Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 02:35 AM EDT

PDB ID	:	6UXO
Title	:	Crystal structure of BAK core domain BH3-groove-dimer in complex with DDM
Authors	:	Cowan, A.D.; Colman, P.M.; Czabotar, P.E.
Deposited on	:	2019-11-07
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9090 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 Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	80	640	408	112	118	2	0	0	0
1	B	78	629	401	110	116	2	0	1	0
1	C	81	644	410	113	119	2	0	0	0
1	D	79	634	405	111	116	2	0	0	0
1	E	80	640	408	112	118	2	0	0	0
1	F	79	634	405	111	116	2	0	0	0
1	G	81	652	415	114	120	3	0	1	0
1	H	78	635	404	112	117	2	0	1	0
1	I	81	644	410	113	119	2	0	0	0
1	J	78	626	399	110	115	2	0	0	0
1	K	79	642	410	112	117	3	0	1	0
1	L	81	655	417	114	121	3	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	GLY	-	expression tag	UNP Q16611
A	65	PRO	-	expression tag	UNP Q16611
A	66	LEU	-	expression tag	UNP Q16611
A	67	GLY	-	expression tag	UNP Q16611
B	64	GLY	-	expression tag	UNP Q16611

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Chain	Residue	Modelled	Actual	Comment	Reference
B	65	PRO	-	expression tag	UNP Q16611
B	66	LEU	-	expression tag	UNP Q16611
B	67	GLY	-	expression tag	UNP Q16611
C	64	GLY	-	expression tag	UNP Q16611
C	65	PRO	-	expression tag	UNP Q16611
C	66	LEU	-	expression tag	UNP Q16611
C	67	GLY	-	expression tag	UNP Q16611
D	64	GLY	-	expression tag	UNP Q16611
D	65	PRO	-	expression tag	UNP Q16611
D	66	LEU	-	expression tag	UNP Q16611
D	67	GLY	-	expression tag	UNP Q16611
E	64	GLY	-	expression tag	UNP Q16611
E	65	PRO	-	expression tag	UNP Q16611
E	66	LEU	-	expression tag	UNP Q16611
E	67	GLY	-	expression tag	UNP Q16611
F	64	GLY	-	expression tag	UNP Q16611
F	65	PRO	-	expression tag	UNP Q16611
F	66	LEU	-	expression tag	UNP Q16611
F	67	GLY	-	expression tag	UNP Q16611
G	64	GLY	-	expression tag	UNP Q16611
G	65	PRO	-	expression tag	UNP Q16611
G	66	LEU	-	expression tag	UNP Q16611
G	67	GLY	-	expression tag	UNP Q16611
H	64	GLY	-	expression tag	UNP Q16611
H	65	PRO	-	expression tag	UNP Q16611
H	66	LEU	-	expression tag	UNP Q16611
H	67	GLY	-	expression tag	UNP Q16611
I	64	GLY	-	expression tag	UNP Q16611
I	65	PRO	-	expression tag	UNP Q16611
I	66	LEU	-	expression tag	UNP Q16611
I	67	GLY	-	expression tag	UNP Q16611
J	64	GLY	-	expression tag	UNP Q16611
J	65	PRO	-	expression tag	UNP Q16611
J	66	LEU	-	expression tag	UNP Q16611
J	67	GLY	-	expression tag	UNP Q16611
K	64	GLY	-	expression tag	UNP Q16611
K	65	PRO	-	expression tag	UNP Q16611
K	66	LEU	-	expression tag	UNP Q16611
K	67	GLY	-	expression tag	UNP Q16611
L	64	GLY	-	expression tag	UNP Q16611
L	65	PRO	-	expression tag	UNP Q16611
L	66	LEU	-	expression tag	UNP Q16611

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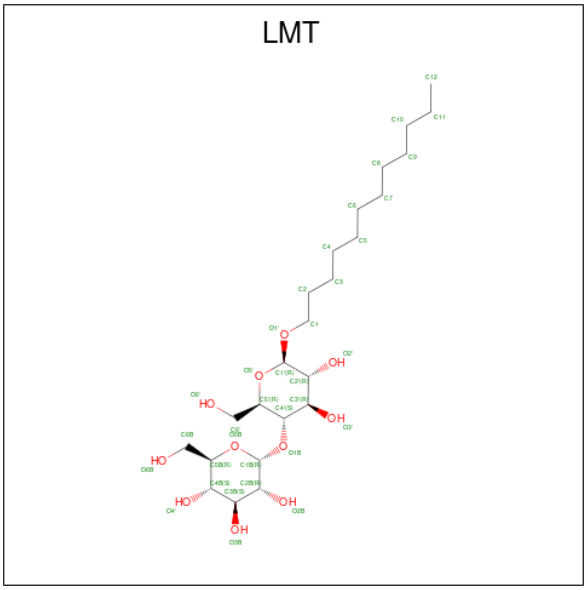
Chain	Residue	Modelled	Actual	Comment	Reference
L	67	GLY	-	expression tag	UNP Q16611

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 23 16 7	0	0
2	B	1	Total C 12 12	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 23 18 5	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 30 19 11	0	0
2	E	1	Total C O 24 18 6	0	0

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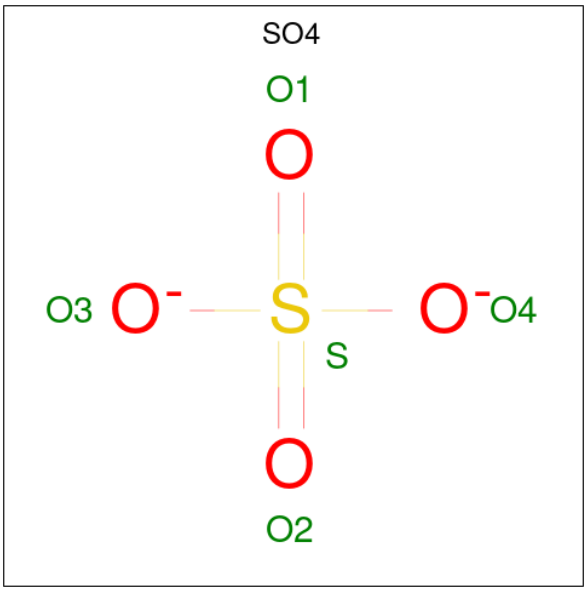
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	F	1	35	24	11	0	0
			Total	C	O		
2	F	1	35	24	11	0	0
			Total	C	O		
2	G	1	70	48	22	0	1
			Total	C	O		
2	G	1	35	24	11	0	0
			Total	C	O		
2	H	1	31	20	11	0	0
			Total	C	O		
2	H	1	35	24	11	0	0
			Total	C	O		
2	I	1	35	24	11	0	0
			Total	C	O		
2	I	1	35	24	11	0	0
			Total	C	O		
2	J	1	35	24	11	0	0
			Total	C	O		
2	J	1	35	24	11	0	0
			Total	C	O		
2	J	1	28	20	8	0	0
			Total	C	O		
2	K	1	35	24	11	0	0
			Total	C	O		
2	K	1	35	24	11	0	0
			Total	C	O		
2	L	1	24	18	6	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	A	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	B	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0
			Total	O	S			
3	E	1	5	4	1		0	0

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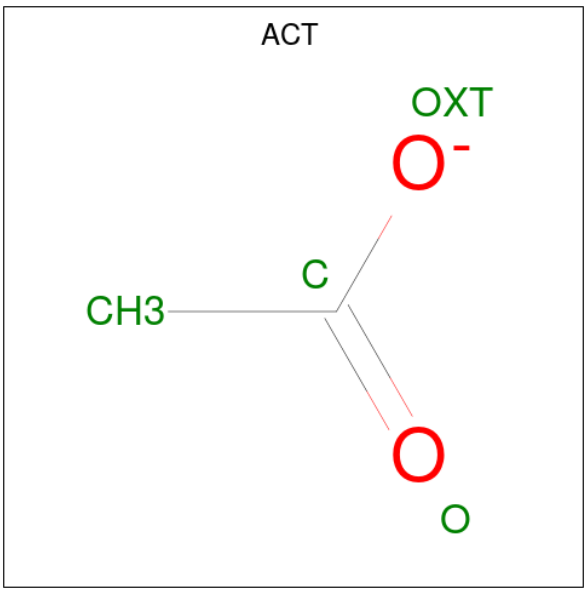
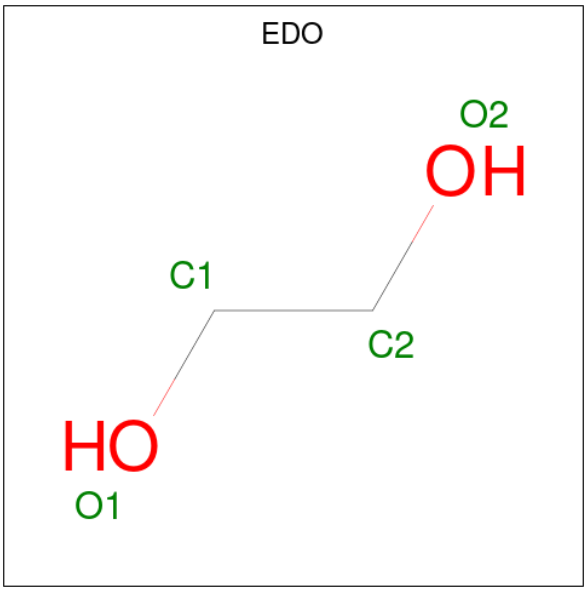
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	E	1	5	4	1		0	0
			Total	O	S			
3	E	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0
			Total	O	S			
3	G	1	5	4	1		0	0
			Total	O	S			
3	G	1	5	4	1		0	0
			Total	O	S			
3	G	1	5	4	1		0	0
			Total	O	S			
3	G	1	5	4	1		0	0
			Total	O	S			
3	H	1	5	4	1		0	0
			Total	O	S			
3	H	1	5	4	1		0	0
			Total	O	S			
3	H	1	5	4	1		0	0
			Total	O	S			
3	I	1	5	4	1		0	0
			Total	O	S			
3	I	1	5	4	1		0	0
			Total	O	S			
3	J	1	5	4	1		0	0
			Total	O	S			
3	J	1	5	4	1		0	0
			Total	O	S			
3	J	1	5	4	1		0	0
			Total	O	S			
3	J	1	5	4	1		0	0
			Total	O	S			
3	K	1	5	4	1		0	0
			Total	O	S			
3	K	1	5	4	1		0	0
			Total	O	S			
3	L	1	5	4	1		0	0
			Total	O	S			
3	L	1	5	4	1		0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
4	C	1	4	2	2	0	0
4	E	1	4	2	2	0	0
4	G	1	4	2	2	0	0
4	I	1	4	2	2	0	0
4	K	1	4	2	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	D	1	4	2	2	0	0
5	E	1	4	2	2	0	0
5	E	1	4	2	2	0	0
5	E	1	4	2	2	0	0
5	F	1	4	2	2	0	0
5	F	1	4	2	2	0	0
5	F	1	4	2	2	0	0
5	F	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	H	1	4	2	2	0	0
			Total	C	O		
5	I	1	4	2	2	0	0
			Total	C	O		
5	I	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	K	1	4	2	2	0	0
			Total	C	O		
5	L	1	4	2	2	0	0
			Total	C	O		
5	L	1	4	2	2	0	0
			Total	C	O		
5	L	1	4	2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	25	25	25	0	0
			Total	O		
6	B	33	33	33	0	0
			Total	O		
6	C	28	28	28	0	0
			Total	O		
6	D	21	21	21	0	0
			Total	O		
6	E	35	35	35	0	0
			Total	O		
6	F	25	25	25	0	0
			Total	O		
6	G	23	23	23	0	0
			Total	O		
6	H	23	23	23	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	I	32	32	32	0	0
			Total	O		
6	J	22	22	22	0	0
			Total	O		
6	K	29	29	29	0	0
			Total	O		
6	L	30	30	30	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.94Å 91.83Å 95.72Å 90.00° 107.52° 90.00°	Depositor
Resolution (Å)	39.45 – 1.80	Depositor
% Data completeness (in resolution range)	99.2 (39.45-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.21 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.212 , 0.250	Depositor
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.140	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9090	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5949e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

91 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	A	201	-	36,36,36	1.09	4 (11%)	47,47,47	1.00	1 (2%)
3	SO4	J	204	-	4,4,4	0.14	0	6,6,6	0.07	0
2	LMT	I	201	-	36,36,36	1.14	6 (16%)	47,47,47	1.01	2 (4%)
3	SO4	F	203	-	4,4,4	0.13	0	6,6,6	0.08	0
5	EDO	B	207	-	3,3,3	0.46	0	2,2,2	0.37	0
5	EDO	E	209	-	3,3,3	0.44	0	2,2,2	0.51	0
5	EDO	H	206	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	J	209	-	3,3,3	0.46	0	2,2,2	0.25	0
5	EDO	F	208	-	3,3,3	0.48	0	2,2,2	0.37	0
3	SO4	J	206	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	D	201	-	4,4,4	0.14	0	6,6,6	0.08	0
2	LMT	D	202	-	23,23,36	1.15	4 (17%)	26,27,47	1.26	3 (11%)
3	SO4	A	205	-	4,4,4	0.13	0	6,6,6	0.10	0
2	LMT	K	201	-	36,36,36	1.18	5 (13%)	47,47,47	1.02	1 (2%)
3	SO4	J	205	-	4,4,4	0.15	0	6,6,6	0.08	0
5	EDO	A	207	-	3,3,3	0.46	0	2,2,2	0.33	0
2	LMT	H	203	-	36,36,36	1.12	3 (8%)	47,47,47	1.10	3 (6%)
5	EDO	E	208	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	F	205	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	J	208	-	3,3,3	0.38	0	2,2,2	0.67	0
5	EDO	L	205	-	3,3,3	0.44	0	2,2,2	0.32	0
5	EDO	B	205	-	3,3,3	0.45	0	2,2,2	0.37	0
2	LMT	C	201	-	36,36,36	1.13	4 (11%)	47,47,47	0.85	0
2	LMT	J	203	-	28,28,36	0.91	1 (3%)	32,34,47	1.11	3 (9%)
3	SO4	H	202	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	B	204	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	E	206	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	G	501	-	4,4,4	0.13	0	6,6,6	0.06	0
5	EDO	I	206	-	3,3,3	0.38	0	2,2,2	0.66	0
3	SO4	G	504	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	K	204	-	4,4,4	0.15	0	6,6,6	0.08	0
4	ACT	C	206	-	3,3,3	1.12	0	3,3,3	1.39	0
5	EDO	F	207	-	3,3,3	0.42	0	2,2,2	0.44	0
2	LMT	L	201	-	24,24,36	1.00	1 (4%)	29,29,47	1.05	2 (6%)
5	EDO	B	209	-	3,3,3	0.46	0	2,2,2	0.36	0
3	SO4	C	202	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	G	503	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	C	204	-	4,4,4	0.13	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	L	206	-	3,3,3	0.45	0	2,2,2	0.50	0
2	LMT	G	506[B]	-	36,36,36	1.18	6 (16%)	47,47,47	1.12	3 (6%)
2	LMT	C	207	-	36,36,36	1.13	3 (8%)	47,47,47	1.25	3 (6%)
5	EDO	I	207	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	L	204	-	3,3,3	0.37	0	2,2,2	1.04	0
3	SO4	C	205	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	D	203	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	K	203	-	4,4,4	0.14	0	6,6,6	0.15	0
5	EDO	F	206	-	3,3,3	0.45	0	2,2,2	0.40	0
3	SO4	A	203	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	A	204	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	F	204	-	4,4,4	0.15	0	6,6,6	0.10	0
5	EDO	K	206	-	3,3,3	0.49	0	2,2,2	0.26	0
2	LMT	E	201	-	36,36,36	1.08	5 (13%)	47,47,47	0.92	0
4	ACT	G	505	-	3,3,3	1.22	0	3,3,3	1.50	0
5	EDO	B	206	-	3,3,3	0.47	0	2,2,2	0.36	0
5	EDO	G	509	-	3,3,3	0.53	0	2,2,2	0.21	0
3	SO4	J	207	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	I	202	-	4,4,4	0.13	0	6,6,6	0.07	0
4	ACT	E	207	-	3,3,3	1.41	0	3,3,3	1.46	0
5	EDO	B	208	-	3,3,3	0.47	0	2,2,2	0.29	0
2	LMT	B	202	-	11,11,36	0.23	0	10,10,47	0.77	0
2	LMT	J	202	-	36,36,36	1.11	4 (11%)	47,47,47	1.10	4 (8%)
3	SO4	I	203	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	H	204	-	4,4,4	0.14	0	6,6,6	0.05	0
2	LMT	K	202	-	36,36,36	1.05	4 (11%)	47,47,47	1.02	2 (4%)
4	ACT	A	206	-	3,3,3	1.25	0	3,3,3	1.42	0
4	ACT	K	205	-	3,3,3	1.46	1 (33%)	3,3,3	1.45	0
4	ACT	I	204	-	3,3,3	0.99	0	3,3,3	1.45	0
3	SO4	E	204	-	4,4,4	0.18	0	6,6,6	0.09	0
2	LMT	F	201	-	36,36,36	1.06	5 (13%)	47,47,47	1.05	4 (8%)
3	SO4	B	203	-	4,4,4	0.13	0	6,6,6	0.08	0
2	LMT	E	202	-	31,31,36	1.21	4 (12%)	42,42,47	1.12	4 (9%)
2	LMT	G	506[A]	-	36,36,36	1.13	6 (16%)	47,47,47	1.09	3 (6%)
3	SO4	D	204	-	4,4,4	0.13	0	6,6,6	0.11	0
5	EDO	E	210	-	3,3,3	0.43	0	2,2,2	0.39	0
3	SO4	H	205	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	L	203	-	4,4,4	0.13	0	6,6,6	0.08	0
2	LMT	H	201	-	32,32,36	1.15	5 (15%)	43,43,47	0.95	2 (4%)
5	EDO	G	508	-	3,3,3	0.49	0	2,2,2	0.34	0
3	SO4	E	205	-	4,4,4	0.13	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LMT	G	507	-	36,36,36	1.12	3 (8%)	47,47,47	1.06	2 (4%)
2	LMT	J	201	-	36,36,36	1.18	4 (11%)	47,47,47	0.96	2 (4%)
3	SO4	C	203	-	4,4,4	0.13	0	6,6,6	0.17	0
2	LMT	C	208	-	36,36,36	1.12	5 (13%)	47,47,47	1.19	6 (12%)
3	SO4	G	502	-	4,4,4	0.12	0	6,6,6	0.14	0
2	LMT	I	205	-	36,36,36	1.10	3 (8%)	47,47,47	0.97	2 (4%)
3	SO4	L	202	-	4,4,4	0.16	0	6,6,6	0.09	0
2	LMT	A	202	-	23,24,36	1.20	2 (8%)	27,31,47	1.28	3 (11%)
2	LMT	F	202	-	36,36,36	1.12	4 (11%)	47,47,47	1.08	2 (4%)
2	LMT	E	203	-	24,24,36	1.00	2 (8%)	29,29,47	1.13	2 (6%)
5	EDO	D	205	-	3,3,3	0.49	0	2,2,2	0.36	0
3	SO4	B	201	-	4,4,4	0.18	0	6,6,6	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	A	201	-	-	6/21/61/61	0/2/2/2
2	LMT	J	203	-	-	16/21/41/61	0/1/1/2
2	LMT	K	202	-	-	13/21/61/61	0/2/2/2
2	LMT	F	201	-	-	9/21/61/61	0/2/2/2
5	EDO	F	206	-	-	0/1/1/1	-
2	LMT	I	201	-	-	16/21/61/61	0/2/2/2
5	EDO	I	206	-	-	0/1/1/1	-
2	LMT	E	202	-	-	11/16/56/61	0/2/2/2
2	LMT	G	506[A]	-	-	13/21/61/61	0/2/2/2
5	EDO	B	207	-	-	0/1/1/1	-
5	EDO	K	206	-	-	0/1/1/1	-
5	EDO	E	209	-	-	0/1/1/1	-
5	EDO	E	210	-	-	1/1/1/1	-
5	EDO	H	206	-	-	1/1/1/1	-
5	EDO	J	209	-	-	0/1/1/1	-
2	LMT	E	201	-	-	7/21/61/61	0/2/2/2
5	EDO	F	208	-	-	1/1/1/1	-
5	EDO	F	207	-	-	1/1/1/1	-
2	LMT	H	201	-	-	4/17/57/61	0/2/2/2
2	LMT	L	201	-	-	6/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	209	-	-	0/1/1/1	-
5	EDO	G	508	-	-	1/1/1/1	-
5	EDO	B	206	-	-	0/1/1/1	-
5	EDO	G	509	-	-	0/1/1/1	-
2	LMT	G	507	-	-	10/21/61/61	0/2/2/2
2	LMT	J	201	-	-	6/21/61/61	0/2/2/2
2	LMT	D	202	-	-	10/15/31/61	0/1/1/2
2	LMT	C	208	-	-	9/21/61/61	0/2/2/2
5	EDO	L	206	-	-	1/1/1/1	-
2	LMT	G	506[B]	-	-	6/21/61/61	0/2/2/2
2	LMT	I	205	-	-	8/21/61/61	0/2/2/2
2	LMT	K	201	-	-	9/21/61/61	0/2/2/2
2	LMT	C	207	-	-	13/21/61/61	0/2/2/2
5	EDO	B	208	-	-	0/1/1/1	-
2	LMT	A	202	-	-	6/12/39/61	1/2/2/2
5	EDO	A	207	-	-	1/1/1/1	-
2	LMT	H	203	-	-	8/21/61/61	0/2/2/2
5	EDO	E	208	-	-	1/1/1/1	-
5	EDO	F	205	-	-	0/1/1/1	-
5	EDO	J	208	-	-	1/1/1/1	-
2	LMT	F	202	-	-	14/21/61/61	0/2/2/2
5	EDO	L	205	-	-	0/1/1/1	-
2	LMT	E	203	-	-	11/15/35/61	0/1/1/2
5	EDO	B	205	-	-	0/1/1/1	-
5	EDO	D	205	-	-	1/1/1/1	-
2	LMT	C	201	-	-	7/21/61/61	0/2/2/2
5	EDO	I	207	-	-	1/1/1/1	-
5	EDO	L	204	-	-	1/1/1/1	-
2	LMT	B	202	-	-	5/9/9/61	-
2	LMT	J	202	-	-	9/21/61/61	0/2/2/2

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	202	LMT	O3'-C3'	-3.04	1.36	1.43
2	G	507	LMT	O2'-C2'	-2.99	1.35	1.43
2	D	202	LMT	O3'-C3'	-2.92	1.37	1.43
2	C	208	LMT	O2'-C2'	-2.91	1.36	1.43
2	A	202	LMT	O2B-C2B	-2.77	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	506[A]	LMT	O2B-C2B	-2.75	1.36	1.43
2	G	507	LMT	O3'-C3'	-2.74	1.36	1.43
2	G	506[A]	LMT	O3'-C3'	-2.74	1.36	1.43
2	G	506[B]	LMT	O3'-C3'	-2.66	1.36	1.43
2	E	201	LMT	O3'-C3'	-2.66	1.36	1.43
2	C	207	LMT	O3'-C3'	-2.63	1.36	1.43
2	F	202	LMT	O3'-C3'	-2.61	1.36	1.43
2	H	203	LMT	O3'-C3'	-2.59	1.36	1.43
2	E	201	LMT	O2'-C2'	-2.58	1.36	1.43
2	I	205	LMT	O2'-C2'	-2.57	1.36	1.43
2	J	201	LMT	O3'-C3'	-2.56	1.37	1.43
2	L	201	LMT	O3'-C3'	-2.55	1.37	1.43
2	E	203	LMT	O3'-C3'	-2.54	1.37	1.43
2	G	506[B]	LMT	O3B-C3B	-2.54	1.37	1.43
2	K	201	LMT	O2B-C2B	-2.54	1.37	1.43
2	C	208	LMT	O3'-C3'	-2.54	1.37	1.43
2	H	201	LMT	O3'-C3'	-2.53	1.37	1.43
2	F	201	LMT	O3'-C3'	-2.50	1.37	1.43
2	I	205	LMT	O3'-C3'	-2.48	1.37	1.43
2	J	201	LMT	O2'-C2'	-2.47	1.37	1.43
2	I	201	LMT	O3'-C3'	-2.47	1.37	1.43
2	E	202	LMT	O3'-C3'	-2.46	1.37	1.43
2	J	202	LMT	O3'-C3'	-2.45	1.37	1.43
2	K	201	LMT	O3'-C3'	-2.45	1.37	1.43
2	G	506[A]	LMT	O3B-C3B	-2.45	1.37	1.43
2	K	202	LMT	O3'-C3'	-2.45	1.37	1.43
2	J	203	LMT	O3'-C3'	-2.44	1.37	1.43
2	G	506[B]	LMT	O2'-C2'	-2.43	1.37	1.43
2	G	506[B]	LMT	O1'-C1'	-2.39	1.36	1.40
2	C	201	LMT	O3'-C3'	-2.36	1.37	1.43
2	J	201	LMT	O3B-C3B	-2.35	1.37	1.43
2	F	201	LMT	O2'-C2'	-2.35	1.37	1.43
2	C	201	LMT	O2'-C2'	-2.34	1.37	1.43
2	F	202	LMT	O3B-C3B	-2.34	1.37	1.43
2	C	207	LMT	O2B-C2B	-2.34	1.37	1.43
2	A	201	LMT	O3B-C3B	-2.33	1.37	1.43
2	C	207	LMT	O3B-C3B	-2.32	1.37	1.43
2	C	201	LMT	O3B-C3B	-2.31	1.37	1.43
2	C	201	LMT	O2B-C2B	-2.30	1.37	1.43
2	I	205	LMT	O3B-C3B	-2.29	1.37	1.43
2	H	201	LMT	O2B-C2B	-2.29	1.37	1.43
2	F	201	LMT	O3B-C3B	-2.28	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	LMT	O3'-C3'	-2.26	1.37	1.43
2	F	201	LMT	O2B-C2B	-2.25	1.37	1.43
2	H	203	LMT	O2B-C2B	-2.25	1.37	1.43
2	E	202	LMT	O3B-C3B	-2.24	1.37	1.43
2	F	202	LMT	O2B-C2B	-2.23	1.37	1.43
2	K	202	LMT	O3B-C3B	-2.22	1.37	1.43
2	I	201	LMT	O3B-C3B	-2.20	1.37	1.43
2	J	201	LMT	O2B-C2B	-2.20	1.37	1.43
2	G	506[A]	LMT	O2'-C2'	-2.20	1.37	1.43
2	K	201	LMT	O1'-C1'	-2.20	1.36	1.40
2	D	202	LMT	C3'-C2'	2.19	1.55	1.52
2	G	507	LMT	O3B-C3B	-2.19	1.37	1.43
2	G	506[B]	LMT	O4'-C4B	-2.19	1.37	1.43
2	K	201	LMT	O3B-C3B	-2.18	1.37	1.43
2	J	202	LMT	O3B-C3B	-2.18	1.37	1.43
2	K	202	LMT	O2B-C2B	-2.17	1.37	1.43
2	H	203	LMT	O3B-C3B	-2.17	1.37	1.43
2	A	201	LMT	O2'-C2'	-2.17	1.37	1.43
2	C	208	LMT	O3B-C3B	-2.17	1.37	1.43
2	H	201	LMT	O3B-C3B	-2.16	1.37	1.43
2	G	506[B]	LMT	O2B-C2B	-2.16	1.37	1.43
2	E	202	LMT	O2'-C2'	-2.15	1.37	1.43
4	K	205	ACT	CH3-C	2.14	1.58	1.49
2	E	201	LMT	O3B-C3B	-2.14	1.37	1.43
2	E	203	LMT	O2'-C2'	-2.14	1.37	1.43
2	E	201	LMT	O4'-C4B	-2.13	1.38	1.43
2	I	201	LMT	O2'-C2'	-2.13	1.38	1.43
2	F	202	LMT	O4'-C4B	-2.13	1.38	1.43
2	I	201	LMT	O2B-C2B	-2.12	1.38	1.43
2	D	202	LMT	O5'-C5'	-2.12	1.40	1.44
2	E	202	LMT	O1'-C1'	-2.11	1.36	1.40
2	I	201	LMT	O4'-C4B	-2.10	1.38	1.43
2	F	201	LMT	O4'-C4B	-2.09	1.38	1.43
2	G	506[A]	LMT	O4'-C4B	-2.09	1.38	1.43
2	K	201	LMT	O2'-C2'	-2.08	1.38	1.43
2	C	208	LMT	O4'-C4B	-2.08	1.38	1.43
2	A	201	LMT	O2B-C2B	-2.07	1.38	1.43
2	C	208	LMT	O2B-C2B	-2.06	1.38	1.43
2	J	202	LMT	O2B-C2B	-2.05	1.38	1.43
2	D	202	LMT	O2'-C2'	-2.05	1.38	1.43
2	E	201	LMT	O2B-C2B	-2.05	1.38	1.43
2	H	201	LMT	O4'-C4B	-2.04	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	LMT	O2'-C2'	-2.03	1.38	1.43
2	G	506[A]	LMT	O5'-C5'	-2.03	1.39	1.44
2	I	201	LMT	O1'-C1'	-2.01	1.36	1.40
2	J	202	LMT	O2'-C2'	-2.00	1.38	1.43
2	K	202	LMT	O4'-C4B	-2.00	1.38	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	202	LMT	O1'-C1'-C2'	3.97	113.16	109.04
2	C	207	LMT	C1'-O5'-C5'	-3.79	106.24	113.69
2	D	202	LMT	C3'-C4'-C5'	-3.42	105.32	111.22
2	G	506[B]	LMT	C3'-C4'-C5'	-3.25	103.48	110.93
2	G	507	LMT	C1-O1'-C1'	3.17	119.10	113.84
2	C	208	LMT	C1-O1'-C1'	3.15	119.07	113.84
2	H	203	LMT	C3'-C4'-C5'	-3.09	103.85	110.93
2	J	202	LMT	C1'-O5'-C5'	-3.08	107.64	113.69
2	G	506[A]	LMT	C1'-O5'-C5'	-3.00	107.80	113.69
2	G	507	LMT	C3'-C4'-C5'	-2.92	104.23	110.93
2	C	208	LMT	O1'-C1'-C2'	2.88	112.81	108.30
2	I	201	LMT	C1'-O5'-C5'	-2.83	108.14	113.69
2	C	207	LMT	C3'-C4'-C5'	-2.82	104.46	110.93
2	E	203	LMT	C3'-C4'-C5'	-2.81	105.23	110.24
2	F	201	LMT	C1-O1'-C1'	2.80	118.48	113.84
2	E	202	LMT	C1'-O5'-C5'	-2.75	108.30	113.69
2	I	205	LMT	C3B-C4B-C5B	-2.72	105.38	110.24
2	K	201	LMT	O6'-C6'-C5'	-2.69	102.06	111.29
2	J	203	LMT	O5'-C5'-C4'	2.66	115.36	109.75
2	F	202	LMT	C3'-C4'-C5'	-2.62	104.91	110.93
2	L	201	LMT	C1'-O5'-C5'	-2.62	108.55	113.69
2	J	202	LMT	C3B-C4B-C5B	-2.61	105.59	110.24
2	C	208	LMT	O5'-C1'-C2'	-2.55	104.95	110.35
2	K	202	LMT	O5'-C5'-C4'	2.53	115.08	109.75
2	L	201	LMT	C3'-C4'-C5'	-2.50	105.78	110.24
2	J	202	LMT	C3'-C4'-C5'	-2.48	105.23	110.93
2	F	202	LMT	C1'-O5'-C5'	-2.47	108.84	113.69
2	E	203	LMT	C1'-O5'-C5'	-2.43	108.92	113.69
2	D	202	LMT	C1'-O5'-C5'	-2.41	110.46	113.13
2	J	201	LMT	C1'-O5'-C5'	-2.40	108.98	113.69
2	I	201	LMT	C3B-C4B-C5B	-2.35	106.05	110.24
2	C	208	LMT	O5B-C5B-C6B	2.34	112.25	106.44
2	C	208	LMT	C3B-C4B-C5B	-2.33	106.09	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	207	LMT	O5'-C5'-C6'	2.31	112.17	106.44
2	C	208	LMT	C3'-C4'-C5'	-2.30	105.65	110.93
2	A	201	LMT	O1'-C1'-C2'	2.29	111.88	108.30
2	G	506[B]	LMT	C1'-O5'-C5'	-2.29	109.19	113.69
2	G	506[A]	LMT	C3B-C4B-C5B	-2.29	106.16	110.24
2	A	202	LMT	O5'-C5'-C4'	2.28	114.55	109.75
2	I	205	LMT	O5B-C5B-C6B	2.25	112.03	106.44
2	E	202	LMT	O5B-C1B-C2B	2.24	115.09	110.35
2	G	506[A]	LMT	O6'-C6'-C5'	-2.22	103.68	111.29
2	H	203	LMT	O5B-C5B-C4B	2.19	113.67	109.69
2	J	202	LMT	O5B-C5B-C6B	2.19	111.88	106.44
2	A	202	LMT	C1'-O5'-C5'	2.18	116.42	113.03
2	K	202	LMT	O5B-C5B-C4B	2.18	113.66	109.69
2	J	203	LMT	C1B-O1B-C4'	2.17	119.06	114.66
2	D	202	LMT	O6'-C6'-C5'	-2.15	106.09	111.78
2	J	203	LMT	O1'-C1'-C2'	2.13	111.64	108.30
2	F	201	LMT	O5'-C1'-C2'	-2.13	105.84	110.35
2	G	506[B]	LMT	O5B-C5B-C4B	2.11	113.53	109.69
2	F	201	LMT	C1'-O5'-C5'	-2.11	109.55	113.69
2	E	202	LMT	O5B-C5B-C4B	2.09	113.49	109.69
2	H	203	LMT	O5B-C5B-C6B	2.08	111.62	106.44
2	H	201	LMT	C1-O1'-C1'	2.07	117.28	113.84
2	F	201	LMT	O5B-C5B-C4B	2.07	113.45	109.69
2	H	201	LMT	O5'-C1'-C2'	-2.05	106.01	110.35
2	J	201	LMT	O5B-C5B-C4B	2.04	113.40	109.69
2	E	202	LMT	O1B-C1B-C2B	2.03	113.35	108.10

There are no chirality outliers.

All (244) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	LMT	C2-C1-O1'-C1'
2	A	202	LMT	C2'-C1'-O1'-C1
2	A	202	LMT	O5'-C1'-O1'-C1
2	C	207	LMT	C2'-C1'-O1'-C1
2	C	207	LMT	O5'-C1'-O1'-C1
2	C	207	LMT	C2-C1-O1'-C1'
2	D	202	LMT	C2'-C1'-O1'-C1
2	D	202	LMT	O5'-C1'-O1'-C1
2	D	202	LMT	C4'-C5'-C6'-O6'
2	D	202	LMT	O5'-C5'-C6'-O6'
2	D	202	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
2	E	202	LMT	O5'-C1'-O1'-C1
2	E	203	LMT	C2'-C1'-O1'-C1
2	E	203	LMT	O5'-C1'-O1'-C1
2	E	203	LMT	C2-C1-O1'-C1'
2	F	201	LMT	C2'-C1'-O1'-C1
2	F	201	LMT	O5'-C1'-O1'-C1
2	F	202	LMT	C2-C1-O1'-C1'
2	G	506[A]	LMT	C2-C1-O1'-C1'
2	G	507	LMT	C2-C1-O1'-C1'
2	H	203	LMT	O5'-C1'-O1'-C1
2	I	201	LMT	C2'-C1'-O1'-C1
2	I	201	LMT	O5'-C1'-O1'-C1
2	I	201	LMT	C2-C1-O1'-C1'
2	J	201	LMT	C2'-C1'-O1'-C1
2	J	201	LMT	O5'-C1'-O1'-C1
2	J	201	LMT	C2-C1-O1'-C1'
2	J	202	LMT	C2'-C1'-O1'-C1
2	J	202	LMT	O5'-C1'-O1'-C1
2	J	203	LMT	O1B-C1B-C2B-O2B
2	J	203	LMT	O5B-C1B-C2B-O2B
2	J	203	LMT	O5B-C1B-O1B-C4'
2	J	203	LMT	C2-C1-O1'-C1'
2	K	201	LMT	C2-C1-O1'-C1'
2	K	202	LMT	O5'-C1'-O1'-C1
2	L	201	LMT	C2-C1-O1'-C1'
2	G	506[B]	LMT	C3'-C4'-O1B-C1B
2	H	203	LMT	O5B-C1B-O1B-C4'
2	H	203	LMT	C2B-C1B-O1B-C4'
2	F	202	LMT	C3'-C4'-O1B-C1B
2	G	506[A]	LMT	O5B-C1B-O1B-C4'
2	E	202	LMT	C2B-C1B-O1B-C4'
2	J	203	LMT	C3'-C4'-O1B-C1B
2	K	202	LMT	C3'-C4'-O1B-C1B
2	J	202	LMT	O5B-C5B-C6B-O6B
2	F	201	LMT	O5B-C5B-C6B-O6B
2	G	507	LMT	O5B-C5B-C6B-O6B
2	C	201	LMT	C5'-C4'-O1B-C1B
2	K	201	LMT	C3'-C4'-O1B-C1B
2	E	203	LMT	O5'-C5'-C6'-O6'
2	E	203	LMT	C4'-C5'-C6'-O6'
2	E	201	LMT	O5B-C5B-C6B-O6B
2	H	201	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
2	C	207	LMT	O5'-C5'-C6'-O6'
2	G	507	LMT	C4B-C5B-C6B-O6B
2	I	205	LMT	C4B-C5B-C6B-O6B
2	J	202	LMT	C4B-C5B-C6B-O6B
2	J	203	LMT	C4'-C5'-C6'-O6'
2	I	201	LMT	O5'-C5'-C6'-O6'
2	K	202	LMT	C4B-C5B-C6B-O6B
2	L	201	LMT	C4'-C5'-C6'-O6'
2	K	202	LMT	O5'-C5'-C6'-O6'
2	G	506[A]	LMT	O5'-C1'-O1'-C1
2	G	506[A]	LMT	O5'-C5'-C6'-O6'
2	J	201	LMT	O5B-C5B-C6B-O6B
2	E	201	LMT	C4B-C5B-C6B-O6B
2	G	506[A]	LMT	C4'-C5'-C6'-O6'
2	K	202	LMT	C4'-C5'-C6'-O6'
2	F	202	LMT	O5B-C5B-C6B-O6B
2	E	202	LMT	C2'-C1'-O1'-C1
2	G	506[A]	LMT	C2'-C1'-O1'-C1
2	H	203	LMT	C2'-C1'-O1'-C1
2	K	202	LMT	C2'-C1'-O1'-C1
2	H	203	LMT	O5'-C5'-C6'-O6'
2	I	205	LMT	O5B-C5B-C6B-O6B
2	C	201	LMT	C4B-C5B-C6B-O6B
2	C	207	LMT	C4'-C5'-C6'-O6'
2	F	201	LMT	C4B-C5B-C6B-O6B
2	H	201	LMT	C4B-C5B-C6B-O6B
2	C	208	LMT	O5B-C5B-C6B-O6B
2	E	202	LMT	O5'-C5'-C6'-O6'
2	H	203	LMT	C7-C8-C9-C10
2	K	202	LMT	O5B-C5B-C6B-O6B
2	L	201	LMT	O5'-C5'-C6'-O6'
2	I	201	LMT	C4'-C5'-C6'-O6'
2	J	201	LMT	O1'-C1-C2-C3
2	K	201	LMT	O5'-C1'-O1'-C1
2	E	202	LMT	O1'-C1-C2-C3
2	C	208	LMT	O1'-C1-C2-C3
2	G	507	LMT	O1'-C1-C2-C3
2	C	207	LMT	O1'-C1-C2-C3
2	D	202	LMT	C5-C6-C7-C8
2	I	201	LMT	C6-C7-C8-C9
2	F	202	LMT	C7-C8-C9-C10
2	I	205	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
2	G	507	LMT	C3-C4-C5-C6
2	J	203	LMT	C2'-C1'-O1'-C1
2	K	201	LMT	C2'-C1'-O1'-C1
2	G	506[A]	LMT	O1'-C1-C2-C3
2	J	203	LMT	C11-C10-C9-C8
2	J	203	LMT	O5'-C5'-C6'-O6'
2	E	203	LMT	C7-C8-C9-C10
2	D	202	LMT	C2-C3-C4-C5
2	L	201	LMT	C3-C4-C5-C6
2	L	201	LMT	C4-C5-C6-C7
2	A	201	LMT	C6-C7-C8-C9
2	J	203	LMT	C3-C4-C5-C6
2	J	203	LMT	C7-C8-C9-C10
2	E	202	LMT	C2-C3-C4-C5
2	F	201	LMT	O1'-C1-C2-C3
2	F	201	LMT	C1-C2-C3-C4
2	E	203	LMT	C6-C7-C8-C9
2	F	202	LMT	C3-C4-C5-C6
2	C	201	LMT	C2-C1-O1'-C1'
2	C	208	LMT	C2-C1-O1'-C1'
2	K	202	LMT	C2-C1-O1'-C1'
2	B	202	LMT	C7-C8-C9-C10
2	C	208	LMT	C11-C10-C9-C8
2	E	201	LMT	C7-C8-C9-C10
2	I	205	LMT	C7-C8-C9-C10
2	E	203	LMT	C1-C2-C3-C4
2	E	201	LMT	C4'-C5'-C6'-O6'
2	G	507	LMT	C2-C3-C4-C5
2	E	202	LMT	C1-C2-C3-C4
2	G	507	LMT	C1-C2-C3-C4
2	K	201	LMT	C4B-C5B-C6B-O6B
2	C	201	LMT	C5-C6-C7-C8
2	G	507	LMT	C4-C5-C6-C7
2	G	506[B]	LMT	C7-C8-C9-C10
5	F	207	EDO	O1-C1-C2-O2
5	L	204	EDO	O1-C1-C2-O2
2	F	202	LMT	C6-C7-C8-C9
2	C	207	LMT	C1-C2-C3-C4
2	I	201	LMT	C11-C10-C9-C8
2	J	201	LMT	C4B-C5B-C6B-O6B
2	F	202	LMT	O5'-C1'-O1'-C1
2	A	201	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	I	201	LMT	C3-C4-C5-C6
2	F	202	LMT	C2'-C1'-O1'-C1
2	K	202	LMT	C7-C8-C9-C10
2	F	202	LMT	C1-C2-C3-C4
2	C	201	LMT	C3'-C4'-O1B-C1B
2	C	208	LMT	C7-C8-C9-C10
2	I	201	LMT	O5B-C1B-O1B-C4'
2	F	201	LMT	C7-C8-C9-C10
2	G	507	LMT	C5-C6-C7-C8
2	I	201	LMT	C5-C6-C7-C8
2	J	202	LMT	C9-C10-C11-C12
2	F	202	LMT	C4B-C5B-C6B-O6B
2	C	208	LMT	C1-C2-C3-C4
2	G	506[B]	LMT	O5B-C5B-C6B-O6B
2	F	201	LMT	C11-C10-C9-C8
2	A	202	LMT	O1'-C1-C2-C3
2	D	202	LMT	C6-C7-C8-C9
2	I	201	LMT	C7-C8-C9-C10
2	A	201	LMT	C3-C4-C5-C6
2	B	202	LMT	C6-C7-C8-C9
2	A	201	LMT	C7-C8-C9-C10
2	G	506[B]	LMT	C9-C10-C11-C12
2	F	202	LMT	C9-C10-C11-C12
2	A	201	LMT	O5B-C5B-C6B-O6B
2	C	201	LMT	O5B-C5B-C6B-O6B
2	K	201	LMT	C5'-C4'-O1B-C1B
2	F	202	LMT	C5-C6-C7-C8
2	I	205	LMT	C9-C10-C11-C12
2	I	205	LMT	O5'-C5'-C6'-O6'
2	C	208	LMT	C9-C10-C11-C12
2	A	202	LMT	C2-C3-C4-C5
2	C	207	LMT	O5B-C1B-O1B-C4'
2	C	207	LMT	C7-C8-C9-C10
2	K	201	LMT	C1-C2-C3-C4
2	E	201	LMT	C6-C7-C8-C9
2	A	202	LMT	C2-C1-O1'-C1'
2	F	201	LMT	C2-C1-O1'-C1'
2	H	201	LMT	C2-C1-O1'-C1'
2	E	203	LMT	O1'-C1-C2-C3
2	K	202	LMT	C9-C10-C11-C12
2	B	202	LMT	C3-C4-C5-C6
2	A	202	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
2	I	201	LMT	C4-C5-C6-C7
2	G	506[A]	LMT	C2-C3-C4-C5
2	E	203	LMT	C5-C6-C7-C8
5	H	206	EDO	O1-C1-C2-O2
2	G	506[A]	LMT	C5'-C4'-O1B-C1B
2	J	202	LMT	C11-C10-C9-C8
2	B	202	LMT	C4-C5-C6-C7
2	J	202	LMT	C3-C4-C5-C6
2	J	203	LMT	O5'-C1'-O1'-C1
2	D	202	LMT	C7-C8-C9-C10
2	I	201	LMT	C5'-C4'-O1B-C1B
2	G	506[A]	LMT	C1-C2-C3-C4
2	J	203	LMT	C5'-C4'-O1B-C1B
2	F	202	LMT	C5'-C4'-O1B-C1B
2	G	506[A]	LMT	C9-C10-C11-C12
2	H	201	LMT	O1'-C1-C2-C3
2	I	201	LMT	O1'-C1-C2-C3
2	K	202	LMT	C5'-C4'-O1B-C1B
2	J	202	LMT	O1'-C1-C2-C3
2	E	201	LMT	C9-C10-C11-C12
2	E	202	LMT	O5B-C1B-O1B-C4'
2	K	202	LMT	C1-C2-C3-C4
2	G	506[A]	LMT	C3'-C4'-O1B-C1B
2	I	205	LMT	C1-C2-C3-C4
2	F	202	LMT	O1'-C1-C2-C3
2	B	202	LMT	C9-C10-C11-C12
2	C	207	LMT	C5'-C4'-O1B-C1B
2	H	203	LMT	C4'-C5'-C6'-O6'
5	E	210	EDO	O1-C1-C2-O2
5	G	508	EDO	O1-C1-C2-O2
2	J	203	LMT	C4-C5-C6-C7
2	C	207	LMT	C2B-C1B-O1B-C4'
2	I	201	LMT	C2B-C1B-O1B-C4'
2	I	205	LMT	C6-C7-C8-C9
2	J	202	LMT	C1-C2-C3-C4
2	C	208	LMT	C4B-C5B-C6B-O6B
2	E	202	LMT	C3-C4-C5-C6
5	A	207	EDO	O1-C1-C2-O2
2	K	201	LMT	C4-C5-C6-C7
2	E	202	LMT	C4'-C5'-C6'-O6'
2	G	506[B]	LMT	O5'-C1'-O1'-C1
2	C	207	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	I	201	LMT	C3'-C4'-O1B-C1B
2	G	507	LMT	C6-C7-C8-C9
2	J	203	LMT	C2-C3-C4-C5
2	K	202	LMT	C11-C10-C9-C8
2	G	506[B]	LMT	C5'-C4'-O1B-C1B
5	J	208	EDO	O1-C1-C2-O2
2	J	203	LMT	C5-C6-C7-C8
2	E	201	LMT	O5'-C5'-C6'-O6'
2	E	203	LMT	C11-C10-C9-C8
2	K	201	LMT	O5B-C5B-C6B-O6B
2	D	202	LMT	C3-C4-C5-C6
5	D	205	EDO	O1-C1-C2-O2
5	E	208	EDO	O1-C1-C2-O2
5	F	208	EDO	O1-C1-C2-O2
5	I	207	EDO	O1-C1-C2-O2
5	L	206	EDO	O1-C1-C2-O2
2	C	207	LMT	C4B-C5B-C6B-O6B
2	E	202	LMT	C5'-C4'-O1B-C1B
2	L	201	LMT	C6-C7-C8-C9
2	C	201	LMT	C3-C4-C5-C6
2	G	506[A]	LMT	C7-C8-C9-C10
2	C	208	LMT	C6-C7-C8-C9
2	H	203	LMT	C9-C10-C11-C12

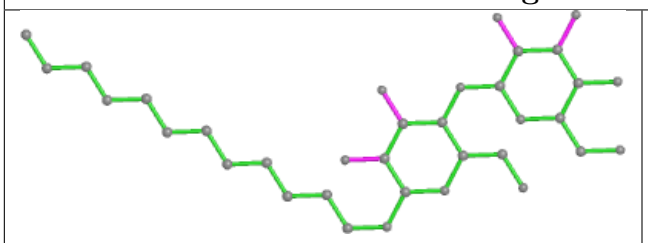
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	202	LMT	C1'-C2'-C3'-C4'-C5'-O5'

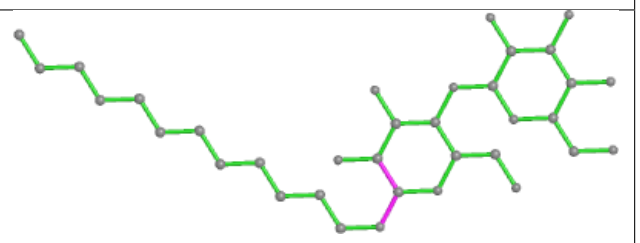
No monomer is involved in short contacts.

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.

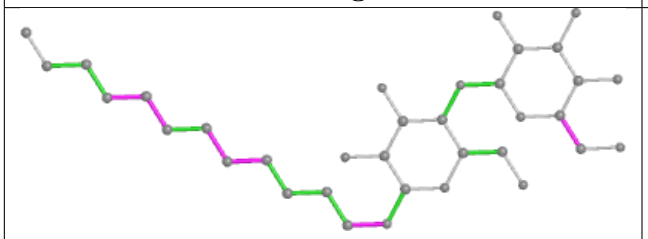
Ligand LMT A 201



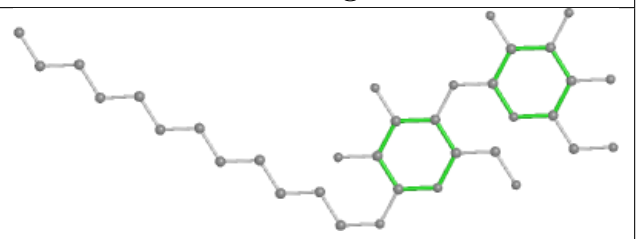
Bond lengths



Bond angles

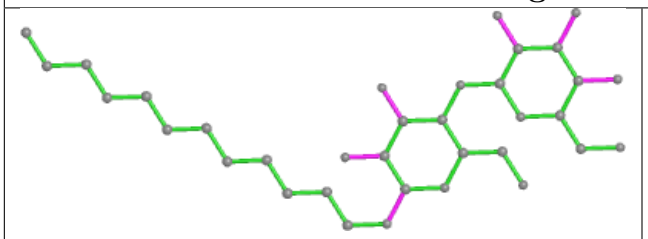


Torsions

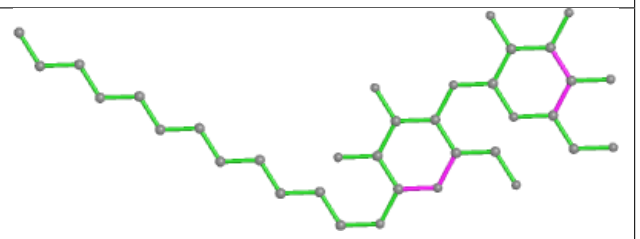


Rings

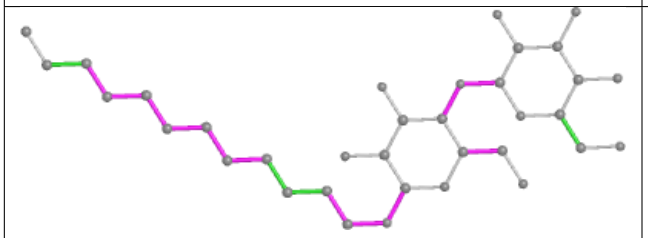
Ligand LMT I 201



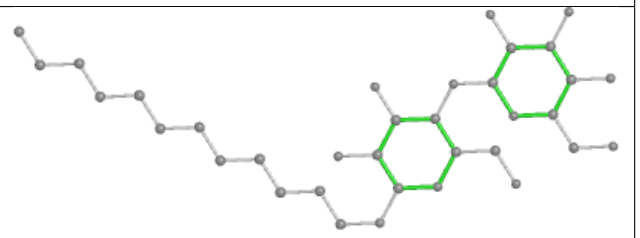
Bond lengths



Bond angles

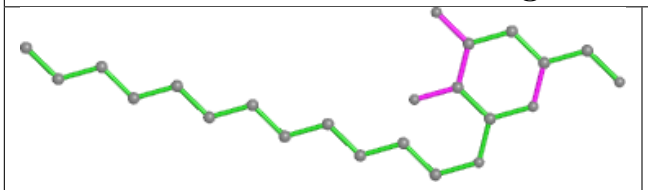


Torsions

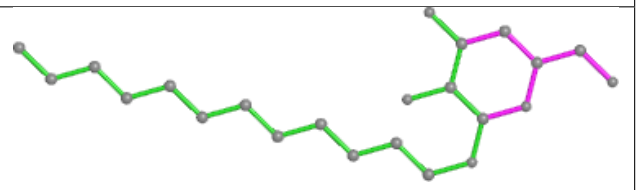


Rings

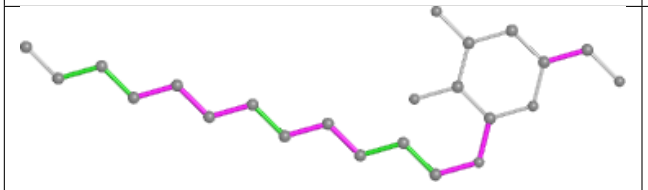
Ligand LMT D 202



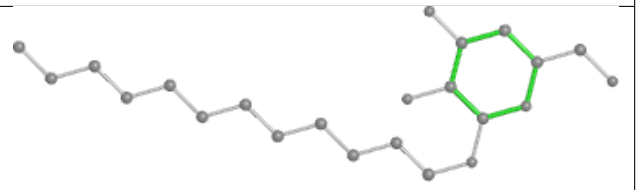
Bond lengths



Bond angles

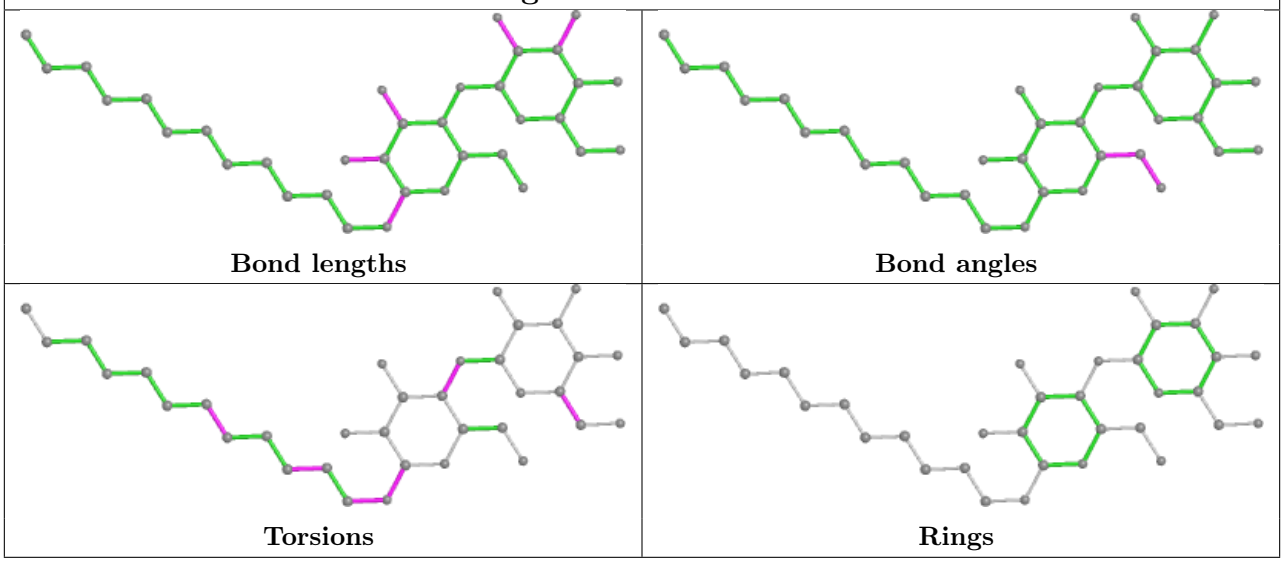


Torsions

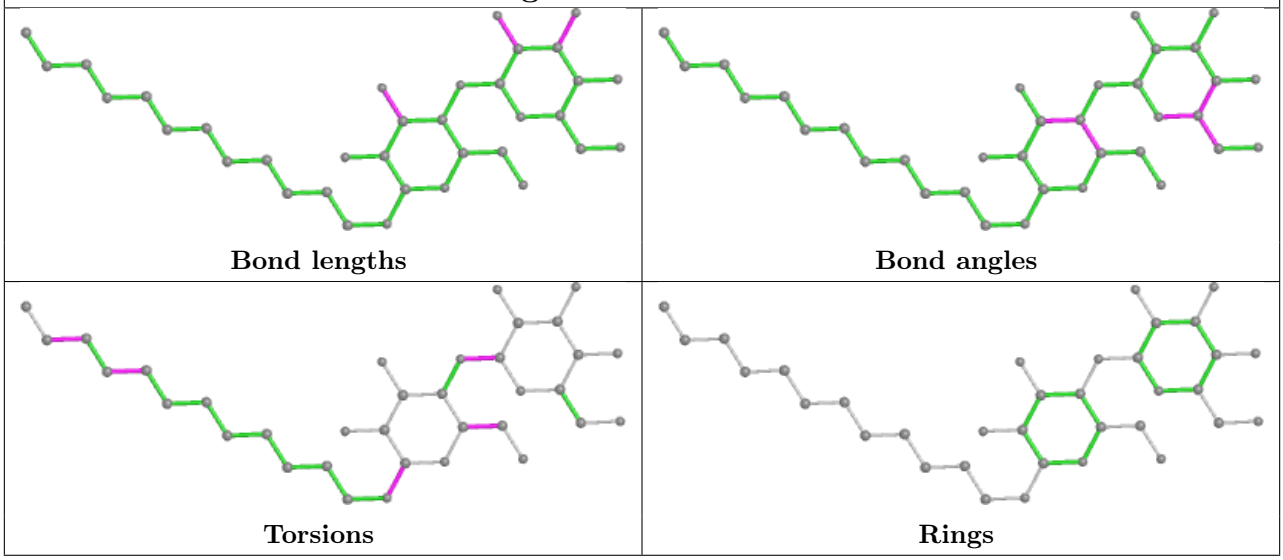


Rings

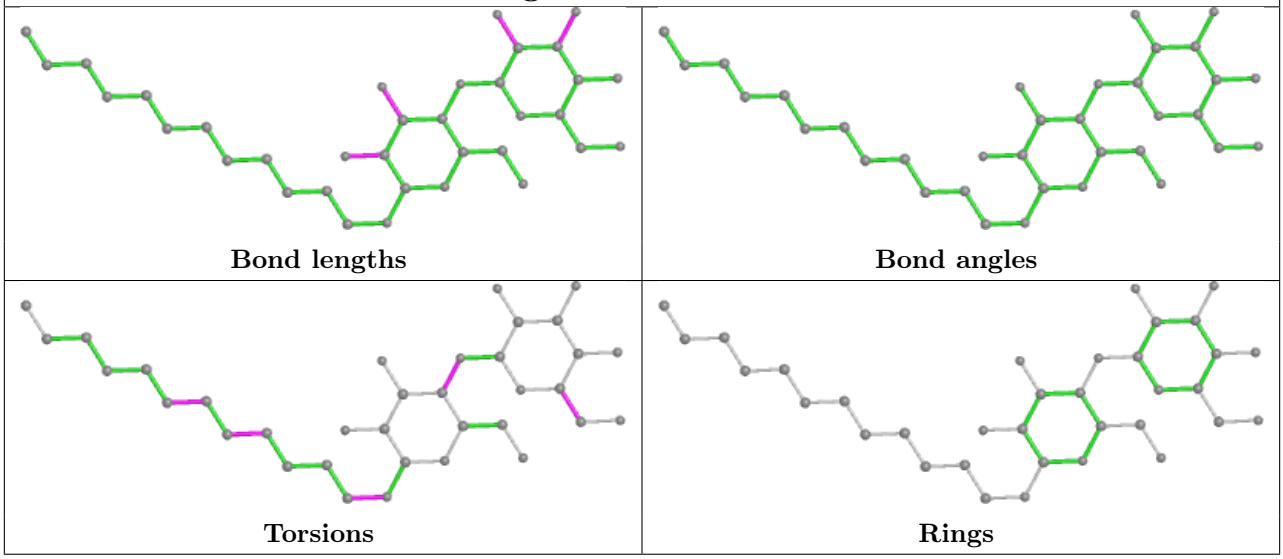
Ligand LMT K 201



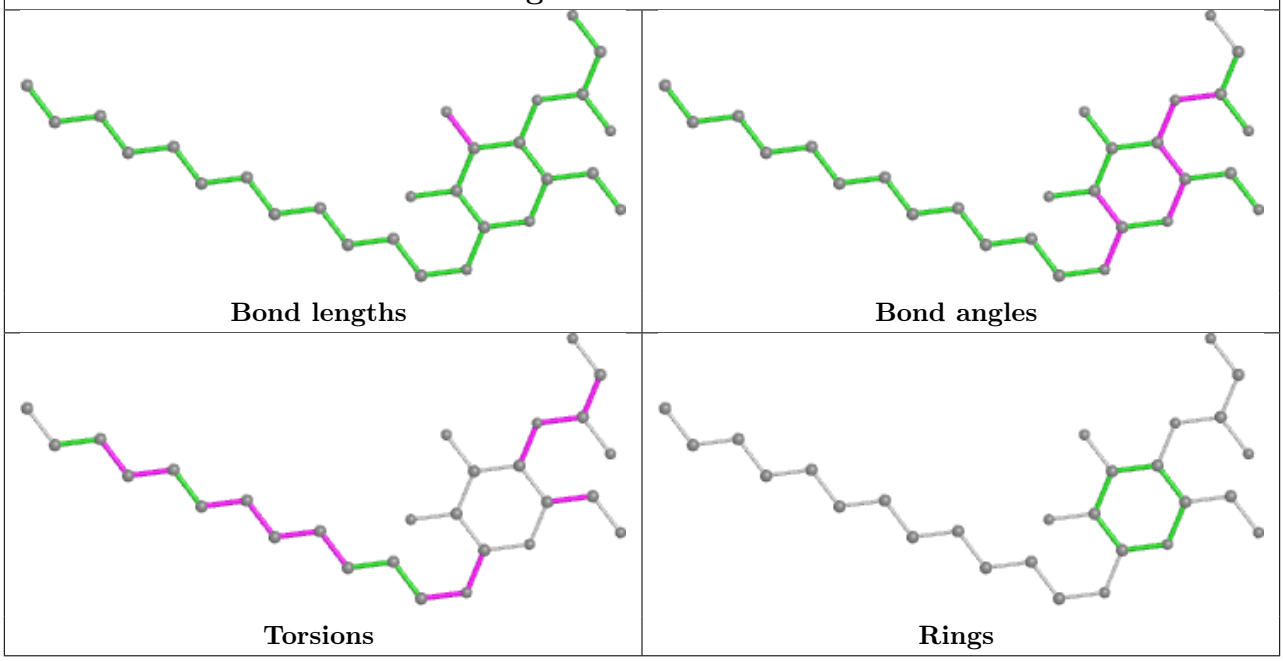
Ligand LMT H 203



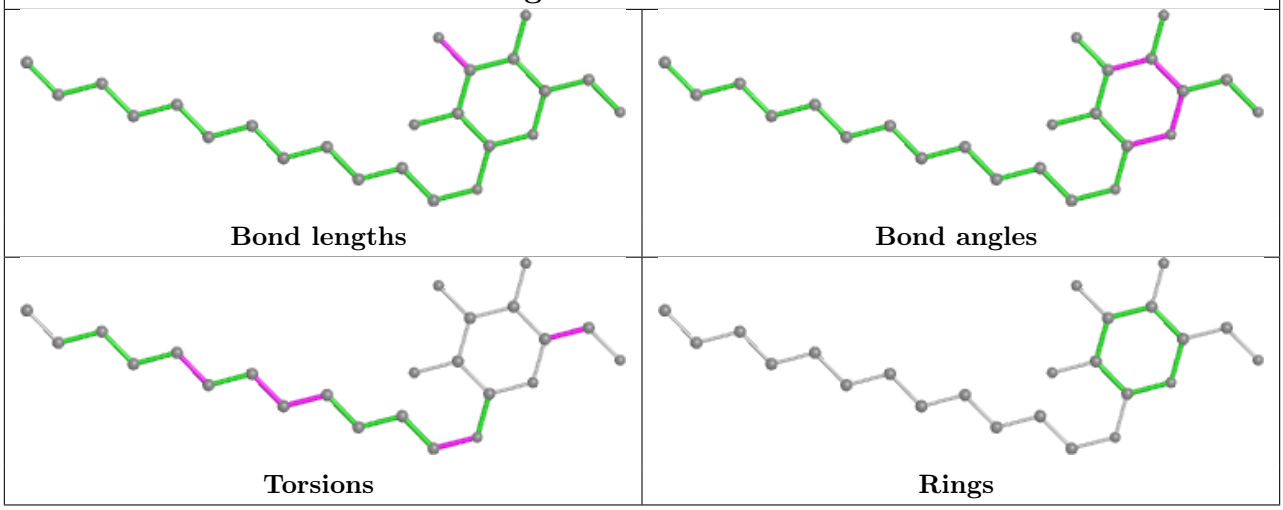
Ligand LMT C 201



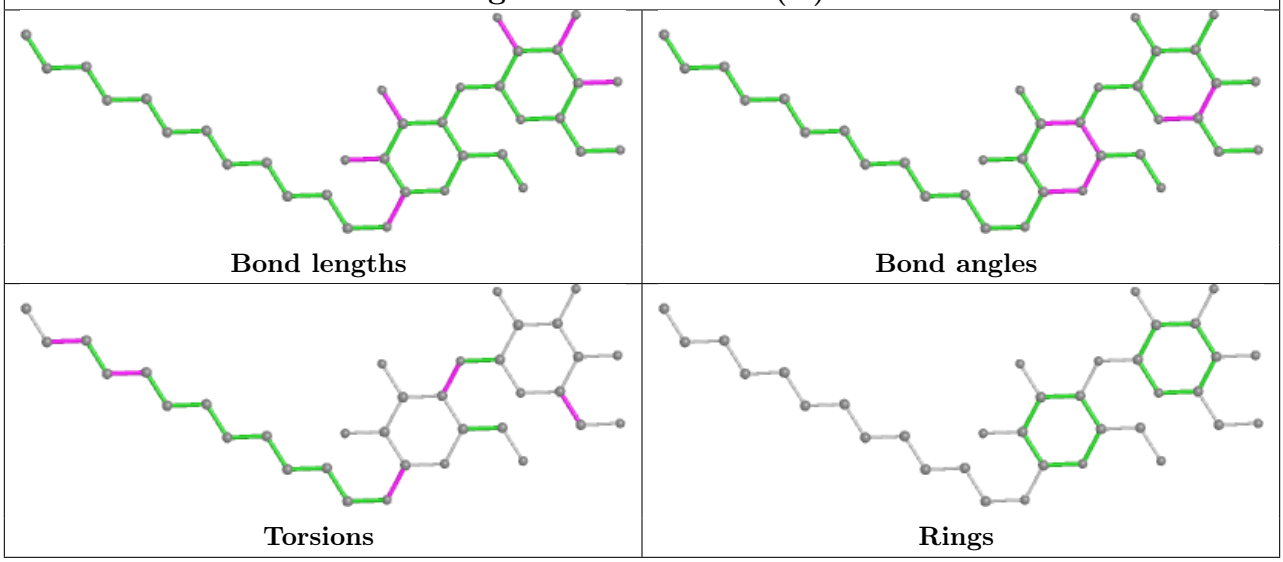
Ligand LMT J 203



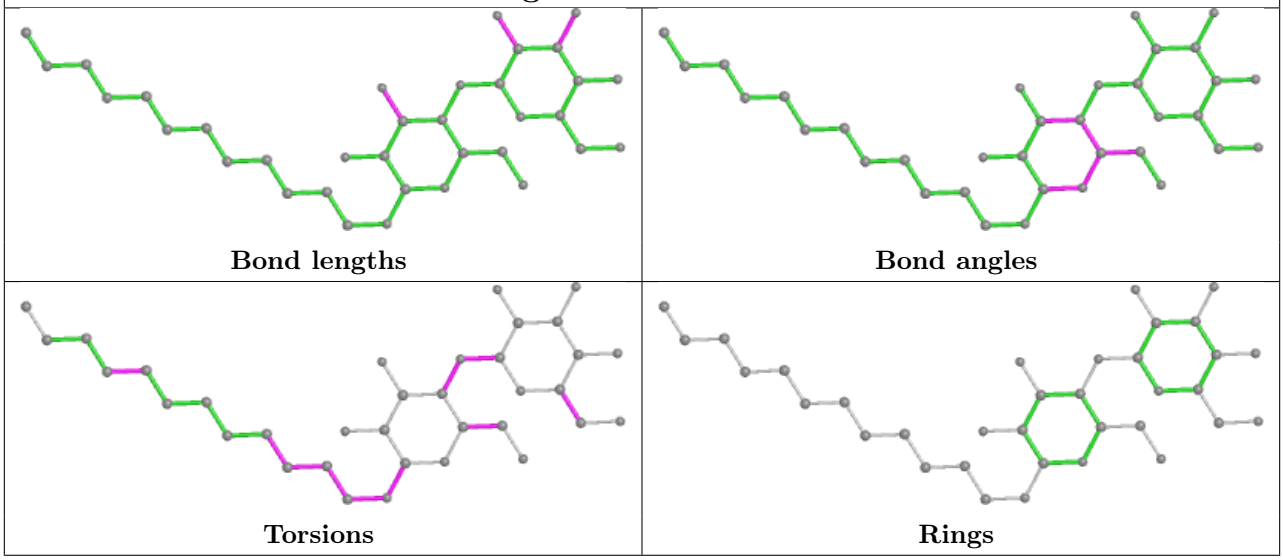
Ligand LMT L 201



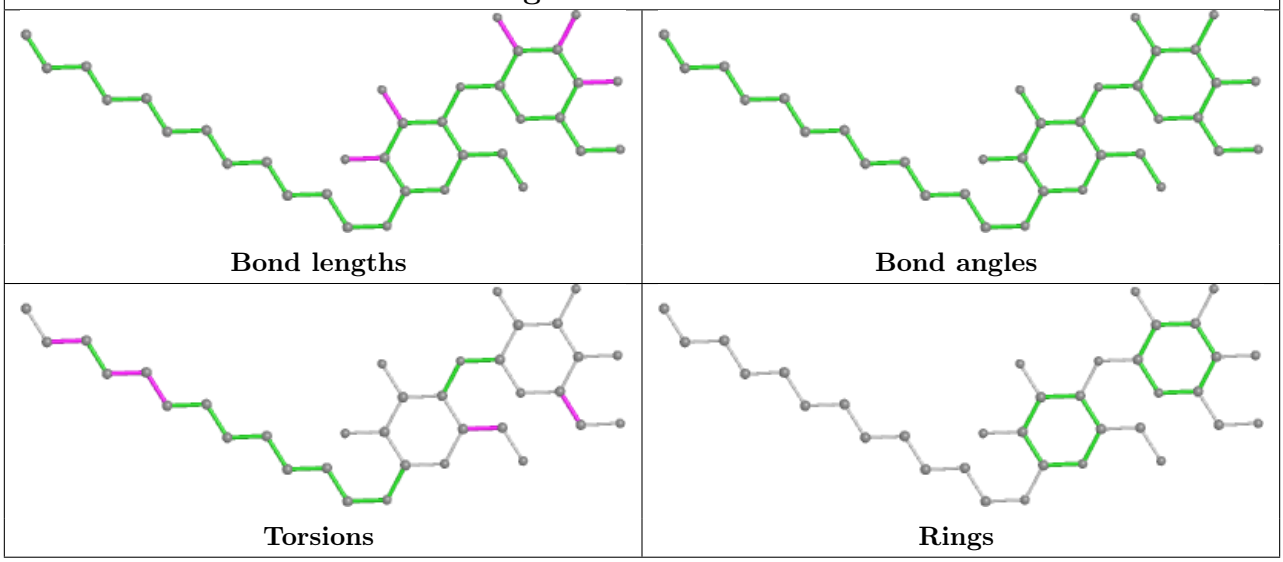
Ligand LMT G 506 (B)



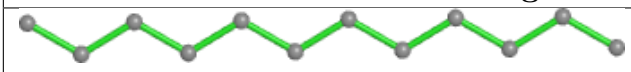
Ligand LMT C 207



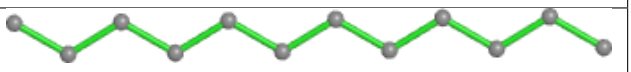
Ligand LMT E 201



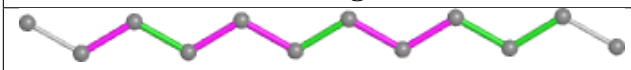
Ligand LMT B 202



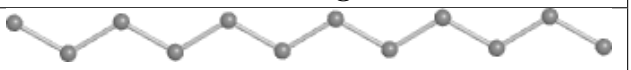
Bond lengths



Bond angles

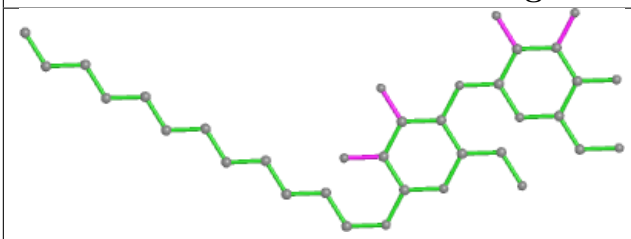


Torsions

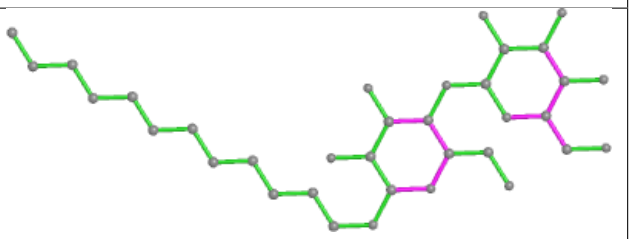


Rings

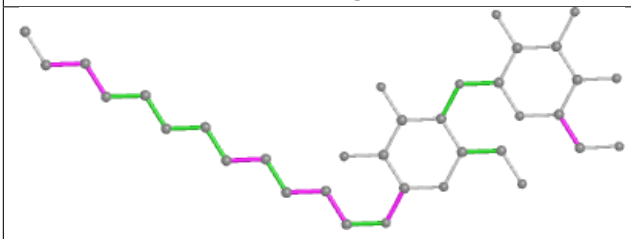
Ligand LMT J 202



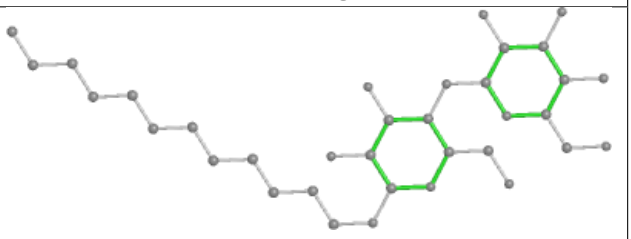
Bond lengths



Bond angles

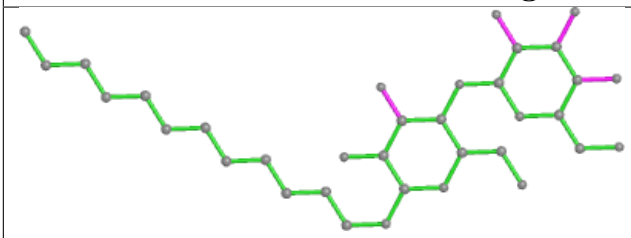


Torsions

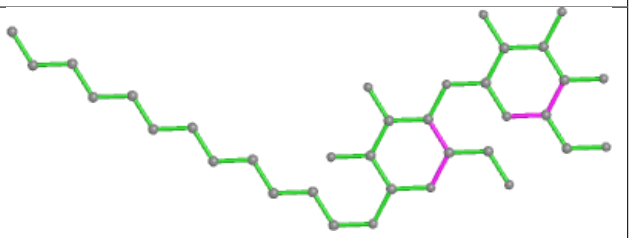


Rings

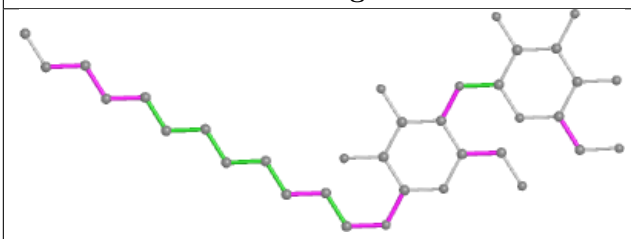
Ligand LMT K 202



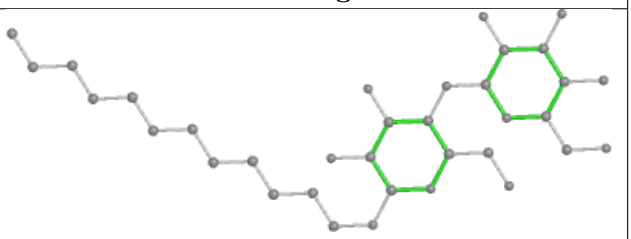
Bond lengths



Bond angles

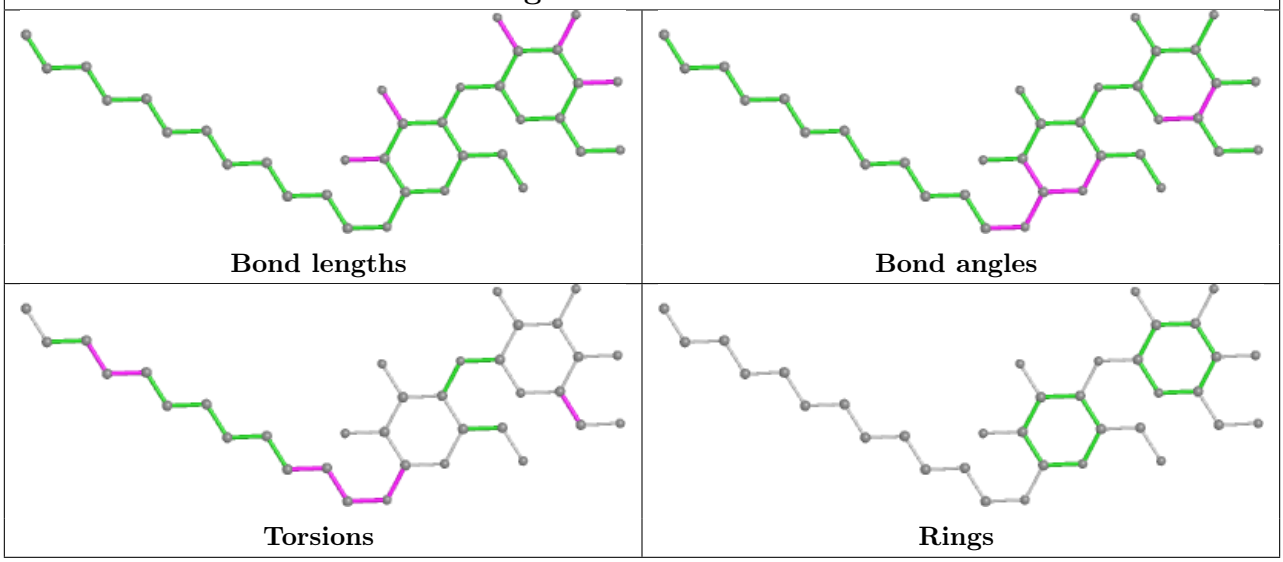


Torsions

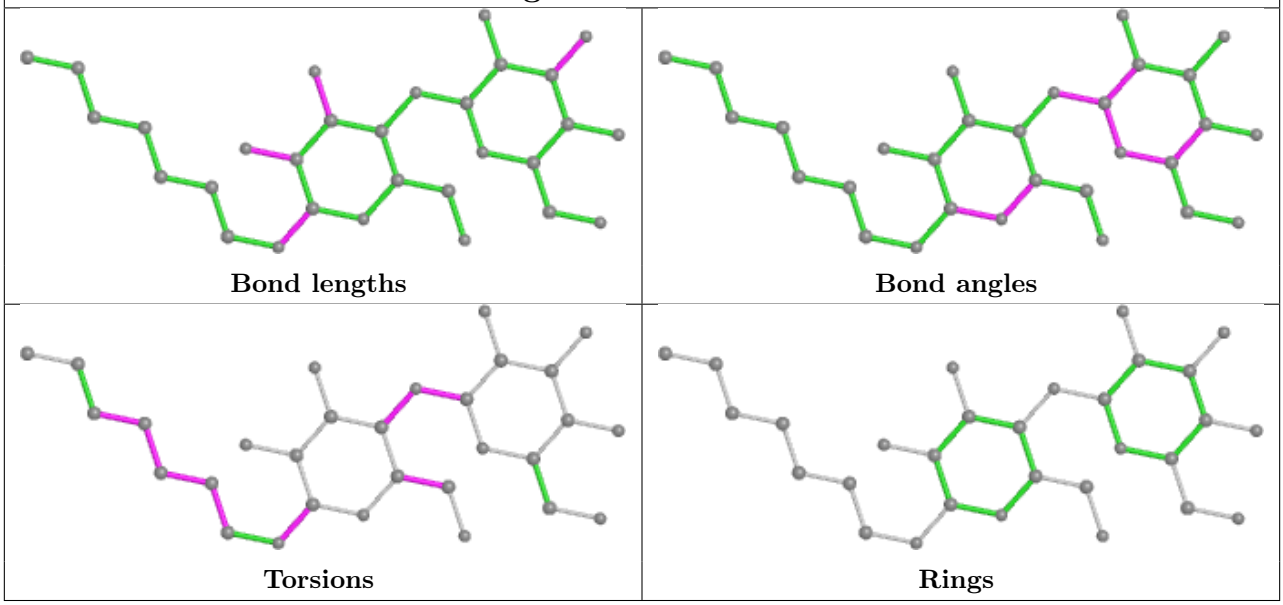


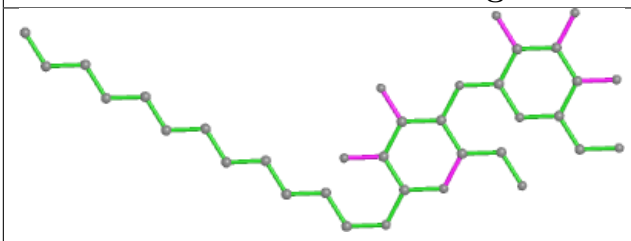
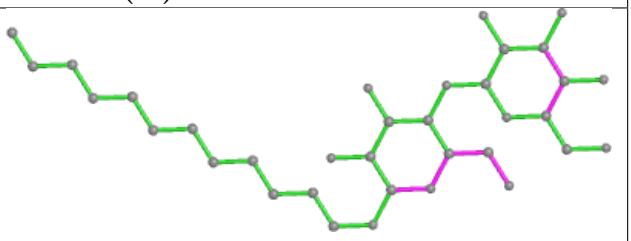
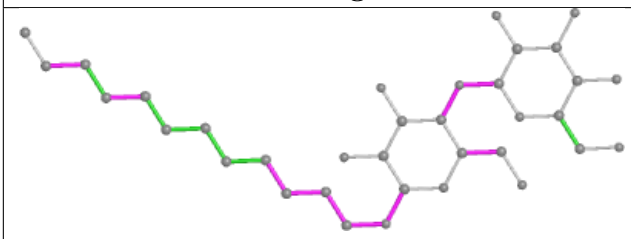
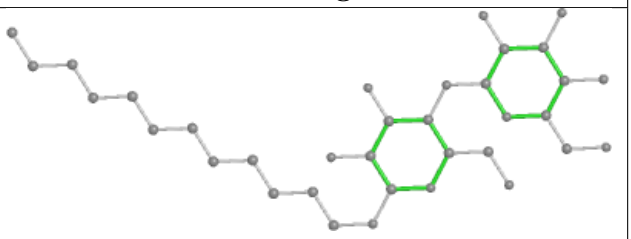
Rings

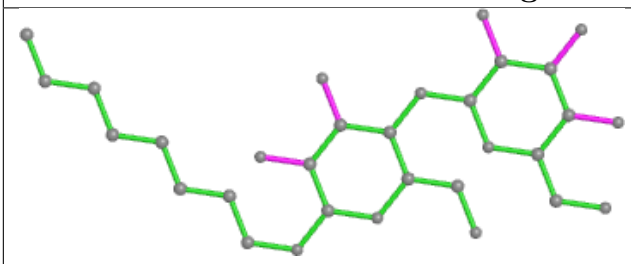
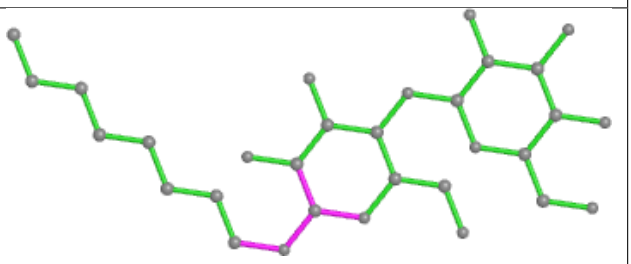
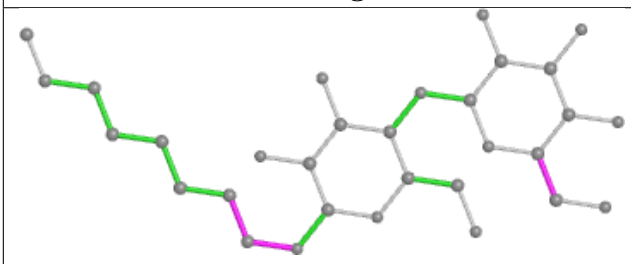
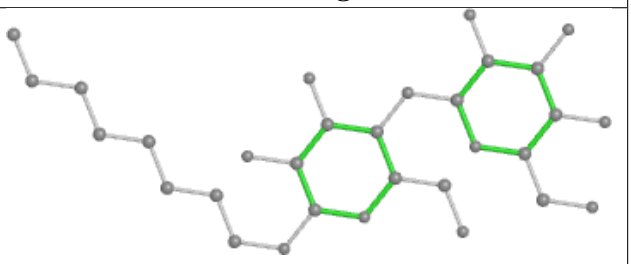
Ligand LMT F 201



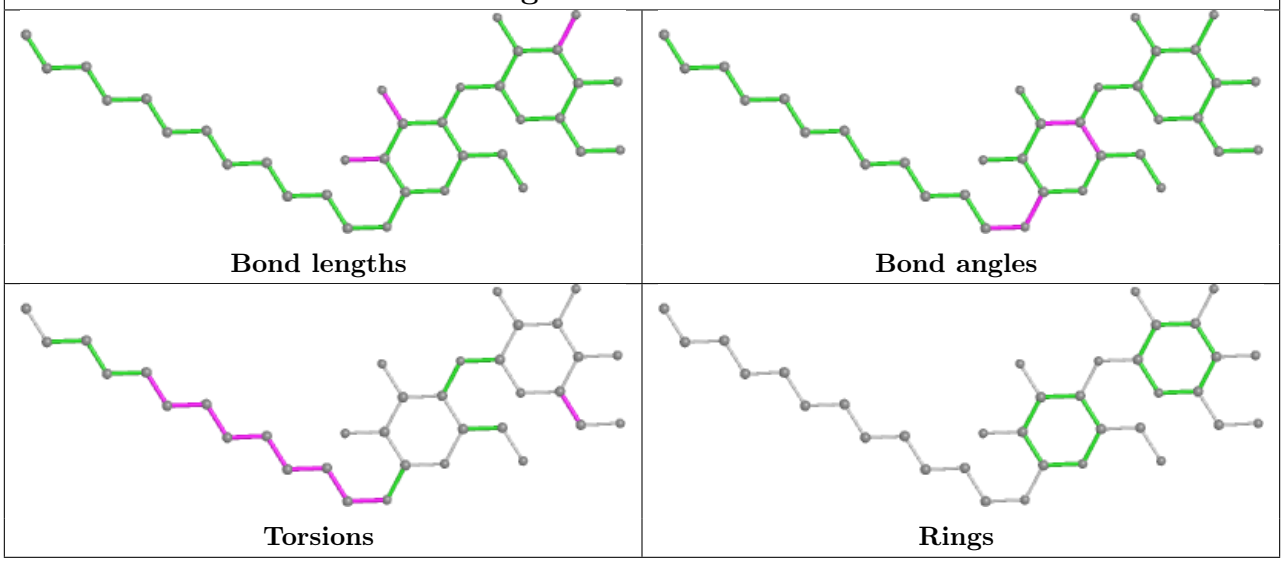
Ligand LMT E 202



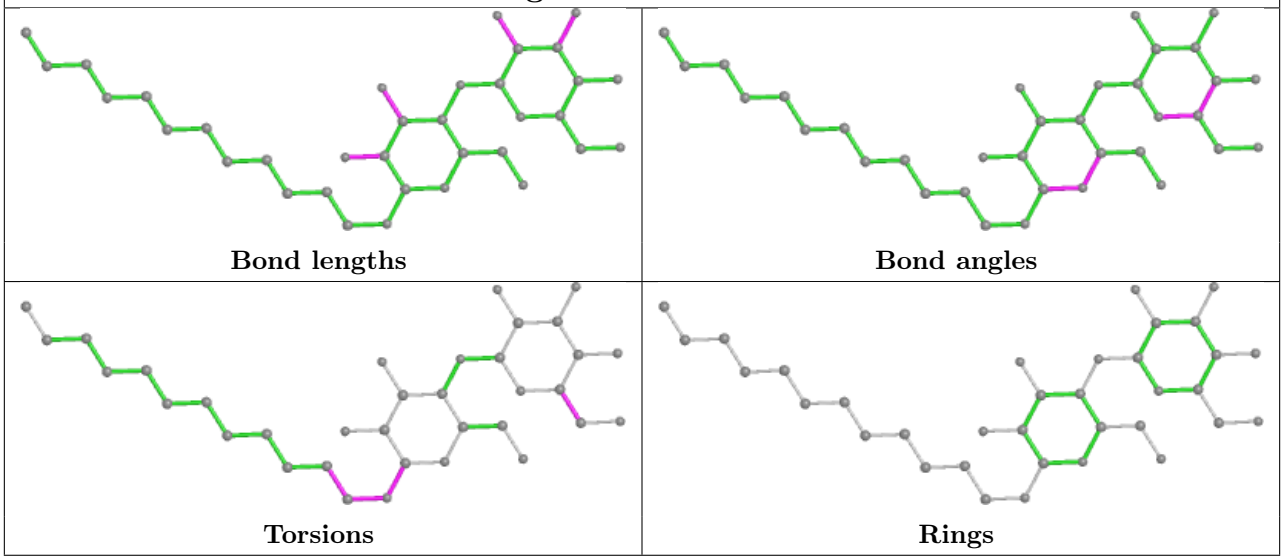
Ligand LMT G 506 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT H 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

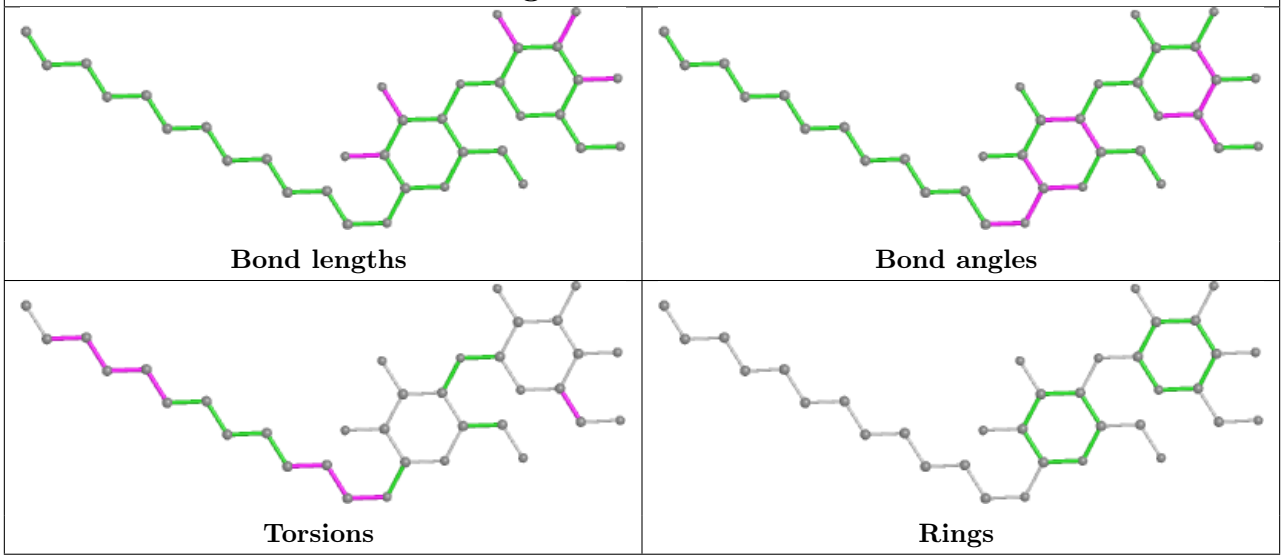
Ligand LMT G 507



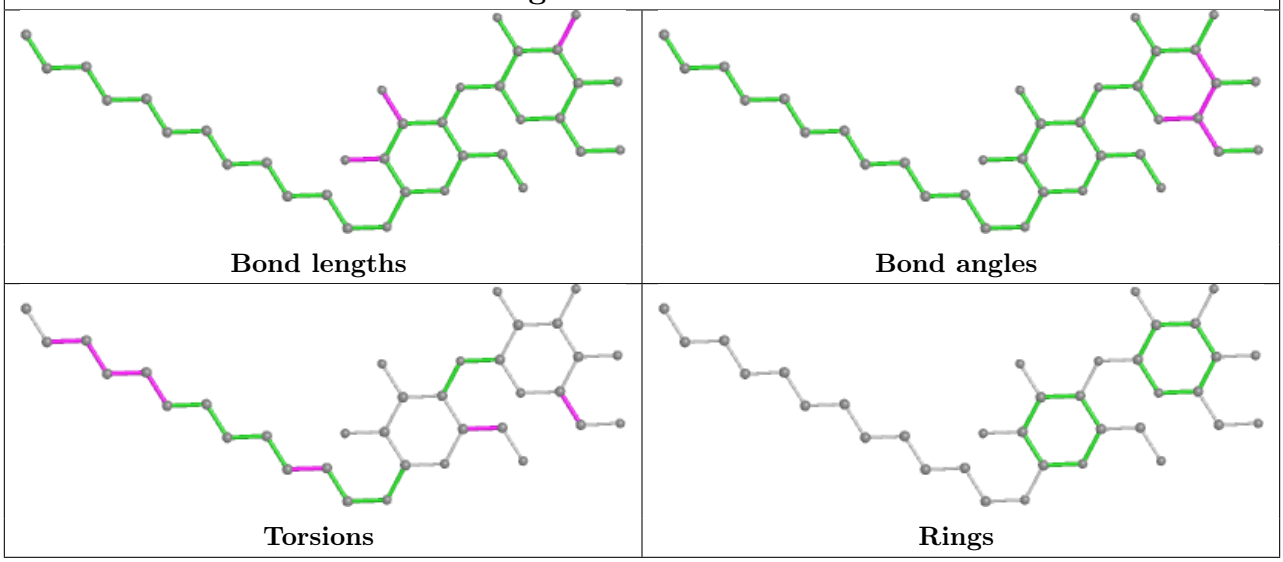
Ligand LMT J 201



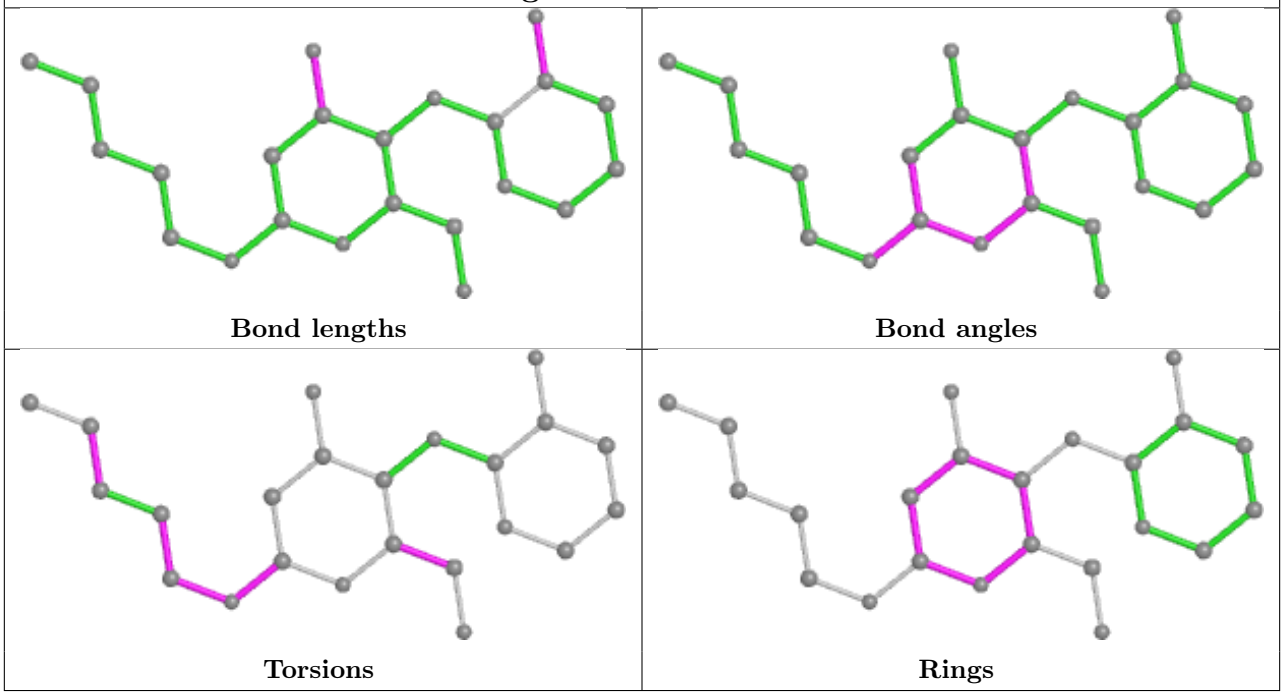
Ligand LMT C 208



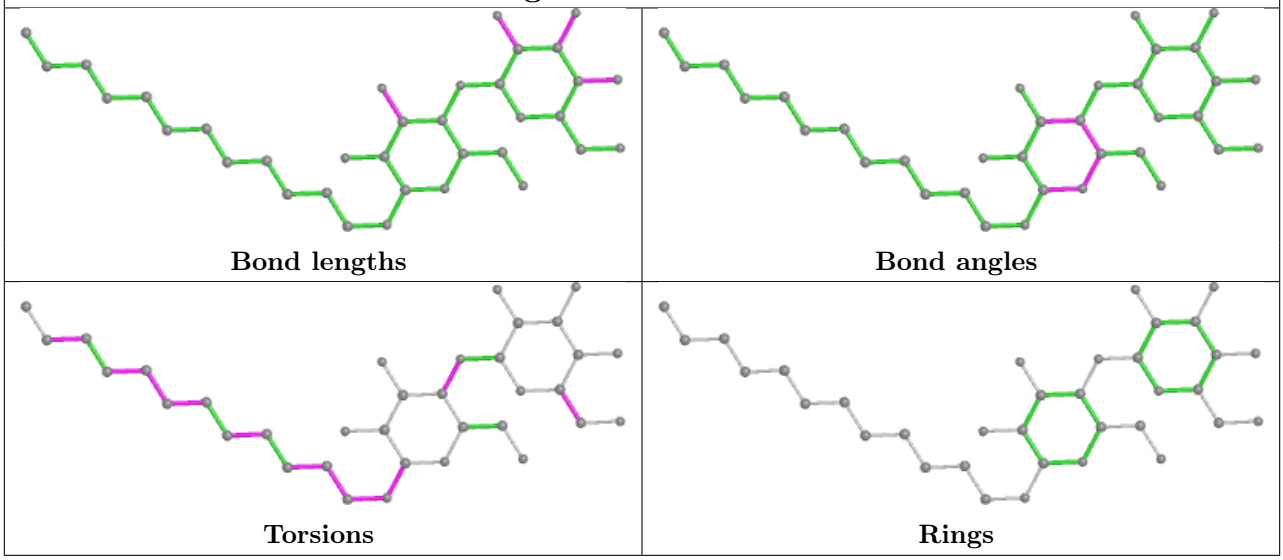
Ligand LMT I 205



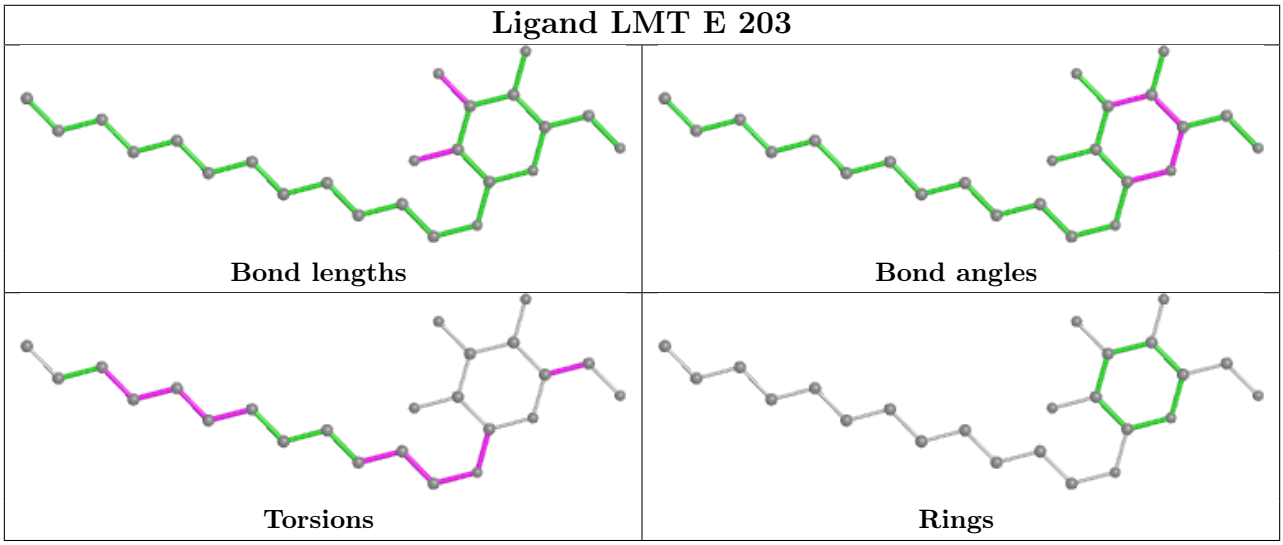
Ligand LMT A 202



Ligand LMT F 202



Ligand LMT E 203



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.