



## wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 07:28 PM JST

PDB ID : 7CZL / pdb\_00007czl  
EMDB ID : EMD-30511  
Title : Structural insights into a dimeric Psb27-photosystem II complex from a cyanobacterium *Thermosynechococcus vulcanus*  
Authors : Pi, X.; Huang, G.; Xiao, Y.  
Deposited on : 2020-09-09  
Resolution : 3.78 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.42

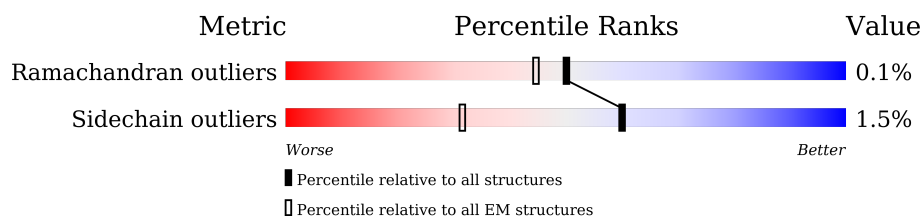
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.78 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)
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  $\geq 3$ , 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	324	99%
1	a	324	98%
2	B	505	95%
2	b	505	96%
3	C	446	8% 100%
3	c	446	7% 100%
4	D	339	100%
4	d	339	100%
5	E	65	12% 100%

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Mol	Chain	Length	Quality of chain
5	e	65	
6	F	31	
6	f	31	
7	H	62	
7	h	62	
8	I	34	
8	i	34	
9	K	37	
9	k	37	
10	L	37	
10	l	37	
11	M	33	
11	m	33	
12	T	30	
12	t	30	
13	Z	62	
13	z	62	
14	Y	30	
14	y	30	
15	N	108	
15	n	108	
16	X	40	
16	x	40	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	401	X	-	-	-
17	CLA	A	402	X	-	-	-
17	CLA	A	403	X	-	-	-
17	CLA	A	405	X	-	-	-
17	CLA	B	601	X	-	-	-
17	CLA	B	602	X	-	-	-
17	CLA	B	603	X	-	-	-
17	CLA	B	604	X	-	-	-
17	CLA	B	605	X	-	-	-
17	CLA	B	606	X	-	-	-
17	CLA	B	607	X	-	-	-
17	CLA	B	608	X	-	-	-
17	CLA	B	609	X	-	-	-
17	CLA	B	610	X	-	-	-
17	CLA	B	611	X	-	-	-
17	CLA	B	612	X	-	-	-
17	CLA	B	613	X	-	-	-
17	CLA	B	614	X	-	-	-
17	CLA	B	615	X	-	-	-
17	CLA	B	616	X	-	-	-
17	CLA	C	501	X	-	-	-
17	CLA	C	502	X	-	-	-
17	CLA	C	503	X	-	-	-
17	CLA	C	504	X	-	-	-
17	CLA	C	505	X	-	-	-
17	CLA	C	506	X	-	-	-
17	CLA	C	507	X	-	-	-
17	CLA	C	508	X	-	-	-
17	CLA	C	509	X	-	-	-
17	CLA	C	510	X	-	-	-
17	CLA	C	511	X	-	-	-
17	CLA	C	512	X	-	-	-
17	CLA	C	513	X	-	-	-
17	CLA	D	404	X	-	-	-
17	CLA	D	405	X	-	-	-
17	CLA	a	5402	X	-	-	-
17	CLA	a	5403	X	-	-	-
17	CLA	a	5404	X	-	-	-
17	CLA	a	5406	X	-	-	-
17	CLA	b	5601	X	-	-	-
17	CLA	b	5602	X	-	-	-
17	CLA	b	5603	X	-	-	-
17	CLA	b	5604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	b	5605	X	-	-	-
17	CLA	b	5606	X	-	-	-
17	CLA	b	5607	X	-	-	-
17	CLA	b	5608	X	-	-	-
17	CLA	b	5609	X	-	-	-
17	CLA	b	5610	X	-	-	-
17	CLA	b	5611	X	-	-	-
17	CLA	b	5612	X	-	-	-
17	CLA	b	5613	X	-	-	-
17	CLA	b	5614	X	-	-	-
17	CLA	b	5615	X	-	-	-
17	CLA	b	5616	X	-	-	-
17	CLA	c	5501	X	-	-	-
17	CLA	c	5502	X	-	-	-
17	CLA	c	5503	X	-	-	-
17	CLA	c	5504	X	-	-	-
17	CLA	c	5505	X	-	-	-
17	CLA	c	5506	X	-	-	-
17	CLA	c	5507	X	-	-	-
17	CLA	c	5508	X	-	-	-
17	CLA	c	5509	X	-	-	-
17	CLA	c	5510	X	-	-	-
17	CLA	c	5511	X	-	-	-
17	CLA	c	5512	X	-	-	-
17	CLA	d	5403	X	-	-	-
17	CLA	d	5404	X	-	-	-
17	CLA	k	5501	X	-	-	-

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 40859 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	324	Total	C	N	O	S	0	0
			2533	1662	414	442	15		
1	a	322	Total	C	N	O	S	0	0
			2523	1656	412	440	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
A	286	THR	ALA	conflict	UNP P51765
a	5279	PRO	ARG	conflict	UNP P51765
a	5286	THR	ALA	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3784	2488	628	655	13		
2	b	484	Total	C	N	O	S	0	0
			3780	2486	628	653	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	ARG	LYS	conflict	UNP D0VWR1
b	5506	ARG	LYS	conflict	UNP D0VWR1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	446	Total	C	N	O	S	0	0
			3412	2240	570	589	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	446	Total	C	N	O	S	0	0
			3412	2240	570	589	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	339	Total	C	N	O	S	0	0
			2693	1786	438	457	12		
4	d	339	Total	C	N	O	S	0	0
			2687	1783	435	457	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	65	Total	C	N	O	0	0
			522	345	81	96		
5	e	65	Total	C	N	O	0	0
			522	345	81	96		

- 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
			242	166	39	36	1		
6	f	28	Total	C	N	O	S	0	0
			219	149	36	33	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	62	Total	C	N	O	S	0	0
			482	324	75	81	2		
7	h	62	Total	C	N	O	S	0	0
			482	324	75	81	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total	C	N	O	S	0	0
			277	189	43	44	1		
8	i	34	Total	C	N	O	S	0	0
			277	189	43	44	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			289	201	42	46		
9	k	34	Total	C	N	O	0	0
			264	186	36	42		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	5033	LEU	PHE	conflict	UNP P19054
k	5039	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	37	Total	C	N	O	0	0
			301	200	48	53		
10	l	37	Total	C	N	O	0	0
			301	200	48	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	33	Total	C	N	O	S	0	0
			258	172	38	47	1		
11	m	33	Total	C	N	O	S	0	0
			258	172	38	47	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	5008	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	62	Total	C	N	O	S	0	0
			442	306	65	69	2		
13	z	62	Total	C	N	O	S	0	0
			442	306	65	69	2		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	29	Total	C	N	O	S	0	0
			215	142	37	33	3		
14	y	29	Total	C	N	O	S	0	0
			215	142	37	33	3		

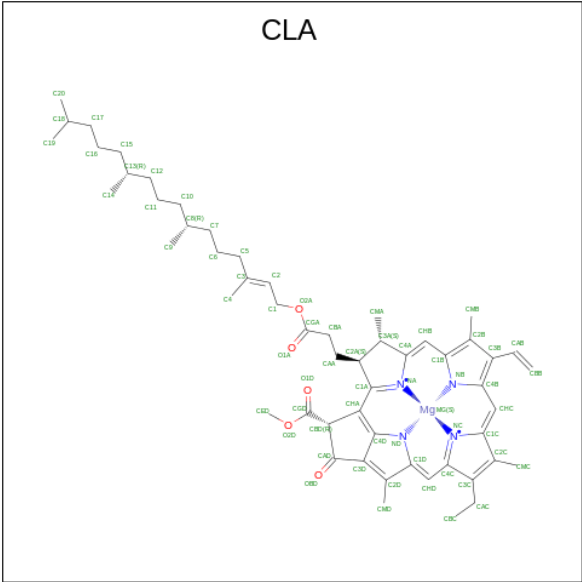
- Molecule 15 is a protein called Psb27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	n	108	Total	C	N	O	S	0	0
			860	536	155	167	2		
15	N	108	Total	C	N	O	S	0	0
			860	536	155	167	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	35	Total	C	N	O	0	0
			254	173	38	43		
16	x	35	Total	C	N	O	0	0
			254	173	38	43		

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	C	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	C	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	D	1	Total 50	C 40	Mg 1	N 4	O 5	0

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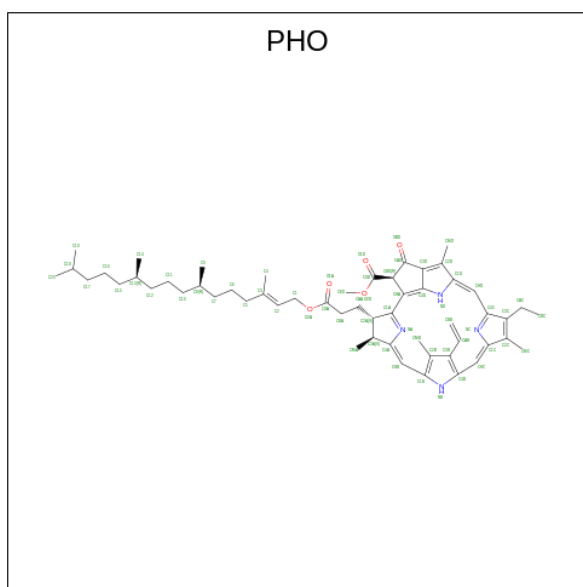
Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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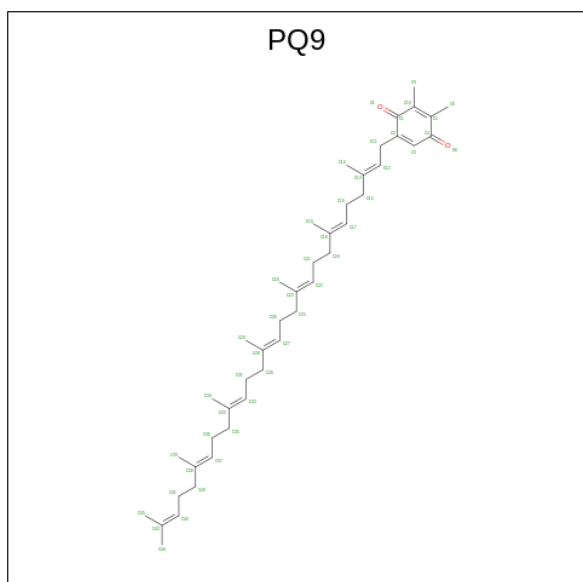
Mol	Chain	Residues	Atoms					AltConf
17	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 18 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



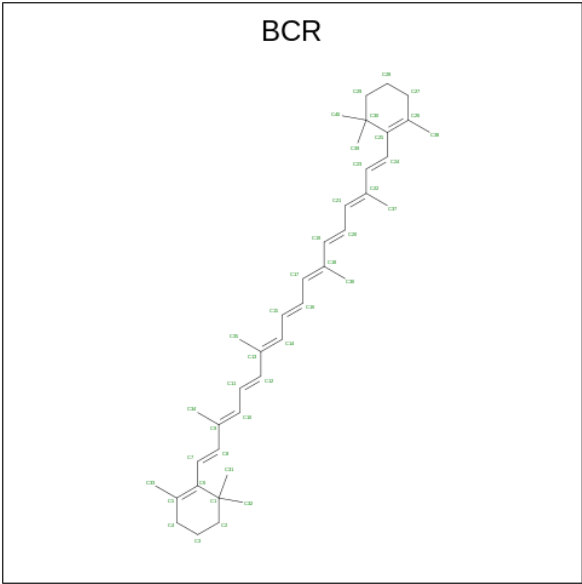
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	N	O	0
			64	55	4	5	
18	D	1	Total	C	N	O	0
			64	55	4	5	
18	a	1	Total	C	N	O	0
			64	55	4	5	
18	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 19 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula:  $C_{43}H_{64}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			45	43	2	
19	D	1	Total	C	O	0
			45	43	2	
19	a	1	Total	C	O	0
			30	28	2	
19	d	1	Total	C	O	0
			45	43	2	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
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	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	H	1	Total	C	0
			40	40	

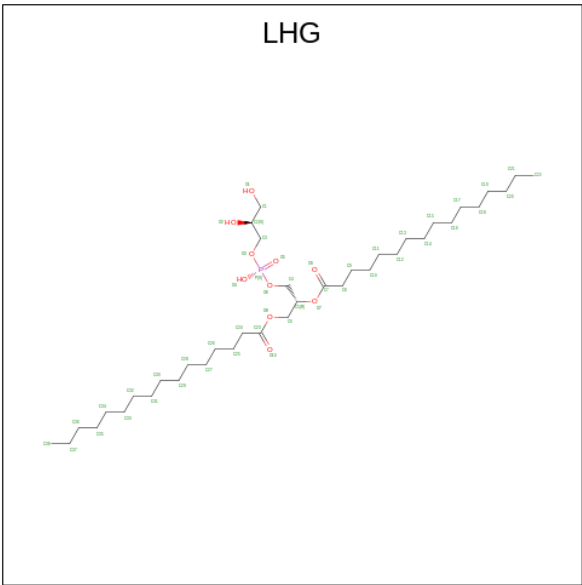
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Mol	Chain	Residues	Atoms	AltConf
20	T	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	d	1	Total C 40 40	0
20	h	1	Total C 40 40	0
20	k	1	Total C 40 40	0
20	t	1	Total C 40 40	0
20	t	1	Total C 40 40	0
20	z	1	Total C 40 40	0
20	Y	1	Total C 40 40	0

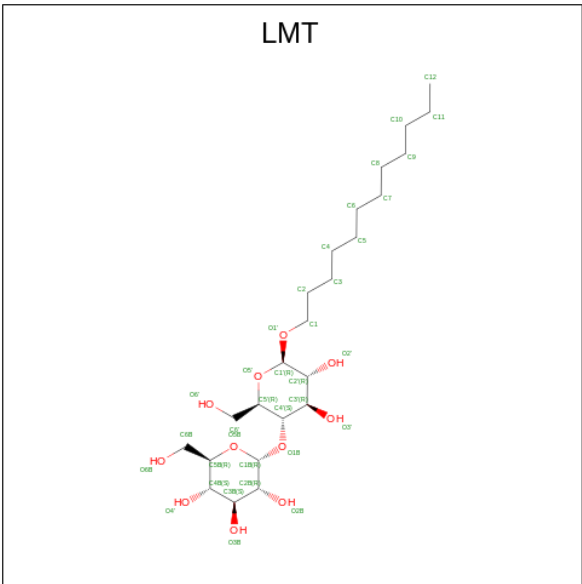
- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).





Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	O	P	0
			39	28	10	1	
21	a	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



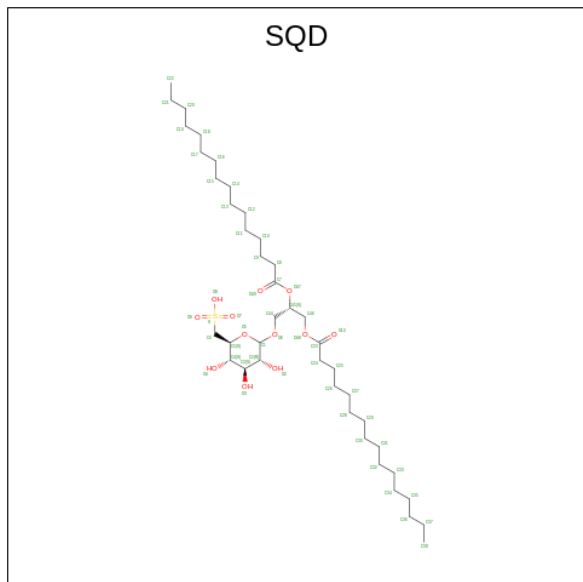
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			35	24	11	

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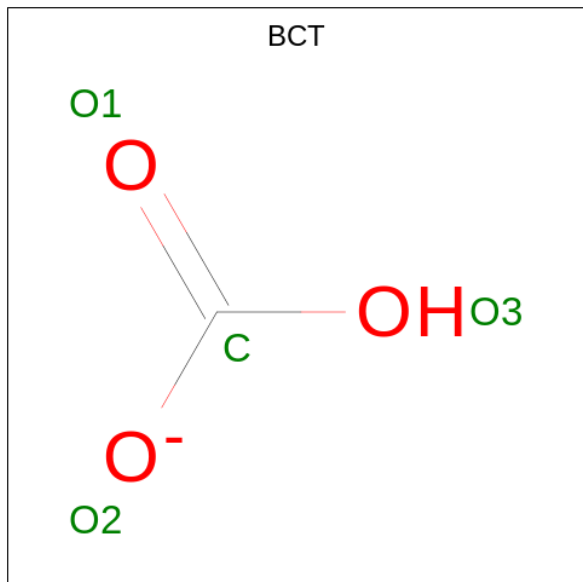
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			35	24	11	
22	M	1	Total	C	O	0
			35	24	11	
22	T	1	Total	C	O	0
			35	24	11	
22	a	1	Total	C	O	0
			35	24	11	
22	m	1	Total	C	O	0
			35	24	11	

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



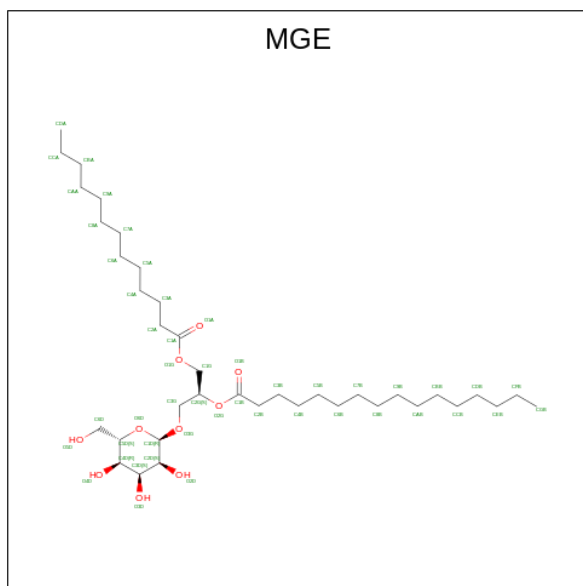
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	S	0
			26	13	12	1	
23	D	1	Total	C	O	S	0
			54	41	12	1	
23	L	1	Total	C	O	S	0
			47	34	12	1	
23	a	1	Total	C	O	S	0
			26	13	12	1	
23	d	1	Total	C	O	S	0
			54	41	12	1	
23	l	1	Total	C	O	S	0
			47	34	12	1	

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



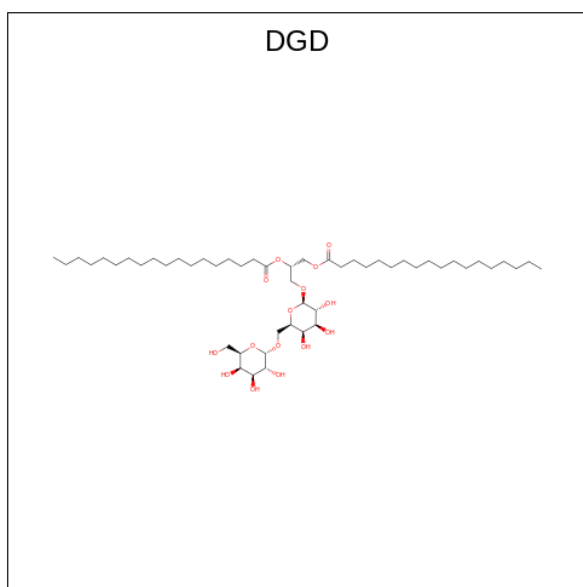
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			4	1	3	
24	a	1	Total	C	O	0
			4	1	3	

- Molecule 25 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula:  $\text{C}_{38}\text{H}_{72}\text{O}_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total 48	C 38	O 10	0
25	B	1	Total 48	C 38	O 10	0
25	C	1	Total 48	C 38	O 10	0
25	D	1	Total 47	C 37	O 10	0
25	D	1	Total 41	C 31	O 10	0
25	D	1	Total 48	C 38	O 10	0
25	b	1	Total 48	C 38	O 10	0
25	c	1	Total 48	C 38	O 10	0
25	d	1	Total 47	C 37	O 10	0
25	d	1	Total 41	C 31	O 10	0
25	d	1	Total 48	C 38	O 10	0
25	l	1	Total 48	C 38	O 10	0
25	m	1	Total 48	C 38	O 10	0
25	m	1	Total 48	C 38	O 10	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
26	C	1	Total	C	O	0
			53	38	15	
26	C	1	Total	C	O	0
			47	32	15	
26	C	1	Total	C	O	0
			57	42	15	
26	H	1	Total	C	O	0
			54	39	15	
26	a	1	Total	C	O	0
			57	42	15	
26	c	1	Total	C	O	0
			53	38	15	
26	c	1	Total	C	O	0
			47	32	15	
26	h	1	Total	C	O	0
			54	39	15	

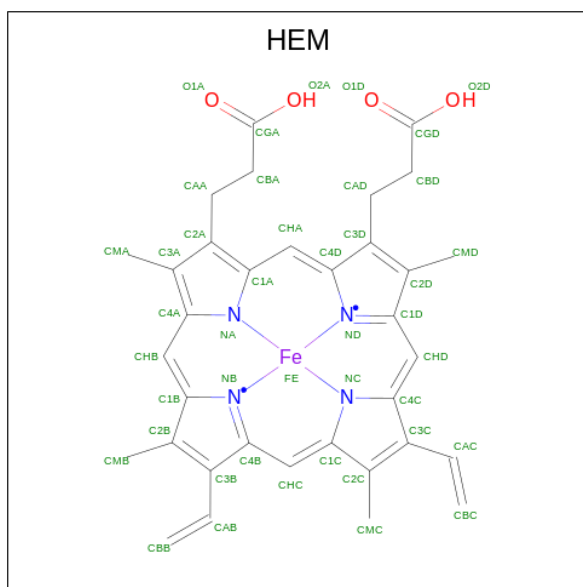
- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	C	1	Total	Ca	0
			1	1	
27	c	1	Total	Ca	0
			1	1	

- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
28	D	1	Total	Fe	0
			1	1	
28	d	1	Total	Fe	0
			1	1	

- Molecule 29 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

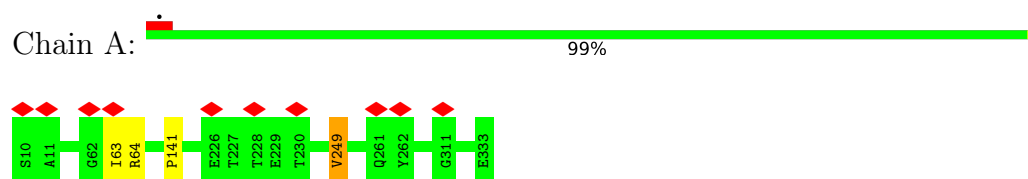
- Molecule 30 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
30	n	1	Total	Cl	0
			1	1	
30	N	1	Total	Cl	0
			1	1	

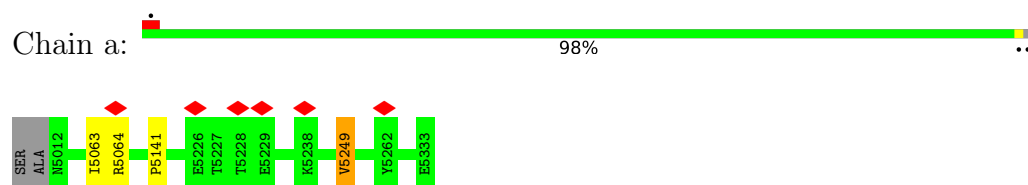
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

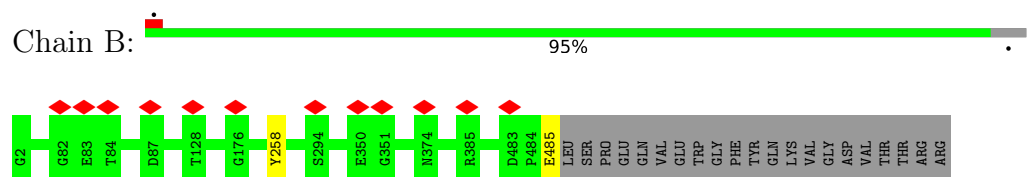
- Molecule 1: Photosystem II protein D1



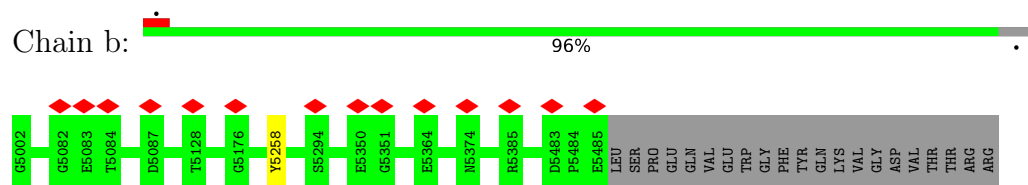
- Molecule 1: Photosystem II protein D1



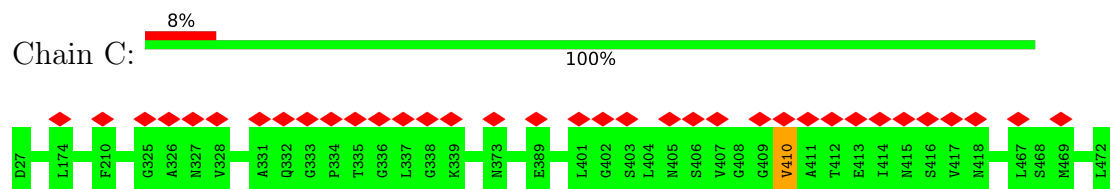
- Molecule 2: Photosystem II CP47 reaction center protein



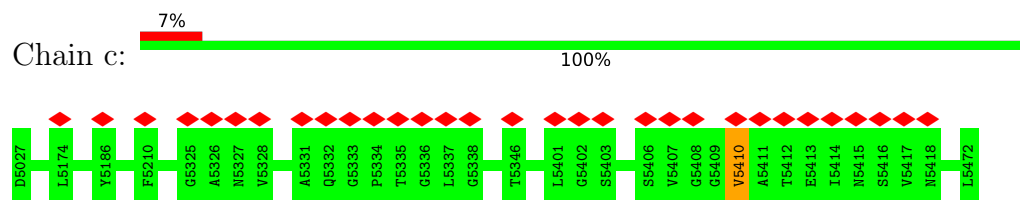
- Molecule 2: Photosystem II CP47 reaction center protein



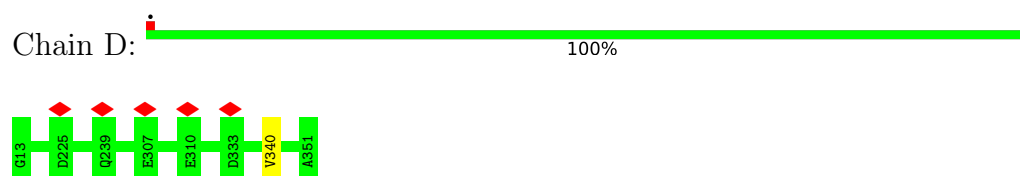
- Molecule 3: Photosystem II CP43 reaction center protein



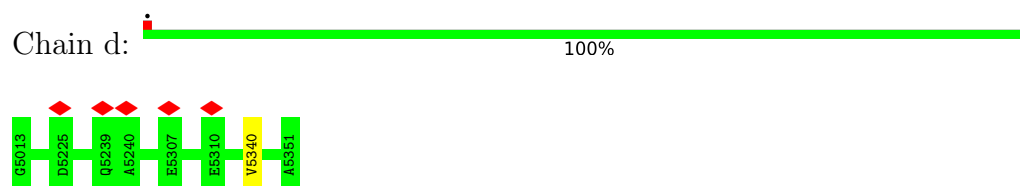
- Molecule 3: Photosystem II CP43 reaction center protein



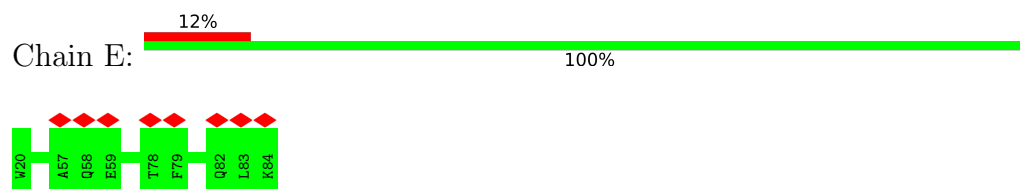
- Molecule 4: Photosystem II D2 protein



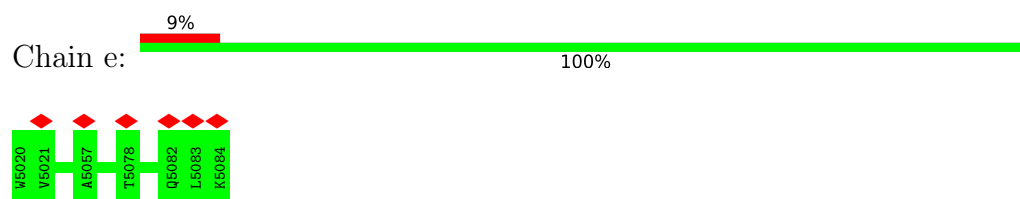
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

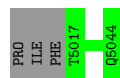
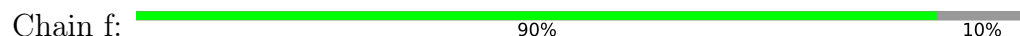


- Molecule 6: Cytochrome b559 subunit beta



There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome b559 subunit beta





- Molecule 7: Photosystem II reaction center protein H

Chain H:  100%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  100%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein I

Chain i:  100%


There are no outlier residues recorded for this chain.

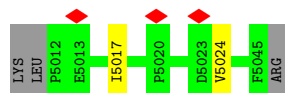
- Molecule 9: Photosystem II reaction center protein K

Chain K:  11% 95% 5%



- Molecule 9: Photosystem II reaction center protein K

Chain k:  8% 86% 5% 8%



- Molecule 10: Photosystem II reaction center protein L

Chain L:  5% 100%



- Molecule 10: Photosystem II reaction center protein L



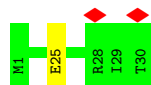
- Molecule 11: Photosystem II reaction center protein M



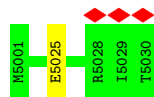
- Molecule 11: Photosystem II reaction center protein M



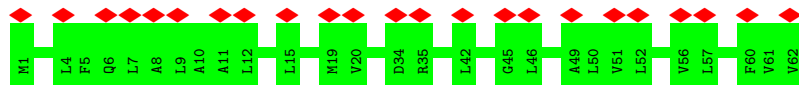
- Molecule 12: Photosystem II reaction center protein T



- Molecule 12: Photosystem II reaction center protein T

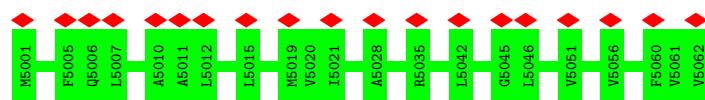


- Molecule 13: Photosystem II reaction center protein Z



- Molecule 13: Photosystem II reaction center protein Z

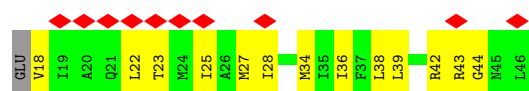




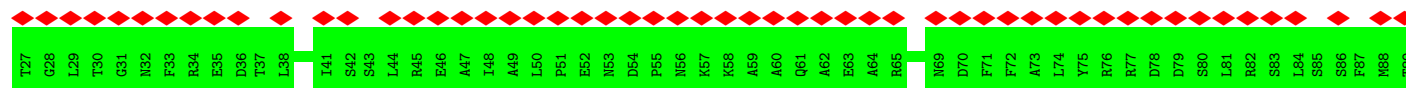
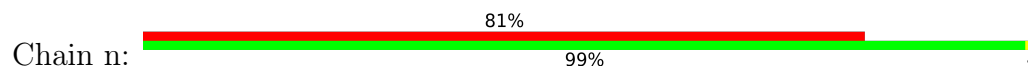
- Molecule 14: Photosystem II reaction center protein Ycf12



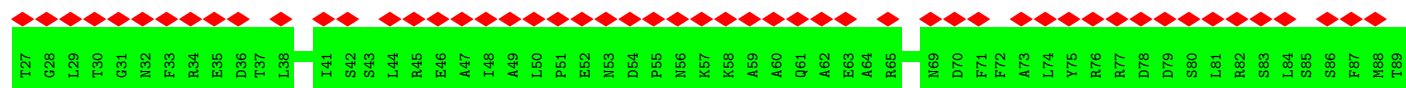
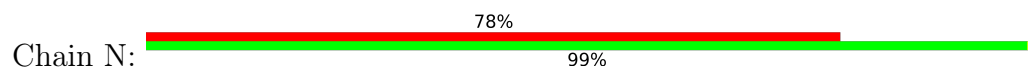
- Molecule 14: Photosystem II reaction center protein Ycf12



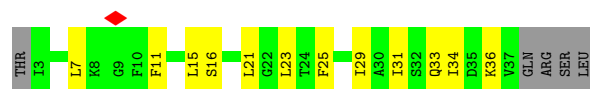
- Molecule 15: Psb27



- Molecule 15: Psb27



- Molecule 16: Photosystem II reaction center protein X



- Molecule 16: Photosystem II reaction center protein X



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.227	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.038	Depositor
Map size ( $\text{\AA}$ )	313.5696, 313.5696, 313.5696	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.30654, 1.30654, 1.30654	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BCT, FE2, HEM, CL, CLA, MGE, PQ9, DGD, BCR, LMT, PHO, LHG, SQD

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	0.53	1/2615 (0.0%)	0.56	1/3568 (0.0%)
1	a	0.52	1/2605 (0.0%)	0.54	1/3554 (0.0%)
2	B	0.54	1/3919 (0.0%)	0.54	0/5343
2	b	0.53	0/3915	0.54	1/5338 (0.0%)
3	C	0.47	0/3524	0.54	1/4804 (0.0%)
3	c	0.47	0/3524	0.54	1/4804 (0.0%)
4	D	0.56	1/2788 (0.0%)	0.55	0/3802
4	d	0.56	1/2782 (0.0%)	0.54	0/3795
5	E	0.42	0/538	0.51	0/737
5	e	0.42	0/538	0.51	0/737
6	F	0.37	0/250	0.47	0/342
6	f	0.37	0/225	0.46	0/308
7	H	0.44	0/495	0.52	0/678
7	h	0.44	0/495	0.52	0/678
8	I	0.49	0/284	0.48	0/384
8	i	0.48	0/284	0.48	0/384
9	K	0.43	0/299	0.52	0/412
9	k	0.44	0/274	0.52	0/379
10	L	0.49	0/308	0.53	0/419
10	l	0.50	0/308	0.53	0/419
11	M	0.46	0/261	0.55	0/356
11	m	0.46	0/261	0.53	0/356
12	T	0.57	0/263	0.51	0/356
12	t	0.57	0/263	0.51	0/356
13	Z	0.30	0/451	0.38	0/620
13	z	0.30	0/451	0.38	0/620
14	Y	0.21	0/216	0.40	0/289
14	y	0.30	0/216	0.87	1/289 (0.3%)
15	N	0.31	0/873	0.46	0/1172
15	n	0.30	0/873	0.44	0/1172
16	X	0.28	0/257	0.46	0/348
16	x	0.25	0/257	0.40	0/348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.49	5/34612 (0.0%)	0.53	6/47167 (0.0%)

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
1	A	0	2
1	a	0	2
9	K	0	2
9	k	0	2
14	y	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	VAL	CB-CG1	-6.56	1.39	1.52
2	B	258	TYR	CD2-CE2	-5.75	1.30	1.39
1	a	5249	VAL	CB-CG1	5.60	1.64	1.52
4	D	340	VAL	C-N	-5.60	1.21	1.34
4	d	5340	VAL	C-N	-5.58	1.21	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	VAL	CG1-CB-CG2	-9.95	94.98	110.90
14	y	28	ILE	C-N-CA	-8.60	104.23	122.30
3	c	5410	VAL	CG1-CB-CG2	-8.48	97.33	110.90
1	a	5249	VAL	CG1-CB-CG2	7.65	123.14	110.90
2	b	5258	TYR	CZ-CE2-CD2	-6.36	114.08	119.80

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	ILE	Mainchain
1	A	64	ARG	Peptide
9	K	17	ILE	Peptide
9	K	24	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	a	5063	ILE	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	322/324 (99%)	300 (93%)	21 (6%)	1 (0%)	37	68
1	a	320/324 (99%)	299 (93%)	20 (6%)	1 (0%)	37	68
2	B	482/505 (95%)	453 (94%)	29 (6%)	0	100	100
2	b	482/505 (95%)	452 (94%)	30 (6%)	0	100	100
3	C	444/446 (100%)	408 (92%)	36 (8%)	0	100	100
3	c	444/446 (100%)	408 (92%)	36 (8%)	0	100	100
4	D	337/339 (99%)	292 (87%)	45 (13%)	0	100	100
4	d	337/339 (99%)	293 (87%)	44 (13%)	0	100	100
5	E	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
5	e	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
6	F	29/31 (94%)	23 (79%)	6 (21%)	0	100	100
6	f	26/31 (84%)	22 (85%)	4 (15%)	0	100	100
7	H	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
7	h	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
8	I	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
8	i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
9	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	k	32/37 (86%)	31 (97%)	1 (3%)	0	100	100
10	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
11	m	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	T	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
12	t	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
13	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
13	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
14	Y	27/30 (90%)	23 (85%)	3 (11%)	1 (4%)	2	23
14	y	27/30 (90%)	24 (89%)	2 (7%)	1 (4%)	2	23
15	N	106/108 (98%)	92 (87%)	13 (12%)	1 (1%)	14	47
15	n	106/108 (98%)	94 (89%)	11 (10%)	1 (1%)	14	47
16	X	33/40 (82%)	31 (94%)	2 (6%)	0	100	100
16	x	33/40 (82%)	31 (94%)	2 (6%)	0	100	100
All	All	4240/4366 (97%)	3875 (91%)	359 (8%)	6 (0%)	50	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	Y	45	ASN
14	y	44	GLY
1	A	141	PRO
1	a	5141	PRO
15	n	124	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/262 (99%)	259 (100%)	1 (0%)	89	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	260/262 (99%)	259 (100%)	1 (0%)	89	93
2	B	379/403 (94%)	378 (100%)	1 (0%)	91	94
2	b	378/403 (94%)	378 (100%)	0	100	100
3	C	340/348 (98%)	339 (100%)	1 (0%)	91	94
3	c	340/348 (98%)	339 (100%)	1 (0%)	91	94
4	D	273/274 (100%)	273 (100%)	0	100	100
4	d	272/274 (99%)	272 (100%)	0	100	100
5	E	55/57 (96%)	55 (100%)	0	100	100
5	e	55/57 (96%)	55 (100%)	0	100	100
6	F	24/25 (96%)	24 (100%)	0	100	100
6	f	22/25 (88%)	22 (100%)	0	100	100
7	H	50/53 (94%)	50 (100%)	0	100	100
7	h	50/53 (94%)	50 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
8	i	31/31 (100%)	31 (100%)	0	100	100
9	K	29/30 (97%)	29 (100%)	0	100	100
9	k	27/30 (90%)	27 (100%)	0	100	100
10	L	34/35 (97%)	34 (100%)	0	100	100
10	l	34/35 (97%)	34 (100%)	0	100	100
11	M	30/30 (100%)	30 (100%)	0	100	100
11	m	30/30 (100%)	30 (100%)	0	100	100
12	T	26/27 (96%)	25 (96%)	1 (4%)	28	53
12	t	26/27 (96%)	25 (96%)	1 (4%)	28	53
13	Z	43/52 (83%)	43 (100%)	0	100	100
13	z	43/52 (83%)	43 (100%)	0	100	100
14	Y	22/23 (96%)	11 (50%)	11 (50%)	0	0
14	y	22/23 (96%)	12 (54%)	10 (46%)	0	0
15	N	92/92 (100%)	92 (100%)	0	100	100
15	n	92/92 (100%)	92 (100%)	0	100	100
16	X	28/33 (85%)	16 (57%)	12 (43%)	0	0
16	x	28/33 (85%)	16 (57%)	12 (43%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3426/3550 (96%)	3374 (98%)	52 (2%)	60 75

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	X	7	LEU
16	X	29	ILE
16	x	34	ILE
16	X	11	PHE
16	X	21	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
9	k	5040	GLN
10	l	5008	GLN
15	n	91	GLN
5	E	23	HIS
4	D	292	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 6 are monoatomic - leaving 140 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
20	BCR	C	514	-	41,41,41	1.29	3 (7%)	56,56,56	1.39	9 (16%)
23	SQD	D	403	-	53,54,54	1.00	5 (9%)	62,65,65	1.54	11 (17%)
20	BCR	c	5514	-	41,41,41	1.35	3 (7%)	56,56,56	1.40	9 (16%)
19	PQ9	A	406	-	45,45,45	0.68	1 (2%)	56,57,57	1.60	15 (26%)
17	CLA	C	506	-	65,73,73	1.43	10 (15%)	76,113,113	1.38	8 (10%)
23	SQD	a	5401	-	25,26,54	1.35	4 (16%)	34,37,65	1.89	7 (20%)
17	CLA	B	608	-	65,73,73	1.47	11 (16%)	76,113,113	1.51	7 (9%)
26	DGD	C	517	3,1	54,54,67	1.20	7 (12%)	68,68,81	1.42	8 (11%)
17	CLA	B	601	20	41,49,73	1.72	8 (19%)	47,84,113	1.66	7 (14%)
26	DGD	c	5515	3	54,54,67	1.20	7 (12%)	68,68,81	1.43	8 (11%)
26	DGD	h	5102	7,2	55,55,67	1.00	3 (5%)	69,69,81	1.49	7 (10%)
29	HEM	F	101	6	41,50,50	1.54	3 (7%)	45,82,82	1.12	2 (4%)
17	CLA	B	609	-	65,73,73	1.47	10 (15%)	76,113,113	1.40	9 (11%)
20	BCR	d	5406	-	41,41,41	1.27	3 (7%)	56,56,56	1.28	7 (12%)
24	BCT	a	5412	28	2,3,3	1.38	0	2,3,3	4.05	2 (100%)
23	SQD	l	5102	-	46,47,54	1.02	5 (10%)	55,58,65	1.72	13 (23%)
22	LMT	m	5102	-	36,36,36	1.18	5 (13%)	47,47,47	1.10	2 (4%)
17	CLA	B	612	-	65,73,73	1.44	11 (16%)	76,113,113	1.54	8 (10%)
21	LHG	a	5409	-	38,38,48	0.76	1 (2%)	41,44,54	1.24	5 (12%)
17	CLA	c	5509	-	47,55,73	1.69	10 (21%)	54,91,113	1.50	9 (16%)
26	DGD	H	102	7,4	55,55,67	1.00	3 (5%)	69,69,81	1.50	7 (10%)
17	CLA	b	5616	-	65,73,73	1.47	12 (18%)	76,113,113	1.46	8 (10%)
20	BCR	A	407	-	41,41,41	1.36	3 (7%)	56,56,56	1.37	9 (16%)
17	CLA	b	5613	-	65,73,73	1.47	13 (20%)	76,113,113	1.52	9 (11%)
17	CLA	c	5505	-	65,73,73	1.44	10 (15%)	76,113,113	1.49	9 (11%)
17	CLA	A	403	-	65,73,73	1.46	11 (16%)	76,113,113	1.46	9 (11%)
21	LHG	A	408	-	38,38,48	0.76	1 (2%)	41,44,54	1.25	5 (12%)
25	MGE	m	5101	-	48,48,48	0.94	2 (4%)	56,56,56	1.13	4 (7%)
17	CLA	a	5402	-	65,73,73	1.48	11 (16%)	76,113,113	1.39	8 (10%)
23	SQD	L	101	-	46,47,54	1.03	6 (13%)	55,58,65	1.63	11 (20%)
17	CLA	D	405	-	50,58,73	1.63	10 (20%)	58,95,113	1.51	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	b	5615	-	65,73,73	1.46	11 (16%)	76,113,113	1.46	7 (9%)
17	CLA	C	503	17	65,73,73	1.44	10 (15%)	76,113,113	1.48	10 (13%)
18	PHO	d	5402	-	51,69,69	1.21	7 (13%)	47,99,99	1.20	6 (12%)
17	CLA	C	513	-	50,58,73	1.60	9 (18%)	58,95,113	1.54	9 (15%)
17	CLA	A	401	-	65,73,73	1.48	11 (16%)	76,113,113	1.39	9 (11%)
17	CLA	c	5510	-	65,73,73	1.48	10 (15%)	76,113,113	1.39	8 (10%)
22	LMT	B	620	-	36,36,36	1.20	5 (13%)	47,47,47	0.95	1 (2%)
17	CLA	c	5503	17	65,73,73	1.43	10 (15%)	76,113,113	1.47	10 (13%)
22	LMT	T	101	12,2	36,36,36	1.10	4 (11%)	47,47,47	1.00	1 (2%)
17	CLA	B	607	-	65,73,73	1.43	10 (15%)	76,113,113	1.51	7 (9%)
23	SQD	d	5407	-	53,54,54	0.99	5 (9%)	62,65,65	1.64	11 (17%)
25	MGE	B	619	-	48,48,48	0.94	2 (4%)	56,56,56	1.14	4 (7%)
25	MGE	d	5408	-	47,47,48	0.97	2 (4%)	55,55,56	1.13	3 (5%)
17	CLA	a	5404	-	65,73,73	1.46	11 (16%)	76,113,113	1.45	9 (11%)
20	BCR	t	5102	-	41,41,41	1.29	3 (7%)	56,56,56	1.22	7 (12%)
25	MGE	A	412	25	48,48,48	0.91	2 (4%)	56,56,56	1.23	5 (8%)
17	CLA	c	5507	-	65,73,73	1.46	11 (16%)	76,113,113	1.44	9 (11%)
25	MGE	D	409	-	41,41,48	1.01	2 (4%)	49,49,56	1.44	8 (16%)
17	CLA	B	606	-	65,73,73	1.43	11 (16%)	76,113,113	1.48	8 (10%)
17	CLA	c	5506	-	65,73,73	1.44	10 (15%)	76,113,113	1.38	8 (10%)
25	MGE	l	5101	-	48,48,48	0.92	2 (4%)	56,56,56	1.23	5 (8%)
17	CLA	b	5606	-	42,50,73	1.75	11 (26%)	48,85,113	1.78	9 (18%)
17	CLA	b	5601	20	41,49,73	1.72	7 (17%)	47,84,113	1.66	7 (14%)
22	LMT	M	101	-	36,36,36	1.26	7 (19%)	47,47,47	1.09	1 (2%)
17	CLA	a	5403	-	65,73,73	1.49	11 (16%)	76,113,113	1.54	8 (10%)
17	CLA	c	5504	-	46,54,73	1.70	10 (21%)	53,90,113	1.56	7 (13%)
20	BCR	T	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.31	7 (12%)
20	BCR	Y	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	5 (8%)
26	DGD	a	5411	-	58,58,67	0.96	3 (5%)	72,72,81	1.53	12 (16%)
17	CLA	d	5403	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	8 (10%)
20	BCR	z	5101	-	41,41,41	1.27	2 (4%)	56,56,56	1.29	8 (14%)
17	CLA	B	602	-	65,73,73	1.46	11 (16%)	76,113,113	1.37	8 (10%)
17	CLA	C	510	-	65,73,73	1.49	10 (15%)	76,113,113	1.40	7 (9%)
17	CLA	b	5611	-	65,73,73	1.54	12 (18%)	76,113,113	1.61	9 (11%)
18	PHO	a	5405	-	51,69,69	1.22	7 (13%)	47,99,99	1.17	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	MGE	D	410	25	48,48,48	0.92	2 (4%)	56,56,56	1.25	4 (7%)
19	PQ9	D	406	-	45,45,45	0.66	2 (4%)	56,57,57	1.84	16 (28%)
19	PQ9	d	5405	-	45,45,45	0.66	2 (4%)	56,57,57	1.84	16 (28%)
17	CLA	B	614	25	56,64,73	1.55	10 (17%)	65,102,113	1.56	7 (10%)
17	CLA	C	509	-	47,55,73	1.70	10 (21%)	54,91,113	1.50	8 (14%)
17	CLA	B	616	-	65,73,73	1.47	12 (18%)	76,113,113	1.46	8 (10%)
25	MGE	m	5103	17	48,48,48	0.91	2 (4%)	56,56,56	1.03	3 (5%)
25	MGE	c	5517	-	48,48,48	0.92	2 (4%)	56,56,56	1.11	5 (8%)
24	BCT	A	411	28	2,3,3	1.37	0	2,3,3	4.05	2 (100%)
17	CLA	A	405	-	55,63,73	1.59	10 (18%)	64,101,113	1.50	7 (10%)
20	BCR	B	618	-	41,41,41	1.31	3 (7%)	56,56,56	1.46	9 (16%)
17	CLA	C	502	17	60,68,73	1.53	11 (18%)	70,107,113	1.56	9 (12%)
17	CLA	b	5603	-	65,73,73	1.45	12 (18%)	76,113,113	1.49	7 (9%)
17	CLA	d	5404	-	50,58,73	1.63	10 (20%)	58,95,113	1.51	8 (13%)
17	CLA	B	613	-	65,73,73	1.48	13 (20%)	76,113,113	1.54	10 (13%)
17	CLA	D	404	-	65,73,73	1.46	10 (15%)	76,113,113	1.41	8 (10%)
17	CLA	b	5614	-	56,64,73	1.54	10 (17%)	65,102,113	1.56	7 (10%)
20	BCR	C	516	-	41,41,41	1.35	4 (9%)	56,56,56	1.40	9 (16%)
20	BCR	b	5619	-	41,41,41	1.39	3 (7%)	56,56,56	1.36	9 (16%)
20	BCR	t	5101	-	41,41,41	1.39	3 (7%)	56,56,56	1.36	10 (17%)
18	PHO	D	402	-	51,69,69	1.21	7 (13%)	47,99,99	1.20	6 (12%)
17	CLA	c	5511	-	51,59,73	1.61	9 (17%)	59,96,113	1.53	7 (11%)
17	CLA	c	5508	-	65,73,73	1.51	12 (18%)	76,113,113	1.53	8 (10%)
17	CLA	C	508	-	65,73,73	1.52	12 (18%)	76,113,113	1.53	8 (10%)
17	CLA	b	5604	-	65,73,73	1.49	12 (18%)	76,113,113	1.48	8 (10%)
17	CLA	b	5608	-	65,73,73	1.44	10 (15%)	76,113,113	1.51	7 (9%)
20	BCR	b	5617	-	41,41,41	1.41	3 (7%)	56,56,56	1.47	10 (17%)
26	DGD	C	519	-	58,58,67	0.96	2 (3%)	72,72,81	1.53	12 (16%)
17	CLA	B	604	-	65,73,73	1.50	12 (18%)	76,113,113	1.48	8 (10%)
20	BCR	H	101	17	41,41,41	1.34	3 (7%)	56,56,56	1.26	6 (10%)
20	BCR	B	617	-	41,41,41	1.41	3 (7%)	56,56,56	1.47	10 (17%)
29	HEM	f	5101	-	41,50,50	1.54	3 (7%)	45,82,82	1.12	2 (4%)
17	CLA	C	511	3	65,73,73	1.44	11 (16%)	76,113,113	1.49	7 (9%)
20	BCR	C	515	-	41,41,41	1.27	2 (4%)	56,56,56	1.29	8 (14%)
17	CLA	C	512	-	51,59,73	1.61	9 (17%)	59,96,113	1.52	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	B	605	-	65,73,73	1.48	12 (18%)	76,113,113	1.48	11 (14%)
20	BCR	c	5513	-	41,41,41	1.30	2 (4%)	56,56,56	1.39	8 (14%)
25	MGE	d	5410	-	48,48,48	0.93	2 (4%)	56,56,56	1.25	5 (8%)
17	CLA	A	402	-	65,73,73	1.48	11 (16%)	76,113,113	1.54	8 (10%)
20	BCR	k	5502	-	41,41,41	1.20	3 (7%)	56,56,56	1.30	6 (10%)
17	CLA	b	5609	-	65,73,73	1.48	10 (15%)	76,113,113	1.40	9 (11%)
17	CLA	B	615	-	65,73,73	1.45	11 (16%)	76,113,113	1.45	7 (9%)
17	CLA	c	5502	17	60,68,73	1.52	11 (18%)	70,107,113	1.55	9 (12%)
17	CLA	c	5512	-	50,58,73	1.61	9 (18%)	58,95,113	1.53	9 (15%)
17	CLA	B	610	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	8 (10%)
17	CLA	b	5607	-	65,73,73	1.43	11 (16%)	76,113,113	1.51	7 (9%)
18	PHO	A	404	-	51,69,69	1.23	7 (13%)	47,99,99	1.17	5 (10%)
17	CLA	b	5605	-	65,73,73	1.48	12 (18%)	76,113,113	1.48	11 (14%)
26	DGD	c	5516	-	48,48,67	1.02	2 (4%)	62,62,81	1.45	7 (11%)
25	MGE	d	5409	-	41,41,48	1.00	2 (4%)	49,49,56	1.44	8 (16%)
26	DGD	C	518	-	48,48,67	1.03	2 (4%)	62,62,81	1.44	7 (11%)
17	CLA	B	611	-	65,73,73	1.54	12 (18%)	76,113,113	1.60	9 (11%)
20	BCR	a	5408	-	41,41,41	1.36	4 (9%)	56,56,56	1.36	9 (16%)
17	CLA	C	501	-	65,73,73	1.46	11 (16%)	76,113,113	1.47	9 (11%)
20	BCR	h	5101	17	41,41,41	1.35	3 (7%)	56,56,56	1.26	6 (10%)
17	CLA	C	507	-	65,73,73	1.46	11 (16%)	76,113,113	1.44	9 (11%)
22	LMT	A	409	-	36,36,36	1.16	6 (16%)	47,47,47	1.11	3 (6%)
22	LMT	a	5410	-	36,36,36	1.19	6 (16%)	47,47,47	1.01	1 (2%)
17	CLA	b	5612	-	65,73,73	1.45	11 (16%)	76,113,113	1.55	8 (10%)
17	CLA	B	603	-	65,73,73	1.45	12 (18%)	76,113,113	1.49	7 (9%)
20	BCR	D	407	-	41,41,41	1.27	3 (7%)	56,56,56	1.27	7 (12%)
20	BCR	b	5618	-	41,41,41	1.30	3 (7%)	56,56,56	1.46	9 (16%)
19	PQ9	a	5407	-	30,30,45	0.79	1 (3%)	38,39,57	1.56	10 (26%)
17	CLA	C	505	-	65,73,73	1.44	10 (15%)	76,113,113	1.48	9 (11%)
17	CLA	a	5406	-	55,63,73	1.59	10 (18%)	64,101,113	1.50	7 (10%)
23	SQD	A	410	-	25,26,54	1.34	4 (16%)	34,37,65	1.83	8 (23%)
25	MGE	D	408	-	47,47,48	0.95	2 (4%)	55,55,56	1.05	3 (5%)
17	CLA	b	5602	-	65,73,73	1.46	11 (16%)	76,113,113	1.37	8 (10%)
17	CLA	C	504	-	46,54,73	1.71	10 (21%)	53,90,113	1.56	7 (13%)
17	CLA	k	5501	3	65,73,73	1.44	11 (16%)	76,113,113	1.48	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	MGE	C	520	-	48,48,48	0.92	2 (4%)	56,56,56	1.11	5 (8%)
25	MGE	b	5620	-	48,48,48	0.94	2 (4%)	56,56,56	1.14	4 (7%)
17	CLA	c	5501	-	65,73,73	1.47	11 (16%)	76,113,113	1.45	9 (11%)
17	CLA	b	5610	-	65,73,73	1.45	10 (15%)	76,113,113	1.48	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
20	BCR	C	514	-	-	12/29/63/63	0/2/2/2
23	SQD	D	403	-	-	22/49/69/69	0/1/1/1
20	BCR	c	5514	-	-	19/29/63/63	0/2/2/2
19	PQ9	A	406	-	-	12/41/61/61	0/1/1/1
17	CLA	C	506	-	1/1/15/20	20/37/115/115	-
23	SQD	a	5401	-	-	10/19/39/69	0/1/1/1
17	CLA	B	608	-	1/1/15/20	11/37/115/115	-
26	DGD	C	517	3,1	-	19/42/82/95	0/2/2/2
17	CLA	B	601	20	1/1/10/20	2/8/86/115	-
26	DGD	c	5515	3	-	19/42/82/95	0/2/2/2
26	DGD	h	5102	7,2	-	21/43/83/95	0/2/2/2
29	HEM	F	101	6	-	1/12/54/54	-
17	CLA	B	609	-	1/1/15/20	21/37/115/115	-
20	BCR	d	5406	-	-	15/29/63/63	0/2/2/2
23	SQD	l	5102	-	-	15/42/62/69	0/1/1/1
22	LMT	m	5102	-	-	9/21/61/61	0/2/2/2
17	CLA	B	612	-	1/1/15/20	19/37/115/115	-
21	LHG	a	5409	-	-	22/43/43/53	-
17	CLA	c	5509	-	1/1/11/20	6/16/94/115	-
26	DGD	H	102	7,4	-	21/43/83/95	0/2/2/2
17	CLA	b	5616	-	1/1/15/20	8/37/115/115	-
20	BCR	A	407	-	-	14/29/63/63	0/2/2/2
17	CLA	b	5613	-	1/1/15/20	18/37/115/115	-
17	CLA	c	5505	-	1/1/15/20	21/37/115/115	-
17	CLA	A	403	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LHG	A	408	-	-	22/43/43/53	-
25	MGE	m	5101	-	-	8/43/63/63	0/1/1/1
17	CLA	a	5402	-	1/1/15/20	12/37/115/115	-
23	SQD	L	101	-	-	23/42/62/69	0/1/1/1
17	CLA	D	405	-	1/1/12/20	9/19/97/115	-
17	CLA	b	5615	-	1/1/15/20	18/37/115/115	-
17	CLA	C	503	17	1/1/15/20	20/37/115/115	-
18	PHO	d	5402	-	-	12/37/103/103	0/5/6/6
17	CLA	C	513	-	1/1/12/20	5/19/97/115	-
17	CLA	A	401	-	1/1/15/20	12/37/115/115	-
17	CLA	c	5510	-	1/1/15/20	8/37/115/115	-
22	LMT	B	620	-	-	7/21/61/61	0/2/2/2
17	CLA	c	5503	17	1/1/15/20	20/37/115/115	-
22	LMT	T	101	12,2	-	10/21/61/61	0/2/2/2
17	CLA	B	607	-	1/1/15/20	18/37/115/115	-
23	SQD	d	5407	-	-	14/49/69/69	0/1/1/1
25	MGE	B	619	-	-	12/43/63/63	0/1/1/1
25	MGE	d	5408	-	-	15/42/62/63	0/1/1/1
17	CLA	a	5404	-	1/1/15/20	13/37/115/115	-
20	BCR	t	5102	-	-	12/29/63/63	0/2/2/2
25	MGE	A	412	25	-	12/43/63/63	0/1/1/1
17	CLA	c	5507	-	1/1/15/20	16/37/115/115	-
25	MGE	D	409	-	-	16/36/56/63	0/1/1/1
17	CLA	B	606	-	1/1/15/20	17/37/115/115	-
17	CLA	c	5506	-	1/1/15/20	20/37/115/115	-
25	MGE	l	5101	-	-	12/43/63/63	0/1/1/1
17	CLA	b	5606	-	1/1/10/20	6/10/88/115	-
17	CLA	b	5601	20	1/1/10/20	2/8/86/115	-
22	LMT	M	101	-	-	8/21/61/61	0/2/2/2
17	CLA	a	5403	-	1/1/15/20	15/37/115/115	-
17	CLA	c	5504	-	1/1/11/20	9/15/93/115	-
20	BCR	T	102	-	-	12/29/63/63	0/2/2/2
20	BCR	Y	101	-	-	11/29/63/63	0/2/2/2
26	DGD	a	5411	-	-	18/46/86/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	d	5403	-	1/1/15/20	22/37/115/115	-
20	BCR	z	5101	-	-	21/29/63/63	0/2/2/2
17	CLA	B	602	-	1/1/15/20	20/37/115/115	-
17	CLA	C	510	-	1/1/15/20	8/37/115/115	-
17	CLA	b	5611	-	1/1/15/20	12/37/115/115	-
18	PHO	a	5405	-	-	15/37/103/103	0/5/6/6
25	MGE	D	410	25	-	17/43/63/63	0/1/1/1
19	PQ9	D	406	-	-	9/41/61/61	0/1/1/1
19	PQ9	d	5405	-	-	9/41/61/61	0/1/1/1
17	CLA	B	614	25	1/1/13/20	12/27/105/115	-
17	CLA	C	509	-	1/1/11/20	6/16/94/115	-
17	CLA	B	616	-	1/1/15/20	8/37/115/115	-
25	MGE	m	5103	17	-	21/43/63/63	0/1/1/1
25	MGE	c	5517	-	-	11/43/63/63	0/1/1/1
17	CLA	A	405	-	1/1/13/20	8/25/103/115	-
20	BCR	B	618	-	-	16/29/63/63	0/2/2/2
17	CLA	C	502	17	1/1/14/20	10/31/109/115	-
17	CLA	b	5603	-	1/1/15/20	12/37/115/115	-
17	CLA	d	5404	-	1/1/12/20	9/19/97/115	-
17	CLA	B	613	-	1/1/15/20	17/37/115/115	-
17	CLA	D	404	-	1/1/15/20	22/37/115/115	-
17	CLA	b	5614	-	1/1/13/20	12/27/105/115	-
20	BCR	C	516	-	-	19/29/63/63	0/2/2/2
20	BCR	b	5619	-	-	10/29/63/63	0/2/2/2
20	BCR	t	5101	-	-	10/29/63/63	0/2/2/2
18	PHO	D	402	-	-	12/37/103/103	0/5/6/6
17	CLA	c	5511	-	1/1/12/20	10/21/99/115	-
17	CLA	c	5508	-	1/1/15/20	13/37/115/115	-
17	CLA	C	508	-	1/1/15/20	13/37/115/115	-
17	CLA	b	5604	-	1/1/15/20	14/37/115/115	-
17	CLA	b	5608	-	1/1/15/20	11/37/115/115	-
20	BCR	b	5617	-	-	14/29/63/63	0/2/2/2
26	DGD	C	519	-	-	18/46/86/95	0/2/2/2
17	CLA	B	604	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	H	101	17	-	10/29/63/63	0/2/2/2
20	BCR	B	617	-	-	14/29/63/63	0/2/2/2
29	HEM	f	5101	-	-	1/12/54/54	-
17	CLA	C	511	3	1/1/15/20	14/37/115/115	-
20	BCR	C	515	-	-	21/29/63/63	0/2/2/2
17	CLA	C	512	-	1/1/12/20	10/21/99/115	-
17	CLA	B	605	-	1/1/15/20	18/37/115/115	-
20	BCR	c	5513	-	-	13/29/63/63	0/2/2/2
25	MGE	d	5410	-	-	14/43/63/63	0/1/1/1
17	CLA	A	402	-	1/1/15/20	15/37/115/115	-
20	BCR	k	5502	-	-	15/29/63/63	0/2/2/2
17	CLA	b	5609	-	1/1/15/20	21/37/115/115	-
17	CLA	B	615	-	1/1/15/20	18/37/115/115	-
17	CLA	c	5502	17	1/1/14/20	10/31/109/115	-
17	CLA	c	5512	-	1/1/12/20	5/19/97/115	-
17	CLA	B	610	-	1/1/15/20	15/37/115/115	-
17	CLA	b	5607	-	1/1/15/20	18/37/115/115	-
18	PHO	A	404	-	-	15/37/103/103	0/5/6/6
17	CLA	b	5605	-	1/1/15/20	18/37/115/115	-
26	DGD	c	5516	-	-	17/36/76/95	0/2/2/2
25	MGE	d	5409	-	-	12/36/56/63	0/1/1/1
26	DGD	C	518	-	-	17/36/76/95	0/2/2/2
17	CLA	B	611	-	1/1/15/20	12/37/115/115	-
20	BCR	a	5408	-	-	14/29/63/63	0/2/2/2
17	CLA	C	501	-	1/1/15/20	15/37/115/115	-
20	BCR	h	5101	17	-	10/29/63/63	0/2/2/2
17	CLA	C	507	-	1/1/15/20	16/37/115/115	-
22	LMT	A	409	-	-	10/21/61/61	0/2/2/2
22	LMT	a	5410	-	-	9/21/61/61	0/2/2/2
17	CLA	b	5612	-	1/1/15/20	19/37/115/115	-
17	CLA	B	603	-	1/1/15/20	12/37/115/115	-
20	BCR	D	407	-	-	15/29/63/63	0/2/2/2
20	BCR	b	5618	-	-	16/29/63/63	0/2/2/2
19	PQ9	a	5407	-	-	7/23/43/61	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	C	505	-	1/1/15/20	21/37/115/115	-
17	CLA	a	5406	-	1/1/13/20	8/25/103/115	-
23	SQD	A	410	-	-	8/19/39/69	0/1/1/1
25	MGE	D	408	-	-	9/42/62/63	0/1/1/1
17	CLA	b	5602	-	1/1/15/20	20/37/115/115	-
17	CLA	C	504	-	1/1/11/20	9/15/93/115	-
17	CLA	k	5501	3	1/1/15/20	14/37/115/115	-
25	MGE	C	520	-	-	11/43/63/63	0/1/1/1
25	MGE	b	5620	-	-	12/43/63/63	0/1/1/1
17	CLA	c	5501	-	1/1/15/20	15/37/115/115	-
17	CLA	b	5610	-	1/1/15/20	15/37/115/115	-

The worst 5 of 970 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	5609	CLA	C4B-NB	6.60	1.41	1.35
17	B	609	CLA	C4B-NB	6.44	1.41	1.35
17	b	5601	CLA	C4B-NB	6.34	1.40	1.35
17	c	5504	CLA	C4B-NB	6.30	1.40	1.35
17	C	504	CLA	C4B-NB	6.30	1.40	1.35

The worst 5 of 1049 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	5403	CLA	C4A-NA-C1A	7.84	110.23	106.71
17	A	402	CLA	C4A-NA-C1A	7.73	110.18	106.71
17	C	508	CLA	C4A-NA-C1A	7.56	110.11	106.71
17	c	5508	CLA	C4A-NA-C1A	7.56	110.11	106.71
17	b	5611	CLA	C4A-NA-C1A	7.46	110.06	106.71

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	401	CLA	ND
17	A	402	CLA	ND
17	A	403	CLA	ND
17	A	405	CLA	ND
17	B	601	CLA	ND

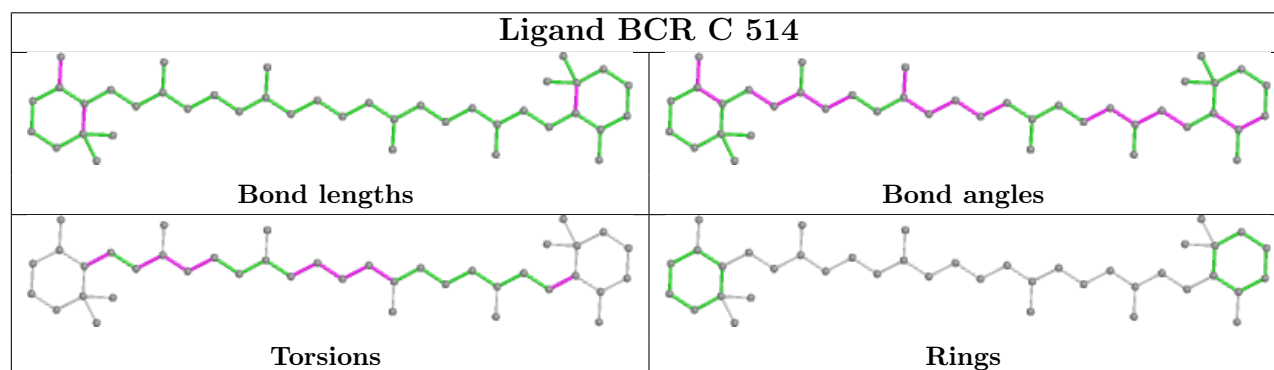
5 of 1877 torsion outliers are listed below:

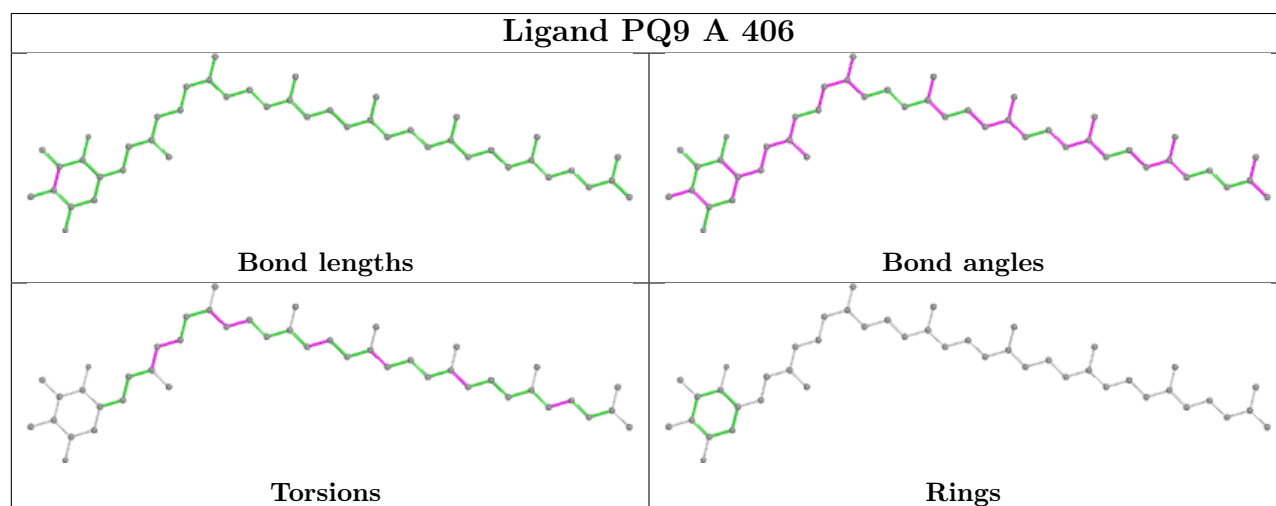
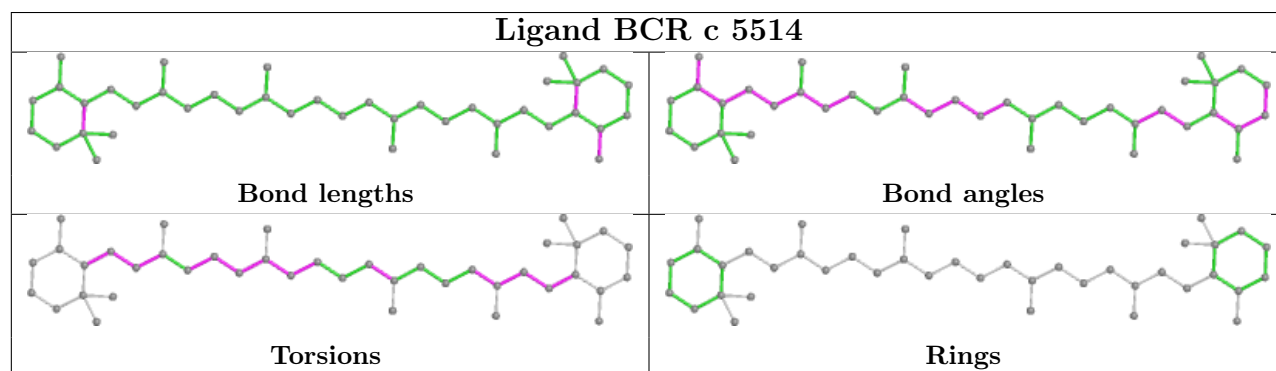
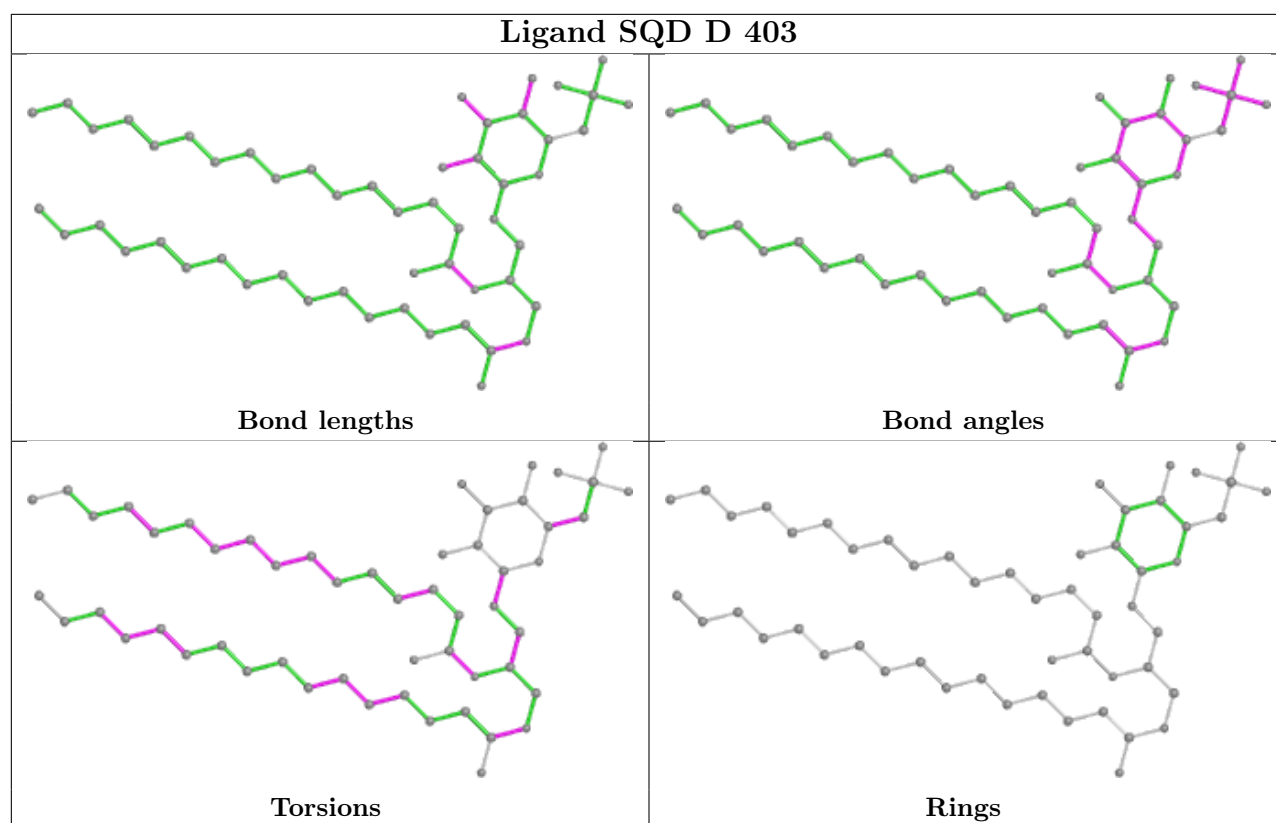
Mol	Chain	Res	Type	Atoms
17	A	403	CLA	CHA-CBD-CGD-O1D
17	A	403	CLA	CHA-CBD-CGD-O2D
17	B	602	CLA	C2-C3-C5-C6
17	B	602	CLA	C4-C3-C5-C6
17	B	603	CLA	CBD-CGD-O2D-CED

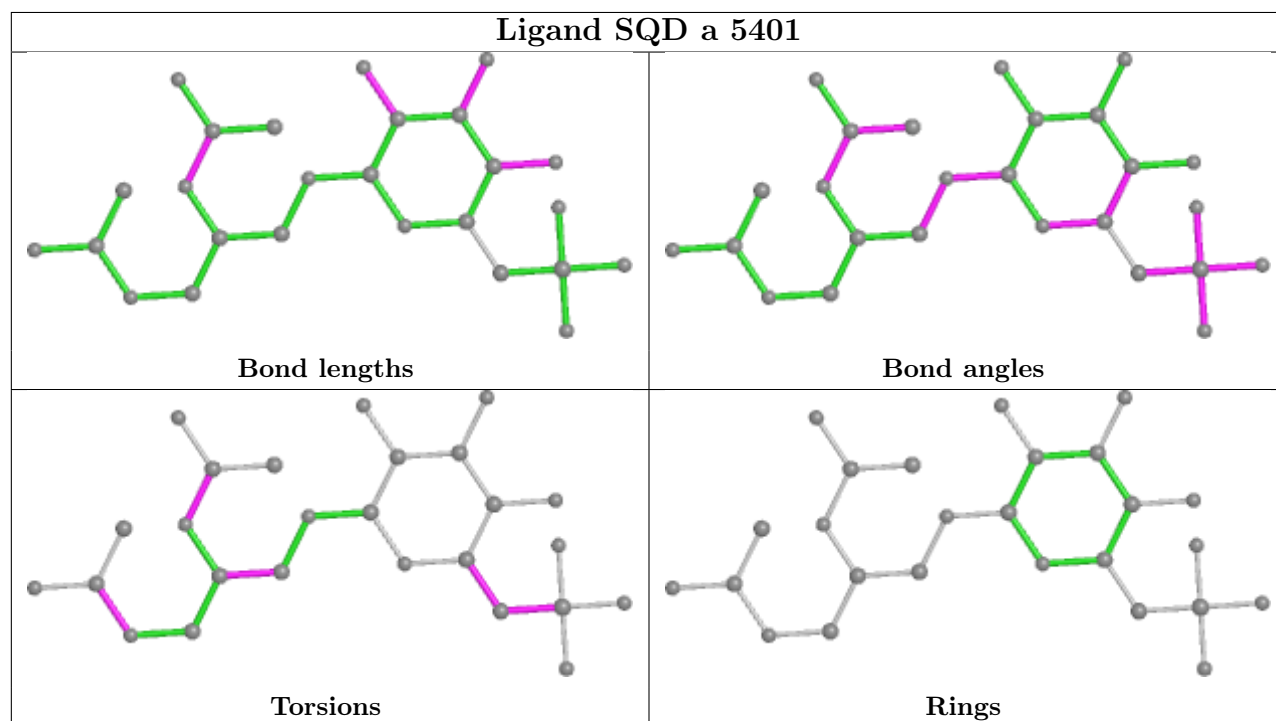
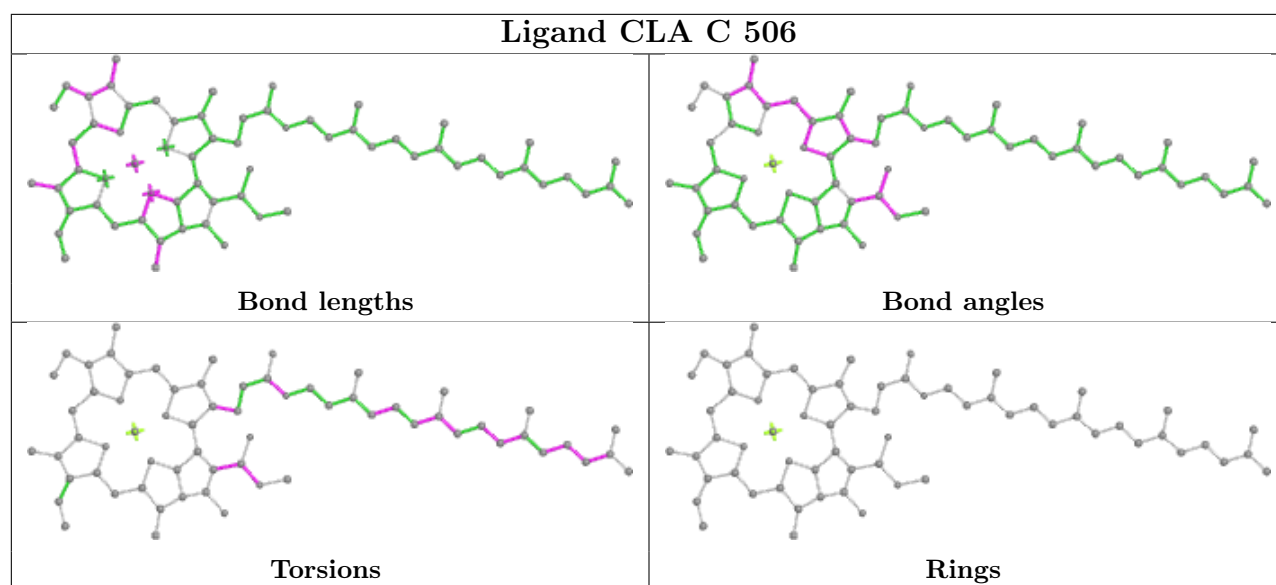
There are no ring outliers.

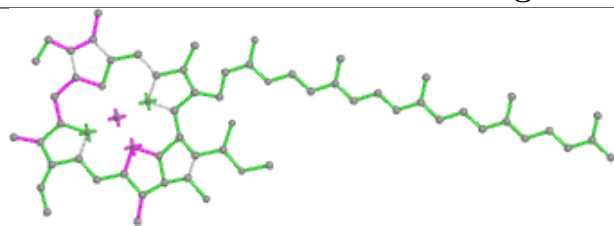
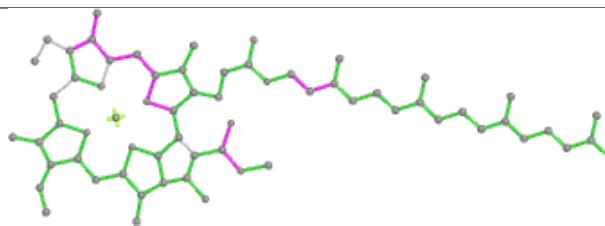
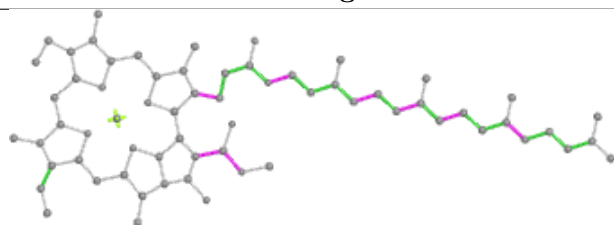
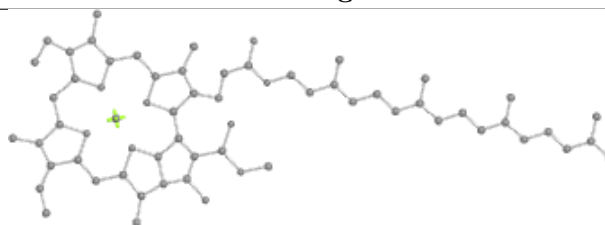
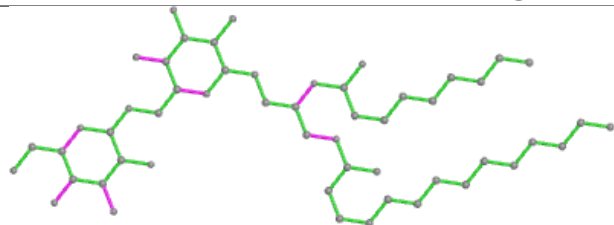
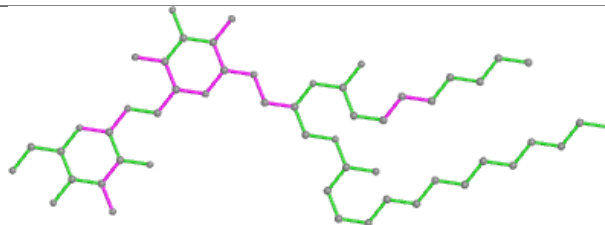
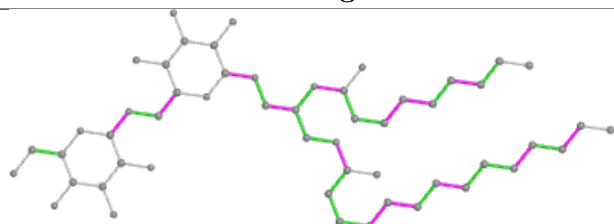
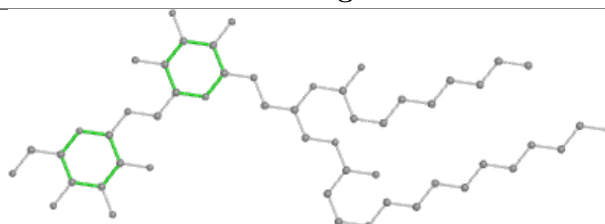
No monomer is involved in short contacts.

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.



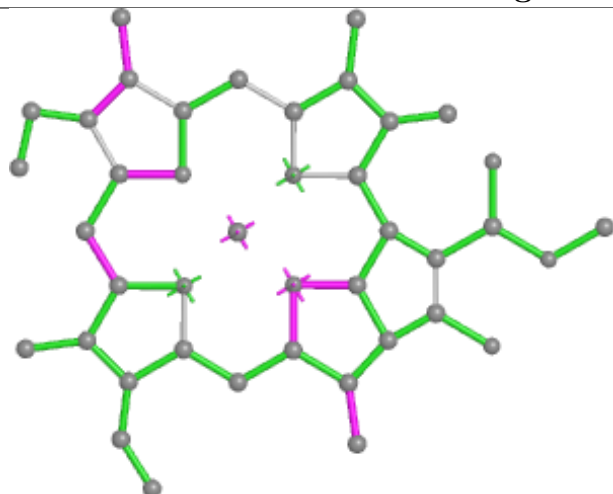




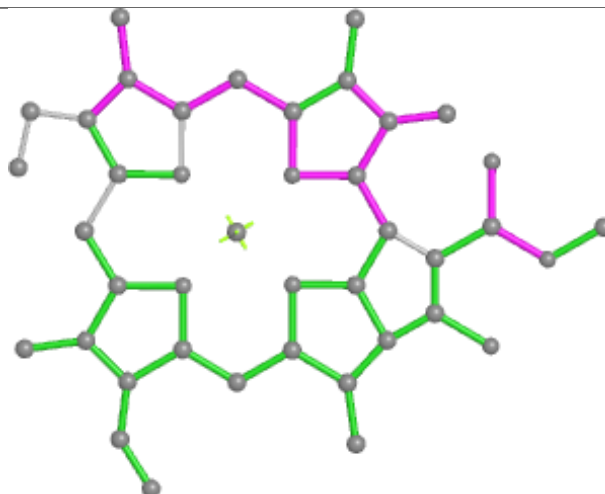
**Ligand CLA B 608****Bond lengths****Bond angles****Torsions****Rings****Ligand DGD C 517****Bond lengths****Bond angles****Torsions****Rings**



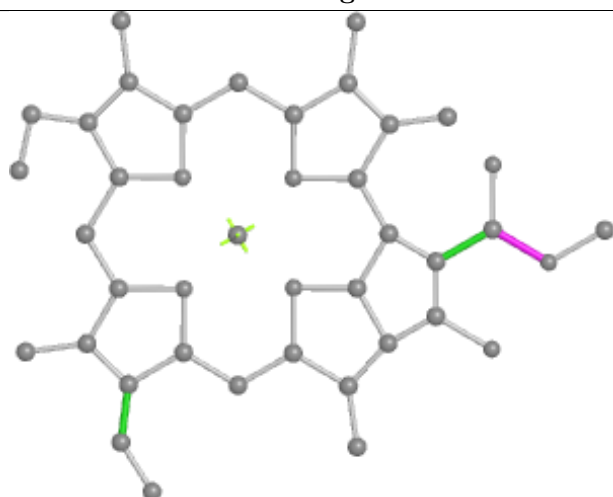
## Ligand CLA B 601



Bond lengths



Bond angles

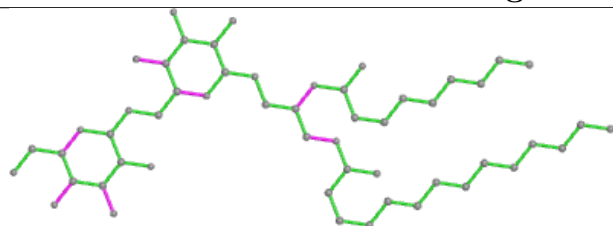


Torsions

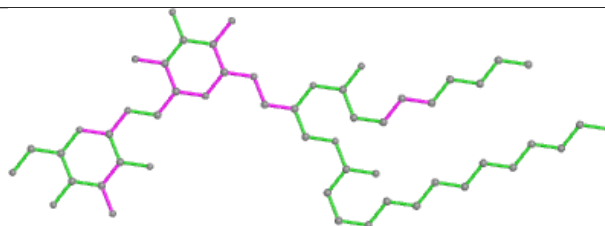


Rings

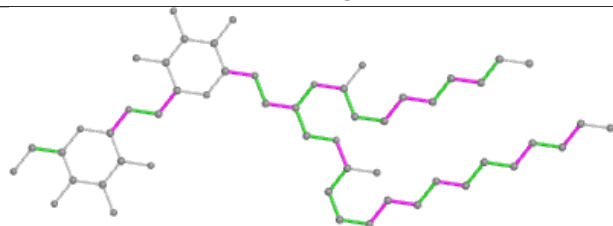
## Ligand DGD c 5515



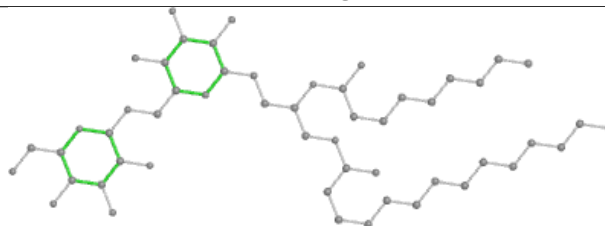
Bond lengths



Bond angles

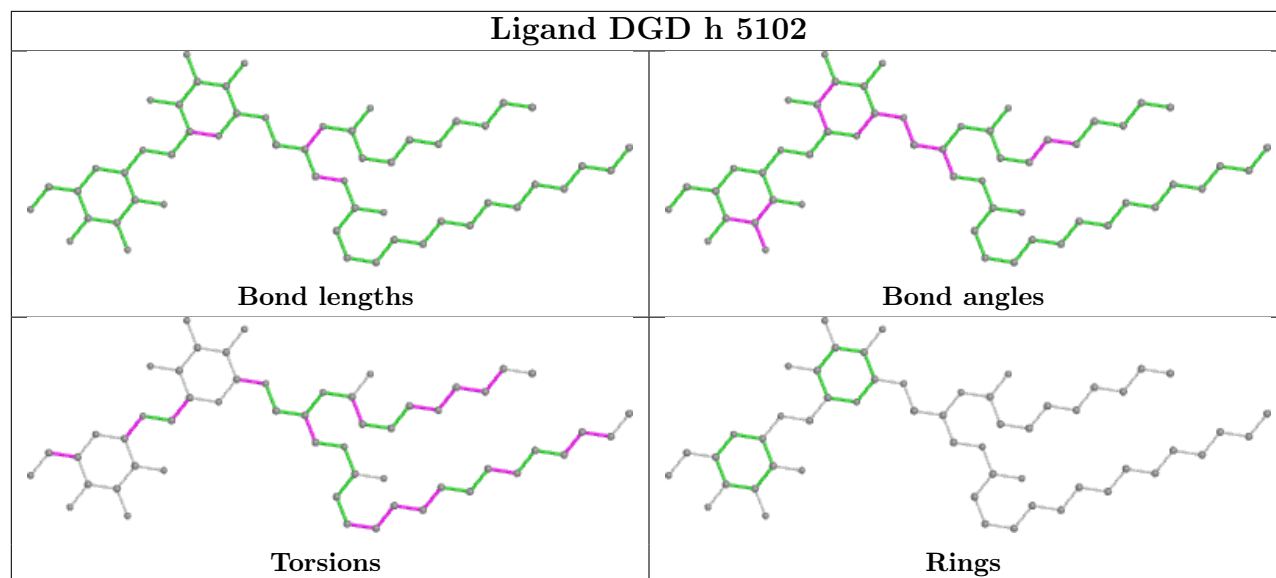


Torsions

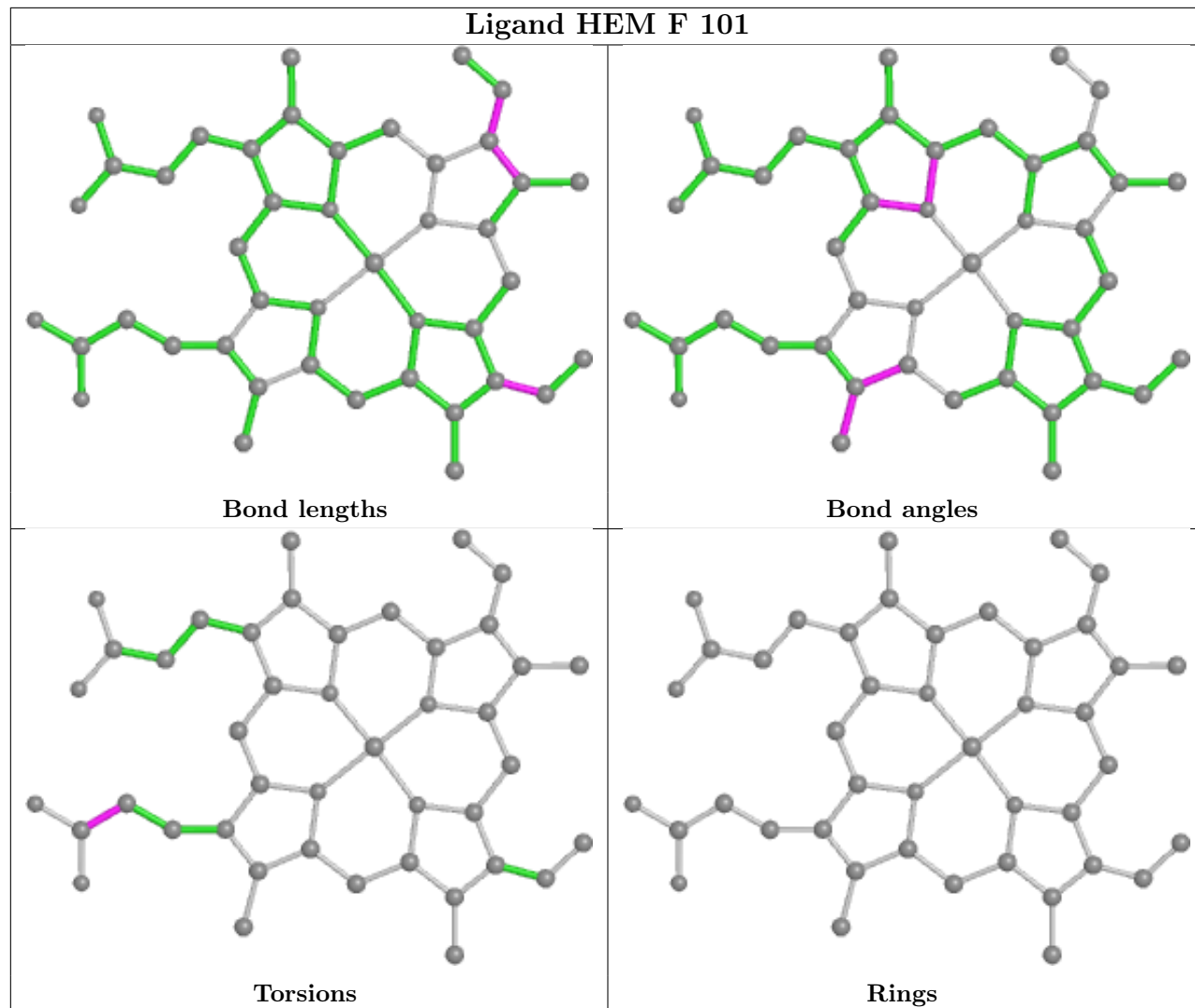


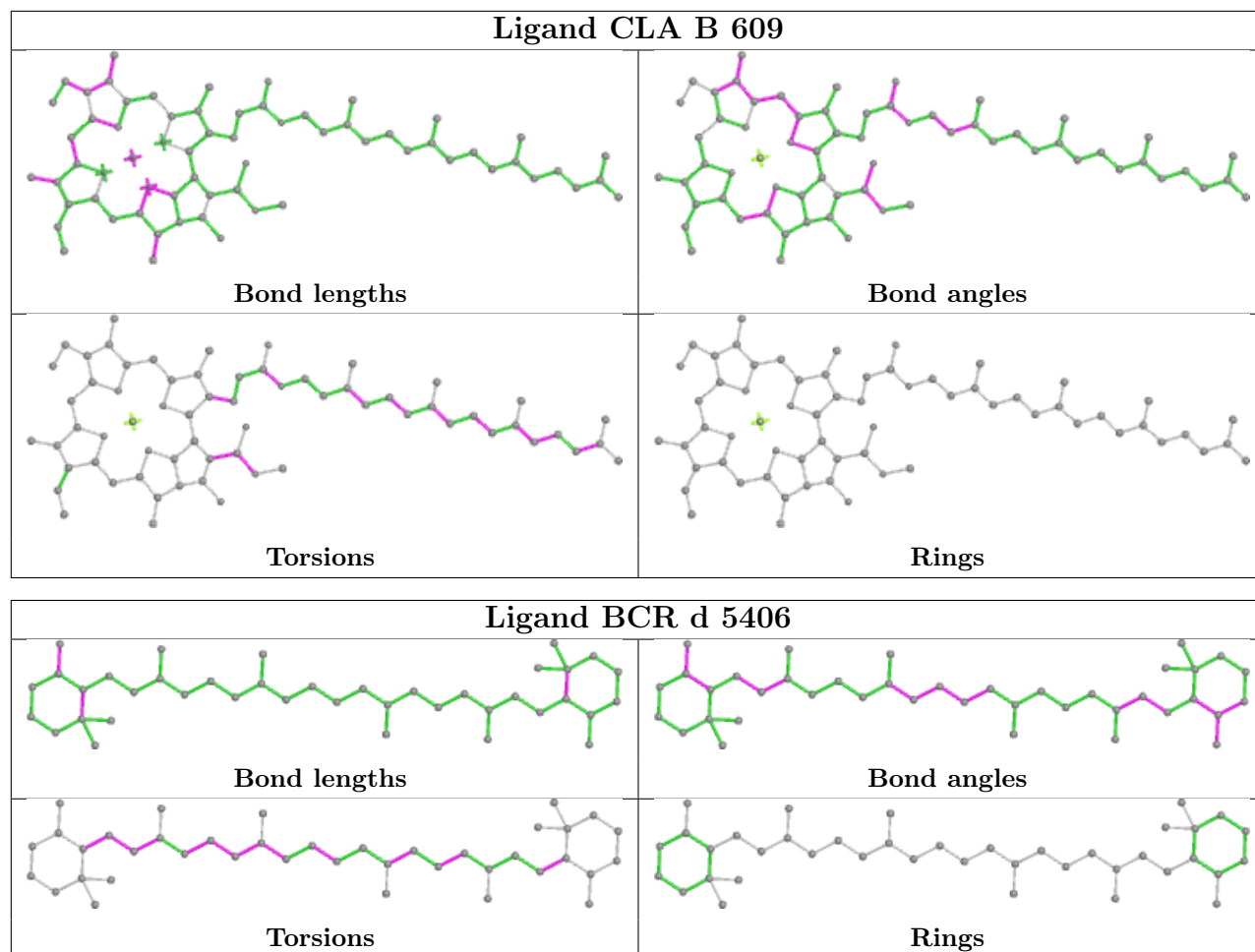
Rings

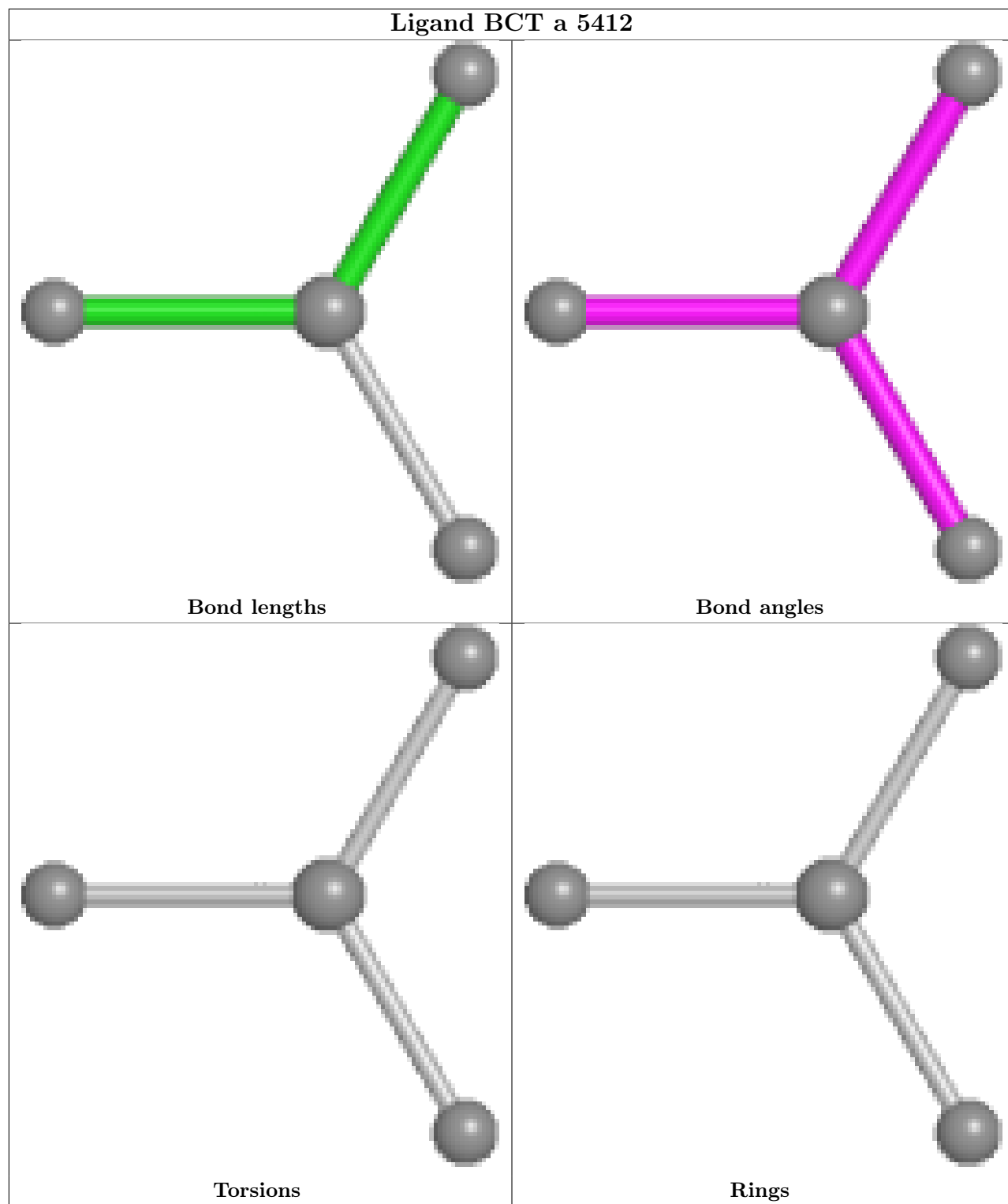
## Ligand DGD h 5102

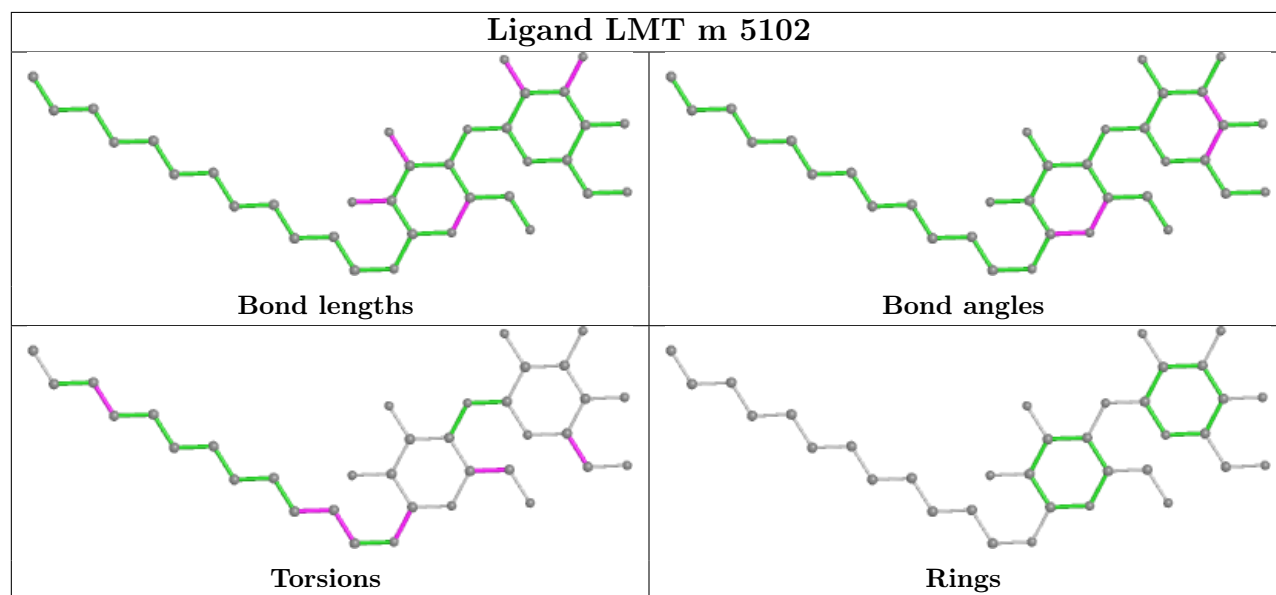
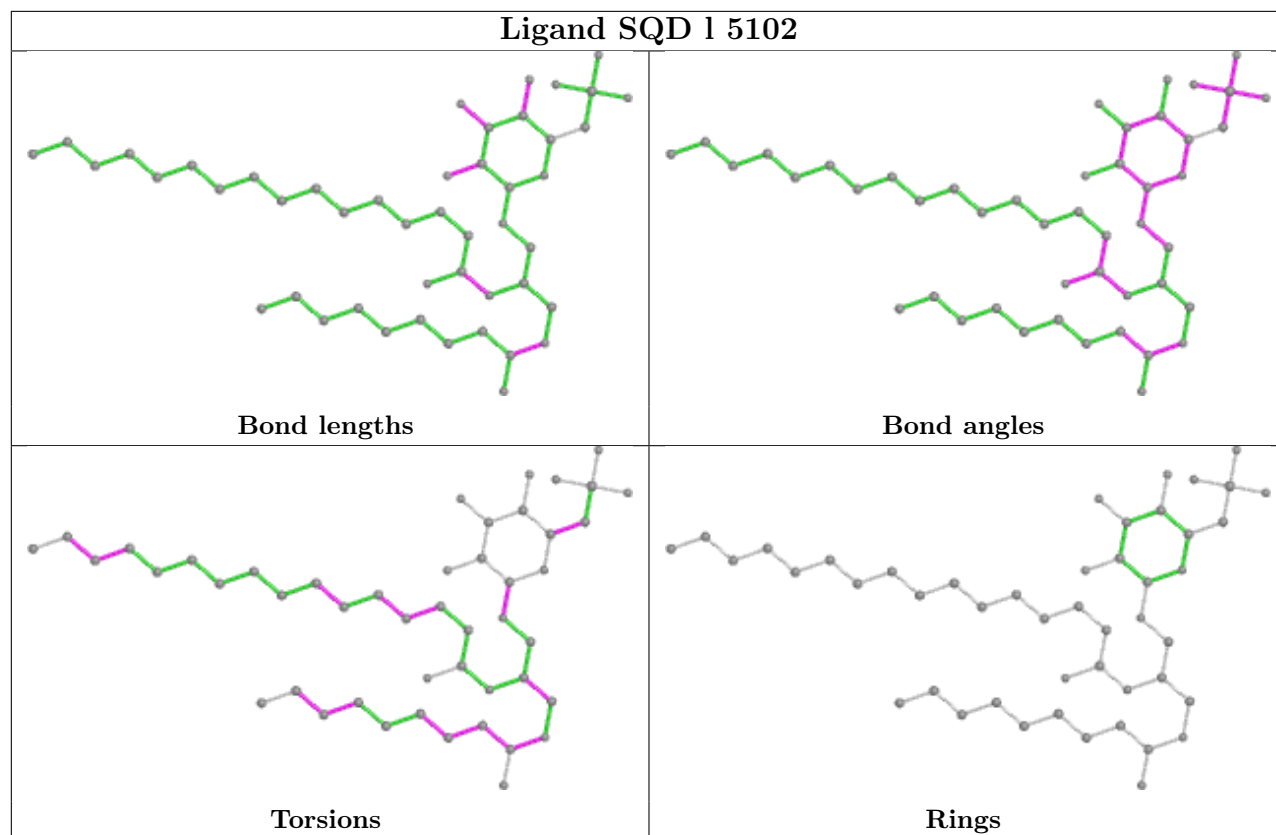


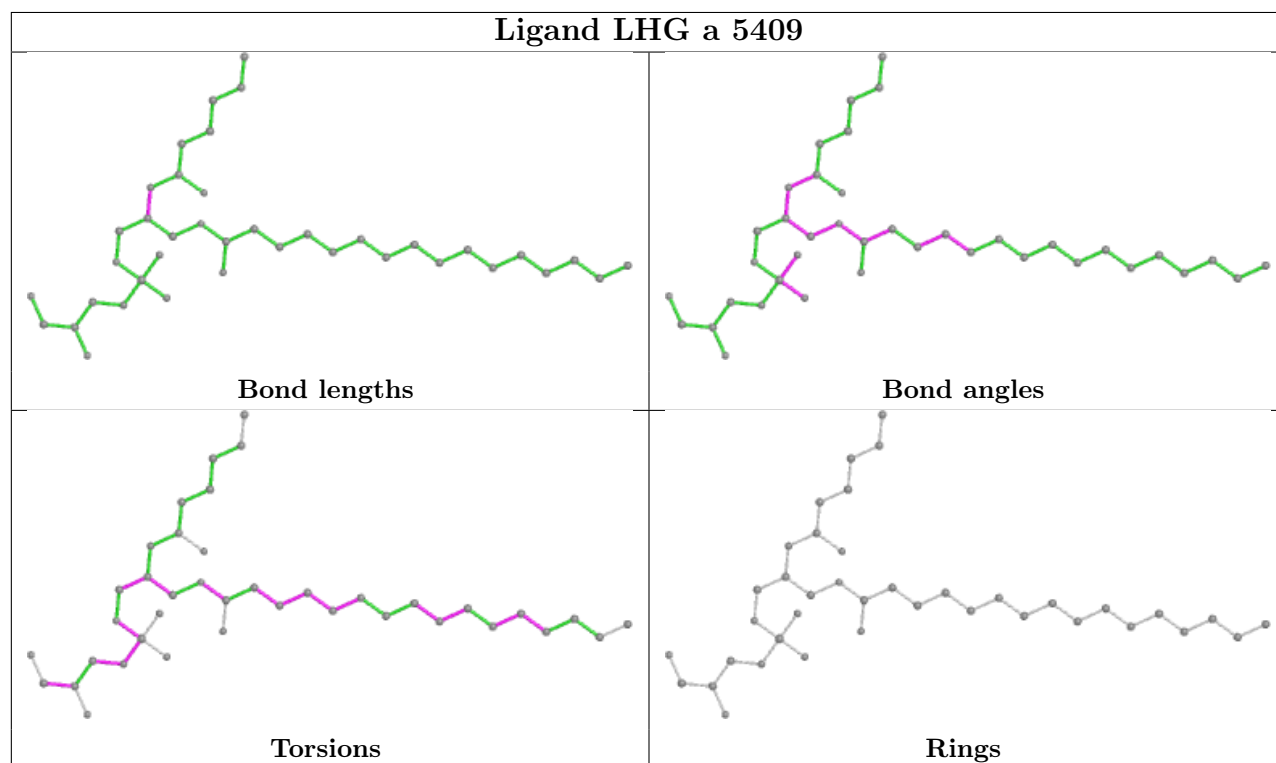
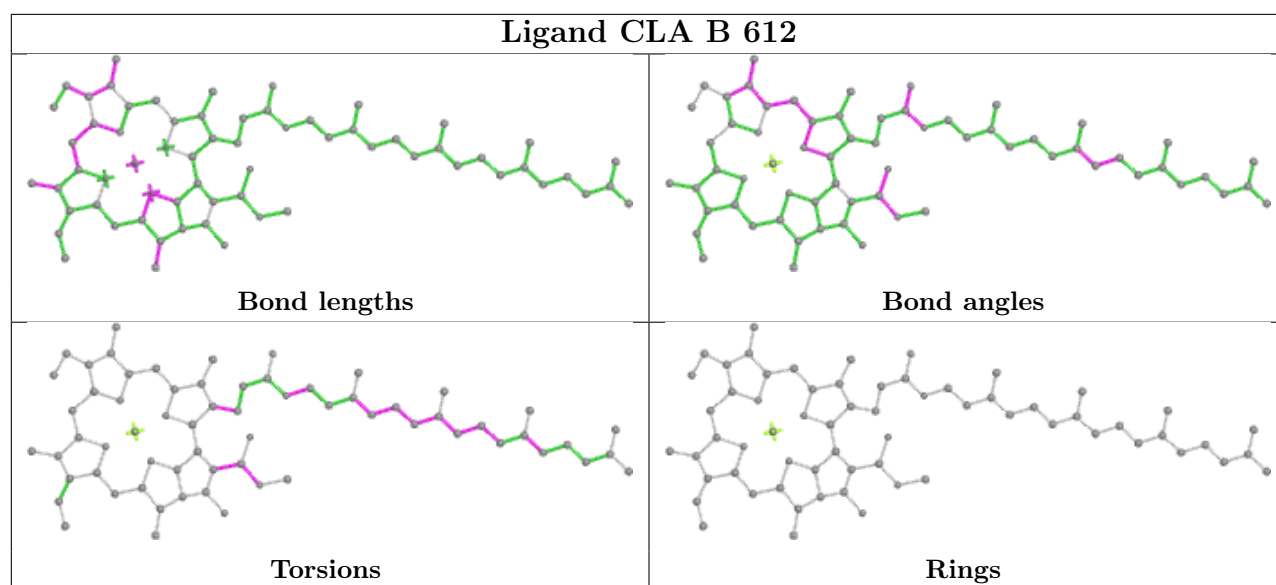
## Ligand HEM F 101

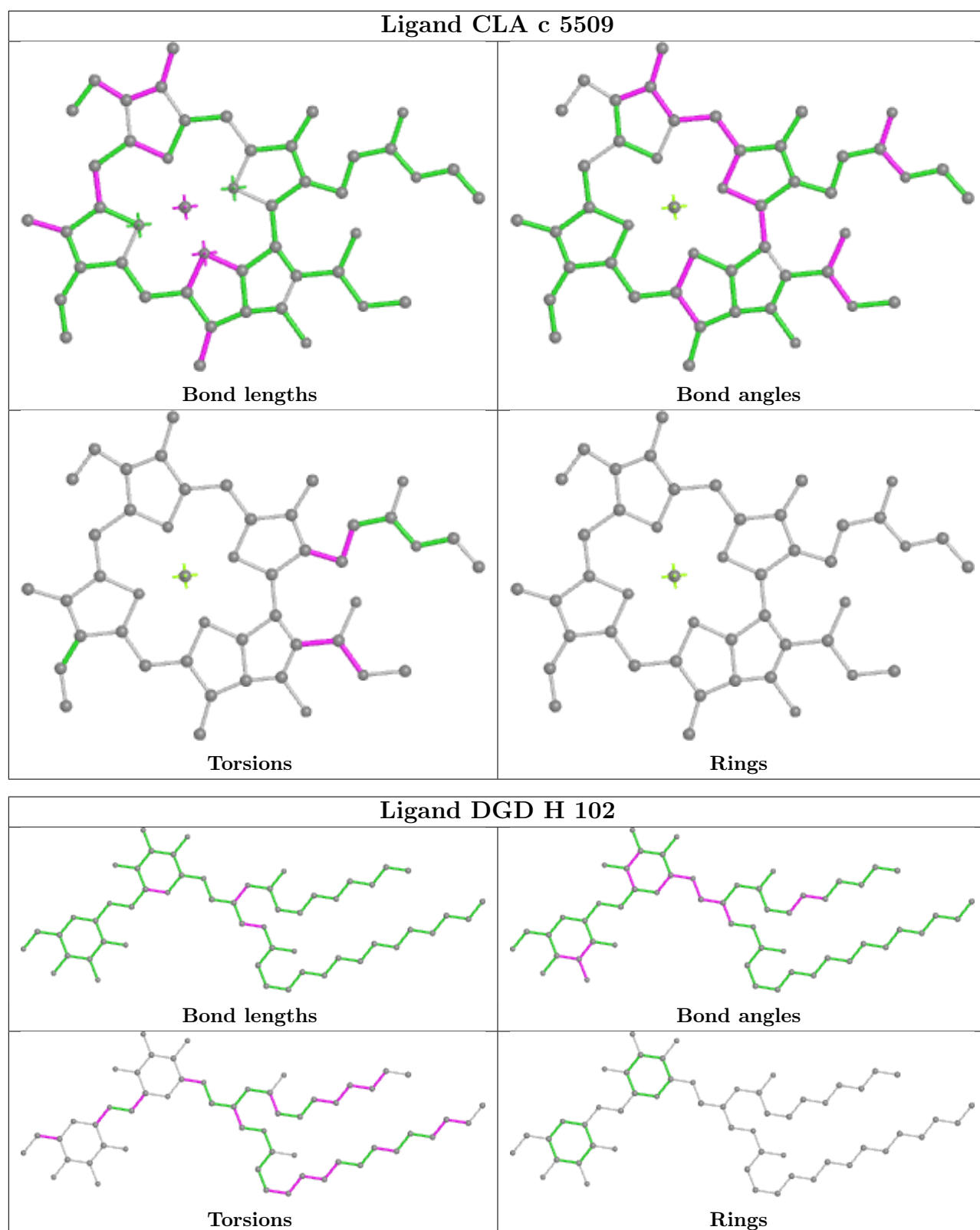


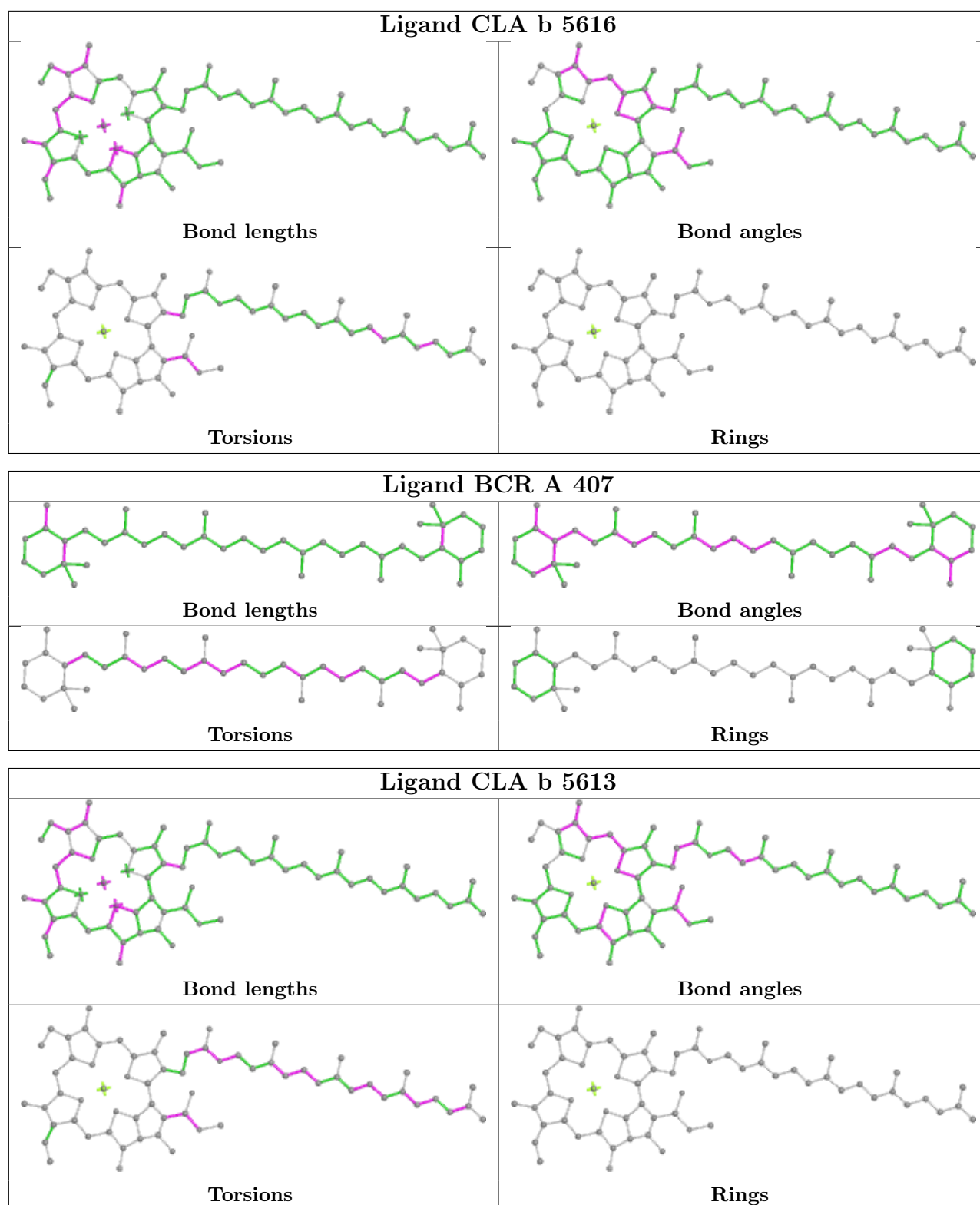




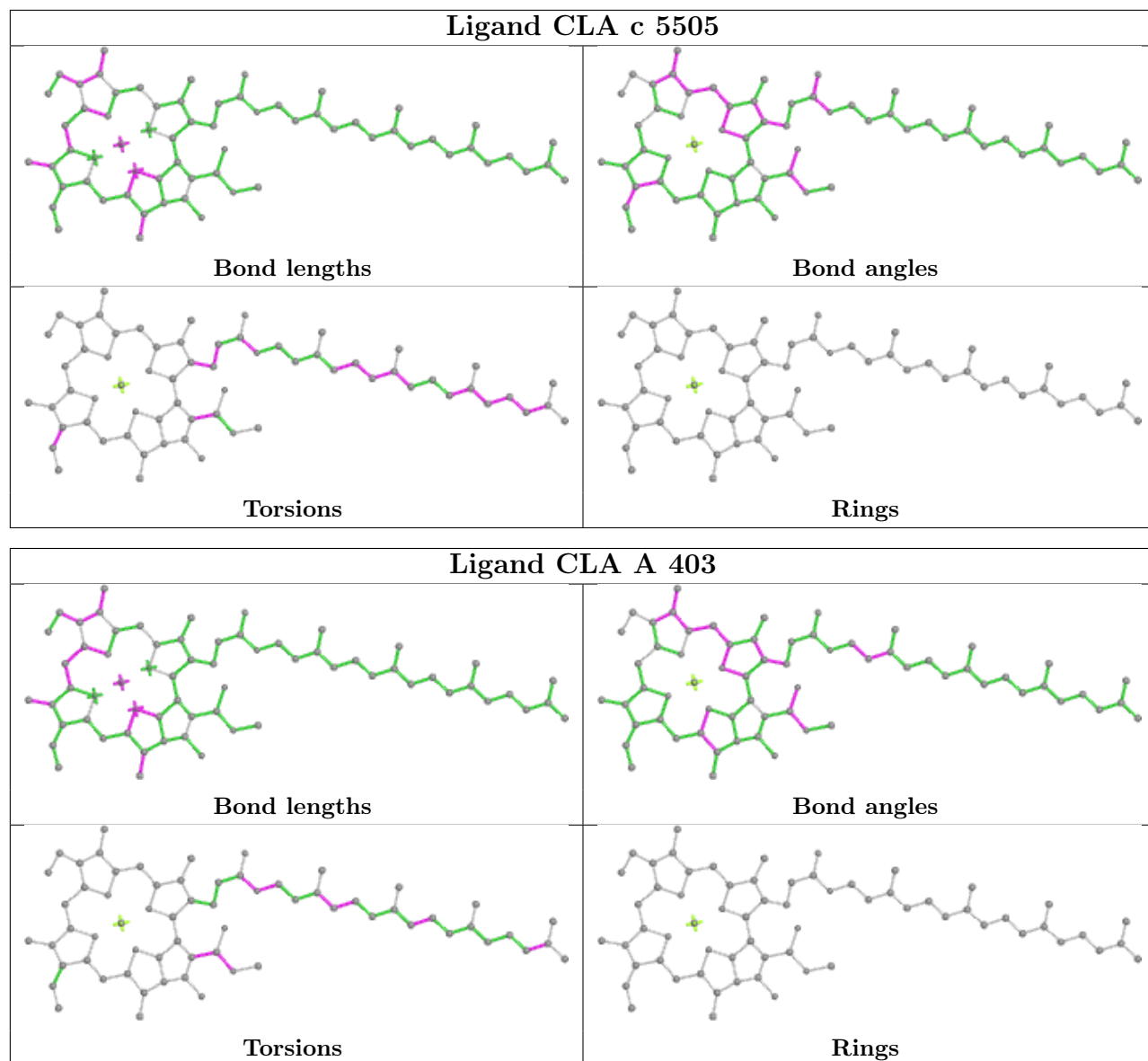


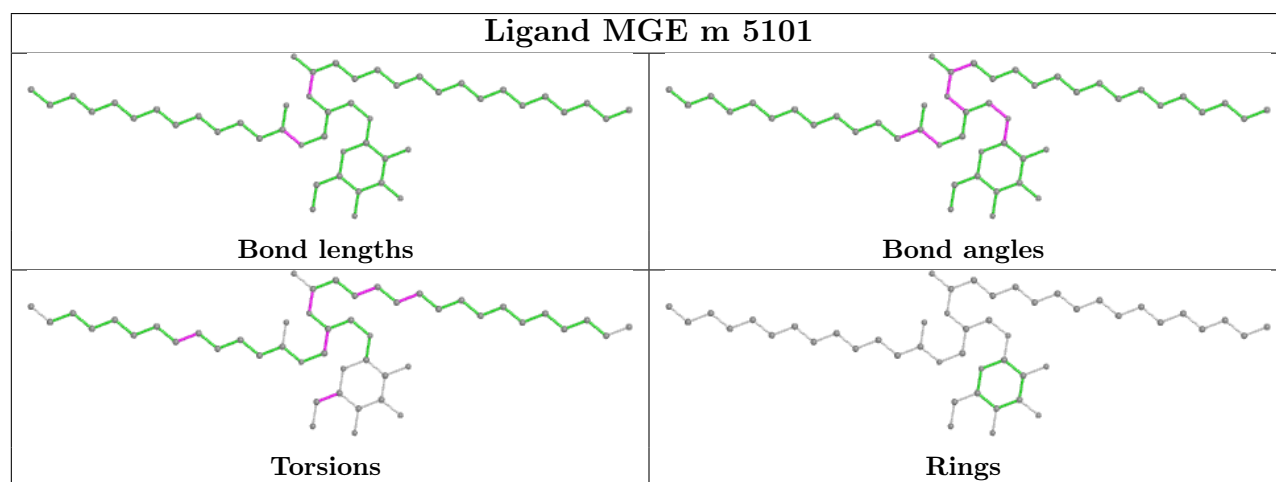
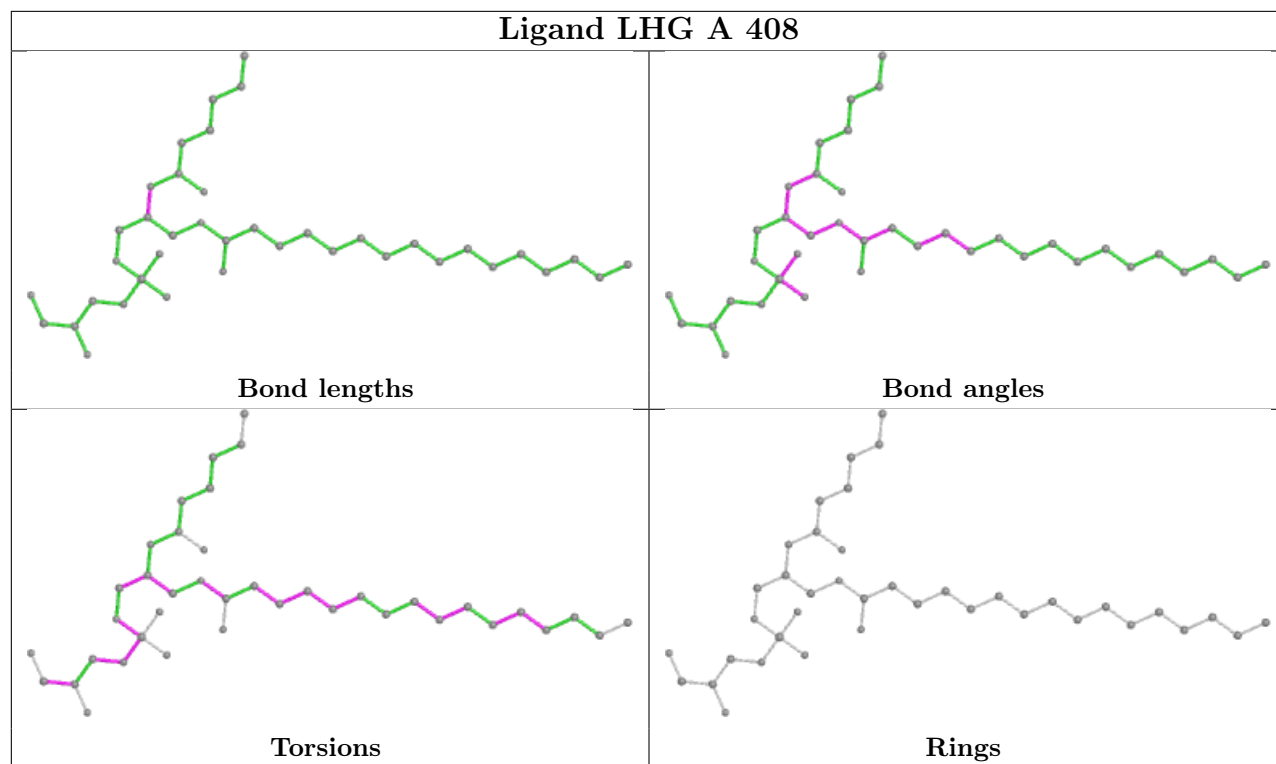


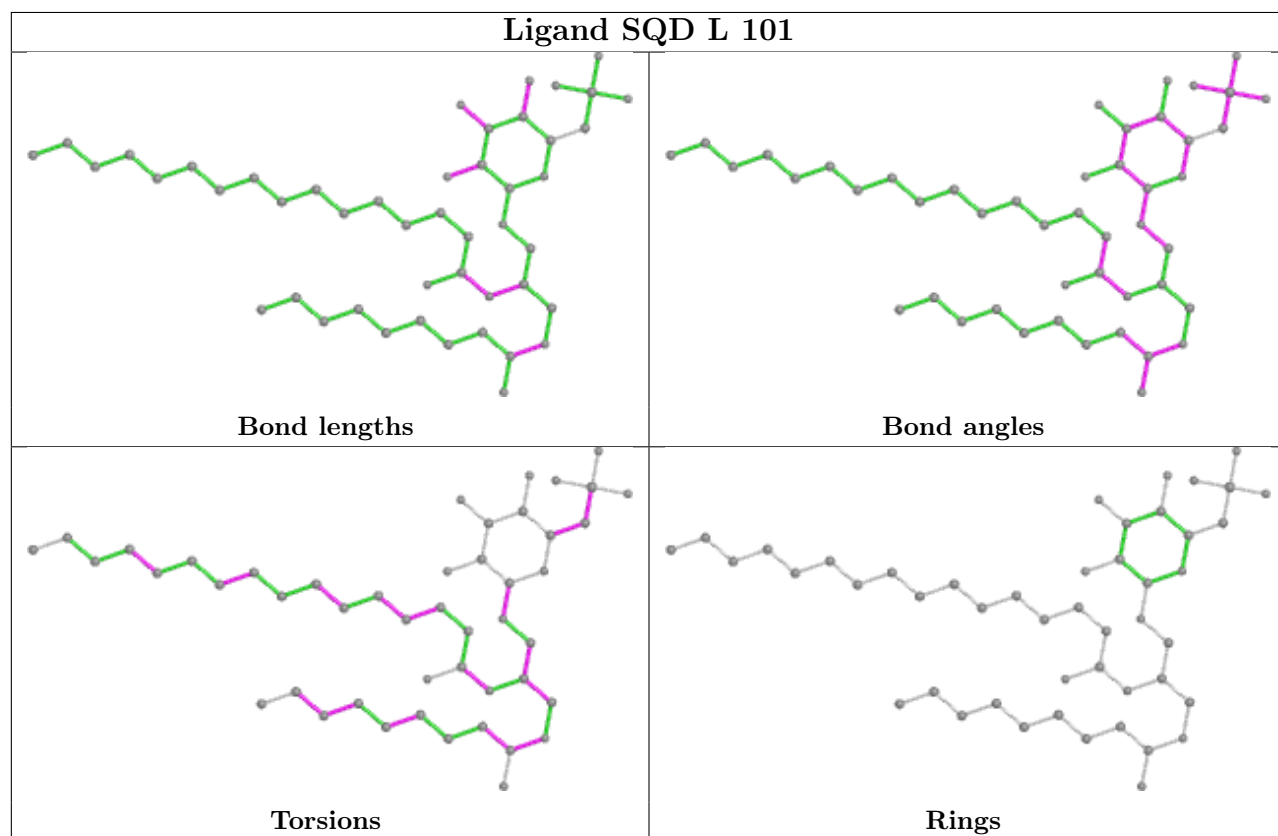
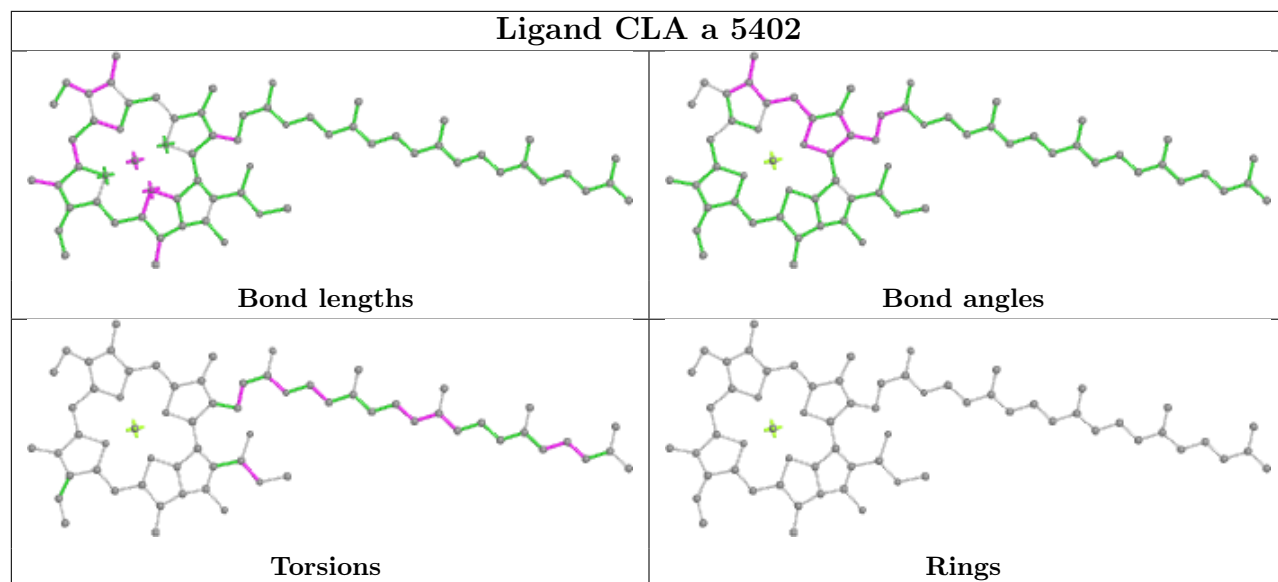


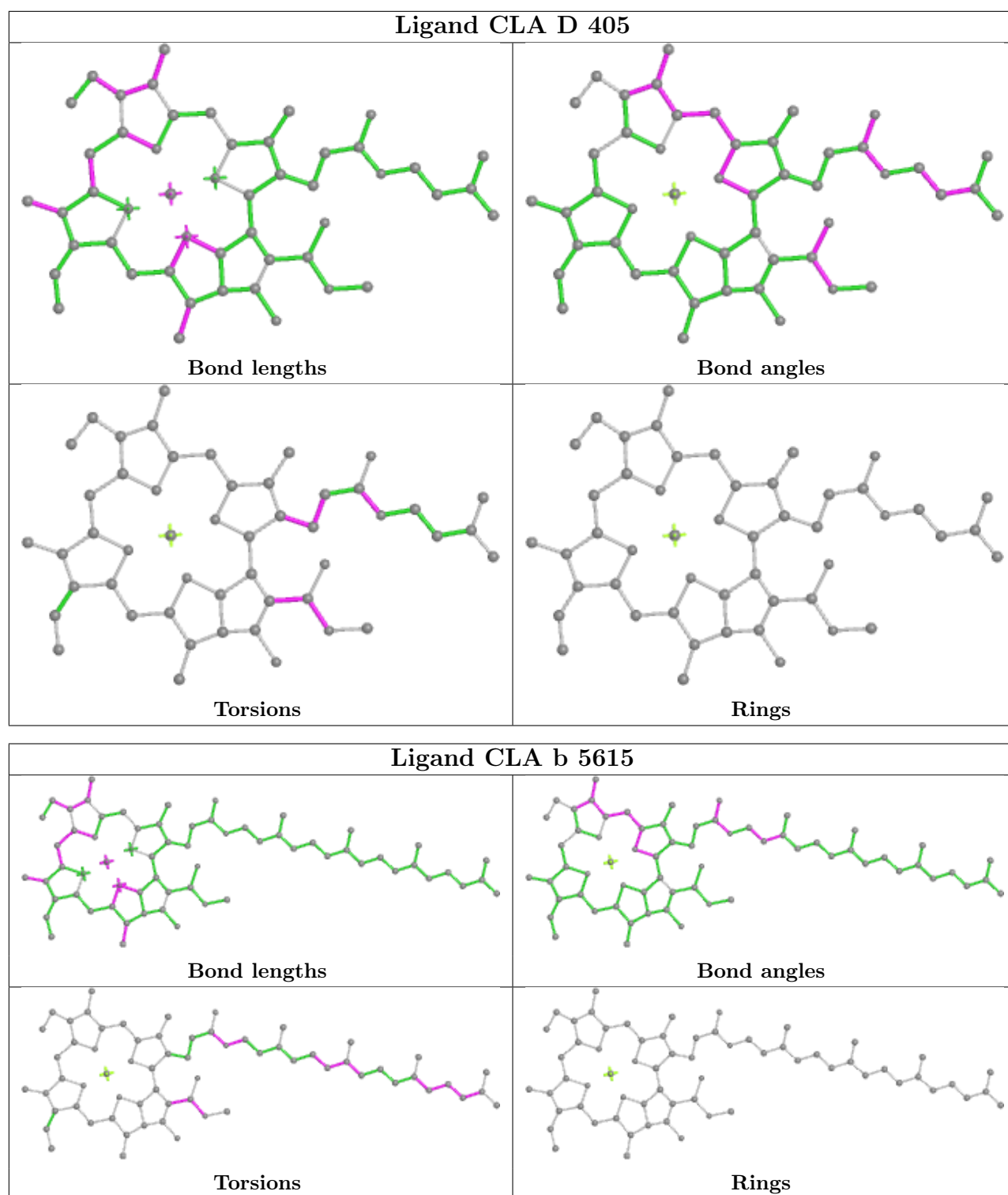


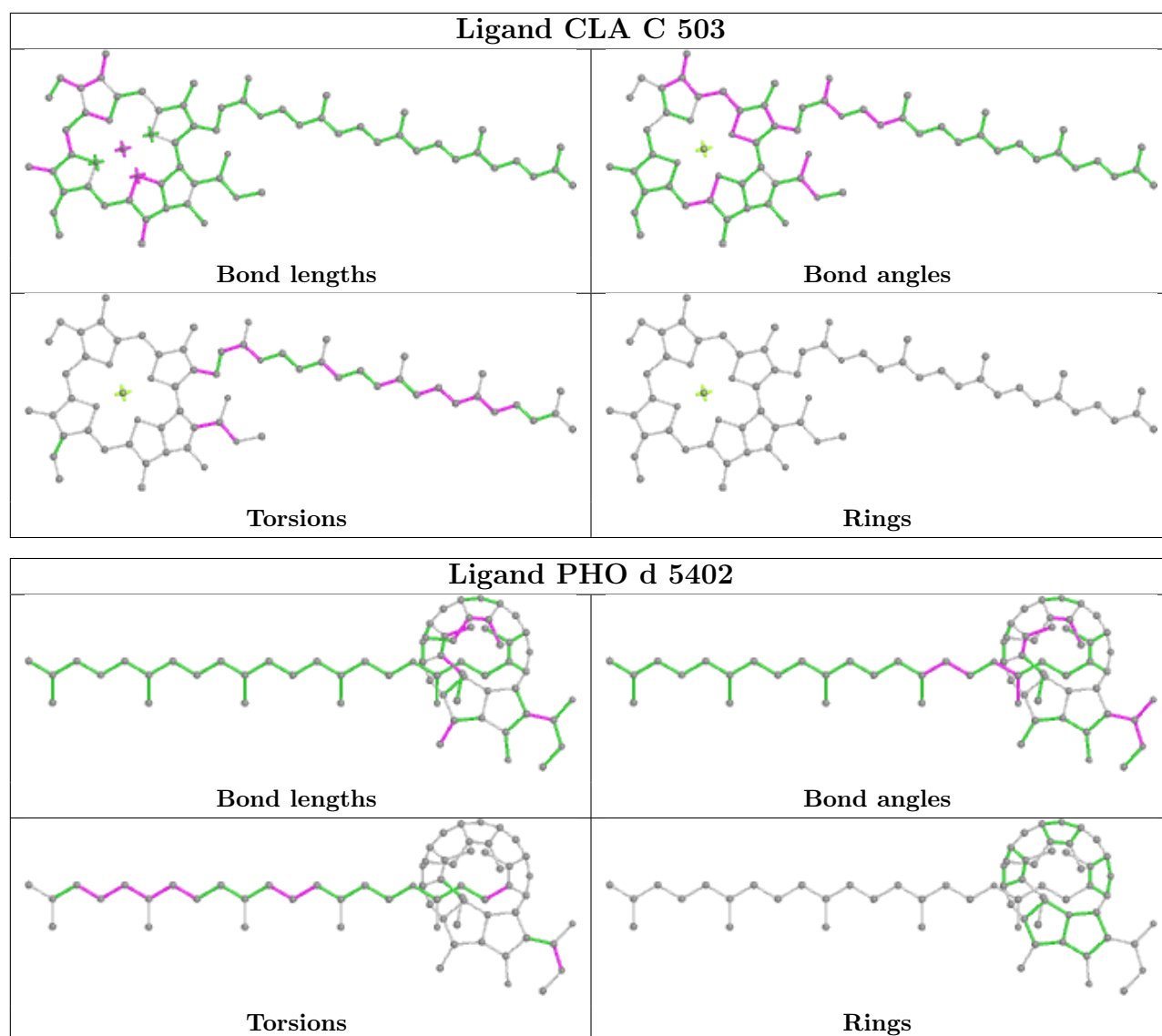




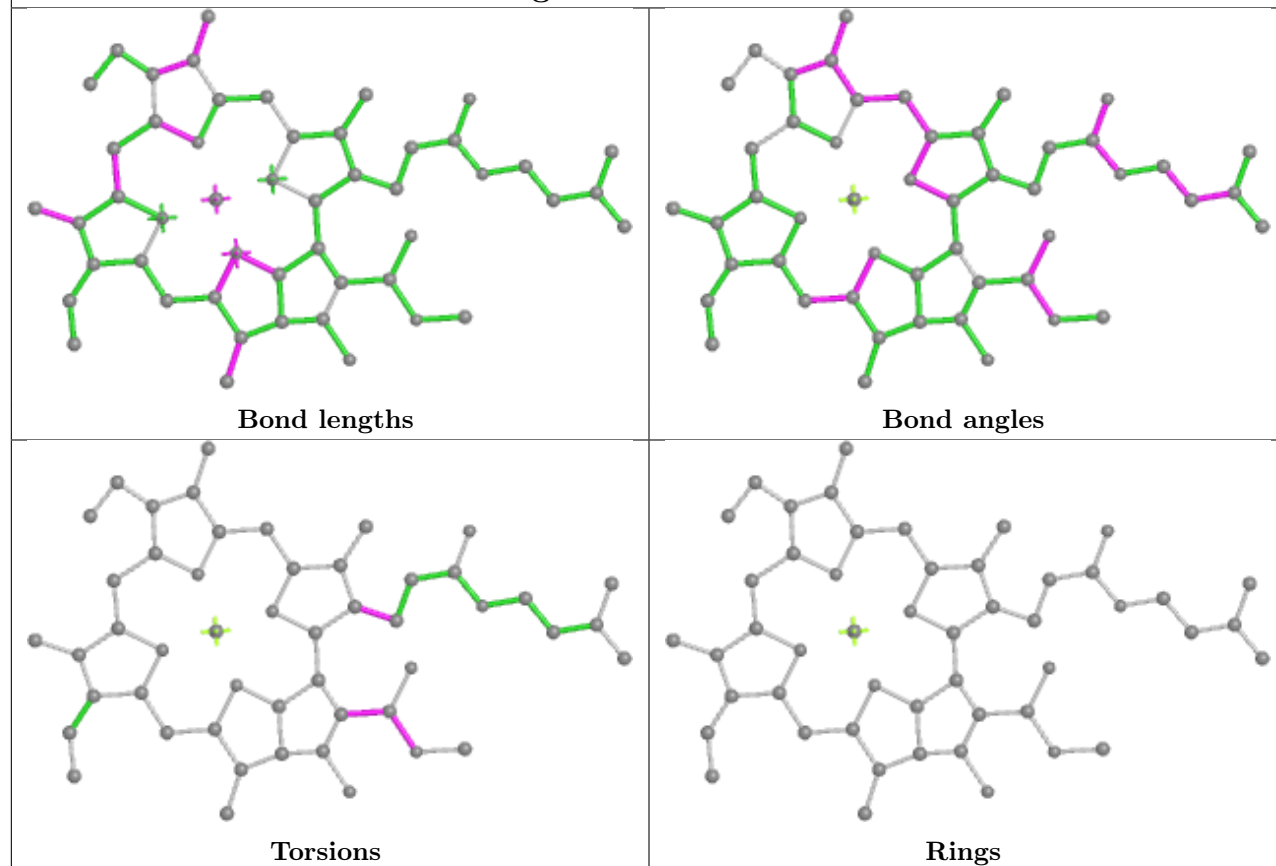




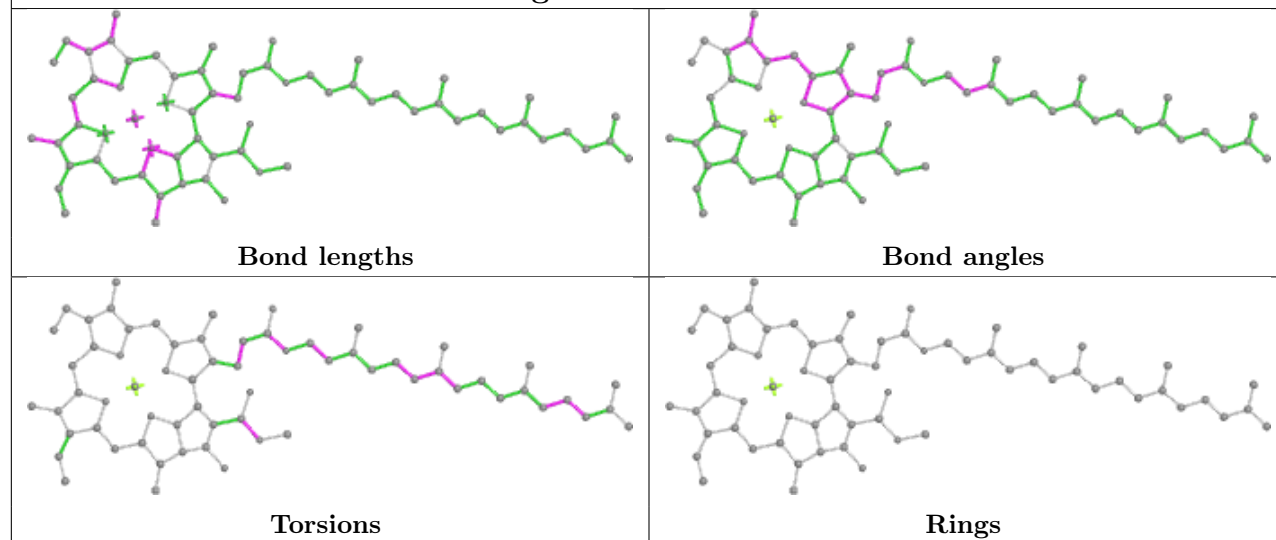


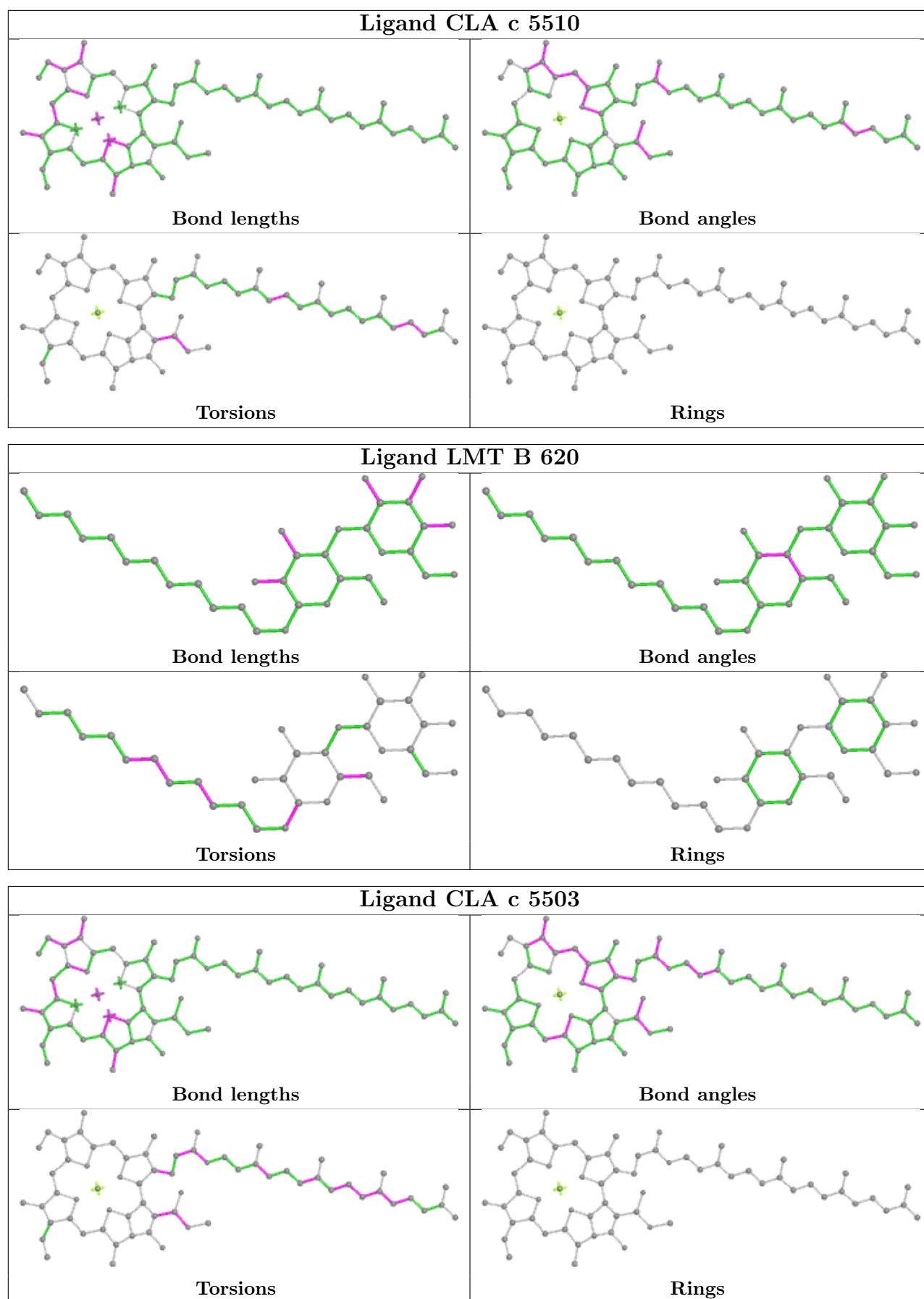


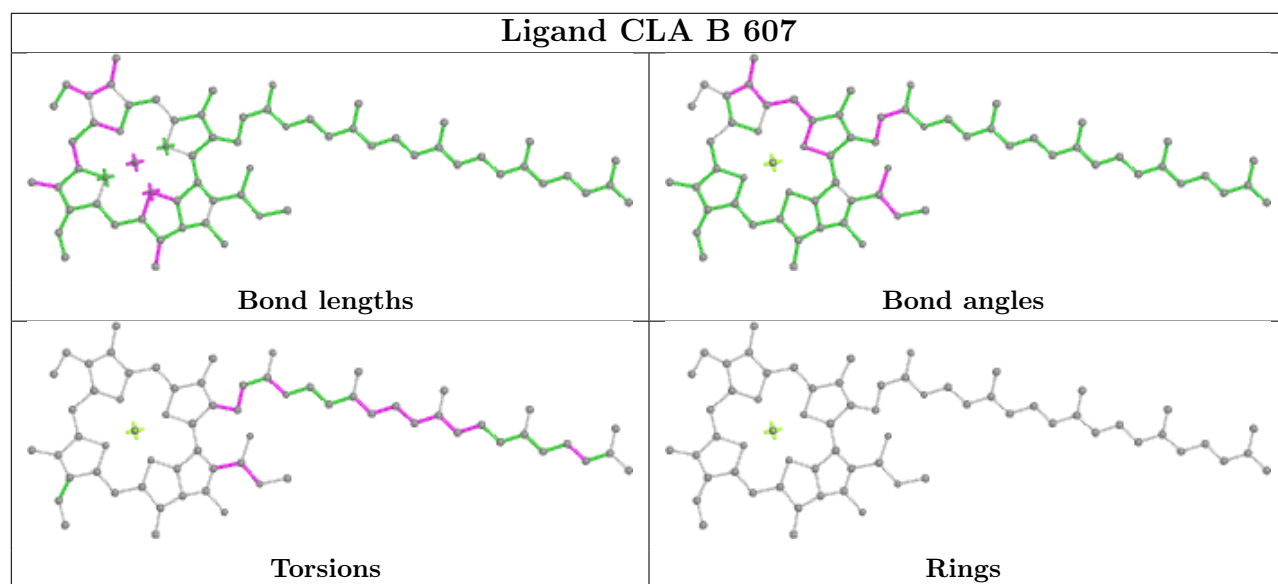
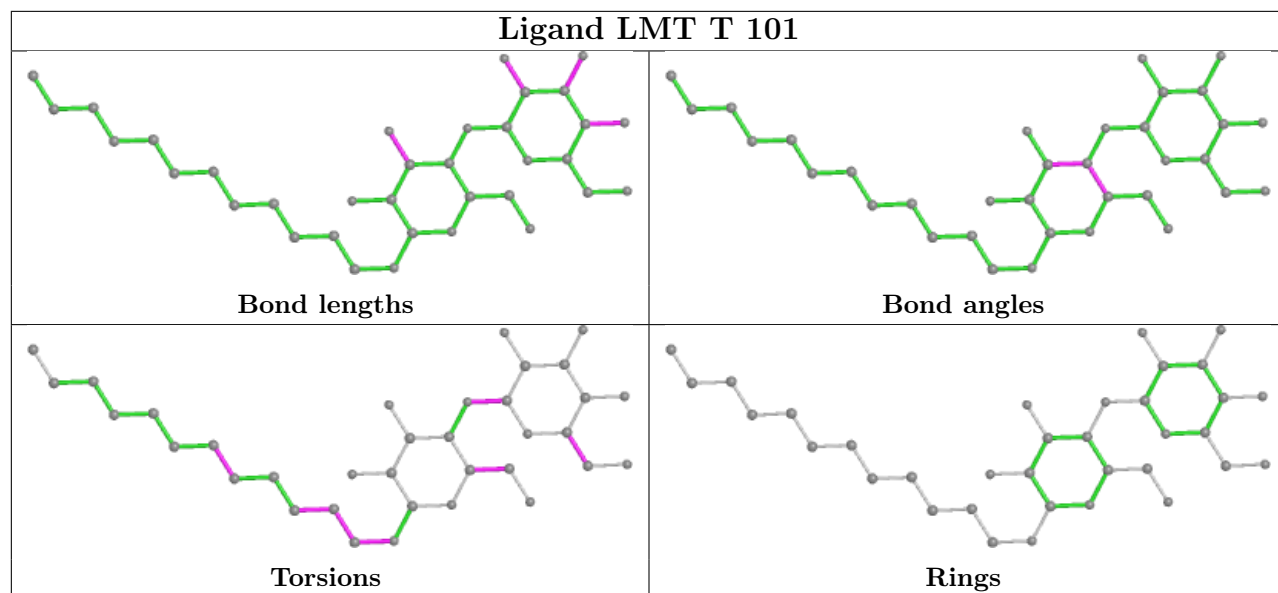
## Ligand CLA C 513



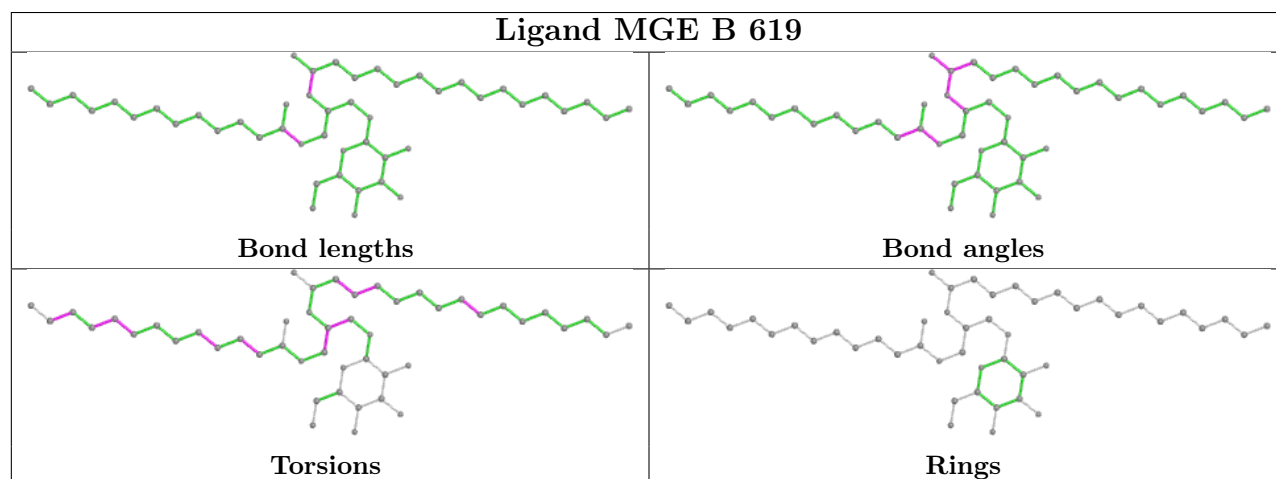
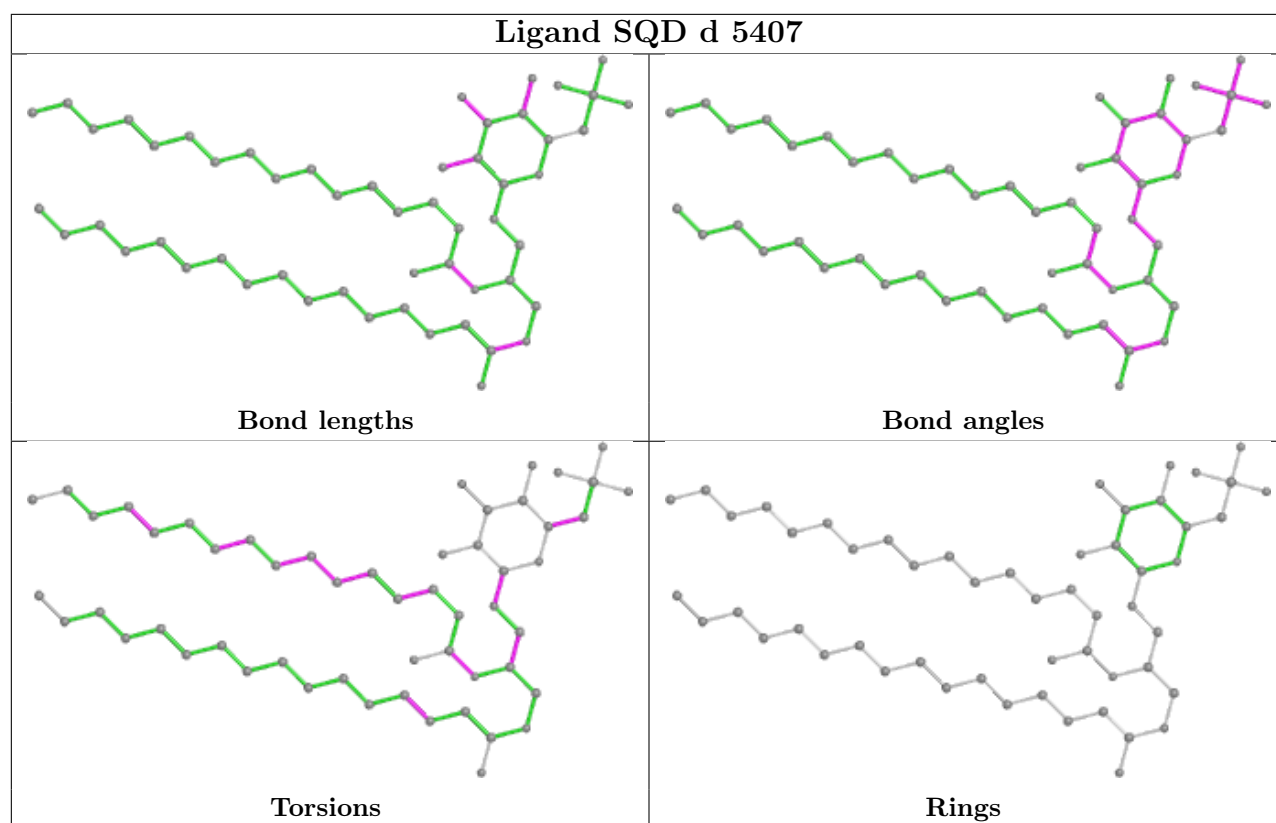
## Ligand CLA A 401

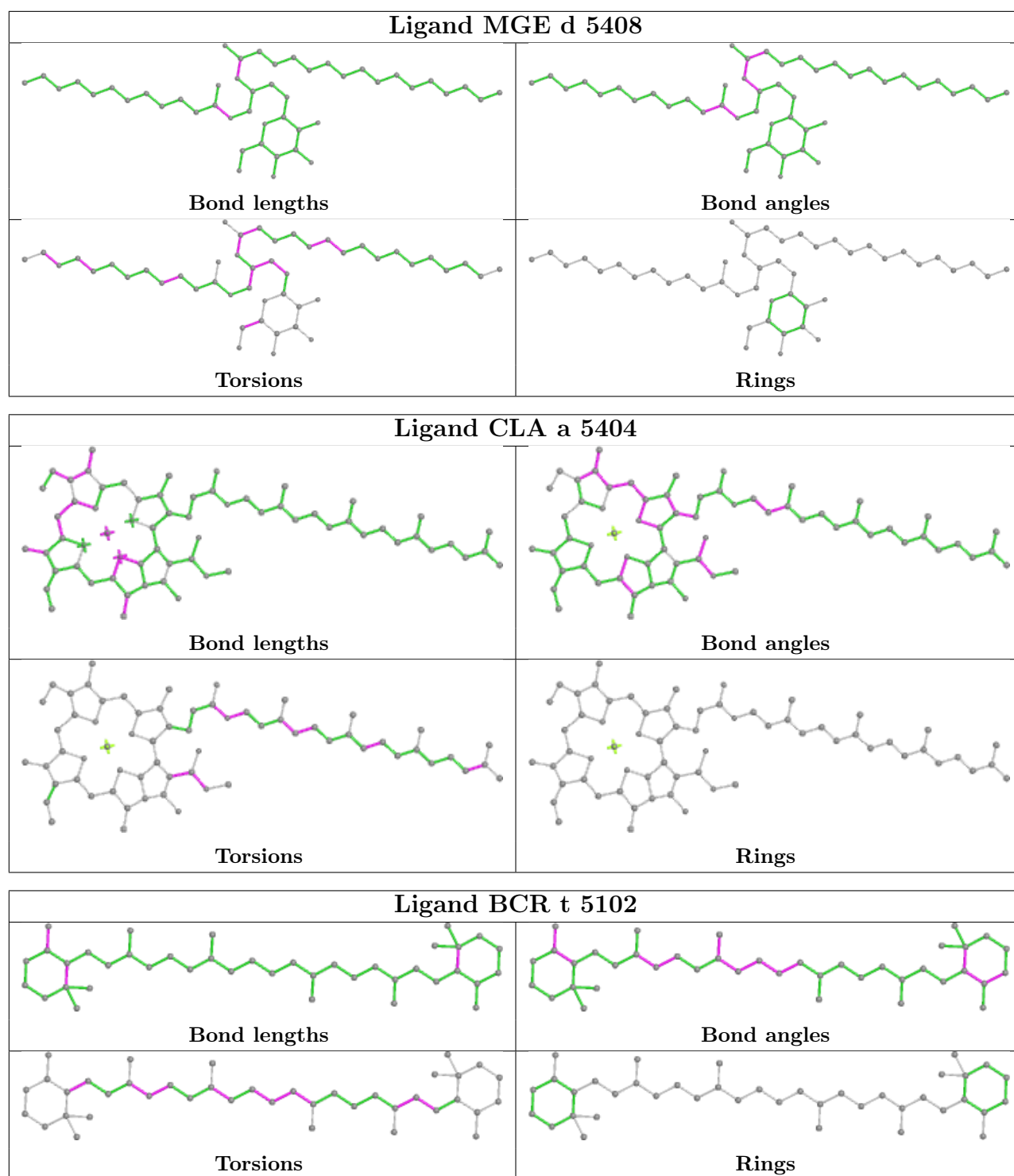


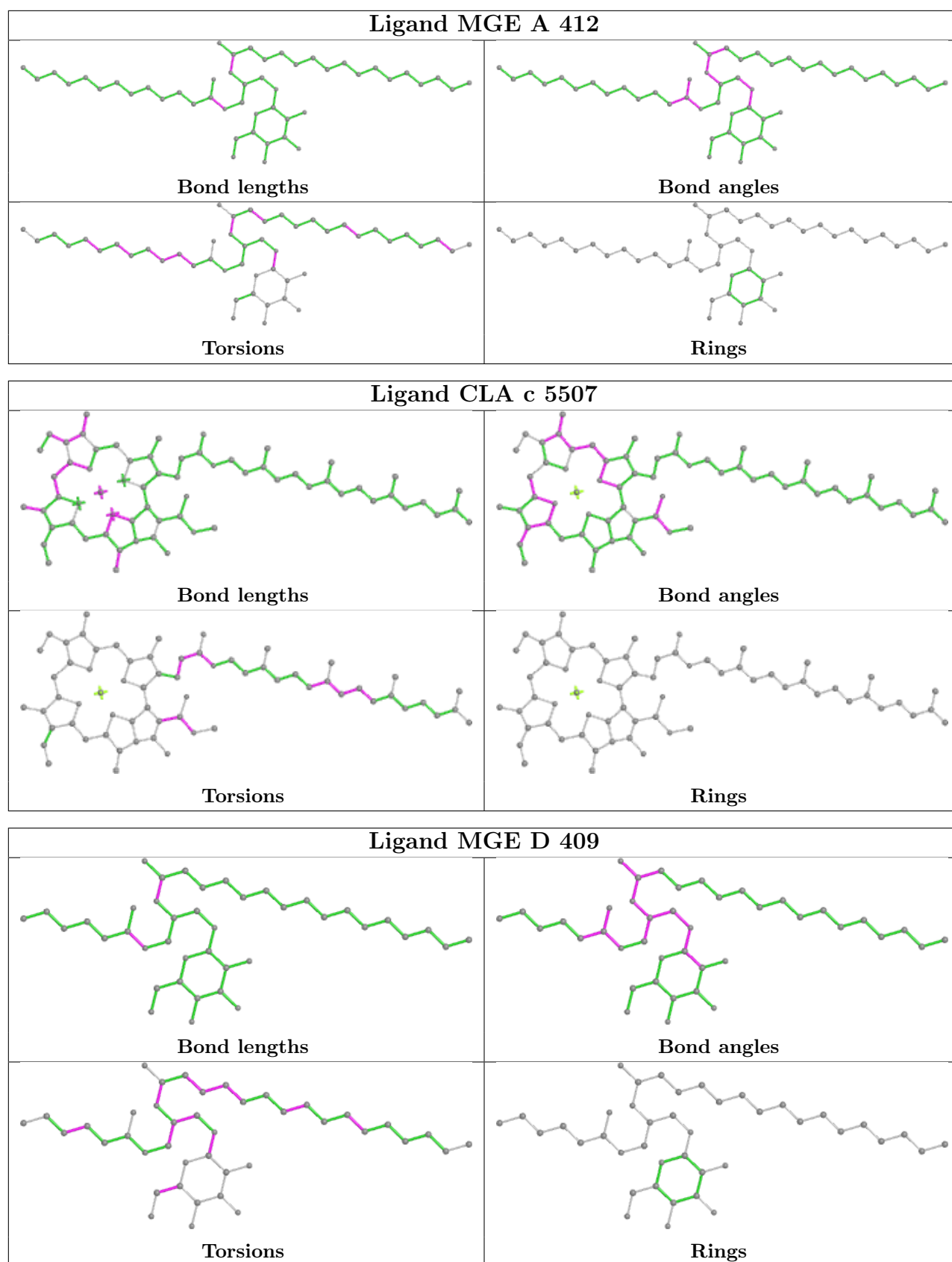


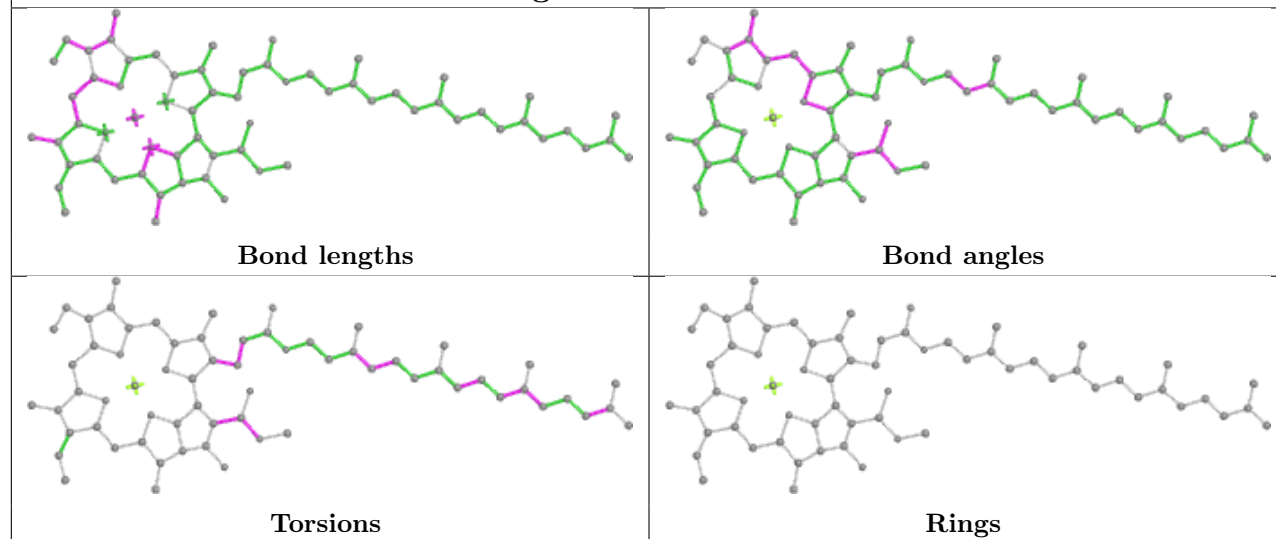
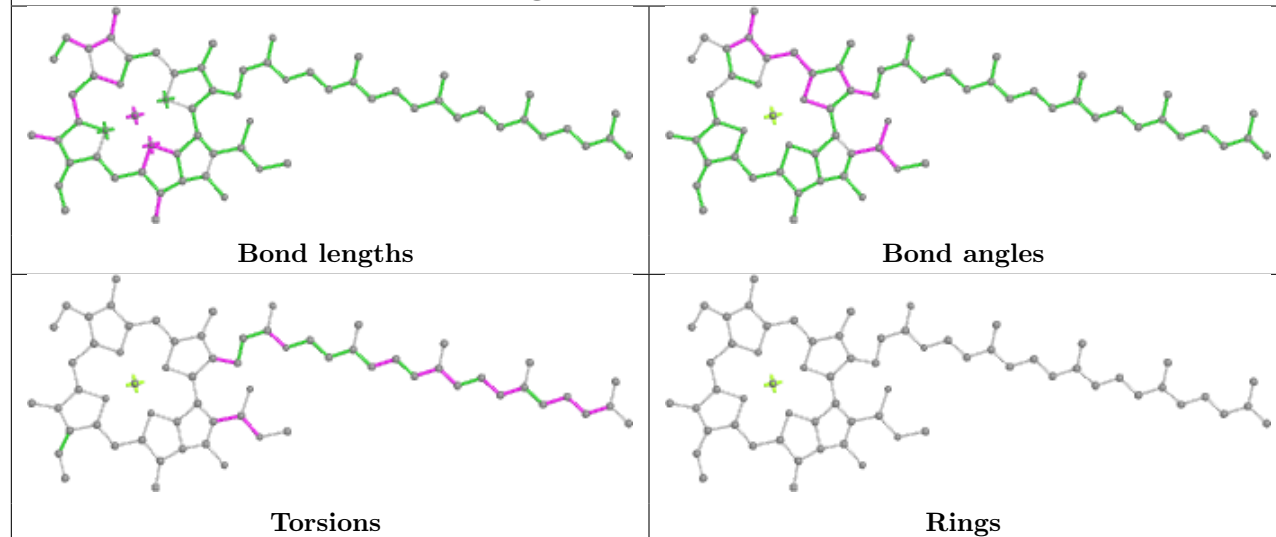
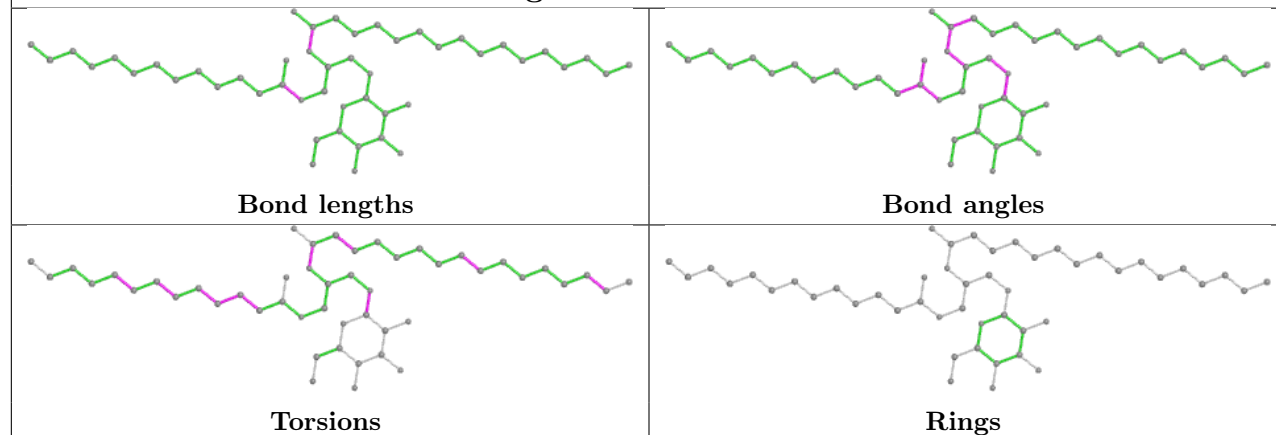


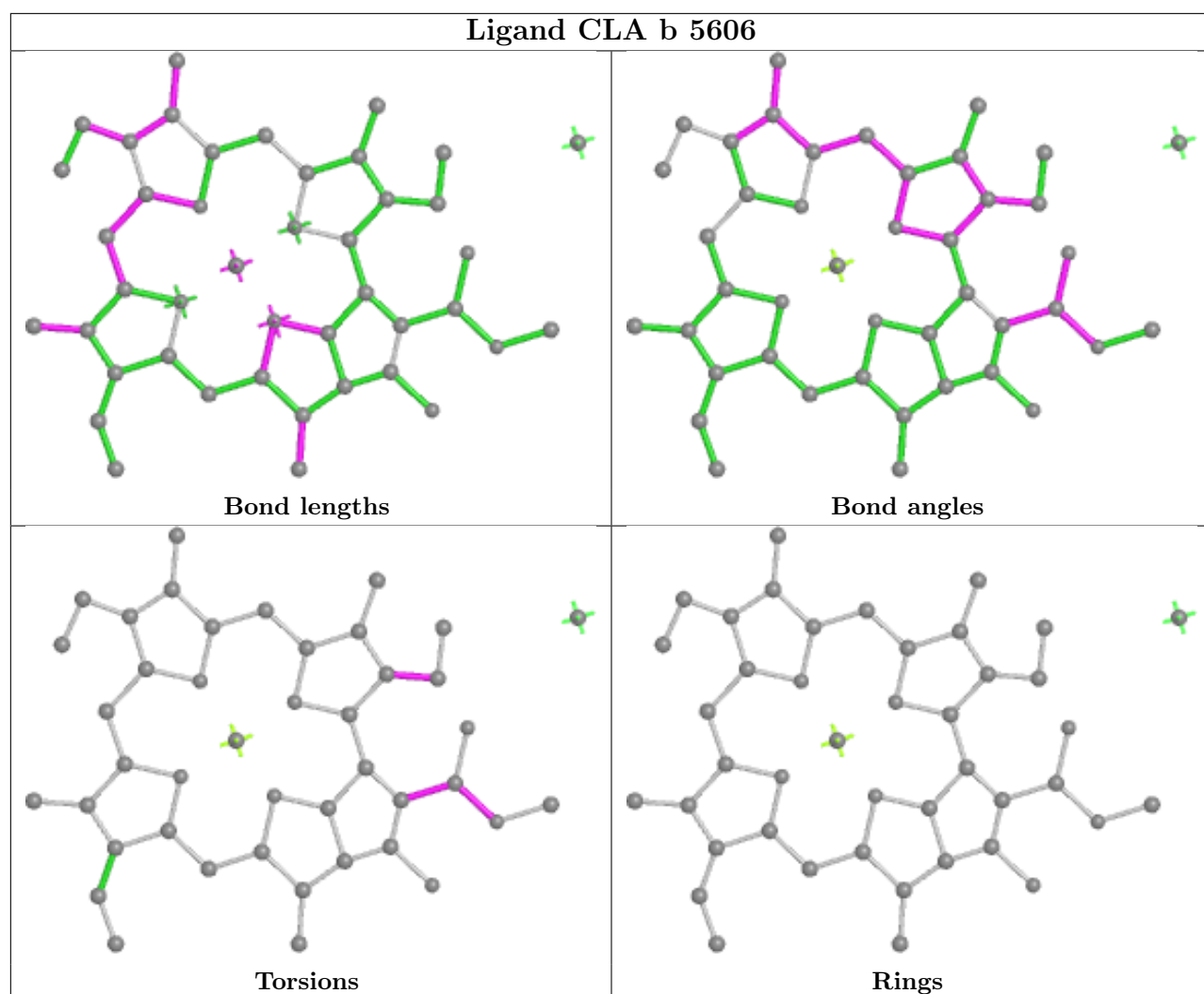


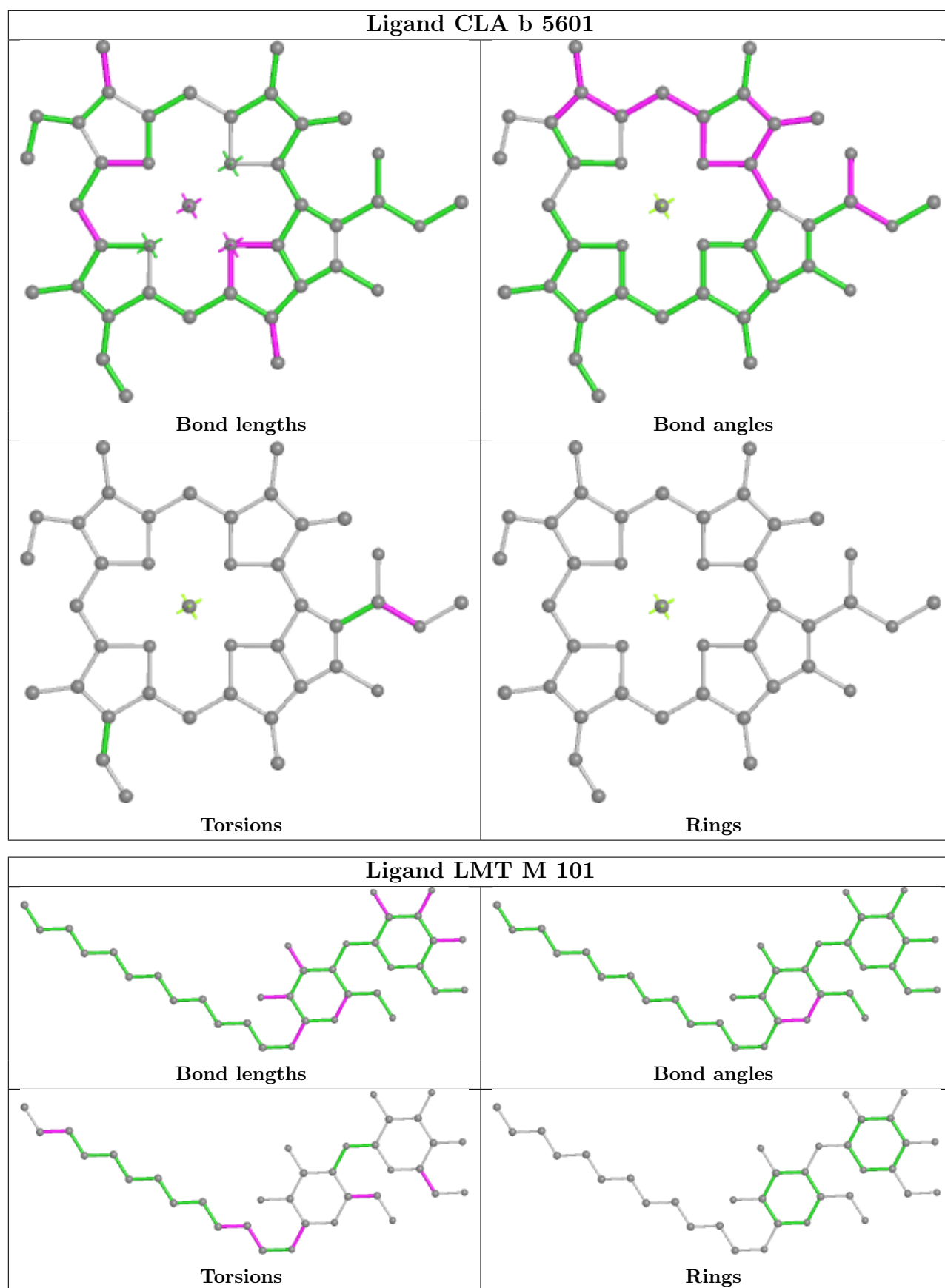


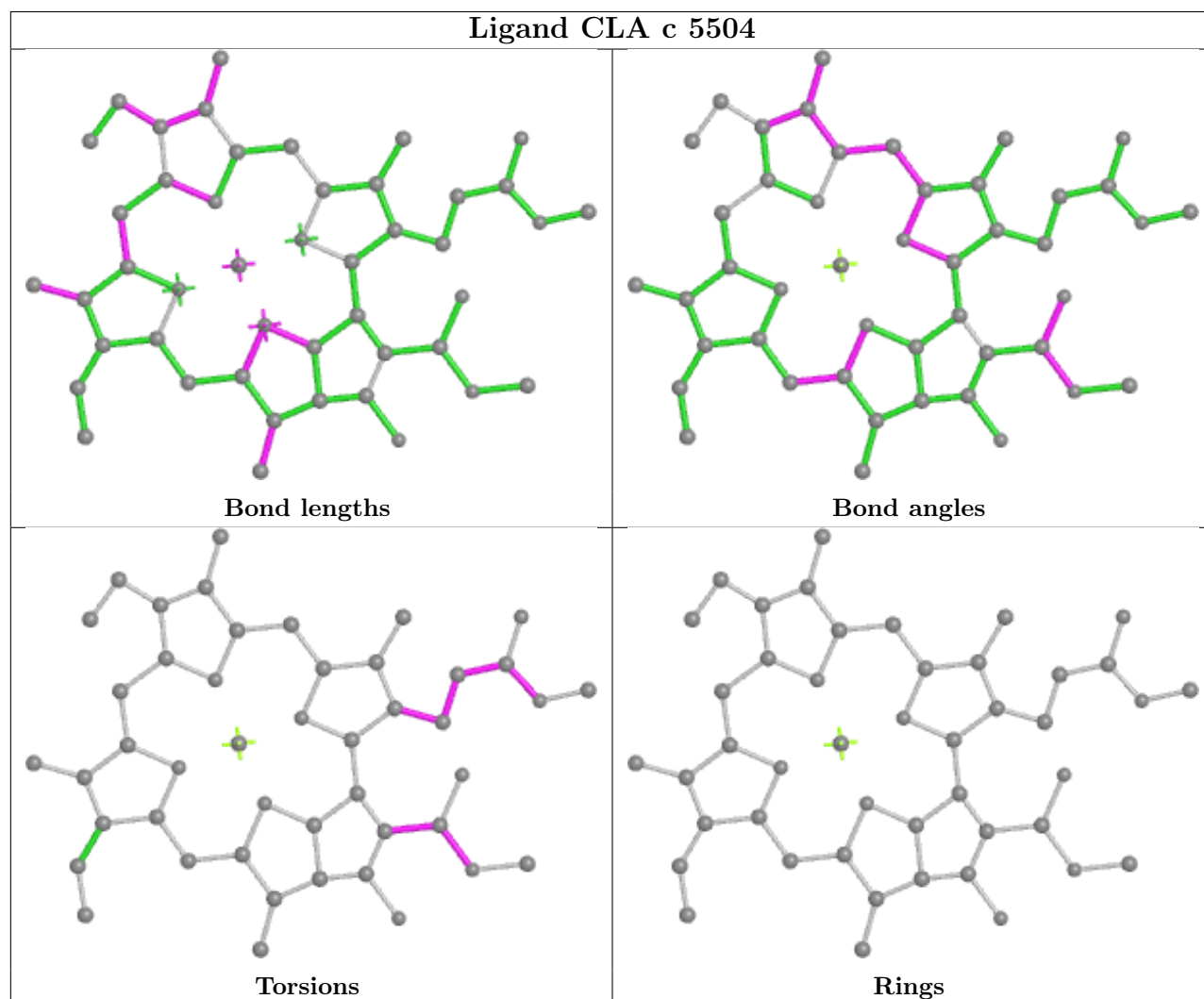
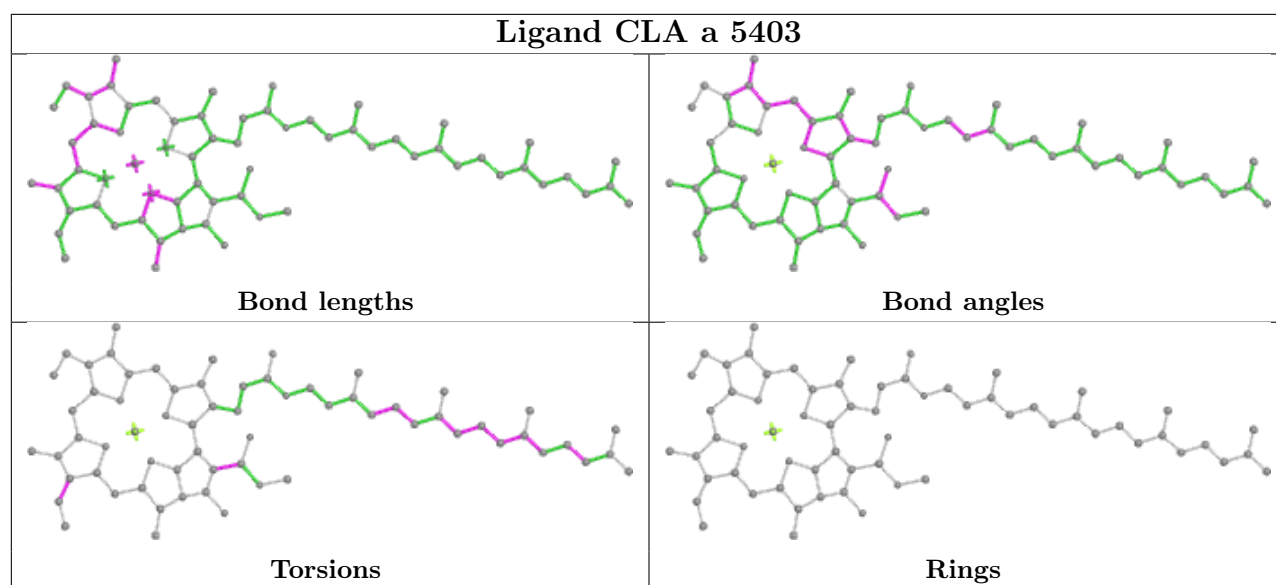


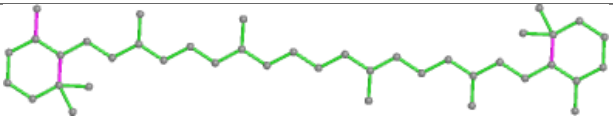
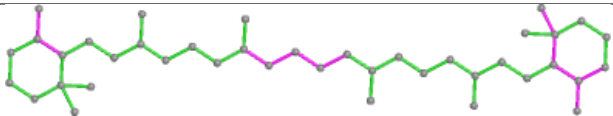
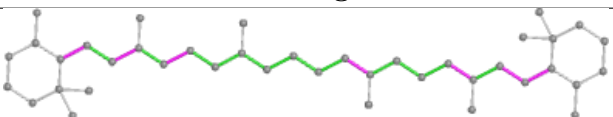
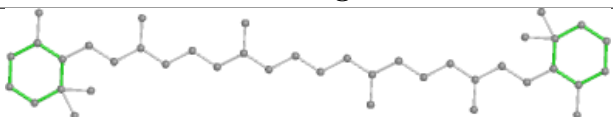


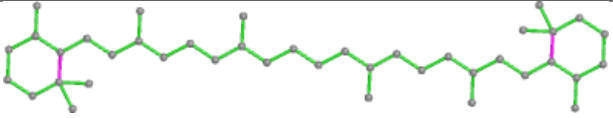
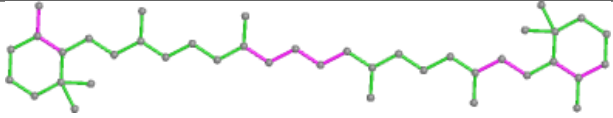
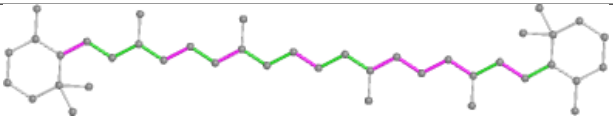
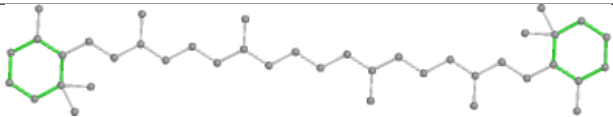
**Ligand CLA B 606****Ligand CLA c 5506****Ligand MGE l 5101**

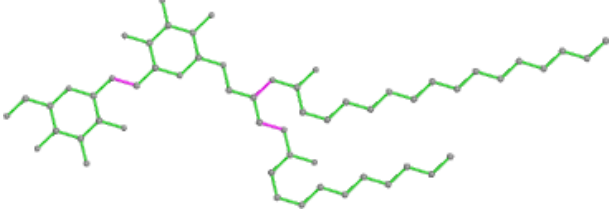
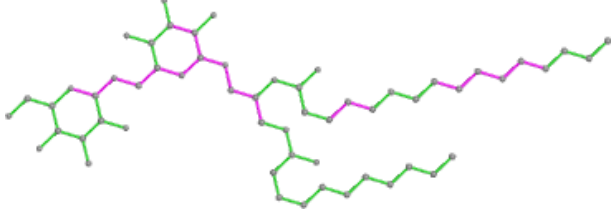
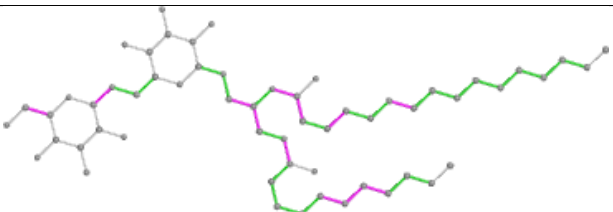
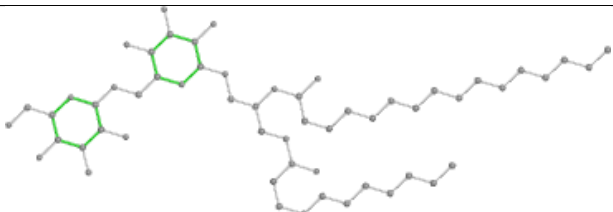




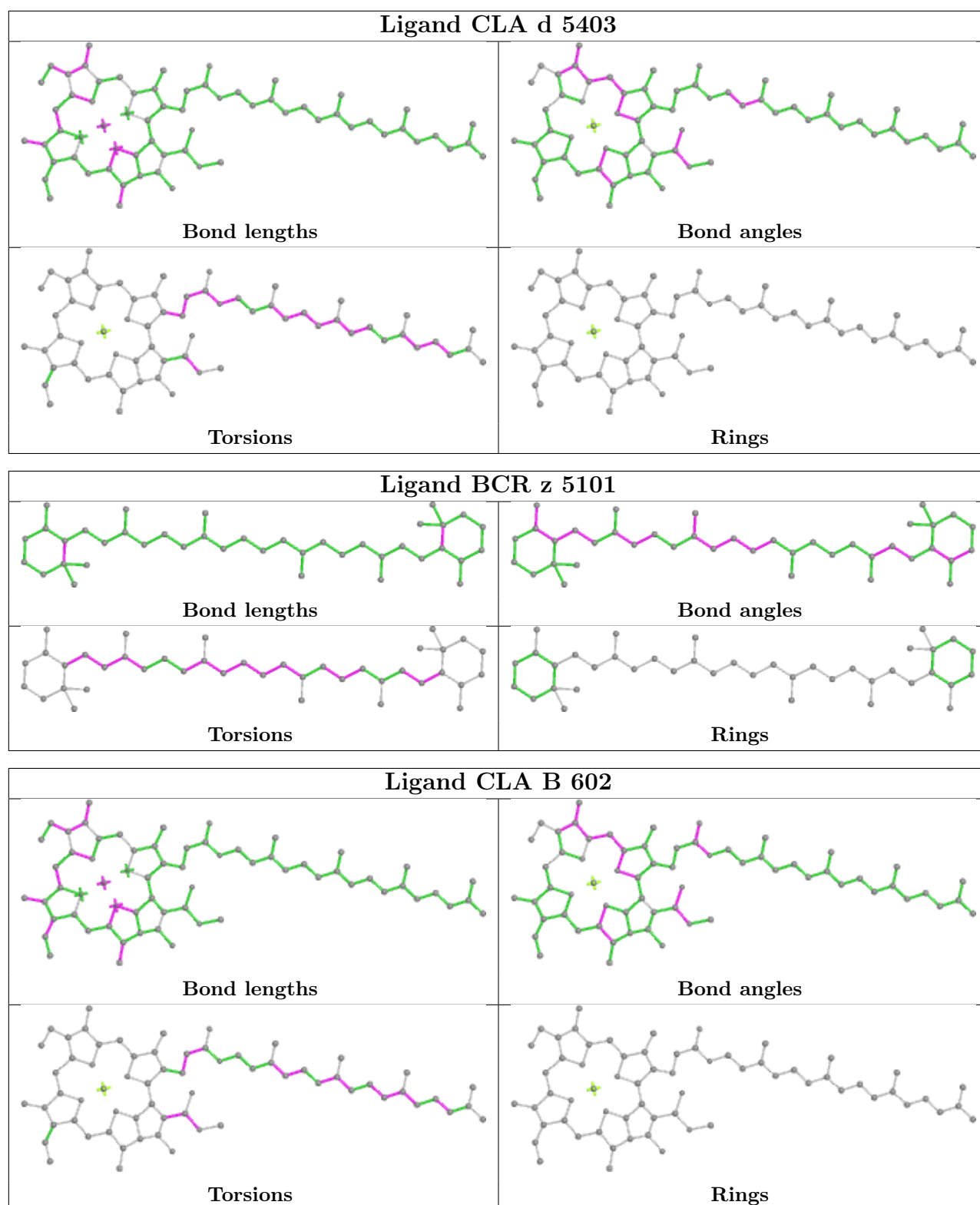


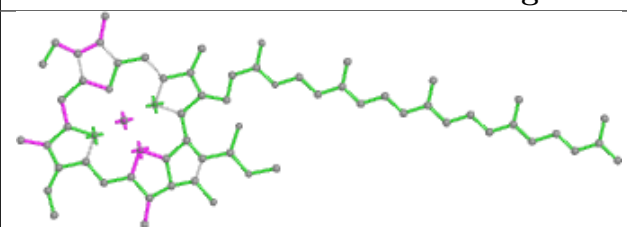
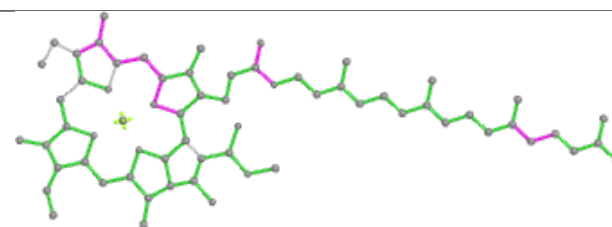
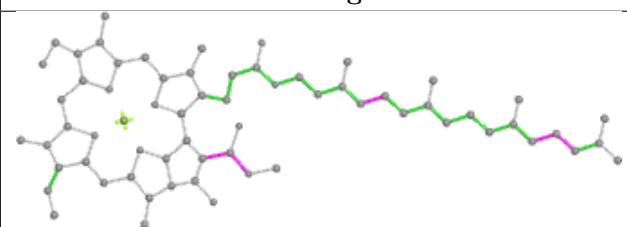
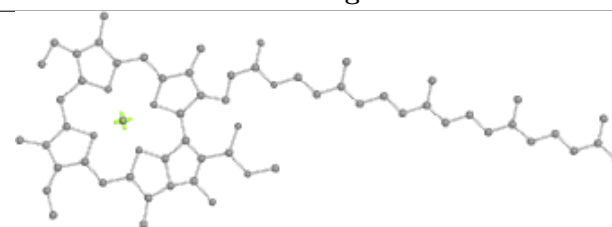
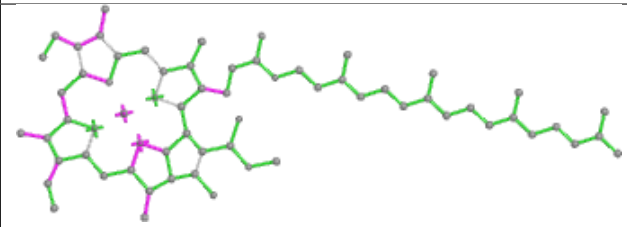
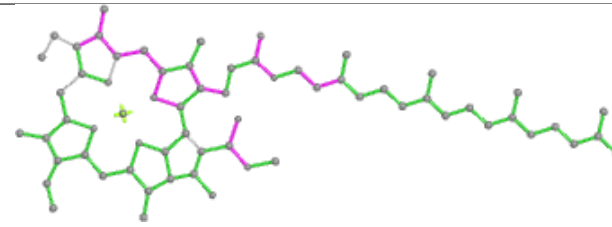
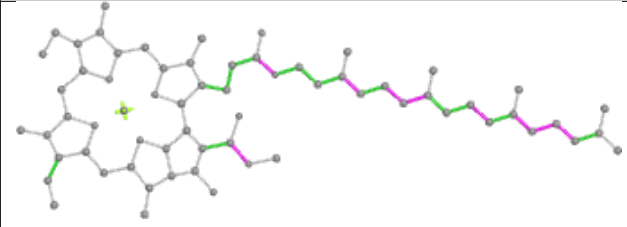
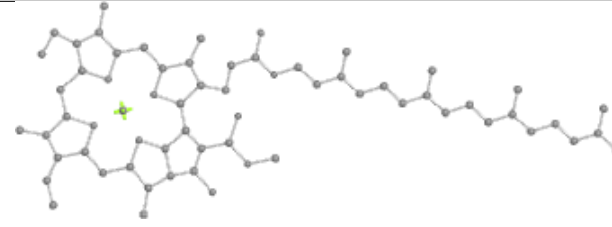
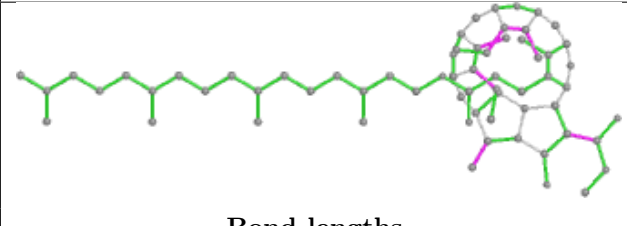
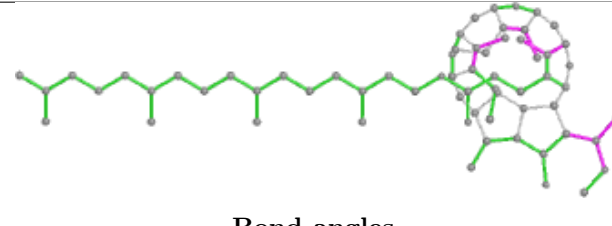
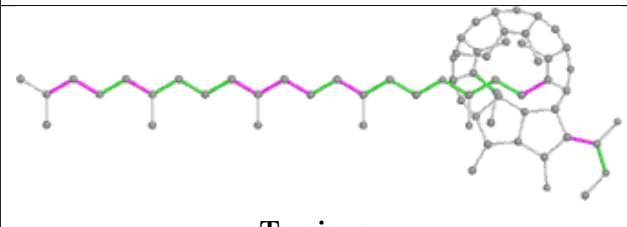
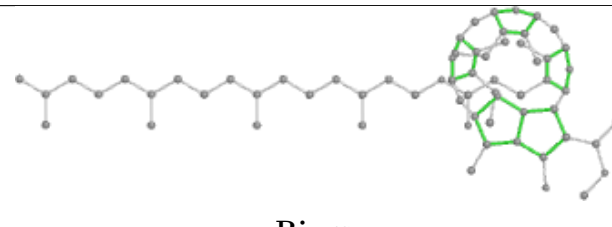
Ligand BCR T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

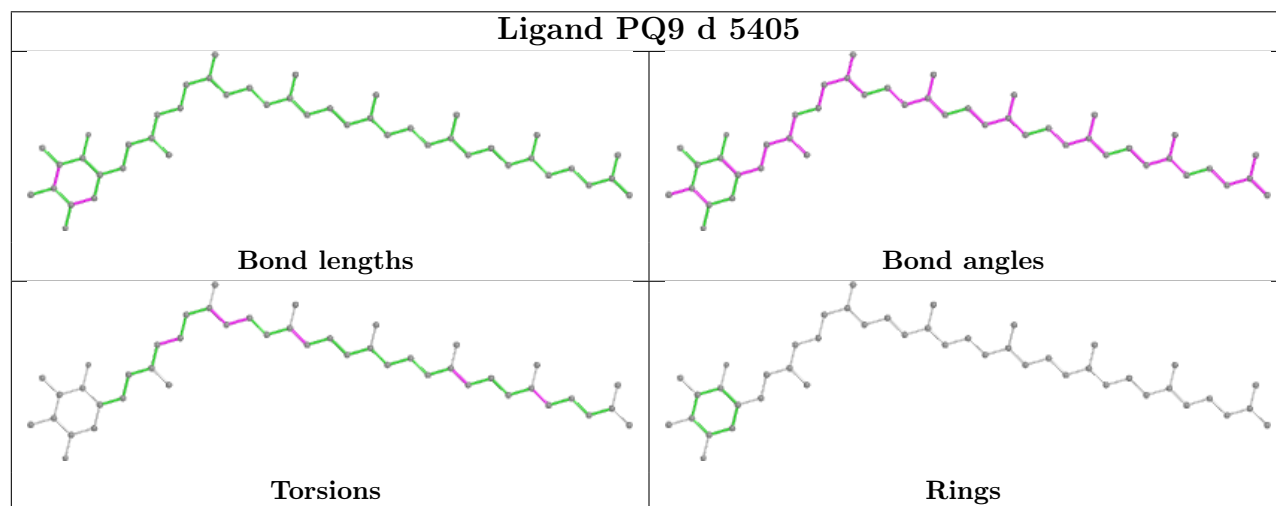
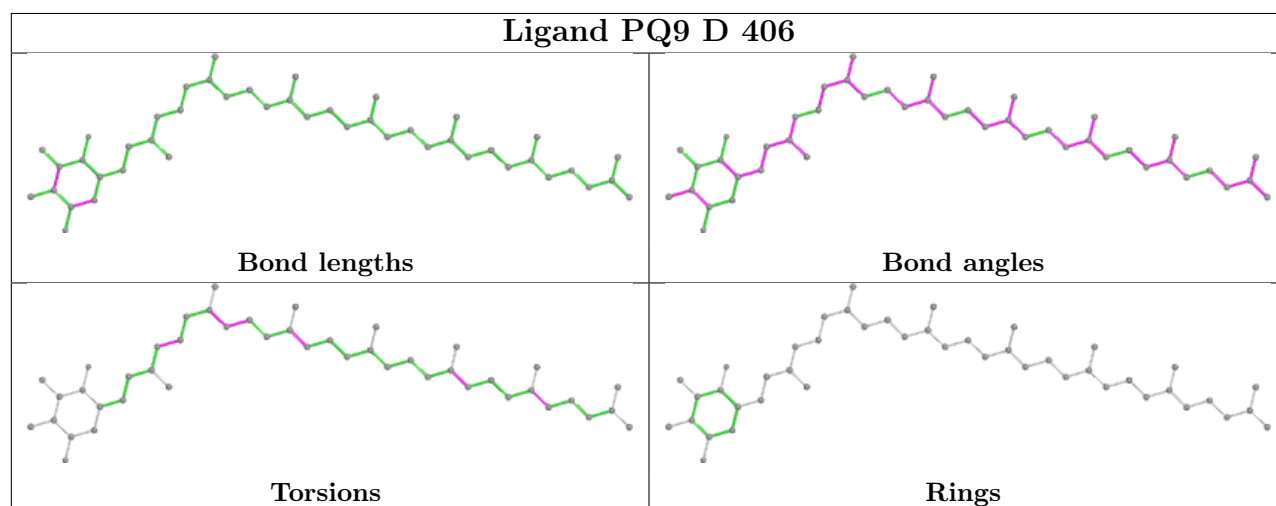
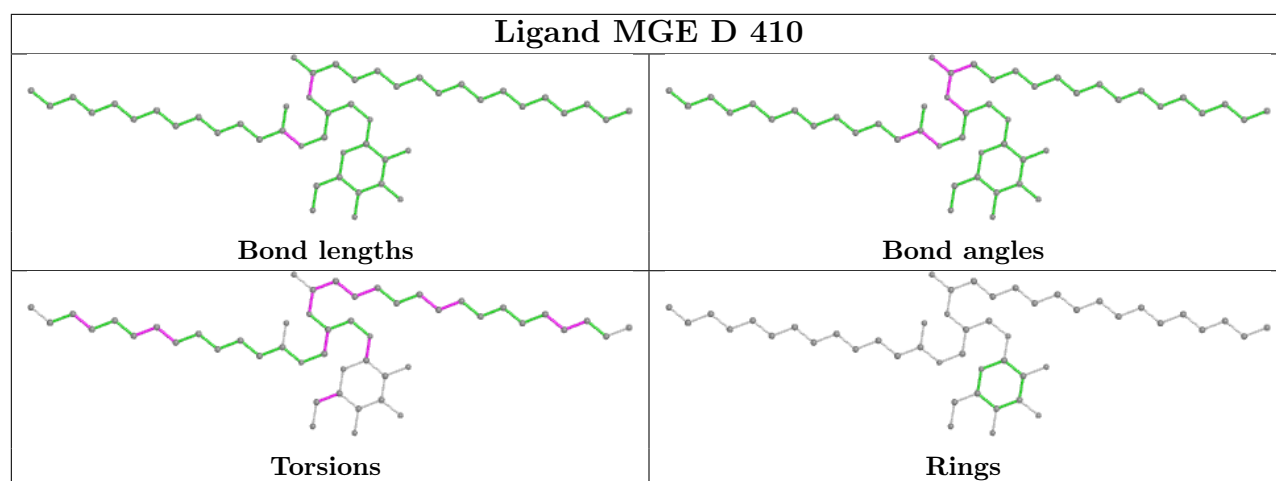
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD a 5411	
	
Bond lengths	Bond angles
	
Torsions	Rings

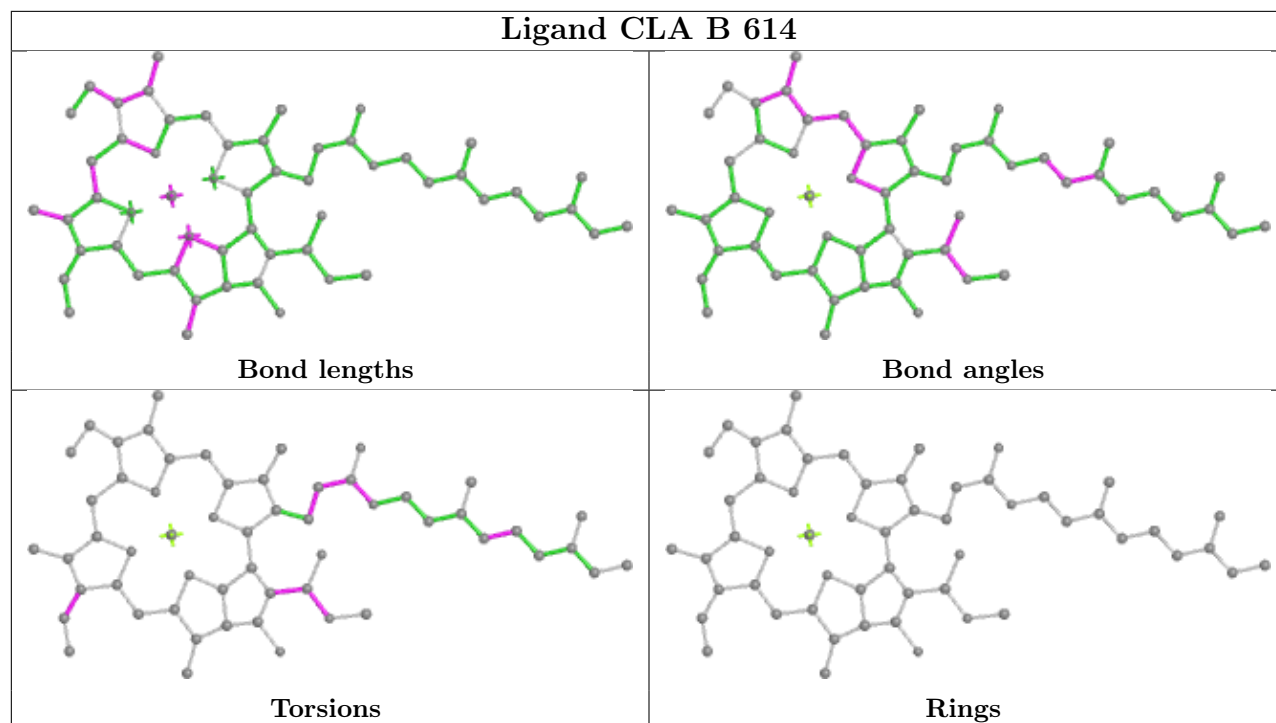




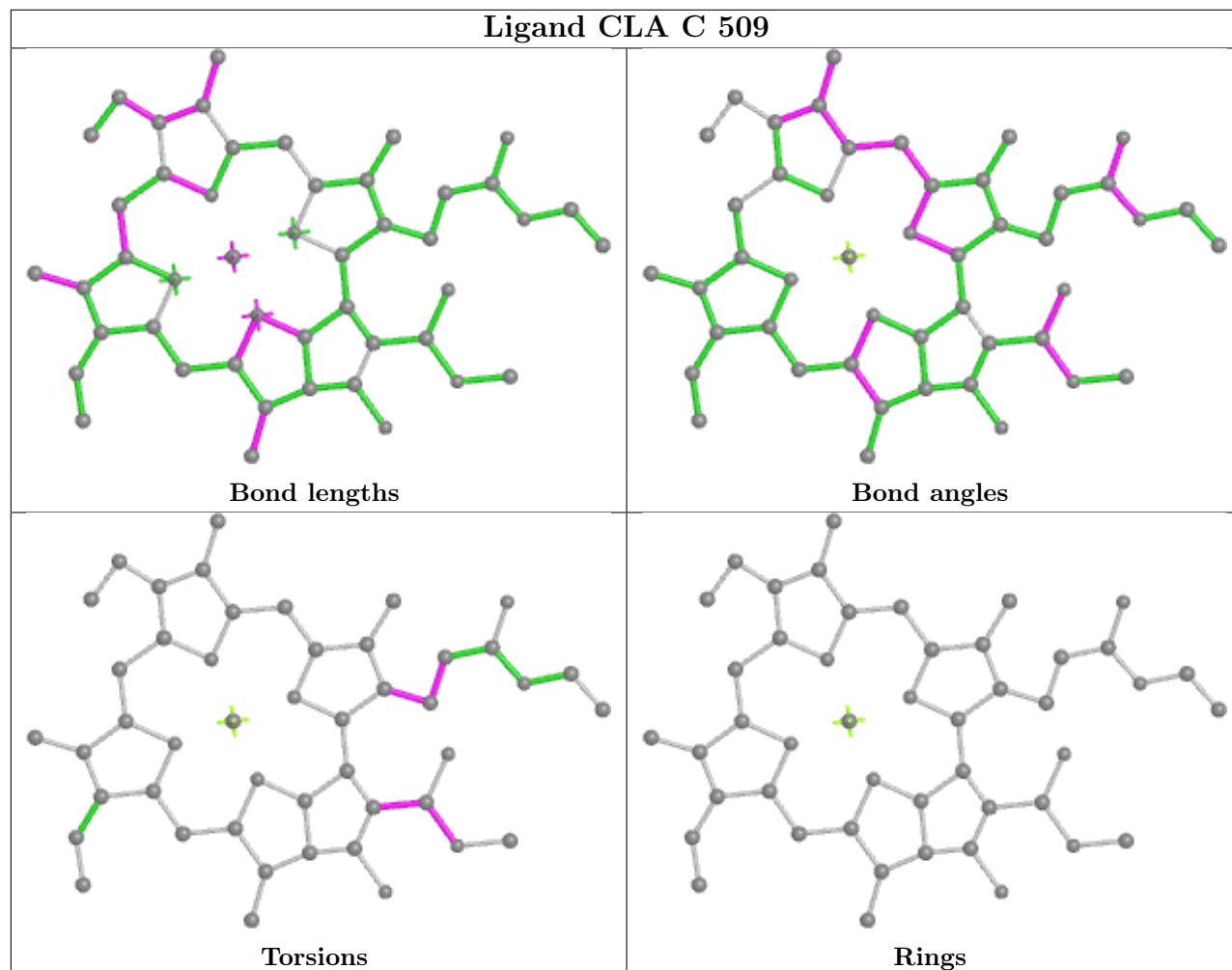
Ligand CLA C 510	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b 5611	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PHO a 5405	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

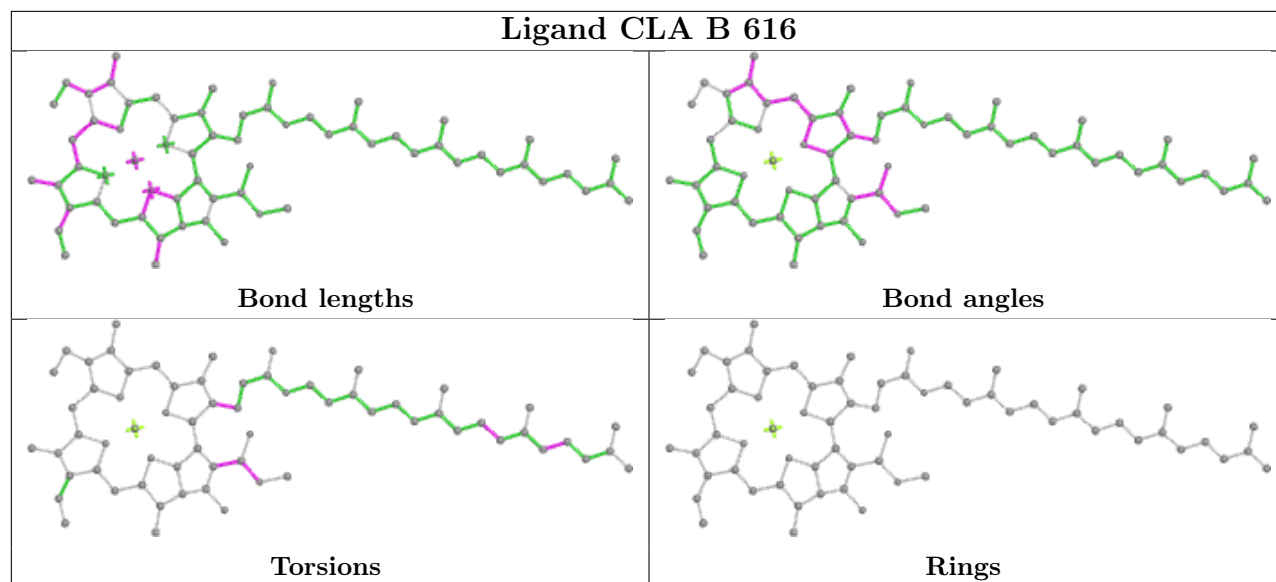
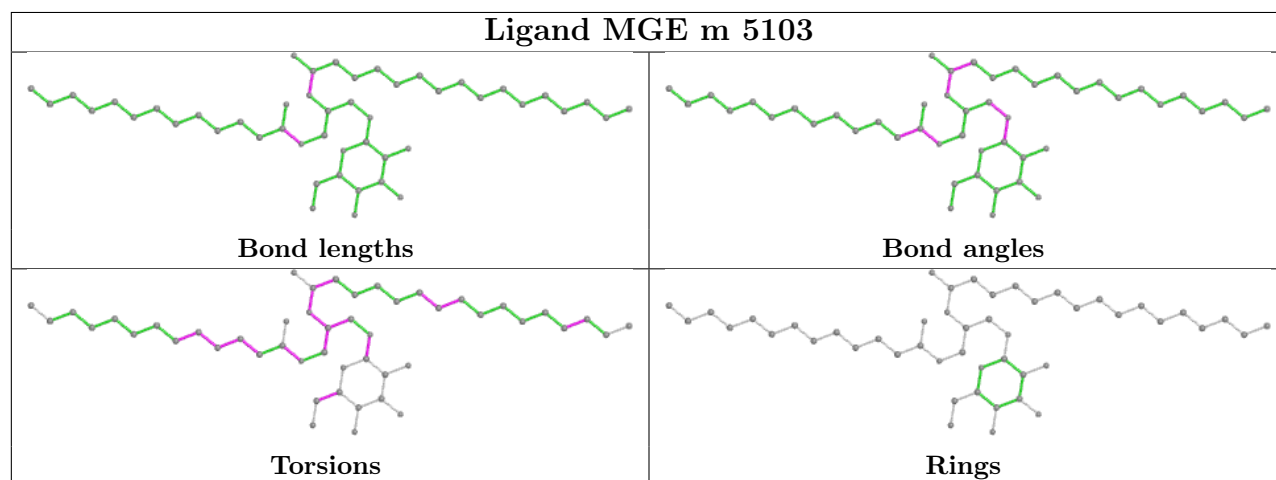
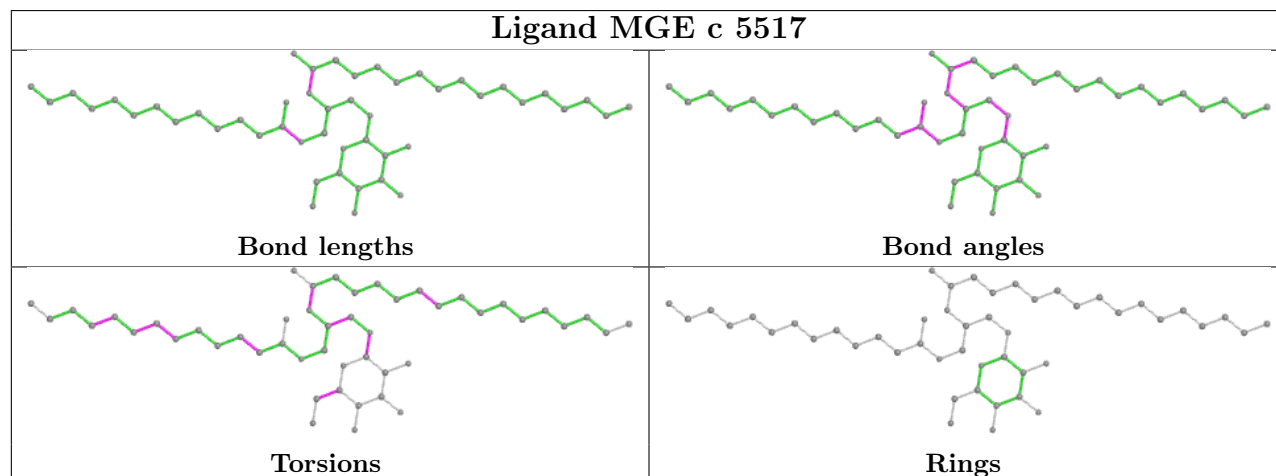


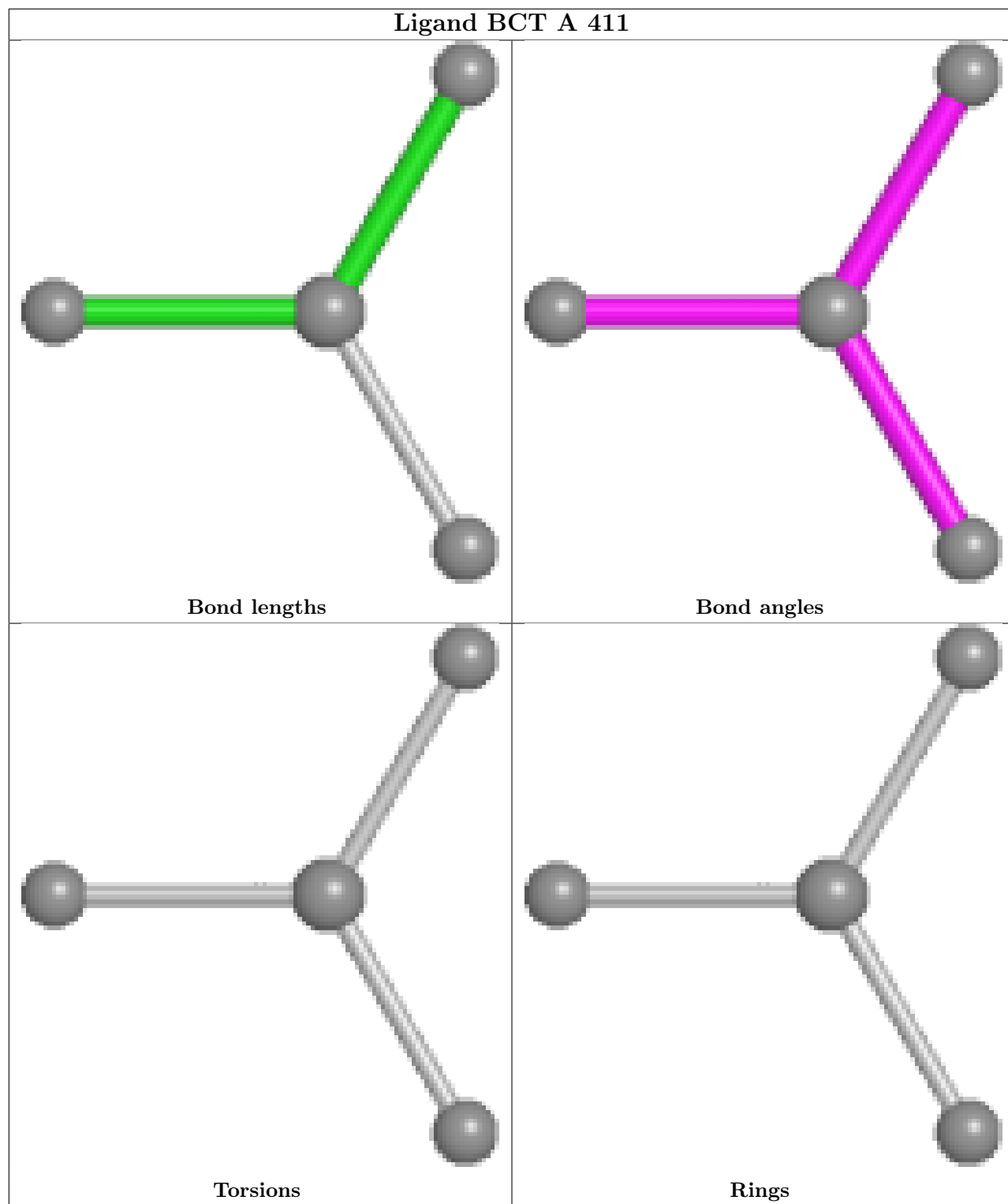
## Ligand CLA B 614

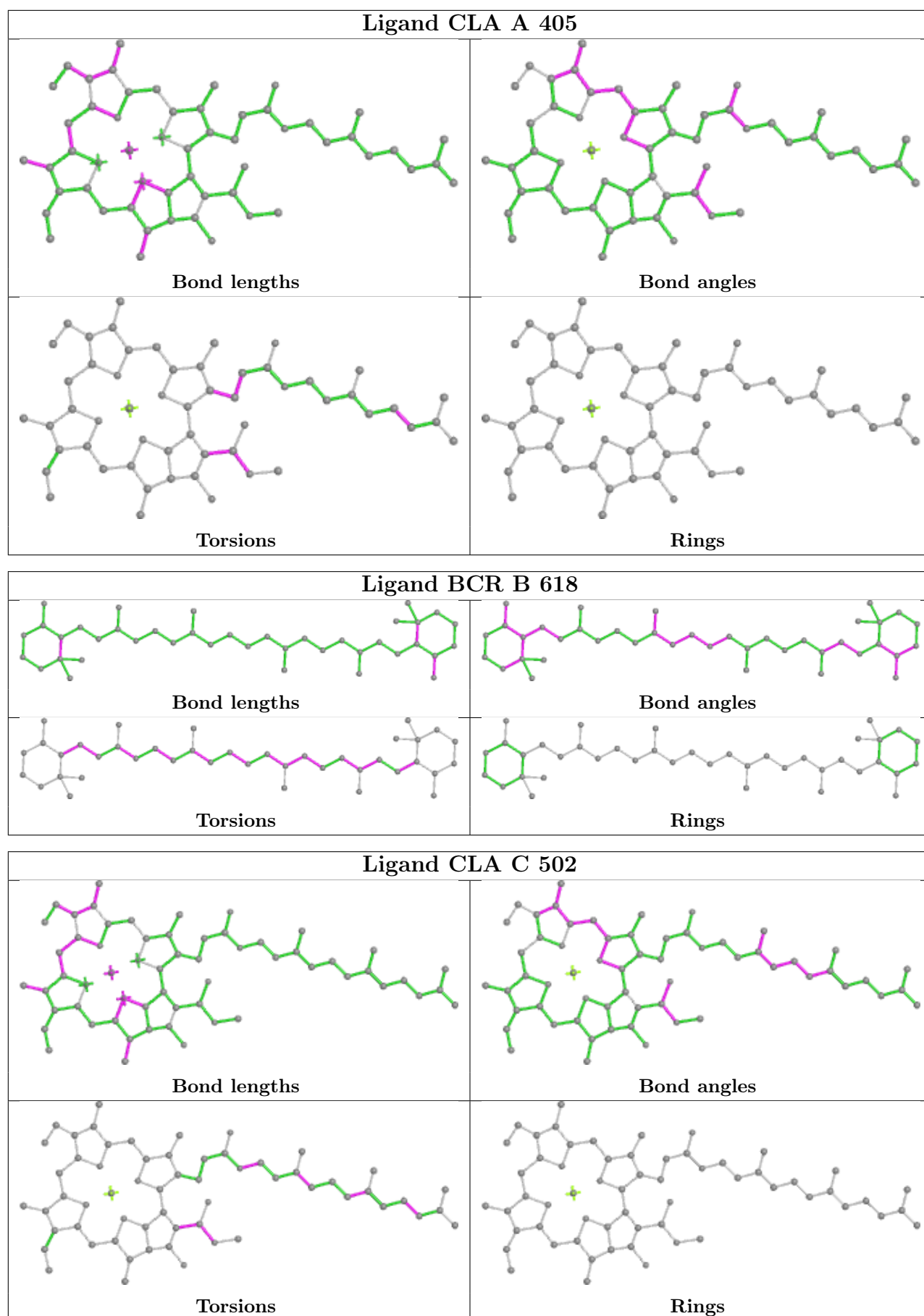


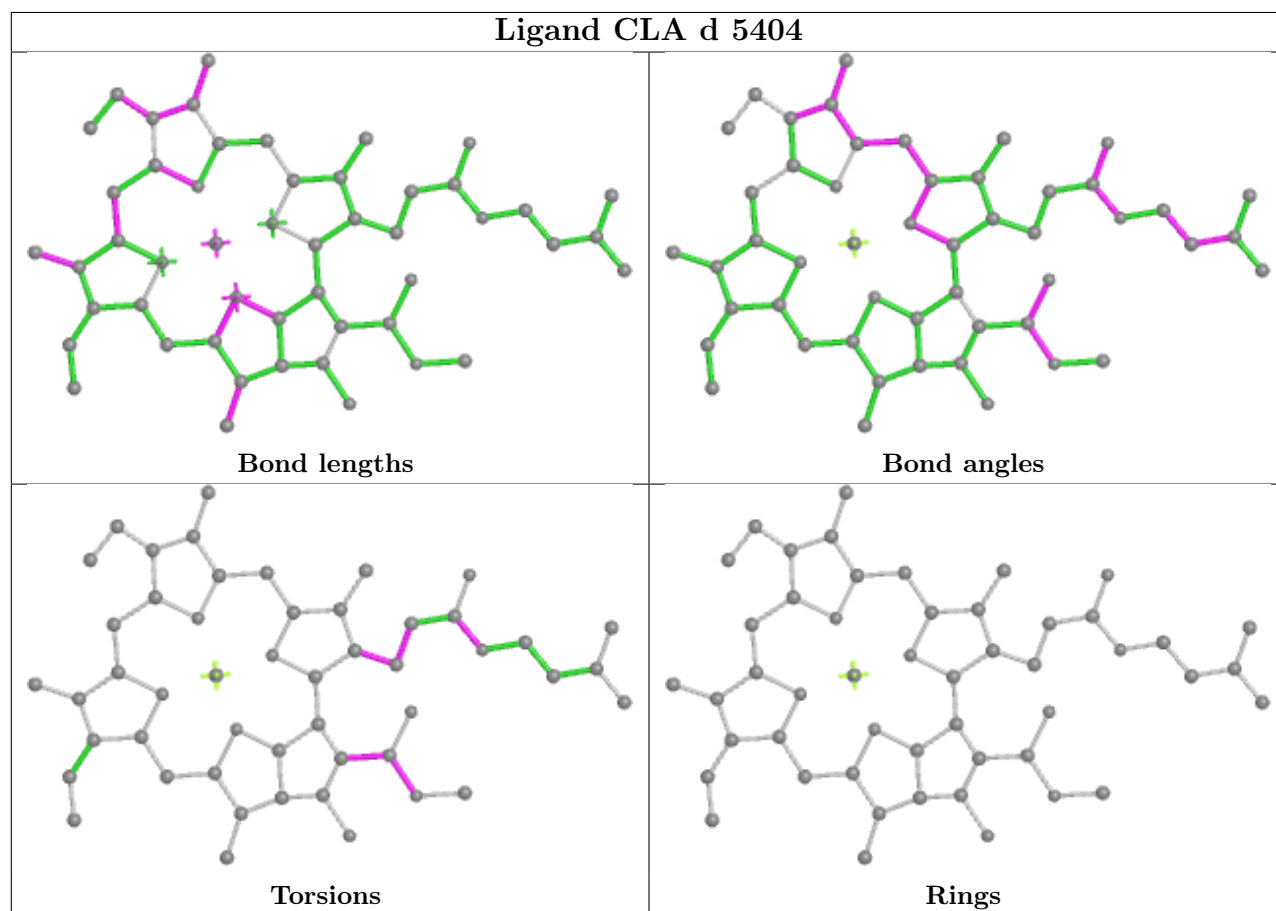
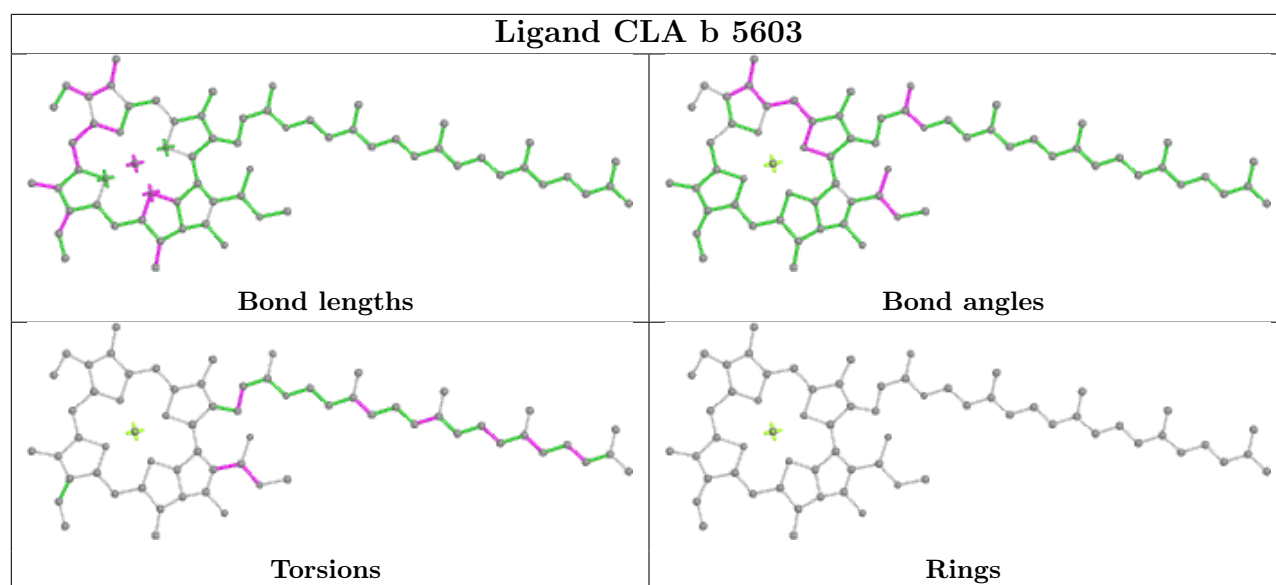
## Ligand CLA C 509



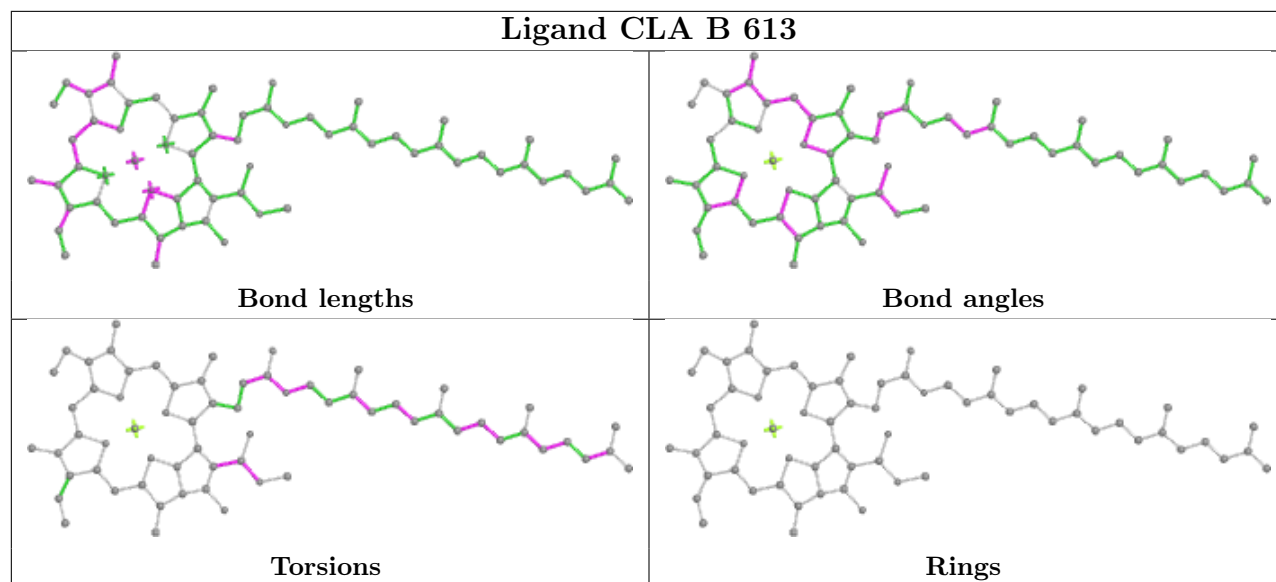
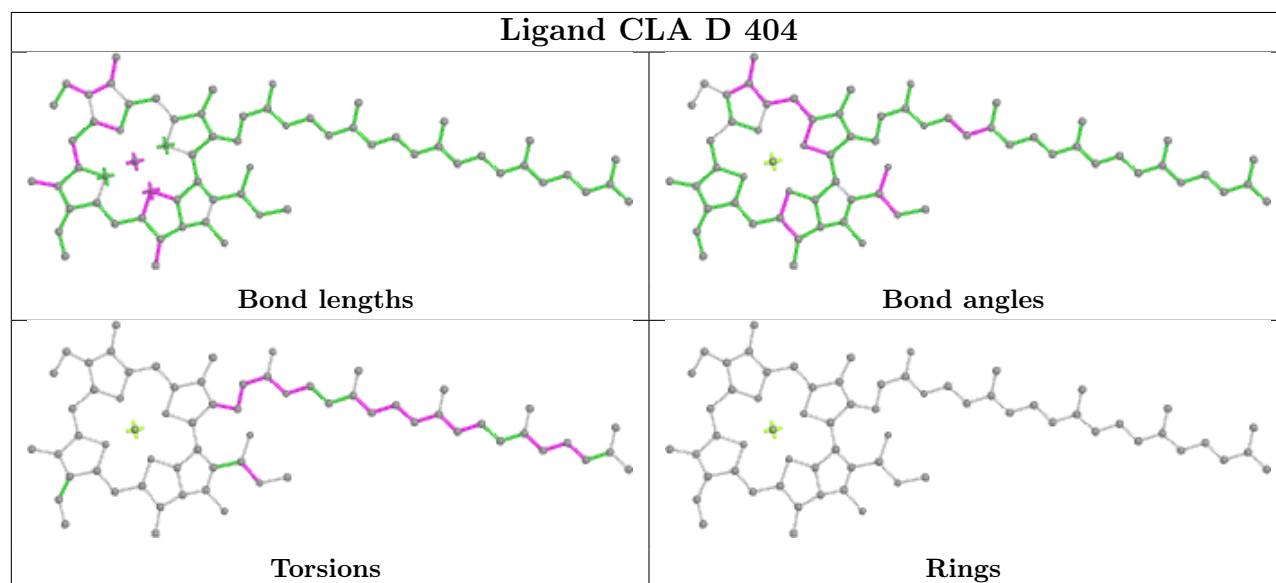
**Ligand CLA B 616****Ligand MGE m 5103****Ligand MGE c 5517**

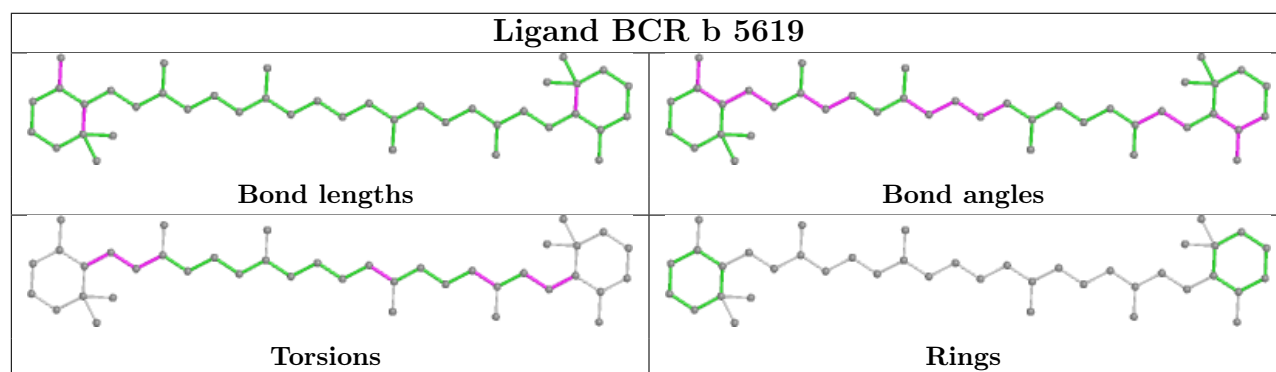
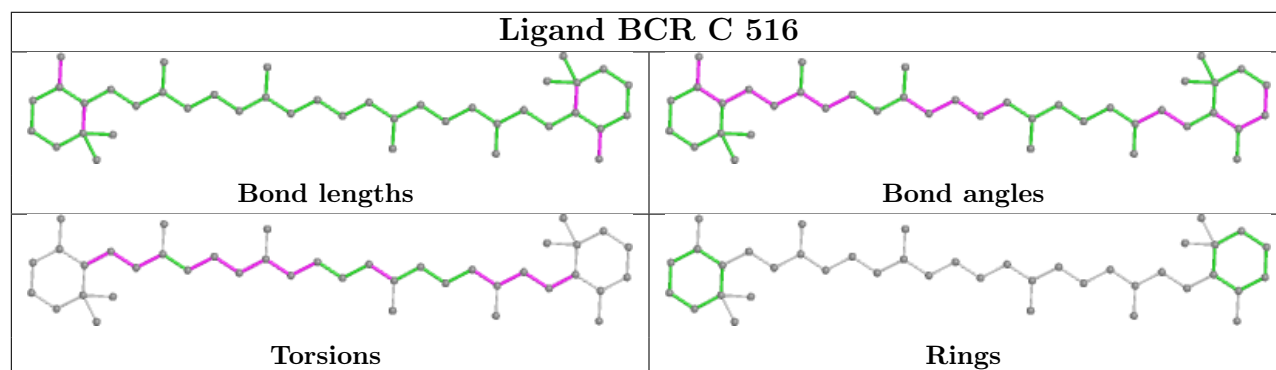
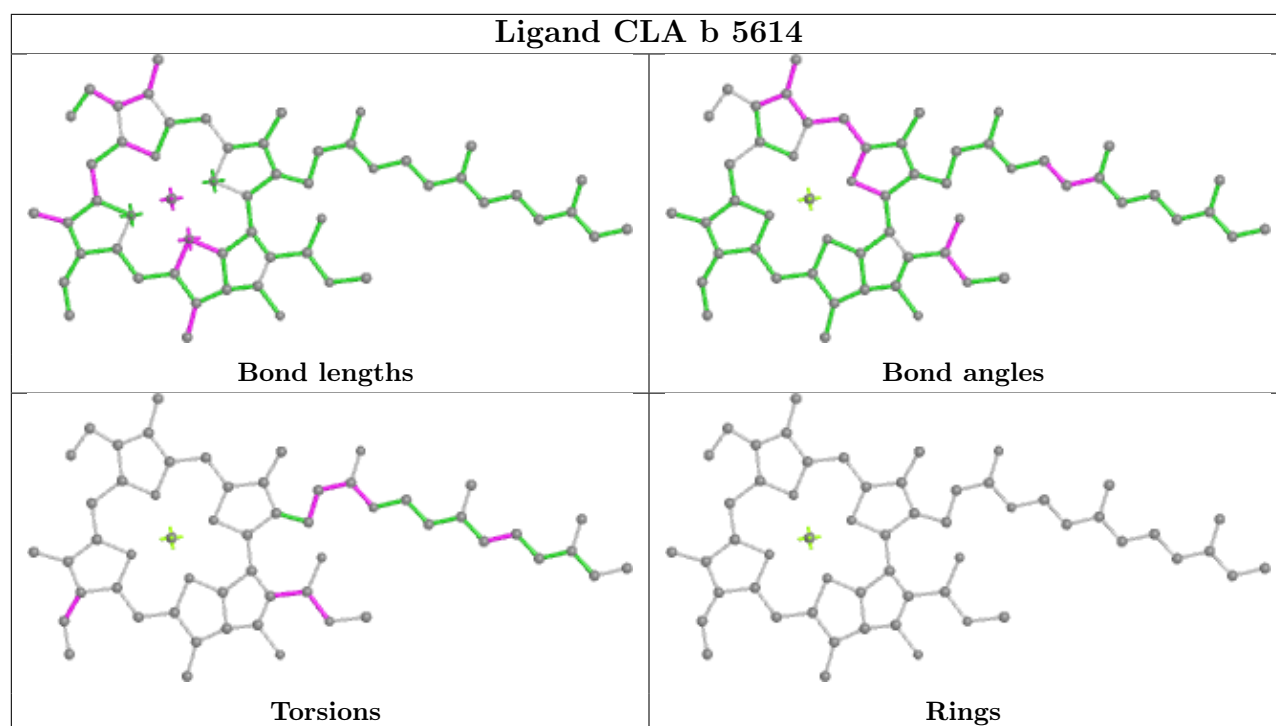


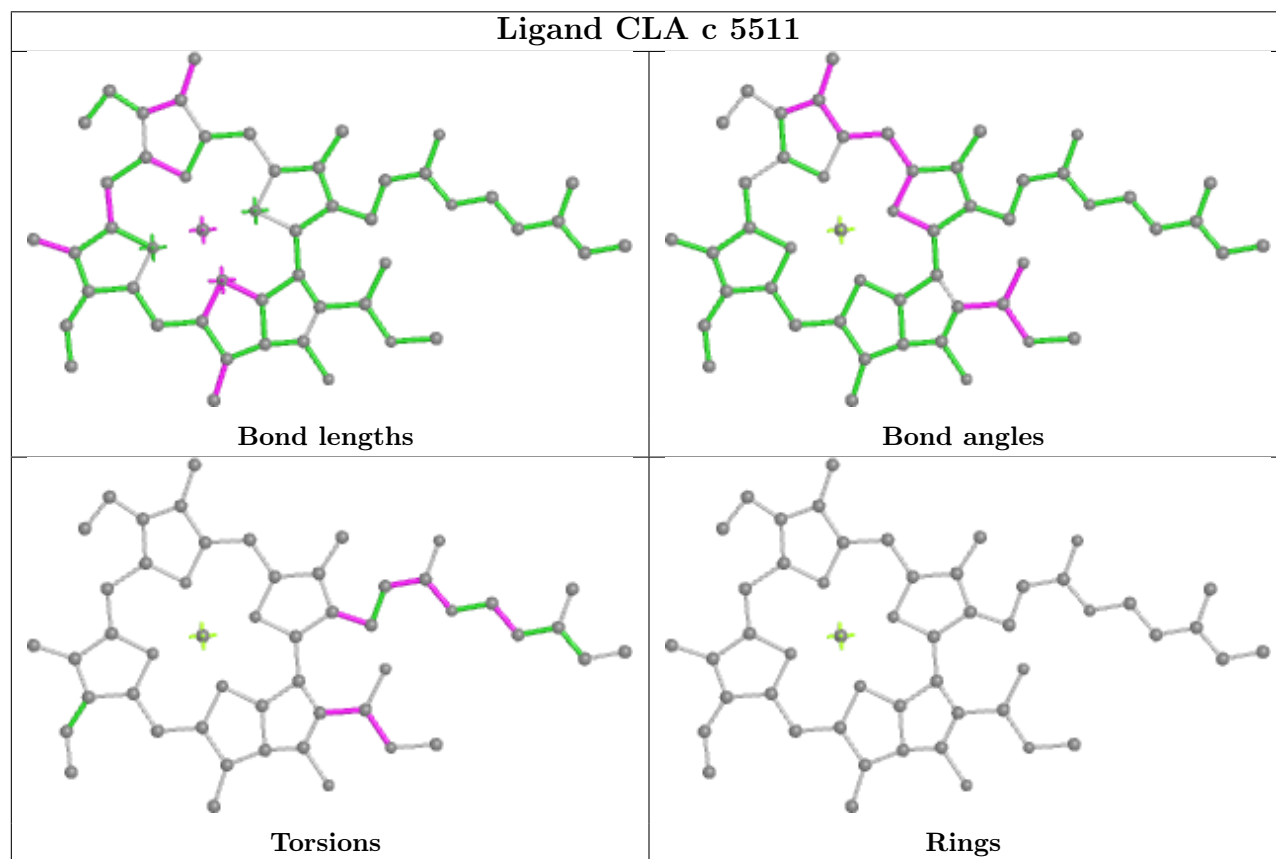
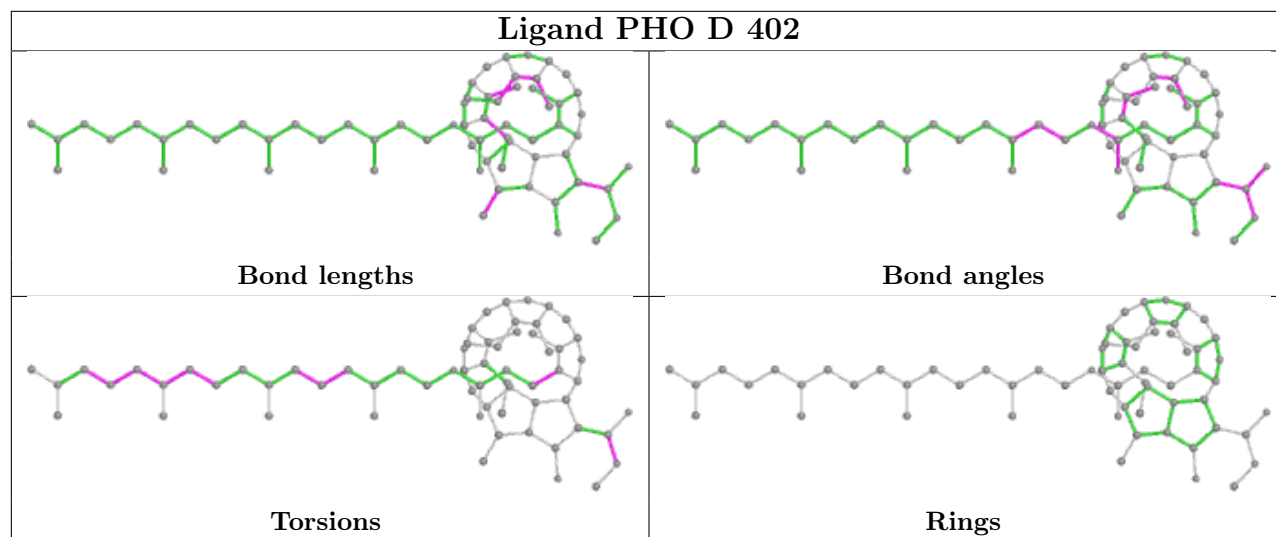
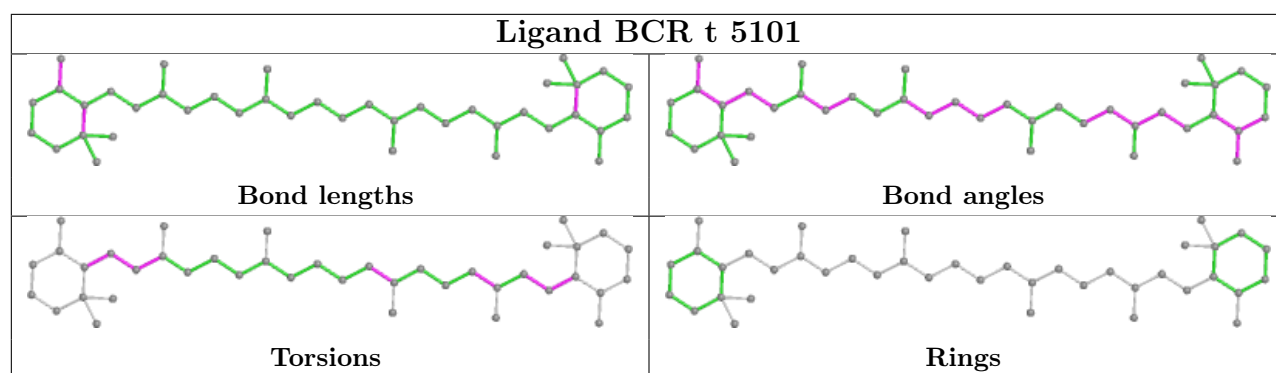


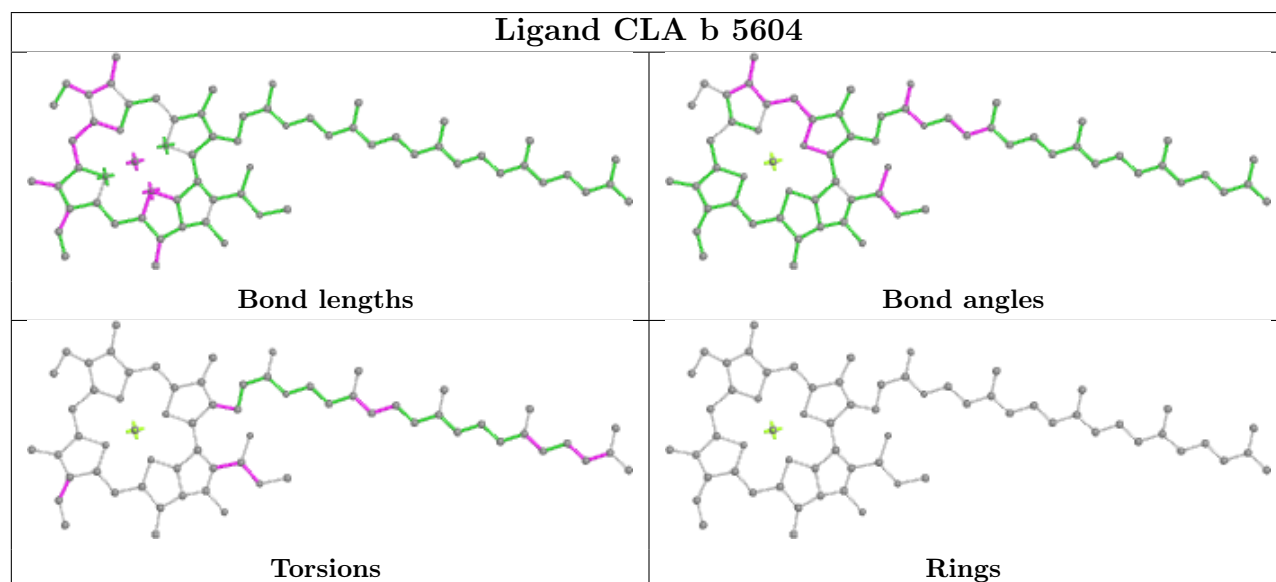
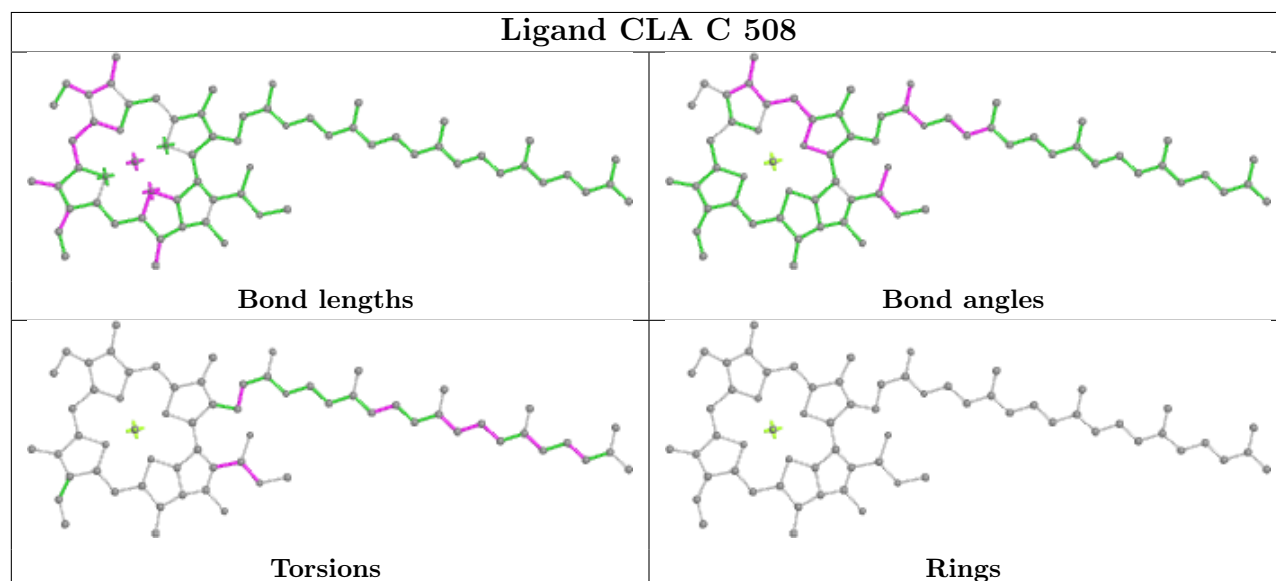
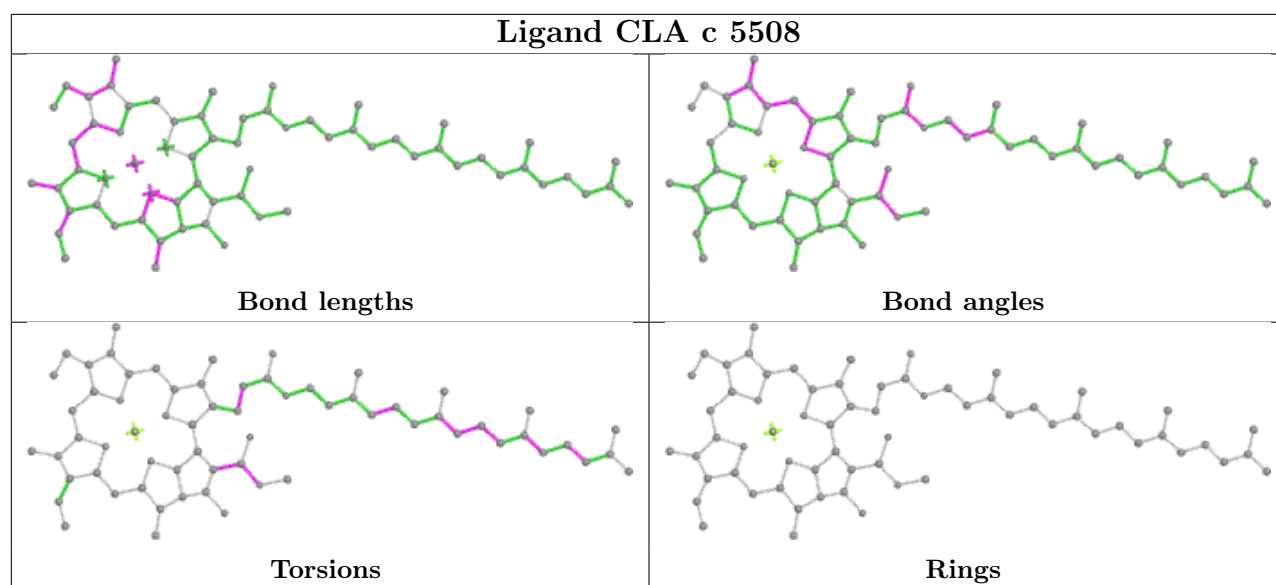


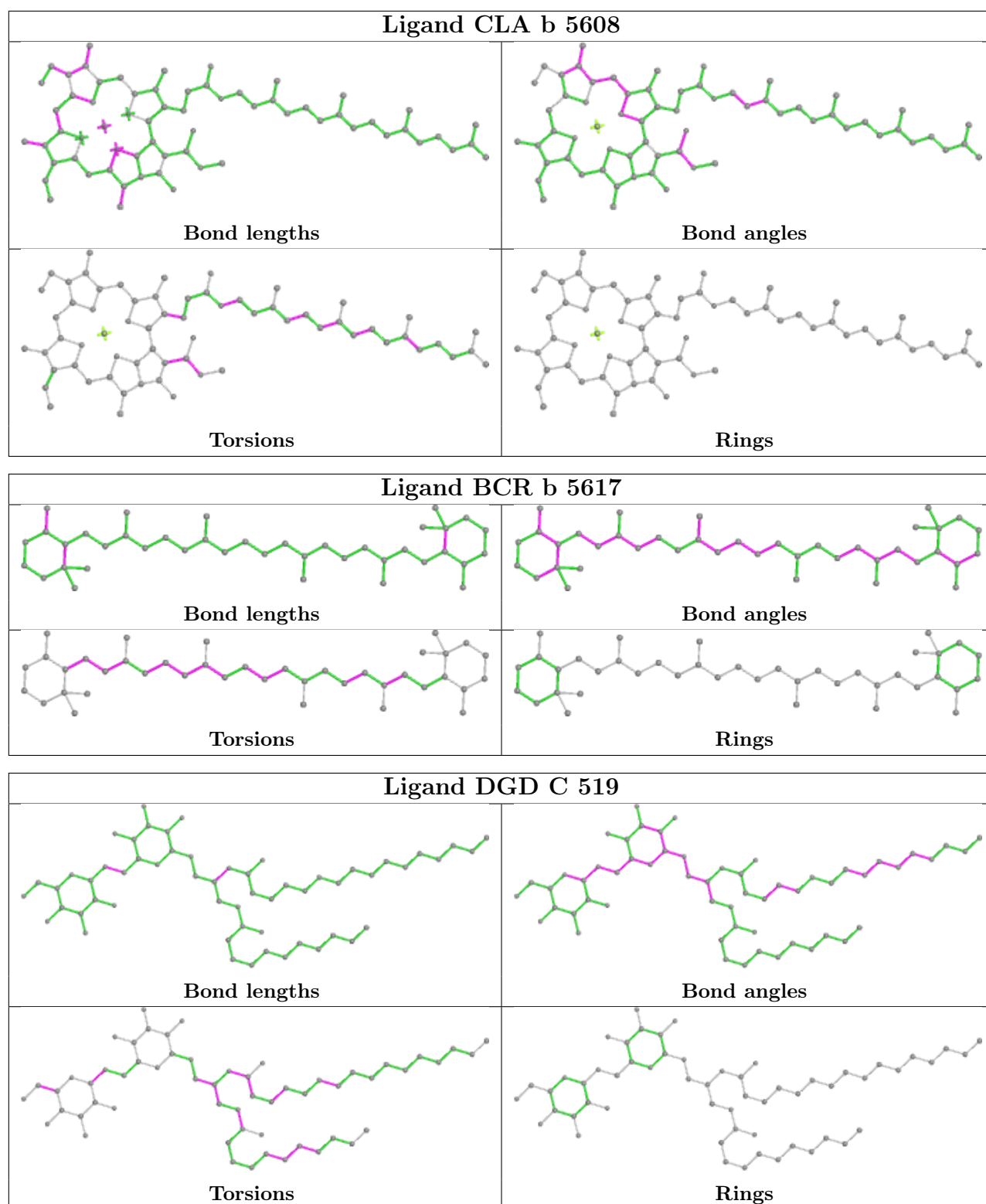


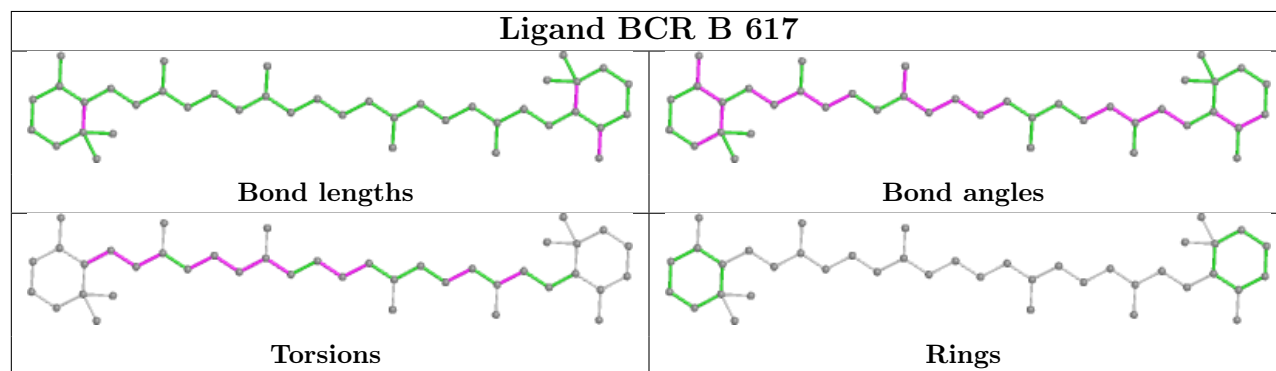
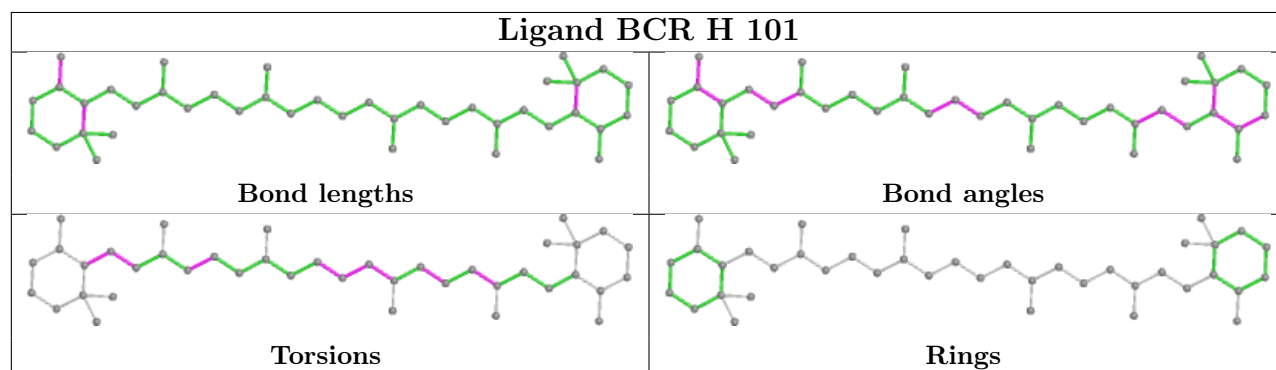
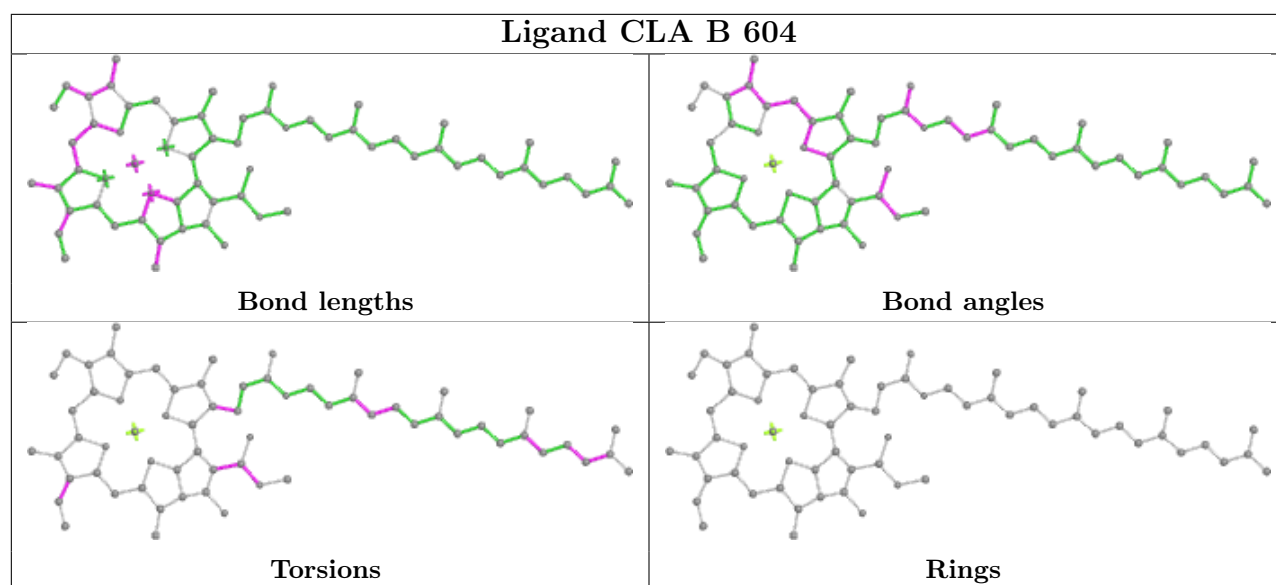
**Ligand CLA B 613****Ligand CLA D 404**

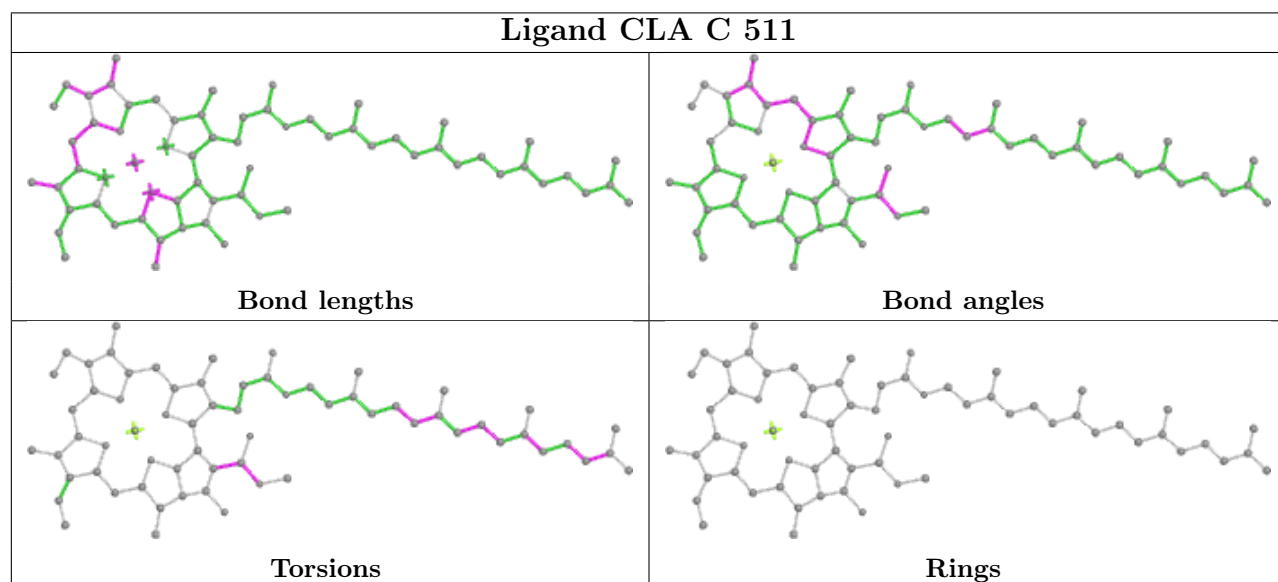
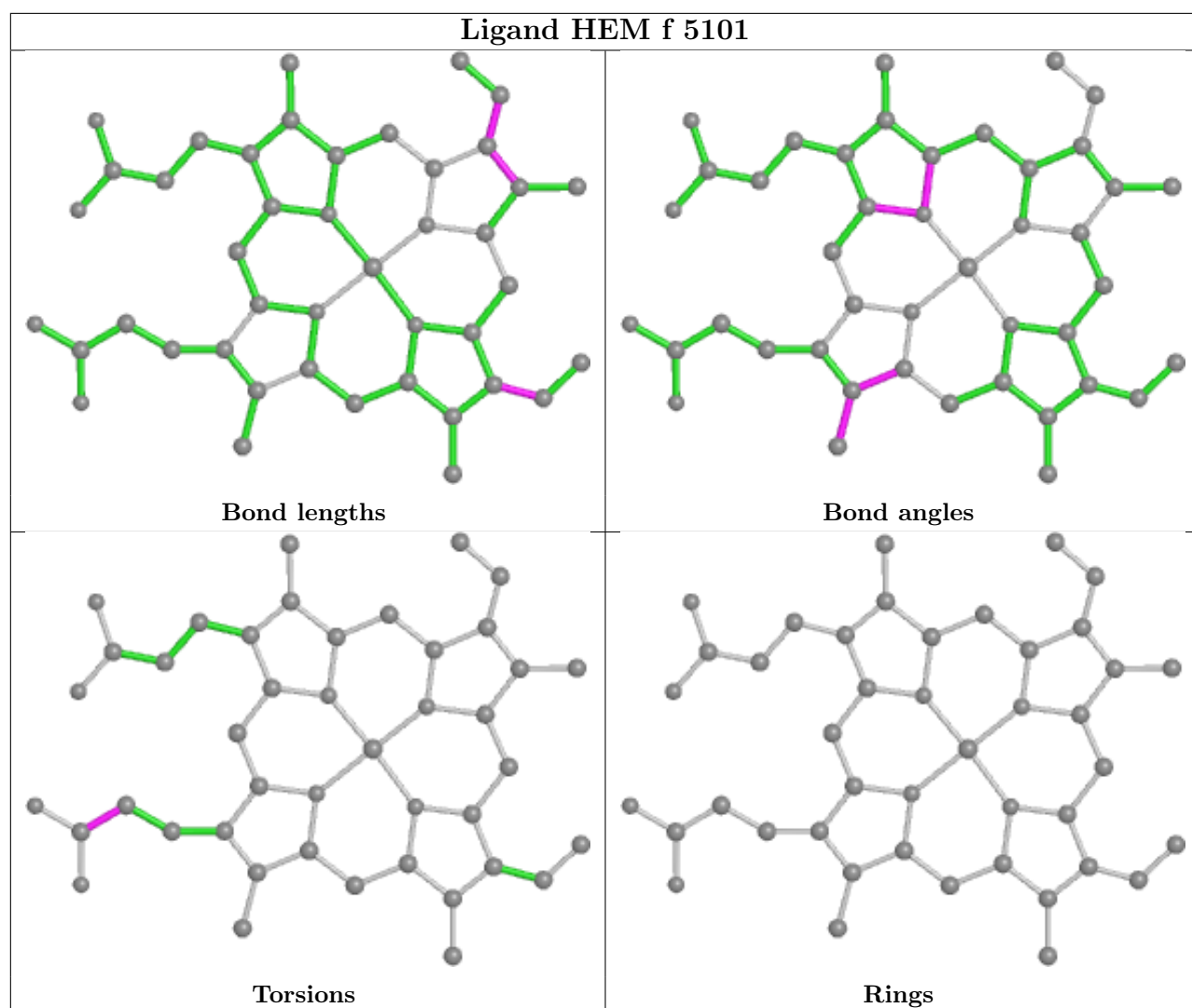


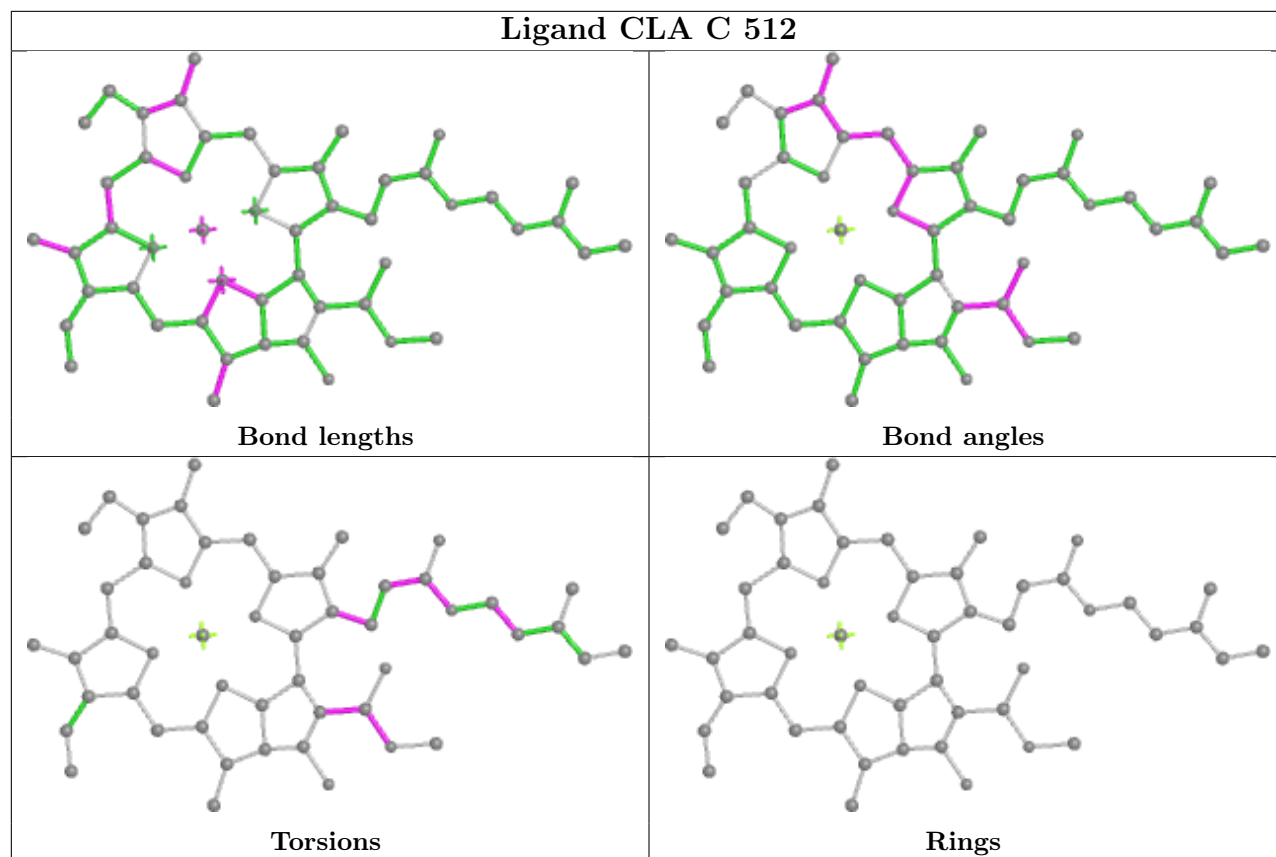
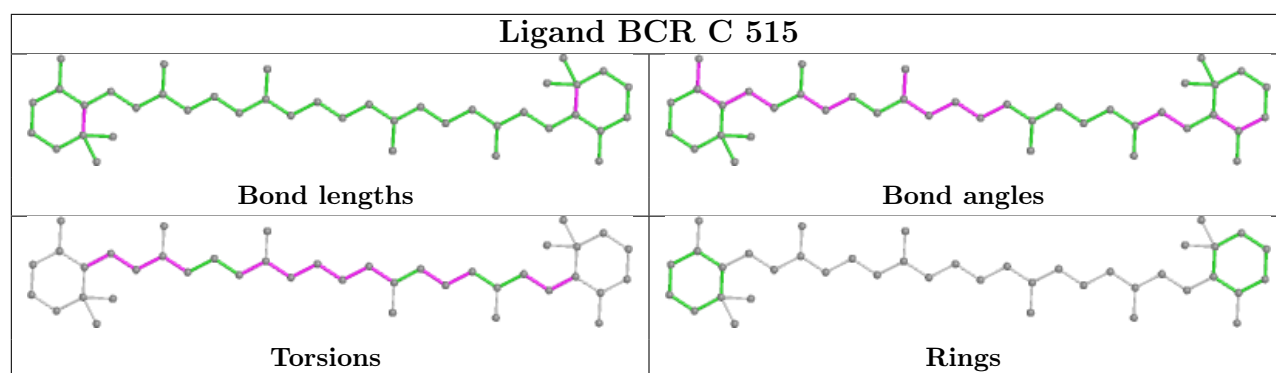




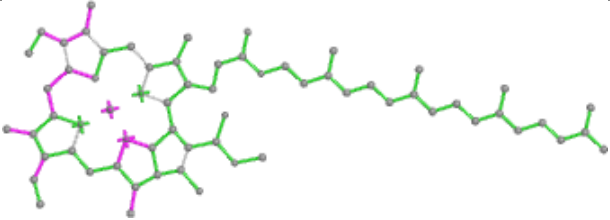
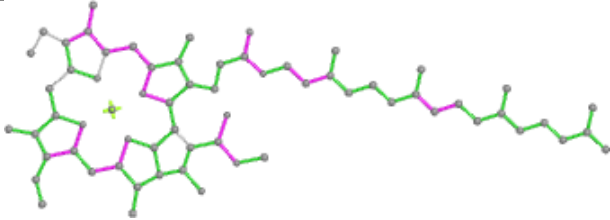
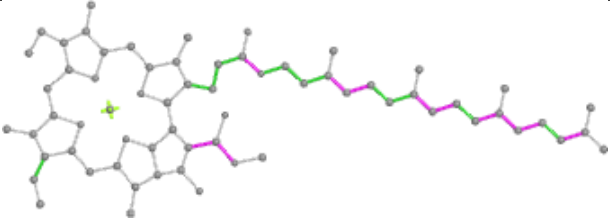
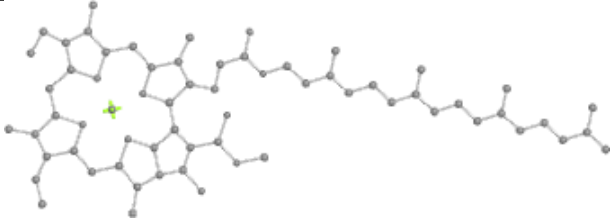
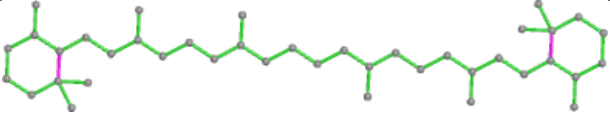
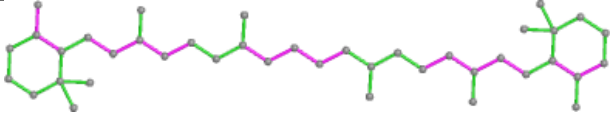
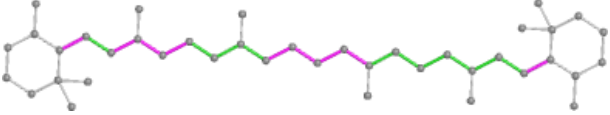
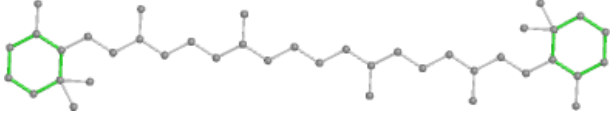
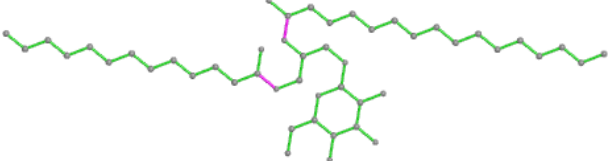
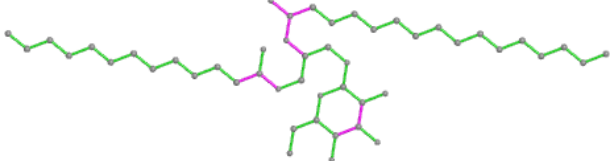
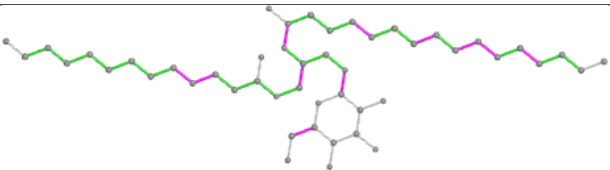
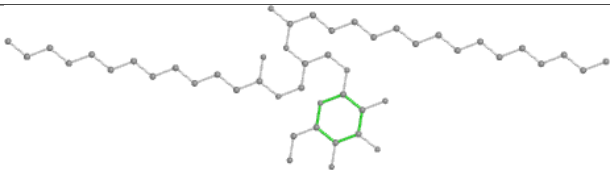


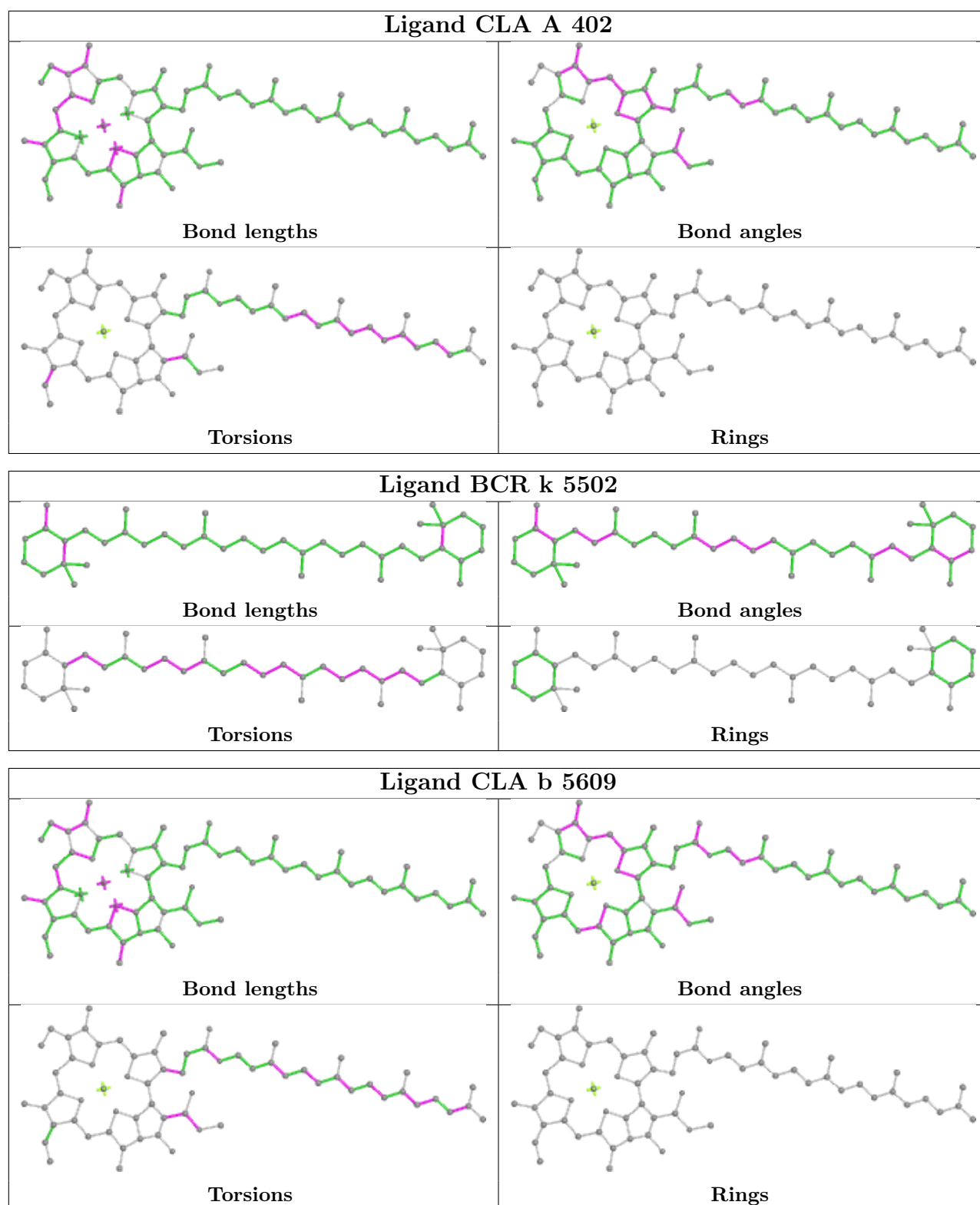


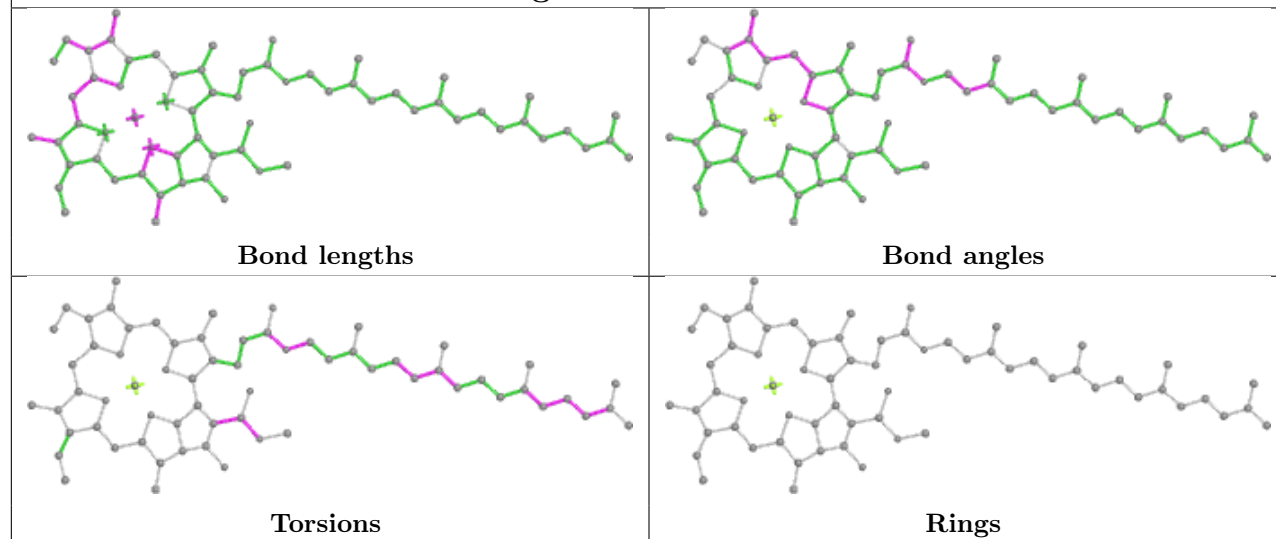
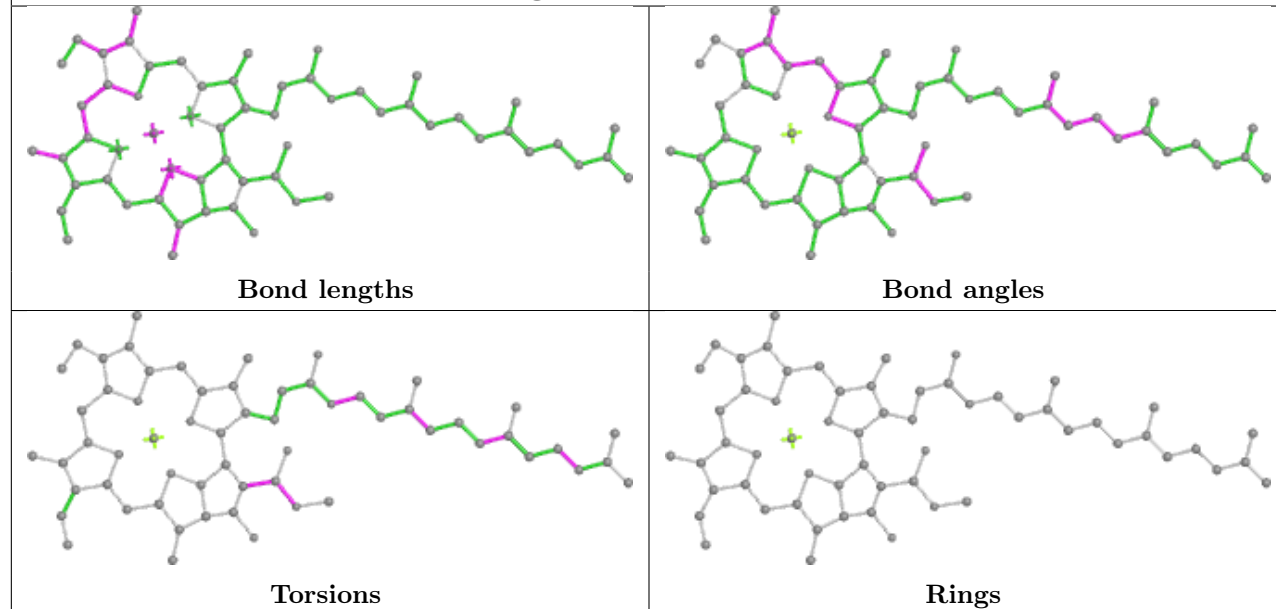


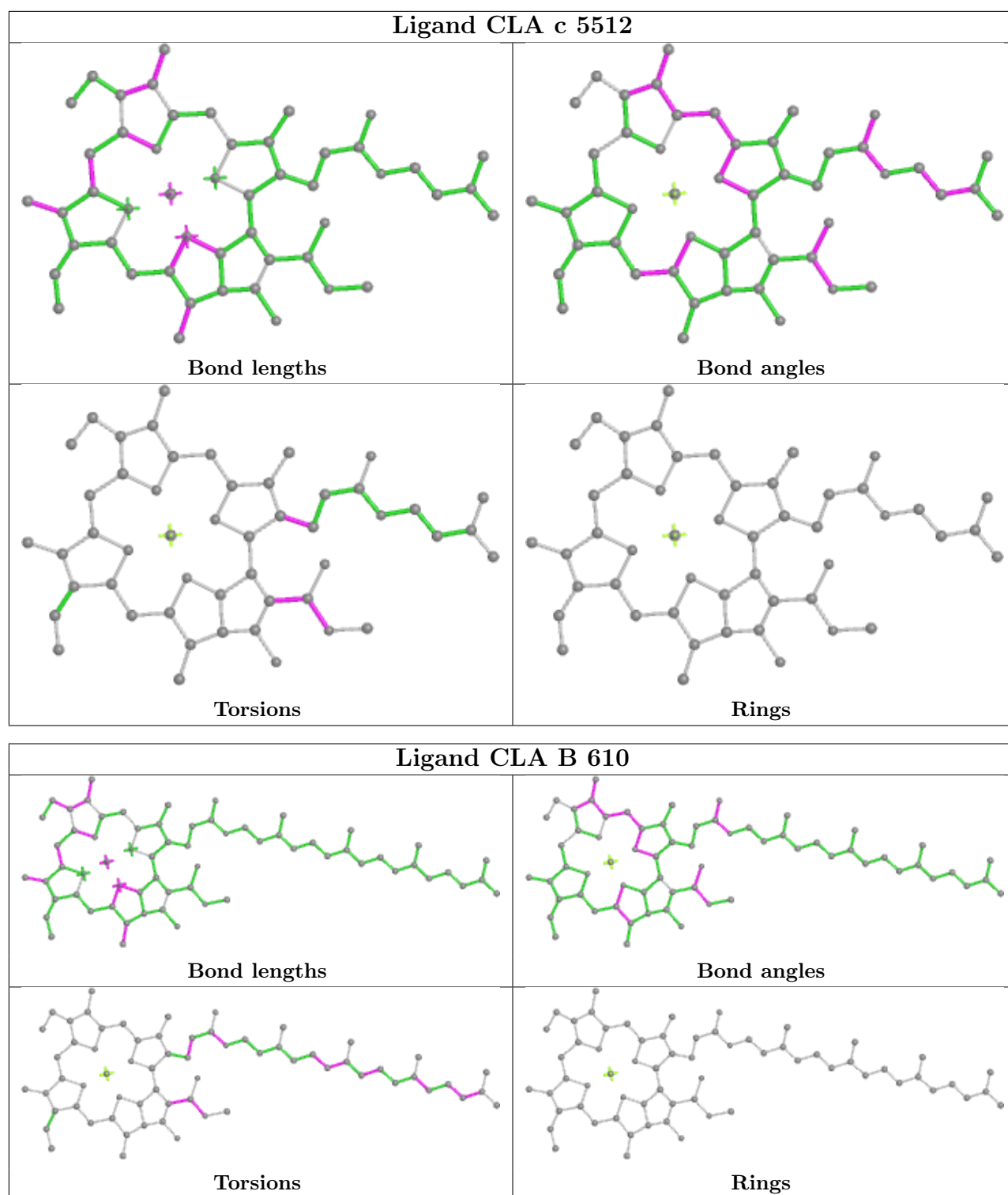


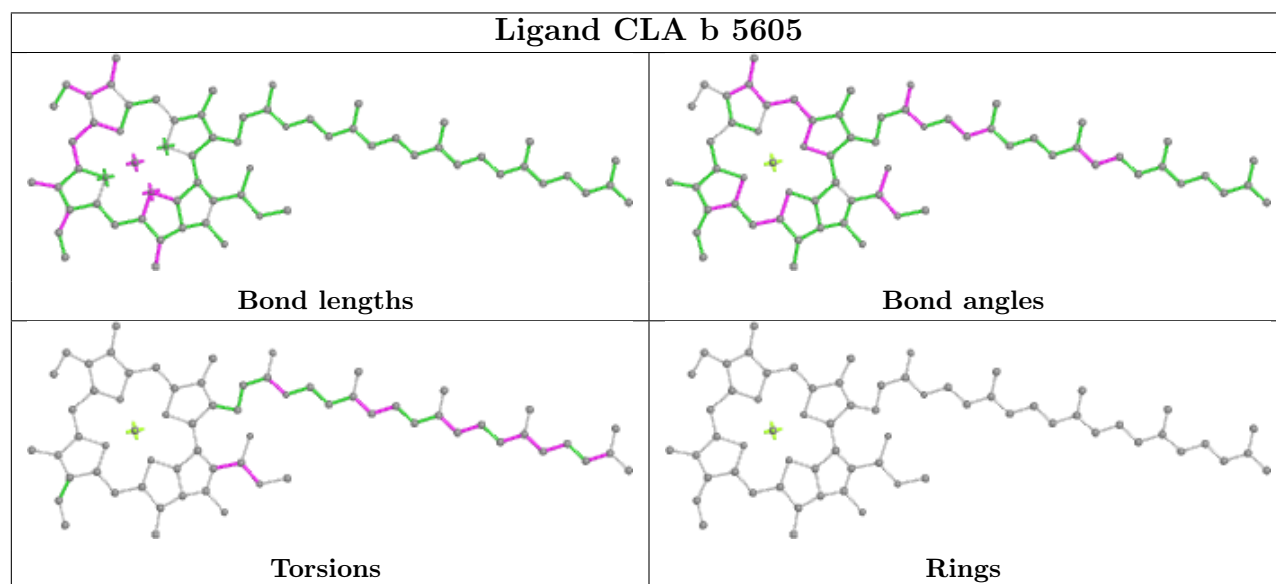
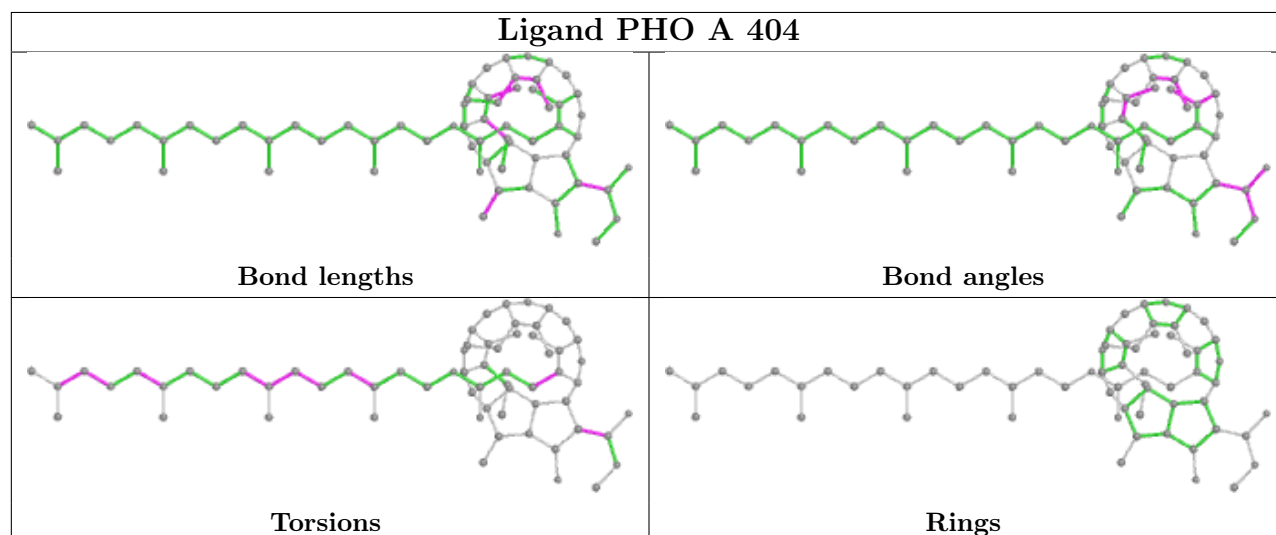
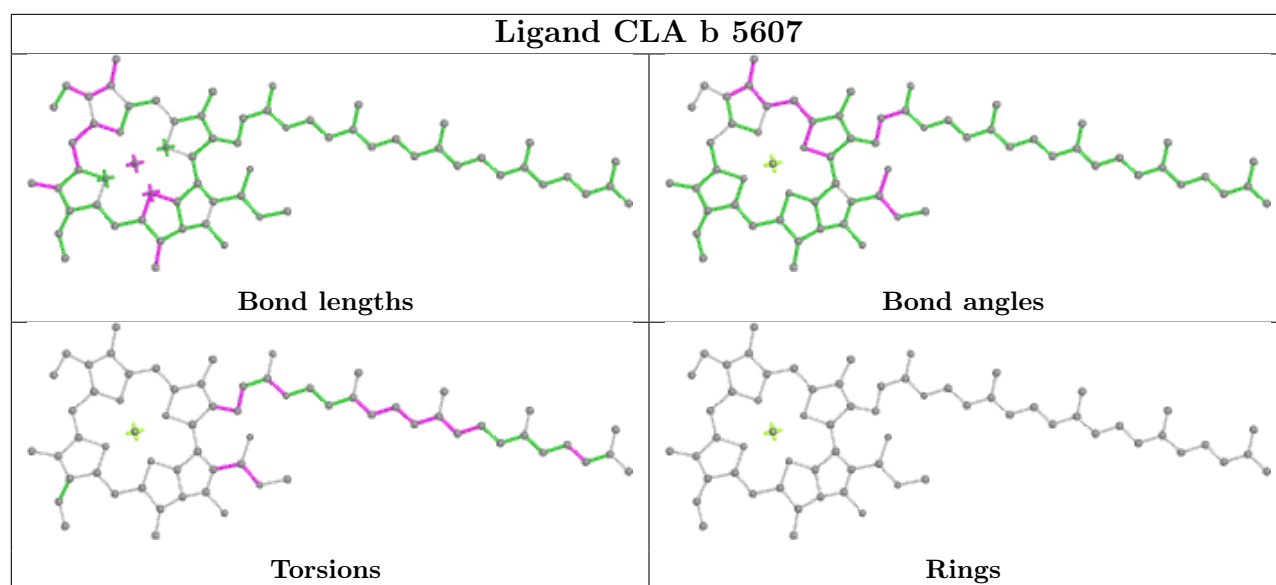


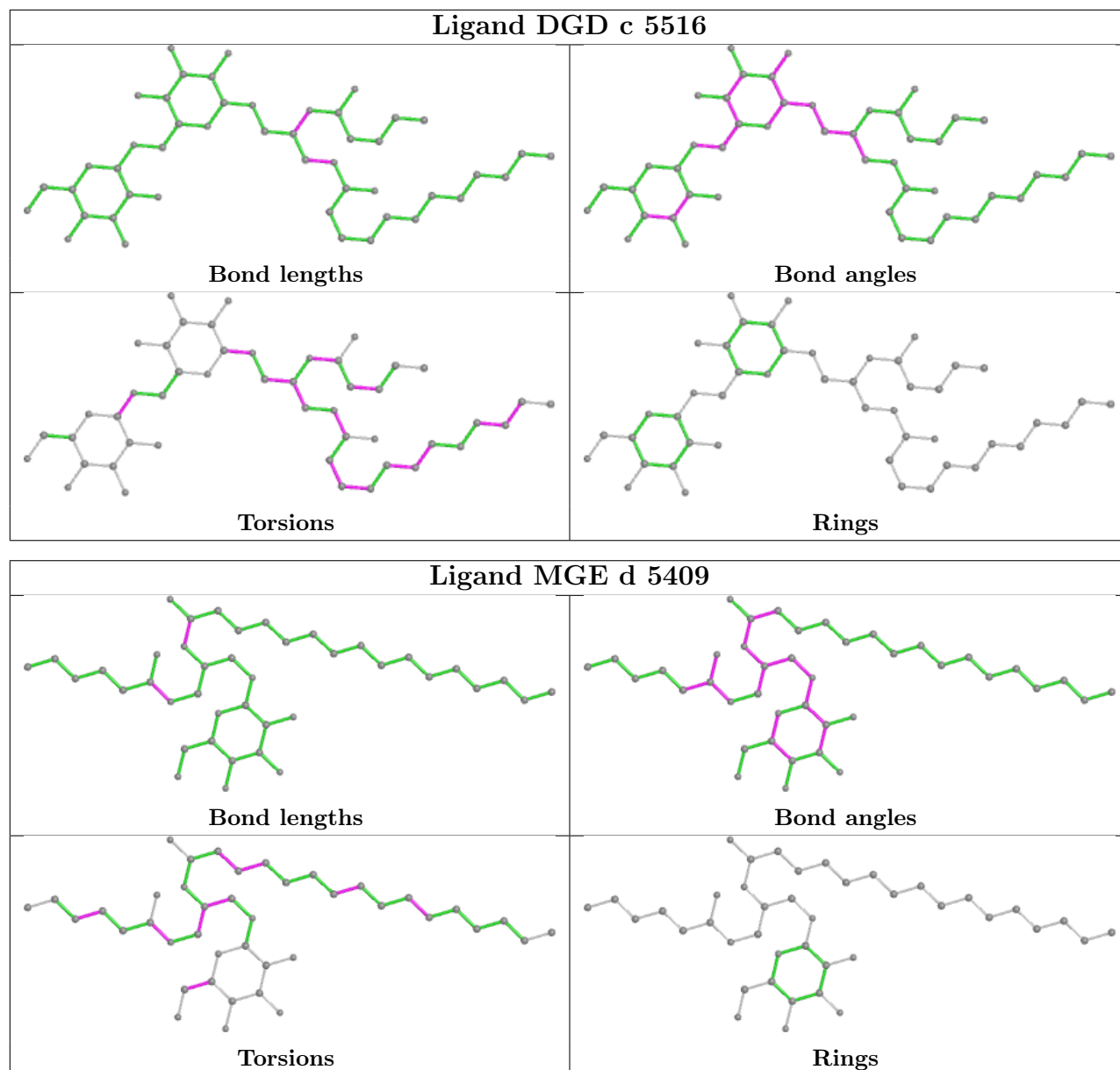
Ligand CLA B 605	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 5513	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand MGE d 5410	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

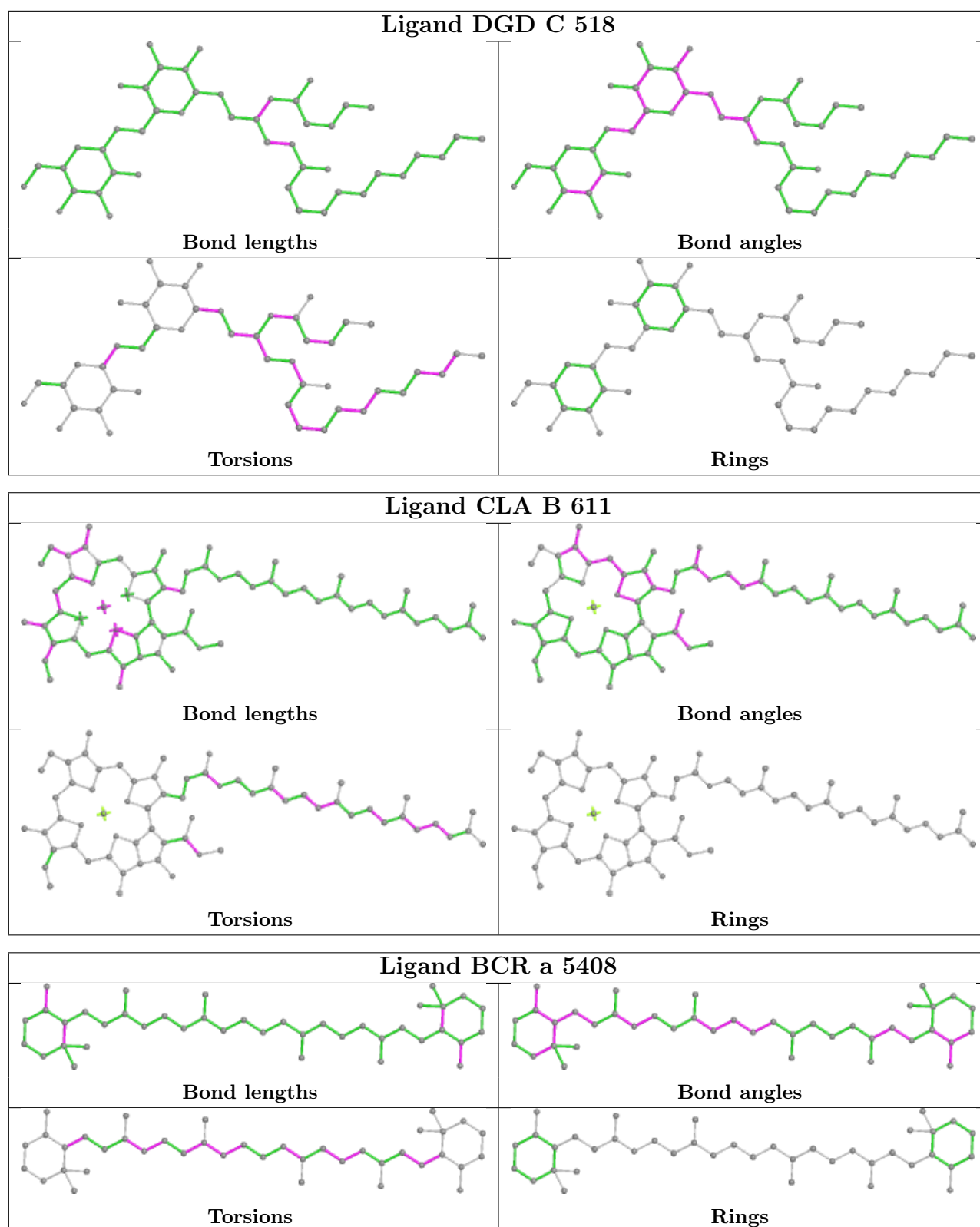


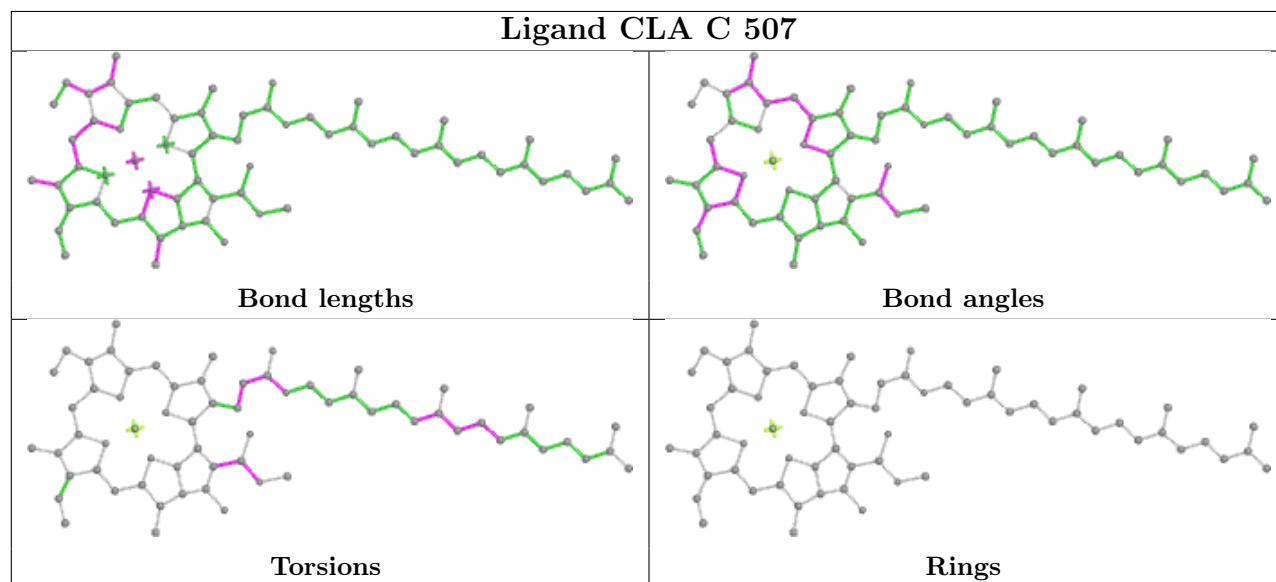
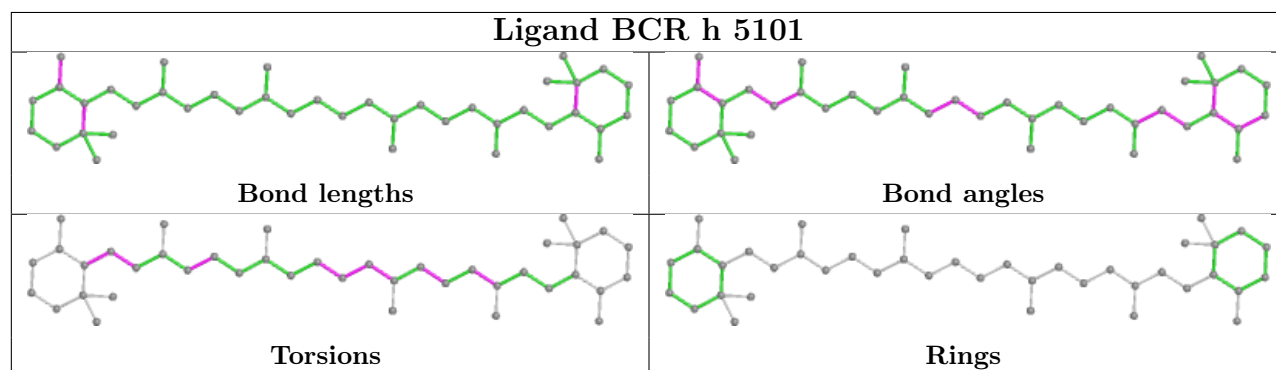
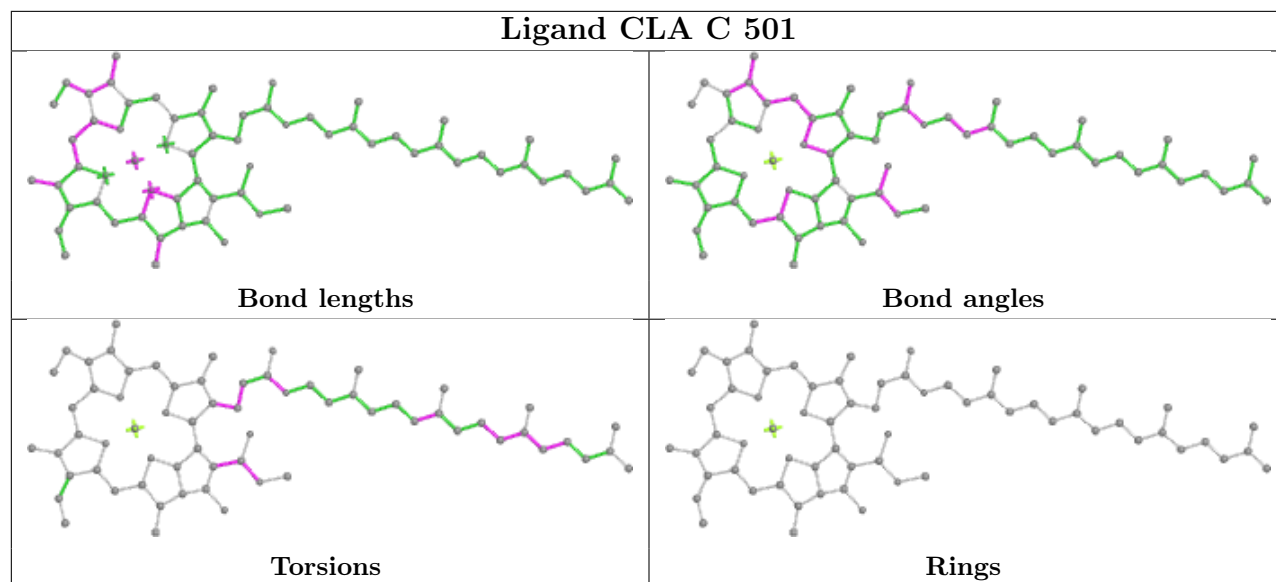
**Ligand CLA B 615****Ligand CLA c 5502**



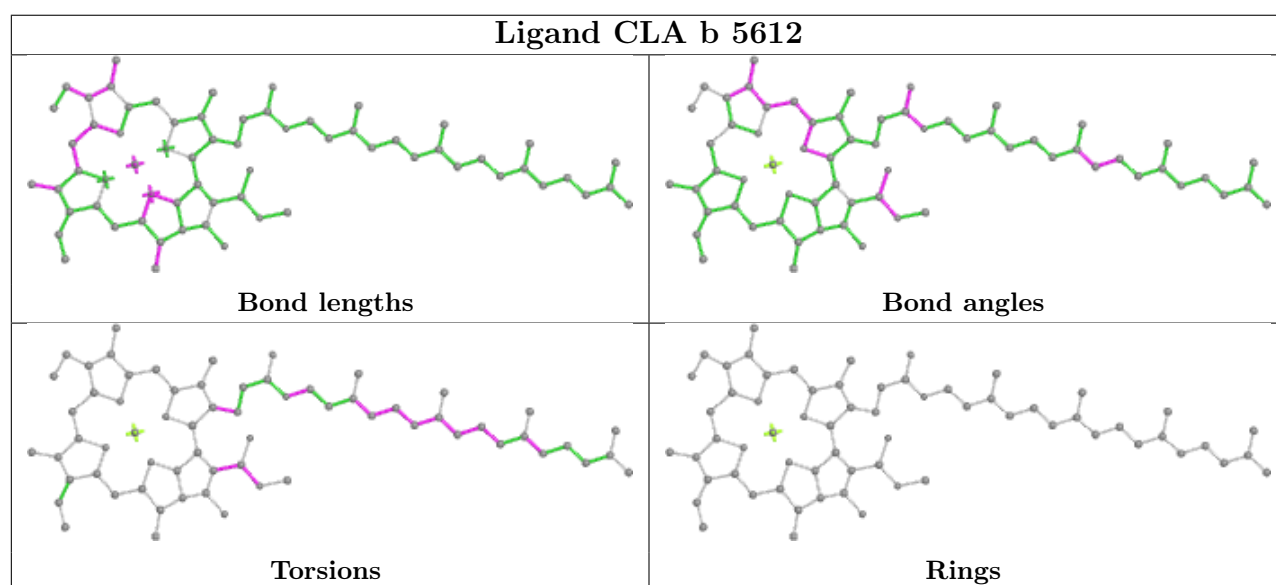
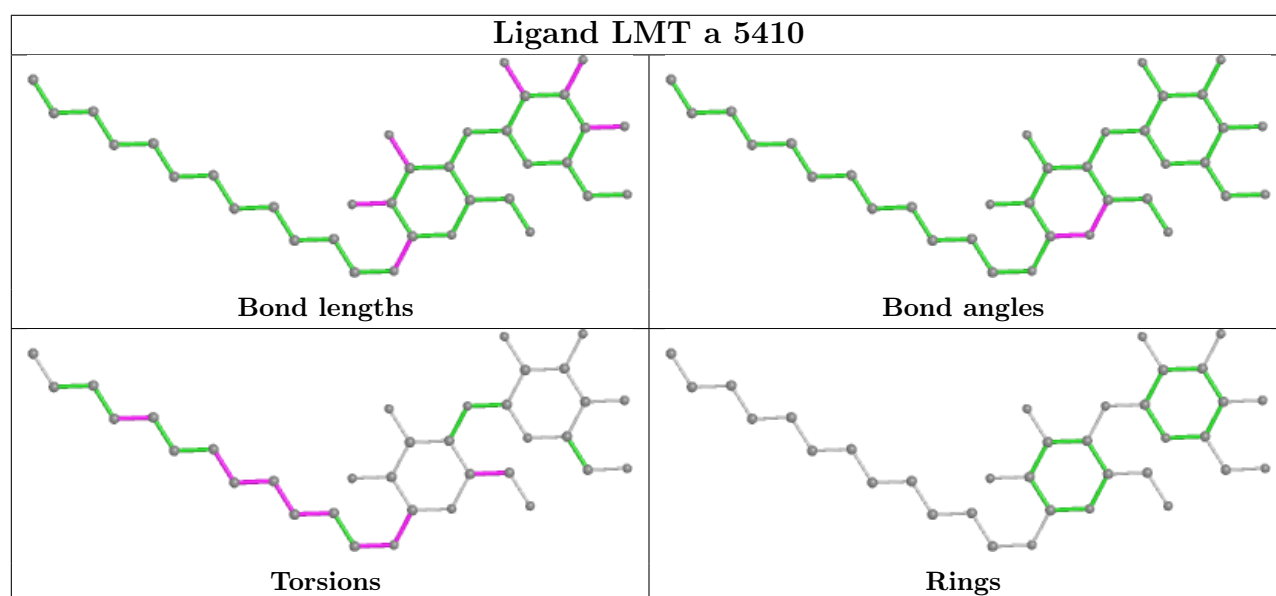
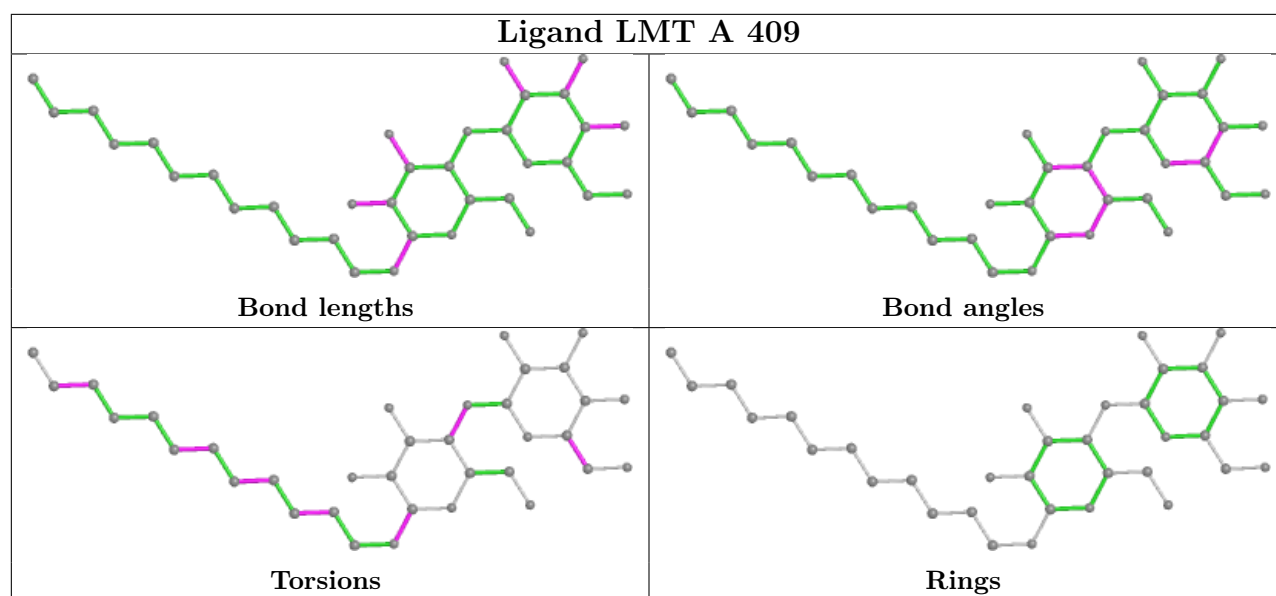


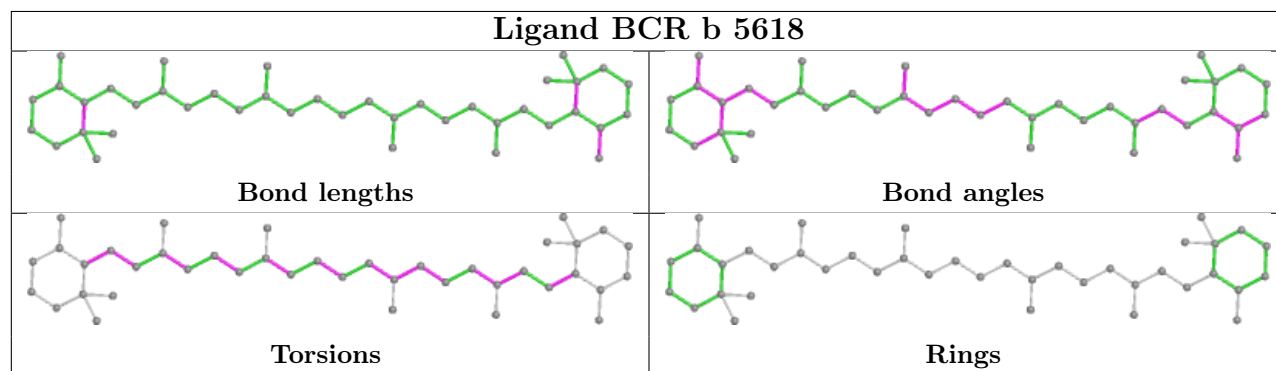
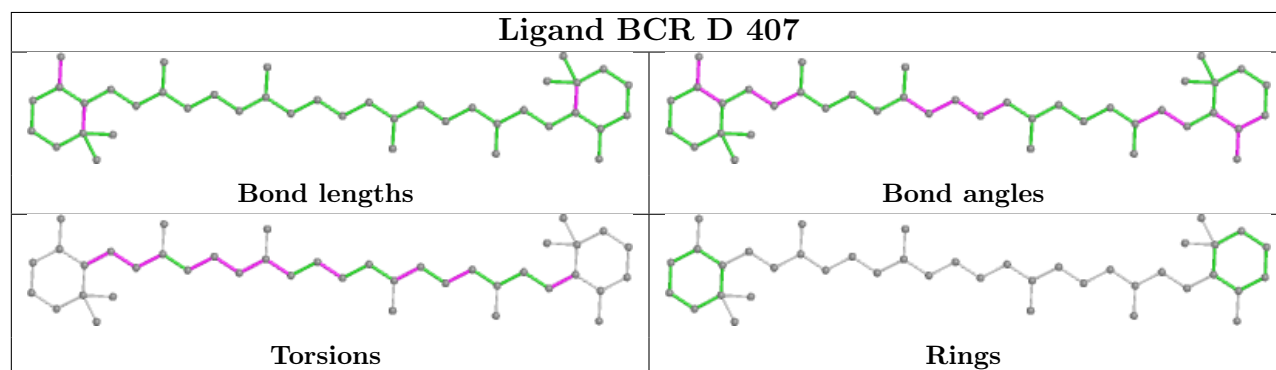
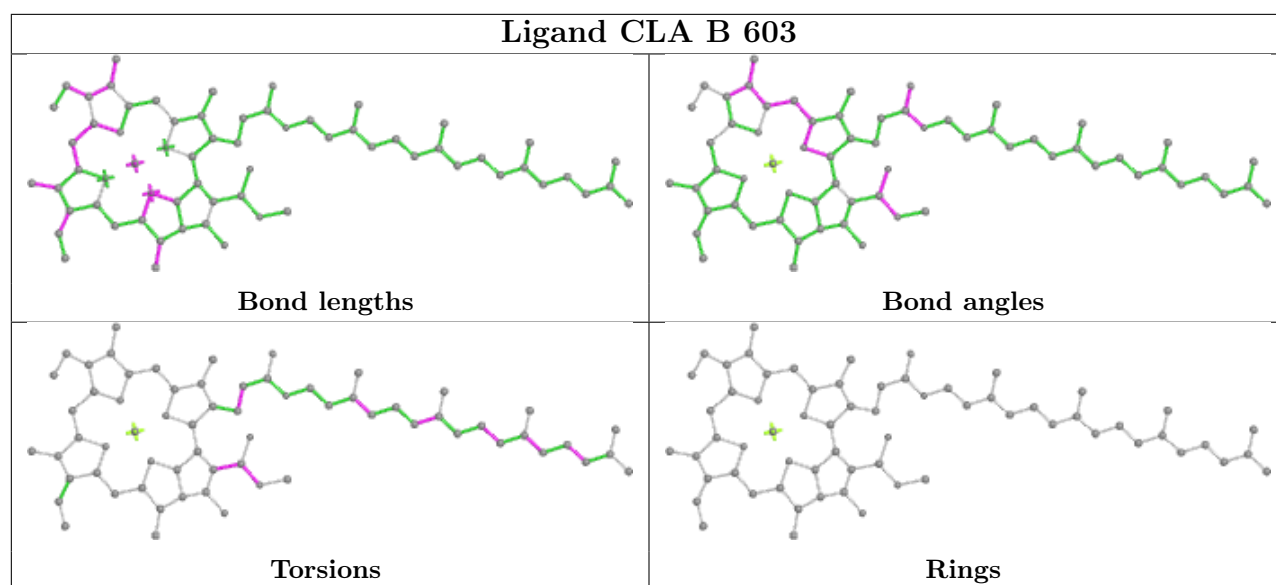


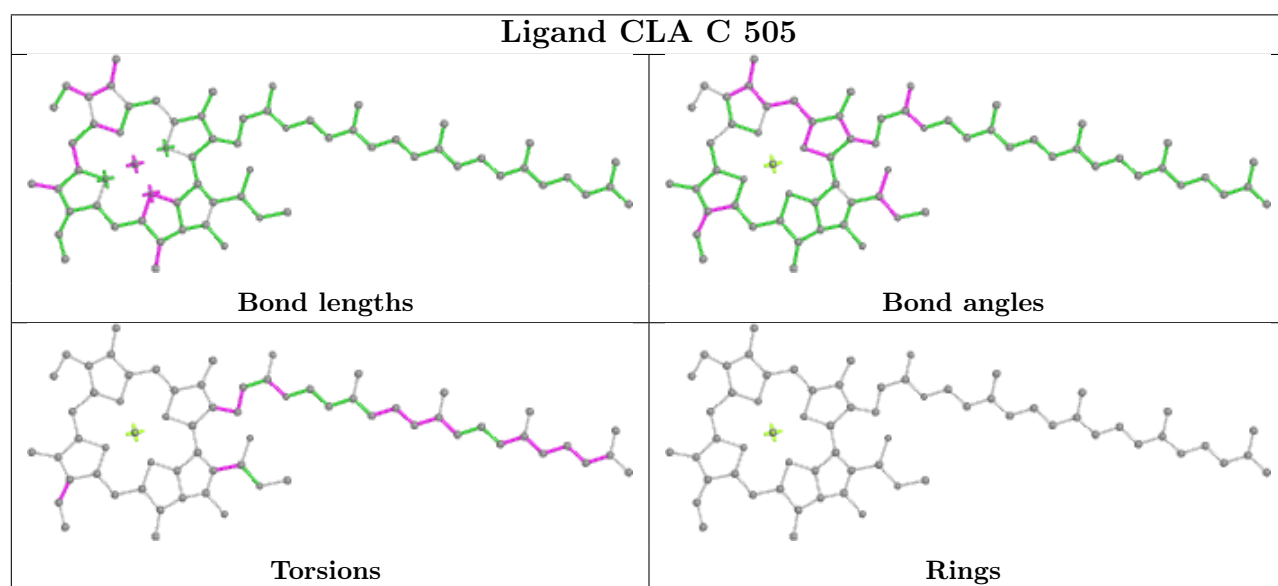
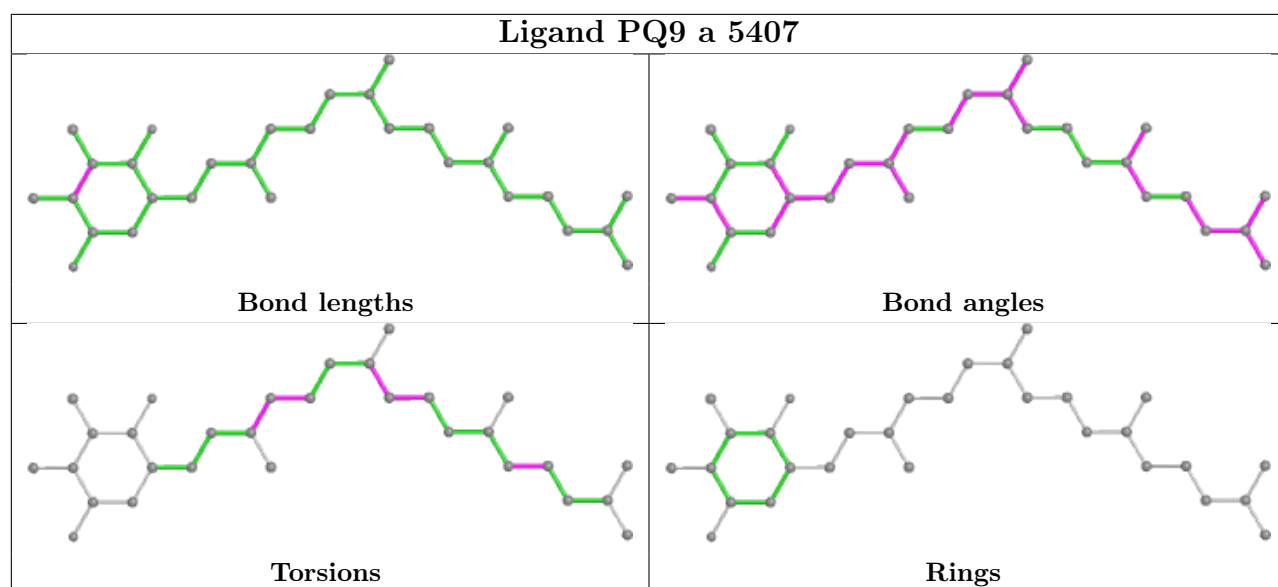


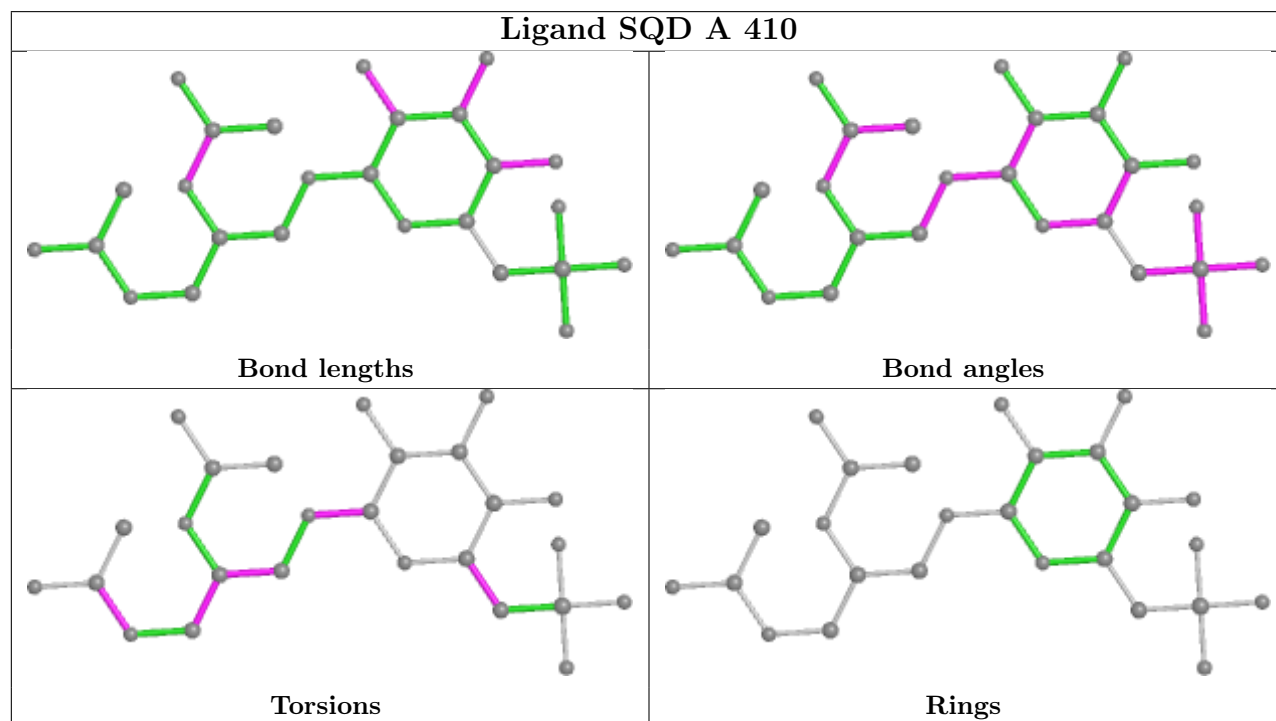
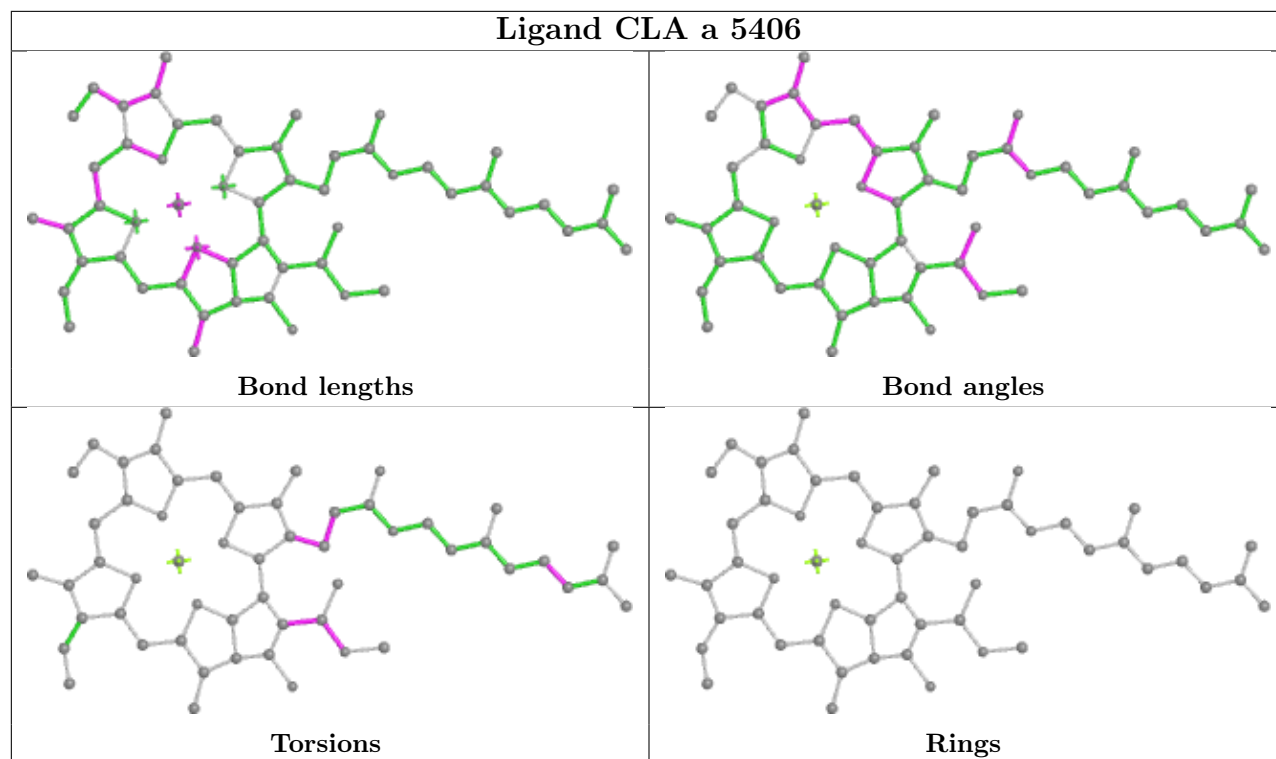


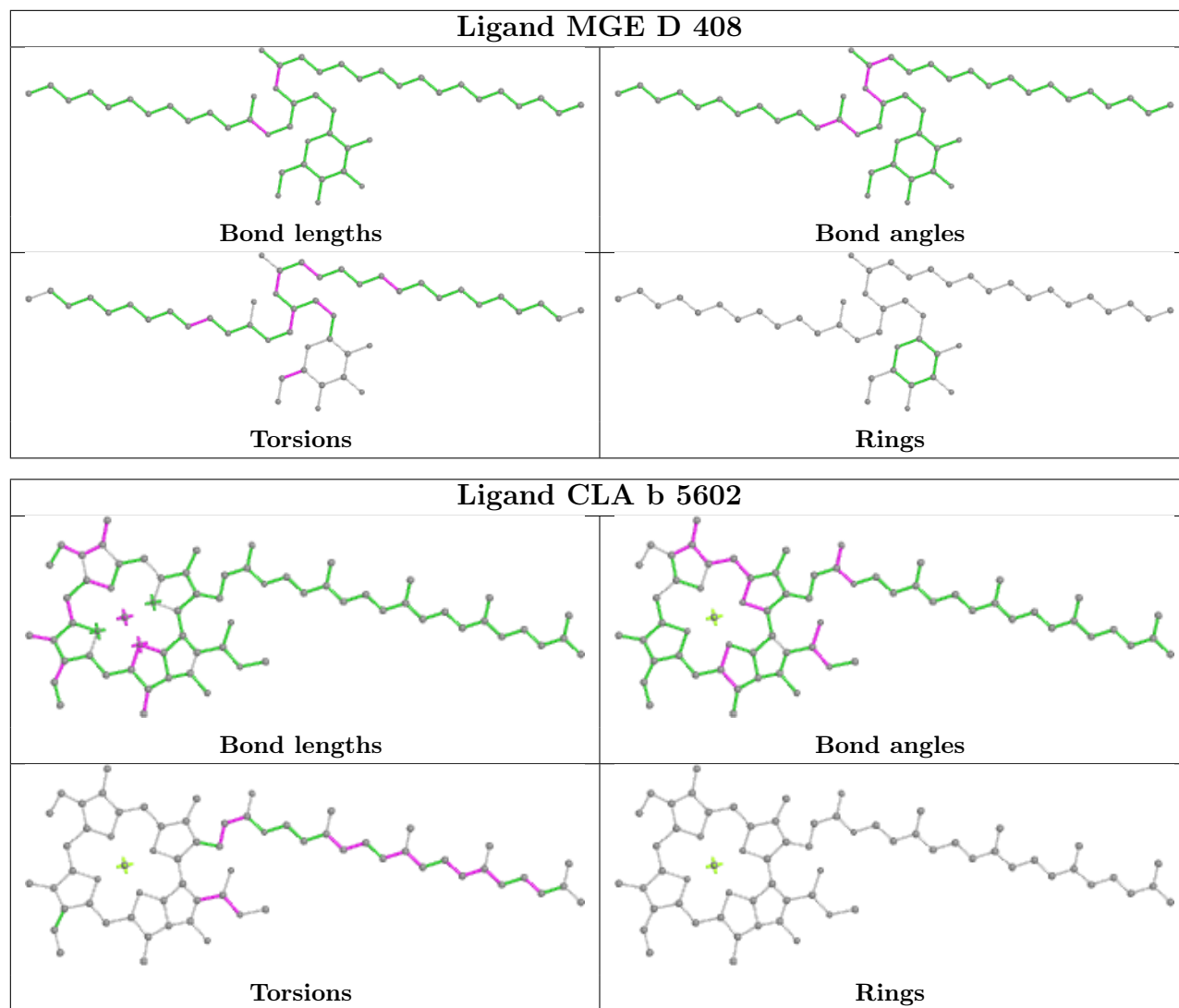




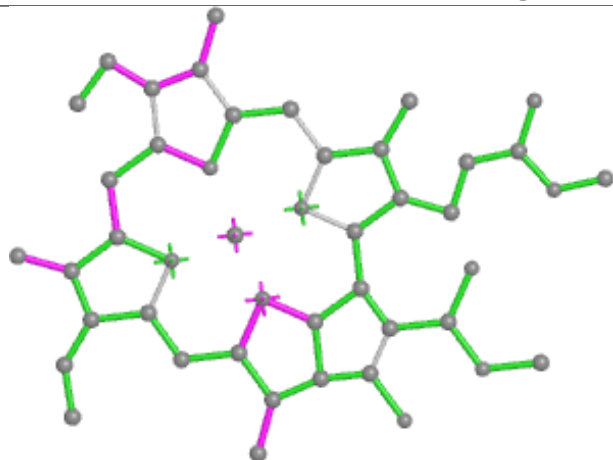




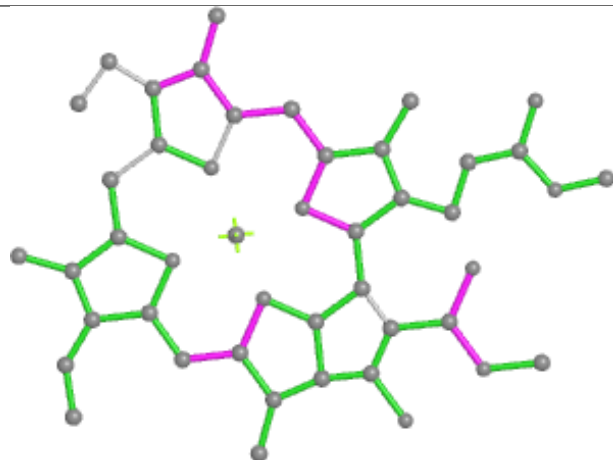




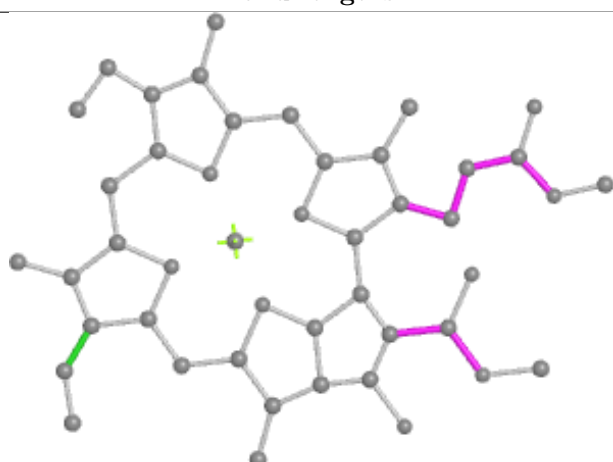
## Ligand CLA C 504



Bond lengths



Bond angles

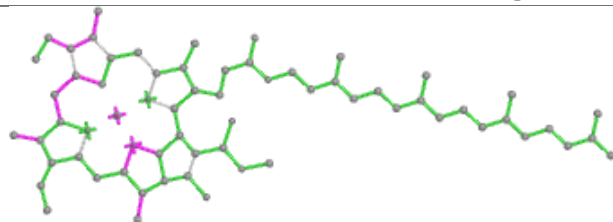


Torsions

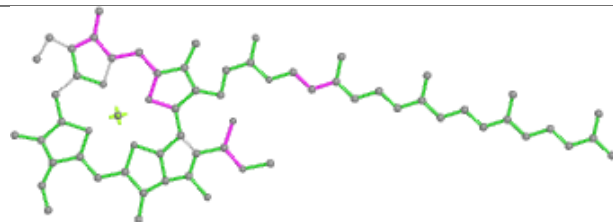


Rings

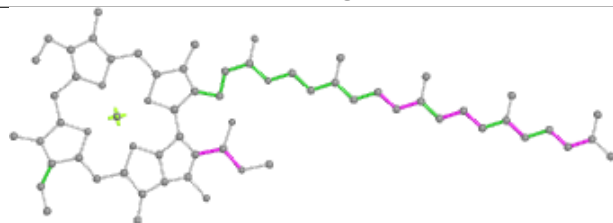
## Ligand CLA k 5501



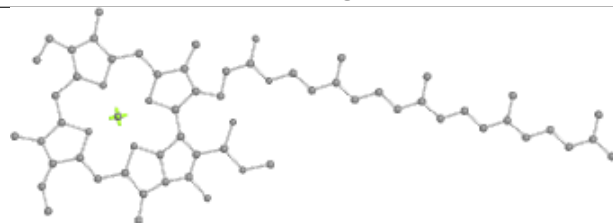
Bond lengths



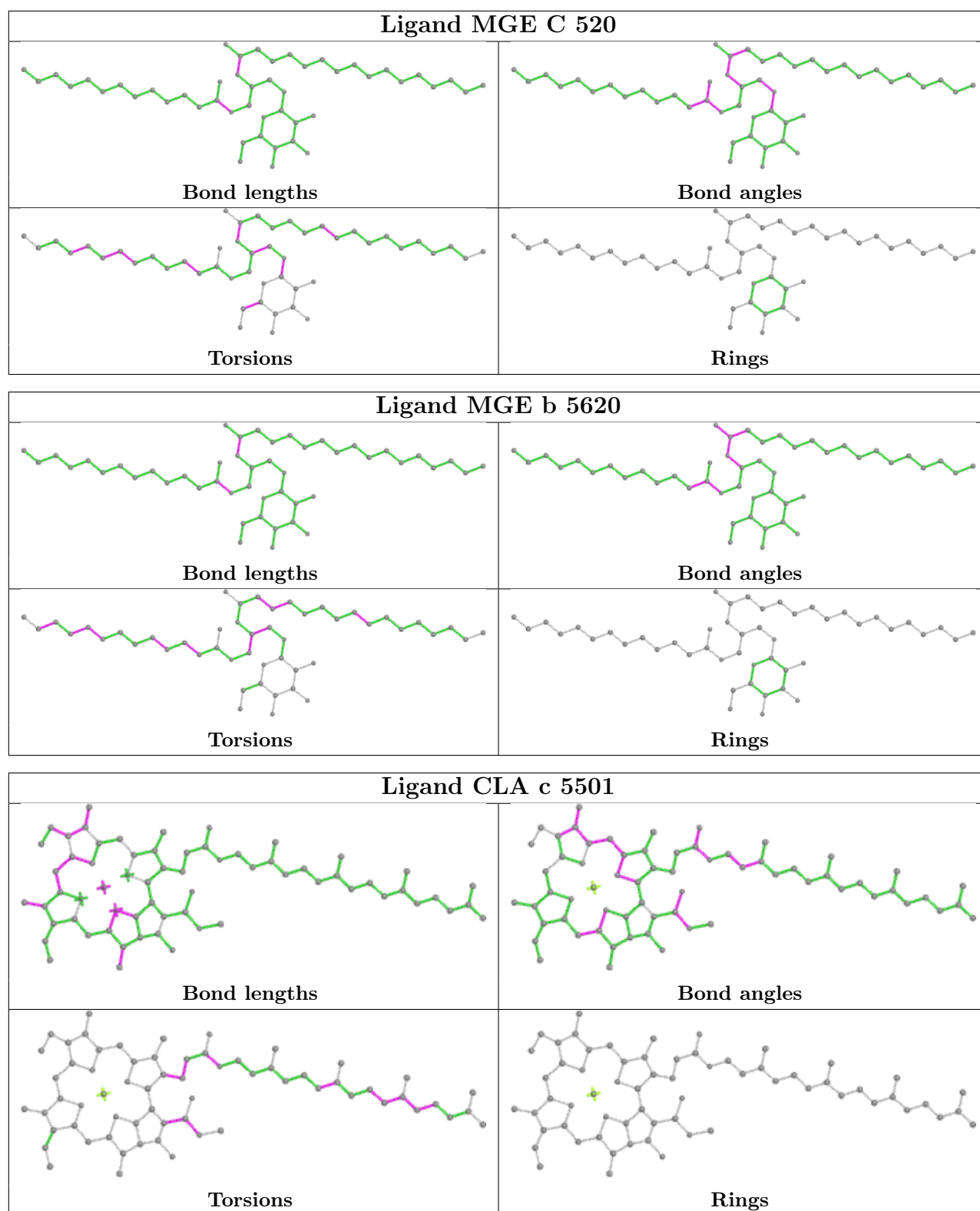
Bond angles

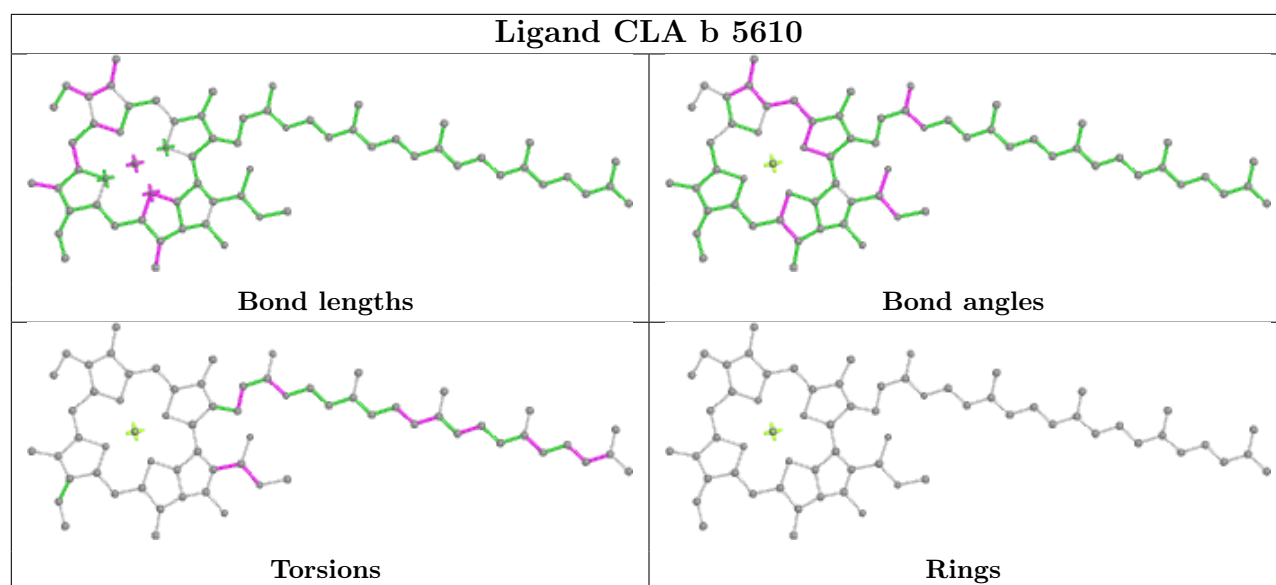


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



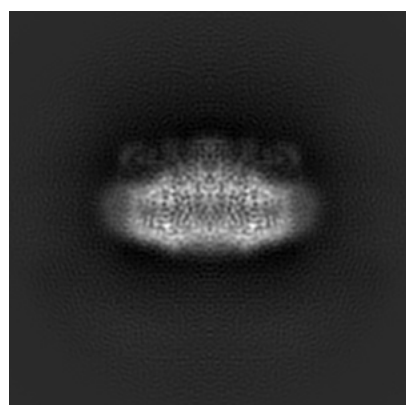
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30511. These allow visual inspection of the internal detail of the map and identification of artifacts.

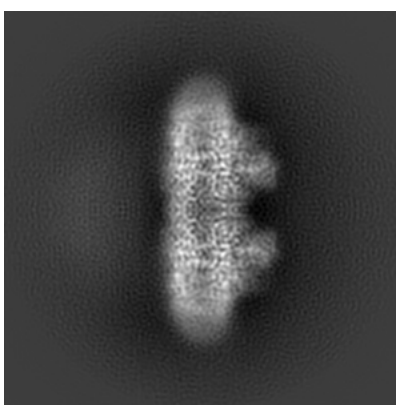
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

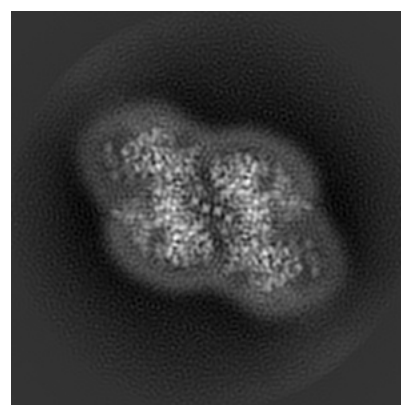
#### 6.1.1 Primary map



X



Y

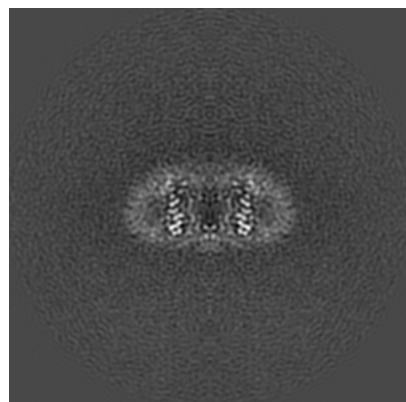


Z

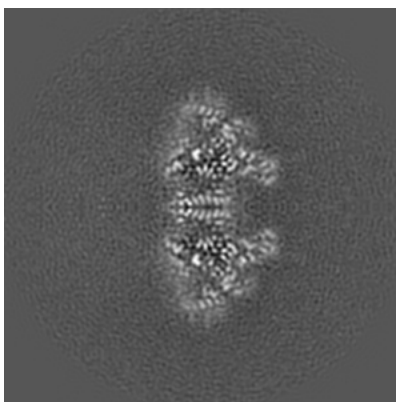
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

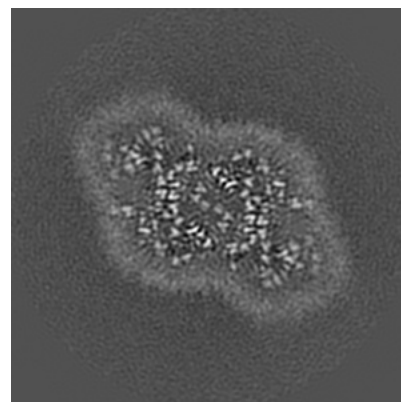
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

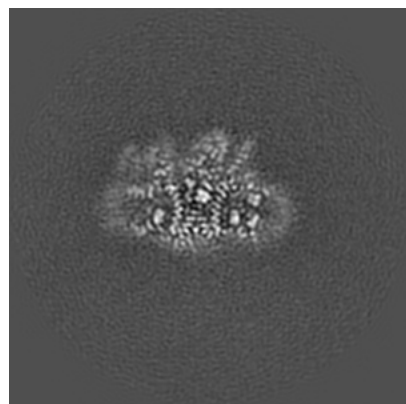


Z Index: 120

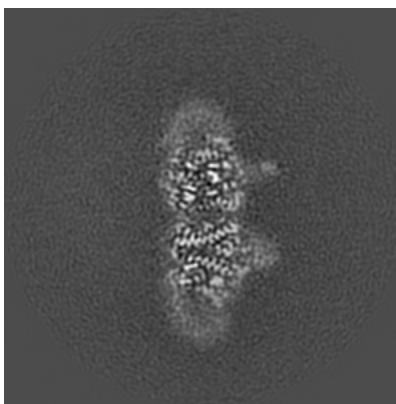
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

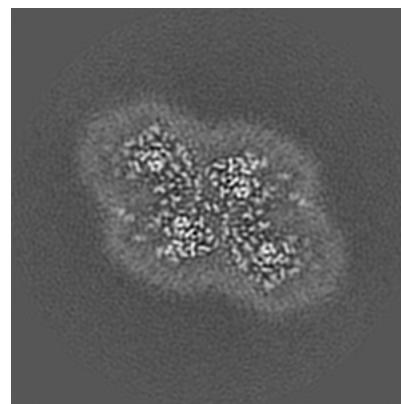
### 6.3.1 Primary map



X Index: 146



Y Index: 144

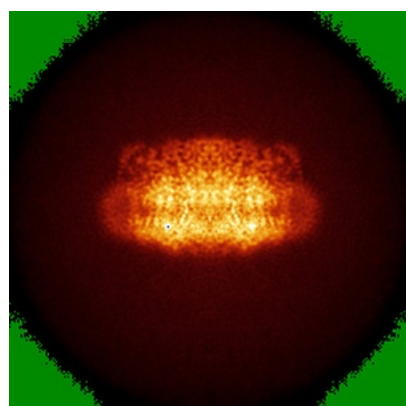


Z Index: 111

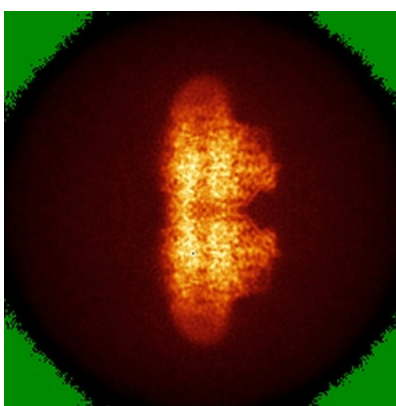
The images above show the largest variance slices of the map in three orthogonal directions.

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

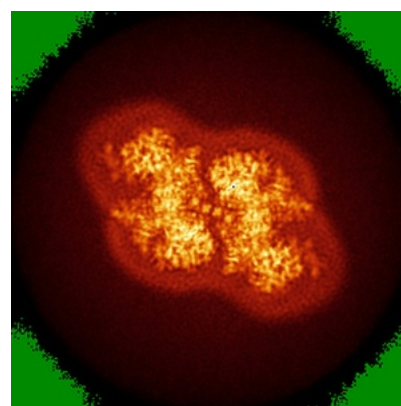
### 6.4.1 Primary map



X



Y

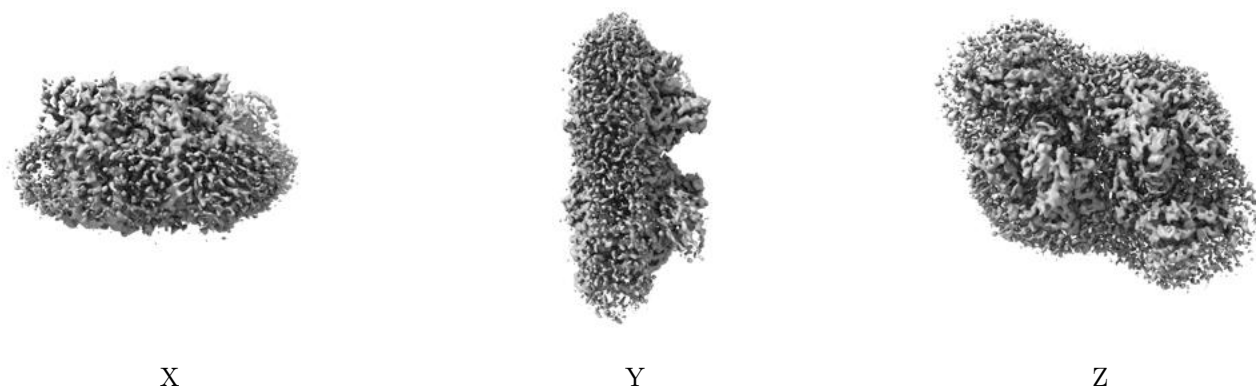


Z

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 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

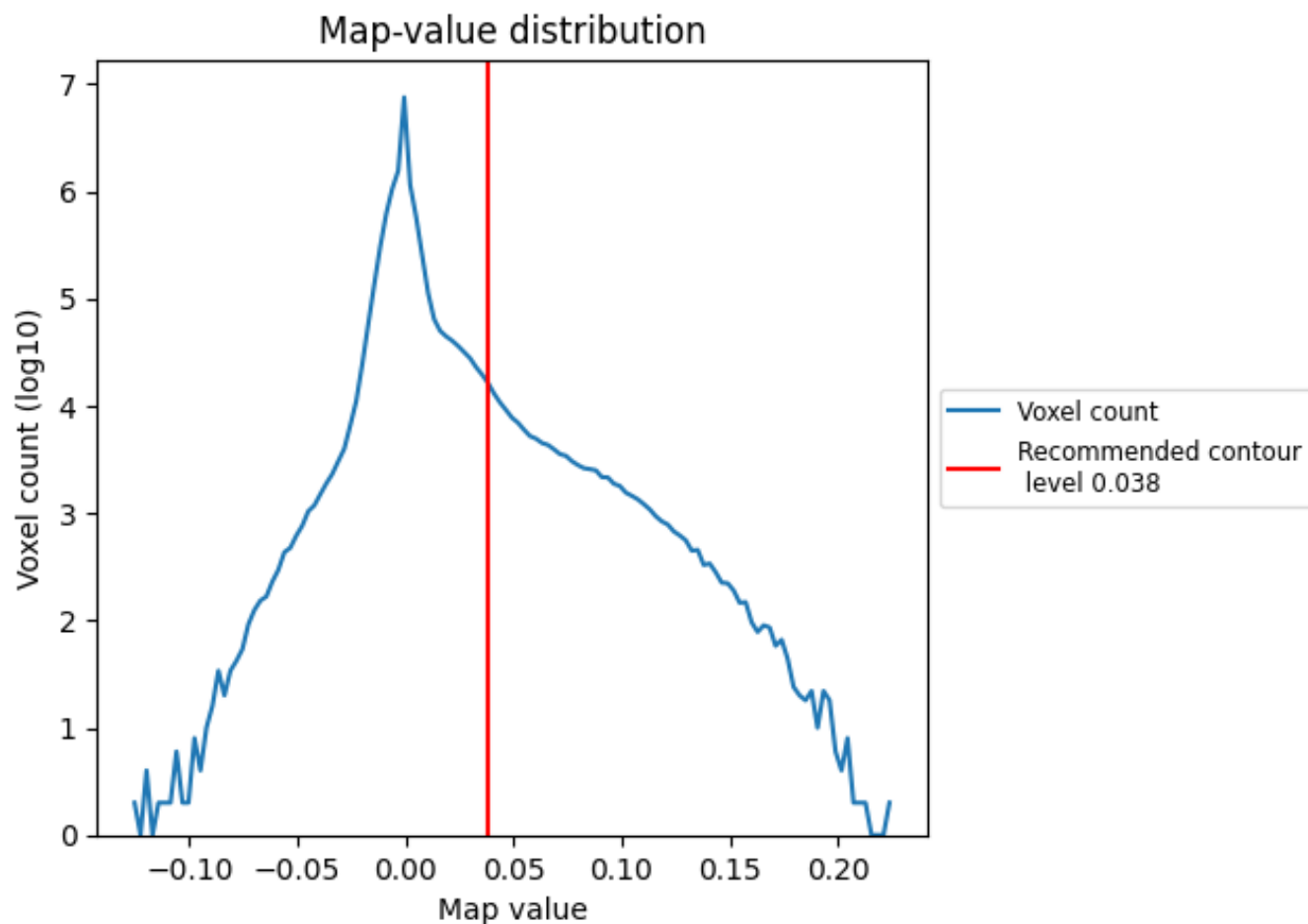
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

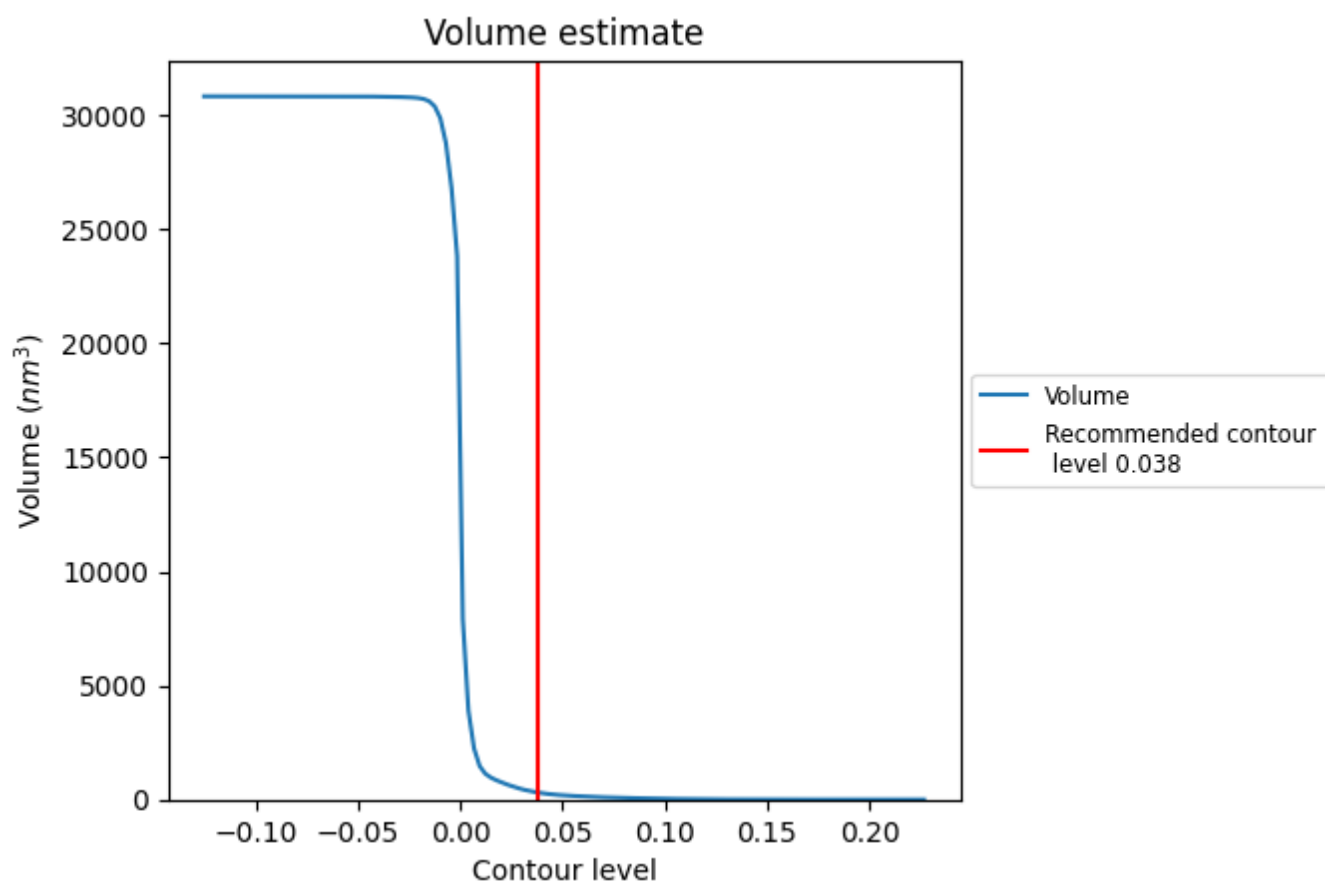
This section contains the results of statistical analysis of the map.

### 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.

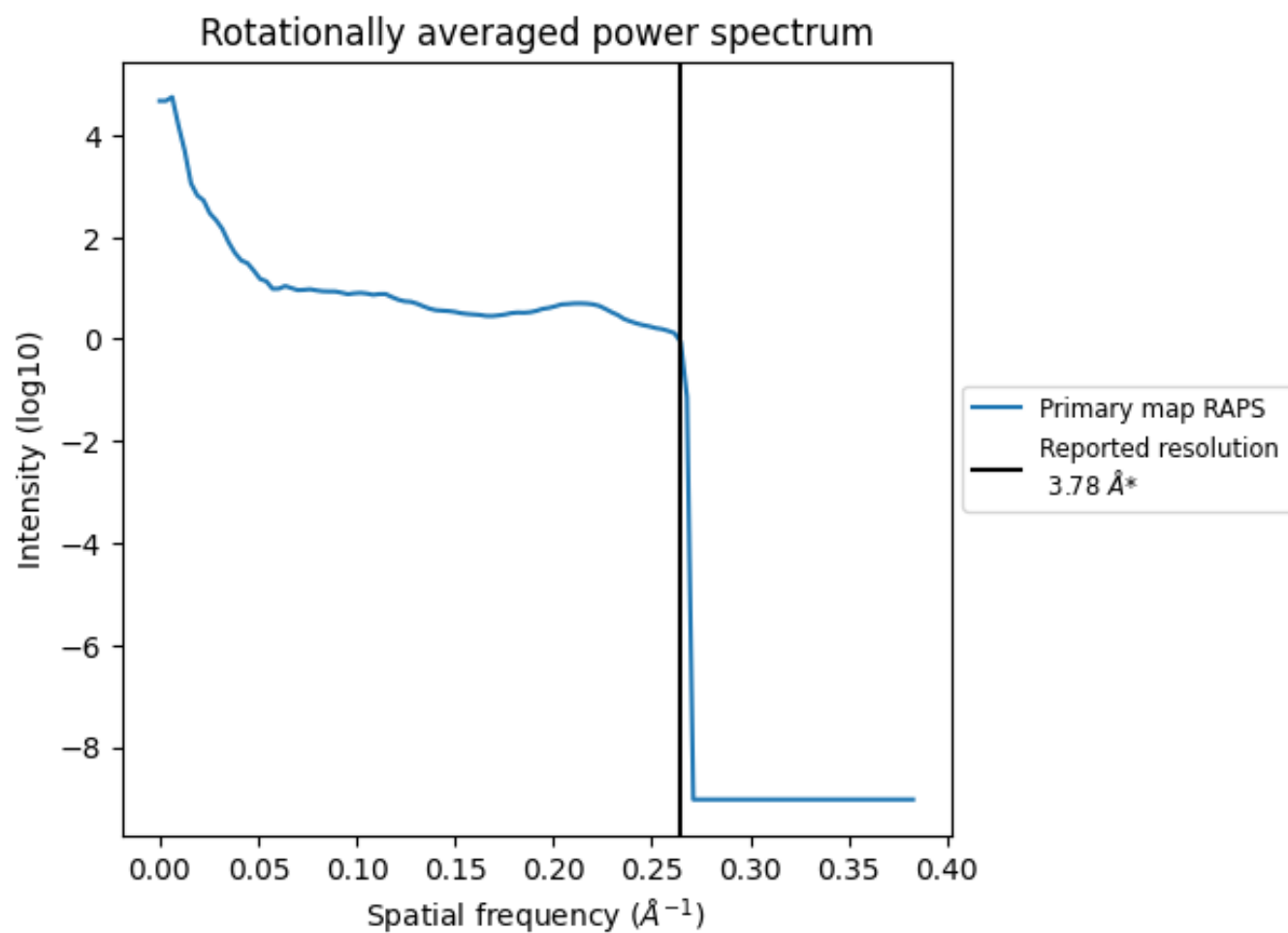
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm<sup>3</sup>; this corresponds to an approximate mass of 277 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 0.265 Å<sup>-1</sup>

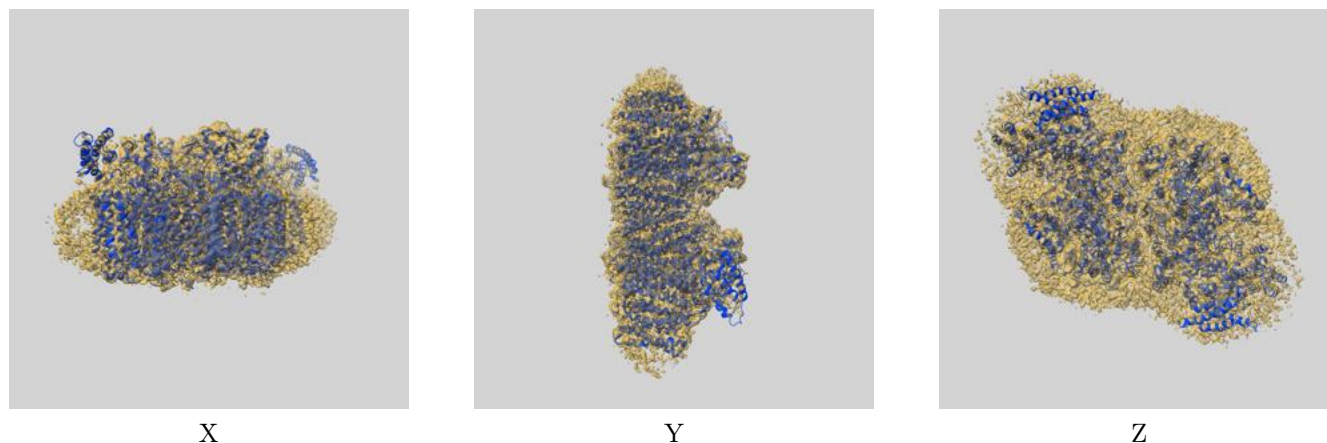
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30511 and PDB model 7CZL. Per-residue inclusion information can be found in section [3](#) on page [23](#).

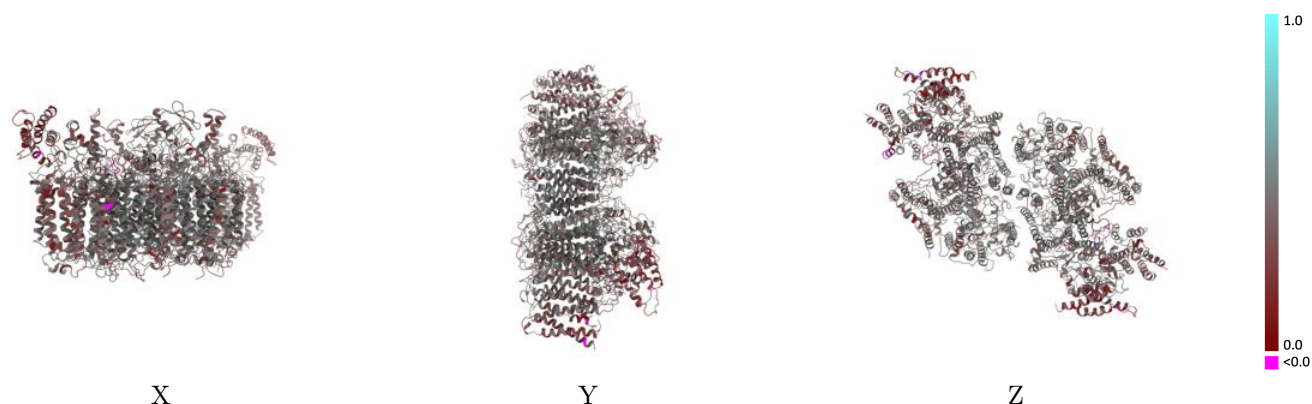
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.038 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.

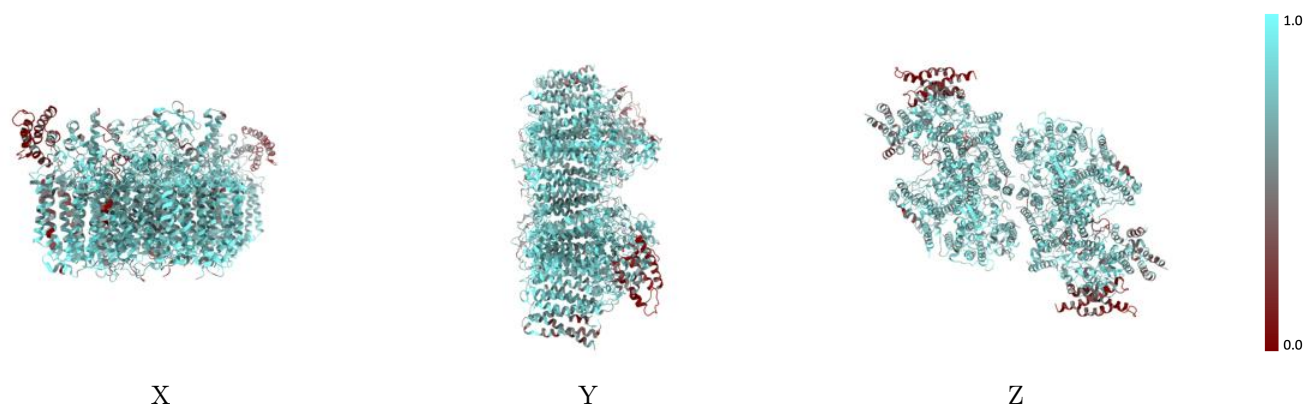


## 9.2 Q-score mapped to coordinate model [i](#)



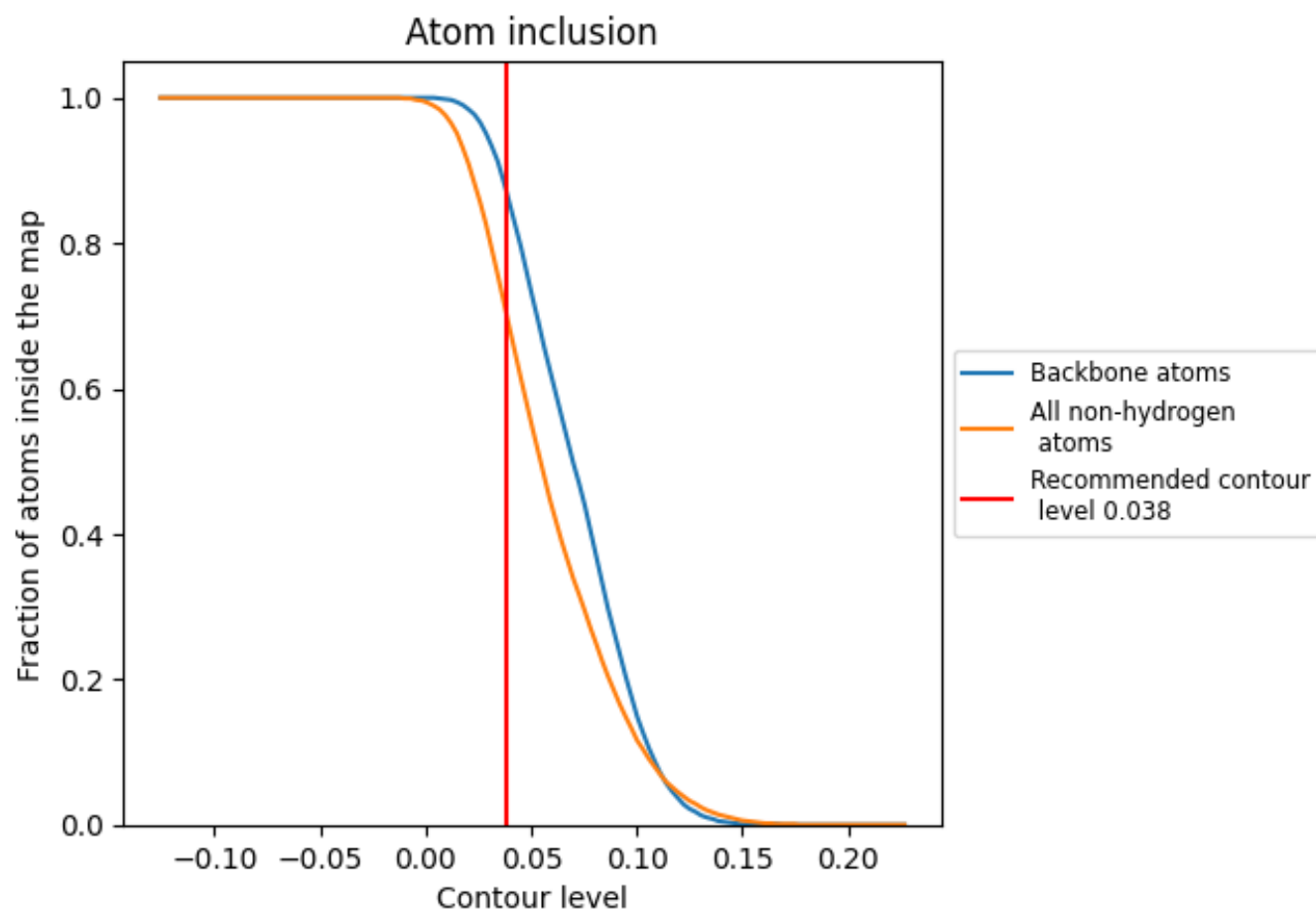
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.038).



































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 71% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.4220
A	 0.7340	 0.4410
B	 0.7710	 0.4490
C	 0.6990	 0.4080
D	 0.7710	 0.4490
E	 0.6800	 0.3720
F	 0.7410	 0.3800
H	 0.7950	 0.4370
I	 0.7650	 0.4150
K	 0.6700	 0.3670
L	 0.6960	 0.4470
M	 0.6060	 0.4270
N	 0.2210	 0.2790
T	 0.6080	 0.4550
X	 0.7360	 0.3700
Y	 0.4900	 0.3980
Z	 0.5290	 0.3190
a	 0.7330	 0.4390
b	 0.7760	 0.4500
c	 0.7080	 0.4070
d	 0.7670	 0.4470
e	 0.6860	 0.3680
f	 0.7410	 0.3550
h	 0.7780	 0.4320
i	 0.7680	 0.4200
k	 0.6530	 0.4010
l	 0.6610	 0.4700
m	 0.5950	 0.4350
n	 0.2060	 0.2740
t	 0.6630	 0.4710
x	 0.7640	 0.3980
y	 0.5020	 0.3350
z	 0.5150	 0.3210

