Full wwPDB EM Validation Report

Aug 26, 2021 – 12:36 pm BST

PDB ID	:	7OO0
EMDB ID	:	EMD-13003
Title	:	Mechanosensitive channel MscS solubilized with DDM in open conformation
Authors	:	Rasmussen, T.; Flegler, V.J.; Boettcher, B.
Deposited on	:	2021-05-26
Resolution	:	3.10 Å(reported)
Based on initial model	:	5AJI

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

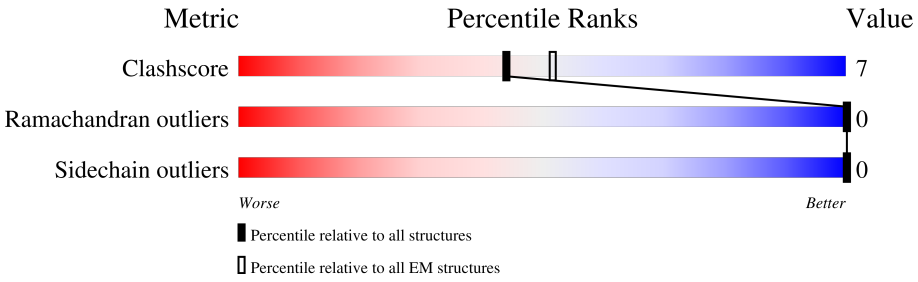
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	294	78% 11% 11%
1	B	294	78% 11% 11%
1	C	294	78% 11% 11%
1	D	294	79% 10% 11%
1	E	294	79% 10% 11%
1	F	294	79% 11% 11%
1	G	294	78% 11% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16016 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Mechanosensitive channel MscS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	262	Total	C	N	O	S	0	0
			1996	1281	349	360	6		
1	B	262	Total	C	N	O	S	0	0
			1996	1281	349	360	6		
1	C	262	Total	C	N	O	S	0	0
			1996	1281	349	360	6		
1	D	262	Total	C	N	O	S	0	0
			1996	1281	349	360	6		
1	E	262	Total	C	N	O	S	0	0
			1996	1281	349	360	6		
1	F	262	Total	C	N	O	S	0	0
			1996	1281	349	360	6		
1	G	262	Total	C	N	O	S	0	0
			1996	1281	349	360	6		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	LEU	-	expression tag	UNP I4SQ31
A	288	GLU	-	expression tag	UNP I4SQ31
A	289	HIS	-	expression tag	UNP I4SQ31
A	290	HIS	-	expression tag	UNP I4SQ31
A	291	HIS	-	expression tag	UNP I4SQ31
A	292	HIS	-	expression tag	UNP I4SQ31
A	293	HIS	-	expression tag	UNP I4SQ31
A	294	HIS	-	expression tag	UNP I4SQ31
B	287	LEU	-	expression tag	UNP I4SQ31
B	288	GLU	-	expression tag	UNP I4SQ31
B	289	HIS	-	expression tag	UNP I4SQ31
B	290	HIS	-	expression tag	UNP I4SQ31
B	291	HIS	-	expression tag	UNP I4SQ31
B	292	HIS	-	expression tag	UNP I4SQ31
B	293	HIS	-	expression tag	UNP I4SQ31
B	294	HIS	-	expression tag	UNP I4SQ31

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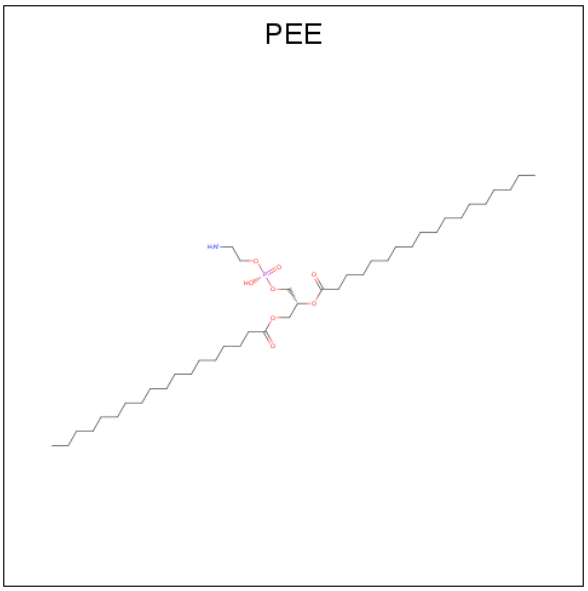
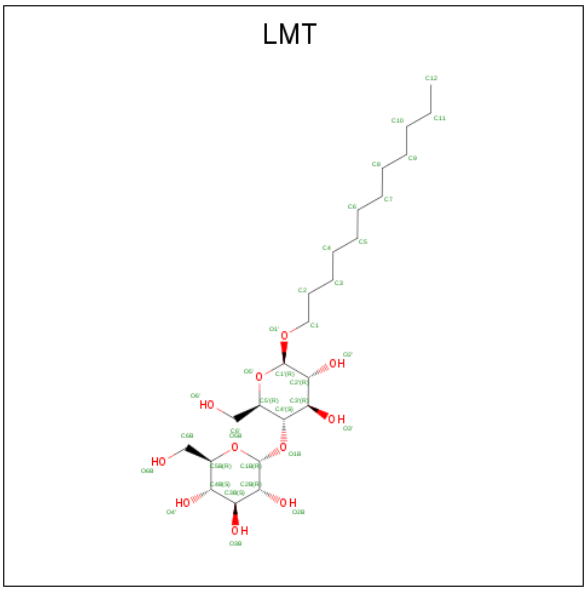
Chain	Residue	Modelled	Actual	Comment	Reference
C	287	LEU	-	expression tag	UNP I4SQ31
C	288	GLU	-	expression tag	UNP I4SQ31
C	289	HIS	-	expression tag	UNP I4SQ31
C	290	HIS	-	expression tag	UNP I4SQ31
C	291	HIS	-	expression tag	UNP I4SQ31
C	292	HIS	-	expression tag	UNP I4SQ31
C	293	HIS	-	expression tag	UNP I4SQ31
C	294	HIS	-	expression tag	UNP I4SQ31
D	287	LEU	-	expression tag	UNP I4SQ31
D	288	GLU	-	expression tag	UNP I4SQ31
D	289	HIS	-	expression tag	UNP I4SQ31
D	290	HIS	-	expression tag	UNP I4SQ31
D	291	HIS	-	expression tag	UNP I4SQ31
D	292	HIS	-	expression tag	UNP I4SQ31
D	293	HIS	-	expression tag	UNP I4SQ31
D	294	HIS	-	expression tag	UNP I4SQ31
E	287	LEU	-	expression tag	UNP I4SQ31
E	288	GLU	-	expression tag	UNP I4SQ31
E	289	HIS	-	expression tag	UNP I4SQ31
E	290	HIS	-	expression tag	UNP I4SQ31
E	291	HIS	-	expression tag	UNP I4SQ31
E	292	HIS	-	expression tag	UNP I4SQ31
E	293	HIS	-	expression tag	UNP I4SQ31
E	294	HIS	-	expression tag	UNP I4SQ31
F	287	LEU	-	expression tag	UNP I4SQ31
F	288	GLU	-	expression tag	UNP I4SQ31
F	289	HIS	-	expression tag	UNP I4SQ31
F	290	HIS	-	expression tag	UNP I4SQ31
F	291	HIS	-	expression tag	UNP I4SQ31
F	292	HIS	-	expression tag	UNP I4SQ31
F	293	HIS	-	expression tag	UNP I4SQ31
F	294	HIS	-	expression tag	UNP I4SQ31
G	287	LEU	-	expression tag	UNP I4SQ31
G	288	GLU	-	expression tag	UNP I4SQ31
G	289	HIS	-	expression tag	UNP I4SQ31
G	290	HIS	-	expression tag	UNP I4SQ31
G	291	HIS	-	expression tag	UNP I4SQ31
G	292	HIS	-	expression tag	UNP I4SQ31
G	293	HIS	-	expression tag	UNP I4SQ31
G	294	HIS	-	expression tag	UNP I4SQ31

- Molecule 2 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	B	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	D	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	E	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	F	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	G	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			245	168	77	
3	A	1	Total	C	O	0
			245	168	77	
3	A	1	Total	C	O	0
			245	168	77	
3	A	1	Total	C	O	0
			245	168	77	
3	A	1	Total	C	O	0
			245	168	77	
3	A	1	Total	C	O	0
			245	168	77	
3	A	1	Total	C	O	0
			245	168	77	
3	B	1	Total	C	O	0
			245	168	77	
3	B	1	Total	C	O	0
			245	168	77	
3	B	1	Total	C	O	0
			245	168	77	
3	B	1	Total	C	O	0
			245	168	77	
3	B	1	Total	C	O	0
			245	168	77	
3	B	1	Total	C	O	0
			245	168	77	
3	B	1	Total	C	O	0
			245	168	77	

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Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total	C	O	0
			245	168	77	
3	C	1	Total	C	O	0
			245	168	77	
3	C	1	Total	C	O	0
			245	168	77	
3	C	1	Total	C	O	0
			245	168	77	
3	C	1	Total	C	O	0
			245	168	77	
3	C	1	Total	C	O	0
			245	168	77	
3	C	1	Total	C	O	0
			245	168	77	
3	D	1	Total	C	O	0
			245	168	77	
3	D	1	Total	C	O	0
			245	168	77	
3	D	1	Total	C	O	0
			245	168	77	
3	D	1	Total	C	O	0
			245	168	77	
3	D	1	Total	C	O	0
			245	168	77	
3	D	1	Total	C	O	0
			245	168	77	
3	D	1	Total	C	O	0
			245	168	77	
3	E	1	Total	C	O	0
			245	168	77	
3	E	1	Total	C	O	0
			245	168	77	
3	E	1	Total	C	O	0
			245	168	77	
3	E	1	Total	C	O	0
			245	168	77	
3	E	1	Total	C	O	0
			245	168	77	
3	E	1	Total	C	O	0
			245	168	77	
3	E	1	Total	C	O	0
			245	168	77	

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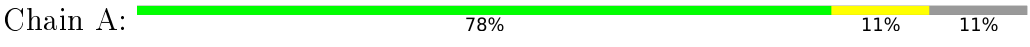
Mol	Chain	Residues	Atoms			AltConf
3	F	1	Total 210	C 144	O 66	0
3	F	1	Total 210	C 144	O 66	0
3	F	1	Total 210	C 144	O 66	0
3	F	1	Total 210	C 144	O 66	0
3	F	1	Total 210	C 144	O 66	0
3	F	1	Total 210	C 144	O 66	0
3	G	1	Total 280	C 192	O 88	0
3	G	1	Total 280	C 192	O 88	0
3	G	1	Total 280	C 192	O 88	0
3	G	1	Total 280	C 192	O 88	0
3	G	1	Total 280	C 192	O 88	0
3	G	1	Total 280	C 192	O 88	0
3	G	1	Total 280	C 192	O 88	0
3	G	1	Total 280	C 192	O 88	0

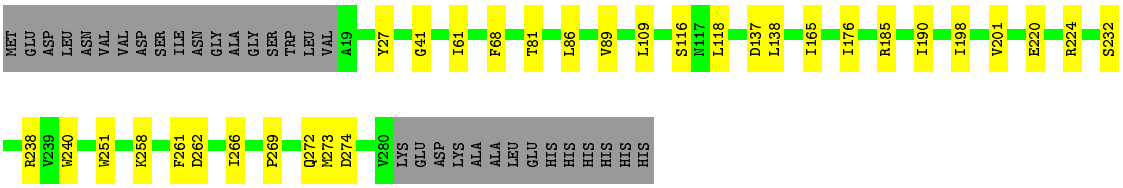
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Mechanosensitive channel MscS

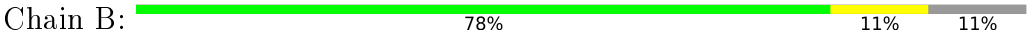
Chain A:

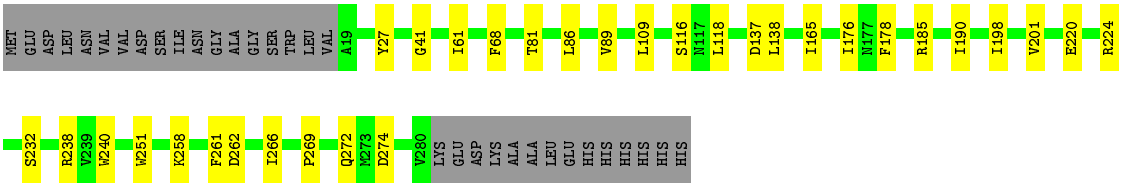




- Molecule 1: Mechanosensitive channel MscS

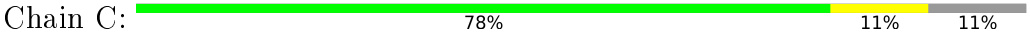
Chain B:

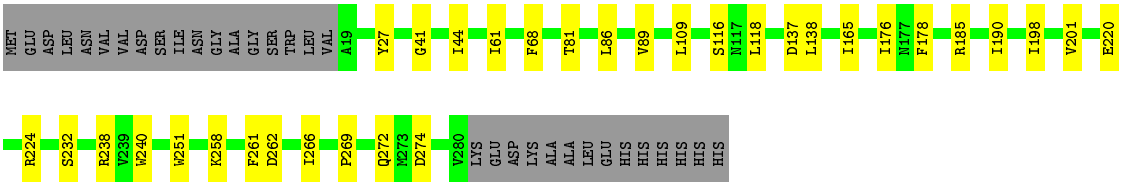




- Molecule 1: Mechanosensitive channel MscS

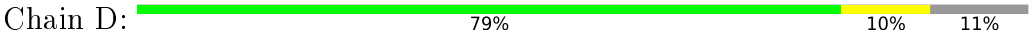
Chain C:

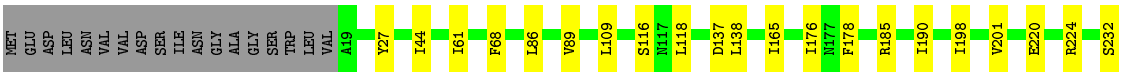


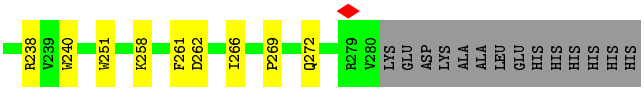


- Molecule 1: Mechanosensitive channel MscS

Chain D:

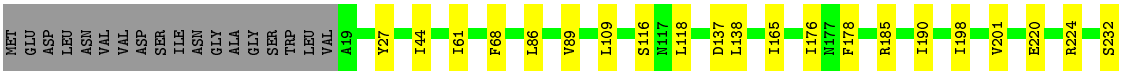


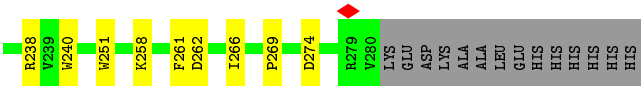




• Molecule 1: Mechanosensitive channel MscS

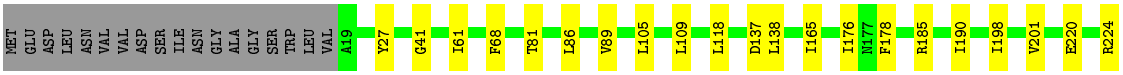
Chain E:





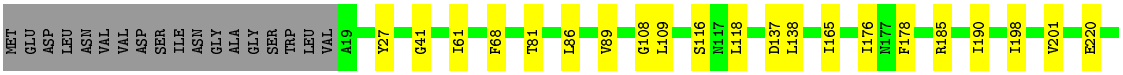
• Molecule 1: Mechanosensitive channel MscS

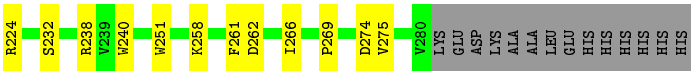
Chain F:



• Molecule 1: Mechanosensitive channel MscS

Chain G:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	841492	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.425	Depositor
Minimum map value	-0.259	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	272.256, 272.256, 272.256	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, 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	0.38	0/2021	0.54	0/2741
1	B	0.38	0/2021	0.53	0/2741
1	C	0.38	0/2021	0.54	0/2741
1	D	0.38	0/2021	0.53	0/2741
1	E	0.38	0/2021	0.53	0/2741
1	F	0.38	0/2021	0.53	0/2741
1	G	0.38	0/2021	0.53	0/2741
All	All	0.38	0/14147	0.53	0/19187

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1996	0	2094	24	0
1	B	1996	0	2094	26	0
1	C	1996	0	2094	26	0
1	D	1996	0	2094	25	0
1	E	1996	0	2094	27	0
1	F	1996	0	2094	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1996	0	2094	26	0
2	A	47	0	71	4	0
2	B	47	0	71	4	0
2	C	47	0	71	4	0
2	D	47	0	71	5	0
2	E	47	0	71	5	0
2	F	47	0	71	4	0
2	G	47	0	71	4	0
3	A	245	0	322	16	0
3	B	245	0	322	19	0
3	C	245	0	322	20	0
3	D	245	0	322	22	0
3	E	245	0	322	24	0
3	F	210	0	276	17	0
3	G	280	0	368	24	0
All	All	16016	0	17409	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (229) 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)
3:D:308:LMT:H6'2	3:E:308:LMT:H2B	1.77	0.67
3:B:308:LMT:H6'2	3:C:308:LMT:H2B	1.75	0.67
1:B:27:TYR:HH	3:B:305:LMT:H2O1	1.43	0.67
3:C:307:LMT:H42	1:D:109:LEU:HD11	1.77	0.67
1:G:109:LEU:HD11	3:G:405:LMT:H42	1.77	0.67
3:D:307:LMT:H42	1:E:109:LEU:HD11	1.77	0.66
3:E:307:LMT:H42	1:F:109:LEU:HD11	1.77	0.66
1:A:109:LEU:HD11	3:G:401:LMT:H42	1.77	0.66
3:B:307:LMT:H42	1:C:109:LEU:HD11	1.77	0.66
3:A:306:LMT:H42	1:B:109:LEU:HD11	1.77	0.66
1:B:198:ILE:HD11	1:C:258:LYS:HG2	1.78	0.65
1:A:272:GLN:NE2	1:G:274:ASP:OD2	2.28	0.65
1:F:258:LYS:NZ	1:F:262:ASP:OD2	2.31	0.64
1:A:258:LYS:NZ	1:A:262:ASP:OD2	2.31	0.63
1:C:258:LYS:NZ	1:C:262:ASP:OD2	2.30	0.62
1:D:27:TYR:HH	3:D:305:LMT:H2O1	1.47	0.62
1:E:258:LYS:NZ	1:E:262:ASP:OD2	2.31	0.62
1:D:258:LYS:NZ	1:D:262:ASP:OD2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:306:LMT:H62	1:F:118:LEU:HD22	1.82	0.62
1:B:258:LYS:NZ	1:B:262:ASP:OD2	2.31	0.61
3:F:307:LMT:H6'2	3:G:402:LMT:H2B	1.82	0.61
3:D:306:LMT:H62	1:E:118:LEU:HD22	1.81	0.61
3:E:308:LMT:H82	3:F:307:LMT:H122	1.83	0.61
1:G:27:TYR:HH	3:G:408:LMT:H2O1	1.49	0.60
1:G:258:LYS:NZ	1:G:262:ASP:OD2	2.31	0.60
3:D:306:LMT:H81	1:E:68:PHE:HD1	1.67	0.60
1:E:198:ILE:HD11	1:F:258:LYS:HG2	1.83	0.59
3:C:308:LMT:H6'2	3:D:308:LMT:H2B	1.83	0.58
3:A:307:LMT:H2B	3:G:402:LMT:H6'2	1.86	0.58
1:F:224:ARG:HG3	1:G:251:TRP:CE3	2.38	0.58
1:G:116:SER:HB2	3:G:401:LMT:H6'1	1.86	0.58
1:E:232:SER:HB3	1:E:269:PRO:HG3	1.88	0.56
3:E:308:LMT:H6'2	3:F:307:LMT:H2B	1.87	0.56
1:F:27:TYR:OH	3:F:305:LMT:O2B	2.24	0.56
1:G:232:SER:HB3	1:G:269:PRO:HG3	1.88	0.56
1:A:232:SER:HB3	1:A:269:PRO:HG3	1.88	0.56
1:A:258:LYS:HG2	1:G:198:ILE:HD11	1.87	0.56
3:E:306:LMT:H81	1:F:68:PHE:HD1	1.71	0.55
1:F:232:SER:HB3	1:F:269:PRO:HG3	1.88	0.55
1:D:198:ILE:HD11	1:E:258:LYS:HG2	1.87	0.55
2:C:302:PEE:H14	3:D:301:LMT:H1B	1.88	0.55
2:D:302:PEE:H14	3:E:301:LMT:H1B	1.88	0.55
1:C:198:ILE:HD11	1:D:258:LYS:HG2	1.87	0.55
2:E:302:PEE:H14	3:F:301:LMT:H1B	1.88	0.55
2:B:302:PEE:H14	3:C:301:LMT:H1B	1.88	0.55
1:B:232:SER:HB3	1:B:269:PRO:HG3	1.88	0.55
1:D:232:SER:HB3	1:D:269:PRO:HG3	1.88	0.54
3:F:306:LMT:H62	1:G:118:LEU:HD22	1.90	0.54
1:F:86:LEU:HD21	3:F:305:LMT:H111	1.89	0.54
1:A:27:TYR:OH	3:A:304:LMT:O2B	2.24	0.54
1:E:86:LEU:HD21	3:E:305:LMT:H111	1.89	0.54
2:F:302:PEE:H14	3:G:403:LMT:H1B	1.88	0.54
3:A:308:LMT:H1B	2:G:404:PEE:H14	1.88	0.54
1:C:232:SER:HB3	1:C:269:PRO:HG3	1.88	0.54
1:D:86:LEU:HD21	3:D:305:LMT:H111	1.89	0.54
1:A:86:LEU:HD21	3:A:304:LMT:H111	1.89	0.54
1:B:116:SER:HB2	3:B:307:LMT:H6'1	1.89	0.54
1:B:274:ASP:OD2	1:C:272:GLN:NE2	2.41	0.53
1:F:27:TYR:HH	3:F:305:LMT:H2O1	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:LEU:HD21	3:G:408:LMT:H111	1.89	0.53
2:A:301:PEE:H14	3:B:301:LMT:H1B	1.88	0.53
1:B:86:LEU:HD21	3:B:305:LMT:H111	1.89	0.53
1:D:86:LEU:HA	1:D:89:VAL:HG22	1.90	0.53
1:B:86:LEU:HA	1:B:89:VAL:HG22	1.90	0.53
1:B:185:ARG:HD2	1:B:238:ARG:HB3	1.91	0.53
1:C:86:LEU:HA	1:C:89:VAL:HG22	1.90	0.53
1:C:274:ASP:OD2	1:D:272:GLN:NE2	2.41	0.53
1:A:86:LEU:HA	1:A:89:VAL:HG22	1.90	0.53
1:C:86:LEU:HD21	3:C:305:LMT:H111	1.89	0.53
1:C:185:ARG:HD2	1:C:238:ARG:HB3	1.91	0.53
1:E:86:LEU:HA	1:E:89:VAL:HG22	1.91	0.53
3:B:308:LMT:H3O2	3:C:308:LMT:H2O1	1.48	0.53
1:D:27:TYR:OH	3:D:305:LMT:O2B	2.24	0.53
3:A:307:LMT:H6'2	3:B:308:LMT:H2B	1.91	0.52
1:F:198:ILE:HD11	1:G:258:LYS:HG2	1.90	0.52
3:F:306:LMT:H81	1:G:68:PHE:HD1	1.73	0.52
1:A:185:ARG:HD2	1:A:238:ARG:HB3	1.91	0.52
3:A:307:LMT:H122	3:G:402:LMT:H82	1.92	0.52
1:E:185:ARG:HD2	1:E:238:ARG:HB3	1.91	0.52
1:E:274:ASP:OD2	1:F:272:GLN:NE2	2.43	0.52
1:F:86:LEU:HA	1:F:89:VAL:HG22	1.90	0.52
1:G:86:LEU:HA	1:G:89:VAL:HG22	1.90	0.52
1:D:185:ARG:HD2	1:D:238:ARG:HB3	1.91	0.52
1:G:27:TYR:OH	3:G:408:LMT:O2B	2.24	0.52
3:B:306:LMT:H81	1:C:68:PHE:HD1	1.75	0.52
1:E:27:TYR:OH	3:E:305:LMT:O2B	2.24	0.52
1:A:198:ILE:HD11	1:B:258:LYS:HG2	1.92	0.51
3:C:308:LMT:H82	3:D:308:LMT:H122	1.91	0.51
1:F:185:ARG:HD2	1:F:238:ARG:HB3	1.91	0.51
1:G:185:ARG:HD2	1:G:238:ARG:HB3	1.91	0.51
3:B:307:LMT:H3'	3:C:307:LMT:O5'	2.10	0.50
2:D:302:PEE:H52	3:E:301:LMT:H12	1.94	0.50
3:E:307:LMT:H3'	3:G:405:LMT:O5'	2.12	0.50
2:E:302:PEE:H52	3:F:301:LMT:H12	1.94	0.49
1:C:224:ARG:HG3	1:D:251:TRP:CE3	2.47	0.49
2:F:302:PEE:H52	3:G:403:LMT:H12	1.94	0.49
2:A:301:PEE:H52	3:B:301:LMT:H12	1.94	0.49
3:A:305:LMT:H62	1:B:118:LEU:HD22	1.93	0.49
2:C:302:PEE:H52	3:D:301:LMT:H12	1.94	0.49
2:B:302:PEE:H18	3:C:301:LMT:H3'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:306:LMT:H62	1:C:118:LEU:HD22	1.94	0.48
2:A:301:PEE:H18	3:B:301:LMT:H3'	1.95	0.48
3:E:308:LMT:O3'	3:F:307:LMT:O2B	2.25	0.48
2:B:302:PEE:H52	3:C:301:LMT:H12	1.94	0.48
2:C:302:PEE:H18	3:D:301:LMT:H3'	1.95	0.48
3:A:308:LMT:H12	2:G:404:PEE:H52	1.94	0.48
1:D:137:ASP:HB3	1:D:176:ILE:HB	1.96	0.48
1:G:138:LEU:HD12	1:G:165:ILE:HD12	1.96	0.48
3:E:308:LMT:H82	3:F:307:LMT:C12	2.44	0.48
1:C:137:ASP:HB3	1:C:176:ILE:HB	1.96	0.48
1:E:224:ARG:HG3	1:F:251:TRP:CE3	2.48	0.48
3:D:307:LMT:H3'	3:E:307:LMT:O5'	2.14	0.47
2:E:302:PEE:H18	3:F:301:LMT:H3'	1.95	0.47
2:F:302:PEE:H18	3:G:403:LMT:H3'	1.95	0.47
3:A:308:LMT:H3'	2:G:404:PEE:H18	1.96	0.47
3:A:306:LMT:H5'	3:A:306:LMT:H1B	1.38	0.47
1:D:138:LEU:HD12	1:D:165:ILE:HD12	1.96	0.47
1:E:137:ASP:HB3	1:E:176:ILE:HB	1.96	0.47
1:A:138:LEU:HD12	1:A:165:ILE:HD12	1.96	0.47
1:C:138:LEU:HD12	1:C:165:ILE:HD12	1.96	0.47
1:F:138:LEU:HD12	1:F:165:ILE:HD12	1.96	0.47
1:G:137:ASP:HB3	1:G:176:ILE:HB	1.96	0.47
2:D:302:PEE:H18	3:E:301:LMT:H3'	1.95	0.47
1:B:137:ASP:HB3	1:B:176:ILE:HB	1.96	0.47
1:B:138:LEU:HD12	1:B:165:ILE:HD12	1.96	0.47
3:D:306:LMT:H12	3:D:306:LMT:H2'	1.56	0.47
3:D:308:LMT:H82	3:E:308:LMT:H122	1.96	0.47
1:E:201:VAL:HG22	1:E:266:ILE:HD13	1.97	0.47
1:A:224:ARG:HG3	1:B:251:TRP:CE3	2.50	0.47
1:E:138:LEU:HD12	1:E:165:ILE:HD12	1.96	0.47
1:F:201:VAL:HG22	1:F:266:ILE:HD13	1.97	0.47
1:E:116:SER:HB2	3:E:307:LMT:H6'1	1.97	0.47
1:F:137:ASP:HB3	1:F:176:ILE:HB	1.96	0.47
1:G:201:VAL:HG22	1:G:266:ILE:HD13	1.97	0.47
1:D:201:VAL:HG22	1:D:266:ILE:HD13	1.97	0.46
3:E:307:LMT:H5'	3:E:307:LMT:H1B	1.38	0.46
1:A:137:ASP:HB3	1:A:176:ILE:HB	1.96	0.46
3:A:305:LMT:H81	1:B:68:PHE:HD1	1.80	0.46
3:G:401:LMT:H5'	3:G:401:LMT:H1B	1.38	0.46
3:G:409:LMT:H2'	3:G:409:LMT:H12	1.56	0.46
1:C:201:VAL:HG22	1:C:266:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HG3	1:C:251:TRP:CE3	2.50	0.46
1:A:251:TRP:CE3	1:G:224:ARG:HG3	2.51	0.45
3:A:305:LMT:H12	3:A:305:LMT:H2'	1.56	0.45
1:A:201:VAL:HG22	1:A:266:ILE:HD13	1.97	0.45
1:B:201:VAL:HG22	1:B:266:ILE:HD13	1.97	0.45
3:B:308:LMT:O3'	3:C:308:LMT:O2B	2.13	0.45
3:C:306:LMT:H62	1:D:118:LEU:HD22	1.98	0.45
1:B:190:ILE:HG21	1:B:261:PHE:HE2	1.82	0.45
1:E:190:ILE:HG21	1:E:261:PHE:HE2	1.82	0.45
3:B:306:LMT:H12	3:B:306:LMT:H2'	1.56	0.45
1:C:190:ILE:HG21	1:C:261:PHE:HE2	1.82	0.44
1:A:118:LEU:HD22	3:G:409:LMT:H62	1.98	0.44
1:A:190:ILE:HG21	1:A:261:PHE:HE2	1.82	0.44
1:B:27:TYR:OH	3:B:305:LMT:O2B	2.24	0.44
1:A:273:MET:O	1:G:275:VAL:HA	2.17	0.44
1:G:190:ILE:HG21	1:G:261:PHE:HE2	1.82	0.44
3:E:306:LMT:H92	3:E:306:LMT:H61	1.84	0.44
3:C:306:LMT:H12	3:C:306:LMT:H2'	1.56	0.44
1:D:116:SER:HB2	3:D:307:LMT:H6'1	2.00	0.44
1:F:190:ILE:HG21	1:F:261:PHE:HE2	1.82	0.44
3:D:306:LMT:H101	1:E:68:PHE:CE1	2.53	0.43
1:E:220:GLU:HG2	1:E:240:TRP:HE1	1.83	0.43
3:A:306:LMT:O5'	3:G:401:LMT:H3'	2.18	0.43
1:B:220:GLU:HG2	1:B:240:TRP:HE1	1.83	0.43
1:D:190:ILE:HG21	1:D:261:PHE:HE2	1.82	0.43
1:D:220:GLU:HG2	1:D:240:TRP:HE1	1.83	0.43
2:E:302:PEE:H28	2:E:302:PEE:H33	1.86	0.43
1:A:220:GLU:HG2	1:A:240:TRP:HE1	1.83	0.43
3:G:409:LMT:H92	3:G:409:LMT:H61	1.84	0.43
3:D:306:LMT:H81	1:E:68:PHE:CD1	2.51	0.43
2:D:302:PEE:H28	2:D:302:PEE:H33	1.86	0.43
1:F:220:GLU:HG2	1:F:240:TRP:HE1	1.83	0.43
1:G:220:GLU:HG2	1:G:240:TRP:HE1	1.83	0.43
3:G:401:LMT:O5'	3:G:405:LMT:H3'	2.18	0.43
1:C:27:TYR:OH	3:C:305:LMT:O2B	2.24	0.43
3:B:308:LMT:H82	3:C:308:LMT:H122	2.00	0.43
3:D:307:LMT:H5'	3:D:307:LMT:H1B	1.38	0.43
3:F:306:LMT:H12	3:F:306:LMT:H2'	1.56	0.42
1:F:105:LEU:HD12	3:G:405:LMT:H52	2.01	0.42
1:A:61:ILE:HD11	2:A:301:PEE:H1	2.01	0.42
1:D:224:ARG:HG3	1:E:251:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:ILE:HD11	2:F:302:PEE:H1	2.01	0.42
3:G:405:LMT:H5'	3:G:405:LMT:H1B	1.38	0.42
1:A:116:SER:HB2	3:A:306:LMT:H6'1	2.00	0.42
1:A:274:ASP:OD2	1:B:272:GLN:NE2	2.52	0.42
1:E:44:ILE:HD13	3:F:304:LMT:H81	2.01	0.42
1:C:220:GLU:HG2	1:C:240:TRP:HE1	1.83	0.42
1:E:61:ILE:HD11	2:E:302:PEE:H1	2.01	0.42
1:G:61:ILE:HD11	2:G:404:PEE:H1	2.01	0.42
3:B:306:LMT:H92	3:B:306:LMT:H61	1.84	0.42
3:E:303:LMT:H91	3:E:303:LMT:H52	2.02	0.42
1:E:27:TYR:HH	3:E:305:LMT:H2O1	1.52	0.42
1:B:61:ILE:HD11	2:B:302:PEE:H1	2.01	0.42
1:D:44:ILE:HD13	3:E:304:LMT:H81	2.02	0.42
1:D:137:ASP:HB2	1:D:178:PHE:HE1	1.85	0.41
3:F:303:LMT:H91	3:F:303:LMT:H52	2.02	0.41
3:B:303:LMT:H91	3:B:303:LMT:H52	2.02	0.41
1:C:61:ILE:HD11	2:C:302:PEE:H1	2.01	0.41
3:C:303:LMT:H91	3:C:303:LMT:H52	2.02	0.41
3:D:303:LMT:H52	3:D:303:LMT:H91	2.02	0.41
1:C:116:SER:HB2	3:C:307:LMT:H6'1	2.03	0.41
1:D:61:ILE:HD11	2:D:302:PEE:H1	2.01	0.41
1:G:41:GLY:HA3	1:G:81:THR:HG21	2.03	0.41
1:G:108:GLY:HA3	3:G:401:LMT:H51	2.03	0.41
3:A:302:LMT:H91	3:A:302:LMT:H52	2.02	0.41
3:C:306:LMT:H81	1:D:68:PHE:HD1	1.86	0.41
1:G:137:ASP:HB2	1:G:178:PHE:HE1	1.85	0.41
1:A:41:GLY:HA3	1:A:81:THR:HG21	2.03	0.41
1:B:137:ASP:HB2	1:B:178:PHE:HE1	1.85	0.41
3:G:406:LMT:H91	3:G:406:LMT:H52	2.02	0.41
1:B:41:GLY:HA3	1:B:81:THR:HG21	2.03	0.41
1:E:137:ASP:HB2	1:E:178:PHE:HE1	1.85	0.41
1:F:137:ASP:HB2	1:F:178:PHE:HE1	1.85	0.41
1:B:220:GLU:HG2	1:B:240:TRP:NE1	2.36	0.40
1:C:44:ILE:HD13	3:D:304:LMT:H81	2.03	0.40
1:C:220:GLU:HG2	1:C:240:TRP:NE1	2.36	0.40
1:C:41:GLY:HA3	1:C:81:THR:HG21	2.03	0.40
1:D:220:GLU:HG2	1:D:240:TRP:NE1	2.36	0.40
3:E:306:LMT:H81	1:F:68:PHE:CD1	2.55	0.40
3:E:306:LMT:H2'	3:E:306:LMT:H12	1.56	0.40
3:F:306:LMT:H61	3:F:306:LMT:H92	1.84	0.40
3:C:307:LMT:H3'	3:D:307:LMT:O5'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:GLU:HG2	1:E:240:TRP:NE1	2.36	0.40
1:C:137:ASP:HB2	1:C:178:PHE:HE1	1.85	0.40
3:C:306:LMT:H92	3:C:306:LMT:H61	1.84	0.40
1:F:41:GLY:HA3	1:F:81:THR:HG21	2.03	0.40
1:A:68:PHE:HD1	3:G:409:LMT:H81	1.86	0.40
1:F:190:ILE:HD12	1:F:190:ILE:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	260/294 (88%)	252 (97%)	8 (3%)	0	100	100
1	B	260/294 (88%)	252 (97%)	8 (3%)	0	100	100
1	C	260/294 (88%)	252 (97%)	8 (3%)	0	100	100
1	D	260/294 (88%)	252 (97%)	8 (3%)	0	100	100
1	E	260/294 (88%)	252 (97%)	8 (3%)	0	100	100
1	F	260/294 (88%)	252 (97%)	8 (3%)	0	100	100
1	G	260/294 (88%)	252 (97%)	8 (3%)	0	100	100
All	All	1820/2058 (88%)	1764 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	212/239 (89%)	212 (100%)	0	100	100
1	B	212/239 (89%)	212 (100%)	0	100	100
1	C	212/239 (89%)	212 (100%)	0	100	100
1	D	212/239 (89%)	212 (100%)	0	100	100
1	E	212/239 (89%)	212 (100%)	0	100	100
1	F	212/239 (89%)	212 (100%)	0	100	100
1	G	212/239 (89%)	212 (100%)	0	100	100
All	All	1484/1673 (89%)	1484 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

56 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LMT	F	304	-	36,36,36	0.09	0	47,47,47	0.37	0
3	LMT	C	304	-	36,36,36	0.09	0	47,47,47	0.37	0
2	PEE	C	302	-	46,46,50	0.27	0	49,51,55	0.26	0
3	LMT	D	301	-	36,36,36	0.11	0	47,47,47	0.37	0
3	LMT	E	306	-	36,36,36	0.10	0	47,47,47	0.21	0
3	LMT	A	306	-	36,36,36	0.09	0	47,47,47	0.22	0
3	LMT	D	307	-	36,36,36	0.09	0	47,47,47	0.22	0
3	LMT	G	402	-	36,36,36	0.10	0	47,47,47	0.35	0
3	LMT	B	303	-	36,36,36	0.09	0	47,47,47	0.18	0
3	LMT	G	401	-	36,36,36	0.09	0	47,47,47	0.22	0
3	LMT	F	303	-	36,36,36	0.08	0	47,47,47	0.18	0
2	PEE	G	404	-	46,46,50	0.27	0	49,51,55	0.26	0
3	LMT	G	405	-	36,36,36	0.09	0	47,47,47	0.22	0
2	PEE	F	302	-	46,46,50	0.27	0	49,51,55	0.26	0
3	LMT	B	308	-	36,36,36	0.11	0	47,47,47	0.36	0
3	LMT	C	308	-	36,36,36	0.11	0	47,47,47	0.35	0
3	LMT	B	304	-	36,36,36	0.10	0	47,47,47	0.37	0
2	PEE	E	302	-	46,46,50	0.27	0	49,51,55	0.26	0
3	LMT	C	307	-	36,36,36	0.09	0	47,47,47	0.22	0
3	LMT	A	303	-	36,36,36	0.10	0	47,47,47	0.37	0
3	LMT	A	307	-	36,36,36	0.10	0	47,47,47	0.36	0
3	LMT	F	307	-	36,36,36	0.11	0	47,47,47	0.36	0
3	LMT	D	305	-	36,36,36	0.09	0	47,47,47	0.26	0
3	LMT	A	302	-	36,36,36	0.09	0	47,47,47	0.18	0
2	PEE	B	302	-	46,46,50	0.27	0	49,51,55	0.26	0
3	LMT	G	409	-	36,36,36	0.11	0	47,47,47	0.21	0
3	LMT	D	308	-	36,36,36	0.11	0	47,47,47	0.36	0
3	LMT	E	301	-	36,36,36	0.11	0	47,47,47	0.38	0
3	LMT	E	307	-	36,36,36	0.10	0	47,47,47	0.22	0
3	LMT	F	305	-	36,36,36	0.08	0	47,47,47	0.26	0
3	LMT	G	408	-	36,36,36	0.08	0	47,47,47	0.26	0
3	LMT	F	306	-	36,36,36	0.10	0	47,47,47	0.21	0
3	LMT	E	305	-	36,36,36	0.08	0	47,47,47	0.26	0
3	LMT	A	305	-	36,36,36	0.11	0	47,47,47	0.21	0
3	LMT	D	306	-	36,36,36	0.11	0	47,47,47	0.21	0
3	LMT	B	306	-	36,36,36	0.11	0	47,47,47	0.21	0
3	LMT	F	301	-	36,36,36	0.11	0	47,47,47	0.38	0
3	LMT	C	301	-	36,36,36	0.11	0	47,47,47	0.38	0
3	LMT	C	303	-	36,36,36	0.08	0	47,47,47	0.18	0
3	LMT	E	304	-	36,36,36	0.09	0	47,47,47	0.37	0
3	LMT	A	304	-	36,36,36	0.08	0	47,47,47	0.27	0
2	PEE	D	302	-	46,46,50	0.27	0	49,51,55	0.26	0
3	LMT	D	304	-	36,36,36	0.10	0	47,47,47	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LMT	C	305	-	36,36,36	0.09	0	47,47,47	0.27	0
3	LMT	B	301	-	36,36,36	0.11	0	47,47,47	0.38	0
3	LMT	B	307	-	36,36,36	0.09	0	47,47,47	0.22	0
3	LMT	G	406	-	36,36,36	0.09	0	47,47,47	0.18	0
3	LMT	A	308	-	36,36,36	0.11	0	47,47,47	0.37	0
3	LMT	B	305	-	36,36,36	0.08	0	47,47,47	0.27	0
3	LMT	G	403	-	36,36,36	0.11	0	47,47,47	0.37	0
3	LMT	D	303	-	36,36,36	0.08	0	47,47,47	0.18	0
3	LMT	G	407	-	36,36,36	0.09	0	47,47,47	0.37	0
3	LMT	E	308	-	36,36,36	0.11	0	47,47,47	0.35	0
2	PEE	A	301	-	46,46,50	0.27	0	49,51,55	0.26	0
3	LMT	C	306	-	36,36,36	0.10	0	47,47,47	0.21	0
3	LMT	E	303	-	36,36,36	0.08	0	47,47,47	0.18	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
3	LMT	F	304	-	-	6/21/61/61	0/2/2/2
3	LMT	C	304	-	-	6/21/61/61	0/2/2/2
2	PEE	C	302	-	-	8/50/50/54	-
3	LMT	D	301	-	-	6/21/61/61	0/2/2/2
3	LMT	E	306	-	-	8/21/61/61	0/2/2/2
3	LMT	A	306	-	-	6/21/61/61	0/2/2/2
3	LMT	D	307	-	-	6/21/61/61	0/2/2/2
3	LMT	G	402	-	-	4/21/61/61	0/2/2/2
3	LMT	B	303	-	-	7/21/61/61	0/2/2/2
3	LMT	G	401	-	-	6/21/61/61	0/2/2/2
3	LMT	F	303	-	-	7/21/61/61	0/2/2/2
2	PEE	G	404	-	-	8/50/50/54	-
3	LMT	G	405	-	-	6/21/61/61	0/2/2/2
2	PEE	F	302	-	-	7/50/50/54	-
3	LMT	B	308	-	-	4/21/61/61	0/2/2/2
3	LMT	C	308	-	-	4/21/61/61	0/2/2/2
3	LMT	B	304	-	-	6/21/61/61	0/2/2/2
2	PEE	E	302	-	-	7/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	C	307	-	-	6/21/61/61	0/2/2/2
3	LMT	A	303	-	-	6/21/61/61	0/2/2/2
3	LMT	A	307	-	-	4/21/61/61	0/2/2/2
3	LMT	F	307	-	-	4/21/61/61	0/2/2/2
3	LMT	D	305	-	-	8/21/61/61	0/2/2/2
3	LMT	A	302	-	-	7/21/61/61	0/2/2/2
2	PEE	B	302	-	-	8/50/50/54	-
3	LMT	G	409	-	-	8/21/61/61	0/2/2/2
3	LMT	D	308	-	-	4/21/61/61	0/2/2/2
3	LMT	E	301	-	-	6/21/61/61	0/2/2/2
3	LMT	E	307	-	-	6/21/61/61	0/2/2/2
3	LMT	F	305	-	-	8/21/61/61	0/2/2/2
3	LMT	G	408	-	-	8/21/61/61	0/2/2/2
3	LMT	F	306	-	-	8/21/61/61	0/2/2/2
3	LMT	E	305	-	-	8/21/61/61	0/2/2/2
3	LMT	A	305	-	-	8/21/61/61	0/2/2/2
3	LMT	D	306	-	-	8/21/61/61	0/2/2/2
3	LMT	B	306	-	-	8/21/61/61	0/2/2/2
3	LMT	F	301	-	-	6/21/61/61	0/2/2/2
3	LMT	C	301	-	-	6/21/61/61	0/2/2/2
3	LMT	C	303	-	-	7/21/61/61	0/2/2/2
3	LMT	E	304	-	-	6/21/61/61	0/2/2/2
3	LMT	A	304	-	-	8/21/61/61	0/2/2/2
2	PEE	D	302	-	-	8/50/50/54	-
3	LMT	D	304	-	-	6/21/61/61	0/2/2/2
3	LMT	C	305	-	-	8/21/61/61	0/2/2/2
3	LMT	B	301	-	-	6/21/61/61	0/2/2/2
3	LMT	B	307	-	-	6/21/61/61	0/2/2/2
3	LMT	G	406	-	-	7/21/61/61	0/2/2/2
3	LMT	A	308	-	-	6/21/61/61	0/2/2/2
3	LMT	B	305	-	-	8/21/61/61	0/2/2/2
3	LMT	G	403	-	-	6/21/61/61	0/2/2/2
3	LMT	D	303	-	-	7/21/61/61	0/2/2/2
3	LMT	G	407	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	E	308	-	-	4/21/61/61	0/2/2/2
2	PEE	A	301	-	-	7/50/50/54	-
3	LMT	C	306	-	-	8/21/61/61	0/2/2/2
3	LMT	E	303	-	-	7/21/61/61	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (368) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	LMT	C2'-C1'-O1'-C1
3	A	303	LMT	O5'-C1'-O1'-C1
3	A	304	LMT	O5'-C1'-O1'-C1
3	A	305	LMT	O5'-C1'-O1'-C1
3	A	306	LMT	C2'-C1'-O1'-C1
3	A	306	LMT	O5'-C1'-O1'-C1
3	A	308	LMT	C2'-C1'-O1'-C1
3	A	308	LMT	O5'-C1'-O1'-C1
3	A	308	LMT	C2-C1-O1'-C1'
3	B	301	LMT	C2'-C1'-O1'-C1
3	B	301	LMT	O5'-C1'-O1'-C1
3	B	301	LMT	C2-C1-O1'-C1'
3	B	304	LMT	C2'-C1'-O1'-C1
3	B	304	LMT	O5'-C1'-O1'-C1
3	B	305	LMT	O5'-C1'-O1'-C1
3	B	306	LMT	O5'-C1'-O1'-C1
3	B	307	LMT	C2'-C1'-O1'-C1
3	B	307	LMT	O5'-C1'-O1'-C1
3	C	301	LMT	C2'-C1'-O1'-C1
3	C	301	LMT	O5'-C1'-O1'-C1
3	C	301	LMT	C2-C1-O1'-C1'
3	C	304	LMT	C2'-C1'-O1'-C1
3	C	304	LMT	O5'-C1'-O1'-C1
3	C	305	LMT	O5'-C1'-O1'-C1
3	C	306	LMT	O5'-C1'-O1'-C1
3	C	307	LMT	C2'-C1'-O1'-C1
3	C	307	LMT	O5'-C1'-O1'-C1
3	D	301	LMT	C2'-C1'-O1'-C1
3	D	301	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
3	D	301	LMT	C2-C1-O1'-C1'
3	D	304	LMT	C2'-C1'-O1'-C1
3	D	304	LMT	O5'-C1'-O1'-C1
3	D	305	LMT	O5'-C1'-O1'-C1
3	D	306	LMT	O5'-C1'-O1'-C1
3	D	307	LMT	C2'-C1'-O1'-C1
3	D	307	LMT	O5'-C1'-O1'-C1
3	E	301	LMT	C2'-C1'-O1'-C1
3	E	301	LMT	O5'-C1'-O1'-C1
3	E	301	LMT	C2-C1-O1'-C1'
3	E	304	LMT	C2'-C1'-O1'-C1
3	E	304	LMT	O5'-C1'-O1'-C1
3	E	305	LMT	O5'-C1'-O1'-C1
3	E	306	LMT	O5'-C1'-O1'-C1
3	E	307	LMT	C2'-C1'-O1'-C1
3	E	307	LMT	O5'-C1'-O1'-C1
3	F	301	LMT	C2'-C1'-O1'-C1
3	F	301	LMT	O5'-C1'-O1'-C1
3	F	301	LMT	C2-C1-O1'-C1'
3	F	304	LMT	C2'-C1'-O1'-C1
3	F	304	LMT	O5'-C1'-O1'-C1
3	F	305	LMT	O5'-C1'-O1'-C1
3	F	306	LMT	O5'-C1'-O1'-C1
3	G	401	LMT	C2'-C1'-O1'-C1
3	G	401	LMT	O5'-C1'-O1'-C1
3	G	403	LMT	C2'-C1'-O1'-C1
3	G	403	LMT	O5'-C1'-O1'-C1
3	G	403	LMT	C2-C1-O1'-C1'
3	G	405	LMT	C2'-C1'-O1'-C1
3	G	405	LMT	O5'-C1'-O1'-C1
3	G	407	LMT	C2'-C1'-O1'-C1
3	G	407	LMT	O5'-C1'-O1'-C1
3	G	408	LMT	O5'-C1'-O1'-C1
3	G	409	LMT	O5'-C1'-O1'-C1
3	A	306	LMT	C5'-C4'-O1B-C1B
3	B	307	LMT	C5'-C4'-O1B-C1B
3	C	307	LMT	C5'-C4'-O1B-C1B
3	D	307	LMT	C5'-C4'-O1B-C1B
3	E	307	LMT	C5'-C4'-O1B-C1B
3	G	401	LMT	C5'-C4'-O1B-C1B
3	G	405	LMT	C5'-C4'-O1B-C1B
3	A	303	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
3	B	304	LMT	O5B-C1B-O1B-C4'
3	C	304	LMT	O5B-C1B-O1B-C4'
3	D	304	LMT	O5B-C1B-O1B-C4'
3	E	304	LMT	O5B-C1B-O1B-C4'
3	F	304	LMT	O5B-C1B-O1B-C4'
3	G	407	LMT	O5B-C1B-O1B-C4'
3	A	304	LMT	O5B-C1B-O1B-C4'
3	B	305	LMT	O5B-C1B-O1B-C4'
3	C	305	LMT	O5B-C1B-O1B-C4'
3	D	305	LMT	O5B-C1B-O1B-C4'
3	E	305	LMT	O5B-C1B-O1B-C4'
3	F	305	LMT	O5B-C1B-O1B-C4'
3	G	408	LMT	O5B-C1B-O1B-C4'
3	A	305	LMT	O5B-C1B-O1B-C4'
3	B	306	LMT	O5B-C1B-O1B-C4'
3	C	306	LMT	O5B-C1B-O1B-C4'
3	D	306	LMT	O5B-C1B-O1B-C4'
3	E	306	LMT	O5B-C1B-O1B-C4'
3	F	306	LMT	O5B-C1B-O1B-C4'
3	G	409	LMT	O5B-C1B-O1B-C4'
3	A	307	LMT	C3'-C4'-O1B-C1B
3	B	308	LMT	C3'-C4'-O1B-C1B
3	C	308	LMT	C3'-C4'-O1B-C1B
3	D	308	LMT	C3'-C4'-O1B-C1B
3	E	308	LMT	C3'-C4'-O1B-C1B
3	F	307	LMT	C3'-C4'-O1B-C1B
3	G	402	LMT	C3'-C4'-O1B-C1B
3	A	305	LMT	C2B-C1B-O1B-C4'
3	B	306	LMT	C2B-C1B-O1B-C4'
3	C	306	LMT	C2B-C1B-O1B-C4'
3	D	306	LMT	C2B-C1B-O1B-C4'
3	E	306	LMT	C2B-C1B-O1B-C4'
3	F	306	LMT	C2B-C1B-O1B-C4'
3	G	409	LMT	C2B-C1B-O1B-C4'
3	A	308	LMT	C3'-C4'-O1B-C1B
3	B	301	LMT	C3'-C4'-O1B-C1B
3	C	301	LMT	C3'-C4'-O1B-C1B
3	D	301	LMT	C3'-C4'-O1B-C1B
3	E	301	LMT	C3'-C4'-O1B-C1B
3	F	301	LMT	C3'-C4'-O1B-C1B
3	G	403	LMT	C3'-C4'-O1B-C1B
2	B	302	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	C	302	PEE	C23-C24-C25-C26
2	D	302	PEE	C23-C24-C25-C26
2	G	404	PEE	C23-C24-C25-C26
2	A	301	PEE	C23-C24-C25-C26
2	E	302	PEE	C23-C24-C25-C26
2	F	302	PEE	C23-C24-C25-C26
3	A	302	LMT	C2'-C1'-O1'-C1
3	A	304	LMT	C2'-C1'-O1'-C1
3	B	303	LMT	C2'-C1'-O1'-C1
3	B	305	LMT	C2'-C1'-O1'-C1
3	C	303	LMT	C2'-C1'-O1'-C1
3	C	305	LMT	C2'-C1'-O1'-C1
3	D	303	LMT	C2'-C1'-O1'-C1
3	D	305	LMT	C2'-C1'-O1'-C1
3	E	303	LMT	C2'-C1'-O1'-C1
3	E	305	LMT	C2'-C1'-O1'-C1
3	F	303	LMT	C2'-C1'-O1'-C1
3	F	305	LMT	C2'-C1'-O1'-C1
3	G	406	LMT	C2'-C1'-O1'-C1
3	G	408	LMT	C2'-C1'-O1'-C1
3	B	305	LMT	C3-C4-C5-C6
3	C	305	LMT	C3-C4-C5-C6
3	D	305	LMT	C3-C4-C5-C6
3	F	305	LMT	C3-C4-C5-C6
3	G	408	LMT	C3-C4-C5-C6
3	A	304	LMT	C3-C4-C5-C6
3	E	305	LMT	C3-C4-C5-C6
3	A	304	LMT	C2-C1-O1'-C1'
3	B	305	LMT	C2-C1-O1'-C1'
3	C	305	LMT	C2-C1-O1'-C1'
3	D	305	LMT	C2-C1-O1'-C1'
3	E	305	LMT	C2-C1-O1'-C1'
3	F	305	LMT	C2-C1-O1'-C1'
3	G	408	LMT	C2-C1-O1'-C1'
3	B	304	LMT	O1'-C1-C2-C3
3	C	304	LMT	O1'-C1-C2-C3
3	D	304	LMT	O1'-C1-C2-C3
3	F	304	LMT	O1'-C1-C2-C3
3	G	407	LMT	O1'-C1-C2-C3
3	A	302	LMT	O5'-C1'-O1'-C1
3	B	303	LMT	O5'-C1'-O1'-C1
3	C	303	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
3	D	303	LMT	O5'-C1'-O1'-C1
3	E	303	LMT	O5'-C1'-O1'-C1
3	F	303	LMT	O5'-C1'-O1'-C1
3	G	406	LMT	O5'-C1'-O1'-C1
3	A	303	LMT	O1'-C1-C2-C3
3	E	304	LMT	O1'-C1-C2-C3
3	A	303	LMT	O5'-C5'-C6'-O6'
3	B	304	LMT	O5'-C5'-C6'-O6'
3	C	304	LMT	O5'-C5'-C6'-O6'
3	D	304	LMT	O5'-C5'-C6'-O6'
3	E	304	LMT	O5'-C5'-C6'-O6'
3	F	304	LMT	O5'-C5'-C6'-O6'
3	G	407	LMT	O5'-C5'-C6'-O6'
3	A	307	LMT	O5B-C5B-C6B-O6B
3	B	308	LMT	O5B-C5B-C6B-O6B
3	C	308	LMT	O5B-C5B-C6B-O6B
3	D	308	LMT	O5B-C5B-C6B-O6B
3	E	308	LMT	O5B-C5B-C6B-O6B
3	F	307	LMT	O5B-C5B-C6B-O6B
3	G	402	LMT	O5B-C5B-C6B-O6B
3	A	304	LMT	O5'-C5'-C6'-O6'
3	B	305	LMT	O5'-C5'-C6'-O6'
3	C	305	LMT	O5'-C5'-C6'-O6'
3	D	305	LMT	O5'-C5'-C6'-O6'
3	E	305	LMT	O5'-C5'-C6'-O6'
3	F	305	LMT	O5'-C5'-C6'-O6'
3	G	408	LMT	O5'-C5'-C6'-O6'
3	A	305	LMT	O5B-C5B-C6B-O6B
3	A	306	LMT	O5'-C5'-C6'-O6'
3	B	306	LMT	O5B-C5B-C6B-O6B
3	B	307	LMT	O5'-C5'-C6'-O6'
3	C	306	LMT	O5B-C5B-C6B-O6B
3	C	307	LMT	O5'-C5'-C6'-O6'
3	D	306	LMT	O5B-C5B-C6B-O6B
3	D	307	LMT	O5'-C5'-C6'-O6'
3	E	306	LMT	O5B-C5B-C6B-O6B
3	E	307	LMT	O5'-C5'-C6'-O6'
3	F	306	LMT	O5B-C5B-C6B-O6B
3	G	401	LMT	O5'-C5'-C6'-O6'
3	G	405	LMT	O5'-C5'-C6'-O6'
3	G	409	LMT	O5B-C5B-C6B-O6B
3	G	403	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
3	F	301	LMT	C5'-C4'-O1B-C1B
3	A	305	LMT	C2'-C1'-O1'-C1
3	B	306	LMT	C2'-C1'-O1'-C1
3	C	306	LMT	C2'-C1'-O1'-C1
3	D	306	LMT	C2'-C1'-O1'-C1
3	E	306	LMT	C2'-C1'-O1'-C1
3	F	306	LMT	C2'-C1'-O1'-C1
3	G	409	LMT	C2'-C1'-O1'-C1
3	A	308	LMT	C5'-C4'-O1B-C1B
3	B	301	LMT	C5'-C4'-O1B-C1B
3	C	301	LMT	C5'-C4'-O1B-C1B
3	D	301	LMT	C5'-C4'-O1B-C1B
3	E	301	LMT	C5'-C4'-O1B-C1B
3	E	308	LMT	C5'-C4'-O1B-C1B
3	F	307	LMT	C5'-C4'-O1B-C1B
3	A	307	LMT	C5'-C4'-O1B-C1B
3	B	308	LMT	C5'-C4'-O1B-C1B
3	C	308	LMT	C5'-C4'-O1B-C1B
3	D	308	LMT	C5'-C4'-O1B-C1B
3	G	402	LMT	C5'-C4'-O1B-C1B
2	A	301	PEE	O3P-C1-C2-C3
2	B	302	PEE	O3P-C1-C2-C3
2	C	302	PEE	O3P-C1-C2-C3
2	D	302	PEE	O3P-C1-C2-C3
2	E	302	PEE	O3P-C1-C2-C3
2	F	302	PEE	O3P-C1-C2-C3
2	G	404	PEE	O3P-C1-C2-C3
3	A	302	LMT	C2-C1-O1'-C1'
3	A	305	LMT	C2-C1-O1'-C1'
3	B	303	LMT	C2-C1-O1'-C1'
3	B	306	LMT	C2-C1-O1'-C1'
3	C	303	LMT	C2-C1-O1'-C1'
3	C	306	LMT	C2-C1-O1'-C1'
3	D	303	LMT	C2-C1-O1'-C1'
3	D	306	LMT	C2-C1-O1'-C1'
3	E	303	LMT	C2-C1-O1'-C1'
3	E	306	LMT	C2-C1-O1'-C1'
3	F	303	LMT	C2-C1-O1'-C1'
3	F	306	LMT	C2-C1-O1'-C1'
3	G	406	LMT	C2-C1-O1'-C1'
3	G	409	LMT	C2-C1-O1'-C1'
3	A	304	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
3	C	305	LMT	C2B-C1B-O1B-C4'
3	F	305	LMT	C2B-C1B-O1B-C4'
3	D	305	LMT	C2B-C1B-O1B-C4'
3	E	305	LMT	C2B-C1B-O1B-C4'
3	G	408	LMT	C2B-C1B-O1B-C4'
3	B	305	LMT	C2B-C1B-O1B-C4'
2	A	301	PEE	C22-C23-C24-C25
2	G	404	PEE	C22-C23-C24-C25
2	B	302	PEE	C22-C23-C24-C25
2	D	302	PEE	C22-C23-C24-C25
2	E	302	PEE	C22-C23-C24-C25
2	F	302	PEE	C22-C23-C24-C25
2	C	302	PEE	C22-C23-C24-C25
3	D	303	LMT	C6-C7-C8-C9
3	B	303	LMT	C6-C7-C8-C9
3	C	303	LMT	C6-C7-C8-C9
3	F	303	LMT	C6-C7-C8-C9
3	G	406	LMT	C6-C7-C8-C9
3	A	302	LMT	C6-C7-C8-C9
3	E	303	LMT	C6-C7-C8-C9
2	A	301	PEE	O3P-C1-C2-O2
2	B	302	PEE	O3P-C1-C2-O2
2	C	302	PEE	O3P-C1-C2-O2
2	D	302	PEE	O3P-C1-C2-O2
2	E	302	PEE	O3P-C1-C2-O2
2	F	302	PEE	O3P-C1-C2-O2
2	G	404	PEE	O3P-C1-C2-O2
3	A	304	LMT	C2-C3-C4-C5
3	D	305	LMT	C2-C3-C4-C5
3	C	305	LMT	C2-C3-C4-C5
3	B	305	LMT	C2-C3-C4-C5
3	E	305	LMT	C2-C3-C4-C5
3	F	305	LMT	C2-C3-C4-C5
3	G	408	LMT	C2-C3-C4-C5
2	A	301	PEE	C1-O3P-P-O4P
2	B	302	PEE	C1-O3P-P-O4P
2	C	302	PEE	C1-O3P-P-O4P
2	D	302	PEE	C1-O3P-P-O4P
2	E	302	PEE	C1-O3P-P-O4P
2	F	302	PEE	C1-O3P-P-O4P
2	G	404	PEE	C1-O3P-P-O4P
2	A	301	PEE	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
2	B	302	PEE	C2-C1-O3P-P
2	C	302	PEE	C2-C1-O3P-P
2	D	302	PEE	C2-C1-O3P-P
2	E	302	PEE	C2-C1-O3P-P
2	F	302	PEE	C2-C1-O3P-P
2	G	404	PEE	C2-C1-O3P-P
2	A	301	PEE	C1-O3P-P-O2P
2	B	302	PEE	C1-O3P-P-O2P
2	C	302	PEE	C1-O3P-P-O2P
2	D	302	PEE	C1-O3P-P-O2P
2	E	302	PEE	C1-O3P-P-O2P
2	F	302	PEE	C1-O3P-P-O2P
2	G	404	PEE	C1-O3P-P-O2P
3	C	301	LMT	O1'-C1-C2-C3
3	B	301	LMT	O1'-C1-C2-C3
3	F	301	LMT	O1'-C1-C2-C3
3	D	301	LMT	O1'-C1-C2-C3
3	A	308	LMT	O1'-C1-C2-C3
3	E	301	LMT	O1'-C1-C2-C3
3	G	403	LMT	O1'-C1-C2-C3
3	D	307	LMT	C2B-C1B-O1B-C4'
3	G	401	LMT	C2B-C1B-O1B-C4'
3	G	405	LMT	C2B-C1B-O1B-C4'
3	A	306	LMT	C2B-C1B-O1B-C4'
3	B	307	LMT	C2B-C1B-O1B-C4'
3	C	307	LMT	C2B-C1B-O1B-C4'
3	E	307	LMT	C2B-C1B-O1B-C4'
3	G	401	LMT	O5B-C1B-O1B-C4'
3	D	307	LMT	O5B-C1B-O1B-C4'
3	A	306	LMT	O5B-C1B-O1B-C4'
3	B	307	LMT	O5B-C1B-O1B-C4'
3	C	307	LMT	O5B-C1B-O1B-C4'
3	E	307	LMT	O5B-C1B-O1B-C4'
3	G	405	LMT	O5B-C1B-O1B-C4'
3	G	406	LMT	O5B-C1B-O1B-C4'
3	A	302	LMT	O5B-C1B-O1B-C4'
3	B	303	LMT	O5B-C1B-O1B-C4'
3	D	303	LMT	O5B-C1B-O1B-C4'
3	E	303	LMT	O5B-C1B-O1B-C4'
3	C	303	LMT	O5B-C1B-O1B-C4'
3	F	303	LMT	O5B-C1B-O1B-C4'
3	G	409	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	C	306	LMT	C1-C2-C3-C4
3	F	306	LMT	C1-C2-C3-C4
3	A	305	LMT	C1-C2-C3-C4
3	B	306	LMT	C1-C2-C3-C4
3	D	306	LMT	C1-C2-C3-C4
3	E	306	LMT	C1-C2-C3-C4
3	B	306	LMT	C6-C7-C8-C9
3	D	306	LMT	C6-C7-C8-C9
3	E	306	LMT	C6-C7-C8-C9
3	A	305	LMT	C6-C7-C8-C9
3	C	306	LMT	C6-C7-C8-C9
3	F	306	LMT	C6-C7-C8-C9
3	G	409	LMT	C6-C7-C8-C9
3	C	303	LMT	C5-C6-C7-C8
3	A	302	LMT	C5-C6-C7-C8
3	D	303	LMT	C5-C6-C7-C8
3	B	303	LMT	C5-C6-C7-C8
3	E	303	LMT	C5-C6-C7-C8
3	F	303	LMT	C5-C6-C7-C8
3	G	406	LMT	C5-C6-C7-C8
3	C	304	LMT	C11-C10-C9-C8
3	A	303	LMT	C11-C10-C9-C8
3	G	407	LMT	C11-C10-C9-C8
3	E	304	LMT	C11-C10-C9-C8
3	B	304	LMT	C11-C10-C9-C8
3	F	304	LMT	C11-C10-C9-C8
3	D	304	LMT	C11-C10-C9-C8
3	A	302	LMT	C2B-C1B-O1B-C4'
3	B	303	LMT	C2B-C1B-O1B-C4'
3	C	303	LMT	C2B-C1B-O1B-C4'
3	D	303	LMT	C2B-C1B-O1B-C4'
3	E	303	LMT	C2B-C1B-O1B-C4'
3	F	303	LMT	C2B-C1B-O1B-C4'
3	G	406	LMT	C2B-C1B-O1B-C4'
3	A	307	LMT	C2-C1-O1'-C1'
3	B	308	LMT	C2-C1-O1'-C1'
3	C	308	LMT	C2-C1-O1'-C1'
3	D	308	LMT	C2-C1-O1'-C1'
3	E	308	LMT	C2-C1-O1'-C1'
3	F	307	LMT	C2-C1-O1'-C1'
3	G	402	LMT	C2-C1-O1'-C1'
2	C	302	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	B	302	PEE	C20-C21-C22-C23
2	D	302	PEE	C20-C21-C22-C23
2	G	404	PEE	C20-C21-C22-C23

There are no ring outliers.

52 monomers are involved in 130 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	304	LMT	1	0
2	C	302	PEE	4	0
3	D	301	LMT	3	0
3	E	306	LMT	5	0
3	A	306	LMT	4	0
3	D	307	LMT	5	0
3	G	402	LMT	3	0
3	B	303	LMT	1	0
3	G	401	LMT	6	0
3	F	303	LMT	1	0
2	G	404	PEE	4	0
3	G	405	LMT	5	0
2	F	302	PEE	4	0
3	B	308	LMT	5	0
3	C	308	LMT	6	0
2	E	302	PEE	5	0
3	C	307	LMT	4	0
3	A	307	LMT	3	0
3	F	307	LMT	5	0
3	D	305	LMT	3	0
3	A	302	LMT	1	0
2	B	302	PEE	4	0
3	G	409	LMT	4	0
3	D	308	LMT	4	0
3	E	301	LMT	3	0
3	E	307	LMT	5	0
3	F	305	LMT	3	0
3	G	408	LMT	3	0
3	F	306	LMT	4	0
3	E	305	LMT	3	0
3	A	305	LMT	3	0
3	D	306	LMT	5	0
3	B	306	LMT	4	0
3	F	301	LMT	3	0

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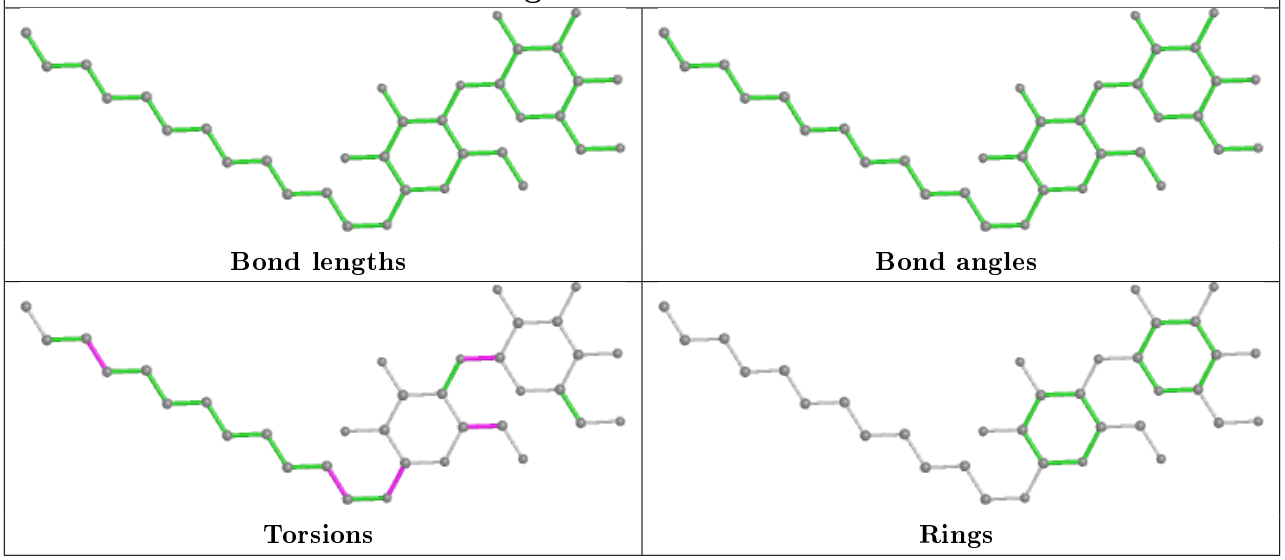
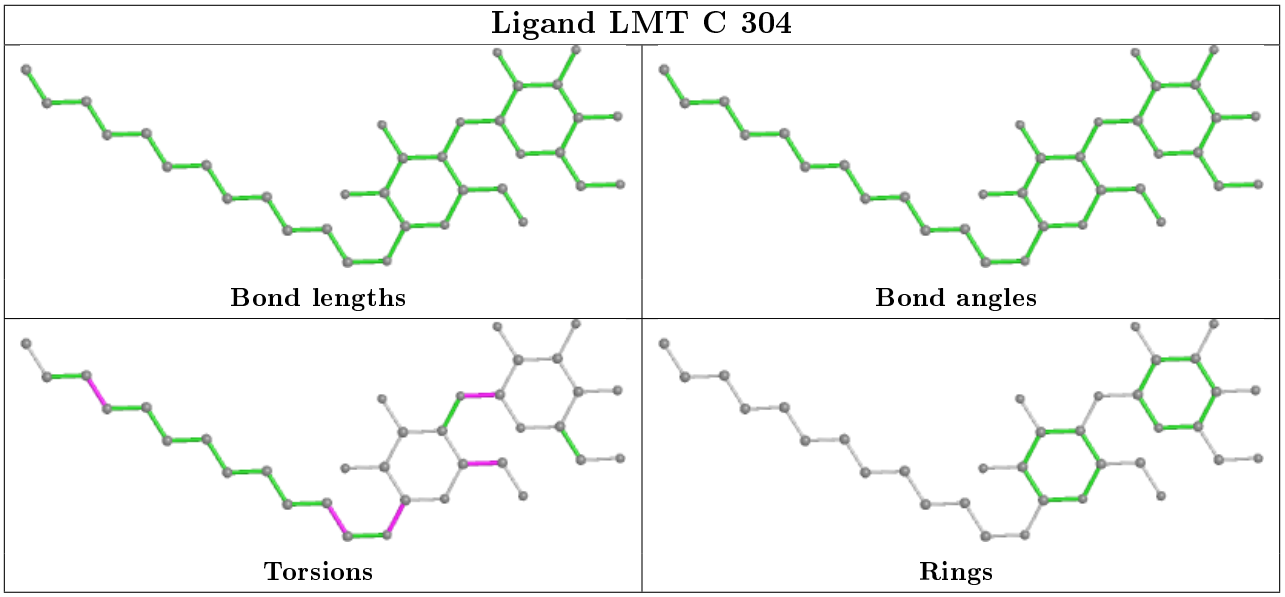
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	LMT	3	0
3	C	303	LMT	1	0
3	E	304	LMT	1	0
3	A	304	LMT	2	0
2	D	302	PEE	5	0
3	D	304	LMT	1	0
3	C	305	LMT	2	0
3	B	301	LMT	3	0
3	B	307	LMT	3	0
3	G	406	LMT	1	0
3	A	308	LMT	3	0
3	B	305	LMT	3	0
3	G	403	LMT	3	0
3	D	303	LMT	1	0
3	E	308	LMT	6	0
2	A	301	PEE	4	0
3	C	306	LMT	4	0
3	E	303	LMT	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.

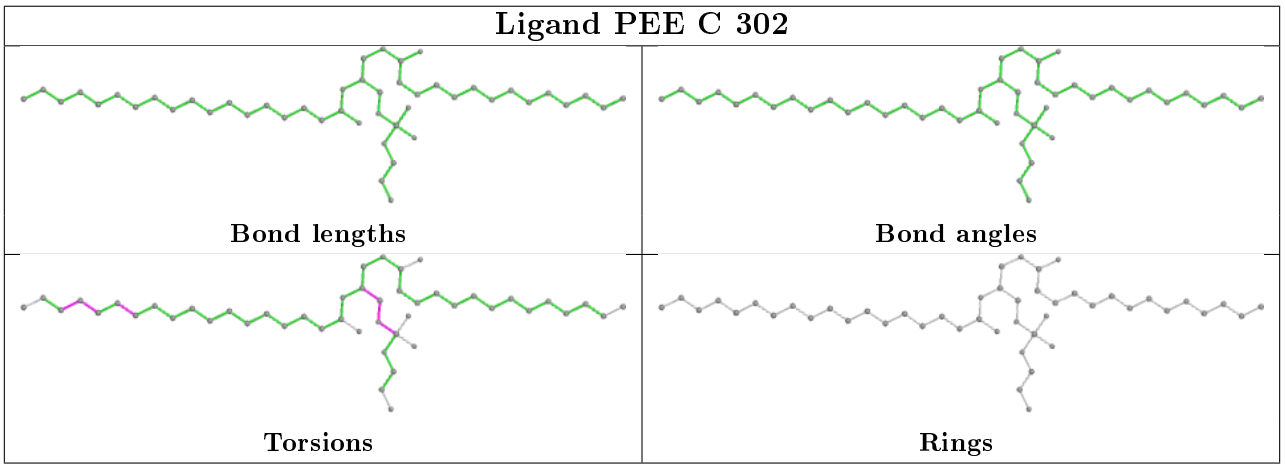
Ligand LMT F 304



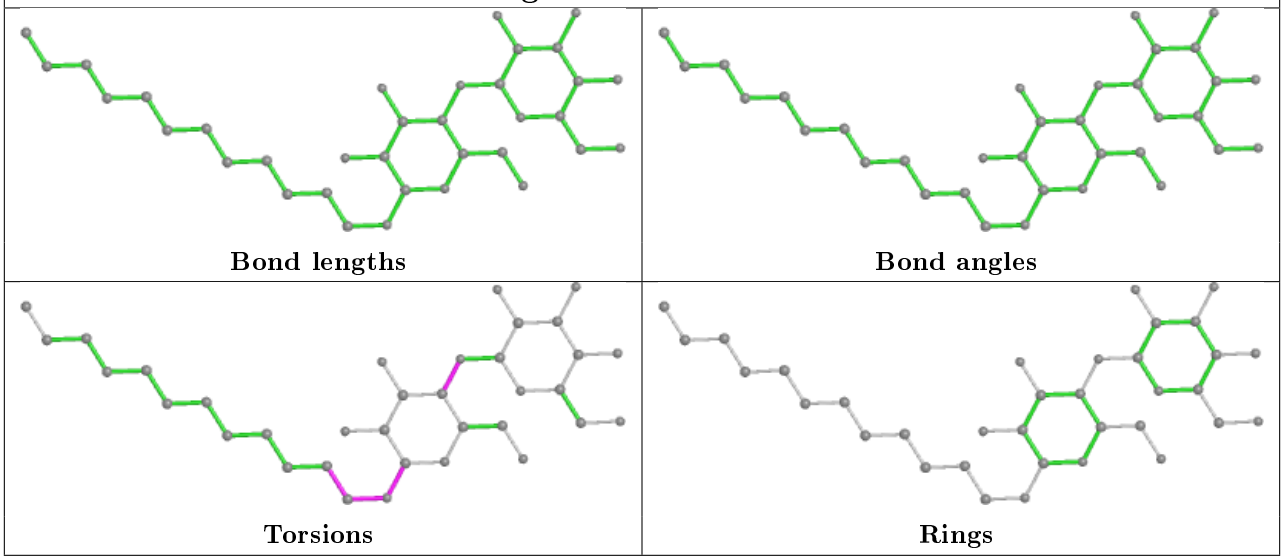
Ligand LMT C 304



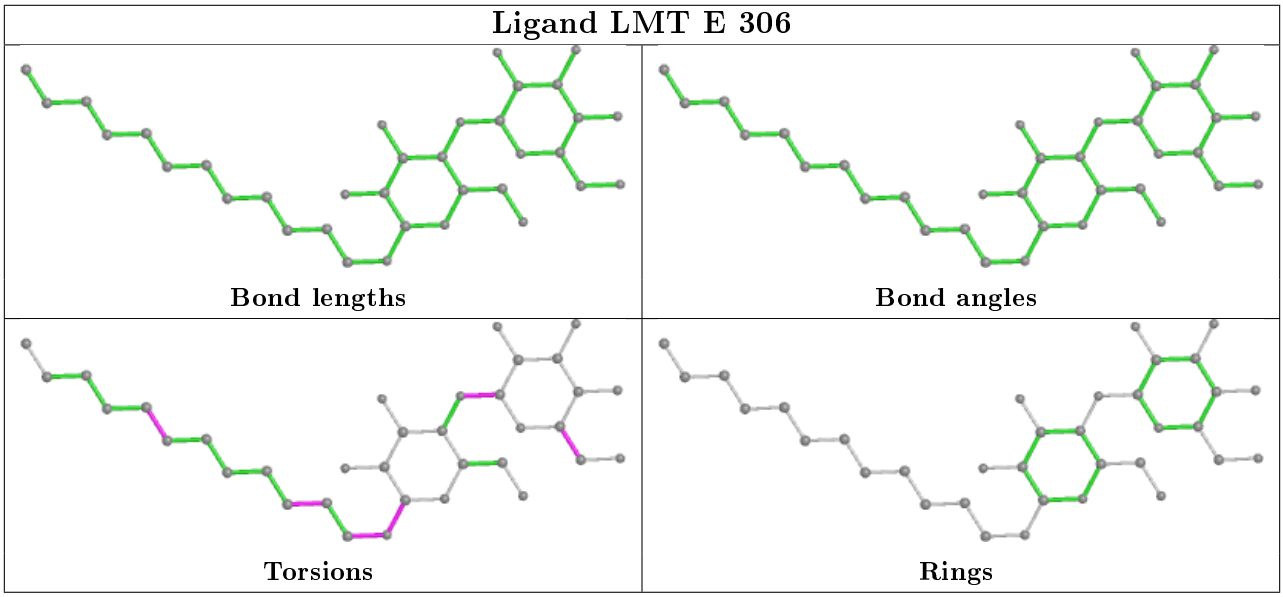
Ligand PEE C 302



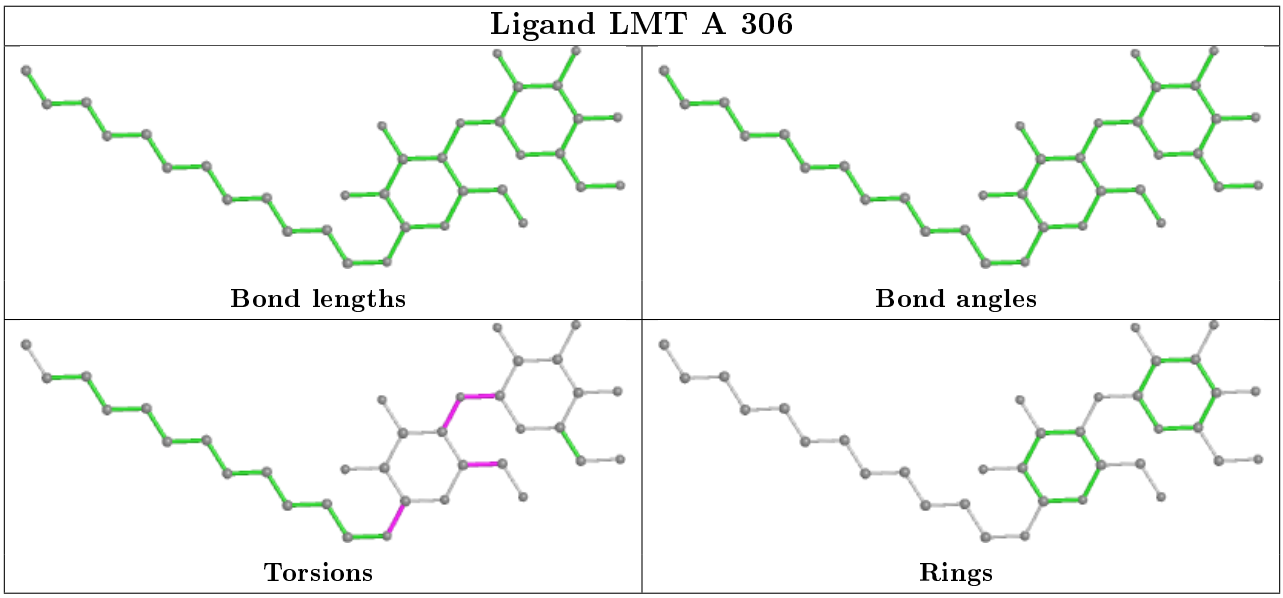
Ligand LMT D 301



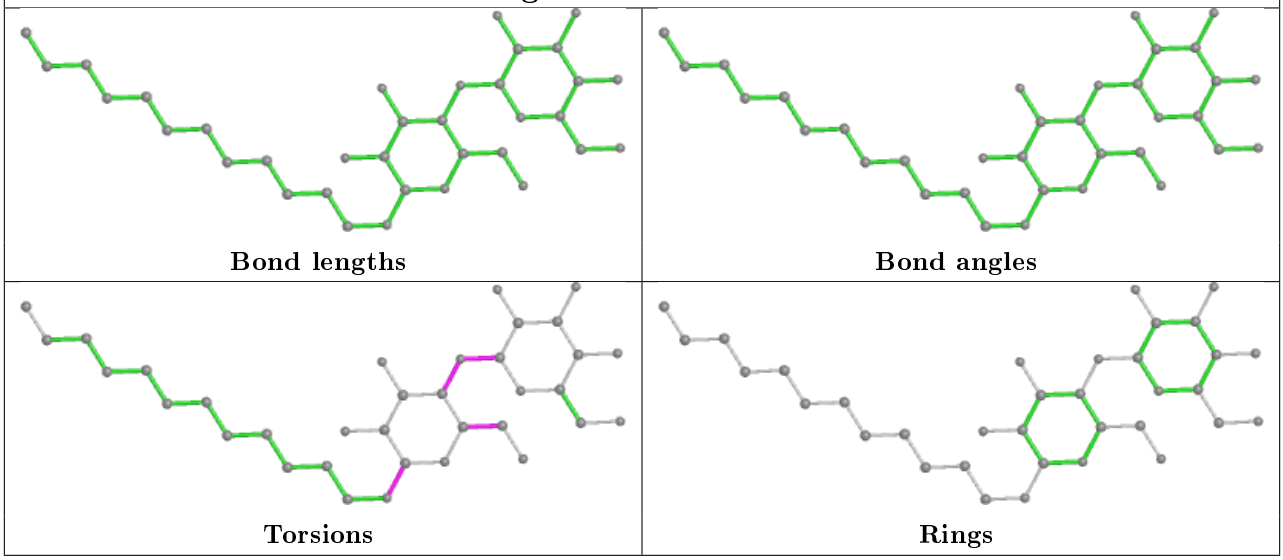
Ligand LMT E 306



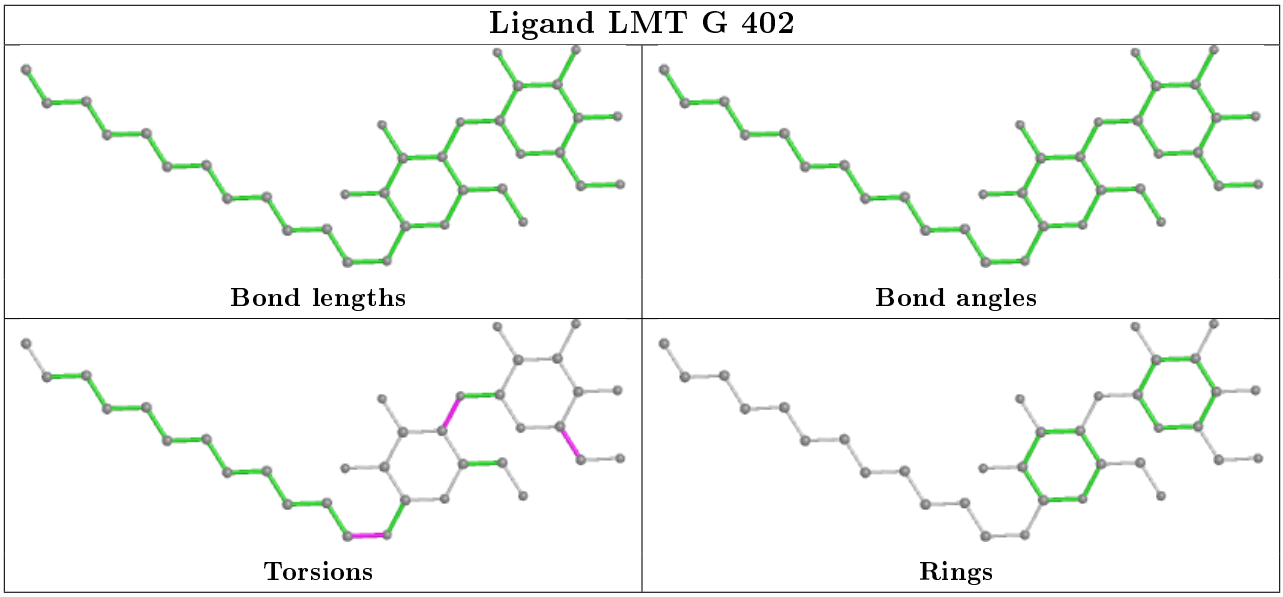
Ligand LMT A 306



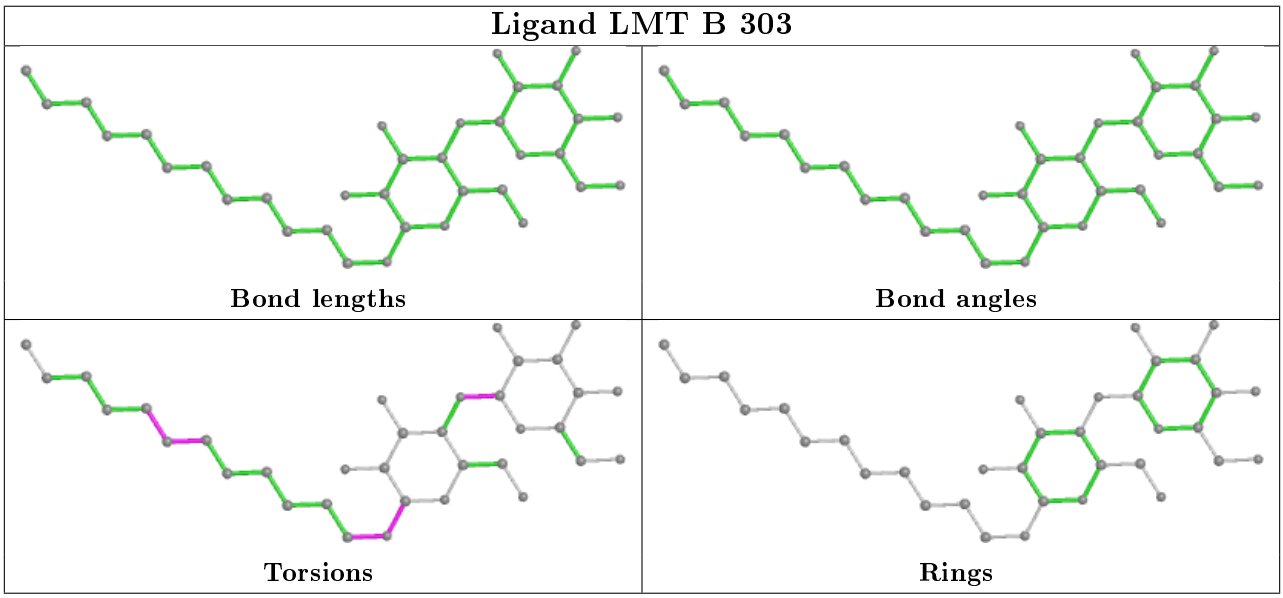
Ligand LMT D 307



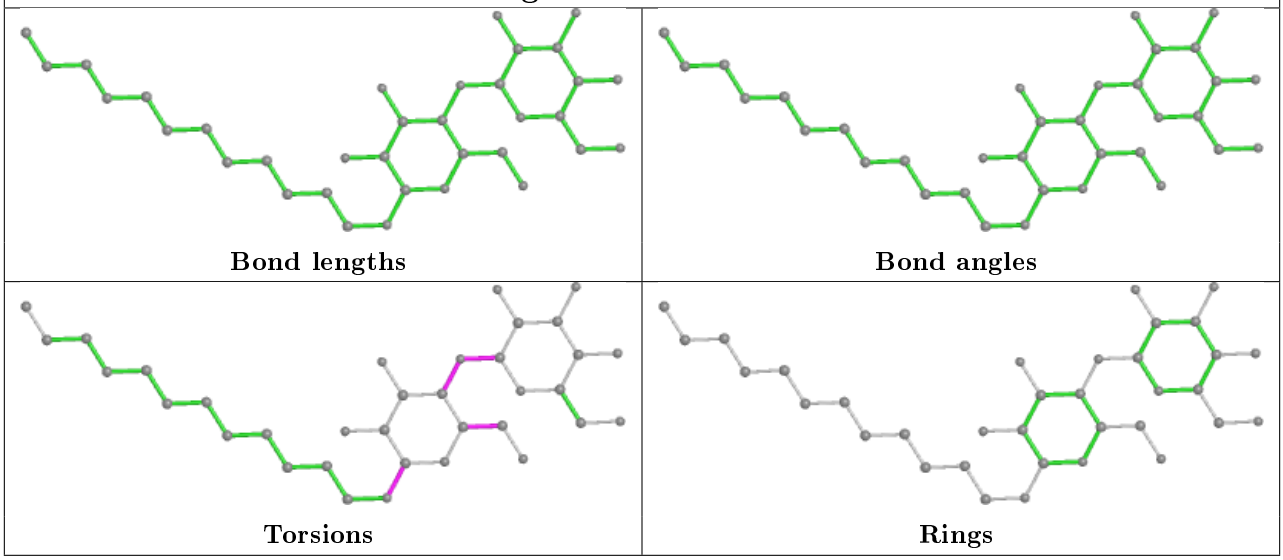
Ligand LMT G 402



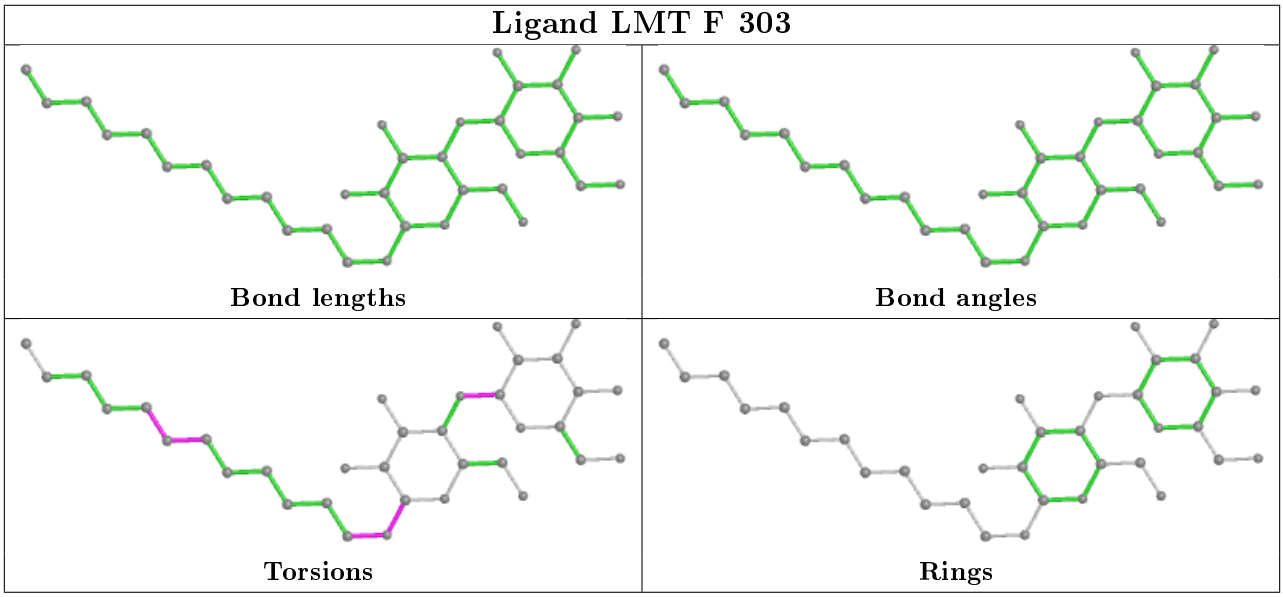
Ligand LMT B 303



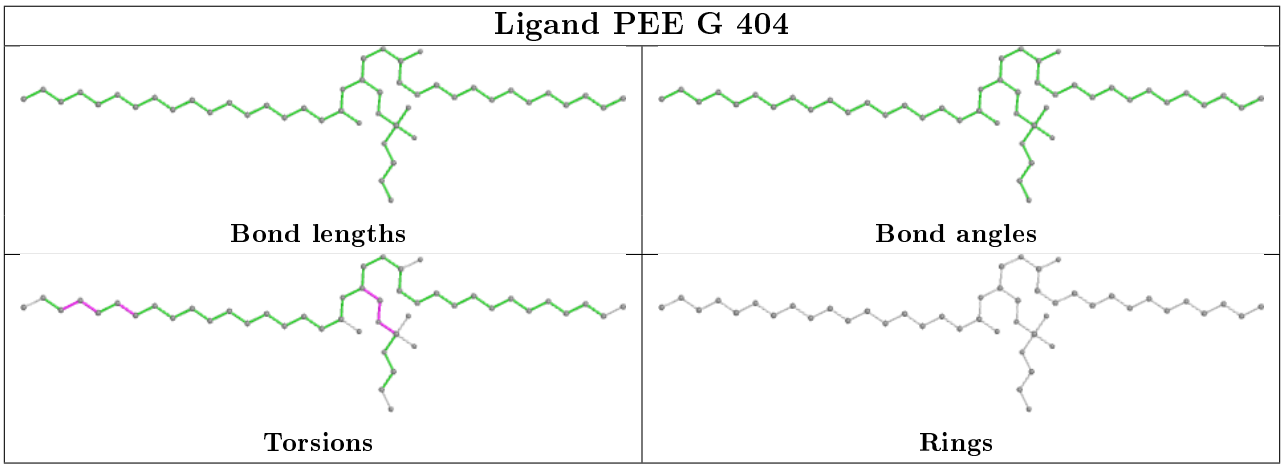
Ligand LMT G 401



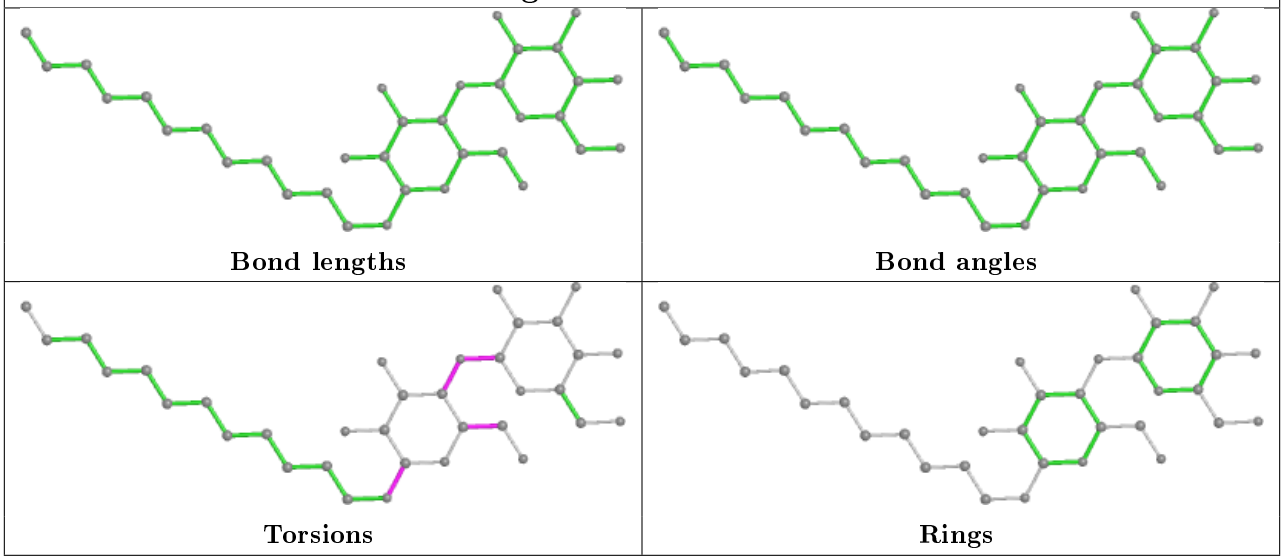
Ligand LMT F 303



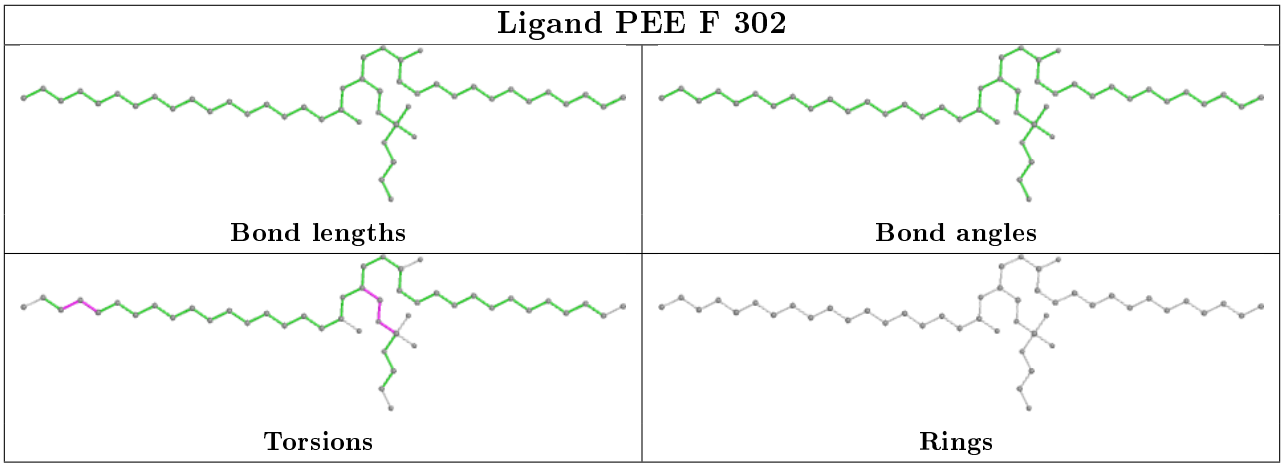
Ligand PEE G 404



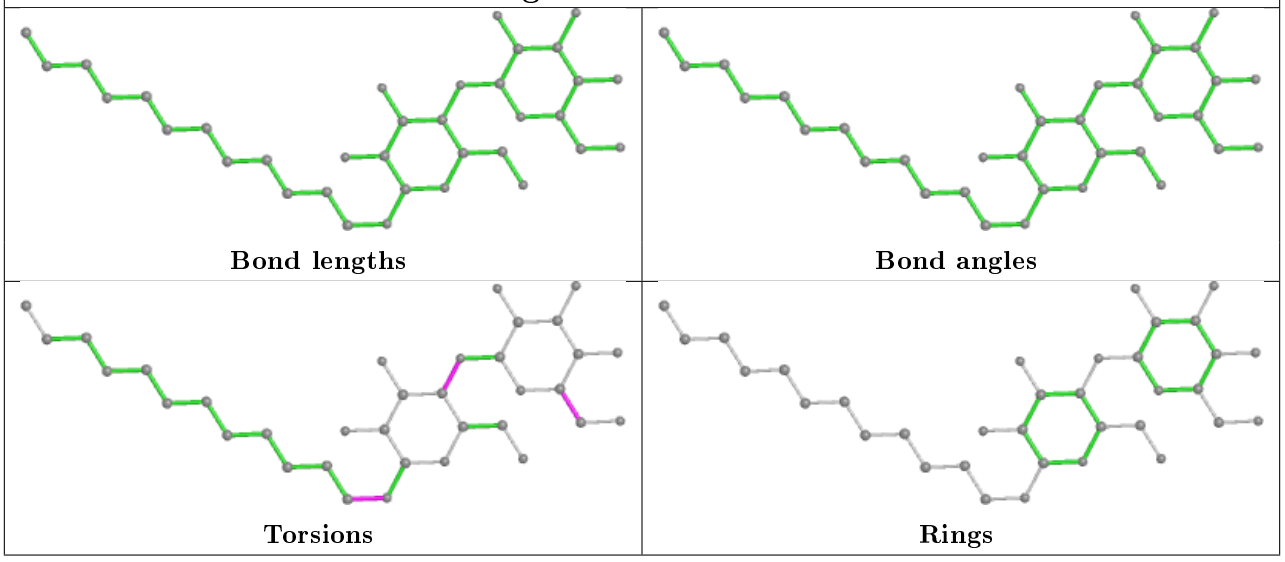
Ligand LMT G 405



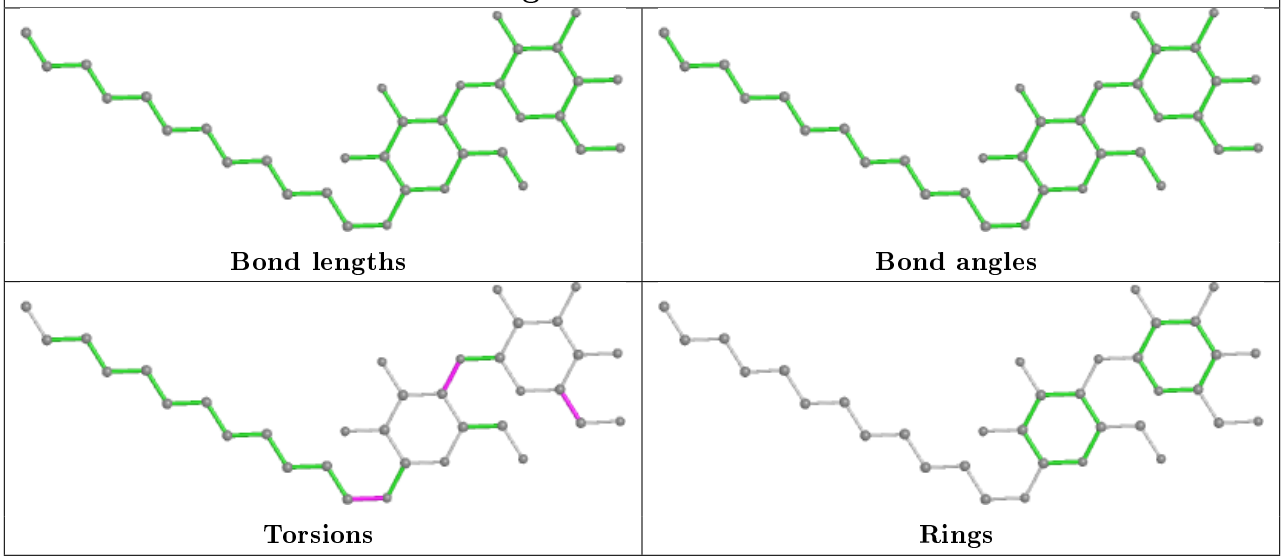
Ligand PEE F 302



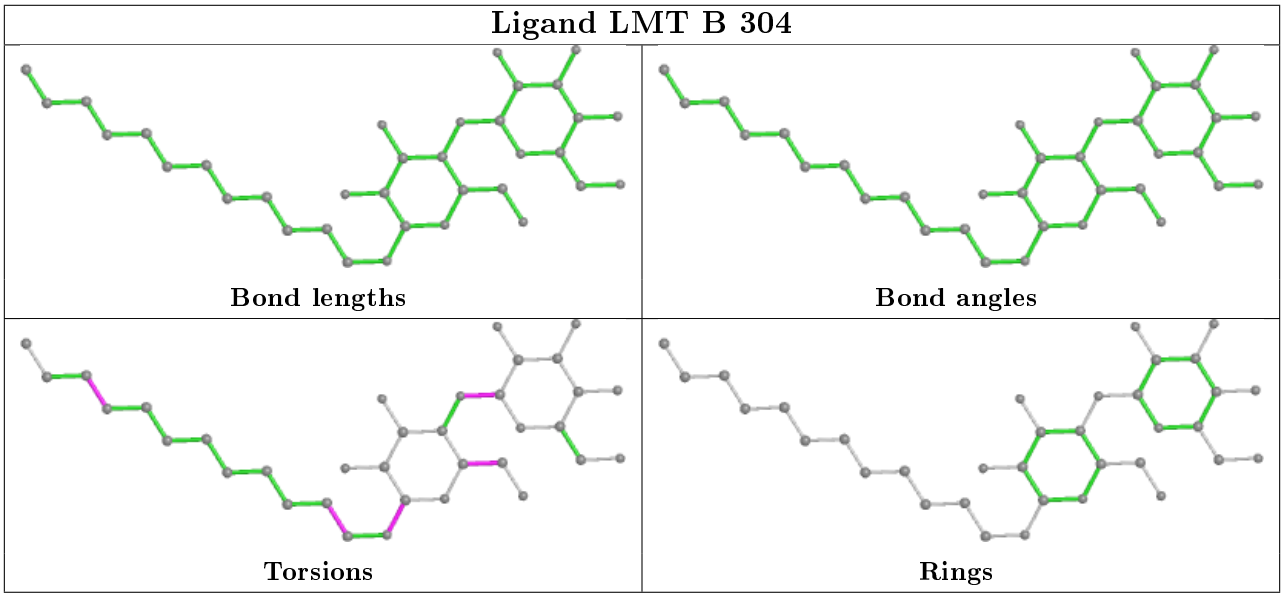
Ligand LMT B 308



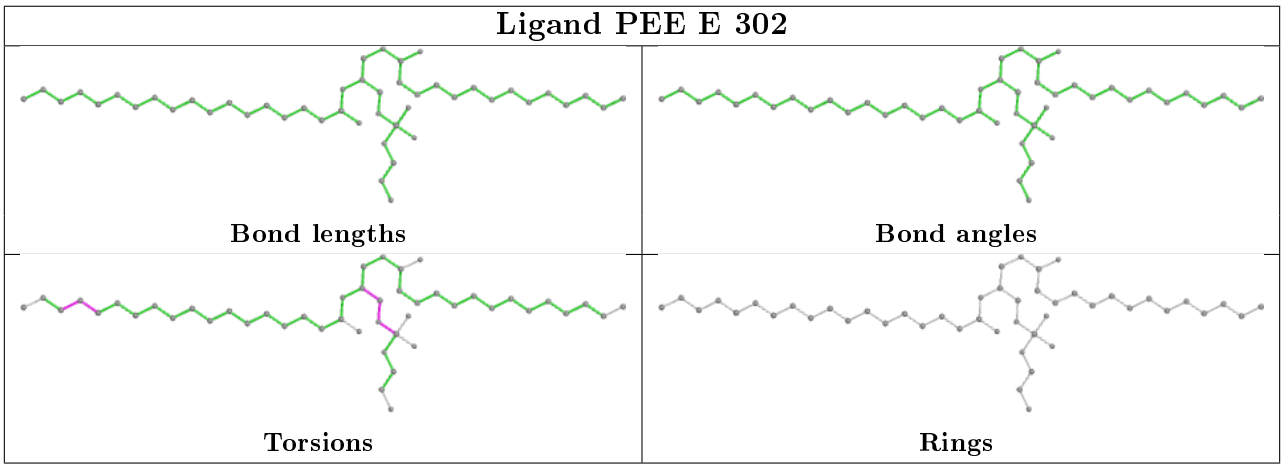
Ligand LMT C 308



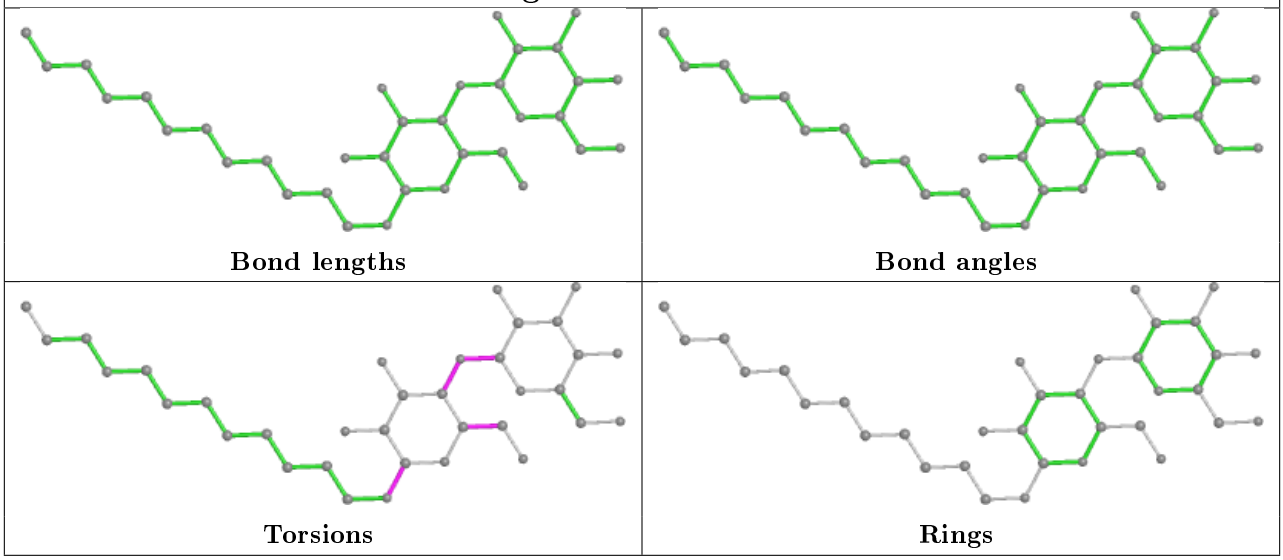
Ligand LMT B 304



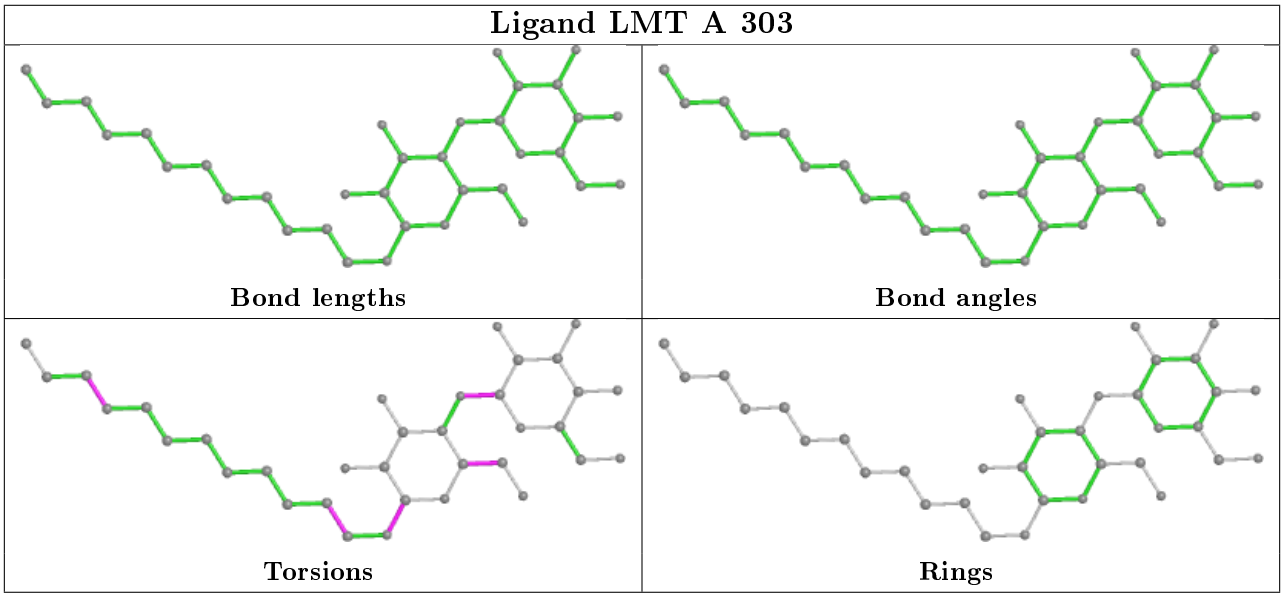
Ligand PEE E 302



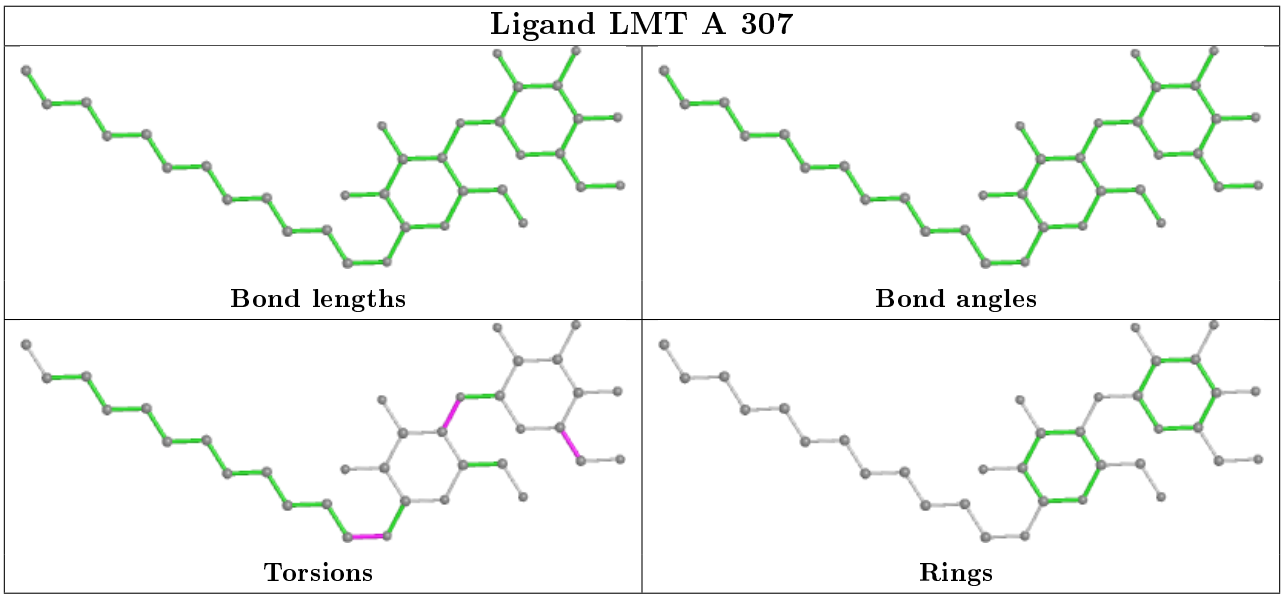
Ligand LMT C 307



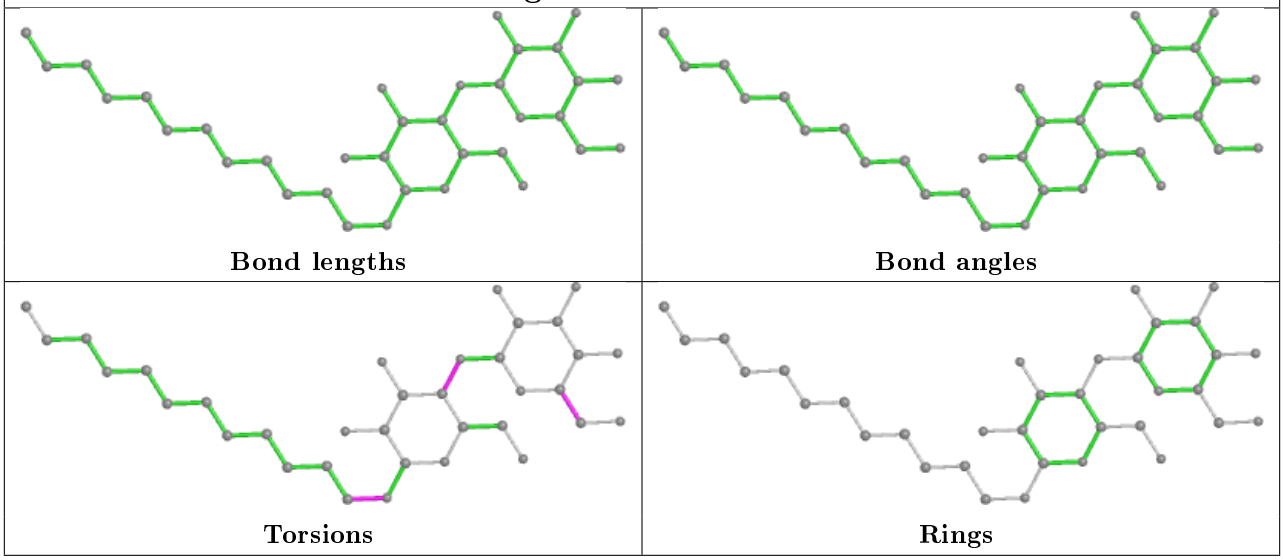
Ligand LMT A 303



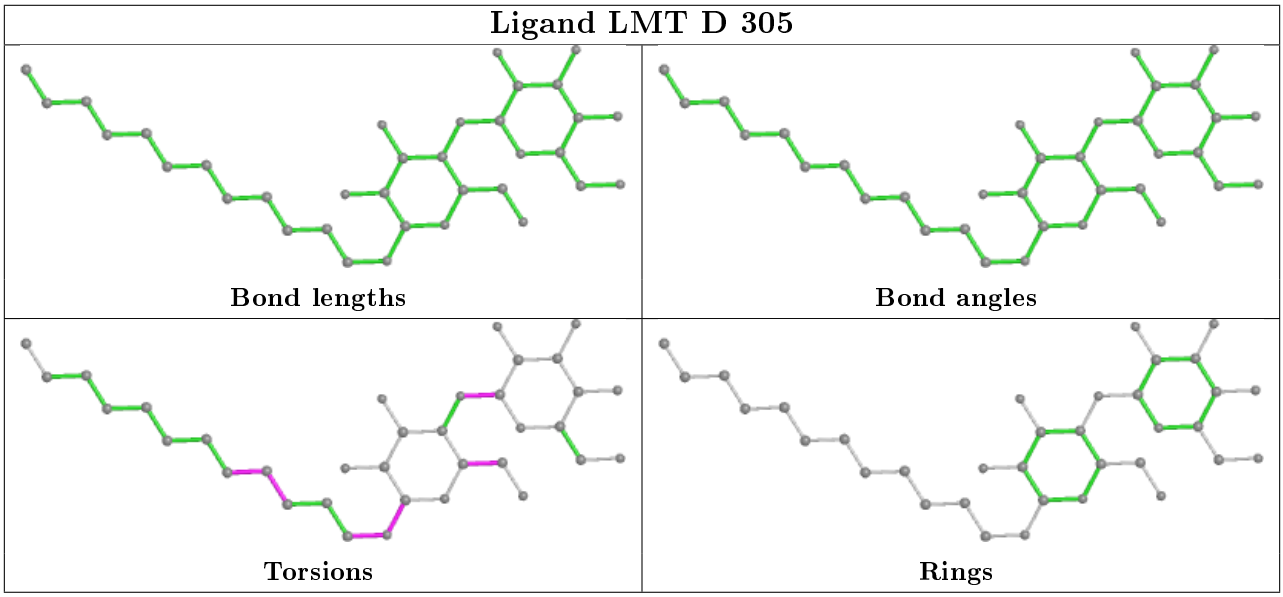
Ligand LMT A 307



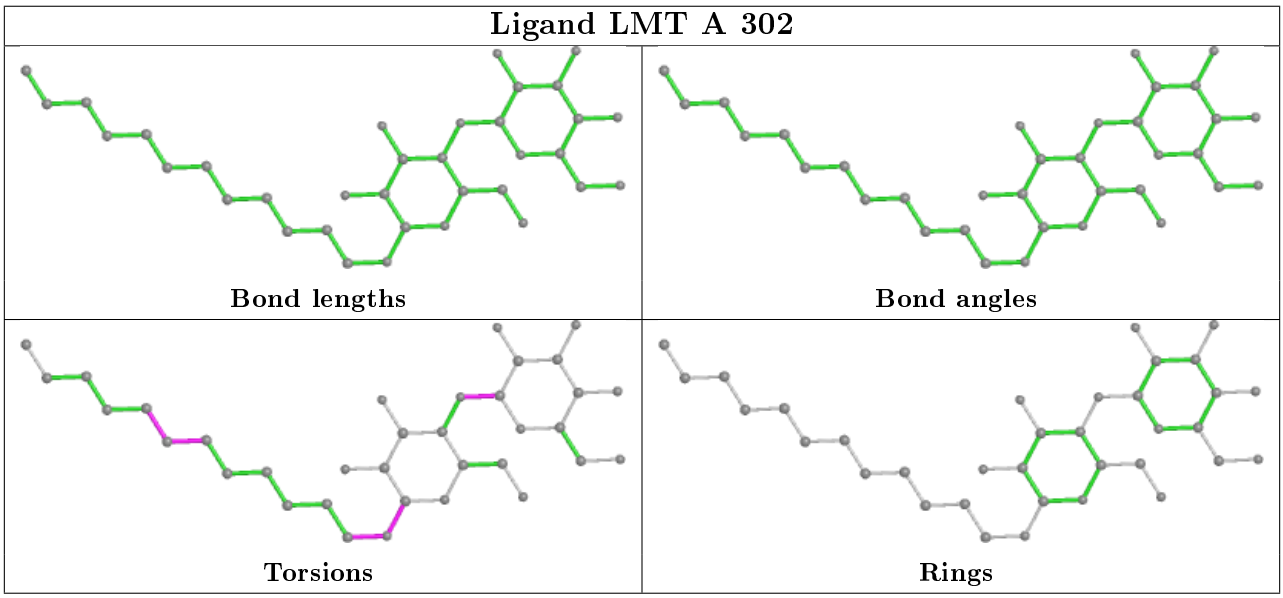
Ligand LMT F 307



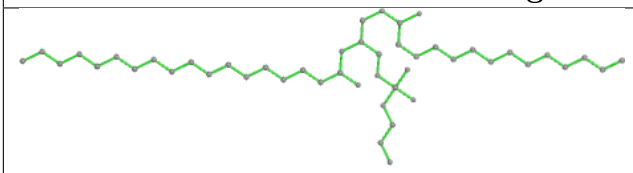
Ligand LMT D 305

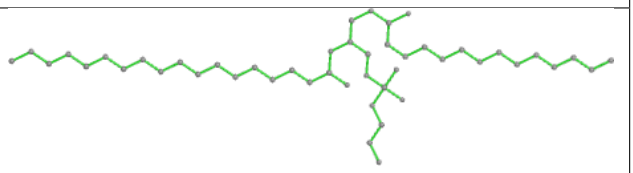


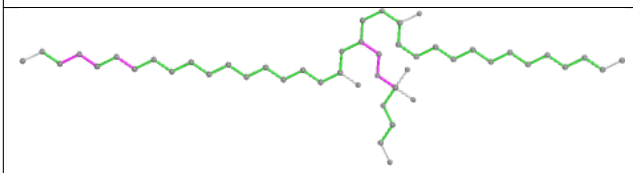
Ligand LMT A 302

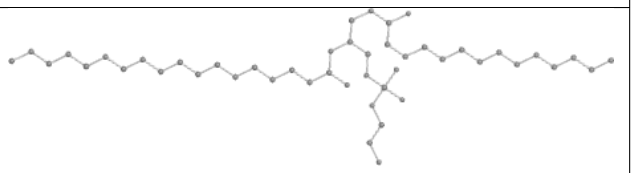


Ligand PEE B 302

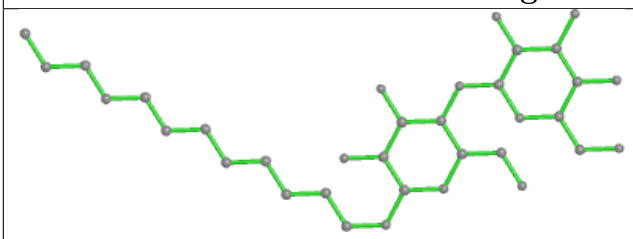

Bond lengths

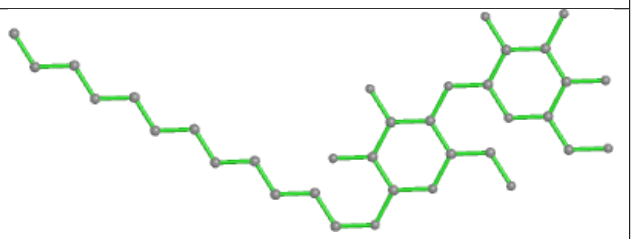

Bond angles

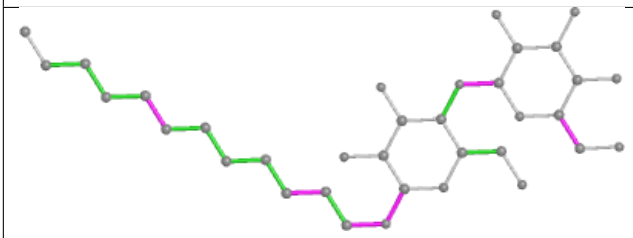

Torsions

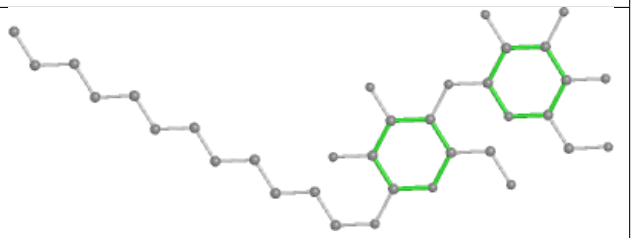

Rings

Ligand LMT G 409

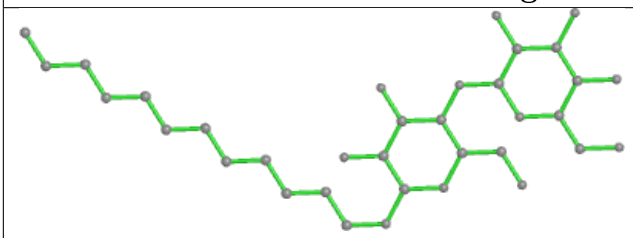

Bond lengths

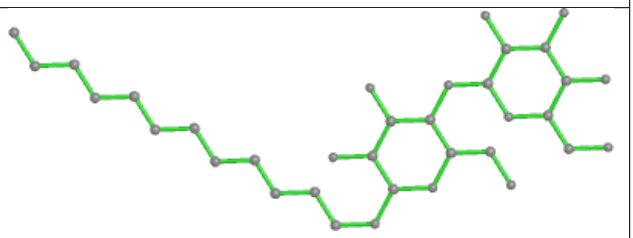

Bond angles

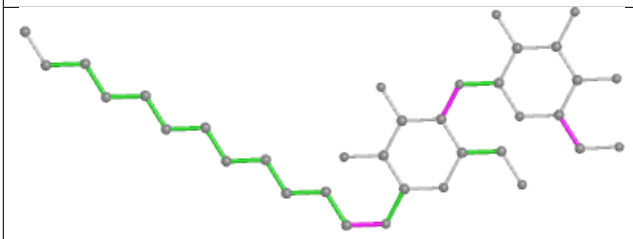

Torsions

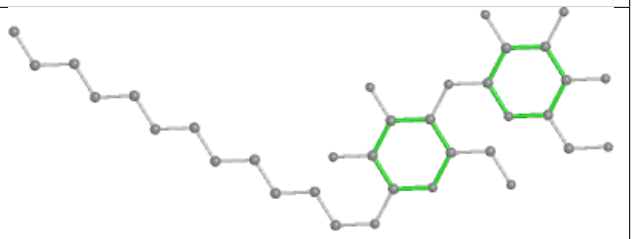

Rings

Ligand LMT D 308

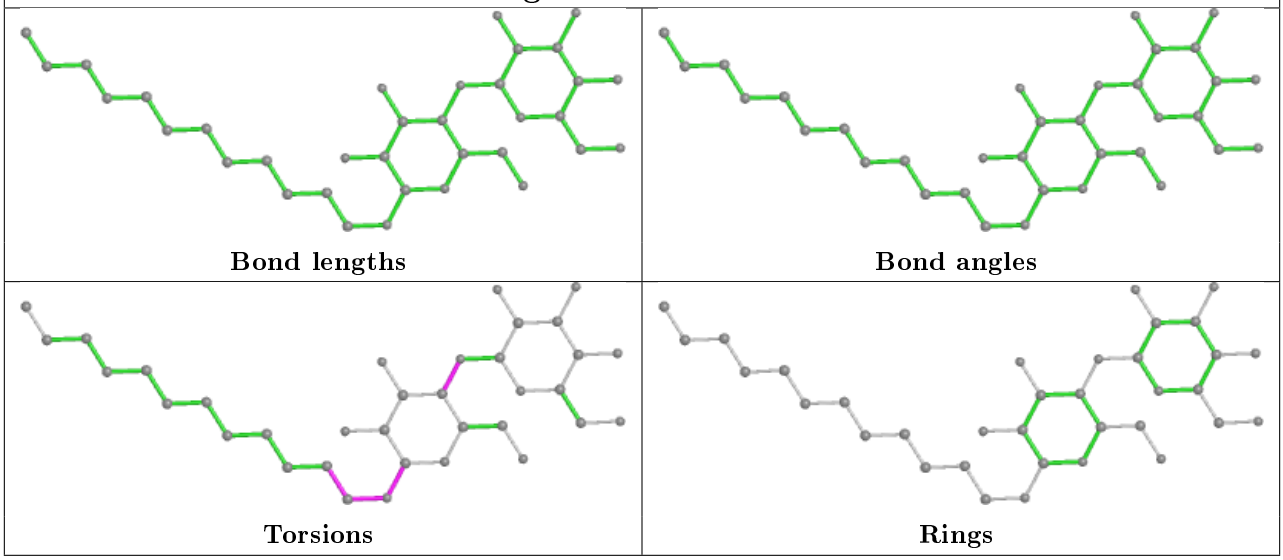

Bond lengths


Bond angles

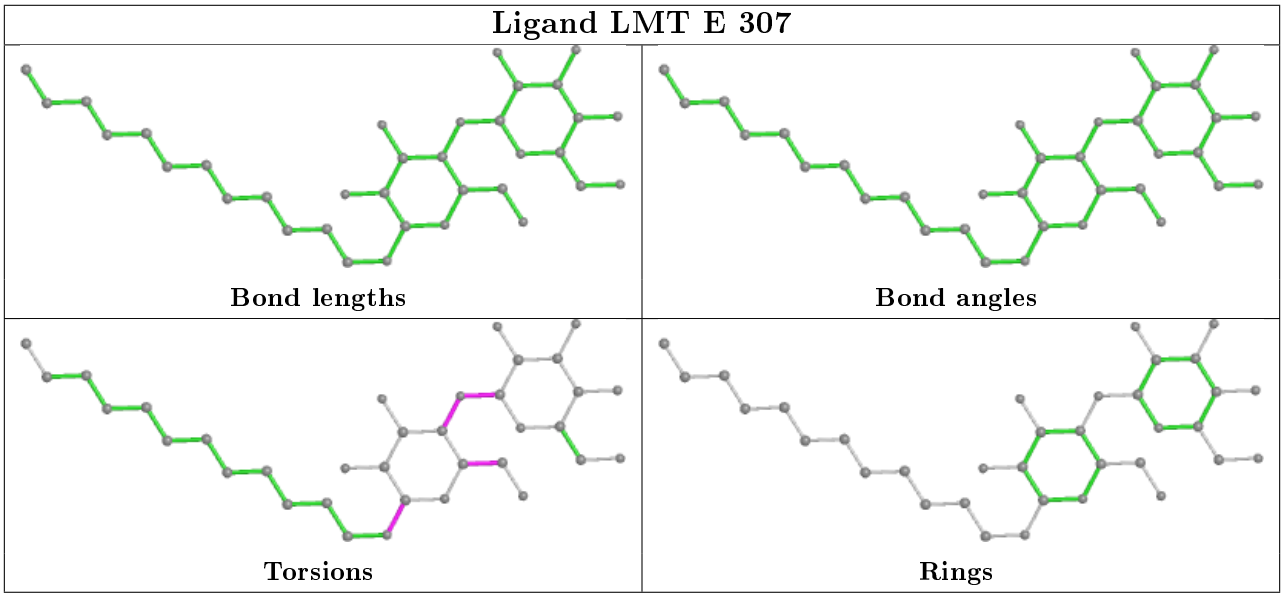

Torsions


Rings

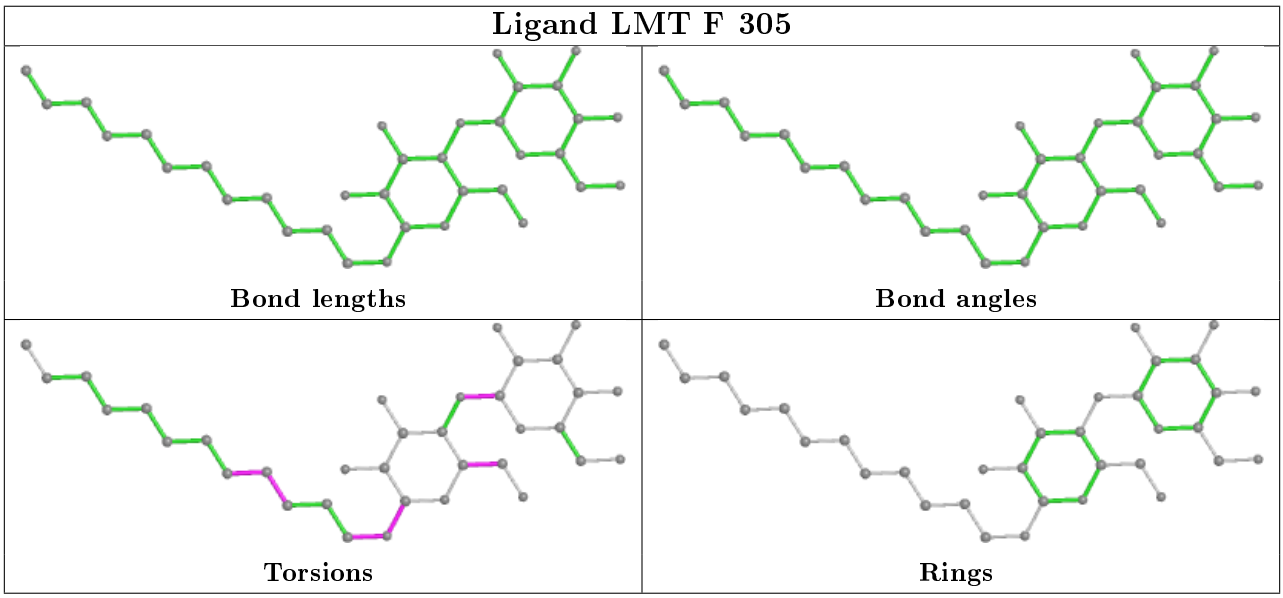
Ligand LMT E 301



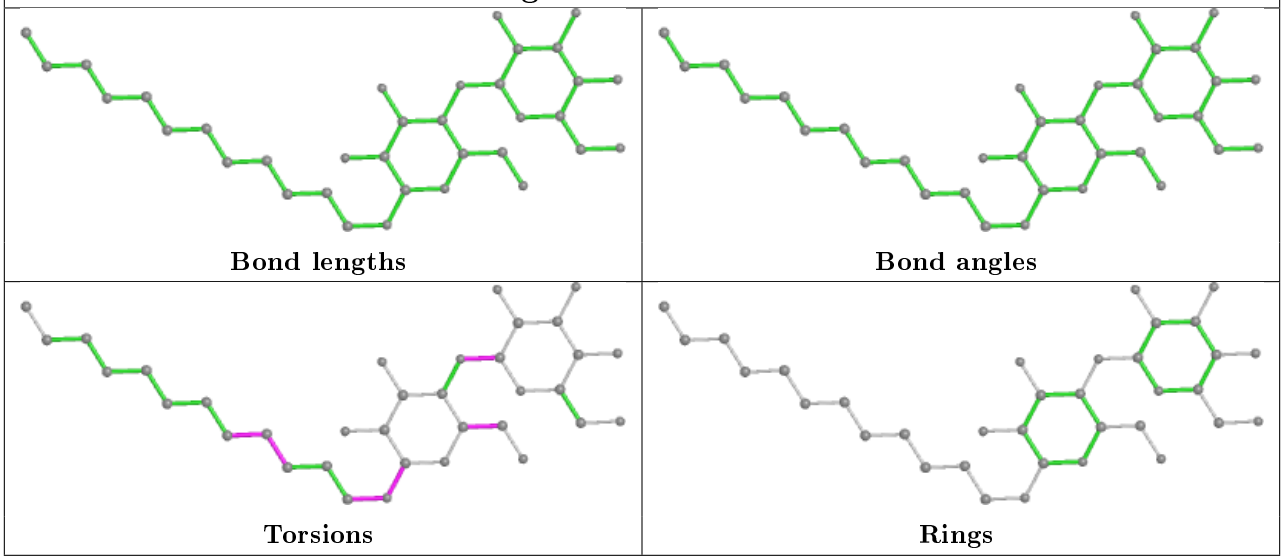
Ligand LMT E 307



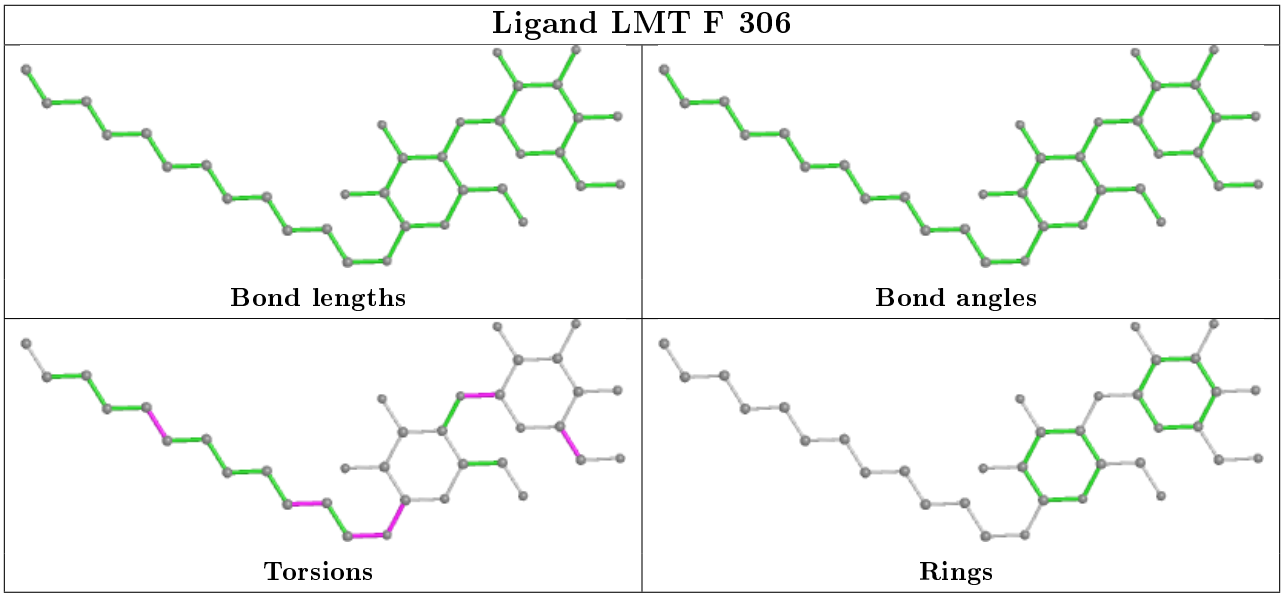
Ligand LMT F 305



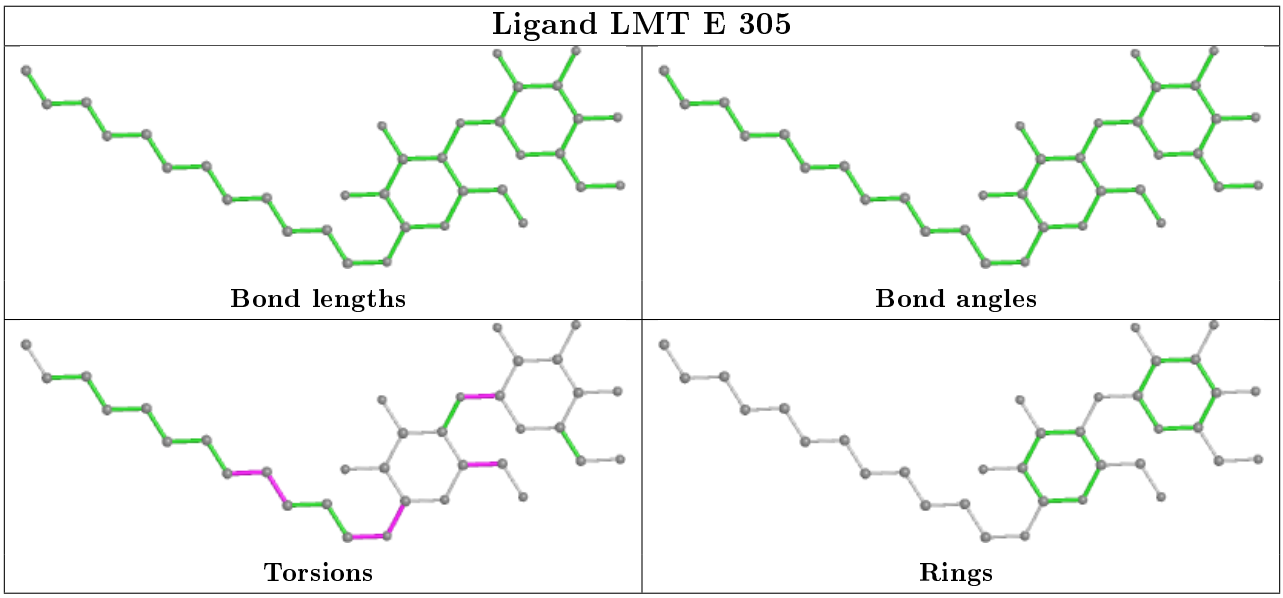
Ligand LMT G 408



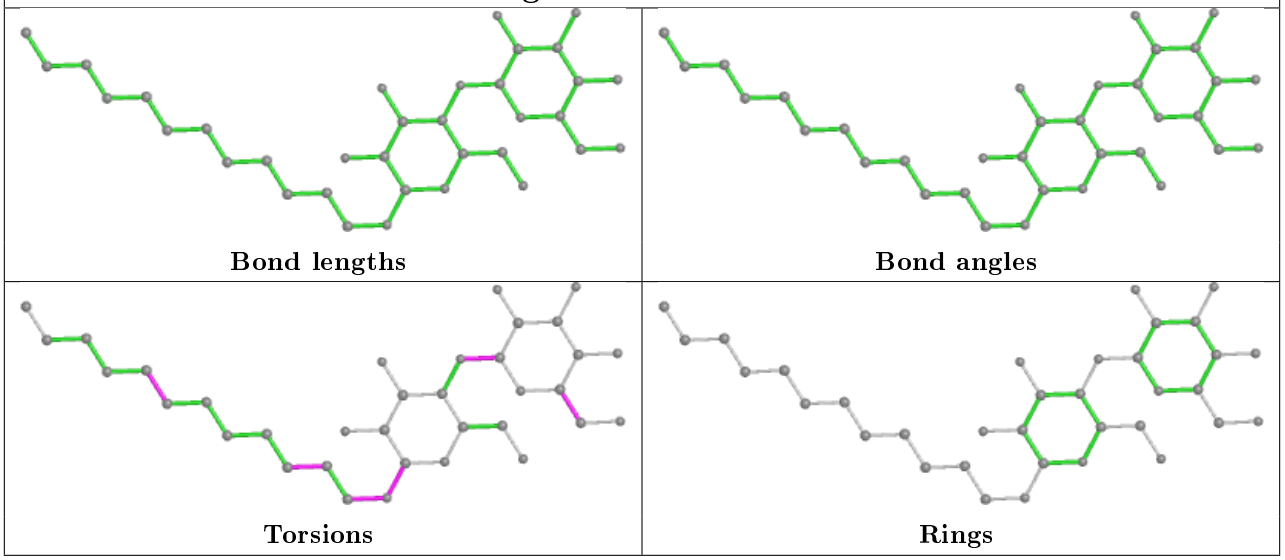
Ligand LMT F 306



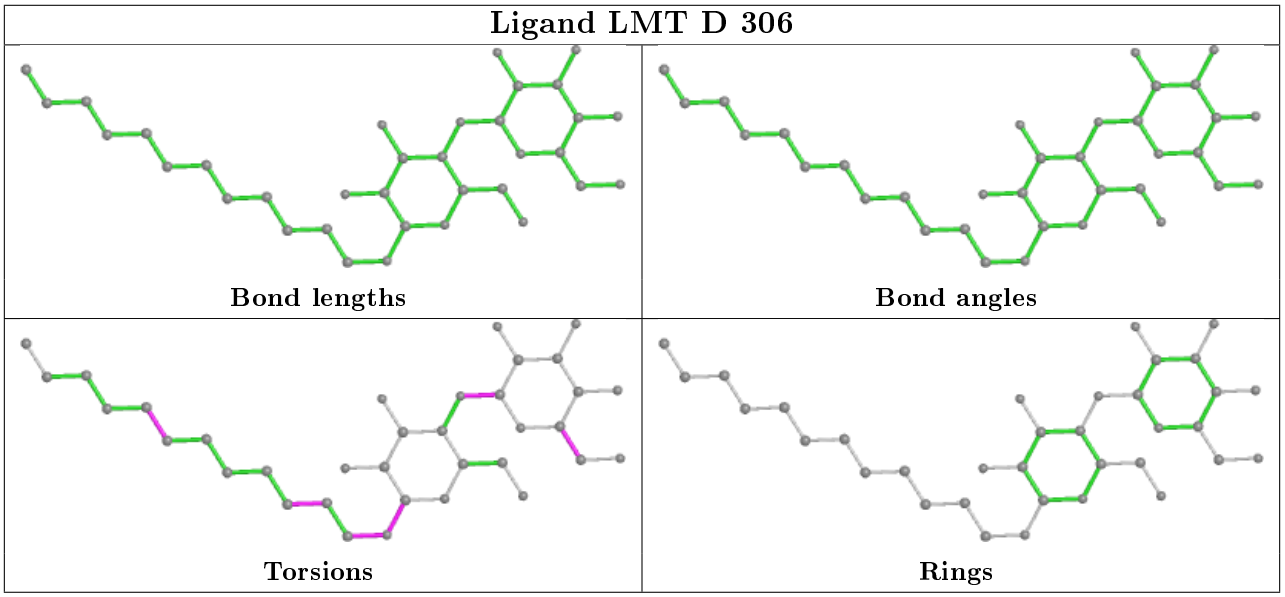
Ligand LMT E 305



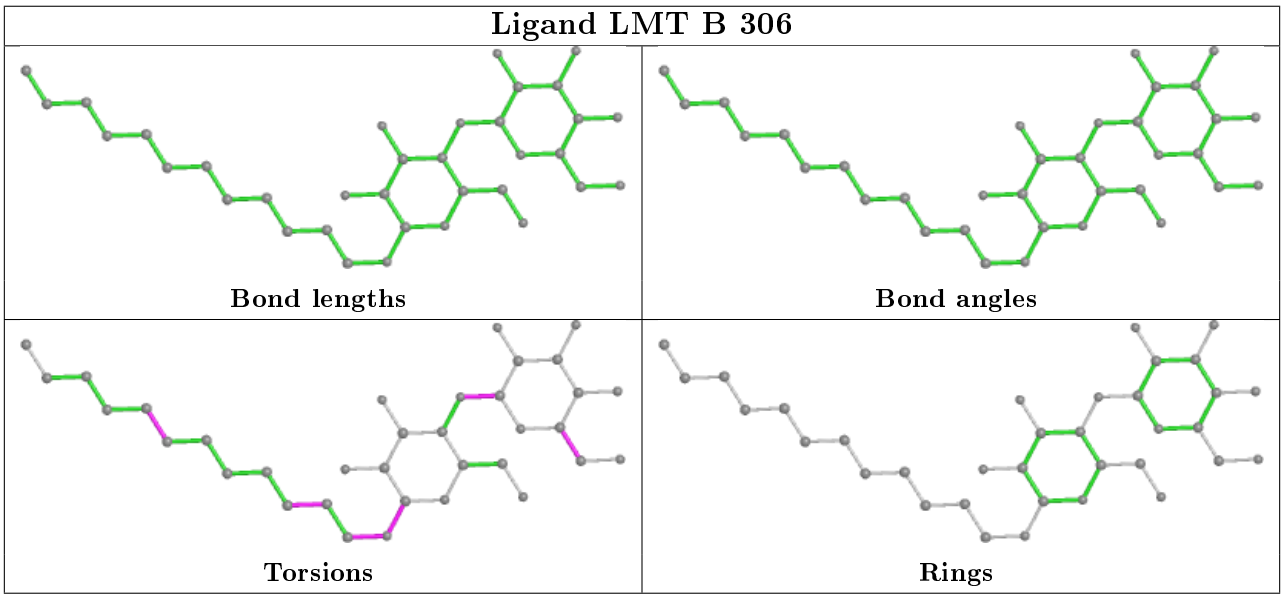
Ligand LMT A 305



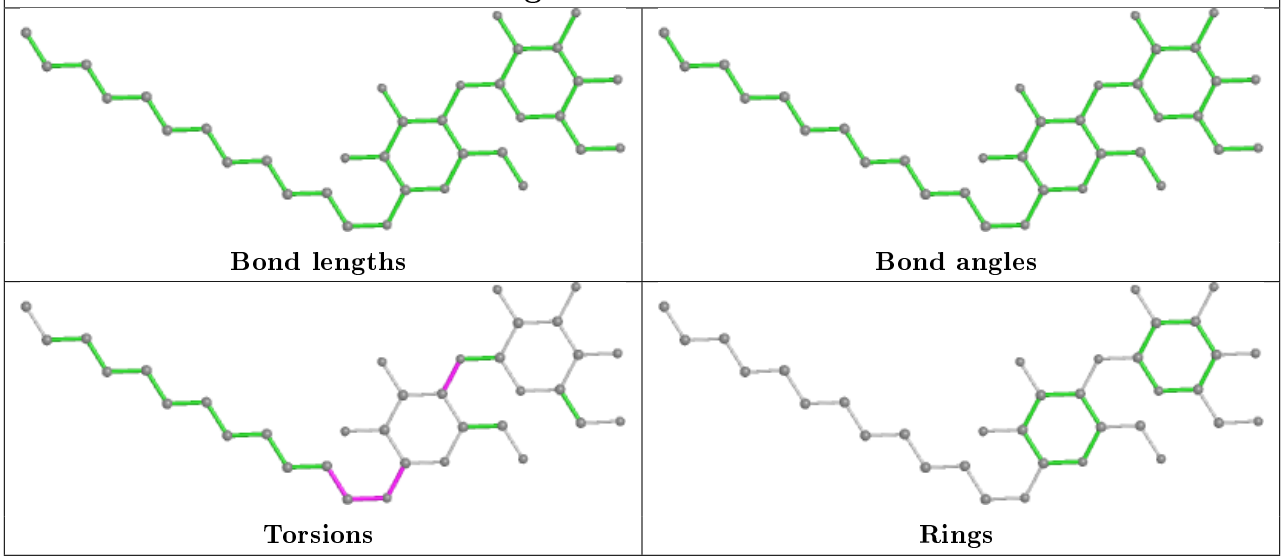
Ligand LMT D 306



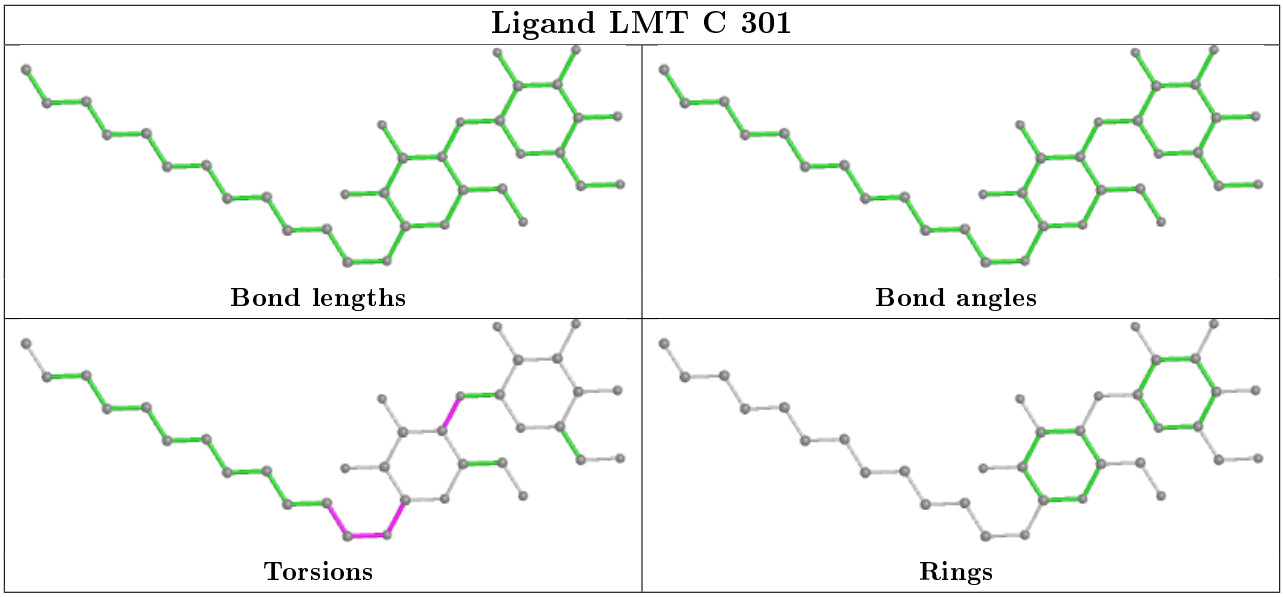
Ligand LMT B 306



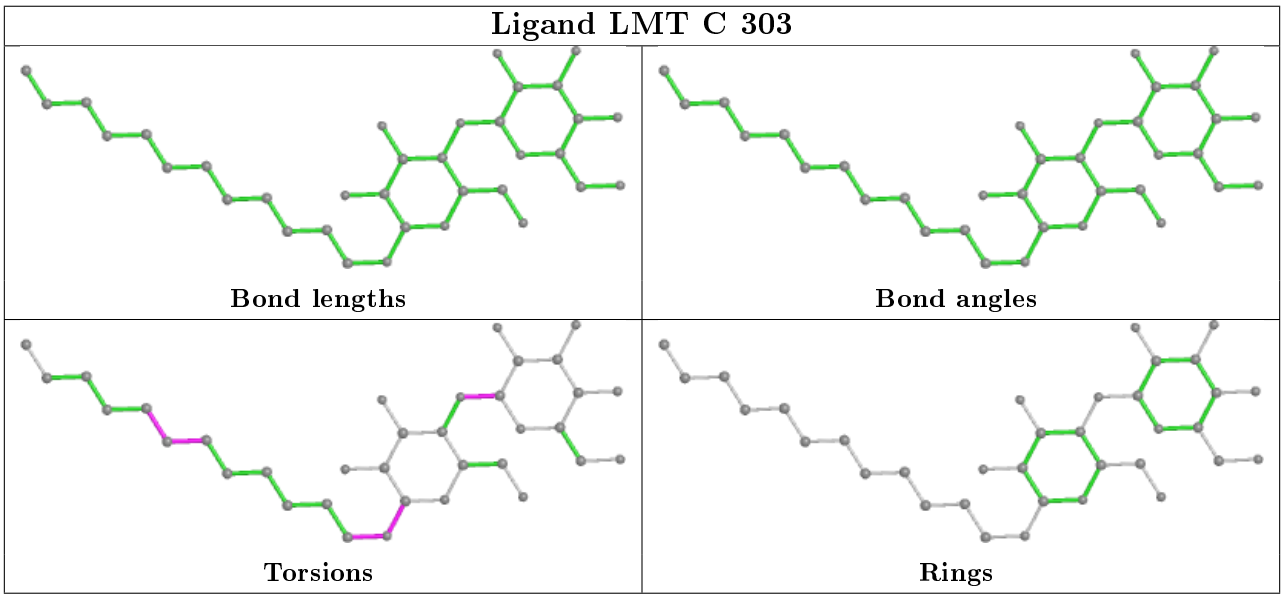
Ligand LMT F 301



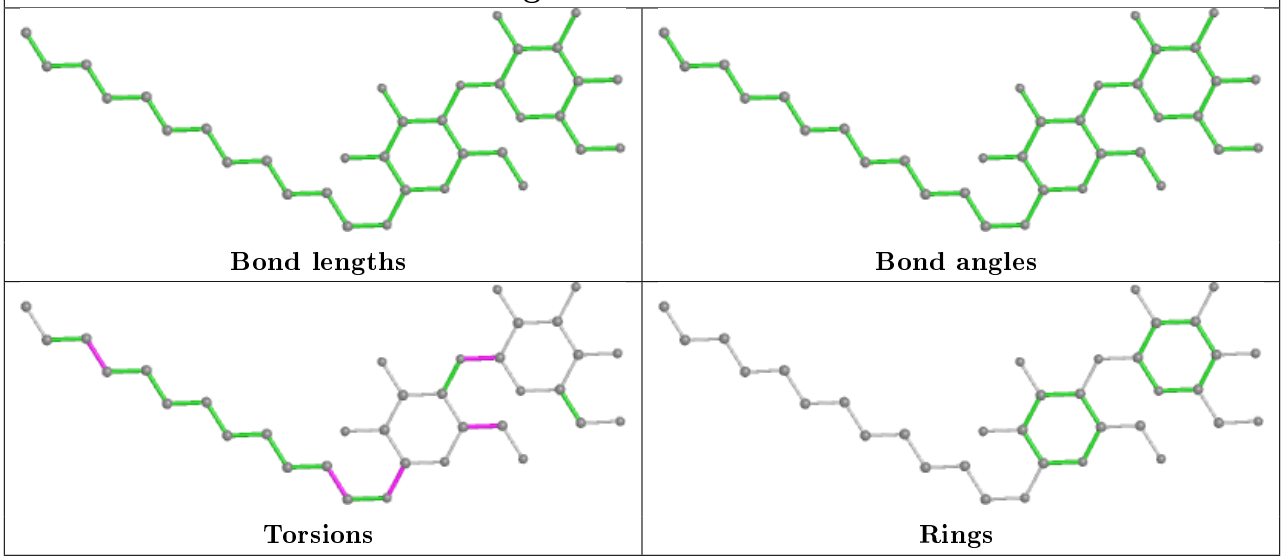
Ligand LMT C 301



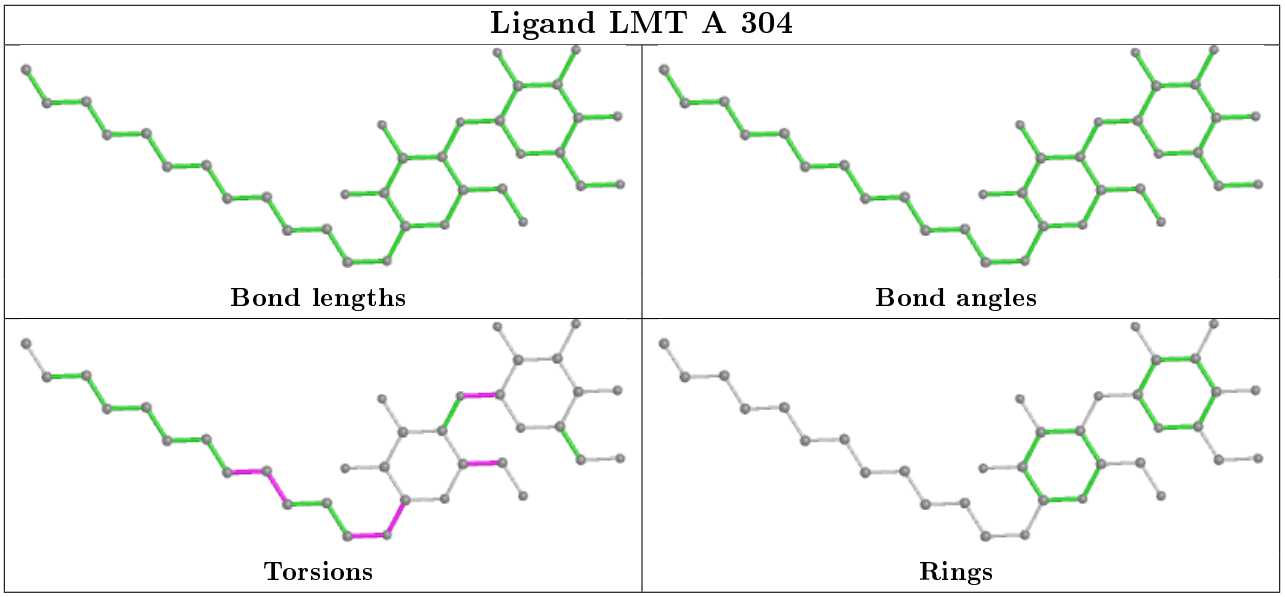
Ligand LMT C 303



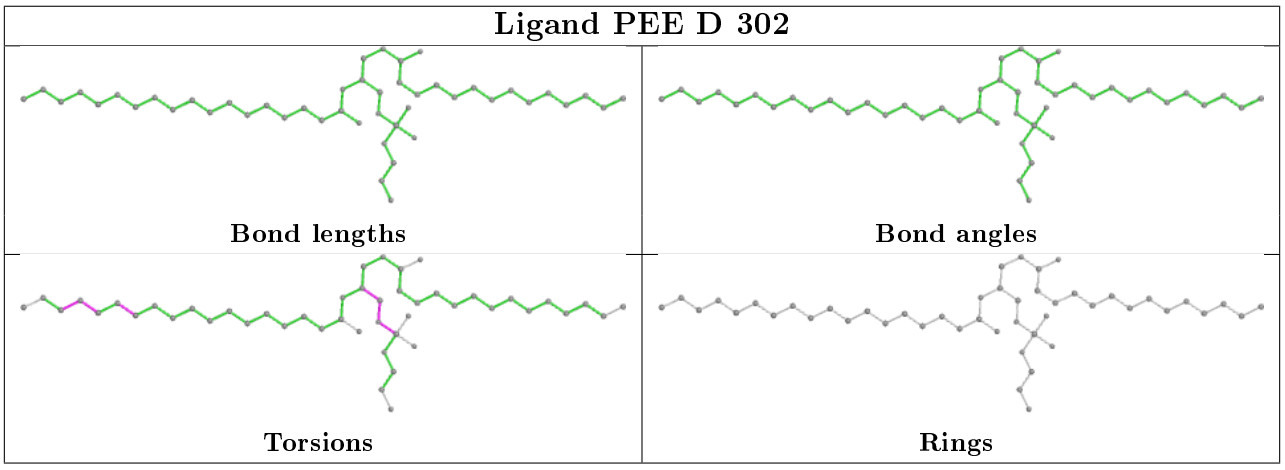
Ligand LMT E 304



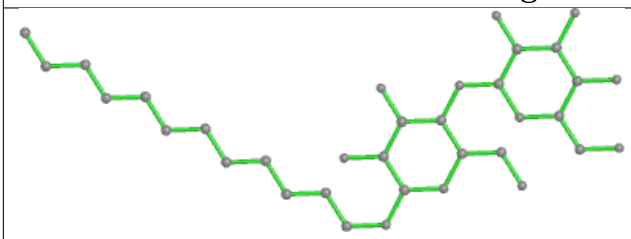
Ligand LMT A 304

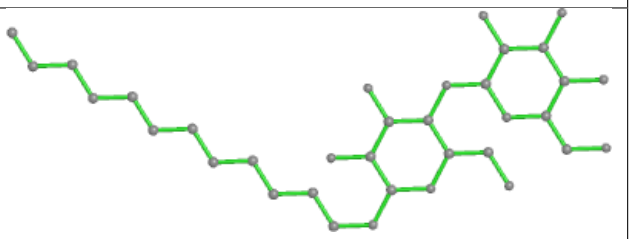


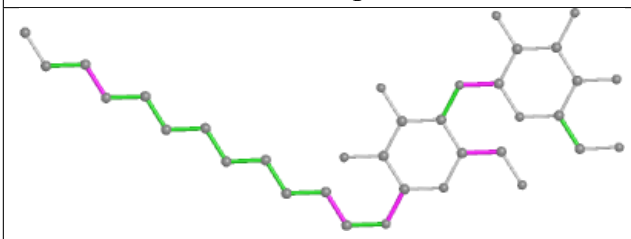
Ligand PEE D 302

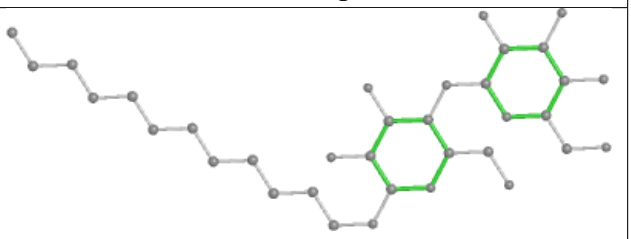


Ligand LMT D 304

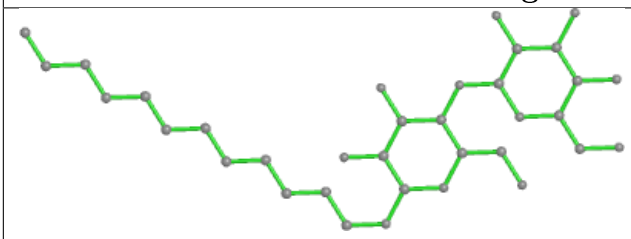

Bond lengths

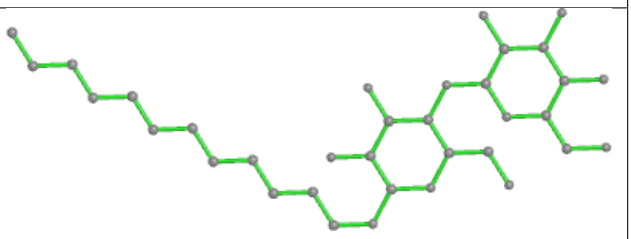

Bond angles

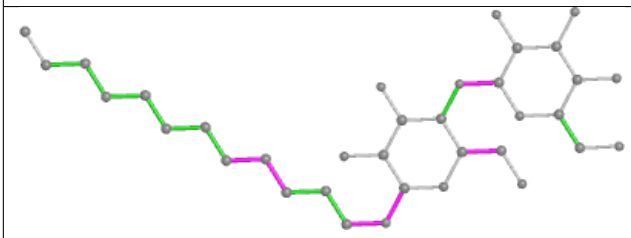

Torsions

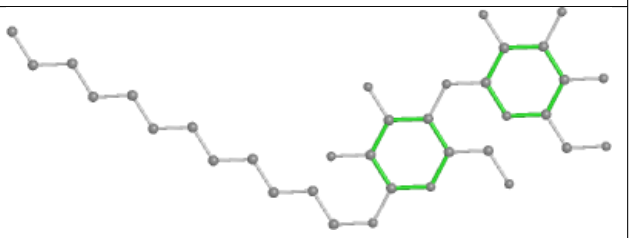

Rings

Ligand LMT C 305

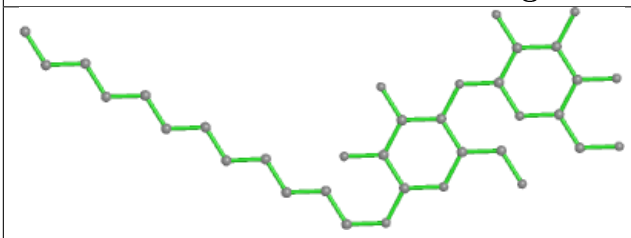

Bond lengths

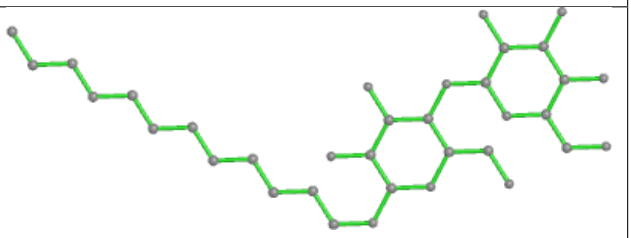

Bond angles

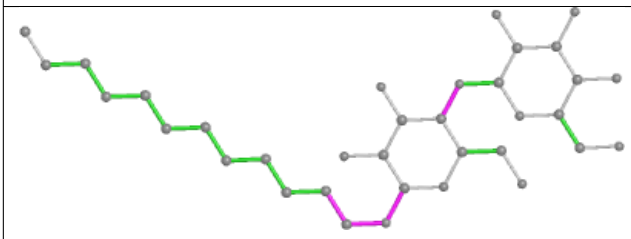

Torsions

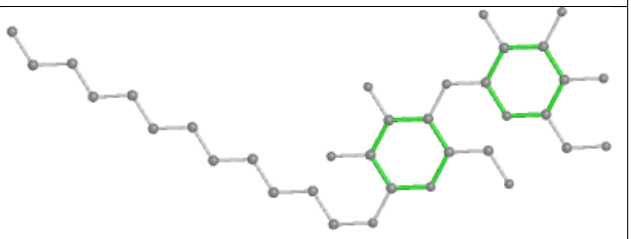

Rings

Ligand LMT B 301

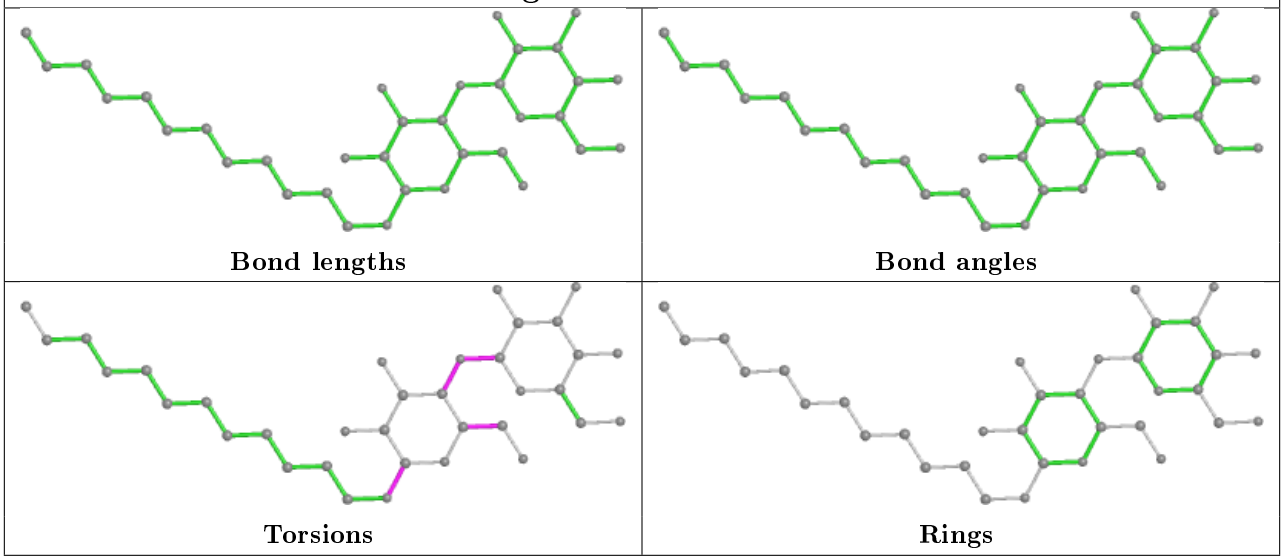

Bond lengths


Bond angles

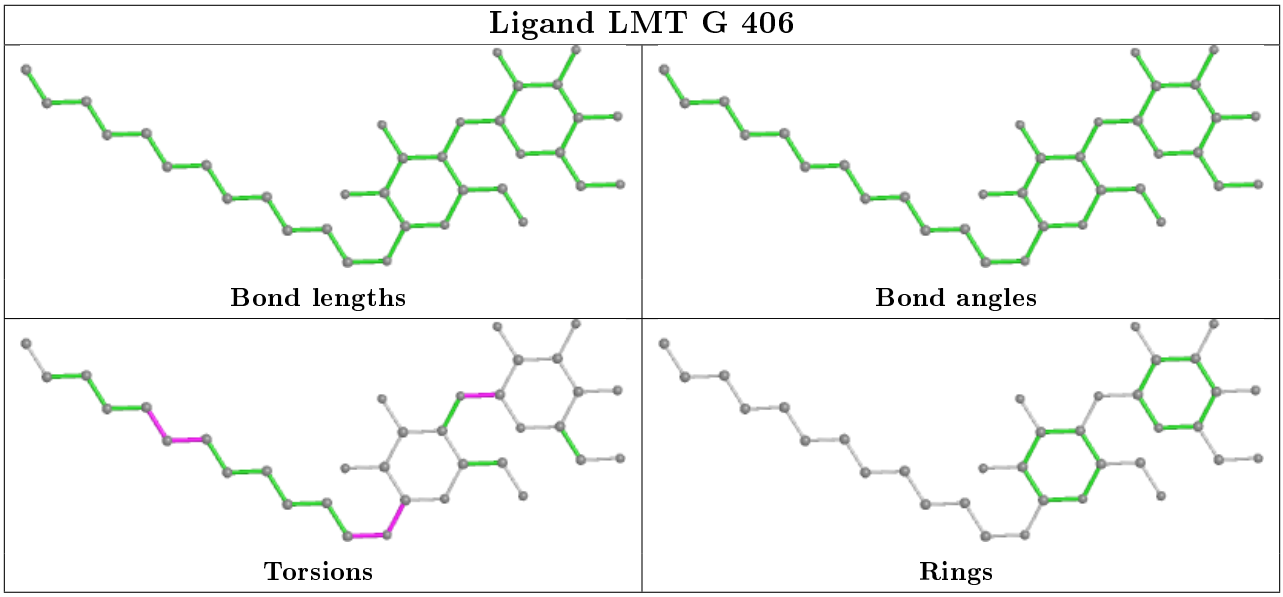

Torsions


Rings

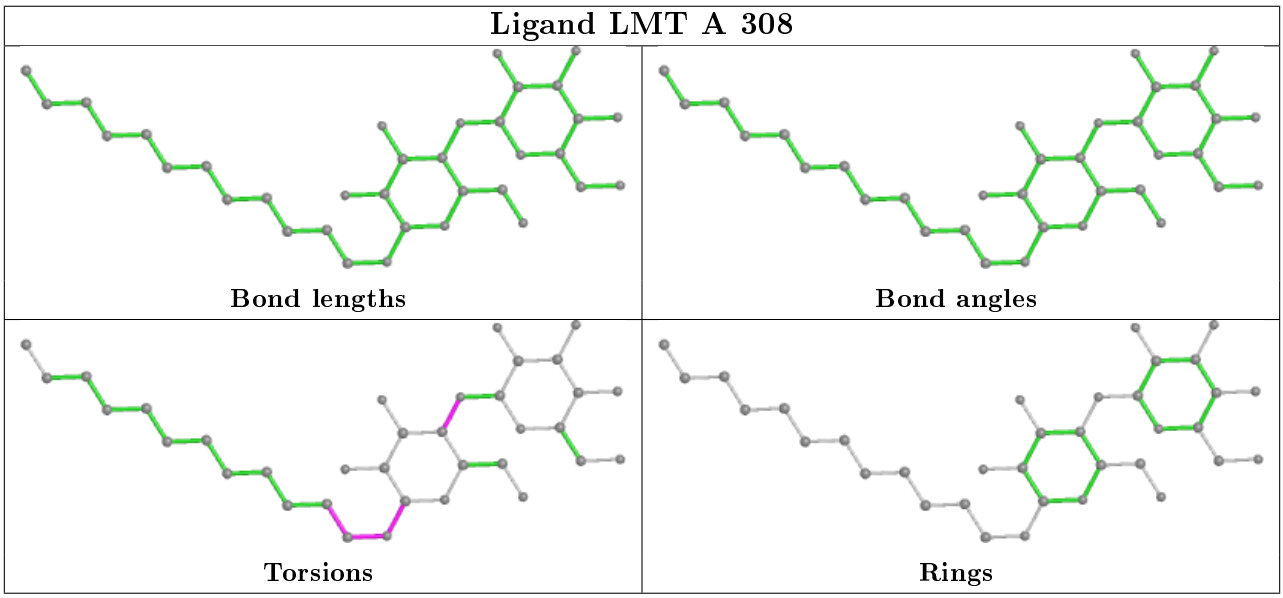
Ligand LMT B 307



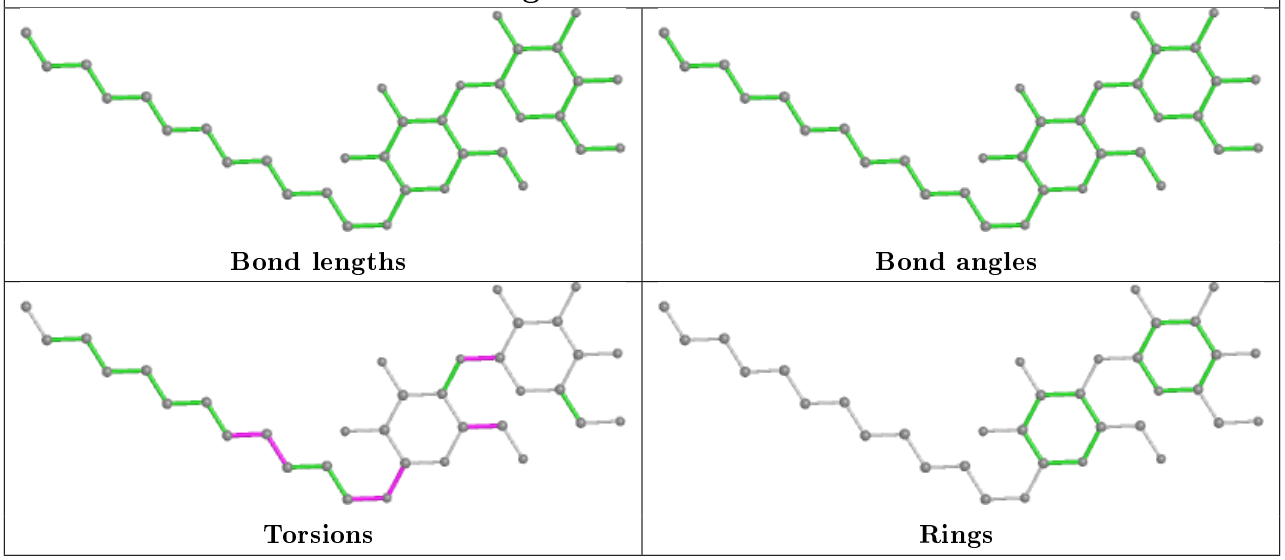
Ligand LMT G 406



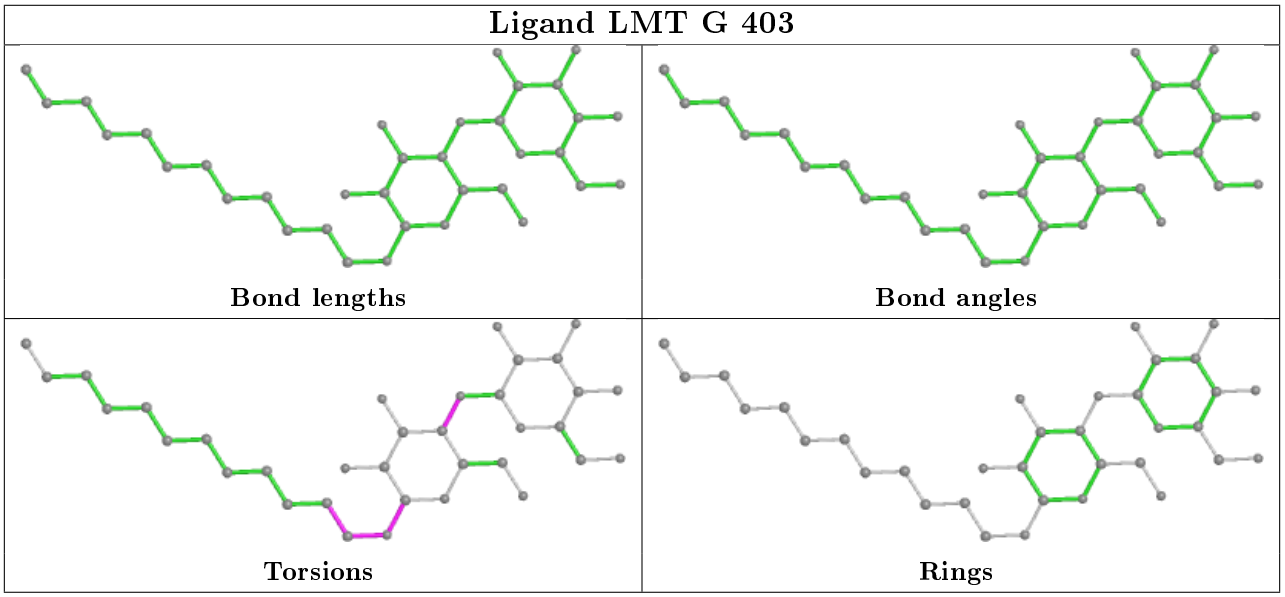
Ligand LMT A 308



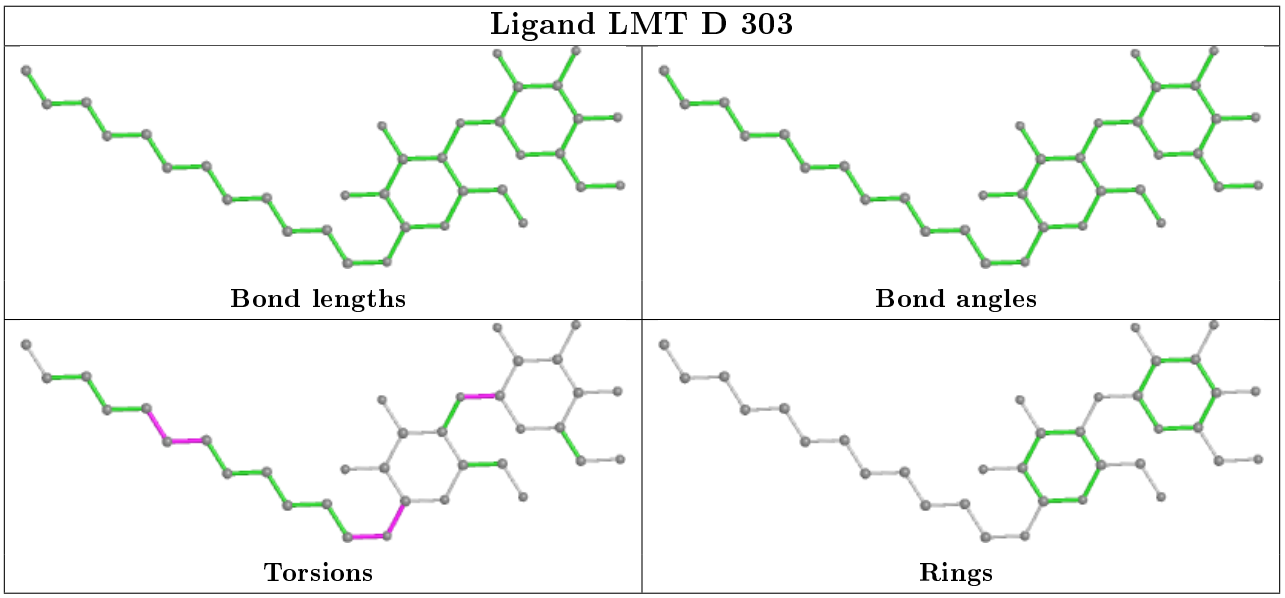
Ligand LMT B 305



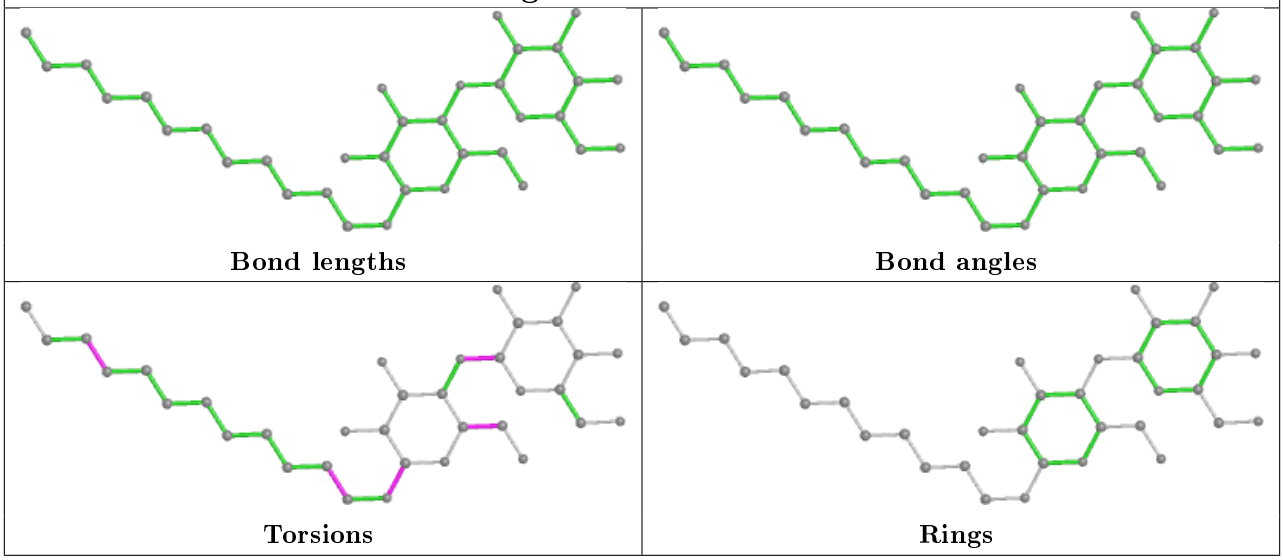
Ligand LMT G 403



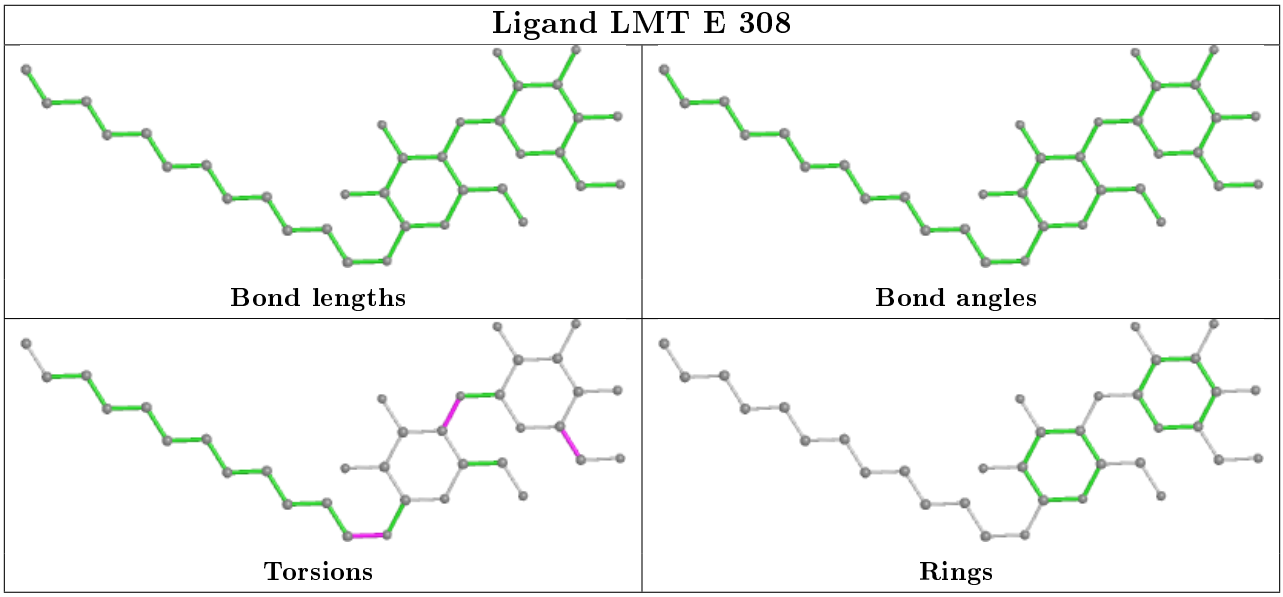
Ligand LMT D 303



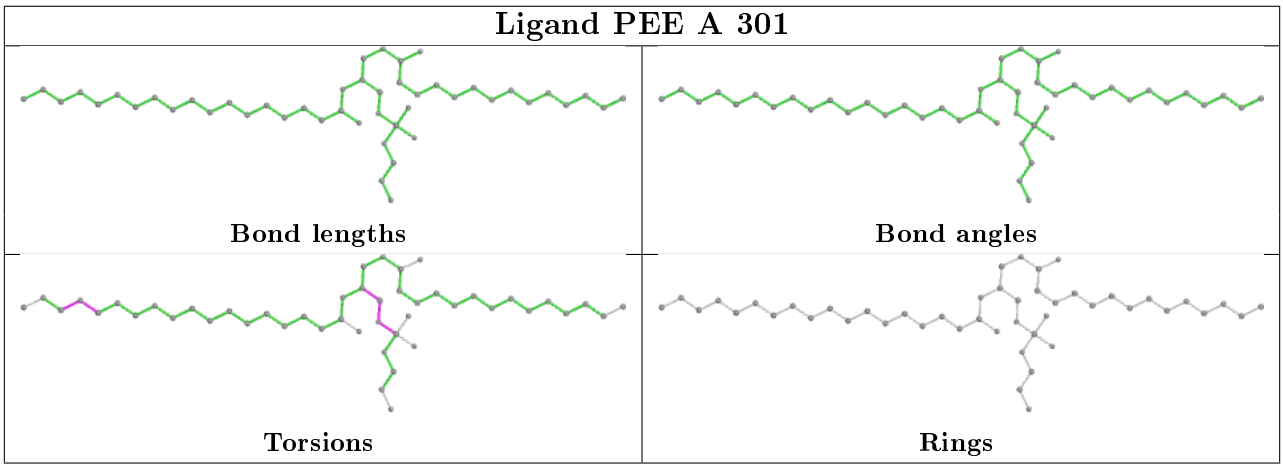
Ligand LMT G 407



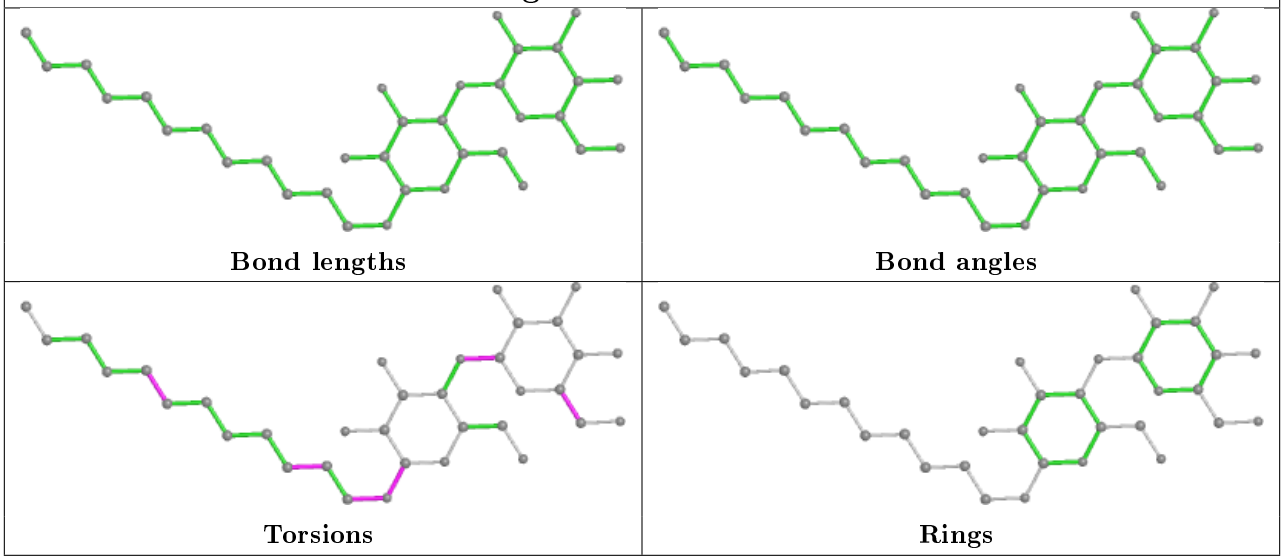
Ligand LMT E 308



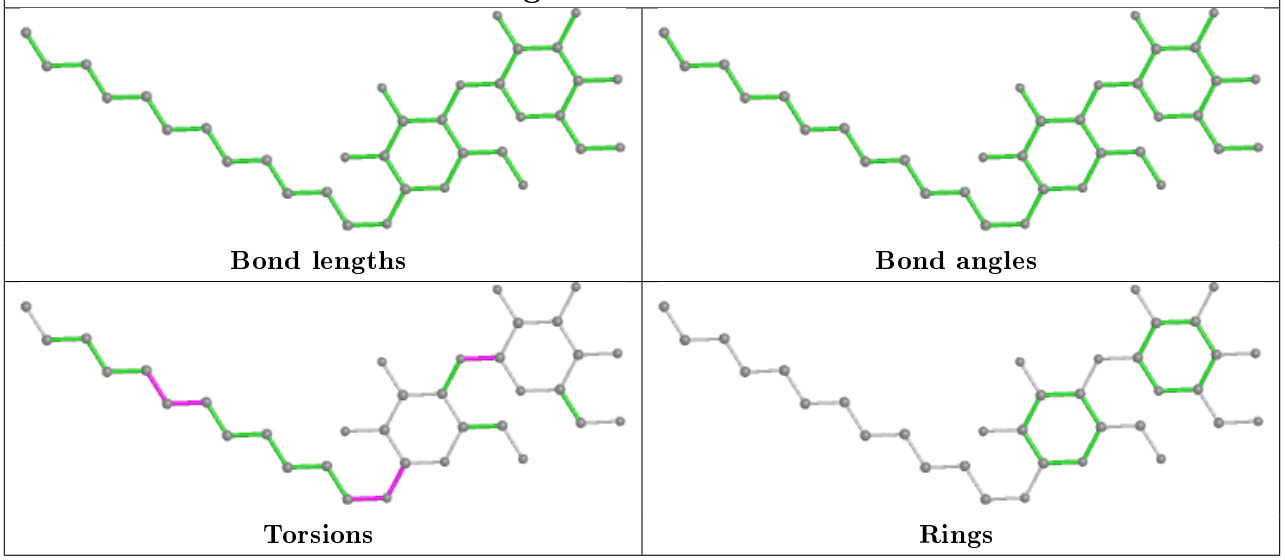
Ligand PEE A 301



Ligand LMT C 306



Ligand LMT E 303



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.

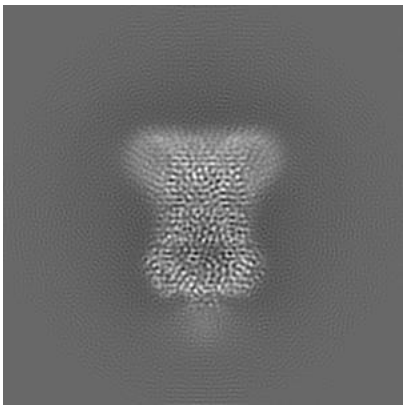
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13003. These allow visual inspection of the internal detail of the map and identification of artifacts.

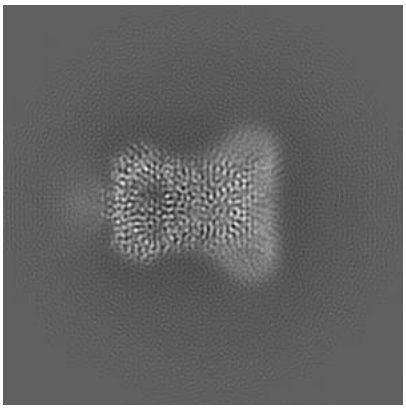
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

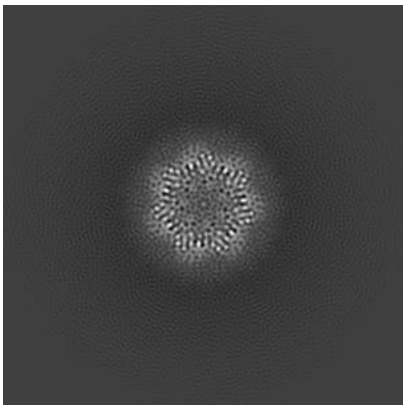
6.1.1 Primary map



X

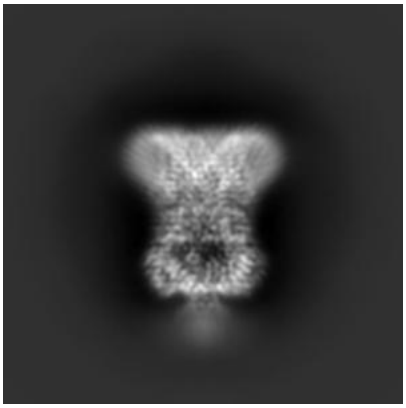


Y

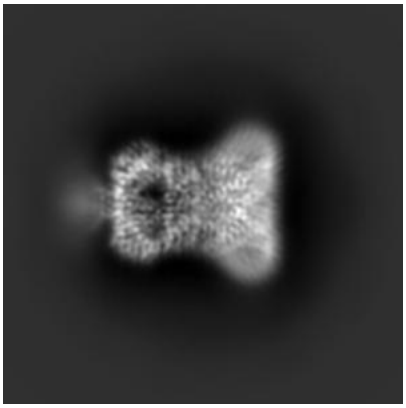


Z

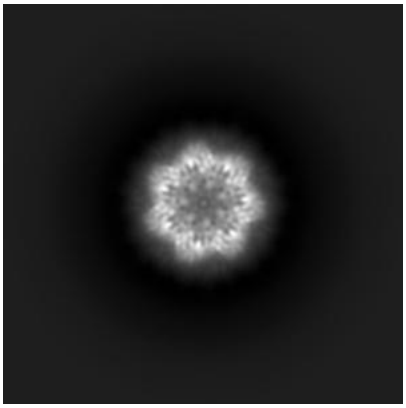
6.1.2 Raw map



X



Y

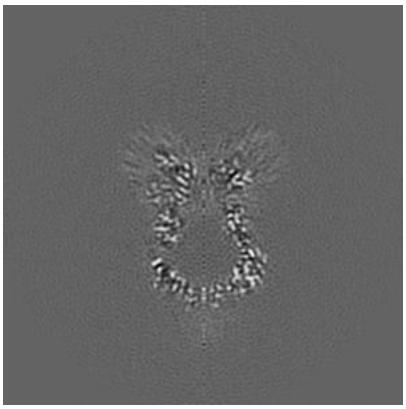


Z

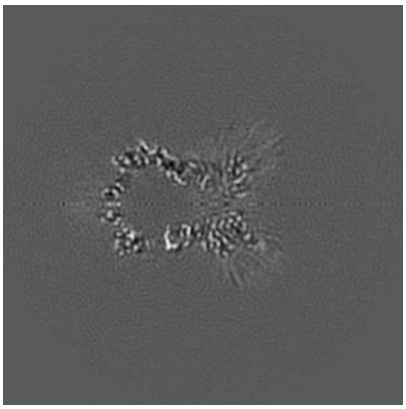
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

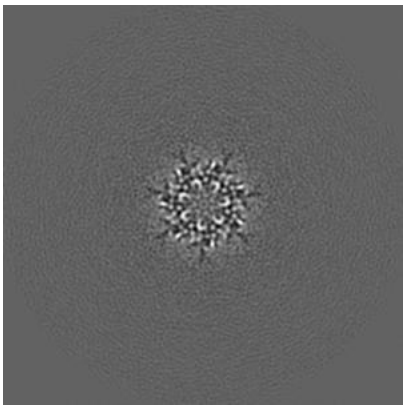
6.2.1 Primary map



X Index: 128

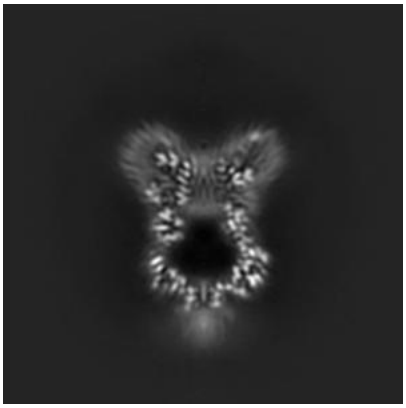


Y Index: 128

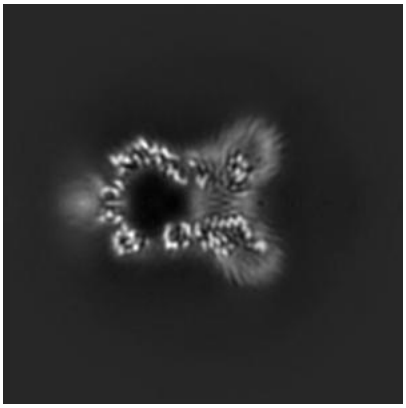


Z Index: 128

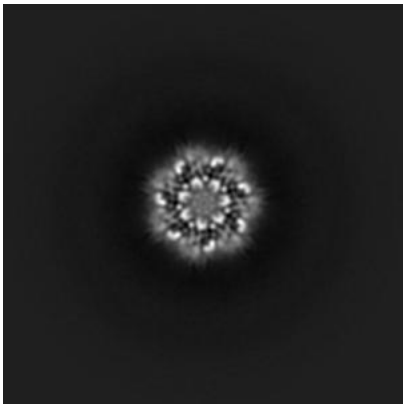
6.2.2 Raw map



X Index: 128



Y Index: 128

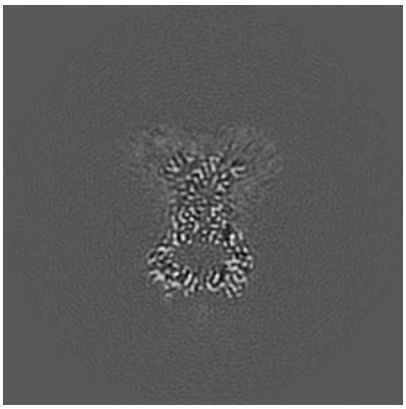


Z Index: 128

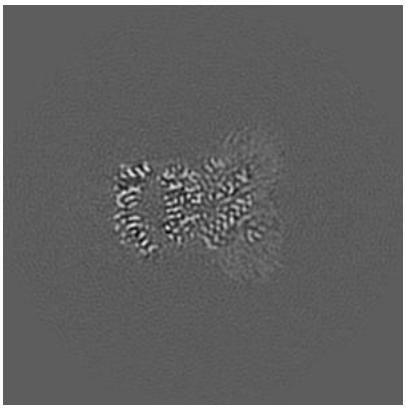
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

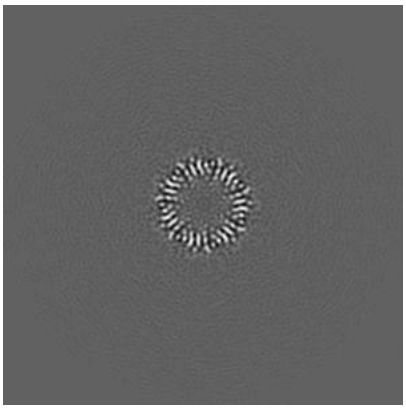
6.3.1 Primary map



X Index: 146

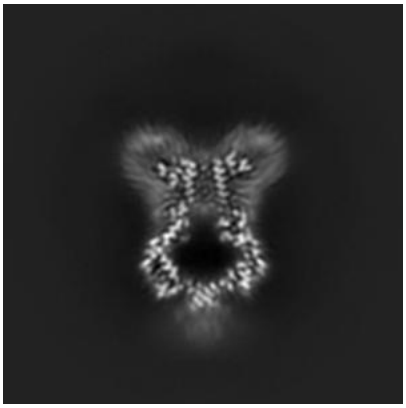


Y Index: 109

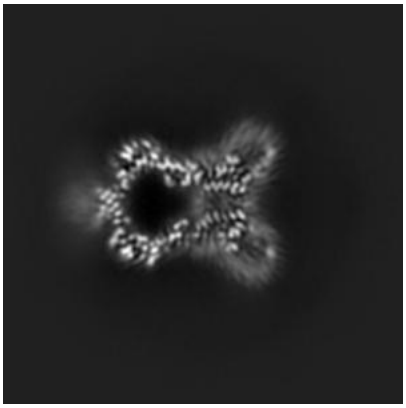


Z Index: 107

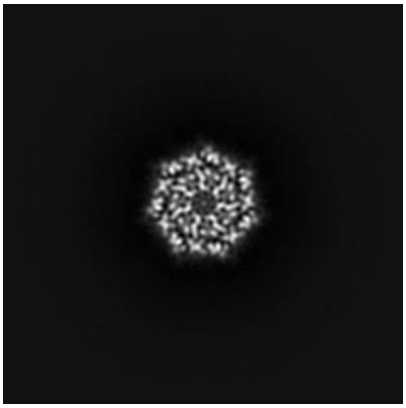
6.3.2 Raw map



X Index: 120



Y Index: 121

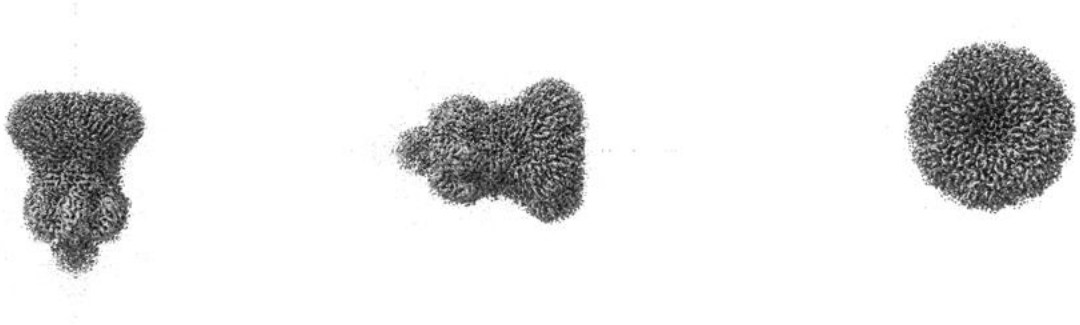


Z Index: 75

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

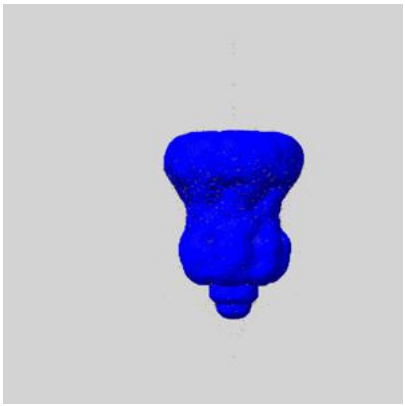
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

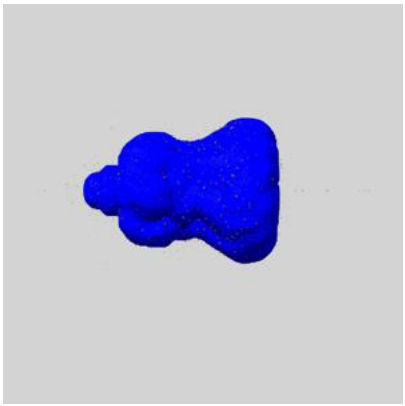
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

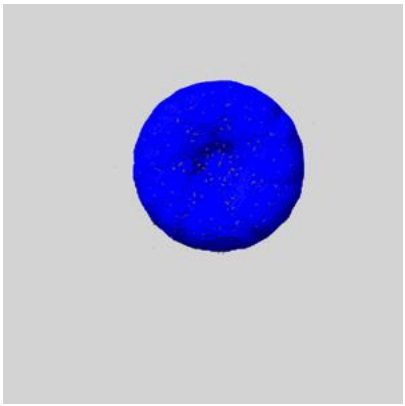
6.5.1 emd_13003_msk_1.map



X



Y

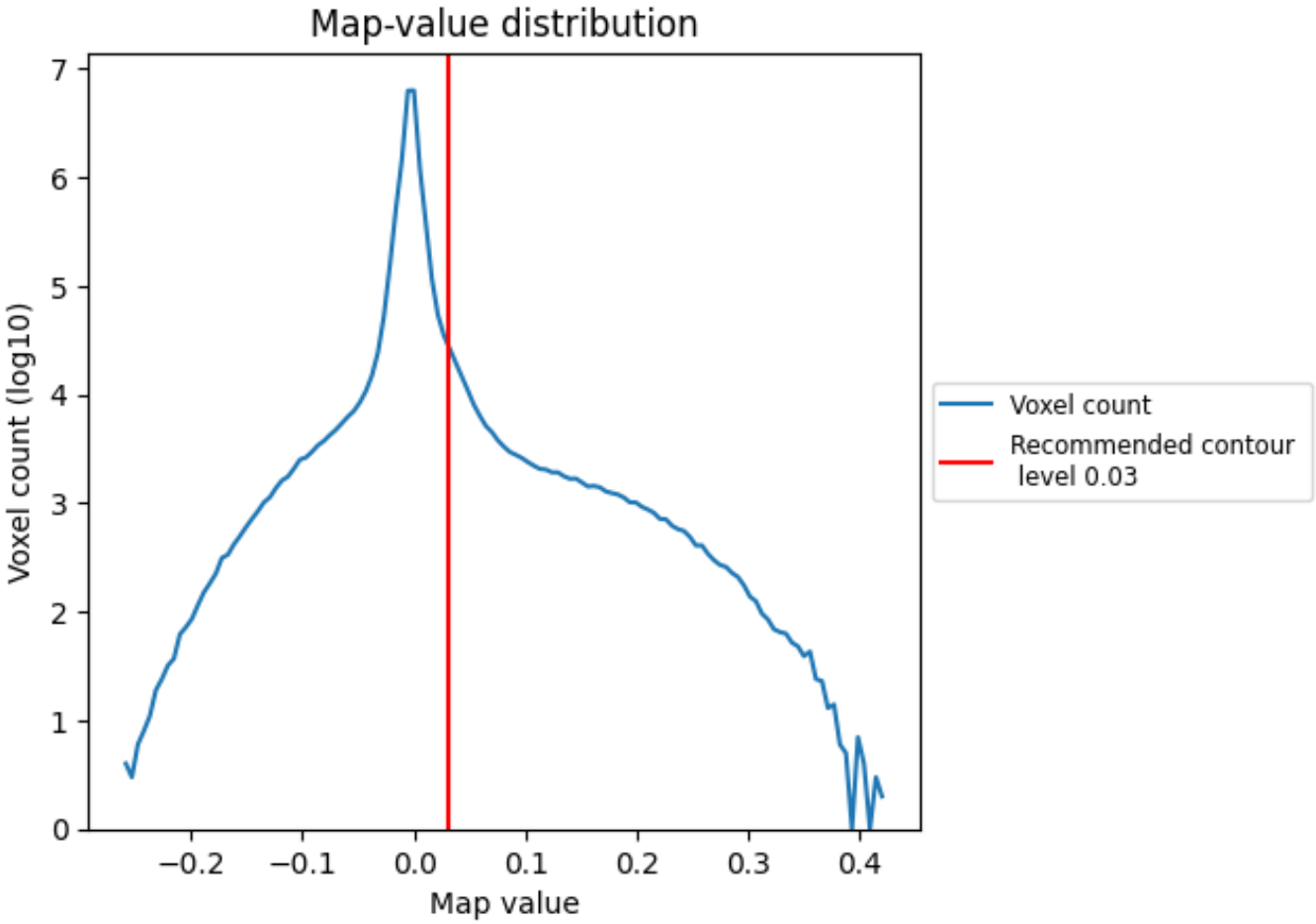


Z

7 Map analysis

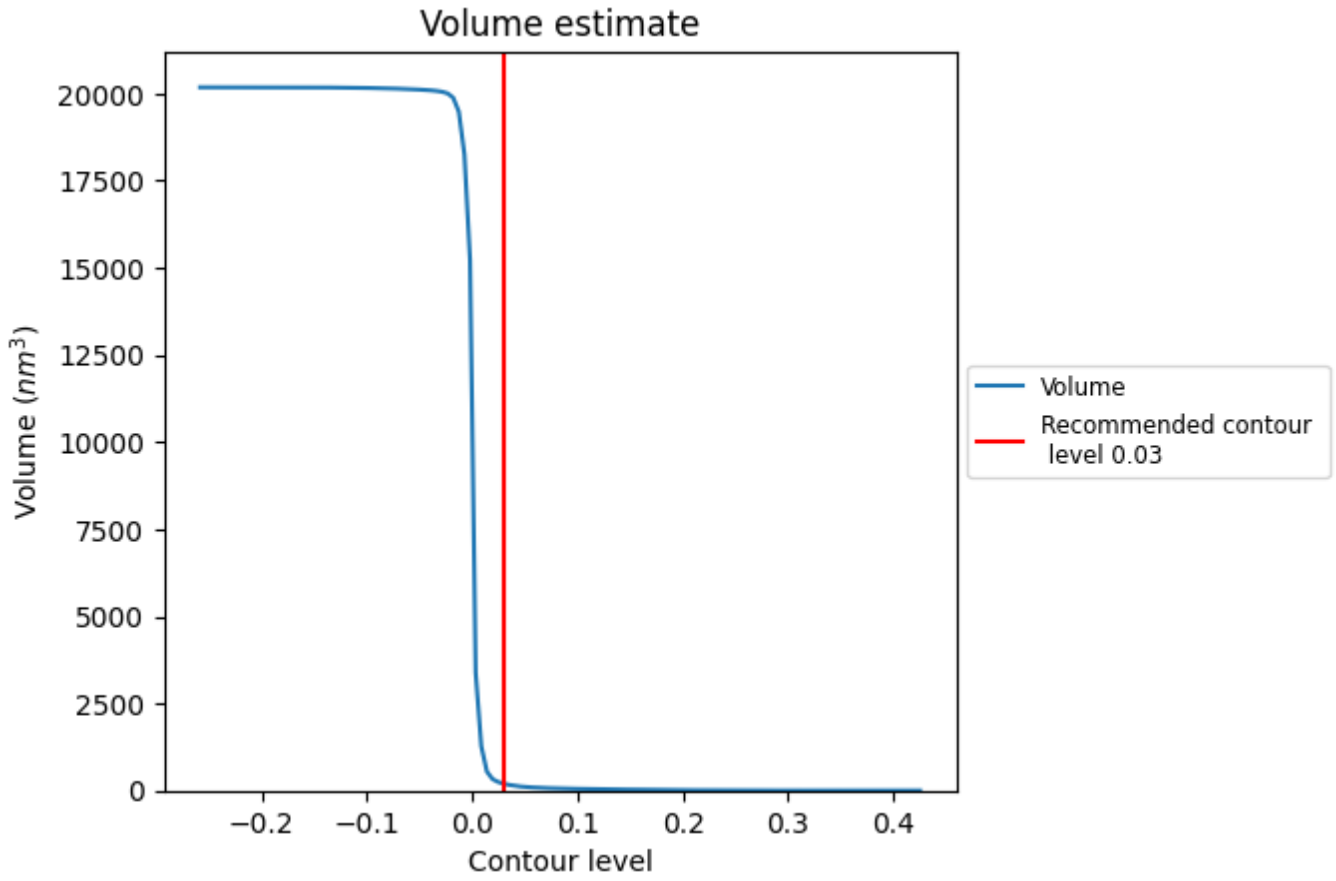
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

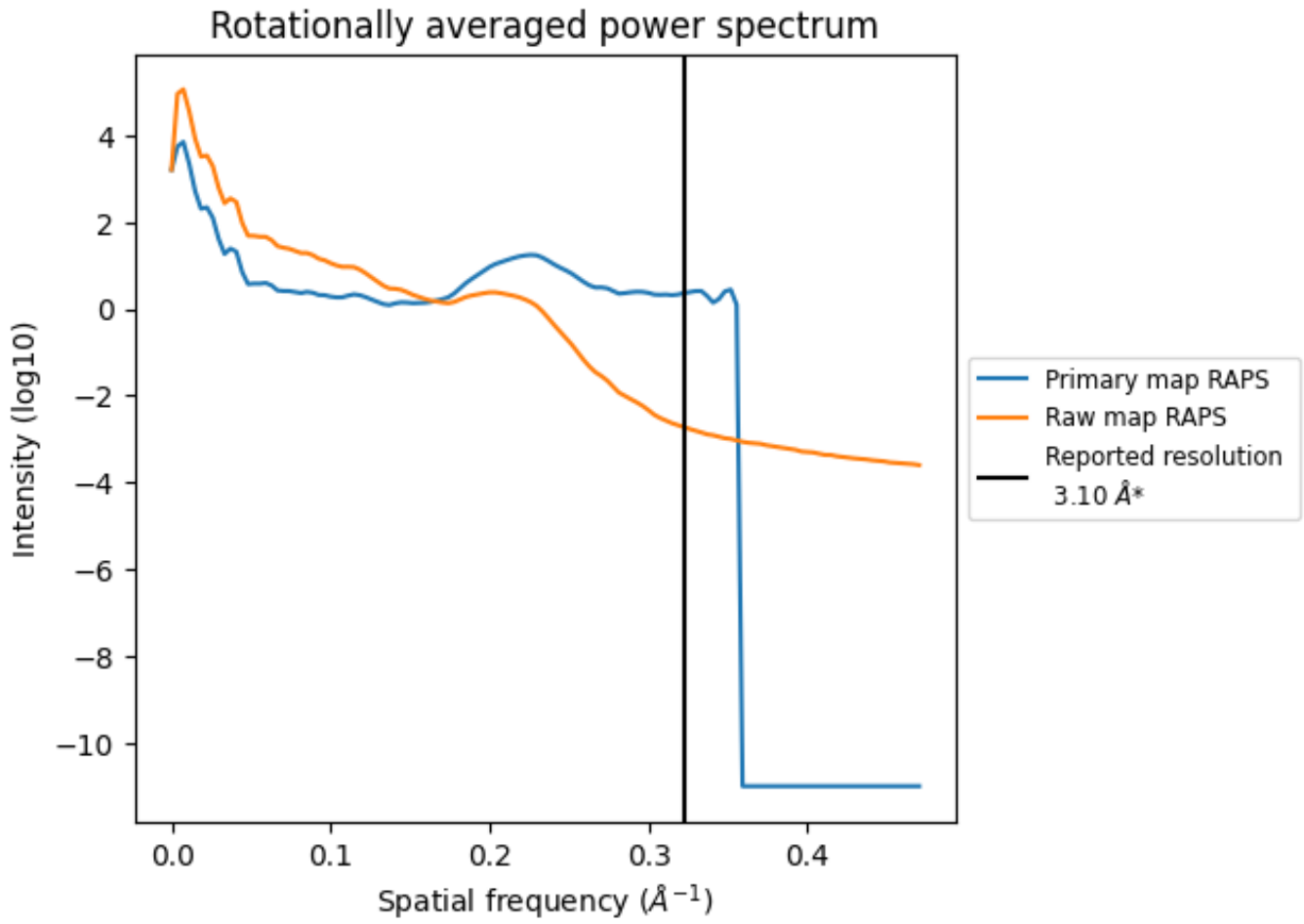
7.2 Volume estimate



The volume at the recommended contour level is 198 nm^3; this corresponds to an approximate mass of 179 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

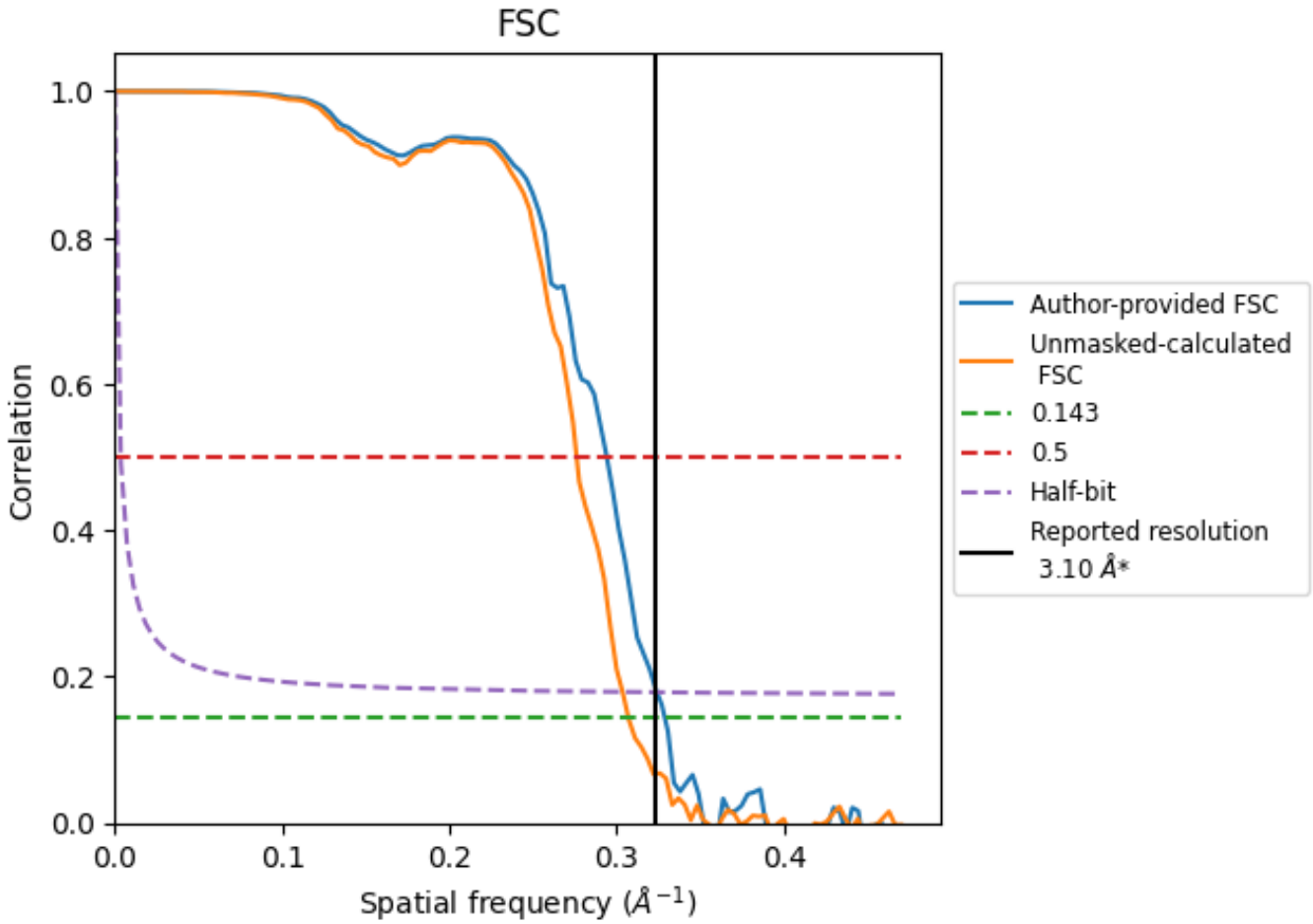


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

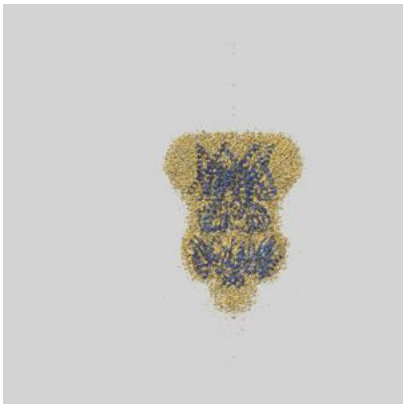
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.40	3.09
Unmasked-calculated*	3.26	3.62	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

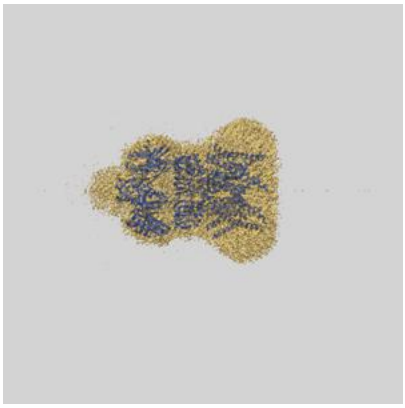
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13003 and PDB model 7OO0. Per-residue inclusion information can be found in section 3 on page 9.

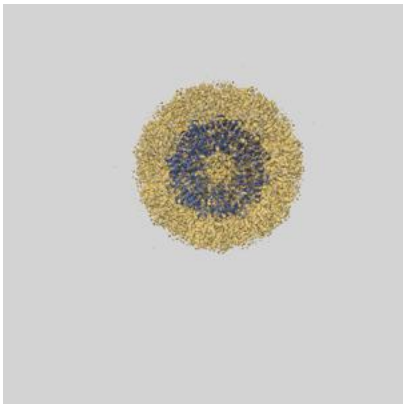
9.1 Map-model overlay



X



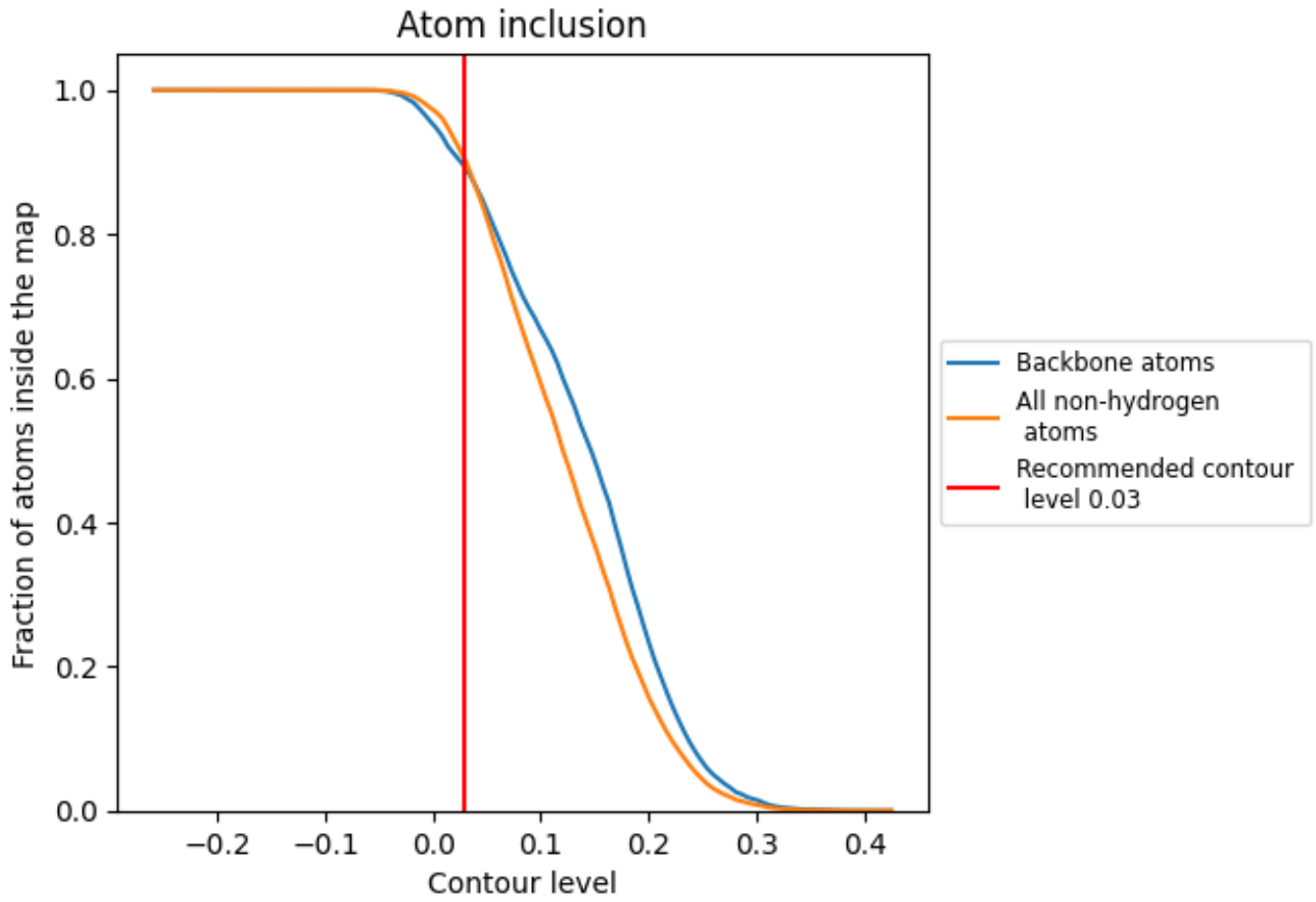
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.