



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 08:12 AM EDT

PDB ID : 8EQM / pdb_00008eqm
EMDB ID : EMD-28539
Title : Structure of a dimeric photosystem II complex acclimated to far-red light
Authors : Gisriel, C.J.; Shen, G.; Flesher, D.A.; Kurashov, V.; Golbeck, J.H.; Brudvig, G.W.; Amin, M.; Bryant, D.A.
Deposited on : 2022-10-08
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

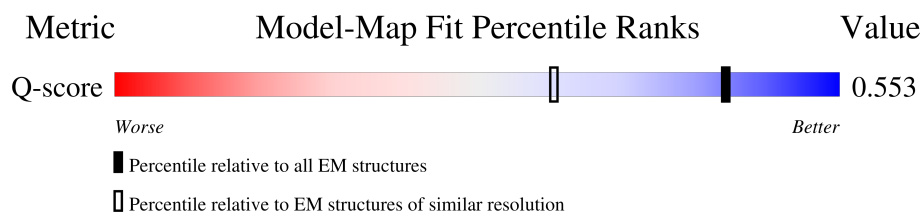
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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ELECTRON MICROSCOPY

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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	8728 (2.10 - 3.10)

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
25	BCT	A	411	-	X	-	-
25	BCT	a	411	-	X	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 42502 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	333	Total	C	N	O	S	0	0
			2630	1723	431	461	15		
1	a	333	Total	C	N	O	S	0	0
			2630	1723	431	461	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	483	Total	C	N	O	S	0	0
			3784	2491	627	653	13		
2	b	483	Total	C	N	O	S	0	0
			3784	2491	627	653	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	453	Total	C	N	O	S	0	0
			3498	2290	591	604	13		
3	c	453	Total	C	N	O	S	0	0
			3498	2290	591	604	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	338	Total	C	N	O	S	1	0
			2709	1797	439	459	14		
4	d	338	Total	C	N	O	S	1	0
			2709	1797	439	459	14		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	48	Total	C	N	O	0	0
			371	246	59	66		
5	e	48	Total	C	N	O	0	0
			371	246	59	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			237	159	41	36	1		
6	f	30	Total	C	N	O	S	0	0
			237	159	41	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			479	318	76	83	2		
7	h	65	Total	C	N	O	S	0	0
			479	318	76	83	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
			261	178	39	43	1		
8	i	34	Total	C	N	O	S	0	0
			261	178	39	43	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
			291	203	45	43		
9	k	37	Total	C	N	O	0	0
			291	203	45	43		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	30	Total	C	N	O	0	0
			245	166	36	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	30	Total	C	N	O	0	0
			245	166	36	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			244	168	34	41	1		
11	m	31	Total	C	N	O	S	0	0
			244	168	34	41	1		

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	182	Total	C	N	O	S	0	0
			1238	788	221	228	1		
12	o	182	Total	C	N	O	S	0	0
			1238	788	221	228	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	30	Total	C	N	O	S	0	0
			236	163	34	37	2		
13	t	30	Total	C	N	O	S	0	0
			236	163	34	37	2		

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	79	Total	C	N	O	0	0
			525	329	96	100		
14	u	79	Total	C	N	O	0	0
			525	329	96	100		

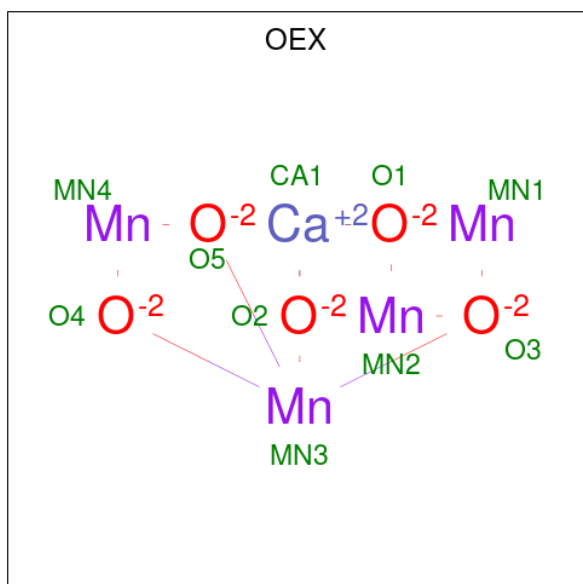
- Molecule 15 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	131	Total	C	N	O	S	0	0
			826	518	153	151	4		
15	v	131	Total	C	N	O	S	0	0
			826	518	153	151	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	35	Total	C	N	O	S	0	0
			261	174	41	44	2		
16	x	35	Total	C	N	O	S	0	0
			261	174	41	44	2		

- Molecule 17 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Ca	Mn	0
			5	1	4	
17	a	1	Total	Ca	Mn	0
			5	1	4	

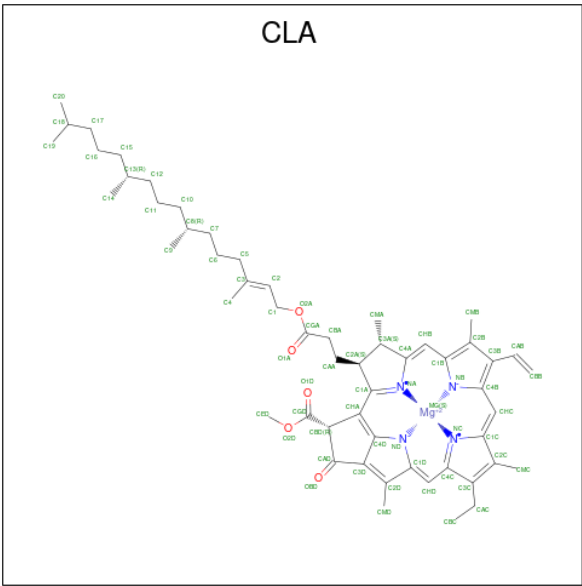
- Molecule 18 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 19 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Cl	0
			1	1	
19	C	1	Total	Cl	0
			1	1	
19	a	1	Total	Cl	0
			1	1	
19	c	1	Total	Cl	0
			1	1	

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	C	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	D	1	Total 45	C 35	Mg 1	N 4	O 5	0

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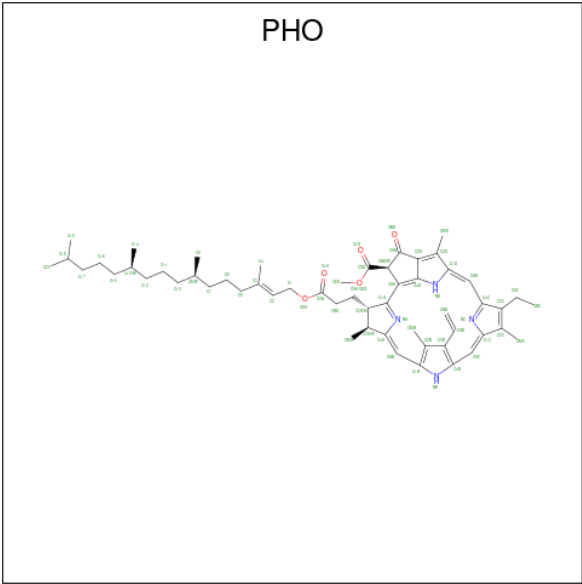
Mol	Chain	Residues	Atoms					AltConf
20	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	c	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 21 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



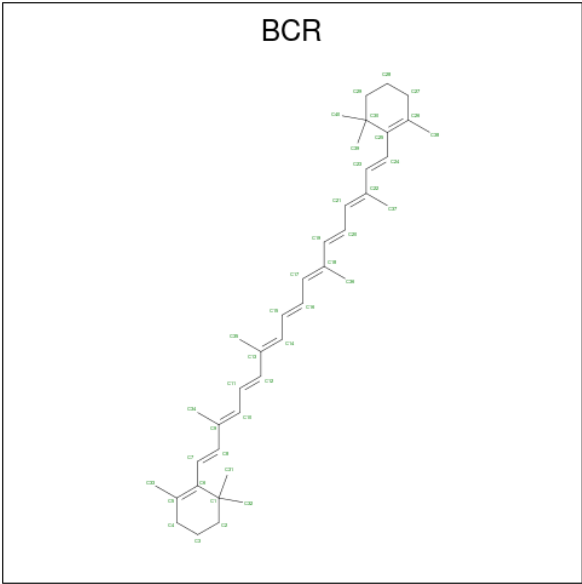
Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	N	O	0
			64	55	4	5	

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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



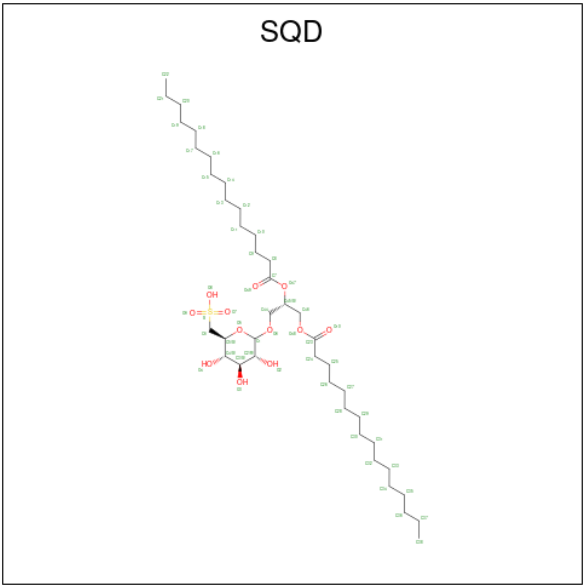
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	C	1	Total	C	0
			40	40	
22	C	1	Total	C	0
			20	20	
22	D	1	Total	C	0
			26	26	
22	a	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms		AltConf
22	b	1	Total	C	0
			40	40	
22	b	1	Total	C	0
			40	40	
22	b	1	Total	C	0
			40	40	
22	c	1	Total	C	0
			40	40	
22	c	1	Total	C	0
			20	20	
22	d	1	Total	C	0
			26	26	

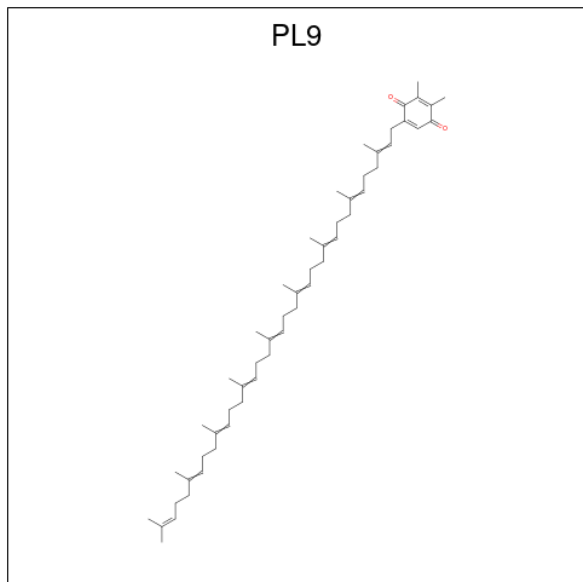
- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	S	0
			52	39	12	1	
23	L	1	Total	C	O	S	0
			54	41	12	1	
23	a	1	Total	C	O	S	0
			52	39	12	1	
23	l	1	Total	C	O	S	0
			54	41	12	1	

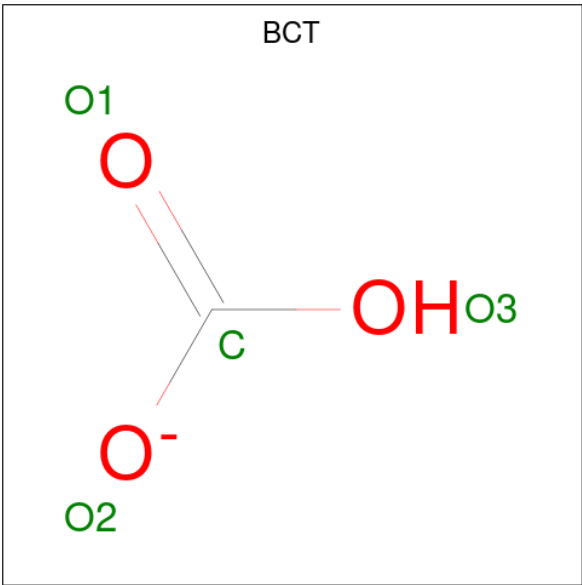
- Molecule 24 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22

,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



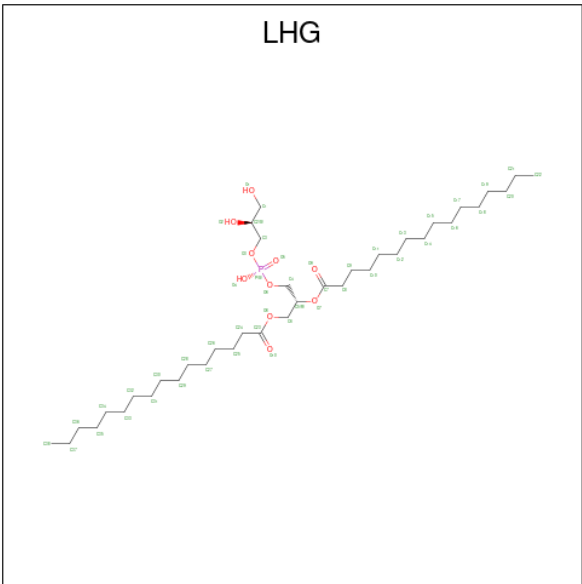
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			20	18	2	
24	D	1	Total	C	O	0
			45	43	2	
24	a	1	Total	C	O	0
			20	18	2	
24	d	1	Total	C	O	0
			45	43	2	

- Molecule 25 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



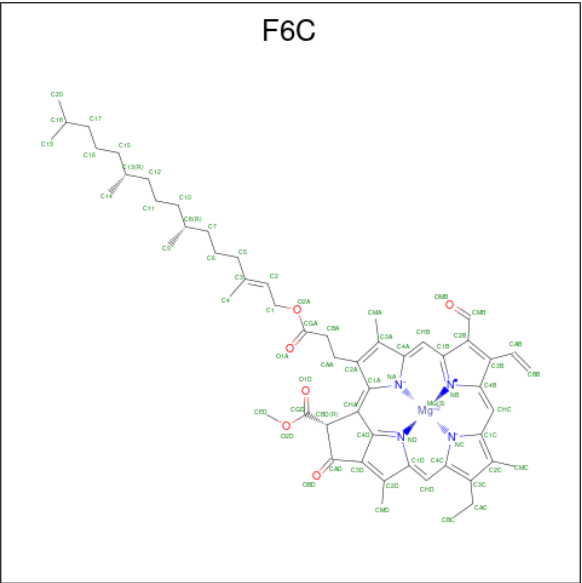
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	D	1	Total	C	O	P	0
			49	38	10	1	
26	D	1	Total	C	O	P	0
			47	36	10	1	
26	L	1	Total	C	O	P	0
			49	38	10	1	
26	a	1	Total	C	O	P	0
			37	26	10	1	
26	d	1	Total	C	O	P	0
			49	38	10	1	
26	d	1	Total	C	O	P	0
			47	36	10	1	
26	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is Chlorophyll F (CCD ID: F6C) (formula: $C_{55}H_{68}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



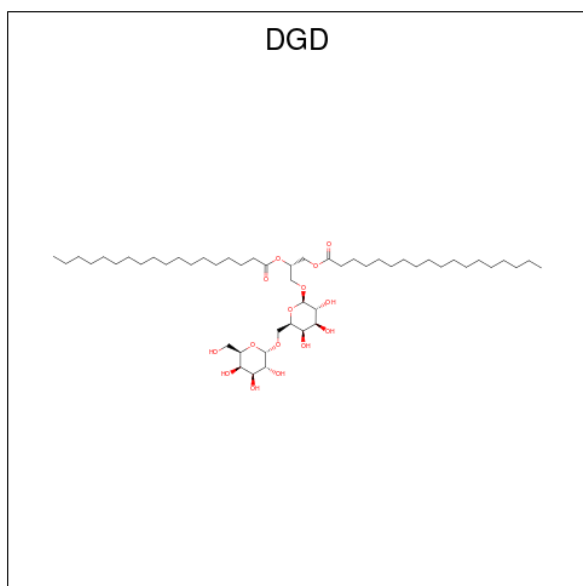
Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	B	1	Total 61	C 50	Mg 1	N 4	O 6	0
27	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	C	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	b	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
27	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	c	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

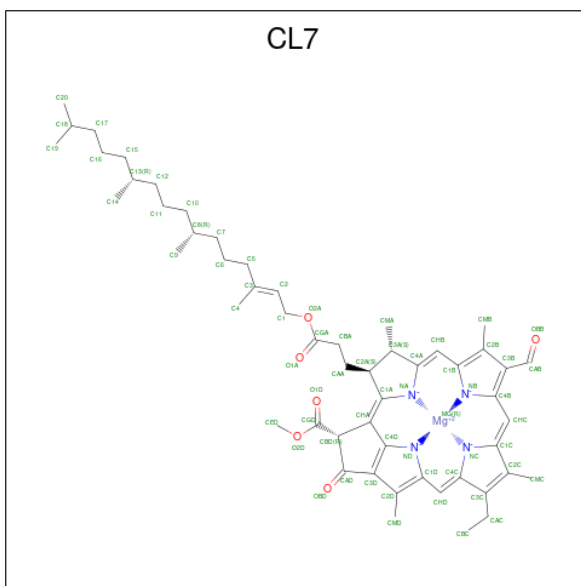
- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	C	1	Total	C	O	0
			49	34	15	
28	C	1	Total	C	O	0
			34	25	9	
28	D	1	Total	C	O	0
			45	36	9	
28	c	1	Total	C	O	0
			49	34	15	
28	c	1	Total	C	O	0
			34	25	9	
28	d	1	Total	C	O	0
			45	36	9	

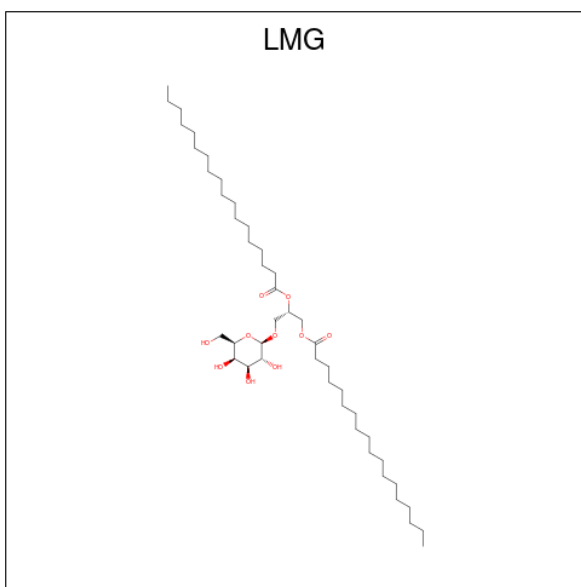
- Molecule 29 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as

"Ligand of Interest" by depositor).



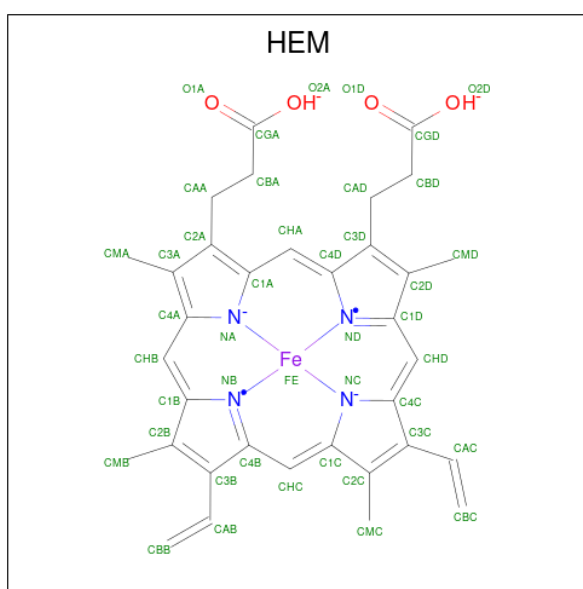
Mol	Chain	Residues	Atoms					AltConf
29	D	1	Total 65	C 54	Mg 1	N 4	O 6	0
29	d	1	Total 65	C 54	Mg 1	N 4	O 6	0

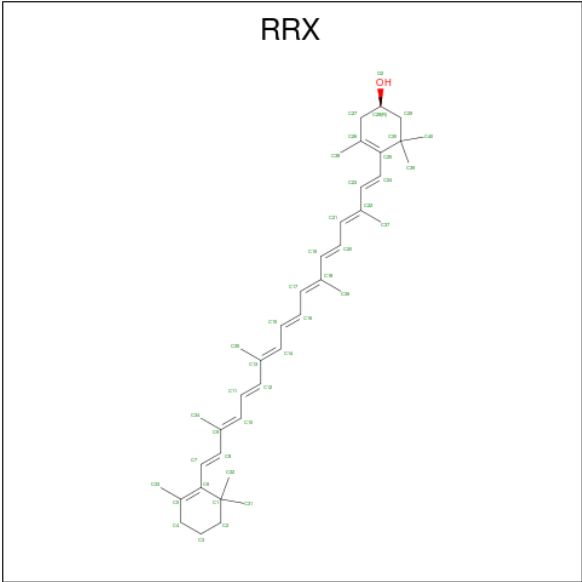
- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
30	D	1	Total	C	O	0
			33	23	10	
30	M	1	Total	C	O	0
			40	30	10	
30	d	1	Total	C	O	0
			33	23	10	
30	m	1	Total	C	O	0
			40	30	10	

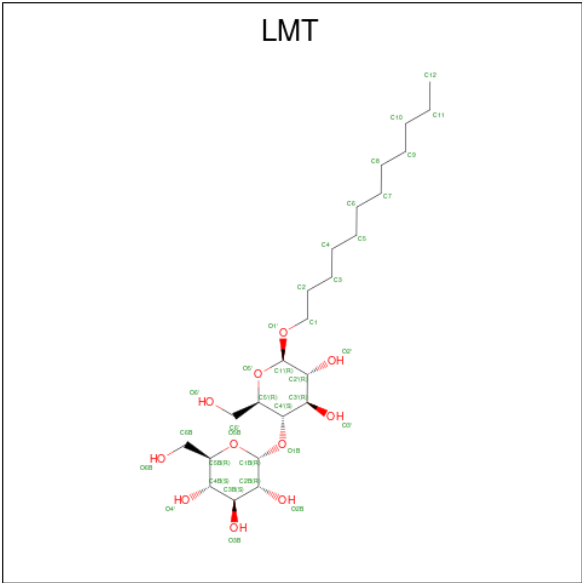
- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms			AltConf
32	H	1	Total	C	O	0
			41	40	1	
32	h	1	Total	C	O	0
			41	40	1	

- Molecule 33 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
33	M	1	Total	C	O	0
			35	24	11	
33	m	1	Total	C	O	0
			35	24	11	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	A	75	Total 75	O 75	0
34	B	69	Total 69	O 69	0
34	C	63	Total 63	O 63	0
34	D	60	Total 60	O 60	0
34	E	1	Total 1	O 1	0
34	F	1	Total 1	O 1	0
34	H	7	Total 7	O 7	0
34	L	6	Total 6	O 6	0
34	M	4	Total 4	O 4	0
34	O	3	Total 3	O 3	0
34	T	5	Total 5	O 5	0
34	X	1	Total 1	O 1	0
34	a	75	Total 75	O 75	0
34	b	69	Total 69	O 69	0
34	c	63	Total 63	O 63	0
34	d	60	Total 60	O 60	0
34	e	1	Total 1	O 1	0
34	f	1	Total 1	O 1	0
34	h	7	Total 7	O 7	0
34	l	6	Total 6	O 6	0
34	m	4	Total 4	O 4	0

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Mol	Chain	Residues	Atoms		AltConf
34	o	3	Total 3	O 3	0
34	t	5	Total 5	O 5	0
34	x	1	Total 1	O 1	0

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.1	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0013	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 132 ligands modelled in this entry, 6 are monoatomic - leaving 126 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	CLA	b	605	2	69,73,73	2.24	20 (28%)	82,113,113	2.59	34 (41%)
20	CLA	c	514	3	49,53,73	2.55	21 (42%)	58,89,113	2.76	24 (41%)
29	CL7	D	401	34	69,73,73	2.28	23 (33%)	80,113,113	2.38	23 (28%)
21	PHO	A	406	-	58,69,69	2.06	11 (18%)	55,99,99	1.65	13 (23%)
20	CLA	B	606	-	59,63,73	2.44	23 (38%)	70,101,113	2.64	25 (35%)
22	BCR	A	408	-	41,41,41	2.68	6 (14%)	56,56,56	6.54	21 (37%)
20	CLA	b	606	-	59,63,73	2.44	23 (38%)	70,101,113	2.64	25 (35%)
20	CLA	A	404	1	69,73,73	2.26	23 (33%)	82,113,113	2.46	25 (30%)
20	CLA	B	605	2	69,73,73	2.24	20 (28%)	82,113,113	2.59	34 (41%)
24	PL9	d	406	-	45,45,55	1.97	11 (24%)	56,57,69	1.56	10 (17%)
20	CLA	d	404	-	49,53,73	2.52	20 (40%)	58,89,113	2.86	22 (37%)
26	LHG	L	101	-	48,48,48	0.94	3 (6%)	51,54,54	1.04	4 (7%)
20	CLA	b	611	2	69,73,73	2.15	20 (28%)	82,113,113	2.41	27 (32%)
30	LMG	D	409	-	33,33,55	1.14	2 (6%)	41,41,63	1.24	4 (9%)
20	CLA	C	510	3	69,73,73	2.21	20 (28%)	82,113,113	2.48	30 (36%)
25	BCT	A	411	18	3,3,3	1.53	1 (33%)	2,3,3	4.50	2 (100%)
23	SQD	L	102	-	52,54,54	0.95	5 (9%)	62,65,65	1.91	13 (20%)
22	BCR	b	616	-	41,41,41	2.60	6 (14%)	56,56,56	6.66	30 (53%)
20	CLA	C	503	3	69,73,73	2.21	20 (28%)	82,113,113	2.53	31 (37%)
27	F6C	b	613	2	72,74,74	2.62	26 (36%)	83,114,114	3.20	31 (37%)
20	CLA	C	505	34	54,58,73	2.46	22 (40%)	64,95,113	2.76	25 (39%)
20	CLA	B	612	2	69,73,73	2.22	21 (30%)	82,113,113	2.58	30 (36%)
20	CLA	c	503	3	69,73,73	2.21	20 (28%)	82,113,113	2.53	31 (37%)
20	CLA	c	511	3	69,73,73	2.22	20 (28%)	82,113,113	2.57	25 (30%)
27	F6C	B	607	34	67,69,74	2.83	30 (44%)	77,108,114	3.23	34 (44%)
20	CLA	c	509	3	64,68,73	2.30	20 (31%)	76,107,113	2.45	30 (39%)
26	LHG	d	408	-	46,46,48	0.94	4 (8%)	49,52,54	1.04	4 (8%)
27	F6C	b	604	2	72,74,74	2.66	24 (33%)	83,114,114	3.16	36 (43%)
22	BCR	B	616	-	41,41,41	2.60	6 (14%)	56,56,56	6.66	29 (51%)
21	PHO	a	406	-	58,69,69	2.06	11 (18%)	55,99,99	1.65	13 (23%)
20	CLA	c	504	3	69,73,73	2.22	22 (31%)	82,113,113	2.51	28 (34%)
22	BCR	d	405	-	25,26,41	2.92	5 (20%)	32,34,56	7.35	12 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	C	517	-	34,34,67	1.19	5 (14%)	42,42,81	1.31	3 (7%)
20	CLA	c	505	34	54,58,73	2.46	22 (40%)	64,95,113	2.75	25 (39%)
20	CLA	D	403	4	64,68,73	2.27	22 (34%)	76,107,113	2.71	22 (28%)
26	LHG	D	408	-	46,46,48	0.95	4 (8%)	49,52,54	1.04	3 (6%)
24	PL9	A	410	-	20,20,55	2.84	7 (35%)	26,27,69	1.93	7 (26%)
20	CLA	B	610	34	69,73,73	2.13	20 (28%)	82,113,113	2.66	30 (36%)
27	F6C	B	604	2	72,74,74	2.66	24 (33%)	83,114,114	3.16	36 (43%)
20	CLA	a	404	1	69,73,73	2.26	23 (33%)	82,113,113	2.47	25 (30%)
21	PHO	d	402	-	58,69,69	2.09	10 (17%)	55,99,99	1.49	8 (14%)
20	CLA	b	609	2	49,53,73	2.54	19 (38%)	58,89,113	2.83	22 (37%)
31	HEM	E	101	5	50,50,50	1.39	7 (14%)	67,82,82	1.15	5 (7%)
33	LMT	M	102	-	36,36,36	1.25	7 (19%)	47,47,47	0.99	0
20	CLA	B	614	2	59,63,73	2.33	21 (35%)	70,101,113	2.62	24 (34%)
20	CLA	C	513	3	49,53,73	2.50	19 (38%)	58,89,113	2.74	22 (37%)
32	RRX	H	102	-	42,42,42	1.33	8 (19%)	56,58,58	1.52	12 (21%)
28	DGD	c	516	-	50,50,67	1.29	8 (16%)	64,64,81	1.47	13 (20%)
26	LHG	l	101	-	48,48,48	0.94	3 (6%)	51,54,54	1.04	4 (7%)
20	CLA	C	514	3	49,53,73	2.55	21 (42%)	58,89,113	2.76	24 (41%)
26	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.33	6 (11%)
20	CLA	b	601	-	49,53,73	2.51	20 (40%)	58,89,113	2.71	22 (37%)
28	DGD	D	410	-	45,45,67	0.90	2 (4%)	53,53,81	1.21	2 (3%)
20	CLA	C	504	3	69,73,73	2.22	22 (31%)	82,113,113	2.51	28 (34%)
22	BCR	B	618	-	41,41,41	2.70	6 (14%)	56,56,56	6.71	21 (37%)
20	CLA	B	611	2	69,73,73	2.15	20 (28%)	82,113,113	2.42	27 (32%)
20	CLA	b	612	2	69,73,73	2.22	21 (30%)	82,113,113	2.58	30 (36%)
20	CLA	c	512	3	54,58,73	2.43	20 (37%)	64,95,113	2.93	26 (40%)
20	CLA	a	405	34	54,58,73	2.46	20 (37%)	64,95,113	2.90	28 (43%)
20	CLA	h	101	2	54,58,73	2.44	20 (37%)	64,95,113	2.86	27 (42%)
20	CLA	c	502	3	64,68,73	2.29	21 (32%)	76,107,113	2.51	22 (28%)
25	BCT	a	411	18	3,3,3	1.53	1 (33%)	2,3,3	4.50	2 (100%)
22	BCR	D	405	-	25,26,41	2.92	5 (20%)	32,34,56	7.36	11 (34%)
20	CLA	c	506	3	64,68,73	2.26	20 (31%)	76,107,113	2.62	27 (35%)
26	LHG	a	412	1	36,36,48	1.06	4 (11%)	39,42,54	1.41	5 (12%)
30	LMG	M	101	-	40,40,55	1.16	4 (10%)	48,48,63	1.29	5 (10%)
23	SQD	a	409	-	50,52,54	0.38	1 (2%)	60,63,65	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	C	507	3	59,63,73	2.48	22 (37%)	70,101,113	2.75	31 (44%)
20	CLA	B	608	2	59,63,73	2.42	20 (33%)	70,101,113	2.58	28 (40%)
20	CLA	c	510	3	69,73,73	2.21	20 (28%)	82,113,113	2.48	30 (36%)
20	CLA	b	614	2	59,63,73	2.33	20 (33%)	70,101,113	2.62	24 (34%)
22	BCR	c	518	-	20,20,41	2.53	3 (15%)	27,27,56	5.86	10 (37%)
32	RRX	h	102	-	42,42,42	1.33	8 (19%)	56,58,58	1.51	12 (21%)
22	BCR	C	518	-	20,20,41	2.54	3 (15%)	27,27,56	5.85	10 (37%)
20	CLA	a	407	1	54,58,73	2.55	23 (42%)	64,95,113	2.75	25 (39%)
24	PL9	a	410	-	20,20,55	2.84	7 (35%)	26,27,69	1.92	7 (26%)
20	CLA	b	602	-	69,73,73	2.26	24 (34%)	82,113,113	2.49	25 (30%)
22	BCR	c	515	-	41,41,41	2.65	6 (14%)	56,56,56	6.82	23 (41%)
26	LHG	A	412	1	36,36,48	1.06	4 (11%)	39,42,54	1.41	5 (12%)
27	F6C	B	613	2	72,74,74	2.61	26 (36%)	83,114,114	3.20	31 (37%)
22	BCR	b	618	-	41,41,41	2.70	6 (14%)	56,56,56	6.72	21 (37%)
24	PL9	D	406	-	45,45,55	1.97	11 (24%)	56,57,69	1.55	10 (17%)
22	BCR	a	408	-	41,41,41	2.67	7 (17%)	56,56,56	6.54	21 (37%)
20	CLA	c	513	3	49,53,73	2.49	19 (38%)	58,89,113	2.74	22 (37%)
20	CLA	A	405	34	54,58,73	2.45	20 (37%)	64,95,113	2.89	28 (43%)
31	HEM	v	201	15	50,50,50	1.41	9 (18%)	67,82,82	1.18	8 (11%)
20	CLA	B	602	-	69,73,73	2.26	23 (33%)	82,113,113	2.49	24 (29%)
20	CLA	B	615	2	64,68,73	2.18	21 (32%)	76,107,113	2.75	27 (35%)
20	CLA	c	507	3	59,63,73	2.48	22 (37%)	70,101,113	2.75	31 (44%)
30	LMG	m	101	-	40,40,55	1.16	4 (10%)	48,48,63	1.29	5 (10%)
20	CLA	C	502	3	64,68,73	2.29	21 (32%)	76,107,113	2.51	22 (28%)
21	PHO	D	402	-	58,69,69	2.09	10 (17%)	55,99,99	1.49	8 (14%)
20	CLA	C	506	3	64,68,73	2.27	20 (31%)	76,107,113	2.62	27 (35%)
28	DGD	c	517	-	34,34,67	1.19	5 (14%)	42,42,81	1.31	3 (7%)
26	LHG	d	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.33	6 (11%)
28	DGD	C	516	-	50,50,67	1.29	9 (18%)	64,64,81	1.47	13 (20%)
31	HEM	V	201	15	50,50,50	1.41	9 (18%)	67,82,82	1.18	8 (11%)
20	CLA	d	403	4	64,68,73	2.26	22 (34%)	76,107,113	2.71	22 (28%)
20	CLA	b	603	-	59,63,73	2.44	23 (38%)	70,101,113	2.66	26 (37%)
20	CLA	C	509	3	64,68,73	2.30	20 (31%)	76,107,113	2.44	30 (39%)
22	BCR	C	515	-	41,41,41	2.65	6 (14%)	56,56,56	6.82	23 (41%)
27	F6C	c	508	34	67,69,74	2.84	29 (43%)	77,108,114	3.23	33 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	601	-	49,53,73	2.51	20 (40%)	58,89,113	2.71	22 (37%)
27	F6C	C	508	34	67,69,74	2.83	30 (44%)	77,108,114	3.23	33 (42%)
30	LMG	d	409	-	33,33,55	1.14	2 (6%)	41,41,63	1.24	4 (9%)
20	CLA	b	615	2	64,68,73	2.18	21 (32%)	76,107,113	2.75	27 (35%)
22	BCR	b	617	-	41,41,41	2.68	6 (14%)	56,56,56	6.62	23 (41%)
20	CLA	b	608	2	59,63,73	2.42	20 (33%)	70,101,113	2.59	28 (40%)
23	SQD	l	102	-	52,54,54	0.95	5 (9%)	62,65,65	1.91	13 (20%)
20	CLA	H	101	2	54,58,73	2.44	20 (37%)	64,95,113	2.86	28 (43%)
31	HEM	e	101	5	50,50,50	1.38	7 (14%)	67,82,82	1.15	5 (7%)
20	CLA	b	610	34	69,73,73	2.13	20 (28%)	82,113,113	2.66	30 (36%)
29	CL7	d	401	34	69,73,73	2.29	23 (33%)	80,113,113	2.38	23 (28%)
33	LMT	m	102	-	36,36,36	1.25	7 (19%)	47,47,47	0.99	0
20	CLA	C	512	3	54,58,73	2.43	20 (37%)	64,95,113	2.93	26 (40%)
20	CLA	A	407	1	54,58,73	2.55	23 (42%)	64,95,113	2.75	26 (40%)
27	F6C	b	607	34	67,69,74	2.83	30 (44%)	77,108,114	3.23	34 (44%)
20	CLA	B	603	-	59,63,73	2.44	23 (38%)	70,101,113	2.67	26 (37%)
22	BCR	B	617	-	41,41,41	2.68	6 (14%)	56,56,56	6.62	23 (41%)
20	CLA	C	511	3	69,73,73	2.22	20 (28%)	82,113,113	2.57	25 (30%)
20	CLA	B	609	2	49,53,73	2.54	19 (38%)	58,89,113	2.83	22 (37%)
23	SQD	A	409	-	50,52,54	0.38	1 (2%)	60,63,65	0.40	0
20	CLA	D	404	-	49,53,73	2.52	20 (40%)	58,89,113	2.86	21 (36%)
28	DGD	d	410	-	45,45,67	0.90	2 (4%)	53,53,81	1.21	2 (3%)

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	CLA	b	605	2	-	12/39/115/115	-
20	CLA	c	514	3	-	3/15/91/115	-
29	CL7	D	401	34	2/2/15/20	12/39/115/115	-
21	PHO	A	406	-	-	17/37/103/103	0/5/6/6
20	CLA	B	606	-	-	7/27/103/115	-
22	BCR	A	408	-	-	6/29/63/63	0/2/2/2
20	CLA	b	606	-	-	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	404	1	-	10/39/115/115	-
20	CLA	B	605	2	-	12/39/115/115	-
24	PL9	d	406	-	-	13/41/61/73	0/1/1/1
20	CLA	d	404	-	-	7/15/91/115	-
26	LHG	L	101	-	-	24/53/53/53	-
20	CLA	b	611	2	-	12/39/115/115	-
30	LMG	D	409	-	-	7/28/48/70	0/1/1/1
20	CLA	C	510	3	-	10/39/115/115	-
23	SQD	L	102	-	-	21/49/69/69	0/1/1/1
22	BCR	b	616	-	-	12/29/63/63	0/2/2/2
20	CLA	C	503	3	-	14/39/115/115	-
27	F6C	b	613	2	1/1/10/16	20/41/97/97	-
20	CLA	C	505	34	-	5/21/97/115	-
20	CLA	B	612	2	-	14/39/115/115	-
20	CLA	c	503	3	-	14/39/115/115	-
20	CLA	c	511	3	-	15/39/115/115	-
27	F6C	B	607	34	1/1/9/16	19/35/91/97	-
20	CLA	c	509	3	-	7/33/109/115	-
26	LHG	d	408	-	-	22/51/51/53	-
27	F6C	b	604	2	1/1/10/16	17/41/97/97	-
22	BCR	B	616	-	-	12/29/63/63	0/2/2/2
21	PHO	a	406	-	-	17/37/103/103	0/5/6/6
20	CLA	c	504	3	-	18/39/115/115	-
22	BCR	d	405	-	-	7/20/37/63	0/1/1/2
28	DGD	C	517	-	-	12/28/48/95	0/1/1/2
20	CLA	c	505	34	-	5/21/97/115	-
20	CLA	D	403	4	-	7/33/109/115	-
26	LHG	D	408	-	-	22/51/51/53	-
24	PL9	A	410	-	-	5/11/31/73	0/1/1/1
20	CLA	B	610	34	-	16/39/115/115	-
27	F6C	B	604	2	1/1/10/16	17/41/97/97	-
20	CLA	a	404	1	-	10/39/115/115	-
21	PHO	d	402	-	-	6/37/103/103	0/5/6/6
20	CLA	b	609	2	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	HEM	E	101	5	-	6/14/54/54	-
33	LMT	M	102	-	-	7/21/61/61	0/2/2/2
20	CLA	B	614	2	-	9/27/103/115	-
20	CLA	C	513	3	-	9/15/91/115	-
32	RRX	H	102	-	-	20/29/65/65	0/2/2/2
28	DGD	c	516	-	-	16/38/78/95	0/2/2/2
26	LHG	l	101	-	-	24/53/53/53	-
20	CLA	C	514	3	-	3/15/91/115	-
26	LHG	D	407	-	-	28/53/53/53	-
20	CLA	b	601	-	-	11/15/91/115	-
28	DGD	D	410	-	-	12/39/59/95	0/1/1/2
20	CLA	C	504	3	-	18/39/115/115	-
22	BCR	B	618	-	-	11/29/63/63	0/2/2/2
20	CLA	B	611	2	-	12/39/115/115	-
20	CLA	b	612	2	-	14/39/115/115	-
20	CLA	c	512	3	-	9/21/97/115	-
20	CLA	a	405	34	-	5/21/97/115	-
20	CLA	h	101	2	-	6/21/97/115	-
20	CLA	c	502	3	-	10/33/109/115	-
22	BCR	D	405	-	-	7/20/37/63	0/1/1/2
20	CLA	c	506	3	-	17/33/109/115	-
26	LHG	a	412	1	-	26/41/41/53	-
30	LMG	M	101	-	-	11/35/55/70	0/1/1/1
23	SQD	a	409	-	-	26/47/67/69	0/1/1/1
20	CLA	C	507	3	-	11/27/103/115	-
20	CLA	B	608	2	-	9/27/103/115	-
20	CLA	c	510	3	-	10/39/115/115	-
20	CLA	b	614	2	-	8/27/103/115	-
22	BCR	c	518	-	-	6/13/30/63	0/1/1/2
32	RRX	h	102	-	-	20/29/65/65	0/2/2/2
22	BCR	C	518	-	-	6/13/30/63	0/1/1/2
20	CLA	a	407	1	-	6/21/97/115	-
27	F6C	B	613	2	1/1/10/16	20/41/97/97	-
20	CLA	b	602	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	c	515	-	-	5/29/63/63	0/2/2/2
24	PL9	a	410	-	-	5/11/31/73	0/1/1/1
26	LHG	A	412	1	-	26/41/41/53	-
22	BCR	b	618	-	-	11/29/63/63	0/2/2/2
24	PL9	D	406	-	-	13/41/61/73	0/1/1/1
22	BCR	a	408	-	-	6/29/63/63	0/2/2/2
20	CLA	c	513	3	-	9/15/91/115	-
20	CLA	A	405	34	-	5/21/97/115	-
31	HEM	v	201	15	-	6/14/54/54	-
20	CLA	B	602	-	-	15/39/115/115	-
20	CLA	B	615	2	-	13/33/109/115	-
20	CLA	c	507	3	-	11/27/103/115	-
30	LMG	m	101	-	-	11/35/55/70	0/1/1/1
20	CLA	C	502	3	-	10/33/109/115	-
21	PHO	D	402	-	-	6/37/103/103	0/5/6/6
20	CLA	C	506	3	-	17/33/109/115	-
28	DGD	c	517	-	-	12/28/48/95	0/1/1/2
26	LHG	d	407	-	-	28/53/53/53	-
28	DGD	C	516	-	-	16/38/78/95	0/2/2/2
31	HEM	V	201	15	-	6/14/54/54	-
20	CLA	d	403	4	-	7/33/109/115	-
20	CLA	b	603	-	-	9/27/103/115	-
27	F6C	c	508	34	1/1/9/16	22/35/91/97	-
20	CLA	C	509	3	-	7/33/109/115	-
22	BCR	C	515	-	-	6/29/63/63	0/2/2/2
20	CLA	B	601	-	-	11/15/91/115	-
27	F6C	C	508	34	1/1/9/16	21/35/91/97	-
30	LMG	d	409	-	-	7/28/48/70	0/1/1/1
20	CLA	b	615	2	-	12/33/109/115	-
22	BCR	b	617	-	-	5/29/63/63	0/2/2/2
20	CLA	b	608	2	-	9/27/103/115	-
23	SQD	l	102	-	-	21/49/69/69	0/1/1/1
20	CLA	H	101	2	-	6/21/97/115	-
31	HEM	e	101	5	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	610	34	-	16/39/115/115	-
29	CL7	d	401	34	2/2/15/20	12/39/115/115	-
33	LMT	m	102	-	-	7/21/61/61	0/2/2/2
20	CLA	C	512	3	-	9/21/97/115	-
20	CLA	A	407	1	-	6/21/97/115	-
27	F6C	b	607	34	1/1/9/16	19/35/91/97	-
20	CLA	B	603	-	-	9/27/103/115	-
22	BCR	B	617	-	-	5/29/63/63	0/2/2/2
20	CLA	C	511	3	-	15/39/115/115	-
20	CLA	B	609	2	-	8/15/91/115	-
23	SQD	A	409	-	-	26/47/67/69	0/1/1/1
20	CLA	D	404	-	-	7/15/91/115	-
28	DGD	d	410	-	-	12/39/59/95	0/1/1/2

The worst 5 of 1819 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	613	F6C	C1A-CHA	9.72	1.51	1.35
27	b	613	F6C	C1A-CHA	9.72	1.51	1.35
27	B	604	F6C	MG-NA	9.21	2.24	2.05
27	b	604	F6C	MG-NA	9.21	2.24	2.05
21	a	406	PHO	C3B-C4B	9.19	1.50	1.41

The worst 5 of 2419 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	BCR	C16-C17-C18	23.63	160.41	127.28
22	B	618	BCR	C16-C17-C18	23.62	160.40	127.28
22	c	518	BCR	C11-C10-C9	23.31	159.97	127.28
22	C	518	BCR	C11-C10-C9	23.27	159.91	127.28
22	C	515	BCR	C16-C17-C18	22.57	158.94	127.28

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	B	604	F6C	NA
27	B	607	F6C	NA
27	B	613	F6C	NA
27	C	508	F6C	NA

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Mol	Chain	Res	Type	Atom
27	b	604	F6C	NA

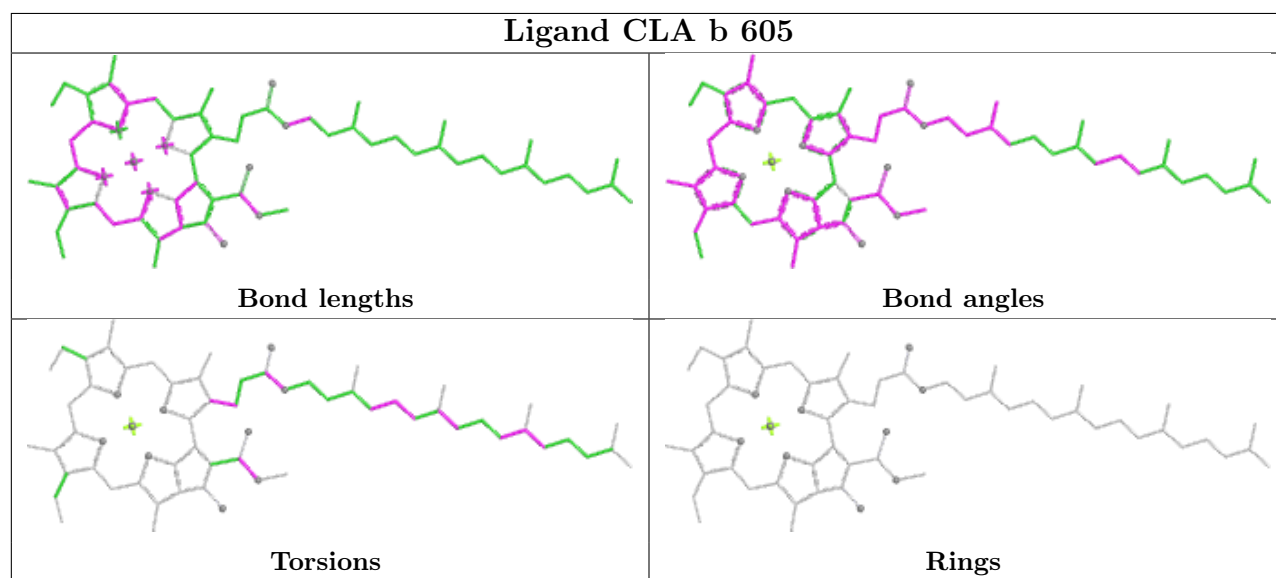
5 of 1460 torsion outliers are listed below:

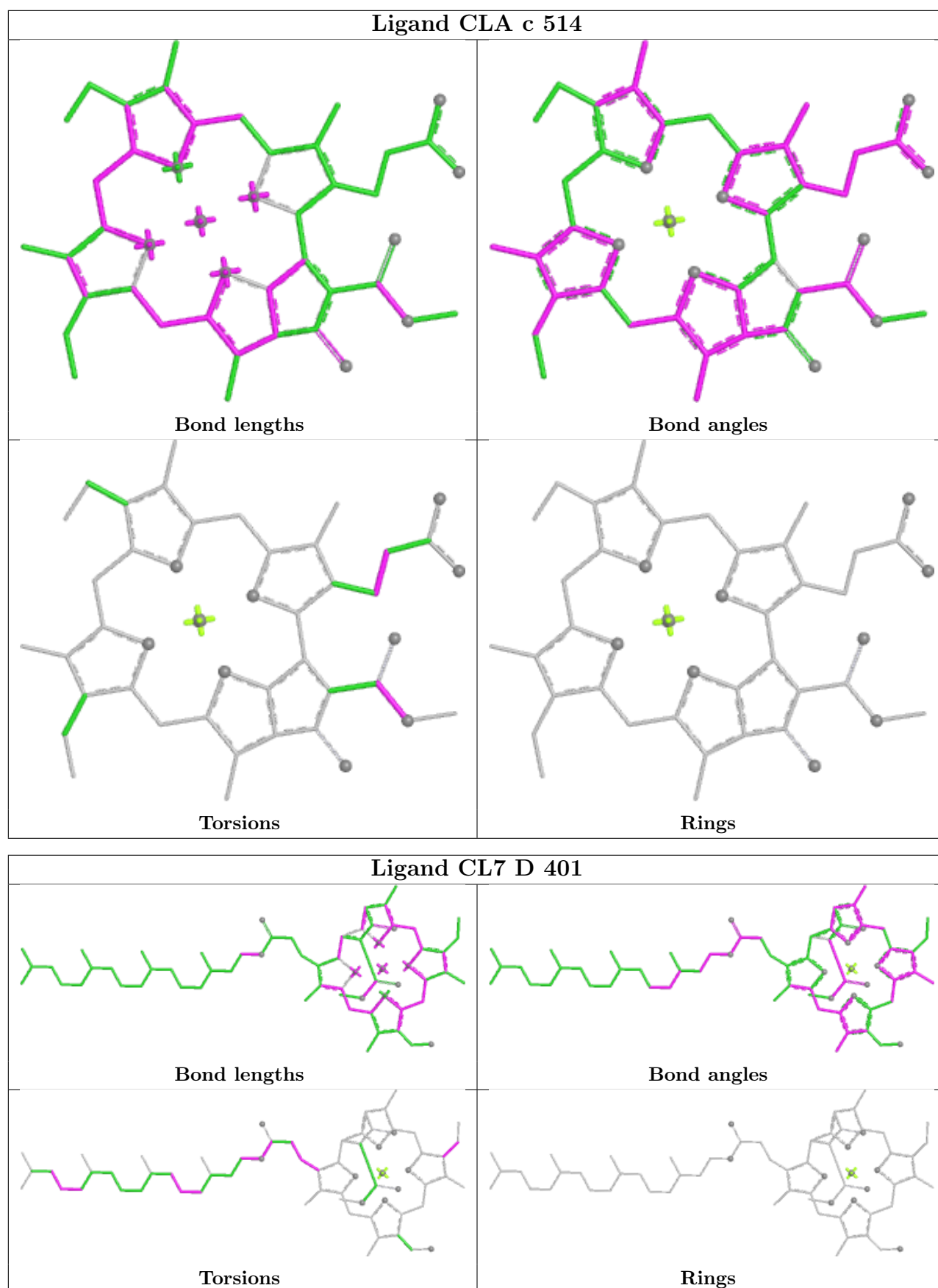
Mol	Chain	Res	Type	Atoms
20	A	404	CLA	CBD-CGD-O2D-CED
20	A	404	CLA	O1D-CGD-O2D-CED
20	A	405	CLA	CBA-CGA-O2A-C1
20	A	405	CLA	O1A-CGA-O2A-C1
20	B	601	CLA	CAD-CBD-CGD-O1D

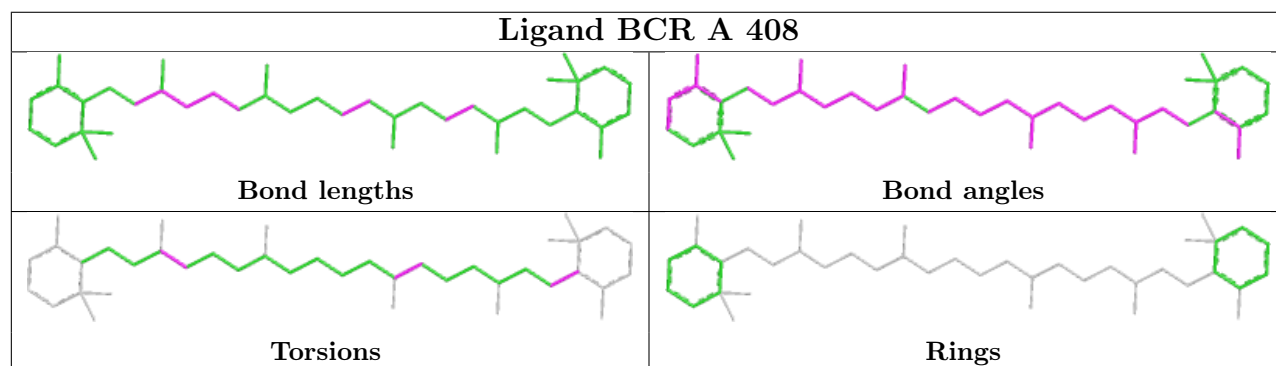
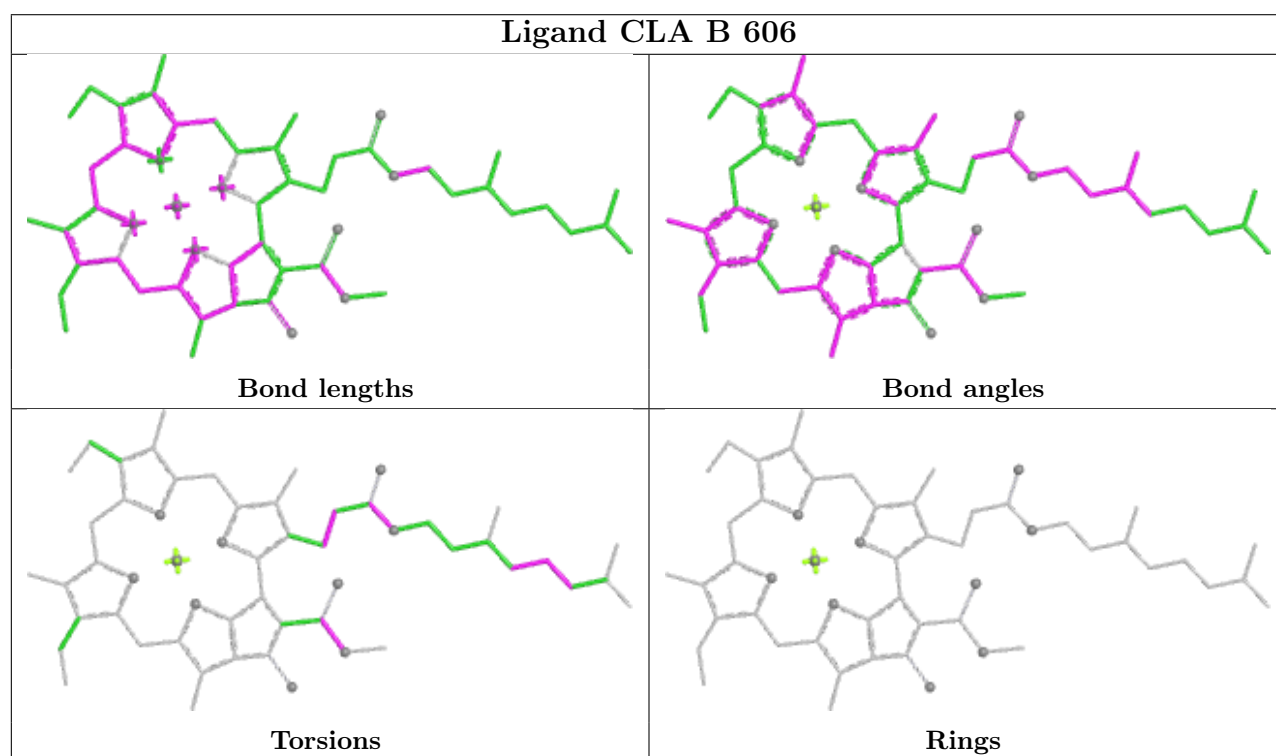
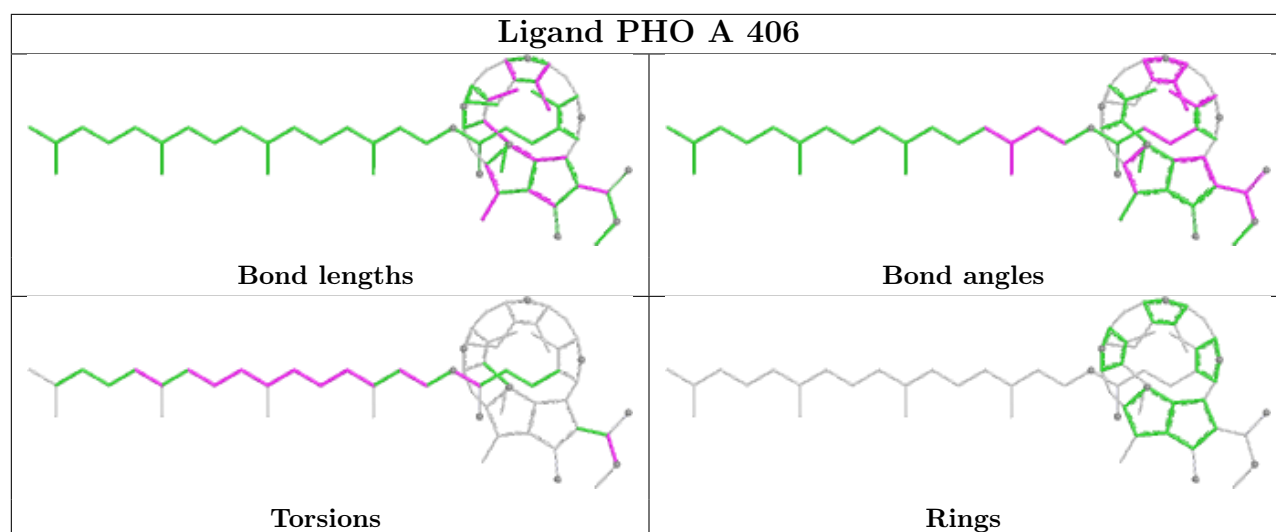
There are no ring outliers.

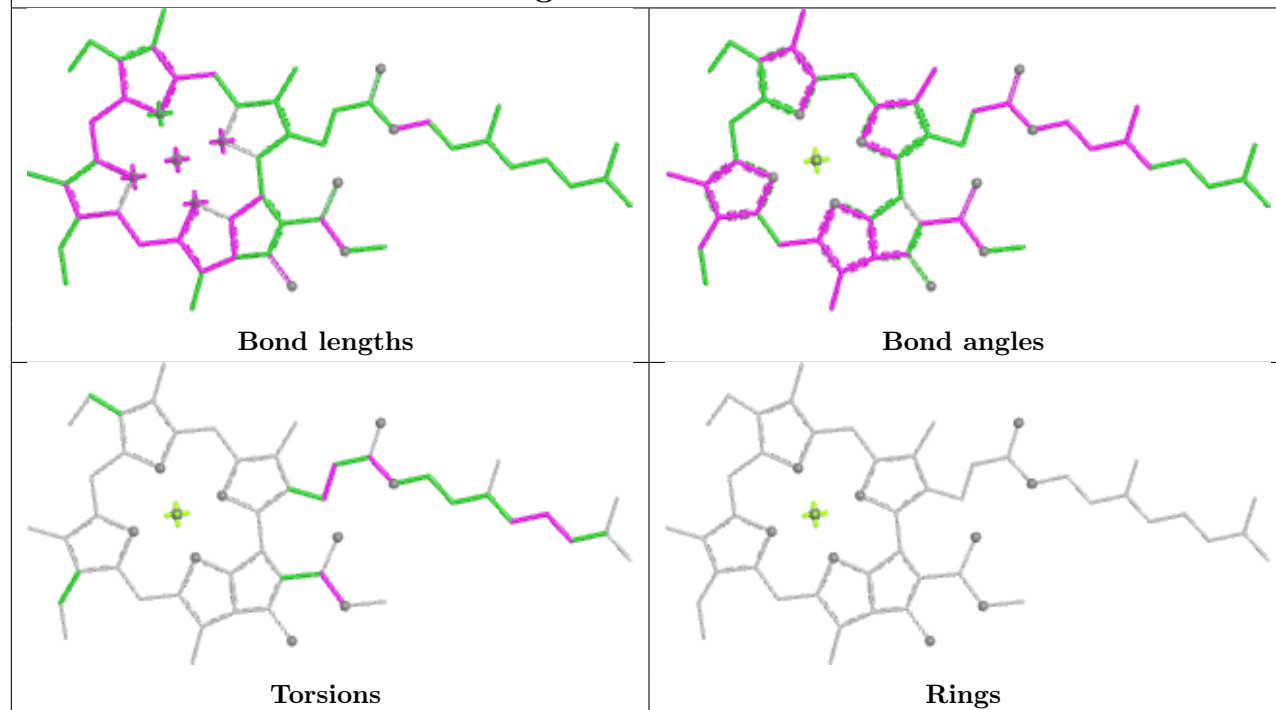
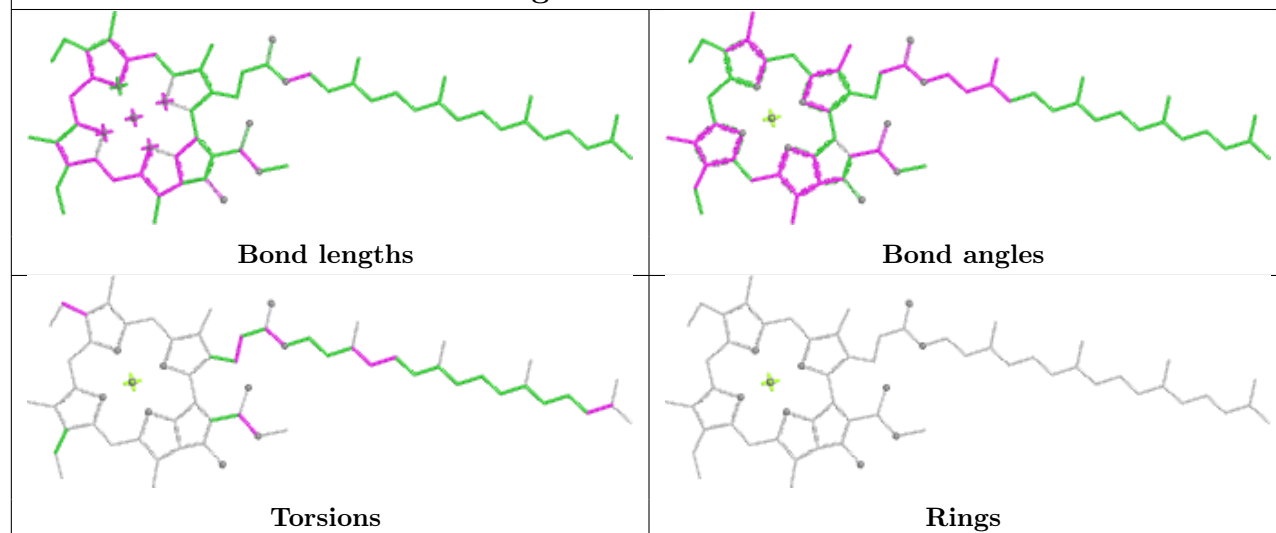
No monomer is involved in short contacts.

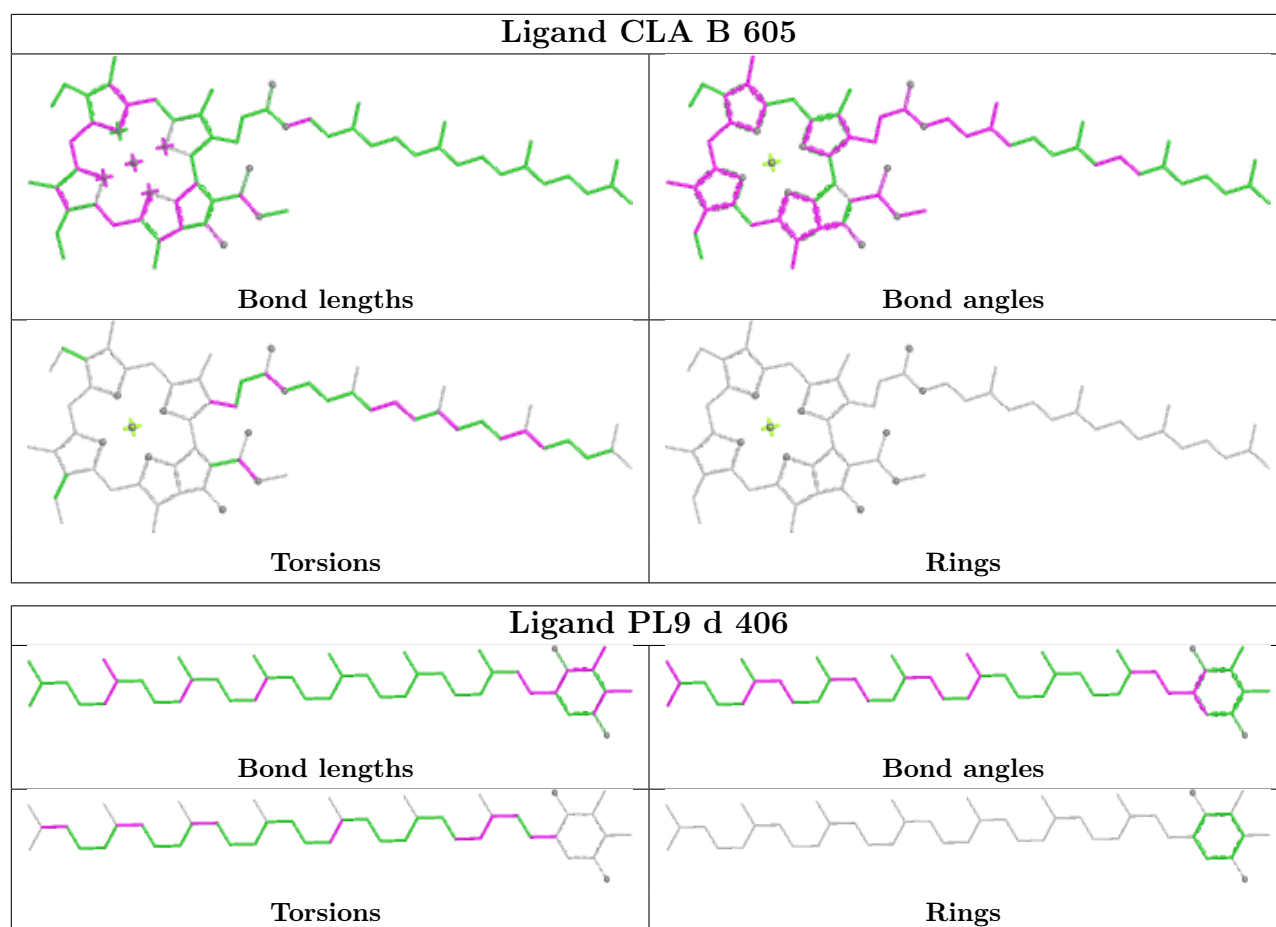
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



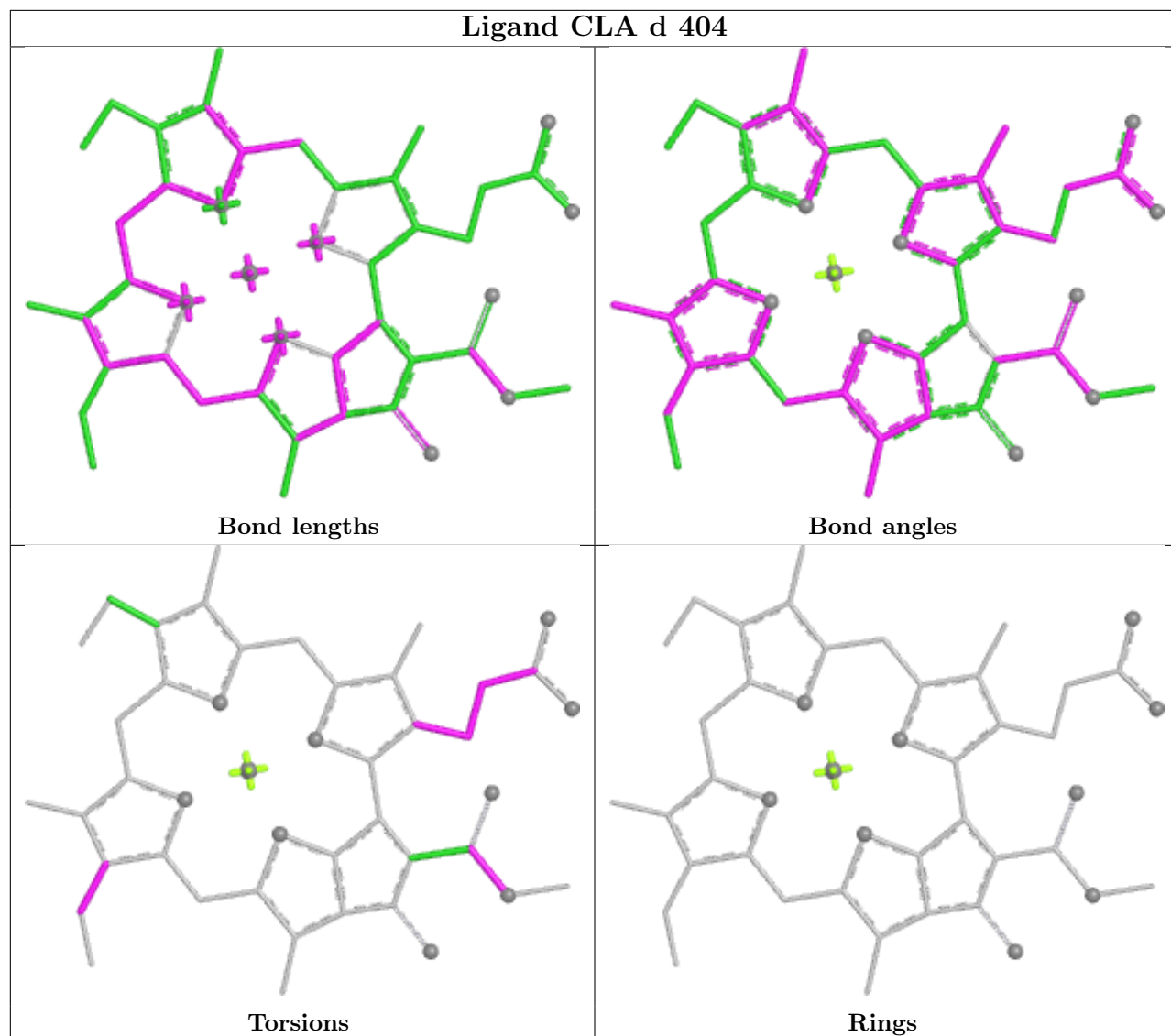


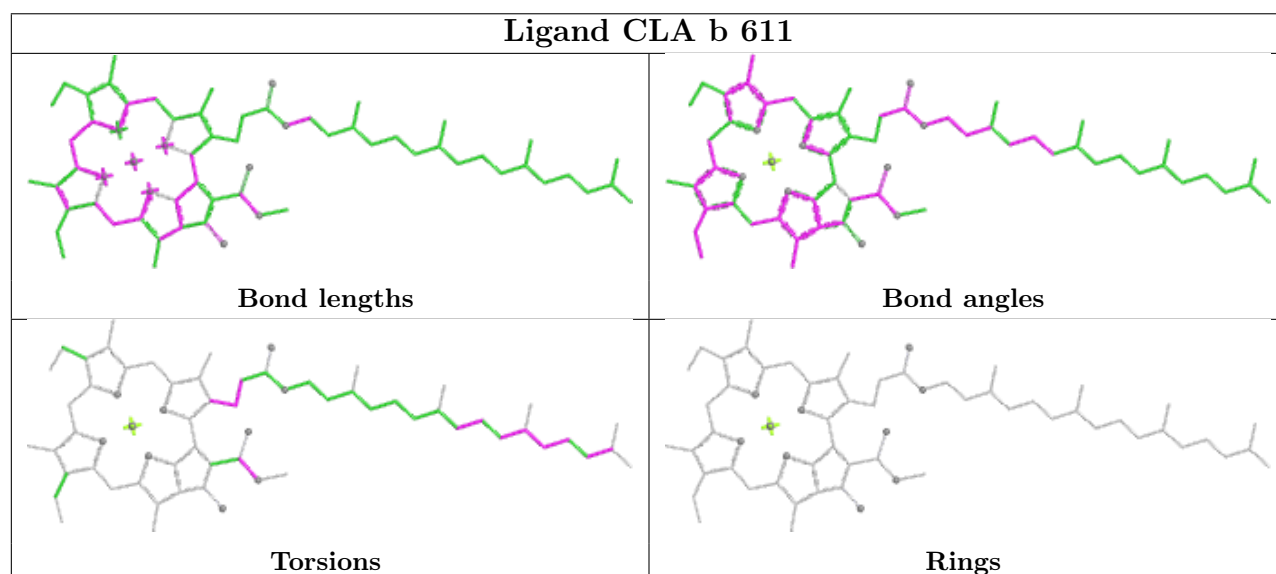
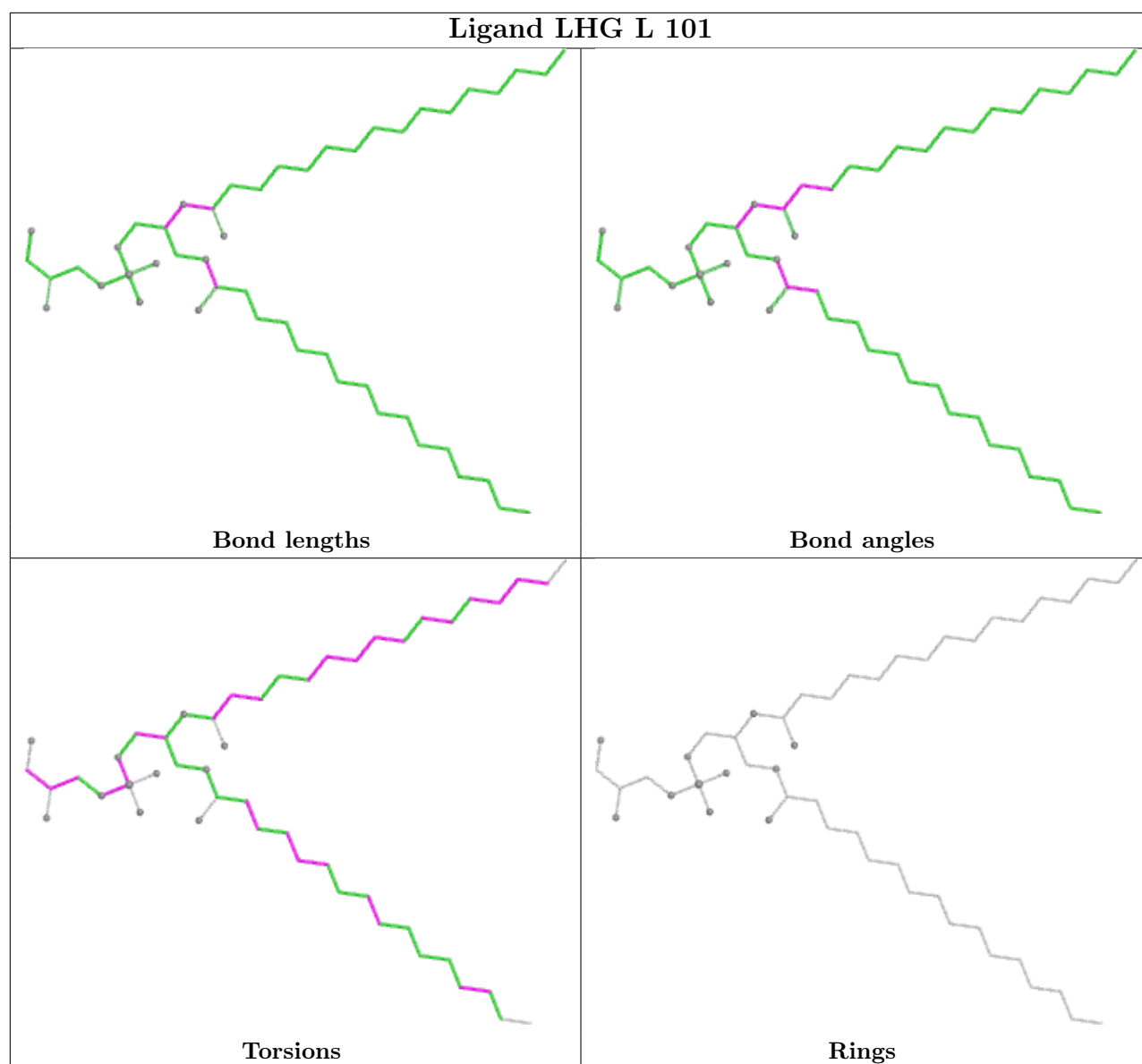


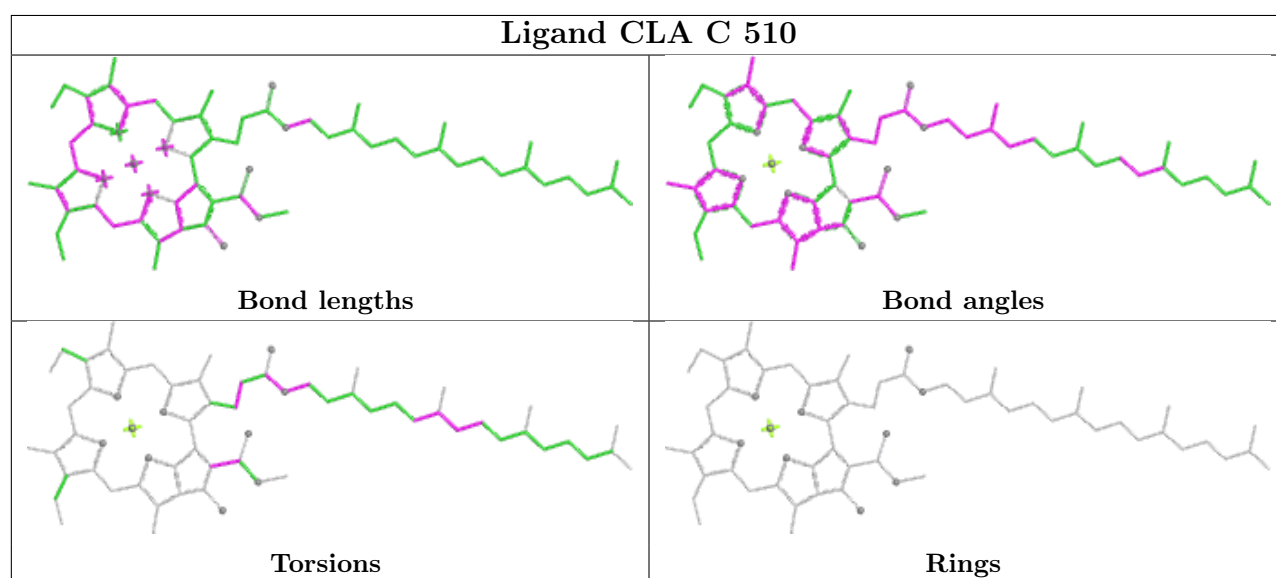
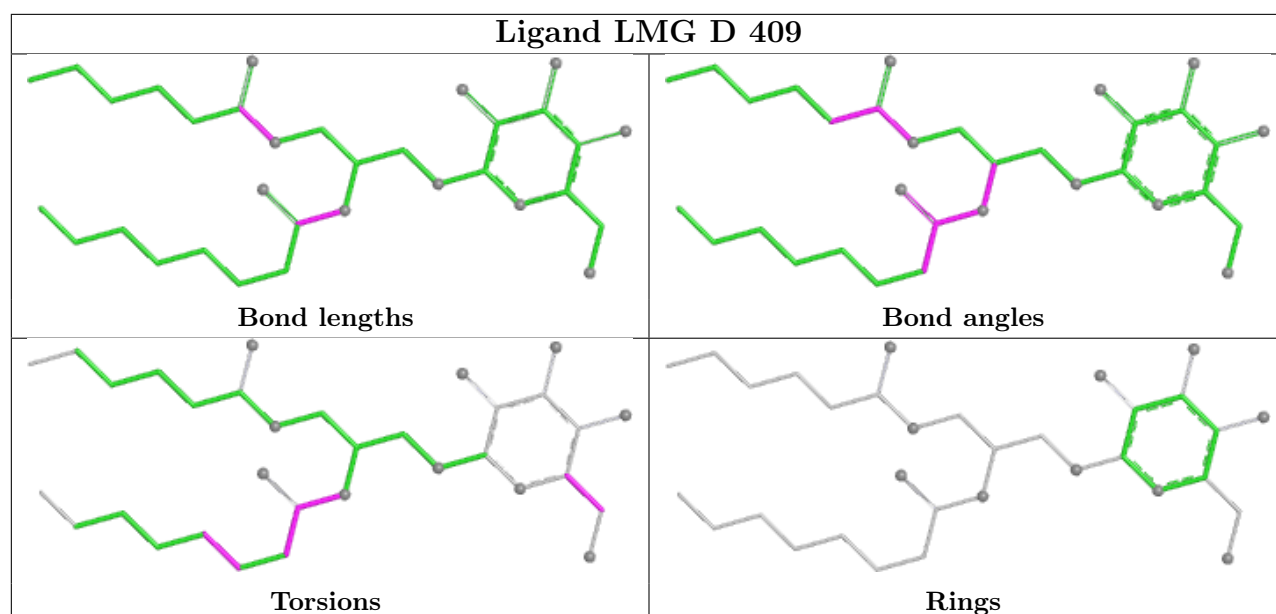
Ligand CLA b 606**Ligand CLA A 404**

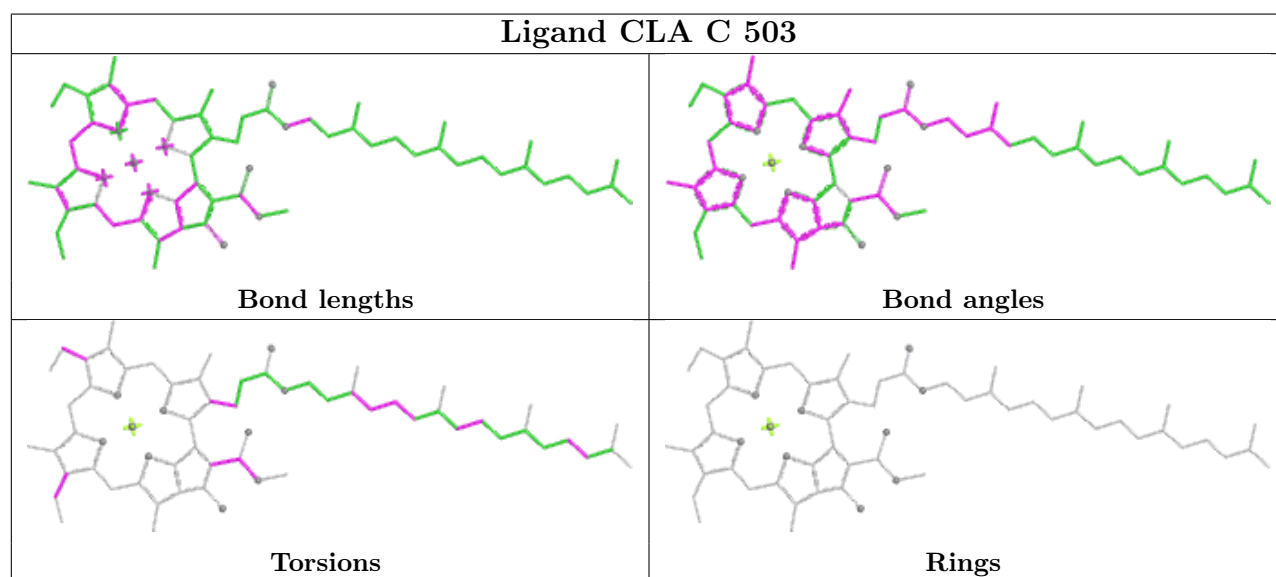
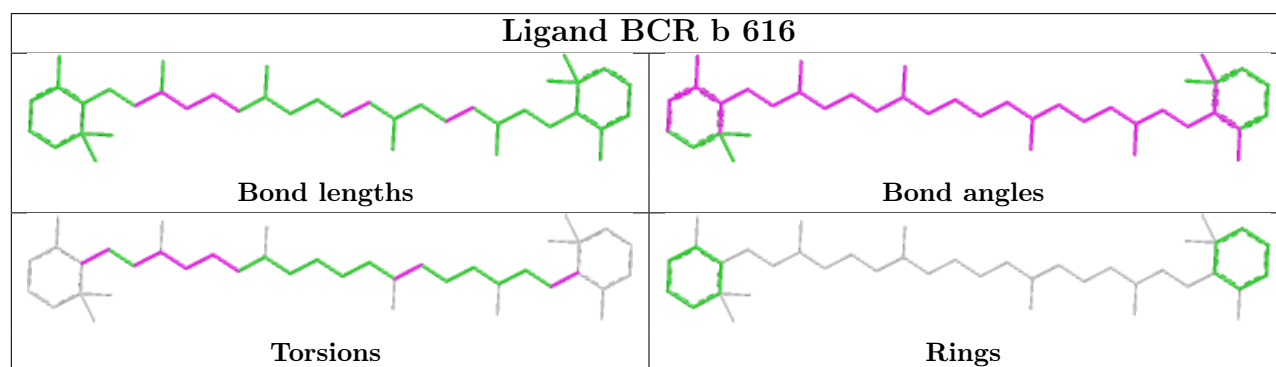
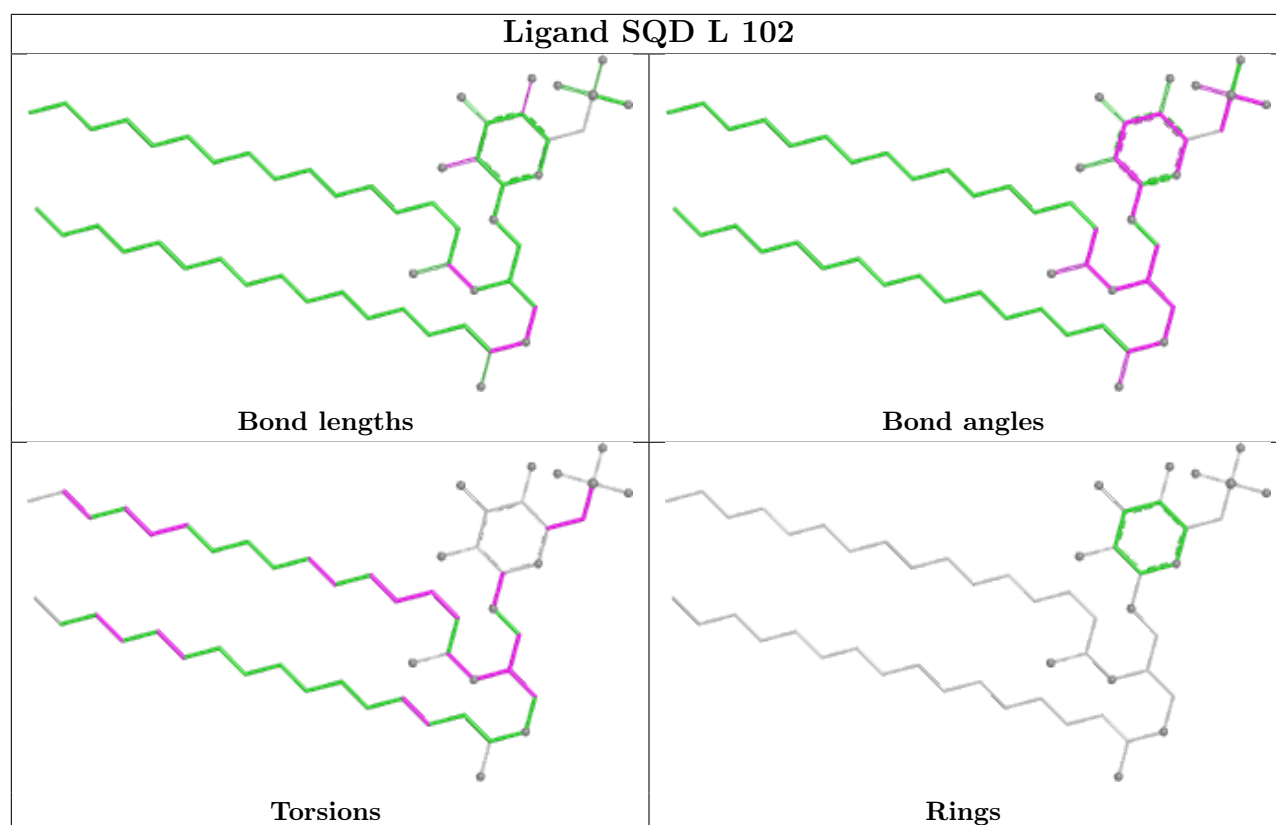


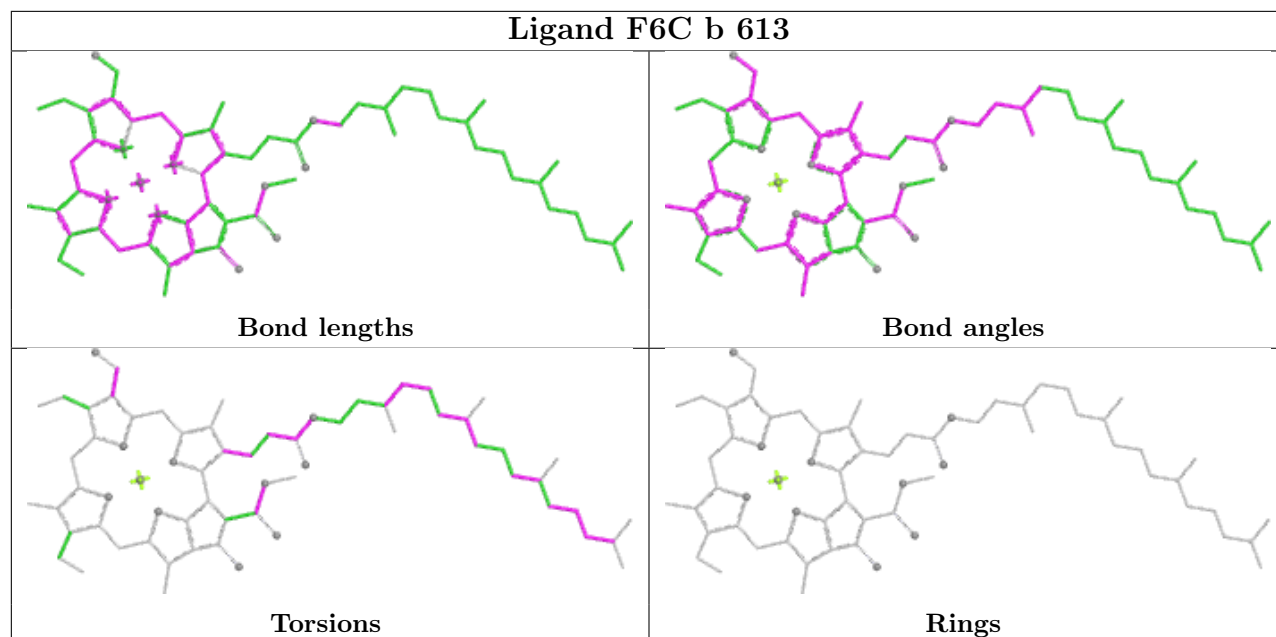
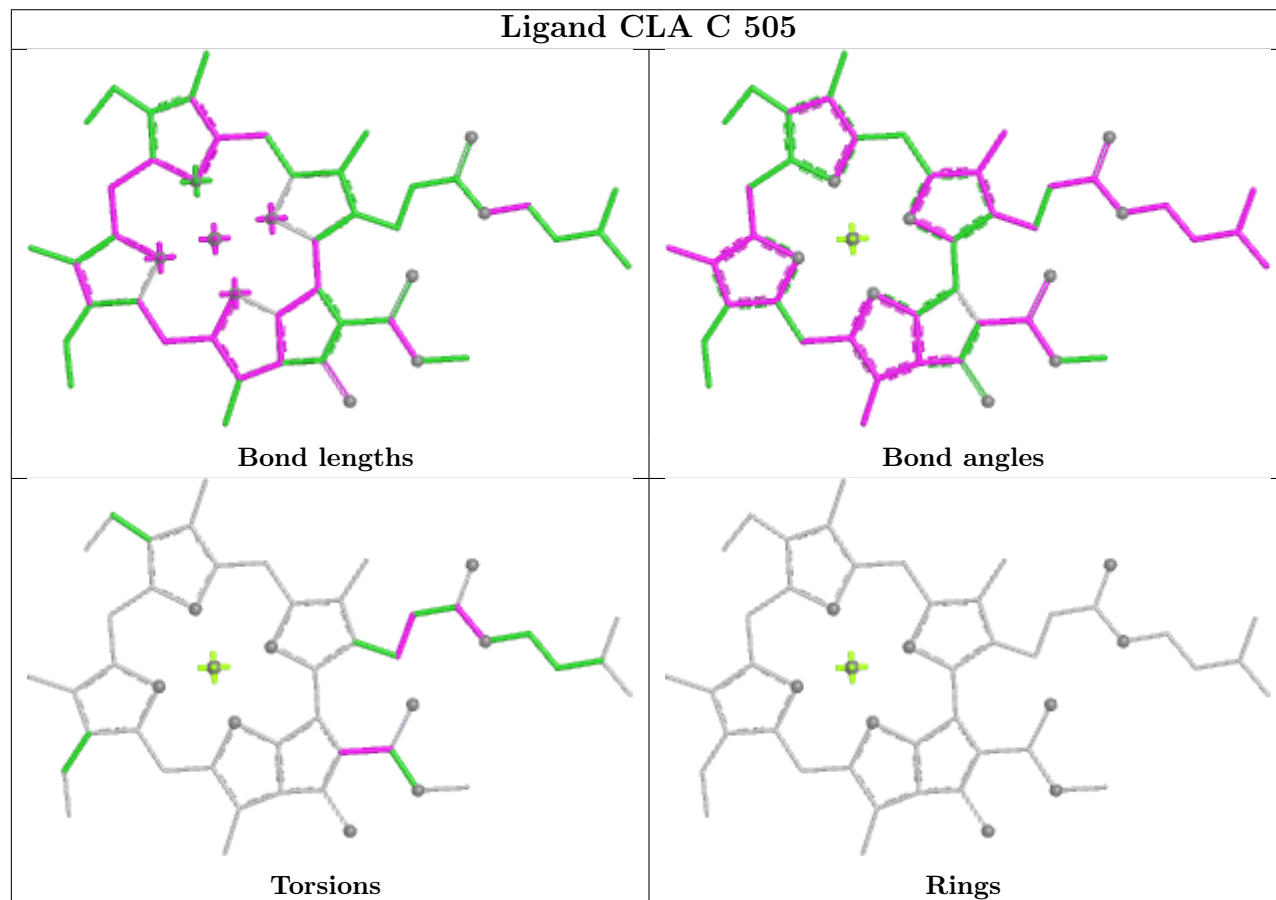
Ligand CLA d 404

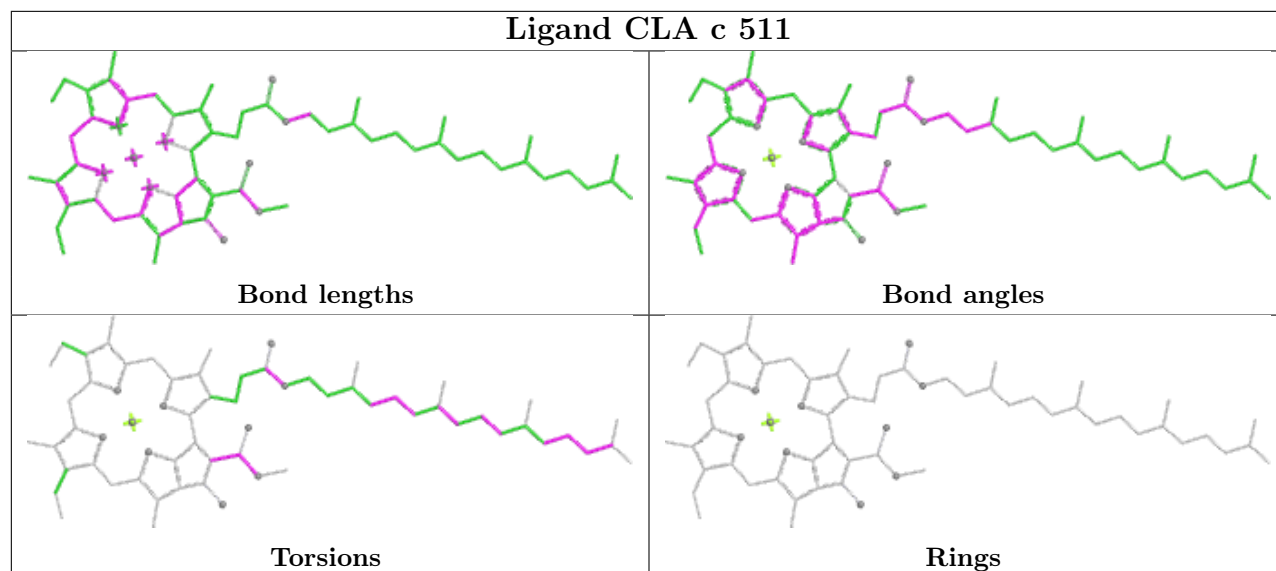
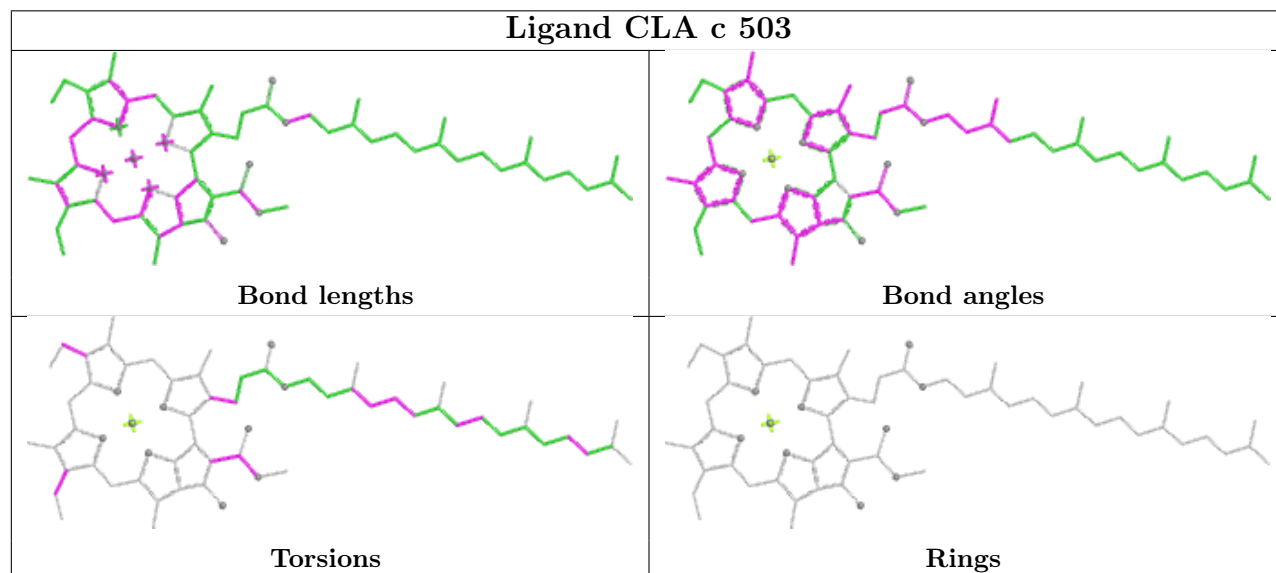
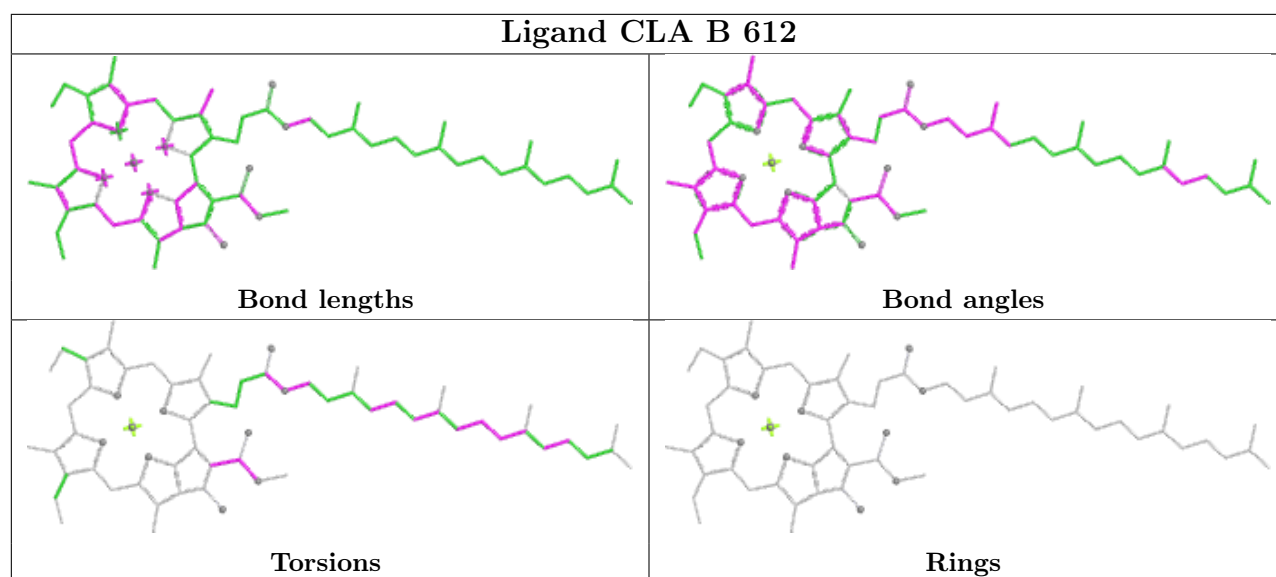


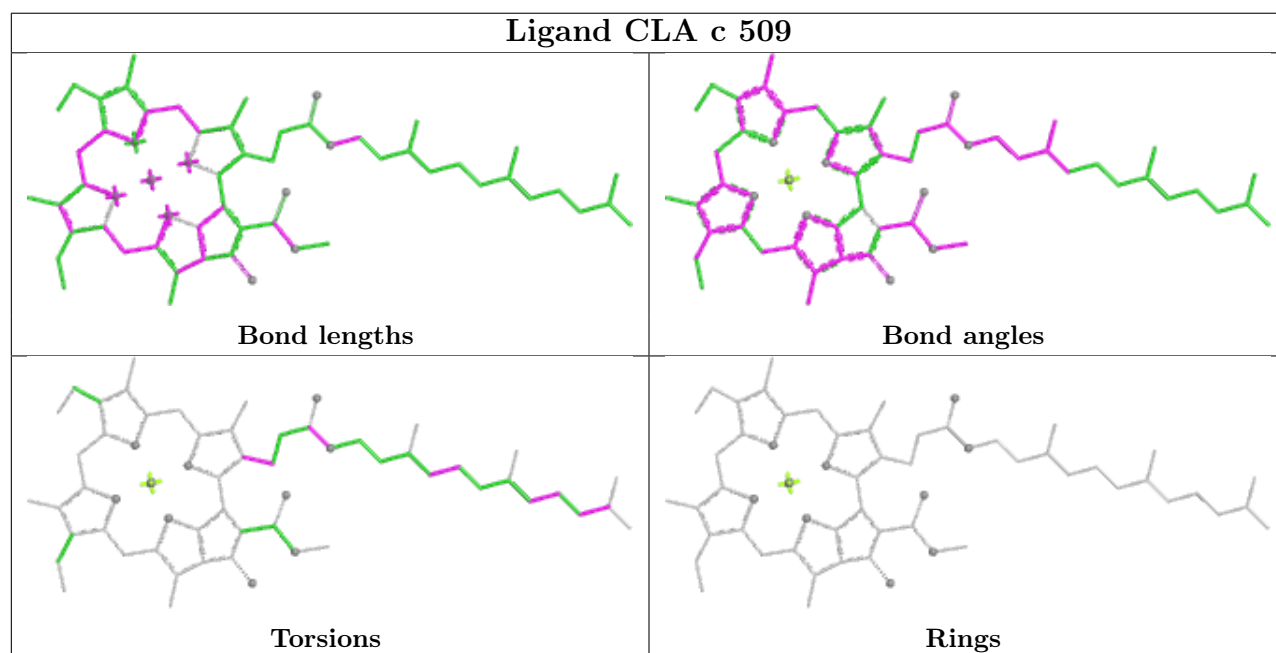
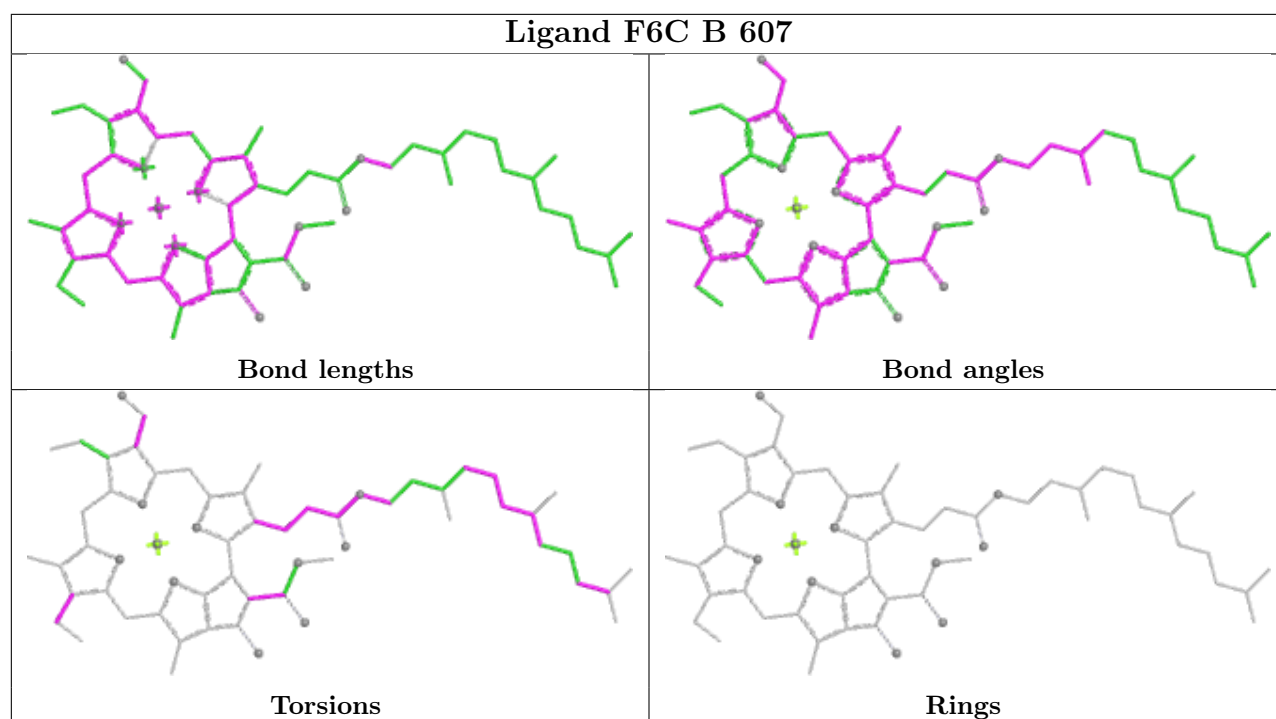


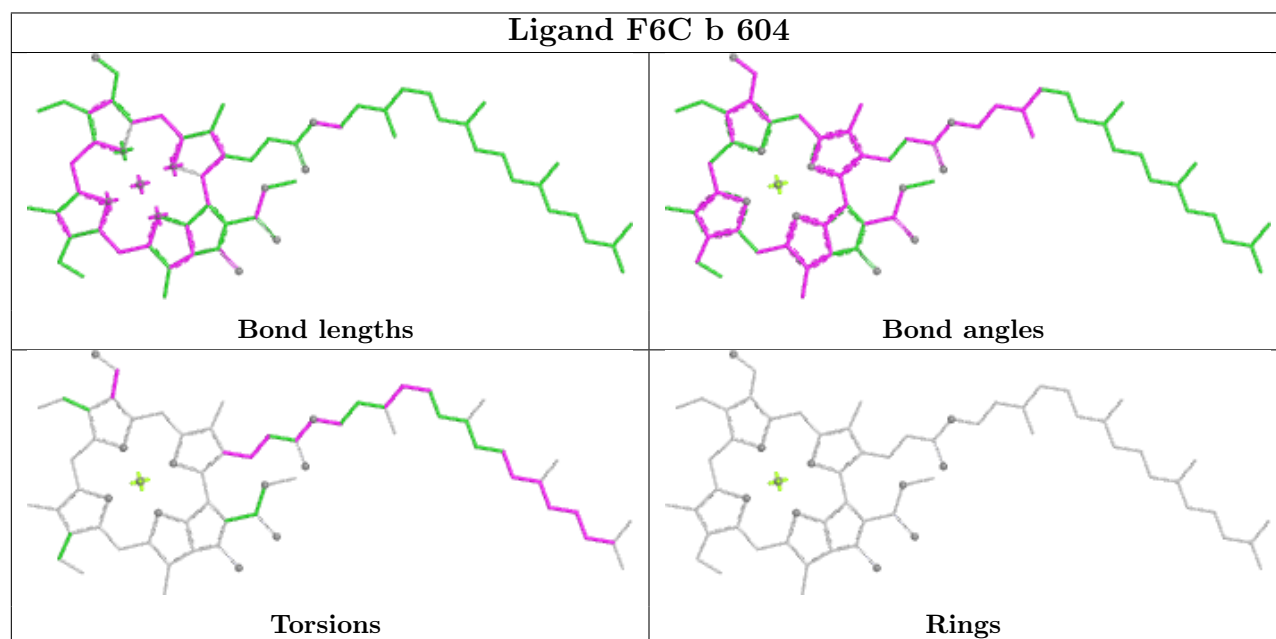
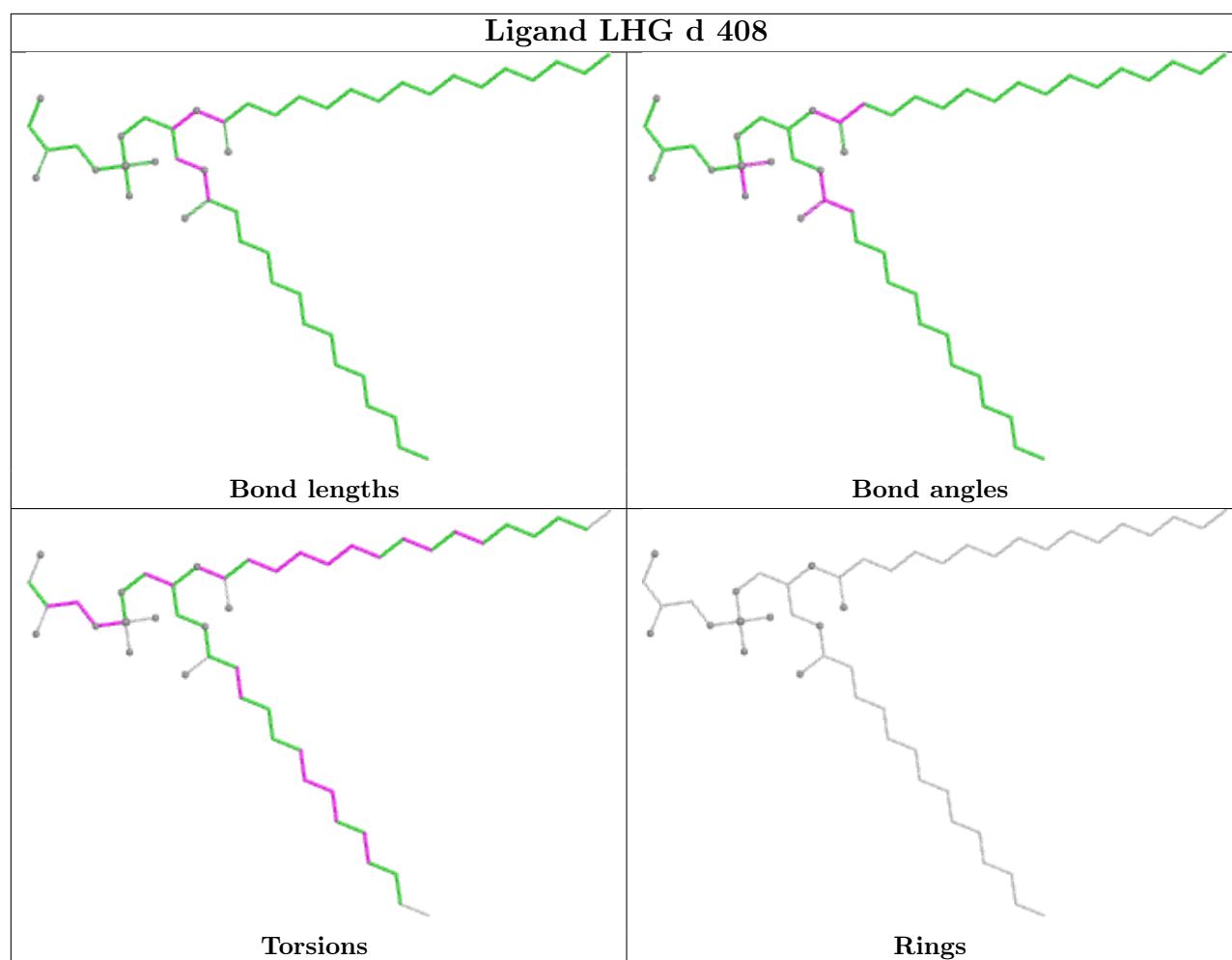


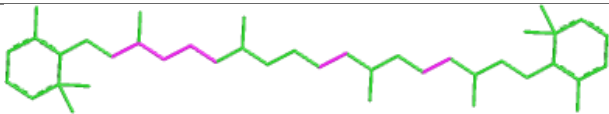
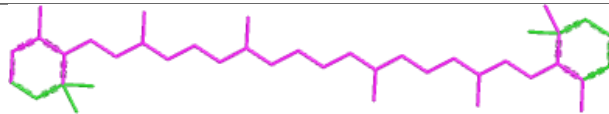
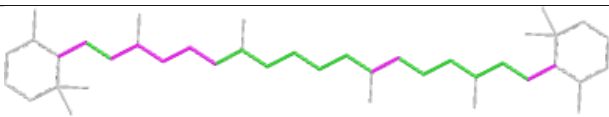
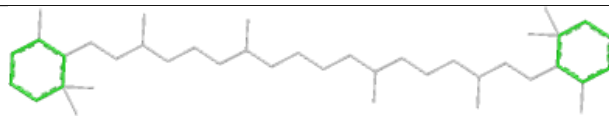


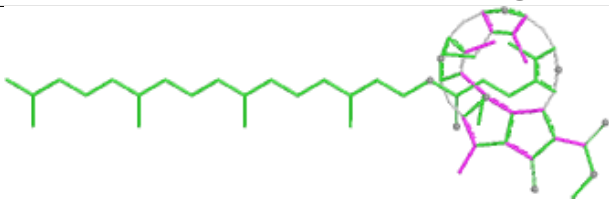
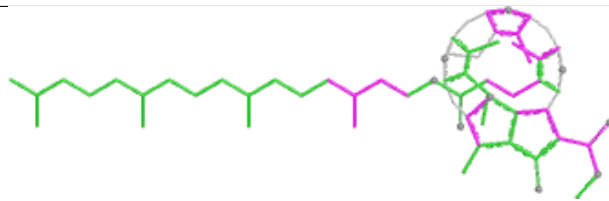
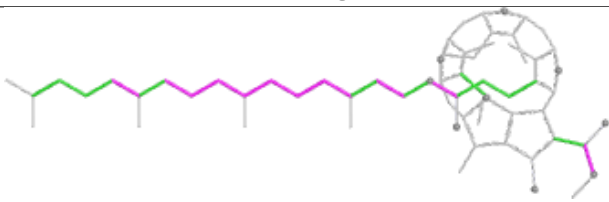
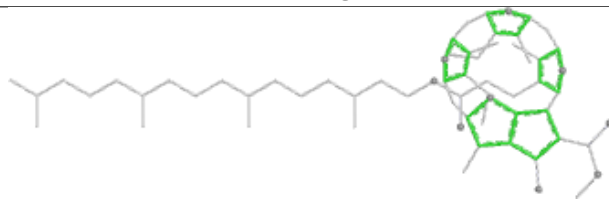
Ligand F6C b 613**Ligand CLA C 505**

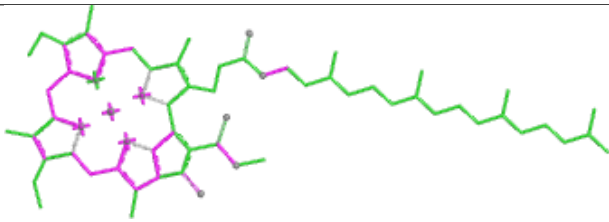
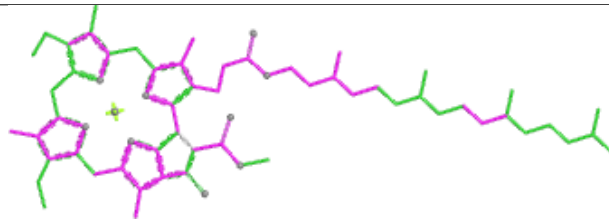
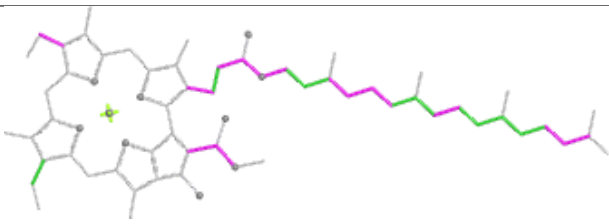
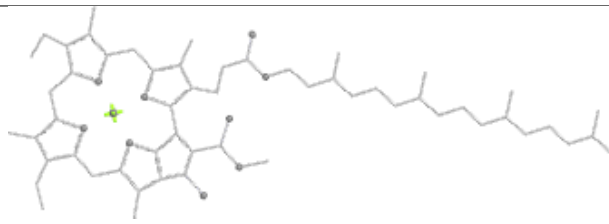


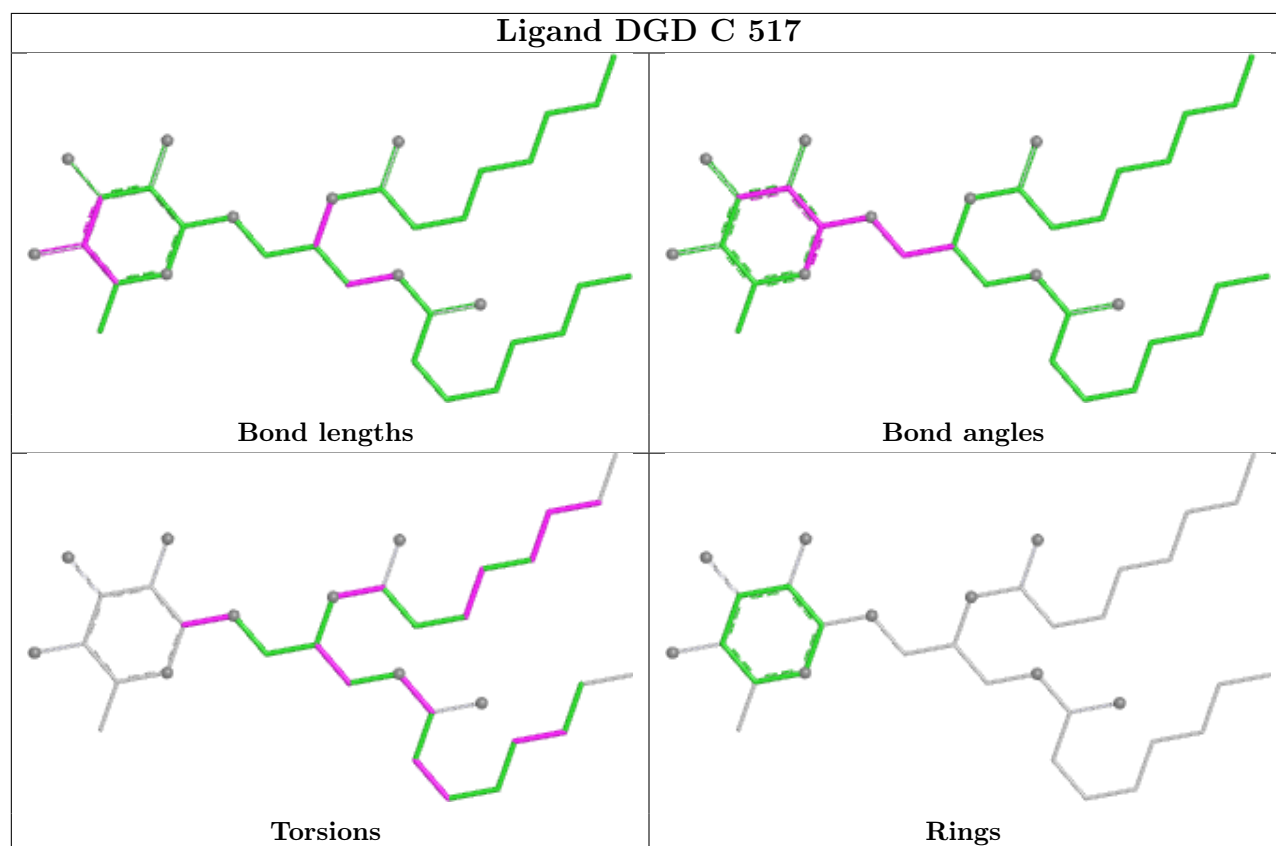
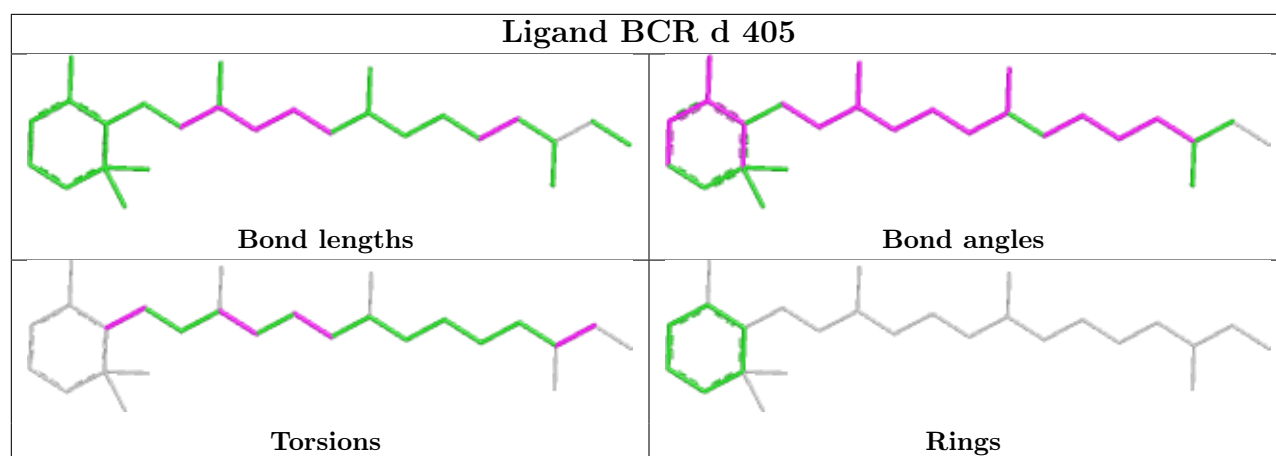




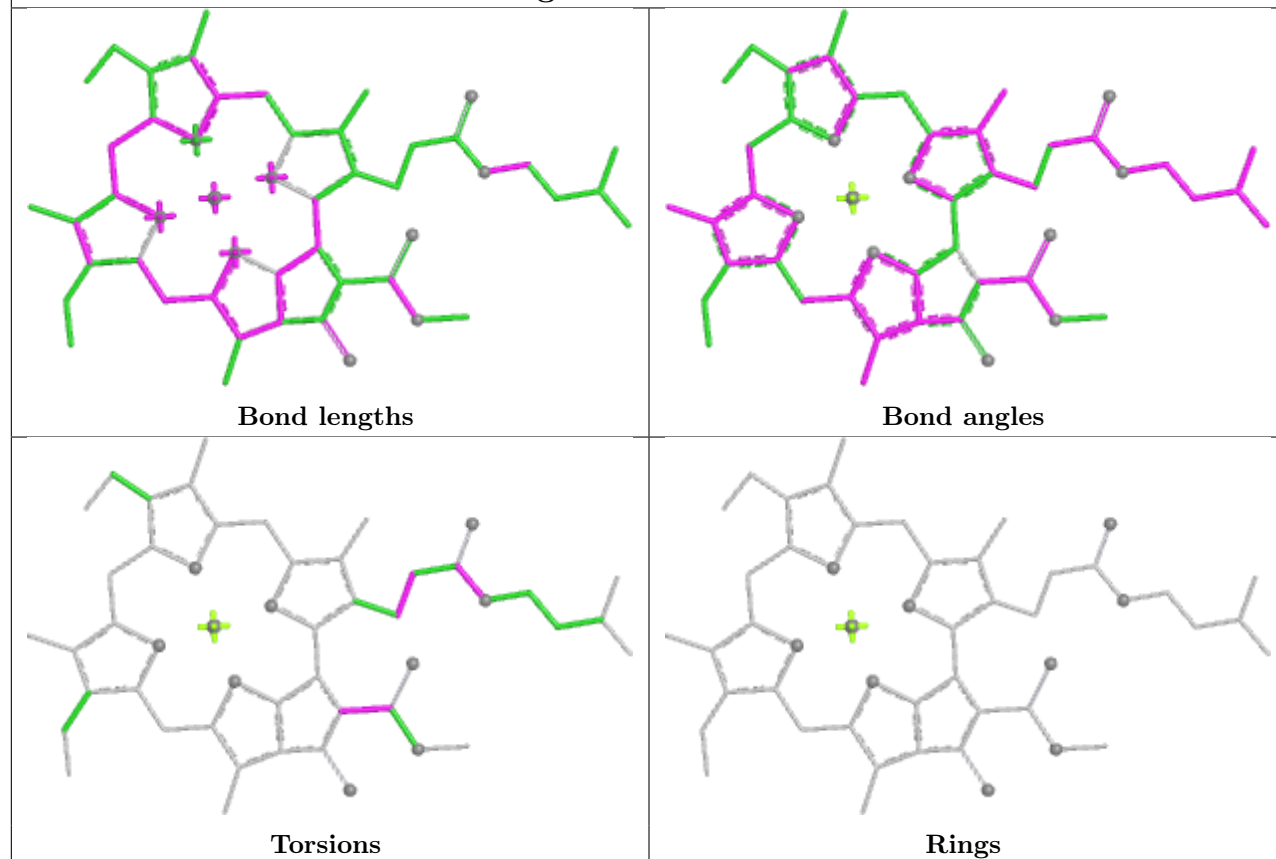
Ligand BCR B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

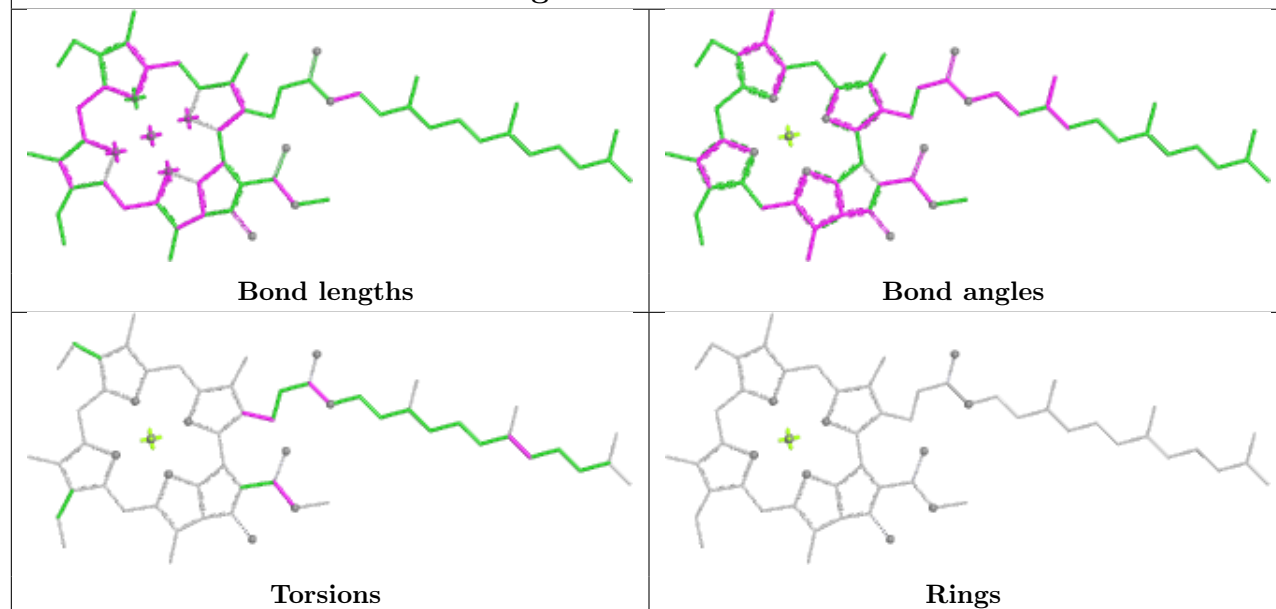
Ligand CLA c 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

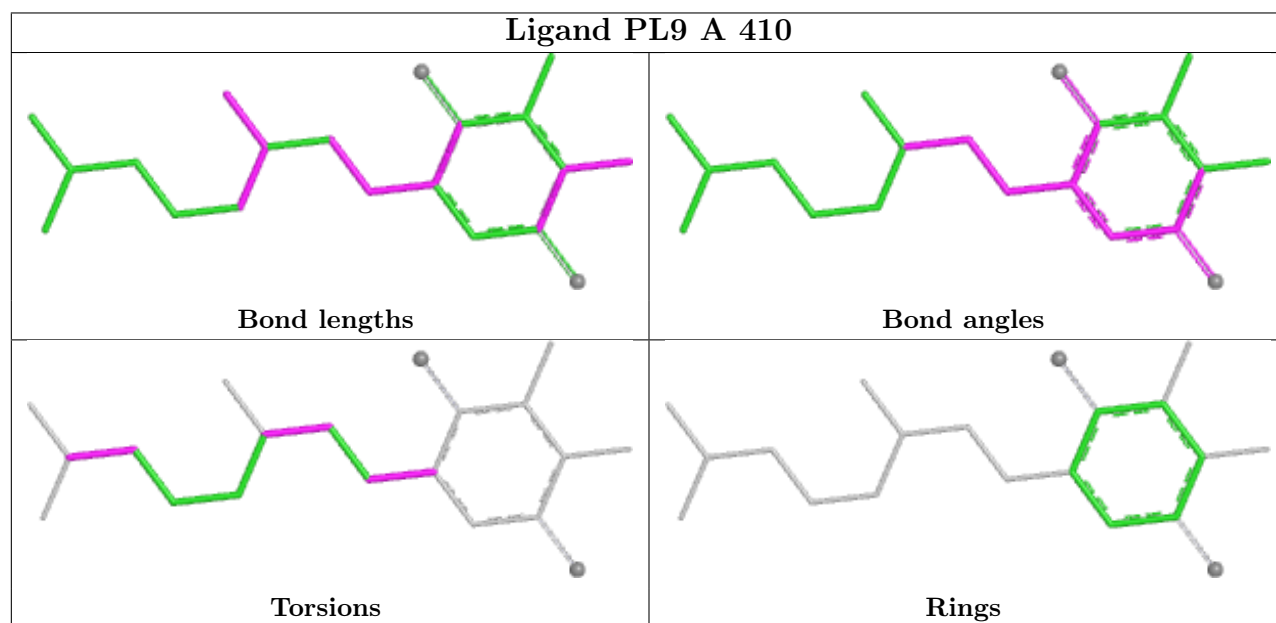
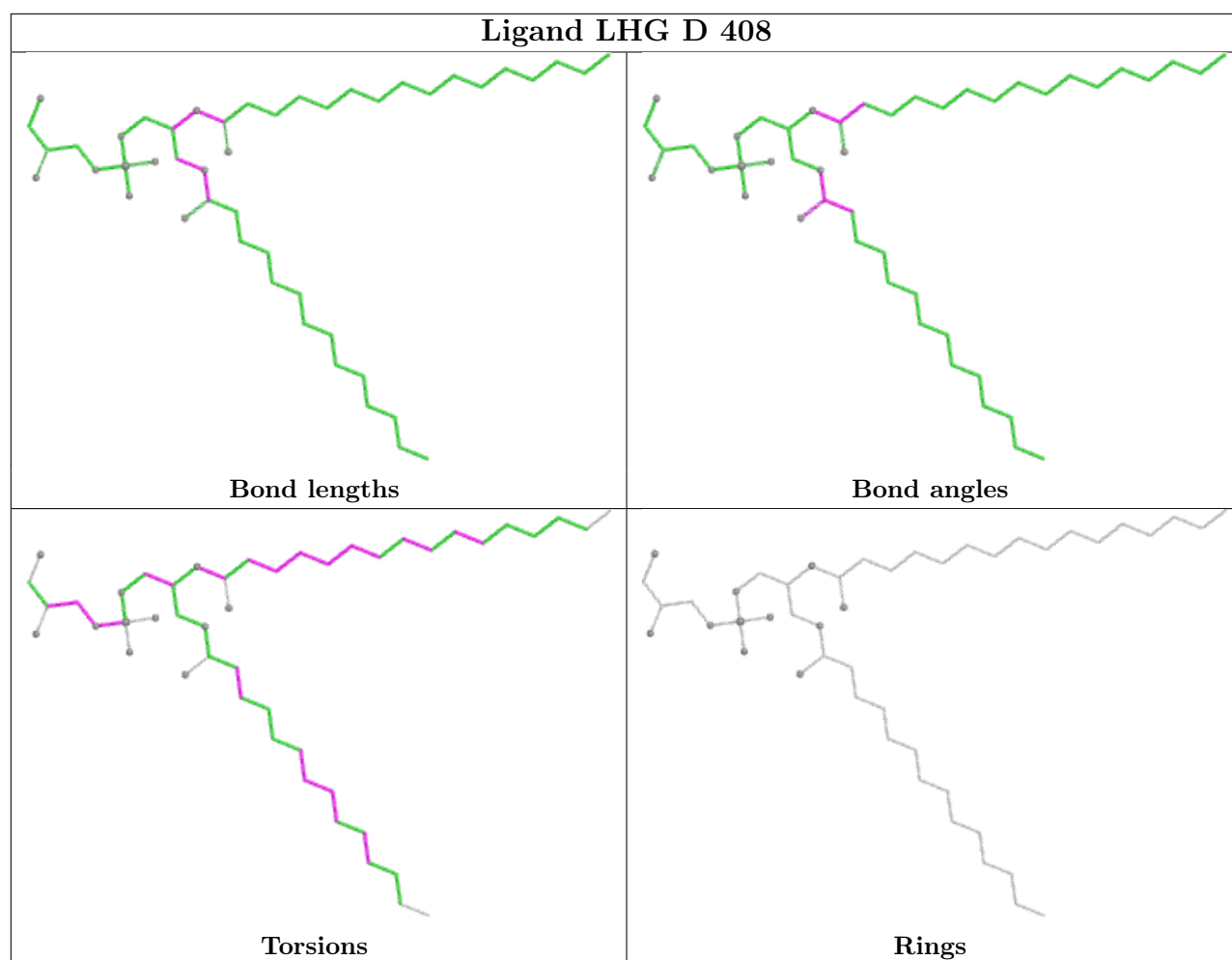


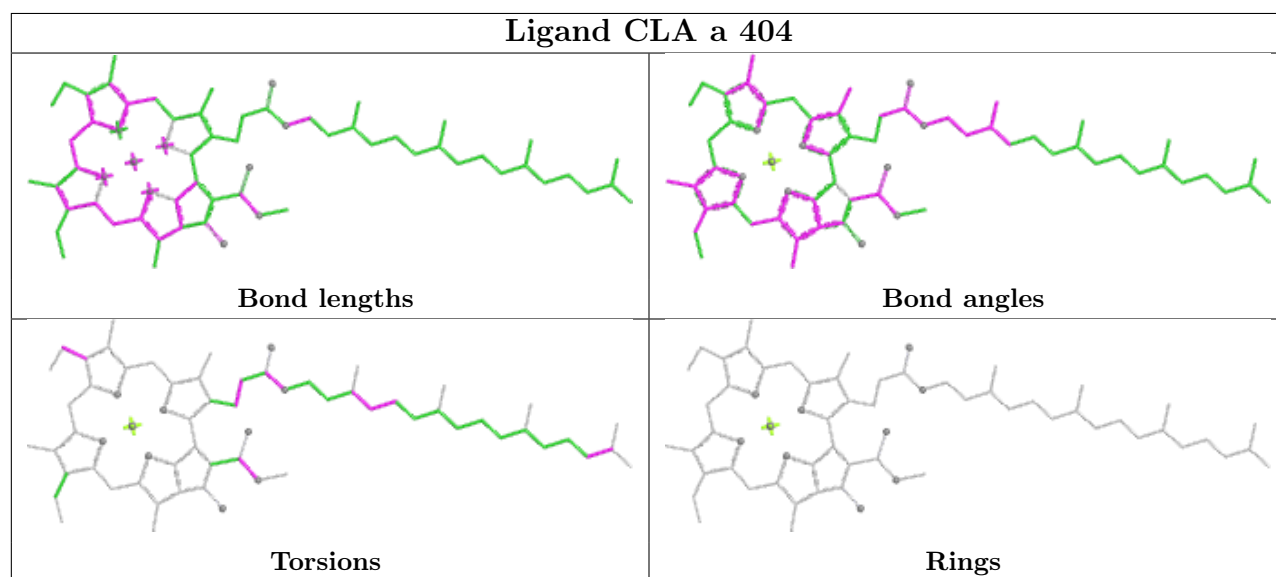
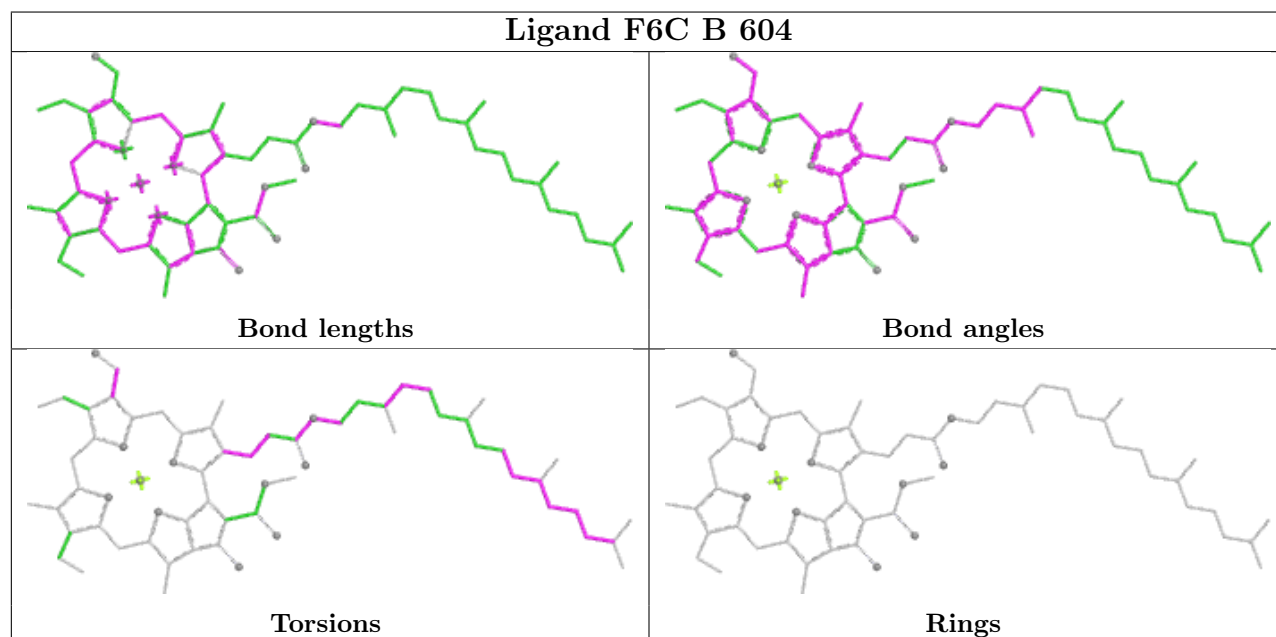
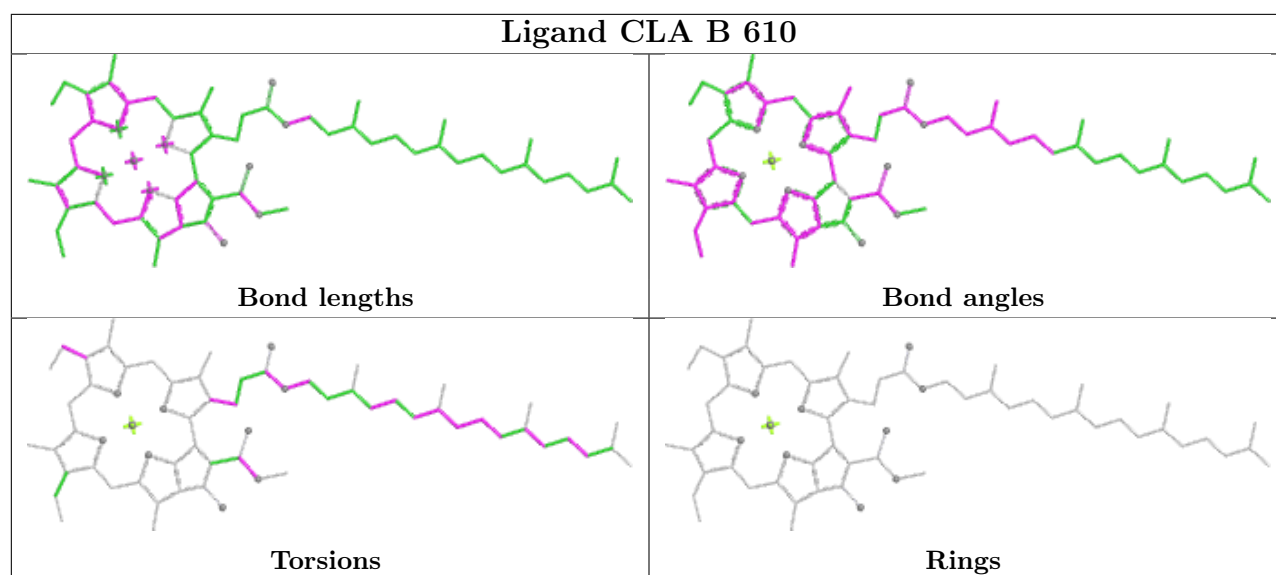
Ligand CLA c 505

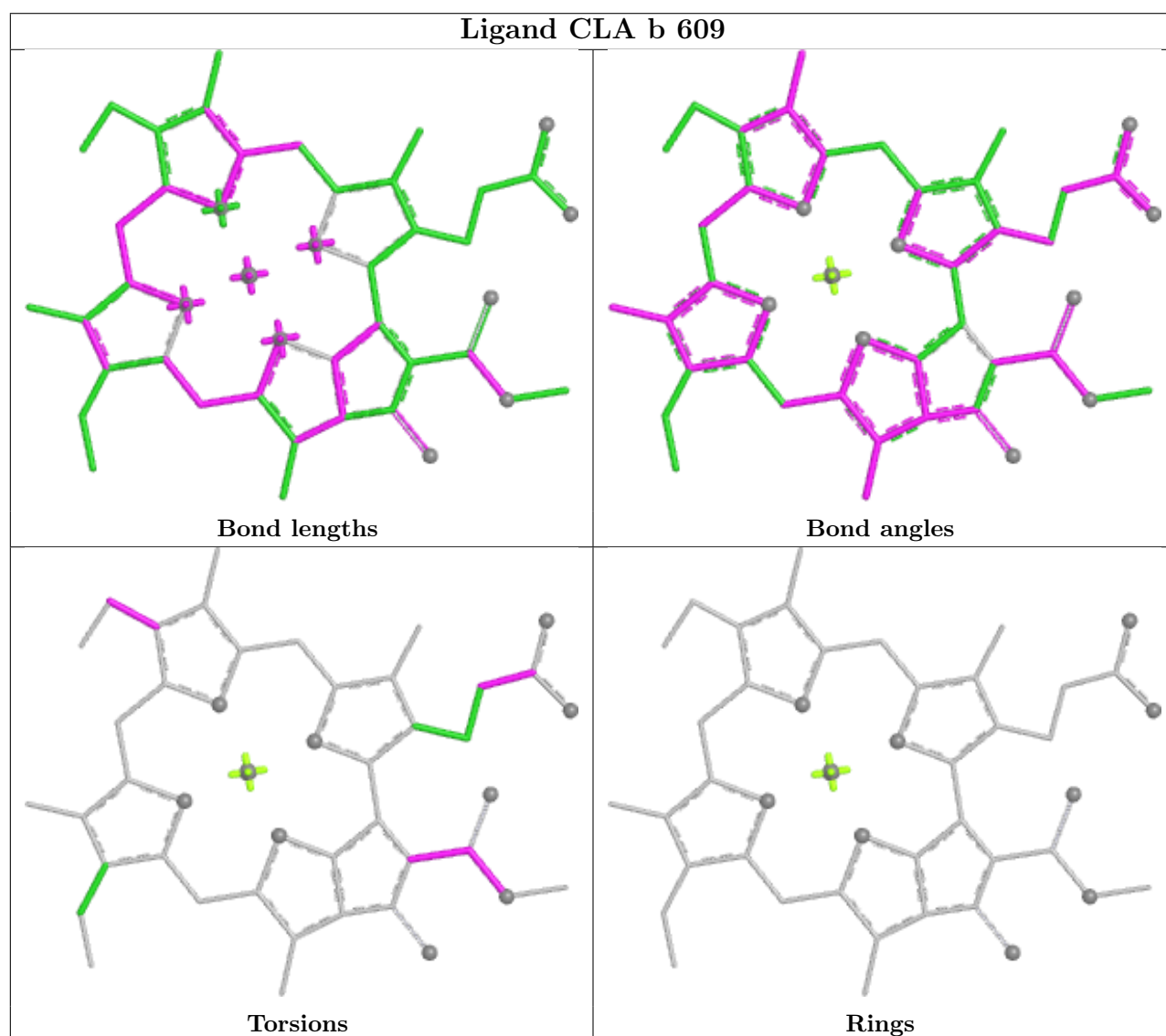
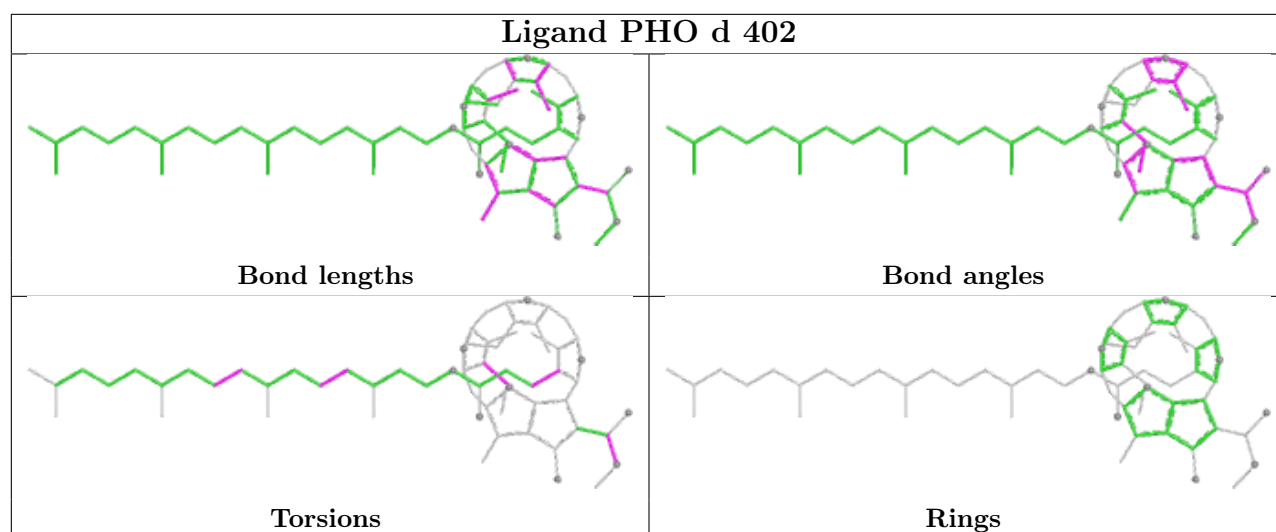


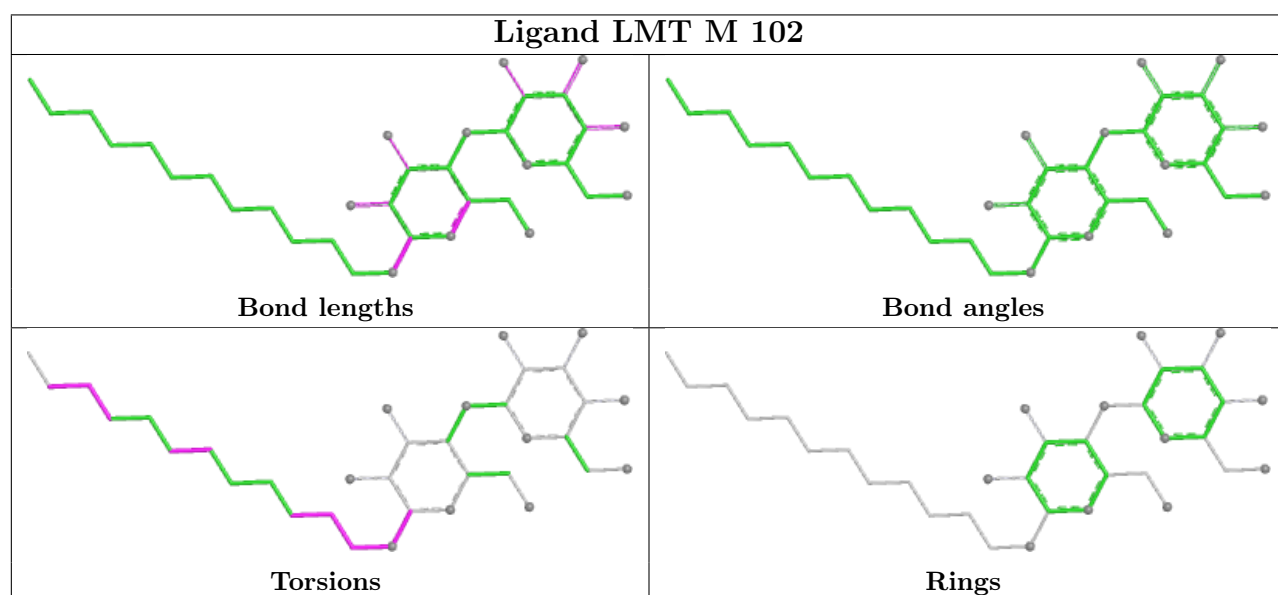
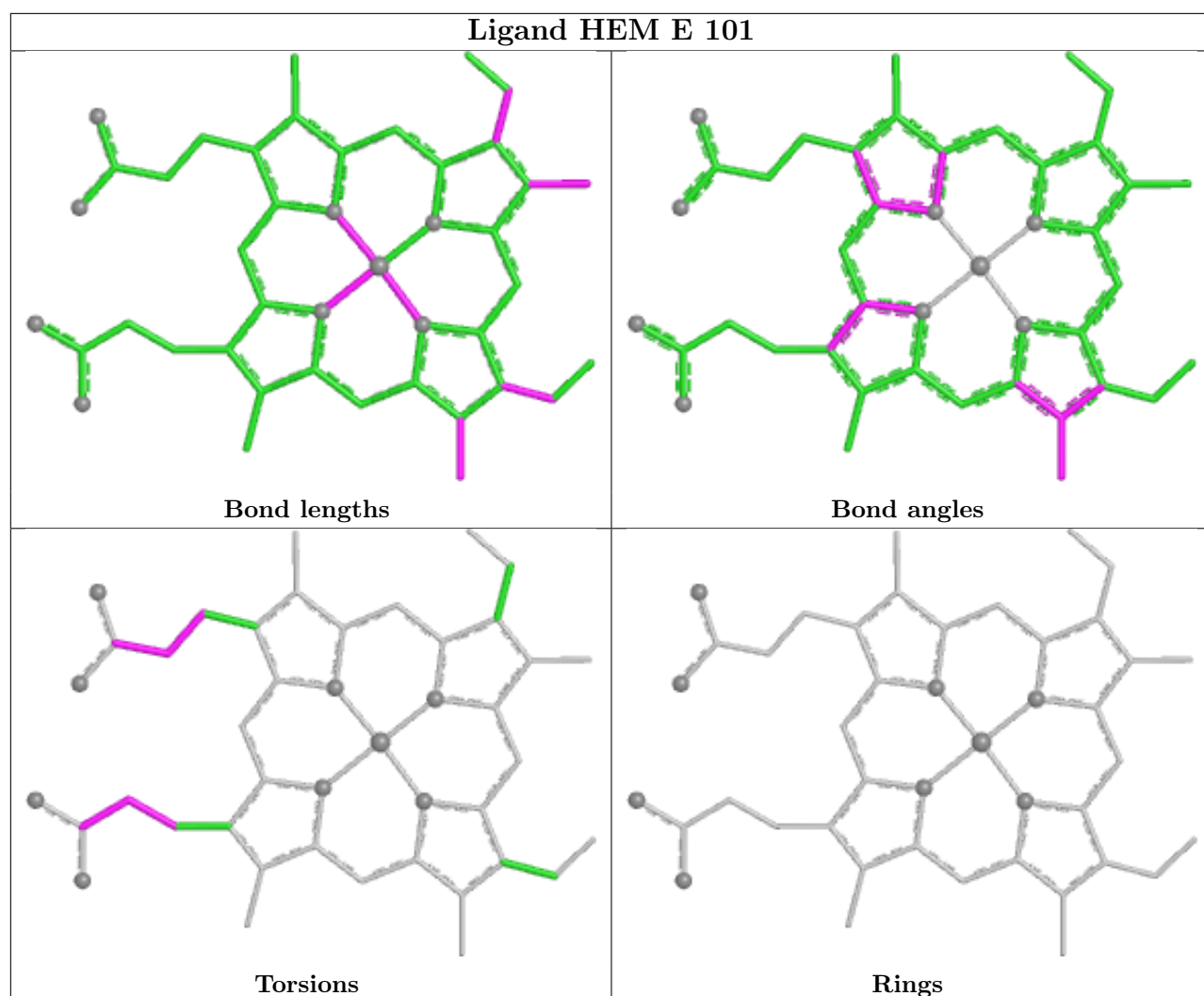
Ligand CLA D 403

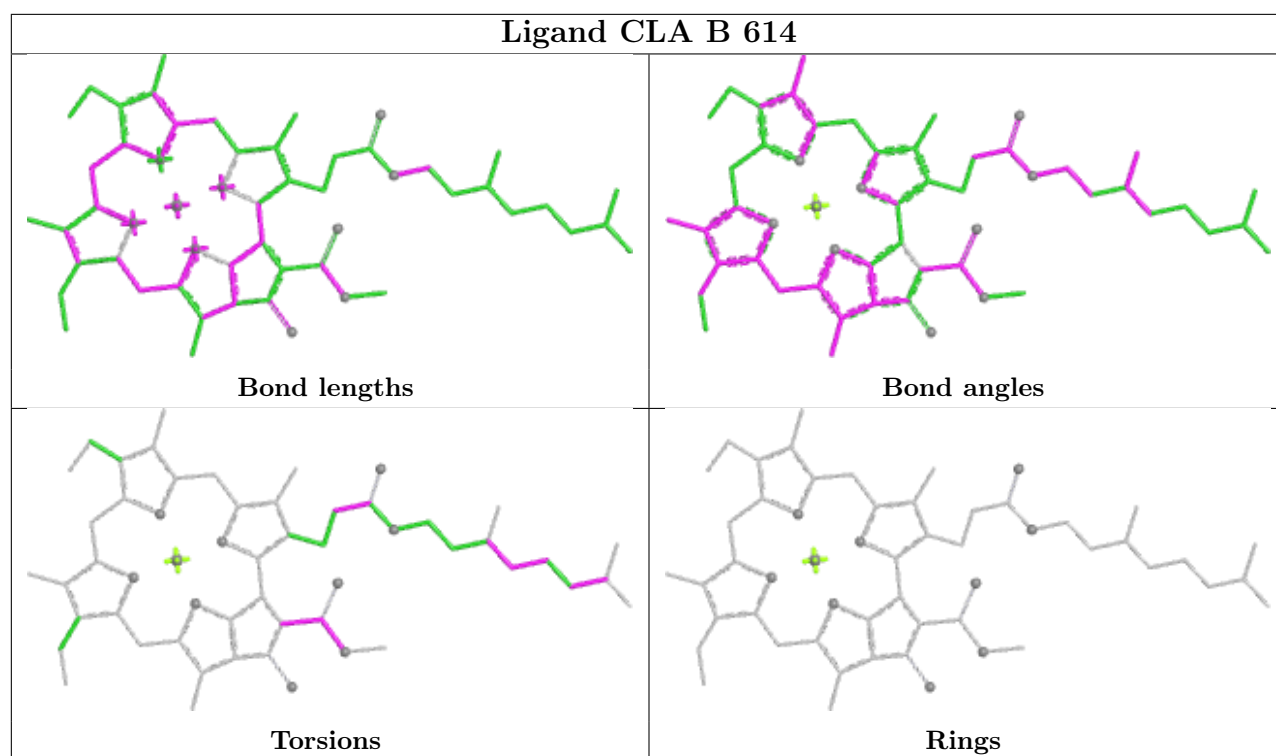


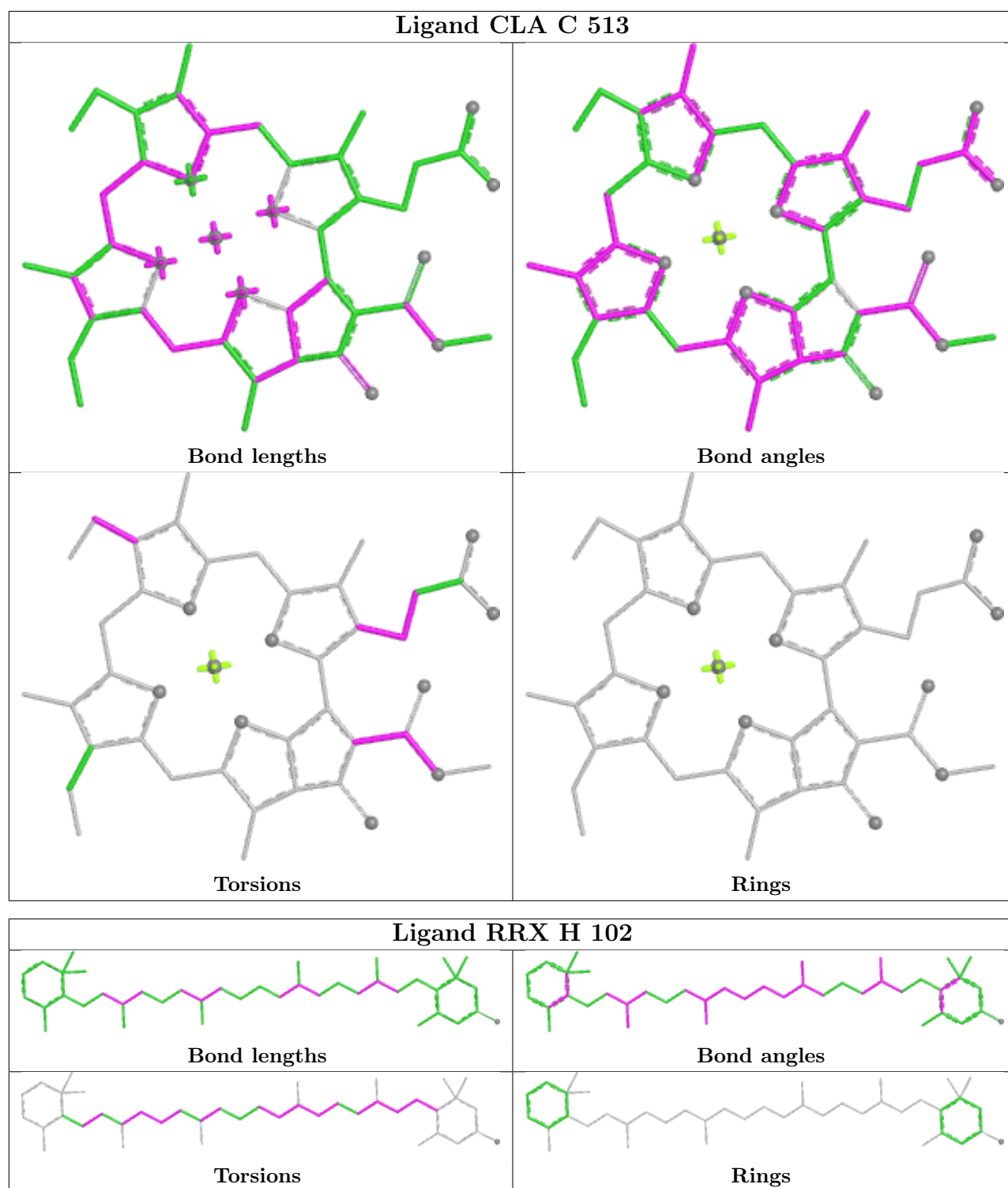


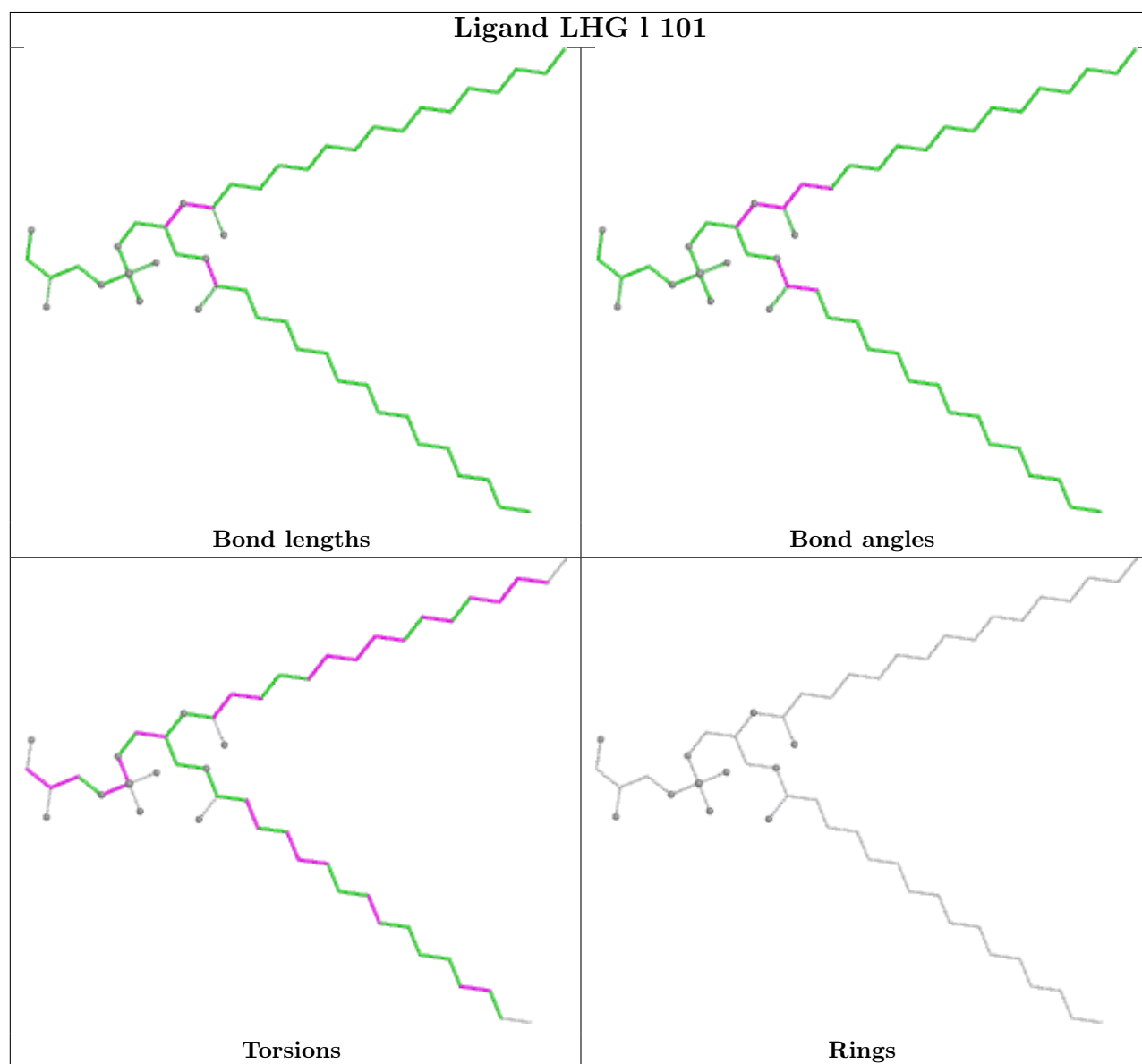
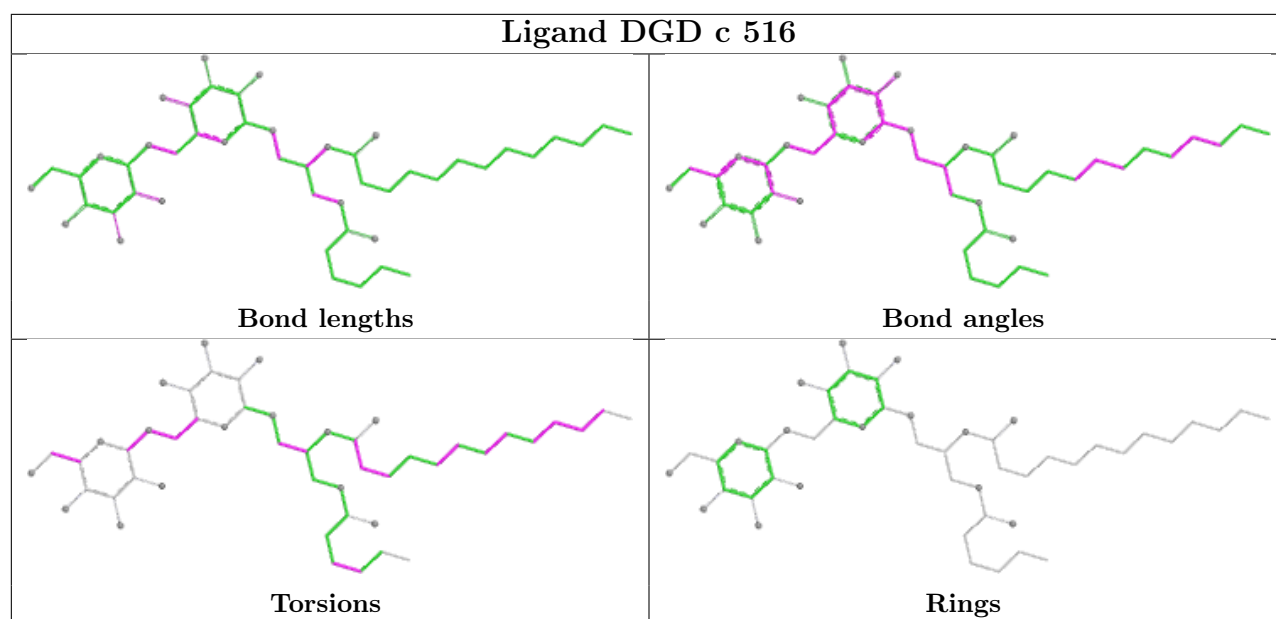


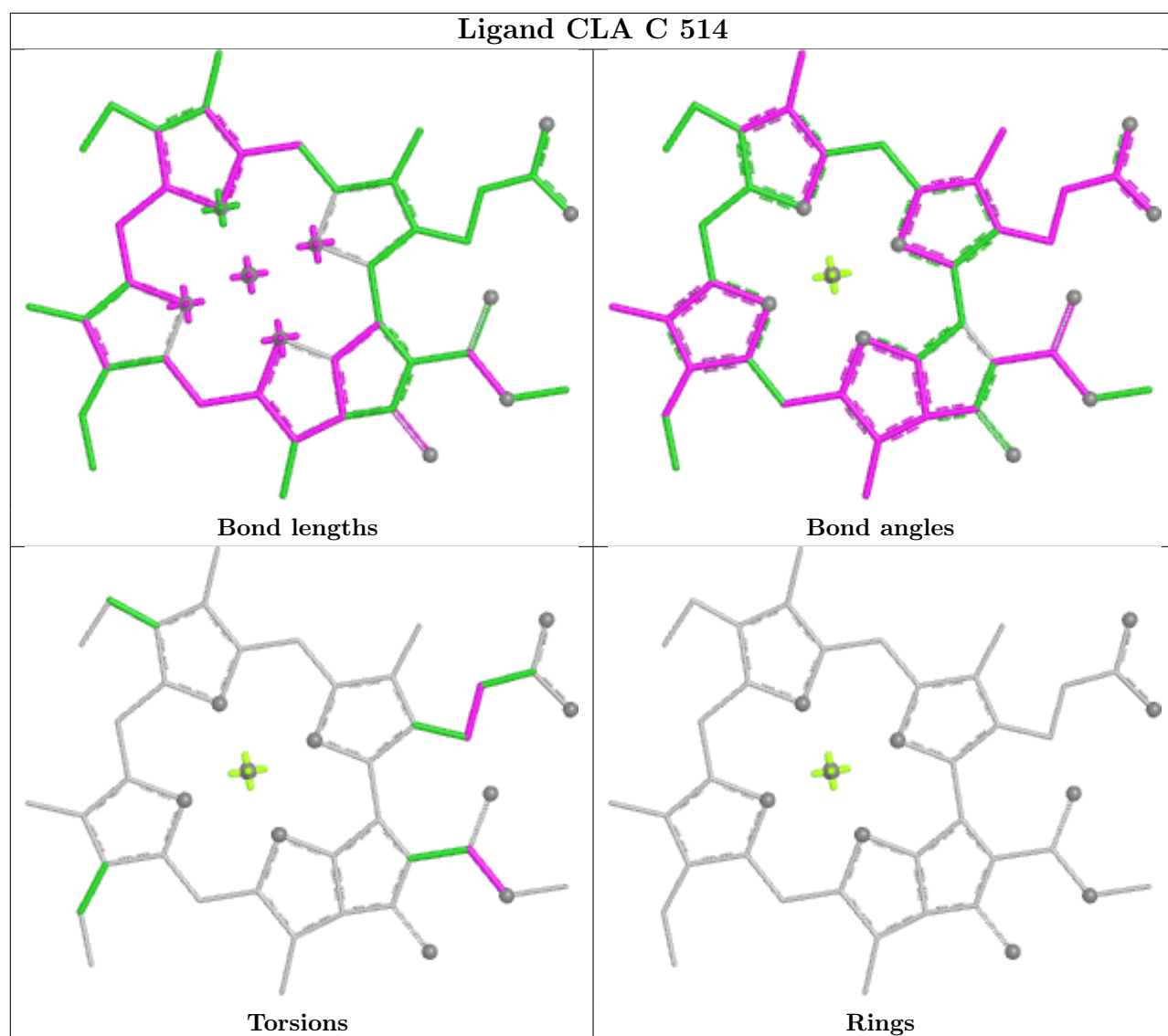


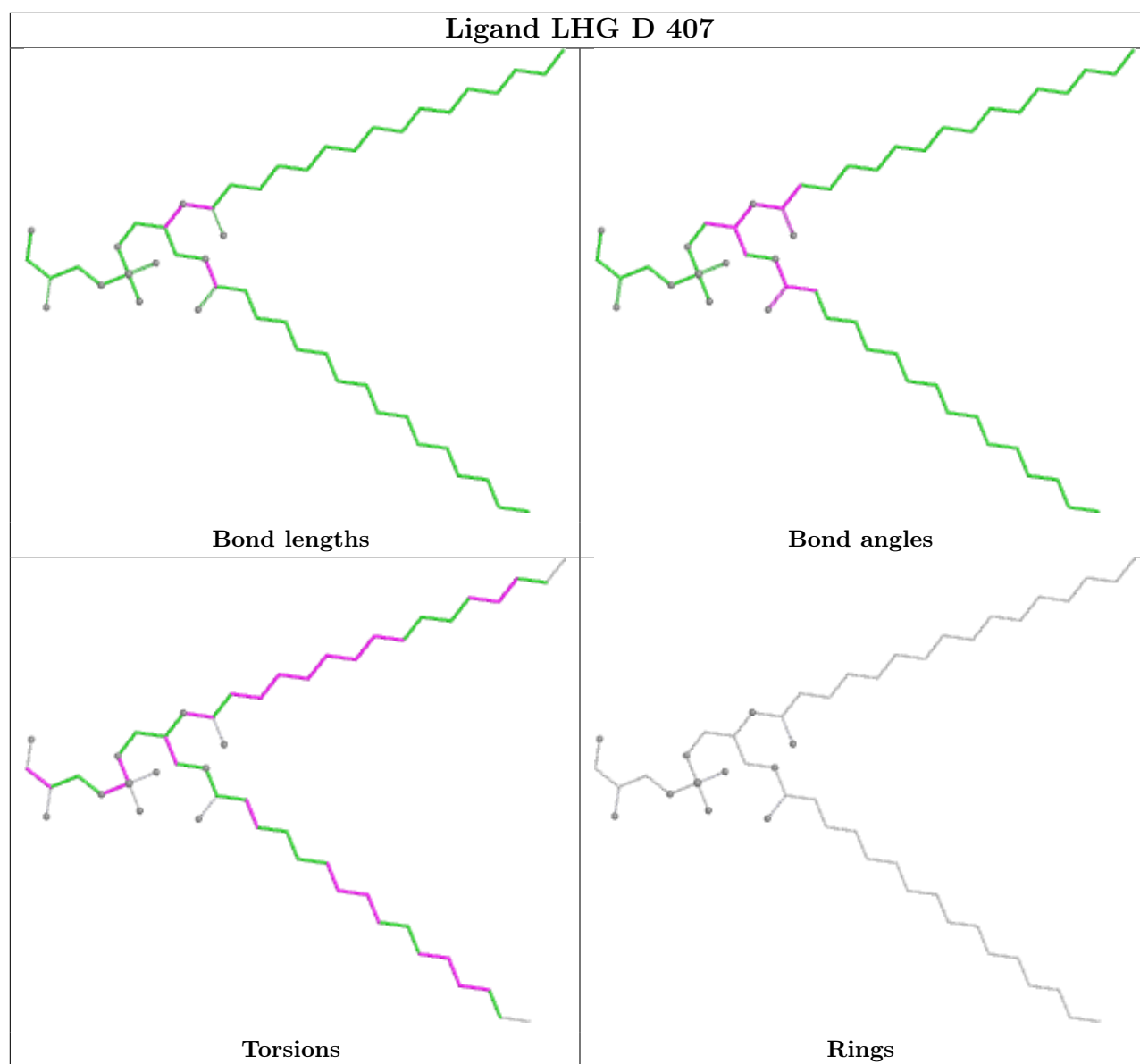




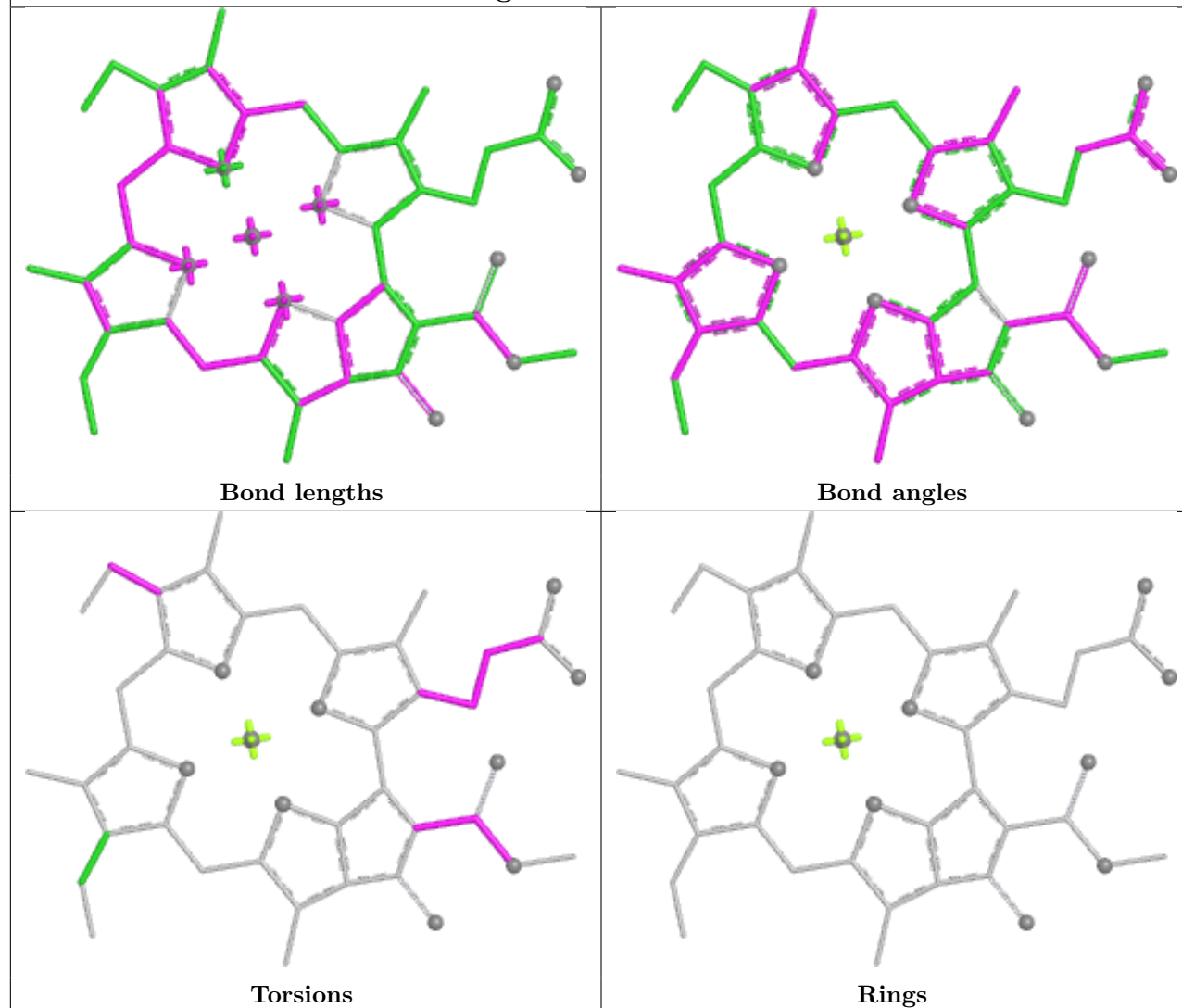




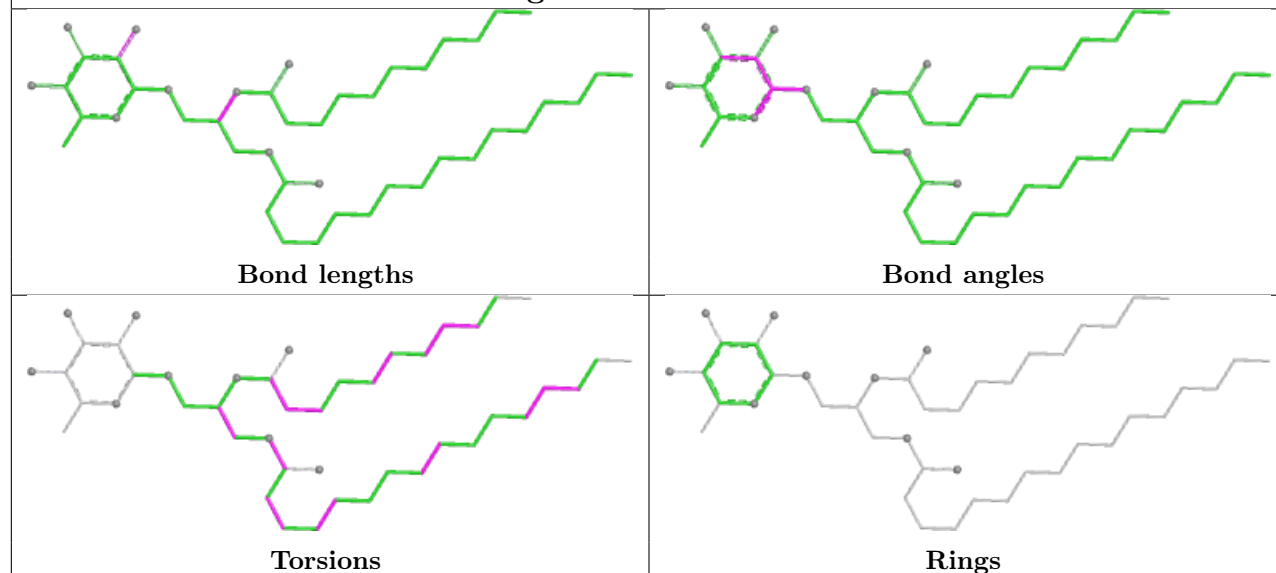


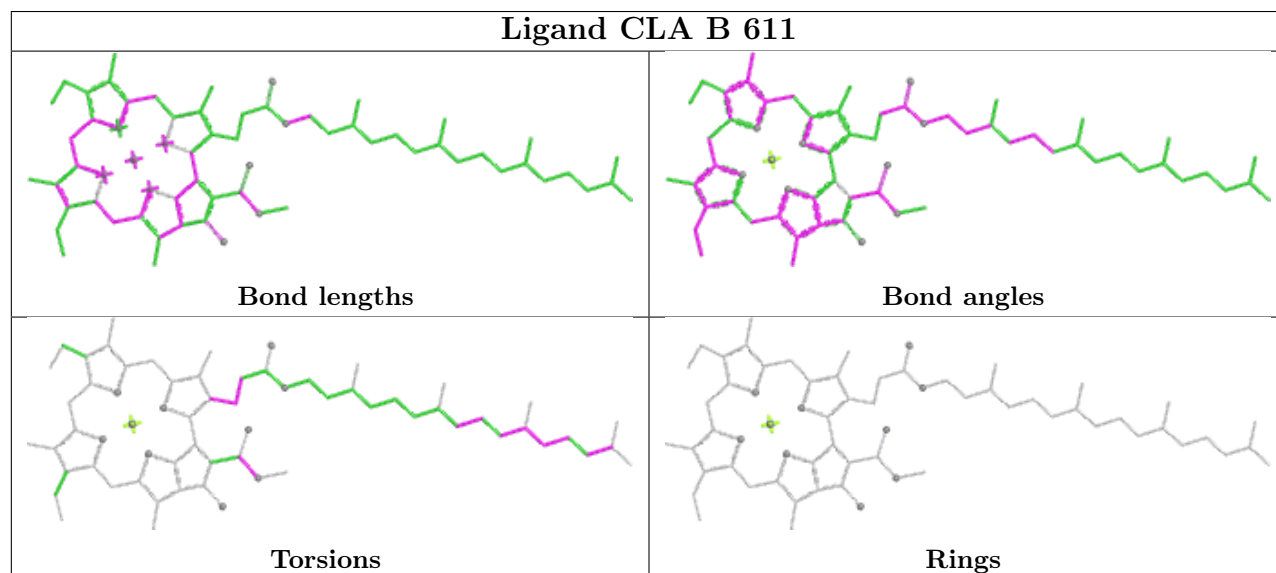
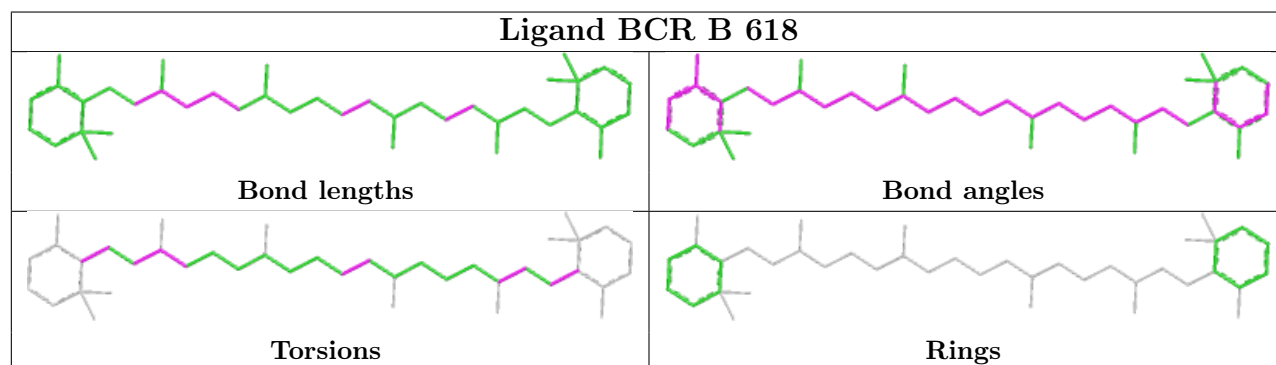
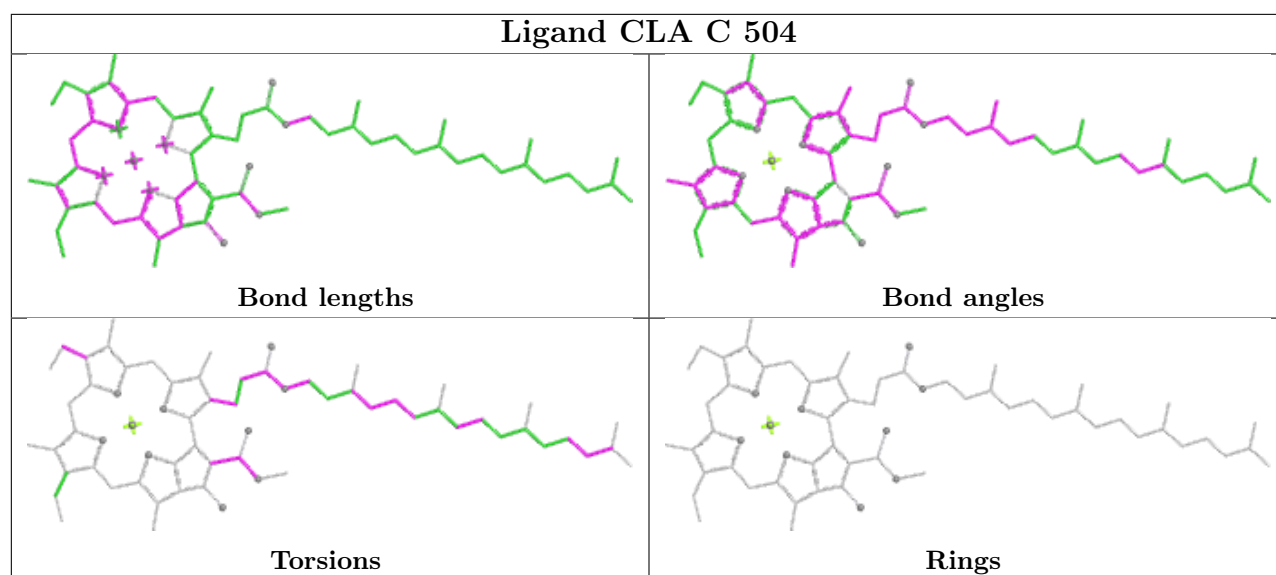


Ligand CLA b 601

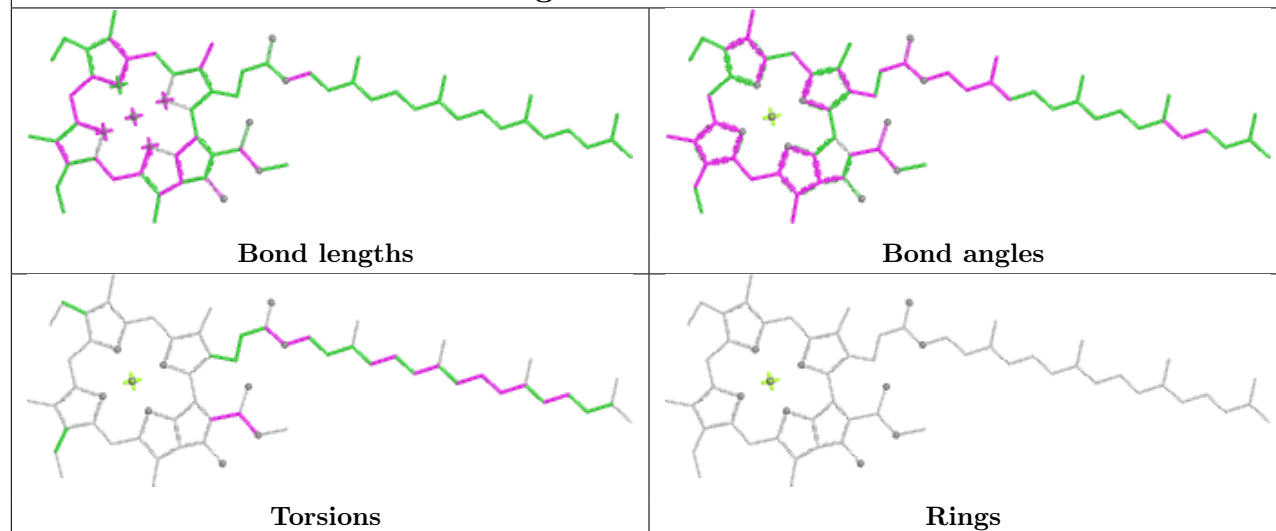


Ligand DGD D 410

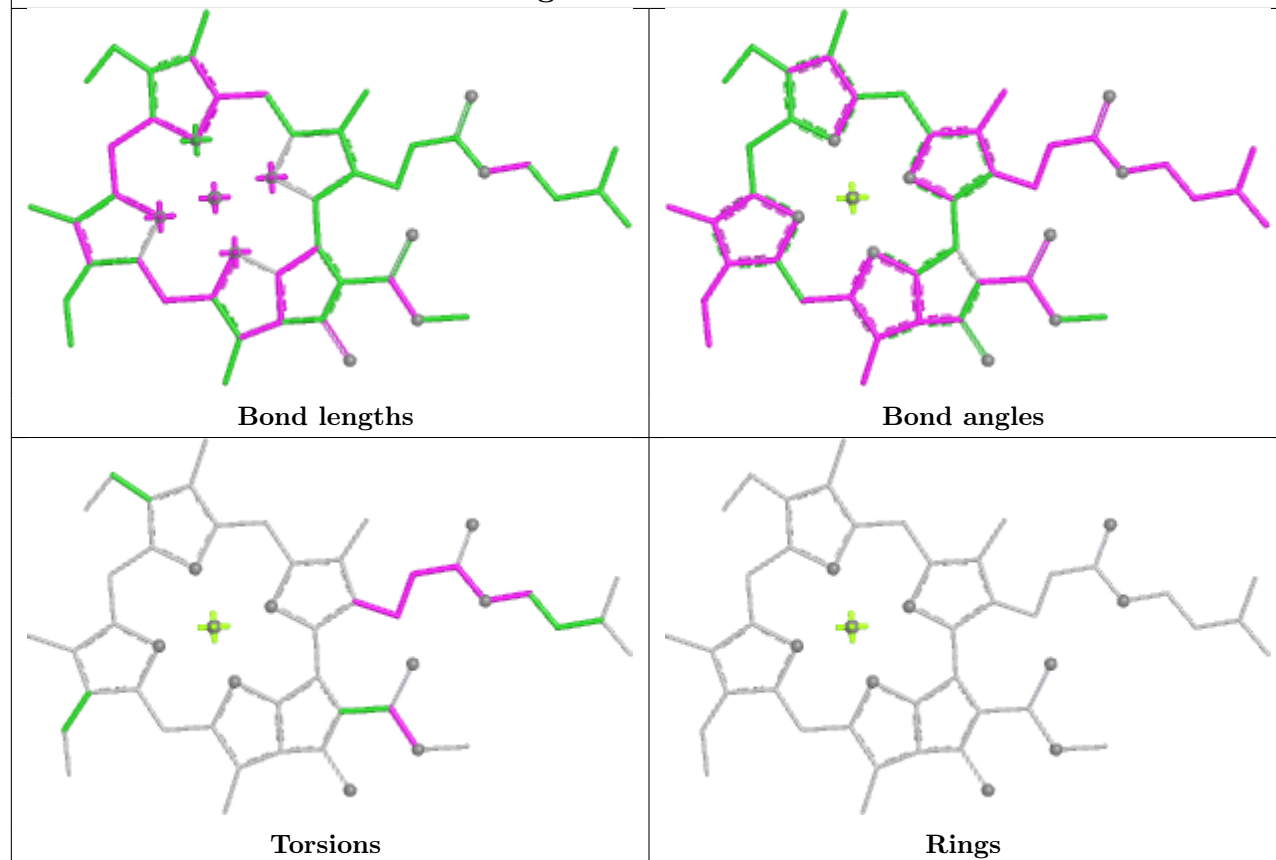


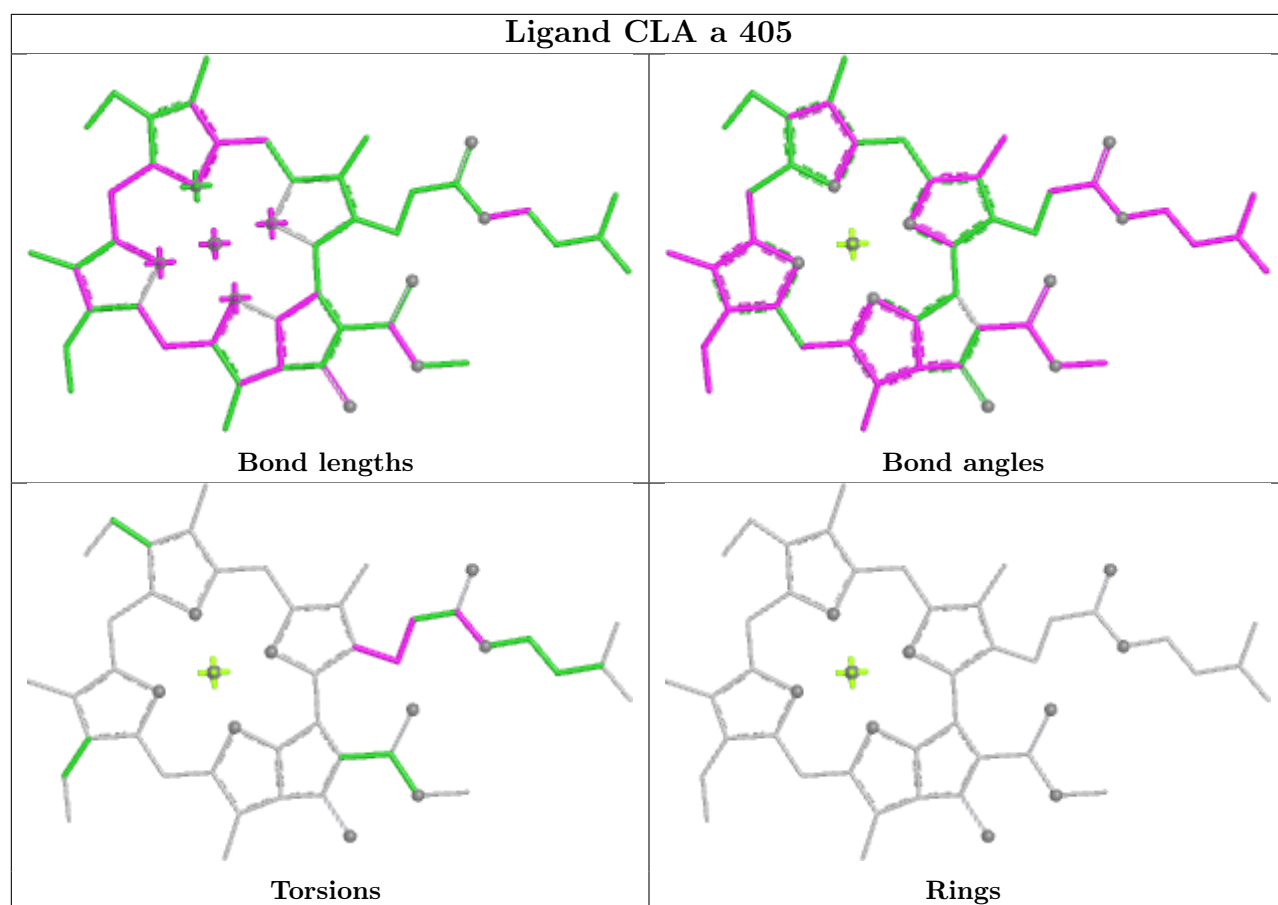


Ligand CLA b 612

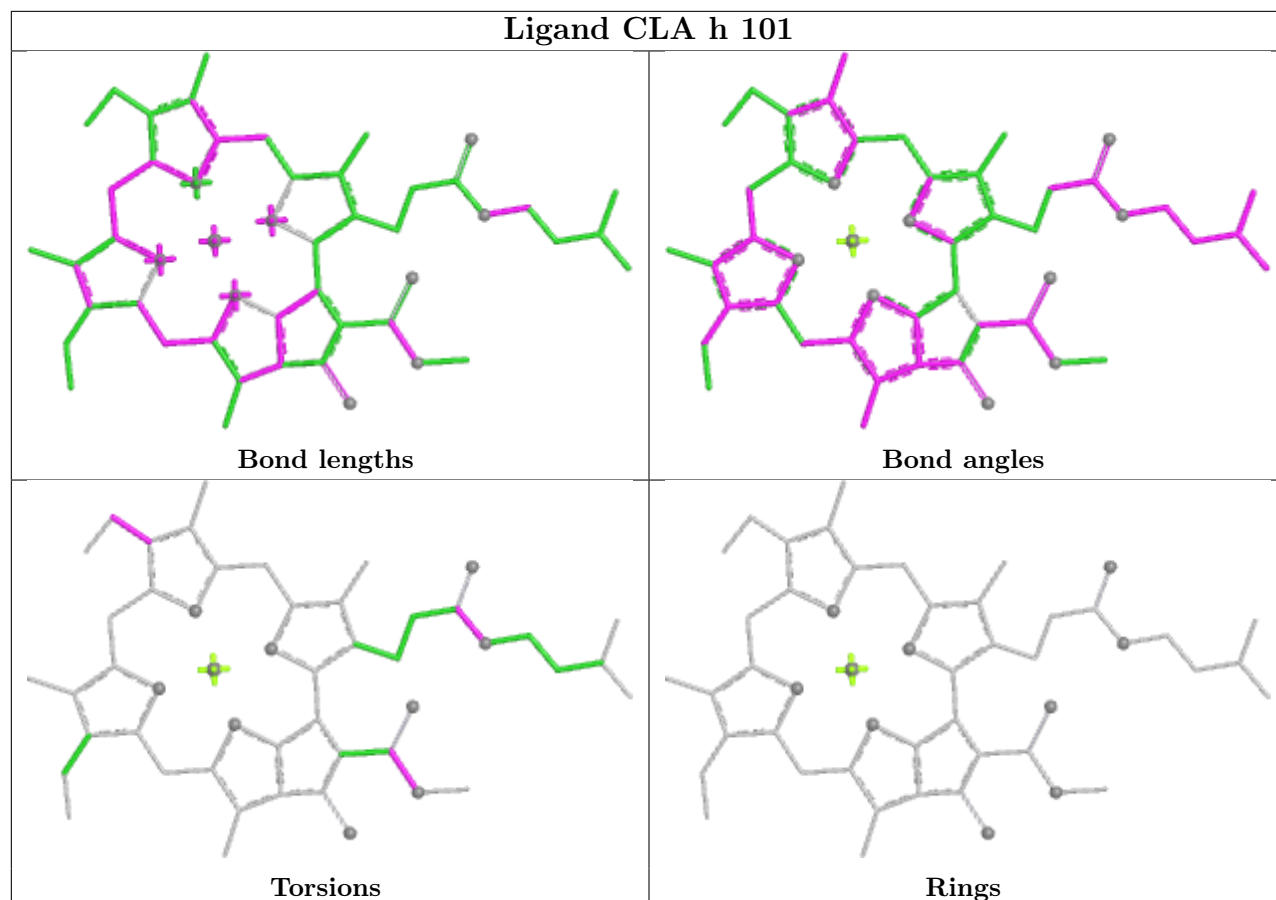


Ligand CLA c 512

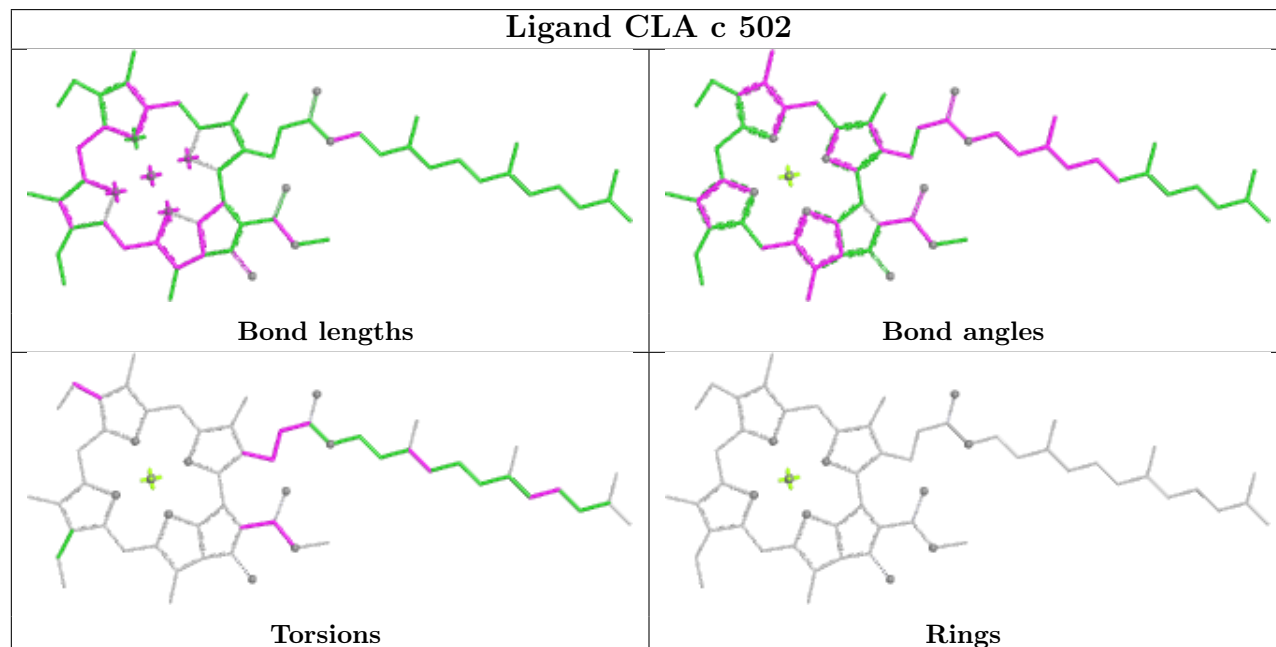


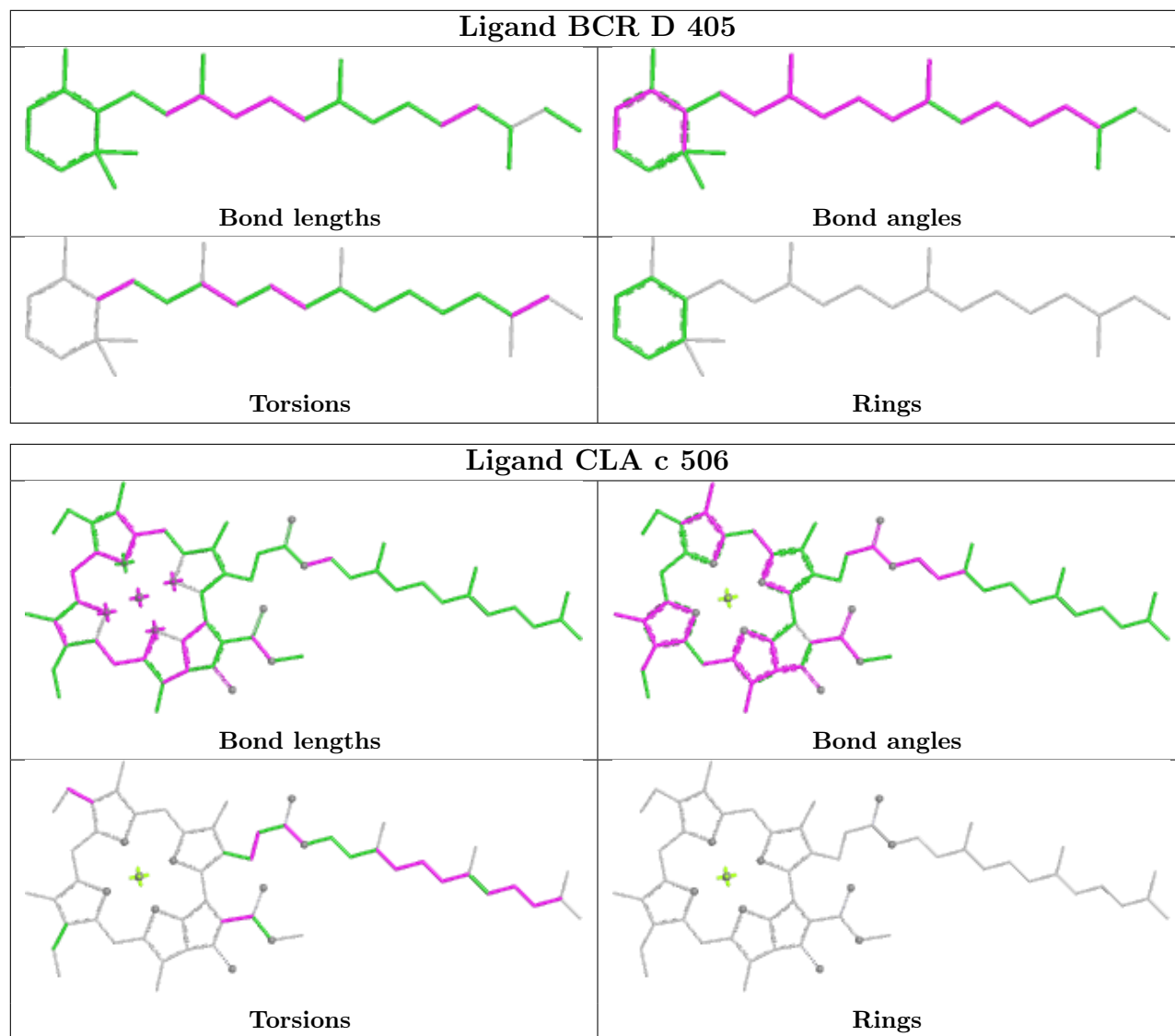


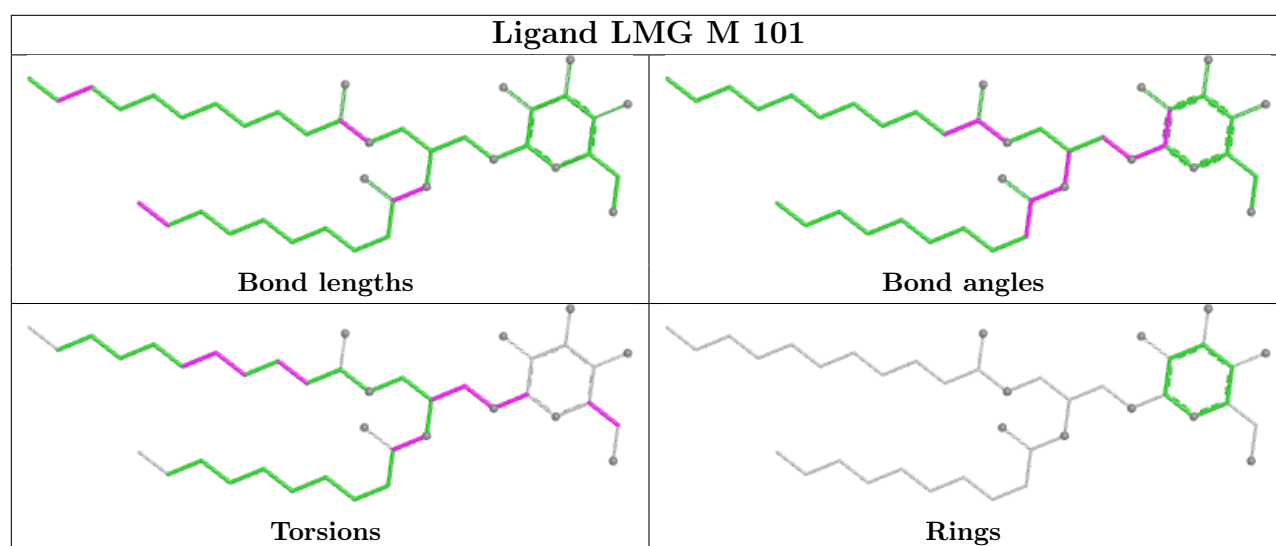
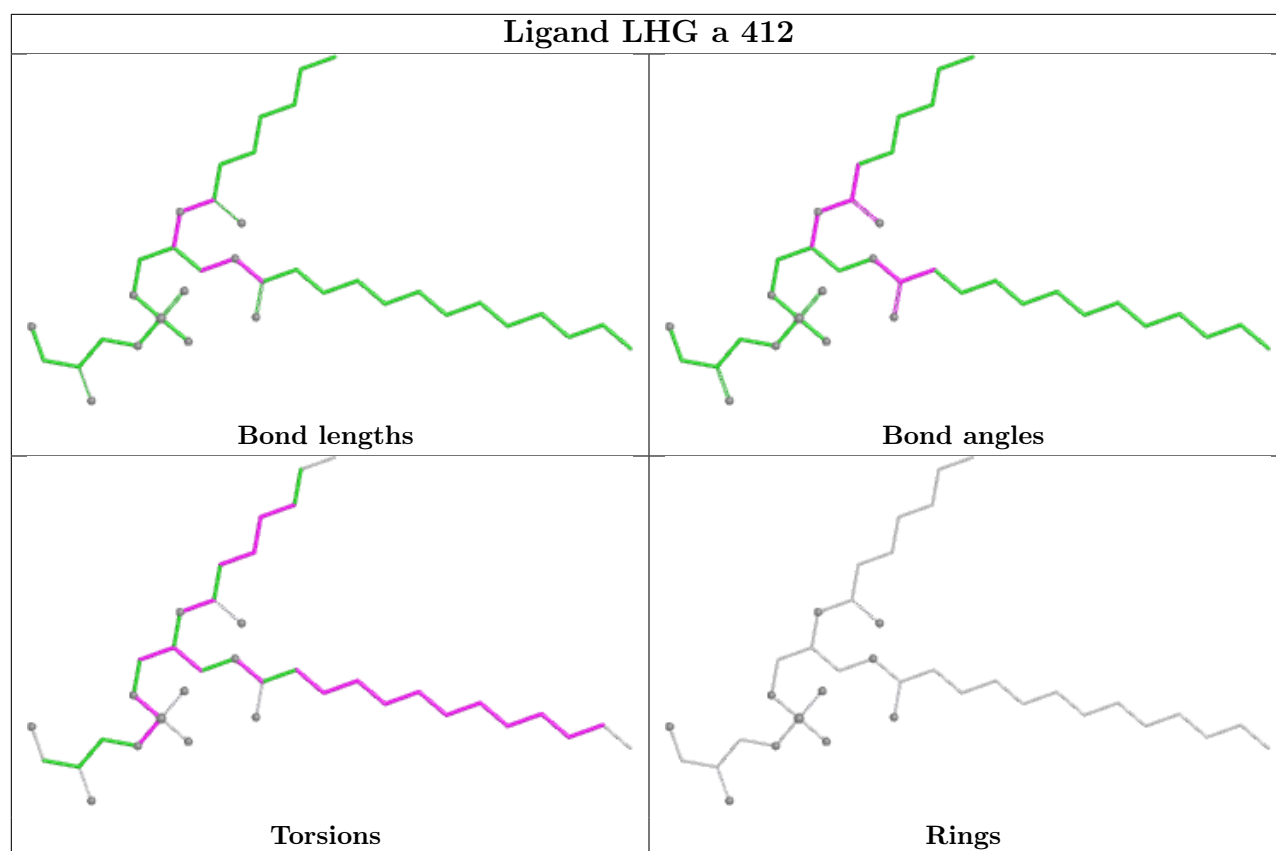
Ligand CLA h 101

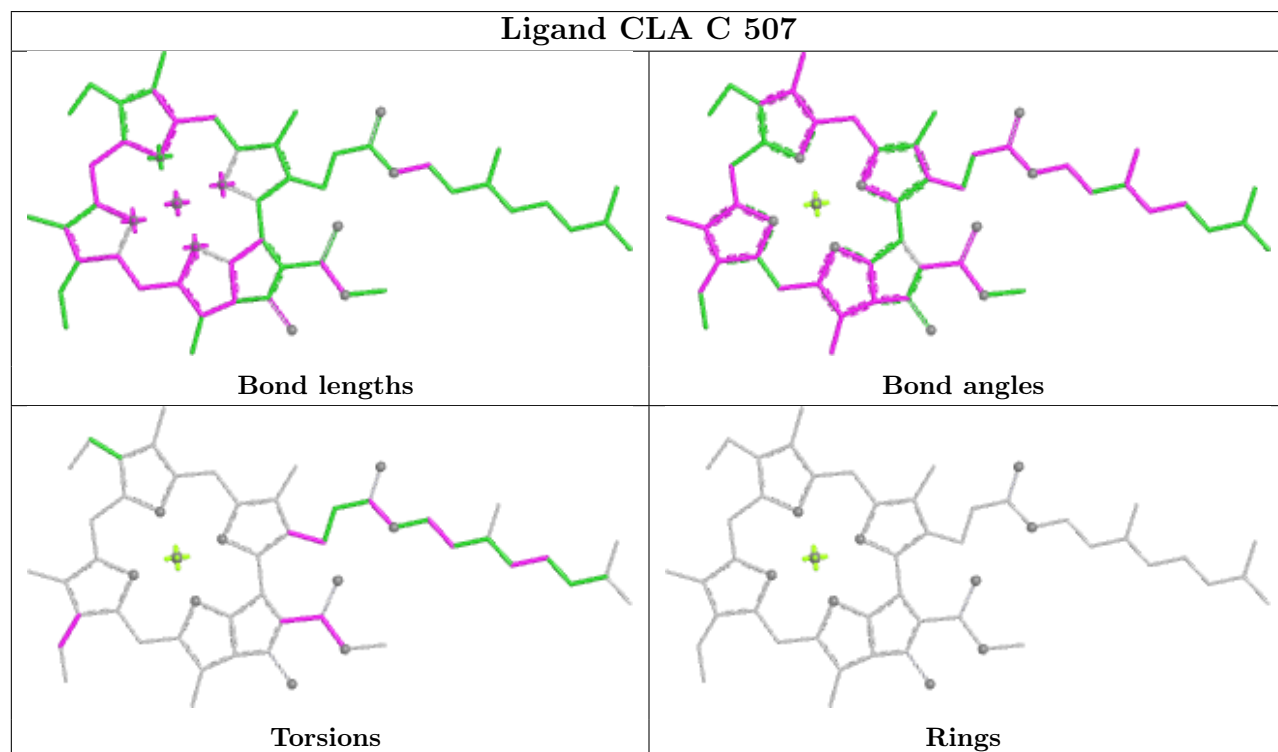
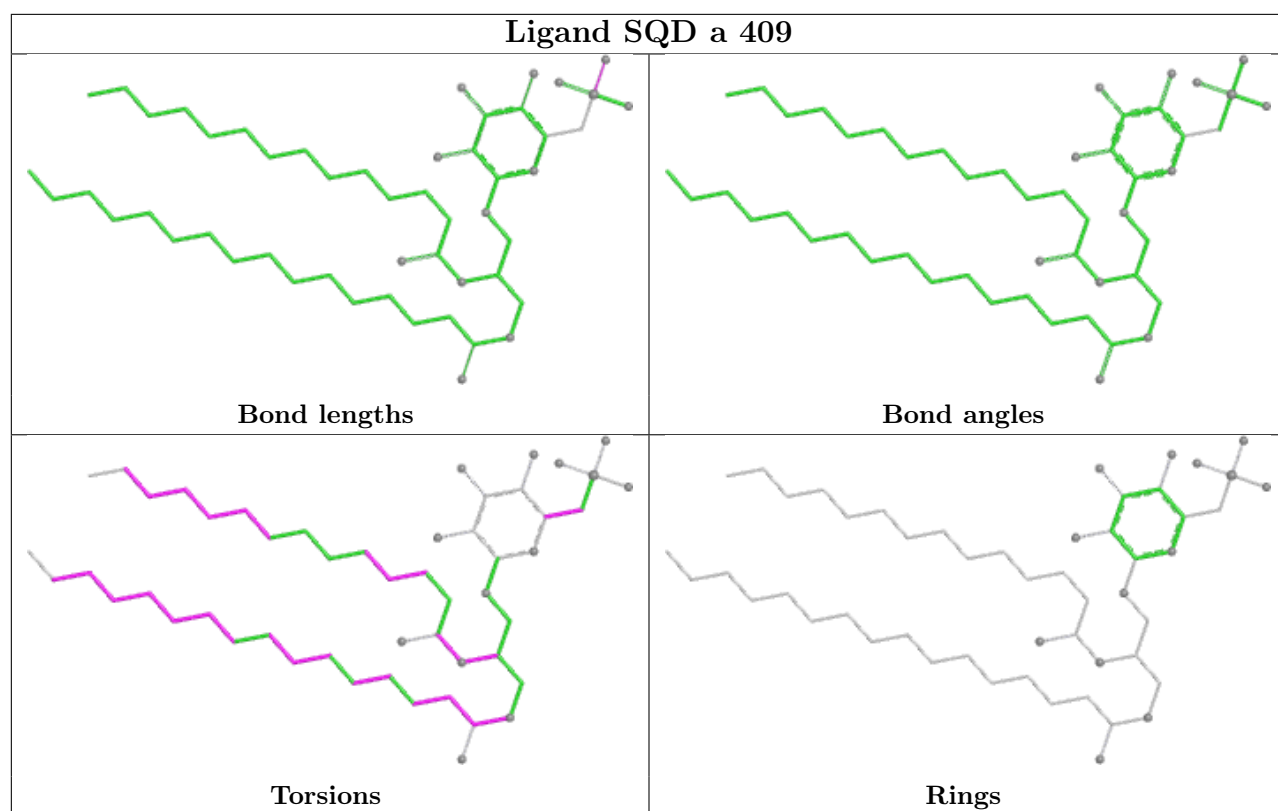


Ligand CLA c 502

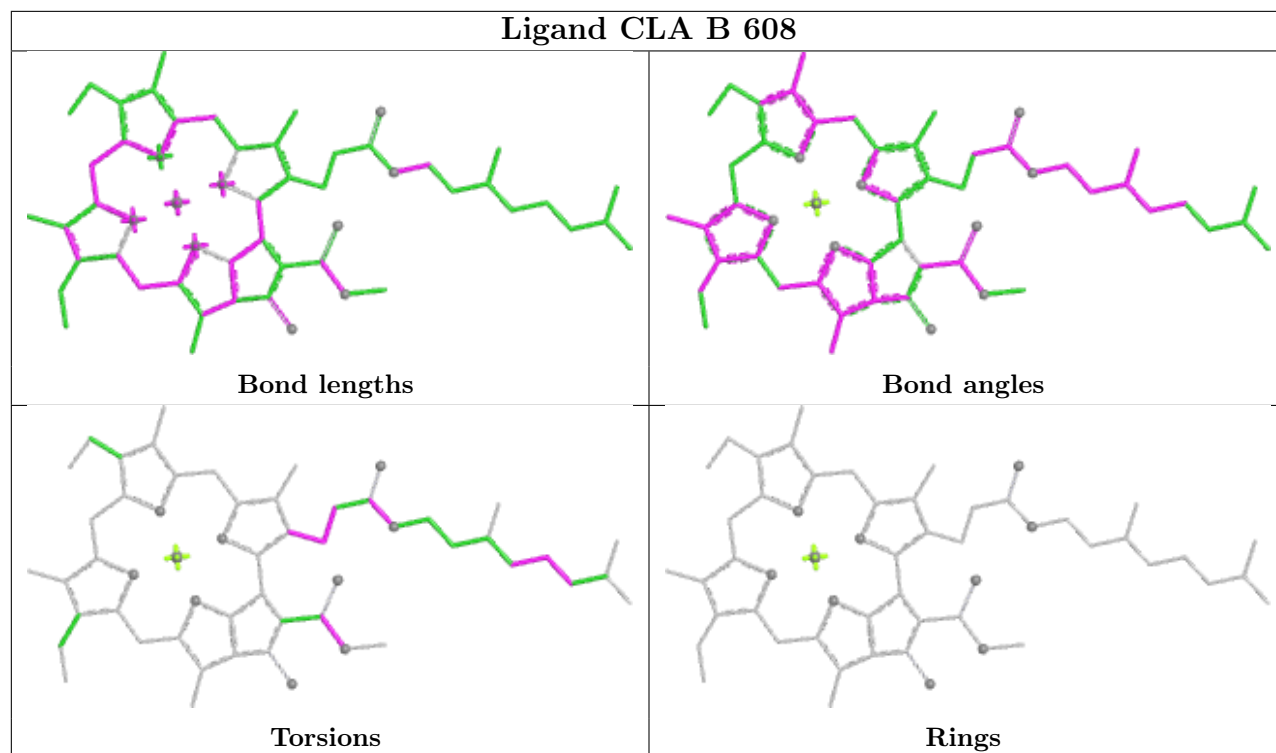




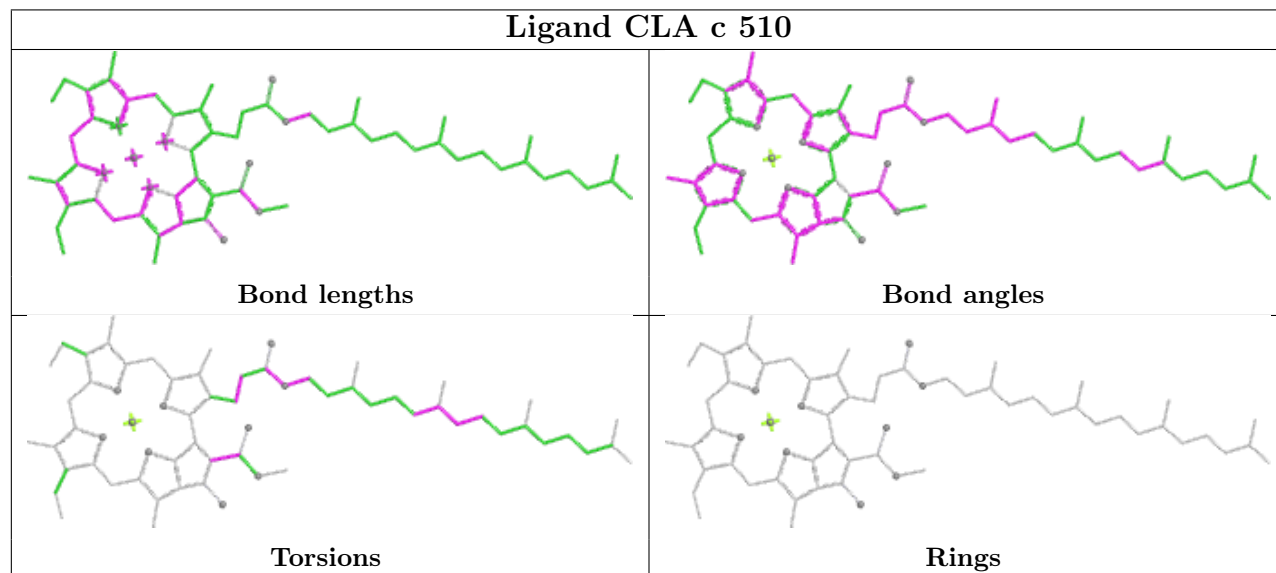


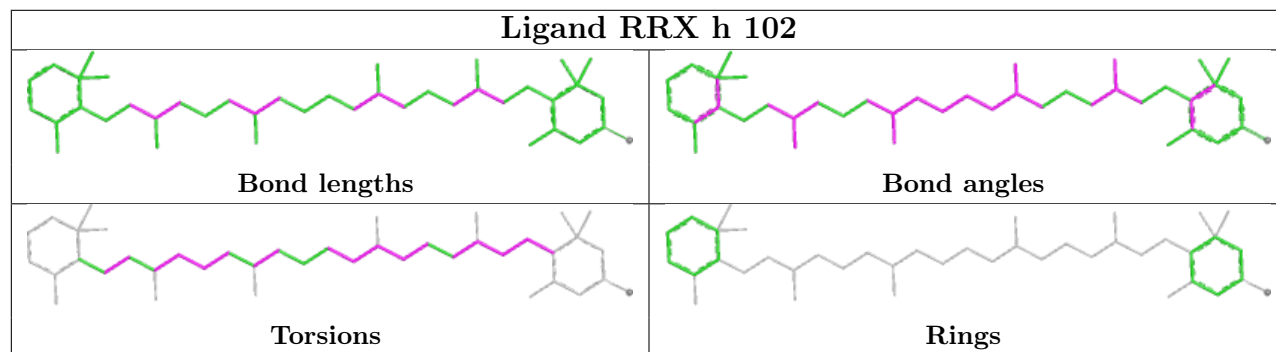
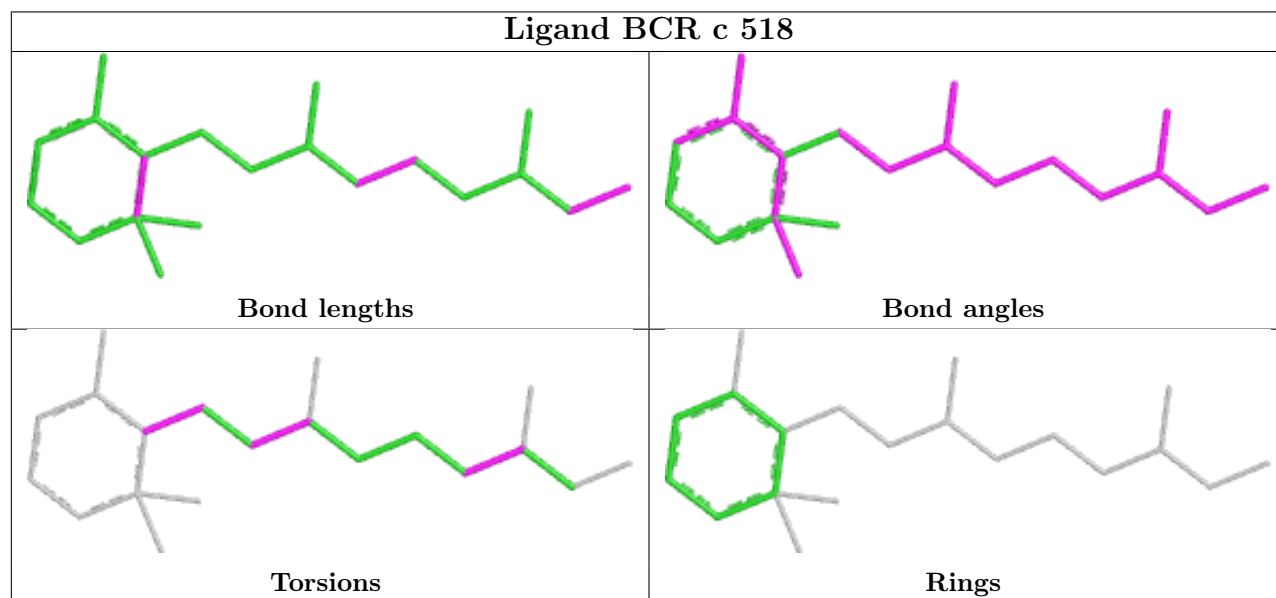
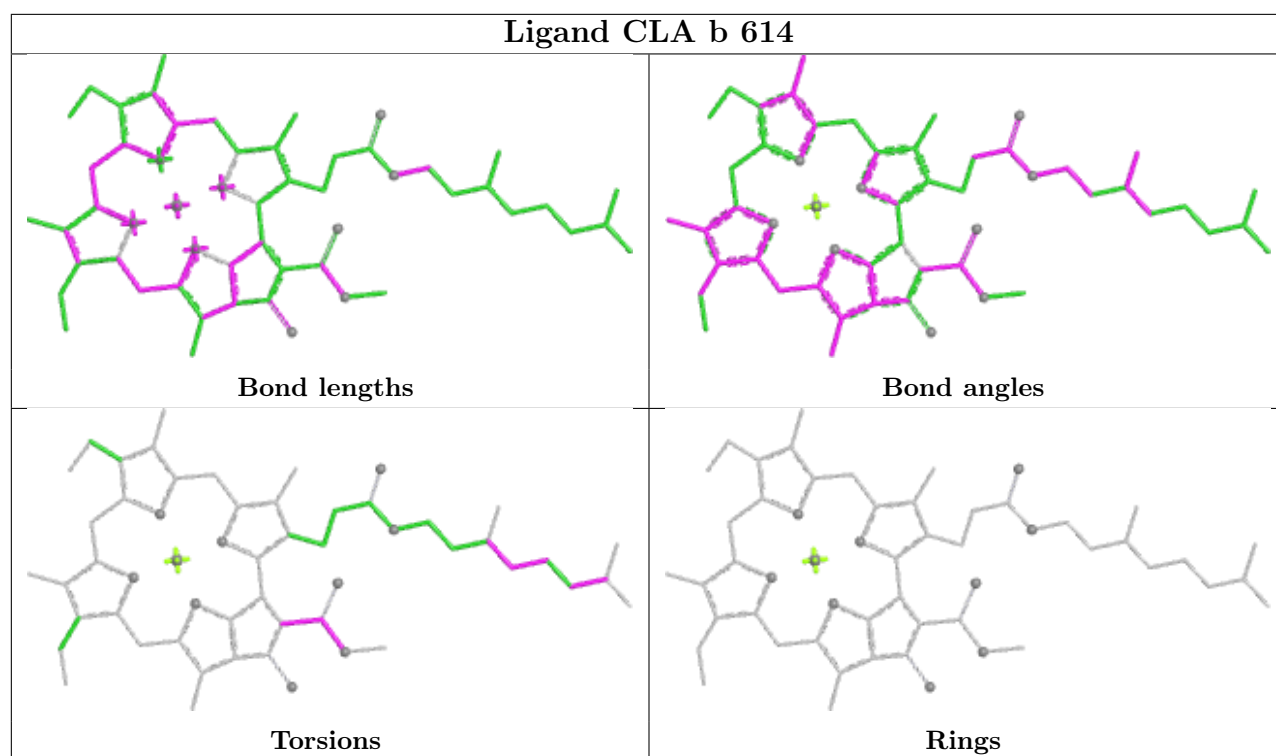


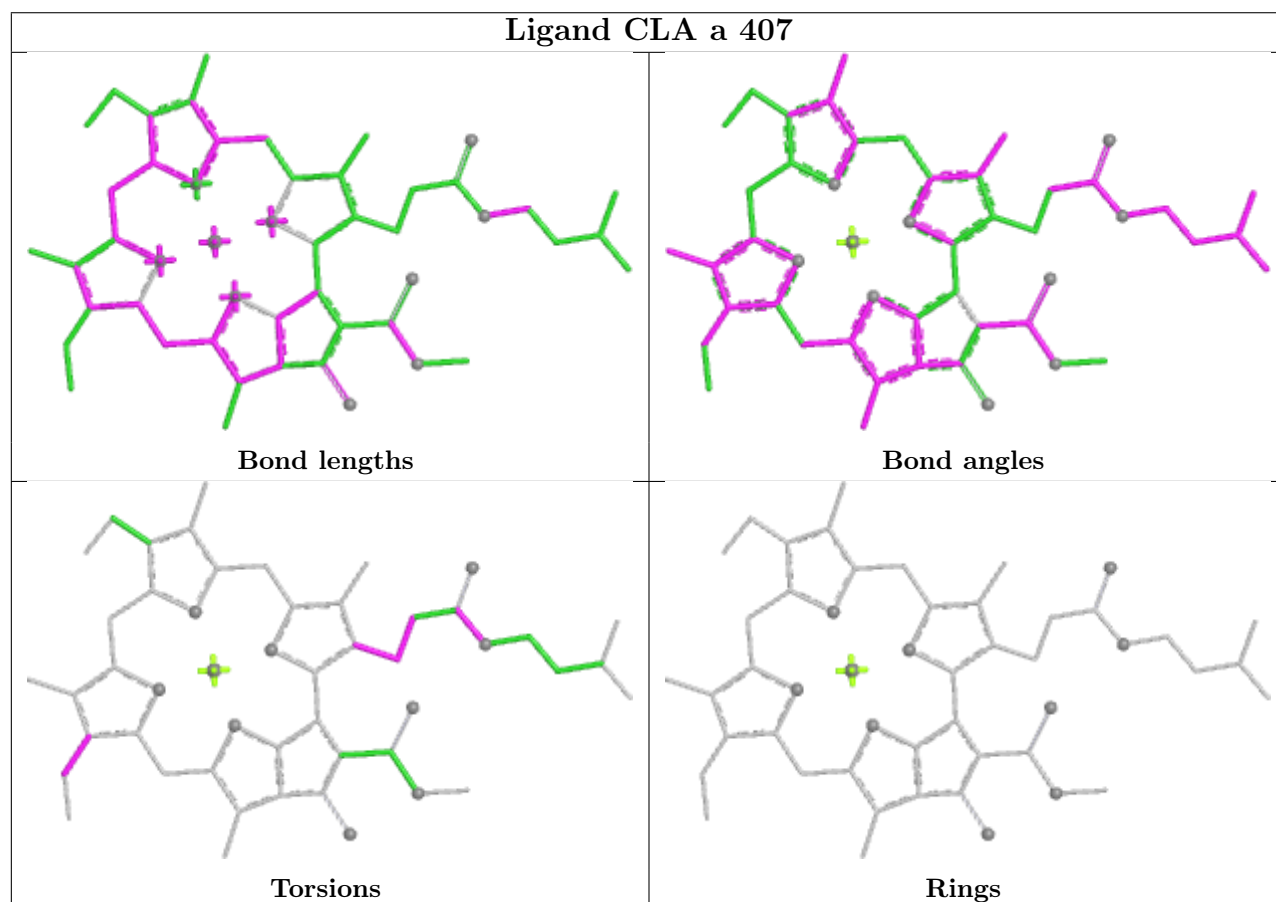
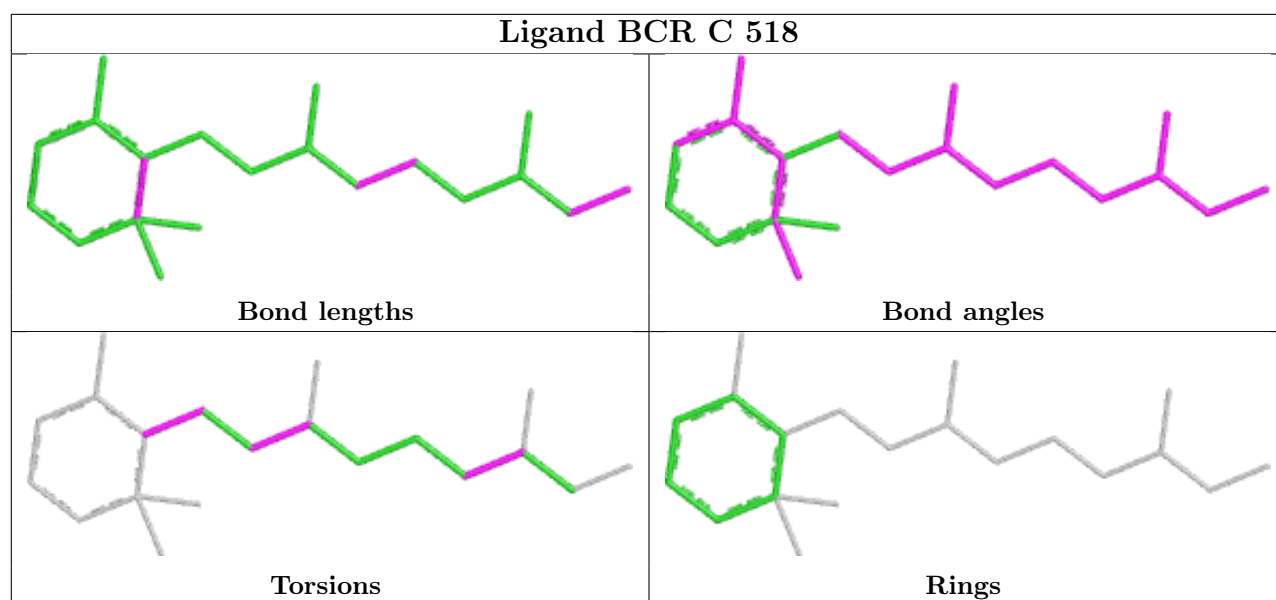
Ligand CLA B 608

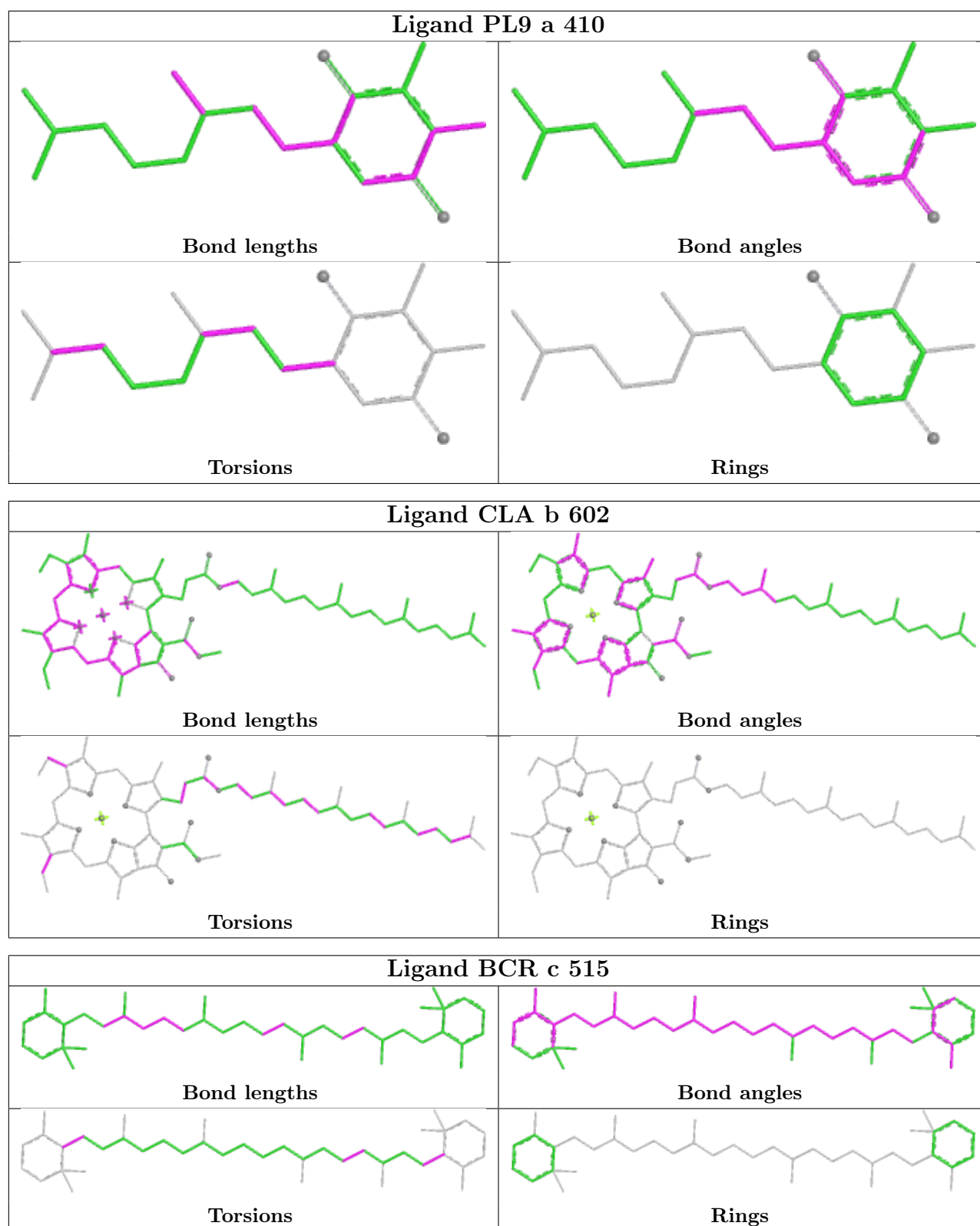


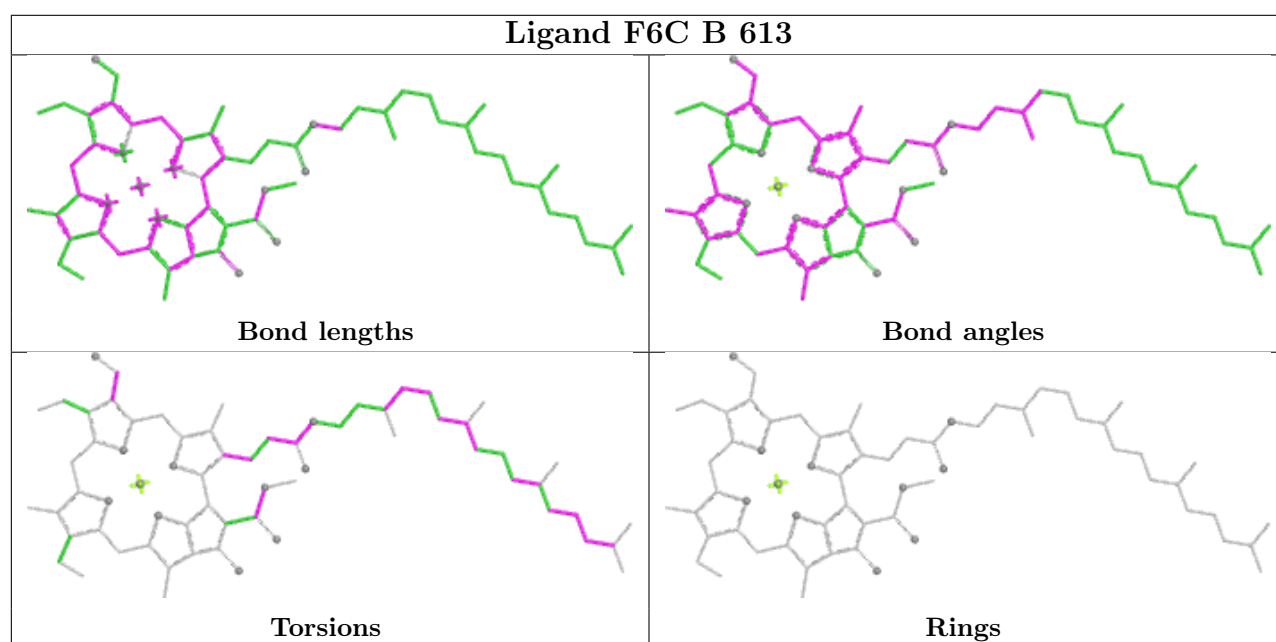
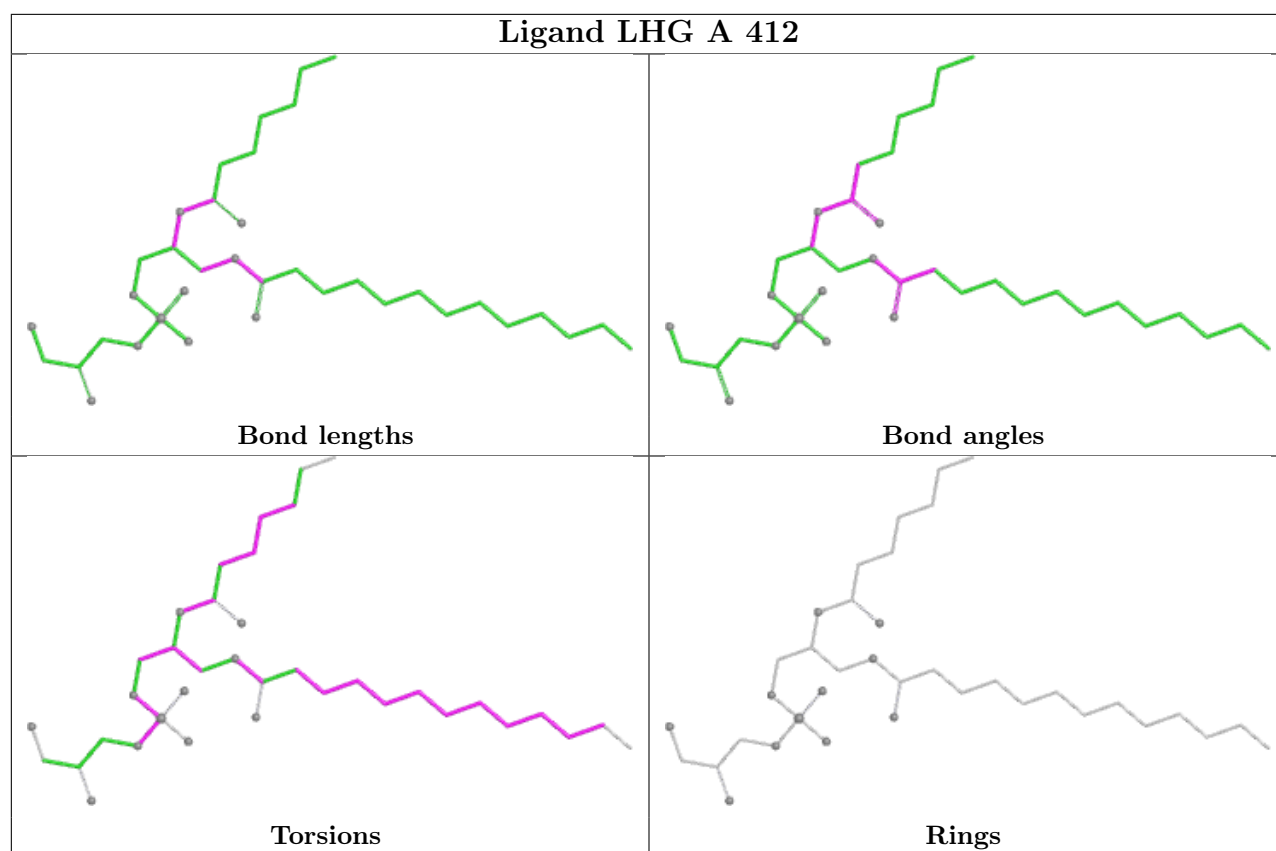
Ligand CLA c 510

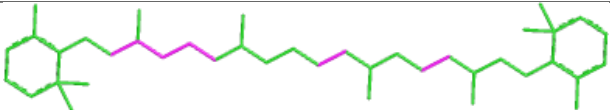
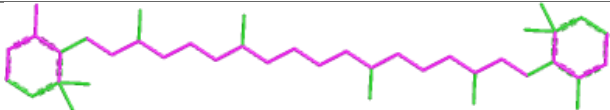
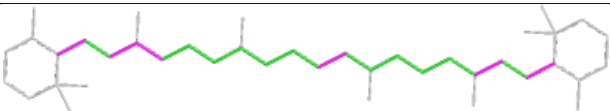
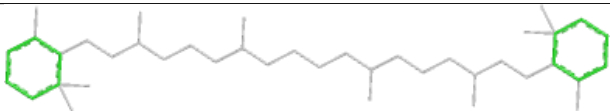
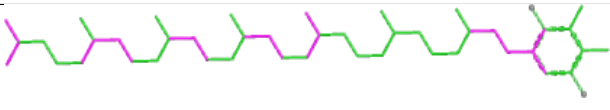
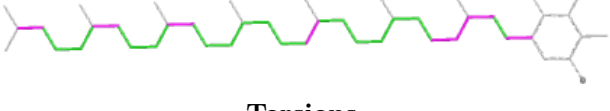
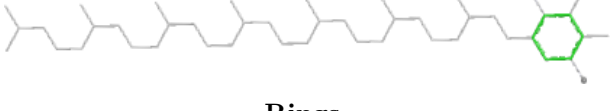
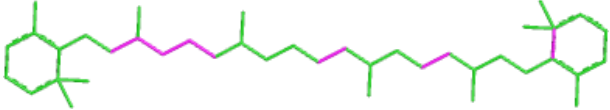
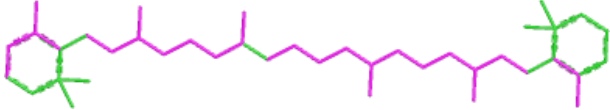
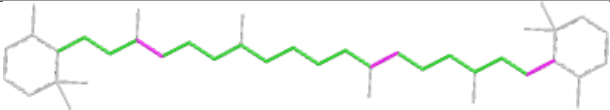
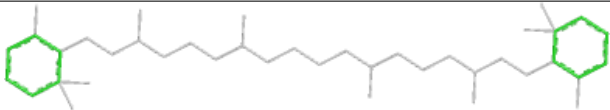




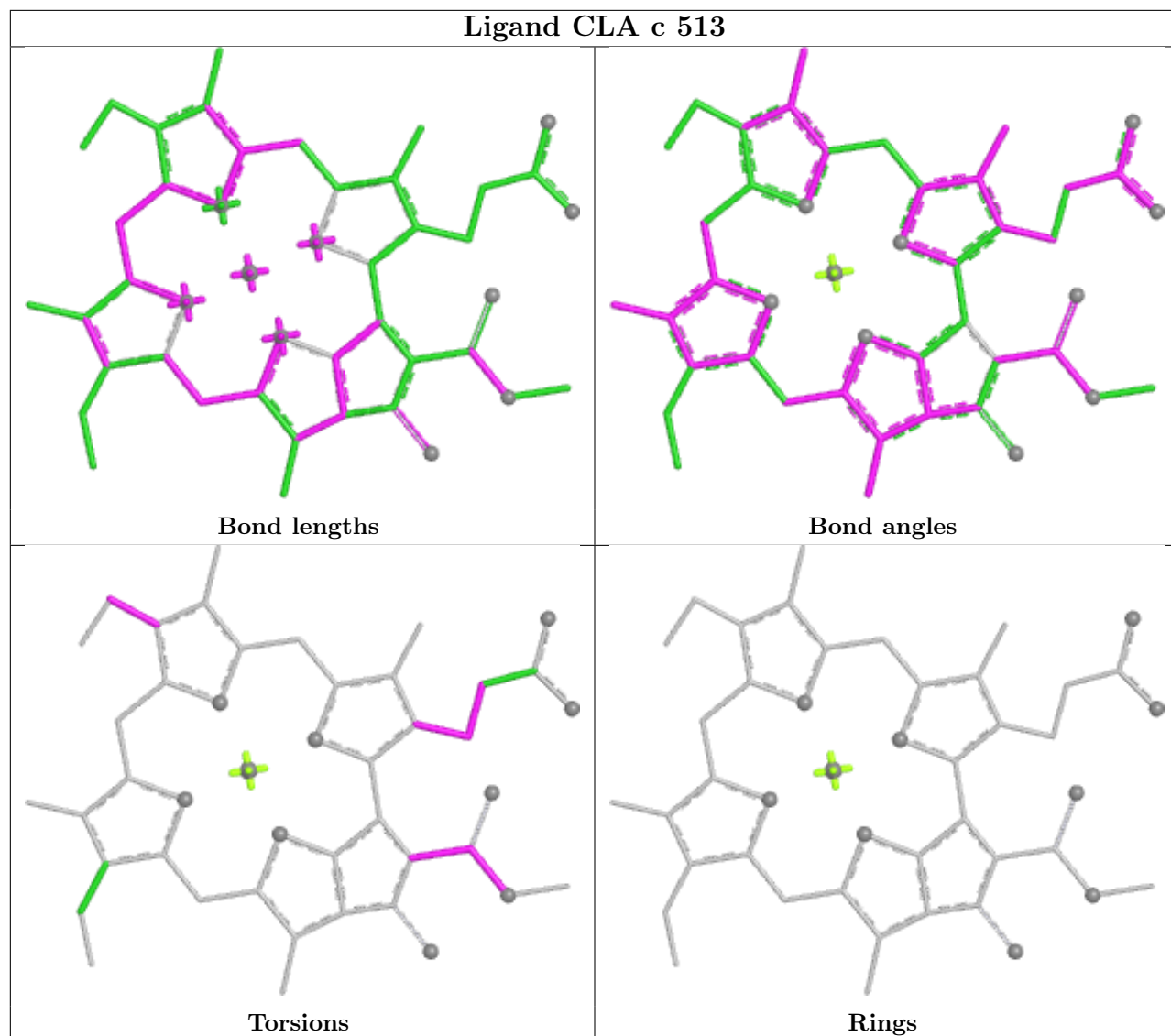


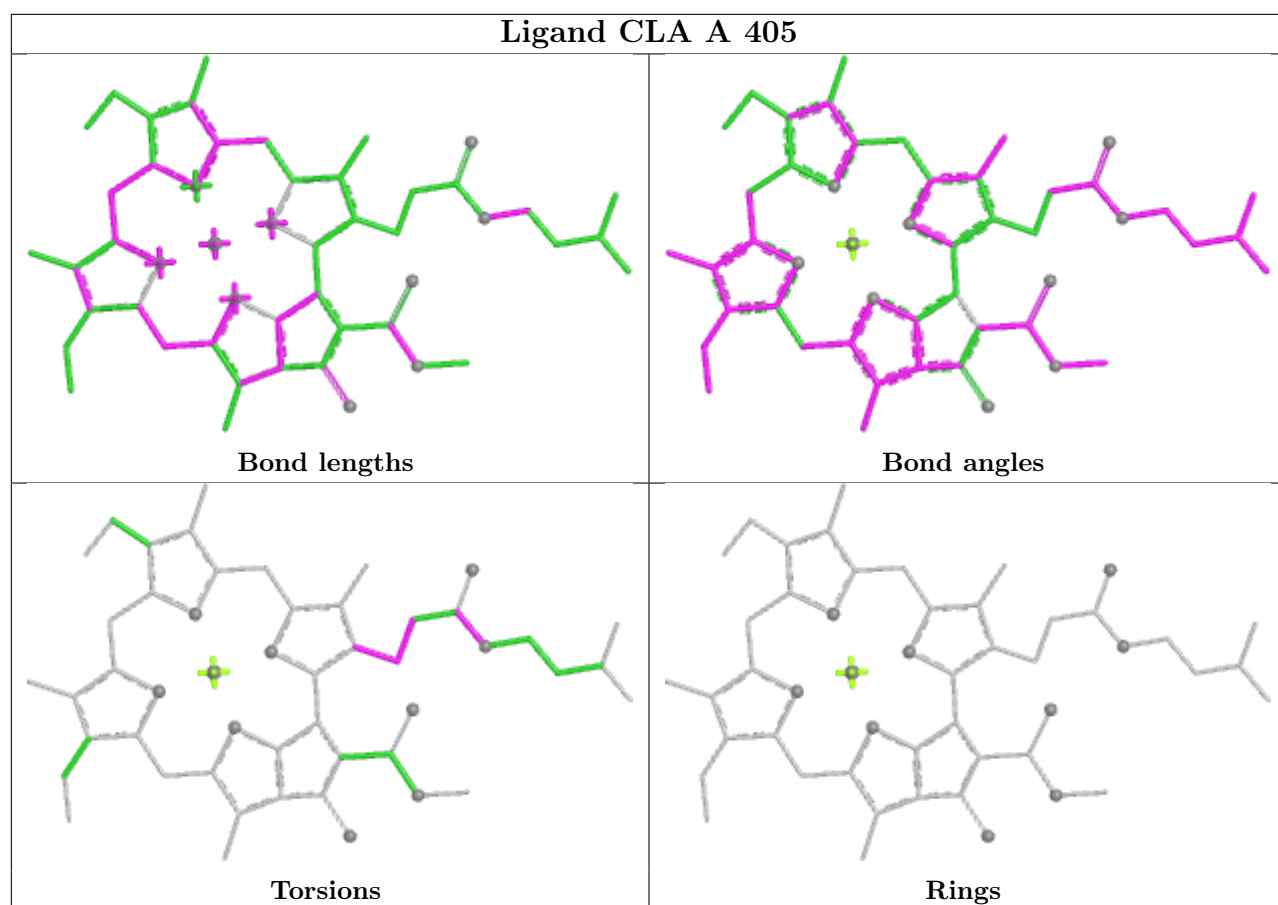


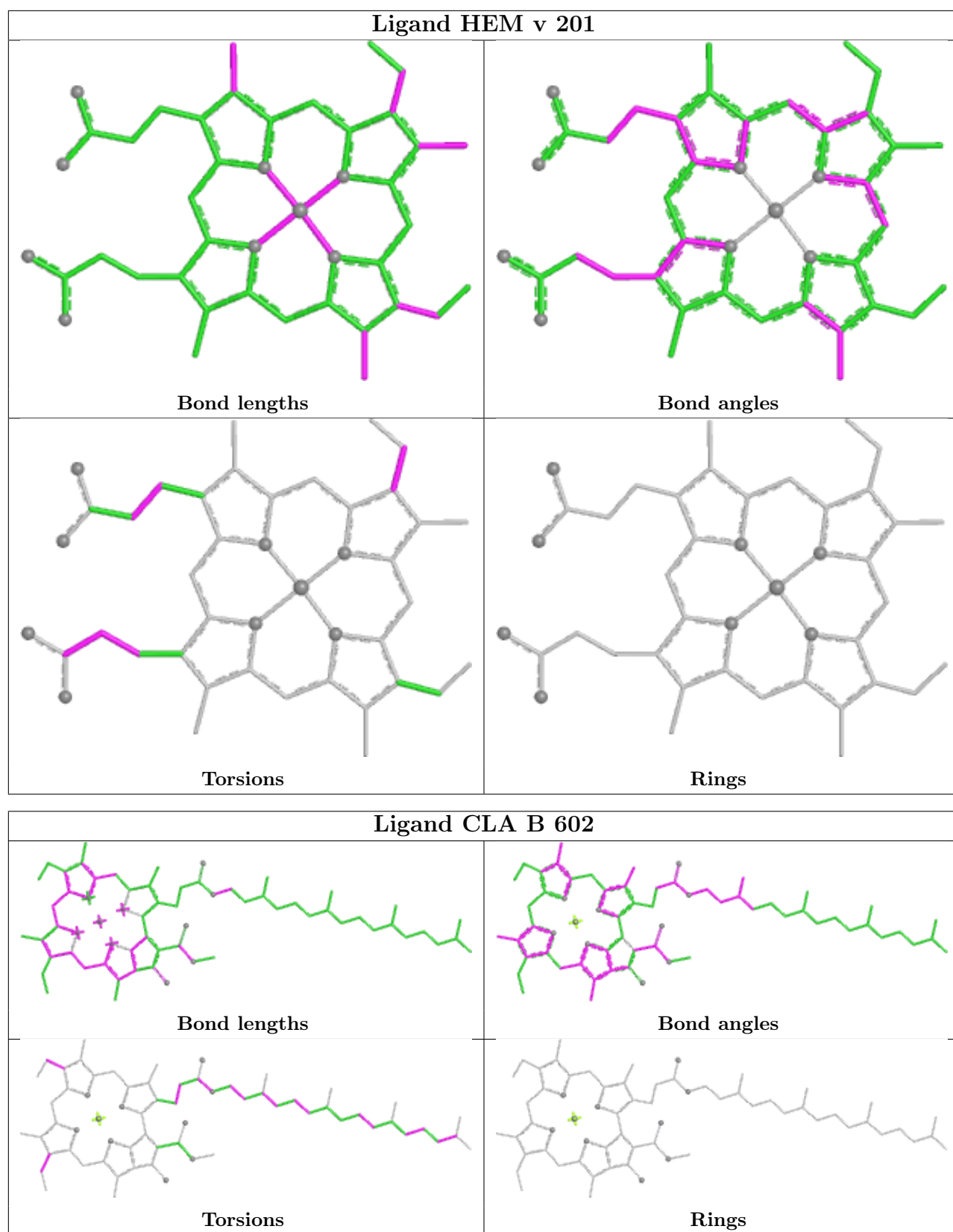


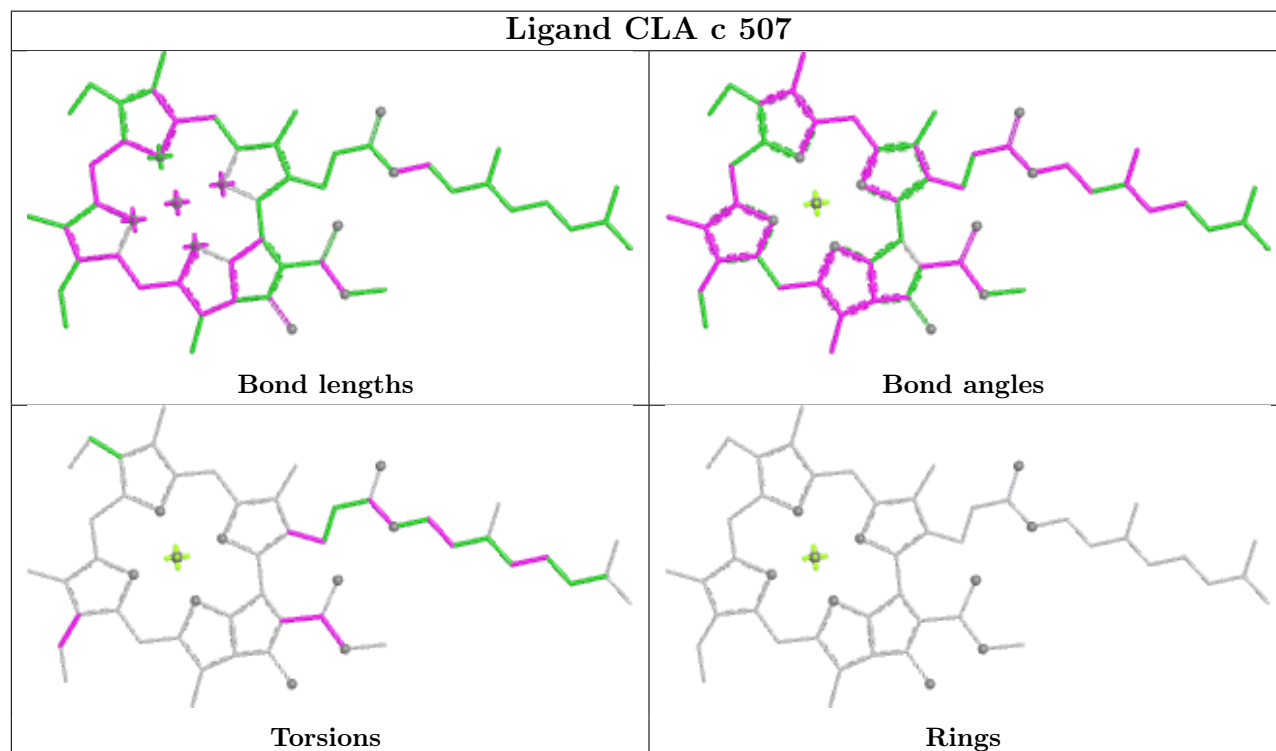
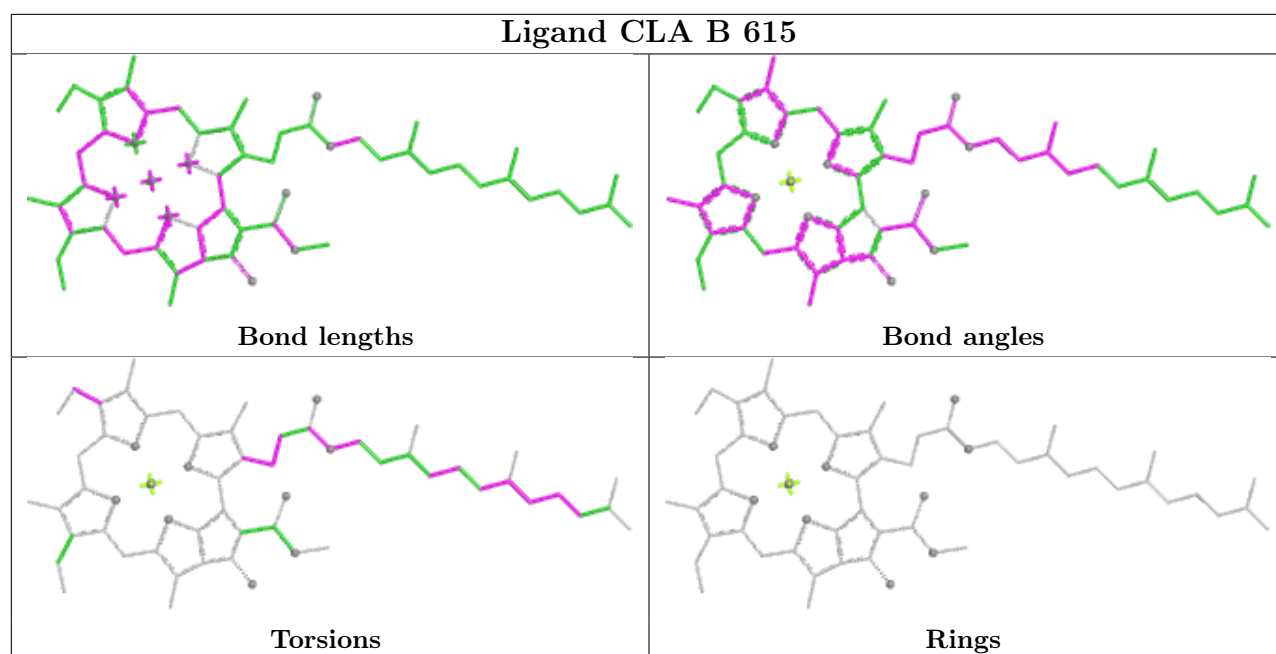
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

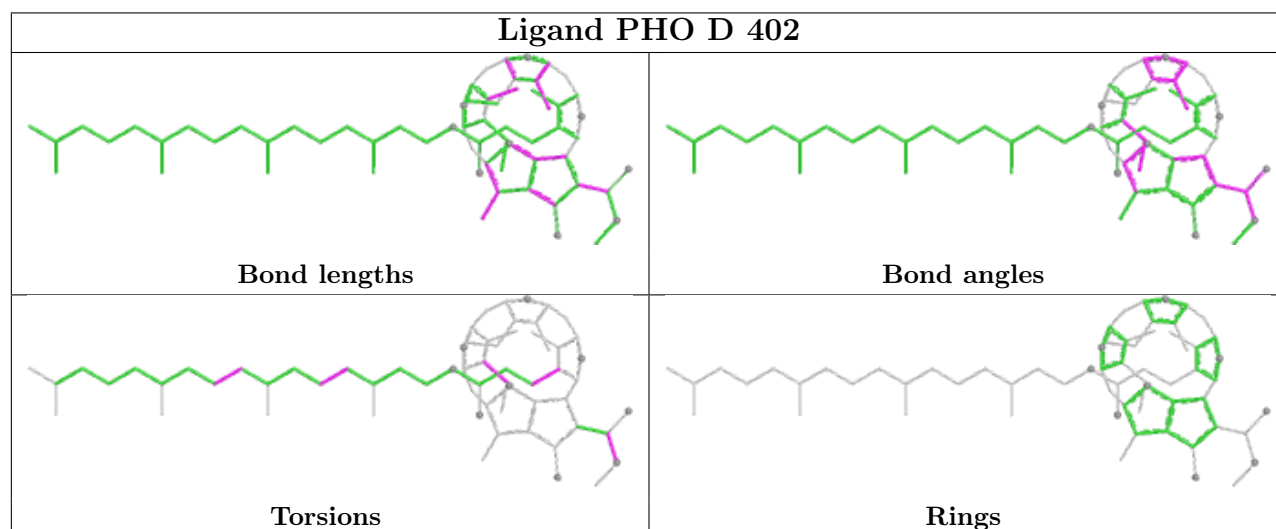
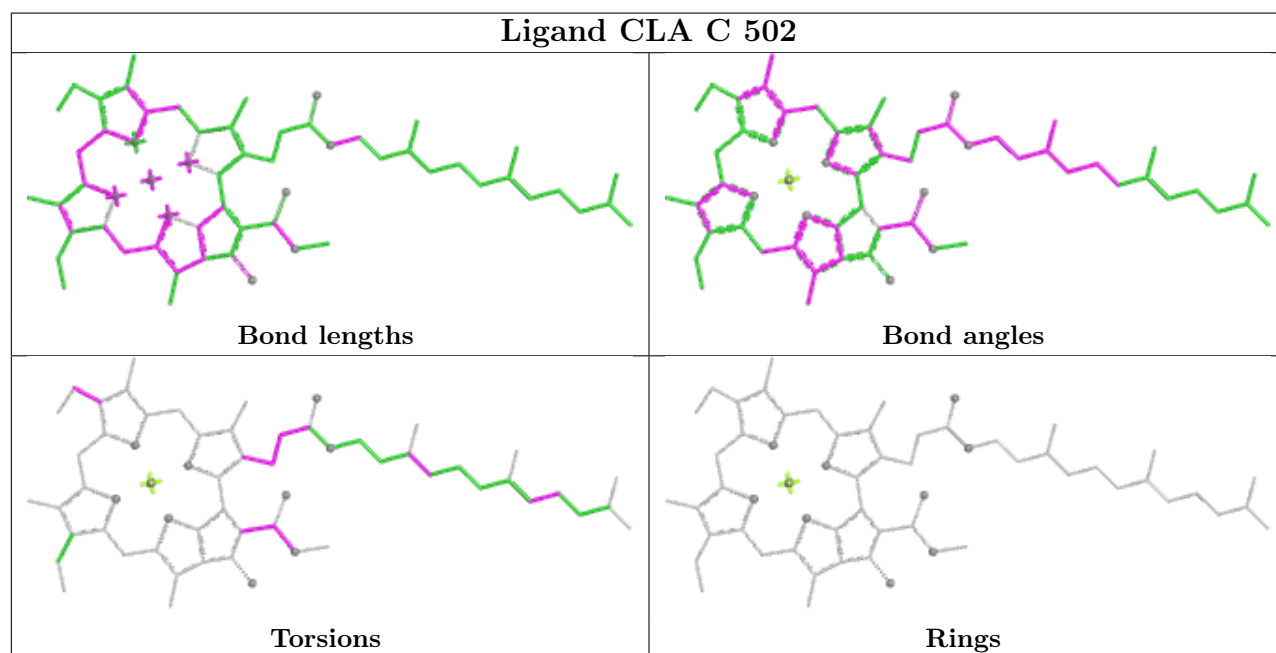
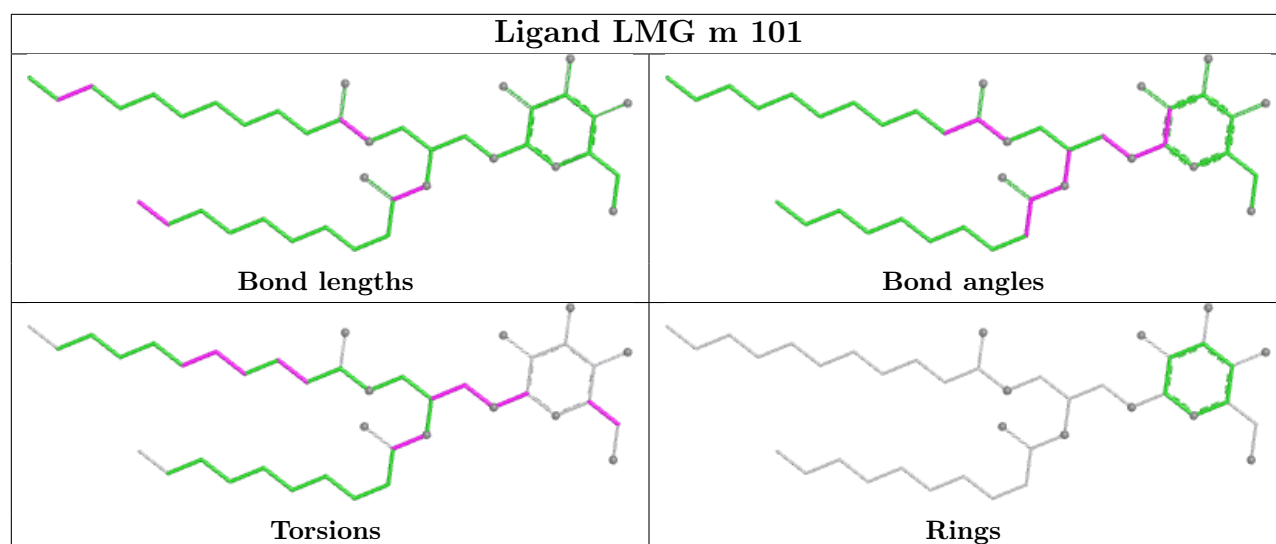
Ligand CLA c 513



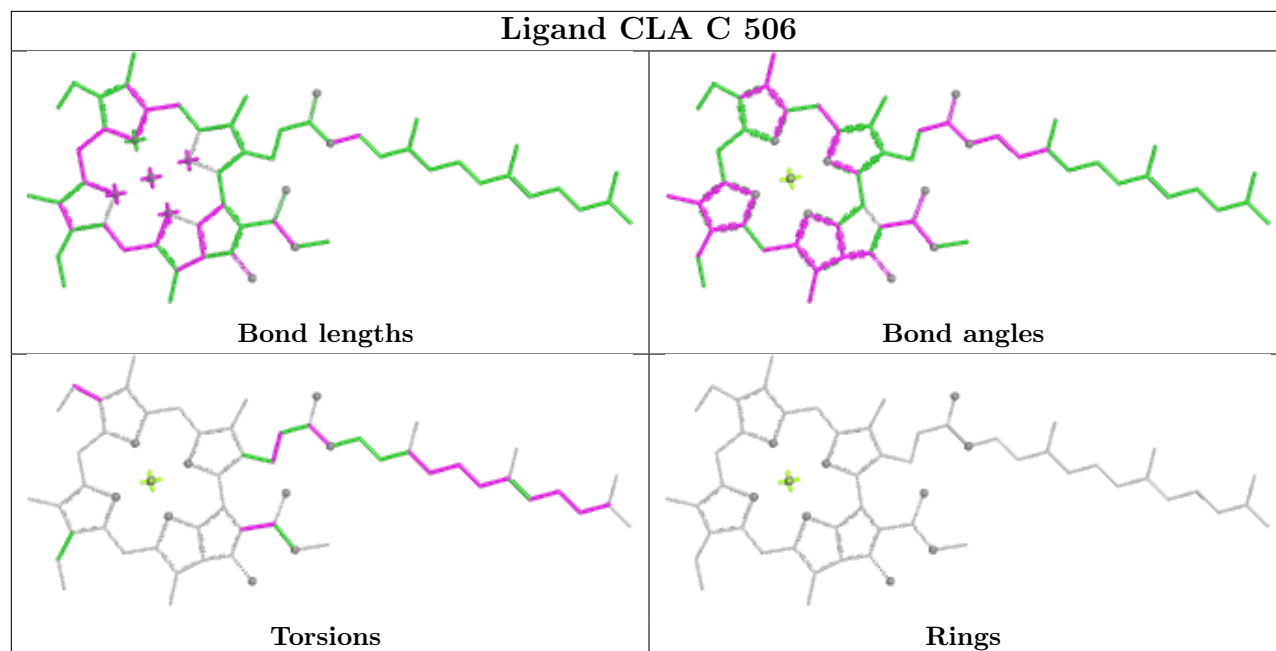




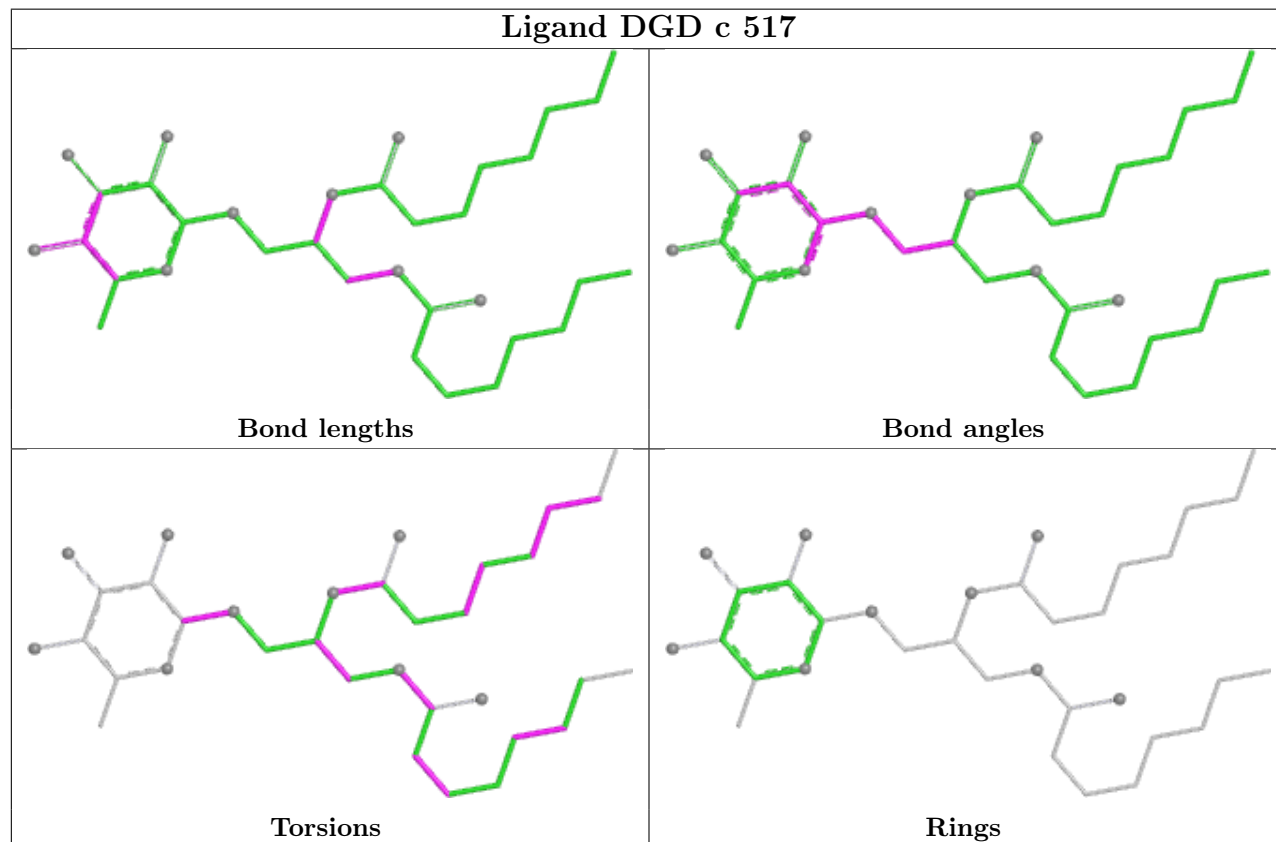


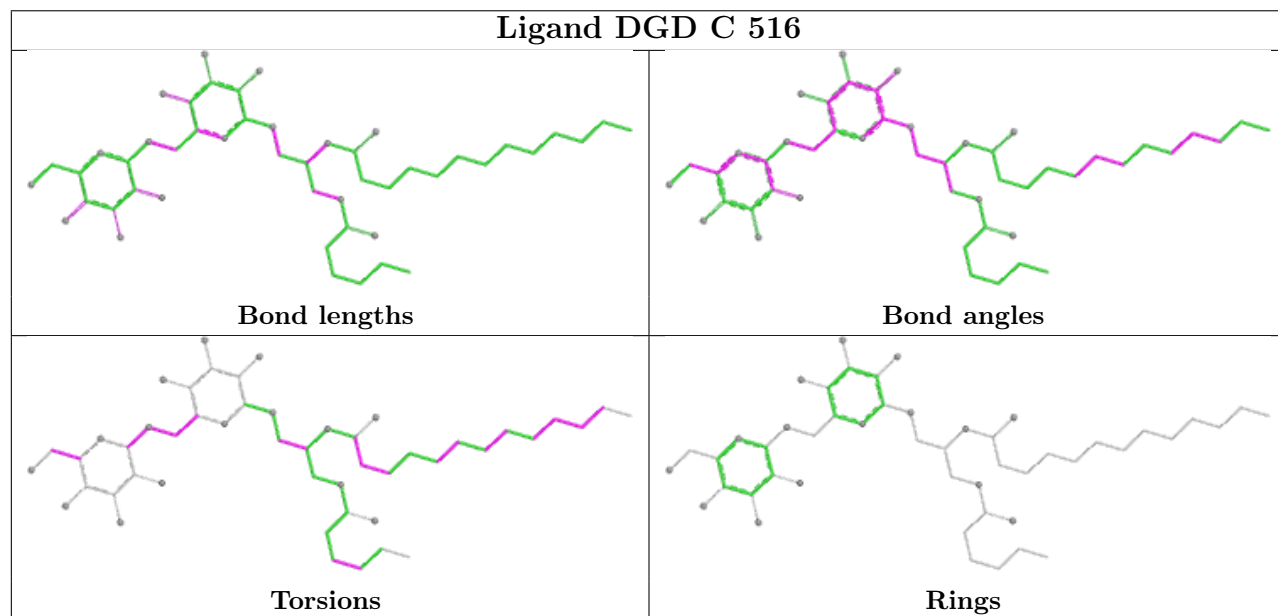
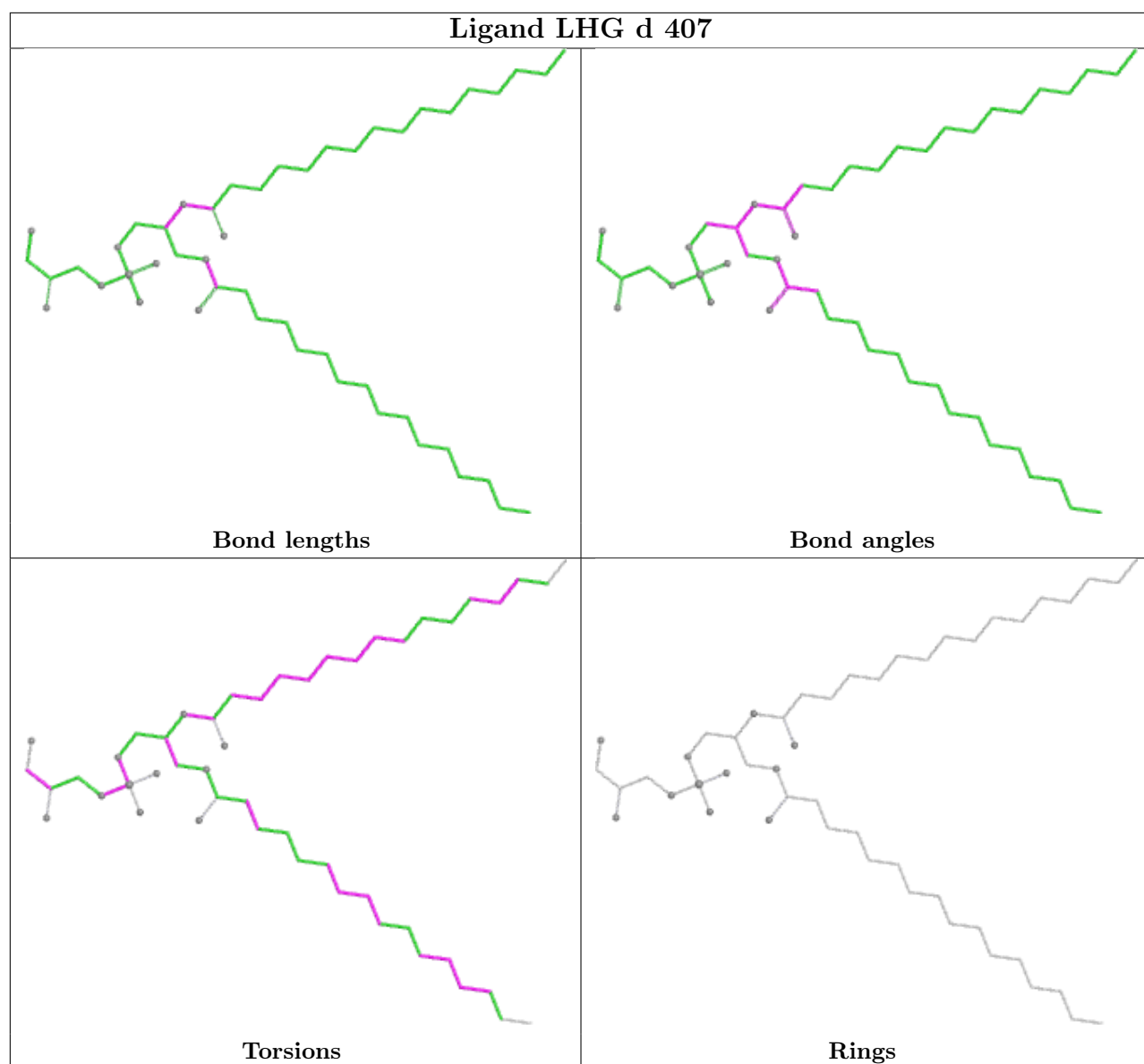


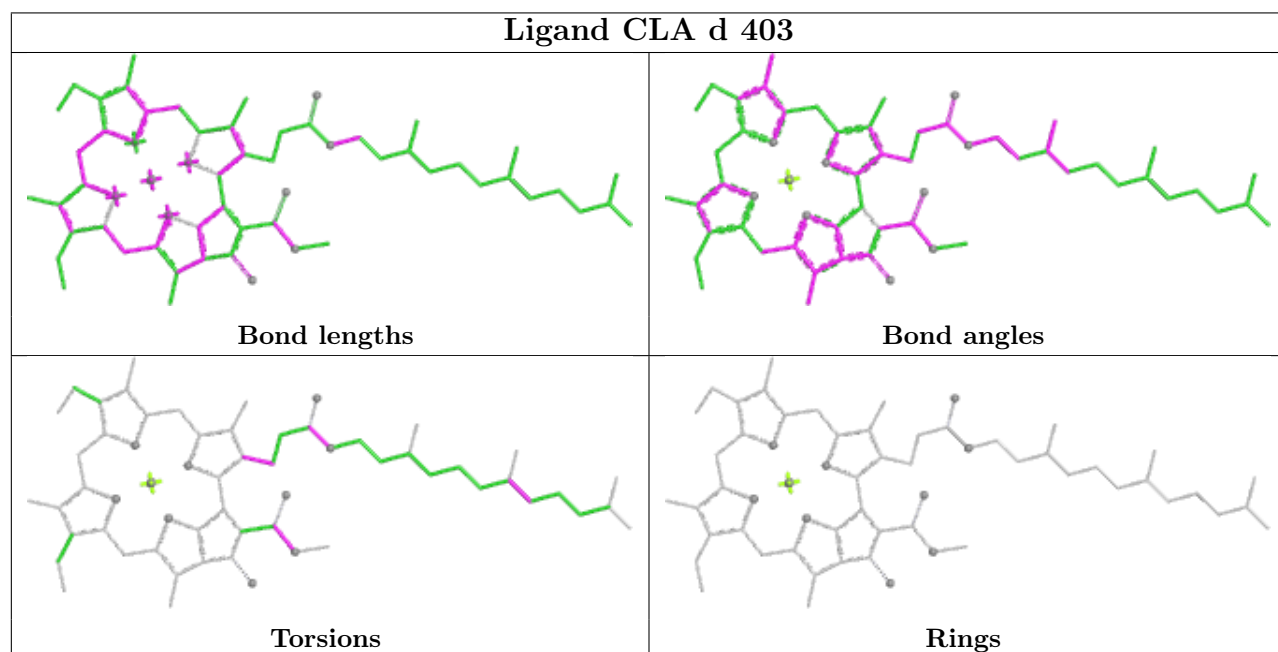
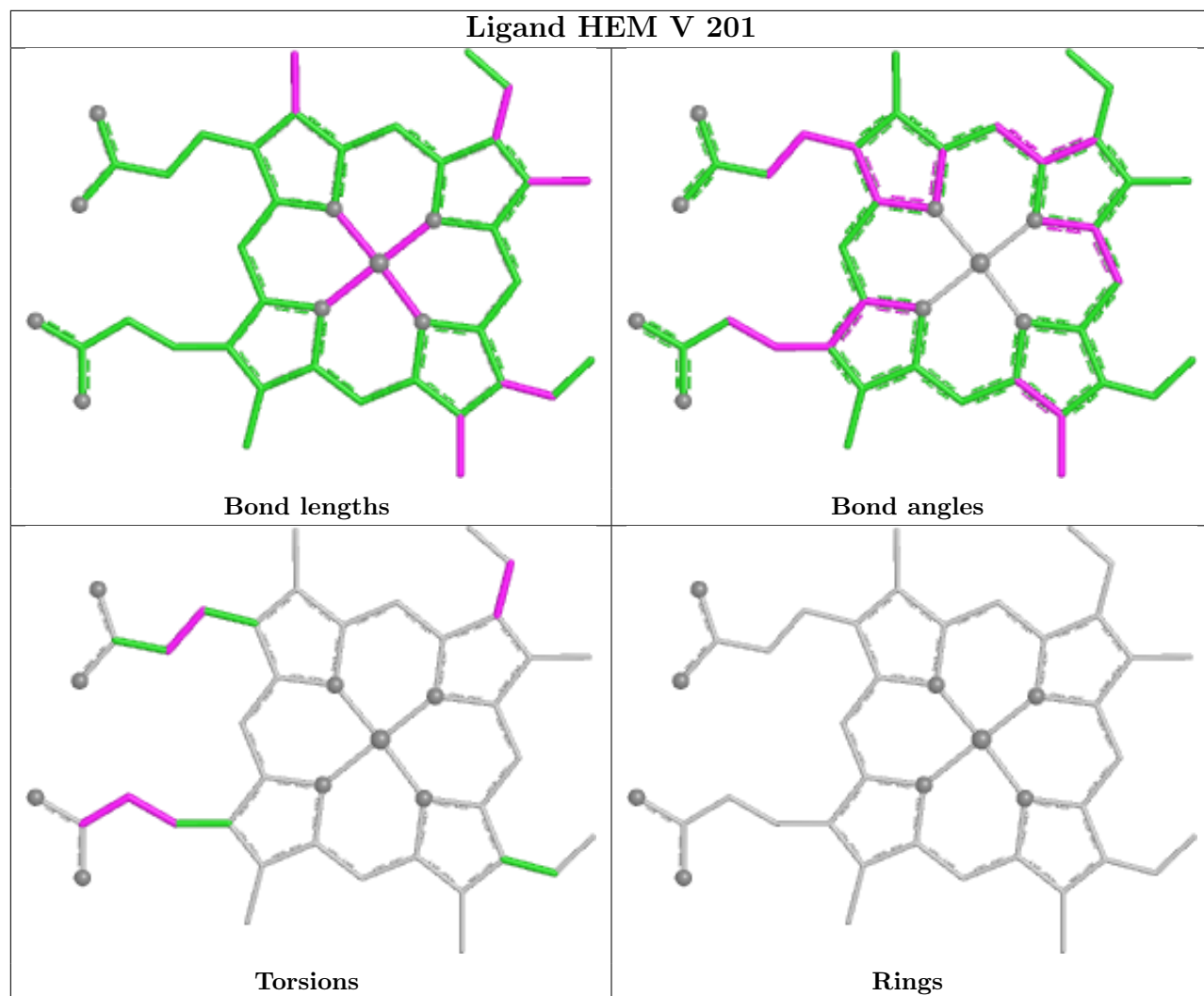
Ligand CLA C 506

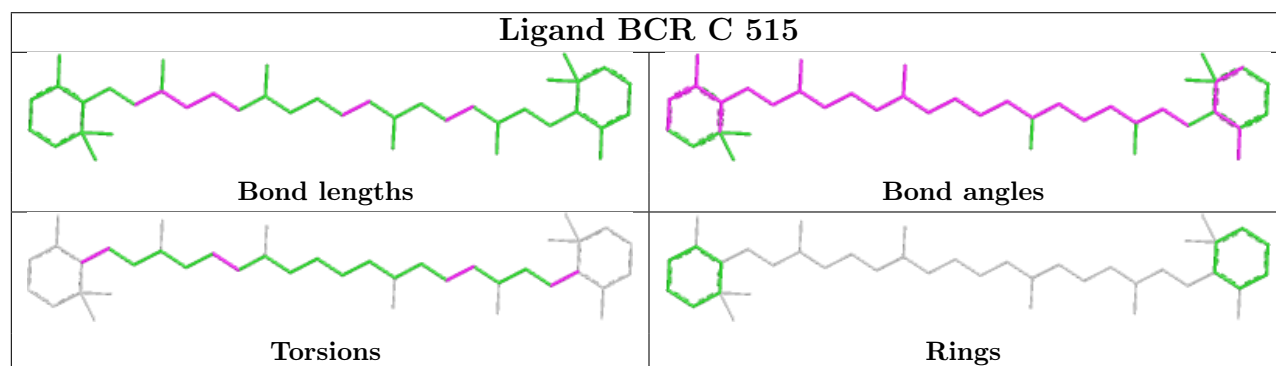
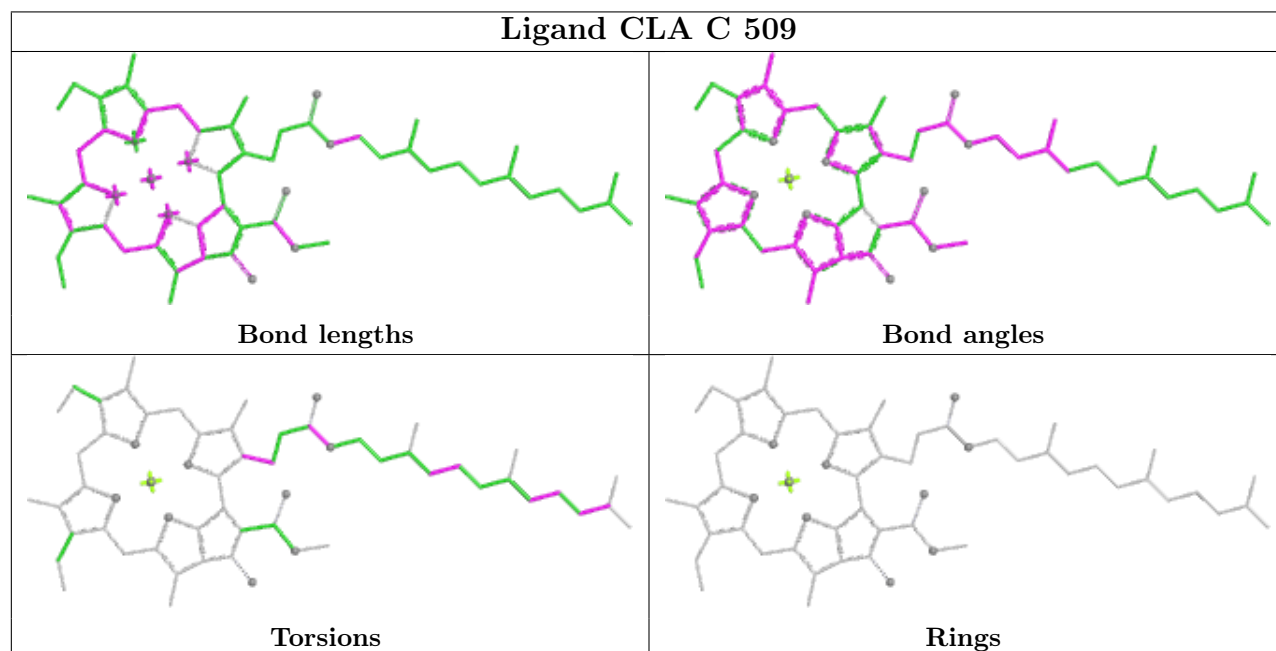
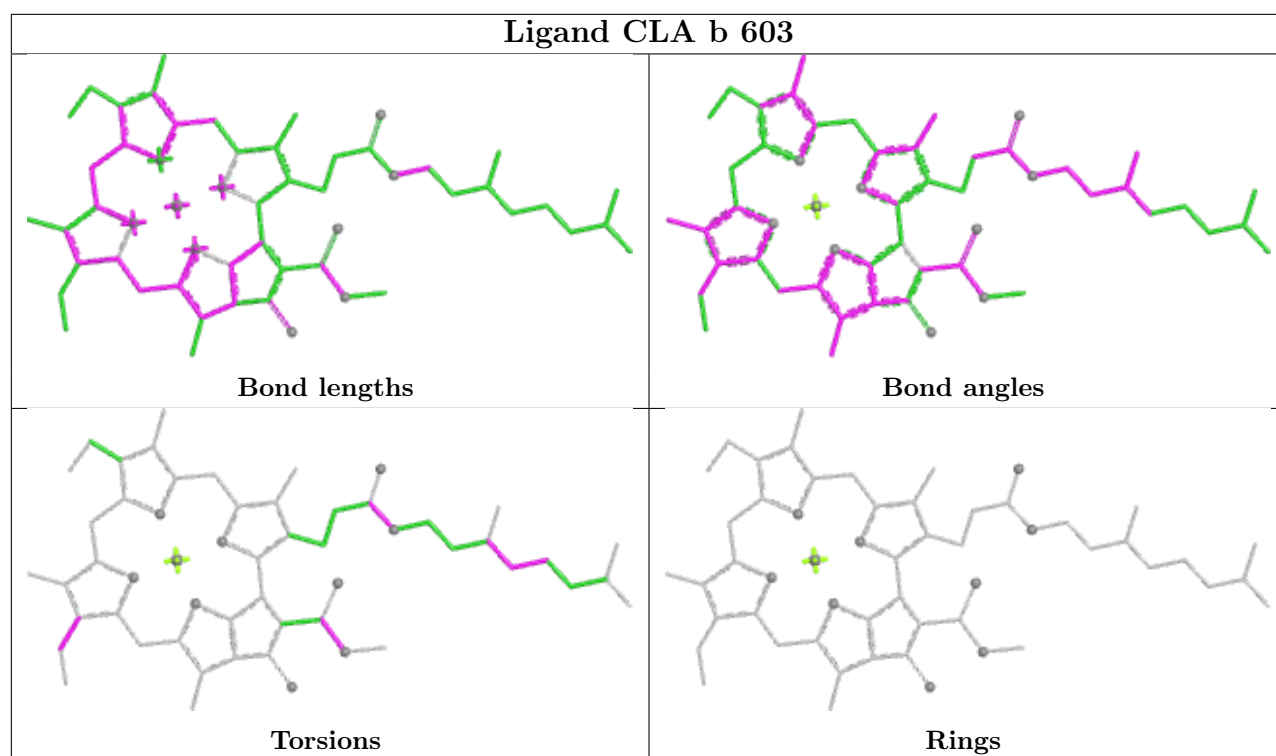


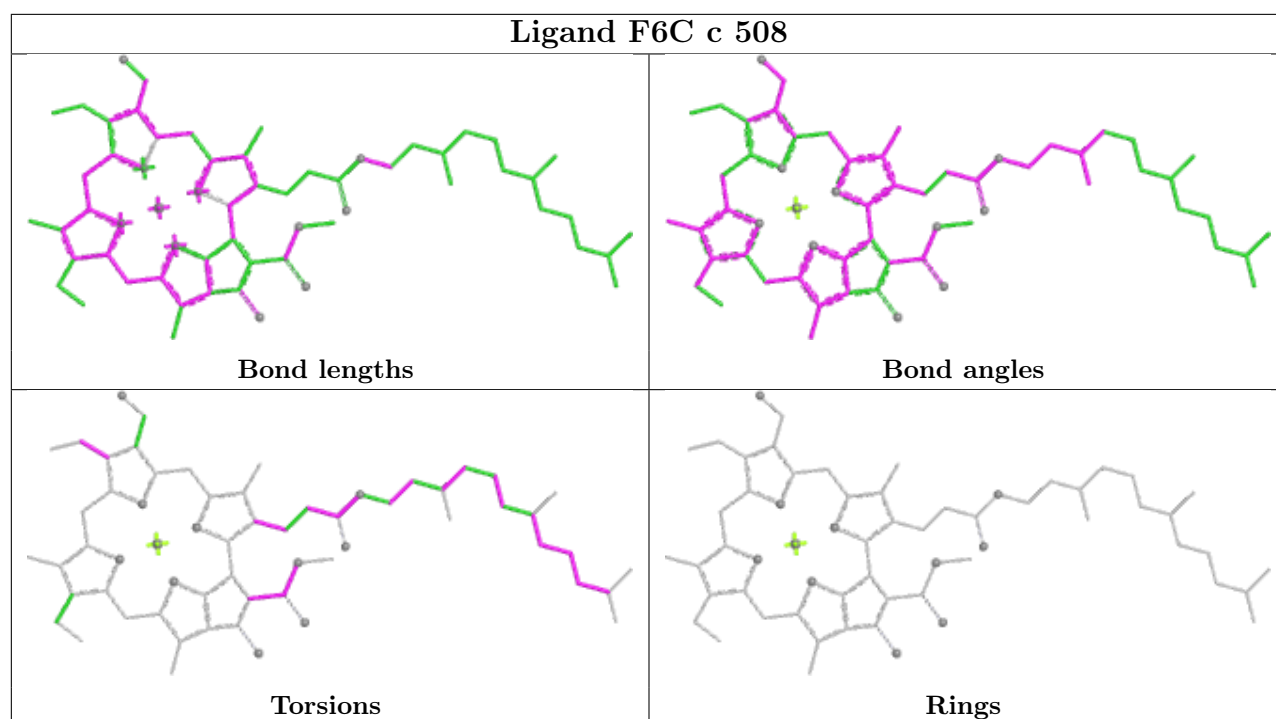
Ligand DGD c 517



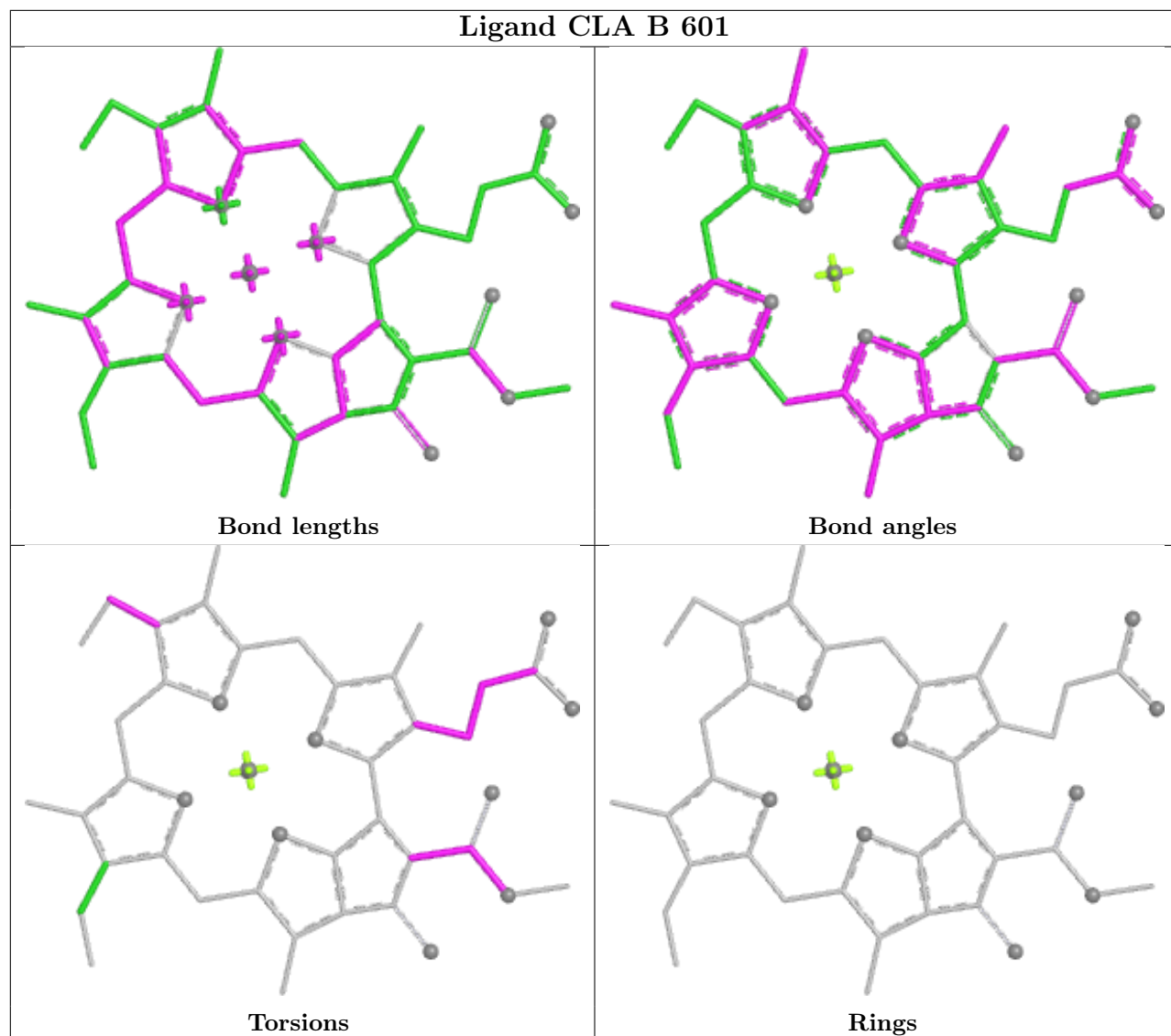


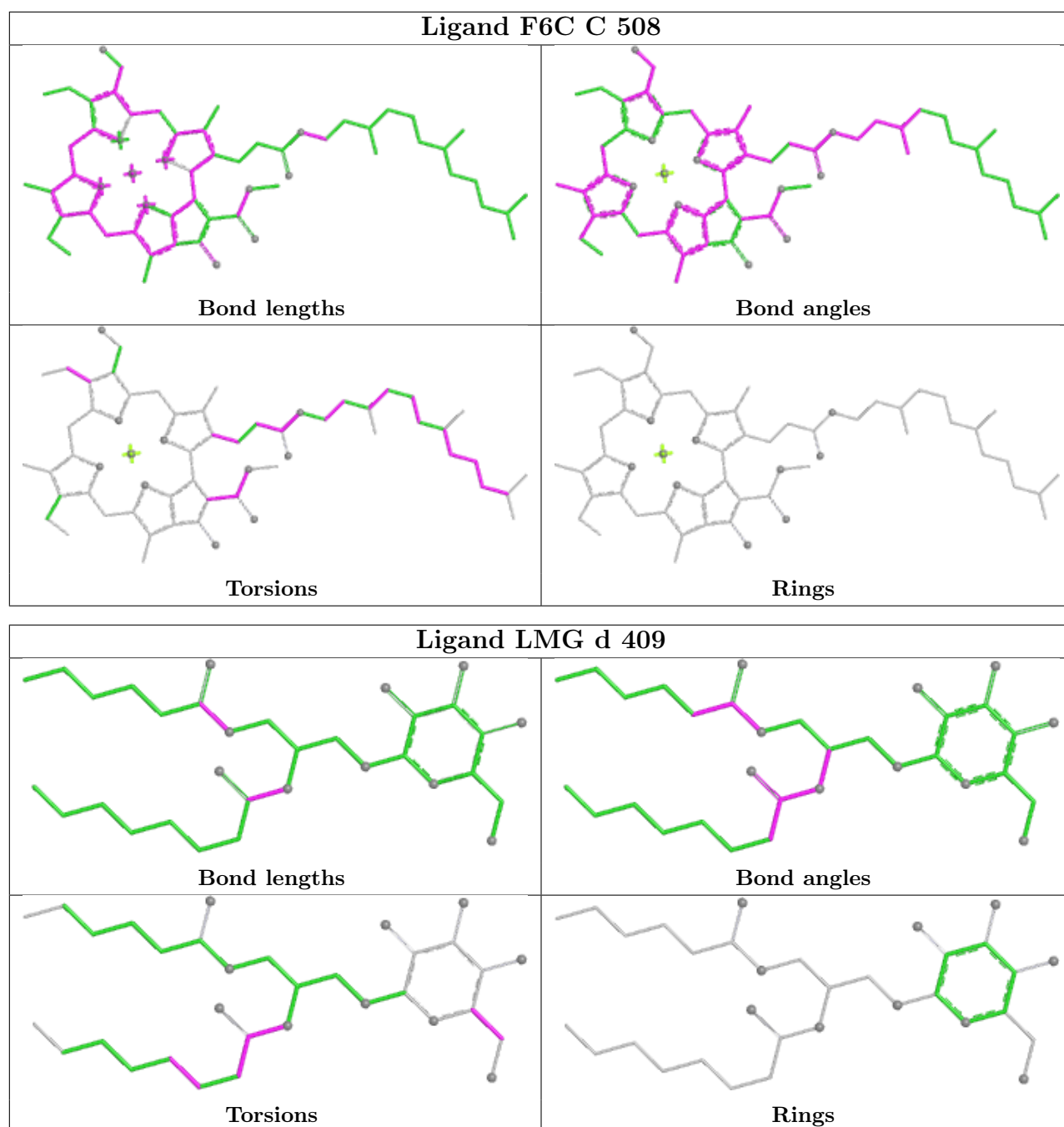


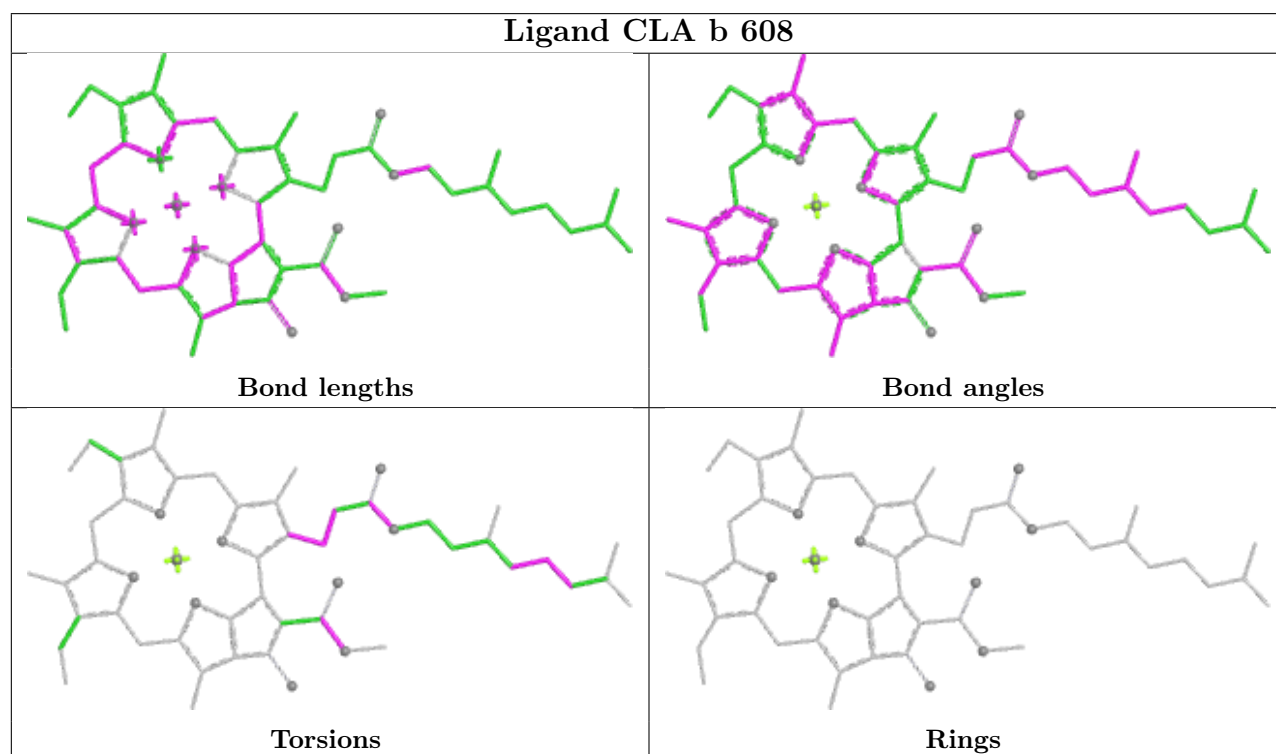
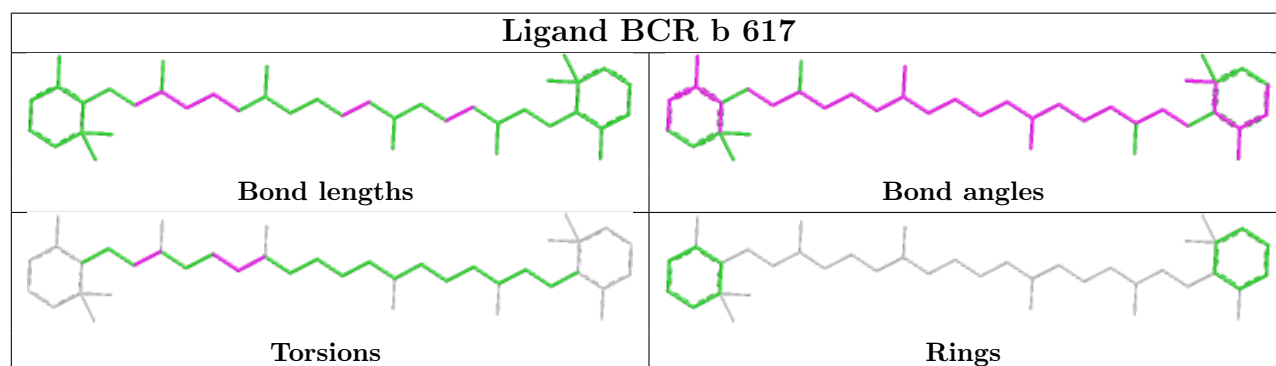
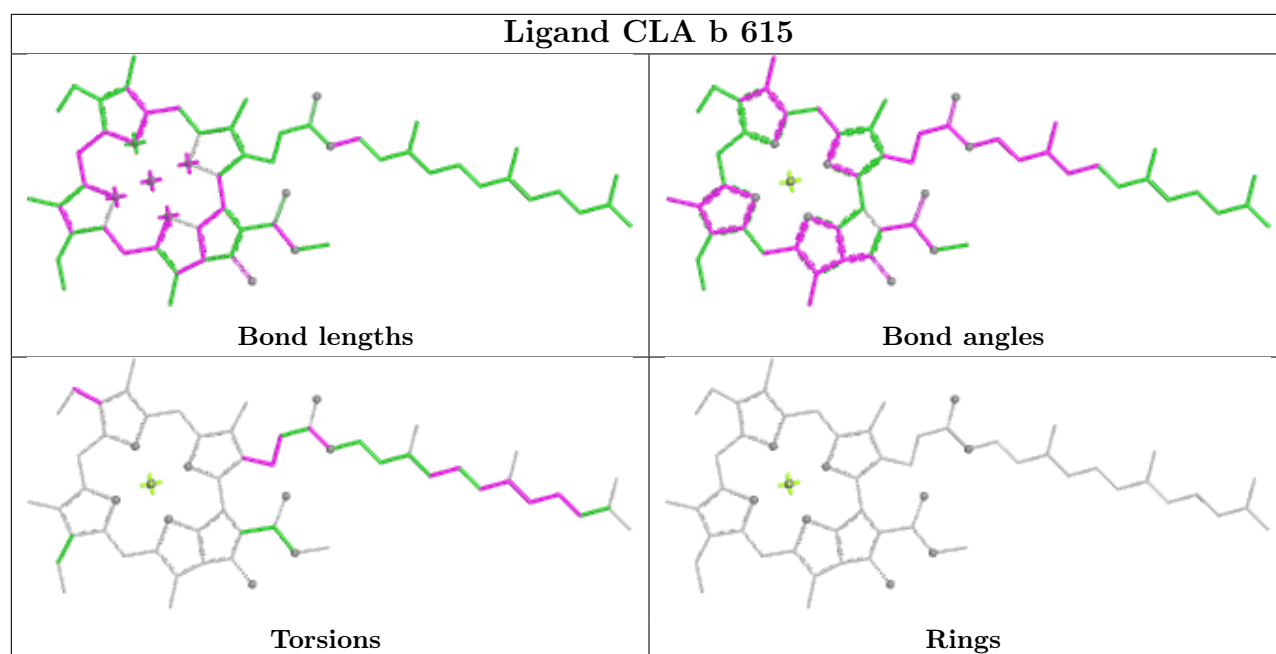


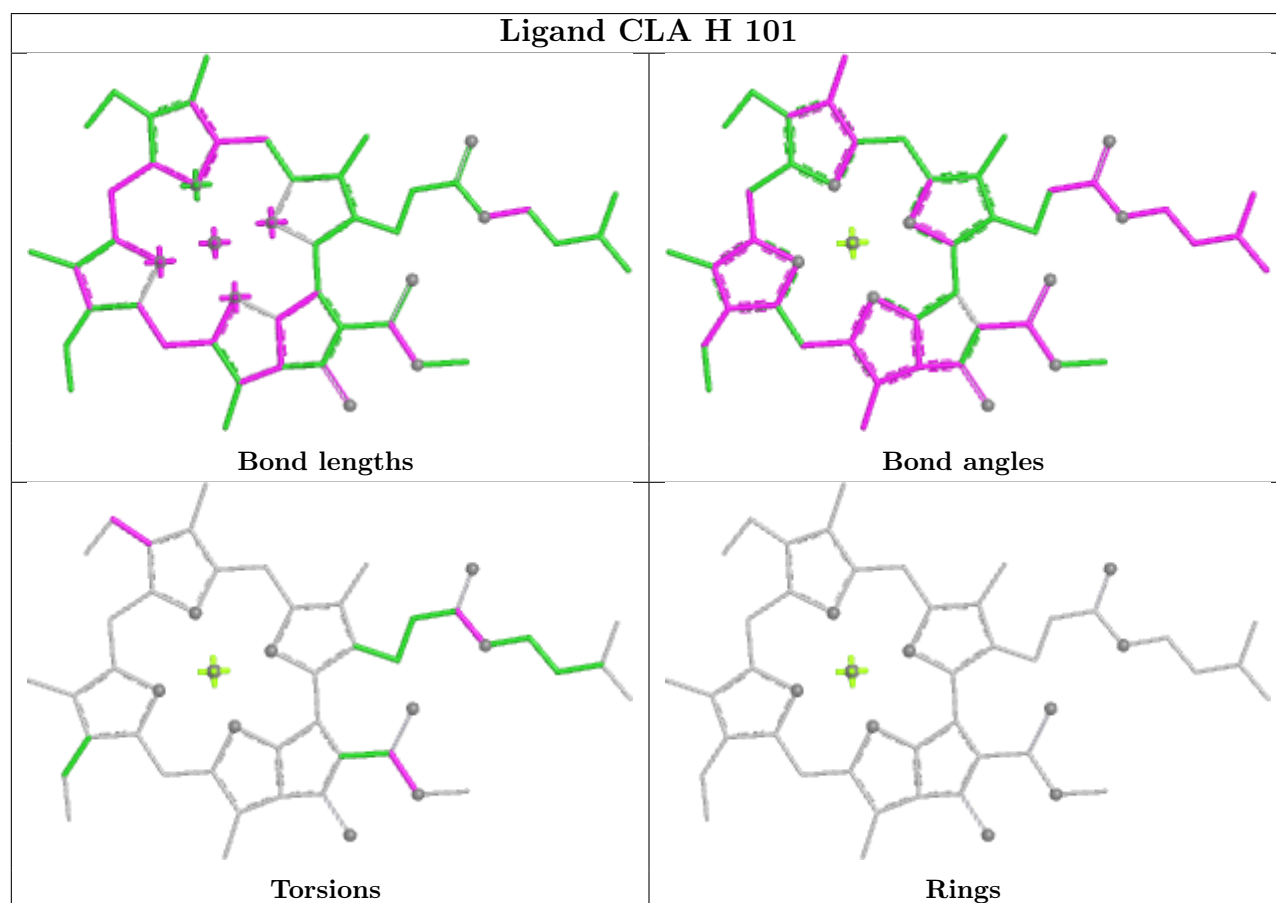
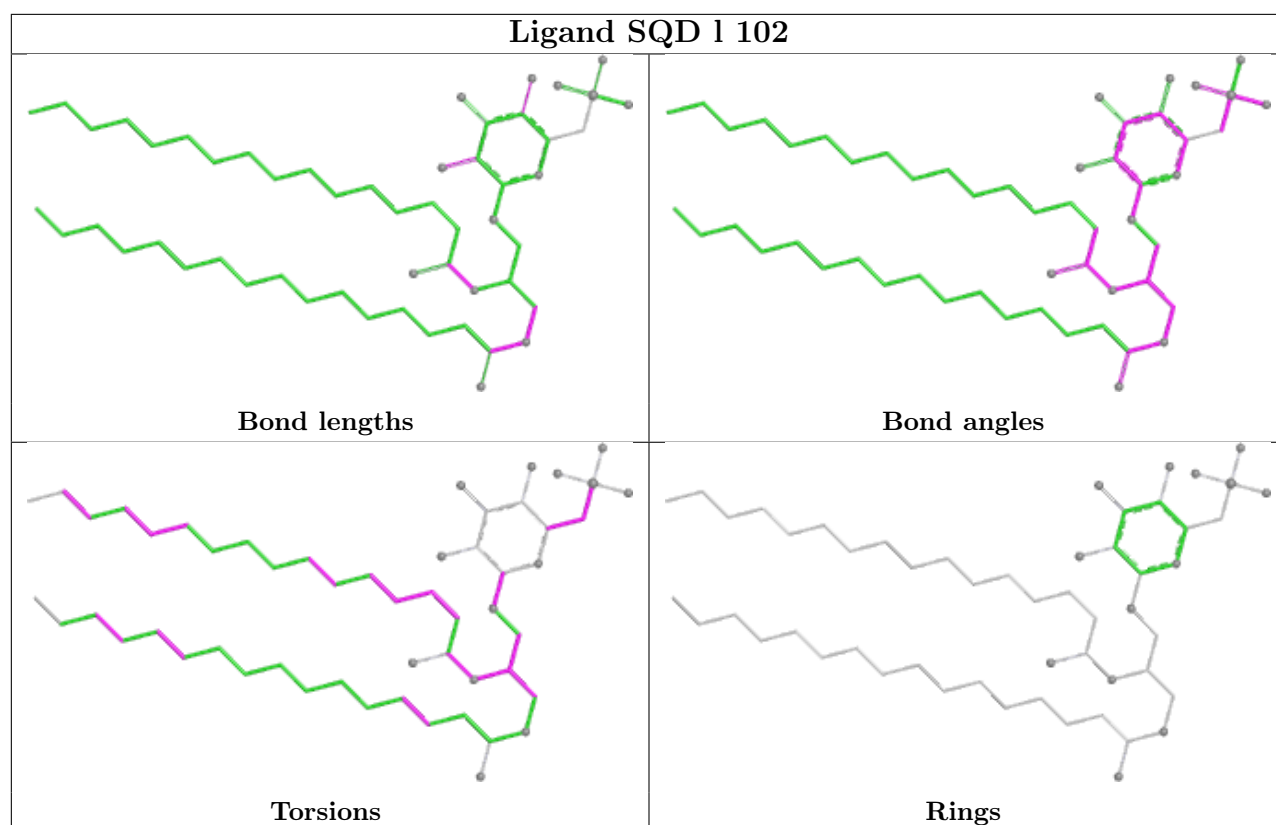


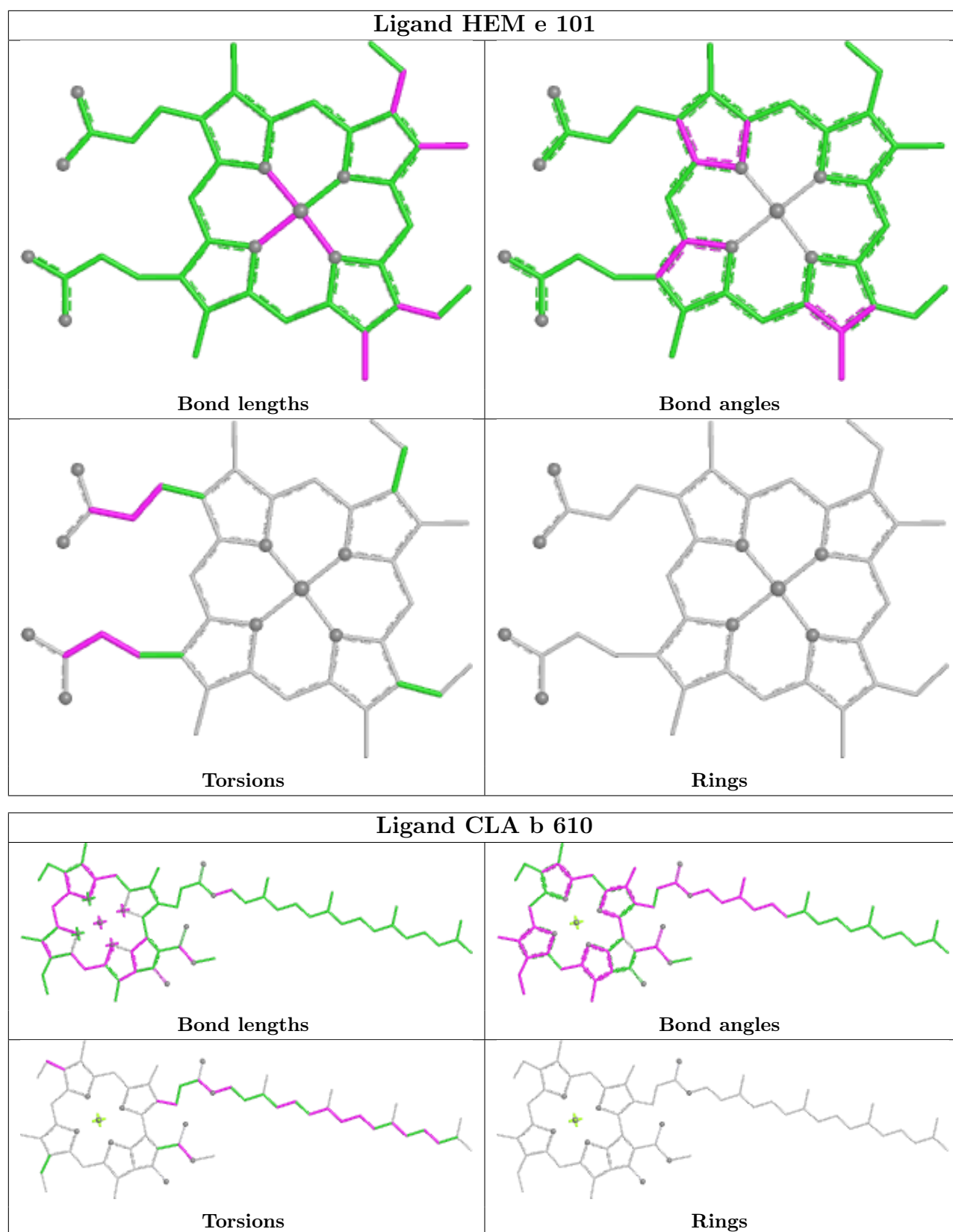
Ligand CLA B 601

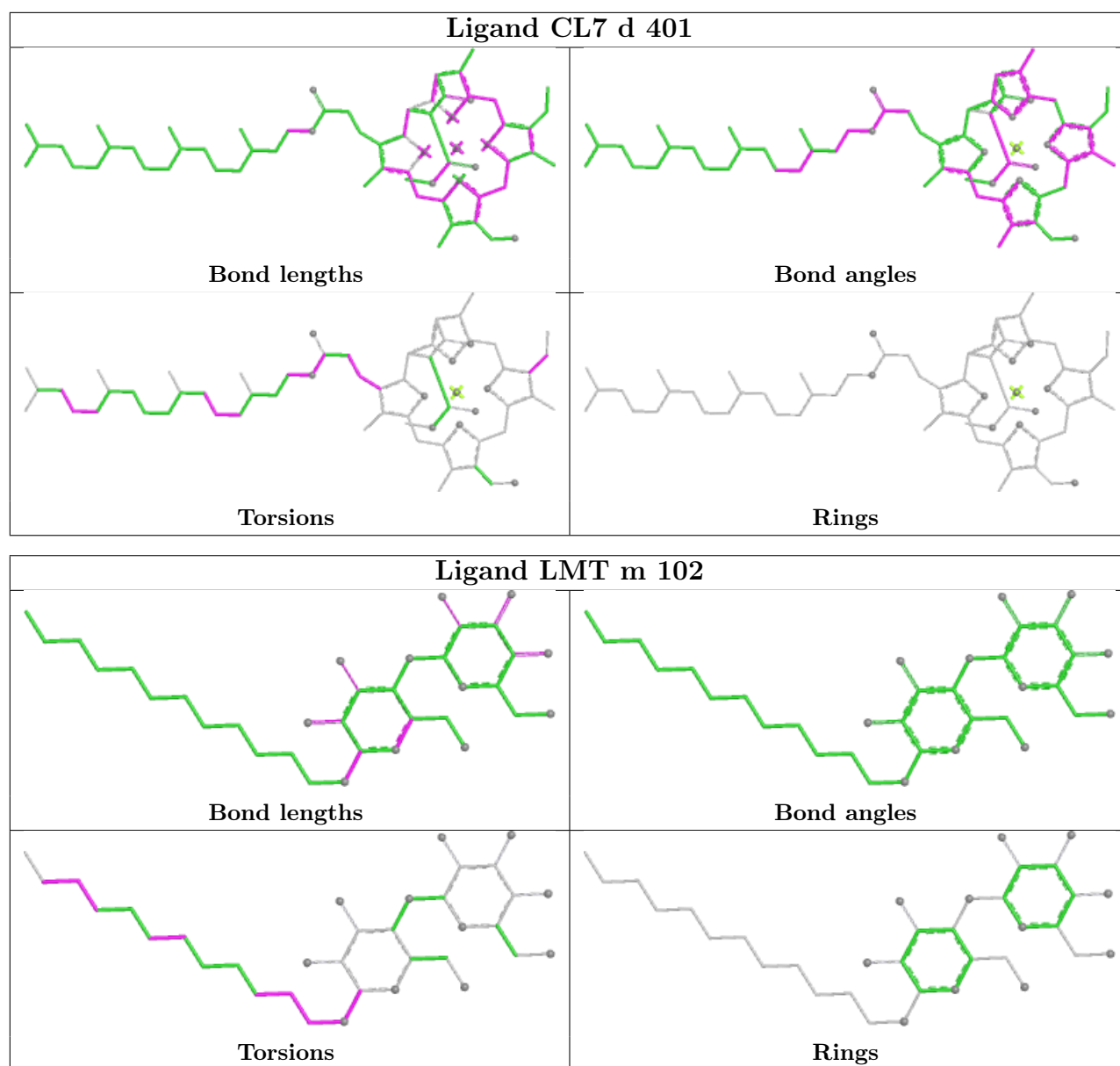


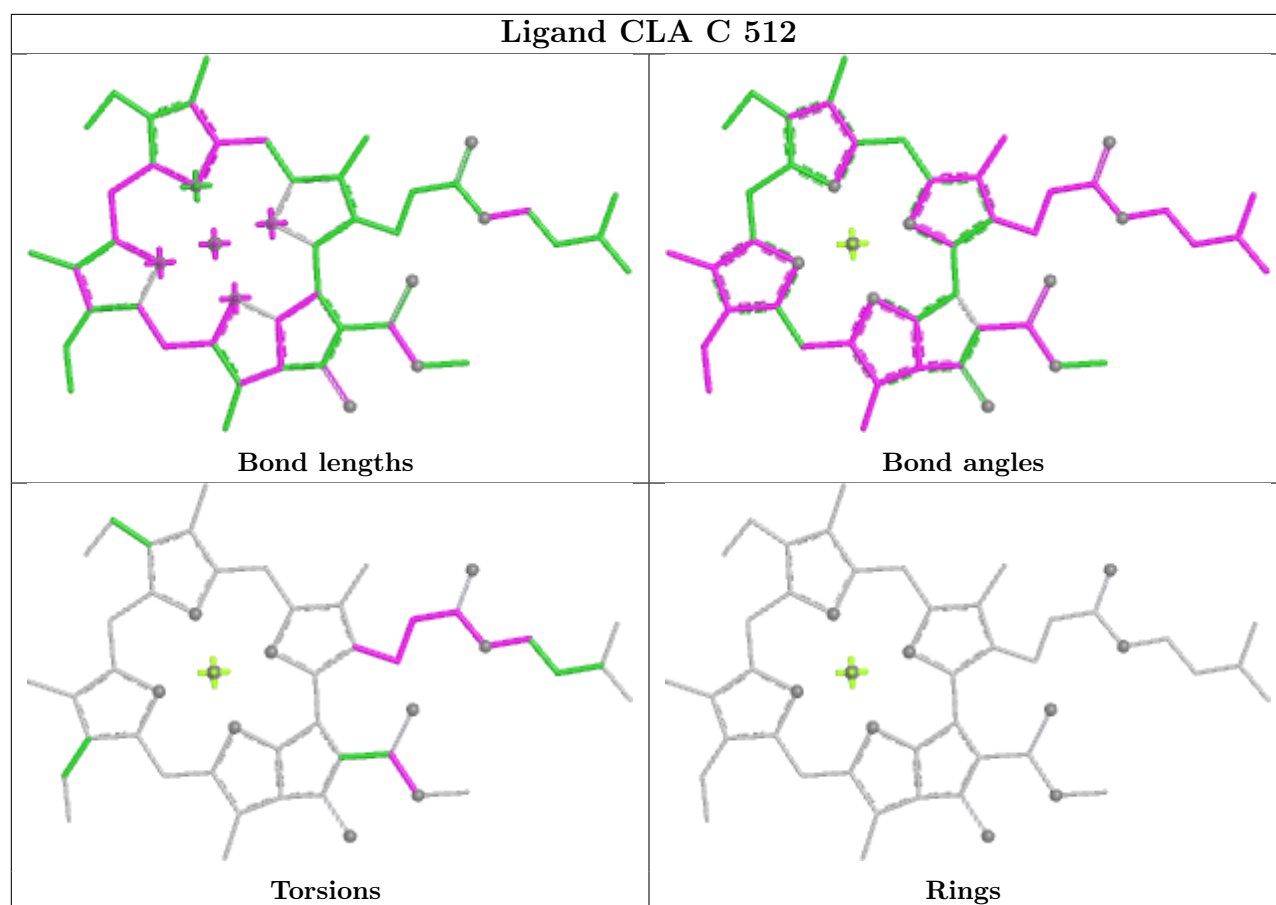




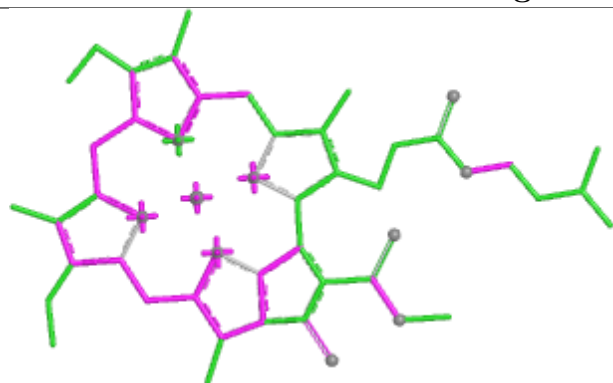




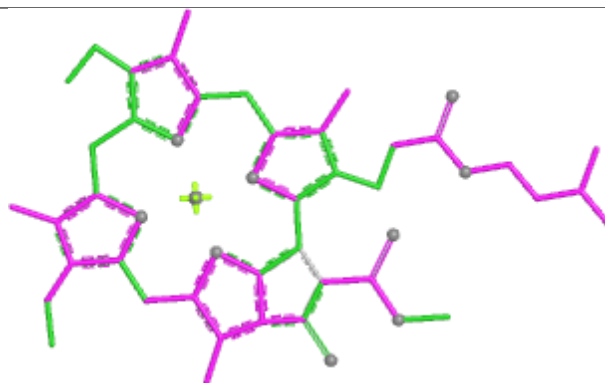




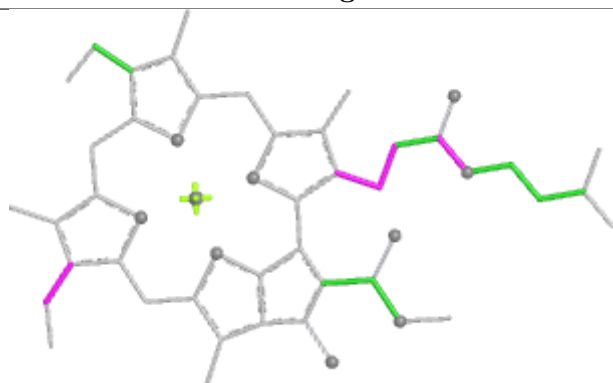
Ligand CLA A 407



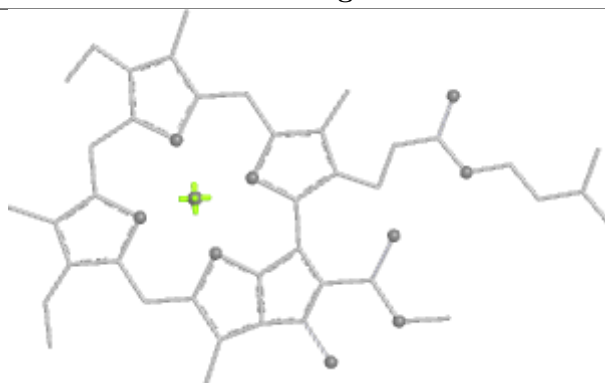
Bond lengths



Bond angles

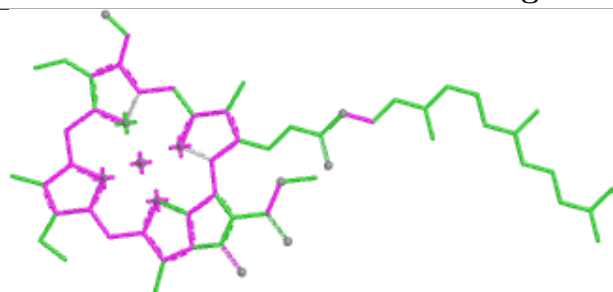


Torsions

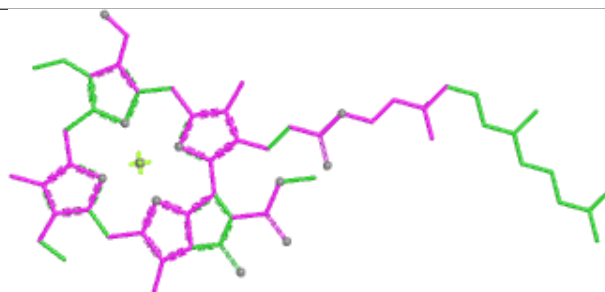


Rings

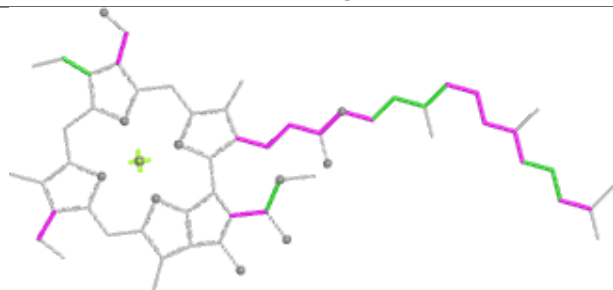
Ligand F6C b 607



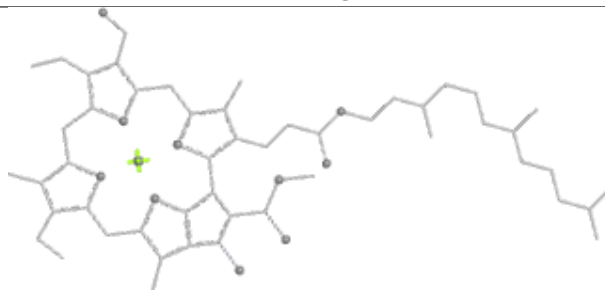
Bond lengths



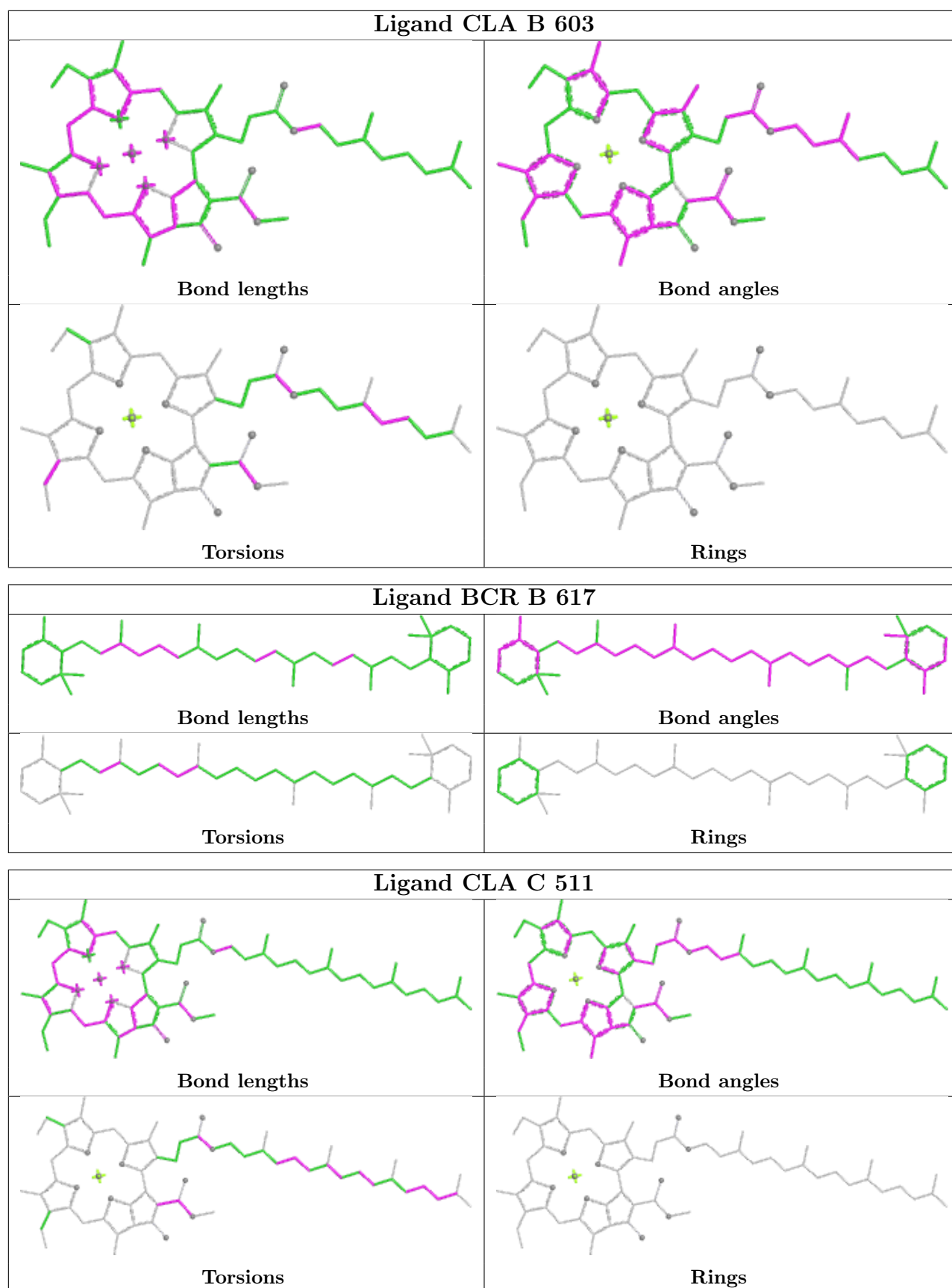
Bond angles



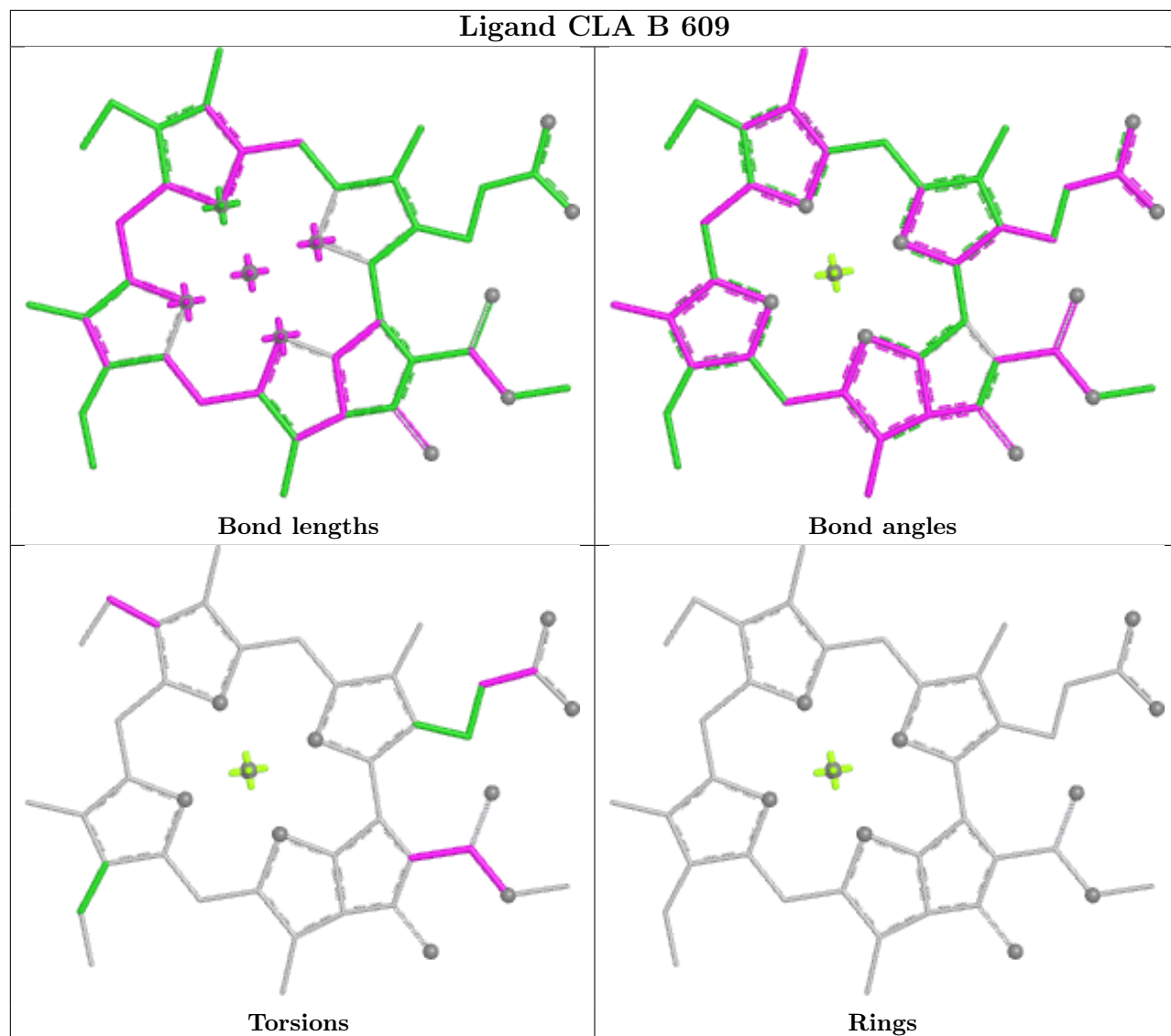
Torsions

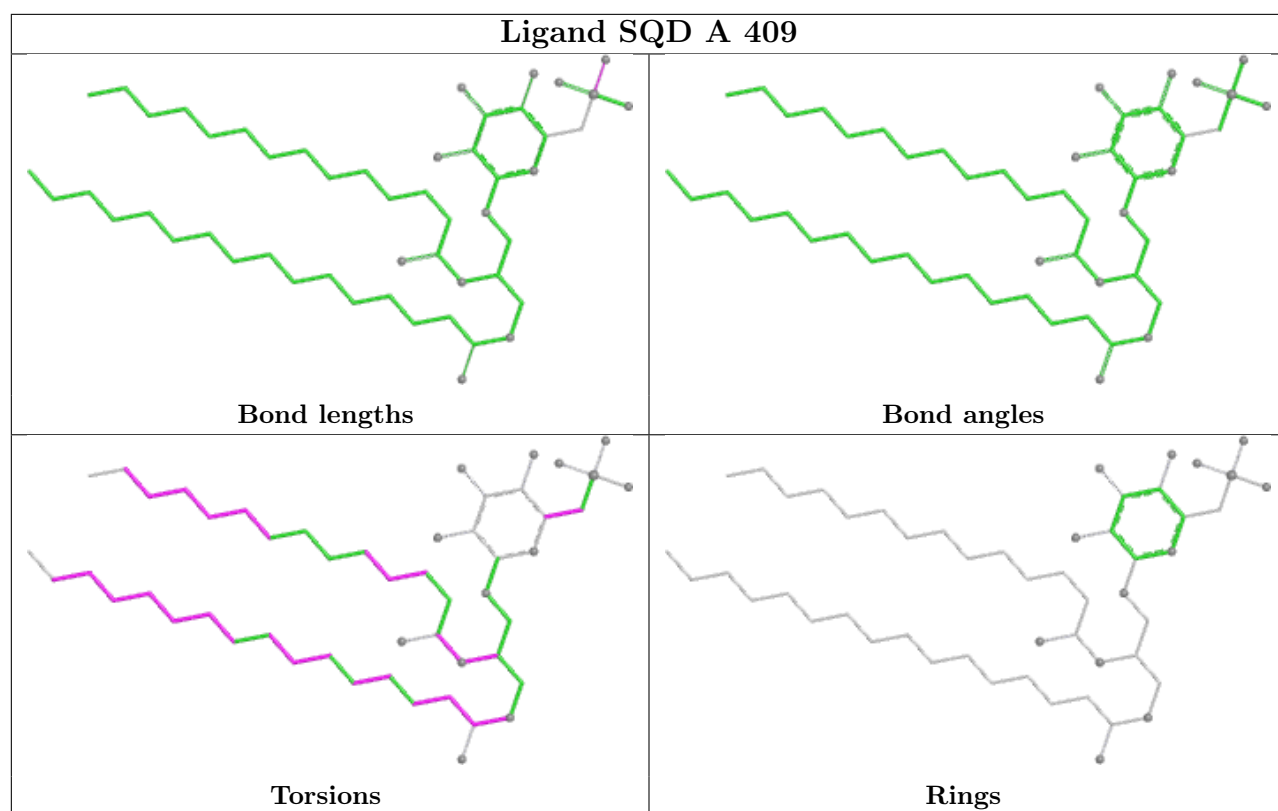


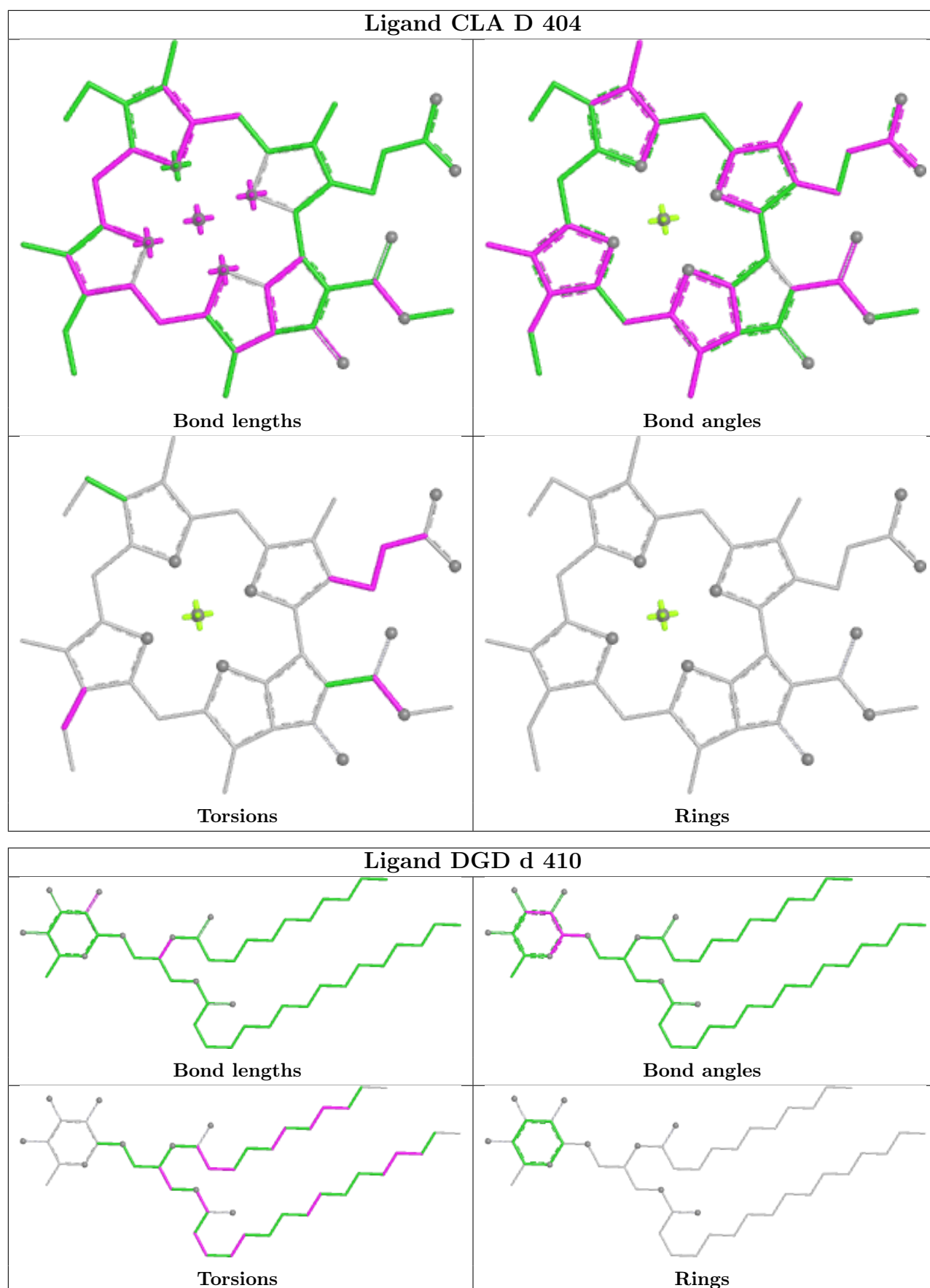
Rings



Ligand CLA B 609







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

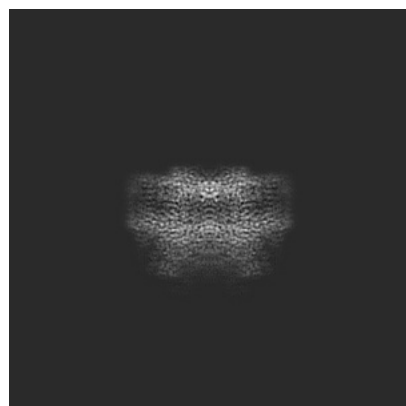
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28539. These allow visual inspection of the internal detail of the map and identification of artifacts.

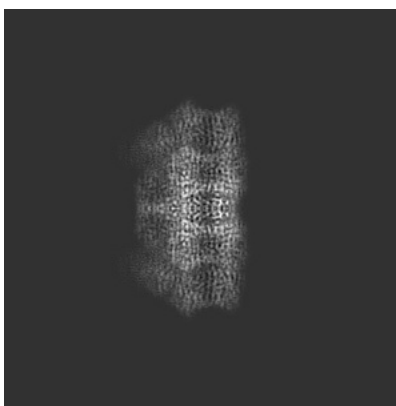
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

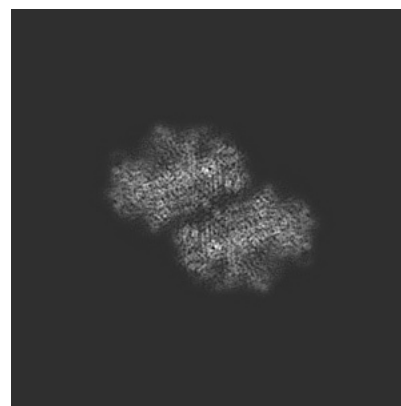
5.1.1 Primary map



X

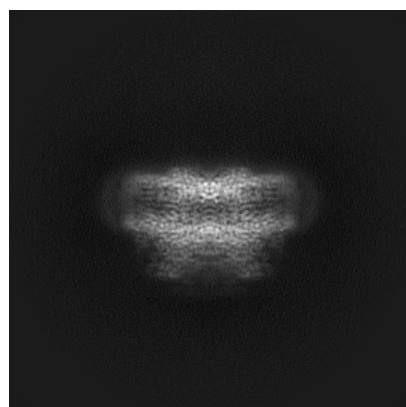


Y

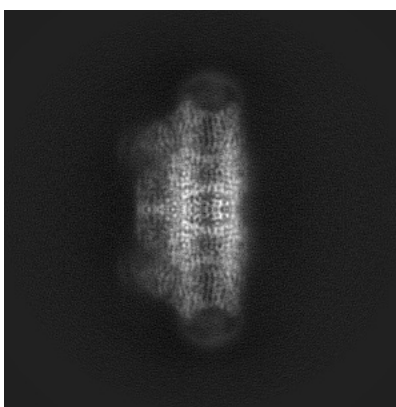


Z

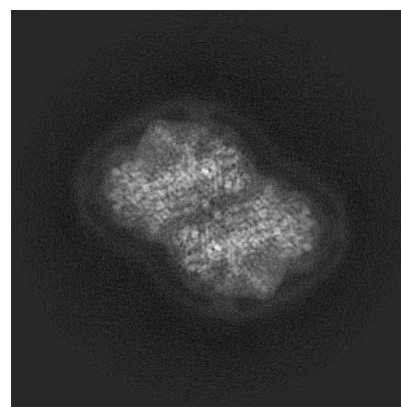
5.1.2 Raw map



X



Y



Z

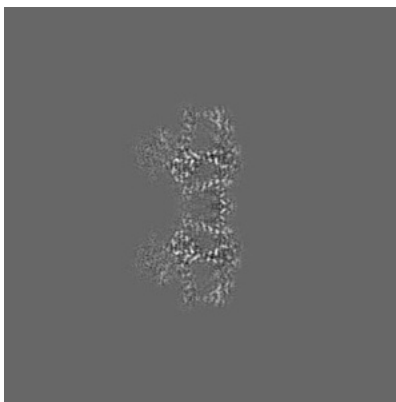
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

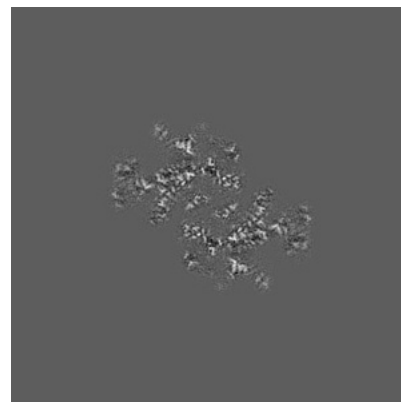
5.2.1 Primary map



X Index: 192

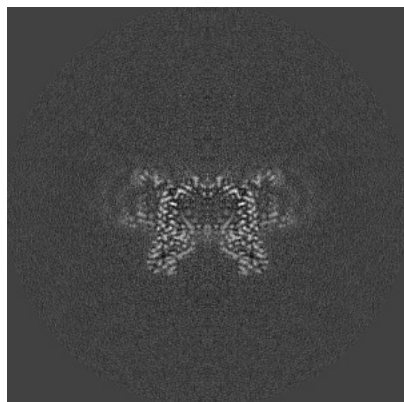


Y Index: 192

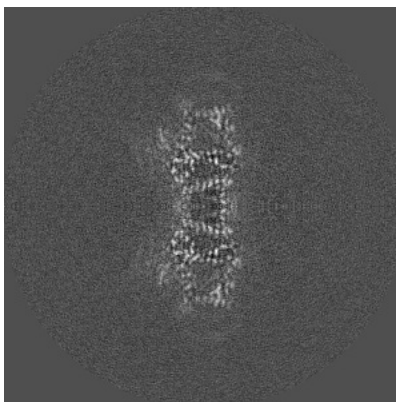


Z Index: 192

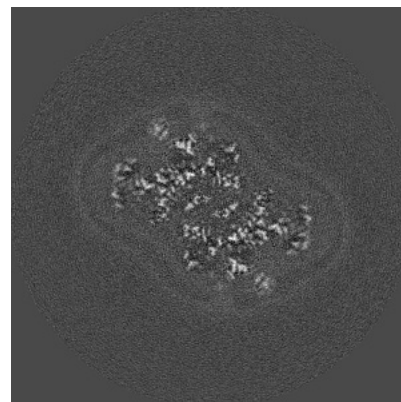
5.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

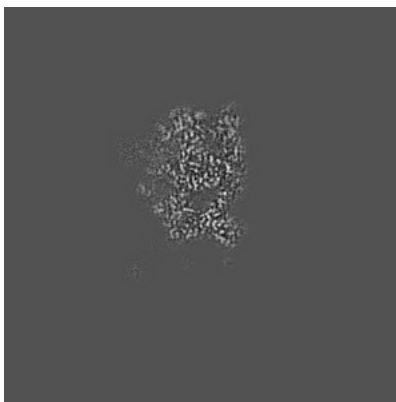
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

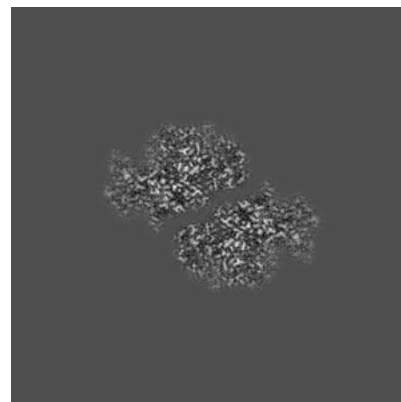
5.3.1 Primary map



X Index: 168

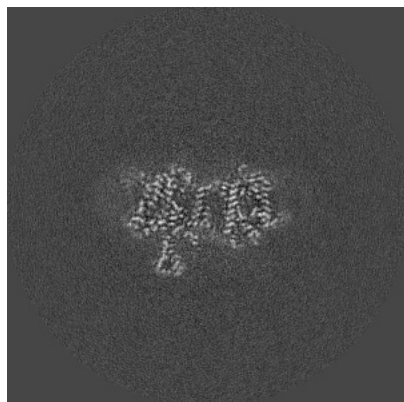


Y Index: 166

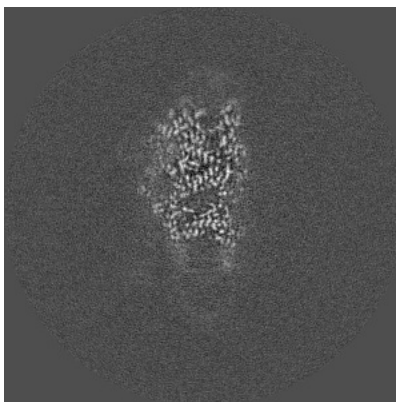


Z Index: 175

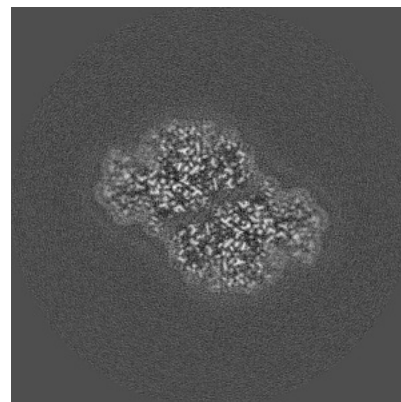
5.3.2 Raw map



X Index: 209



Y Index: 167

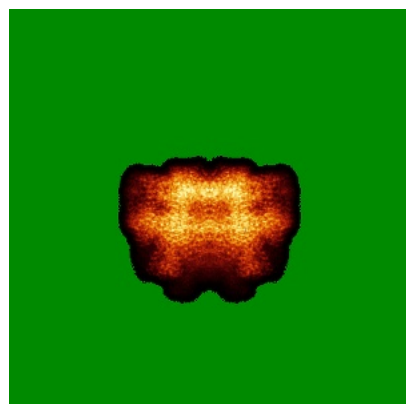


Z Index: 175

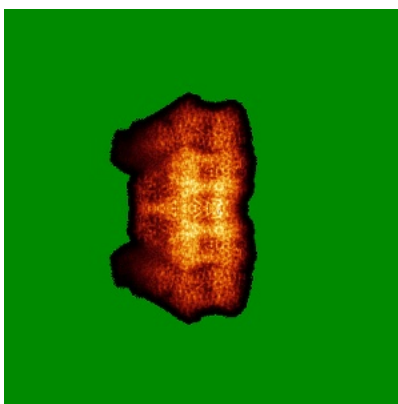
The images above show the largest variance slices of the map in three orthogonal directions.

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

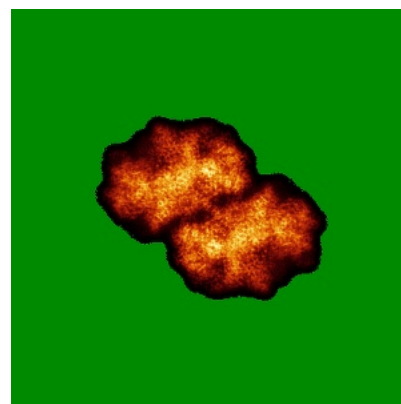
5.4.1 Primary map



X

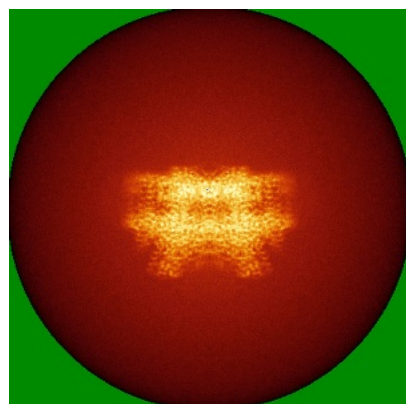


Y

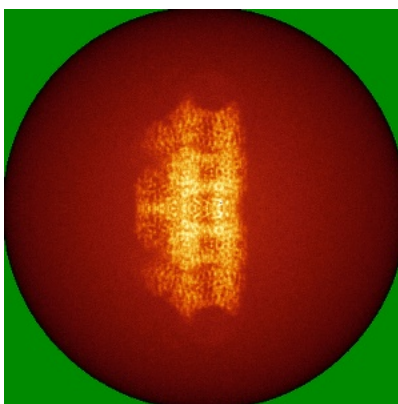


Z

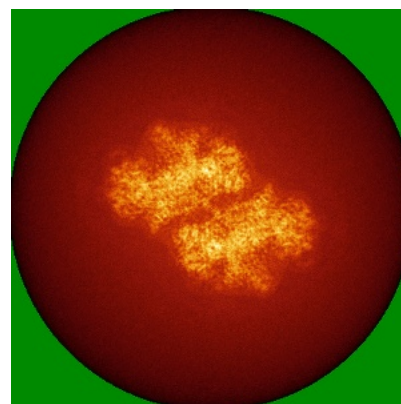
5.4.2 Raw map



X



Y

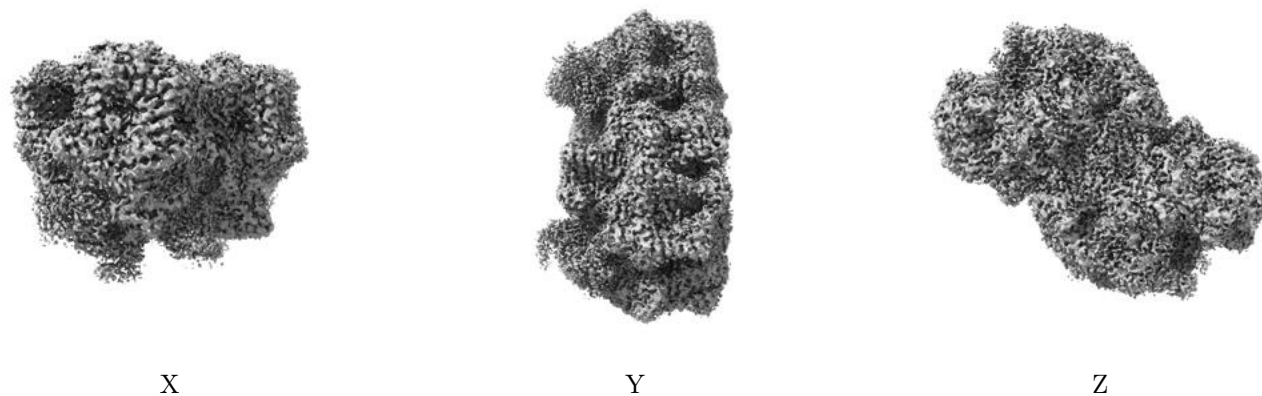


Z

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

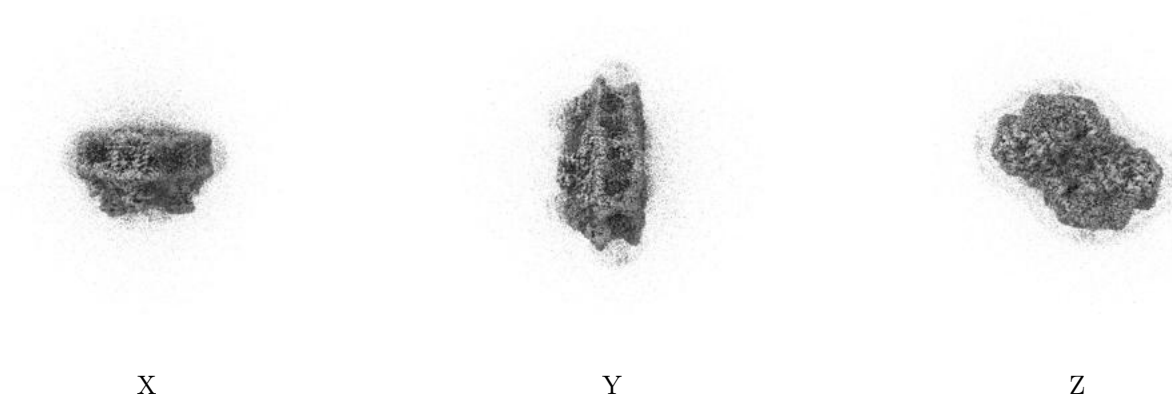
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



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

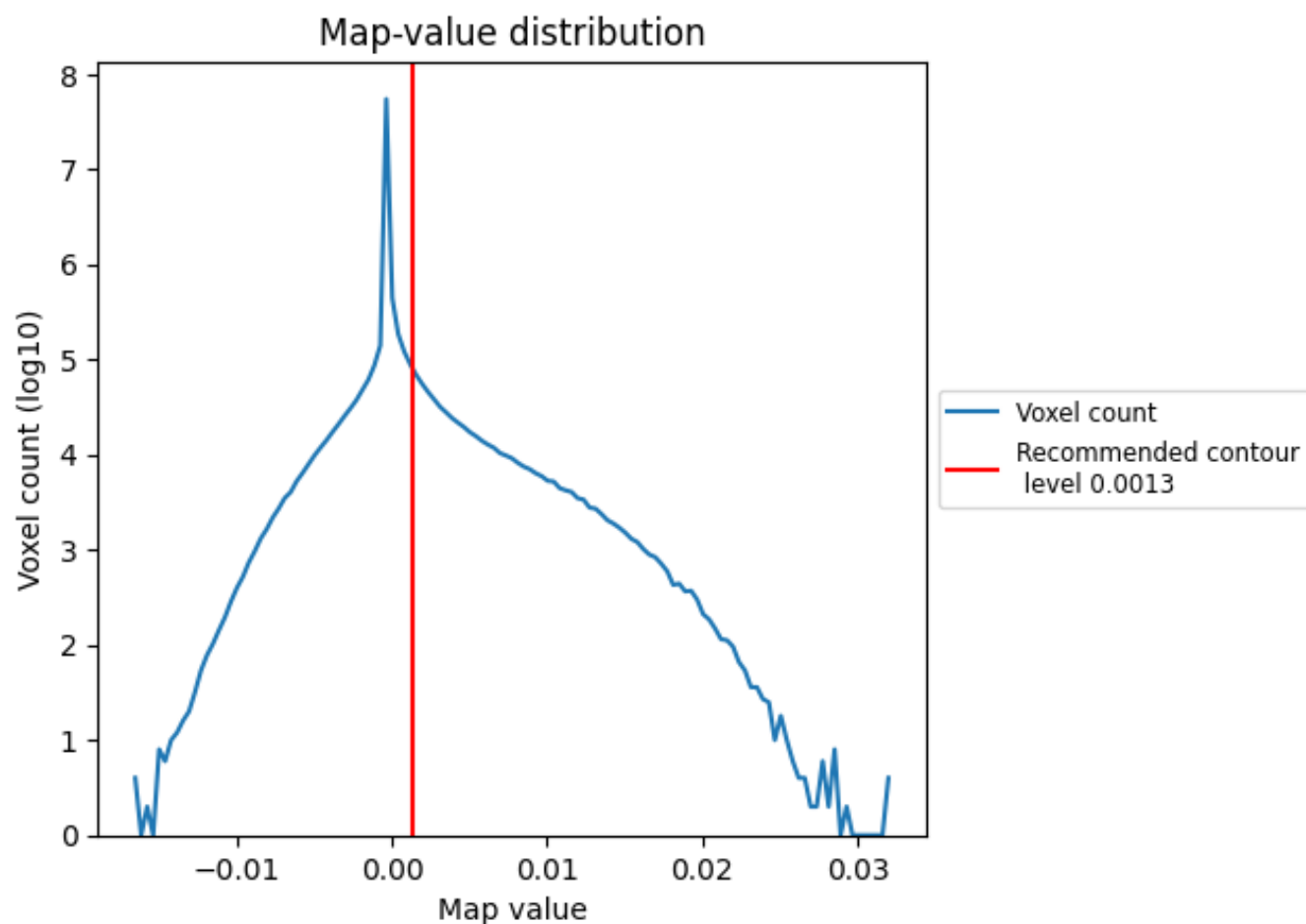
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

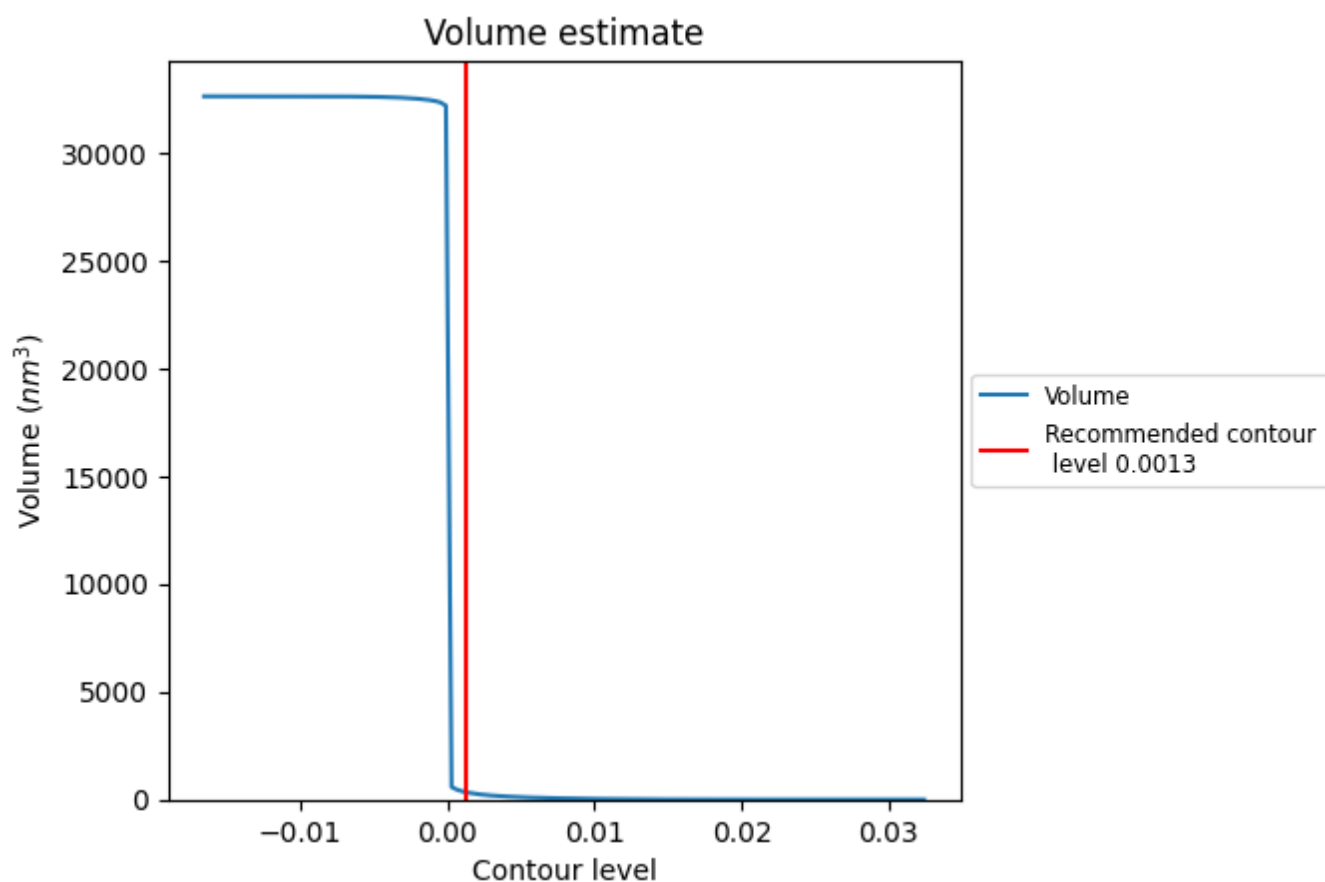
This section contains the results of statistical analysis of the map.

6.1 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.

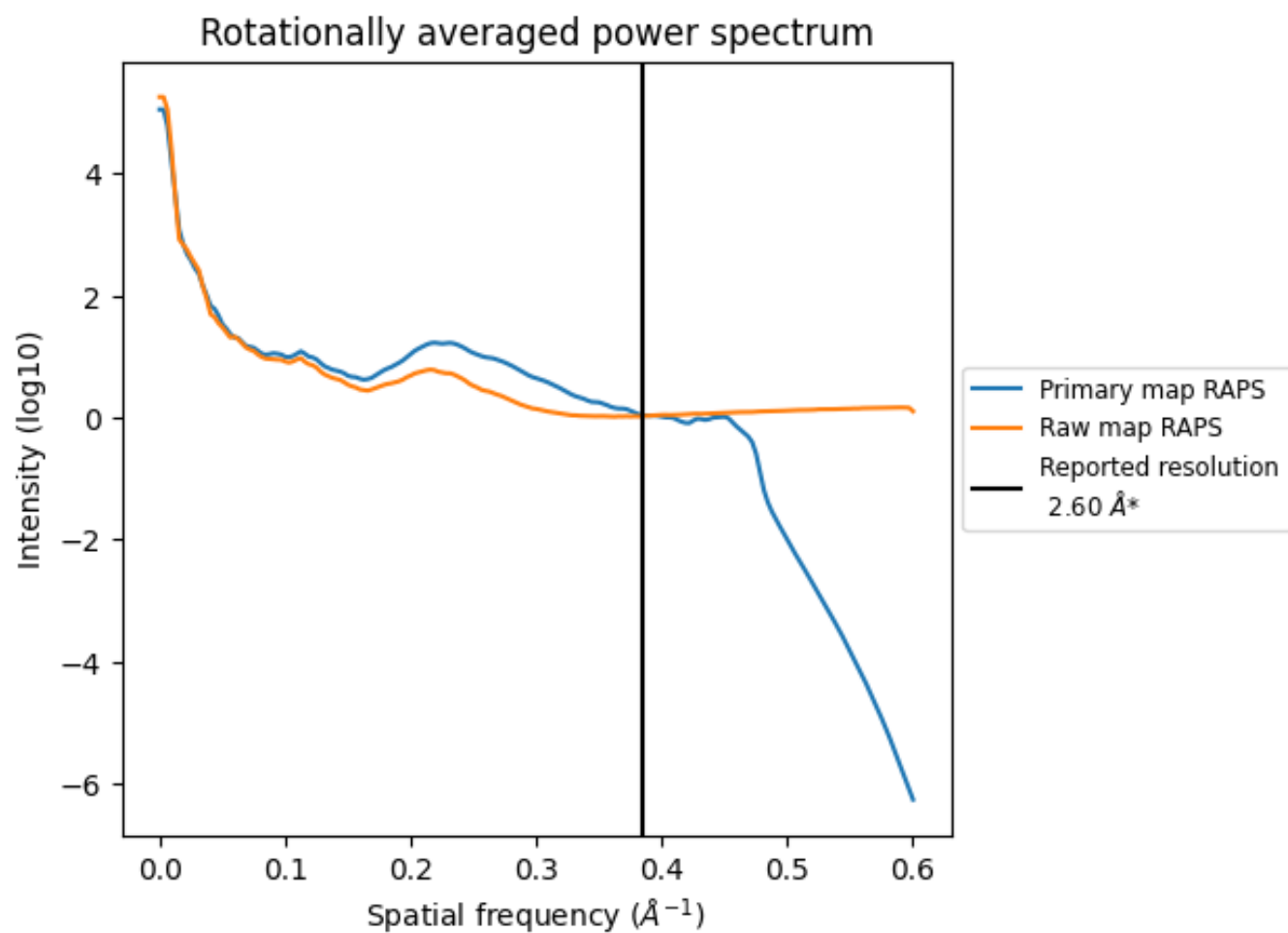
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 340 nm^3 ; this corresponds to an approximate mass of 308 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.

6.3 Rotationally averaged power spectrum ⓘ

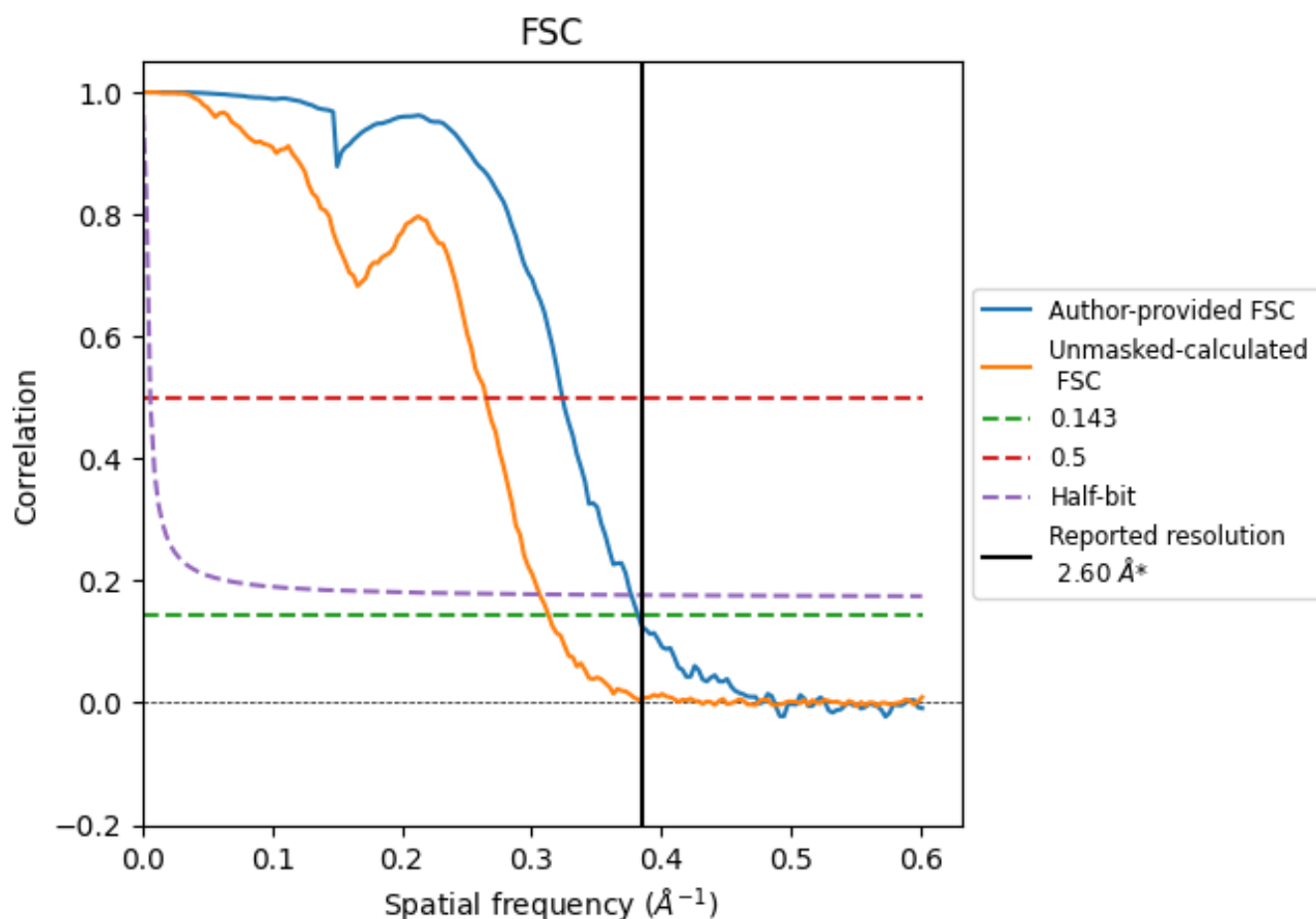


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

7 Fourier-Shell correlation [i](#)

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

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

7.2 Resolution estimates [i](#)

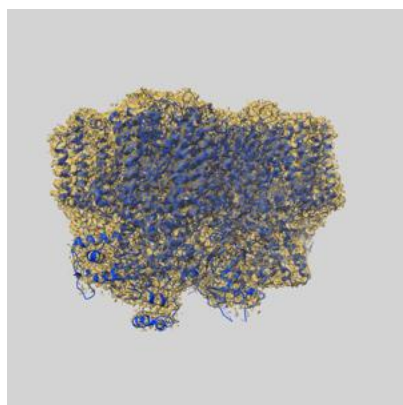
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	3.09	2.65
Unmasked-calculated*	3.19	3.78	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.6 by more than 10 %

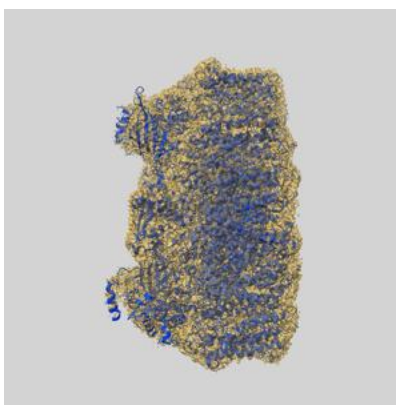
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28539 and PDB model 8EQM. Per-residue inclusion information can be found in section ?? on page ??.

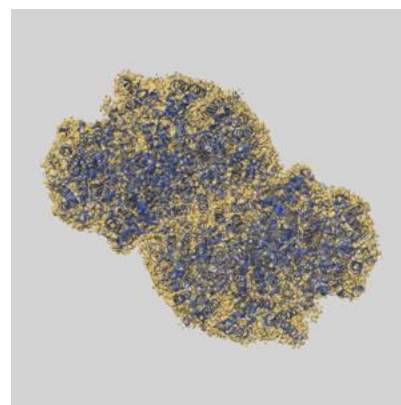
8.1 Map-model overlay [i](#)



X



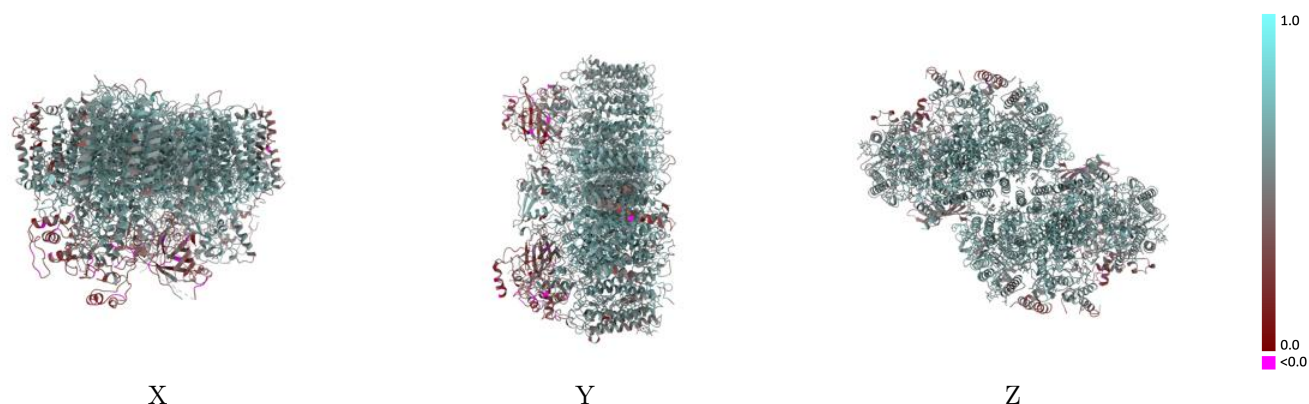
Y



Z

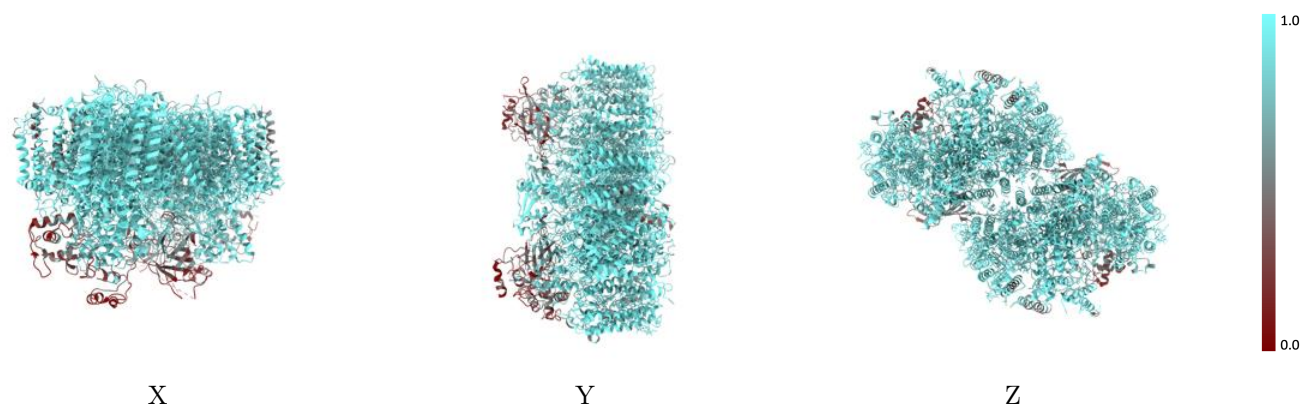
The images above show the 3D surface view of the map at the recommended contour level 0.0013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



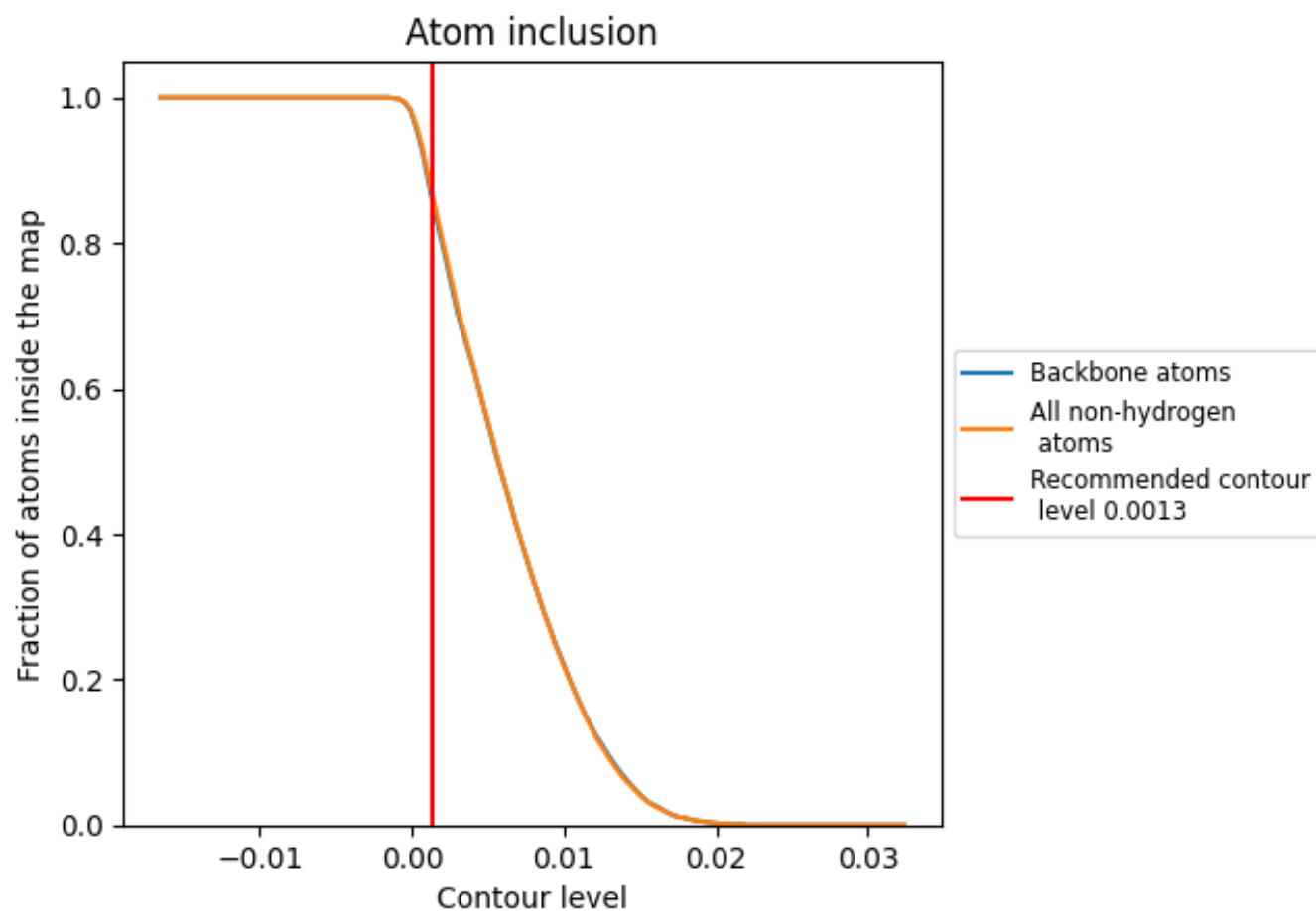
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.0013).

8.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8720	 0.5530
A	 0.9650	 0.6260
B	 0.9450	 0.6120
C	 0.9310	 0.5520
D	 0.9650	 0.6280
E	 0.9000	 0.4990
F	 0.8840	 0.4900
H	 0.8870	 0.5460
I	 0.9420	 0.5700
K	 0.8250	 0.4550
L	 0.9480	 0.6220
M	 0.9340	 0.5750
O	 0.4790	 0.3290
T	 0.9230	 0.5840
U	 0.3330	 0.2590
V	 0.4180	 0.2930
X	 0.6370	 0.3290
a	 0.9650	 0.6260
b	 0.9450	 0.6110
c	 0.9300	 0.5520
d	 0.9650	 0.6290
e	 0.9000	 0.4980
f	 0.8880	 0.4910
h	 0.8910	 0.5510
i	 0.9420	 0.5750
k	 0.8250	 0.4510
l	 0.9480	 0.6210
m	 0.9280	 0.5740
o	 0.4760	 0.3280
t	 0.9180	 0.5830
u	 0.3280	 0.2570
v	 0.4220	 0.2930
x	 0.6490	 0.3270

