



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 03:34 PM UTC

PDB ID : 7OJF / pdb_00007ojf
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

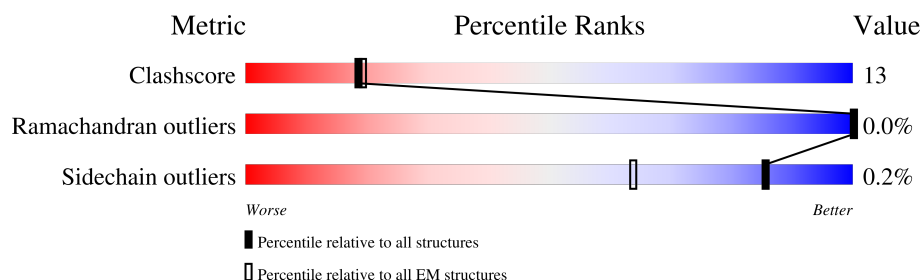
1 Overall quality at a glance

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.



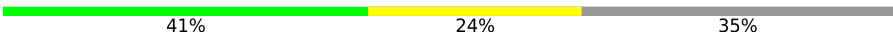
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	72% 17% 11%
1	B	155	69% 20% 11%
1	C	155	71% 18% 11%
1	D	155	72% 17% 11%
1	E	155	74% 15% 11%
1	F	155	68% 21% 11%
1	G	155	68% 21% 11%
1	H	155	70% 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	 41% 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.

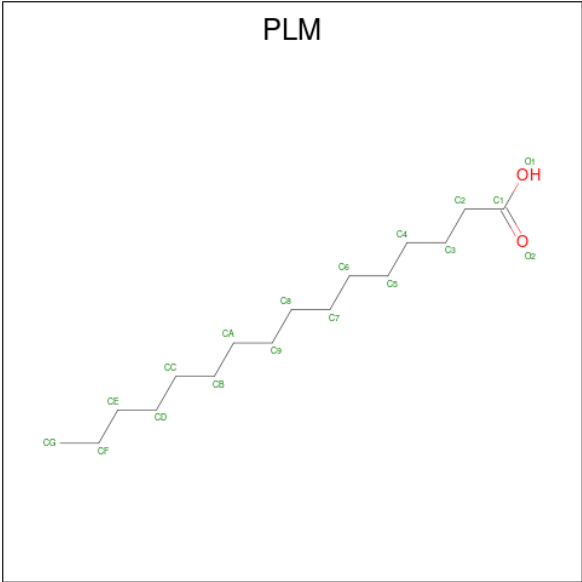
- Molecule 1 is a protein called Outer membrane lipoprotein slyB.

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		

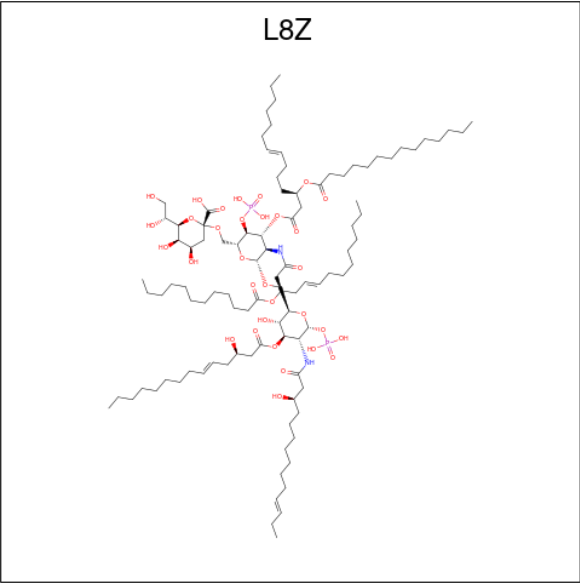
- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



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-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 (CCD ID: L8Z) (formula: C₁₀₂H₁₈₂N₂O₃₂P₂).



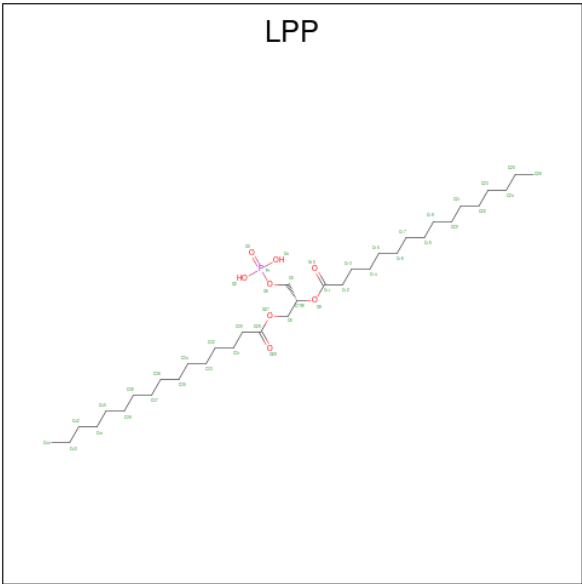
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	B	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	C	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	D	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	E	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	F	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	G	1	Total	C	N	O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

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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 (CCD ID: LPP) (formula: C₃₅H₆₉O₈P).



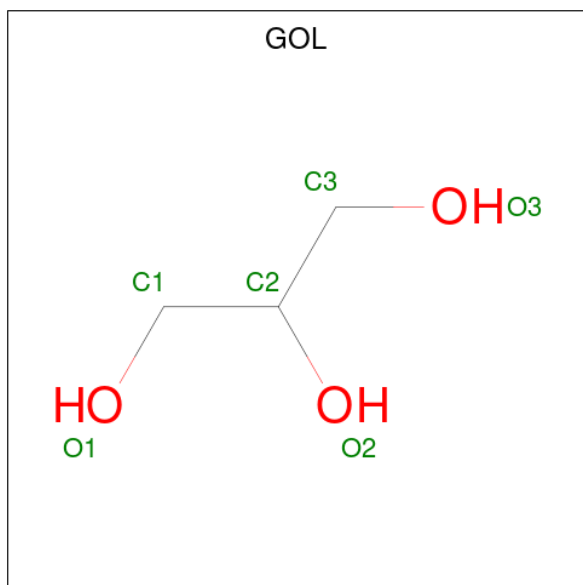
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			44	35	8	1	
5	B	1	Total	C	O	P	0
			44	35	8	1	
5	C	1	Total	C	O	P	0
			44	35	8	1	
5	D	1	Total	C	O	P	0
			44	35	8	1	
5	F	1	Total	C	O	P	0
			44	35	8	1	
5	G	1	Total	C	O	P	0
			44	35	8	1	
5	H	1	Total	C	O	P	0
			44	35	8	1	
5	I	1	Total	C	O	P	0
			44	35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

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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 (CCD ID: 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
			5	3	2		
6	D	1	Total	C	O		0
			5	3	2		
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
			5	3	2		
6	H	1	Total	C	O		0
			5	3	2		

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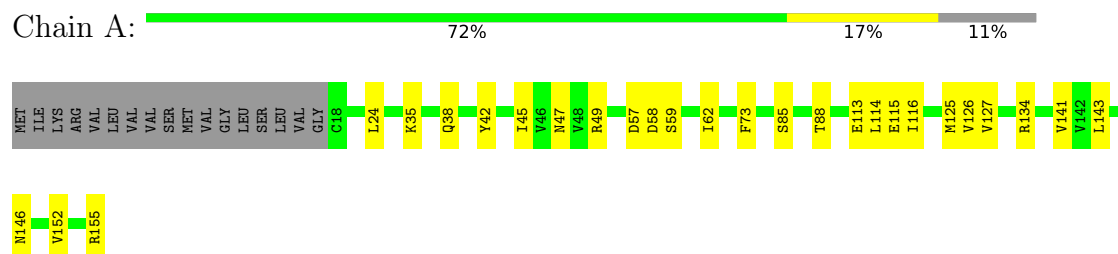
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Mol	Chain	Residues	Atoms			AltConf
6	J	1	Total	C	O	0
			5	3	2	
6	J	1	Total	C	O	0
			5	3	2	
6	K	1	Total	C	O	0
			5	3	2	
6	M	1	Total	C	O	0
			5	3	2	
6	M	1	Total	C	O	0
			5	3	2	

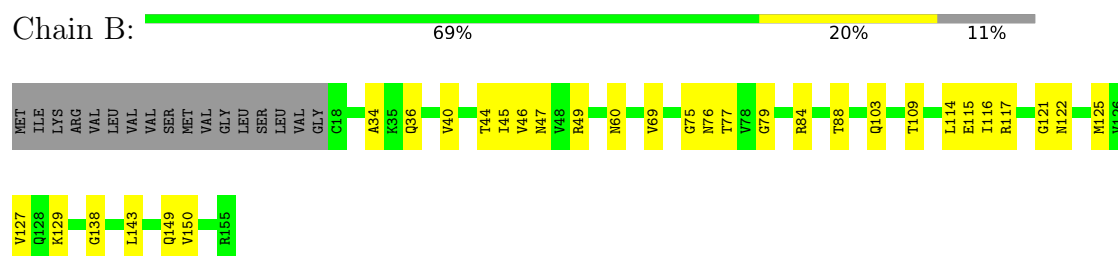
3 Residue-property plots [i](#)

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.

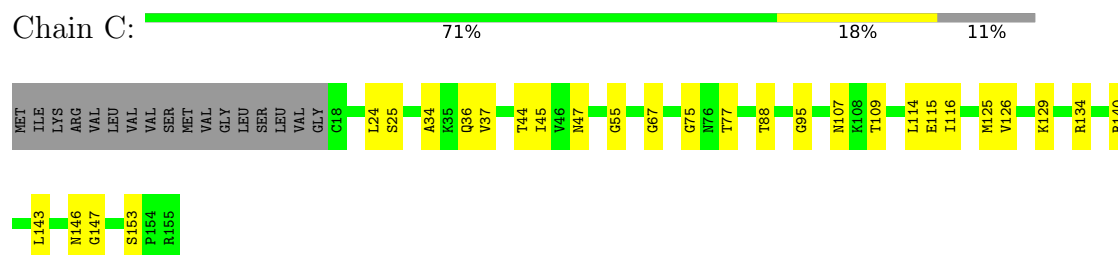
- Molecule 1: Outer membrane lipoprotein slyB



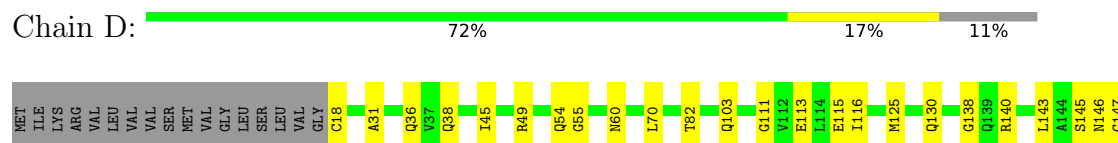
- Molecule 1: Outer membrane lipoprotein slyB



- Molecule 1: Outer membrane lipoprotein slyB



- Molecule 1: Outer membrane lipoprotein slyB



S148
P154
R155

- Molecule 1: Outer membrane lipoprotein slyB

Chain E:  74% 15% 11%

MET ILE LYS ARG VAL LEU VAL VAL SER SER MET MET VAL GLY LEU LEU SER LEU VAL VAL GLY C18 A31 T45 V46 R49 S59 N60 V61 I62 S85 T88 S104 V112 E113 L114 E115 I116 M125 V126 V127 G138 Q139 R140 V141 V142 L143 V150 S153 P154 R155

- Molecule 1: Outer membrane lipoprotein slyB

Chain F:  68% 21% 11%

MET ILE LYS ARG VAL LEU VAL VAL SER SER MET MET VAL GLY LEU LEU SER LEU VAL VAL GLY C18 S25 G26 L24 A34 Q38 T44 I45 V46 N47 V48 R49 P50 S59 N60 V61 V69 G75 T88 Q100 T109 E115 I116 R117 M125 V126 K129 T133 G138

V142 L143 A144 S145 N146 G147 S148 S153 P154 R155

- Molecule 1: Outer membrane lipoprotein slyB

Chain G:  68% 21% 11%

MET ILE LYS ARG VAL LEU VAL VAL SER SER MET MET VAL GLY LEU LEU SER LEU VAL VAL GLY C18 V19 T23 L24 S25 V28 Q36 Y42 I45 V46 R49 Q52 T53 Q54 Q55 D58 S59 N60 G63 N107 K108 T109 E113 L114 E115 I116 M125 V126 V127 Q128 K129

G138 Q139 R140 V141 L143 R155

- Molecule 1: Outer membrane lipoprotein slyB

Chain H:  70% 19% 11%

MET ILE LYS ARG VAL LEU VAL VAL SER SER MET MET VAL GLY LEU LEU SER LEU VAL VAL GLY C18 N21 A34 K35 Q36 T45 V46 N47 V48 R49 I53 Q54 S55 S56 D57 D58 S59 N60 V69 L70 H76 R84 N107 K108 T109 Q110 G111 V112 E113 L114 E115 M125 V126

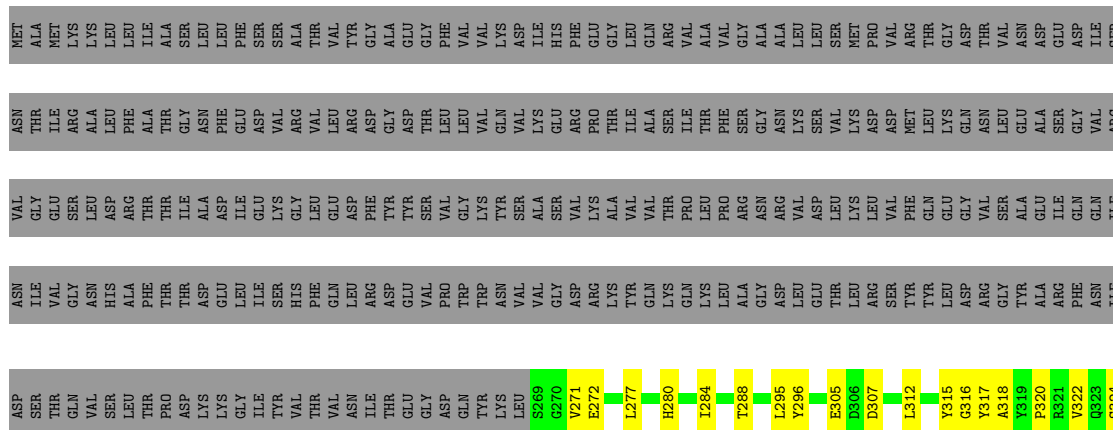
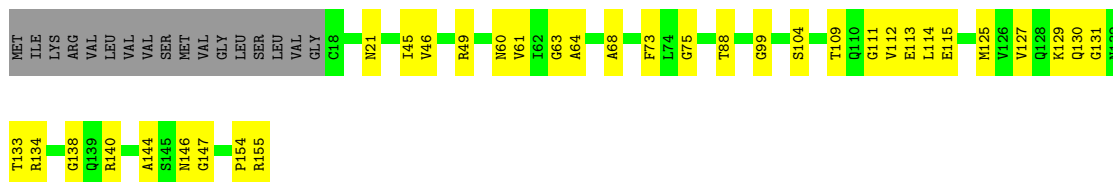
Q130 G138 N146 Q149 R155

- Molecule 1: Outer membrane lipoprotein slyB

Chain I:  68% 21% 11%

MET ILE LYS ARG VAL LEU VAL VAL SER SER MET MET VAL GLY LEU LEU SER LEU VAL VAL GLY C18 D22 G26 Q36 V37 Q38 T45 N45 R49 P50 V51 Q52 N60 G63 V69 G79 G80 G81 T82 Q103 S104 T109 Q110 G111 V112 E113 L114 E115 I116 M125 V126 V127

Q128 K129 Q130 T133 L143 A144 S145 N146 G147 V150 P154 R155



N325	P326	V335	K336	L337	R338	V339	R340	V341	D342	A343	G344	N345	R346	F347	Y348	V349	R350	K351	L352	F354	N357	S360	K361	V364	L365	R366	R367	E368	M369	R370	Q371	M372	E373	G374	A375	W376	L377	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	N459	G460	T461	Y465	Y468	S484	R488	F494	Q495	A499	D503	F504	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	F586	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	D698	L699	V706	G707	G708	N709					
I719	T720	P721	T722	F723	F724	V733	S736	M741	G742	T743	V744	W745	D746	T747	W748	W749	Y754	Y757	Y760	I766	R767	M768	G771	W776	V784	F785	S786	Y787	A788	D797	Q803	F804	N805	K808	T809	TRP																

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	NONE	Depositor
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: L8Z, LPP, PLM, 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	0.38	0/973	0.52	0/1317
1	B	0.38	0/973	0.55	0/1317
1	C	0.38	0/973	0.54	0/1317
1	D	0.40	0/973	0.51	0/1317
1	E	0.41	0/973	0.55	0/1317
1	F	0.42	0/973	0.63	0/1317
1	G	0.39	0/973	0.54	0/1317
1	H	0.39	0/973	0.52	0/1317
1	I	0.41	0/973	0.55	0/1317
1	J	0.39	0/973	0.52	0/1317
1	K	0.41	0/973	0.55	0/1317
1	L	0.40	0/973	0.55	0/1317
1	M	0.39	0/973	0.55	0/1317
2	N	0.31	1/4243 (0.0%)	0.54	0/5751
All	All	0.38	1/16892 (0.0%)	0.54	0/22872

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	586	PHE	C-O	-5.69	1.21	1.23

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	23	0
1	B	967	0	963	29	0
1	C	967	0	963	23	0
1	D	967	0	963	22	0
1	E	967	0	963	21	0
1	F	967	0	963	25	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	19	0
1	L	967	0	963	28	0
1	M	967	0	963	33	0
2	N	4139	0	3882	164	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	479	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 479 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	1.07
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%)	18	53
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%)	102 (100%)	0	100	100
1	C	102/117 (87%)	102 (100%)	0	100	100
1	D	102/117 (87%)	102 (100%)	0	100	100
1	E	102/117 (87%)	101 (99%)	1 (1%)	68	75
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%)	101 (99%)	1 (1%)	68	75
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%)	439 (100%)	2 (0%)	81	82
All	All	1767/2209 (80%)	1763 (100%)	4 (0%)	85	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	60	ASN
1	H	60	ASN
2	N	563	ASN
2	N	607	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	520	ASN
2	N	523	ASN
1	G	132	ASN
1	F	122	ASN
2	N	561	GLN

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 oligosaccharides 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	$\# Z > 2$
6	GOL	D	205	-	4,4,5	1.20	0	4,4,5	0.96	0
3	PLM	J	201	1	15,16,17	0.45	0	14,15,17	0.31	0
6	GOL	F	204	-	4,4,5	0.60	0	4,4,5	1.33	0
6	GOL	H	205	-	4,4,5	0.97	0	4,4,5	1.08	0
5	LPP	A	203	-	43,43,43	1.62	4 (9%)	46,48,48	1.07	5 (10%)
5	LPP	L	203	-	43,43,43	1.60	4 (9%)	46,48,48	1.04	5 (10%)
3	PLM	L	201	1	15,16,17	0.49	0	14,15,17	0.36	0
4	L8Z	J	203	-	138,140,140	1.95	26 (18%)	164,176,176	2.23	34 (20%)
5	LPP	I	203	-	43,43,43	1.68	3 (6%)	46,48,48	0.98	4 (8%)
5	LPP	H	204	-	43,43,43	1.65	3 (6%)	46,48,48	0.98	4 (8%)
4	L8Z	E	1002	-	138,140,140	1.98	27 (19%)	164,176,176	2.27	35 (21%)
4	L8Z	B	202	-	138,140,140	2.03	30 (21%)	164,176,176	2.10	31 (18%)
5	LPP	G	203	-	43,43,43	1.66	3 (6%)	46,48,48	1.08	5 (10%)
3	PLM	I	201	1	15,16,17	0.53	0	14,15,17	0.33	0
4	L8Z	I	202	-	138,140,140	1.99	27 (19%)	164,176,176	2.16	32 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLM	G	201	1	15,16,17	0.41	0	14,15,17	0.34	0
4	L8Z	K	202	-	138,140,140	1.98	28 (20%)	164,176,176	2.49	32 (19%)
5	LPP	F	203	-	43,43,43	1.59	3 (6%)	46,48,48	1.00	5 (10%)
6	GOL	A	204	-	4,4,5	1.09	0	4,4,5	1.34	1 (25%)
4	L8Z	M	204	-	138,140,140	1.93	27 (19%)	164,176,176	2.19	30 (18%)
6	GOL	K	204	-	4,4,5	1.18	0	4,4,5	1.00	0
5	LPP	B	203	-	43,43,43	1.63	3 (6%)	46,48,48	1.02	5 (10%)
4	L8Z	G	202	-	138,140,140	1.97	31 (22%)	164,176,176	2.36	36 (21%)
3	PLM	M	202	1	15,16,17	0.53	0	14,15,17	0.30	0
3	PLM	F	201	1	15,16,17	0.57	0	14,15,17	0.32	0
4	L8Z	C	203	-	138,140,140	2.00	27 (19%)	164,176,176	2.29	34 (20%)
3	PLM	C	201	1	15,16,17	0.52	0	14,15,17	0.29	0
6	GOL	D	202	-	4,4,5	0.98	0	4,4,5	1.39	0
3	PLM	K	201	1	15,16,17	0.53	0	14,15,17	0.30	0
3	PLM	A	201	1	15,16,17	0.55	0	14,15,17	0.34	0
4	L8Z	F	202	-	138,140,140	2.04	32 (23%)	164,176,176	2.32	33 (20%)
4	L8Z	D	203	-	138,140,140	1.94	25 (18%)	164,176,176	2.27	31 (18%)
5	LPP	C	204	-	43,43,43	1.61	3 (6%)	46,48,48	1.07	4 (8%)
3	PLM	B	201	1	15,16,17	0.41	0	14,15,17	0.31	0
5	LPP	M	205	-	43,43,43	1.76	3 (6%)	46,48,48	1.01	3 (6%)
3	PLM	D	201	1	15,16,17	0.44	0	14,15,17	0.31	0
4	L8Z	A	202	-	138,140,140	2.03	27 (19%)	164,176,176	2.18	36 (21%)
5	LPP	K	203	-	43,43,43	1.63	3 (6%)	46,48,48	0.94	4 (8%)
6	GOL	C	202	-	4,4,5	1.08	0	4,4,5	1.25	0
4	L8Z	H	203	-	138,140,140	1.97	29 (21%)	164,176,176	2.27	33 (20%)
3	PLM	H	201	1	15,16,17	0.50	0	14,15,17	0.40	0
6	GOL	M	203	-	4,4,5	1.29	0	4,4,5	1.02	0
4	L8Z	L	202	-	138,140,140	2.05	28 (20%)	164,176,176	2.22	35 (21%)
6	GOL	H	202	-	4,4,5	1.21	0	4,4,5	1.04	0
3	PLM	E	1001	1	15,16,17	0.41	0	14,15,17	0.35	0
6	GOL	M	201	-	4,4,5	1.28	0	4,4,5	1.33	0
5	LPP	J	204	-	43,43,43	1.67	3 (6%)	46,48,48	0.99	5 (10%)
6	GOL	E	1003	-	4,4,5	1.23	0	4,4,5	1.29	0
6	GOL	J	202	-	4,4,5	1.30	0	4,4,5	1.09	0
5	LPP	D	204	-	43,43,43	1.69	3 (6%)	46,48,48	0.93	4 (8%)
6	GOL	J	205	-	4,4,5	1.13	0	4,4,5	1.33	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
6	GOL	D	205	-	-	2/2/2/4	-
3	PLM	J	201	1	-	4/14/14/15	-
6	GOL	F	204	-	-	2/2/2/4	-
6	GOL	H	205	-	-	2/2/2/4	-
5	LPP	A	203	-	-	22/45/45/45	-
5	LPP	L	203	-	-	21/45/45/45	-
3	PLM	L	201	1	-	4/14/14/15	-
4	L8Z	J	203	-	-	50/140/199/199	0/3/3/3
5	LPP	I	203	-	-	21/45/45/45	-
5	LPP	H	204	-	-	19/45/45/45	-
4	L8Z	E	1002	-	-	63/140/199/199	0/3/3/3
4	L8Z	B	202	-	-	53/140/199/199	0/3/3/3
5	LPP	G	203	-	-	20/45/45/45	-
3	PLM	I	201	1	-	2/14/14/15	-
4	L8Z	I	202	-	-	69/140/199/199	0/3/3/3
3	PLM	G	201	1	-	4/14/14/15	-
4	L8Z	K	202	-	-	51/140/199/199	0/3/3/3
5	LPP	F	203	-	-	23/45/45/45	-
6	GOL	A	204	-	-	2/2/2/4	-
4	L8Z	M	204	-	-	61/140/199/199	0/3/3/3
6	GOL	K	204	-	-	0/2/2/4	-
5	LPP	B	203	-	-	22/45/45/45	-
4	L8Z	G	202	-	-	64/140/199/199	0/3/3/3
3	PLM	M	202	1	-	4/14/14/15	-
3	PLM	F	201	1	-	5/14/14/15	-
4	L8Z	C	203	-	-	59/140/199/199	0/3/3/3
3	PLM	C	201	1	-	4/14/14/15	-
6	GOL	D	202	-	-	0/2/2/4	-
3	PLM	K	201	1	-	3/14/14/15	-
3	PLM	A	201	1	-	7/14/14/15	-
4	L8Z	F	202	-	-	50/140/199/199	0/3/3/3
4	L8Z	D	203	-	-	47/140/199/199	0/3/3/3
5	LPP	C	204	-	-	23/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	B	201	1	-	4/14/14/15	-
5	LPP	M	205	-	-	19/45/45/45	-
3	PLM	D	201	1	-	4/14/14/15	-
4	L8Z	A	202	-	-	64/140/199/199	0/3/3/3
5	LPP	K	203	-	-	15/45/45/45	-
6	GOL	C	202	-	-	2/2/2/4	-
4	L8Z	H	203	-	-	59/140/199/199	0/3/3/3
3	PLM	H	201	1	-	3/14/14/15	-
6	GOL	M	203	-	-	0/2/2/4	-
4	L8Z	L	202	-	-	60/140/199/199	0/3/3/3
6	GOL	H	202	-	-	0/2/2/4	-
3	PLM	E	1001	1	-	5/14/14/15	-
6	GOL	M	201	-	-	2/2/2/4	-
5	LPP	J	204	-	-	18/45/45/45	-
6	GOL	E	1003	-	-	2/2/2/4	-
6	GOL	J	202	-	-	0/2/2/4	-
5	LPP	D	204	-	-	20/45/45/45	-
6	GOL	J	205	-	-	0/2/2/4	-

The worst 5 of 402 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	202	L8Z	C2E-C1G	8.81	1.75	1.54
5	M	205	LPP	P1-O5	8.67	1.87	1.60
5	I	203	LPP	P1-O5	8.64	1.87	1.60
5	H	204	LPP	P1-O5	8.49	1.87	1.60
5	J	204	LPP	P1-O5	8.44	1.87	1.60

The worst 5 of 486 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	202	L8Z	O61-C2E-O62	-12.83	74.56	109.97
4	K	202	L8Z	O61-C2E-C3D	11.40	135.72	107.23
4	G	202	L8Z	O61-C2E-O62	-10.19	81.84	109.97
4	L	202	L8Z	O61-C2E-O62	-8.99	85.15	109.97
4	F	202	L8Z	C22-C1A-N21	8.90	128.41	116.25

There are no chirality outliers.

5 of 1060 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:

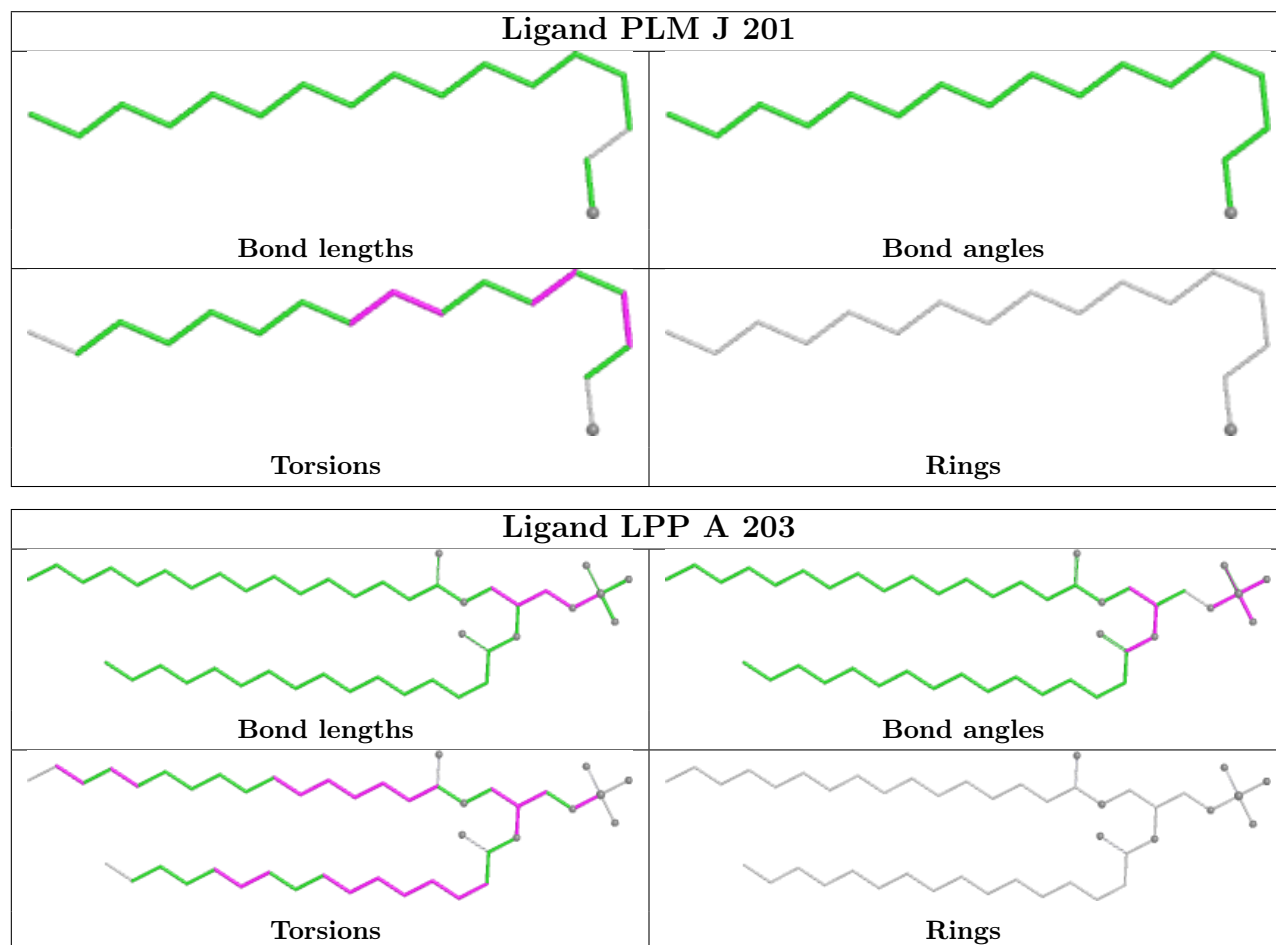
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	203	LPP	2	0
5	L	203	LPP	3	0
3	L	201	PLM	1	0
4	J	203	L8Z	2	0
5	I	203	LPP	1	0
5	H	204	LPP	5	0
4	E	1002	L8Z	3	0
4	B	202	L8Z	1	0
5	G	203	LPP	1	0
3	I	201	PLM	2	0
4	I	202	L8Z	3	0
3	G	201	PLM	1	0
4	K	202	L8Z	2	0
5	F	203	LPP	2	0
4	M	204	L8Z	3	0
5	B	203	LPP	3	0
4	G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

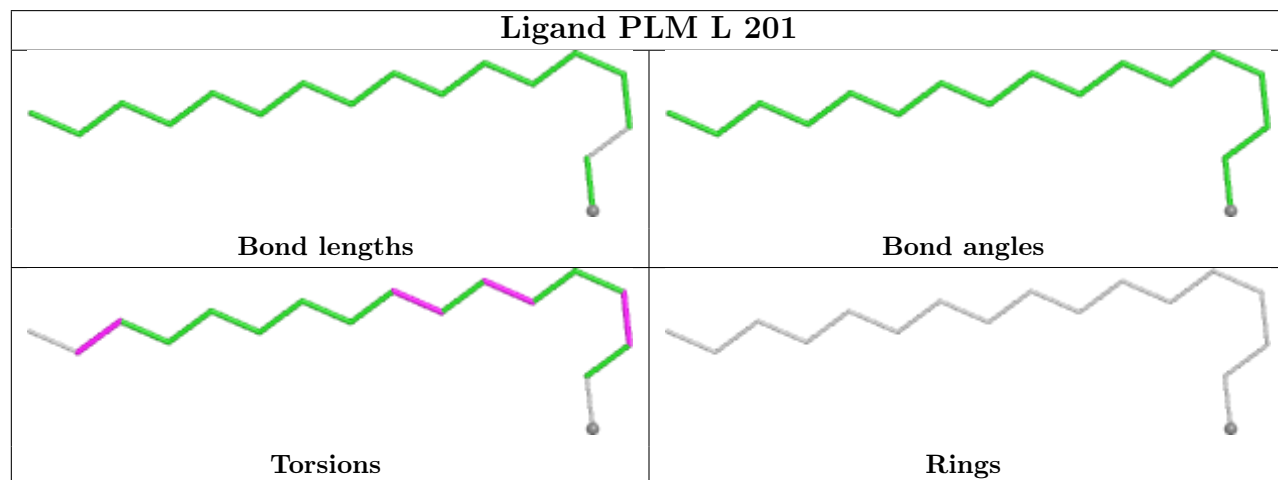
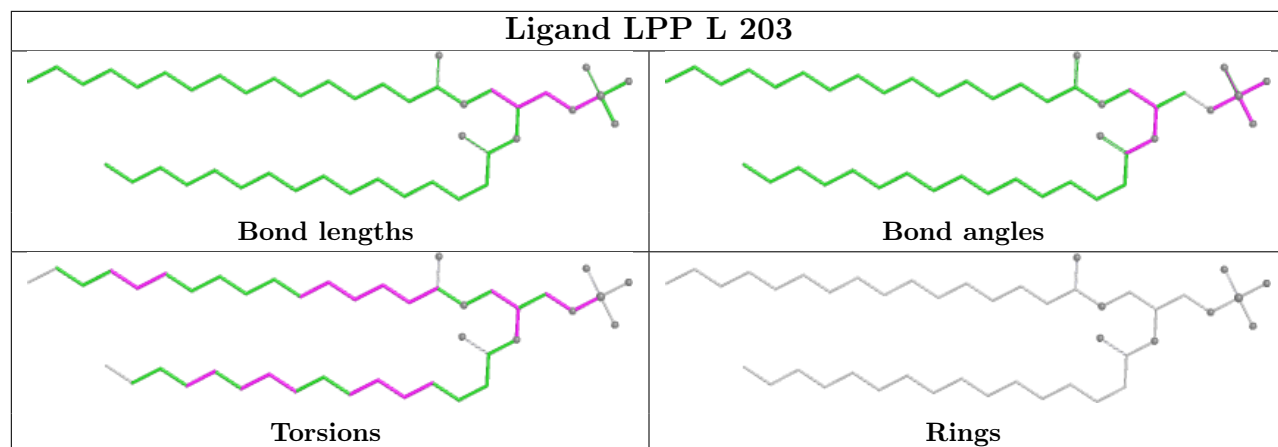
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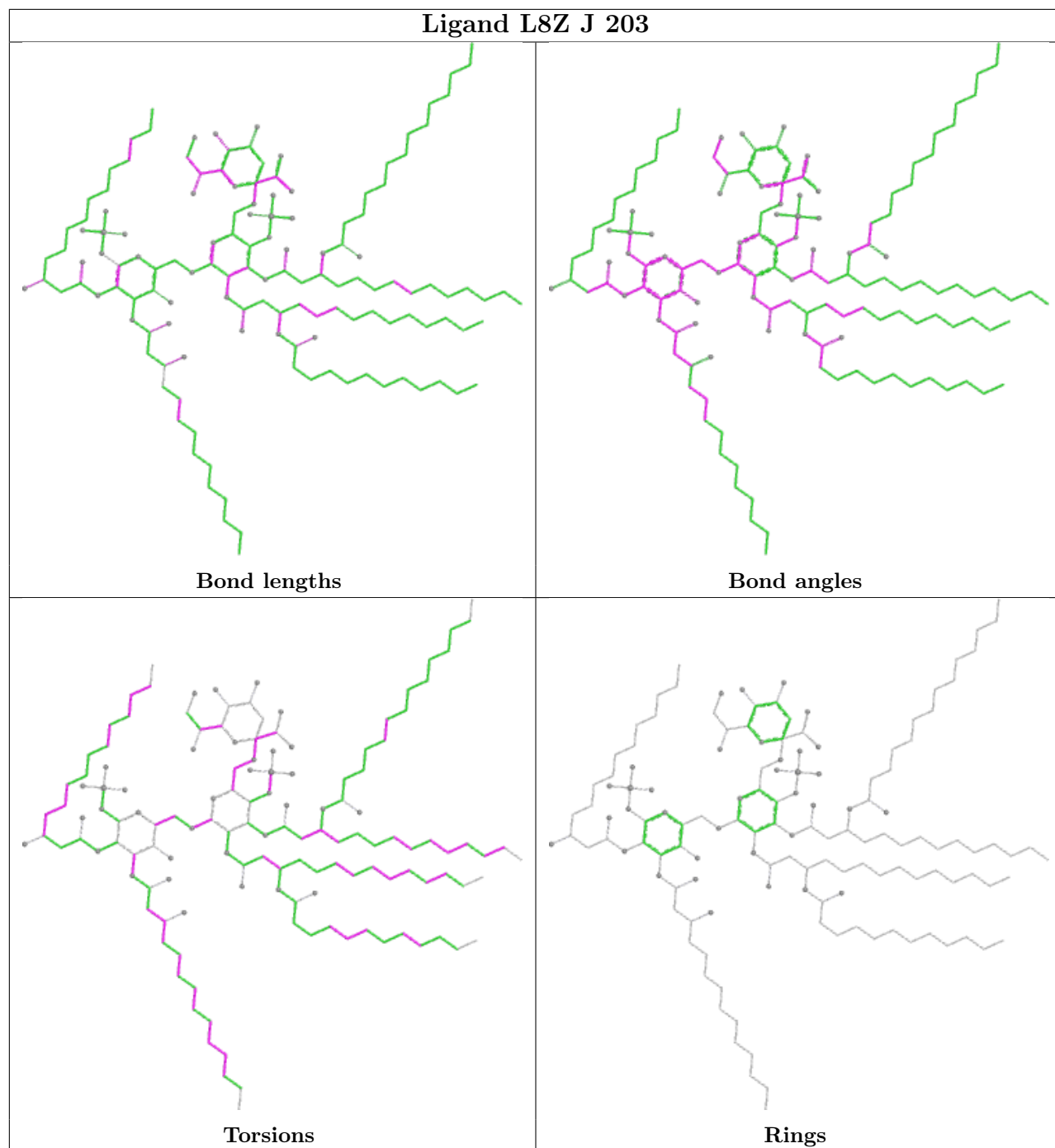
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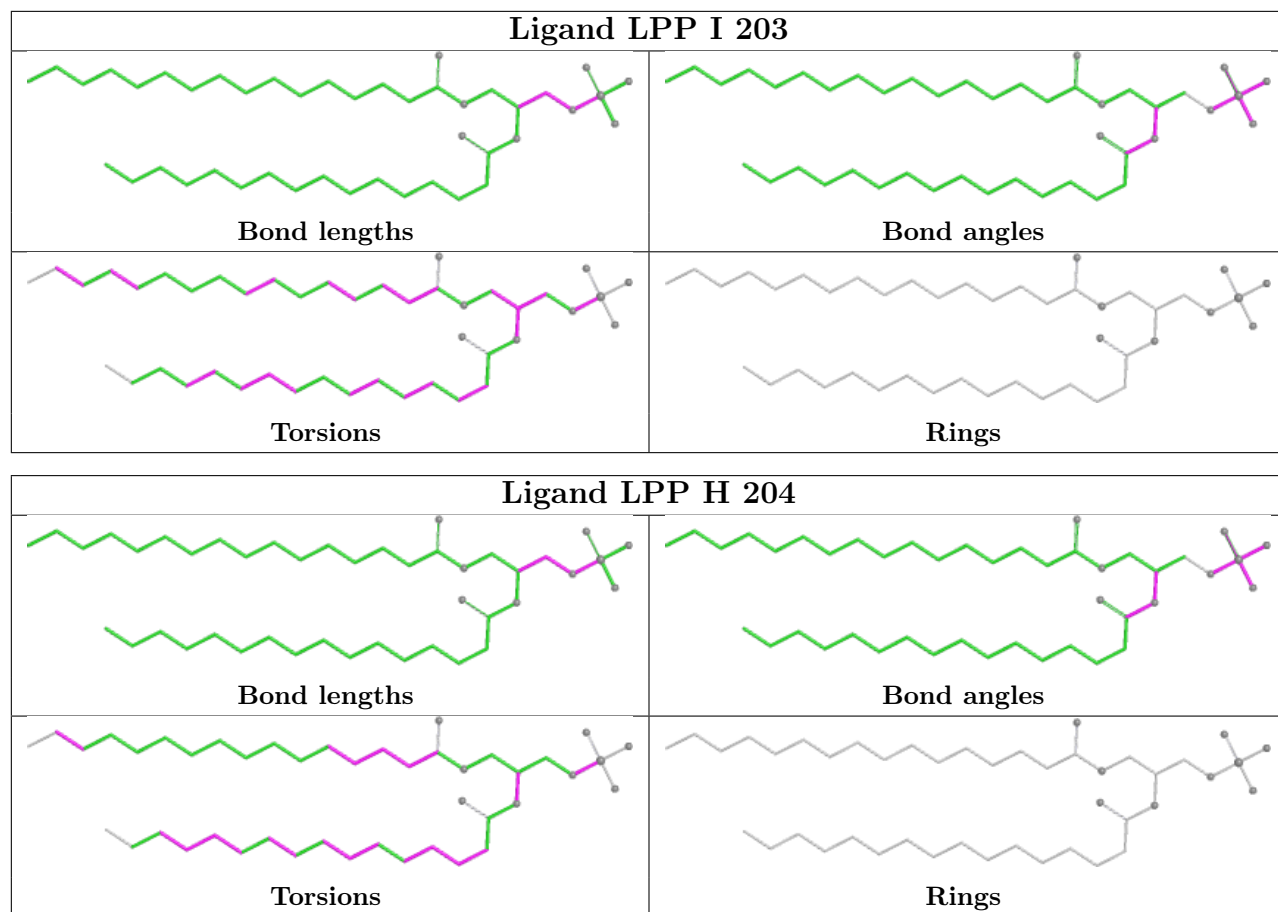
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	204	LPP	1	0

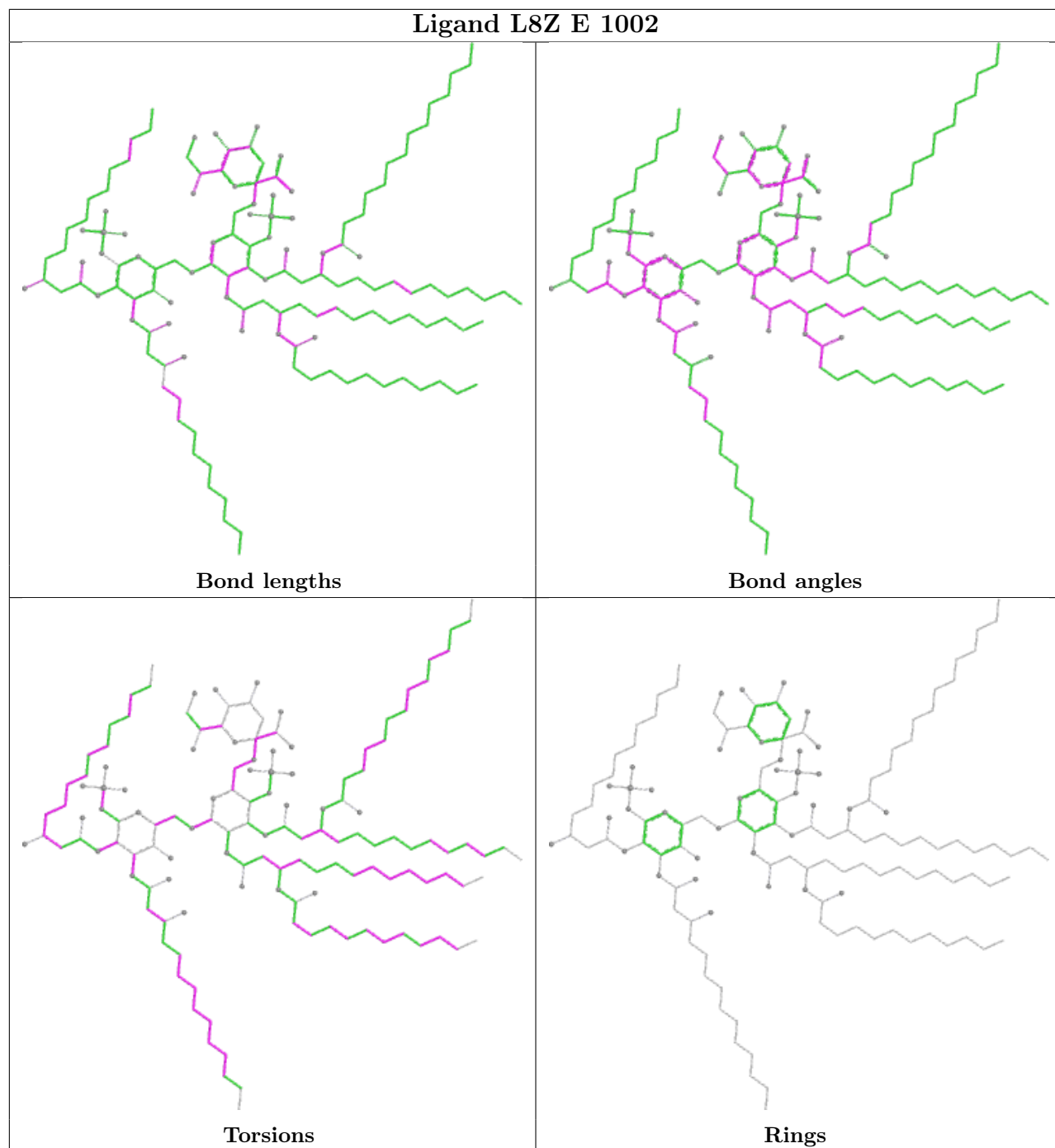
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

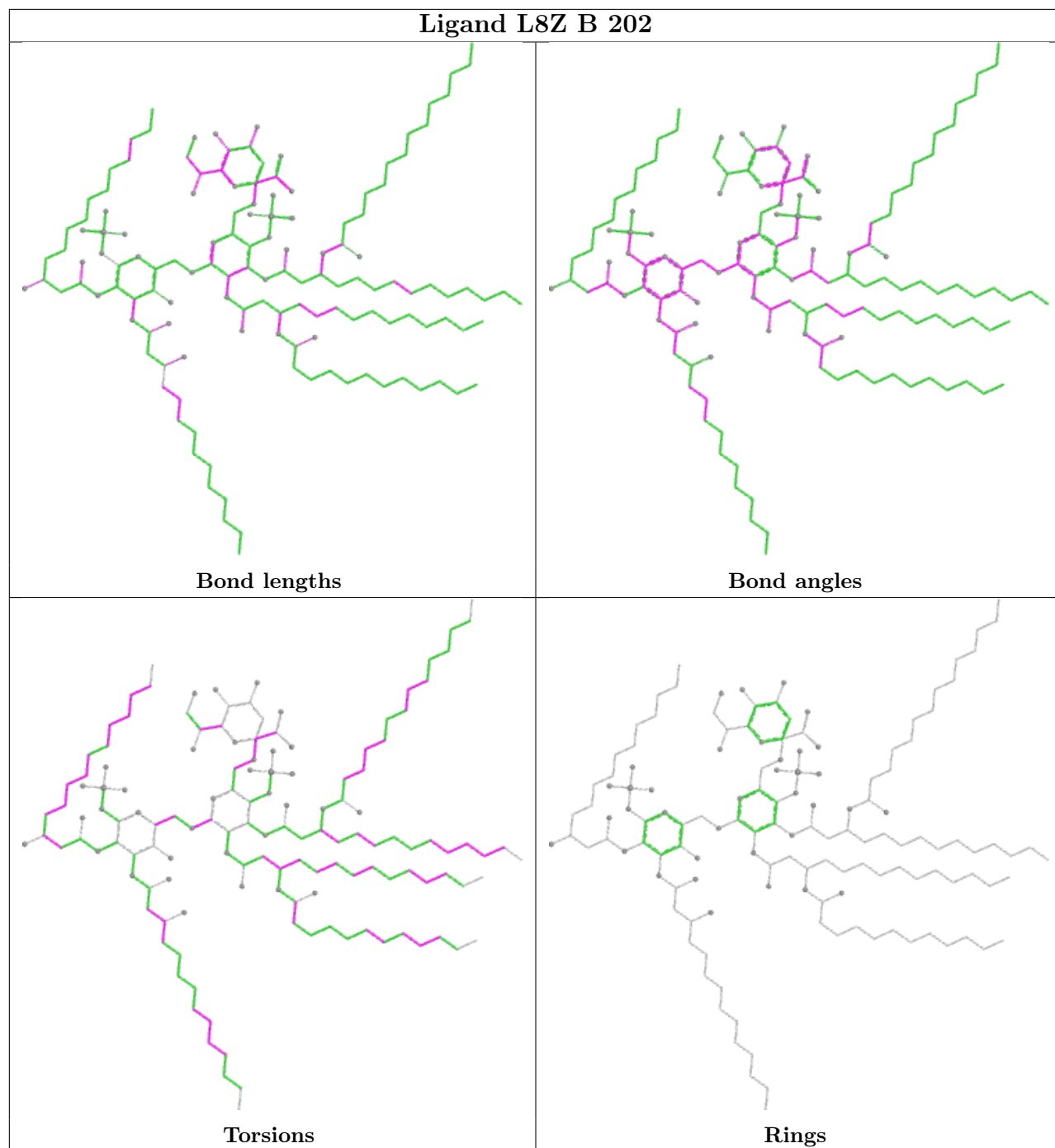


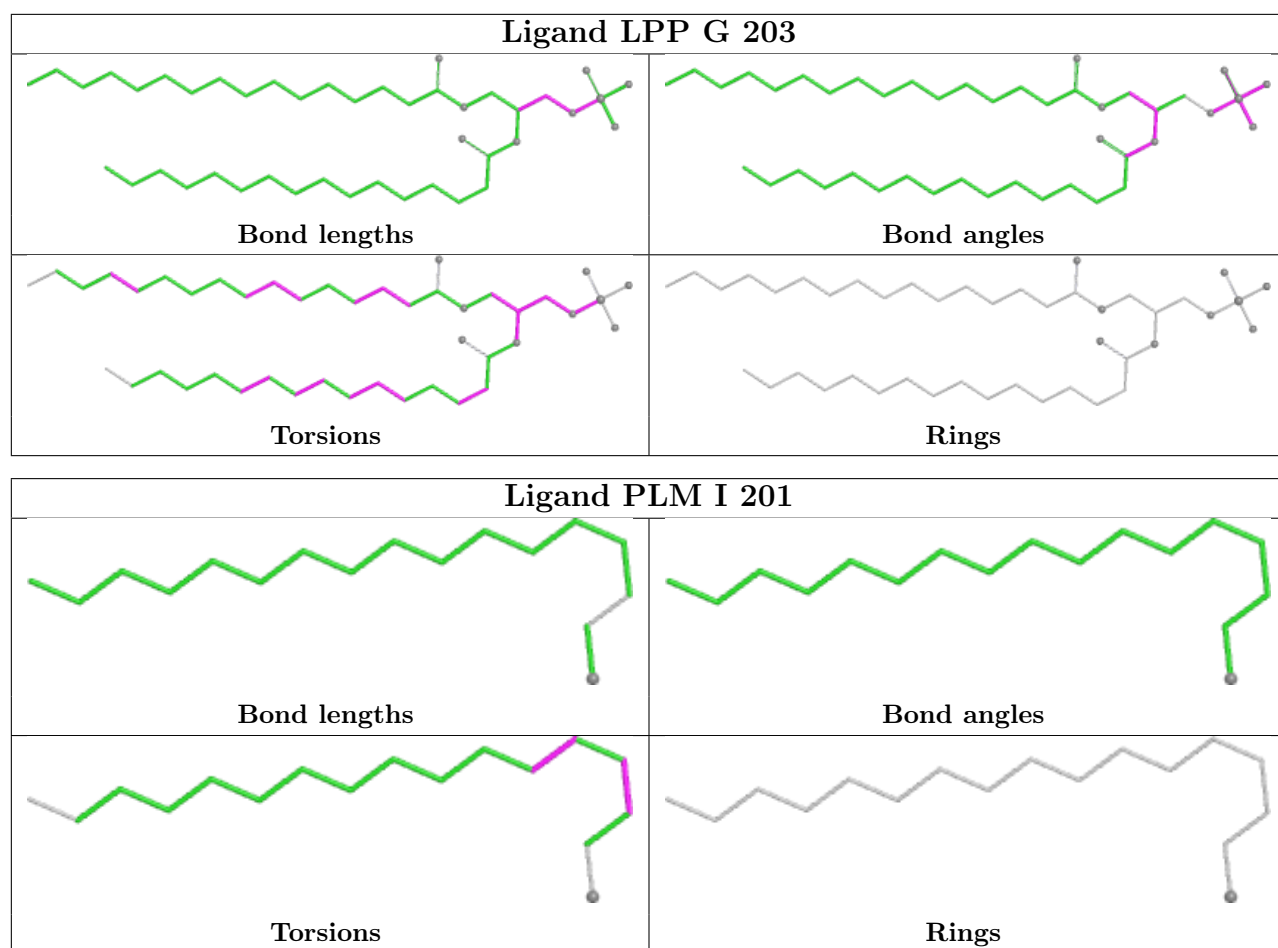




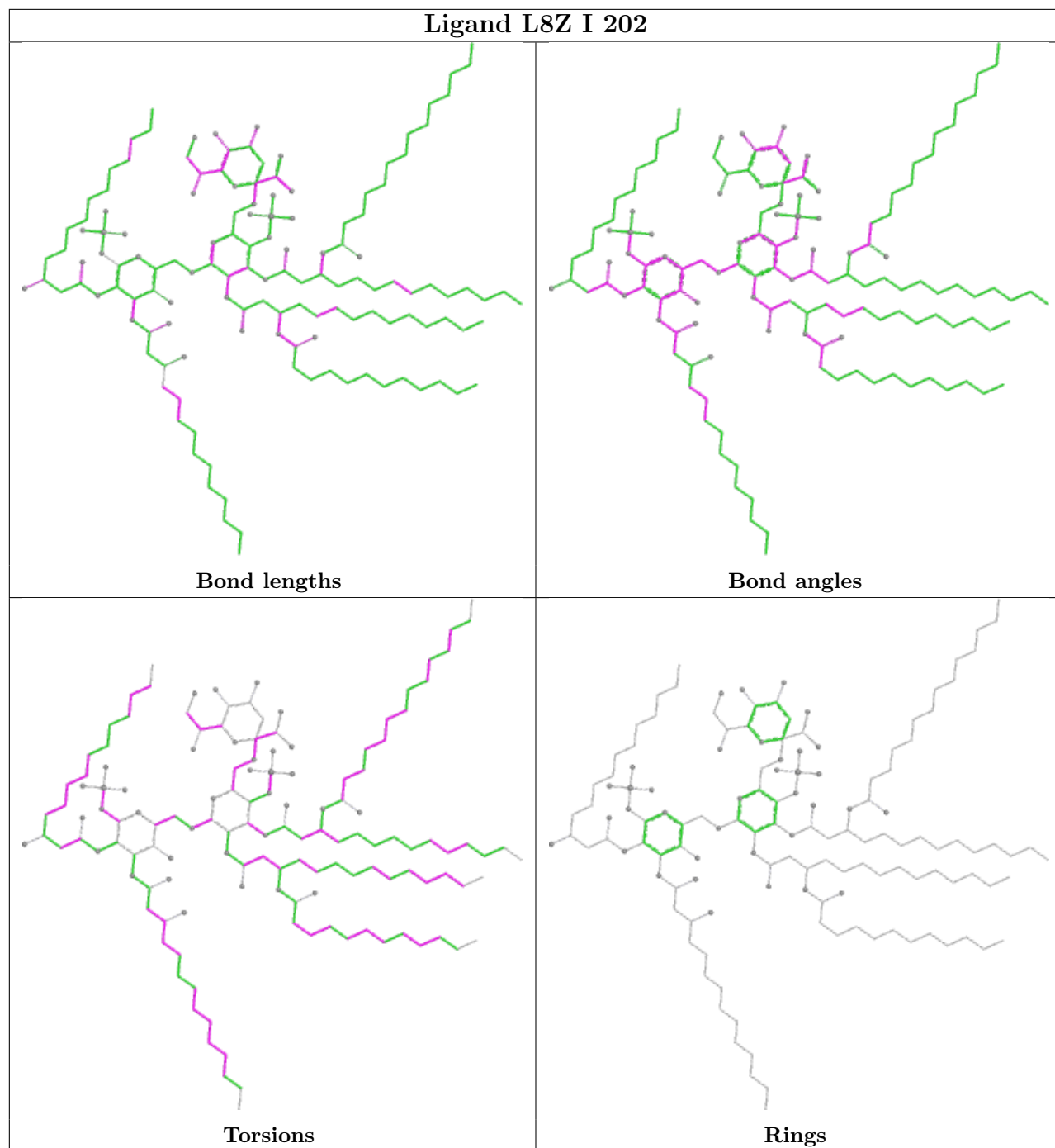


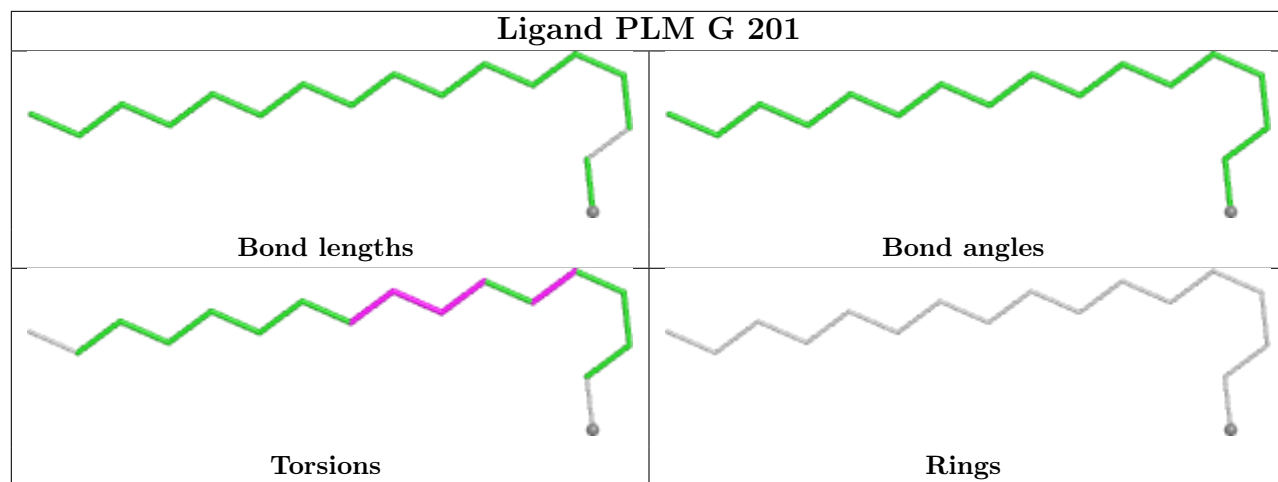


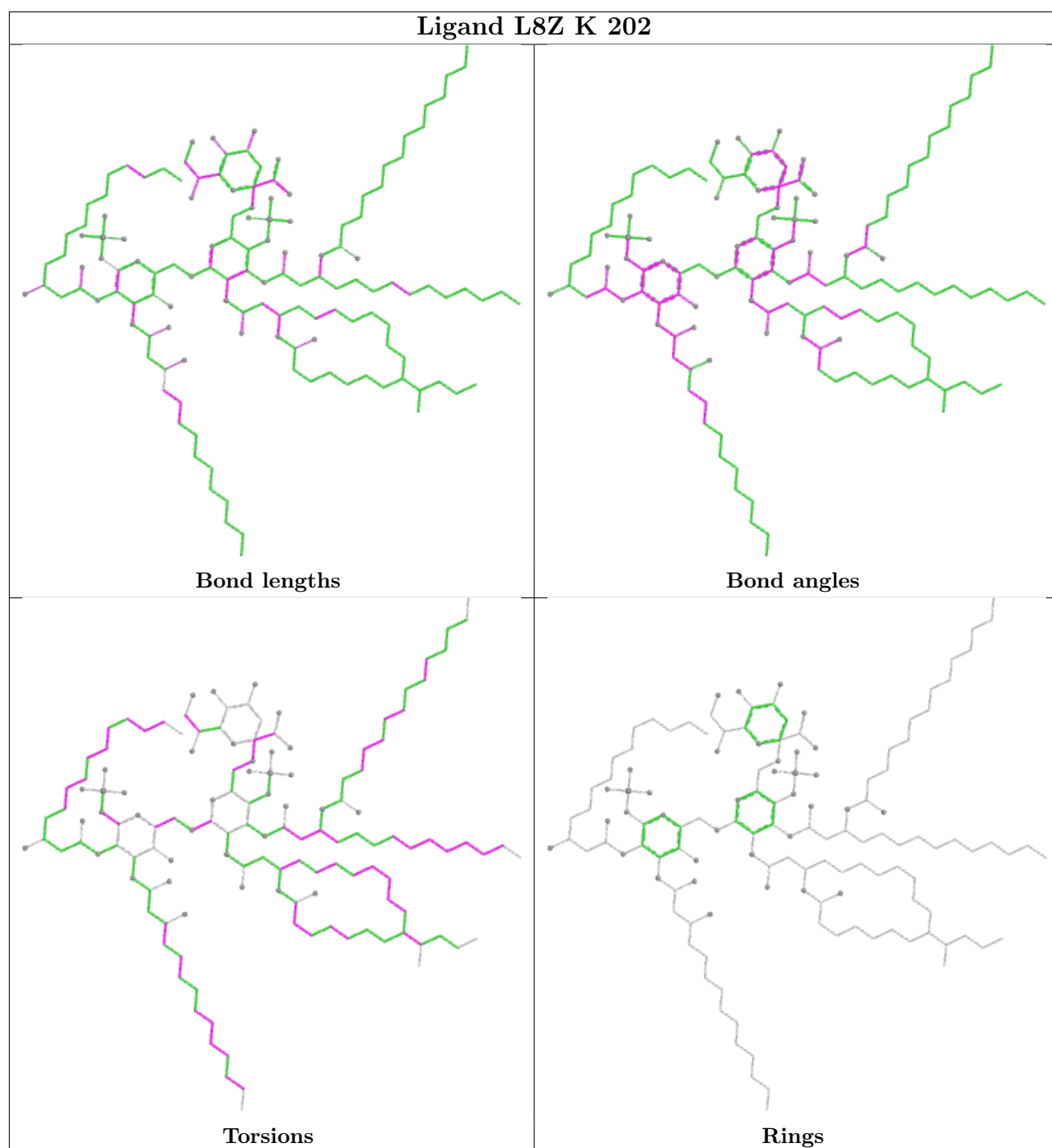


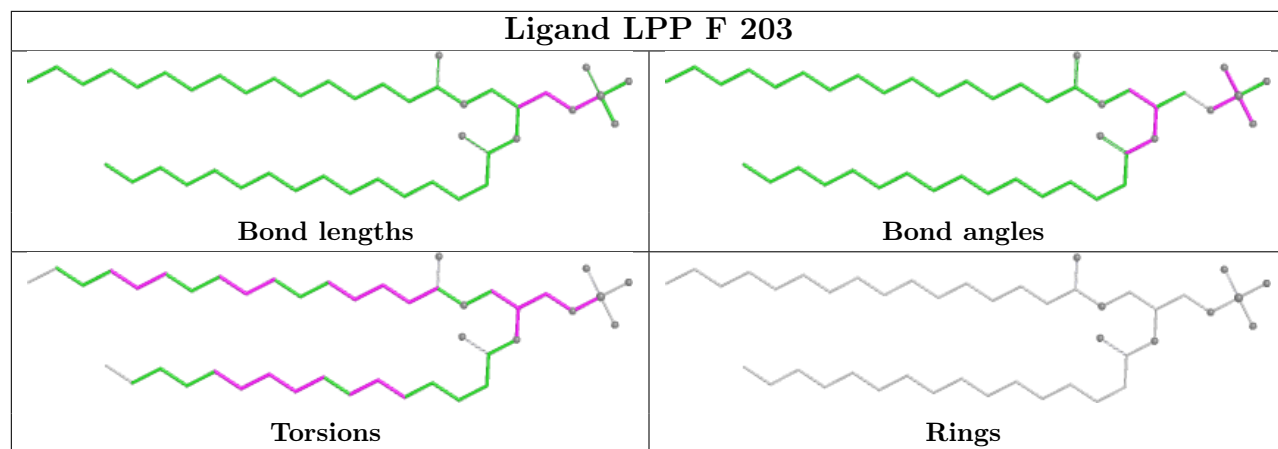


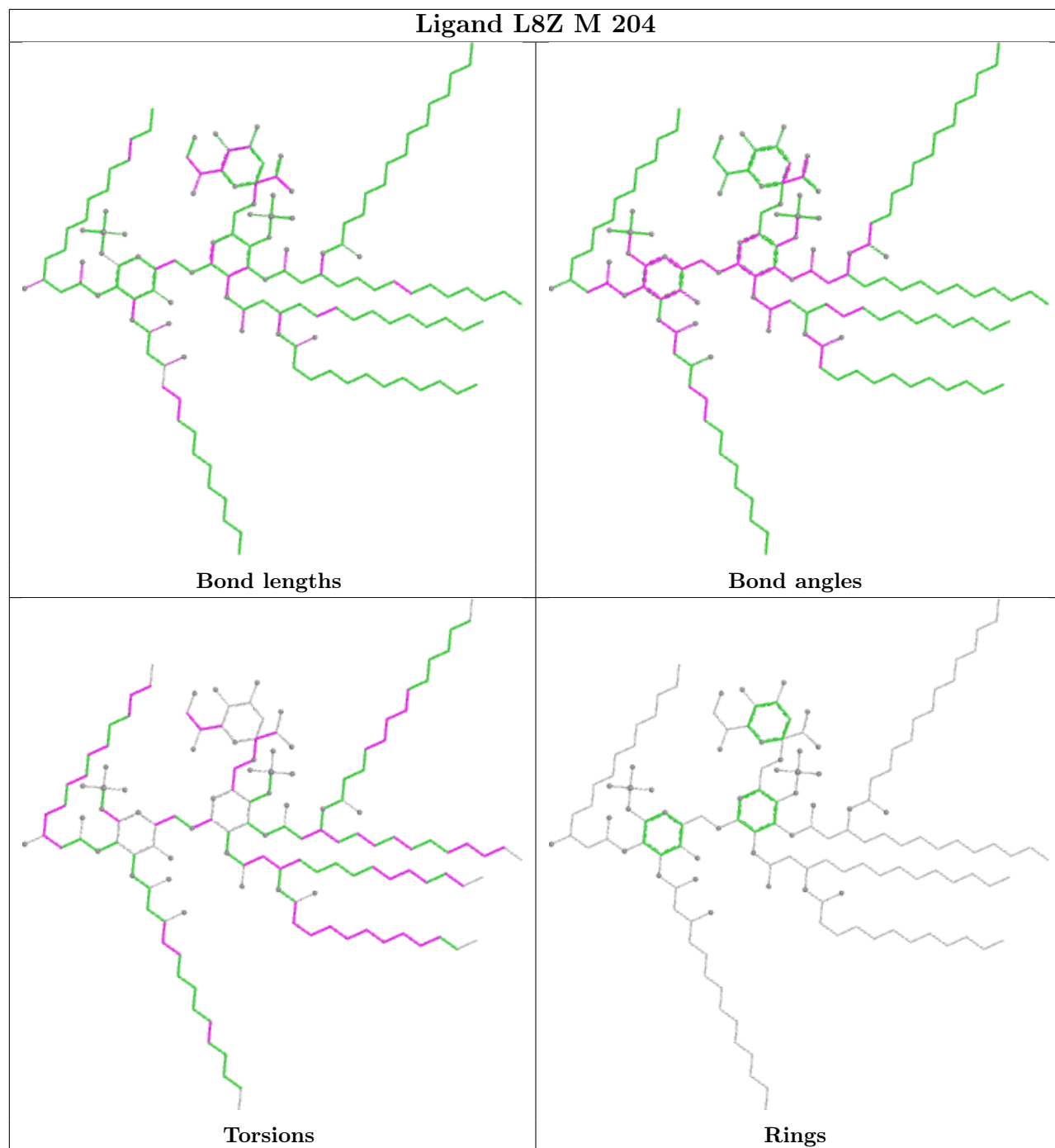
Ligand L8Z I 202

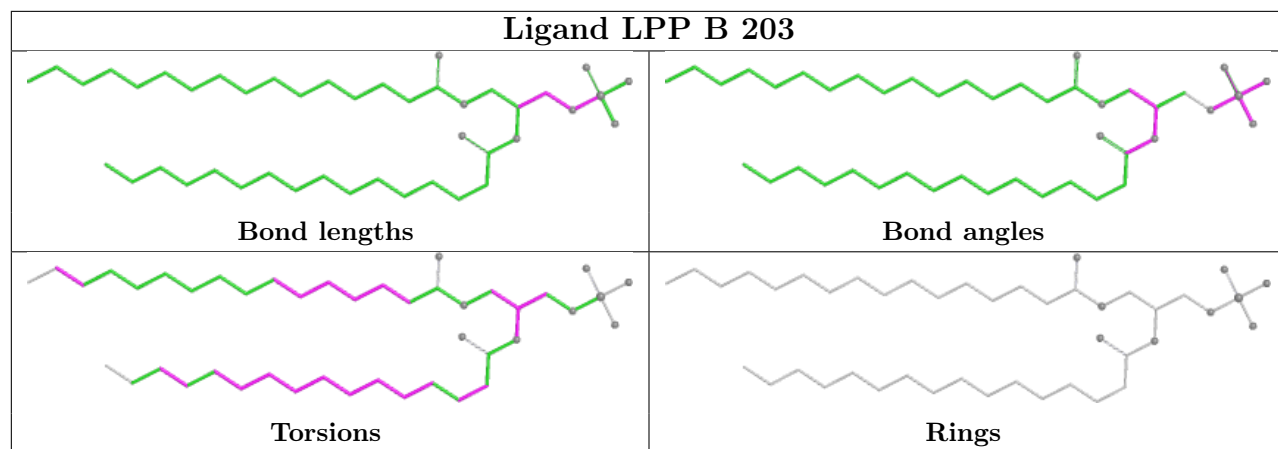


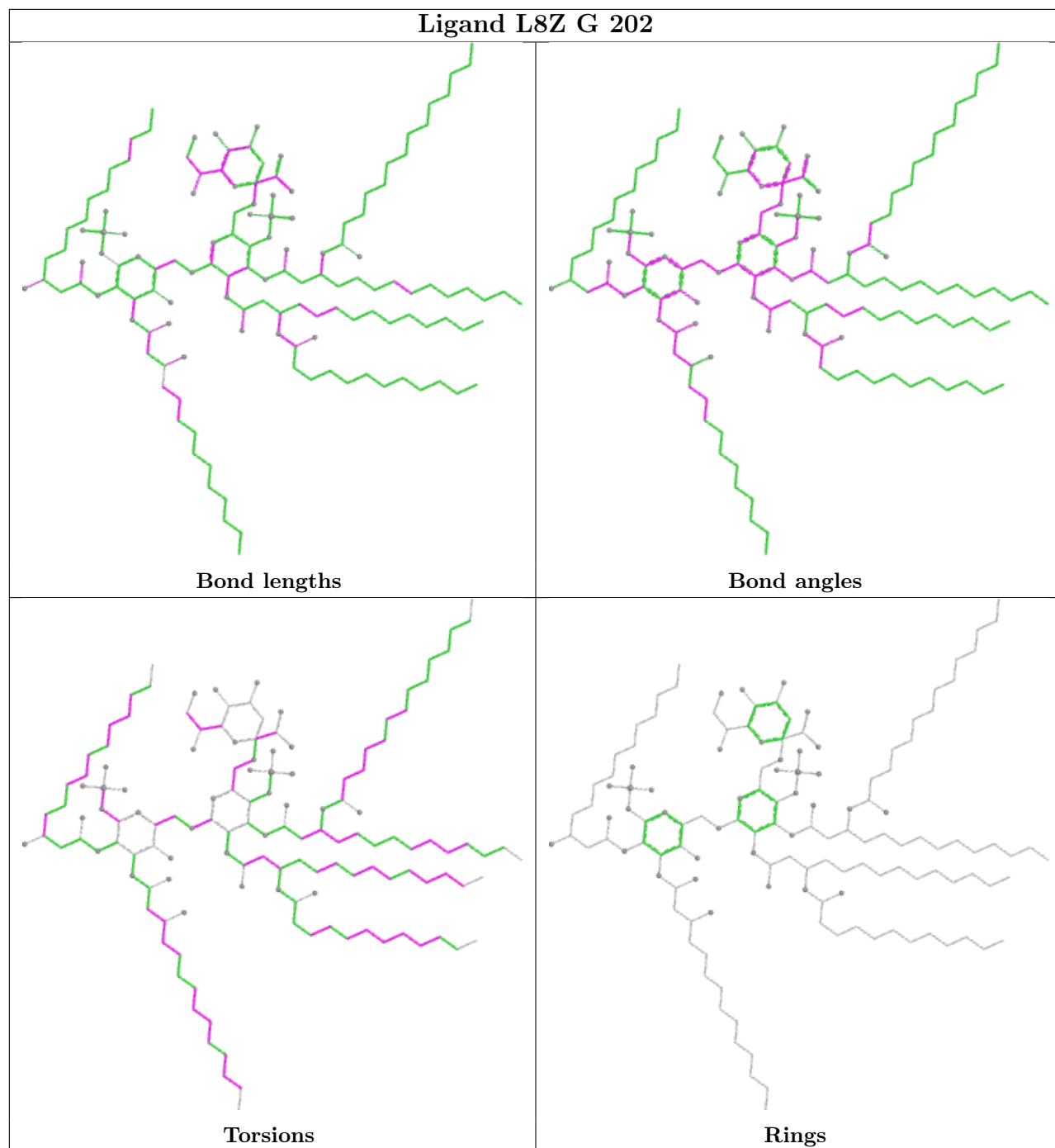


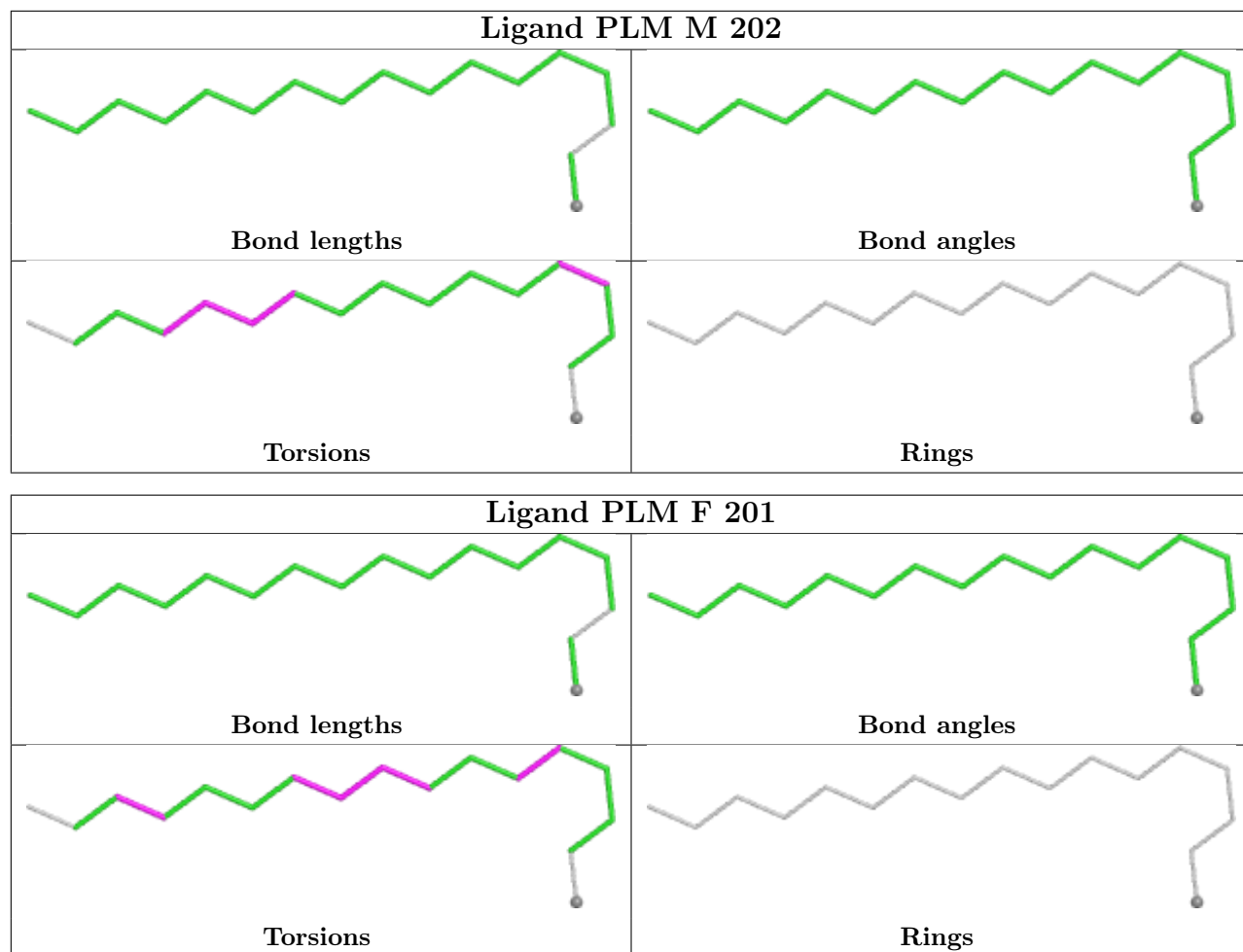


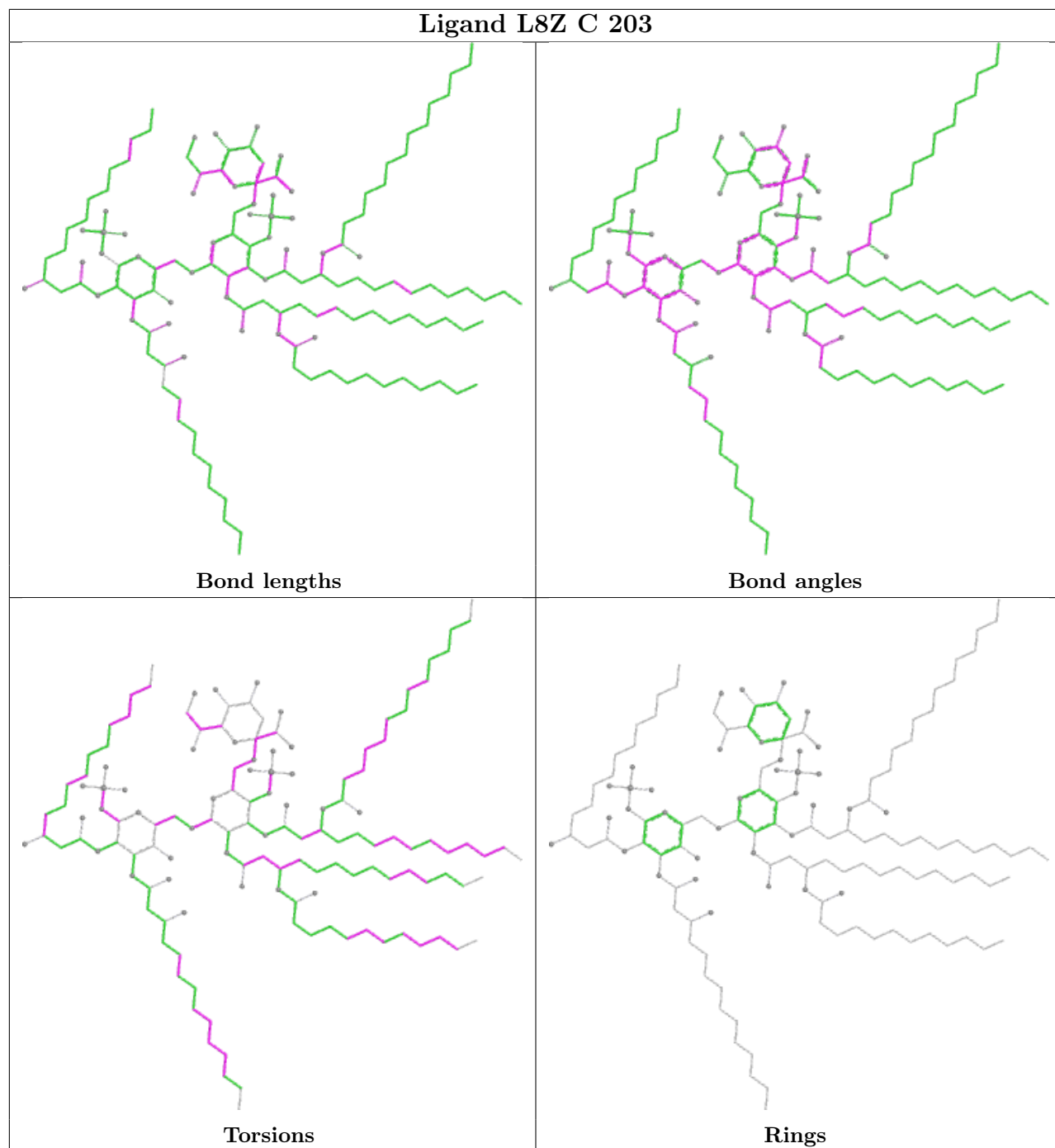


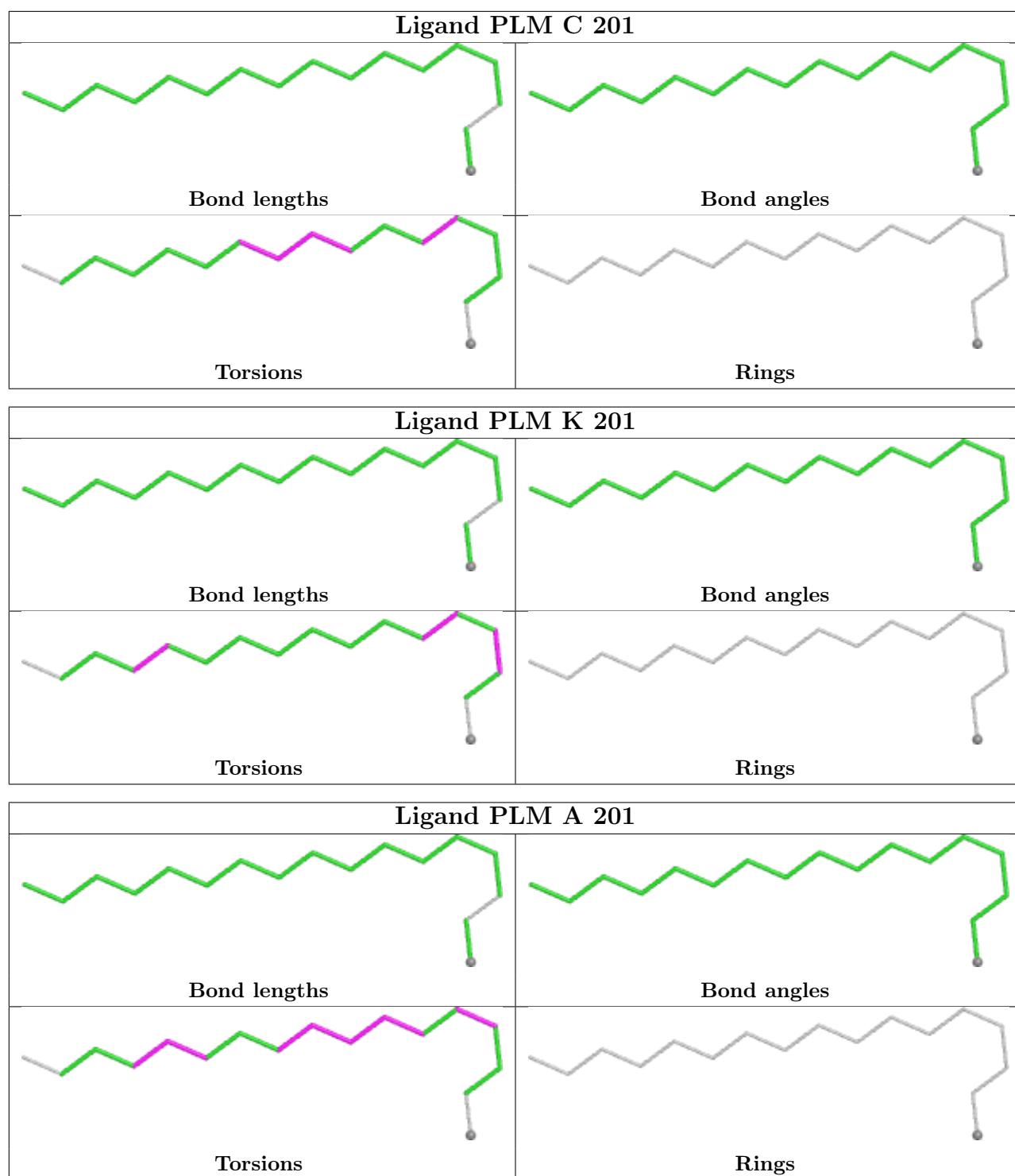


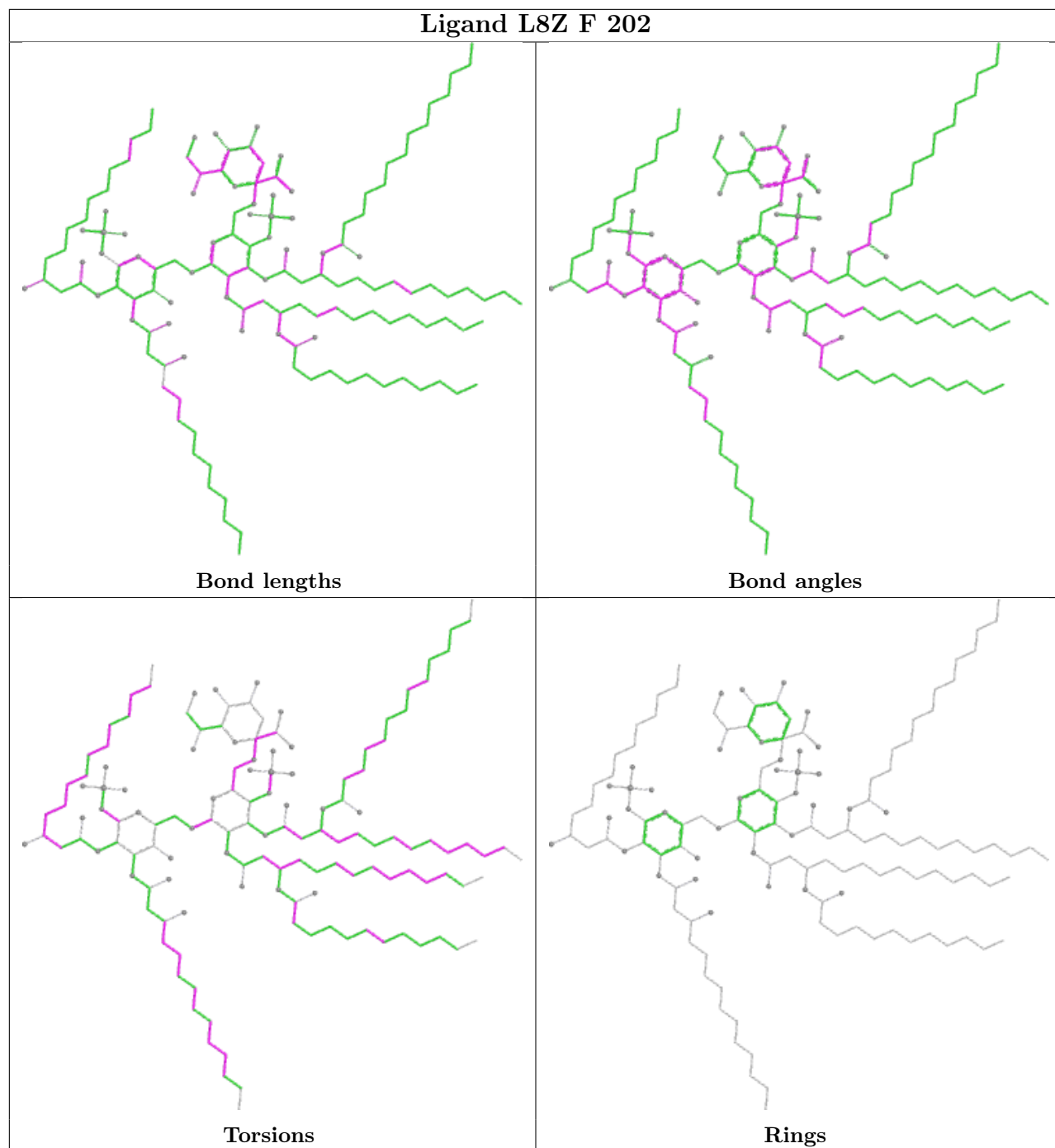


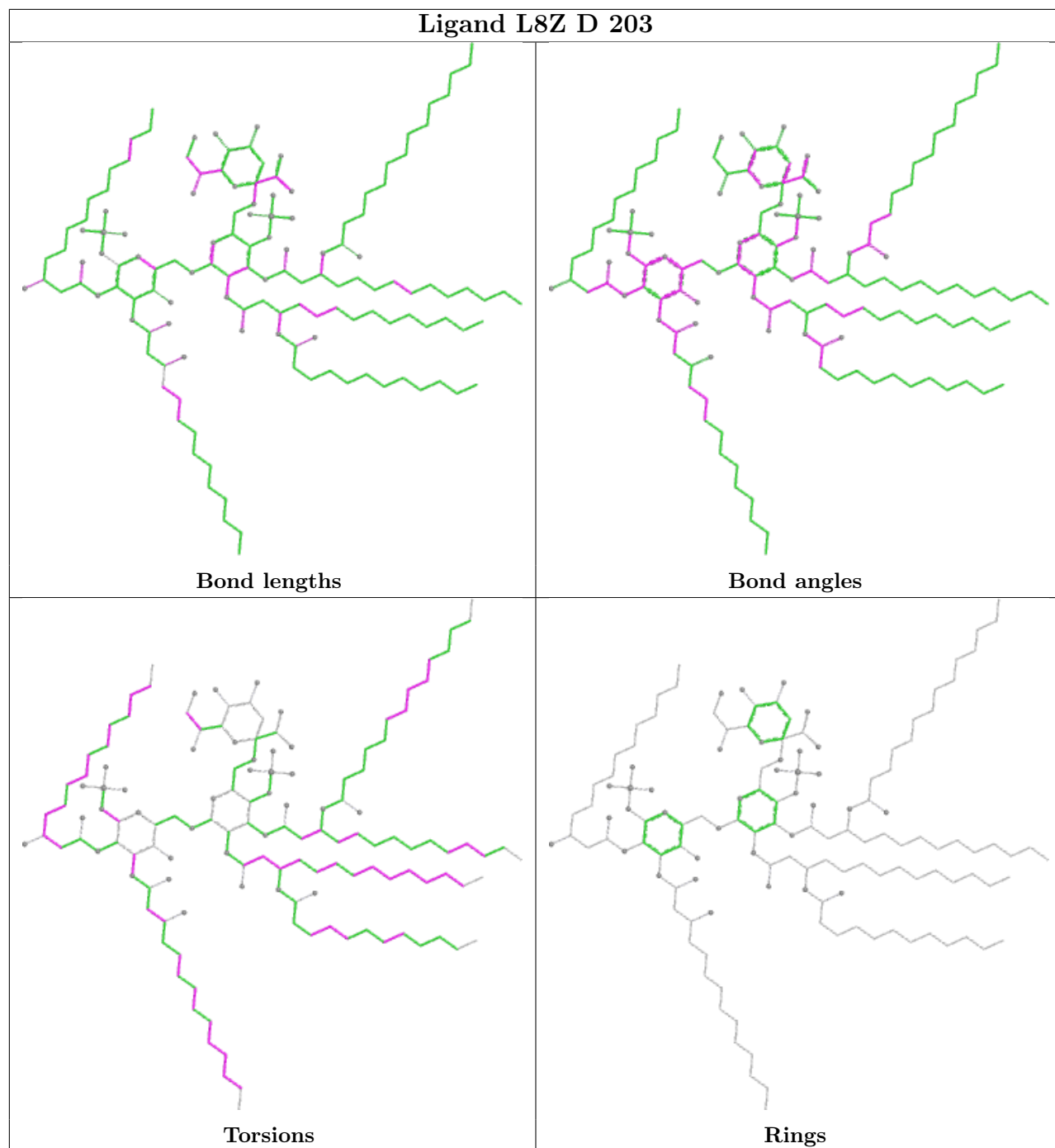


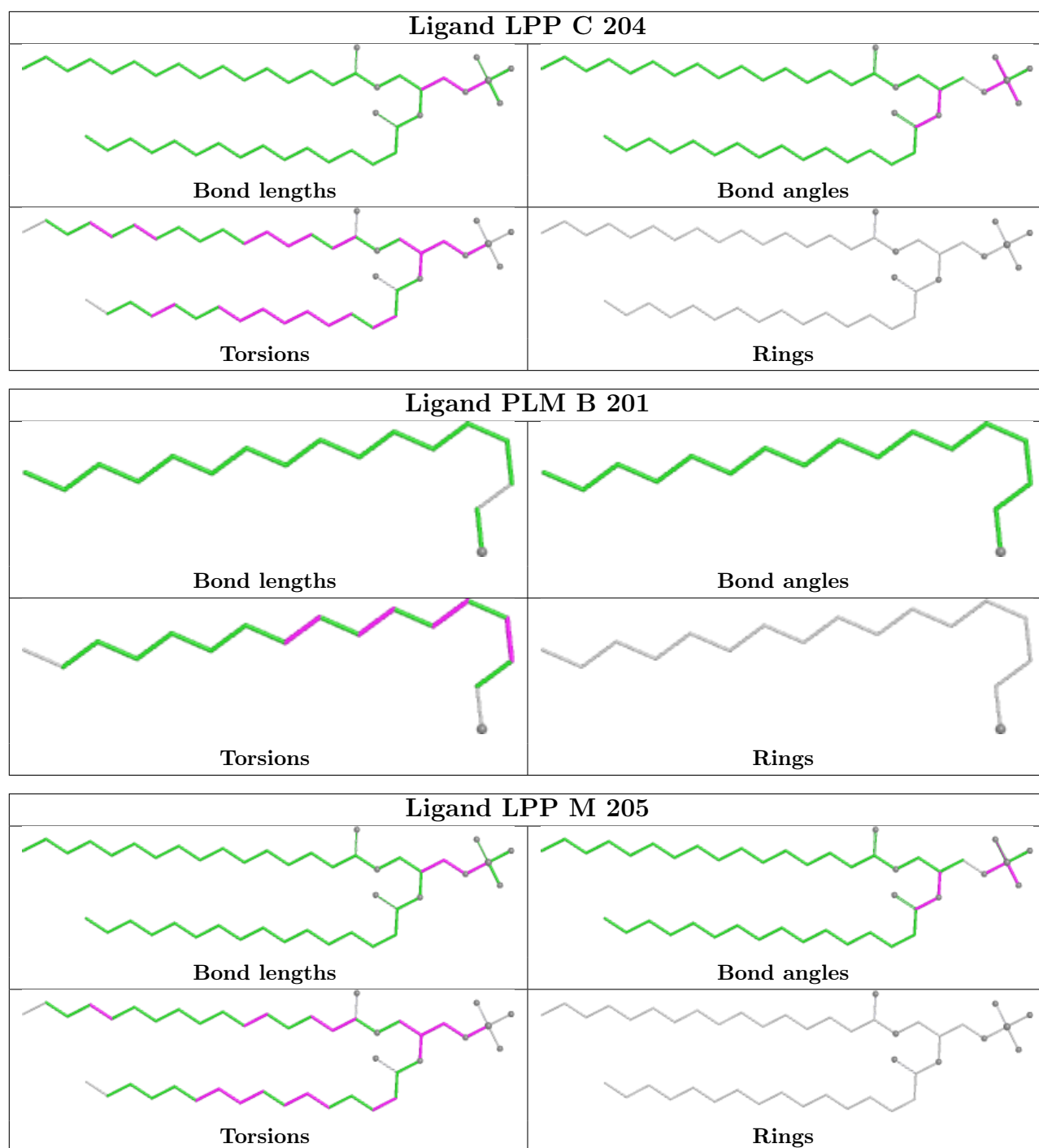


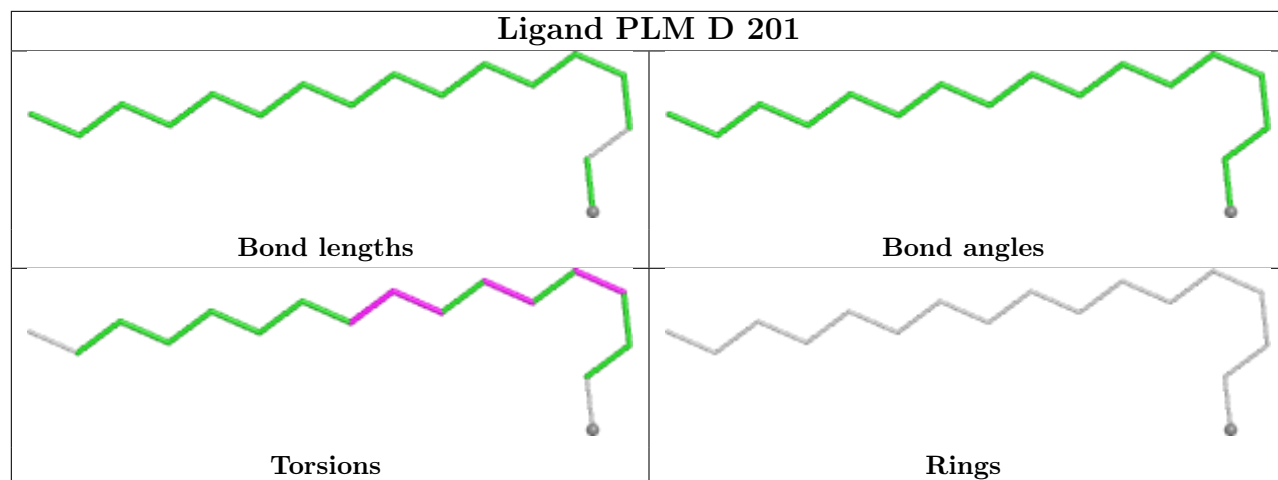


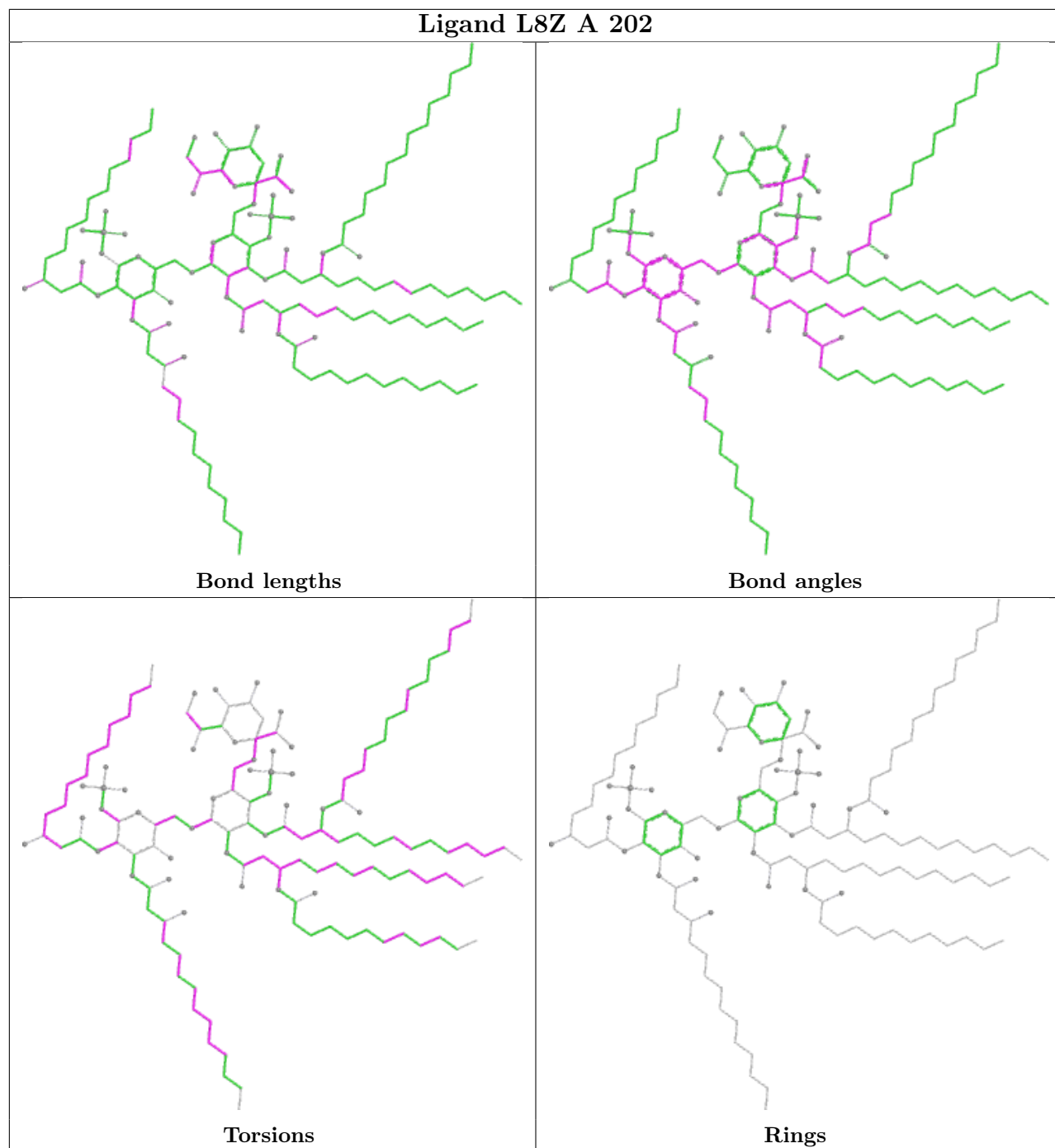


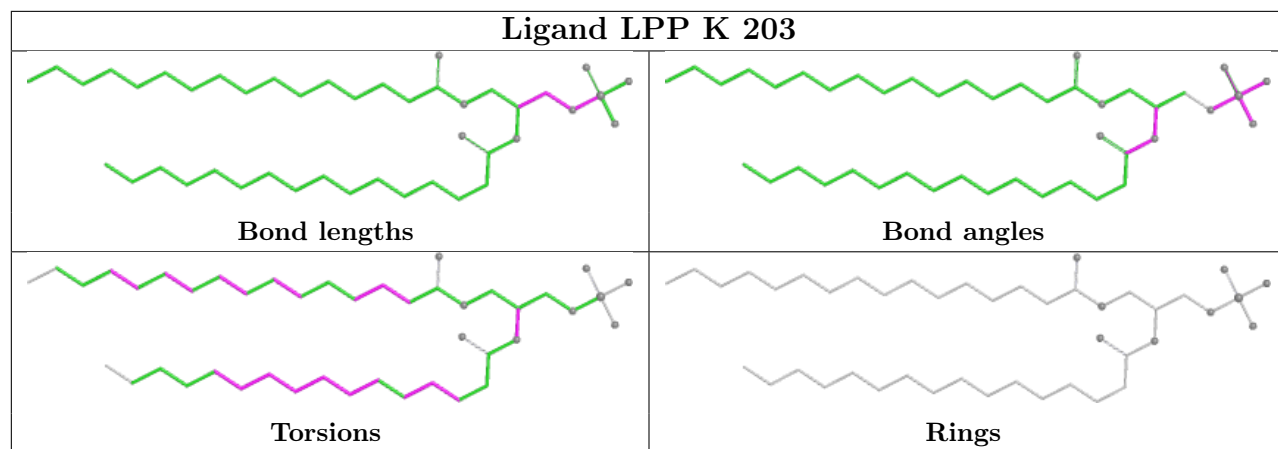


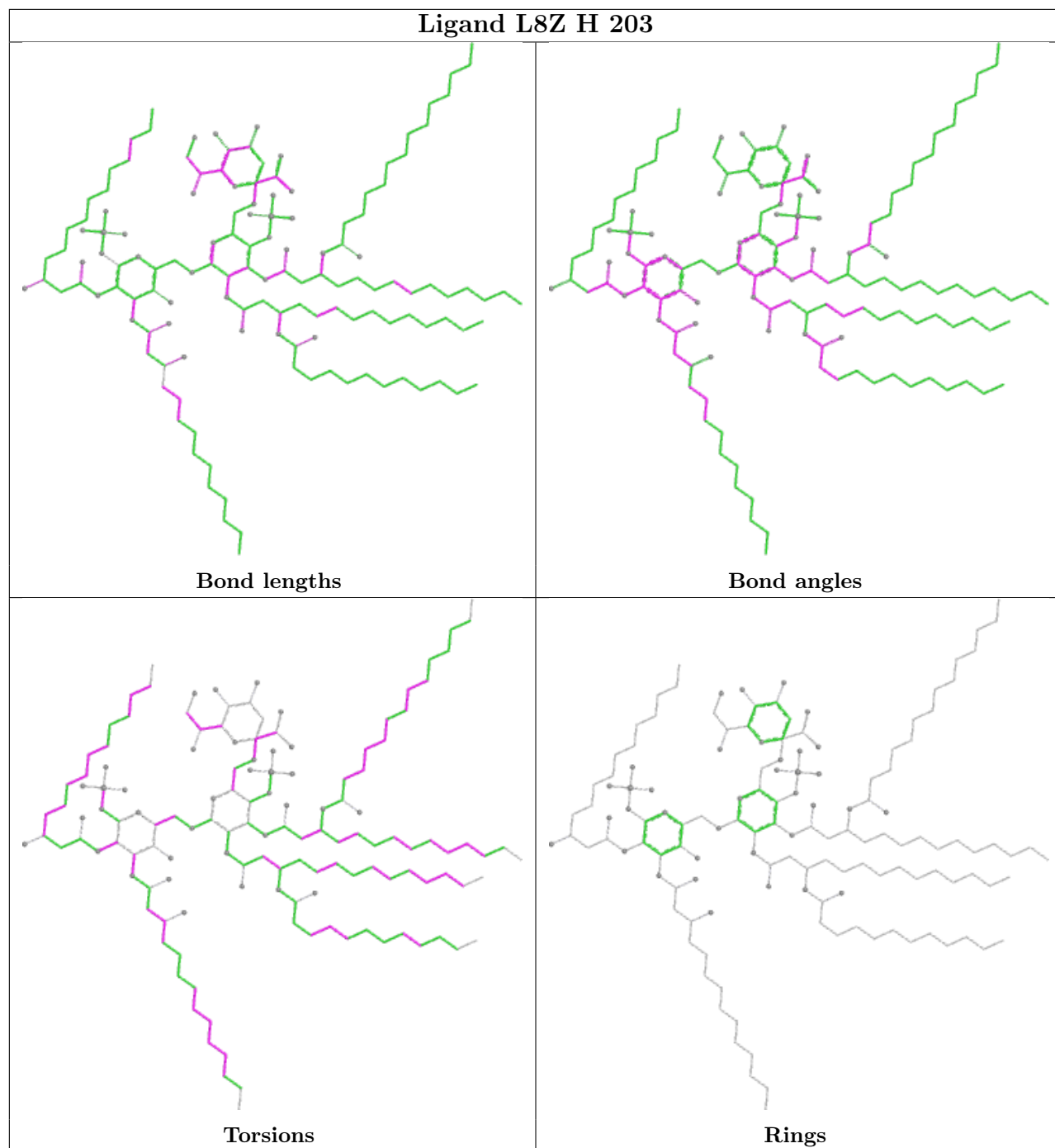


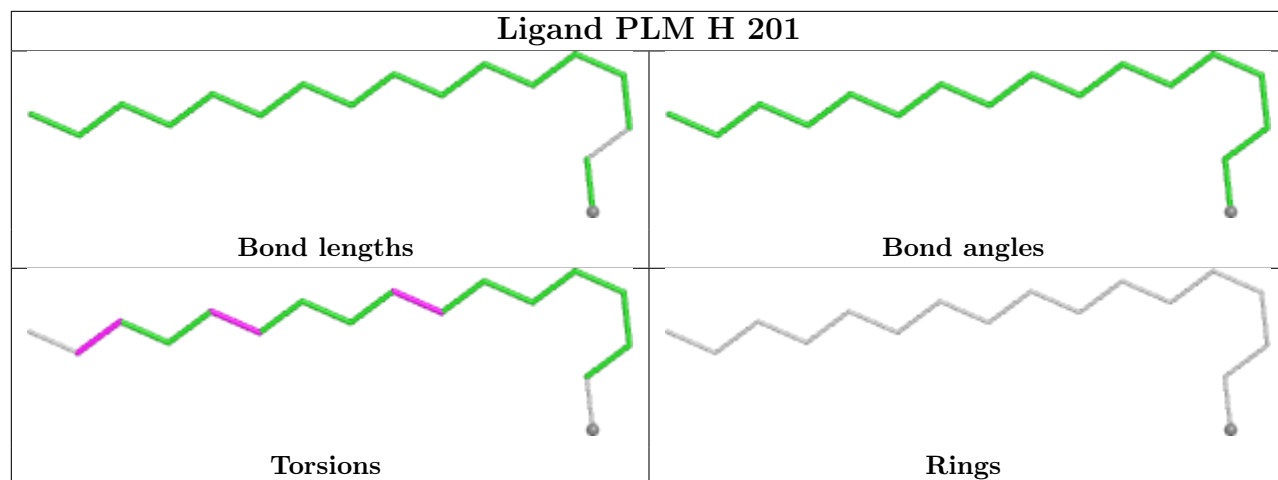


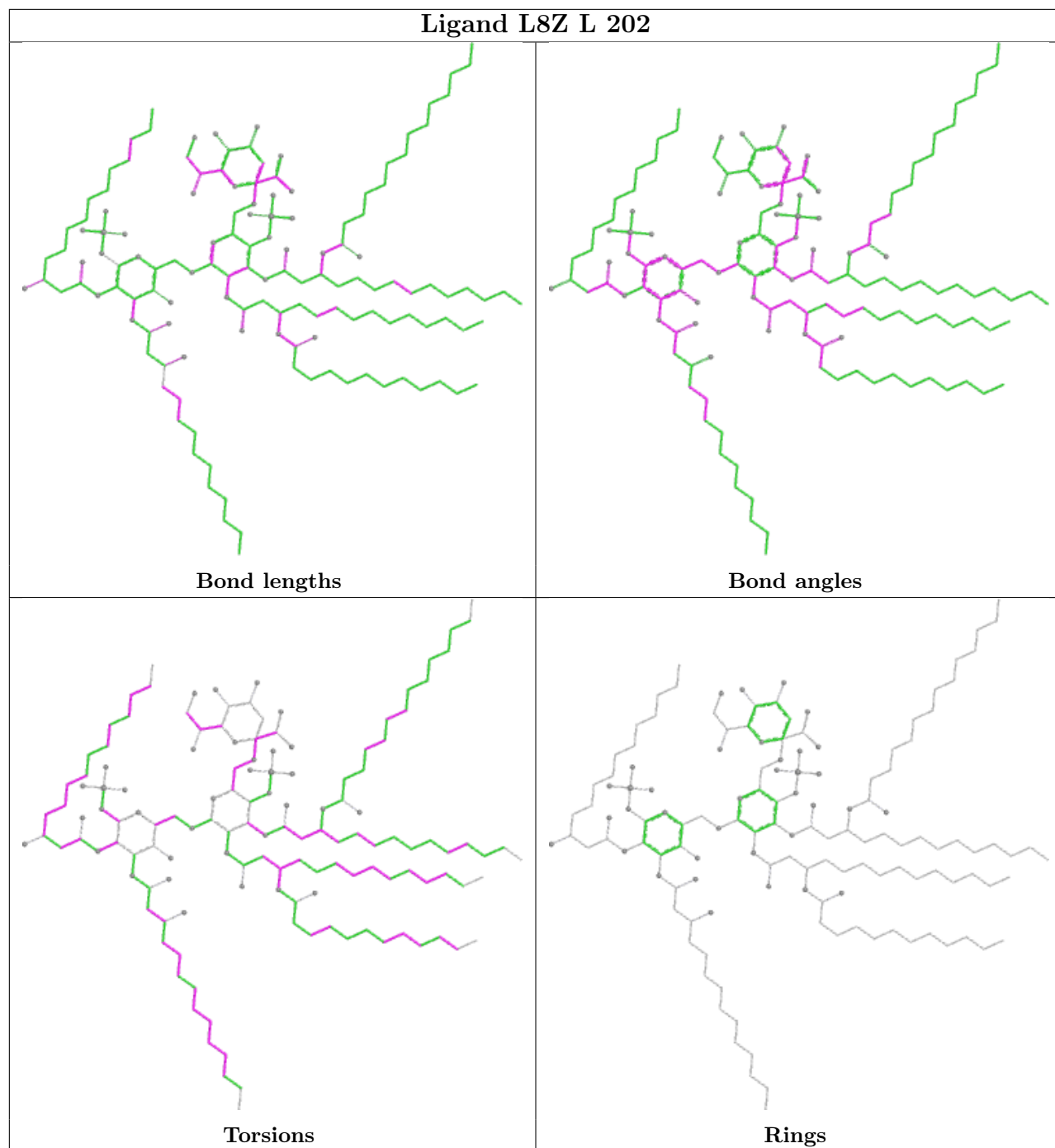


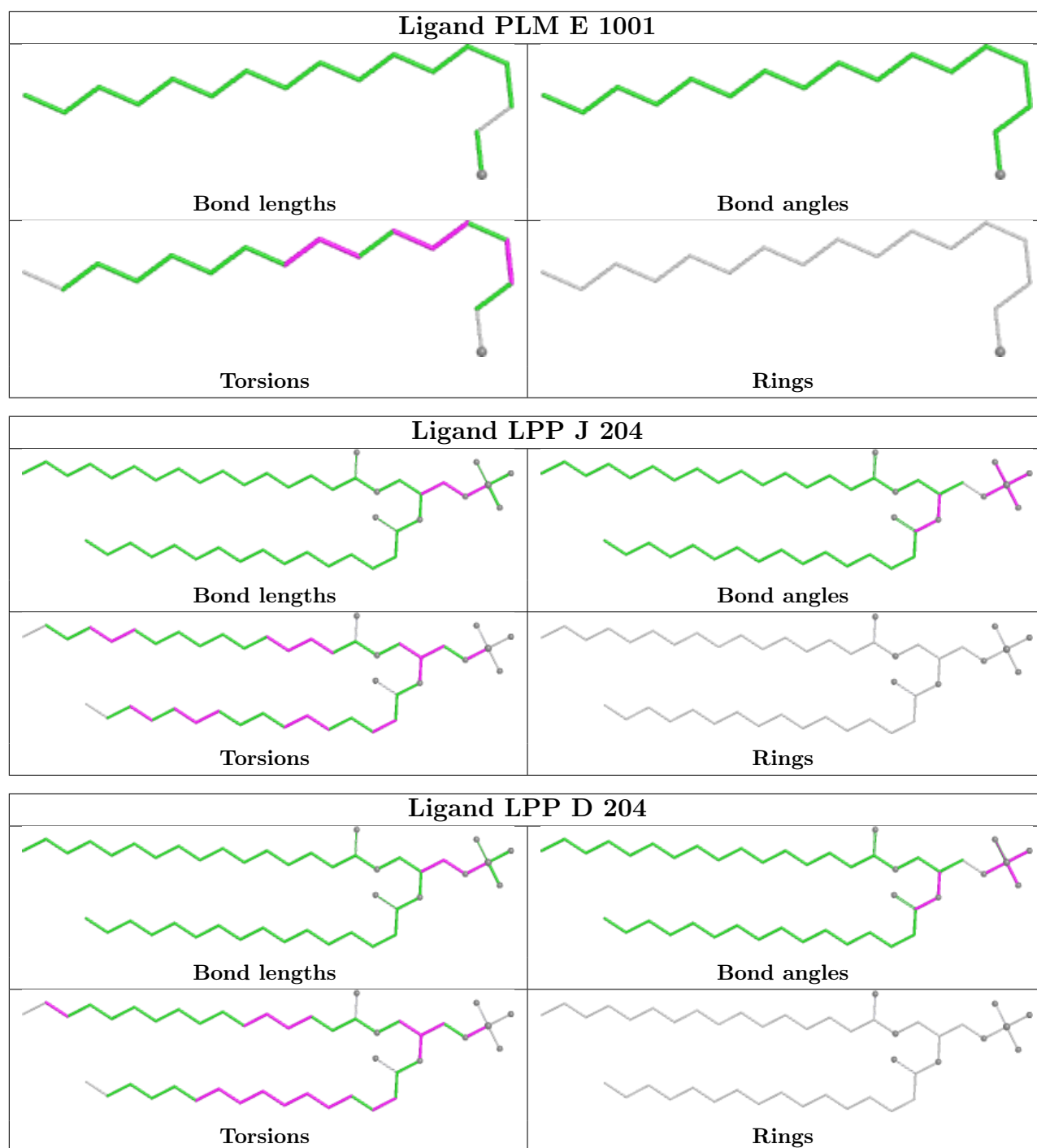












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.