



wwPDB EM Validation Summary Report ⓘ

Jul 24, 2025 – 06:55 PM JST

PDB ID : 9IOX / pdb_00009iox
EMDB ID : EMD-60748
Title : Cryo-EM structure of a TEF30-associated intermediate PSII core dimer complex, type II, from Chlamydomonas reinhardtii
Authors : Wang, Y.; Wang, C.; Li, A.; Liu, Z.
Deposited on : 2024-07-09
Resolution : 3.30 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) : 2.44

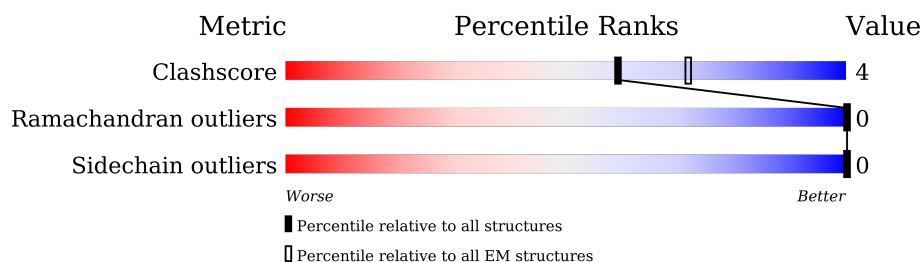
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	<div> <div>10%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	a	327	<div> <div>9%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
2	B	480	<div> <div>6%</div> <div>93%</div> <div>7%</div> </div>
2	b	480	<div> <div>6%</div> <div>92%</div> <div>8%</div> </div>
3	C	450	<div> <div>12%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>
3	c	450	<div> <div>12%</div> <div>91%</div> <div>7%</div> <div>•</div> </div>
4	D	351	<div> <div>6%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>
4	d	351	<div> <div>6%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	74	
5	e	74	
6	F	31	
6	f	31	
7	G	195	
7	g	195	
8	H	71	
8	h	71	
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	28	
13	t	28	
14	V	31	
14	v	31	
15	X	32	
15	x	32	
16	Z	61	
16	z	61	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	402	X	-	-	-
18	CLA	A	403	X	-	-	-
18	CLA	A	405	X	-	-	-
18	CLA	B	501	X	-	-	-
18	CLA	B	502	X	-	-	-
18	CLA	B	503	X	-	-	-
18	CLA	B	504	X	-	-	-
18	CLA	B	505	X	-	-	-
18	CLA	B	506	X	-	-	-
18	CLA	B	507	X	-	-	-
18	CLA	B	508	X	-	-	-
18	CLA	B	509	X	-	-	-
18	CLA	B	510	X	-	-	-
18	CLA	B	511	X	-	-	-
18	CLA	B	512	X	-	-	-
18	CLA	B	513	X	-	-	-
18	CLA	B	514	X	-	-	-
18	CLA	B	515	X	-	-	-
18	CLA	B	516	X	-	-	-
18	CLA	C	502	X	-	-	-
18	CLA	C	503	X	-	-	-
18	CLA	C	504	X	-	-	-
18	CLA	C	505	X	-	-	-
18	CLA	C	506	X	-	-	-
18	CLA	C	507	X	-	-	-
18	CLA	C	508	X	-	-	-
18	CLA	C	509	X	-	-	-
18	CLA	C	510	X	-	-	-
18	CLA	C	511	X	-	-	-
18	CLA	C	512	X	-	-	-
18	CLA	C	513	X	-	-	-
18	CLA	C	514	X	-	-	-
18	CLA	D	401	X	-	-	-
18	CLA	D	404	X	-	-	-
18	CLA	D	405	X	-	-	-
18	CLA	a	402	X	-	-	-
18	CLA	a	403	X	-	-	-
18	CLA	a	405	X	-	-	-
18	CLA	b	501	X	-	-	-
18	CLA	b	502	X	-	-	-
18	CLA	b	503	X	-	-	-
18	CLA	b	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	b	505	X	-	-	-
18	CLA	b	506	X	-	-	-
18	CLA	b	507	X	-	-	-
18	CLA	b	508	X	-	-	-
18	CLA	b	509	X	-	-	-
18	CLA	b	510	X	-	-	-
18	CLA	b	511	X	-	-	-
18	CLA	b	512	X	-	-	-
18	CLA	b	513	X	-	-	-
18	CLA	b	514	X	-	-	-
18	CLA	b	515	X	-	-	-
18	CLA	b	516	X	-	-	-
18	CLA	c	503	X	-	-	-
18	CLA	c	504	X	-	-	-
18	CLA	c	505	X	-	-	-
18	CLA	c	506	X	-	-	-
18	CLA	c	507	X	-	-	-
18	CLA	c	508	X	-	-	-
18	CLA	c	509	X	-	-	-
18	CLA	c	510	X	-	-	-
18	CLA	c	511	X	-	-	-
18	CLA	c	512	X	-	-	-
18	CLA	c	513	X	-	-	-
18	CLA	c	514	X	-	-	-
18	CLA	c	515	X	-	-	-
18	CLA	d	401	X	-	-	-
18	CLA	d	404	X	-	-	-
18	CLA	d	405	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 41854 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	74	Total	C	N	O	0	0
			602	395	99	108		
5	e	74	Total	C	N	O	0	0
			602	395	99	108		

- 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	169	Total	C	N	O	S	0	0
			1368	856	245	260	7		
7	g	169	Total	C	N	O	S	0	0
			1368	856	245	260	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	71	Total	C	N	O	S	0	0
			546	366	81	97	2		
8	h	71	Total	C	N	O	S	0	0
			546	366	81	97	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	28	Total	C	N	O	S	0	0
			231	160	34	36	1		
13	t	28	Total	C	N	O	S	0	0
			231	160	34	36	1		

- 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 Chloroplast photosystem II subunit X.

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

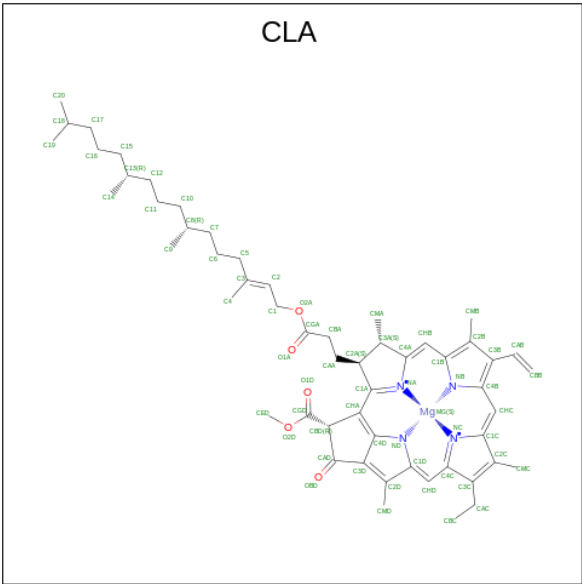
- Molecule 16 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 17 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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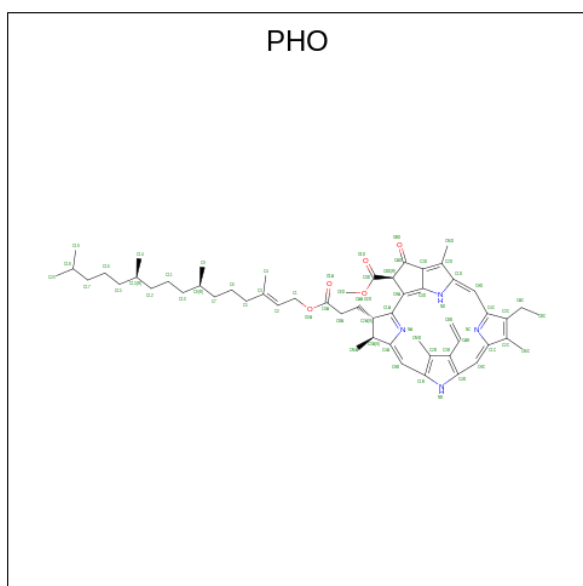
Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total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

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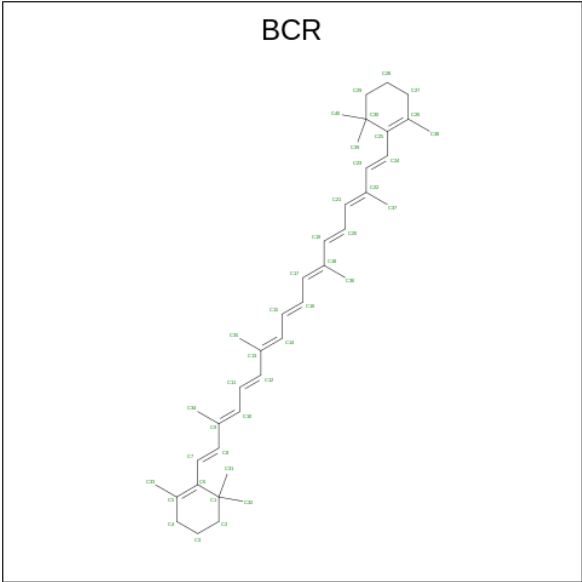
Mol	Chain	Residues	Atoms					AltConf
18	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 19 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
19	A	1	Total	C	N	O		0
			64	55	4	5		
19	D	1	Total	C	N	O		0
			64	55	4	5		
19	a	1	Total	C	N	O		0
			64	55	4	5		
19	d	1	Total	C	N	O		0
			64	55	4	5		

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



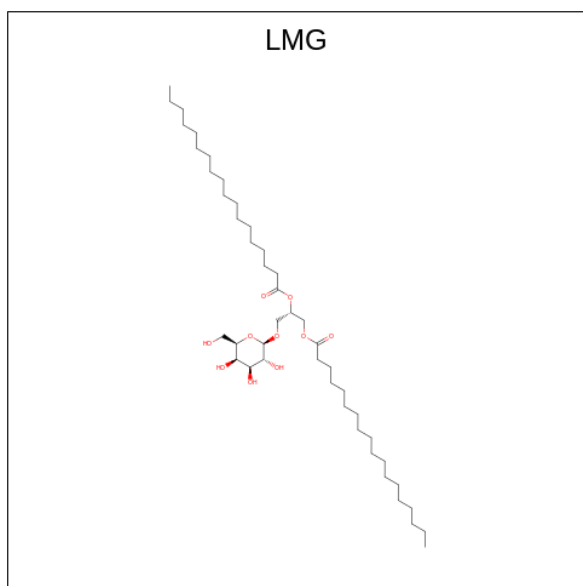
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	D	1	Total	C	0
			40	40	
20	K	1	Total	C	0
			40	40	
20	X	1	Total	C	0
			40	40	
20	a	1	Total	C	0
			40	40	
20	b	1	Total	C	0
			40	40	
20	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
20	c	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	d	1	Total C 40 40	0
20	k	1	Total C 40 40	0
20	x	1	Total C 40 40	0
20	z	1	Total C 40 40	0

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



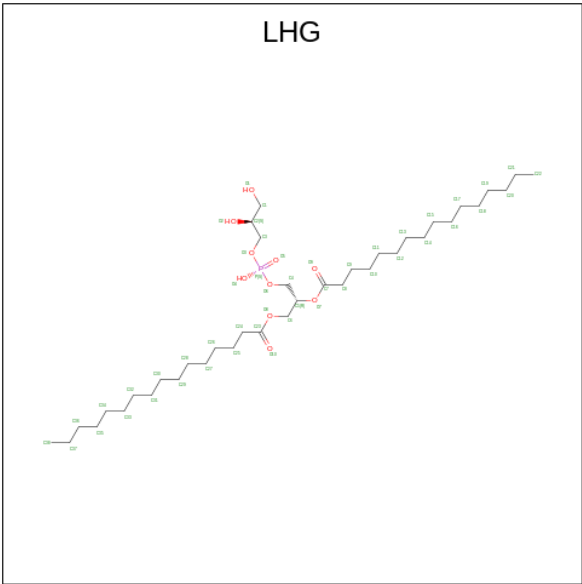
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C O 46 36 10	0
21	B	1	Total C O 42 32 10	0
21	C	1	Total C O 51 41 10	0
21	D	1	Total C O 46 36 10	0
21	D	1	Total C O 48 38 10	0

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

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



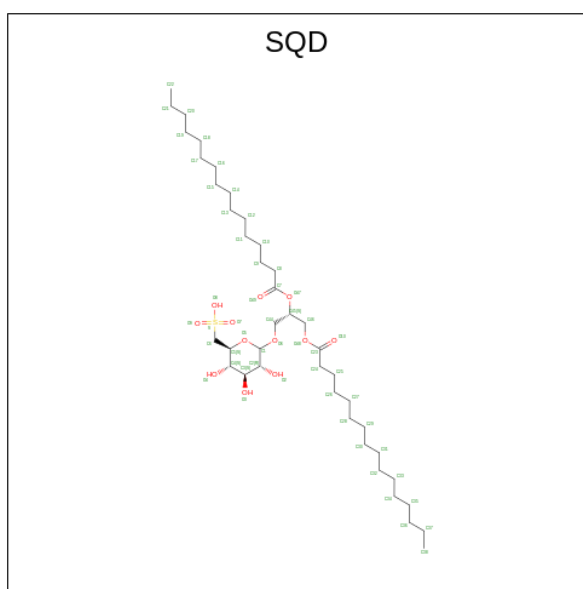
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			43	32	10	1	
22	A	1	Total	C	O	P	0
			44	33	10	1	
22	B	1	Total	C	O	P	0
			44	33	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			49	38	10	1	
22	L	1	Total	C	O	P	0
			49	38	10	1	

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

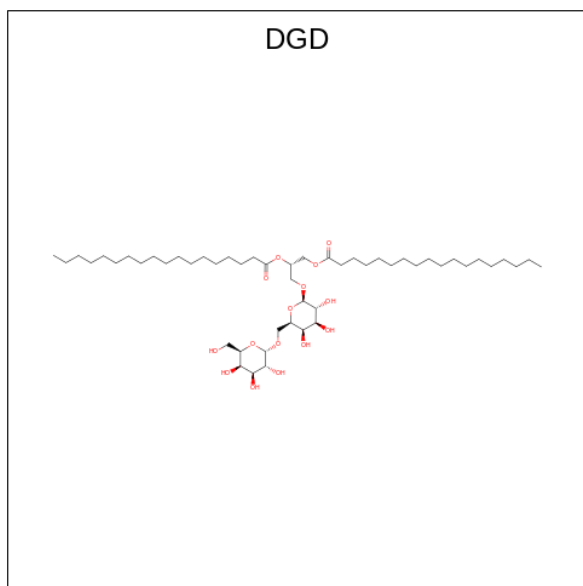
- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

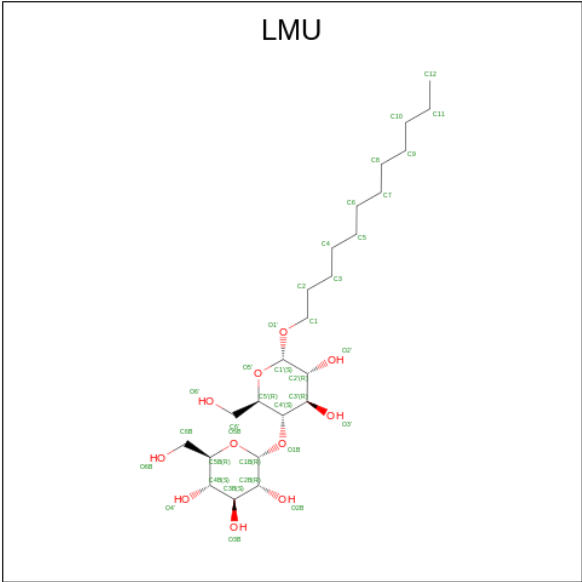
- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



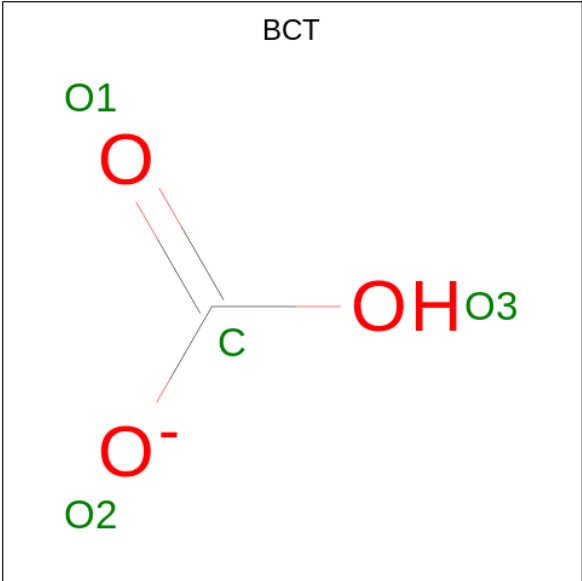
Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total	C	O	0
			53	38	15	
24	C	1	Total	C	O	0
			49	34	15	
24	C	1	Total	C	O	0
			59	44	15	
24	c	1	Total	C	O	0
			53	38	15	
24	c	1	Total	C	O	0
			49	34	15	
24	c	1	Total	C	O	0
			59	44	15	

- Molecule 25 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



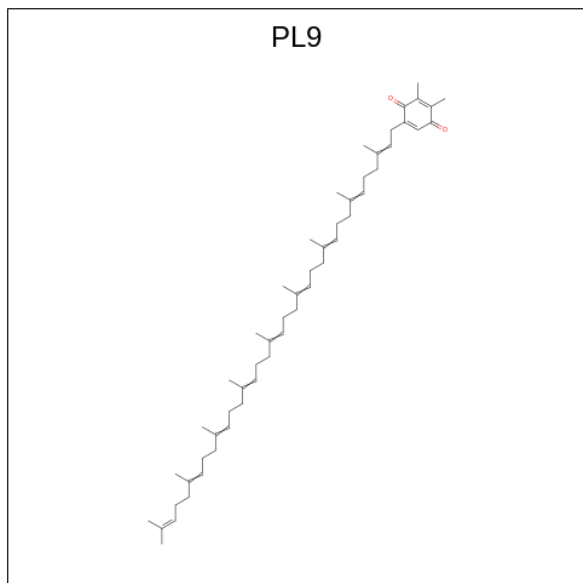
Mol	Chain	Residues	Atoms			AltConf
26	D	1	Total	C	O	0
			4	1	3	

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

- Molecule 27 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
27	D	1	Total	C	O	0
			55	53	2	
27	d	1	Total	C	O	0
			55	53	2	

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

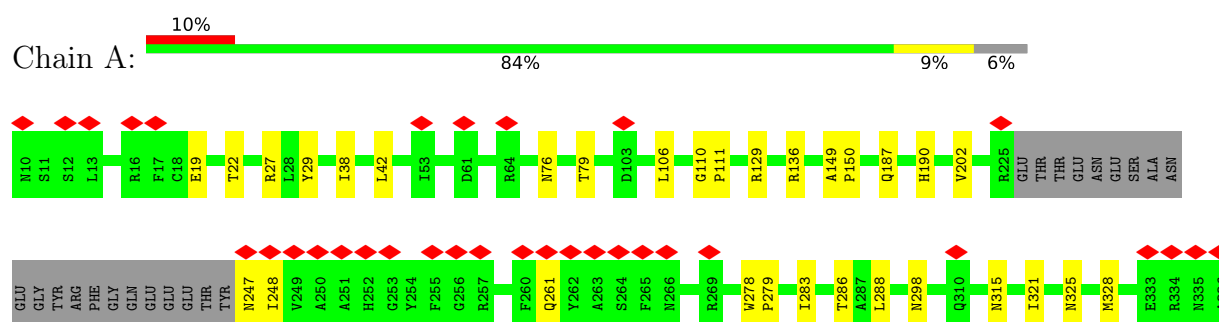


Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	e	1	Total 43	C 34	Fe 1	N 4	O 4	0

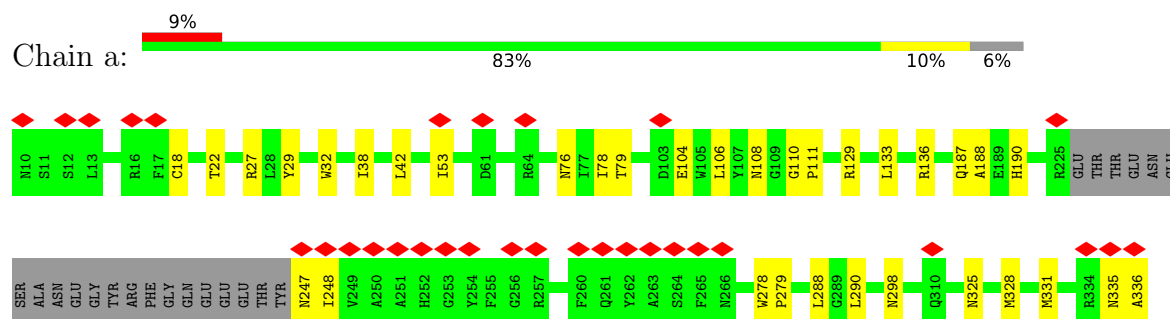
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

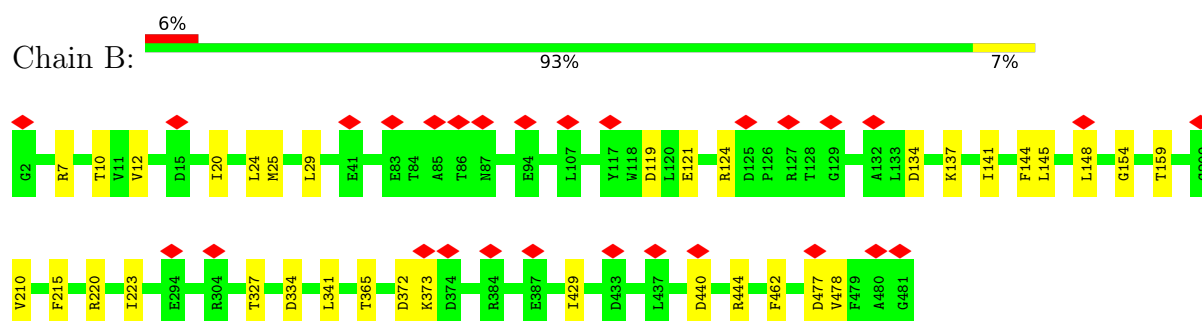
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

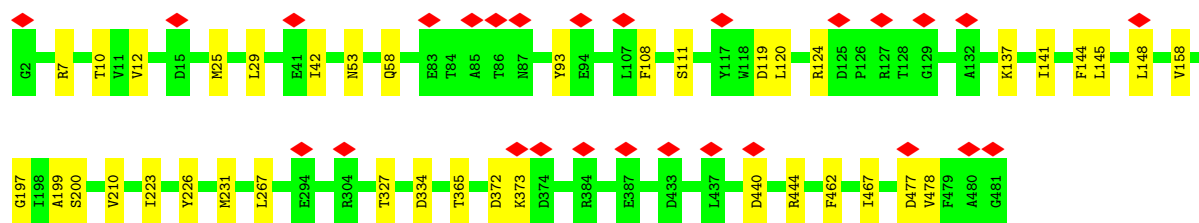


- Molecule 2: Photosystem II CP47 reaction center protein

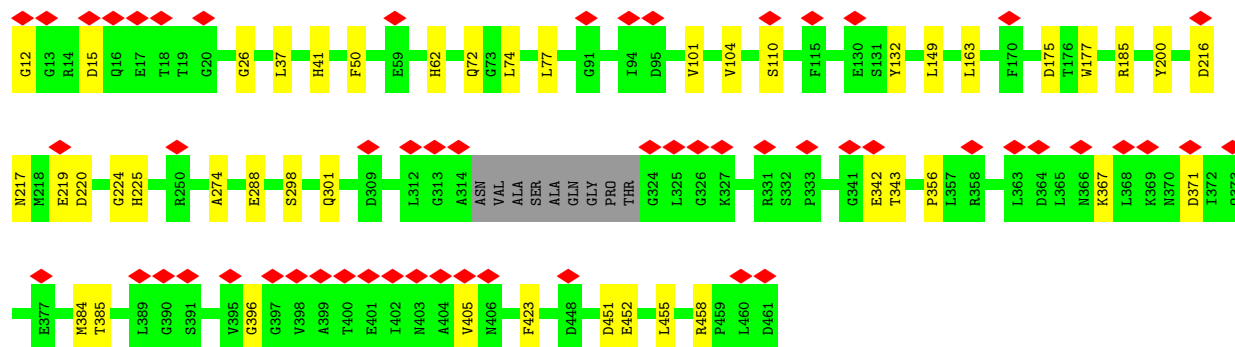
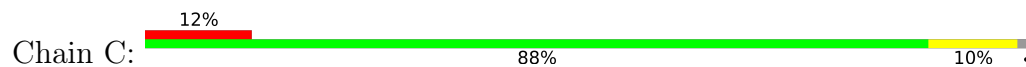


- Molecule 2: Photosystem II CP47 reaction center protein

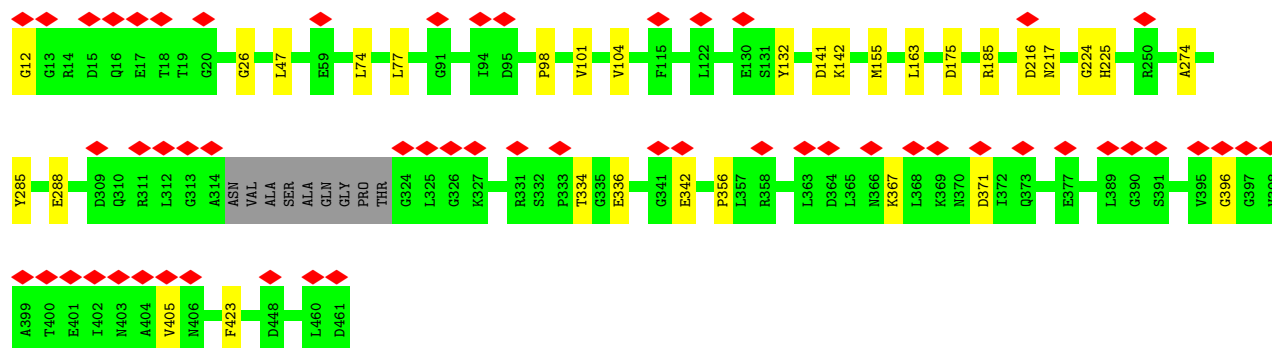
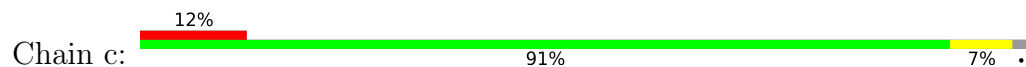




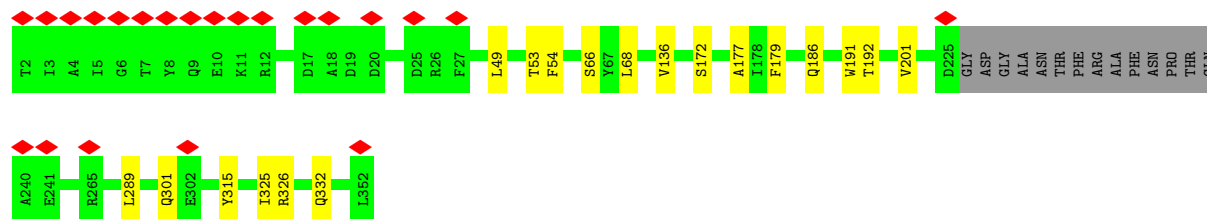
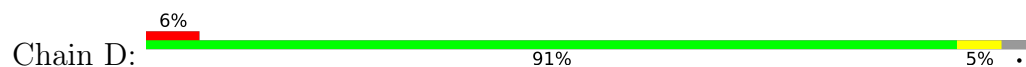
• Molecule 3: Photosystem II CP43 reaction center protein



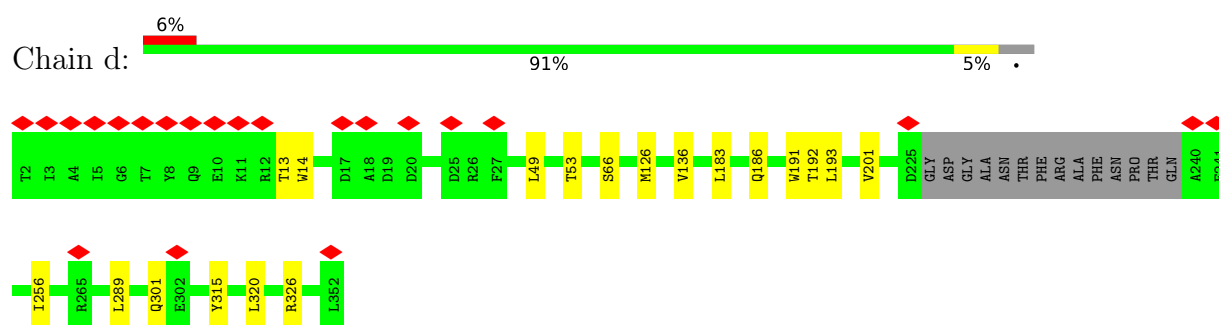
• Molecule 3: Photosystem II CP43 reaction center protein



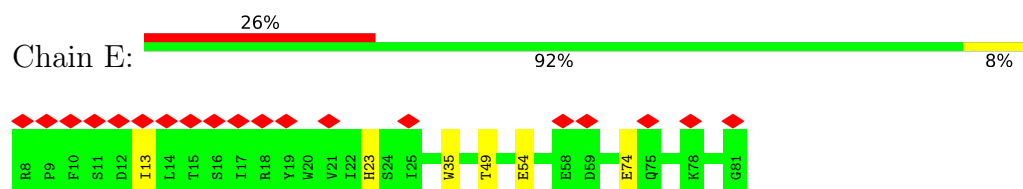
• Molecule 4: Photosystem II D2 protein



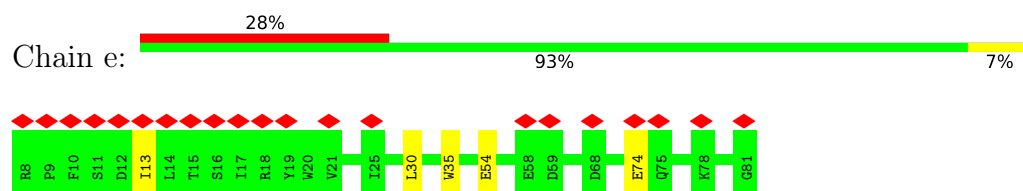
• Molecule 4: Photosystem II D2 protein



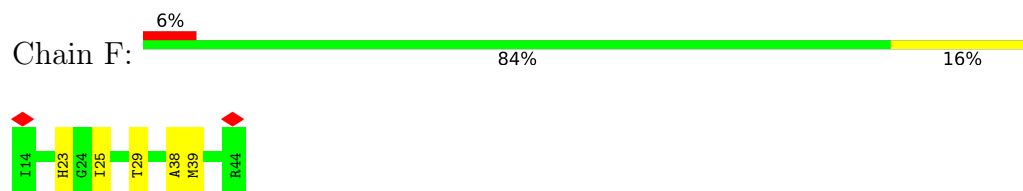
- Molecule 5: Cytochrome b559 subunit alpha



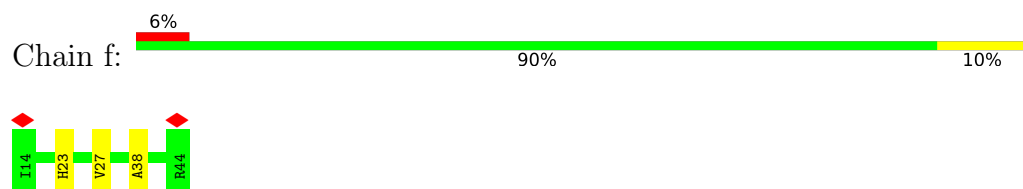
- Molecule 5: Cytochrome b559 subunit alpha



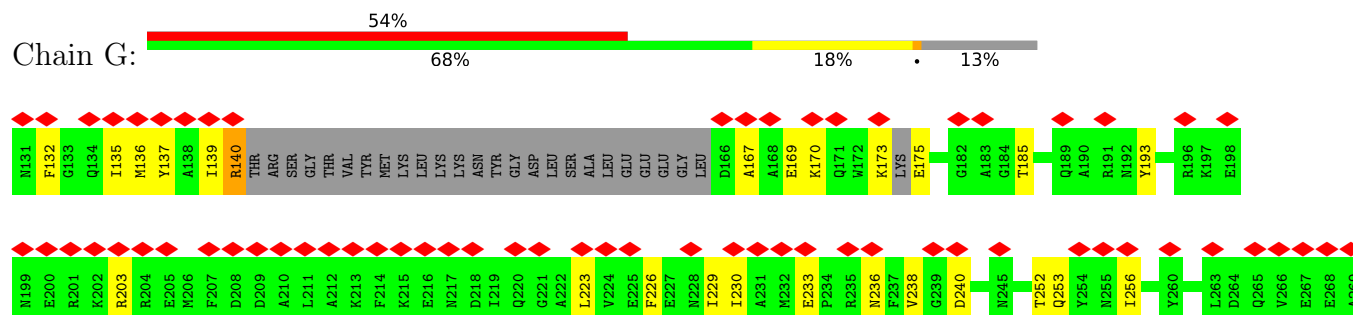
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta

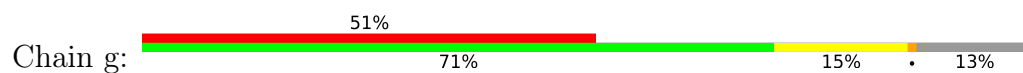


- Molecule 7: PDZ domain-containing protein

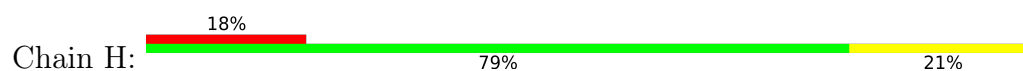




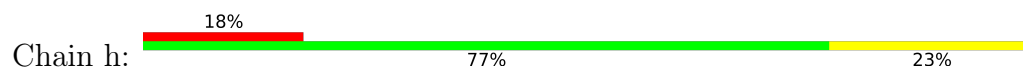
• Molecule 7: PDZ domain-containing protein



• Molecule 8: Photosystem II reaction center protein H



• Molecule 8: Photosystem II reaction center protein H



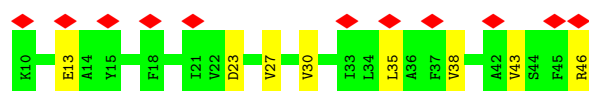
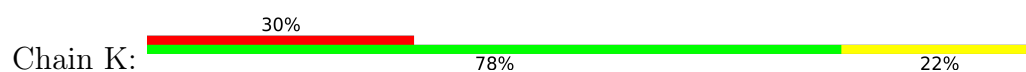
• Molecule 9: Photosystem II reaction center protein I



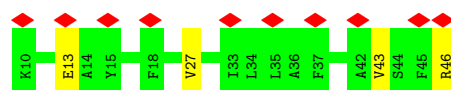
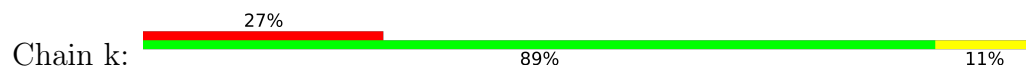
• Molecule 9: Photosystem II reaction center protein I



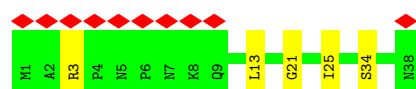
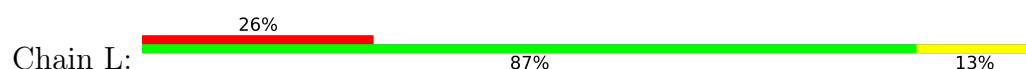
• Molecule 10: Photosystem II reaction center protein K



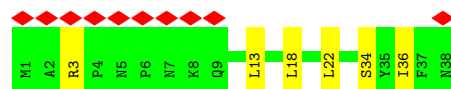
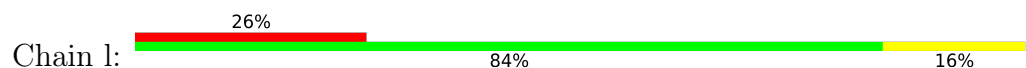
• Molecule 10: Photosystem II reaction center protein K



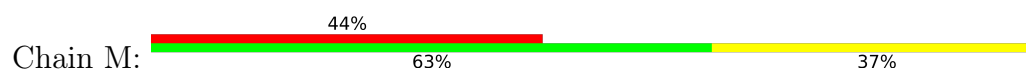
• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



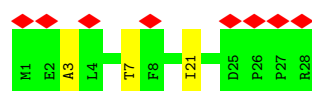
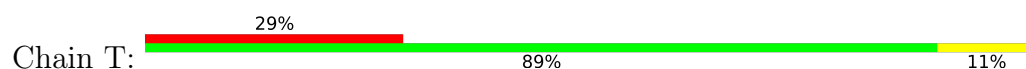
• Molecule 12: Photosystem II reaction center protein M



• Molecule 12: Photosystem II reaction center protein M



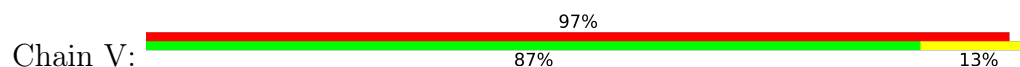
• Molecule 13: Photosystem II reaction center protein T



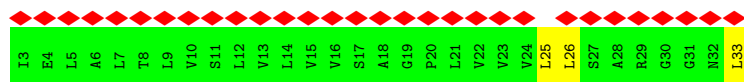
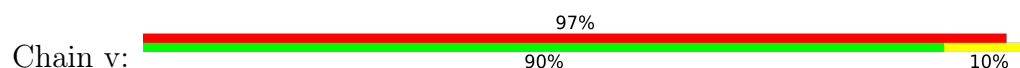
- Molecule 13: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein Psb30



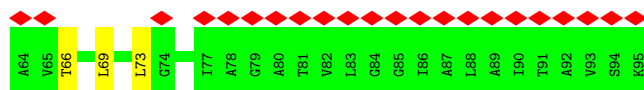
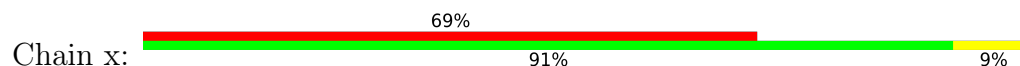
- Molecule 14: Photosystem II reaction center protein Psb30



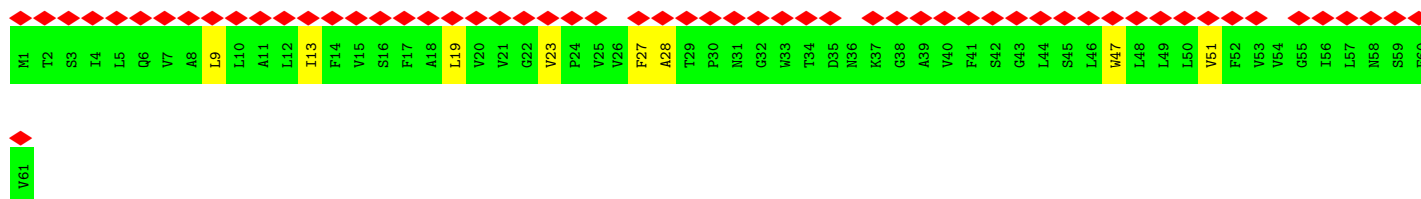
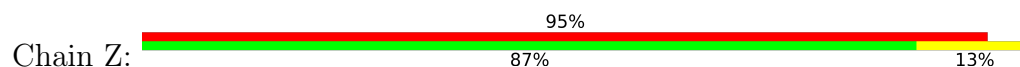
- Molecule 15: Chloroplast photosystem II subunit X



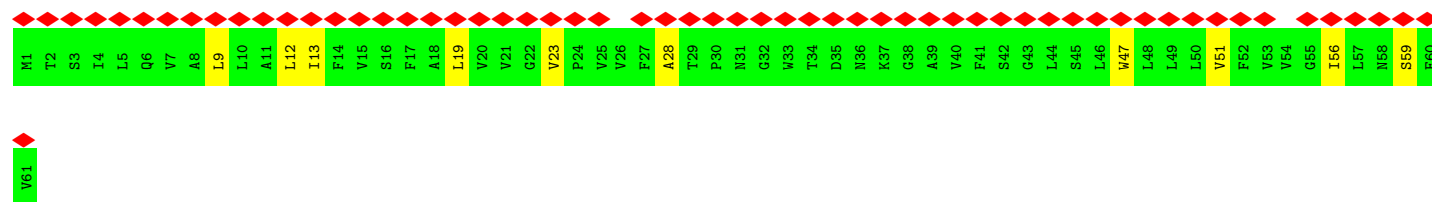
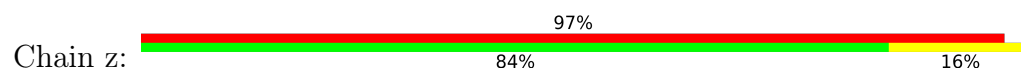
- Molecule 15: Chloroplast photosystem II subunit X



- Molecule 16: Photosystem II reaction center protein Z



- Molecule 16: 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	33509	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	0.770	Depositor
Minimum map value	-0.485	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.165	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: SQD, BCT, LMG, FE2, LHG, HEM, DGD, CLA, PL9, LMU, PHO, BCR

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	0.14	0/2463	0.32	0/3358
1	a	0.14	0/2463	0.31	0/3358
2	B	0.12	0/3883	0.28	0/5286
2	b	0.12	0/3883	0.28	0/5286
3	C	0.12	0/3563	0.29	0/4851
3	c	0.12	0/3563	0.28	0/4851
4	D	0.12	0/2777	0.29	0/3787
4	d	0.13	0/2777	0.29	0/3787
5	E	0.18	0/620	0.33	0/846
5	e	0.13	0/620	0.33	0/846
6	F	0.28	0/258	0.40	0/349
6	f	0.16	0/258	0.39	0/349
7	G	0.24	0/1390	0.40	0/1864
7	g	0.24	0/1390	0.44	0/1864
8	H	0.13	0/558	0.29	0/763
8	h	0.14	0/558	0.29	0/763
9	I	0.18	0/283	0.39	0/383
9	i	0.22	0/283	0.38	0/383
10	K	0.16	0/309	0.44	0/425
10	k	0.16	0/309	0.37	0/425
11	L	0.16	0/322	0.30	0/437
11	l	0.16	0/322	0.32	0/437
12	M	0.19	0/214	0.47	0/293
12	m	0.15	0/214	0.39	0/293
13	T	0.19	0/238	0.34	0/322
13	t	0.19	0/238	0.37	0/322
14	V	0.11	0/216	0.26	0/296
14	v	0.13	0/216	0.30	0/296
15	X	0.11	0/215	0.24	0/292
15	x	0.13	0/215	0.25	0/292
16	Z	0.16	0/469	0.37	0/644
16	z	0.15	0/469	0.40	0/644

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.15	0/35556	0.31	0/48392

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
7	g	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	140	ARG	Sidechain
7	g	140	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2327	27	0
1	a	2388	0	2327	27	0
2	B	3755	0	3642	24	0
2	b	3755	0	3642	27	0
3	C	3444	0	3319	34	0
3	c	3444	0	3319	25	0
4	D	2686	0	2585	19	0
4	d	2686	0	2585	17	0
5	E	602	0	593	6	0
5	e	602	0	593	6	0
6	F	251	0	263	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	251	0	263	4	0
7	G	1368	0	1323	30	0
7	g	1368	0	1327	23	0
8	H	546	0	575	12	0
8	h	546	0	575	13	0
9	I	275	0	287	1	0
9	i	275	0	287	1	0
10	K	297	0	308	7	0
10	k	297	0	308	4	0
11	L	314	0	327	4	0
11	l	314	0	327	5	0
12	M	210	0	231	8	0
12	m	210	0	231	6	0
13	T	231	0	240	2	0
13	t	231	0	240	2	0
14	V	216	0	250	4	0
14	v	216	0	250	3	0
15	X	214	0	240	0	0
15	x	214	0	240	2	0
16	Z	458	0	490	10	0
16	z	458	0	490	9	0
17	A	1	0	0	0	0
17	a	1	0	0	0	0
18	A	174	0	170	3	0
18	B	1020	0	1113	7	0
18	C	845	0	936	7	0
18	D	195	0	216	5	0
18	a	174	0	170	1	0
18	b	1020	0	1113	7	0
18	c	845	0	936	7	0
18	d	195	0	216	5	0
19	A	64	0	74	0	0
19	D	64	0	74	0	0
19	a	64	0	74	0	0
19	d	64	0	74	0	0
20	A	80	0	112	5	0
20	B	120	0	168	3	0
20	C	120	0	168	16	0
20	D	40	0	56	2	0
20	K	40	0	56	4	0
20	X	40	0	56	2	0
20	a	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	b	80	0	112	1	0
20	c	80	0	112	9	0
20	d	40	0	56	1	0
20	k	40	0	56	4	0
20	x	40	0	56	4	0
20	z	40	0	56	6	0
21	A	46	0	62	0	0
21	B	42	0	54	0	0
21	C	51	0	72	0	0
21	D	94	0	128	1	0
21	b	42	0	54	0	0
21	c	97	0	134	0	0
21	d	46	0	62	0	0
21	h	48	0	66	1	0
22	A	87	0	117	1	0
22	B	93	0	135	0	0
22	D	49	0	74	0	0
22	L	49	0	74	0	0
22	X	49	0	74	0	0
22	a	87	0	117	1	0
22	b	93	0	135	0	0
22	d	49	0	74	0	0
22	l	49	0	74	1	0
22	x	49	0	74	0	0
23	C	51	0	69	0	0
23	c	51	0	69	0	0
24	C	161	0	196	0	0
24	c	161	0	196	0	0
25	C	35	0	46	0	0
25	c	35	0	46	0	0
26	D	4	0	0	0	0
26	d	4	0	0	0	0
27	D	55	0	80	0	0
27	d	55	0	80	0	0
28	F	43	0	30	6	0
28	e	43	0	30	5	0
All	All	41854	0	42712	370	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 4.

The worst 5 of 370 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)
2:b:119:ASP:OD1	2:b:124:ARG:NH1	2.17	0.78
1:a:104:GLU:OE2	1:a:108:ASN:ND2	2.17	0.77
2:B:119:ASP:OD1	2:B:124:ARG:NH1	2.19	0.76
2:B:148:LEU:HD22	2:B:210:VAL:HG22	1.68	0.76
2:B:121:GLU:O	8:H:31:ARG:NH1	2.20	0.75

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%)	289 (96%)	13 (4%)	0	100	100
1	a	302/327 (92%)	289 (96%)	13 (4%)	0	100	100
2	B	478/480 (100%)	467 (98%)	11 (2%)	0	100	100
2	b	478/480 (100%)	464 (97%)	14 (3%)	0	100	100
3	C	437/450 (97%)	428 (98%)	9 (2%)	0	100	100
3	c	437/450 (97%)	428 (98%)	9 (2%)	0	100	100
4	D	333/351 (95%)	319 (96%)	14 (4%)	0	100	100
4	d	333/351 (95%)	323 (97%)	10 (3%)	0	100	100
5	E	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
5	e	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
6	F	29/31 (94%)	29 (100%)	0	0	100	100
6	f	29/31 (94%)	29 (100%)	0	0	100	100
7	G	163/195 (84%)	158 (97%)	5 (3%)	0	100	100
7	g	163/195 (84%)	161 (99%)	2 (1%)	0	100	100
8	H	69/71 (97%)	66 (96%)	3 (4%)	0	100	100
8	h	69/71 (97%)	67 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	34 (94%)	2 (6%)	0	100	100
11	l	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
12	M	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
12	m	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
13	T	26/28 (93%)	24 (92%)	2 (8%)	0	100	100
13	t	26/28 (93%)	24 (92%)	2 (8%)	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	X	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
15	x	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
16	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
16	z	59/61 (97%)	59 (100%)	0	0	100	100
All	All	4310/4534 (95%)	4184 (97%)	126 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	65/65 (100%)	65 (100%)	0	100	100
5	e	65/65 (100%)	65 (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	140/162 (86%)	140 (100%)	0	100	100
7	g	140/162 (86%)	140 (100%)	0	100	100
8	H	61/61 (100%)	61 (100%)	0	100	100
8	h	61/61 (100%)	61 (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	25/25 (100%)	25 (100%)	0	100	100
13	t	25/25 (100%)	25 (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	X	22/22 (100%)	22 (100%)	0	100	100
15	x	22/22 (100%)	22 (100%)	0	100	100
16	Z	51/51 (100%)	51 (100%)	0	100	100
16	z	51/51 (100%)	51 (100%)	0	100	100
All	All	3560/3672 (97%)	3560 (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 10 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	292	ASN
7	g	134	GLN
10	k	40	GLN
1	a	76	ASN
1	a	322	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
18	CLA	C	509	-	65,73,73	1.52	6 (9%)	76,113,113	1.21	6 (7%)
18	CLA	C	503	-	65,73,73	1.51	7 (10%)	76,113,113	1.27	9 (11%)
18	CLA	B	510	-	65,73,73	1.49	5 (7%)	76,113,113	1.29	8 (10%)
18	CLA	b	504	-	65,73,73	1.52	6 (9%)	76,113,113	1.24	8 (10%)
18	CLA	b	501	-	65,73,73	1.53	7 (10%)	76,113,113	1.20	8 (10%)
18	CLA	c	511	-	65,73,73	1.52	5 (7%)	76,113,113	1.25	7 (9%)
20	BCR	x	102	-	41,41,41	0.70	0	56,56,56	2.13	24 (42%)
20	BCR	B	518	-	41,41,41	0.78	0	56,56,56	1.95	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	d	404	-	65,73,73	1.52	6 (9%)	76,113,113	1.20	6 (7%)
20	BCR	B	517	-	41,41,41	0.81	0	56,56,56	2.13	22 (39%)
18	CLA	c	503	-	65,73,73	1.51	7 (10%)	76,113,113	1.15	5 (6%)
18	CLA	C	506	-	65,73,73	1.50	6 (9%)	76,113,113	1.18	9 (11%)
18	CLA	b	513	-	65,73,73	1.50	6 (9%)	76,113,113	1.22	7 (9%)
19	PHO	A	404	-	51,69,69	1.01	4 (7%)	47,99,99	1.17	6 (12%)
22	LHG	a	407	-	42,42,48	1.01	2 (4%)	45,48,54	1.04	2 (4%)
18	CLA	B	505	-	65,73,73	1.52	5 (7%)	76,113,113	1.15	6 (7%)
18	CLA	B	506	-	65,73,73	1.52	7 (10%)	76,113,113	1.20	8 (10%)
22	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
18	CLA	b	510	-	65,73,73	1.49	6 (9%)	76,113,113	1.27	9 (11%)
18	CLA	b	511	-	65,73,73	1.51	6 (9%)	76,113,113	1.26	9 (11%)
18	CLA	A	405	-	60,68,73	1.58	6 (10%)	70,107,113	1.24	9 (12%)
26	BCT	d	403	17	2,3,3	1.25	0	2,3,3	4.18	1 (50%)
24	DGD	C	518	-	54,54,67	0.94	2 (3%)	68,68,81	0.94	3 (4%)
22	LHG	x	101	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
18	CLA	b	514	-	45,53,73	1.79	6 (13%)	52,89,113	1.43	8 (15%)
28	HEM	F	101	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.44	6 (13%)
18	CLA	A	402	-	65,73,73	1.51	7 (10%)	76,113,113	1.20	10 (13%)
18	CLA	d	405	-	65,73,73	1.53	6 (9%)	76,113,113	1.25	9 (11%)
20	BCR	k	101	-	41,41,41	0.66	0	56,56,56	2.18	23 (41%)
18	CLA	a	402	-	65,73,73	1.52	6 (9%)	76,113,113	1.23	10 (13%)
19	PHO	d	402	-	51,69,69	1.00	3 (5%)	47,99,99	1.04	4 (8%)
20	BCR	b	517	-	41,41,41	0.81	0	56,56,56	2.12	22 (39%)
21	LMG	B	520	-	42,42,55	1.02	2 (4%)	50,50,63	0.95	2 (4%)
18	CLA	C	512	3	65,73,73	1.54	6 (9%)	76,113,113	1.18	8 (10%)
24	DGD	c	518	-	54,54,67	0.93	2 (3%)	68,68,81	0.94	3 (4%)
18	CLA	C	507	-	65,73,73	1.52	7 (10%)	76,113,113	1.22	8 (10%)
18	CLA	b	509	-	65,73,73	1.52	6 (9%)	76,113,113	1.23	10 (13%)
18	CLA	B	512	-	65,73,73	1.52	6 (9%)	76,113,113	1.28	7 (9%)
18	CLA	d	401	-	65,73,73	1.54	7 (10%)	76,113,113	1.17	9 (11%)
18	CLA	B	516	-	65,73,73	1.52	7 (10%)	76,113,113	1.21	7 (9%)
24	DGD	C	519	-	50,50,67	0.99	2 (4%)	64,64,81	0.88	2 (3%)
18	CLA	D	405	-	65,73,73	1.52	5 (7%)	76,113,113	1.24	8 (10%)
20	BCR	d	406	-	41,41,41	0.79	0	56,56,56	2.00	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	b	518	-	41,41,41	0.79	0	56,56,56	1.95	18 (32%)
18	CLA	c	514	-	65,73,73	1.52	7 (10%)	76,113,113	1.27	8 (10%)
18	CLA	C	511	-	65,73,73	1.52	7 (10%)	76,113,113	1.21	7 (9%)
21	LMG	d	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.91	2 (3%)
18	CLA	b	515	-	65,73,73	1.52	6 (9%)	76,113,113	1.27	8 (10%)
25	LMU	c	522	-	36,36,36	1.15	2 (5%)	47,47,47	0.84	1 (2%)
22	LHG	B	521	-	43,43,48	1.01	2 (4%)	46,49,54	0.91	2 (4%)
18	CLA	A	403	-	49,57,73	1.75	6 (12%)	55,93,113	1.40	7 (12%)
18	CLA	C	504	-	65,73,73	1.52	6 (9%)	76,113,113	1.19	8 (10%)
20	BCR	C	517	-	41,41,41	0.73	0	56,56,56	1.93	17 (30%)
18	CLA	B	504	-	65,73,73	1.52	6 (9%)	76,113,113	1.23	7 (9%)
19	PHO	a	404	-	51,69,69	1.01	4 (7%)	47,99,99	1.17	6 (12%)
18	CLA	a	405	-	60,68,73	1.58	6 (10%)	70,107,113	1.26	9 (12%)
21	LMG	D	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.93	2 (3%)
18	CLA	b	506	-	65,73,73	1.52	7 (10%)	76,113,113	1.19	8 (10%)
25	LMU	C	522	-	36,36,36	1.15	2 (5%)	47,47,47	0.85	1 (2%)
18	CLA	B	509	-	65,73,73	1.53	7 (10%)	76,113,113	1.17	8 (10%)
24	DGD	c	519	-	50,50,67	0.99	2 (4%)	64,64,81	0.86	2 (3%)
18	CLA	B	502	-	65,73,73	1.52	5 (7%)	76,113,113	1.20	7 (9%)
27	PL9	D	407	-	55,55,55	1.01	3 (5%)	68,69,69	1.55	12 (17%)
18	CLA	D	401	-	65,73,73	1.54	7 (10%)	76,113,113	1.15	8 (10%)
20	BCR	A	406	-	41,41,41	0.81	1 (2%)	56,56,56	2.05	20 (35%)
20	BCR	c	516	-	41,41,41	0.80	1 (2%)	56,56,56	2.26	21 (37%)
20	BCR	B	519	-	41,41,41	0.75	0	56,56,56	1.93	18 (32%)
22	LHG	b	521	-	48,48,48	0.94	2 (4%)	51,54,54	0.91	2 (3%)
20	BCR	D	406	-	41,41,41	0.79	0	56,56,56	2.00	18 (32%)
18	CLA	b	512	-	65,73,73	1.52	6 (9%)	76,113,113	1.28	7 (9%)
21	LMG	c	502	-	46,46,55	0.99	2 (4%)	54,54,63	1.00	3 (5%)
22	LHG	b	520	-	43,43,48	1.00	2 (4%)	46,49,54	0.90	2 (4%)
20	BCR	a	406	-	41,41,41	0.81	1 (2%)	56,56,56	2.10	21 (37%)
18	CLA	c	505	-	65,73,73	1.52	6 (9%)	76,113,113	1.19	8 (10%)
18	CLA	B	501	-	65,73,73	1.54	5 (7%)	76,113,113	1.21	8 (10%)
21	LMG	c	521	-	51,51,55	0.94	2 (3%)	59,59,63	0.92	2 (3%)
21	LMG	b	519	-	42,42,55	1.02	2 (4%)	50,50,63	0.96	2 (4%)
18	CLA	b	507	-	65,73,73	1.51	5 (7%)	76,113,113	1.17	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCT	D	403	17	2,3,3	1.25	0	2,3,3	4.19	2 (100%)
18	CLA	b	502	-	65,73,73	1.51	6 (9%)	76,113,113	1.19	7 (9%)
23	SQD	C	501	-	50,51,54	1.21	4 (8%)	59,62,65	1.08	5 (8%)
24	DGD	c	520	-	60,60,67	0.91	2 (3%)	74,74,81	0.87	2 (2%)
20	BCR	X	102	-	41,41,41	0.70	0	56,56,56	2.15	25 (44%)
18	CLA	c	506	-	65,73,73	1.52	6 (9%)	76,113,113	1.19	8 (10%)
20	BCR	K	101	-	41,41,41	0.66	0	56,56,56	2.16	24 (42%)
18	CLA	c	509	-	65,73,73	1.50	6 (9%)	76,113,113	1.20	6 (7%)
18	CLA	B	511	-	65,73,73	1.51	6 (9%)	76,113,113	1.27	9 (11%)
18	CLA	B	514	-	45,53,73	1.80	5 (11%)	52,89,113	1.48	8 (15%)
18	CLA	b	508	-	65,73,73	1.50	6 (9%)	76,113,113	1.10	8 (10%)
20	BCR	C	515	-	41,41,41	0.77	0	56,56,56	2.09	20 (35%)
18	CLA	c	515	-	65,73,73	1.51	6 (9%)	76,113,113	1.17	8 (10%)
18	CLA	D	404	-	65,73,73	1.51	6 (9%)	76,113,113	1.19	6 (7%)
18	CLA	B	503	-	65,73,73	1.52	7 (10%)	76,113,113	1.21	7 (9%)
18	CLA	B	507	-	65,73,73	1.53	6 (9%)	76,113,113	1.19	8 (10%)
18	CLA	b	505	-	65,73,73	1.51	6 (9%)	76,113,113	1.15	6 (7%)
18	CLA	c	508	-	65,73,73	1.52	7 (10%)	76,113,113	1.22	8 (10%)
18	CLA	b	503	-	65,73,73	1.52	7 (10%)	76,113,113	1.25	7 (9%)
21	LMG	D	410	-	48,48,55	0.97	2 (4%)	56,56,63	0.95	2 (3%)
22	LHG	A	409	-	43,43,48	1.00	2 (4%)	46,49,54	0.91	2 (4%)
22	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	0.92	2 (3%)
18	CLA	c	507	-	65,73,73	1.51	6 (9%)	76,113,113	1.18	8 (10%)
18	CLA	C	508	-	65,73,73	1.50	6 (9%)	76,113,113	1.22	8 (10%)
18	CLA	a	403	-	49,57,73	1.73	6 (12%)	55,93,113	1.41	8 (14%)
20	BCR	C	516	-	41,41,41	0.80	1 (2%)	56,56,56	2.24	22 (39%)
21	LMG	h	101	-	48,48,55	0.98	3 (6%)	56,56,63	1.02	3 (5%)
18	CLA	B	508	-	65,73,73	1.51	7 (10%)	76,113,113	1.11	5 (6%)
28	HEM	e	101	6,5	41,50,50	1.50	4 (9%)	45,82,82	1.45	5 (11%)
18	CLA	C	502	-	65,73,73	1.51	7 (10%)	76,113,113	1.15	6 (7%)
19	PHO	D	402	-	51,69,69	1.01	4 (7%)	47,99,99	1.04	4 (8%)
18	CLA	c	513	3	65,73,73	1.54	6 (9%)	76,113,113	1.18	8 (10%)
18	CLA	C	510	-	65,73,73	1.52	5 (7%)	76,113,113	1.23	6 (7%)
22	LHG	a	408	-	43,43,48	1.00	2 (4%)	46,49,54	0.92	2 (4%)
21	LMG	A	407	-	46,46,55	0.99	2 (4%)	54,54,63	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PL9	d	407	-	55,55,55	1.01	3 (5%)	68,69,69	1.55	12 (17%)
20	BCR	A	410	-	41,41,41	0.75	0	56,56,56	1.93	17 (30%)
21	LMG	C	521	-	51,51,55	0.94	2 (3%)	59,59,63	0.92	2 (3%)
18	CLA	C	513	-	65,73,73	1.53	7 (10%)	76,113,113	1.25	8 (10%)
22	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	0.91	2 (3%)
24	DGD	C	520	-	60,60,67	0.91	2 (3%)	74,74,81	0.87	2 (2%)
18	CLA	B	513	-	65,73,73	1.49	6 (9%)	76,113,113	1.20	8 (10%)
18	CLA	c	512	-	65,73,73	1.54	6 (9%)	76,113,113	1.21	7 (9%)
18	CLA	C	505	-	65,73,73	1.53	6 (9%)	76,113,113	1.20	8 (10%)
23	SQD	c	501	-	50,51,54	1.21	4 (8%)	59,62,65	1.14	4 (6%)
18	CLA	c	504	-	65,73,73	1.51	7 (10%)	76,113,113	1.28	9 (11%)
18	CLA	B	515	-	65,73,73	1.51	5 (7%)	76,113,113	1.27	8 (10%)
22	LHG	A	408	-	42,42,48	1.01	2 (4%)	45,48,54	1.03	2 (4%)
18	CLA	c	510	-	65,73,73	1.51	6 (9%)	76,113,113	1.21	6 (7%)
20	BCR	z	101	-	41,41,41	0.79	0	56,56,56	2.07	21 (37%)
18	CLA	b	516	-	65,73,73	1.53	7 (10%)	76,113,113	1.21	7 (9%)
22	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
20	BCR	c	517	-	41,41,41	0.74	0	56,56,56	1.87	16 (28%)
22	LHG	B	522	-	48,48,48	0.94	2 (4%)	51,54,54	0.91	2 (3%)
22	LHG	X	101	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
18	CLA	C	514	-	65,73,73	1.52	5 (7%)	76,113,113	1.16	8 (10%)

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
18	CLA	C	509	-	1/1/15/20	9/37/115/115	-
18	CLA	C	503	-	1/1/15/20	11/37/115/115	-
18	CLA	B	510	-	1/1/15/20	10/37/115/115	-
18	CLA	b	504	-	1/1/15/20	17/37/115/115	-
18	CLA	b	501	-	1/1/15/20	18/37/115/115	-
18	CLA	c	511	-	1/1/15/20	16/37/115/115	-
20	BCR	x	102	-	-	5/29/63/63	0/2/2/2
20	BCR	B	518	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	d	404	-	1/1/15/20	8/37/115/115	-
20	BCR	B	517	-	-	4/29/63/63	0/2/2/2
18	CLA	c	503	-	1/1/15/20	13/37/115/115	-
18	CLA	C	506	-	1/1/15/20	18/37/115/115	-
18	CLA	b	513	-	1/1/15/20	12/37/115/115	-
19	PHO	A	404	-	-	11/37/103/103	0/5/6/6
22	LHG	a	407	-	-	13/47/47/53	-
18	CLA	B	505	-	1/1/15/20	15/37/115/115	-
18	CLA	B	506	-	1/1/15/20	13/37/115/115	-
22	LHG	d	408	-	-	6/53/53/53	-
18	CLA	b	510	-	1/1/15/20	10/37/115/115	-
18	CLA	b	511	-	1/1/15/20	17/37/115/115	-
18	CLA	A	405	-	1/1/14/20	4/31/109/115	-
24	DGD	C	518	-	-	5/42/82/95	0/2/2/2
22	LHG	x	101	-	-	17/53/53/53	-
18	CLA	b	514	-	1/1/11/20	2/13/91/115	-
28	HEM	F	101	6,5	-	5/12/54/54	-
18	CLA	A	402	-	1/1/15/20	10/37/115/115	-
18	CLA	d	405	-	1/1/15/20	18/37/115/115	-
20	BCR	k	101	-	-	2/29/63/63	0/2/2/2
18	CLA	a	402	-	1/1/15/20	9/37/115/115	-
19	PHO	d	402	-	-	9/37/103/103	0/5/6/6
20	BCR	b	517	-	-	4/29/63/63	0/2/2/2
21	LMG	B	520	-	-	4/37/57/70	0/1/1/1
18	CLA	C	512	3	1/1/15/20	11/37/115/115	-
24	DGD	c	518	-	-	5/42/82/95	0/2/2/2
18	CLA	C	507	-	1/1/15/20	16/37/115/115	-
18	CLA	b	509	-	1/1/15/20	18/37/115/115	-
18	CLA	B	512	-	1/1/15/20	11/37/115/115	-
18	CLA	d	401	-	1/1/15/20	9/37/115/115	-
18	CLA	B	516	-	1/1/15/20	9/37/115/115	-
24	DGD	C	519	-	-	8/38/78/95	0/2/2/2
18	CLA	D	405	-	1/1/15/20	15/37/115/115	-
20	BCR	d	406	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	b	518	-	-	4/29/63/63	0/2/2/2
18	CLA	c	514	-	1/1/15/20	10/37/115/115	-
18	CLA	C	511	-	1/1/15/20	12/37/115/115	-
21	LMG	d	409	-	-	7/41/61/70	0/1/1/1
18	CLA	b	515	-	1/1/15/20	7/37/115/115	-
25	LMU	c	522	-	-	7/21/61/61	0/2/2/2
22	LHG	B	521	-	-	7/48/48/53	-
18	CLA	A	403	-	1/1/11/20	7/18/96/115	-
18	CLA	C	504	-	1/1/15/20	16/37/115/115	-
20	BCR	C	517	-	-	4/29/63/63	0/2/2/2
18	CLA	B	504	-	1/1/15/20	15/37/115/115	-
19	PHO	a	404	-	-	10/37/103/103	0/5/6/6
18	CLA	a	405	-	1/1/14/20	4/31/109/115	-
21	LMG	D	409	-	-	8/41/61/70	0/1/1/1
18	CLA	b	506	-	1/1/15/20	14/37/115/115	-
25	LMU	C	522	-	-	8/21/61/61	0/2/2/2
18	CLA	B	509	-	1/1/15/20	18/37/115/115	-
24	DGD	c	519	-	-	8/38/78/95	0/2/2/2
18	CLA	B	502	-	1/1/15/20	10/37/115/115	-
27	PL9	D	407	-	-	10/53/73/73	0/1/1/1
18	CLA	D	401	-	1/1/15/20	9/37/115/115	-
20	BCR	A	406	-	-	4/29/63/63	0/2/2/2
20	BCR	c	516	-	-	3/29/63/63	0/2/2/2
20	BCR	B	519	-	-	4/29/63/63	0/2/2/2
22	LHG	b	521	-	-	9/53/53/53	-
20	BCR	D	406	-	-	4/29/63/63	0/2/2/2
18	CLA	b	512	-	1/1/15/20	11/37/115/115	-
21	LMG	c	502	-	-	5/41/61/70	0/1/1/1
22	LHG	b	520	-	-	7/48/48/53	-
20	BCR	a	406	-	-	4/29/63/63	0/2/2/2
18	CLA	c	505	-	1/1/15/20	17/37/115/115	-
18	CLA	B	501	-	1/1/15/20	17/37/115/115	-
21	LMG	c	521	-	-	9/46/66/70	0/1/1/1
21	LMG	b	519	-	-	4/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	507	-	1/1/15/20	13/37/115/115	-
18	CLA	b	502	-	1/1/15/20	10/37/115/115	-
23	SQD	C	501	-	-	13/46/66/69	0/1/1/1
24	DGD	c	520	-	-	4/48/88/95	0/2/2/2
20	BCR	X	102	-	-	5/29/63/63	0/2/2/2
18	CLA	c	506	-	1/1/15/20	10/37/115/115	-
20	BCR	K	101	-	-	2/29/63/63	0/2/2/2
18	CLA	c	509	-	1/1/15/20	8/37/115/115	-
18	CLA	B	511	-	1/1/15/20	17/37/115/115	-
18	CLA	B	514	-	1/1/11/20	2/13/91/115	-
18	CLA	b	508	-	1/1/15/20	10/37/115/115	-
20	BCR	C	515	-	-	6/29/63/63	0/2/2/2
18	CLA	c	515	-	1/1/15/20	12/37/115/115	-
18	CLA	D	404	-	1/1/15/20	8/37/115/115	-
18	CLA	B	503	-	1/1/15/20	10/37/115/115	-
18	CLA	B	507	-	1/1/15/20	13/37/115/115	-
18	CLA	b	505	-	1/1/15/20	14/37/115/115	-
18	CLA	c	508	-	1/1/15/20	16/37/115/115	-
18	CLA	b	503	-	1/1/15/20	10/37/115/115	-
21	LMG	D	410	-	-	11/43/63/70	0/1/1/1
22	LHG	A	409	-	-	17/48/48/53	-
22	LHG	l	101	-	-	12/53/53/53	-
18	CLA	c	507	-	1/1/15/20	17/37/115/115	-
18	CLA	C	508	-	1/1/15/20	8/37/115/115	-
18	CLA	a	403	-	1/1/11/20	9/18/96/115	-
20	BCR	C	516	-	-	3/29/63/63	0/2/2/2
21	LMG	h	101	-	-	11/43/63/70	0/1/1/1
18	CLA	B	508	-	1/1/15/20	10/37/115/115	-
28	HEM	e	101	6,5	-	5/12/54/54	-
18	CLA	C	502	-	1/1/15/20	13/37/115/115	-
19	PHO	D	402	-	-	9/37/103/103	0/5/6/6
18	CLA	c	513	3	1/1/15/20	11/37/115/115	-
18	CLA	C	510	-	1/1/15/20	14/37/115/115	-
22	LHG	a	408	-	-	17/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMG	A	407	-	-	5/41/61/70	0/1/1/1
27	PL9	d	407	-	-	11/53/73/73	0/1/1/1
20	BCR	A	410	-	-	4/29/63/63	0/2/2/2
21	LMG	C	521	-	-	9/46/66/70	0/1/1/1
18	CLA	C	513	-	1/1/15/20	10/37/115/115	-
22	LHG	L	101	-	-	14/53/53/53	-
24	DGD	C	520	-	-	4/48/88/95	0/2/2/2
18	CLA	B	513	-	1/1/15/20	12/37/115/115	-
18	CLA	c	512	-	1/1/15/20	15/37/115/115	-
18	CLA	C	505	-	1/1/15/20	10/37/115/115	-
23	SQD	c	501	-	-	10/46/66/69	0/1/1/1
18	CLA	c	504	-	1/1/15/20	11/37/115/115	-
18	CLA	B	515	-	1/1/15/20	7/37/115/115	-
22	LHG	A	408	-	-	13/47/47/53	-
18	CLA	c	510	-	1/1/15/20	9/37/115/115	-
20	BCR	z	101	-	-	6/29/63/63	0/2/2/2
18	CLA	b	516	-	1/1/15/20	7/37/115/115	-
22	LHG	D	408	-	-	6/53/53/53	-
20	BCR	c	517	-	-	4/29/63/63	0/2/2/2
22	LHG	B	522	-	-	9/53/53/53	-
22	LHG	X	101	-	-	16/53/53/53	-
18	CLA	C	514	-	1/1/15/20	12/37/115/115	-

The worst 5 of 537 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	501	CLA	C4B-NB	7.92	1.42	1.35
18	B	509	CLA	C4B-NB	7.88	1.42	1.35
18	c	512	CLA	C4B-NB	7.86	1.42	1.35
18	D	401	CLA	C4B-NB	7.86	1.42	1.35
18	C	505	CLA	C4B-NB	7.82	1.42	1.35

The worst 5 of 1078 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	z	101	BCR	C3-C4-C5	-6.13	103.14	114.08
20	C	515	BCR	C3-C4-C5	-6.01	103.35	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	516	BCR	C3-C4-C5	-5.85	103.63	114.08
20	c	516	BCR	C30-C25-C26	-5.77	114.49	122.61
20	K	101	BCR	C28-C27-C26	-5.76	103.79	114.08

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	402	CLA	ND
18	A	403	CLA	ND
18	A	405	CLA	ND
18	B	501	CLA	ND
18	B	502	CLA	ND

5 of 1272 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	B	501	CLA	C1A-C2A-CAA-CBA
18	B	501	CLA	CHA-CBD-CGD-O1D
18	B	501	CLA	CHA-CBD-CGD-O2D
18	B	501	CLA	CAD-CBD-CGD-O1D
18	B	501	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

53 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	503	CLA	1	0
18	b	501	CLA	1	0
20	x	102	BCR	4	0
20	B	518	BCR	1	0
18	d	404	CLA	5	0
18	c	503	CLA	1	0
18	b	513	CLA	2	0
22	a	407	LHG	1	0
18	B	505	CLA	1	0
18	B	506	CLA	1	0
28	F	101	HEM	6	0
18	A	402	CLA	3	0
20	k	101	BCR	4	0
18	a	402	CLA	1	0
18	C	512	CLA	3	0
18	C	507	CLA	1	0

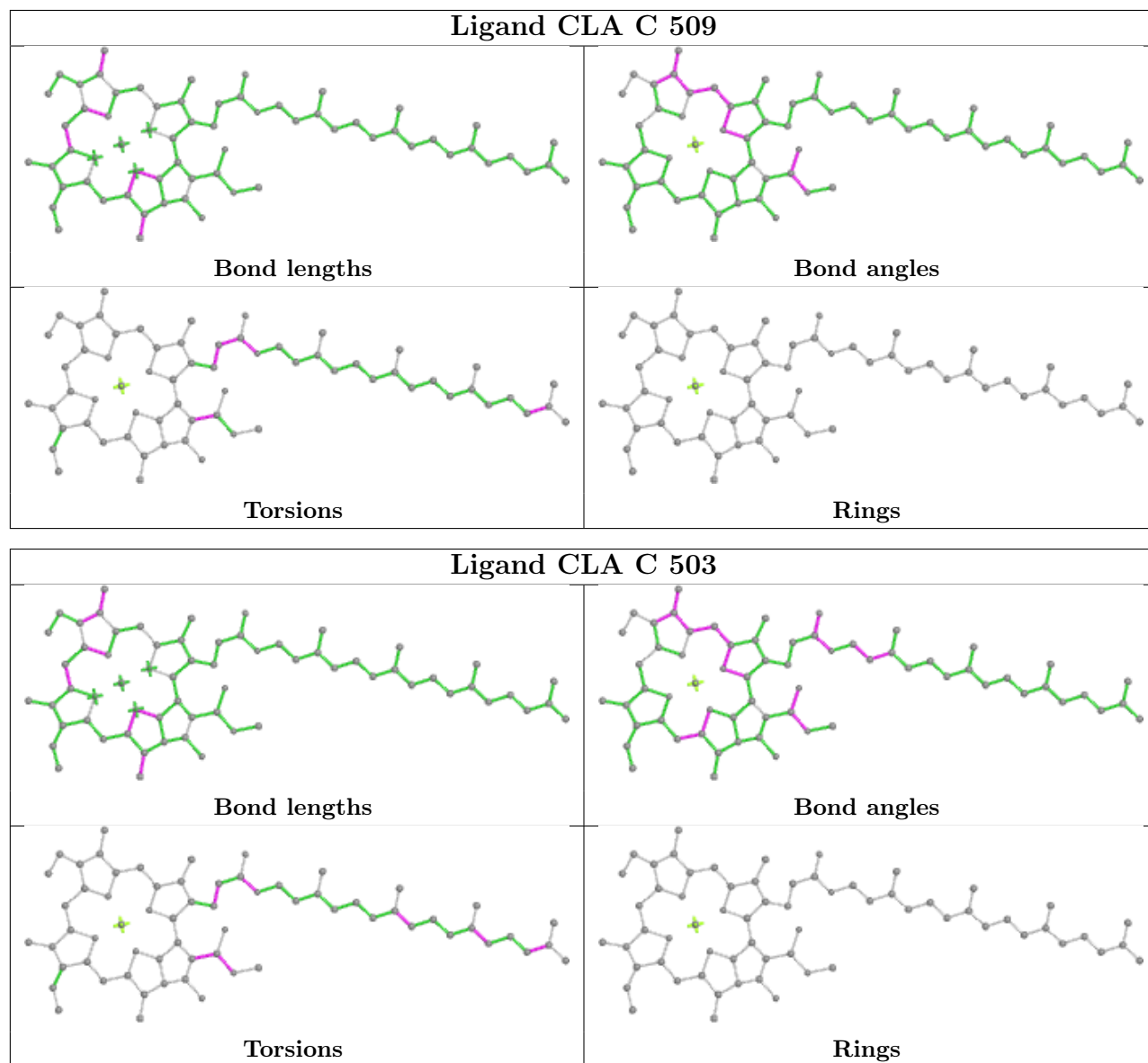
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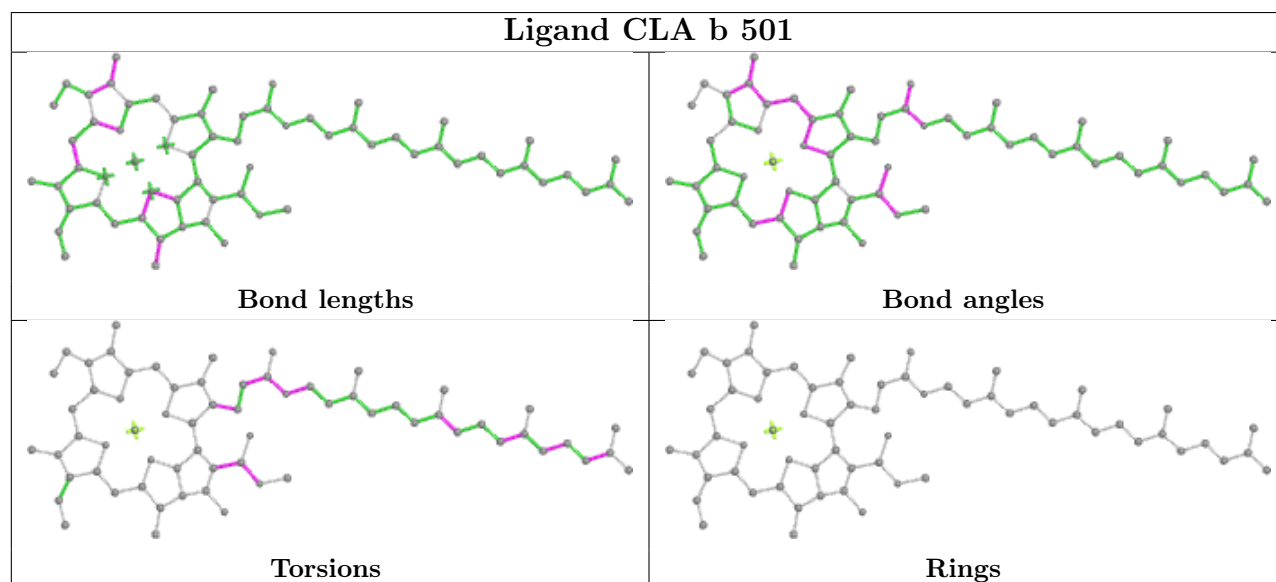
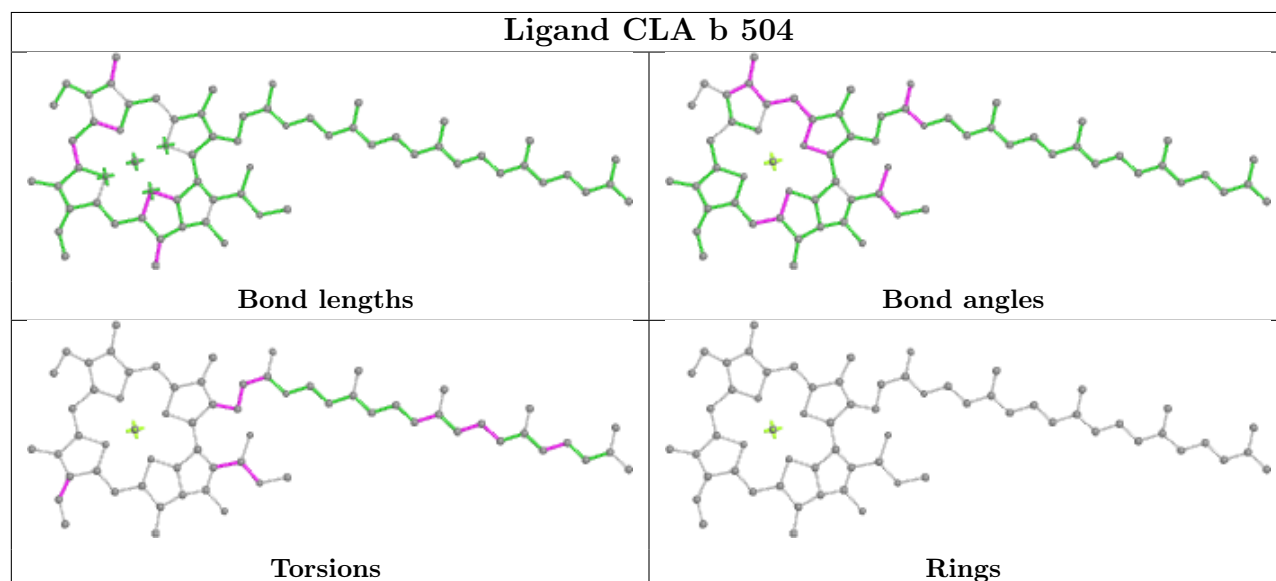
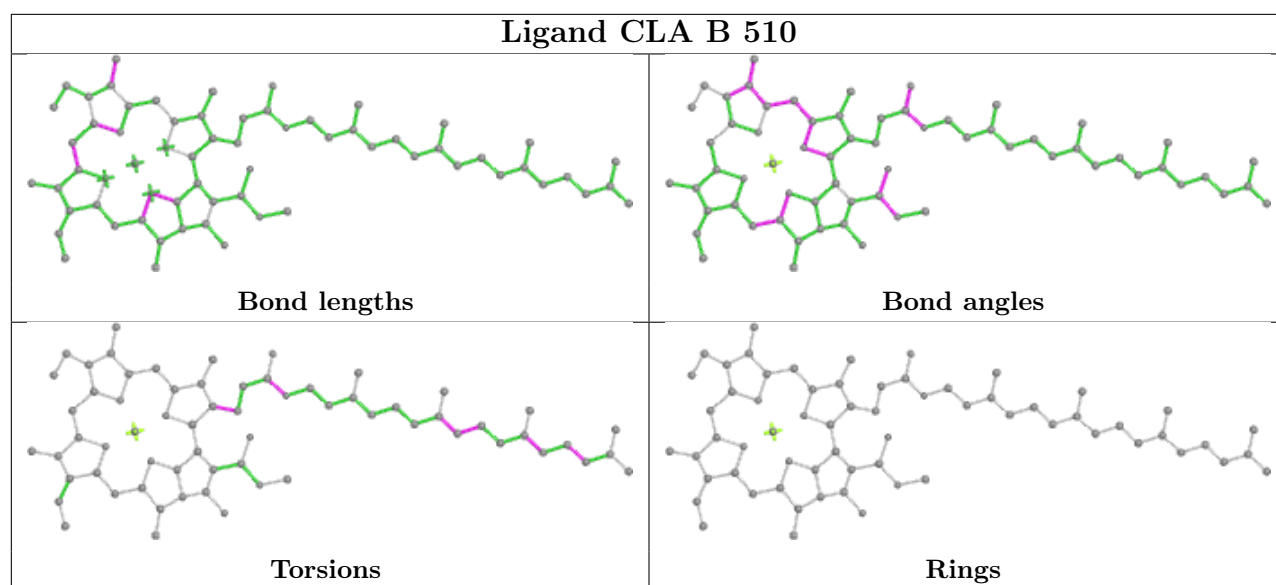
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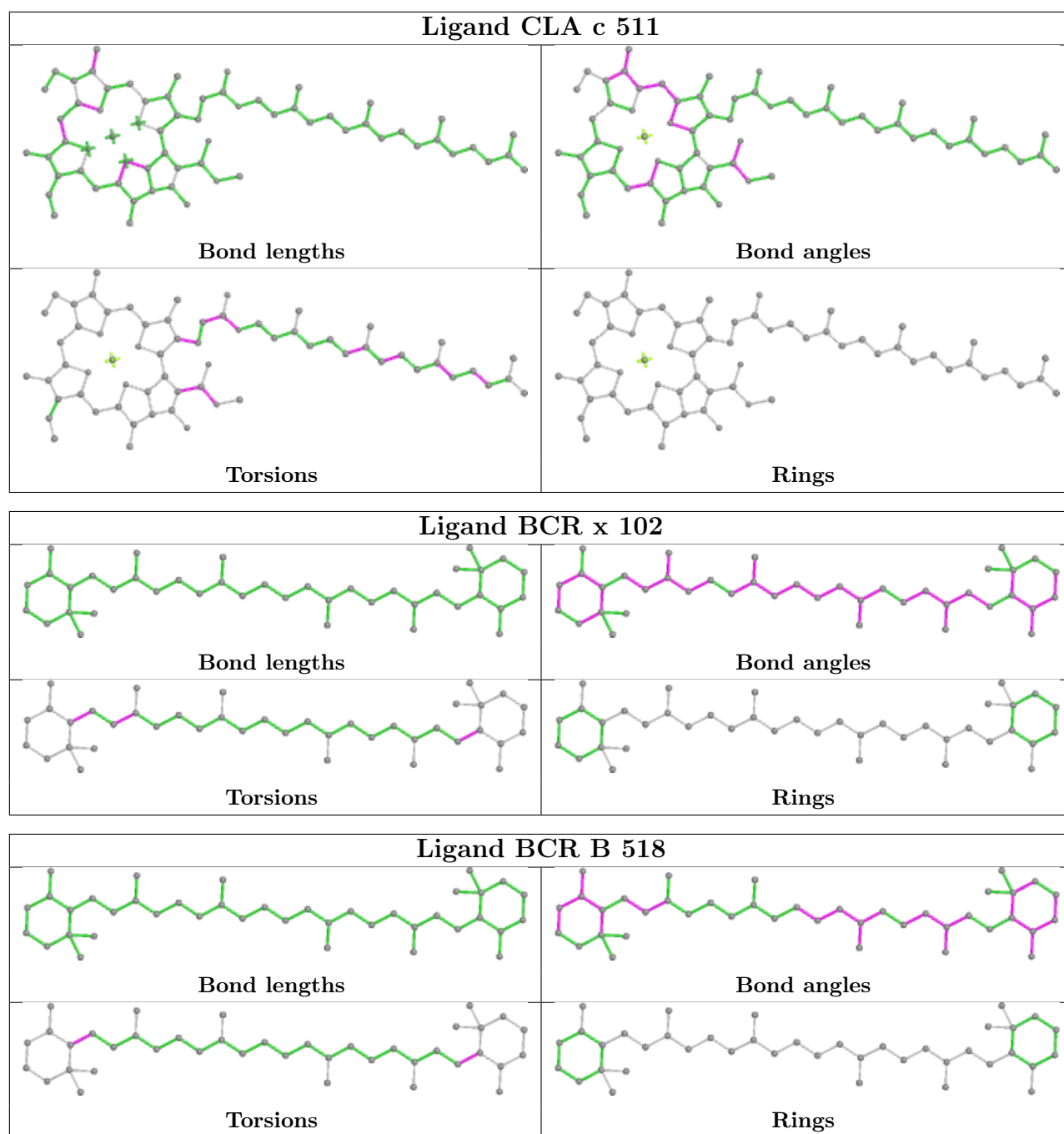
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b	509	CLA	1	0
20	d	406	BCR	1	0
20	b	518	BCR	1	0
20	C	517	BCR	4	0
18	b	506	CLA	1	0
18	B	509	CLA	2	0
18	B	502	CLA	1	0
20	A	406	BCR	3	0
20	c	516	BCR	5	0
20	B	519	BCR	2	0
20	D	406	BCR	2	0
20	a	406	BCR	4	0
18	B	501	CLA	1	0
18	b	507	CLA	1	0
18	b	502	CLA	1	0
20	X	102	BCR	2	0
20	K	101	BCR	4	0
20	C	515	BCR	8	0
18	c	515	CLA	1	0
18	D	404	CLA	5	0
18	b	505	CLA	1	0
21	D	410	LMG	1	0
22	l	101	LHG	1	0
18	c	507	CLA	1	0
20	C	516	BCR	4	0
21	h	101	LMG	1	0
28	e	101	HEM	5	0
18	C	502	CLA	1	0
18	c	513	CLA	1	0
20	A	410	BCR	2	0
18	B	513	CLA	2	0
18	c	512	CLA	1	0
18	c	504	CLA	2	0
22	A	408	LHG	1	0
20	z	101	BCR	6	0
20	c	517	BCR	4	0
18	C	514	CLA	1	0

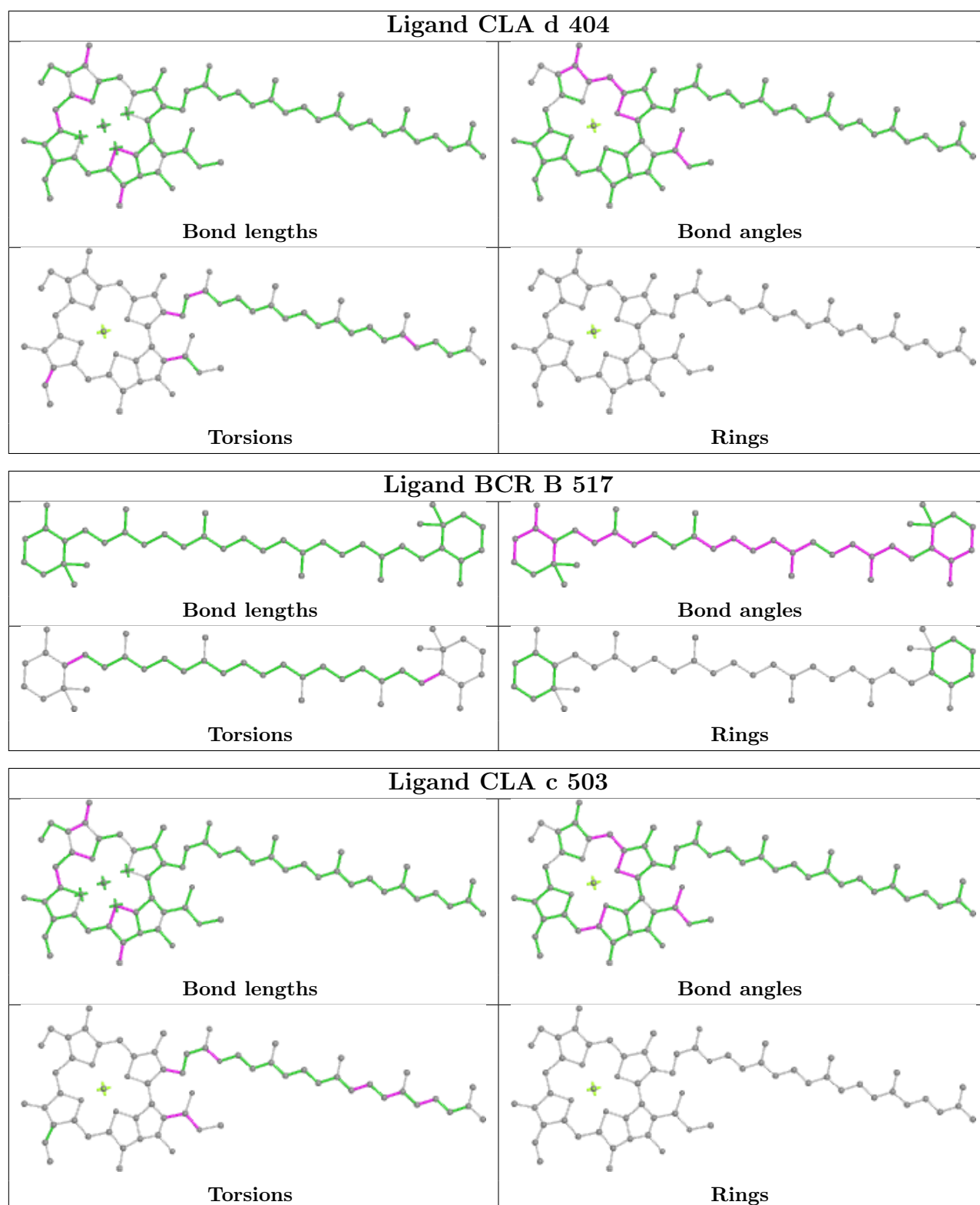
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

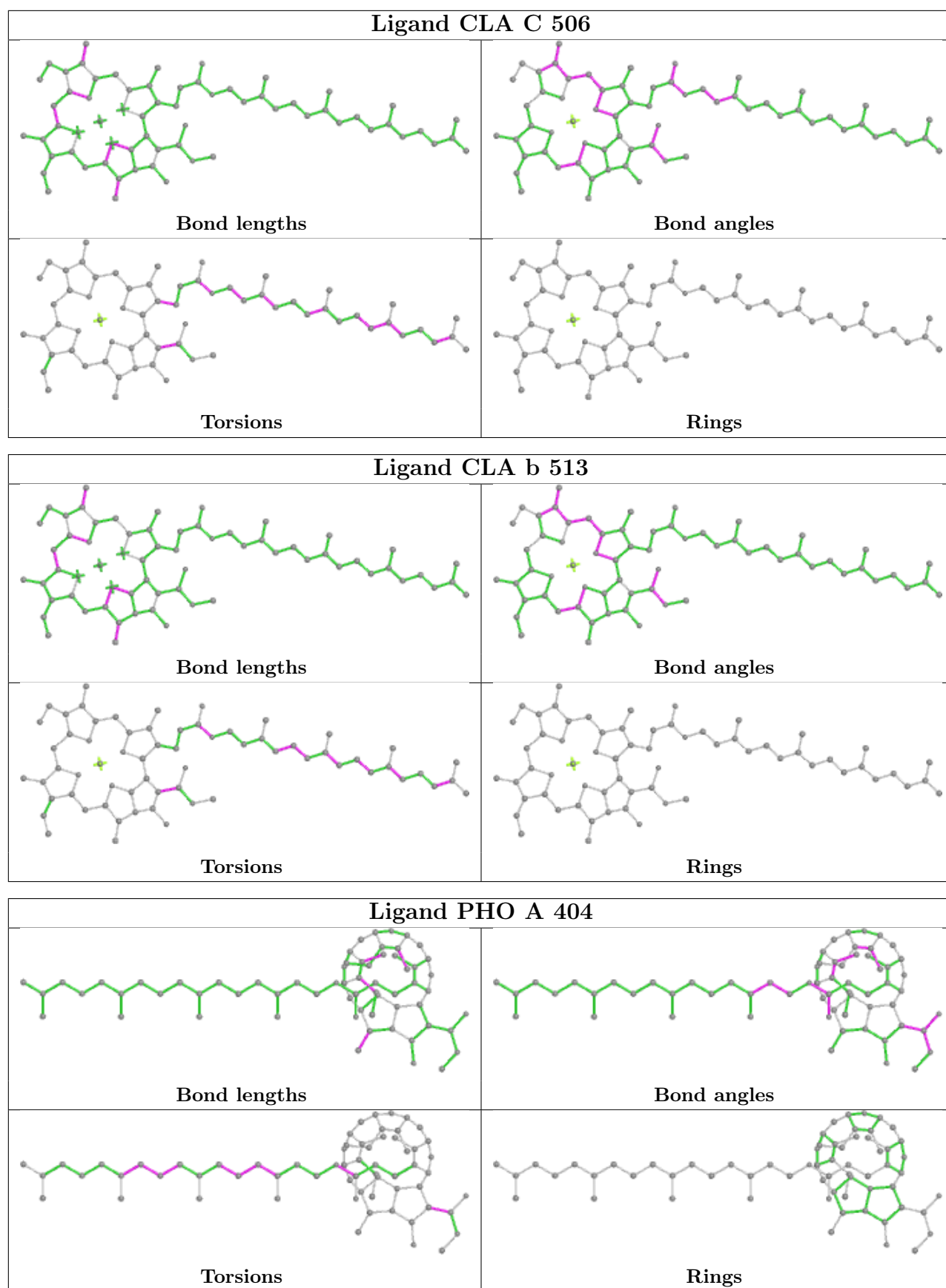
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

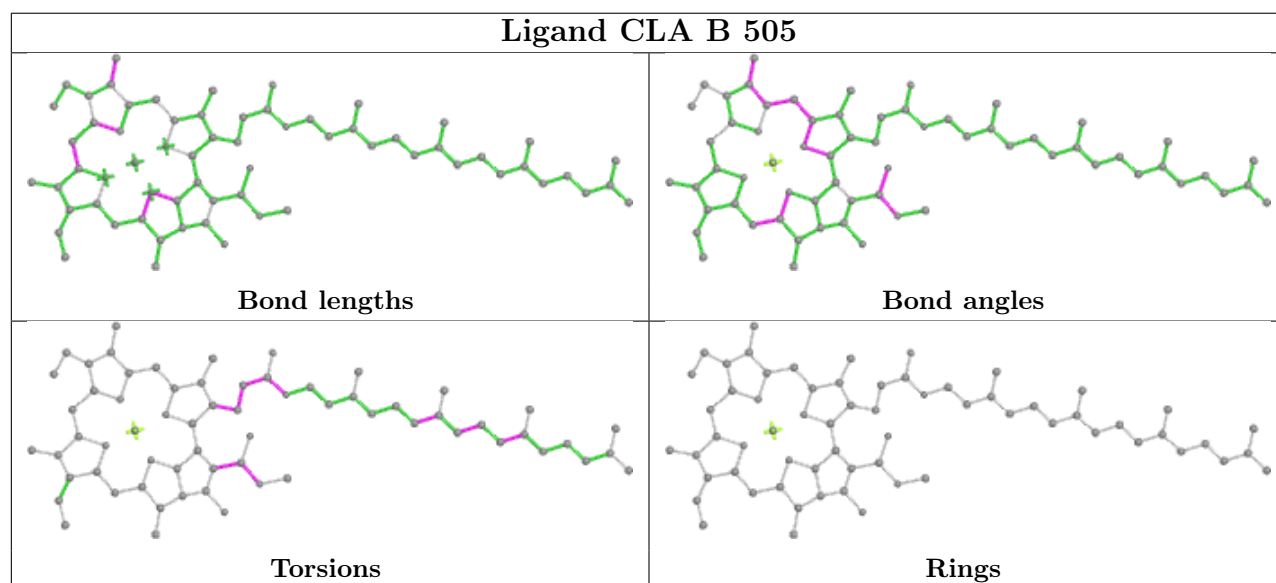
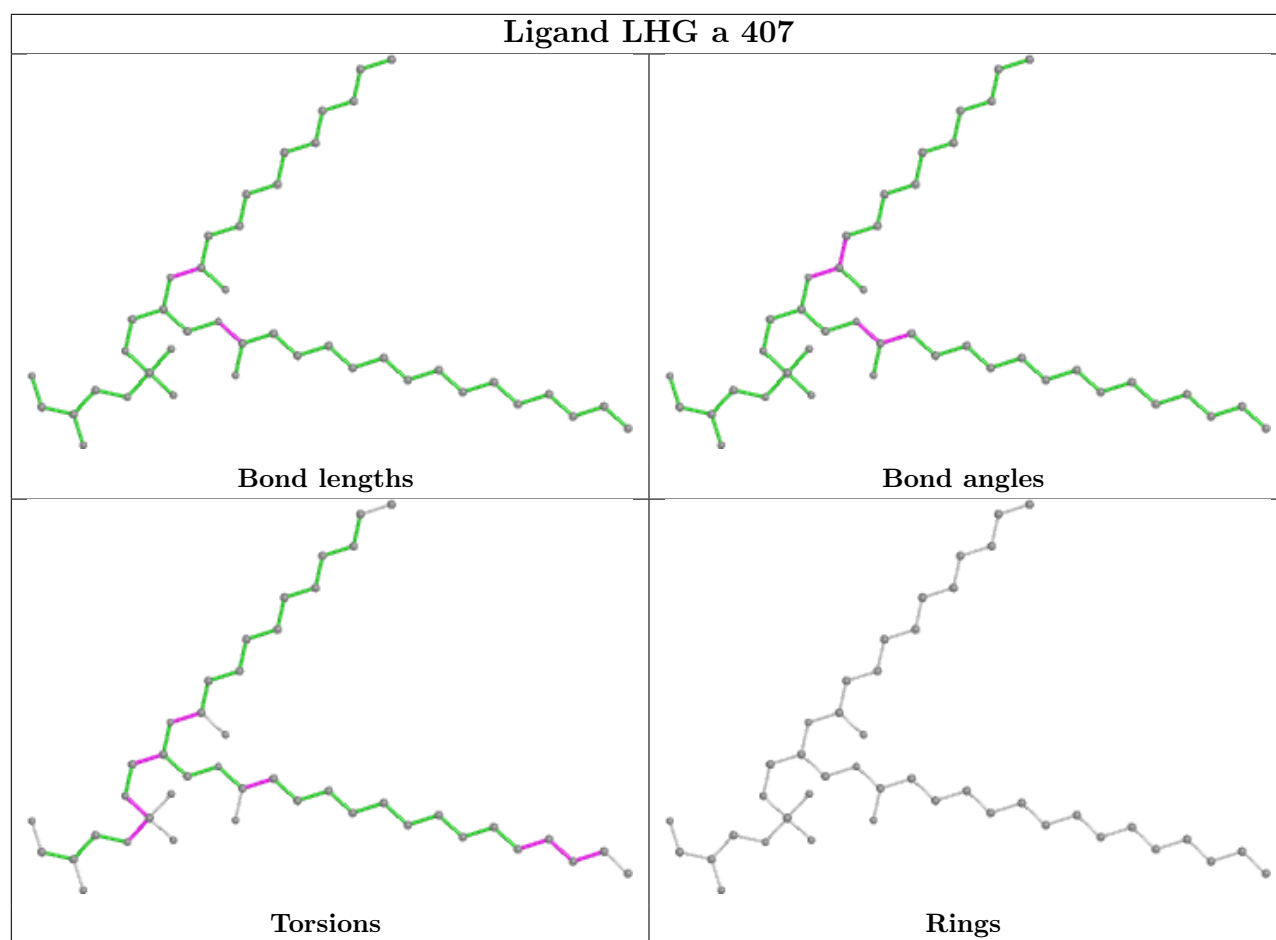


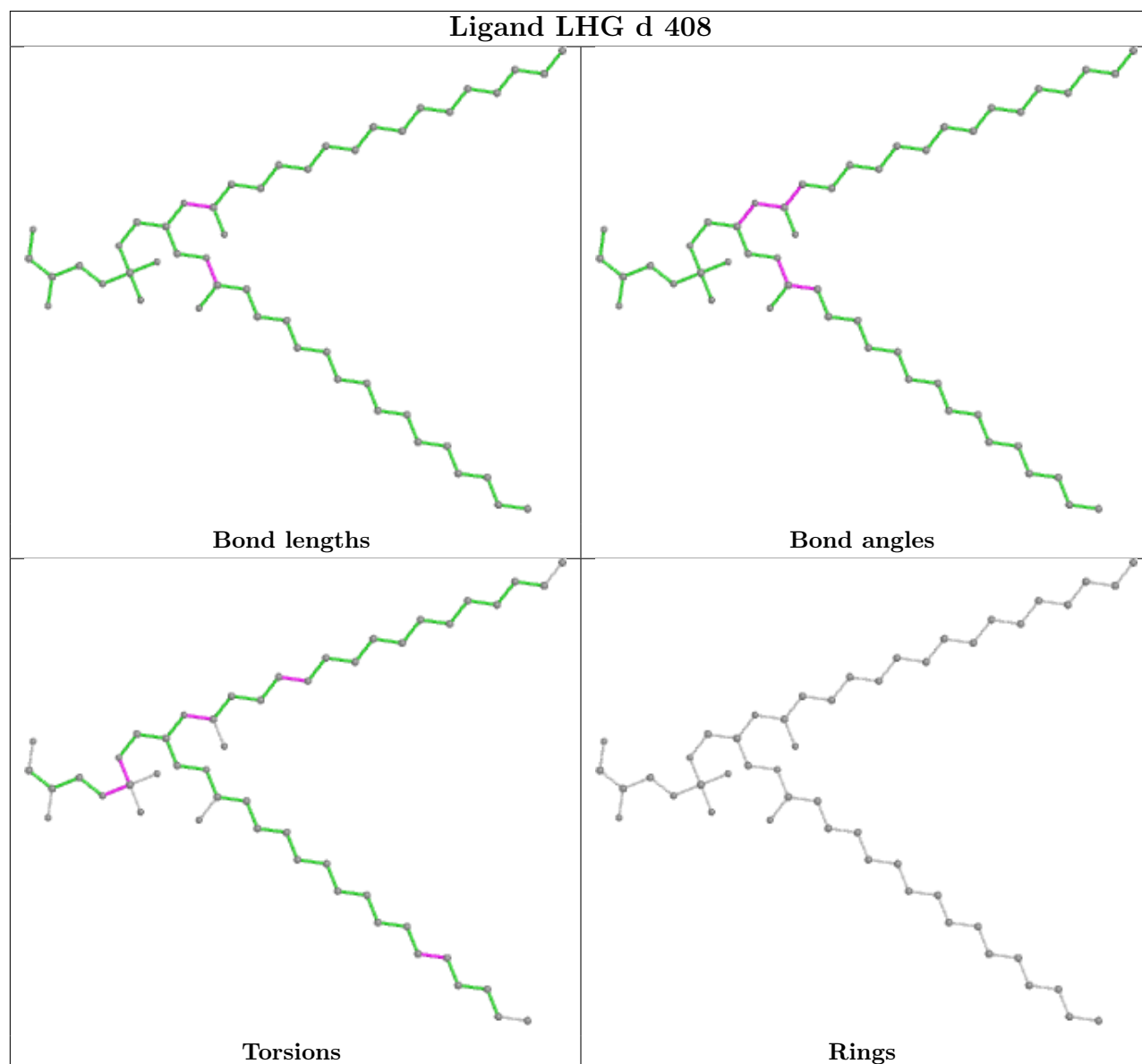
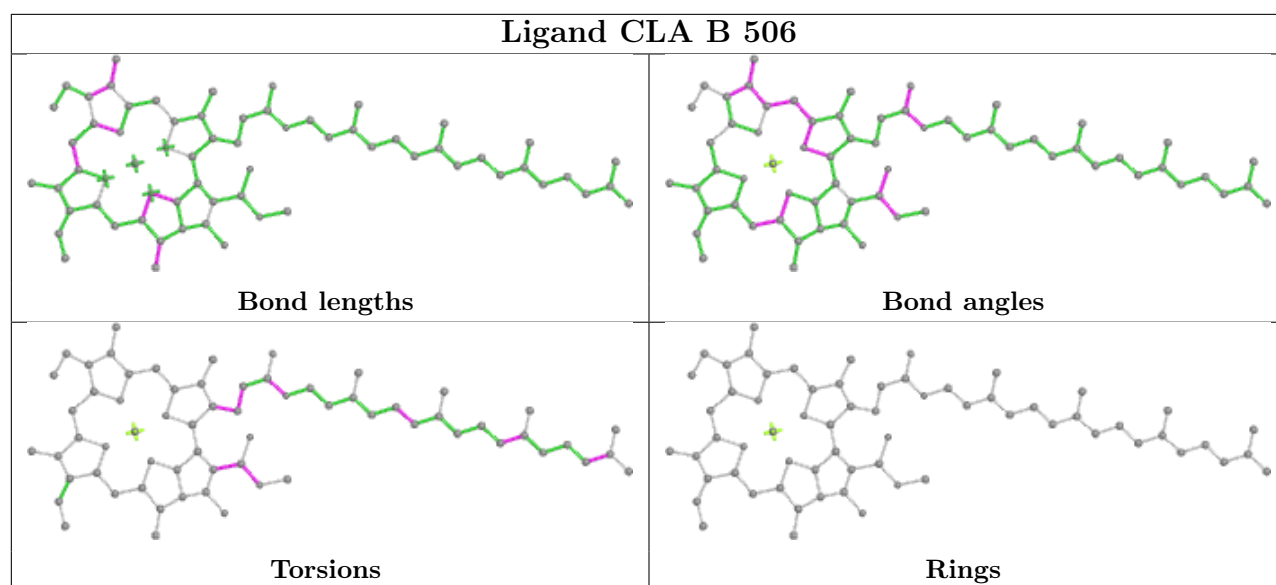


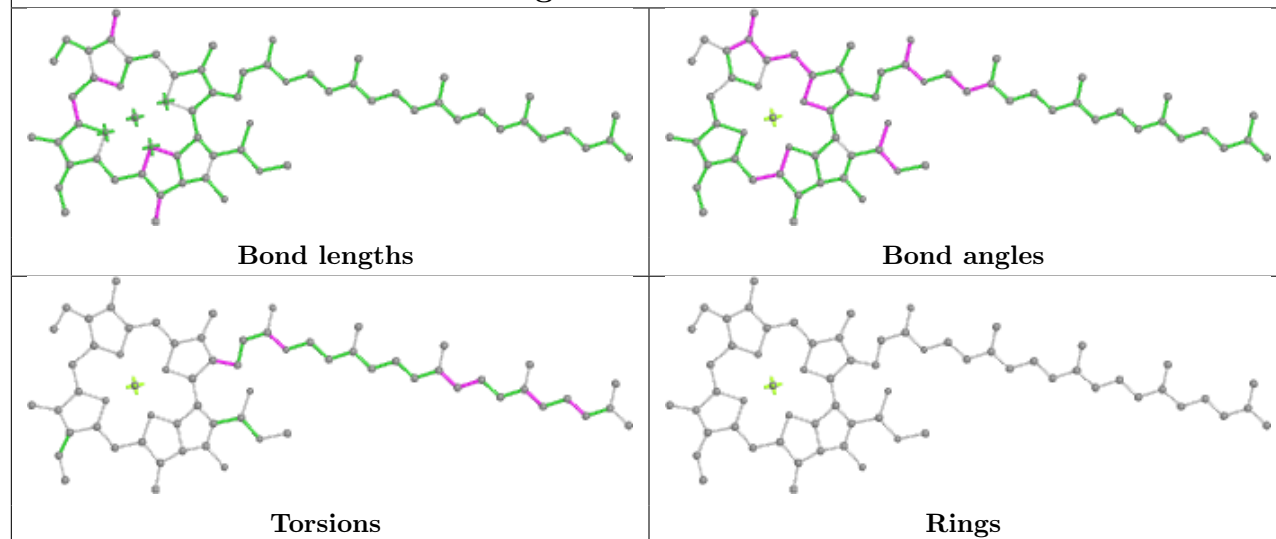
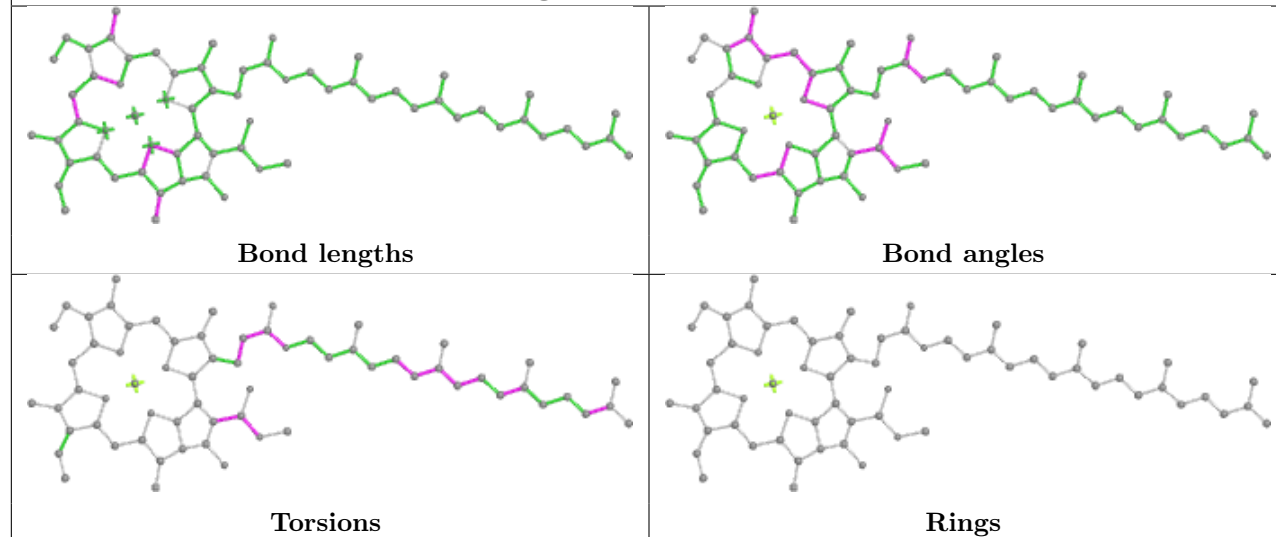


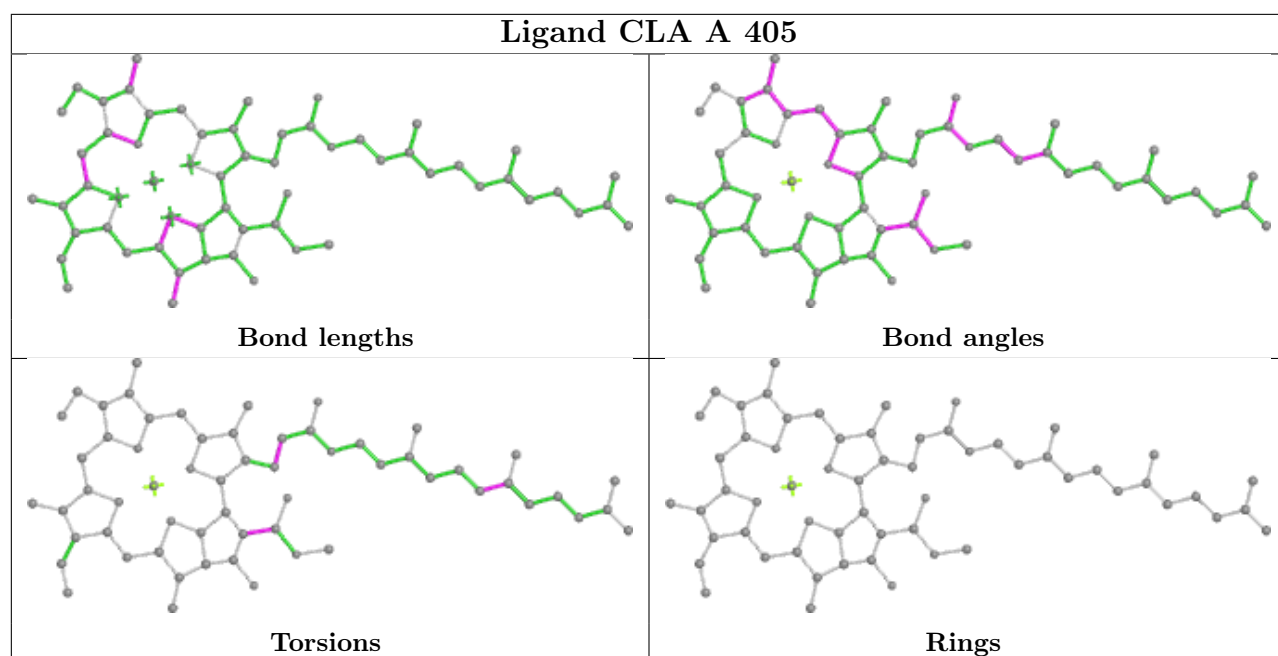


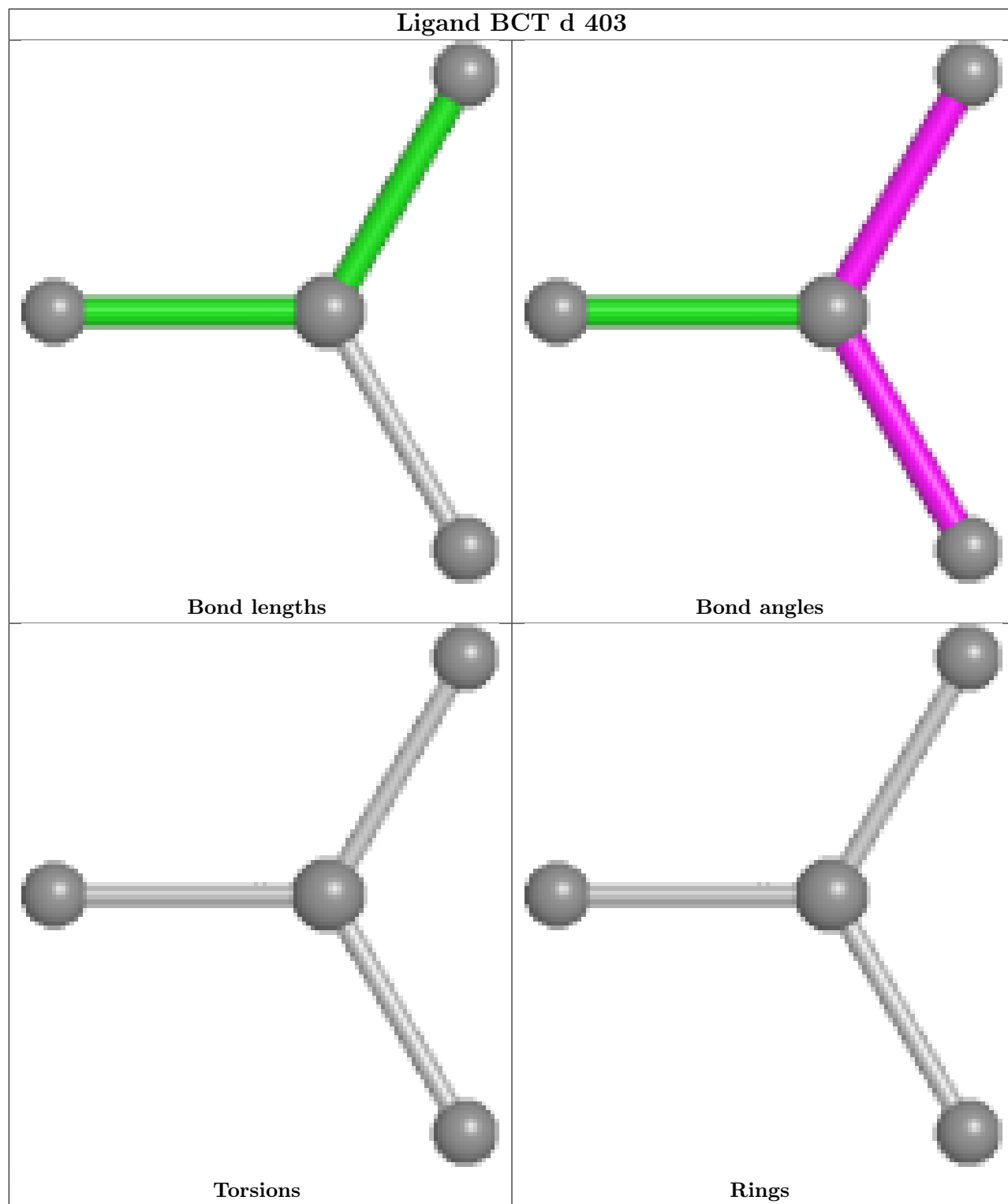


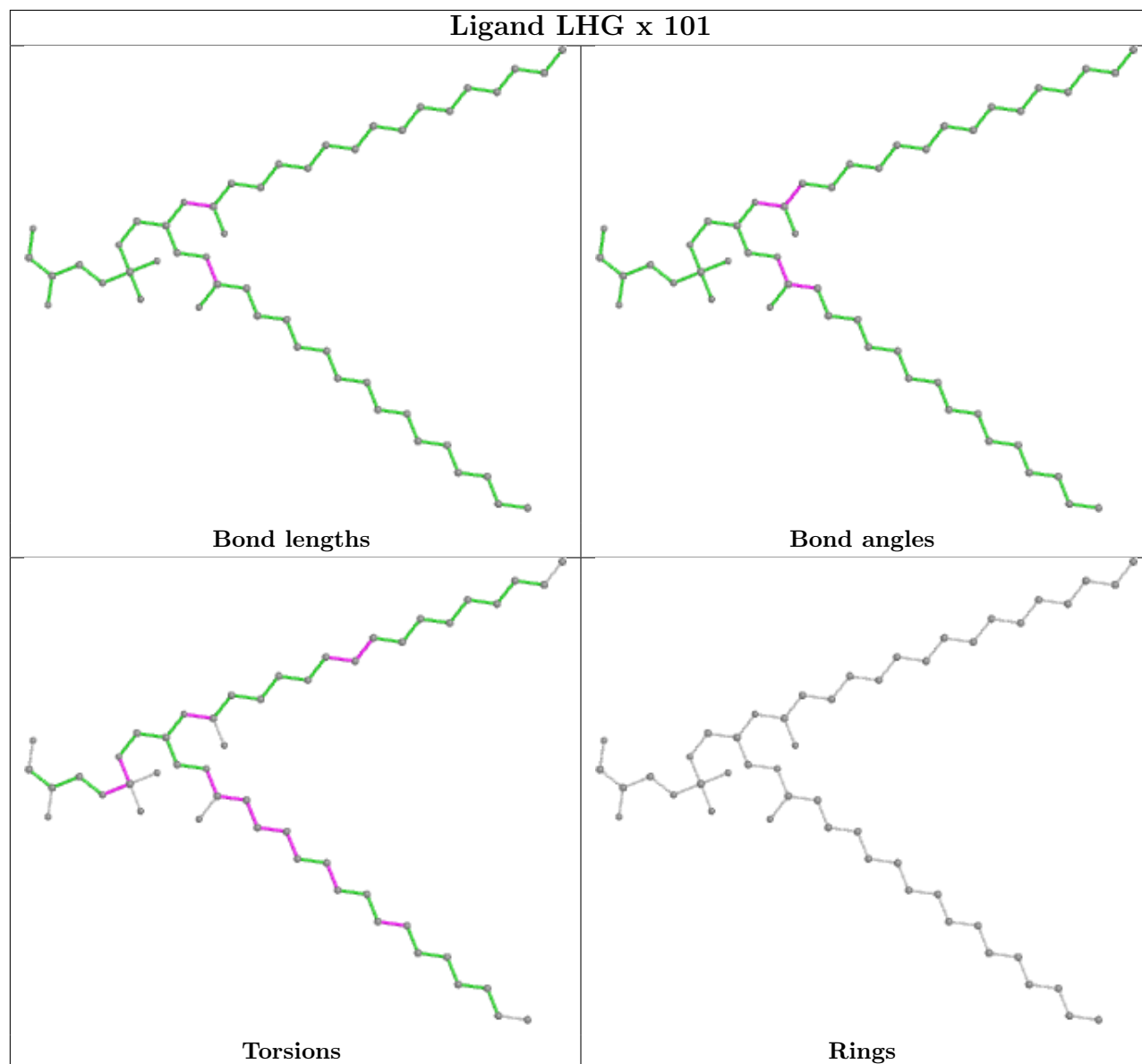
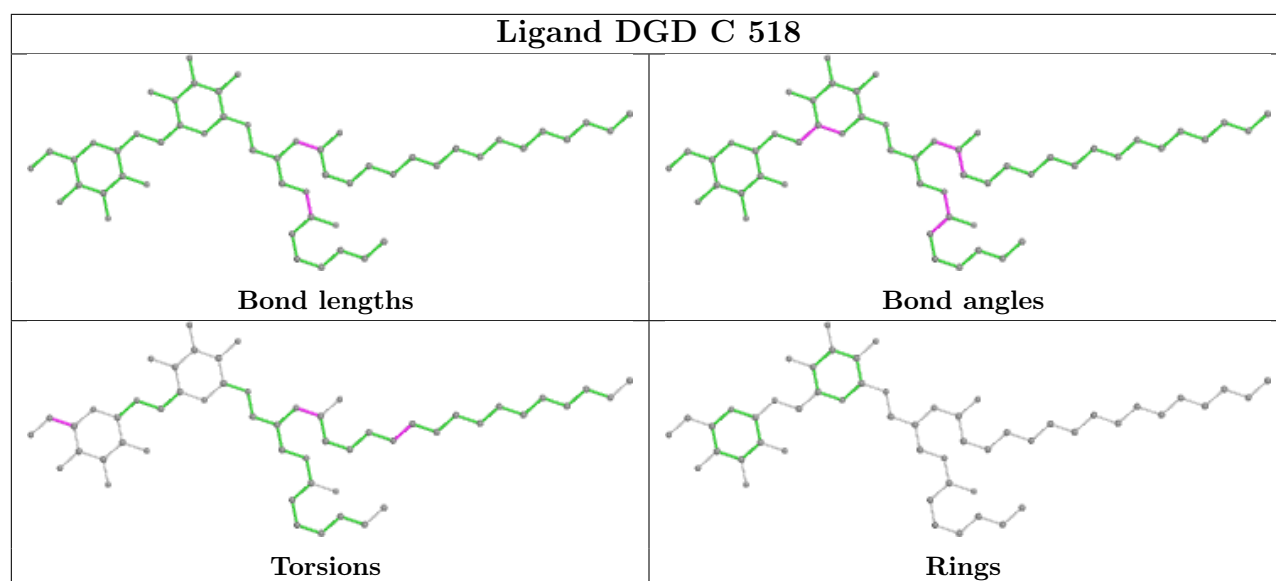




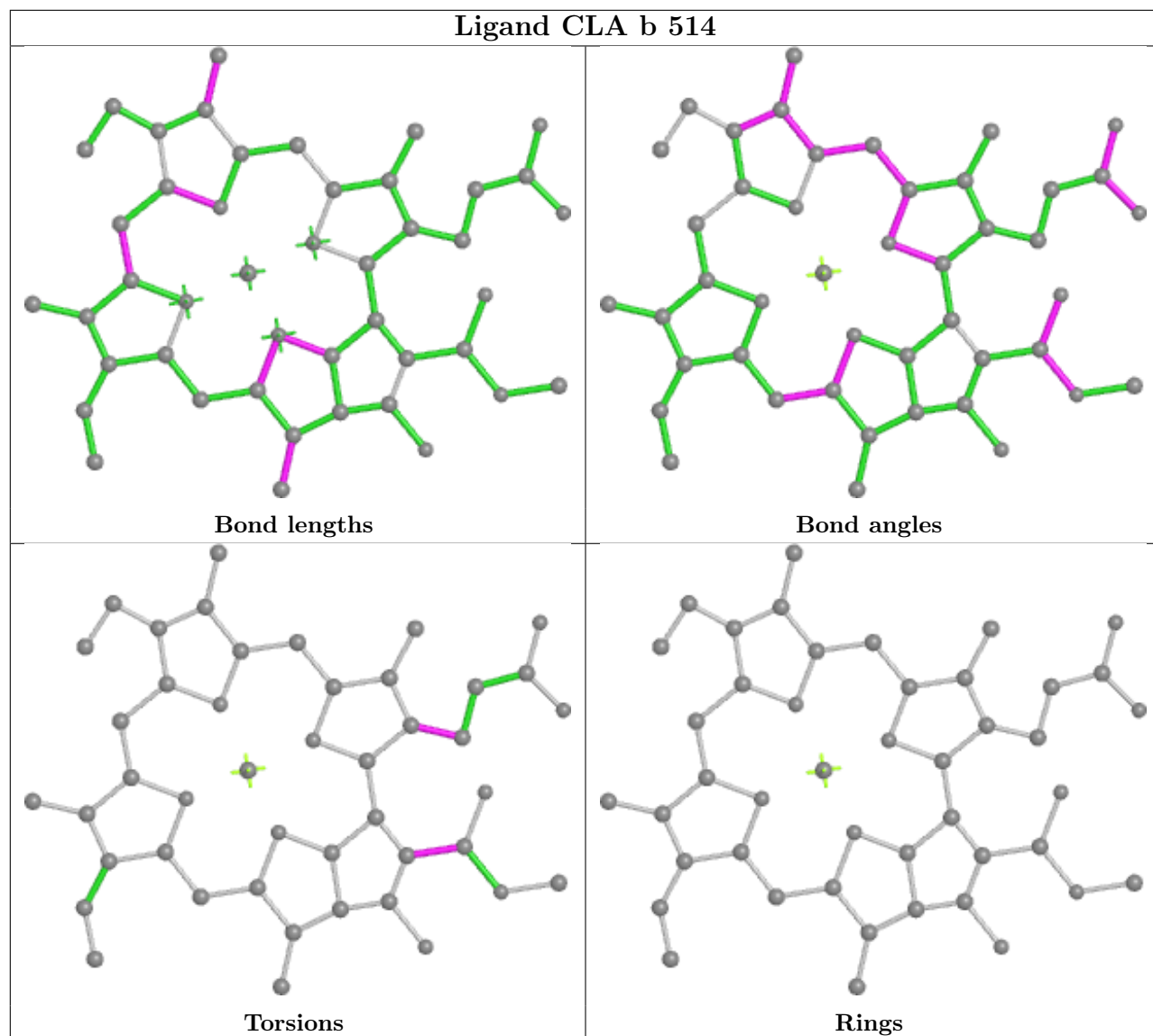
Ligand CLA b 510**Ligand CLA b 511**

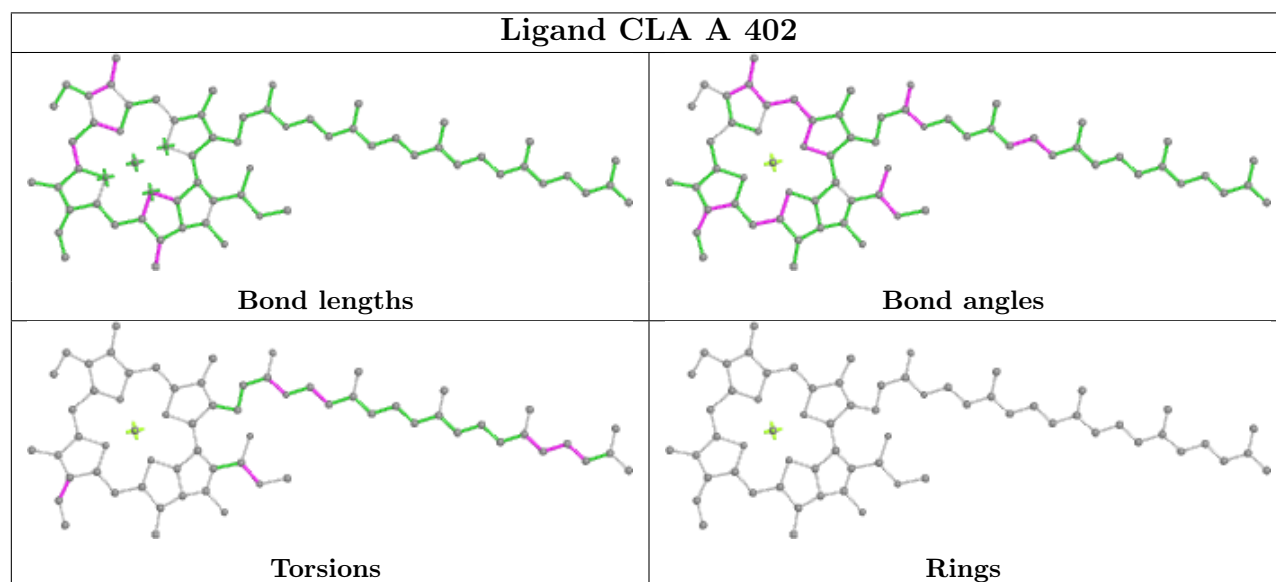
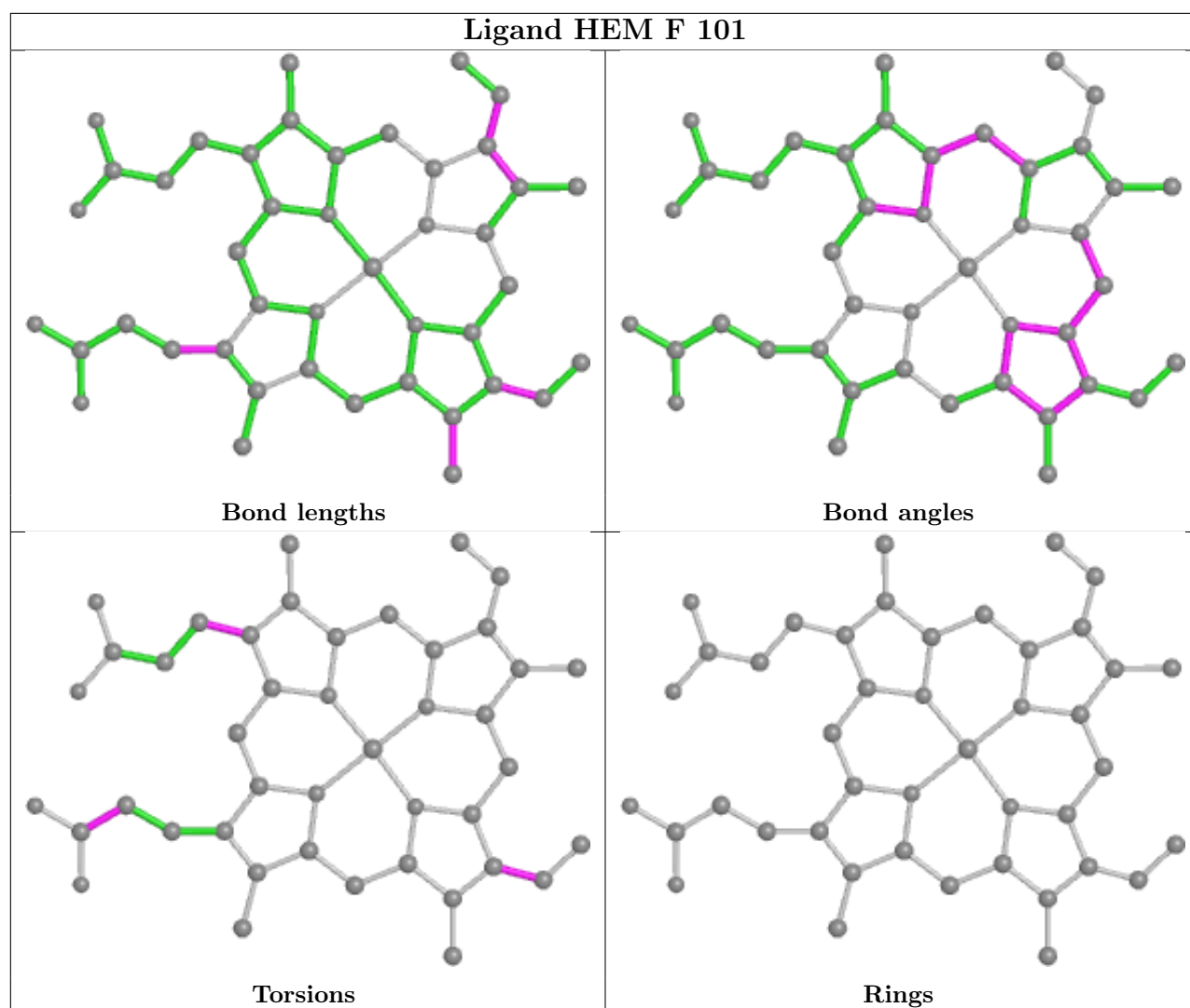


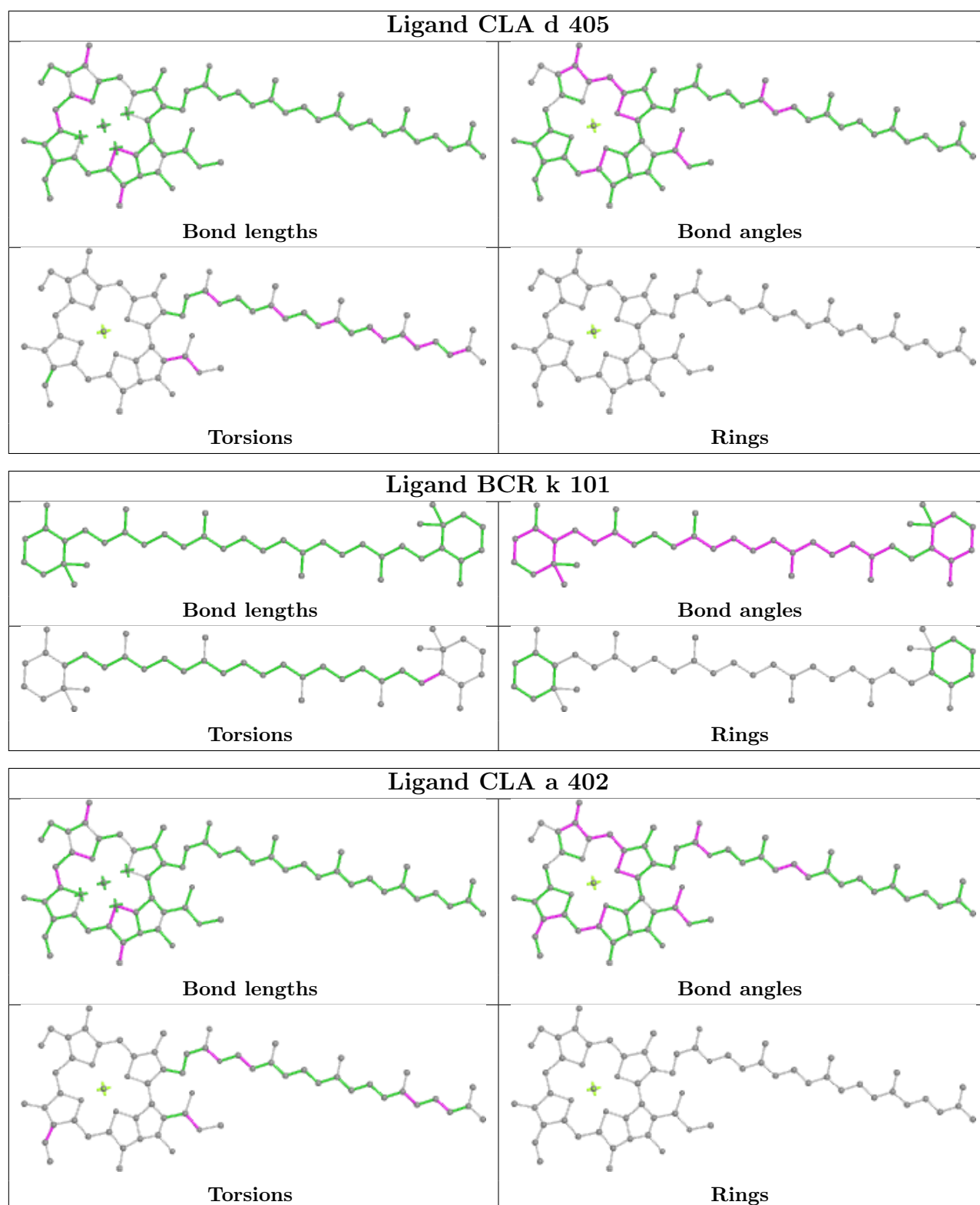


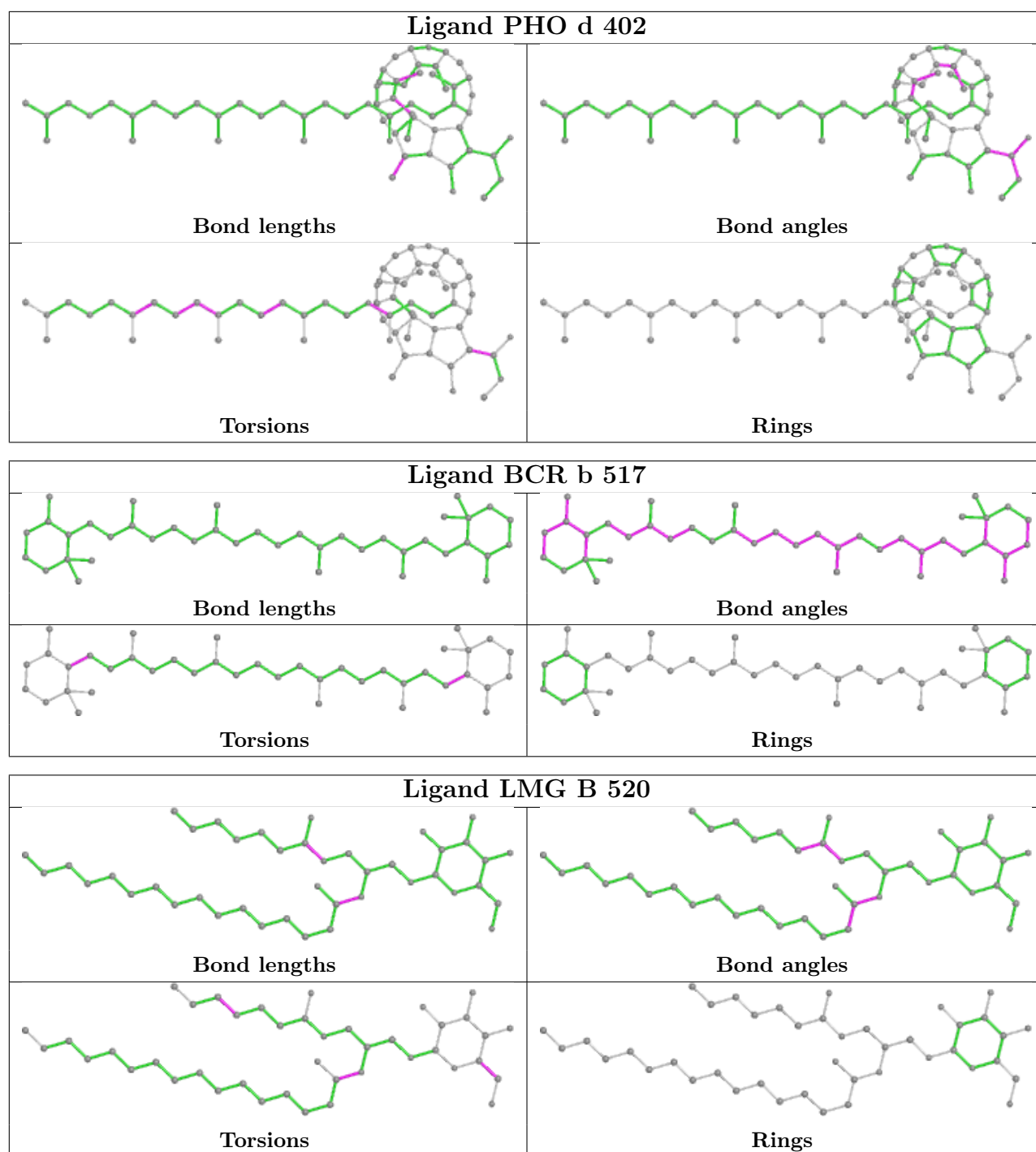


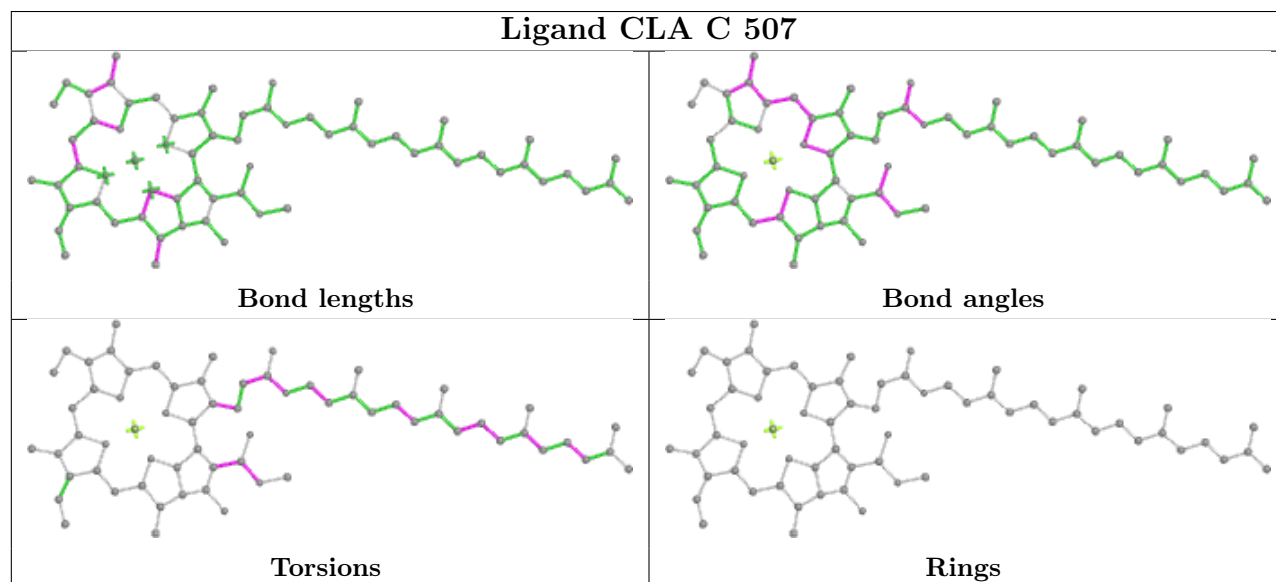
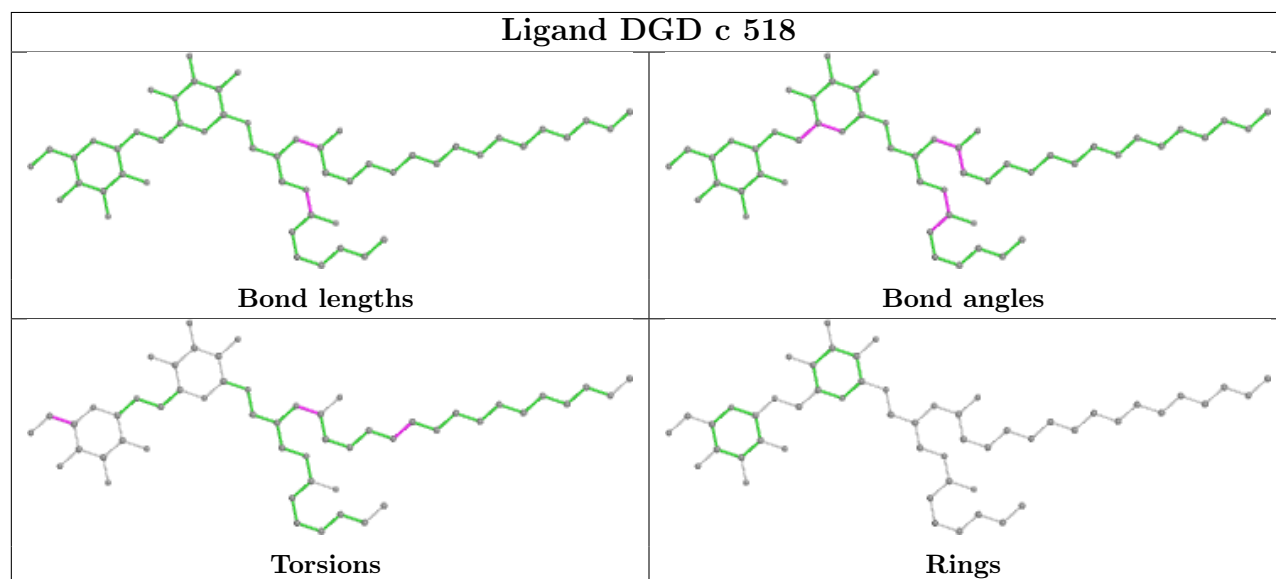
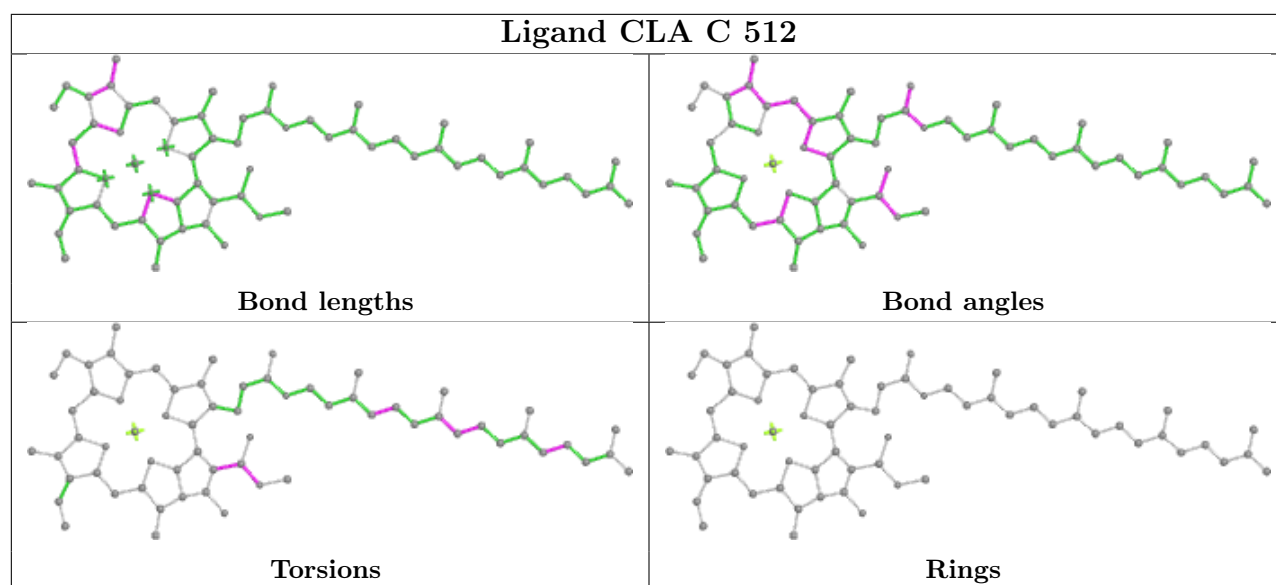
Ligand CLA b 514

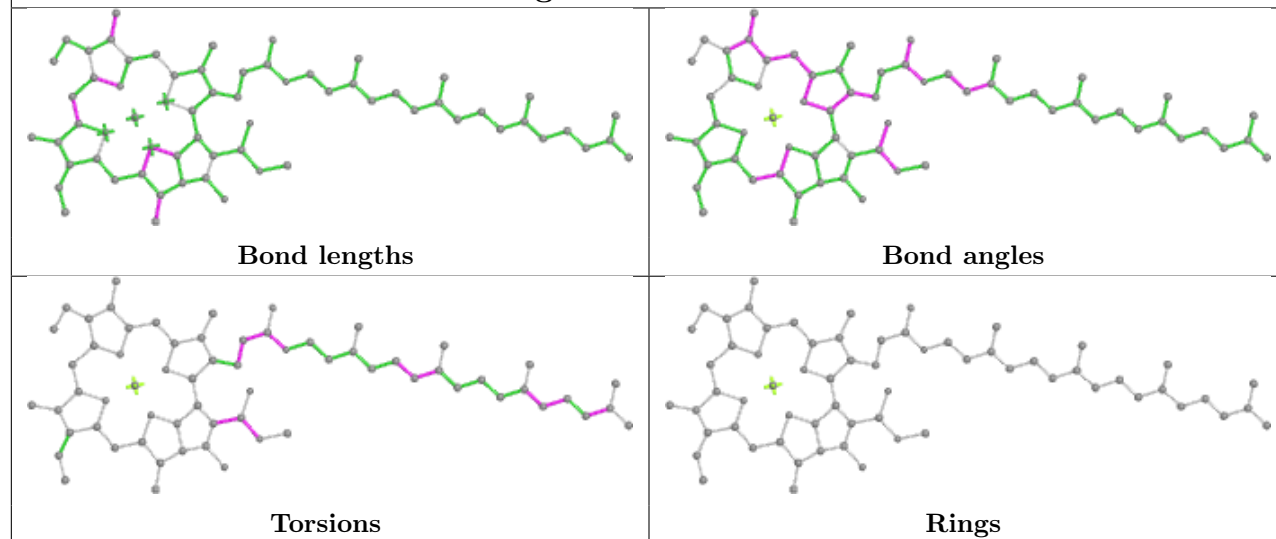
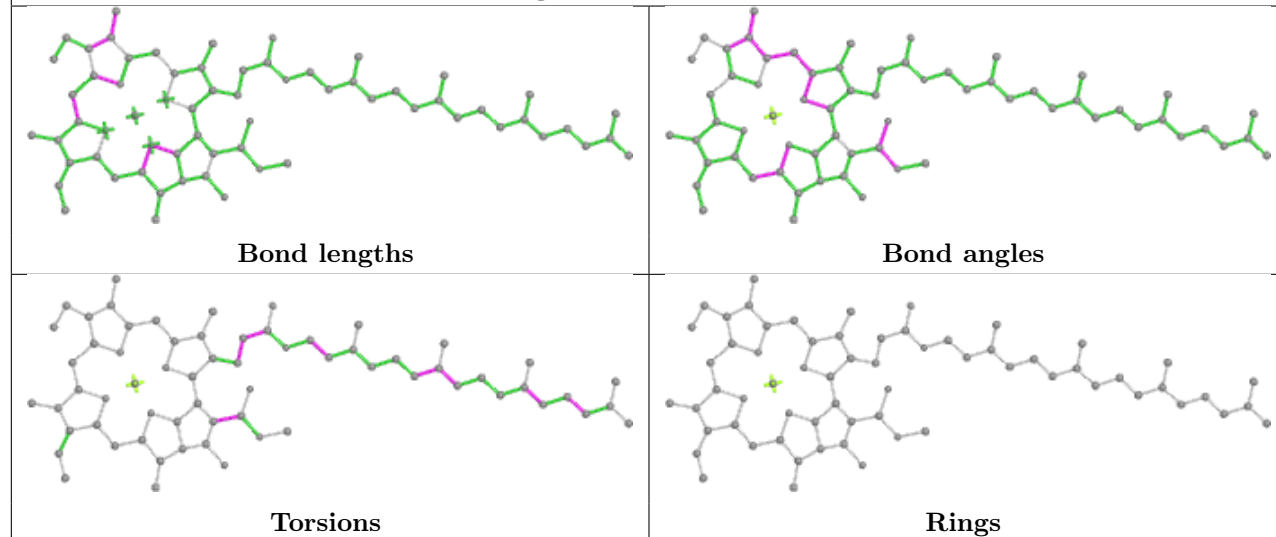
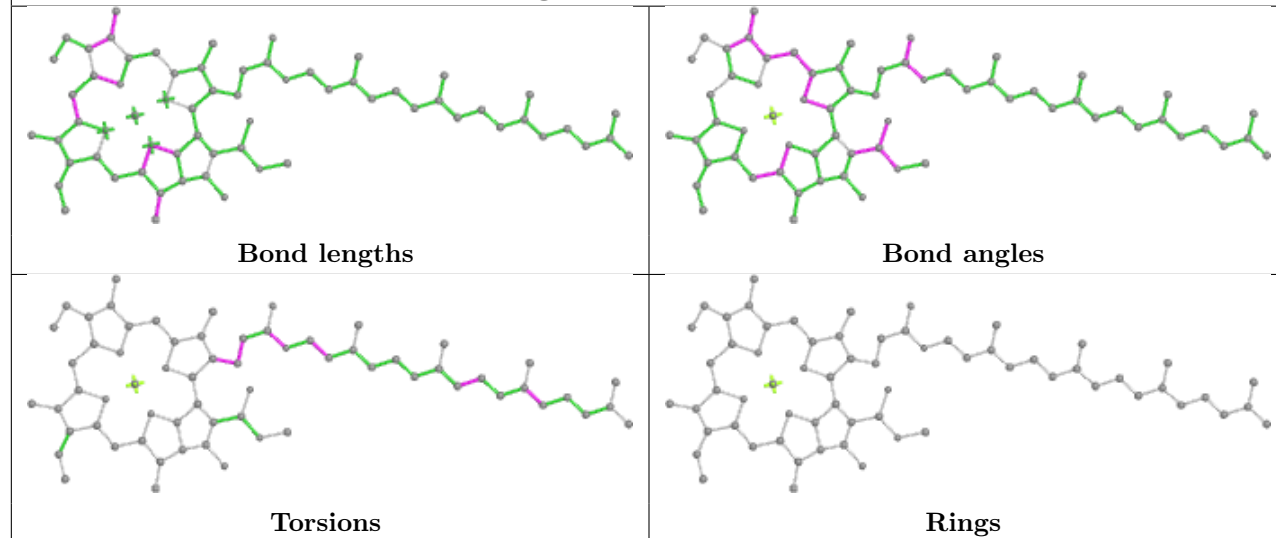


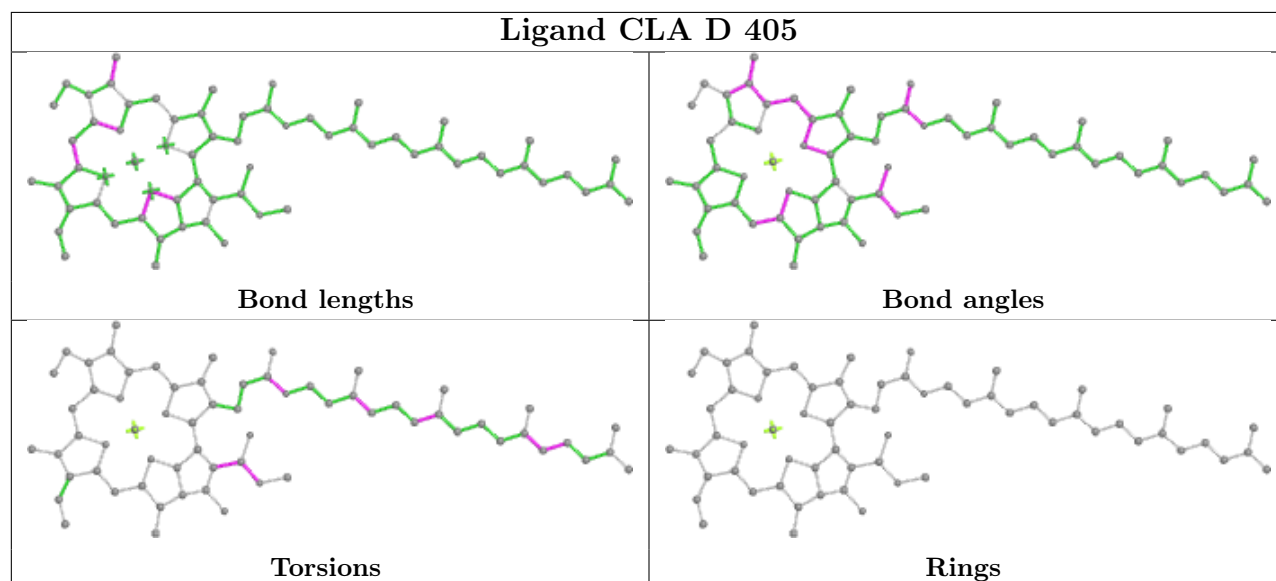
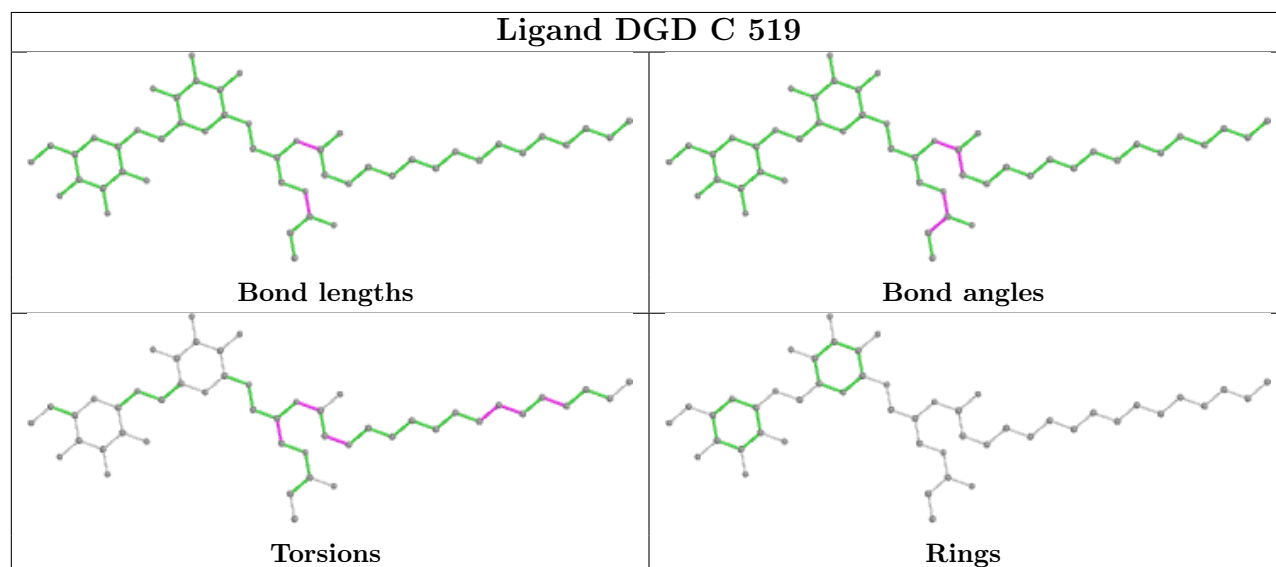
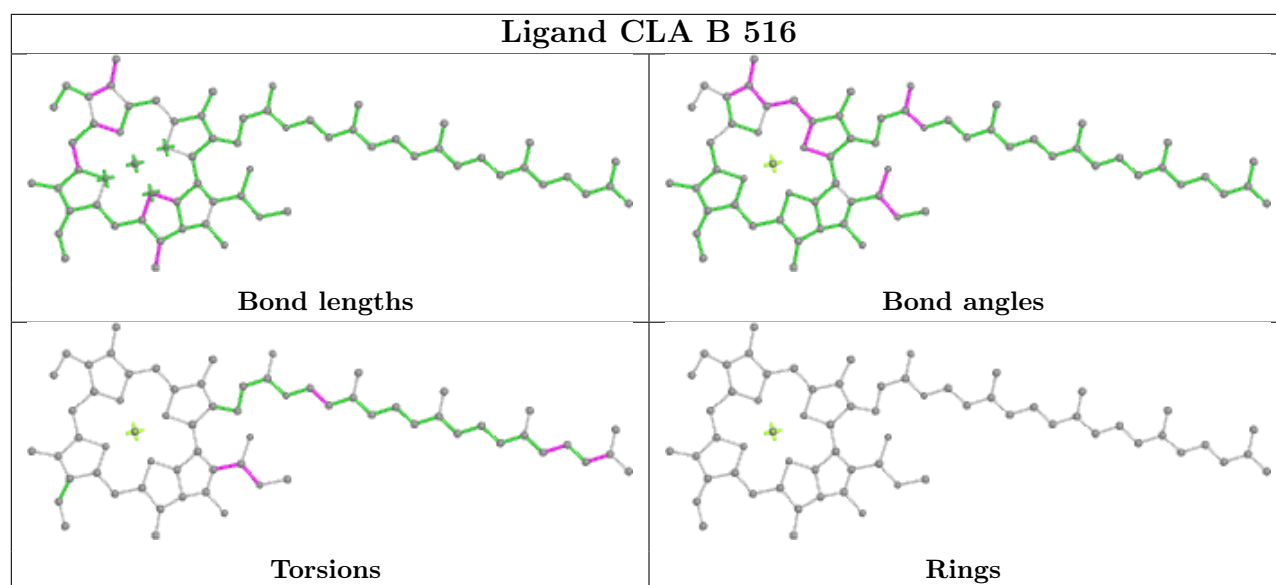


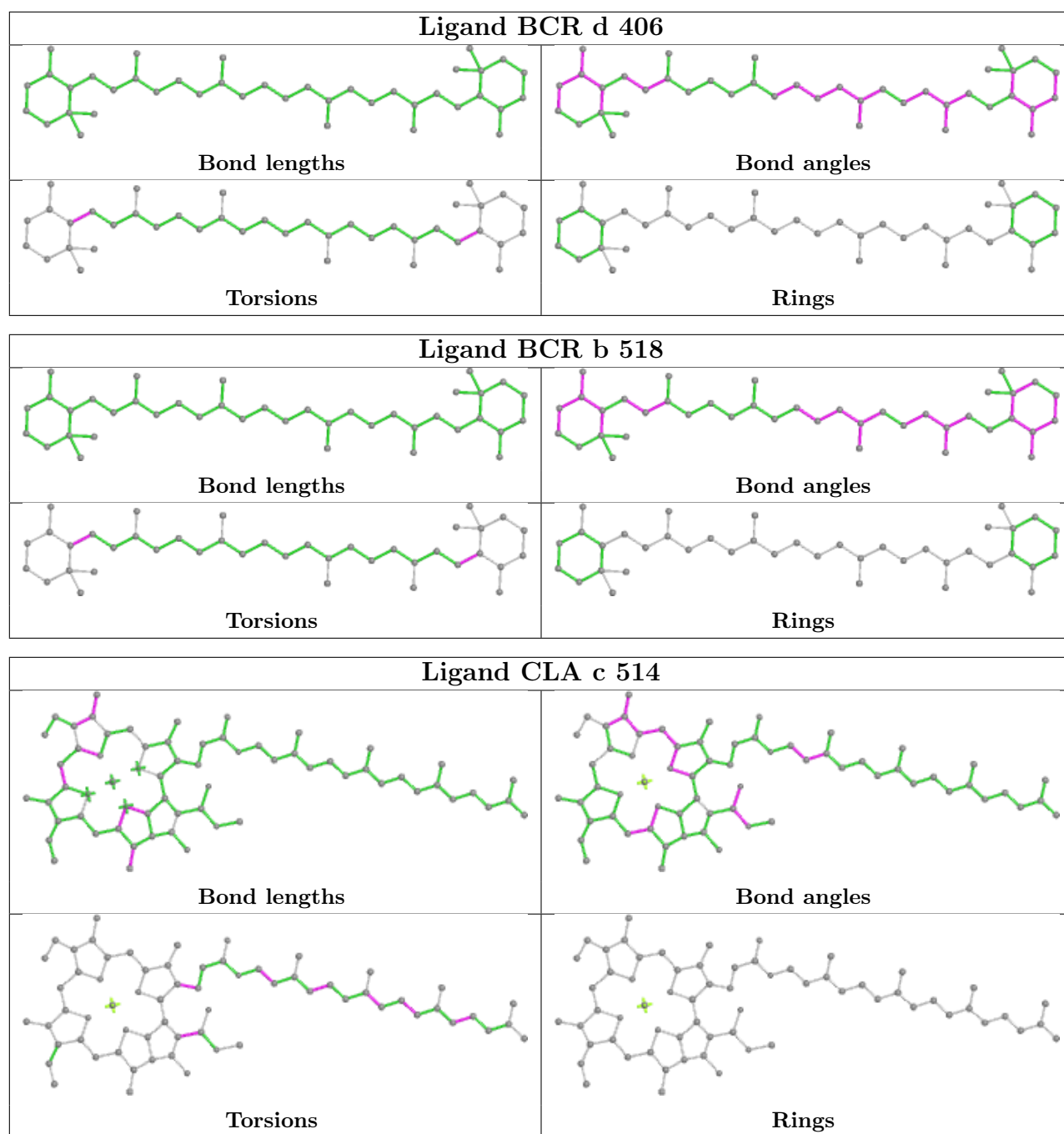


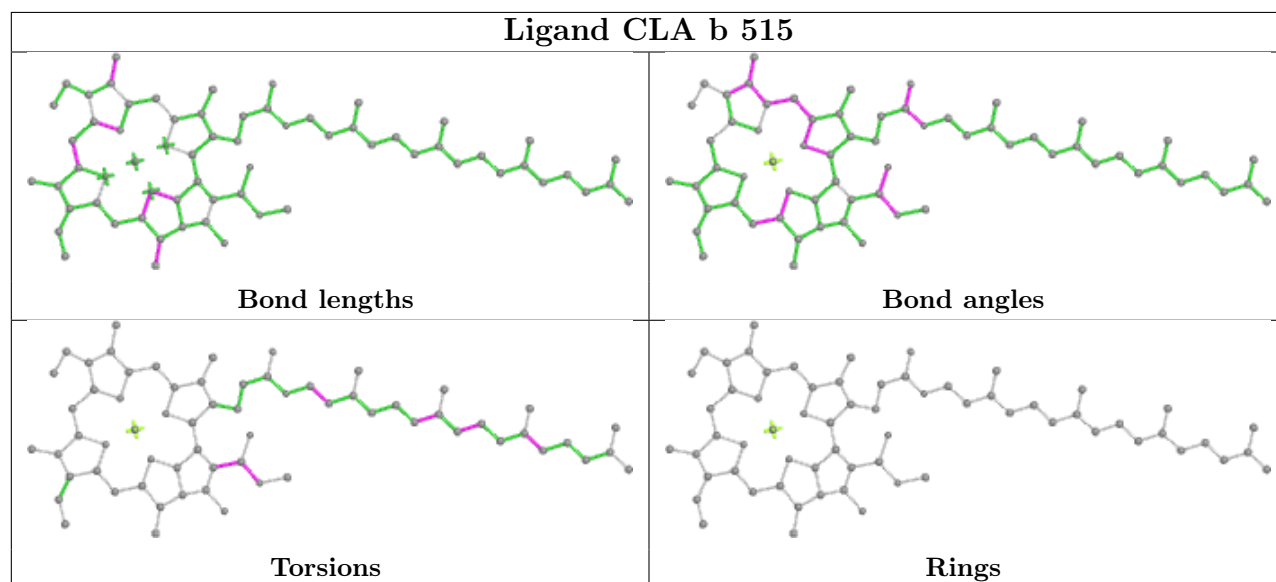
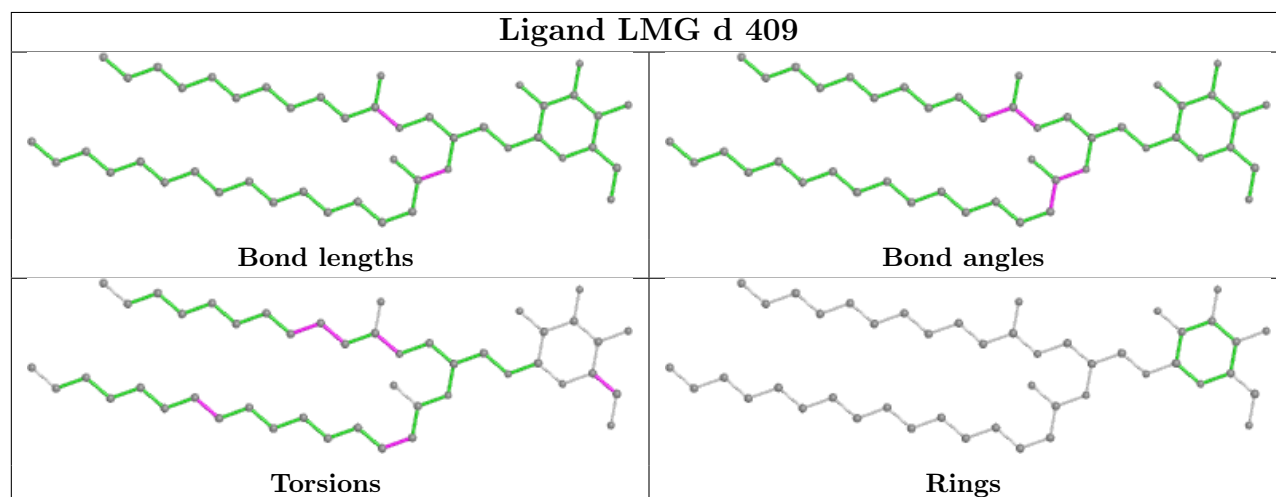
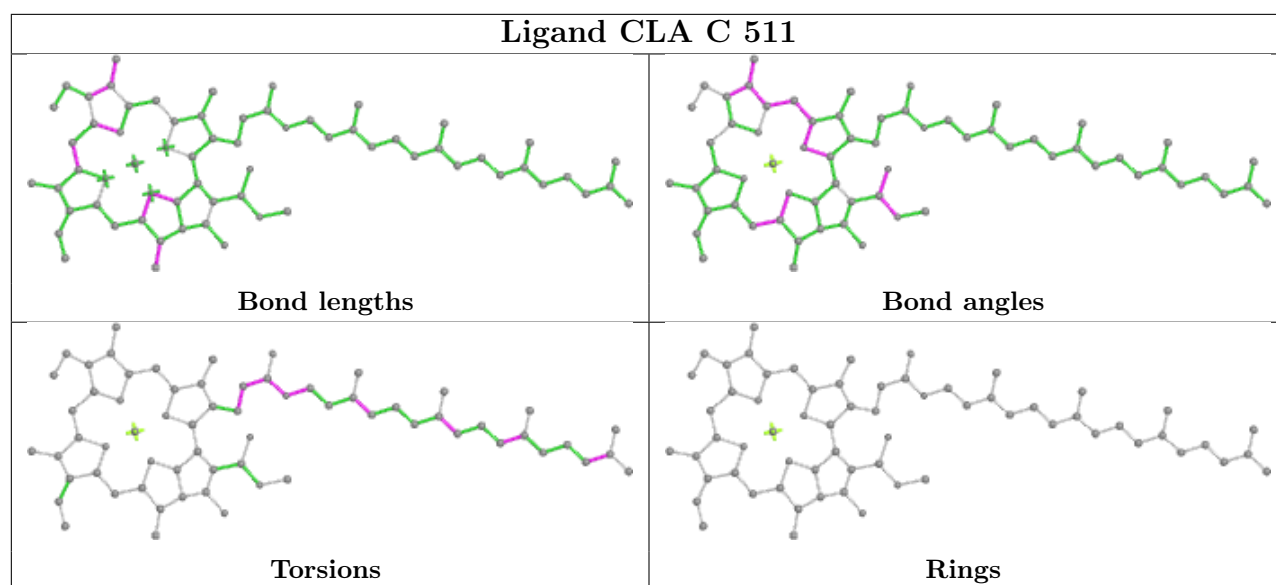


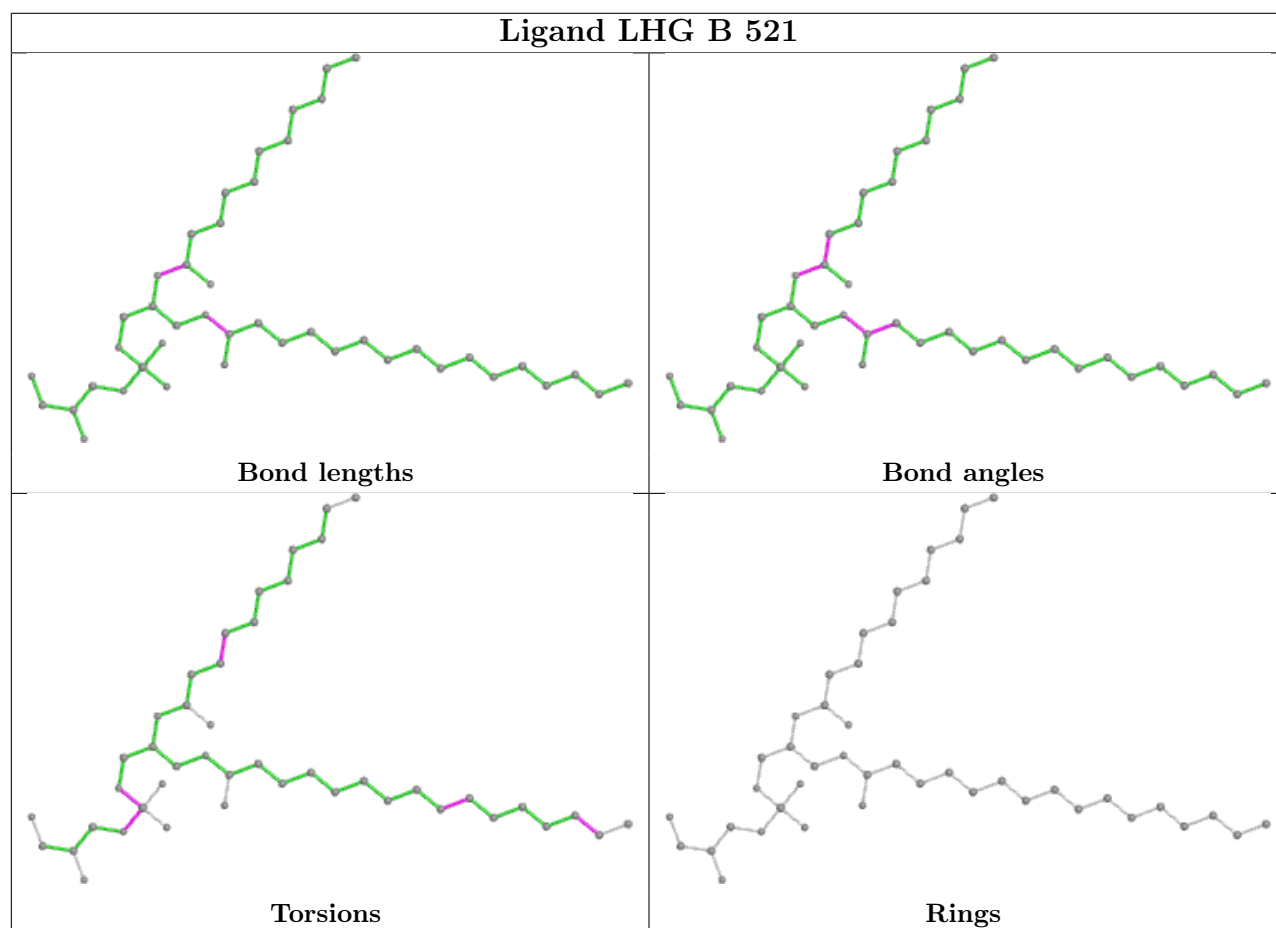
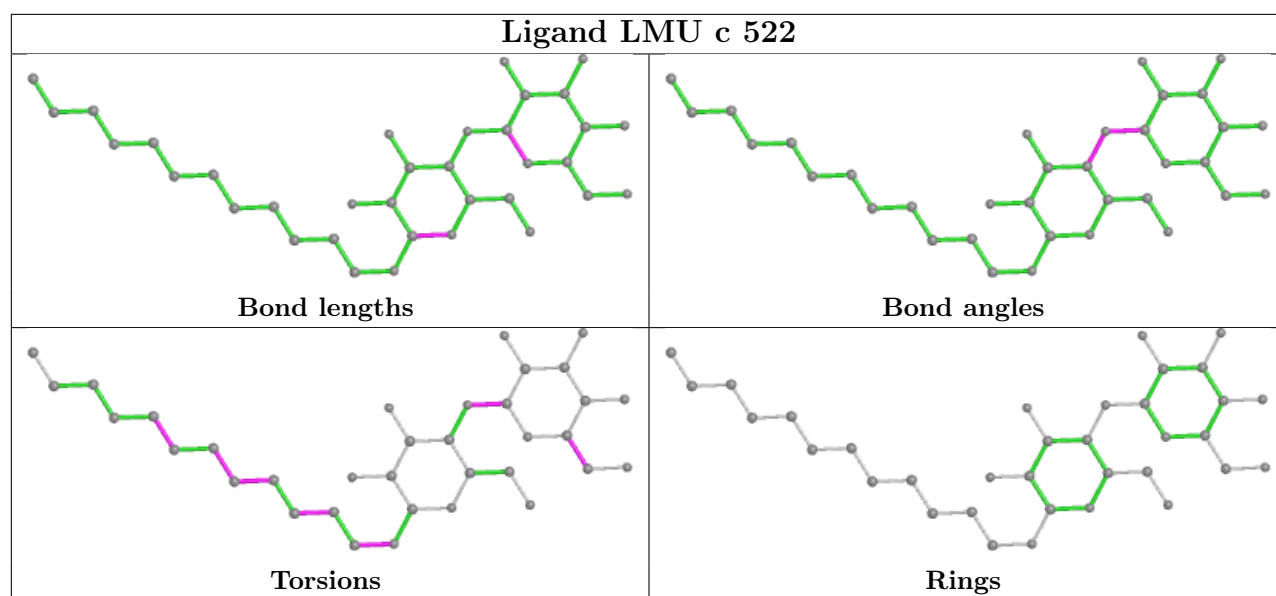


Ligand CLA b 509**Ligand CLA B 512****Ligand CLA d 401**

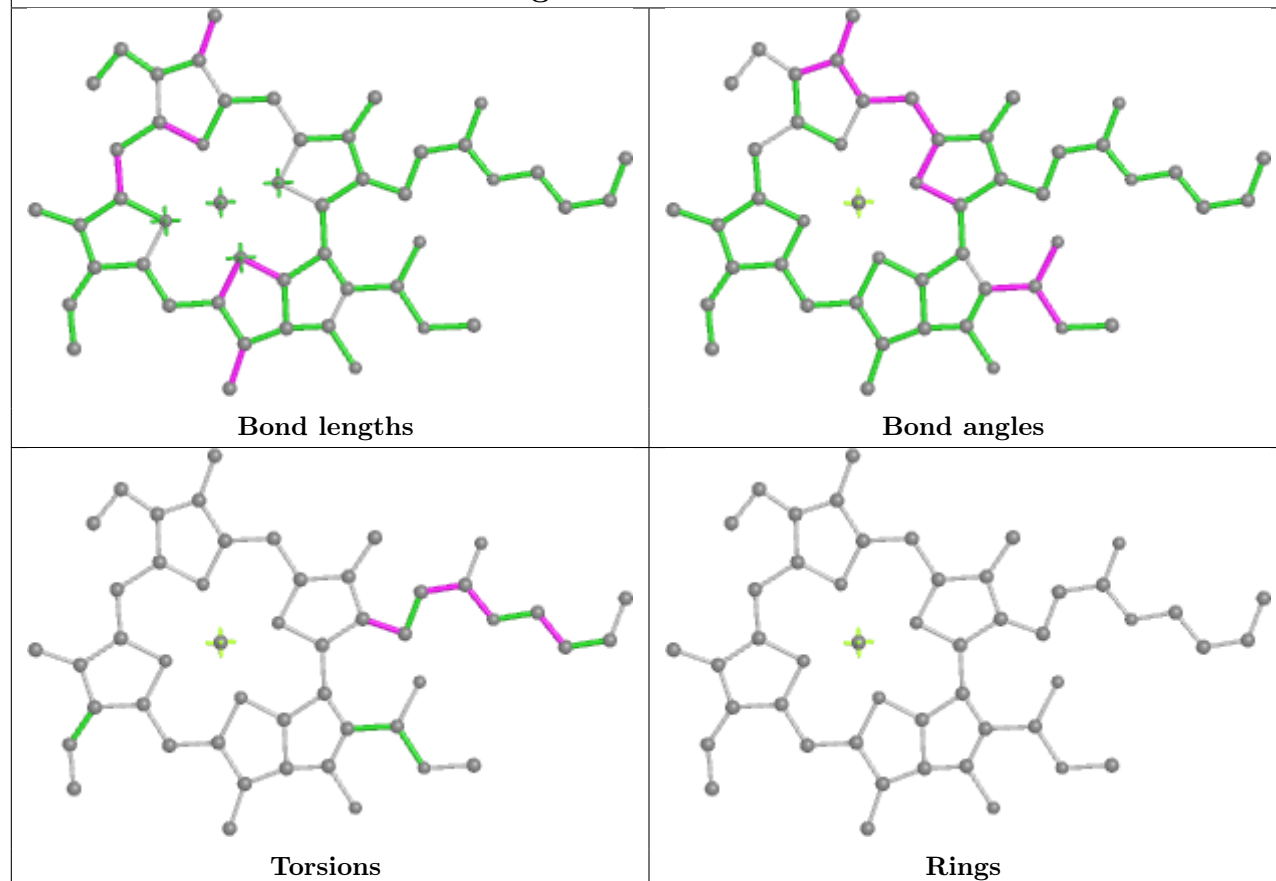




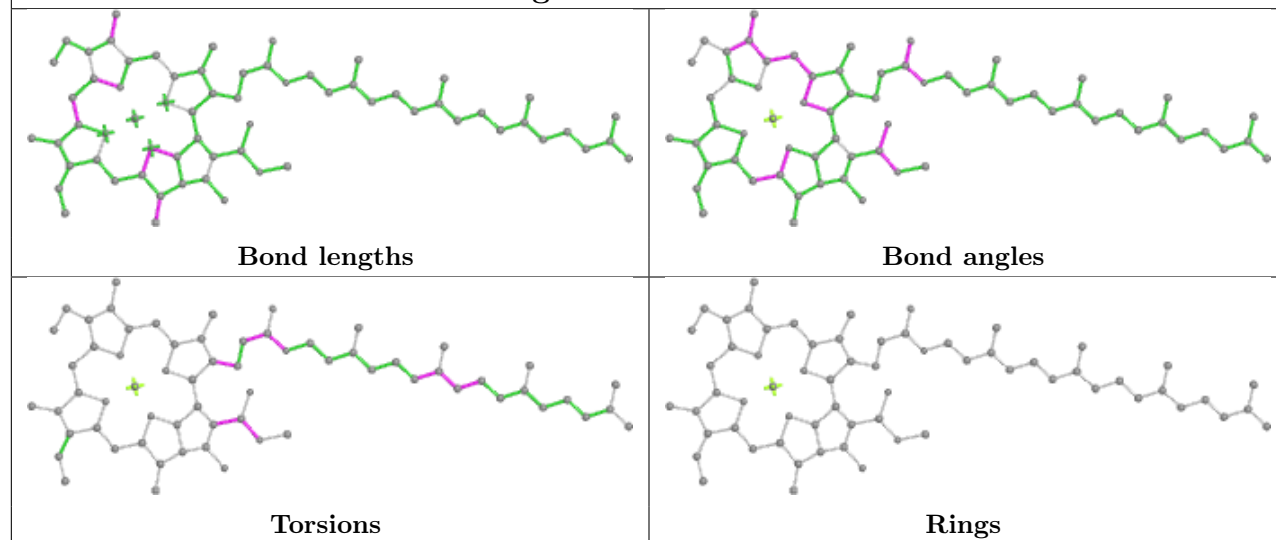


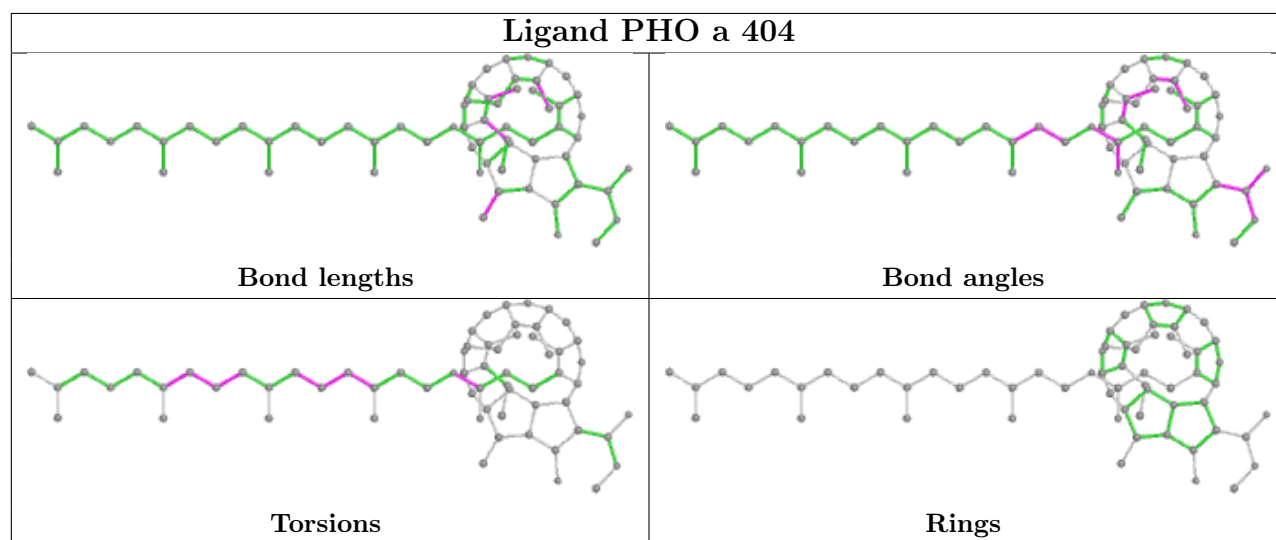
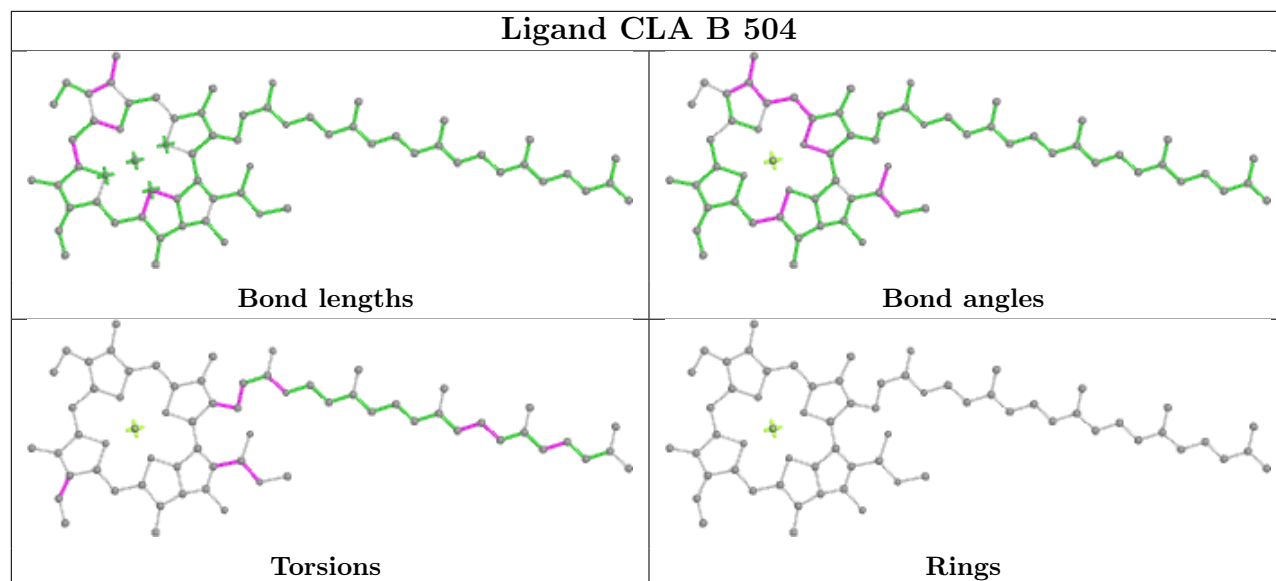
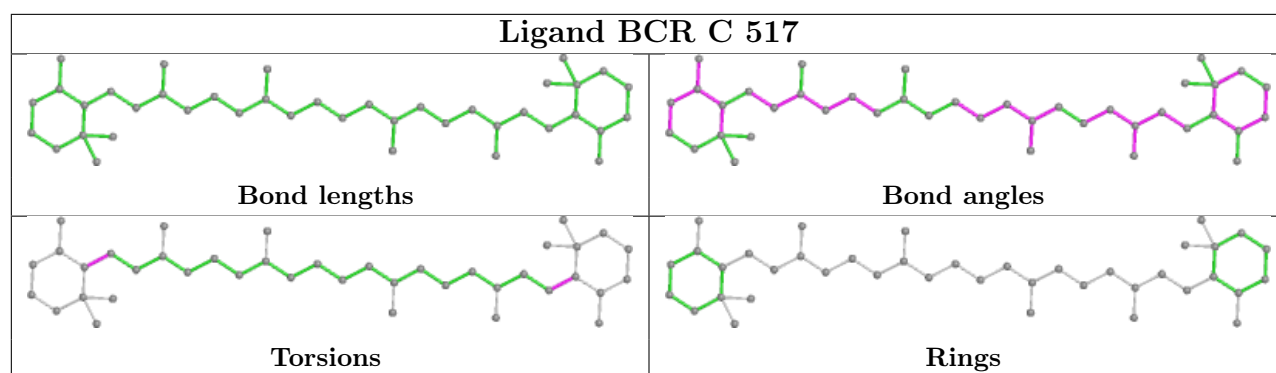


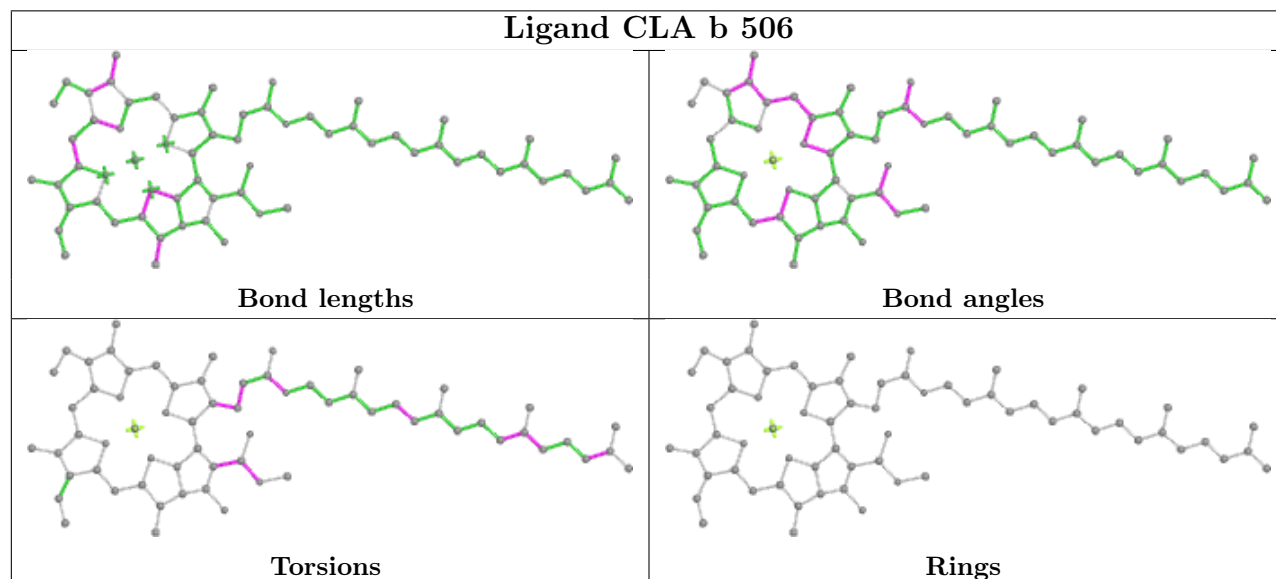
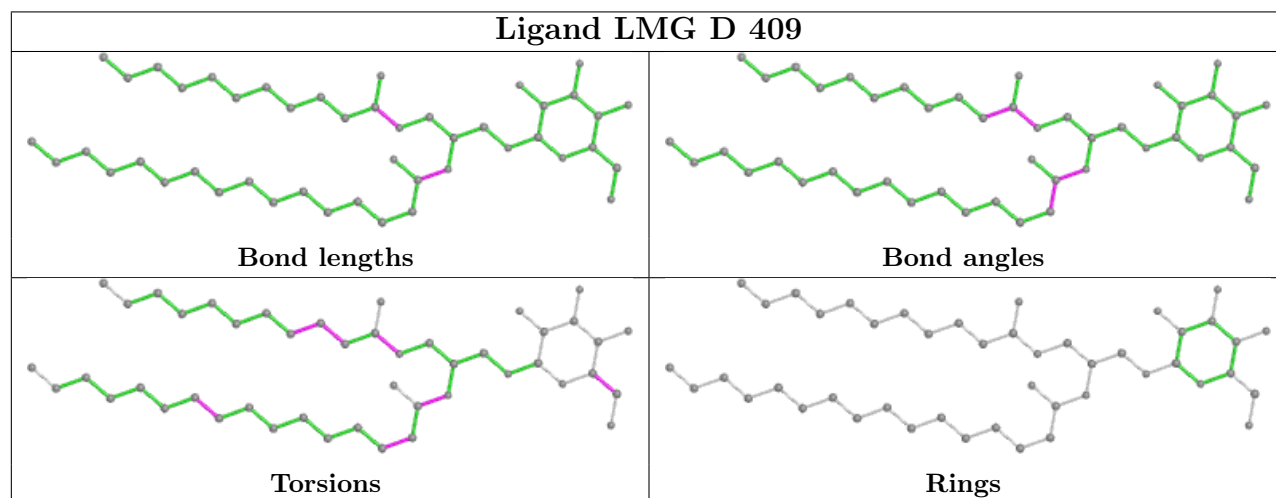
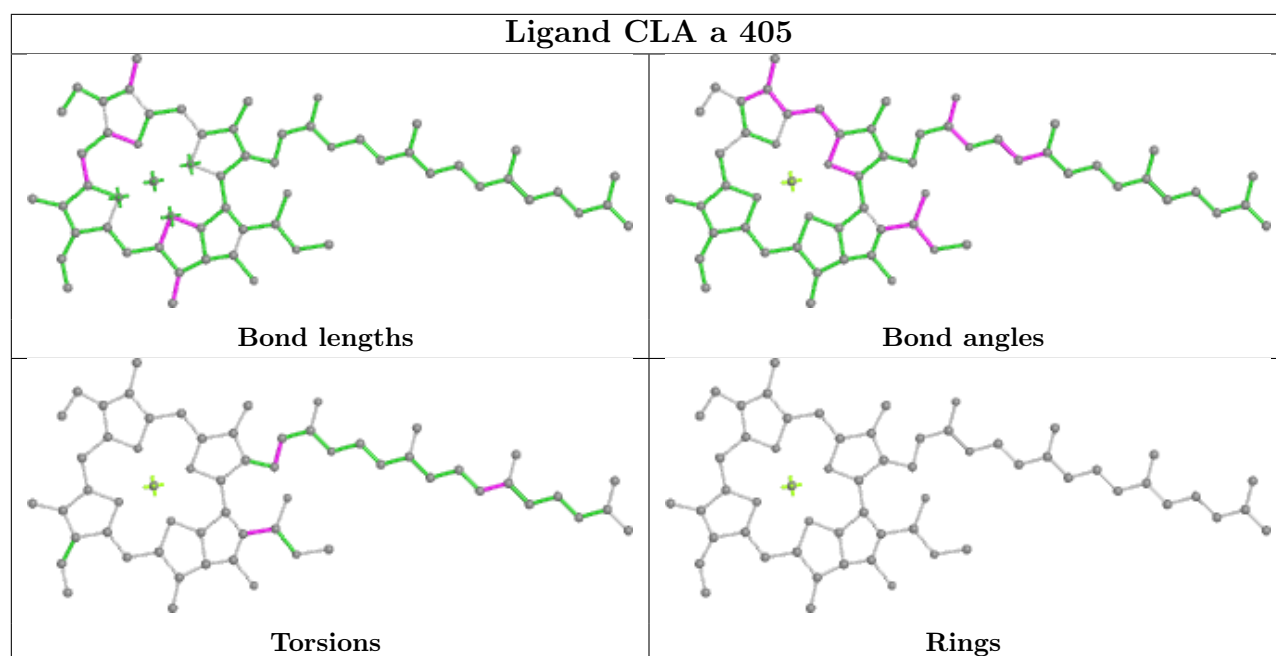
Ligand CLA A 403

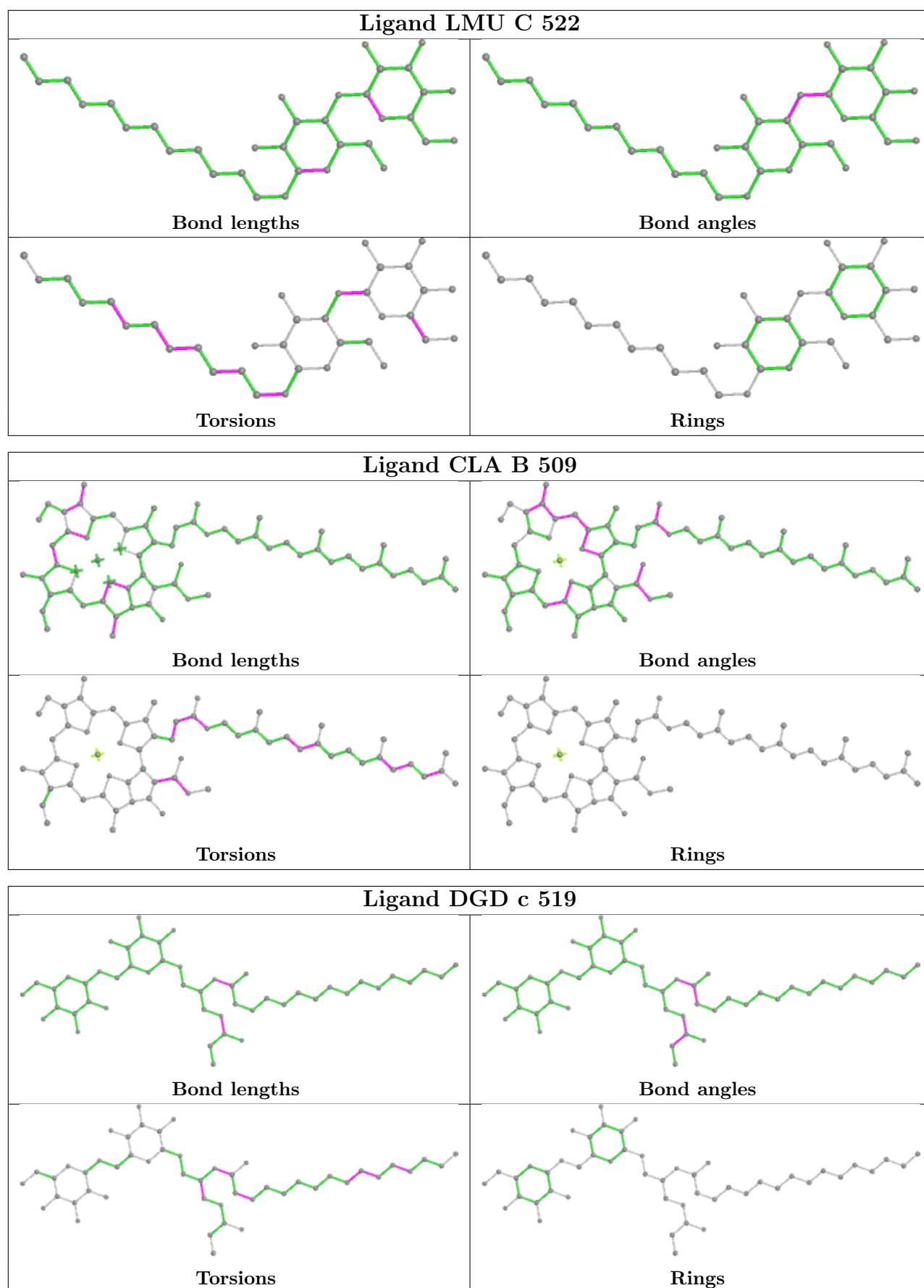


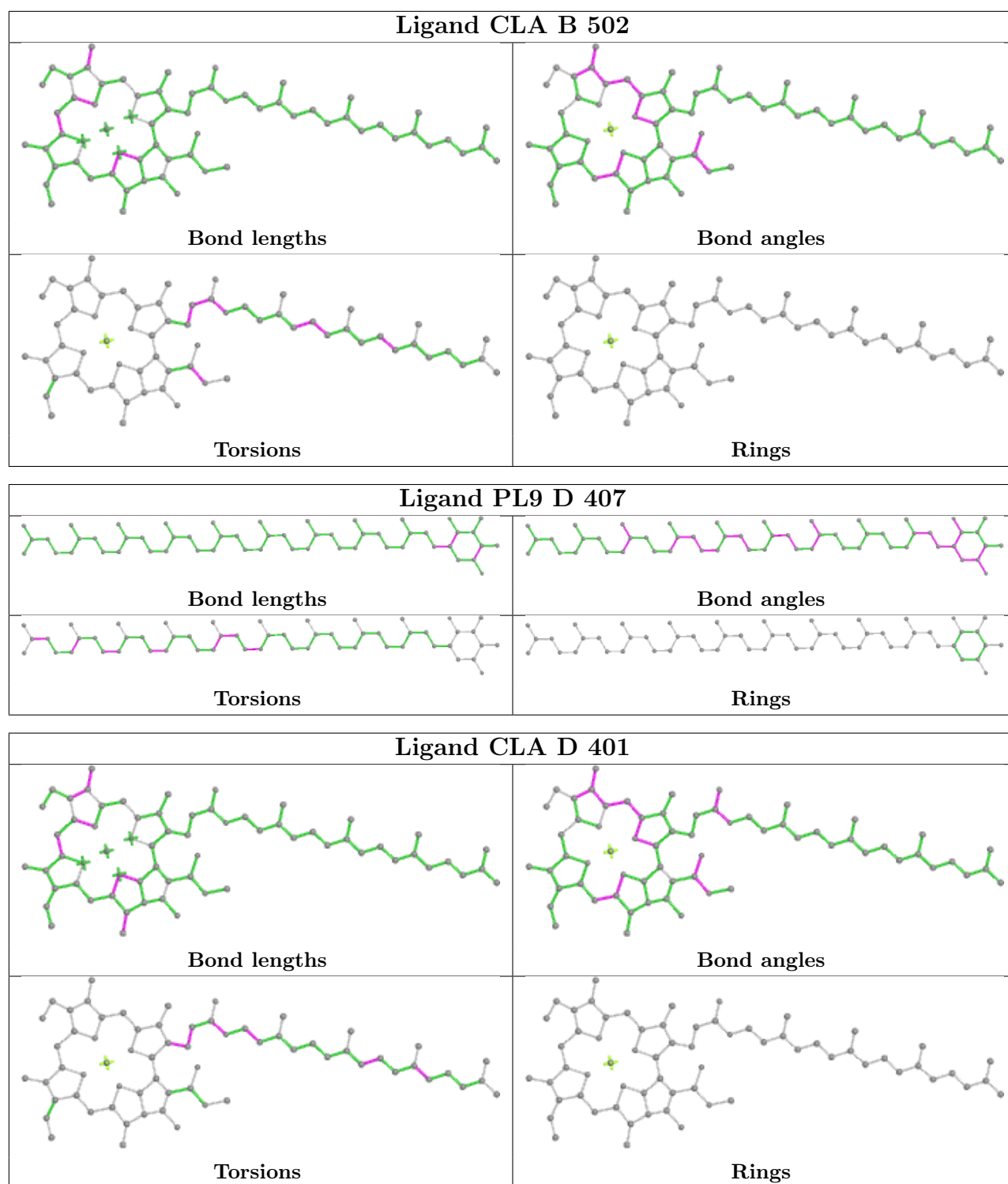
Ligand CLA C 504

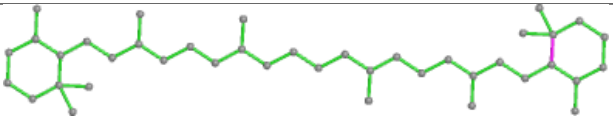
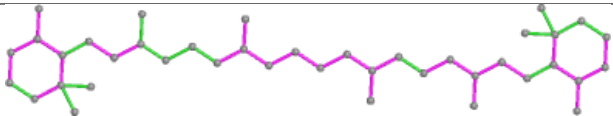
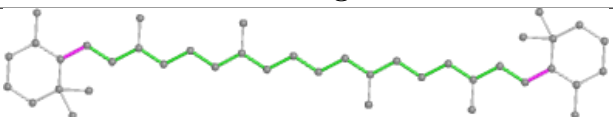
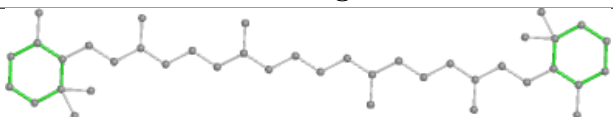


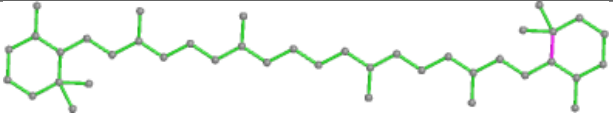
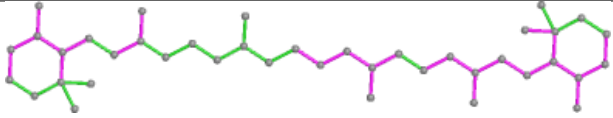
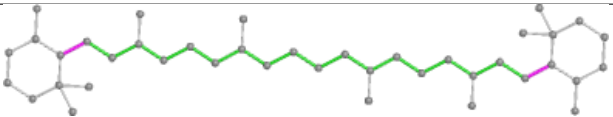
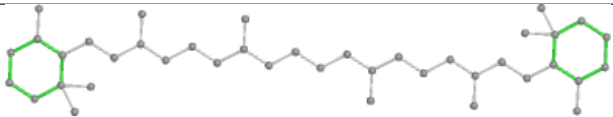


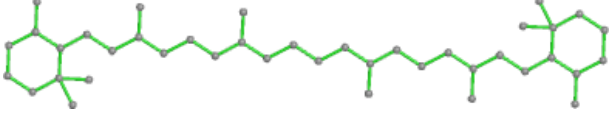
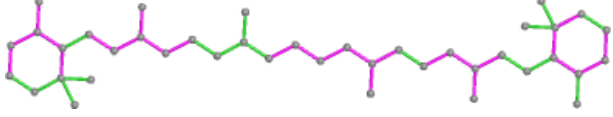
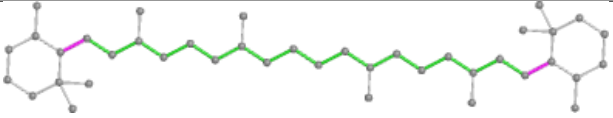
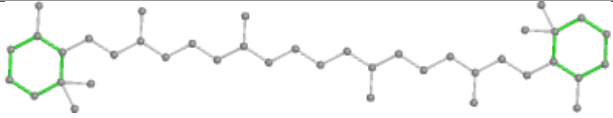




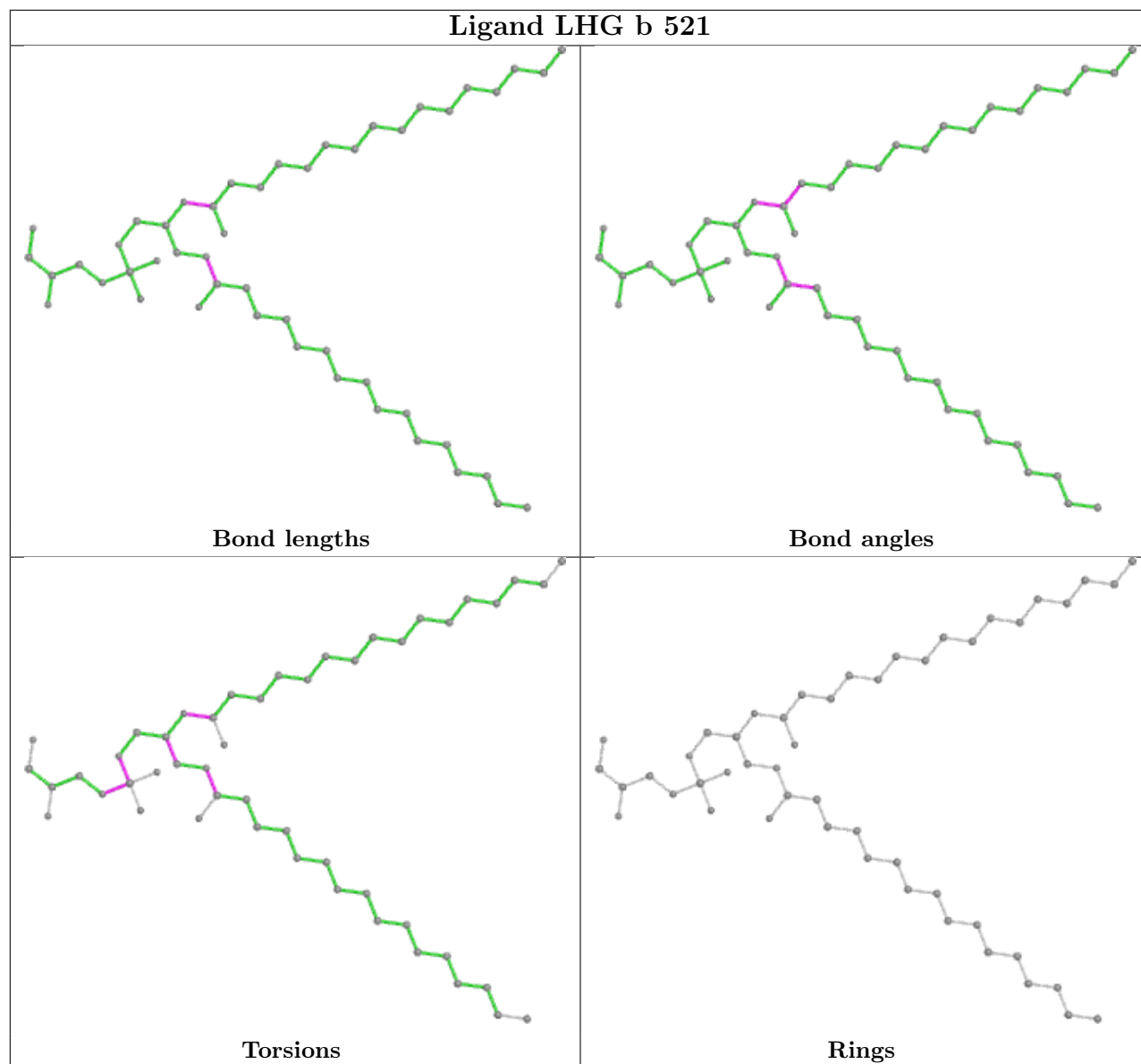


Ligand BCR A 406	
	Bond lengths
	Bond angles
	Torsions
	Rings

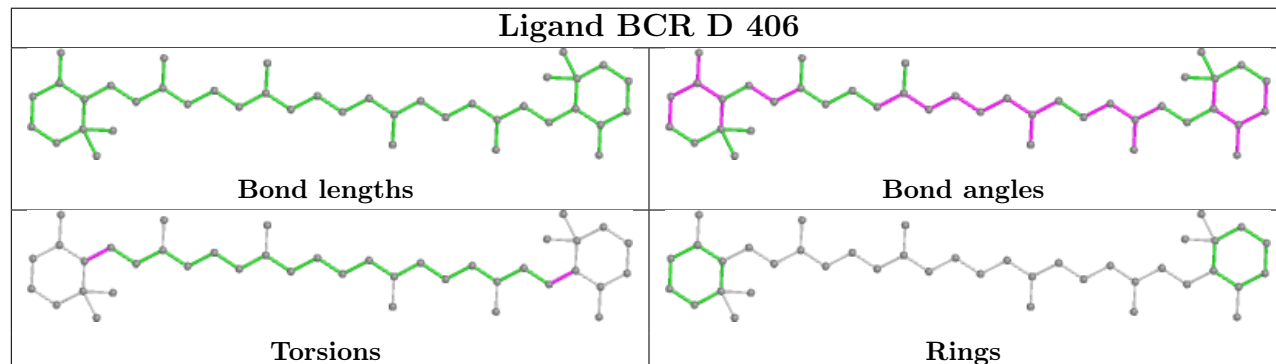
Ligand BCR c 516	
	Bond lengths
	Bond angles
	Torsions
	Rings

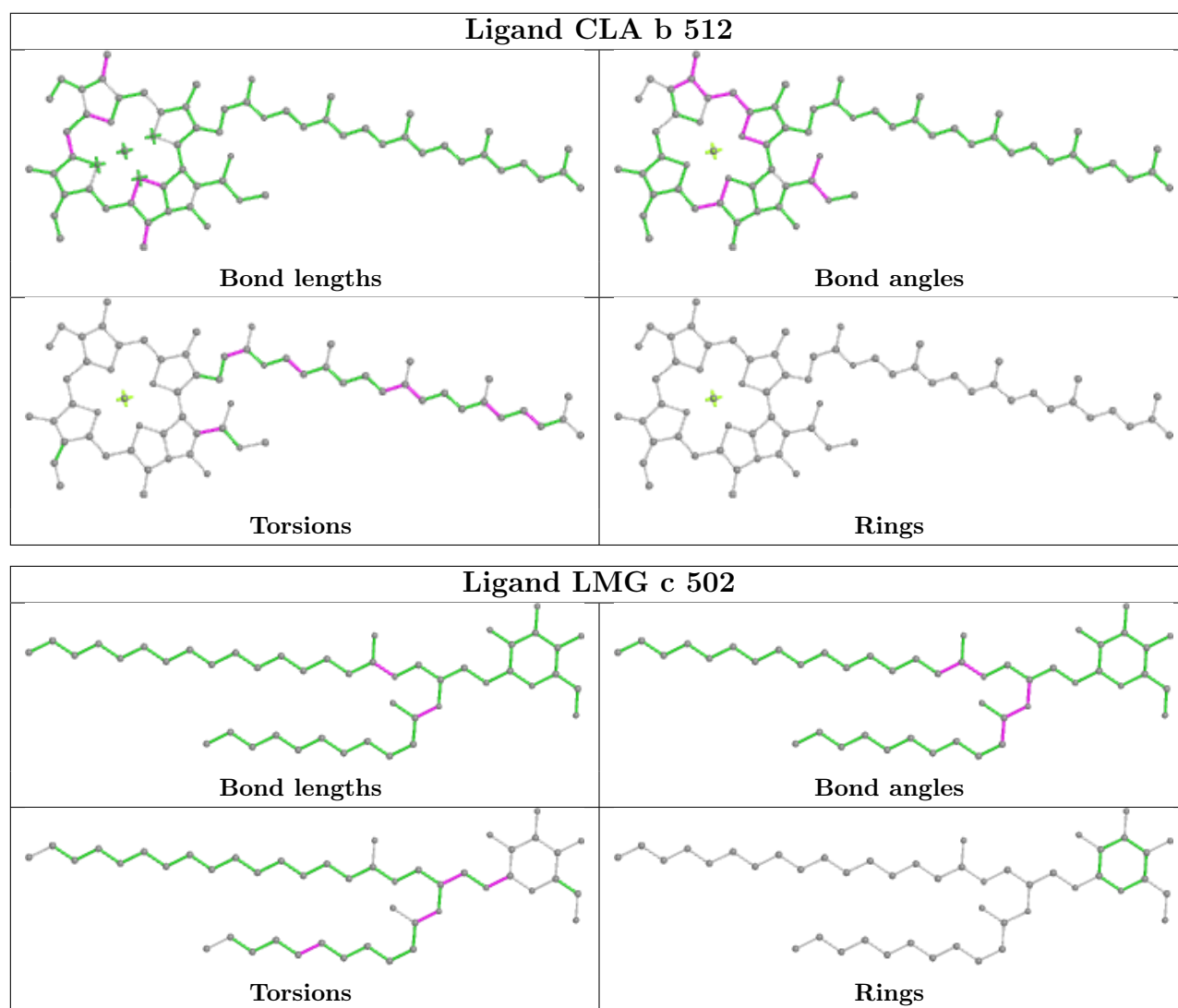
Ligand BCR B 519	
	Bond lengths
	Bond angles
	Torsions
	Rings

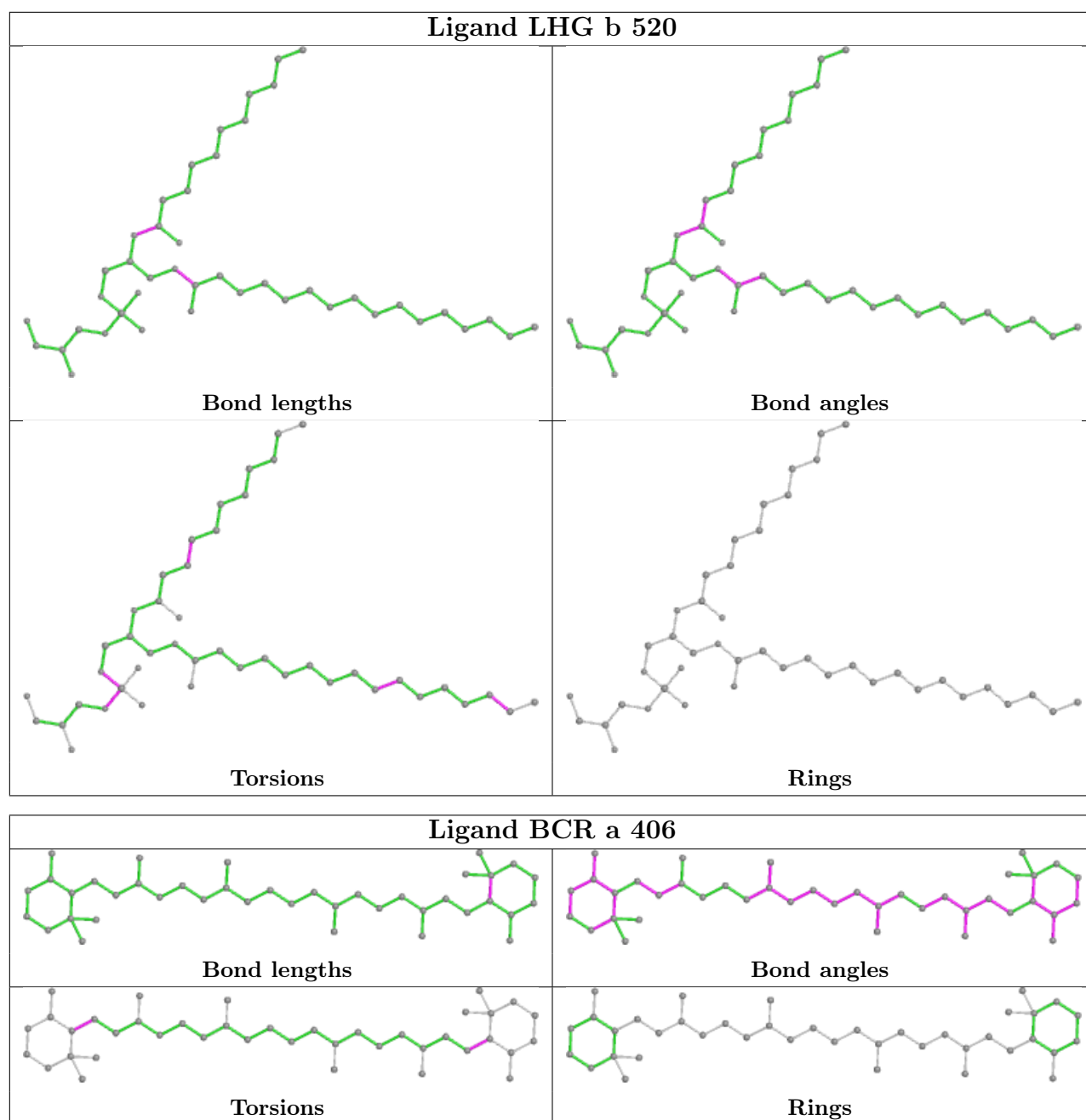
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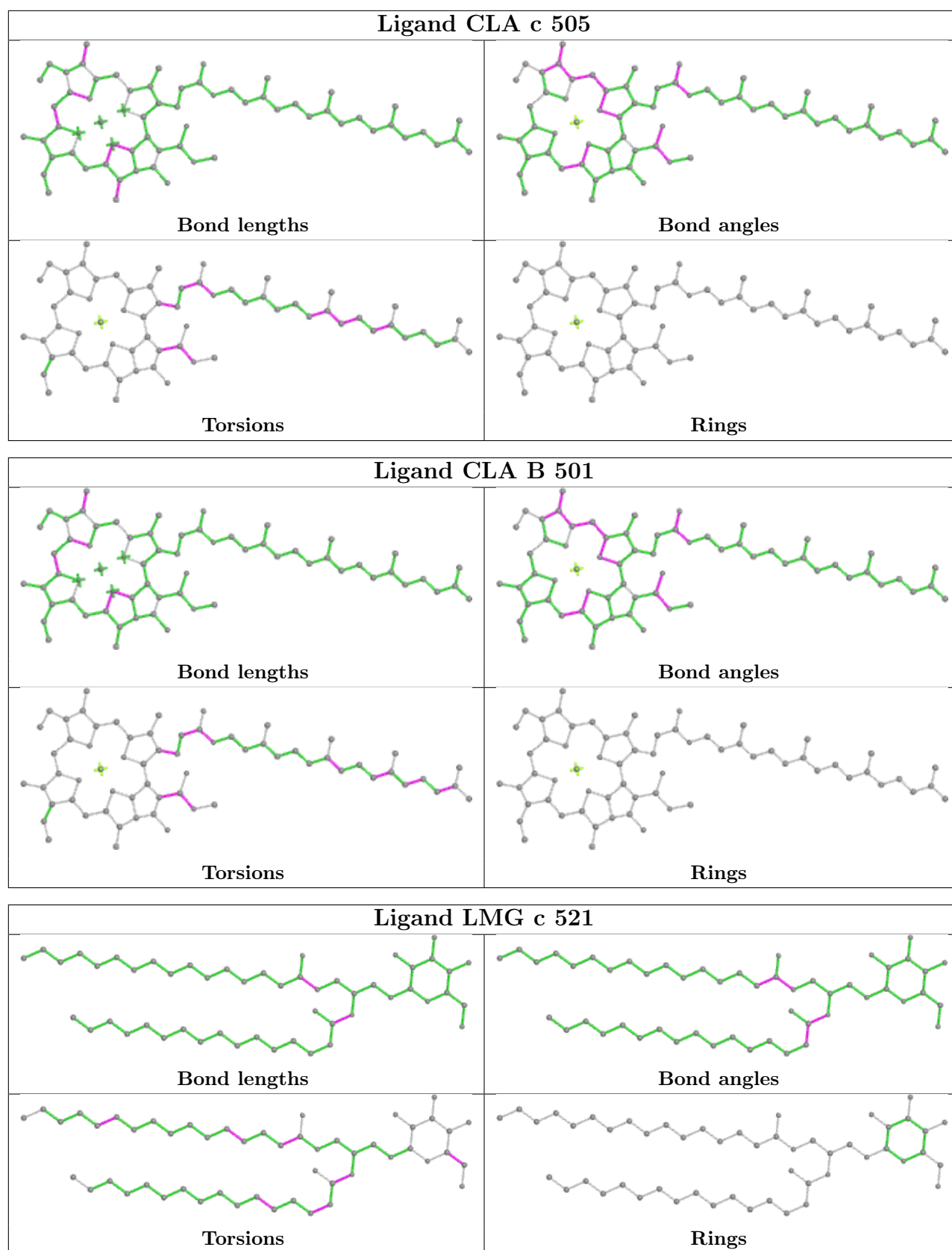


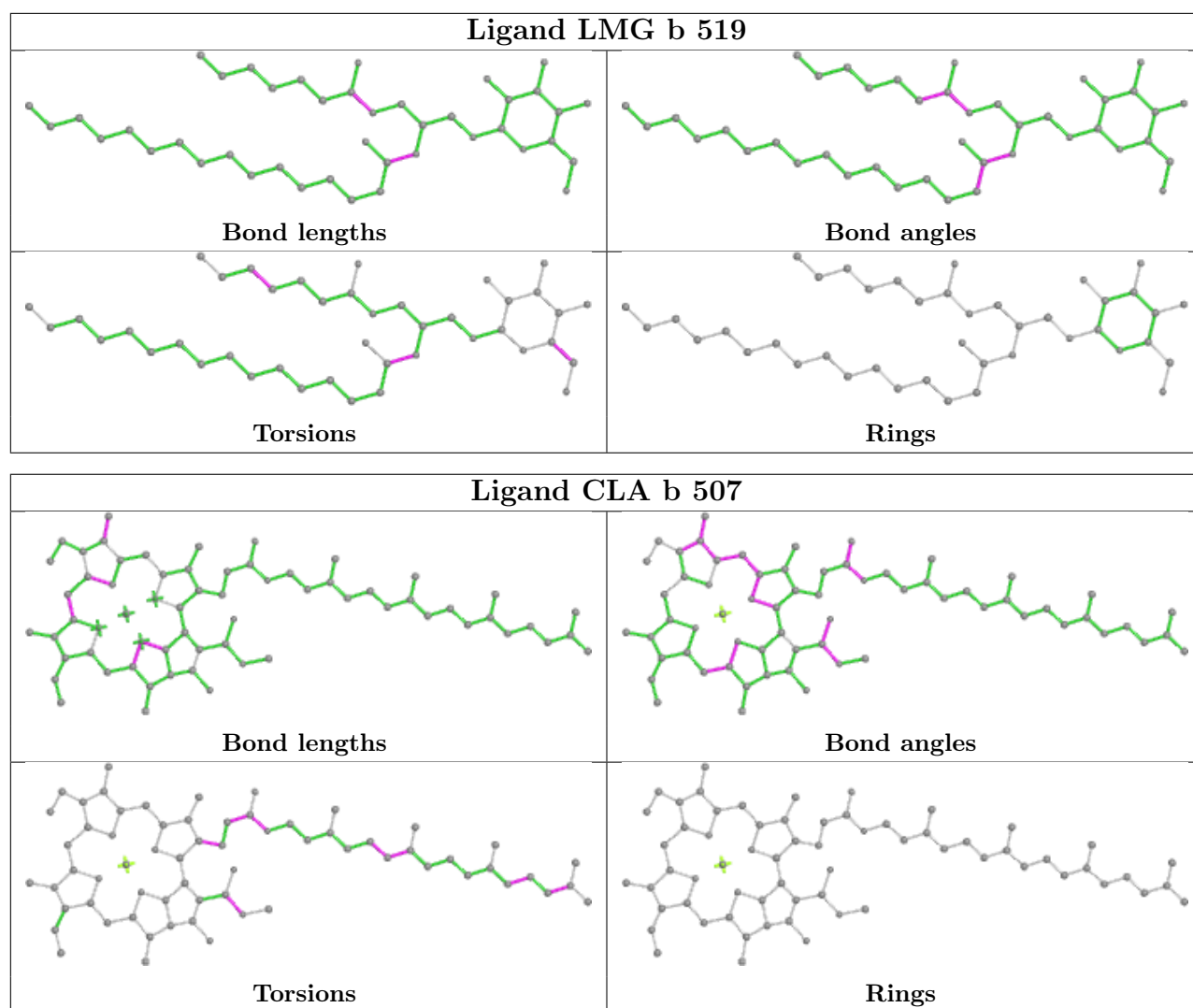
Ligand BCR D 406

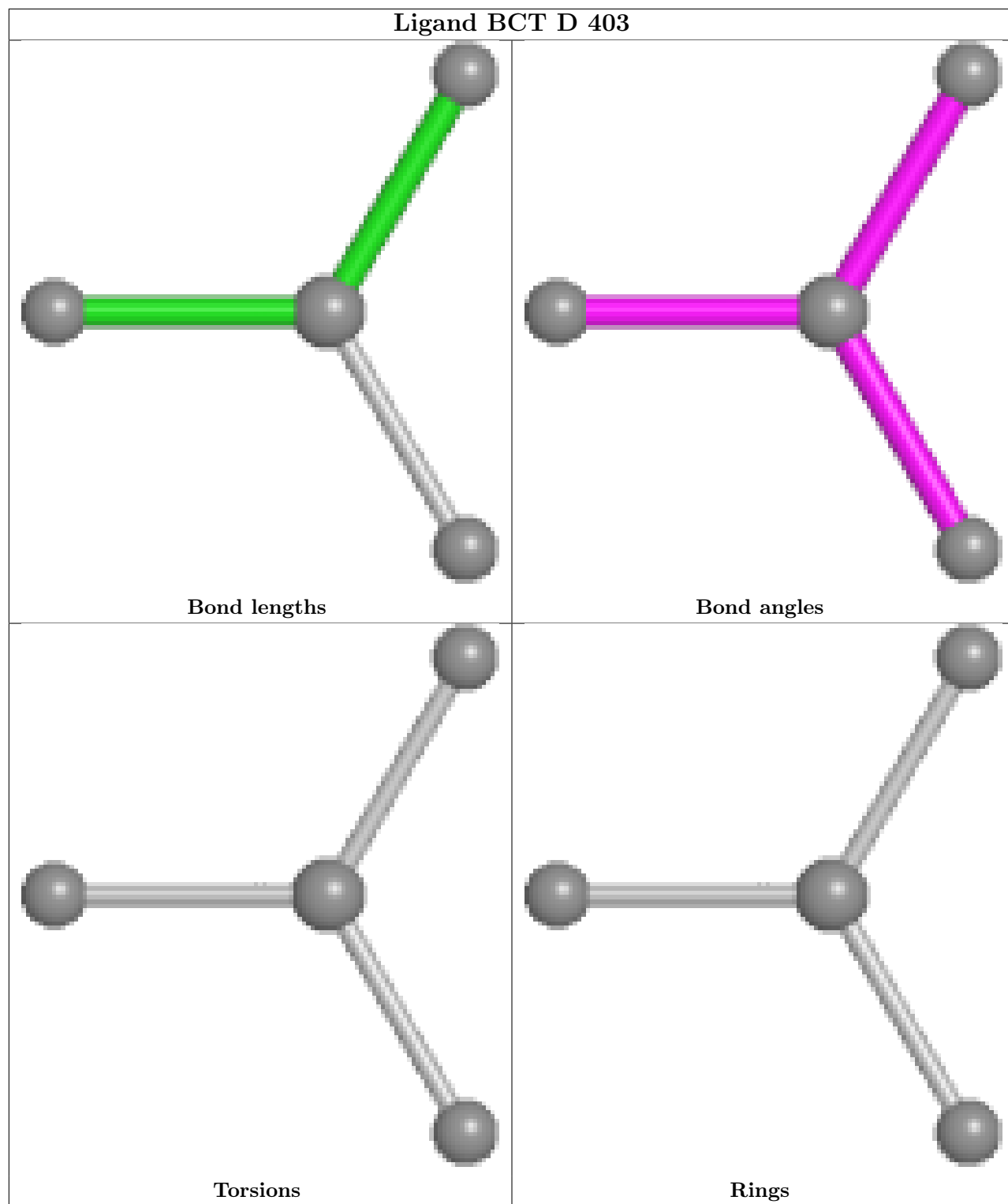


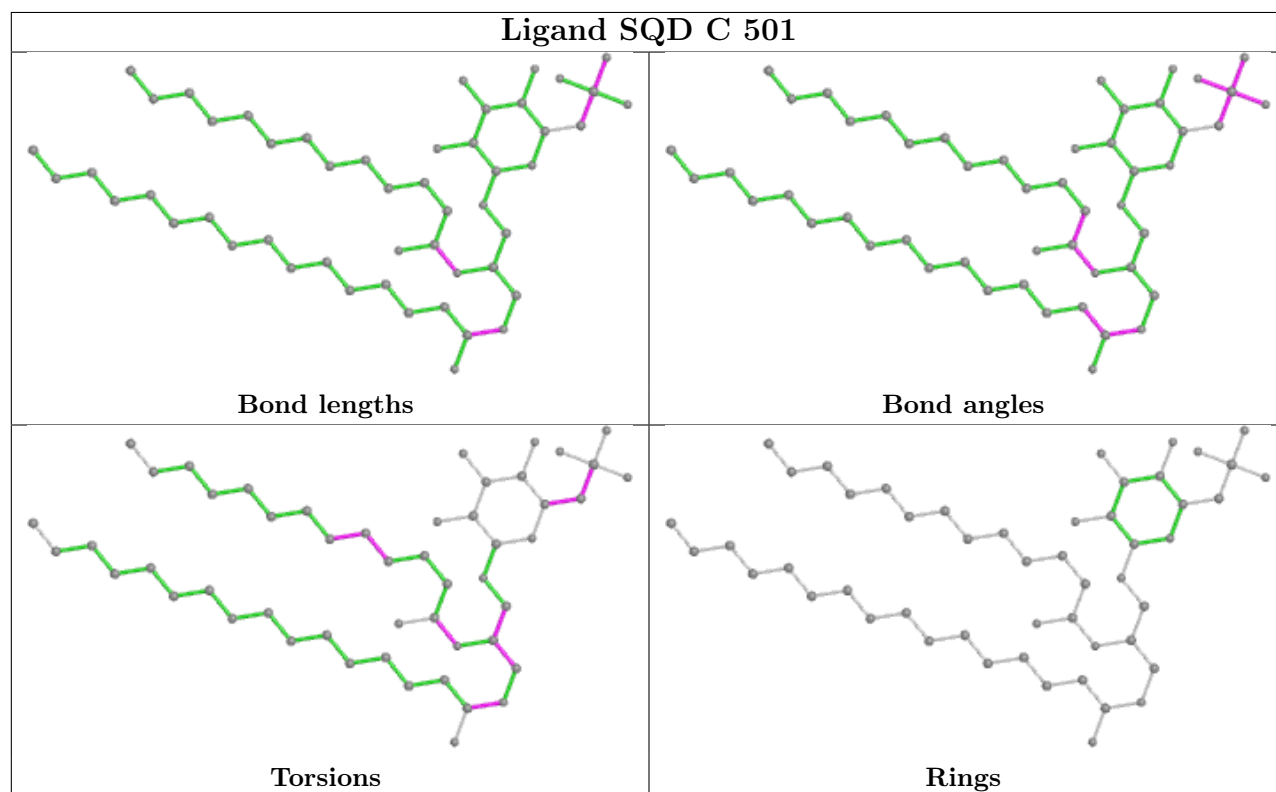
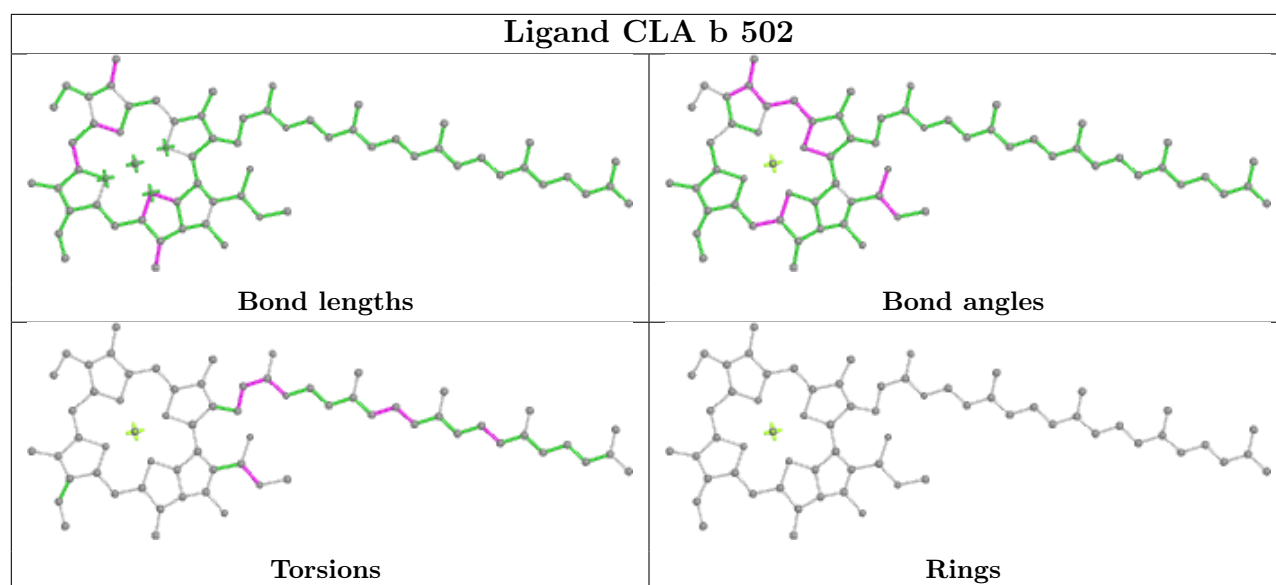


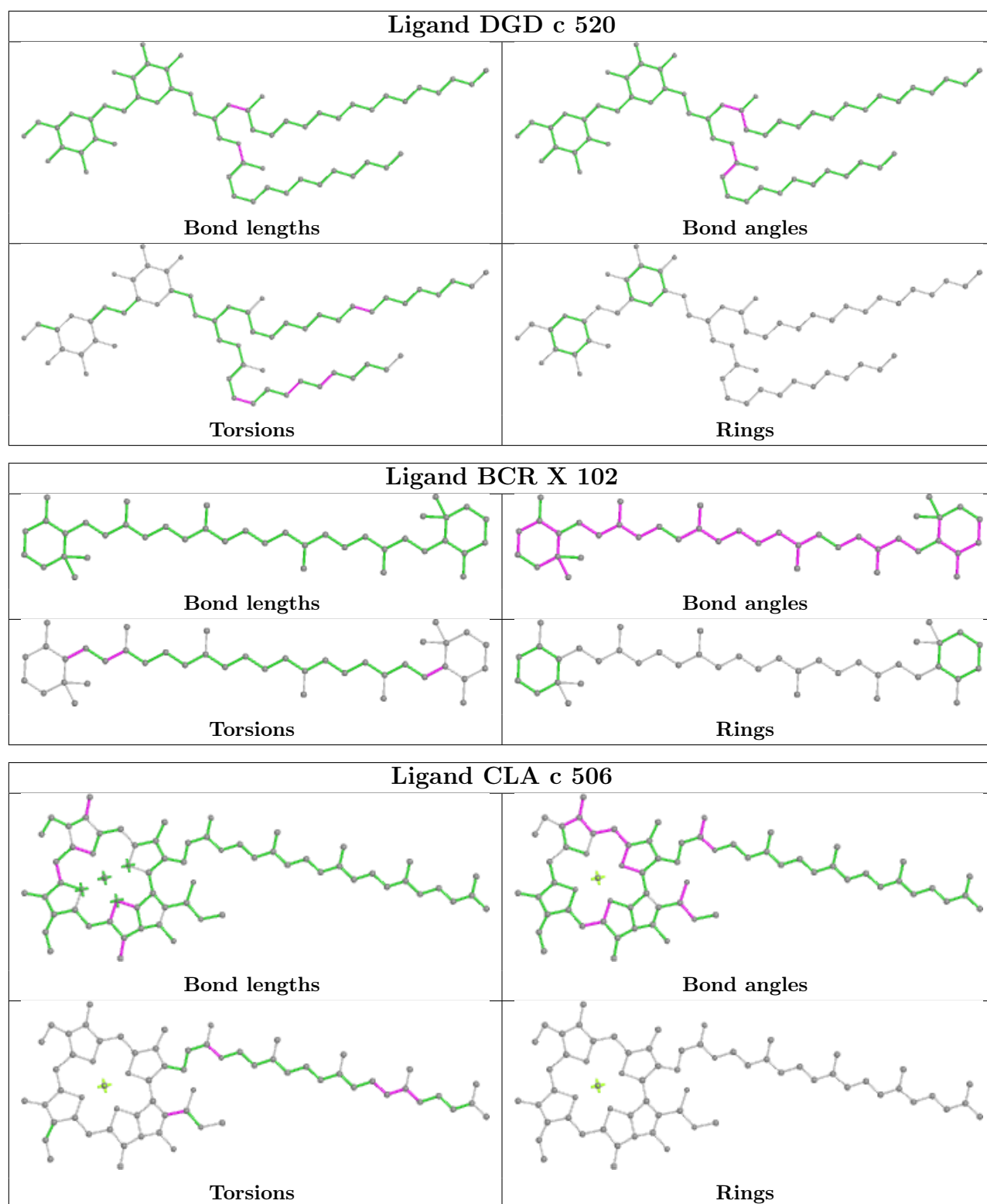


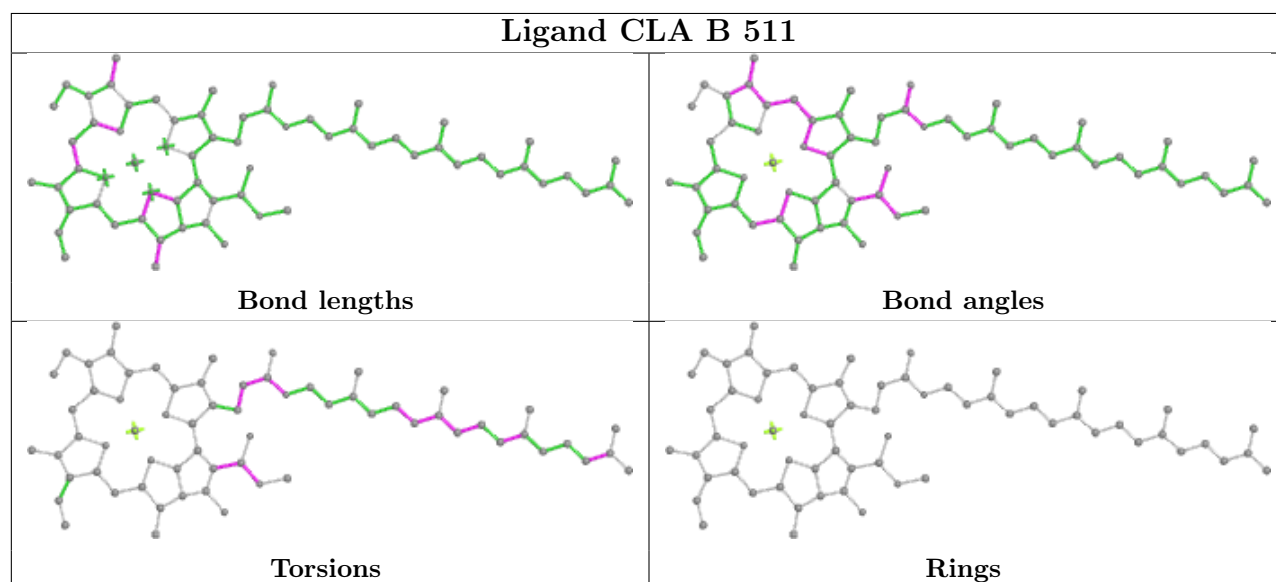
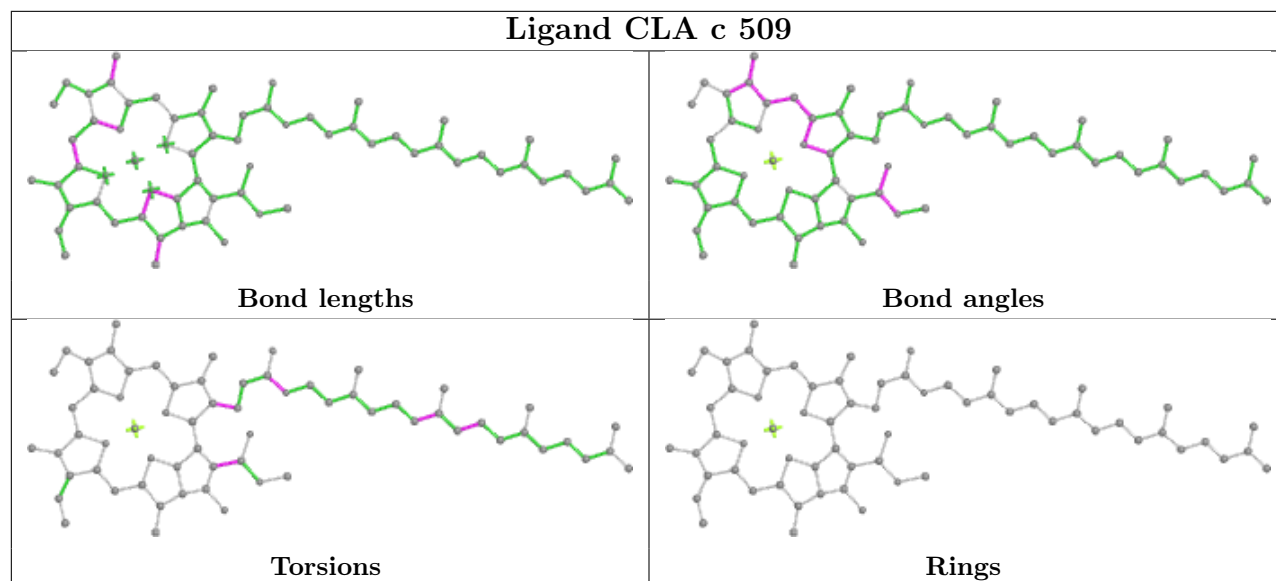
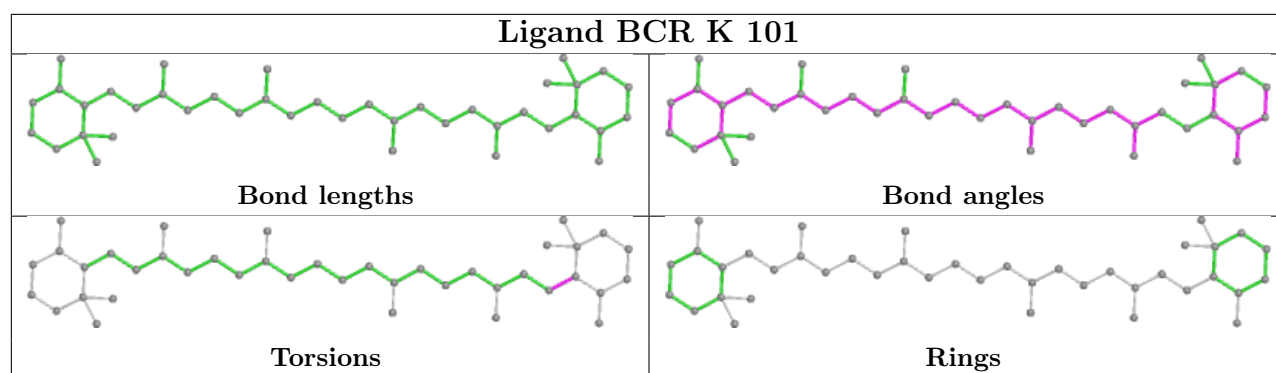




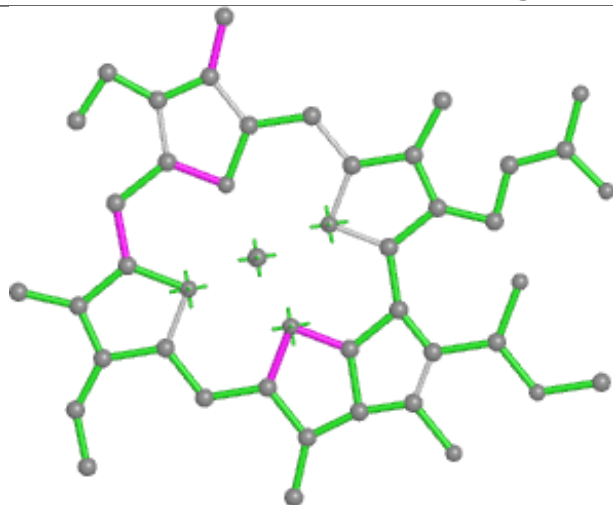




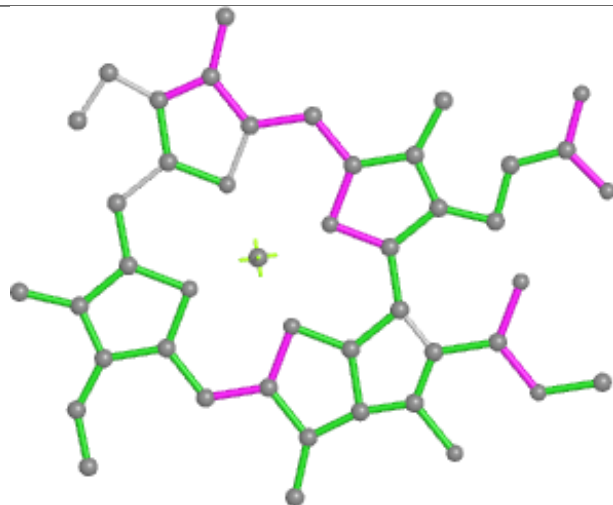




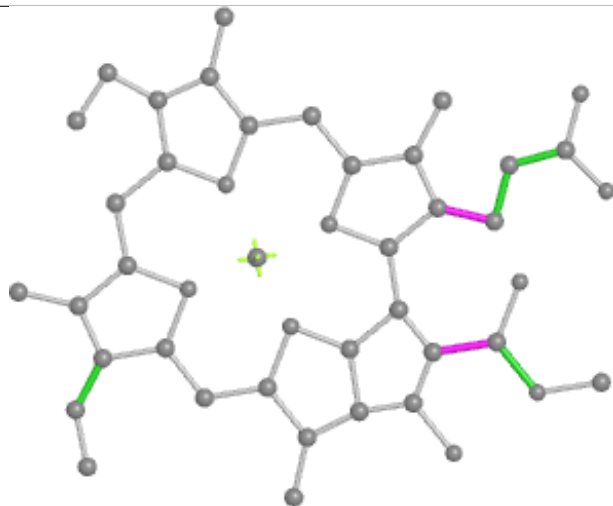
Ligand CLA B 514



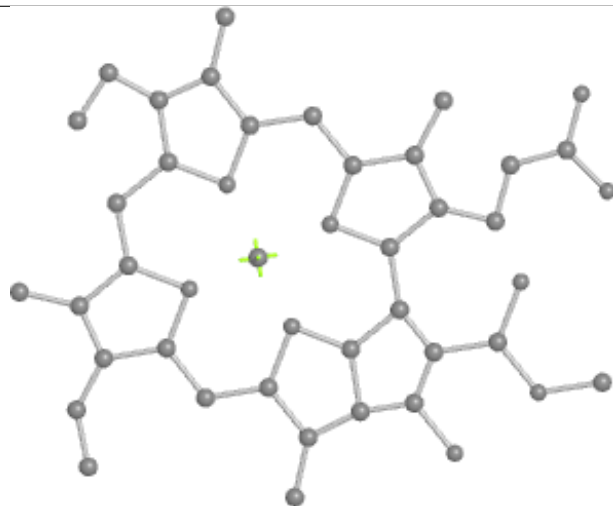
Bond lengths



Bond angles

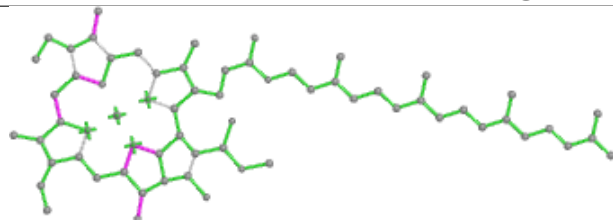


Torsions

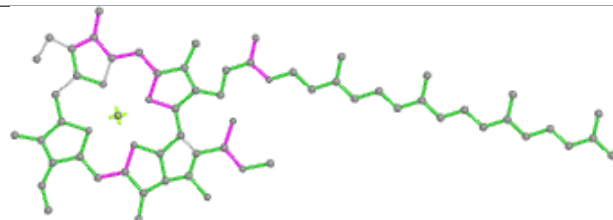


Rings

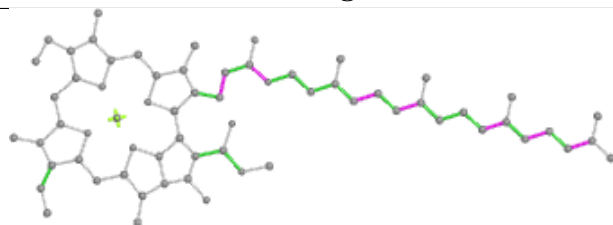
Ligand CLA b 508



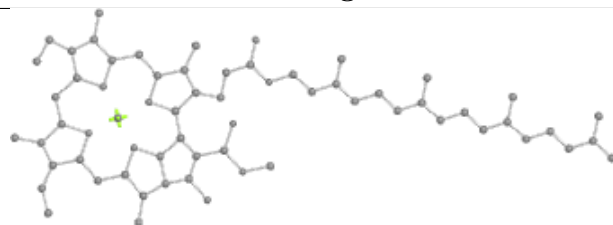
Bond lengths



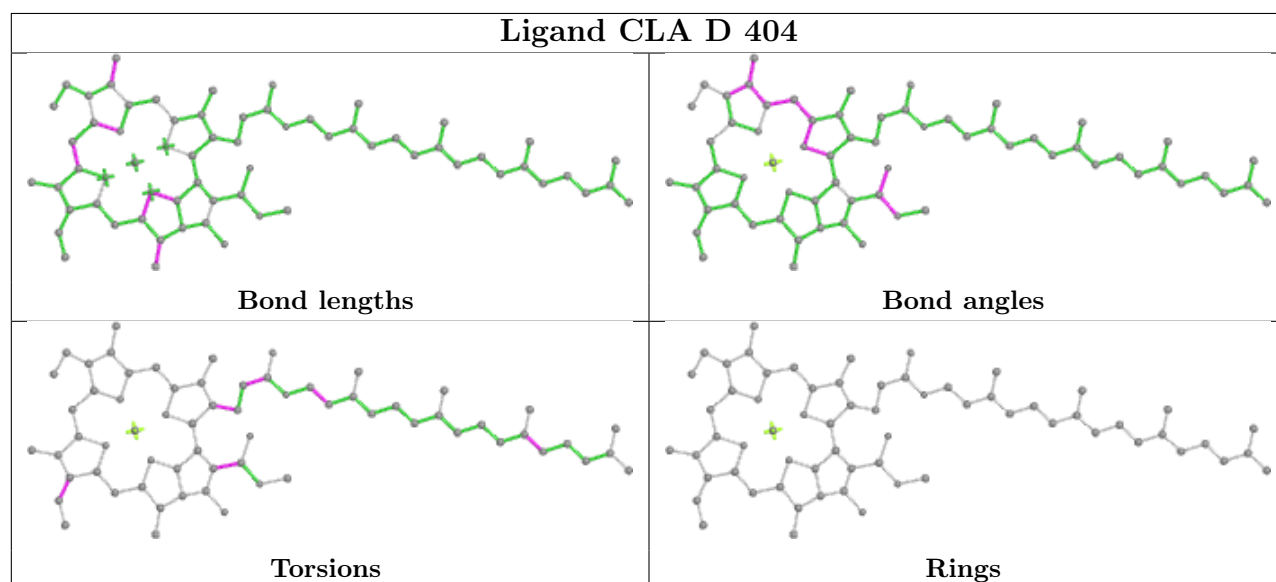
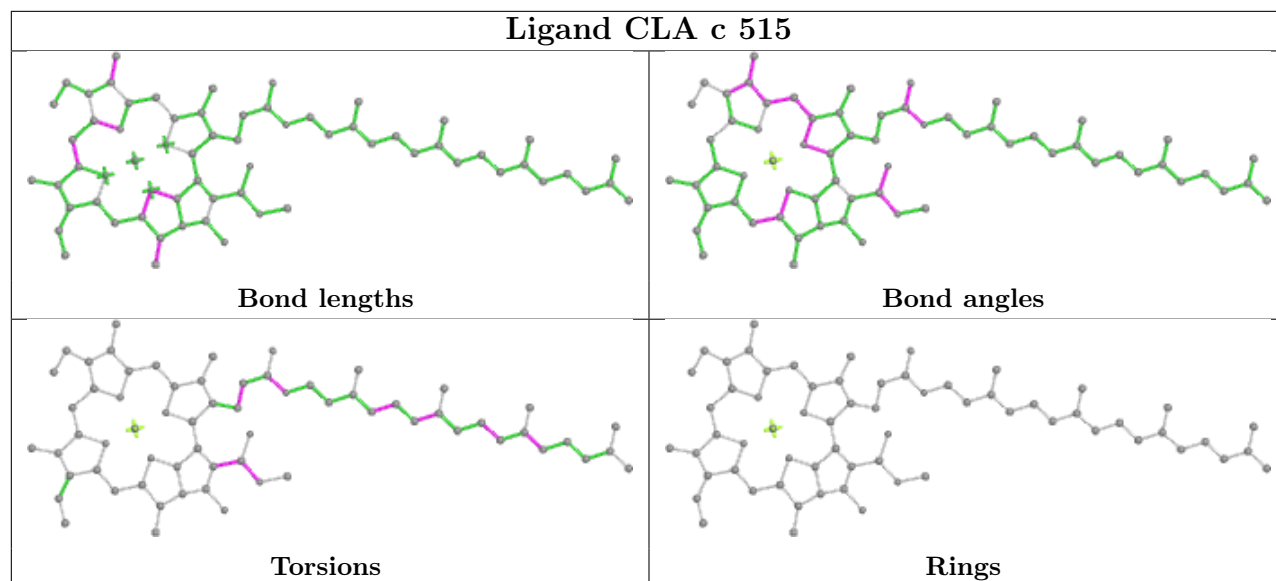
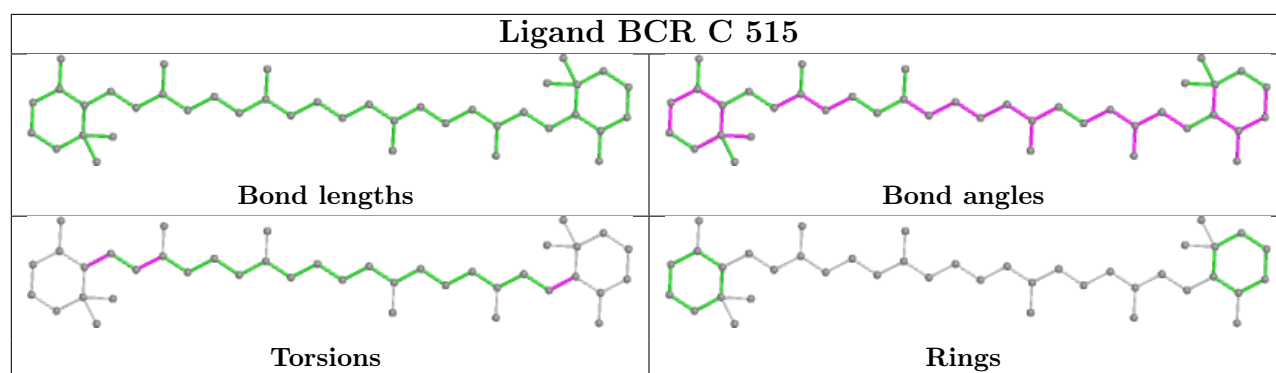
Bond angles

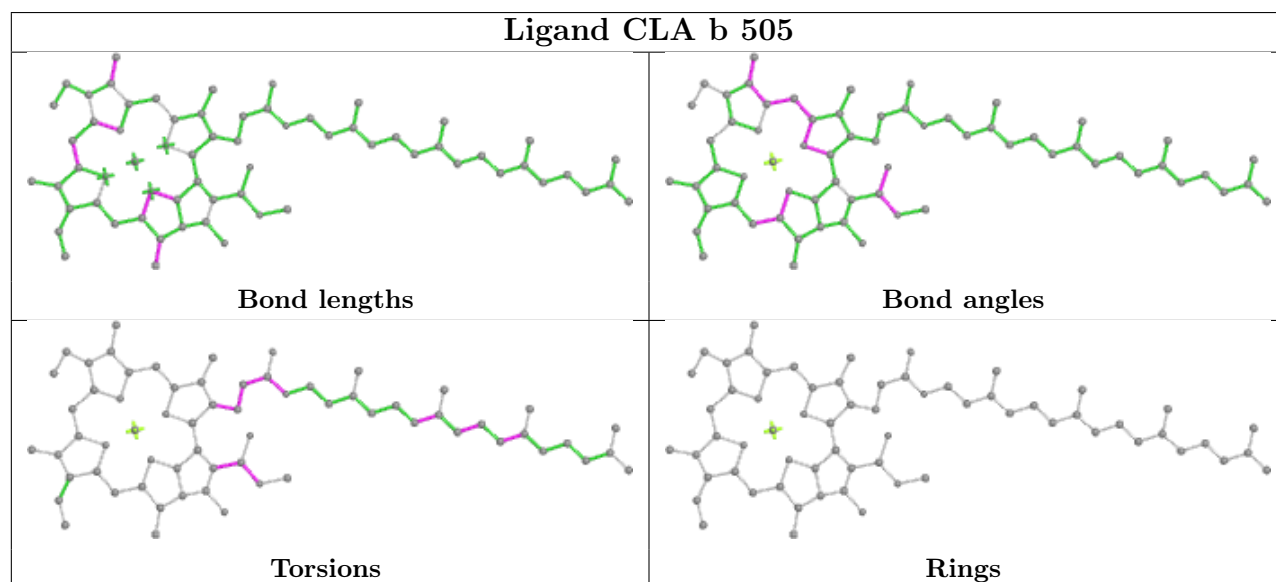
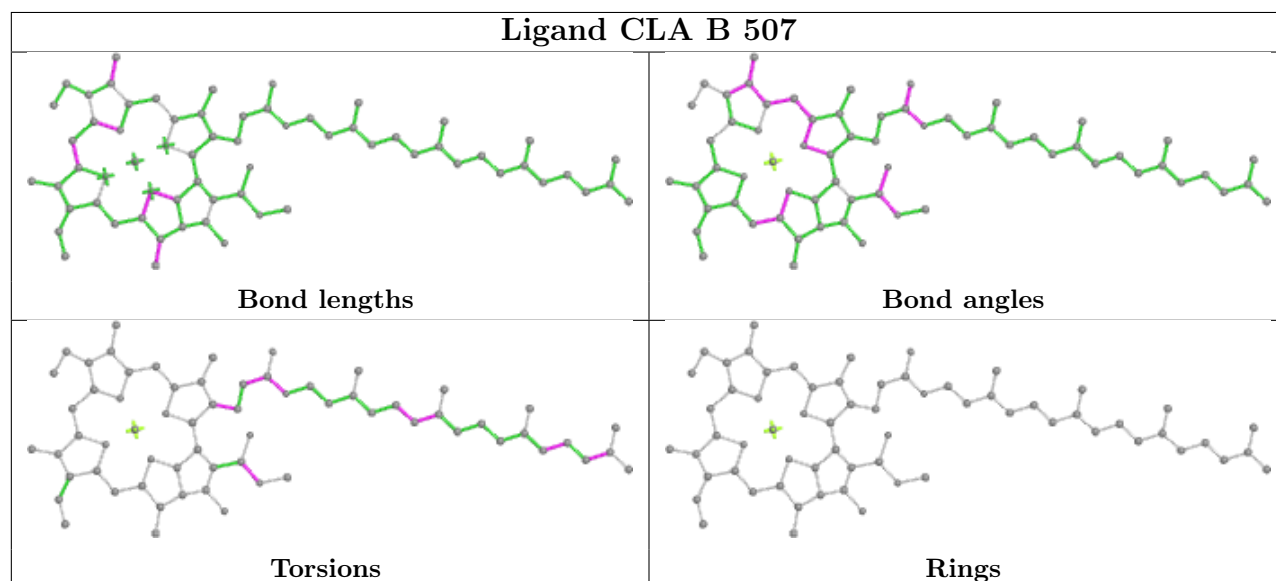
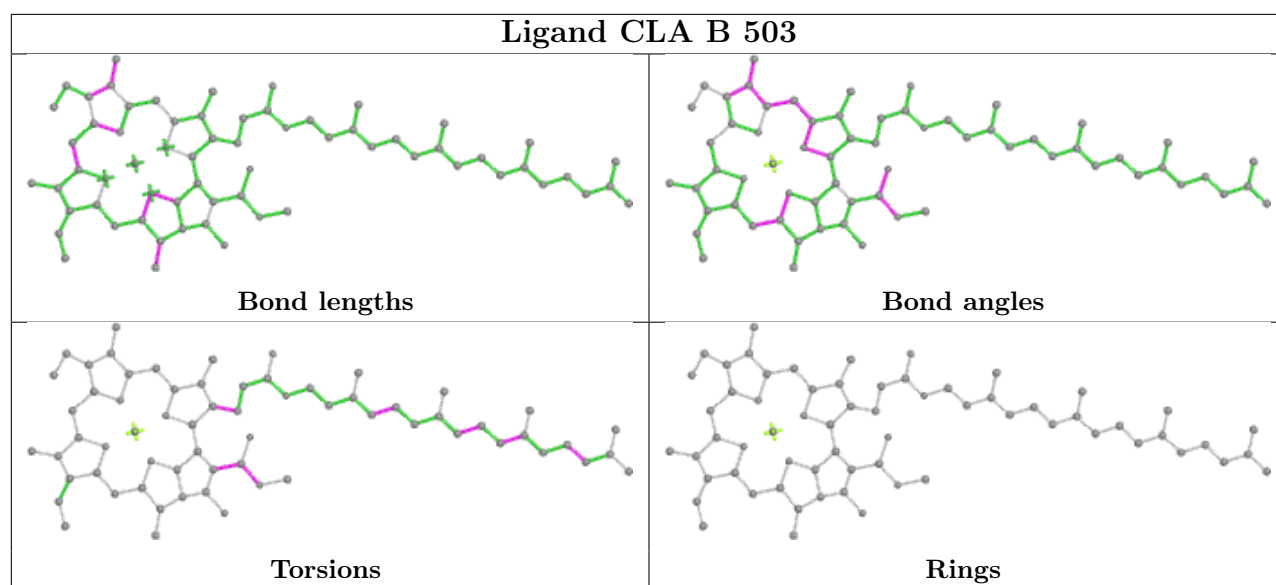


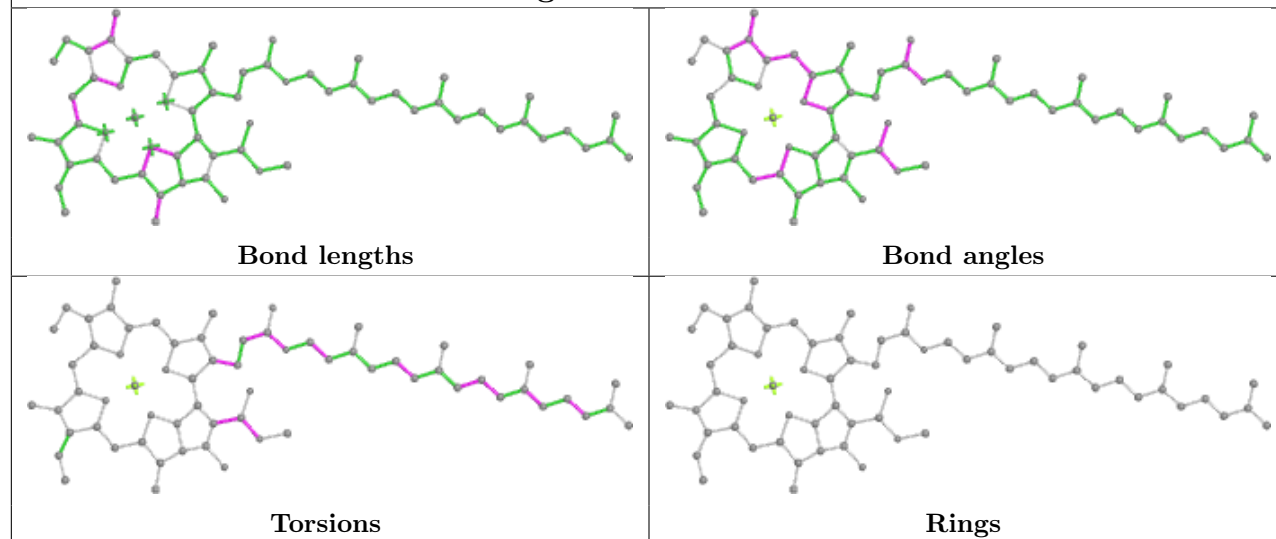
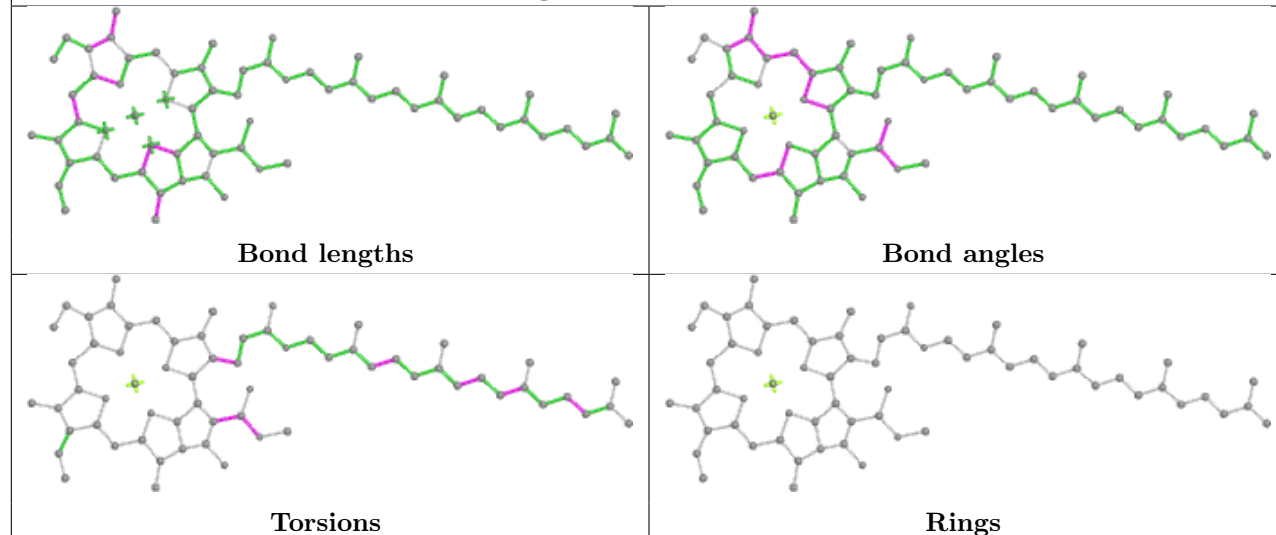
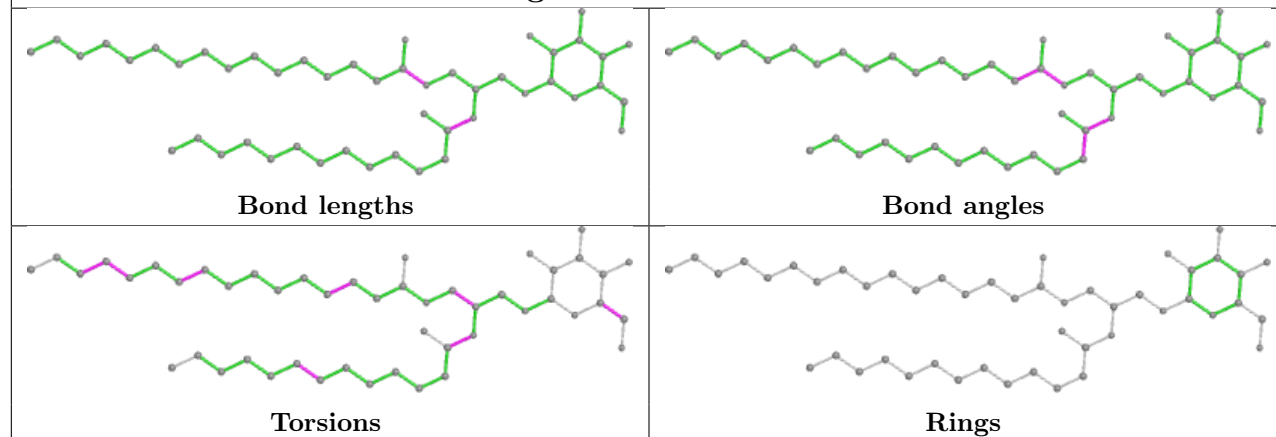
Torsions

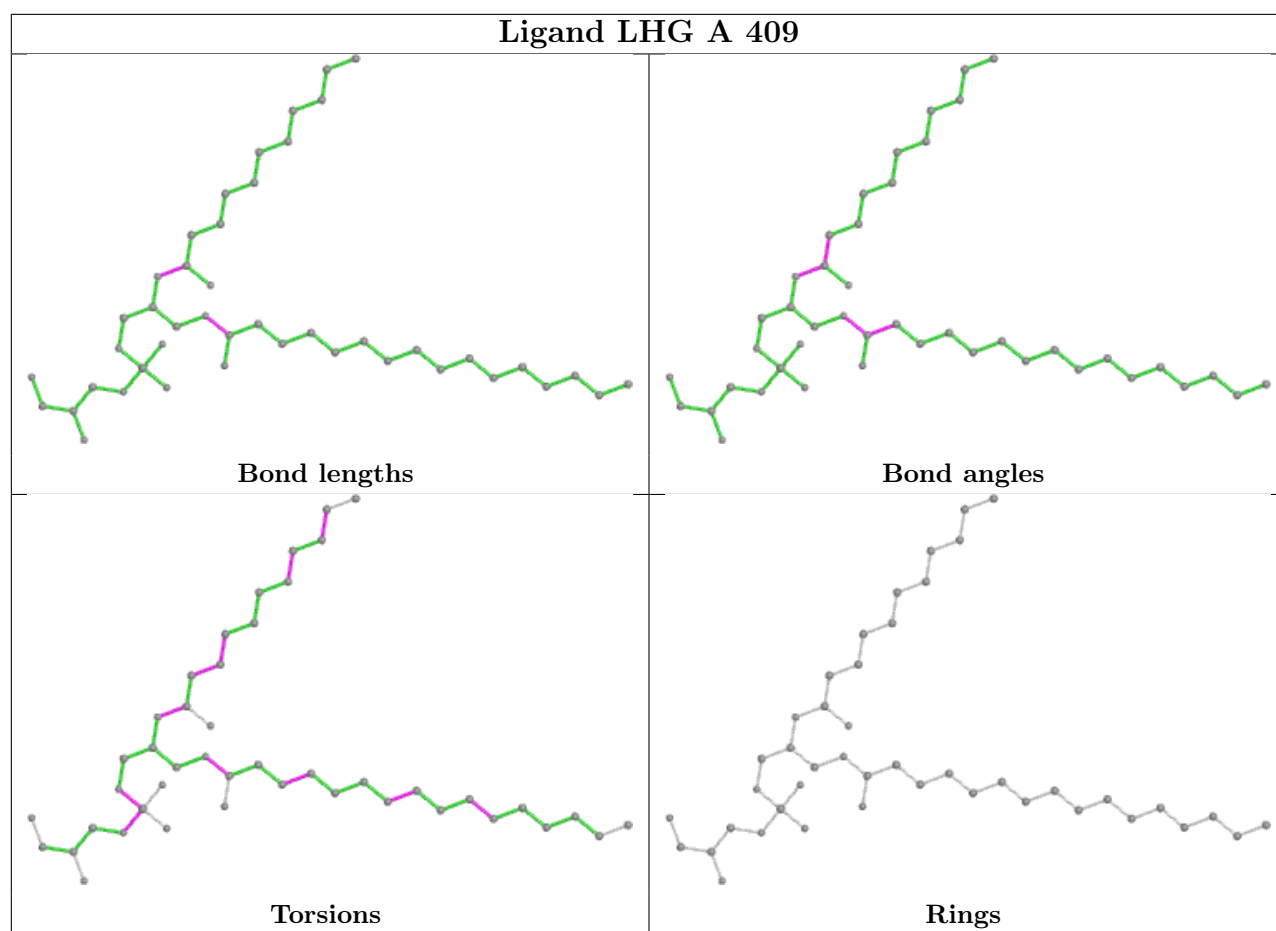


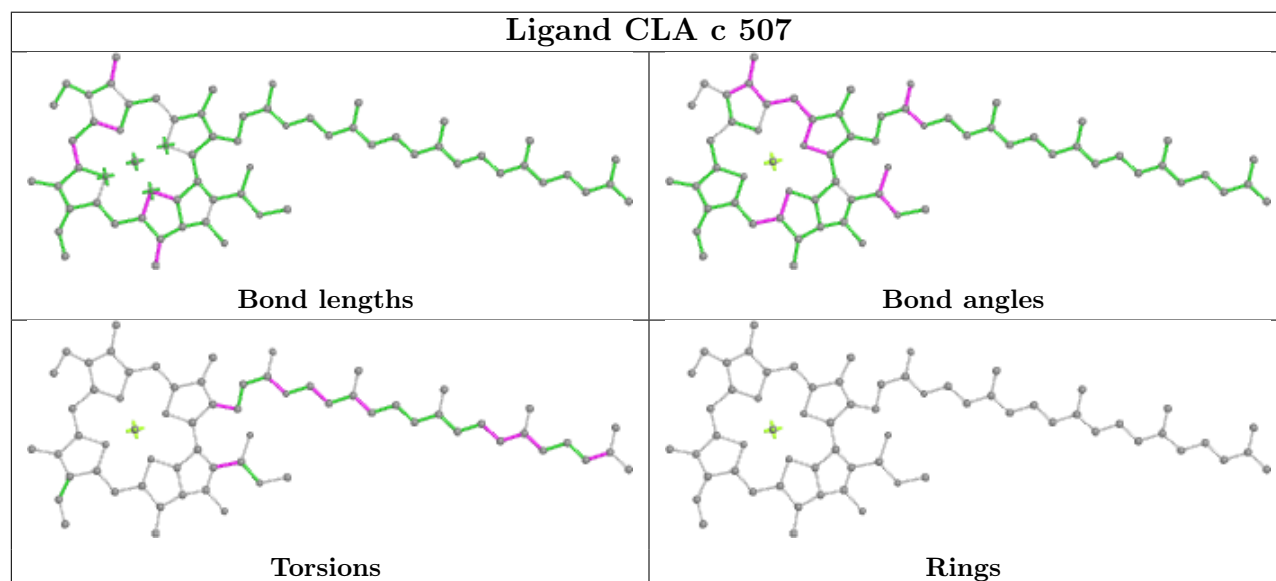
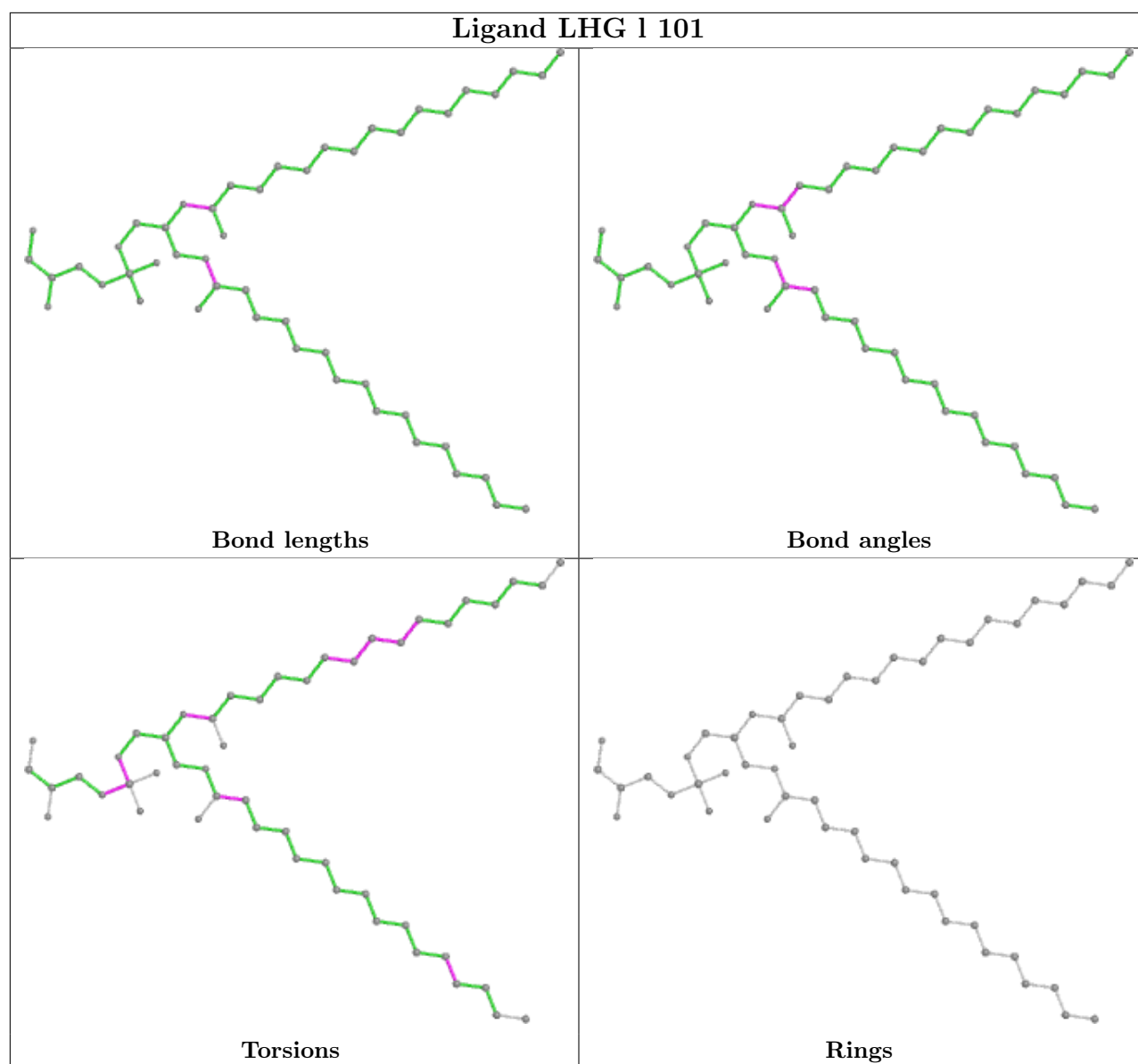
Rings



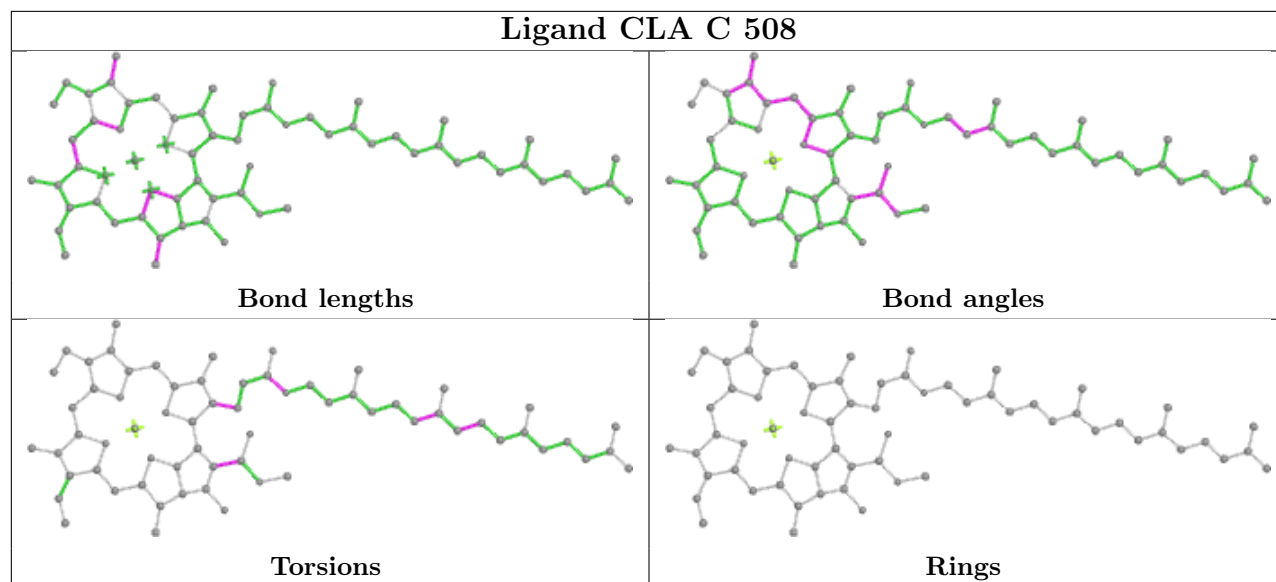


Ligand CLA c 508**Ligand CLA b 503****Ligand LMG D 410**

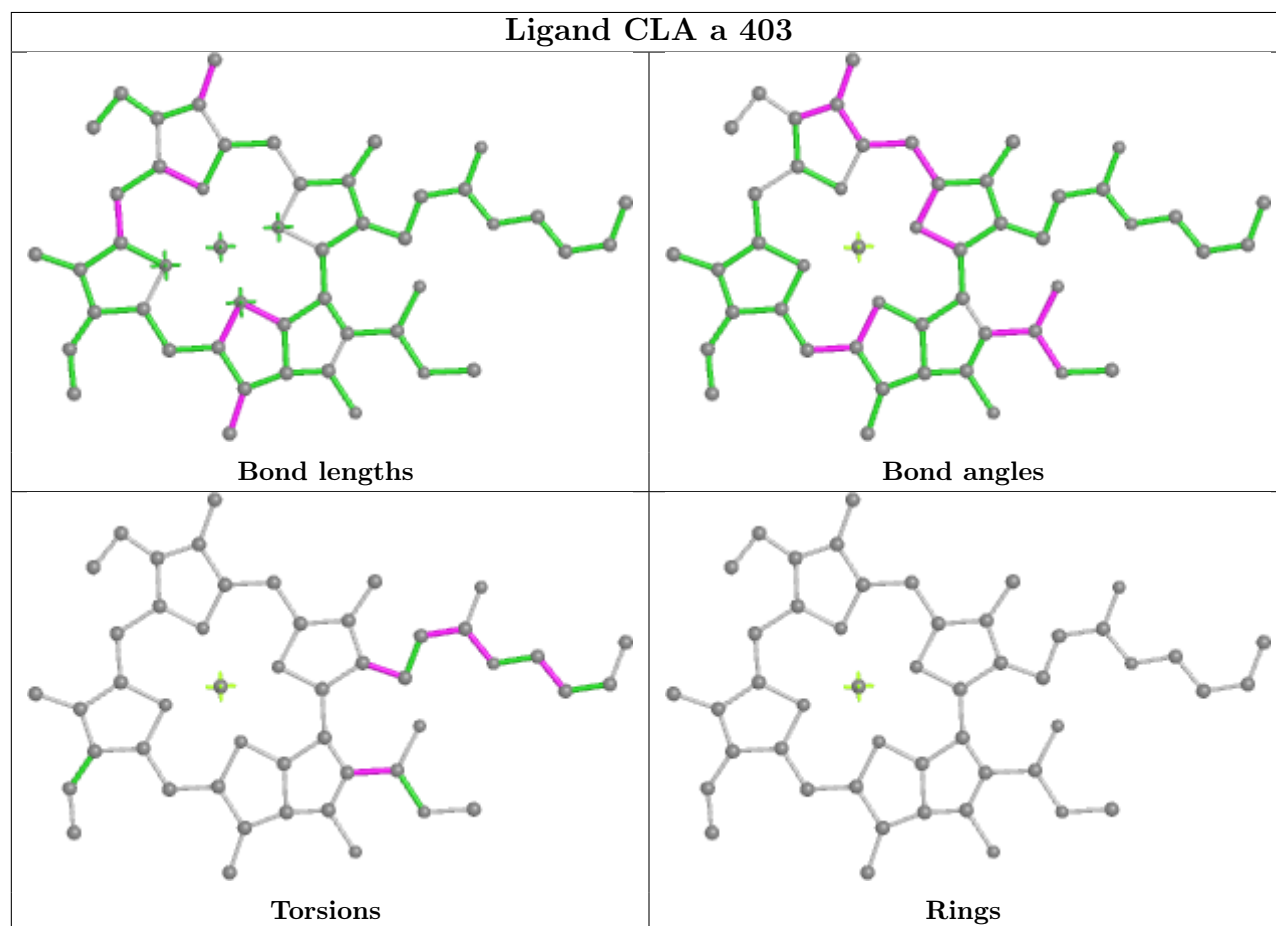


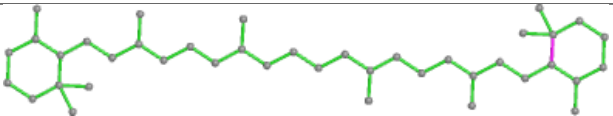
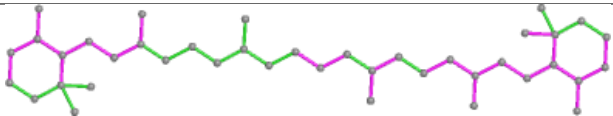
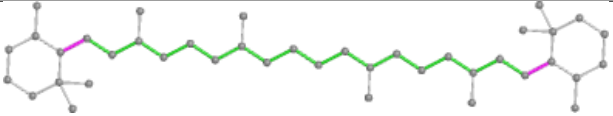
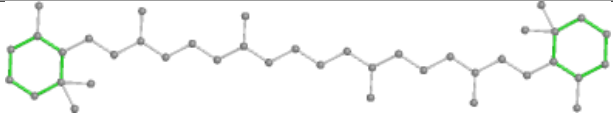


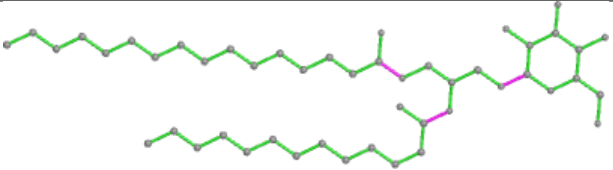
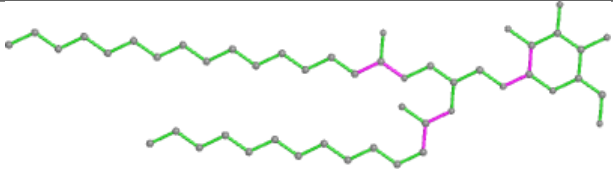
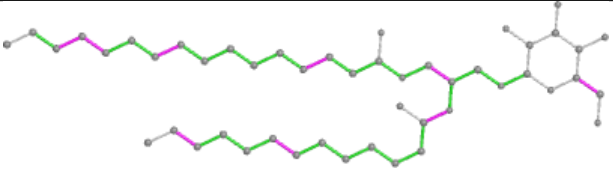

Ligand CLA C 508

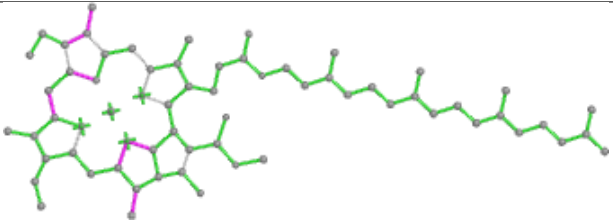
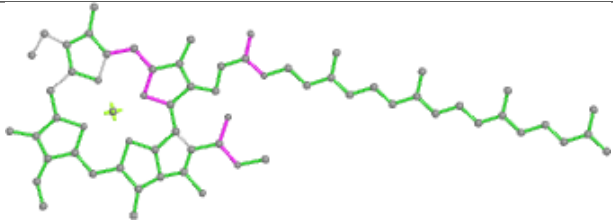
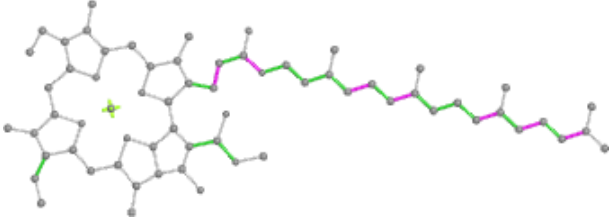
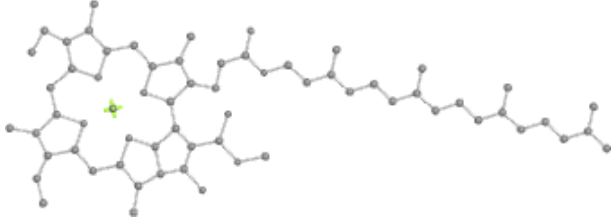


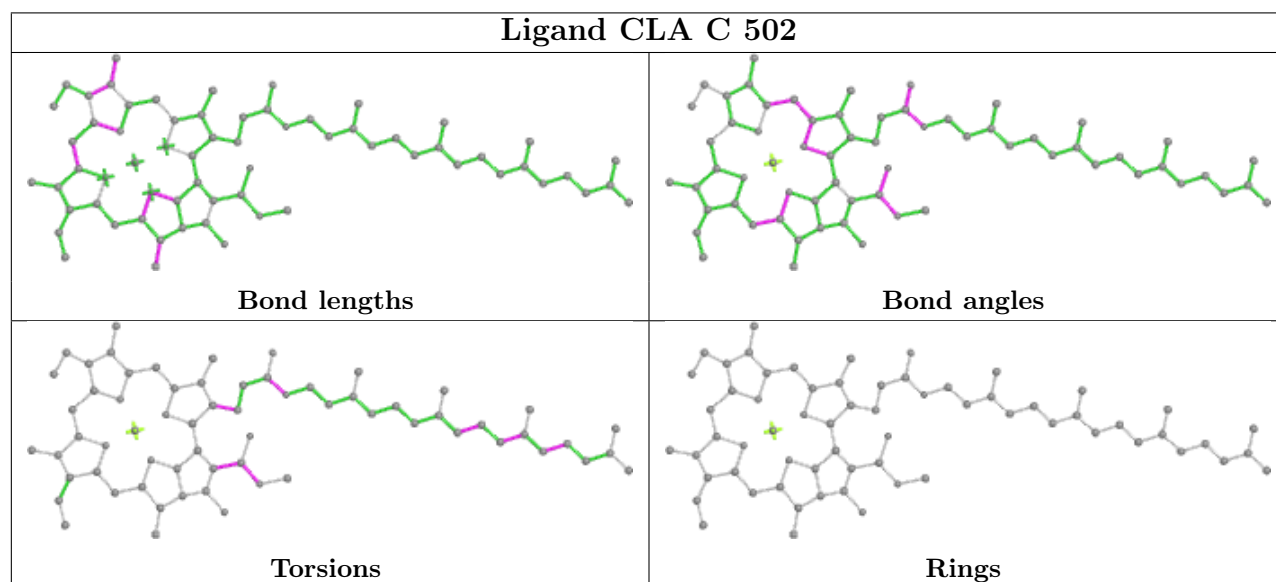
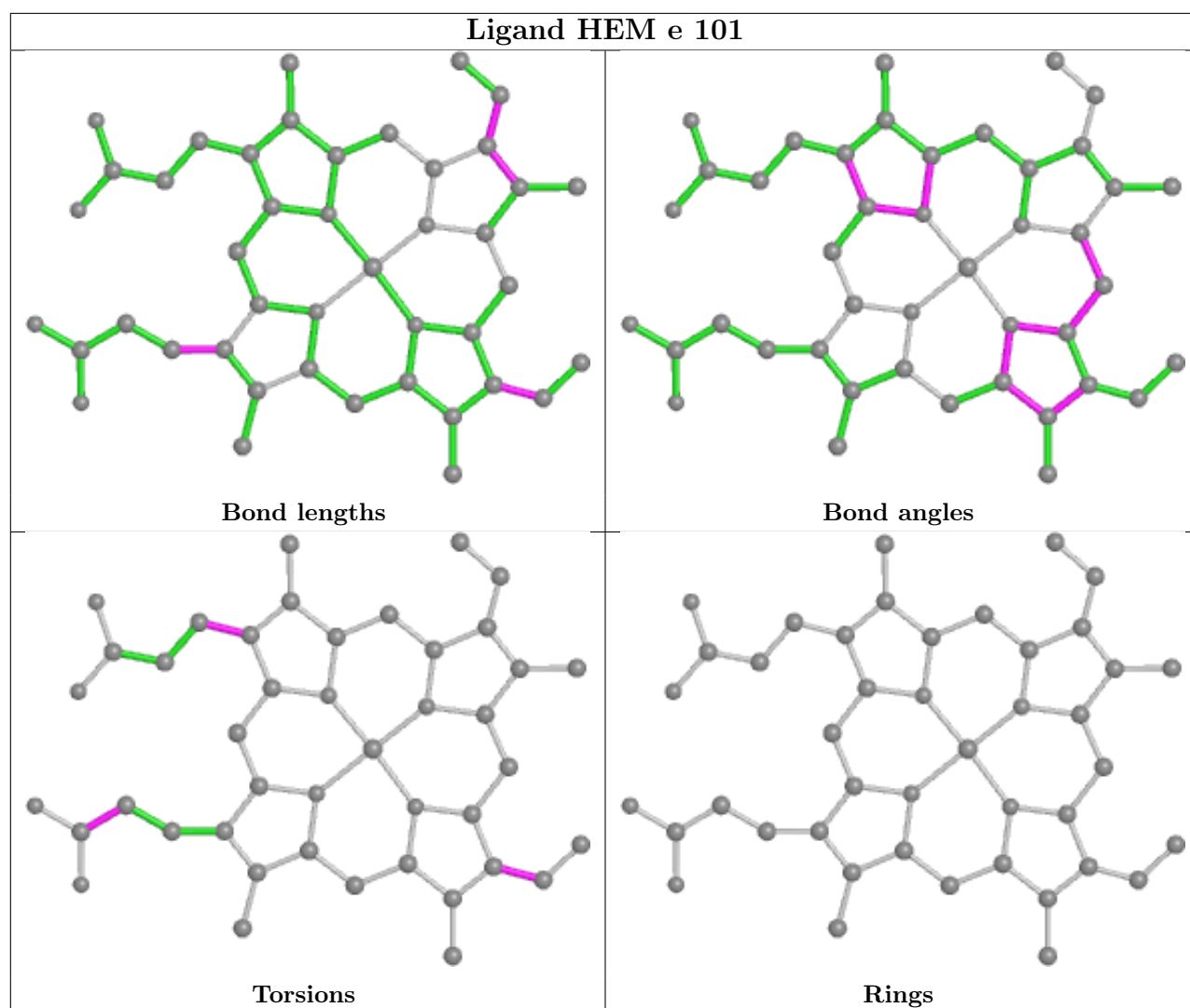
Ligand CLA a 403

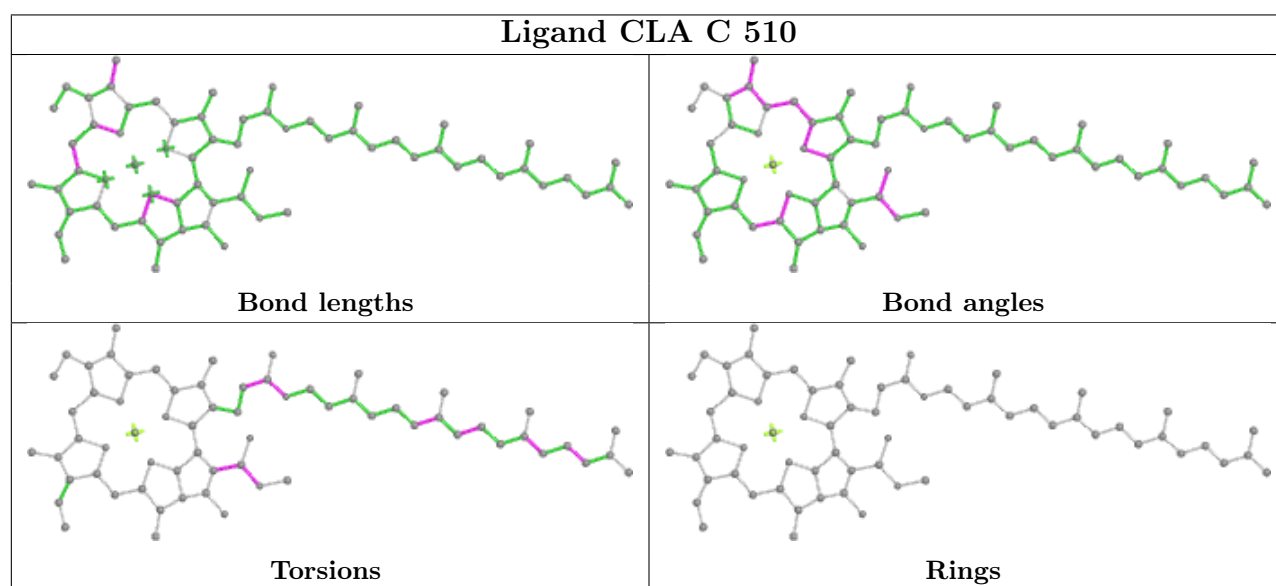
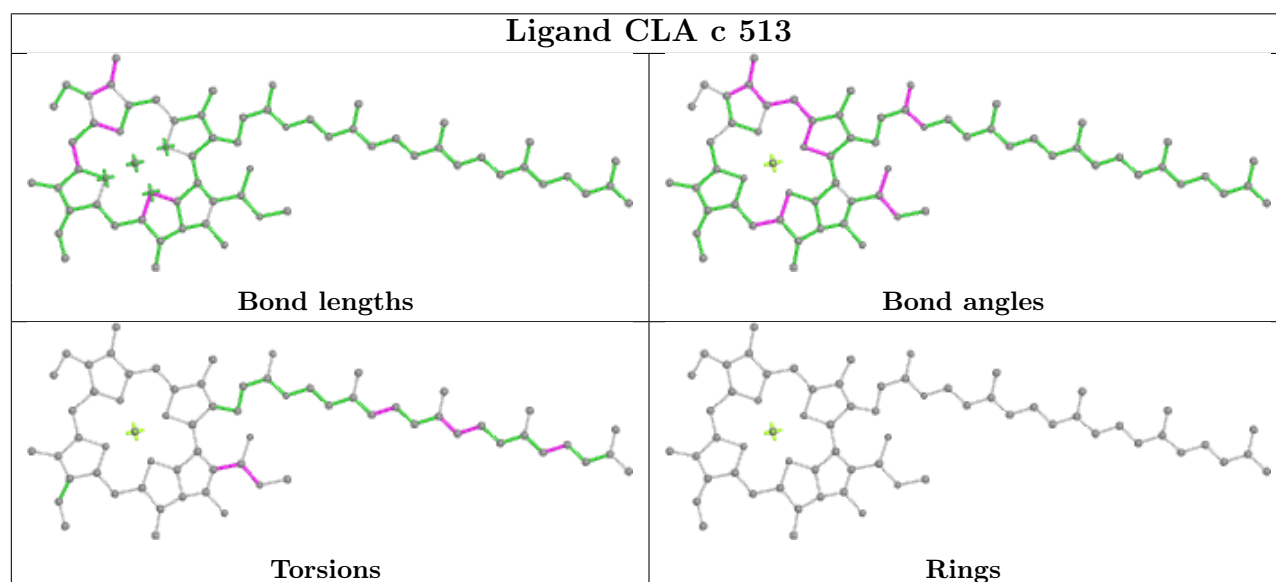
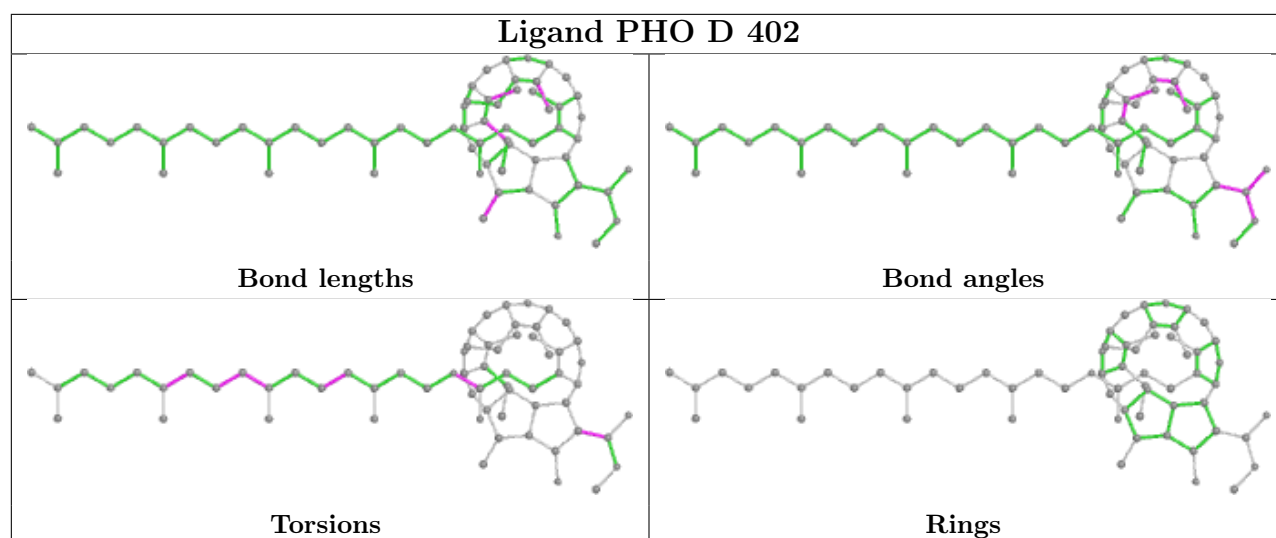


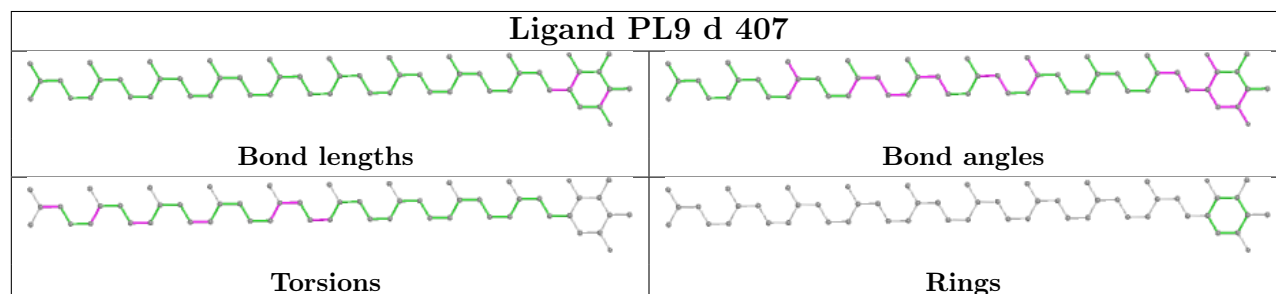
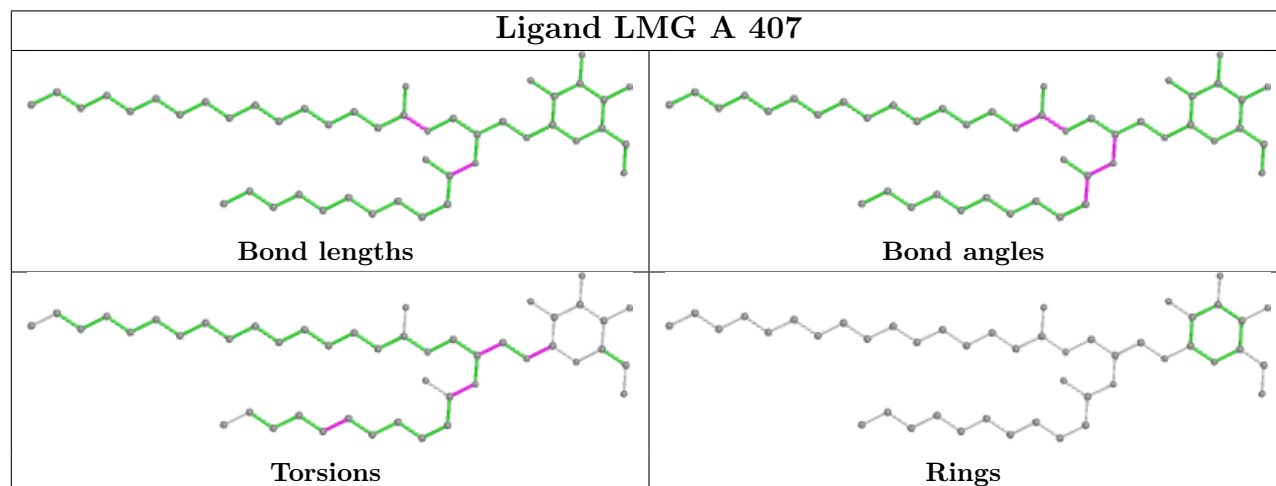
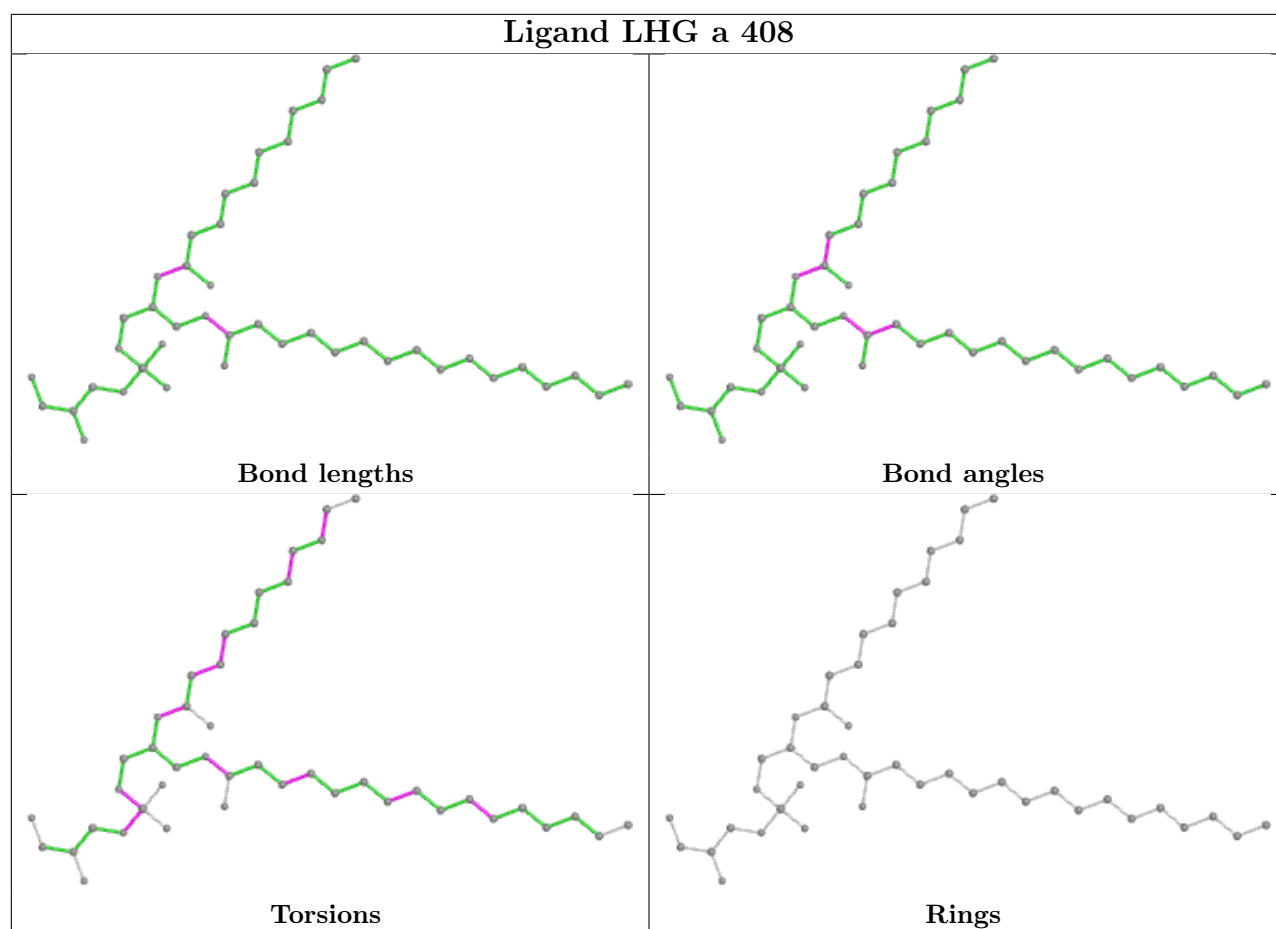
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

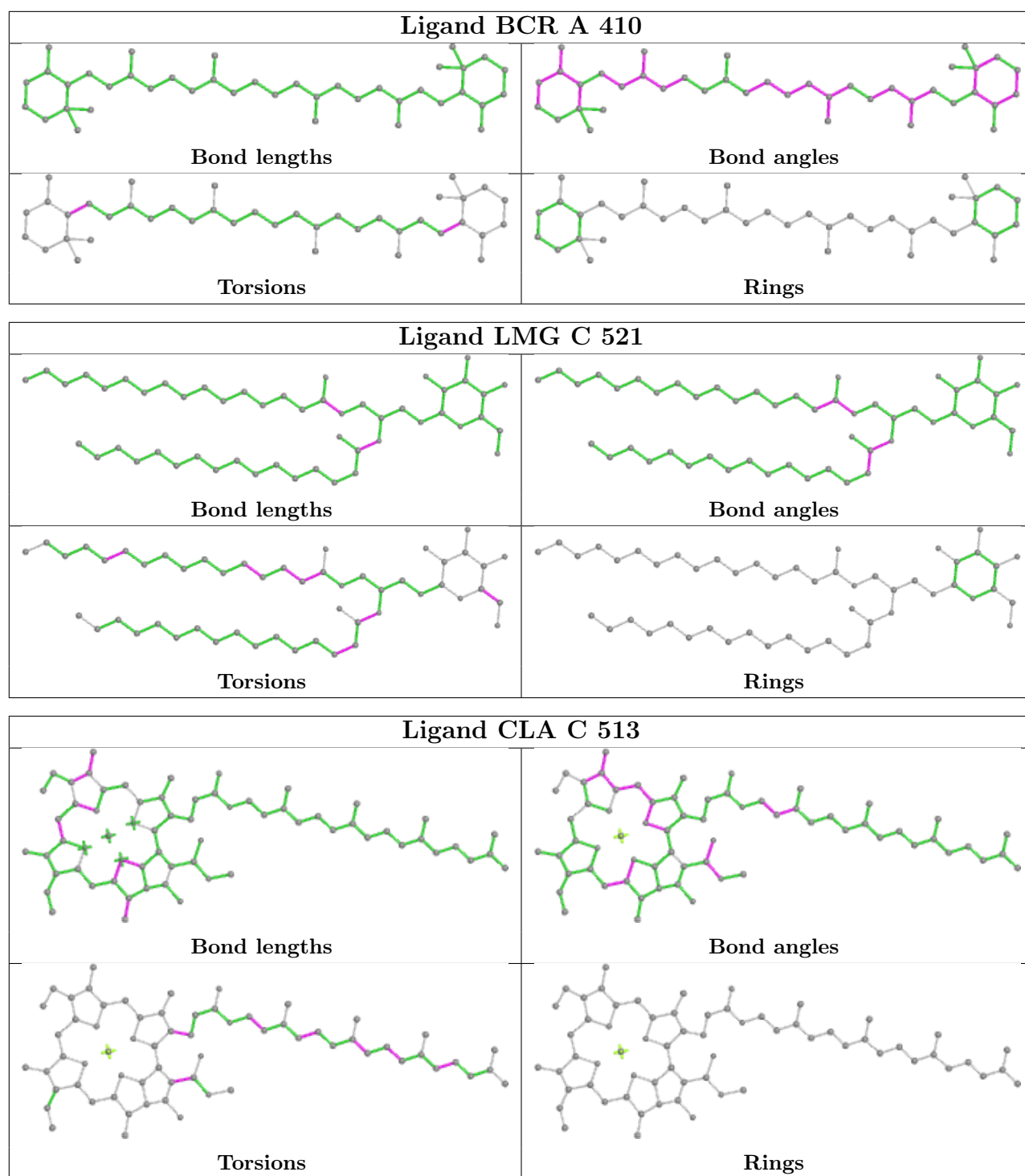
Ligand LMG h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

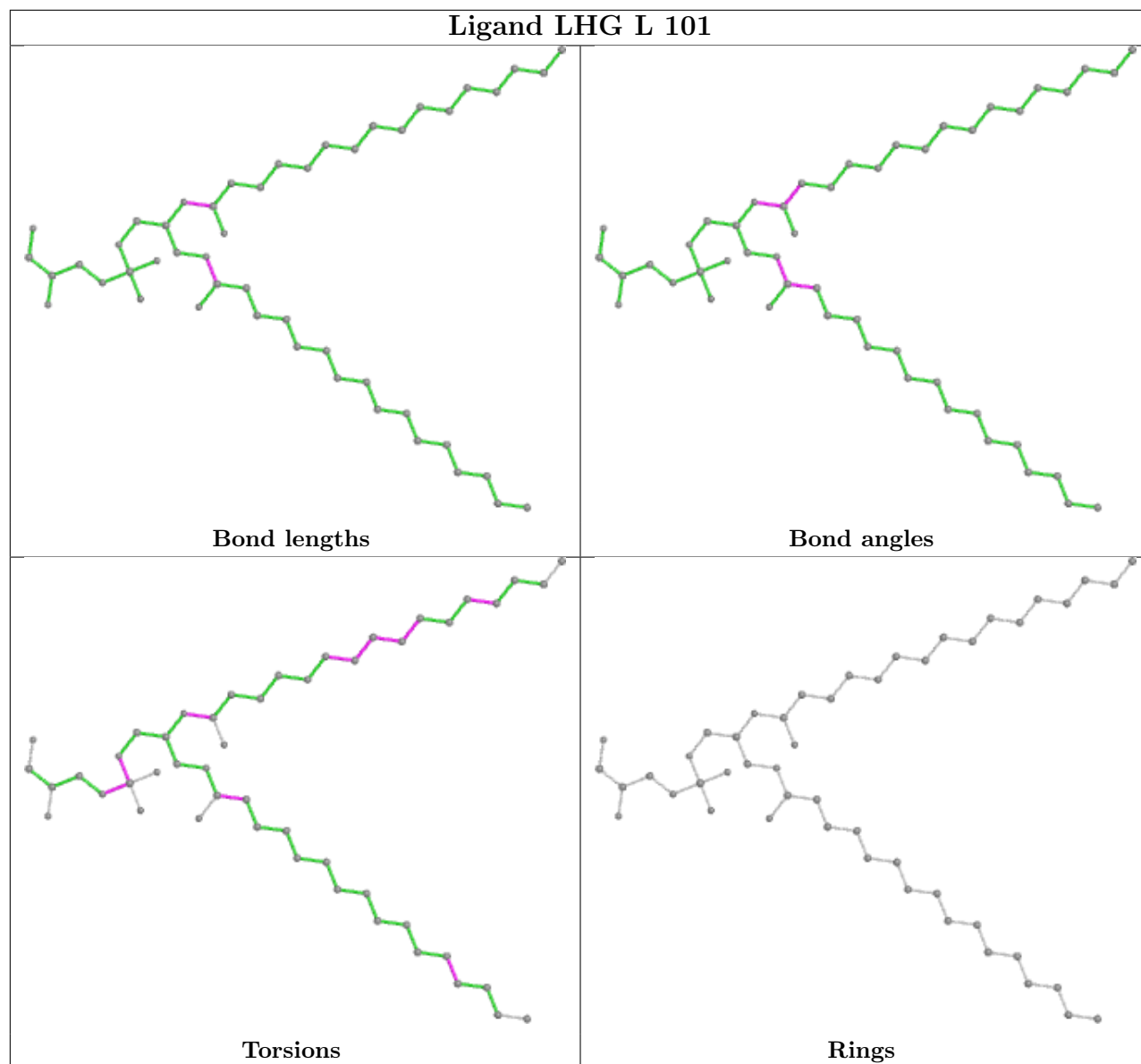




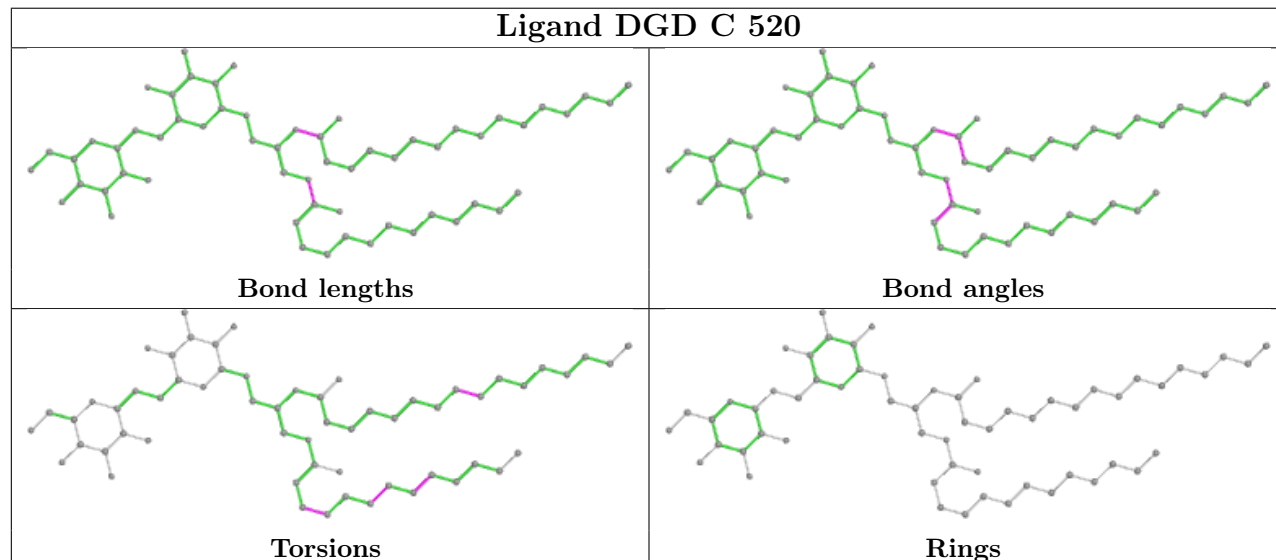


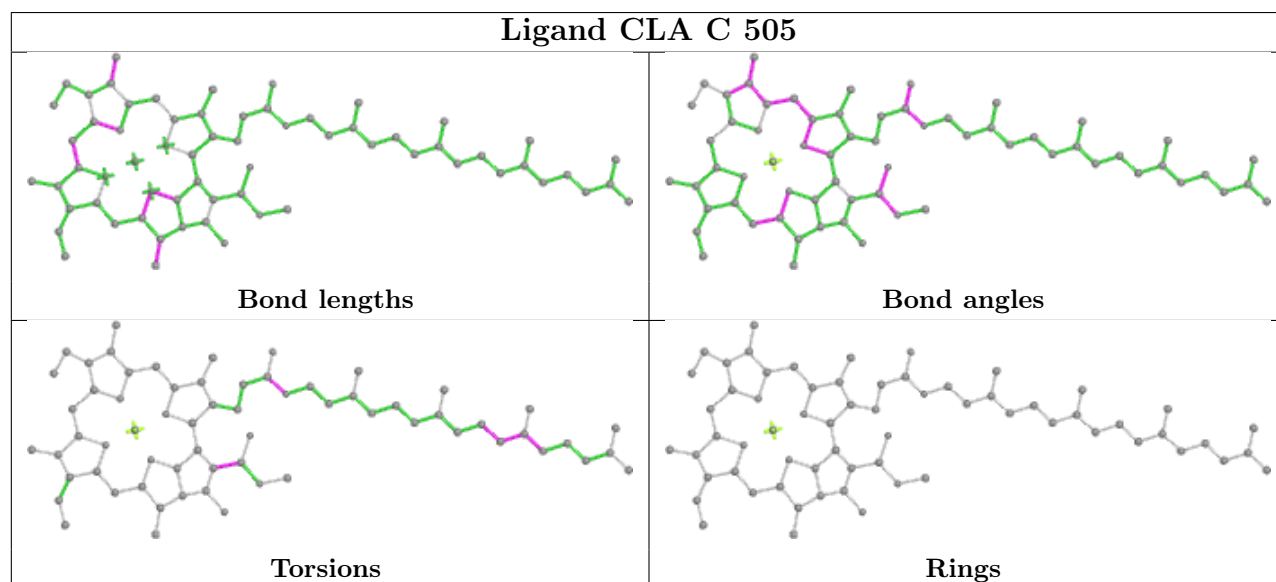
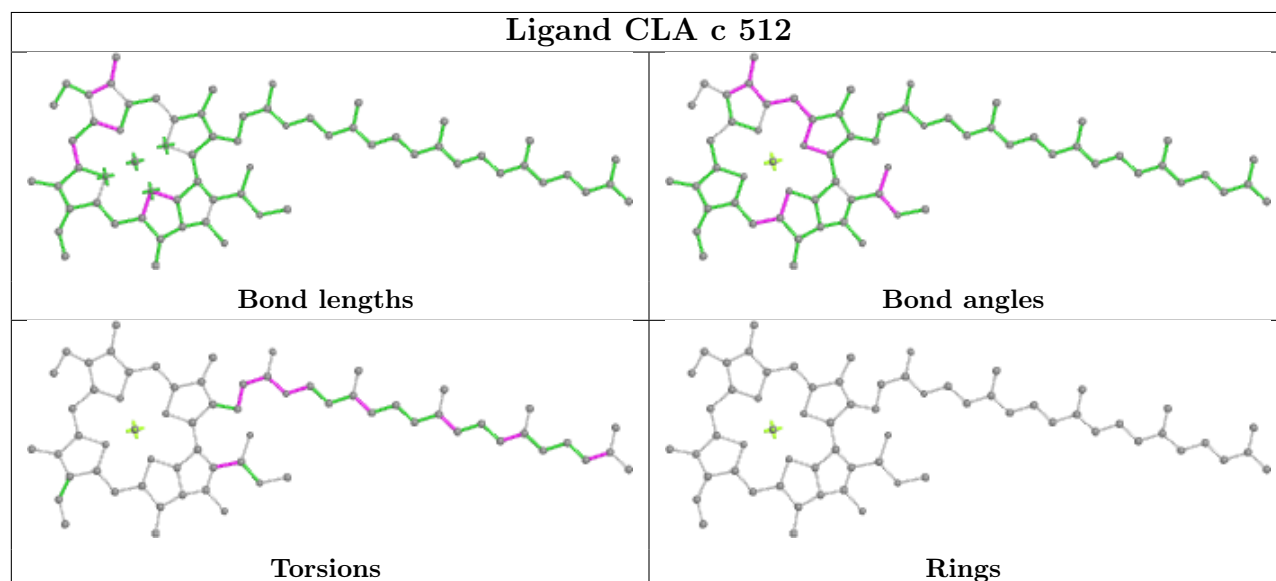
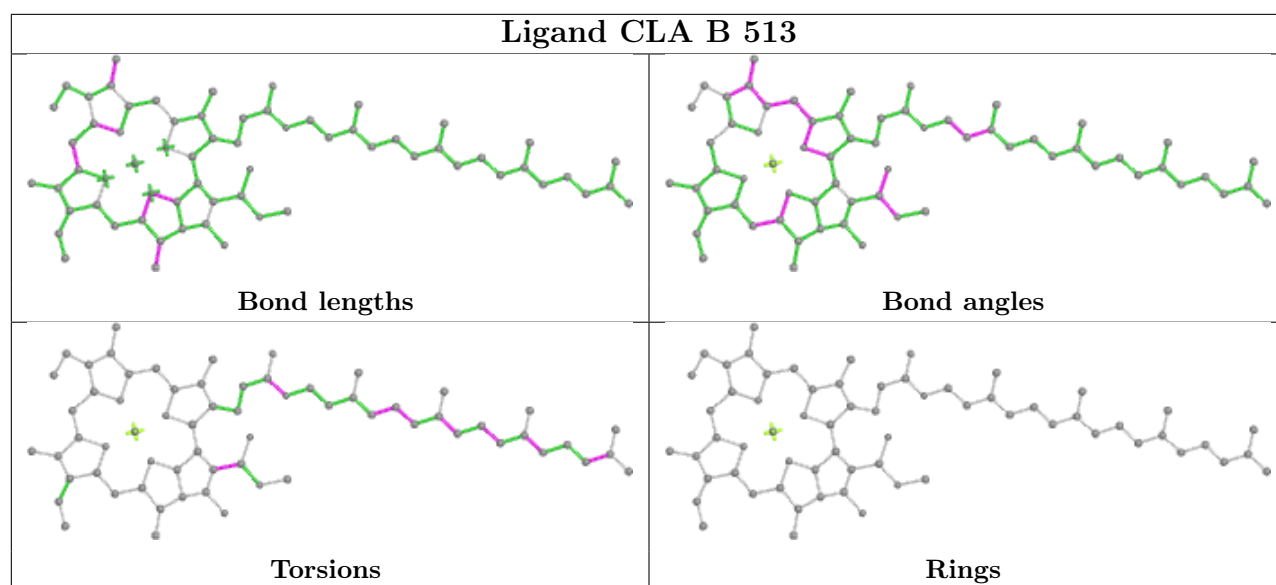


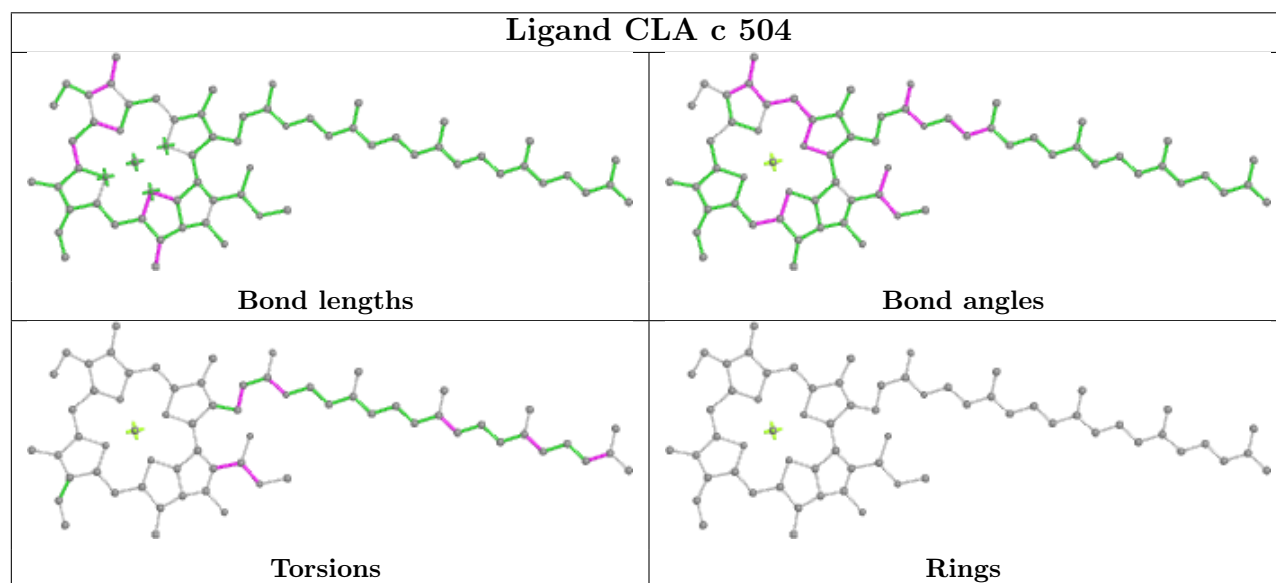
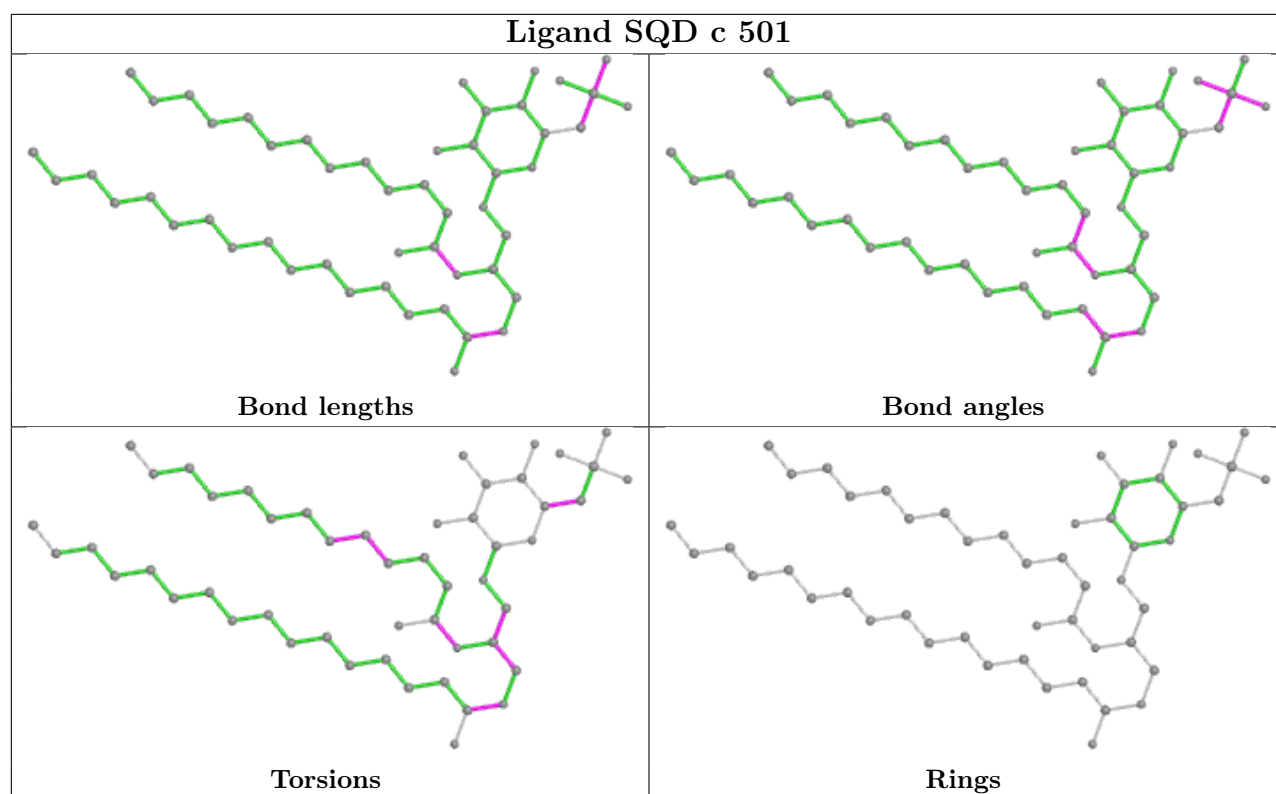
Ligand LHG L 101

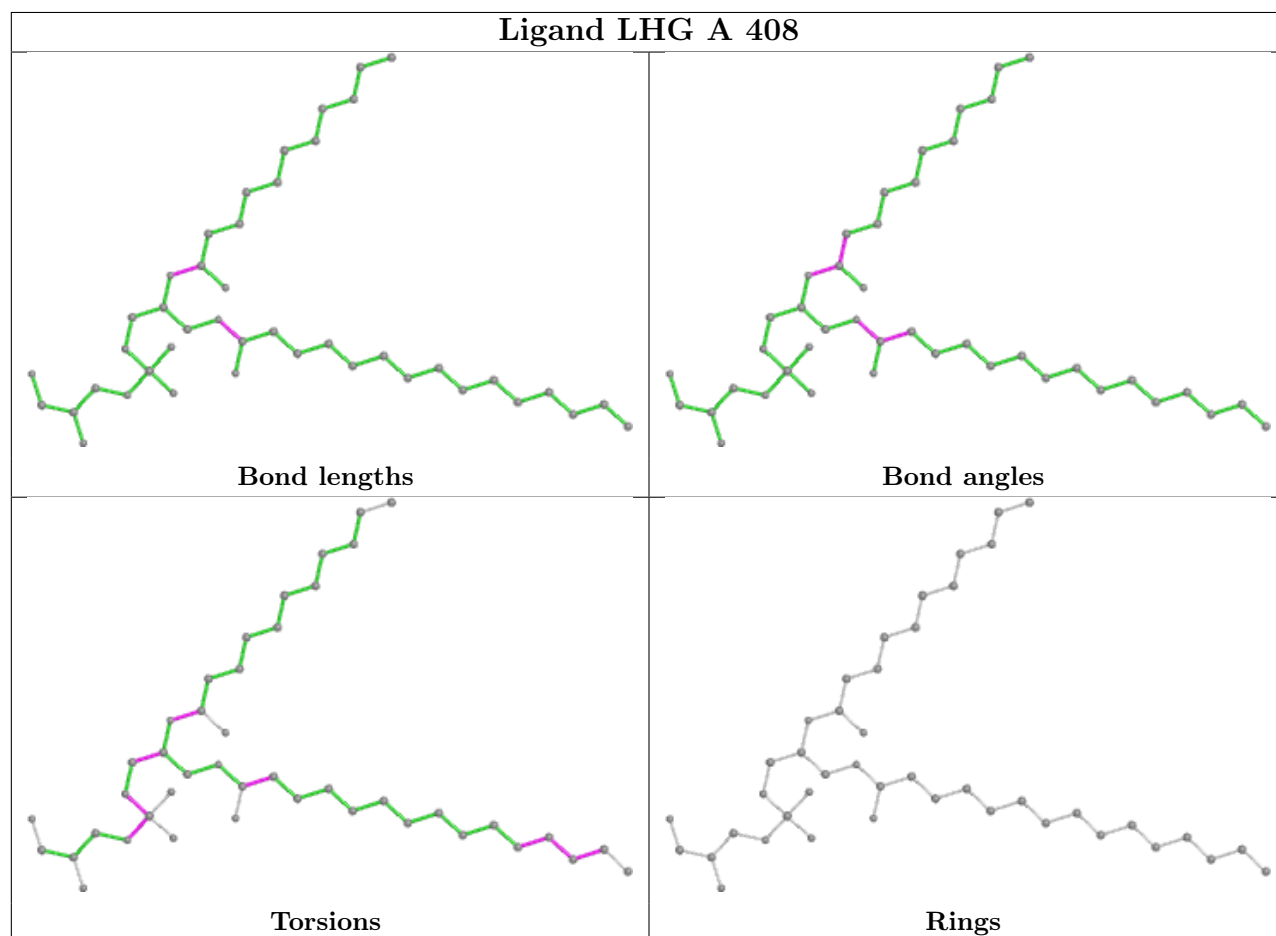
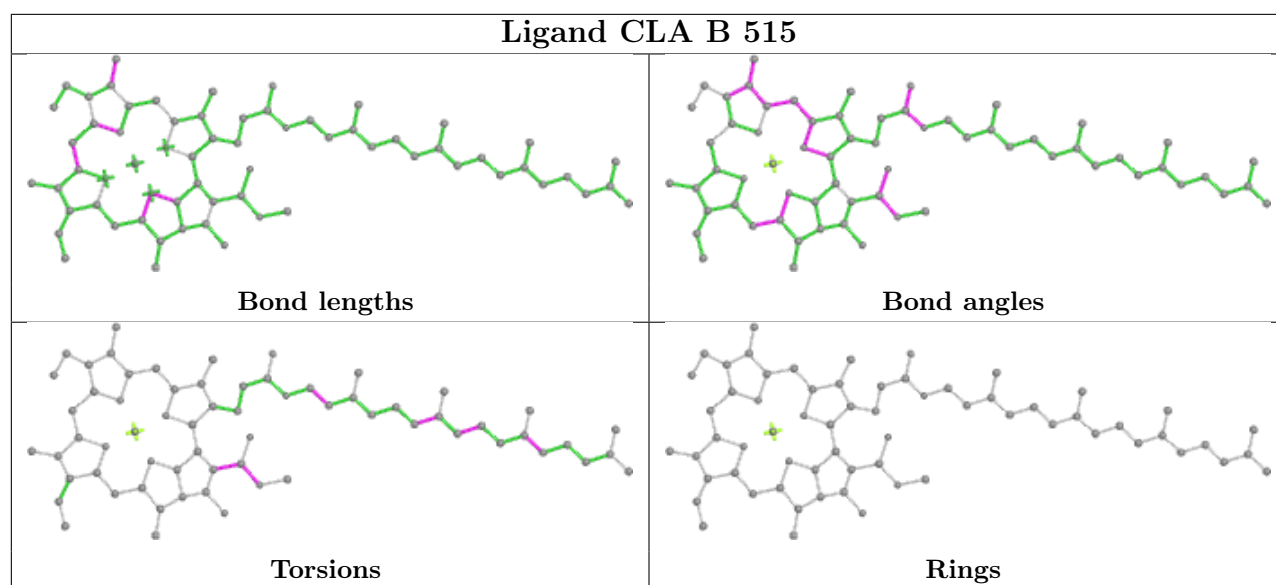


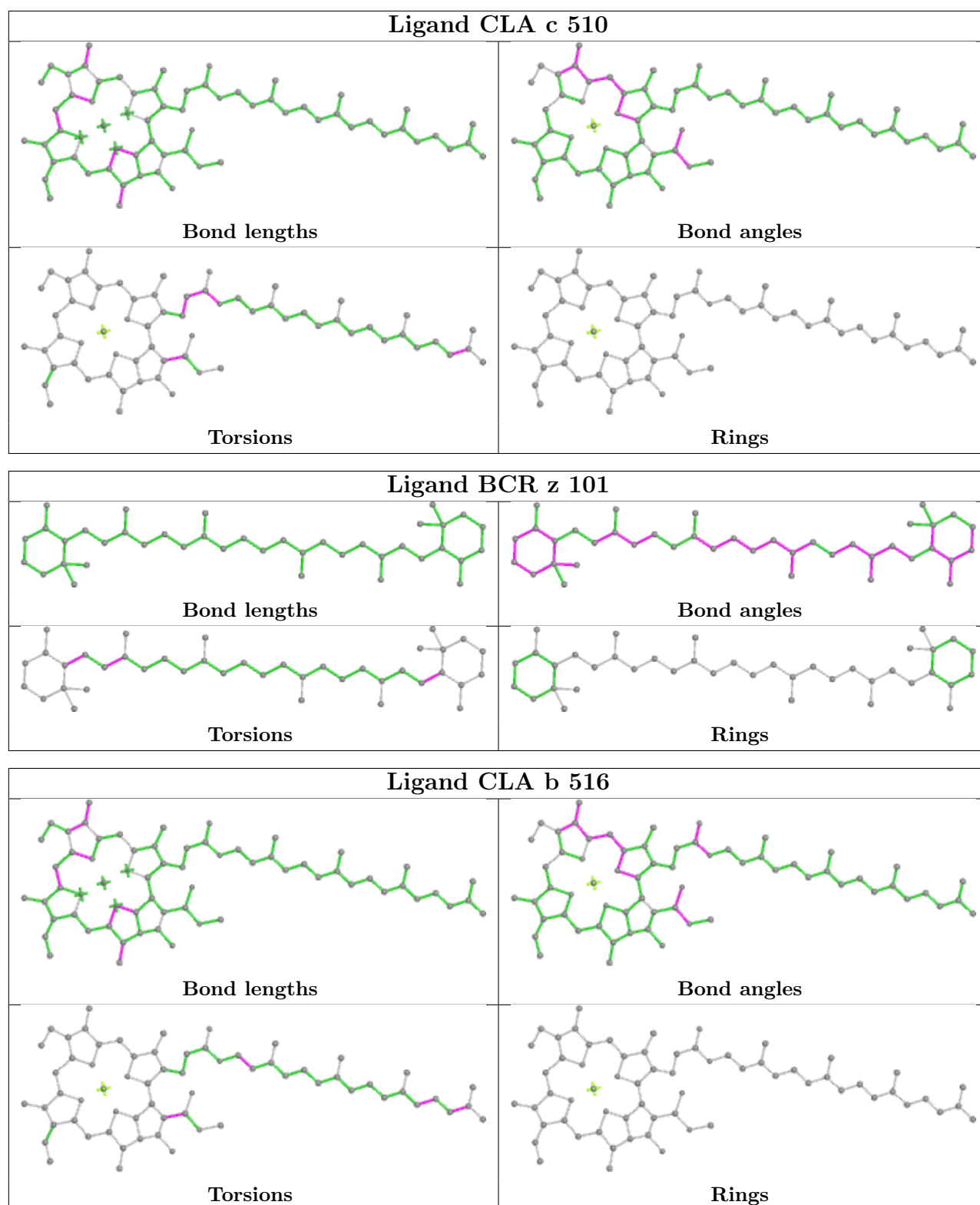
Ligand DGD C 520

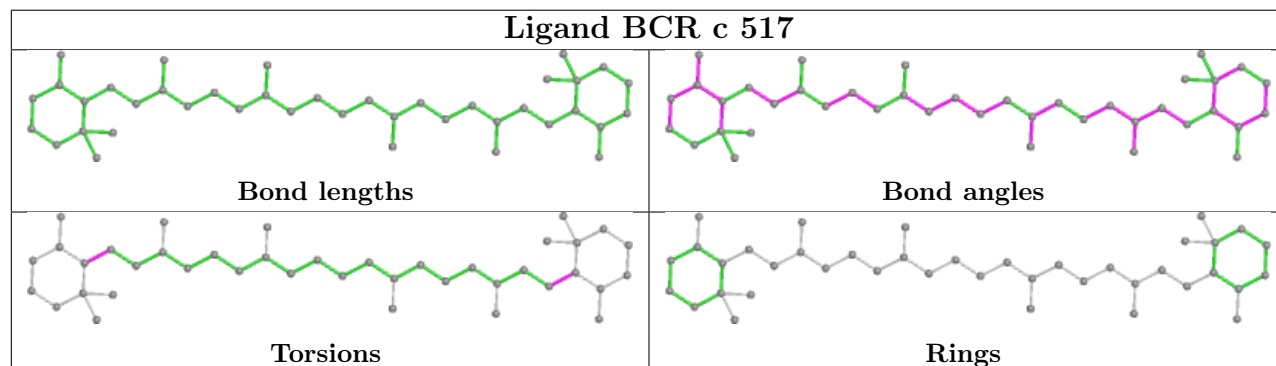
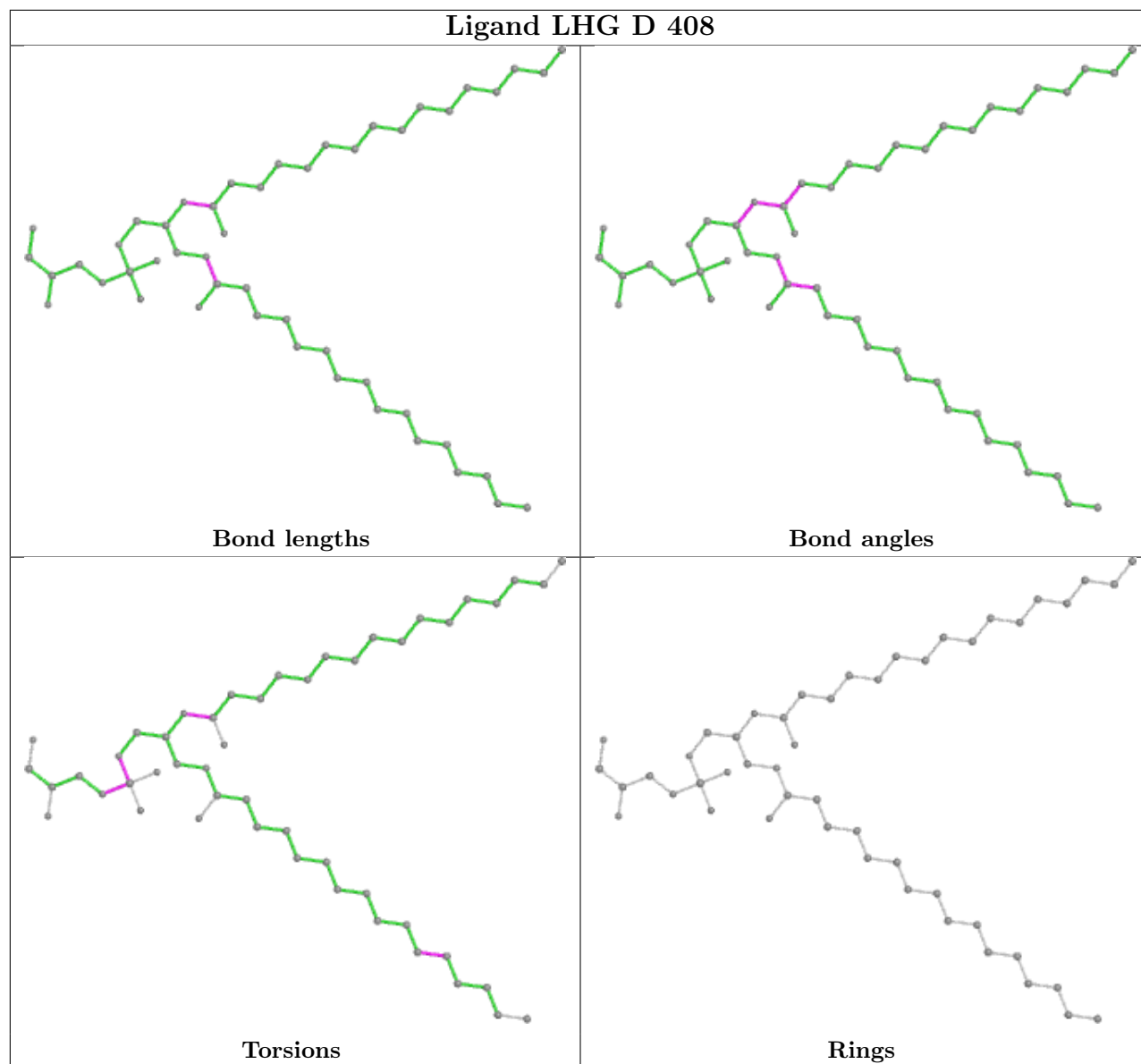


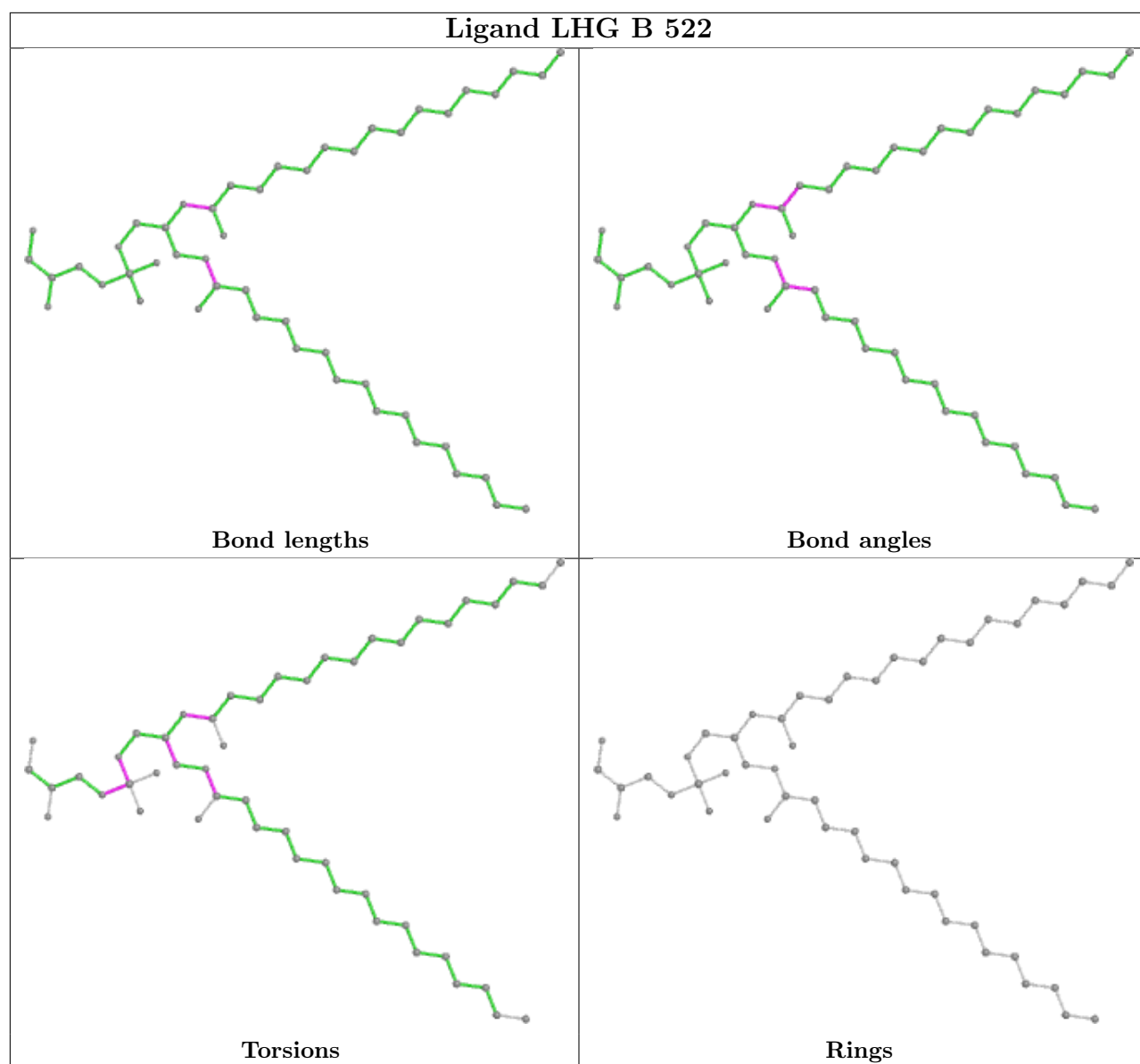


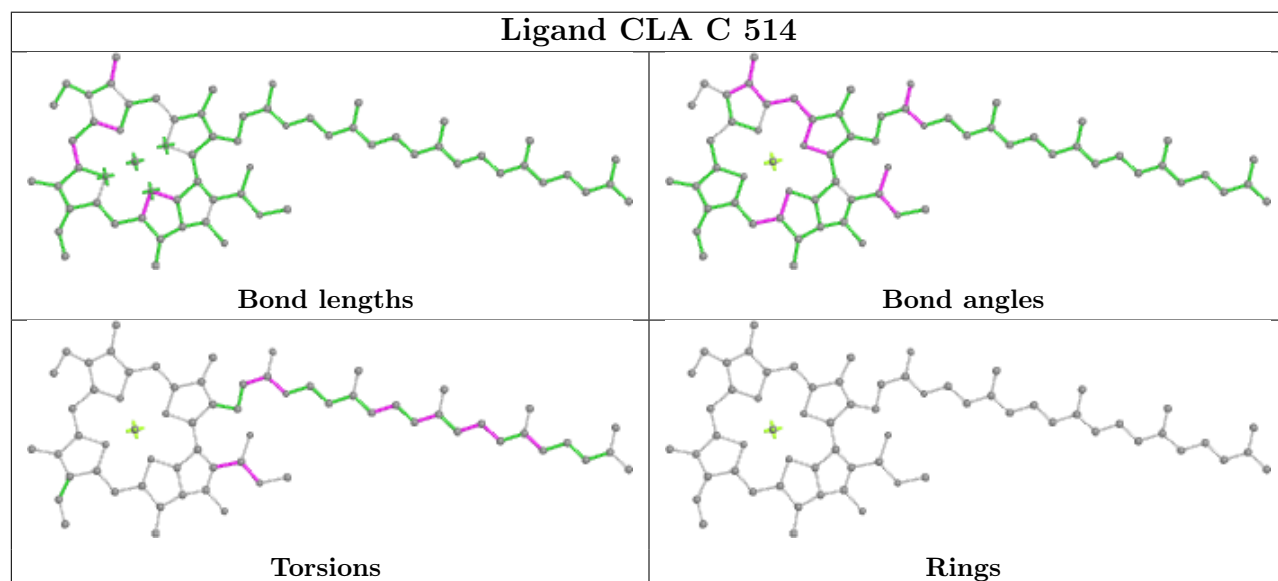
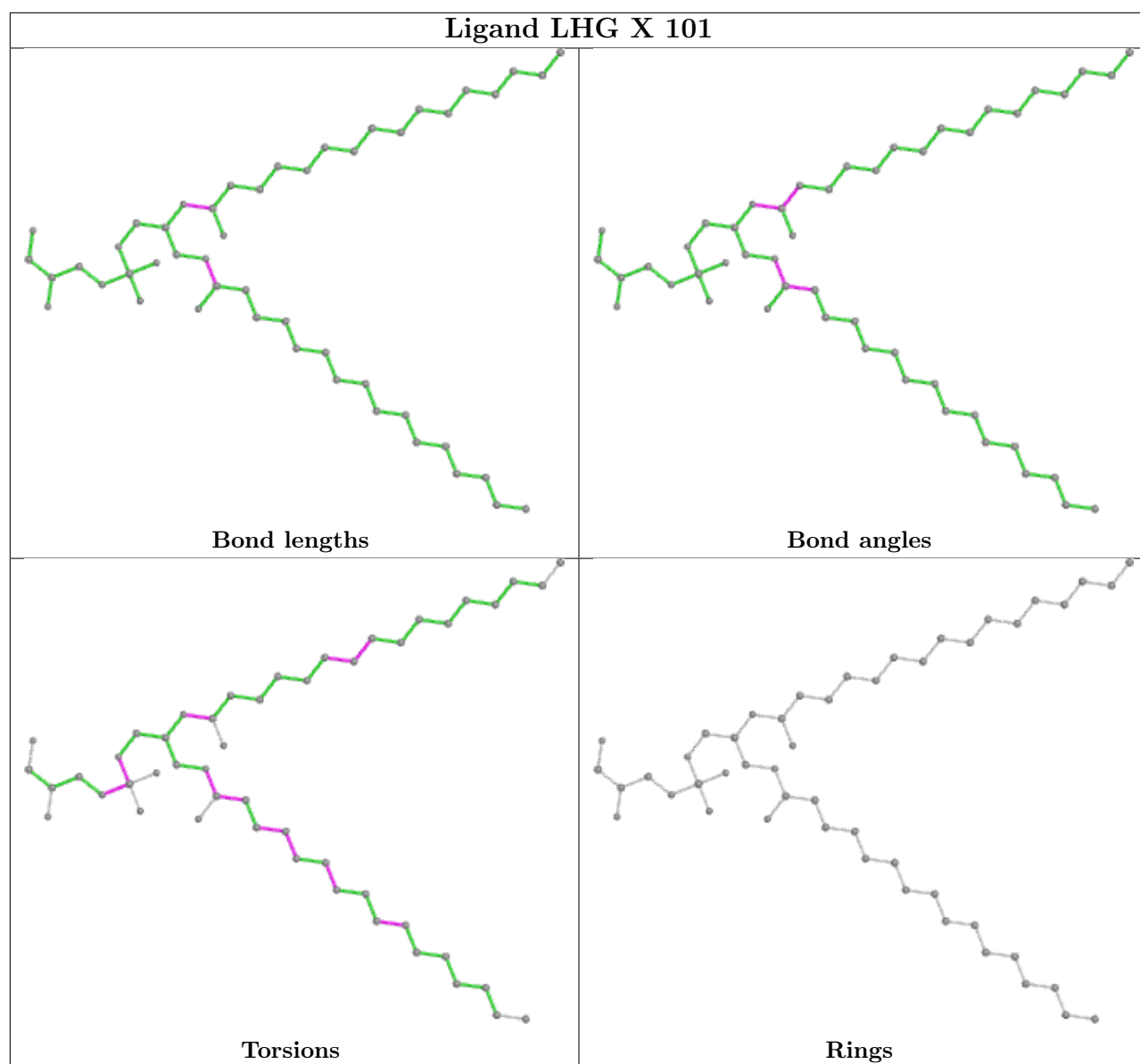












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

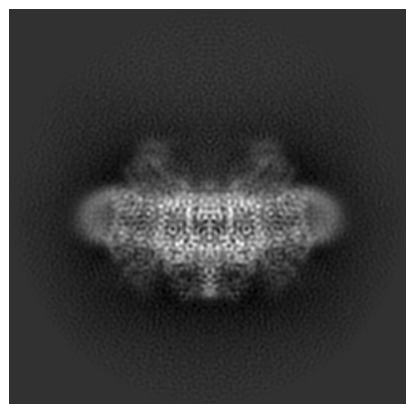
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60748. These allow visual inspection of the internal detail of the map and identification of artifacts.

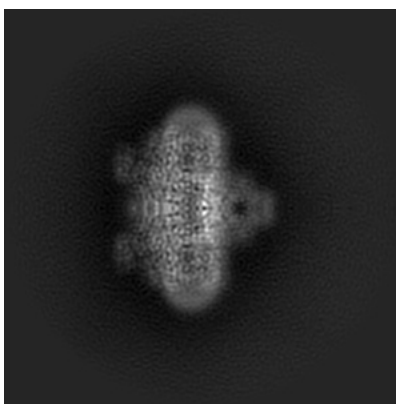
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

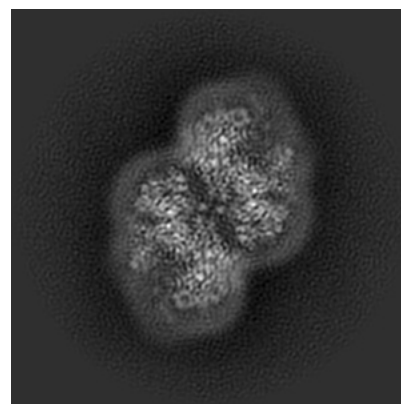
6.1.1 Primary map



X

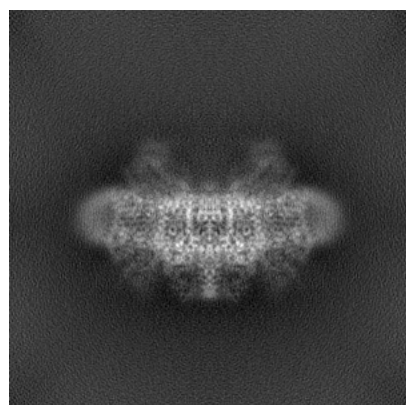


Y

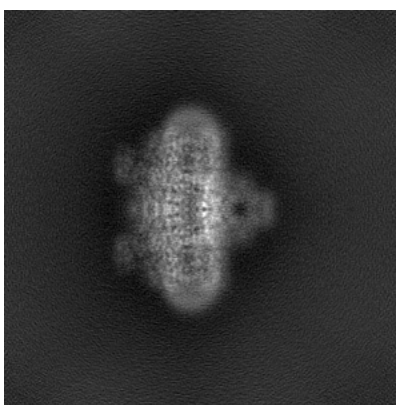


Z

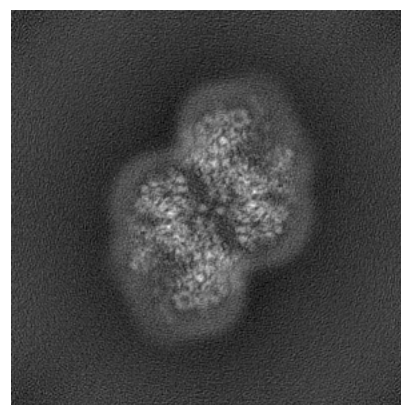
6.1.2 Raw map



X



Y

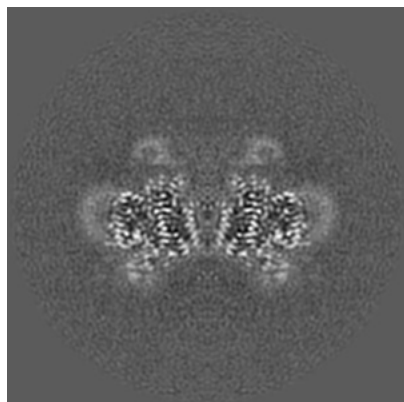


Z

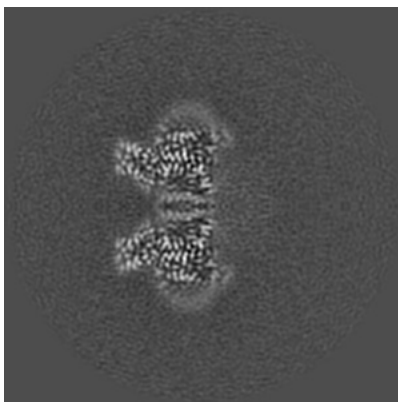
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

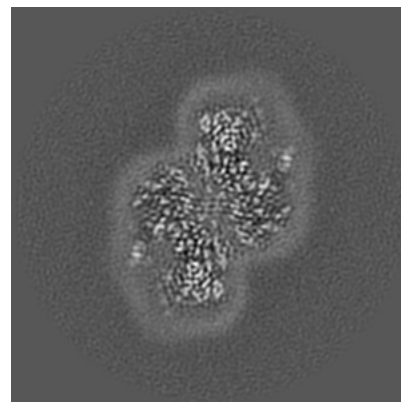
6.2.1 Primary map



X Index: 150

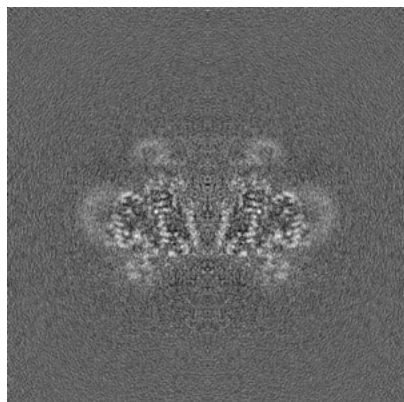


Y Index: 150

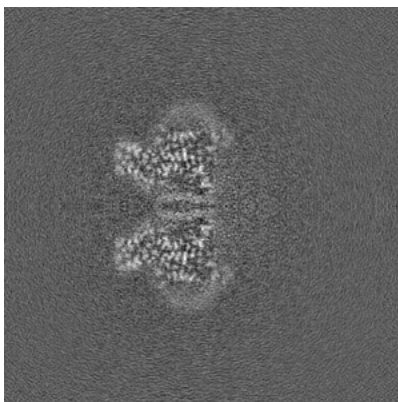


Z Index: 150

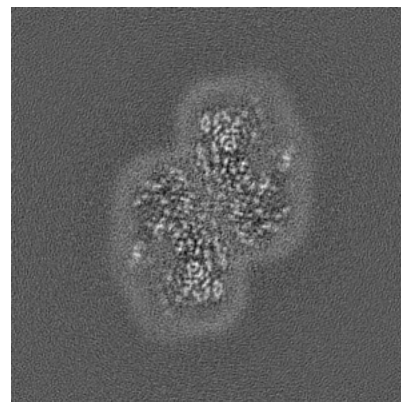
6.2.2 Raw map



X Index: 150



Y Index: 150

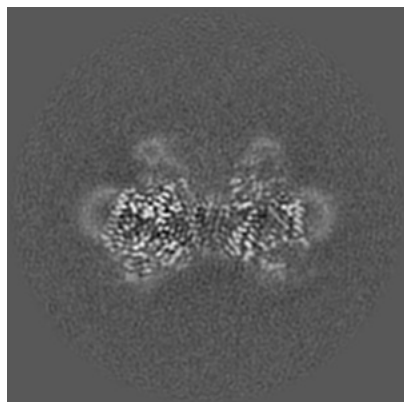


Z Index: 150

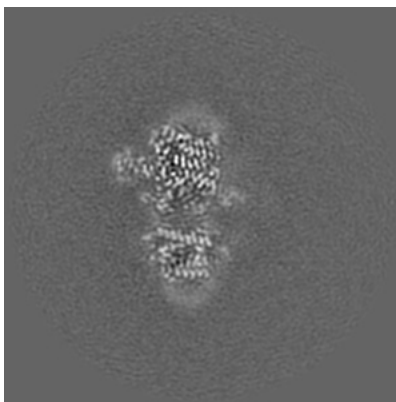
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

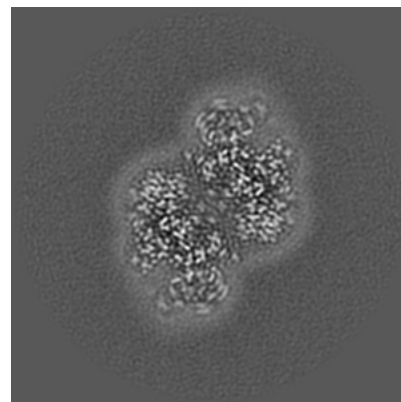
6.3.1 Primary map



X Index: 147

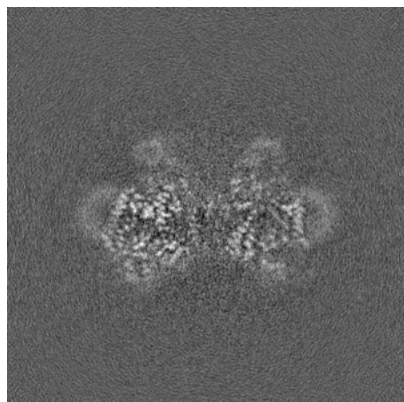


Y Index: 166

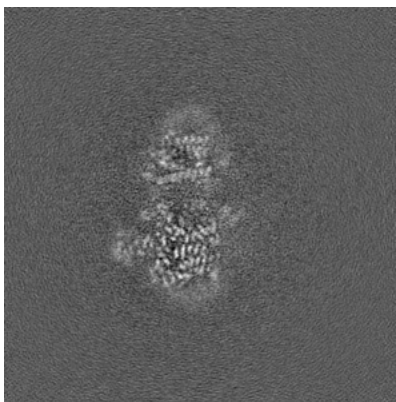


Z Index: 128

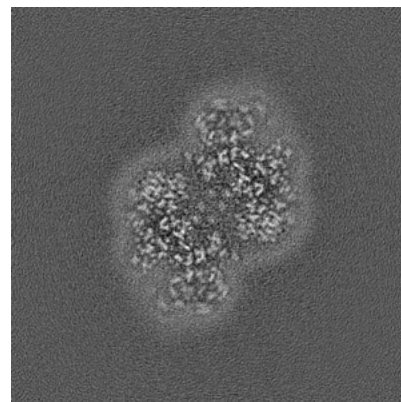
6.3.2 Raw map



X Index: 147



Y Index: 134

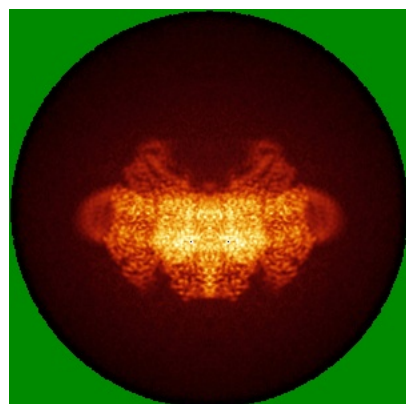


Z Index: 128

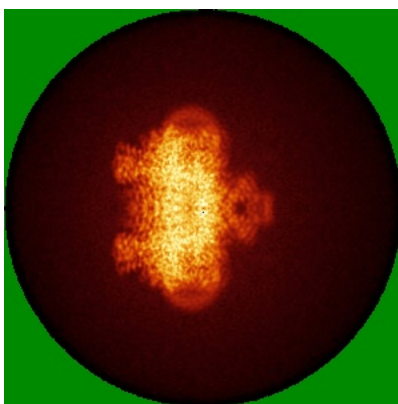
The images above show the largest variance slices of the map in three orthogonal directions.

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

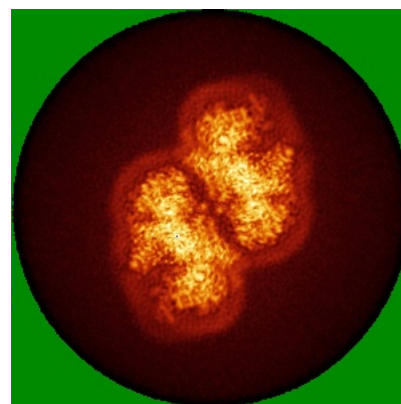
6.4.1 Primary map



X

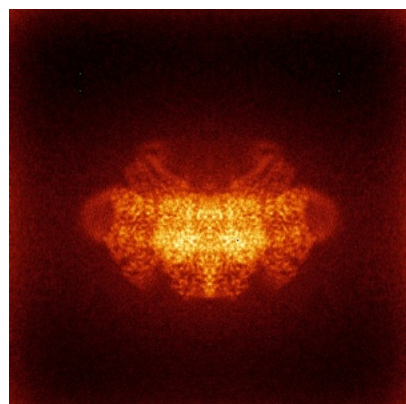


Y

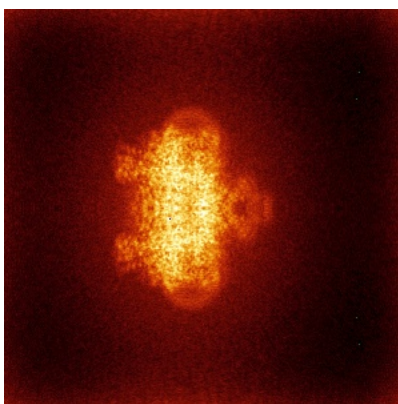


Z

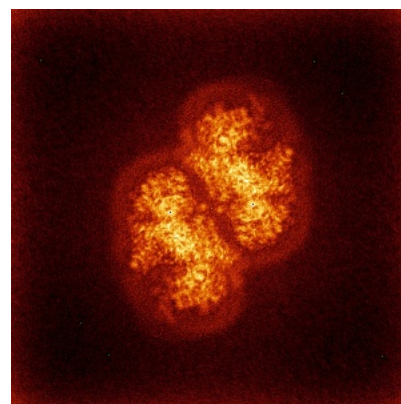
6.4.2 Raw map



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.

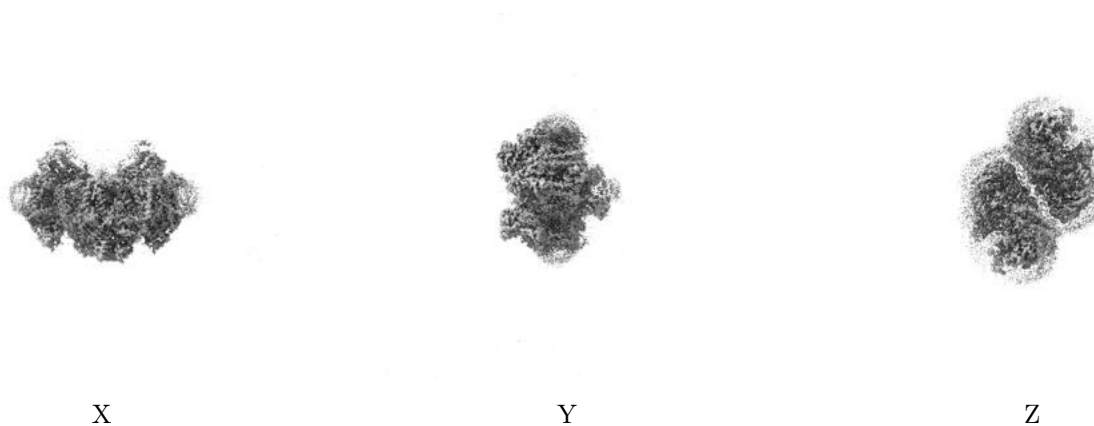
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.165. 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.

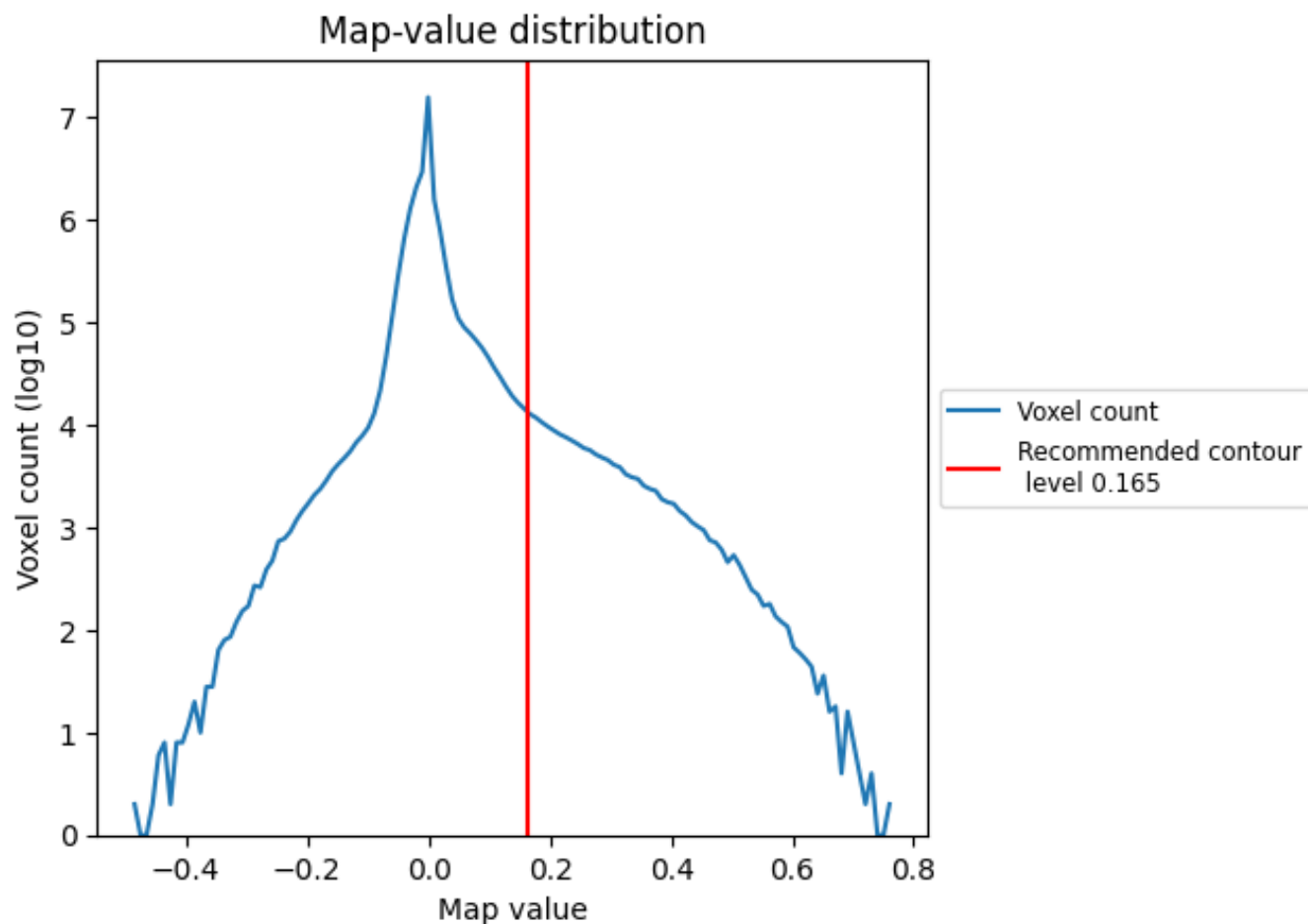
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

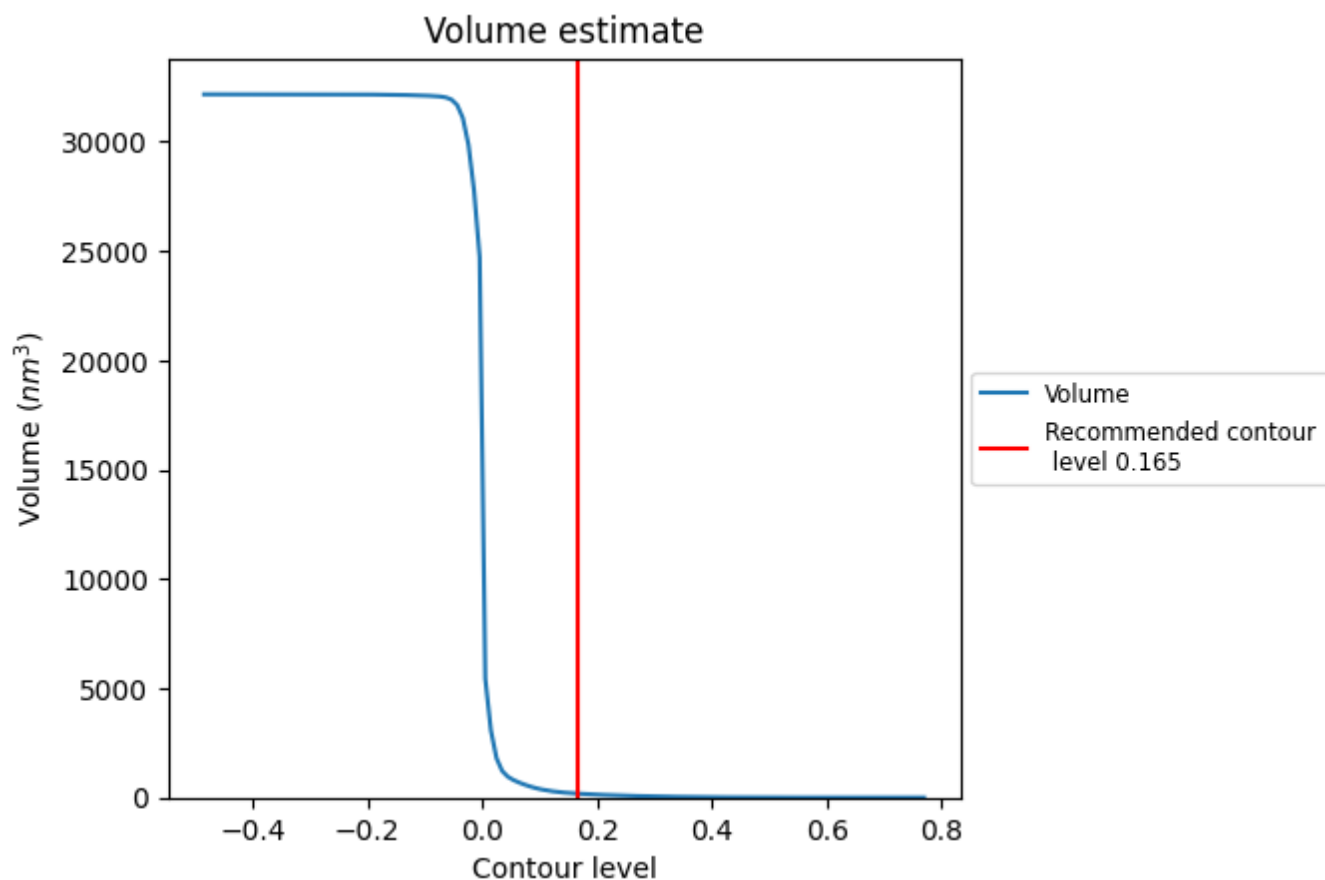
This section contains the results of statistical analysis of the map.

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.

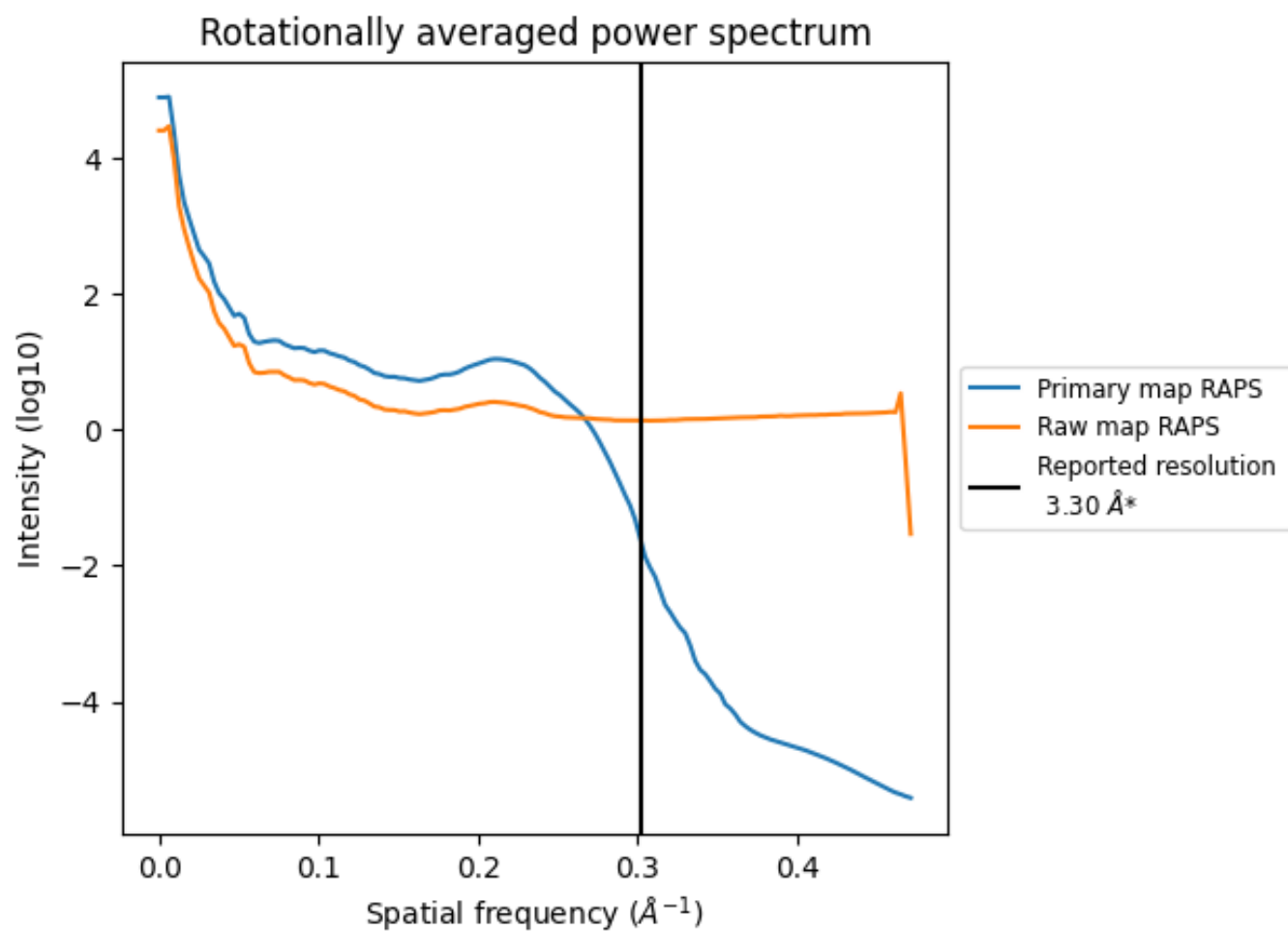
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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 ⓘ

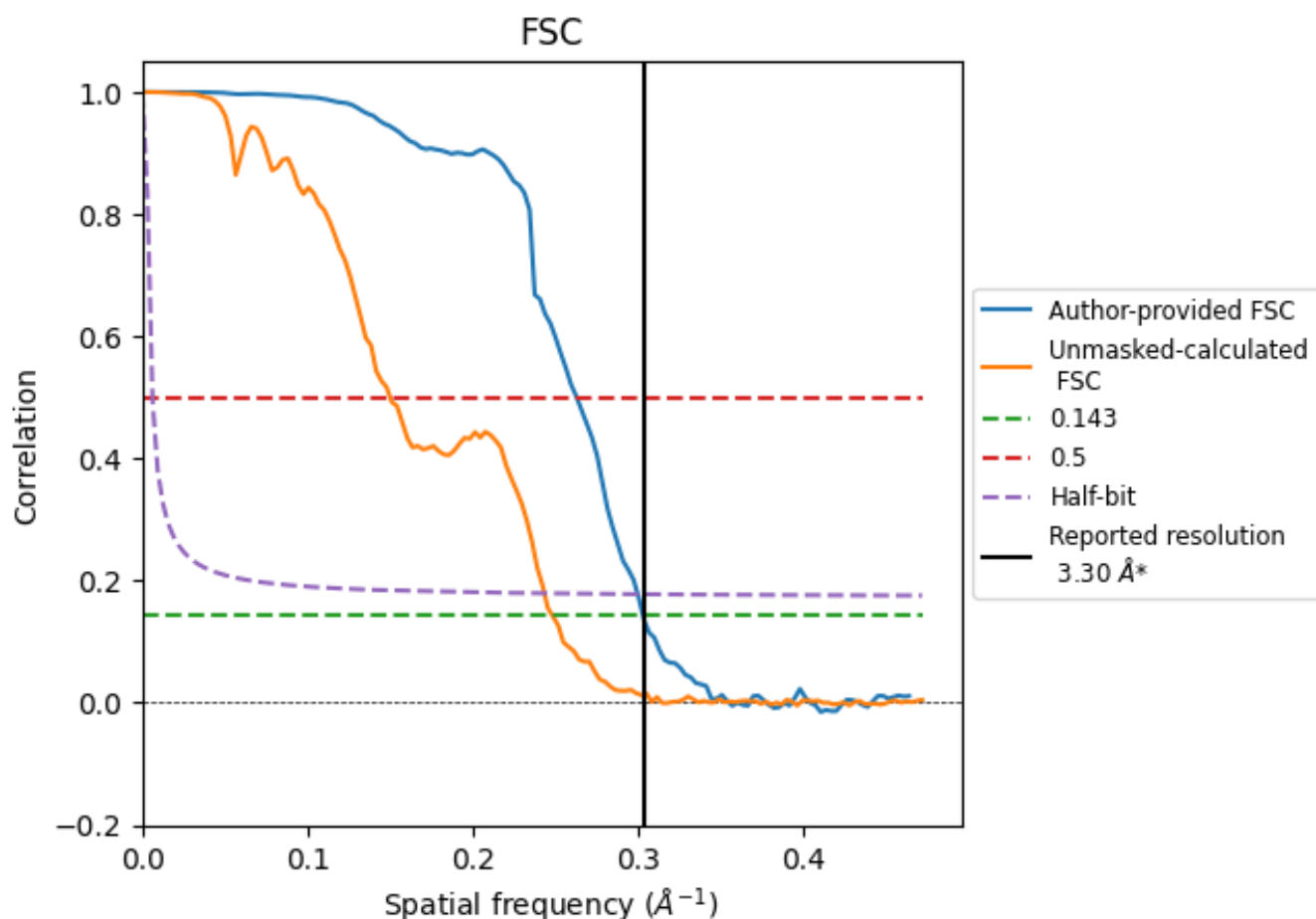


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

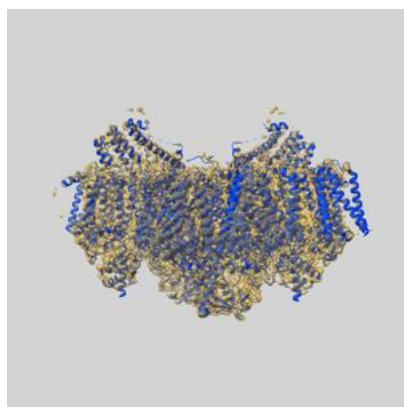
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.81	3.34
Unmasked-calculated*	4.03	6.67	4.11

*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 4.03 differs from the reported value 3.3 by more than 10 %

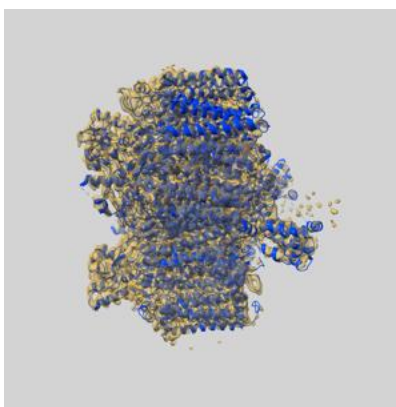
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60748 and PDB model 9IOX. Per-residue inclusion information can be found in section [3](#) on page [22](#).

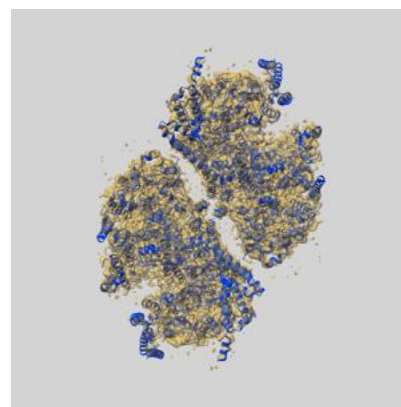
9.1 Map-model overlay [i](#)



X



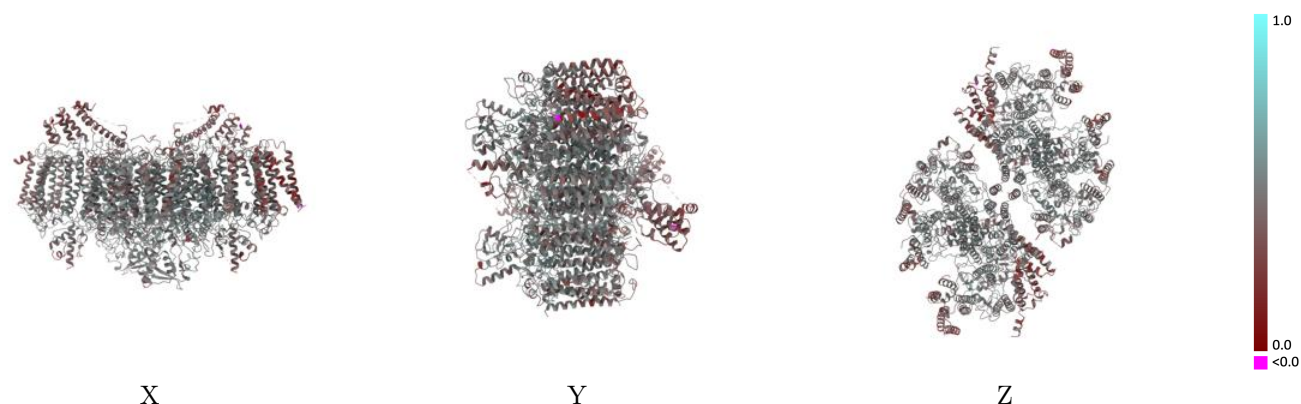
Y



Z

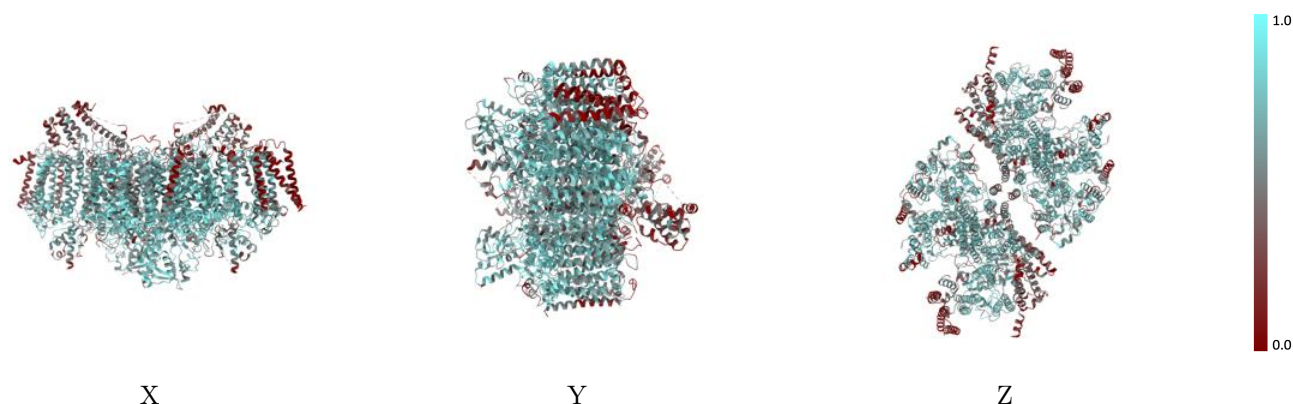
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



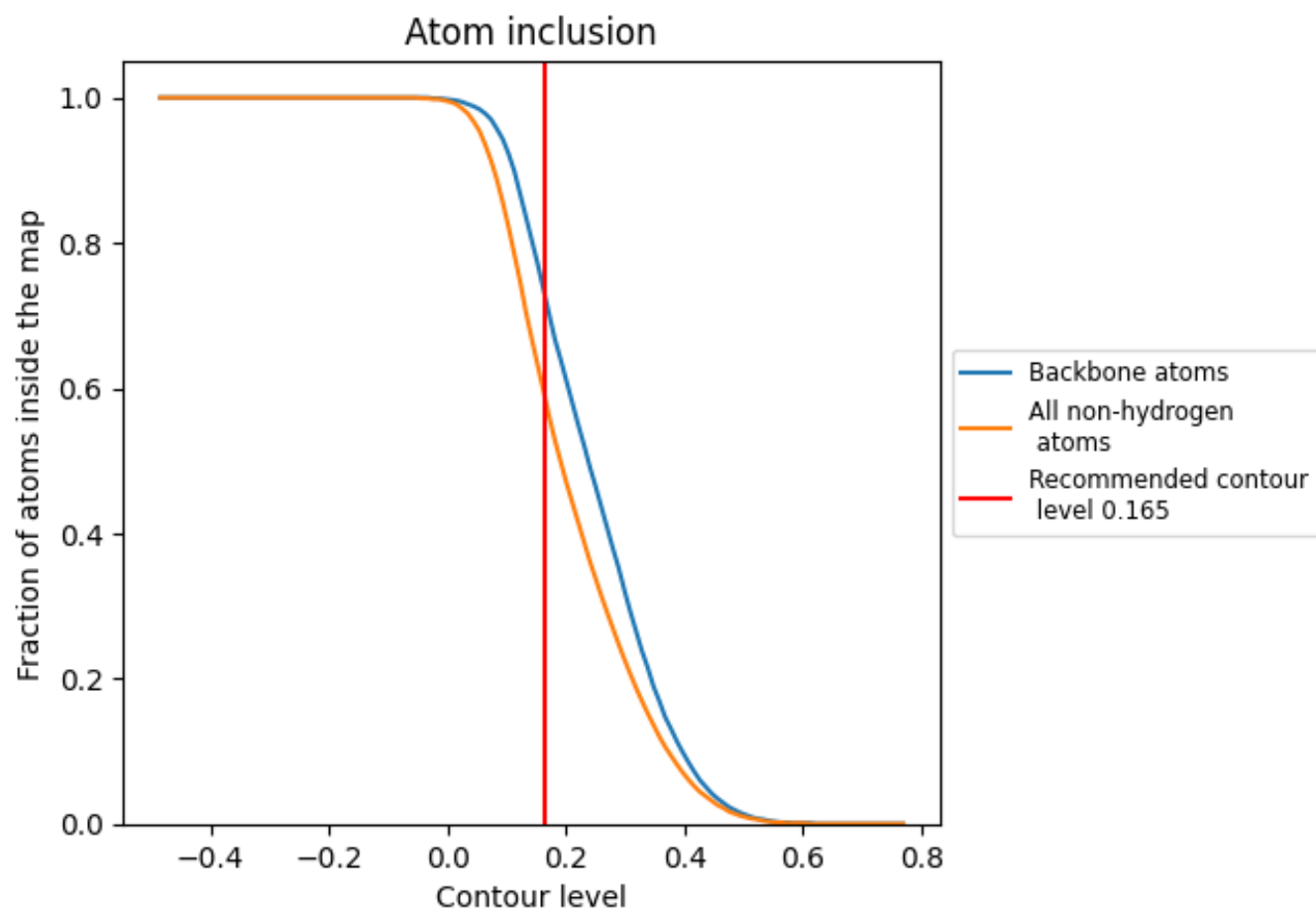
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.165).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 59% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.4630
A	 0.6460	 0.4890
B	 0.6580	 0.4850
C	 0.5900	 0.4630
D	 0.7080	 0.5100
E	 0.5470	 0.4150
F	 0.6250	 0.4380
G	 0.3550	 0.3560
H	 0.5530	 0.4260
I	 0.5510	 0.4500
K	 0.4230	 0.4270
L	 0.4920	 0.4720
M	 0.4330	 0.4330
T	 0.4560	 0.4420
V	 0.0930	 0.3270
X	 0.2470	 0.4050
Z	 0.0970	 0.2960
a	 0.6650	 0.4930
b	 0.6650	 0.4890
c	 0.5930	 0.4640
d	 0.7090	 0.5090
e	 0.5450	 0.4210
f	 0.6380	 0.4230
g	 0.3580	 0.3580
h	 0.5480	 0.4380
i	 0.5590	 0.4530
k	 0.4170	 0.4300
l	 0.4890	 0.4720
m	 0.4330	 0.4270
t	 0.4510	 0.4390
v	 0.0890	 0.3280
x	 0.2570	 0.4110
z	 0.0910	 0.2970

