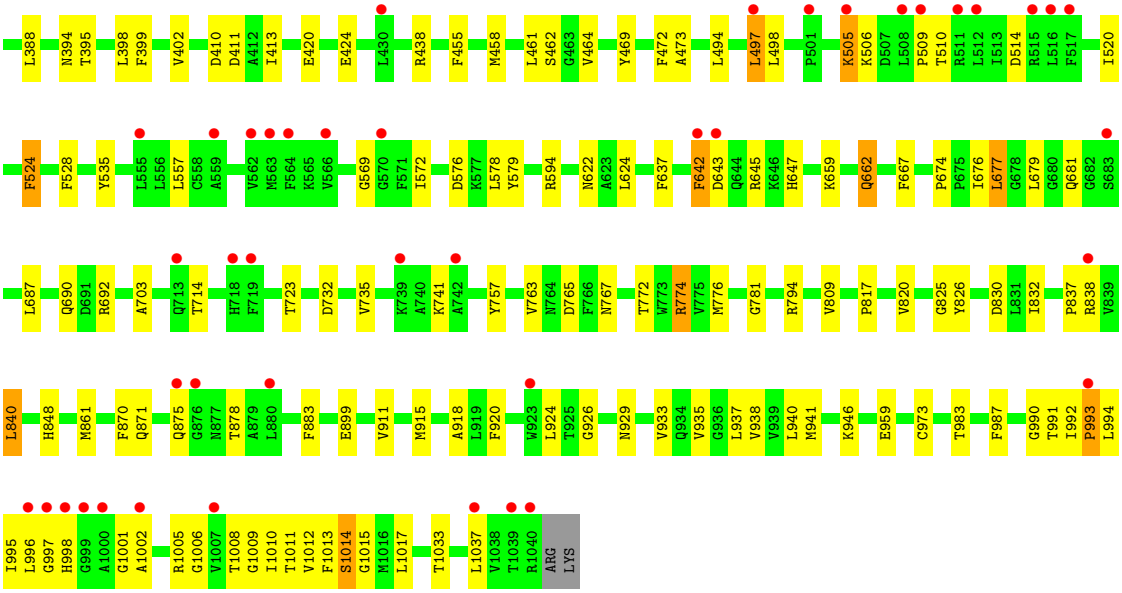




• Molecule 1: Efflux pump membrane transporter






L388 N394 T395 L398 F399 V402 D410 D411 A412 I413 E420 E424 L430 R438 F455 M458 L461 S462 G463 V464 Y469 F472 A473 L494 L497 L498 P501 K505 K506 D507 L508 P509 T510 R511 L512 I513 D514 R515 L516 F517 I520
F524 F528 Y535 L555 L556 L557 C558 A559 V562 M563 F564 K565 V566 G569 G570 F571 I572 D576 K577 L578 Y579 R594 N622 A623 L624 F637 F642 D643 Q644 R645 K646 H647 K659 Q662 F667 P674 P675 I676 L677 G678 L679 G680 Q681 G682 S683
L687 Q690 D691 R692 A703 Q713 T714 H718 F719 T723 D732 V735 K739 A740 K741 A742 Y757 V763 N764 D765 F766 N767 T772 W773 R774 V775 M776 G781 R794 V809 P817 V820 G825 Y826 D830 L831 I832 P837 R838 V839
L840 H848 M861 F870 Q871 Q875 G876 N877 T878 A879 L880 F883 E899 V911 M915 A918 L919 F920 W923 L924 T925 G926 N929 V933 Q934 V935 G936 L937 V938 V939 L940 M941 K946 E959 C973 T983 F987 G990 T991 I992 P993 L994
I995 L996 G997 H998 G999 A1000 G1001 A1002 R1005 G1006 V1007 T1008 G1009 I1010 T1011 V1012 F1013 S1014 G1015 M1016 L1017 T1033 L1037 V1038 T1039 R1040 ARG LYS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PTY, GOL, LMT

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%)

The worst 5 of 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

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1042/1042 (100%)	1010 (97%)	28 (3%)	4 (0%)	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

5 of 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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	853/851 (100%)	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

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	77	MET
1	F	677	LEU
1	D	854	LYS
1	F	662	GLN
1	F	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	872	GLN
1	F	134	GLN
1	E	110	GLN
1	F	743	GLN
1	F	115	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

116 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LMT	C	1107	-	36,36,36	1.15	3 (8%)	47,47,47	1.21	4 (8%)
2	LMT	E	1109	-	36,36,36	1.09	2 (5%)	47,47,47	1.09	4 (8%)
2	LMT	E	1110	-	36,36,36	1.02	1 (2%)	47,47,47	0.90	1 (2%)
2	LMT	C	1102	-	36,36,36	1.12	2 (5%)	47,47,47	1.05	3 (6%)
4	GOL	A	1115	-	5,5,5	1.66	2 (40%)	5,5,5	0.90	0
2	LMT	A	1107	-	36,36,36	1.04	2 (5%)	47,47,47	1.11	2 (4%)
3	PTY	E	1114	-	45,45,49	0.93	3 (6%)	48,50,54	1.06	2 (4%)
2	LMT	F	1112	-	5,5,36	0.22	0	4,4,47	0.66	0
3	PTY	B	1111	-	45,45,49	0.94	3 (6%)	48,50,54	0.98	2 (4%)
2	LMT	E	1101	-	36,36,36	1.14	5 (13%)	47,47,47	1.12	4 (8%)
2	LMT	F	1108	-	12,12,36	0.29	0	11,11,47	0.91	0
4	GOL	D	1114	-	5,5,5	1.07	1 (20%)	5,5,5	1.35	1 (20%)
2	LMT	F	1106	-	36,36,36	1.07	2 (5%)	47,47,47	1.37	7 (14%)
3	PTY	F	1114	-	36,36,49	0.88	2 (5%)	37,37,54	1.05	2 (5%)
2	LMT	D	1104	-	36,36,36	1.25	3 (8%)	47,47,47	1.19	5 (10%)
4	GOL	B	1115	-	5,5,5	0.88	0	5,5,5	1.63	2 (40%)
2	LMT	A	1105	-	36,36,36	1.18	2 (5%)	47,47,47	1.19	5 (10%)
4	GOL	D	1116	-	5,5,5	1.18	1 (20%)	5,5,5	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	F	1119	-	5,5,5	1.31	0	5,5,5	1.44	1 (20%)
2	LMT	F	1110	-	36,36,36	1.11	3 (8%)	47,47,47	1.34	6 (12%)
4	GOL	A	1117	-	5,5,5	0.92	0	5,5,5	0.98	0
4	GOL	C	1114	-	5,5,5	1.32	1 (20%)	5,5,5	1.20	0
4	GOL	C	1115	-	5,5,5	1.46	0	5,5,5	1.39	1 (20%)
4	GOL	F	1117	-	5,5,5	1.53	2 (40%)	5,5,5	1.69	1 (20%)
2	LMT	B	1108	-	11,11,36	0.21	0	10,10,47	0.73	0
2	LMT	B	1102	-	36,36,36	1.19	3 (8%)	47,47,47	1.29	2 (4%)
3	PTY	D	1113	-	47,47,49	0.96	2 (4%)	50,52,54	1.09	2 (4%)
2	LMT	E	1105	-	36,36,36	1.03	1 (2%)	47,47,47	1.08	4 (8%)
2	LMT	B	1106	-	36,36,36	1.06	2 (5%)	47,47,47	1.07	4 (8%)
2	LMT	A	1104	-	36,36,36	1.28	3 (8%)	47,47,47	1.15	3 (6%)
2	LMT	D	1107	-	36,36,36	1.14	4 (11%)	47,47,47	1.26	4 (8%)
2	LMT	D	1106	-	36,36,36	1.05	3 (8%)	47,47,47	1.23	6 (12%)
2	LMT	D	1102	-	36,36,36	1.05	2 (5%)	47,47,47	1.10	2 (4%)
2	LMT	C	1108	-	36,36,36	1.16	4 (11%)	47,47,47	1.51	6 (12%)
2	LMT	F	1105	-	36,36,36	1.12	3 (8%)	47,47,47	1.24	6 (12%)
2	LMT	D	1101	-	36,36,36	1.13	3 (8%)	47,47,47	1.03	2 (4%)
2	LMT	B	1104	-	36,36,36	1.09	4 (11%)	47,47,47	1.16	2 (4%)
2	LMT	C	1109	-	36,36,36	1.08	3 (8%)	47,47,47	1.08	3 (6%)
2	LMT	D	1112	-	36,36,36	1.13	3 (8%)	47,47,47	1.28	5 (10%)
2	LMT	D	1103	-	36,36,36	1.19	4 (11%)	47,47,47	1.20	3 (6%)
2	LMT	D	1108	-	36,36,36	1.07	3 (8%)	47,47,47	0.94	1 (2%)
2	LMT	A	1111	-	36,36,36	1.23	6 (16%)	47,47,47	1.20	5 (10%)
4	GOL	E	1120	-	5,5,5	0.71	0	5,5,5	1.34	1 (20%)
2	LMT	C	1104	-	36,36,36	1.10	4 (11%)	47,47,47	1.12	3 (6%)
2	LMT	A	1103	-	36,36,36	1.01	3 (8%)	47,47,47	1.18	4 (8%)
4	GOL	C	1119	-	5,5,5	1.02	0	5,5,5	1.17	0
4	GOL	F	1118	-	5,5,5	1.28	0	5,5,5	0.82	0
4	GOL	A	1114	-	5,5,5	1.57	1 (20%)	5,5,5	0.81	0
2	LMT	F	1101	-	36,36,36	1.10	3 (8%)	47,47,47	1.08	2 (4%)
4	GOL	C	1116	-	5,5,5	1.09	0	5,5,5	1.33	0
2	LMT	B	1103	-	36,36,36	0.94	2 (5%)	47,47,47	0.93	0
2	LMT	E	1111	-	11,11,36	0.17	0	10,10,47	0.72	0
4	GOL	B	1113	-	5,5,5	1.11	0	5,5,5	0.81	0
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	$\#\|Z\|>2$
2	LMT	E	1112	-	36,36,36	1.07	3 (8%)	47,47,47	1.22	5 (10%)
2	LMT	E	1107	-	36,36,36	1.09	1 (2%)	47,47,47	1.07	3 (6%)
4	GOL	C	1120	-	5,5,5	0.94	0	5,5,5	0.89	0
2	LMT	A	1102	-	36,36,36	0.94	1 (2%)	47,47,47	1.07	2 (4%)
2	LMT	D	1109	-	36,36,36	1.11	3 (8%)	47,47,47	1.15	5 (10%)
2	LMT	C	1103	-	36,36,36	1.08	2 (5%)	47,47,47	1.22	6 (12%)
2	LMT	B	1107	-	15,15,36	0.44	0	14,14,47	0.72	0
2	LMT	E	1102	-	36,36,36	1.21	3 (8%)	47,47,47	1.24	6 (12%)
4	GOL	C	1117	-	5,5,5	0.71	0	5,5,5	0.81	0
4	GOL	F	1116	-	5,5,5	1.84	1 (20%)	5,5,5	1.14	0
4	GOL	E	1116	-	5,5,5	1.64	2 (40%)	5,5,5	1.22	0
2	LMT	F	1113	-	36,36,36	1.02	3 (8%)	47,47,47	0.96	3 (6%)
2	LMT	B	1110	-	36,36,36	1.13	4 (11%)	47,47,47	1.02	3 (6%)
4	GOL	A	1120	-	5,5,5	0.86	0	5,5,5	1.98	2 (40%)
4	GOL	F	1120	-	5,5,5	0.59	0	5,5,5	1.43	1 (20%)
2	LMT	F	1102	-	36,36,36	1.07	3 (8%)	47,47,47	1.01	3 (6%)
2	LMT	E	1104	-	36,36,36	1.11	2 (5%)	47,47,47	1.00	2 (4%)
4	GOL	E	1122	-	5,5,5	3.13	3 (60%)	5,5,5	1.98	1 (20%)
2	LMT	F	1111	-	16,16,36	0.52	0	15,15,47	0.67	0
2	LMT	C	1110	-	36,36,36	1.05	1 (2%)	47,47,47	1.51	9 (19%)
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	1112	-	36,36,36	1.16	5 (13%)	47,47,47	1.34	6 (12%)
2	LMT	B	1109	-	36,36,36	0.99	2 (5%)	47,47,47	1.06	3 (6%)
4	GOL	E	1123	-	5,5,5	1.56	2 (40%)	5,5,5	0.95	0
4	GOL	A	1119	-	5,5,5	1.91	2 (40%)	5,5,5	1.09	0
4	GOL	A	1116	-	5,5,5	1.86	2 (40%)	5,5,5	0.92	0
2	LMT	E	1103	-	36,36,36	1.11	3 (8%)	47,47,47	1.20	7 (14%)
3	PTY	A	1112	-	45,45,49	0.92	3 (6%)	48,50,54	1.02	2 (4%)
2	LMT	F	1107	-	36,36,36	1.13	3 (8%)	47,47,47	1.06	3 (6%)
2	LMT	D	1111	-	36,36,36	1.09	4 (11%)	47,47,47	1.15	3 (6%)
2	LMT	E	1108	-	36,36,36	1.22	5 (13%)	47,47,47	1.09	2 (4%)
2	LMT	A	1101	-	36,36,36	1.18	4 (11%)	47,47,47	1.15	5 (10%)
2	LMT	A	1110	-	25,25,36	0.99	1 (4%)	30,30,47	1.09	2 (6%)
3	PTY	B	1112	-	47,47,49	0.92	3 (6%)	50,52,54	1.06	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LMT	E	1106	-	36,36,36	1.12	5 (13%)	47,47,47	1.39	7 (14%)
2	LMT	F	1103	-	36,36,36	1.22	3 (8%)	47,47,47	1.24	8 (17%)
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%)
4	GOL	E	1118	-	5,5,5	1.51	1 (20%)	5,5,5	0.72	0
2	LMT	C	1101	-	36,36,36	1.14	1 (2%)	47,47,47	1.04	3 (6%)
2	LMT	F	1104	-	36,36,36	1.12	2 (5%)	47,47,47	1.42	5 (10%)
2	LMT	A	1106	-	36,36,36	1.14	4 (11%)	47,47,47	1.35	6 (12%)
2	LMT	A	1108	-	35,35,36	1.14	4 (11%)	46,46,47	1.12	3 (6%)
2	LMT	E	1113	-	9,9,36	0.25	0	8,8,47	0.73	0
4	GOL	A	1118	-	5,5,5	1.49	1 (20%)	5,5,5	1.22	0
4	GOL	A	1121	-	5,5,5	1.04	0	5,5,5	1.07	1 (20%)
2	LMT	B	1101	-	36,36,36	1.02	1 (2%)	47,47,47	1.10	5 (10%)
2	LMT	A	1109	-	36,36,36	1.07	2 (5%)	47,47,47	0.83	0
4	GOL	B	1114	-	5,5,5	0.89	0	5,5,5	0.96	0
4	GOL	D	1117	-	5,5,5	1.12	0	5,5,5	0.99	0
2	LMT	F	1109	-	36,36,36	1.02	1 (2%)	47,47,47	1.10	3 (6%)
2	LMT	B	1105	-	36,36,36	1.14	4 (11%)	47,47,47	1.22	5 (10%)
4	GOL	D	1115	-	5,5,5	1.54	1 (20%)	5,5,5	1.13	0
3	PTY	E	1115	-	47,47,49	0.97	3 (6%)	50,52,54	0.96	2 (4%)
2	LMT	C	1106	-	36,36,36	1.08	4 (11%)	47,47,47	1.07	3 (6%)
2	LMT	C	1105	-	36,36,36	0.92	1 (2%)	47,47,47	1.30	6 (12%)
4	GOL	E	1117	-	5,5,5	1.12	0	5,5,5	0.76	0
2	LMT	D	1110	-	9,9,36	0.34	0	8,8,47	0.81	0
4	GOL	C	1118	-	5,5,5	2.43	1 (20%)	5,5,5	0.68	0
4	GOL	E	1119	-	5,5,5	1.20	1 (20%)	5,5,5	1.72	1 (20%)
3	PTY	C	1113	-	47,47,49	0.98	3 (6%)	50,52,54	1.15	4 (8%)

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	C	1107	-	-	3/21/61/61	0/2/2/2
2	LMT	E	1109	-	-	6/21/61/61	0/2/2/2
2	LMT	E	1110	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	C	1102	-	-	6/21/61/61	0/2/2/2
4	GOL	A	1115	-	-	2/4/4/4	-
2	LMT	A	1107	-	-	13/21/61/61	0/2/2/2
3	PTY	E	1114	-	-	28/49/49/53	-
2	LMT	F	1112	-	-	2/3/3/61	-
3	PTY	B	1111	-	-	24/49/49/53	-
2	LMT	E	1101	-	-	4/21/61/61	0/2/2/2
2	LMT	F	1108	-	-	5/10/10/61	-
4	GOL	D	1114	-	-	1/4/4/4	-
2	LMT	F	1106	-	-	12/21/61/61	0/2/2/2
3	PTY	F	1114	-	-	17/36/36/53	-
2	LMT	D	1104	-	-	10/21/61/61	0/2/2/2
4	GOL	B	1115	-	-	2/4/4/4	-
2	LMT	A	1105	-	-	12/21/61/61	0/2/2/2
4	GOL	D	1116	-	-	2/4/4/4	-
4	GOL	F	1119	-	-	4/4/4/4	-
2	LMT	F	1110	-	-	12/21/61/61	0/2/2/2
4	GOL	A	1117	-	-	1/4/4/4	-
4	GOL	C	1114	-	-	1/4/4/4	-
4	GOL	C	1115	-	-	2/4/4/4	-
4	GOL	F	1117	-	-	1/4/4/4	-
2	LMT	B	1108	-	-	3/9/9/61	-
2	LMT	B	1102	-	-	13/21/61/61	0/2/2/2
3	PTY	D	1113	-	-	23/51/51/53	-
2	LMT	E	1105	-	-	13/21/61/61	0/2/2/2
2	LMT	B	1106	-	-	10/21/61/61	0/2/2/2
2	LMT	A	1104	-	-	4/21/61/61	0/2/2/2
2	LMT	D	1107	-	-	11/21/61/61	0/2/2/2
2	LMT	D	1106	-	-	10/21/61/61	0/2/2/2
2	LMT	D	1102	-	-	2/21/61/61	0/2/2/2
2	LMT	C	1108	-	-	13/21/61/61	0/2/2/2
2	LMT	F	1105	-	-	14/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	B	1104	-	-	8/21/61/61	0/2/2/2
2	LMT	C	1109	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	D	1112	-	-	13/21/61/61	0/2/2/2
2	LMT	D	1103	-	-	6/21/61/61	0/2/2/2
2	LMT	D	1108	-	-	10/21/61/61	0/2/2/2
2	LMT	A	1111	-	-	9/21/61/61	0/2/2/2
4	GOL	E	1120	-	-	0/4/4/4	-
2	LMT	C	1104	-	-	7/21/61/61	0/2/2/2
2	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
4	GOL	C	1119	-	-	4/4/4/4	-
4	GOL	F	1118	-	-	4/4/4/4	-
4	GOL	A	1114	-	-	3/4/4/4	-
2	LMT	F	1101	-	-	7/21/61/61	0/2/2/2
4	GOL	C	1116	-	-	4/4/4/4	-
2	LMT	B	1103	-	-	10/21/61/61	0/2/2/2
2	LMT	E	1111	-	-	8/9/9/61	-
4	GOL	B	1113	-	-	1/4/4/4	-
2	LMT	D	1105	-	-	11/21/61/61	0/2/2/2
2	LMT	E	1112	-	-	9/21/61/61	0/2/2/2
2	LMT	E	1107	-	-	8/21/61/61	0/2/2/2
4	GOL	C	1120	-	-	2/4/4/4	-
2	LMT	A	1102	-	-	3/21/61/61	0/2/2/2
2	LMT	D	1109	-	-	13/21/61/61	0/2/2/2
2	LMT	C	1103	-	-	12/21/61/61	0/2/2/2
2	LMT	B	1107	-	-	9/13/13/61	-
2	LMT	E	1102	-	-	14/21/61/61	0/2/2/2
4	GOL	C	1117	-	-	2/4/4/4	-
4	GOL	F	1116	-	-	2/4/4/4	-
4	GOL	E	1116	-	-	4/4/4/4	-
2	LMT	F	1113	-	-	9/21/61/61	0/2/2/2
2	LMT	B	1110	-	-	8/21/61/61	0/2/2/2
4	GOL	A	1120	-	-	4/4/4/4	-
4	GOL	F	1120	-	-	1/4/4/4	-
2	LMT	F	1102	-	-	6/21/61/61	0/2/2/2
2	LMT	E	1104	-	-	7/21/61/61	0/2/2/2
4	GOL	E	1122	-	-	0/4/4/4	-
2	LMT	F	1111	-	-	8/14/14/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	C	1110	-	-	9/21/61/61	0/2/2/2
4	GOL	A	1113	-	-	4/4/4/4	-
4	GOL	E	1121	-	-	2/4/4/4	-
2	LMT	C	1112	-	-	13/21/61/61	0/2/2/2
2	LMT	B	1109	-	-	12/21/61/61	0/2/2/2
4	GOL	E	1123	-	-	4/4/4/4	-
4	GOL	A	1119	-	-	1/4/4/4	-
4	GOL	A	1116	-	-	4/4/4/4	-
2	LMT	E	1103	-	-	7/21/61/61	0/2/2/2
3	PTY	A	1112	-	-	22/49/49/53	-
2	LMT	F	1107	-	-	13/21/61/61	0/2/2/2
2	LMT	D	1111	-	-	12/21/61/61	0/2/2/2
2	LMT	E	1108	-	-	16/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	9/21/61/61	0/2/2/2
2	LMT	A	1110	-	-	11/17/37/61	0/1/1/2
3	PTY	B	1112	-	-	33/51/51/53	-
2	LMT	E	1106	-	-	7/21/61/61	0/2/2/2
2	LMT	F	1103	-	-	10/21/61/61	0/2/2/2
2	LMT	C	1111	-	-	14/21/61/61	0/2/2/2
3	PTY	F	1115	-	-	21/51/51/53	-
4	GOL	E	1118	-	-	1/4/4/4	-
2	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	F	1104	-	-	6/21/61/61	0/2/2/2
2	LMT	A	1106	-	-	12/21/61/61	0/2/2/2
2	LMT	A	1108	-	-	7/20/60/61	0/2/2/2
2	LMT	E	1113	-	-	2/7/7/61	-
4	GOL	A	1118	-	-	2/4/4/4	-
4	GOL	A	1121	-	-	2/4/4/4	-
2	LMT	B	1101	-	-	11/21/61/61	0/2/2/2
2	LMT	A	1109	-	-	9/21/61/61	0/2/2/2
4	GOL	B	1114	-	-	4/4/4/4	-
4	GOL	D	1117	-	-	2/4/4/4	-
2	LMT	F	1109	-	-	8/21/61/61	0/2/2/2
2	LMT	B	1105	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	1115	-	-	4/4/4/4	-
3	PTY	E	1115	-	-	24/51/51/53	-
2	LMT	C	1106	-	-	11/21/61/61	0/2/2/2
2	LMT	C	1105	-	-	7/21/61/61	0/2/2/2
4	GOL	E	1117	-	-	2/4/4/4	-
2	LMT	D	1110	-	-	2/7/7/61	-
4	GOL	C	1118	-	-	2/4/4/4	-
4	GOL	E	1119	-	-	4/4/4/4	-
3	PTY	C	1113	-	-	23/51/51/53	-

The worst 5 of 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

The worst 5 of 280 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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

There are no ring outliers.

80 monomers are involved in 202 short contacts:

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

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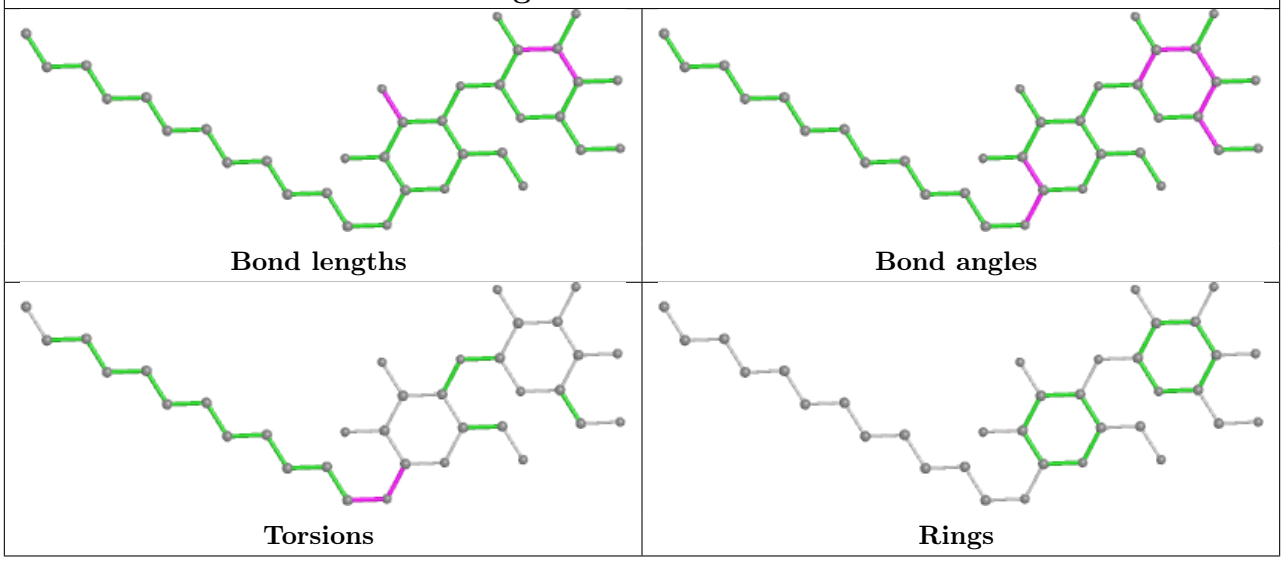
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1103	LMT	3	0
2	B	1107	LMT	1	0
2	E	1102	LMT	1	0
4	C	1117	GOL	1	0
4	F	1116	GOL	1	0
4	E	1116	GOL	5	0
2	F	1113	LMT	1	0
2	F	1102	LMT	3	0
4	E	1122	GOL	1	0
2	F	1111	LMT	3	0
4	E	1121	GOL	2	0
2	C	1112	LMT	4	0
2	B	1109	LMT	1	0
4	A	1119	GOL	1	0
4	A	1116	GOL	1	0
2	E	1103	LMT	7	0
3	A	1112	PTY	4	0
2	F	1107	LMT	1	0
2	E	1108	LMT	11	0
2	A	1110	LMT	5	0
3	B	1112	PTY	2	0
2	E	1106	LMT	1	0
2	F	1103	LMT	7	0
2	C	1111	LMT	3	0
3	F	1115	PTY	1	0
2	C	1101	LMT	2	0
2	F	1104	LMT	1	0
2	A	1106	LMT	1	0
2	A	1108	LMT	2	0
2	E	1113	LMT	1	0
4	A	1121	GOL	2	0
2	B	1101	LMT	3	0
4	B	1114	GOL	1	0
2	F	1109	LMT	1	0
3	E	1115	PTY	2	0
4	C	1118	GOL	3	0
4	E	1119	GOL	1	0
3	C	1113	PTY	1	0

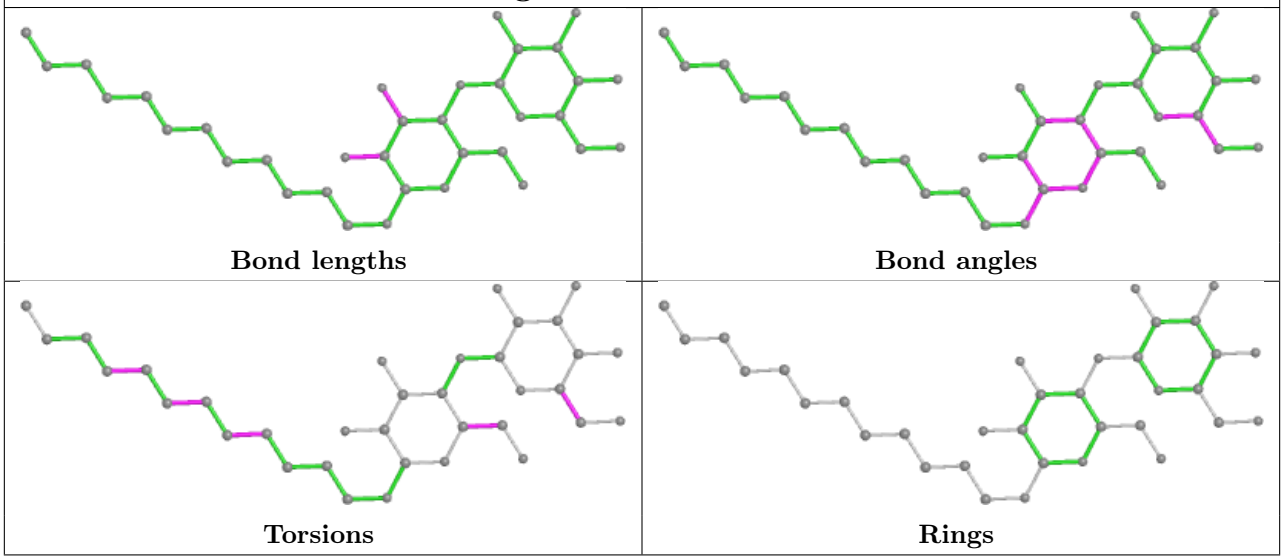
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

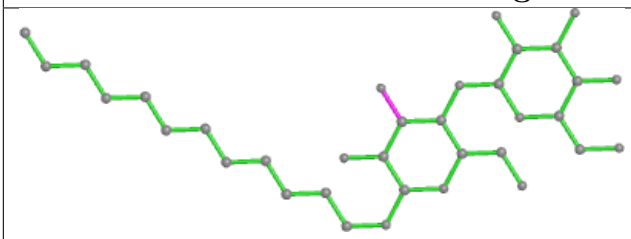
Ligand LMT C 1107



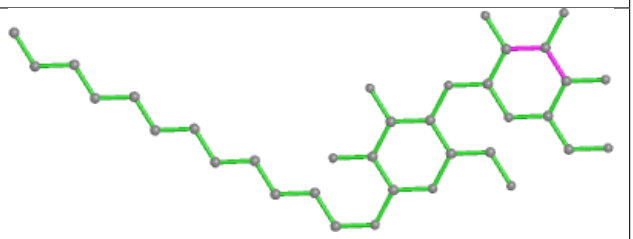
Ligand LMT E 1109



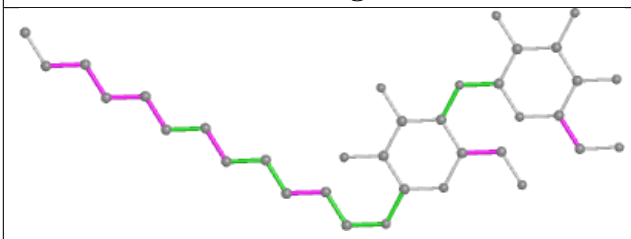
Ligand LMT E 1110



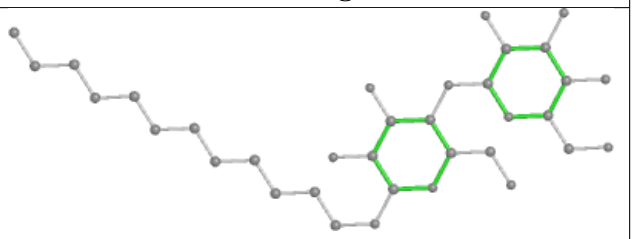
Bond lengths



Bond angles

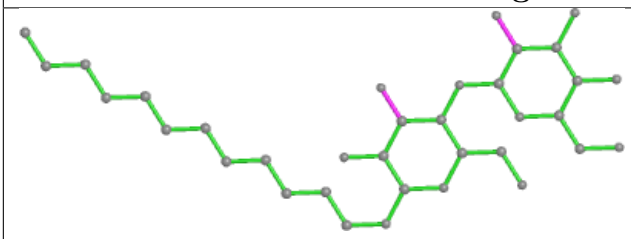


Torsions

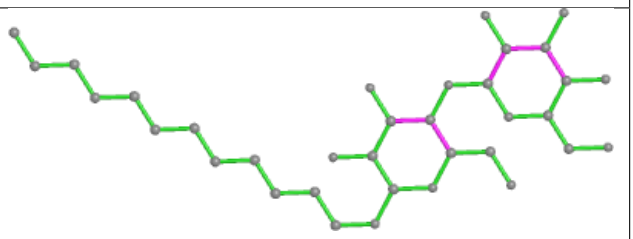


Rings

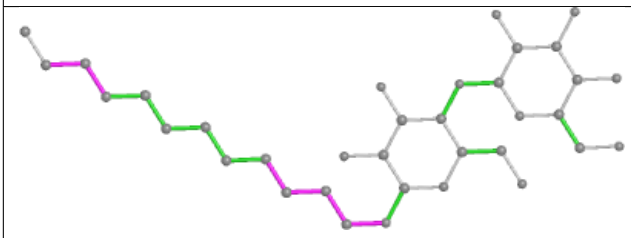
Ligand LMT C 1102



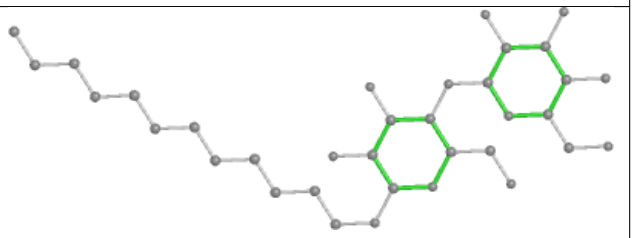
Bond lengths



Bond angles

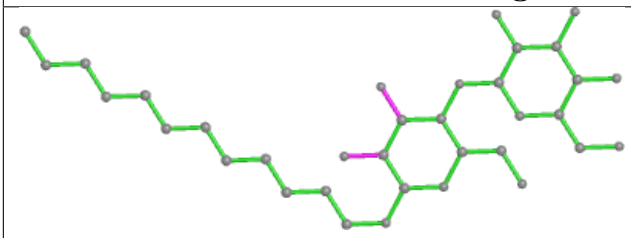


Torsions

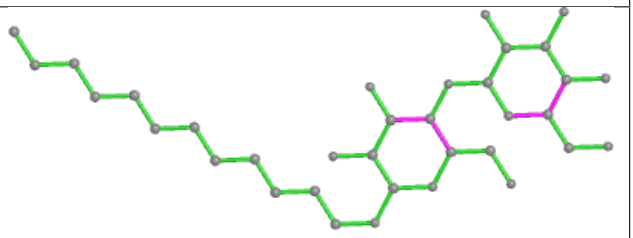


Rings

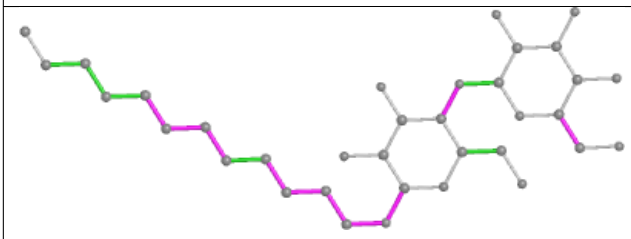
Ligand LMT A 1107



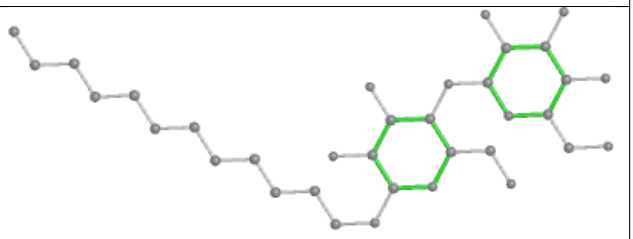
Bond lengths



Bond angles

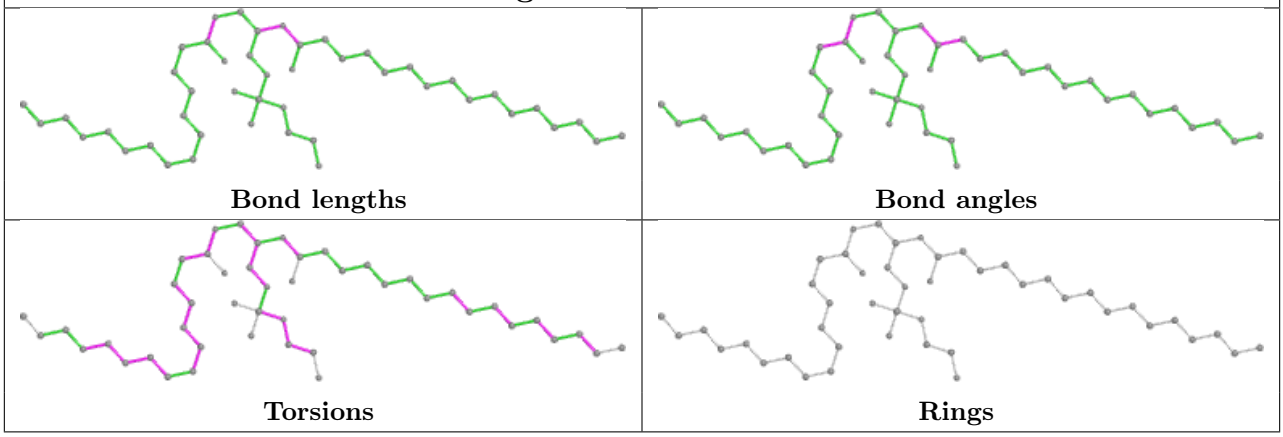


Torsions

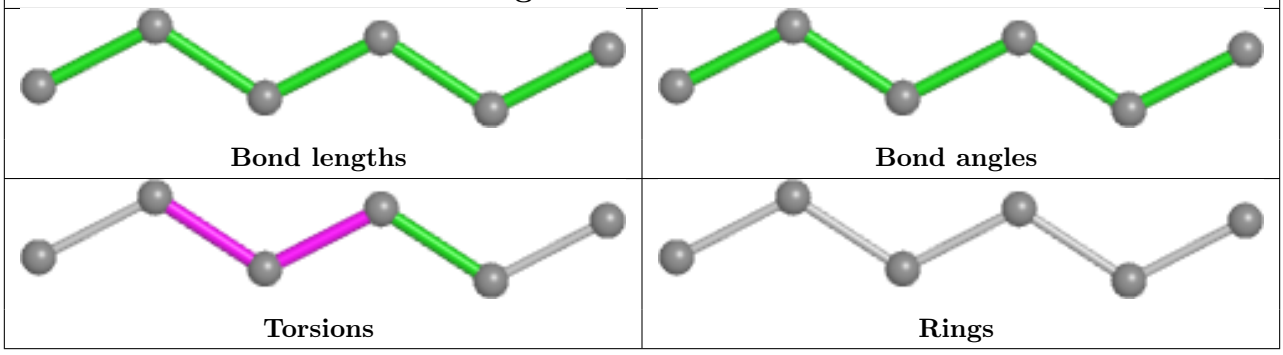


Rings

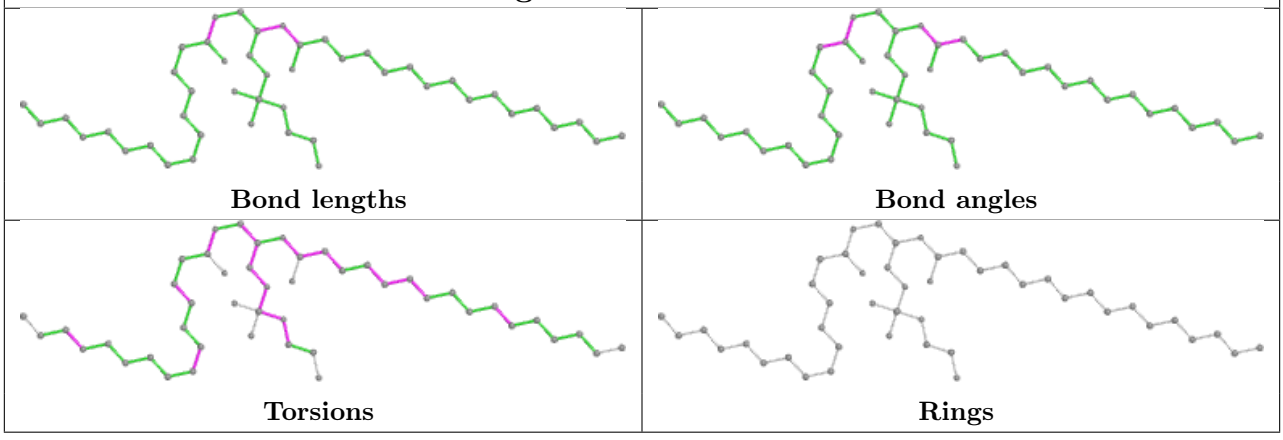
Ligand PTY E 1114



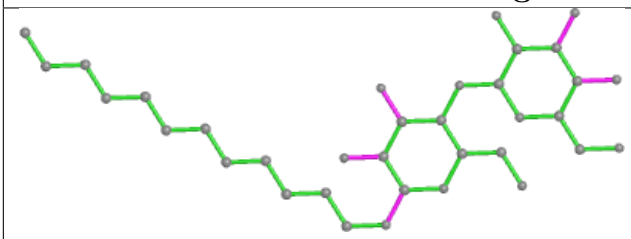
Ligand LMT F 1112



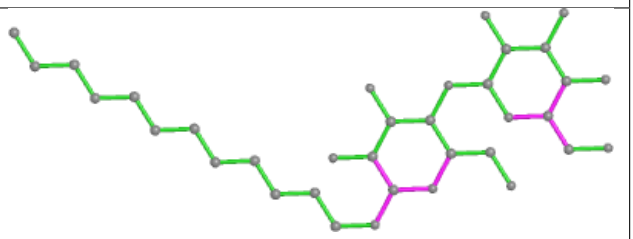
Ligand PTY B 1111



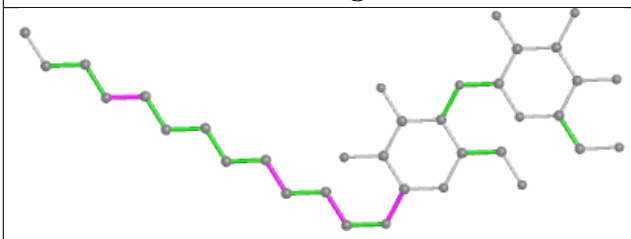
Ligand LMT E 1101



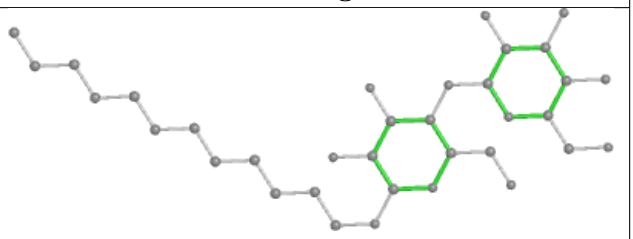
Bond lengths



Bond angles

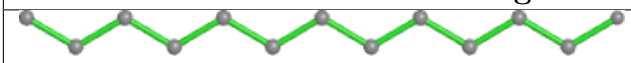


Torsions

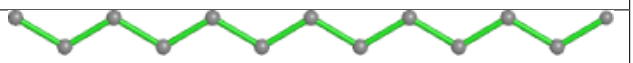


Rings

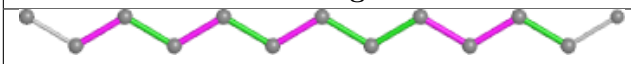
Ligand LMT F 1108



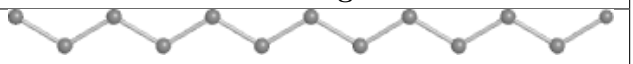
Bond lengths



Bond angles

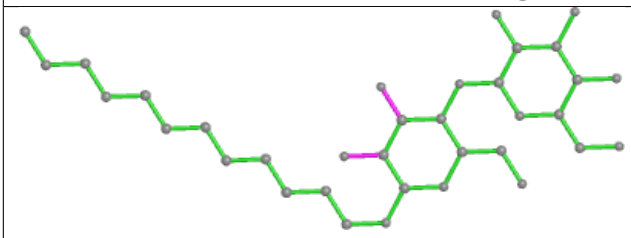


Torsions

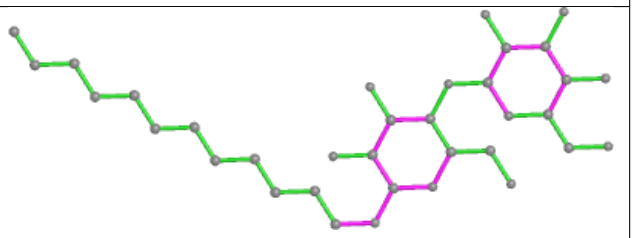


Rings

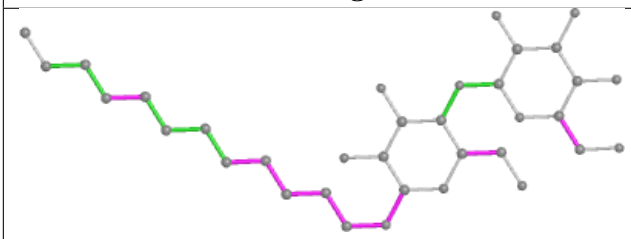
Ligand LMT F 1106



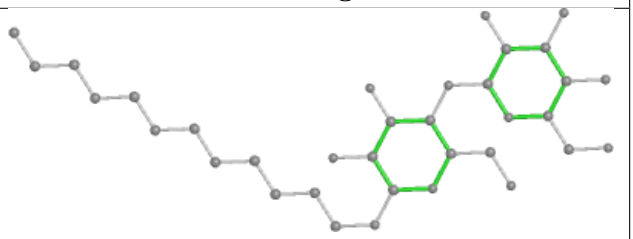
Bond lengths



Bond angles

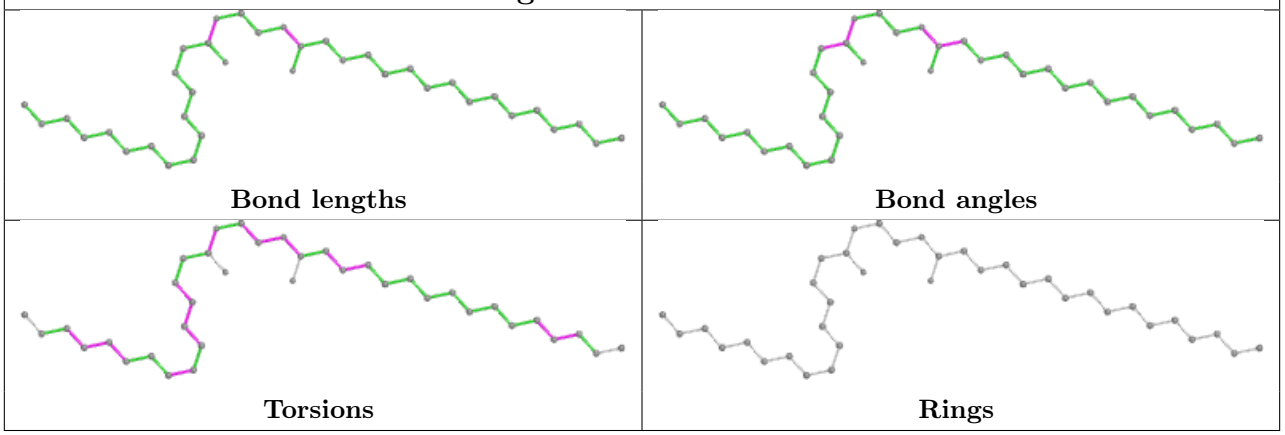


Torsions

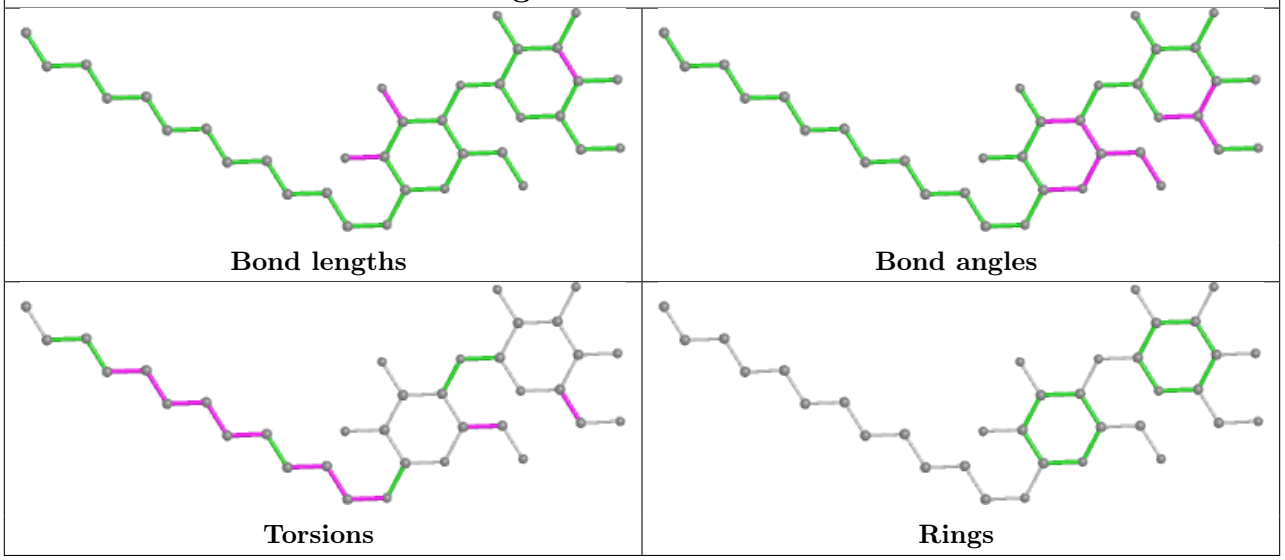


Rings

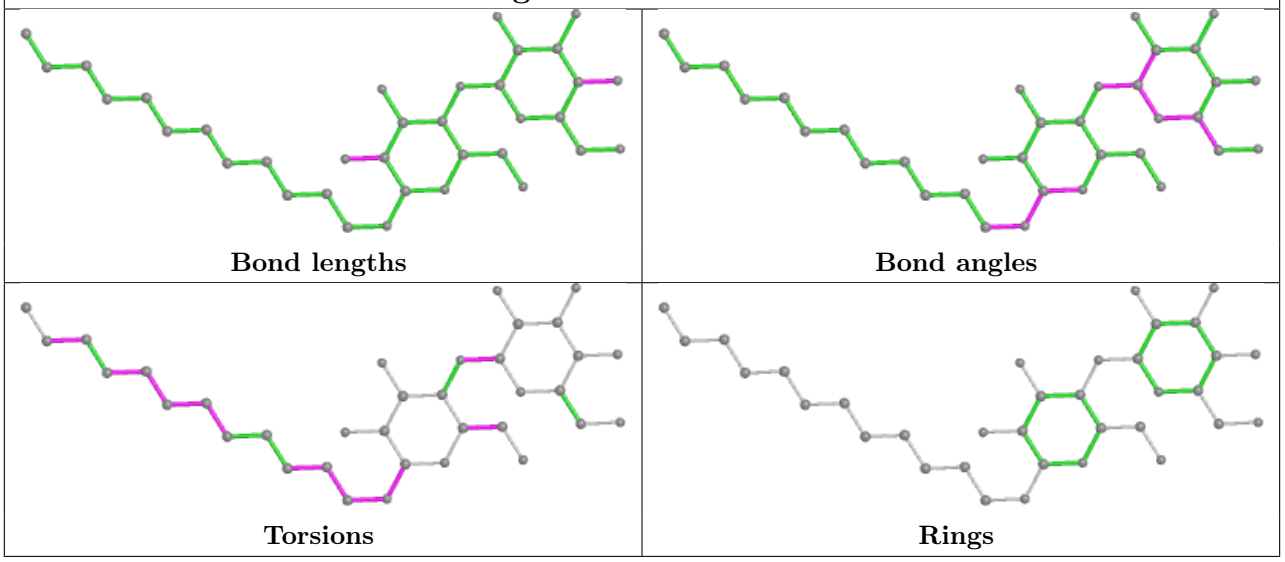
Ligand PTY F 1114



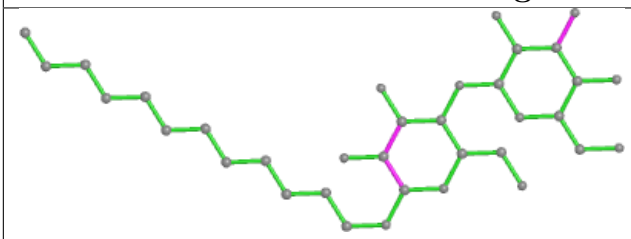
Ligand LMT D 1104



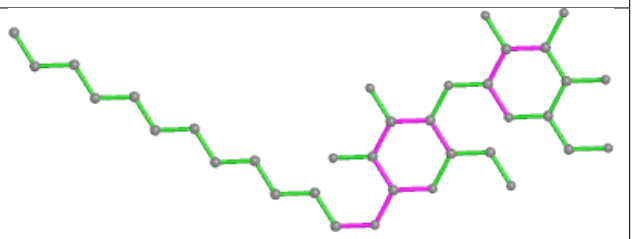
Ligand LMT A 1105



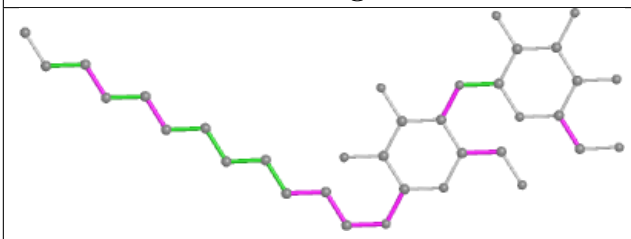
Ligand LMT F 1110



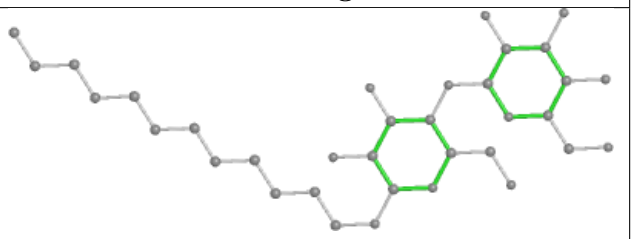
Bond lengths



Bond angles

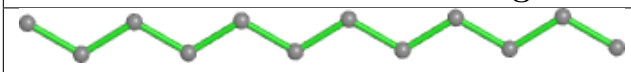


Torsions

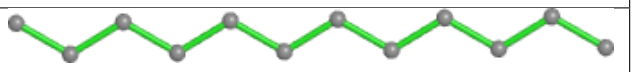


Rings

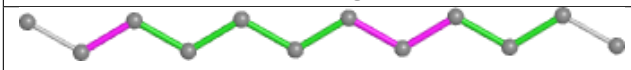
Ligand LMT B 1108



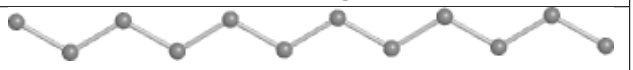
Bond lengths



Bond angles

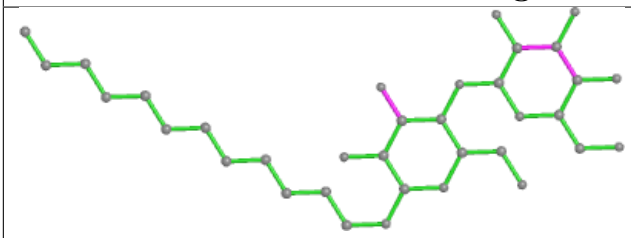


Torsions

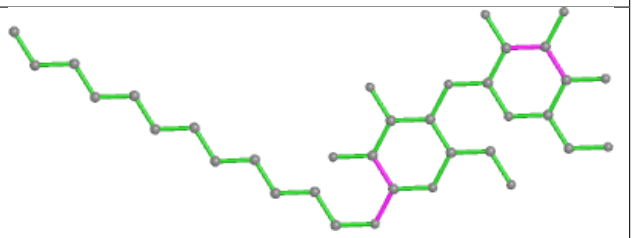


Rings

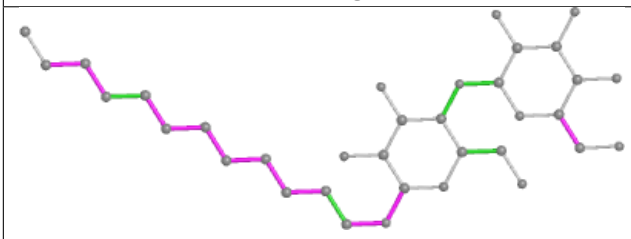
Ligand LMT B 1102



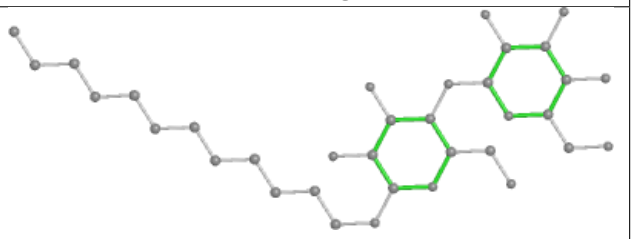
Bond lengths



Bond angles

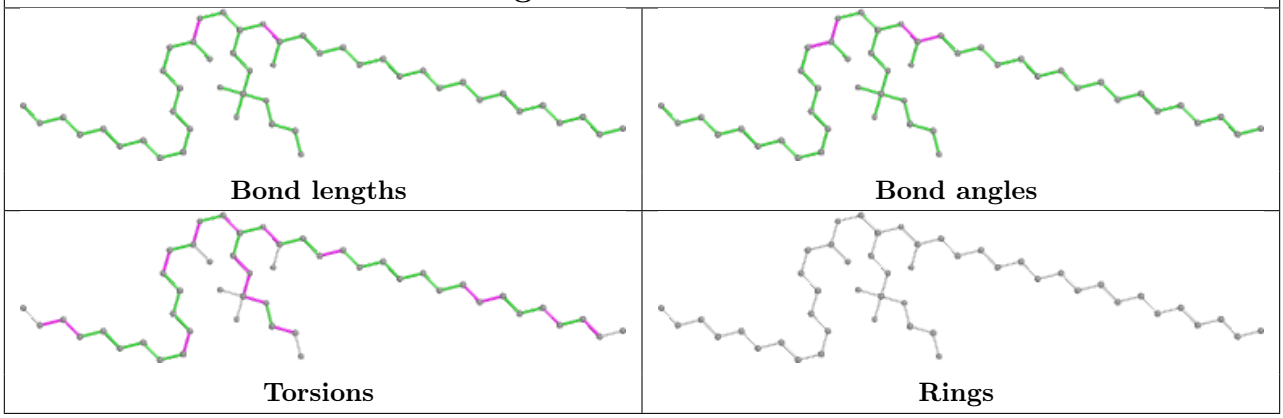


Torsions

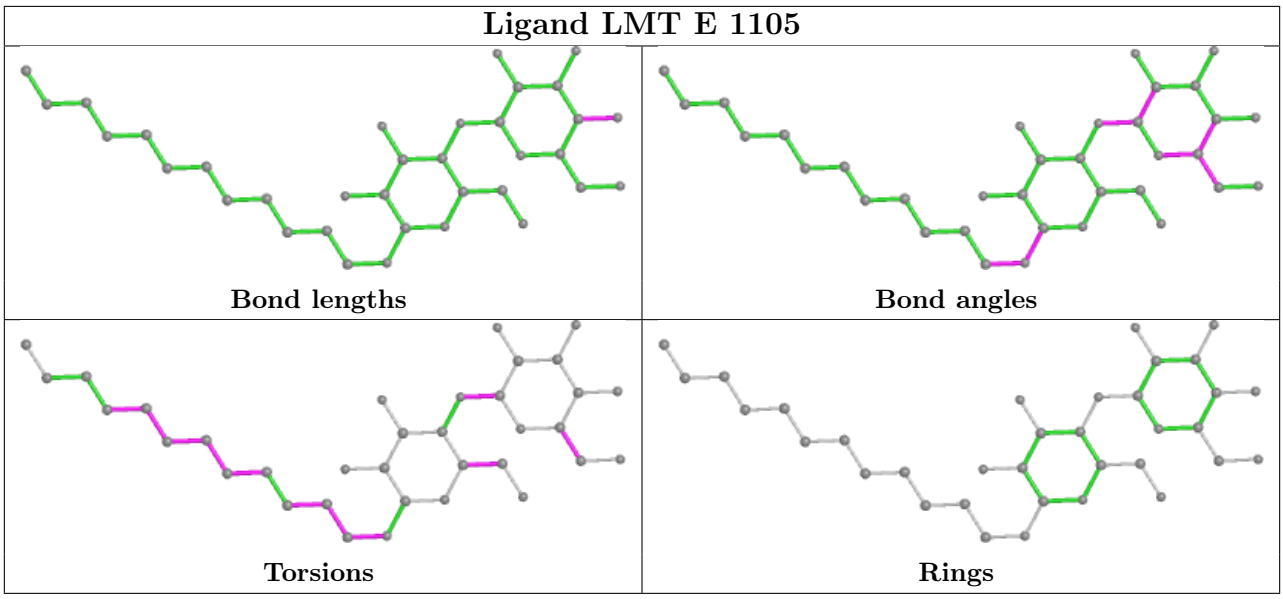


Rings

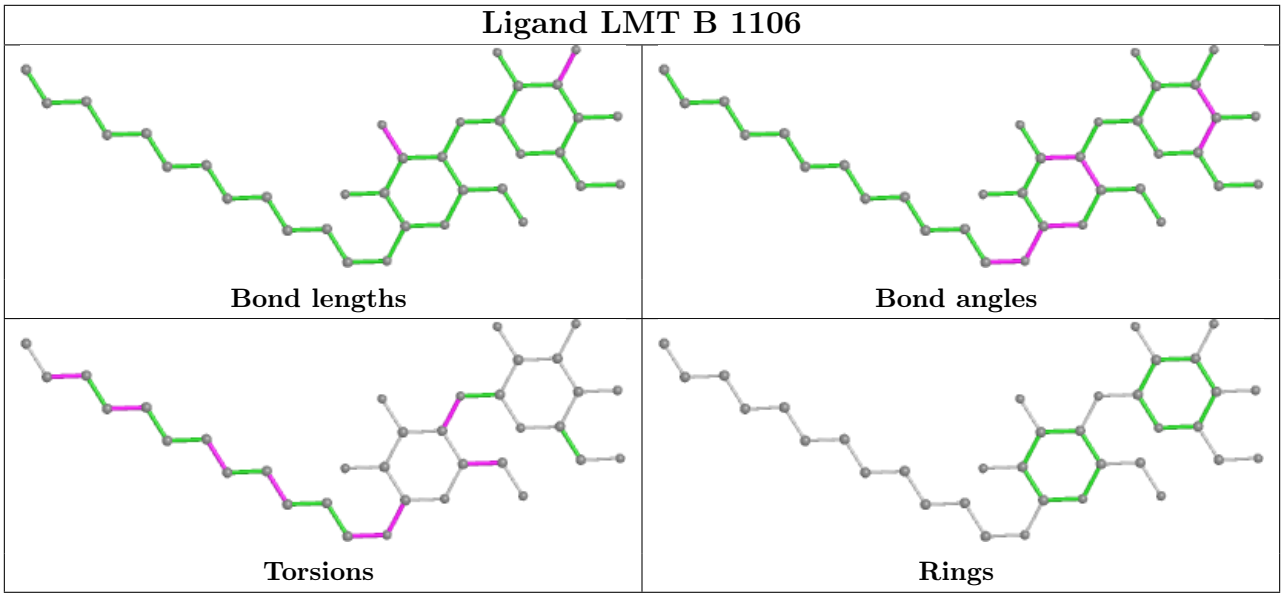
Ligand PTY D 1113



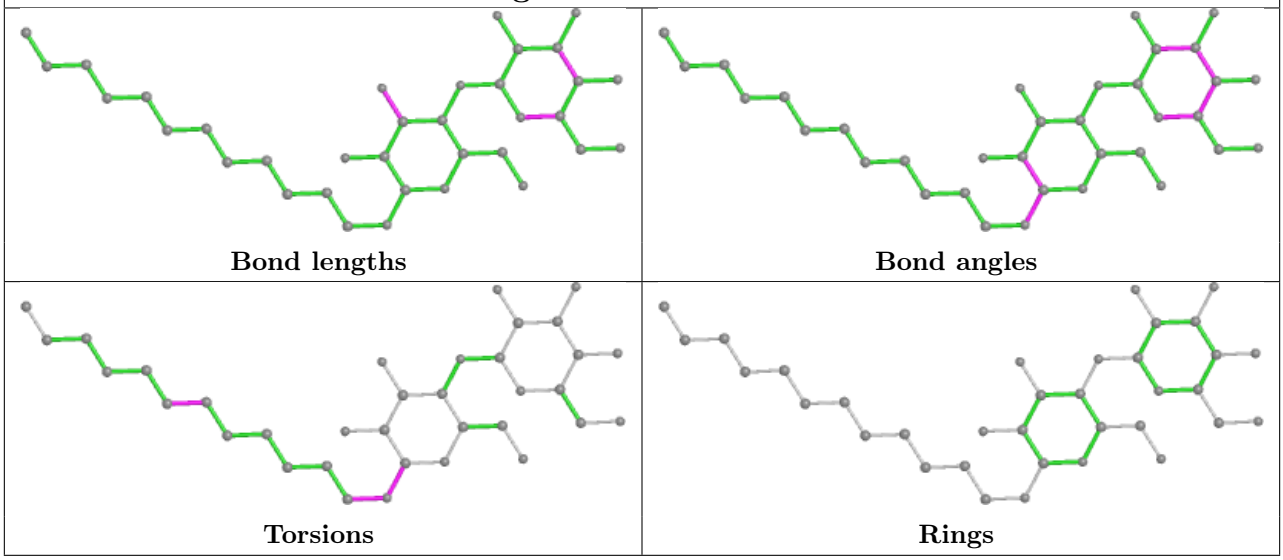
Ligand LMT E 1105



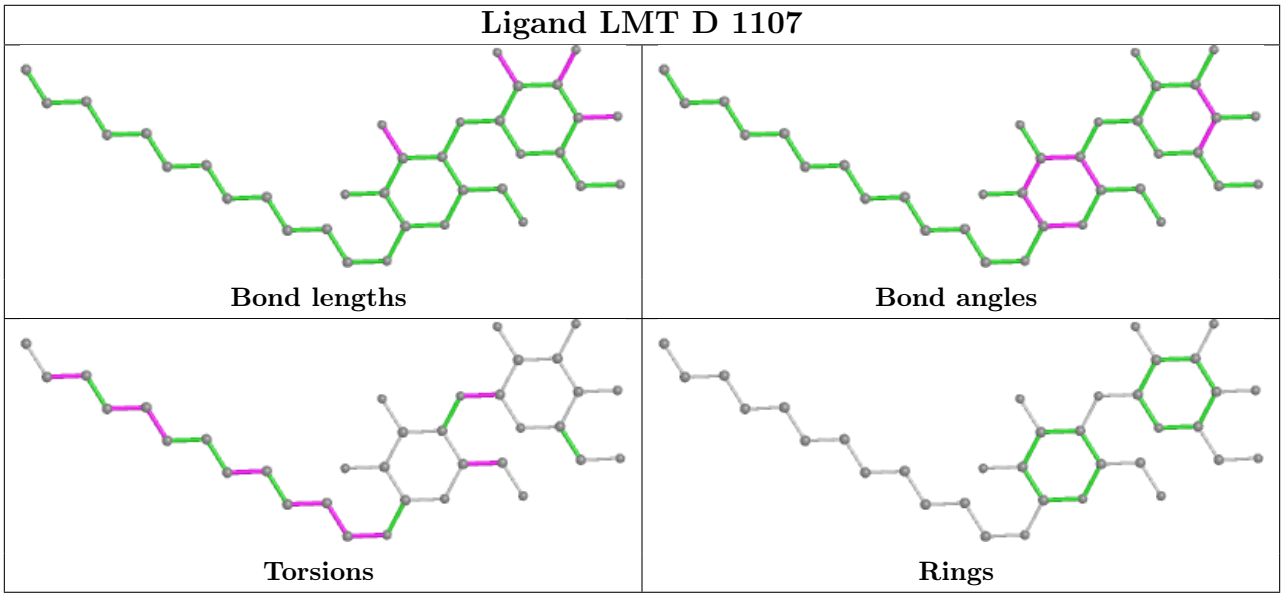
Ligand LMT B 1106



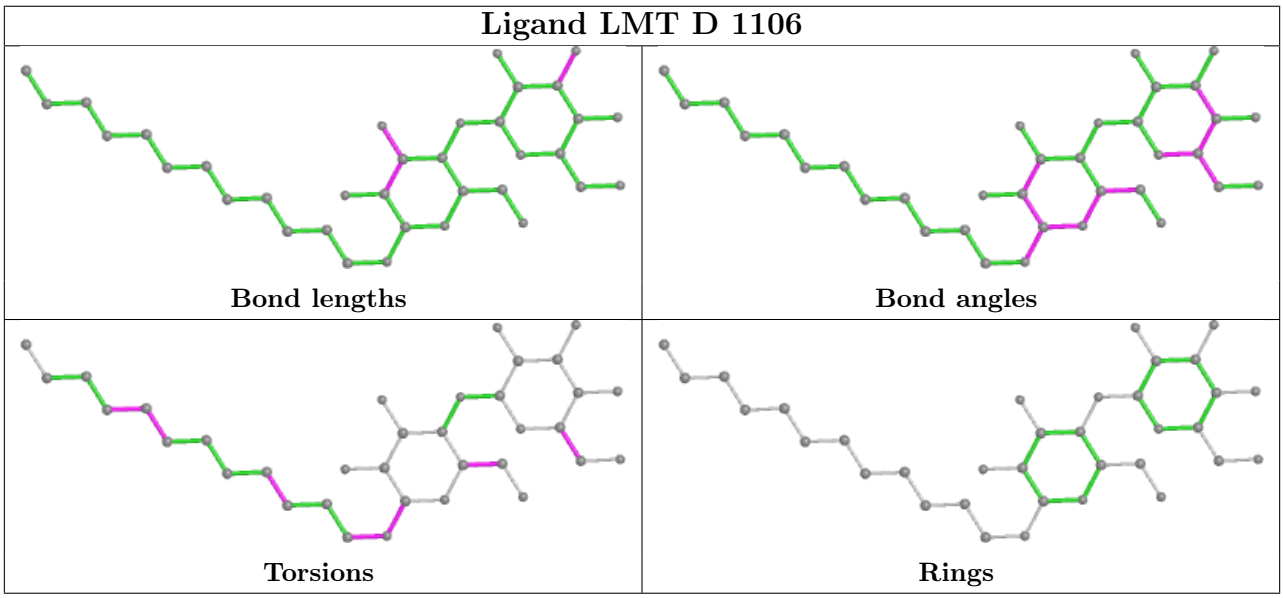
Ligand LMT A 1104



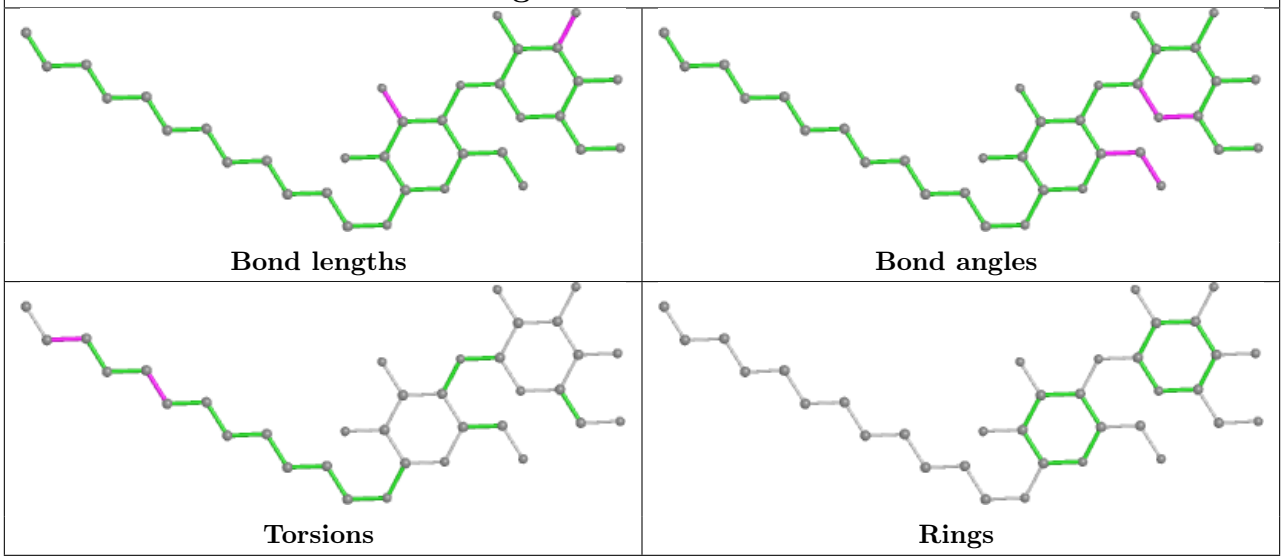
Ligand LMT D 1107



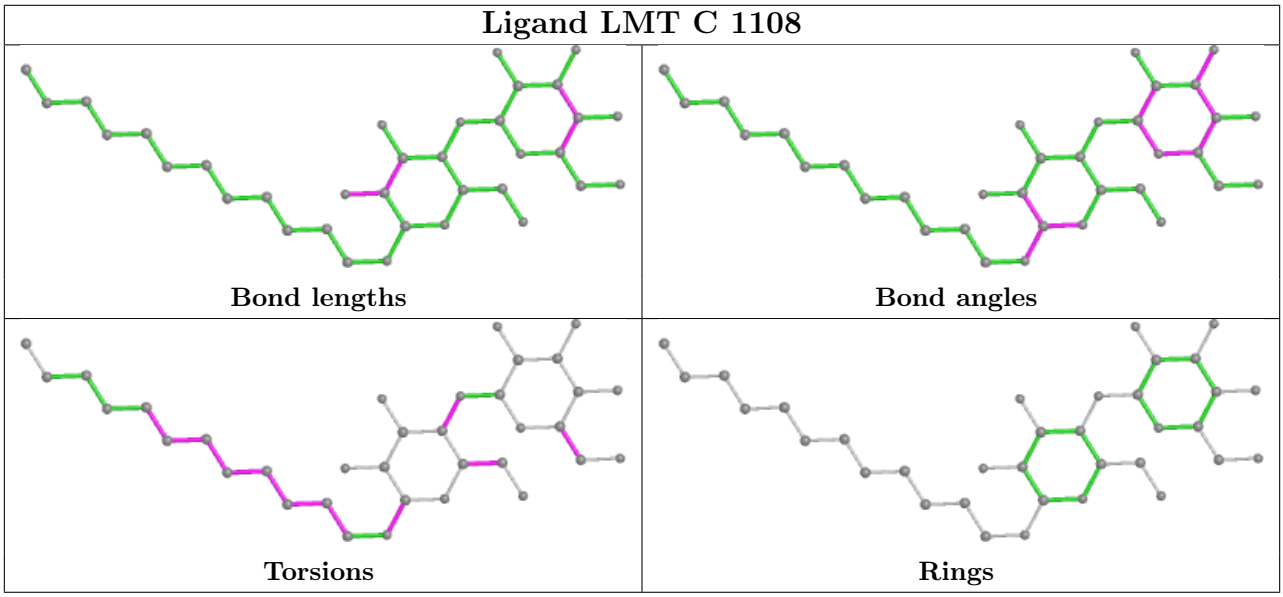
Ligand LMT D 1106



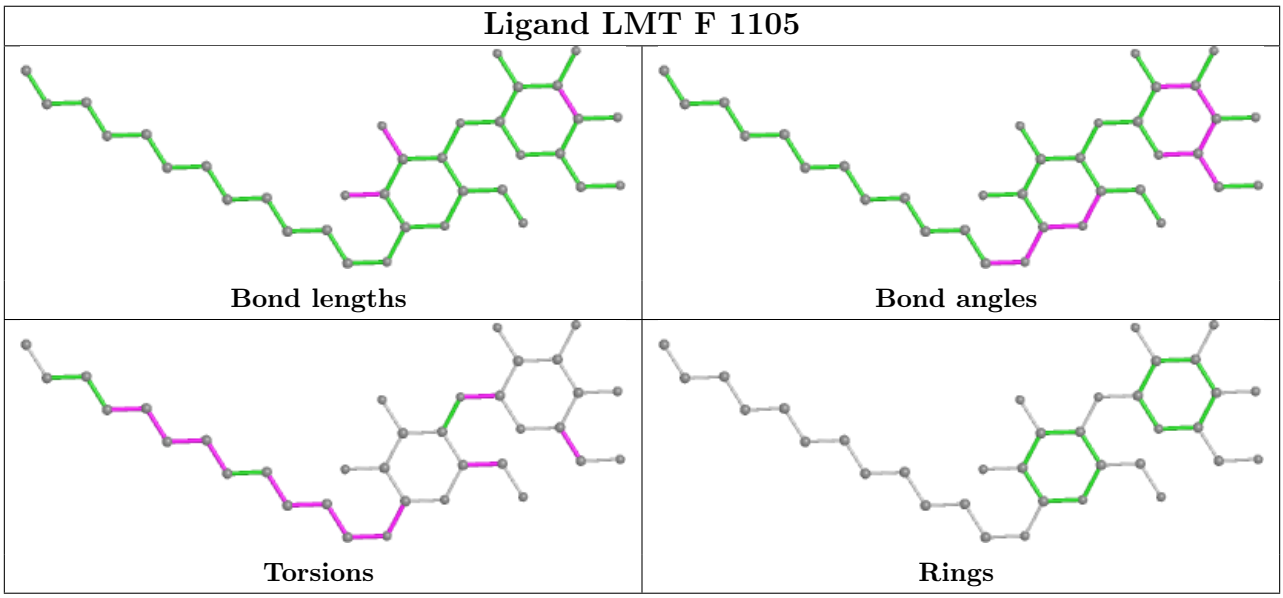
Ligand LMT D 1102



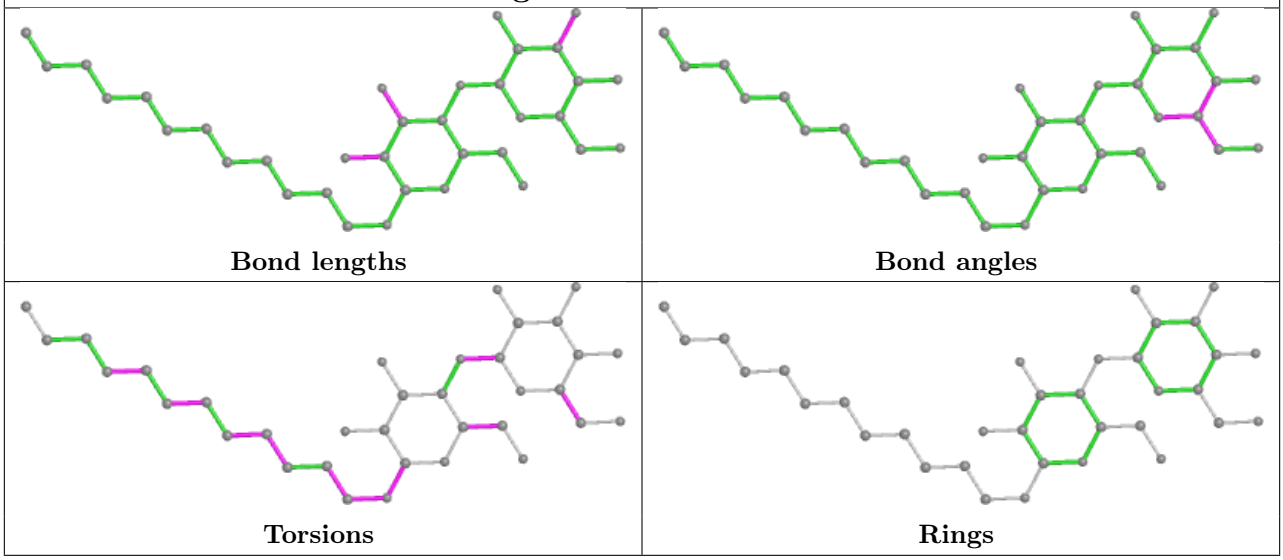
Ligand LMT C 1108



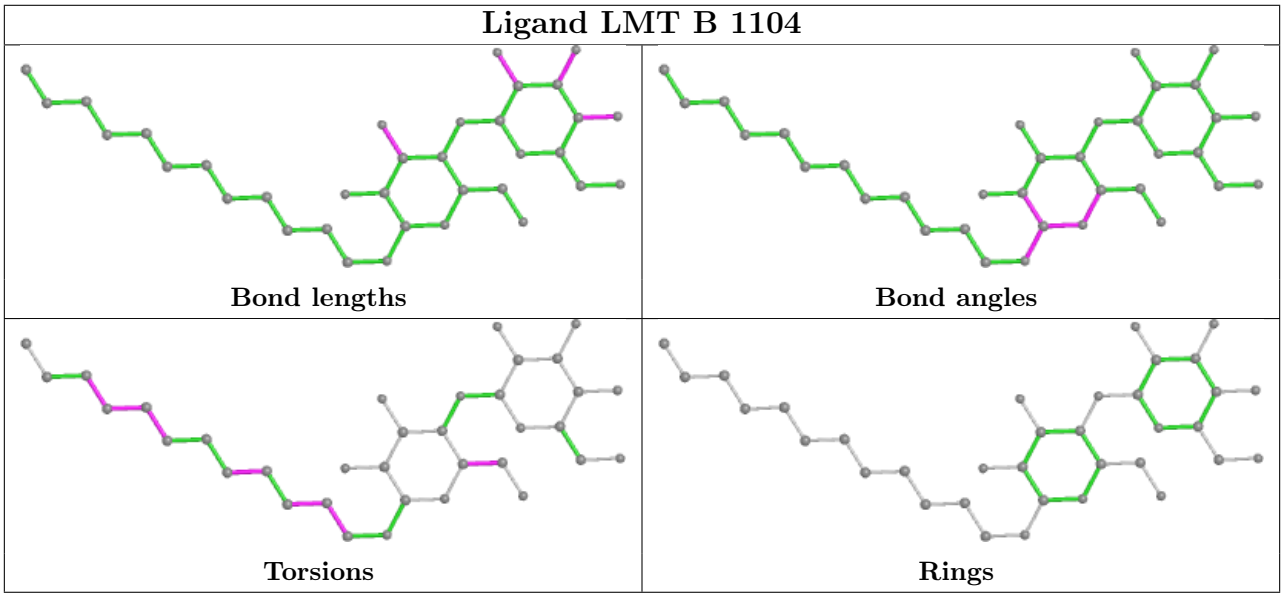
Ligand LMT F 1105



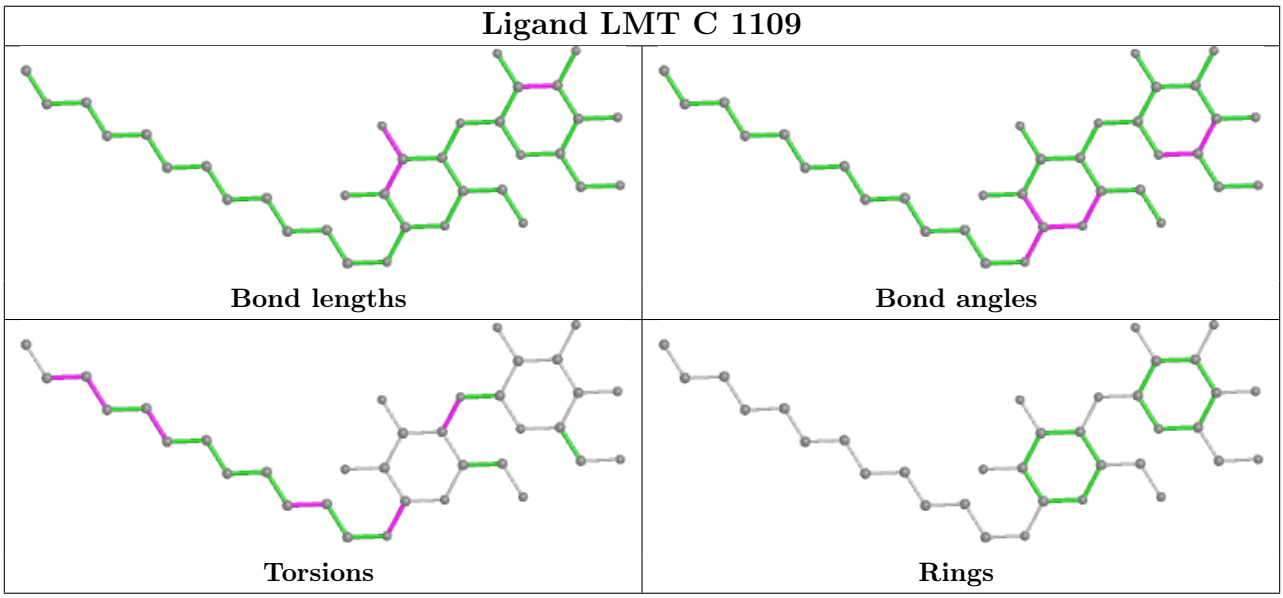
Ligand LMT D 1101



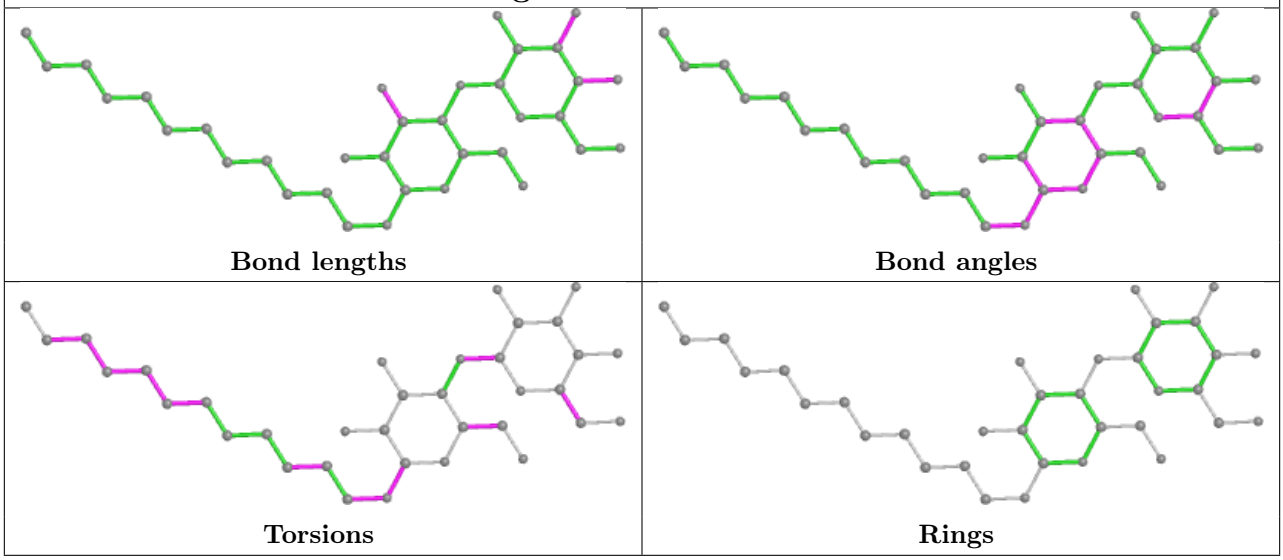
Ligand LMT B 1104



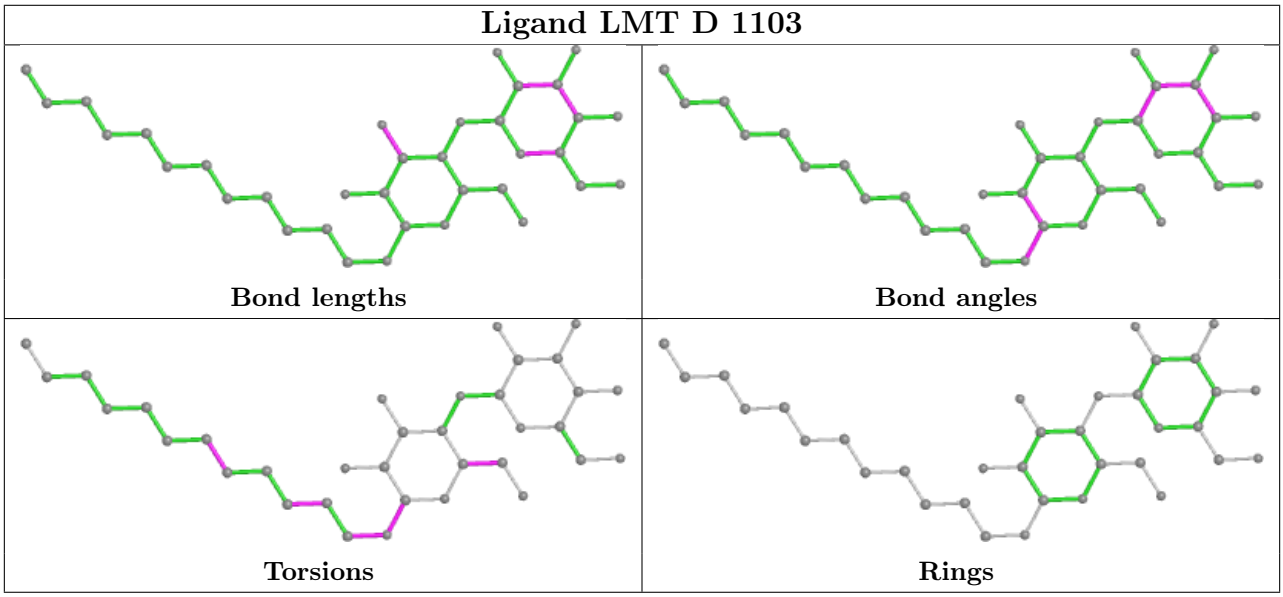
Ligand LMT C 1109



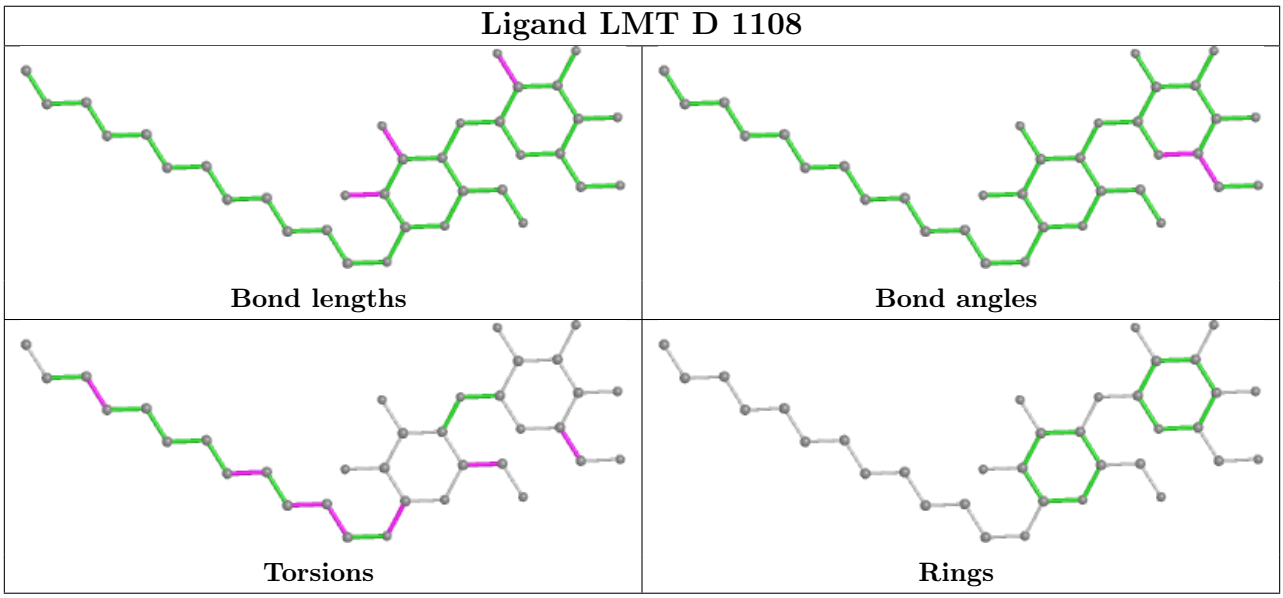
Ligand LMT D 1112



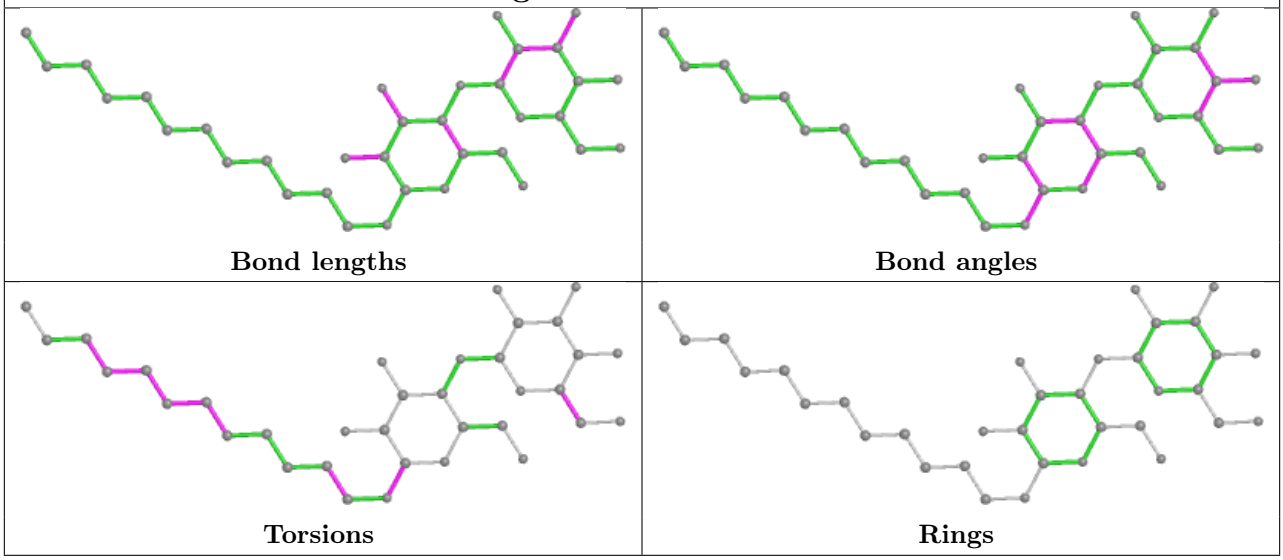
Ligand LMT D 1103



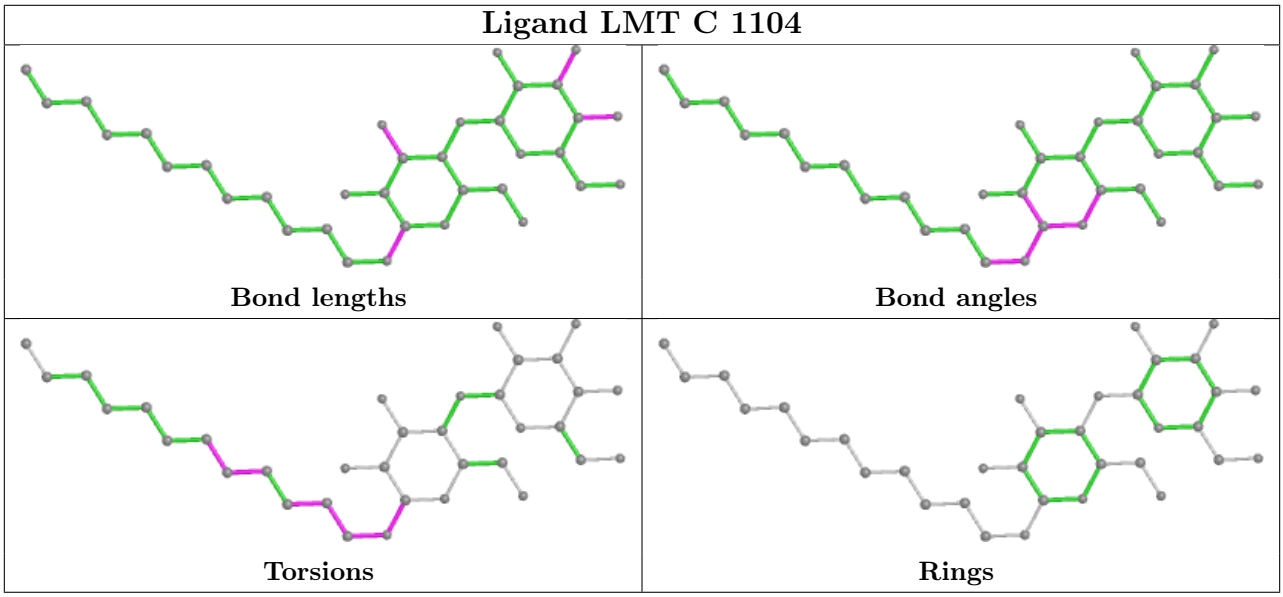
Ligand LMT D 1108



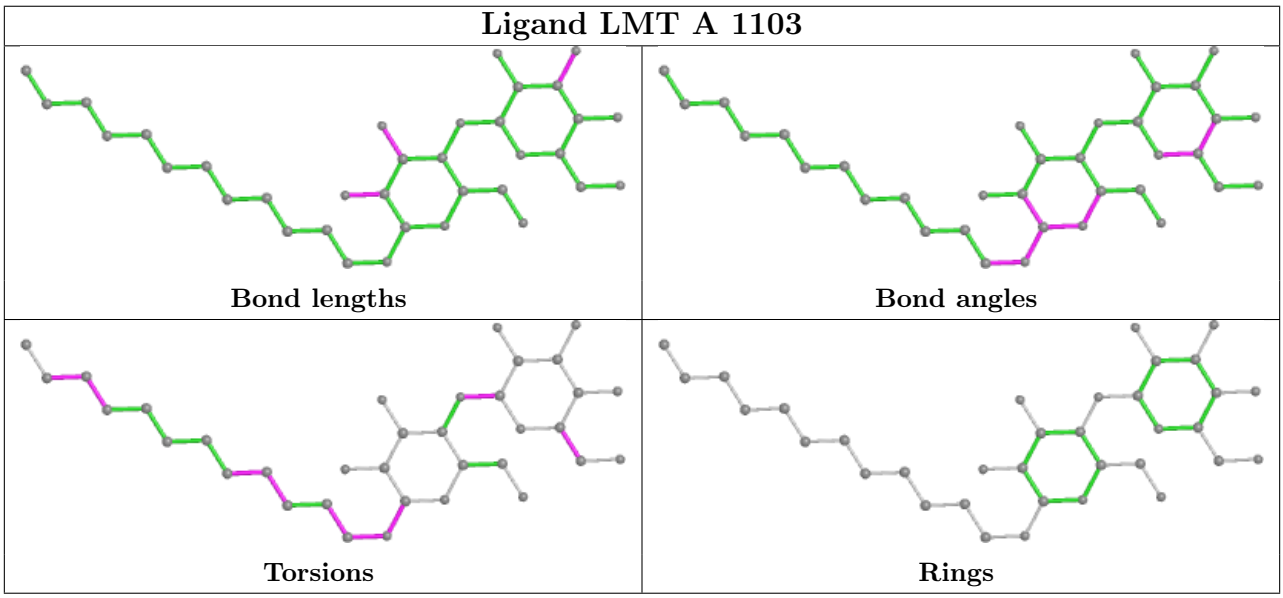
Ligand LMT A 1111



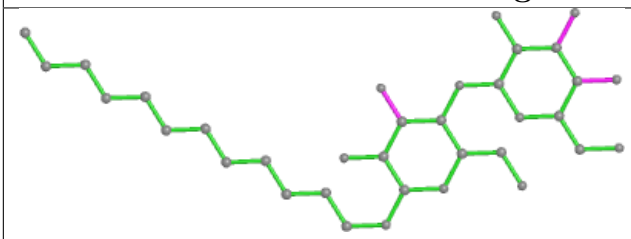
Ligand LMT C 1104



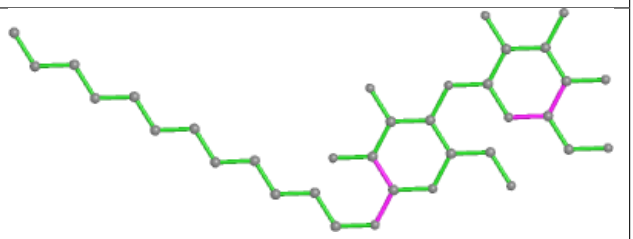
Ligand LMT A 1103



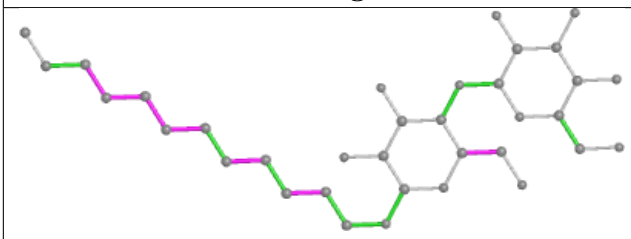
Ligand LMT F 1101



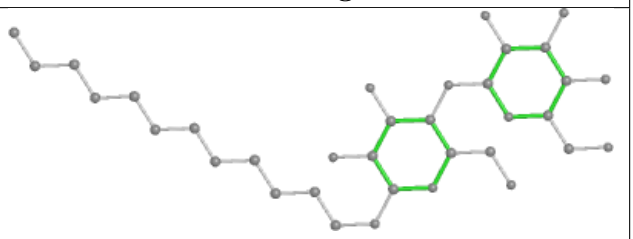
Bond lengths



Bond angles

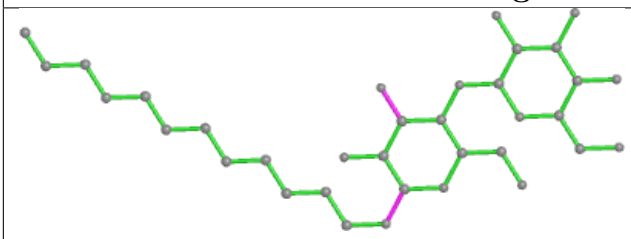


Torsions

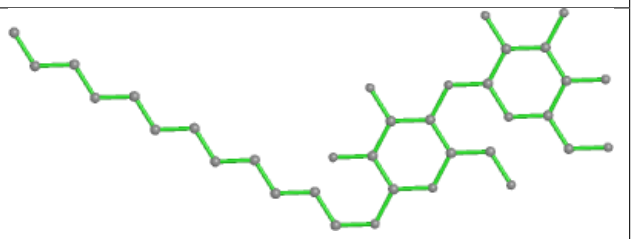


Rings

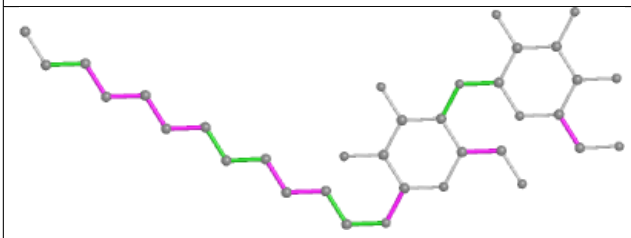
Ligand LMT B 1103



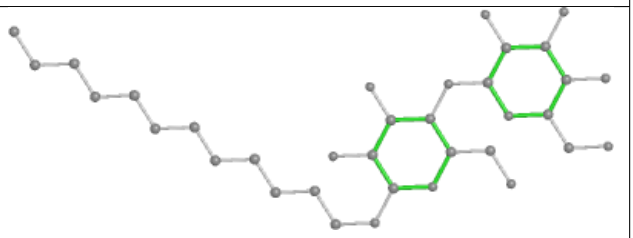
Bond lengths



Bond angles

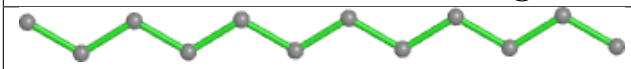


Torsions

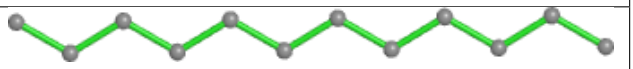


Rings

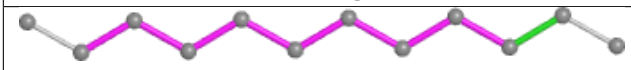
Ligand LMT E 1111



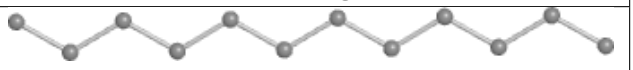
Bond lengths



Bond angles

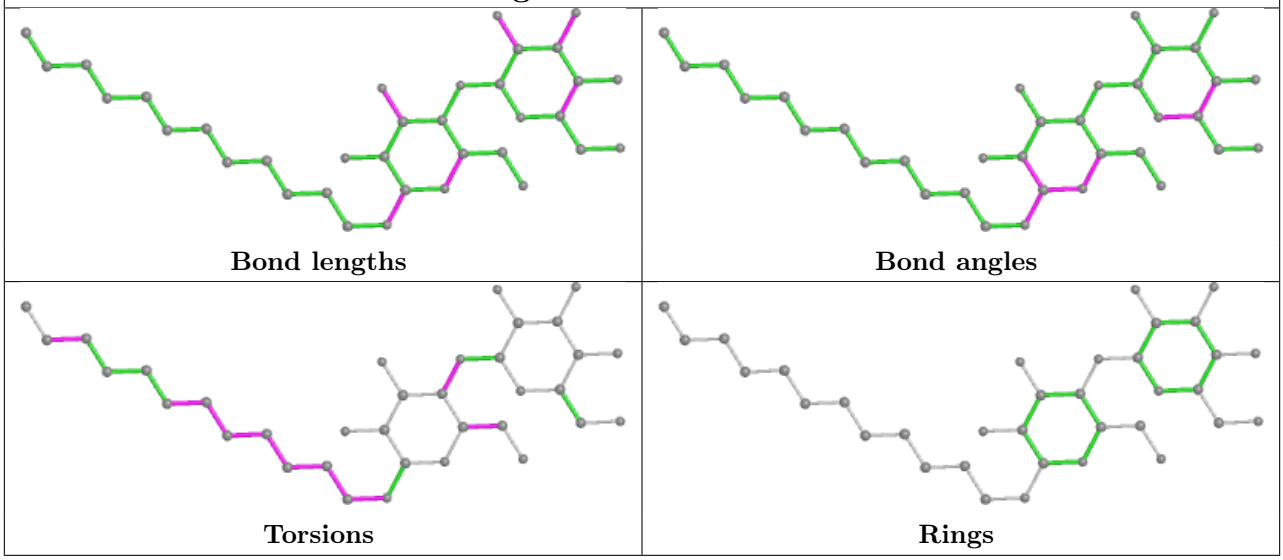


Torsions

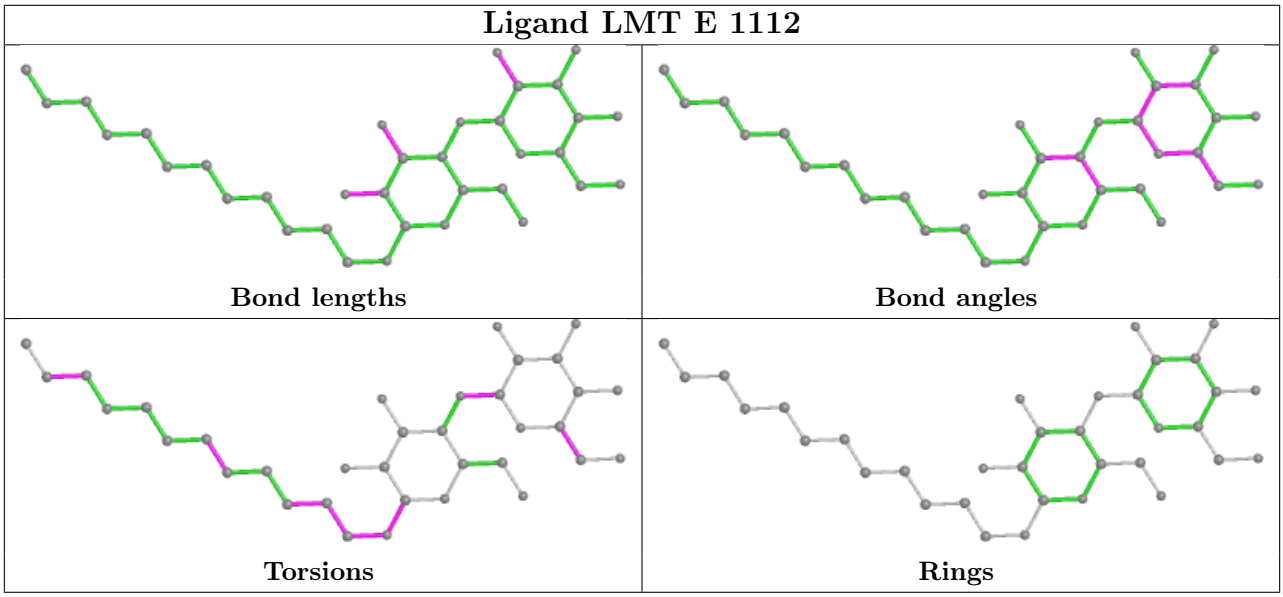


Rings

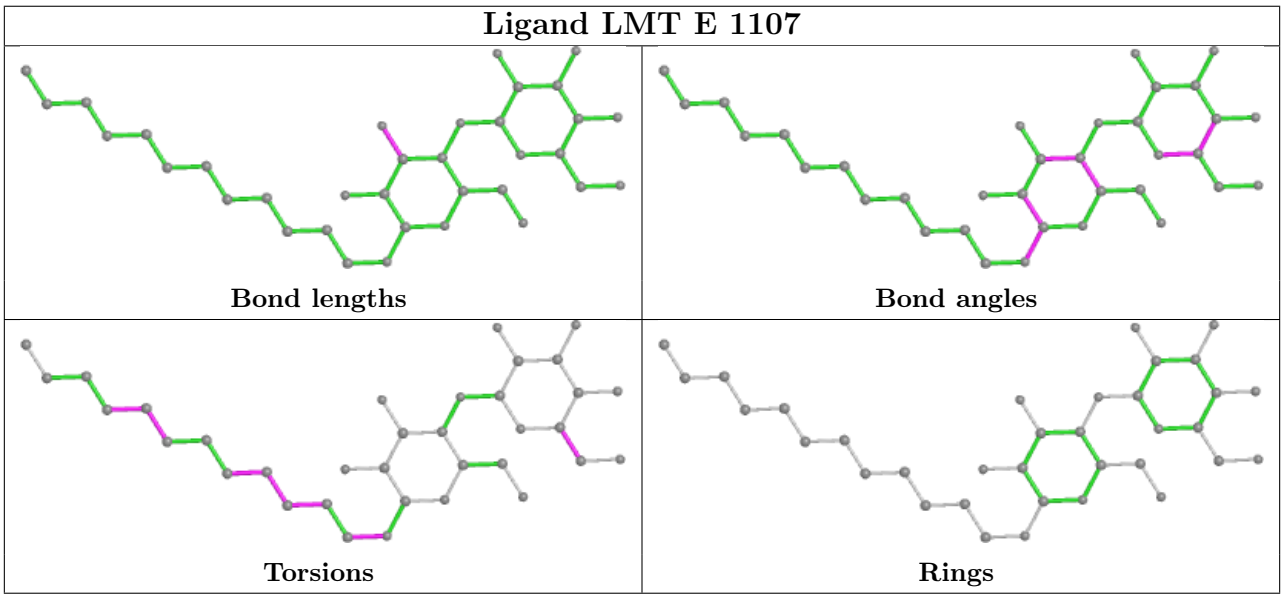
Ligand LMT D 1105



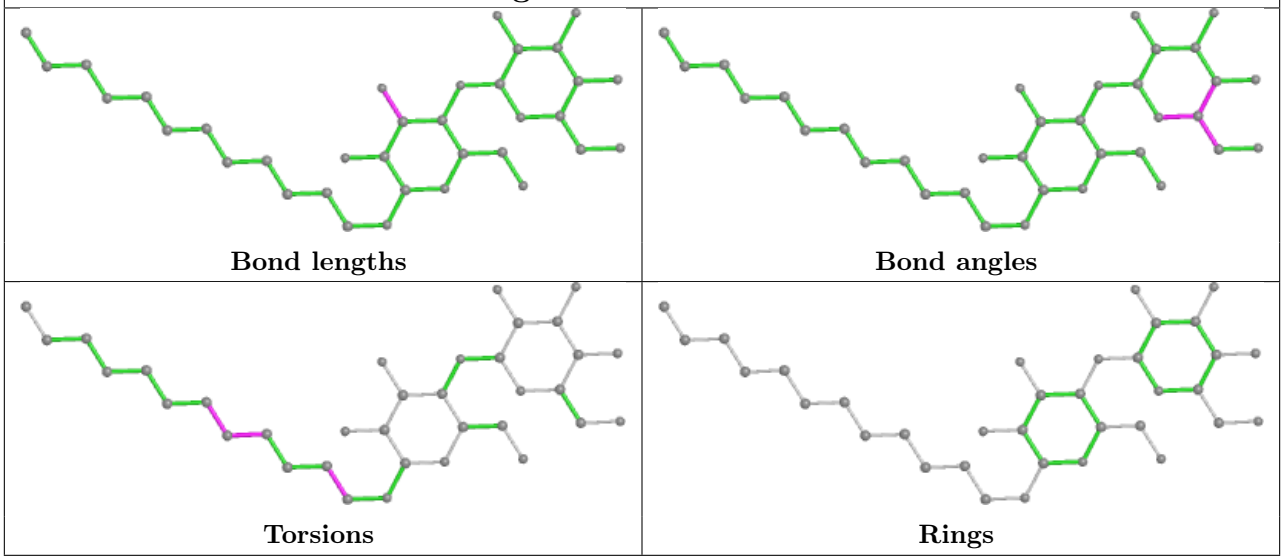
Ligand LMT E 1112



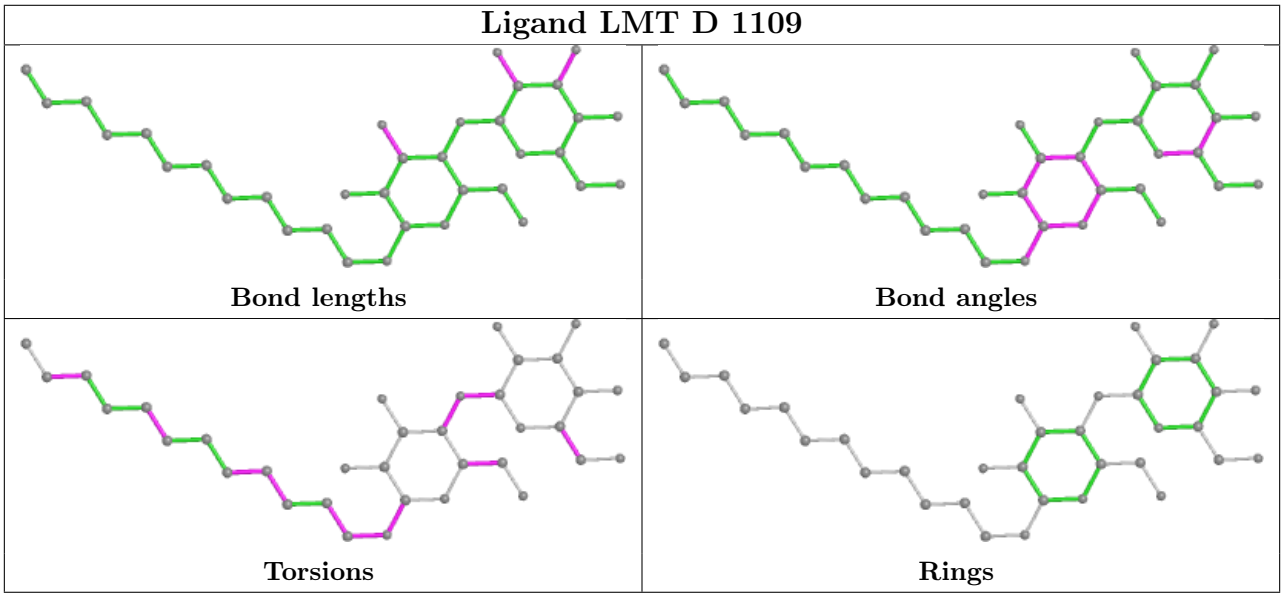
Ligand LMT E 1107



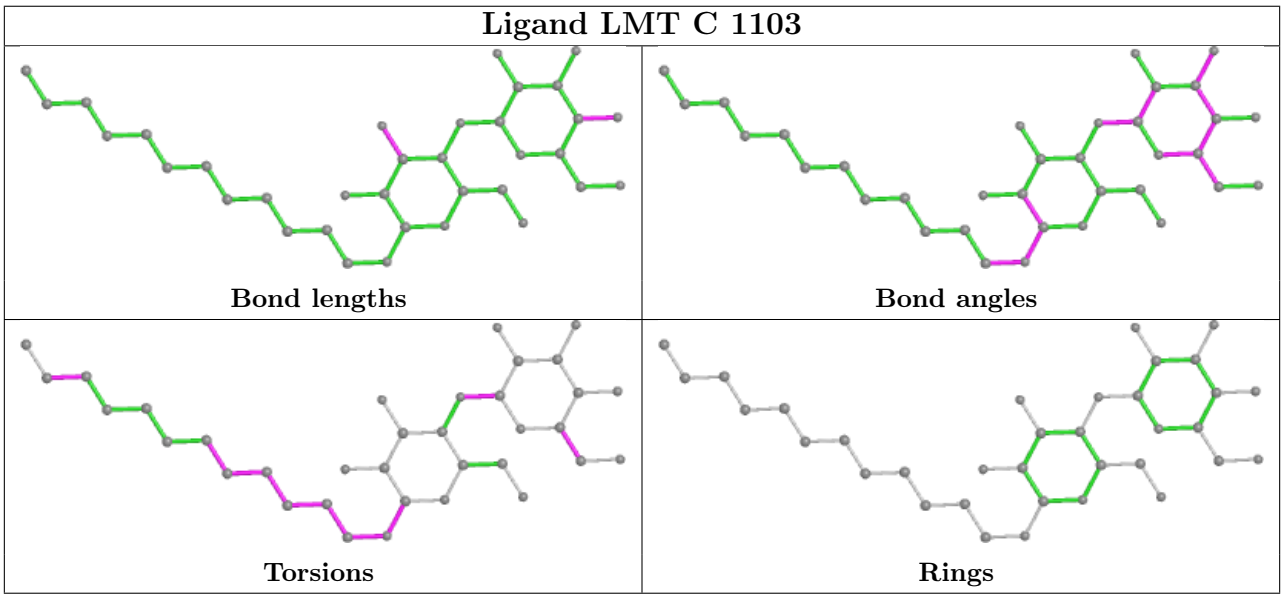
Ligand LMT A 1102



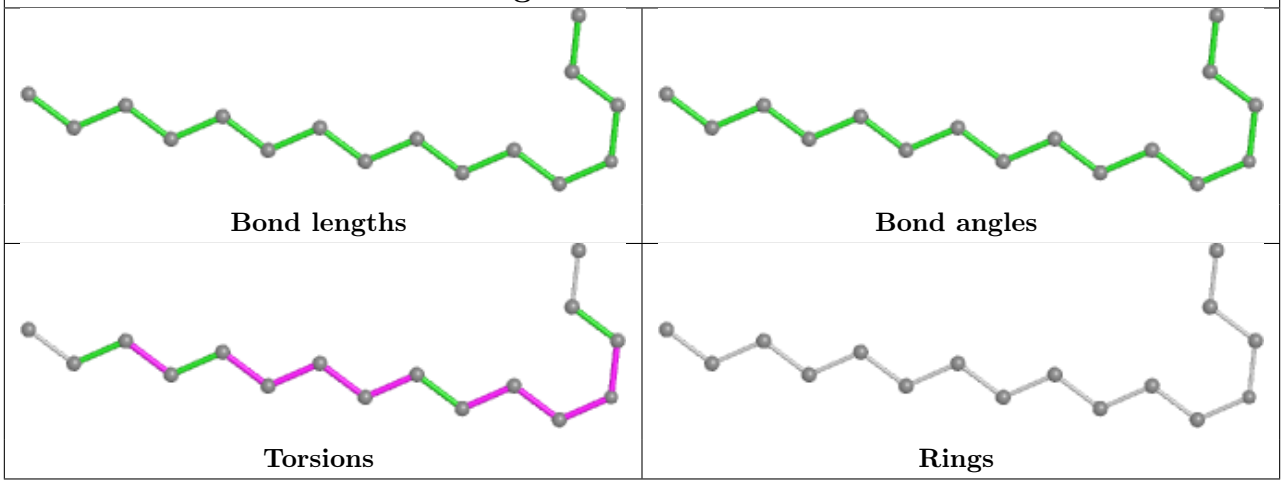
Ligand LMT D 1109



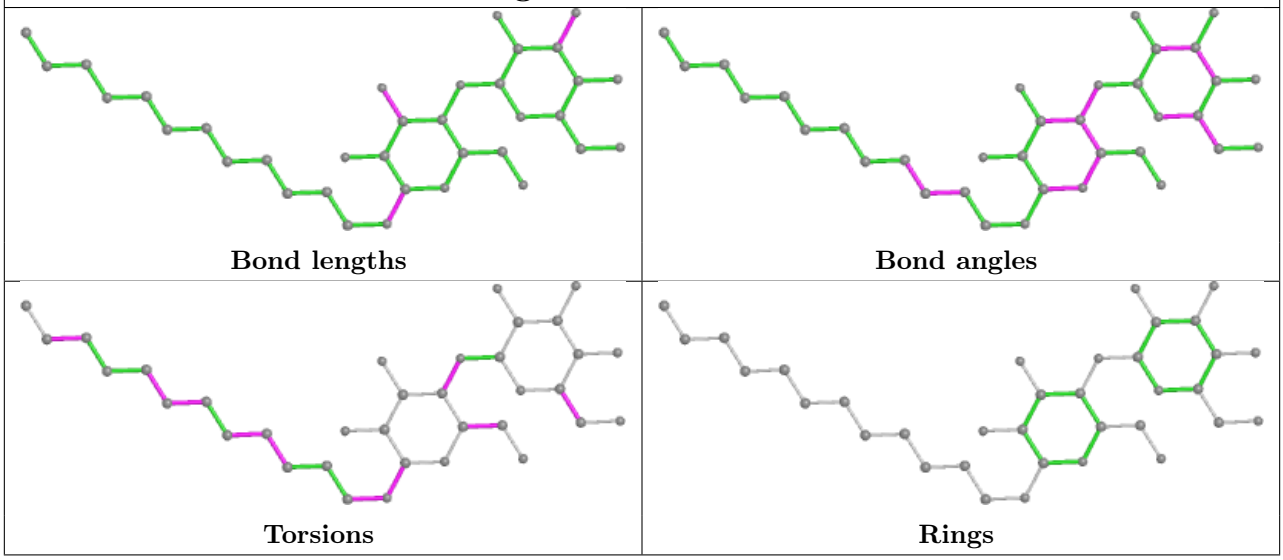
Ligand LMT C 1103



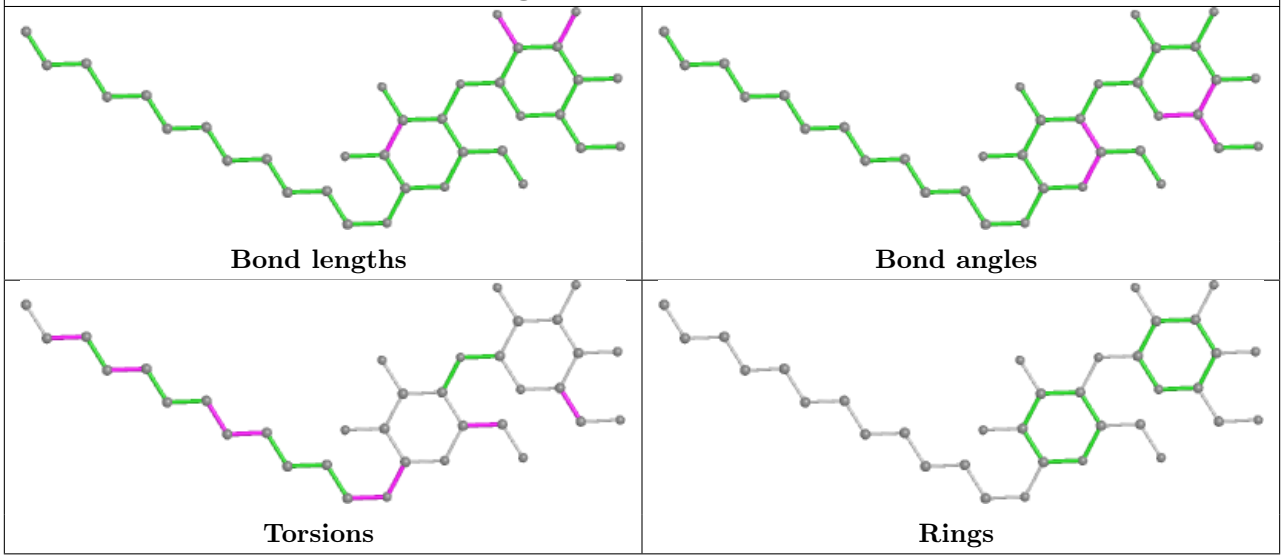
Ligand LMT B 1107



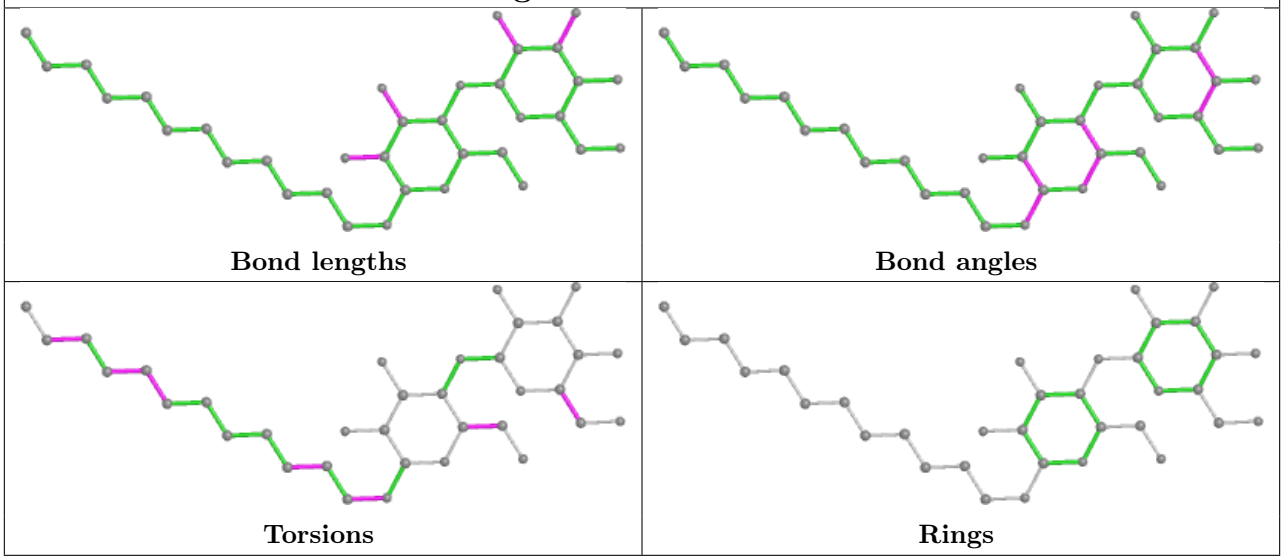
Ligand LMT E 1102



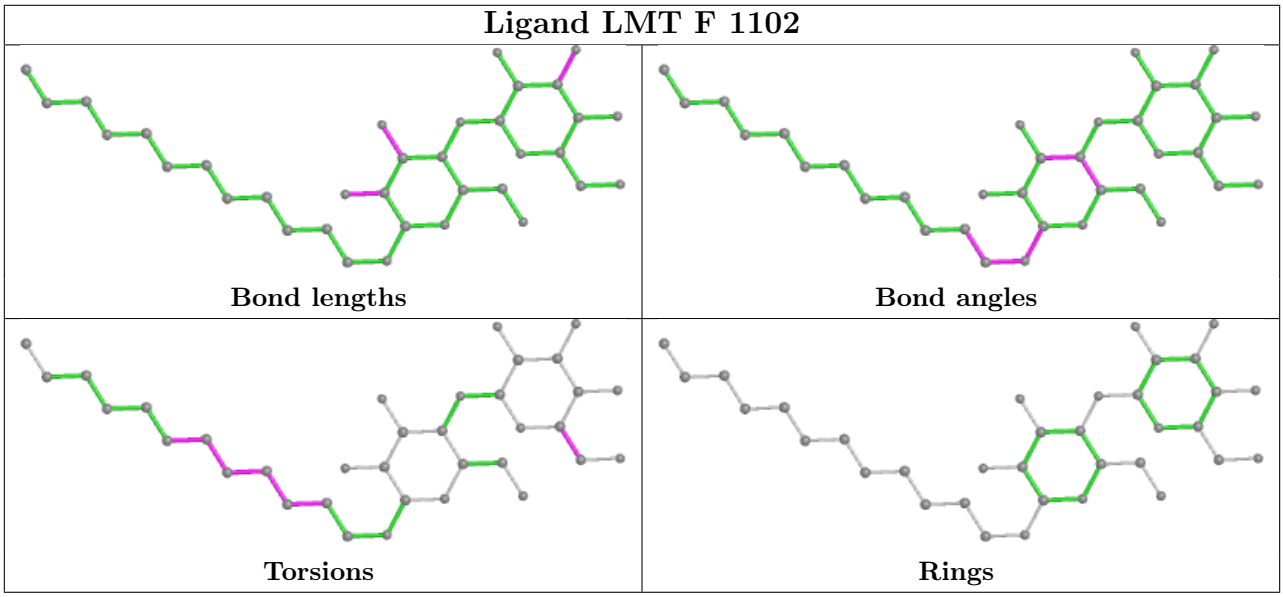
Ligand LMT F 1113



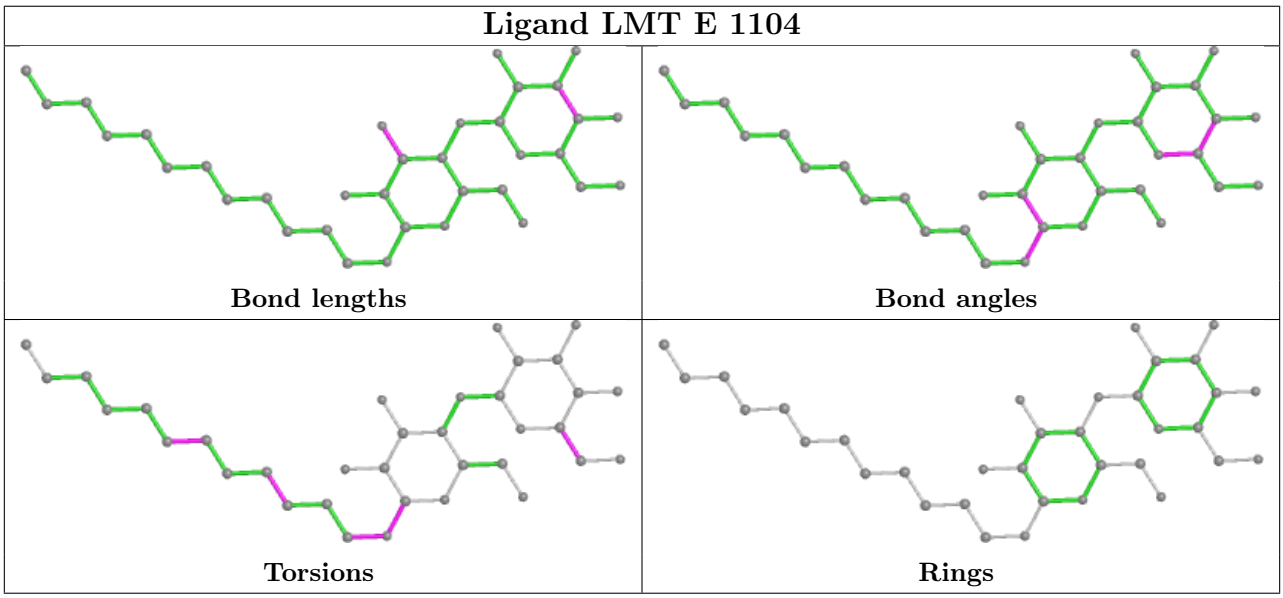
Ligand LMT B 1110



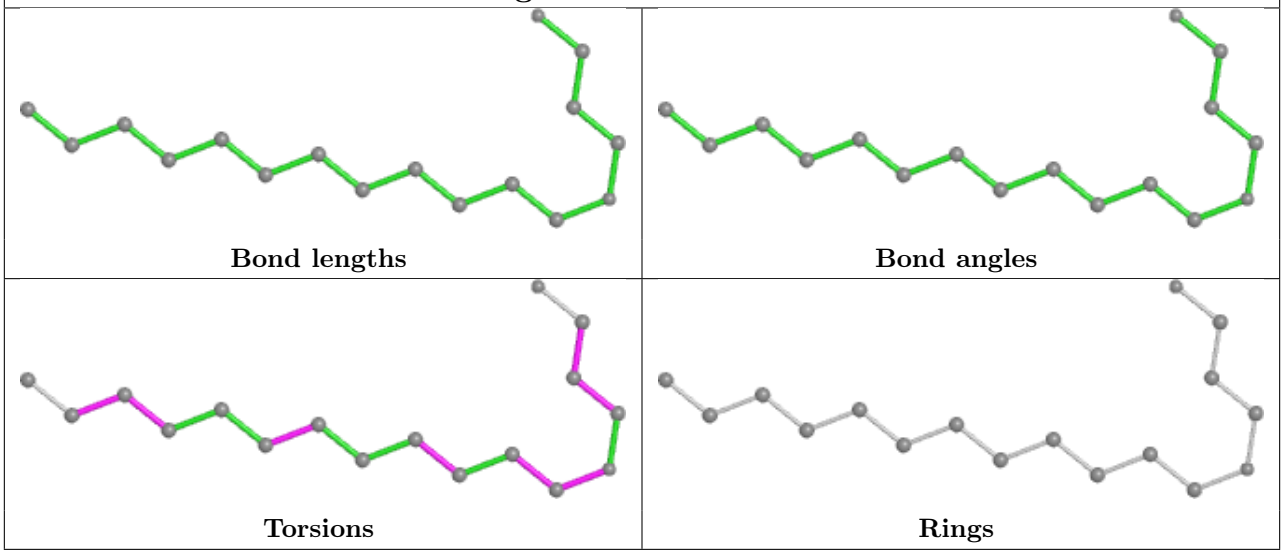
Ligand LMT F 1102



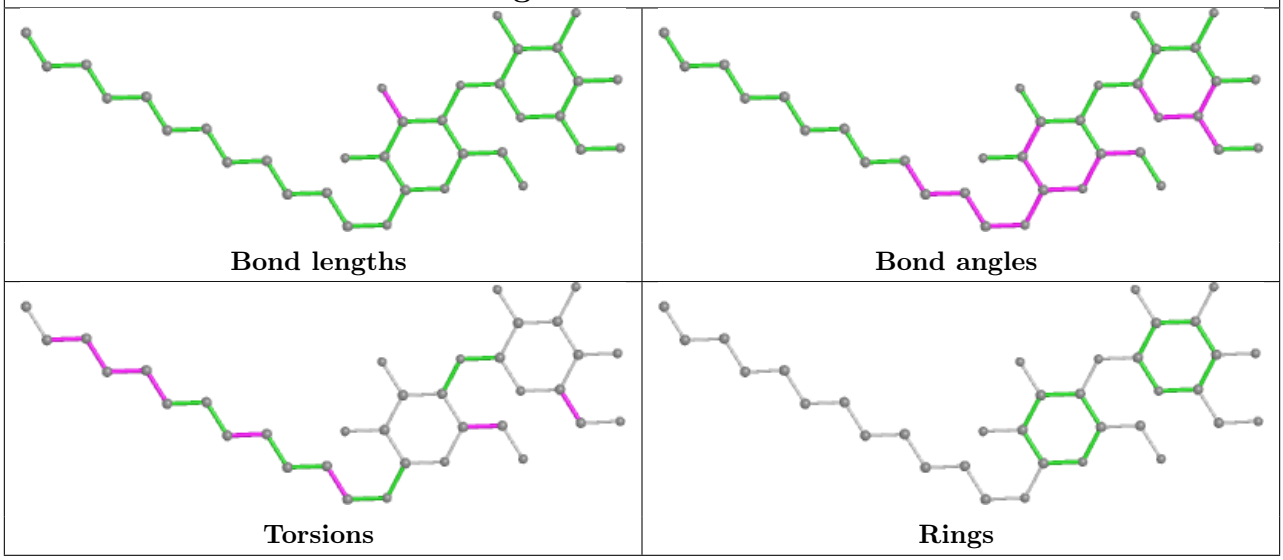
Ligand LMT E 1104



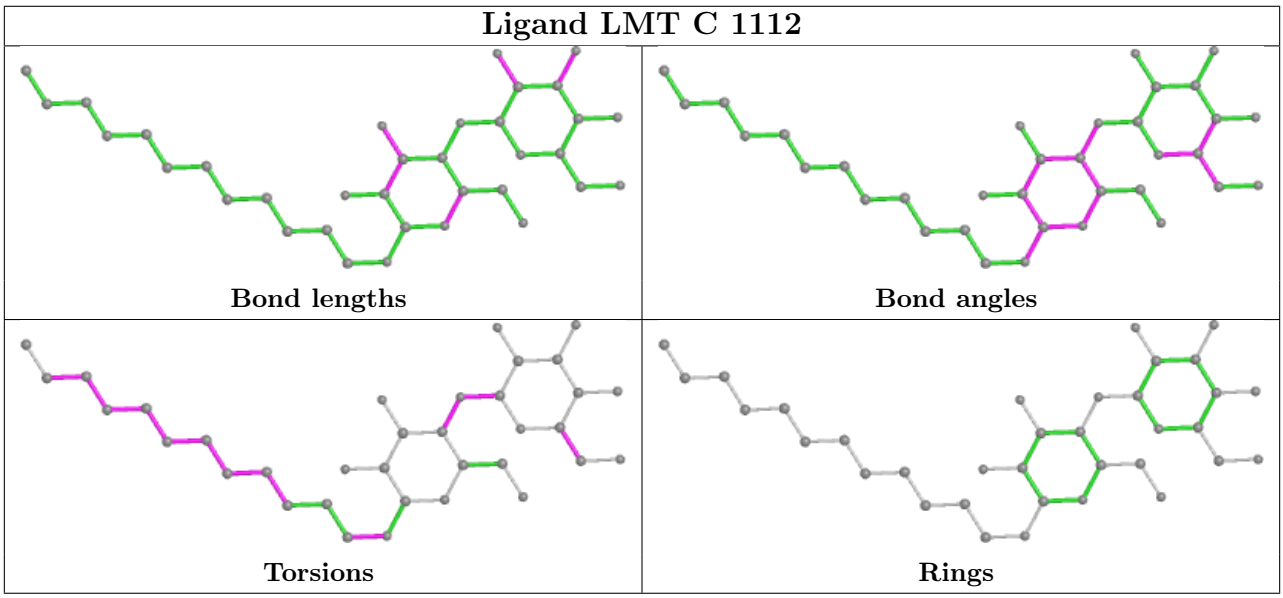
Ligand LMT F 1111



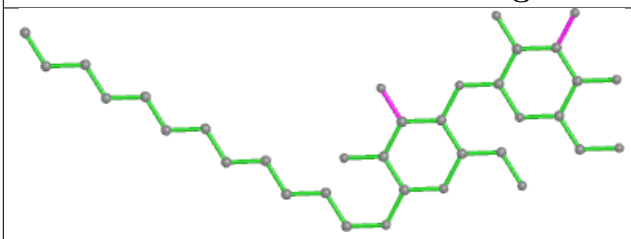
Ligand LMT C 1110

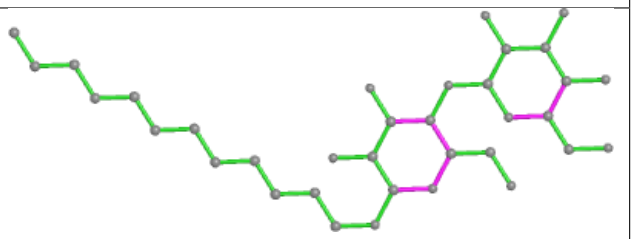


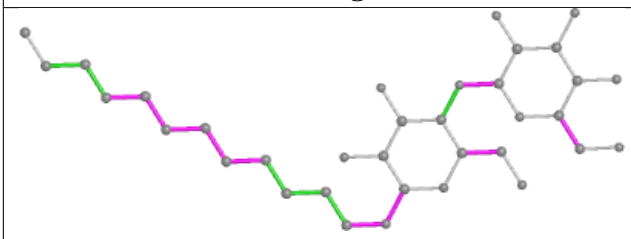
Ligand LMT C 1112

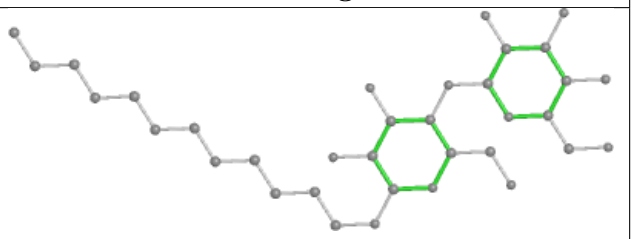


Ligand LMT B 1109

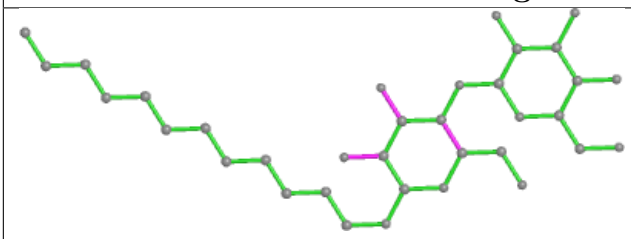

Bond lengths

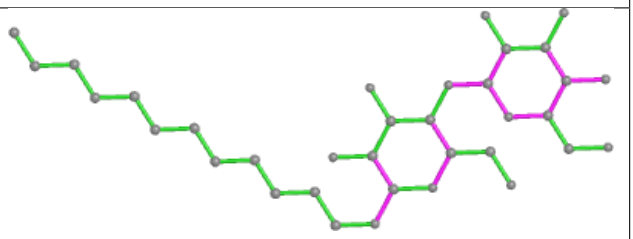

Bond angles

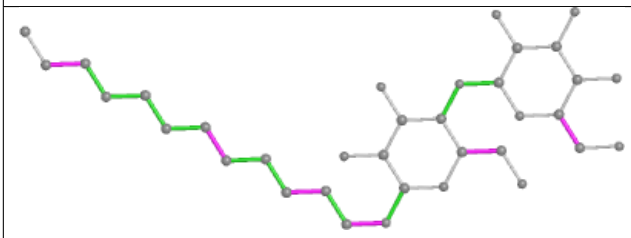

Torsions

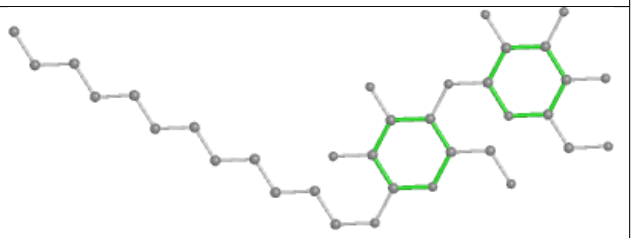

Rings

Ligand LMT E 1103

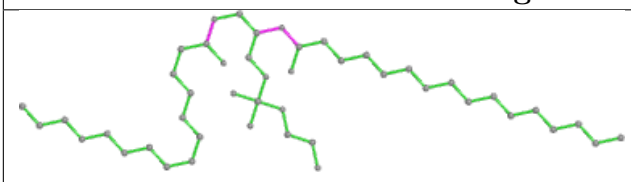

Bond lengths

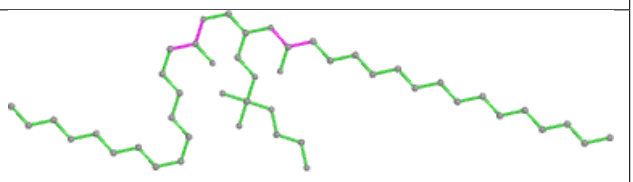

Bond angles

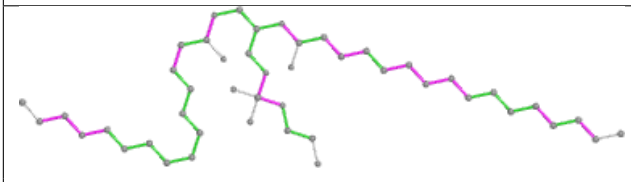

Torsions

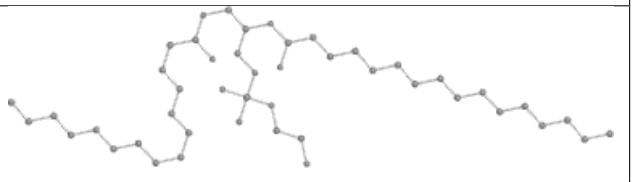

Rings

Ligand PTY A 1112

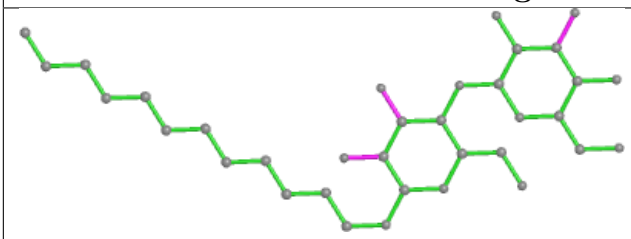

Bond lengths


Bond angles

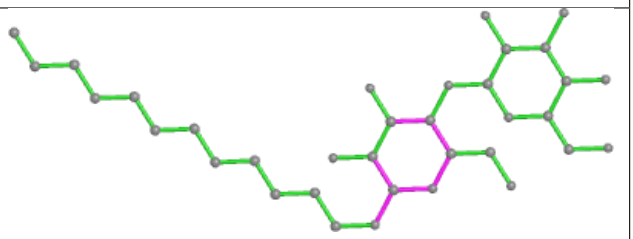

Torsions


Rings

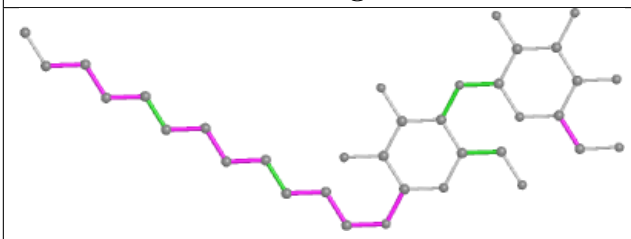
Ligand LMT F 1107



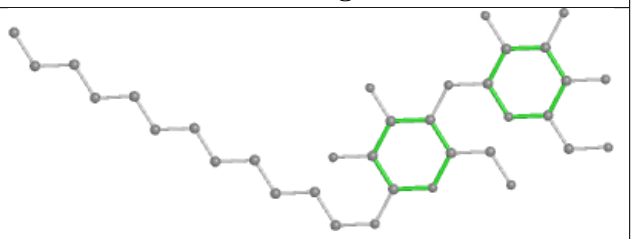
Bond lengths



Bond angles

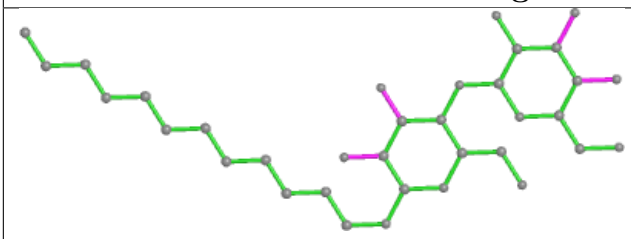


Torsions

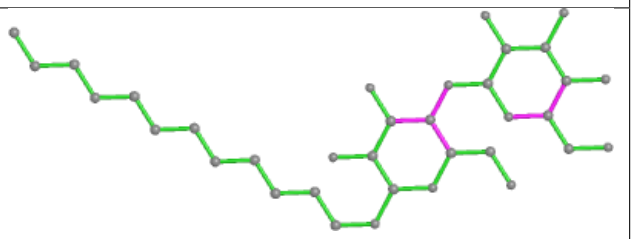


Rings

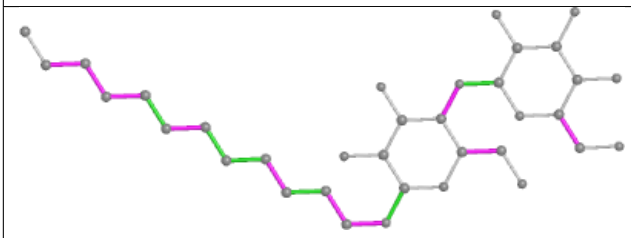
Ligand LMT D 1111



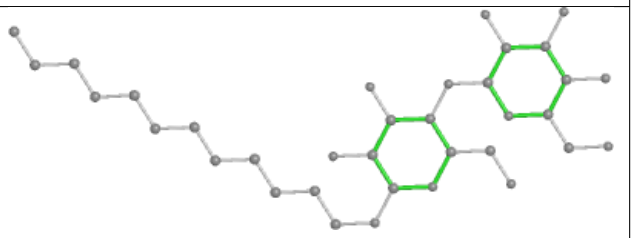
Bond lengths



Bond angles

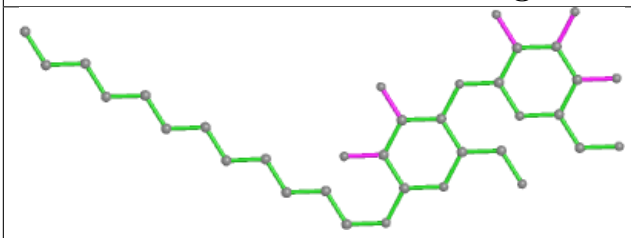


Torsions

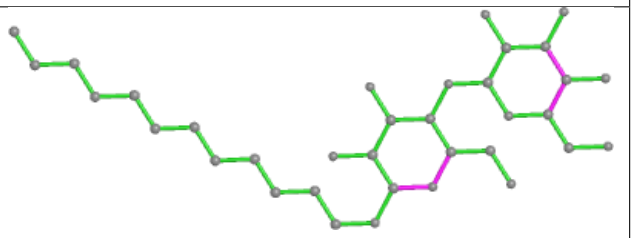


Rings

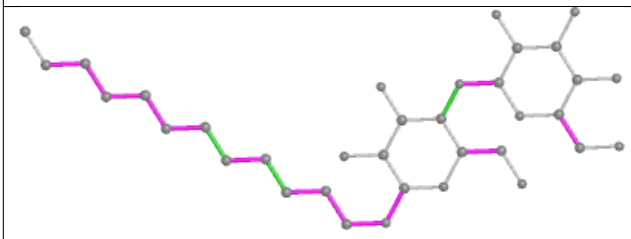
Ligand LMT E 1108



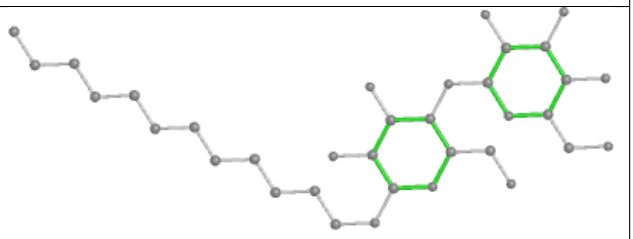
Bond lengths



Bond angles

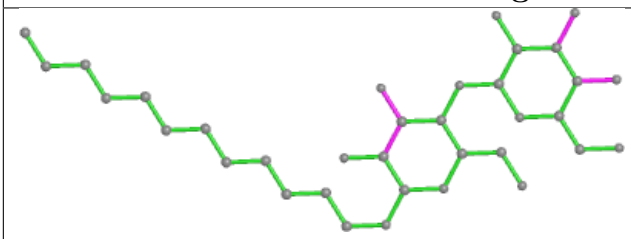


Torsions

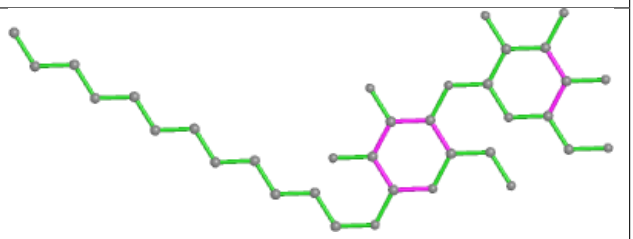


Rings

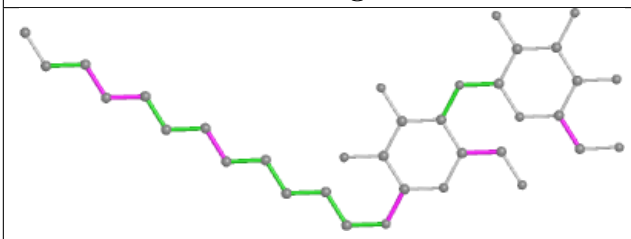
Ligand LMT A 1101



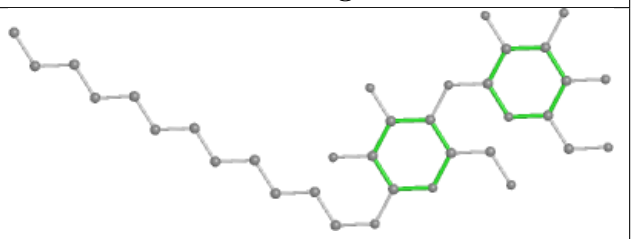
Bond lengths



Bond angles

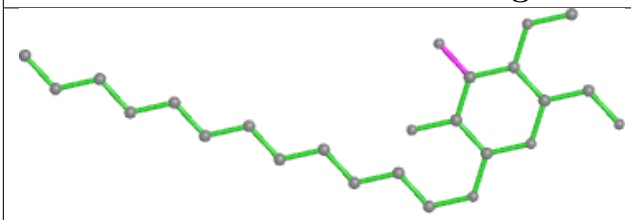


Torsions

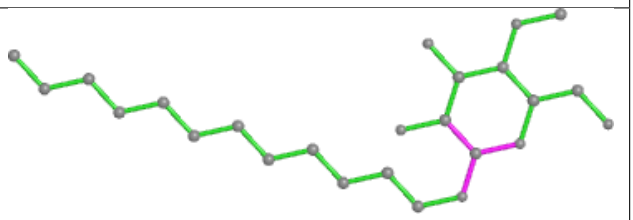


Rings

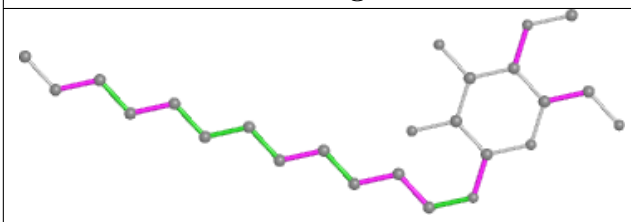
Ligand LMT A 1110



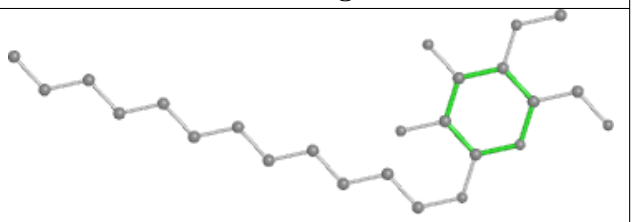
Bond lengths



Bond angles

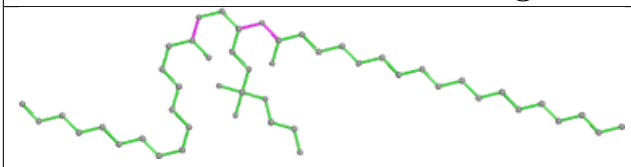


Torsions

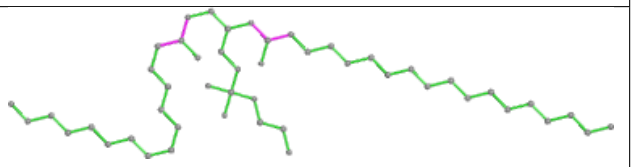


Rings

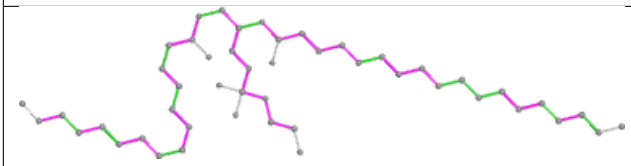
Ligand PTY B 1112



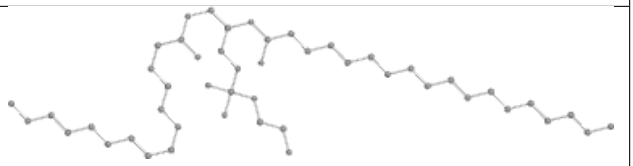
Bond lengths



Bond angles

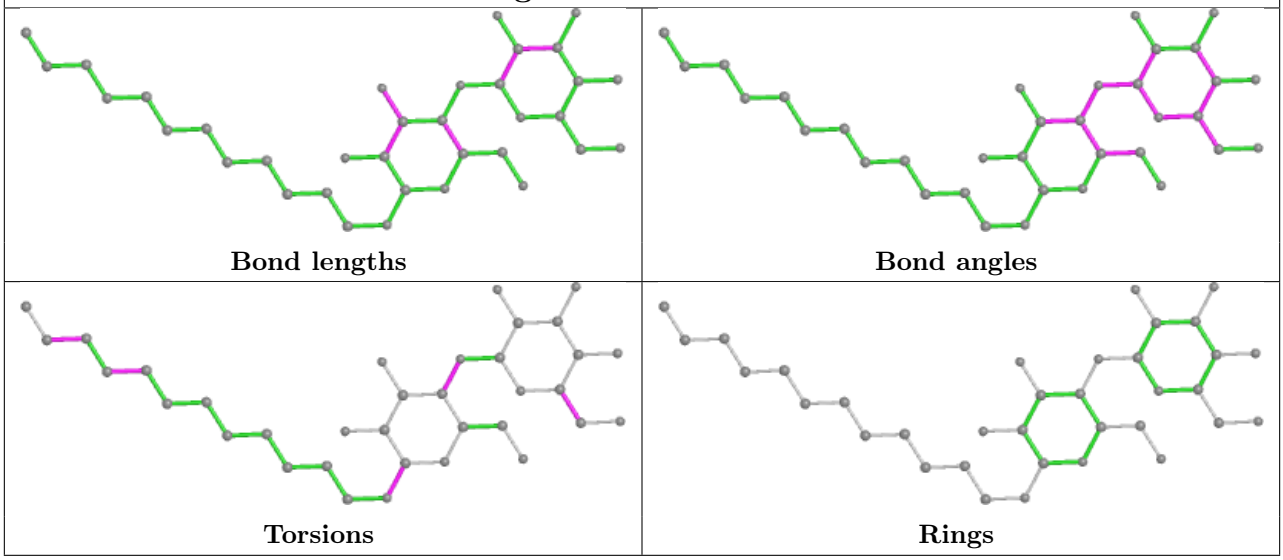


Torsions

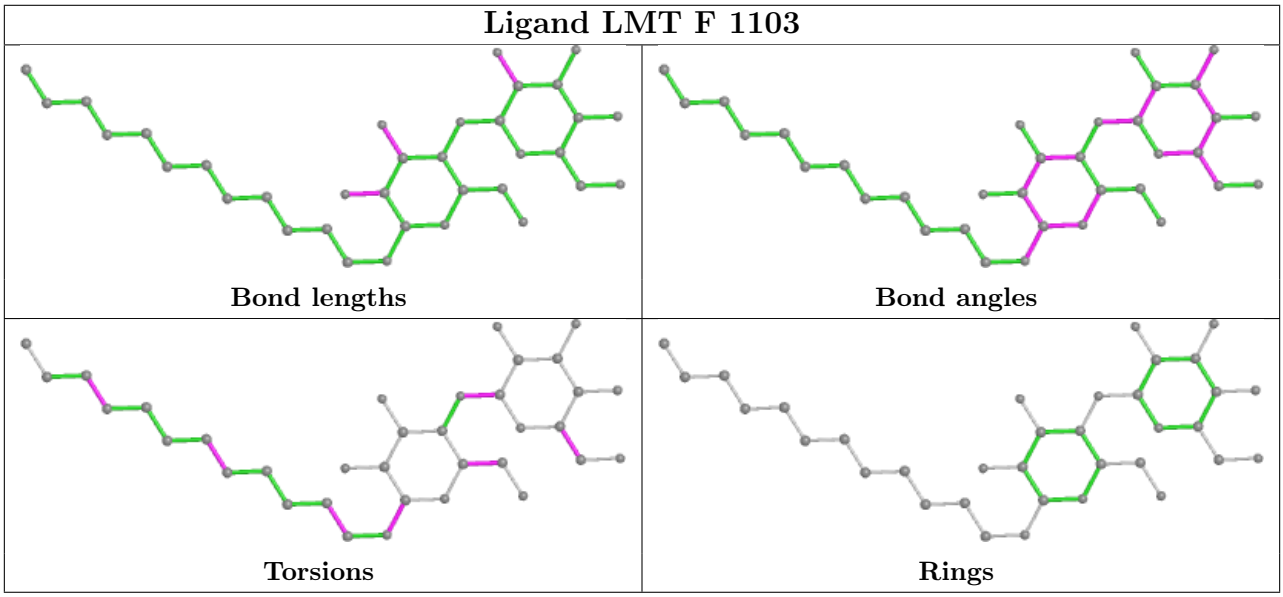


Rings

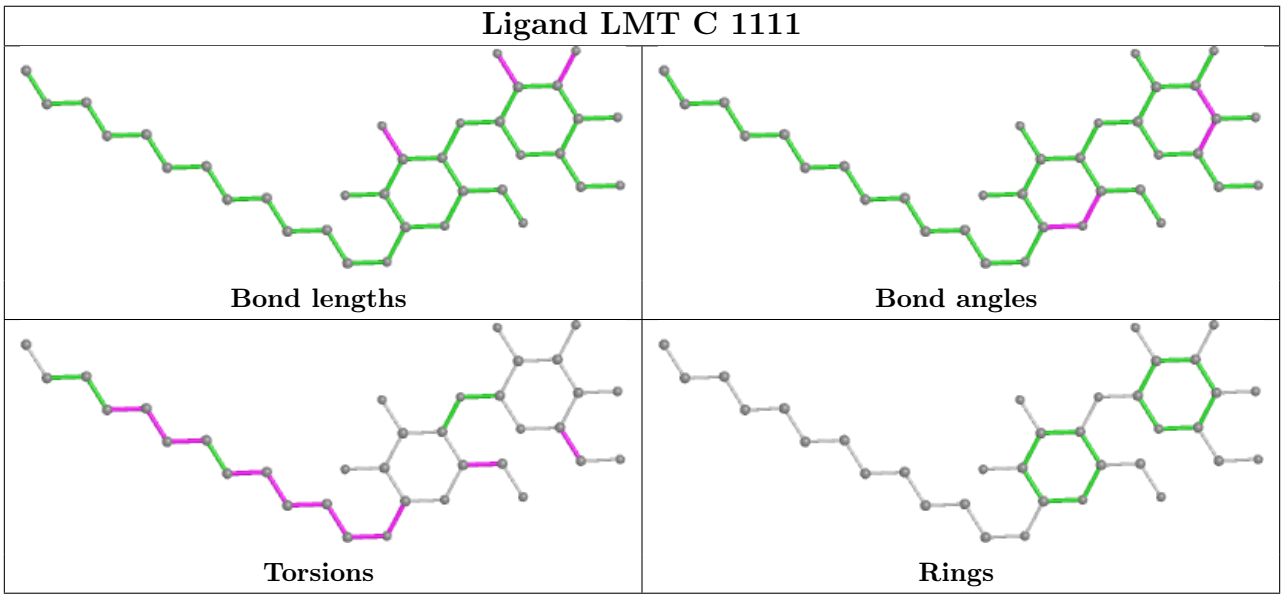
Ligand LMT E 1106



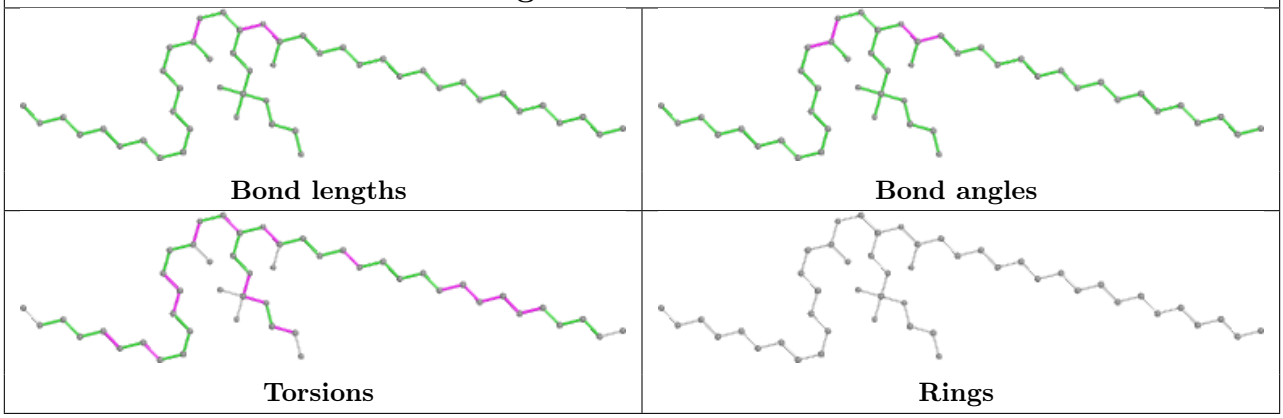
Ligand LMT F 1103



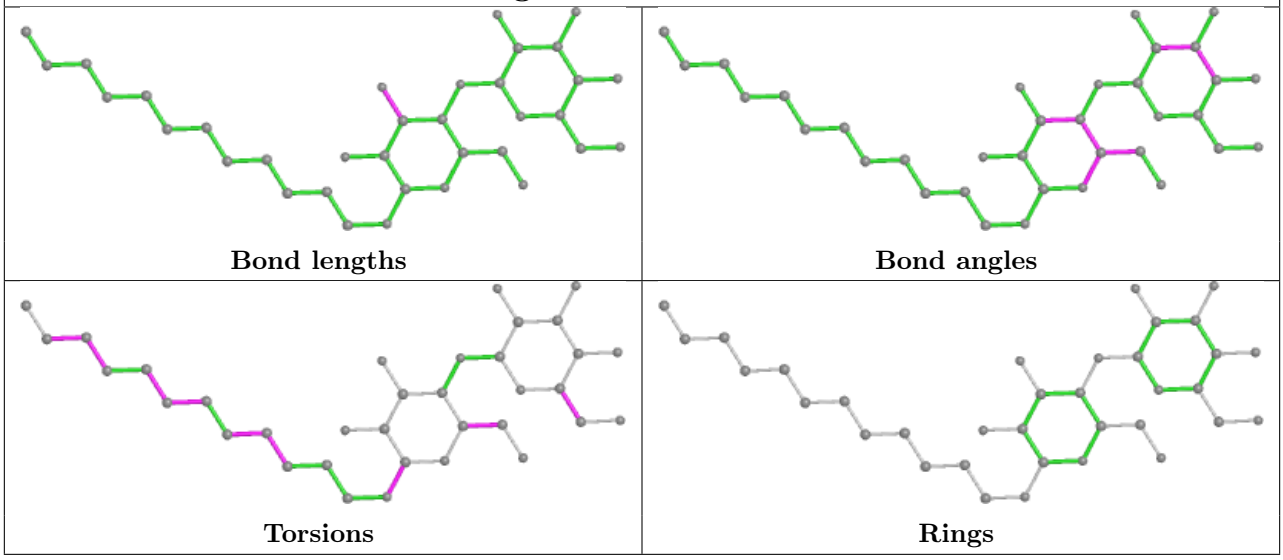
Ligand LMT C 1111



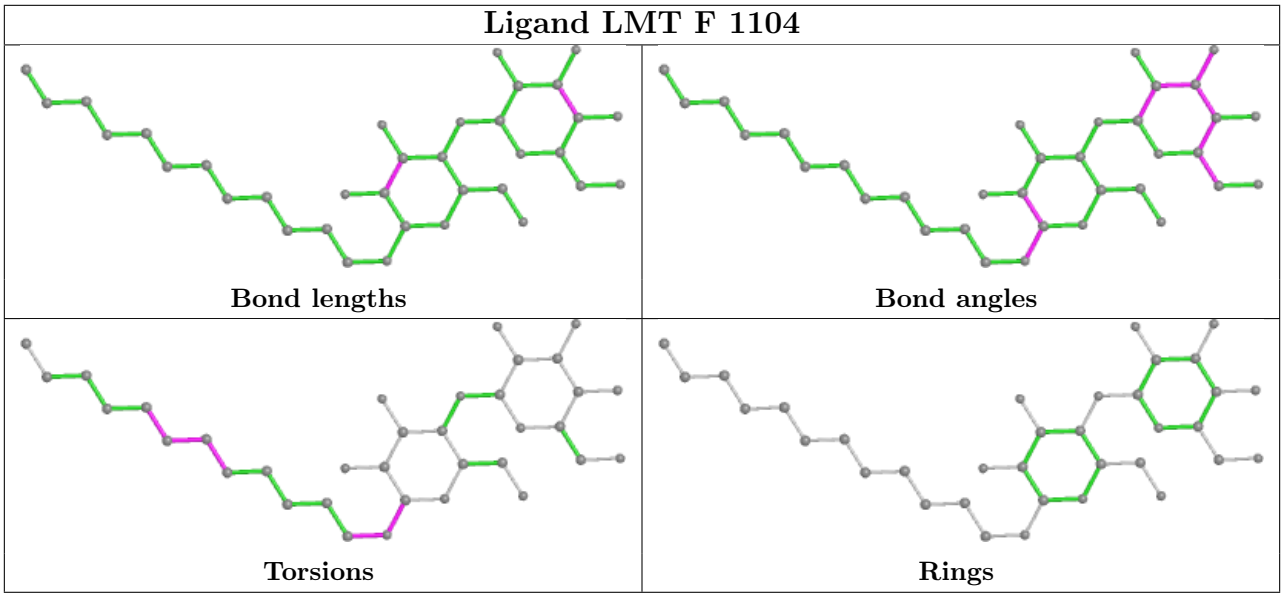
Ligand PTY F 1115



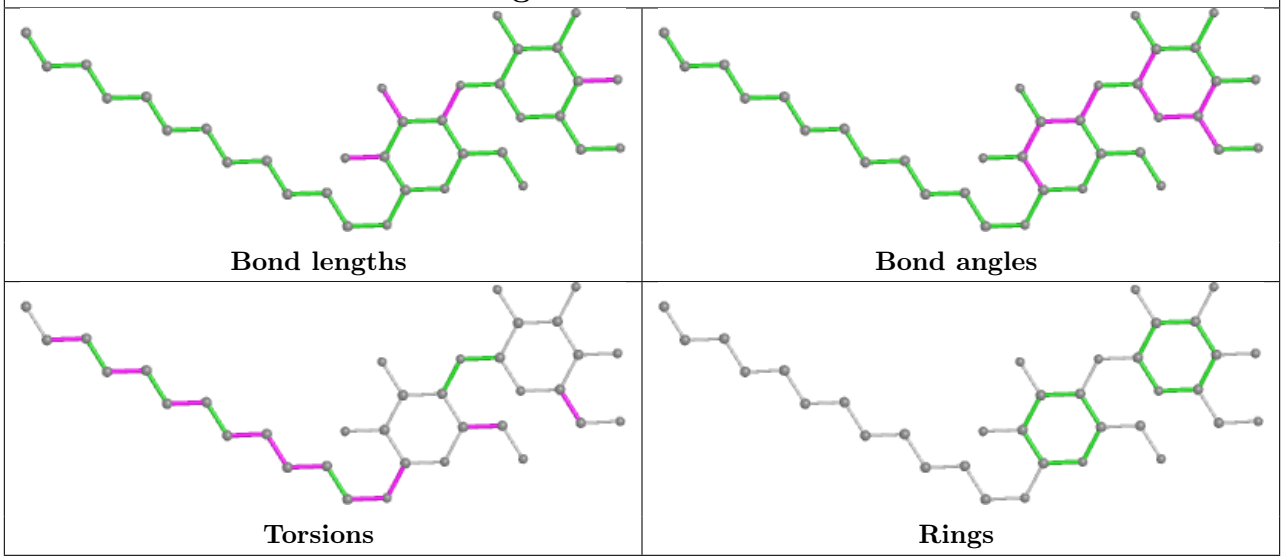
Ligand LMT C 1101



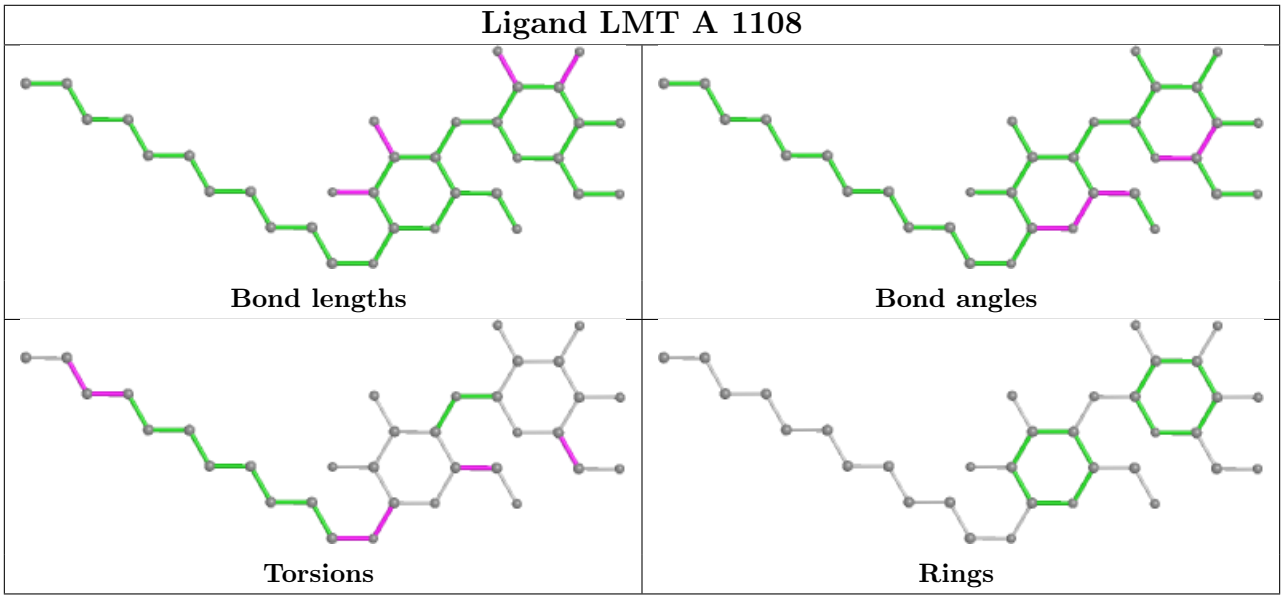
Ligand LMT F 1104



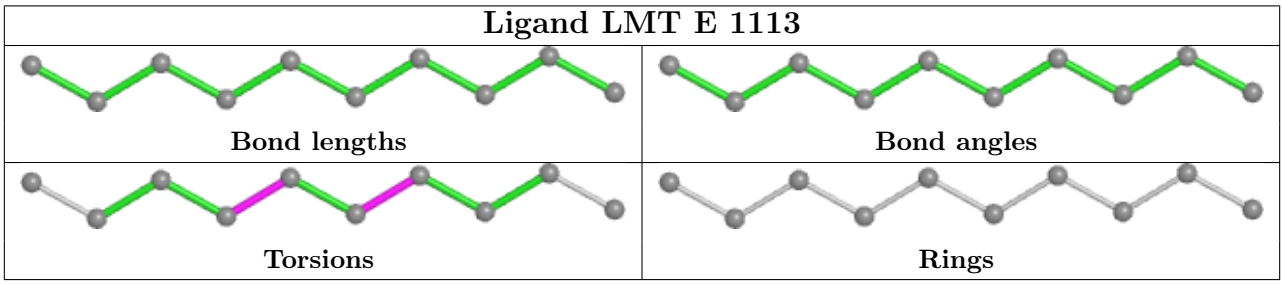
Ligand LMT A 1106



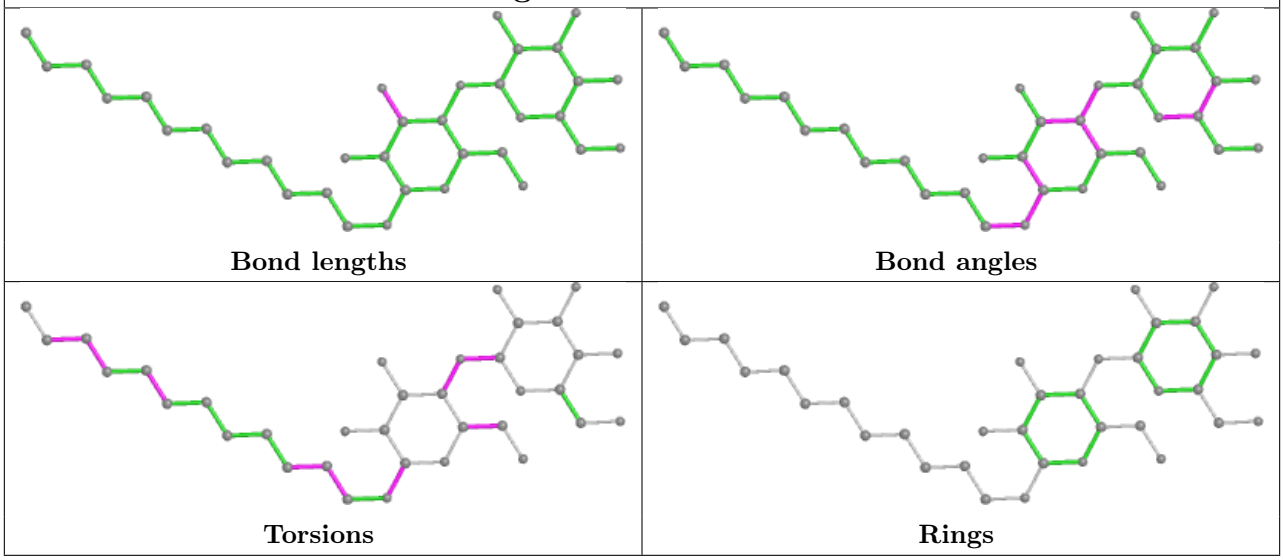
Ligand LMT A 1108



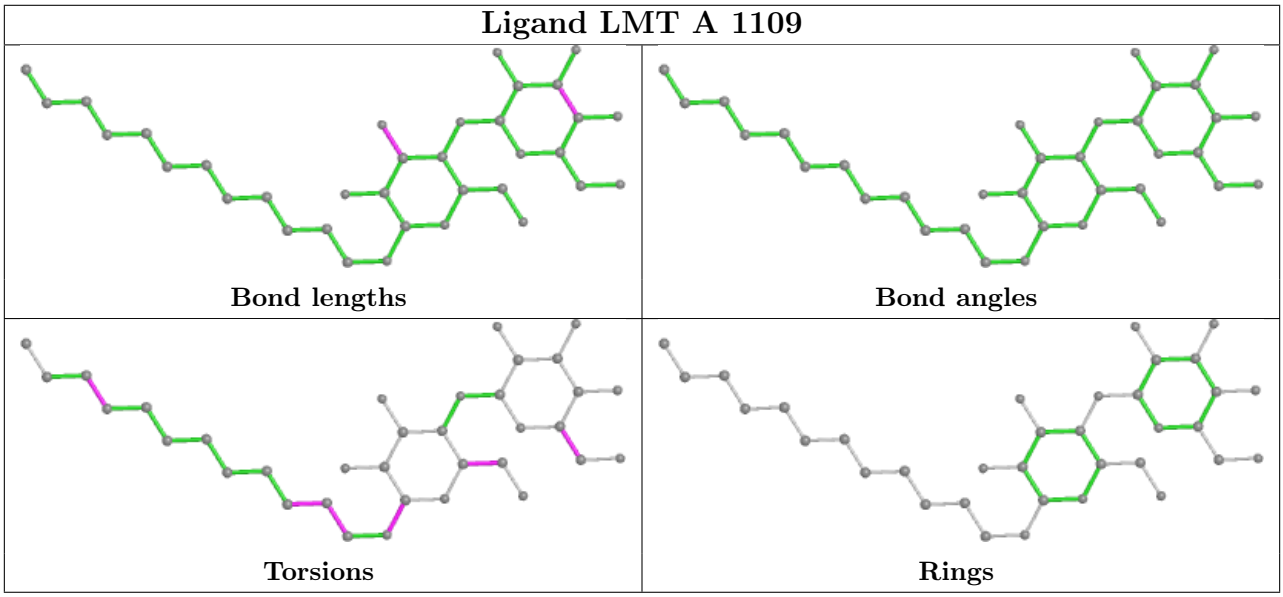
Ligand LMT E 1113



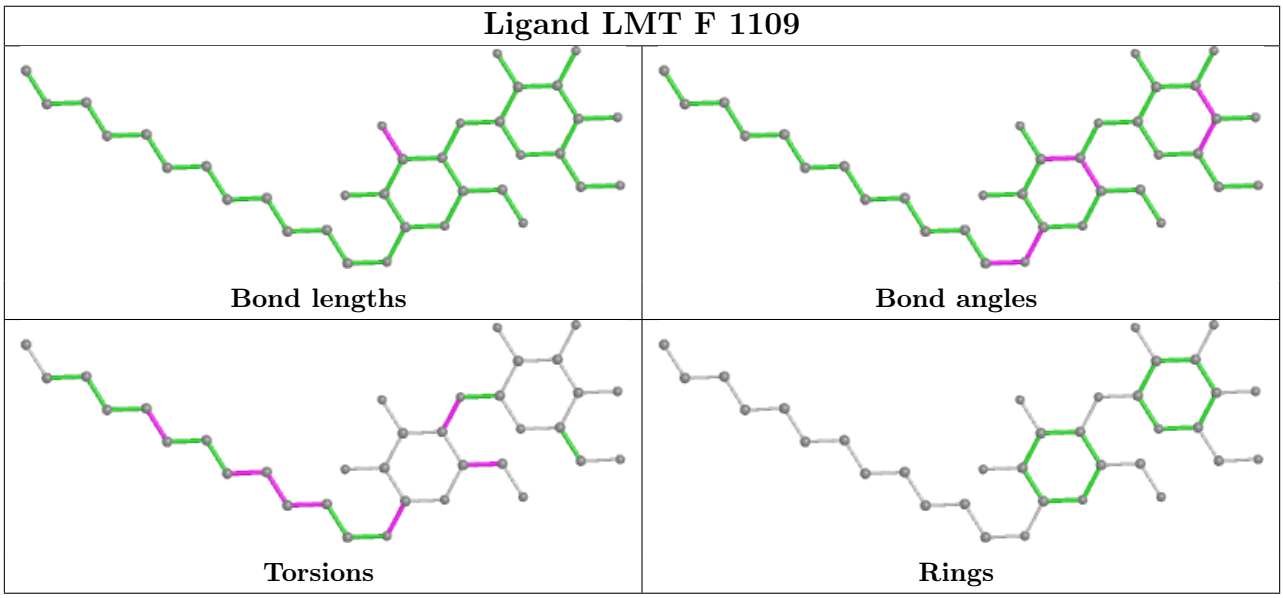
Ligand LMT B 1101



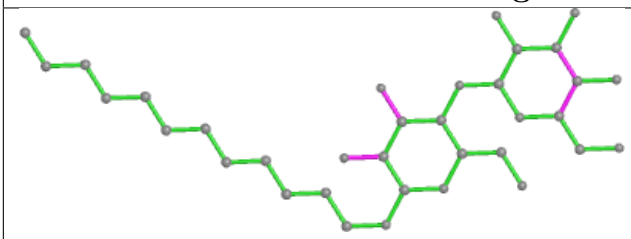
Ligand LMT A 1109



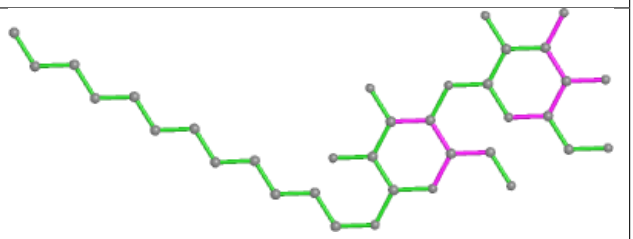
Ligand LMT F 1109



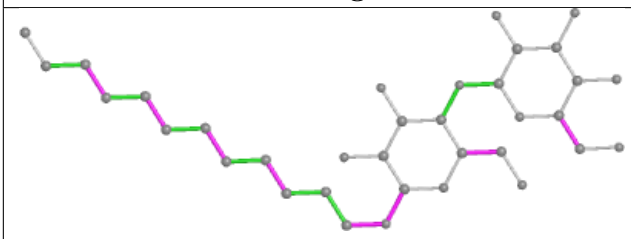
Ligand LMT B 1105



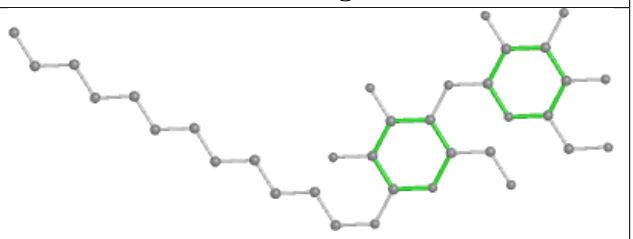
Bond lengths



Bond angles

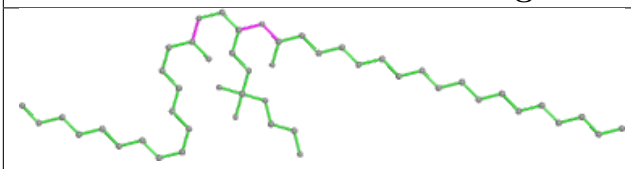


Torsions

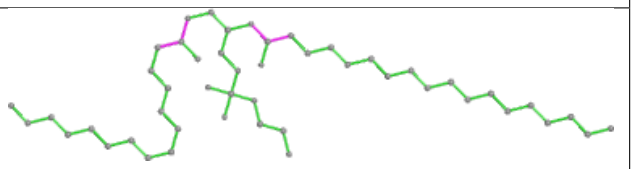


Rings

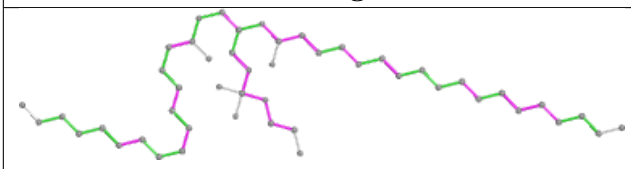
Ligand PTY E 1115



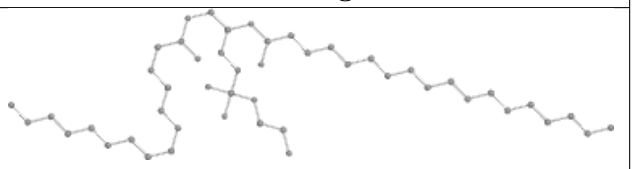
Bond lengths



Bond angles

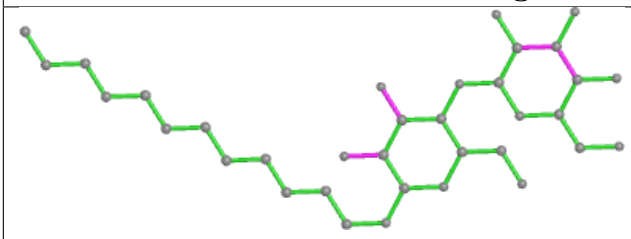


Torsions

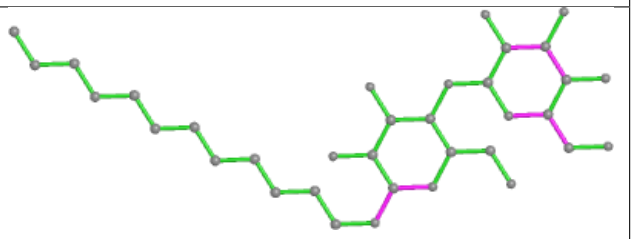


Rings

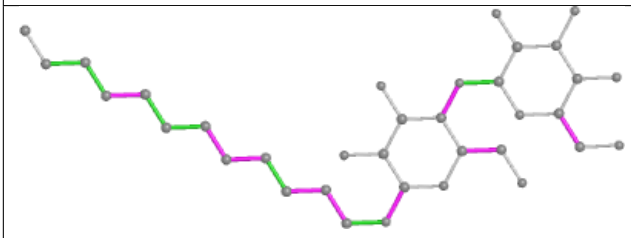
Ligand LMT C 1106



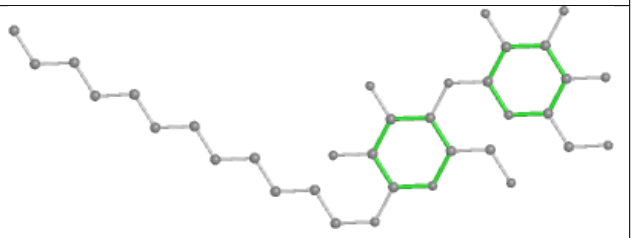
Bond lengths



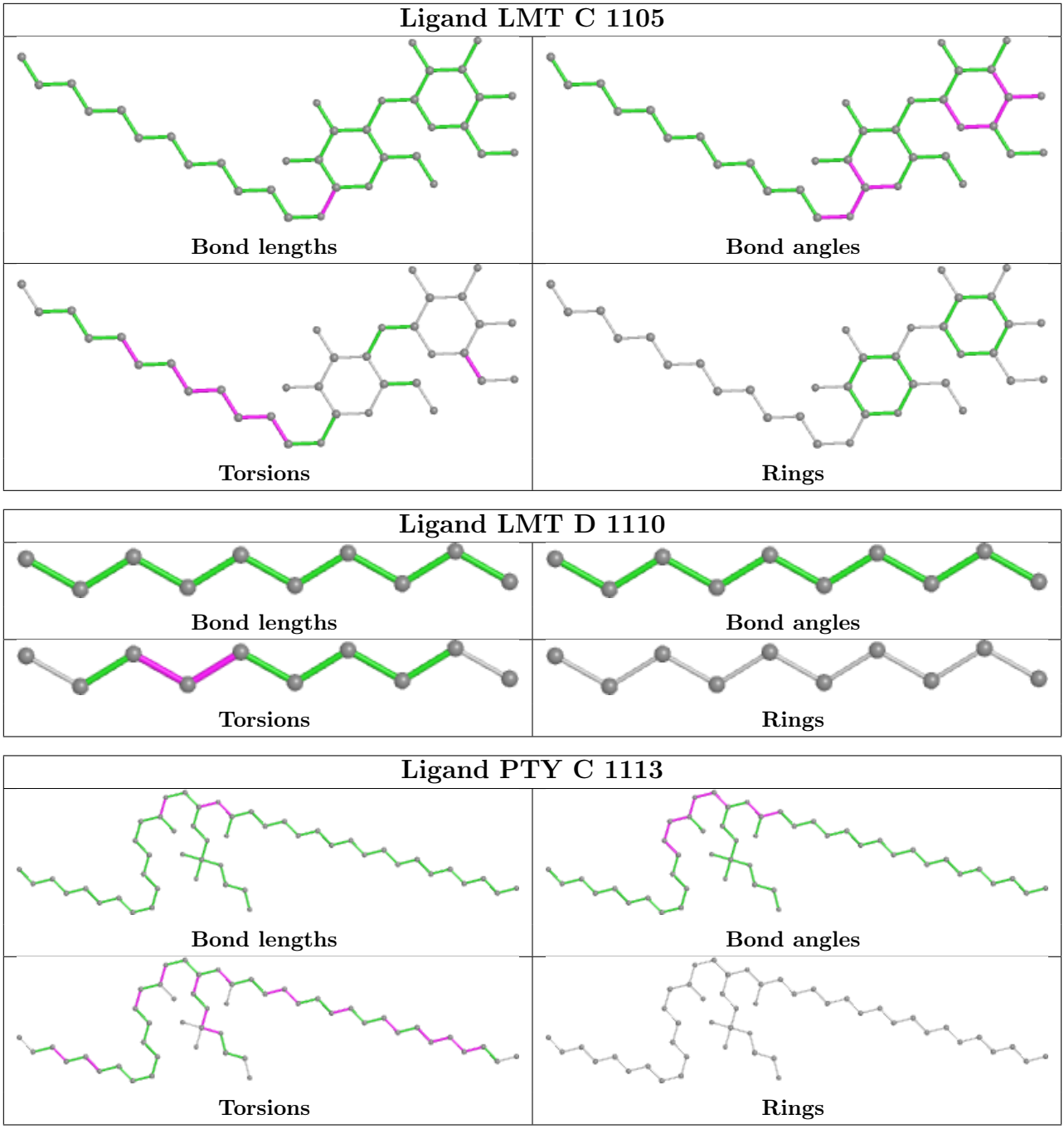
Bond angles



Torsions



Rings



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1041/1042 (99%)	0.07	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

The worst 5 of 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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

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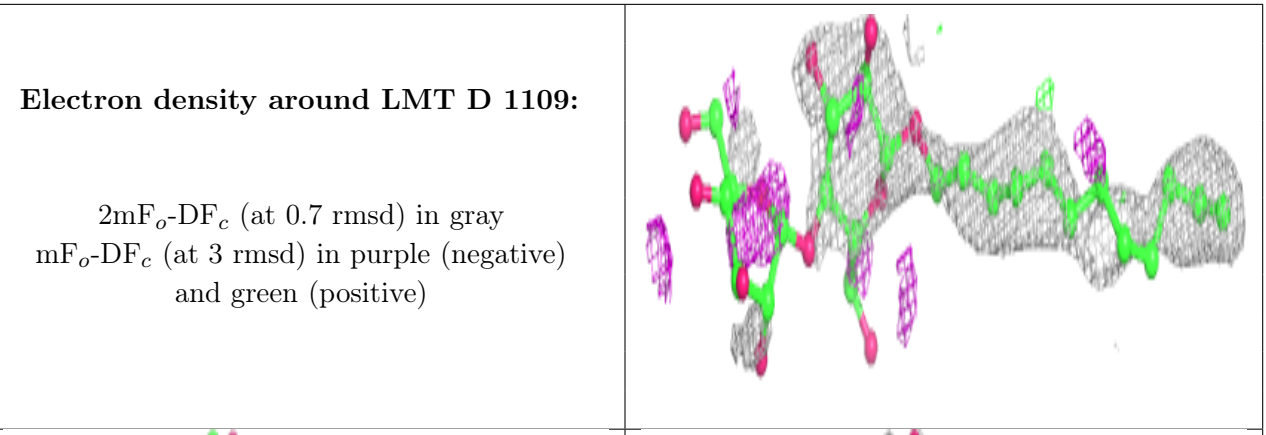
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	A	1104	35/35	0.83	0.16	32,58,66,67	0
4	GOL	E	1122	6/6	0.84	0.15	44,49,53,60	0
4	GOL	A	1117	6/6	0.84	0.10	62,69,71,72	0
4	GOL	C	1120	6/6	0.85	0.12	50,57,65,67	0
2	LMT	A	1103	35/35	0.85	0.16	54,65,82,86	0
2	LMT	F	1113	35/35	0.85	0.20	51,83,101,103	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
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.

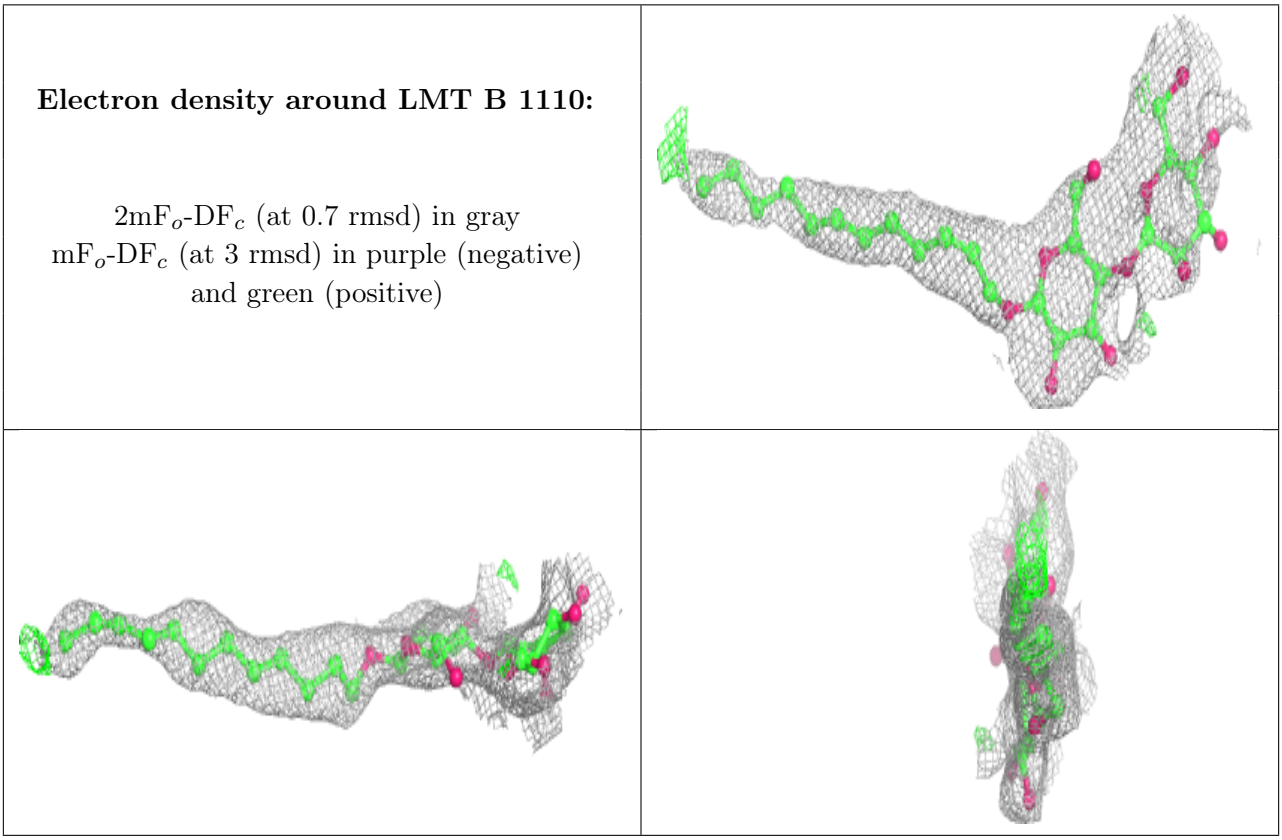
Electron density around LMT D 1109:

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



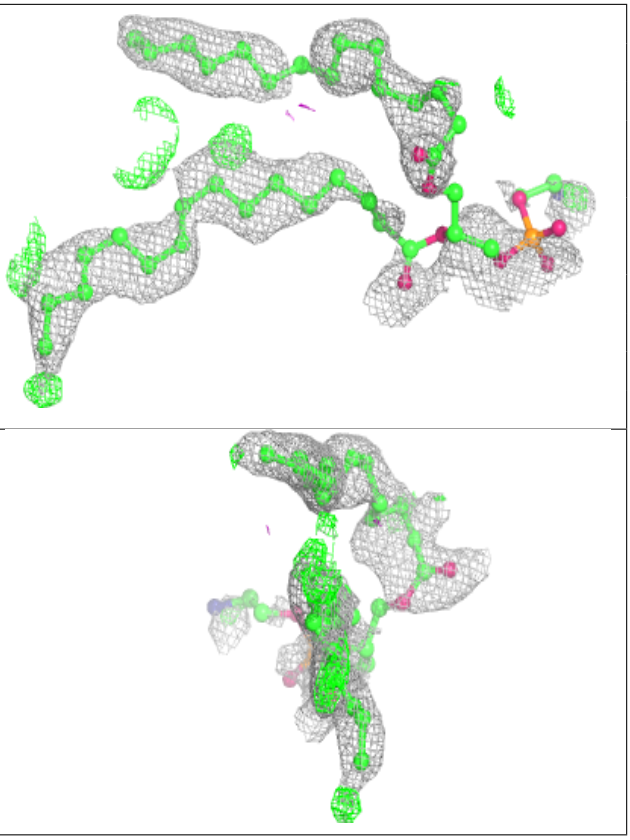
Electron density around LMT B 1110:

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



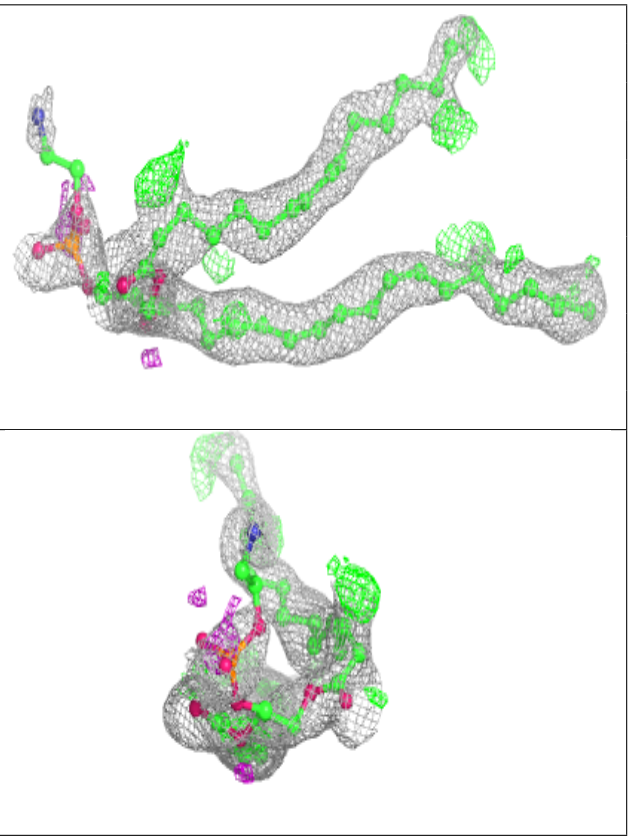
Electron density around PTY E 1114:

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



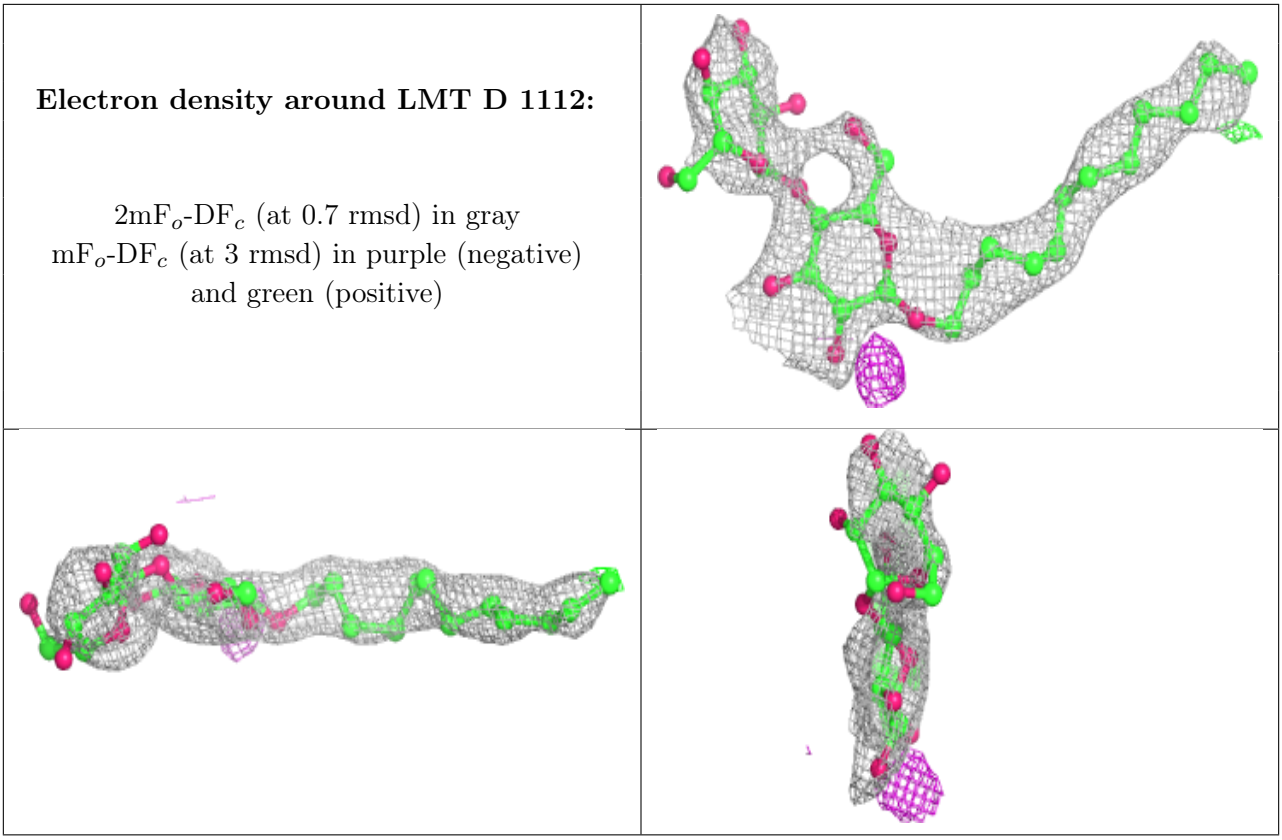
Electron density around PTY E 1115:

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



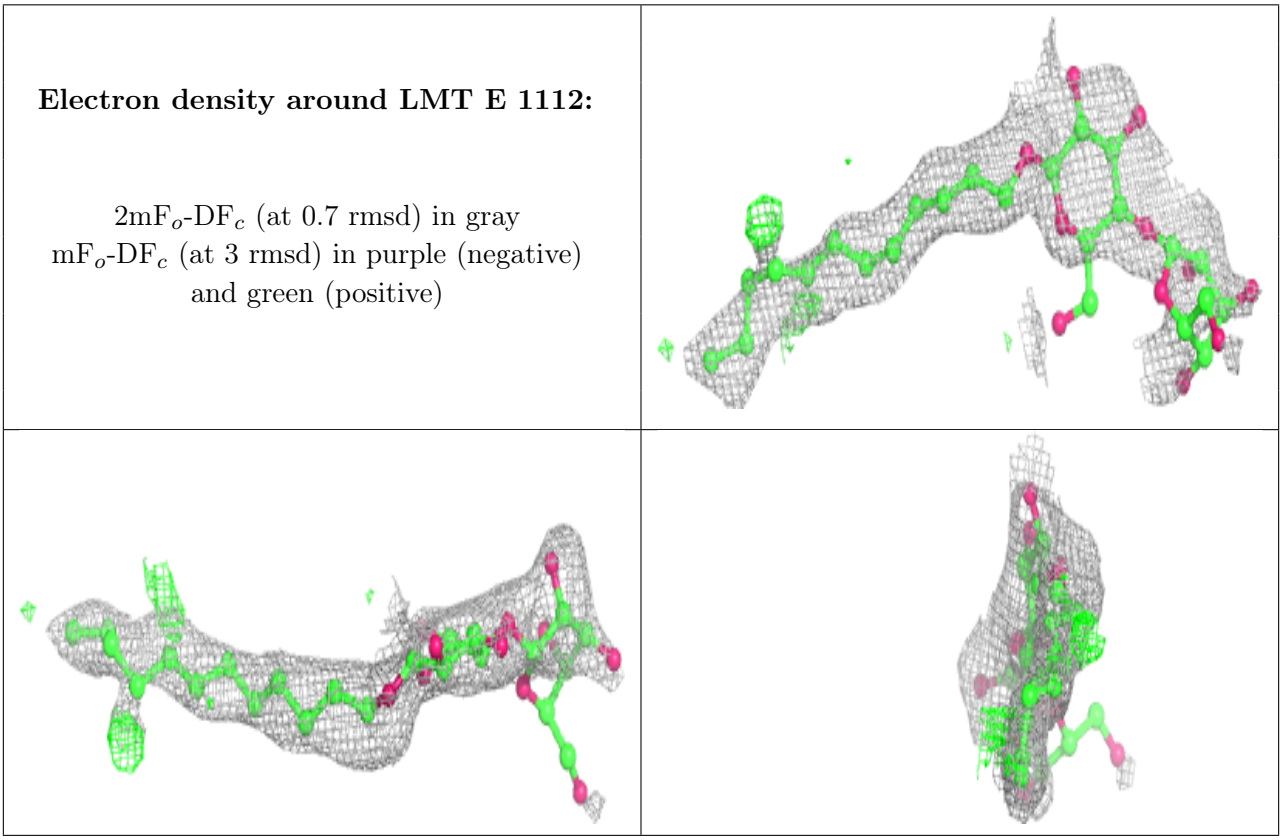
Electron density around LMT D 1112:

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



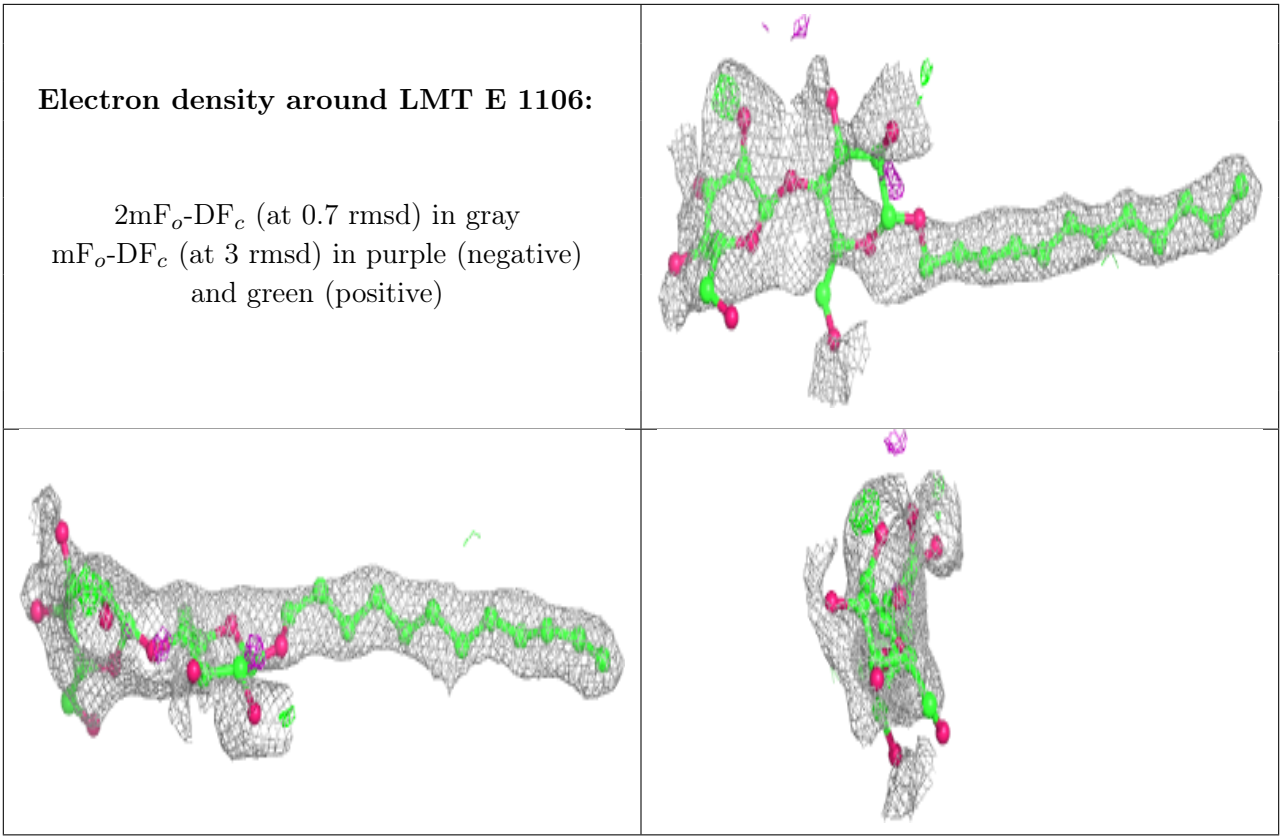
Electron density around LMT E 1112:

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



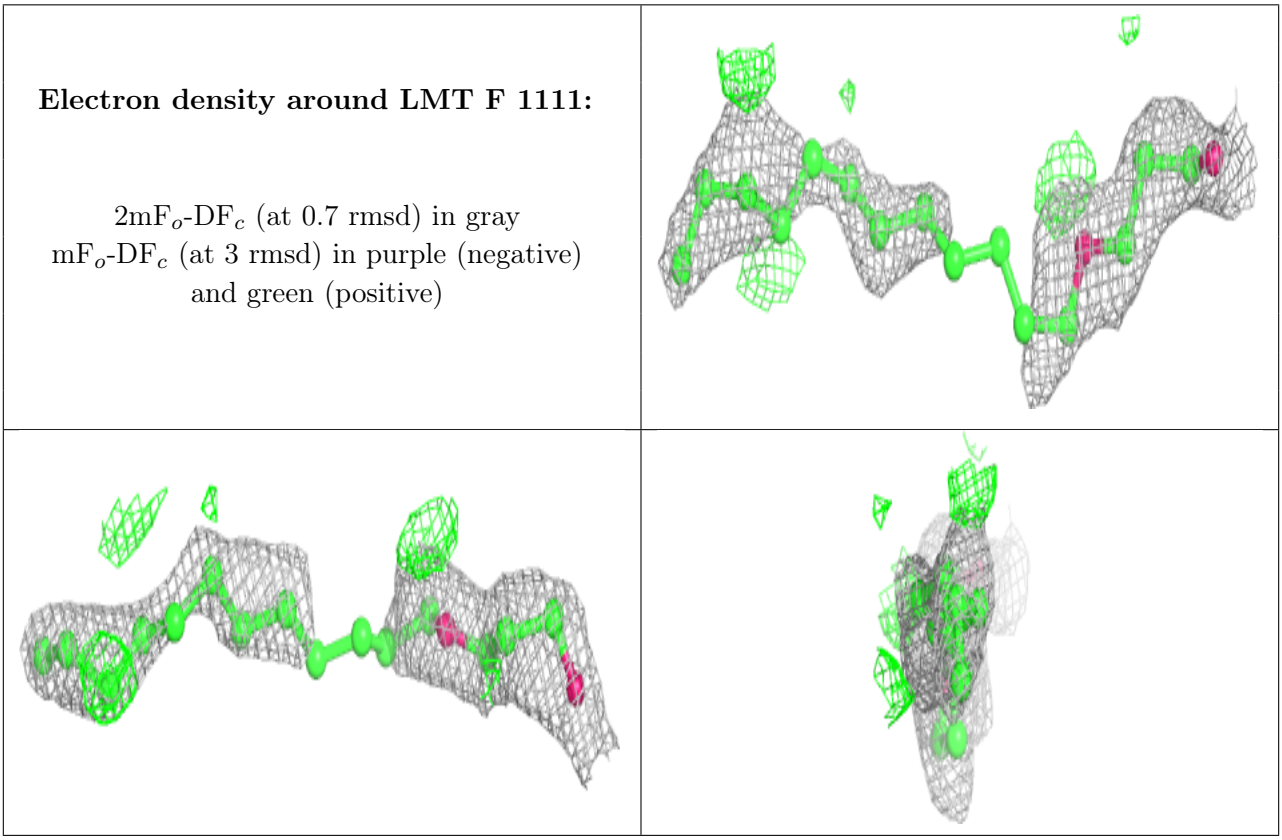
Electron density around LMT E 1106:

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



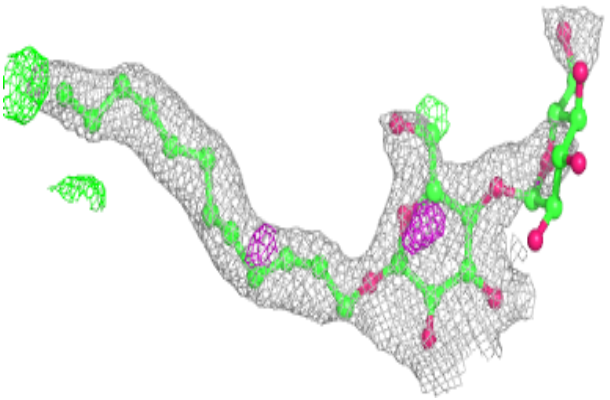
Electron density around LMT F 1111:

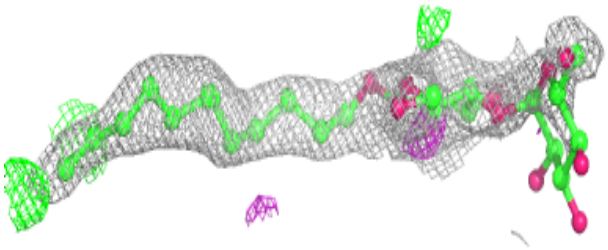
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

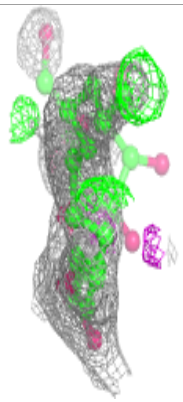


Electron density around LMT A 1107:

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

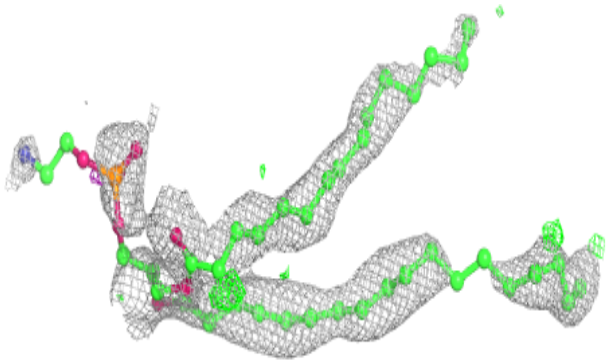


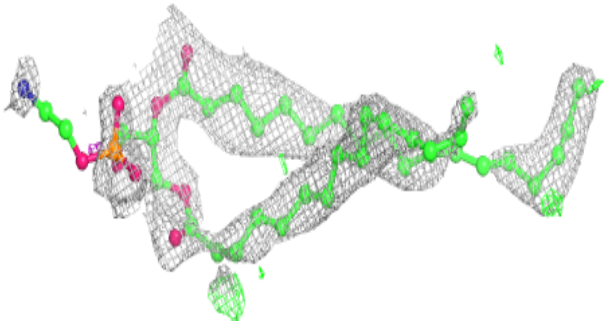




Electron density around PTY D 1113:

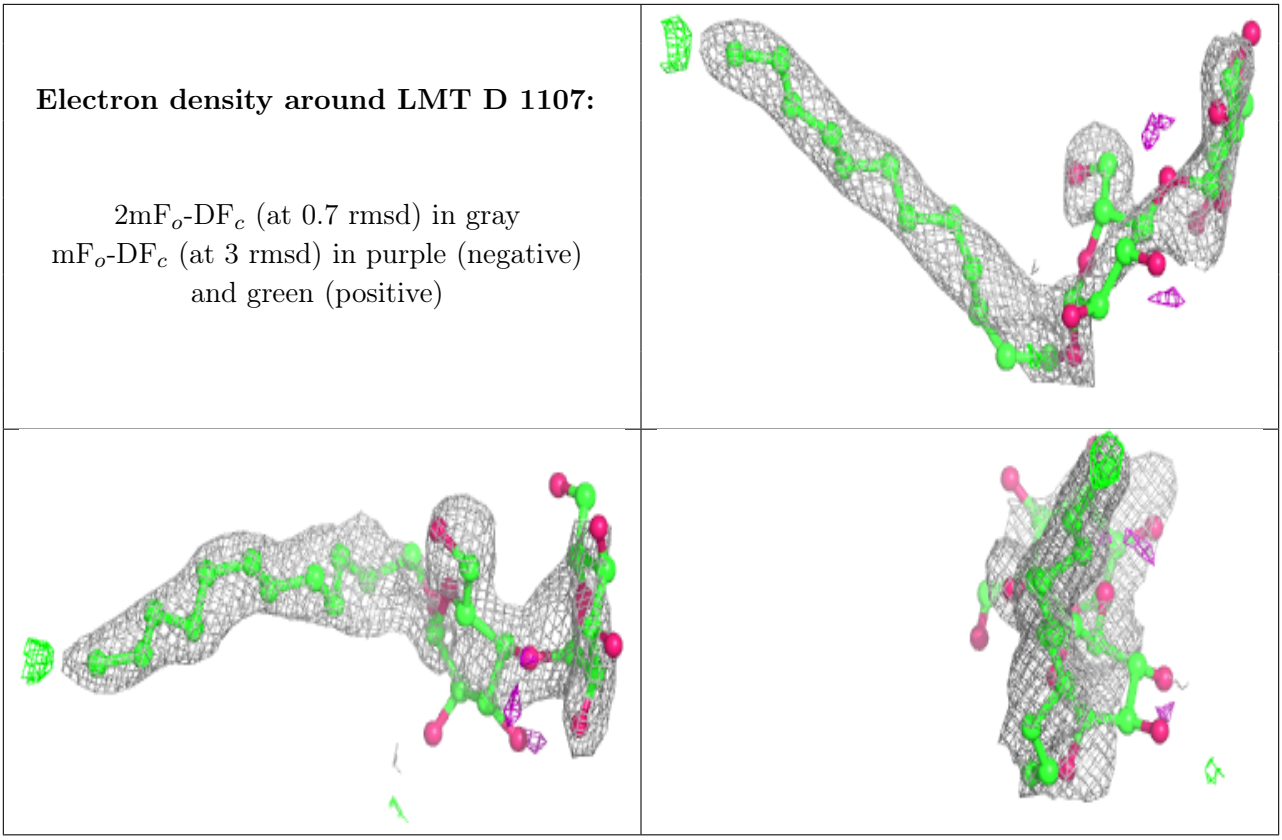
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





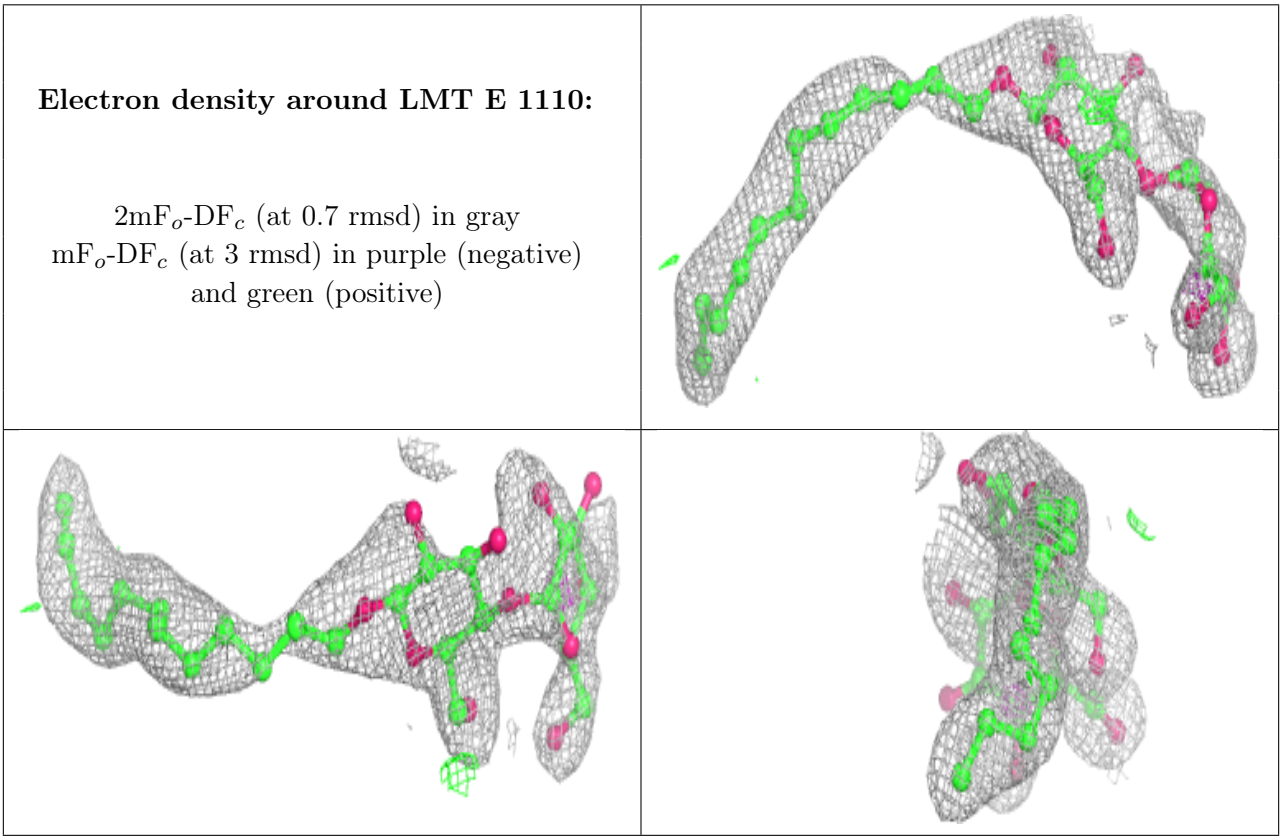
Electron density around LMT D 1107:

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



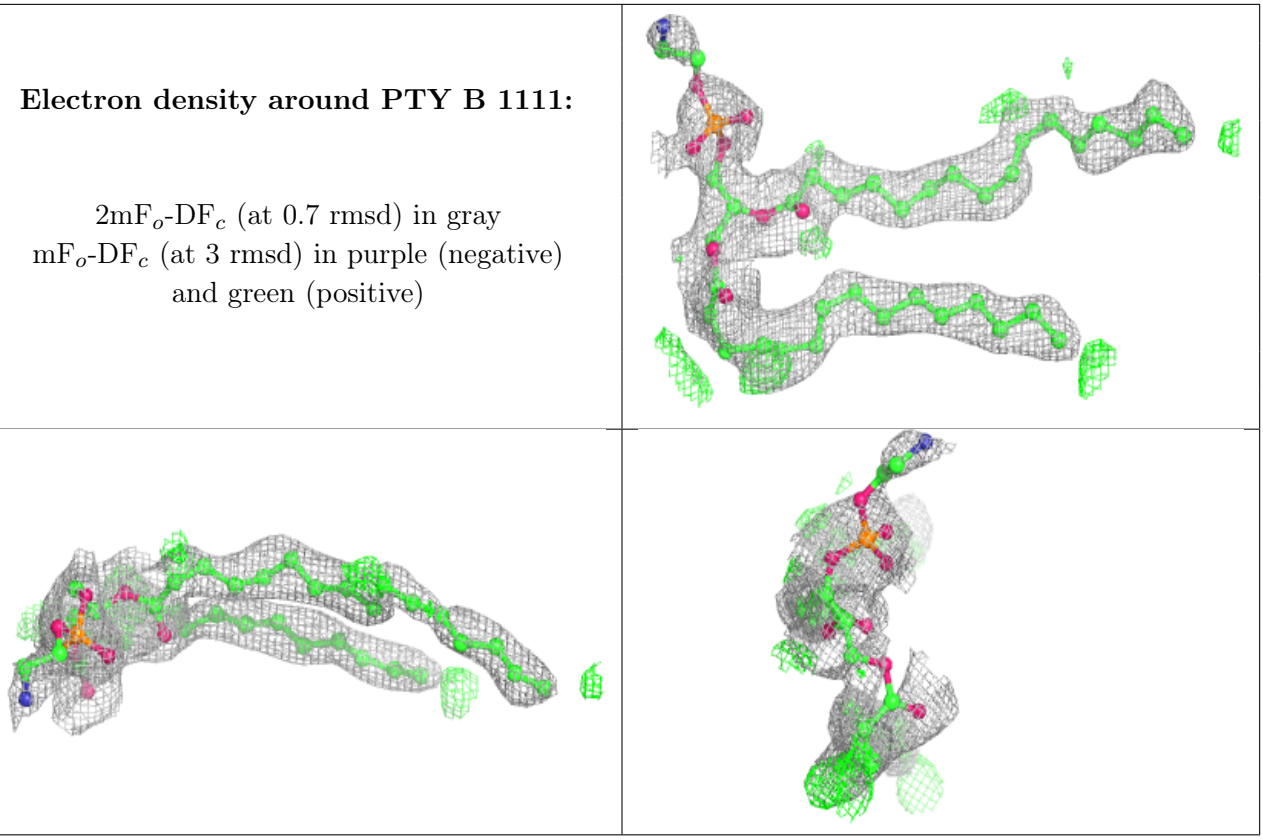
Electron density around LMT E 1110:

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



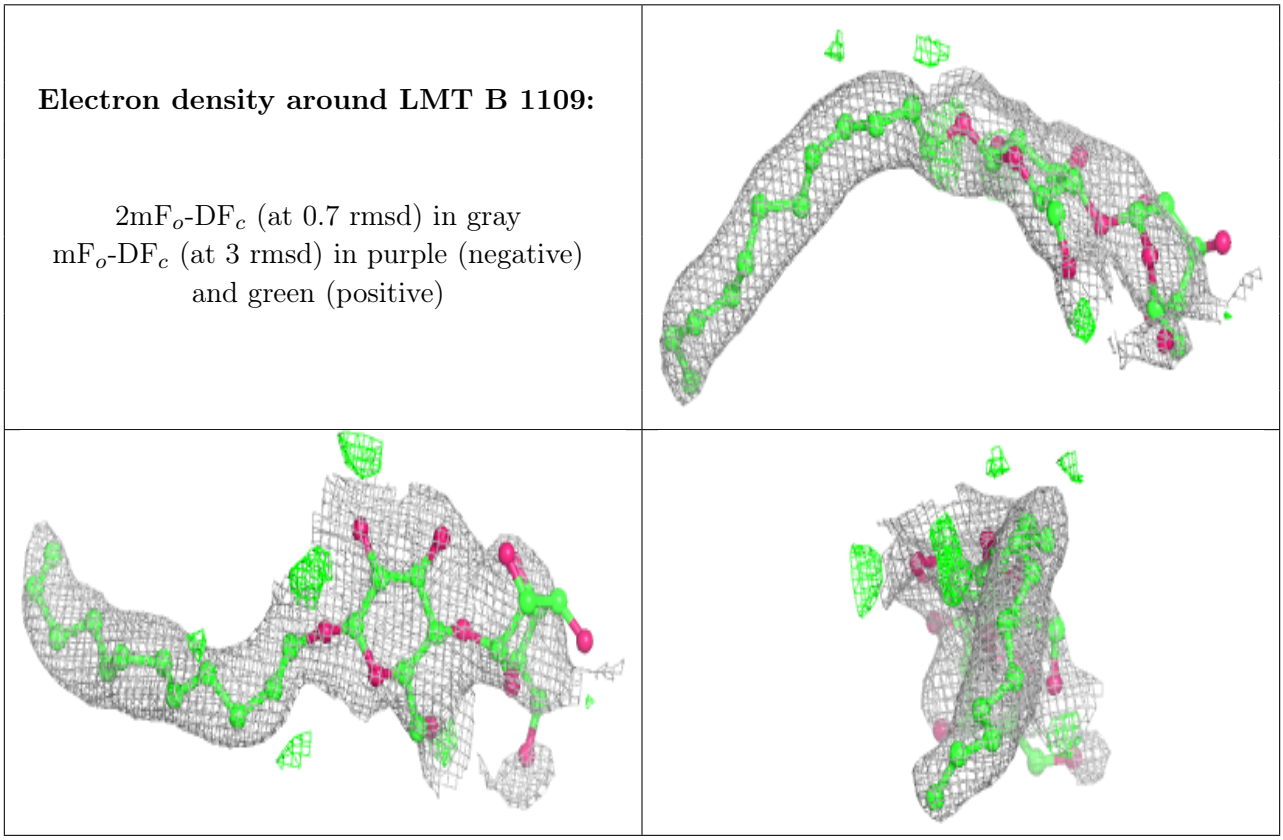
Electron density around PTY B 1111:

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



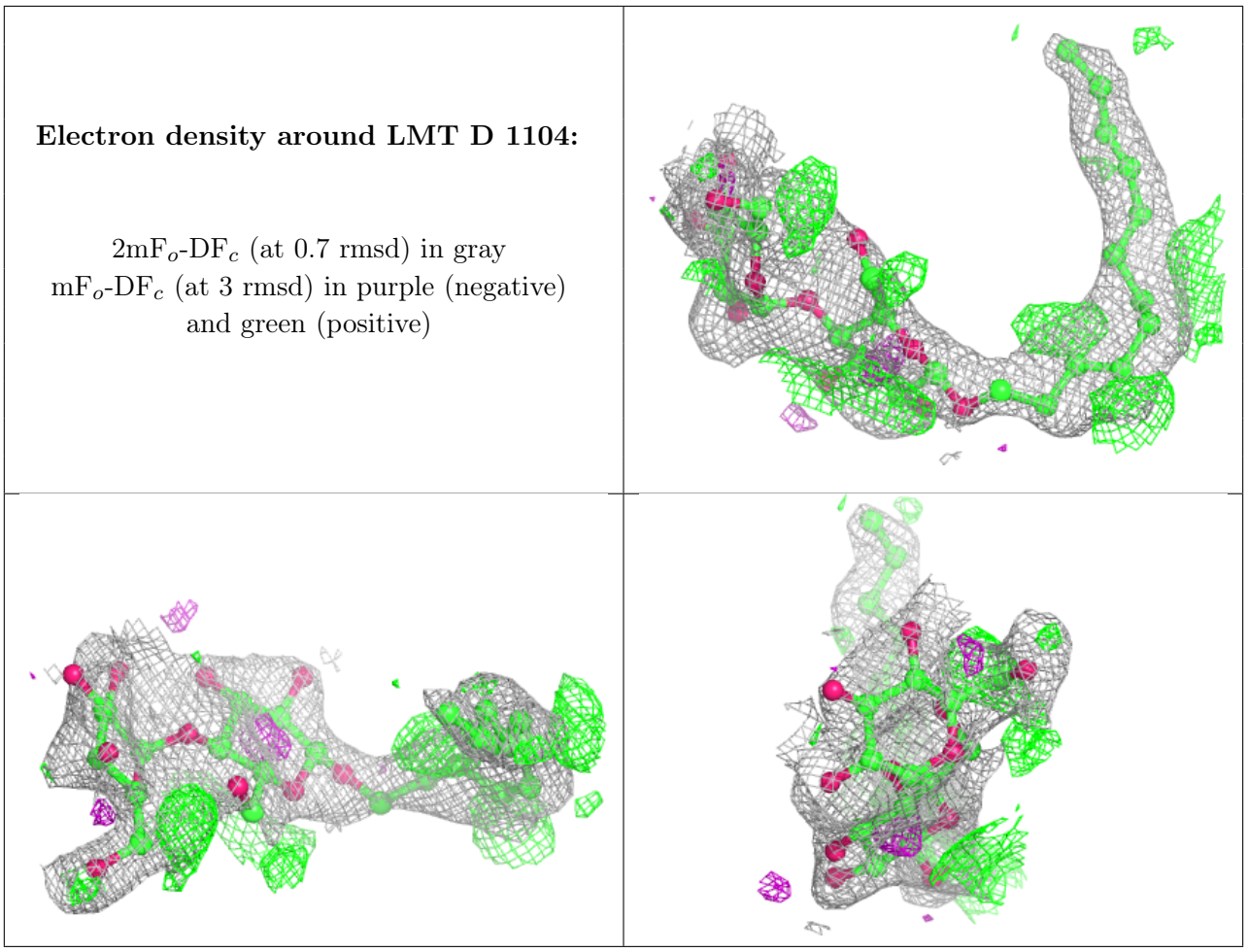
Electron density around LMT B 1109:

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



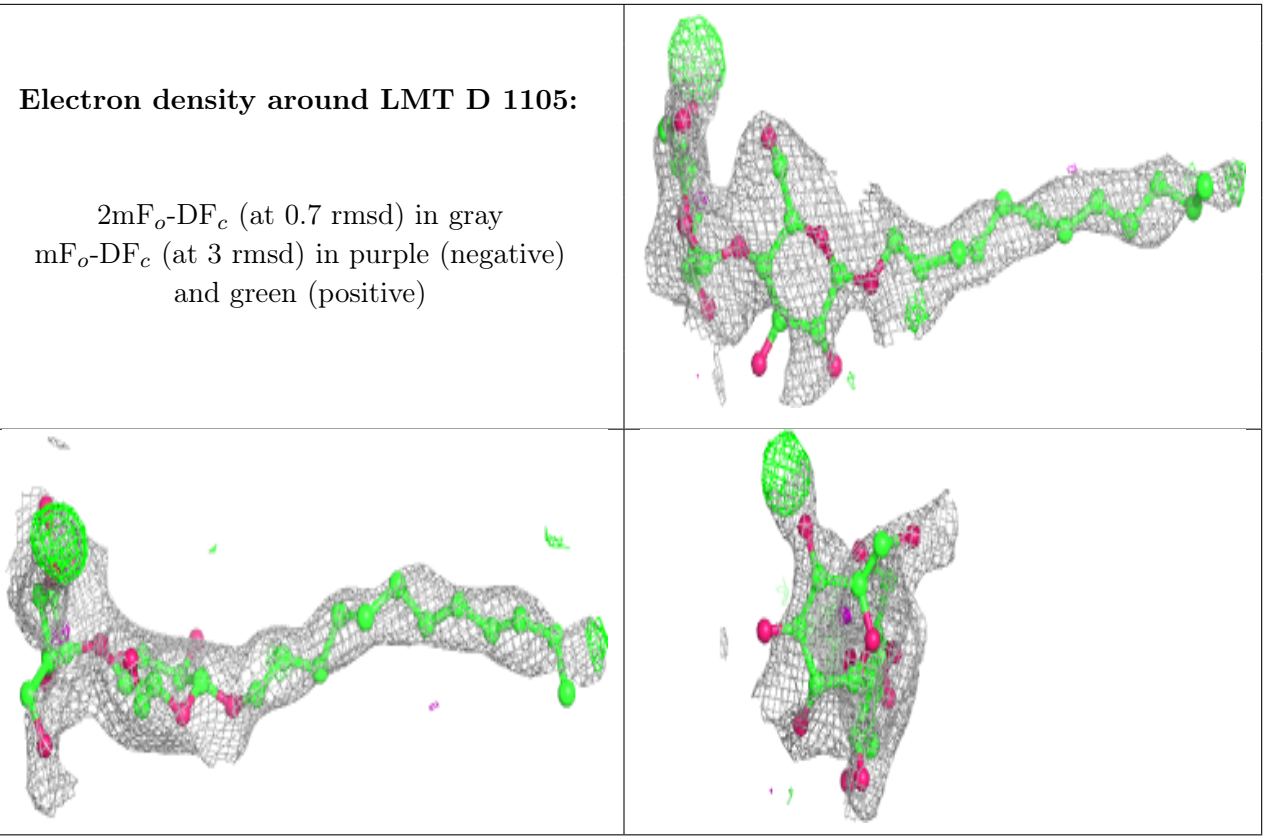
Electron density around LMT D 1104:

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



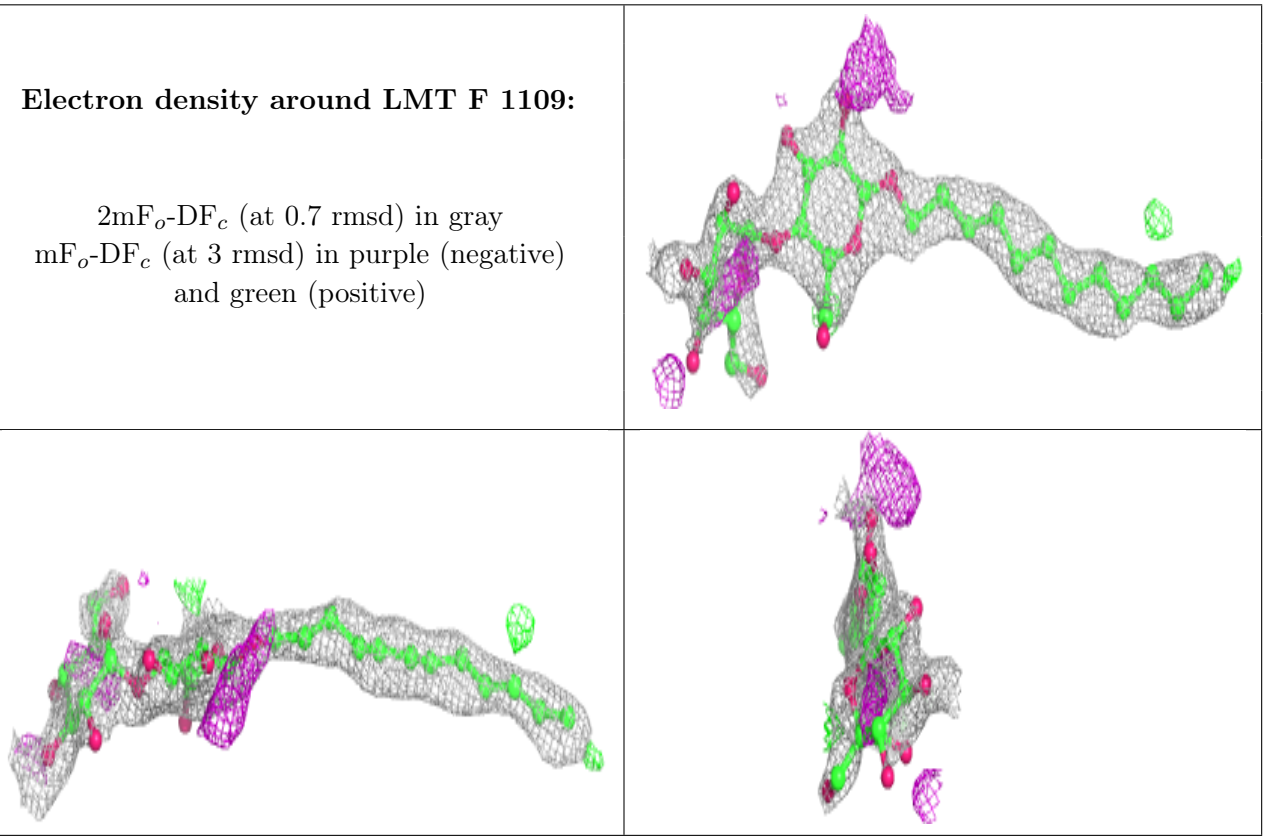
Electron density around LMT D 1105:

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



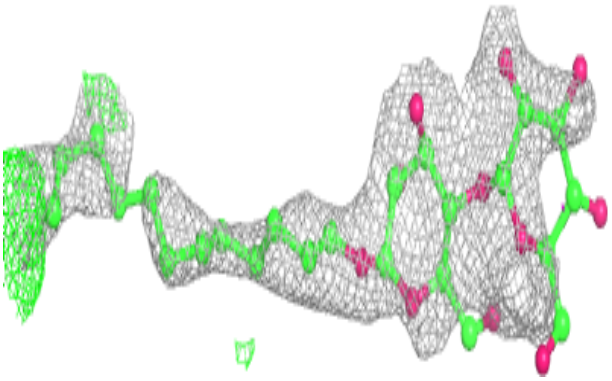
Electron density around LMT F 1109:

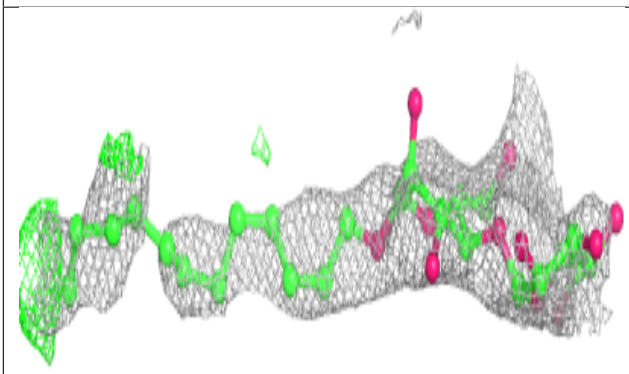
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

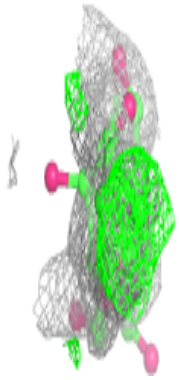


Electron density around LMT A 1101:

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

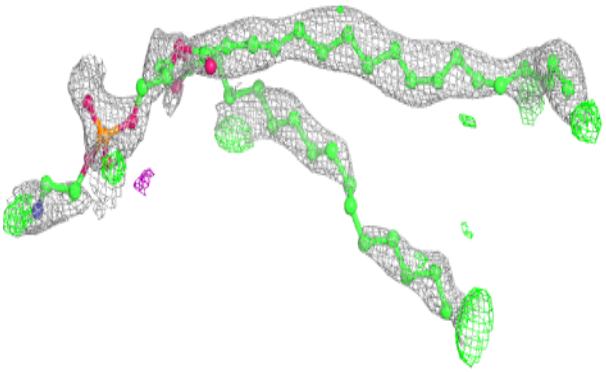


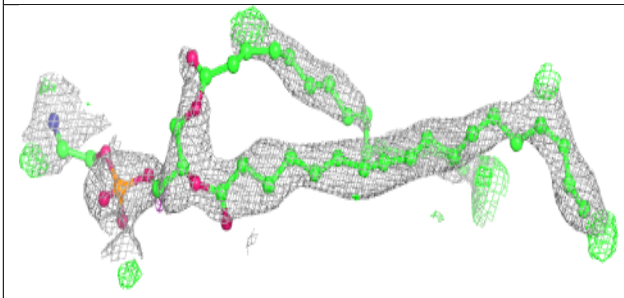


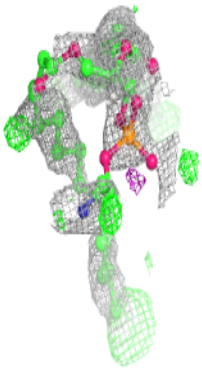


Electron density around PTY F 1115:

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

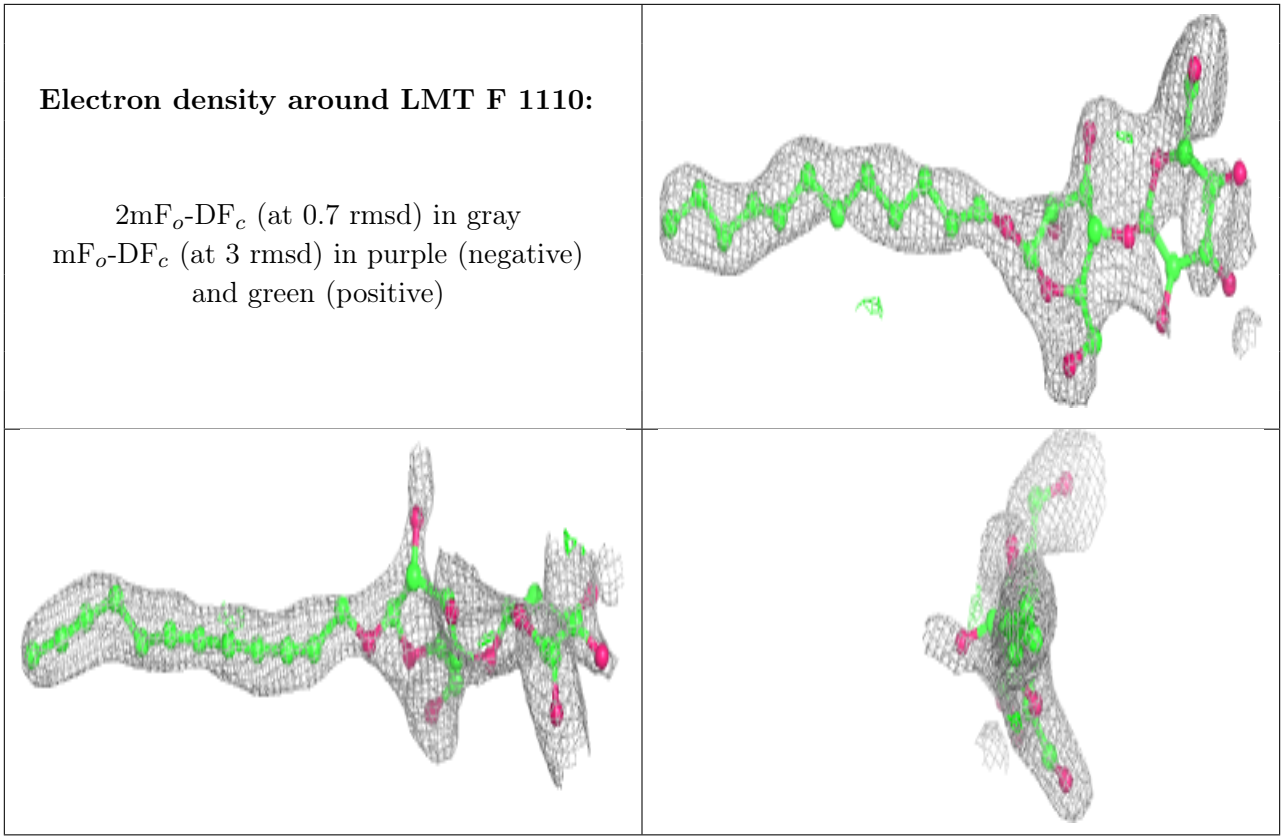






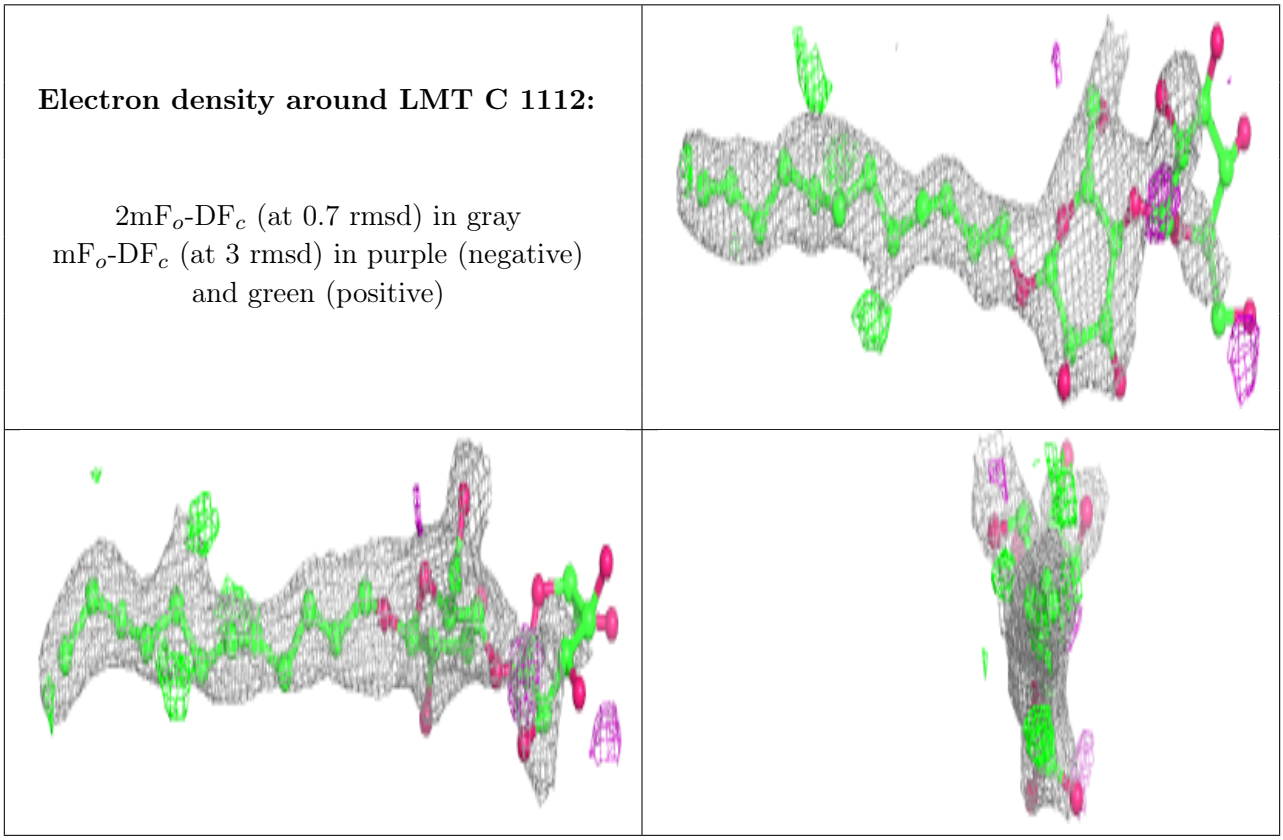
Electron density around LMT F 1110:

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



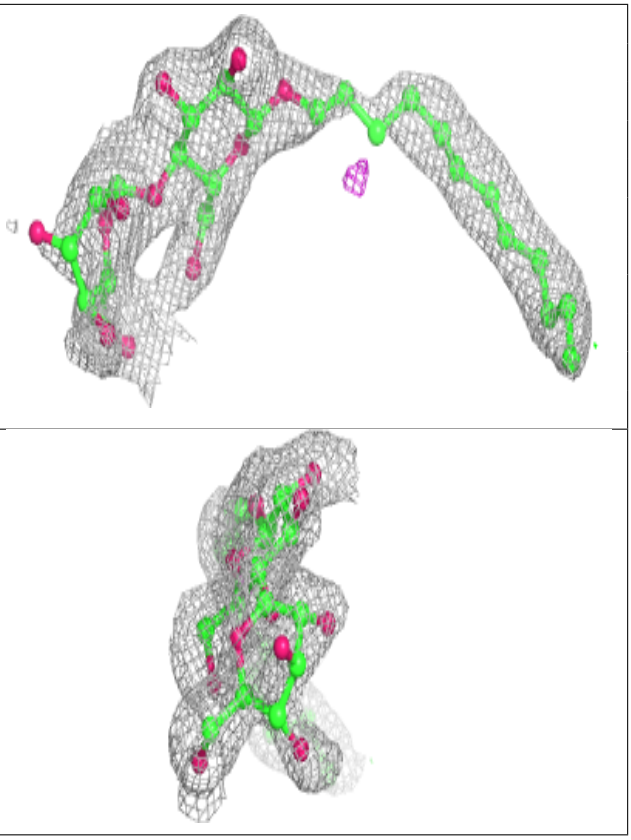
Electron density around LMT C 1112:

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



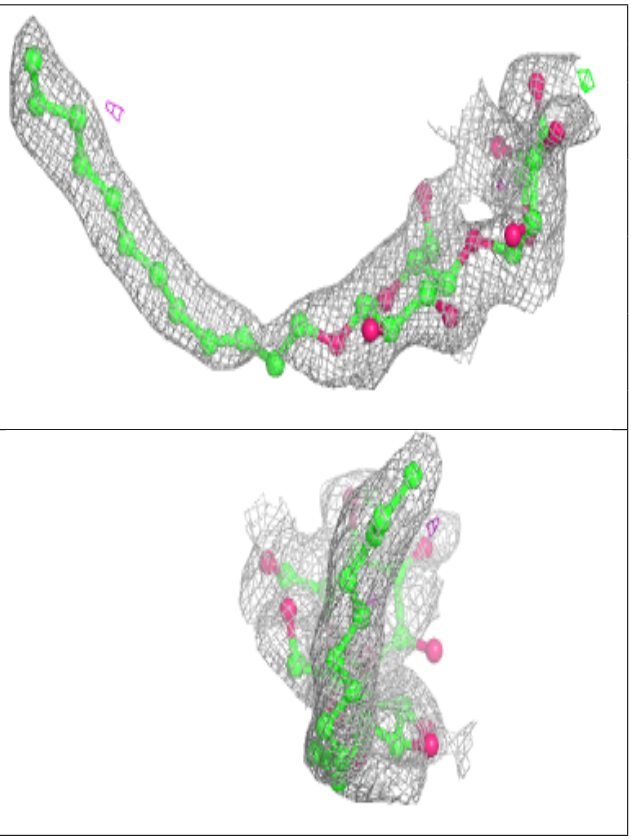
Electron density around LMT A 1109:

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



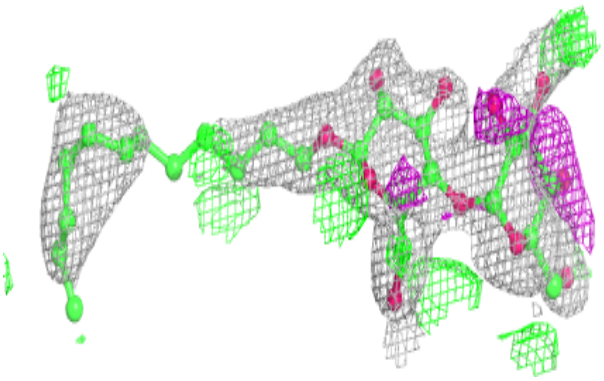
Electron density around LMT D 1108:

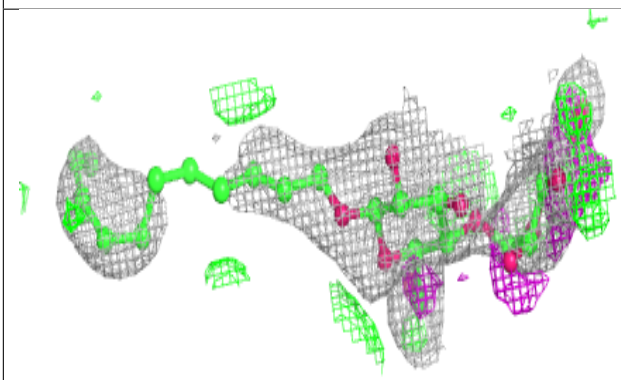
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

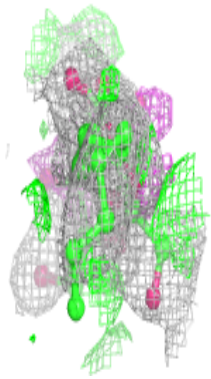


Electron density around LMT F 1103:

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

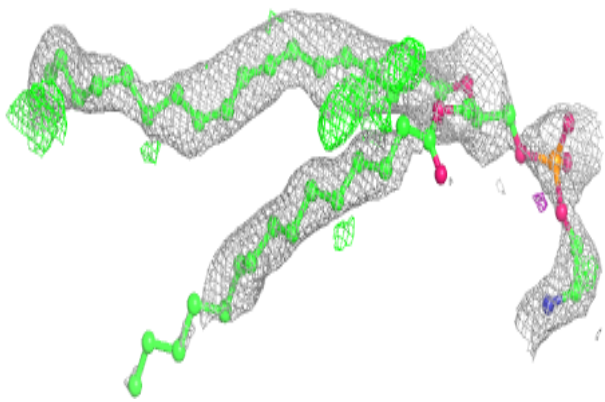


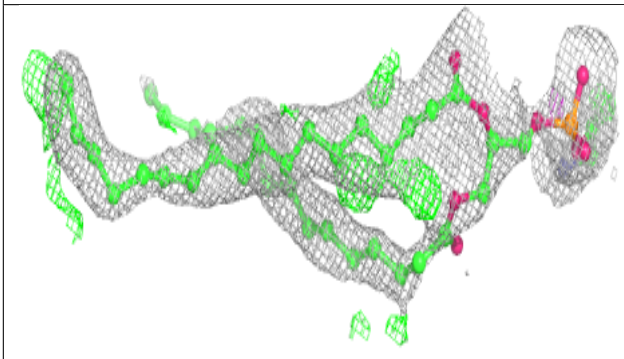


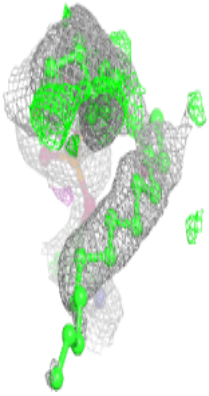


Electron density around PTY C 1113:

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

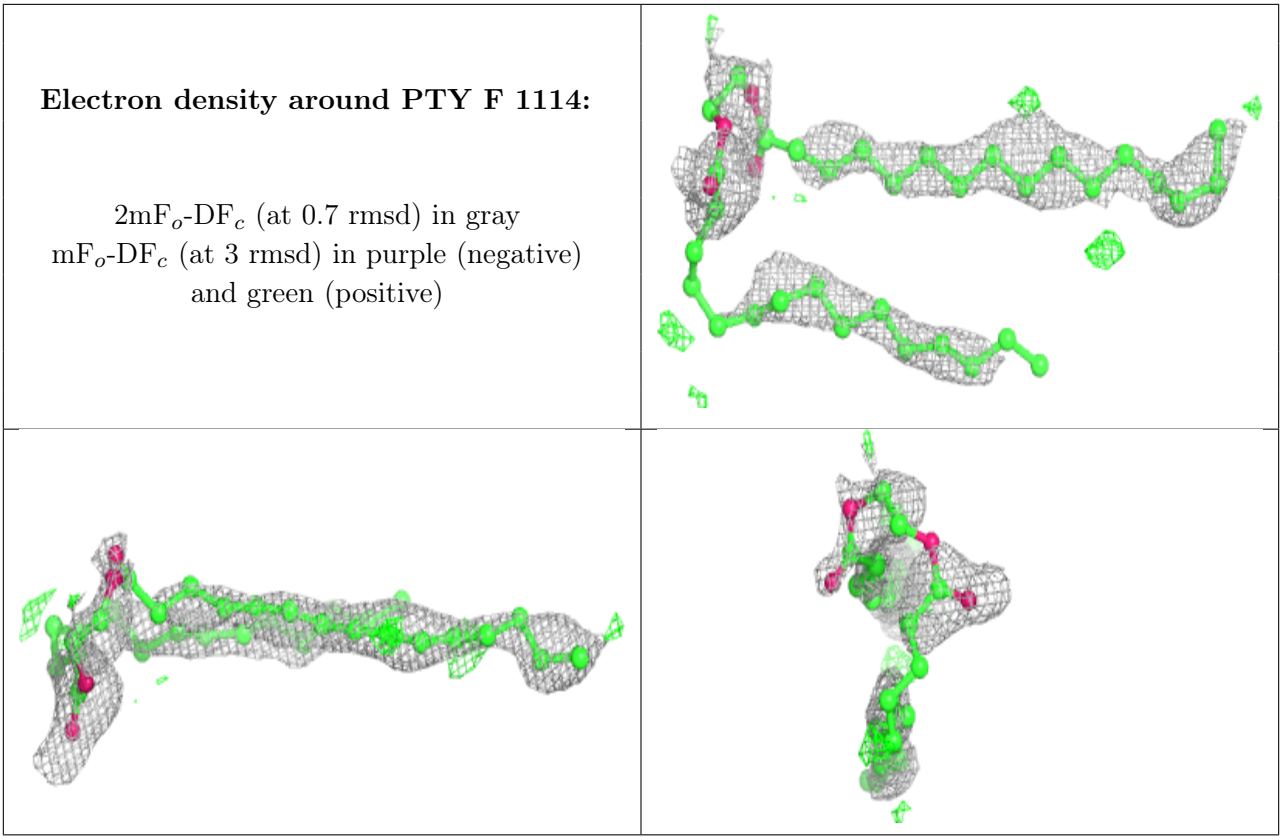






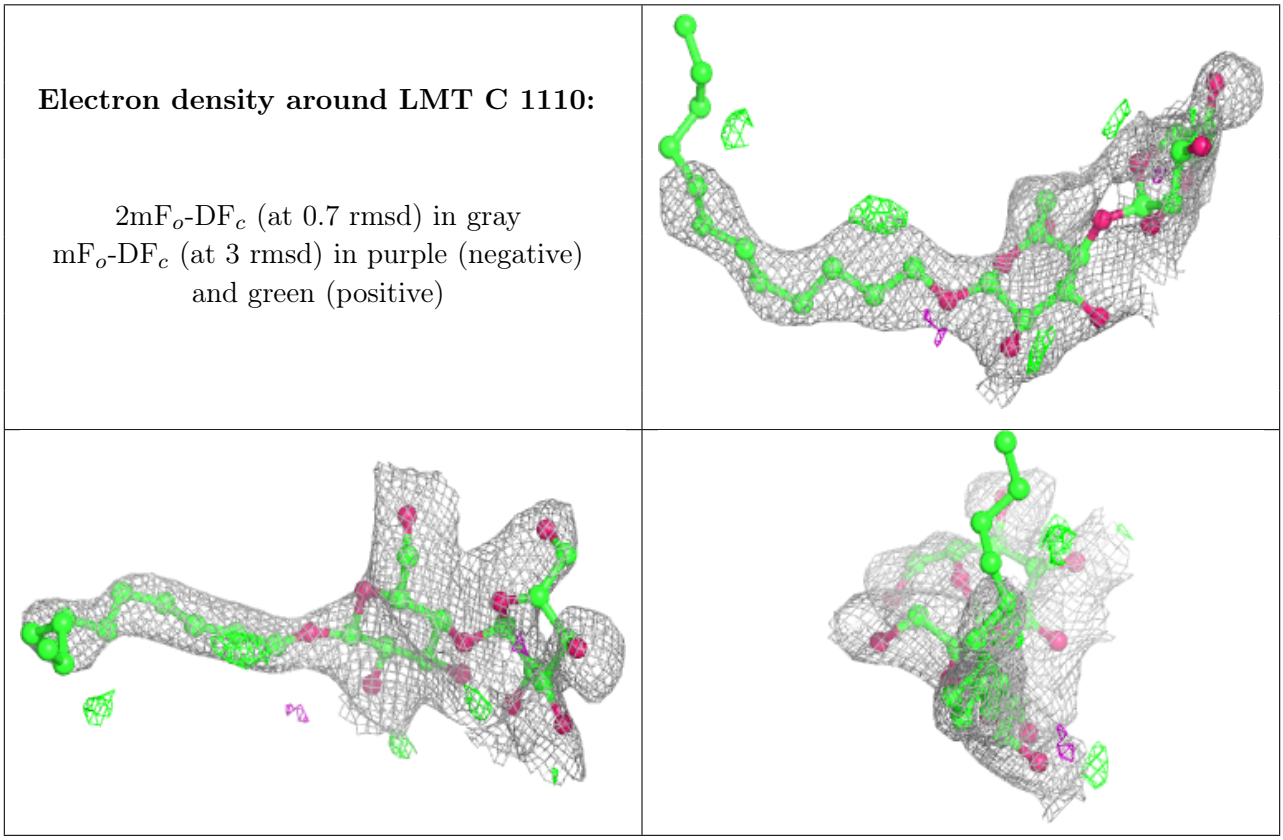
Electron density around PTY F 1114:

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



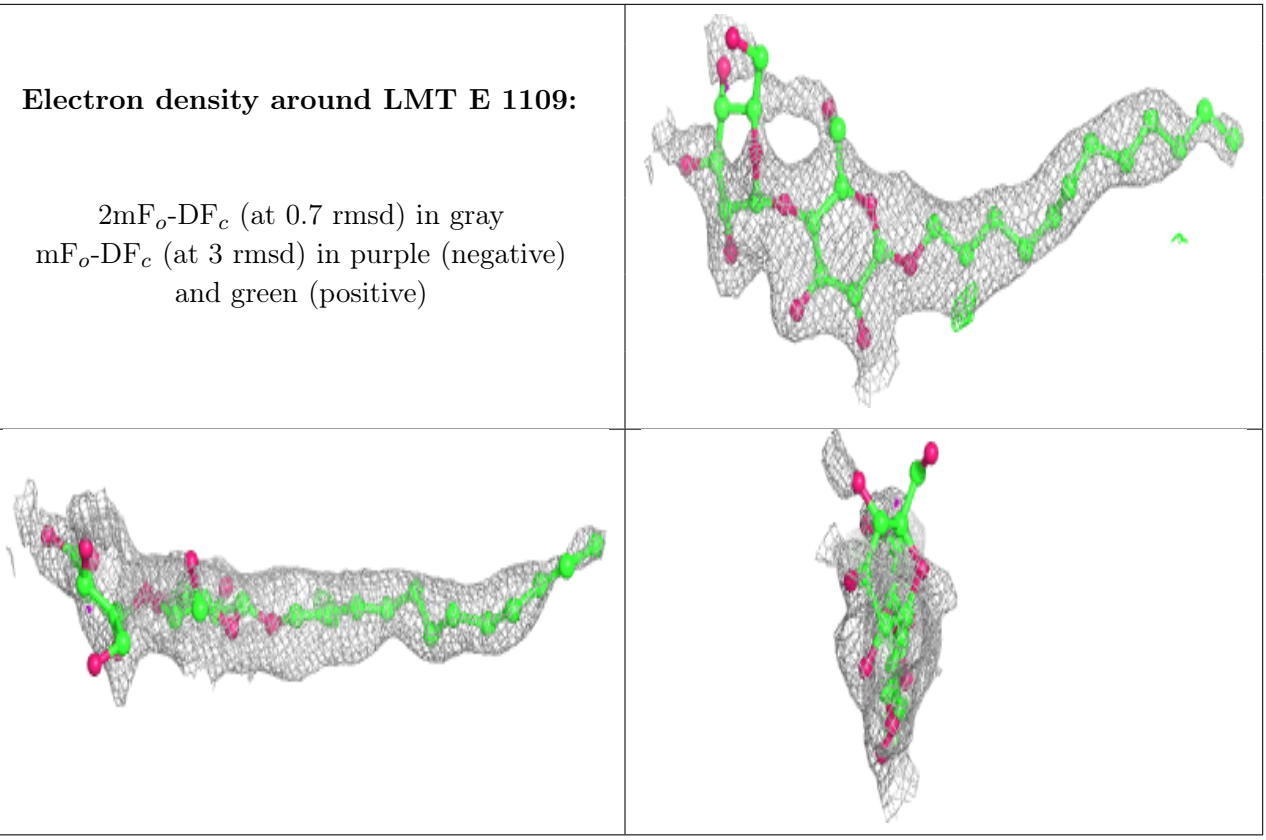
Electron density around LMT C 1110:

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



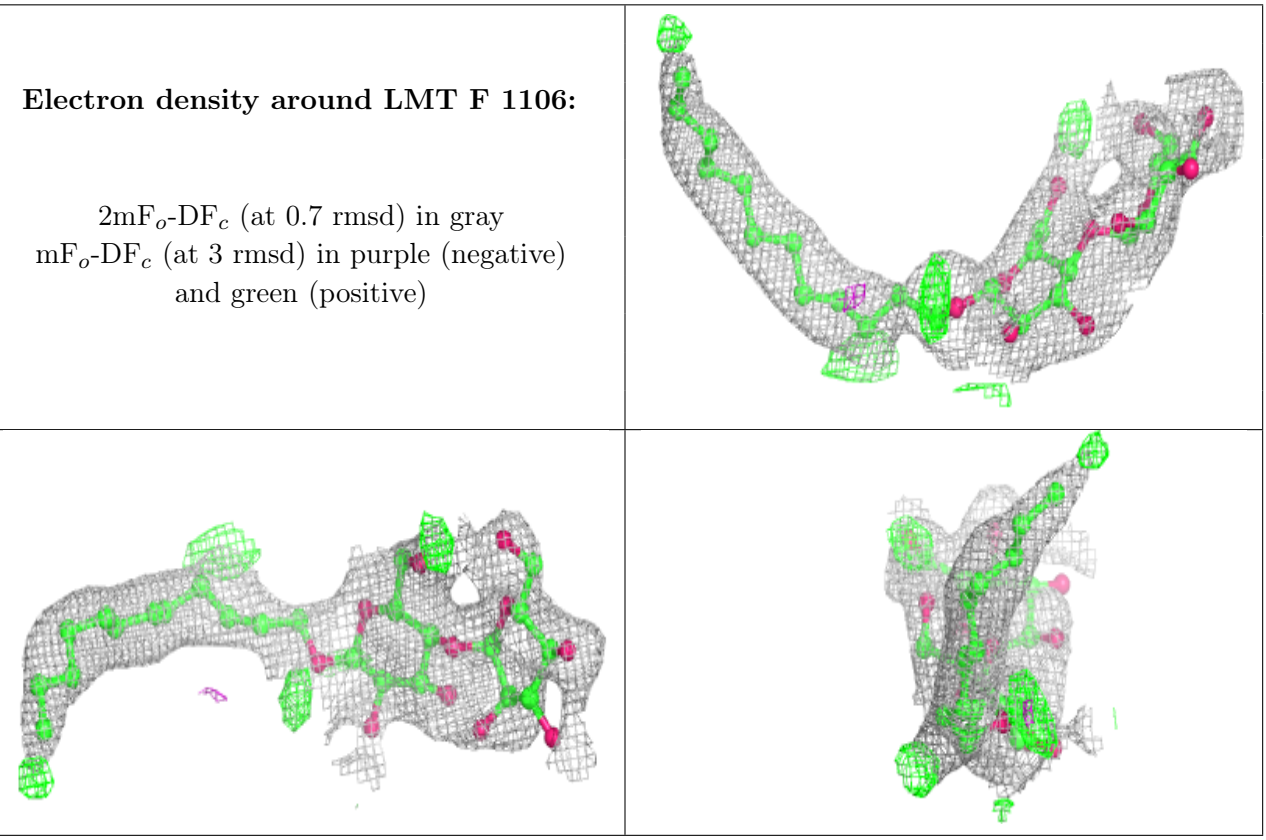
Electron density around LMT E 1109:

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



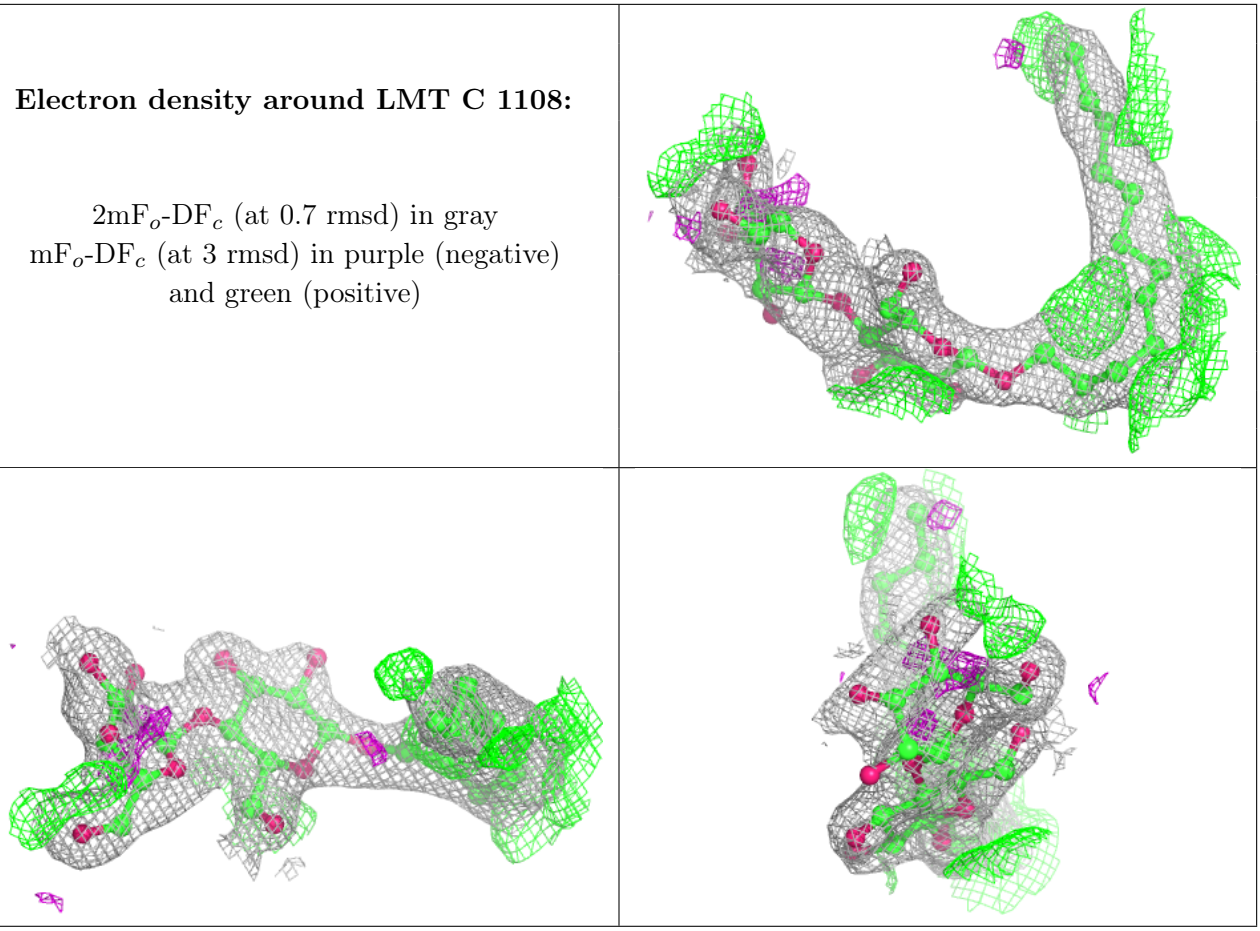
Electron density around LMT F 1106:

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



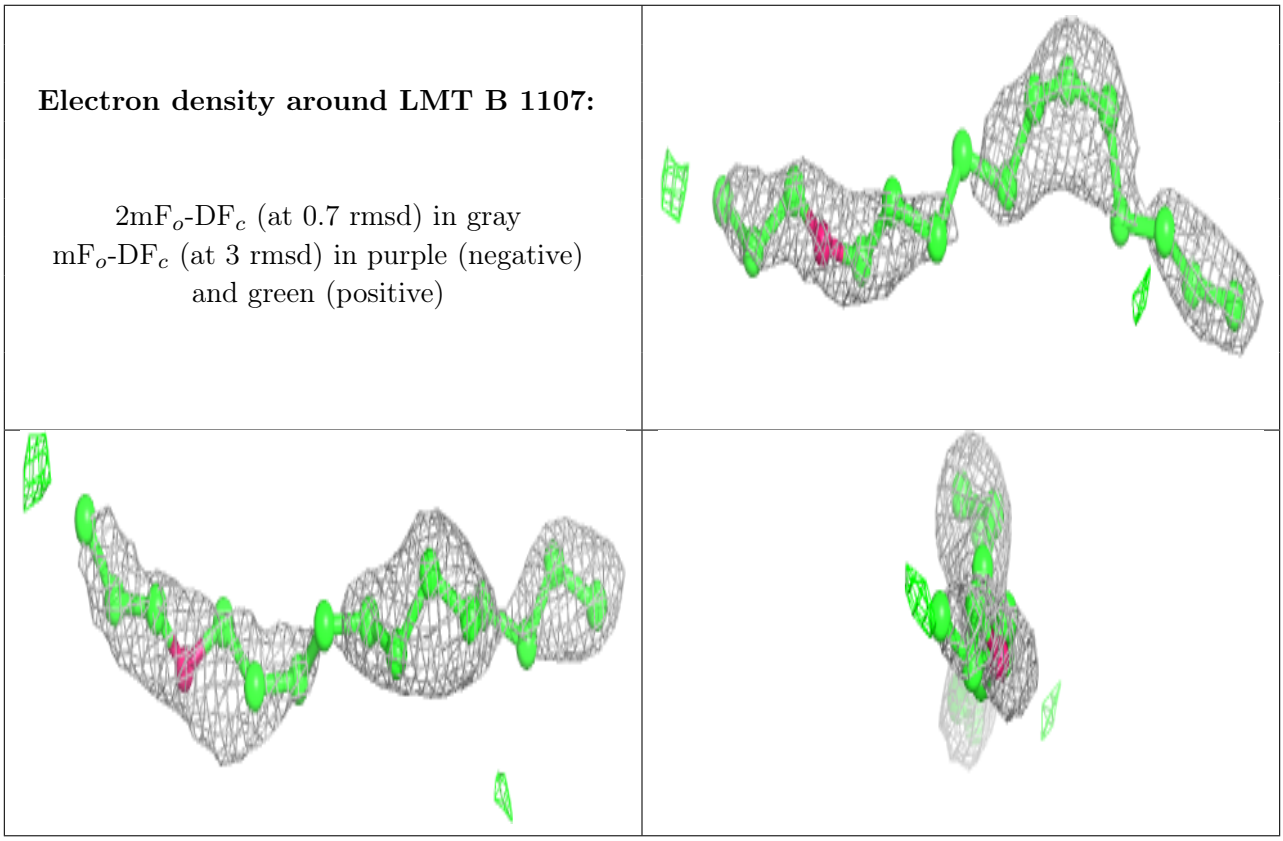
Electron density around LMT C 1108:

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



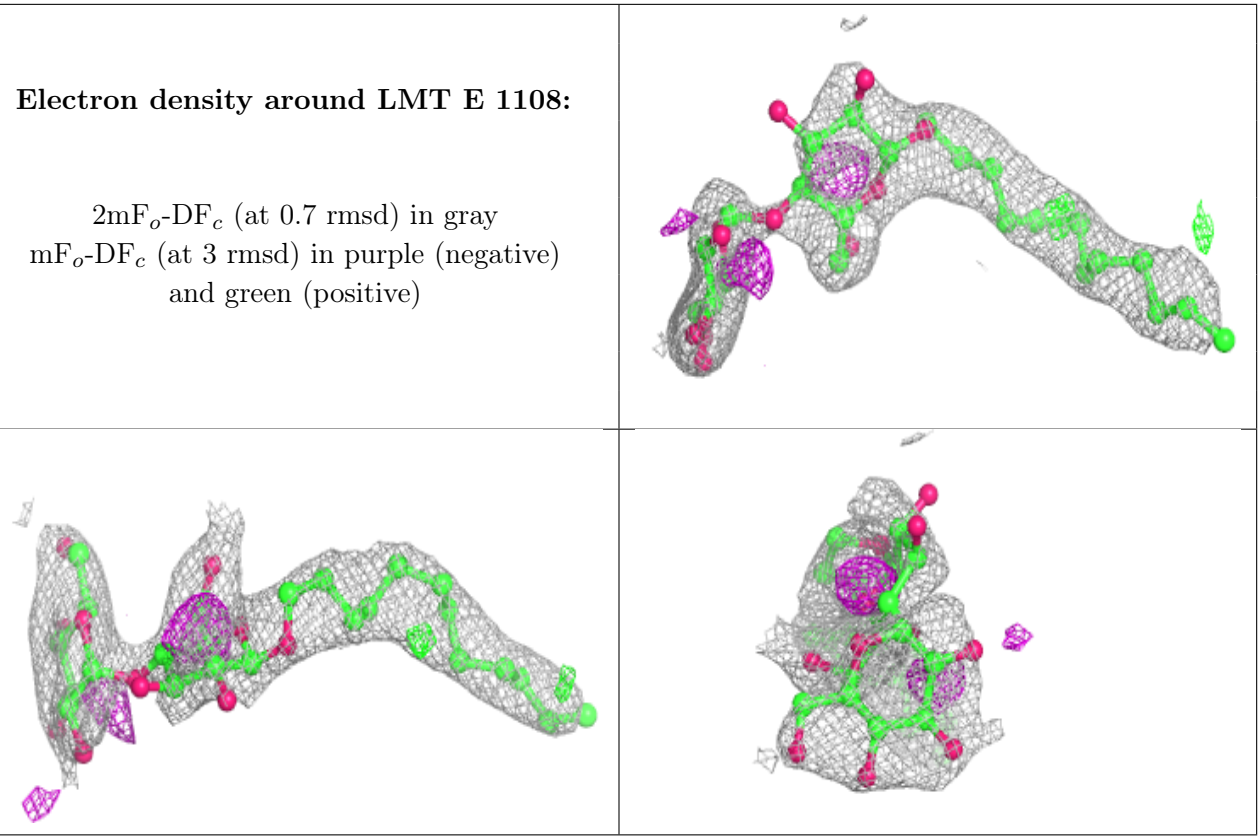
Electron density around LMT B 1107:

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



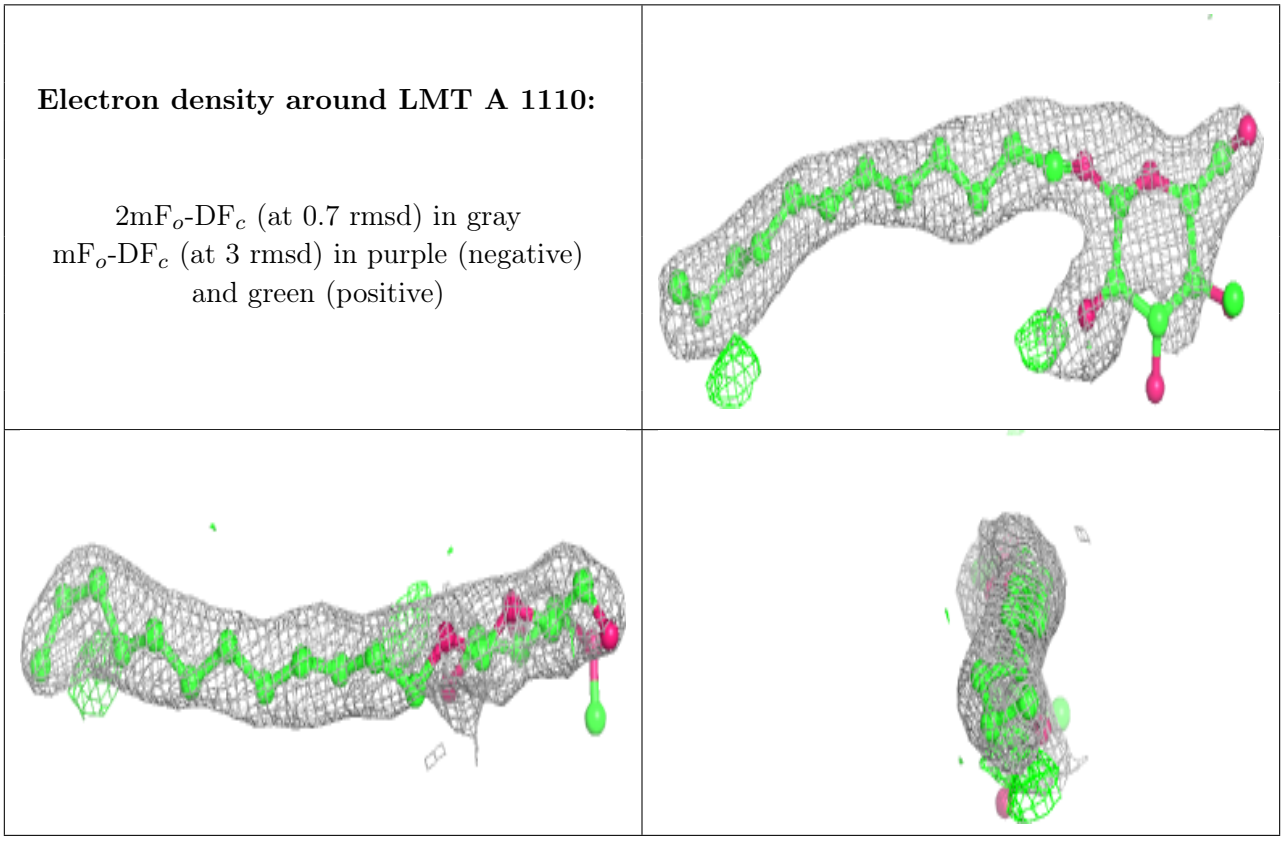
Electron density around LMT E 1108:

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



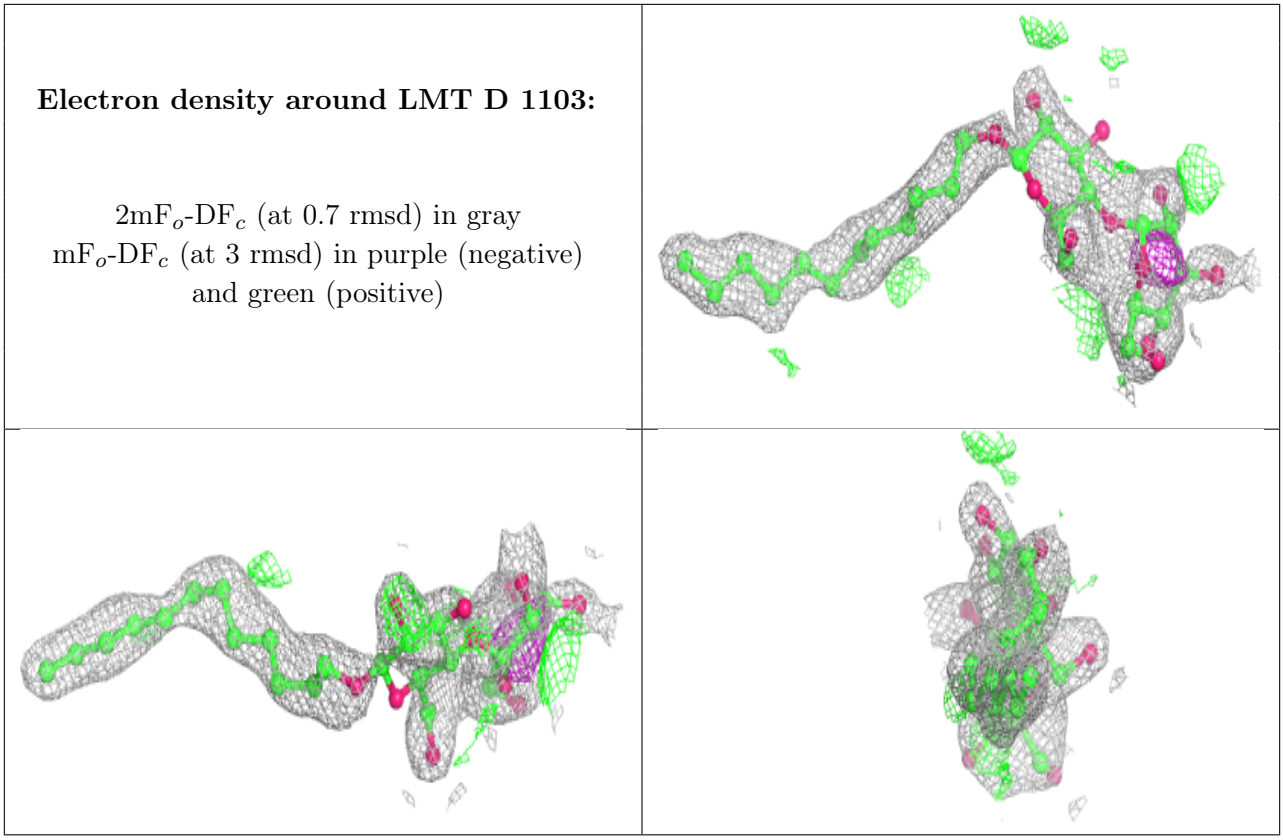
Electron density around LMT A 1110:

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



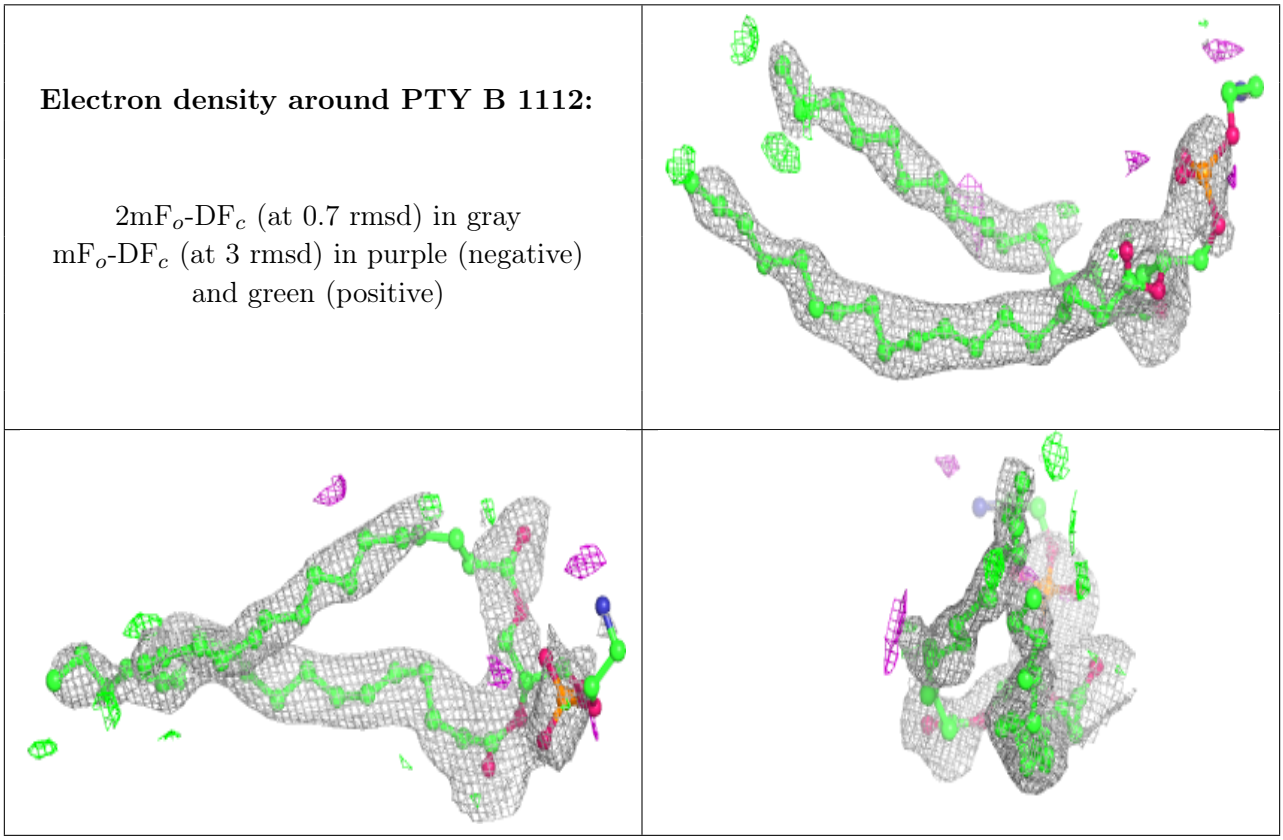
Electron density around LMT D 1103:

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



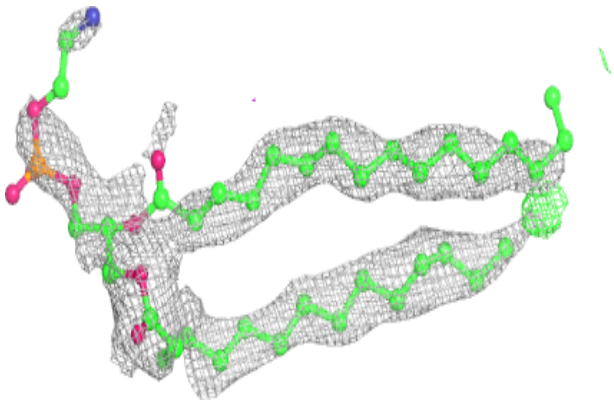
Electron density around PTY B 1112:

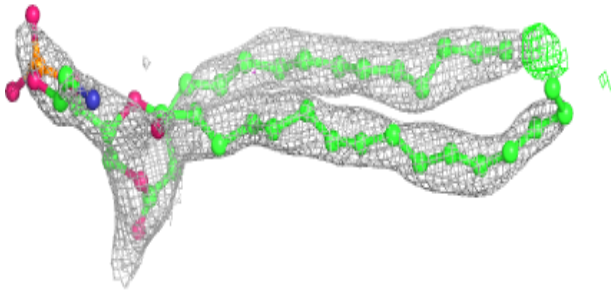
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

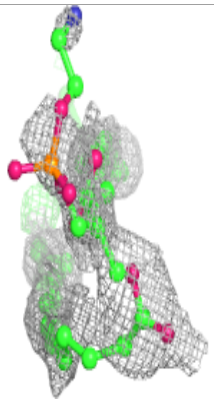


Electron density around PTY A 1112:

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

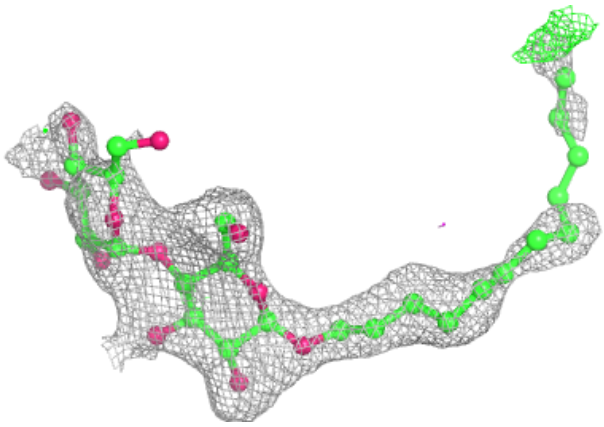


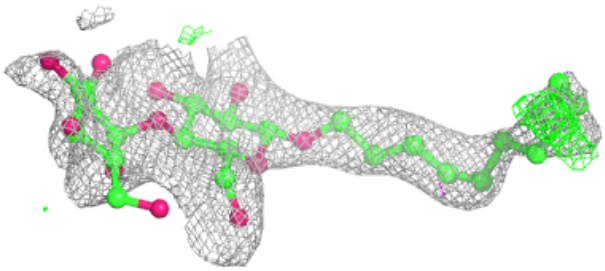


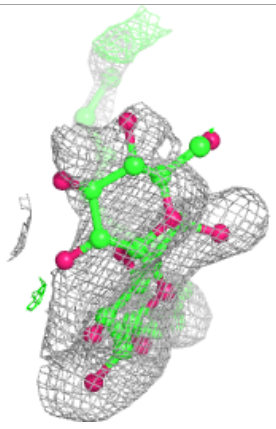


Electron density around LMT D 1106:

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

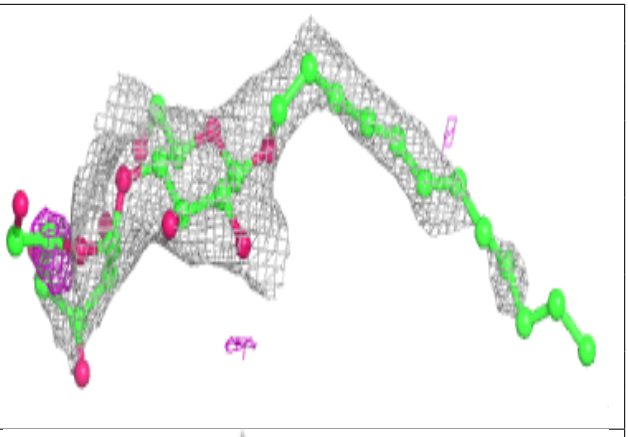


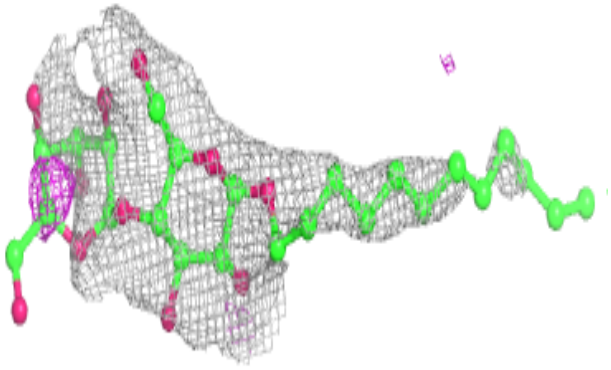


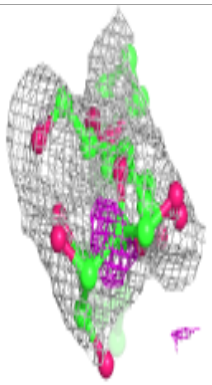


Electron density around LMT B 1101:

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

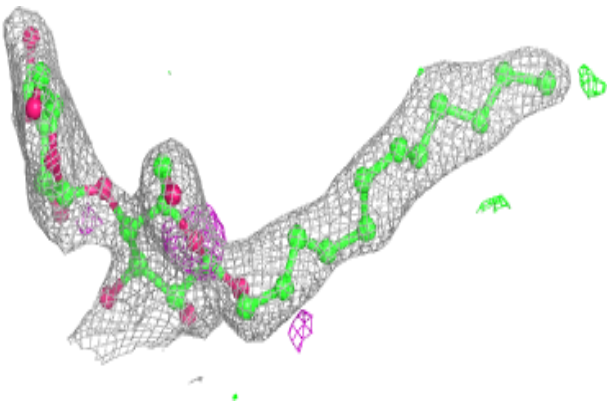


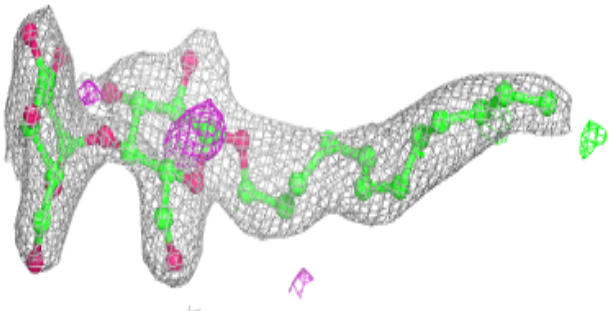


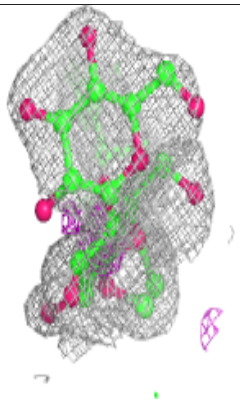


Electron density around LMT C 1111:

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

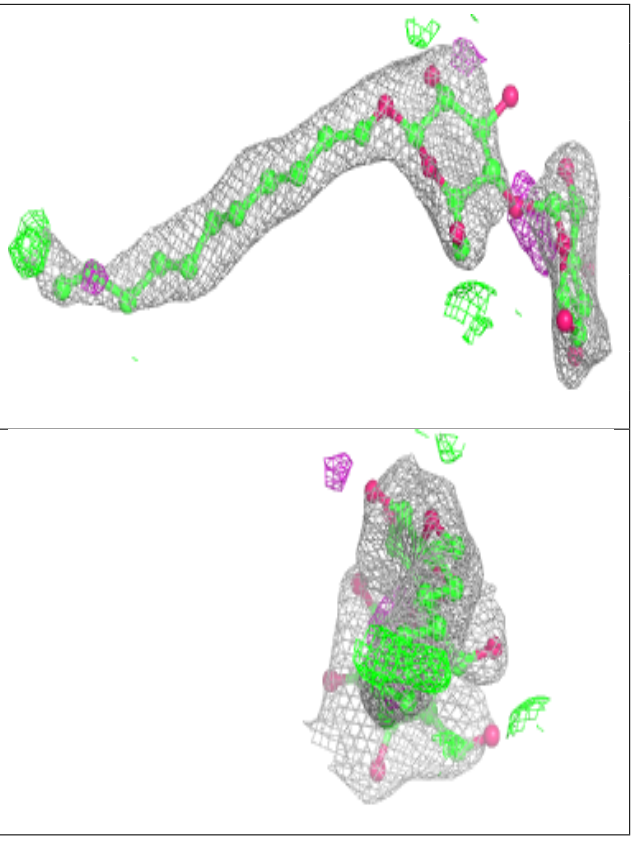


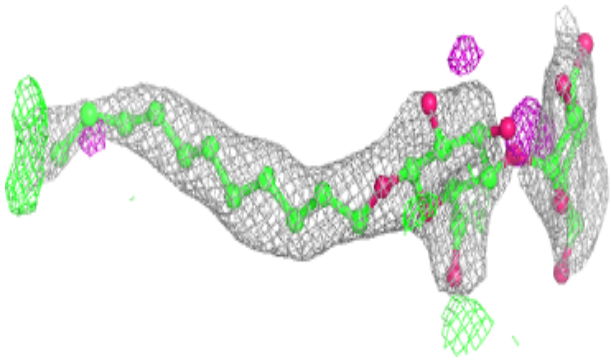




Electron density around LMT A 1108:

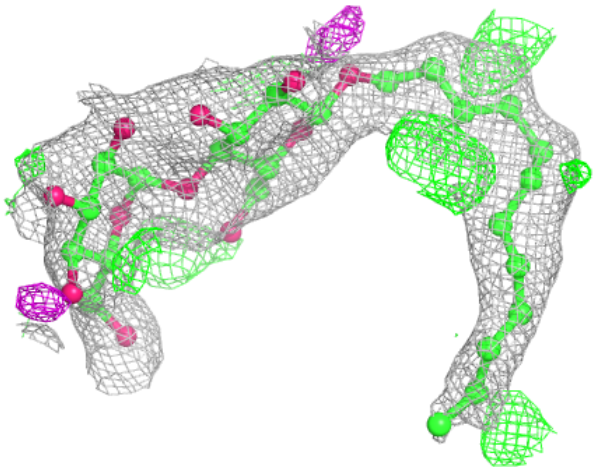
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

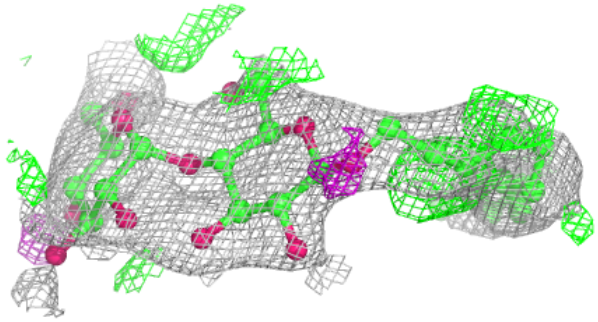


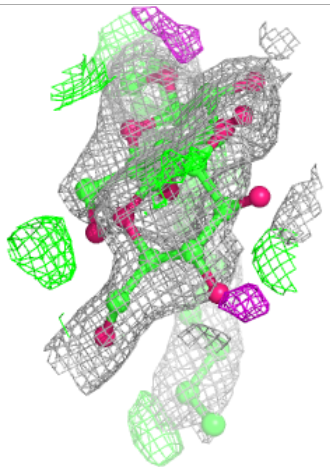


Electron density around LMT E 1105:

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

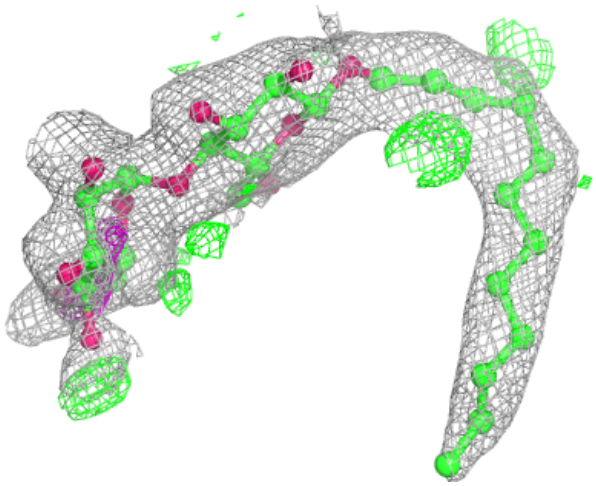


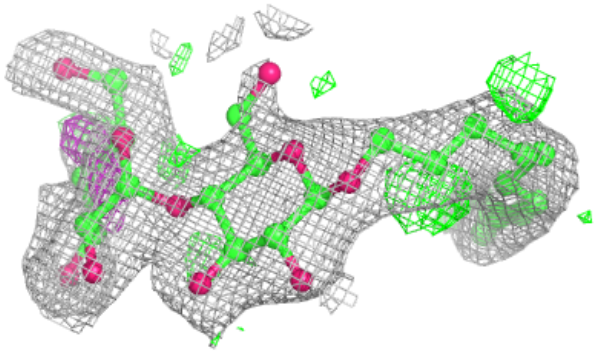




Electron density around LMT B 1105:

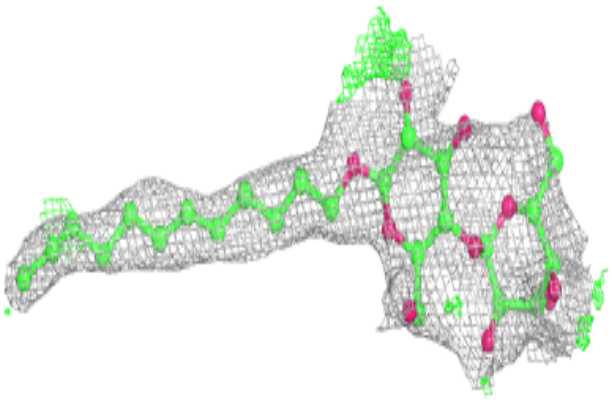
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

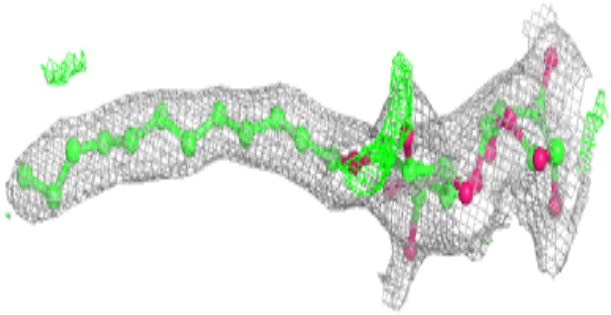


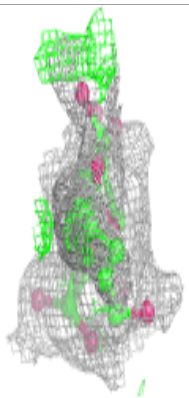


Electron density around LMT C 1109:

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

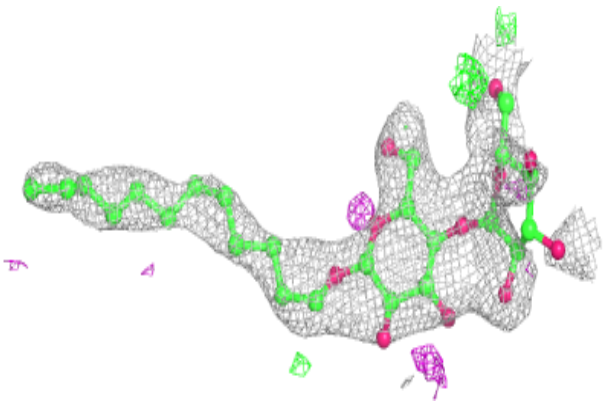


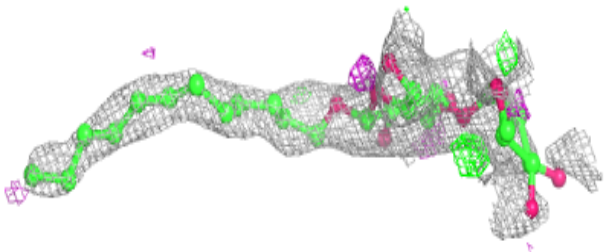


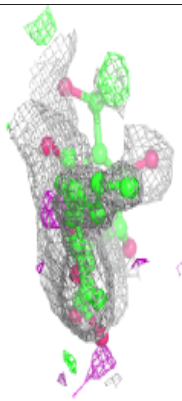


Electron density around LMT C 1101:

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

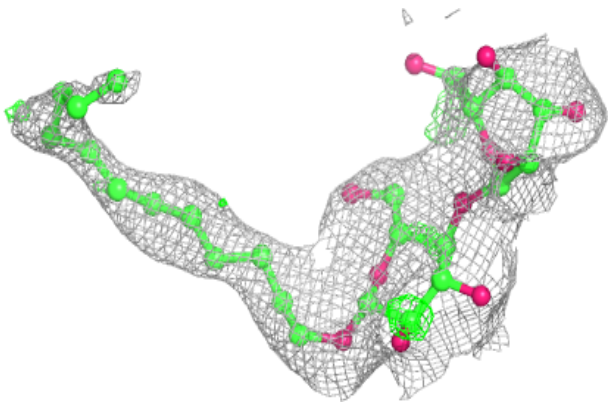


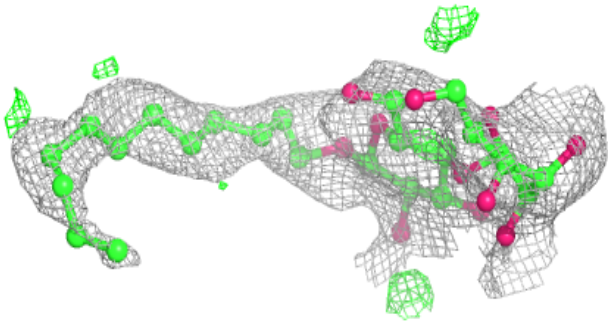


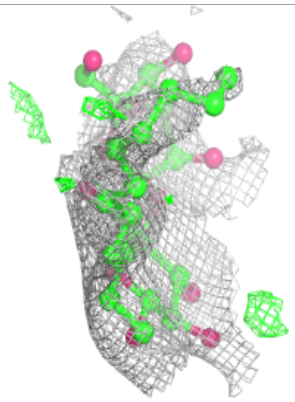


Electron density around LMT F 1107:

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

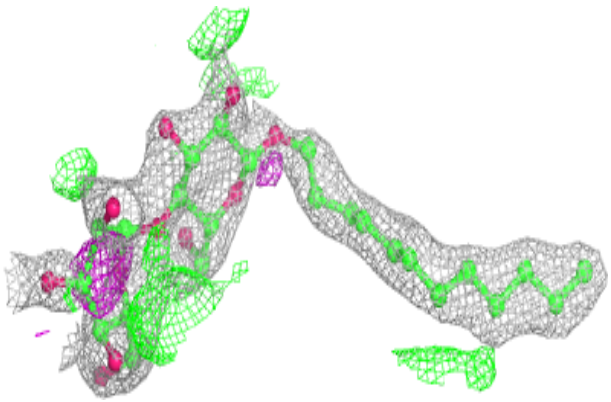


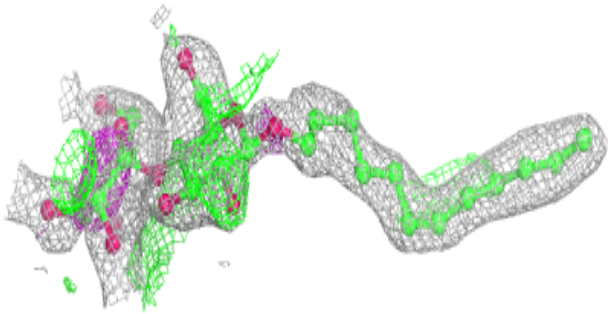


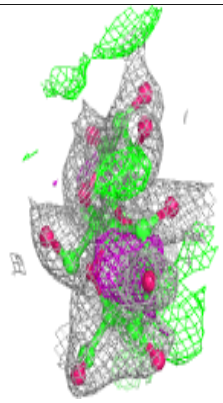


Electron density around LMT C 1107:

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

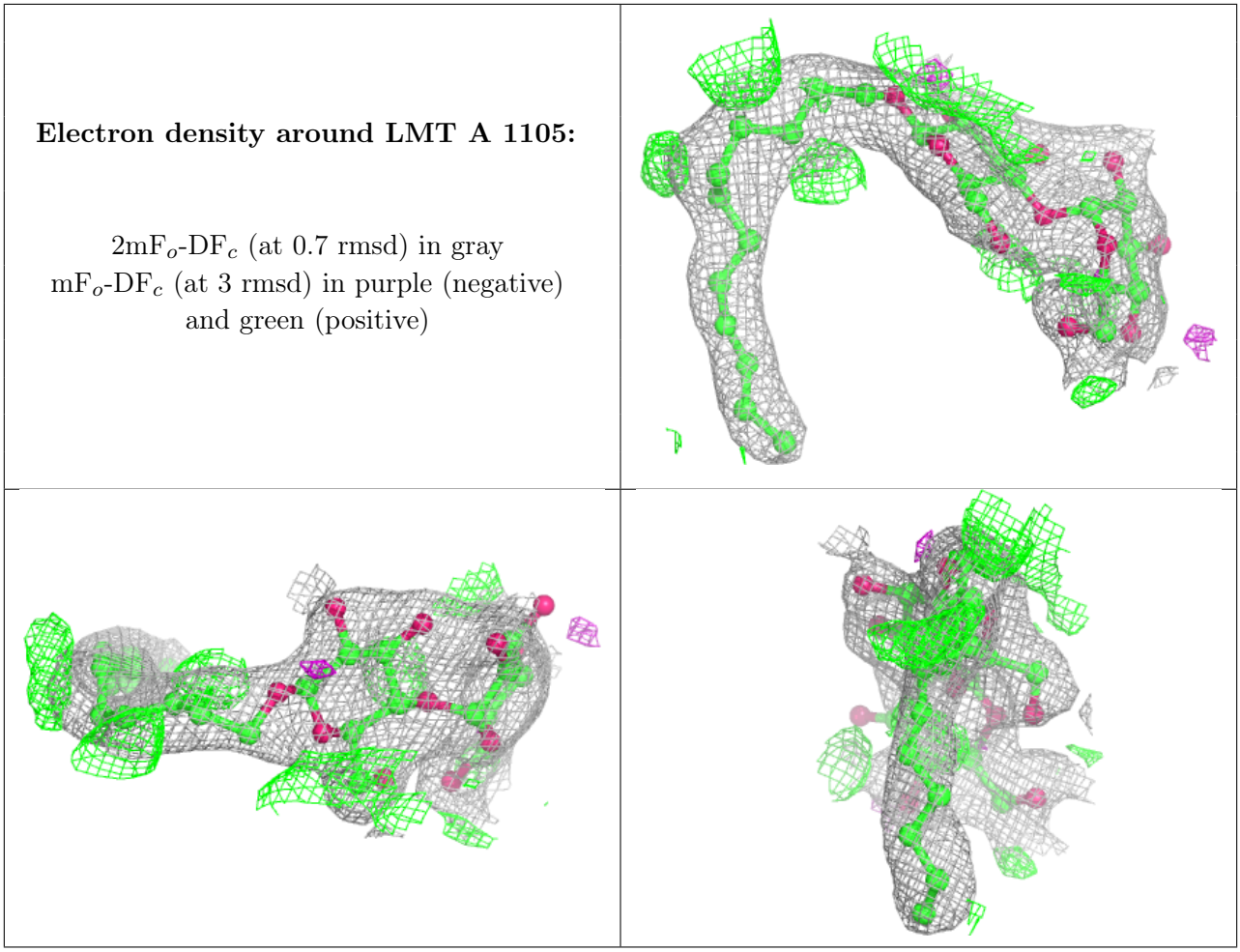






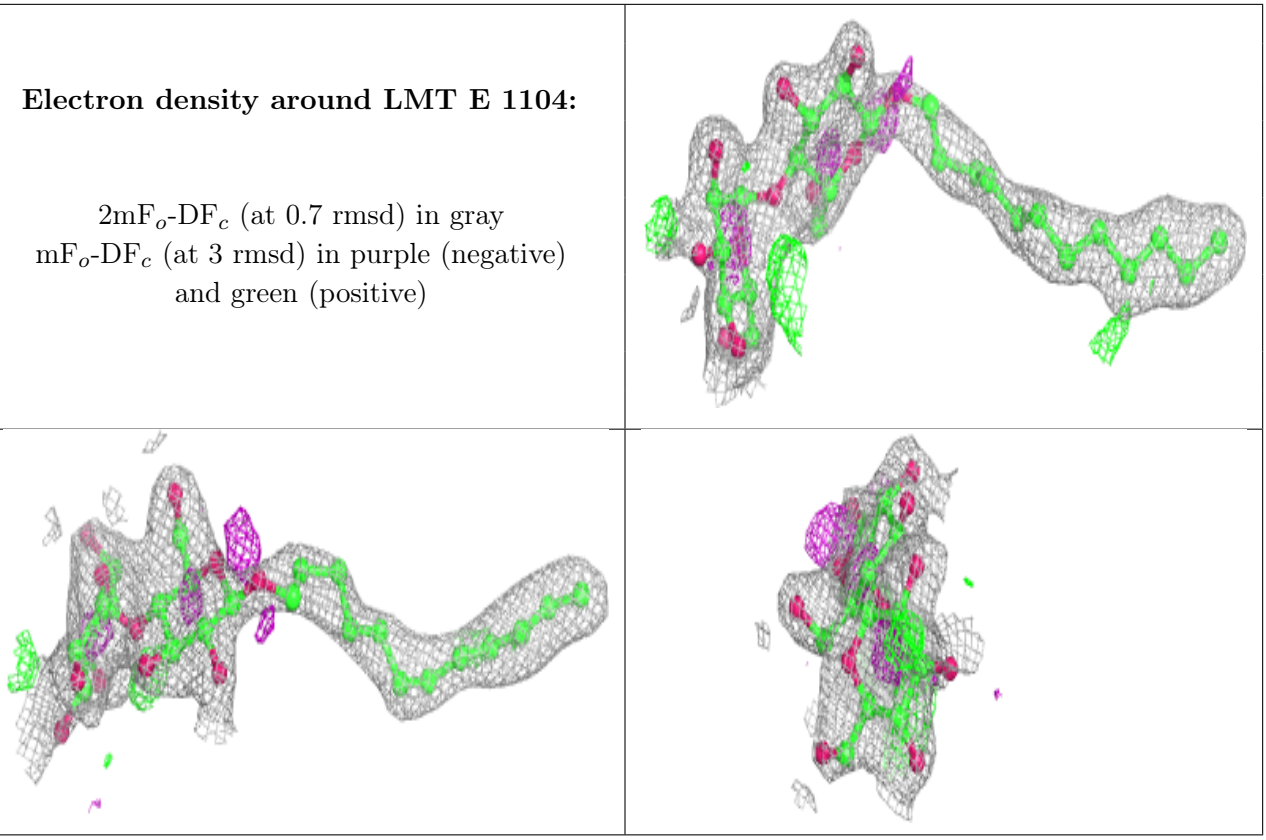
Electron density around LMT A 1105:

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



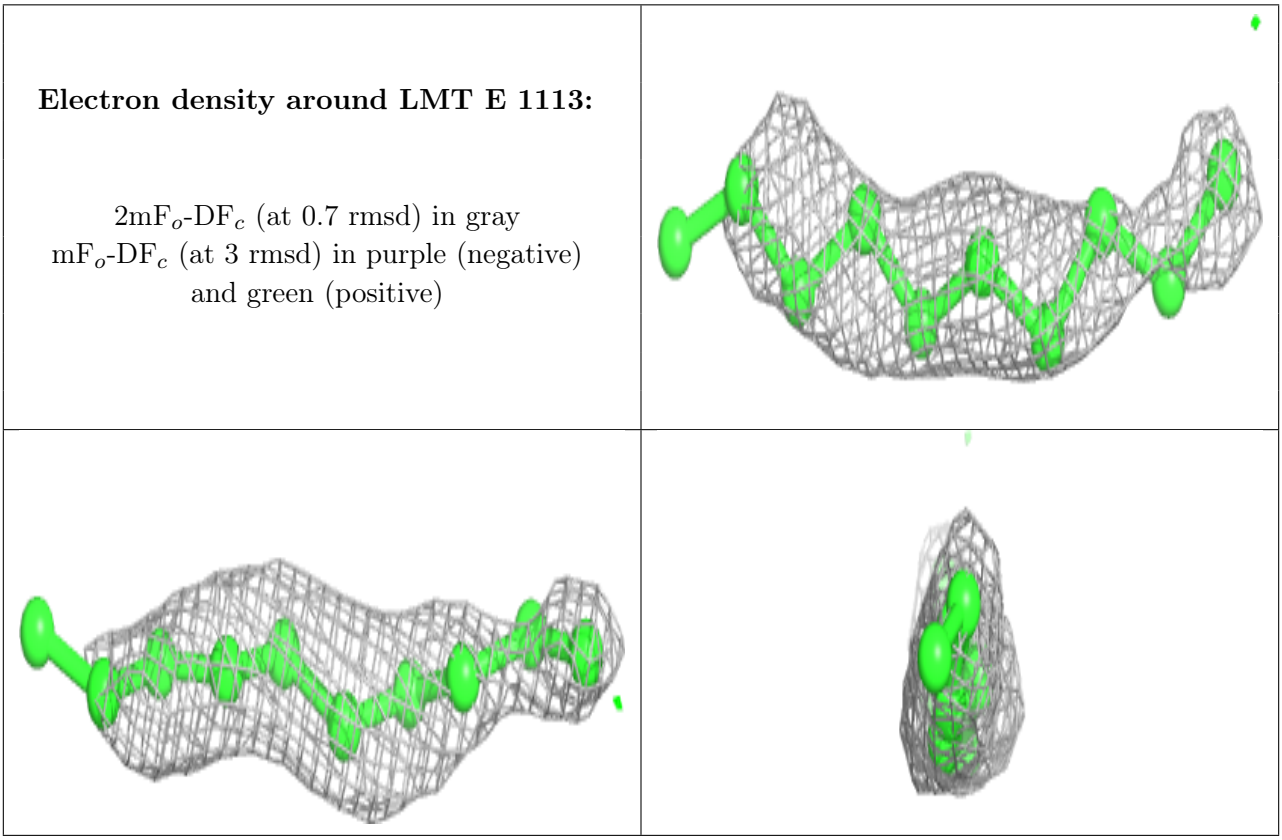
Electron density around LMT E 1104:

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



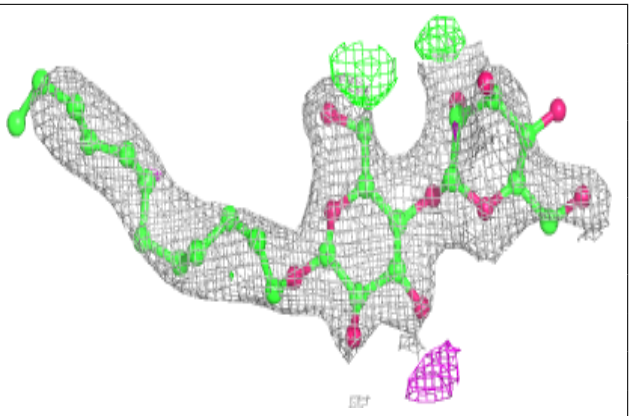
Electron density around LMT E 1113:

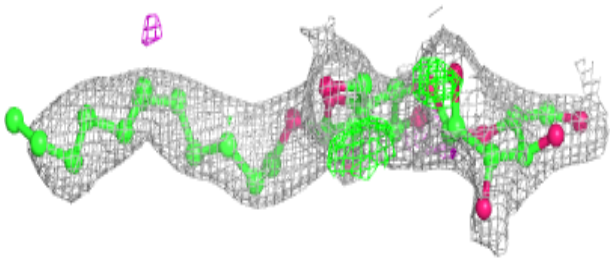
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

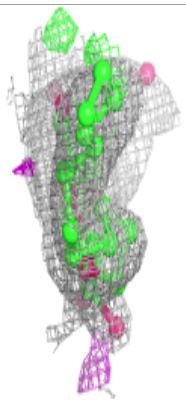


Electron density around LMT E 1102:

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

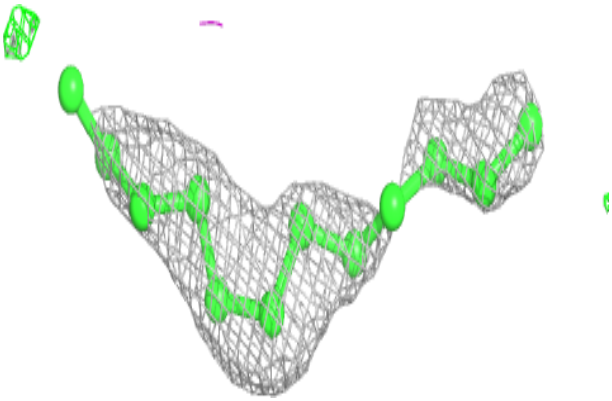


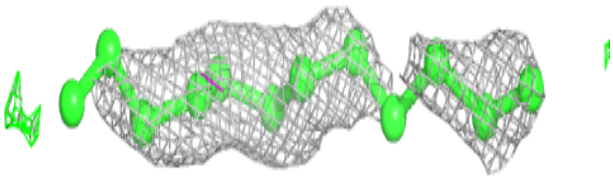




Electron density around LMT E 1111:

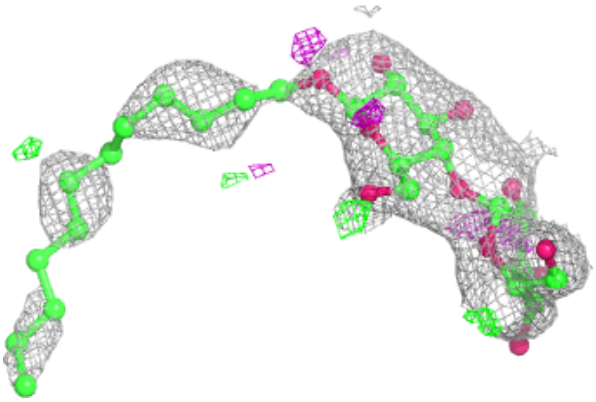
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

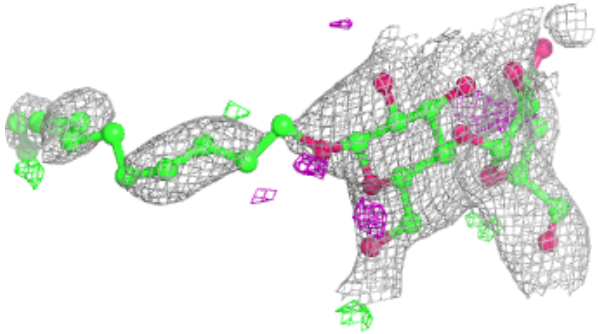


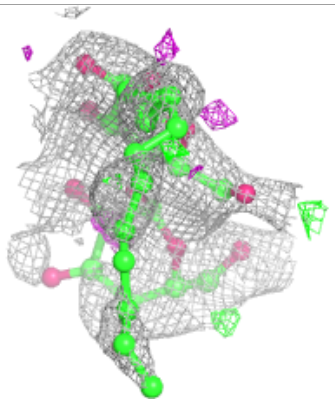


Electron density around LMT A 1106:

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

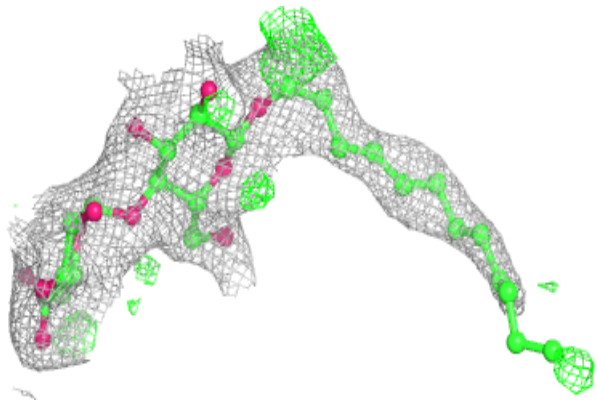


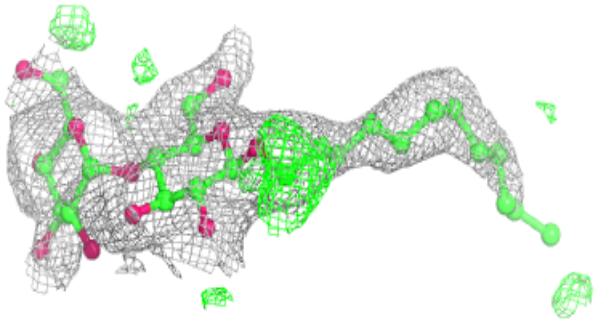


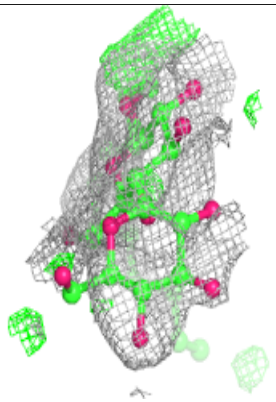


Electron density around LMT B 1106:

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

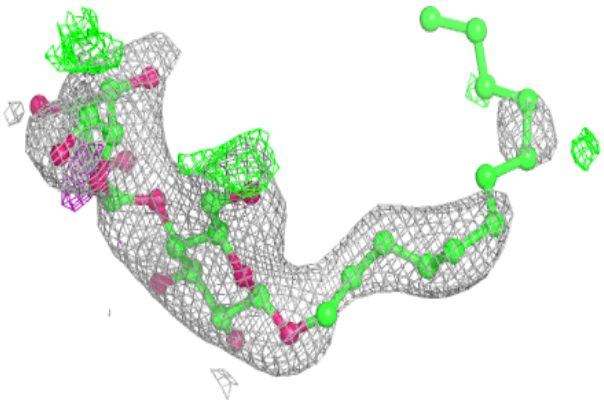


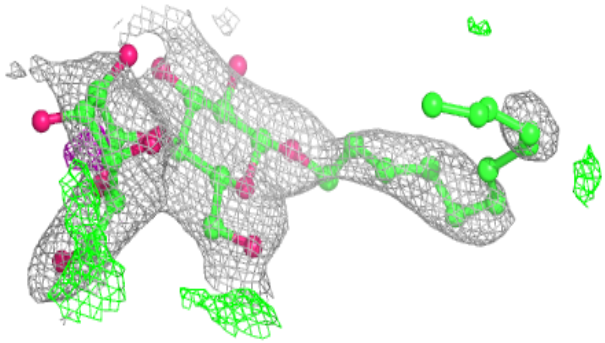


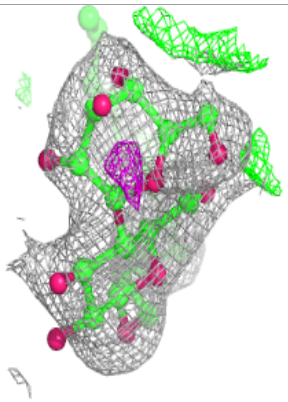


Electron density around LMT E 1107:

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

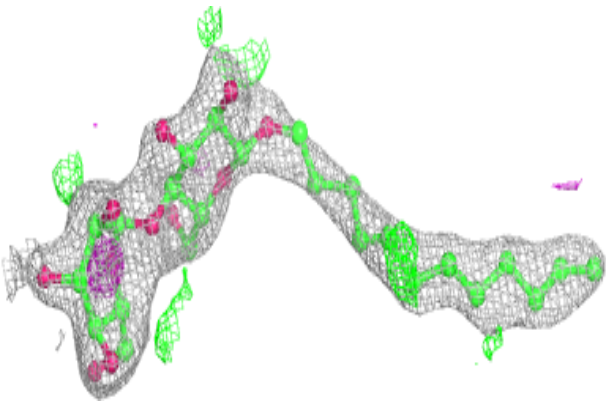


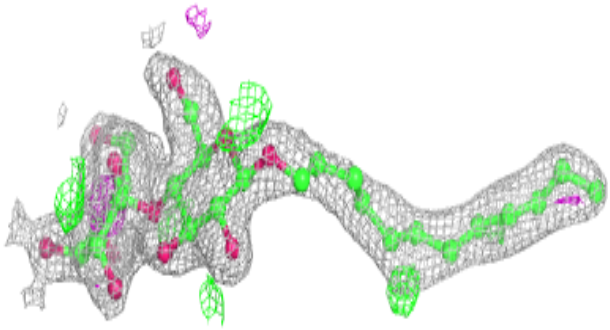


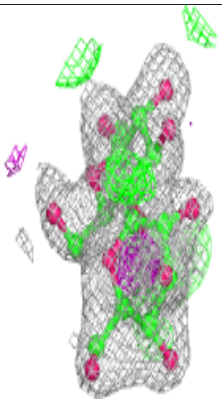


Electron density around LMT B 1102:

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

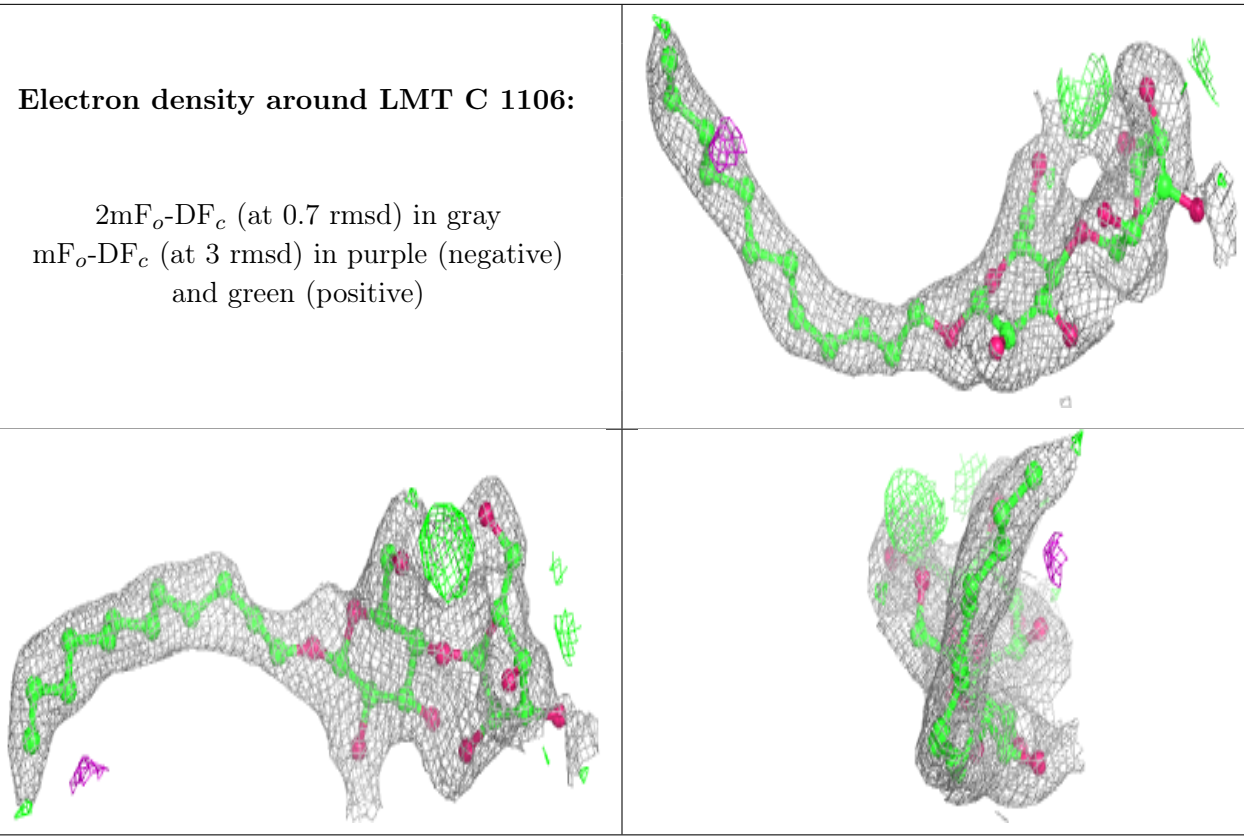






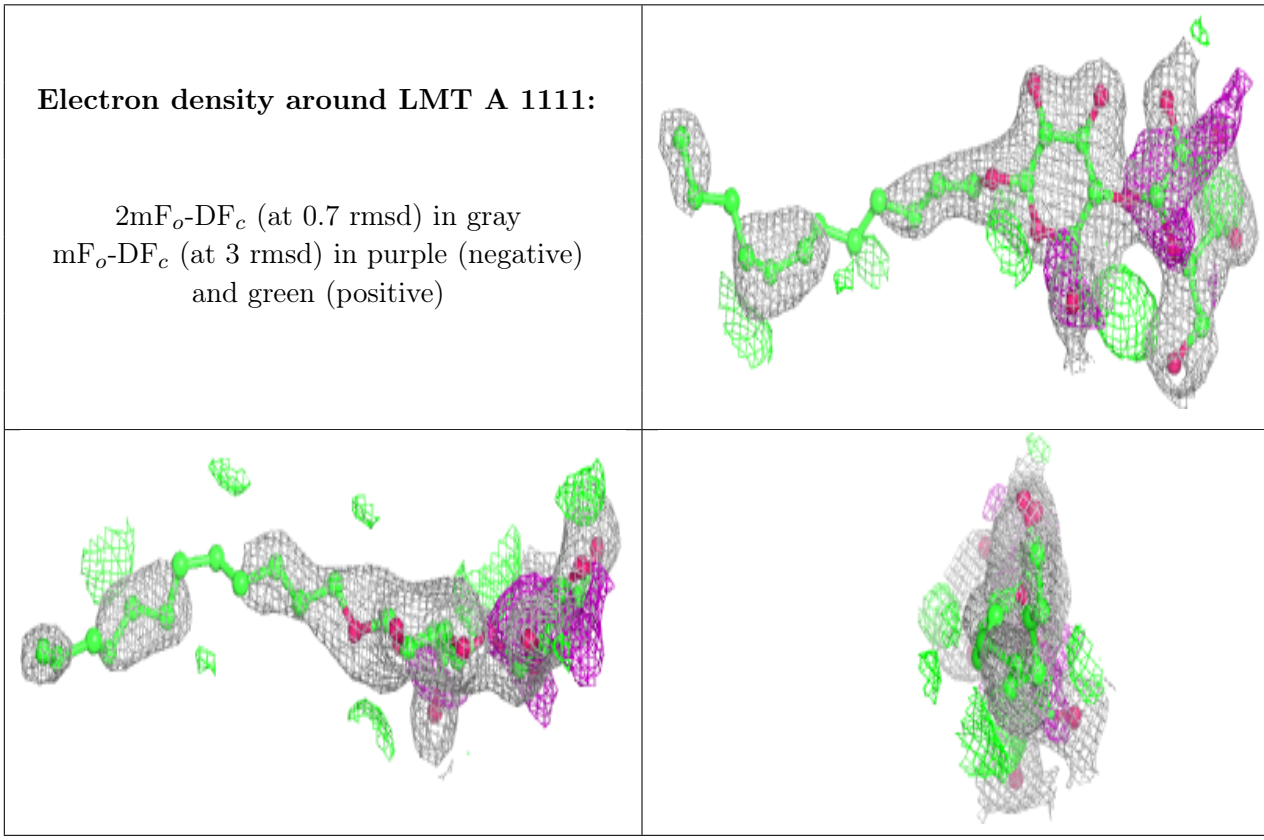
Electron density around LMT C 1106:

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



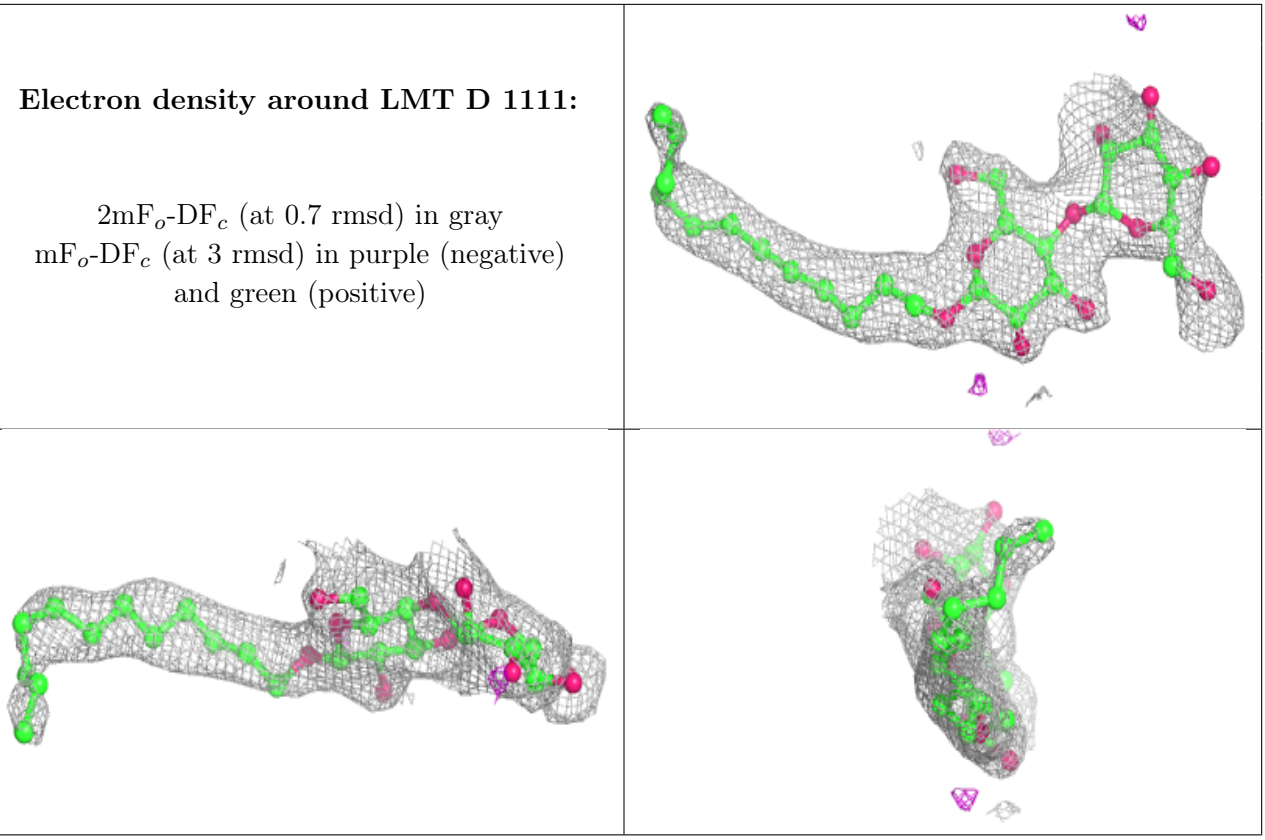
Electron density around LMT A 1111:

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



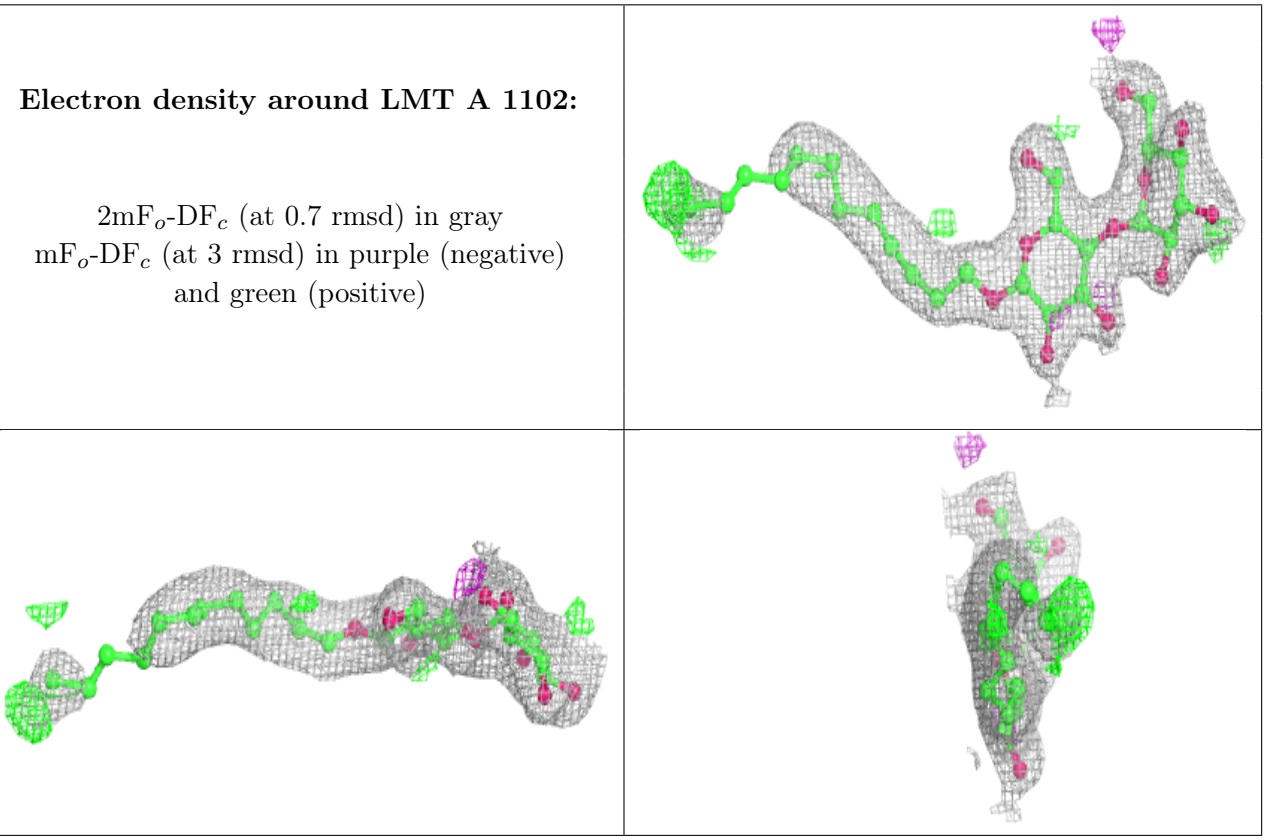
Electron density around LMT D 1111:

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



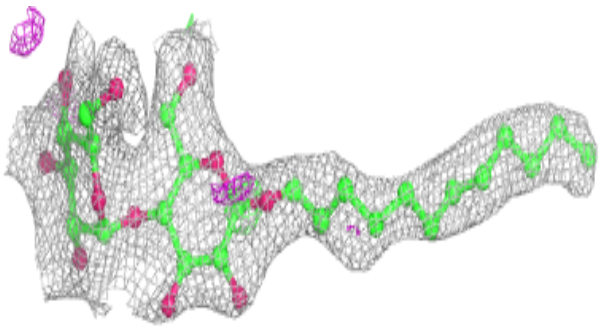
Electron density around LMT A 1102:

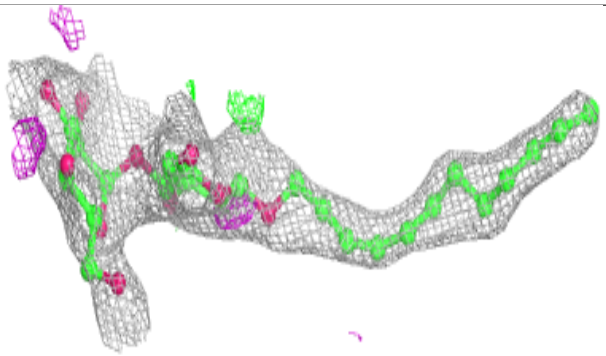
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

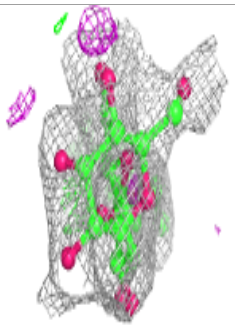


Electron density around LMT D 1101:

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

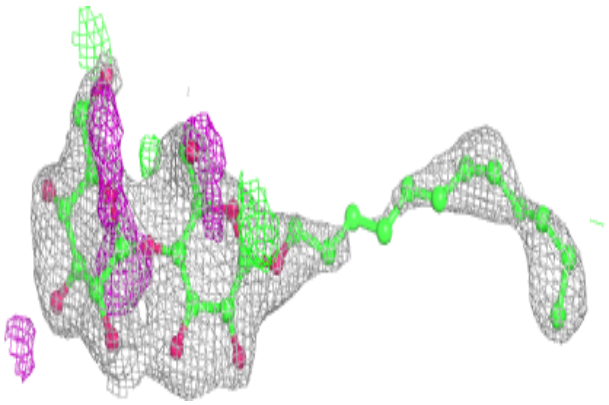


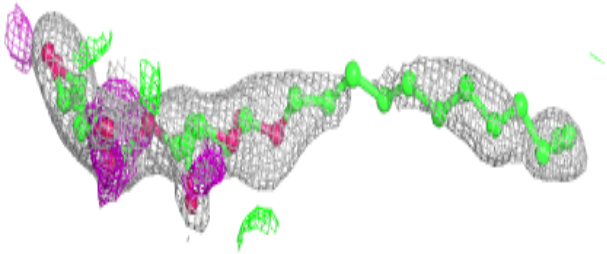


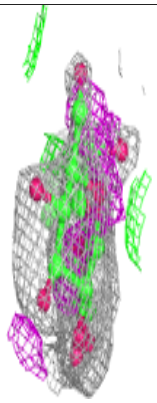


Electron density around LMT D 1102:

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

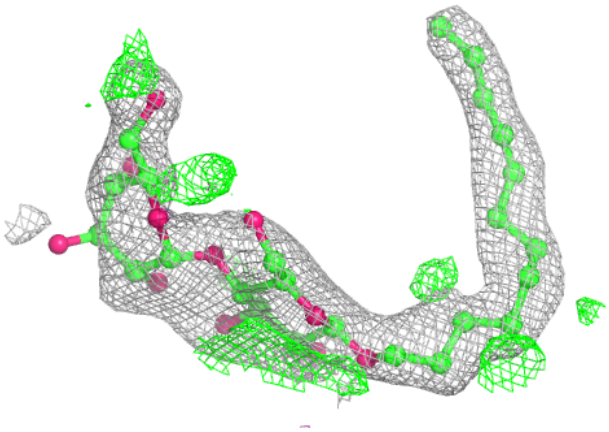


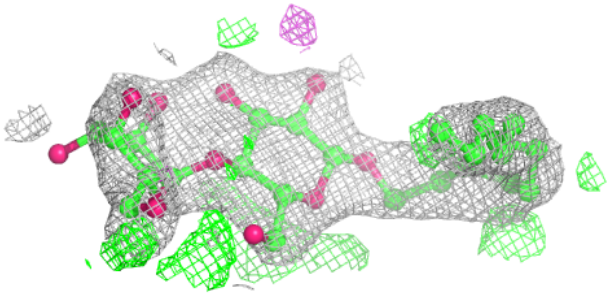


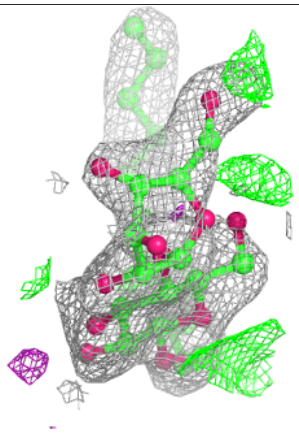


Electron density around LMT F 1105:

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

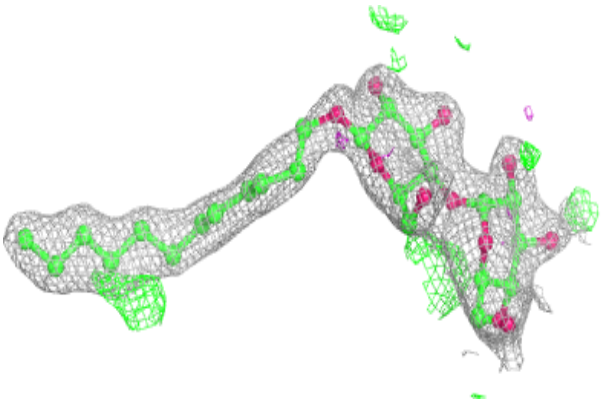


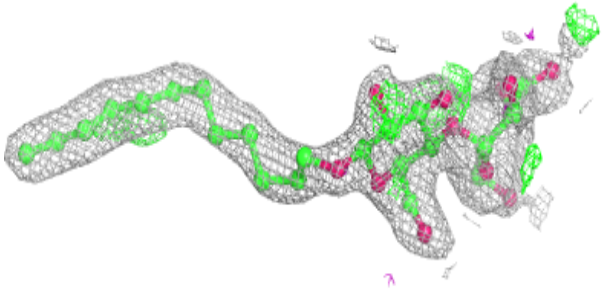


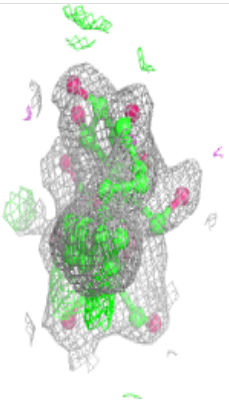


Electron density around LMT A 1104:

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

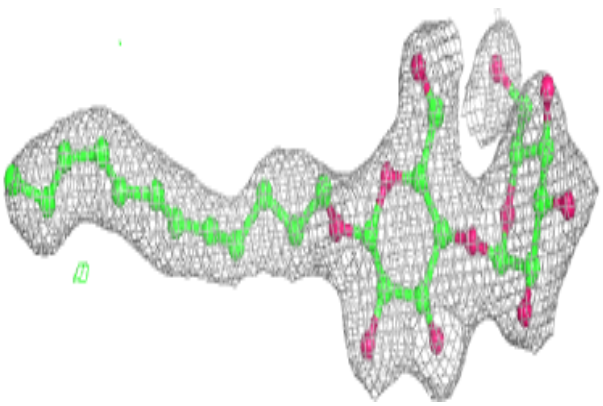


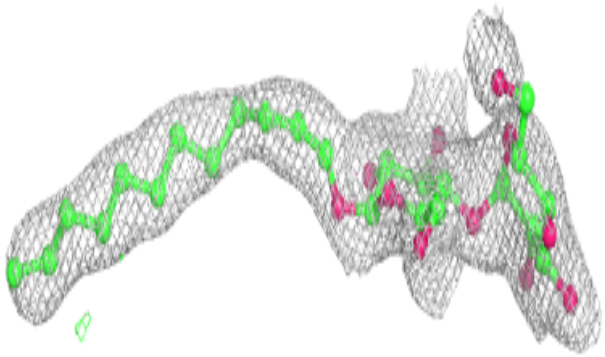


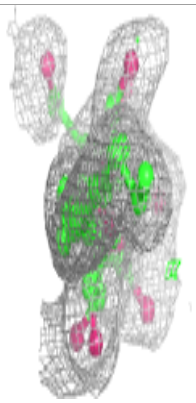


Electron density around LMT A 1103:

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

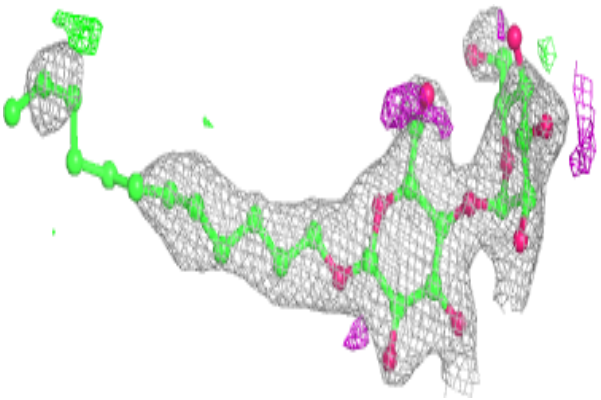


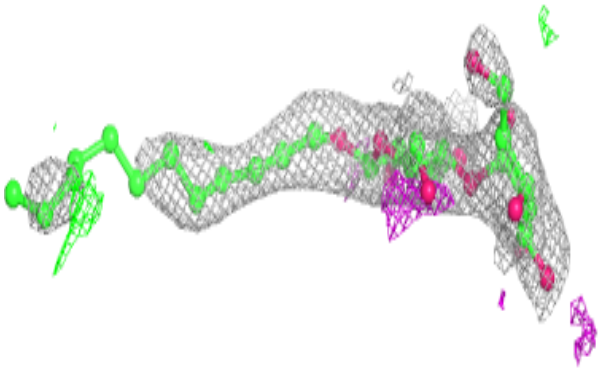


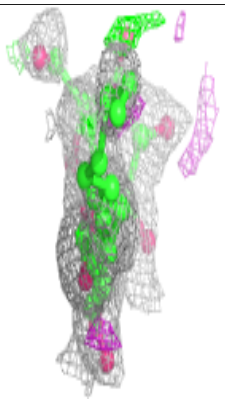


Electron density around LMT F 1113:

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

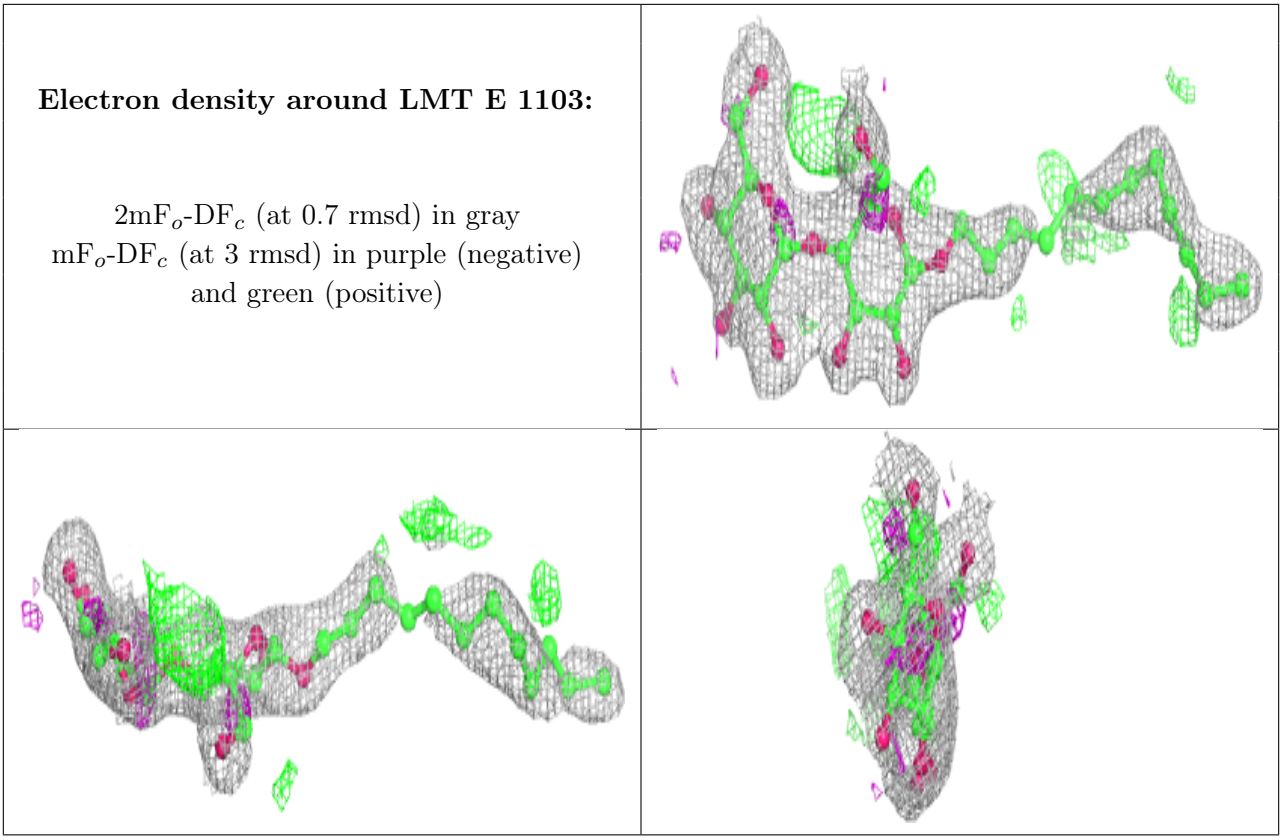






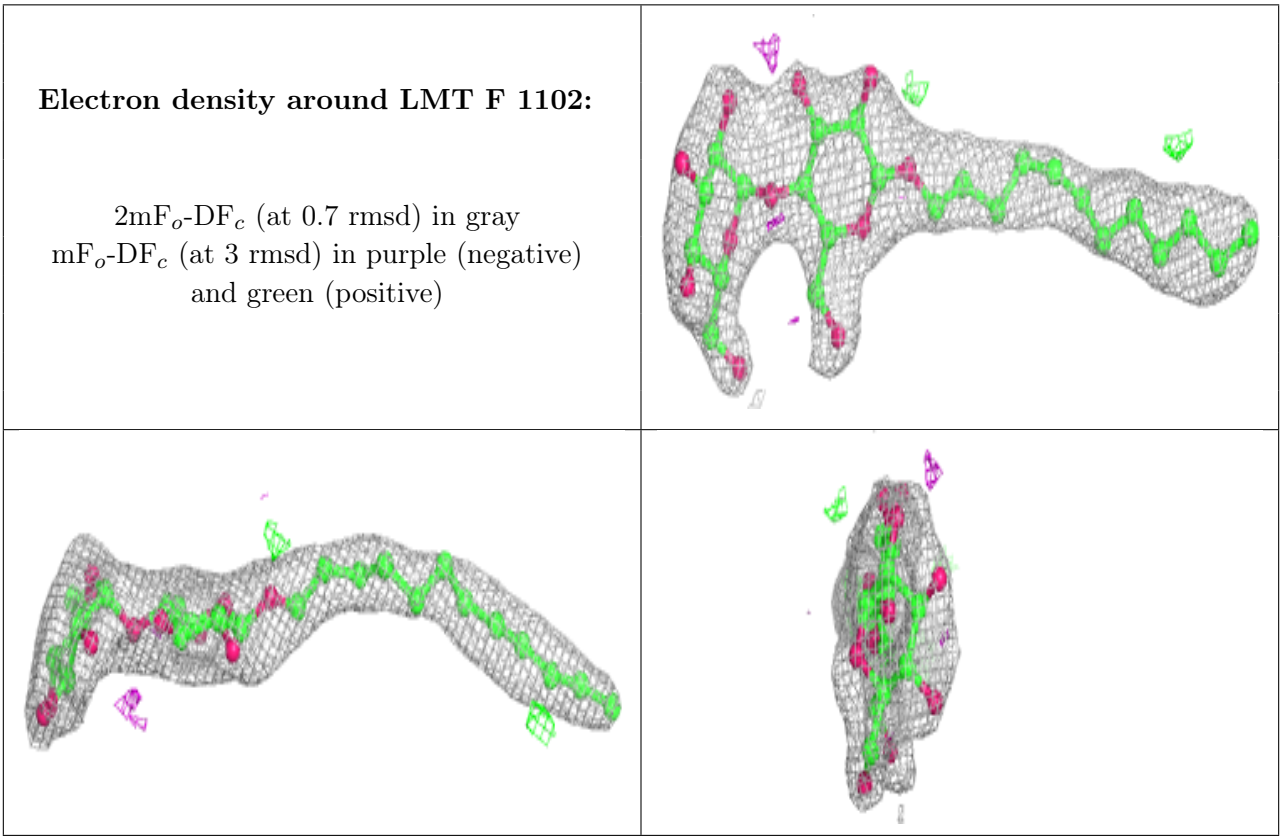
Electron density around LMT E 1103:

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



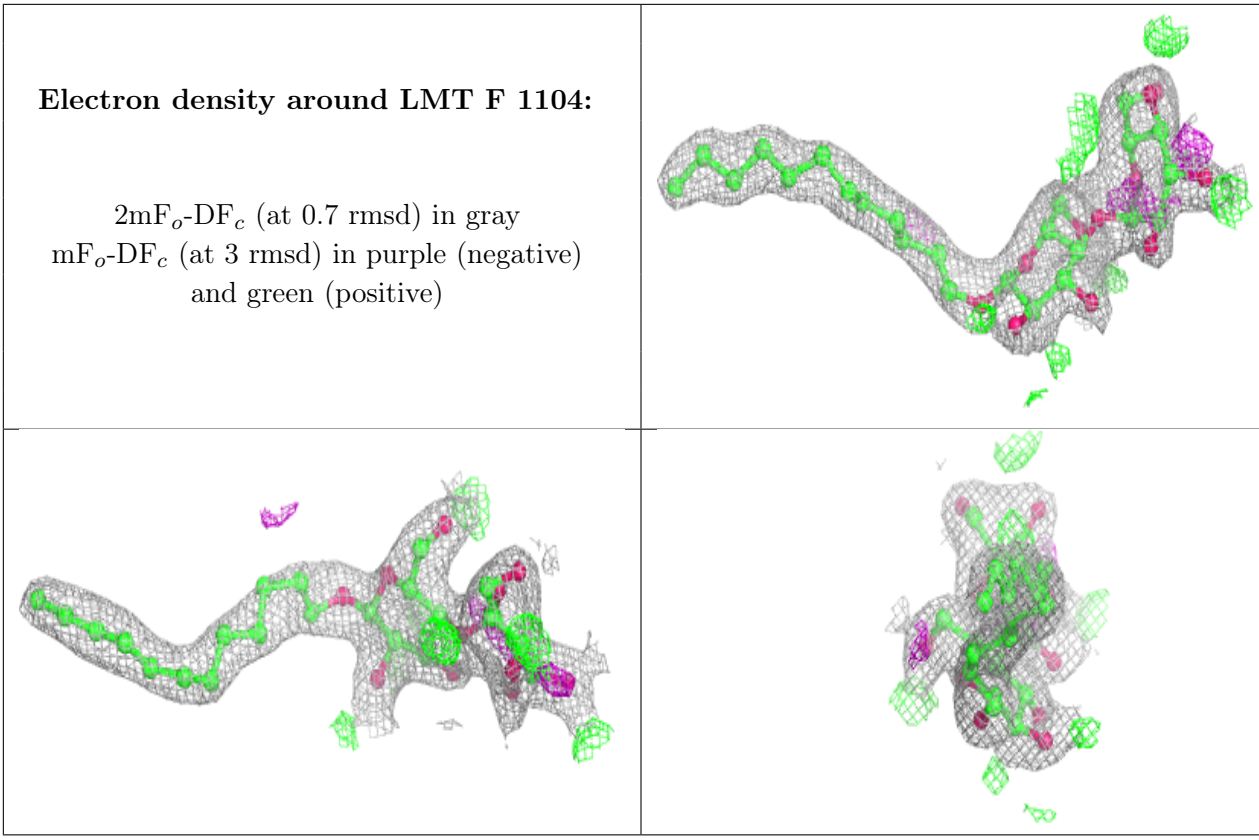
Electron density around LMT F 1102:

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



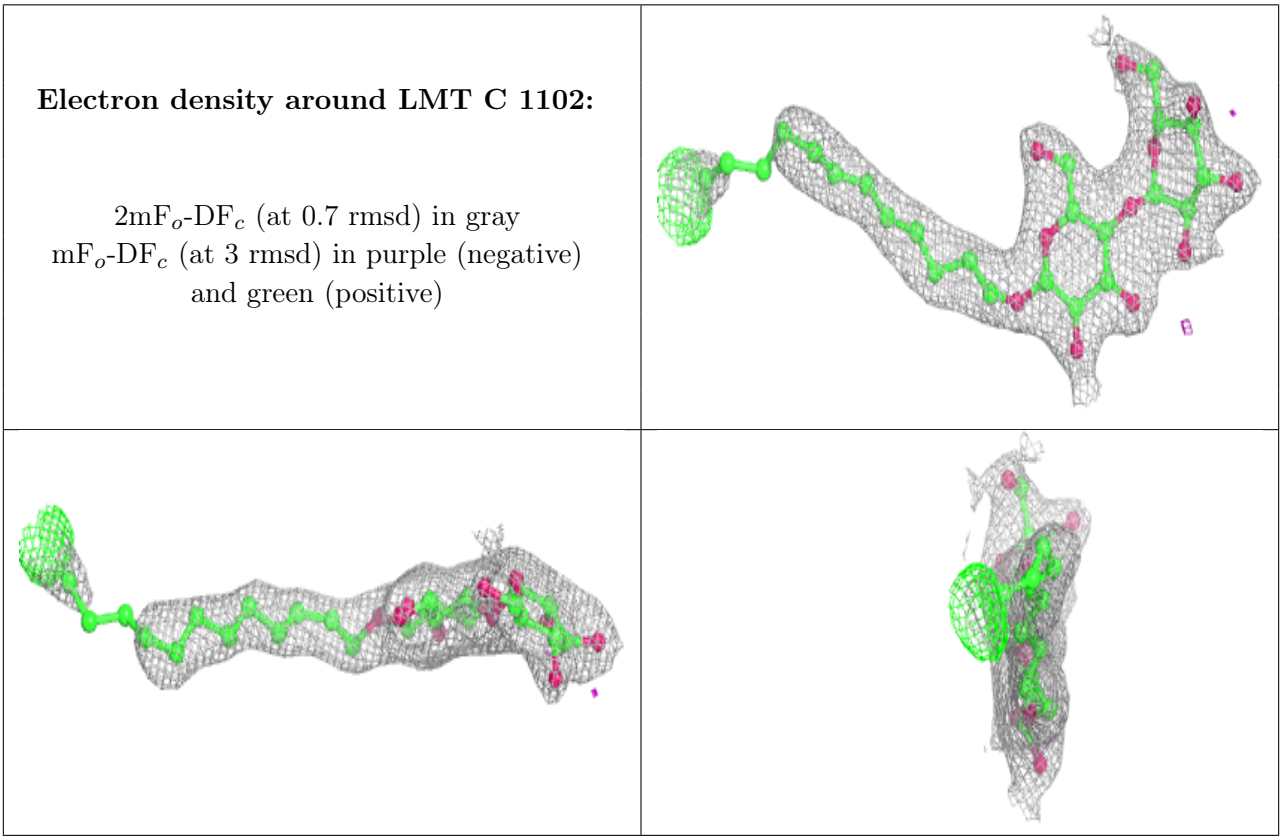
Electron density around LMT F 1104:

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



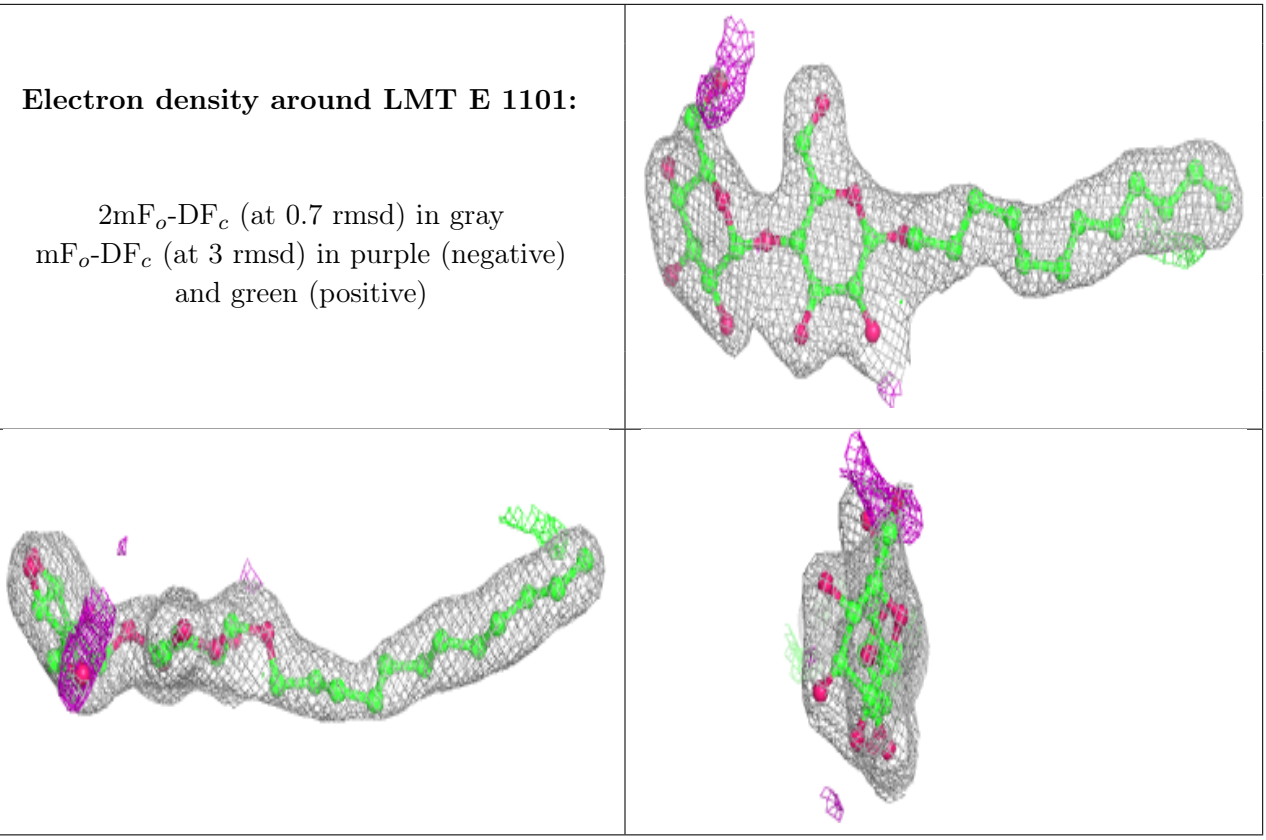
Electron density around LMT C 1102:

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



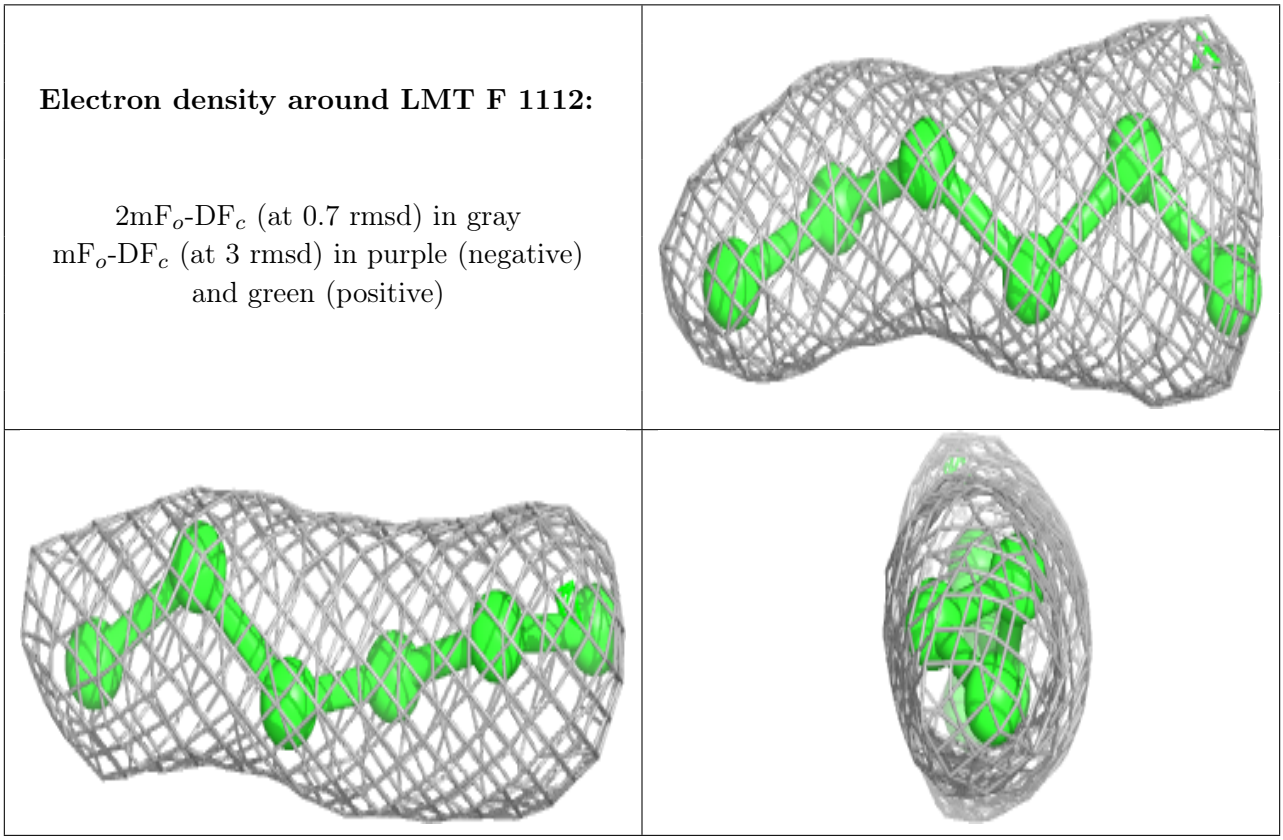
Electron density around LMT E 1101:

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



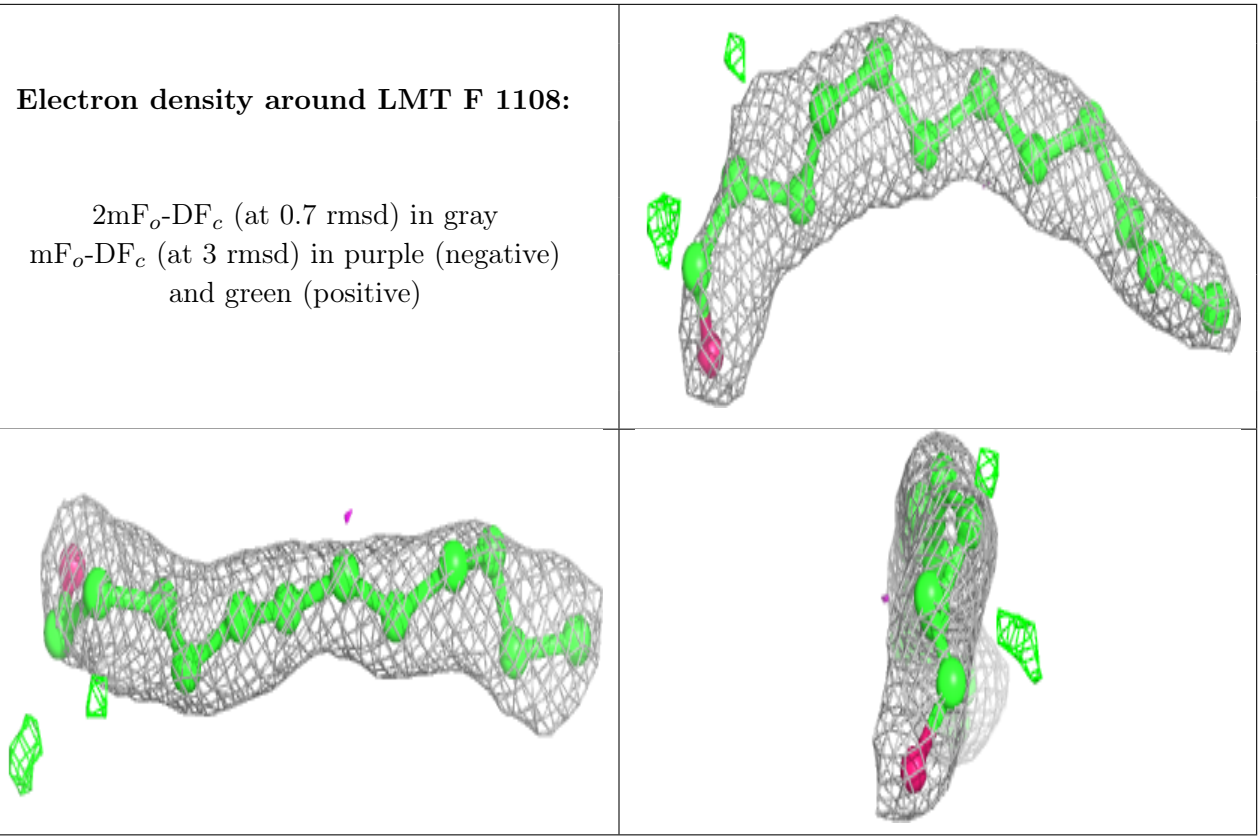
Electron density around LMT F 1112:

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



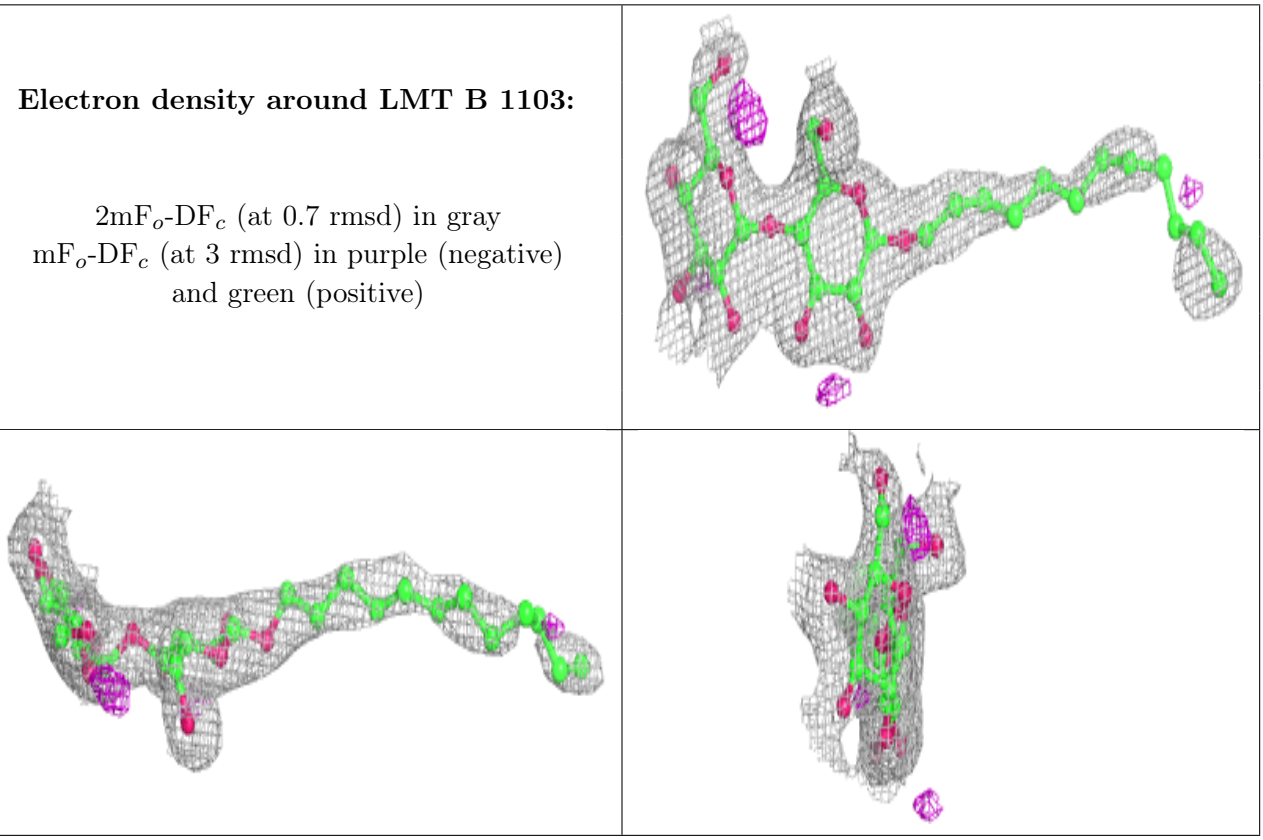
Electron density around LMT F 1108:

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



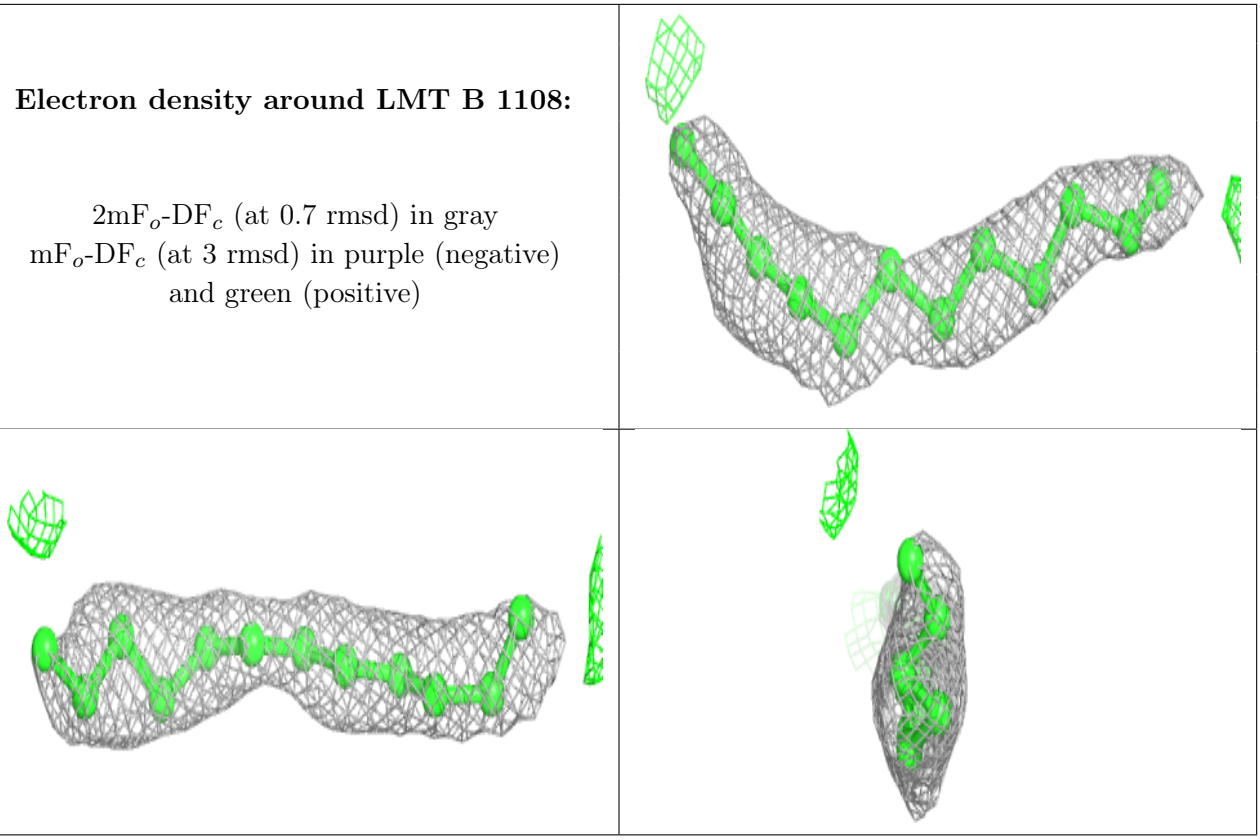
Electron density around LMT B 1103:

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



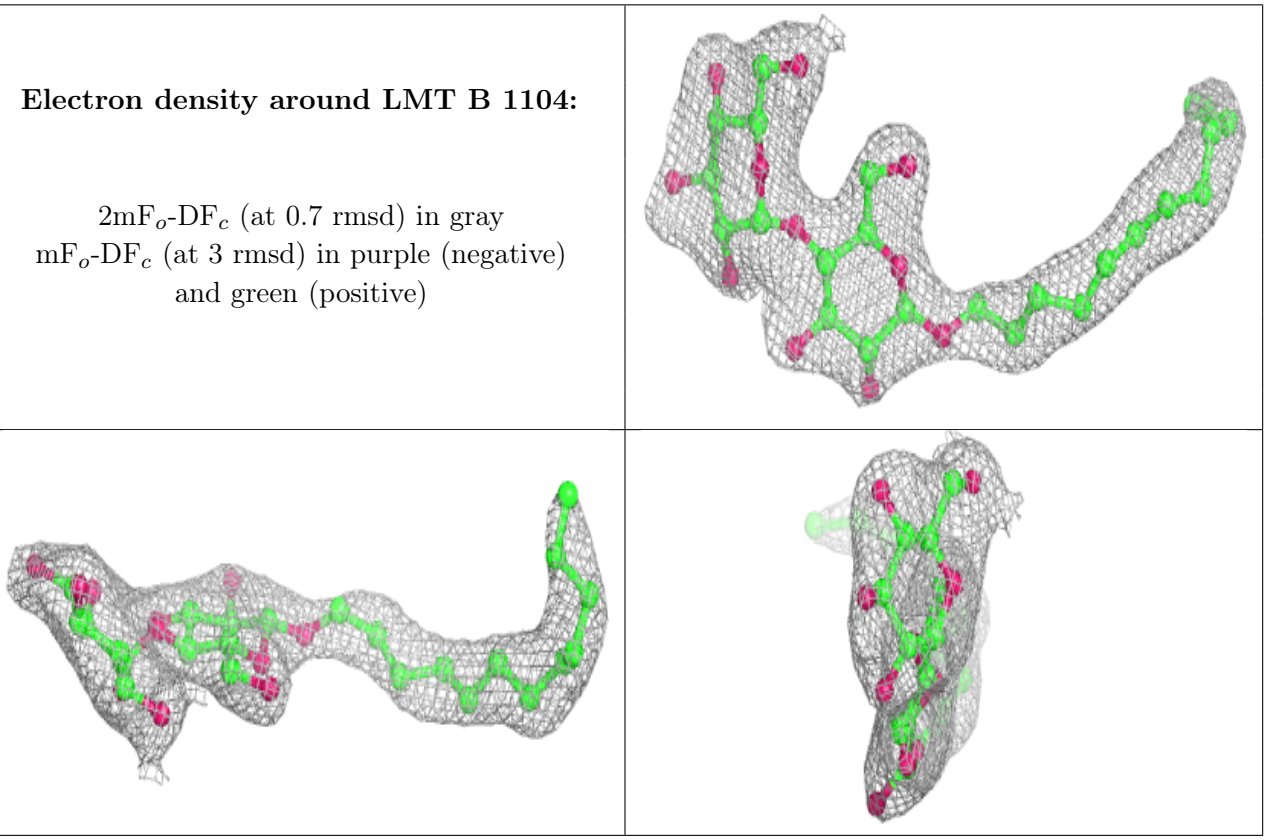
Electron density around LMT B 1108:

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



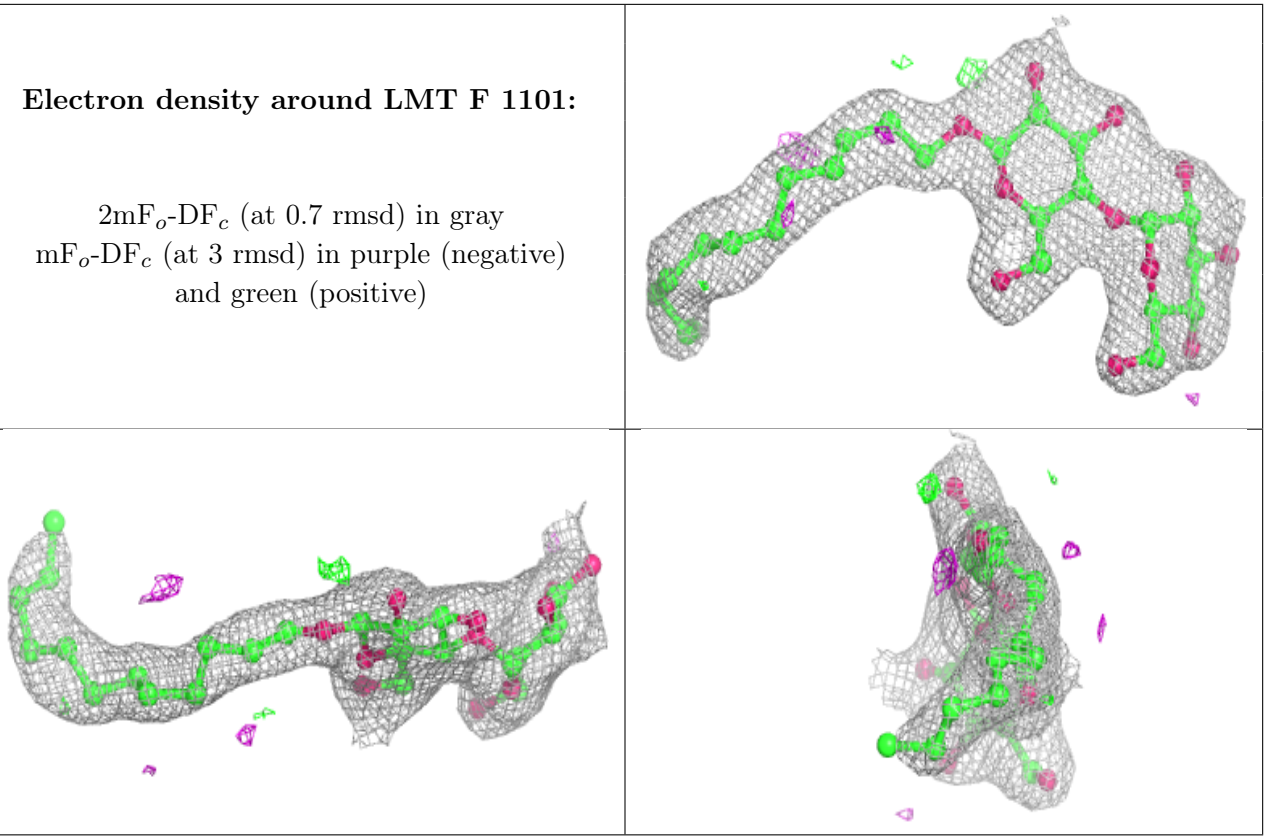
Electron density around LMT B 1104:

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



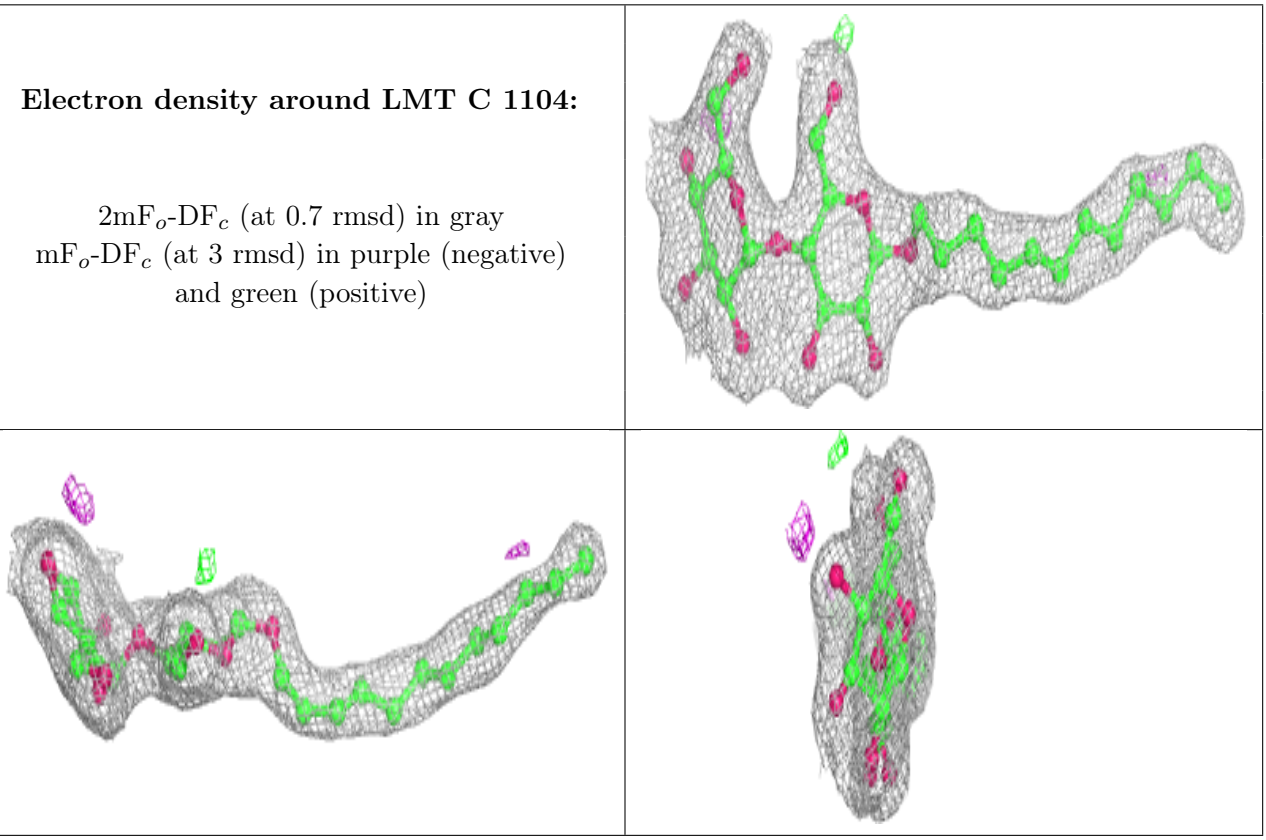
Electron density around LMT F 1101:

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



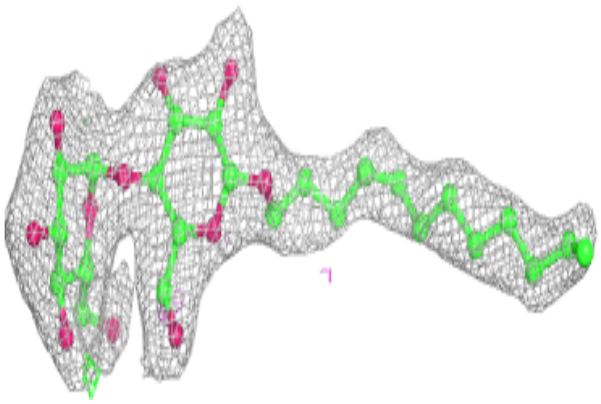
Electron density around LMT C 1104:

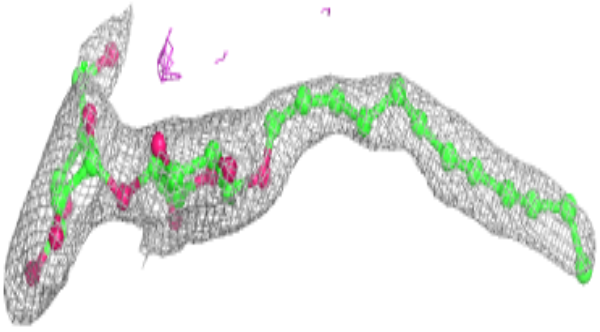
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

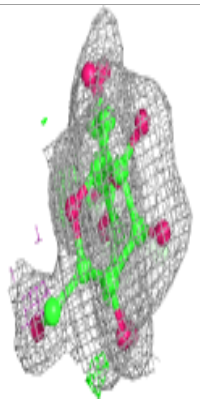


Electron density around LMT C 1103:

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

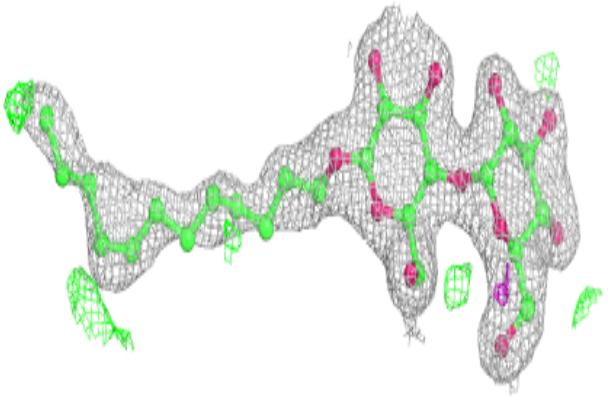


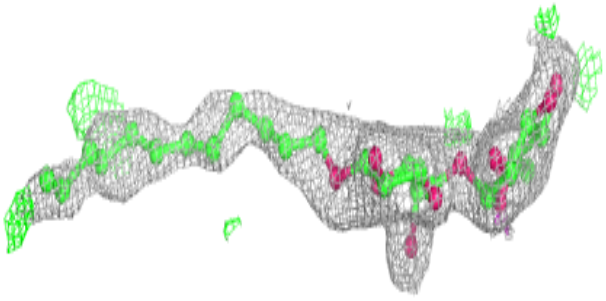


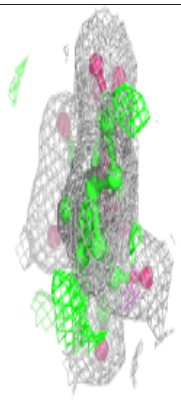


Electron density around LMT C 1105:

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

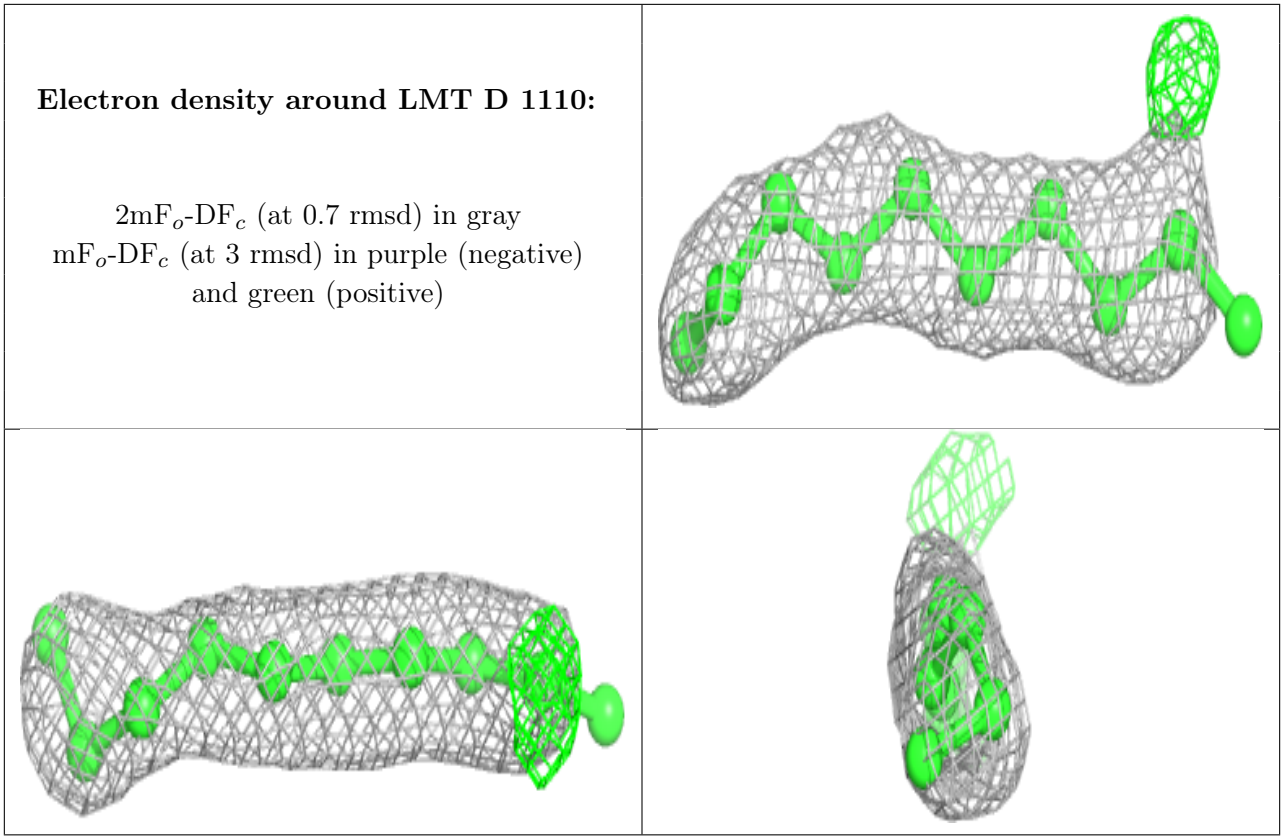






Electron density around LMT D 1110:

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



6.5 Other polymers (i)

There are no such residues in this entry.