



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 05:23 PM JST

PDB ID : 7YML / pdb_00007yml
EMDB ID : EMD-33931
Title : Structure of photosynthetic LH1-RC super-complex of Rhodobacter capsulatus
Authors : Tani, K.; Kanno, R.; Ji, X.-C.; Satoh, I.; Kobayashi, Y.; Nagashima, K.V.P.; Hall, M.; Yu, L.-J.; Kimura, Y.; Mizoguchi, A.; Humbel, B.M.; Madigan, M.T.; Wang-Otomo, Z.-Y.
Deposited on : 2022-07-28
Resolution : 2.60 Å (reported)
Based on initial model : 7F0L

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

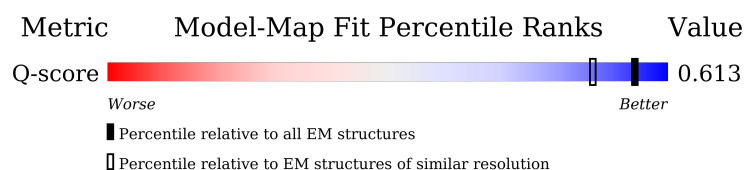
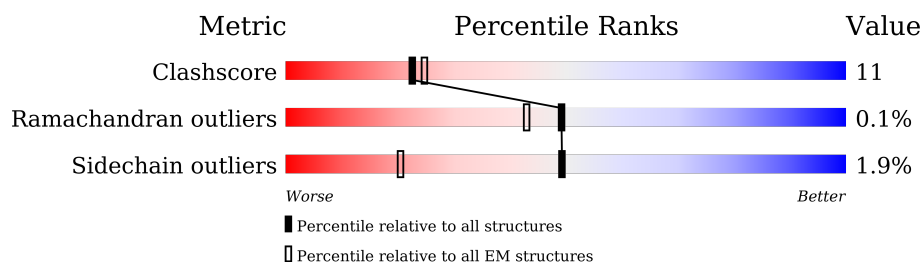
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	282	
2	M	307	
3	H	253	
4	A	58	

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Mol	Chain	Length	Quality of chain
4	D	58	
4	F	58	
4	I	58	
4	K	58	
4	O	58	
4	Q	58	
4	S	58	
4	V	58	
4	Y	58	
5	B	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	W	49	
5	Z	49	
6	X	78	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 18554 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	1	0
			2239	1501	356	365	17		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	304	Total	C	N	O	S	0	0
			2417	1608	392	404	13		

- Molecule 3 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	248	Total	C	N	O	S	0	0
			1956	1246	329	371	10		

- Molecule 4 is a protein called Light-harvesting protein B-870 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	44	Total	C	N	O	S	0	0
			374	262	58	53	1		
4	D	56	Total	C	N	O	S	0	0
			457	315	73	68	1		
4	F	54	Total	C	N	O	S	0	0
			447	309	71	66	1		
4	I	56	Total	C	N	O	S	0	0
			457	315	73	68	1		
4	K	55	Total	C	N	O	S	0	0
			452	312	72	67	1		
4	O	56	Total	C	N	O	S	0	0
			453	312	72	68	1		
4	Q	56	Total	C	N	O	S	0	0
			457	315	73	68	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	S	56	Total	C	N	O	1	0
			462	318	76	68		
4	V	56	Total	C	N	O	0	0
			457	315	73	68		
4	Y	42	Total	C	N	O	0	0
			335	228	56	51		

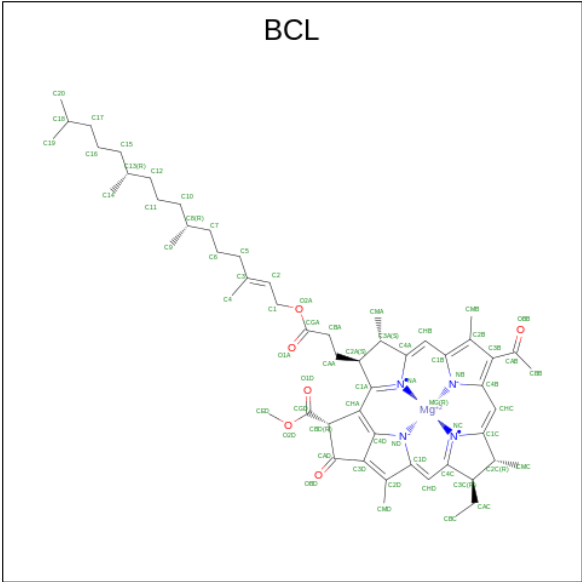
- Molecule 5 is a protein called Light-harvesting protein B-870 beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	44	Total	C	N	O	0	0
			346	229	55	60		
5	E	44	Total	C	N	O	0	0
			346	229	55	60		
5	G	43	Total	C	N	O	0	0
			338	225	54	57		
5	J	44	Total	C	N	O	0	0
			346	229	55	60		
5	N	43	Total	C	N	O	0	0
			338	225	54	57		
5	P	43	Total	C	N	O	0	0
			338	225	54	57		
5	R	43	Total	C	N	O	0	0
			334	223	54	55		
5	T	43	Total	C	N	O	0	0
			338	225	54	57		
5	W	41	Total	C	N	O	0	0
			309	204	52	51		
5	Z	31	Total	C	N	O	0	0
			224	150	36	36		

- Molecule 6 is a protein called Photosynthetic reaction center PufX protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	X	65	Total	C	N	O	0	0
			502	333	79	86		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



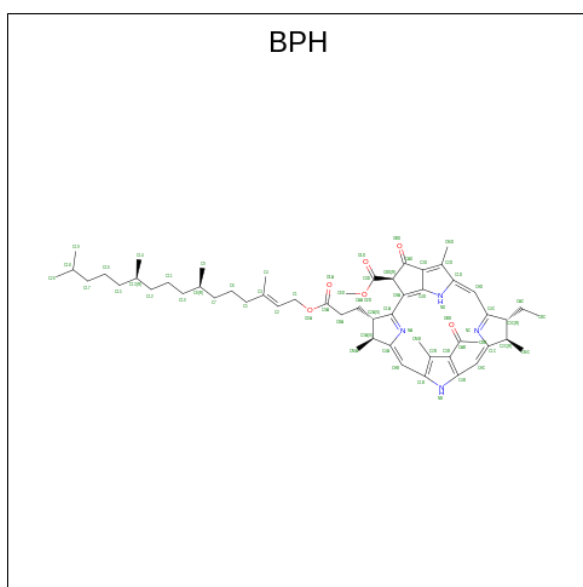
Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 61	C 50	Mg 1	N 4	O 6	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0

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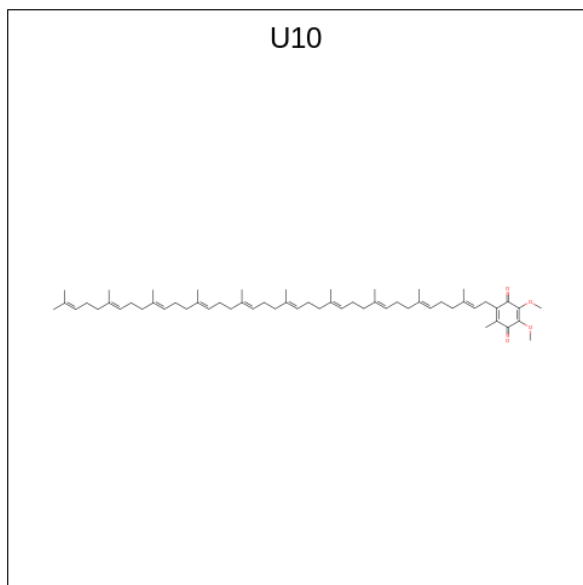
Mol	Chain	Residues	Atoms					AltConf
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



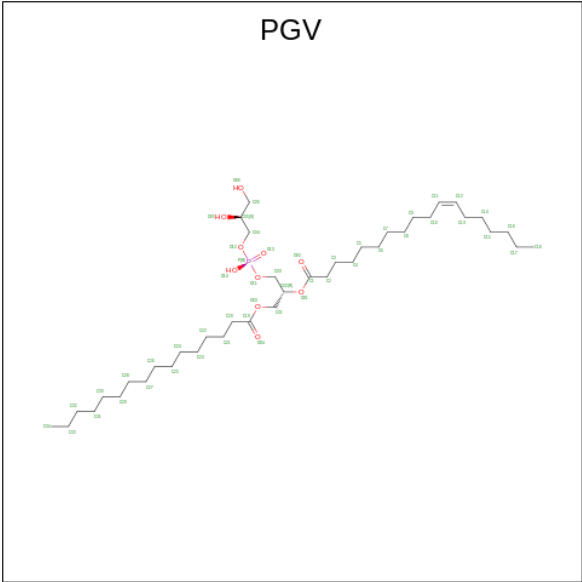
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	N	O	0
			65	55	4	6	
8	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



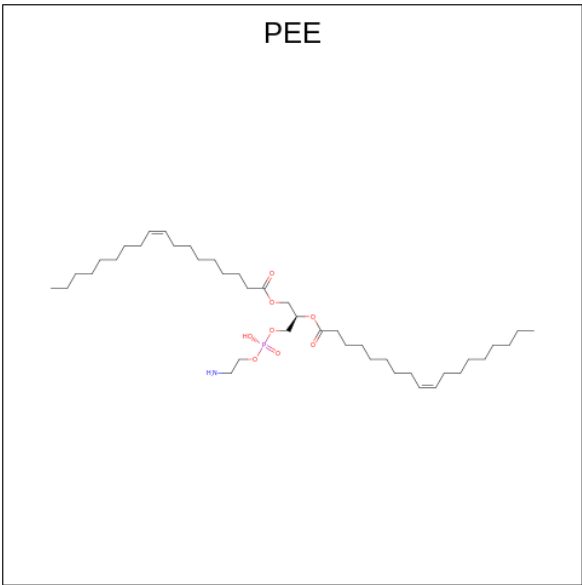
Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			48	44	4	
9	L	1	Total	C	O	0
			63	59	4	
9	M	1	Total	C	O	0
			20	16	4	
9	M	1	Total	C	O	0
			48	44	4	

- Molecule 10 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



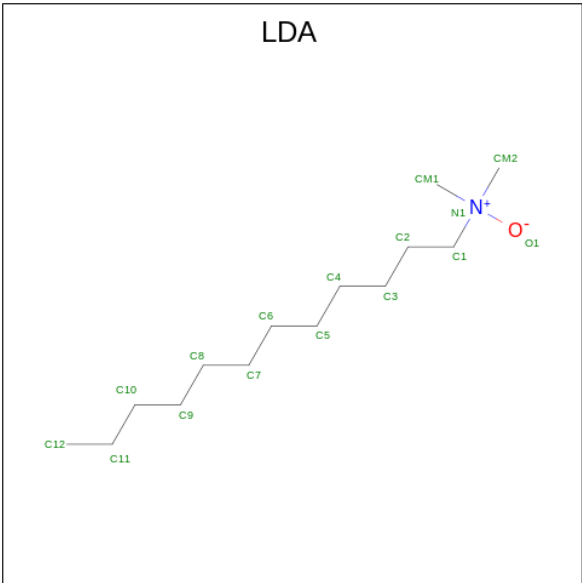
Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	O	P	0
			39	28	10	1	
10	M	1	Total	C	O	P	0
			36	25	10	1	
10	M	1	Total	C	O	P	0
			45	34	10	1	
10	M	1	Total	C	O	P	0
			35	24	10	1	
10	M	1	Total	C	O	P	0
			38	27	10	1	
10	H	1	Total	C	O	P	0
			43	32	10	1	
10	H	1	Total	C	O	P	0
			34	23	10	1	
10	Q	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



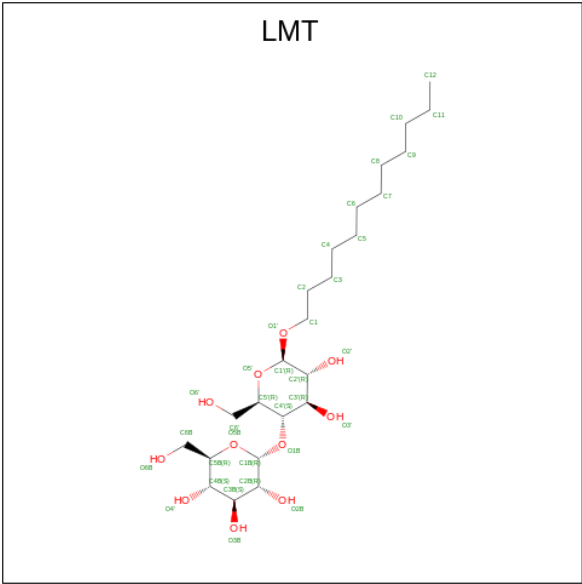
Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	

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Mol	Chain	Residues	Atoms				AltConf
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	H	1	Total	C	N	O	0
			16	14	1	1	
12	H	1	Total	C	N	O	0
			14	12	1	1	
12	D	1	Total	C	N	O	0
			16	14	1	1	
12	O	1	Total	C	N	O	0
			16	14	1	1	
12	Q	1	Total	C	N	O	0
			9	7	1	1	
12	Q	1	Total	C	N	O	0
			12	10	1	1	

- Molecule 13 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			35	24	11	
13	L	1	Total	C	O	0
			34	23	11	

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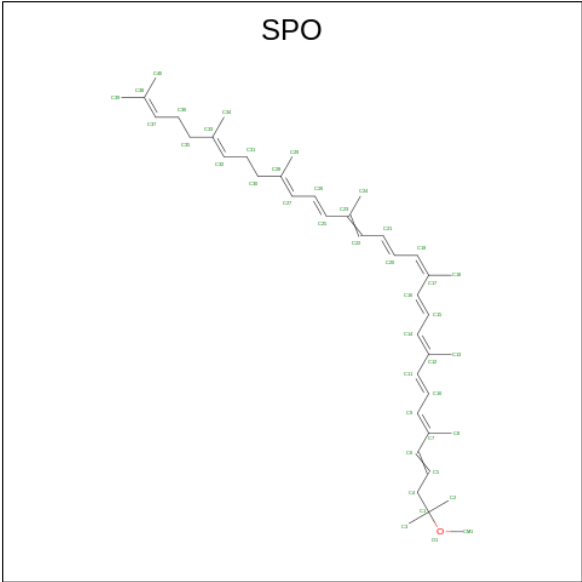
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Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			35	24	11	
13	M	1	Total	C	O	0
			24	13	11	
13	M	1	Total	C	O	0
			35	24	11	
13	M	1	Total	C	O	0
			35	24	11	
13	M	1	Total	C	O	0
			32	21	11	
13	M	1	Total	C	O	0
			33	22	11	
13	A	1	Total	C	O	0
			32	21	11	
13	I	1	Total	C	O	0
			35	24	11	
13	K	1	Total	C	O	0
			35	24	11	
13	Q	1	Total	C	O	0
			35	24	11	
13	S	1	Total	C	O	0
			26	15	11	
13	S	1	Total	C	O	0
			33	22	11	
13	Y	1	Total	C	O	0
			28	17	11	
13	Y	1	Total	C	O	0
			27	16	11	
13	X	1	Total	C	O	0
			35	24	11	
13	X	1	Total	C	O	0
			35	24	11	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total	Fe	0
			1	1	

- Molecule 15 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



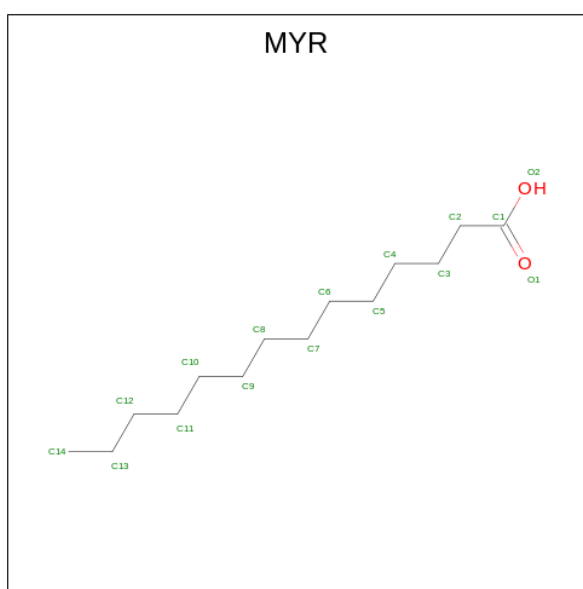
Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	E	1	Total	C	O	0
			42	41	1	
15	F	1	Total	C	O	0
			42	41	1	
15	G	1	Total	C	O	0
			42	41	1	
15	I	1	Total	C	O	0
			42	41	1	
15	I	1	Total	C	O	0
			42	41	1	
15	N	1	Total	C	O	0
			42	41	1	
15	O	1	Total	C	O	0
			42	41	1	
15	O	1	Total	C	O	0
			42	41	1	
15	P	1	Total	C	O	0
			42	41	1	
15	R	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
15	S	1	Total	C	O	0
			42	41	1	
15	S	1	Total	C	O	0
			42	41	1	
15	T	1	Total	C	O	0
			42	41	1	
15	W	1	Total	C	O	0
			42	41	1	

- Molecule 16 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
16	F	1	Total	C	O	0
			16	14	2	

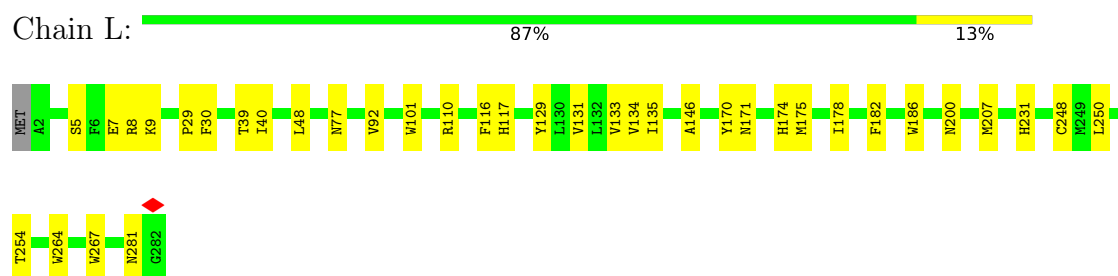
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	L	4	Total	O	0
			4	4	
17	M	3	Total	O	0
			3	3	

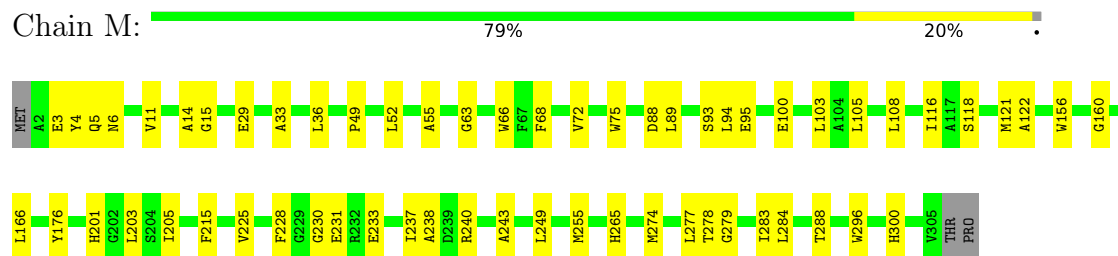
3 Residue-property plots

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

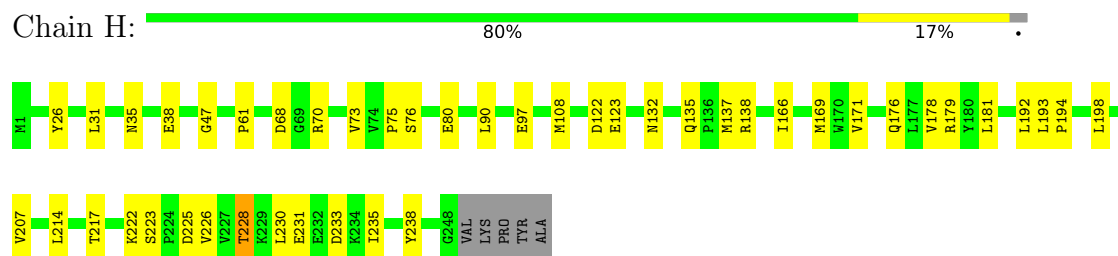
- Molecule 1: Reaction center protein L chain



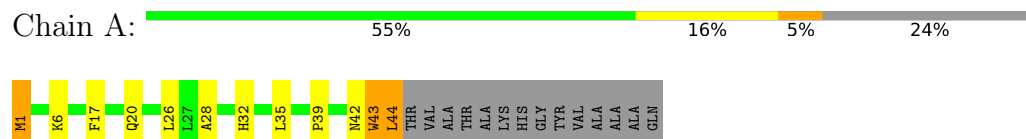
- Molecule 2: Reaction center protein M chain



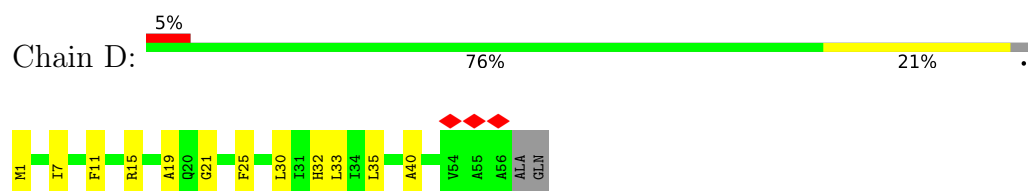
- Molecule 3: Photosynthetic reaction center H subunit



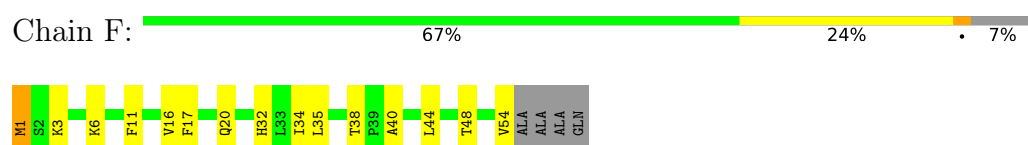
- Molecule 4: Light-harvesting protein B-870 alpha chain



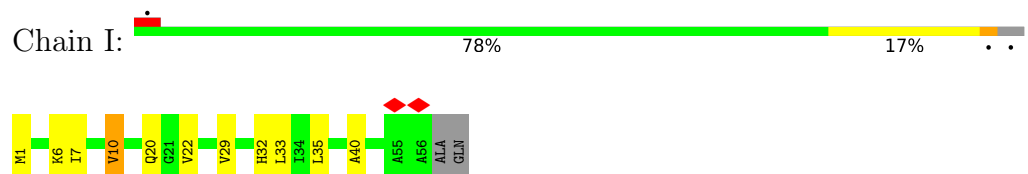
- Molecule 4: Light-harvesting protein B-870 alpha chain



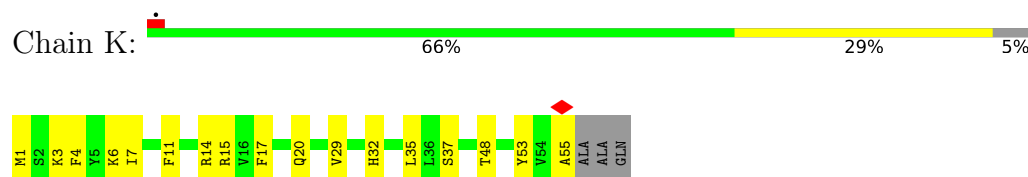
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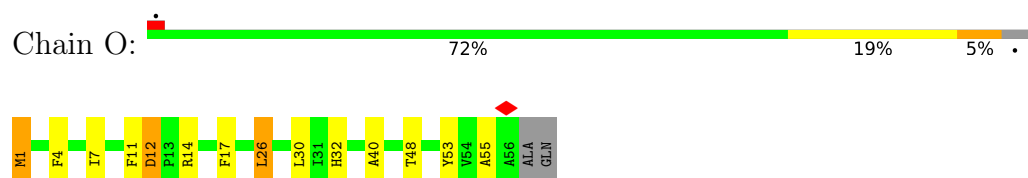
- Molecule 4: Light-harvesting protein B-870 alpha chain



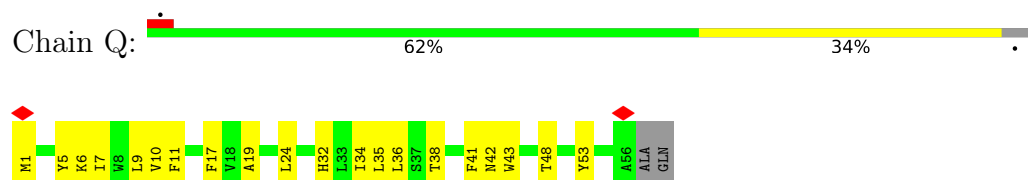
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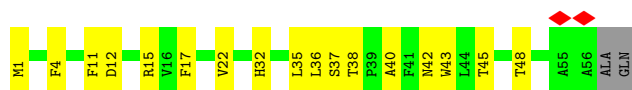


- Molecule 4: Light-harvesting protein B-870 alpha chain

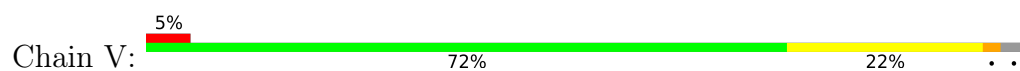


- Molecule 4: Light-harvesting protein B-870 alpha chain





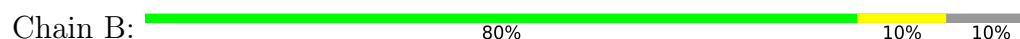
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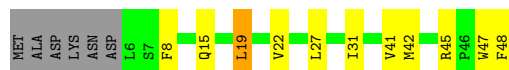
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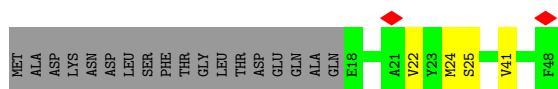
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- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 6: Photosynthetic reaction center PufX protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224431	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.191	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	Depositor
Map size ($\text{\AA}$)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, BCL, SPO, PEE, FME, LMT, U10, PGV, BPH, LDA, FE

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	L	0.28	0/2328	0.29	0/3180
2	M	0.27	0/2507	0.28	0/3425
3	H	0.22	0/2006	0.25	0/2728
4	A	0.25	0/377	0.26	0/514
4	D	0.28	0/462	0.27	0/631
4	F	0.28	0/452	0.25	0/617
4	I	0.26	0/462	0.25	0/631
4	K	0.25	0/457	0.24	0/624
4	O	0.22	0/458	0.21	0/627
4	Q	0.19	0/462	0.21	0/631
4	S	0.18	0/473	0.26	0/645
4	V	0.15	0/462	0.24	0/631
4	Y	0.08	0/345	0.22	0/472
5	B	0.20	0/356	0.22	0/486
5	E	0.23	0/356	0.25	0/486
5	G	0.22	0/348	0.24	0/475
5	J	0.24	0/356	0.22	0/486
5	N	0.22	0/348	0.23	0/475
5	P	0.21	0/348	0.25	0/475
5	R	0.17	0/344	0.21	0/470
5	T	0.17	0/348	0.21	0/475
5	W	0.13	0/318	0.23	0/435
5	Z	0.07	0/229	0.22	0/313
6	X	0.21	0/519	0.25	0/700
All	All	0.24	0/15121	0.26	0/20632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2239	0	2184	33	0
2	M	2417	0	2327	54	0
3	H	1956	0	1923	31	0
4	A	374	0	396	9	0
4	D	457	0	480	13	0
4	F	447	0	470	12	0
4	I	457	0	480	11	0
4	K	452	0	475	17	0
4	O	453	0	469	15	0
4	Q	457	0	480	14	0
4	S	462	0	486	16	0
4	V	457	0	480	13	0
4	Y	335	0	351	12	0
5	B	346	0	337	5	0
5	E	346	0	337	8	0
5	G	338	0	333	12	0
5	J	346	0	337	8	0
5	N	338	0	333	10	0
5	P	338	0	333	9	0
5	R	334	0	329	8	0
5	T	338	0	333	7	0
5	W	309	0	292	8	0
5	Z	224	0	217	3	0
6	X	502	0	488	4	0
7	A	61	0	61	3	0
7	B	66	0	74	4	0
7	D	66	0	74	8	0
7	E	66	0	74	3	0
7	F	132	0	148	8	0
7	G	66	0	74	8	0
7	I	66	0	74	6	0
7	J	66	0	74	6	0
7	K	66	0	74	7	0
7	L	132	0	148	2	0
7	M	132	0	148	8	0
7	N	66	0	74	7	0
7	O	66	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	66	0	74	8	0
7	Q	66	0	74	0	0
7	R	66	0	74	4	0
7	S	66	0	74	5	0
7	T	66	0	74	5	0
7	V	66	0	74	6	0
7	W	66	0	74	6	0
7	Y	66	0	74	3	0
7	Z	66	0	74	3	0
8	L	65	0	76	3	0
8	M	65	0	76	8	0
9	L	111	0	153	10	0
9	M	68	0	82	6	0
10	H	77	0	92	5	0
10	L	39	0	47	5	0
10	M	154	0	188	14	0
10	Q	35	0	40	5	0
11	L	46	0	69	3	0
12	D	16	0	31	3	0
12	H	30	0	55	3	0
12	L	16	0	31	2	0
12	M	64	0	124	5	0
12	O	16	0	31	1	0
12	Q	21	0	34	3	0
13	A	32	0	37	3	0
13	I	35	0	46	3	0
13	K	35	0	46	2	0
13	L	104	0	133	6	0
13	M	159	0	189	15	0
13	Q	35	0	46	2	0
13	S	59	0	64	8	0
13	X	70	0	92	1	0
13	Y	55	0	56	2	0
14	M	1	0	0	0	0
15	D	126	0	180	17	0
15	E	42	0	60	6	0
15	F	42	0	60	5	0
15	G	42	0	60	3	0
15	I	84	0	120	13	0
15	M	42	0	60	6	0
15	N	42	0	60	6	0
15	O	84	0	120	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	42	0	60	5	0
15	R	42	0	60	6	0
15	S	84	0	120	14	0
15	T	42	0	60	3	0
15	W	42	0	60	8	0
16	F	16	0	27	2	0
17	L	4	0	0	0	0
17	M	3	0	0	0	0
All	All	18554	0	19452	429	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 11.

The worst 5 of 429 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:D:11:PHE:HZ	4:F:17:PHE:HD2	1.21	0.85
4:F:1:FME:HCN	4:F:3:LYS:H	1.41	0.84
4:D:25:PHE:HB2	7:D:102:BCL:H43	1.61	0.81
4:O:40:ALA:O	5:P:45:ARG:NH1	2.18	0.77
10:L:305:PGV:H51	10:L:305:PGV:H232	1.67	0.76

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	L	280/282 (99%)	274 (98%)	6 (2%)	0	100	100
2	M	302/307 (98%)	293 (97%)	9 (3%)	0	100	100
3	H	246/253 (97%)	240 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
4	D	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	F	52/58 (90%)	52 (100%)	0	0	100	100
4	I	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	K	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	O	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	Q	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
4	S	55/58 (95%)	51 (93%)	4 (7%)	0	100	100
4	V	54/58 (93%)	51 (94%)	2 (4%)	1 (2%)	6	13
4	Y	40/58 (69%)	40 (100%)	0	0	100	100
5	B	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	E	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	G	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	J	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	41/49 (84%)	41 (100%)	0	0	100	100
5	W	39/49 (80%)	38 (97%)	1 (3%)	0	100	100
5	Z	29/49 (59%)	29 (100%)	0	0	100	100
6	X	63/78 (81%)	60 (95%)	3 (5%)	0	100	100
All	All	1802/1990 (91%)	1753 (97%)	48 (3%)	1 (0%)	49	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	V	2	SER

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	L	227/227 (100%)	226 (100%)	1 (0%)	84	93
2	M	236/239 (99%)	234 (99%)	2 (1%)	73	88
3	H	213/217 (98%)	211 (99%)	2 (1%)	70	87
4	A	39/47 (83%)	36 (92%)	3 (8%)	12	27
4	D	46/47 (98%)	45 (98%)	1 (2%)	45	72
4	F	46/47 (98%)	45 (98%)	1 (2%)	45	72
4	I	46/47 (98%)	45 (98%)	1 (2%)	45	72
4	K	46/47 (98%)	46 (100%)	0	100	100
4	O	45/47 (96%)	43 (96%)	2 (4%)	25	50
4	Q	46/47 (98%)	45 (98%)	1 (2%)	45	72
4	S	47/47 (100%)	47 (100%)	0	100	100
4	V	46/47 (98%)	44 (96%)	2 (4%)	26	51
4	Y	35/47 (74%)	33 (94%)	2 (6%)	18	40
5	B	35/39 (90%)	34 (97%)	1 (3%)	37	65
5	E	35/39 (90%)	34 (97%)	1 (3%)	37	65
5	G	34/39 (87%)	33 (97%)	1 (3%)	37	65
5	J	35/39 (90%)	33 (94%)	2 (6%)	18	40
5	N	34/39 (87%)	34 (100%)	0	100	100
5	P	34/39 (87%)	33 (97%)	1 (3%)	37	65
5	R	33/39 (85%)	31 (94%)	2 (6%)	17	37
5	T	34/39 (87%)	34 (100%)	0	100	100
5	W	28/39 (72%)	28 (100%)	0	100	100
5	Z	20/39 (51%)	20 (100%)	0	100	100
6	X	50/62 (81%)	48 (96%)	2 (4%)	28	55
All	All	1490/1605 (93%)	1462 (98%)	28 (2%)	49	75

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	6	LEU
6	X	53	MET
4	O	26	LEU
4	Y	31	ILE

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Mol	Chain	Res	Type
4	O	12	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
5	N	15	GLN
5	W	17	GLN
4	V	20	GLN
3	H	135	GLN
5	J	17	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	FME	V	1	4	8,9,10	0.55	0	7,9,11	0.93	1 (14%)
4	FME	F	1	4	8,9,10	0.49	0	7,9,11	1.18	1 (14%)
4	FME	K	1	4	8,9,10	0.53	0	7,9,11	0.97	1 (14%)
4	FME	O	1	4	8,9,10	0.51	0	7,9,11	1.06	1 (14%)
4	FME	I	1	4	8,9,10	0.52	0	7,9,11	0.95	1 (14%)
4	FME	Q	1	4	8,9,10	0.53	0	7,9,11	0.96	1 (14%)
4	FME	S	1	4	5,6,10	0.82	0	3,6,11	0.75	0
4	FME	A	1	4	8,9,10	0.52	0	7,9,11	0.92	1 (14%)
4	FME	D	1	4	8,9,10	0.51	0	7,9,11	1.02	1 (14%)

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	FME	V	1	4	-	1/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	K	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	S	1	4	-	1/2/5/11	-
4	FME	A	1	4	-	1/7/9/11	-
4	FME	D	1	4	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1	FME	O-C-CA	-2.59	118.00	124.78
4	F	1	FME	O-C-CA	-2.53	118.16	124.78
4	D	1	FME	O-C-CA	-2.52	118.18	124.78
4	I	1	FME	O-C-CA	-2.45	118.35	124.78
4	V	1	FME	O-C-CA	-2.43	118.42	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	F	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA
4	S	1	FME	O1-CN-N-CA
4	I	1	FME	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	V	1	FME	1	0
4	F	1	FME	1	0
4	O	1	FME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	FME	1	0
4	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 1 is monoatomic - leaving 88 for Mogul analysis.

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$
7	BCL	F	101	16	69,74,74	1.85	17 (24%)	83,115,115	2.46	22 (26%)
12	LDA	M	419	-	12,15,15	2.09	1 (8%)	14,17,17	0.46	0
15	SPO	D	105	-	40,41,41	0.67	0	47,50,50	1.75	13 (27%)
15	SPO	N	101	-	40,41,41	0.67	0	47,50,50	1.95	16 (34%)
7	BCL	F	103	4	69,74,74	1.79	19 (27%)	83,115,115	2.59	24 (28%)
12	LDA	Q	104	-	8,11,15	2.54	1 (12%)	10,13,17	0.44	0
7	BCL	A	101	4	64,69,74	1.91	17 (26%)	77,109,115	2.53	24 (31%)
13	LMT	M	410	-	36,36,36	0.36	0	47,47,47	0.86	2 (4%)
13	LMT	A	102	-	33,33,36	0.47	0	44,44,47	0.97	2 (4%)
9	U10	L	303	-	48,48,63	0.70	2 (4%)	58,61,79	0.60	0
7	BCL	R	102	5	69,74,74	1.80	19 (27%)	83,115,115	2.45	24 (28%)
7	BCL	E	102	5	69,74,74	1.80	19 (27%)	83,115,115	2.47	25 (30%)
7	BCL	T	102	5	69,74,74	1.82	18 (26%)	83,115,115	2.45	22 (26%)
15	SPO	G	102	-	40,41,41	0.67	0	47,50,50	1.99	14 (29%)
15	SPO	O	104	-	40,41,41	0.67	0	47,50,50	1.87	15 (31%)
7	BCL	W	102	5	69,74,74	1.83	17 (24%)	83,115,115	2.39	23 (27%)
8	BPH	L	302	-	59,70,70	0.82	4 (6%)	61,101,101	0.97	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LMT	K	101	-	36,36,36	0.40	0	47,47,47	0.84	1 (2%)
12	LDA	Q	102	-	5,8,15	3.23	1 (20%)	7,10,17	0.33	0
7	BCL	N	102	5	69,74,74	1.79	18 (26%)	83,115,115	2.45	24 (28%)
7	BCL	P	102	5	69,74,74	1.78	18 (26%)	83,115,115	2.45	25 (30%)
7	BCL	Q	105	4	69,74,74	1.79	19 (27%)	83,115,115	2.61	26 (31%)
13	LMT	L	308	-	36,36,36	0.35	0	47,47,47	0.72	0
10	PGV	H	303	-	42,42,50	0.98	2 (4%)	44,48,56	1.15	4 (9%)
15	SPO	R	101	-	40,41,41	0.68	0	47,50,50	3.72	16 (34%)
10	PGV	M	415	-	37,37,50	1.06	2 (5%)	40,43,56	1.12	3 (7%)
12	LDA	H	302	-	10,13,15	2.28	1 (10%)	12,15,17	0.47	0
7	BCL	J	101	5	69,74,74	1.80	19 (27%)	83,115,115	2.41	26 (31%)
13	LMT	S	101	-	27,27,36	0.44	0	37,38,47	0.86	2 (5%)
7	BCL	B	101	5	69,74,74	1.81	20 (28%)	83,115,115	2.45	25 (30%)
15	SPO	W	101	-	40,41,41	0.65	0	47,50,50	1.77	12 (25%)
7	BCL	D	102	4	69,74,74	1.80	19 (27%)	83,115,115	2.63	27 (32%)
7	BCL	K	102	4	69,74,74	1.79	19 (27%)	83,115,115	2.62	27 (32%)
7	BCL	L	301	1	69,74,74	1.79	19 (27%)	83,115,115	2.56	26 (31%)
9	U10	L	304	-	63,63,63	0.64	2 (3%)	76,79,79	0.58	0
13	LMT	S	102	-	34,34,36	0.37	0	45,45,47	0.72	1 (2%)
10	PGV	L	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.11	2 (4%)
10	PGV	M	414	-	34,34,50	1.09	2 (5%)	37,40,56	1.15	3 (8%)
11	PEE	L	306	-	45,45,50	0.77	2 (4%)	48,50,55	0.54	0
12	LDA	D	104	-	12,15,15	2.06	1 (8%)	14,17,17	0.61	0
15	SPO	O	103	-	40,41,41	0.63	0	47,50,50	1.62	10 (21%)
10	PGV	Q	103	-	34,34,50	1.11	2 (5%)	37,40,56	1.14	3 (8%)
15	SPO	D	101	-	40,41,41	0.64	0	47,50,50	1.58	11 (23%)
13	LMT	Y	103	-	28,28,36	0.45	0	39,39,47	0.75	1 (2%)
10	PGV	M	402	-	35,35,50	1.07	2 (5%)	38,41,56	1.14	3 (7%)
15	SPO	M	408	-	40,41,41	0.64	0	47,50,50	1.75	12 (25%)
15	SPO	P	101	-	40,41,41	0.65	0	47,50,50	1.81	14 (29%)
13	LMT	L	309	-	35,35,36	0.39	0	46,46,47	0.72	1 (2%)
13	LMT	M	409	-	25,25,36	0.48	0	36,36,47	0.99	1 (2%)
16	MYR	F	102	7	15,15,15	0.56	0	15,15,15	0.54	0
13	LMT	X	102	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
15	SPO	S	105	-	40,41,41	0.62	0	47,50,50	1.83	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	M	404	2	69,74,74	1.81	20 (28%)	83,115,115	2.60	26 (31%)
15	SPO	T	101	-	40,41,41	0.63	0	47,50,50	1.75	12 (25%)
9	U10	M	407	-	48,48,63	0.73	2 (4%)	58,61,79	0.60	1 (1%)
12	LDA	L	307	-	12,15,15	2.09	1 (8%)	14,17,17	0.49	0
15	SPO	F	104	-	40,41,41	0.65	0	47,50,50	1.98	14 (29%)
13	LMT	M	412	-	33,33,36	0.38	0	44,44,47	0.81	1 (2%)
7	BCL	L	310	1	69,74,74	1.79	18 (26%)	83,115,115	2.43	25 (30%)
7	BCL	Y	102	4	69,74,74	1.85	17 (24%)	83,115,115	2.41	24 (28%)
15	SPO	I	103	-	40,41,41	0.65	0	47,50,50	1.68	12 (25%)
7	BCL	Z	101	5	69,74,74	1.89	17 (24%)	83,115,115	2.40	23 (27%)
13	LMT	M	411	-	36,36,36	0.35	0	47,47,47	0.74	1 (2%)
13	LMT	Q	101	-	36,36,36	0.45	0	47,47,47	0.82	1 (2%)
7	BCL	O	102	4	69,74,74	1.78	19 (27%)	83,115,115	2.63	26 (31%)
15	SPO	D	103	-	40,41,41	0.67	0	47,50,50	1.80	13 (27%)
7	BCL	G	101	5	69,74,74	1.80	19 (27%)	83,115,115	2.40	22 (26%)
7	BCL	I	102	4	69,74,74	1.78	20 (28%)	83,115,115	2.62	27 (32%)
7	BCL	S	103	4	69,74,74	1.80	19 (27%)	83,115,115	2.66	25 (30%)
13	LMT	L	311	-	36,36,36	0.37	0	47,47,47	0.93	1 (2%)
10	PGV	H	304	-	33,33,50	1.10	2 (6%)	36,39,56	1.14	2 (5%)
12	LDA	M	418	-	12,15,15	2.08	1 (8%)	14,17,17	0.53	0
7	BCL	V	101	4	69,74,74	1.79	18 (26%)	83,115,115	2.54	26 (31%)
15	SPO	S	104	-	40,41,41	0.66	0	47,50,50	1.82	14 (29%)
13	LMT	Y	101	-	29,29,36	0.42	0	40,40,47	0.75	1 (2%)
15	SPO	E	101	-	40,41,41	0.66	0	47,50,50	2.08	14 (29%)
13	LMT	I	101	-	36,36,36	0.32	0	47,47,47	1.03	4 (8%)
7	BCL	M	403	2	69,74,74	1.83	18 (26%)	83,115,115	2.40	21 (25%)
9	U10	M	401	-	20,20,63	0.99	2 (10%)	24,27,79	0.82	0
8	BPH	M	405	-	59,70,70	0.77	3 (5%)	61,101,101	0.97	4 (6%)
13	LMT	X	101	-	36,36,36	0.43	0	47,47,47	0.90	2 (4%)
12	LDA	H	301	-	12,15,15	2.11	1 (8%)	14,17,17	0.49	0
15	SPO	I	104	-	40,41,41	0.67	0	47,50,50	1.80	16 (34%)
13	LMT	M	417	-	34,34,36	0.38	0	45,45,47	0.68	1 (2%)
12	LDA	M	416	-	12,15,15	2.09	1 (8%)	14,17,17	0.47	0
12	LDA	M	420	-	12,15,15	2.10	1 (8%)	14,17,17	0.58	0
10	PGV	M	413	-	44,44,50	0.97	2 (4%)	47,50,56	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LDA	O	101	-	12,15,15	2.06	1 (8%)	14,17,17	0.53	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
7	BCL	F	101	16	-	16/41/137/137	-
12	LDA	M	419	-	-	2/13/13/13	-
15	SPO	D	105	-	-	4/47/47/47	-
15	SPO	N	101	-	-	9/47/47/47	-
7	BCL	F	103	4	-	10/41/137/137	-
12	LDA	Q	104	-	-	2/9/9/13	-
7	BCL	A	101	4	-	12/35/131/137	-
13	LMT	M	410	-	-	5/21/61/61	0/2/2/2
13	LMT	A	102	-	-	6/18/58/61	0/2/2/2
9	U10	L	303	-	-	12/45/69/87	0/1/1/1
7	BCL	R	102	5	-	14/41/137/137	-
7	BCL	E	102	5	-	13/41/137/137	-
7	BCL	T	102	5	-	11/41/137/137	-
15	SPO	G	102	-	-	13/47/47/47	-
15	SPO	O	104	-	-	4/47/47/47	-
7	BCL	W	102	5	-	14/41/137/137	-
8	BPH	L	302	-	-	6/37/105/105	0/5/6/6
13	LMT	K	101	-	-	4/21/61/61	0/2/2/2
12	LDA	Q	102	-	-	0/6/6/13	-
7	BCL	N	102	5	-	15/41/137/137	-
7	BCL	P	102	5	-	10/41/137/137	-
7	BCL	Q	105	4	-	15/41/137/137	-
13	LMT	L	308	-	-	1/21/61/61	0/2/2/2
10	PGV	H	303	-	-	10/47/47/55	-
15	SPO	R	101	-	-	9/47/47/47	-
10	PGV	M	415	-	-	9/42/42/55	-
12	LDA	H	302	-	-	2/11/11/13	-
7	BCL	J	101	5	-	14/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	S	101	-	-	6/12/52/61	0/2/2/2
7	BCL	B	101	5	-	11/41/137/137	-
15	SPO	W	101	-	-	3/47/47/47	-
7	BCL	D	102	4	-	14/41/137/137	-
7	BCL	K	102	4	-	10/41/137/137	-
7	BCL	L	301	1	-	8/41/137/137	-
9	U10	L	304	-	-	17/63/87/87	0/1/1/1
13	LMT	S	102	-	-	4/19/59/61	0/2/2/2
10	PGV	L	305	-	-	15/43/43/55	-
10	PGV	M	414	-	-	7/39/39/55	-
11	PEE	L	306	-	-	12/49/49/54	-
12	LDA	D	104	-	-	9/13/13/13	-
15	SPO	O	103	-	-	1/47/47/47	-
10	PGV	Q	103	-	-	11/39/39/55	-
15	SPO	D	101	-	-	6/47/47/47	-
13	LMT	Y	103	-	-	6/13/53/61	0/2/2/2
10	PGV	M	402	-	-	16/40/40/55	-
15	SPO	M	408	-	-	4/47/47/47	-
15	SPO	P	101	-	-	5/47/47/47	-
13	LMT	L	309	-	-	8/20/60/61	0/2/2/2
13	LMT	M	409	-	-	1/10/50/61	0/2/2/2
16	MYR	F	102	7	-	5/13/13/13	-
13	LMT	X	102	-	-	4/21/61/61	0/2/2/2
15	SPO	S	105	-	-	5/47/47/47	-
7	BCL	M	404	2	-	7/41/137/137	-
15	SPO	T	101	-	-	4/47/47/47	-
9	U10	M	407	-	-	5/45/69/87	0/1/1/1
12	LDA	L	307	-	-	2/13/13/13	-
15	SPO	F	104	-	-	10/47/47/47	-
13	LMT	M	412	-	-	1/18/58/61	0/2/2/2
7	BCL	L	310	1	-	8/41/137/137	-
7	BCL	Y	102	4	-	10/41/137/137	-
15	SPO	I	103	-	-	4/47/47/47	-
7	BCL	Z	101	5	-	12/41/137/137	-
13	LMT	M	411	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	Q	101	-	-	8/21/61/61	0/2/2/2
7	BCL	O	102	4	-	11/41/137/137	-
15	SPO	D	103	-	-	6/47/47/47	-
7	BCL	G	101	5	-	15/41/137/137	-
7	BCL	I	102	4	-	9/41/137/137	-
7	BCL	S	103	4	-	8/41/137/137	-
13	LMT	L	311	-	-	6/21/61/61	0/2/2/2
10	PGV	H	304	-	-	18/38/38/55	-
12	LDA	M	418	-	-	2/13/13/13	-
7	BCL	V	101	4	-	12/41/137/137	-
15	SPO	S	104	-	-	4/47/47/47	-
13	LMT	Y	101	-	-	3/14/54/61	0/2/2/2
15	SPO	E	101	-	-	14/47/47/47	-
13	LMT	I	101	-	-	6/21/61/61	0/2/2/2
7	BCL	M	403	2	-	17/41/137/137	-
9	U10	M	401	-	-	4/12/36/87	0/1/1/1
8	BPH	M	405	-	-	5/37/105/105	0/5/6/6
13	LMT	X	101	-	-	6/21/61/61	0/2/2/2
12	LDA	H	301	-	-	7/13/13/13	-
15	SPO	I	104	-	-	4/47/47/47	-
13	LMT	M	417	-	-	7/19/59/61	0/2/2/2
12	LDA	M	416	-	-	1/13/13/13	-
12	LDA	M	420	-	-	3/13/13/13	-
10	PGV	M	413	-	-	15/49/49/55	-
12	LDA	O	101	-	-	2/13/13/13	-

The worst 5 of 506 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	301	LDA	O1-N1	-7.29	1.25	1.42
12	M	420	LDA	O1-N1	-7.24	1.25	1.42
12	M	419	LDA	O1-N1	-7.22	1.25	1.42
12	Q	102	LDA	O1-N1	-7.21	1.25	1.42
12	M	416	LDA	O1-N1	-7.20	1.25	1.42

The worst 5 of 909 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	101	SPO	C2-C1-C4	-15.71	86.74	110.86
15	R	101	SPO	C3-C1-C4	-14.76	88.19	110.86
7	S	103	BCL	C2B-C1B-NB	10.92	117.55	110.23
7	F	103	BCL	C2B-C1B-NB	10.86	117.51	110.23
7	O	102	BCL	C2B-C1B-NB	10.80	117.47	110.23

There are no chirality outliers.

5 of 688 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	403	BCL	C1A-C2A-CAA-CBA
7	M	403	BCL	C3A-C2A-CAA-CBA
7	A	101	BCL	C2C-C3C-CAC-CBC
7	A	101	BCL	C4C-C3C-CAC-CBC
7	D	102	BCL	C1A-C2A-CAA-CBA

There are no ring outliers.

82 monomers are involved in 286 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	101	BCL	7	0
12	M	419	LDA	2	0
15	D	105	SPO	7	0
15	N	101	SPO	6	0
7	F	103	BCL	1	0
12	Q	104	LDA	2	0
7	A	101	BCL	3	0
13	M	410	LMT	3	0
13	A	102	LMT	3	0
9	L	303	U10	3	0
7	R	102	BCL	4	0
7	E	102	BCL	3	0
7	T	102	BCL	5	0
15	G	102	SPO	3	0
15	O	104	SPO	10	0
7	W	102	BCL	6	0
8	L	302	BPH	3	0
13	K	101	LMT	2	0
12	Q	102	LDA	1	0
7	N	102	BCL	7	0
7	P	102	BCL	8	0
13	L	308	LMT	2	0

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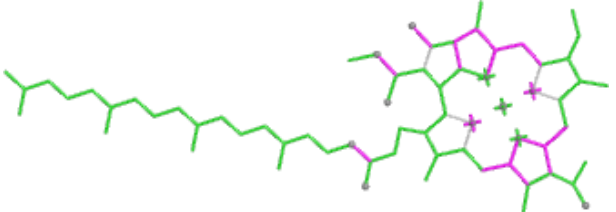
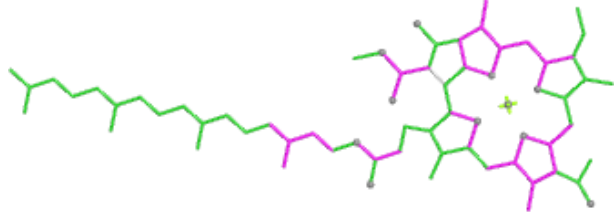
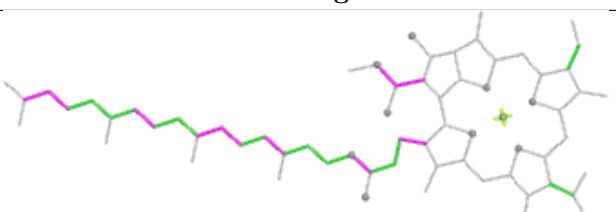
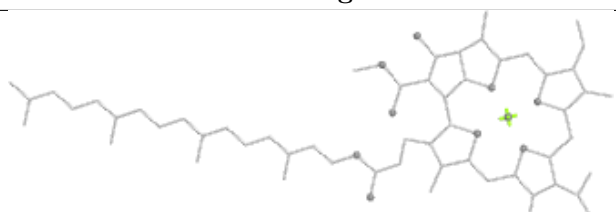
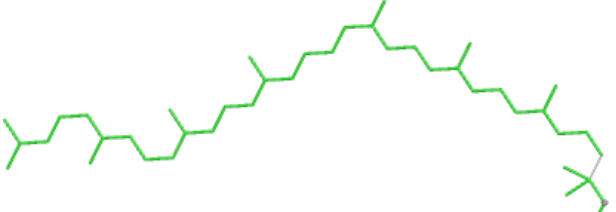
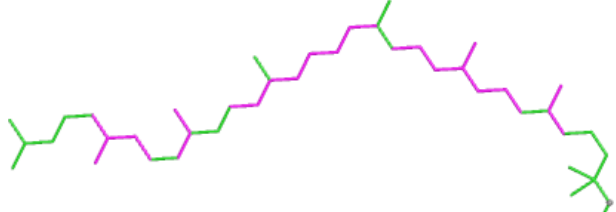
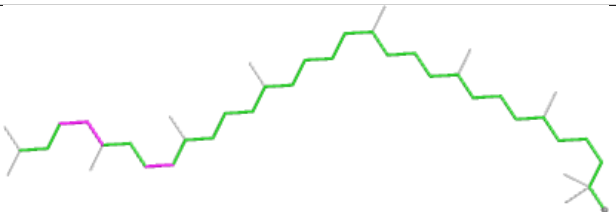
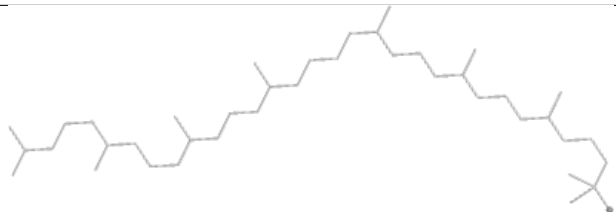
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	303	PGV	2	0
15	R	101	SPO	6	0
10	M	415	PGV	5	0
7	J	101	BCL	6	0
13	S	101	LMT	3	0
7	B	101	BCL	4	0
15	W	101	SPO	8	0
7	D	102	BCL	8	0
7	K	102	BCL	7	0
9	L	304	U10	7	0
13	S	102	LMT	6	0
10	L	305	PGV	5	0
10	M	414	PGV	2	0
11	L	306	PEE	3	0
12	D	104	LDA	3	0
15	O	103	SPO	5	0
10	Q	103	PGV	5	0
15	D	101	SPO	6	0
13	Y	103	LMT	1	0
10	M	402	PGV	3	0
15	M	408	SPO	6	0
15	P	101	SPO	5	0
13	M	409	LMT	3	0
16	F	102	MYR	2	0
15	S	105	SPO	6	0
7	M	404	BCL	3	0
15	T	101	SPO	3	0
9	M	407	U10	3	0
12	L	307	LDA	2	0
15	F	104	SPO	5	0
13	M	412	LMT	6	0
7	L	310	BCL	2	0
7	Y	102	BCL	3	0
15	I	103	SPO	4	0
7	Z	101	BCL	3	0
13	M	411	LMT	1	0
13	Q	101	LMT	2	0
7	O	102	BCL	4	0
15	D	103	SPO	4	0
7	G	101	BCL	8	0
7	I	102	BCL	6	0
7	S	103	BCL	5	0

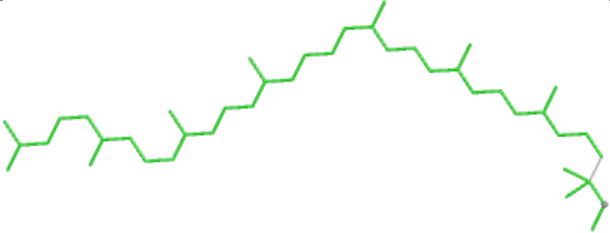
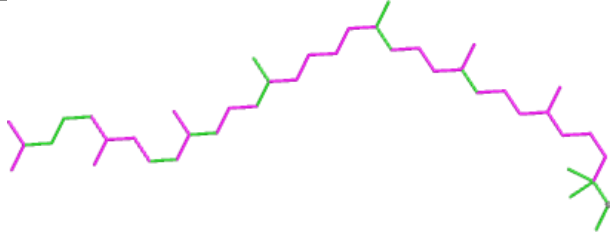
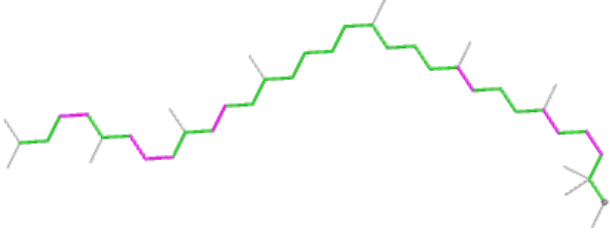
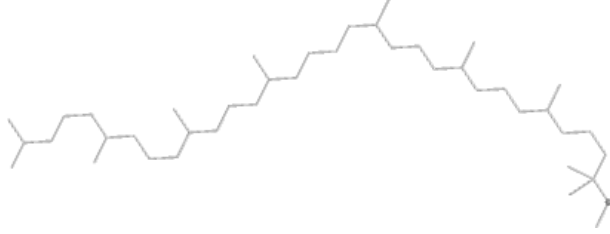
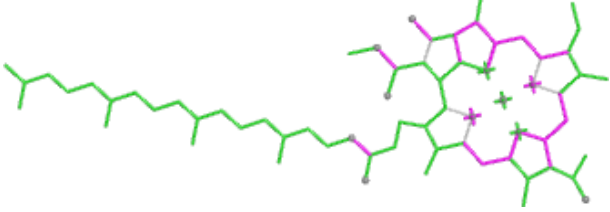
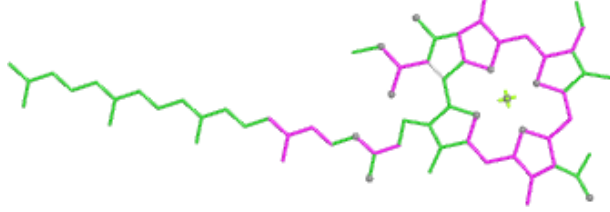
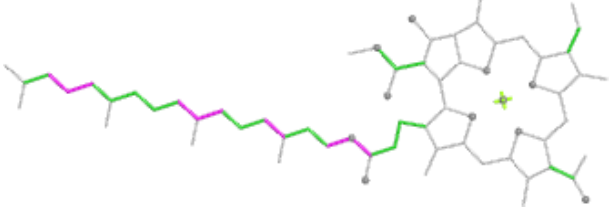
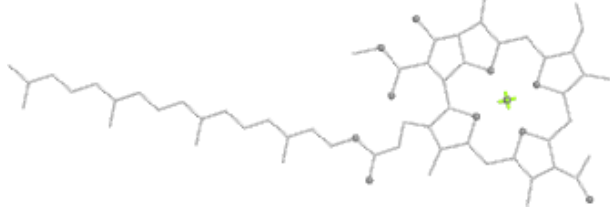
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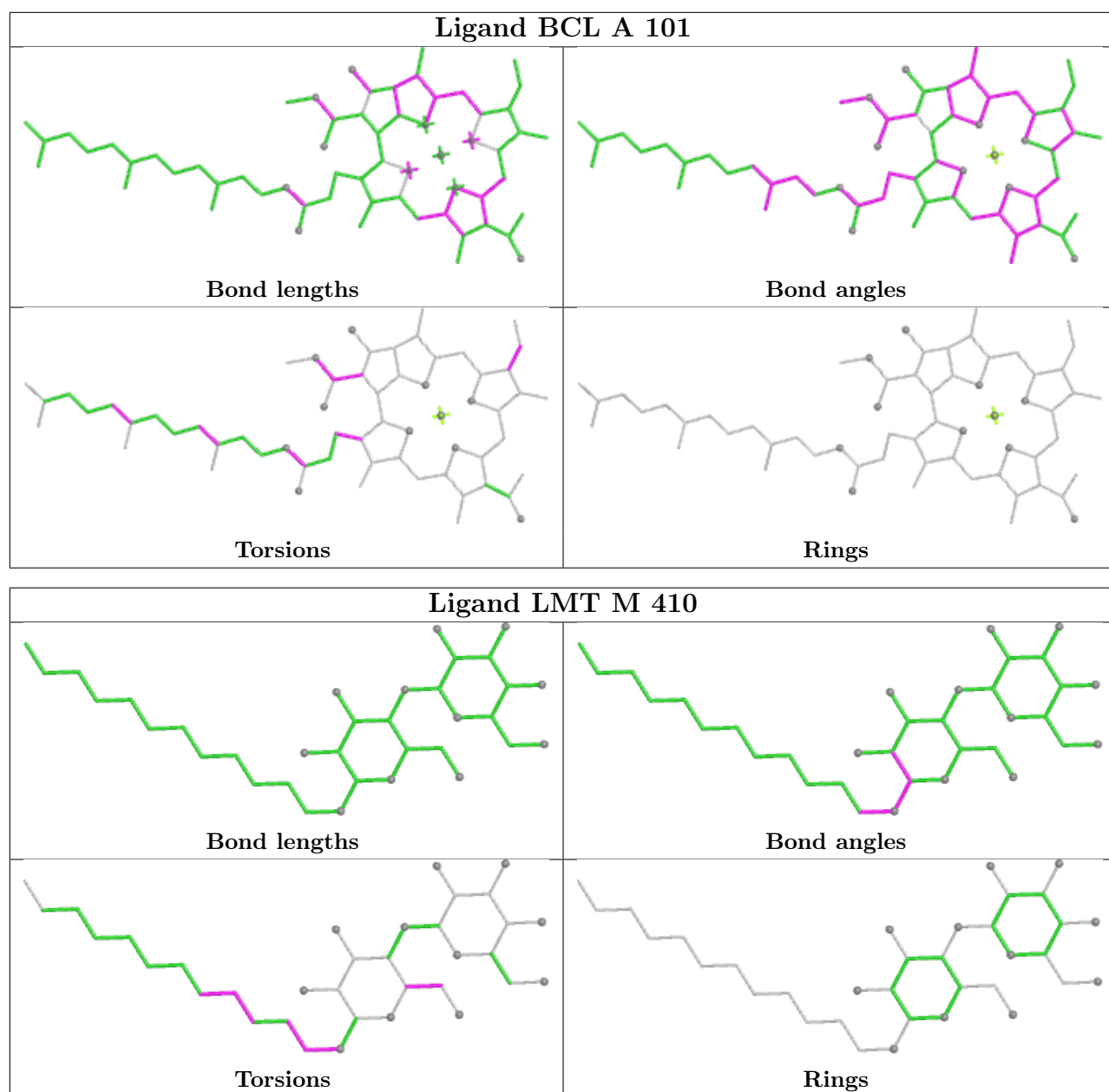
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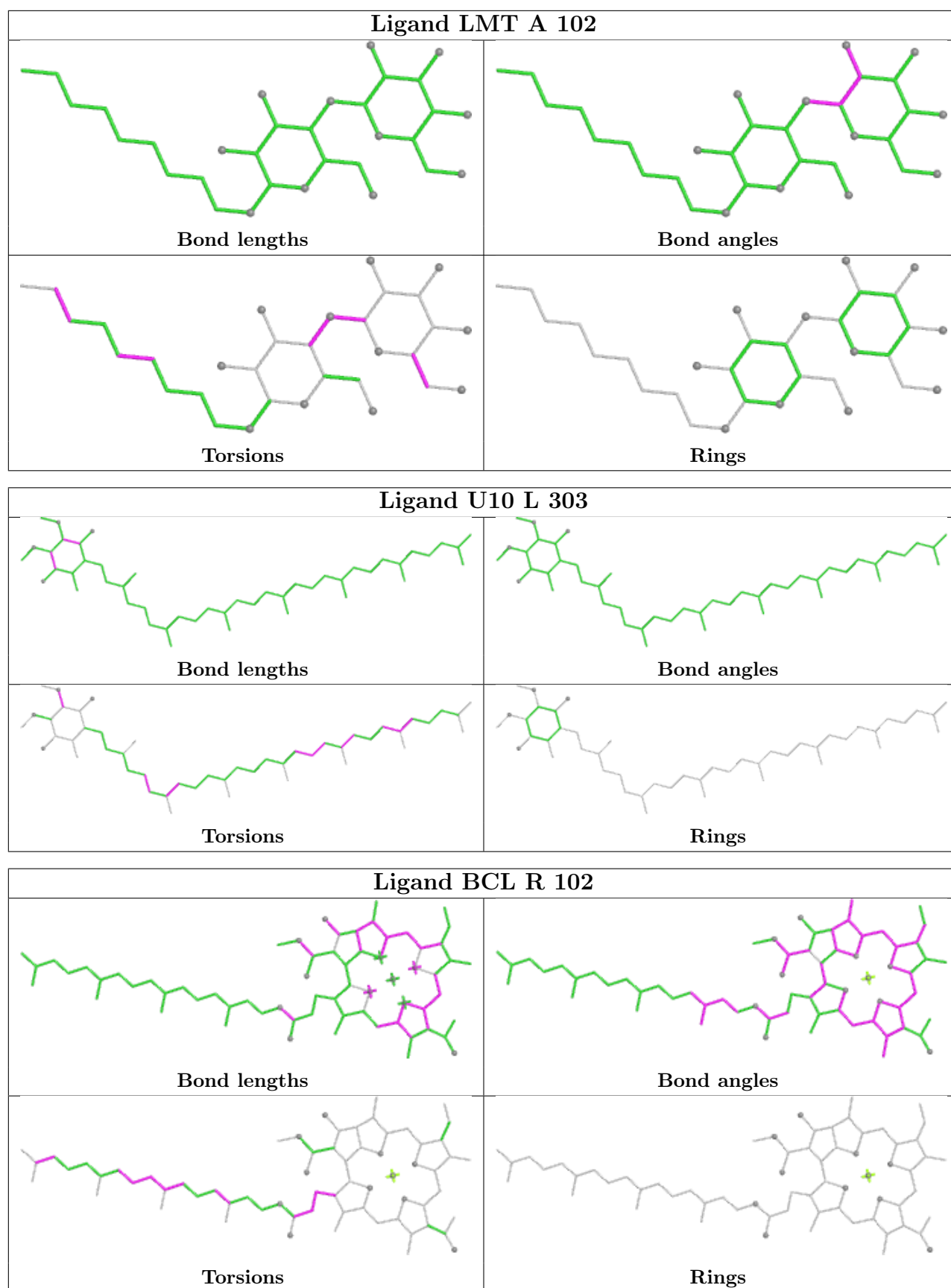
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	311	LMT	4	0
10	H	304	PGV	3	0
12	M	418	LDA	1	0
7	V	101	BCL	6	0
15	S	104	SPO	8	0
13	Y	101	LMT	1	0
15	E	101	SPO	6	0
13	I	101	LMT	3	0
7	M	403	BCL	6	0
9	M	401	U10	3	0
8	M	405	BPH	8	0
13	X	101	LMT	1	0
12	H	301	LDA	3	0
15	I	104	SPO	9	0
13	M	417	LMT	2	0
12	M	420	LDA	3	0
10	M	413	PGV	5	0
12	O	101	LDA	1	0

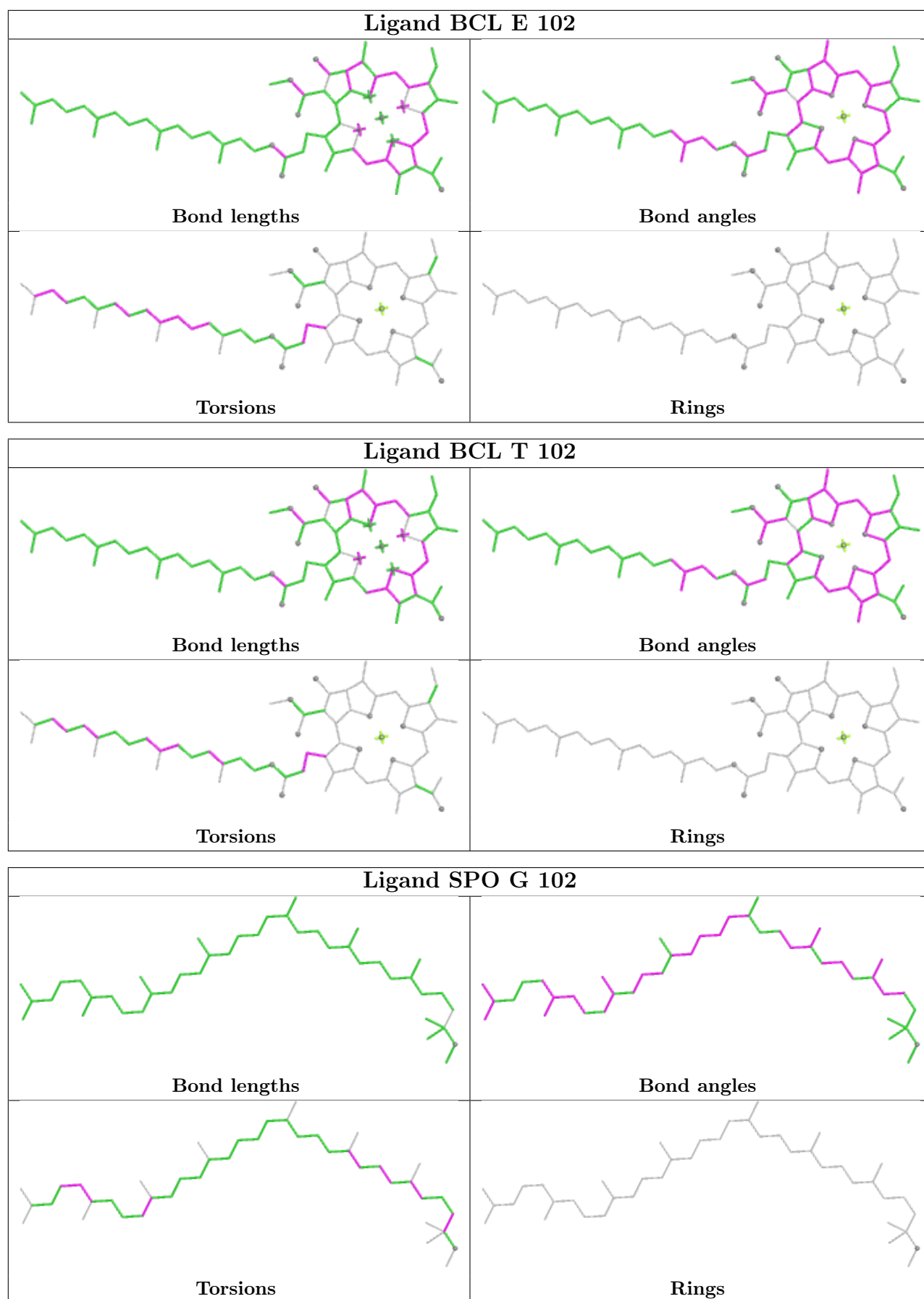
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

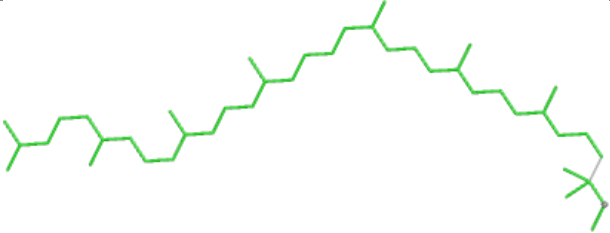
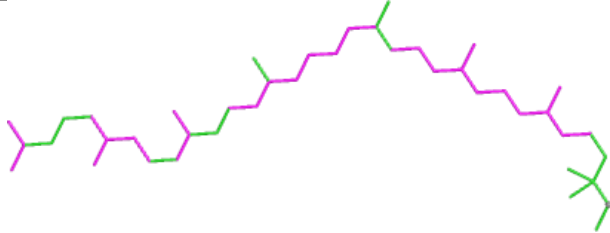
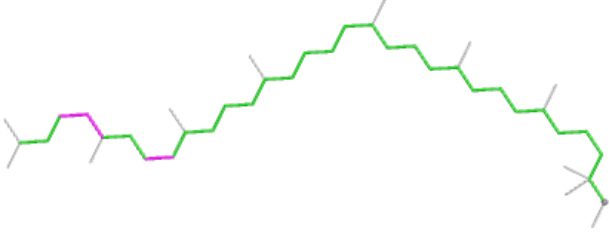
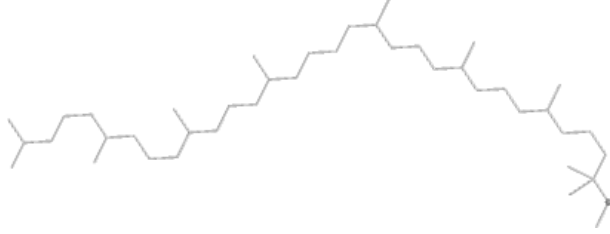
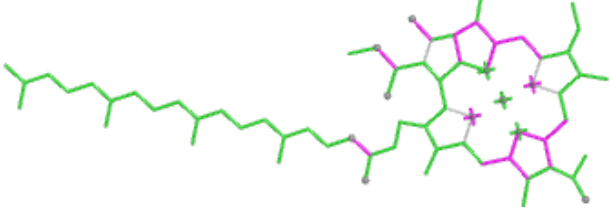
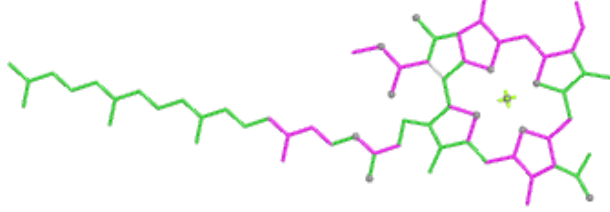
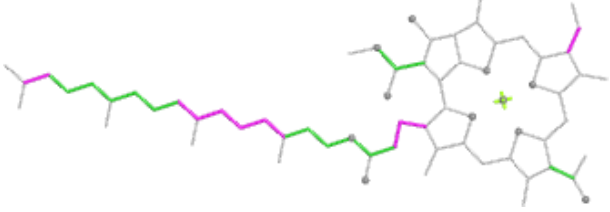
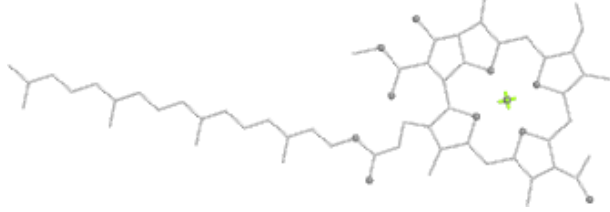
Ligand BCL F 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO D 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

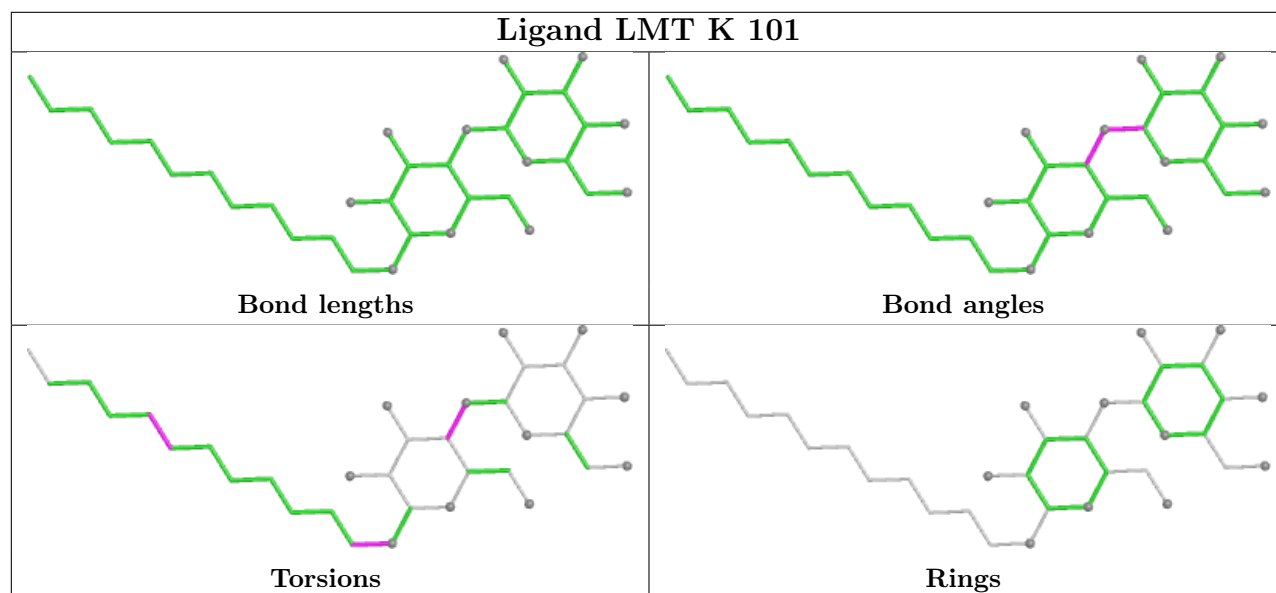
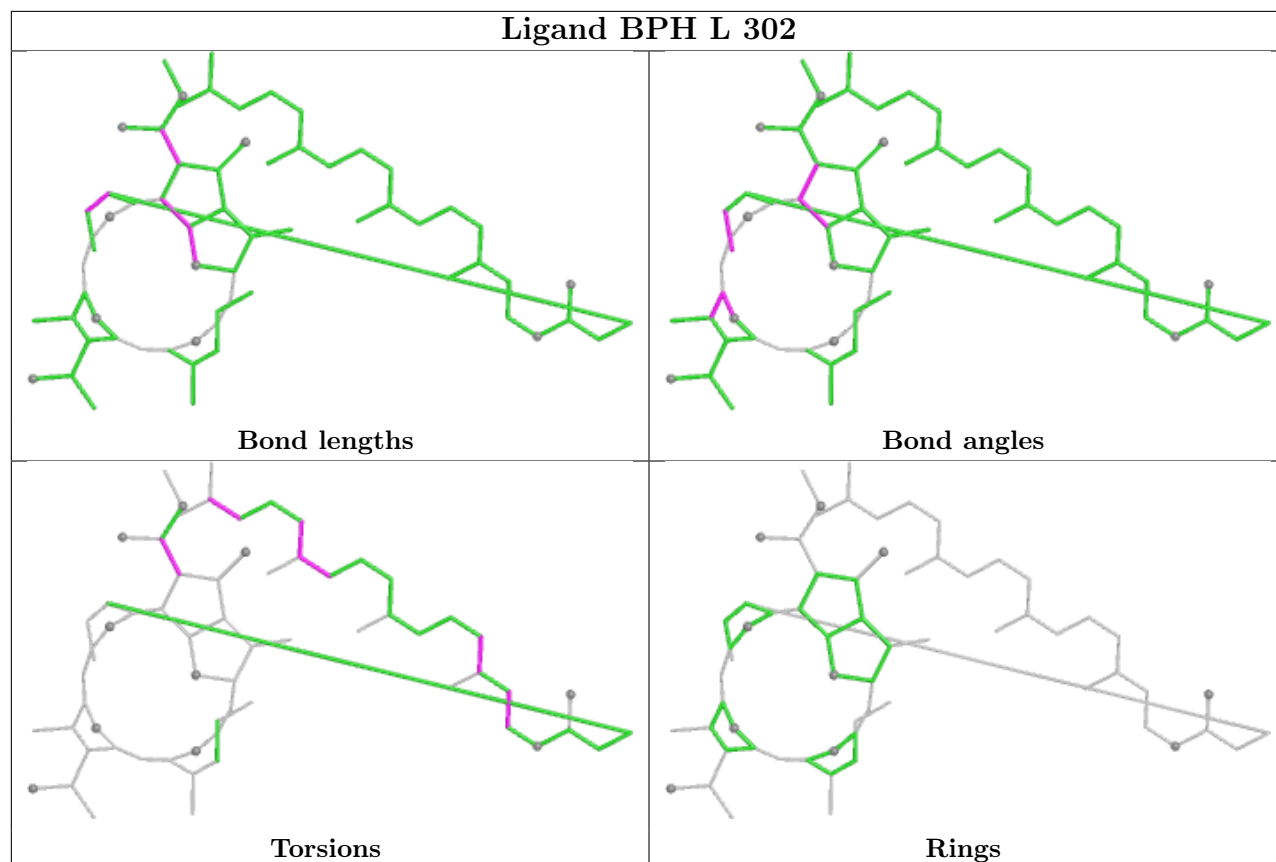
Ligand SPO N 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL F 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

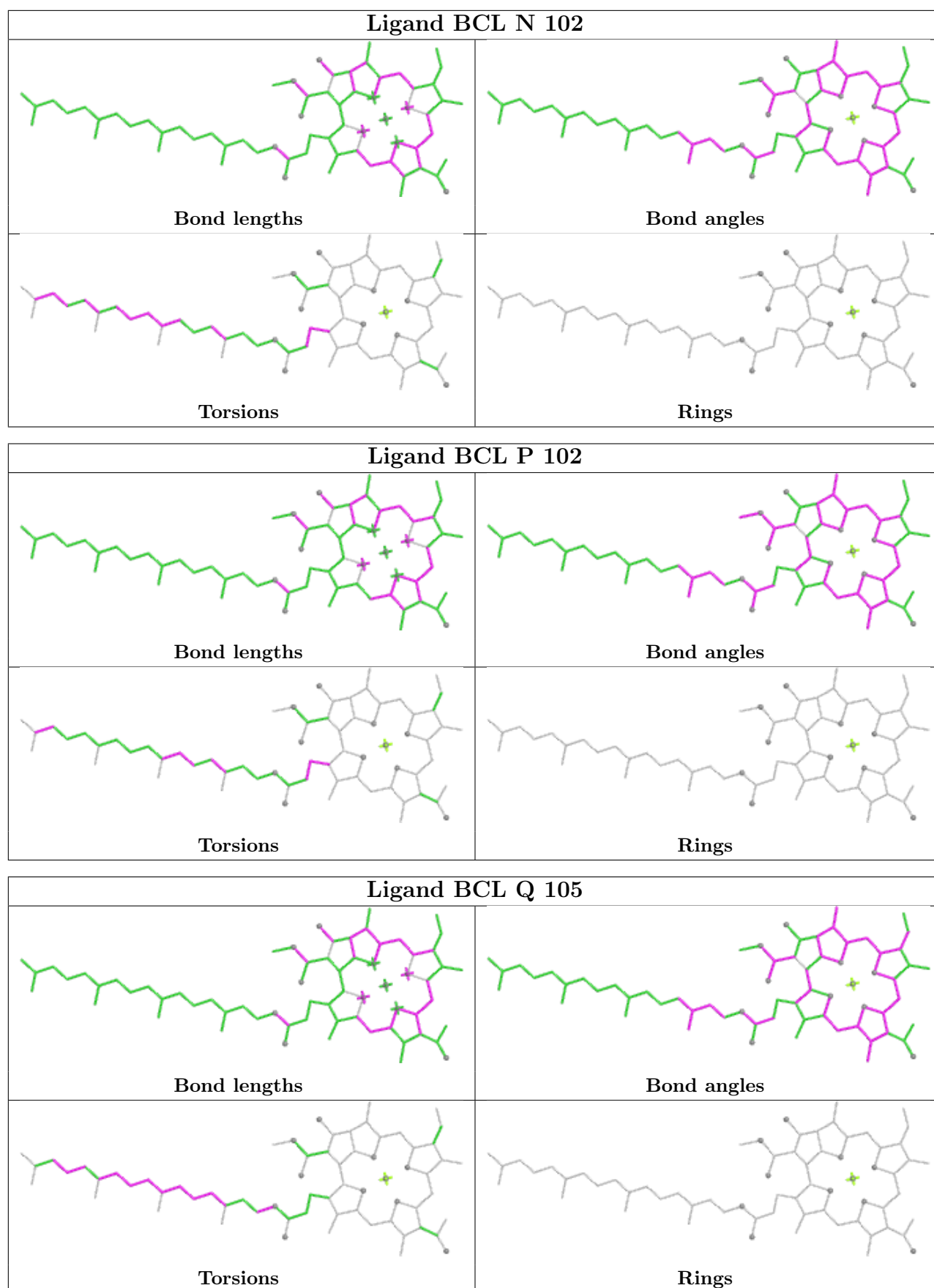


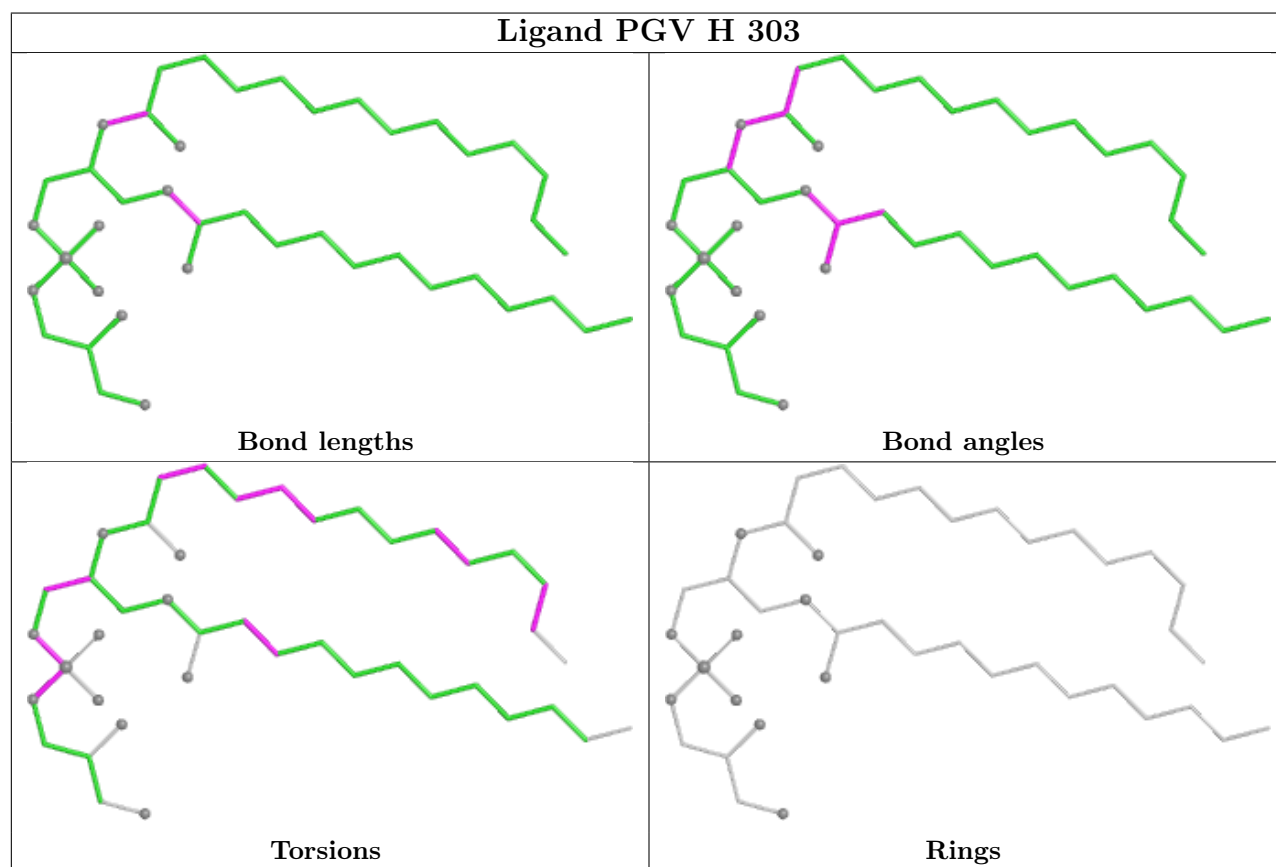
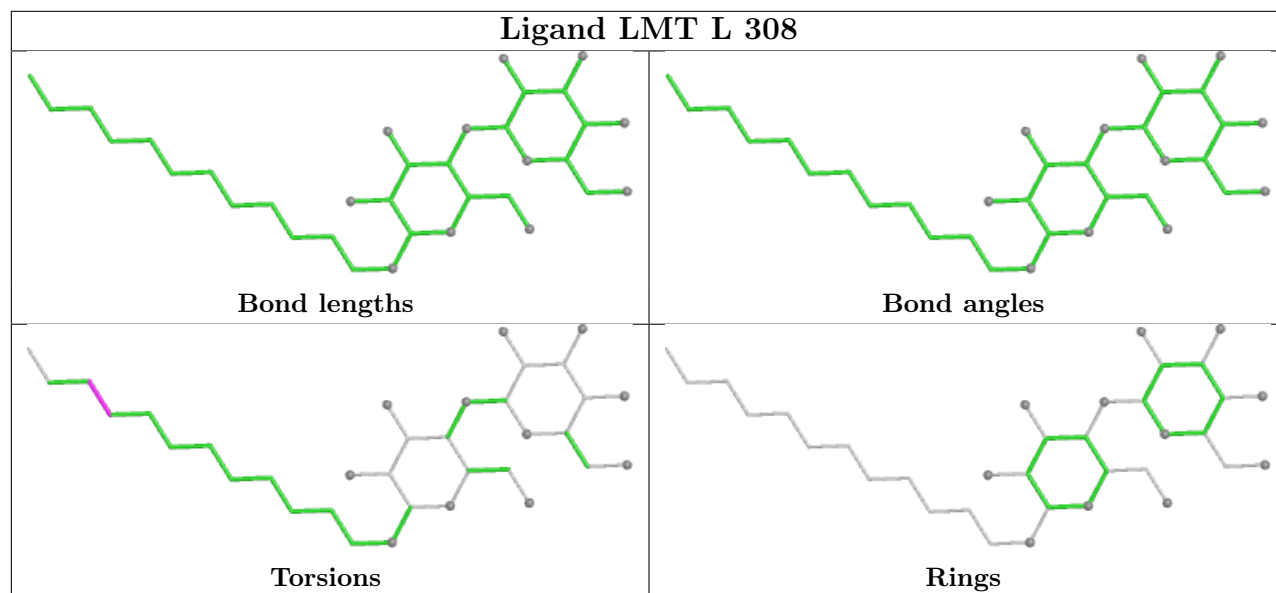


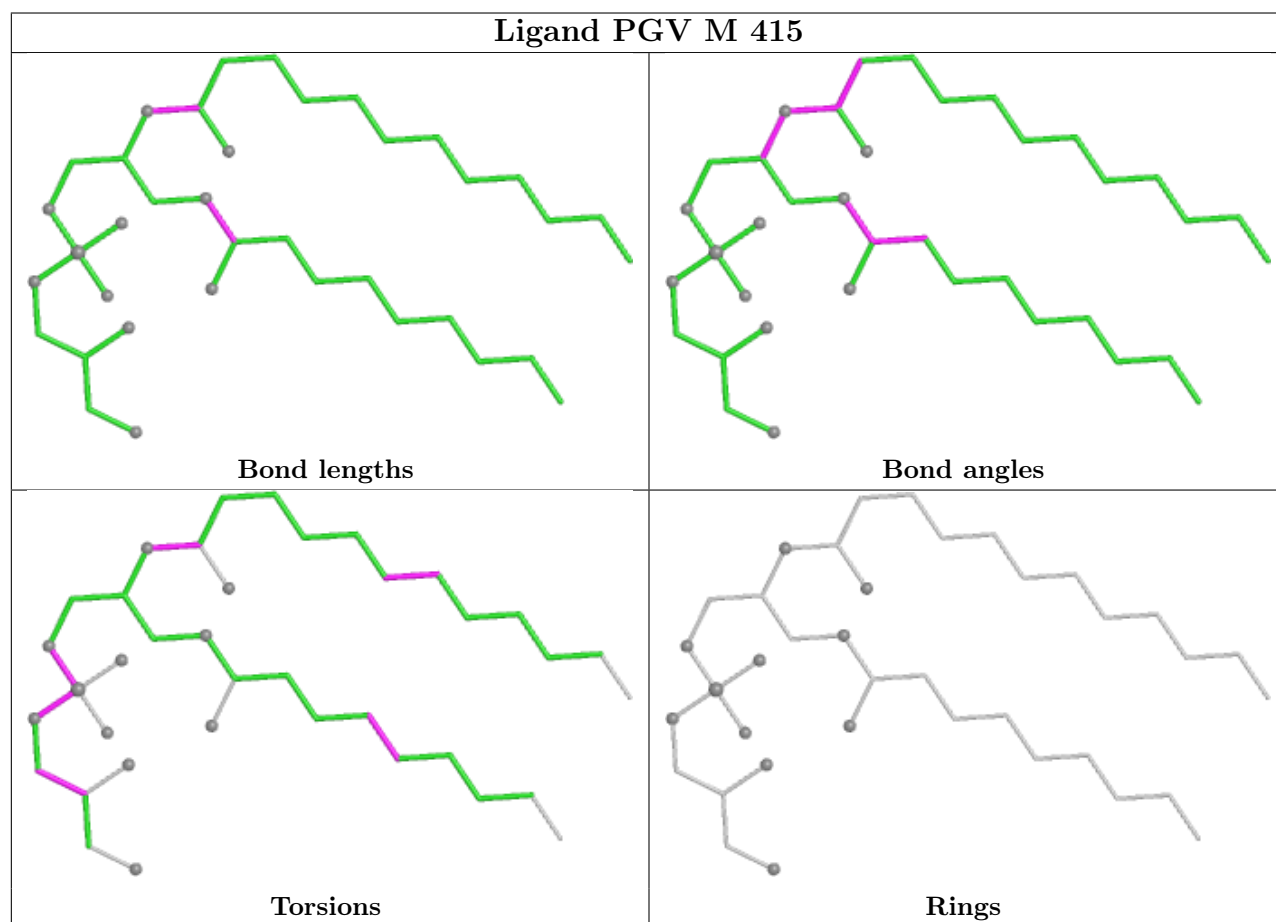
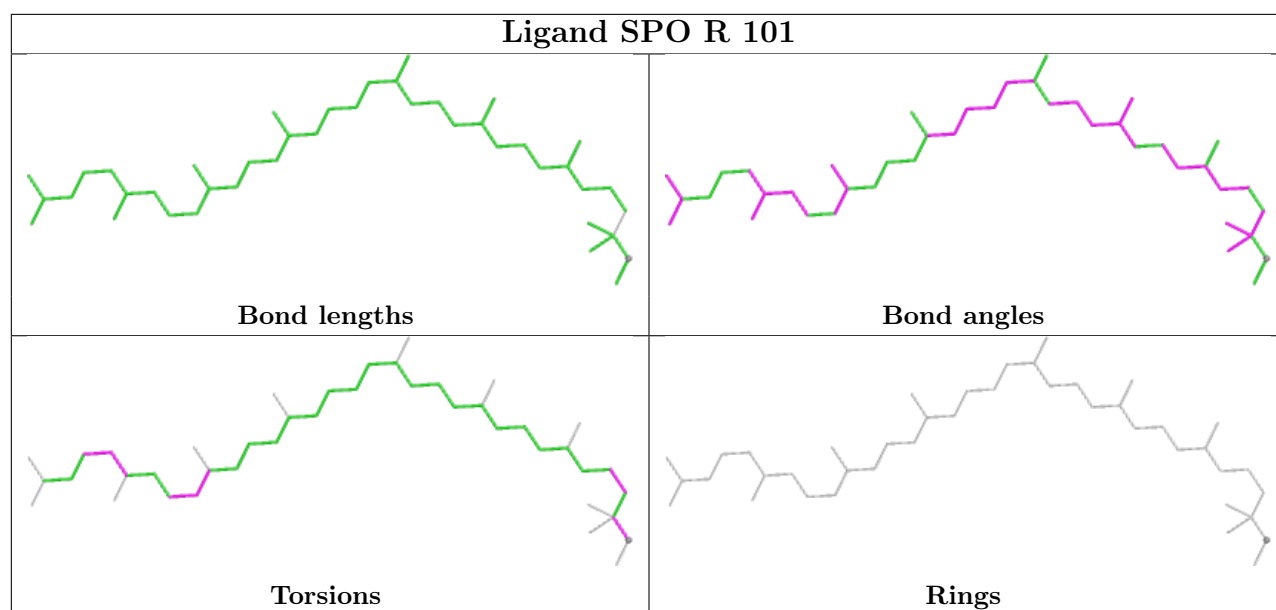


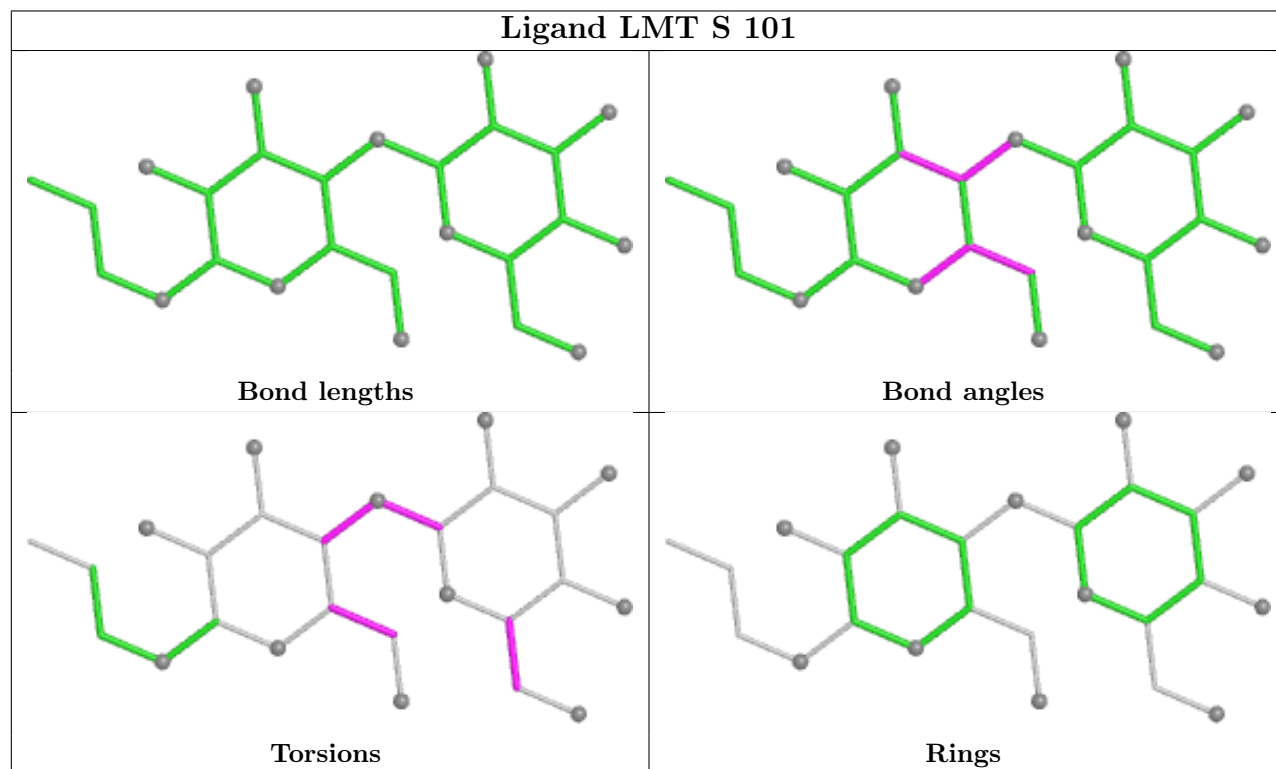
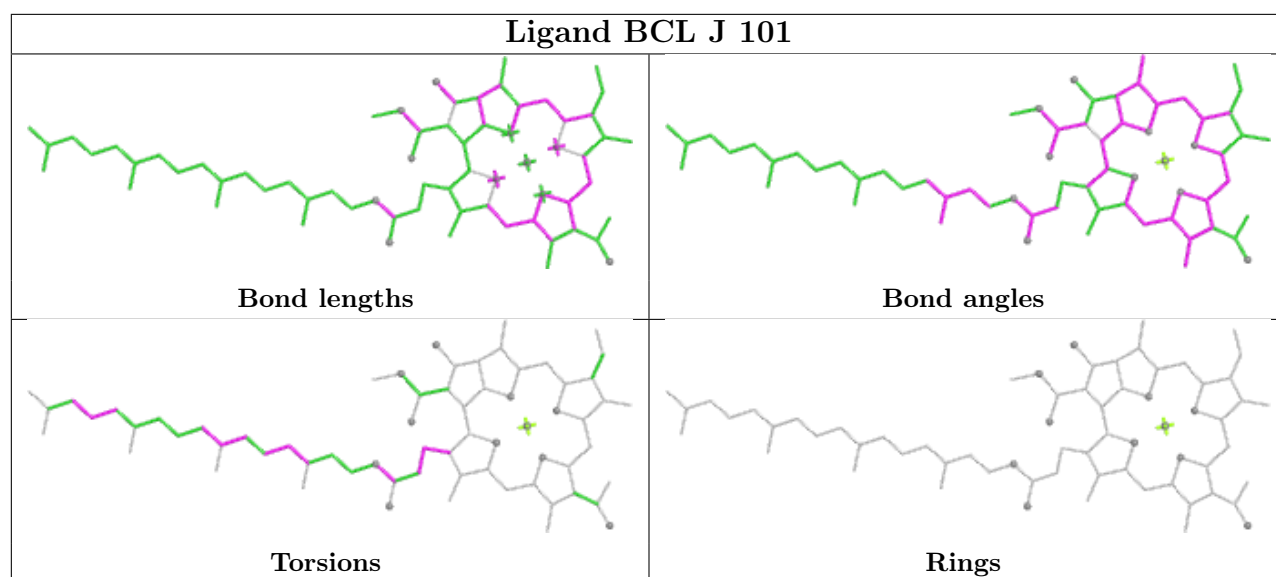
Ligand SPO O 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL W 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

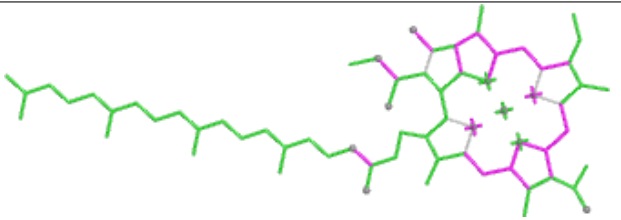
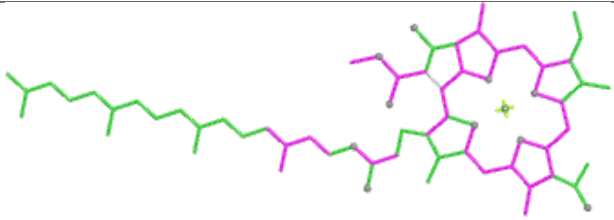
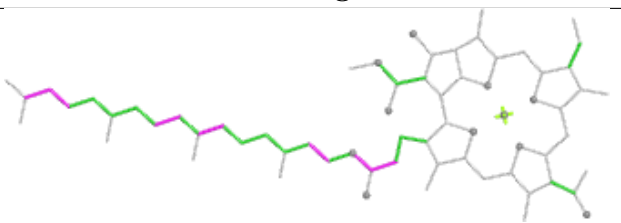
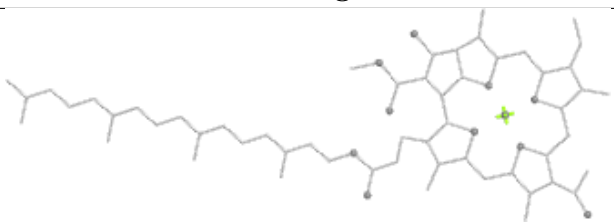


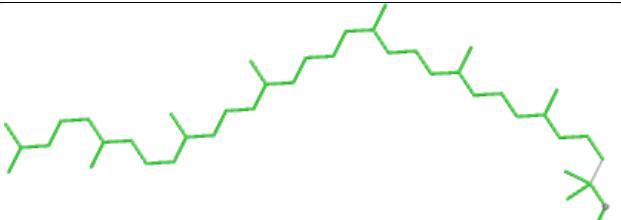
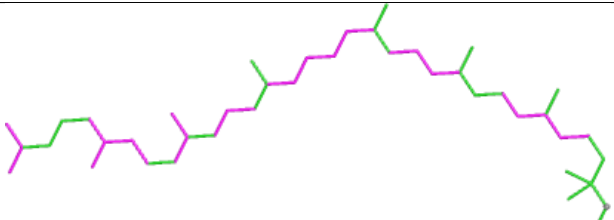
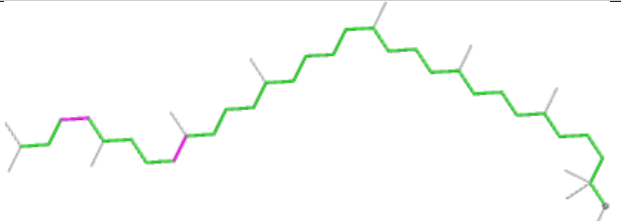


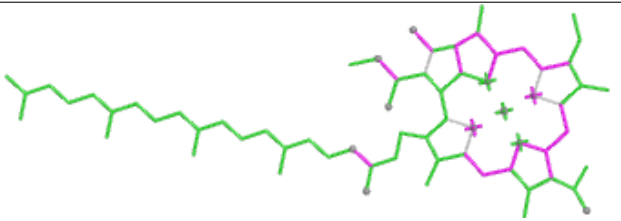
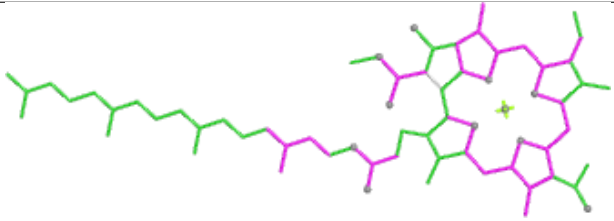
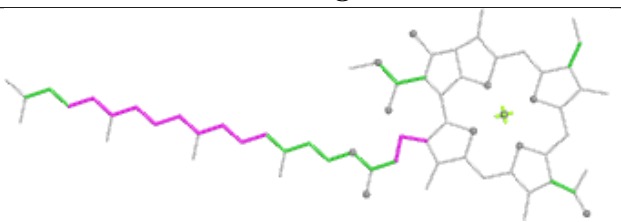
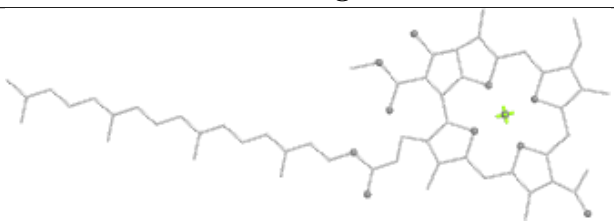


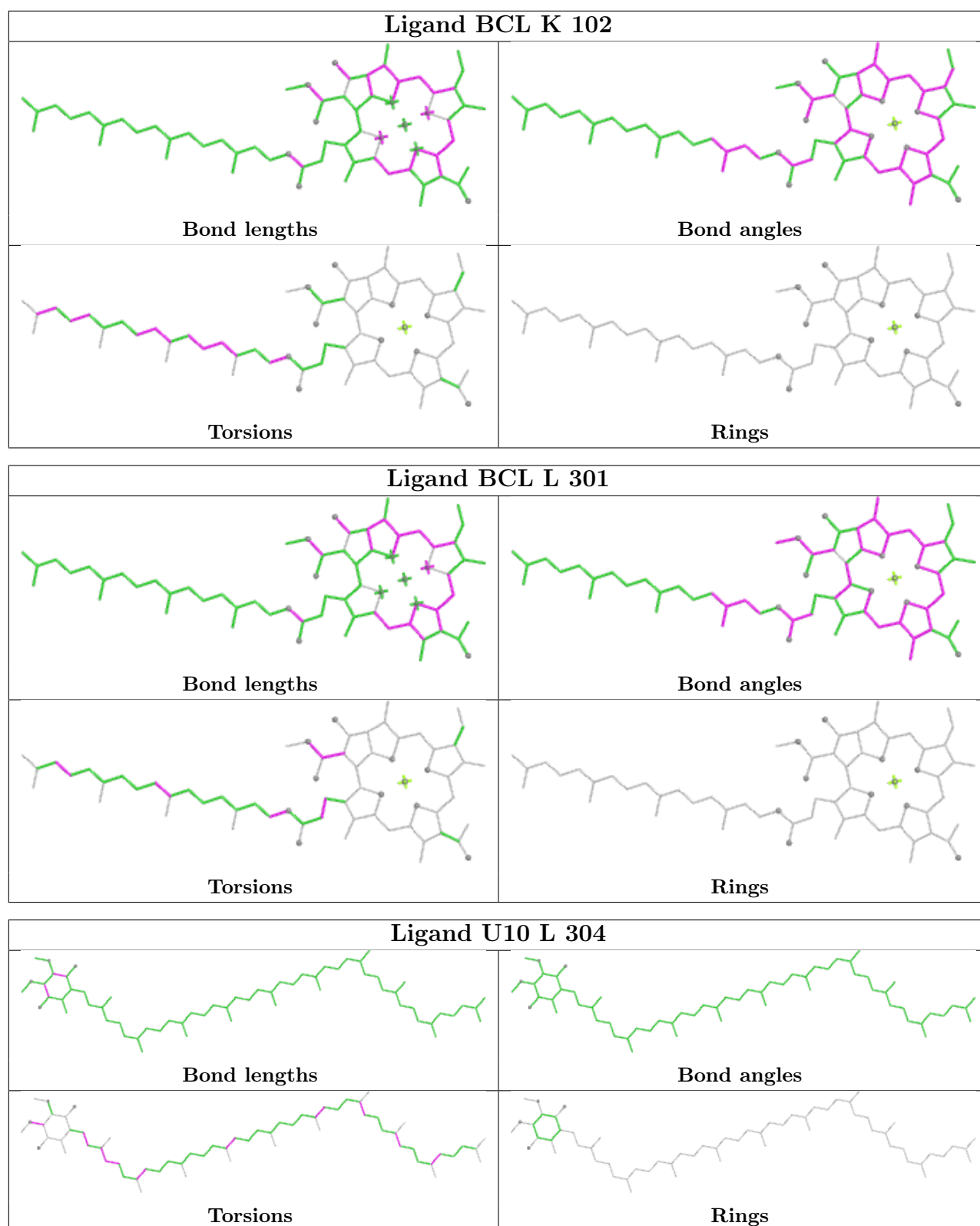


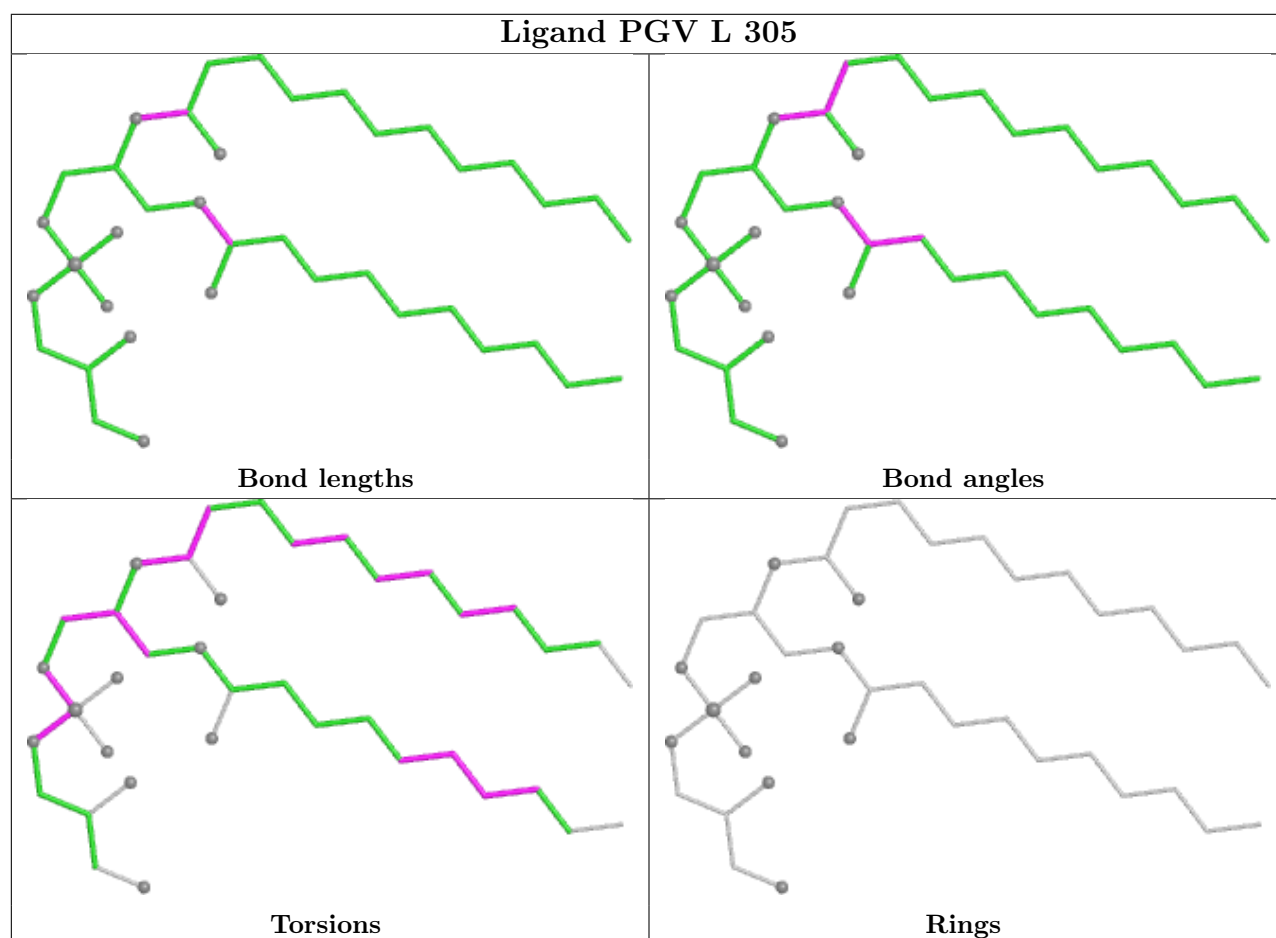
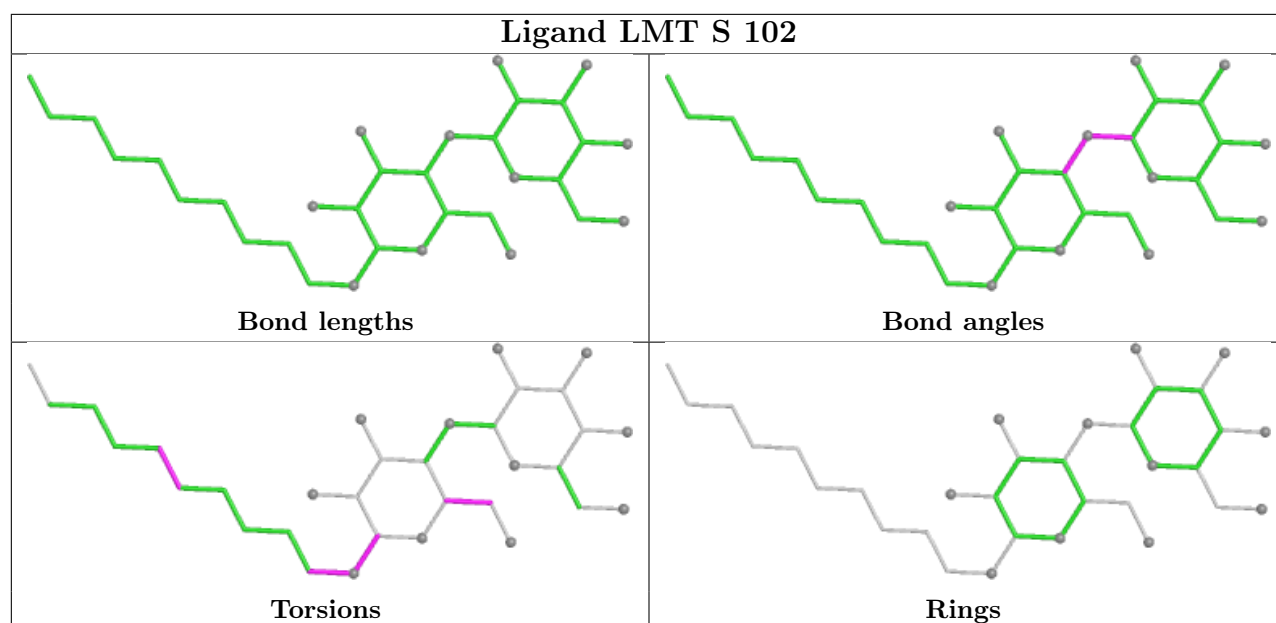


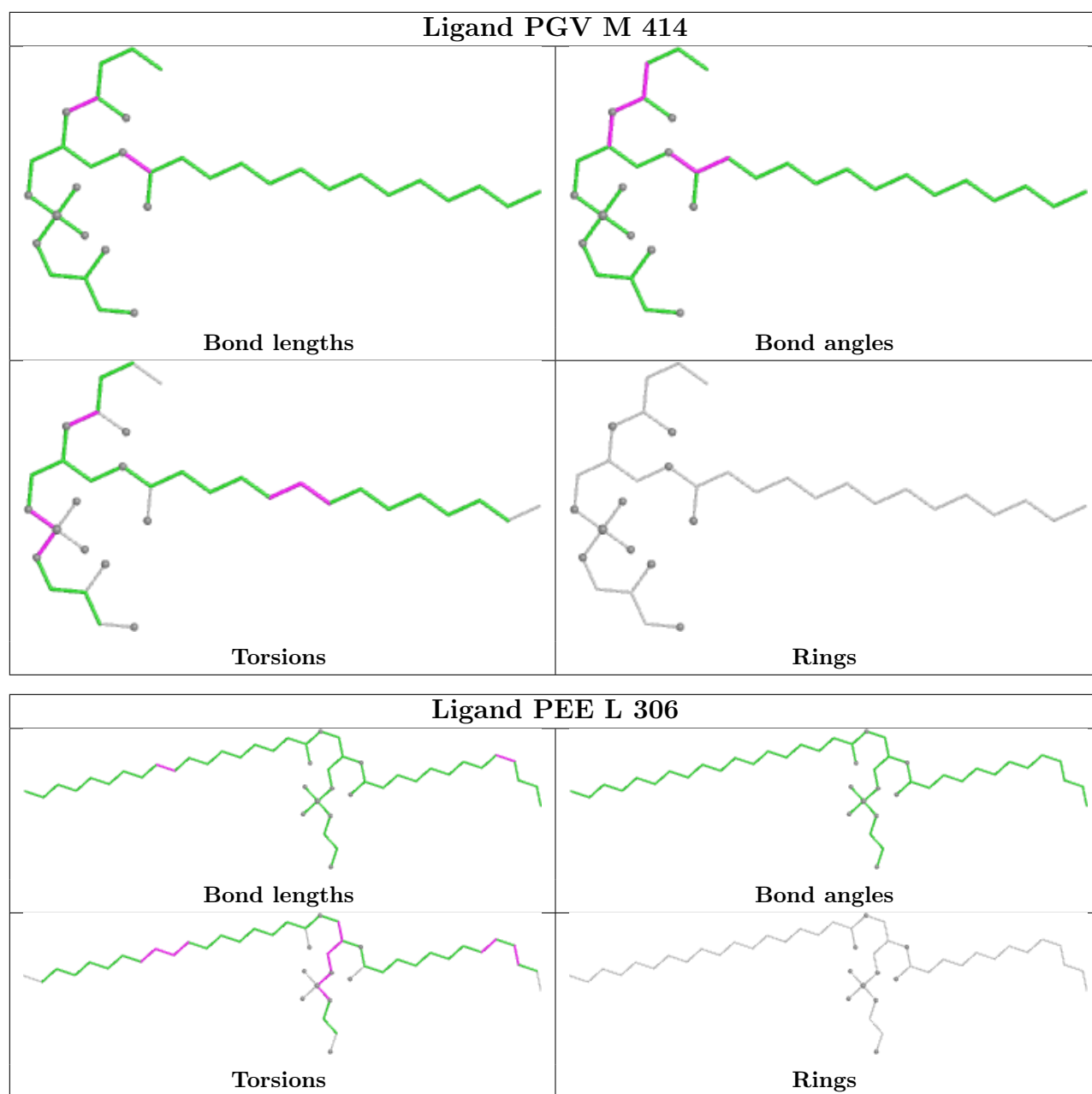
Ligand BCL B 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

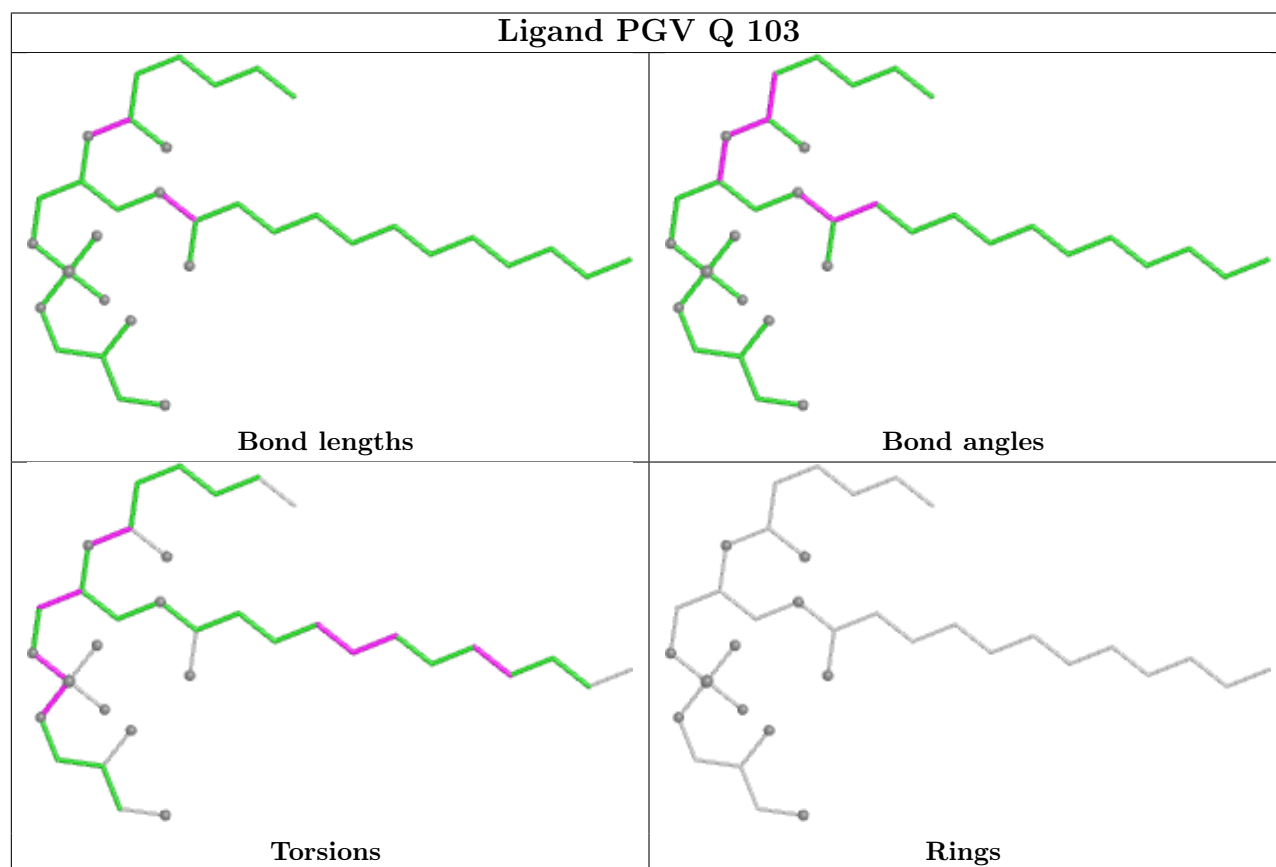
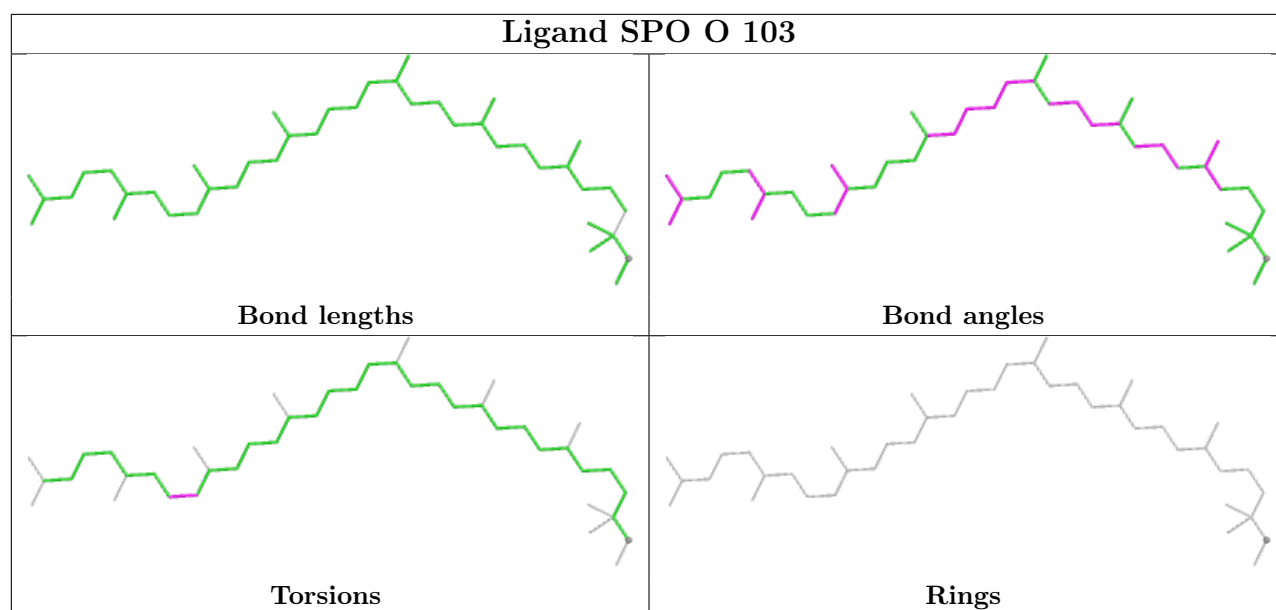
Ligand SPO W 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

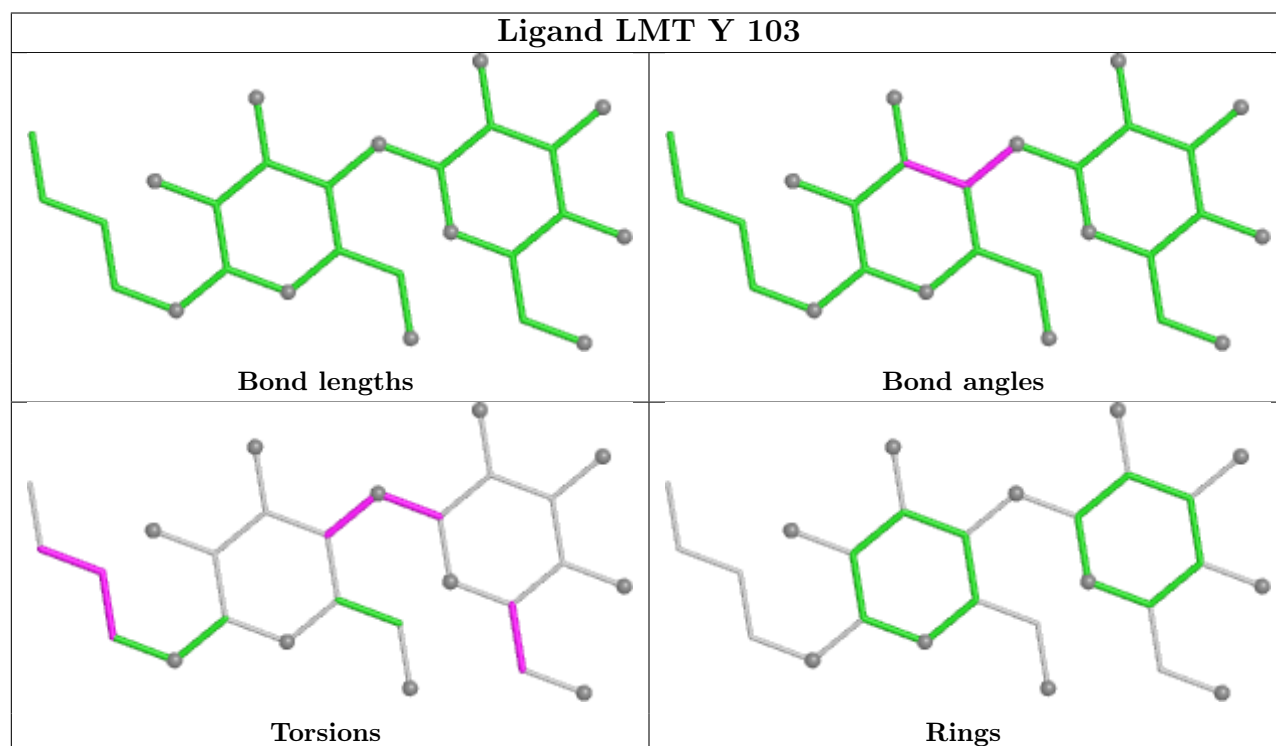
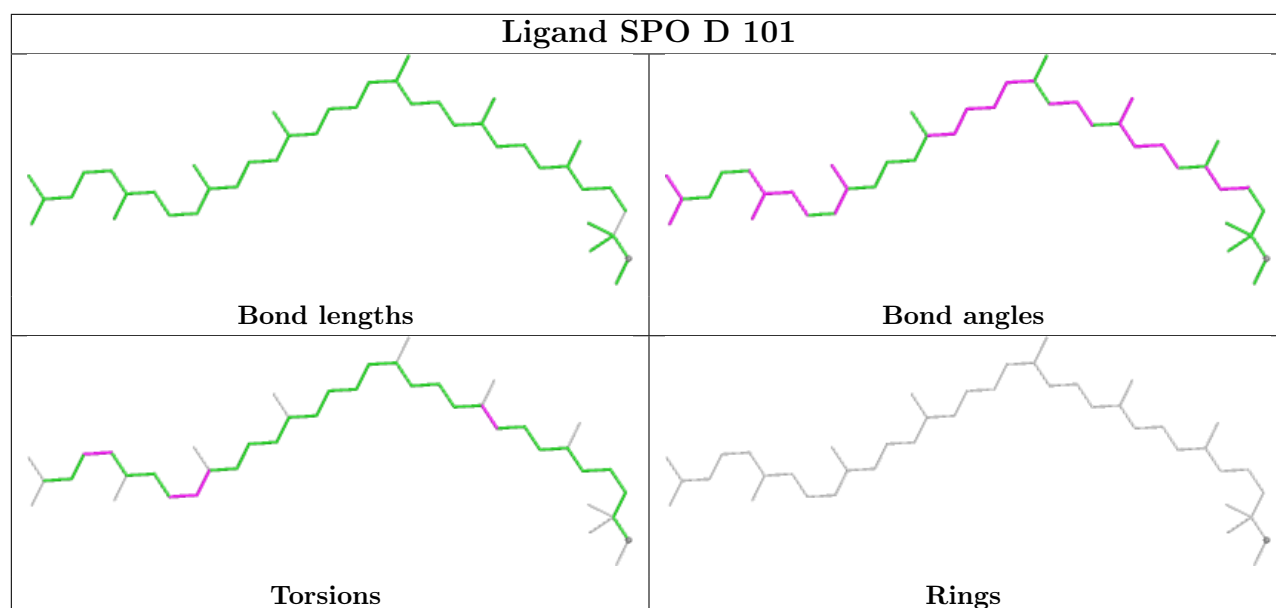
Ligand BCL D 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

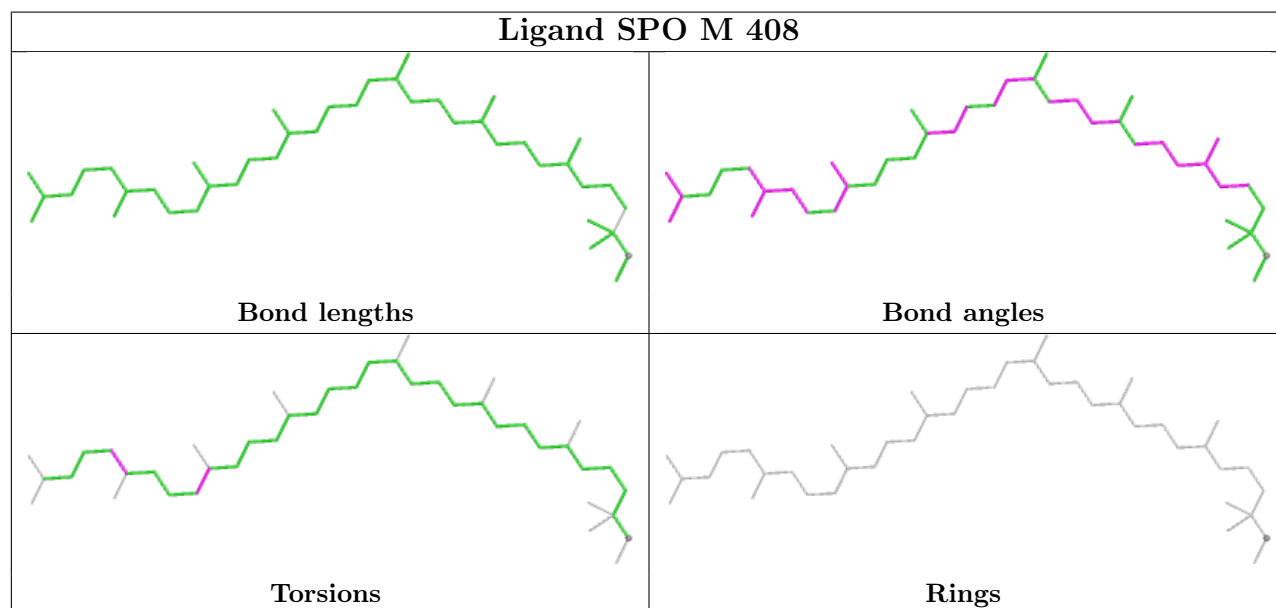
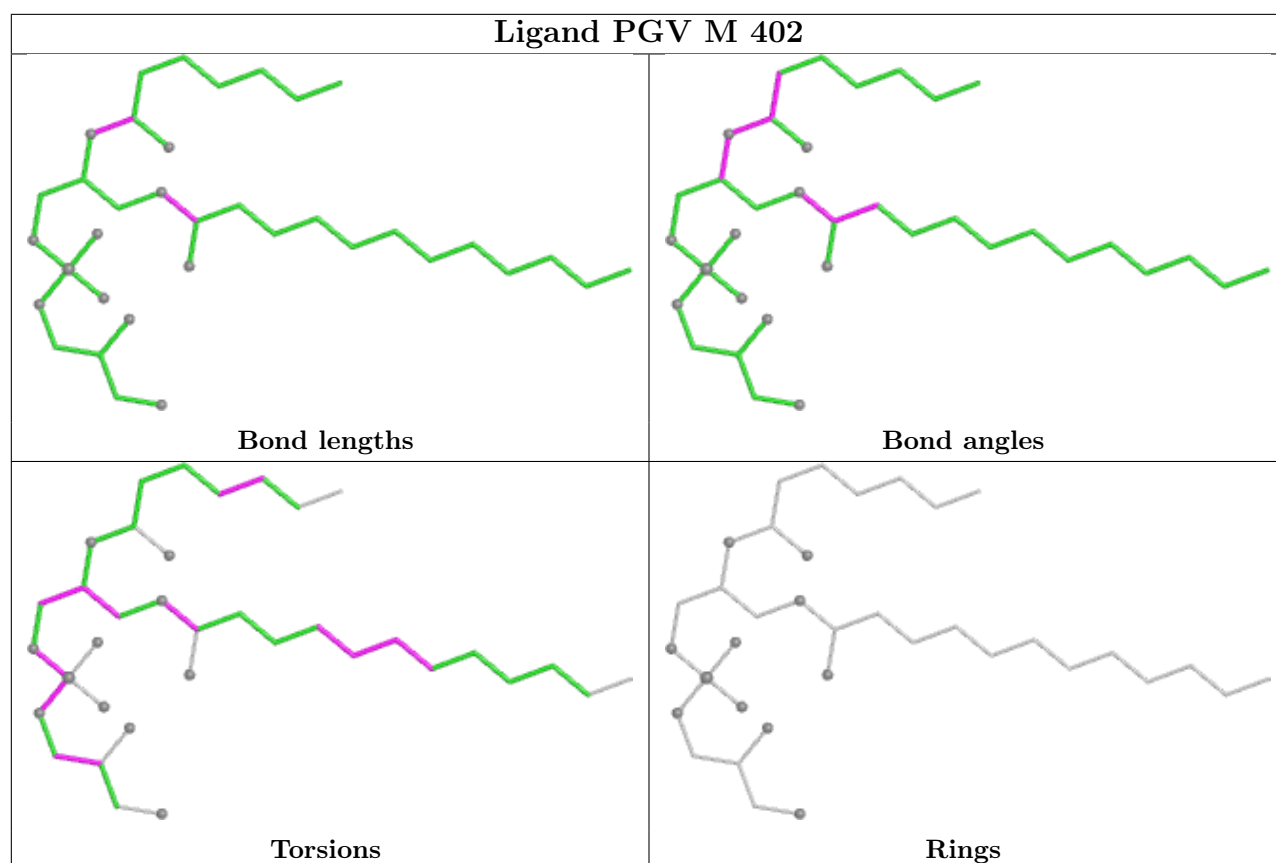


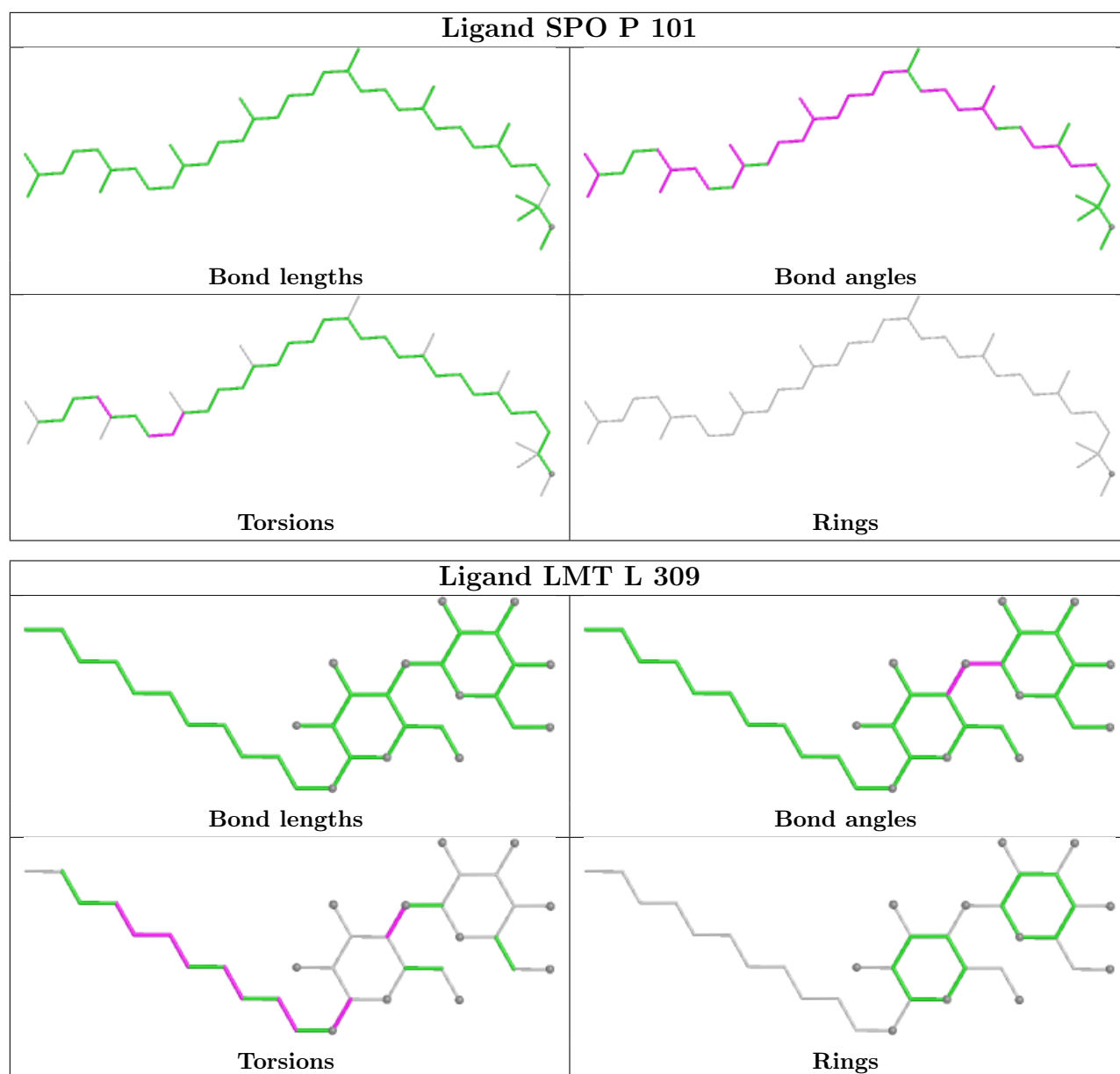


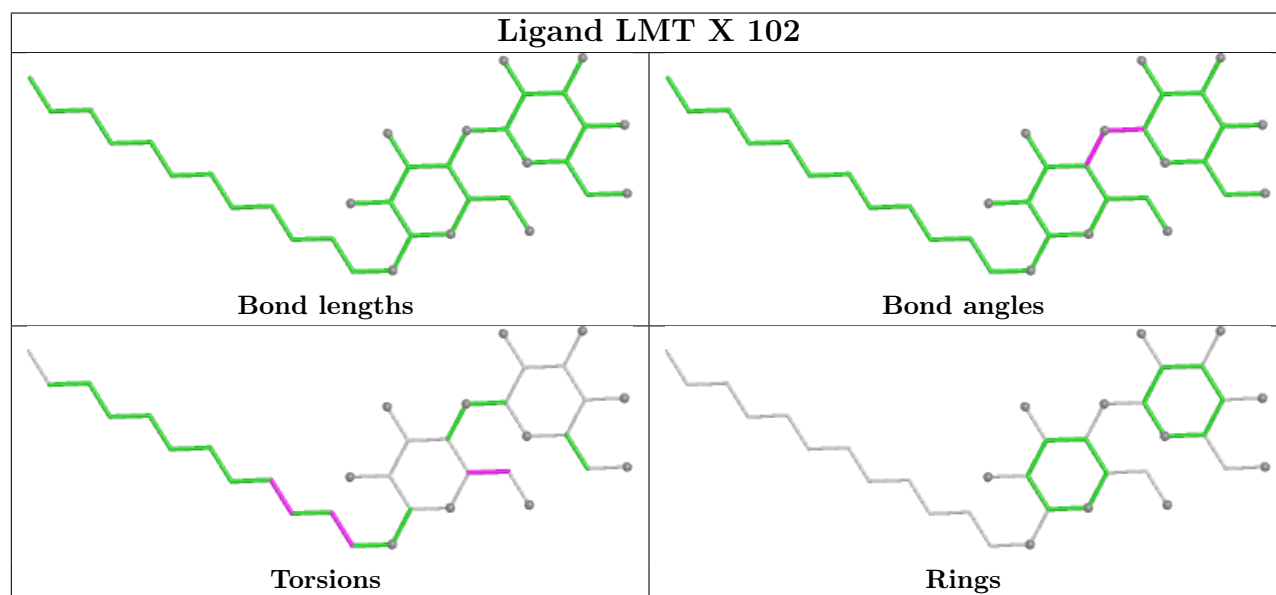
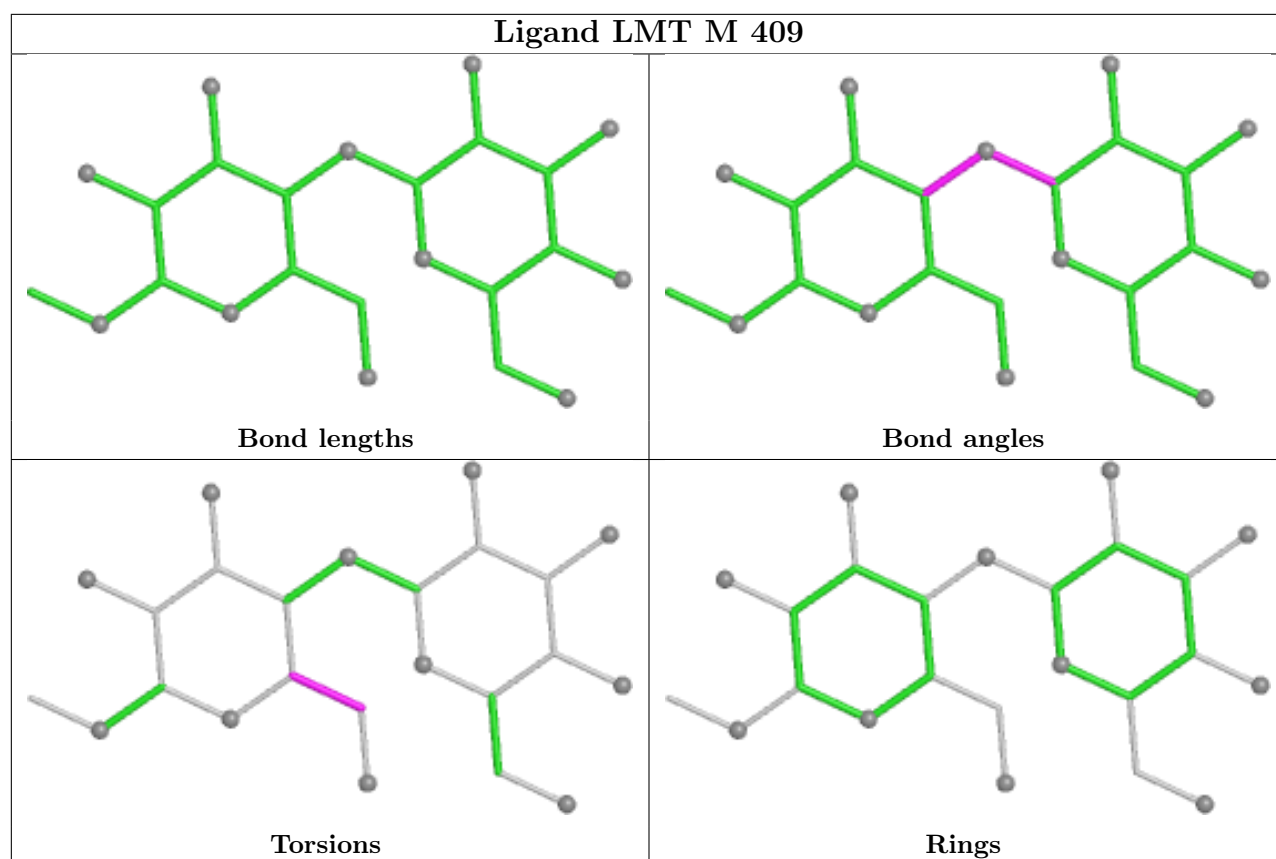


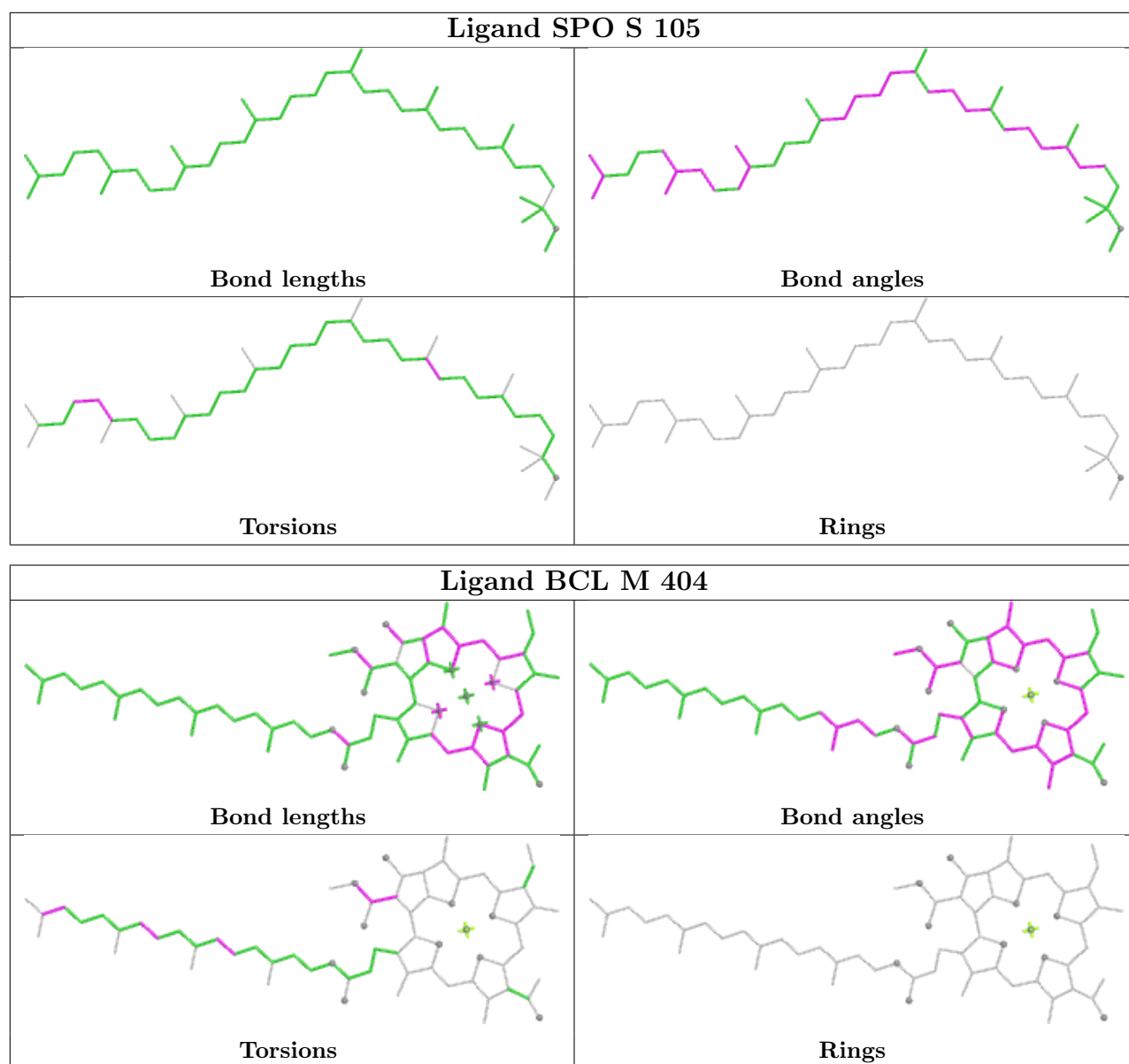


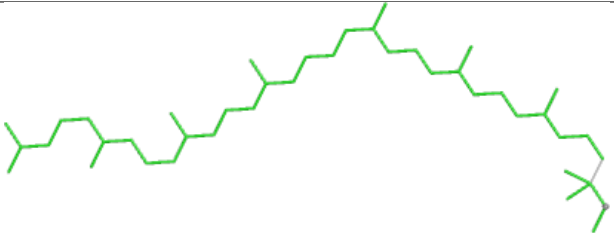
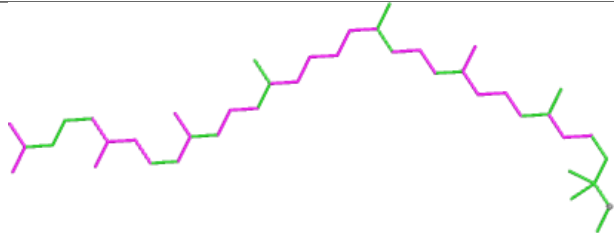
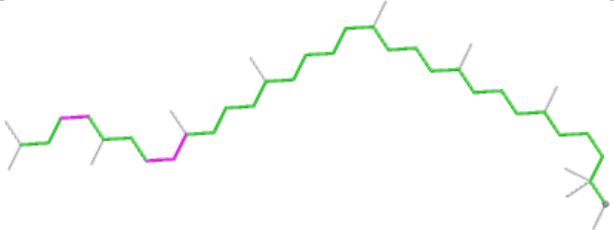
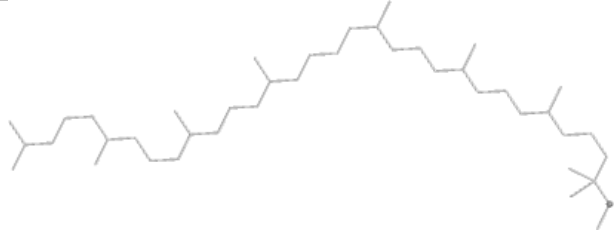


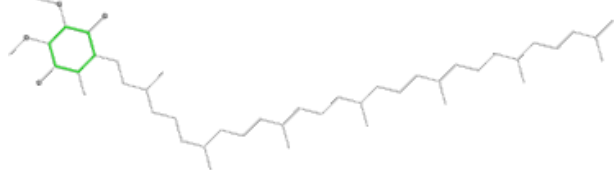


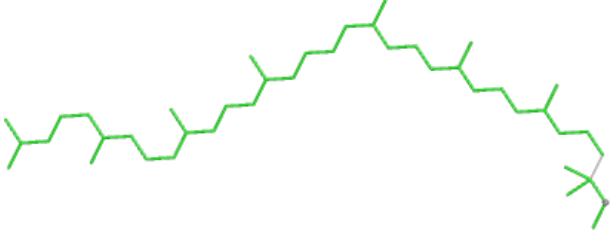
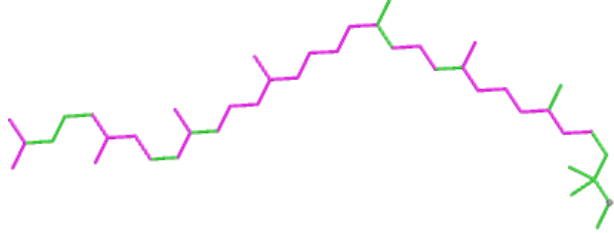
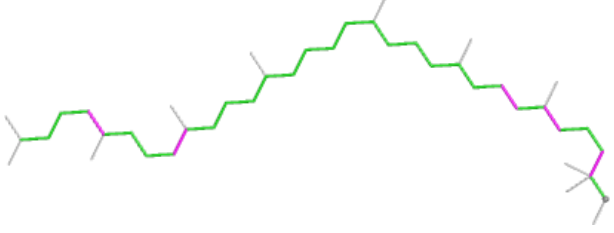
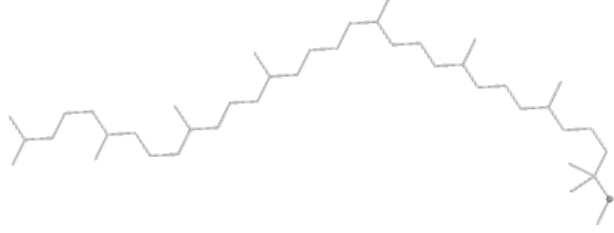


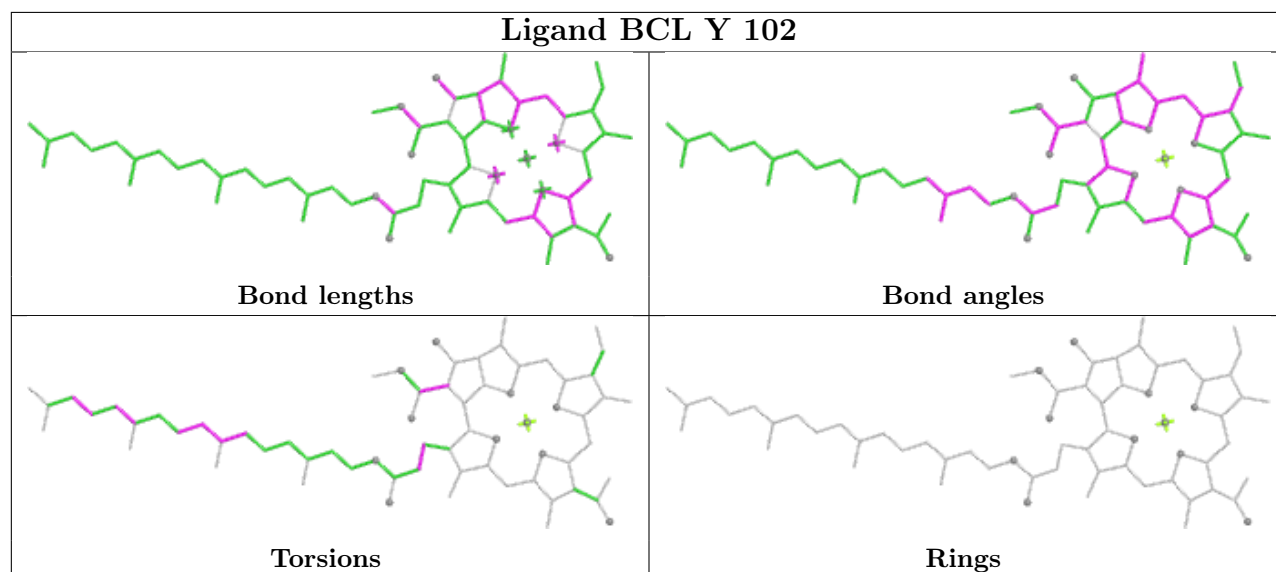
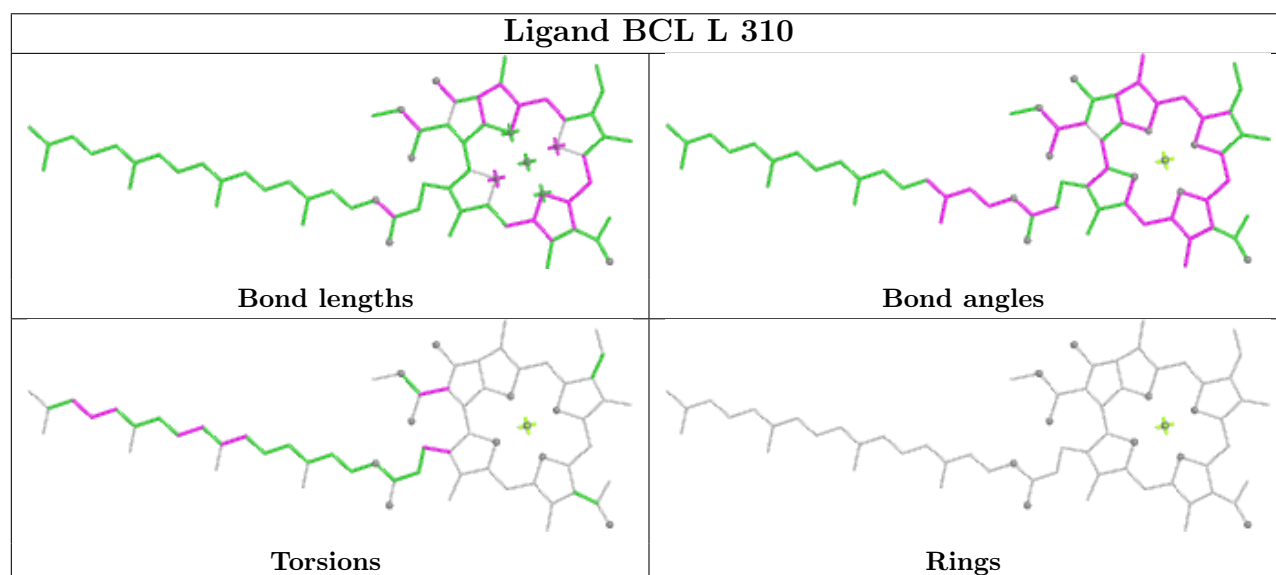
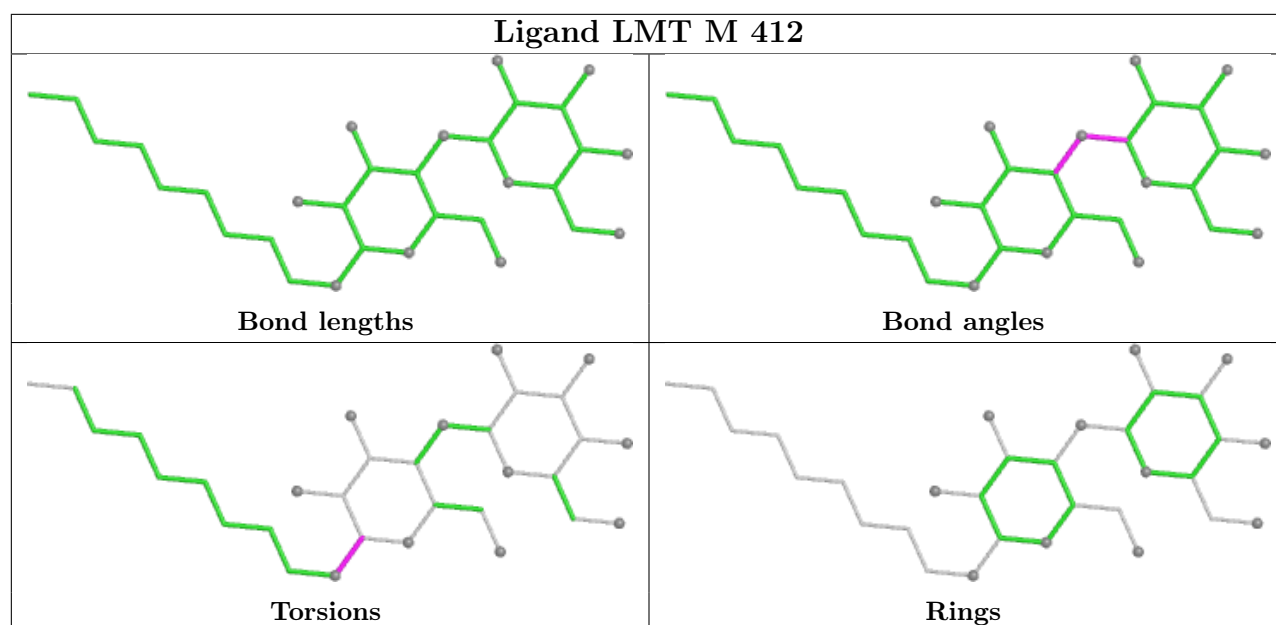


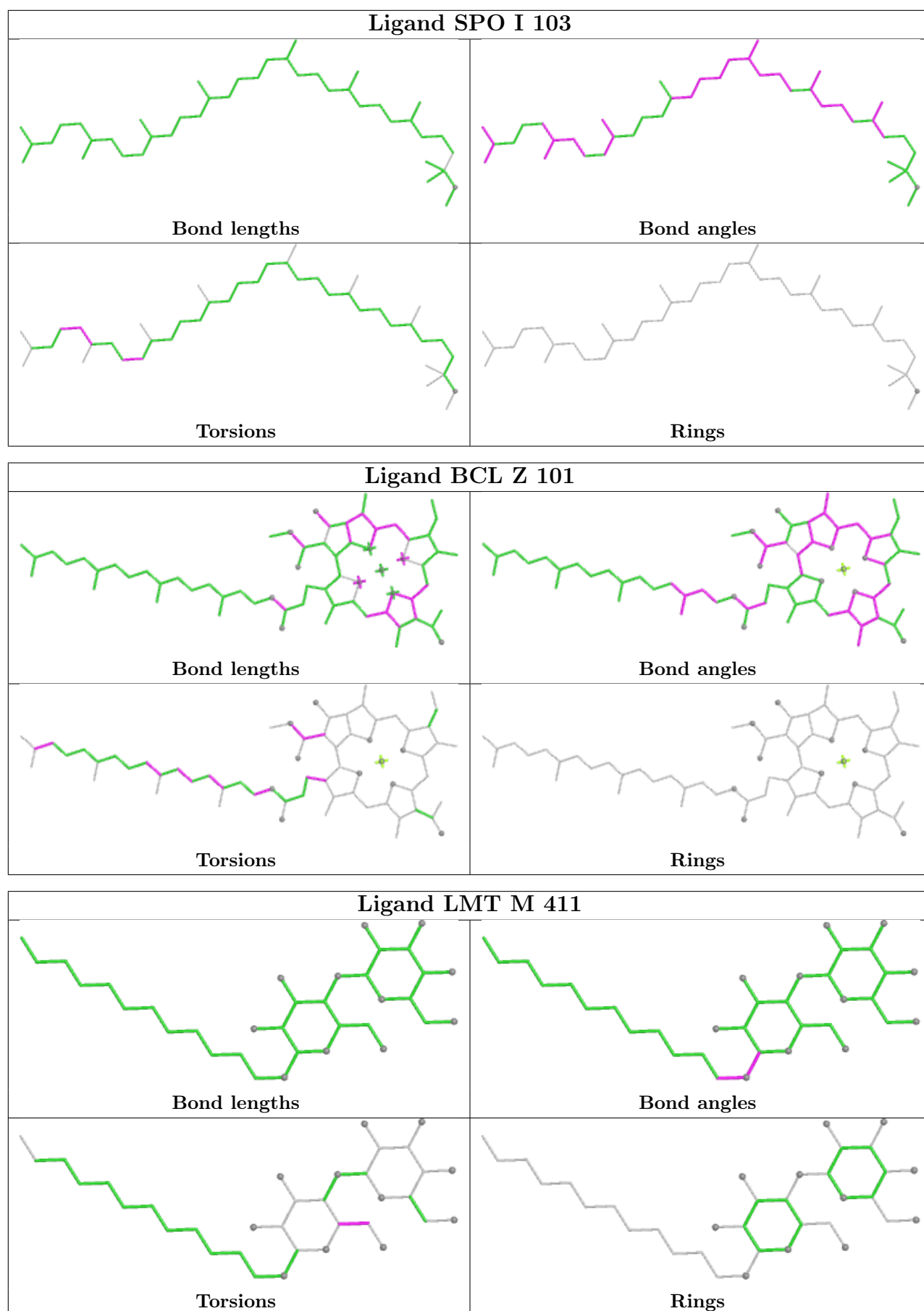


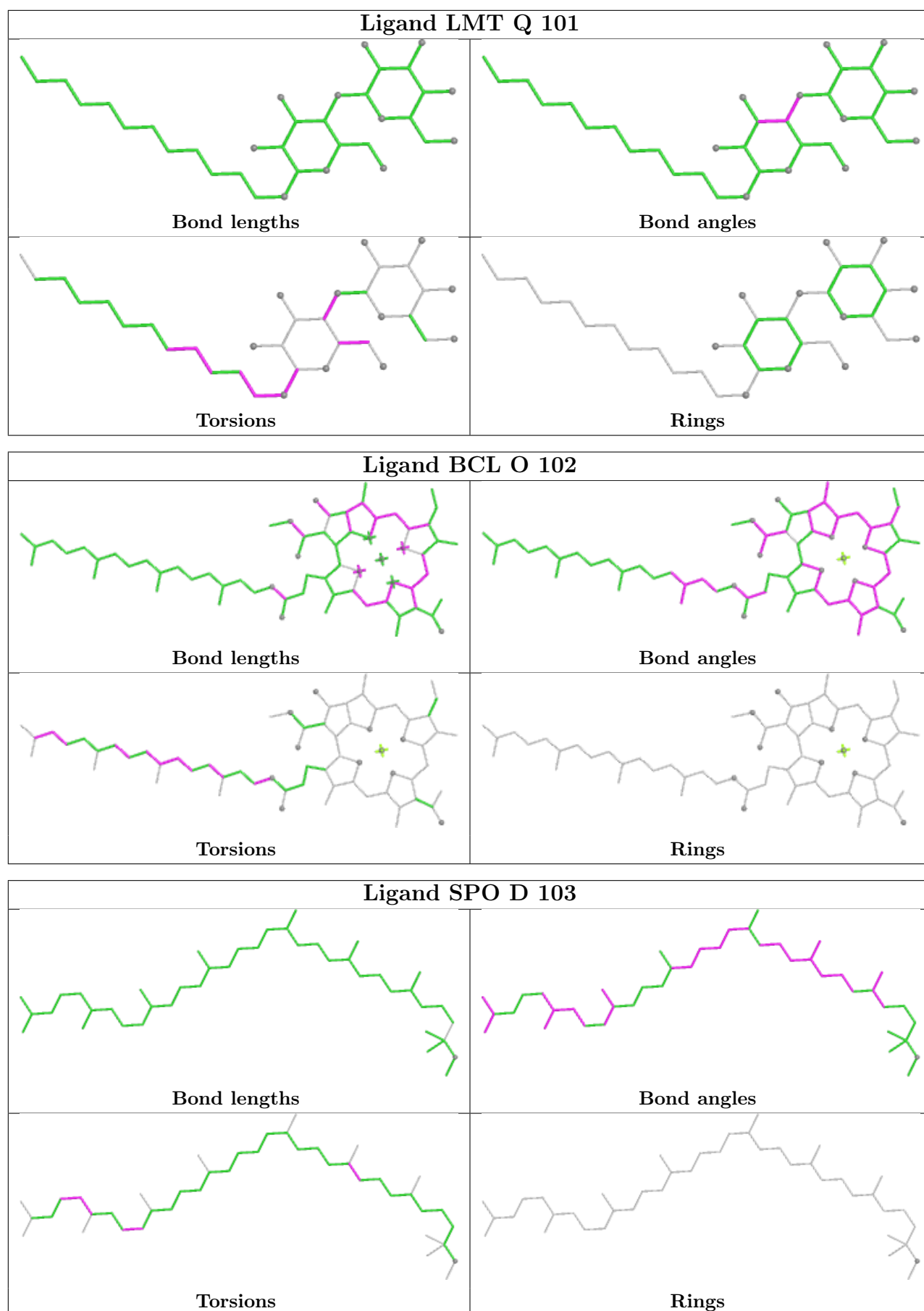
Ligand SPO T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

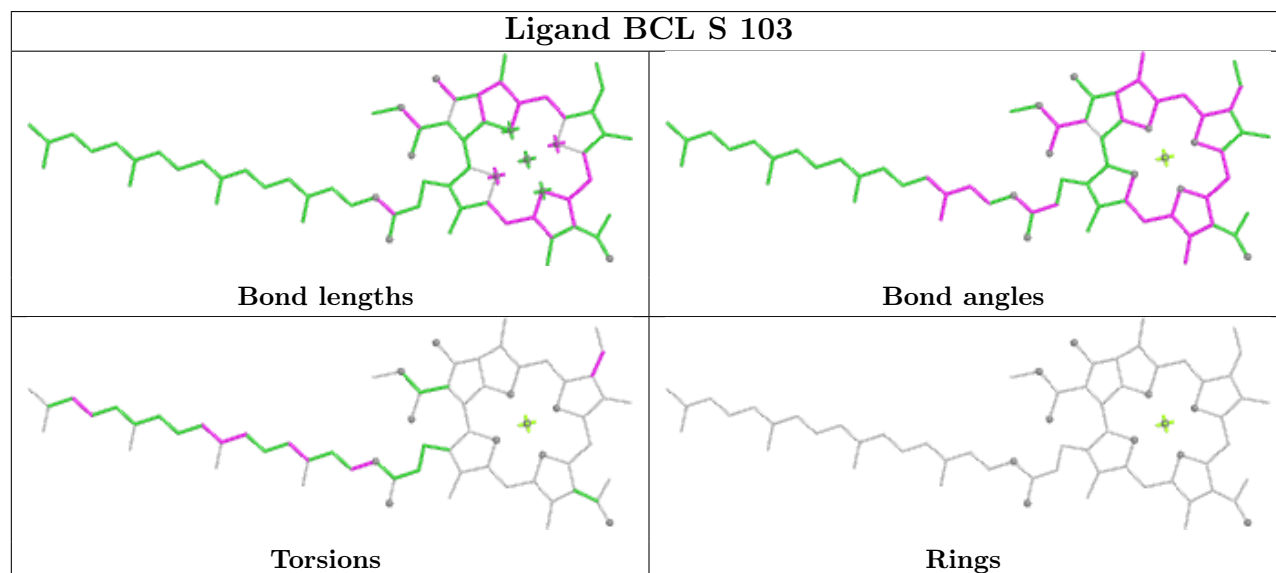
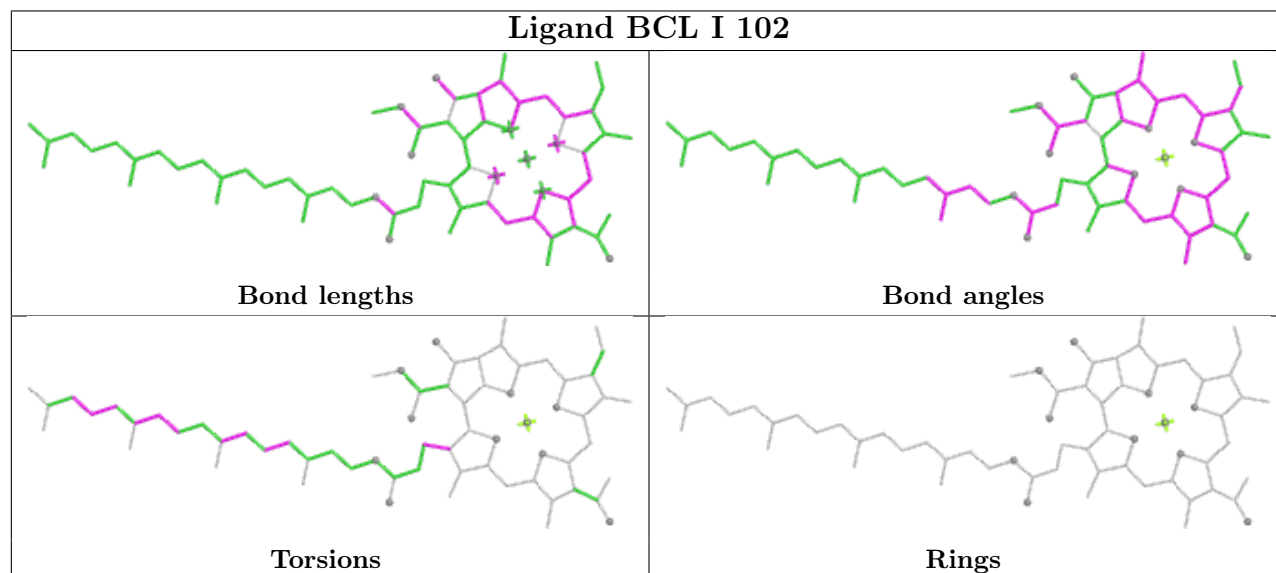
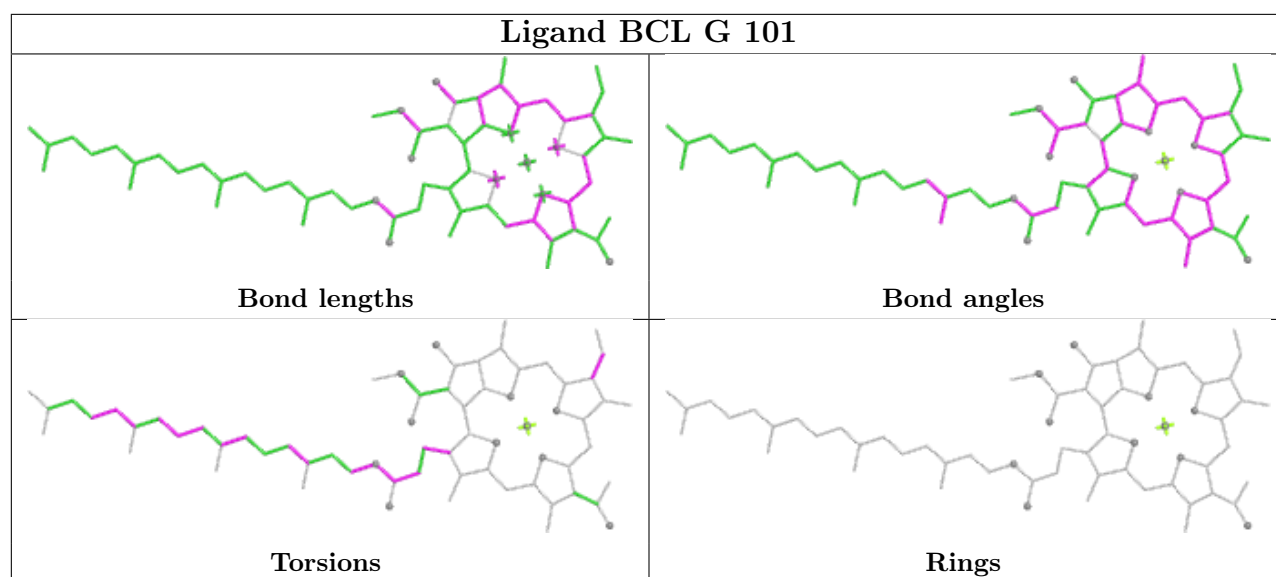
Ligand U10 M 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

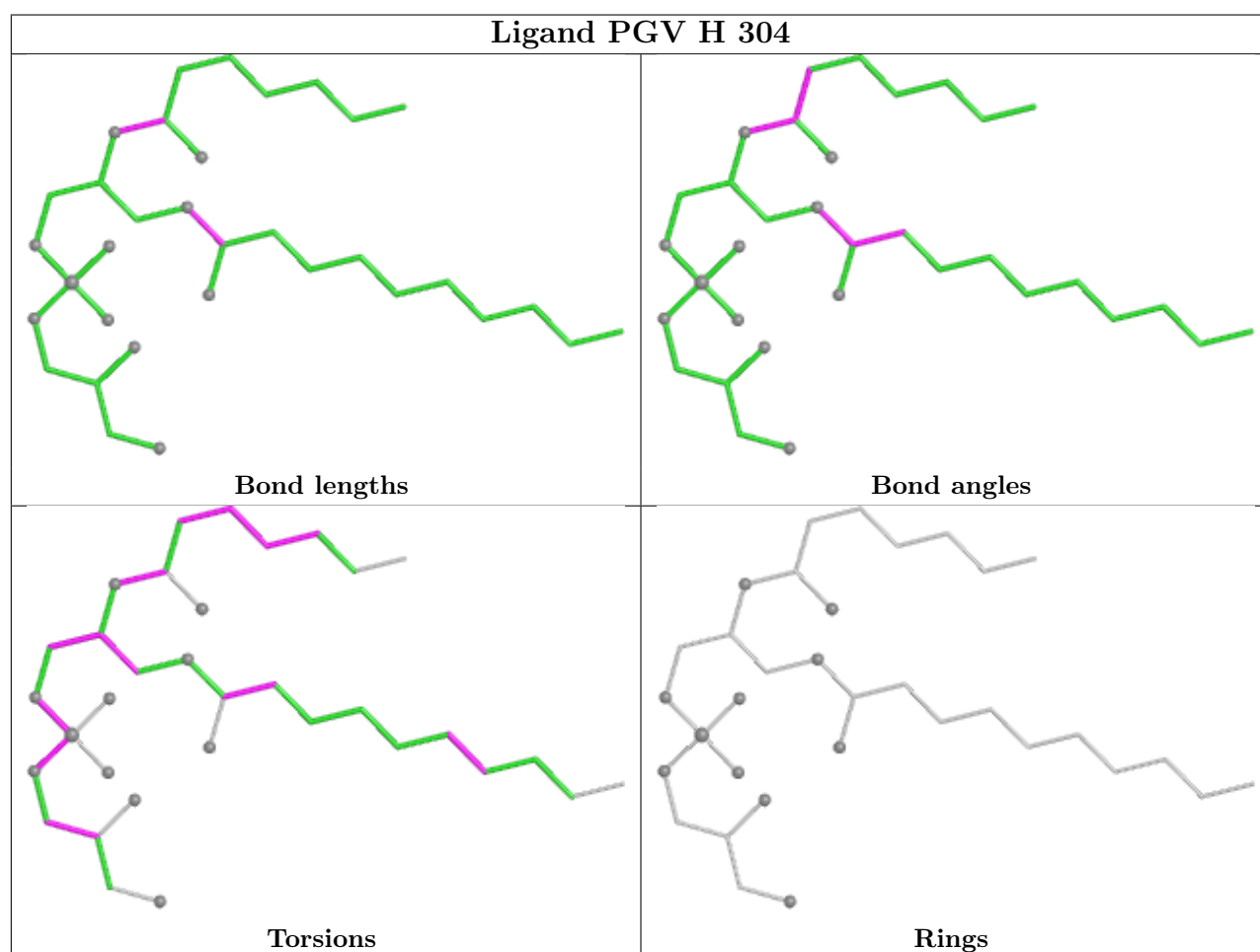
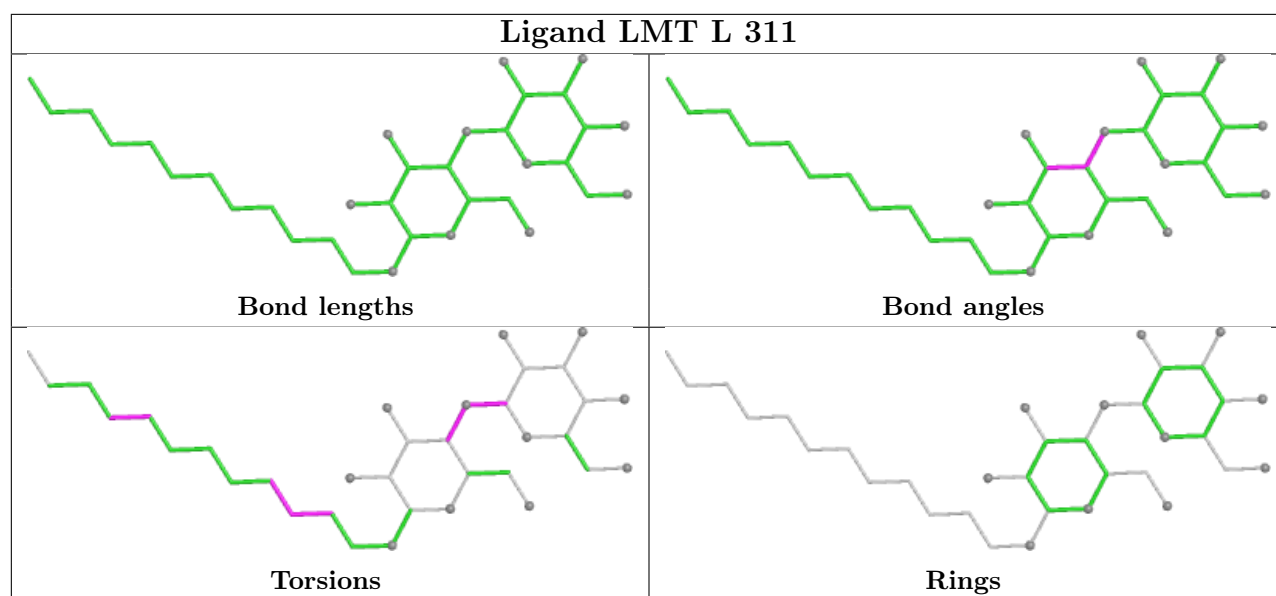
Ligand SPO F 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

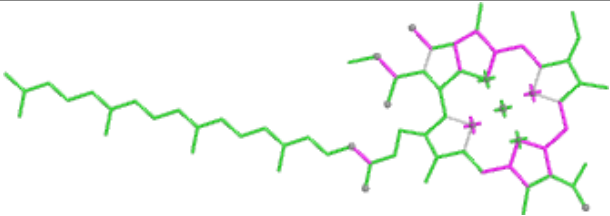
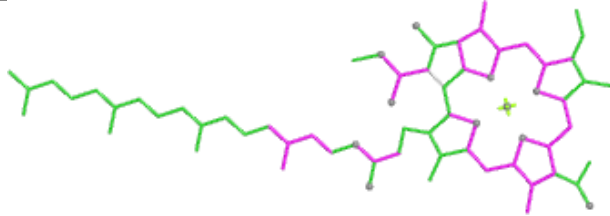
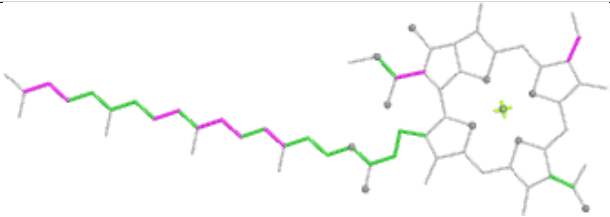
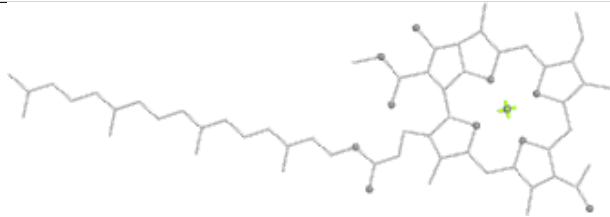
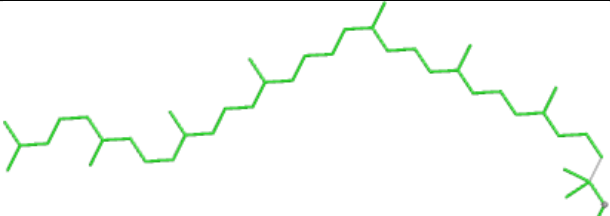
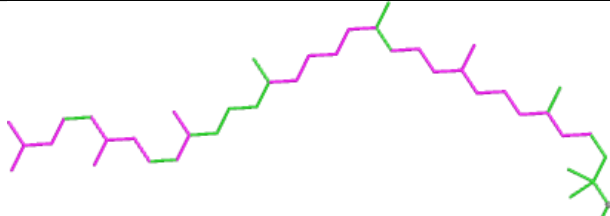
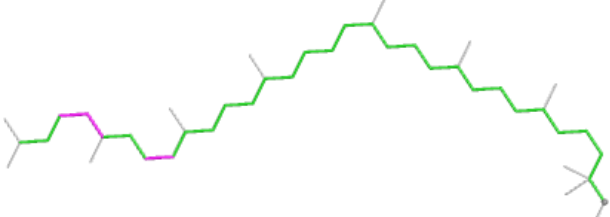
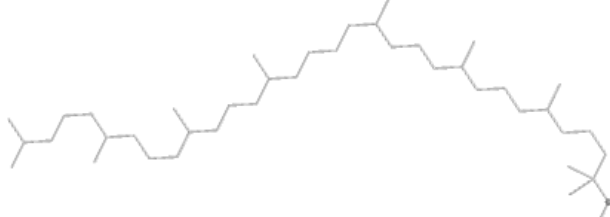


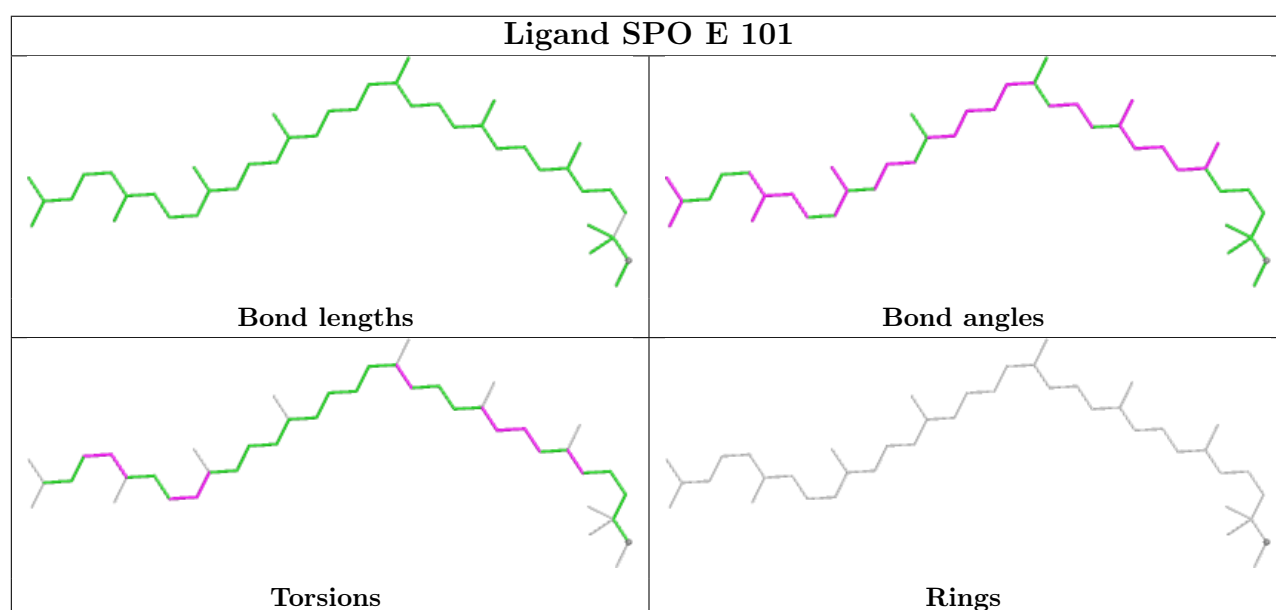
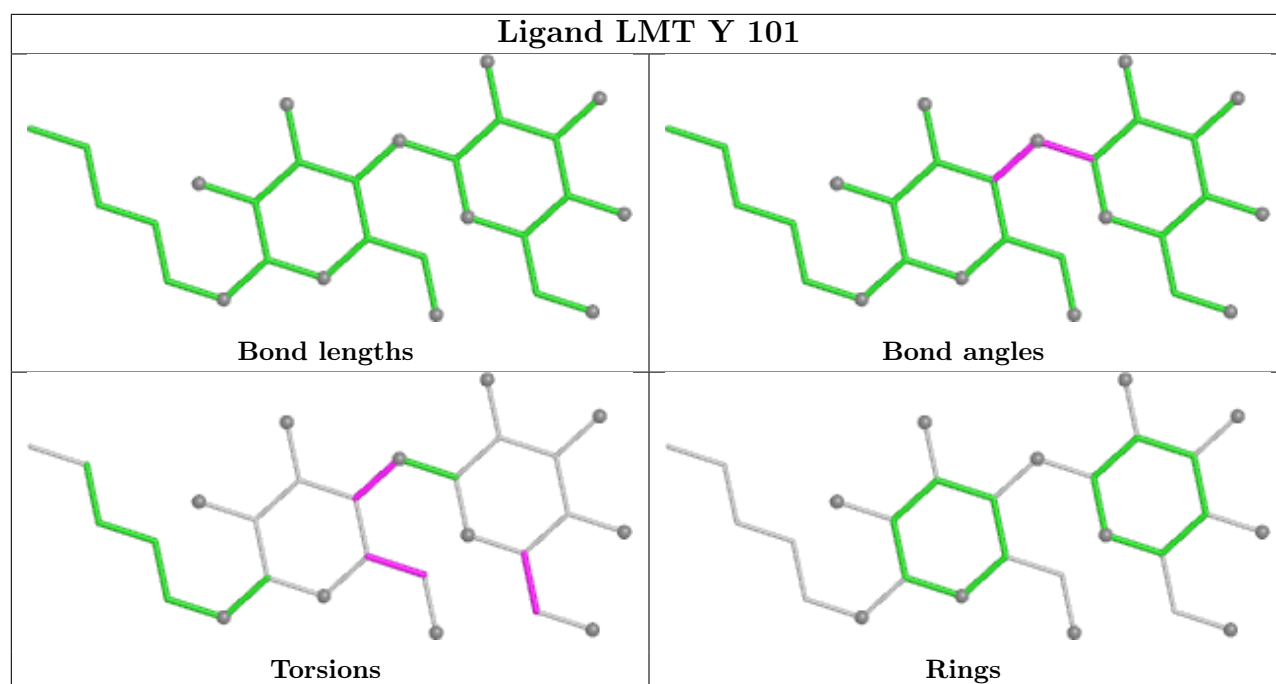


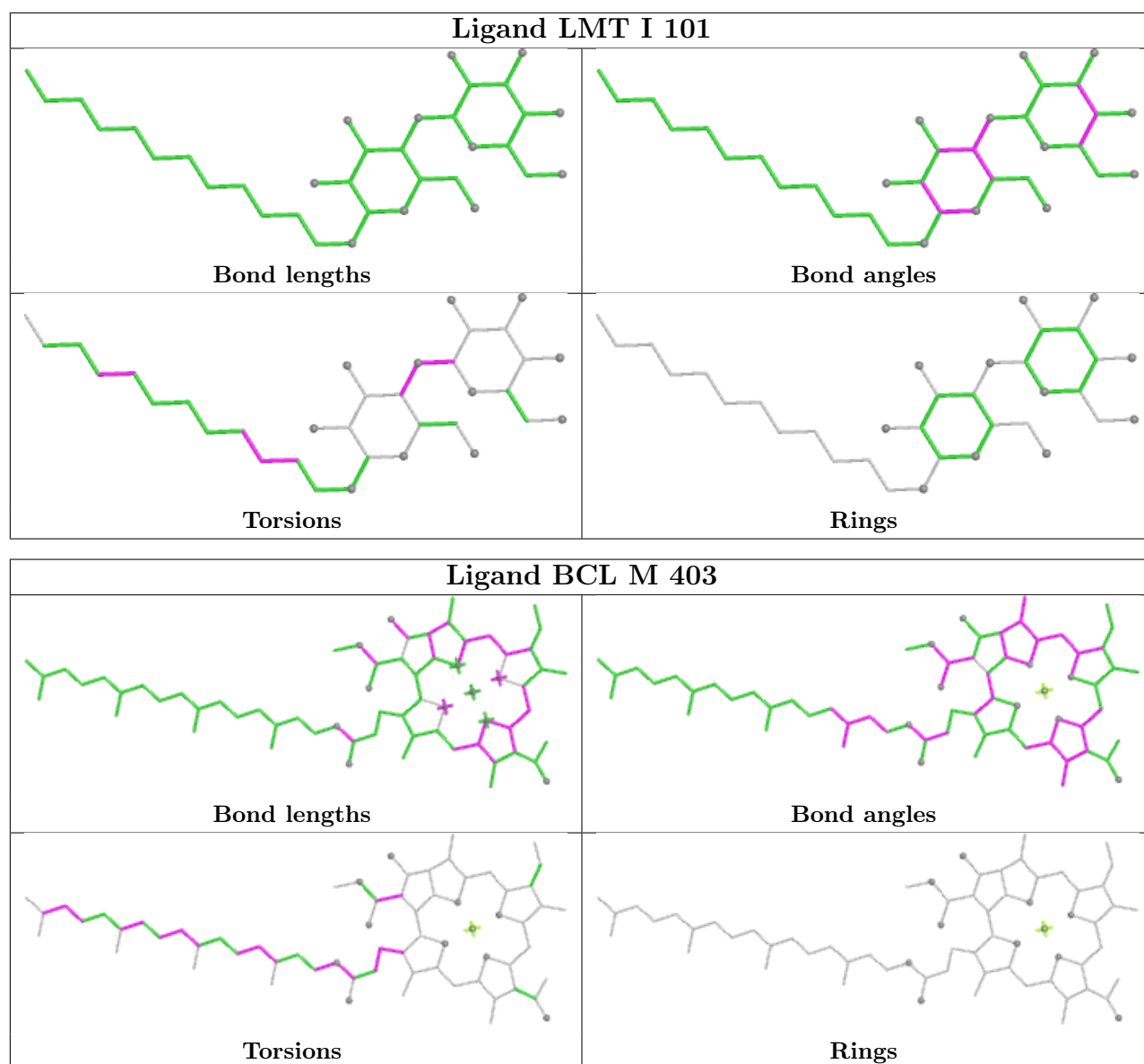




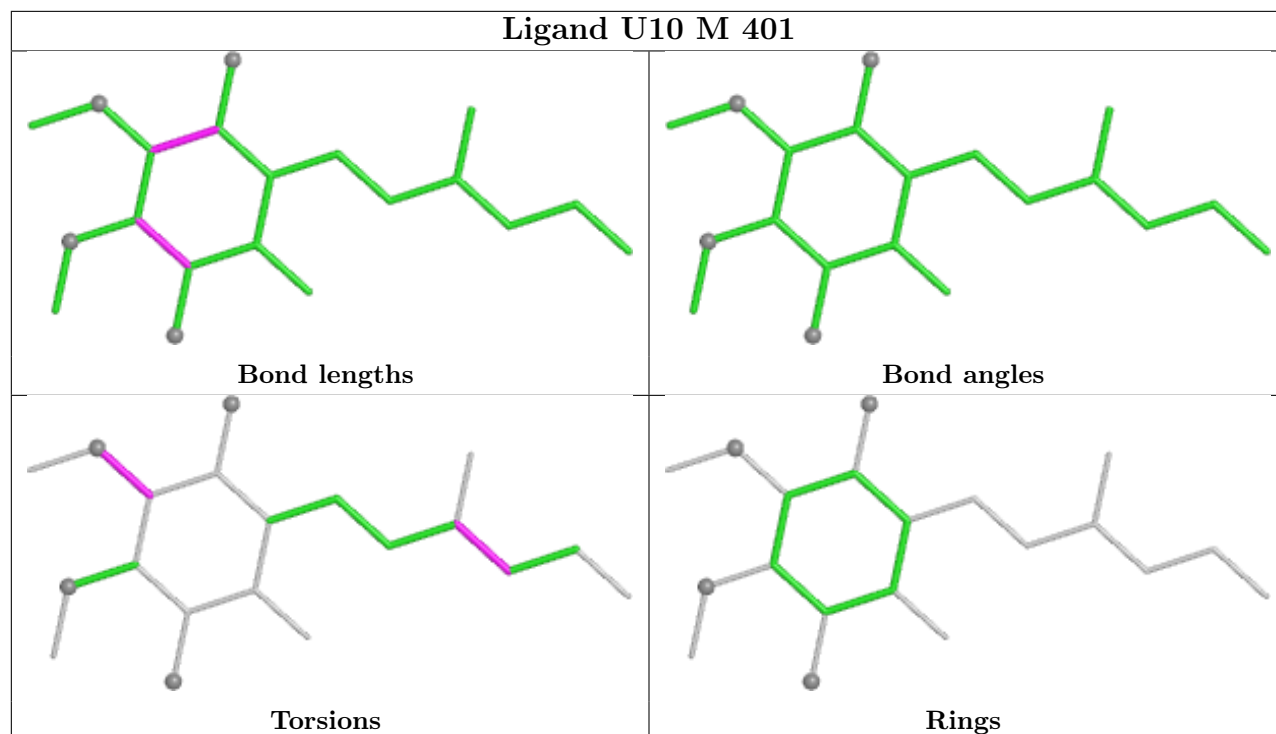


Ligand BCL V 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO S 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

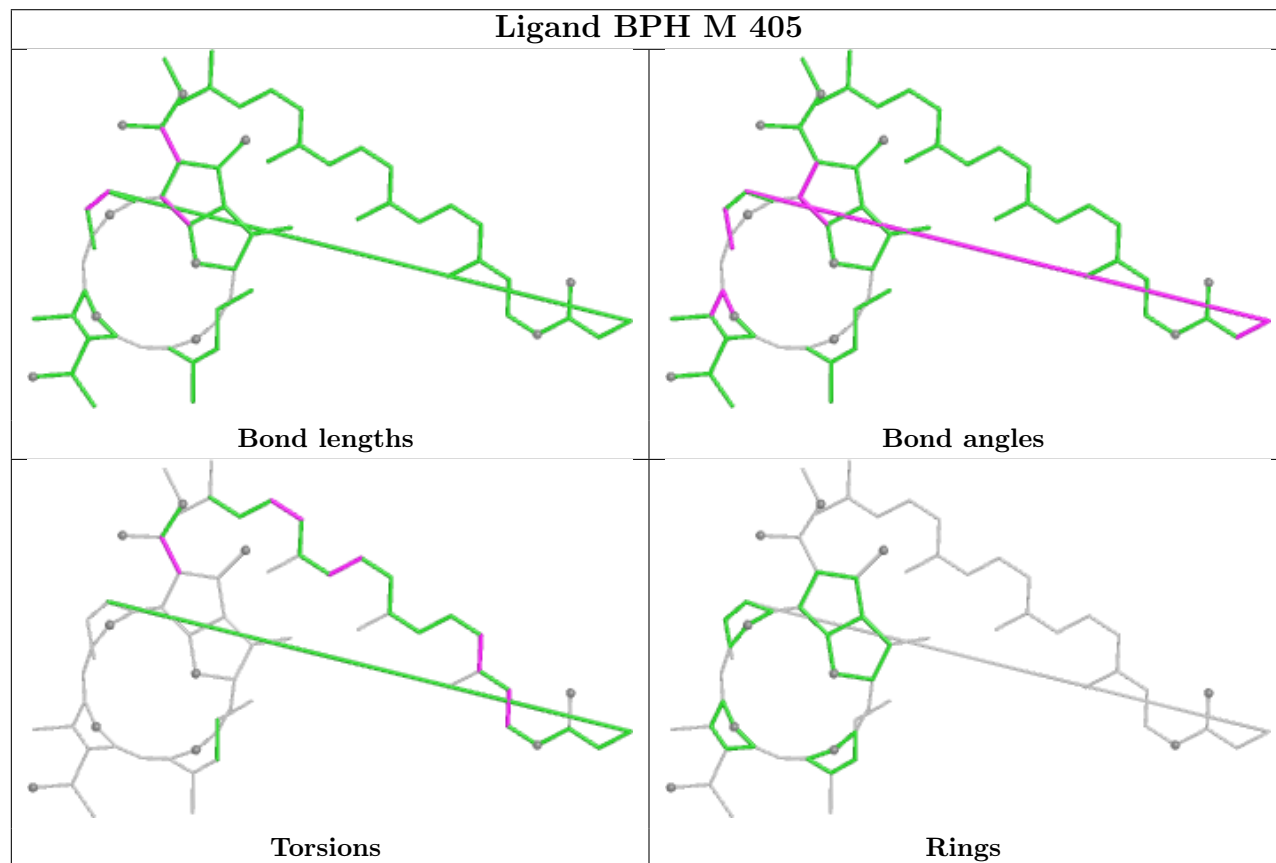


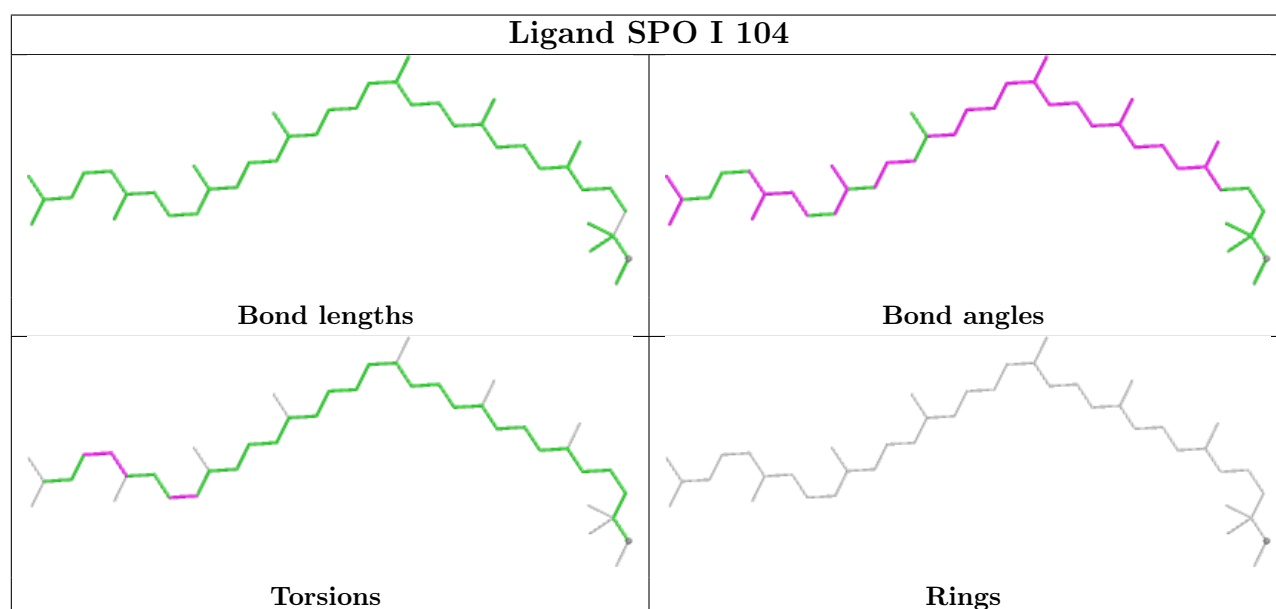
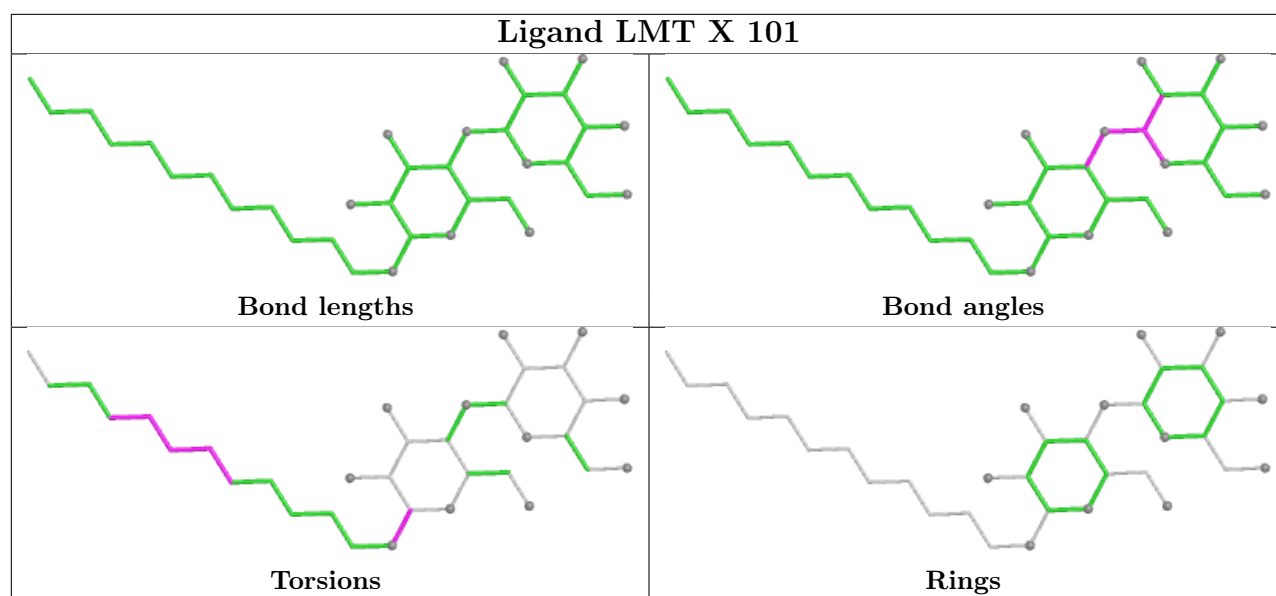


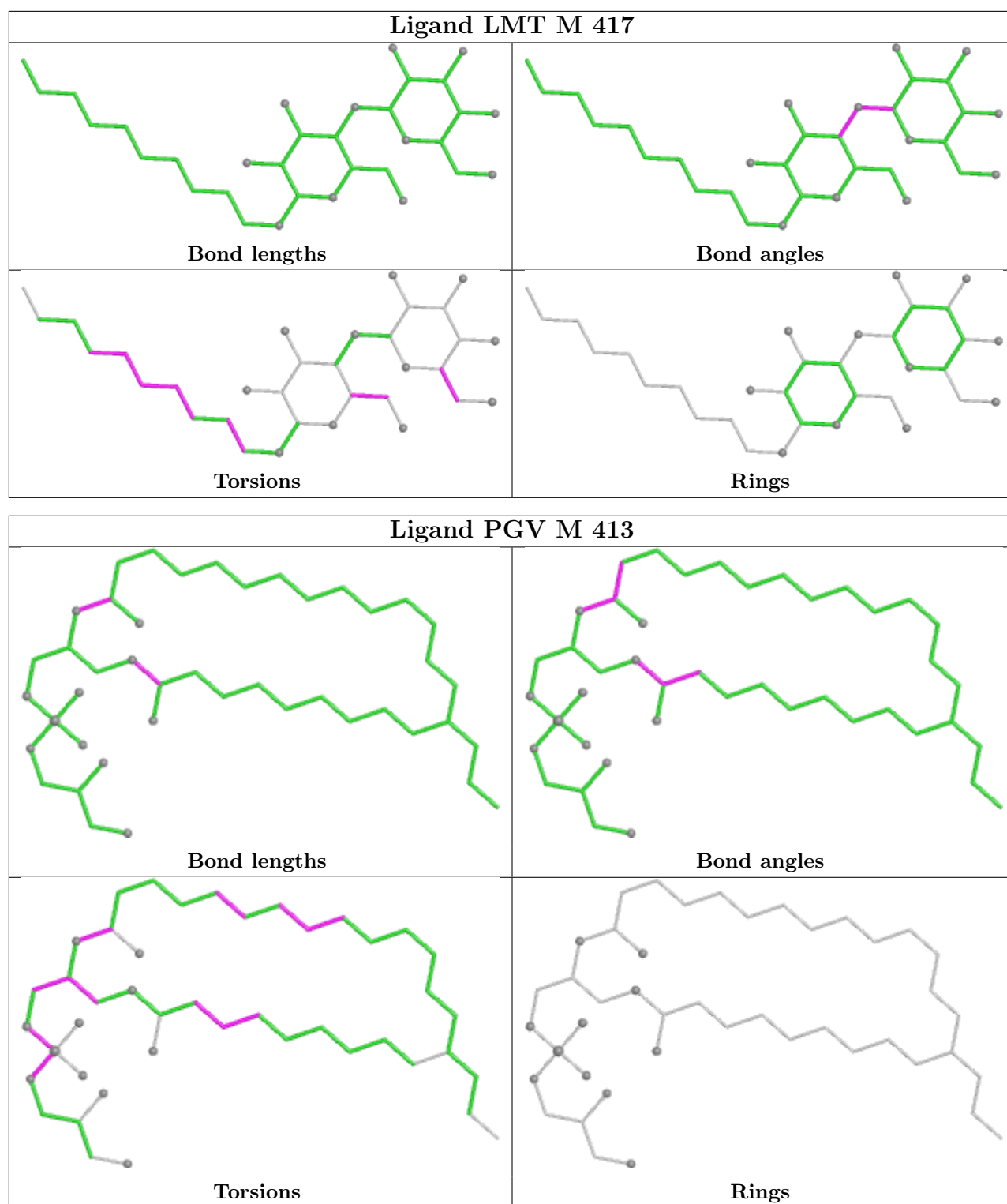
Ligand U10 M 401



Ligand BPH M 405







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

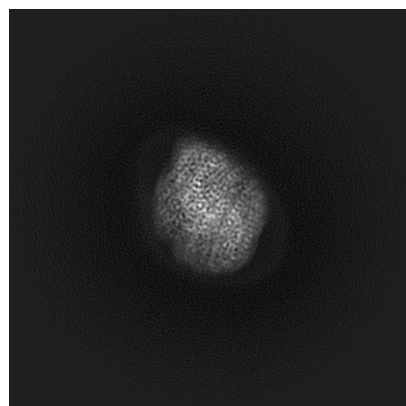
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33931. These allow visual inspection of the internal detail of the map and identification of artifacts.

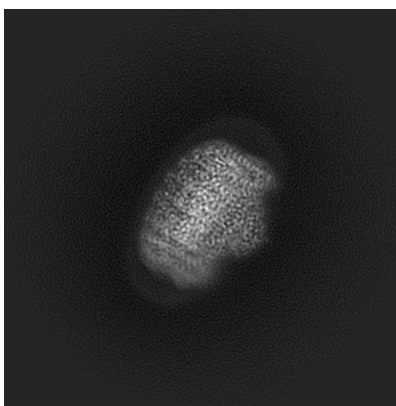
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

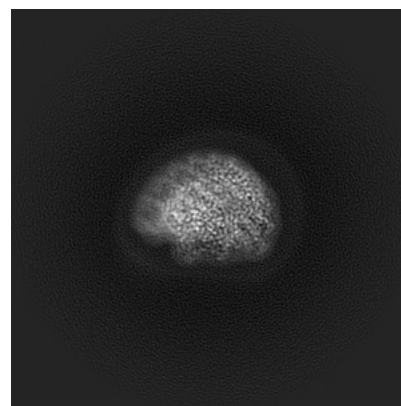
6.1.1 Primary map



X

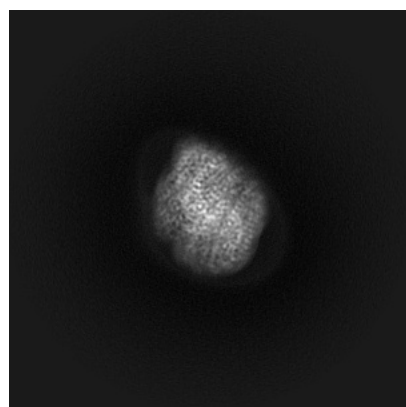


Y

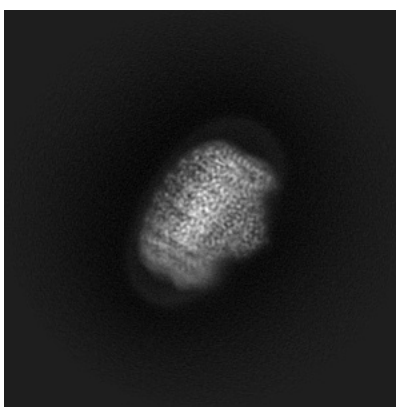


Z

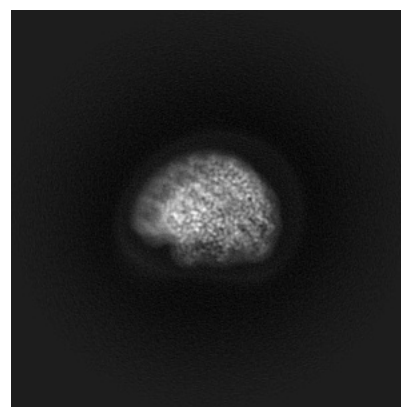
6.1.2 Raw map



X



Y

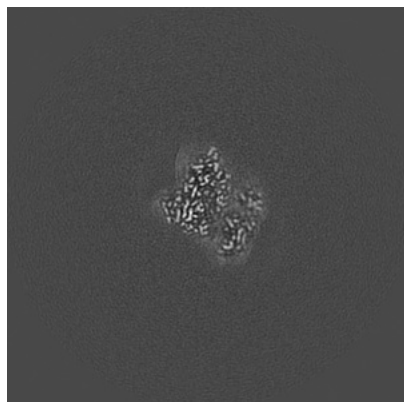


Z

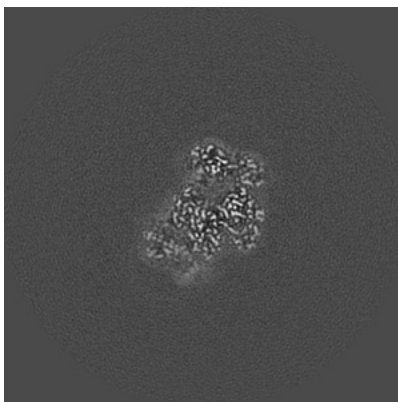
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

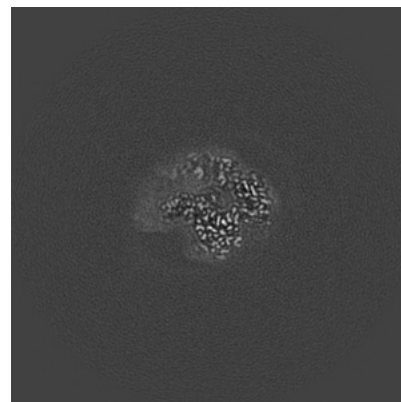
6.2.1 Primary map



X Index: 200

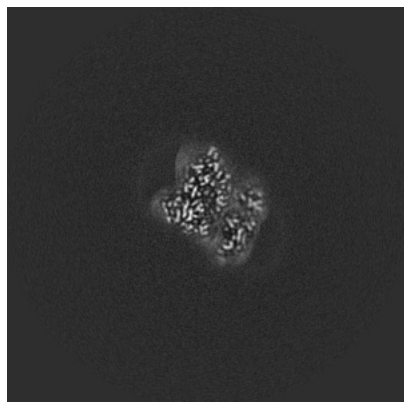


Y Index: 200

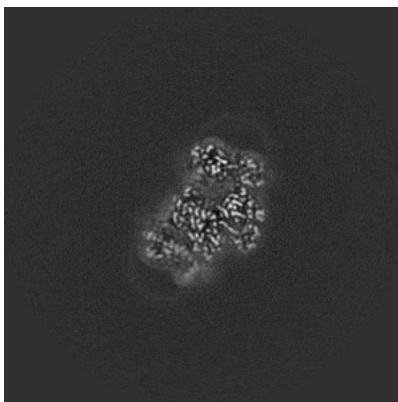


Z Index: 200

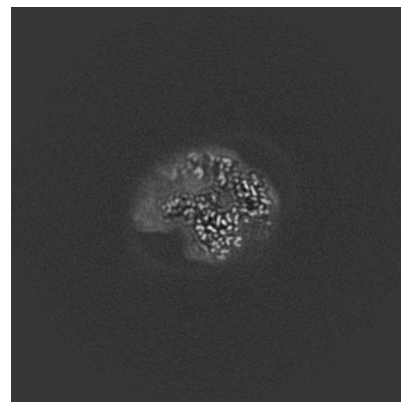
6.2.2 Raw map



X Index: 200



Y Index: 200

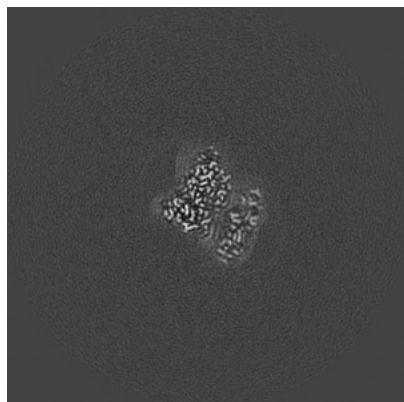


Z Index: 200

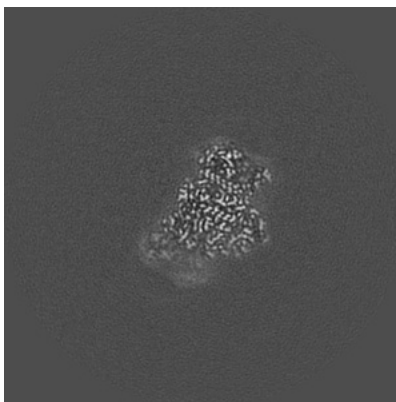
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

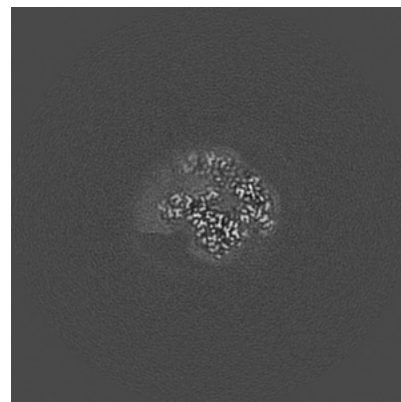
6.3.1 Primary map



X Index: 198

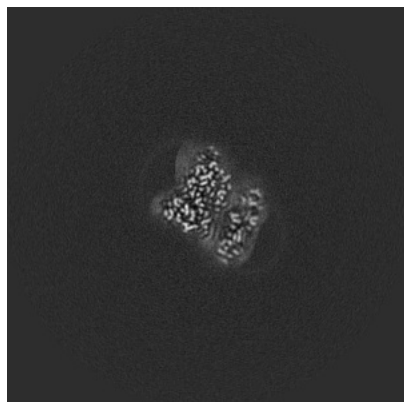


Y Index: 190

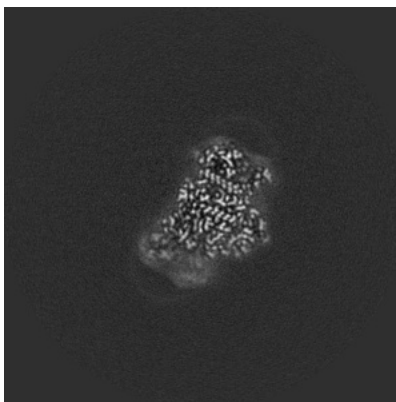


Z Index: 203

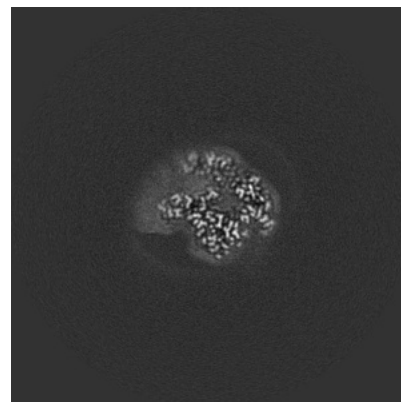
6.3.2 Raw map



X Index: 198



Y Index: 190

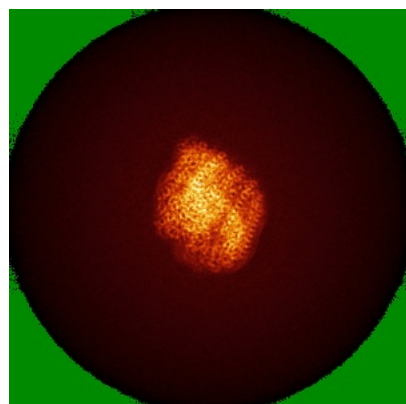


Z Index: 203

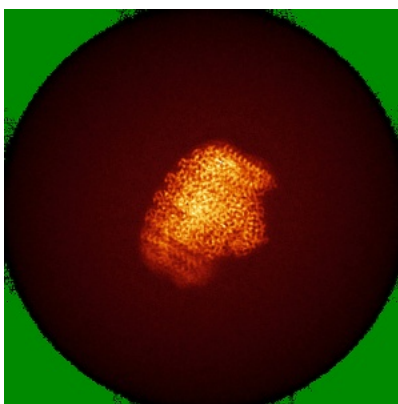
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

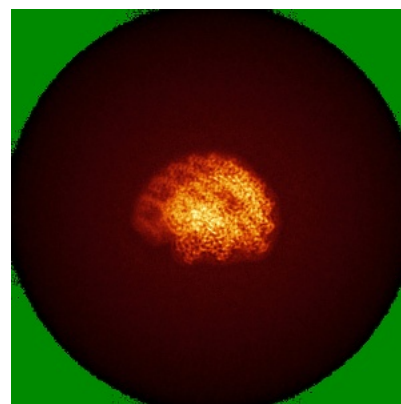
6.4.1 Primary map



X

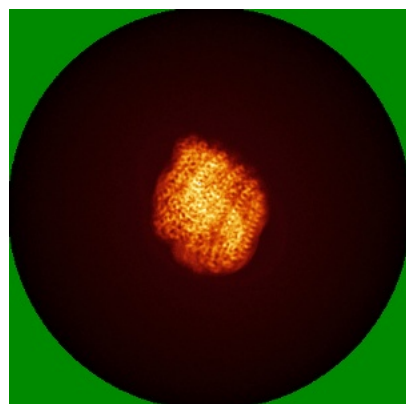


Y

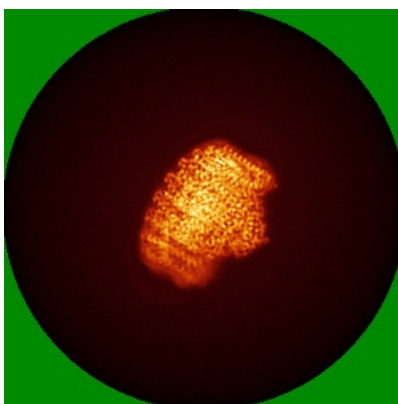


Z

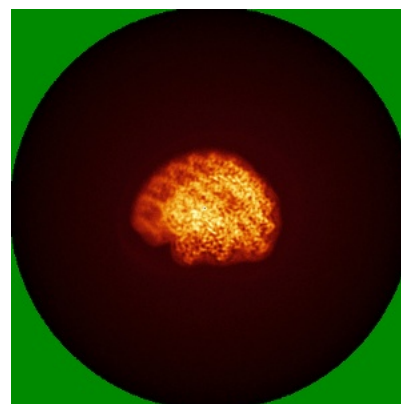
6.4.2 Raw map



X



Y

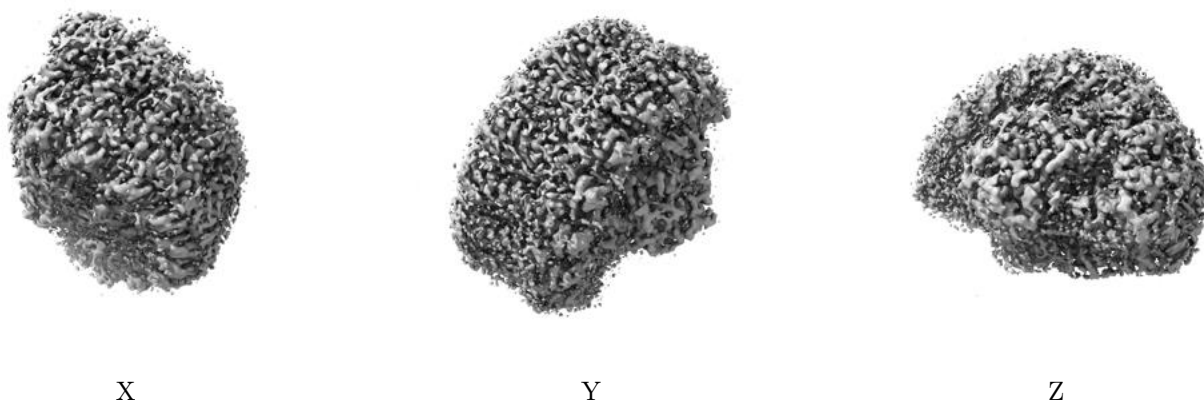


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

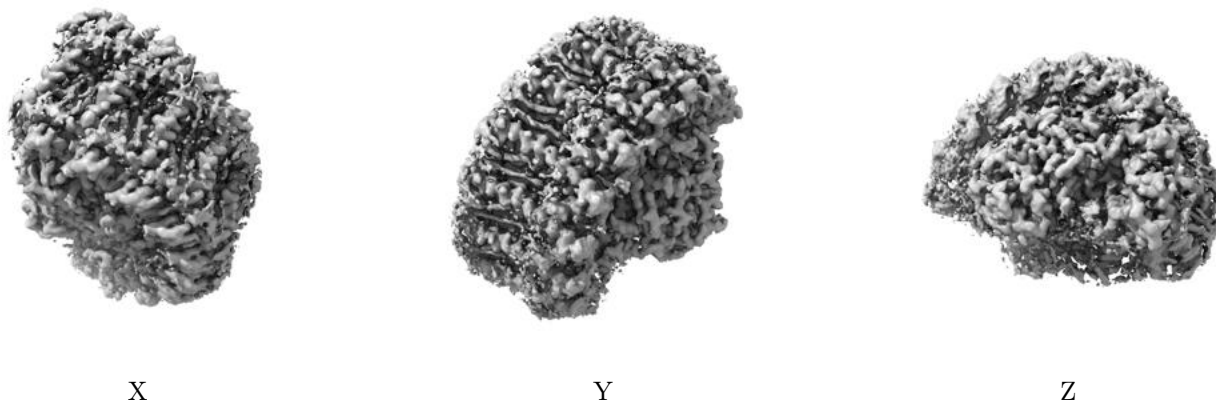
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

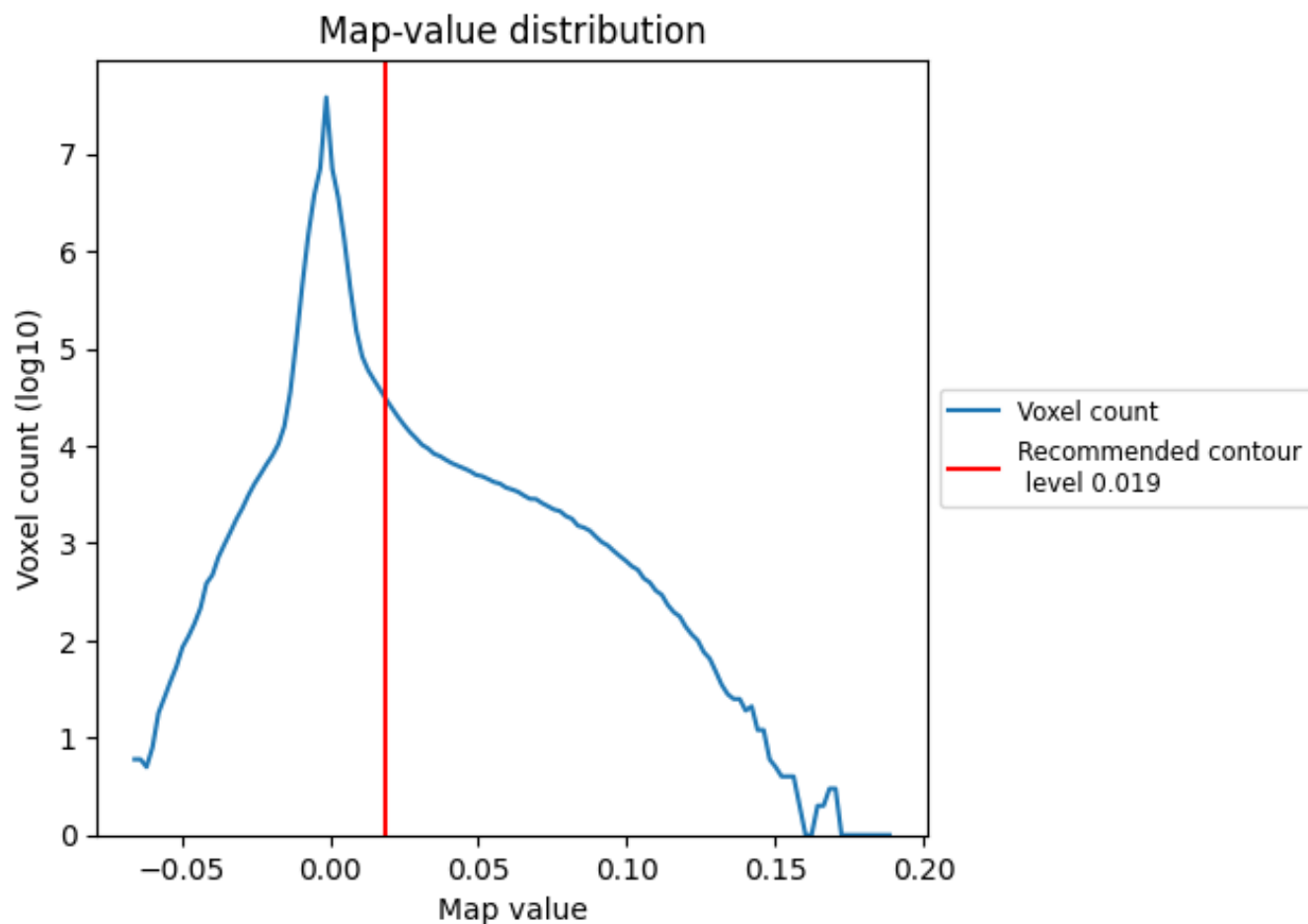
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

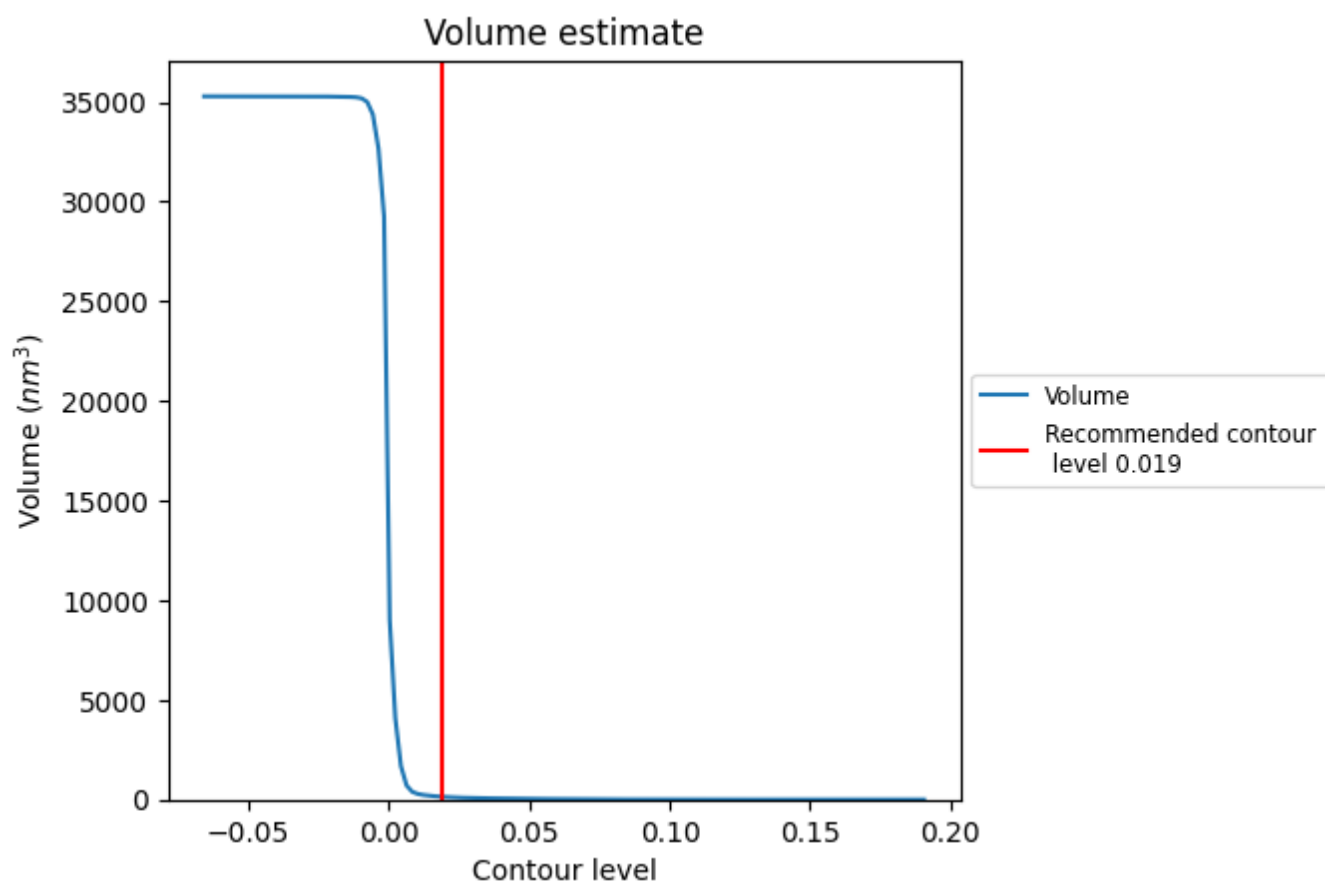
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

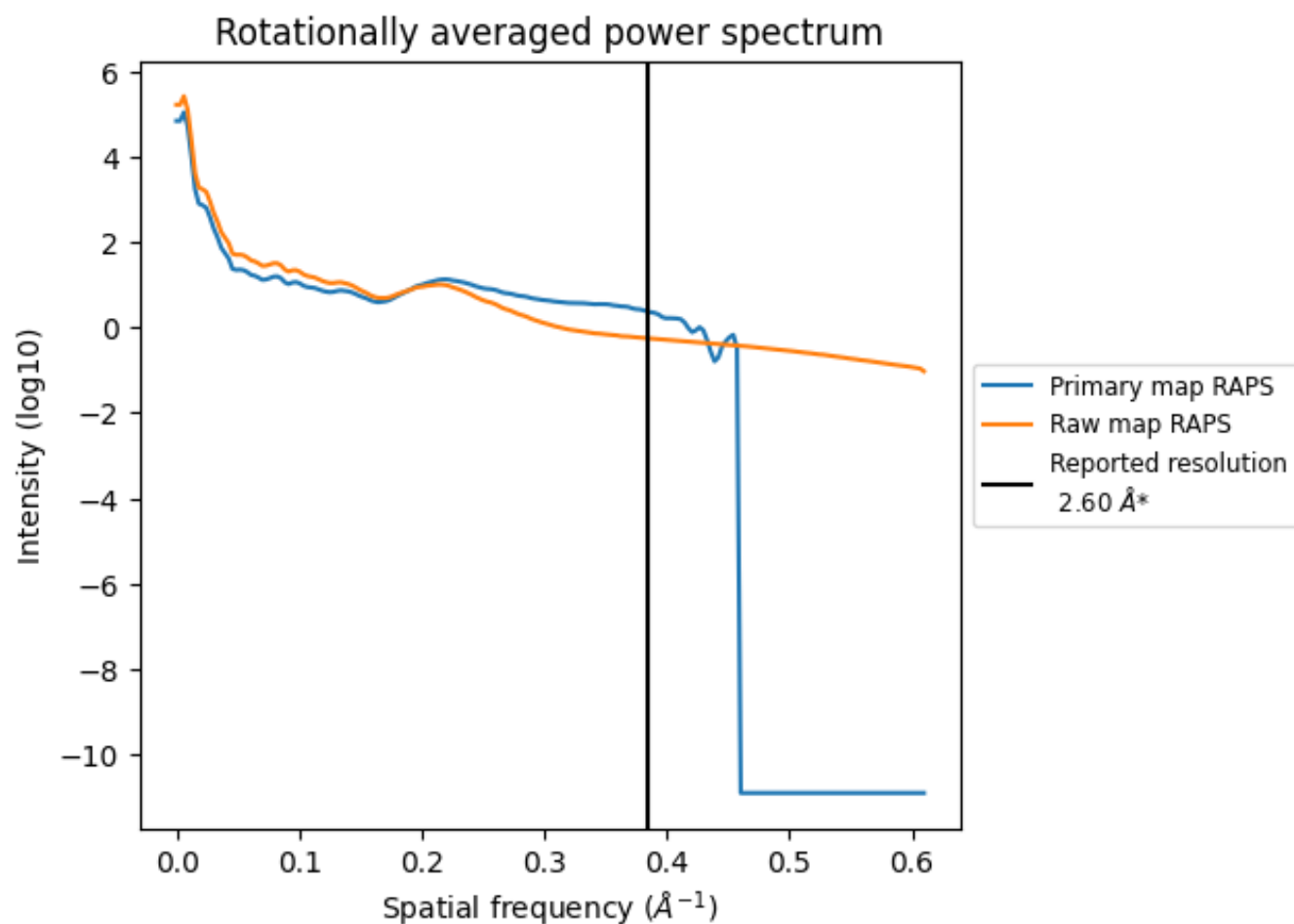
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm^3 ; this corresponds to an approximate mass of 125 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

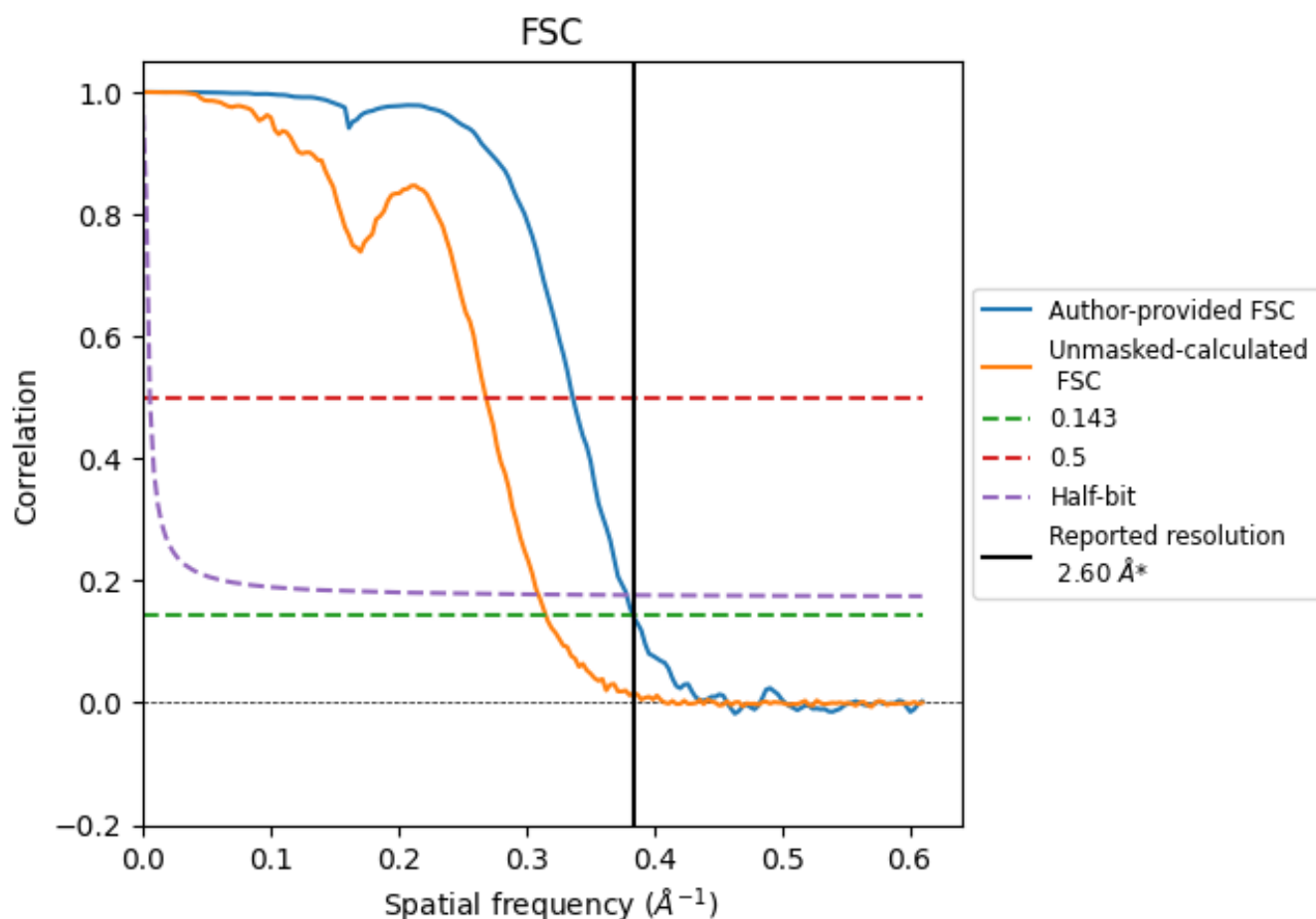


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

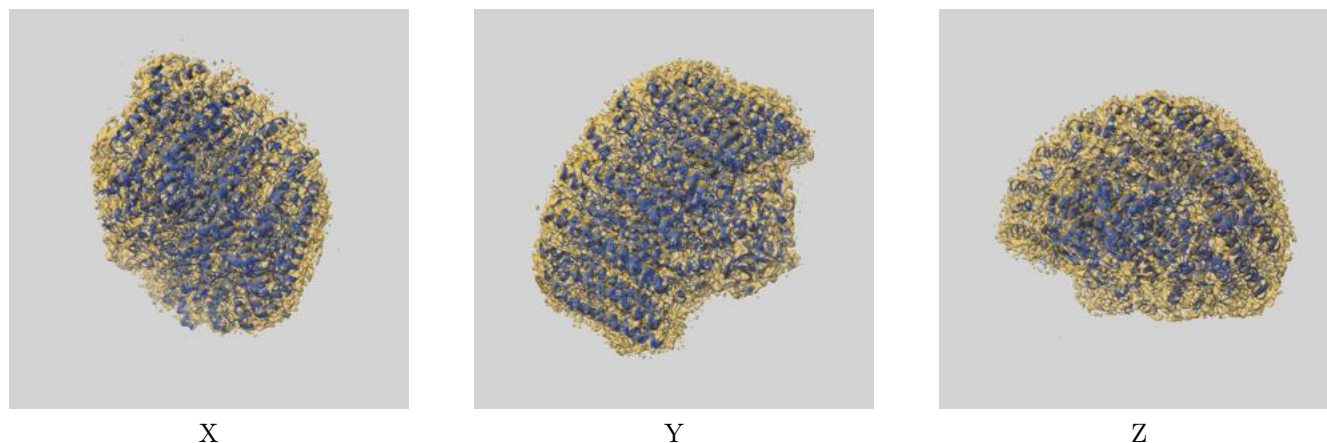
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.97	2.64
Unmasked-calculated*	3.17	3.72	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

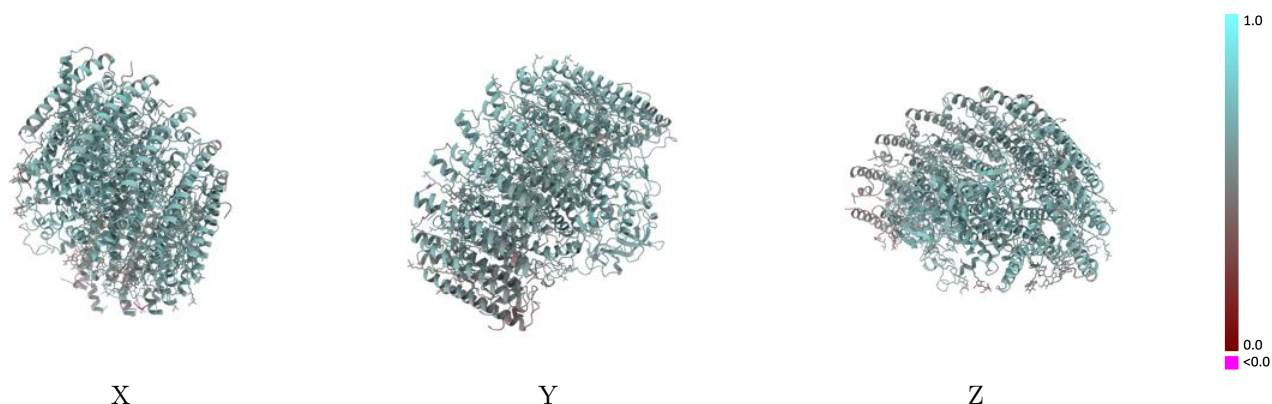
This section contains information regarding the fit between EMDB map EMD-33931 and PDB model 7YML. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



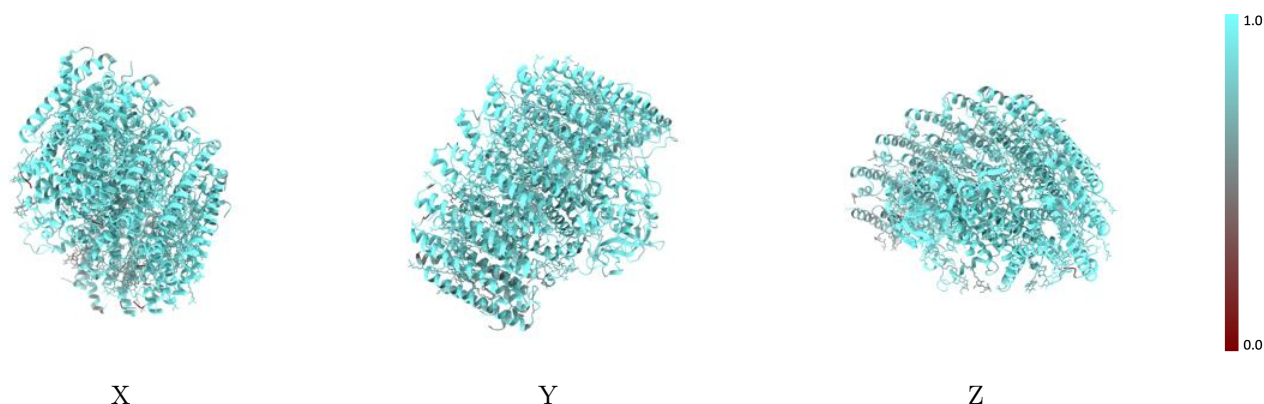
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



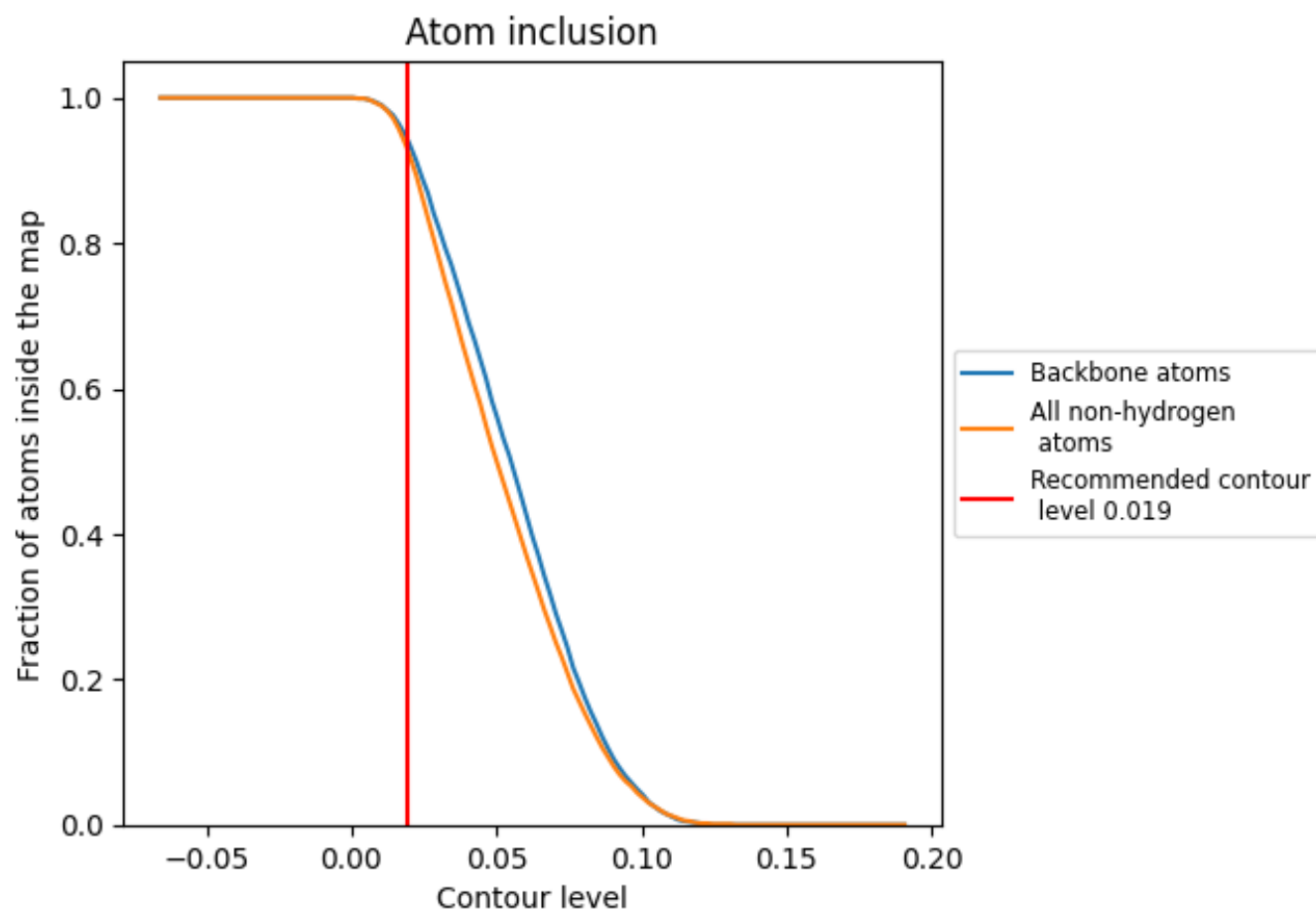
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.6130
A	 0.9610	 0.6030
B	 0.9350	 0.5990
D	 0.9530	 0.6350
E	 0.9480	 0.6210
F	 0.9730	 0.6430
G	 0.9660	 0.6390
H	 0.9480	 0.6270
I	 0.9380	 0.6340
J	 0.9550	 0.6250
K	 0.9650	 0.6230
L	 0.9630	 0.6550
M	 0.9590	 0.6470
N	 0.9310	 0.6180
O	 0.9360	 0.6260
P	 0.9310	 0.6000
Q	 0.8920	 0.5800
R	 0.9190	 0.5840
S	 0.8880	 0.5580
T	 0.9040	 0.5780
V	 0.8530	 0.5280
W	 0.8600	 0.5320
X	 0.9320	 0.6100
Y	 0.7180	 0.4540
Z	 0.6650	 0.3590

