wwPDB EM Validation Summary Report

Dec 17, 2023 – 04:15 pm GMT

PDB ID	:	7OJF
EMDB ID	:	EMD-12949
Title	:	CRYO-EM STRUCTURE OF SLYB13-BAMA FROM ESCHERICHIA COLI
Authors	:	Nguyen, V.S.; Remaut, H.
Deposited on	:	2021-05-14
Resolution	:	3.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

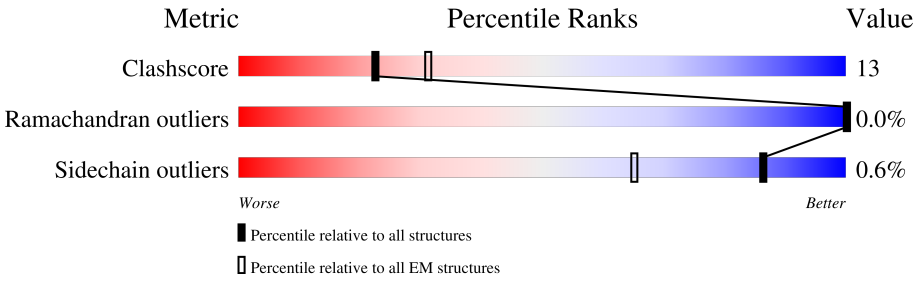
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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%

Mol	Chain	Length	Quality of chain
1	A	155	72% 17% 11%
1	B	155	69% 19% • 11%
1	C	155	71% 17% • 11%
1	D	155	73% 15% • 11%
1	E	155	74% 15% • 11%
1	F	155	68% 21% 11%
1	G	155	68% 21% 11%
1	H	155	69% 19% • 11%
1	I	155	68% 21% 11%

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Mol	Chain	Length	Quality of chain
1	J	155	77% 12% 11%
1	K	155	75% 14% 11%
1	L	155	67% 22% 11%
1	M	155	65% 25% 11%
2	N	810	40% 24% 35%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19318 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.

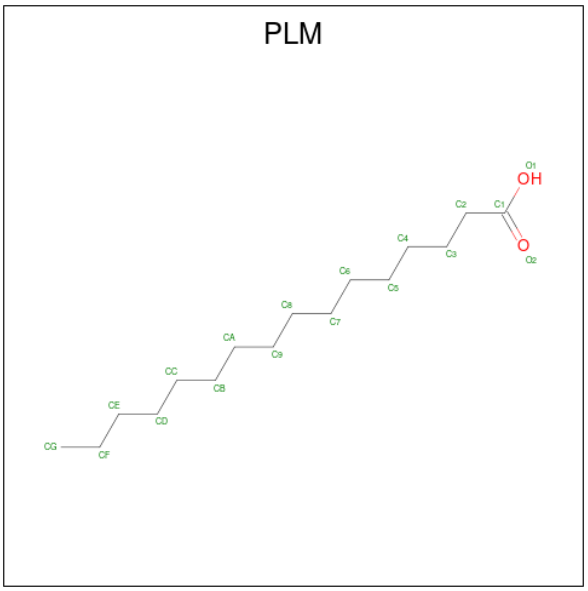
- Molecule 1 is a protein called Outer membrane lipoprotein slyB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	B	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	C	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	D	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	E	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	F	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	G	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	H	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	I	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	J	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	K	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	L	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	M	138	Total	C	N	O	S	0	0
			967	584	181	199	3		

- Molecule 2 is a protein called Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	525	Total	C	N	O	S	0	0
			4139	2614	691	820	14		

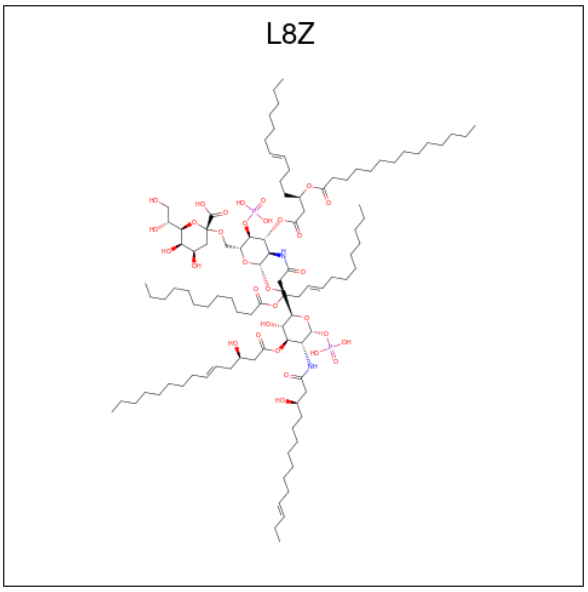
- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 17 16 1	0
3	B	1	Total C O 17 16 1	0
3	C	1	Total C O 17 16 1	0
3	D	1	Total C O 17 16 1	0
3	E	1	Total C O 17 16 1	0
3	F	1	Total C O 17 16 1	0
3	G	1	Total C O 17 16 1	0
3	H	1	Total C O 17 16 1	0
3	I	1	Total C O 17 16 1	0
3	J	1	Total C O 17 16 1	0
3	K	1	Total C O 17 16 1	0
3	L	1	Total C O 17 16 1	0
3	M	1	Total C O 17 16 1	0

- Molecule 4 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[[(2 {R},3 {S}

,4 {R},5 {R},6 {R})-5-[[({E},3 {R})-3-dodecanoyloxytetradec-5-enoyl]amino]-6-[[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[[({E},3 {R})-3-oxidanyltetradec-11-enoyl]amino]-4-[({E},3 {R})-3-oxidanyltetradec-5-enoyl]oxy-6-phosphonooxy-oxan-2-yl]methoxy]-3-phosphonooxy-4-[({E},3 {R})-3-tetradecanoyloxytetradec-7-enoyl]oxy-oxan-2-yl]methoxy]-4,5-bis(oxidanyl)oxane-2-carboxylic acid (three-letter code: L8Z) (formula: $C_{102}H_{182}N_2O_{32}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	B	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	C	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	D	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	E	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	F	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	G	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	H	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	I	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	J	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	K	1	Total	C	N	O	P	0
			138	102	2	32	2	

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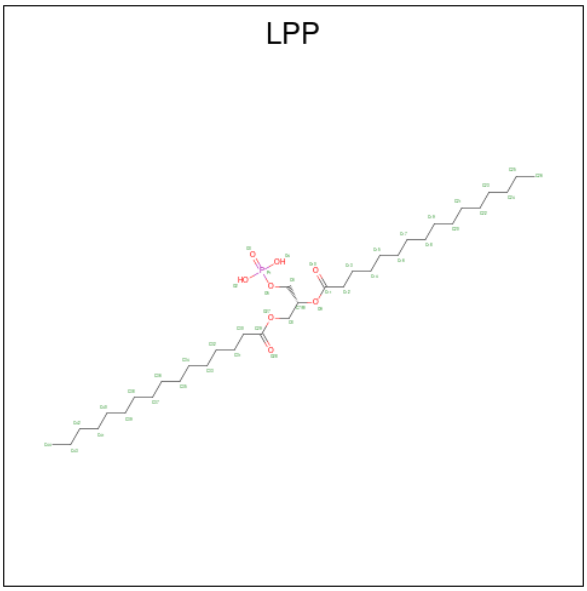
Mol	Chain	Residues	Atoms					AltConf
4	L	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	M	1	Total	C	N	O	P	0
			138	102	2	32	2	

- Molecule 5 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			44	35	8	1	
5	B	1	Total	C	O	P	0
			44	35	8	1	
5	C	1	Total	C	O	P	0
			44	35	8	1	
5	D	1	Total	C	O	P	0
			44	35	8	1	
5	F	1	Total	C	O	P	0
			44	35	8	1	
5	G	1	Total	C	O	P	0
			44	35	8	1	
5	H	1	Total	C	O	P	0
			44	35	8	1	
5	I	1	Total	C	O	P	0
			44	35	8	1	
5	J	1	Total	C	O	P	0
			44	35	8	1	

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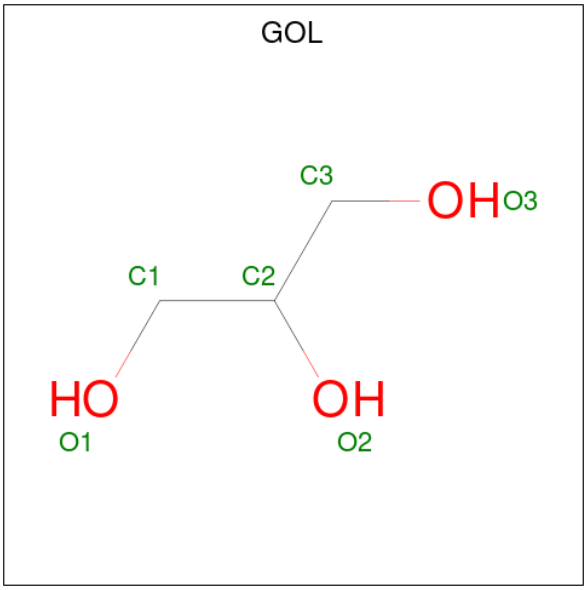
Mol	Chain	Residues	Atoms	AltConf
5	K	1	Total C O P 44 35 8 1	0
5	L	1	Total C O P 44 35 8 1	0
5	M	1	Total C O P 44 35 8 1	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 5 3 2	0
6	C	1	Total C O 5 3 2	0
6	D	1	Total C O 5 3 2	0
6	D	1	Total C O 5 3 2	0
6	E	1	Total C O 5 3 2	0
6	F	1	Total C O 5 3 2	0
6	H	1	Total C O 5 3 2	0
6	H	1	Total C O 5 3 2	0

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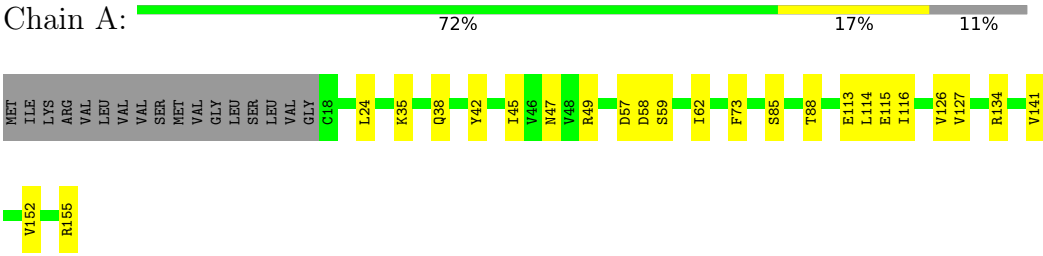
Mol	Chain	Residues	Atoms			AltConf
6	J	1	Total	C	O	0
			5	3	2	
6	J	1	Total	C	O	0
			5	3	2	
6	K	1	Total	C	O	0
			5	3	2	
6	M	1	Total	C	O	0
			5	3	2	
6	M	1	Total	C	O	0
			5	3	2	

3 Residue-property plots

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. 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. 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.

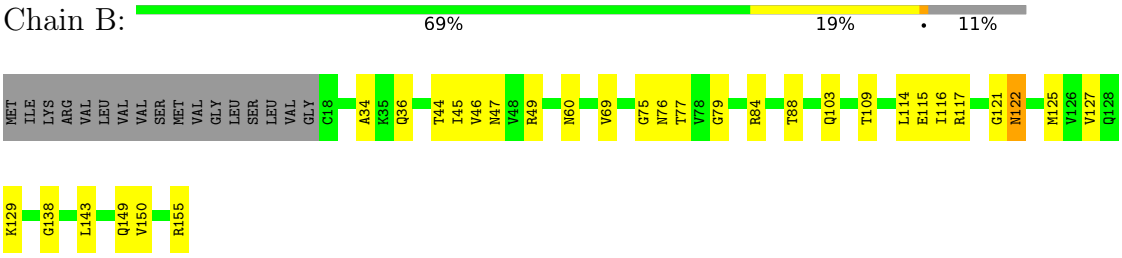
• Molecule 1: Outer membrane lipoprotein slyB

Chain A:



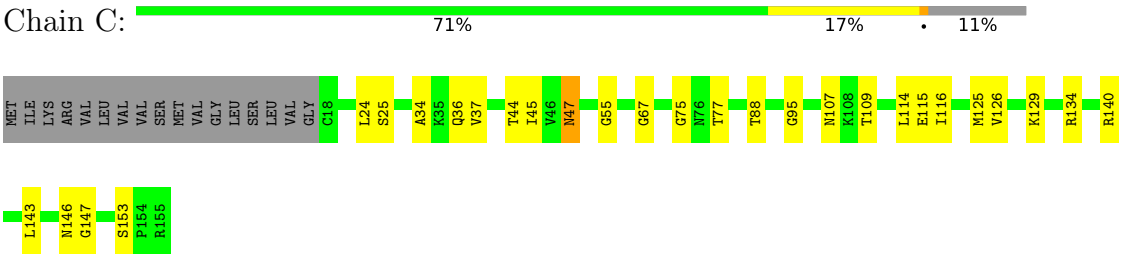
• Molecule 1: Outer membrane lipoprotein slyB

Chain B:



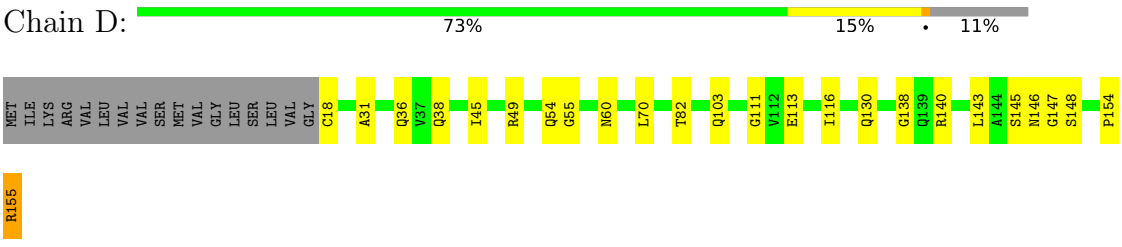
• Molecule 1: Outer membrane lipoprotein slyB

Chain C:



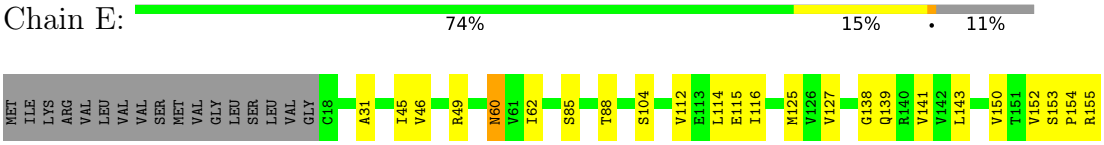
• Molecule 1: Outer membrane lipoprotein slyB

Chain D:



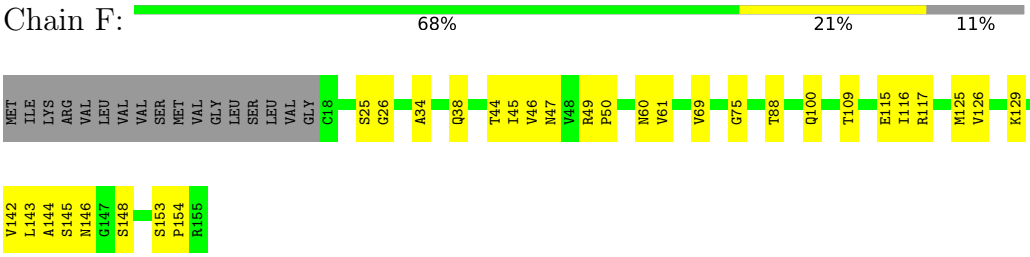
• Molecule 1: Outer membrane lipoprotein slyB

Chain E:



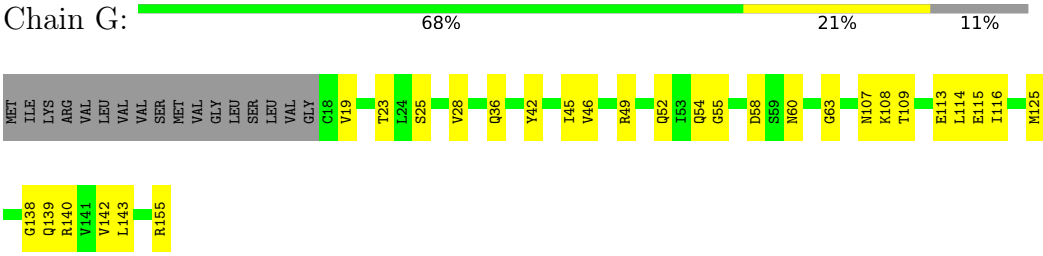
• Molecule 1: Outer membrane lipoprotein slyB

Chain F:



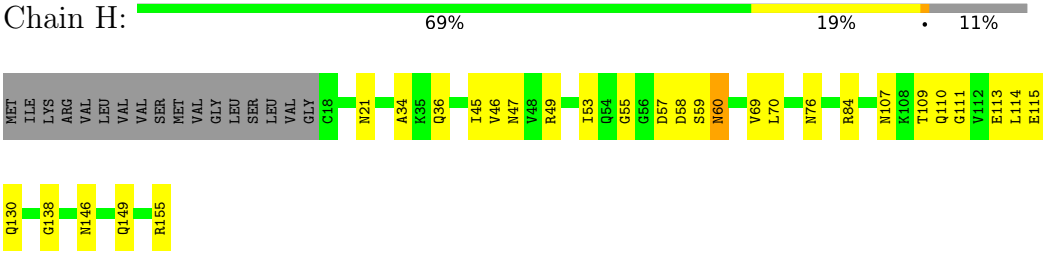
• Molecule 1: Outer membrane lipoprotein slyB

Chain G:



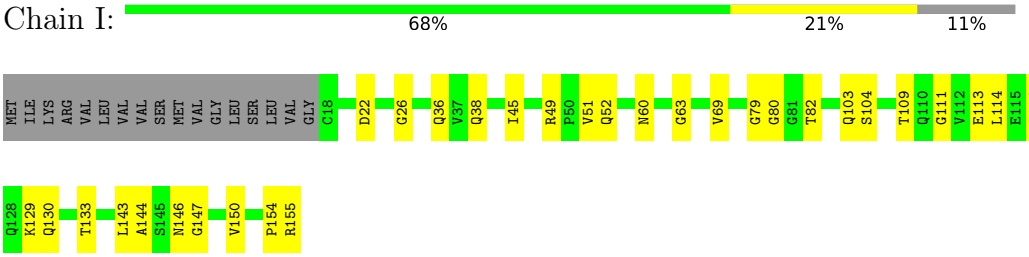
• Molecule 1: Outer membrane lipoprotein slyB

Chain H:



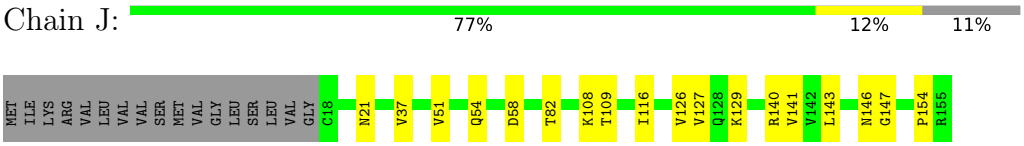
• Molecule 1: Outer membrane lipoprotein slyB

Chain I:



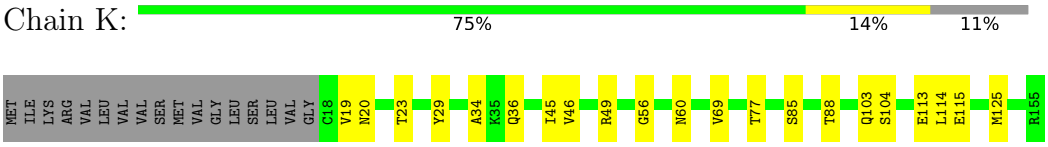
• Molecule 1: Outer membrane lipoprotein slyB

Chain J:



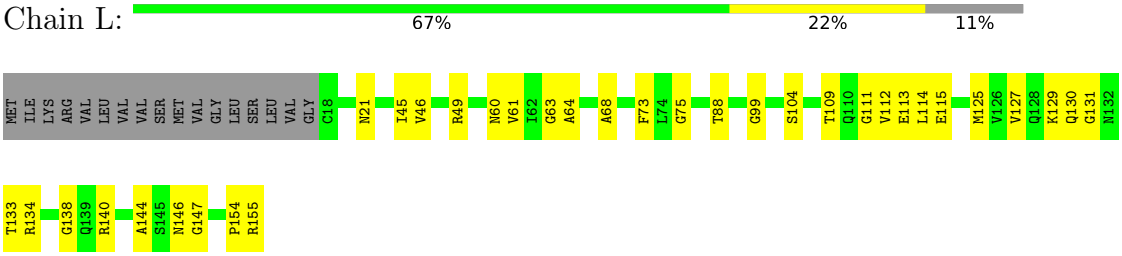
• Molecule 1: Outer membrane lipoprotein slyB

Chain K:



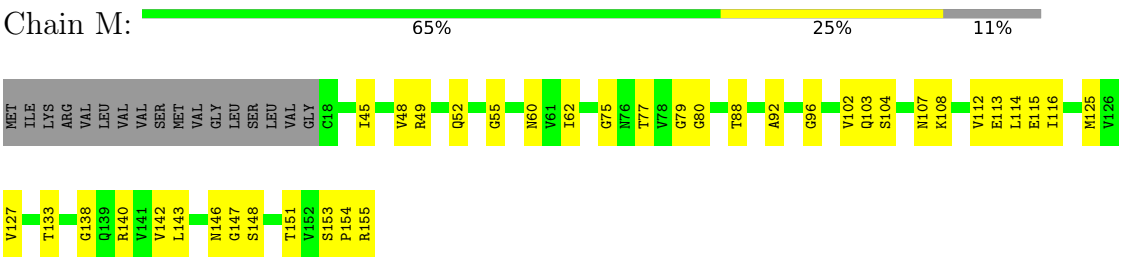
• Molecule 1: Outer membrane lipoprotein slyB

Chain L:



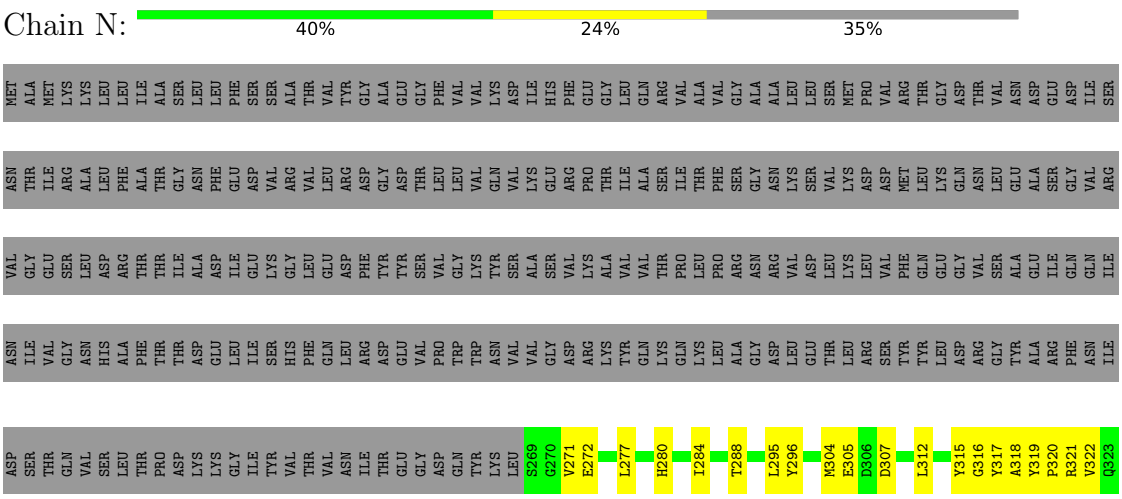
• Molecule 1: Outer membrane lipoprotein slyB

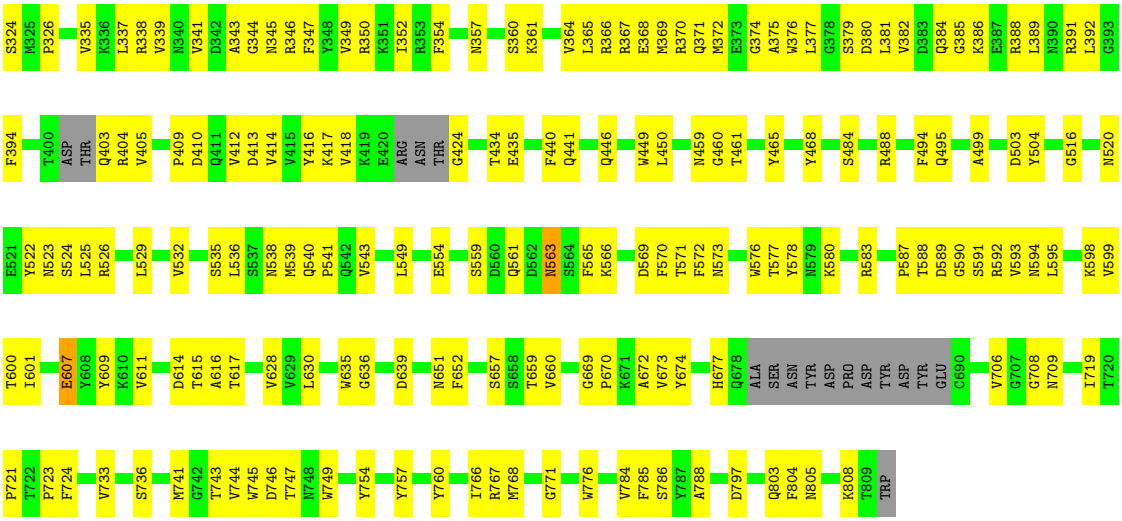
Chain M:



• Molecule 2: Outer membrane protein assembly factor BamA

Chain N:




S324 M325 P326 V335 K336 L337 R338 V339 N340 V341 D342 A343 G344 N345 R346 F347 Y348 V349 R350 K351 I352 R353 F354 N357 S360 K361 V364 L365 R366 R367 E368 M369 R370 Q371 M372 E373 G374 A375 W376 L377 G378 S379 D380 L381 V382 D383 Q384 G385 K386 E387 R388 L389 N390 R391 L392 G393
F394 T400 ASP THR Q403 R404 V405 P409 D410 Q411 V412 D413 V414 V415 Y416 K417 V418 K419 E420 ARG ASN THR G424 T434 E435 F440 Q441 Q446 W449 L450 M459 G460 T461 Y465 Y468 S484 R488 F494 Q495 A499 D503 Y504 G516 N520
E521 Y522 N523 S524 L525 R526 L529 V532 S535 L536 S537 N538 M539 Q540 P541 Q542 V543 L549 E554 S559 D560 Q561 D562 N563 S564 F565 K566 D569 F570 T571 F572 N573 W576 T577 Y578 N579 K580 R583 P587 T588 D589 G590 S591 R592 V593 N594 L595 K598 V599
T600 I601 E607 Y608 Y609 K610 V611 D614 T615 A616 T617 V628 V629 L630 W635 G636 D639 N651 F652 S657 S658 T659 V660 G669 P670 K671 A672 V673 Y674 H677 Q678 ALA SER ASN TYR ASP PRO ASP TYR ASP TYR GLU G690 V706 G707 G708 N709 I719 T720
P721 T722 P723 F724 V733 S736 M741 G742 T743 V744 W745 D746 T747 N748 W749 Y754 Y757 Y760 I766 R767 M768 G771 W776 V784 F785 S786 Y787 A788 D797 Q803 F804 N805 K808 T809 TRP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73756	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LPP, GOL, L8Z, PLM

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	0.43	0/973	0.56	0/1317
1	B	0.46	0/973	0.58	0/1317
1	C	0.45	0/973	0.57	0/1317
1	D	0.45	0/973	0.55	0/1317
1	E	0.49	1/973 (0.1%)	0.58	0/1317
1	F	0.46	0/973	0.63	0/1317
1	G	0.45	0/973	0.58	0/1317
1	H	0.45	0/973	0.56	0/1317
1	I	0.46	0/973	0.57	0/1317
1	J	0.45	0/973	0.57	0/1317
1	K	0.47	0/973	0.57	0/1317
1	L	0.44	0/973	0.57	0/1317
1	M	0.44	0/973	0.58	0/1317
2	N	0.37	0/4243	0.57	0/5751
All	All	0.44	1/16892 (0.0%)	0.57	0/22872

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	152	VAL	C-N	-5.18	1.22	1.34

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	967	0	963	20	0
1	B	967	0	963	26	0
1	C	967	0	963	23	0
1	D	967	0	963	21	0
1	E	967	0	963	20	0
1	F	967	0	963	24	0
1	G	967	0	963	25	0
1	H	967	0	963	33	0
1	I	967	0	963	30	0
1	J	967	0	963	15	0
1	K	967	0	963	18	0
1	L	967	0	963	28	0
1	M	967	0	963	32	0
2	N	4139	0	3882	161	0
3	A	17	0	31	1	0
3	B	17	0	31	0	0
3	C	17	0	31	2	0
3	D	17	0	31	2	0
3	E	17	0	31	0	0
3	F	17	0	31	0	0
3	G	17	0	31	1	0
3	H	17	0	31	1	0
3	I	17	0	31	2	0
3	J	17	0	31	0	0
3	K	17	0	31	1	0
3	L	17	0	31	1	0
3	M	17	0	31	2	0
4	A	138	0	0	1	0
4	B	138	0	0	1	0
4	C	138	0	0	2	0
4	D	138	0	0	2	0
4	E	138	0	0	3	0
4	F	138	0	0	1	0
4	G	138	0	0	2	0
4	H	138	0	0	2	0
4	I	138	0	0	3	0
4	J	138	0	0	2	0
4	K	138	0	0	2	0
4	L	138	0	0	4	0
4	M	138	0	0	3	0
5	A	44	0	67	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	44	0	67	3	0
5	C	44	0	67	3	0
5	D	44	0	67	0	0
5	F	44	0	67	2	0
5	G	44	0	67	1	0
5	H	44	0	67	5	0
5	I	44	0	67	1	0
5	J	44	0	67	1	0
5	K	44	0	67	2	0
5	L	44	0	67	3	0
5	M	44	0	67	3	0
6	A	5	0	4	0	0
6	C	5	0	5	0	0
6	D	10	0	10	1	0
6	E	5	0	5	0	0
6	F	5	0	5	0	0
6	H	10	0	10	0	0
6	J	10	0	10	0	0
6	K	5	0	5	0	0
6	M	10	0	10	0	0
All	All	19318	0	17672	466	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 13.

The worst 5 of 466 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)
4:L:202:L8Z:C1G	4:L:202:L8Z:C2E	1.75	1.60
1:H:59:SER:C	1:H:60:ASN:HD22	1.62	1.02
2:N:312:LEU:HB3	2:N:320:PRO:HB3	1.56	0.84
2:N:594:ASN:HB3	2:N:614:ASP:HB3	1.60	0.81
2:N:357:ASN:HD22	2:N:360:SER:HB3	1.46	0.81

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	136/155 (88%)	123 (90%)	13 (10%)	0	100	100
1	B	136/155 (88%)	125 (92%)	11 (8%)	0	100	100
1	C	136/155 (88%)	127 (93%)	9 (7%)	0	100	100
1	D	136/155 (88%)	127 (93%)	9 (7%)	0	100	100
1	E	136/155 (88%)	123 (90%)	13 (10%)	0	100	100
1	F	136/155 (88%)	122 (90%)	13 (10%)	1 (1%)	22	60
1	G	136/155 (88%)	125 (92%)	11 (8%)	0	100	100
1	H	136/155 (88%)	128 (94%)	8 (6%)	0	100	100
1	I	136/155 (88%)	126 (93%)	10 (7%)	0	100	100
1	J	136/155 (88%)	121 (89%)	15 (11%)	0	100	100
1	K	136/155 (88%)	124 (91%)	12 (9%)	0	100	100
1	L	136/155 (88%)	124 (91%)	12 (9%)	0	100	100
1	M	136/155 (88%)	122 (90%)	14 (10%)	0	100	100
2	N	517/810 (64%)	445 (86%)	72 (14%)	0	100	100
All	All	2285/2825 (81%)	2062 (90%)	222 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	61	VAL

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	102/117 (87%)	102 (100%)	0	100 100
1	B	102/117 (87%)	100 (98%)	2 (2%)	55 74
1	C	102/117 (87%)	101 (99%)	1 (1%)	76 86
1	D	102/117 (87%)	101 (99%)	1 (1%)	76 86
1	E	102/117 (87%)	101 (99%)	1 (1%)	76 86
1	F	102/117 (87%)	102 (100%)	0	100 100
1	G	102/117 (87%)	102 (100%)	0	100 100
1	H	102/117 (87%)	100 (98%)	2 (2%)	55 74
1	I	102/117 (87%)	102 (100%)	0	100 100
1	J	102/117 (87%)	102 (100%)	0	100 100
1	K	102/117 (87%)	102 (100%)	0	100 100
1	L	102/117 (87%)	102 (100%)	0	100 100
1	M	102/117 (87%)	102 (100%)	0	100 100
2	N	441/688 (64%)	438 (99%)	3 (1%)	84 90
All	All	1767/2209 (80%)	1757 (99%)	10 (1%)	86 91

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	321	ARG
2	N	563	ASN
2	N	607	GLU
1	D	155	ARG
1	E	60	ASN

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

Mol	Chain	Res	Type
1	I	60	ASN
2	N	523	ASN
1	J	21	ASN
2	N	561	GLN
1	M	60	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

51 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	PLM	M	202	1	16,16,17	0.59	0	15,15,17	0.41	0
4	L8Z	I	202	-	138,140,140	1.96	27 (19%)	162,176,176	2.09	30 (18%)
6	GOL	H	202	-	3,4,5	0.92	0	1,4,5	0.63	0
4	L8Z	G	202	-	138,140,140	1.93	28 (20%)	162,176,176	2.29	35 (21%)
5	LPP	B	203	-	43,43,43	1.61	3 (6%)	47,48,48	1.00	5 (10%)
3	PLM	D	201	1	16,16,17	0.50	0	15,15,17	0.39	0
4	L8Z	C	203	-	138,140,140	1.94	26 (18%)	162,176,176	2.22	30 (18%)
6	GOL	M	201	-	3,4,5	1.08	0	1,4,5	0.82	0
5	LPP	H	204	-	43,43,43	1.63	3 (6%)	47,48,48	0.96	4 (8%)
6	GOL	H	205	-	3,4,5	0.63	0	1,4,5	0.28	0
6	GOL	D	205	-	3,4,5	0.97	0	1,4,5	0.45	0
5	LPP	G	203	-	43,43,43	1.64	3 (6%)	47,48,48	1.05	5 (10%)
6	GOL	K	204	-	3,4,5	0.86	0	1,4,5	0.33	0
4	L8Z	E	1002	-	138,140,140	1.93	27 (19%)	162,176,176	2.19	33 (20%)
3	PLM	A	201	1	16,16,17	0.58	0	15,15,17	0.43	0
3	PLM	L	201	1	16,16,17	0.53	0	15,15,17	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	L8Z	M	204	-	138,140,140	1.90	26 (18%)	162,176,176	2.13	27 (16%)
3	PLM	K	201	1	16,16,17	0.57	0	15,15,17	0.41	0
4	L8Z	K	202	-	138,140,140	1.93	27 (19%)	162,176,176	2.44	32 (19%)
6	GOL	J	205	-	3,4,5	1.02	0	1,4,5	0.80	0
4	L8Z	L	202	-	138,140,140	1.99	27 (19%)	162,176,176	2.14	33 (20%)
5	LPP	K	203	-	43,43,43	1.61	3 (6%)	47,48,48	0.92	4 (8%)
3	PLM	G	201	1	16,16,17	0.45	0	15,15,17	0.43	0
4	L8Z	A	202	-	138,140,140	1.97	26 (18%)	162,176,176	2.12	34 (20%)
3	PLM	B	201	1	16,16,17	0.47	0	15,15,17	0.39	0
5	LPP	J	204	-	43,43,43	1.66	3 (6%)	47,48,48	0.97	4 (8%)
6	GOL	J	202	-	3,4,5	0.95	0	1,4,5	0.99	0
6	GOL	D	202	-	3,4,5	1.02	0	1,4,5	0.62	0
4	L8Z	J	203	-	138,140,140	1.89	25 (18%)	162,176,176	2.20	31 (19%)
3	PLM	E	1001	1	16,16,17	0.48	0	15,15,17	0.43	0
5	LPP	A	203	-	43,43,43	1.61	4 (9%)	47,48,48	1.05	5 (10%)
6	GOL	A	204	-	3,4,5	1.05	0	1,4,5	0.01	0
3	PLM	J	201	1	16,16,17	0.51	0	15,15,17	0.40	0
5	LPP	I	203	-	43,43,43	1.66	3 (6%)	47,48,48	0.96	4 (8%)
3	PLM	F	201	1	16,16,17	0.63	0	15,15,17	0.42	0
5	LPP	C	204	-	43,43,43	1.59	3 (6%)	47,48,48	1.05	4 (8%)
5	LPP	L	203	-	43,43,43	1.58	4 (9%)	47,48,48	1.01	5 (10%)
6	GOL	E	1003	-	3,4,5	1.05	0	1,4,5	1.43	0
6	GOL	M	203	-	3,4,5	1.09	0	1,4,5	0.76	0
5	LPP	D	204	-	43,43,43	1.67	3 (6%)	47,48,48	0.91	4 (8%)
6	GOL	F	204	-	3,4,5	0.65	0	1,4,5	0.33	0
4	L8Z	D	203	-	138,140,140	1.91	24 (17%)	162,176,176	2.20	30 (18%)
4	L8Z	F	202	-	138,140,140	2.00	33 (23%)	162,176,176	2.24	30 (18%)
6	GOL	C	202	-	3,4,5	0.80	0	1,4,5	0.30	0
3	PLM	I	201	1	16,16,17	0.56	0	15,15,17	0.42	0
3	PLM	C	201	1	16,16,17	0.57	0	15,15,17	0.39	0
4	L8Z	H	203	-	138,140,140	1.94	28 (20%)	162,176,176	2.16	31 (19%)
5	LPP	F	203	-	43,43,43	1.58	3 (6%)	47,48,48	0.97	4 (8%)
5	LPP	M	205	-	43,43,43	1.74	3 (6%)	47,48,48	1.00	3 (6%)
3	PLM	H	201	1	16,16,17	0.56	0	15,15,17	0.48	0
4	L8Z	B	202	-	138,140,140	1.98	30 (21%)	162,176,176	2.03	28 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	M	202	1	-	4/13/14/15	-
4	L8Z	I	202	-	-	68/140/199/199	0/3/3/3
6	GOL	H	202	-	-	0/2/2/4	-
4	L8Z	G	202	-	-	66/140/199/199	0/3/3/3
5	LPP	B	203	-	-	22/45/45/45	-
3	PLM	D	201	1	-	4/13/14/15	-
4	L8Z	C	203	-	-	60/140/199/199	0/3/3/3
6	GOL	M	201	-	-	2/2/2/4	-
5	LPP	H	204	-	-	19/45/45/45	-
6	GOL	H	205	-	-	2/2/2/4	-
6	GOL	D	205	-	-	2/2/2/4	-
5	LPP	G	203	-	-	20/45/45/45	-
6	GOL	K	204	-	-	1/2/2/4	-
4	L8Z	E	1002	-	-	62/140/199/199	0/3/3/3
3	PLM	A	201	1	-	7/13/14/15	-
3	PLM	L	201	1	-	4/13/14/15	-
4	L8Z	M	204	-	-	60/140/199/199	0/3/3/3
3	PLM	K	201	1	-	3/13/14/15	-
4	L8Z	K	202	-	-	53/140/199/199	0/3/3/3
6	GOL	J	205	-	-	0/2/2/4	-
4	L8Z	L	202	-	-	59/140/199/199	0/3/3/3
5	LPP	K	203	-	-	15/45/45/45	-
3	PLM	G	201	1	-	4/13/14/15	-
4	L8Z	A	202	-	-	65/140/199/199	0/3/3/3
3	PLM	B	201	1	-	4/13/14/15	-
5	LPP	J	204	-	-	18/45/45/45	-
6	GOL	J	202	-	-	0/2/2/4	-
6	GOL	D	202	-	-	0/2/2/4	-
4	L8Z	J	203	-	-	50/140/199/199	0/3/3/3
3	PLM	E	1001	1	-	5/13/14/15	-
5	LPP	A	203	-	-	22/45/45/45	-
6	GOL	A	204	-	-	2/2/2/4	-
3	PLM	J	201	1	-	4/13/14/15	-
5	LPP	I	203	-	-	21/45/45/45	-
3	PLM	F	201	1	-	5/13/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LPP	C	204	-	-	23/45/45/45	-
5	LPP	L	203	-	-	21/45/45/45	-
6	GOL	E	1003	-	-	2/2/2/4	-
6	GOL	M	203	-	-	0/2/2/4	-
5	LPP	D	204	-	-	20/45/45/45	-
6	GOL	F	204	-	-	2/2/2/4	-
4	L8Z	D	203	-	-	49/140/199/199	0/3/3/3
4	L8Z	F	202	-	-	52/140/199/199	0/3/3/3
6	GOL	C	202	-	-	2/2/2/4	-
3	PLM	I	201	1	-	2/13/14/15	-
3	PLM	C	201	1	-	4/13/14/15	-
4	L8Z	H	203	-	-	55/140/199/199	0/3/3/3
5	LPP	F	203	-	-	23/45/45/45	-
5	LPP	M	205	-	-	19/45/45/45	-
3	PLM	H	201	1	-	3/13/14/15	-
4	L8Z	B	202	-	-	55/140/199/199	0/3/3/3

The worst 5 of 392 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	205	LPP	P1-O5	8.53	1.87	1.60
5	I	203	LPP	P1-O5	8.50	1.87	1.60
5	H	204	LPP	P1-O5	8.35	1.87	1.60
5	J	204	LPP	P1-O5	8.30	1.87	1.60
5	K	203	LPP	P1-O5	8.18	1.86	1.60

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	202	L8Z	O61-C2E-O62	-12.79	74.56	110.07
4	K	202	L8Z	O61-C2E-C3D	11.00	135.72	107.31
4	G	202	L8Z	O61-C2E-O62	-10.17	81.84	110.07
4	F	202	L8Z	C22-C1A-N21	9.22	128.41	116.33
4	L	202	L8Z	O61-C2E-O62	-8.98	85.15	110.07

There are no chirality outliers.

5 of 1065 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1001	PLM	C1-C2-C3-C4
3	I	201	PLM	C1-C2-C3-C4
3	J	201	PLM	C1-C2-C3-C4
4	A	202	L8Z	C1A-C22-C32-C42
4	A	202	L8Z	C1A-C22-C32-O32

There are no ring outliers.

34 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	202	PLM	2	0
4	I	202	L8Z	3	0
4	G	202	L8Z	2	0
5	B	203	LPP	3	0
3	D	201	PLM	2	0
4	C	203	L8Z	2	0
5	H	204	LPP	5	0
5	G	203	LPP	1	0
4	E	1002	L8Z	3	0
3	A	201	PLM	1	0
3	L	201	PLM	1	0
4	M	204	L8Z	3	0
3	K	201	PLM	1	0
4	K	202	L8Z	2	0
4	L	202	L8Z	4	0
5	K	203	LPP	2	0
3	G	201	PLM	1	0
4	A	202	L8Z	1	0
5	J	204	LPP	1	0
6	D	202	GOL	1	0
4	J	203	L8Z	2	0
5	A	203	LPP	2	0
5	I	203	LPP	1	0
5	C	204	LPP	3	0
5	L	203	LPP	3	0
4	D	203	L8Z	2	0
4	F	202	L8Z	1	0
3	I	201	PLM	2	0
3	C	201	PLM	2	0
4	H	203	L8Z	2	0
5	F	203	LPP	2	0
5	M	205	LPP	3	0
3	H	201	PLM	1	0

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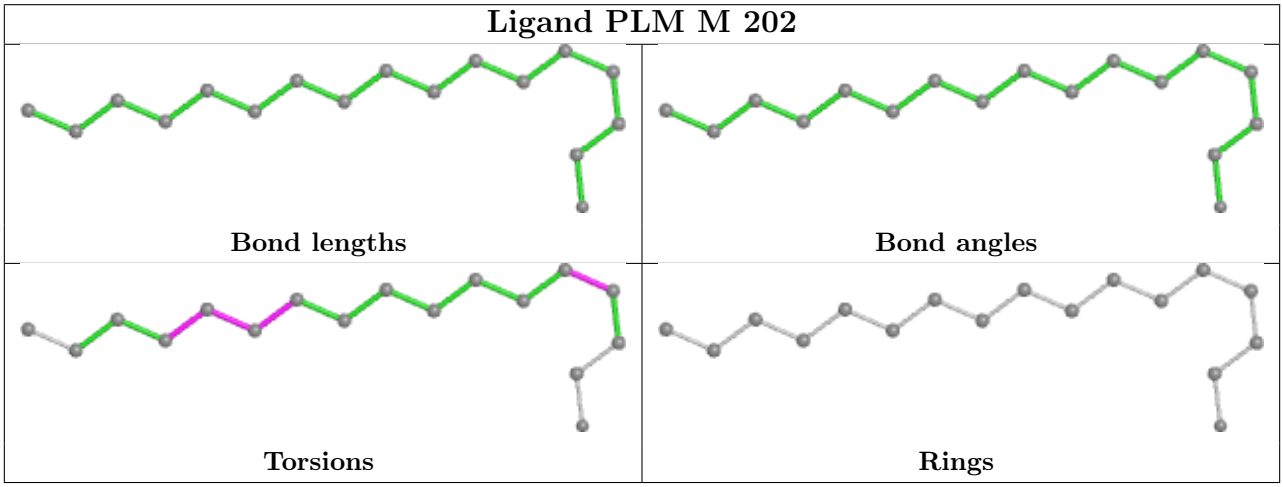
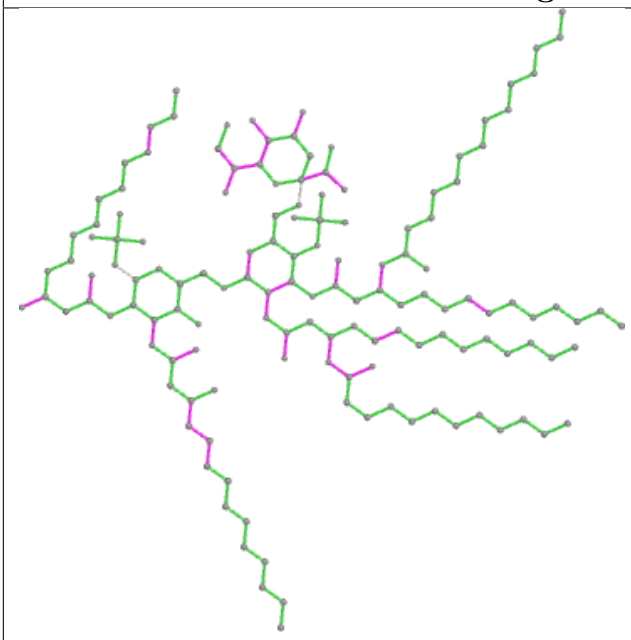
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	L8Z	1	0

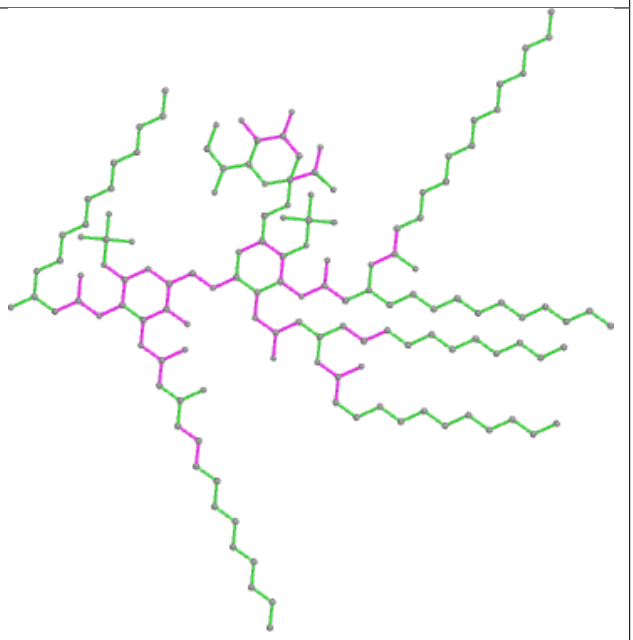
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



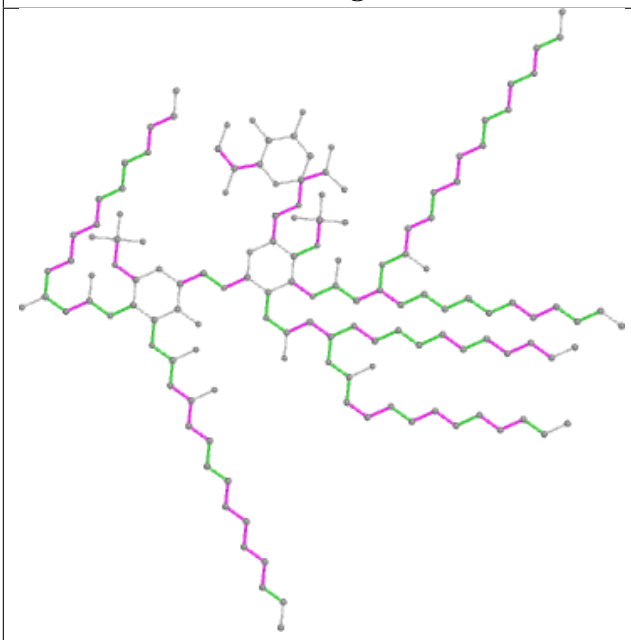
Ligand L8Z I 202



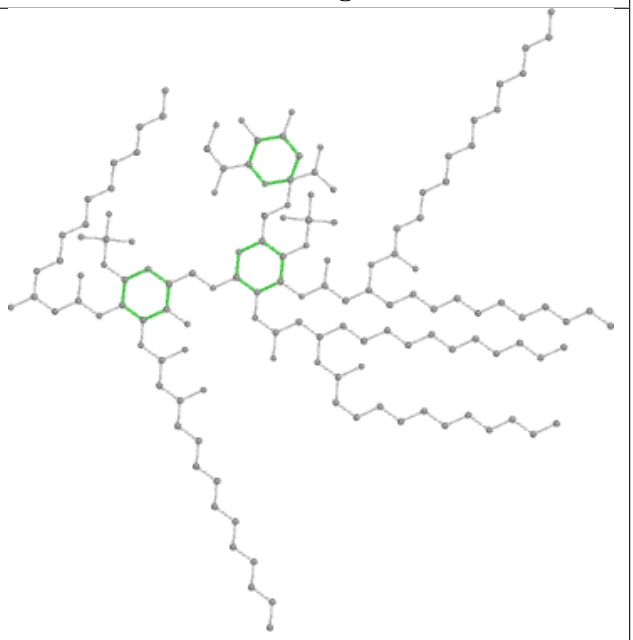
Bond lengths



Bond angles

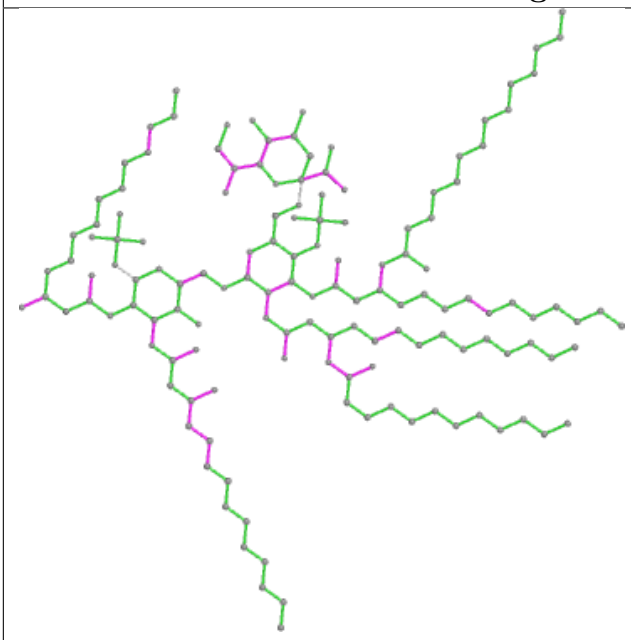


Torsions

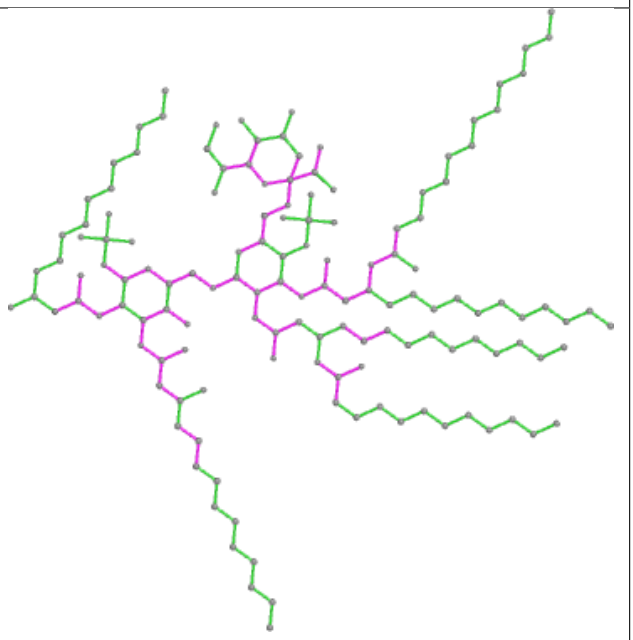


Rings

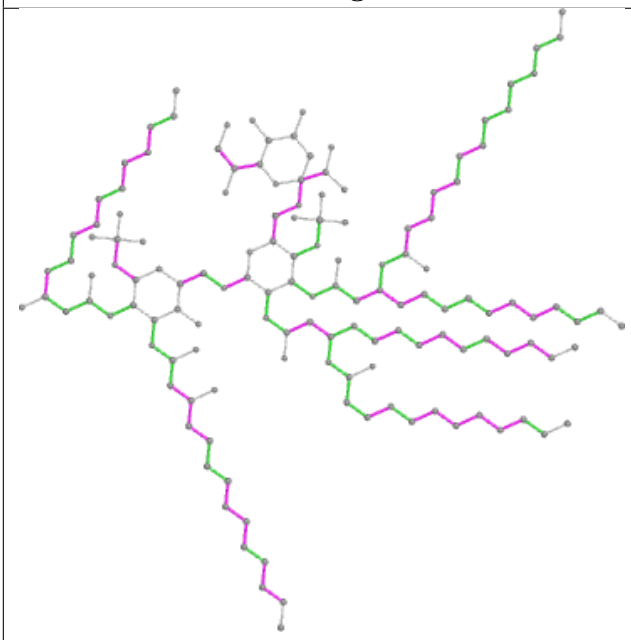
Ligand L8Z G 202



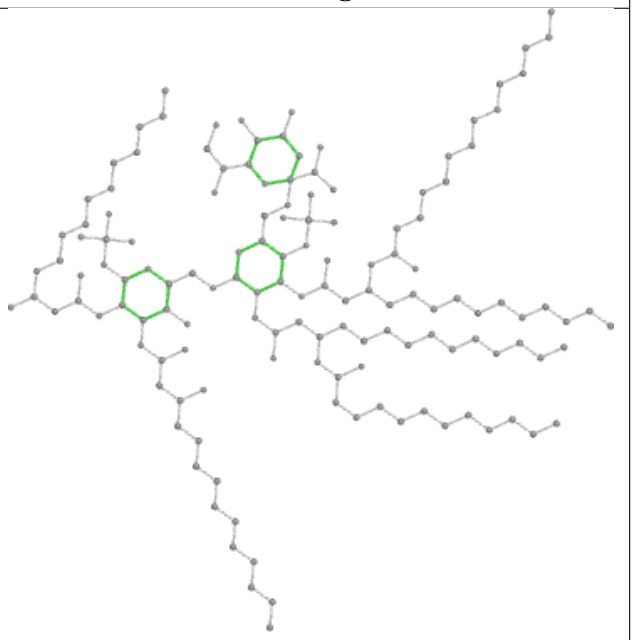
Bond lengths



Bond angles

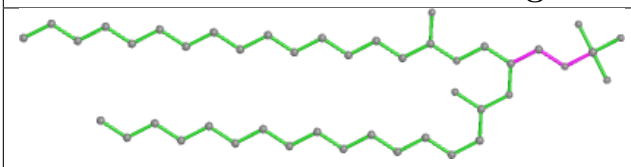


Torsions



Rings

Ligand LPP B 203



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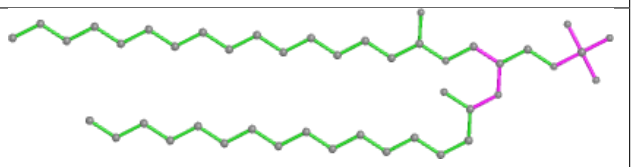
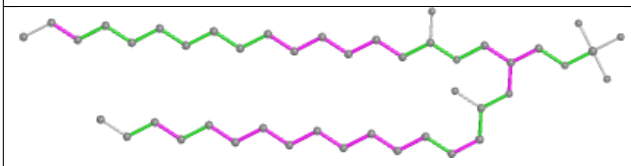


Bond angles



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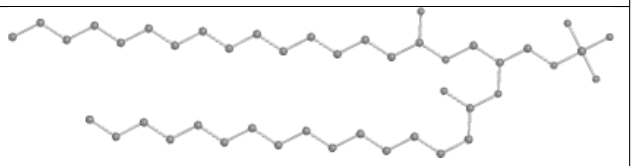
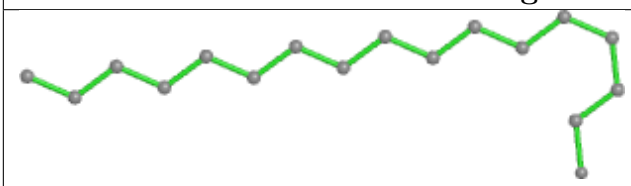
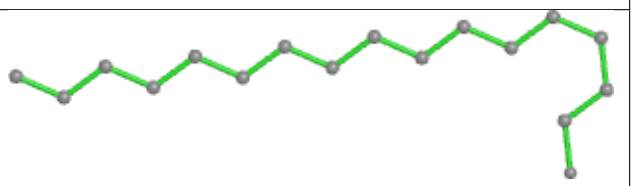


Rings

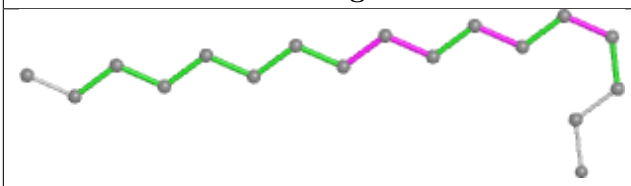
Ligand PLM D 201



Bond lengths



Bond angles



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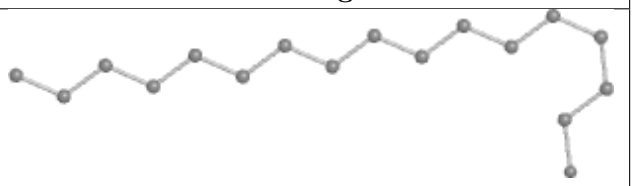
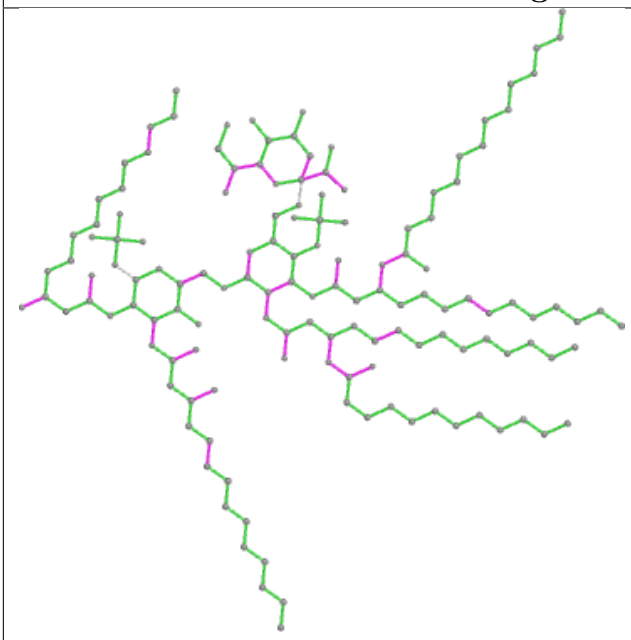
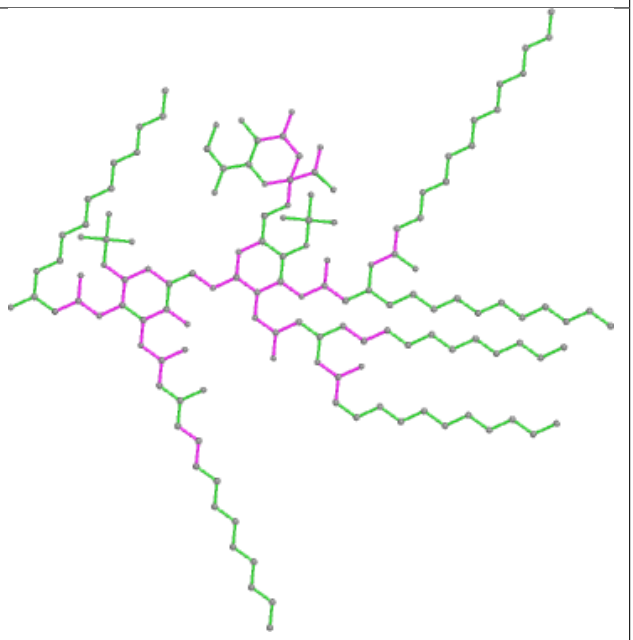


Rings

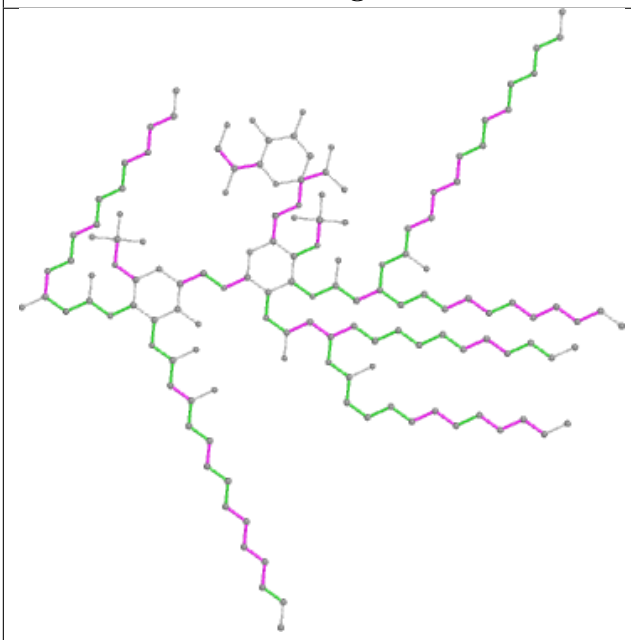
Ligand L8Z C 203



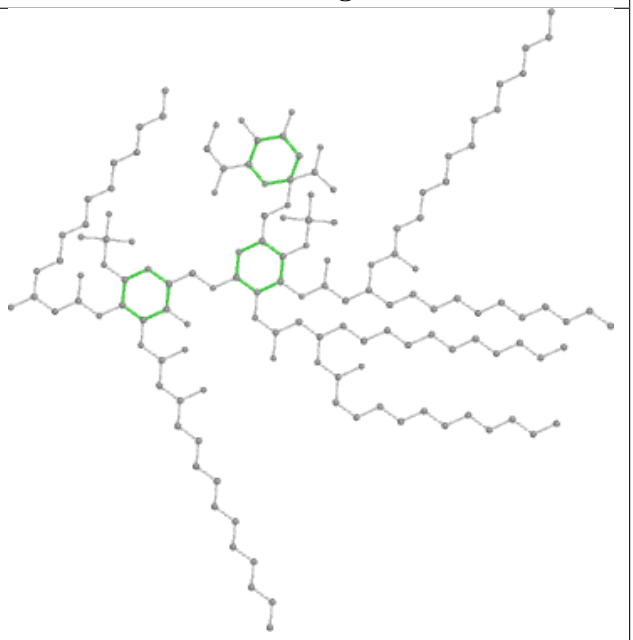
Bond lengths



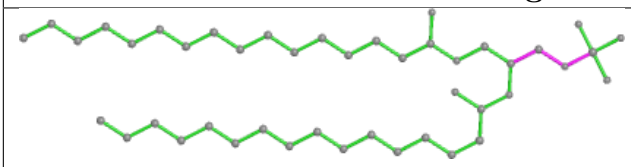
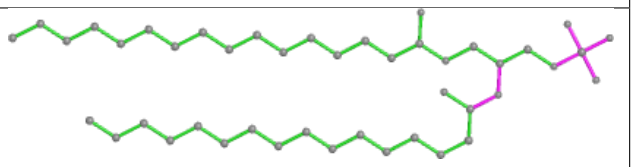
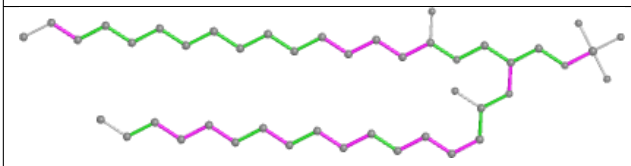
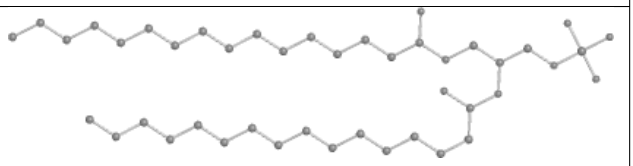
Bond angles

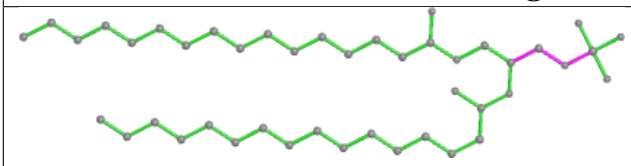
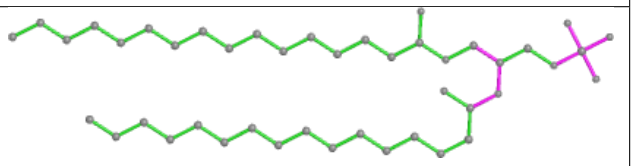
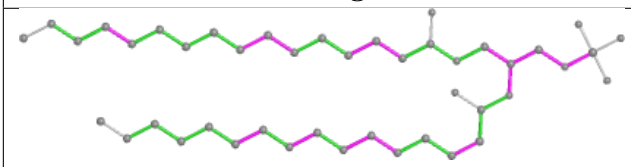
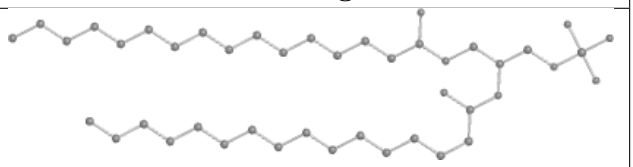


Torsions

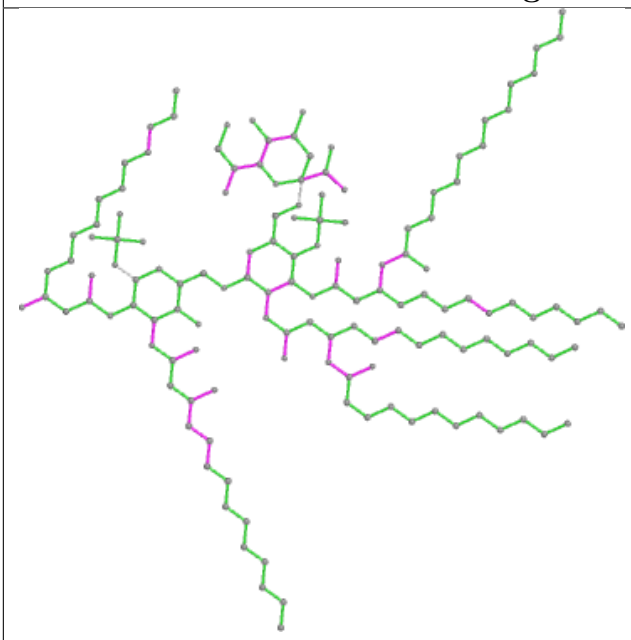


Rings

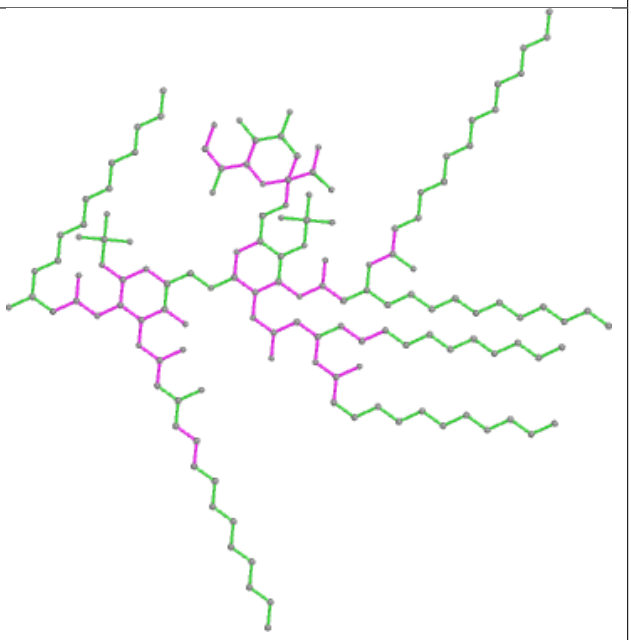
Ligand LPP H 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LPP G 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

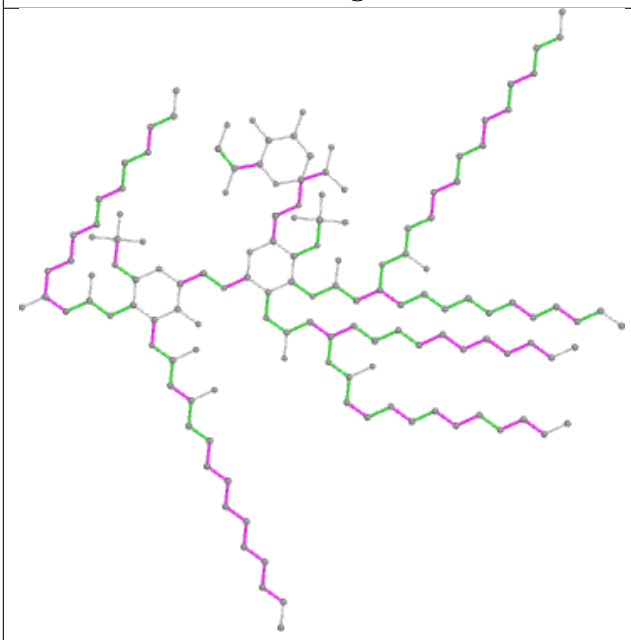
Ligand L8Z E 1002



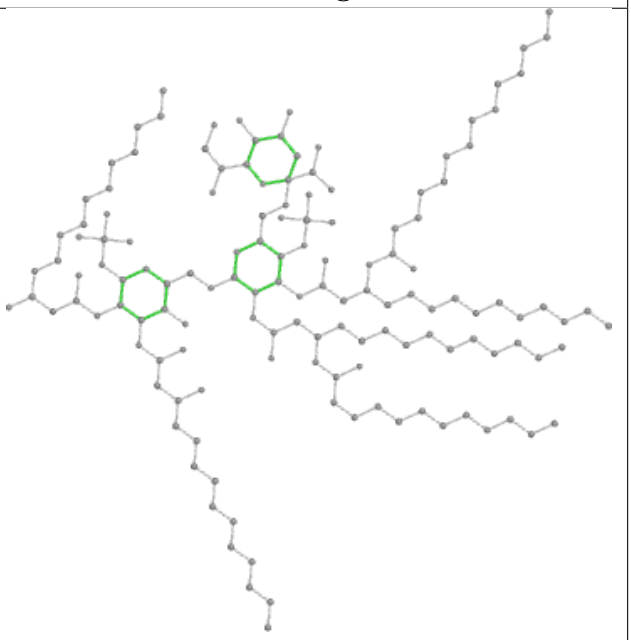
Bond lengths



Bond angles

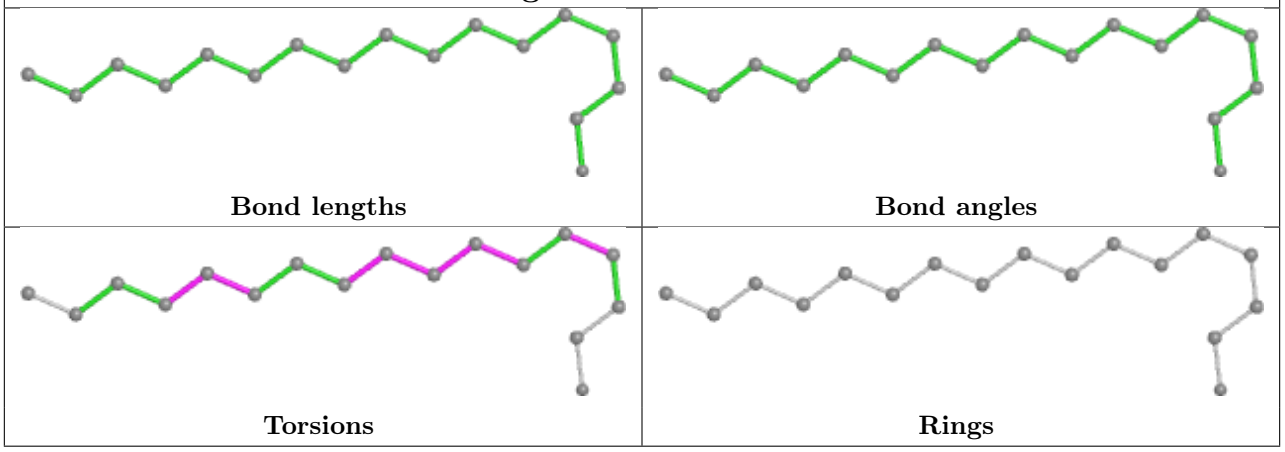


Torsions



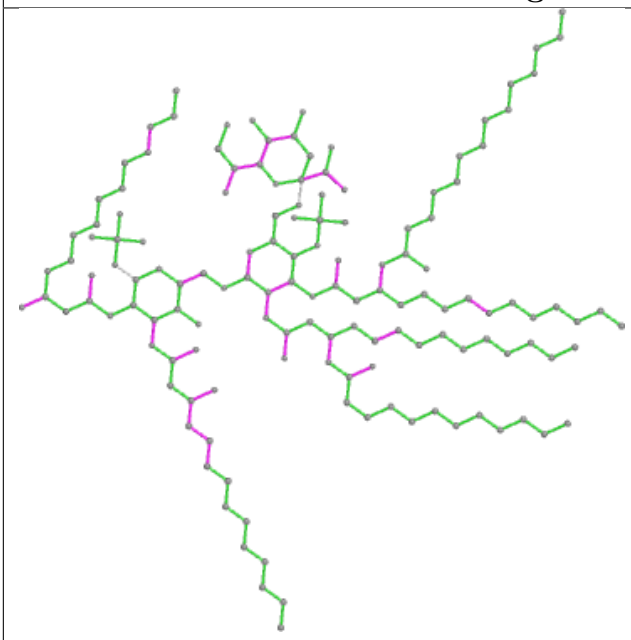
Rings

Ligand PLM A 201



Ligand PLM L 201

Ligand L8Z M 204



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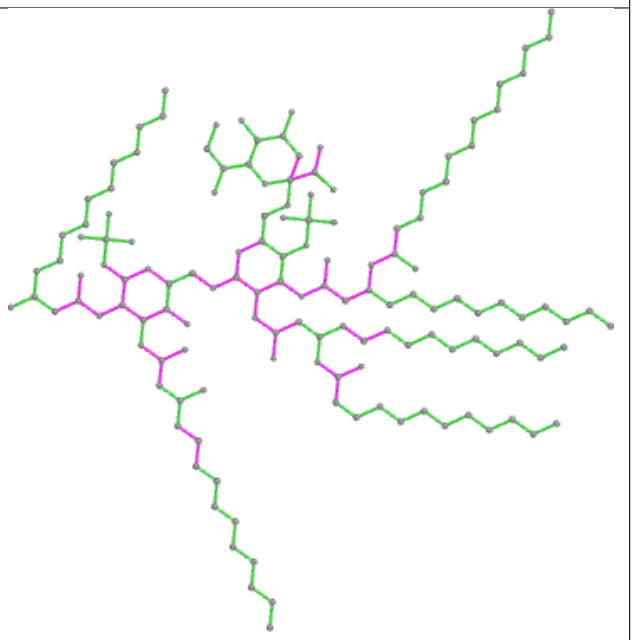
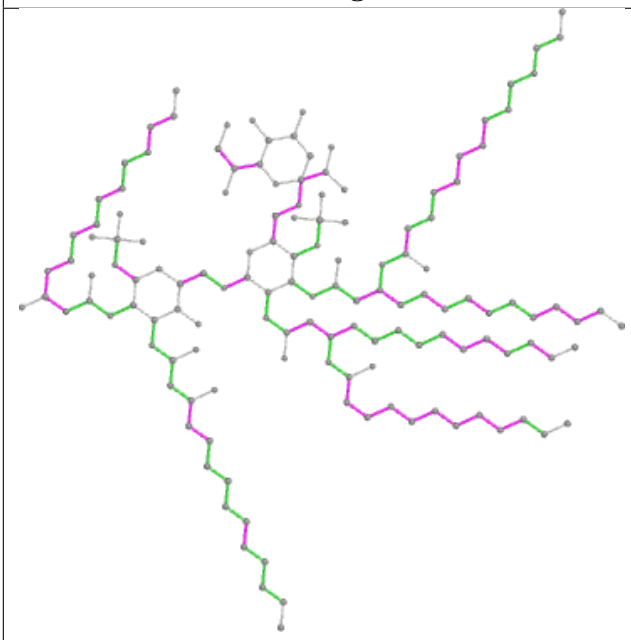


Bond angles



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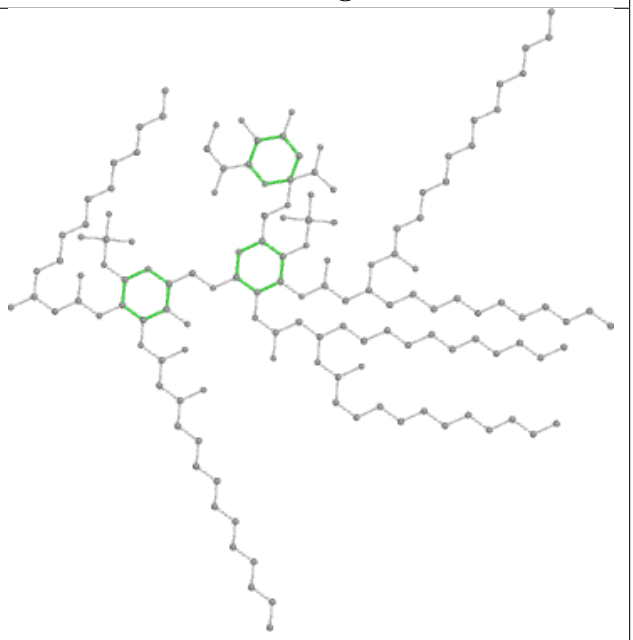
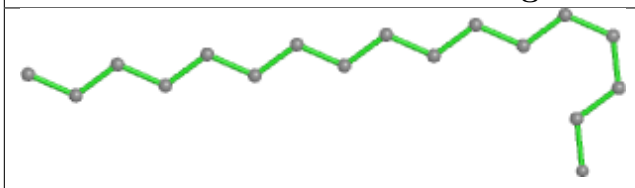


Rings

Ligand PLM K 201



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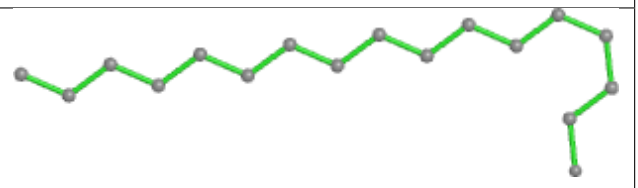
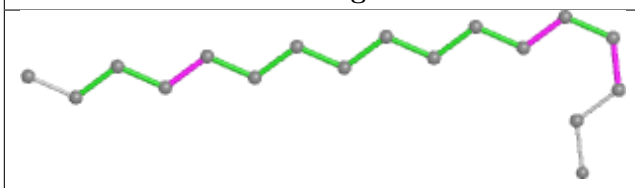


Bond angles



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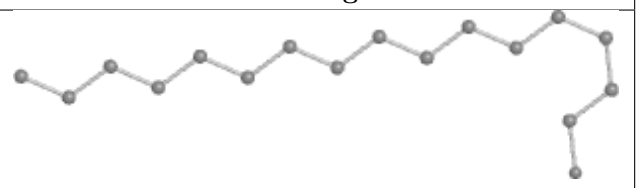
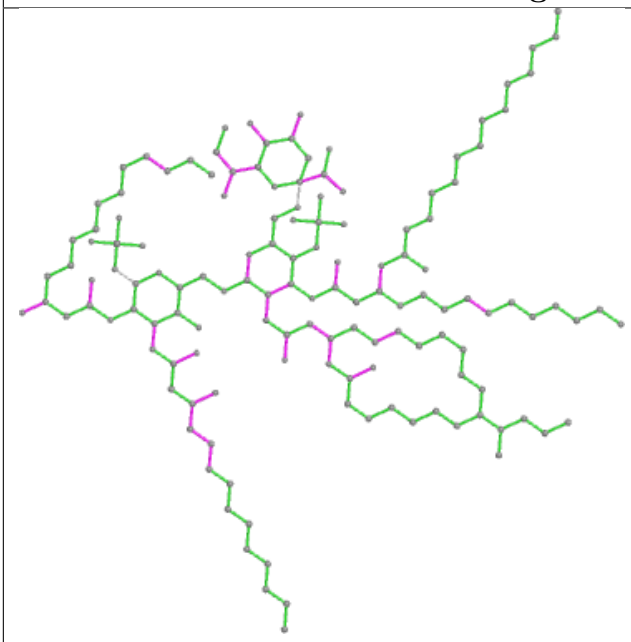
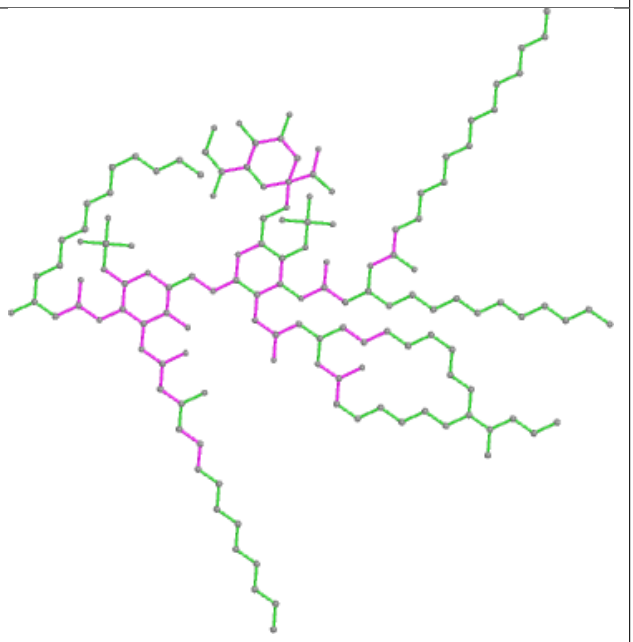


Rings

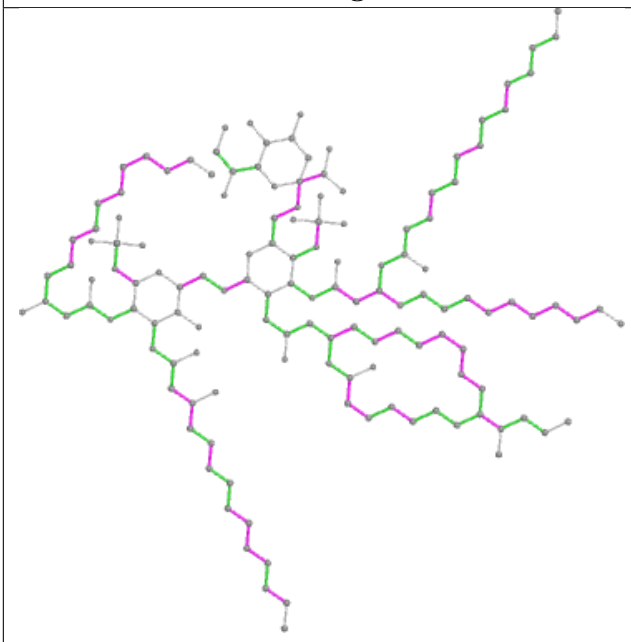
Ligand L8Z K 202



Bond lengths



Bond angles



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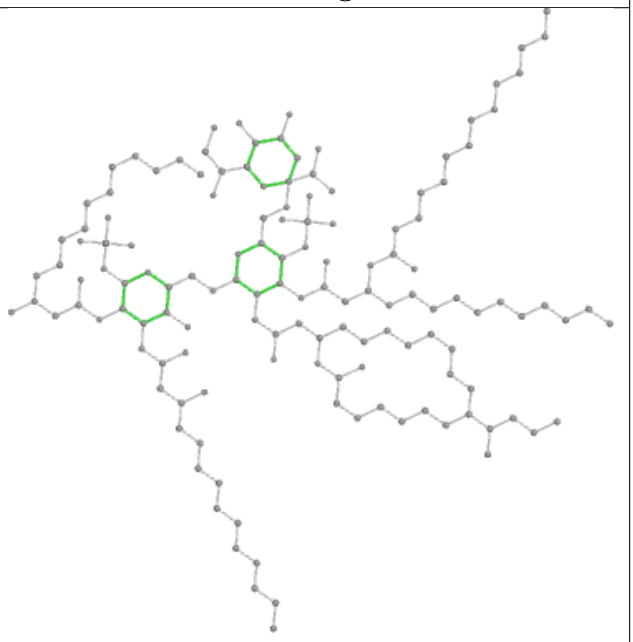
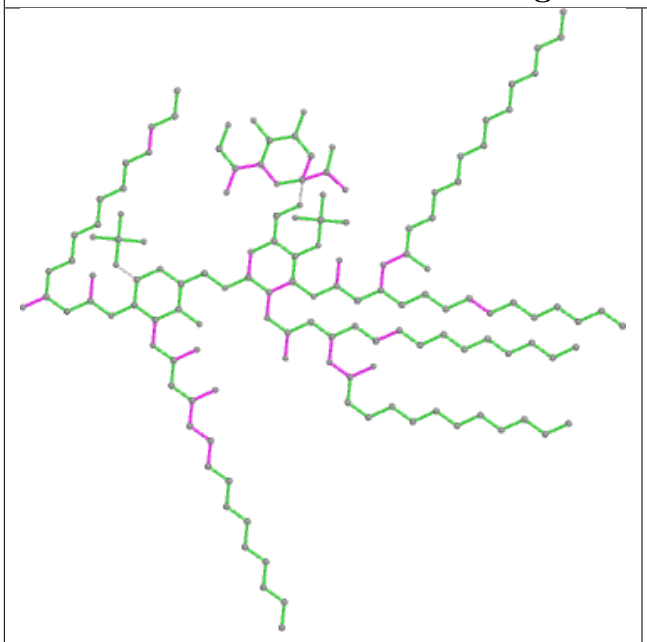


Rings

Ligand L8Z L 202



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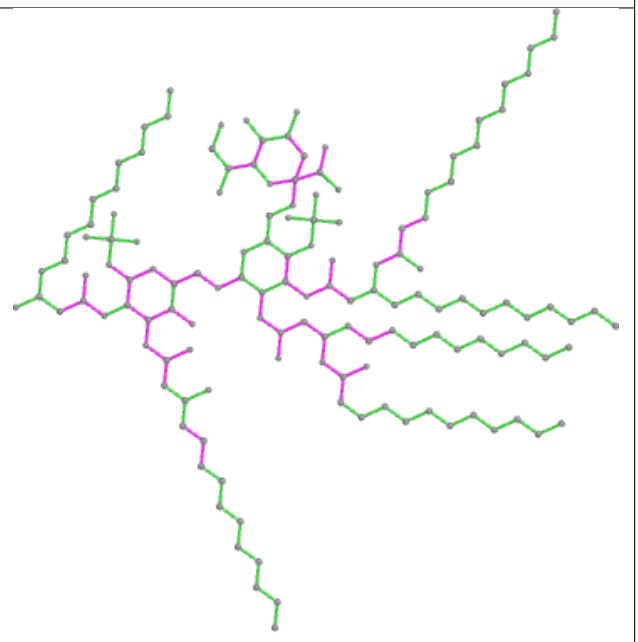
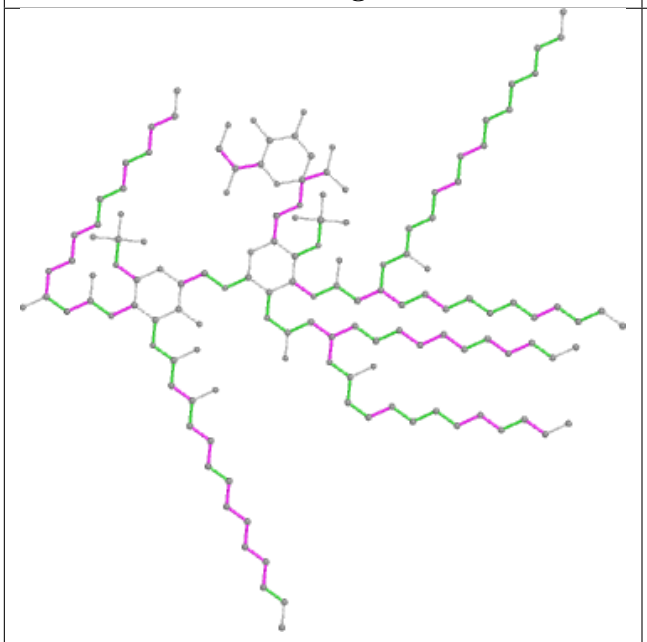


Bond angles



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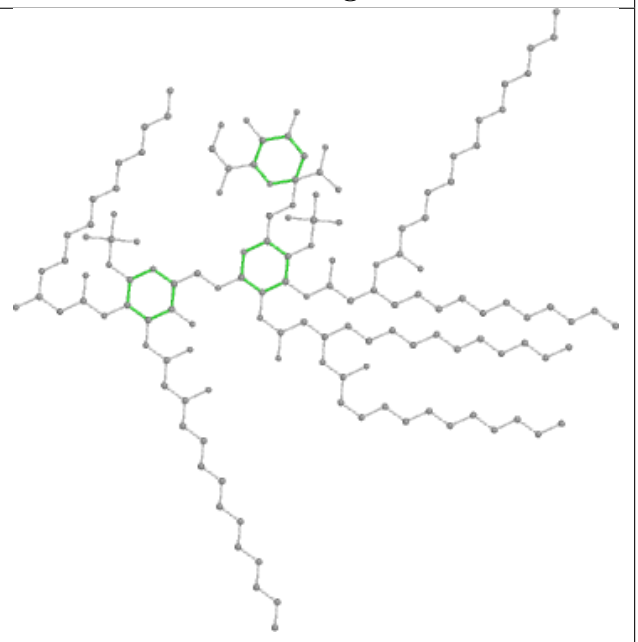
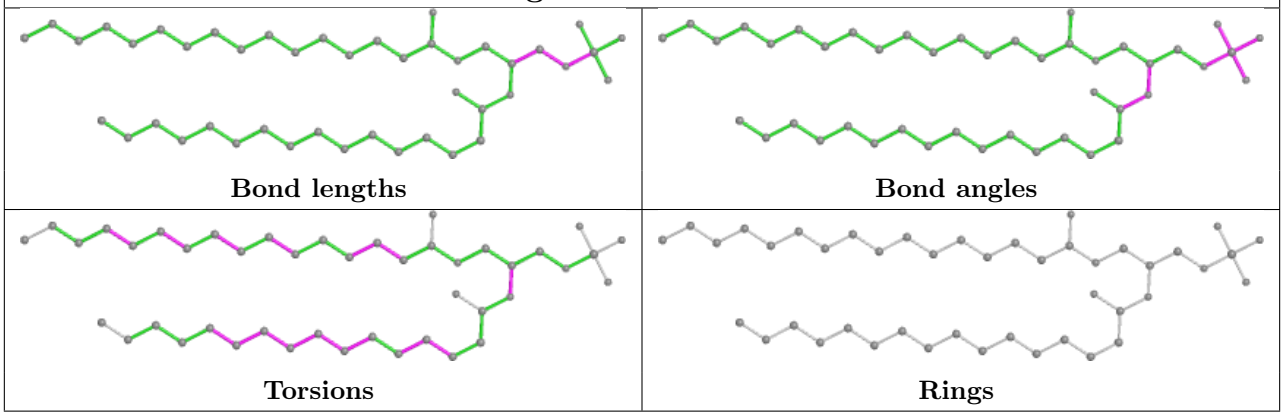
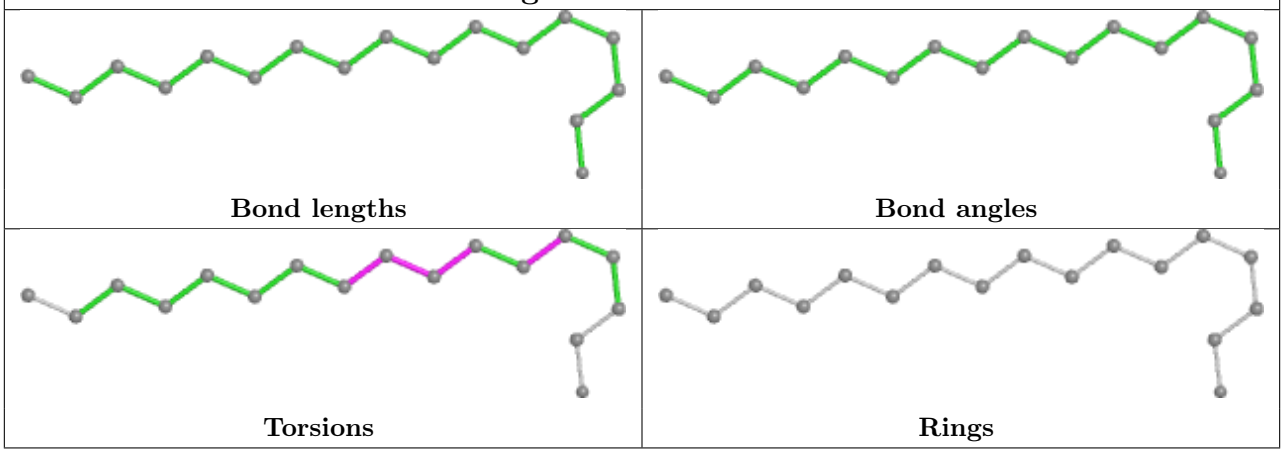


Rings

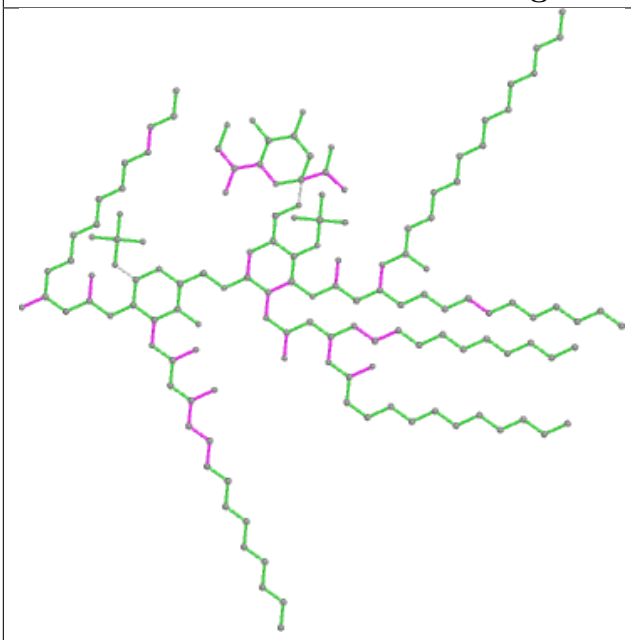
Ligand LPP K 203



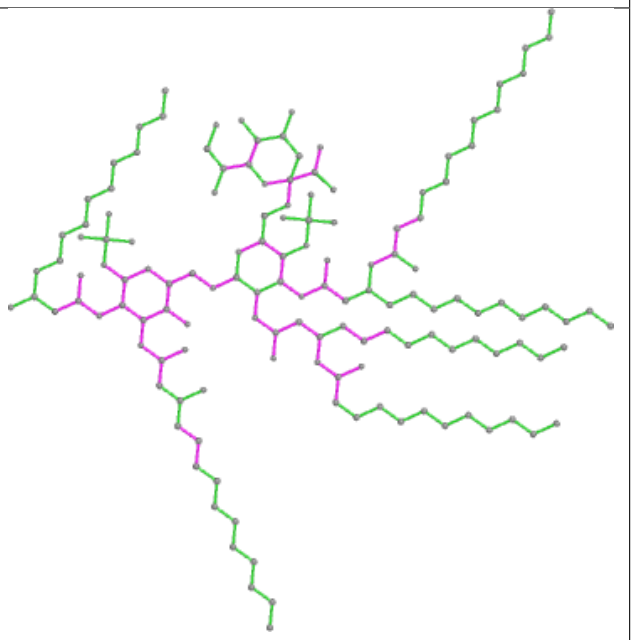
Ligand PLM G 201



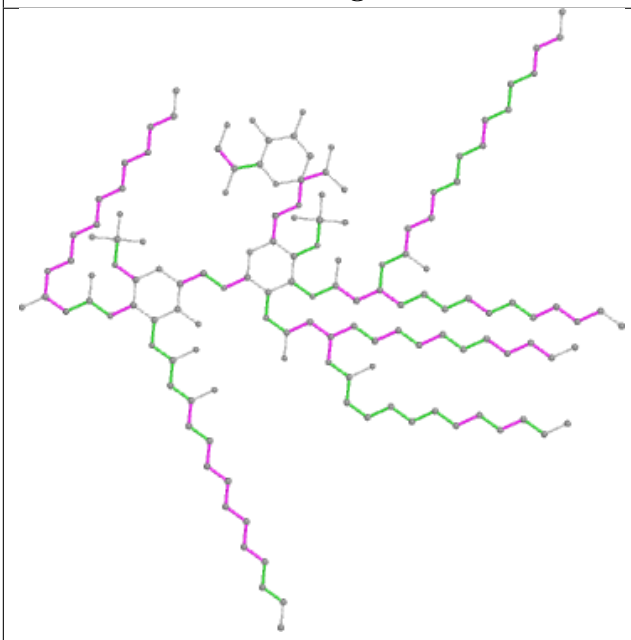
Ligand L8Z A 202



Bond lengths



Bond angles



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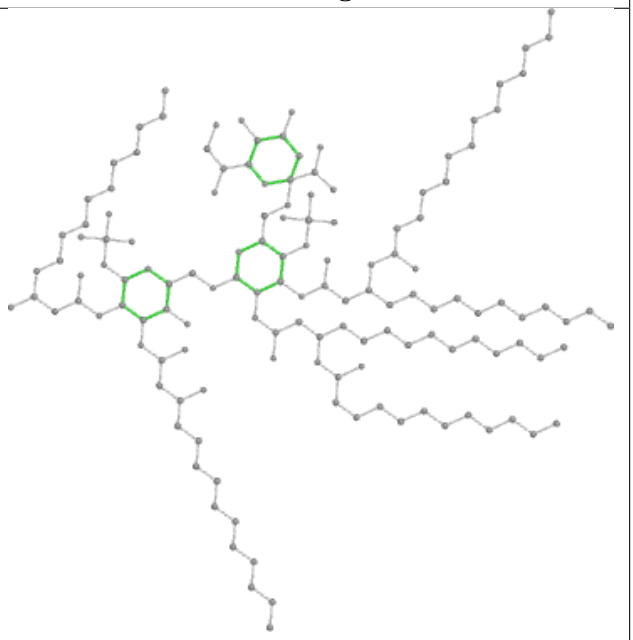
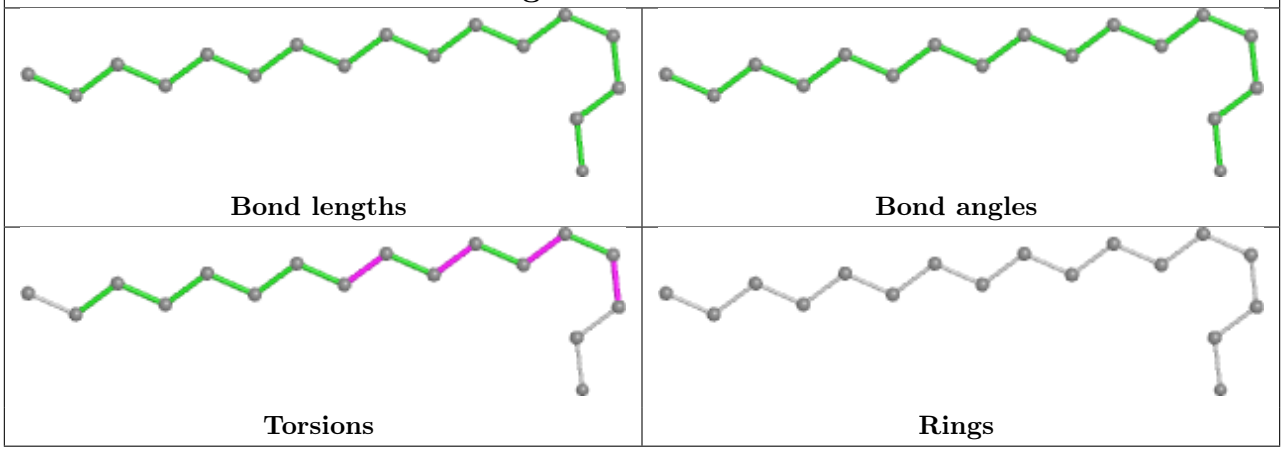
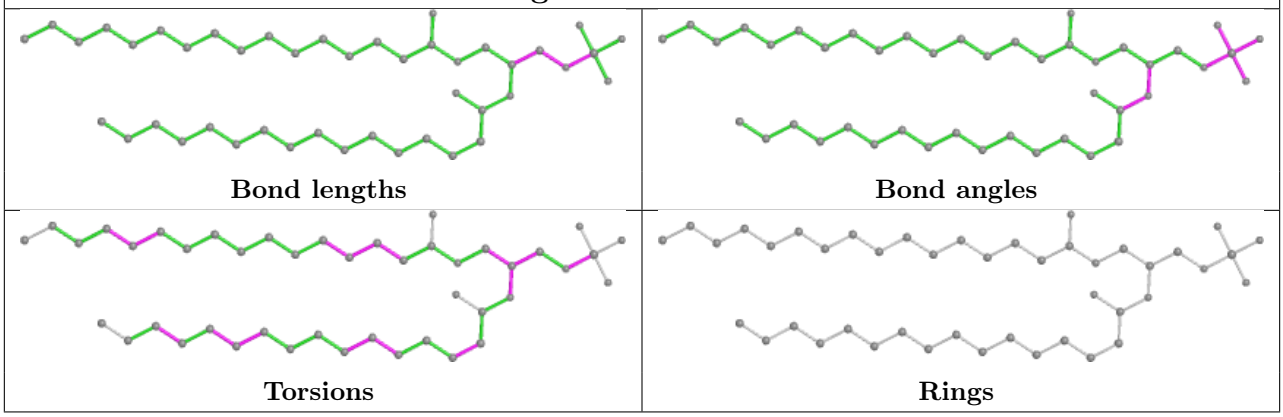


Rings

Ligand PLM B 201



Ligand LPP J 204



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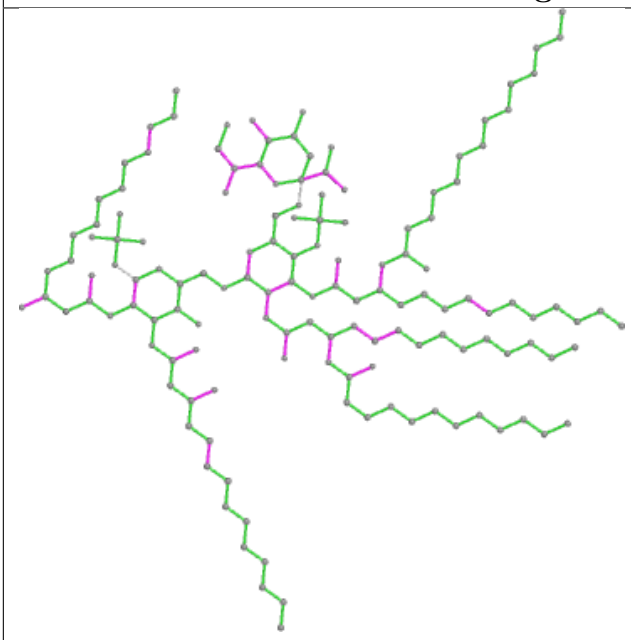
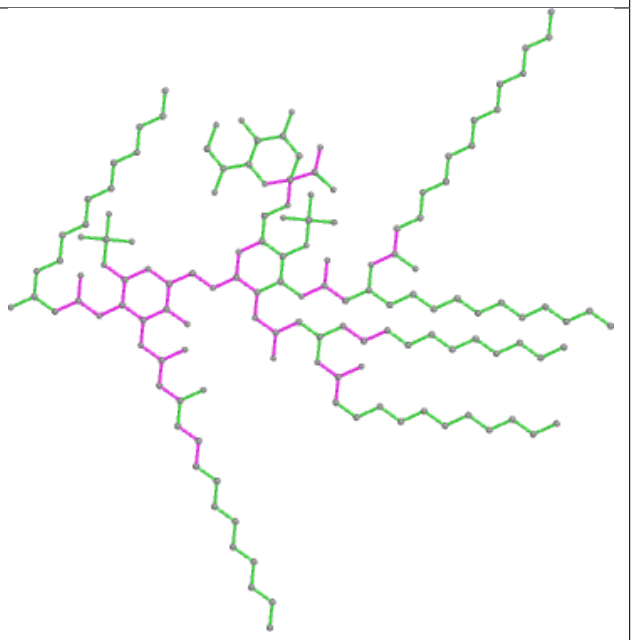
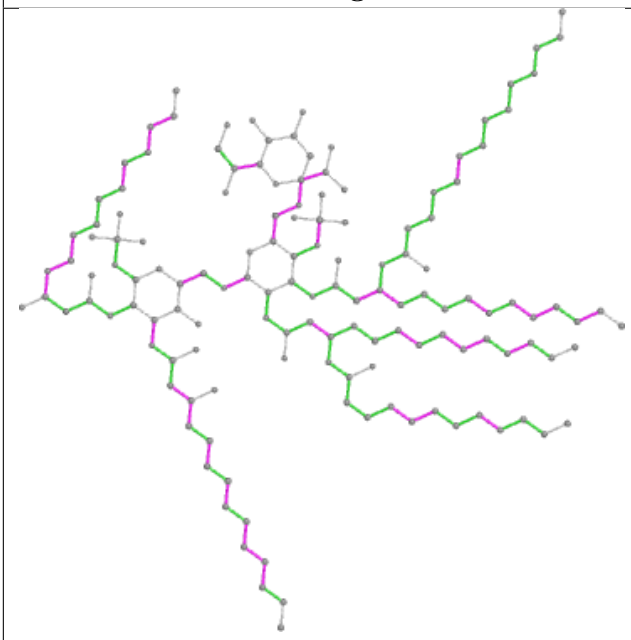


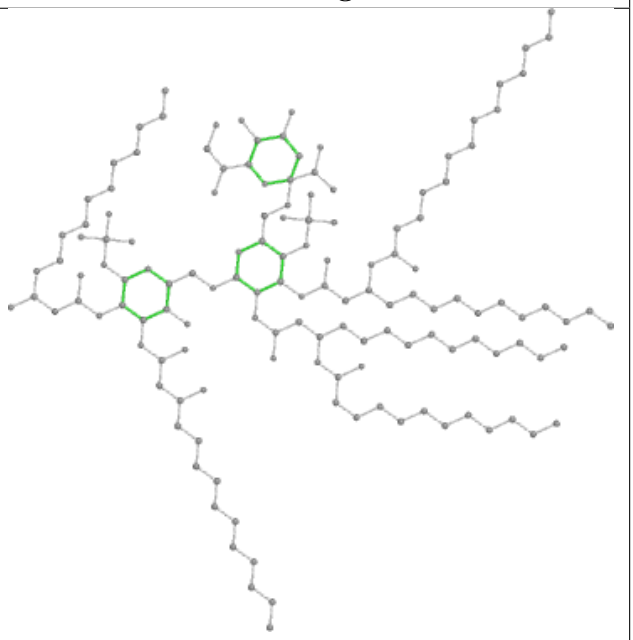
Bond lengths



Bond angles

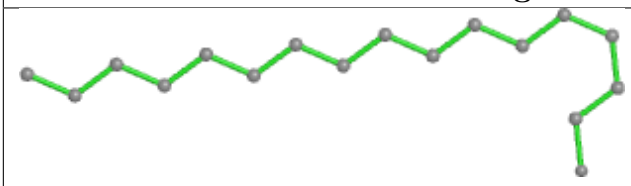


Torsions

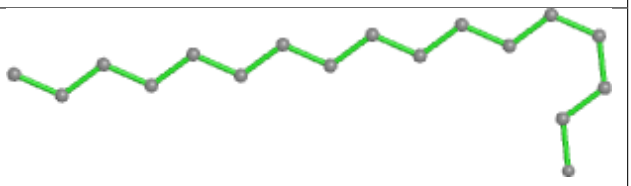


Rings

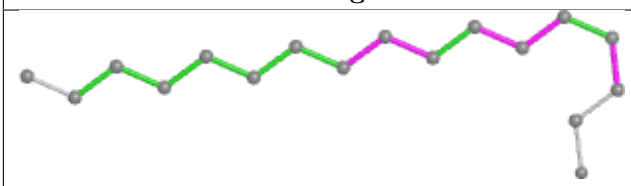
Ligand PLM E 1001



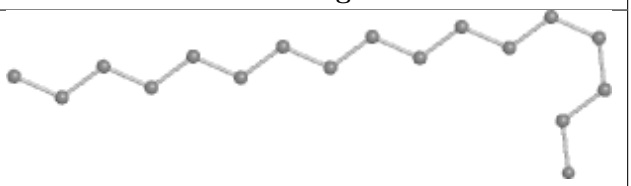
Bond lengths



Bond angles

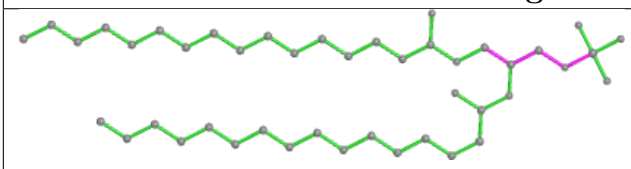


Torsions



Rings

Ligand LPP A 203



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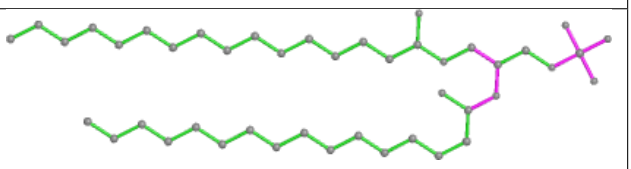
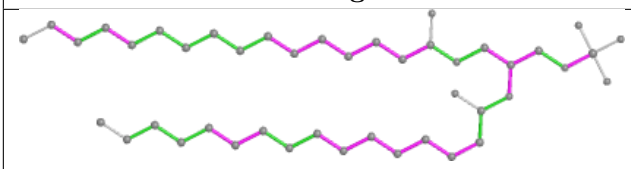


Bond angles



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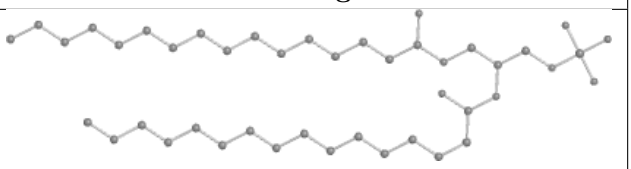
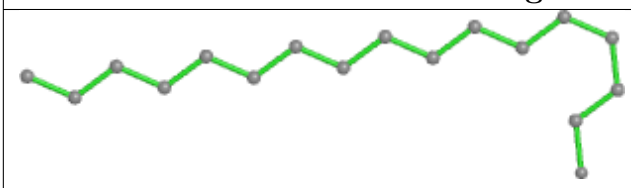
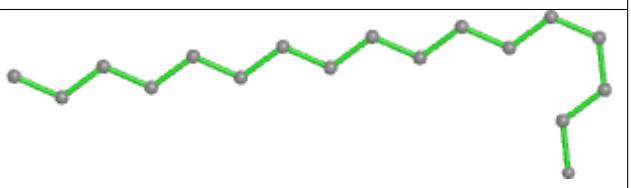


Rings

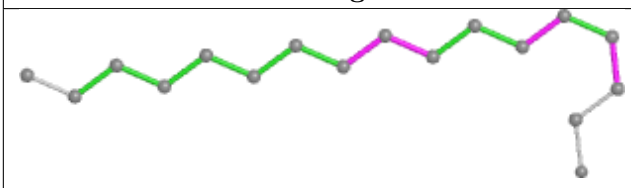
Ligand PLM J 201



Bond lengths



Bond angles



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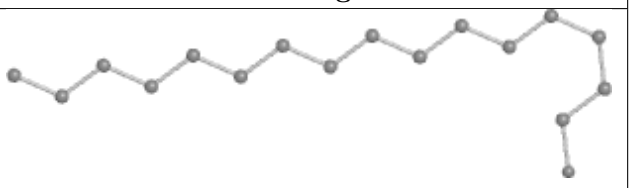
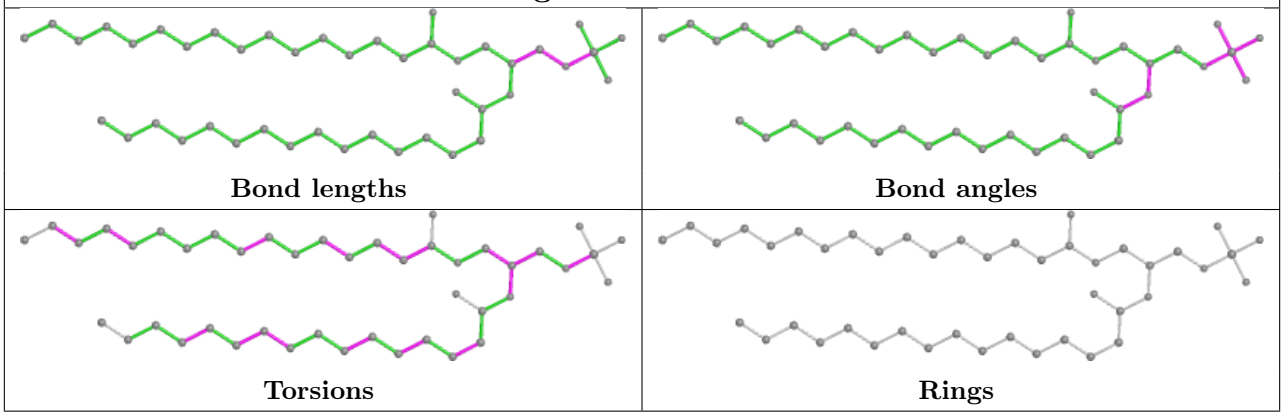
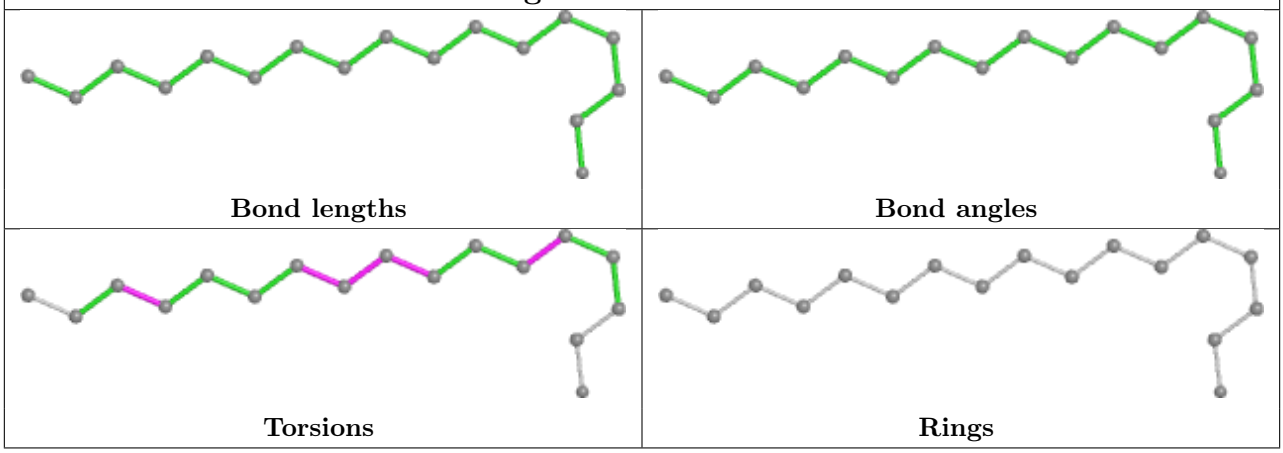


Rings

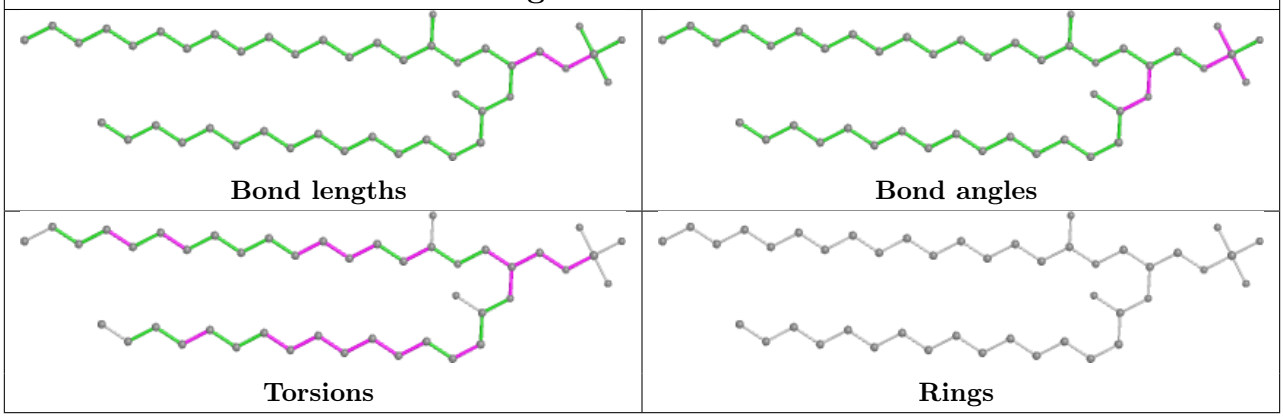
Ligand LPP I 203

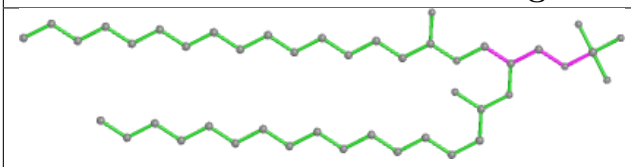
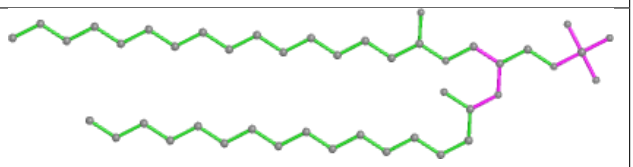
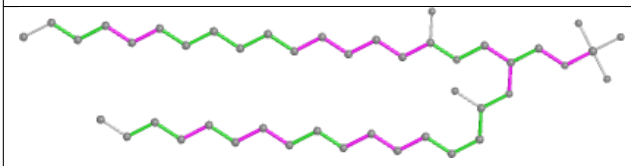
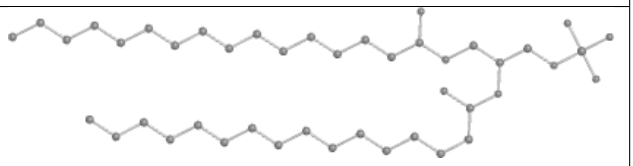


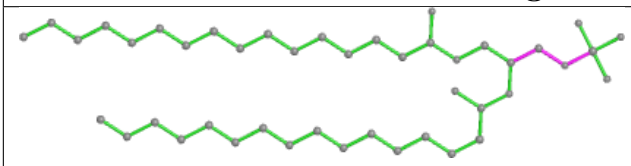
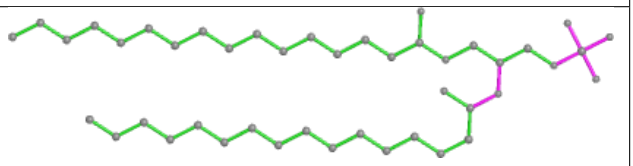
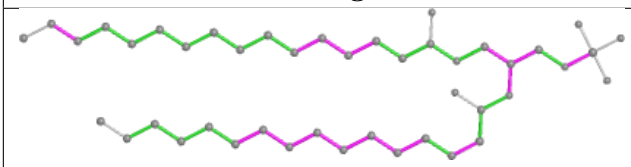
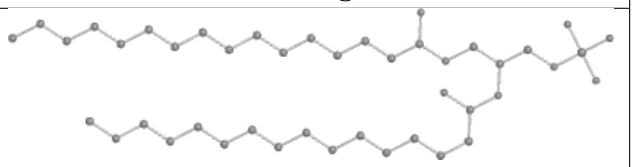
Ligand PLM F 201



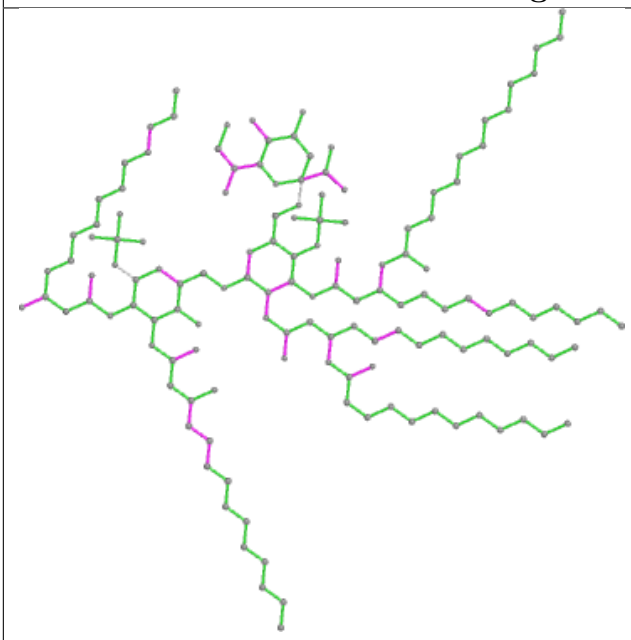
Ligand LPP C 204



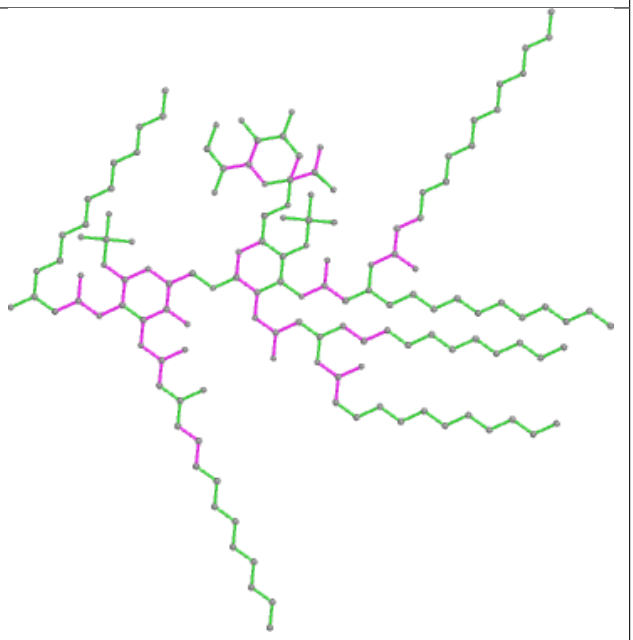
Ligand LPP L 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LPP D 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

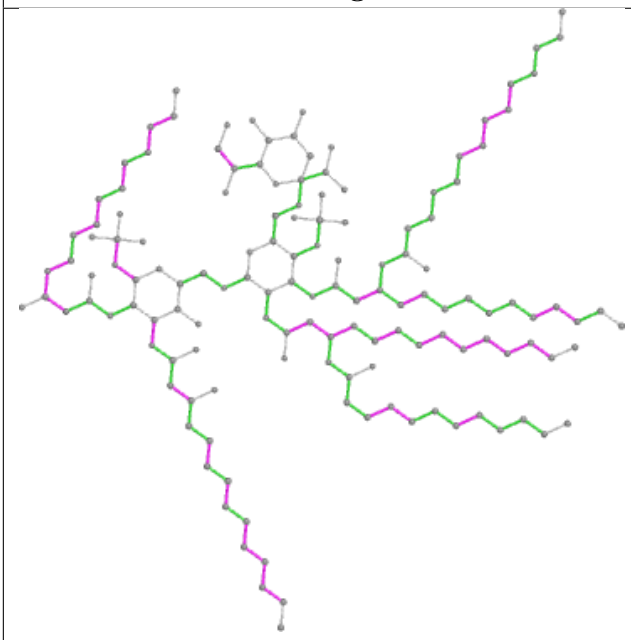
Ligand L8Z D 203



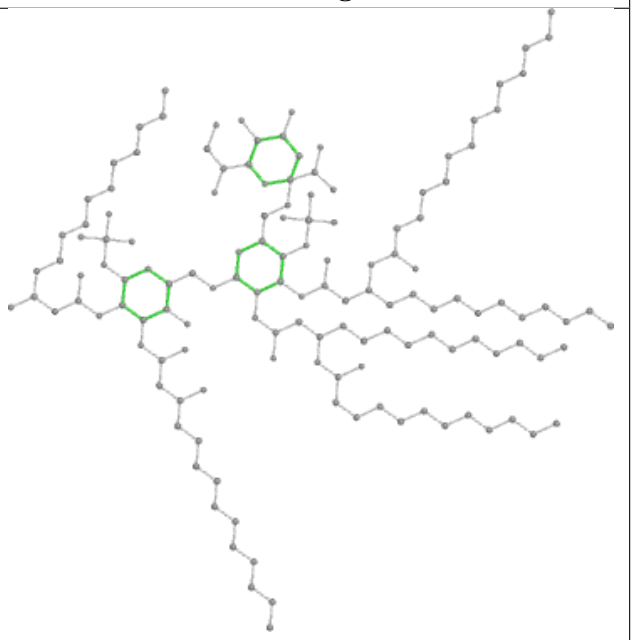
Bond lengths



Bond angles

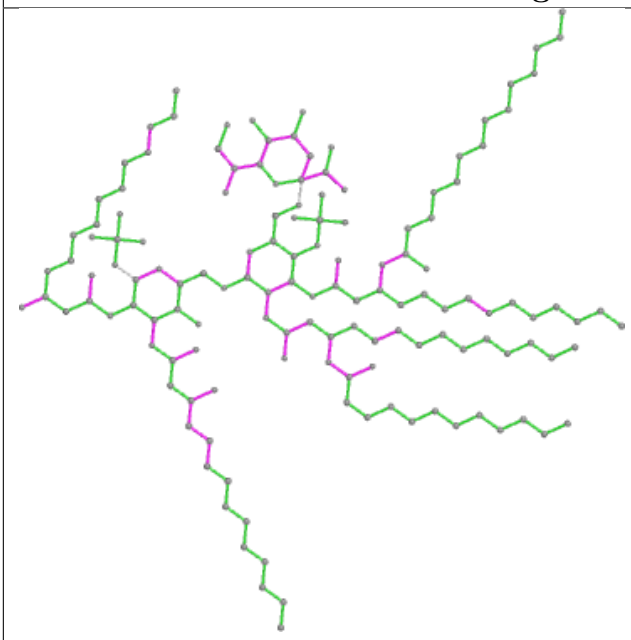


Torsions

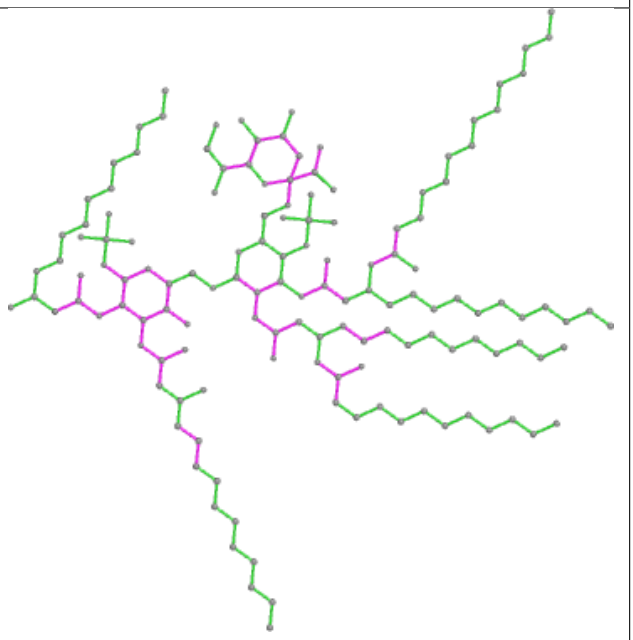


Rings

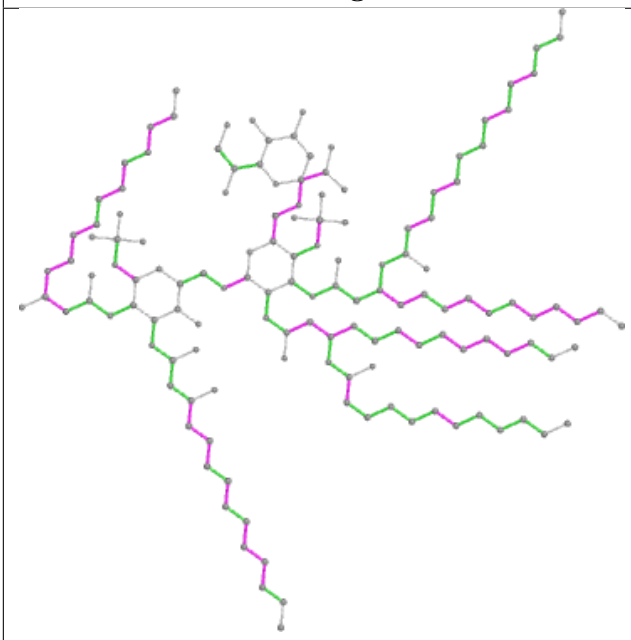
Ligand L8Z F 202



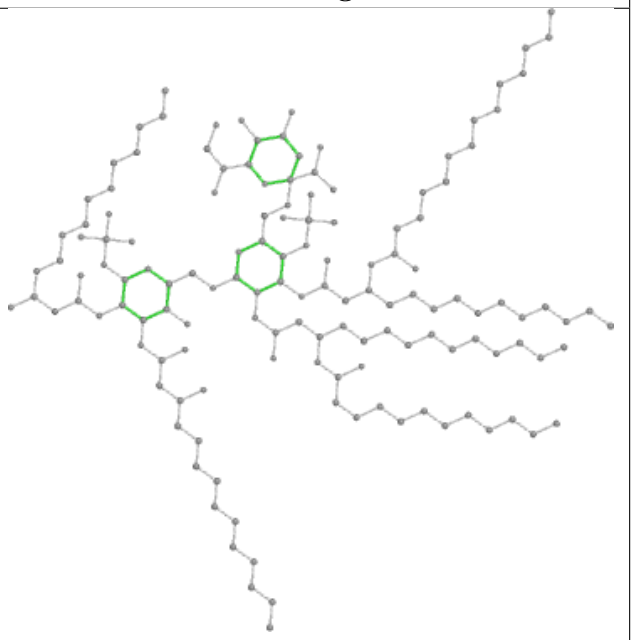
Bond lengths



Bond angles

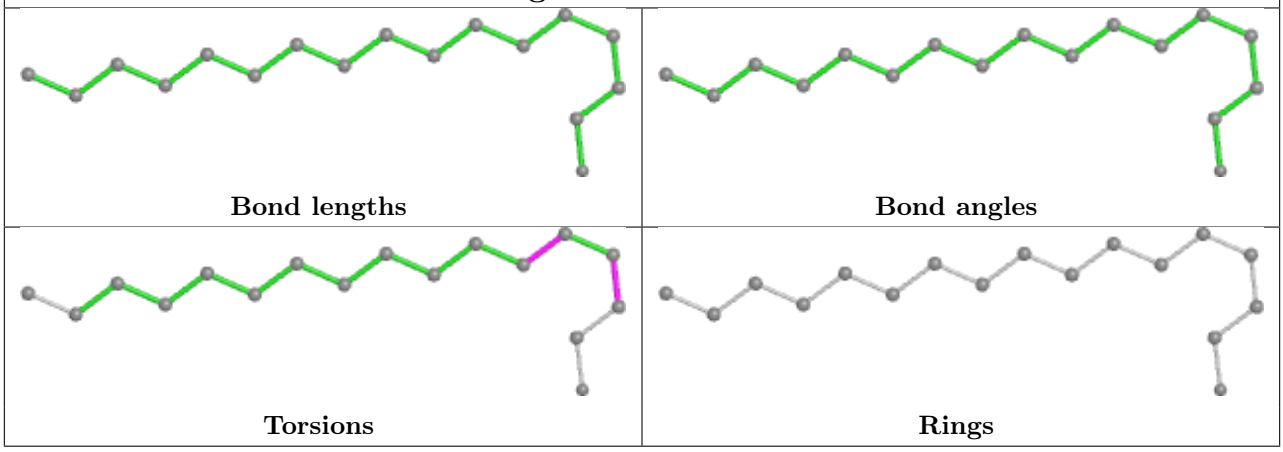


Torsions

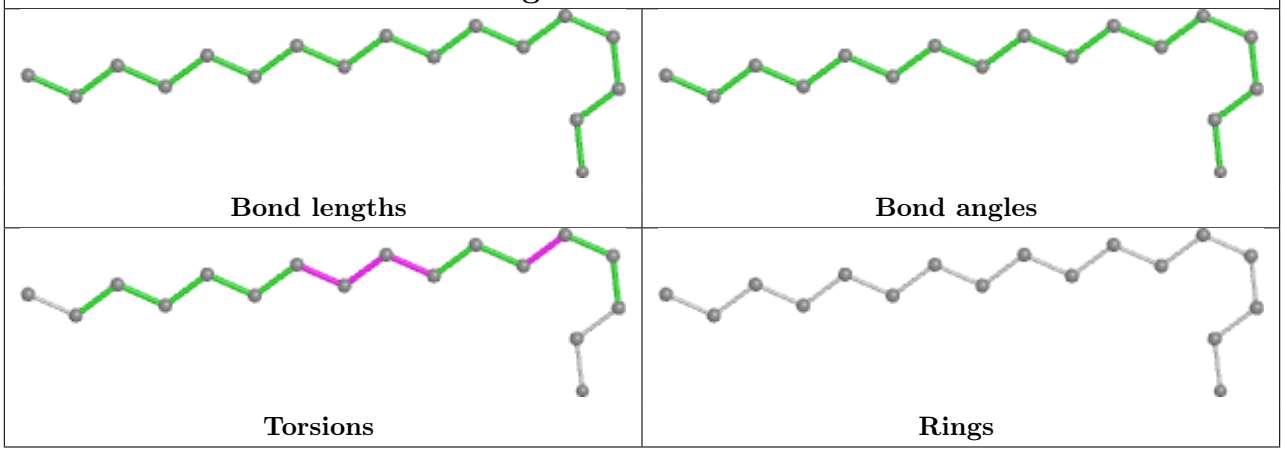


Rings

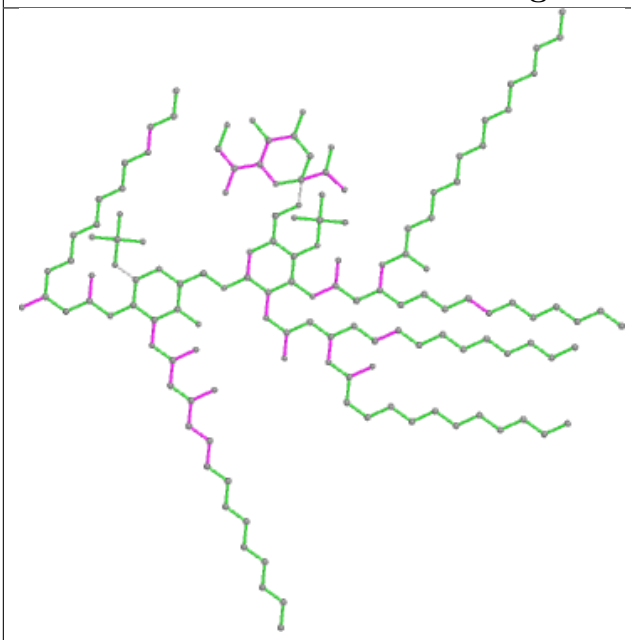
Ligand PLM I 201



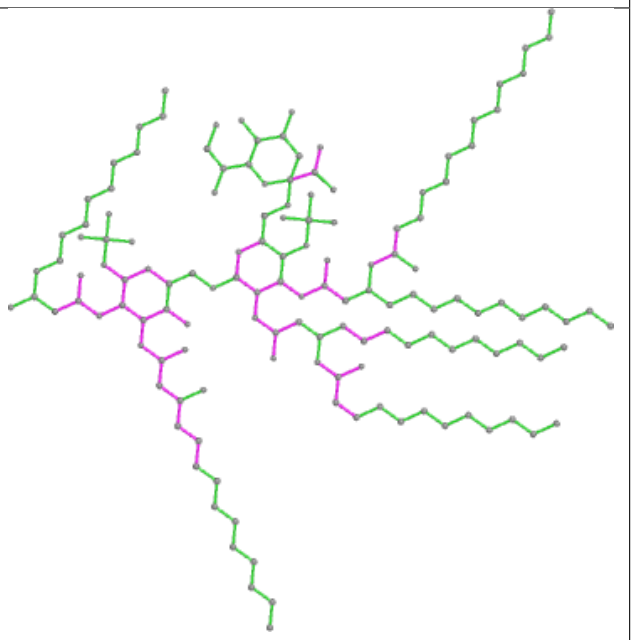
Ligand PLM C 201



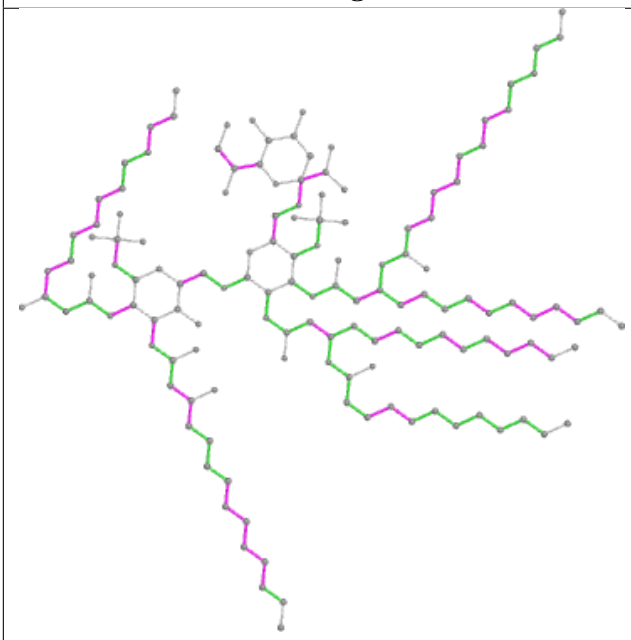
Ligand L8Z H 203



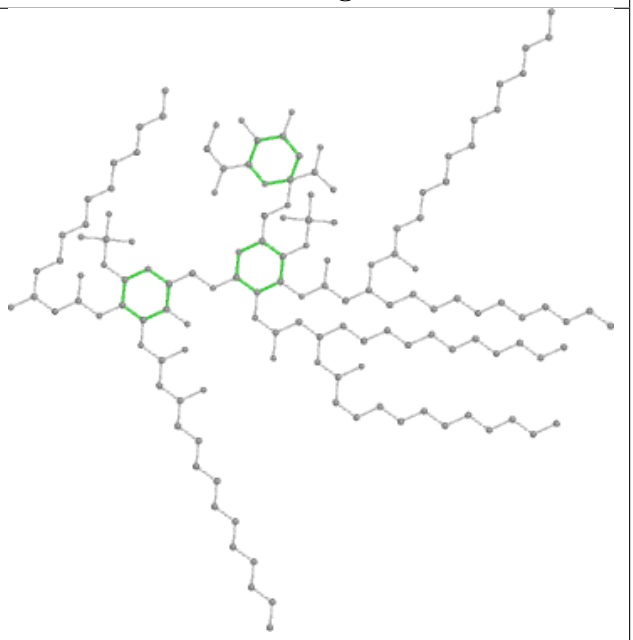
Bond lengths



Bond angles

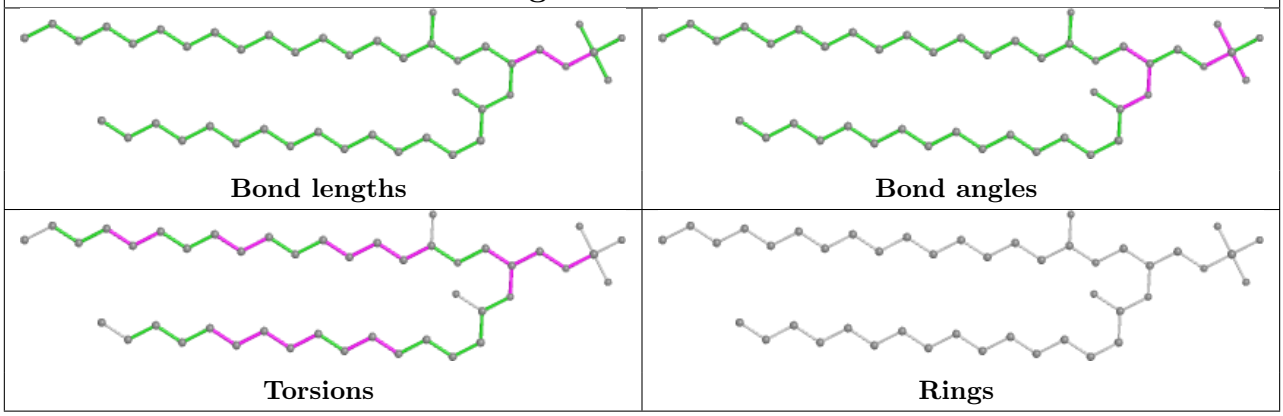


Torsions

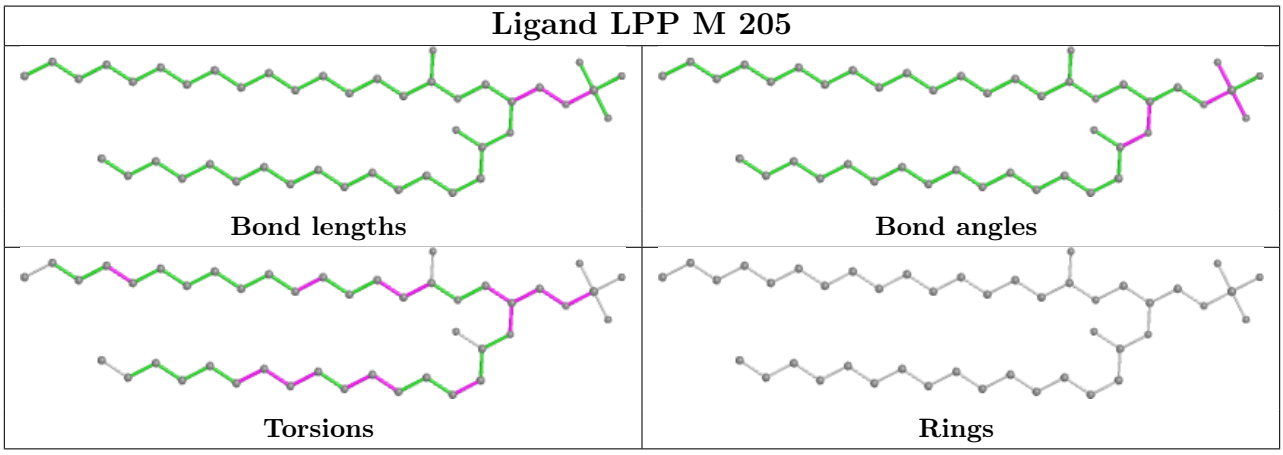


Rings

Ligand LPP F 203



Ligand LPP M 205



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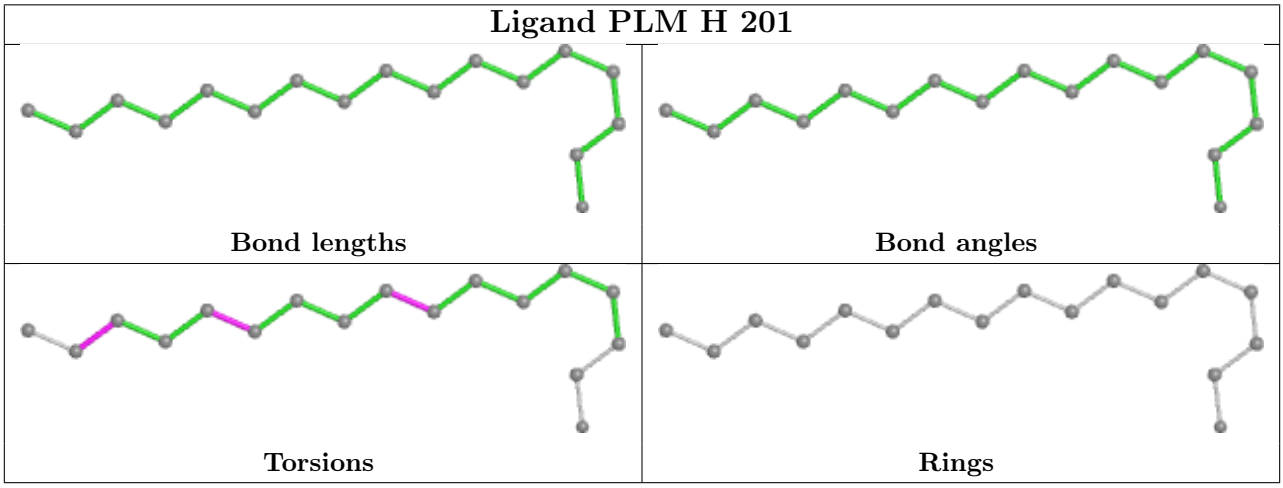
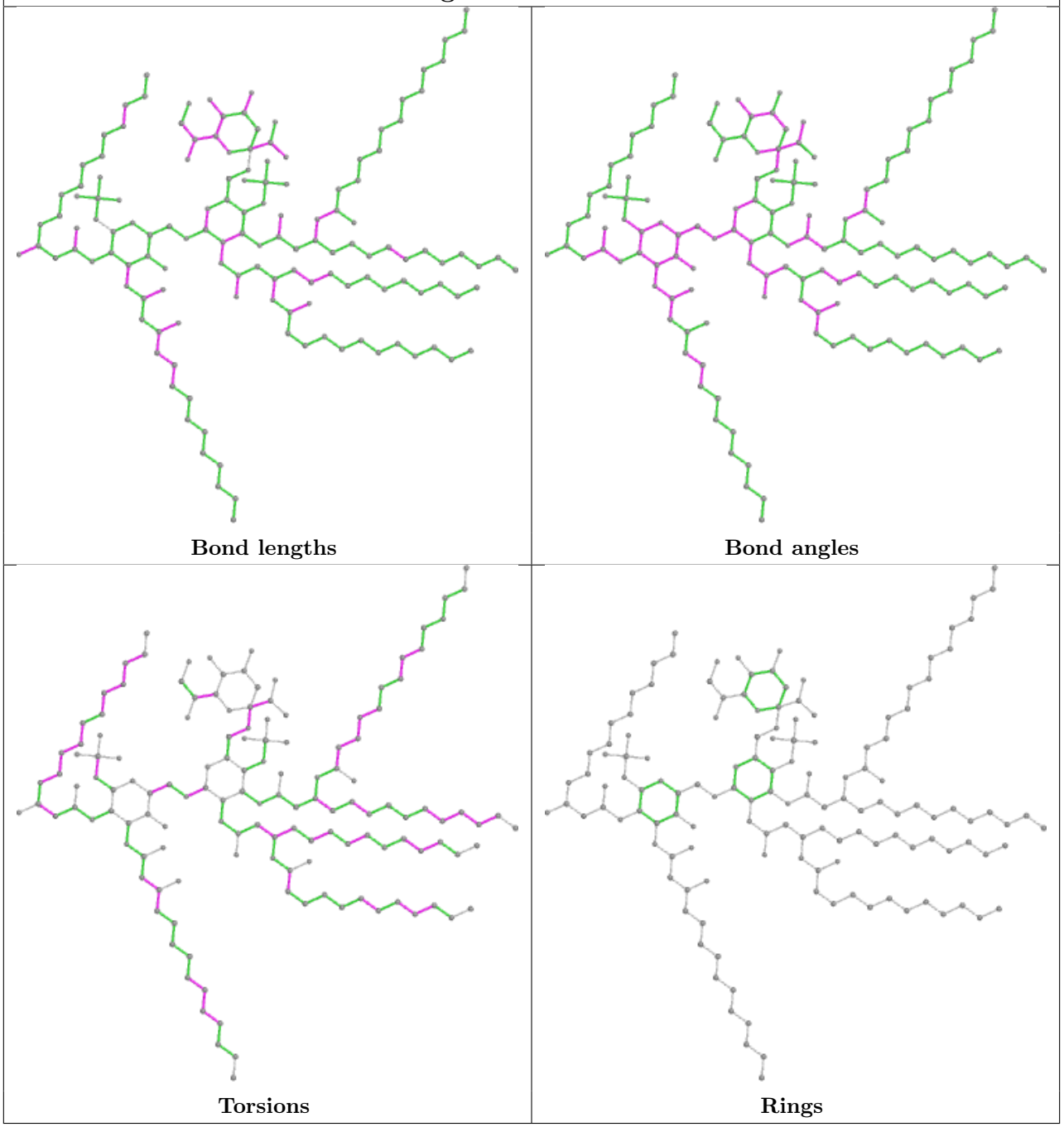


Ligand L8Z B 202



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.