



wwPDB EM Validation Summary Report ⓘ

Jul 18, 2022 – 05:07 pm BST

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 ⓘ 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 ⓘ](#)) 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) : 2.29

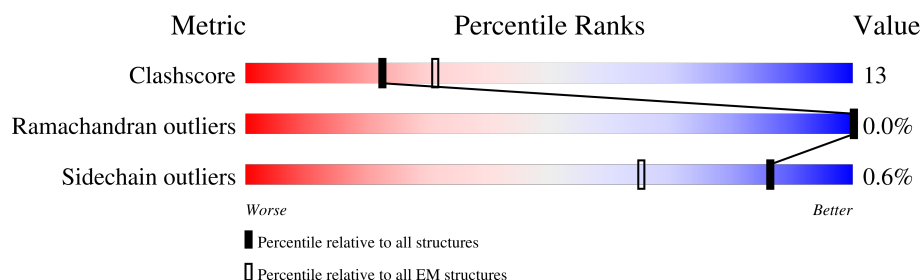
1 Overall quality at a glance

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.







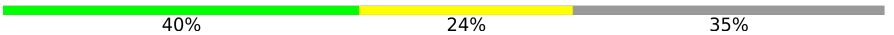
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	155	
1	B	155	
1	C	155	
1	D	155	
1	E	155	
1	F	155	
1	G	155	
1	H	155	
1	I	155	

Continued on next page...

Continued from previous page...

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

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.

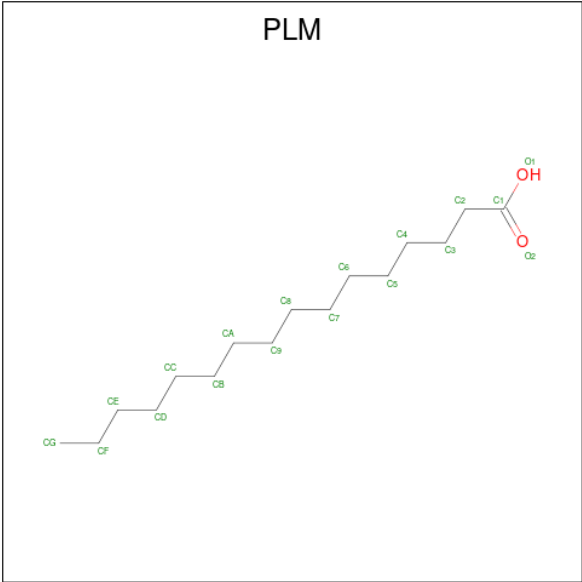
- Molecule 1 is a protein called Outer membrane lipoprotein slyB.

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		

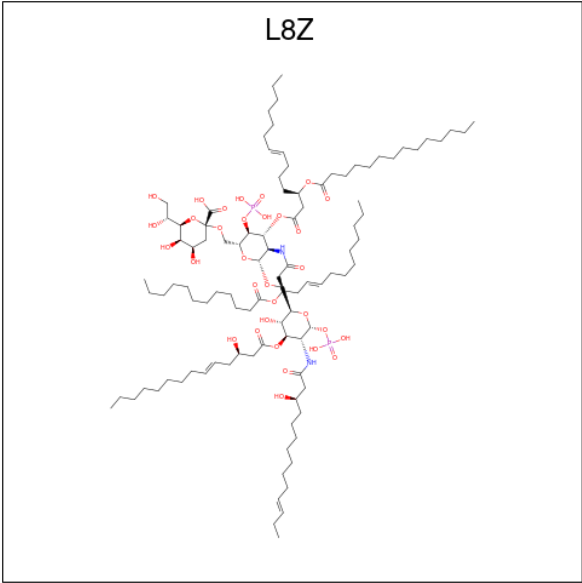
- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



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

- 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-phosphonoxy-oxan-2-yl]methoxy]-3-phosphonoxy-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: C₁₀₂H₁₈₂N₂O₃₂P₂).



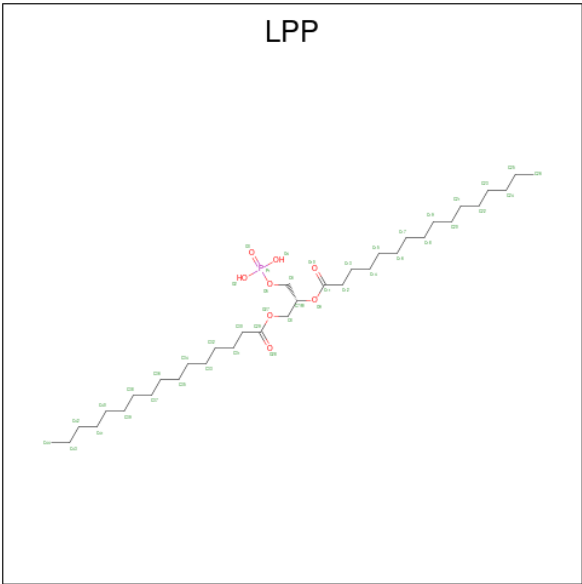
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	B	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	C	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	D	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	E	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	F	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	G	1	Total	C	N	O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

Continued on next page...

Continued from previous page...

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: C₃₅H₆₉O₈P).



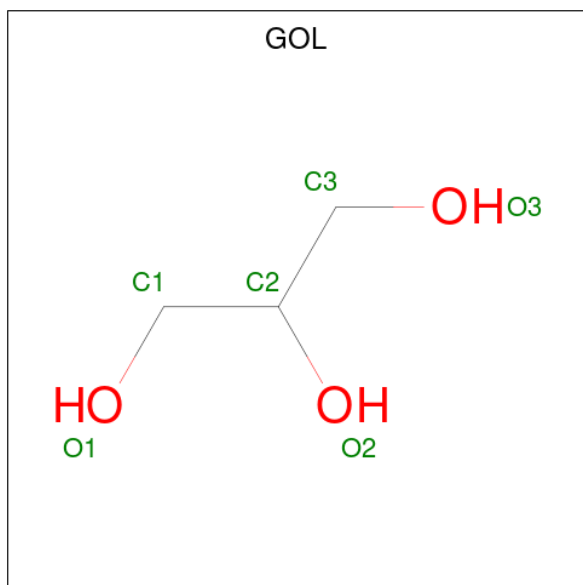
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			44	35	8	1	
5	B	1	Total	C	O	P	0
			44	35	8	1	
5	C	1	Total	C	O	P	0
			44	35	8	1	
5	D	1	Total	C	O	P	0
			44	35	8	1	
5	F	1	Total	C	O	P	0
			44	35	8	1	
5	G	1	Total	C	O	P	0
			44	35	8	1	
5	H	1	Total	C	O	P	0
			44	35	8	1	
5	I	1	Total	C	O	P	0
			44	35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

Continued on next page...

Continued from previous page...

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

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



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			5	3	2	
6	C	1	Total	C	O	0
			5	3	2	
6	D	1	Total	C	O	0
			10	6	4	
6	D	1	Total	C	O	0
			10	6	4	
6	E	1	Total	C	O	0
			5	3	2	
6	F	1	Total	C	O	0
			5	3	2	
6	H	1	Total	C	O	0
			10	6	4	
6	H	1	Total	C	O	0
			10	6	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
6	J	1	Total	C	O	0
			10	6	4	
6	J	1	Total	C	O	0
			10	6	4	
6	K	1	Total	C	O	0
			5	3	2	
6	M	1	Total	C	O	0
			10	6	4	
6	M	1	Total	C	O	0
			10	6	4	

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. 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.

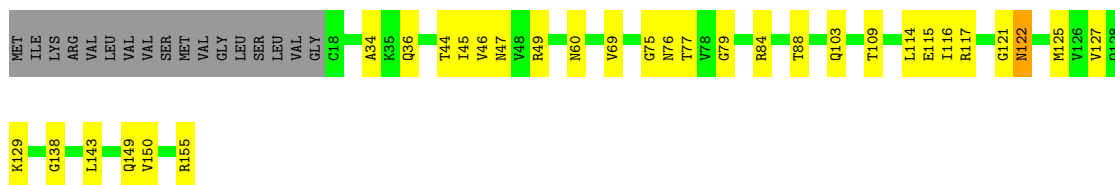
- Molecule 1: Outer membrane lipoprotein slyB

Chain A: 



- Molecule 1: Outer membrane lipoprotein slyB

Chain B: 



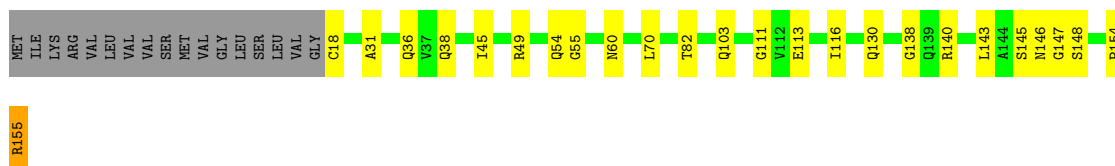
- Molecule 1: Outer membrane lipoprotein slyB

Chain C: 



- Molecule 1: Outer membrane lipoprotein slyB

Chain D: 



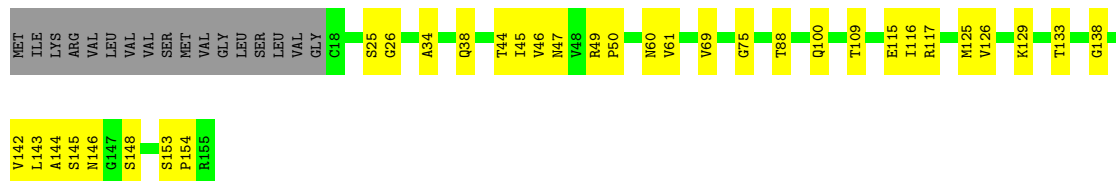
- Molecule 1: Outer membrane lipoprotein slyB

Chain E:  74% 15% 11%



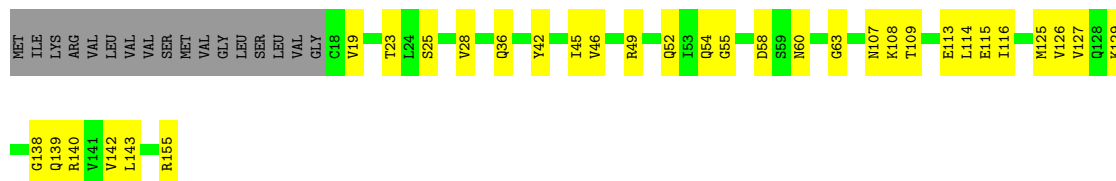
- Molecule 1: Outer membrane lipoprotein slyB

Chain F:  68% 21% 11%



- Molecule 1: Outer membrane lipoprotein slyB

Chain G:  68% 21% 11%



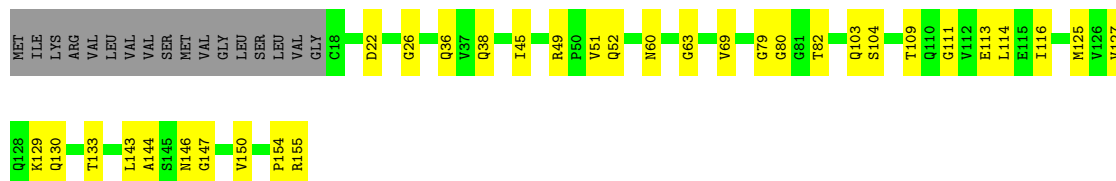
- Molecule 1: Outer membrane lipoprotein slyB

Chain H:  69% 19% 11%



- Molecule 1: Outer membrane lipoprotein slyB

Chain I:  68% 21% 11%



- Molecule 1: Outer membrane lipoprotein slyB

MET	ILE	LYS	ARG	VAL	LEU	VAL	VAL	SER	MET	GLY	GLY	LEU	SER	LEU	VAL	VAL	GLY	C18	N21	V37	V51	Q54	D58	T82	K108	T109	I116	V126	V127	Q128	K129	R140	V141	V142	L143	N146	G147	P154	R155
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Chain K: 75% 14% 11%

MET	TLE	LVS	ARG	VAL	LEV	VAL	VAL	SER	MET	VAL	GLY	LEV	SER	LEV	VAL	GLY	C18	N20	T23	Y29	A34	K35	Q36	I45	V46	V69	T77	S85	T88	Q103	S104	E113	L114	E115	M125
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------

- Chain L:  67% 22% 11%

T133	T134	G138	G139	R140	A144	S145	N146	G147	P154	R155	MET	ILE	LYS	ARG	VAL	LEU	VAL	VAL	SER	MET	VAL	GLY	LEU	SER	LEU	VAL	GLY	C18	N21	I45	V46	R49	N60	V61	I62	G63	A64	A68	F73	L74	G75	T88	G89	S104	T109	G110	G111	V112	E113	L114	E115	M125	V126	V127	G128	K129	Q130	G131	V132
------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Chain M:  65% 25% 11%

V127	T133	G138	Q139	R140	V141	V142	L143	N146	G147	S148	T151	V152	S153	P154	R155	NET	L1E	L1YS	ARG	VAL	LEU	VAL	VAL	SER	NET	VAL	GLY	LEU	SER	LEU	GLY	C18	T45	V48	R49	Q52	G55	N60	P63	I62	G75	H76	T77	H76	G79	G80	T88	A92	G95	V102	Q103	S104	M107	K108	V112	E113	L114	E115	I116	M125
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------

- Chain N: 40% 24% 35%

ASP	SER	THR	GLN	VAL	ASN	ASN	VAL	ASN	THR	MET
THR	THR	GLN	VAL	ASN	ASN	ILE	GLY	ILE	THR	ALA
VAL	VAL	ASN	VAL	ASN	ASN	GLY	SER	ARG	ARG	LYS
SER	SER	ASN	VAL	ASN	ASN	HIS	ASP	LEU	PHE	LEU
LEU	LEU	ALA	VAL	ASN	ALA	ALA	ARG	ASP	THR	ILE
THR	THR	PRO	THR	THR	THR	PHE	THR	ALA	ALA	ALA
ASP	ASP	THR	THR	THR	THR	THR	ILE	GLY	SER	SER
LYS	LYS	VAL	VAL	ASN	ASN	ASP	ASP	ASN	LEU	LEU
GLY	GLY	VAL	VAL	GLU	GLU	LEU	ASP	PHE	GLU	PHE
ILE	ILE	THR	THR	ILE	ILE	ILE	GLU	ASP	SER	SER
THR	THR	VAL	VAL	HIS	SER	SER	LYS	VAL	VAL	THR
THR	THR	THR	THR	THR	THR	PHE	GLY	ARG	ALA	THR
VAL	VAL	VAL	VAL	GLN	GLN	VAL	GLU	LEU	VAL	VAL
ASN	ASN	VAL	VAL	LEU	LEU	ARG	PHE	ASP	ARG	TYR
ILE	ILE	THR	THR	ASP	ASP	THR	THR	GLY	GLY	ALA
THR	THR	GLU	GLU	GLU	GLU	TYR	TYR	ASP	GLY	ALA
GLY	GLY	VAL	VAL	VAL	VAL	SER	VAL	THR	THR	GLY
ASP	ASP	GLN	GLN	PRO	PRO	VAL	VAL	LEU	LEU	PHE
GLN	GLN	TRP	TRP	TRP	TRP	GLY	SER	GLU	GLU	VAL
LYS	LYS	ASN	ASN	ASN	ASN	VAL	TYR	VAL	VAL	HIS
LEU	LEU	VAL	VAL	VAL	VAL	ALA	ALA	LYS	LYS	ILE
\$269	\$270	\$271	\$272	\$273	\$274	\$275	\$276	\$277	\$278	\$279
\$280	\$281	\$282	\$283	\$284	\$285	\$286	\$287	\$288	\$289	\$290
\$291	\$292	\$293	\$294	\$295	\$296	\$297	\$298	\$299	\$300	\$301
\$302	\$303	\$304	\$305	\$306	\$307	\$308	\$309	\$310	\$311	\$312
\$313	\$314	\$315	\$316	\$317	\$318	\$319	\$320	\$321	\$322	\$323
\$324	\$325	\$326	\$327	\$328	\$329	\$330	\$331	\$332	\$333	\$334
\$335	\$336	\$337	\$338	\$339	\$340	\$341	\$342	\$343	\$344	\$345
\$346	\$347	\$348	\$349	\$350	\$351	\$352	\$353	\$354	\$355	\$356
\$357	\$358	\$359	\$360	\$361	\$362	\$363	\$364	\$365	\$366	\$367
\$368	\$369	\$370	\$371	\$372	\$373	\$374	\$375	\$376	\$377	\$378
\$379	\$380	\$381	\$382	\$383	\$384	\$385	\$386	\$387	\$388	\$389
\$390	\$391	\$392	\$393	\$394	\$395	\$396	\$397	\$398	\$399	\$400
\$401	\$402	\$403	\$404	\$405	\$406	\$407	\$408	\$409	\$410	\$411
\$412	\$413	\$414	\$415	\$416	\$417	\$418	\$419	\$420	\$421	\$422
\$423	\$424	\$425	\$426	\$427	\$428	\$429	\$430	\$431	\$432	\$433
\$434	\$435	\$436	\$437	\$438	\$439	\$440	\$441	\$442	\$443	\$444
\$445	\$446	\$447	\$448	\$449	\$450	\$451	\$452	\$453	\$454	\$455
\$456	\$457	\$458	\$459	\$460	\$461	\$462	\$463	\$464	\$465	\$466
\$467	\$468	\$469	\$470	\$471	\$472	\$473	\$474	\$475	\$476	\$477
\$478	\$479	\$480	\$481	\$482	\$483	\$484	\$485	\$486	\$487	\$488
\$489	\$490	\$491	\$492	\$493	\$494	\$495	\$496	\$497	\$498	\$499
\$500	\$501	\$502	\$503	\$504	\$505	\$506	\$507	\$508	\$509	\$510
\$511	\$512	\$513	\$514	\$515	\$516	\$517	\$518	\$519	\$520	\$521
\$522	\$523	\$524	\$525	\$526	\$527	\$528	\$529	\$530	\$531	\$532
\$533	\$534	\$535	\$536	\$537	\$538	\$539	\$540	\$541	\$542	\$543
\$544	\$545	\$546	\$547	\$548	\$549	\$550	\$551	\$552	\$553	\$554
\$555	\$556	\$557	\$558	\$559	\$560	\$561	\$562	\$563	\$564	\$565
\$566	\$567	\$568	\$569	\$570	\$571	\$572	\$573	\$574	\$575	

S324	F394	E521	T600	P721
R325	T400	Y522	I601	T722
P326	ASP	N523	E607	P723
	THR	S524	Y608	F724
V335	Q403	L525	Y609	
K336	R404	R526	K610	V733
L337	V405		V611	S736
R338		L529		
V339		V532	D614	M741
N340	P409		T615	G742
V341	D410	S535	A616	T743
D342	Q411	L536	T617	V744
A343	V412	S537		V745
G344	D413	N538	V628	D746
N345	V414	M539	V629	T747
R346	V415	Q540	L630	N748
F347	V416	P541		V749
Y348	K417	D542	W635	
V349	V418	V543	G636	Y754
R350	K419			
R351	E420	L549	D639	Y757
I352	ARG			
R353	ASN	E554	N651	Y760
F354	THR		F652	
	G424	S559		I766
N357		D560	S657	R767
	T434	Q561	S658	M768
S360	E435	D562	T659	
K361		N563	V660	G771
	F440	S564		
V364	Q441	F565	G669	W776
L365		K566	P670	
R366	Q446		K671	V784
R367		D569	A672	F785
E368	W449	F570	V673	S786
M369	L450	T571	Y674	Y787
R370		F572		A788
Q371	M459	N573	H677	
M372	G460		Q678	D797
E373	T461	W576	ALA	
G374		T577	SER	Q803
A375	Y465	Y578	ASN	F804
W376		R579	TYR	N805
L377	Y468	K580	ASP	
G378		R583	PRD	R808
S379	S484		TYR	T809
D380		P587	TYR	TRP
L381	R488	T588	GLU	
V382	F494	D589	G690	
D383	Q495	G590		
Q384		S591	V706	
G385	A499	R592	G707	
K386		V593	G708	
E387	D503	N594	N709	
R388	Y504	L595		
L389			I719	
K390	G516	K598	T720	
R391		V599		
L392				
G393				

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

Continued on next page...

Continued from previous page...

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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 ⓘ

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 ⓘ

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 ⓘ

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	$\# Z > 2$
4	L8Z	C	203	-	138,140,140	1.94	26 (18%)	162,176,176	2.22	30 (18%)
4	L8Z	I	202	-	138,140,140	1.96	27 (19%)	162,176,176	2.09	30 (18%)
5	LPP	G	203	-	43,43,43	1.64	3 (6%)	47,48,48	1.05	5 (10%)
6	GOL	D	202	-	3,4,5	1.02	0	1,4,5	0.62	0
4	L8Z	E	1002	-	138,140,140	1.93	27 (19%)	162,176,176	2.19	33 (20%)
5	LPP	L	203	-	43,43,43	1.58	4 (9%)	47,48,48	1.01	5 (10%)
3	PLM	F	201	1	16,16,17	0.63	0	15,15,17	0.42	0
3	PLM	E	1001	1	16,16,17	0.48	0	15,15,17	0.43	0
3	PLM	K	201	1	16,16,17	0.57	0	15,15,17	0.41	0
3	PLM	J	201	1	16,16,17	0.51	0	15,15,17	0.40	0
5	LPP	H	204	-	43,43,43	1.63	3 (6%)	47,48,48	0.96	4 (8%)
5	LPP	M	205	-	43,43,43	1.74	3 (6%)	47,48,48	1.00	3 (6%)
4	L8Z	L	202	-	138,140,140	1.99	27 (19%)	162,176,176	2.14	33 (20%)
3	PLM	B	201	1	16,16,17	0.47	0	15,15,17	0.39	0
3	PLM	H	201	1	16,16,17	0.56	0	15,15,17	0.48	0
5	LPP	B	203	-	43,43,43	1.61	3 (6%)	47,48,48	1.00	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	K	204	-	3,4,5	0.86	0	1,4,5	0.33	0
4	L8Z	B	202	-	138,140,140	1.98	30 (21%)	162,176,176	2.03	28 (17%)
3	PLM	A	201	1	16,16,17	0.58	0	15,15,17	0.43	0
3	PLM	C	201	1	16,16,17	0.57	0	15,15,17	0.39	0
4	L8Z	K	202	-	138,140,140	1.93	27 (19%)	162,176,176	2.44	32 (19%)
5	LPP	A	203	-	43,43,43	1.61	4 (9%)	47,48,48	1.05	5 (10%)
5	LPP	I	203	-	43,43,43	1.66	3 (6%)	47,48,48	0.96	4 (8%)
3	PLM	G	201	1	16,16,17	0.45	0	15,15,17	0.43	0
5	LPP	F	203	-	43,43,43	1.58	3 (6%)	47,48,48	0.97	4 (8%)
4	L8Z	F	202	-	138,140,140	2.00	33 (23%)	162,176,176	2.24	30 (18%)
4	L8Z	H	203	-	138,140,140	1.94	28 (20%)	162,176,176	2.16	31 (19%)
6	GOL	J	205	-	3,4,5	1.02	0	1,4,5	0.80	0
4	L8Z	A	202	-	138,140,140	1.97	26 (18%)	162,176,176	2.12	34 (20%)
6	GOL	H	202	-	3,4,5	0.92	0	1,4,5	0.63	0
6	GOL	M	201	-	3,4,5	1.08	0	1,4,5	0.82	0
4	L8Z	J	203	-	138,140,140	1.89	25 (18%)	162,176,176	2.20	31 (19%)
6	GOL	M	203	-	3,4,5	1.09	0	1,4,5	0.76	0
6	GOL	D	205	-	3,4,5	0.97	0	1,4,5	0.45	0
6	GOL	J	202	-	3,4,5	0.95	0	1,4,5	0.99	0
4	L8Z	G	202	-	138,140,140	1.93	28 (20%)	162,176,176	2.29	35 (21%)
5	LPP	J	204	-	43,43,43	1.66	3 (6%)	47,48,48	0.97	4 (8%)
3	PLM	M	202	1	16,16,17	0.59	0	15,15,17	0.41	0
6	GOL	H	205	-	3,4,5	0.63	0	1,4,5	0.28	0
6	GOL	C	202	-	3,4,5	0.80	0	1,4,5	0.30	0
5	LPP	D	204	-	43,43,43	1.67	3 (6%)	47,48,48	0.91	4 (8%)
5	LPP	C	204	-	43,43,43	1.59	3 (6%)	47,48,48	1.05	4 (8%)
5	LPP	K	203	-	43,43,43	1.61	3 (6%)	47,48,48	0.92	4 (8%)
6	GOL	A	204	-	3,4,5	1.05	0	1,4,5	0.01	0
6	GOL	E	1003	-	3,4,5	1.05	0	1,4,5	1.43	0
3	PLM	I	201	1	16,16,17	0.56	0	15,15,17	0.42	0
3	PLM	D	201	1	16,16,17	0.50	0	15,15,17	0.39	0
4	L8Z	D	203	-	138,140,140	1.91	24 (17%)	162,176,176	2.20	30 (18%)
4	L8Z	M	204	-	138,140,140	1.90	26 (18%)	162,176,176	2.13	27 (16%)
6	GOL	F	204	-	3,4,5	0.65	0	1,4,5	0.33	0
3	PLM	L	201	1	16,16,17	0.53	0	15,15,17	0.45	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
4	L8Z	C	203	-	-	60/140/199/199	0/3/3/3
4	L8Z	I	202	-	-	68/140/199/199	0/3/3/3
5	LPP	G	203	-	-	20/45/45/45	-
6	GOL	D	202	-	-	0/2/2/4	-
4	L8Z	E	1002	-	-	62/140/199/199	0/3/3/3
5	LPP	L	203	-	-	21/45/45/45	-
3	PLM	F	201	1	-	5/13/14/15	-
3	PLM	E	1001	1	-	5/13/14/15	-
3	PLM	K	201	1	-	3/13/14/15	-
3	PLM	J	201	1	-	4/13/14/15	-
5	LPP	H	204	-	-	19/45/45/45	-
5	LPP	M	205	-	-	19/45/45/45	-
4	L8Z	L	202	-	-	59/140/199/199	0/3/3/3
3	PLM	B	201	1	-	4/13/14/15	-
3	PLM	H	201	1	-	3/13/14/15	-
5	LPP	B	203	-	-	22/45/45/45	-
6	GOL	K	204	-	-	1/2/2/4	-
4	L8Z	B	202	-	-	55/140/199/199	0/3/3/3
3	PLM	A	201	1	-	7/13/14/15	-
3	PLM	C	201	1	-	4/13/14/15	-
4	L8Z	K	202	-	-	53/140/199/199	0/3/3/3
5	LPP	A	203	-	-	22/45/45/45	-
5	LPP	I	203	-	-	21/45/45/45	-
3	PLM	G	201	1	-	4/13/14/15	-
5	LPP	F	203	-	-	23/45/45/45	-
4	L8Z	F	202	-	-	52/140/199/199	0/3/3/3
4	L8Z	H	203	-	-	55/140/199/199	0/3/3/3
6	GOL	J	205	-	-	0/2/2/4	-
4	L8Z	A	202	-	-	65/140/199/199	0/3/3/3
6	GOL	H	202	-	-	0/2/2/4	-
6	GOL	M	201	-	-	2/2/2/4	-
4	L8Z	J	203	-	-	50/140/199/199	0/3/3/3
6	GOL	M	203	-	-	0/2/2/4	-
6	GOL	D	205	-	-	2/2/2/4	-
6	GOL	J	202	-	-	0/2/2/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	L8Z	G	202	-	-	66/140/199/199	0/3/3/3
5	LPP	J	204	-	-	18/45/45/45	-
3	PLM	M	202	1	-	4/13/14/15	-
6	GOL	H	205	-	-	2/2/2/4	-
6	GOL	C	202	-	-	2/2/2/4	-
5	LPP	D	204	-	-	20/45/45/45	-
5	LPP	C	204	-	-	23/45/45/45	-
5	LPP	K	203	-	-	15/45/45/45	-
6	GOL	A	204	-	-	2/2/2/4	-
6	GOL	E	1003	-	-	2/2/2/4	-
3	PLM	I	201	1	-	2/13/14/15	-
3	PLM	D	201	1	-	4/13/14/15	-
4	L8Z	D	203	-	-	49/140/199/199	0/3/3/3
4	L8Z	M	204	-	-	60/140/199/199	0/3/3/3
6	GOL	F	204	-	-	2/2/2/4	-
3	PLM	L	201	1	-	4/13/14/15	-

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(°)	Ideal(°)
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:

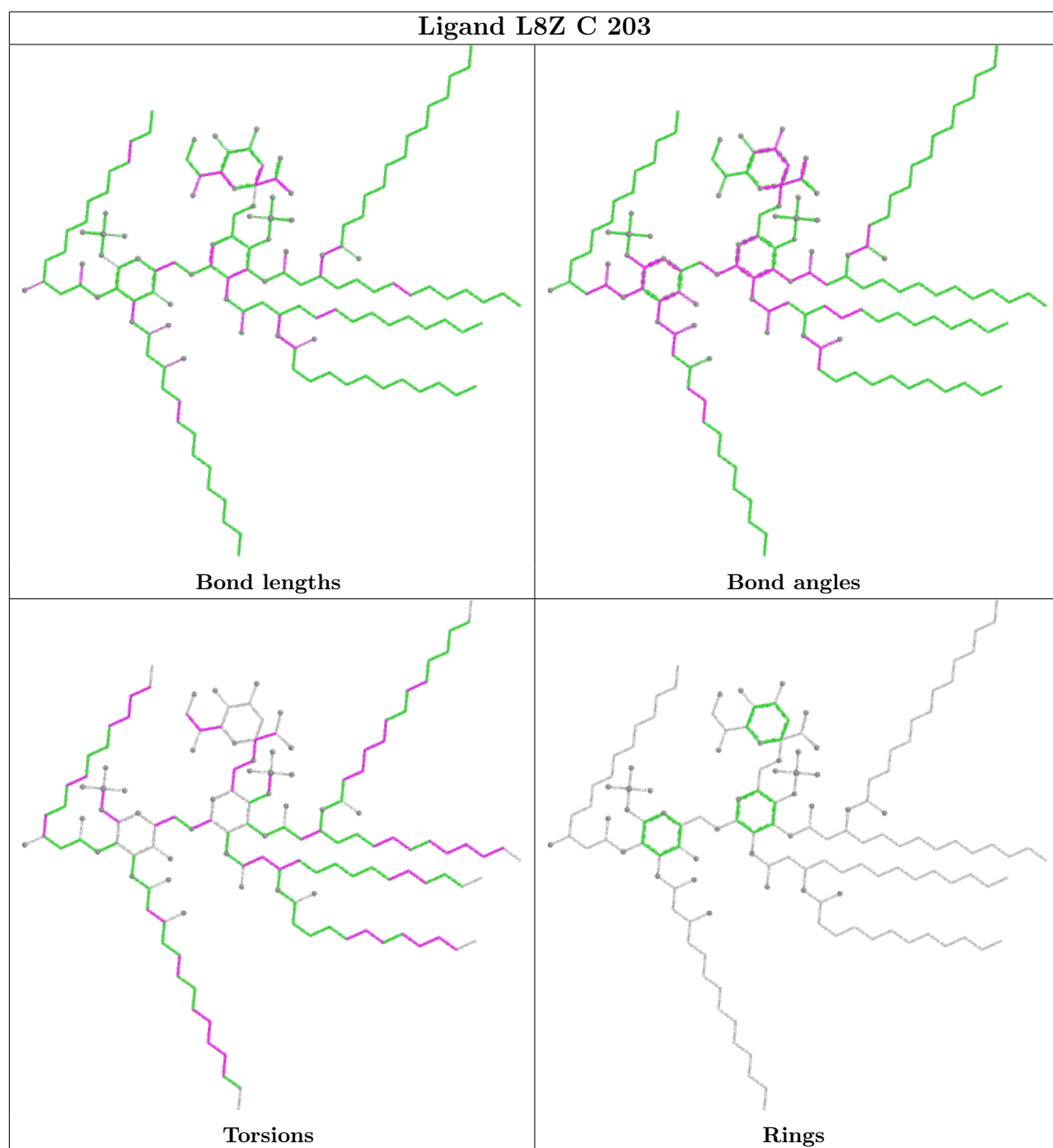
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	203	L8Z	2	0
4	I	202	L8Z	3	0
5	G	203	LPP	1	0
6	D	202	GOL	1	0
4	E	1002	L8Z	3	0
5	L	203	LPP	3	0
3	K	201	PLM	1	0
5	H	204	LPP	5	0
5	M	205	LPP	3	0
4	L	202	L8Z	4	0
3	H	201	PLM	1	0
5	B	203	LPP	3	0
4	B	202	L8Z	1	0
3	A	201	PLM	1	0
3	C	201	PLM	2	0
4	K	202	L8Z	2	0
5	A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

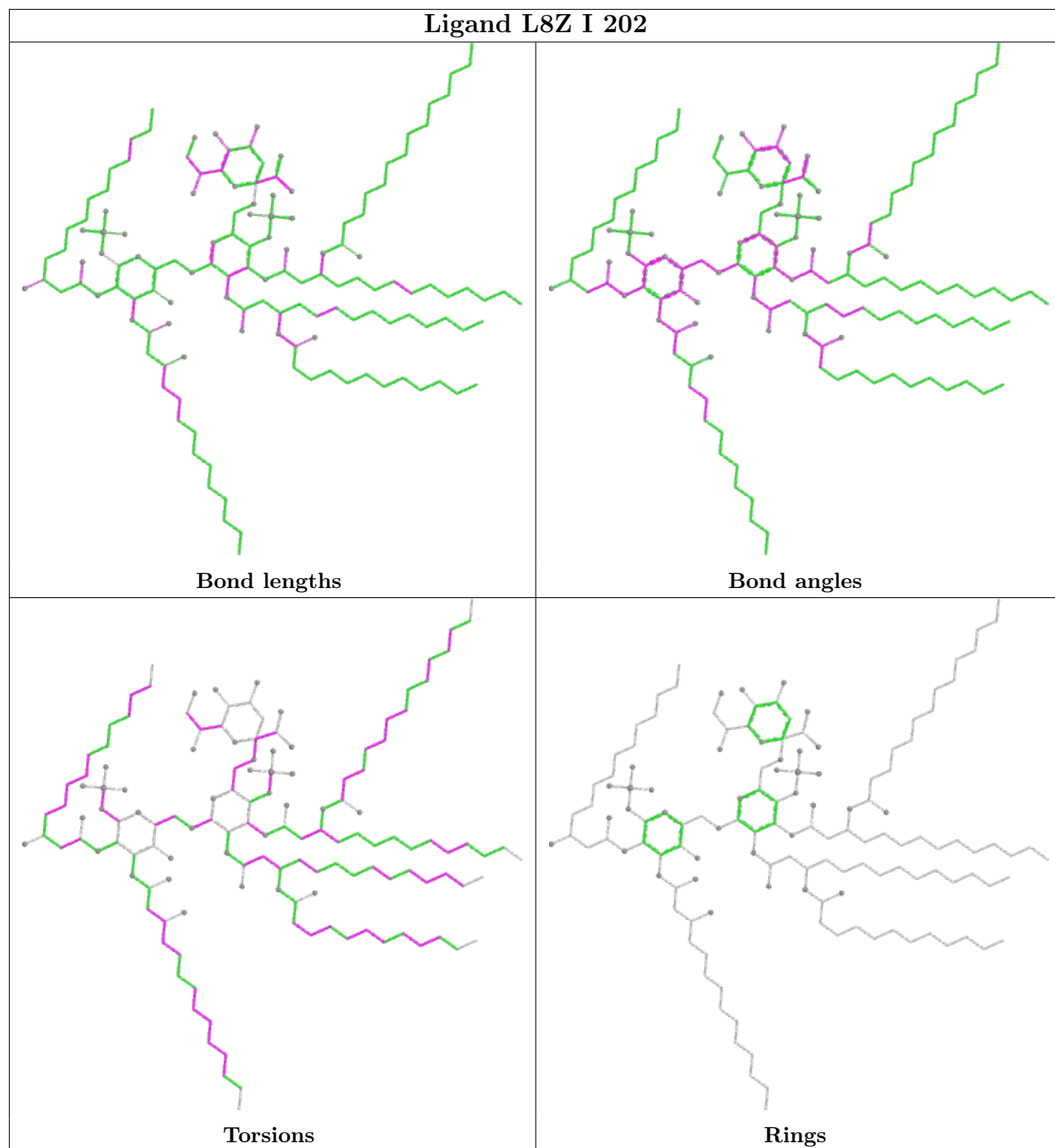
Continued on next page...

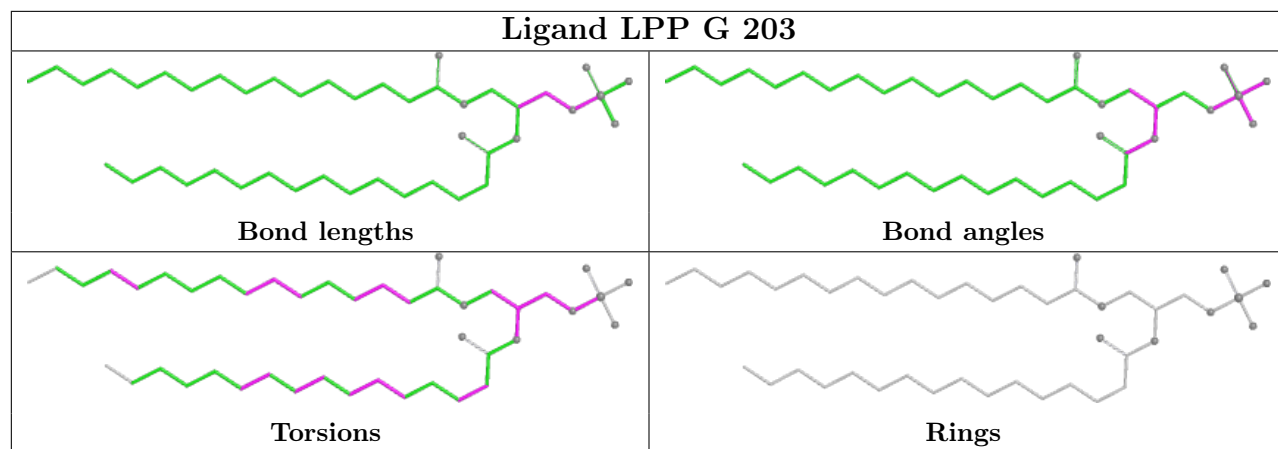
Continued from previous page...

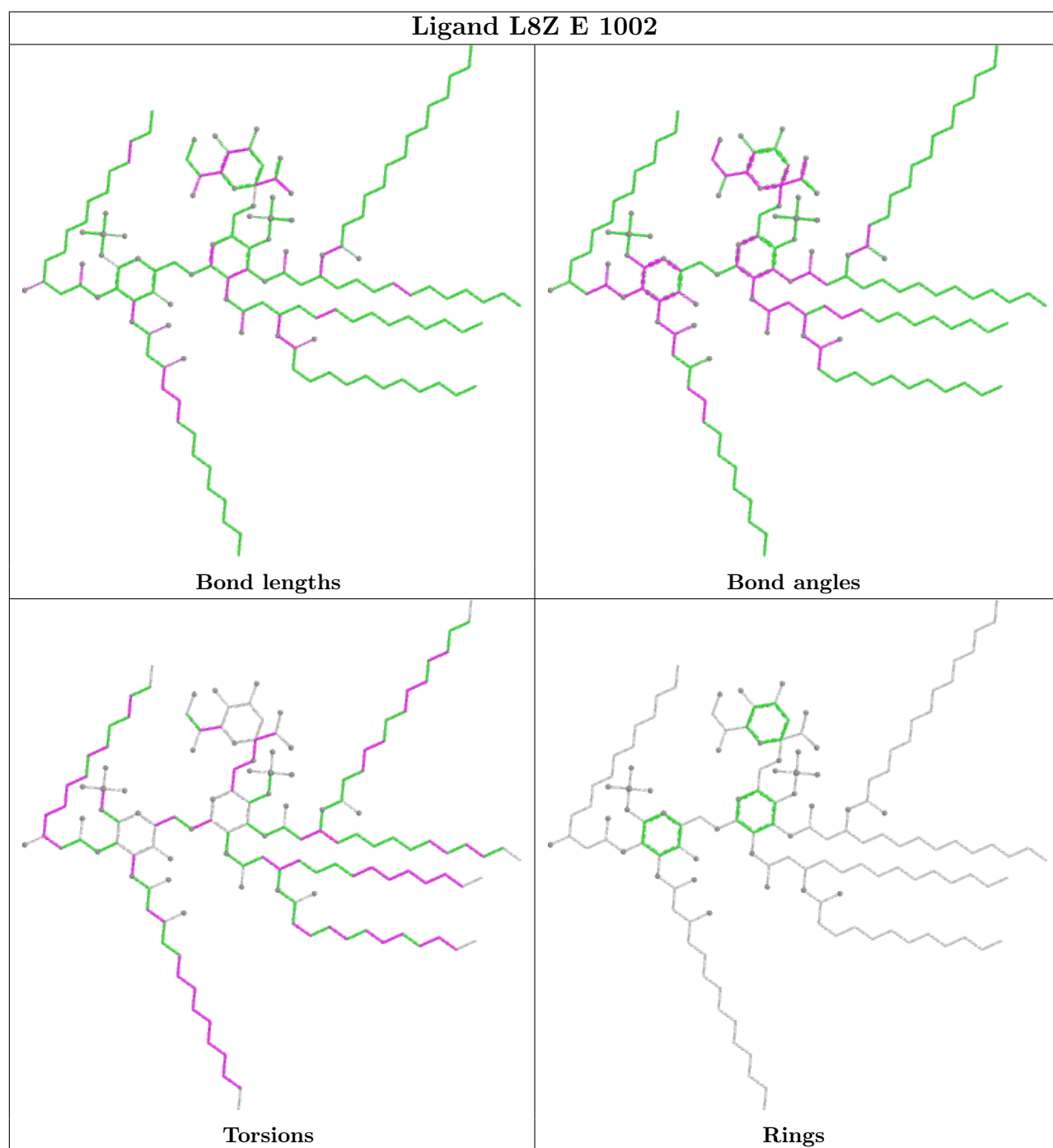
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	201	PLM	1	0

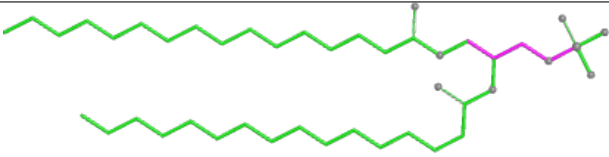
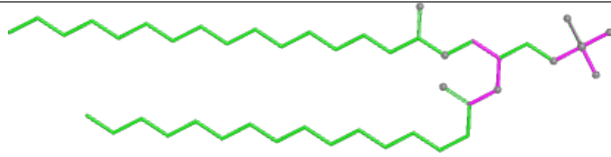
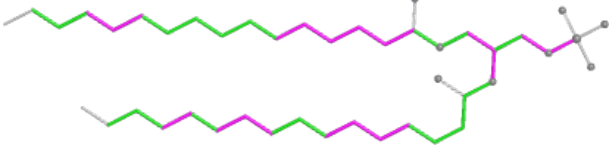
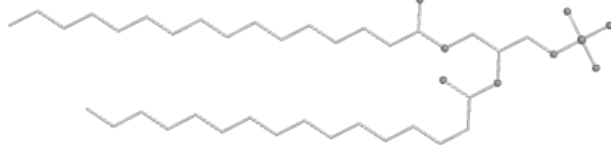
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

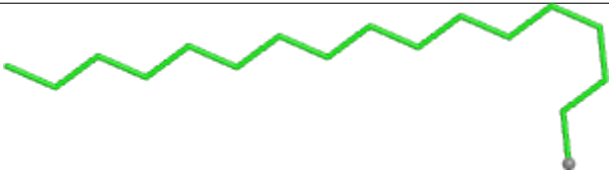
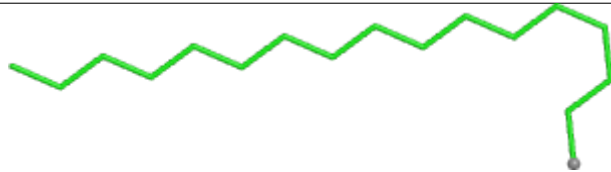
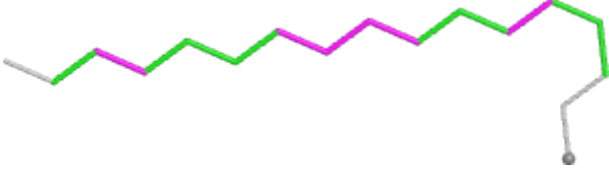
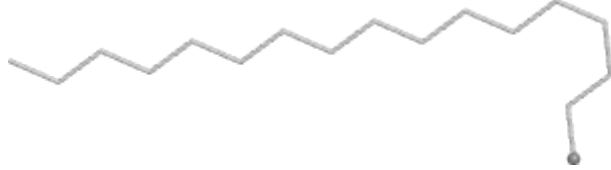


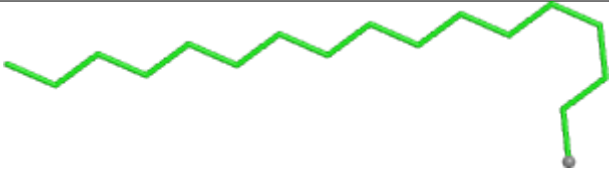
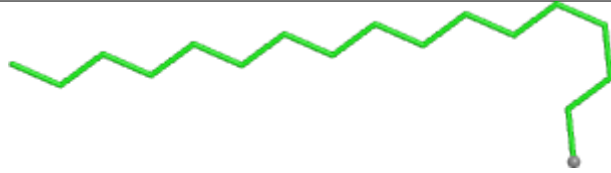
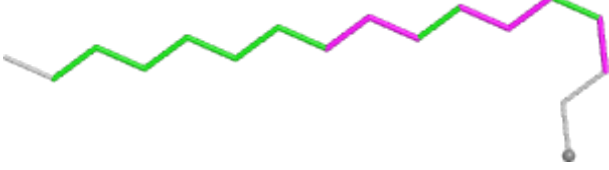
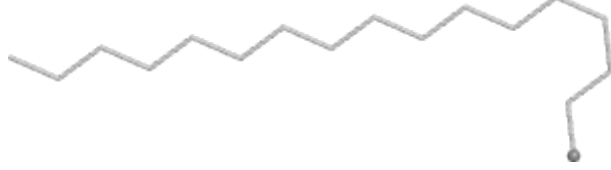


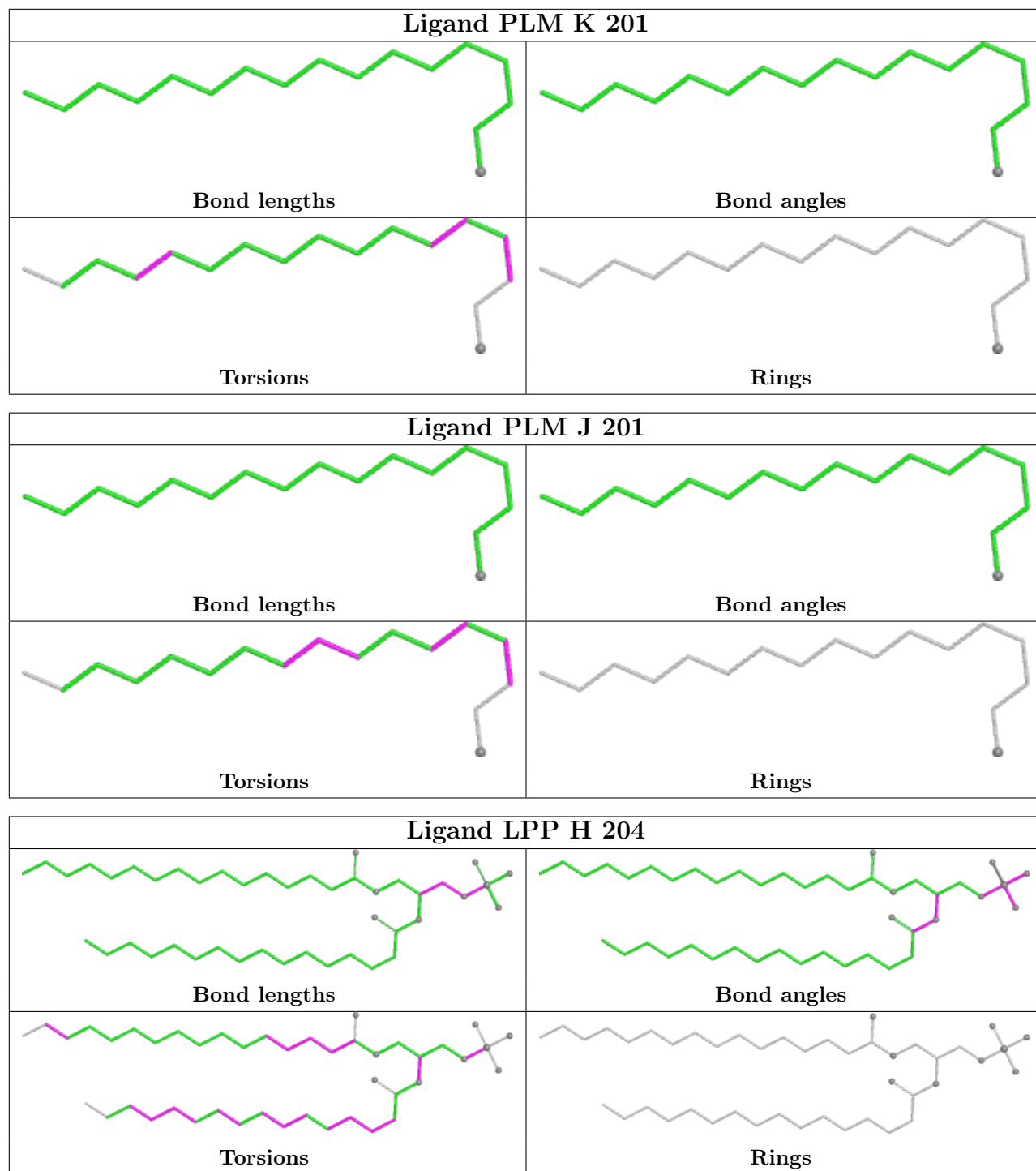


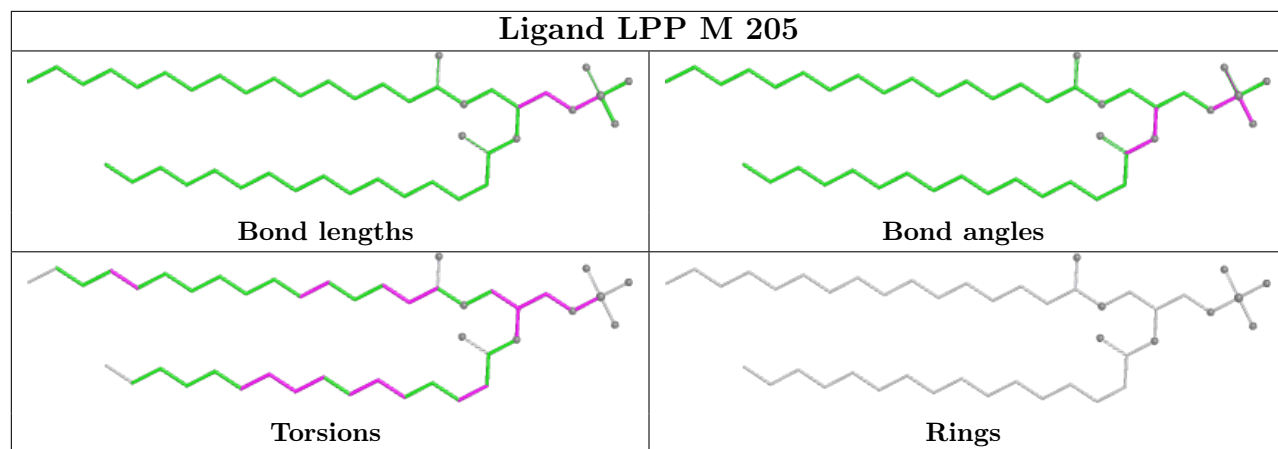


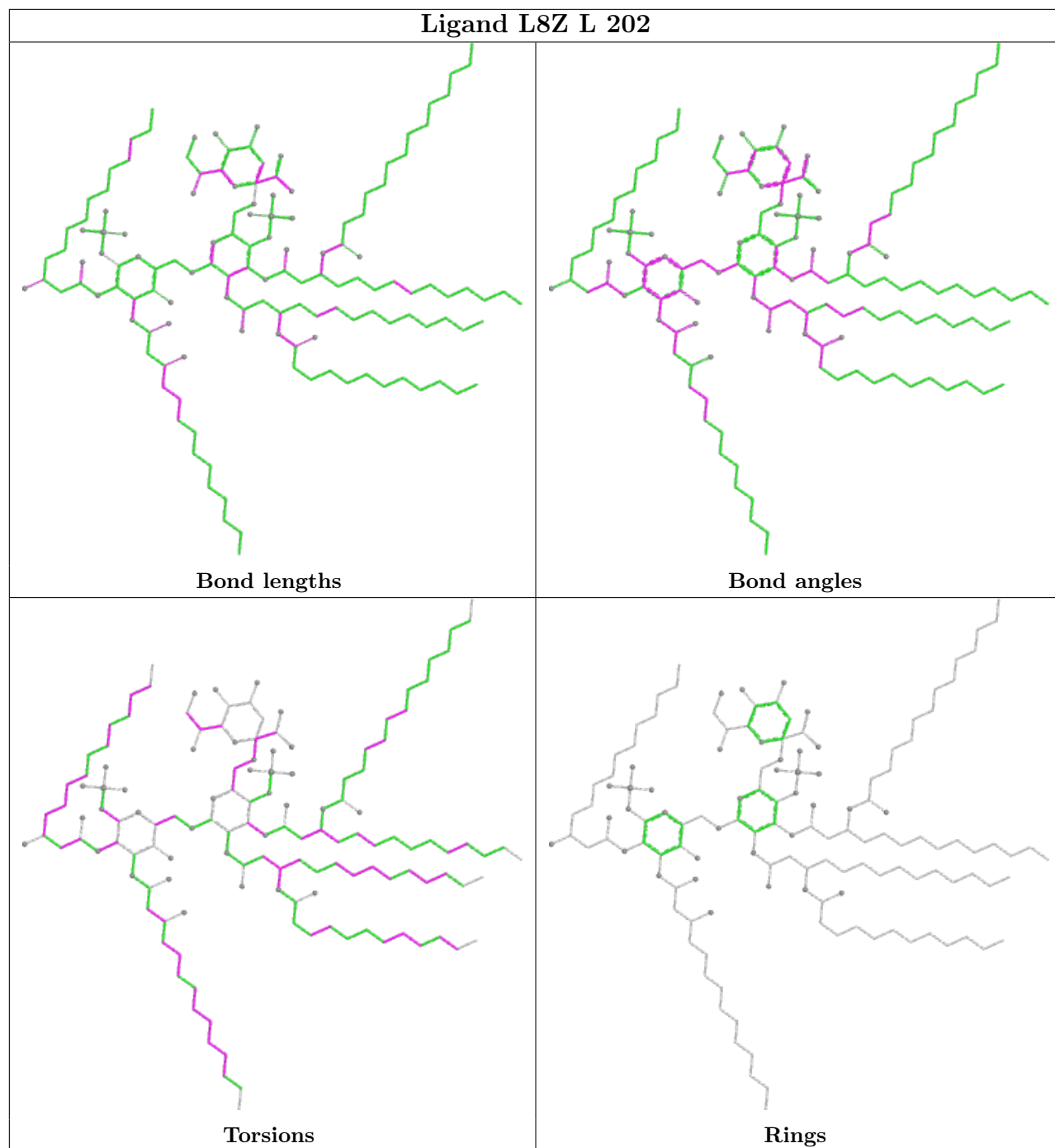
Ligand LPP L 203	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

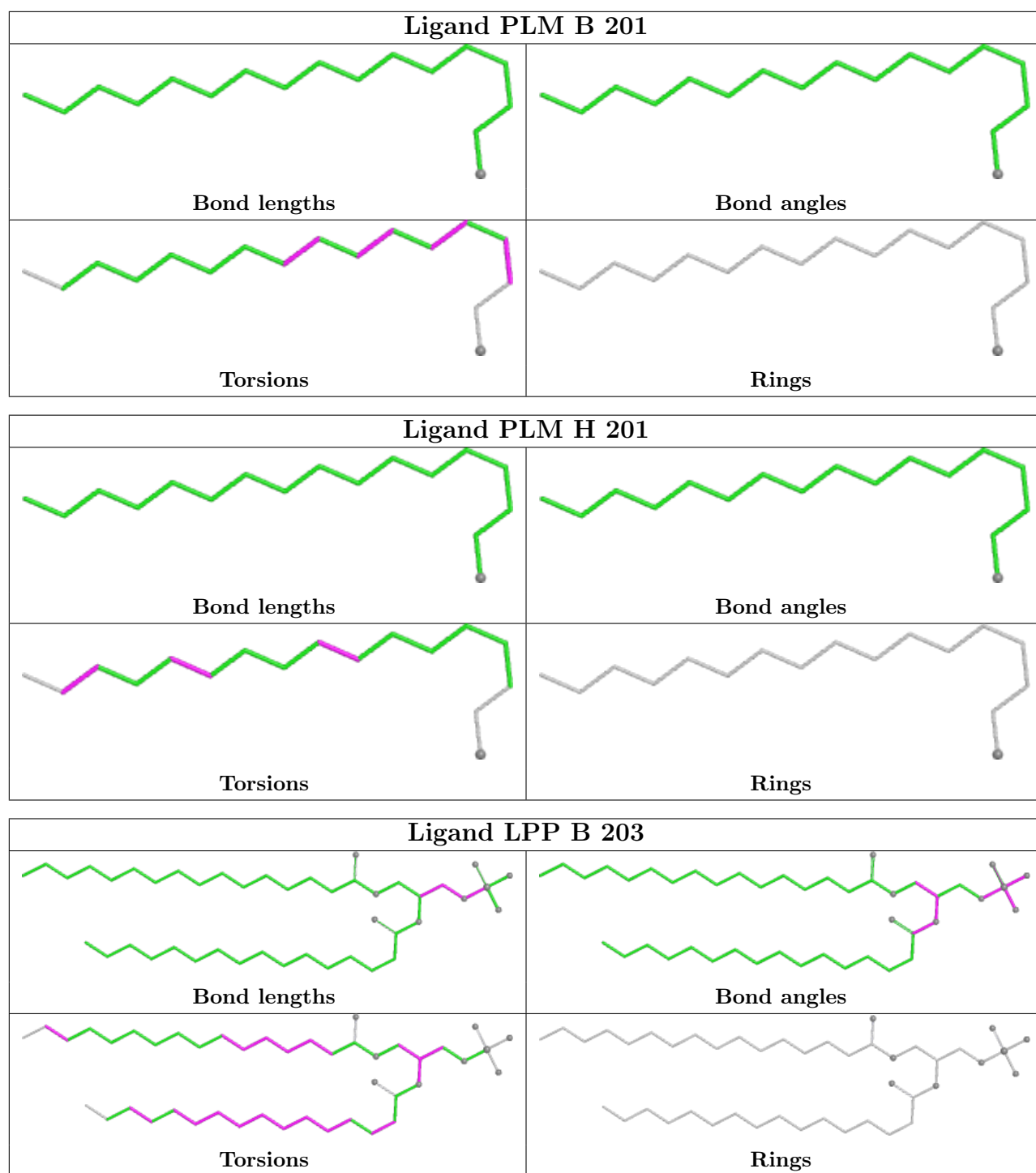
Ligand PLM F 201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

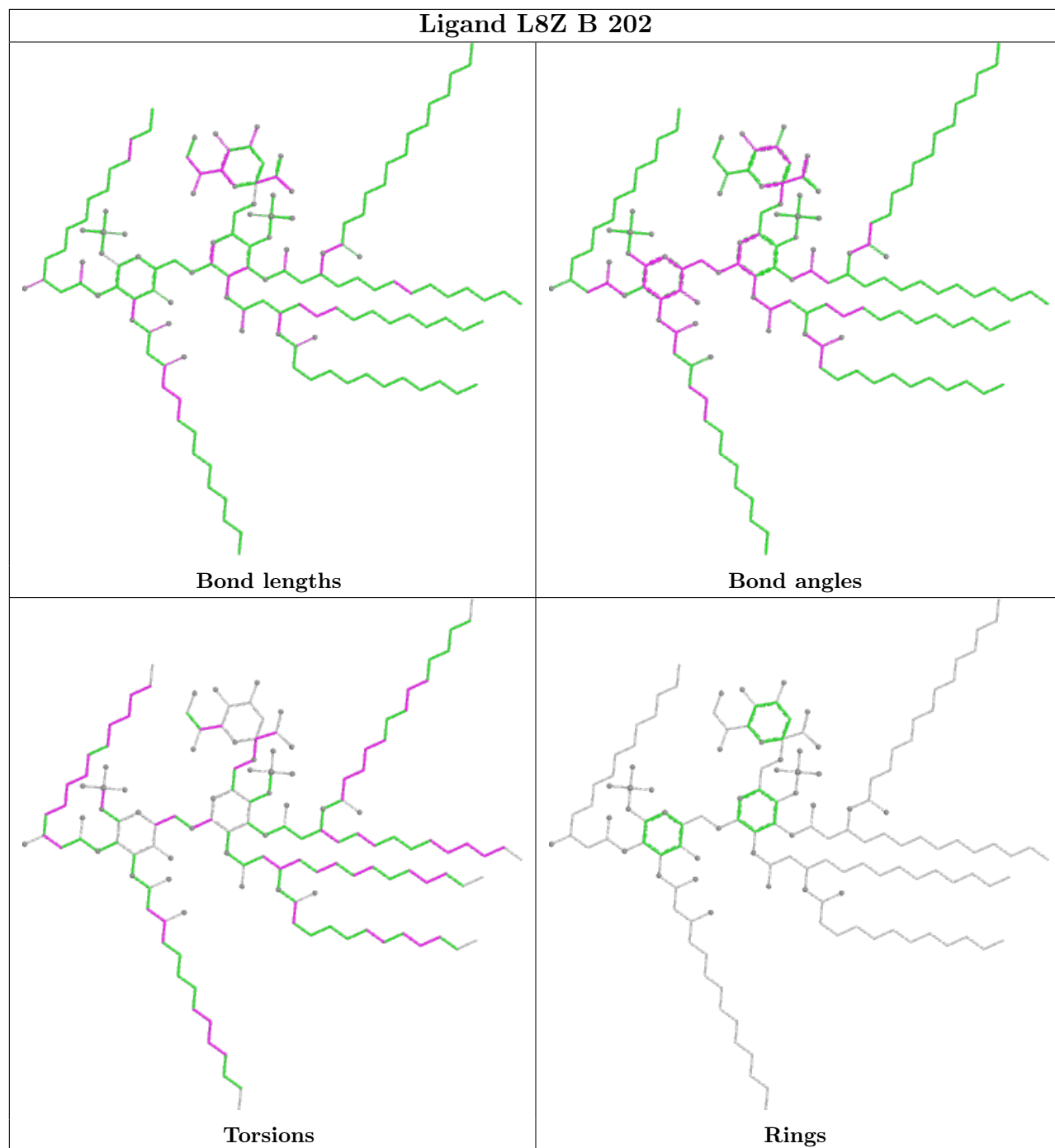
Ligand PLM E 1001	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

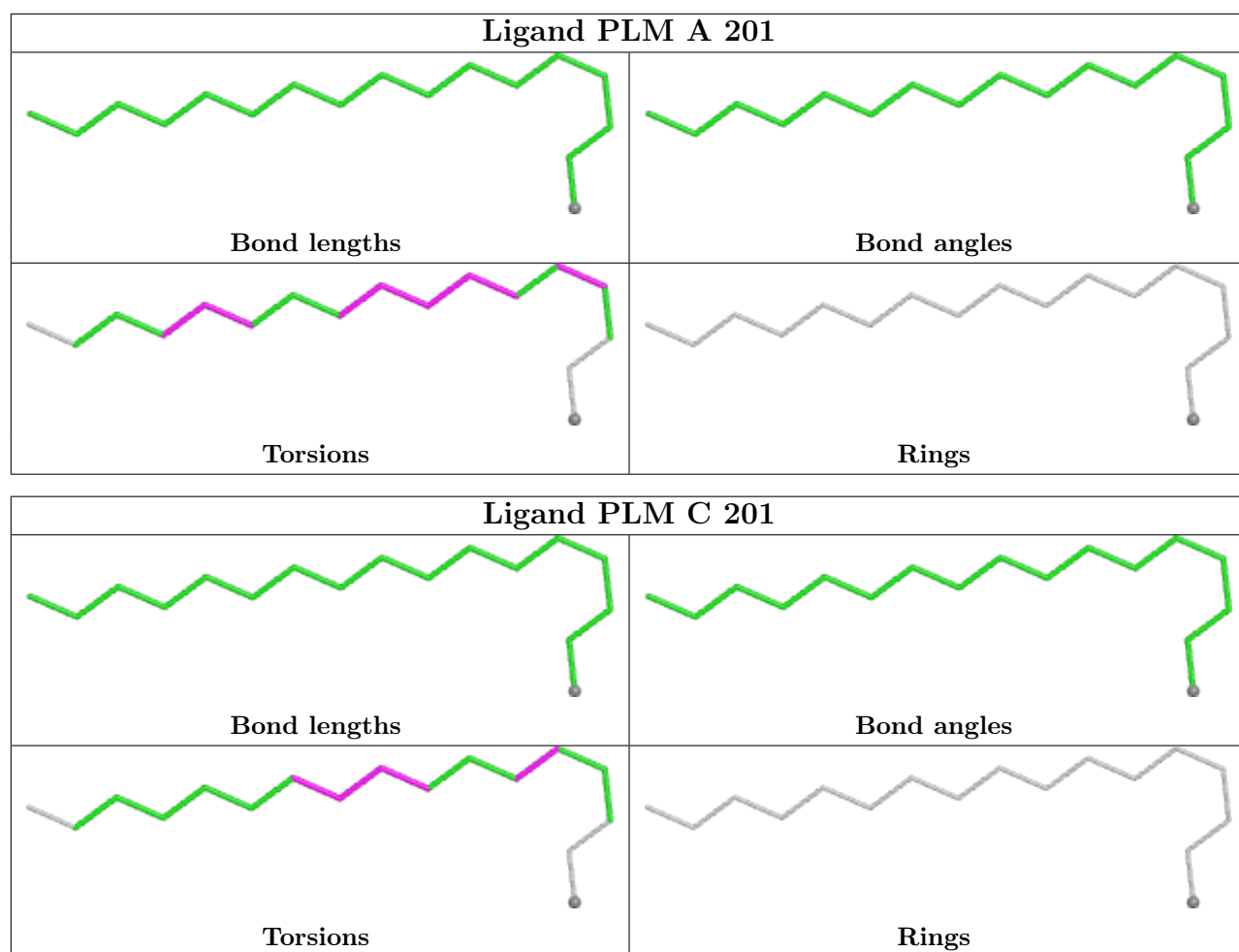


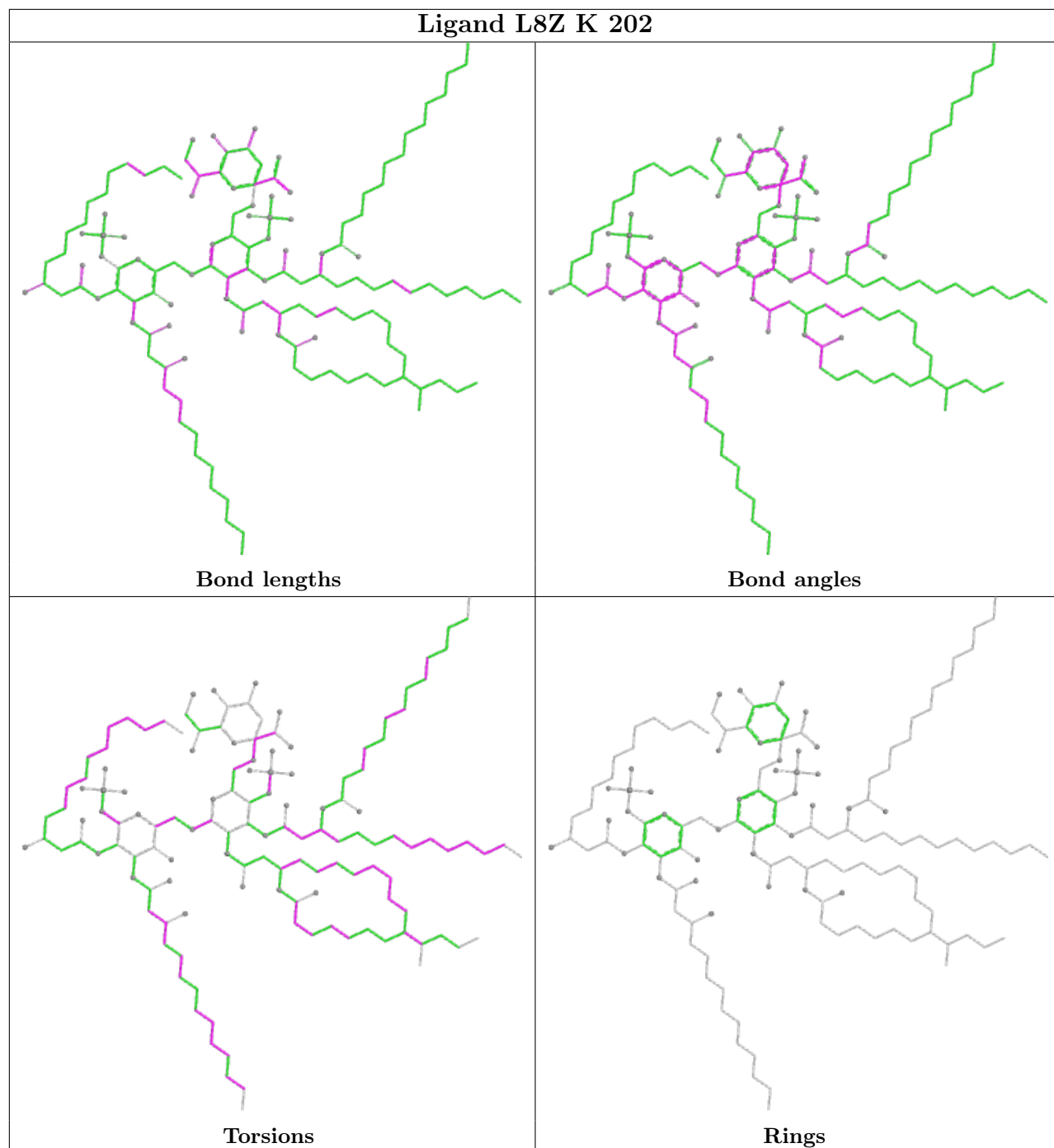


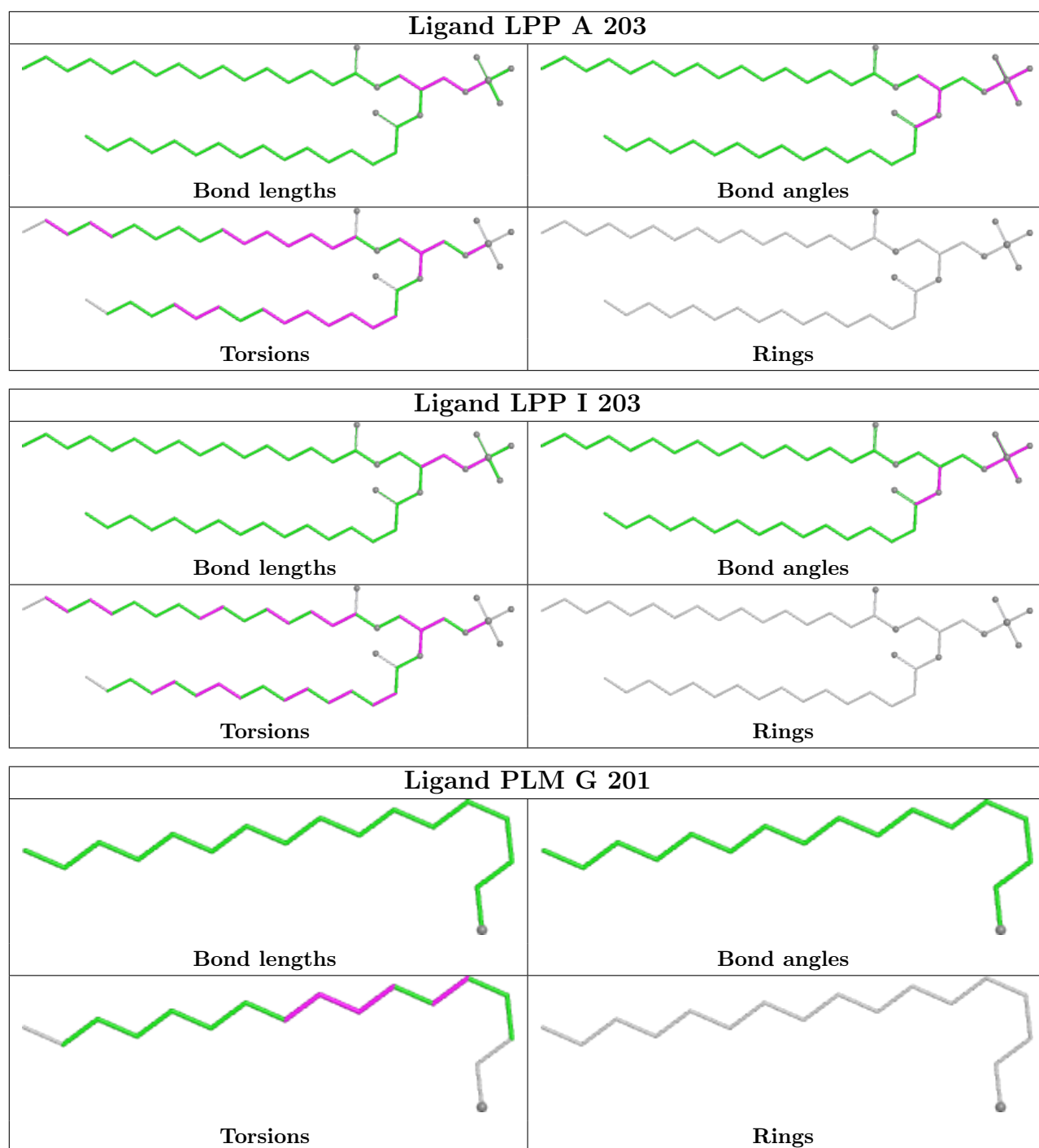


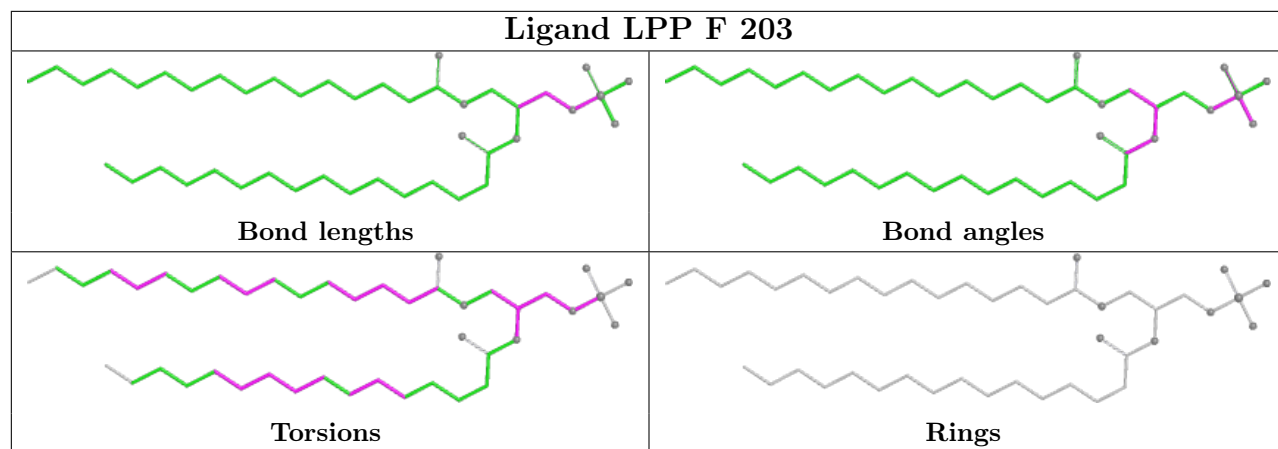


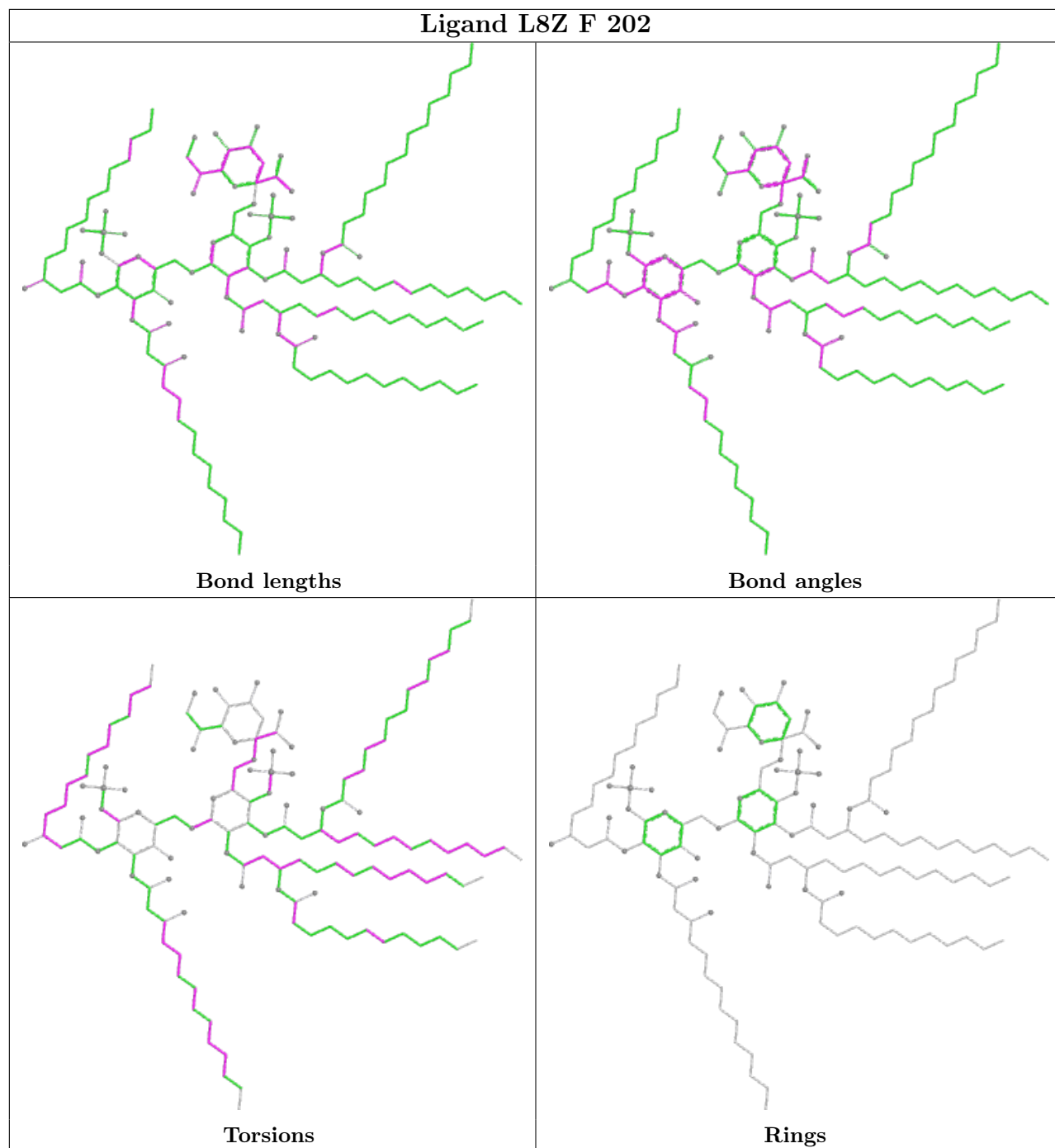


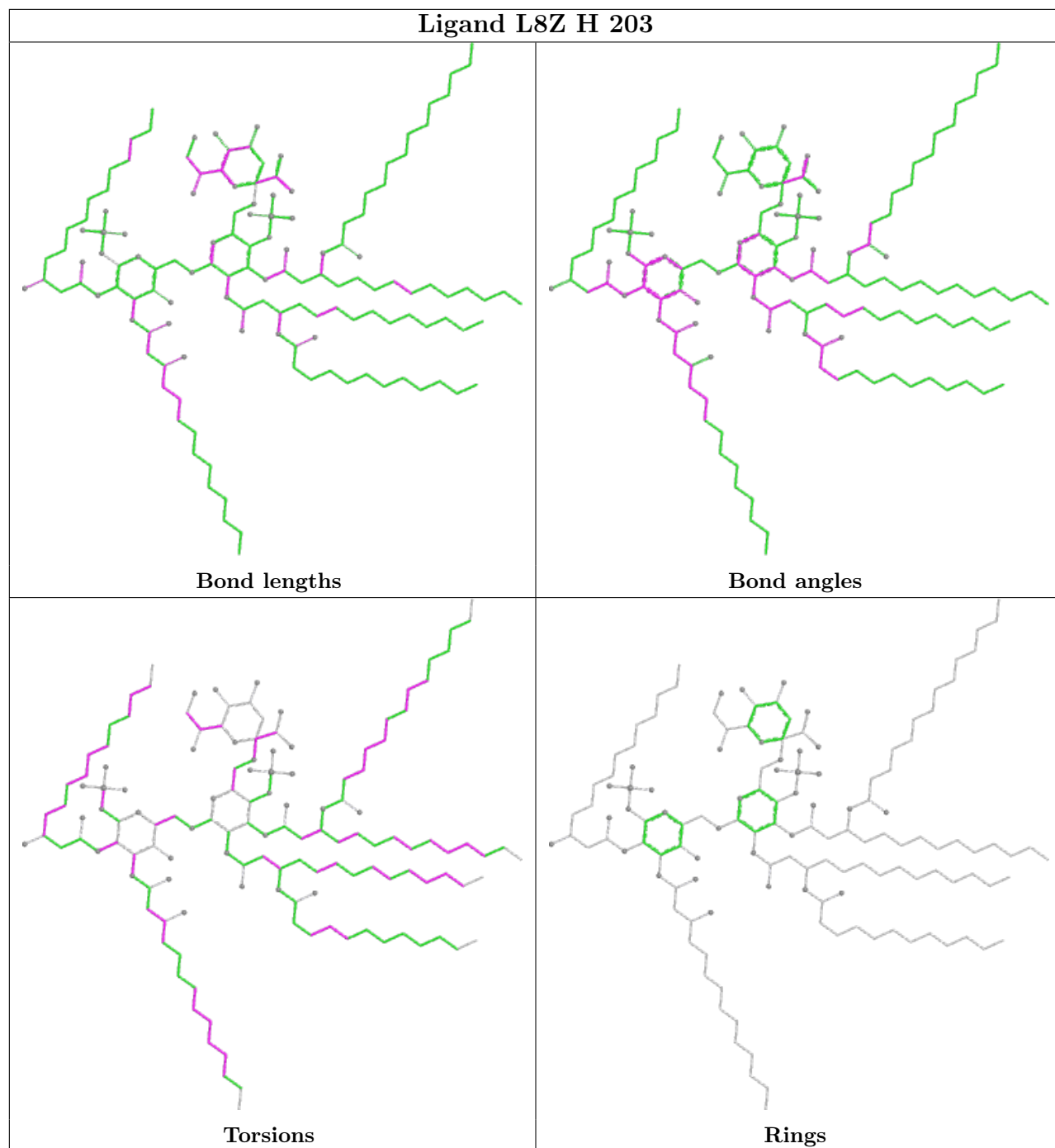


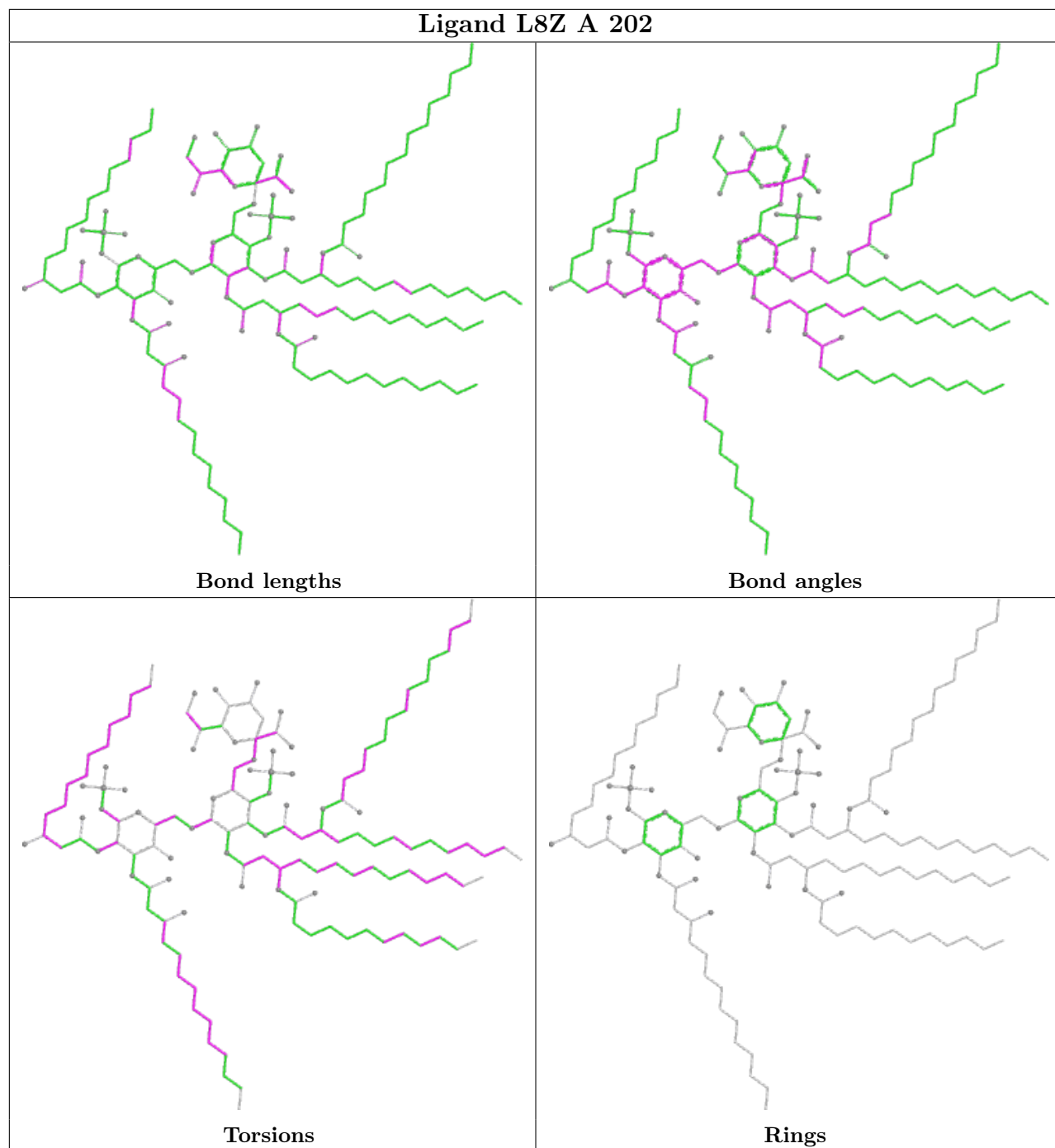


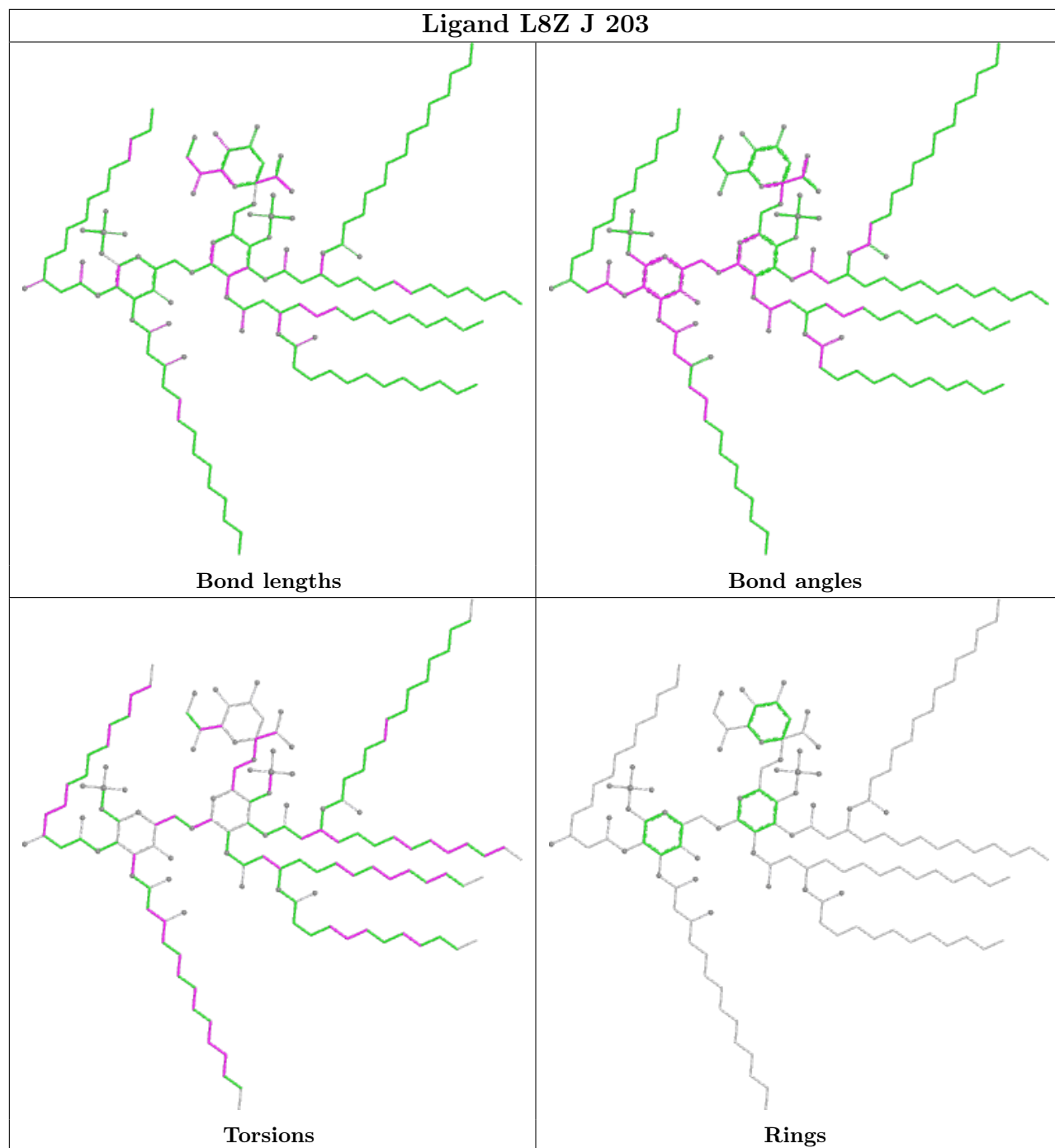


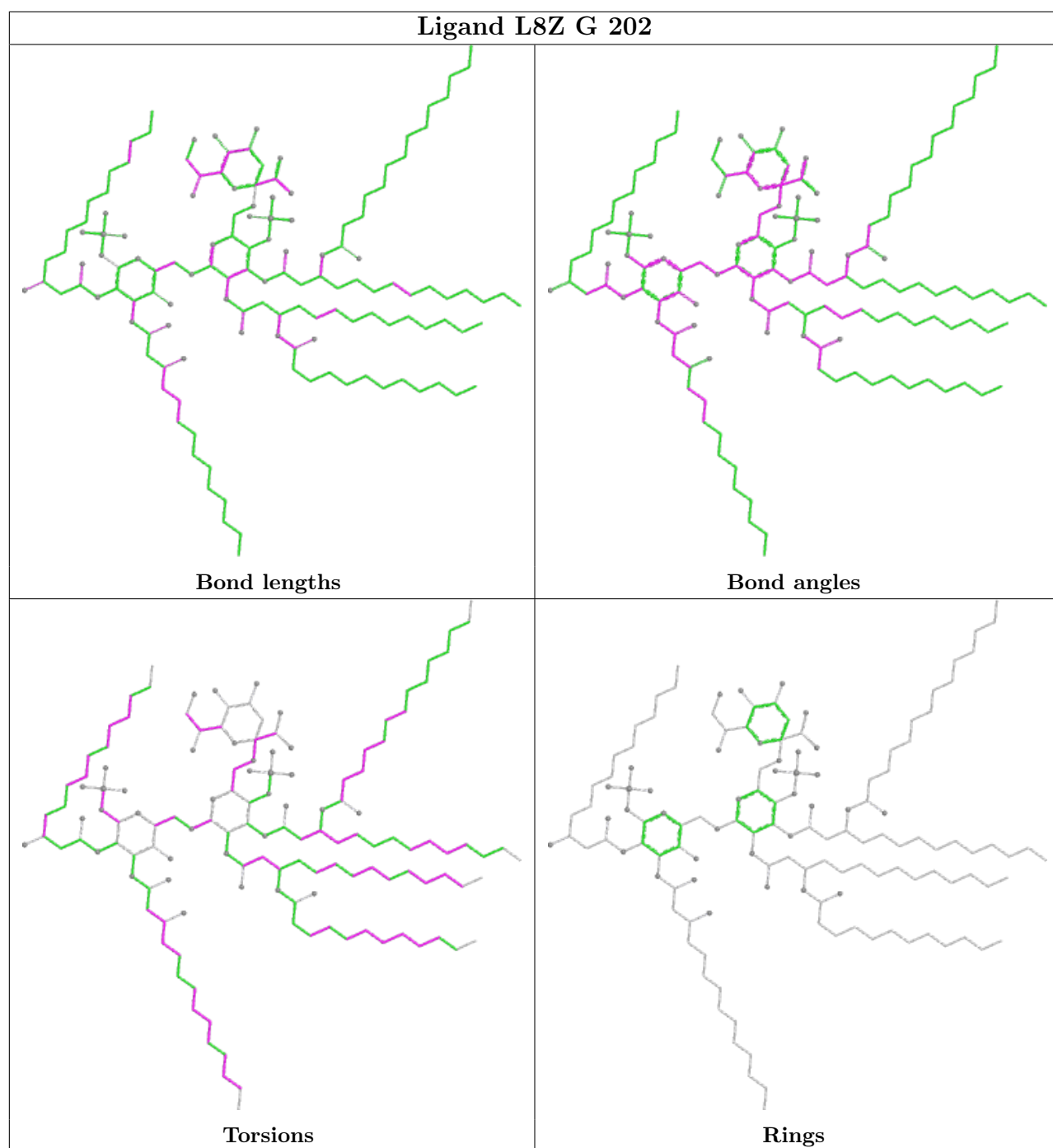


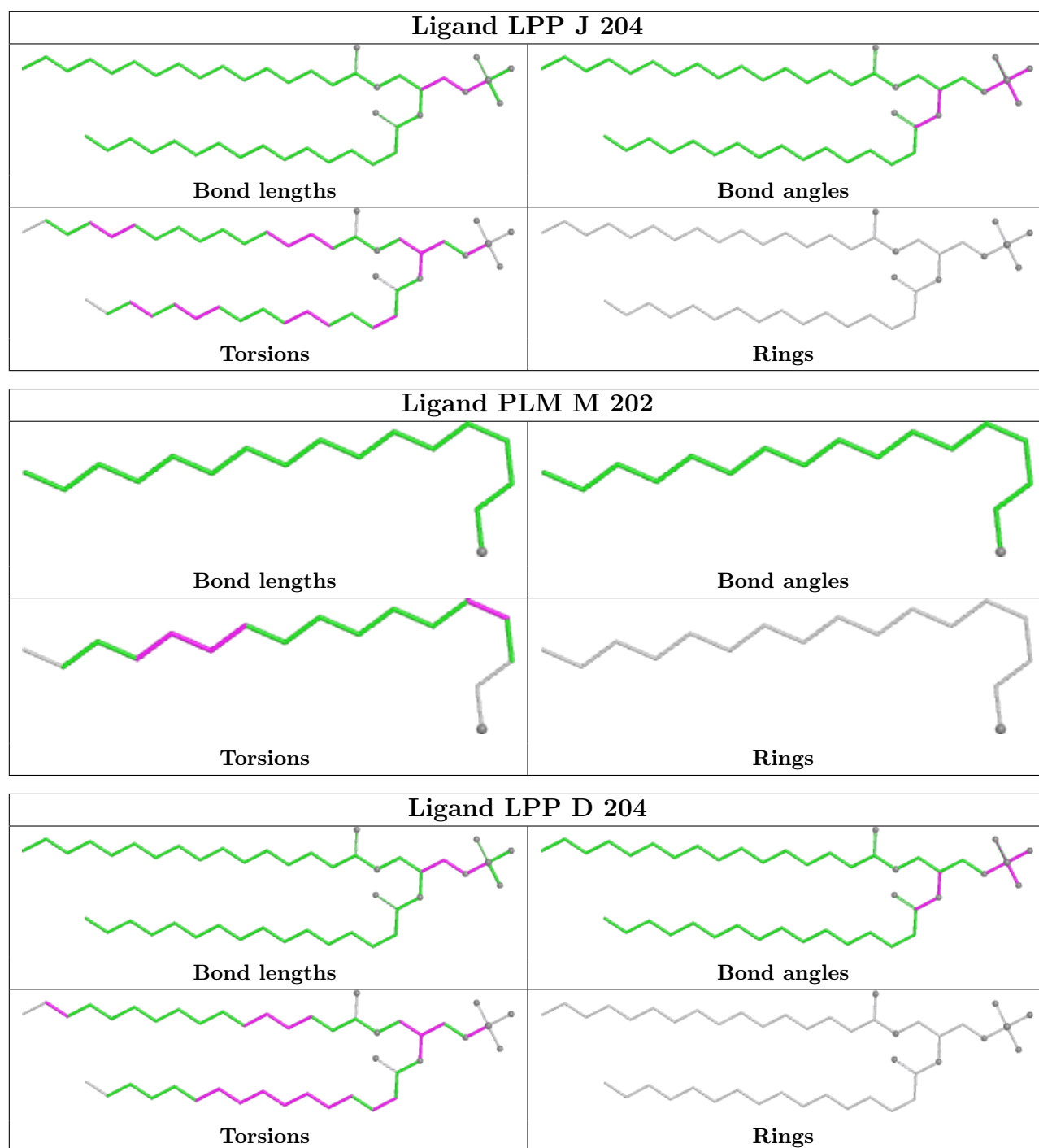


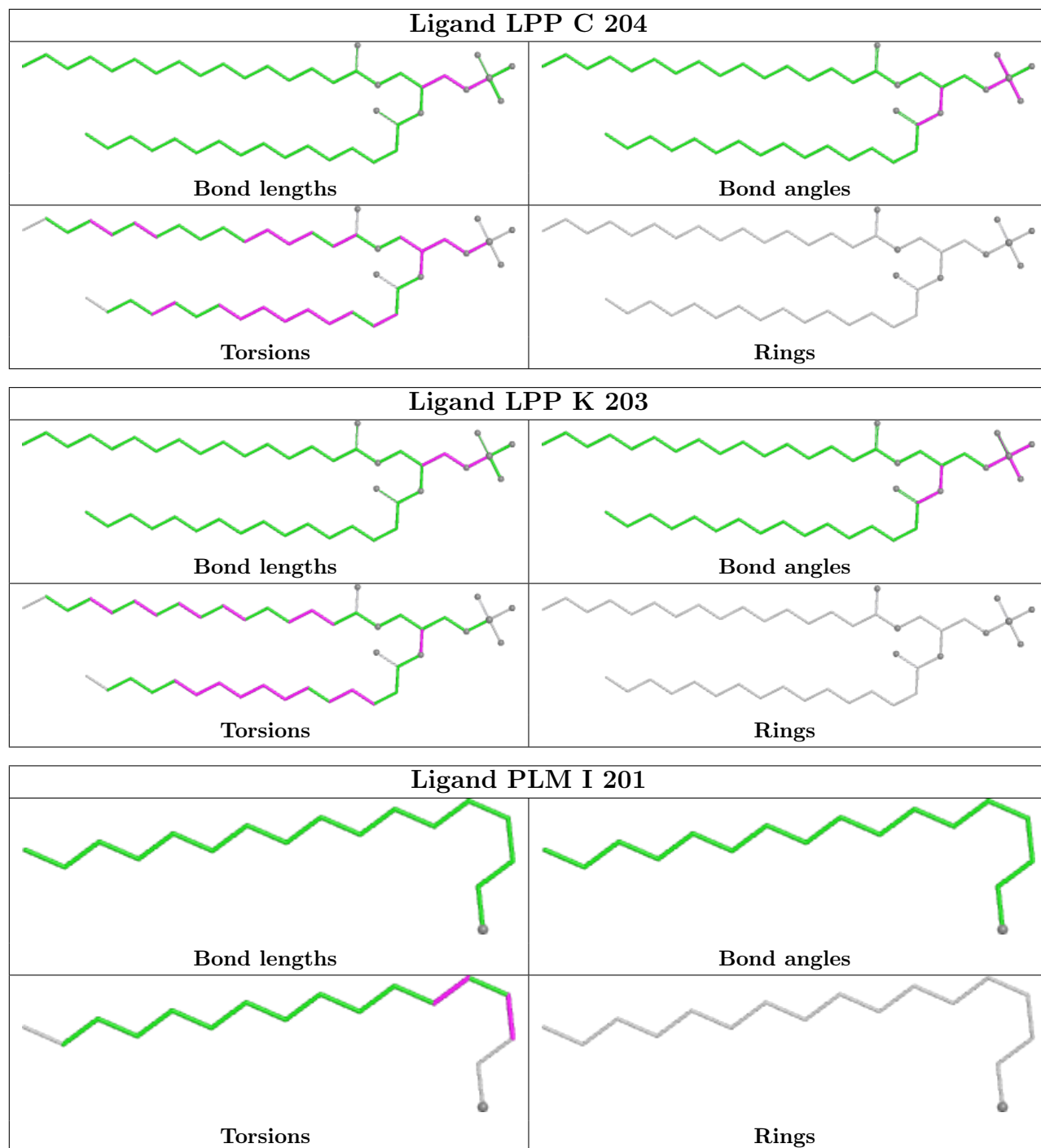


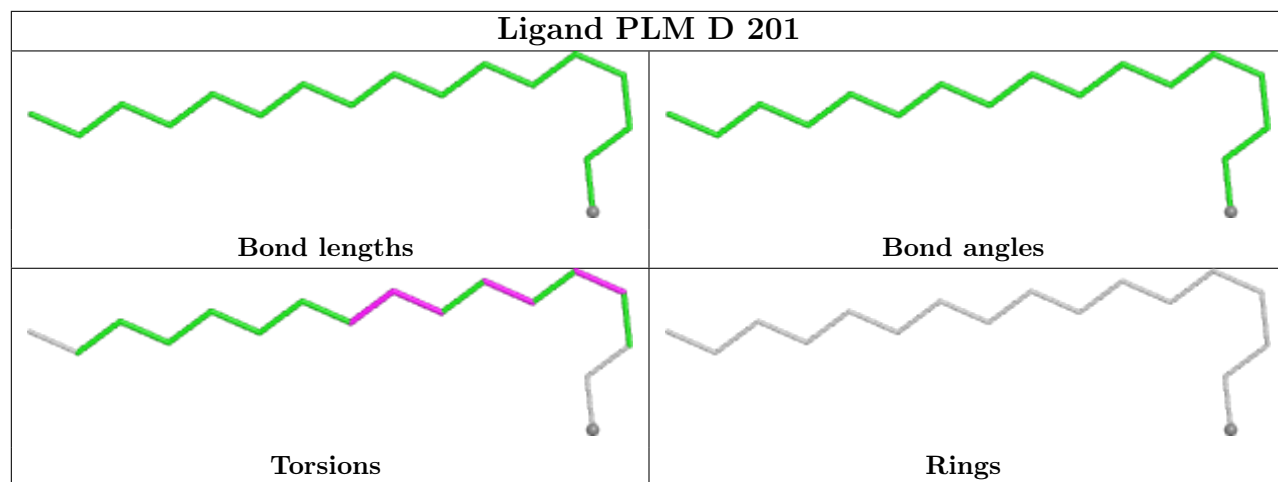


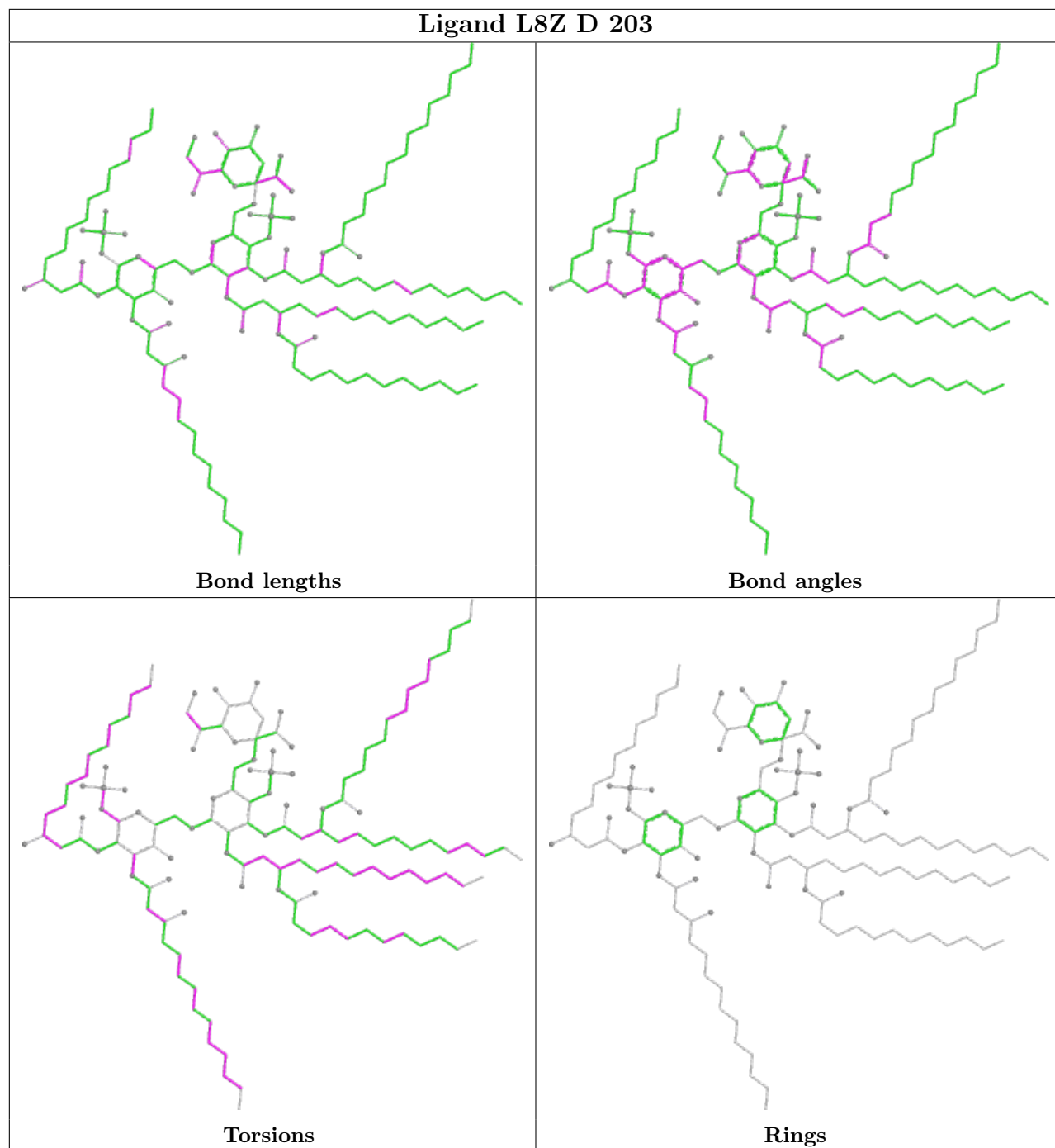


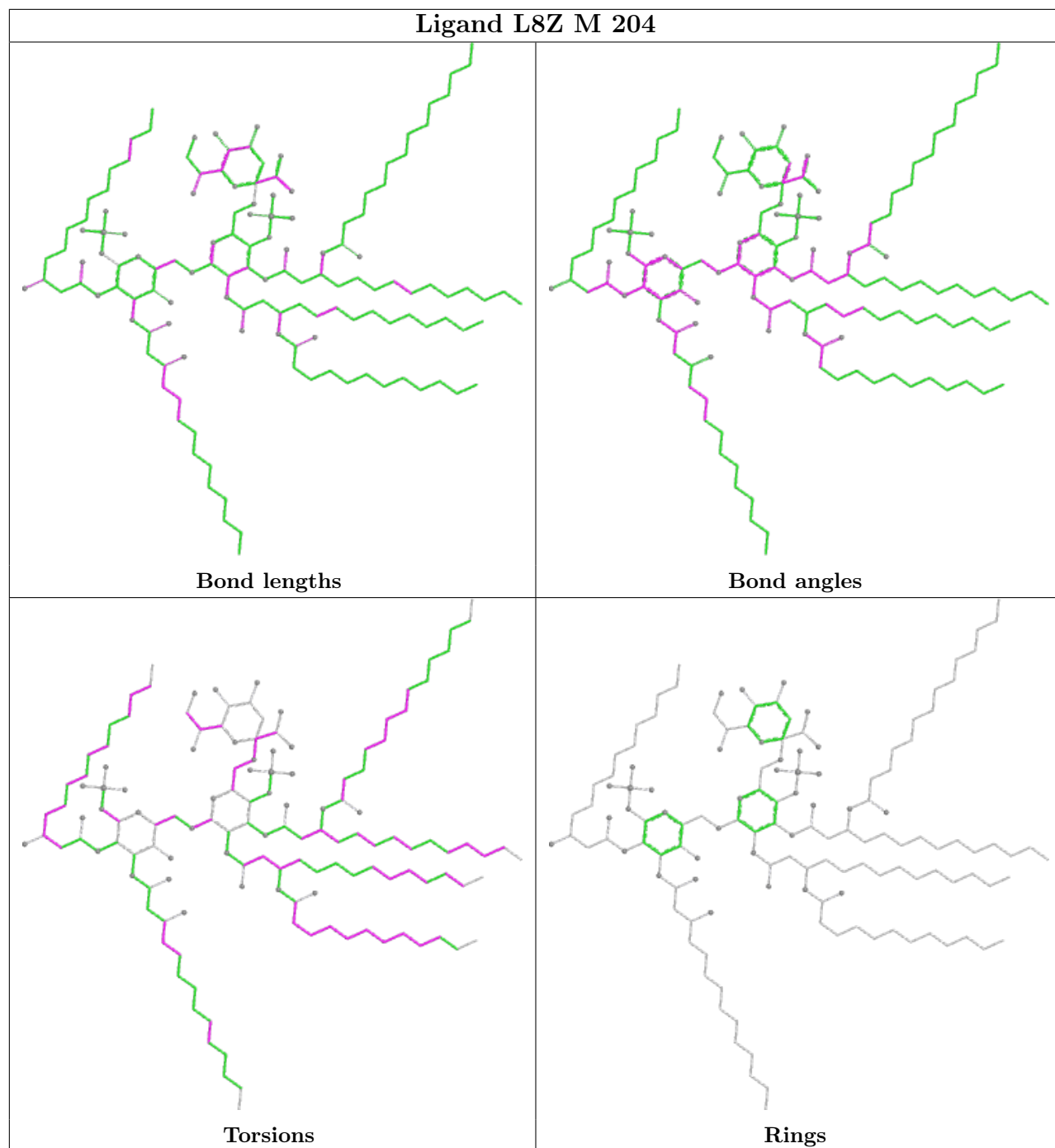


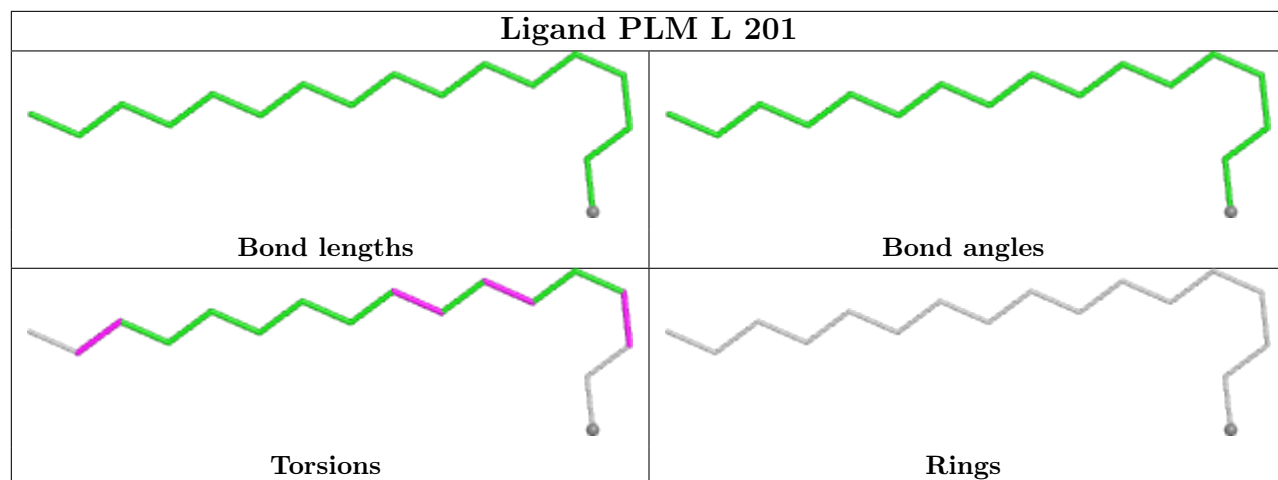












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.