



wwPDB EM Validation Summary Report ⓘ

May 6, 2025 – 12:22 PM JST

PDB ID : 9IMN / pdb_00009imn
EMDB ID : EMD-60694
Title : Cryo-EM structure of a TEF30-associated intermediate PSII core dimer complex, type I, from *Chlamydomonas reinhardtii*
Authors : Wang, Y.; Wang, C.; Li, A.; Liu, Z.
Deposited on : 2024-07-03
Resolution : 2.97 Å(reported)

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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

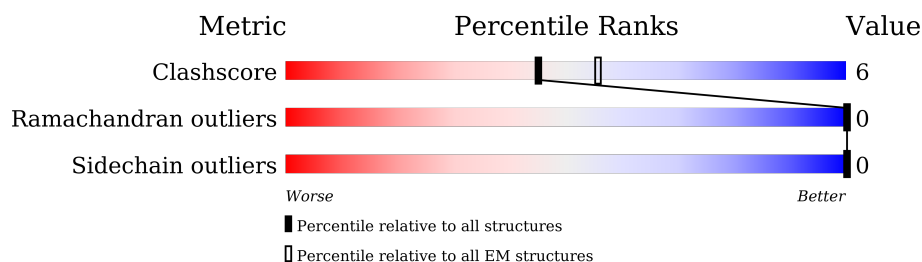
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	327	 82% 12% 6%
1	a	327	 82% 12% 6%
2	B	480	 87% 13%
2	b	480	 90% 10%
3	C	450	 85% 13% .
3	c	450	 89% 9% .
4	D	351	 85% 11% .
4	d	351	 87% 9% .

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Mol	Chain	Length	Quality of chain
5	E	75	
5	e	75	
6	F	31	
6	f	31	
7	G	240	
7	g	240	
8	H	69	
8	h	69	
9	I	34	
9	i	34	
10	K	37	
10	k	37	
11	L	38	
11	l	38	
12	M	27	
12	m	27	
13	T	31	
13	t	31	
14	V	31	
14	v	31	
15	W	19	
15	w	19	
16	X	32	
16	x	32	
17	Z	61	

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Mol	Chain	Length	Quality of chain
17	z	61	<div> <div>62%</div> <div>92%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	A	404	X	-	-	-
19	CLA	A	406	X	-	-	-
19	CLA	B	501	X	-	-	-
19	CLA	B	502	X	-	-	-
19	CLA	B	503	X	-	-	-
19	CLA	B	504	X	-	-	-
19	CLA	B	506	X	-	-	-
19	CLA	B	507	X	-	-	-
19	CLA	B	508	X	-	-	-
19	CLA	B	509	X	-	-	-
19	CLA	B	510	X	-	-	-
19	CLA	B	511	X	-	-	-
19	CLA	B	512	X	-	-	-
19	CLA	B	513	X	-	-	-
19	CLA	B	514	X	-	-	-
19	CLA	B	515	X	-	-	-
19	CLA	B	516	X	-	-	-
19	CLA	C	502	X	-	-	-
19	CLA	C	503	X	-	-	-
19	CLA	C	504	X	-	-	-
19	CLA	C	505	X	-	-	-
19	CLA	C	506	X	-	-	-
19	CLA	C	507	X	-	-	-
19	CLA	C	508	X	-	-	-
19	CLA	C	509	X	-	-	-
19	CLA	C	510	X	-	-	-
19	CLA	C	511	X	-	-	-
19	CLA	C	512	X	-	-	-
19	CLA	C	513	X	-	-	-
19	CLA	C	514	X	-	-	-
19	CLA	D	403	X	-	-	-
19	CLA	D	404	X	-	-	-
19	CLA	a	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	403	X	-	-	-
19	CLA	a	404	X	-	-	-
19	CLA	a	406	X	-	-	-
19	CLA	b	501	X	-	-	-
19	CLA	b	502	X	-	-	-
19	CLA	b	503	X	-	-	-
19	CLA	b	504	X	-	-	-
19	CLA	b	505	X	-	-	-
19	CLA	b	506	X	-	-	-
19	CLA	b	507	X	-	-	-
19	CLA	b	508	X	-	-	-
19	CLA	b	509	X	-	-	-
19	CLA	b	510	X	-	-	-
19	CLA	b	511	X	-	-	-
19	CLA	b	512	X	-	-	-
19	CLA	b	513	X	-	-	-
19	CLA	b	514	X	-	-	-
19	CLA	b	515	X	-	-	-
19	CLA	b	516	X	-	-	-
19	CLA	c	503	X	-	-	-
19	CLA	c	504	X	-	-	-
19	CLA	c	505	X	-	-	-
19	CLA	c	506	X	-	-	-
19	CLA	c	507	X	-	-	-
19	CLA	c	508	X	-	-	-
19	CLA	c	509	X	-	-	-
19	CLA	c	510	X	-	-	-
19	CLA	c	511	X	-	-	-
19	CLA	c	512	X	-	-	-
19	CLA	c	513	X	-	-	-
19	CLA	c	514	X	-	-	-
19	CLA	c	515	X	-	-	-
19	CLA	d	403	X	-	-	-
19	CLA	d	404	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 42392 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2388	1568	395	410	15		
1	a	306	Total	C	N	O	S	0	0
			2388	1568	395	410	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		
2	b	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	441	Total	C	N	O	S	0	0
			3444	2256	574	597	17		
3	c	441	Total	C	N	O	S	0	0
			3444	2256	574	597	17		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	337	Total	C	N	O	S	0	0
			2686	1777	439	458	12		
4	d	337	Total	C	N	O	S	0	0
			2686	1777	439	458	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total	C	N	O	0	0
			610	399	101	110		
5	e	75	Total	C	N	O	0	0
			610	399	101	110		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	31	Total	C	N	O	S	0	0
			251	171	42	37	1		
6	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

- Molecule 7 is a protein called PDZ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	182	Total	C	N	O	S	0	0
			1464	913	266	278	7		
7	g	182	Total	C	N	O	S	0	0
			1464	913	266	278	7		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	69	Total	C	N	O	S	0	0
			530	355	78	95	2		
8	h	69	Total	C	N	O	S	0	0
			530	355	78	95	2		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		
9	i	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			297	209	43	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			297	209	43	45		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	38	Total	C	N	O	S	0	0
			314	210	51	52	1		
11	l	38	Total	C	N	O	S	0	0
			314	210	51	52	1		

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	27	Total	C	N	O	0	0
			210	146	29	35		
12	m	27	Total	C	N	O	0	0
			210	146	29	35		

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	31	Total	C	N	O	S	0	0
			256	177	38	39	2		
13	t	31	Total	C	N	O	S	0	0
			256	177	38	39	2		

- Molecule 14 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	31	Total	C	N	O	0	0
			216	143	35	38		
14	v	31	Total	C	N	O	0	0
			216	143	35	38		

- Molecule 15 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	19	Total	C	N	O	S	0	0
			156	113	22	20	1		
15	w	19	Total	C	N	O	S	0	0
			156	113	22	20	1		

- Molecule 16 is a protein called Chloroplast photosystem II subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	32	Total	C	N	O	0	0
			214	140	35	39		
16	x	32	Total	C	N	O	0	0
			214	140	35	39		

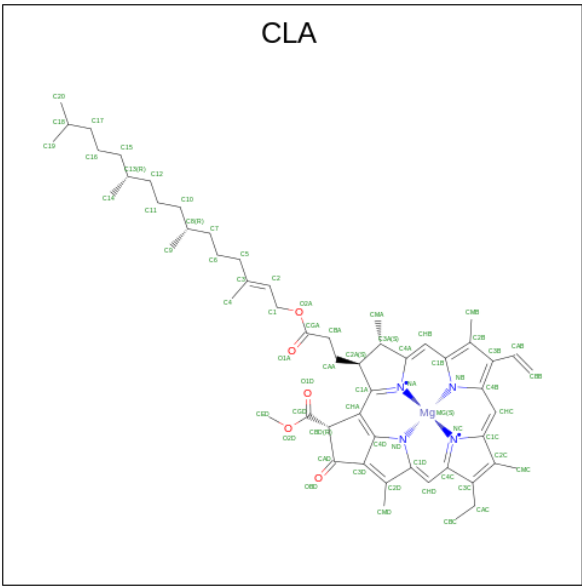
- Molecule 17 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
17	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 18 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Fe	0
			1	1	
18	a	1	Total	Fe	0
			1	1	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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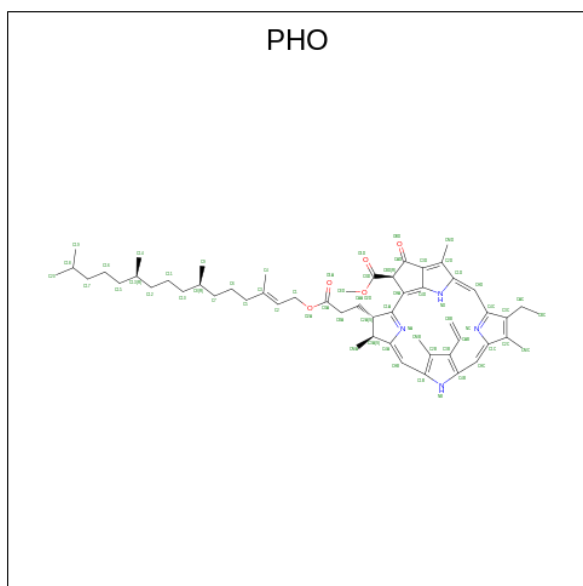
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

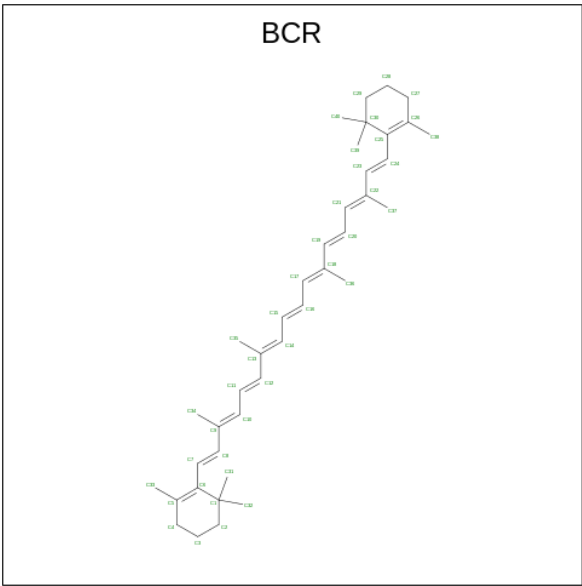
- Molecule 20 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	N	O	0
			64	55	4	5	
20	D	1	Total	C	N	O	0
			64	55	4	5	
20	a	1	Total	C	N	O	0
			64	55	4	5	
20	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand

of Interest" by depositor).



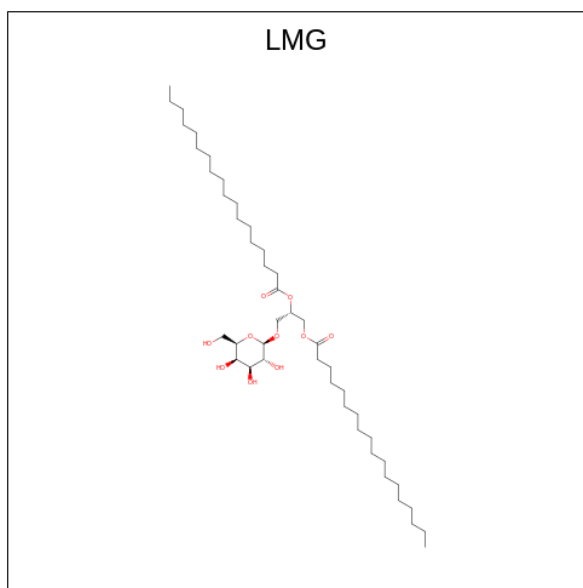
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	D	1	Total C 40 40	0
21	H	1	Total C 40 40	0
21	V	1	Total C 40 40	0
21	W	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
21	c	1	Total C 40 40	0
21	c	1	Total C 40 40	0
21	c	1	Total C 40 40	0
21	d	1	Total C 40 40	0
21	h	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	w	1	Total C 40 40	0

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



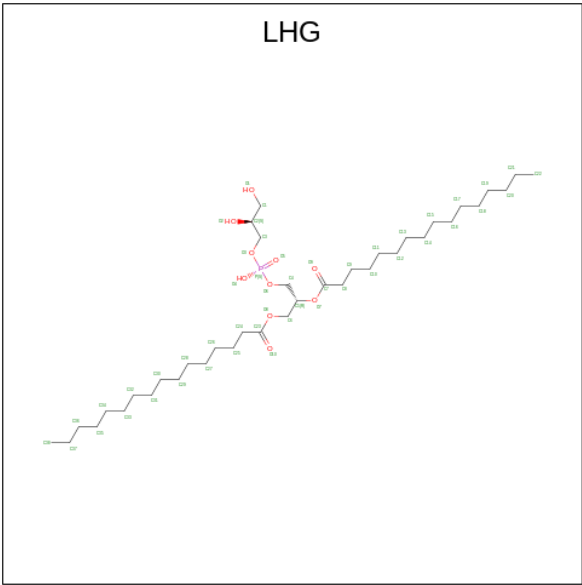
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C O 46 36 10	0
22	B	1	Total C O 42 32 10	0
22	C	1	Total C O 51 41 10	0
22	F	1	Total C O 46 36 10	0

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Mol	Chain	Residues	Atoms			AltConf
22	H	1	Total	C	O	0
			48	38	10	
22	b	1	Total	C	O	0
			42	32	10	
22	c	1	Total	C	O	0
			46	36	10	
22	c	1	Total	C	O	0
			51	41	10	
22	f	1	Total	C	O	0
			46	36	10	
22	h	1	Total	C	O	0
			48	38	10	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



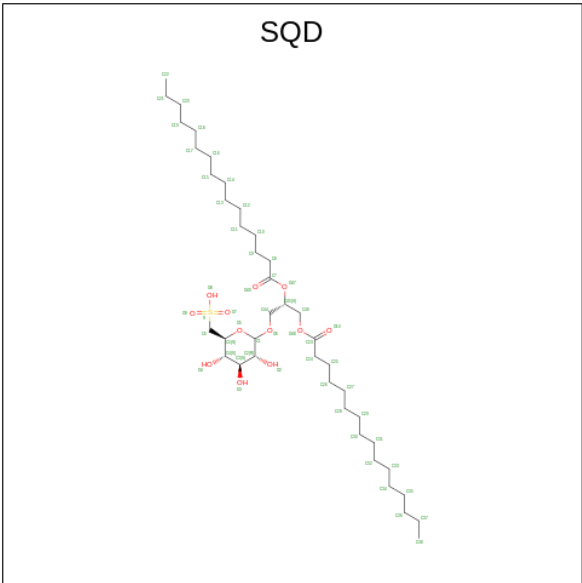
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			43	32	10	1	
23	A	1	Total	C	O	P	0
			44	33	10	1	
23	B	1	Total	C	O	P	0
			44	33	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	D	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
23	L	1	Total	C	O	P	0
			49	38	10	1	
23	X	1	Total	C	O	P	0
			49	38	10	1	
23	a	1	Total	C	O	P	0
			43	32	10	1	
23	a	1	Total	C	O	P	0
			44	33	10	1	
23	b	1	Total	C	O	P	0
			49	38	10	1	
23	d	1	Total	C	O	P	0
			44	33	10	1	
23	d	1	Total	C	O	P	0
			49	38	10	1	
23	l	1	Total	C	O	P	0
			49	38	10	1	
23	x	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



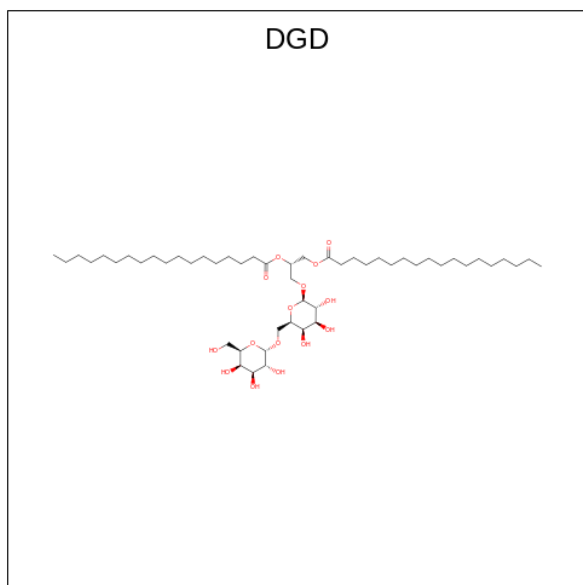
Mol	Chain	Residues	Atoms				AltConf
24	C	1	Total	C	O	S	0
			51	38	12	1	

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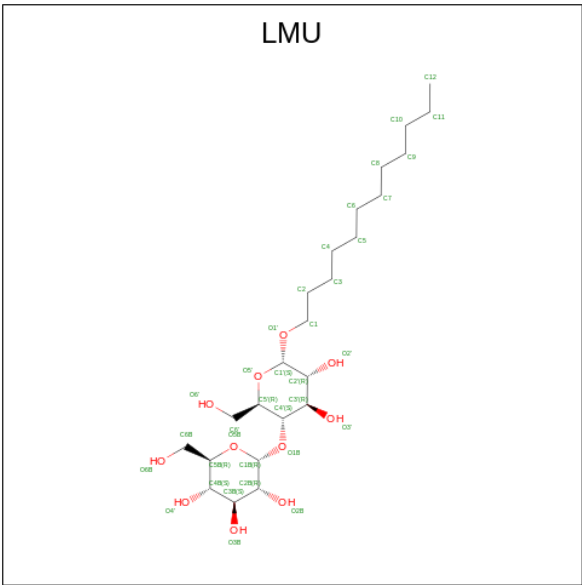
Mol	Chain	Residues	Atoms				AltConf
24	c	1	Total	C	O	S	0
			51	38	12	1	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



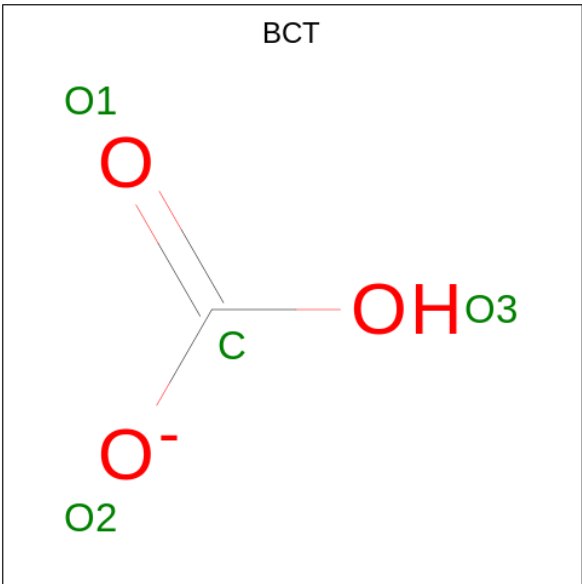
Mol	Chain	Residues	Atoms			AltConf
25	C	1	Total	C	O	0
			53	38	15	
25	C	1	Total	C	O	0
			49	34	15	
25	C	1	Total	C	O	0
			59	44	15	
25	c	1	Total	C	O	0
			53	38	15	
25	c	1	Total	C	O	0
			49	34	15	
25	c	1	Total	C	O	0
			59	44	15	

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	C	1	Total	C	O	0
			35	24	11	
26	c	1	Total	C	O	0
			35	24	11	

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



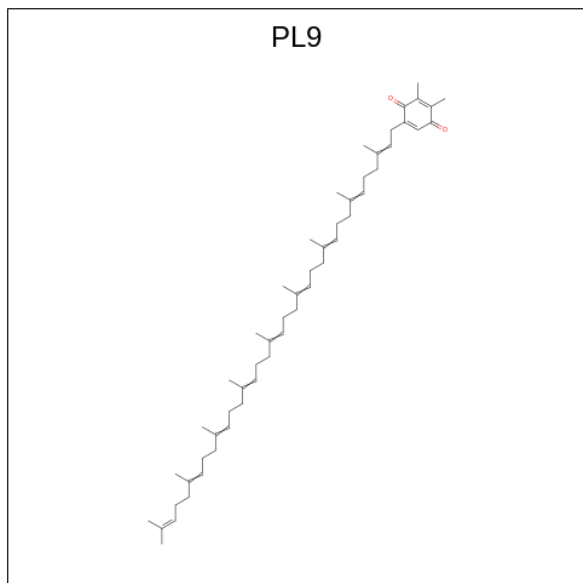
Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total	C	O	0
			4	1	3	

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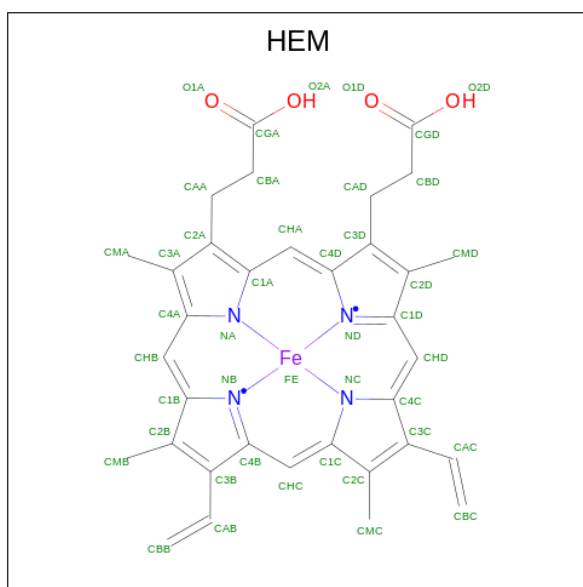
Mol	Chain	Residues	Atoms			AltConf
27	d	1	Total	C	O	0
			4	1	3	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).

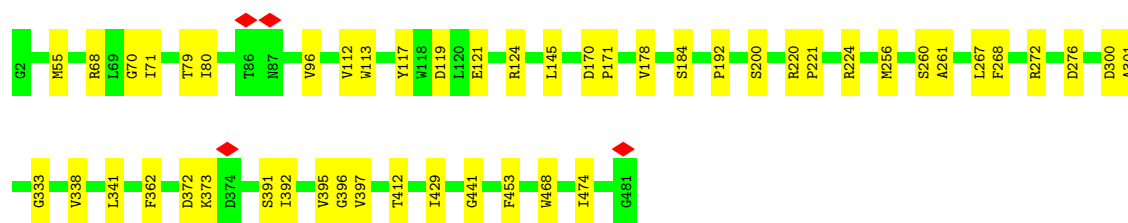


Mol	Chain	Residues	Atoms			AltConf
28	D	1	Total	C	O	0
			55	53	2	
28	d	1	Total	C	O	0
			55	53	2	

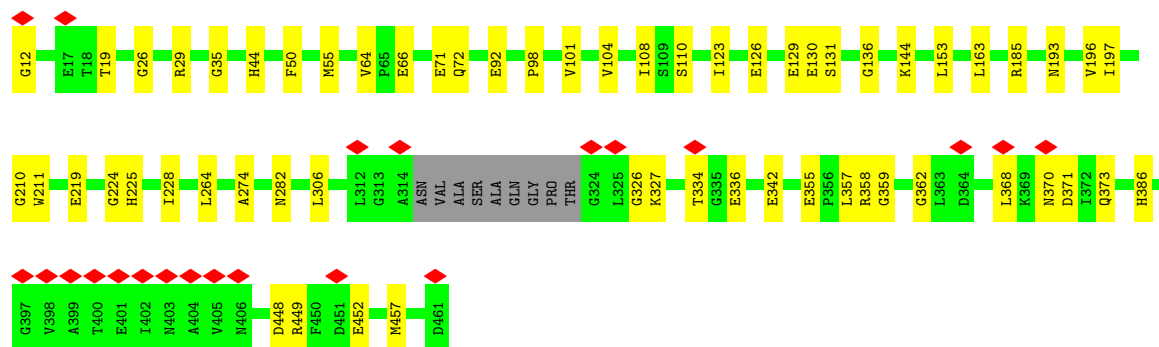
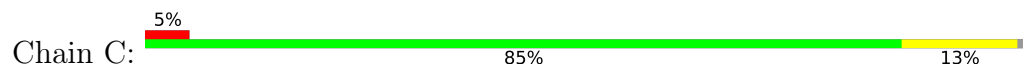
- Molecule 29 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



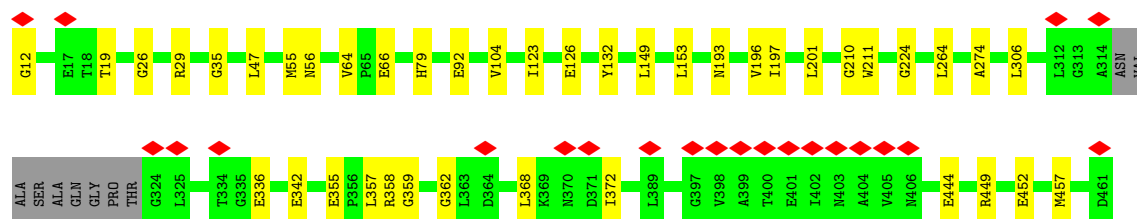
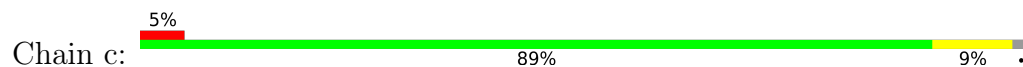
Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	e	1	Total 43	C 34	Fe 1	N 4	O 4	0



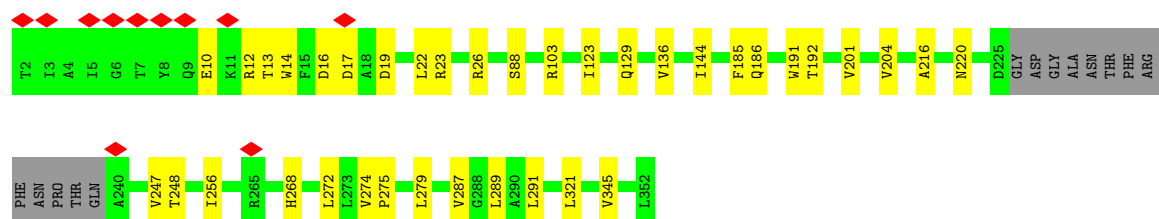
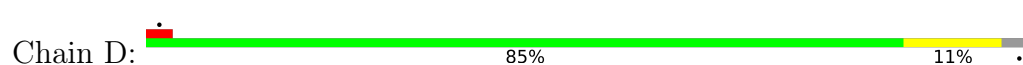
• Molecule 3: Photosystem II CP43 reaction center protein



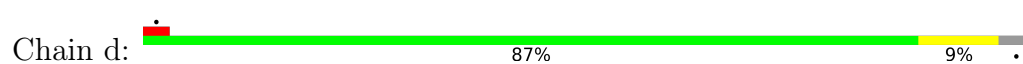
• Molecule 3: Photosystem II CP43 reaction center protein

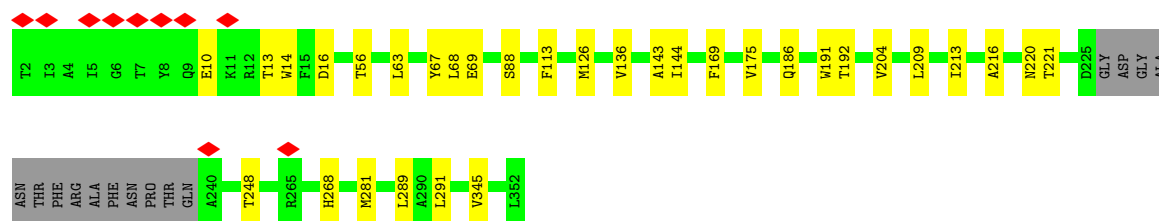


• Molecule 4: Photosystem II D2 protein

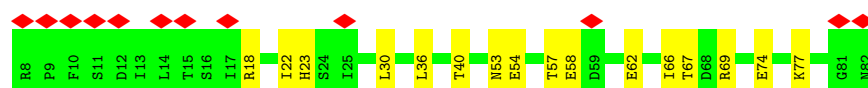
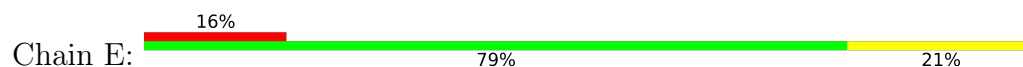


• Molecule 4: Photosystem II D2 protein

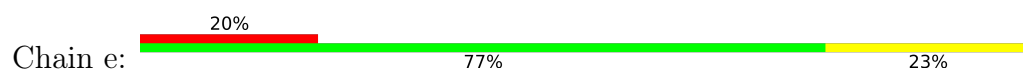




• Molecule 5: Cytochrome b559 subunit alpha



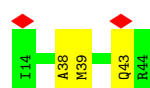
• Molecule 5: Cytochrome b559 subunit alpha



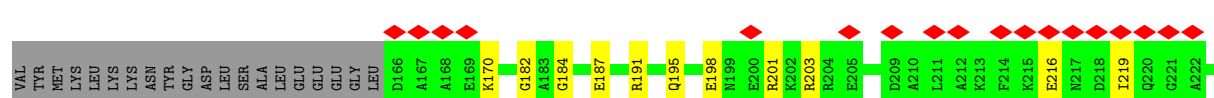
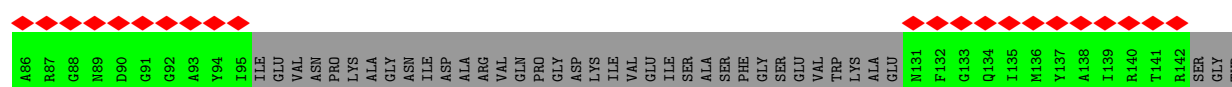
• Molecule 6: Cytochrome b559 subunit beta

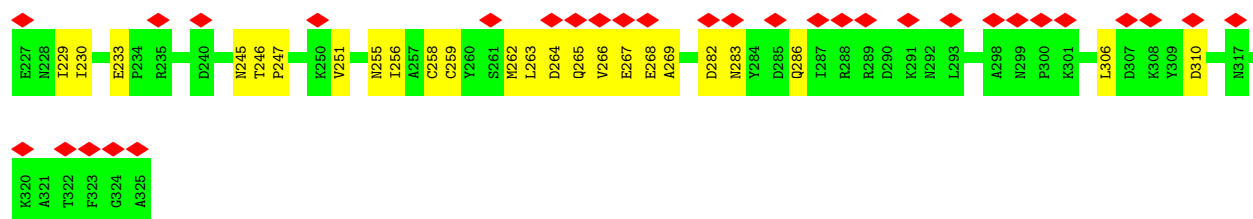


• Molecule 6: Cytochrome b559 subunit beta

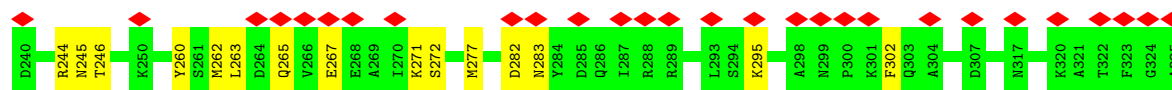
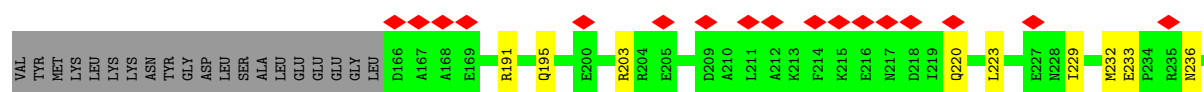
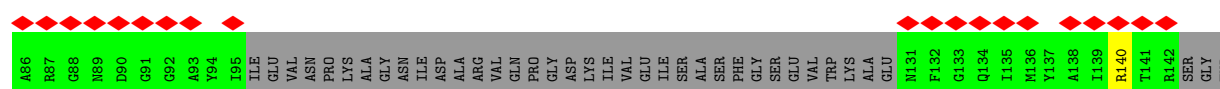


• Molecule 7: PDZ domain-containing protein

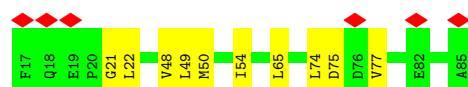
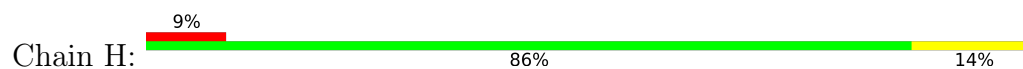




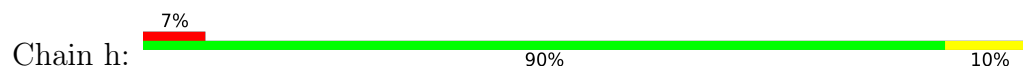
• Molecule 7: PDZ domain-containing protein



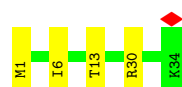
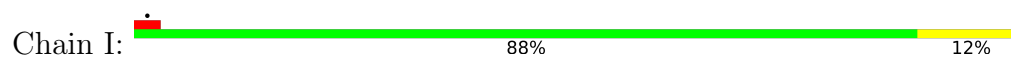
• Molecule 8: Photosystem II reaction center protein H



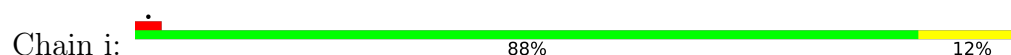
• Molecule 8: Photosystem II reaction center protein H



• Molecule 9: Photosystem II reaction center protein I

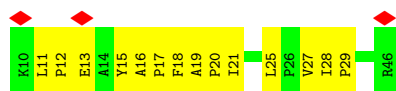


• Molecule 9: Photosystem II reaction center protein I

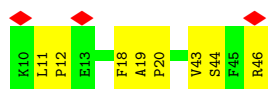
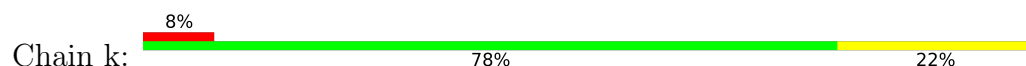




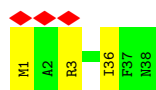
- Molecule 10: Photosystem II reaction center protein K



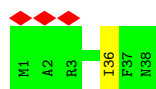
- Molecule 10: Photosystem II reaction center protein K



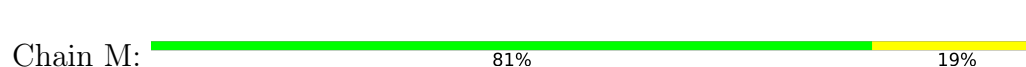
- Molecule 11: Photosystem II reaction center protein L



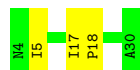
- Molecule 11: Photosystem II reaction center protein L



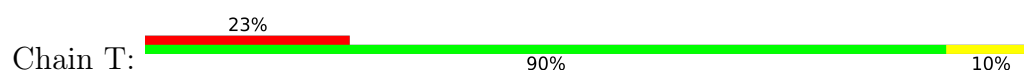
- Molecule 12: Photosystem II reaction center protein M



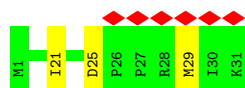
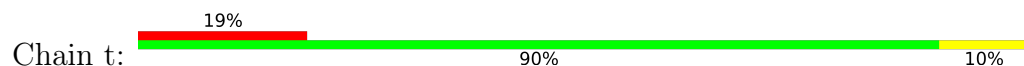
- Molecule 12: Photosystem II reaction center protein M



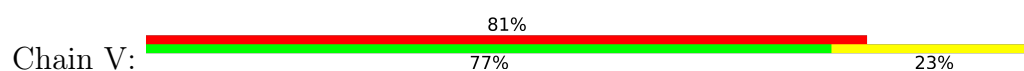
- Molecule 13: Photosystem II reaction center protein T



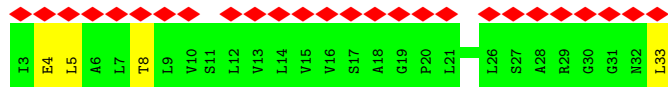
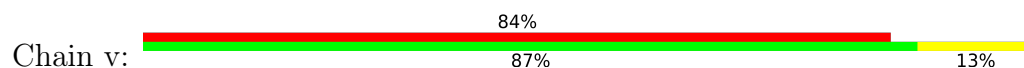
- Molecule 13: Photosystem II reaction center protein T



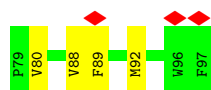
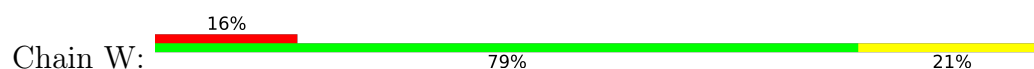
- Molecule 14: Photosystem II reaction center protein Psb30



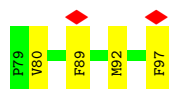
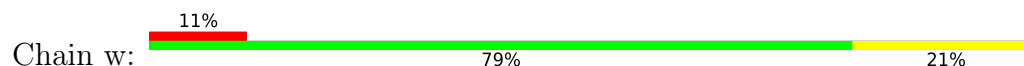
- Molecule 14: Photosystem II reaction center protein Psb30



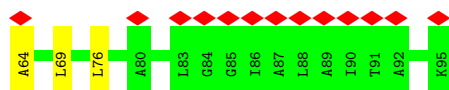
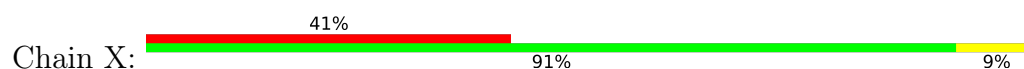
- Molecule 15: Photosystem II reaction center W protein, chloroplastic



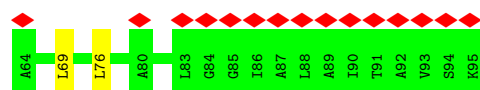
- Molecule 15: Photosystem II reaction center W protein, chloroplastic



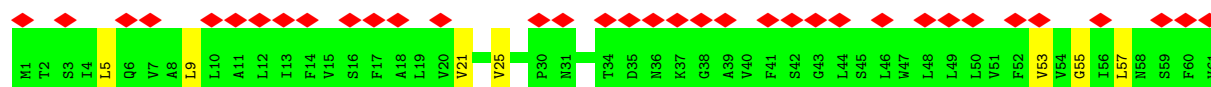
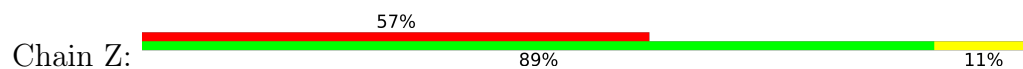
- Molecule 16: Chloroplast photosystem II subunit X



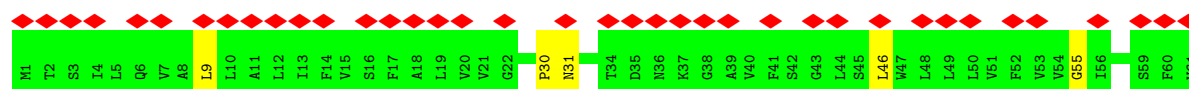
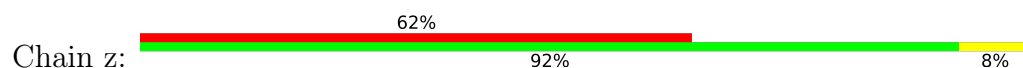
• Molecule 16: Chloroplast photosystem II subunit X



• Molecule 17: Photosystem II reaction center protein Z



• Molecule 17: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61267	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.008	Depositor
Minimum map value	-0.544	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.16	Depositor
Map size (\AA)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, SQD, LMU, FE2, DGD, BCT, HEM, PHO, LMG, BCR, PL9, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.19	0/2463	0.30	0/3358
1	a	0.18	0/2463	0.26	0/3358
2	B	0.17	0/3883	0.29	0/5286
2	b	0.16	0/3883	0.24	0/5286
3	C	0.15	0/3563	0.28	0/4851
3	c	0.14	0/3563	0.25	0/4851
4	D	0.18	0/2777	0.28	0/3787
4	d	0.18	0/2777	0.26	0/3787
5	E	0.15	0/628	0.31	0/857
5	e	0.12	0/628	0.27	0/857
6	F	0.16	0/258	0.36	0/349
6	f	0.17	0/258	0.47	0/349
7	G	0.12	0/1487	0.32	0/1993
7	g	0.10	0/1487	0.26	0/1993
8	H	0.13	0/542	0.27	0/742
8	h	0.14	0/542	0.28	0/742
9	I	0.18	0/283	0.27	0/383
9	i	0.18	0/283	0.22	0/383
10	K	0.13	0/309	0.33	0/425
10	k	0.12	0/309	0.31	0/425
11	L	0.21	0/322	0.28	0/437
11	l	0.19	0/322	0.26	0/437
12	M	0.14	0/214	0.36	0/293
12	m	0.15	0/214	0.25	0/293
13	T	0.18	0/263	0.26	0/354
13	t	0.17	0/263	0.24	0/354
14	V	0.12	0/216	0.28	0/296
14	v	0.09	0/216	0.24	0/296
15	W	0.79	0/164	1.14	0/225
15	w	0.80	0/164	1.15	0/225
16	X	0.11	0/215	0.23	0/292
16	x	0.09	0/215	0.21	0/292

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Z	0.14	0/469	0.27	0/644
17	z	0.12	0/469	0.24	0/644
All	All	0.17	0/36112	0.29	0/49144

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2327	27	0
1	a	2388	0	2327	28	0
2	B	3755	0	3642	46	0
2	b	3755	0	3642	38	0
3	C	3444	0	3319	47	0
3	c	3444	0	3319	39	0
4	D	2686	0	2585	31	0
4	d	2686	0	2585	30	0
5	E	610	0	599	12	0
5	e	610	0	599	14	0
6	F	251	0	263	4	0
6	f	251	0	263	7	0
7	G	1464	0	1422	26	0
7	g	1464	0	1422	18	0
8	H	530	0	553	10	0
8	h	530	0	553	7	0
9	I	275	0	287	11	0
9	i	275	0	287	10	0
10	K	297	0	308	11	0
10	k	297	0	308	7	0
11	L	314	0	327	2	0
11	l	314	0	327	1	0
12	M	210	0	231	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	m	210	0	231	2	0
13	T	256	0	273	3	0
13	t	256	0	273	3	0
14	V	216	0	250	10	0
14	v	216	0	250	3	0
15	W	156	0	156	10	0
15	w	156	0	156	9	0
16	X	214	0	240	3	0
16	x	214	0	240	3	0
17	Z	458	0	490	11	0
17	z	458	0	490	8	0
18	A	1	0	0	0	0
18	a	1	0	0	0	0
19	A	239	0	242	0	0
19	B	1020	0	1113	17	0
19	C	845	0	936	14	0
19	D	130	0	144	6	0
19	a	239	0	242	4	0
19	b	1020	0	1113	11	0
19	c	845	0	936	14	0
19	d	130	0	144	5	0
20	A	64	0	74	1	0
20	D	64	0	74	2	0
20	a	64	0	74	0	0
20	d	64	0	74	1	0
21	A	40	0	56	9	0
21	B	80	0	112	7	0
21	C	120	0	168	21	0
21	D	40	0	56	1	0
21	H	40	0	56	7	0
21	V	40	0	56	4	0
21	W	40	0	56	8	0
21	a	40	0	56	5	0
21	b	80	0	112	10	0
21	c	120	0	168	18	0
21	d	40	0	56	1	0
21	h	40	0	56	6	0
21	k	40	0	56	2	0
21	w	40	0	56	7	0
22	A	46	0	62	0	0
22	B	42	0	54	0	0
22	C	51	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	46	0	62	0	0
22	H	48	0	66	2	0
22	b	42	0	54	0	0
22	c	97	0	134	0	0
22	f	46	0	62	0	0
22	h	48	0	66	1	0
23	A	87	0	117	1	0
23	B	93	0	135	1	0
23	D	49	0	74	1	0
23	L	49	0	74	0	0
23	X	49	0	74	0	0
23	a	87	0	117	0	0
23	b	49	0	74	1	0
23	d	93	0	135	1	0
23	l	49	0	74	0	0
23	x	49	0	74	0	0
24	C	51	0	69	0	0
24	c	51	0	69	0	0
25	C	161	0	196	1	0
25	c	161	0	196	0	0
26	C	35	0	46	0	0
26	c	35	0	46	0	0
27	D	4	0	0	1	0
27	d	4	0	0	1	0
28	D	55	0	80	0	0
28	d	55	0	80	1	0
29	F	43	0	30	6	0
29	e	43	0	30	5	0
All	All	42392	0	43252	518	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 6.

The worst 5 of 518 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)
9:I:6:ILE:CD1	15:W:80:VAL:HG13	1.85	1.07
9:i:6:ILE:HD11	15:w:80:VAL:HG13	1.30	1.05
9:i:6:ILE:CD1	15:w:80:VAL:HG13	1.85	1.05
9:I:6:ILE:CD1	15:W:80:VAL:CG1	2.33	1.05
9:i:6:ILE:CD1	15:w:80:VAL:CG1	2.35	1.04

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/327 (92%)	296 (98%)	6 (2%)	0	100	100
1	a	302/327 (92%)	295 (98%)	7 (2%)	0	100	100
2	B	478/480 (100%)	464 (97%)	14 (3%)	0	100	100
2	b	478/480 (100%)	465 (97%)	13 (3%)	0	100	100
3	C	437/450 (97%)	426 (98%)	11 (2%)	0	100	100
3	c	437/450 (97%)	424 (97%)	13 (3%)	0	100	100
4	D	333/351 (95%)	327 (98%)	6 (2%)	0	100	100
4	d	333/351 (95%)	325 (98%)	8 (2%)	0	100	100
5	E	73/75 (97%)	73 (100%)	0	0	100	100
5	e	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	F	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	f	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	G	176/240 (73%)	172 (98%)	4 (2%)	0	100	100
7	g	176/240 (73%)	174 (99%)	2 (1%)	0	100	100
8	H	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
8	h	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	25/27 (93%)	25 (100%)	0	0	100	100
12	m	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
13	T	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	t	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
14	V	29/31 (94%)	29 (100%)	0	0	100	100
14	v	29/31 (94%)	29 (100%)	0	0	100	100
15	W	17/19 (90%)	17 (100%)	0	0	100	100
15	w	17/19 (90%)	17 (100%)	0	0	100	100
16	X	30/32 (94%)	30 (100%)	0	0	100	100
16	x	30/32 (94%)	30 (100%)	0	0	100	100
17	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
17	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
All	All	4374/4666 (94%)	4275 (98%)	99 (2%)	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	A	248/266 (93%)	248 (100%)	0	100	100
1	a	248/266 (93%)	248 (100%)	0	100	100
2	B	382/382 (100%)	382 (100%)	0	100	100
2	b	382/382 (100%)	382 (100%)	0	100	100
3	C	346/352 (98%)	346 (100%)	0	100	100
3	c	346/352 (98%)	346 (100%)	0	100	100
4	D	270/280 (96%)	270 (100%)	0	100	100
4	d	270/280 (96%)	270 (100%)	0	100	100
5	E	66/66 (100%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	66/66 (100%)	66 (100%)	0	100	100
6	F	25/25 (100%)	25 (100%)	0	100	100
6	f	25/25 (100%)	25 (100%)	0	100	100
7	G	148/195 (76%)	148 (100%)	0	100	100
7	g	148/195 (76%)	148 (100%)	0	100	100
8	H	59/59 (100%)	59 (100%)	0	100	100
8	h	59/59 (100%)	59 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	K	31/31 (100%)	31 (100%)	0	100	100
10	k	31/31 (100%)	31 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	23/23 (100%)	23 (100%)	0	100	100
12	m	23/23 (100%)	23 (100%)	0	100	100
13	T	28/28 (100%)	28 (100%)	0	100	100
13	t	28/28 (100%)	28 (100%)	0	100	100
14	V	25/25 (100%)	25 (100%)	0	100	100
14	v	25/25 (100%)	25 (100%)	0	100	100
15	W	15/15 (100%)	15 (100%)	0	100	100
15	w	15/15 (100%)	15 (100%)	0	100	100
16	X	22/22 (100%)	22 (100%)	0	100	100
16	x	22/22 (100%)	22 (100%)	0	100	100
17	Z	51/51 (100%)	51 (100%)	0	100	100
17	z	51/51 (100%)	51 (100%)	0	100	100
All	All	3610/3772 (96%)	3610 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	164	GLN

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Mol	Chain	Res	Type
4	D	186	GLN
11	l	5	ASN
2	b	331	ASN
3	c	56	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 2 are monoatomic - leaving 134 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$
19	CLA	c	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.27	9 (11%)
19	CLA	c	508	-	65,73,73	1.52	7 (10%)	76,113,113	1.20	7 (9%)
21	BCR	a	407	-	41,41,41	0.76	0	56,56,56	1.93	19 (33%)
19	CLA	B	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.23	8 (10%)
19	CLA	c	511	-	65,73,73	1.49	9 (13%)	76,113,113	1.24	7 (9%)
19	CLA	C	509	-	65,73,73	1.50	8 (12%)	76,113,113	1.19	7 (9%)
19	CLA	c	514	-	65,73,73	1.50	7 (10%)	76,113,113	1.28	7 (9%)
25	DGD	C	520	-	60,60,67	0.88	2 (3%)	74,74,81	0.87	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	C	502	-	65,73,73	1.51	7 (10%)	76,113,113	1.17	9 (11%)
19	CLA	b	509	-	65,73,73	1.51	7 (10%)	76,113,113	1.21	9 (11%)
19	CLA	b	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.23	9 (11%)
19	CLA	b	513	-	65,73,73	1.49	8 (12%)	76,113,113	1.25	8 (10%)
19	CLA	c	515	-	65,73,73	1.50	6 (9%)	76,113,113	1.22	7 (9%)
22	LMG	H	102	-	48,48,55	0.95	2 (4%)	56,56,63	0.95	2 (3%)
28	PL9	d	406	-	55,55,55	1.32	5 (9%)	68,69,69	1.50	12 (17%)
19	CLA	B	510	-	65,73,73	1.47	7 (10%)	76,113,113	1.29	9 (11%)
19	CLA	d	404	-	65,73,73	1.49	7 (10%)	76,113,113	1.25	9 (11%)
21	BCR	V	101	-	41,41,41	0.66	0	56,56,56	2.19	24 (42%)
19	CLA	b	514	-	45,53,73	1.77	6 (13%)	52,89,113	1.46	7 (13%)
23	LHG	a	408	-	42,42,48	0.98	2 (4%)	45,48,54	1.02	2 (4%)
19	CLA	B	516	-	65,73,73	1.50	8 (12%)	76,113,113	1.22	8 (10%)
19	CLA	C	505	-	65,73,73	1.51	7 (10%)	76,113,113	1.23	7 (9%)
27	BCT	D	402	18	2,3,3	1.28	0	2,3,3	4.12	2 (100%)
26	LMU	c	523	-	36,36,36	1.18	2 (5%)	47,47,47	0.89	1 (2%)
19	CLA	A	402	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	8 (10%)
19	CLA	B	512	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	8 (10%)
19	CLA	a	402	-	65,73,73	1.48	8 (12%)	76,113,113	1.27	9 (11%)
25	DGD	C	519	-	50,50,67	0.97	2 (4%)	64,64,81	0.92	2 (3%)
24	SQD	C	501	-	50,51,54	1.21	4 (8%)	59,62,65	1.09	5 (8%)
20	PHO	a	405	-	51,69,69	1.03	5 (9%)	47,99,99	1.21	6 (12%)
19	CLA	a	404	-	49,57,73	1.72	8 (16%)	55,93,113	1.39	8 (14%)
23	LHG	B	521	-	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
21	BCR	C	516	-	41,41,41	0.79	0	56,56,56	1.83	17 (30%)
22	LMG	C	521	-	51,51,55	0.93	2 (3%)	59,59,63	0.88	2 (3%)
19	CLA	B	506	-	65,73,73	1.50	7 (10%)	76,113,113	1.20	8 (10%)
21	BCR	h	101	-	41,41,41	0.70	0	56,56,56	2.09	23 (41%)
23	LHG	x	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	3 (5%)
21	BCR	A	407	-	41,41,41	0.76	0	56,56,56	1.88	17 (30%)
29	HEM	F	102	5,6	41,50,50	1.49	4 (9%)	45,82,82	1.39	5 (11%)
25	DGD	c	520	-	50,50,67	0.97	2 (4%)	64,64,81	0.92	2 (3%)
19	CLA	C	506	-	65,73,73	1.48	7 (10%)	76,113,113	1.16	7 (9%)
23	LHG	D	407	-	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
19	CLA	c	507	-	65,73,73	1.49	7 (10%)	76,113,113	1.19	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	b	503	-	65,73,73	1.50	8 (12%)	76,113,113	1.26	8 (10%)
19	CLA	b	516	-	65,73,73	1.48	8 (12%)	76,113,113	1.27	7 (9%)
19	CLA	a	406	-	60,68,73	1.54	7 (11%)	70,107,113	1.29	8 (11%)
21	BCR	b	518	-	41,41,41	0.74	0	56,56,56	1.91	19 (33%)
19	CLA	b	501	-	65,73,73	1.52	7 (10%)	76,113,113	1.20	7 (9%)
24	SQD	c	501	-	50,51,54	1.21	4 (8%)	59,62,65	1.09	5 (8%)
23	LHG	b	520	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
21	BCR	B	518	-	41,41,41	0.74	0	56,56,56	1.92	20 (35%)
21	BCR	b	517	-	41,41,41	0.76	1 (2%)	56,56,56	2.04	20 (35%)
19	CLA	b	502	-	65,73,73	1.49	6 (9%)	76,113,113	1.22	8 (10%)
28	PL9	D	406	-	55,55,55	1.34	5 (9%)	68,69,69	1.50	12 (17%)
26	LMU	C	522	-	36,36,36	1.17	2 (5%)	47,47,47	0.89	1 (2%)
19	CLA	B	509	-	65,73,73	1.51	7 (10%)	76,113,113	1.19	9 (11%)
19	CLA	b	510	-	65,73,73	1.47	6 (9%)	76,113,113	1.31	9 (11%)
19	CLA	C	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.24	7 (9%)
19	CLA	B	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.27	8 (10%)
19	CLA	B	508	-	65,73,73	1.49	7 (10%)	76,113,113	1.22	9 (11%)
19	CLA	B	501	-	65,73,73	1.52	6 (9%)	76,113,113	1.19	7 (9%)
19	CLA	b	515	-	65,73,73	1.51	7 (10%)	76,113,113	1.22	9 (11%)
19	CLA	a	403	-	65,73,73	1.53	8 (12%)	76,113,113	1.28	9 (11%)
23	LHG	B	520	-	43,43,48	0.99	2 (4%)	46,49,54	0.93	2 (4%)
25	DGD	c	519	-	54,54,67	0.93	2 (3%)	68,68,81	0.98	3 (4%)
19	CLA	C	512	3	65,73,73	1.53	6 (9%)	76,113,113	1.19	8 (10%)
19	CLA	B	502	-	65,73,73	1.50	6 (9%)	76,113,113	1.25	8 (10%)
19	CLA	c	510	-	65,73,73	1.50	8 (12%)	76,113,113	1.19	7 (9%)
19	CLA	B	514	-	45,53,73	1.76	6 (13%)	52,89,113	1.46	7 (13%)
21	BCR	d	405	-	41,41,41	0.76	0	56,56,56	1.98	17 (30%)
19	CLA	d	403	-	65,73,73	1.50	8 (12%)	76,113,113	1.22	7 (9%)
29	HEM	e	101	5,6	41,50,50	1.49	3 (7%)	45,82,82	1.38	5 (11%)
21	BCR	c	516	-	41,41,41	0.79	1 (2%)	56,56,56	1.93	19 (33%)
22	LMG	f	101	-	46,46,55	0.97	2 (4%)	54,54,63	0.94	2 (3%)
19	CLA	b	512	-	65,73,73	1.47	7 (10%)	76,113,113	1.30	8 (10%)
19	CLA	B	515	-	65,73,73	1.50	8 (12%)	76,113,113	1.23	9 (11%)
19	CLA	c	505	-	65,73,73	1.51	7 (10%)	76,113,113	1.23	9 (11%)
23	LHG	d	407	-	43,43,48	0.99	2 (4%)	46,49,54	0.93	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	505	-	65,73,73	1.53	8 (12%)	76,113,113	1.15	6 (7%)
21	BCR	W	101	-	41,41,41	0.84	2 (4%)	56,56,56	2.30	20 (35%)
25	DGD	c	521	-	60,60,67	0.89	2 (3%)	74,74,81	0.87	2 (2%)
22	LMG	A	408	-	46,46,55	0.99	3 (6%)	54,54,63	1.03	3 (5%)
22	LMG	b	519	-	42,42,55	0.99	2 (4%)	50,50,63	1.03	3 (6%)
21	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	2.04	19 (33%)
19	CLA	b	506	-	65,73,73	1.50	7 (10%)	76,113,113	1.19	8 (10%)
20	PHO	A	405	-	51,69,69	1.03	5 (9%)	47,99,99	1.21	6 (12%)
21	BCR	D	405	-	41,41,41	0.77	0	56,56,56	1.98	17 (30%)
19	CLA	D	404	-	65,73,73	1.50	7 (10%)	76,113,113	1.24	7 (9%)
19	CLA	c	503	-	65,73,73	1.51	7 (10%)	76,113,113	1.19	8 (10%)
21	BCR	C	517	-	41,41,41	0.75	1 (2%)	56,56,56	1.93	17 (30%)
22	LMG	c	502	-	46,46,55	0.99	2 (4%)	54,54,63	1.02	3 (5%)
21	BCR	H	101	-	41,41,41	0.69	0	56,56,56	2.10	23 (41%)
21	BCR	c	517	-	41,41,41	0.81	1 (2%)	56,56,56	1.84	16 (28%)
19	CLA	A	404	-	49,57,73	1.72	8 (16%)	55,93,113	1.41	9 (16%)
22	LMG	c	522	-	51,51,55	0.93	2 (3%)	59,59,63	0.88	2 (3%)
19	CLA	c	509	-	65,73,73	1.47	7 (10%)	76,113,113	1.25	8 (10%)
19	CLA	c	513	3	65,73,73	1.52	6 (9%)	76,113,113	1.19	7 (9%)
27	BCT	d	402	18	2,3,3	1.27	0	2,3,3	4.13	2 (100%)
21	BCR	c	518	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
19	CLA	C	508	-	65,73,73	1.47	7 (10%)	76,113,113	1.25	8 (10%)
19	CLA	B	513	-	65,73,73	1.48	8 (12%)	76,113,113	1.25	8 (10%)
19	CLA	b	505	-	65,73,73	1.50	8 (12%)	76,113,113	1.17	8 (10%)
21	BCR	k	101	-	41,41,41	0.70	0	56,56,56	1.91	20 (35%)
20	PHO	D	401	-	51,69,69	1.03	5 (9%)	47,99,99	1.09	4 (8%)
19	CLA	b	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.28	8 (10%)
19	CLA	b	507	-	65,73,73	1.52	7 (10%)	76,113,113	1.26	8 (10%)
19	CLA	b	508	-	65,73,73	1.50	7 (10%)	76,113,113	1.22	8 (10%)
23	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.98	2 (3%)
23	LHG	A	409	-	42,42,48	0.98	2 (4%)	45,48,54	1.02	2 (4%)
22	LMG	F	101	-	46,46,55	0.97	2 (4%)	54,54,63	0.96	2 (3%)
19	CLA	D	403	-	65,73,73	1.49	8 (12%)	76,113,113	1.23	6 (7%)
22	LMG	h	102	-	48,48,55	0.96	2 (4%)	56,56,63	1.04	2 (3%)
19	CLA	B	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.22	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	c	512	-	65,73,73	1.51	9 (13%)	76,113,113	1.23	7 (9%)
23	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	0.89	2 (3%)
23	LHG	X	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.02	3 (5%)
19	CLA	A	406	-	60,68,73	1.55	7 (11%)	70,107,113	1.28	9 (12%)
23	LHG	A	410	-	43,43,48	1.00	2 (4%)	46,49,54	0.93	2 (4%)
21	BCR	w	101	-	41,41,41	0.84	1 (2%)	56,56,56	2.24	18 (32%)
19	CLA	B	507	-	65,73,73	1.51	7 (10%)	76,113,113	1.26	8 (10%)
23	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	0.89	2 (3%)
19	CLA	c	506	-	65,73,73	1.49	7 (10%)	76,113,113	1.23	7 (9%)
22	LMG	B	519	-	42,42,55	0.99	2 (4%)	50,50,63	1.03	3 (6%)
23	LHG	a	409	-	43,43,48	1.00	2 (4%)	46,49,54	0.93	2 (4%)
19	CLA	C	504	-	65,73,73	1.51	7 (10%)	76,113,113	1.22	9 (11%)
19	CLA	C	513	-	65,73,73	1.50	7 (10%)	76,113,113	1.28	7 (9%)
21	BCR	B	517	-	41,41,41	0.76	1 (2%)	56,56,56	2.05	20 (35%)
19	CLA	C	503	-	65,73,73	1.48	9 (13%)	76,113,113	1.29	9 (11%)
19	CLA	C	507	-	65,73,73	1.51	6 (9%)	76,113,113	1.23	7 (9%)
19	CLA	C	510	-	65,73,73	1.49	7 (10%)	76,113,113	1.26	7 (9%)
20	PHO	d	401	-	51,69,69	1.03	5 (9%)	47,99,99	1.10	4 (8%)
19	CLA	C	514	-	65,73,73	1.50	5 (7%)	76,113,113	1.21	7 (9%)
25	DGD	C	518	-	54,54,67	0.93	2 (3%)	68,68,81	0.97	3 (4%)
19	CLA	A	403	-	65,73,73	1.53	8 (12%)	76,113,113	1.29	9 (11%)

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
19	CLA	c	504	-	1/1/15/20	19/37/115/115	-
19	CLA	c	508	-	1/1/15/20	17/37/115/115	-
21	BCR	a	407	-	-	4/29/63/63	0/2/2/2
19	CLA	B	503	-	1/1/15/20	14/37/115/115	-
19	CLA	c	511	-	1/1/15/20	15/37/115/115	-
19	CLA	C	509	-	1/1/15/20	12/37/115/115	-
19	CLA	c	514	-	1/1/15/20	14/37/115/115	-
25	DGD	C	520	-	-	10/48/88/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	C	502	-	1/1/15/20	11/37/115/115	-
19	CLA	b	509	-	1/1/15/20	18/37/115/115	-
19	CLA	b	511	-	1/1/15/20	21/37/115/115	-
19	CLA	b	513	-	1/1/15/20	14/37/115/115	-
19	CLA	c	515	-	1/1/15/20	15/37/115/115	-
22	LMG	H	102	-	-	12/43/63/70	0/1/1/1
28	PL9	d	406	-	-	7/53/73/73	0/1/1/1
19	CLA	B	510	-	1/1/15/20	9/37/115/115	-
19	CLA	d	404	-	1/1/15/20	20/37/115/115	-
21	BCR	V	101	-	-	2/29/63/63	0/2/2/2
19	CLA	b	514	-	1/1/11/20	7/13/91/115	-
23	LHG	a	408	-	-	11/47/47/53	-
19	CLA	B	516	-	1/1/15/20	10/37/115/115	-
19	CLA	C	505	-	1/1/15/20	12/37/115/115	-
26	LMU	c	523	-	-	8/21/61/61	0/2/2/2
19	CLA	A	402	-	1/1/15/20	8/37/115/115	-
19	CLA	B	512	-	1/1/15/20	12/37/115/115	-
19	CLA	a	402	-	1/1/15/20	10/37/115/115	-
25	DGD	C	519	-	-	7/38/78/95	0/2/2/2
24	SQD	C	501	-	-	9/46/66/69	0/1/1/1
20	PHO	a	405	-	-	12/37/103/103	0/5/6/6
19	CLA	a	404	-	1/1/11/20	9/18/96/115	-
23	LHG	B	521	-	-	10/53/53/53	-
21	BCR	C	516	-	-	5/29/63/63	0/2/2/2
22	LMG	C	521	-	-	5/46/66/70	0/1/1/1
19	CLA	B	506	-	1/1/15/20	8/37/115/115	-
21	BCR	h	101	-	-	5/29/63/63	0/2/2/2
23	LHG	x	101	-	-	11/53/53/53	-
21	BCR	A	407	-	-	4/29/63/63	0/2/2/2
29	HEM	F	102	5,6	-	4/12/54/54	-
25	DGD	c	520	-	-	7/38/78/95	0/2/2/2
19	CLA	C	506	-	1/1/15/20	15/37/115/115	-
23	LHG	D	407	-	-	12/53/53/53	-
19	CLA	c	507	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	503	-	1/1/15/20	13/37/115/115	-
19	CLA	b	516	-	1/1/15/20	11/37/115/115	-
19	CLA	a	406	-	1/1/14/20	9/31/109/115	-
21	BCR	b	518	-	-	4/29/63/63	0/2/2/2
19	CLA	b	501	-	1/1/15/20	15/37/115/115	-
24	SQD	c	501	-	-	9/46/66/69	0/1/1/1
23	LHG	b	520	-	-	10/53/53/53	-
21	BCR	B	518	-	-	4/29/63/63	0/2/2/2
21	BCR	b	517	-	-	4/29/63/63	0/2/2/2
19	CLA	b	502	-	1/1/15/20	10/37/115/115	-
28	PL9	D	406	-	-	8/53/73/73	0/1/1/1
26	LMU	C	522	-	-	9/21/61/61	0/2/2/2
19	CLA	B	509	-	1/1/15/20	18/37/115/115	-
19	CLA	b	510	-	1/1/15/20	10/37/115/115	-
19	CLA	C	511	-	1/1/15/20	14/37/115/115	-
19	CLA	B	504	-	1/1/15/20	15/37/115/115	-
19	CLA	B	508	-	1/1/15/20	9/37/115/115	-
19	CLA	B	501	-	1/1/15/20	16/37/115/115	-
19	CLA	b	515	-	1/1/15/20	5/37/115/115	-
19	CLA	a	403	-	1/1/15/20	10/37/115/115	-
23	LHG	B	520	-	-	11/48/48/53	-
25	DGD	c	519	-	-	5/42/82/95	0/2/2/2
19	CLA	C	512	3	1/1/15/20	17/37/115/115	-
19	CLA	B	502	-	1/1/15/20	10/37/115/115	-
19	CLA	c	510	-	1/1/15/20	12/37/115/115	-
19	CLA	B	514	-	1/1/11/20	7/13/91/115	-
21	BCR	d	405	-	-	4/29/63/63	0/2/2/2
19	CLA	d	403	-	1/1/15/20	7/37/115/115	-
29	HEM	e	101	5,6	-	3/12/54/54	-
21	BCR	c	516	-	-	4/29/63/63	0/2/2/2
22	LMG	f	101	-	-	5/41/61/70	0/1/1/1
19	CLA	b	512	-	1/1/15/20	12/37/115/115	-
19	CLA	B	515	-	1/1/15/20	4/37/115/115	-
19	CLA	c	505	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	d	407	-	-	11/48/48/53	-
19	CLA	B	505	-	-	19/37/115/115	-
21	BCR	W	101	-	-	2/29/63/63	0/2/2/2
25	DGD	c	521	-	-	9/48/88/95	0/2/2/2
22	LMG	A	408	-	-	7/41/61/70	0/1/1/1
22	LMG	b	519	-	-	4/37/57/70	0/1/1/1
21	BCR	C	515	-	-	4/29/63/63	0/2/2/2
19	CLA	b	506	-	1/1/15/20	11/37/115/115	-
20	PHO	A	405	-	-	12/37/103/103	0/5/6/6
21	BCR	D	405	-	-	4/29/63/63	0/2/2/2
19	CLA	D	404	-	1/1/15/20	20/37/115/115	-
19	CLA	c	503	-	1/1/15/20	12/37/115/115	-
21	BCR	C	517	-	-	4/29/63/63	0/2/2/2
22	LMG	c	502	-	-	7/41/61/70	0/1/1/1
21	BCR	H	101	-	-	5/29/63/63	0/2/2/2
21	BCR	c	517	-	-	5/29/63/63	0/2/2/2
19	CLA	A	404	-	1/1/11/20	7/18/96/115	-
22	LMG	c	522	-	-	4/46/66/70	0/1/1/1
19	CLA	c	509	-	1/1/15/20	7/37/115/115	-
19	CLA	c	513	3	1/1/15/20	11/37/115/115	-
21	BCR	c	518	-	-	4/29/63/63	0/2/2/2
19	CLA	C	508	-	1/1/15/20	7/37/115/115	-
19	CLA	B	513	-	1/1/15/20	14/37/115/115	-
19	CLA	b	505	-	1/1/15/20	19/37/115/115	-
21	BCR	k	101	-	-	2/29/63/63	0/2/2/2
20	PHO	D	401	-	-	9/37/103/103	0/5/6/6
19	CLA	b	504	-	1/1/15/20	15/37/115/115	-
19	CLA	b	507	-	1/1/15/20	15/37/115/115	-
19	CLA	b	508	-	1/1/15/20	8/37/115/115	-
23	LHG	d	408	-	-	9/53/53/53	-
23	LHG	A	409	-	-	6/47/47/53	-
22	LMG	F	101	-	-	5/41/61/70	0/1/1/1
19	CLA	D	403	-	1/1/15/20	8/37/115/115	-
22	LMG	h	102	-	-	10/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	511	-	1/1/15/20	21/37/115/115	-
19	CLA	c	512	-	1/1/15/20	14/37/115/115	-
23	LHG	L	101	-	-	9/53/53/53	-
23	LHG	X	101	-	-	9/53/53/53	-
19	CLA	A	406	-	1/1/14/20	9/31/109/115	-
23	LHG	A	410	-	-	13/48/48/53	-
21	BCR	w	101	-	-	10/29/63/63	0/2/2/2
19	CLA	B	507	-	1/1/15/20	14/37/115/115	-
23	LHG	l	101	-	-	8/53/53/53	-
19	CLA	c	506	-	1/1/15/20	11/37/115/115	-
22	LMG	B	519	-	-	4/37/57/70	0/1/1/1
23	LHG	a	409	-	-	14/48/48/53	-
19	CLA	C	504	-	1/1/15/20	18/37/115/115	-
19	CLA	C	513	-	1/1/15/20	14/37/115/115	-
21	BCR	B	517	-	-	4/29/63/63	0/2/2/2
19	CLA	C	503	-	1/1/15/20	18/37/115/115	-
19	CLA	C	507	-	1/1/15/20	16/37/115/115	-
19	CLA	C	510	-	1/1/15/20	15/37/115/115	-
20	PHO	d	401	-	-	9/37/103/103	0/5/6/6
19	CLA	C	514	-	1/1/15/20	14/37/115/115	-
25	DGD	C	518	-	-	3/42/82/95	0/2/2/2
19	CLA	A	403	-	1/1/15/20	13/37/115/115	-

The worst 5 of 626 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	403	CLA	C4B-NB	7.68	1.42	1.35
19	B	501	CLA	C4B-NB	7.68	1.42	1.35
19	A	403	CLA	C4B-NB	7.66	1.42	1.35
19	b	501	CLA	C4B-NB	7.66	1.42	1.35
19	C	512	CLA	C4B-NB	7.65	1.42	1.35

The worst 5 of 1074 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	w	101	BCR	C7-C8-C9	-5.78	117.49	126.23
19	B	512	CLA	C4A-NA-C1A	5.78	109.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	101	BCR	C38-C26-C25	-5.69	118.13	124.53
19	b	512	CLA	C4A-NA-C1A	5.63	109.24	106.71
19	C	503	CLA	C4A-NA-C1A	5.48	109.17	106.71

5 of 69 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	402	CLA	ND
19	A	403	CLA	ND
19	A	404	CLA	ND
19	A	406	CLA	ND
19	B	501	CLA	ND

5 of 1327 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	403	CLA	C3A-C2A-CAA-CBA
19	A	406	CLA	C1A-C2A-CAA-CBA
19	A	406	CLA	C3A-C2A-CAA-CBA
19	B	501	CLA	C1A-C2A-CAA-CBA
19	B	501	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

78 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	c	504	CLA	2	0
19	c	508	CLA	2	0
21	a	407	BCR	5	0
19	C	509	CLA	1	0
19	C	502	CLA	3	0
19	b	513	CLA	2	0
19	c	515	CLA	1	0
22	H	102	LMG	2	0
28	d	406	PL9	1	0
19	d	404	CLA	2	0
21	V	101	BCR	4	0
19	B	516	CLA	1	0
19	C	505	CLA	1	0
27	D	402	BCT	1	0
19	B	512	CLA	1	0
19	a	402	CLA	1	0

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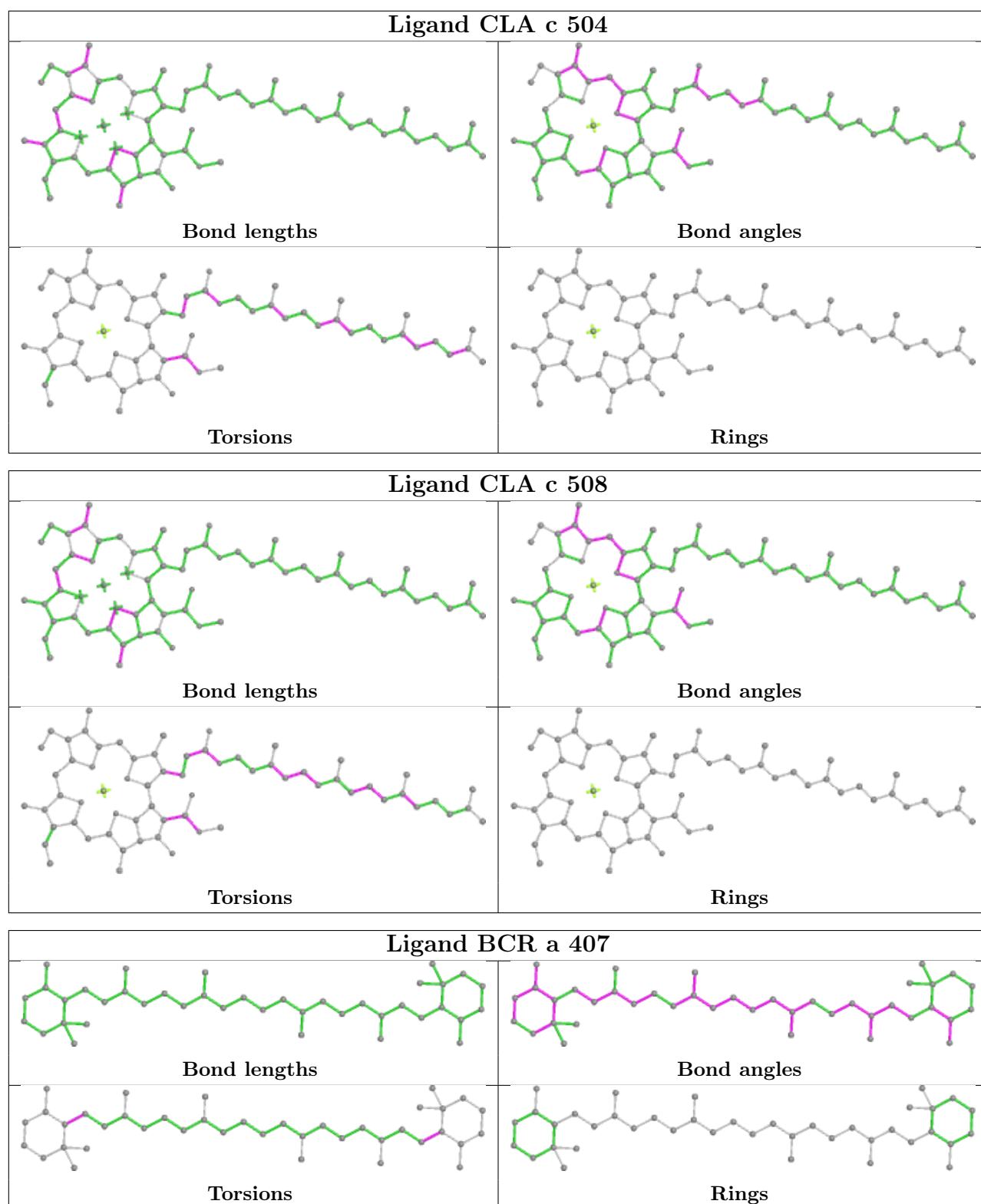
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	404	CLA	2	0
23	B	521	LHG	1	0
21	C	516	BCR	8	0
19	B	506	CLA	3	0
21	h	101	BCR	6	0
21	A	407	BCR	9	0
29	F	102	HEM	6	0
23	D	407	LHG	1	0
19	b	516	CLA	1	0
21	b	518	BCR	4	0
19	b	501	CLA	1	0
23	b	520	LHG	1	0
21	B	518	BCR	3	0
21	b	517	BCR	6	0
19	b	502	CLA	3	0
19	B	509	CLA	2	0
19	B	504	CLA	2	0
19	B	501	CLA	1	0
19	b	515	CLA	1	0
19	a	403	CLA	1	0
19	C	512	CLA	5	0
19	B	502	CLA	3	0
19	c	510	CLA	1	0
21	d	405	BCR	1	0
19	d	403	CLA	3	0
29	e	101	HEM	5	0
21	c	516	BCR	6	0
19	b	512	CLA	1	0
19	B	505	CLA	1	0
21	W	101	BCR	8	0
21	C	515	BCR	6	0
19	b	506	CLA	1	0
20	A	405	PHO	1	0
21	D	405	BCR	1	0
19	D	404	CLA	1	0
19	c	503	CLA	2	0
21	C	517	BCR	7	0
21	H	101	BCR	7	0
21	c	517	BCR	7	0
19	c	513	CLA	4	0
27	d	402	BCT	1	0
21	c	518	BCR	5	0

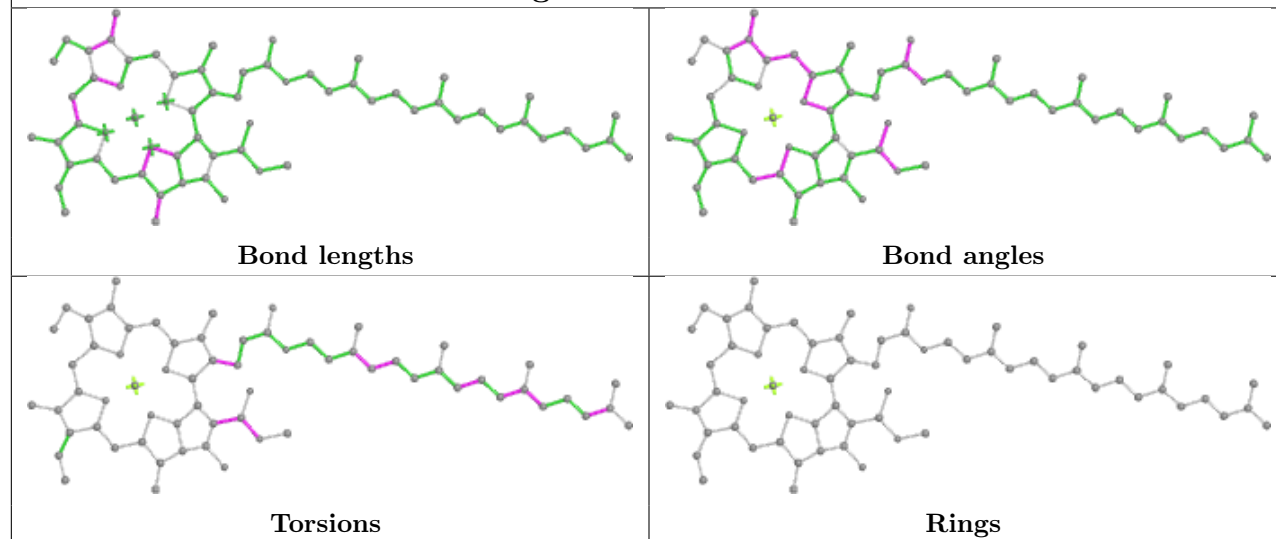
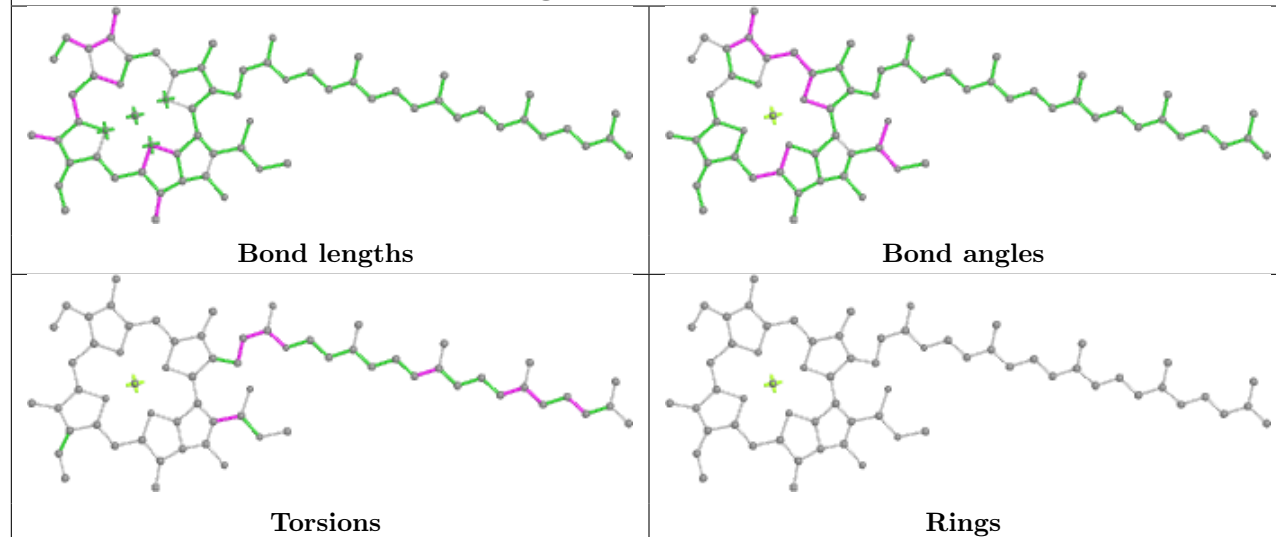
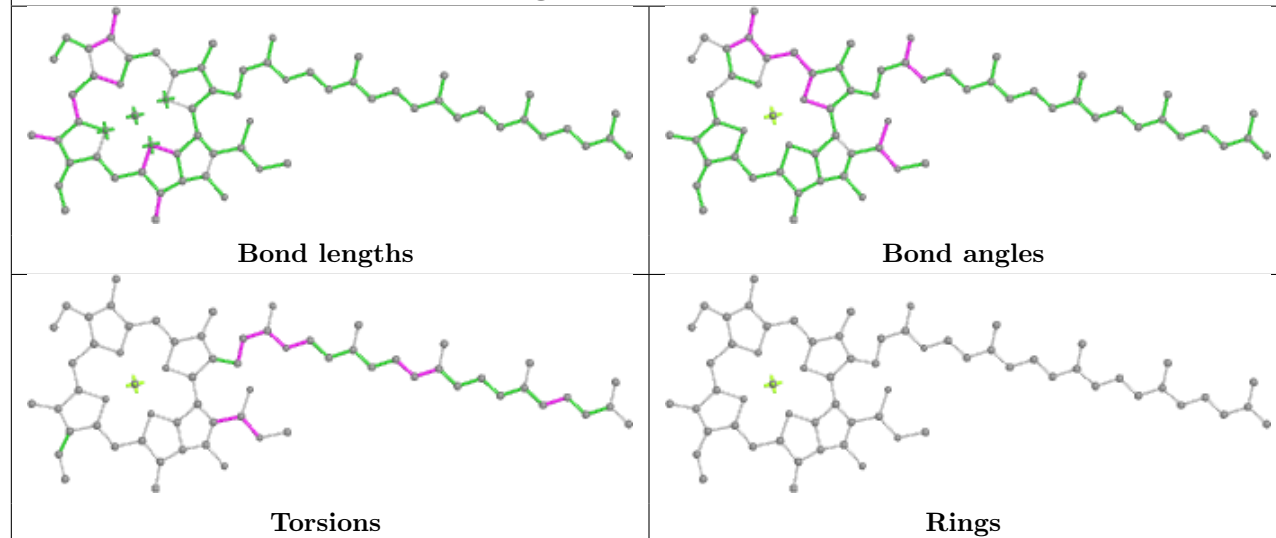
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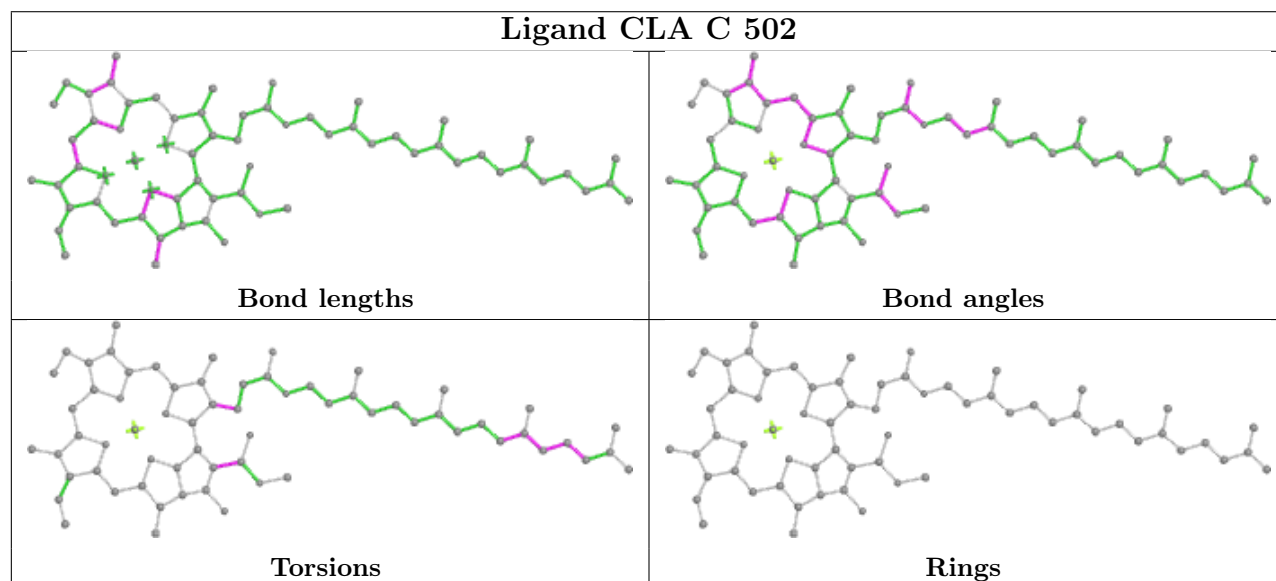
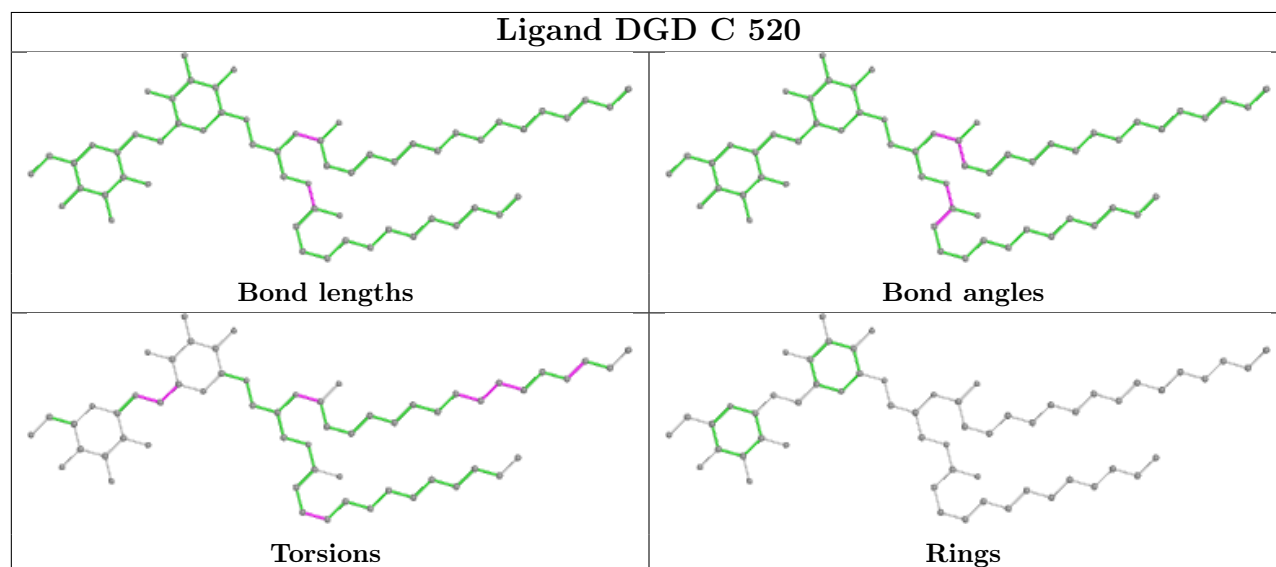
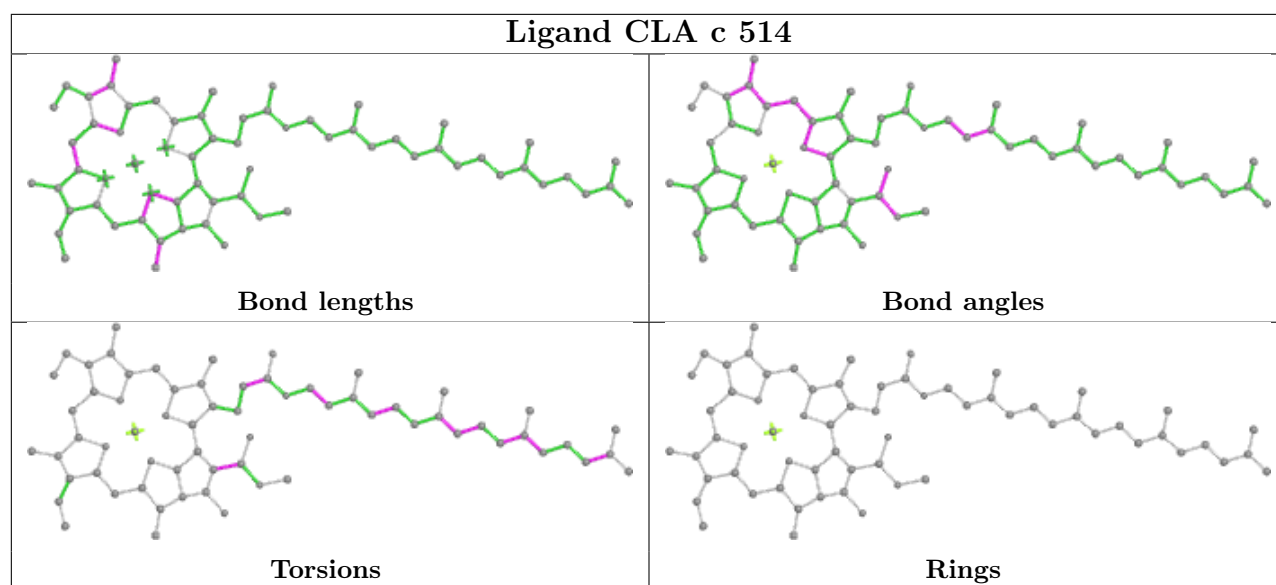
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	513	CLA	4	0
21	k	101	BCR	2	0
20	D	401	PHO	2	0
19	b	504	CLA	2	0
19	b	507	CLA	1	0
23	d	408	LHG	1	0
23	A	409	LHG	1	0
19	D	403	CLA	5	0
22	h	102	LMG	1	0
19	c	512	CLA	1	0
21	w	101	BCR	7	0
19	B	507	CLA	1	0
19	c	506	CLA	1	0
21	B	517	BCR	4	0
19	C	503	CLA	1	0
19	C	507	CLA	1	0
19	C	510	CLA	1	0
20	d	401	PHO	1	0
19	C	514	CLA	1	0
25	C	518	DGD	1	0

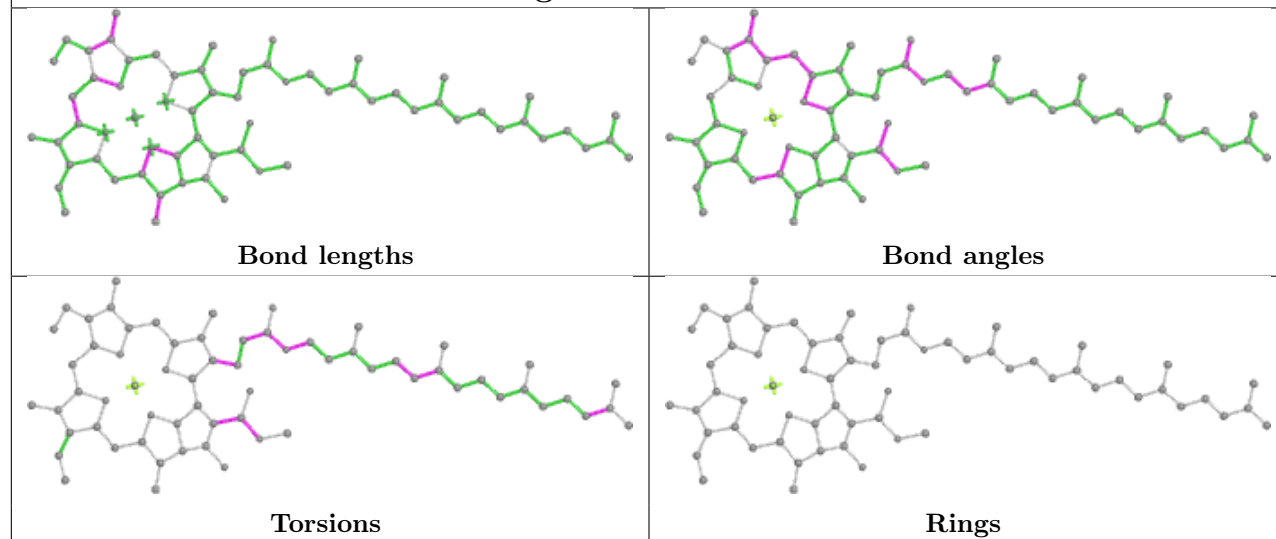
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



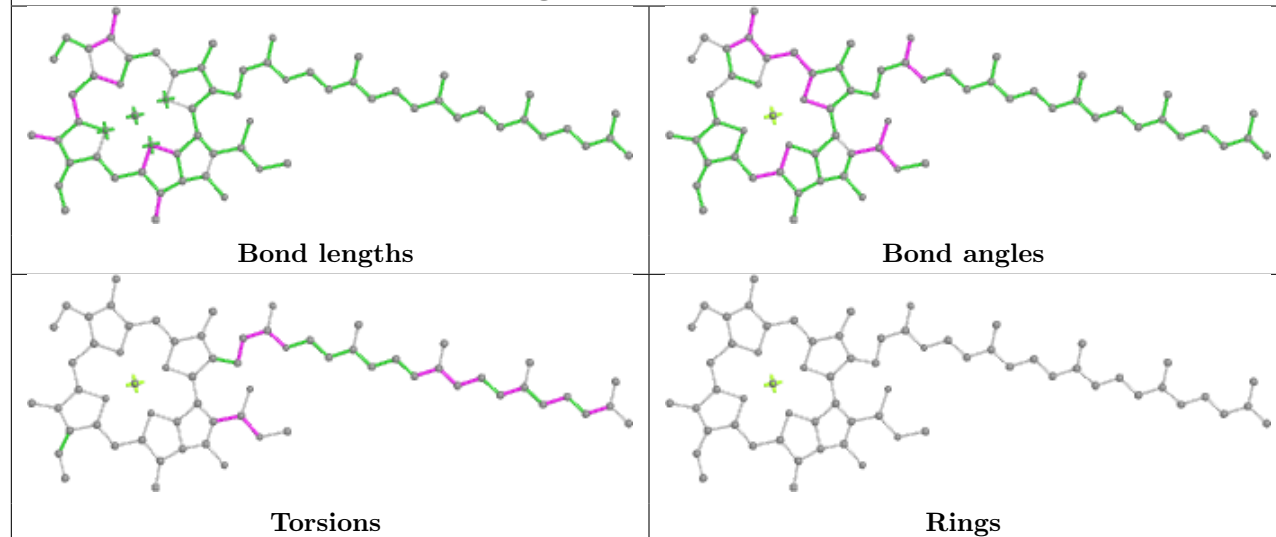
Ligand CLA B 503**Ligand CLA c 511****Ligand CLA C 509**



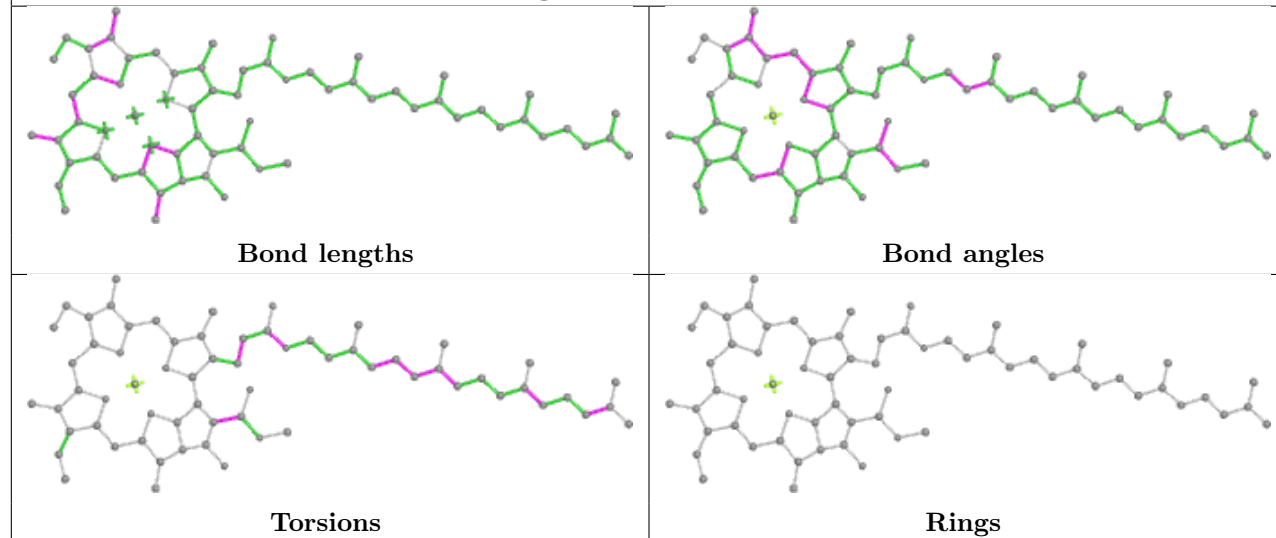
Ligand CLA b 509

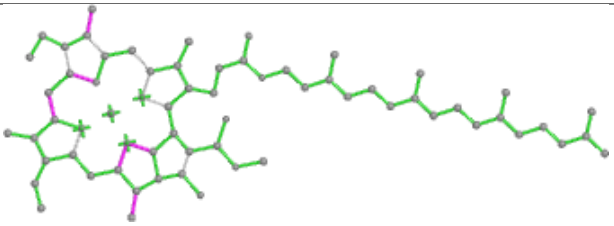
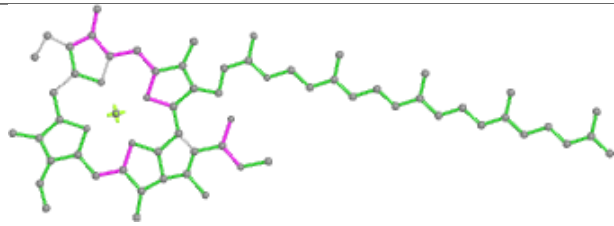
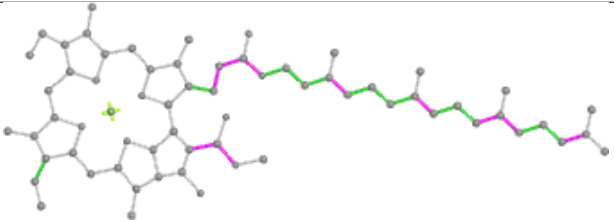
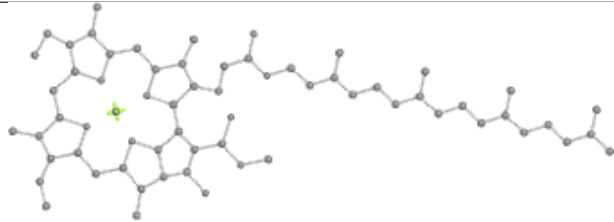


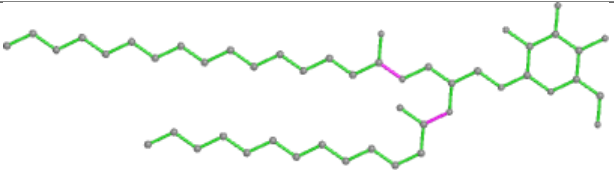
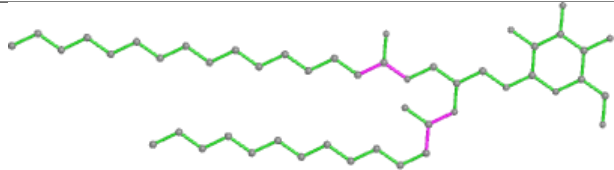
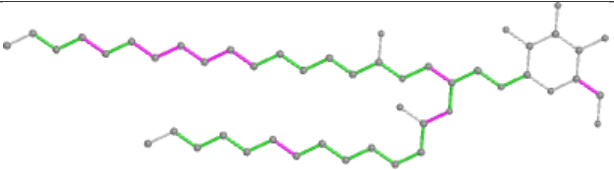
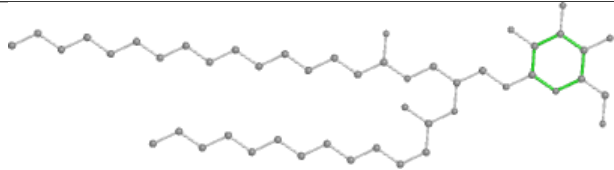
Ligand CLA b 511

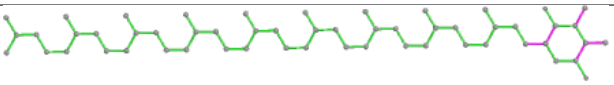
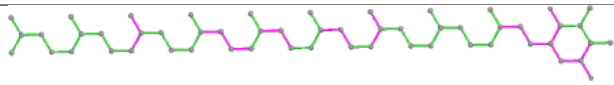
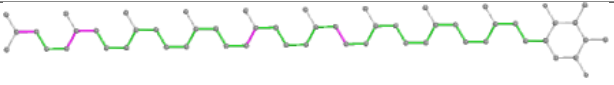
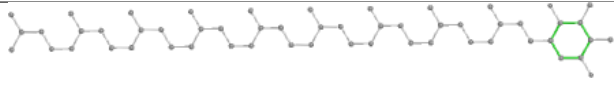


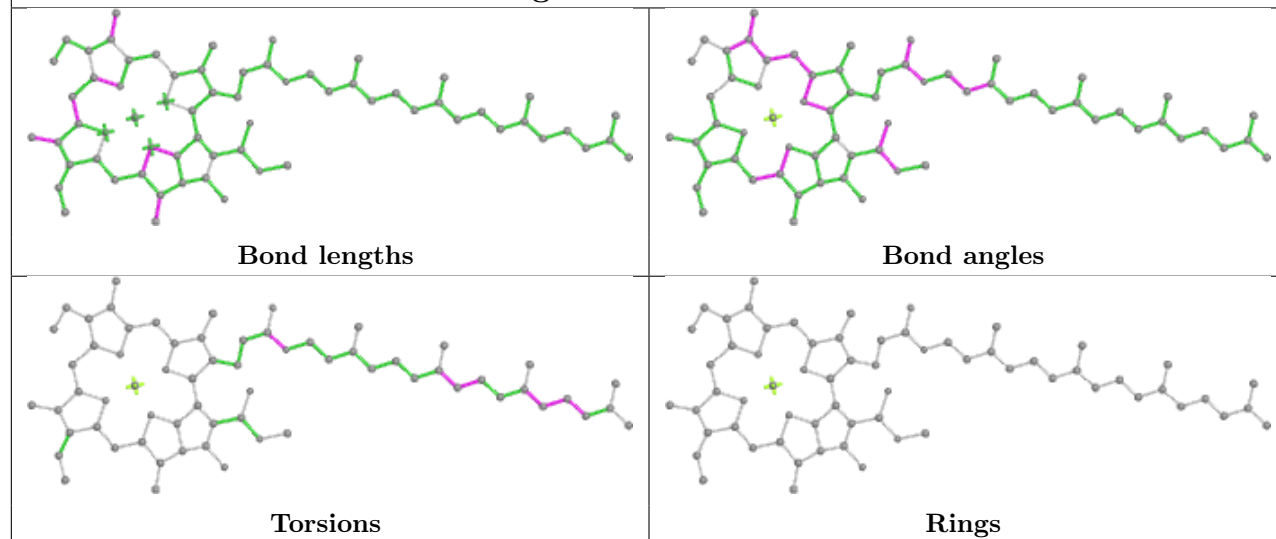
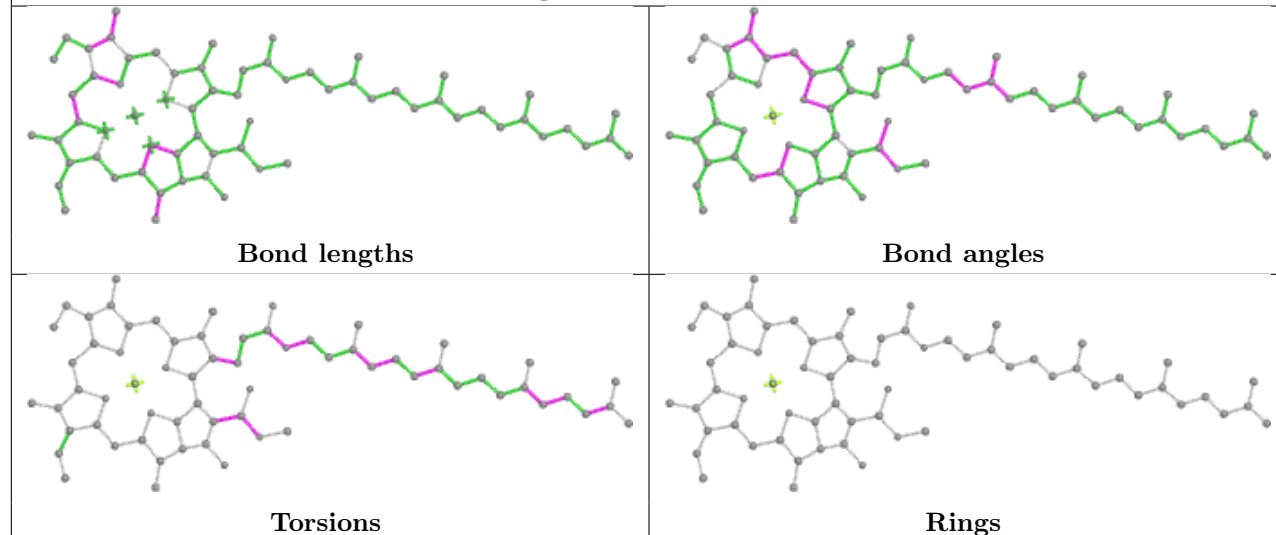
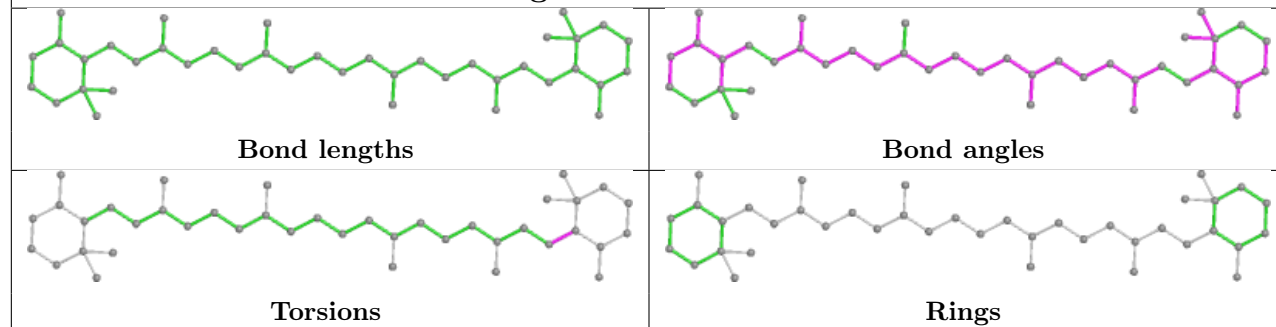
Ligand CLA b 513



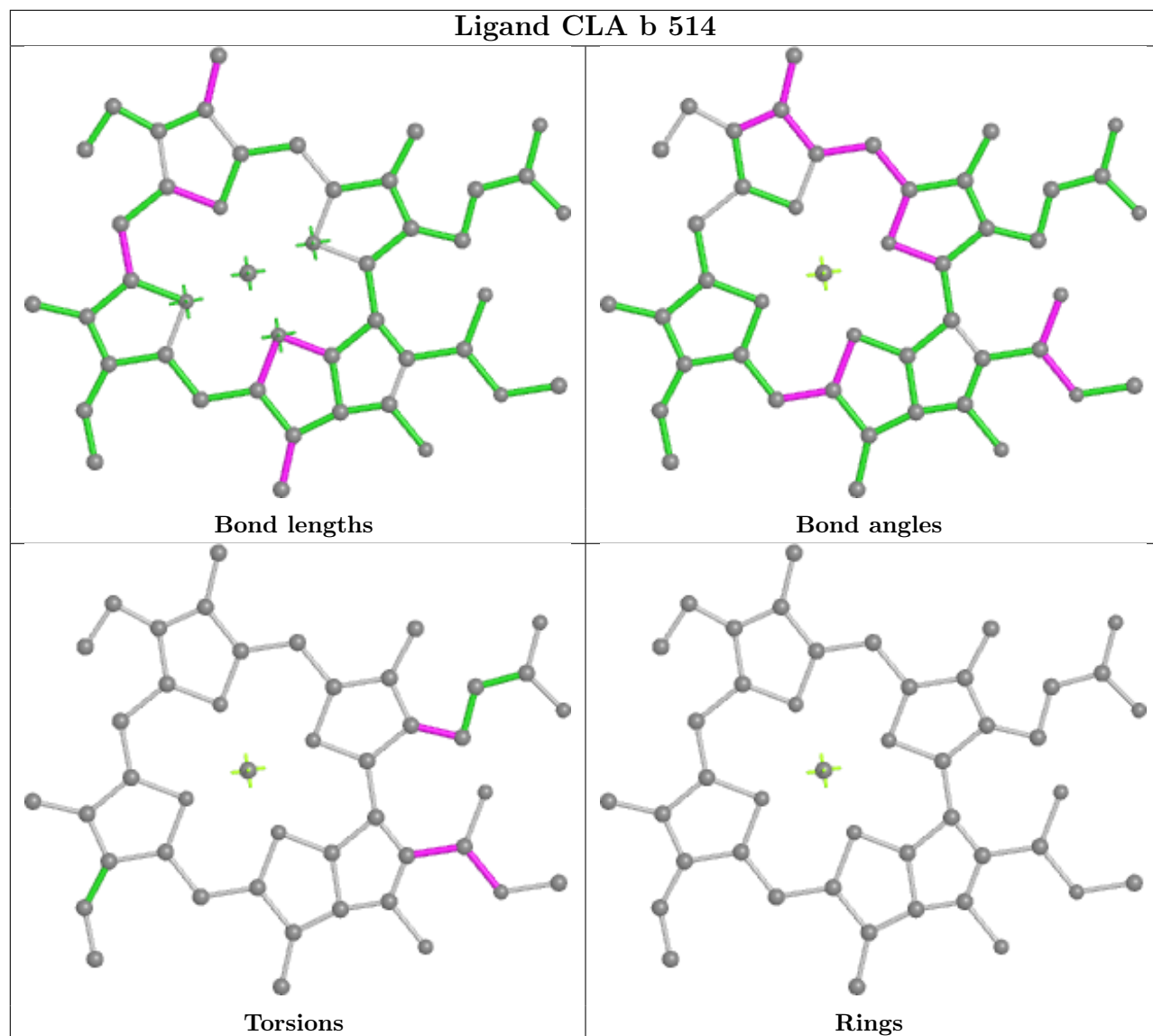
Ligand CLA c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

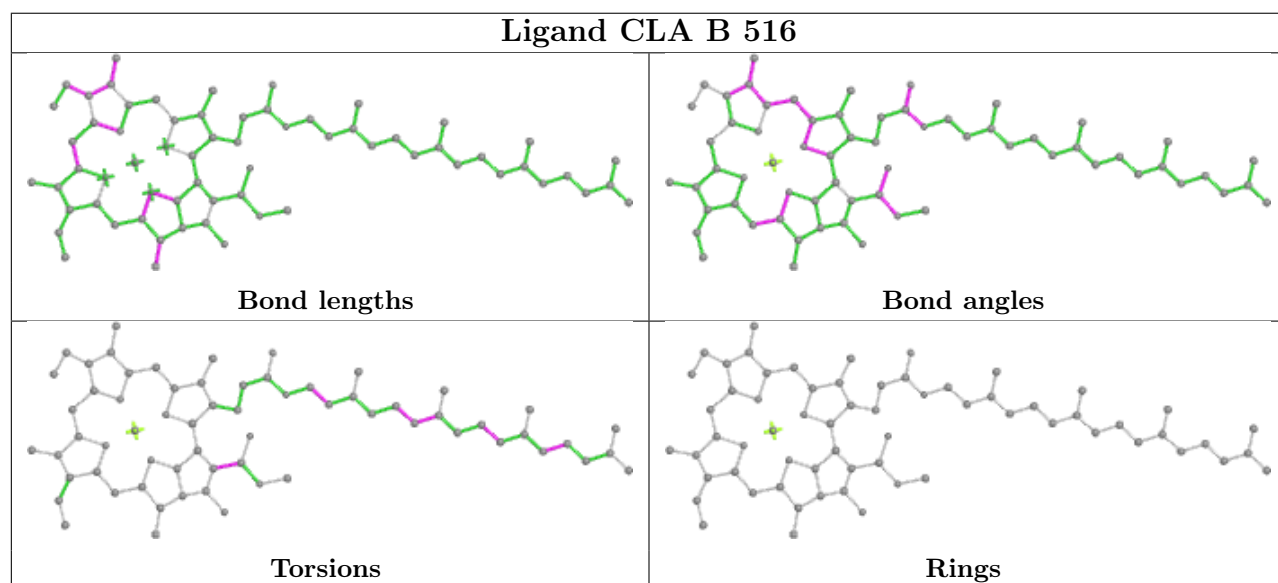
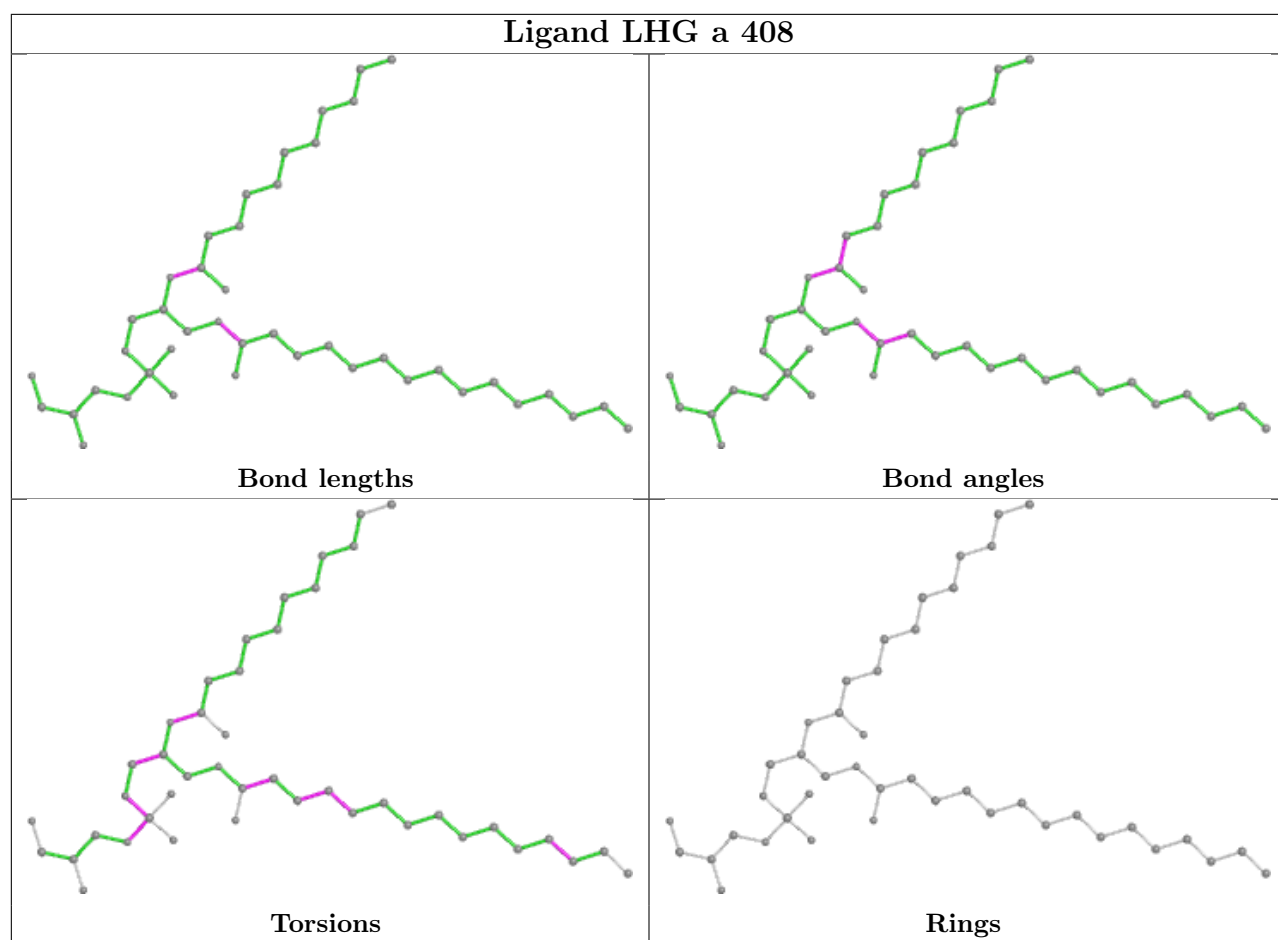
Ligand LMG H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

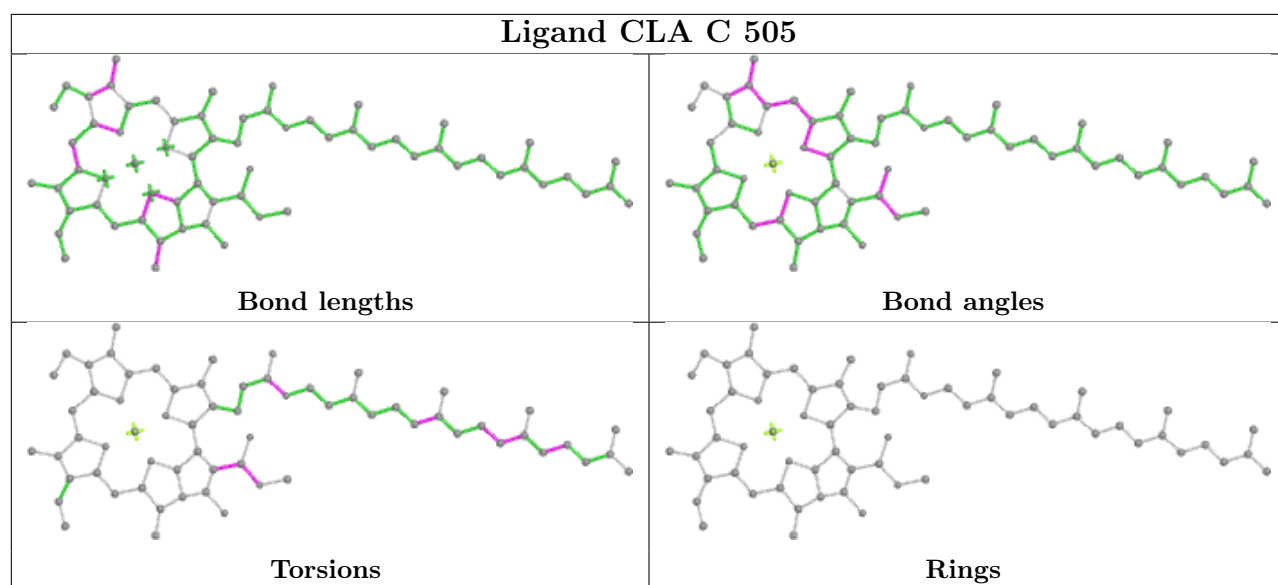
Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

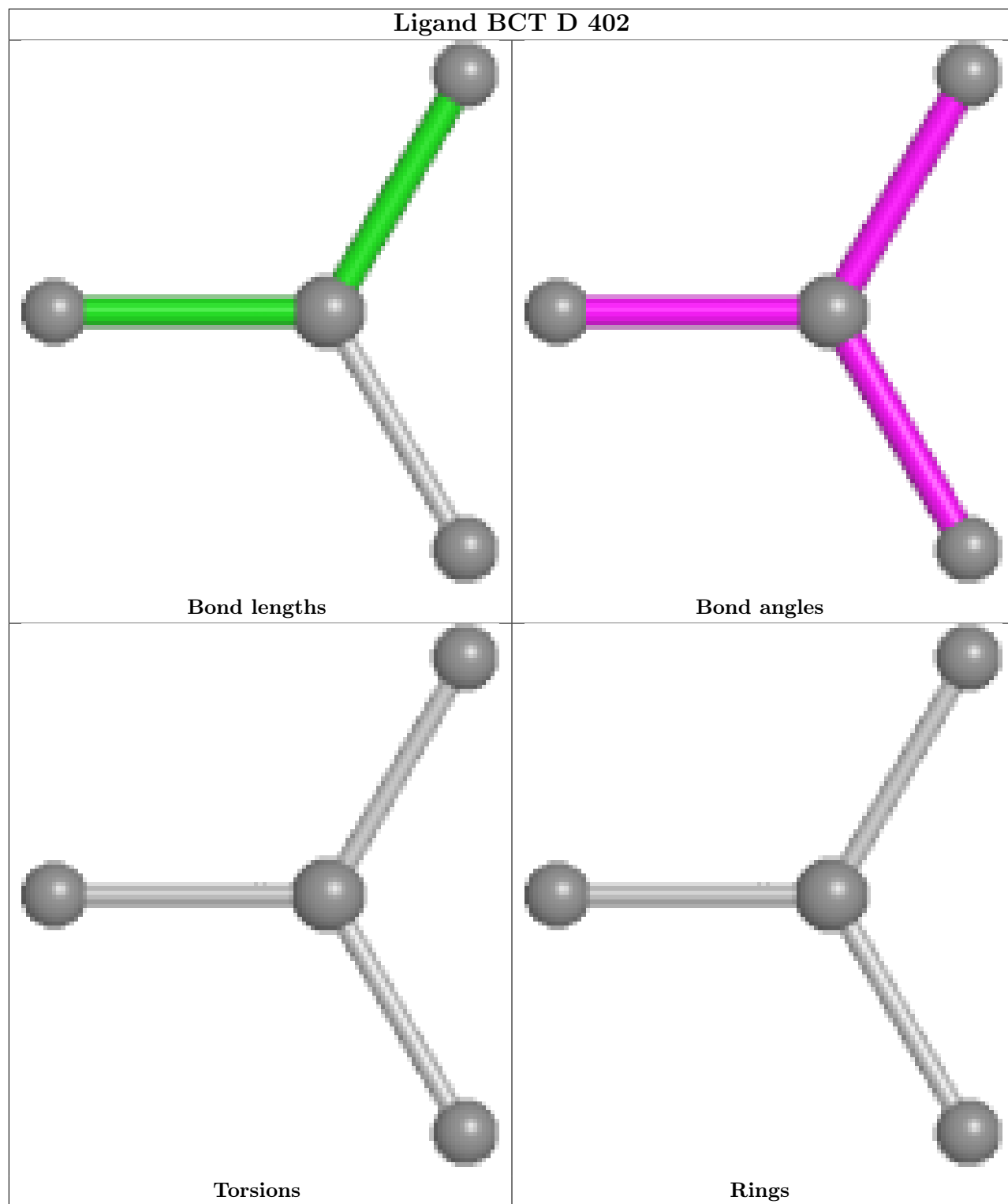
Ligand CLA B 510**Ligand CLA d 404****Ligand BCR V 101**

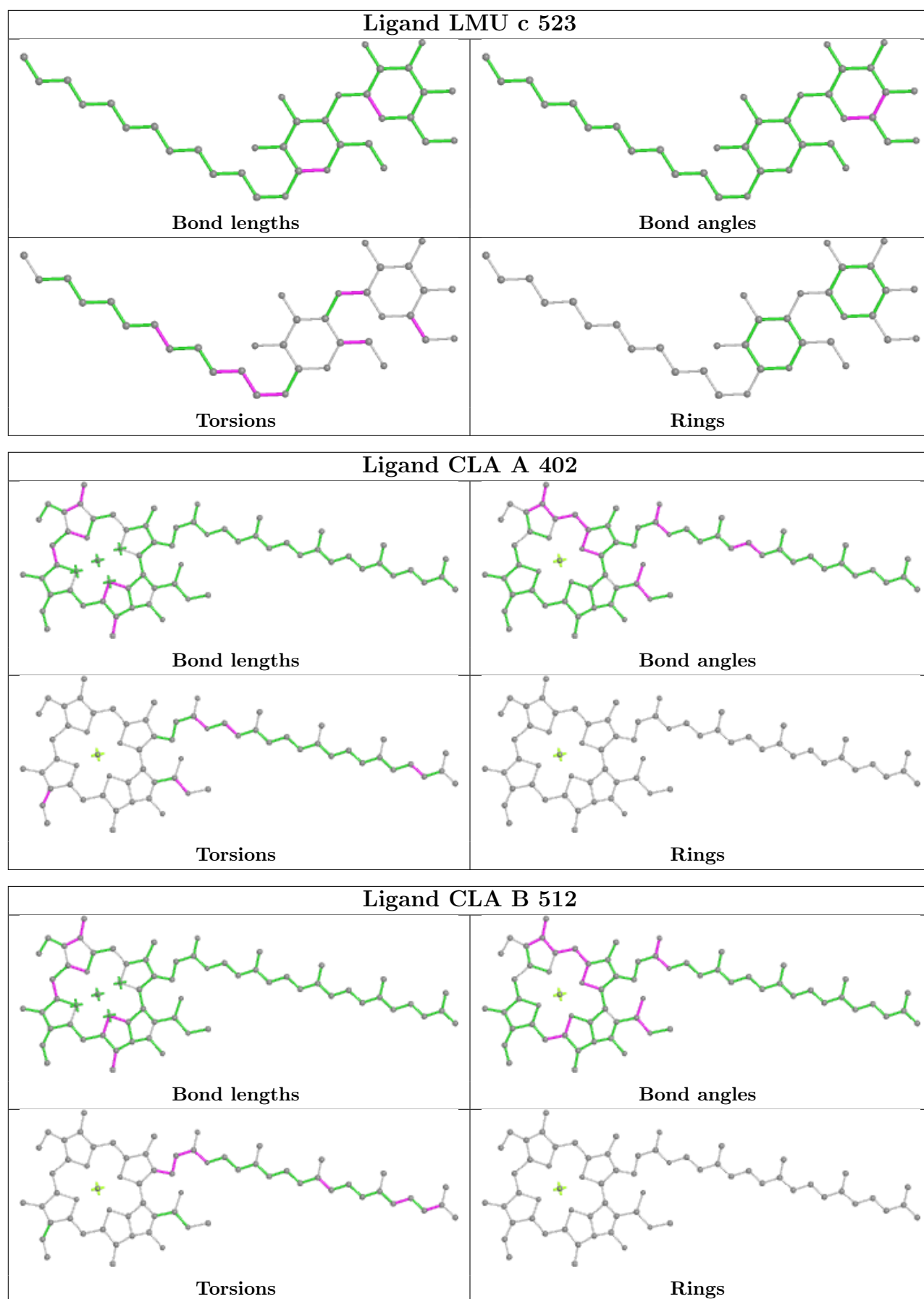
Ligand CLA b 514

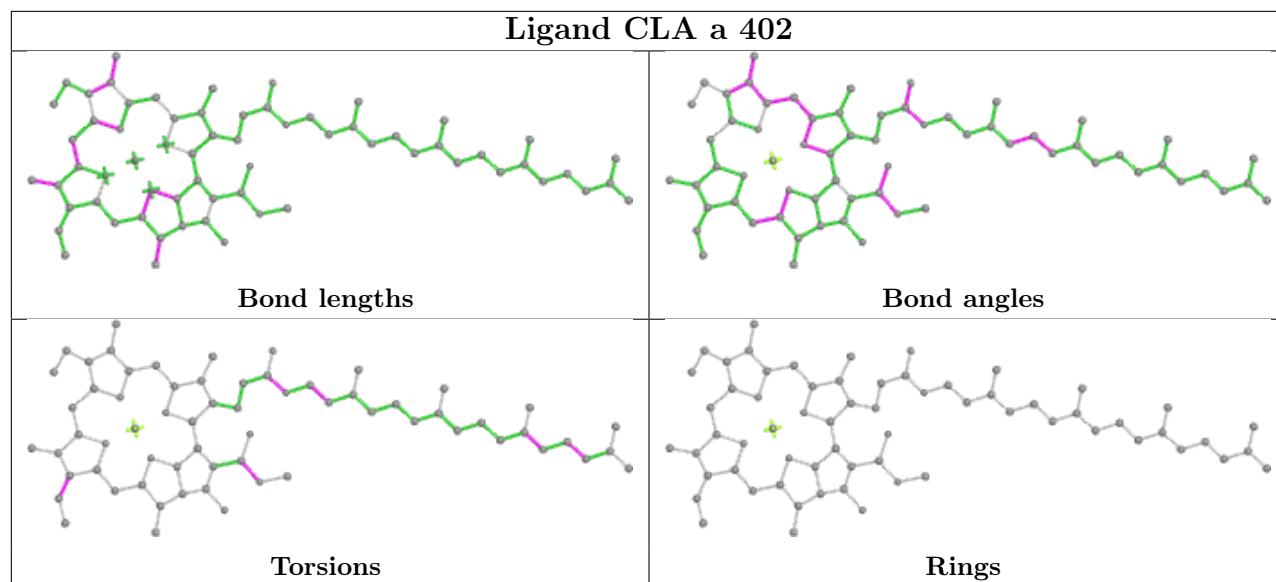
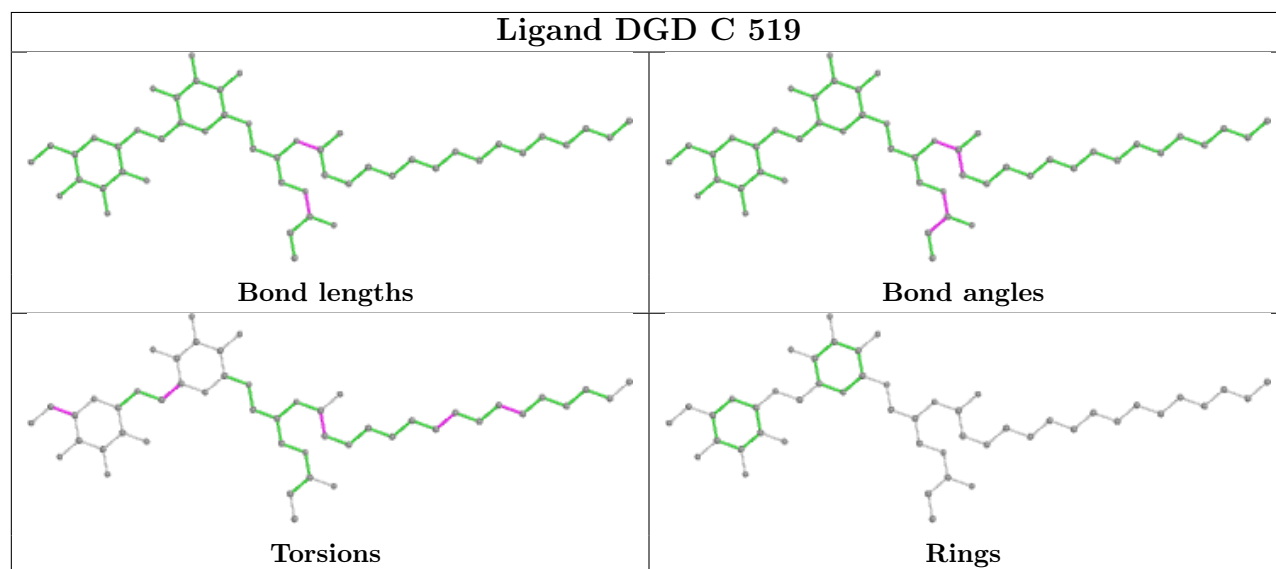


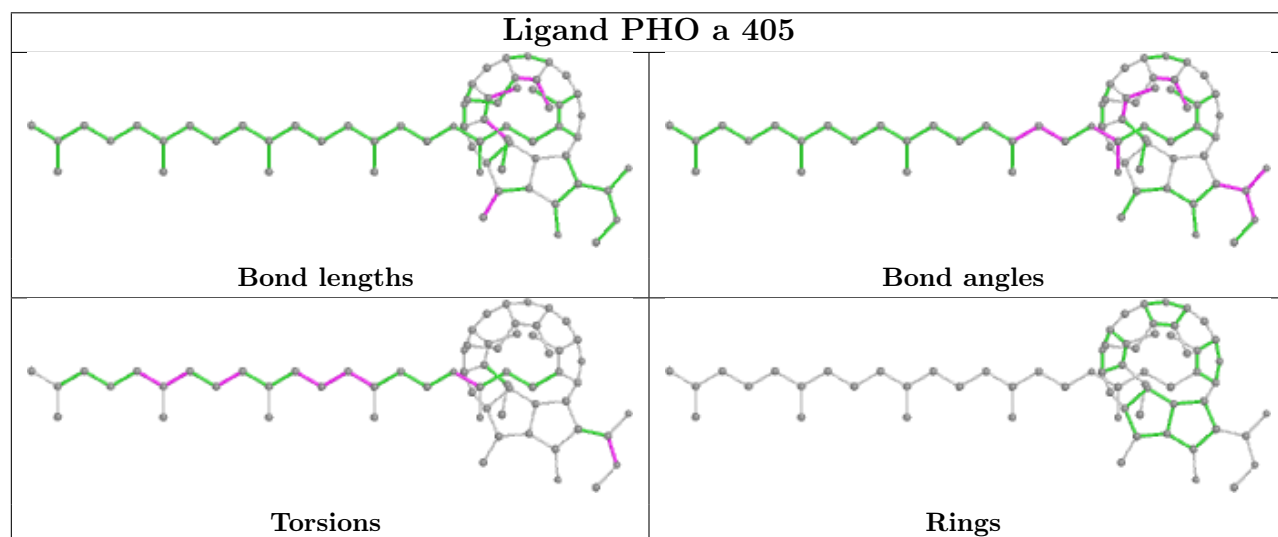
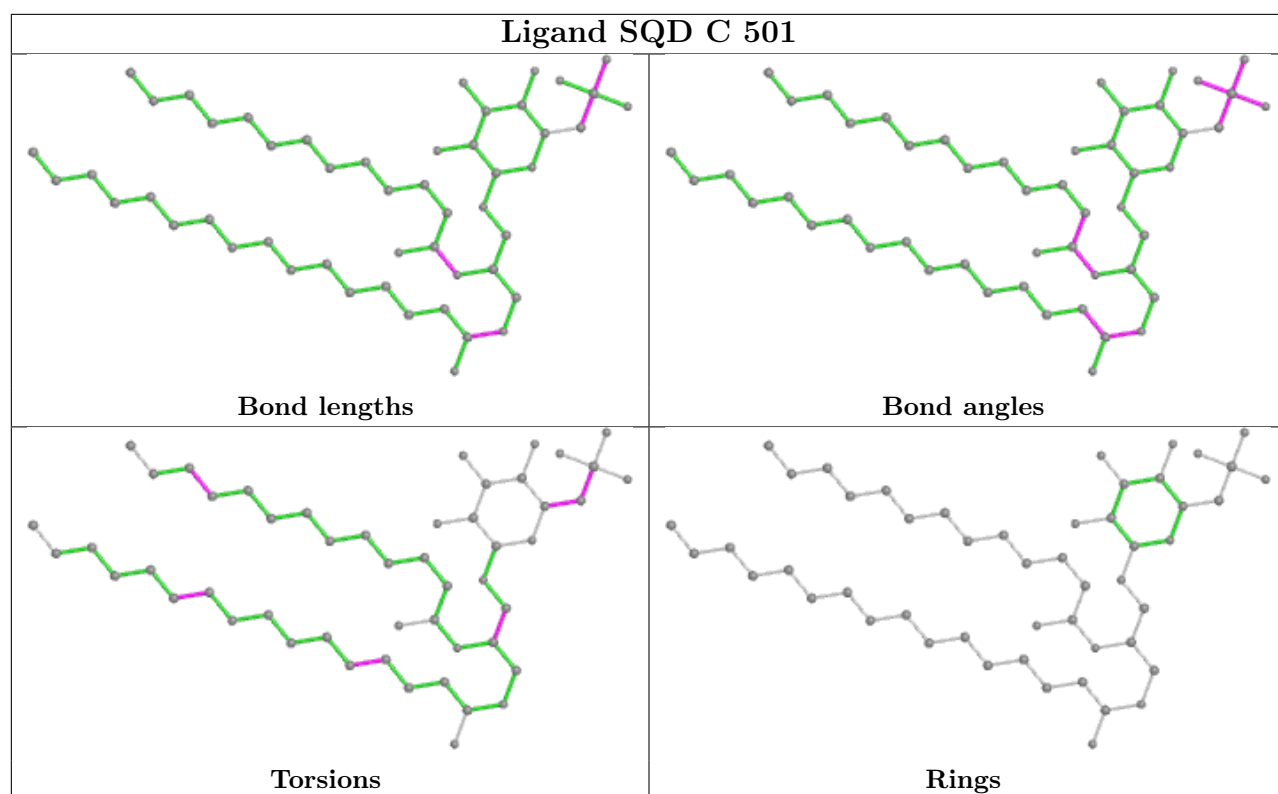


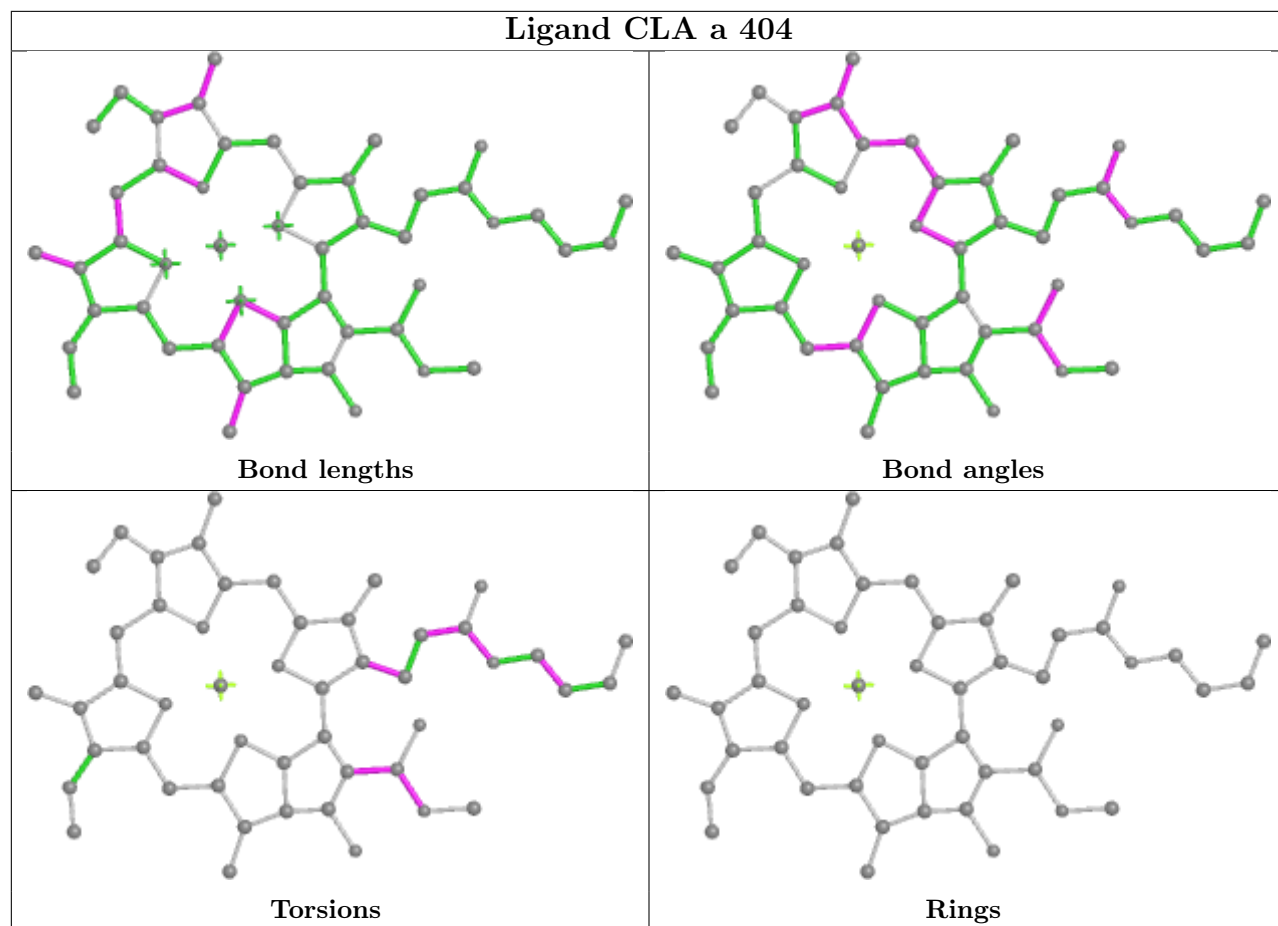


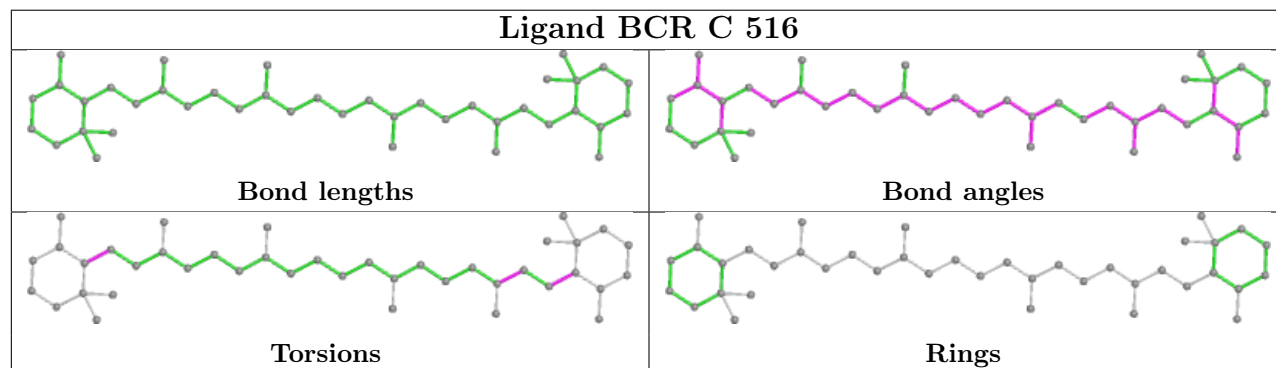
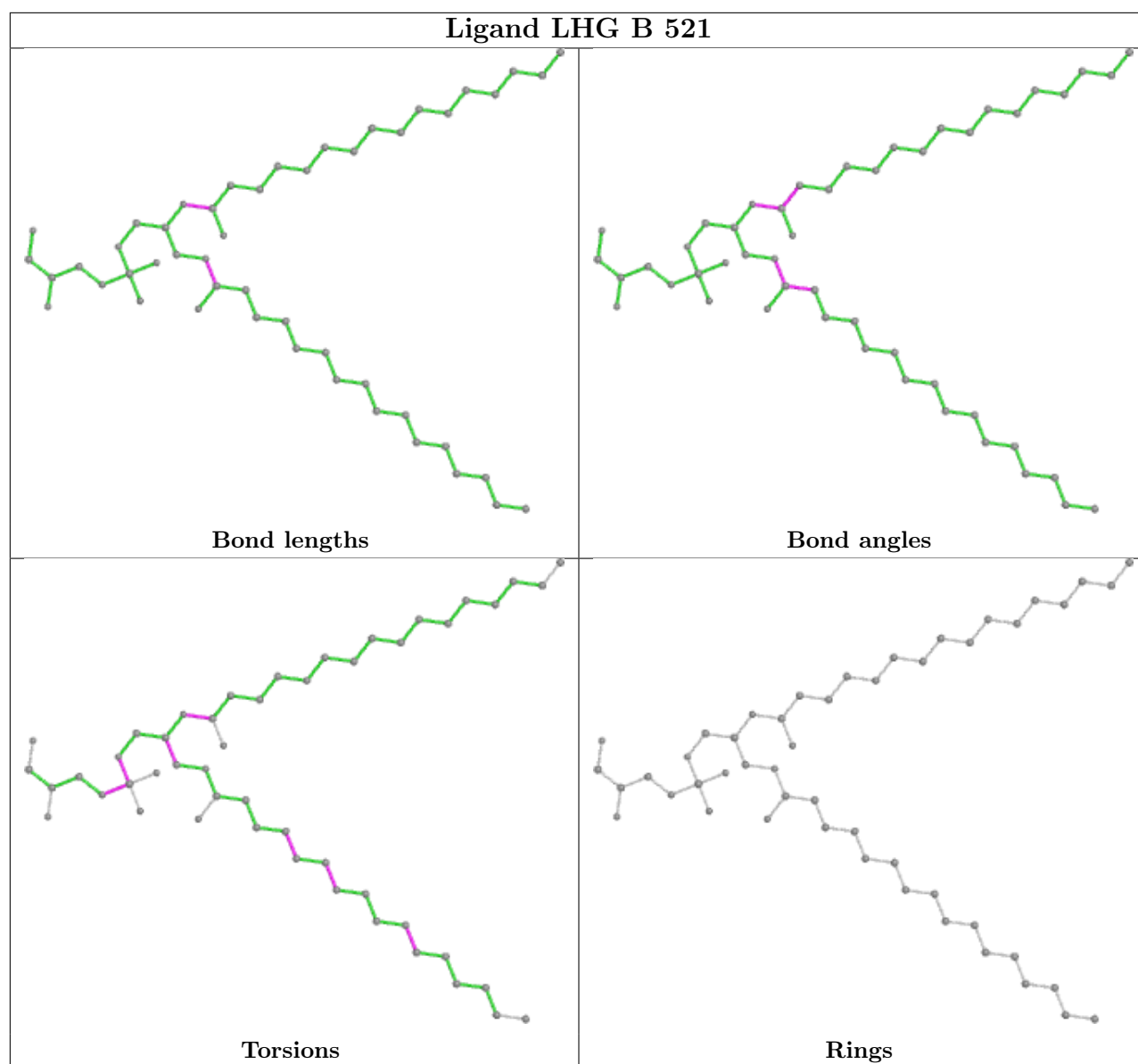


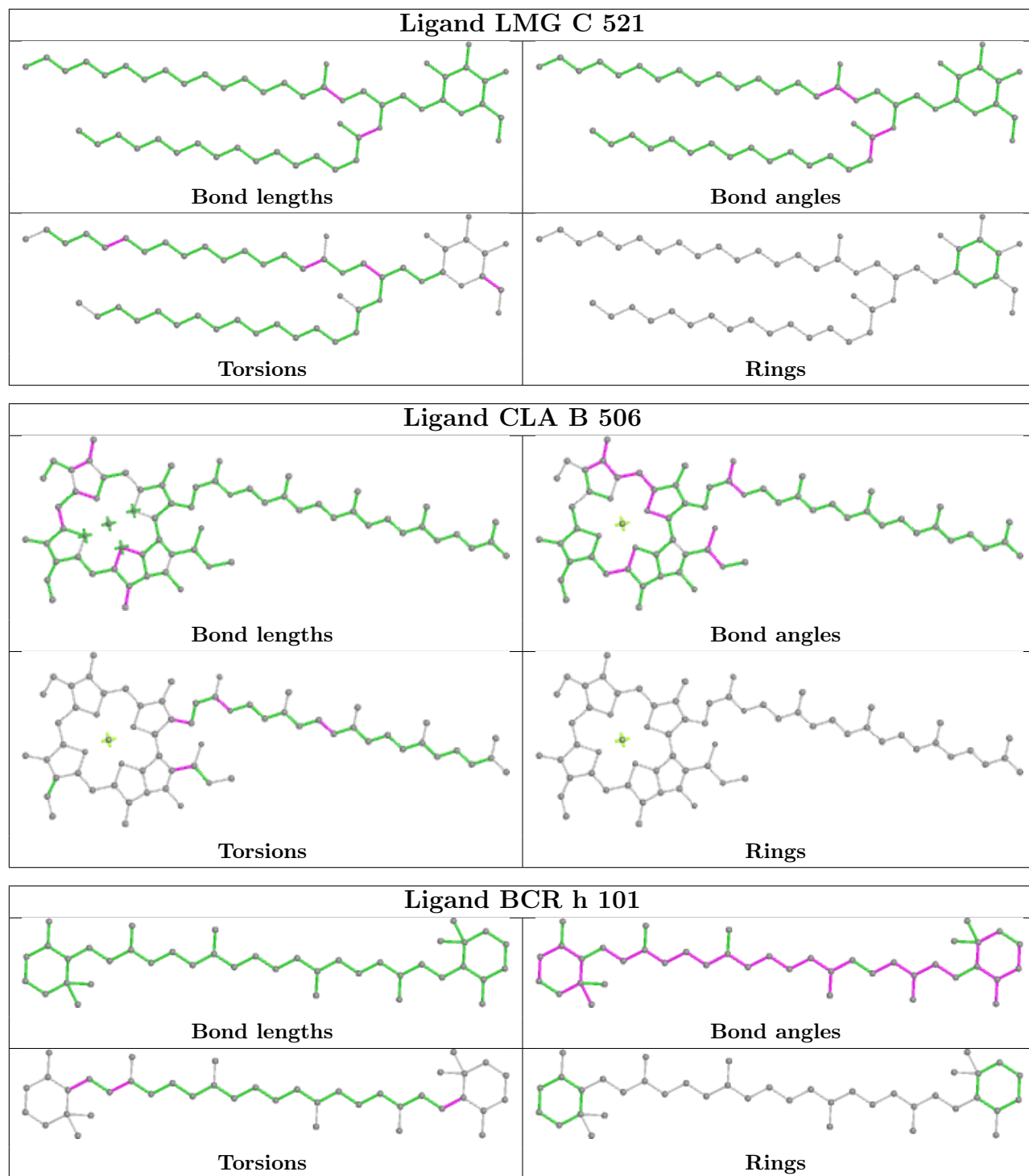


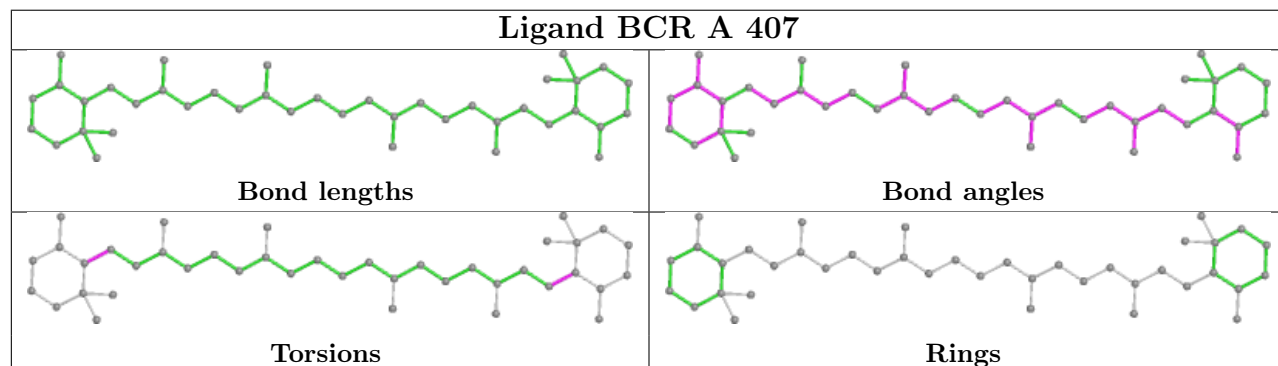
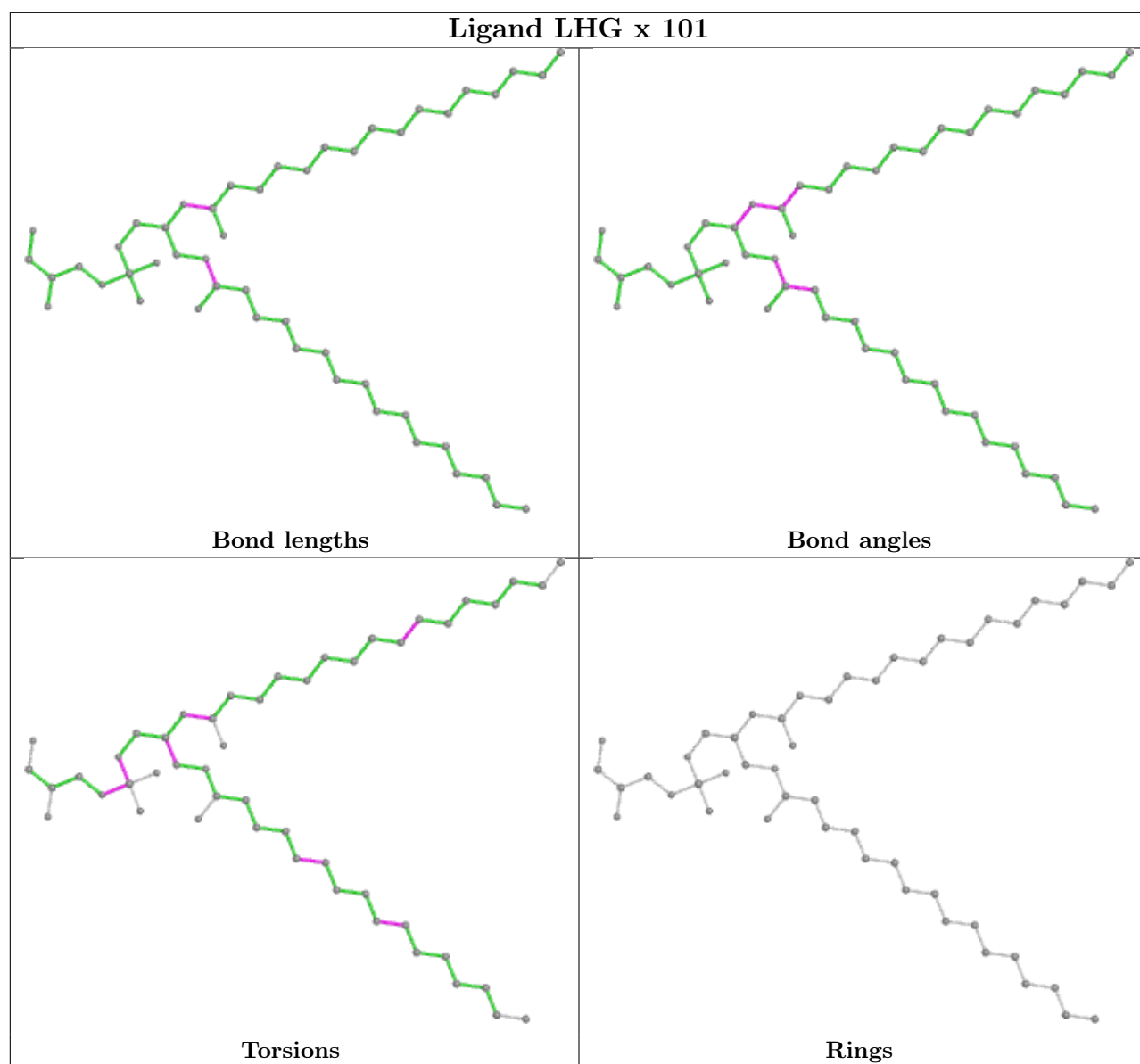
Ligand CLA a 402**Ligand DGD C 519**

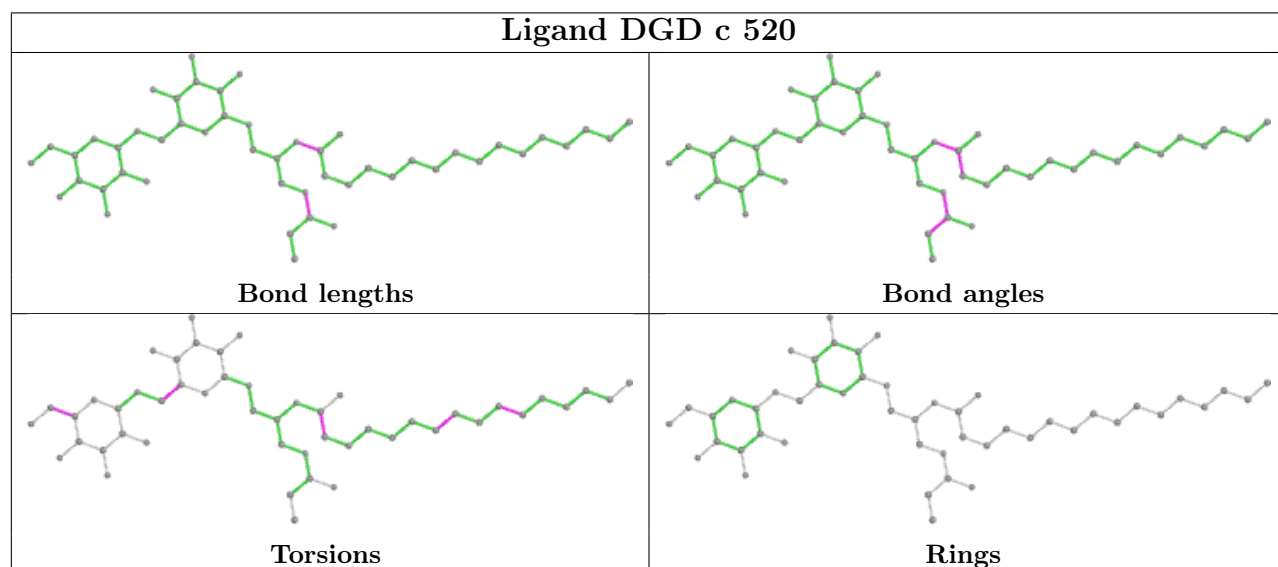
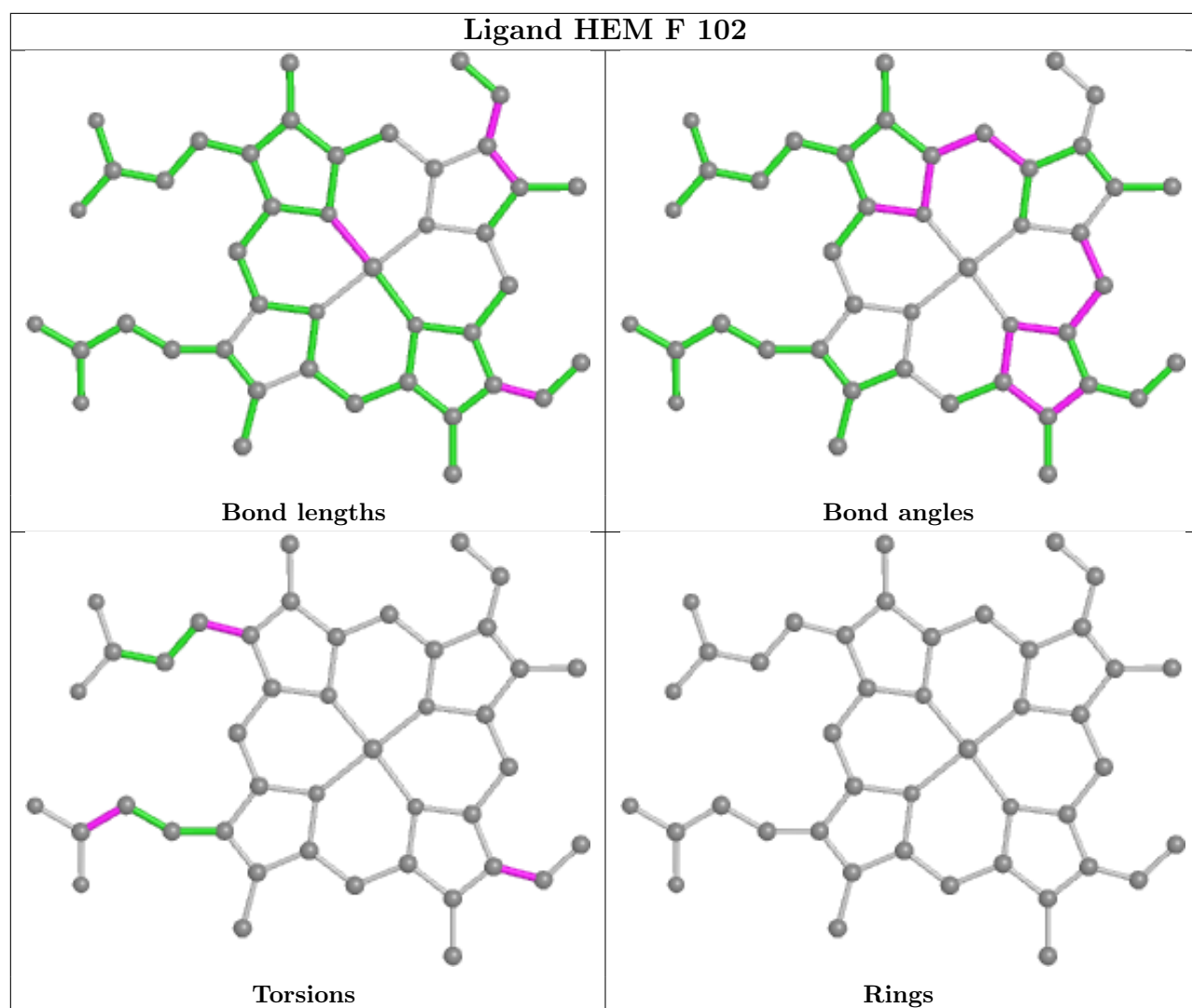


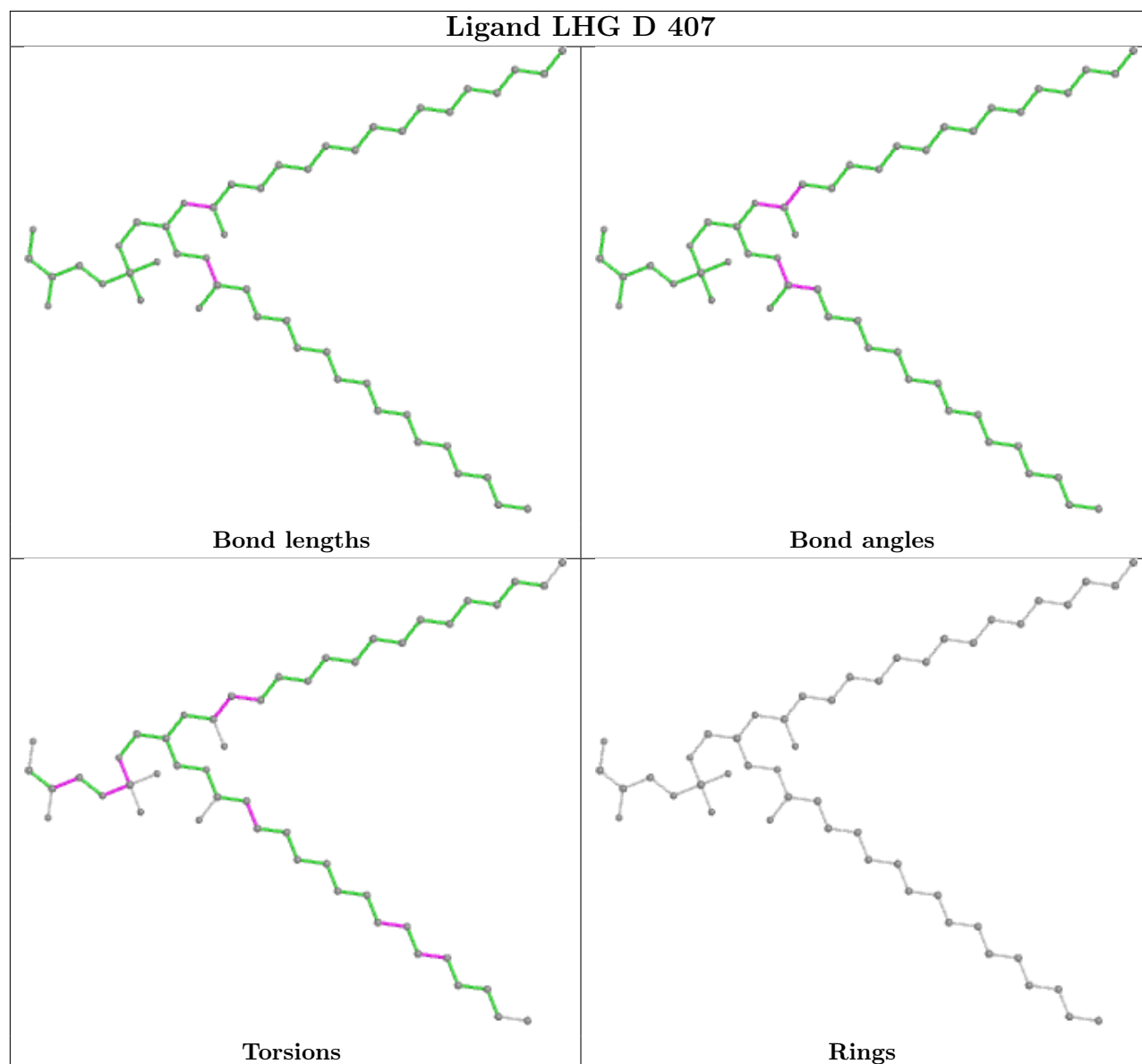
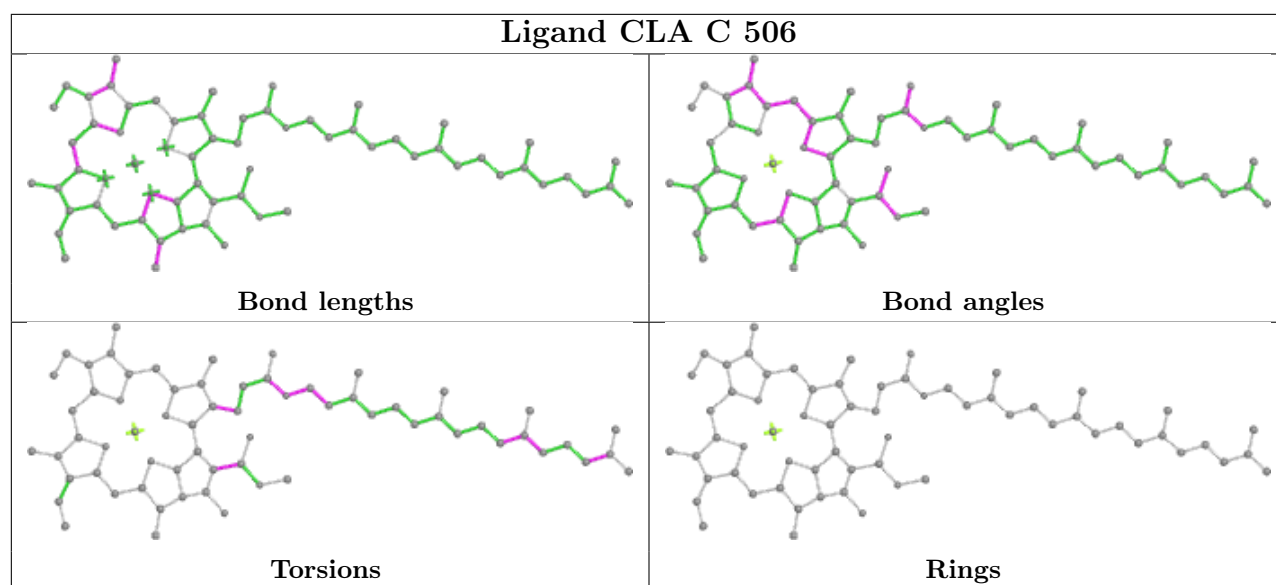




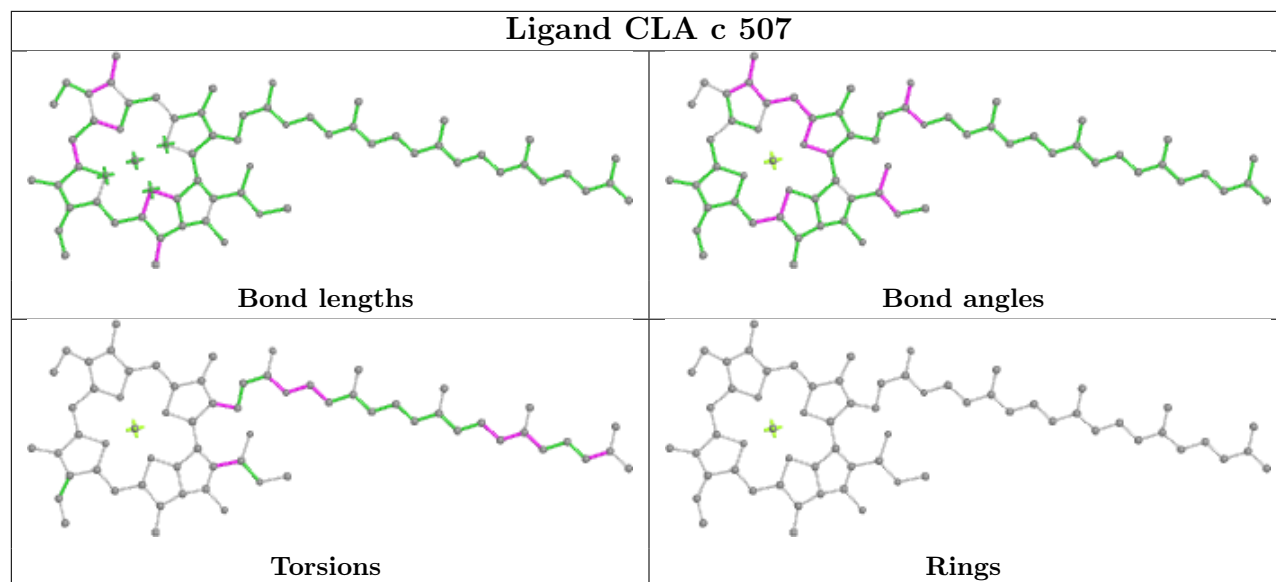




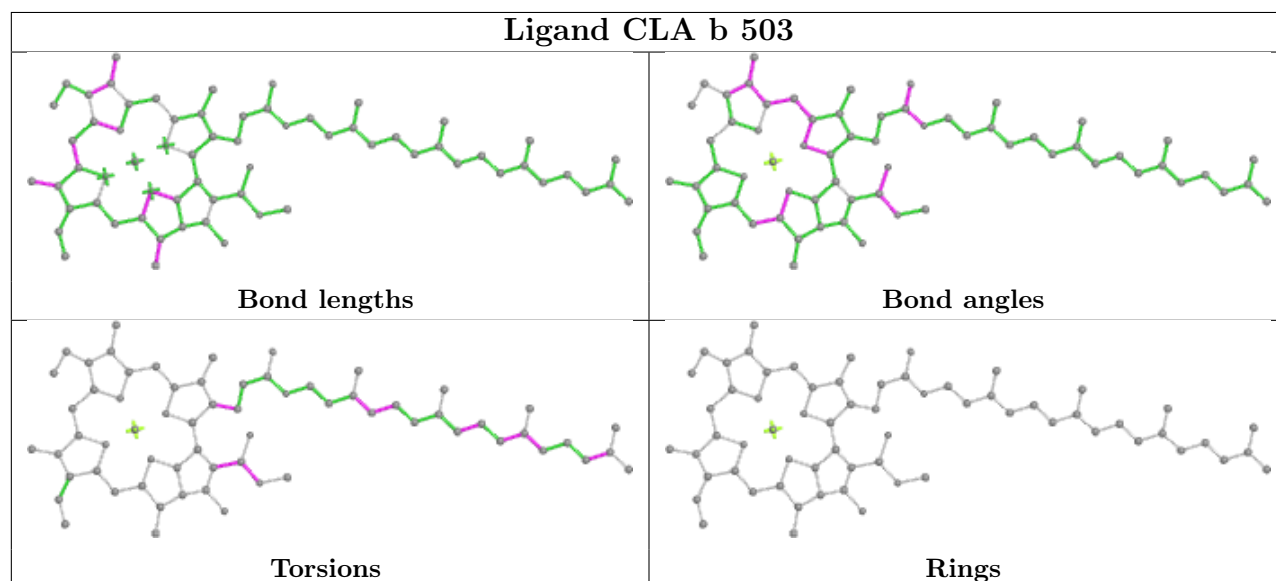




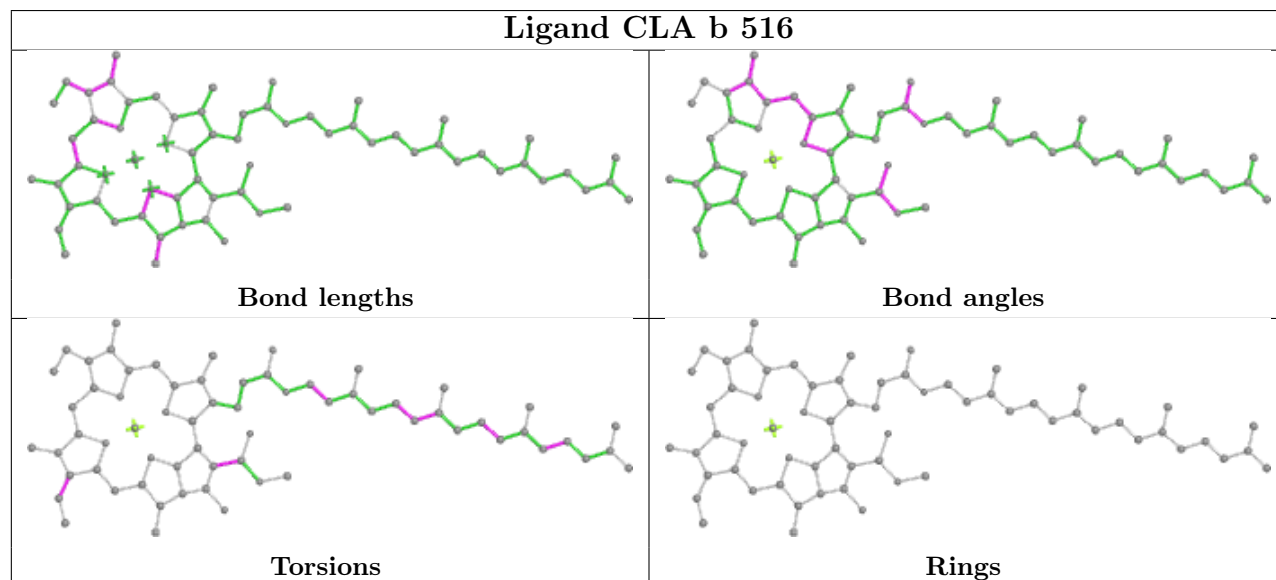
Ligand CLA c 507

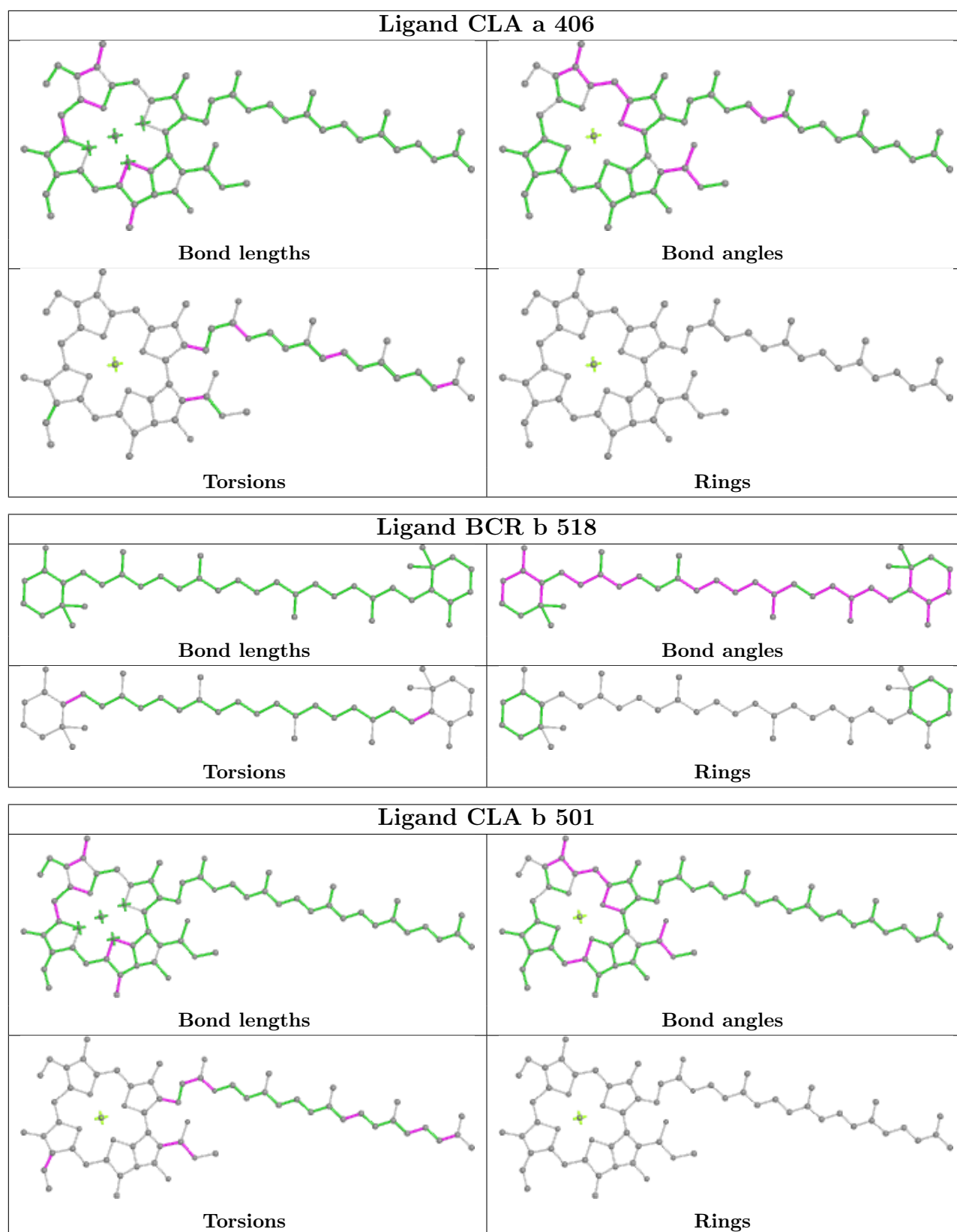


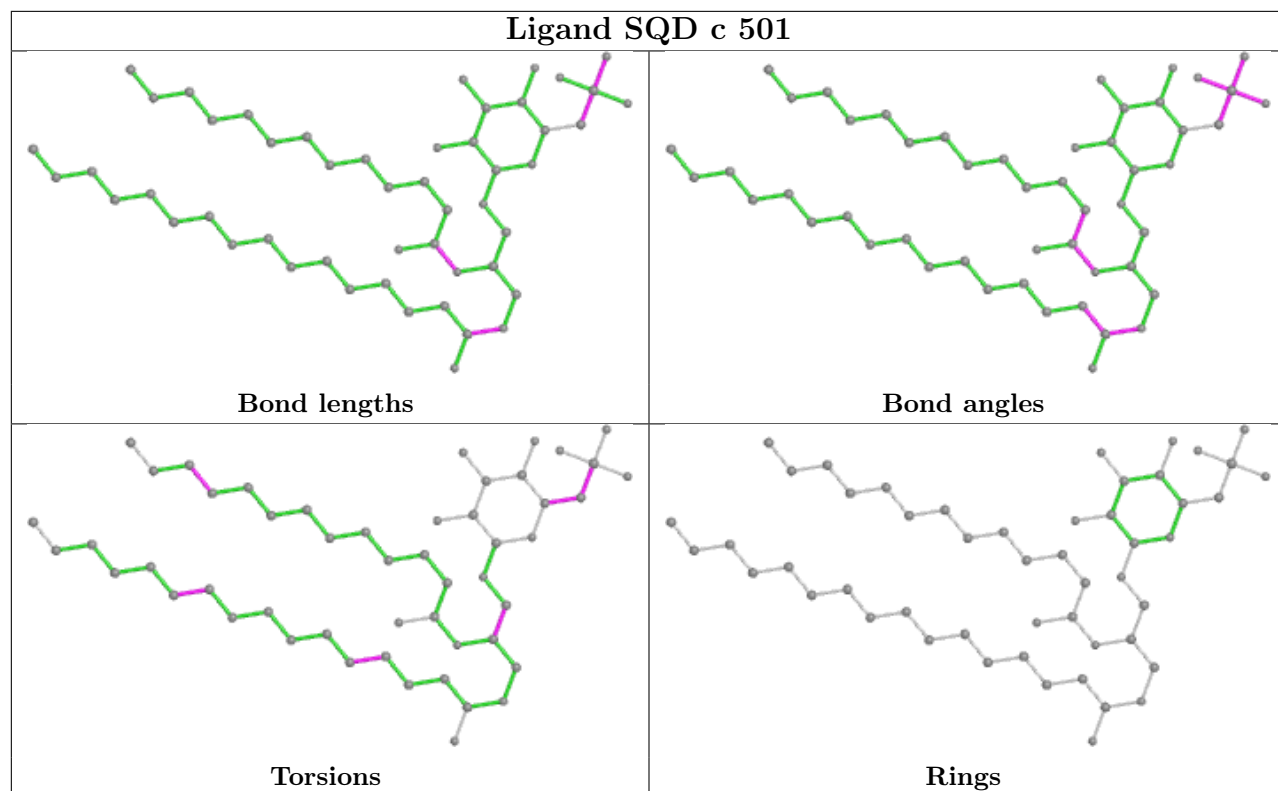
Ligand CLA b 503



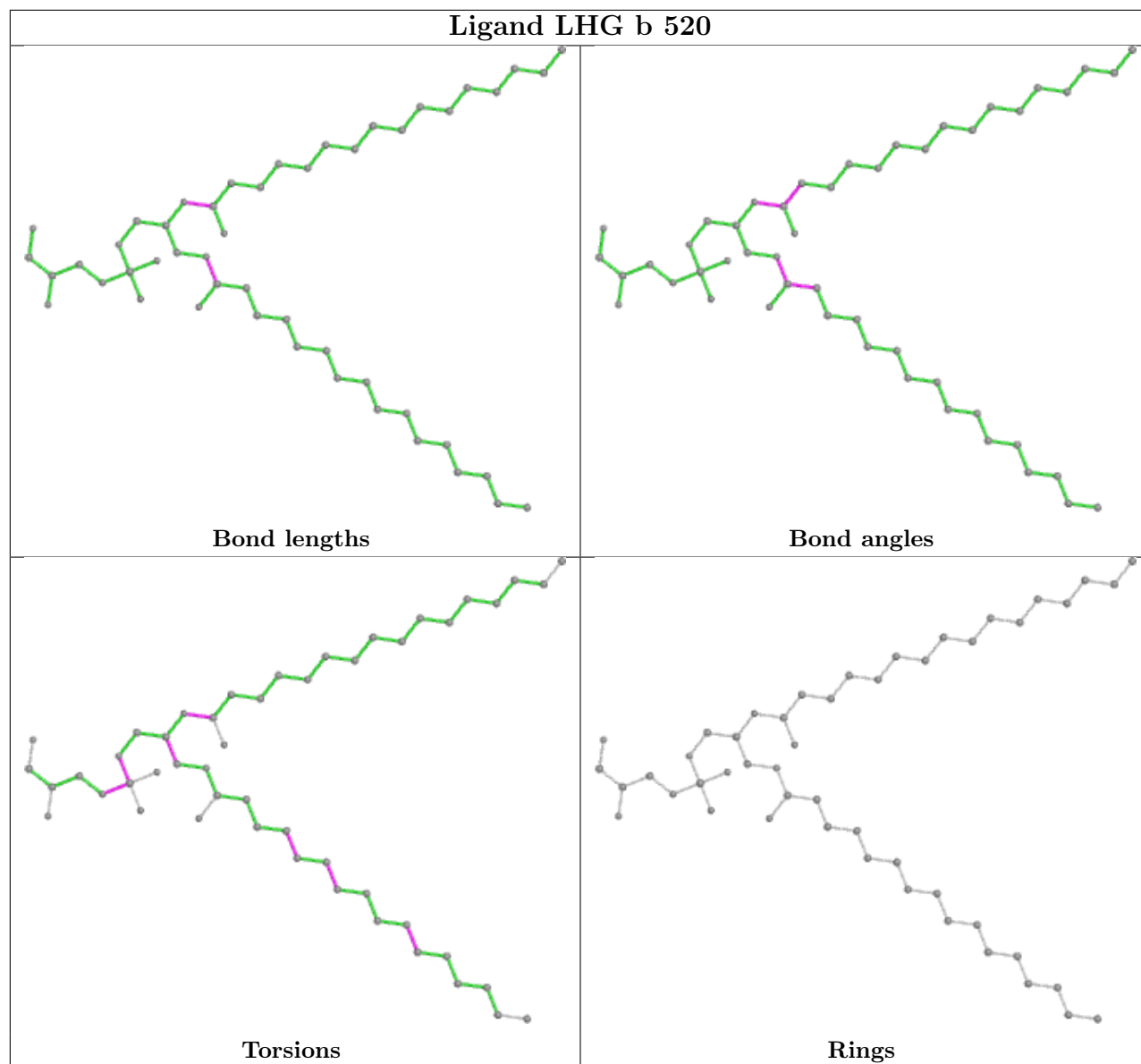
Ligand CLA b 516



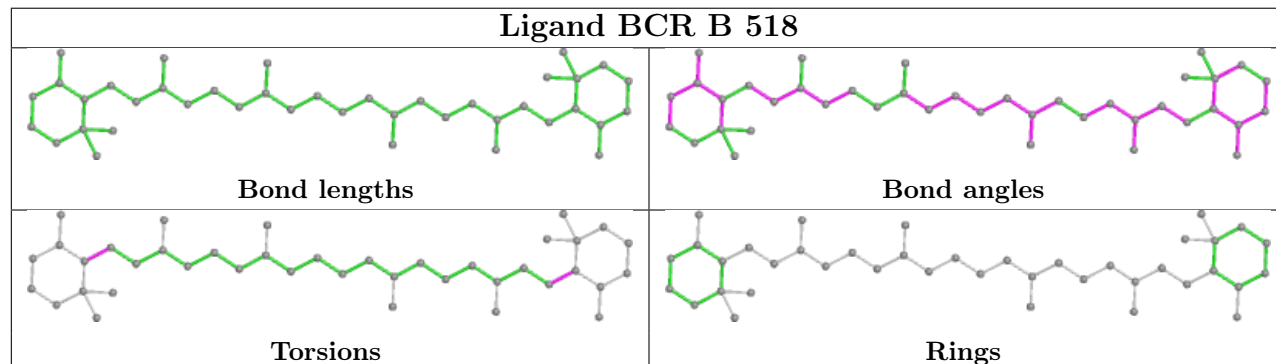


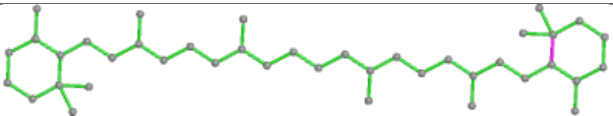
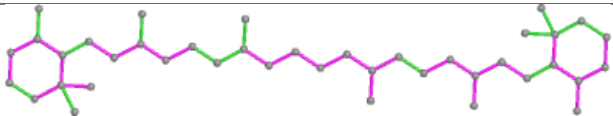
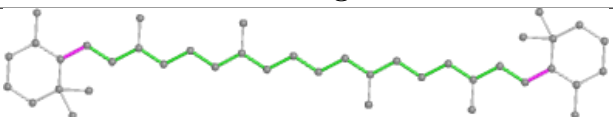
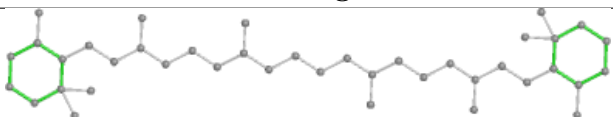


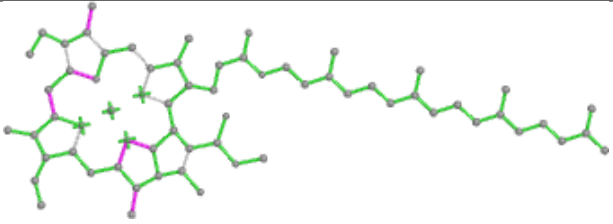
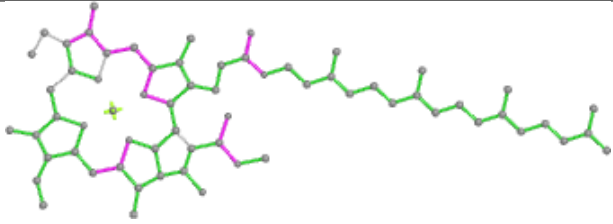
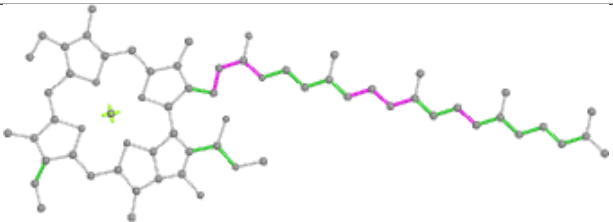
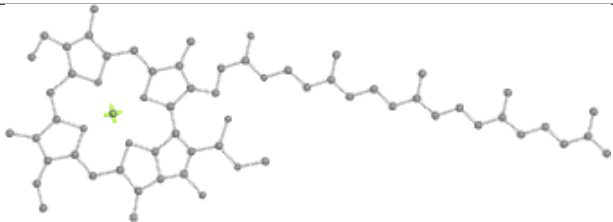
Ligand LHG b 520

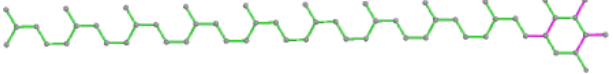
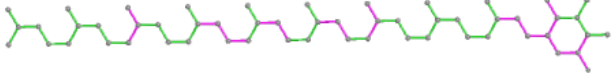
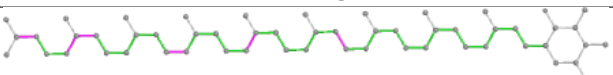
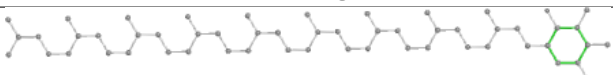


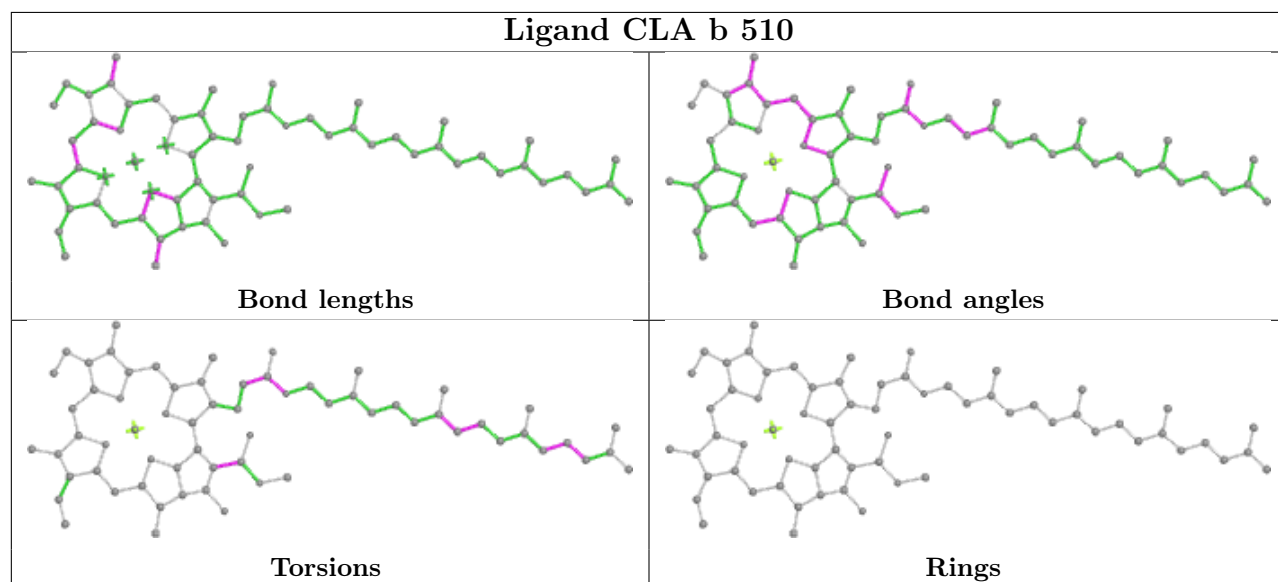
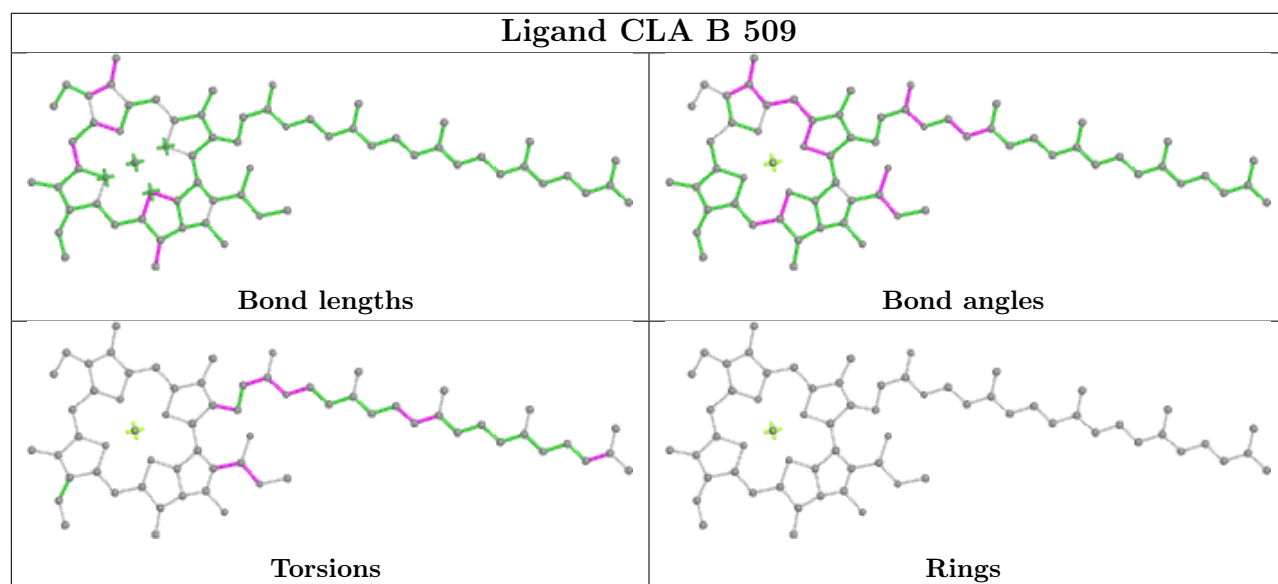
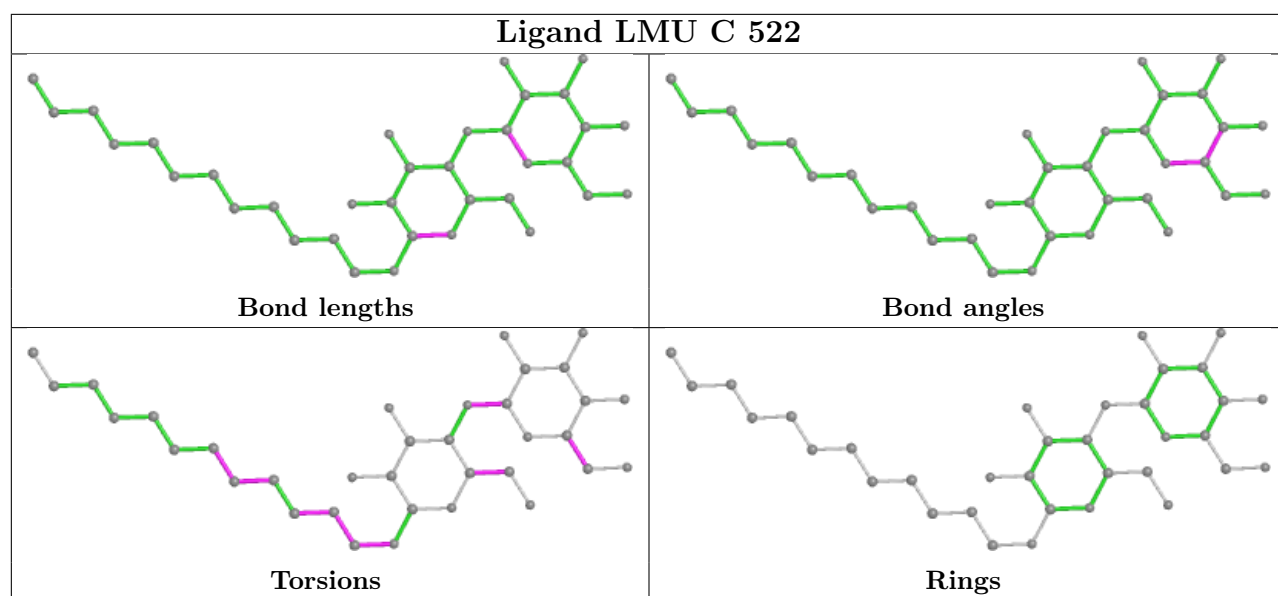
Ligand BCR B 518

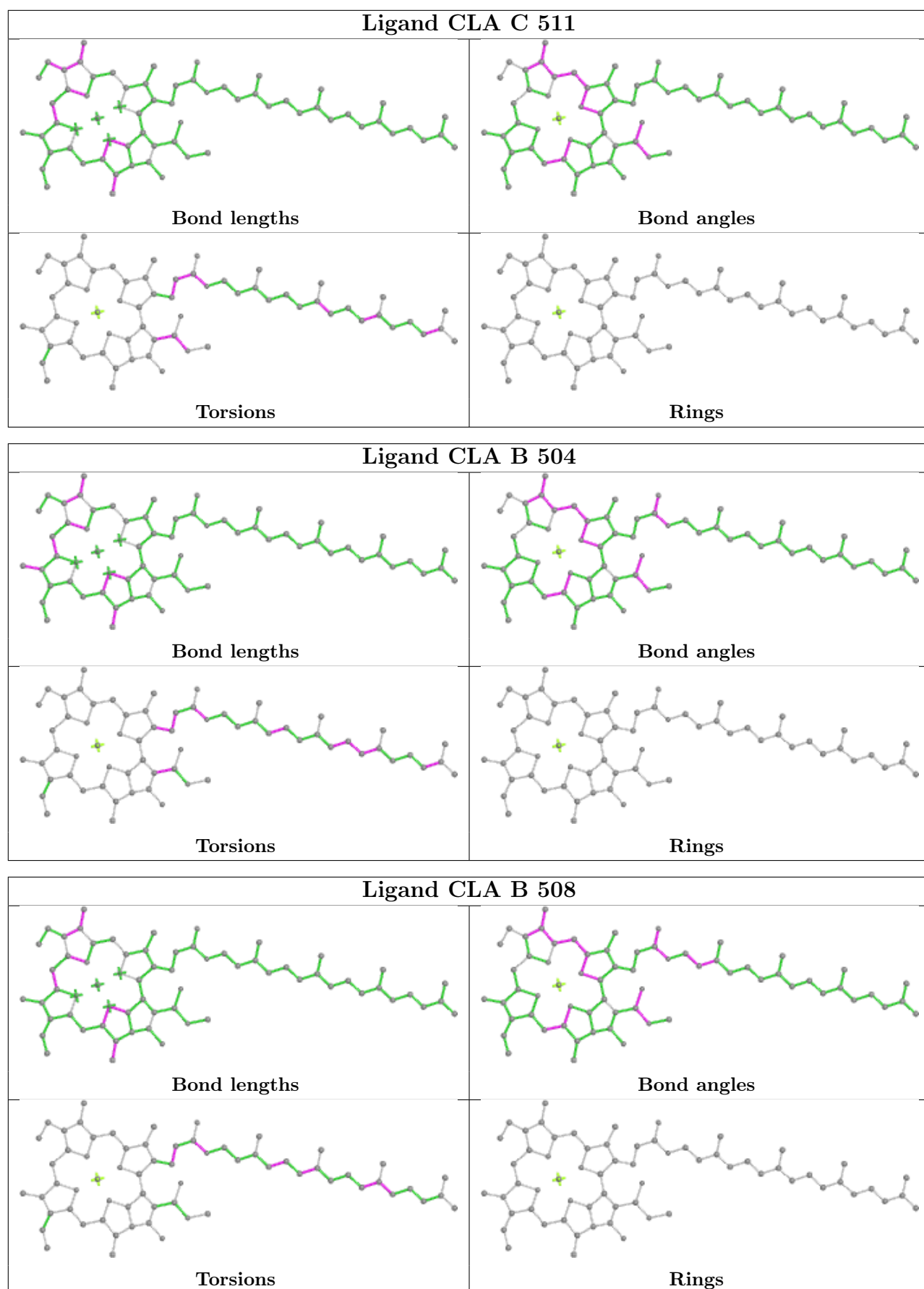


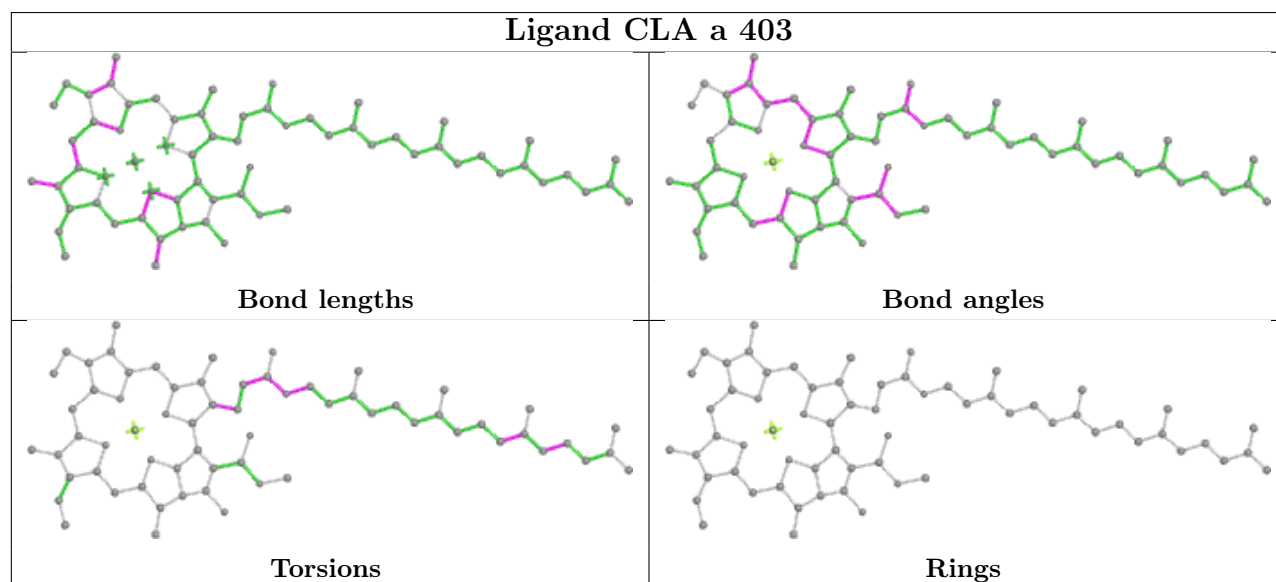
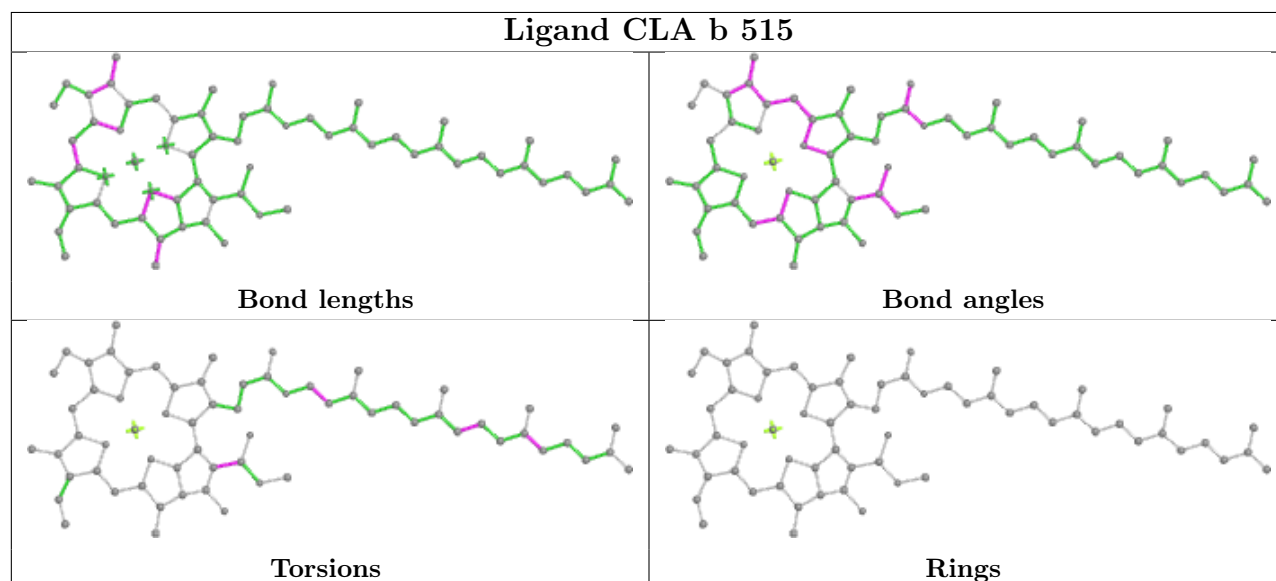
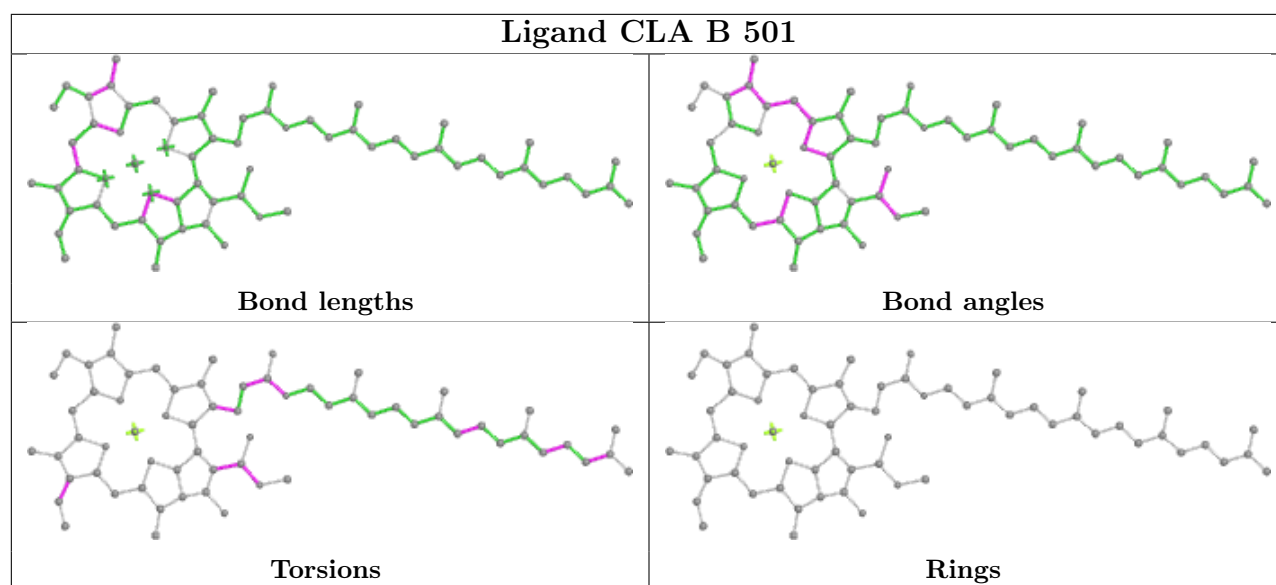
Ligand BCR b 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

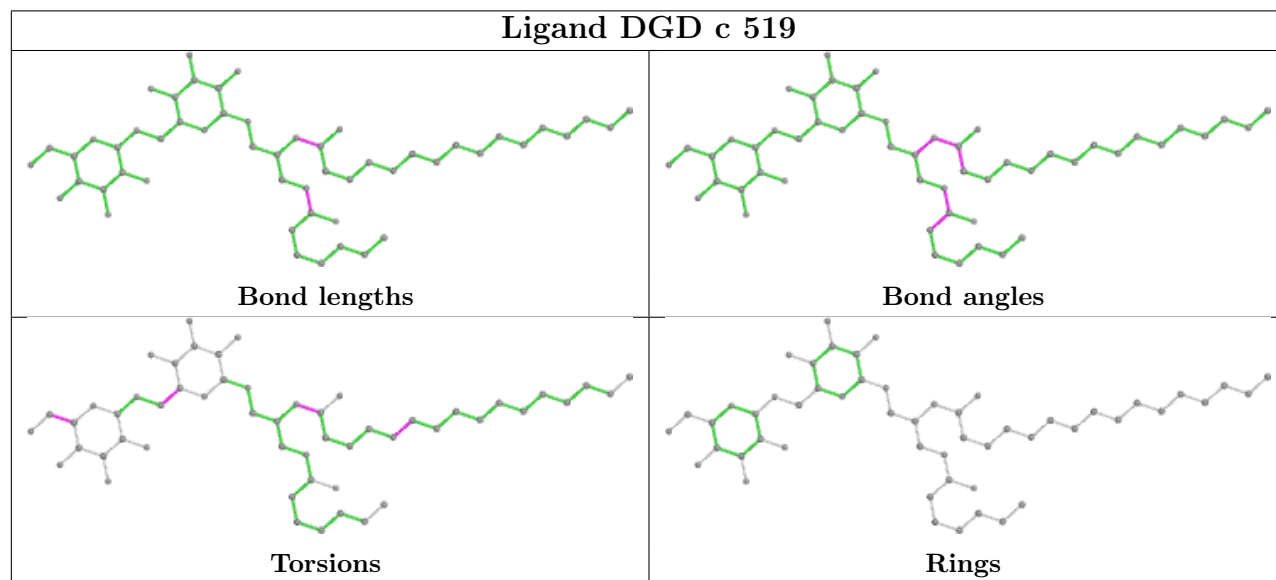
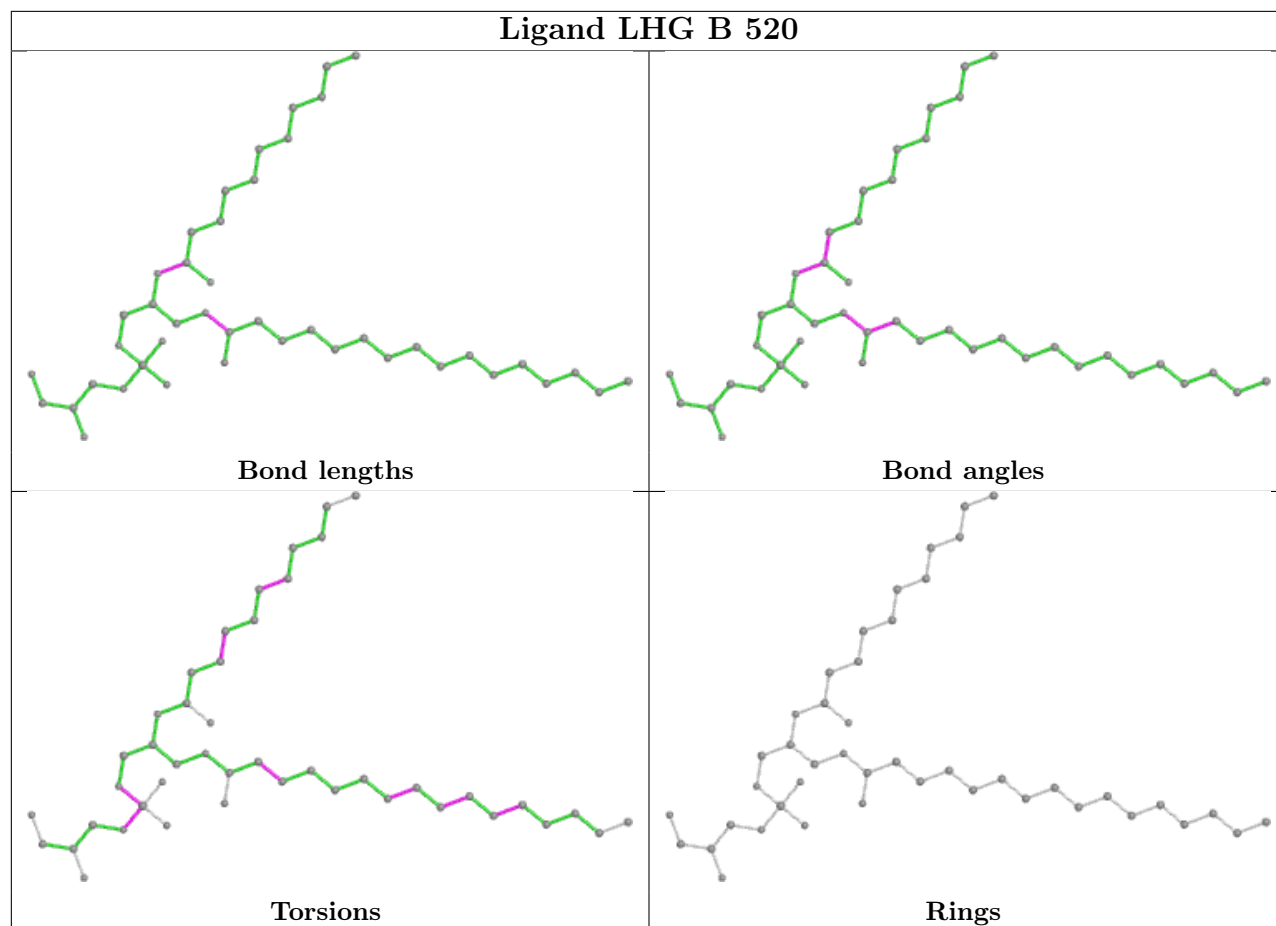
Ligand CLA b 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

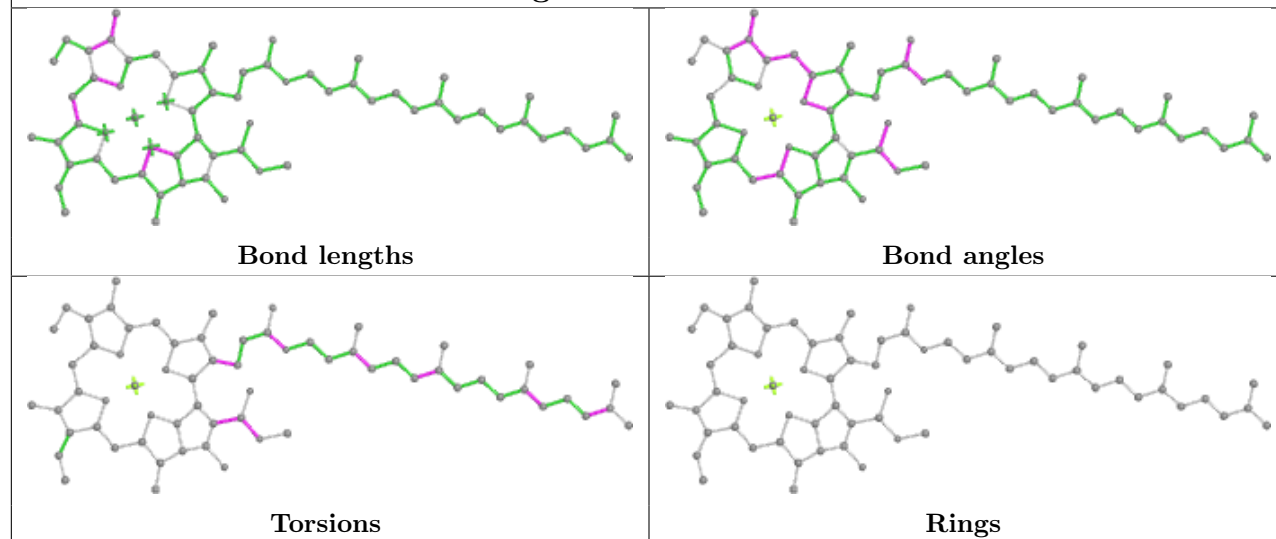
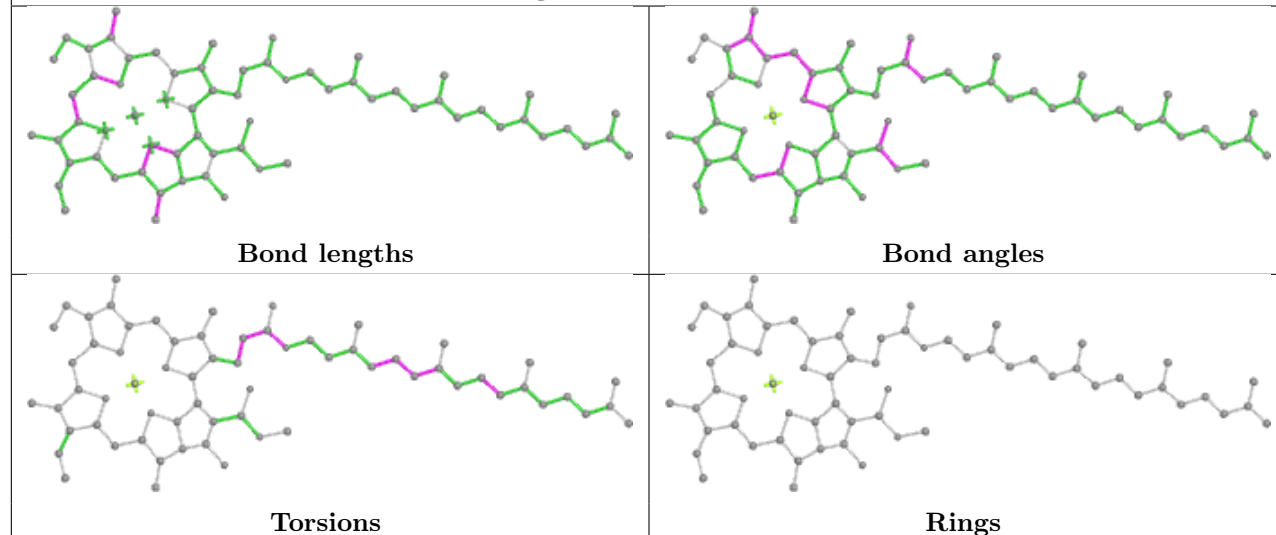
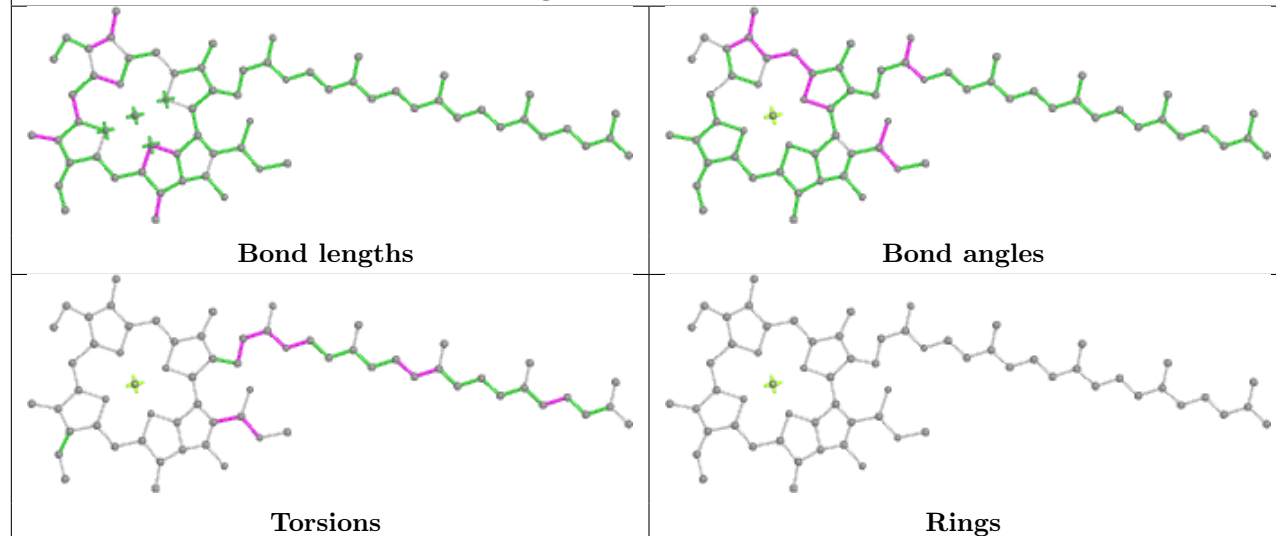
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings



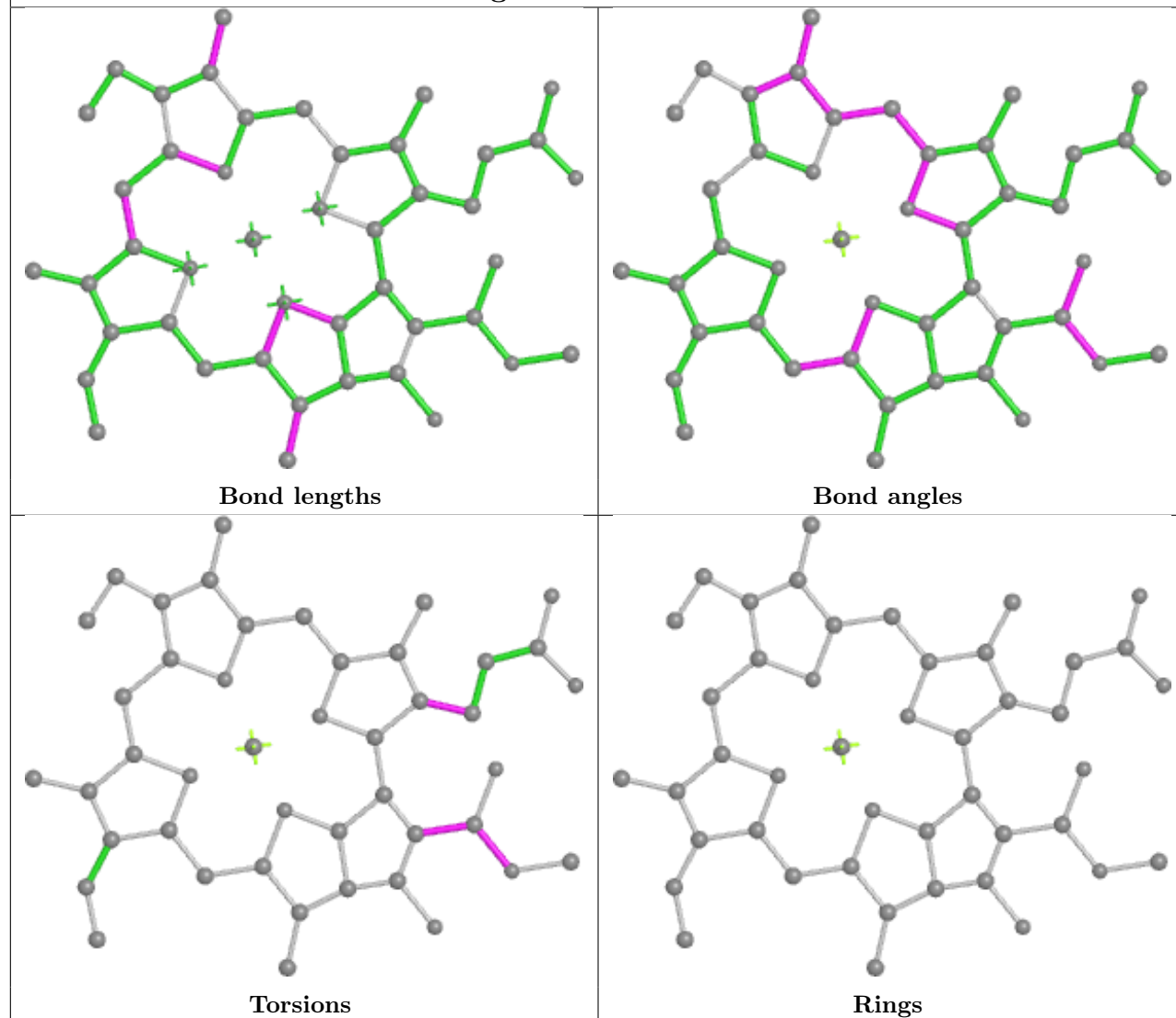




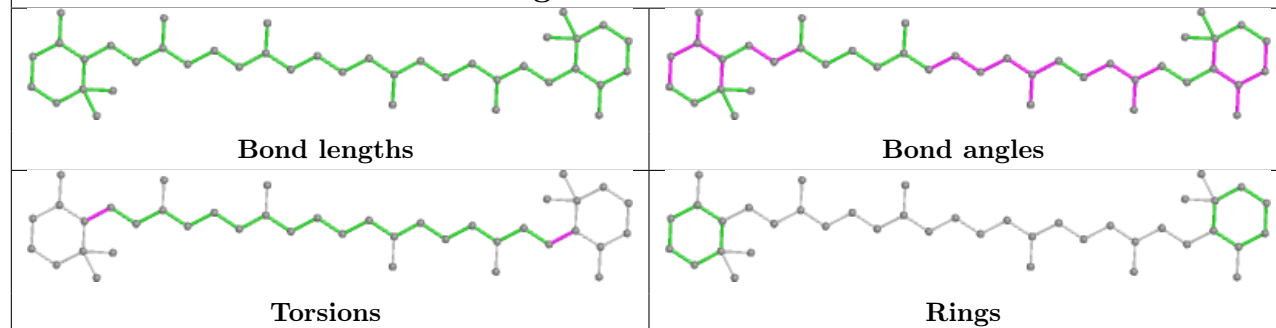


Ligand CLA C 512**Ligand CLA B 502****Ligand CLA c 510**

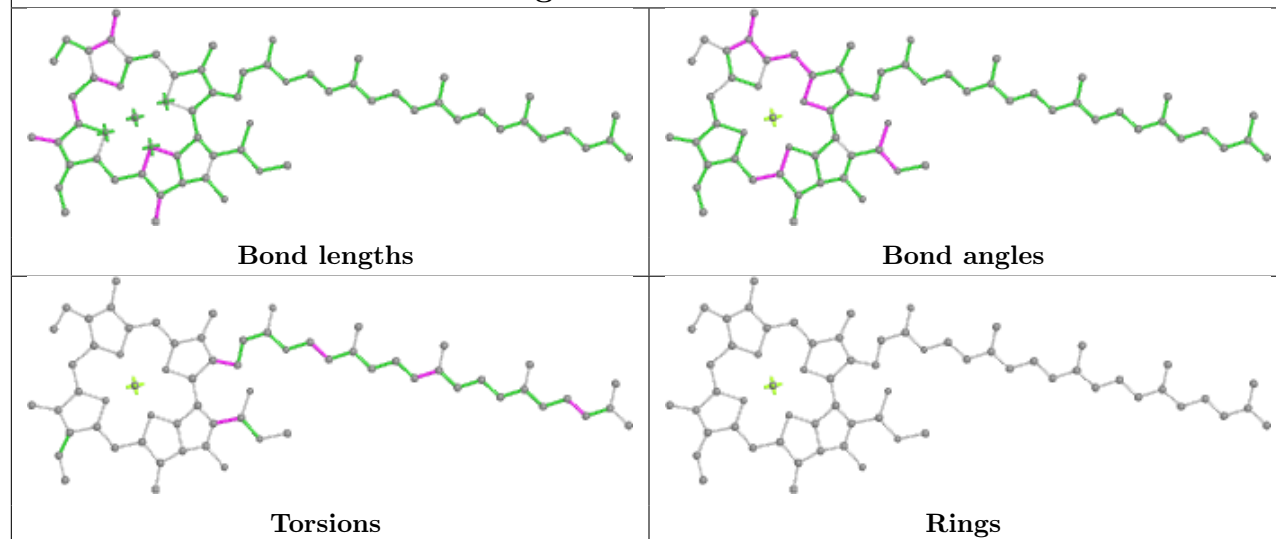
Ligand CLA B 514



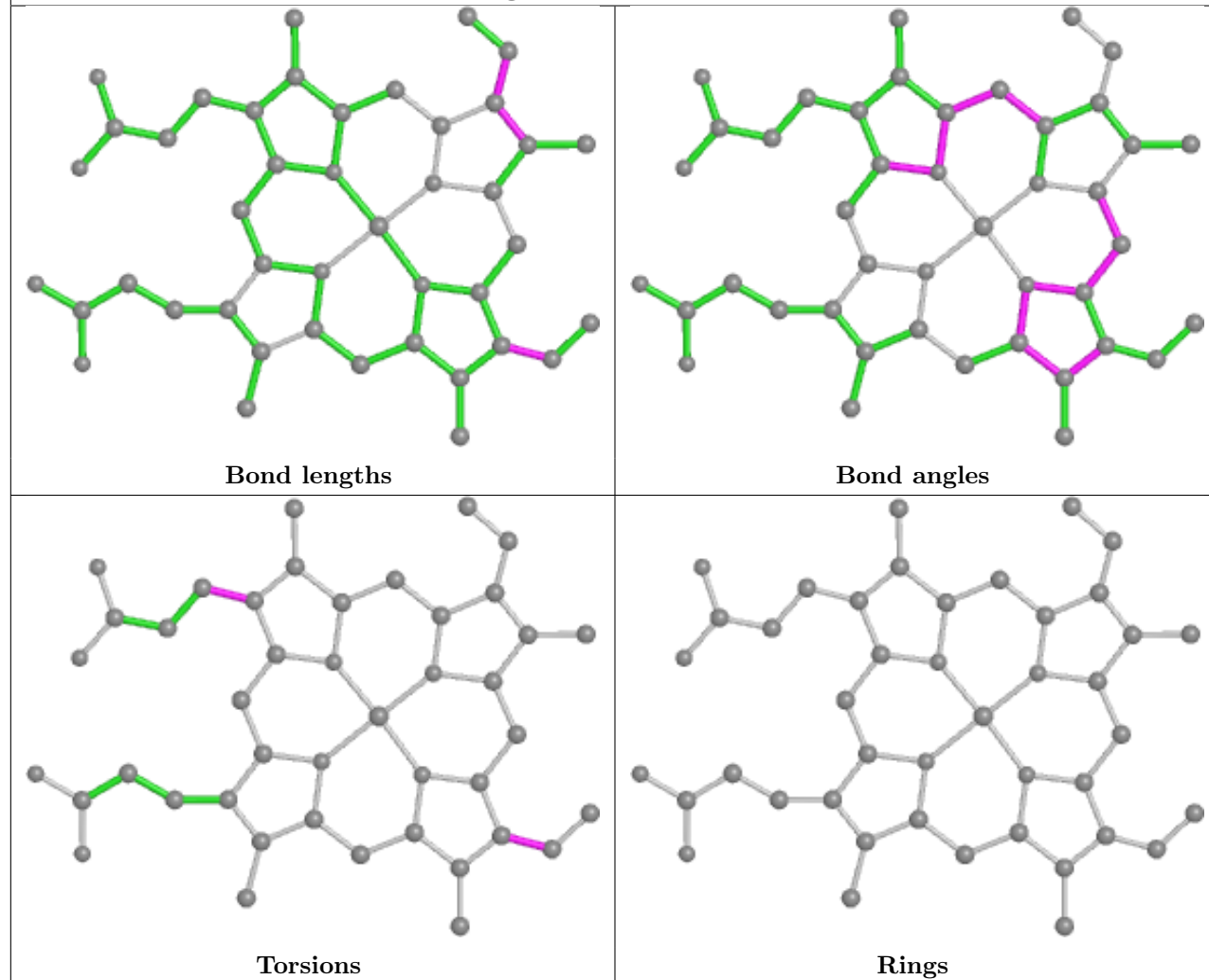
Ligand BCR d 405

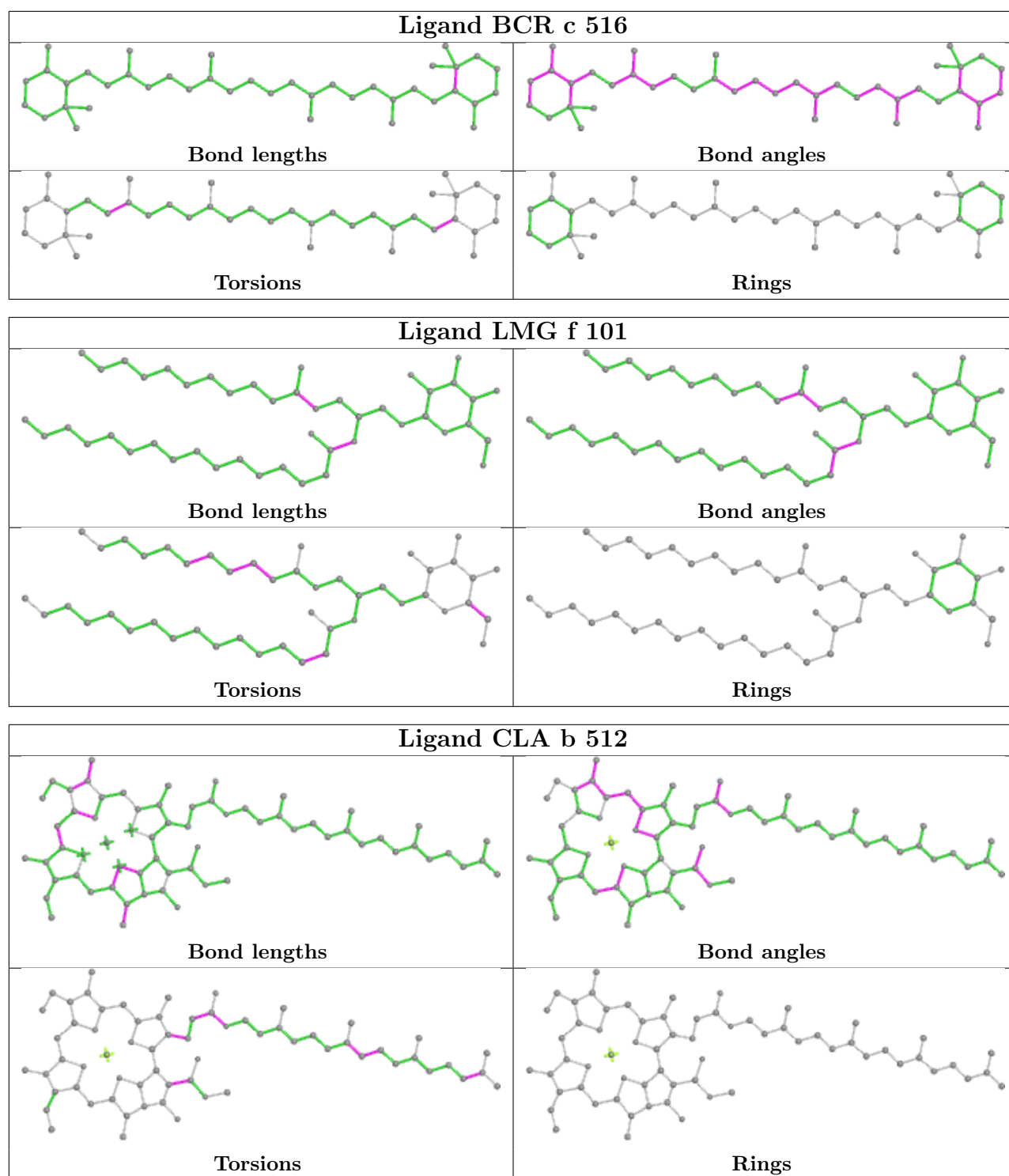


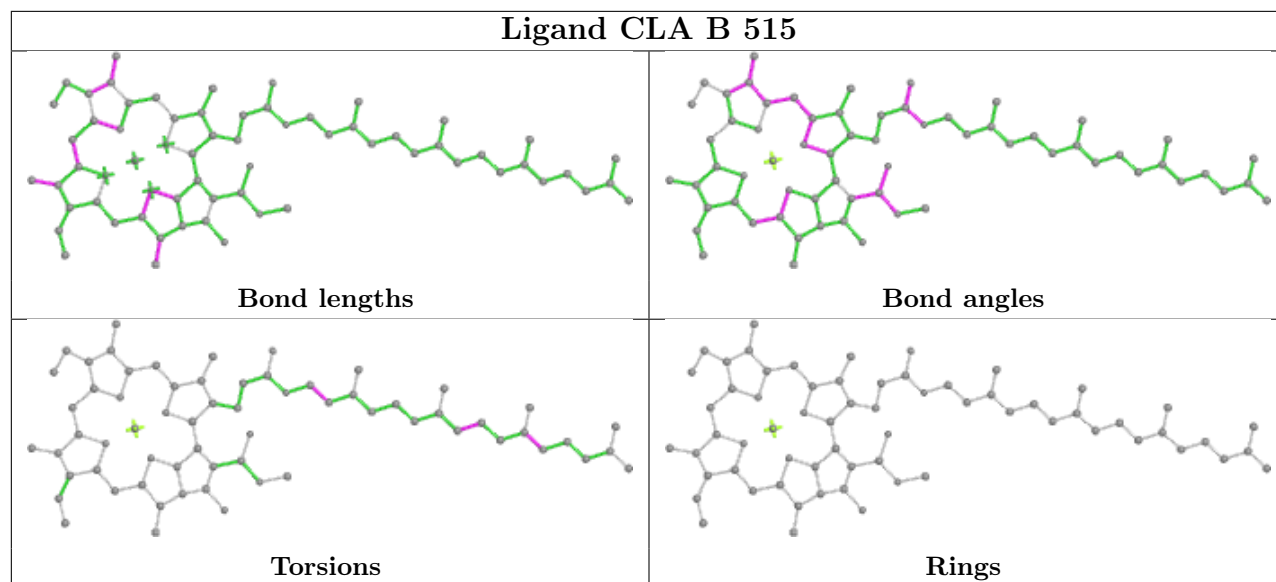
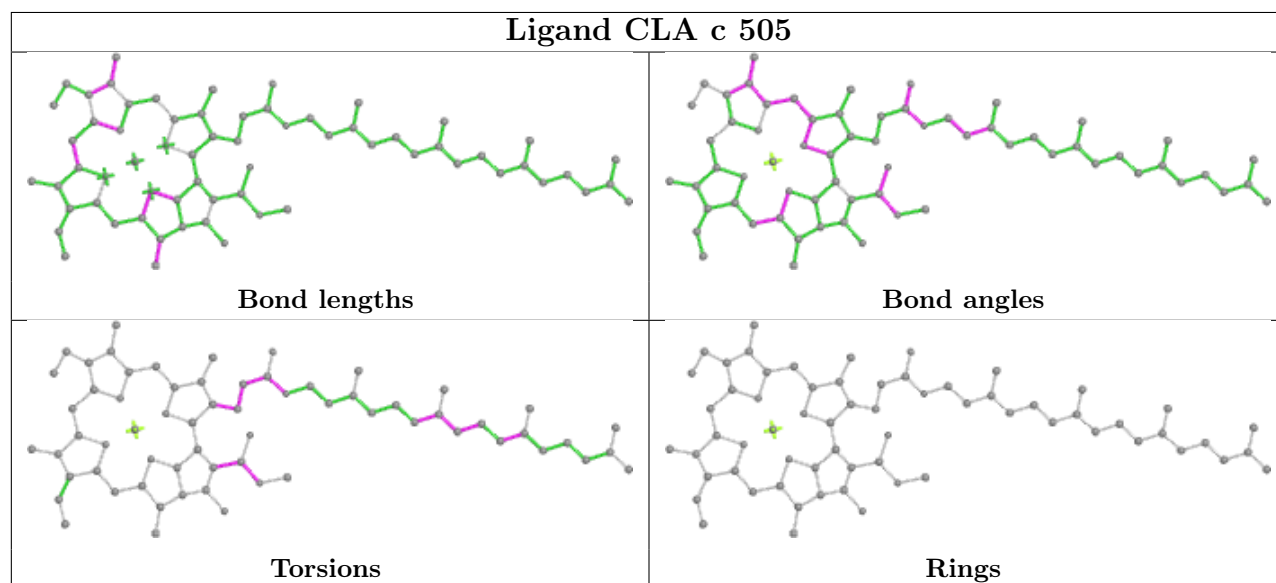
Ligand CLA d 403



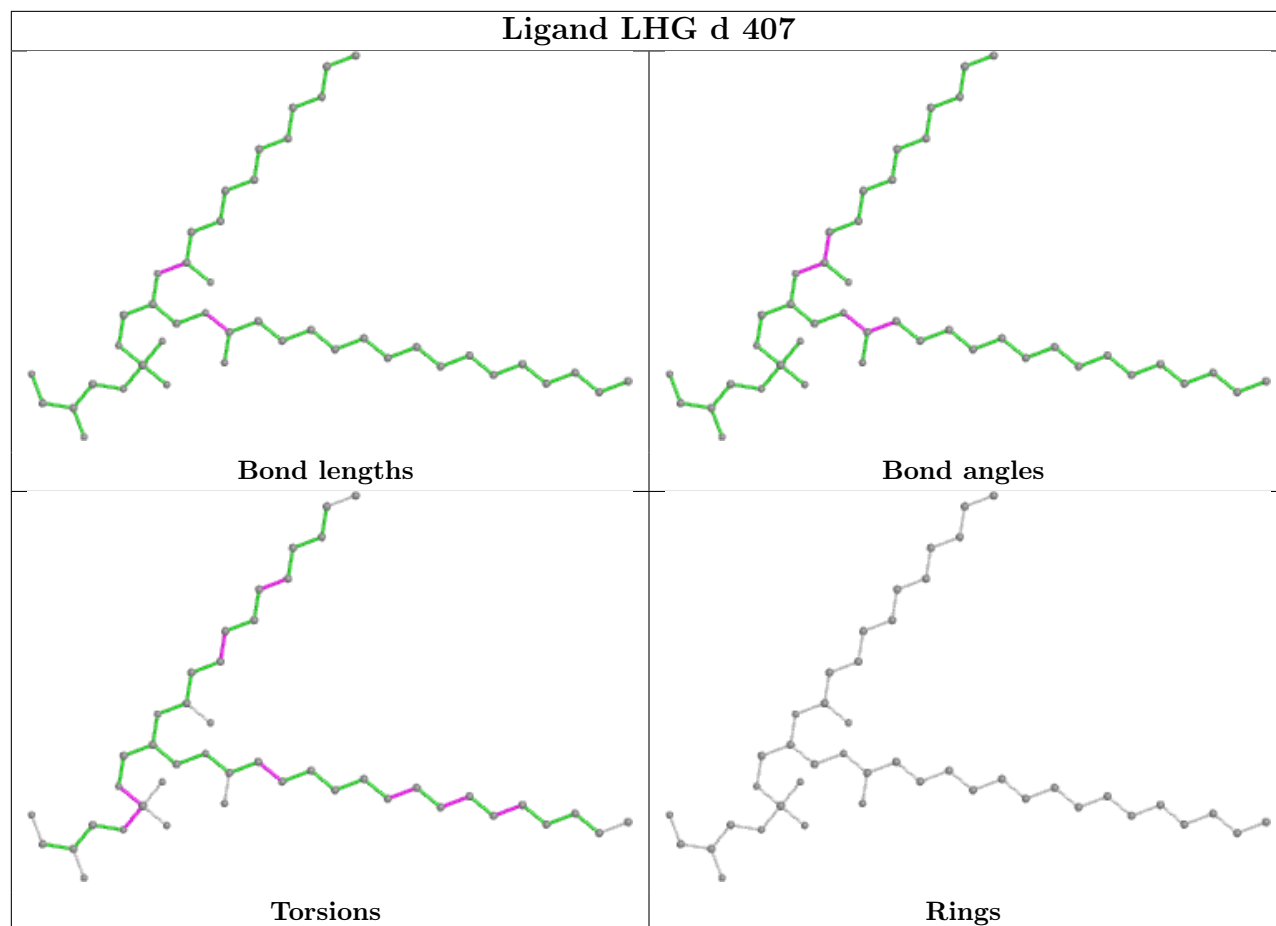
Ligand HEM e 101



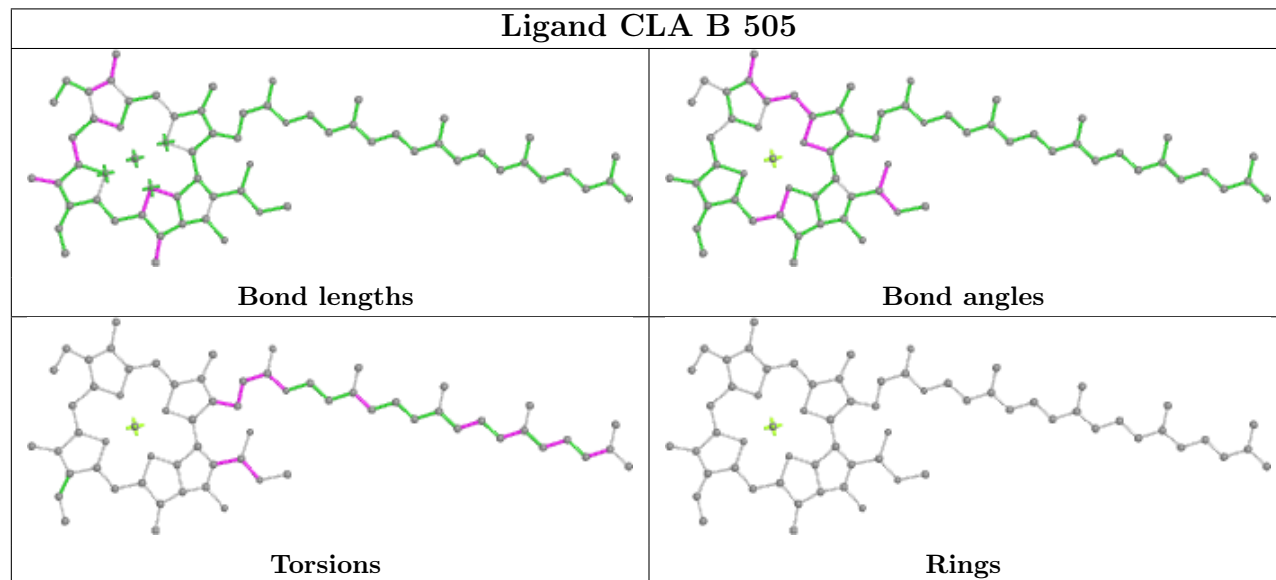


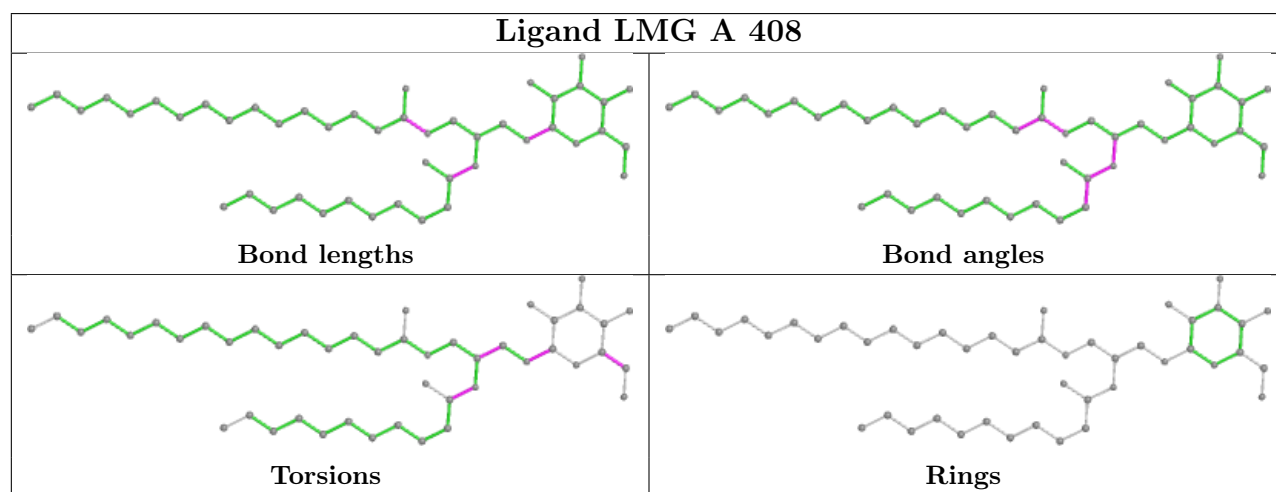
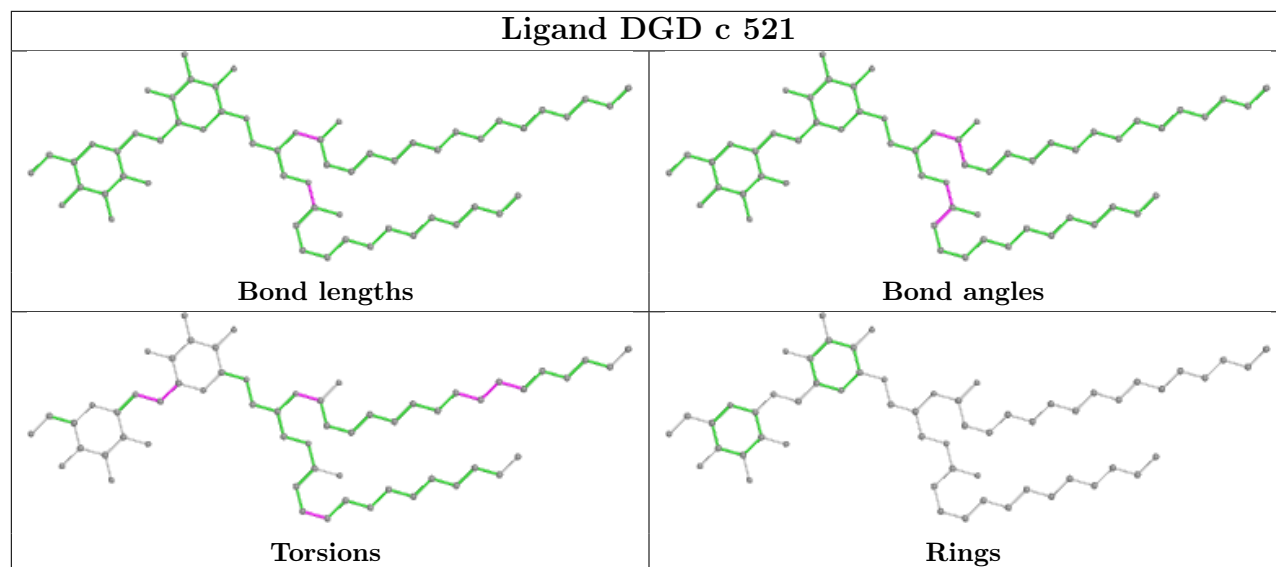
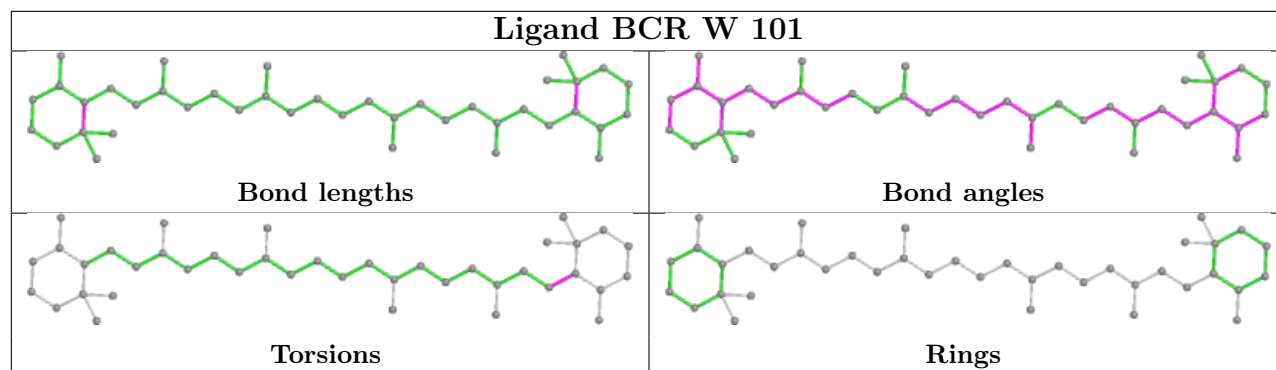
Ligand CLA B 515**Ligand CLA c 505**

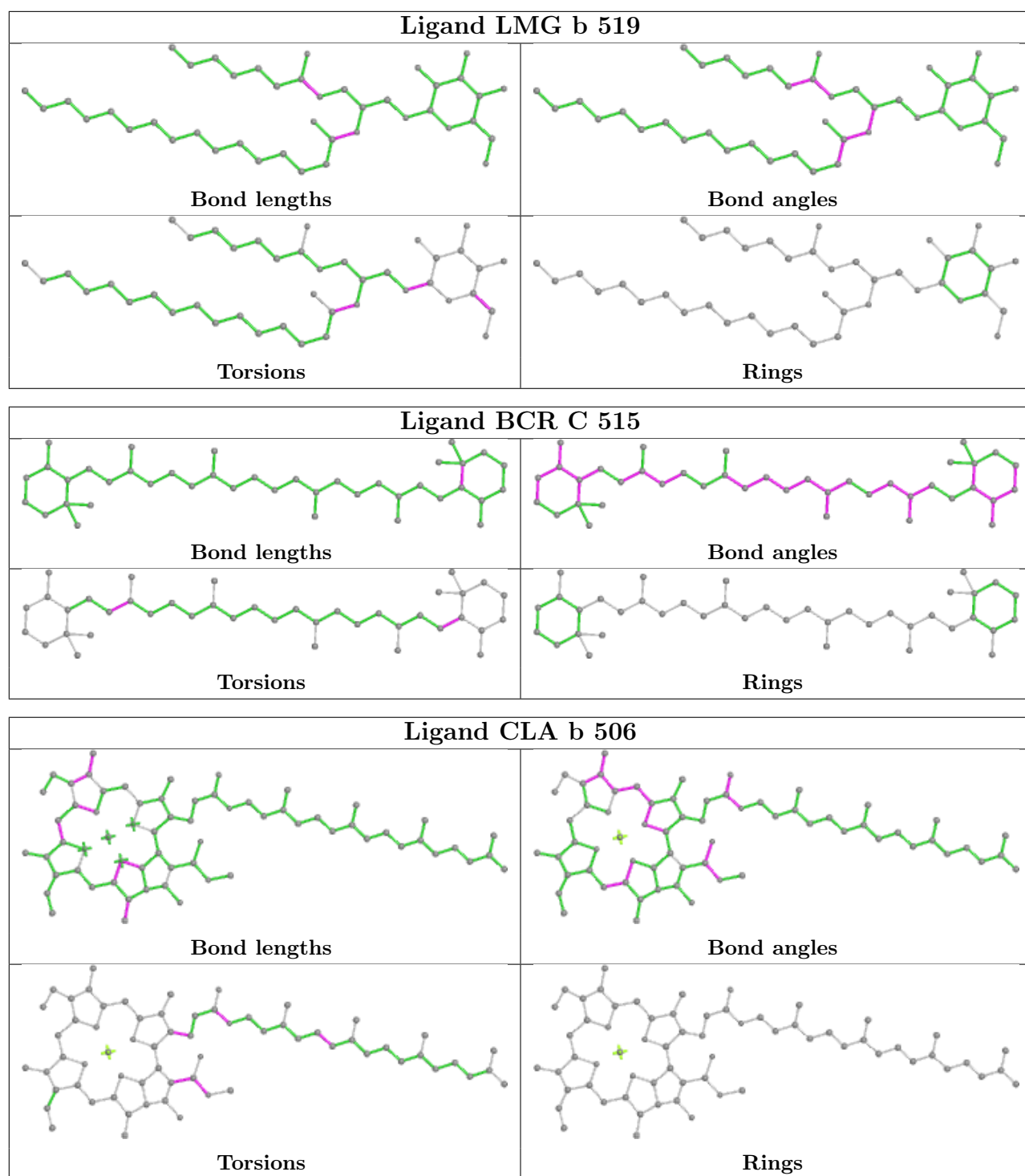
Ligand LHG d 407

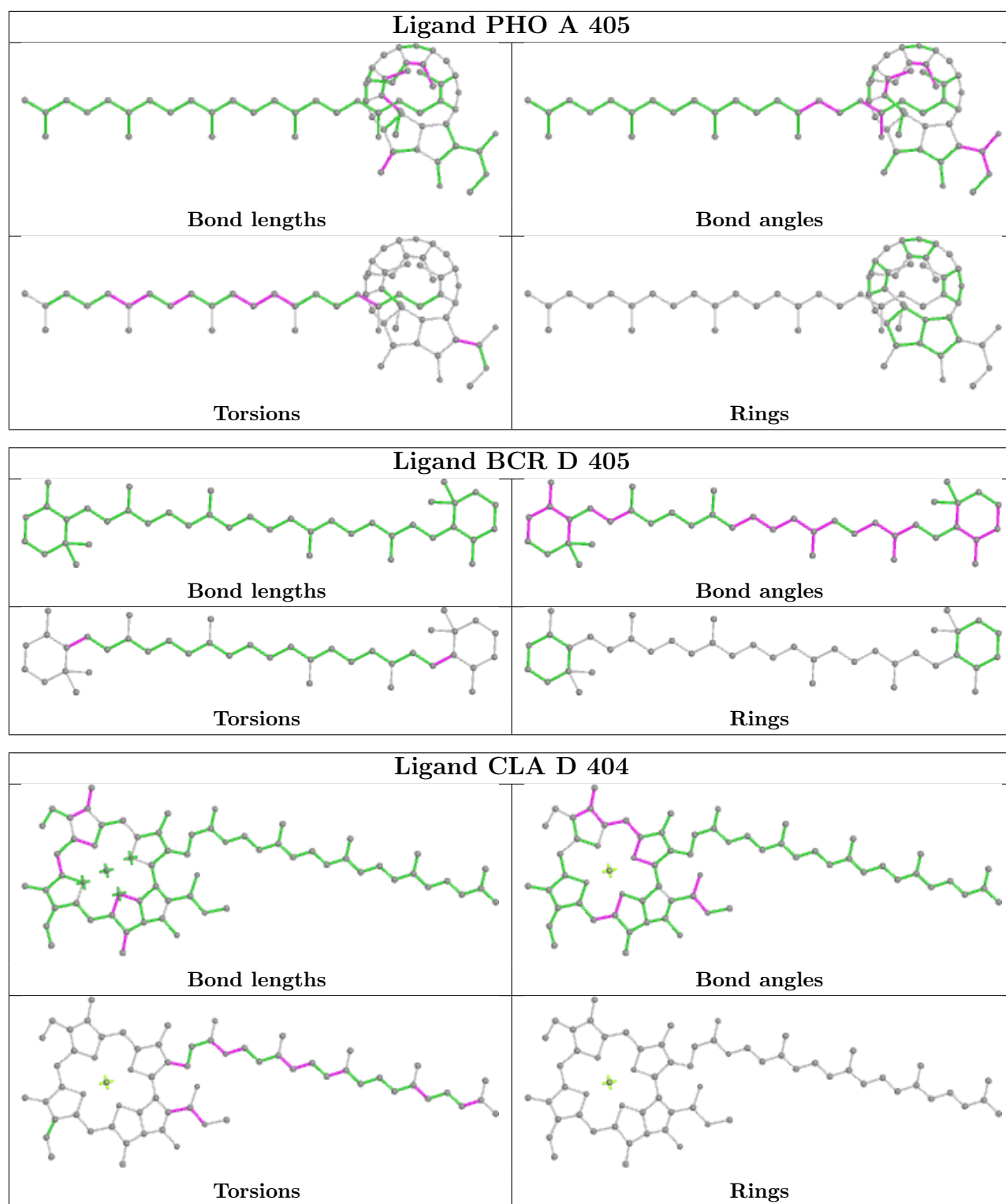


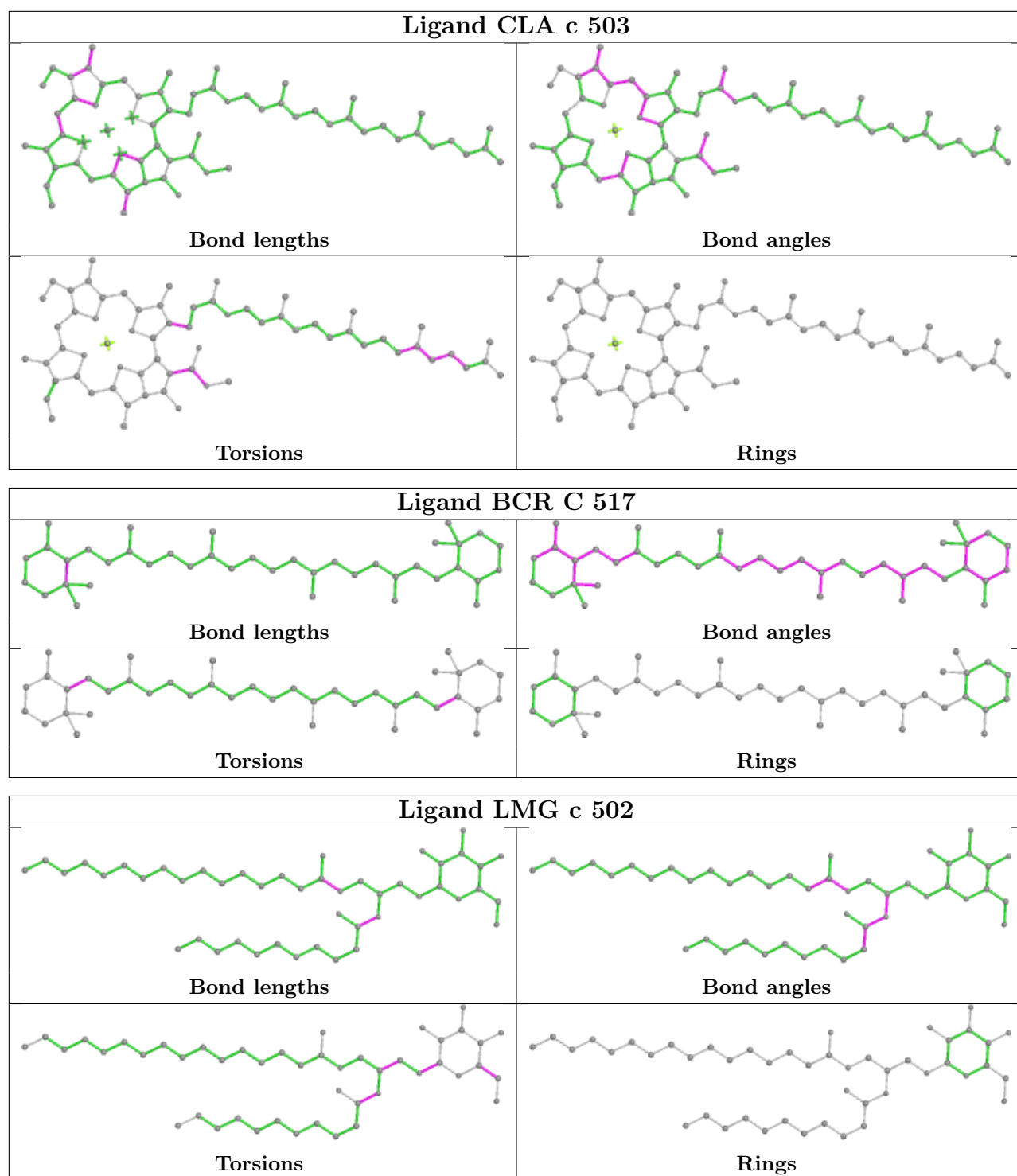
Ligand CLA B 505

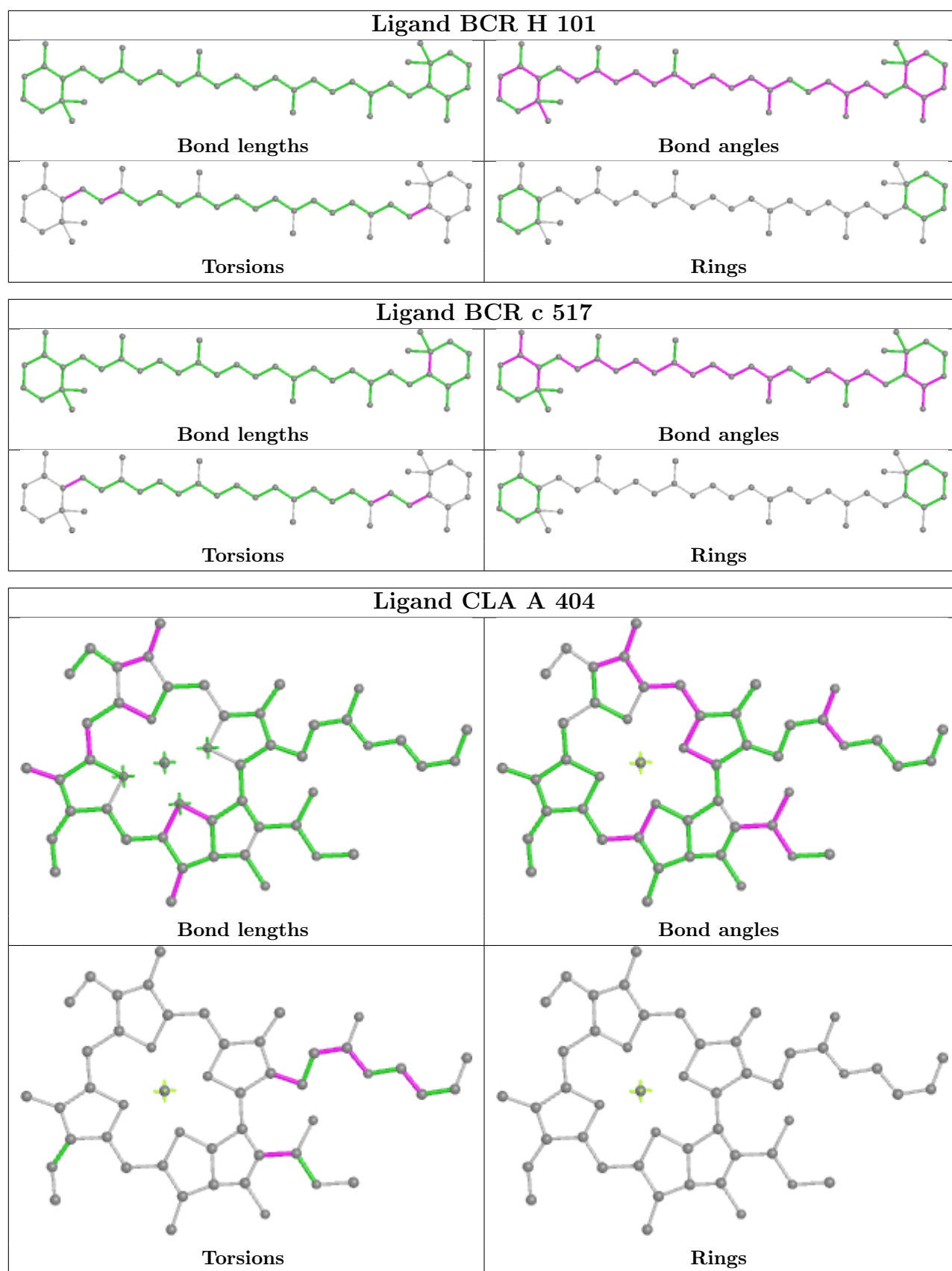


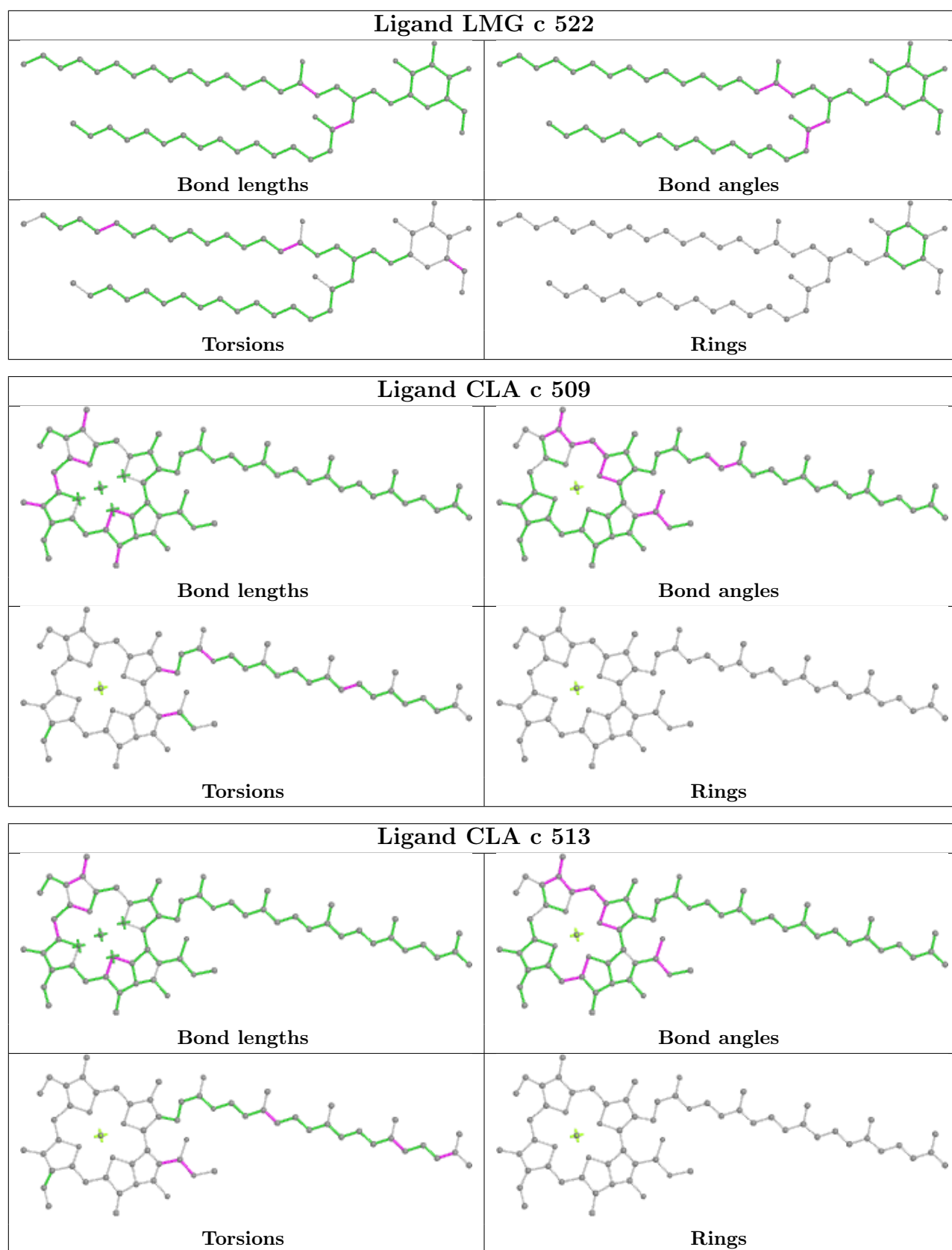


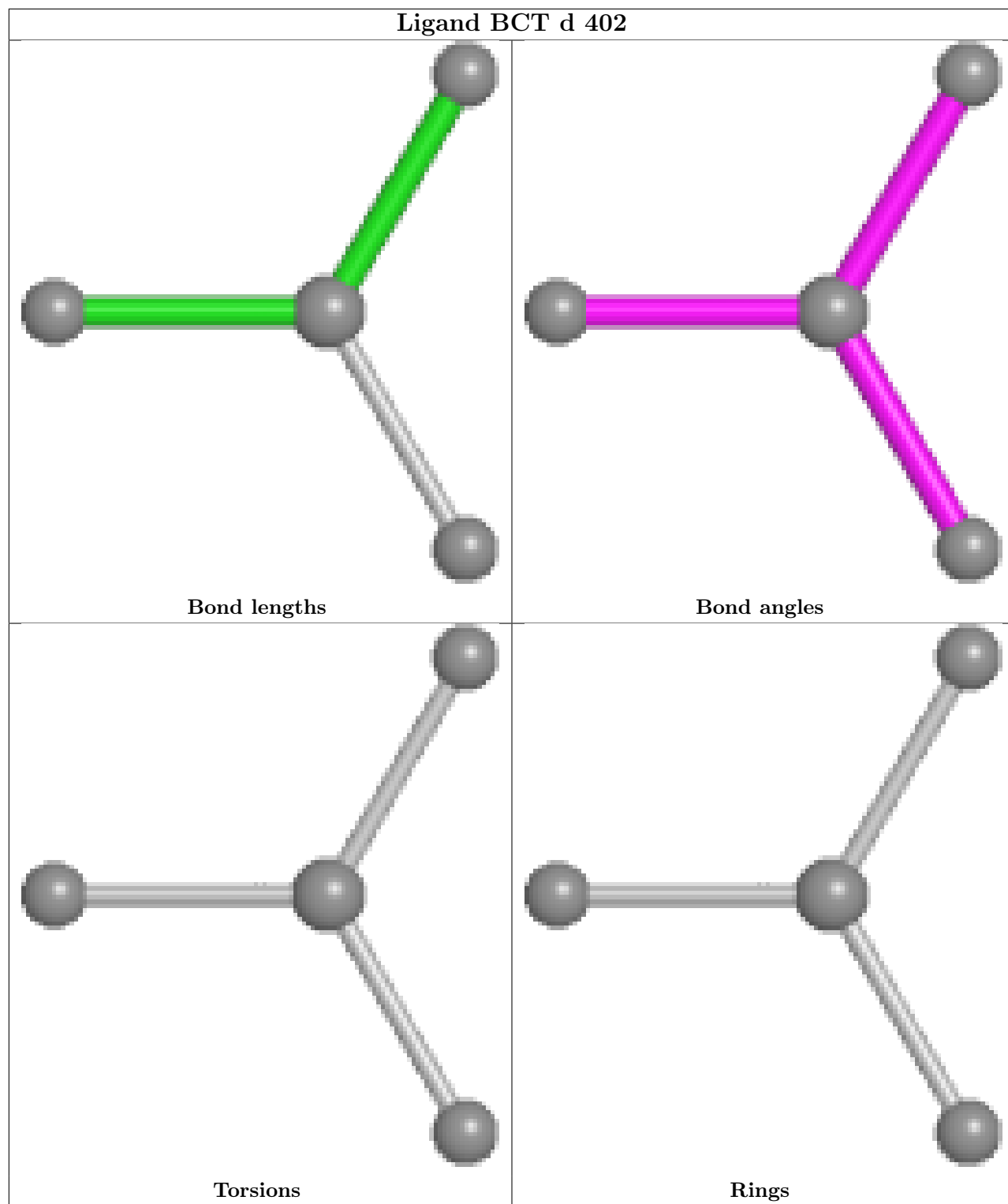


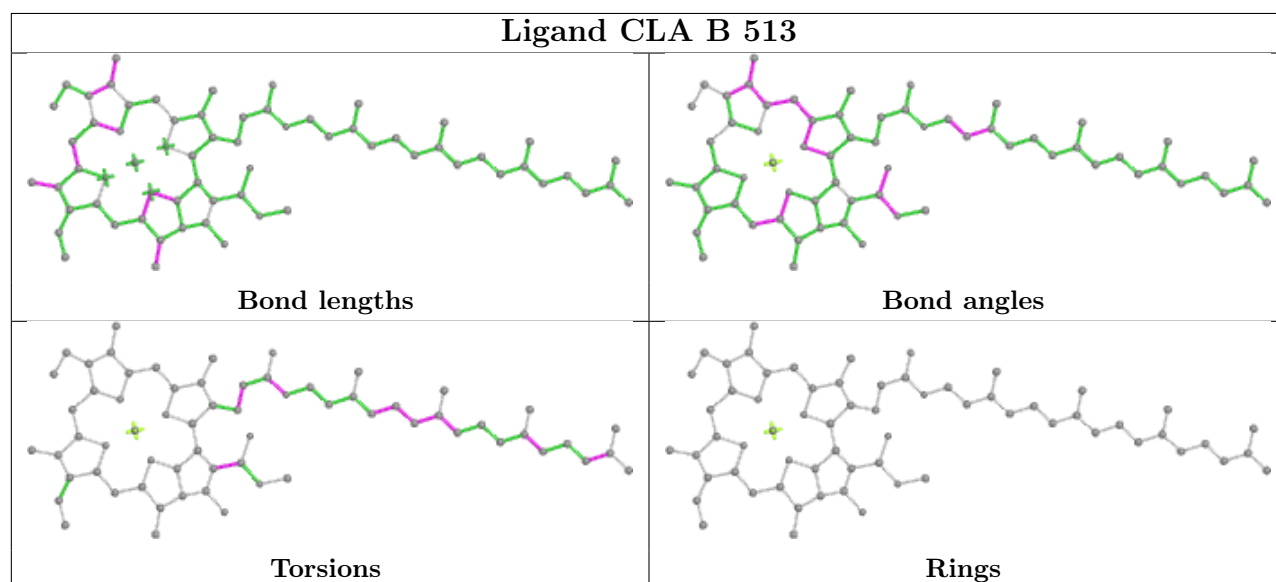
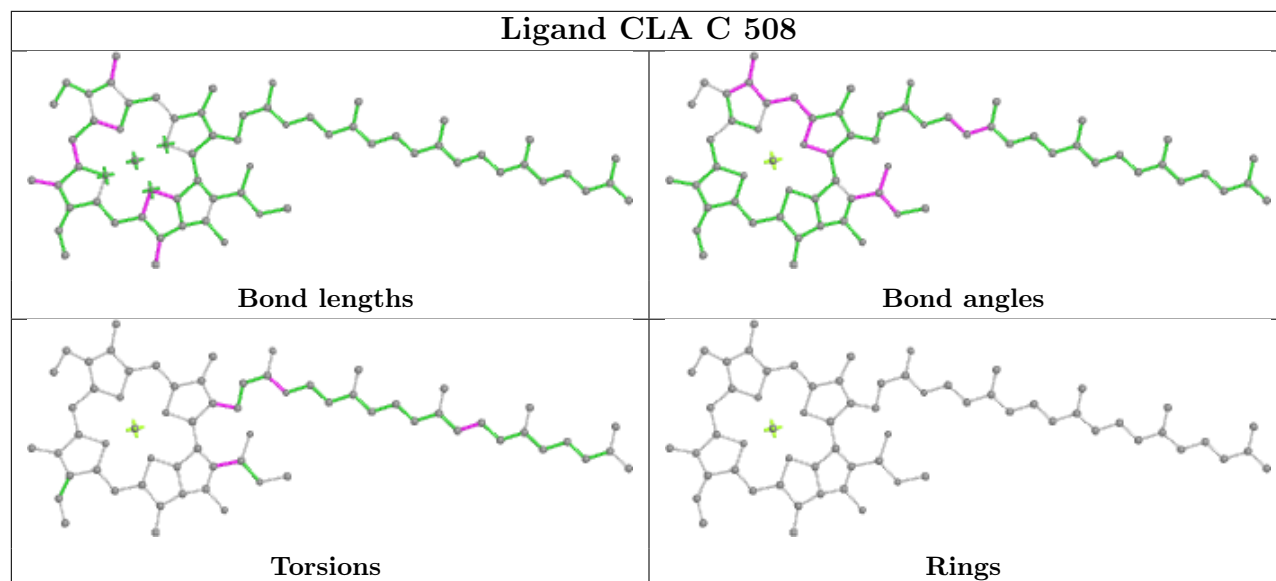
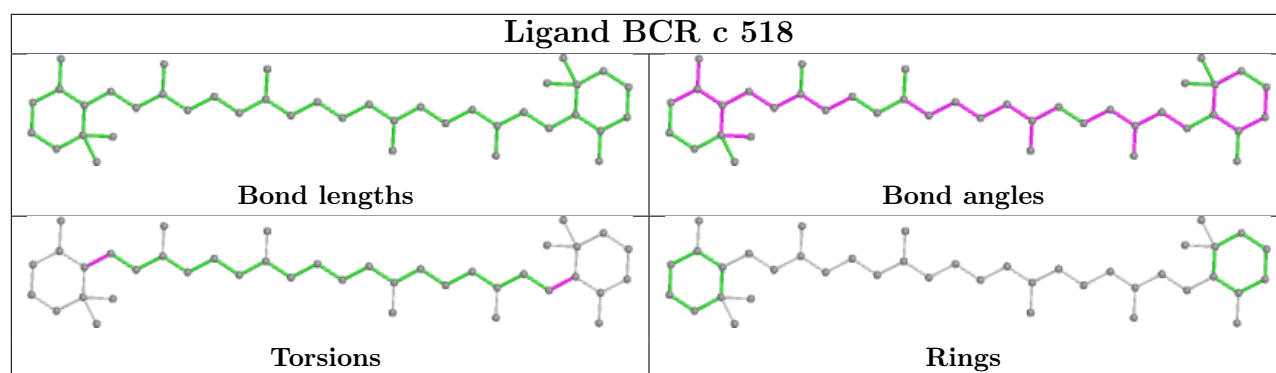


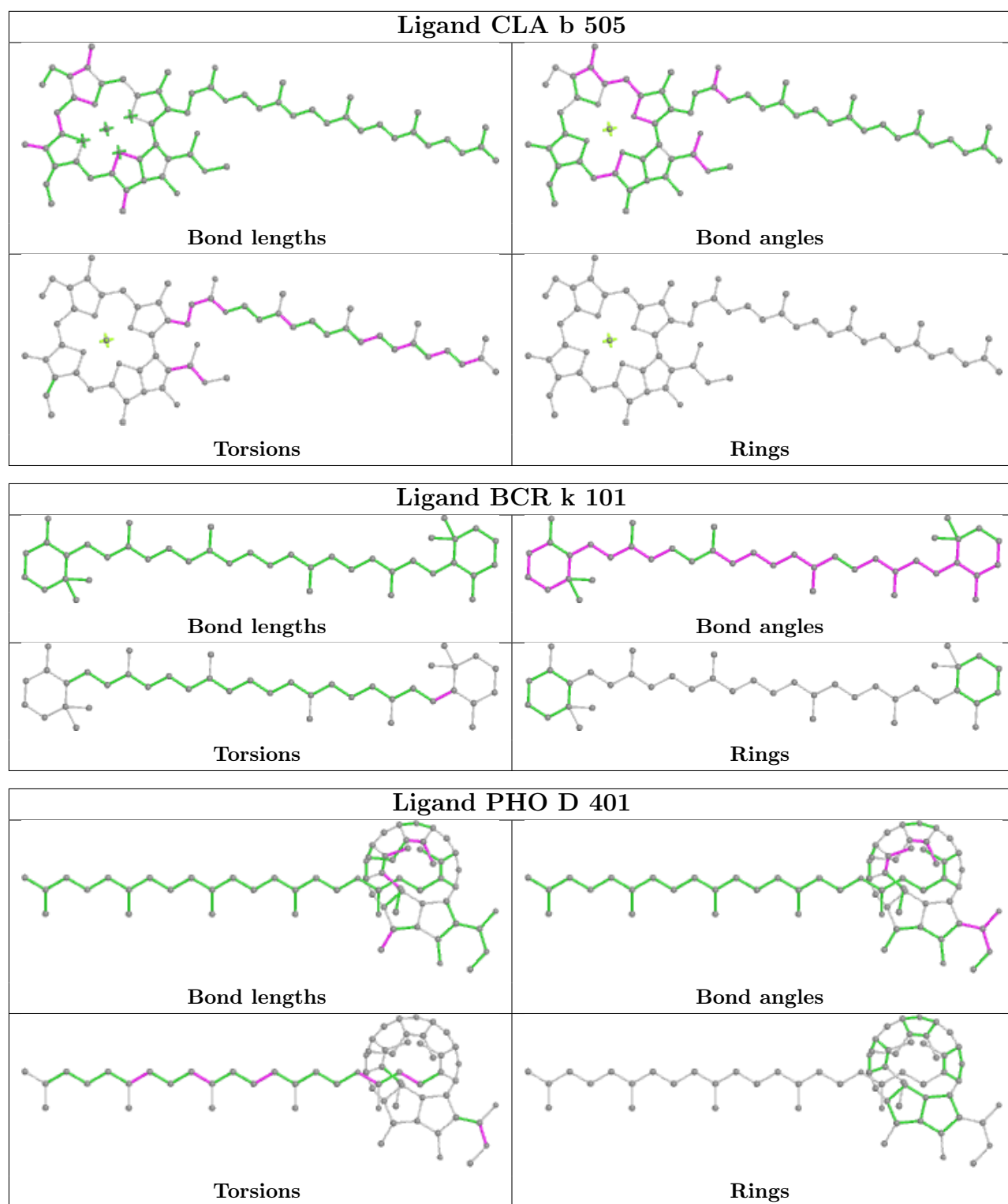




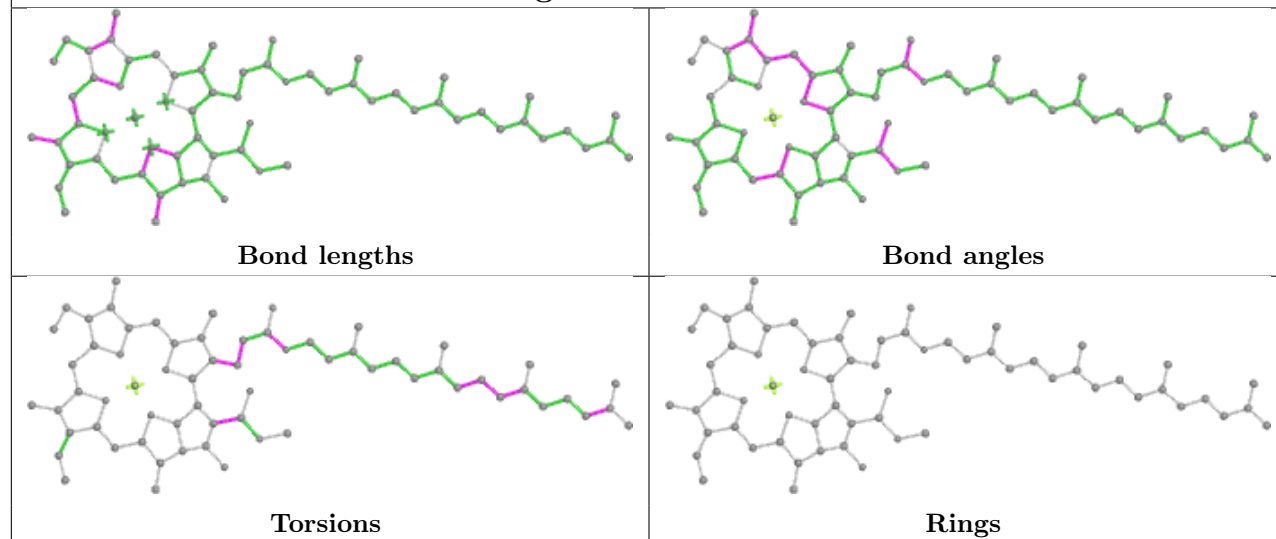




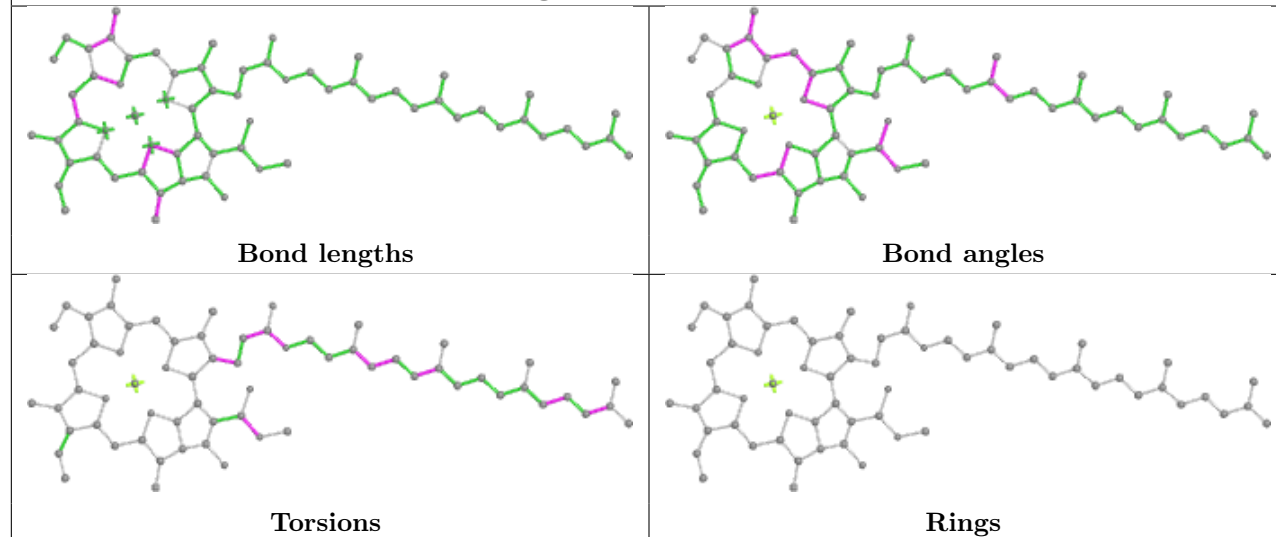




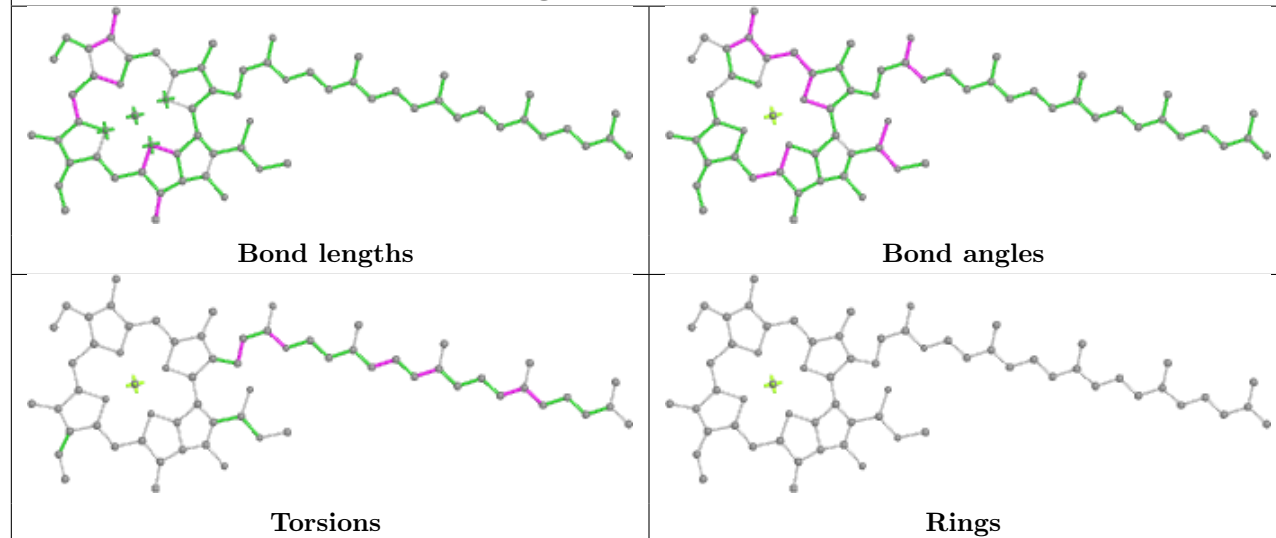
Ligand CLA b 504

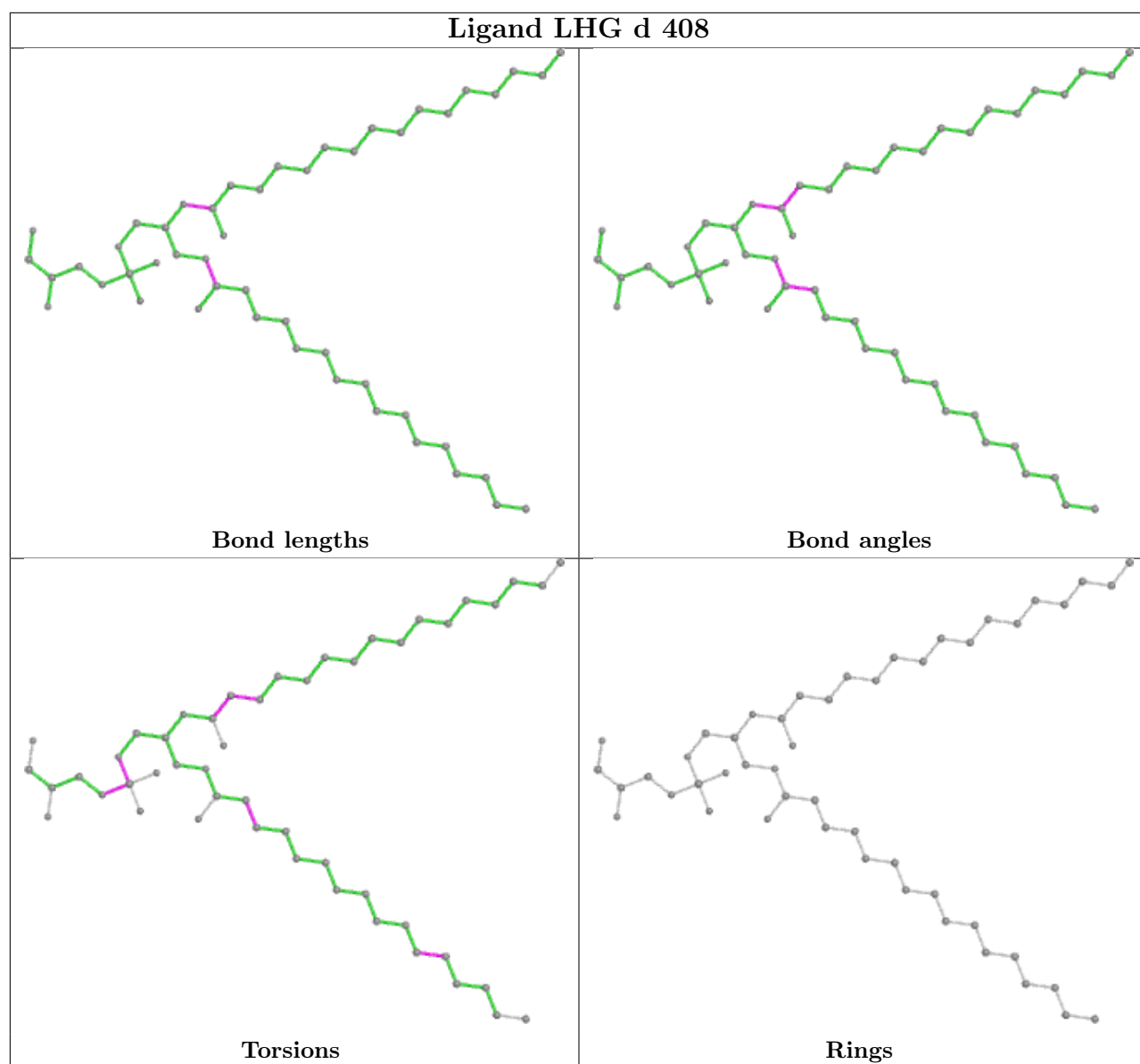


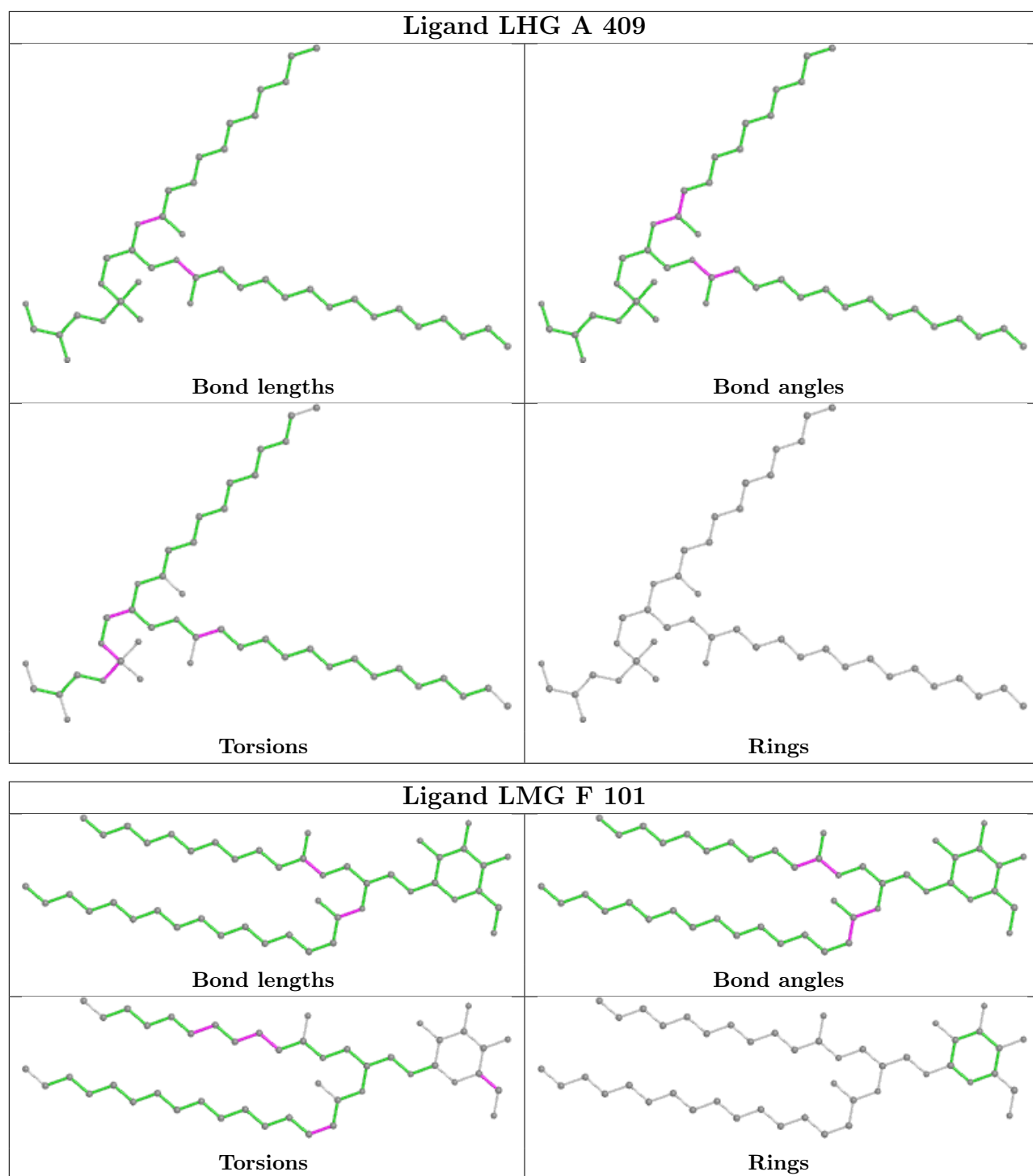
Ligand CLA b 507

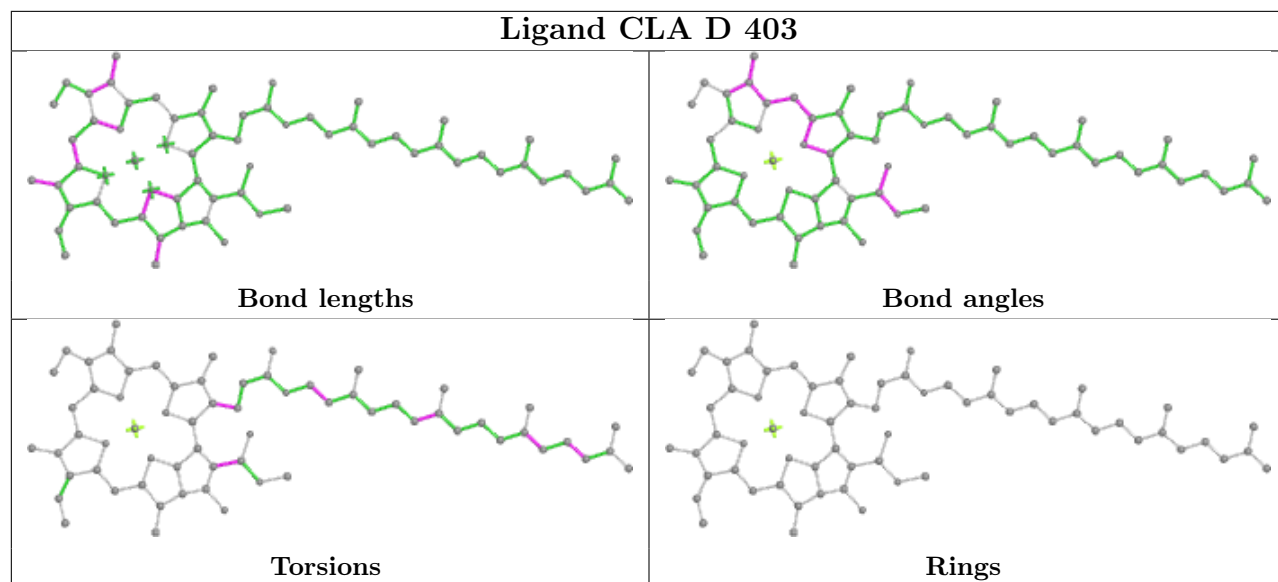
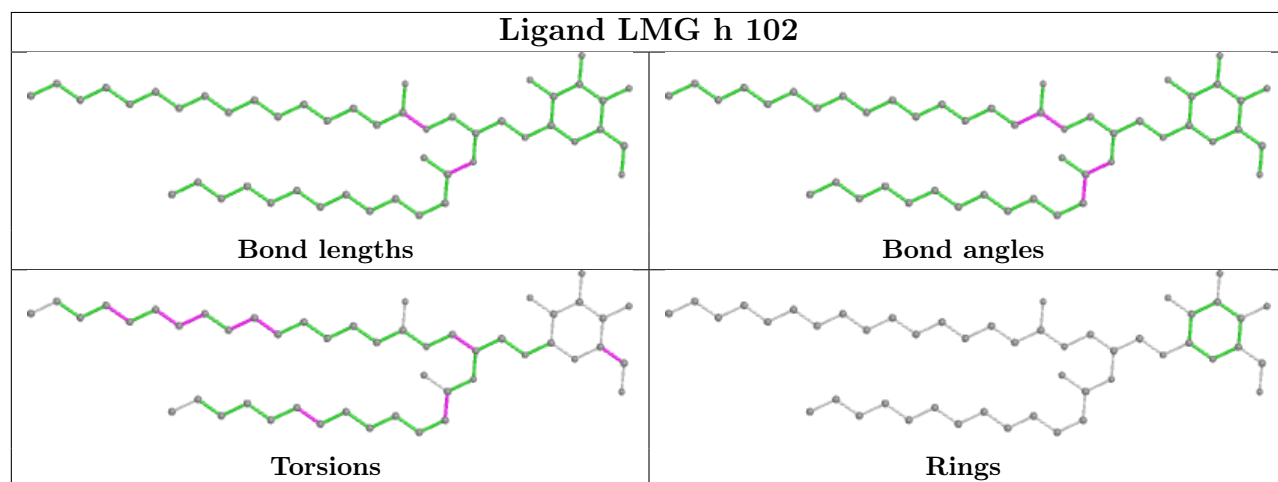
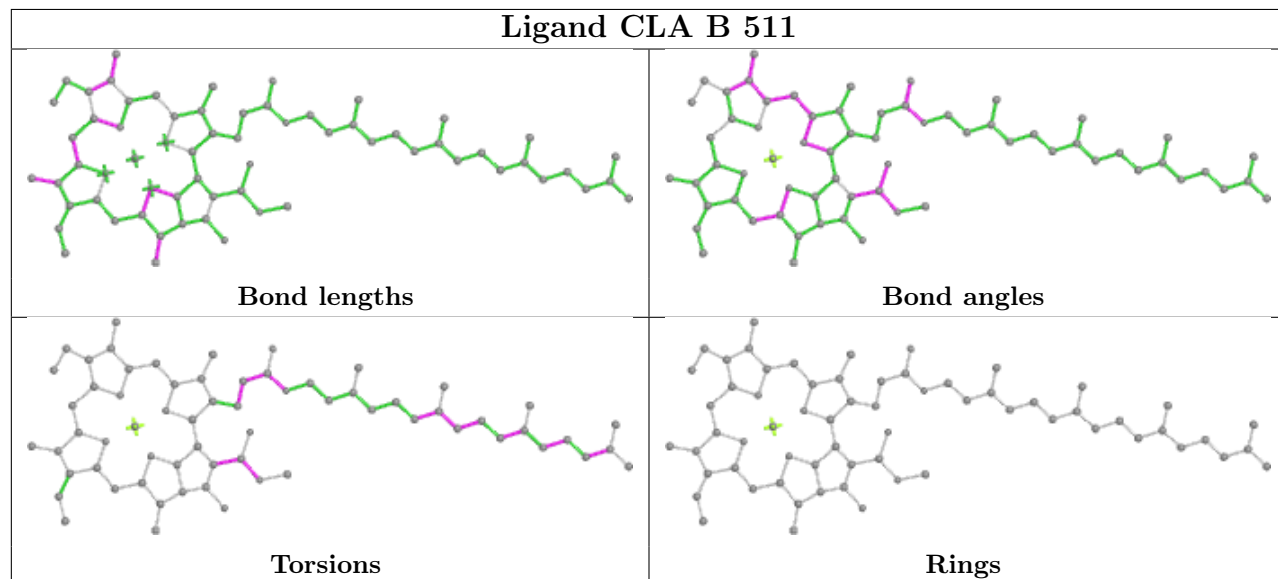


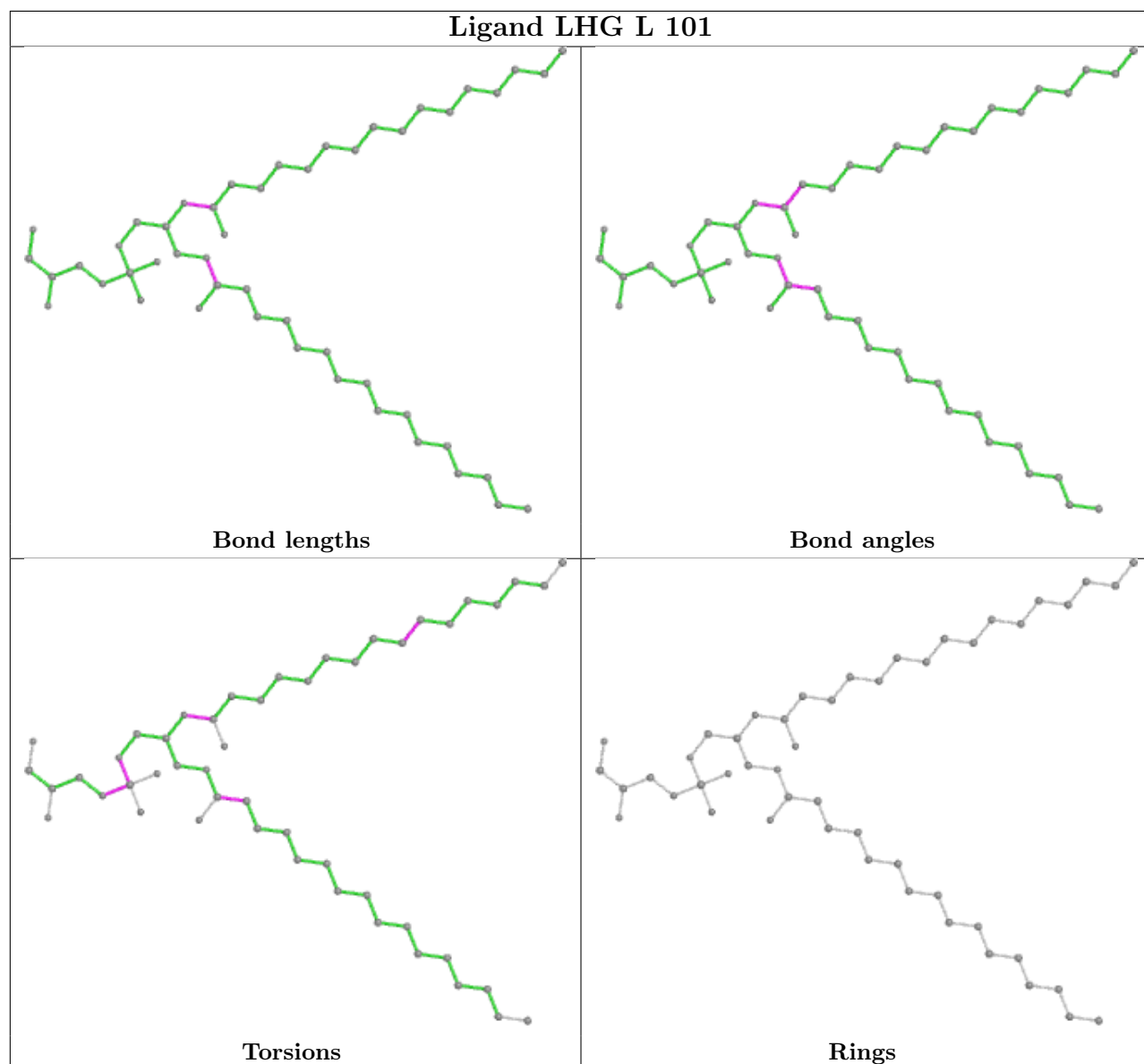
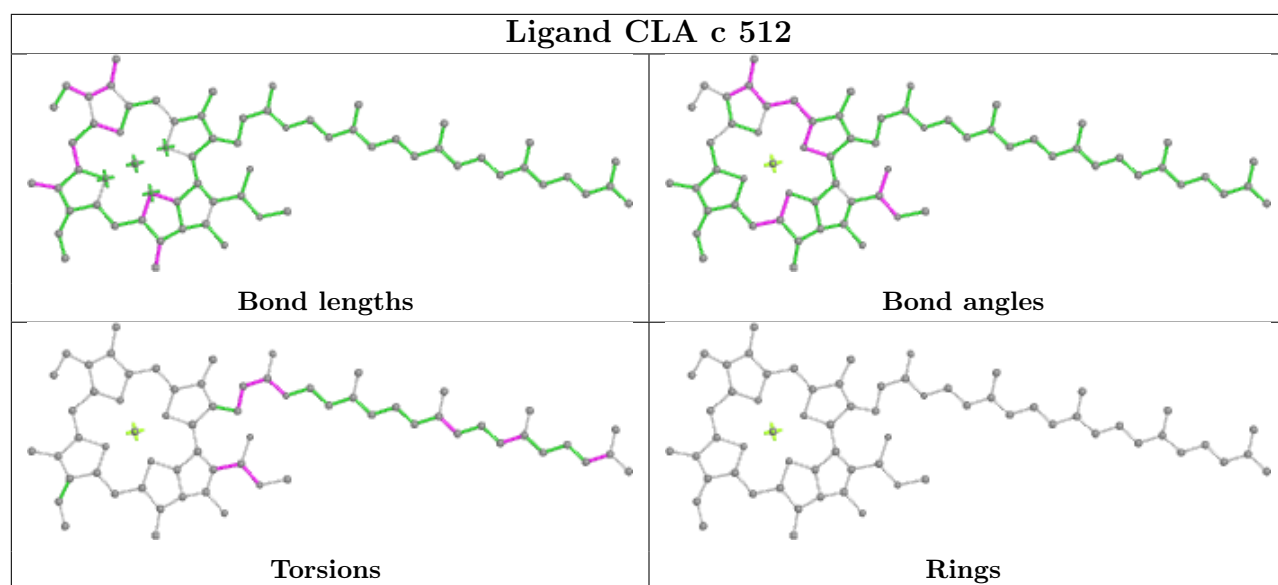
Ligand CLA b 508

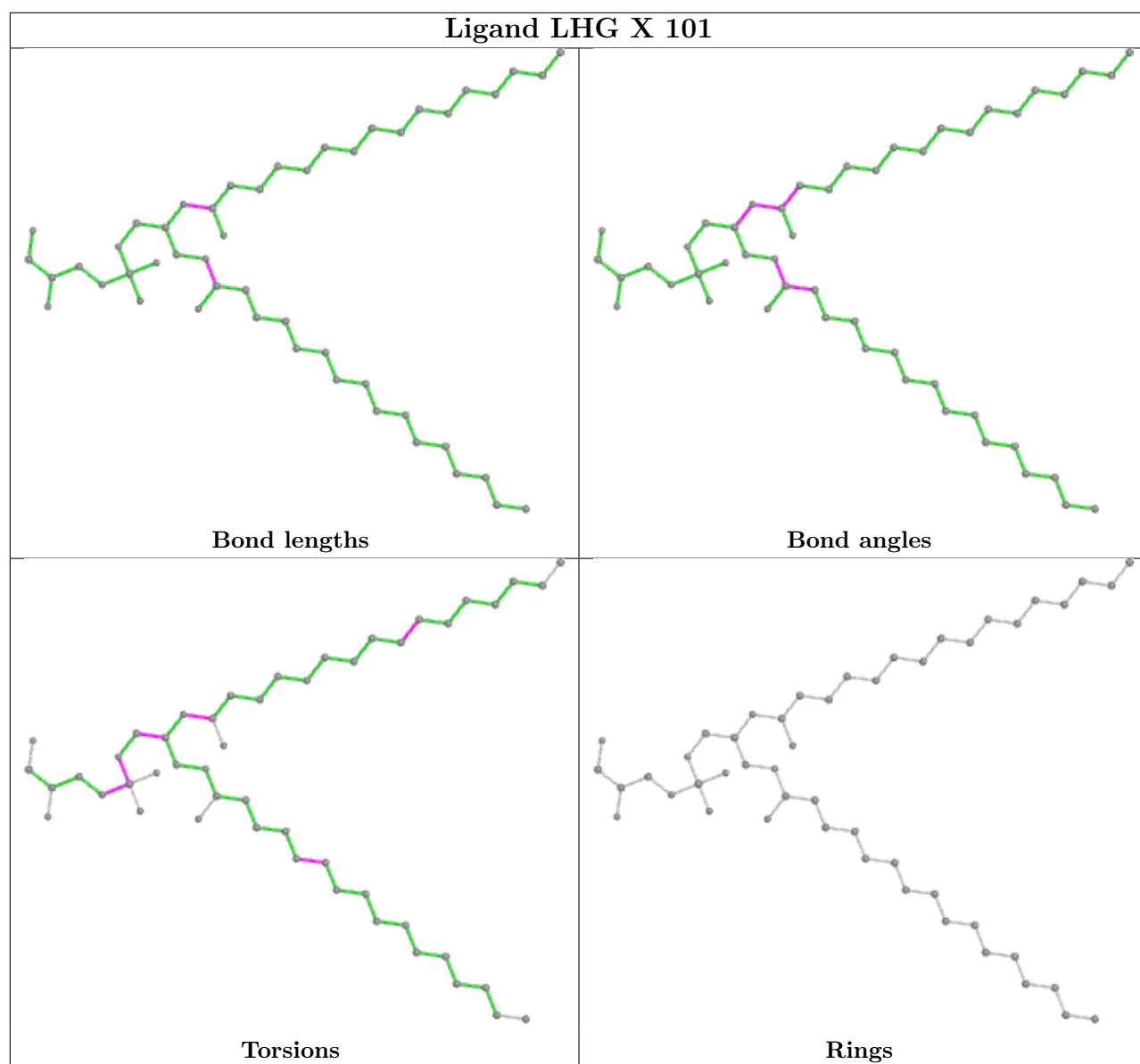


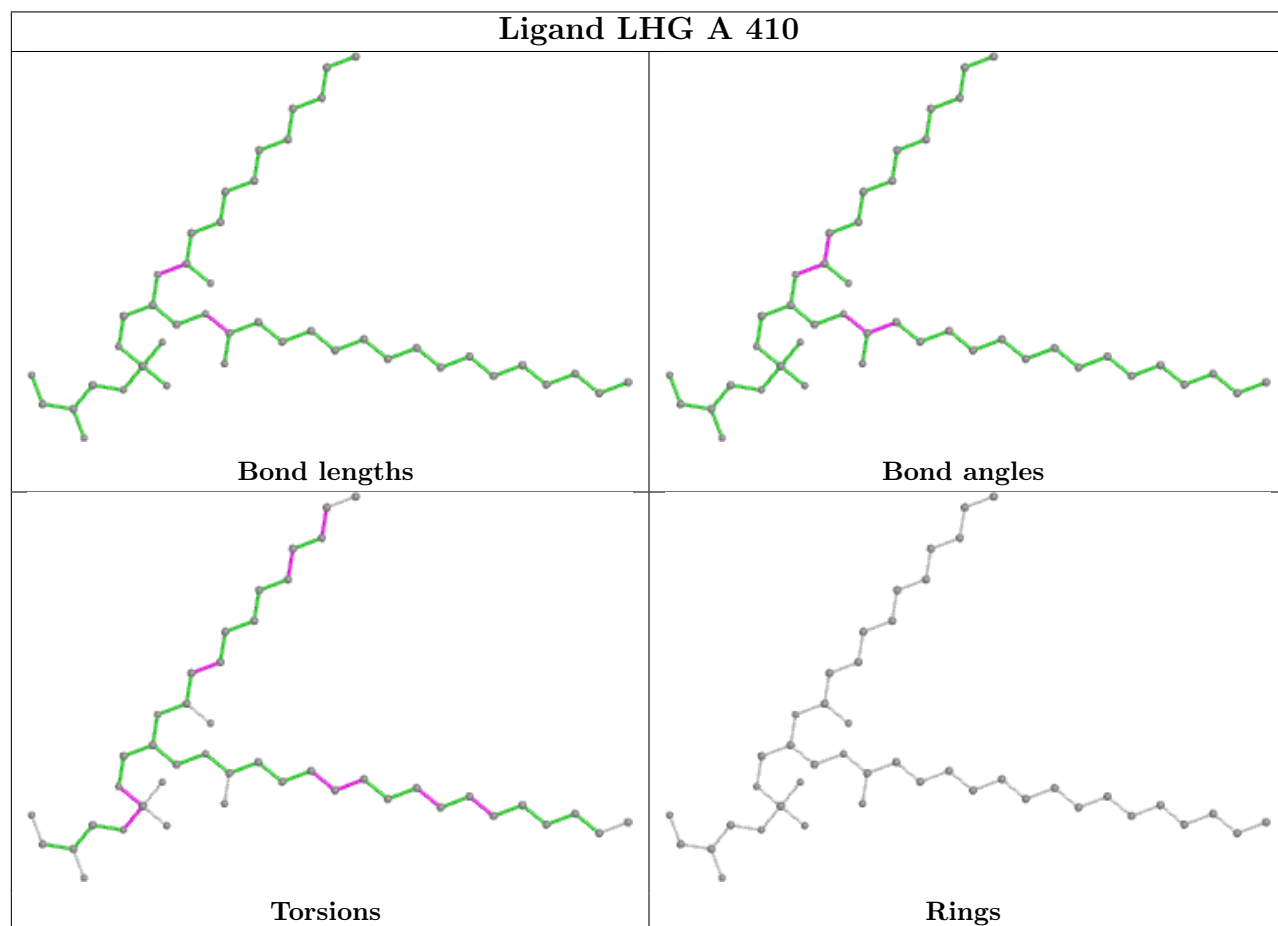
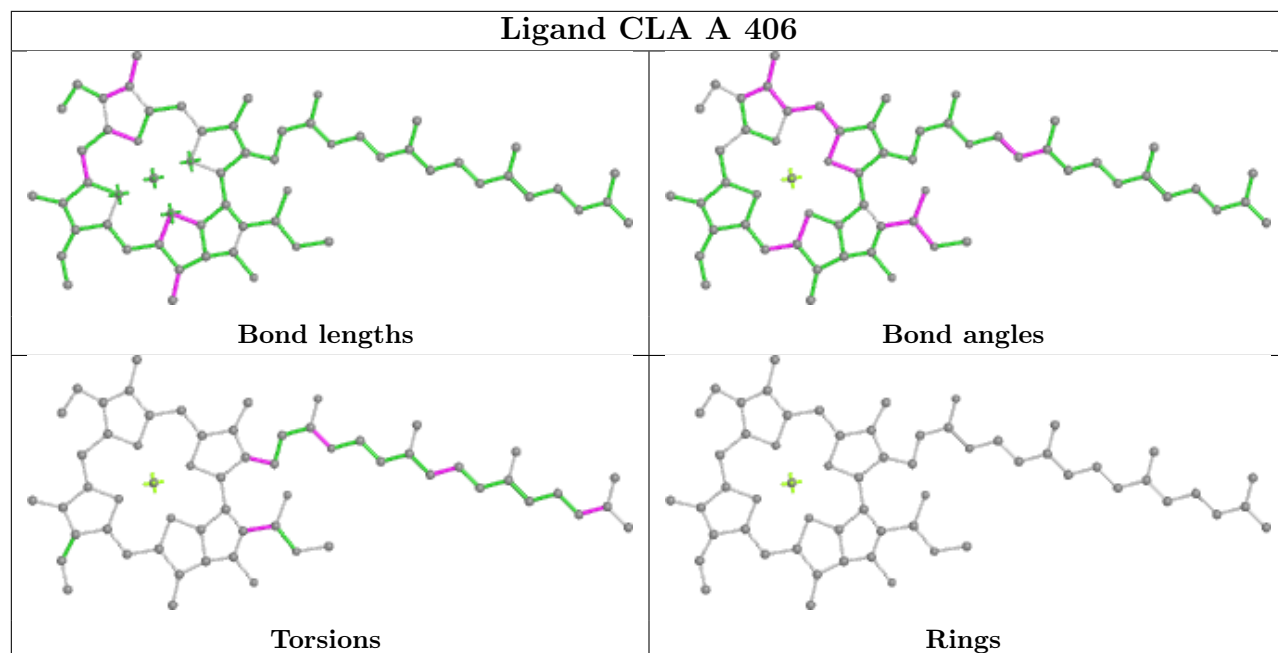


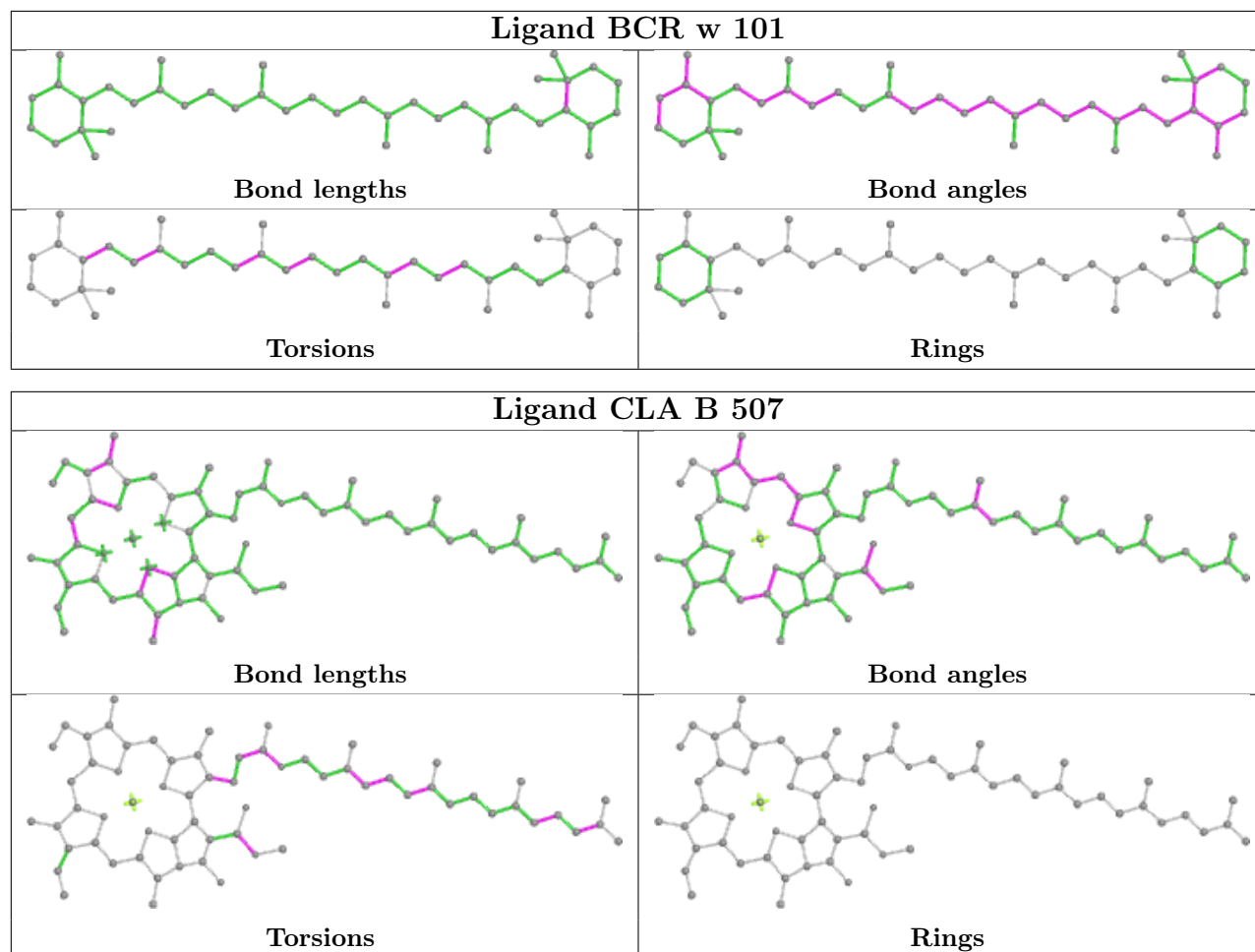


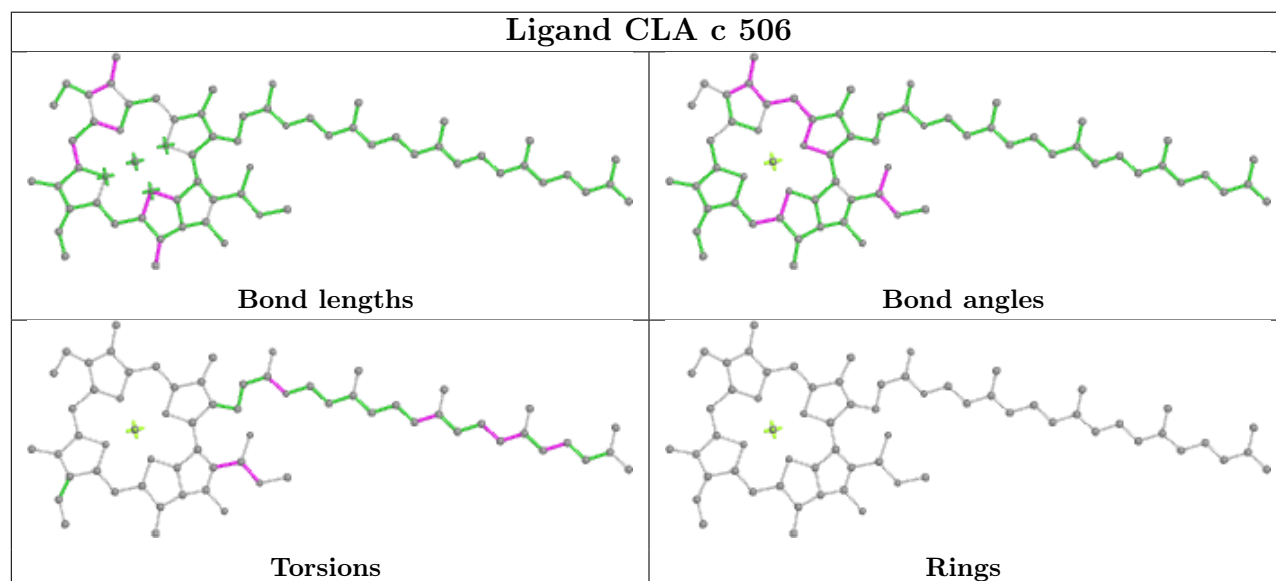
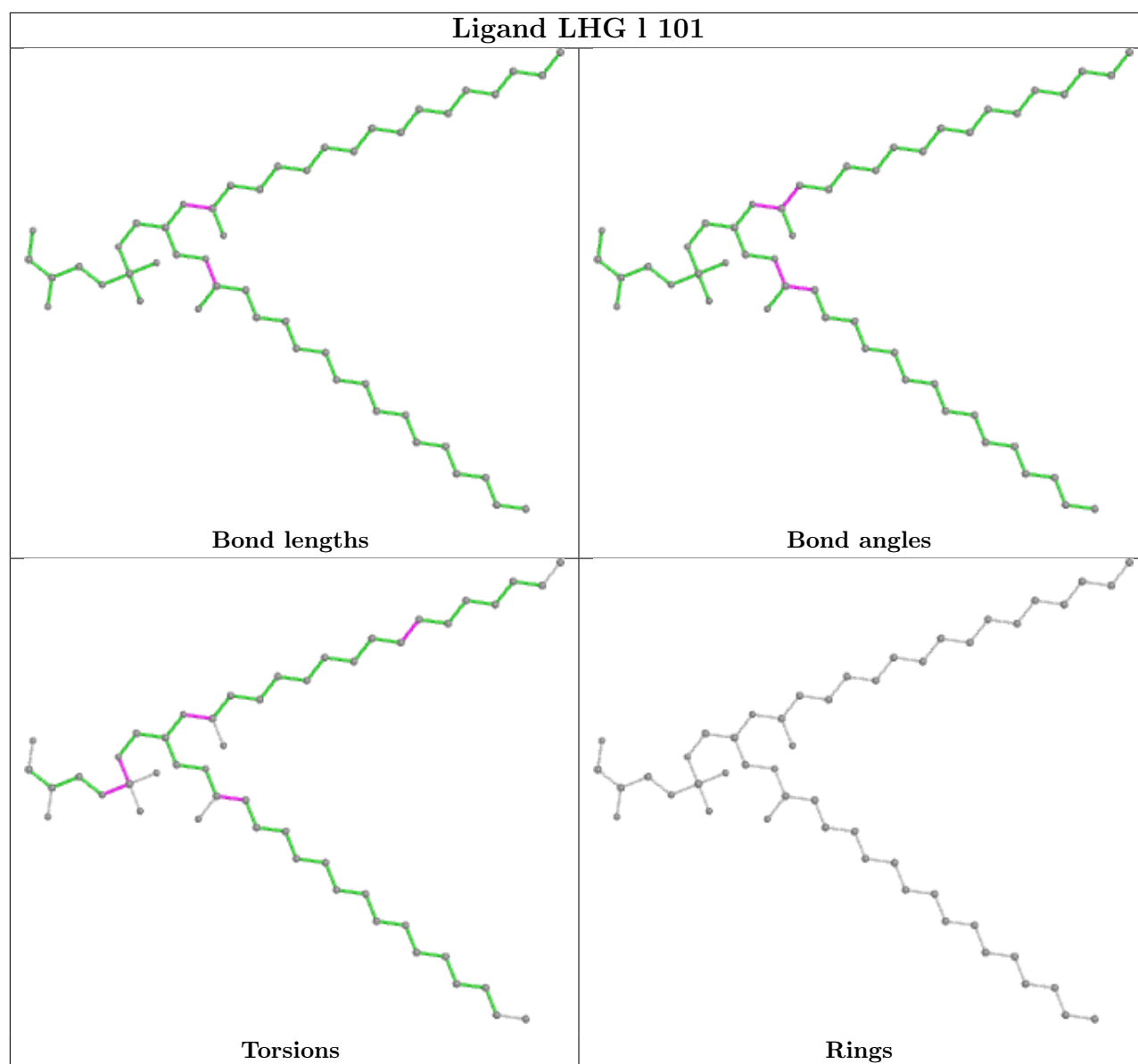
Ligand CLA D 403**Ligand LMG h 102****Ligand CLA B 511**

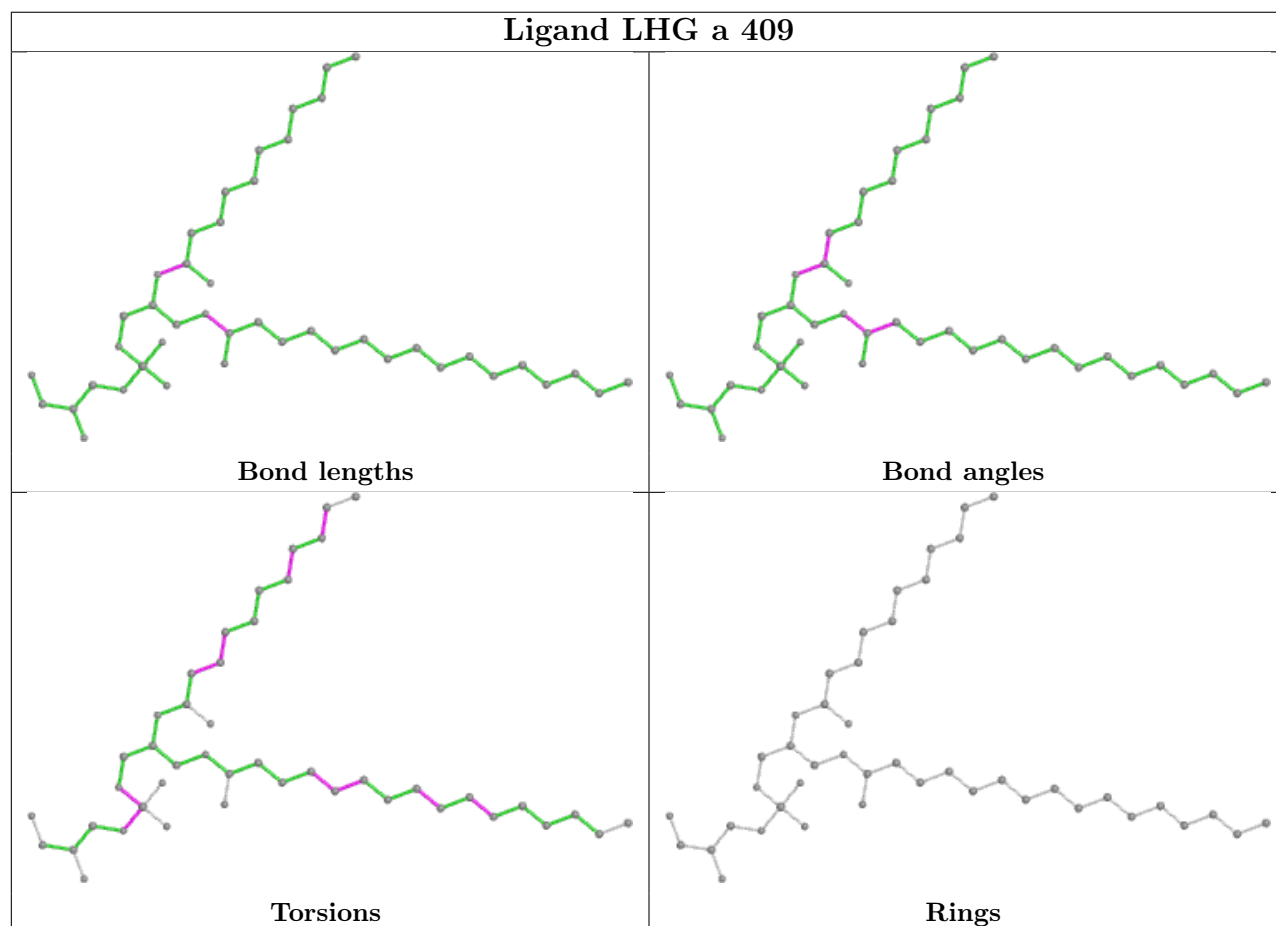
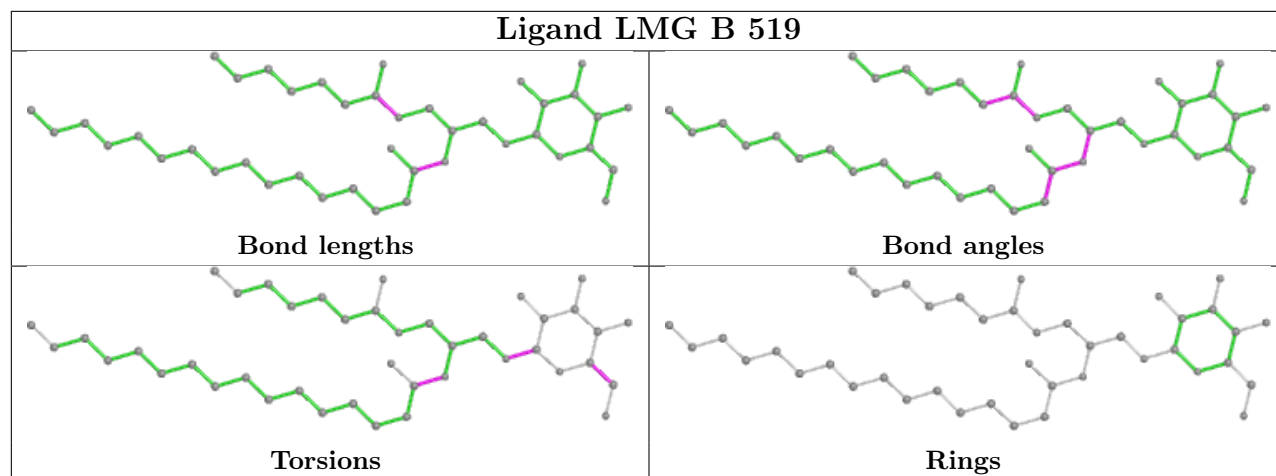


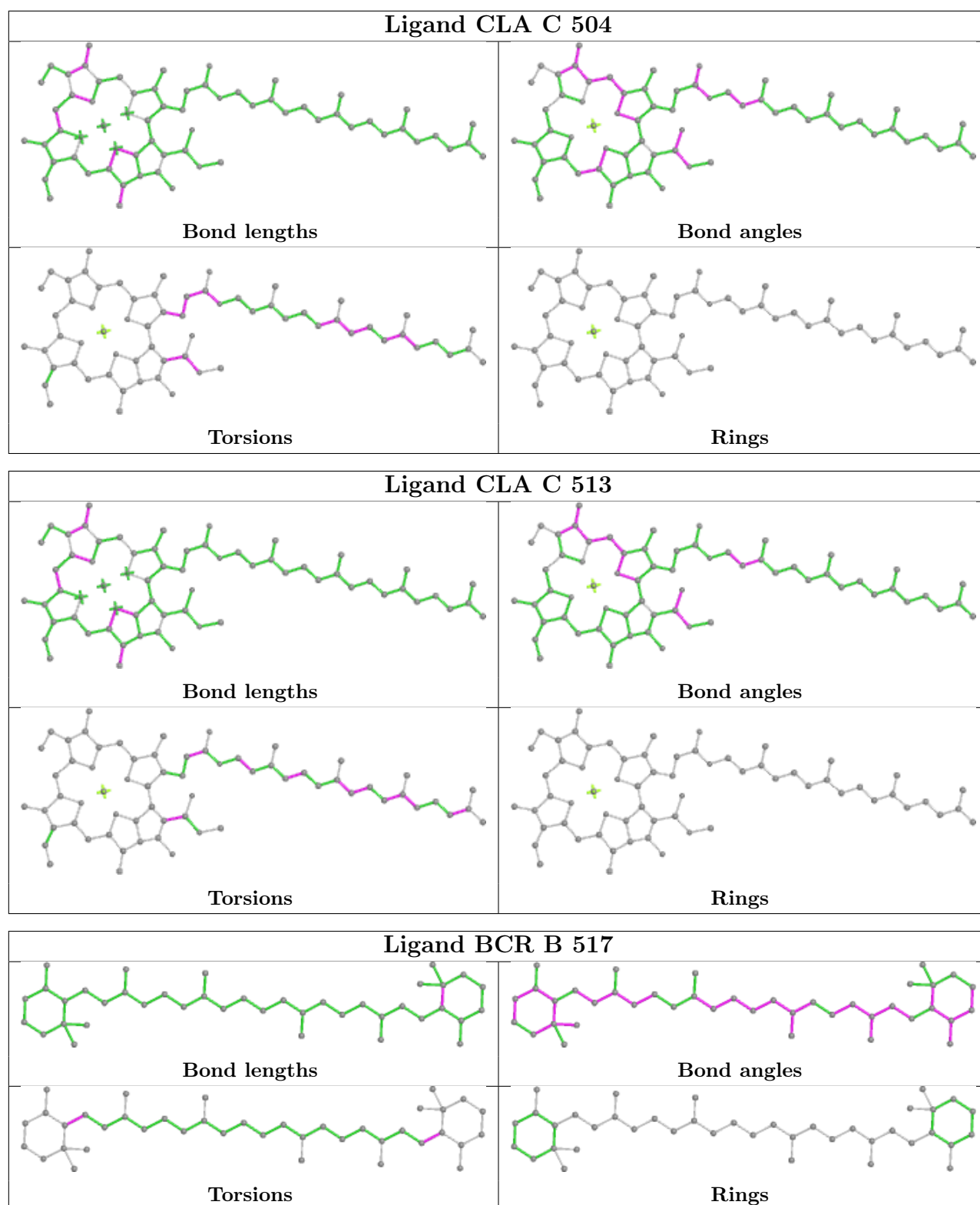


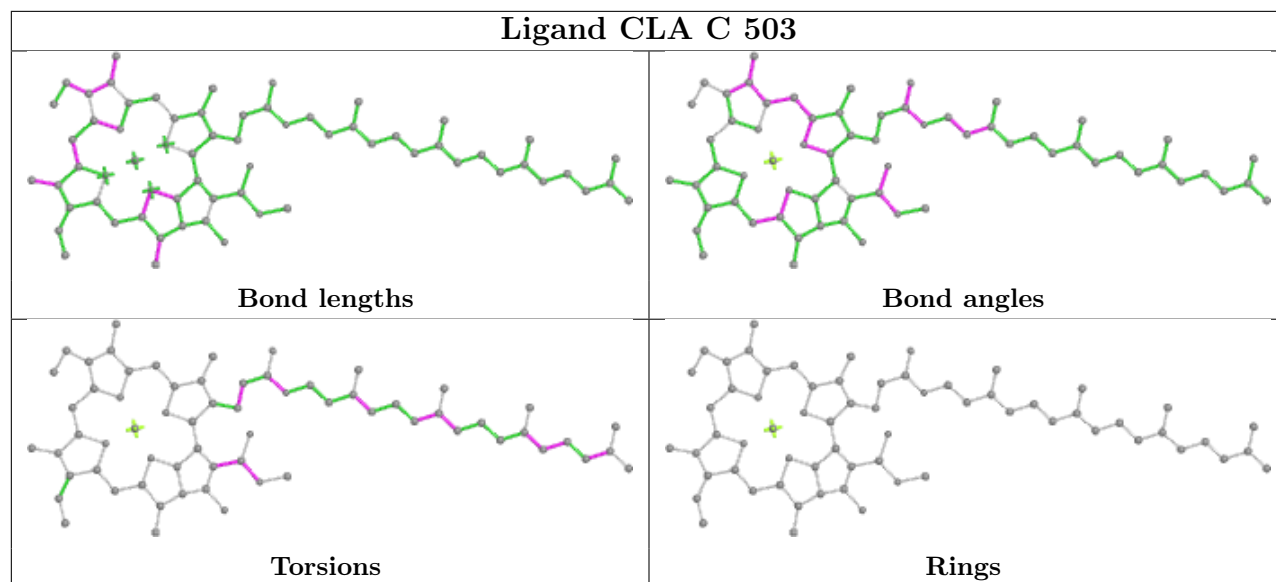
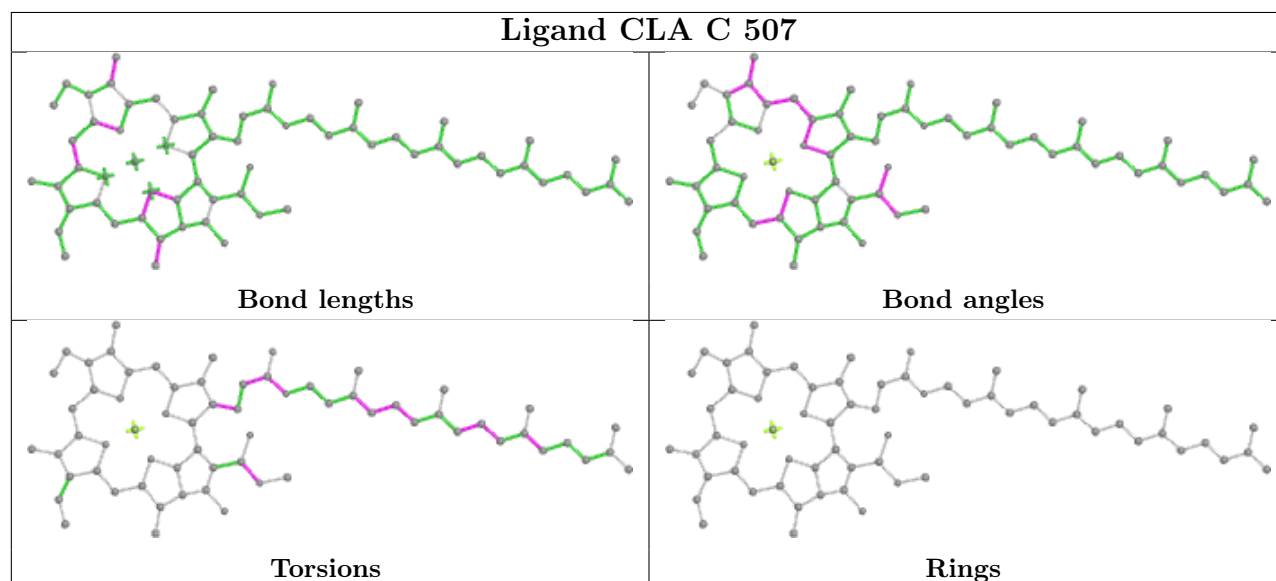
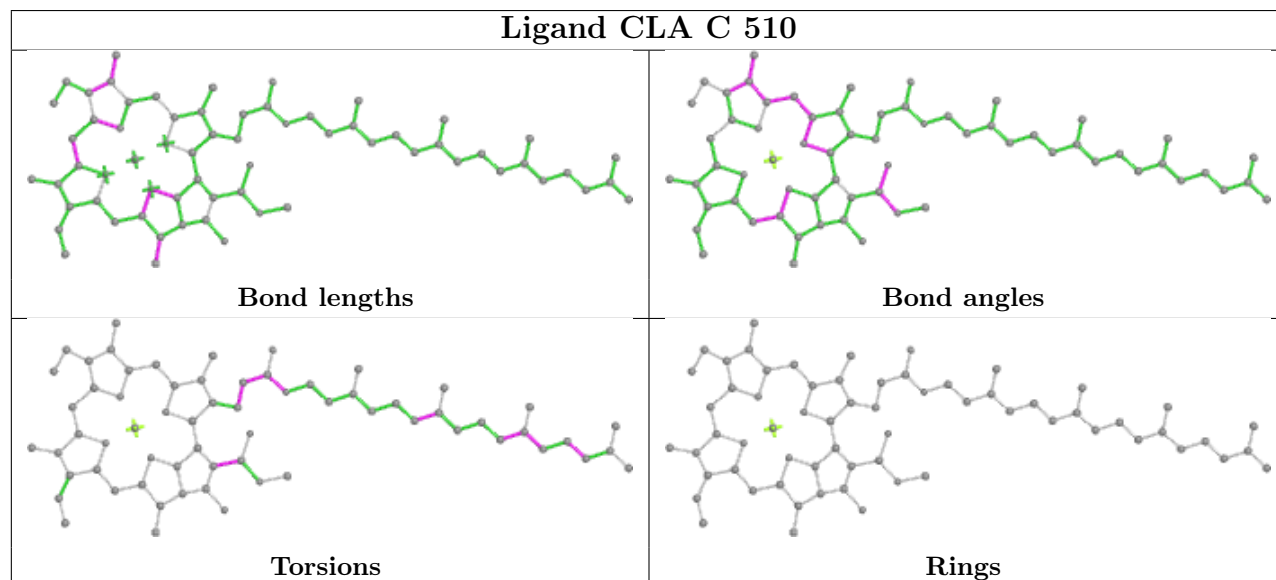


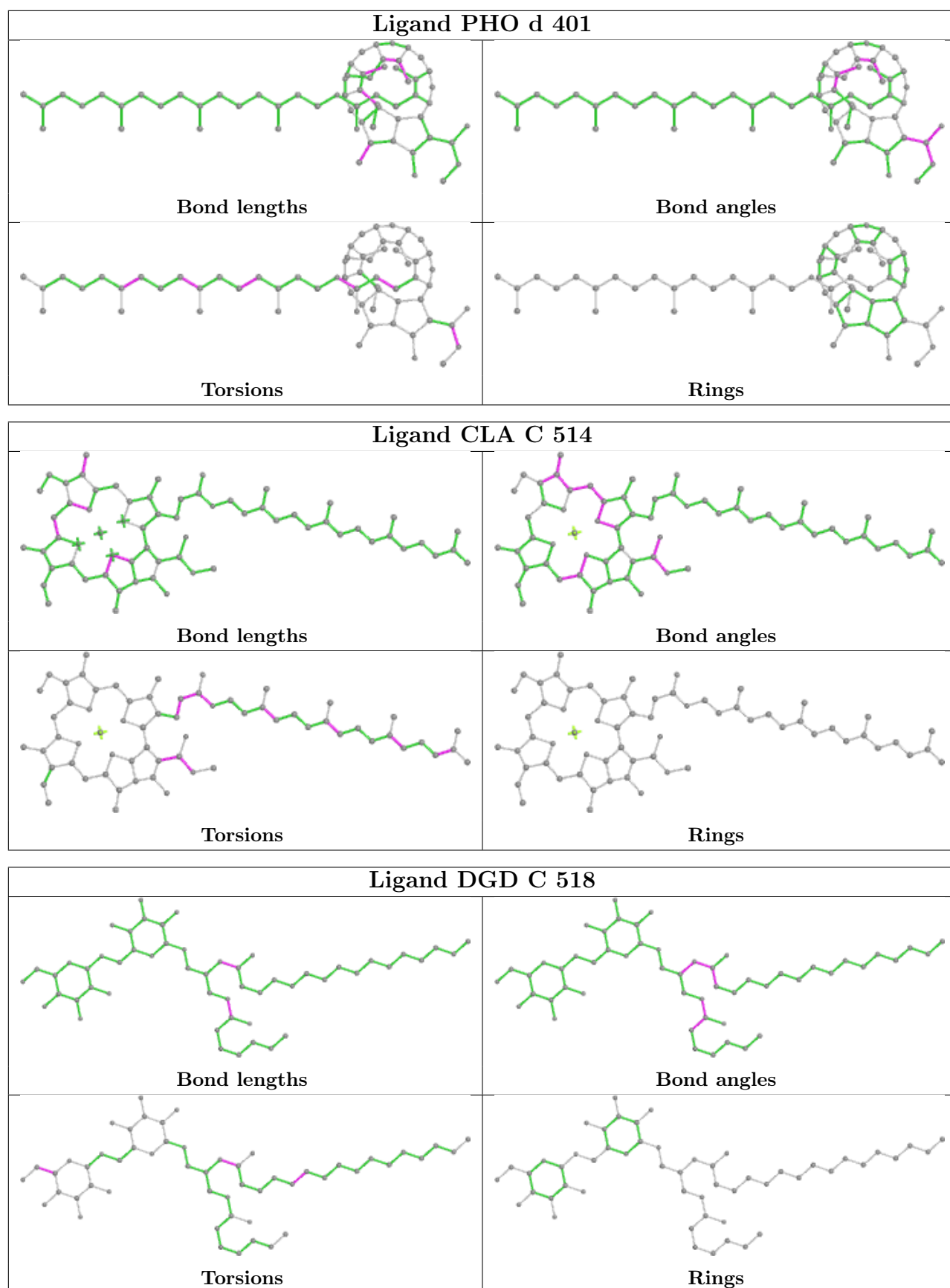


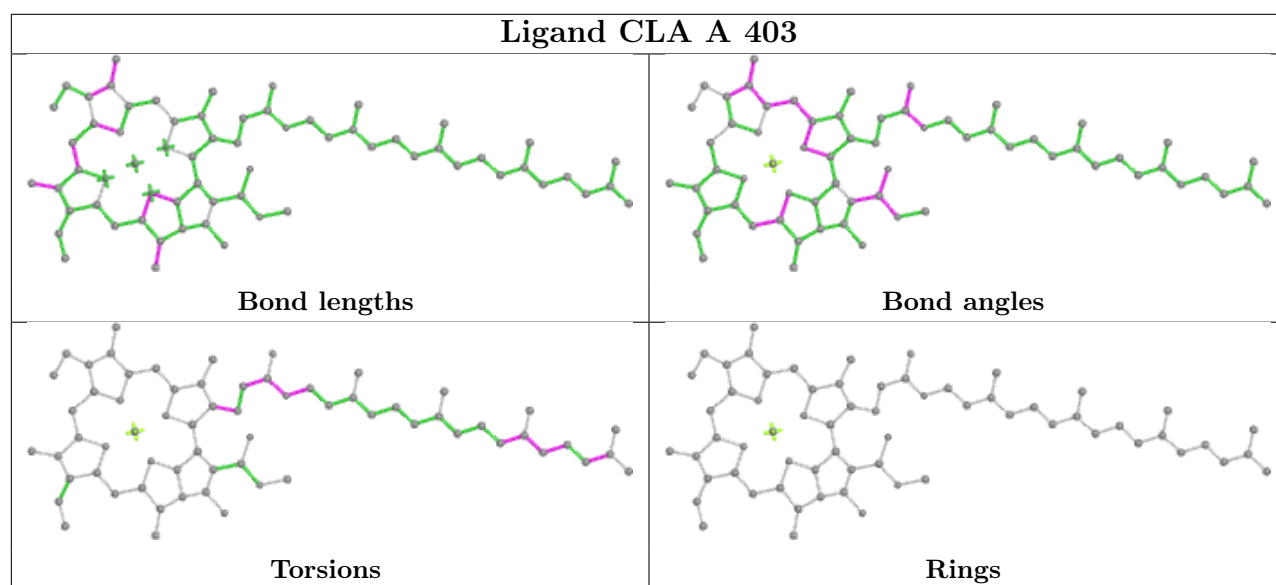






Ligand CLA C 503**Ligand CLA C 507****Ligand CLA C 510**





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.

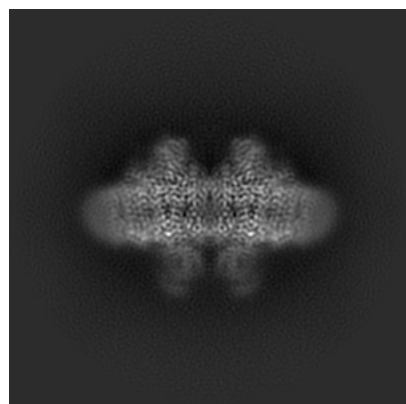
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60694. These allow visual inspection of the internal detail of the map and identification of artifacts.

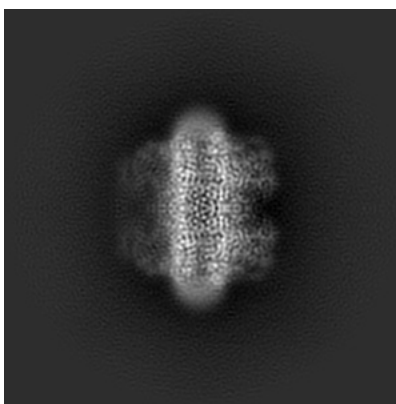
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

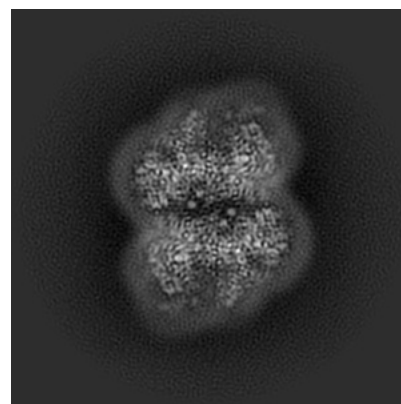
6.1.1 Primary map



X

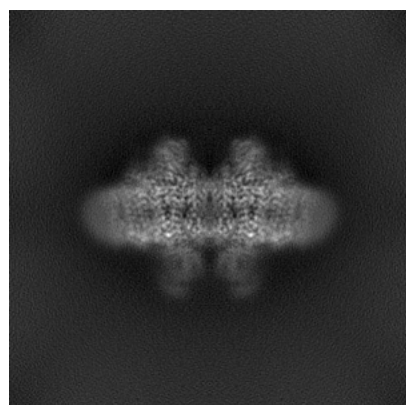


Y

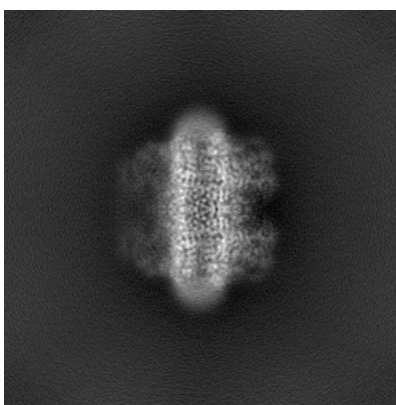


Z

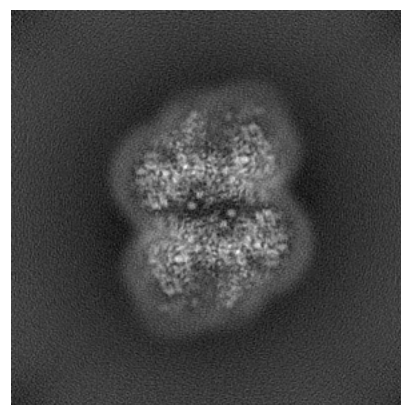
6.1.2 Raw map



X



Y

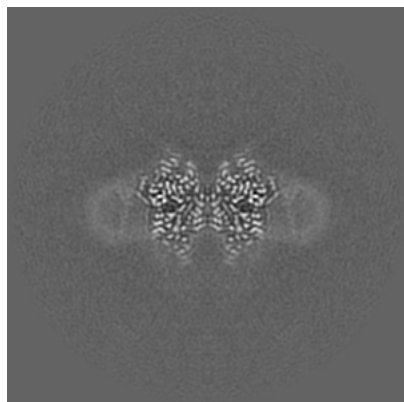


Z

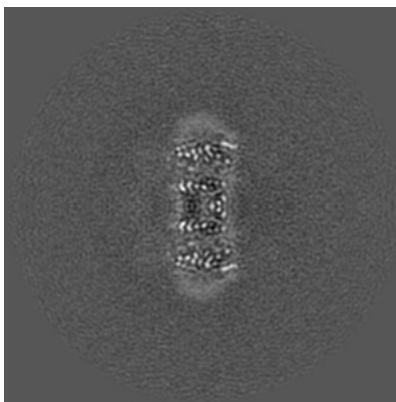
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

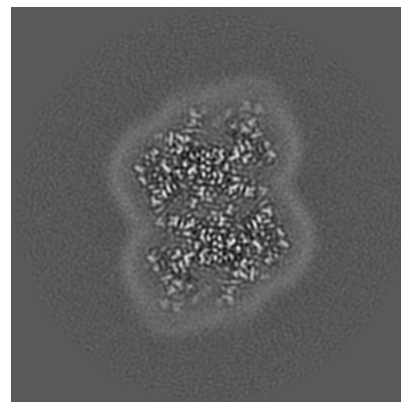
6.2.1 Primary map



X Index: 150

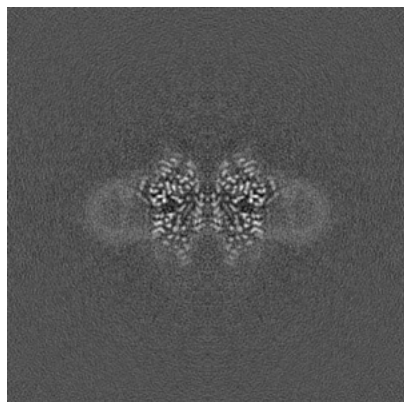


Y Index: 150

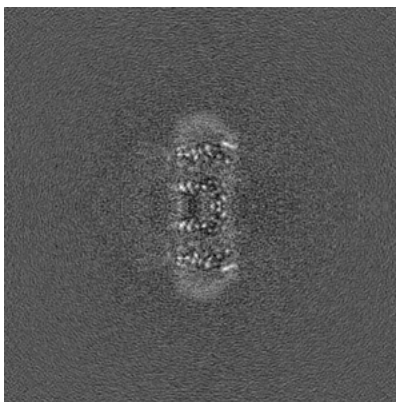


Z Index: 150

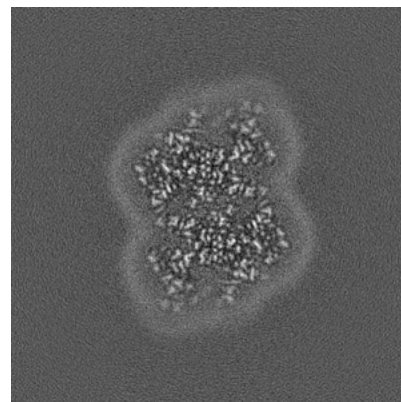
6.2.2 Raw map



X Index: 150



Y Index: 150

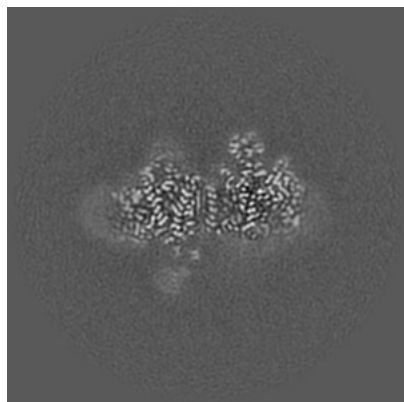


Z Index: 150

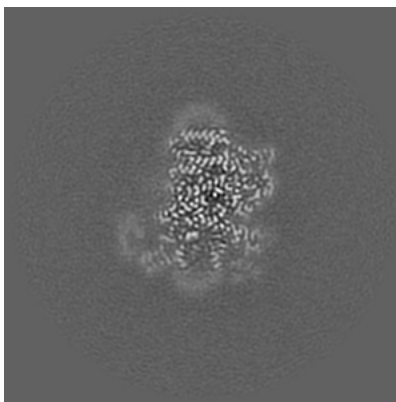
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

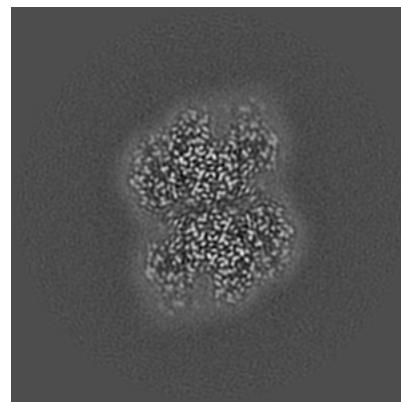
6.3.1 Primary map



X Index: 133

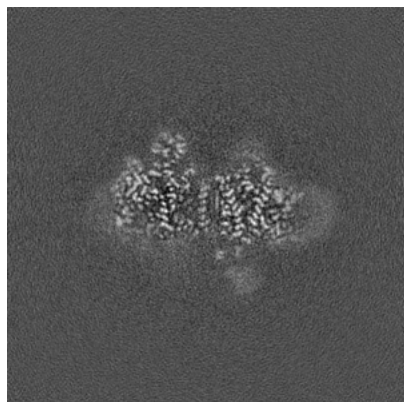


Y Index: 122

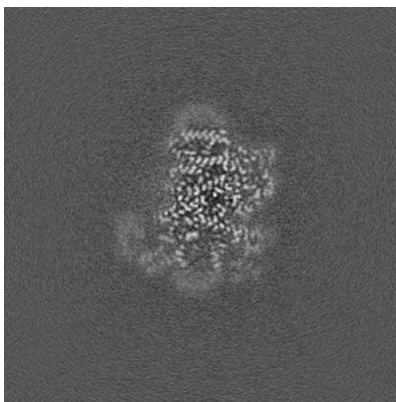


Z Index: 162

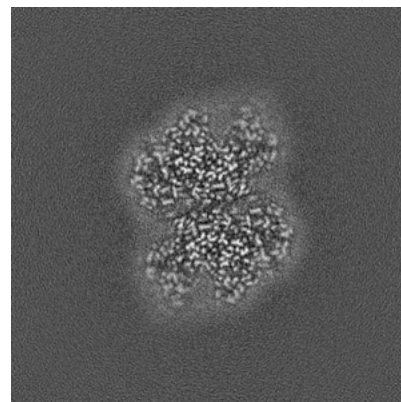
6.3.2 Raw map



X Index: 167



Y Index: 122

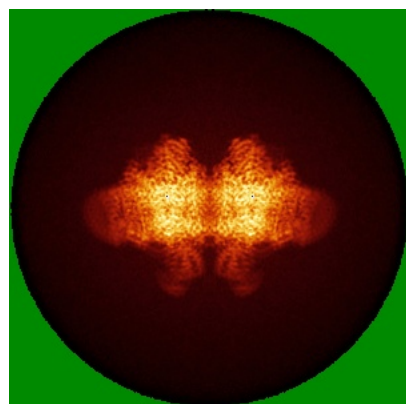


Z Index: 163

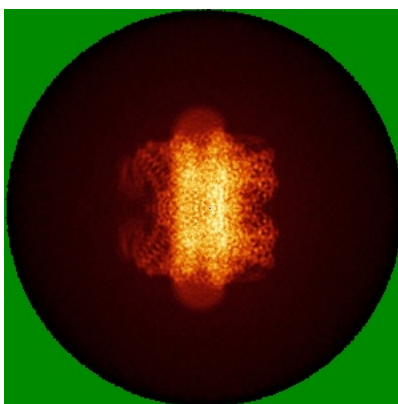
The images above show the largest variance slices of the map in three orthogonal directions.

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

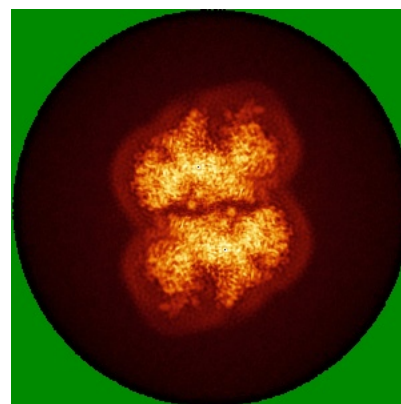
6.4.1 Primary map



X

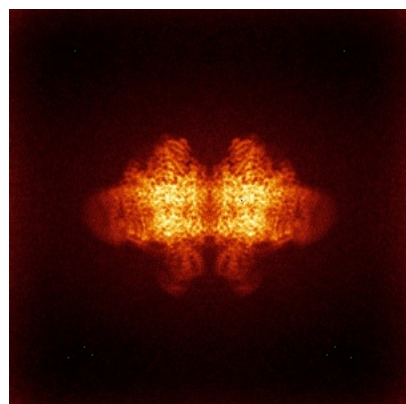


Y

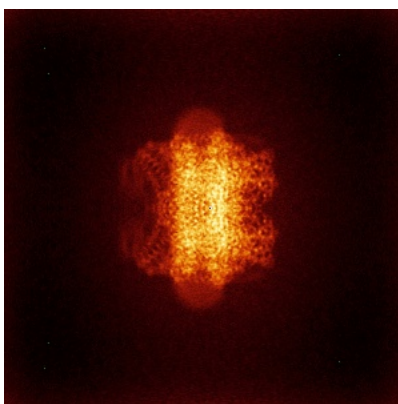


Z

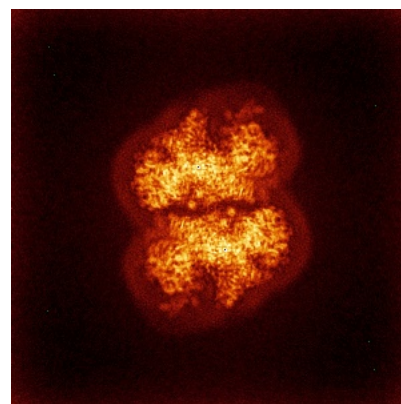
6.4.2 Raw map



X



Y

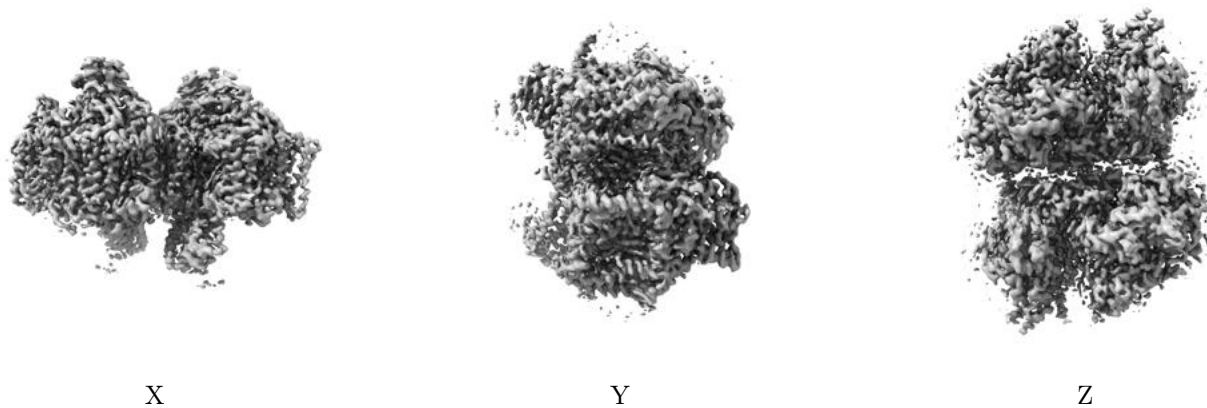


Z

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.

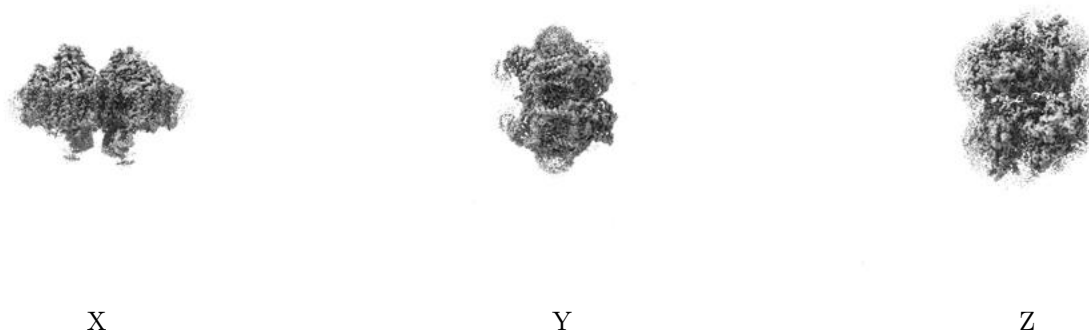
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

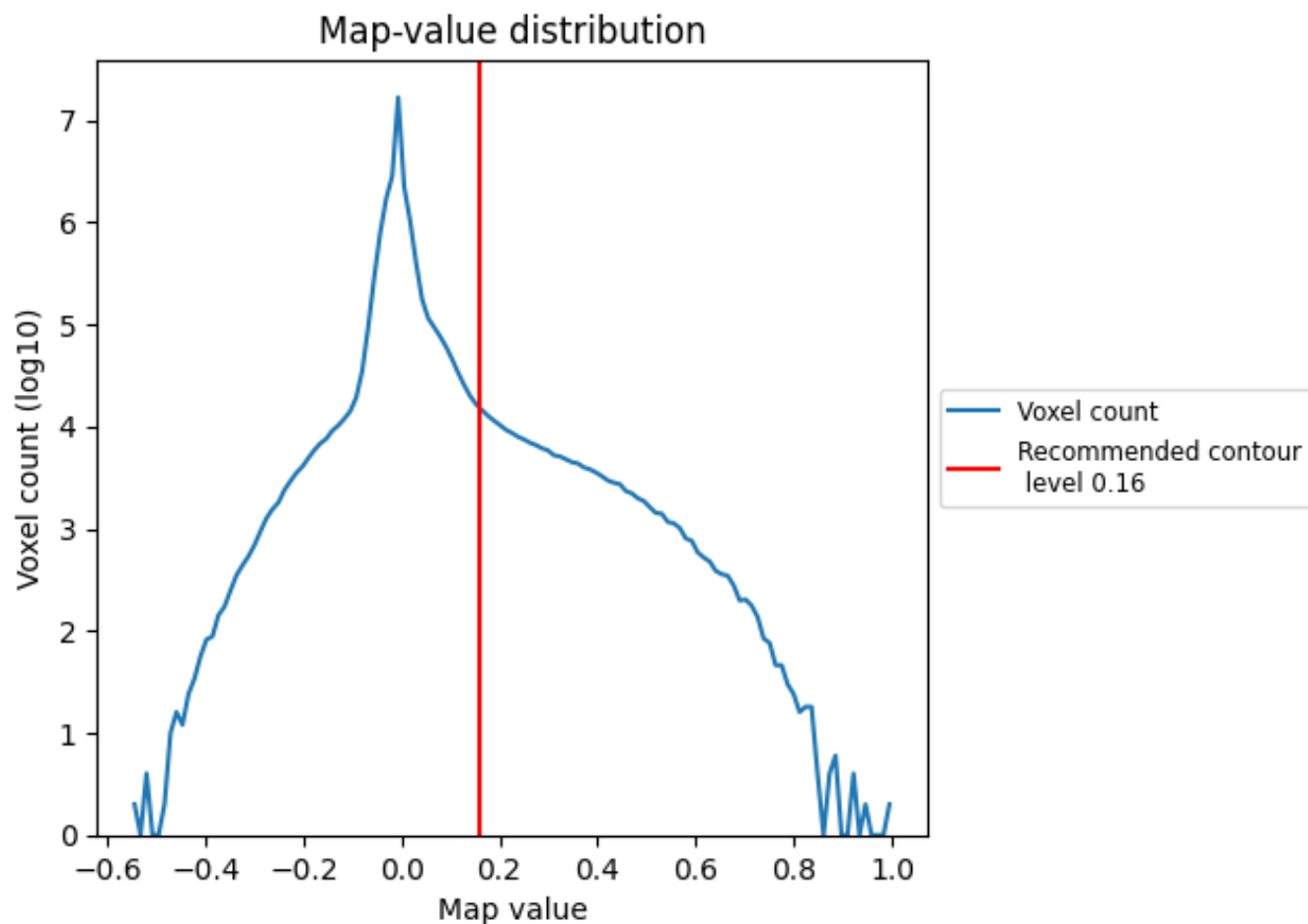
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

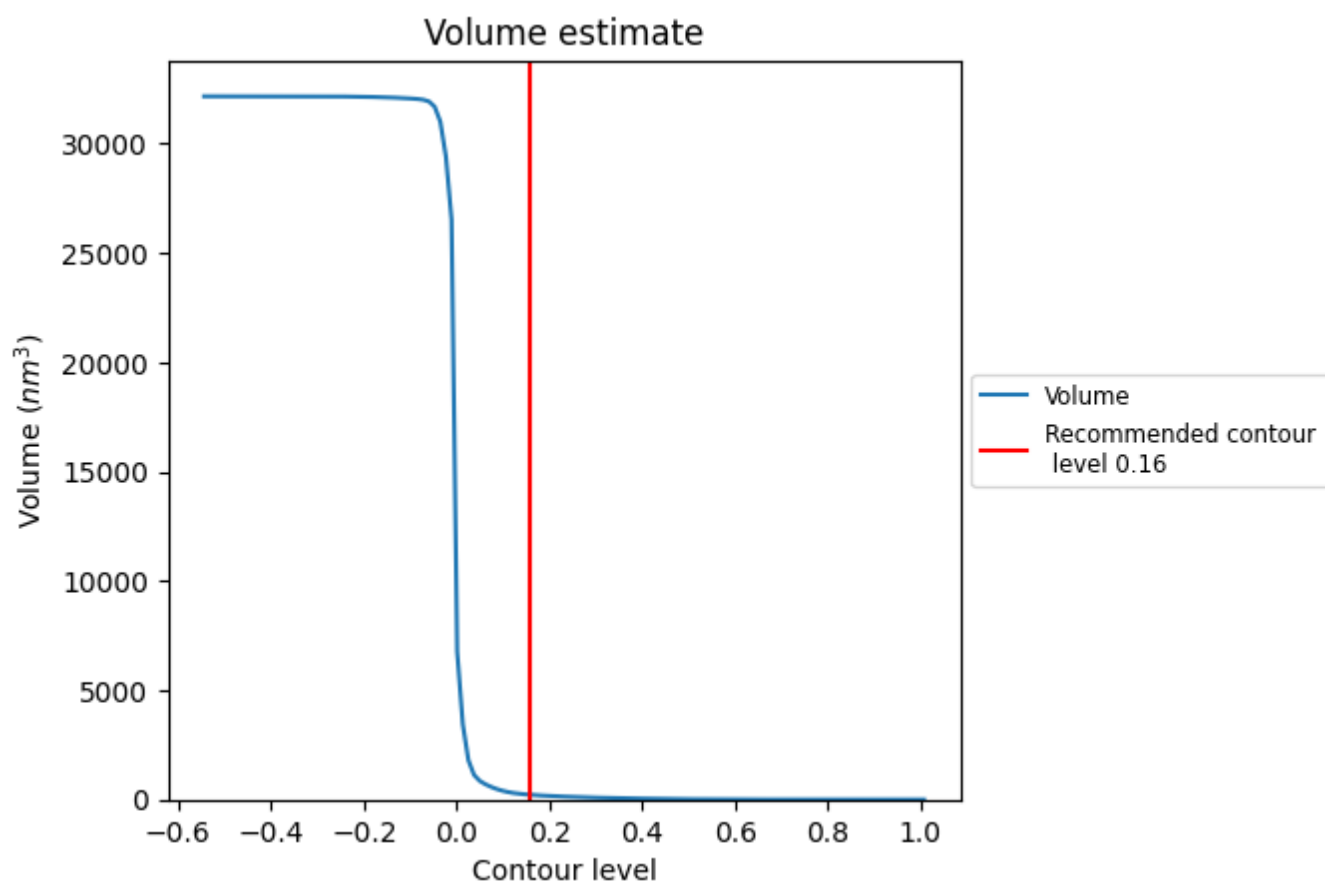
This section contains the results of statistical analysis of the map.

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.

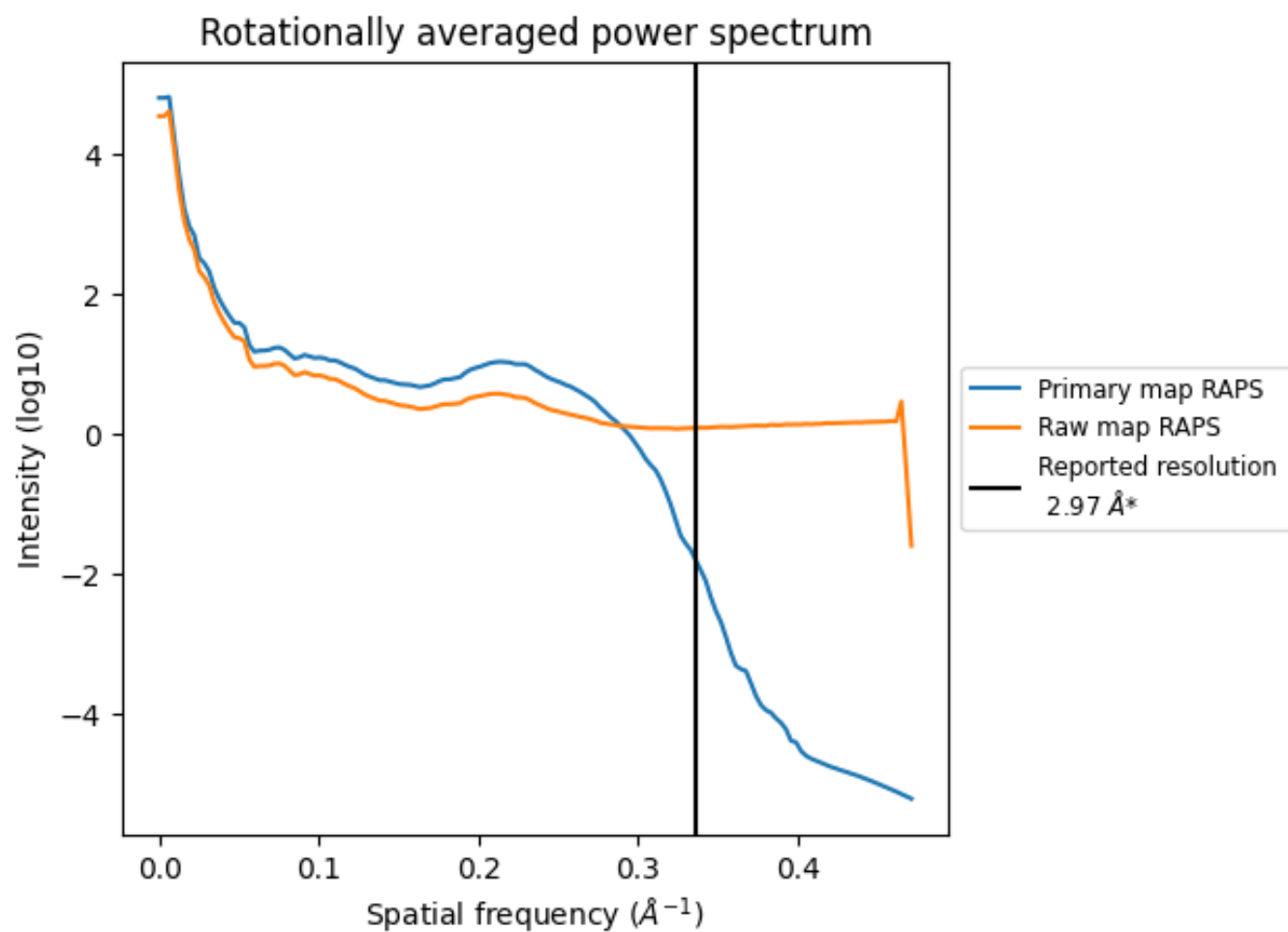
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 217 nm³; this corresponds to an approximate mass of 196 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 ⓘ

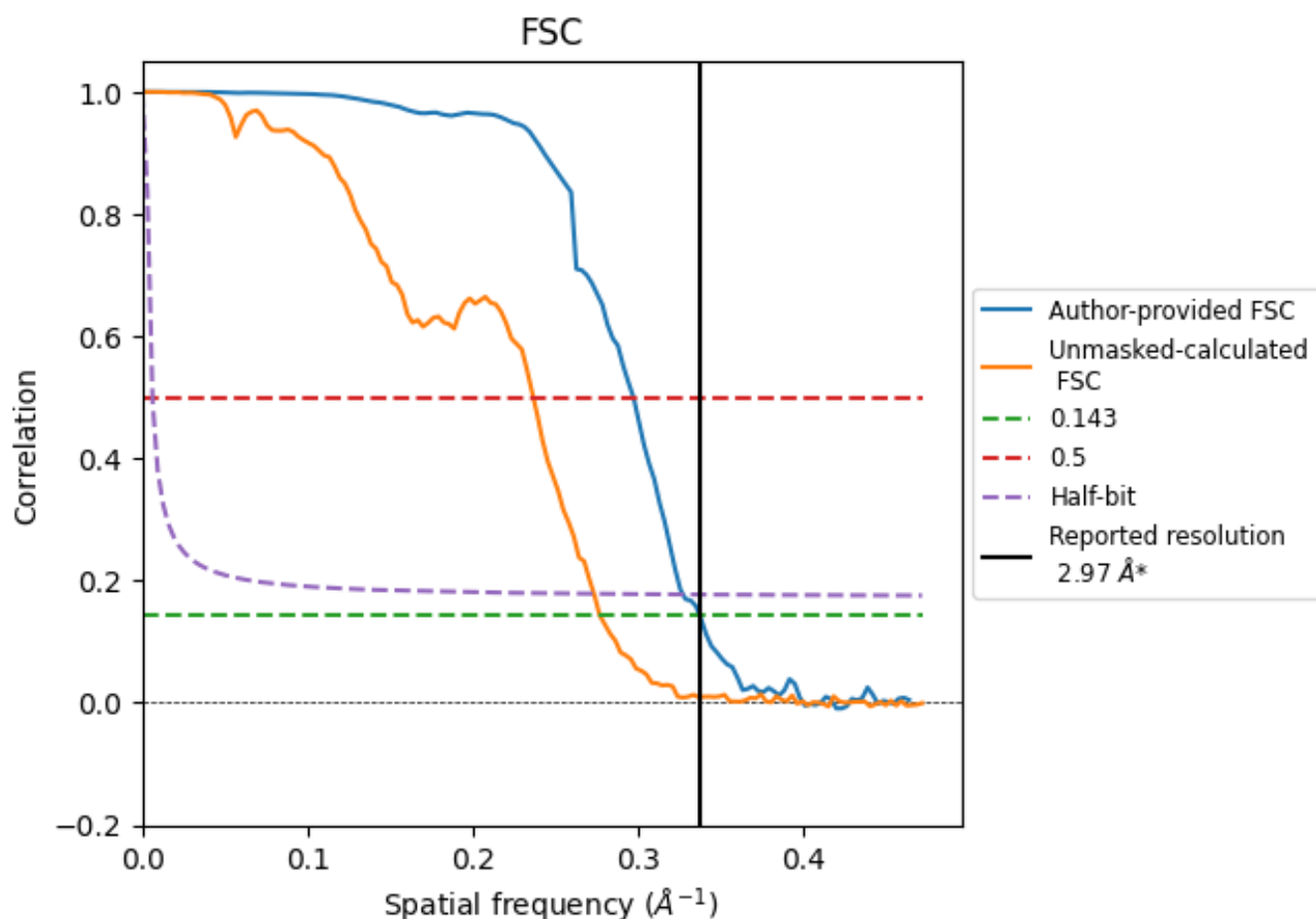


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

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 0.337 \AA^{-1}

8.2 Resolution estimates [i](#)

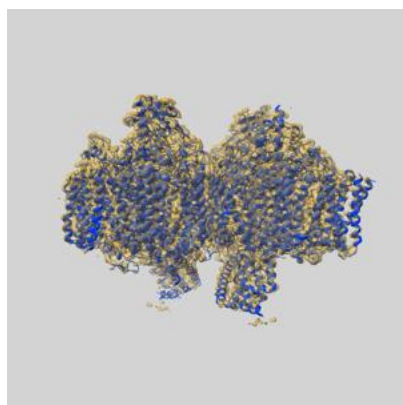
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.37	3.06
Unmasked-calculated*	3.61	4.23	3.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 2.97 by more than 10 %

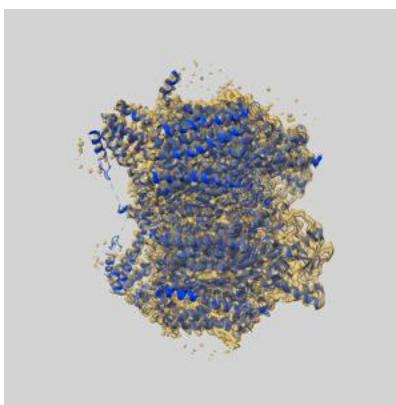
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60694 and PDB model 9IMN. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

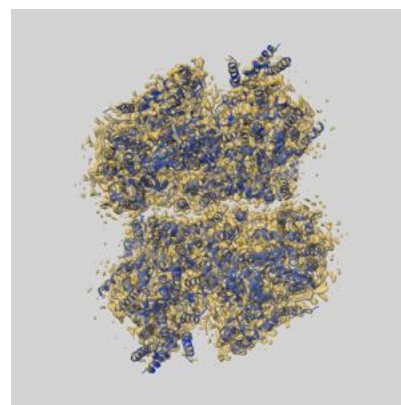
9.1 Map-model overlay [i](#)



X



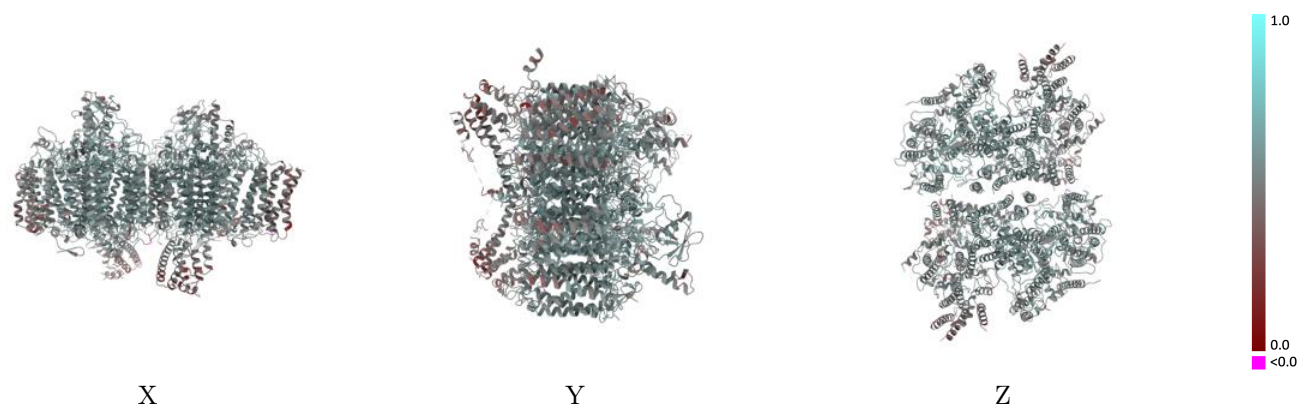
Y



Z

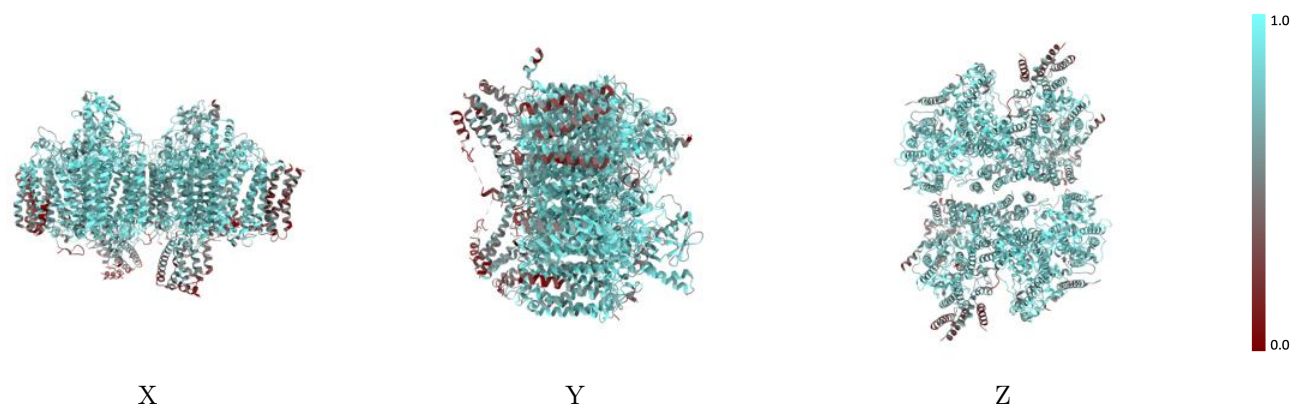
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



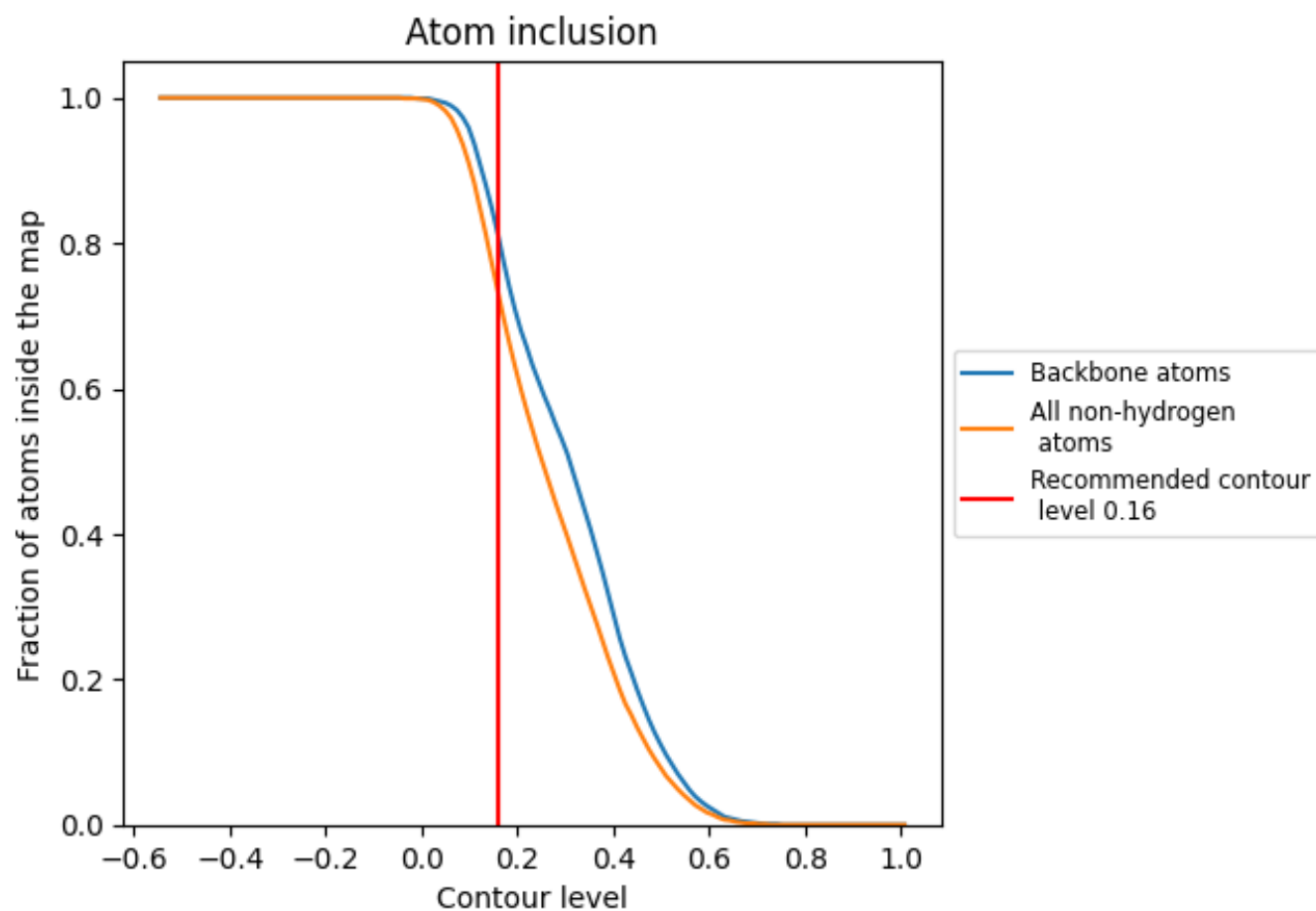
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.5340
A	 0.7970	 0.5650
B	 0.8200	 0.5560
C	 0.7180	 0.5270
D	 0.8410	 0.5710
E	 0.6720	 0.4780
F	 0.6710	 0.5120
G	 0.4790	 0.4310
H	 0.7150	 0.5290
I	 0.7430	 0.5360
K	 0.6310	 0.4870
L	 0.7500	 0.5430
M	 0.7600	 0.5420
T	 0.6330	 0.5230
V	 0.2830	 0.4370
W	 0.4710	 0.4890
X	 0.3760	 0.4700
Z	 0.3620	 0.4110
a	 0.8090	 0.5660
b	 0.8210	 0.5580
c	 0.7170	 0.5310
d	 0.8440	 0.5740
e	 0.6660	 0.4880
f	 0.6750	 0.5120
g	 0.4920	 0.4390
h	 0.7030	 0.5310
i	 0.7460	 0.5380
k	 0.6010	 0.4930
l	 0.7640	 0.5480
m	 0.7500	 0.5500
t	 0.6730	 0.5380
v	 0.2710	 0.4280
w	 0.4710	 0.4830
x	 0.3760	 0.4730
z	 0.3680	 0.4210

