



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 06:39 PM UTC

PDB ID : 7XXF / pdb_00007xxf
EMDB ID : EMD-33501
Title : Structure of photosynthetic LH1-RC super-complex of Rhodospila globiformis
Authors : Tani, K.; Kanno, R.; Kurosawa, K.; Takaichi, S.; Nagashima, K.V.P.; Hall, M.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2022-05-30
Resolution : 2.24 Å (reported)
Based on initial model : 5Y5S

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

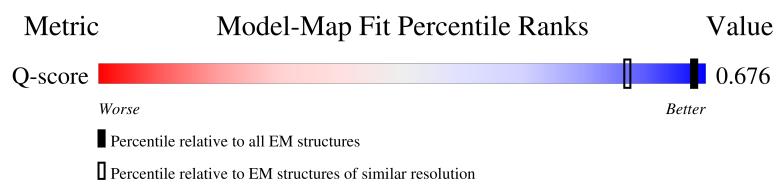
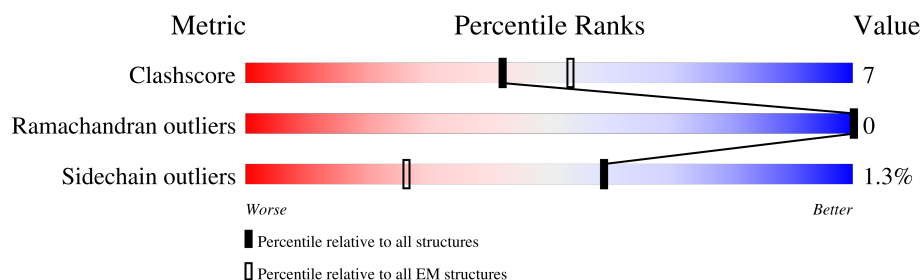
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.24 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.



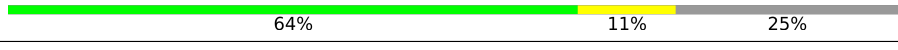
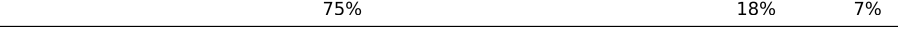
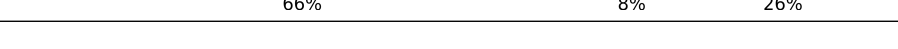
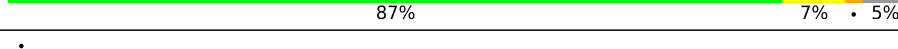
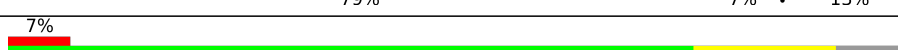
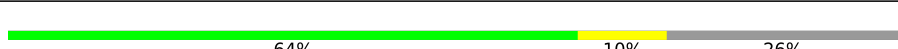
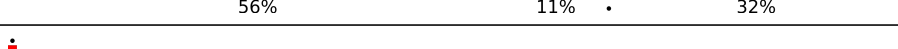
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3381 (1.75 - 2.74)

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	C	344	 91% 8%
2	L	275	 86% 13% .
3	M	326	 83% 14% ..

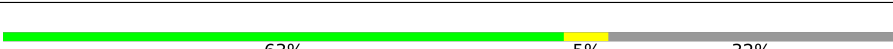
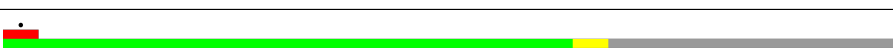
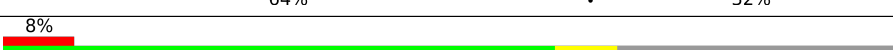
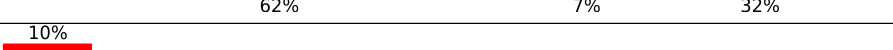
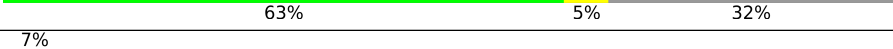
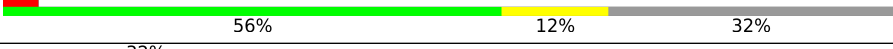
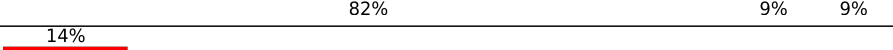
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Mol	Chain	Length	Quality of chain
4	H	258	
5	1	61	
5	3	61	
5	5	61	
5	7	61	
5	9	61	
5	A	61	
5	D	61	
5	F	61	
5	I	61	
5	K	61	
5	O	61	
5	Q	61	
5	S	61	
5	U	61	
5	W	61	
5	Y	61	
6	0	73	
6	2	73	
6	4	73	
6	6	73	
6	8	73	
6	B	73	
6	E	73	
6	G	73	

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Mol	Chain	Length	Quality of chain
6	J	73	
6	N	73	
6	P	73	
6	R	73	
6	T	73	
6	V	73	
6	X	73	
6	Z	73	
7	a	22	
7	b	22	
7	c	22	
7	d	22	
7	e	22	
7	f	22	
7	g	22	
7	h	22	
7	i	22	
7	j	22	
7	k	22	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 29826 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	343	Total	C	N	O	S	0	0
			2655	1683	471	481	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	274	Total	C	N	O	S	0	0
			2177	1469	353	347	8		

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	320	Total	C	N	O	S	1	0
			2550	1714	421	404	11		

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	258	Total	C	N	O	S	0	0
			2000	1284	332	376	8		

- Molecule 5 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	D	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	F	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	I	46	Total	C	N	O	S	0	0
			394	270	66	56	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	O	45	Total	C	N	O	S	0	0
			389	267	65	55	2		
5	Q	45	Total	C	N	O	S	0	0
			389	267	65	55	2		
5	S	58	Total	C	N	O	S	0	0
			475	321	82	69	3		
5	U	53	Total	C	N	O	S	0	0
			443	299	77	64	3		
5	W	57	Total	C	N	O	S	0	0
			470	318	81	68	3		
5	Y	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	1	46	Total	C	N	O	S	0	0
			395	270	67	56	2		
5	3	57	Total	C	N	O	S	0	0
			472	321	79	69	3		
5	5	45	Total	C	N	O	S	0	0
			389	267	65	55	2		
5	7	45	Total	C	N	O	S	0	0
			389	267	65	55	2		
5	9	45	Total	C	N	O	S	1	0
			392	270	64	56	2		

- Molecule 6 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	B	50	Total	C	N	O	0	0
			396	268	62	66		
6	E	50	Total	C	N	O	0	0
			396	268	62	66		
6	G	50	Total	C	N	O	0	0
			396	268	62	66		
6	J	50	Total	C	N	O	0	0
			396	268	62	66		
6	N	50	Total	C	N	O	0	0
			396	268	62	66		
6	P	50	Total	C	N	O	0	0
			396	268	62	66		
6	R	50	Total	C	N	O	0	0
			396	268	62	66		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	50	Total	C	N	O	0	0
			396	268	62	66		
6	V	50	Total	C	N	O	0	0
			396	268	62	66		
6	X	50	Total	C	N	O	0	0
			396	268	62	66		
6	Z	50	Total	C	N	O	0	0
			396	268	62	66		
6	2	50	Total	C	N	O	0	0
			396	268	62	66		
6	4	50	Total	C	N	O	0	0
			396	268	62	66		
6	6	50	Total	C	N	O	0	0
			396	268	62	66		
6	8	50	Total	C	N	O	0	0
			396	268	62	66		
6	0	50	Total	C	N	O	0	0
			396	268	62	66		

- Molecule 7 is a protein called Light-harvesting protein LH1 Gamma-like.

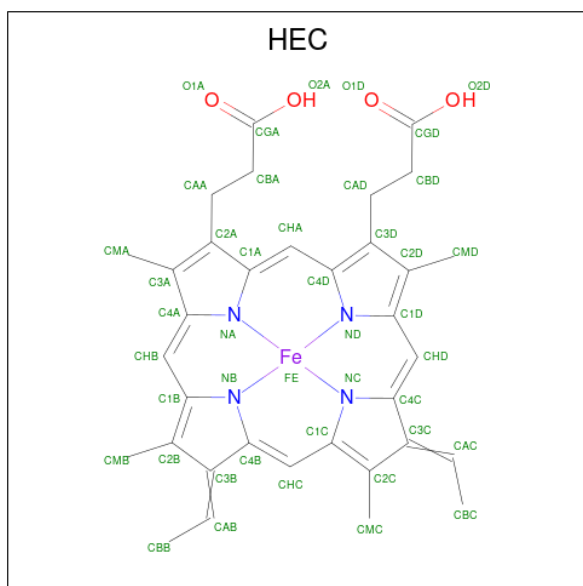
Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	b	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	c	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	d	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	e	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	f	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	g	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	h	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	i	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	j	22	Total	C	N	O	S	0	0
			177	120	28	26	3		

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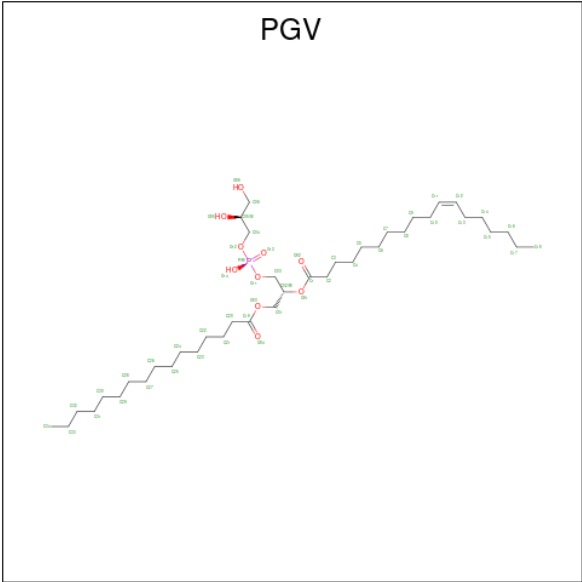
Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	22	Total	C	N	O	S	0	0
			177	120	28	26	3		

- Molecule 8 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
8	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 9 is (1R)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY](HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



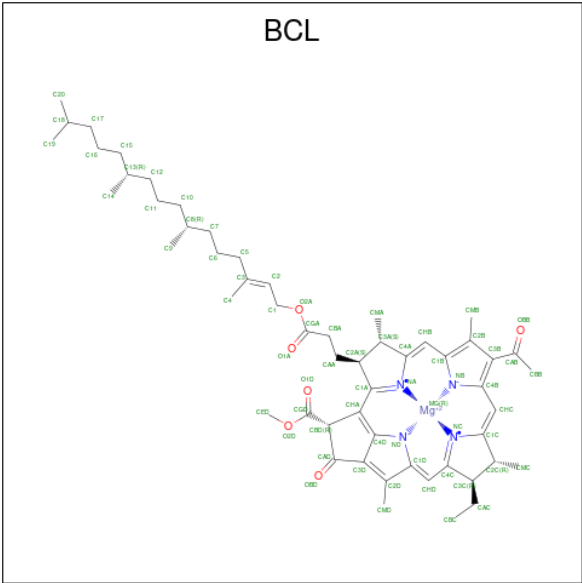
Mol	Chain	Residues	Atoms				AltConf
9	C	1	Total	C	O	P	0
			44	33	10	1	
9	C	1	Total	C	O	P	0
			42	31	10	1	
9	C	1	Total	C	O	P	0
			38	29	8	1	
9	L	1	Total	C	O	P	0
			43	32	10	1	
9	L	1	Total	C	O	P	0
			44	33	10	1	
9	L	1	Total	C	O	P	0
			37	26	10	1	
9	L	1	Total	C	O	P	0
			33	22	10	1	
9	L	1	Total	C	O	P	0
			34	23	10	1	
9	M	1	Total	C	O	P	0
			51	40	10	1	
9	M	1	Total	C	O	P	0
			33	22	10	1	
9	H	1	Total	C	O	P	0
			36	25	10	1	
9	H	1	Total	C	O	P	0
			36	25	10	1	
9	D	1	Total	C	O	P	0
			33	22	10	1	
9	F	1	Total	C	O	P	0
			39	29	9	1	

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Mol	Chain	Residues	Atoms				AltConf
9	K	1	Total	C	O	P	0
			39	28	10	1	
9	5	1	Total	C	O	P	0
			37	28	8	1	
9	5	1	Total	C	O	P	0
			37	28	8	1	
9	5	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 10 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	D	1	Total 66	C 55	Mg 1	N 4	O 6	0

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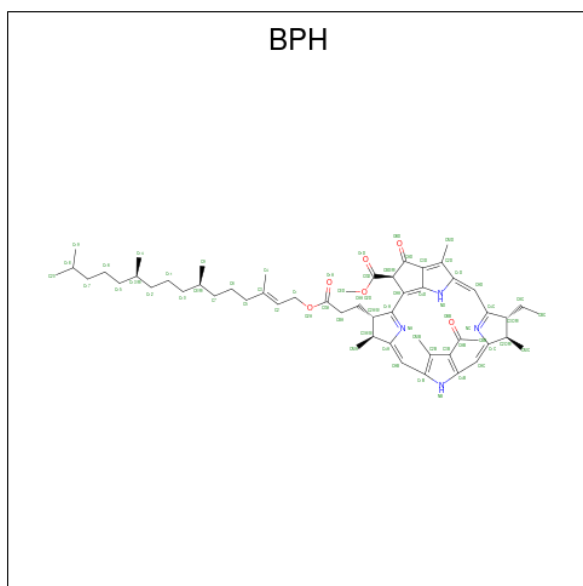
Mol	Chain	Residues	Atoms					AltConf
10	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	2	1	Total 66	C 55	Mg 1	N 4	O 6	0

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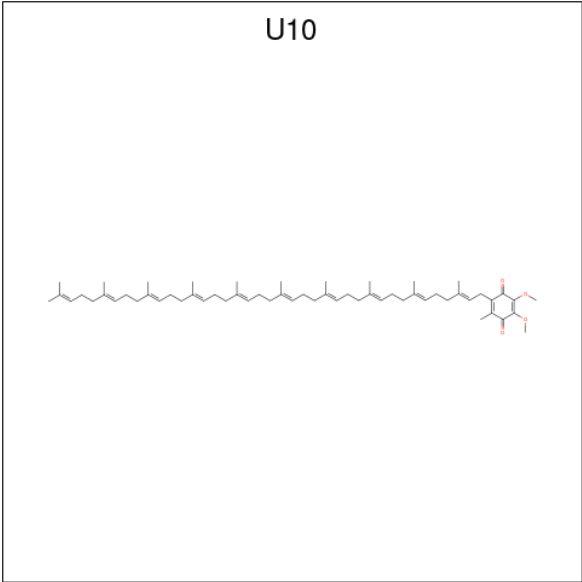
Mol	Chain	Residues	Atoms					AltConf
10	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 11 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



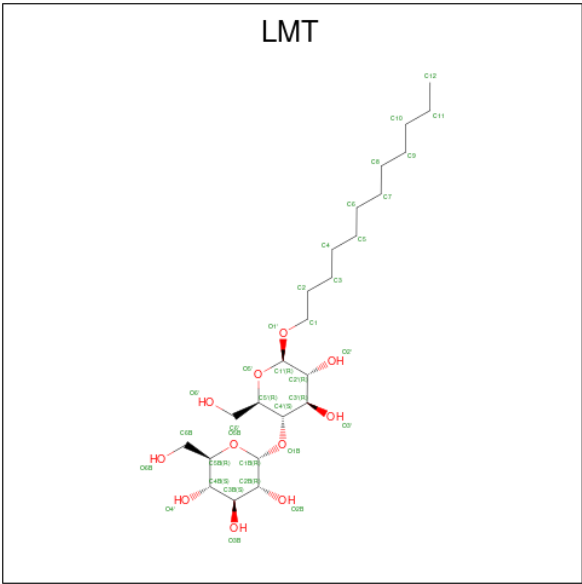
Mol	Chain	Residues	Atoms				AltConf
11	L	1	Total	C	N	O	0
			65	55	4	6	
11	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			36	32	4	
12	L	1	Total	C	O	0
			15	11	4	
12	L	1	Total	C	O	0
			35	31	4	
12	7	1	Total	C	O	0
			63	59	4	

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

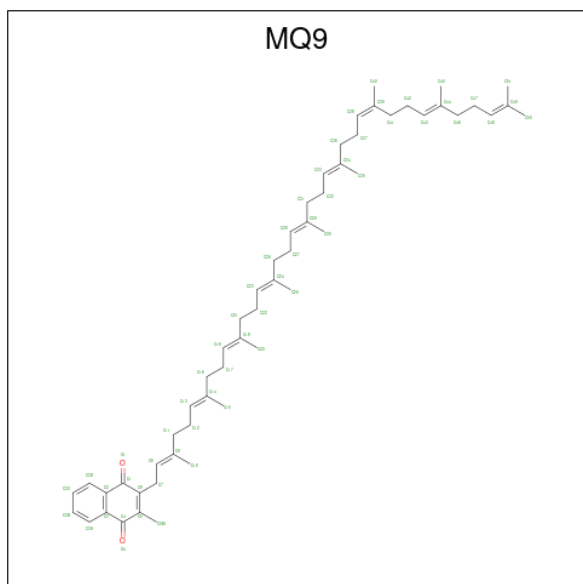


Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			30	19	11	
13	L	1	Total	C	O	0
			35	24	11	
13	I	1	Total	C	O	0
			33	22	11	
13	1	1	Total	C	O	0
			35	24	11	
13	3	1	Total	C	O	0
			31	20	11	

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

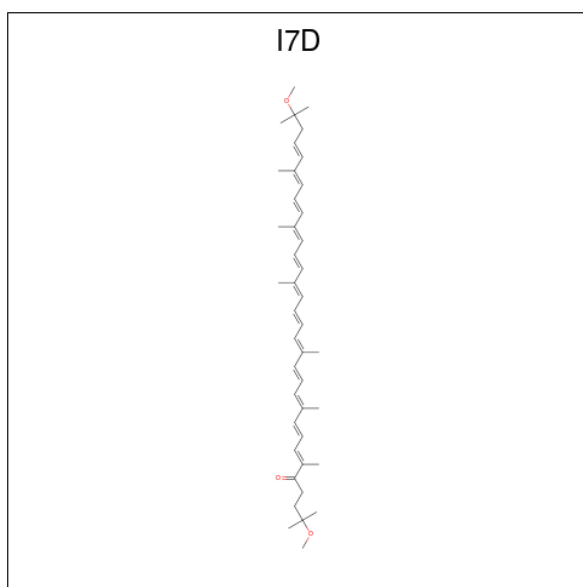
Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total	Fe	0
			1	1	

- Molecule 15 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			39	37	2	

- Molecule 16 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E},26 {E},28 {E})-2,31-dimethoxy-2,6,10,14,19,23,27,31-octamethyl-dotriaconta-6,8,10,12,14,16,18,20,22,24,26,28-dodecaen-5-one (CCD ID: I7D) (formula: C₄₂H₆₀O₃) (labeled as "Ligand of Interest" by depositor).



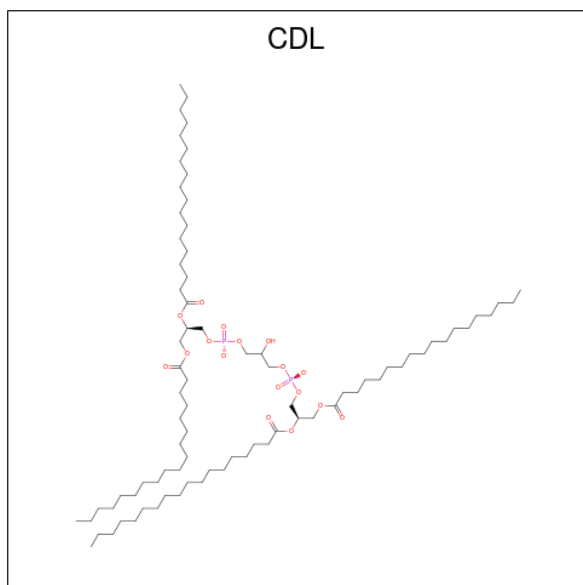
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			45	42	3	
16	A	1	Total	C	O	0
			45	42	3	
16	D	1	Total	C	O	0
			45	42	3	
16	E	1	Total	C	O	0
			45	42	3	
16	I	1	Total	C	O	0
			45	42	3	
16	K	1	Total	C	O	0
			45	42	3	
16	N	1	Total	C	O	0
			45	42	3	
16	Q	1	Total	C	O	0
			45	42	3	
16	R	1	Total	C	O	0
			45	42	3	
16	T	1	Total	C	O	0
			45	42	3	
16	V	1	Total	C	O	0
			45	42	3	
16	X	1	Total	C	O	0
			45	42	3	
16	1	1	Total	C	O	0
			45	42	3	
16	3	1	Total	C	O	0
			45	42	3	

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Mol	Chain	Residues	Atoms			AltConf
16	4	1	Total	C	O	0
			45	42	3	
16	6	1	Total	C	O	0
			45	42	3	
16	8	1	Total	C	O	0
			45	42	3	

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



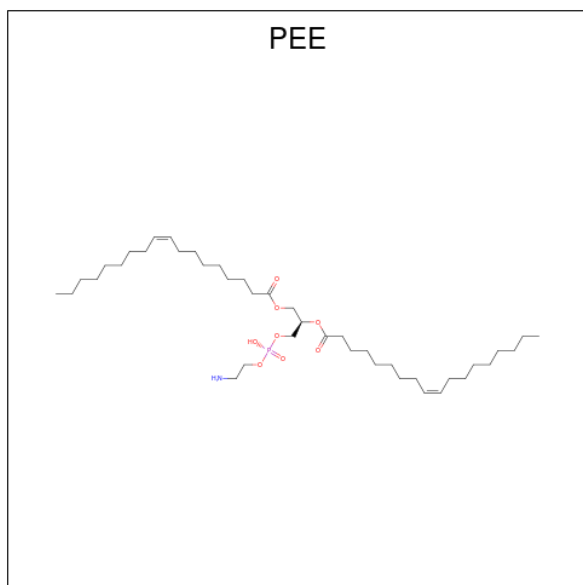
Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total	C	O	P	0
			35	17	16	2	
17	M	1	Total	C	O	P	0
			69	50	17	2	
17	H	1	Total	C	O	P	0
			72	53	17	2	
17	A	1	Total	C	O	P	0
			58	39	17	2	
17	T	1	Total	C	O	P	0
			72	53	17	2	
17	2	1	Total	C	O	P	0
			72	53	17	2	
17	6	1	Total	C	O	P	0
			69	50	17	2	
17	6	1	Total	C	O	P	0
			63	44	17	2	

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Mol	Chain	Residues	Atoms				AltConf
17	0	1	Total	C	O	P	0
			63	44	17	2	

- Molecule 18 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
18	M	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	C	136	Total	O	0
			136	136	
19	L	65	Total	O	0
			65	65	
19	M	81	Total	O	0
			81	81	
19	H	81	Total	O	0
			81	81	
19	A	4	Total	O	0
			4	4	
19	B	7	Total	O	0
			7	7	
19	D	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
19	E	3	Total 3	O 3	0
19	F	4	Total 4	O 4	0
19	G	2	Total 2	O 2	0
19	I	6	Total 6	O 6	0
19	J	3	Total 3	O 3	0
19	K	3	Total 3	O 3	0
19	N	4	Total 4	O 4	0
19	O	7	Total 7	O 7	0
19	P	5	Total 5	O 5	0
19	Q	9	Total 9	O 9	0
19	R	12	Total 12	O 12	0
19	S	16	Total 16	O 16	0
19	T	6	Total 6	O 6	0
19	U	8	Total 8	O 8	0
19	V	5	Total 5	O 5	0
19	W	11	Total 11	O 11	0
19	X	3	Total 3	O 3	0
19	Y	6	Total 6	O 6	0
19	Z	3	Total 3	O 3	0
19	1	2	Total 2	O 2	0
19	2	4	Total 4	O 4	0

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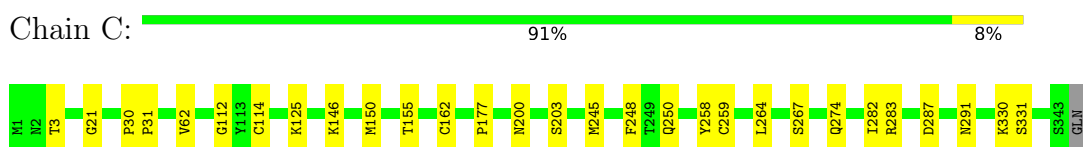
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Mol	Chain	Residues	Atoms		AltConf
19	3	7	Total 7	O 7	0
19	4	7	Total 7	O 7	0
19	5	3	Total 3	O 3	0
19	6	4	Total 4	O 4	0
19	7	7	Total 7	O 7	0
19	8	2	Total 2	O 2	0
19	9	7	Total 7	O 7	0
19	0	1	Total 1	O 1	0
19	b	1	Total 1	O 1	0

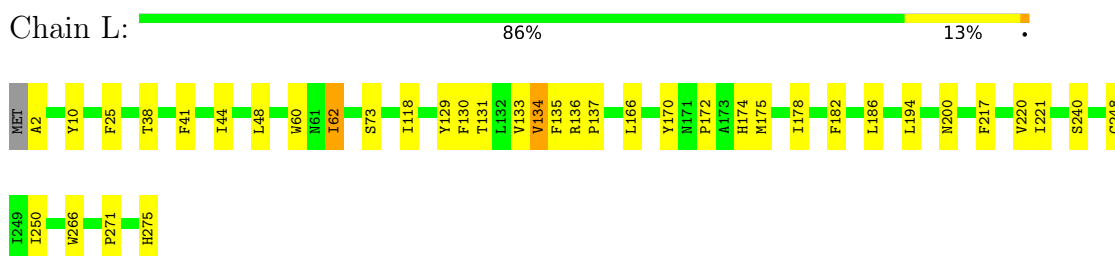
3 Residue-property plots

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.

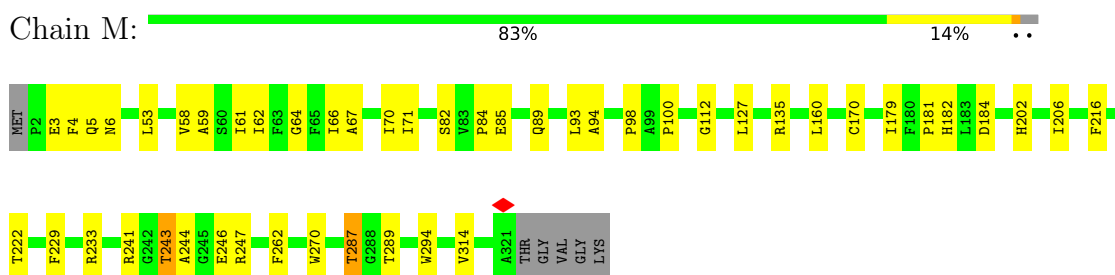
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



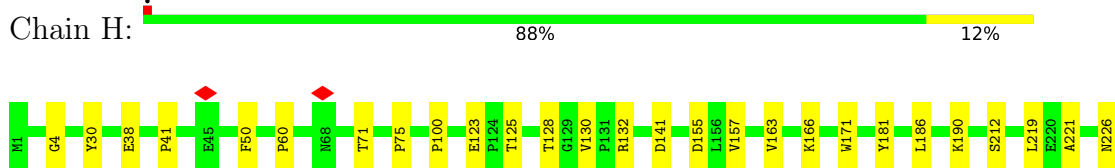
- Molecule 2: Reaction center protein L chain

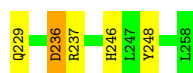


- Molecule 3: Reaction center protein M chain



- Molecule 4: Photosynthetic reaction center H subunit

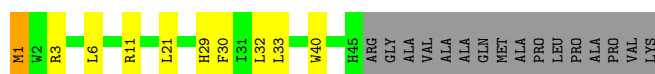




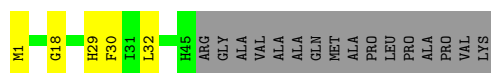
- Molecule 5: Light-harvesting protein



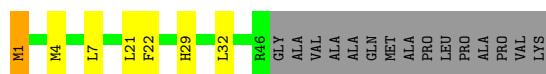
- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein

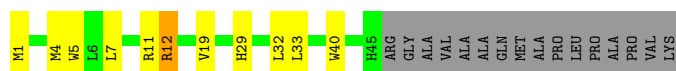


- Molecule 5: Light-harvesting protein

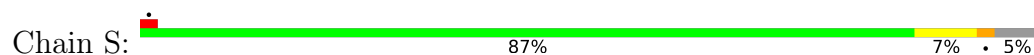


- Molecule 5: Light-harvesting protein

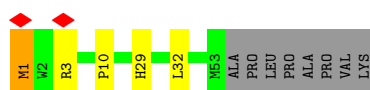
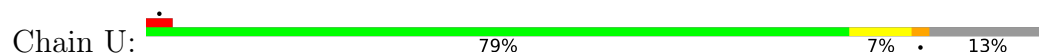




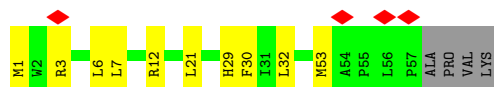
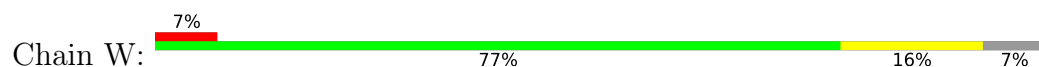
- Molecule 5: Light-harvesting protein



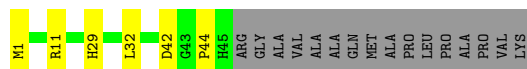
- Molecule 5: Light-harvesting protein



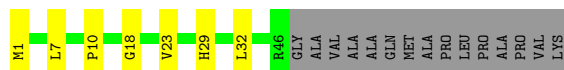
- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein

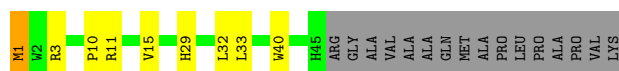


- Molecule 5: Light-harvesting protein

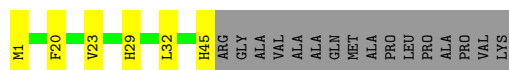


- Molecule 5: Light-harvesting protein

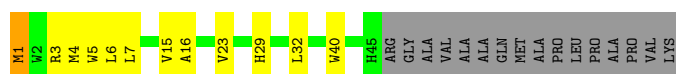




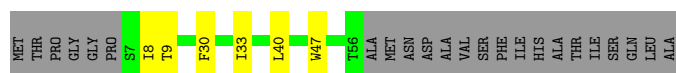
- Molecule 5: Light-harvesting protein



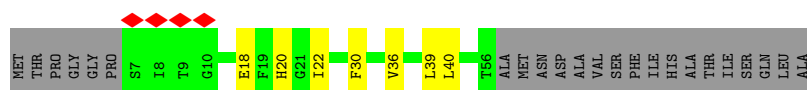
- Molecule 5: Light-harvesting protein



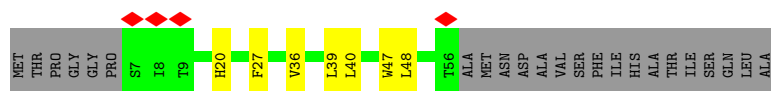
- Molecule 6: Light-harvesting protein



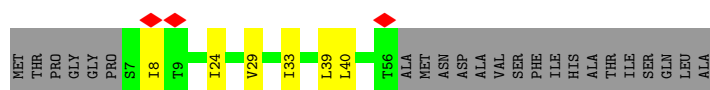
- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein

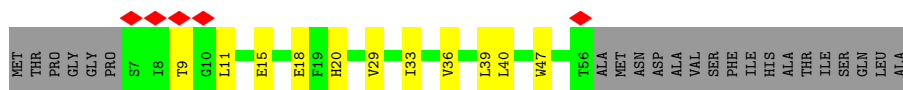


- Molecule 6: Light-harvesting protein

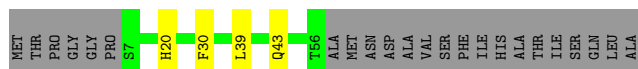


- Molecule 6: Light-harvesting protein





- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein



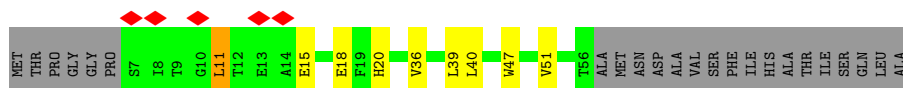
- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein



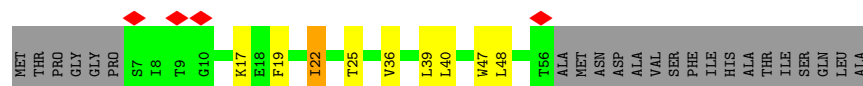
- Molecule 6: Light-harvesting protein



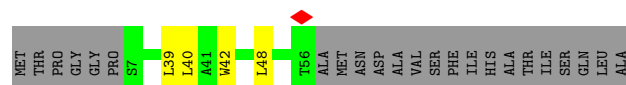
- Molecule 6: Light-harvesting protein



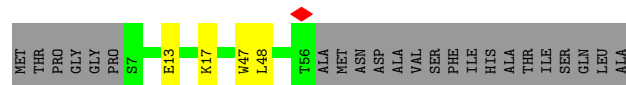
- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein



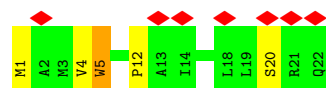
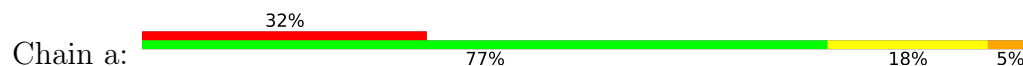
- Molecule 6: Light-harvesting protein



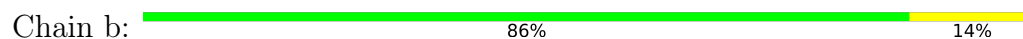
- Molecule 6: Light-harvesting protein



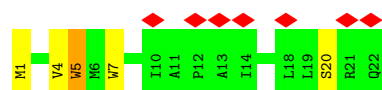
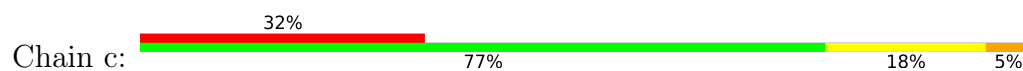
- Molecule 7: Light-harvesting protein LH1 Gamma-like



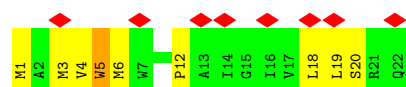
- Molecule 7: Light-harvesting protein LH1 Gamma-like



• Molecule 7: Light-harvesting protein LH1 Gamma-like



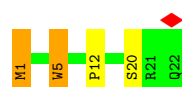
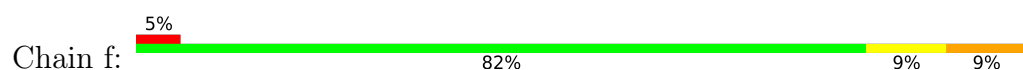
• Molecule 7: Light-harvesting protein LH1 Gamma-like



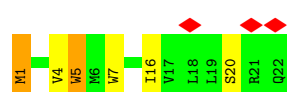
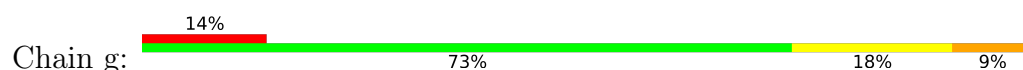
• Molecule 7: Light-harvesting protein LH1 Gamma-like



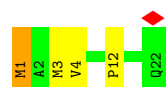
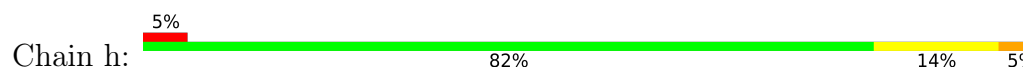
• Molecule 7: Light-harvesting protein LH1 Gamma-like



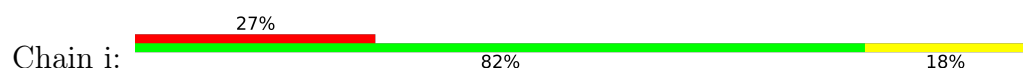
• Molecule 7: Light-harvesting protein LH1 Gamma-like

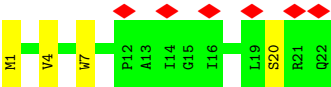


• Molecule 7: Light-harvesting protein LH1 Gamma-like

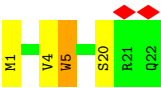
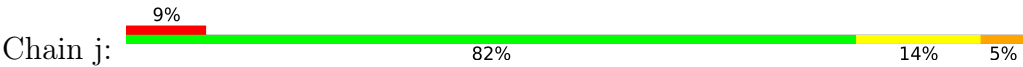


• Molecule 7: Light-harvesting protein LH1 Gamma-like





• Molecule 7: Light-harvesting protein LH1 Gamma-like



• Molecule 7: Light-harvesting protein LH1 Gamma-like



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128119	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)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.316	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	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: U10, PEE, BPH, MQ9, BCL, FE, FME, HEC, PGV, I7D, CDL, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	C	0.14	0/2730	0.28	0/3730
2	L	0.14	0/2266	0.30	0/3102
3	M	0.14	0/2652	0.29	0/3624
4	H	0.12	0/2053	0.27	0/2800
5	1	0.11	0/398	0.25	0/542
5	3	0.13	0/478	0.26	0/651
5	5	0.12	0/393	0.21	0/536
5	7	0.11	0/393	0.25	0/536
5	9	0.13	0/395	0.25	0/539
5	A	0.13	0/387	0.26	0/528
5	D	0.12	0/387	0.26	0/528
5	F	0.12	0/387	0.22	0/528
5	I	0.11	0/398	0.22	0/543
5	K	0.11	0/387	0.24	0/528
5	O	0.12	0/393	0.22	0/536
5	Q	0.13	0/393	0.25	0/536
5	S	0.12	0/481	0.24	0/657
5	U	0.13	0/447	0.28	0/608
5	W	0.11	0/476	0.24	0/650
5	Y	0.12	0/387	0.26	0/528
6	0	0.11	0/410	0.22	0/563
6	2	0.10	0/410	0.21	0/563
6	4	0.10	0/410	0.21	0/563
6	6	0.12	0/410	0.23	0/563
6	8	0.10	0/410	0.21	0/563
6	B	0.10	0/410	0.19	0/563
6	E	0.11	0/410	0.20	0/563
6	G	0.11	0/410	0.20	0/563
6	J	0.11	0/410	0.20	0/563
6	N	0.11	0/410	0.22	0/563
6	P	0.12	0/410	0.22	0/563
6	R	0.11	0/410	0.20	0/563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	T	0.11	0/410	0.22	0/563
6	V	0.10	0/410	0.21	0/563
6	X	0.12	0/410	0.24	0/563
6	Z	0.11	0/410	0.22	0/563
7	a	0.10	0/171	0.25	0/232
7	b	0.11	0/171	0.27	0/232
7	c	0.10	0/171	0.28	0/232
7	d	0.11	0/171	0.28	0/232
7	e	0.11	0/171	0.27	0/232
7	f	0.12	0/171	0.25	0/232
7	g	0.11	0/171	0.25	0/232
7	h	0.10	0/171	0.26	0/232
7	i	0.11	0/171	0.28	0/232
7	j	0.10	0/171	0.25	0/232
7	k	0.12	0/171	0.32	0/232
All	All	0.12	0/24722	0.26	0/33790

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	C	2655	0	2591	26	0
2	L	2177	0	2130	34	0
3	M	2550	0	2503	38	0
4	H	2000	0	1985	20	0
5	1	395	0	409	6	0
5	3	472	0	491	12	0
5	5	389	0	401	7	0
5	7	389	0	401	7	0
5	9	392	0	406	10	0
5	A	384	0	396	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	384	0	396	10	0
5	F	384	0	396	4	0
5	I	394	0	403	8	0
5	K	384	0	396	6	0
5	O	389	0	401	9	0
5	Q	389	0	401	7	0
5	S	475	0	493	5	0
5	U	443	0	458	6	0
5	W	470	0	488	8	0
5	Y	384	0	396	4	0
6	0	396	0	394	3	0
6	2	396	0	394	9	0
6	4	396	0	394	7	0
6	6	396	0	394	4	0
6	8	396	0	394	4	0
6	B	396	0	394	7	0
6	E	396	0	394	8	0
6	G	396	0	394	9	0
6	J	396	0	394	7	0
6	N	396	0	394	11	0
6	P	396	0	394	6	0
6	R	396	0	394	3	0
6	T	396	0	394	5	0
6	V	396	0	394	4	0
6	X	396	0	394	8	0
6	Z	396	0	394	7	0
7	a	177	0	194	6	0
7	b	177	0	194	2	0
7	c	177	0	194	7	0
7	d	177	0	194	10	0
7	e	177	0	194	7	0
7	f	177	0	194	4	0
7	g	177	0	194	9	0
7	h	177	0	194	4	0
7	i	177	0	194	3	0
7	j	177	0	194	4	0
7	k	177	0	194	9	0
8	C	172	0	120	9	0
9	5	111	0	132	6	0
9	C	124	0	155	7	0
9	D	33	0	36	1	0
9	F	39	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	72	0	83	2	0
9	K	39	0	48	1	0
9	L	191	0	241	15	0
9	M	84	0	112	4	0
10	0	66	0	74	4	0
10	1	66	0	74	1	0
10	2	66	0	74	3	0
10	3	66	0	74	3	0
10	4	66	0	74	4	0
10	5	66	0	74	3	0
10	6	66	0	74	2	0
10	7	66	0	74	0	0
10	8	66	0	74	4	0
10	9	66	0	74	4	0
10	A	66	0	74	3	0
10	B	66	0	74	5	0
10	D	66	0	74	3	0
10	E	66	0	74	5	0
10	F	66	0	74	2	0
10	G	66	0	74	10	0
10	I	66	0	74	3	0
10	J	66	0	74	4	0
10	K	66	0	74	3	0
10	L	132	0	148	3	0
10	M	132	0	148	5	0
10	N	66	0	74	7	0
10	O	66	0	74	1	0
10	P	66	0	74	7	0
10	Q	66	0	74	1	0
10	R	66	0	74	6	0
10	S	66	0	74	1	0
10	T	66	0	74	3	0
10	U	66	0	74	1	0
10	V	66	0	74	3	0
10	W	66	0	74	1	0
10	X	66	0	74	6	0
10	Y	66	0	74	2	0
10	Z	66	0	74	5	0
11	L	65	0	76	4	0
11	M	65	0	76	9	0
12	7	63	0	90	9	0
12	L	86	0	98	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	35	0	46	1	0
13	3	31	0	35	8	0
13	I	33	0	39	3	0
13	L	65	0	79	4	0
14	M	1	0	0	0	0
15	M	39	0	47	3	0
16	1	45	0	0	0	0
16	3	45	0	0	0	0
16	4	45	0	0	0	0
16	6	45	0	0	1	0
16	8	45	0	0	0	0
16	A	45	0	0	0	0
16	D	45	0	0	0	0
16	E	45	0	0	0	0
16	I	45	0	0	0	0
16	K	45	0	0	0	0
16	M	45	0	0	0	0
16	N	45	0	0	0	0
16	Q	45	0	0	0	0
16	R	45	0	0	0	0
16	T	45	0	0	0	0
16	V	45	0	0	0	0
16	X	45	0	0	0	0
17	0	63	0	70	3	0
17	2	72	0	88	4	0
17	6	132	0	152	9	0
17	A	58	0	60	1	0
17	H	72	0	88	4	0
17	M	104	0	102	7	0
17	T	72	0	88	4	0
18	M	44	0	62	3	0
19	0	1	0	0	0	0
19	1	2	0	0	0	0
19	2	4	0	0	0	0
19	3	7	0	0	0	0
19	4	7	0	0	0	0
19	5	3	0	0	0	0
19	6	4	0	0	0	0
19	7	7	0	0	0	0
19	8	2	0	0	0	0
19	9	7	0	0	0	0
19	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	7	0	0	0	0
19	C	136	0	0	0	0
19	D	3	0	0	0	0
19	E	3	0	0	0	0
19	F	4	0	0	0	0
19	G	2	0	0	0	0
19	H	81	0	0	1	0
19	I	6	0	0	0	0
19	J	3	0	0	0	0
19	K	3	0	0	0	0
19	L	65	0	0	0	0
19	M	81	0	0	0	0
19	N	4	0	0	0	0
19	O	7	0	0	0	0
19	P	5	0	0	0	0
19	Q	9	0	0	0	0
19	R	12	0	0	0	0
19	S	16	0	0	0	0
19	T	6	0	0	0	0
19	U	8	0	0	0	0
19	V	5	0	0	0	0
19	W	11	0	0	0	0
19	X	3	0	0	0	0
19	Y	6	0	0	0	0
19	Z	3	0	0	0	0
19	b	1	0	0	0	0
All	All	29826	0	29312	395	0

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

The worst 5 of 395 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)
1:C:162:CYS:SG	8:C:402:HEC:CAC	2.01	1.46
1:C:114:CYS:SG	8:C:401:HEC:CAC	2.04	1.45
1:C:259:CYS:SG	8:C:403:HEC:CAC	2.04	1.45
2:L:2:ALA:N	9:L:311:PGV:H1	1.58	1.00
3:M:287:THR:HB	3:M:294:TRP:HE1	1.45	0.80

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	C	341/344 (99%)	332 (97%)	9 (3%)	0	100	100
2	L	272/275 (99%)	268 (98%)	4 (2%)	0	100	100
3	M	319/326 (98%)	313 (98%)	6 (2%)	0	100	100
4	H	256/258 (99%)	248 (97%)	8 (3%)	0	100	100
5	1	44/61 (72%)	43 (98%)	1 (2%)	0	100	100
5	3	53/61 (87%)	52 (98%)	1 (2%)	0	100	100
5	5	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	7	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	9	44/61 (72%)	43 (98%)	1 (2%)	0	100	100
5	A	43/61 (70%)	41 (95%)	2 (5%)	0	100	100
5	D	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	F	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	I	44/61 (72%)	43 (98%)	1 (2%)	0	100	100
5	K	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	O	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	Q	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	S	56/61 (92%)	55 (98%)	1 (2%)	0	100	100
5	U	51/61 (84%)	49 (96%)	2 (4%)	0	100	100
5	W	55/61 (90%)	53 (96%)	2 (4%)	0	100	100
5	Y	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
6	0	48/73 (66%)	45 (94%)	3 (6%)	0	100	100
6	2	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	4	48/73 (66%)	45 (94%)	3 (6%)	0	100	100
6	6	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	8	48/73 (66%)	46 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	E	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	G	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	J	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	N	48/73 (66%)	45 (94%)	3 (6%)	0	100	100
6	P	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	R	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	T	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	V	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	X	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	Z	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
7	a	20/22 (91%)	20 (100%)	0	0	100	100
7	b	20/22 (91%)	20 (100%)	0	0	100	100
7	c	20/22 (91%)	20 (100%)	0	0	100	100
7	d	20/22 (91%)	19 (95%)	1 (5%)	0	100	100
7	e	20/22 (91%)	20 (100%)	0	0	100	100
7	f	20/22 (91%)	20 (100%)	0	0	100	100
7	g	20/22 (91%)	20 (100%)	0	0	100	100
7	h	20/22 (91%)	19 (95%)	1 (5%)	0	100	100
7	i	20/22 (91%)	20 (100%)	0	0	100	100
7	j	20/22 (91%)	20 (100%)	0	0	100	100
7	k	20/22 (91%)	20 (100%)	0	0	100	100
All	All	2910/3589 (81%)	2827 (97%)	83 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	283/284 (100%)	283 (100%)	0	100	100
2	L	214/215 (100%)	209 (98%)	5 (2%)	44	53
3	M	251/254 (99%)	246 (98%)	5 (2%)	48	58
4	H	212/212 (100%)	210 (99%)	2 (1%)	70	78
5	1	40/50 (80%)	40 (100%)	0	100	100
5	3	48/50 (96%)	48 (100%)	0	100	100
5	5	40/50 (80%)	40 (100%)	0	100	100
5	7	40/50 (80%)	39 (98%)	1 (2%)	42	50
5	9	40/50 (80%)	38 (95%)	2 (5%)	22	22
5	A	39/50 (78%)	39 (100%)	0	100	100
5	D	39/50 (78%)	39 (100%)	0	100	100
5	F	39/50 (78%)	39 (100%)	0	100	100
5	I	40/50 (80%)	40 (100%)	0	100	100
5	K	39/50 (78%)	38 (97%)	1 (3%)	40	48
5	O	40/50 (80%)	39 (98%)	1 (2%)	42	50
5	Q	40/50 (80%)	38 (95%)	2 (5%)	22	22
5	S	47/50 (94%)	47 (100%)	0	100	100
5	U	44/50 (88%)	44 (100%)	0	100	100
5	W	47/50 (94%)	47 (100%)	0	100	100
5	Y	39/50 (78%)	38 (97%)	1 (3%)	40	48
6	0	40/57 (70%)	40 (100%)	0	100	100
6	2	40/57 (70%)	40 (100%)	0	100	100
6	4	40/57 (70%)	38 (95%)	2 (5%)	22	22
6	6	40/57 (70%)	40 (100%)	0	100	100
6	8	40/57 (70%)	40 (100%)	0	100	100
6	B	40/57 (70%)	40 (100%)	0	100	100
6	E	40/57 (70%)	40 (100%)	0	100	100
6	G	40/57 (70%)	40 (100%)	0	100	100
6	J	40/57 (70%)	40 (100%)	0	100	100
6	N	40/57 (70%)	40 (100%)	0	100	100
6	P	40/57 (70%)	40 (100%)	0	100	100
6	R	40/57 (70%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	40/57 (70%)	40 (100%)	0	100	100
6	V	40/57 (70%)	40 (100%)	0	100	100
6	X	40/57 (70%)	39 (98%)	1 (2%)	42	50
6	Z	40/57 (70%)	39 (98%)	1 (2%)	42	50
7	a	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	b	17/17 (100%)	17 (100%)	0	100	100
7	c	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	d	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	e	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	f	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	g	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	h	17/17 (100%)	17 (100%)	0	100	100
7	i	17/17 (100%)	17 (100%)	0	100	100
7	j	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	k	17/17 (100%)	15 (88%)	2 (12%)	5	2
All	All	2448/2864 (86%)	2415 (99%)	33 (1%)	59	71

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	f	5	TRP
7	g	5	TRP
7	k	5	TRP
5	K	3	ARG
4	H	236	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
6	8	43	GLN
7	h	22	GLN
7	k	22	GLN
7	g	22	GLN
6	N	20	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

27 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	$\# Z > 2$
5	FME	A	1	5	8,9,10	0.53	0	8,9,11	0.95	1 (12%)
5	FME	K	1	5	8,9,10	0.54	0	8,9,11	1.06	1 (12%)
5	FME	F	1	5	8,9,10	0.56	0	8,9,11	0.93	1 (12%)
5	FME	7	1	5	8,9,10	0.55	0	8,9,11	1.04	1 (12%)
5	FME	U	1	5	8,9,10	0.56	0	8,9,11	0.89	1 (12%)
5	FME	S	1	5	8,9,10	0.53	0	8,9,11	0.93	1 (12%)
7	FME	j	1	7	8,9,10	0.54	0	8,9,11	1.00	1 (12%)
7	FME	i	1	7	8,9,10	0.54	0	8,9,11	1.04	1 (12%)
7	FME	h	1	7	8,9,10	0.54	0	8,9,11	0.95	1 (12%)
5	FME	3	1	5	8,9,10	0.55	0	8,9,11	0.95	1 (12%)
7	FME	d	1	7	8,9,10	0.55	0	8,9,11	0.90	1 (12%)
5	FME	9	1	5	8,9,10	0.53	0	8,9,11	0.90	1 (12%)
5	FME	Q	1	5	8,9,10	0.49	0	8,9,11	1.17	1 (12%)
7	FME	a	1	7	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
7	FME	g	1	7	8,9,10	0.54	0	8,9,11	0.94	1 (12%)
7	FME	k	1	7	8,9,10	0.57	0	8,9,11	0.91	1 (12%)
5	FME	I	1	5	8,9,10	0.55	0	8,9,11	1.11	1 (12%)
7	FME	c	1	7	8,9,10	0.55	0	8,9,11	1.12	1 (12%)
5	FME	1	1	5	8,9,10	0.54	0	8,9,11	1.04	1 (12%)
5	FME	D	1	5	8,9,10	0.54	0	8,9,11	1.14	1 (12%)
7	FME	b	1	7	8,9,10	0.55	0	8,9,11	0.89	1 (12%)
5	FME	O	1	5	8,9,10	0.57	0	8,9,11	0.94	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FME	Y	1	5	8,9,10	0.57	0	8,9,11	0.88	1 (12%)
7	FME	f	1	7	8,9,10	0.54	0	8,9,11	0.92	1 (12%)
7	FME	e	1	7	8,9,10	0.56	0	8,9,11	0.95	1 (12%)
5	FME	W	1	5	8,9,10	0.55	0	8,9,11	0.88	1 (12%)
5	FME	5	1	5	8,9,10	0.56	0	8,9,11	0.87	1 (12%)

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
5	FME	A	1	5	-	1/7/9/11	-
5	FME	K	1	5	-	3/7/9/11	-
5	FME	F	1	5	-	1/7/9/11	-
5	FME	7	1	5	-	4/7/9/11	-
5	FME	U	1	5	-	1/7/9/11	-
5	FME	S	1	5	-	1/7/9/11	-
7	FME	j	1	7	-	1/7/9/11	-
7	FME	i	1	7	-	0/7/9/11	-
7	FME	h	1	7	-	2/7/9/11	-
5	FME	3	1	5	-	0/7/9/11	-
7	FME	d	1	7	-	2/7/9/11	-
5	FME	9	1	5	-	1/7/9/11	-
5	FME	Q	1	5	-	1/7/9/11	-
7	FME	a	1	7	-	3/7/9/11	-
7	FME	g	1	7	-	4/7/9/11	-
7	FME	k	1	7	-	0/7/9/11	-
5	FME	I	1	5	-	0/7/9/11	-
7	FME	c	1	7	-	2/7/9/11	-
5	FME	1	1	5	-	2/7/9/11	-
5	FME	D	1	5	-	1/7/9/11	-
7	FME	b	1	7	-	3/7/9/11	-
5	FME	O	1	5	-	0/7/9/11	-
5	FME	Y	1	5	-	2/7/9/11	-
7	FME	f	1	7	-	1/7/9/11	-
7	FME	e	1	7	-	1/7/9/11	-
5	FME	W	1	5	-	2/7/9/11	-
5	FME	5	1	5	-	3/7/9/11	-

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	1	FME	O-C-CA	-2.89	117.33	124.77
5	D	1	FME	O-C-CA	-2.81	117.54	124.77
5	I	1	FME	O-C-CA	-2.80	117.58	124.77
5	K	1	FME	O-C-CA	-2.71	117.79	124.77
5	1	1	FME	O-C-CA	-2.69	117.86	124.77

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	FME	O1-CN-N-CA
5	K	1	FME	CB-CA-N-CN
5	U	1	FME	O1-CN-N-CA
5	Y	1	FME	O1-CN-N-CA
5	Y	1	FME	CB-CA-N-CN

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	FME	1	0
5	U	1	FME	2	0
5	S	1	FME	1	0
7	h	1	FME	1	0
5	9	1	FME	2	0
7	g	1	FME	1	0
5	I	1	FME	1	0
5	D	1	FME	2	0
5	O	1	FME	1	0
7	f	1	FME	1	0
5	5	1	FME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 98 ligands modelled in this entry, 1 is monoatomic - leaving 97 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
10	BCL	D	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.27	23 (29%)
9	PGV	5	104	-	36,36,50	1.09	2 (5%)	39,42,56	1.02	2 (5%)
9	PGV	C	406	-	41,41,50	1.02	2 (4%)	44,47,56	1.21	3 (6%)
16	I7D	3	101	-	44,44,44	1.67	10 (22%)	50,56,56	2.14	12 (24%)
10	BCL	4	102	-	69,74,74	1.76	17 (24%)	79,115,115	2.23	23 (29%)
12	U10	L	307	-	35,35,63	0.80	2 (5%)	43,45,79	0.79	1 (2%)
11	BPH	M	404	-	59,70,70	0.79	3 (5%)	59,101,101	0.90	3 (5%)
16	I7D	D	101	-	44,44,44	1.65	10 (22%)	50,56,56	2.17	12 (24%)
13	LMT	1	103	-	36,36,36	0.37	0	47,47,47	0.75	2 (4%)
18	PEE	M	409	-	43,43,50	0.80	2 (4%)	46,48,55	0.58	0
17	CDL	A	101	-	57,57,99	1.13	4 (7%)	63,69,111	1.28	7 (11%)
10	BCL	6	103	-	69,74,74	1.78	18 (26%)	79,115,115	2.18	22 (27%)
9	PGV	L	305	-	43,43,50	0.97	2 (4%)	46,49,56	1.03	3 (6%)
16	I7D	8	101	-	44,44,44	1.66	10 (22%)	50,56,56	2.45	15 (30%)
10	BCL	S	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.30	24 (30%)
8	HEC	C	403	1	46,50,50	1.75	10 (21%)	58,82,82	1.65	11 (18%)
9	PGV	L	304	-	42,42,50	0.97	2 (4%)	45,48,56	1.15	4 (8%)
16	I7D	N	101	-	44,44,44	1.66	10 (22%)	50,56,56	2.18	14 (28%)
17	CDL	M	407	-	34,34,99	1.44	3 (8%)	39,45,111	1.45	5 (12%)
17	CDL	2	101	-	71,71,99	1.10	4 (5%)	77,83,111	1.10	5 (6%)
10	BCL	M	402	-	69,74,74	1.78	18 (26%)	79,115,115	2.19	23 (29%)
16	I7D	Q	101	-	44,44,44	1.66	10 (22%)	50,56,56	2.15	12 (24%)
10	BCL	X	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.20	22 (27%)
10	BCL	J	101	-	69,74,74	1.76	17 (24%)	79,115,115	2.17	21 (26%)
13	LMT	3	103	-	32,32,36	0.40	0	43,43,47	0.86	1 (2%)
10	BCL	N	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.22	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	I7D	X	101	-	44,44,44	1.68	10 (22%)	50,56,56	2.23	12 (24%)
10	BCL	P	101	-	69,74,74	1.75	17 (24%)	79,115,115	2.19	23 (29%)
10	BCL	I	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.27	24 (30%)
15	MQ9	M	405	-	40,40,59	0.41	0	49,52,75	0.52	1 (2%)
16	I7D	6	102	-	44,44,44	1.68	10 (22%)	50,56,56	2.24	14 (28%)
9	PGV	C	405	-	43,43,50	1.00	2 (4%)	46,49,56	1.13	4 (8%)
16	I7D	I	101	-	44,44,44	1.67	10 (22%)	50,56,56	2.21	12 (24%)
10	BCL	M	403	-	69,74,74	1.77	17 (24%)	79,115,115	2.27	24 (30%)
11	BPH	L	302	-	59,70,70	0.80	2 (3%)	59,101,101	0.88	2 (3%)
10	BCL	L	301	-	69,74,74	1.77	16 (23%)	79,115,115	2.23	24 (30%)
10	BCL	Z	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.20	22 (27%)
9	PGV	L	312	-	33,33,50	1.11	2 (6%)	36,39,56	1.24	4 (11%)
9	PGV	5	101	-	36,36,50	1.08	2 (5%)	39,41,56	1.20	4 (10%)
12	U10	L	306	-	15,15,63	1.15	2 (13%)	20,21,79	0.94	1 (5%)
16	I7D	4	101	-	44,44,44	1.66	10 (22%)	50,56,56	2.21	13 (26%)
10	BCL	0	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.16	22 (27%)
9	PGV	L	311	-	32,32,50	1.15	2 (6%)	35,38,56	1.29	4 (11%)
8	HEC	C	402	1	46,50,50	1.74	10 (21%)	58,82,82	1.58	11 (18%)
10	BCL	T	102	-	69,74,74	1.76	18 (26%)	79,115,115	2.18	22 (27%)
8	HEC	C	401	1	46,50,50	1.74	10 (21%)	58,82,82	1.66	15 (25%)
16	I7D	A	103	-	44,44,44	1.65	10 (22%)	50,56,56	2.23	12 (24%)
16	I7D	T	101	-	44,44,44	1.66	10 (22%)	50,56,56	2.19	13 (26%)
16	I7D	1	101	-	44,44,44	1.67	10 (22%)	50,56,56	2.25	13 (26%)
17	CDL	0	101	-	62,62,99	1.16	4 (6%)	68,74,111	1.20	6 (8%)
9	PGV	M	410	-	50,50,50	0.90	2 (4%)	53,56,56	1.07	4 (7%)
16	I7D	M	406	-	44,44,44	1.64	8 (18%)	50,56,56	2.20	9 (18%)
9	PGV	K	103	-	38,38,50	1.06	2 (5%)	41,44,56	1.05	2 (4%)
10	BCL	L	309	-	69,74,74	1.76	17 (24%)	79,115,115	2.23	23 (29%)
10	BCL	G	101	-	69,74,74	1.76	17 (24%)	79,115,115	2.19	22 (27%)
10	BCL	A	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.25	23 (29%)
10	BCL	5	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.24	25 (31%)
10	BCL	B	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.19	23 (29%)
10	BCL	K	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.30	23 (29%)
10	BCL	8	102	-	69,74,74	1.76	17 (24%)	79,115,115	2.17	24 (30%)
10	BCL	V	102	-	69,74,74	1.76	18 (26%)	79,115,115	2.19	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCL	Y	101	-	69,74,74	1.79	16 (23%)	79,115,115	2.27	23 (29%)
10	BCL	E	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.22	21 (26%)
13	LMT	L	313	-	36,36,36	0.36	0	47,47,47	0.74	2 (4%)
17	CDL	H	303	-	71,71,99	1.09	4 (5%)	77,83,111	1.10	6 (7%)
16	I7D	K	101	-	44,44,44	1.66	10 (22%)	50,56,56	2.15	12 (24%)
16	I7D	V	101	-	44,44,44	1.65	10 (22%)	50,56,56	2.22	12 (24%)
16	I7D	E	101	-	44,44,44	1.66	10 (22%)	50,56,56	2.19	13 (26%)
10	BCL	F	101	-	69,74,74	1.77	18 (26%)	79,115,115	2.33	24 (30%)
9	PGV	M	411	-	32,32,50	1.14	2 (6%)	35,38,56	1.24	3 (8%)
9	PGV	F	102	-	38,38,50	1.06	2 (5%)	41,43,56	1.02	2 (4%)
9	PGV	H	301	-	35,35,50	1.10	2 (5%)	38,41,56	1.18	3 (7%)
9	PGV	D	103	-	32,32,50	1.14	2 (6%)	35,38,56	1.22	4 (11%)
17	CDL	M	408	-	68,68,99	1.11	4 (5%)	74,80,111	1.10	4 (5%)
10	BCL	R	102	-	69,74,74	1.76	17 (24%)	79,115,115	2.22	23 (29%)
10	BCL	7	402	-	69,74,74	1.78	17 (24%)	79,115,115	2.23	22 (27%)
9	PGV	C	407	-	37,37,50	1.10	2 (5%)	40,42,56	1.25	4 (10%)
12	U10	L	303	-	36,36,63	0.78	2 (5%)	45,46,79	0.70	1 (2%)
10	BCL	2	102	-	69,74,74	1.76	17 (24%)	79,115,115	2.20	22 (27%)
9	PGV	5	103	-	36,36,50	1.08	2 (5%)	39,41,56	1.12	3 (7%)
8	HEC	C	404	1	46,50,50	1.74	10 (21%)	58,82,82	1.62	11 (18%)
12	U10	7	401	-	63,63,63	0.60	2 (3%)	78,79,79	0.59	1 (1%)
13	LMT	L	308	-	31,31,36	0.38	0	42,42,47	0.69	0
16	I7D	R	101	-	44,44,44	1.66	10 (22%)	50,56,56	2.16	13 (26%)
17	CDL	T	103	-	71,71,99	1.08	4 (5%)	77,83,111	1.16	6 (7%)
10	BCL	Q	102	-	69,74,74	1.78	19 (27%)	79,115,115	2.28	24 (30%)
10	BCL	W	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.27	24 (30%)
10	BCL	U	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.24	24 (30%)
10	BCL	1	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.31	26 (32%)
17	CDL	6	101	-	68,68,99	1.12	4 (5%)	74,80,111	1.12	5 (6%)
9	PGV	L	310	-	36,36,50	1.08	2 (5%)	39,42,56	1.14	3 (7%)
9	PGV	H	302	-	35,35,50	1.09	2 (5%)	38,41,56	1.20	4 (10%)
10	BCL	O	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.34	24 (30%)
13	LMT	I	103	-	34,34,36	0.38	0	45,45,47	0.76	1 (2%)
10	BCL	9	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.24	23 (29%)
17	CDL	6	104	-	62,62,99	1.16	4 (6%)	68,74,111	1.28	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCL	3	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.23	24 (30%)

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
10	BCL	D	102	-	-	12/41/137/137	-
9	PGV	5	104	-	-	10/41/41/55	-
9	PGV	C	406	-	-	13/46/46/55	-
16	I7D	3	101	-	-	5/54/54/54	-
10	BCL	4	102	-	-	17/41/137/137	-
12	U10	L	307	-	-	3/30/54/87	0/1/1/1
11	BPH	M	404	-	-	1/37/105/105	0/5/6/6
16	I7D	D	101	-	-	3/54/54/54	-
13	LMT	1	103	-	-	2/21/61/61	0/2/2/2
18	PEE	M	409	-	-	7/47/47/54	-
17	CDL	A	101	-	-	17/67/67/110	-
10	BCL	6	103	-	-	8/41/137/137	-
9	PGV	L	305	-	-	10/48/48/55	-
16	I7D	8	101	-	-	10/54/54/54	-
10	BCL	S	101	-	-	10/41/137/137	-
8	HEC	C	403	1	-	6/14/54/54	-
9	PGV	L	304	-	-	15/47/47/55	-
16	I7D	N	101	-	-	8/54/54/54	-
17	CDL	M	407	-	-	10/43/43/110	-
17	CDL	2	101	-	-	20/82/82/110	-
10	BCL	M	402	-	-	5/41/137/137	-
16	I7D	Q	101	-	-	4/54/54/54	-
10	BCL	X	102	-	-	13/41/137/137	-
10	BCL	J	101	-	-	15/41/137/137	-
13	LMT	3	103	-	-	4/17/57/61	0/2/2/2
10	BCL	N	102	-	-	14/41/137/137	-
16	I7D	X	101	-	-	6/54/54/54	-
10	BCL	P	101	-	-	13/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	I	102	-	-	8/41/137/137	-
15	MQ9	M	405	-	-	0/31/51/73	0/2/2/2
16	I7D	6	102	-	-	2/54/54/54	-
9	PGV	C	405	-	-	6/48/48/55	-
16	I7D	I	101	-	-	5/54/54/54	-
10	BCL	M	403	-	-	4/41/137/137	-
11	BPH	L	302	-	-	4/37/105/105	0/5/6/6
10	BCL	L	301	-	-	9/41/137/137	-
10	BCL	Z	101	-	-	15/41/137/137	-
9	PGV	L	312	-	-	12/38/38/55	-
9	PGV	5	101	-	-	12/40/40/55	-
12	U10	L	306	-	-	1/6/30/87	0/1/1/1
16	I7D	4	101	-	-	5/54/54/54	-
10	BCL	0	102	-	-	17/41/137/137	-
9	PGV	L	311	-	-	12/37/37/55	-
8	HEC	C	402	1	-	8/14/54/54	-
10	BCL	T	102	-	-	9/41/137/137	-
8	HEC	C	401	1	-	8/14/54/54	-
16	I7D	A	103	-	-	4/54/54/54	-
16	I7D	T	101	-	-	5/54/54/54	-
16	I7D	1	101	-	-	4/54/54/54	-
17	CDL	0	101	-	-	31/73/73/110	-
9	PGV	M	410	-	-	14/55/55/55	-
16	I7D	M	406	-	-	4/54/54/54	-
9	PGV	K	103	-	-	7/43/43/55	-
10	BCL	L	309	-	-	11/41/137/137	-
10	BCL	G	101	-	-	14/41/137/137	-
10	BCL	A	102	-	-	11/41/137/137	-
10	BCL	5	102	-	-	10/41/137/137	-
10	BCL	B	101	-	-	10/41/137/137	-
10	BCL	K	102	-	-	8/41/137/137	-
10	BCL	8	102	-	-	16/41/137/137	-
10	BCL	V	102	-	-	13/41/137/137	-
10	BCL	Y	101	-	-	12/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	E	102	-	-	16/41/137/137	-
13	LMT	L	313	-	-	4/21/61/61	0/2/2/2
17	CDL	H	303	-	-	27/82/82/110	-
16	I7D	K	101	-	-	6/54/54/54	-
16	I7D	V	101	-	-	6/54/54/54	-
16	I7D	E	101	-	-	3/54/54/54	-
10	BCL	F	101	-	-	11/41/137/137	-
9	PGV	M	411	-	-	11/37/37/55	-
9	PGV	F	102	-	-	6/42/42/55	-
9	PGV	H	301	-	-	8/40/40/55	-
9	PGV	D	103	-	-	10/37/37/55	-
17	CDL	M	408	-	-	23/79/79/110	-
10	BCL	R	102	-	-	14/41/137/137	-
10	BCL	7	402	-	-	10/41/137/137	-
9	PGV	C	407	-	-	7/39/39/55	-
12	U10	L	303	-	-	5/31/55/87	0/1/1/1
10	BCL	2	102	-	-	14/41/137/137	-
9	PGV	5	103	-	-	10/40/40/55	-
8	HEC	C	404	1	-	6/14/54/54	-
12	U10	7	401	-	-	14/63/87/87	0/1/1/1
13	LMT	L	308	-	-	4/16/56/61	0/2/2/2
16	I7D	R	101	-	-	1/54/54/54	-
17	CDL	T	103	-	-	23/82/82/110	-
10	BCL	Q	102	-	-	8/41/137/137	-
10	BCL	W	101	-	-	9/41/137/137	-
10	BCL	U	101	-	-	9/41/137/137	-
10	BCL	1	102	-	-	4/41/137/137	-
17	CDL	6	101	-	-	27/79/79/110	-
9	PGV	L	310	-	-	8/41/41/55	-
9	PGV	H	302	-	-	11/40/40/55	-
10	BCL	O	101	-	-	15/41/137/137	-
13	LMT	I	103	-	-	9/19/59/61	0/2/2/2
10	BCL	9	101	-	-	12/41/137/137	-
17	CDL	6	104	-	-	28/73/73/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	3	102	-	-	7/41/137/137	-

The worst 5 of 912 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	101	I7D	C35-C36	6.63	1.50	1.32
16	6	102	I7D	C35-C36	6.59	1.50	1.32
16	8	101	I7D	C35-C36	6.51	1.50	1.32
16	I	101	I7D	C35-C36	6.49	1.50	1.32
16	E	101	I7D	C35-C36	6.49	1.50	1.32

The worst 5 of 1217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	406	I7D	C37-C36-C35	-9.79	111.16	124.91
16	V	101	I7D	C37-C36-C35	-9.20	111.99	124.91
16	1	101	I7D	C37-C36-C35	-9.04	112.21	124.91
16	8	101	I7D	C36-C35-C33	-8.98	112.33	125.89
16	4	101	I7D	C37-C36-C35	-8.94	112.36	124.91

There are no chirality outliers.

5 of 958 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	401	HEC	C2B-C3B-CAB-CBB
8	C	401	HEC	C4B-C3B-CAB-CBB
8	C	401	HEC	C2C-C3C-CAC-CBC
8	C	401	HEC	C4C-C3C-CAC-CBC
8	C	402	HEC	C2B-C3B-CAB-CBB

There are no ring outliers.

75 monomers are involved in 224 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	102	BCL	3	0
10	4	102	BCL	4	0
12	L	307	U10	5	0
11	M	404	BPH	9	0
13	1	103	LMT	1	0
18	M	409	PEE	3	0
17	A	101	CDL	1	0

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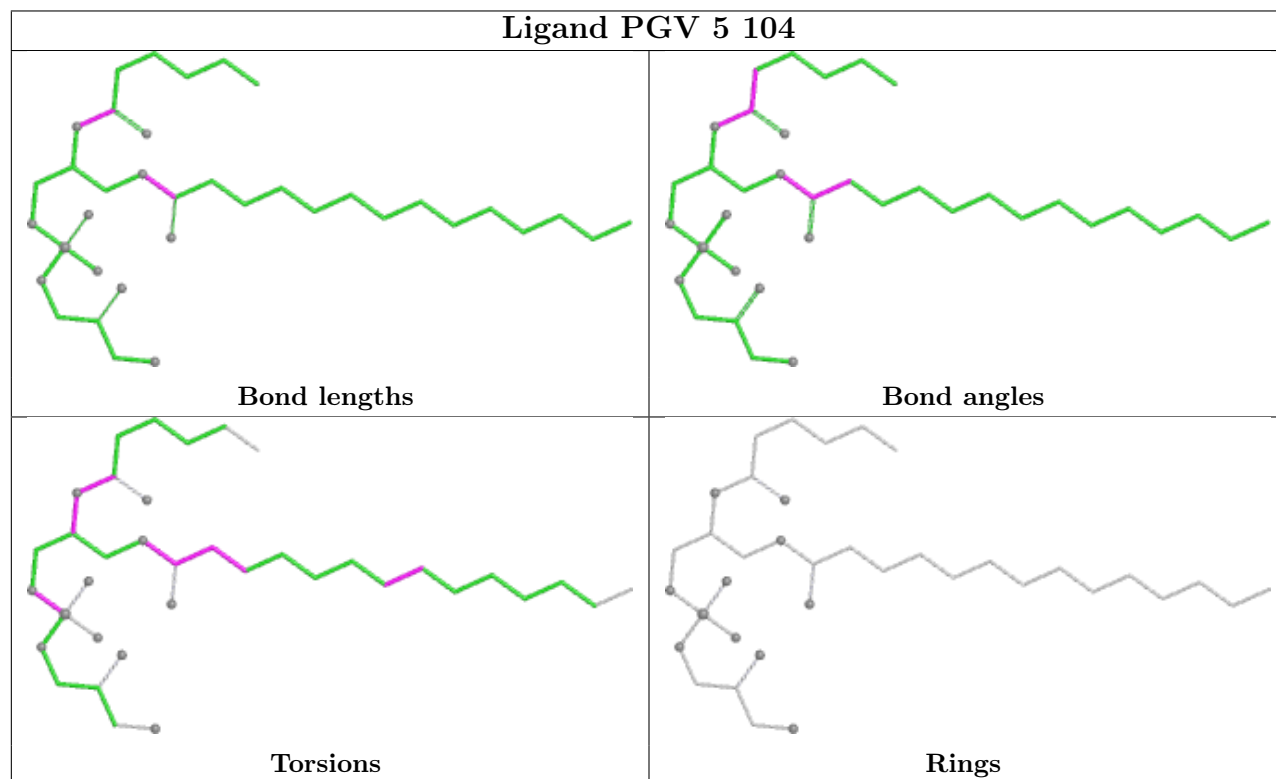
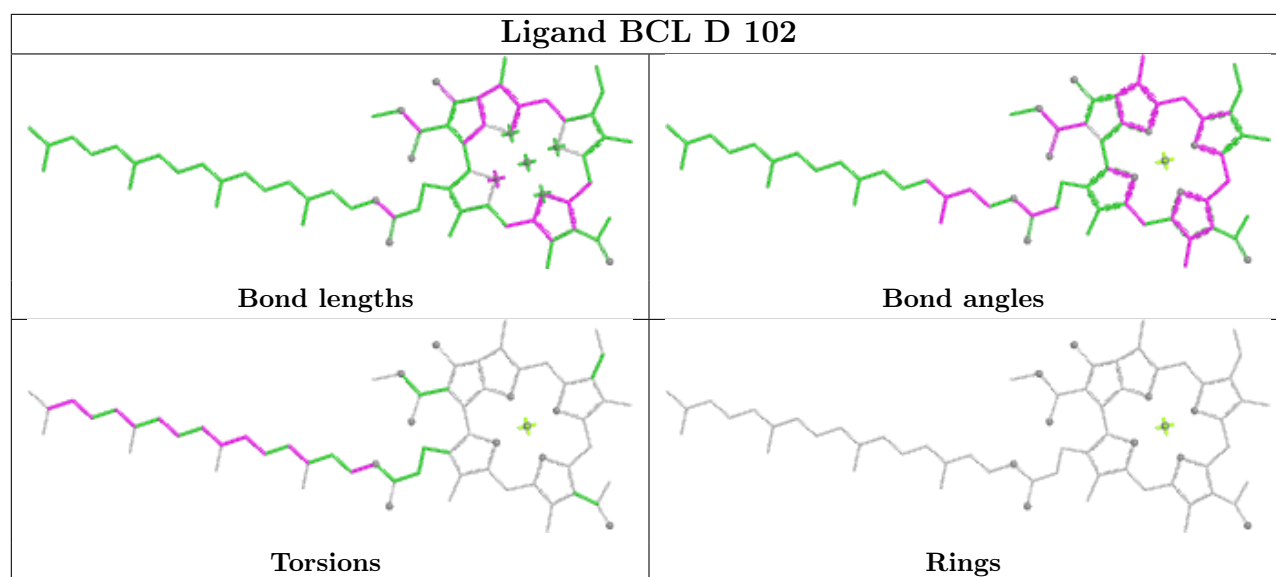
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	6	103	BCL	2	0
9	L	305	PGV	3	0
10	S	101	BCL	1	0
8	C	403	HEC	3	0
9	L	304	PGV	3	0
17	M	407	CDL	1	0
17	2	101	CDL	4	0
10	M	402	BCL	2	0
10	X	102	BCL	6	0
10	J	101	BCL	4	0
13	3	103	LMT	8	0
10	N	102	BCL	7	0
10	P	101	BCL	7	0
10	I	102	BCL	3	0
15	M	405	MQ9	3	0
16	6	102	I7D	1	0
9	C	405	PGV	2	0
10	M	403	BCL	3	0
11	L	302	BPH	4	0
10	L	301	BCL	1	0
10	Z	101	BCL	5	0
9	L	312	PGV	2	0
9	5	101	PGV	3	0
12	L	306	U10	1	0
10	0	102	BCL	4	0
9	L	311	PGV	7	0
8	C	402	HEC	3	0
10	T	102	BCL	3	0
8	C	401	HEC	2	0
17	0	101	CDL	3	0
9	M	410	PGV	3	0
9	K	103	PGV	1	0
10	L	309	BCL	2	0
10	G	101	BCL	10	0
10	A	102	BCL	3	0
10	5	102	BCL	3	0
10	B	101	BCL	5	0
10	K	102	BCL	3	0
10	8	102	BCL	4	0
10	V	102	BCL	3	0
10	Y	101	BCL	2	0
10	E	102	BCL	5	0

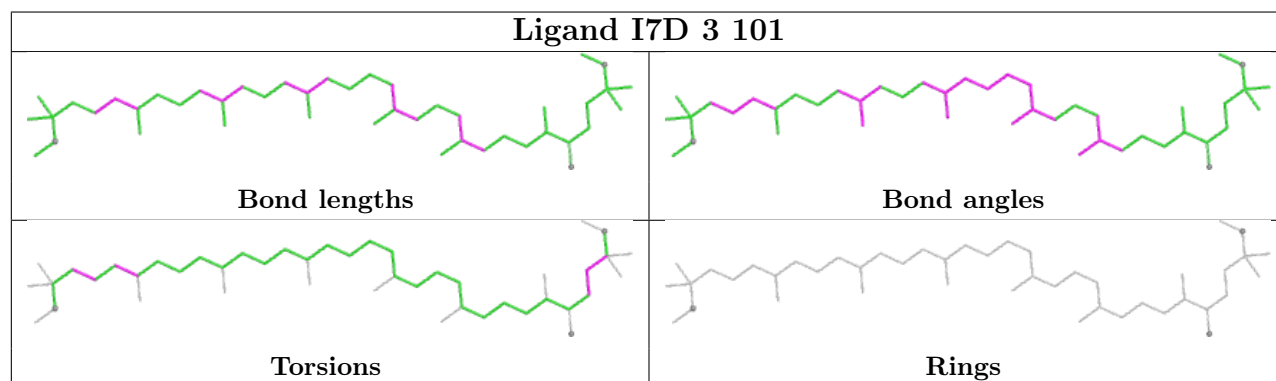
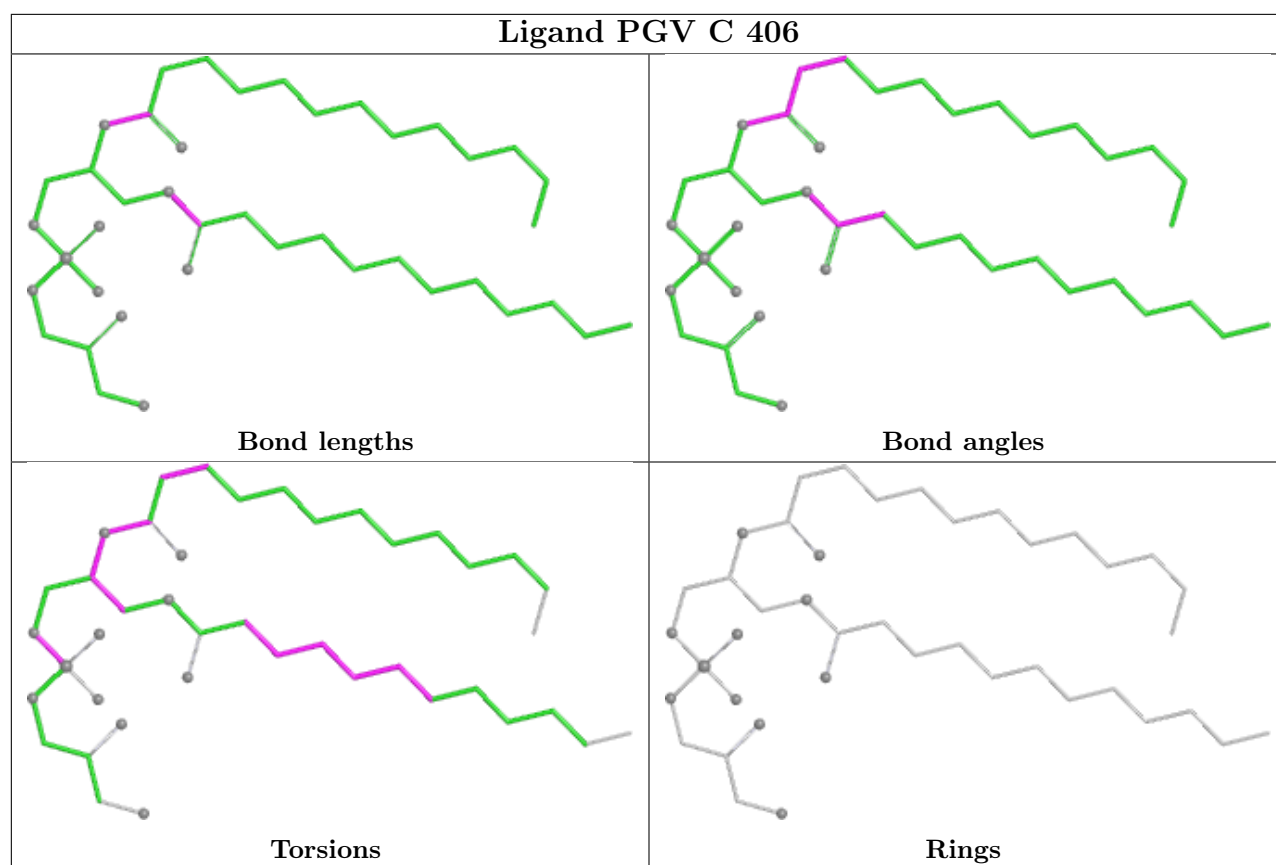
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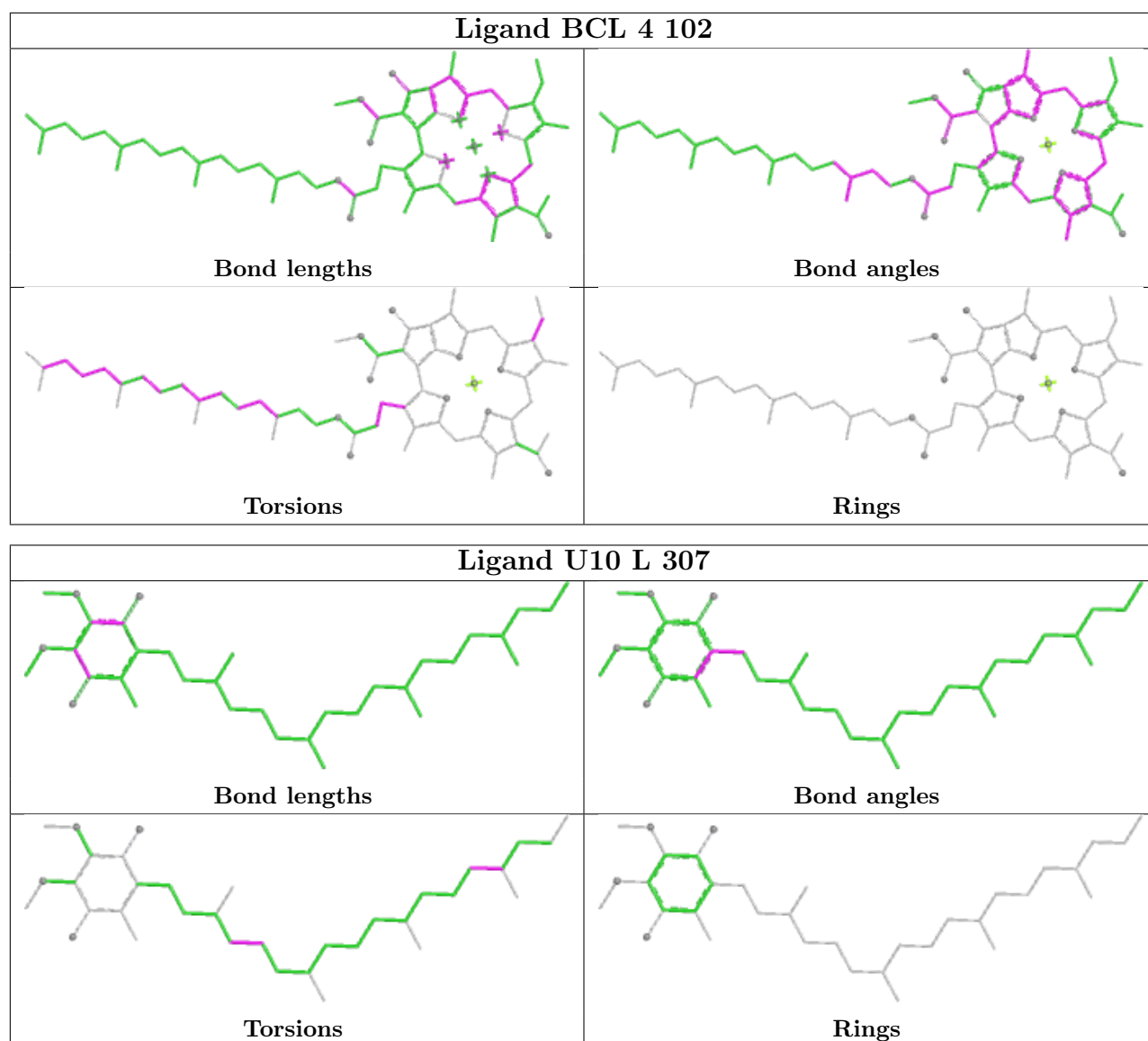
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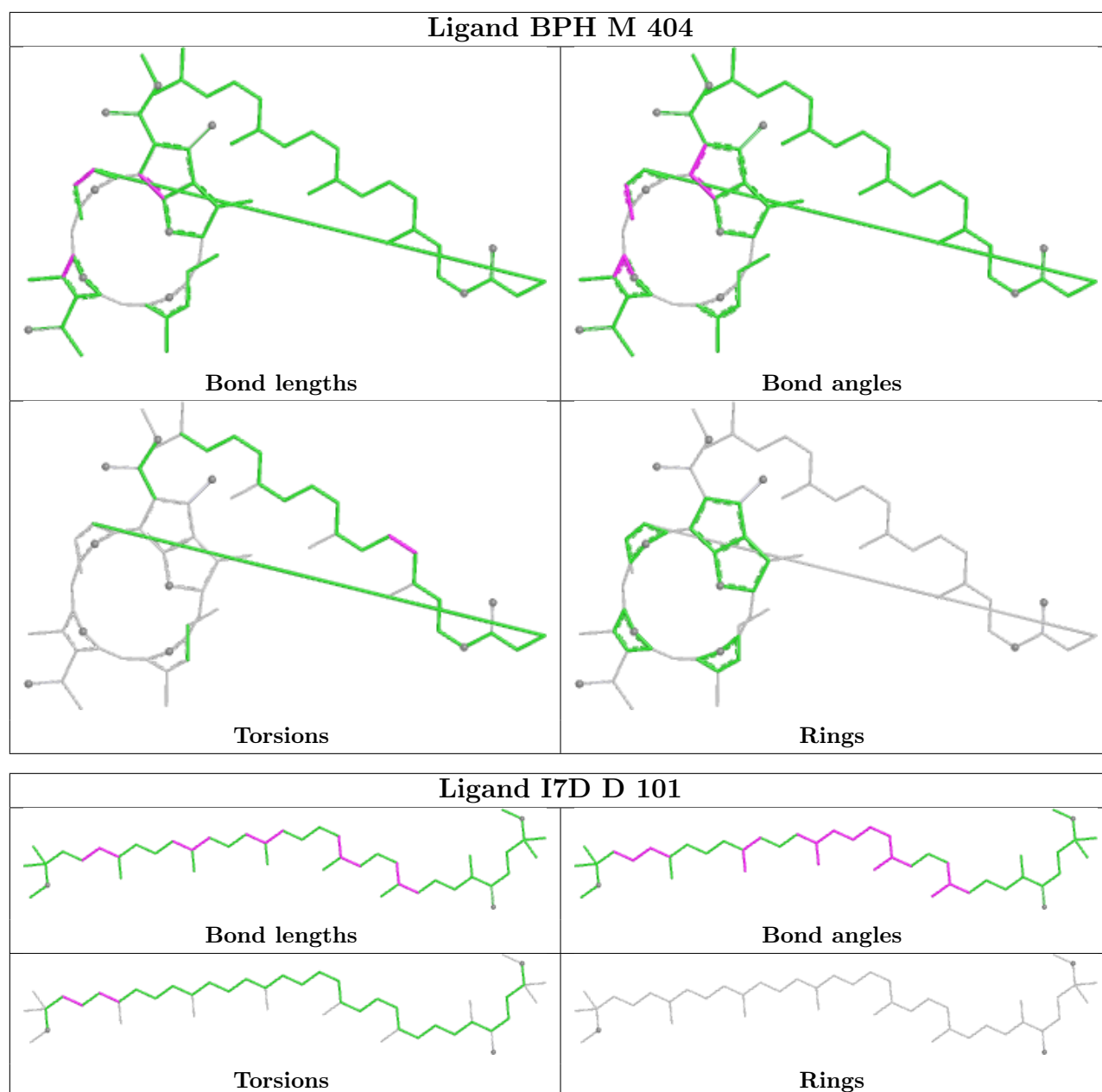
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	313	LMT	2	0
17	H	303	CDL	4	0
10	F	101	BCL	2	0
9	M	411	PGV	1	0
9	F	102	PGV	1	0
9	H	301	PGV	2	0
9	D	103	PGV	1	0
17	M	408	CDL	6	0
10	R	102	BCL	6	0
9	C	407	PGV	5	0
10	2	102	BCL	3	0
9	5	103	PGV	3	0
8	C	404	HEC	1	0
12	7	401	U10	9	0
13	L	308	LMT	2	0
17	T	103	CDL	4	0
10	Q	102	BCL	1	0
10	W	101	BCL	1	0
10	U	101	BCL	1	0
10	1	102	BCL	1	0
17	6	101	CDL	6	0
10	O	101	BCL	1	0
13	I	103	LMT	3	0
10	9	101	BCL	4	0
17	6	104	CDL	3	0
10	3	102	BCL	3	0

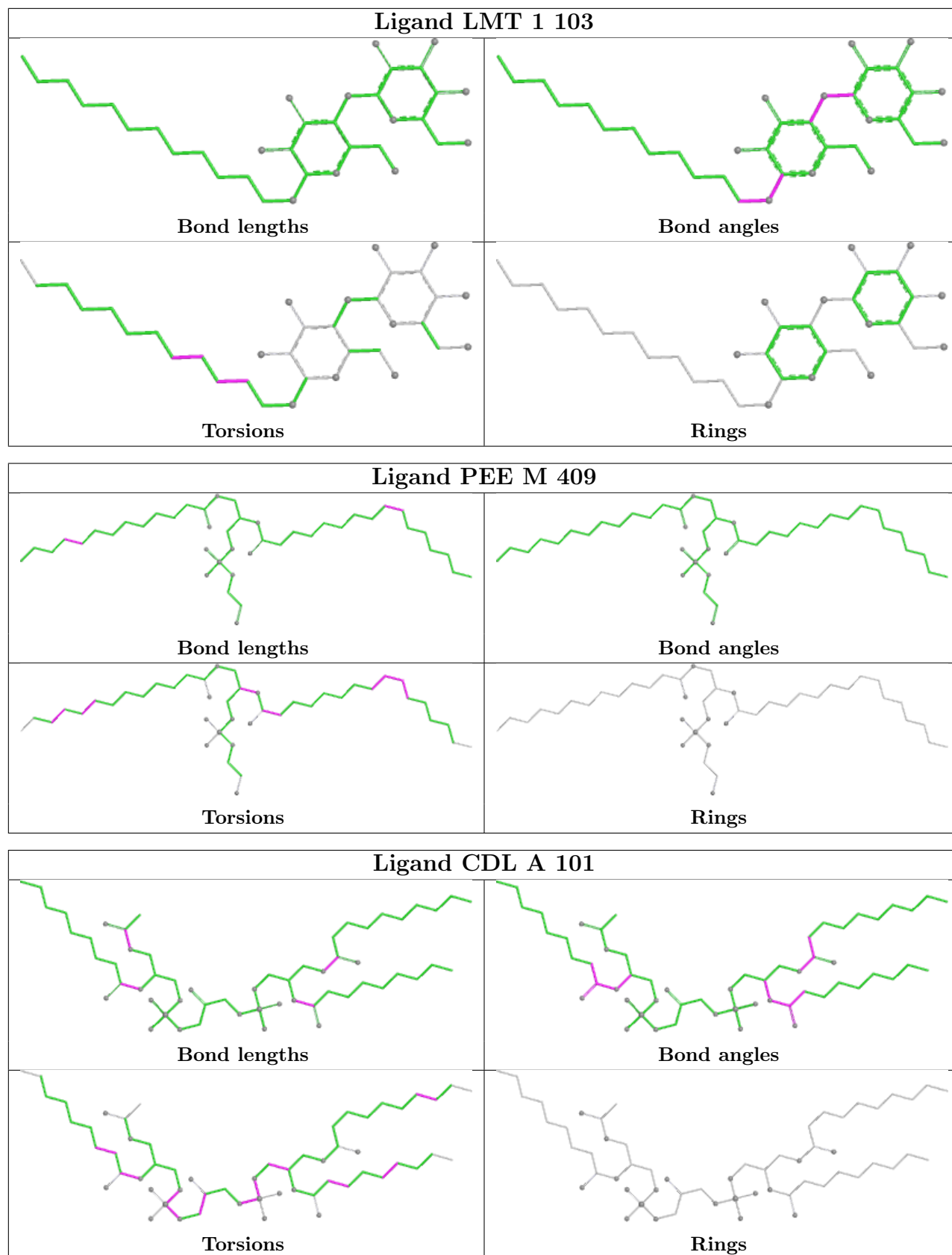
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

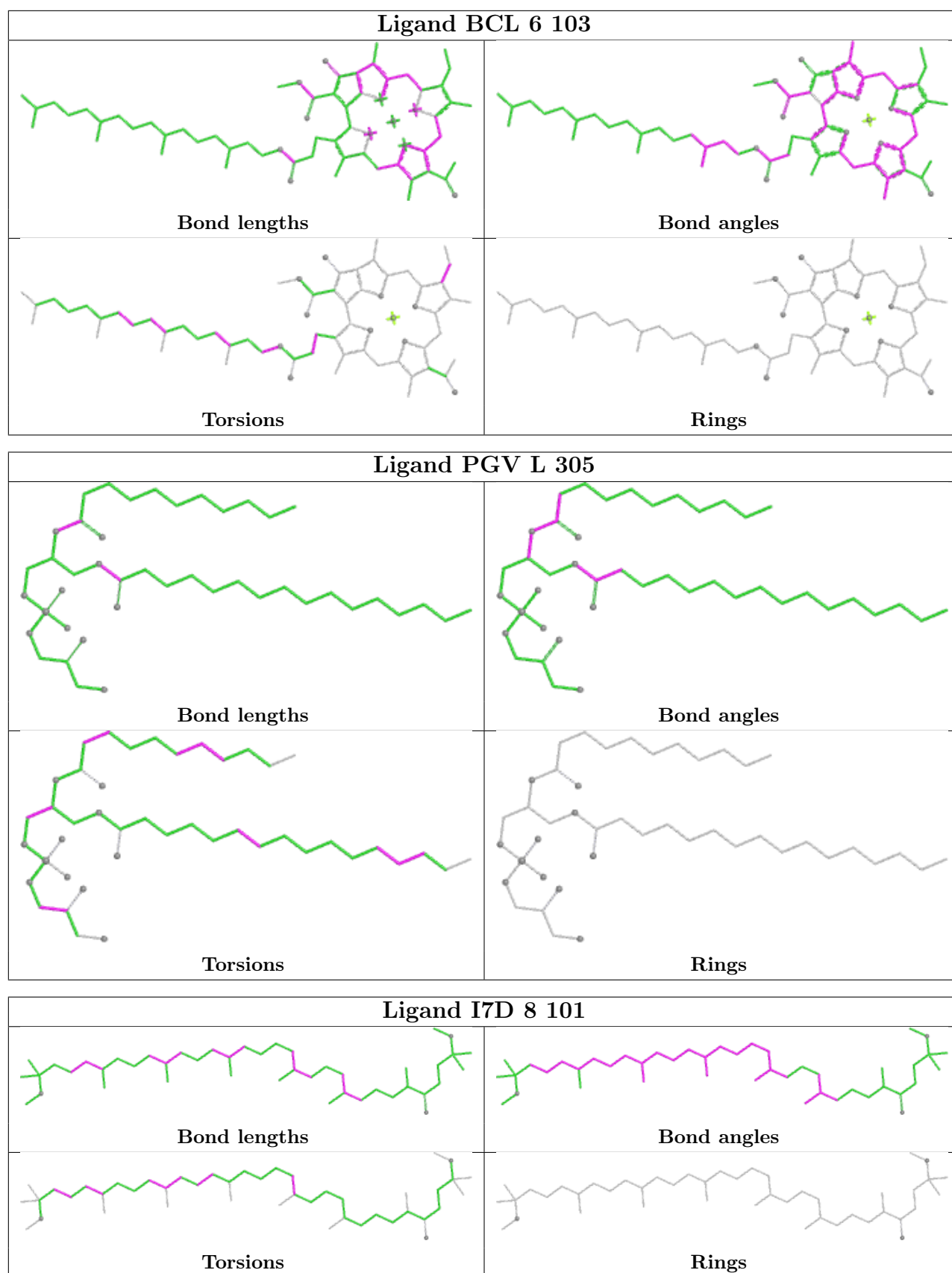


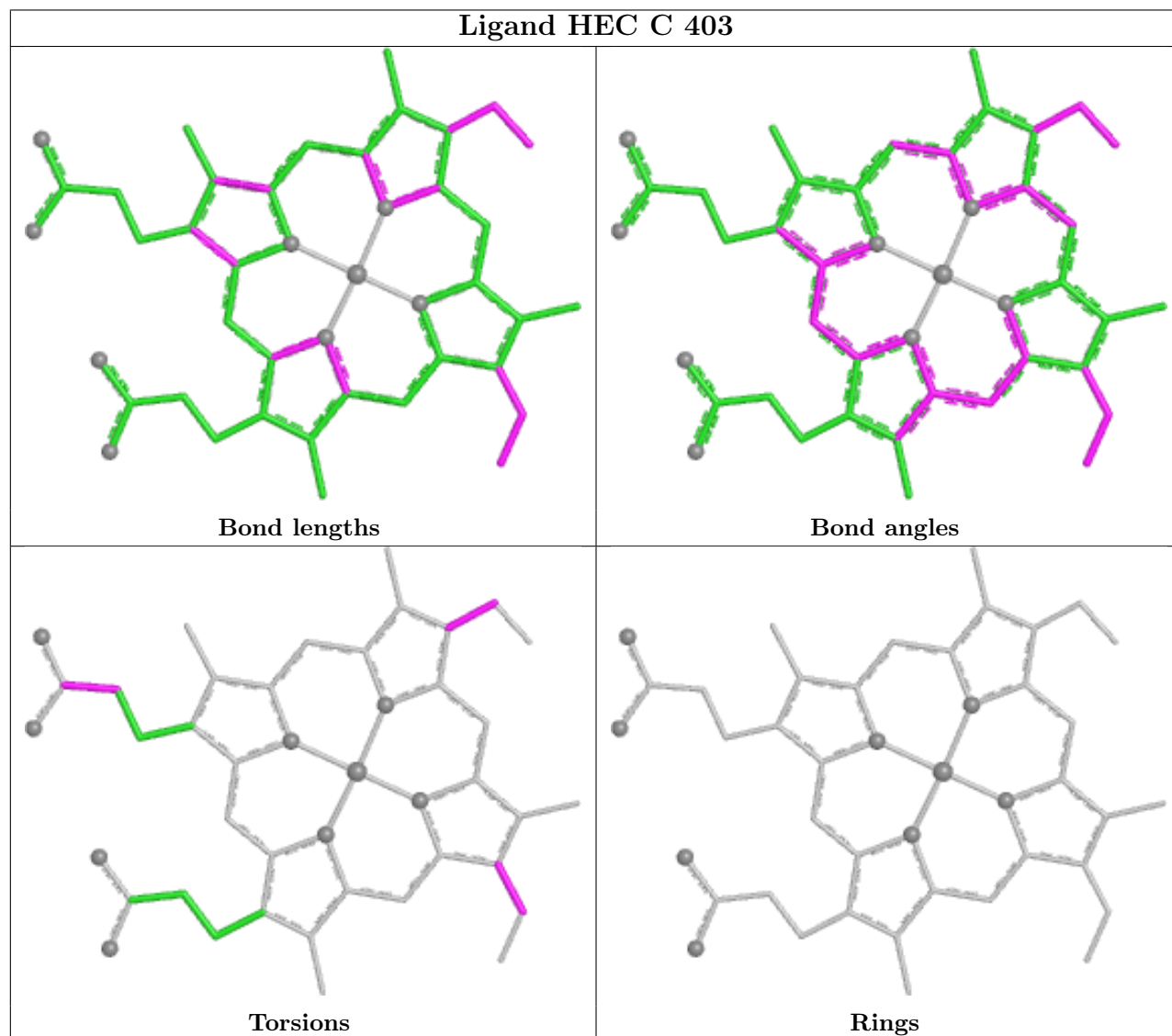
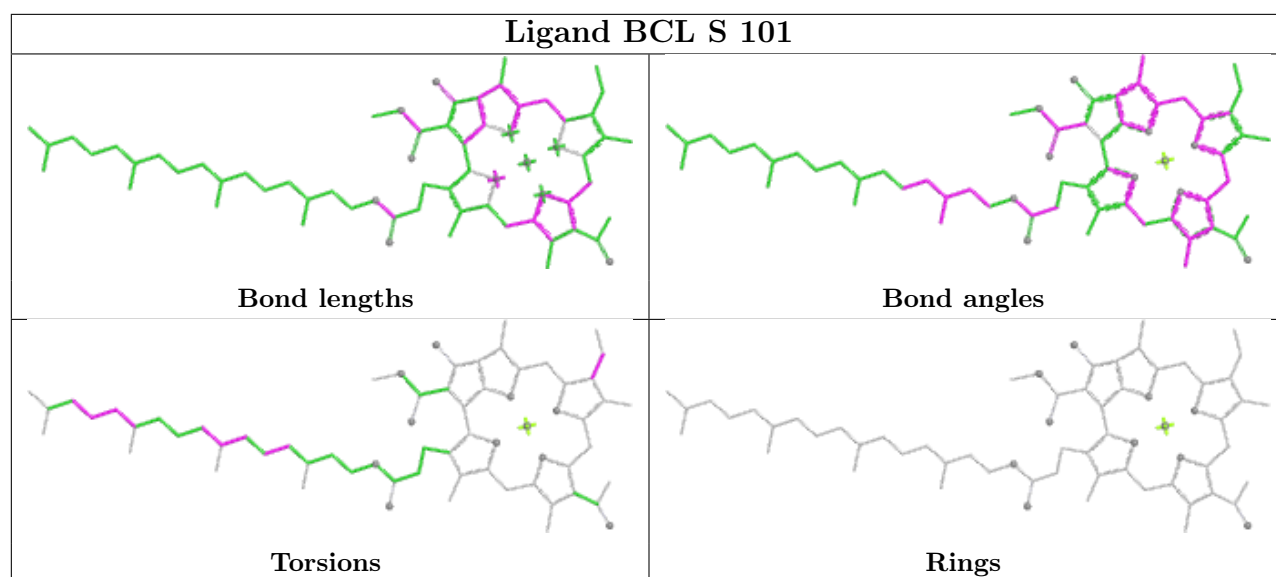


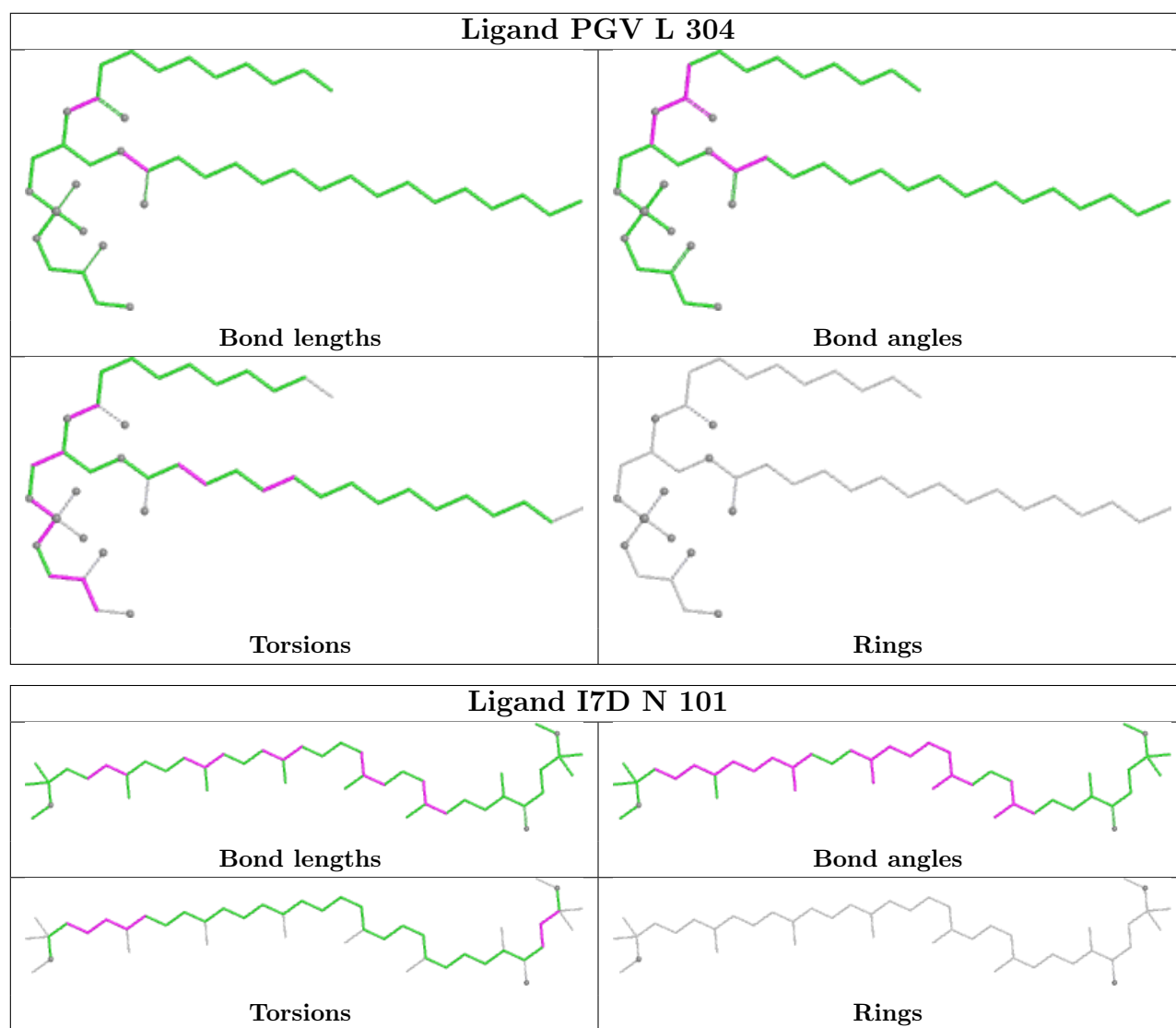


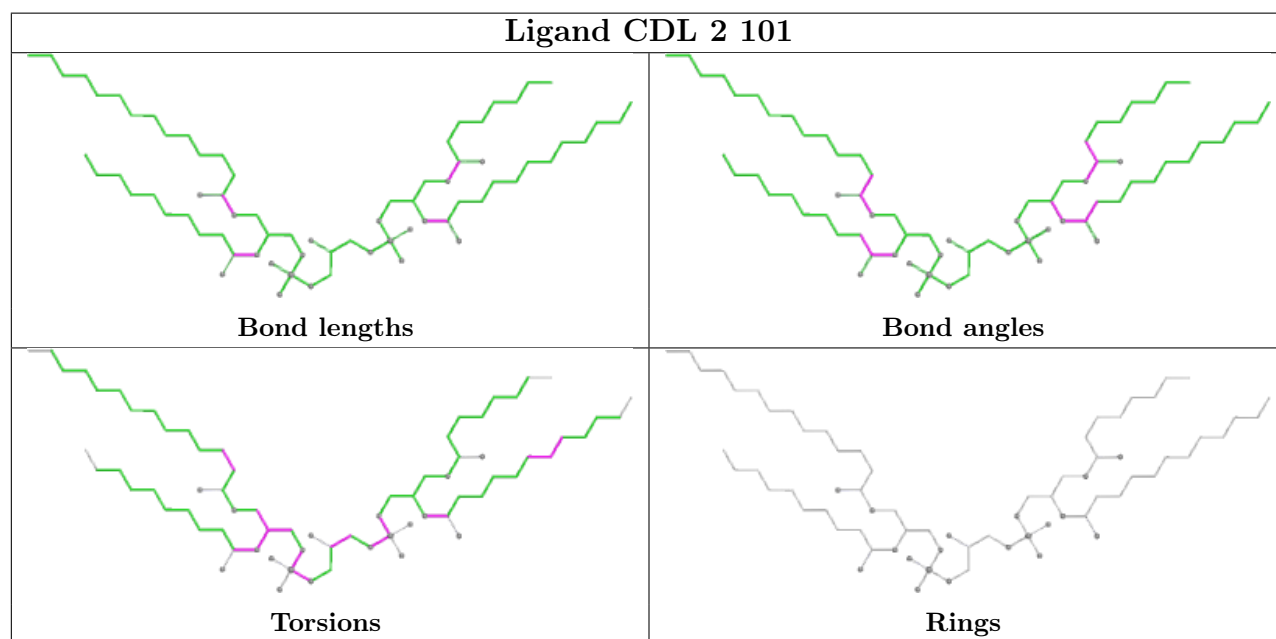
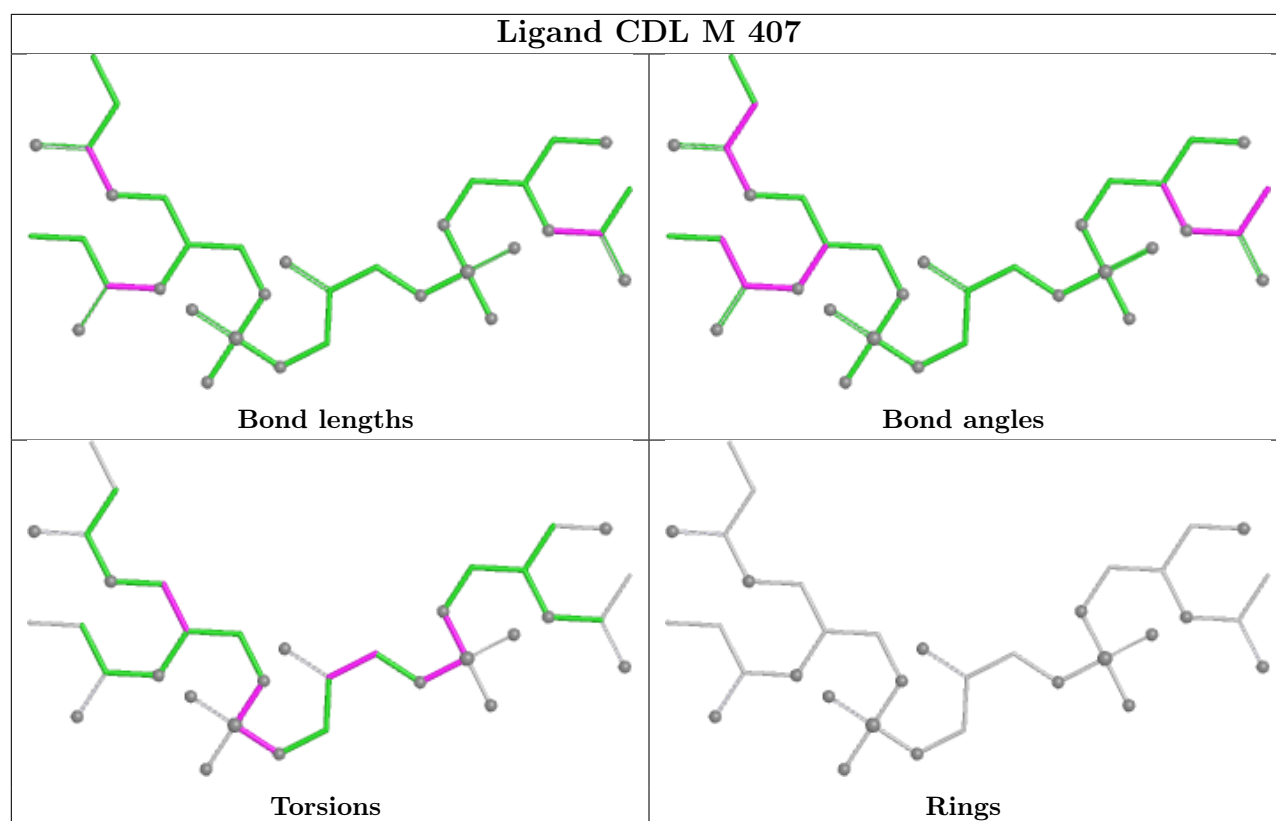


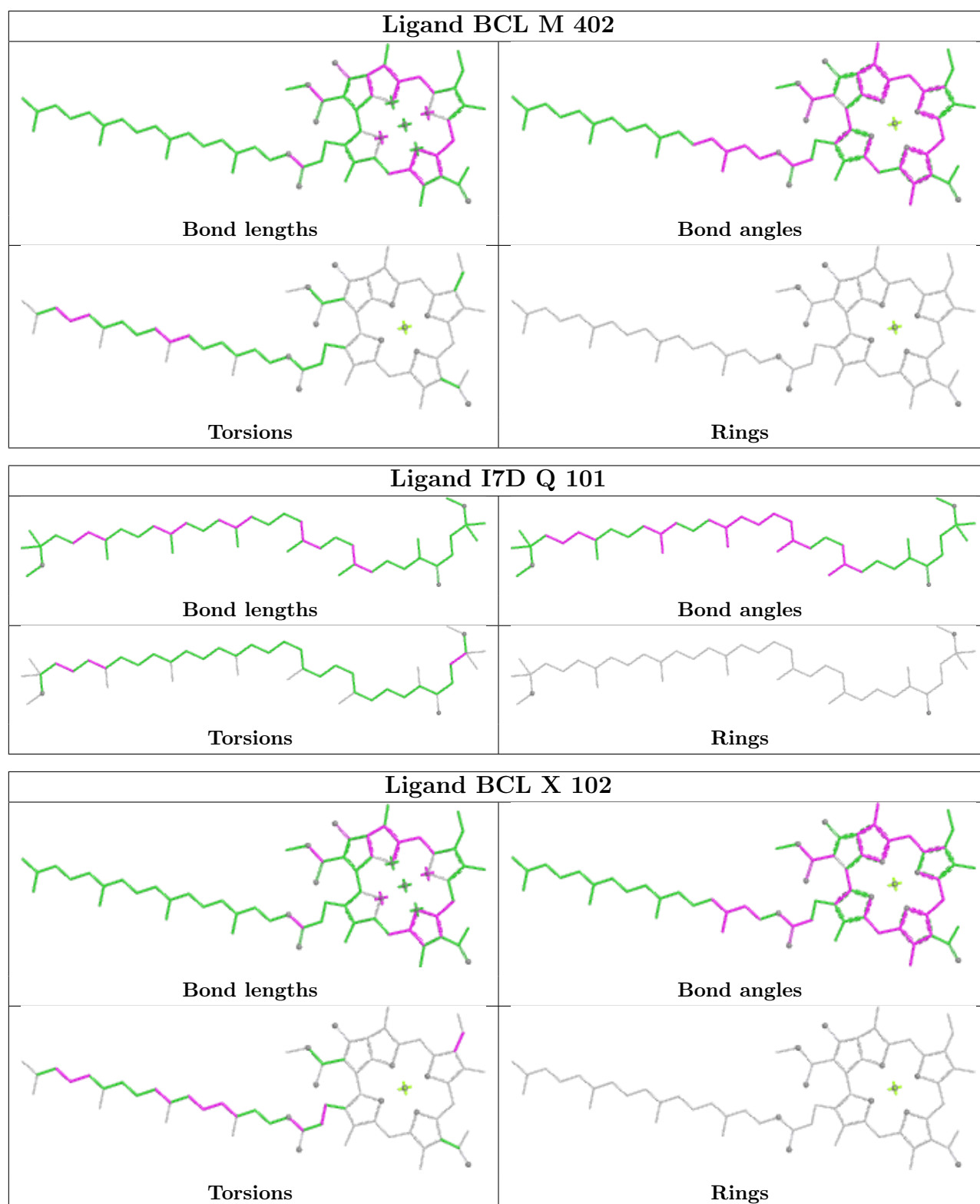


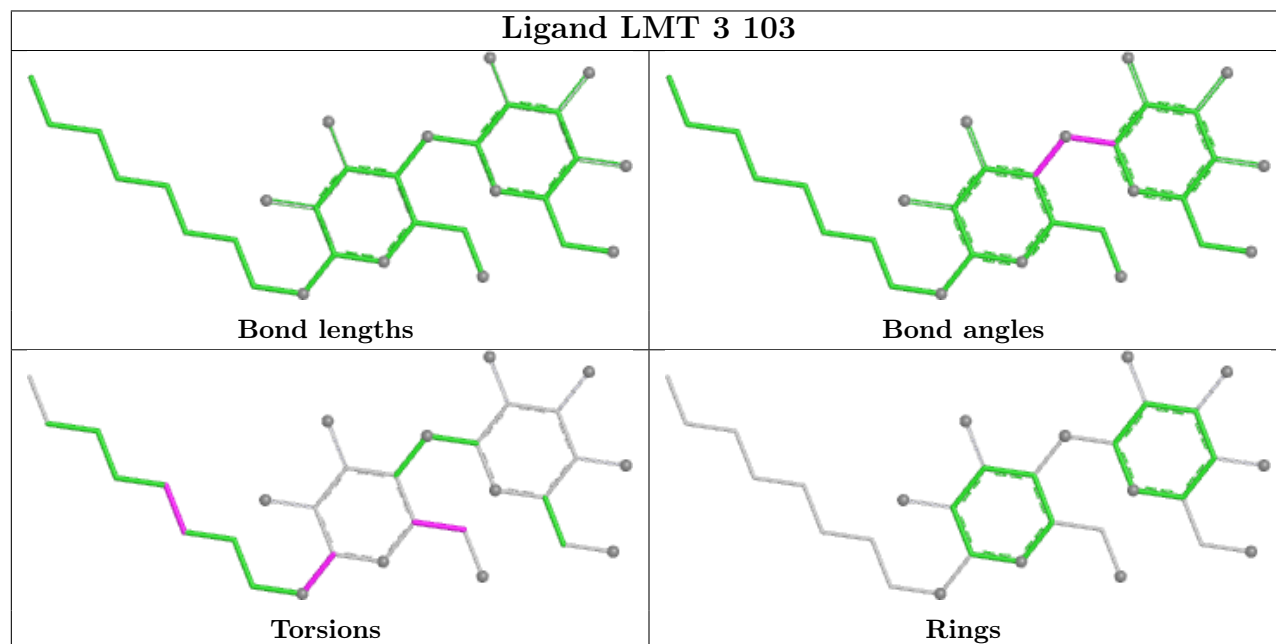
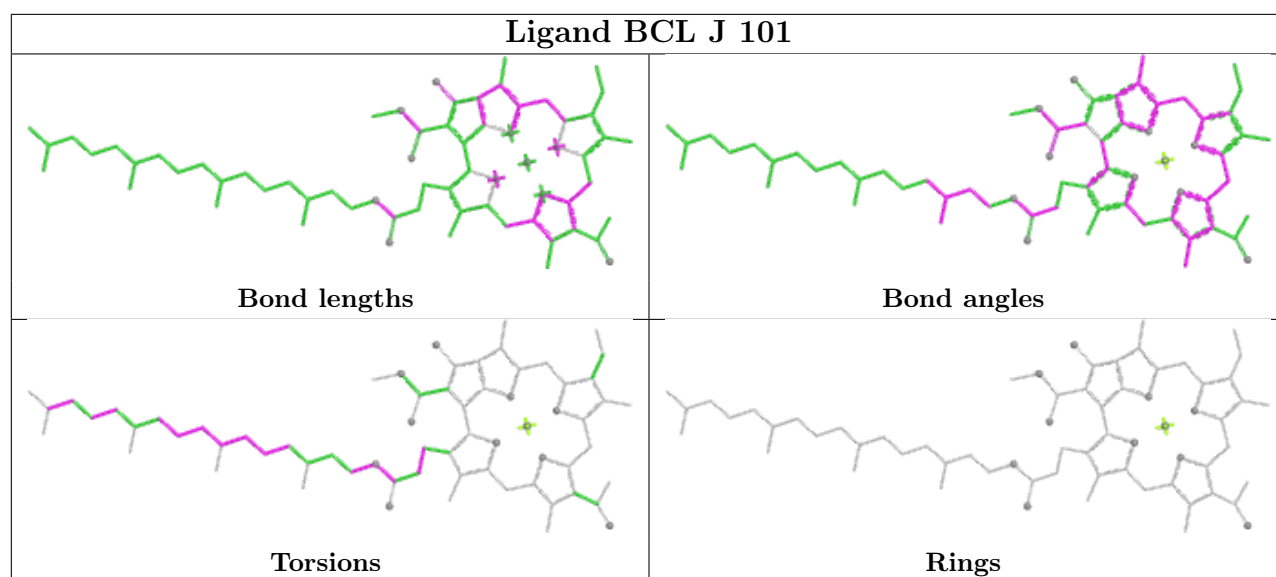


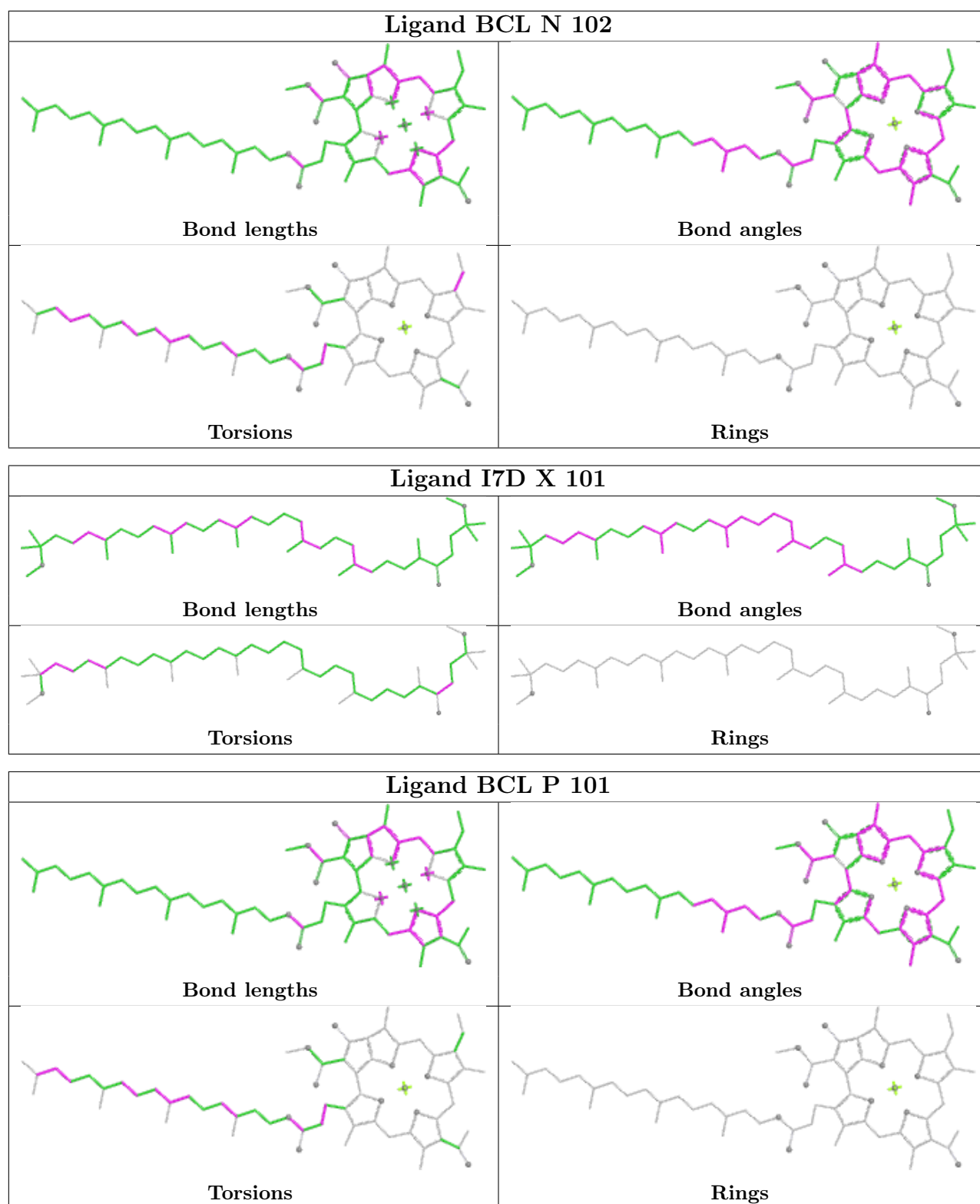


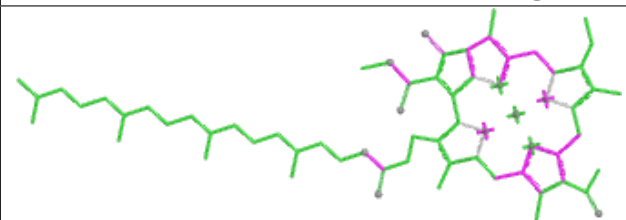
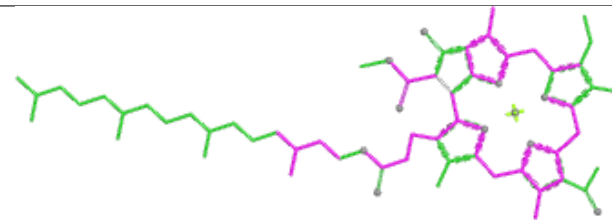
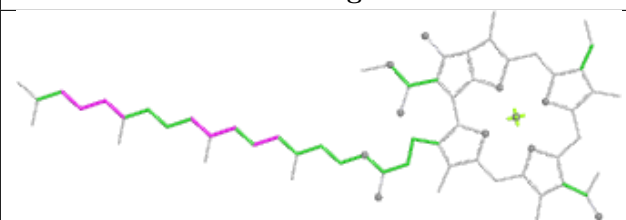
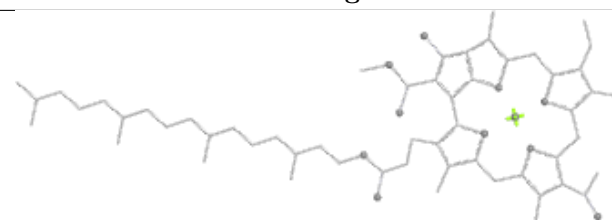


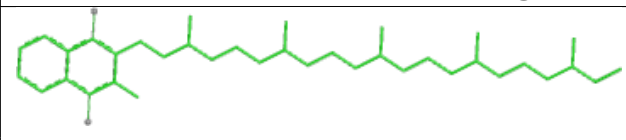
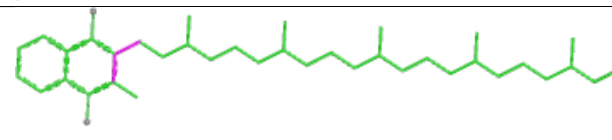
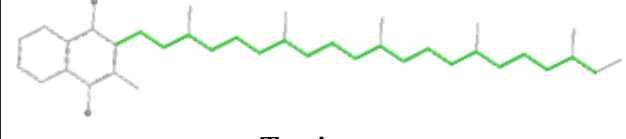
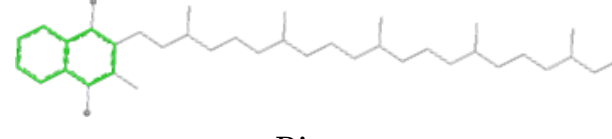


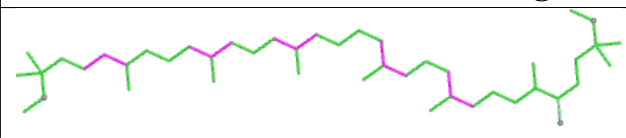
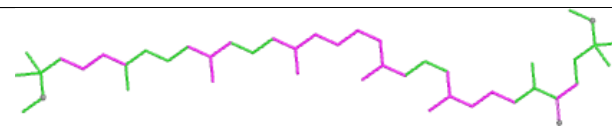
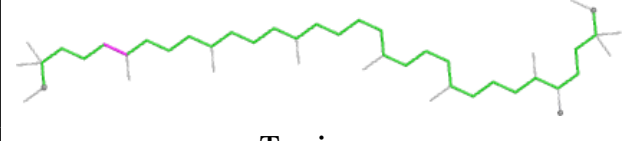
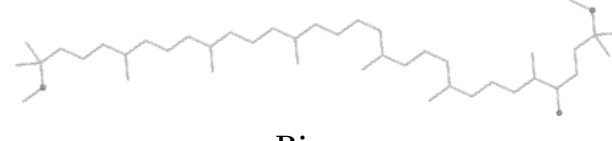


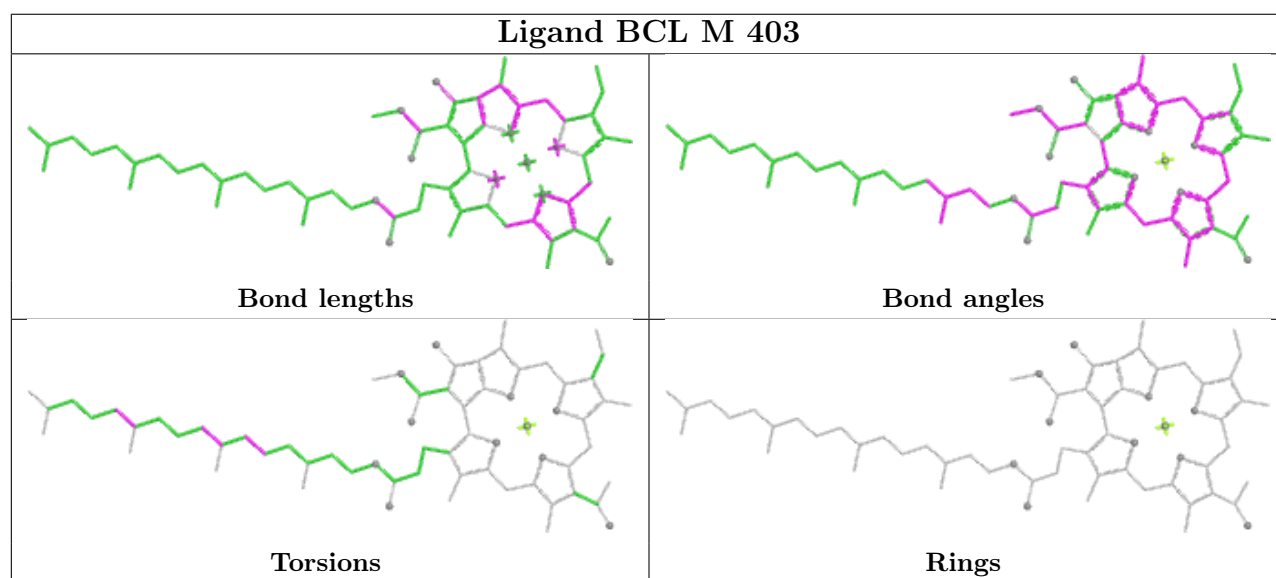
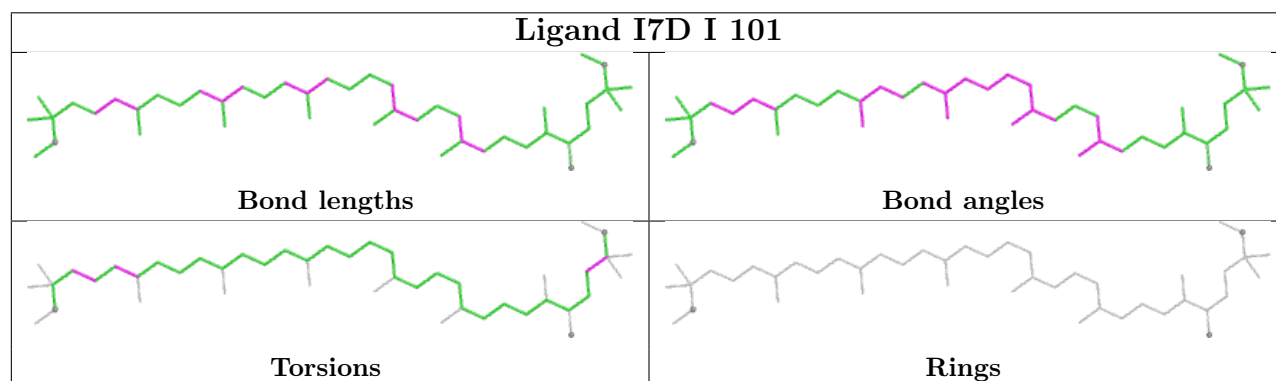
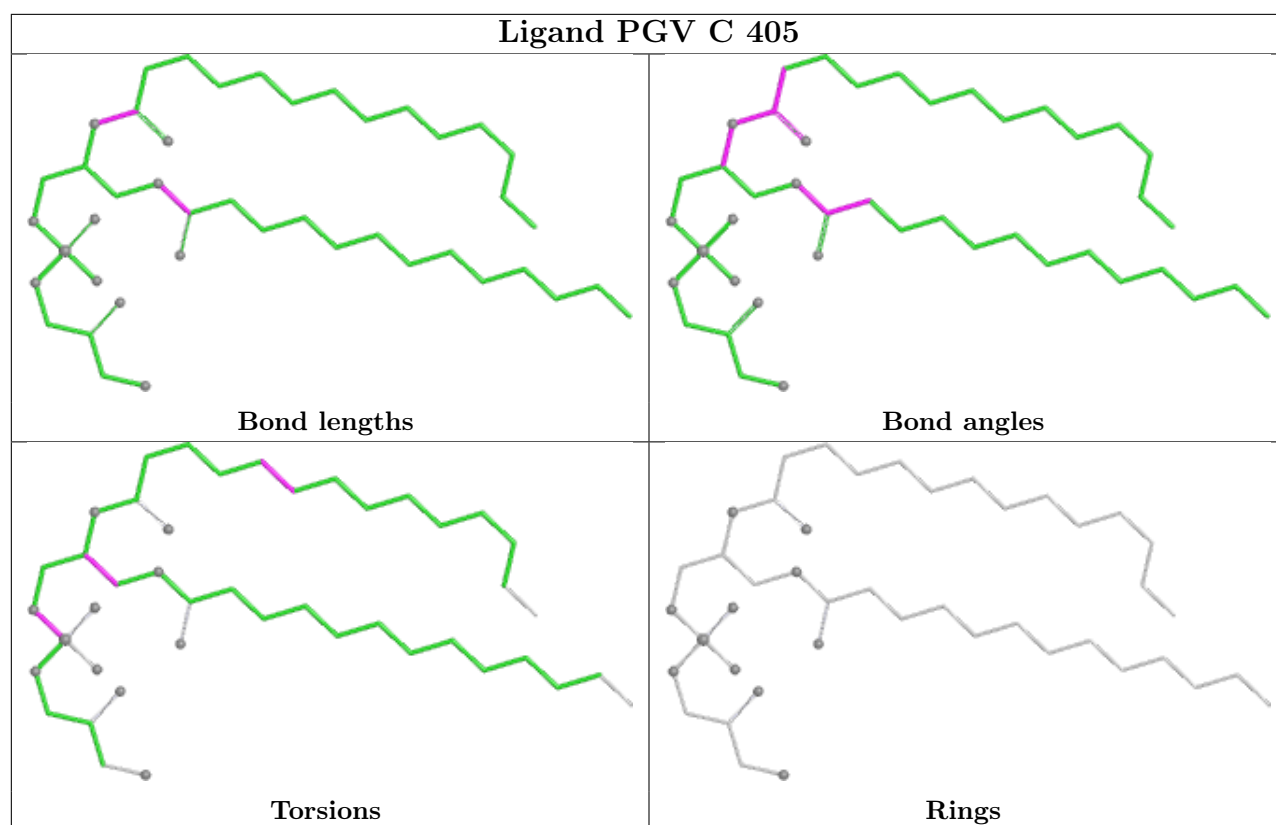


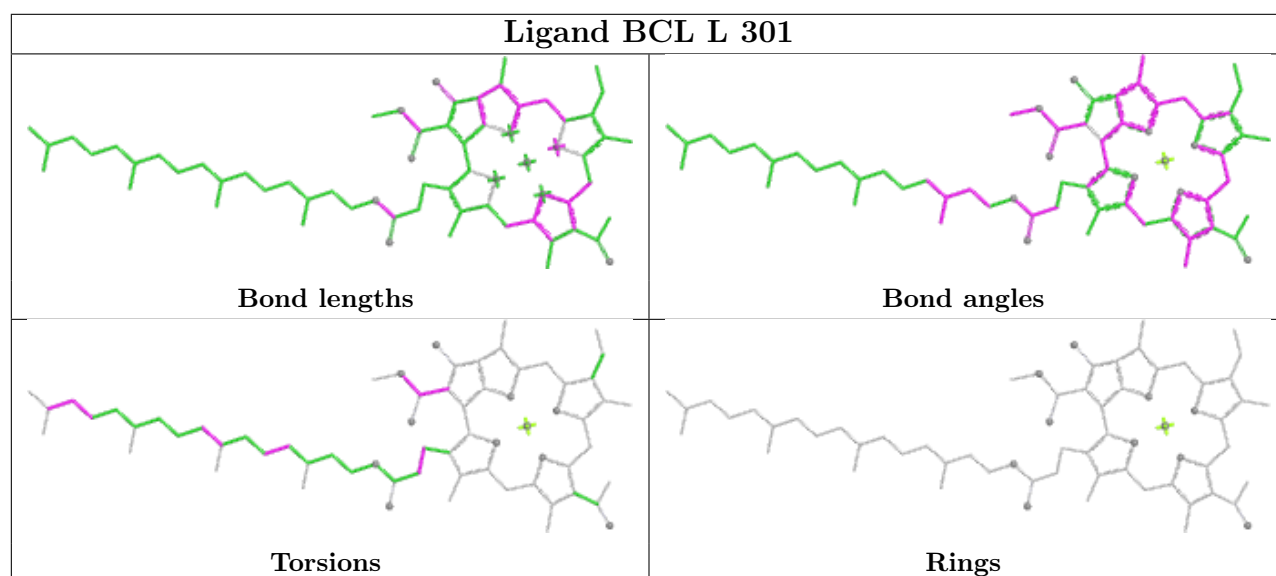
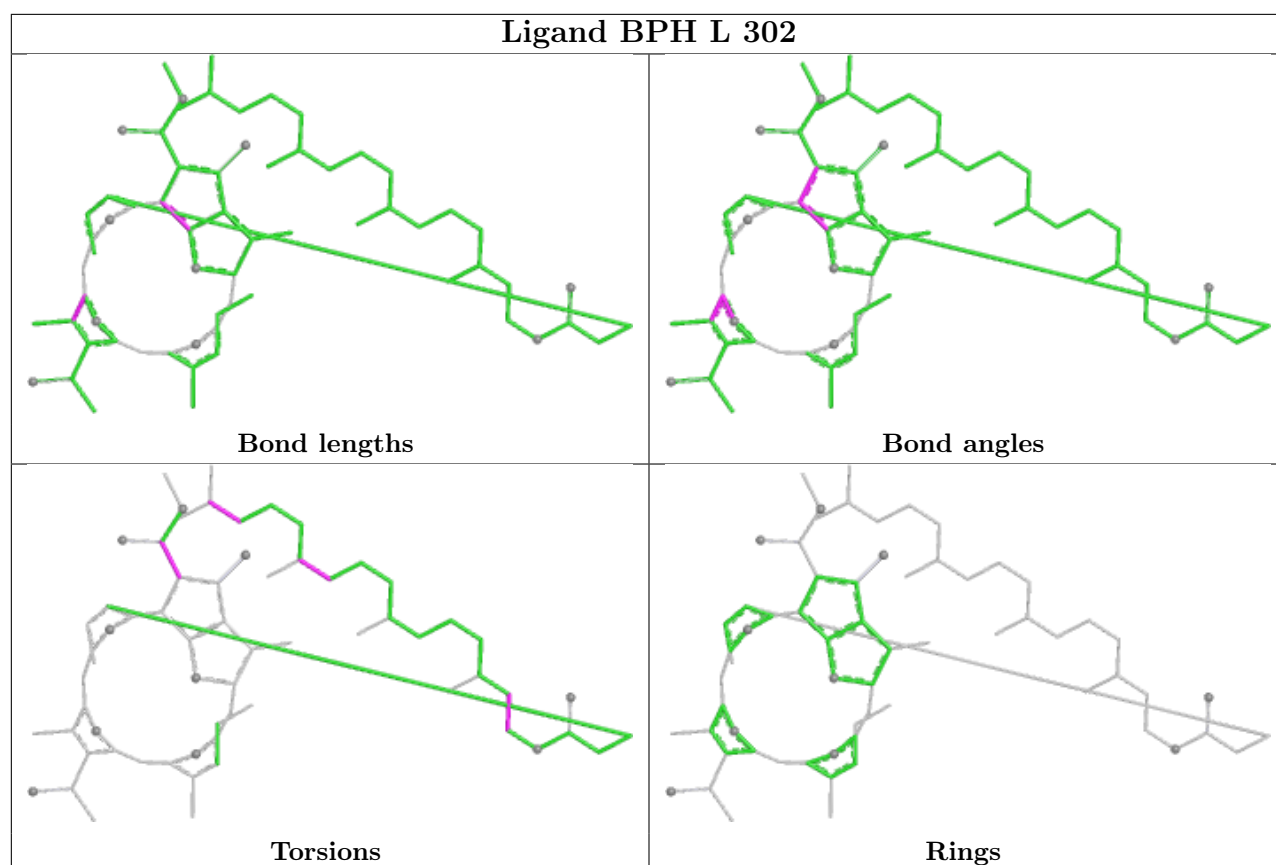


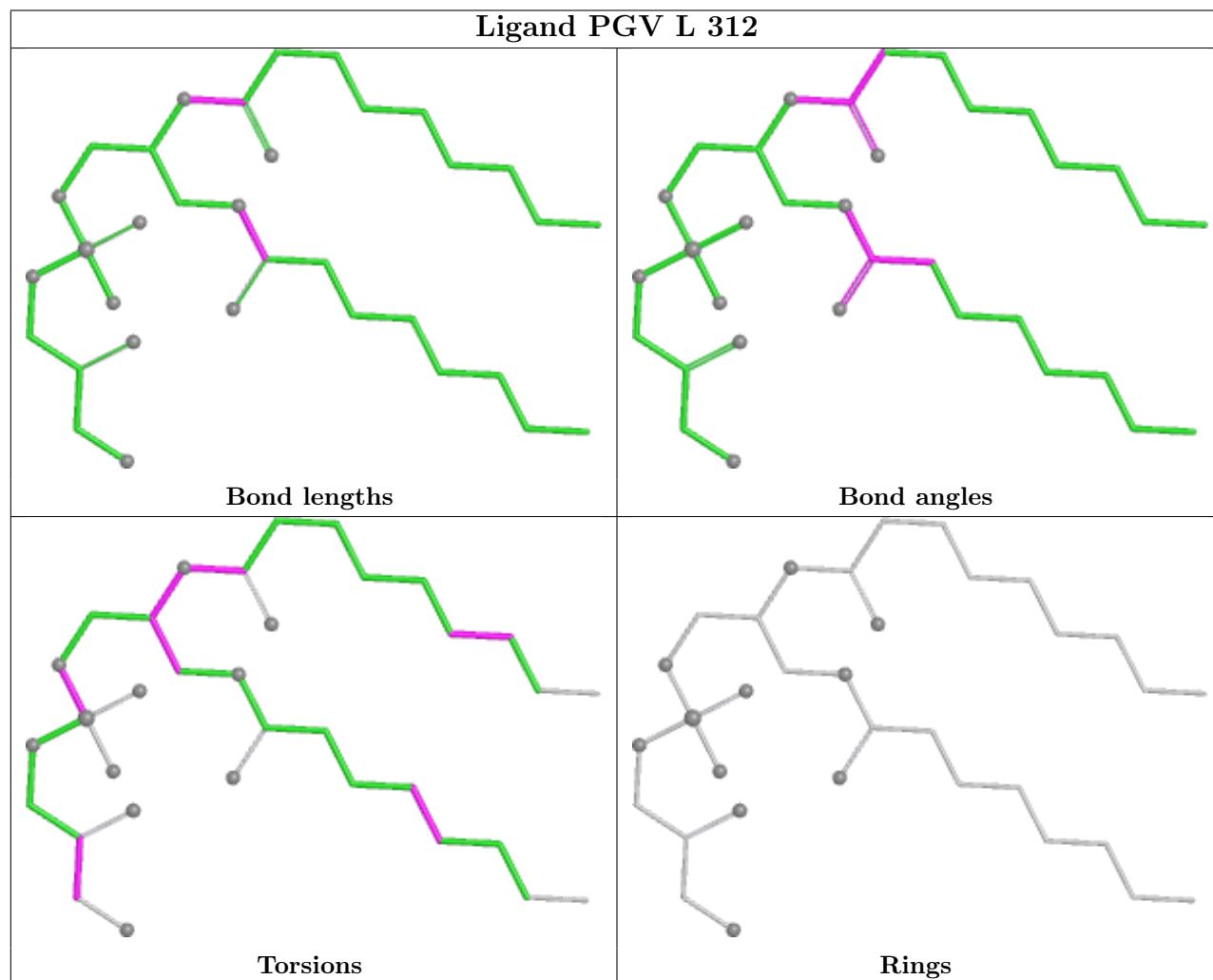
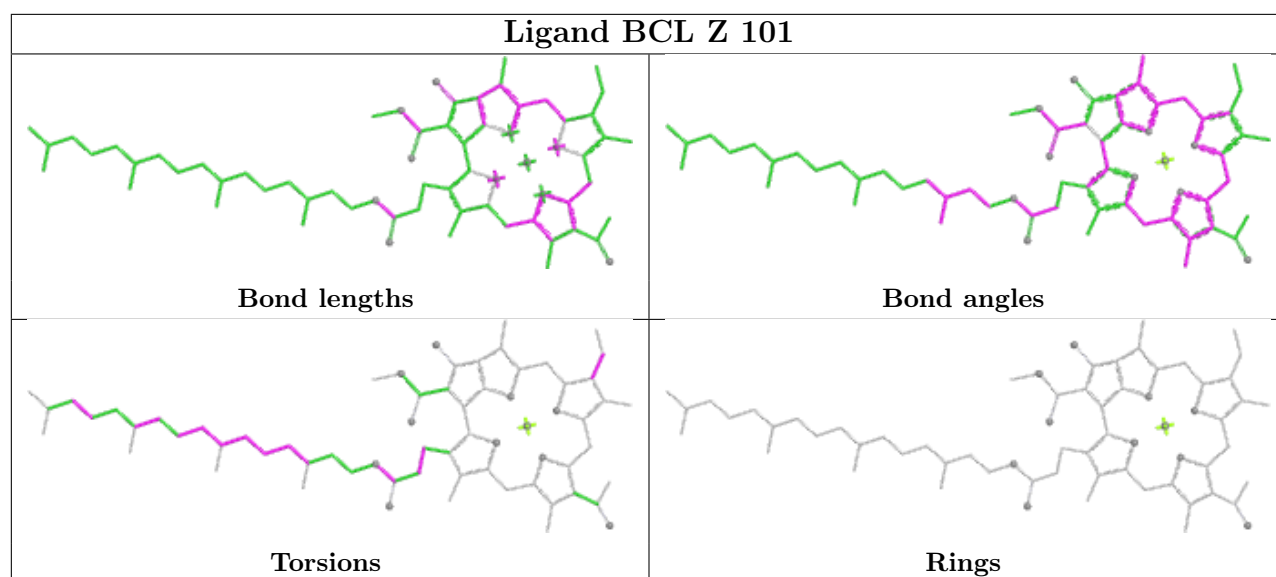
Ligand BCL I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

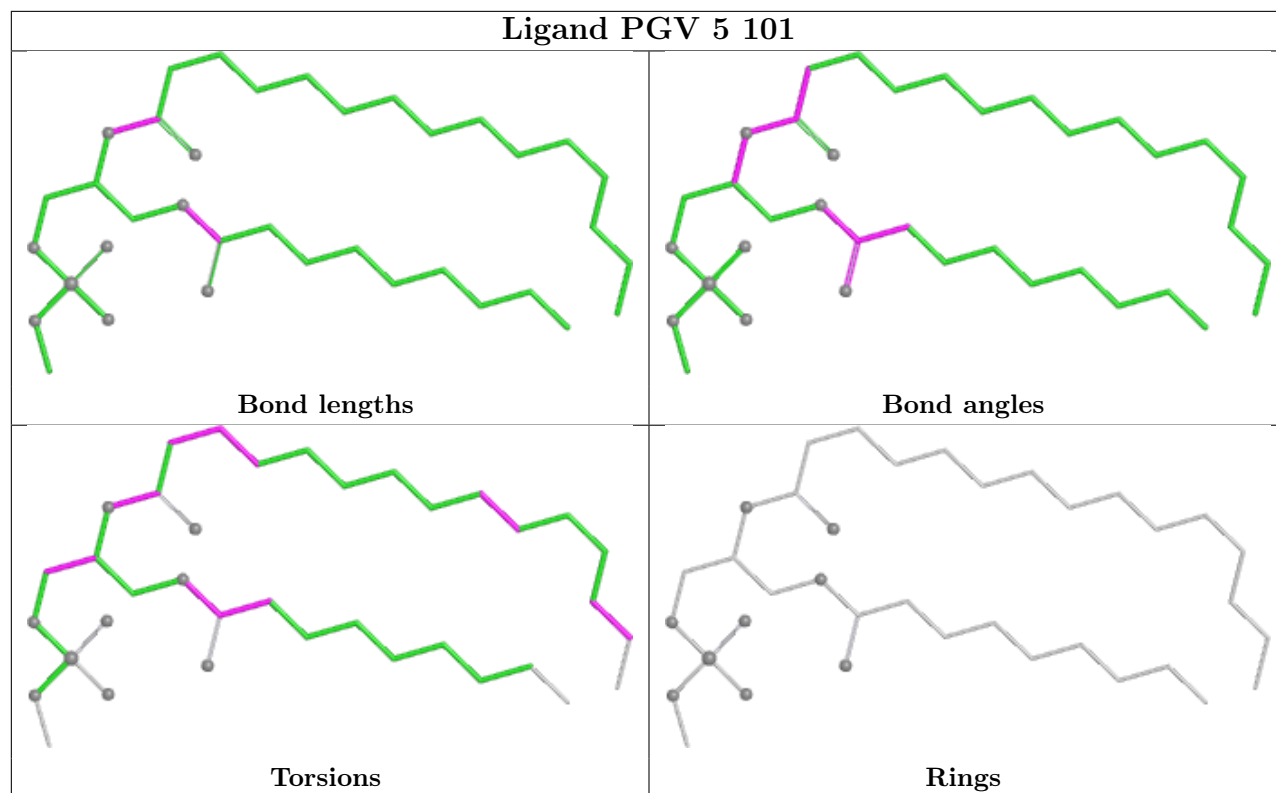
Ligand MQ9 M 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand I7D 6 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

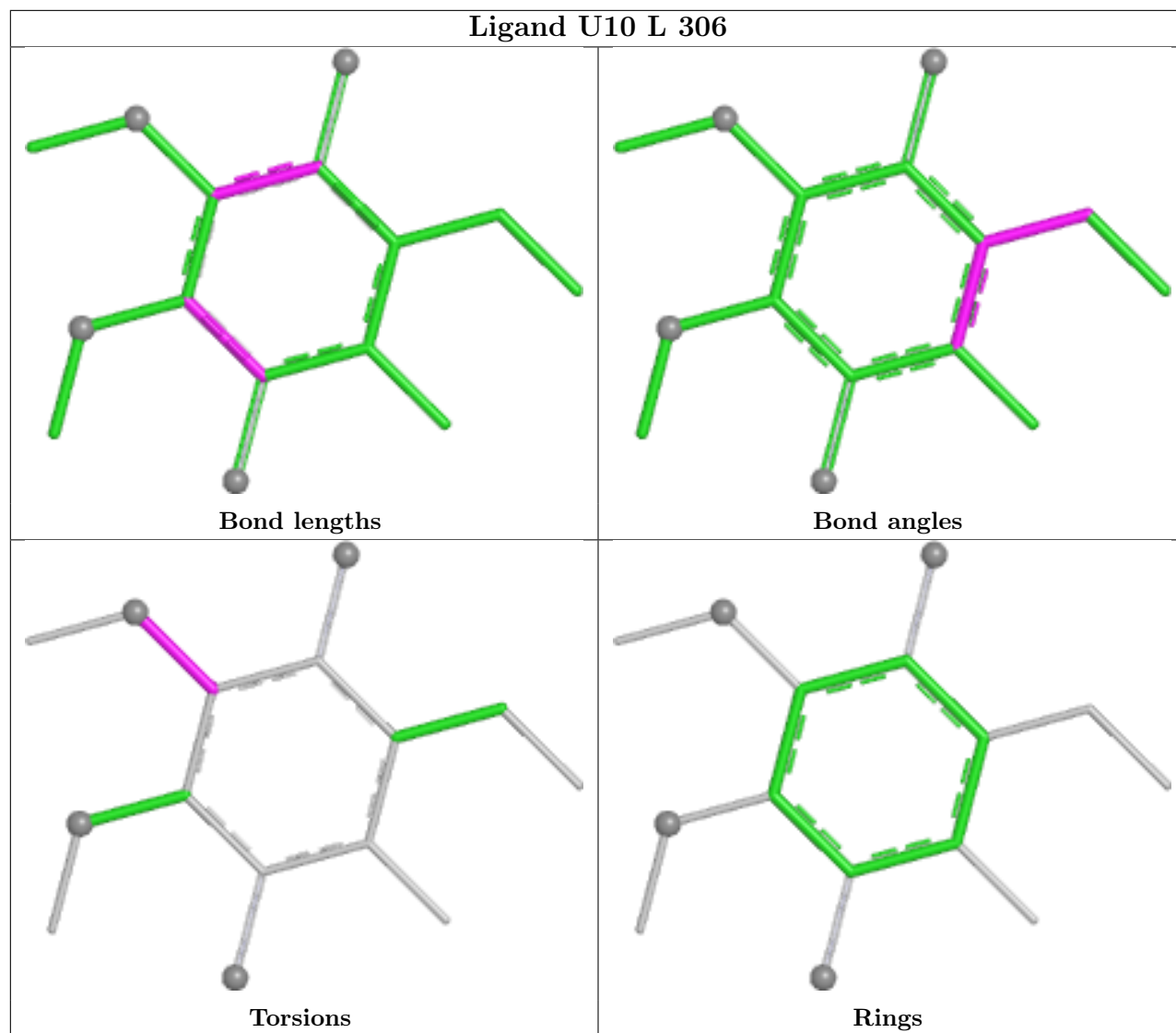




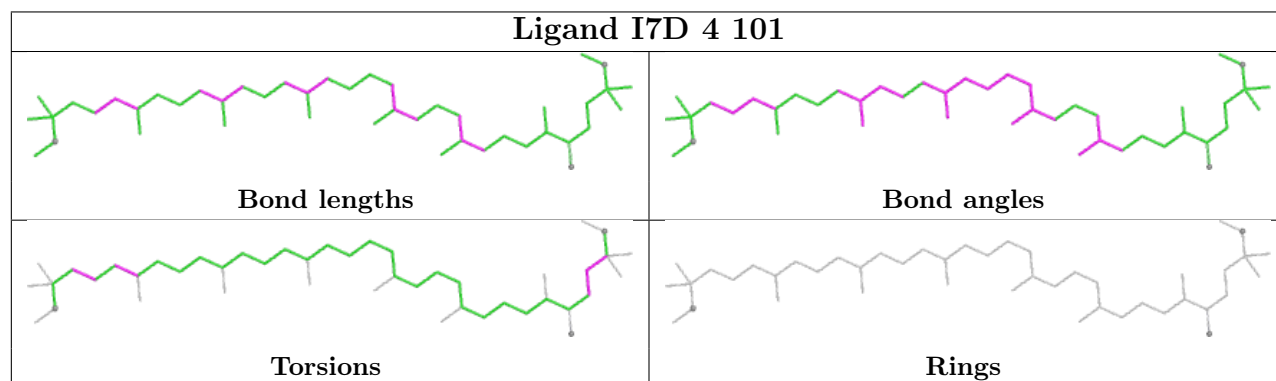


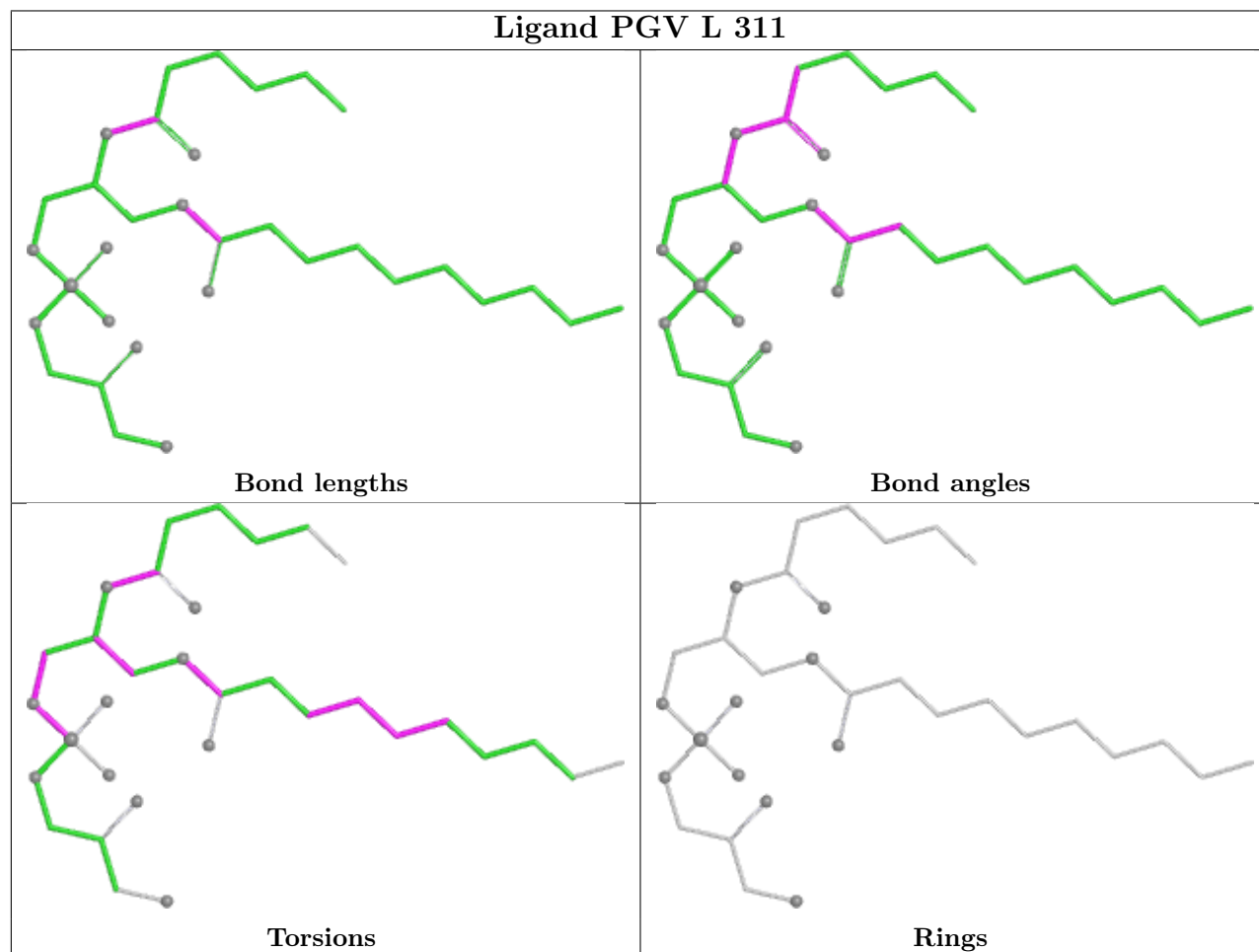
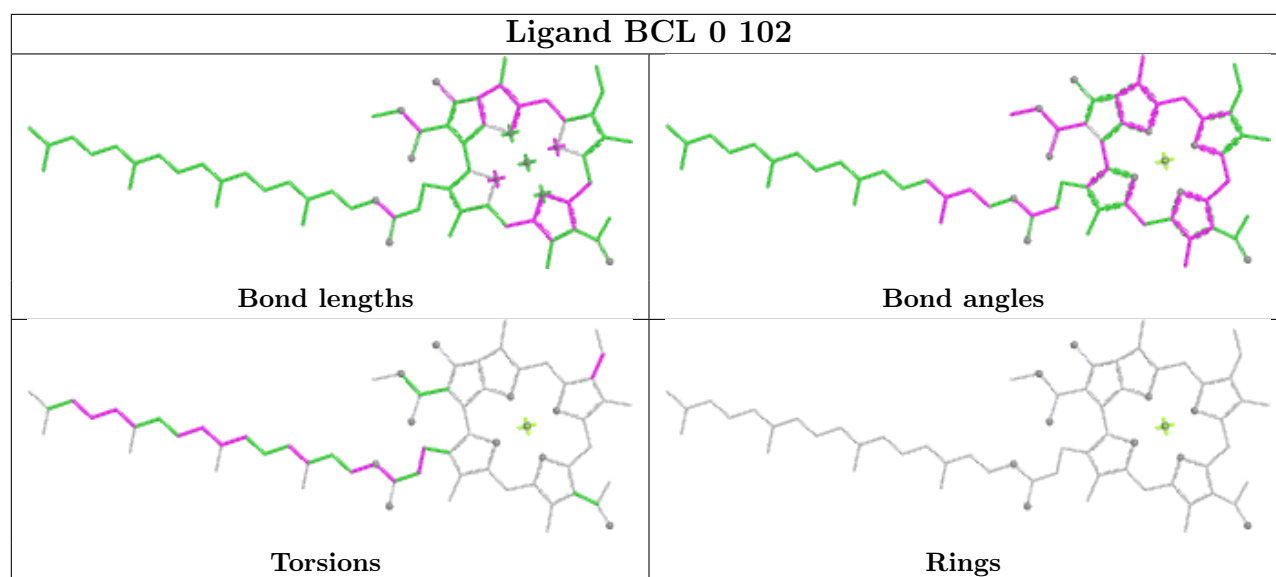


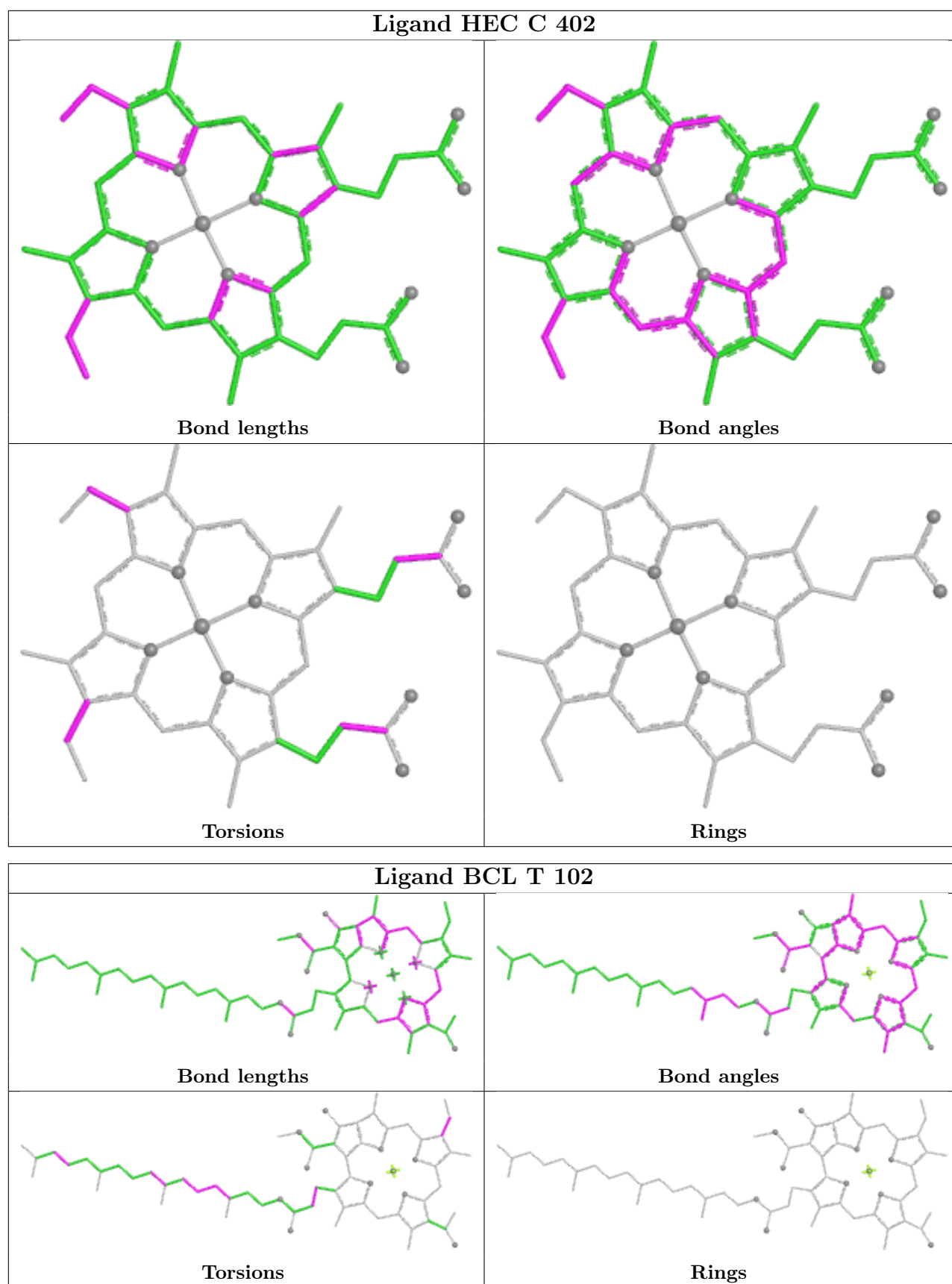
Ligand U10 L 306



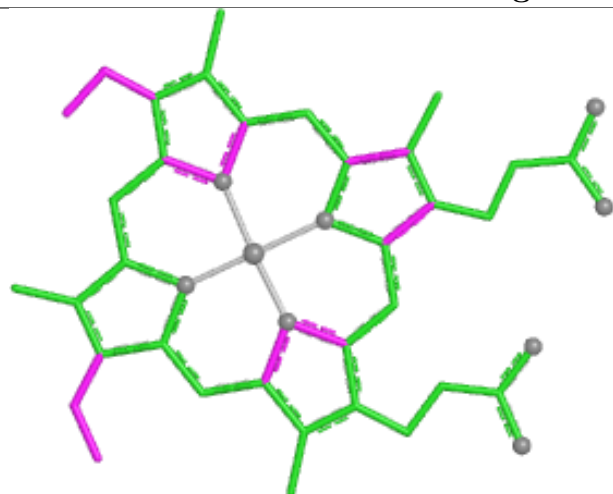
Ligand I7D 4 101



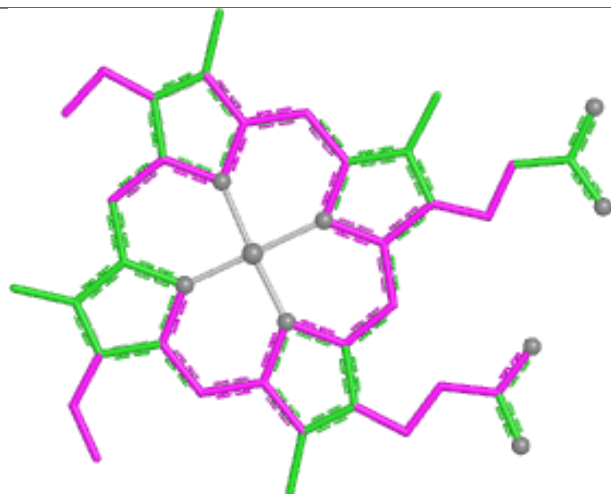




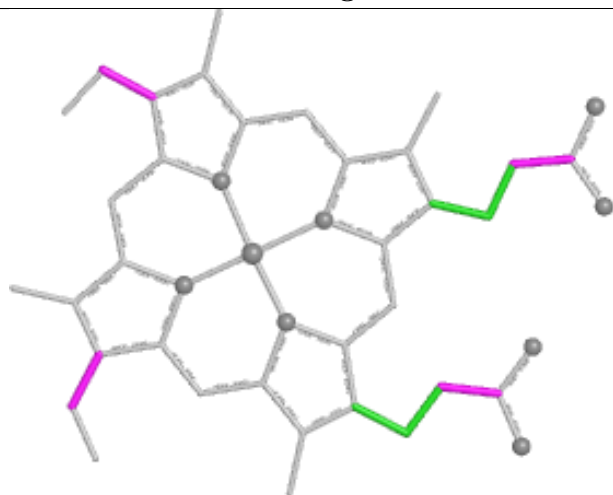
Ligand HEC C 401



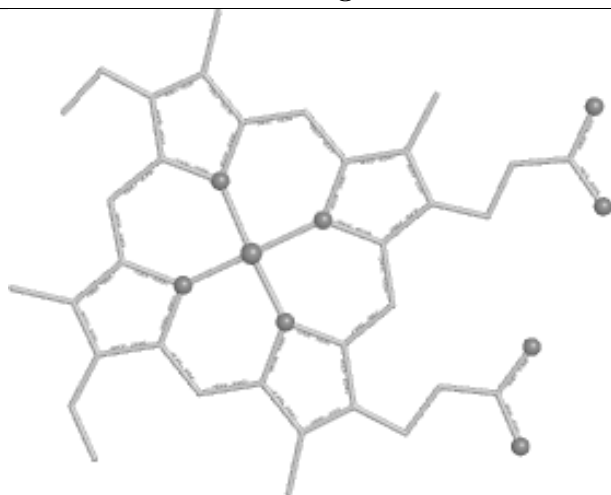
Bond lengths



Bond angles

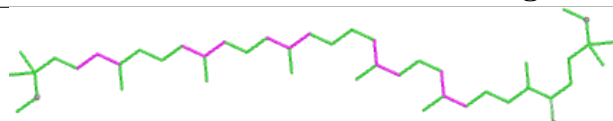


Torsions

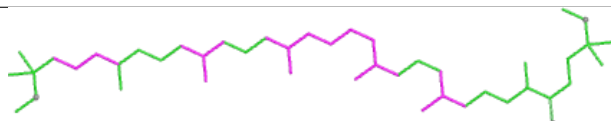


Rings

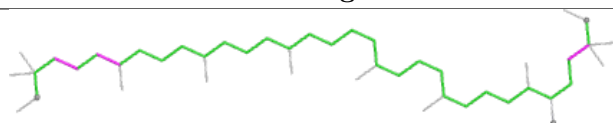
Ligand I7D A 103



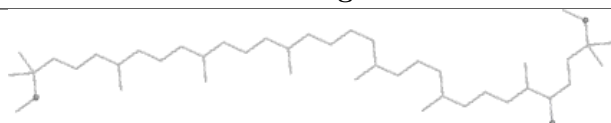
Bond lengths



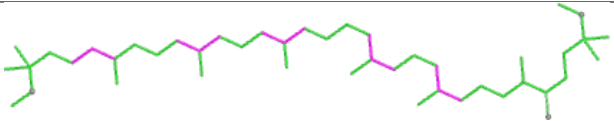
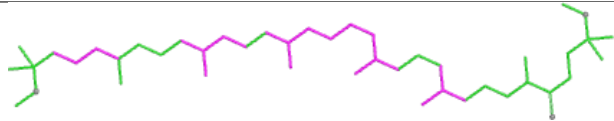
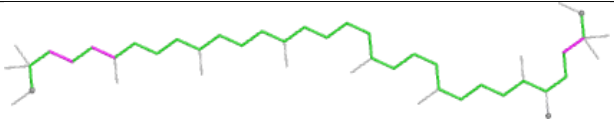
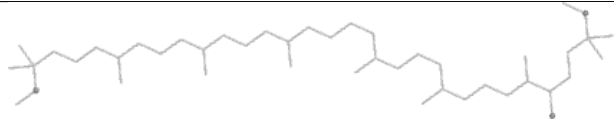
Bond angles

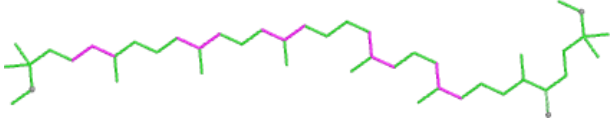
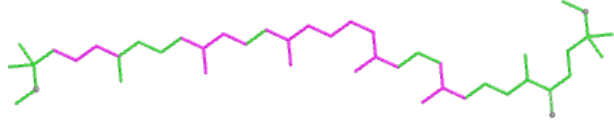
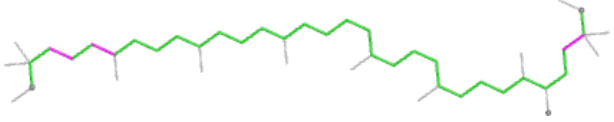
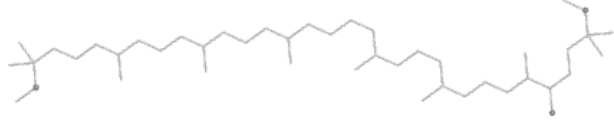


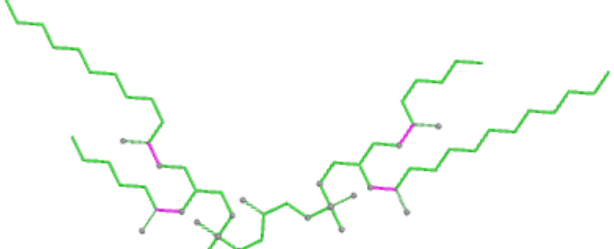
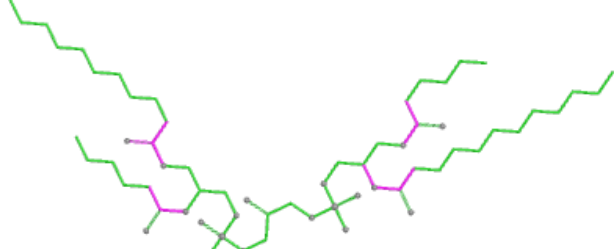
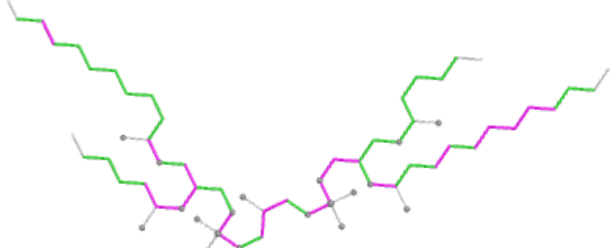
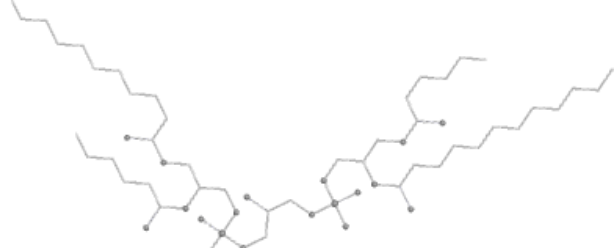
Torsions

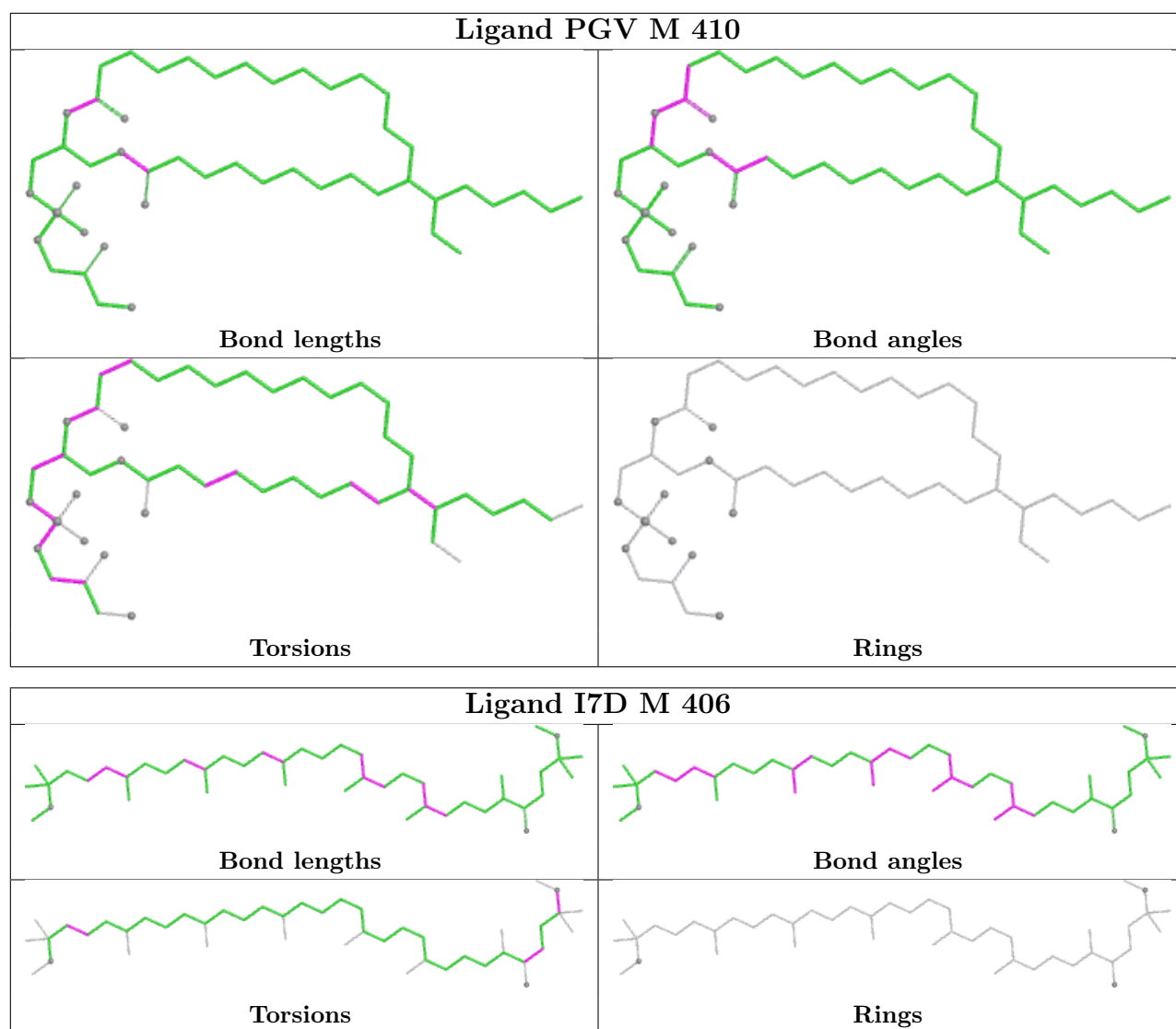


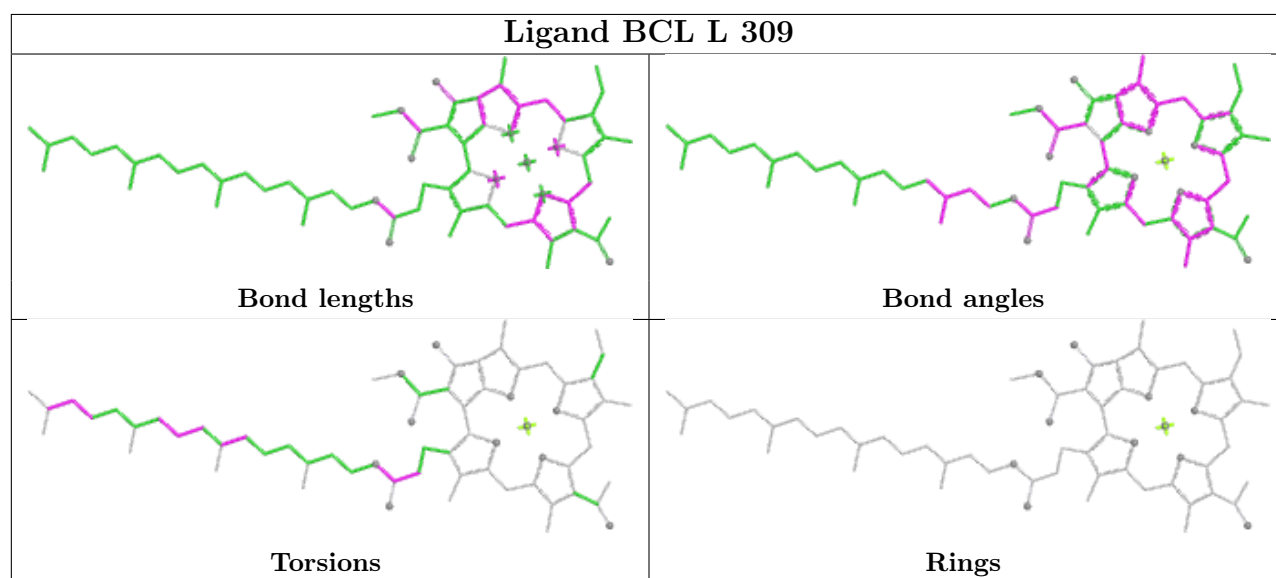
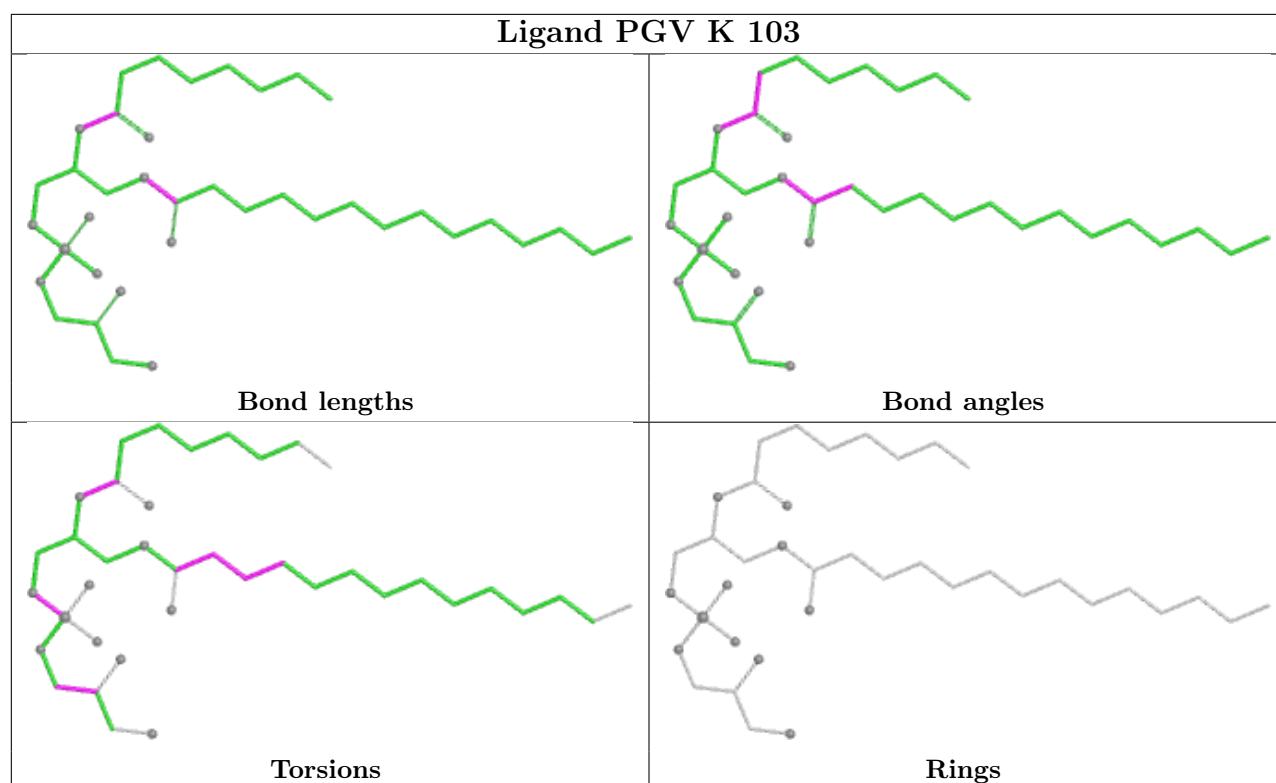
Rings

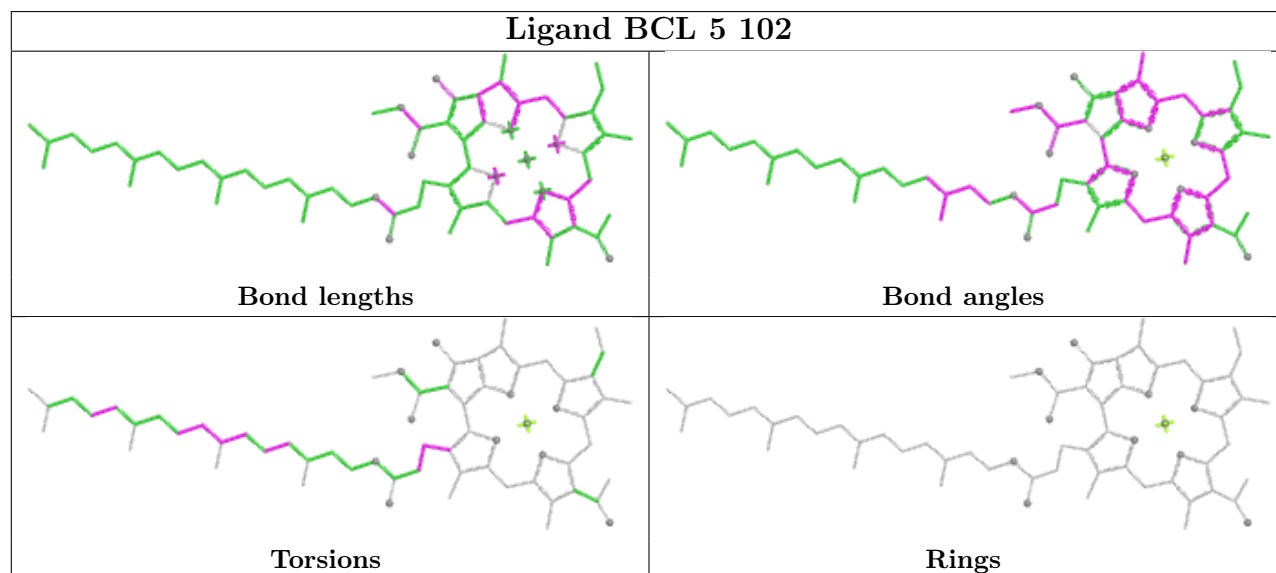
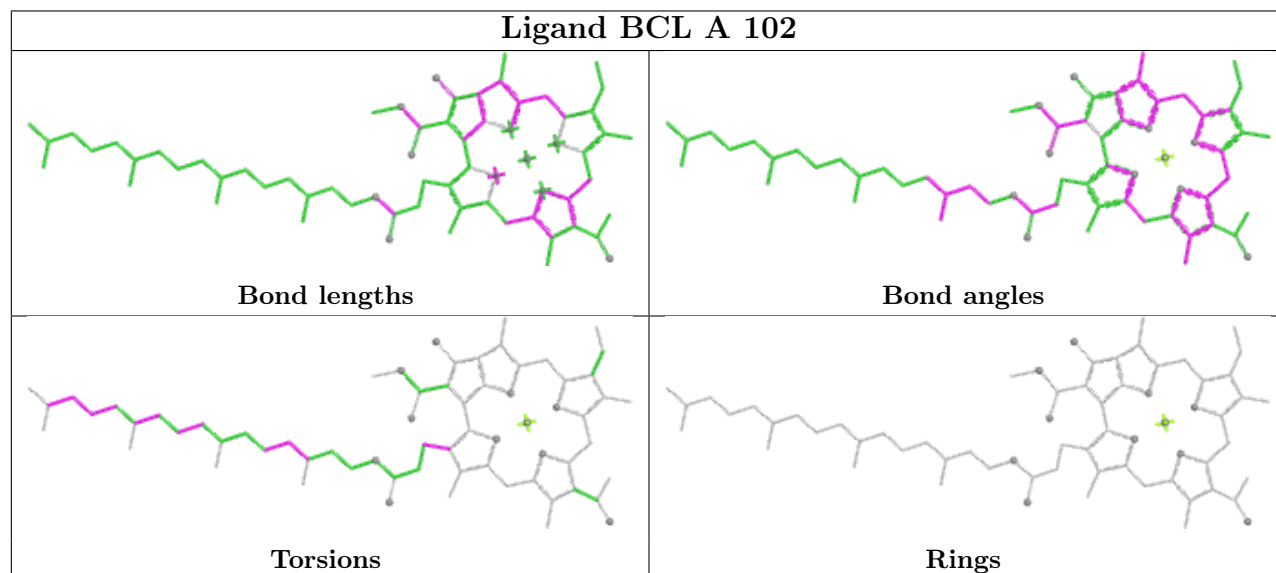
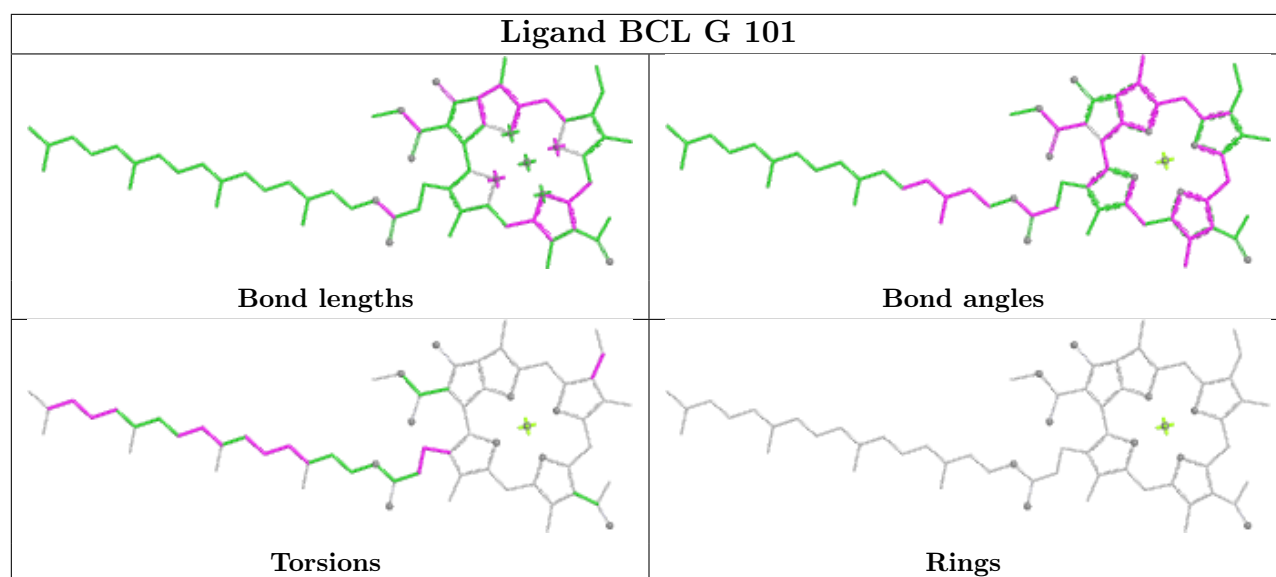
Ligand I7D T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

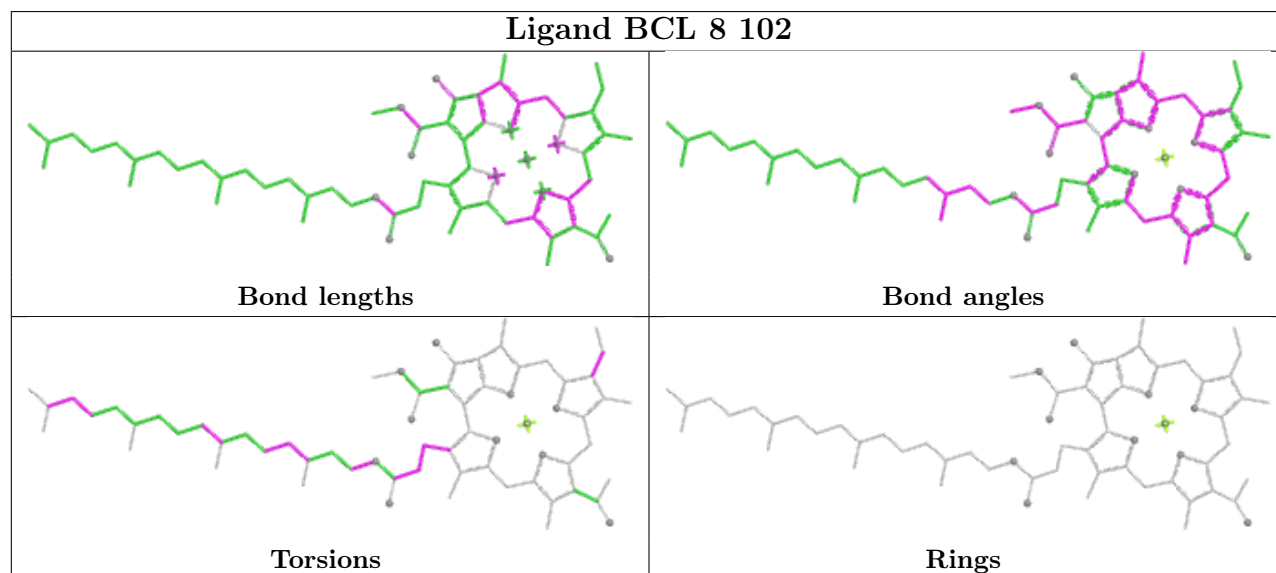
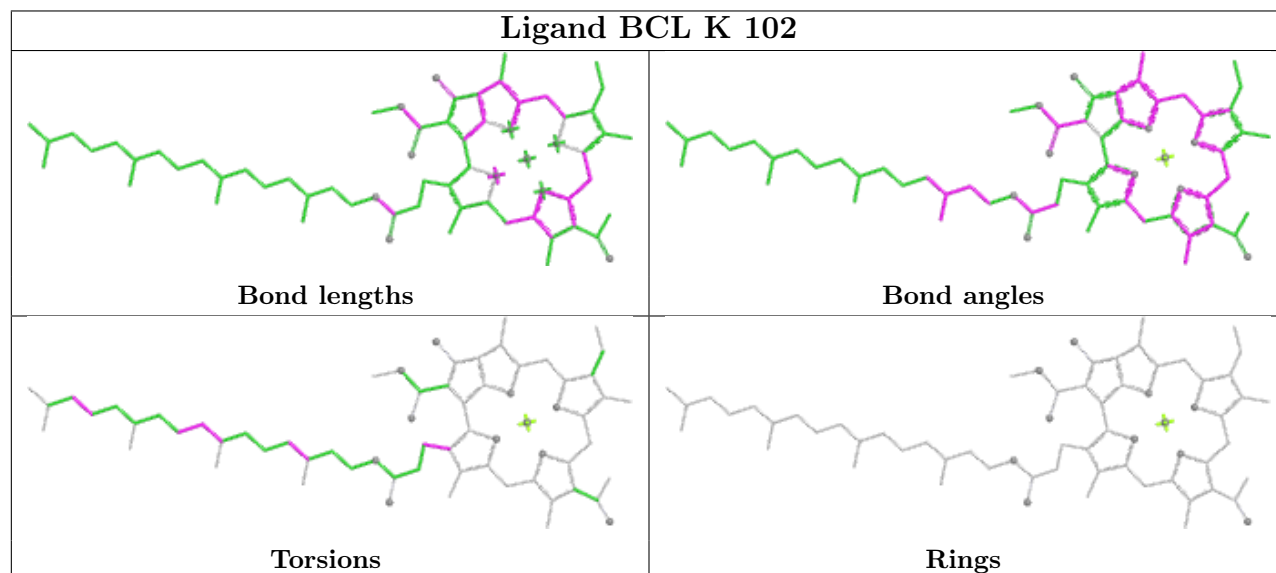
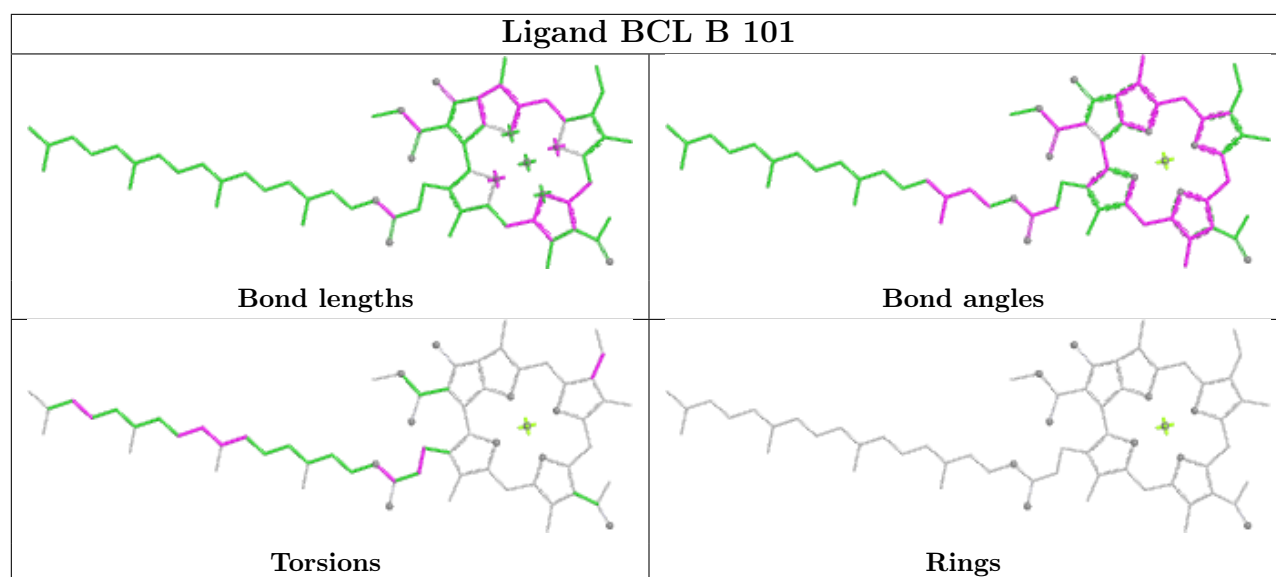
Ligand I7D 1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

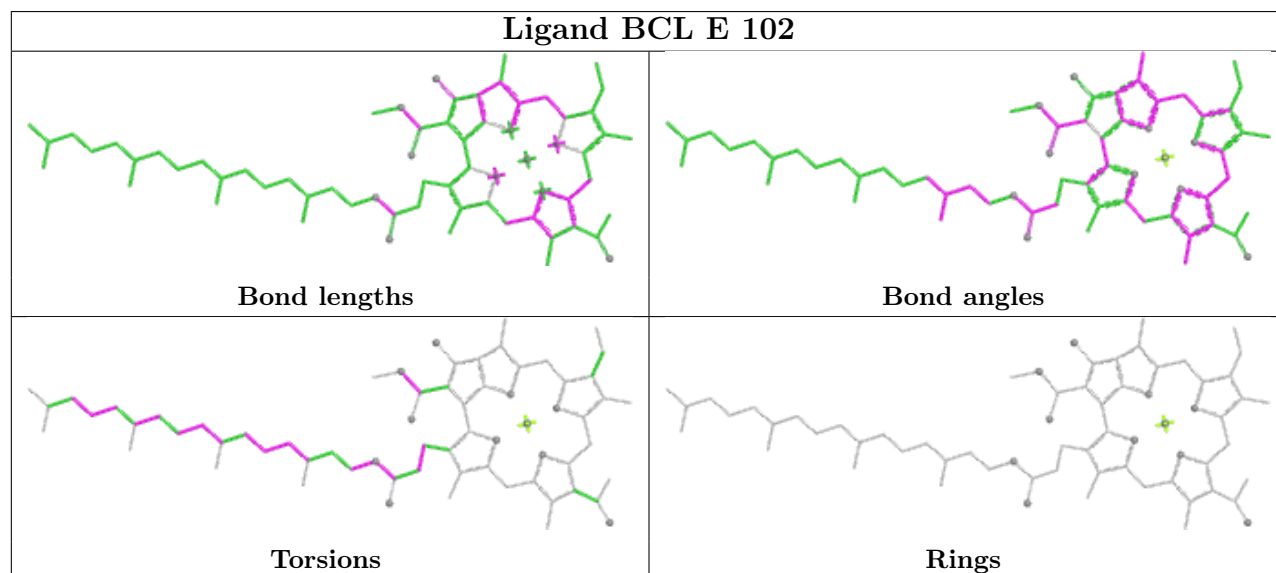
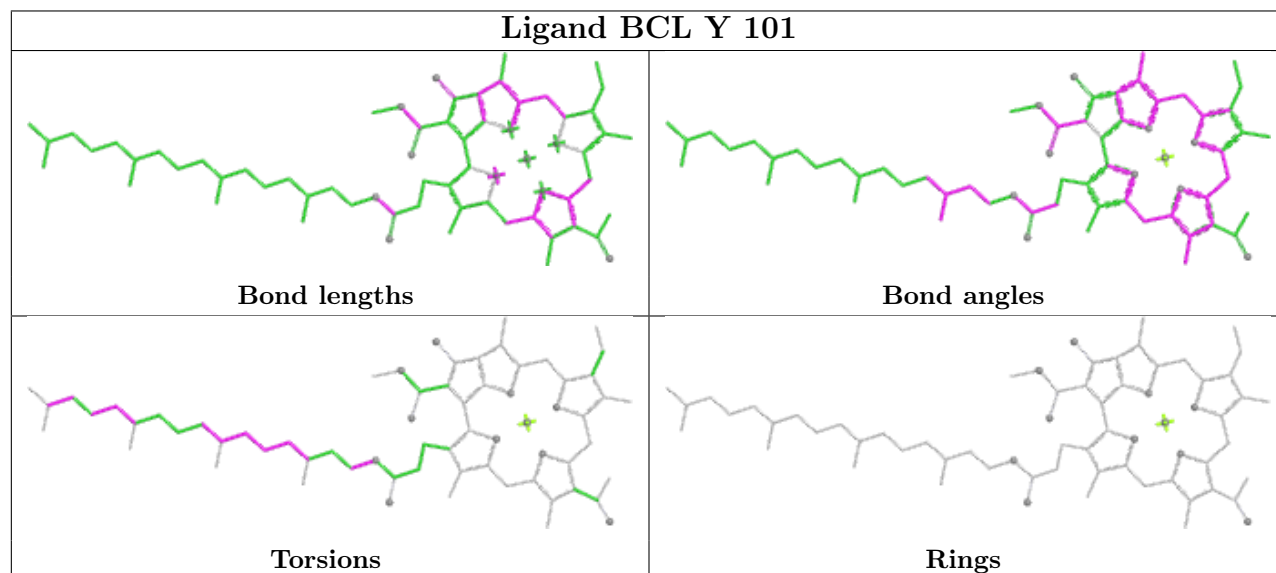
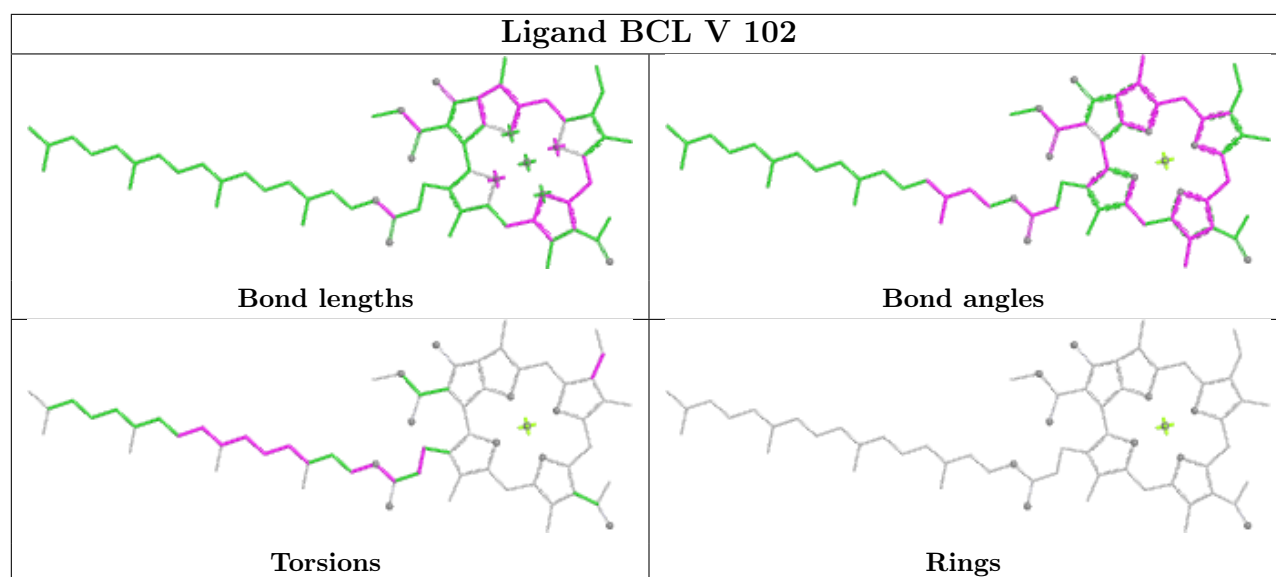
Ligand CDL 0 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

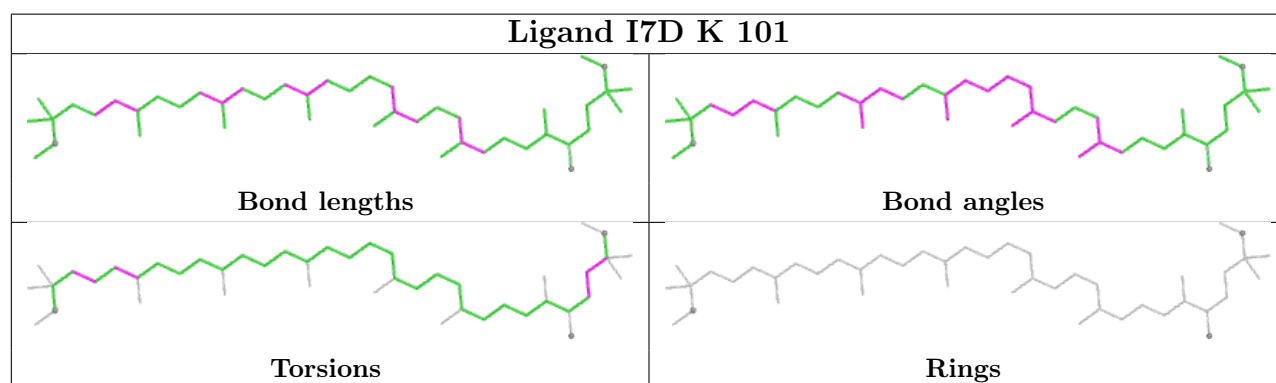
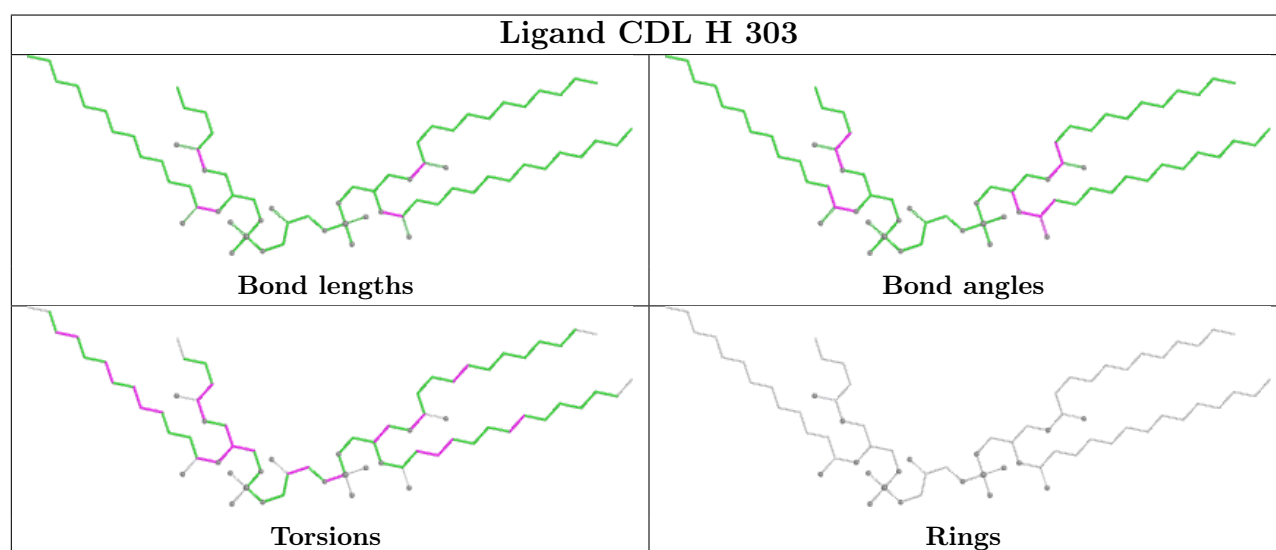
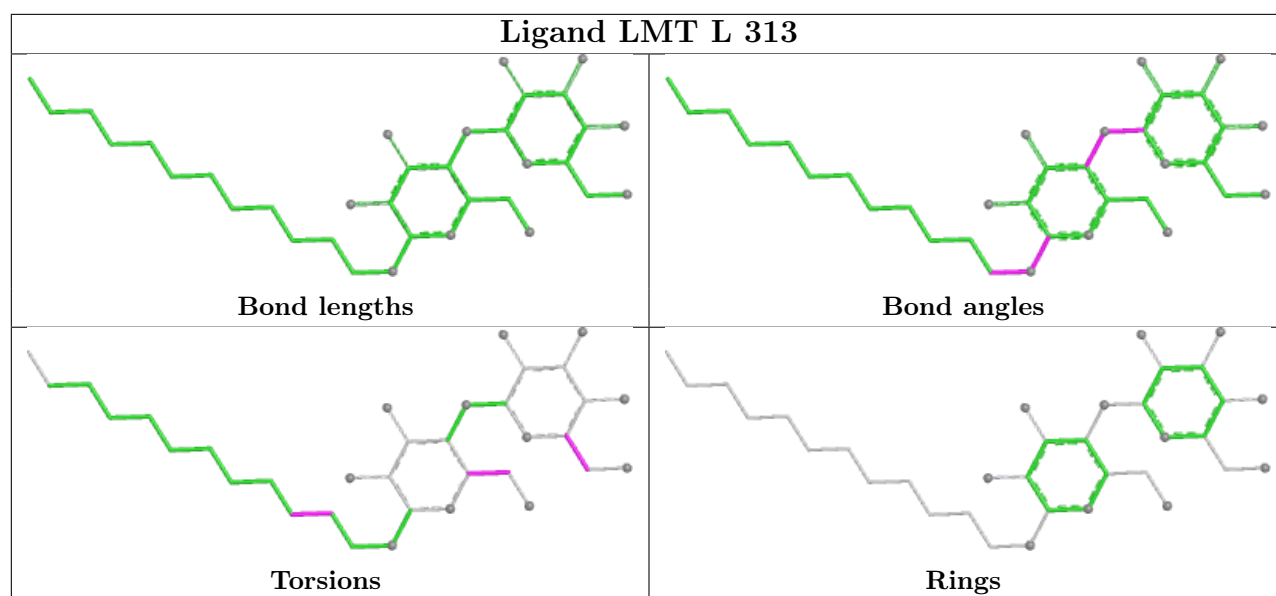


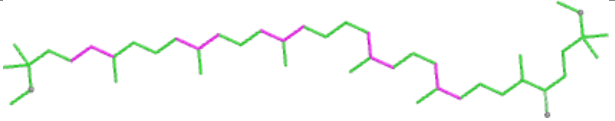
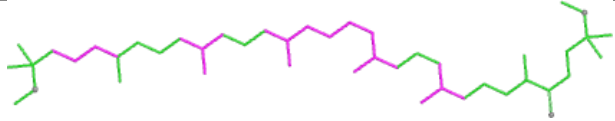
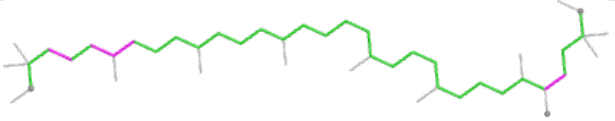
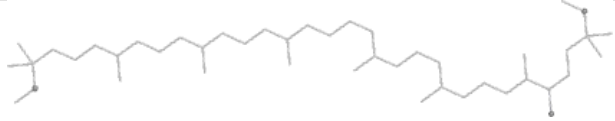
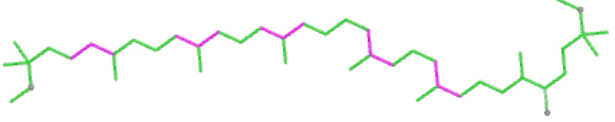
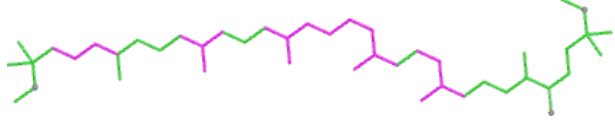
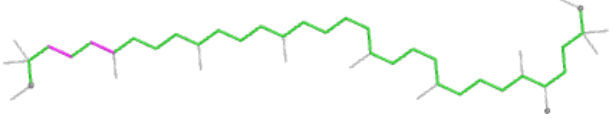
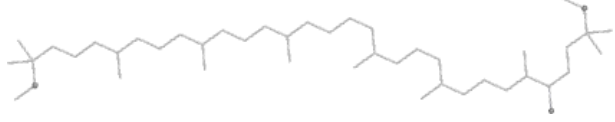
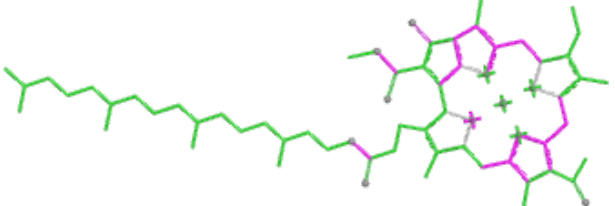
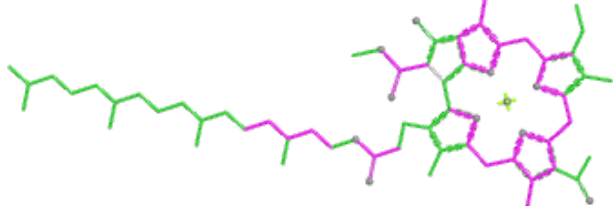
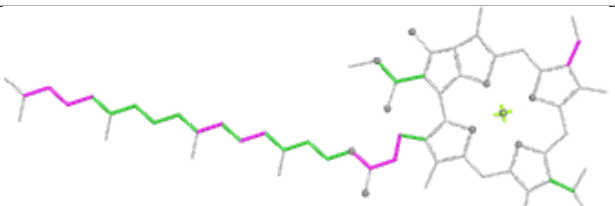
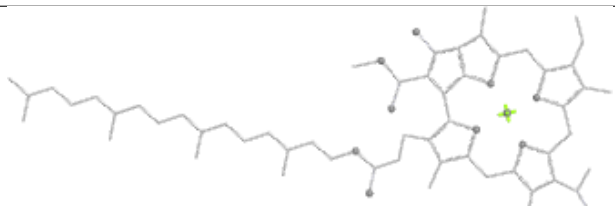


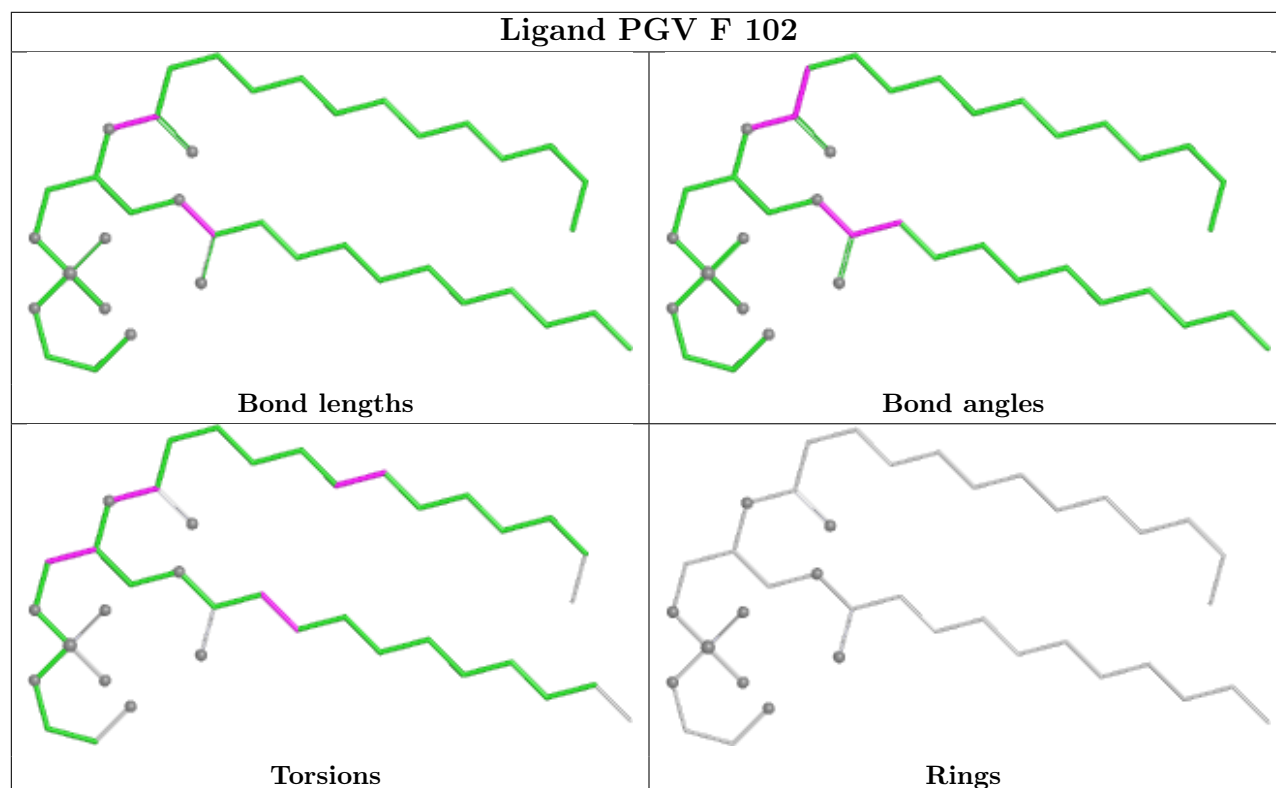
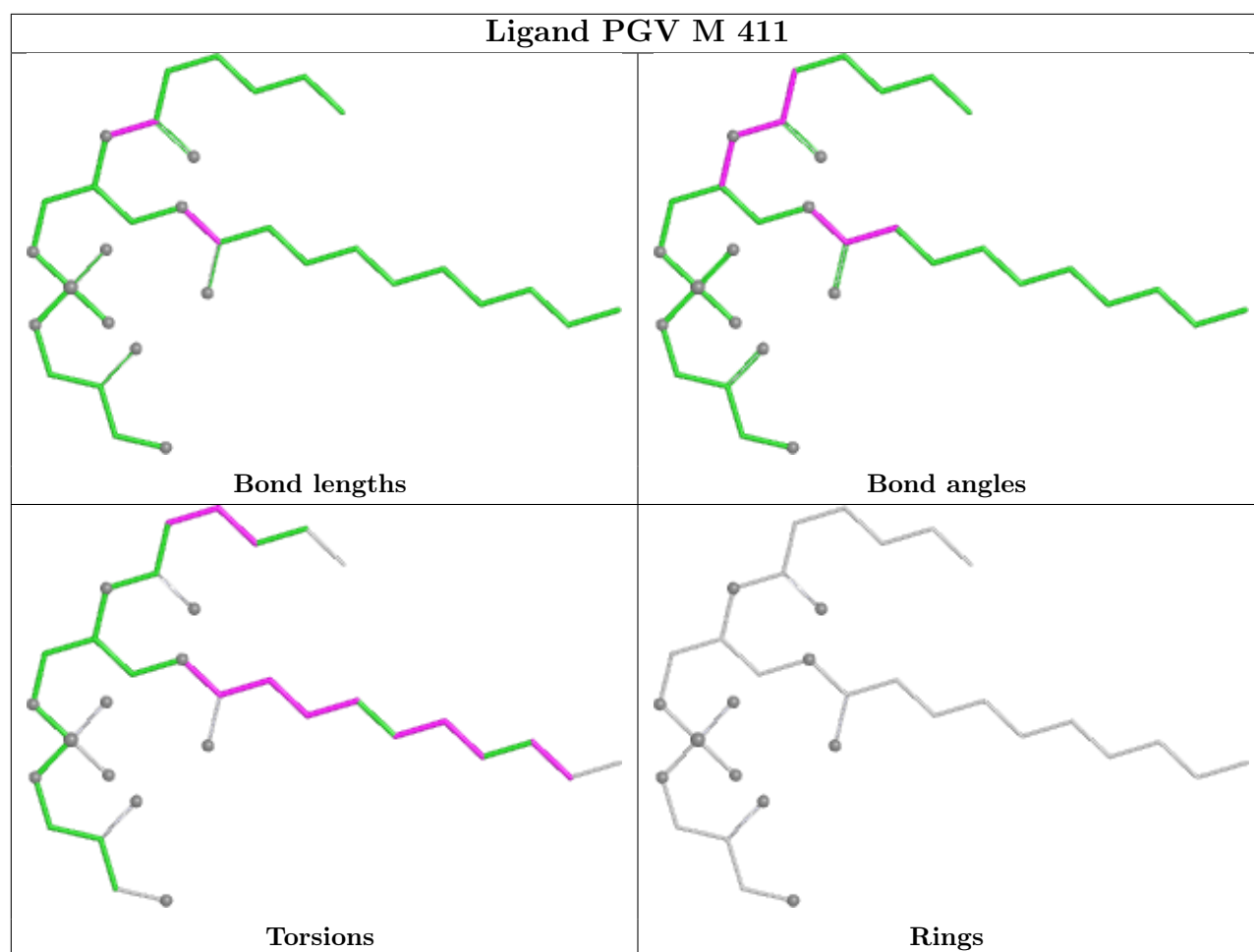


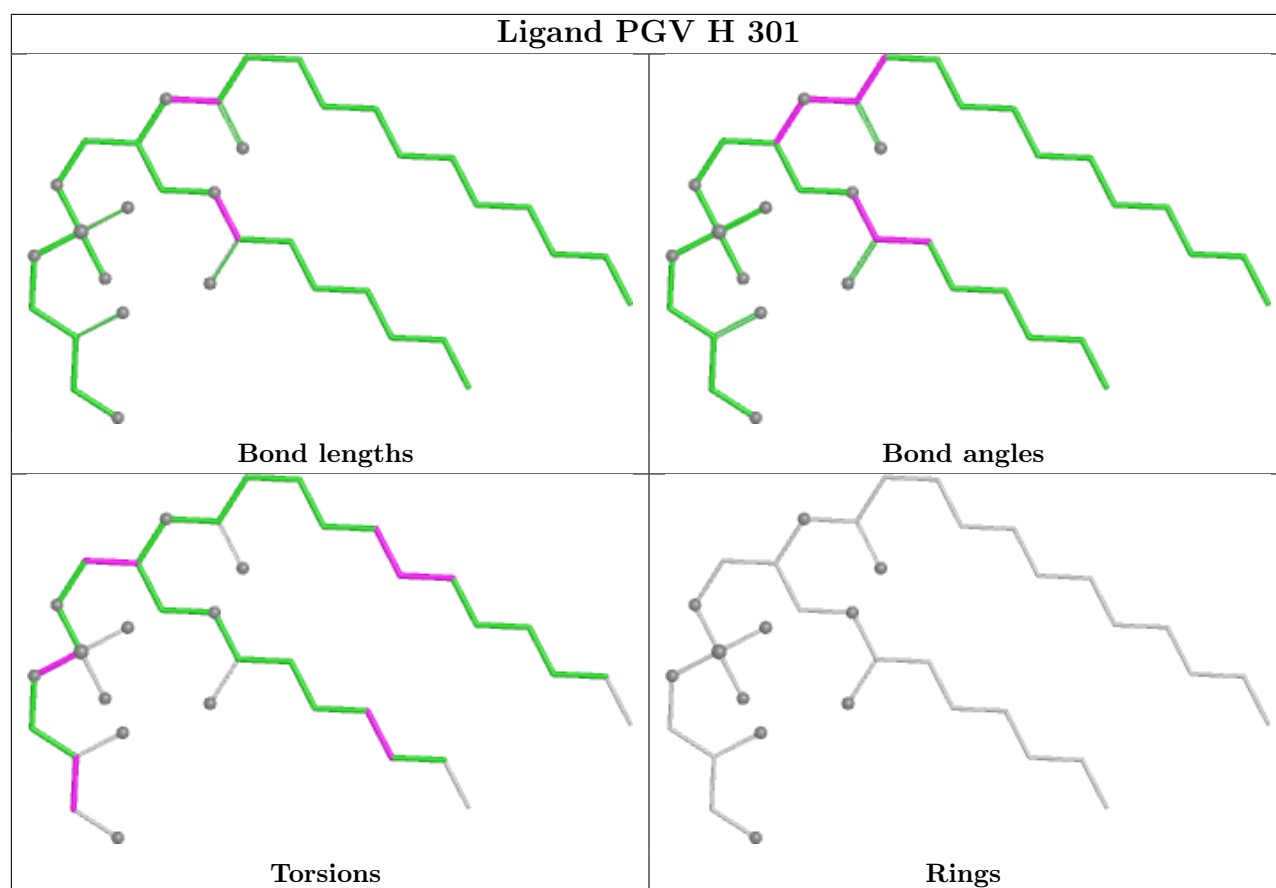


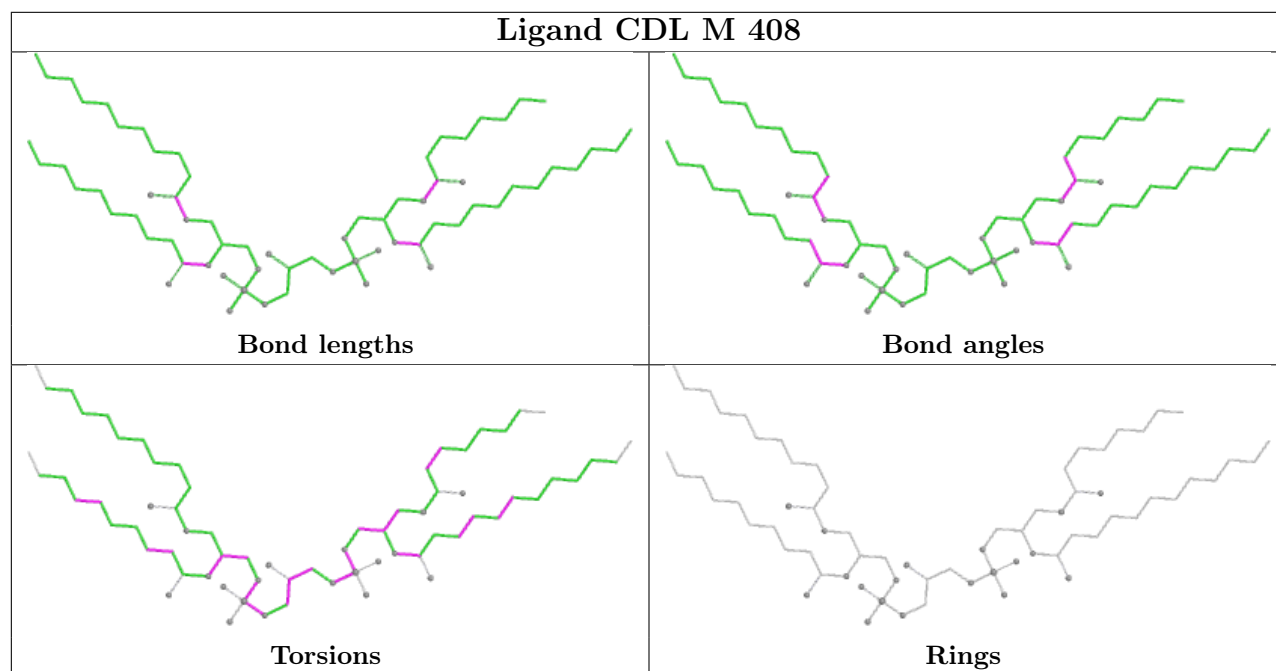
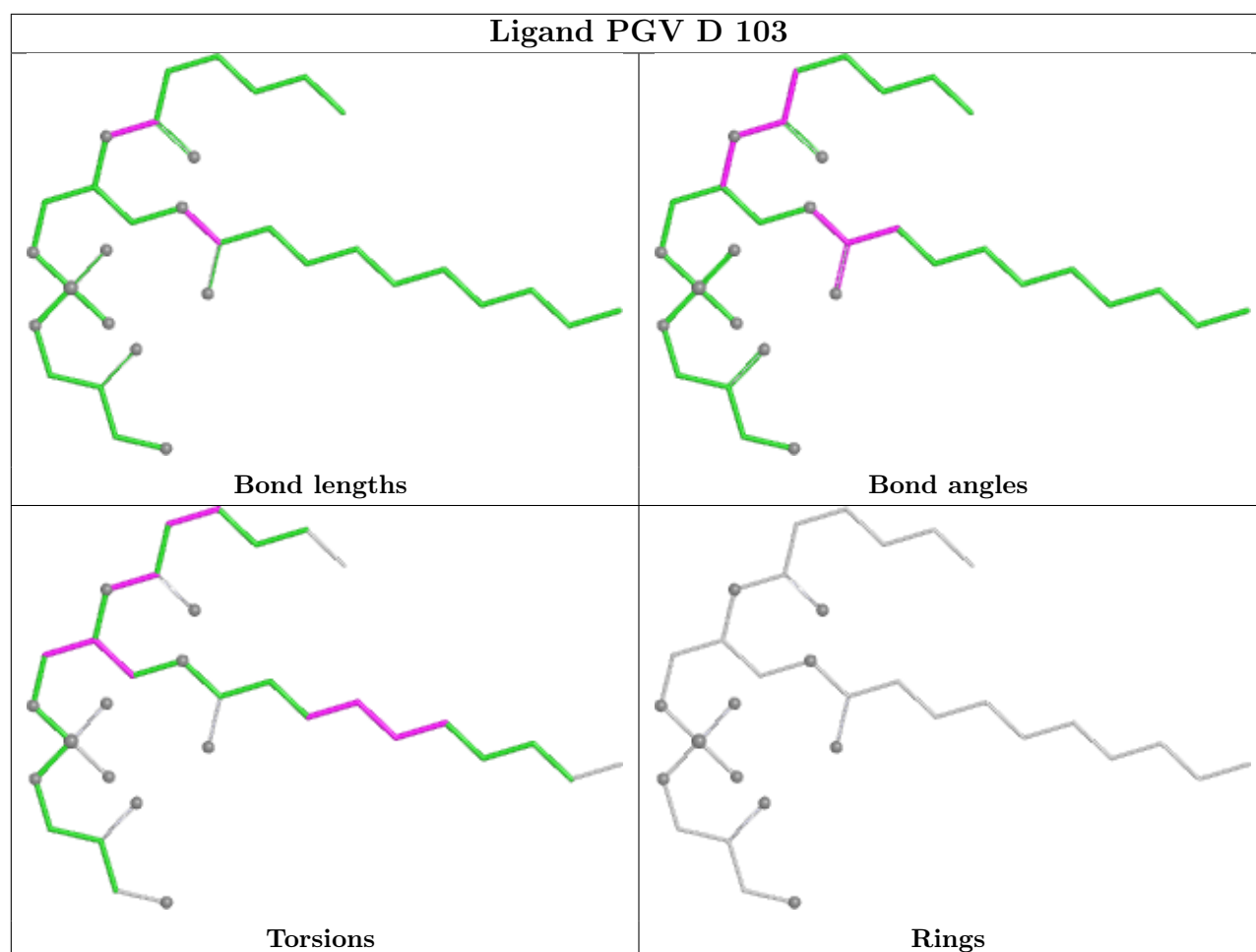


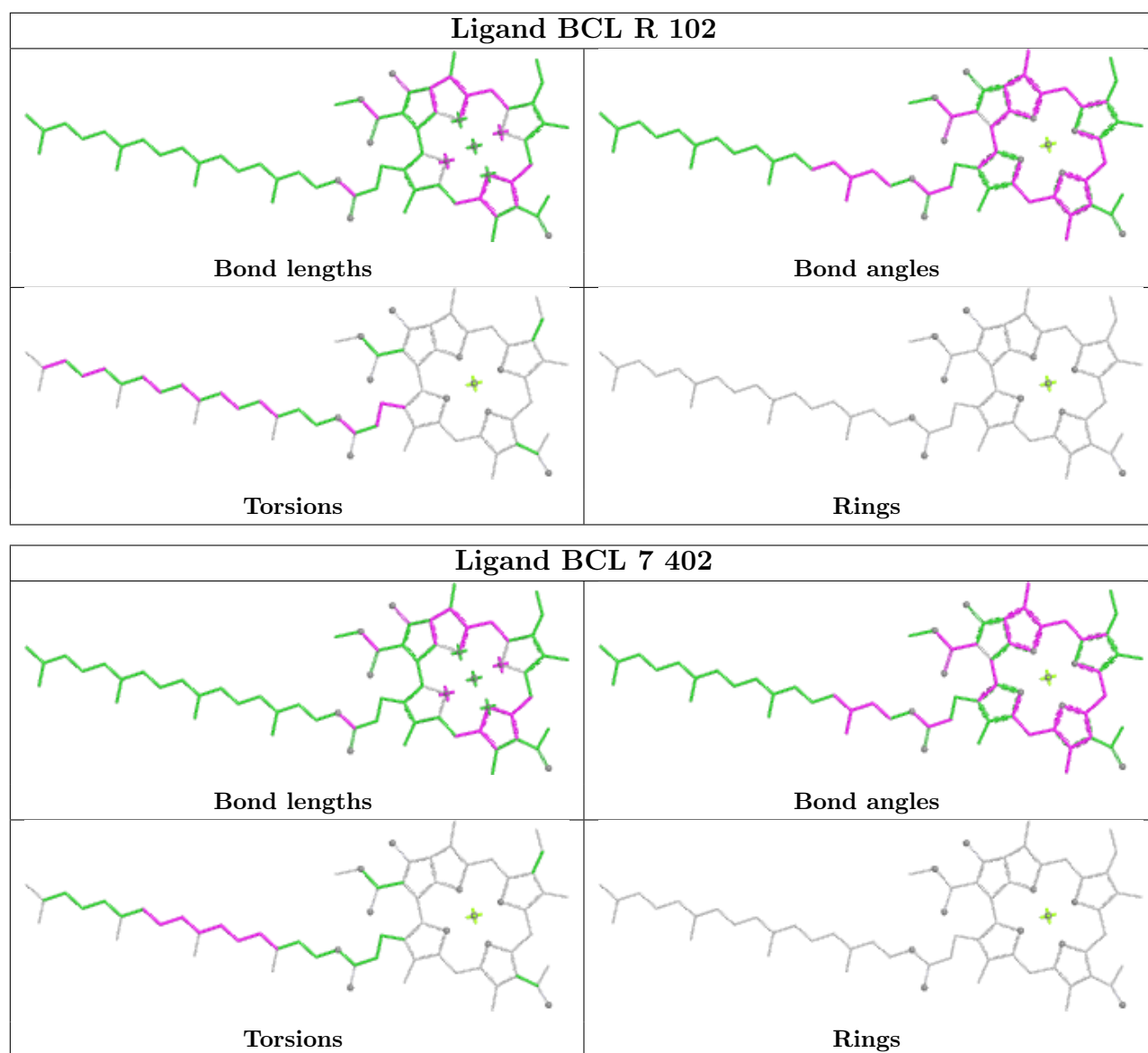


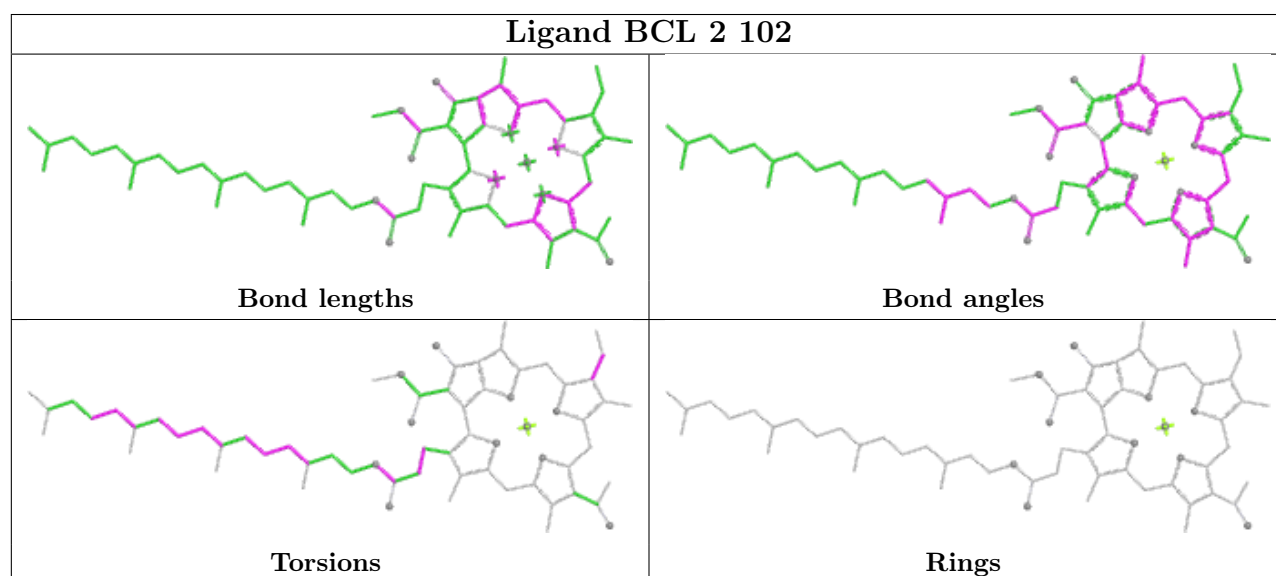
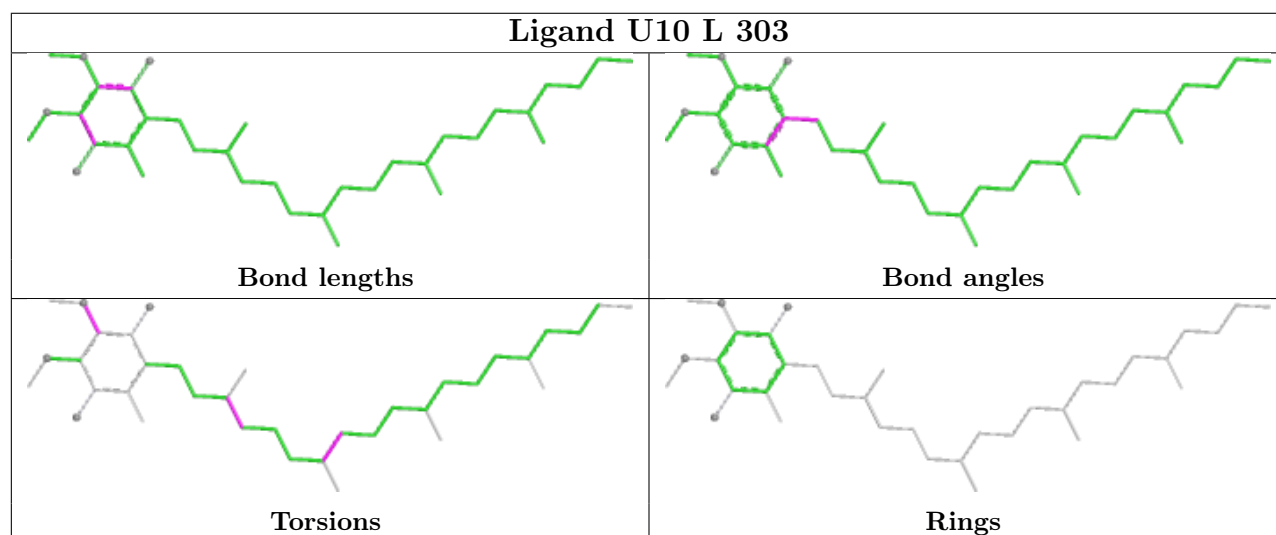
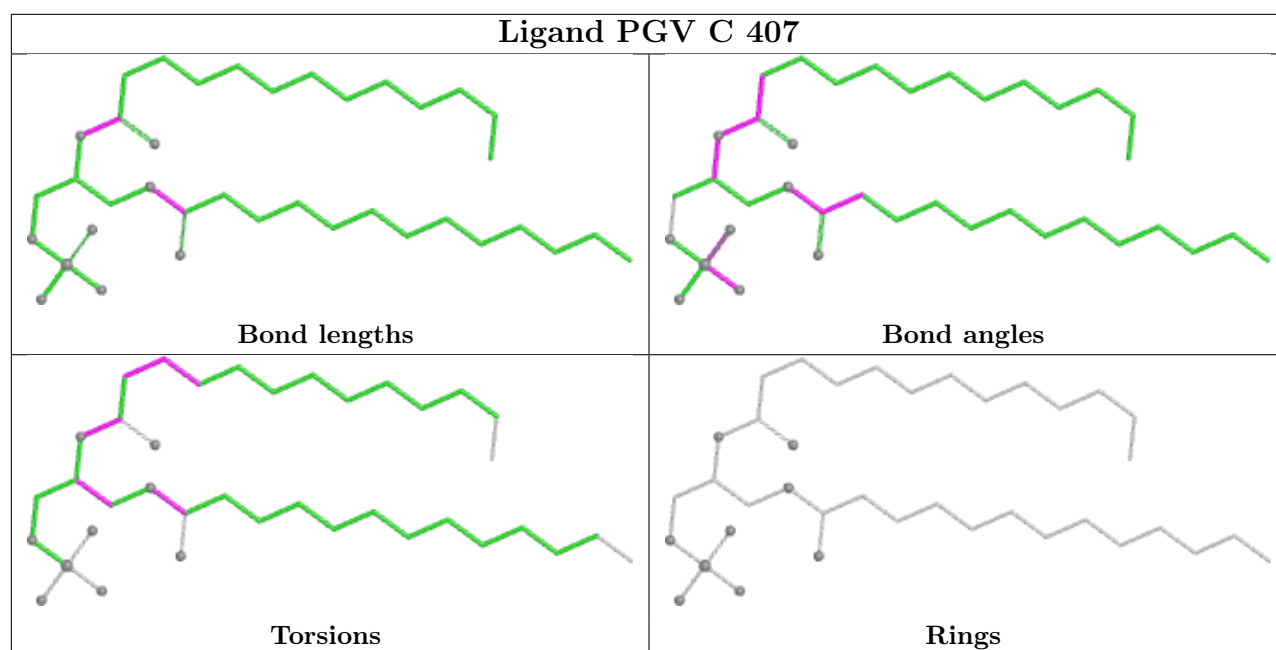
Ligand I7D V 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand I7D E 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL F 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

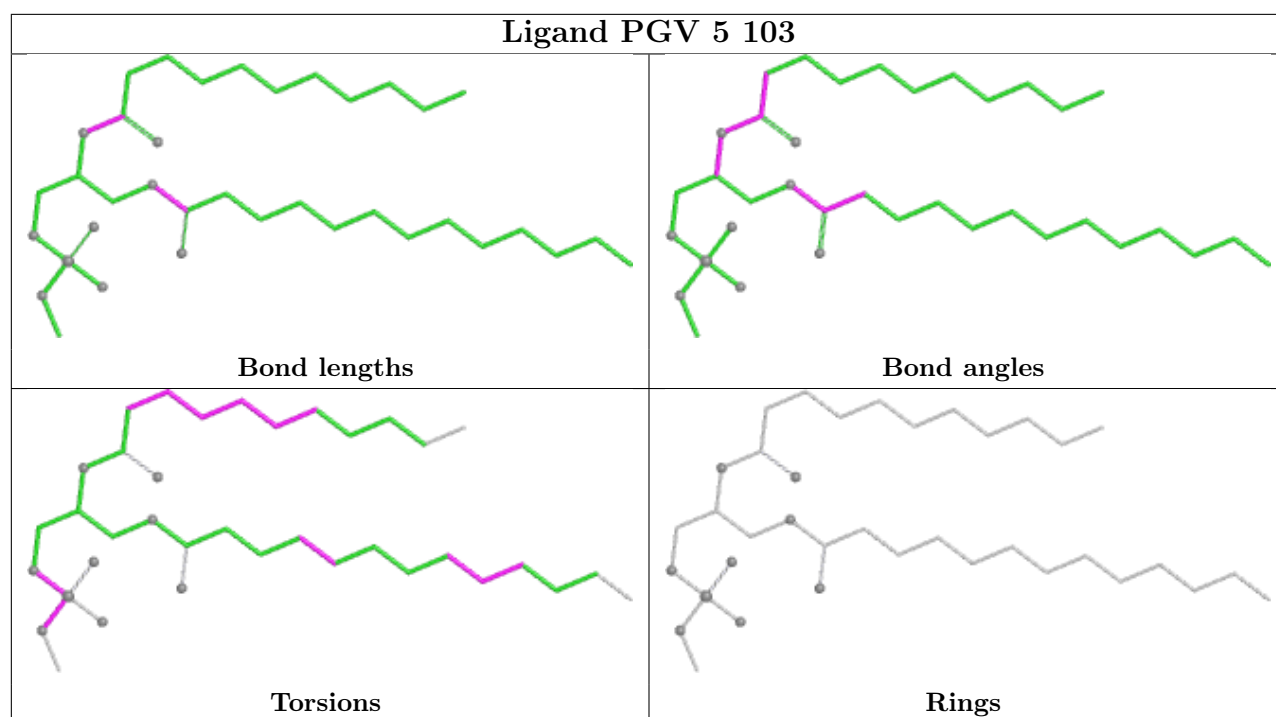




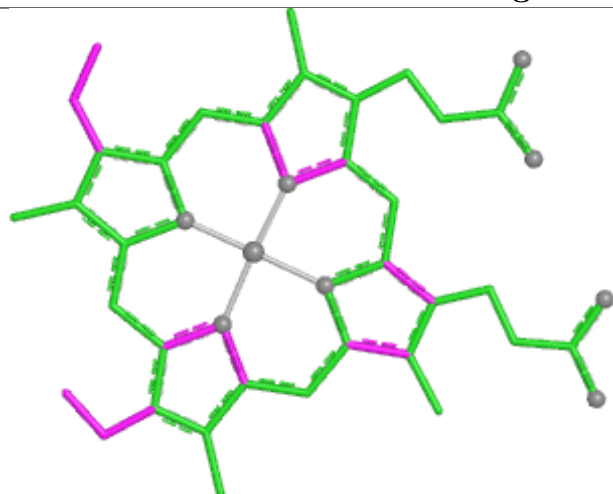




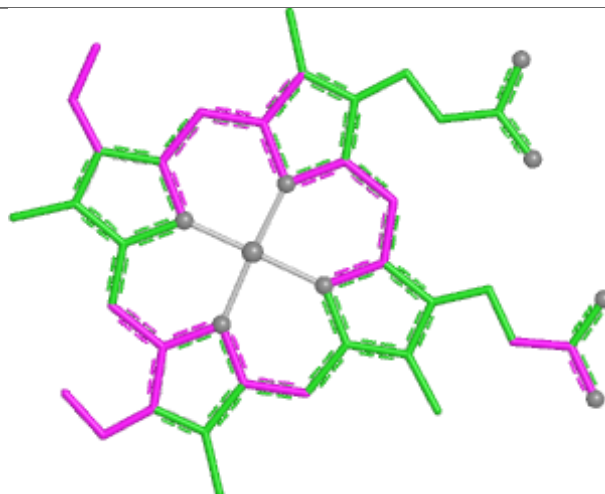




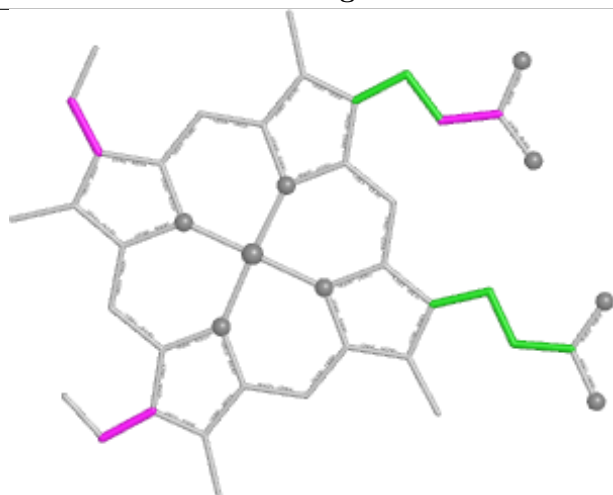
Ligand HEC C 404



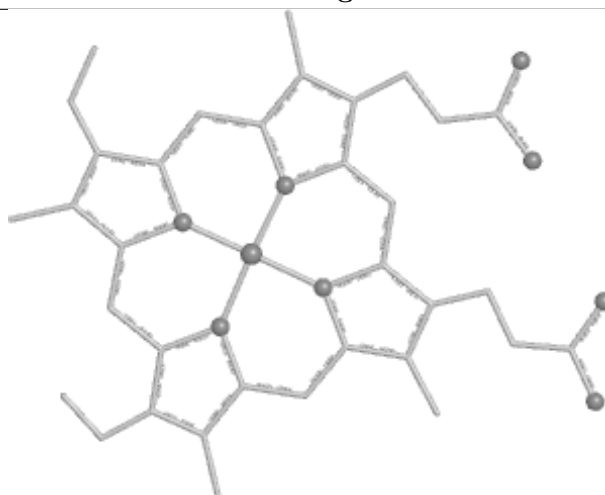
Bond lengths



Bond angles

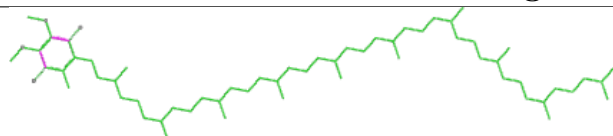


Torsions

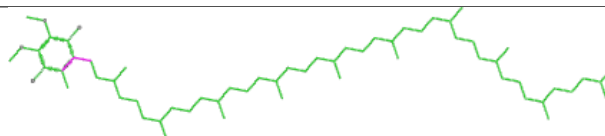


Rings

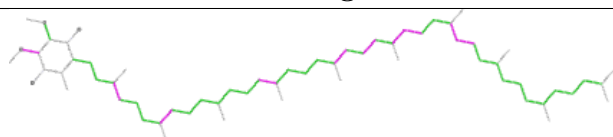
Ligand U10 7 401



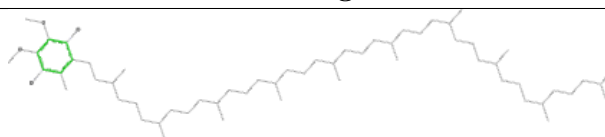
Bond lengths



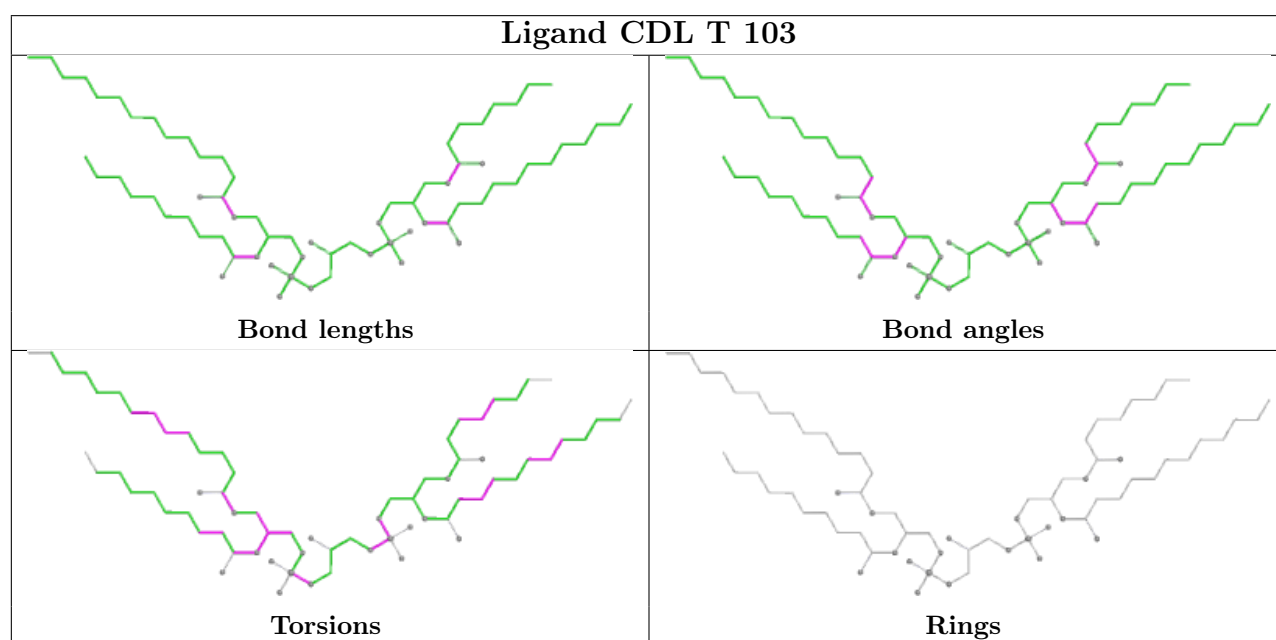
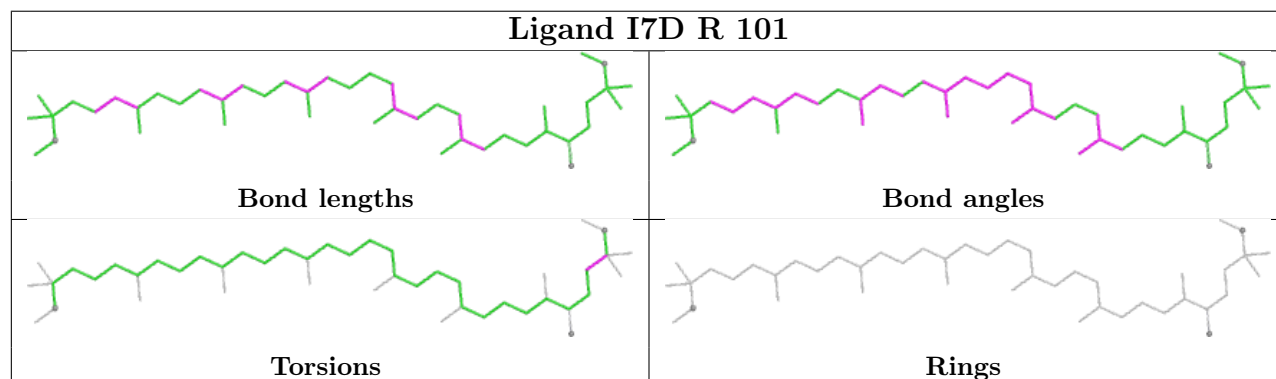
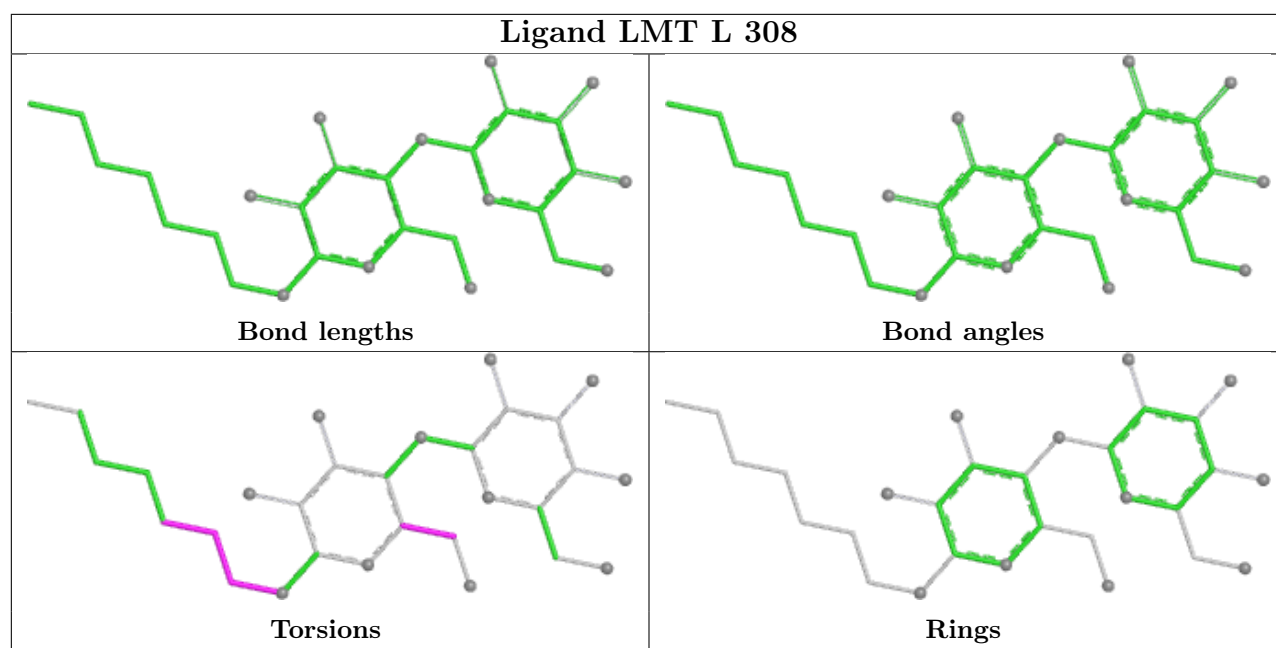
Bond angles

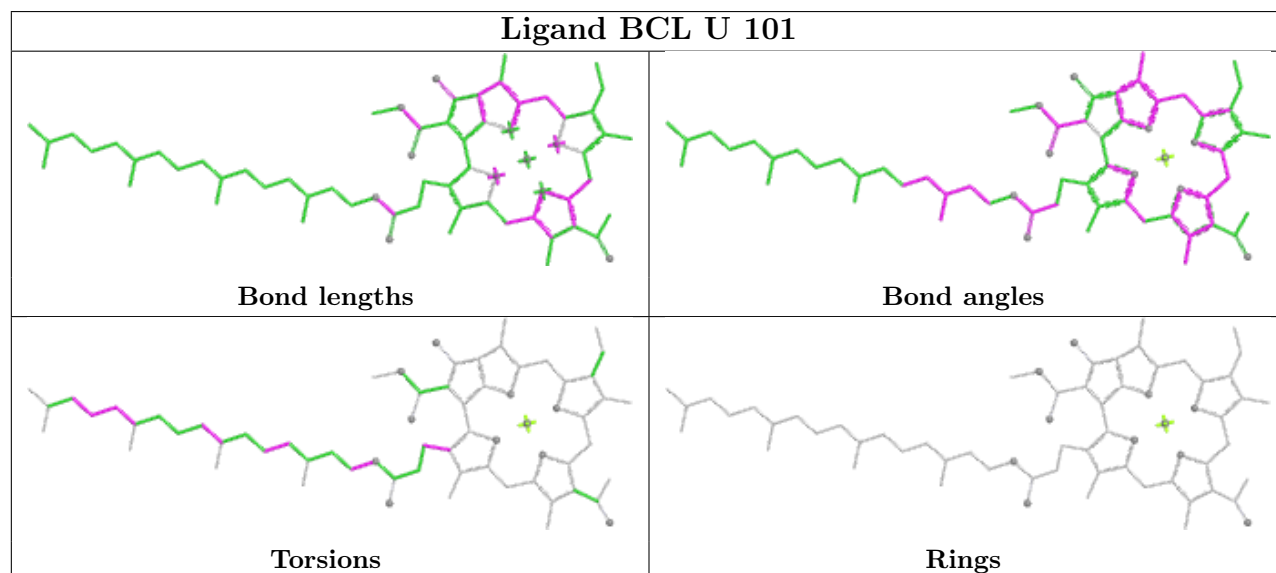
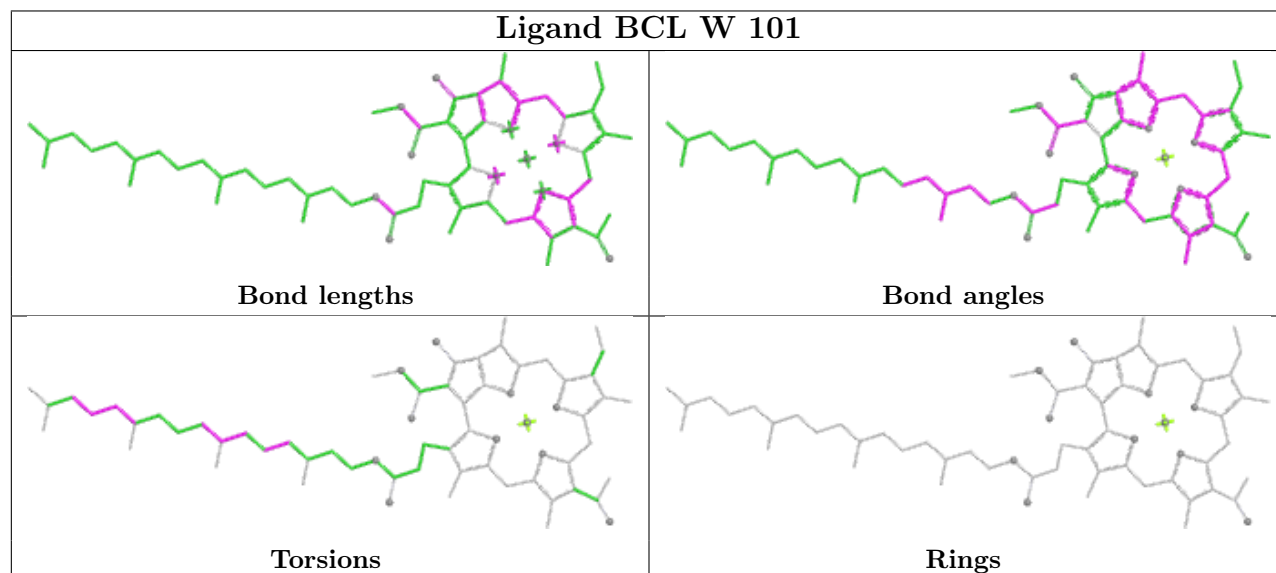
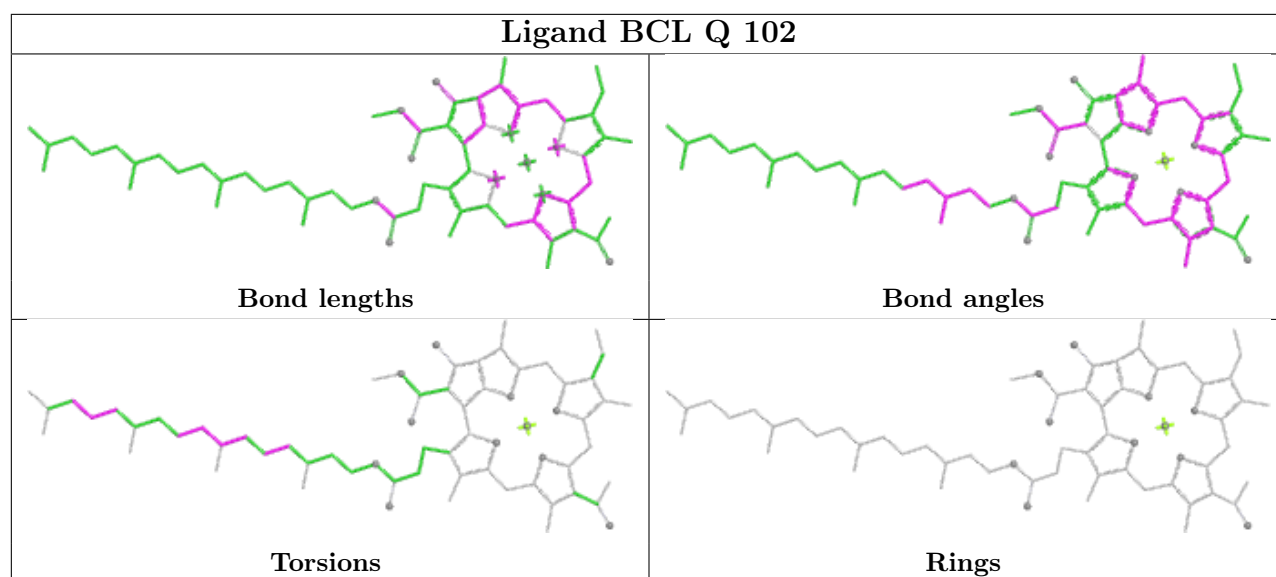


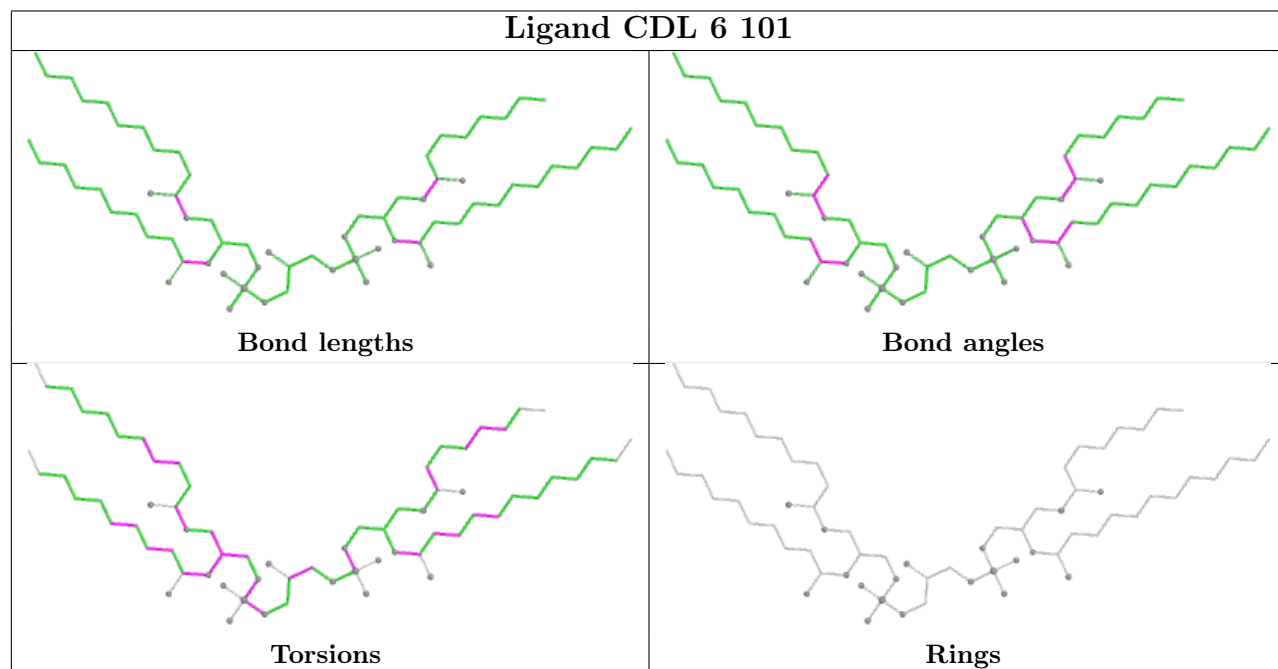
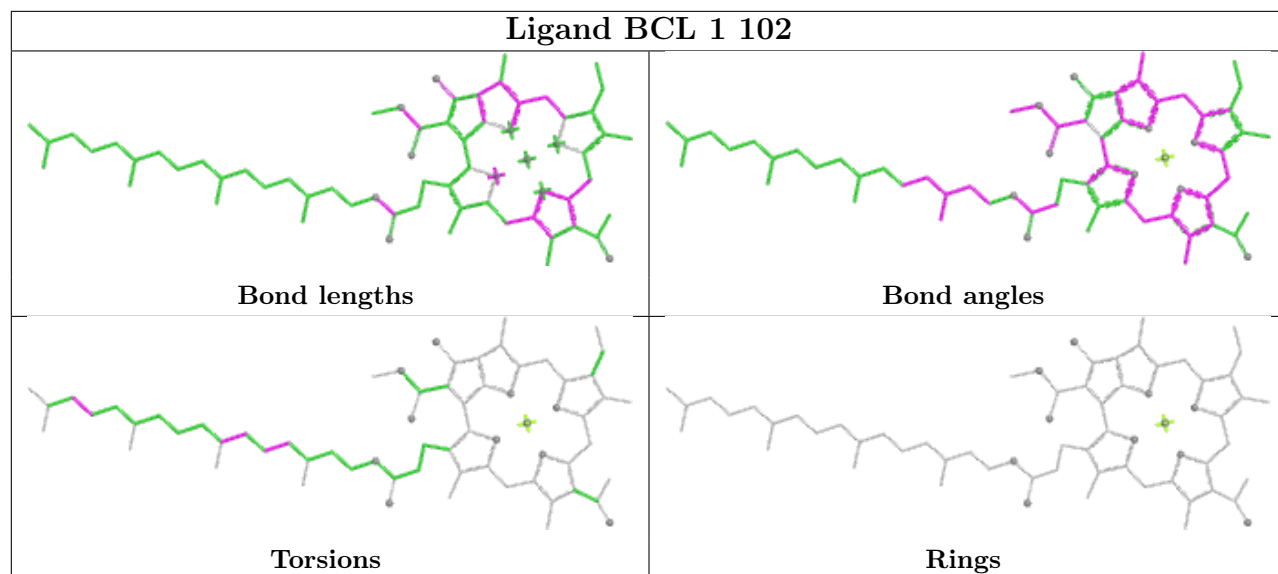
Torsions

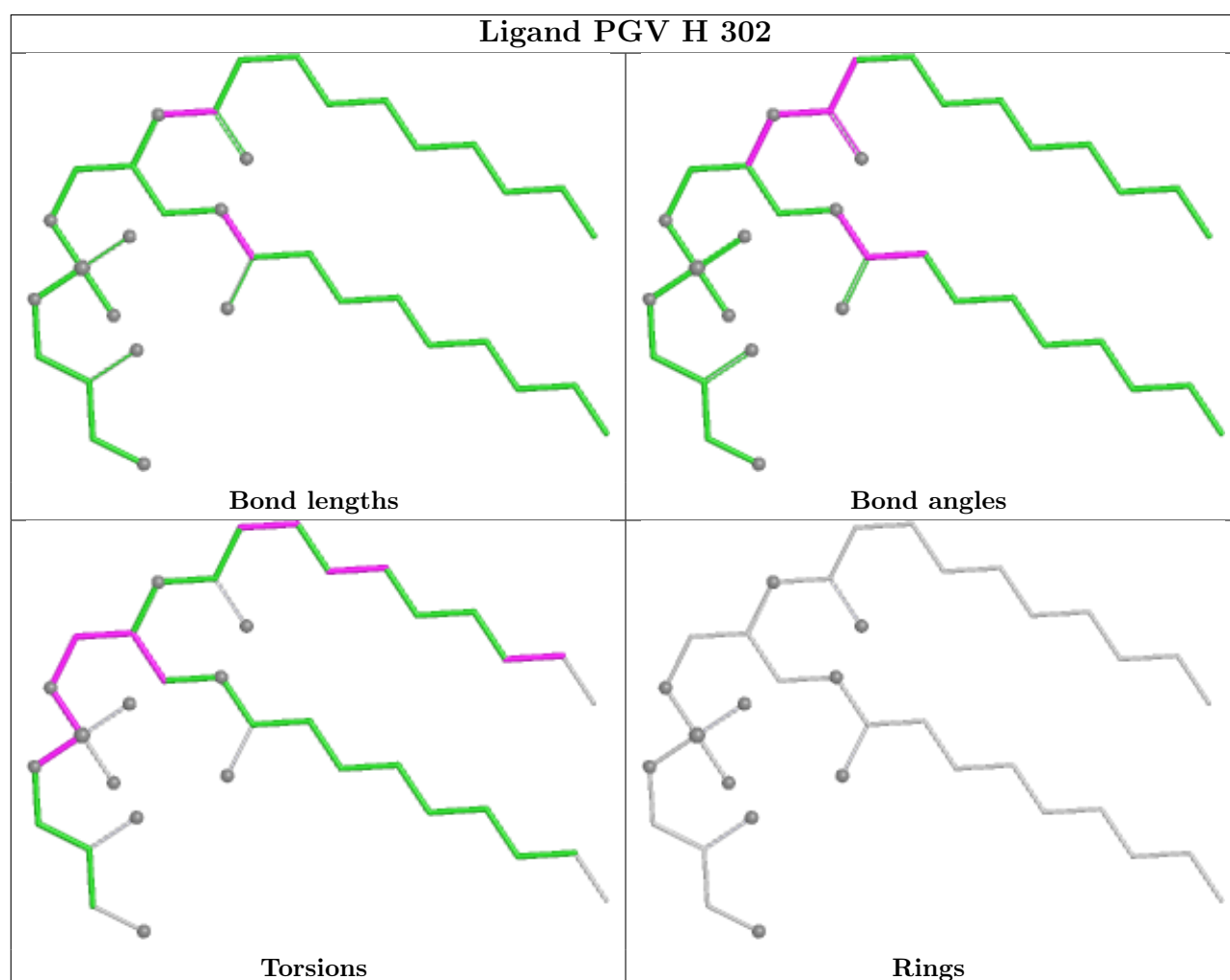
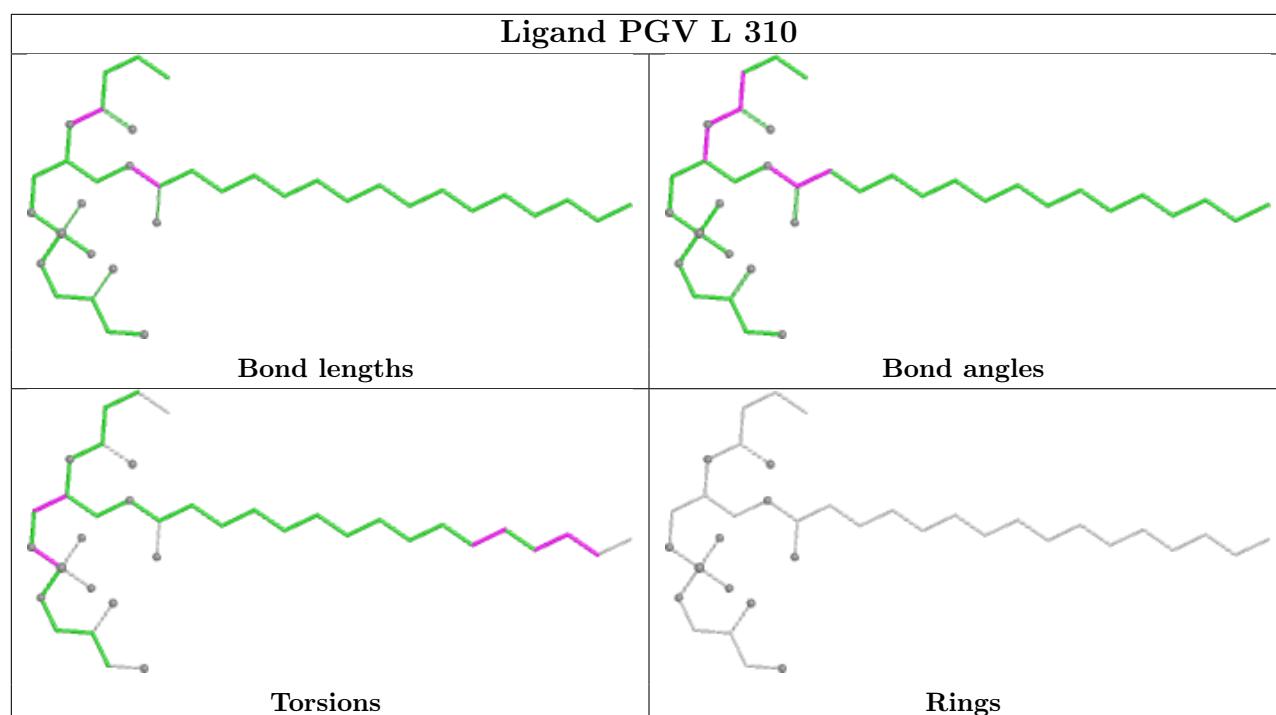


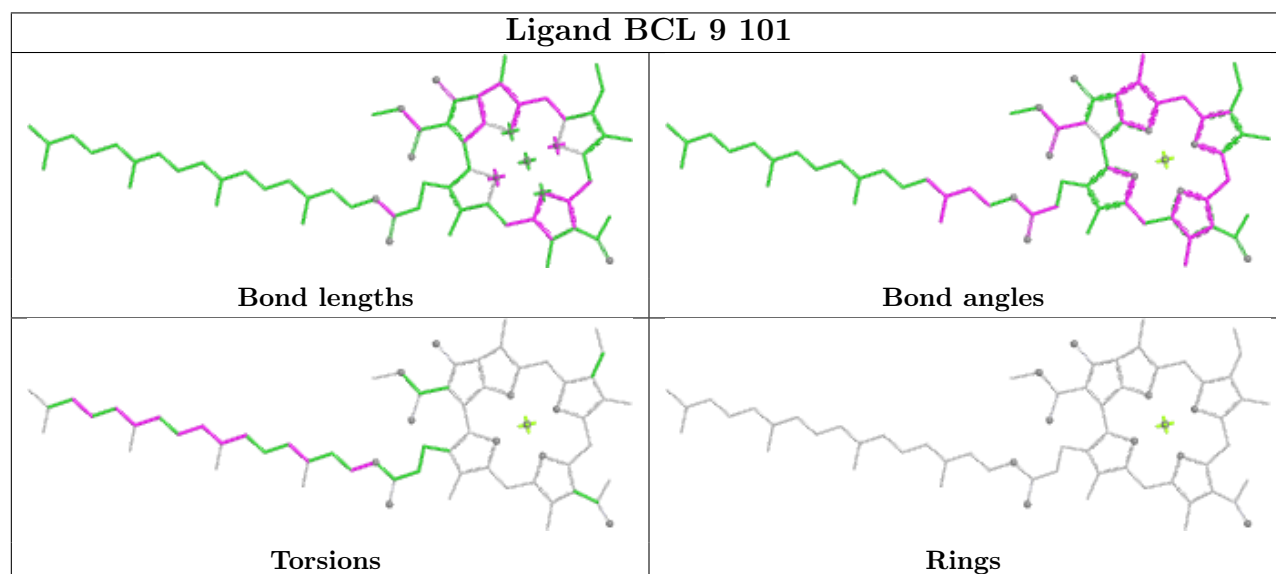
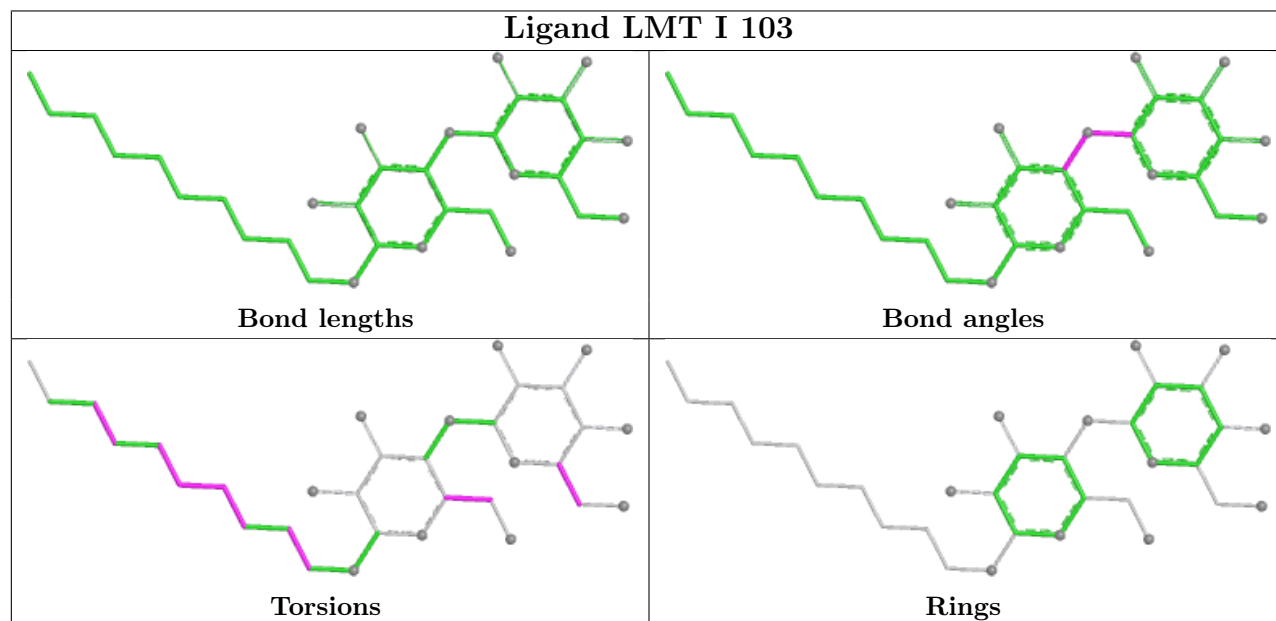
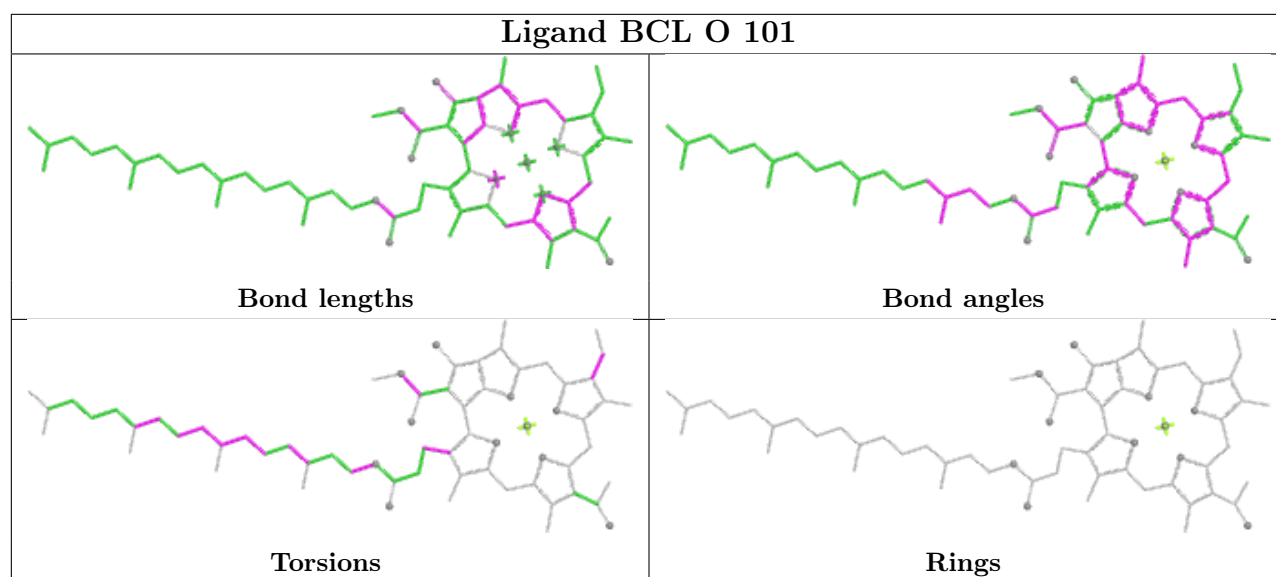
Rings

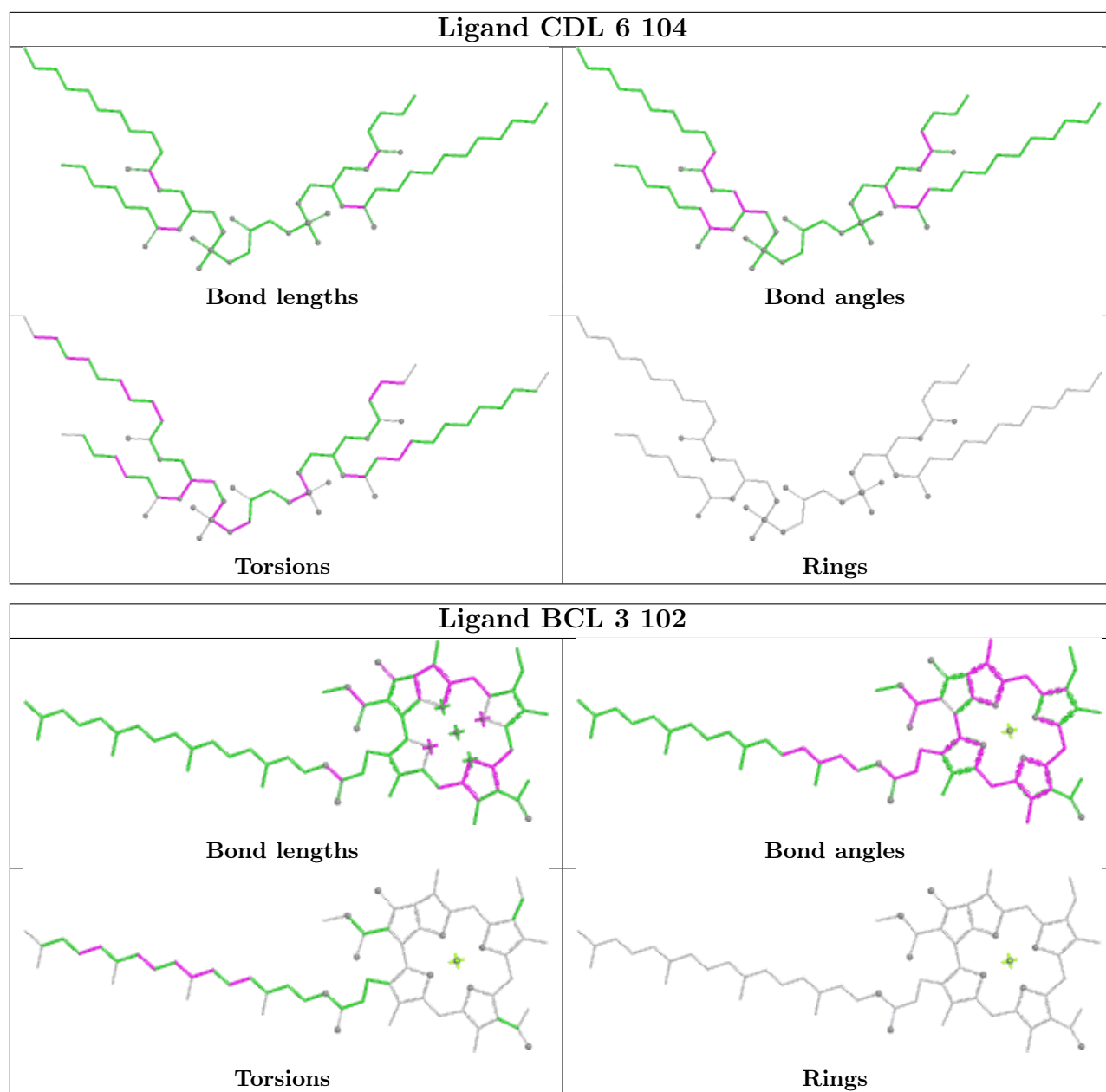












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

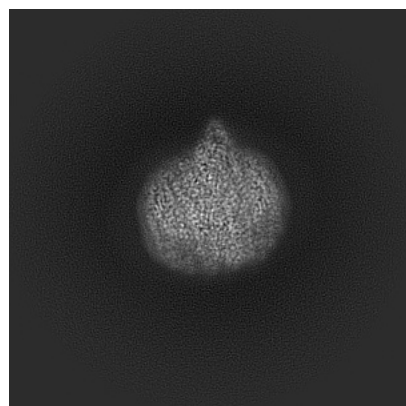
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33501. These allow visual inspection of the internal detail of the map and identification of artifacts.

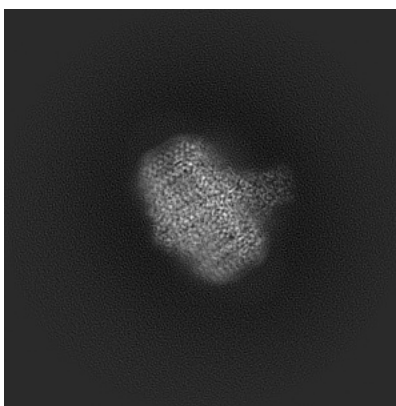
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

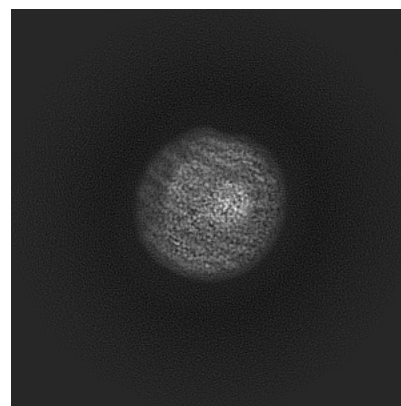
6.1.1 Primary map



X

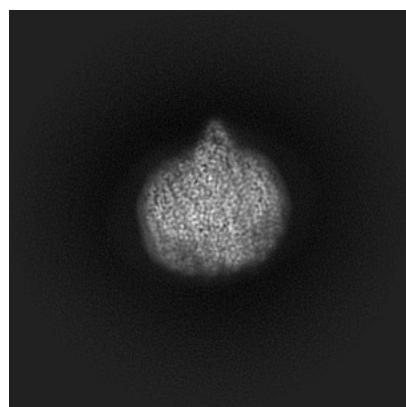


Y

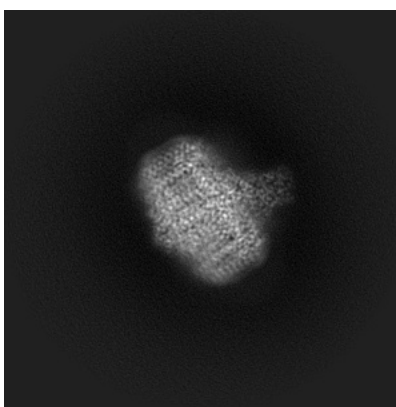


Z

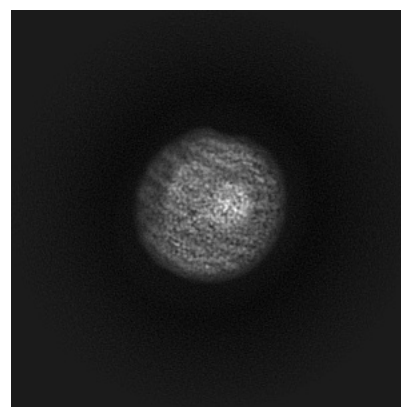
6.1.2 Raw map



X



Y

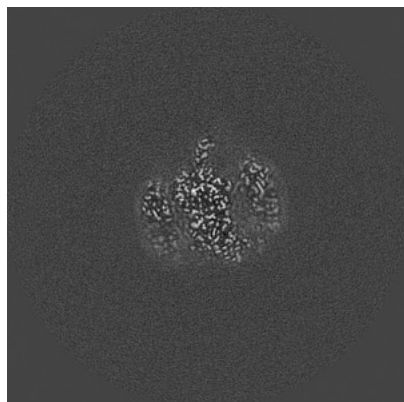


Z

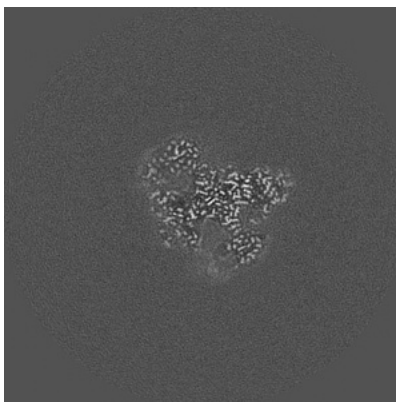
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

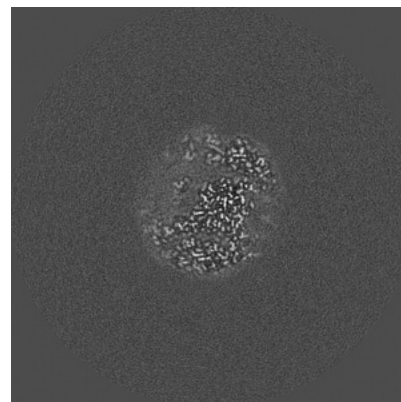
6.2.1 Primary map



X Index: 200

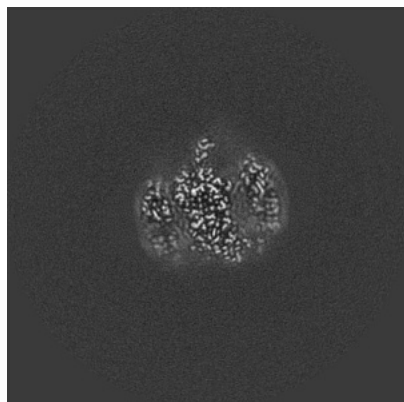


Y Index: 200

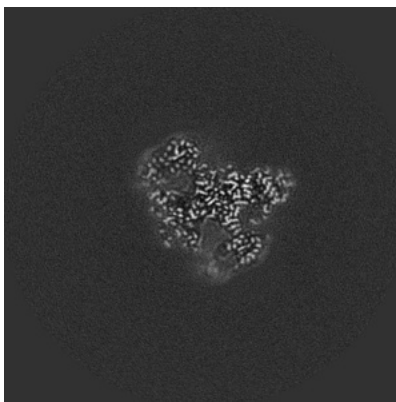


Z Index: 200

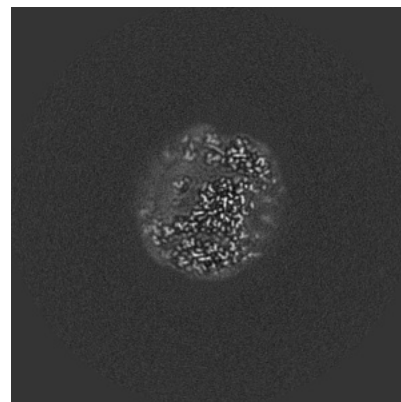
6.2.2 Raw map



X Index: 200



Y Index: 200

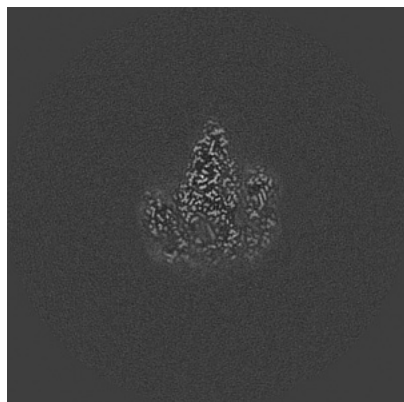


Z Index: 200

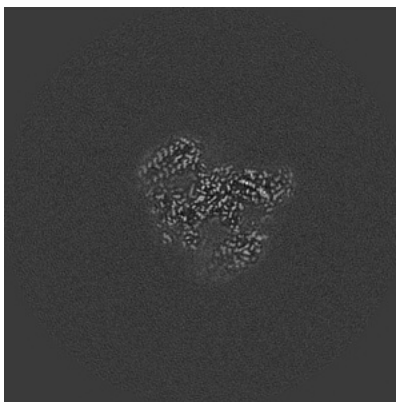
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

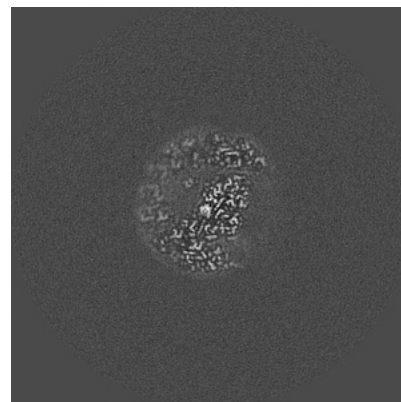
6.3.1 Primary map



X Index: 217

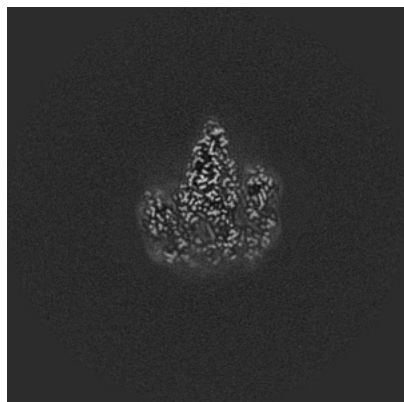


Y Index: 203

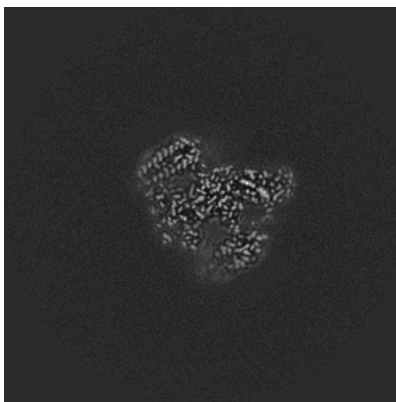


Z Index: 209

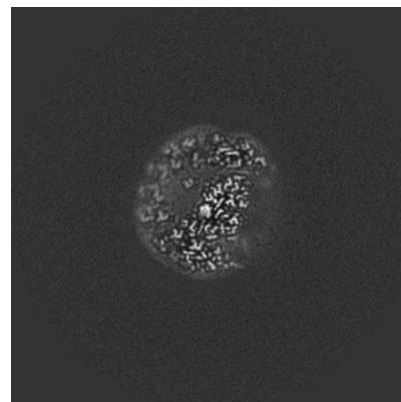
6.3.2 Raw map



X Index: 217



Y Index: 203

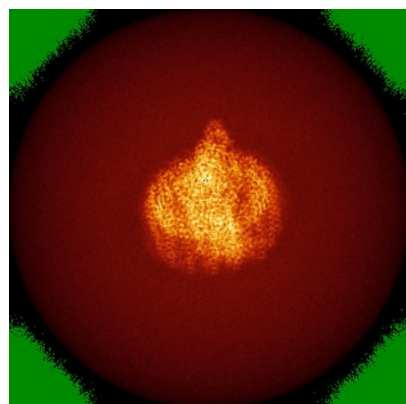


Z Index: 209

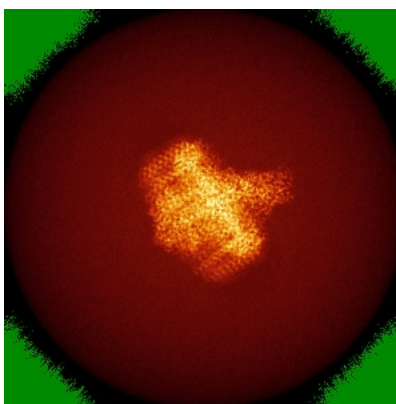
The images above show the largest variance slices of the map in three orthogonal directions.

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

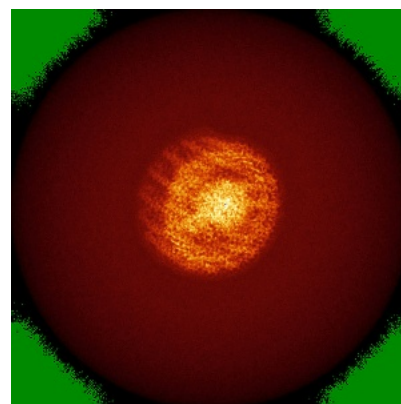
6.4.1 Primary map



X

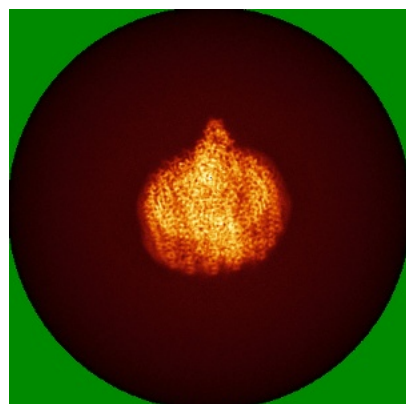


Y

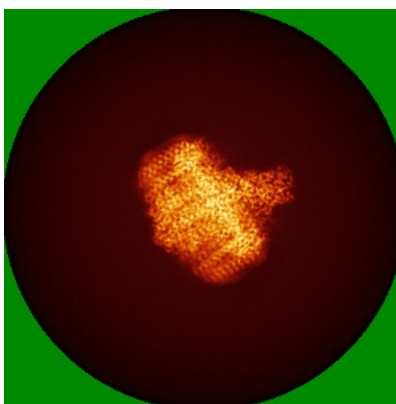


Z

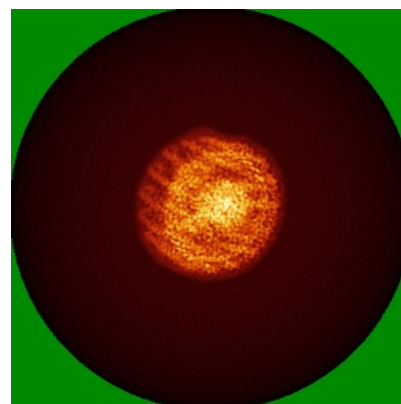
6.4.2 Raw map



X



Y

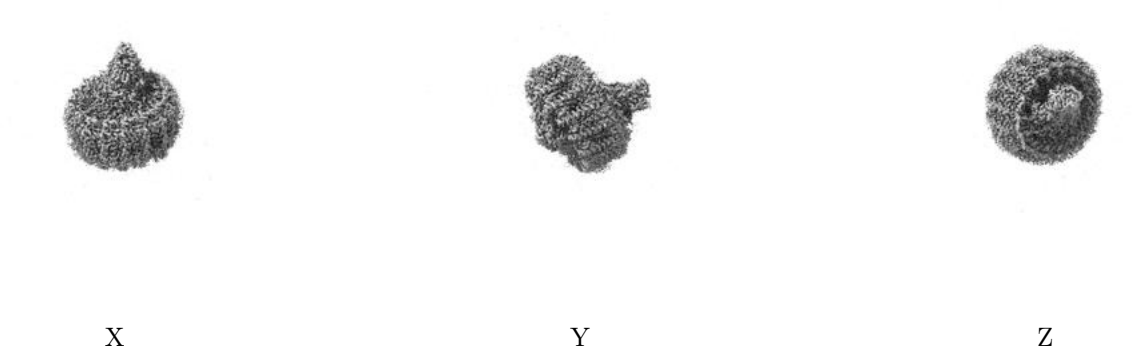


Z

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.

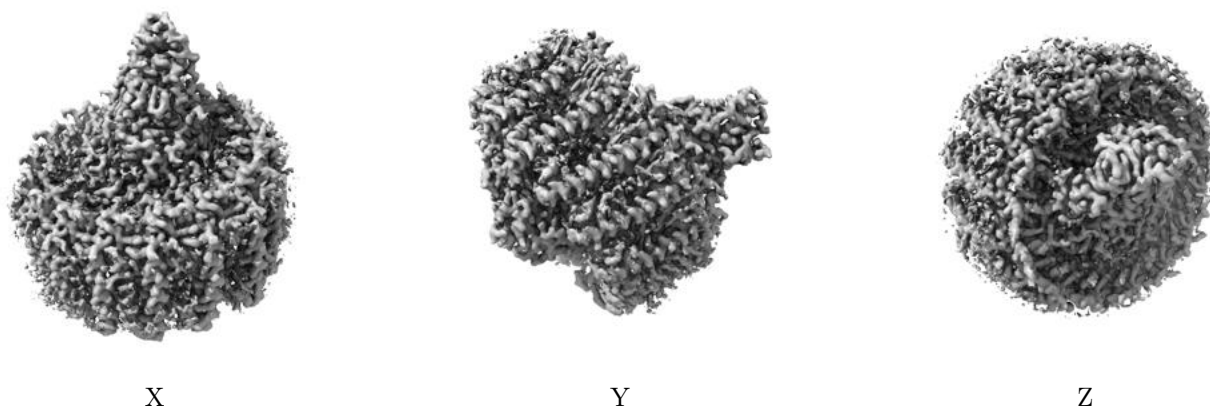
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

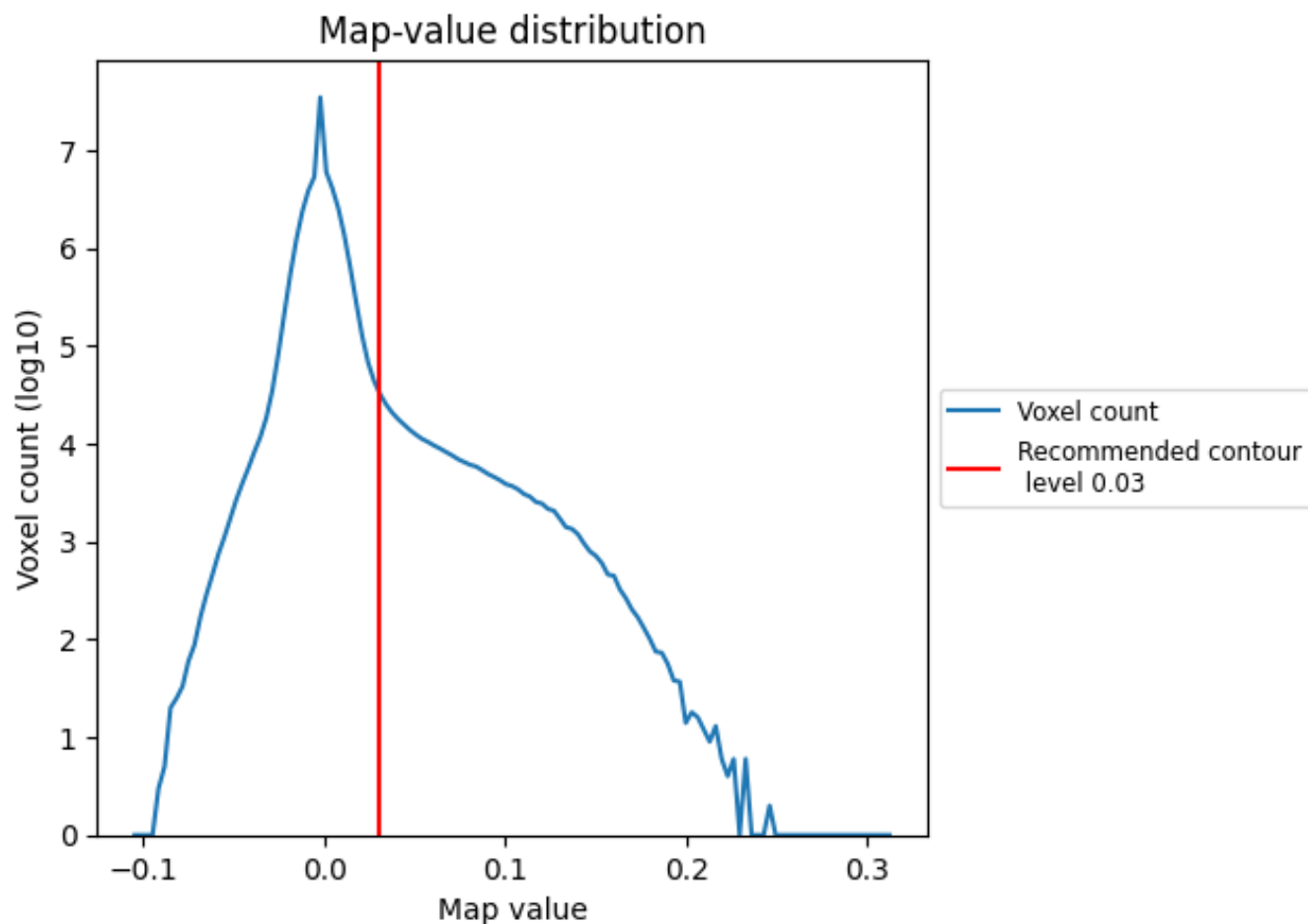
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

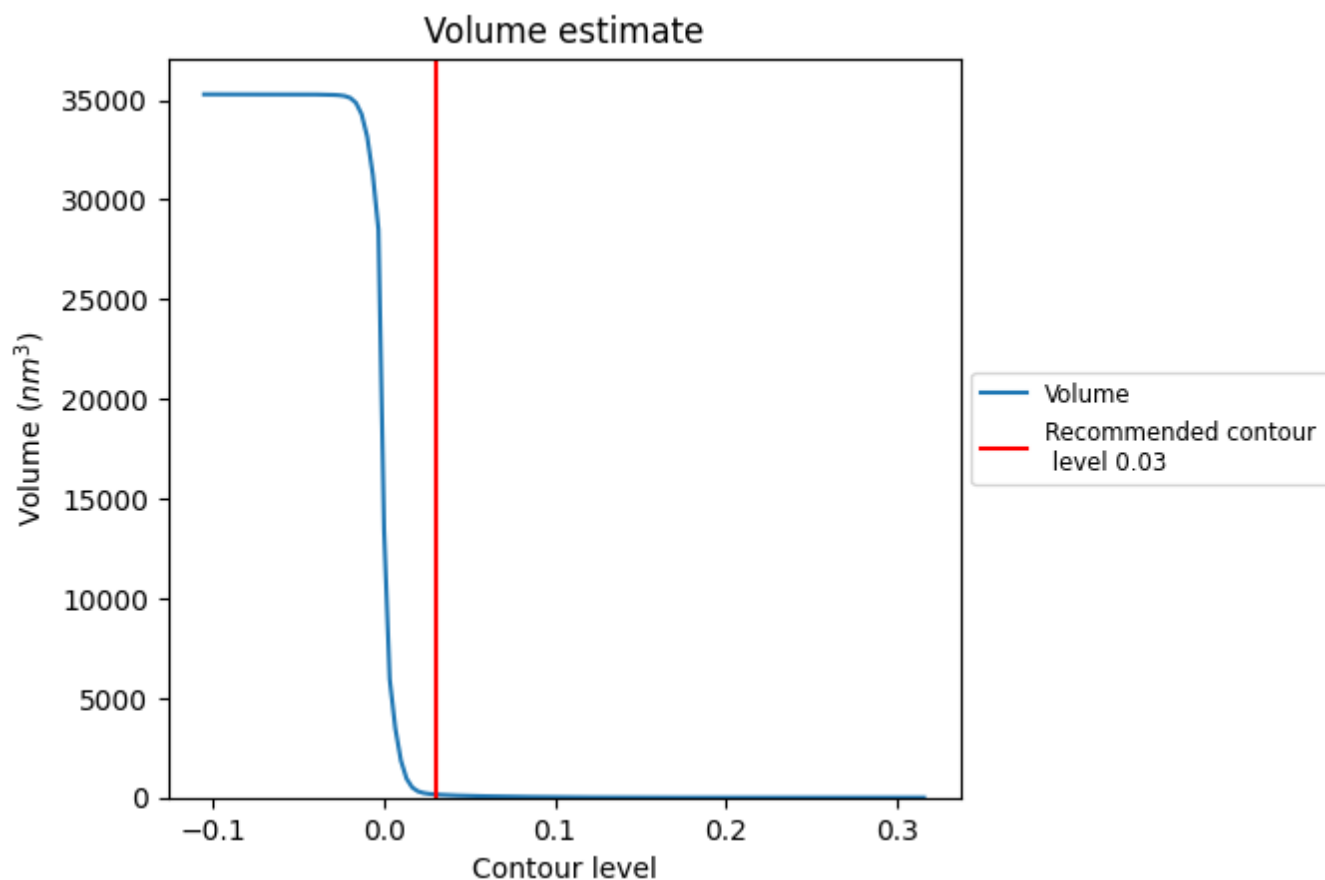
This section contains the results of statistical analysis of the map.

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.

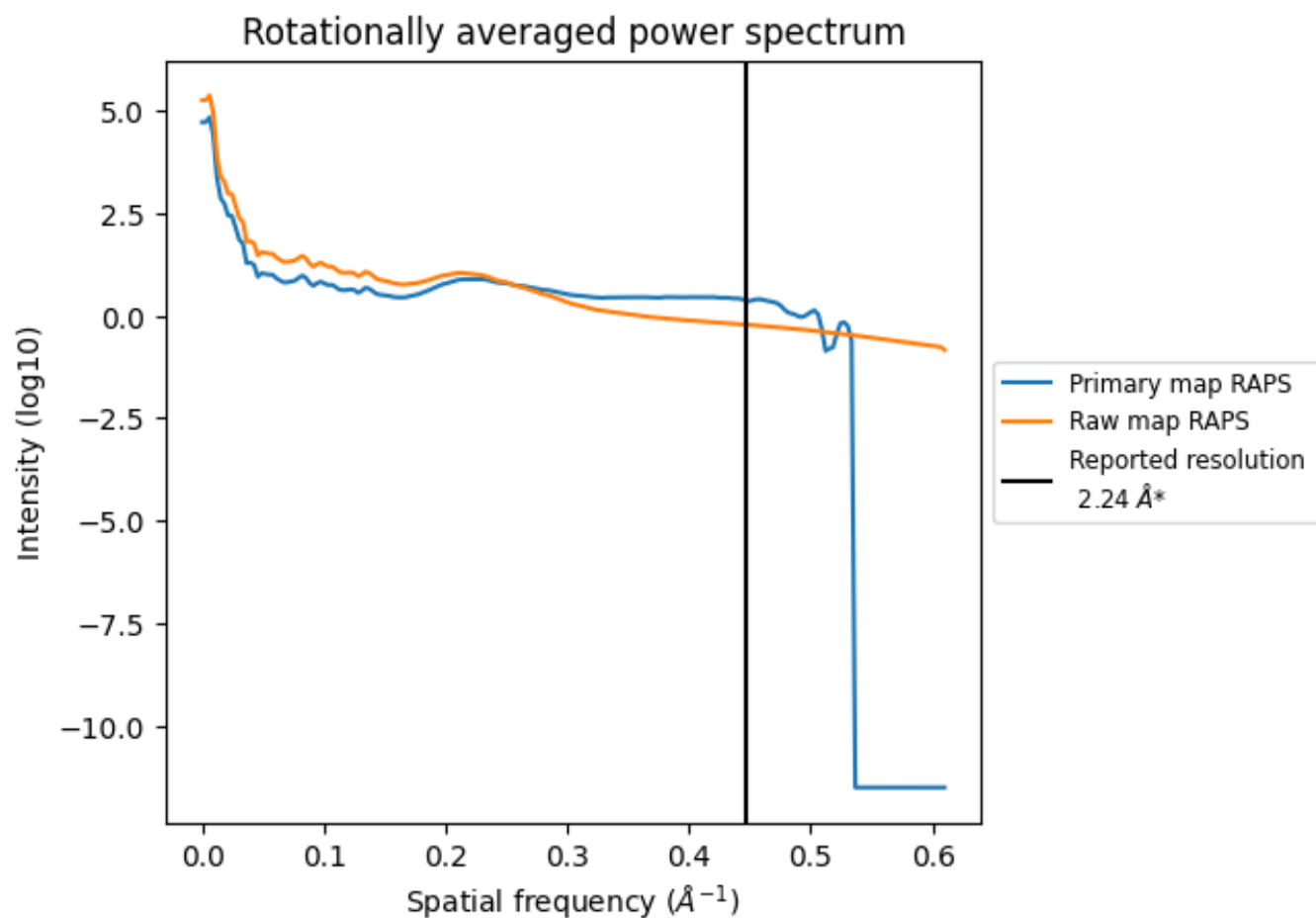
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm^3 ; this corresponds to an approximate mass of 142 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 ⓘ

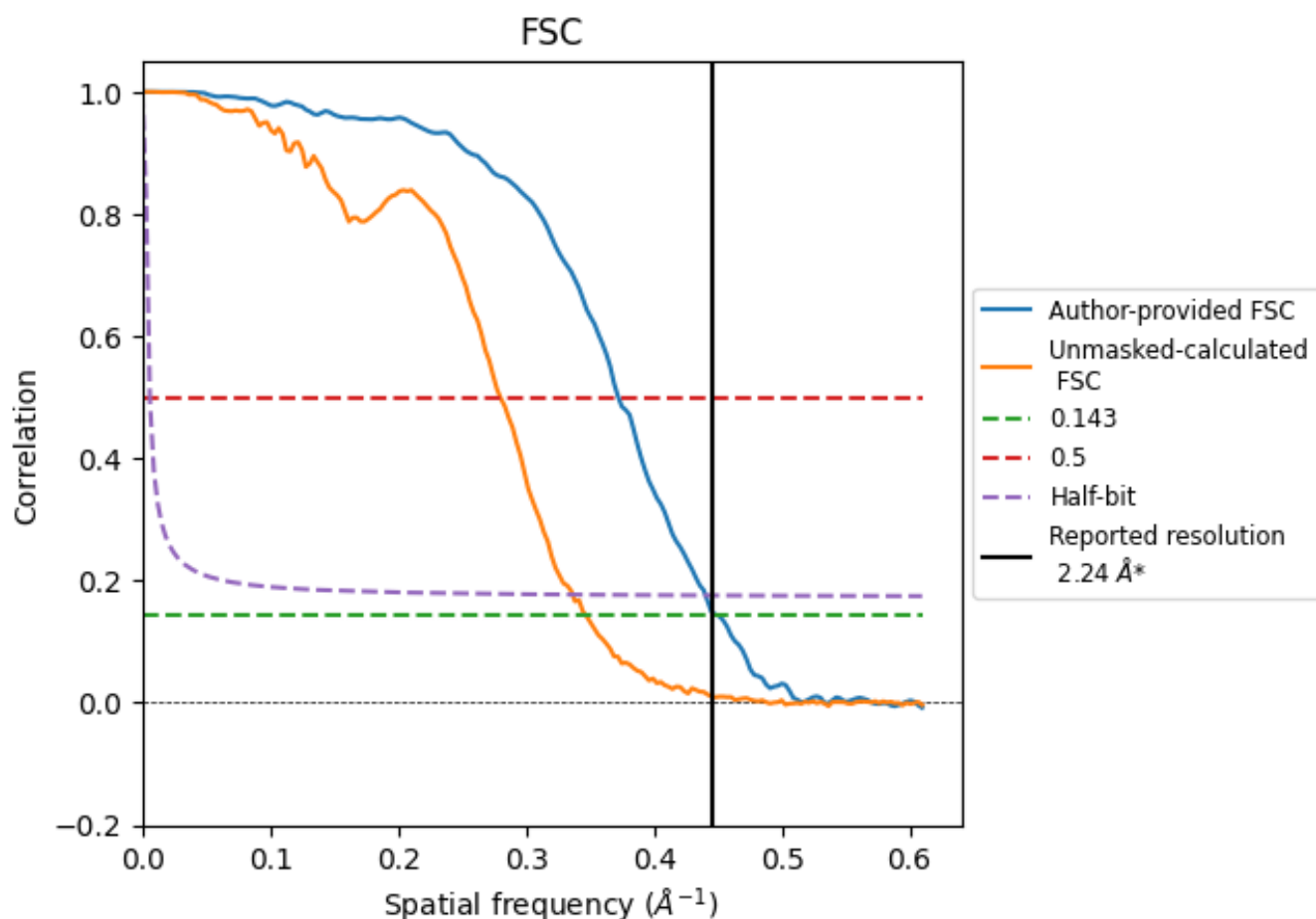


*Reported resolution corresponds to spatial frequency of 0.446 Å⁻¹

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 $0.446 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

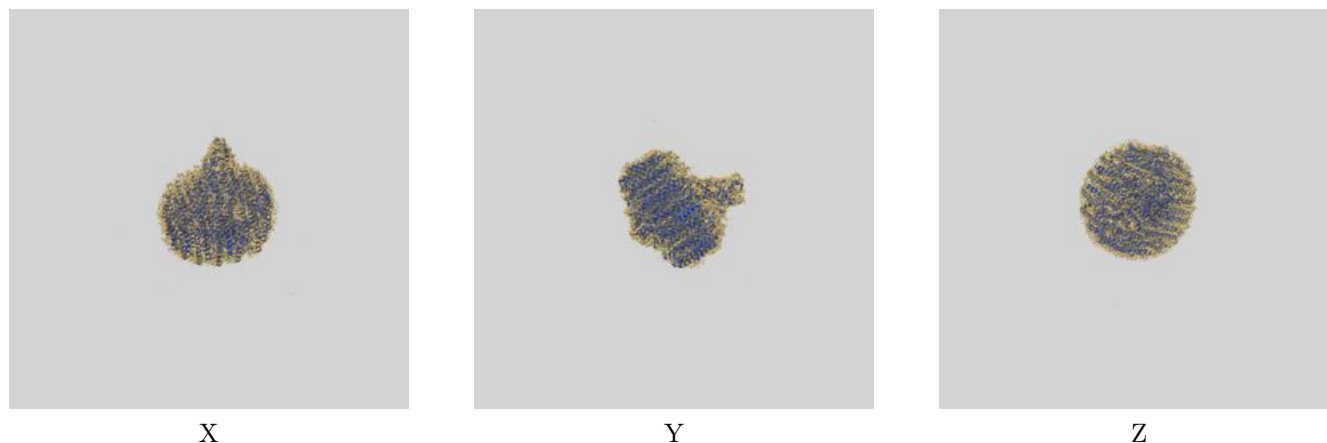
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.22	2.69	2.27
Unmasked-calculated*	2.88	3.57	2.97

*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 2.88 differs from the reported value 2.24 by more than 10 %

9 Map-model fit [i](#)

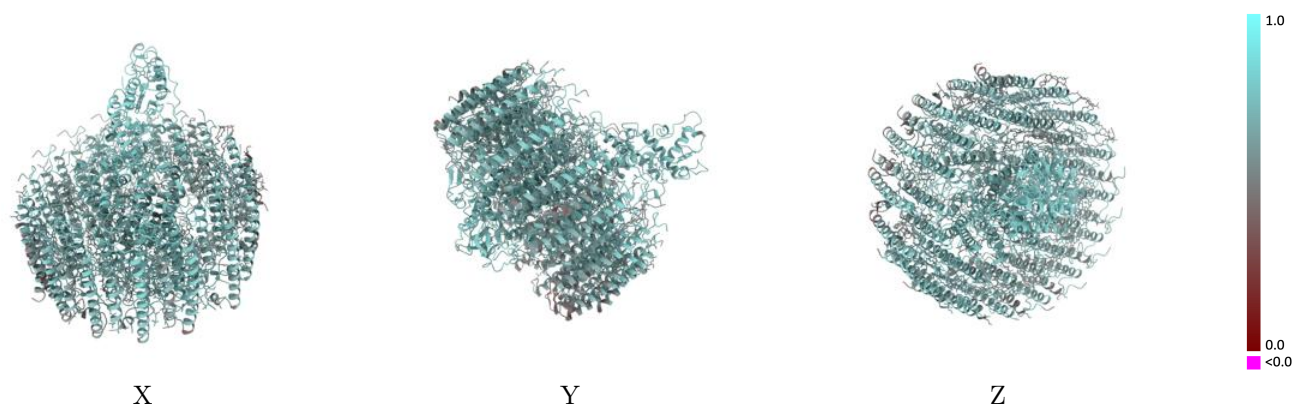
This section contains information regarding the fit between EMDB map EMD-33501 and PDB model 7XXF. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



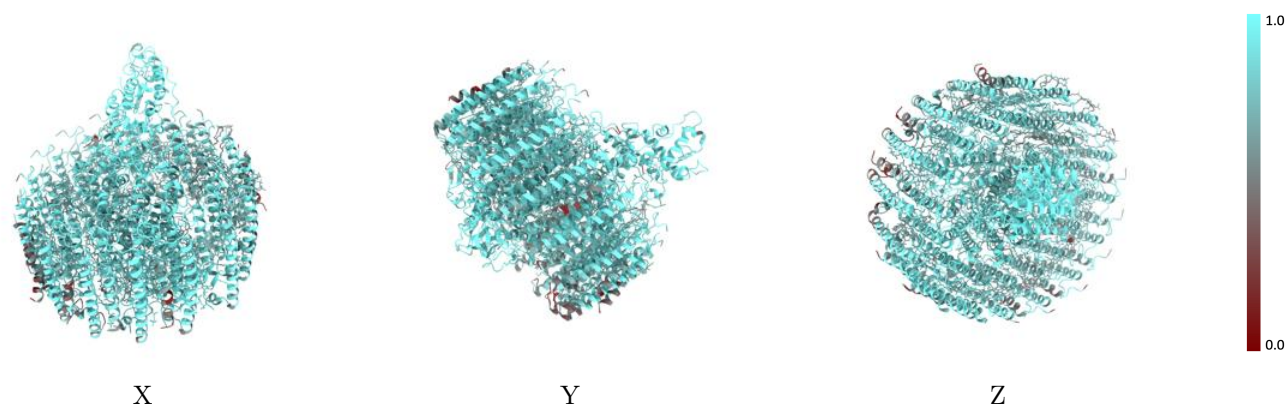
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



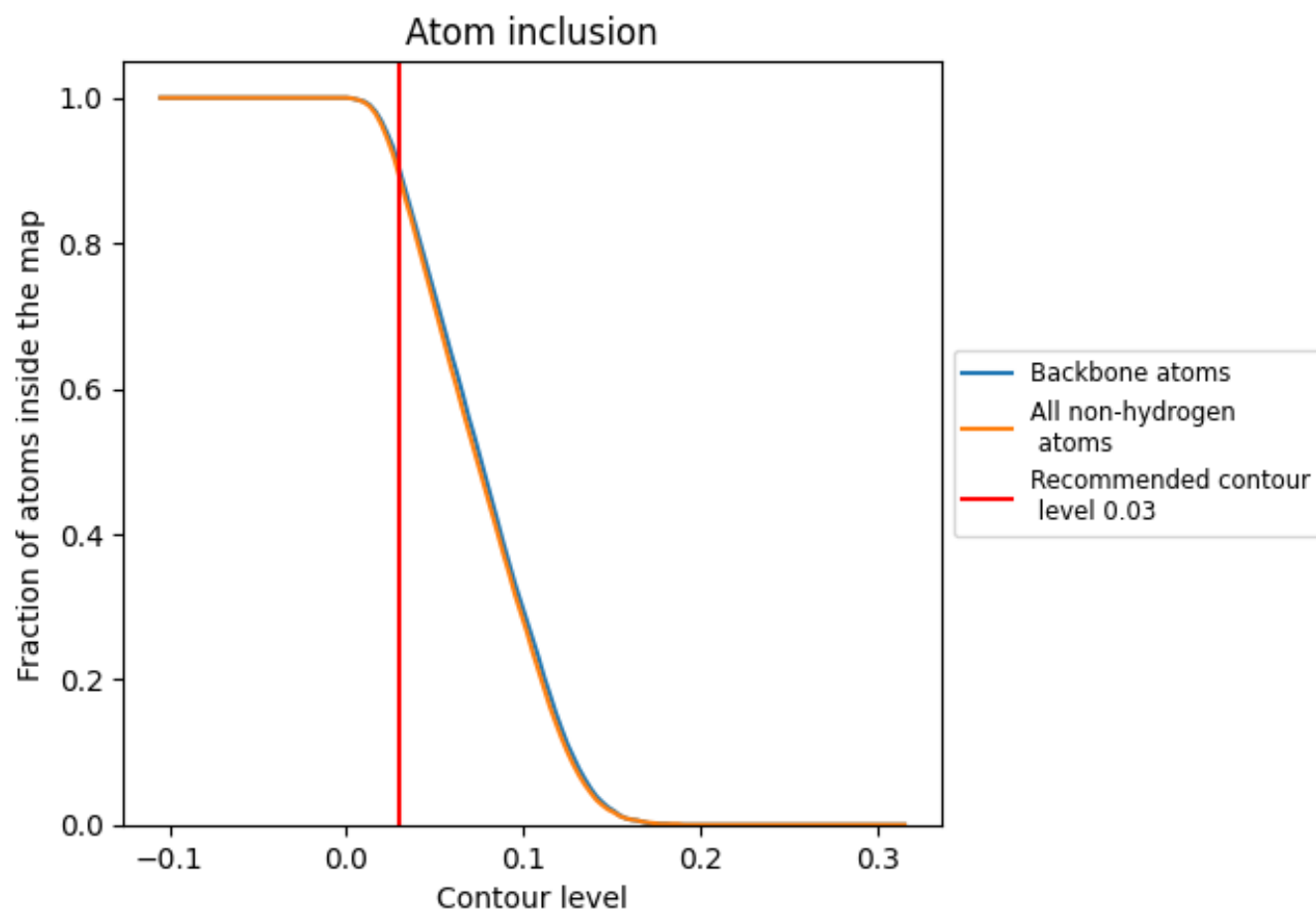
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.6760
0	 0.8830	 0.6580
1	 0.8970	 0.6610
2	 0.8000	 0.6200
3	 0.8760	 0.6530
4	 0.8550	 0.6490
5	 0.9020	 0.6750
6	 0.8410	 0.6380
7	 0.9080	 0.6750
8	 0.8690	 0.6580
9	 0.9380	 0.7020
A	 0.8920	 0.6700
B	 0.9050	 0.6820
C	 0.9680	 0.7240
D	 0.9040	 0.6730
E	 0.8750	 0.6610
F	 0.9390	 0.6820
G	 0.8720	 0.6590
H	 0.9370	 0.6960
I	 0.8910	 0.6690
J	 0.8450	 0.6430
K	 0.8860	 0.6530
L	 0.9620	 0.7280
M	 0.9680	 0.7290
N	 0.8610	 0.6580
O	 0.9430	 0.6890
P	 0.9110	 0.6720
Q	 0.9300	 0.6860
R	 0.8950	 0.6780
S	 0.9080	 0.6710
T	 0.7890	 0.6170
U	 0.8660	 0.6510
V	 0.8130	 0.6360
W	 0.8630	 0.6590
X	 0.8190	 0.6330



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Chain	Atom inclusion	Q-score
Y	 0.8870	 0.6590
Z	 0.8560	 0.6430
a	 0.5780	 0.5470
b	 0.8150	 0.6400
c	 0.6010	 0.5570
d	 0.4510	 0.5070
e	 0.4970	 0.5040
f	 0.8210	 0.6180
g	 0.6880	 0.5940
h	 0.8270	 0.6330
i	 0.5670	 0.5550
j	 0.6470	 0.5740
k	 0.5140	 0.4980