



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:24 PM UTC

PDB ID : 5TIS / pdb_00005tis

Title : Room temperature XFEL structure of the native, doubly-illuminated photo-system II complex

Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Fuller, F.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Hussein, R.; Zhang, M.; Douthit, L.; Kubin, M.; de Lichtenberg, C.; Pham, L.V.; Nilsson, H.; Cheah, M.H.; Shevela, D.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Pastor, E.; Weninger, C.; Fransson, T.; Lassalle, L.; Braeuer, P.; Aller, P.; Docker, P.T.; Andi, B.; Orville, A.M.; Glowina, J.M.; Nelson, S.; Sikorski, M.; Zhu, D.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Watermann, D.G.; Evans, G.; Wernet, P.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.

Deposited on : 2016-10-03

Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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>.

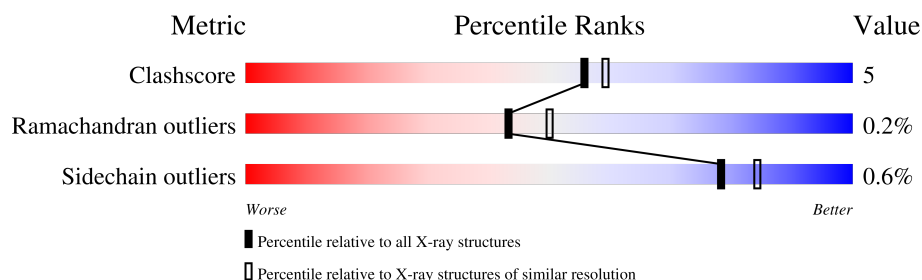
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

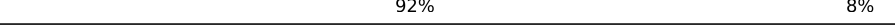
Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	

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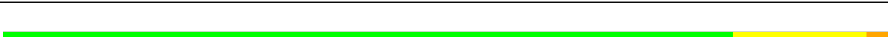
MolProbity : 4-5-2 with Phenix2.0
 Mogul : 2022.3.0, CSD as543be (2022)
 Xtriage (Phenix) : 2.0
 EDS : **FAILED**
 Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	B	510	 90% 9% .
2	b	510	 90% 9% .
3	C	461	 91% 7% .
3	c	461	 89% 9% .
4	D	352	 87% 10% .
4	d	352	 87% 10% .
5	E	84	 81% 15% .
5	e	84	 75% 23% .
6	F	45	 76% 24%
6	f	45	 69% 7% 24%
7	H	66	 91% 8% .
7	h	66	 89% 6% 5%
8	I	38	 95% . .
8	i	38	 92% . 5%
9	J	40	 88% . 10%
9	j	40	 82% 8% 10%
10	K	46	 72% 9% 20%
10	k	46	 74% 7% 20%
11	L	37	 92% 8%
11	l	37	 95% 5%
12	M	36	 89% . 8%
12	m	36	 86% 6% 8%
13	O	272	 79% 10% 10%
13	o	272	 78% 12% 10%
14	T	32	 78% 16% 6%

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Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	613	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	615	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606[A]	X	-	-	-
25	CLA	b	606[B]	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	402	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 51757 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2625	1719	431	460	15			
1	a	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	5	0
			4005	2629	667	696	13			
2	b	504	Total	C	N	O	S	0	2	0
			3982	2613	665	691	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	1	0
			3494	2287	585	609	13			
3	c	451	Total	C	N	O	S	0	1	0
			3494	2286	587	608	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			
4	d	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			670	437	109	124			
5	e	82	Total	C	N	O	0	1	0
			671	438	108	125			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	37	Total	C	N	O	S	0	0	0
			304	206	47	50	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			269	178	39	51	1			
12	m	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	2	0
			1888	1179	320	385	4			
13	o	244	Total	C	N	O	S	0	2	0
			1888	1179	320	385	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1070	680	178	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			200	131	35	31	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			281	188	45	48				
18	x	38	Total	C	N	O		0	1	0
			285	192	46	47				

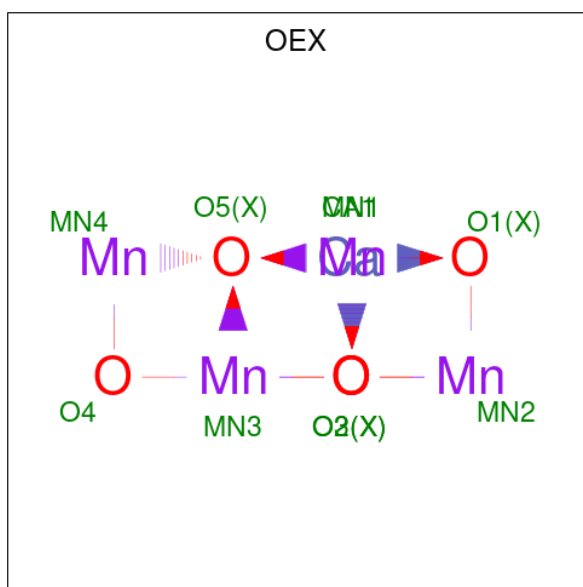
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			478	328	72	76	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			273	186	47	40				
20	r	34	Total	C	N	O		0	0	0
			270	183	47	40				

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

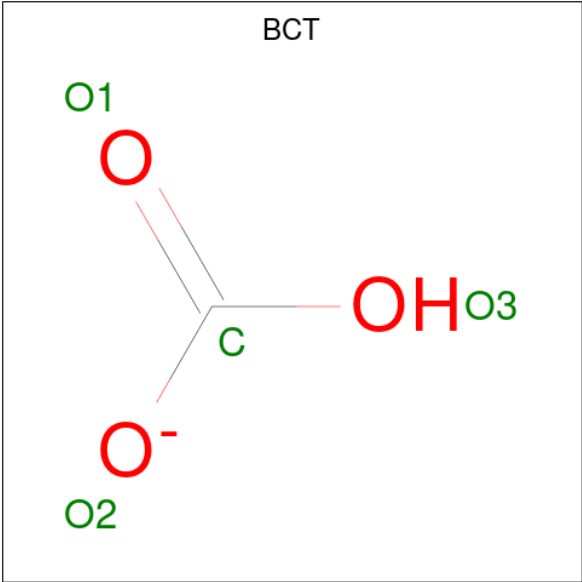
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		
22	a	1	Total	Fe	0	0
			1	1		

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

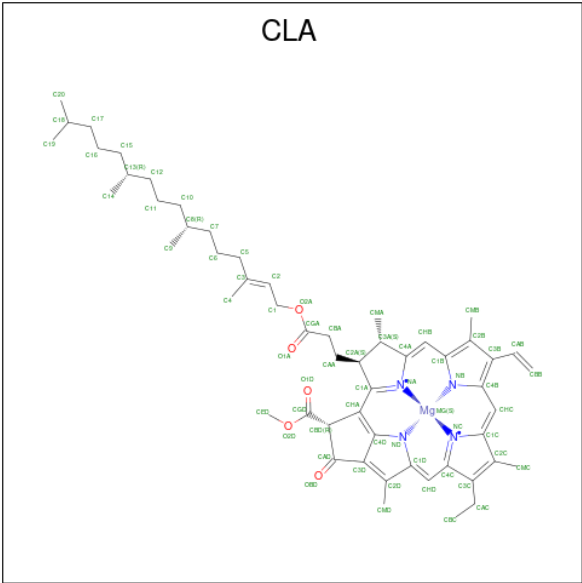
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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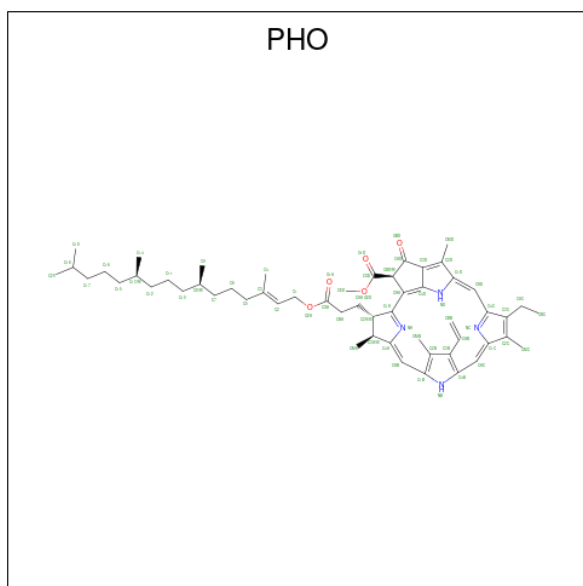
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	1
			129	110	1	8	10		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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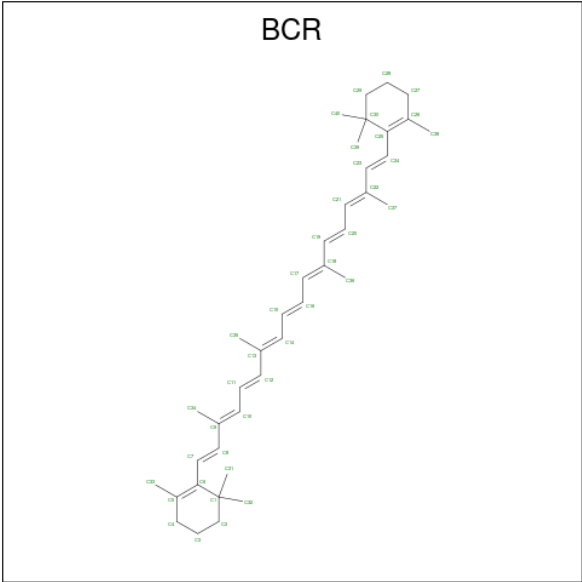
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



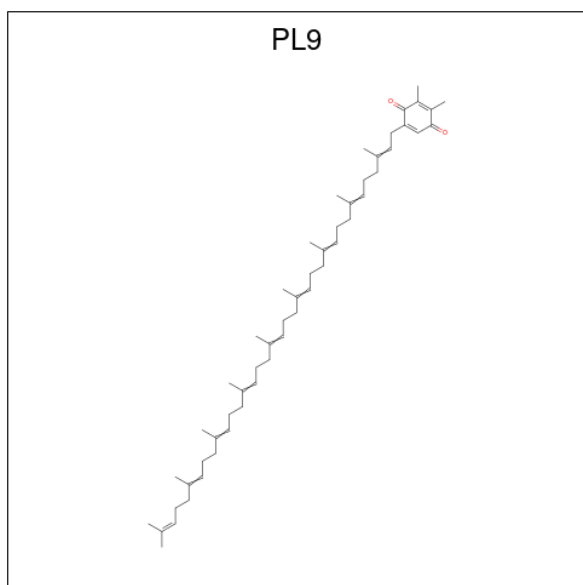
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



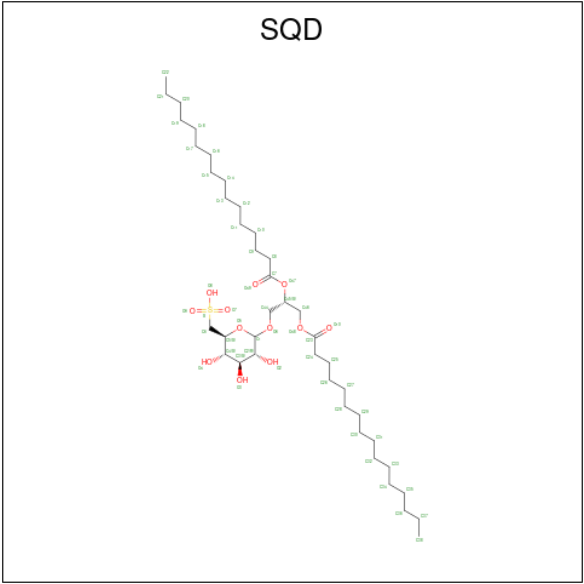
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



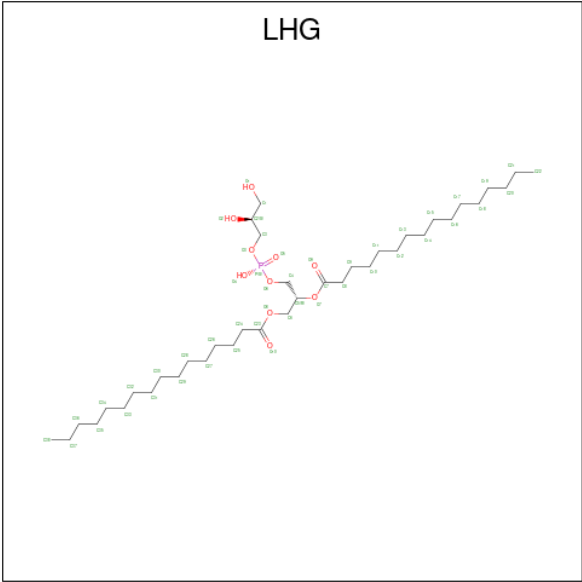
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	D	1	Total	C	O	S	0	0
			47	34	12	1		
29	L	1	Total	C	O	S	0	0
			49	36	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O		0	0
			40	35	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).

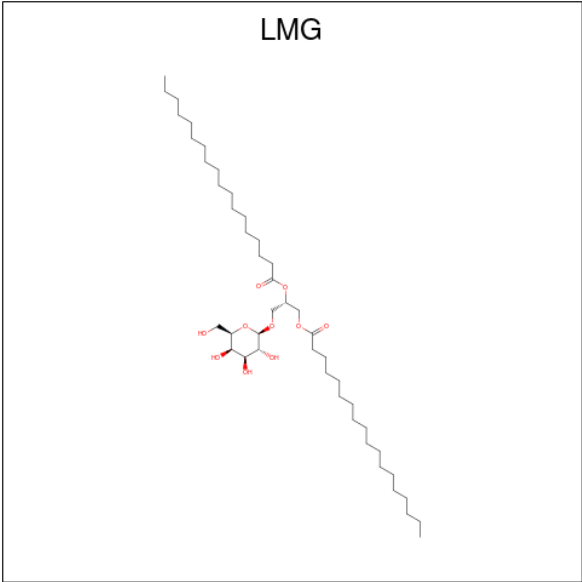


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			47	36	10	1		
30	A	1	Total	C	O	P	0	0
			49	38	10	1		
30	B	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	1	Total	C	O	P	0	0
			39	28	10	1		
30	a	1	Total	C	O	P	0	0
			42	31	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

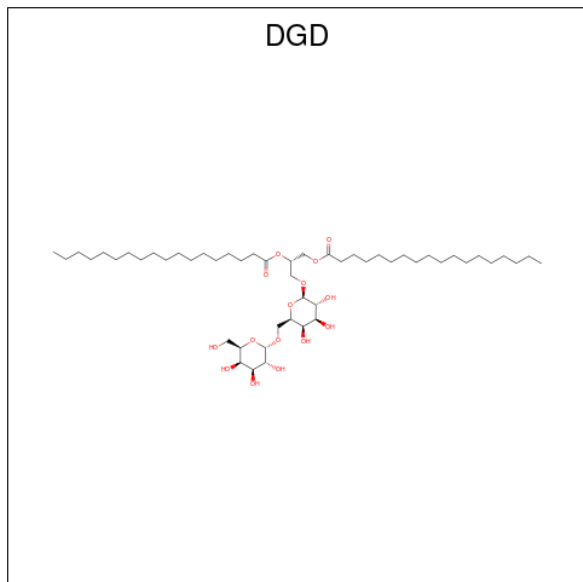
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	2	Total C O 29 27 2	0	0
31	B	2	Total C 26 26	0	0
31	C	2	Total C O 33 31 2	0	0
31	D	2	Total C 28 28	0	0
31	E	1	Total C O 12 10 2	0	0
31	H	1	Total C 7 7	0	0
31	I	2	Total C O 27 25 2	0	0
31	J	2	Total C O 23 21 2	0	0
31	M	2	Total C O 32 30 2	0	0
31	T	2	Total C 26 26	0	0
31	a	2	Total C O 29 27 2	0	0
31	b	2	Total C 28 28	0	0
31	c	3	Total C O 40 34 6	0	0
31	d	1	Total C 17 17	0	0
31	i	1	Total C O 20 18 2	0	0
31	j	2	Total C O 27 25 2	0	0
31	m	2	Total C O 25 23 2	0	0
31	t	1	Total C 18 18	0	0
31	x	1	Total C 16 16	0	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



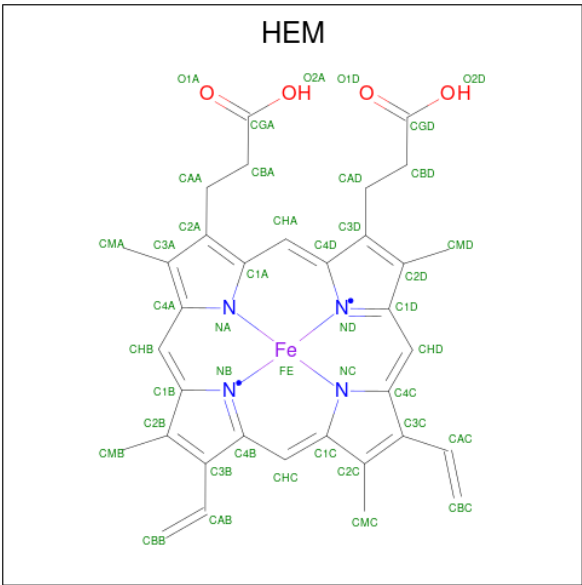
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	b	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			34	24	10		
32	d	1	Total	C	O	0	0
			51	41	10		
32	d	1	Total	C	O	0	0
			38	36	2		
32	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



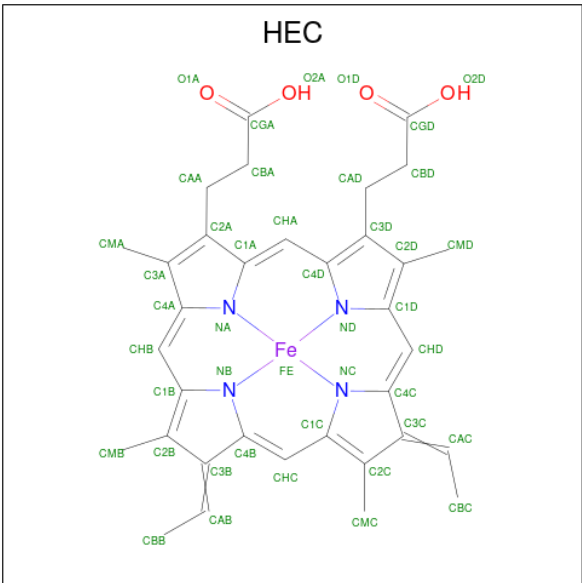
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

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



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
35	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	86	Total O 86 86	0	0
36	B	109	Total O 109 109	0	0
36	C	95	Total O 95 95	0	0
36	D	82	Total O 82 82	0	0
36	E	14	Total O 14 14	0	0
36	F	3	Total O 3 3	0	0
36	H	11	Total O 11 11	0	0
36	I	3	Total O 3 3	0	0
36	J	5	Total O 5 5	0	0
36	K	2	Total O 2 2	0	0
36	L	3	Total O 3 3	0	0
36	M	5	Total O 5 5	0	0
36	O	72	Total O 72 72	0	0
36	T	9	Total O 9 9	0	0
36	U	22	Total O 22 22	0	0
36	V	42	Total O 42 42	0	0
36	X	5	Total O 5 5	0	0
36	Z	3	Total O 3 3	0	0
36	a	90	Total O 90 90	0	0
36	b	129	Total O 129 129	0	0
36	c	95	Total O 95 95	0	0

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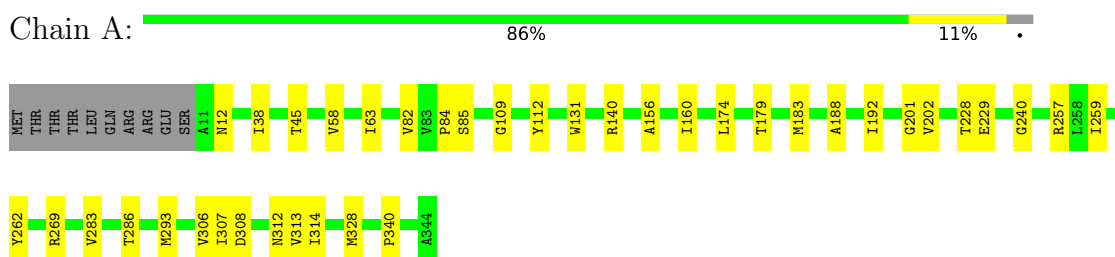
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	d	87	Total 87	O 87	0	0
36	e	9	Total 9	O 9	0	0
36	f	2	Total 2	O 2	0	0
36	h	13	Total 13	O 13	0	0
36	i	6	Total 6	O 6	0	0
36	j	2	Total 2	O 2	0	0
36	k	4	Total 4	O 4	0	0
36	l	10	Total 10	O 10	0	0
36	m	10	Total 10	O 10	0	0
36	o	69	Total 69	O 69	0	0
36	t	4	Total 4	O 4	0	0
36	u	34	Total 34	O 34	0	0
36	v	37	Total 37	O 37	0	0
36	y	1	Total 1	O 1	0	0
36	x	4	Total 4	O 4	0	0
36	z	1	Total 1	O 1	0	0
36	r	1	Total 1	O 1	0	0

3 Residue-property plots

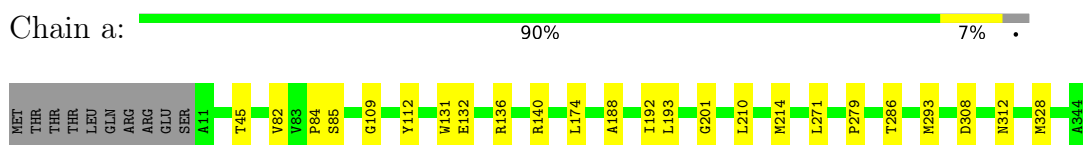
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

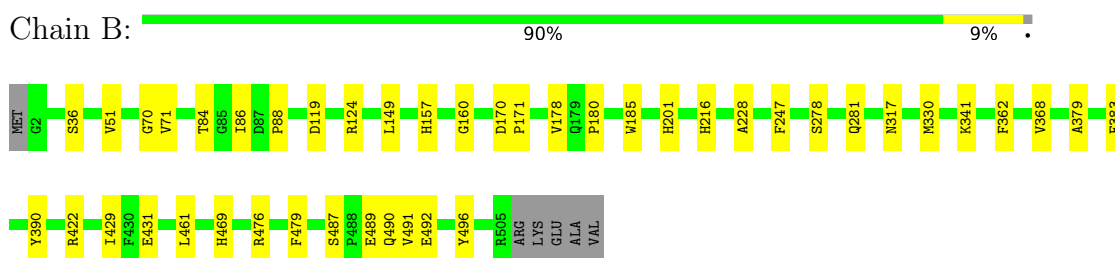
- Molecule 1: Photosystem II protein D1 1



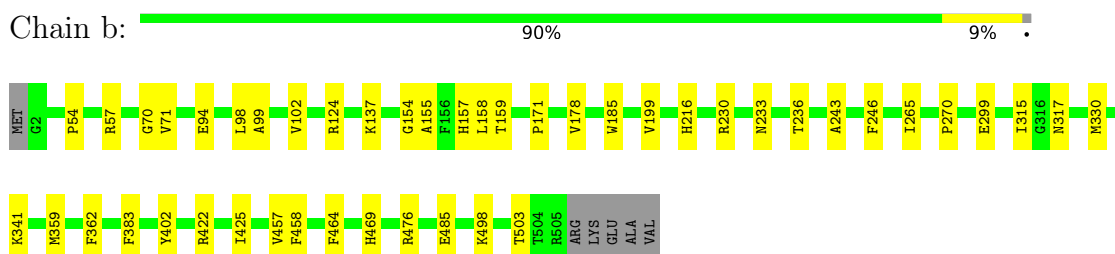
- Molecule 1: Photosystem II protein D1 1



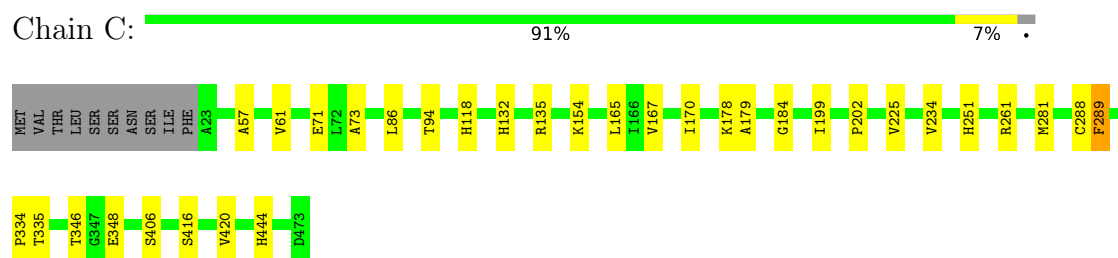
- Molecule 2: Photosystem II CP47 reaction center protein



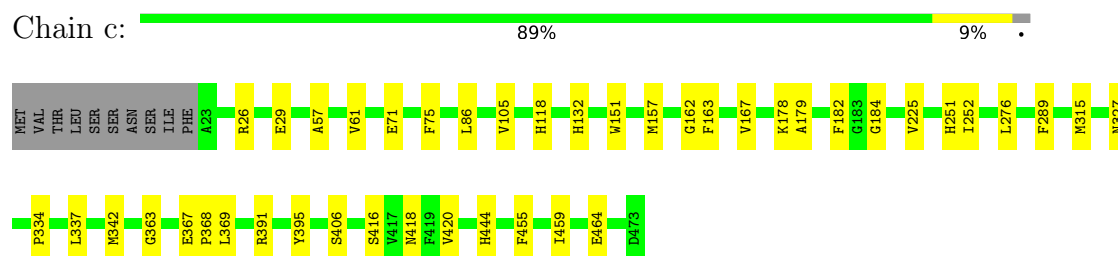
- Molecule 2: Photosystem II CP47 reaction center protein



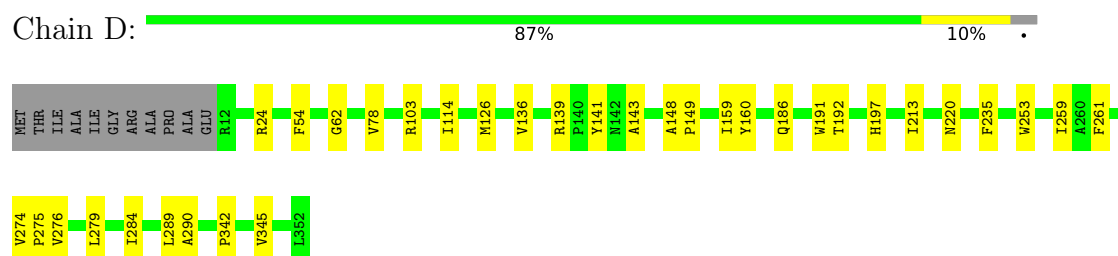
- Molecule 3: Photosystem II CP43 reaction center protein



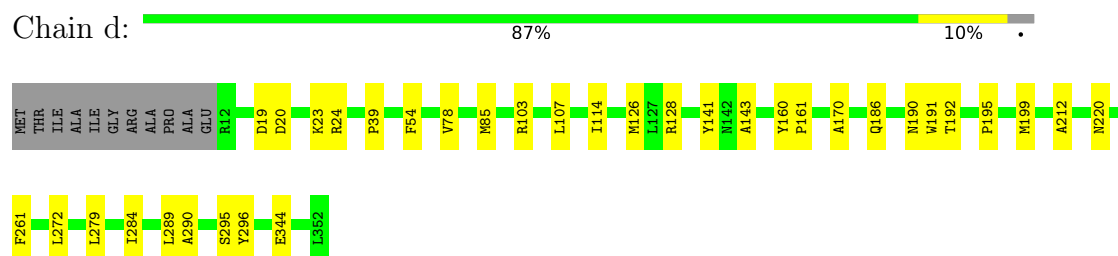
- Molecule 3: Photosystem II CP43 reaction center protein



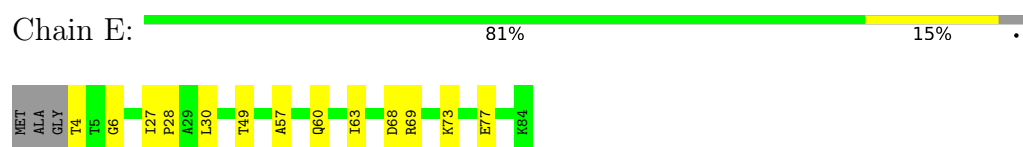
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



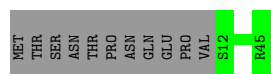
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  75% 23% .



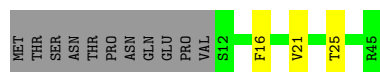
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  76% 24%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  69% 7% 24%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  91% 8% .

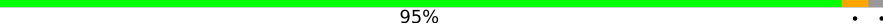


- Molecule 7: Photosystem II reaction center protein H

Chain h:  89% 6% 5%



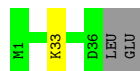
- Molecule 8: Photosystem II reaction center protein I

Chain I:  95% . .



- Molecule 8: Photosystem II reaction center protein I

Chain i:  92% . 5%



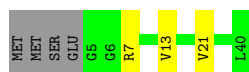
- Molecule 9: Photosystem II reaction center protein J

Chain J:  88% 10%



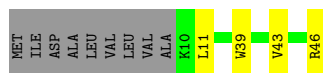
- Molecule 9: Photosystem II reaction center protein J

Chain j:  82% 8% 10%



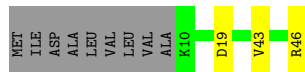
- Molecule 10: Photosystem II reaction center protein K

Chain K:  72% 9% 20%



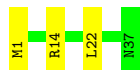
- Molecule 10: Photosystem II reaction center protein K

Chain k:  74% 7% 20%

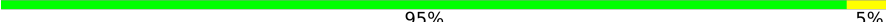


- Molecule 11: Photosystem II reaction center protein L

Chain L:  92% 8%



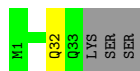
- Molecule 11: Photosystem II reaction center protein L

Chain l:  95% 5%



- Molecule 12: Photosystem II reaction center protein M

Chain M:  89% 8%

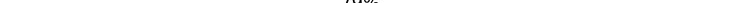


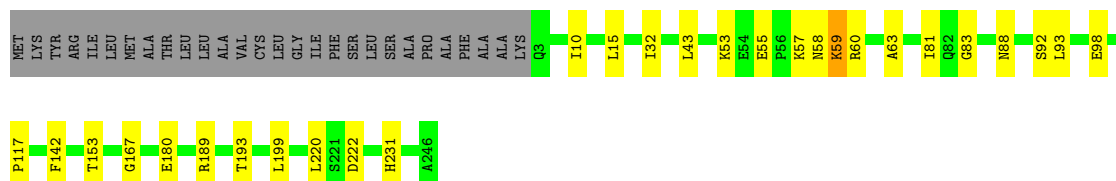
- Molecule 12: Photosystem II reaction center protein M

Chain m:  86% 6% 8%



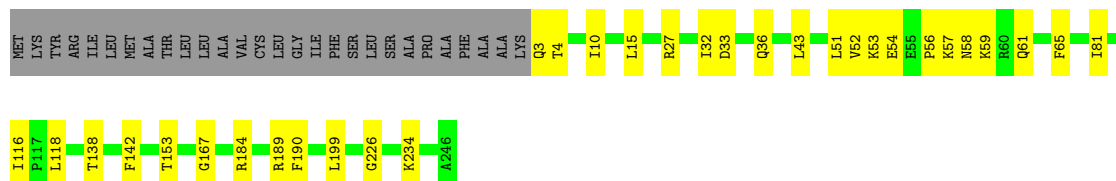
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  79% 10% 10%

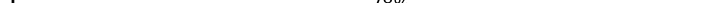


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 



- Molecule 14: Photosystem II reaction center protein T

Chain T:  78% 16% 6%



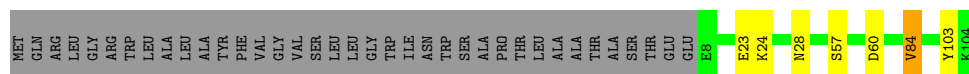
- Molecule 14: Photosystem II reaction center protein T

Chain t: 84% 9% 6%



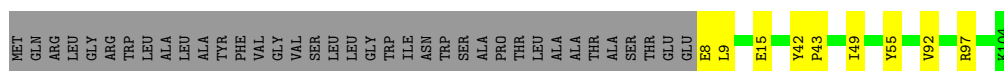
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 67% .. 28%

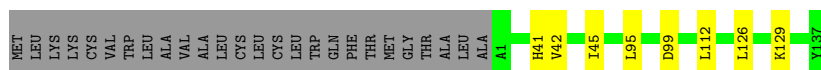
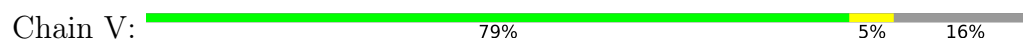


- Molecule 15: Photosystem II 12 kDa extrinsic protein

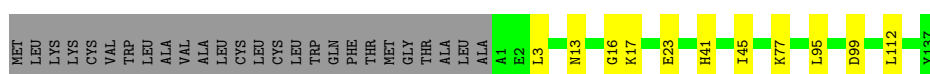
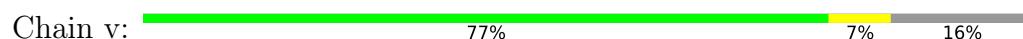
Chain u: 66% 7% 28%



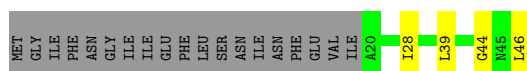
- Molecule 16: Cytochrome c-550



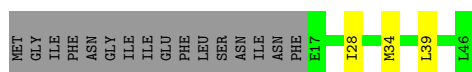
- Molecule 16: Cytochrome c-550



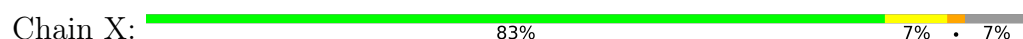
- Molecule 17: Photosystem II reaction center protein Ycf12



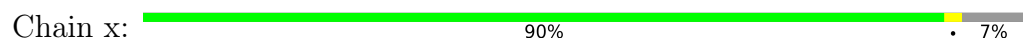
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein

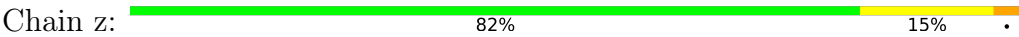


- Molecule 19: Photosystem II reaction center protein Z





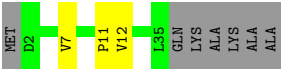
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.87Å 223.14Å 310.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 2.25	Depositor
% Data completeness (in resolution range)	99.9 (44.28-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.24Å)	Xtriage
Refinement program	PHENIX dev_2481	Depositor
R, R_{free}	0.193 , 0.231	Depositor
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.255	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51757	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.10	0/2713	0.28	0/3700
1	a	0.10	0/2707	0.28	0/3692
2	B	0.10	0/4155	0.26	0/5661
2	b	0.10	0/4125	0.27	0/5621
3	C	0.09	0/3607	0.25	0/4911
3	c	0.10	0/3610	0.25	0/4914
4	D	0.10	0/2812	0.28	0/3832
4	d	0.10	0/2811	0.27	0/3830
5	E	0.09	0/689	0.26	0/940
5	e	0.19	0/693	0.25	0/945
6	F	0.08	0/284	0.23	0/387
6	f	0.10	0/284	0.22	0/387
7	H	0.11	0/523	0.26	0/713
7	h	0.09	0/511	0.25	0/697
8	I	0.10	0/301	0.28	0/407
8	i	0.09	0/293	0.24	0/396
9	J	0.07	0/263	0.23	0/356
9	j	0.08	0/263	0.22	0/356
10	K	0.11	0/303	0.27	0/416
10	k	0.11	0/303	0.28	0/416
11	L	0.09	0/311	0.25	0/422
11	l	0.09	0/311	0.25	0/422
12	M	0.08	0/262	0.20	0/358
12	m	0.09	0/253	0.22	0/346
13	O	0.10	0/1925	0.28	0/2610
13	o	0.12	0/1925	0.35	0/2609
14	T	0.09	0/257	0.24	0/349
14	t	0.08	0/257	0.25	0/349
15	U	0.14	0/785	0.27	0/1064
15	u	0.10	0/785	0.27	0/1064
16	V	0.09	0/1085	0.23	0/1473
16	v	0.08	0/1094	0.23	0/1484

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.09	0/201	0.28	0/268
17	y	0.08	0/225	0.24	0/301
18	X	0.07	0/284	0.18	0/384
18	x	0.06	0/291	0.16	0/392
19	Z	0.07	0/490	0.22	0/669
19	z	0.09	0/489	0.25	0/669
20	R	0.10	0/279	0.27	0/383
20	r	0.09	0/276	0.25	0/379
All	All	0.10	0/43035	0.27	0/58572

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2625	0	2524	26	0
1	a	2622	0	2519	17	0
2	B	4005	0	3865	35	0
2	b	3982	0	3842	39	0
3	C	3494	0	3417	24	0
3	c	3494	0	3420	30	0
4	D	2717	0	2621	26	0
4	d	2716	0	2621	28	0
5	E	670	0	655	9	0
5	e	671	0	657	13	0
6	F	275	0	282	0	0
6	f	275	0	282	2	0
7	H	510	0	532	4	0
7	h	498	0	518	4	0
8	I	304	0	322	2	0
8	i	296	0	311	1	0
9	J	257	0	268	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	257	0	268	1	0
10	K	293	0	305	3	0
10	k	293	0	305	2	0
11	L	304	0	316	4	0
11	l	304	0	316	3	0
12	M	269	0	280	0	0
12	m	260	0	275	1	0
13	O	1888	0	1865	15	0
13	o	1888	0	1865	17	0
14	T	258	0	261	4	0
14	t	258	0	261	4	0
15	U	774	0	773	5	0
15	u	774	0	773	6	0
16	V	1064	0	1073	4	0
16	v	1070	0	1086	6	0
17	Y	200	0	226	4	0
17	y	224	0	252	3	0
18	X	281	0	312	3	0
18	x	285	0	320	1	0
19	Z	479	0	516	4	0
19	z	478	0	516	7	0
20	R	273	0	305	4	0
20	r	270	0	296	3	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	4	0	0	0	0
24	a	4	0	0	0	0
25	A	249	0	264	10	0
25	B	1040	0	1152	38	0
25	C	845	0	936	27	0
25	D	130	0	144	6	0
25	a	260	0	288	8	0
25	b	1086	0	1187	31	0
25	c	839	0	919	21	0
25	d	130	0	144	6	0
26	A	64	0	74	2	0
26	D	64	0	74	0	0
26	a	128	0	148	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	40	0	56	2	0
27	B	120	0	168	11	0
27	C	80	0	112	4	0
27	D	40	0	56	4	0
27	H	40	0	56	1	0
27	K	40	0	56	2	0
27	T	40	0	56	3	0
27	Y	40	0	56	4	0
27	a	40	0	56	2	0
27	b	120	0	168	1	0
27	c	160	0	224	11	0
27	d	40	0	56	2	0
27	h	40	0	56	3	0
27	t	40	0	56	3	0
28	A	55	0	80	3	0
28	D	55	0	80	0	0
28	a	55	0	80	3	0
28	d	55	0	80	1	0
29	A	106	0	148	2	0
29	B	108	0	156	6	0
29	D	90	0	111	3	0
29	L	49	0	65	3	0
29	a	54	0	78	0	0
29	b	40	0	67	3	0
29	f	41	0	49	1	0
30	A	96	0	141	3	0
30	B	49	0	74	4	0
30	D	49	0	74	3	0
30	L	49	0	74	1	0
30	a	81	0	108	2	0
30	d	98	0	148	5	0
30	l	49	0	74	1	0
31	A	29	0	0	0	0
31	B	26	0	0	0	0
31	C	33	0	0	0	0
31	D	28	0	0	0	0
31	E	12	0	0	0	0
31	H	7	0	0	0	0
31	I	27	0	0	0	0
31	J	23	0	0	0	0
31	M	32	0	0	0	0
31	T	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	29	0	0	0	0
31	b	28	0	0	0	0
31	c	40	0	0	0	0
31	d	17	0	0	0	0
31	i	20	0	0	0	0
31	j	27	0	0	0	0
31	m	25	0	0	0	0
31	t	18	0	0	0	0
31	x	16	0	0	0	0
32	B	153	0	216	3	0
32	C	147	0	204	2	0
32	D	51	0	72	1	0
32	a	51	0	72	0	0
32	b	51	0	72	0	0
32	c	71	0	82	0	0
32	d	89	0	142	4	0
32	m	51	0	72	1	0
33	C	186	0	246	4	0
33	H	62	0	82	1	0
33	c	186	0	246	4	0
33	h	62	0	82	1	0
34	E	43	0	30	3	0
34	e	43	0	30	3	0
35	V	43	0	30	0	0
35	v	43	0	29	0	0
36	A	86	0	0	1	0
36	B	109	0	0	0	0
36	C	95	0	0	0	0
36	D	82	0	0	0	0
36	E	14	0	0	0	0
36	F	3	0	0	0	0
36	H	11	0	0	0	0
36	I	3	0	0	1	0
36	J	5	0	0	1	0
36	K	2	0	0	0	0
36	L	3	0	0	0	0
36	M	5	0	0	0	0
36	O	72	0	0	1	0
36	T	9	0	0	0	0
36	U	22	0	0	0	0
36	V	42	0	0	0	0
36	X	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	Z	3	0	0	0	0
36	a	90	0	0	0	0
36	b	129	0	0	4	0
36	c	95	0	0	2	0
36	d	87	0	0	1	0
36	e	9	0	0	0	0
36	f	2	0	0	0	0
36	h	13	0	0	0	0
36	i	6	0	0	0	0
36	j	2	0	0	0	0
36	k	4	0	0	0	0
36	l	10	0	0	0	0
36	m	10	0	0	0	0
36	o	69	0	0	0	0
36	r	1	0	0	0	0
36	t	4	0	0	0	0
36	u	34	0	0	3	0
36	v	37	0	0	0	0
36	x	4	0	0	0	0
36	y	1	0	0	0	0
36	z	1	0	0	0	0
All	All	51757	0	51377	474	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 474 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:157:HIS:HE1	25:b:606[A]:CLA:NA	1.76	0.84
2:B:157:HIS:HE1	25:B:606:CLA:NA	1.78	0.81
2:b:359:MET:SD	36:b:703:HOH:O	2.44	0.75
3:C:165:LEU:HD21	25:C:507:CLA:HAB	1.67	0.74
2:b:315:ILE:HD13	2:b:359:MET:HE3	1.69	0.74

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	333/344 (97%)	327 (98%)	5 (2%)	1 (0%)	36	40
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	507/510 (99%)	498 (98%)	9 (2%)	0	100	100
2	b	504/510 (99%)	491 (97%)	13 (3%)	0	100	100
3	C	450/461 (98%)	439 (98%)	10 (2%)	1 (0%)	43	50
3	c	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	43	50
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	6
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	35/38 (92%)	32 (91%)	3 (9%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	30 (94%)	1 (3%)	1 (3%)	3	1
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	244/272 (90%)	235 (96%)	8 (3%)	1 (0%)	30	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	244/272 (90%)	229 (94%)	11 (4%)	4 (2%)	7	4
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
16	v	136/163 (83%)	130 (96%)	5 (4%)	1 (1%)	18	17
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	1 (3%)	1 (3%)	4	2
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	3
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5700 (92%)	5108 (97%)	137 (3%)	13 (0%)	43	50

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	53	LYS
13	o	58	ASN
3	C	416	SER
3	c	416	SER
13	o	59	LYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	271/280 (97%)	269 (99%)	2 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	407/407 (100%)	404 (99%)	3 (1%)	76	82
2	b	403/407 (99%)	401 (100%)	2 (0%)	81	87
3	C	353/362 (98%)	352 (100%)	1 (0%)	86	90
3	c	353/362 (98%)	352 (100%)	1 (0%)	86	90
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	276/283 (98%)	275 (100%)	1 (0%)	84	89
5	E	73/73 (100%)	72 (99%)	1 (1%)	59	70
5	e	73/73 (100%)	72 (99%)	1 (1%)	59	70
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	61
7	h	53/55 (96%)	53 (100%)	0	100	100
8	I	33/34 (97%)	32 (97%)	1 (3%)	36	45
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	8
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	29 (97%)	1 (3%)	33	42
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	209/228 (92%)	208 (100%)	1 (0%)	81	87
13	o	209/228 (92%)	207 (99%)	2 (1%)	68	77
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	83 (99%)	1 (1%)	63	74
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	74
16	V	117/138 (85%)	116 (99%)	1 (1%)	70	79
16	v	118/138 (86%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	20/37 (54%)	20 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	52 (100%)	0	100	100
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	36
20	R	29/33 (88%)	28 (97%)	1 (3%)	32	40
20	r	28/33 (85%)	28 (100%)	0	100	100
All	All	4359/4654 (94%)	4333 (99%)	26 (1%)	78	84

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	485	GLU
5	e	5	THR
19	z	9	LEU
4	d	272	LEU
9	j	13	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	327	ASN
13	o	155	ASN
3	c	418	ASN
4	d	350	ASN
13	O	82	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	M	1	12	8,9,10	0.97	0	8,9,11	0.92	0
14	FME	t	1	14	8,9,10	0.99	0	8,9,11	0.98	0
14	FME	T	1	14	8,9,10	0.95	0	8,9,11	1.11	1 (12%)
8	FME	i	1	8	8,9,10	0.99	0	8,9,11	0.87	0
8	FME	I	1	8	8,9,10	0.98	0	8,9,11	0.89	0
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	0.85	0

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
12	FME	M	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.26	113.87	109.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	i	1	FME	O-C-CA-CB
12	M	1	FME	N-CA-CB-CG
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE
12	M	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 6 are monoatomic and 33 are unknown - leaving 151 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
35	HEC	V	201	16	46,50,50	1.88	7 (15%)	58,82,82	1.14	2 (3%)
26	PHO	A	608	-	58,69,69	2.19	10 (17%)	55,99,99	1.43	6 (10%)
29	SQD	B	624	-	52,54,54	0.95	2 (3%)	62,65,65	1.56	10 (16%)
29	SQD	D	409	-	45,47,54	1.02	2 (4%)	55,58,65	1.51	9 (16%)
25	CLA	b	601	36	69,73,73	1.13	7 (10%)	82,113,113	1.18	4 (4%)
27	BCR	b	617	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	6 (10%)
25	CLA	B	611	-	69,73,73	1.12	7 (10%)	82,113,113	1.22	7 (8%)
33	DGD	C	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.38	10 (12%)
27	BCR	C	516	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
29	SQD	f	101	-	39,41,54	1.09	3 (7%)	49,52,65	1.49	9 (18%)
32	LMG	D	407	-	51,51,55	0.72	0	59,59,63	1.31	5 (8%)
21	OEX	A	601	36,1,3	0,15,15	-	-	-	-	-
25	CLA	c	512	-	69,73,73	1.13	7 (10%)	82,113,113	1.25	6 (7%)
32	LMG	a	614	-	51,51,55	0.73	1 (1%)	59,59,63	1.33	7 (11%)
27	BCR	a	611	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
25	CLA	b	606[A]	-	69,73,73	1.12	7 (10%)	82,113,113	1.16	4 (4%)
27	BCR	c	515	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	6 (10%)
28	PL9	a	612	-	55,55,55	0.96	3 (5%)	68,69,69	1.51	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	b	621	-	39,39,54	0.88	2 (5%)	41,41,65	1.15	2 (4%)
30	LHG	A	618	-	48,48,48	0.64	2 (4%)	51,54,54	1.27	6 (11%)
33	DGD	c	518	-	63,63,67	0.84	1 (1%)	77,77,81	1.35	8 (10%)
30	LHG	B	623	-	48,48,48	0.62	1 (2%)	51,54,54	1.29	6 (11%)
25	CLA	C	509	-	69,73,73	1.13	5 (7%)	82,113,113	1.22	6 (7%)
25	CLA	B	605	-	69,73,73	1.10	6 (8%)	82,113,113	1.16	5 (6%)
25	CLA	b	611	-	69,73,73	1.13	7 (10%)	82,113,113	1.23	7 (8%)
25	CLA	b	602	-	69,73,73	1.12	6 (8%)	82,113,113	1.21	7 (8%)
30	LHG	l	101	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
29	SQD	a	613	-	52,54,54	0.95	3 (5%)	62,65,65	1.42	8 (12%)
34	HEM	e	101	6,5	50,50,50	1.53	6 (12%)	67,82,82	1.24	4 (5%)
25	CLA	b	608	-	69,73,73	1.11	6 (8%)	82,113,113	1.15	6 (7%)
29	SQD	A	612	-	50,52,54	0.97	3 (6%)	60,63,65	1.44	9 (15%)
27	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
28	PL9	A	611	-	55,55,55	0.97	4 (7%)	68,69,69	1.49	12 (17%)
25	CLA	c	503	-	69,73,73	1.12	6 (8%)	82,113,113	1.25	4 (4%)
32	LMG	c	520	-	34,34,55	0.85	0	42,42,63	1.25	4 (9%)
25	CLA	b	616	-	51,55,73	1.29	7 (13%)	60,91,113	1.36	6 (10%)
30	LHG	A	614	-	46,46,48	0.63	1 (2%)	49,52,54	1.26	5 (10%)
32	LMG	b	620	-	51,51,55	0.71	0	59,59,63	1.34	7 (11%)
25	CLA	b	604	-	69,73,73	1.14	6 (8%)	82,113,113	1.30	6 (7%)
25	CLA	C	503	-	69,73,73	1.12	6 (8%)	82,113,113	1.20	5 (6%)
25	CLA	b	605	-	69,73,73	1.12	6 (8%)	82,113,113	1.18	6 (7%)
25	CLA	c	504	36	64,68,73	1.16	7 (10%)	76,107,113	1.20	5 (6%)
25	CLA	b	613	-	69,73,73	1.14	6 (8%)	82,113,113	1.24	6 (7%)
35	HEC	v	201	16	46,50,50	1.87	7 (15%)	58,82,82	1.07	2 (3%)
27	BCR	b	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	5 (8%)
30	LHG	D	406	-	48,48,48	0.62	2 (4%)	51,54,54	1.27	6 (11%)
25	CLA	C	504	-	69,73,73	1.13	6 (8%)	82,113,113	1.23	5 (6%)
25	CLA	A	609	-	58,62,73	1.21	7 (12%)	68,99,113	1.25	6 (8%)
30	LHG	a	616	-	38,38,48	0.69	1 (2%)	41,44,54	1.19	3 (7%)
27	BCR	d	403	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	4 (7%)
33	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.35	9 (11%)
33	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.41	10 (12%)
25	CLA	B	602	-	69,73,73	1.13	6 (8%)	82,113,113	1.18	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	L	102	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
27	BCR	T	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
25	CLA	B	616	-	69,73,73	1.13	6 (8%)	82,113,113	1.25	5 (6%)
25	CLA	c	509	-	69,73,73	1.12	6 (8%)	82,113,113	1.22	5 (6%)
27	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
33	DGD	C	517	-	63,63,67	0.82	1 (1%)	77,77,81	1.34	9 (11%)
25	CLA	c	510	-	69,73,73	1.13	6 (8%)	82,113,113	1.21	4 (4%)
25	CLA	a	615	36	69,73,73	1.13	5 (7%)	82,113,113	1.14	7 (8%)
25	CLA	B	615	-	69,73,73	1.14	6 (8%)	82,113,113	1.21	5 (6%)
25	CLA	B	607	36	69,73,73	1.12	5 (7%)	82,113,113	1.11	6 (7%)
25	CLA	C	507	-	69,73,73	1.13	6 (8%)	82,113,113	1.22	6 (7%)
25	CLA	D	403	-	69,73,73	1.13	6 (8%)	82,113,113	1.24	9 (10%)
25	CLA	C	502	-	69,73,73	1.13	6 (8%)	82,113,113	1.20	5 (6%)
25	CLA	c	511	3	69,73,73	1.12	5 (7%)	82,113,113	1.15	6 (7%)
32	LMG	B	620	-	51,51,55	0.72	0	59,59,63	1.34	6 (10%)
25	CLA	B	604	-	69,73,73	1.14	7 (10%)	82,113,113	1.27	6 (7%)
25	CLA	B	601	36	69,73,73	1.13	6 (8%)	82,113,113	1.21	6 (7%)
25	CLA	a	610	-	69,73,73	1.13	6 (8%)	82,113,113	1.20	6 (7%)
32	LMG	c	519	-	37,37,55	0.85	1 (2%)	45,45,63	1.35	6 (13%)
27	BCR	h	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	5 (8%)
26	PHO	D	401	-	58,69,69	2.17	9 (15%)	55,99,99	1.44	5 (9%)
26	PHO	a	608	-	58,69,69	2.17	9 (15%)	55,99,99	1.44	7 (12%)
32	LMG	B	626	-	51,51,55	0.71	0	59,59,63	1.30	5 (8%)
25	CLA	d	402	-	69,73,73	1.12	7 (10%)	82,113,113	1.18	6 (7%)
30	LHG	a	617	-	41,41,48	0.68	2 (4%)	44,47,54	1.34	6 (13%)
25	CLA	c	506	-	69,73,73	1.12	7 (10%)	82,113,113	1.16	5 (6%)
25	CLA	C	510	-	69,73,73	1.11	6 (8%)	82,113,113	1.22	7 (8%)
25	CLA	b	615	-	69,73,73	1.14	7 (10%)	82,113,113	1.21	5 (6%)
25	CLA	b	607	36	69,73,73	1.11	6 (8%)	82,113,113	1.13	5 (6%)
29	SQD	L	101	-	47,49,54	0.99	3 (6%)	57,60,65	1.52	10 (17%)
25	CLA	b	606[B]	-	69,73,73	1.12	7 (10%)	82,113,113	1.16	4 (4%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.19	7 (12%)
25	CLA	B	609	-	69,73,73	1.13	6 (8%)	82,113,113	1.19	6 (7%)
25	CLA	C	506	-	69,73,73	1.13	6 (8%)	82,113,113	1.20	5 (6%)
25	CLA	b	610	36	69,73,73	1.12	6 (8%)	82,113,113	1.20	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	606	-	69,73,73	1.12	6 (8%)	82,113,113	1.11	6 (7%)
25	CLA	C	511	-	69,73,73	1.13	6 (8%)	82,113,113	1.19	5 (6%)
32	LMG	d	407	-	51,51,55	0.73	1 (1%)	59,59,63	1.34	7 (11%)
33	DGD	c	517	-	63,63,67	0.89	2 (3%)	77,77,81	1.37	7 (9%)
25	CLA	B	603	-	69,73,73	1.11	6 (8%)	82,113,113	1.12	5 (6%)
27	BCR	D	404	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	6 (10%)
32	LMG	m	102	-	51,51,55	0.72	1 (1%)	59,59,63	1.36	7 (11%)
27	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	6 (10%)
25	CLA	A	606	-	69,73,73	1.12	6 (8%)	82,113,113	1.10	6 (7%)
29	SQD	D	408	-	41,43,54	1.07	3 (7%)	51,54,65	1.57	9 (17%)
27	BCR	C	515	-	41,41,41	1.10	2 (4%)	56,56,56	1.19	5 (8%)
29	SQD	A	616	-	52,54,54	0.96	2 (3%)	62,65,65	1.43	9 (14%)
25	CLA	d	401	-	69,73,73	1.12	7 (10%)	82,113,113	1.13	5 (6%)
25	CLA	C	512	3	69,73,73	1.14	6 (8%)	82,113,113	1.15	6 (7%)
25	CLA	b	609	-	69,73,73	1.13	6 (8%)	82,113,113	1.19	5 (6%)
27	BCR	Y	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.15	4 (7%)
30	LHG	d	406	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
21	OEX	a	601	36,1,3	0,15,15	-	-	-	-	-
25	CLA	C	513	-	69,73,73	1.13	7 (10%)	82,113,113	1.23	5 (6%)
24	BCT	a	605	22	3,3,3	3.79	1 (33%)	2,3,3	1.93	1 (50%)
25	CLA	B	613	-	69,73,73	1.13	6 (8%)	82,113,113	1.27	8 (9%)
25	CLA	c	508	-	68,72,73	1.13	5 (7%)	80,111,113	1.21	7 (8%)
25	CLA	a	607	36	69,73,73	1.13	7 (10%)	82,113,113	1.15	6 (7%)
32	LMG	B	621	-	51,51,55	0.72	1 (1%)	59,59,63	1.32	7 (11%)
27	BCR	t	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	6 (10%)
25	CLA	b	603	-	69,73,73	1.11	7 (10%)	82,113,113	1.14	5 (6%)
25	CLA	c	505	-	69,73,73	1.12	7 (10%)	82,113,113	1.18	4 (4%)
24	BCT	A	605	22	3,3,3	3.78	1 (33%)	2,3,3	1.94	1 (50%)
34	HEM	E	101	6,5	50,50,50	1.50	8 (16%)	67,82,82	1.10	1 (1%)
25	CLA	c	507	36	69,73,73	1.12	7 (10%)	82,113,113	1.26	5 (6%)
25	CLA	b	612	-	69,73,73	1.12	6 (8%)	82,113,113	1.20	5 (6%)
25	CLA	C	514	-	69,73,73	1.12	6 (8%)	82,113,113	1.18	5 (6%)
25	CLA	D	402	-	69,73,73	1.12	6 (8%)	82,113,113	1.12	5 (6%)
27	BCR	c	522	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	5 (8%)
32	LMG	C	501	-	48,48,55	0.73	0	56,56,63	1.30	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	d	405	-	48,48,48	0.62	1 (2%)	51,54,54	1.30	6 (11%)
25	CLA	B	610	36	69,73,73	1.13	7 (10%)	82,113,113	1.18	6 (7%)
32	LMG	C	520	-	48,48,55	0.76	0	56,56,63	1.33	6 (10%)
28	PL9	d	404	-	55,55,55	0.95	3 (5%)	68,69,69	1.46	12 (17%)
25	CLA	B	608	-	69,73,73	1.12	6 (8%)	82,113,113	1.16	4 (4%)
25	CLA	C	505	36	69,73,73	1.13	7 (10%)	82,113,113	1.17	7 (8%)
32	LMG	C	521	-	51,51,55	0.78	1 (1%)	59,59,63	1.35	6 (10%)
33	DGD	h	102	-	63,63,67	0.87	1 (1%)	77,77,81	1.35	7 (9%)
25	CLA	b	614	-	69,73,73	1.11	5 (7%)	82,113,113	1.20	6 (7%)
25	CLA	C	508	36	69,73,73	1.12	6 (8%)	82,113,113	1.26	6 (7%)
25	CLA	c	501	-	69,73,73	1.13	6 (8%)	82,113,113	1.23	7 (8%)
25	CLA	B	606	-	69,73,73	1.13	8 (11%)	82,113,113	1.21	5 (6%)
25	CLA	B	614	-	69,73,73	1.12	5 (7%)	82,113,113	1.12	6 (7%)
27	BCR	B	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	5 (8%)
26	PHO	a	609	-	58,69,69	2.18	9 (15%)	55,99,99	1.42	6 (10%)
25	CLA	c	502	-	69,73,73	1.13	6 (8%)	82,113,113	1.20	6 (7%)
25	CLA	c	513	-	69,73,73	1.12	6 (8%)	82,113,113	1.18	6 (7%)
28	PL9	D	405	-	55,55,55	0.94	3 (5%)	68,69,69	1.49	13 (19%)
33	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.39	9 (11%)
25	CLA	B	612	-	69,73,73	1.10	6 (8%)	82,113,113	1.23	6 (7%)
27	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.17	5 (8%)
25	CLA	A	613	36	69,73,73	1.11	6 (8%)	82,113,113	1.14	6 (7%)
25	CLA	A	607	36	69,73,73	1.14	7 (10%)	82,113,113	1.15	7 (8%)
27	BCR	c	521	-	41,41,41	1.12	2 (4%)	56,56,56	1.16	5 (8%)
27	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	3 (5%)
32	LMG	d	408	-	36,36,55	0.31	0	35,35,63	1.38	3 (8%)
27	BCR	H	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.19	5 (8%)
29	SQD	B	625	-	52,54,54	0.96	3 (5%)	62,65,65	1.43	8 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEC	V	201	16	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	A	608	-	-	5/37/103/103	0/5/6/6
29	SQD	B	624	-	-	26/49/69/69	0/1/1/1
29	SQD	D	409	-	-	20/42/62/69	0/1/1/1
25	CLA	b	601	36	1/1/15/20	14/39/115/115	-
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
25	CLA	B	611	-	1/1/15/20	7/39/115/115	-
33	DGD	C	519	-	-	17/51/91/95	0/2/2/2
27	BCR	C	516	-	-	3/29/63/63	0/2/2/2
29	SQD	f	101	-	-	8/36/56/69	0/1/1/1
32	LMG	D	407	-	-	14/46/66/70	0/1/1/1
25	CLA	c	512	-	1/1/15/20	13/39/115/115	-
32	LMG	a	614	-	-	19/46/66/70	0/1/1/1
27	BCR	a	611	-	-	3/29/63/63	0/2/2/2
25	CLA	b	606[A]	-	1/1/15/20	13/39/115/115	-
27	BCR	c	515	-	-	2/29/63/63	0/2/2/2
28	PL9	a	612	-	-	3/53/73/73	0/1/1/1
29	SQD	b	621	-	-	9/41/41/69	-
30	LHG	A	618	-	-	20/53/53/53	-
33	DGD	c	518	-	-	15/51/91/95	0/2/2/2
30	LHG	B	623	-	-	18/53/53/53	-
25	CLA	C	509	-	1/1/15/20	8/39/115/115	-
25	CLA	B	605	-	1/1/15/20	8/39/115/115	-
25	CLA	b	611	-	1/1/15/20	3/39/115/115	-
25	CLA	b	602	-	1/1/15/20	9/39/115/115	-
30	LHG	l	101	-	-	19/53/53/53	-
29	SQD	a	613	-	-	22/49/69/69	0/1/1/1
34	HEM	e	101	6,5	-	4/14/54/54	-
25	CLA	b	608	-	1/1/15/20	7/39/115/115	-
29	SQD	A	612	-	-	14/47/67/69	0/1/1/1
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2
28	PL9	A	611	-	-	13/53/73/73	0/1/1/1
25	CLA	c	503	-	1/1/15/20	13/39/115/115	-
32	LMG	c	520	-	-	18/29/49/70	0/1/1/1
25	CLA	b	616	-	1/1/11/20	6/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	A	614	-	-	16/51/51/53	-
32	LMG	b	620	-	-	19/46/66/70	0/1/1/1
25	CLA	b	604	-	1/1/15/20	12/39/115/115	-
25	CLA	C	503	-	1/1/15/20	9/39/115/115	-
25	CLA	b	605	-	1/1/15/20	8/39/115/115	-
25	CLA	c	504	36	1/1/14/20	5/33/109/115	-
25	CLA	b	613	-	1/1/15/20	11/39/115/115	-
35	HEC	v	201	16	-	2/14/54/54	-
27	BCR	b	618	-	-	10/29/63/63	0/2/2/2
30	LHG	D	406	-	-	17/53/53/53	-
25	CLA	C	504	-	1/1/15/20	9/39/115/115	-
25	CLA	A	609	-	1/1/12/20	4/26/102/115	-
30	LHG	a	616	-	-	17/43/43/53	-
27	BCR	d	403	-	-	4/29/63/63	0/2/2/2
33	DGD	H	102	-	-	13/51/91/95	0/2/2/2
33	DGD	c	516	-	-	20/51/91/95	0/2/2/2
25	CLA	B	602	-	1/1/15/20	2/39/115/115	-
30	LHG	L	102	-	-	19/53/53/53	-
27	BCR	T	101	-	-	8/29/63/63	0/2/2/2
25	CLA	B	616	-	1/1/15/20	14/39/115/115	-
25	CLA	c	509	-	1/1/15/20	11/39/115/115	-
27	BCR	K	101	-	-	3/29/63/63	0/2/2/2
33	DGD	C	517	-	-	23/51/91/95	0/2/2/2
25	CLA	c	510	-	1/1/15/20	12/39/115/115	-
25	CLA	a	615	36	1/1/15/20	8/39/115/115	-
25	CLA	B	615	-	1/1/15/20	7/39/115/115	-
25	CLA	B	607	36	1/1/15/20	8/39/115/115	-
25	CLA	C	507	-	1/1/15/20	12/39/115/115	-
25	CLA	D	403	-	1/1/15/20	8/39/115/115	-
25	CLA	C	502	-	1/1/15/20	12/39/115/115	-
25	CLA	c	511	3	1/1/15/20	11/39/115/115	-
32	LMG	B	620	-	-	17/46/66/70	0/1/1/1
25	CLA	B	604	-	1/1/15/20	8/39/115/115	-
25	CLA	B	601	36	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	610	-	1/1/15/20	5/39/115/115	-
32	LMG	c	519	-	-	12/31/51/70	0/1/1/1
27	BCR	h	101	-	-	6/29/63/63	0/2/2/2
26	PHO	D	401	-	-	4/37/103/103	0/5/6/6
26	PHO	a	608	-	-	6/37/103/103	0/5/6/6
32	LMG	B	626	-	-	25/46/66/70	0/1/1/1
25	CLA	d	402	-	1/1/15/20	9/39/115/115	-
30	LHG	a	617	-	-	19/46/46/53	-
25	CLA	c	506	-	1/1/15/20	19/39/115/115	-
25	CLA	C	510	-	1/1/15/20	5/39/115/115	-
25	CLA	b	615	-	1/1/15/20	5/39/115/115	-
25	CLA	b	607	36	1/1/15/20	11/39/115/115	-
29	SQD	L	101	-	-	22/44/64/69	0/1/1/1
25	CLA	b	606[B]	-	1/1/15/20	8/39/115/115	-
27	BCR	A	610	-	-	4/29/63/63	0/2/2/2
25	CLA	B	609	-	1/1/15/20	7/39/115/115	-
25	CLA	C	506	-	1/1/15/20	7/39/115/115	-
25	CLA	b	610	36	1/1/15/20	11/39/115/115	-
25	CLA	a	606	-	1/1/15/20	3/39/115/115	-
25	CLA	C	511	-	1/1/15/20	9/39/115/115	-
32	LMG	d	407	-	-	18/46/66/70	0/1/1/1
33	DGD	c	517	-	-	20/51/91/95	0/2/2/2
25	CLA	B	603	-	1/1/15/20	10/39/115/115	-
27	BCR	D	404	-	-	2/29/63/63	0/2/2/2
32	LMG	m	102	-	-	22/46/66/70	0/1/1/1
27	BCR	c	514	-	-	1/29/63/63	0/2/2/2
25	CLA	A	606	-	1/1/15/20	10/39/115/115	-
29	SQD	D	408	-	-	9/38/58/69	0/1/1/1
27	BCR	C	515	-	-	1/29/63/63	0/2/2/2
29	SQD	A	616	-	-	14/49/69/69	0/1/1/1
25	CLA	d	401	-	1/1/15/20	10/39/115/115	-
25	CLA	C	512	3	1/1/15/20	7/39/115/115	-
25	CLA	b	609	-	1/1/15/20	12/39/115/115	-
27	BCR	Y	101	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	d	406	-	-	23/53/53/53	-
25	CLA	C	513	-	1/1/15/20	15/39/115/115	-
25	CLA	B	613	-	1/1/15/20	12/39/115/115	-
25	CLA	c	508	-	1/1/14/20	7/38/114/115	-
25	CLA	a	607	36	1/1/15/20	9/39/115/115	-
32	LMG	B	621	-	-	20/46/66/70	0/1/1/1
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
25	CLA	b	603	-	1/1/15/20	12/39/115/115	-
25	CLA	c	505	-	1/1/15/20	16/39/115/115	-
34	HEM	E	101	6,5	-	3/14/54/54	-
25	CLA	c	507	36	1/1/15/20	13/39/115/115	-
25	CLA	b	612	-	1/1/15/20	13/39/115/115	-
25	CLA	C	514	-	1/1/15/20	14/39/115/115	-
25	CLA	D	402	-	1/1/15/20	6/39/115/115	-
27	BCR	c	522	-	-	4/29/63/63	0/2/2/2
32	LMG	C	501	-	-	23/43/63/70	0/1/1/1
30	LHG	d	405	-	-	23/53/53/53	-
25	CLA	B	610	36	1/1/15/20	7/39/115/115	-
32	LMG	C	520	-	-	22/43/63/70	0/1/1/1
28	PL9	d	404	-	-	8/53/73/73	0/1/1/1
25	CLA	B	608	-	1/1/15/20	10/39/115/115	-
25	CLA	C	505	36	1/1/15/20	7/39/115/115	-
32	LMG	C	521	-	-	21/46/66/70	0/1/1/1
33	DGD	h	102	-	-	15/51/91/95	0/2/2/2
25	CLA	b	614	-	1/1/15/20	16/39/115/115	-
25	CLA	C	508	36	1/1/15/20	15/39/115/115	-
25	CLA	c	501	-	1/1/15/20	5/39/115/115	-
25	CLA	B	606	-	1/1/15/20	14/39/115/115	-
25	CLA	B	614	-	1/1/15/20	20/39/115/115	-
27	BCR	B	619	-	-	3/29/63/63	0/2/2/2
26	PHO	a	609	-	-	10/37/103/103	0/5/6/6
25	CLA	c	502	-	1/1/15/20	12/39/115/115	-
25	CLA	c	513	-	1/1/15/20	13/39/115/115	-
28	PL9	D	405	-	-	7/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	C	518	-	-	21/51/91/95	0/2/2/2
25	CLA	B	612	-	1/1/15/20	6/39/115/115	-
27	BCR	B	617	-	-	4/29/63/63	0/2/2/2
25	CLA	A	613	36	1/1/15/20	4/39/115/115	-
25	CLA	A	607	36	1/1/15/20	9/39/115/115	-
27	BCR	c	521	-	-	6/29/63/63	0/2/2/2
27	BCR	b	619	-	-	5/29/63/63	0/2/2/2
32	LMG	d	408	-	-	18/32/32/70	-
27	BCR	H	101	-	-	5/29/63/63	0/2/2/2
29	SQD	B	625	-	-	25/49/69/69	0/1/1/1

The worst 5 of 625 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	C1B-C2B	9.85	1.50	1.39
26	a	609	PHO	C1B-C2B	9.65	1.50	1.39
26	a	608	PHO	C1B-C2B	9.60	1.50	1.39
26	D	401	PHO	C1B-C2B	9.57	1.50	1.39
26	a	609	PHO	C3B-C4B	8.90	1.50	1.41

The worst 5 of 893 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	C4A-NA-C1A	6.80	109.78	106.68
26	D	401	PHO	C4D-CHA-CBD	-6.48	105.35	108.45
25	B	604	CLA	C4A-NA-C1A	6.38	109.59	106.68
25	c	503	CLA	C4A-NA-C1A	6.36	109.58	106.68
25	C	508	CLA	C4A-NA-C1A	6.30	109.56	106.68

5 of 71 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	609	CLA	ND
25	A	613	CLA	ND
25	B	601	CLA	ND

5 of 1629 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB
25	B	608	CLA	C6-C7-C8-C9

There are no ring outliers.

124 monomers are involved in 247 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	608	PHO	2	0
29	B	624	SQD	4	0
29	D	409	SQD	1	0
25	b	601	CLA	2	0
25	B	611	CLA	1	0
33	C	519	DGD	1	0
27	C	516	BCR	2	0
29	f	101	SQD	1	0
32	D	407	LMG	1	0
25	c	512	CLA	3	0
27	a	611	BCR	2	0
25	b	606[A]	CLA	4	0
27	c	515	BCR	3	0
28	a	612	PL9	3	0
29	b	621	SQD	3	0
30	A	618	LHG	3	0
33	c	518	DGD	1	0
30	B	623	LHG	4	0
25	C	509	CLA	4	0
25	B	605	CLA	4	0
25	b	611	CLA	3	0
25	b	602	CLA	3	0
30	l	101	LHG	1	0
34	e	101	HEM	3	0
25	b	608	CLA	1	0
27	B	618	BCR	3	0
28	A	611	PL9	3	0
25	b	604	CLA	3	0
25	C	503	CLA	1	0
25	b	605	CLA	1	0
27	b	618	BCR	1	0
30	D	406	LHG	3	0
25	C	504	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	609	CLA	1	0
27	d	403	BCR	2	0
33	H	102	DGD	1	0
33	c	516	DGD	1	0
25	B	602	CLA	1	0
30	L	102	LHG	1	0
27	T	101	BCR	3	0
25	B	616	CLA	1	0
25	c	509	CLA	2	0
27	K	101	BCR	2	0
33	C	517	DGD	1	0
25	c	510	CLA	1	0
25	B	615	CLA	5	0
25	B	607	CLA	1	0
25	C	507	CLA	2	0
25	D	403	CLA	2	0
25	C	502	CLA	3	0
25	c	511	CLA	2	0
32	B	620	LMG	1	0
25	B	604	CLA	3	0
25	B	601	CLA	5	0
25	a	610	CLA	1	0
27	h	101	BCR	3	0
26	a	608	PHO	2	0
32	B	626	LMG	1	0
25	d	402	CLA	2	0
30	a	617	LHG	2	0
25	c	506	CLA	2	0
25	C	510	CLA	3	0
25	b	615	CLA	3	0
25	b	607	CLA	1	0
29	L	101	SQD	3	0
25	b	606[B]	CLA	3	0
27	A	610	BCR	2	0
25	B	609	CLA	5	0
25	C	506	CLA	3	0
25	b	610	CLA	3	0
25	a	606	CLA	3	0
25	C	511	CLA	2	0
32	d	407	LMG	1	0
33	c	517	DGD	2	0
25	B	603	CLA	2	0

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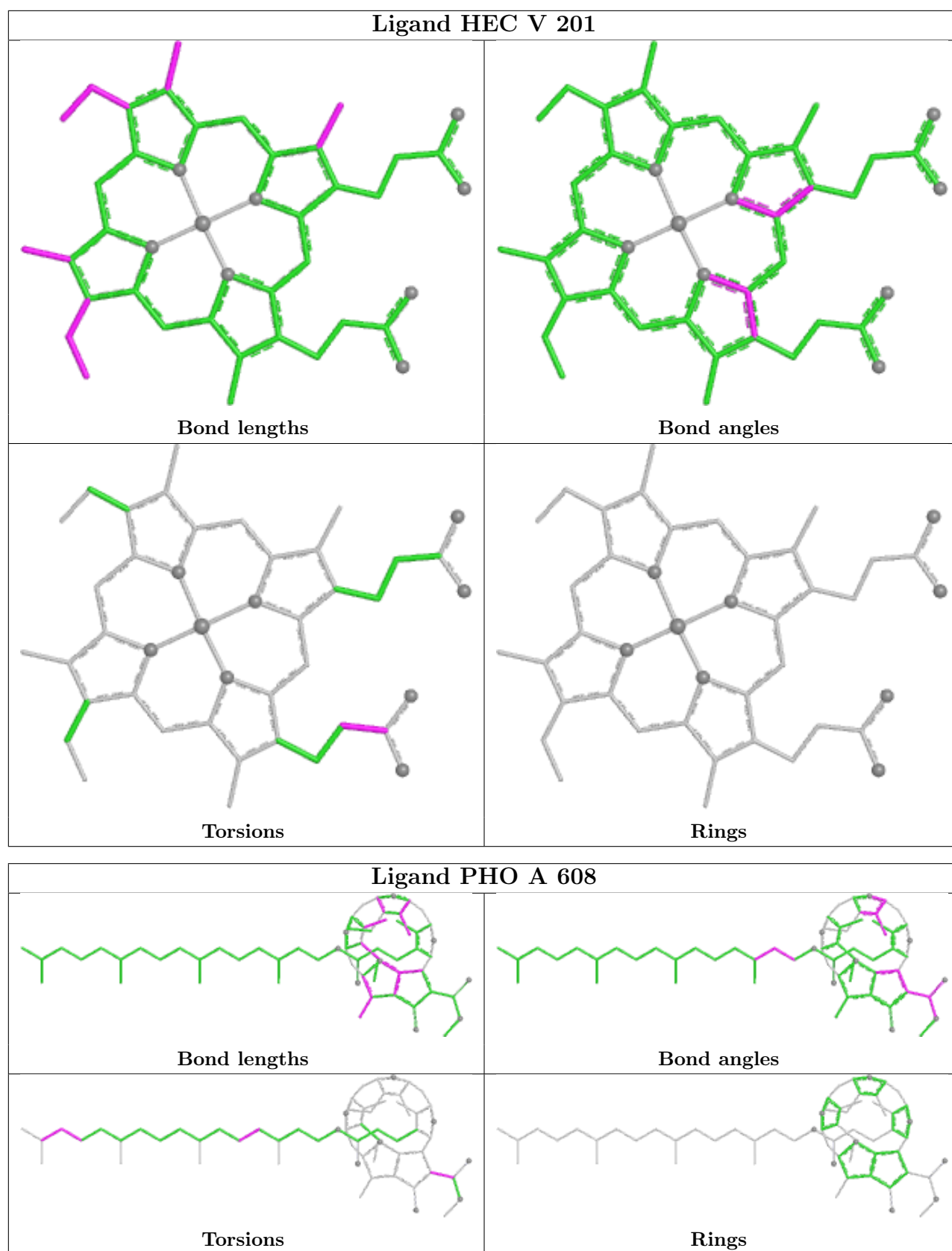
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27	D	404	BCR	4	0
32	m	102	LMG	1	0
27	c	514	BCR	3	0
25	A	606	CLA	4	0
29	D	408	SQD	2	0
27	C	515	BCR	2	0
29	A	616	SQD	2	0
25	d	401	CLA	4	0
25	b	609	CLA	3	0
27	Y	101	BCR	4	0
30	d	406	LHG	3	0
25	C	513	CLA	4	0
25	B	613	CLA	3	0
25	c	508	CLA	3	0
25	a	607	CLA	4	0
32	B	621	LMG	1	0
27	t	101	BCR	3	0
25	b	603	CLA	1	0
25	c	505	CLA	4	0
34	E	101	HEM	3	0
25	c	507	CLA	3	0
25	b	612	CLA	1	0
25	C	514	CLA	2	0
25	D	402	CLA	4	0
27	c	522	BCR	2	0
32	C	501	LMG	1	0
30	d	405	LHG	2	0
25	B	610	CLA	1	0
28	d	404	PL9	1	0
25	B	608	CLA	2	0
25	C	505	CLA	2	0
32	C	521	LMG	1	0
33	h	102	DGD	1	0
25	b	614	CLA	3	0
25	C	508	CLA	3	0
25	c	501	CLA	2	0
25	B	606	CLA	3	0
25	B	614	CLA	6	0
27	B	619	BCR	4	0
26	a	609	PHO	3	0
25	c	513	CLA	1	0
33	C	518	DGD	2	0

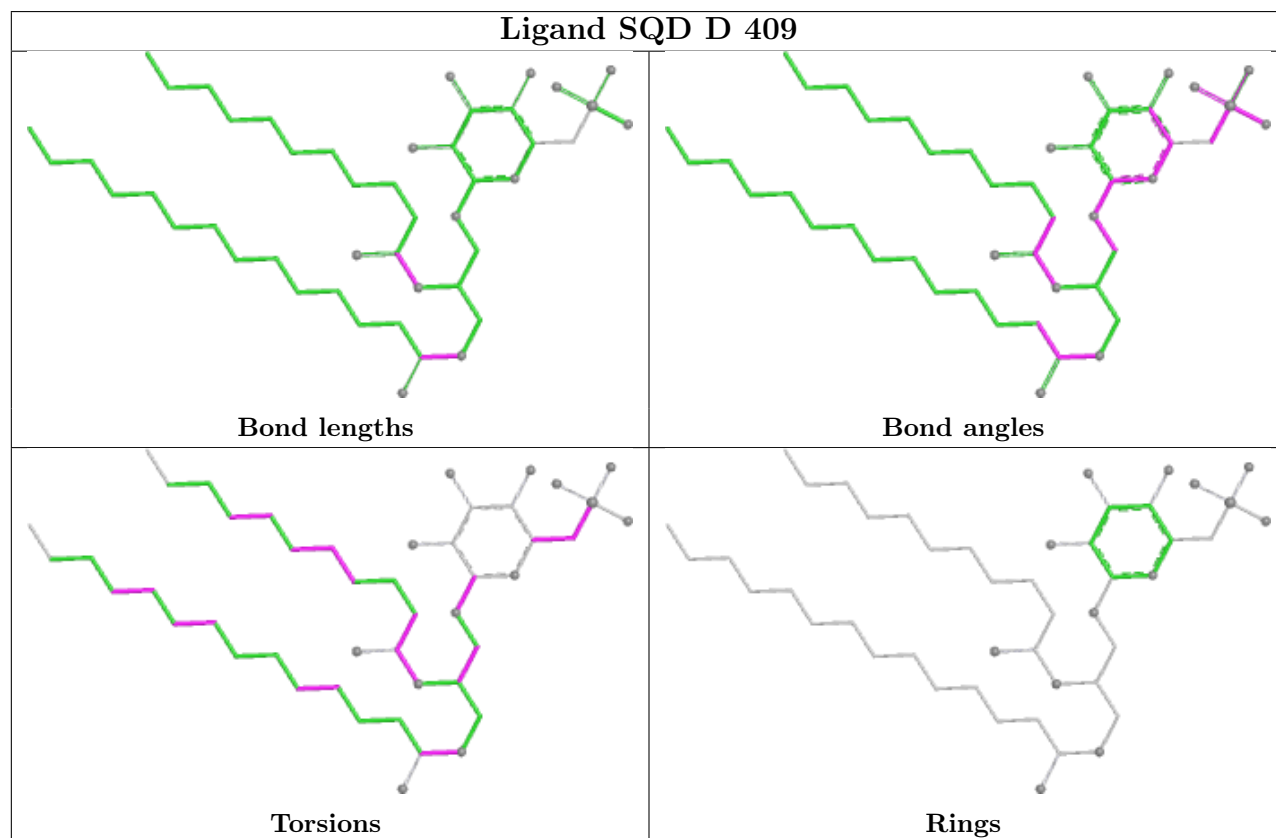
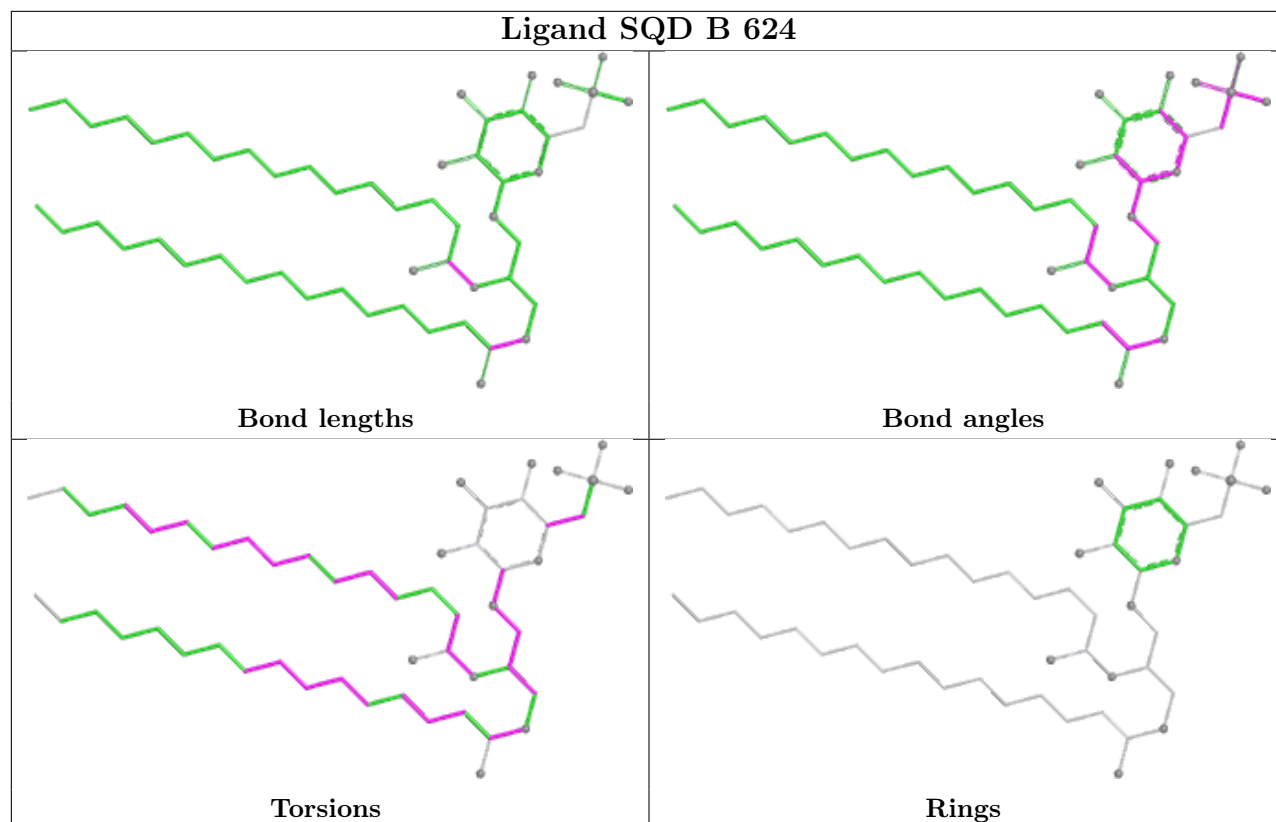
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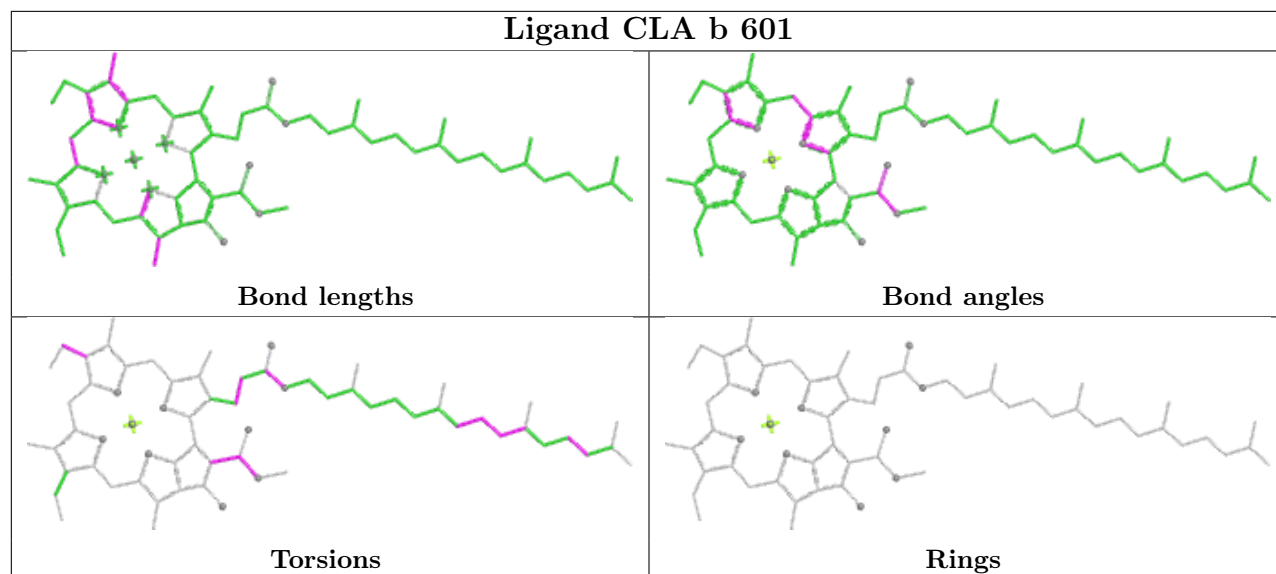
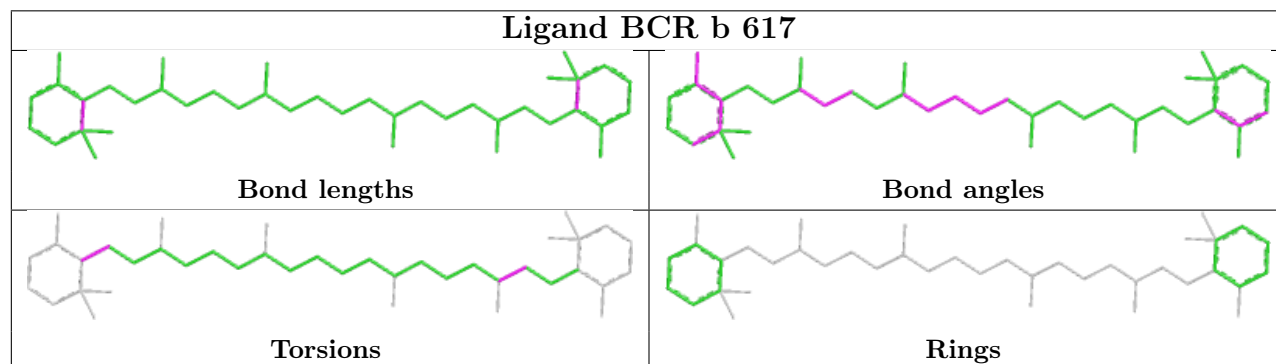
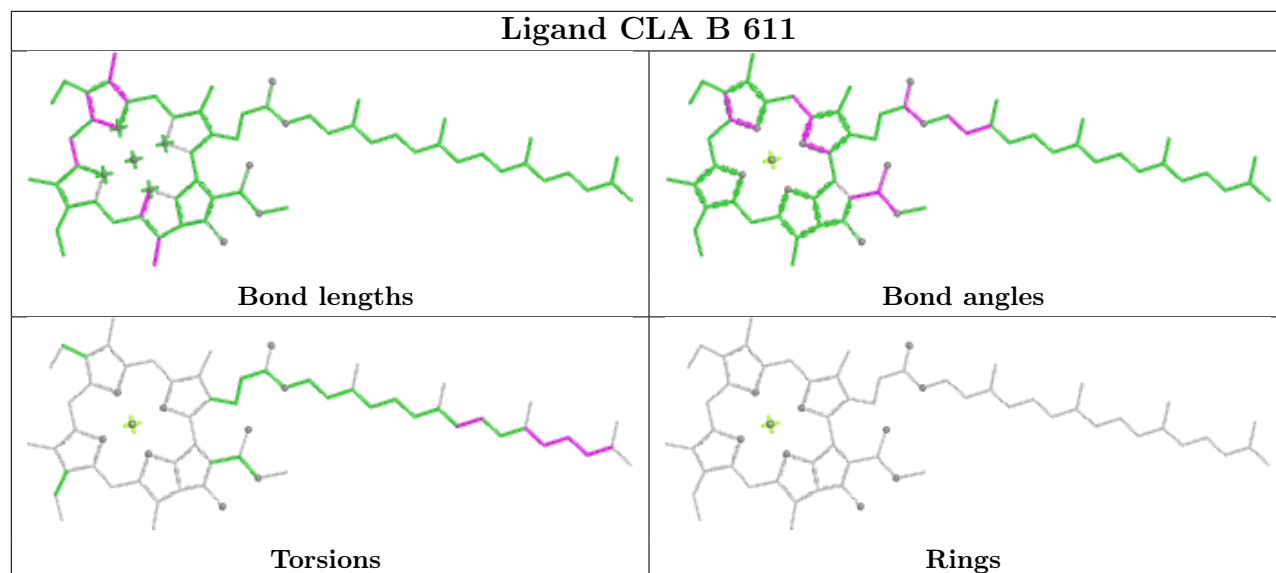
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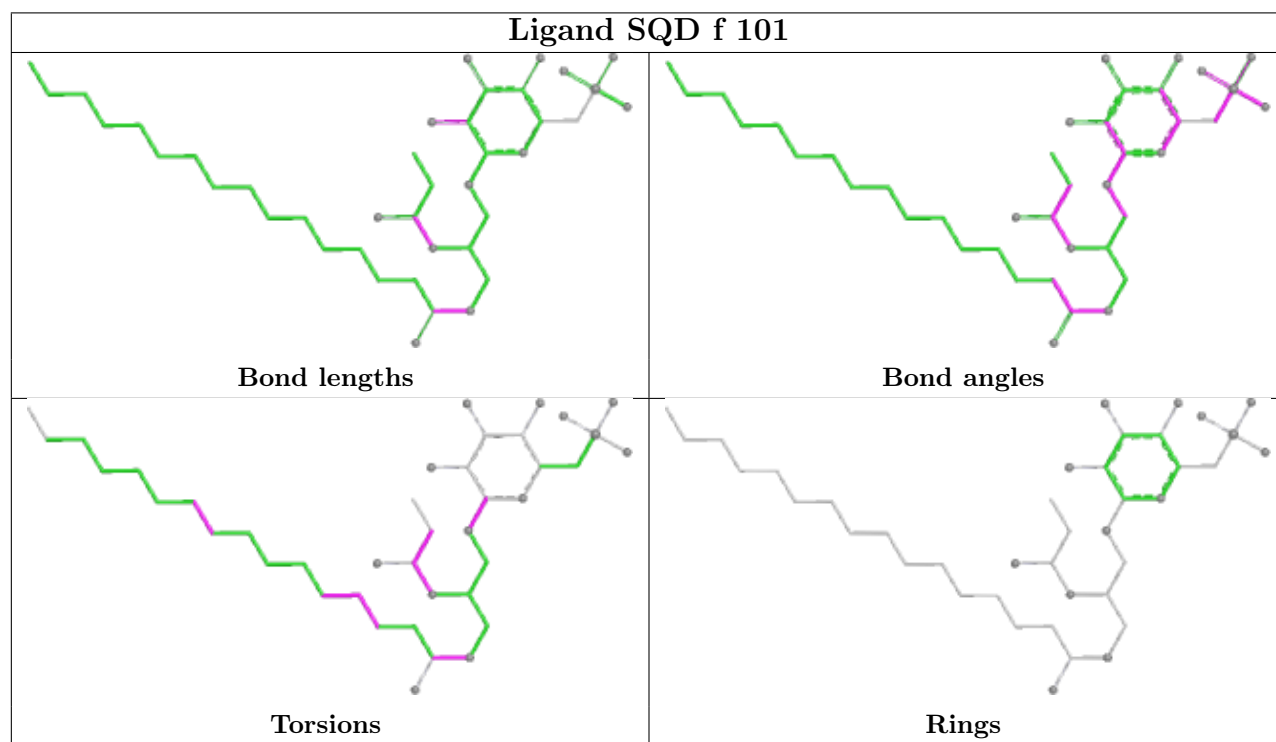
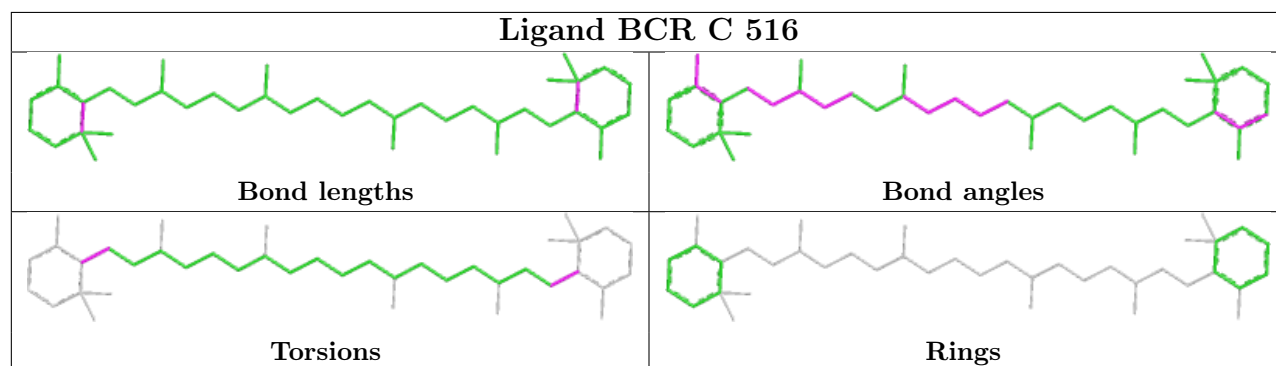
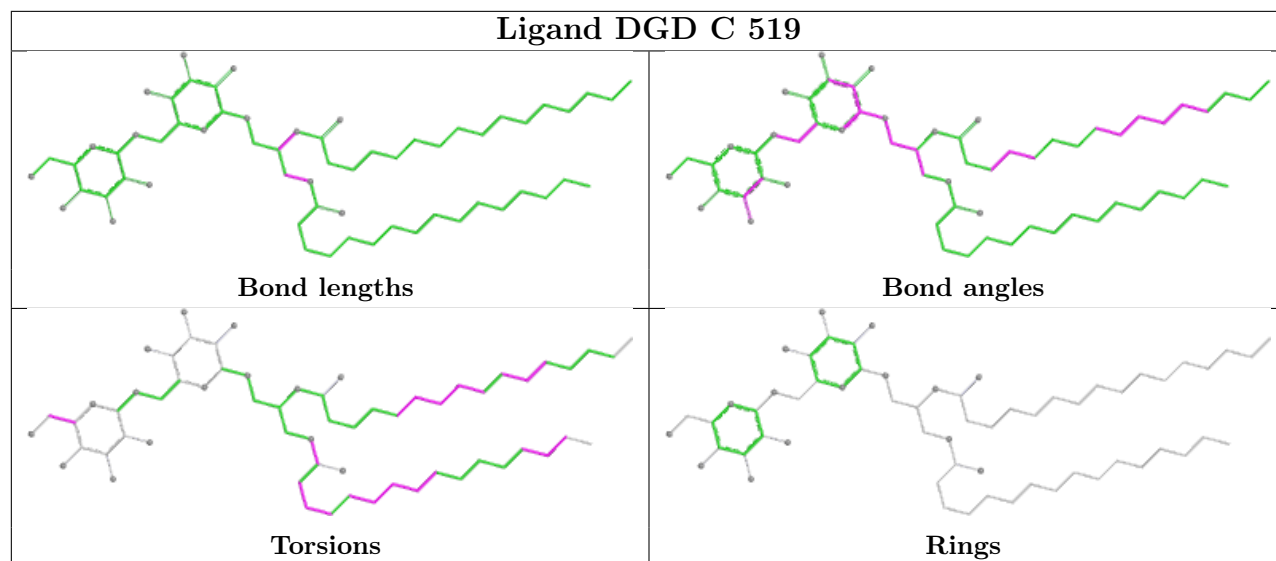
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	617	BCR	4	0
25	A	613	CLA	1	0
25	A	607	CLA	5	0
27	c	521	BCR	3	0
32	d	408	LMG	3	0
27	H	101	BCR	1	0
29	B	625	SQD	2	0

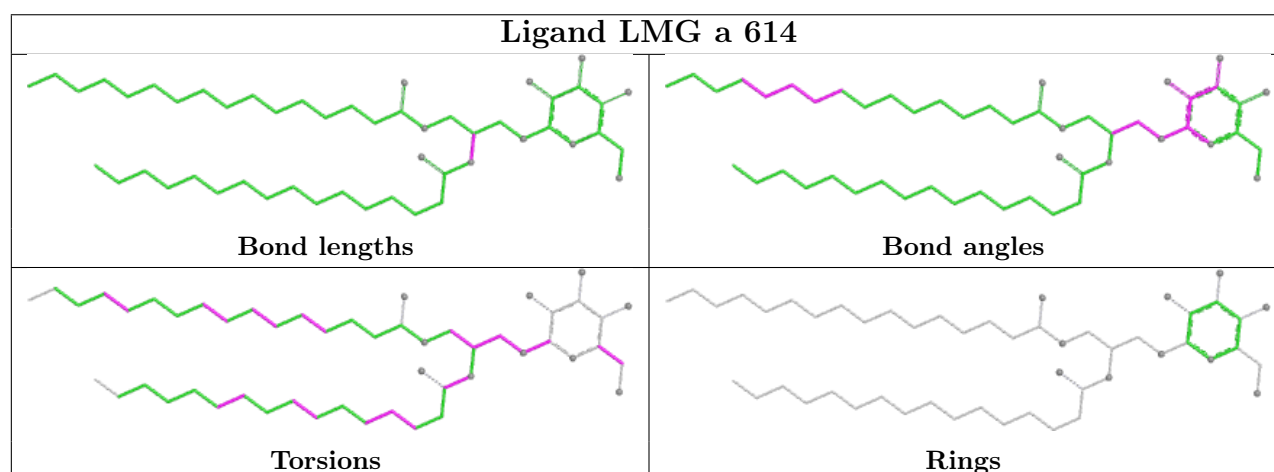
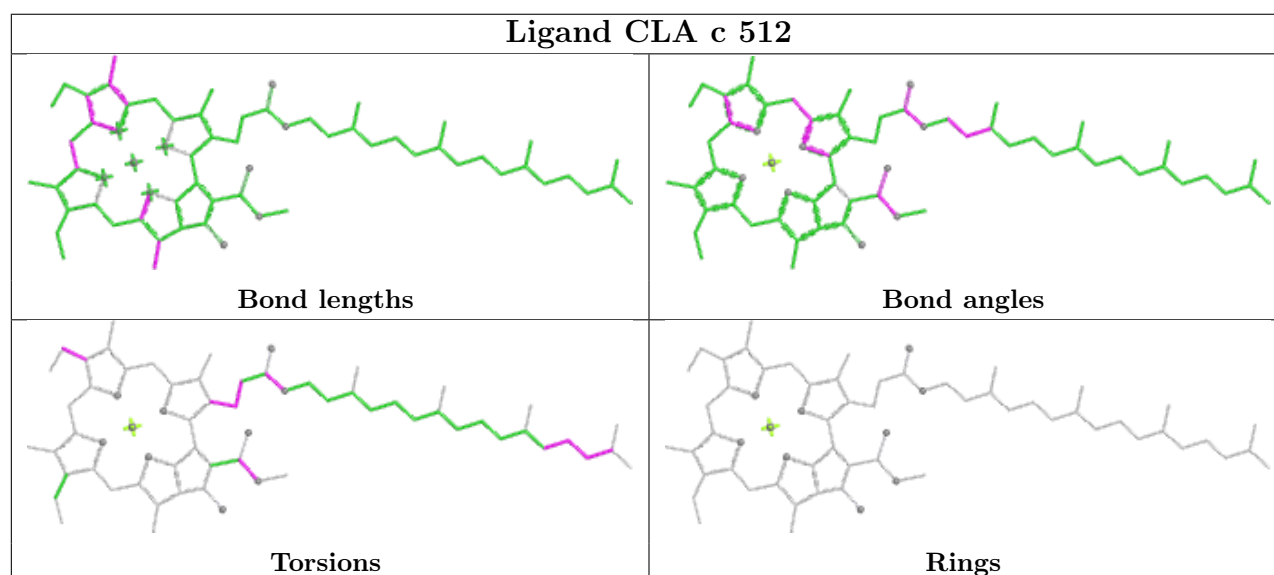
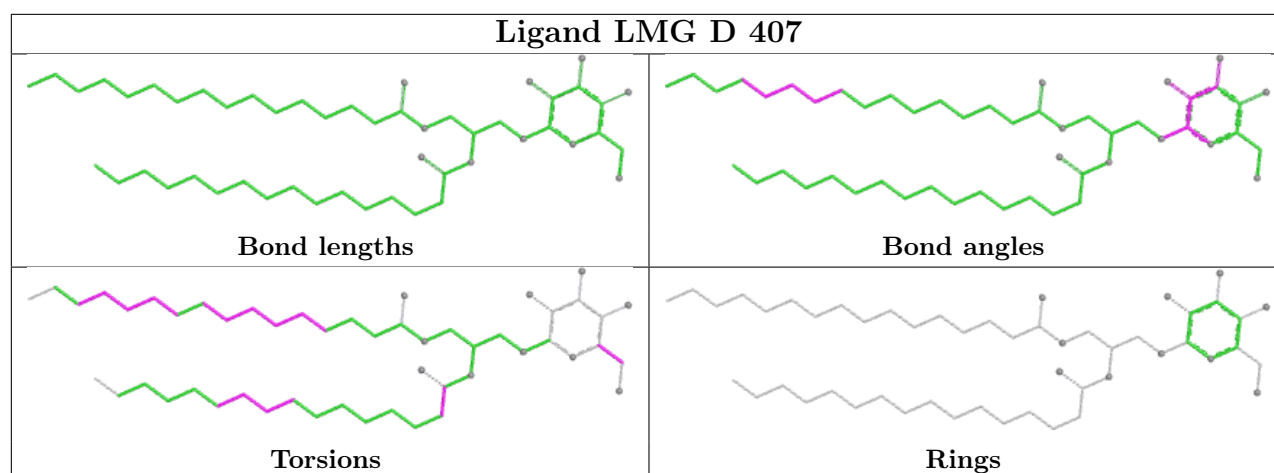
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

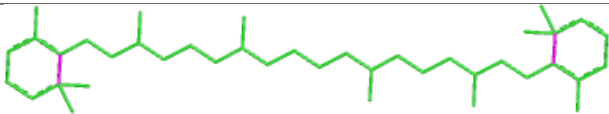
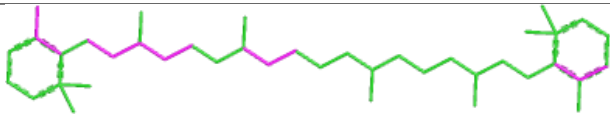
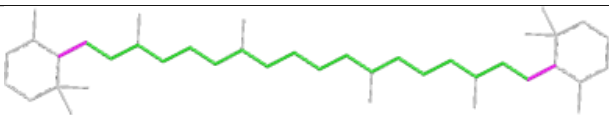
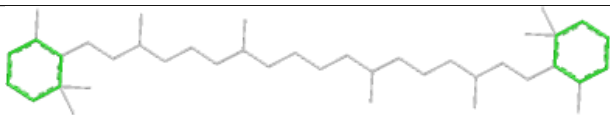


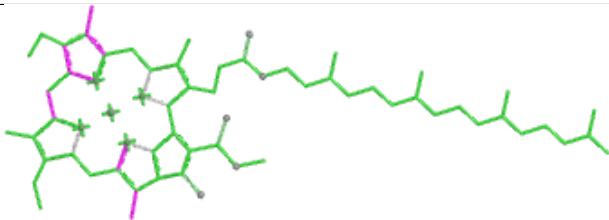
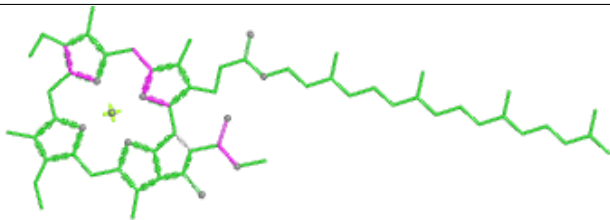
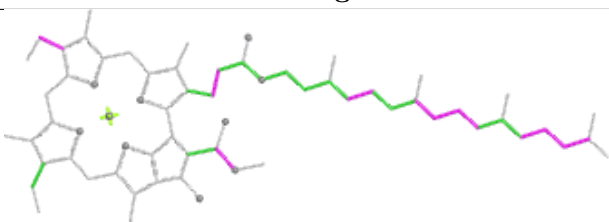
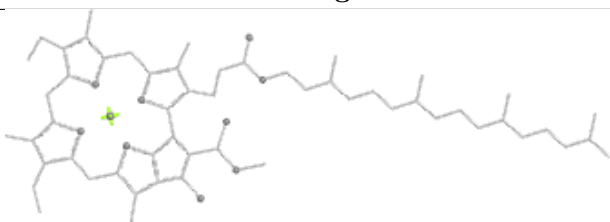


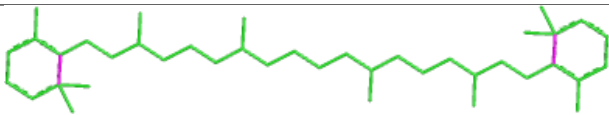
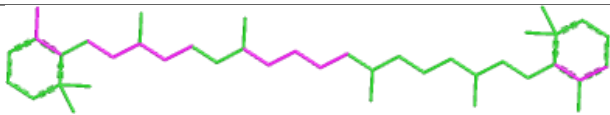
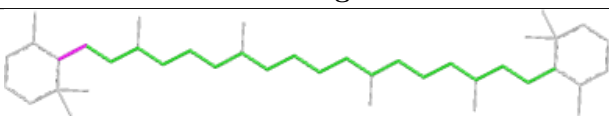
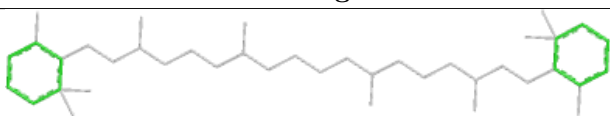
Ligand CLA b 601**Ligand BCR b 617****Ligand CLA B 611**

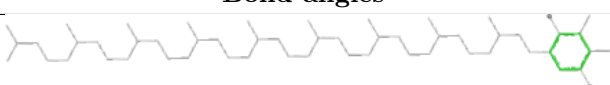


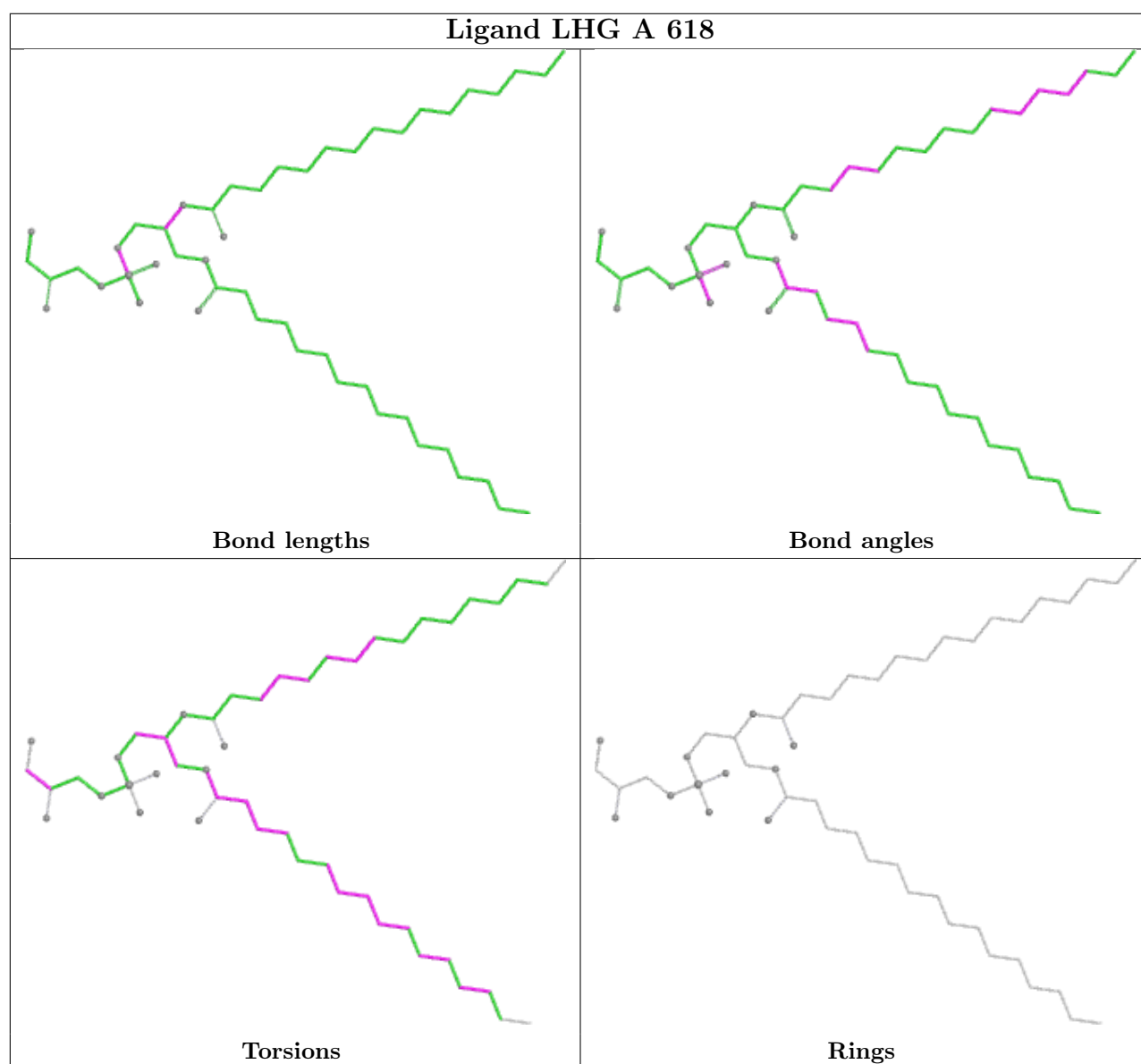
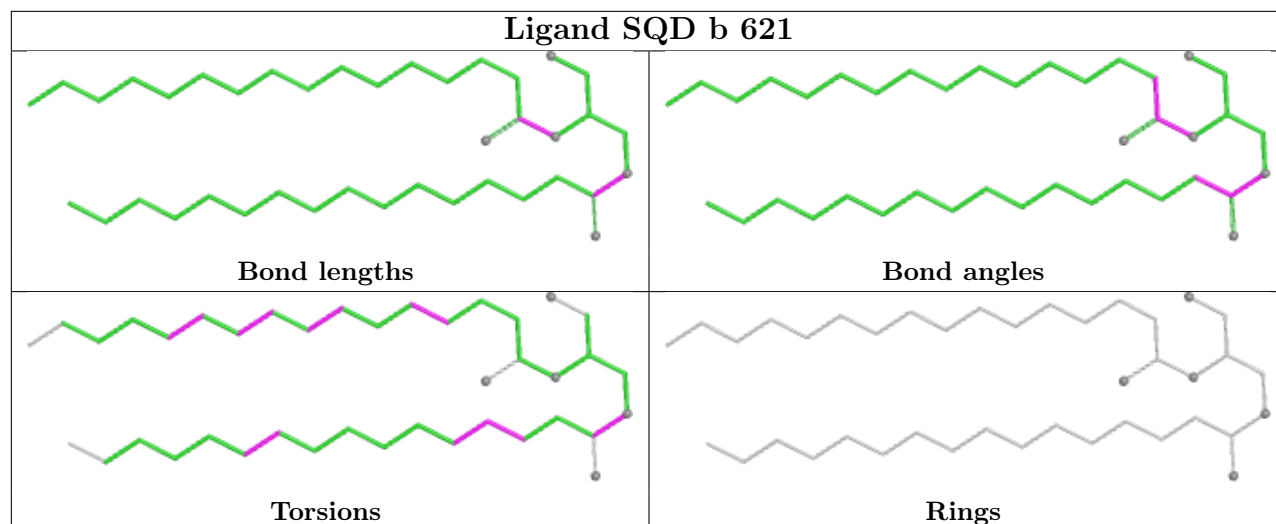


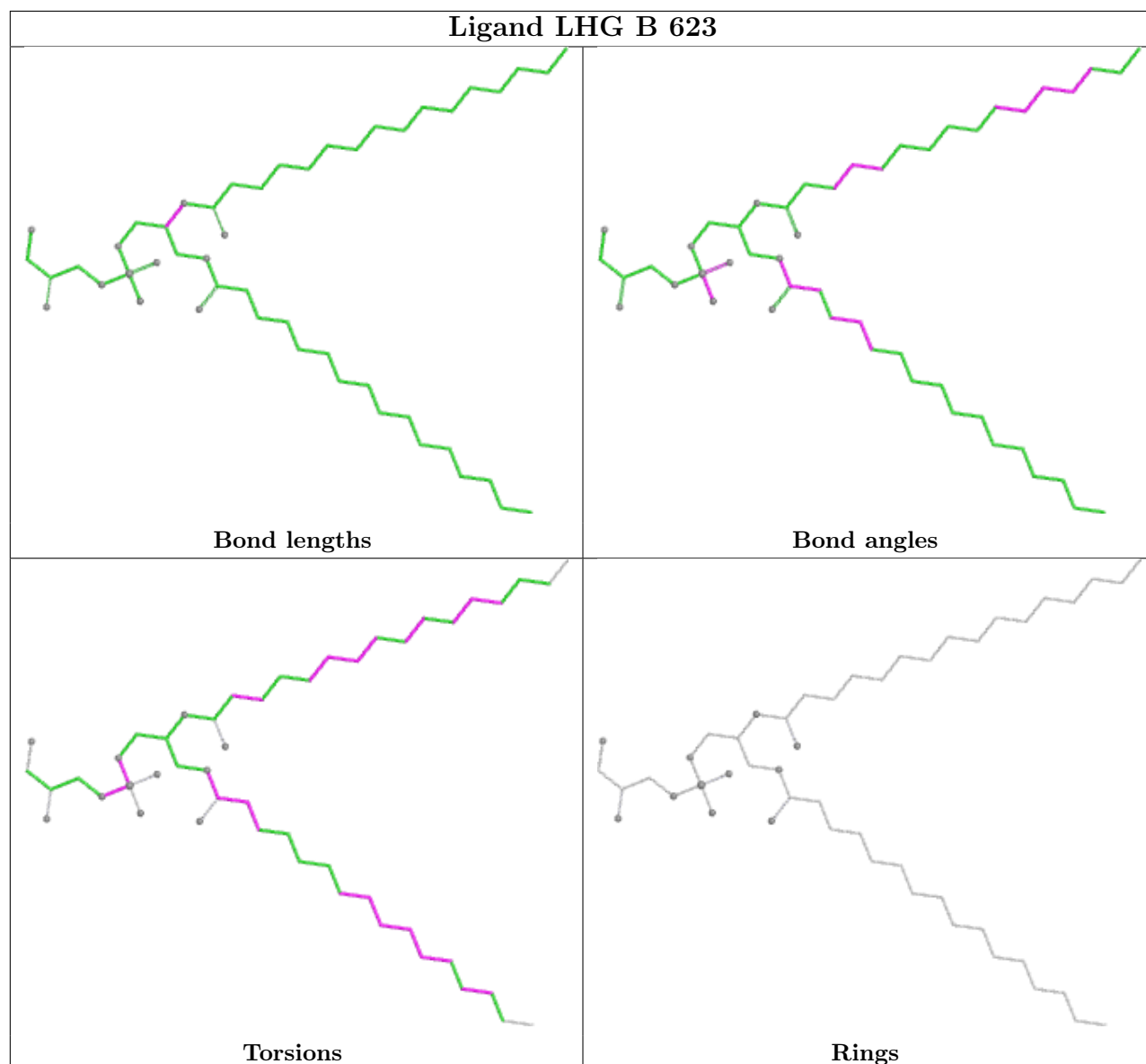
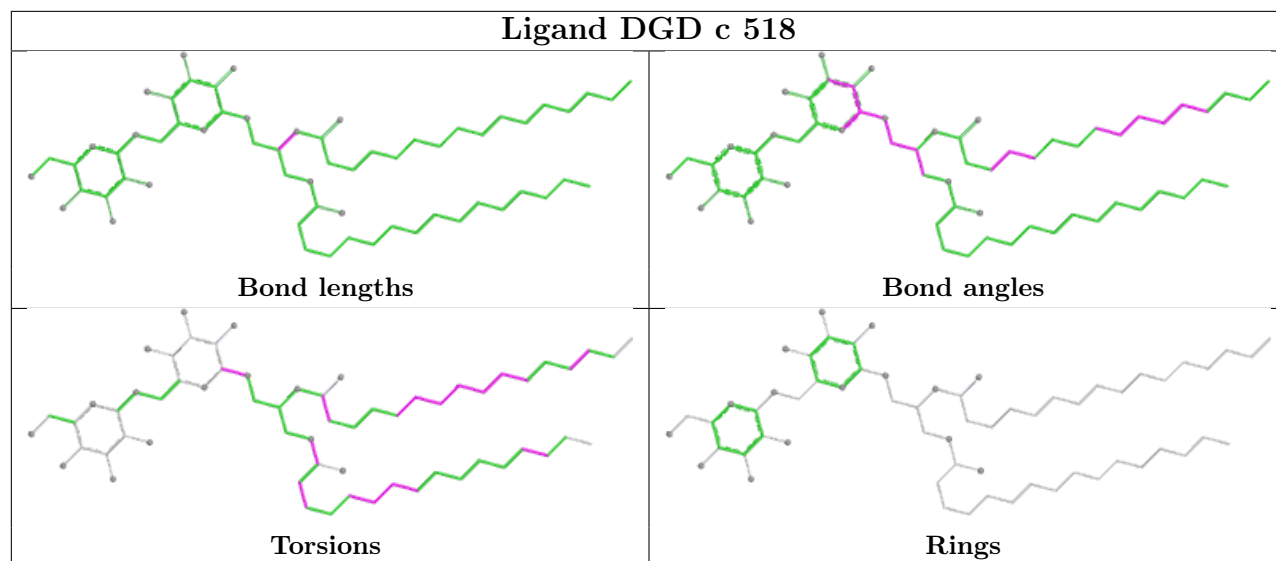
Ligand BCR a 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

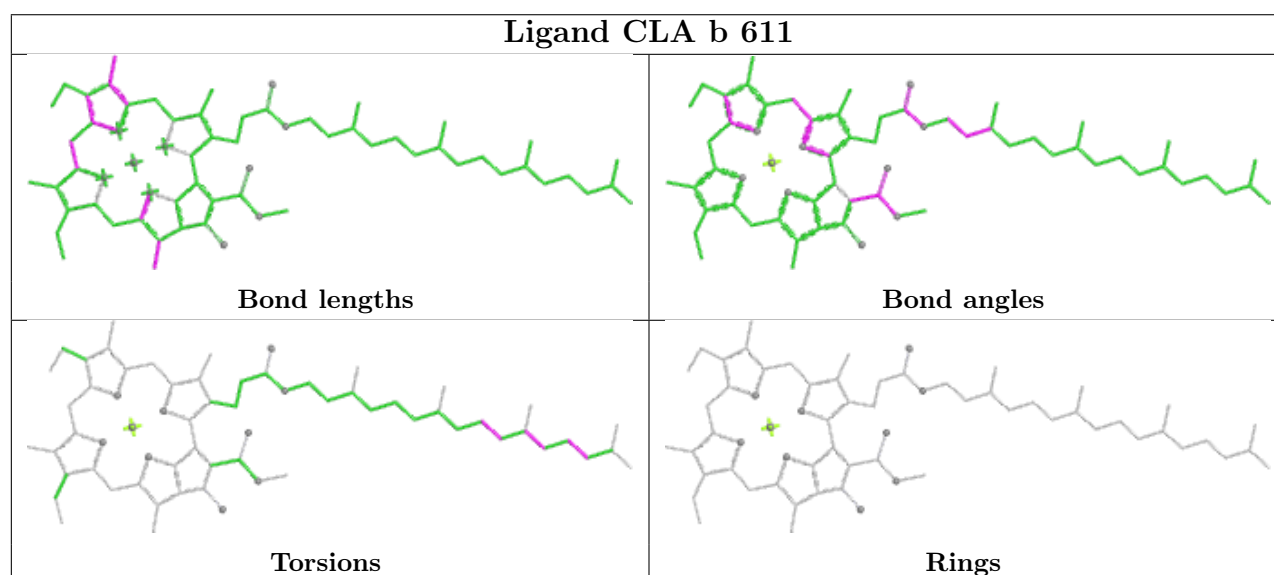
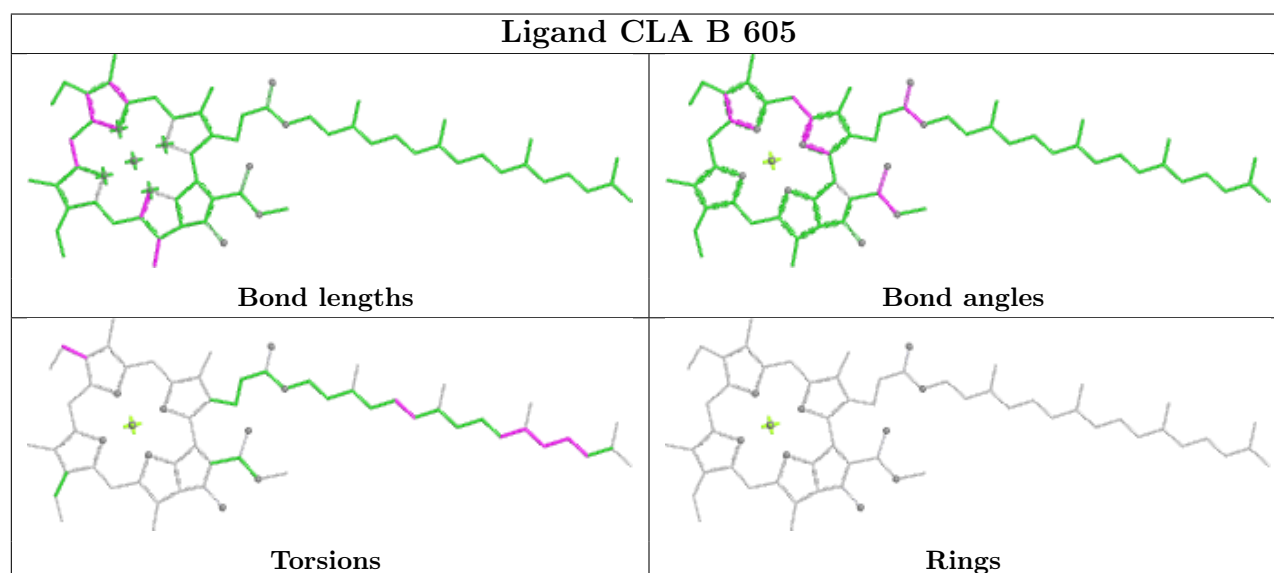
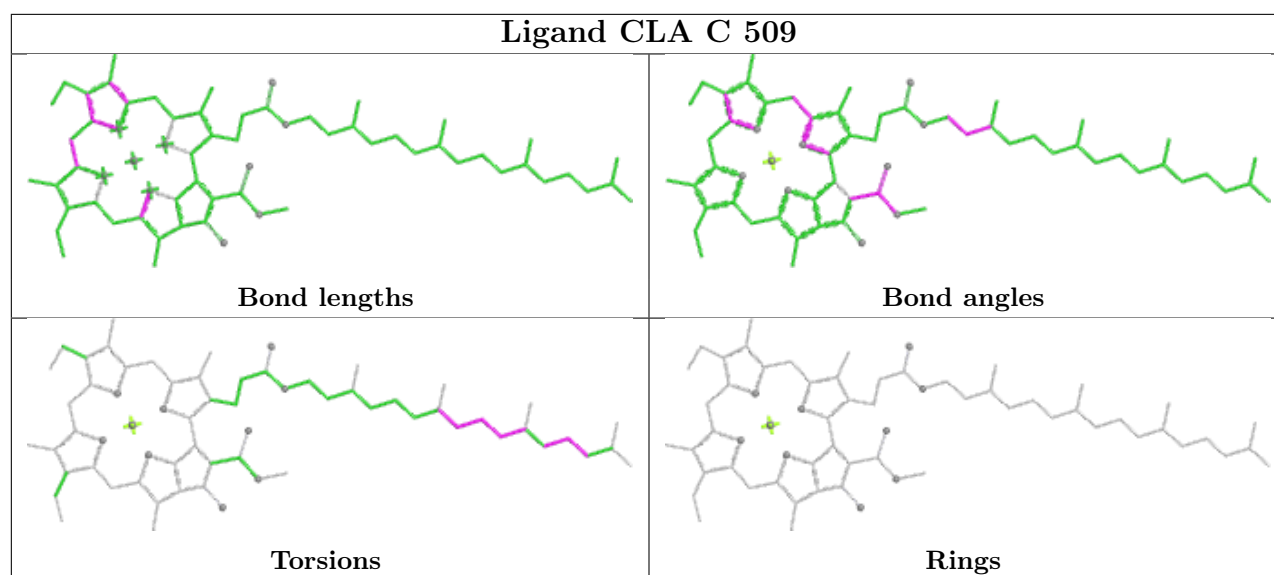
Ligand CLA b 606 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

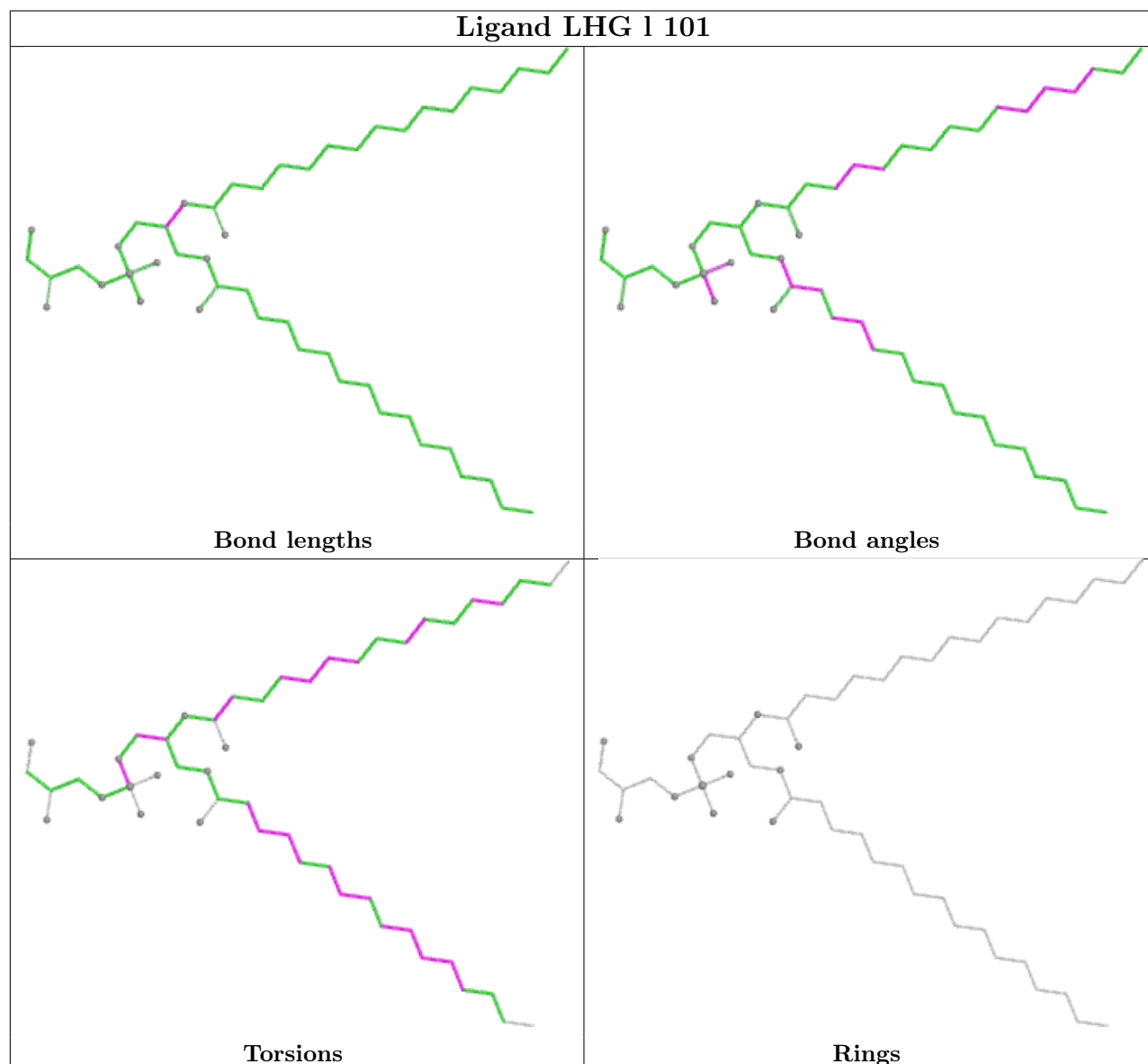
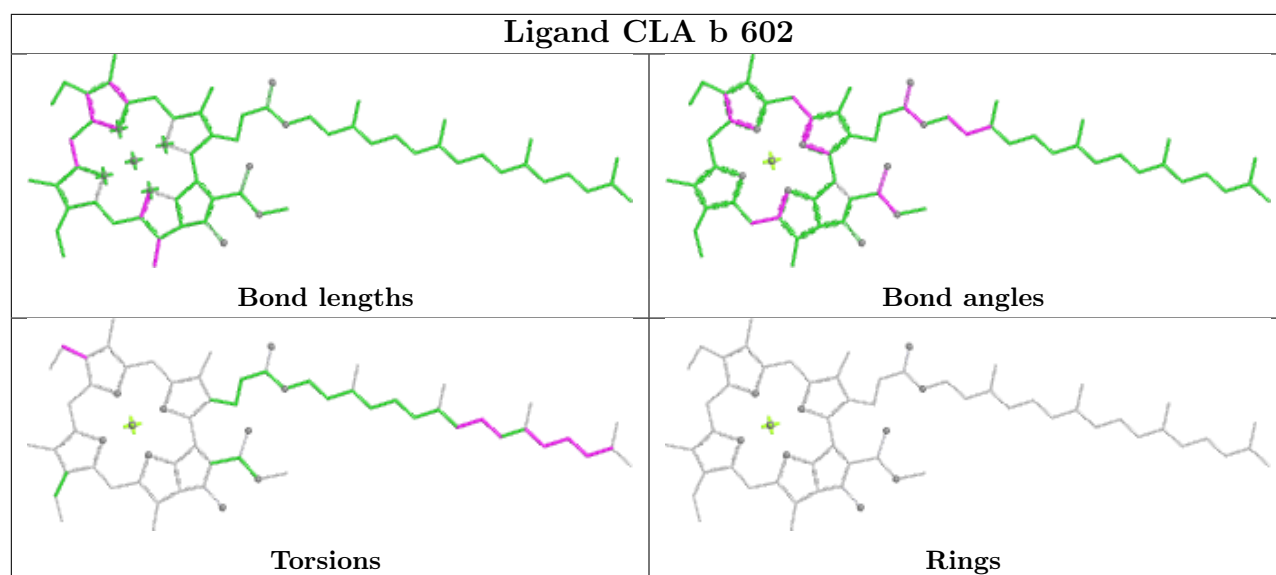
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

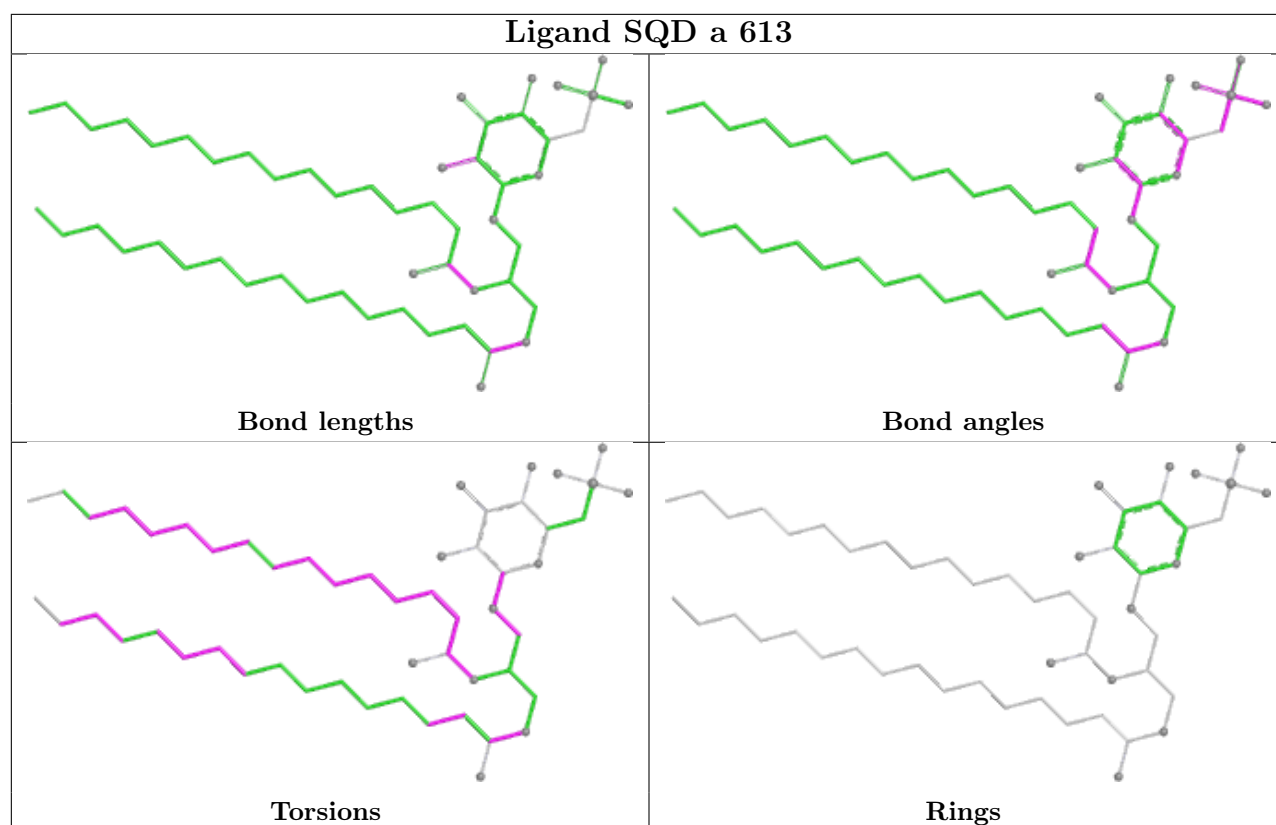
Ligand PL9 a 612	
	
Bond lengths	Bond angles
	
Torsions	Rings



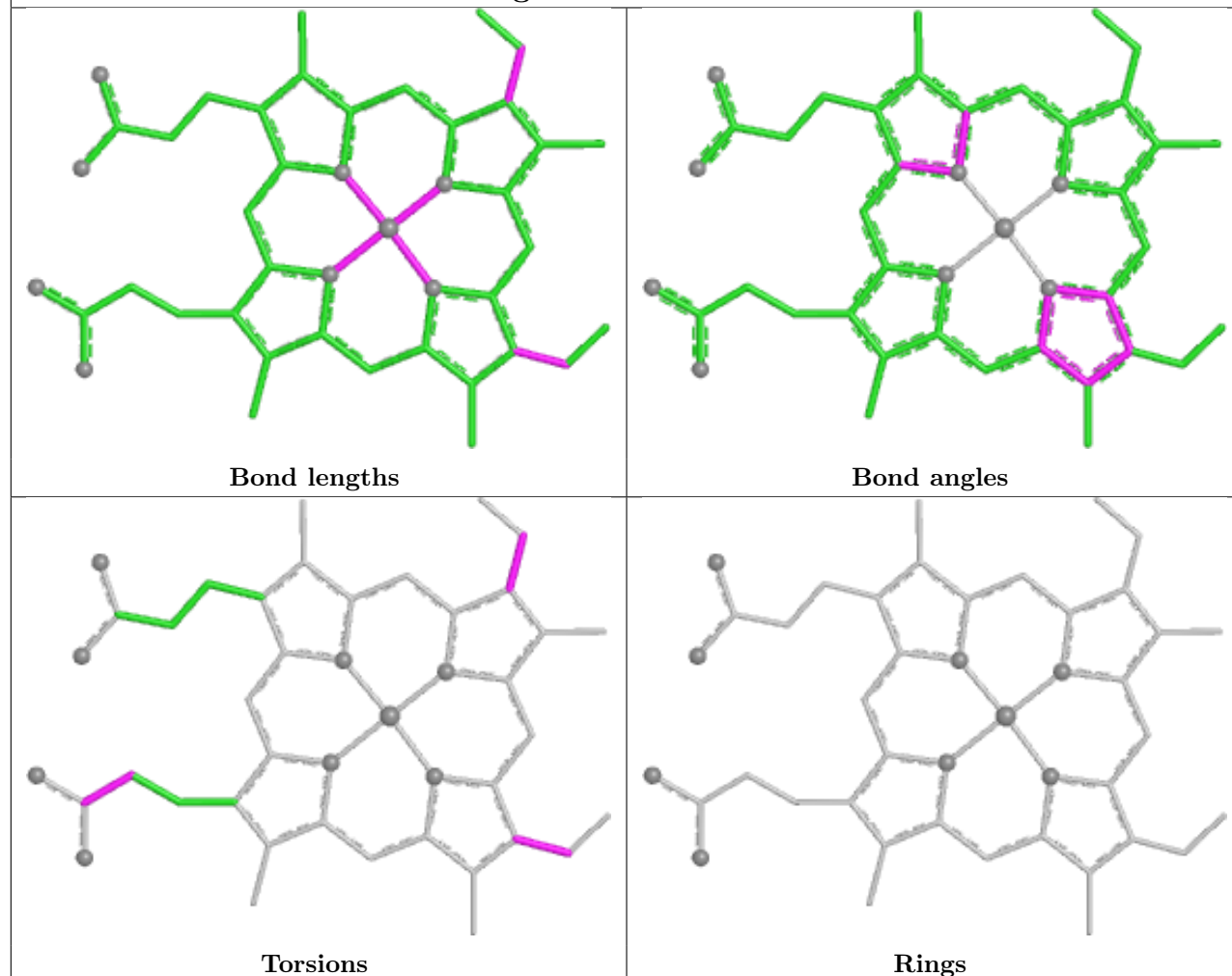




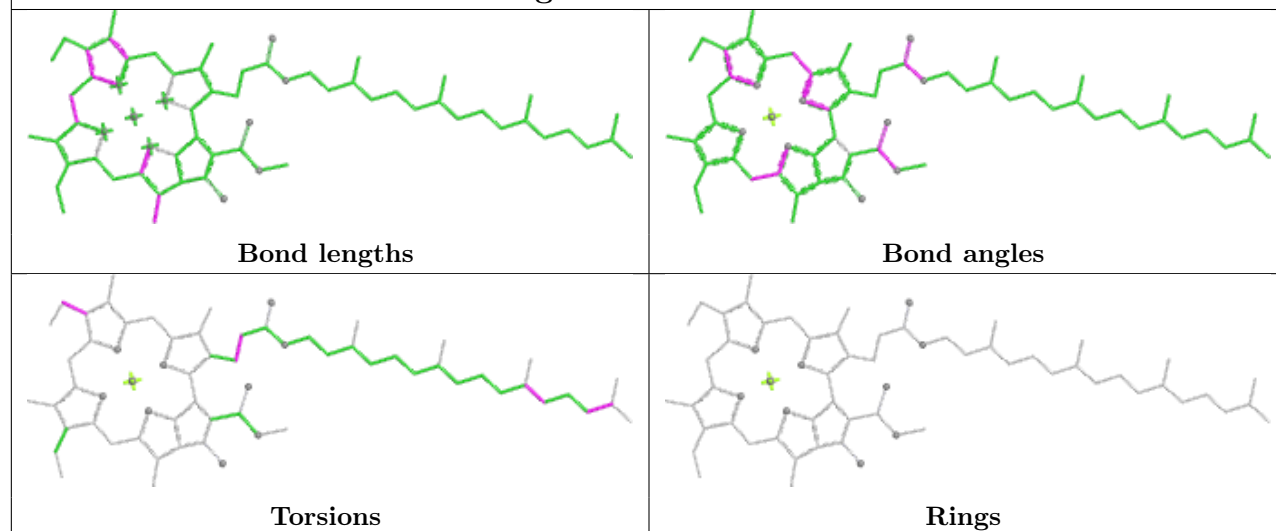


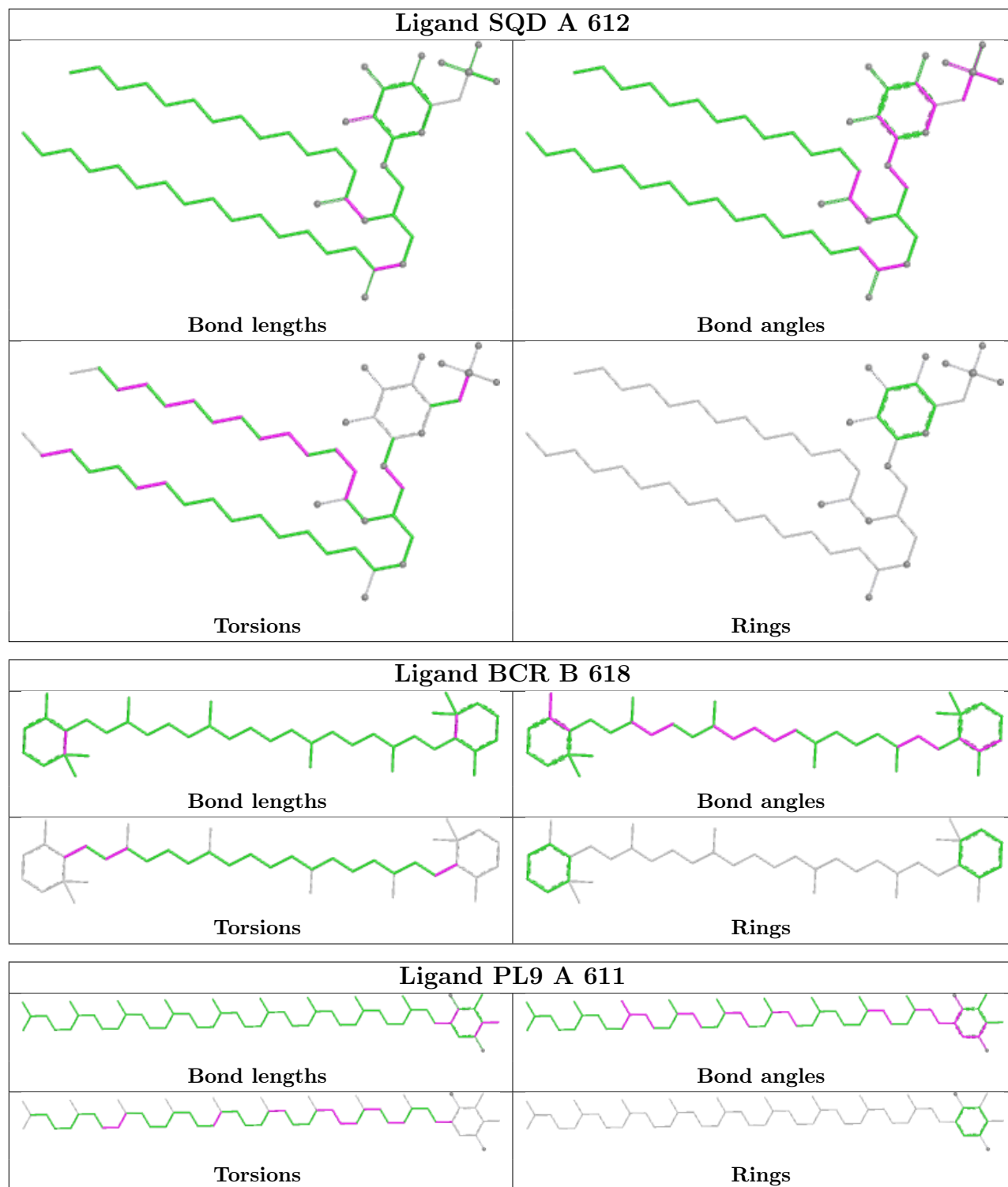


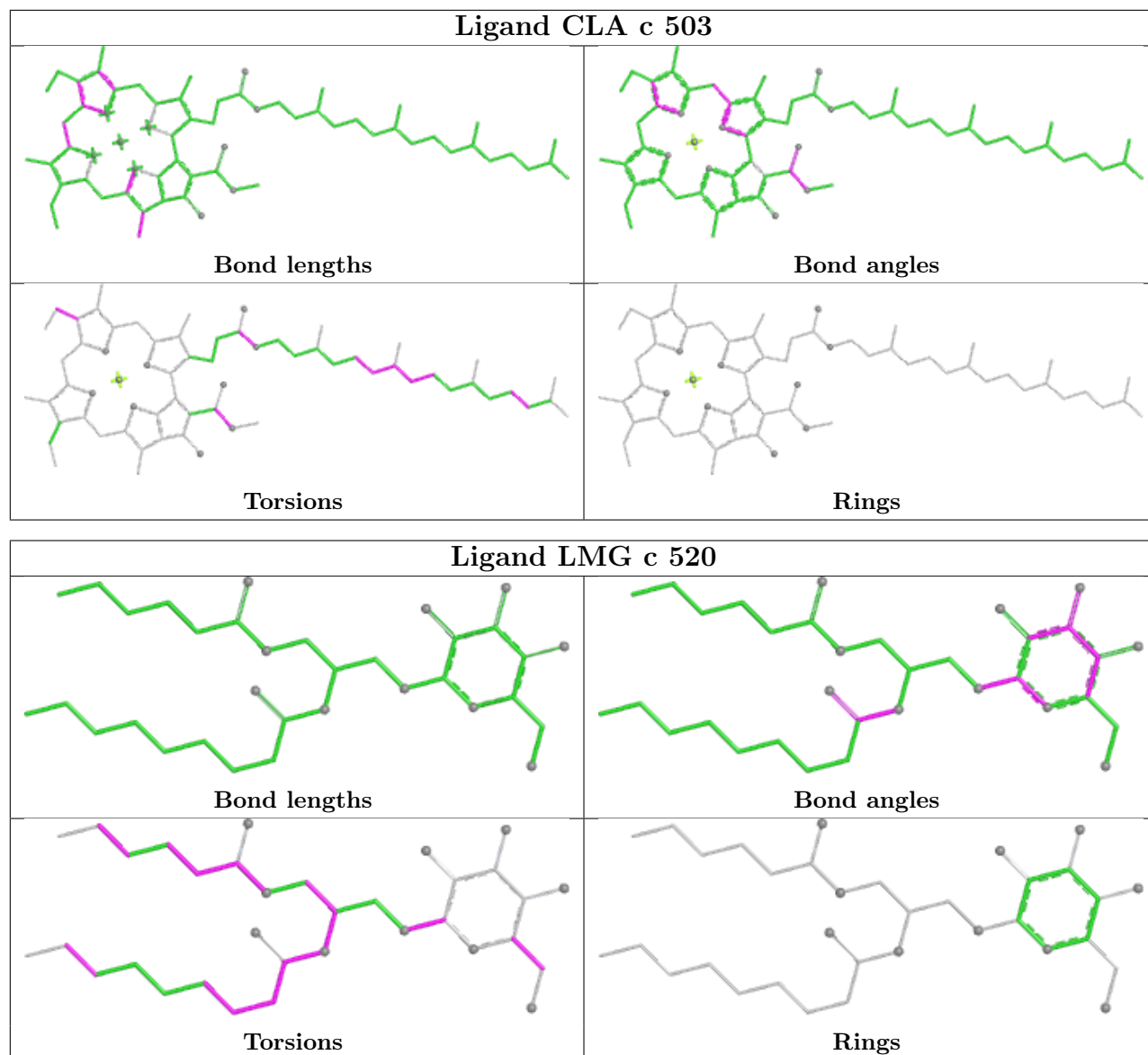
Ligand HEM e 101



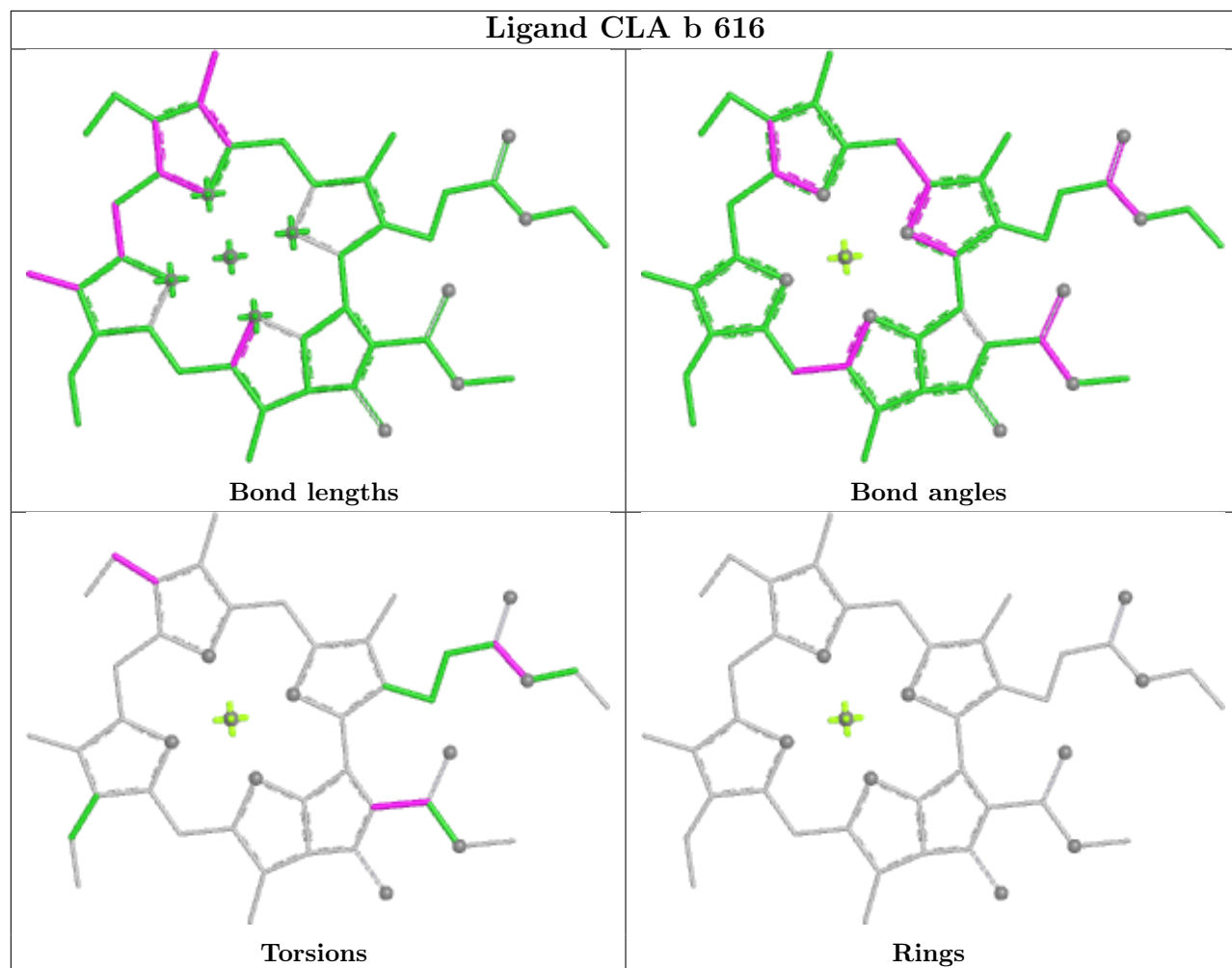
Ligand CLA b 608

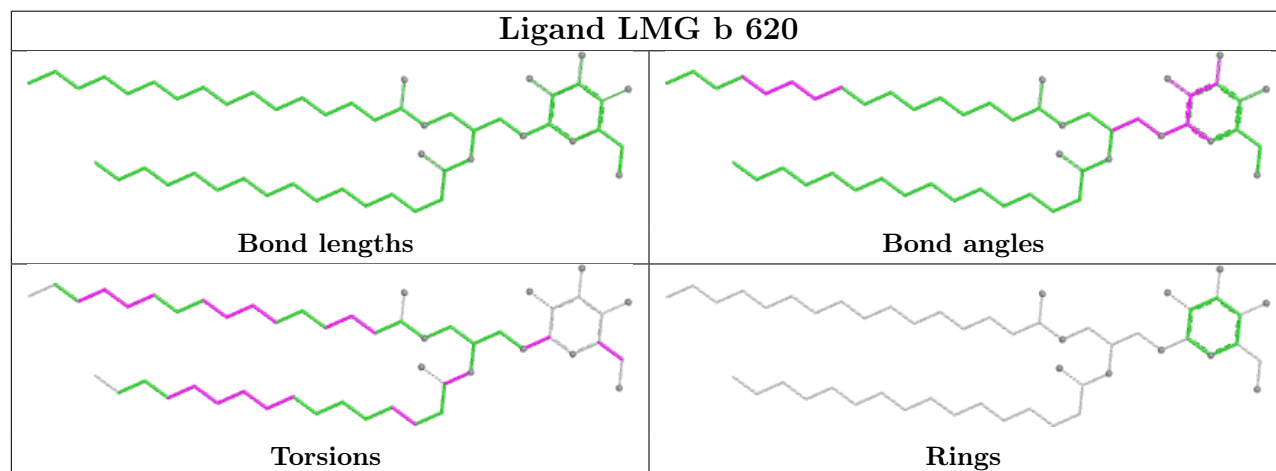
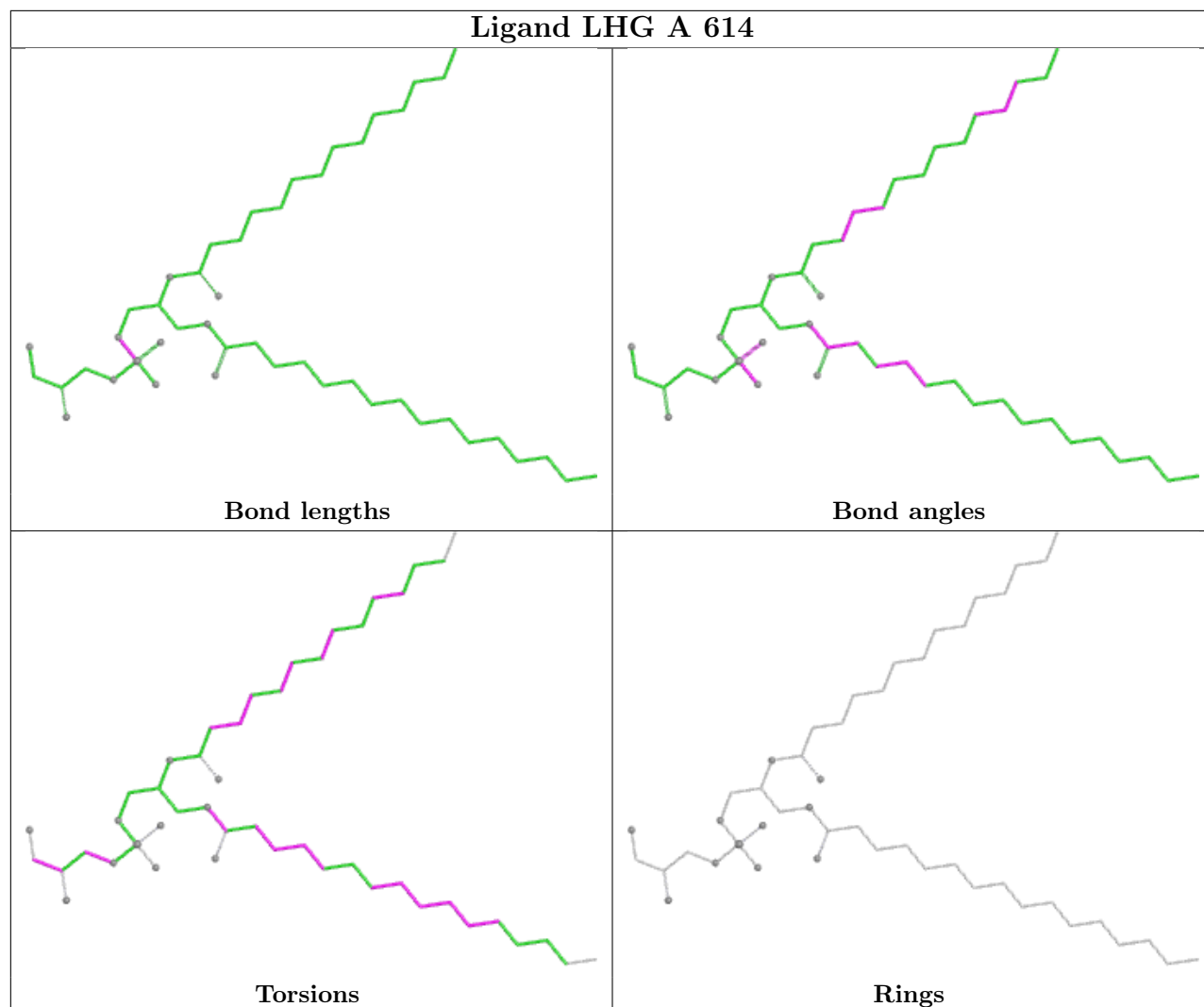


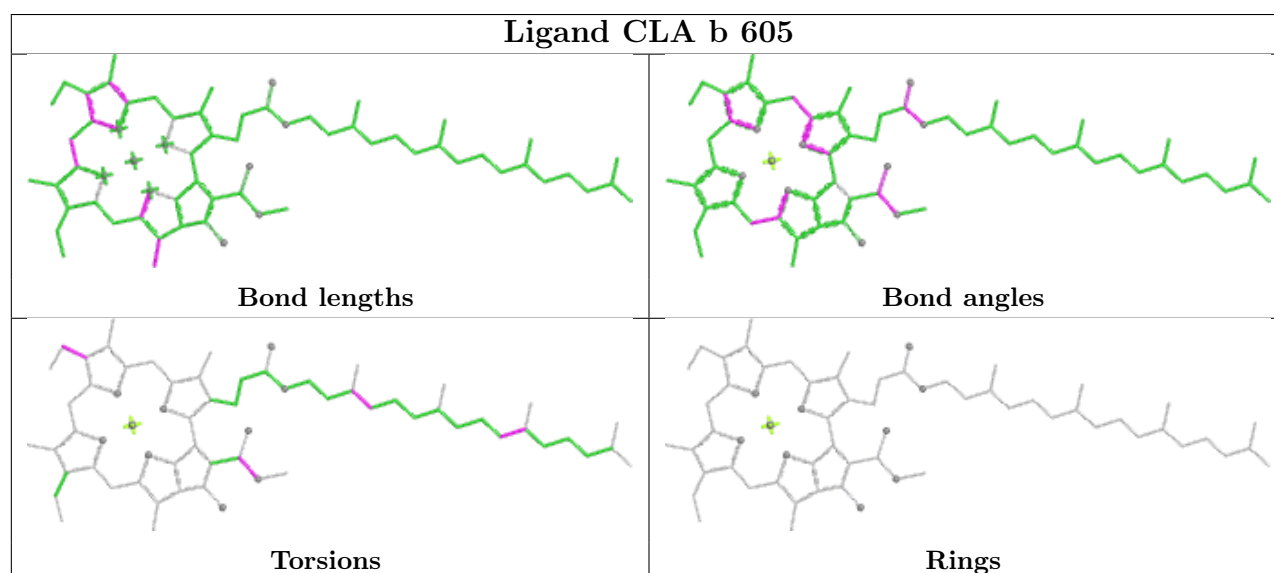
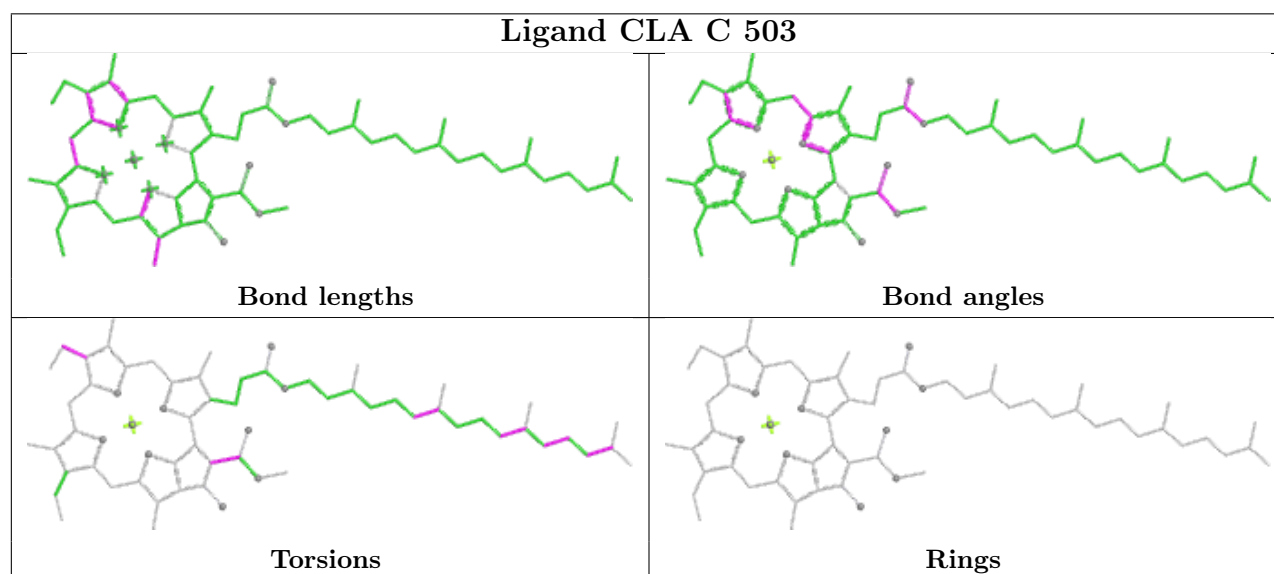
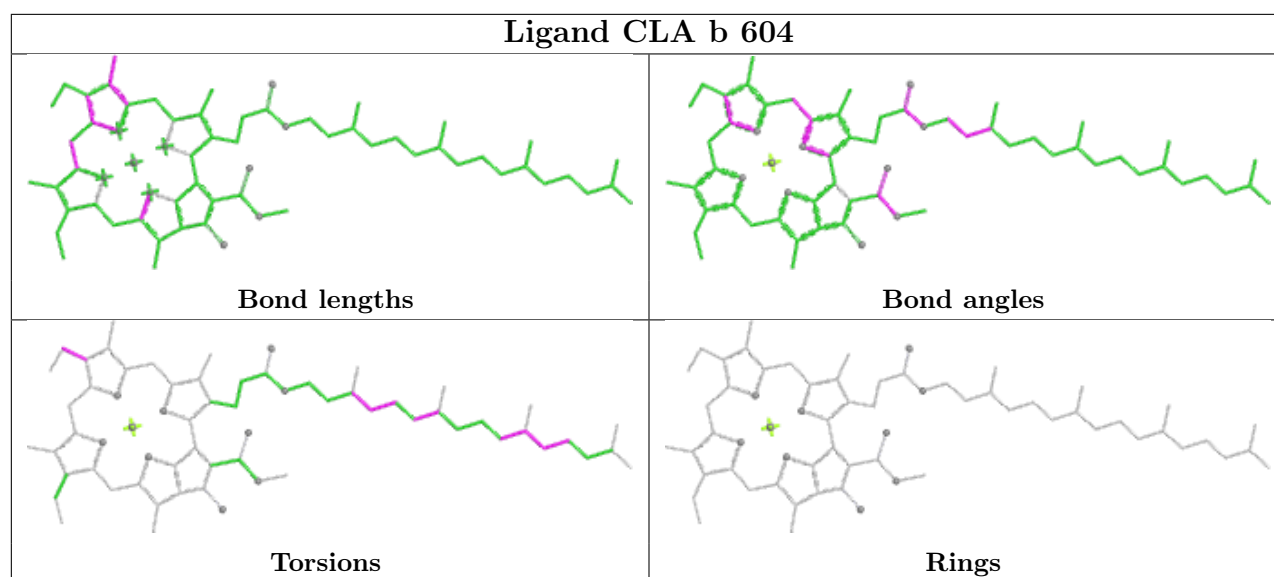


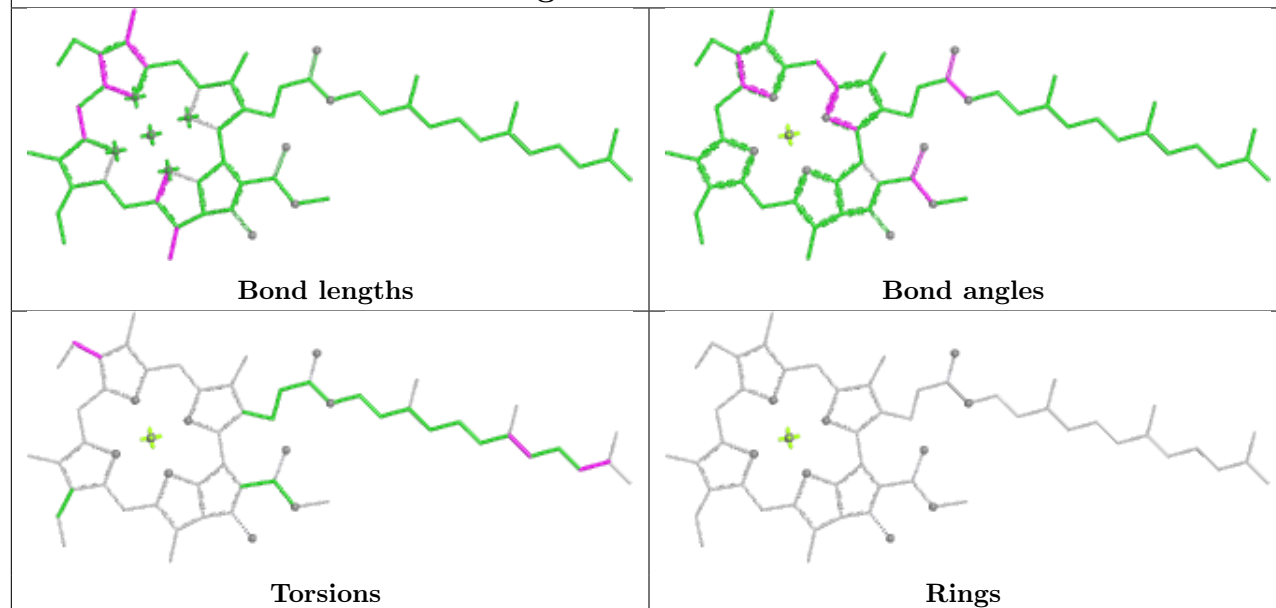
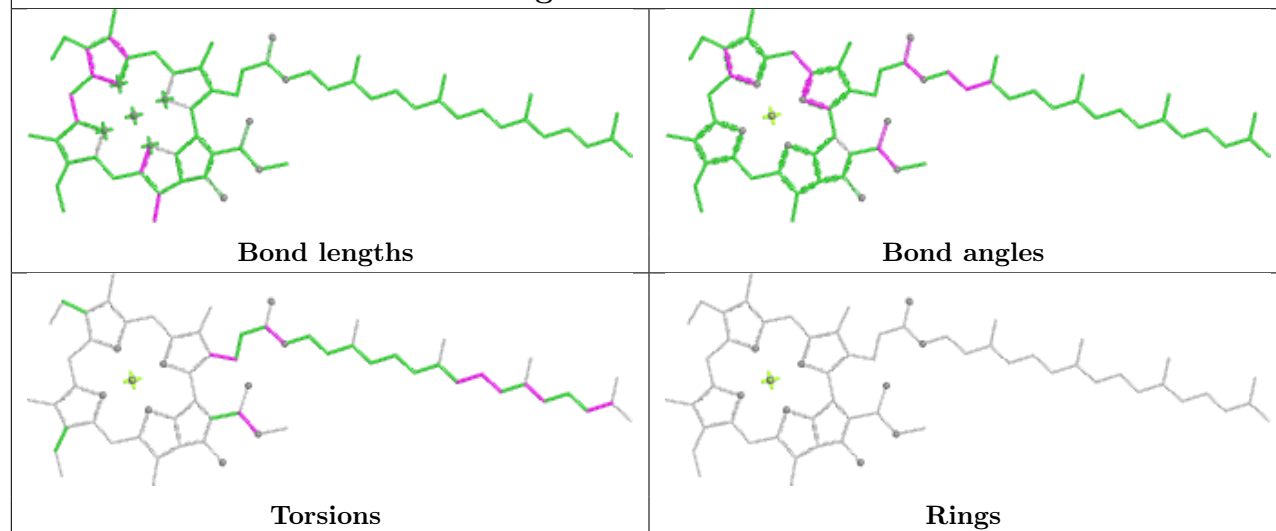


Ligand CLA b 616

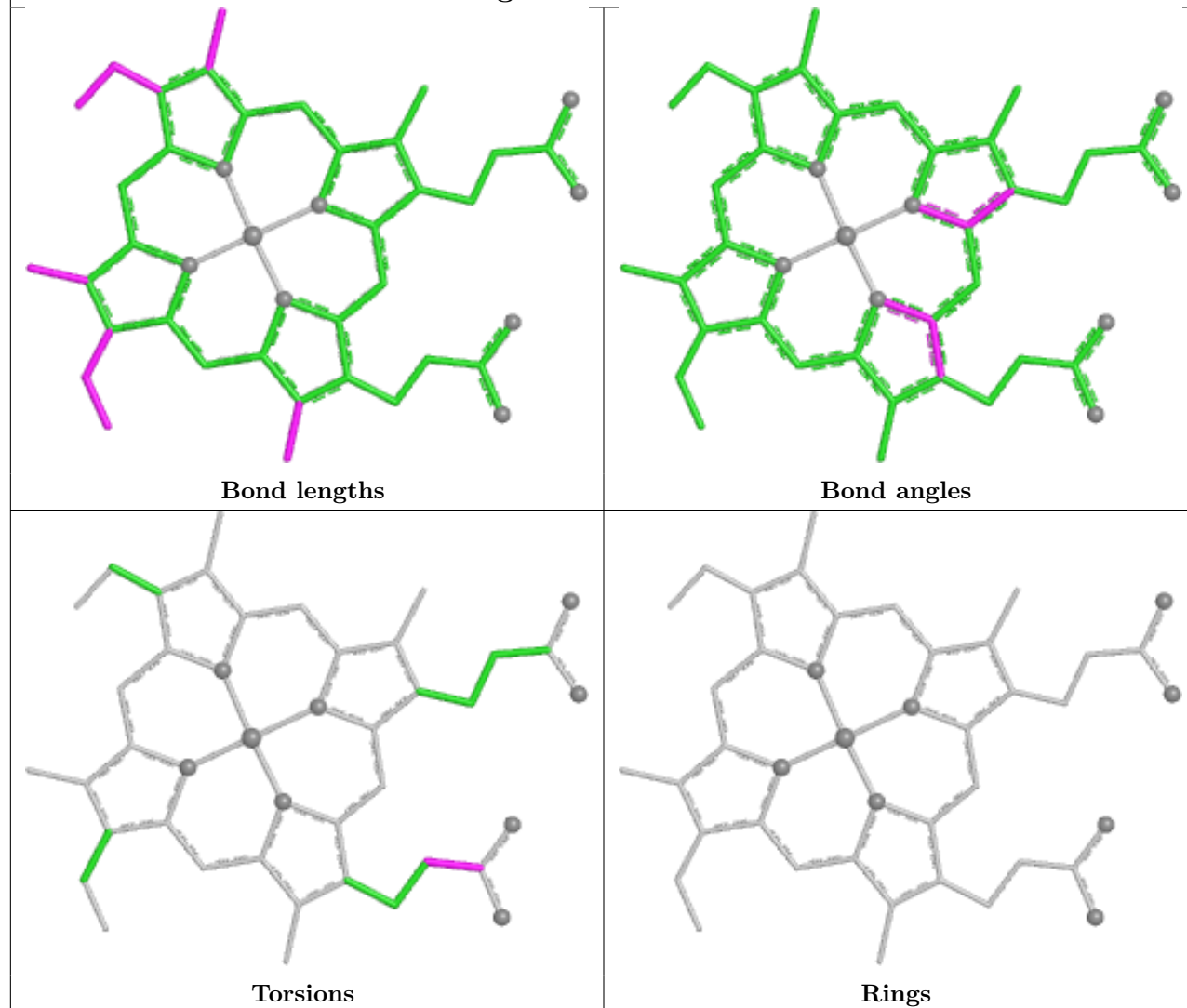




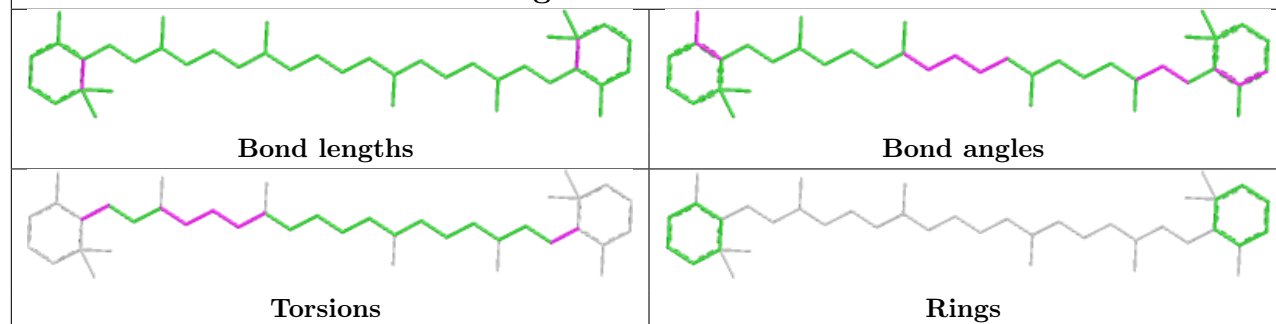


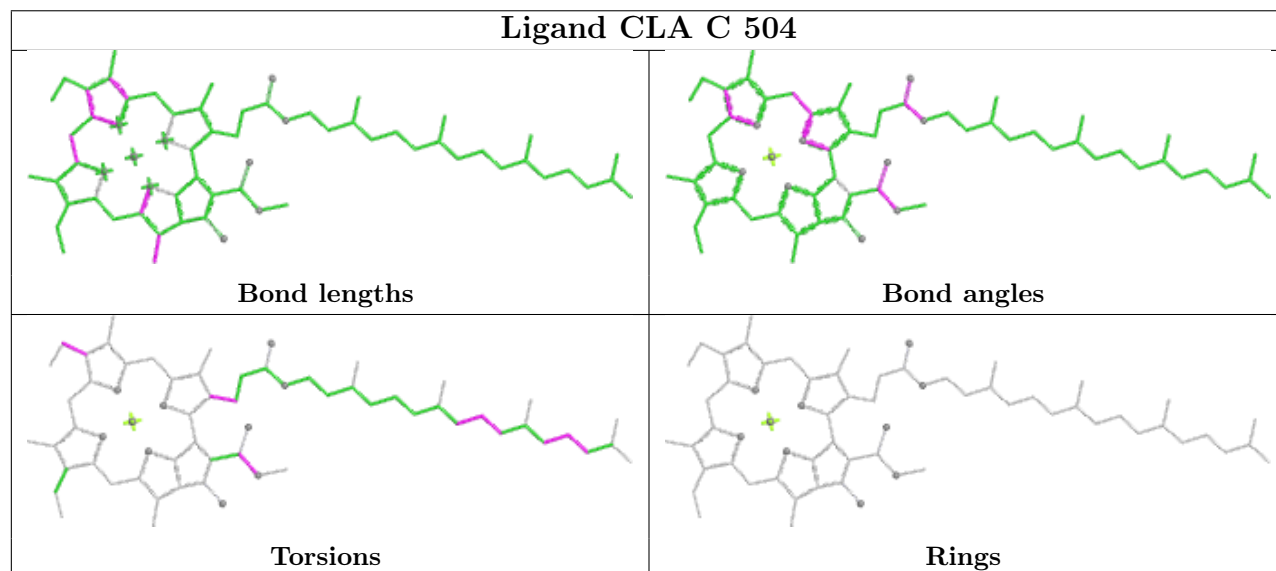
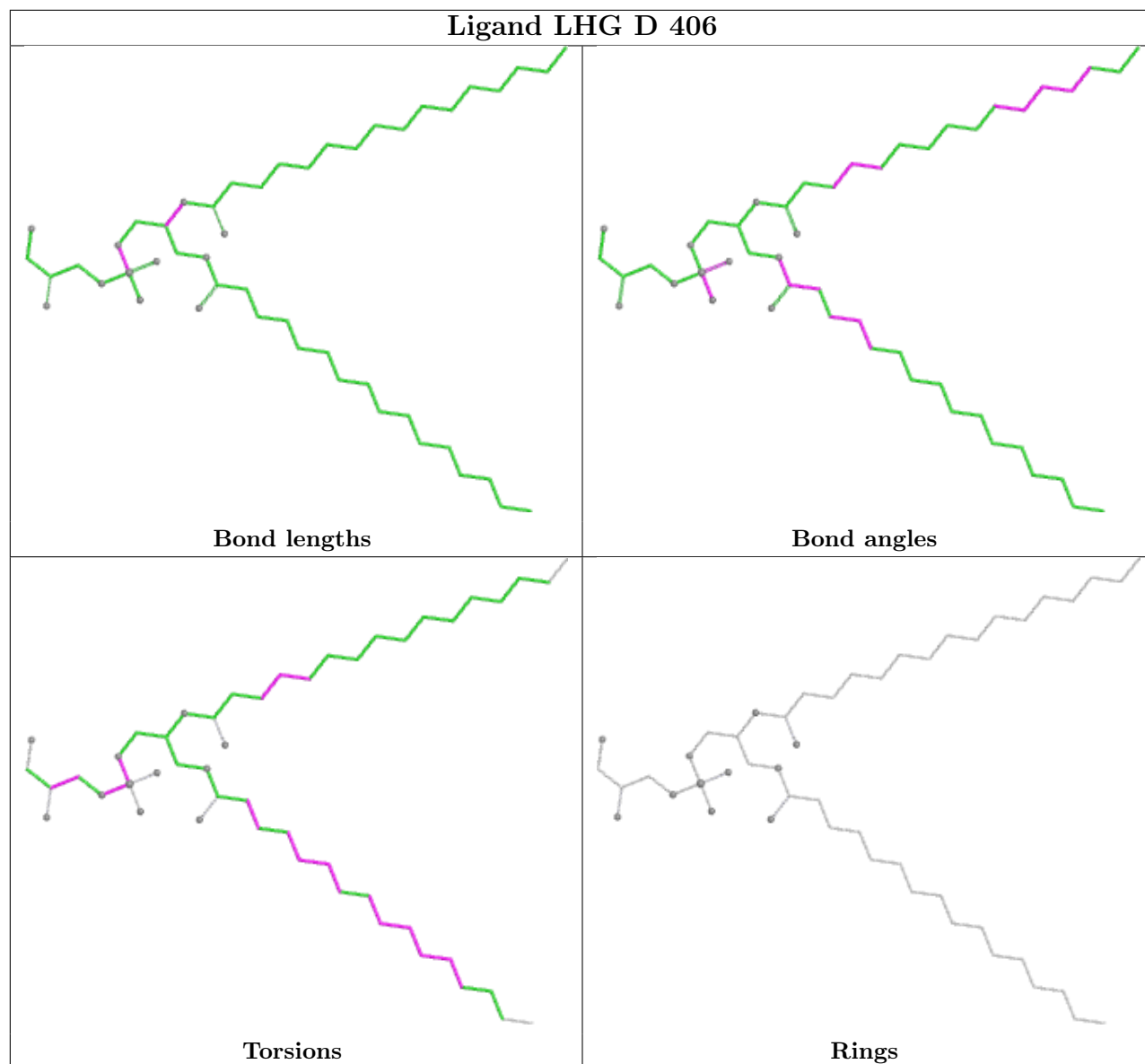
Ligand CLA c 504**Ligand CLA b 613**

Ligand HEC v 201

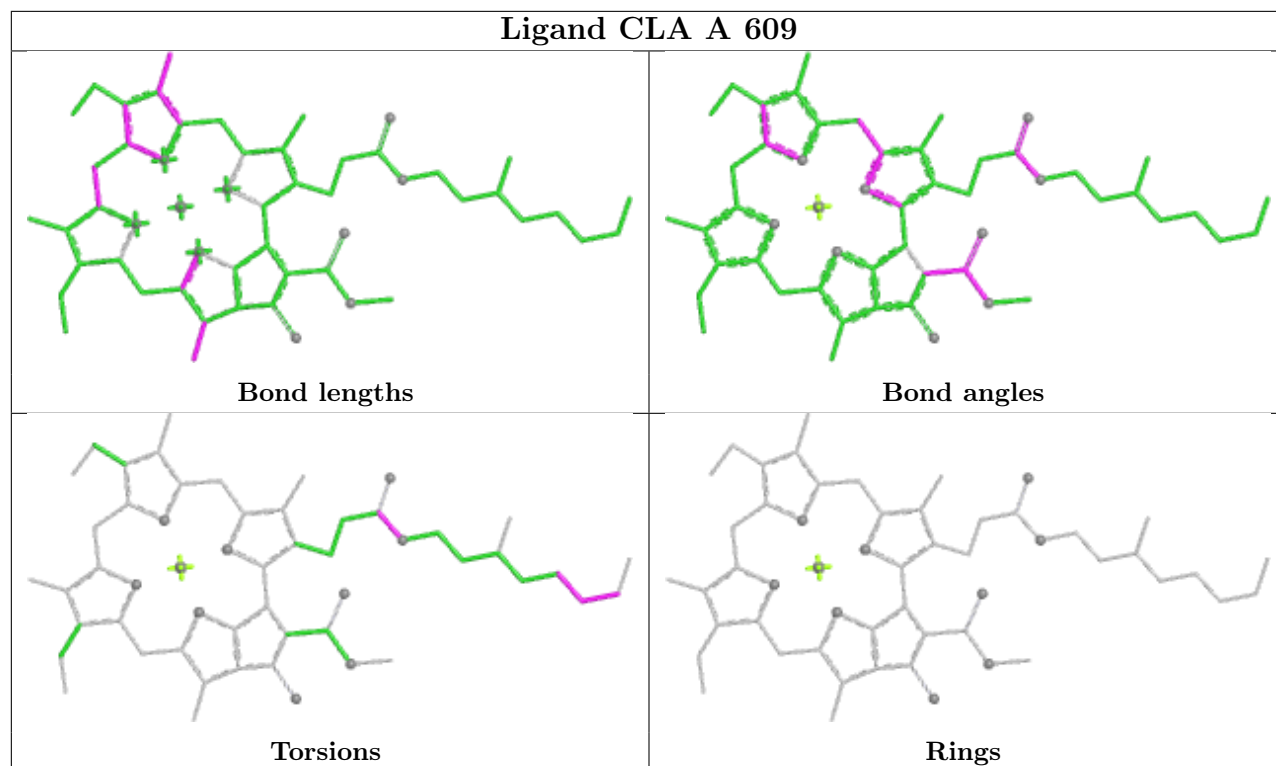


Ligand BCR b 618

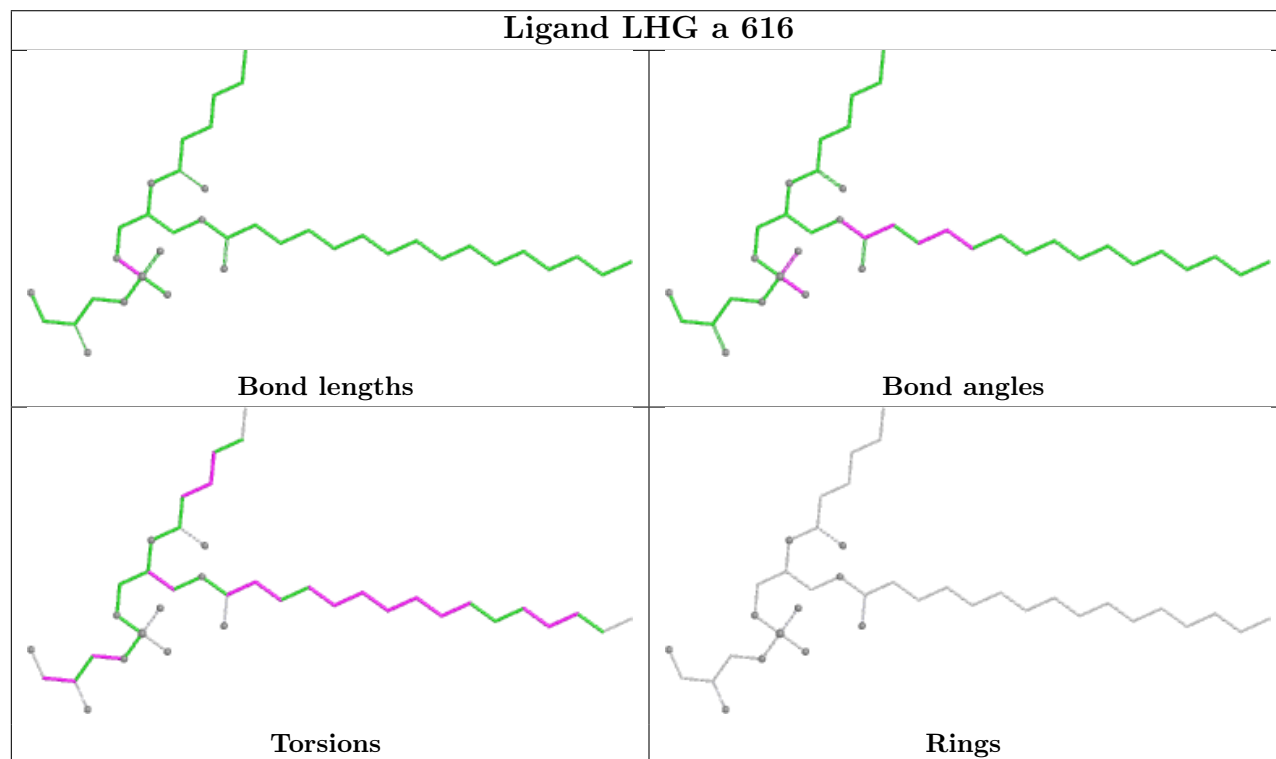


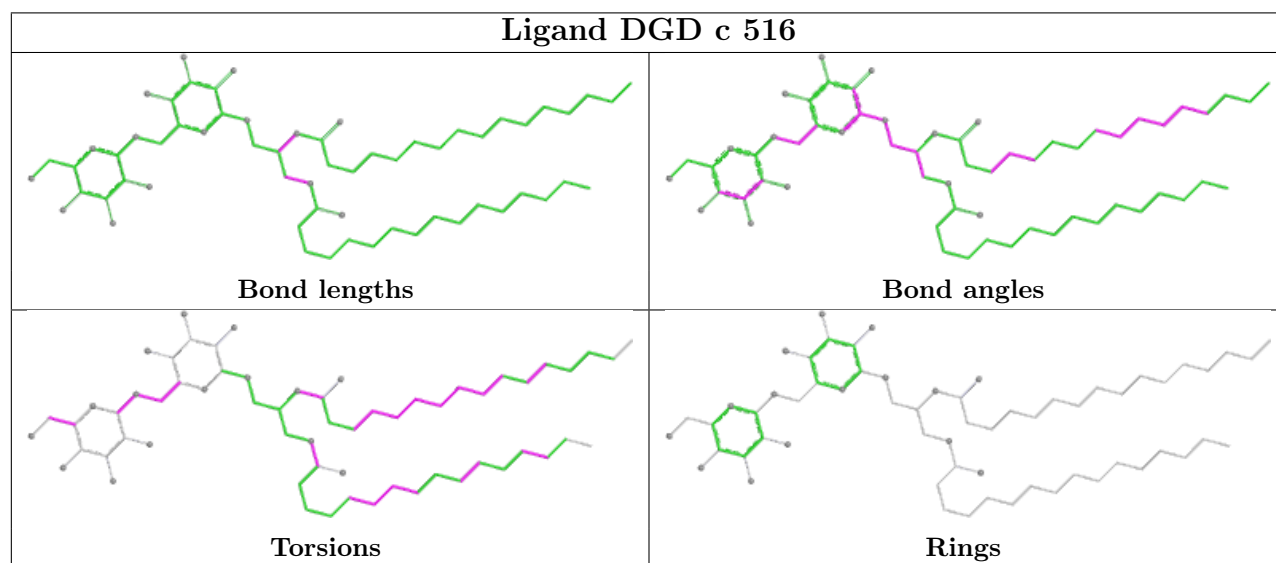
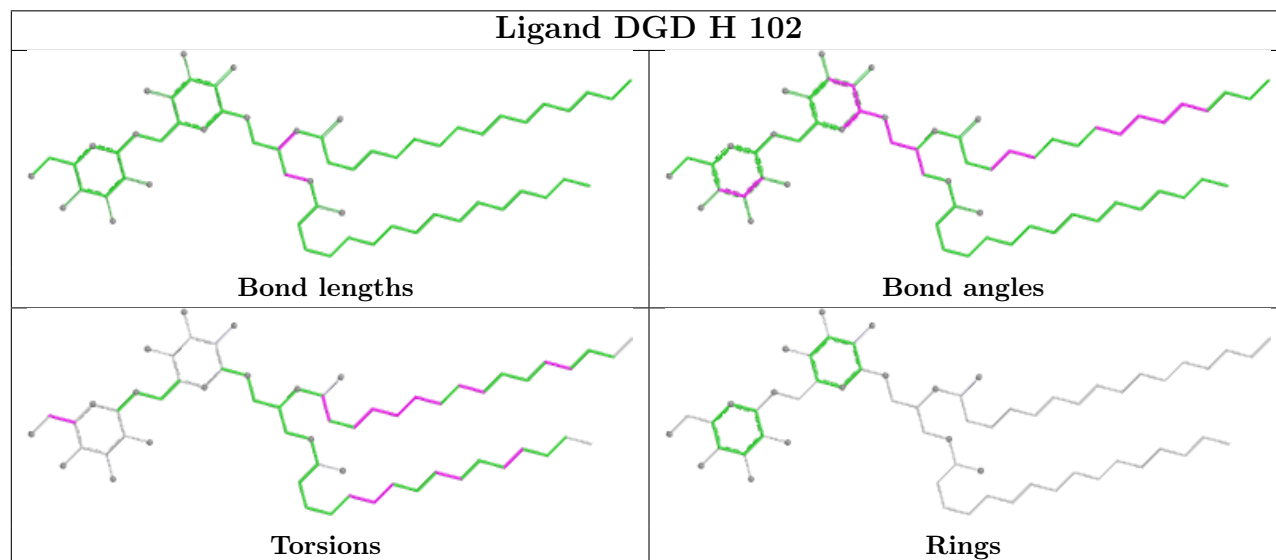
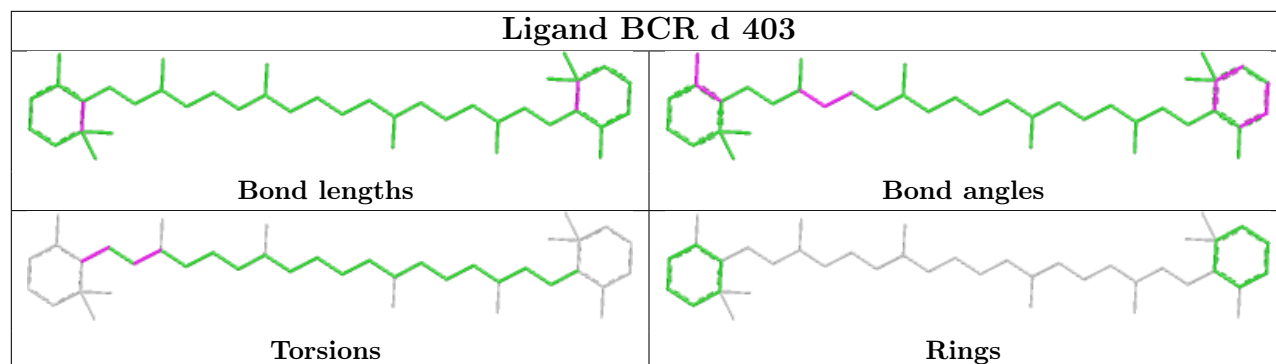


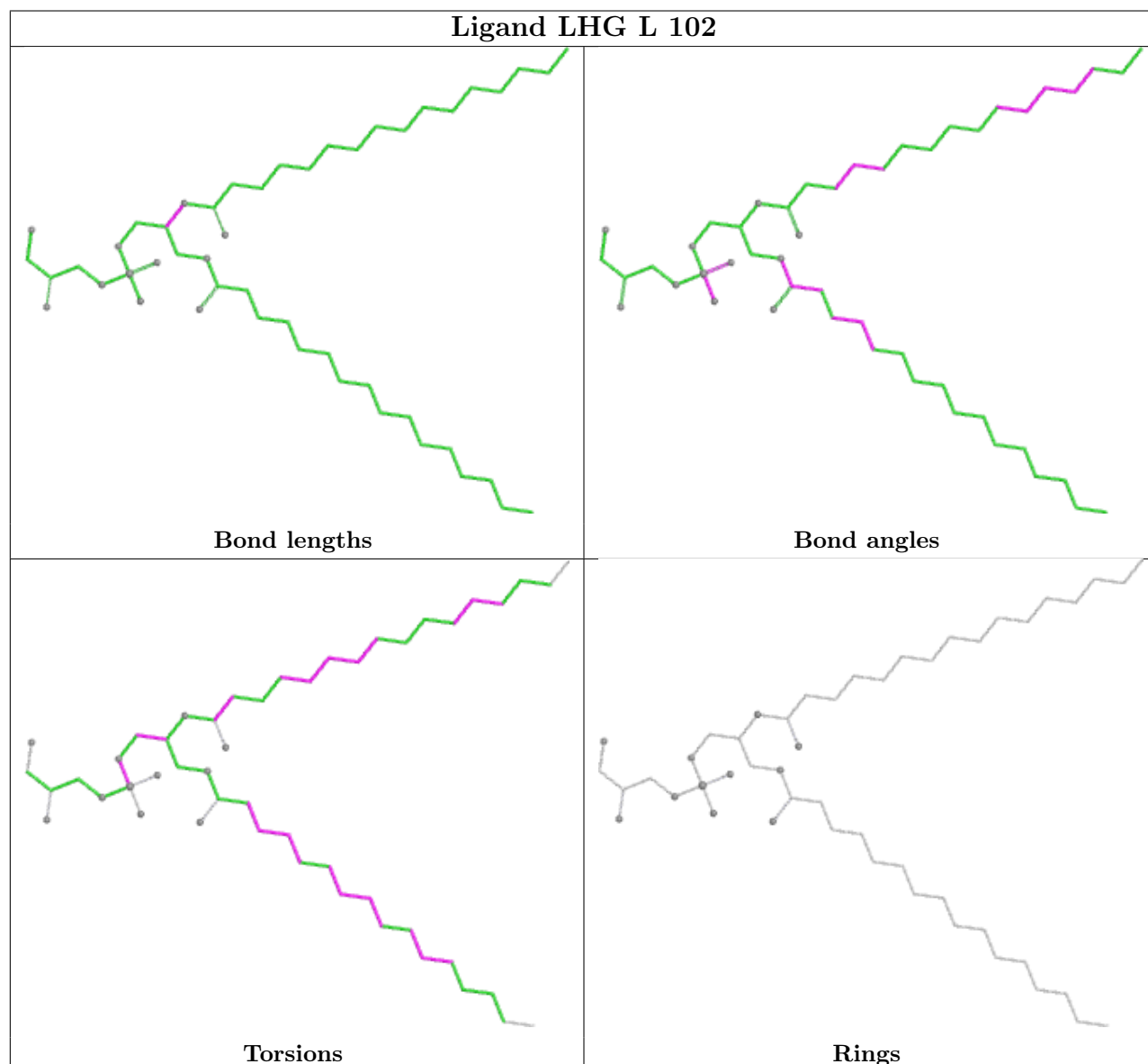
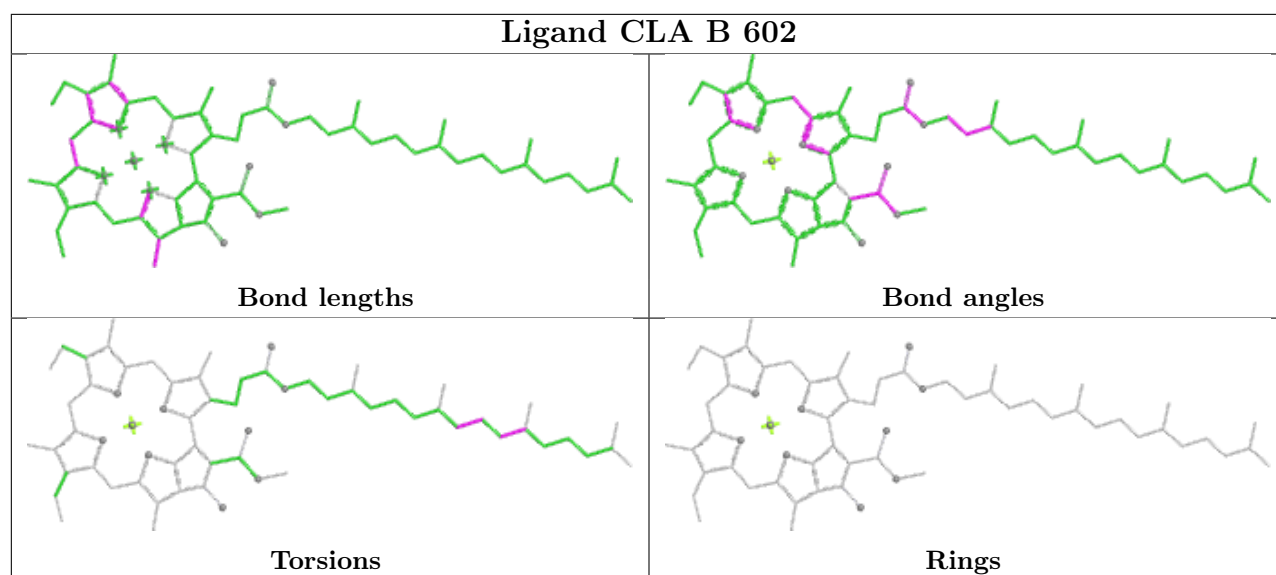
Ligand CLA A 609

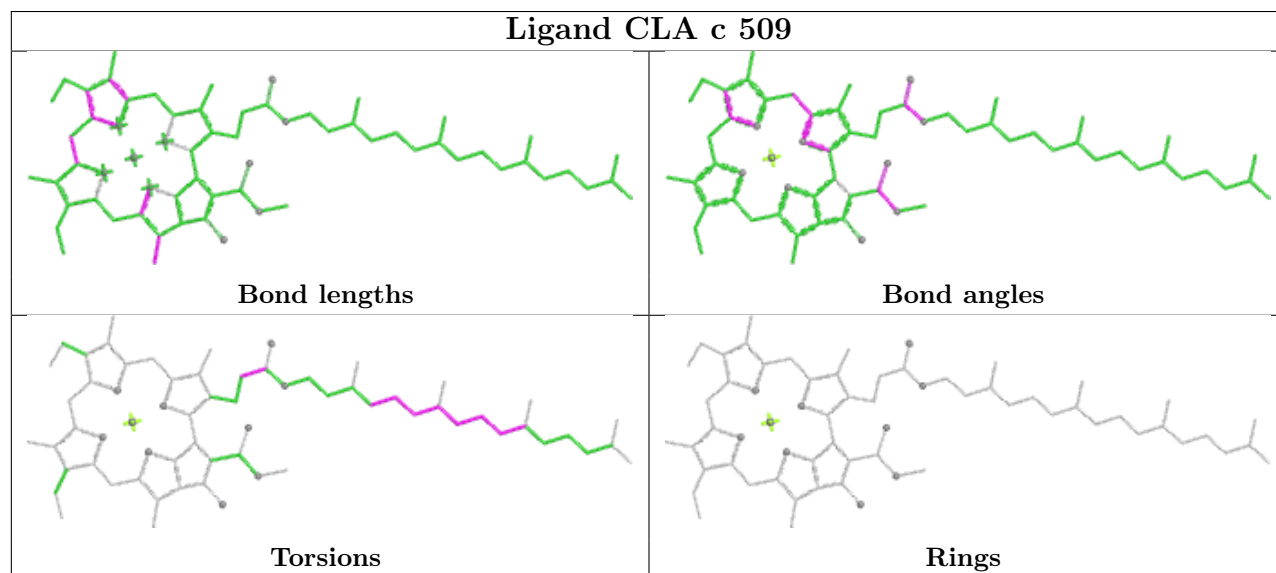
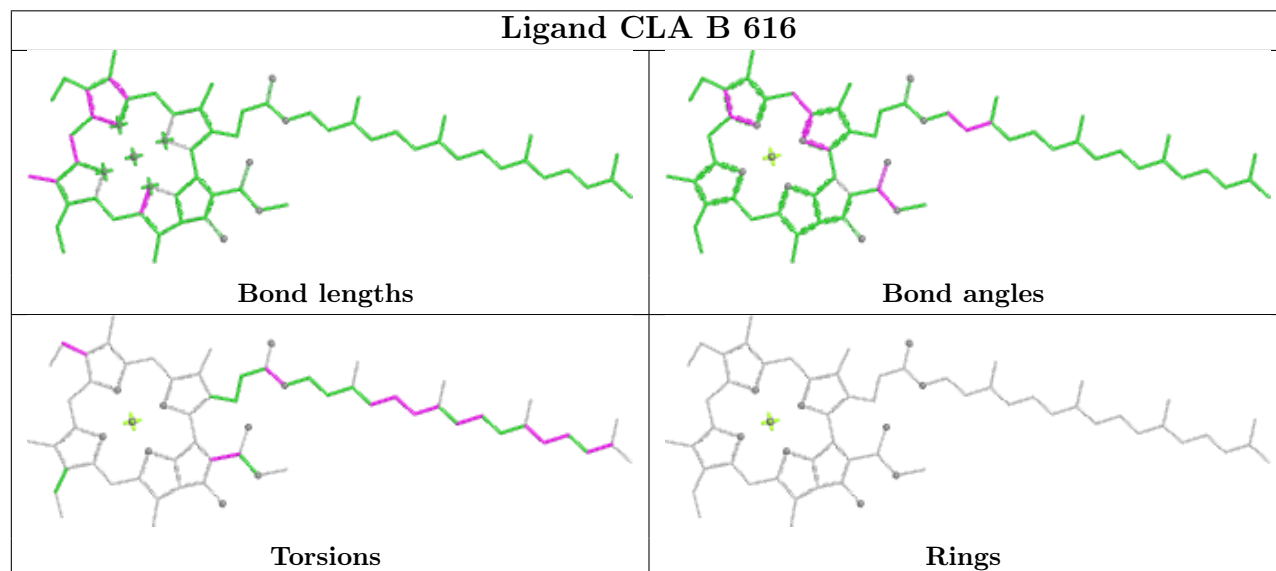
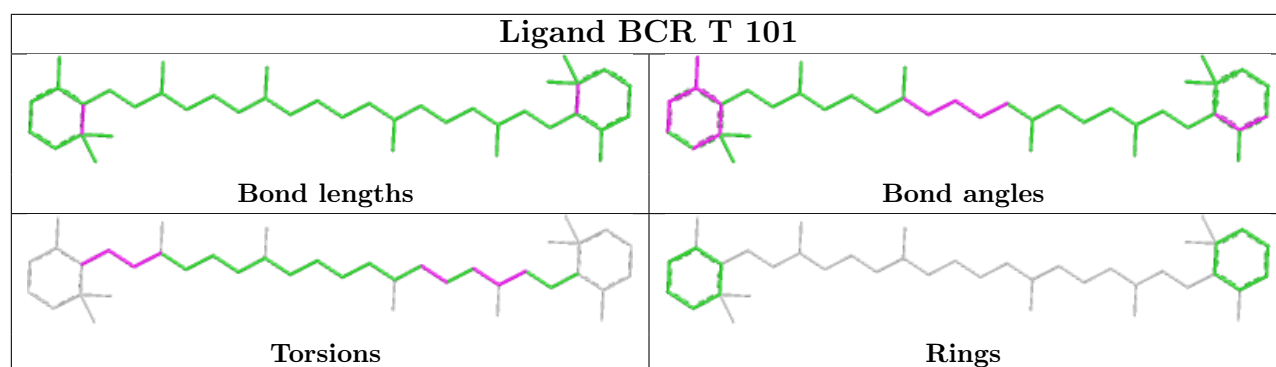


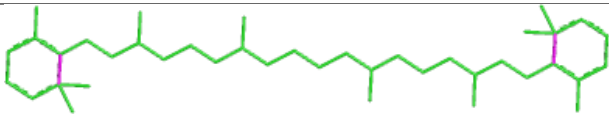
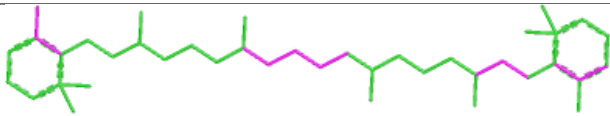
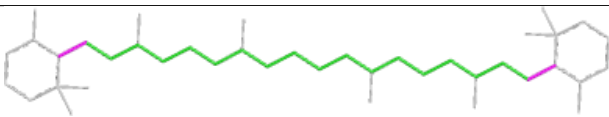
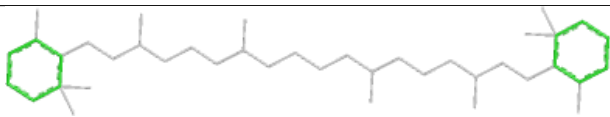
Ligand LHG a 616

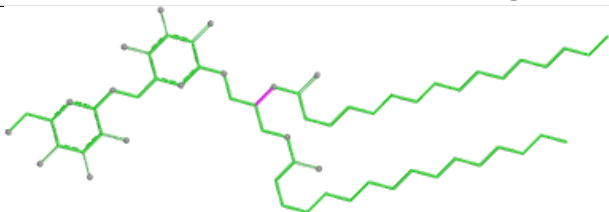
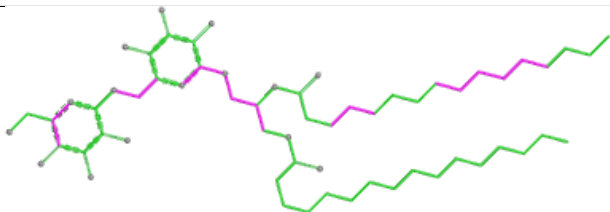
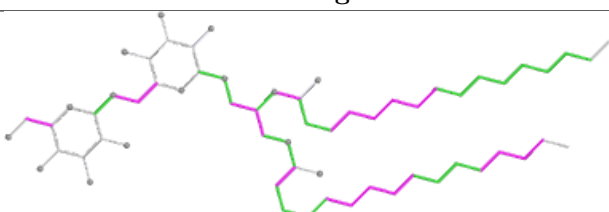
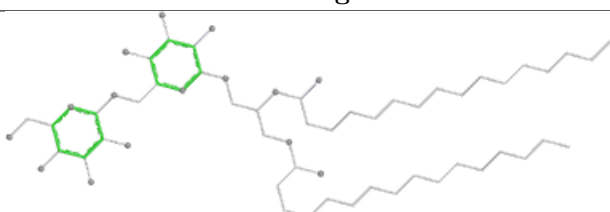


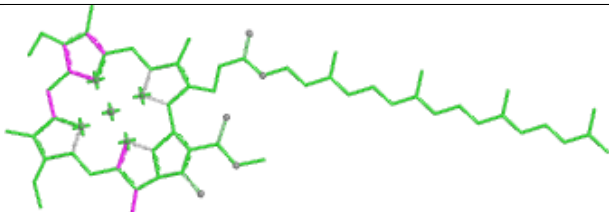
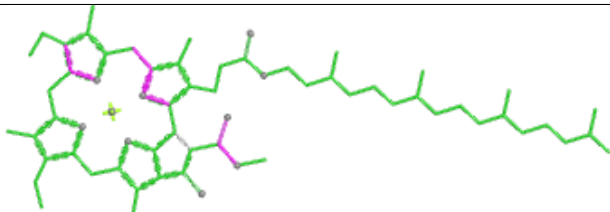
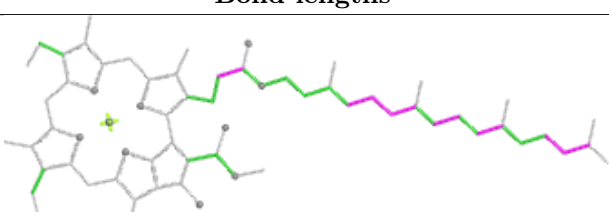
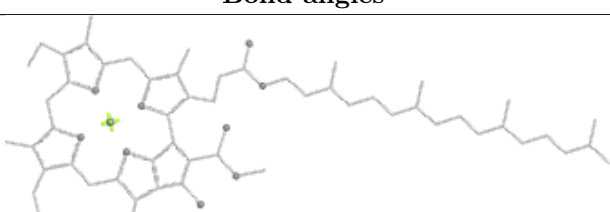


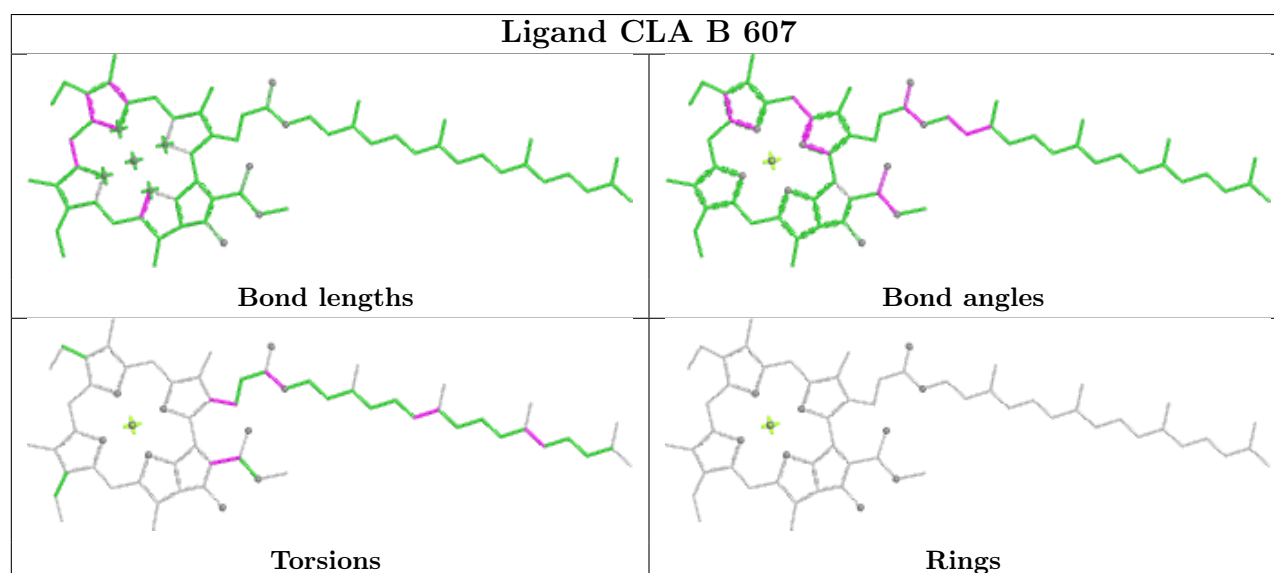
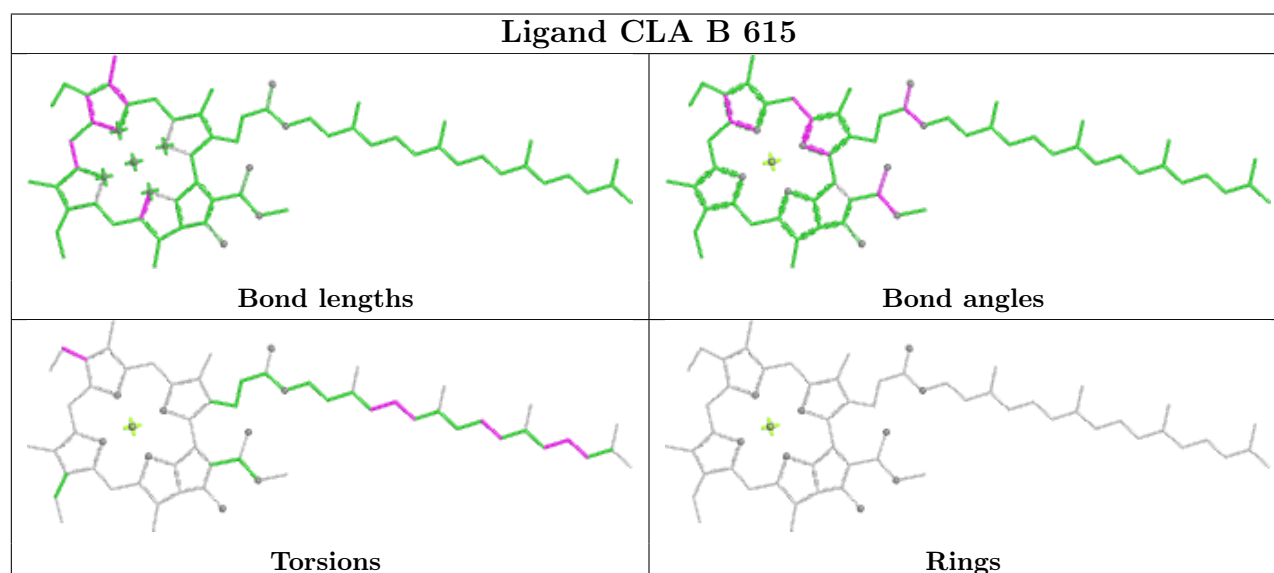
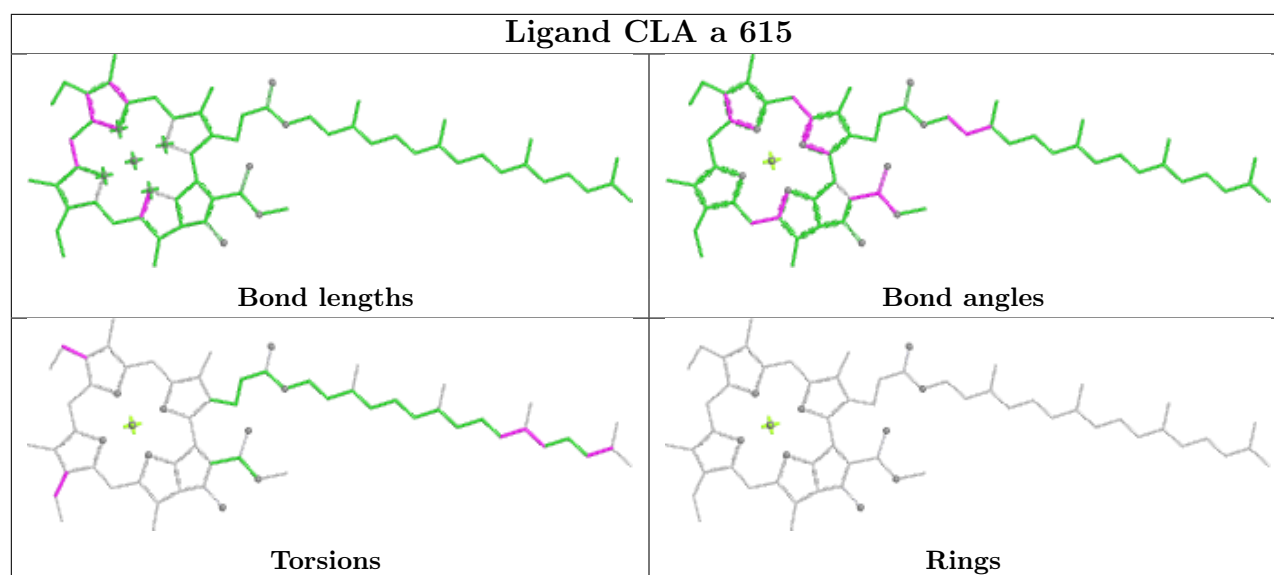




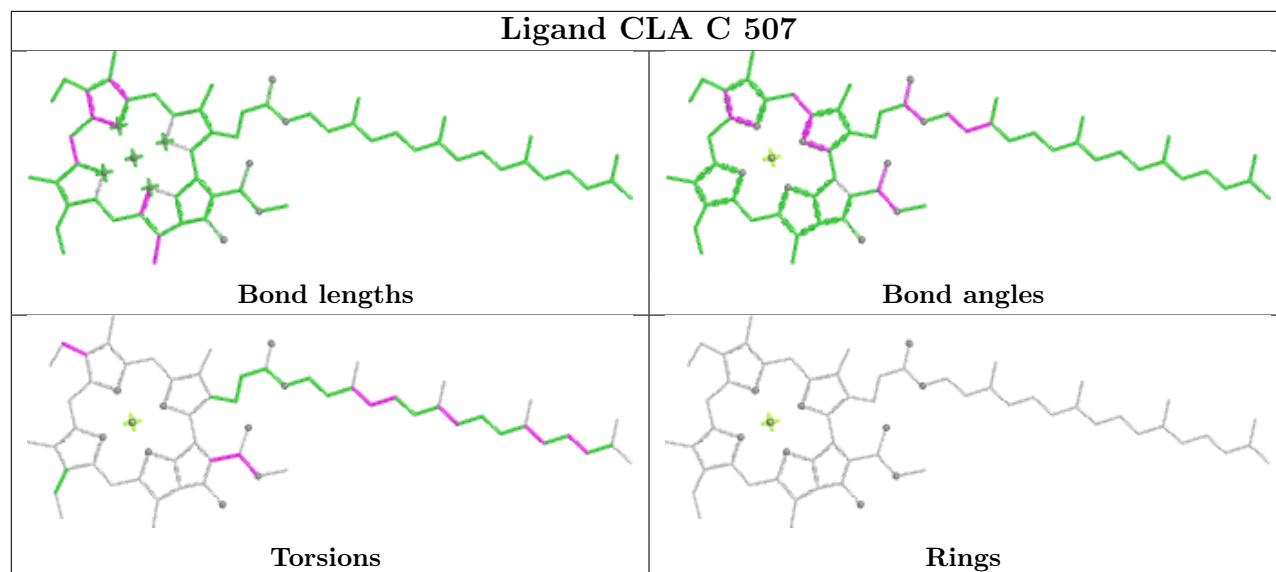
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

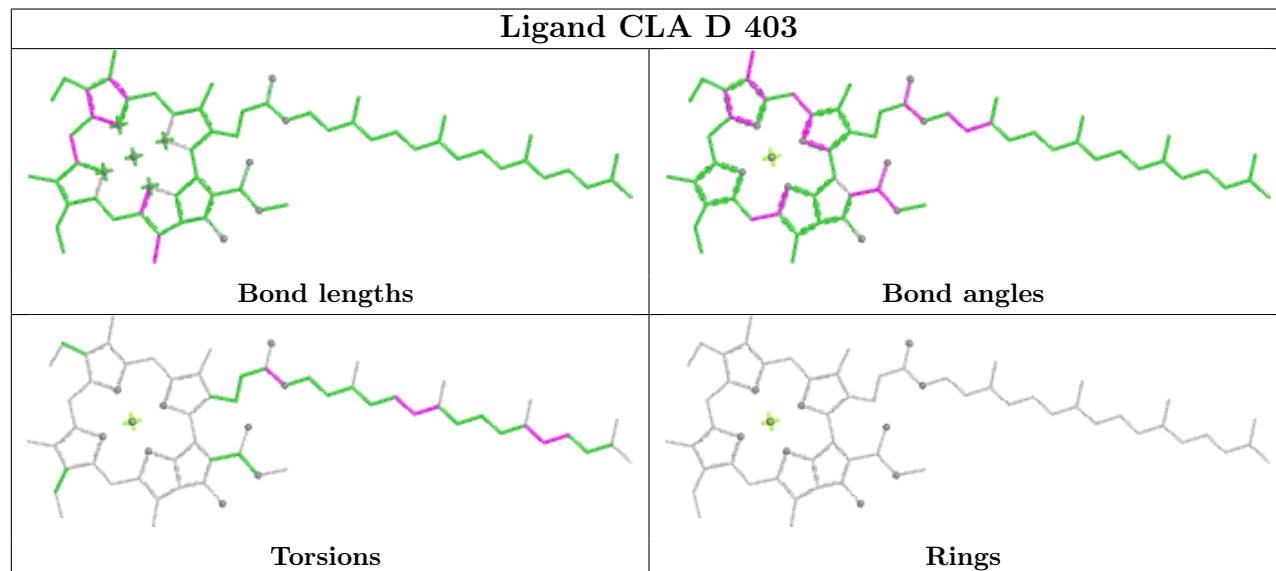
Ligand CLA c 510	
	
Bond lengths	Bond angles
	
Torsions	Rings



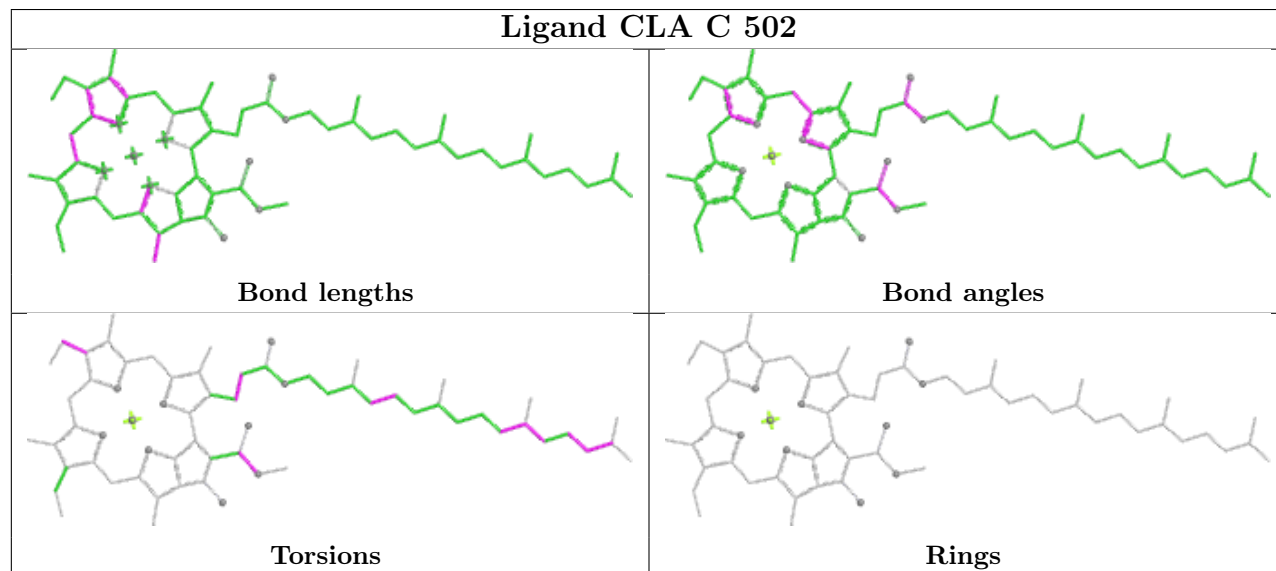
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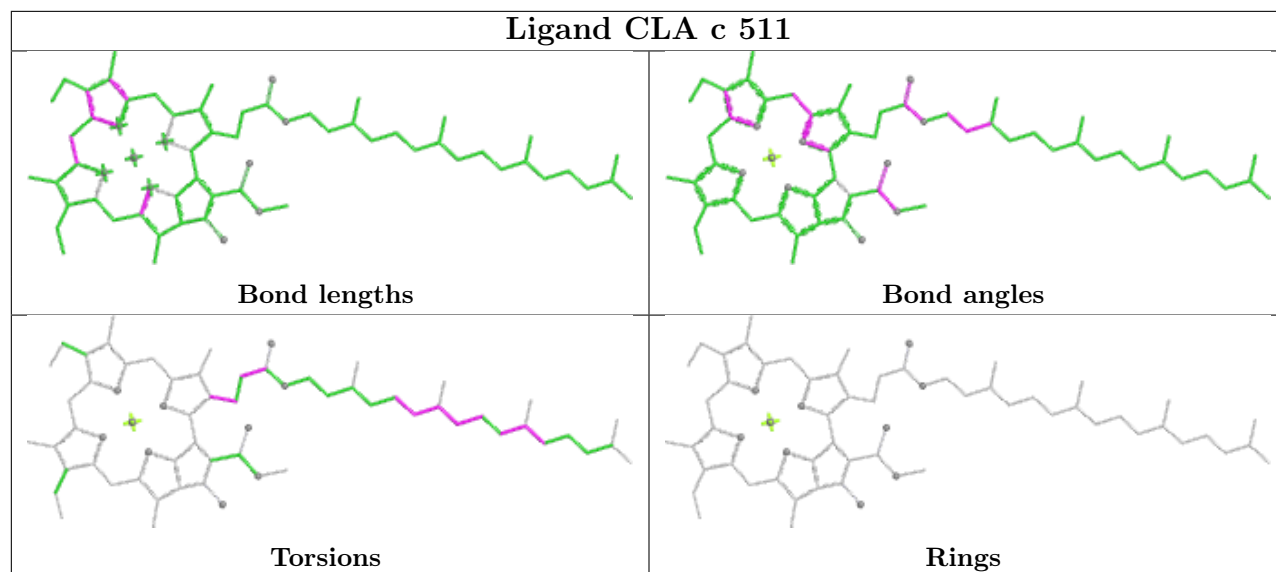
Ligand CLA D 403



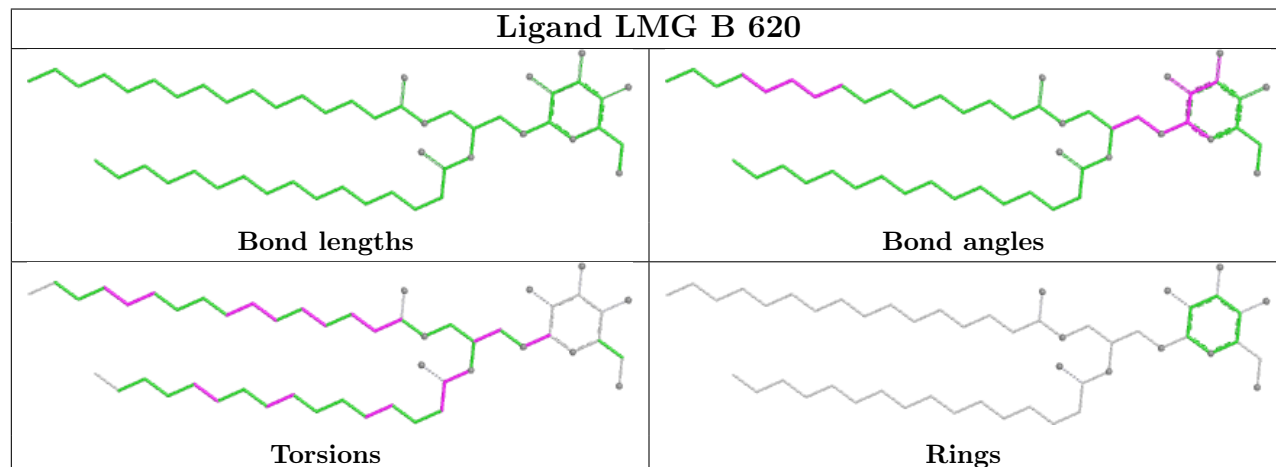
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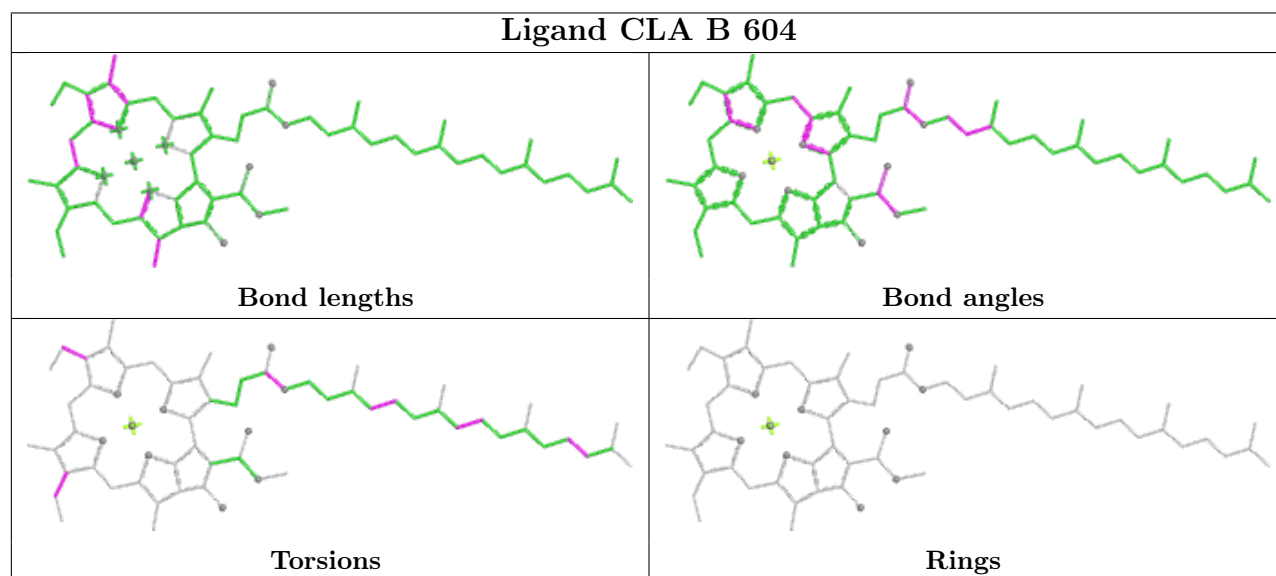
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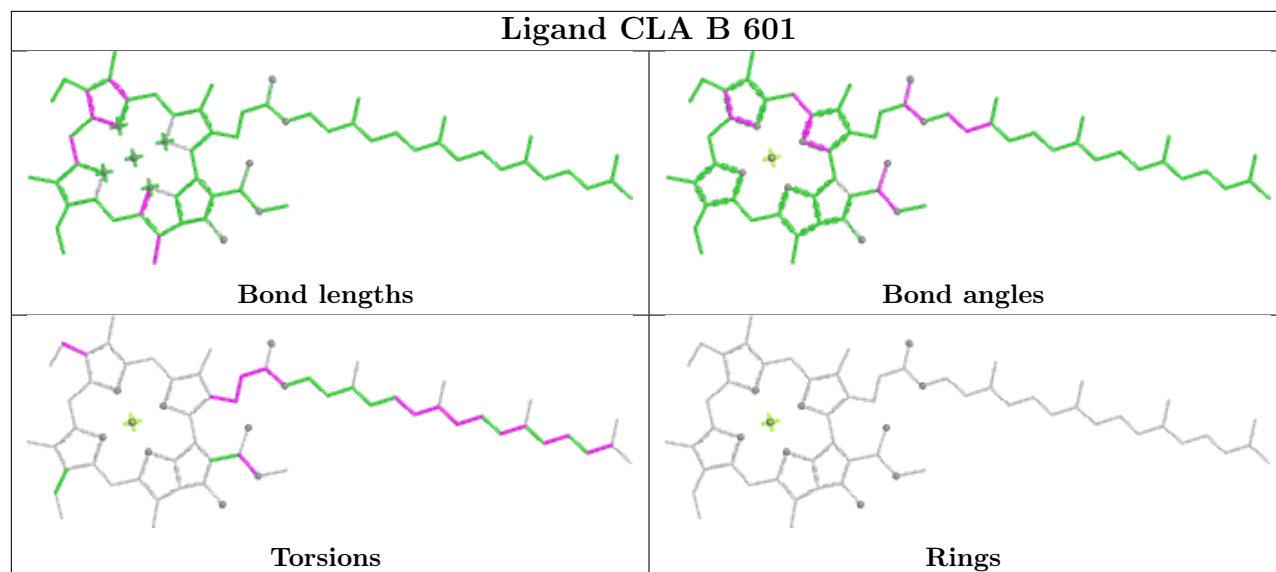
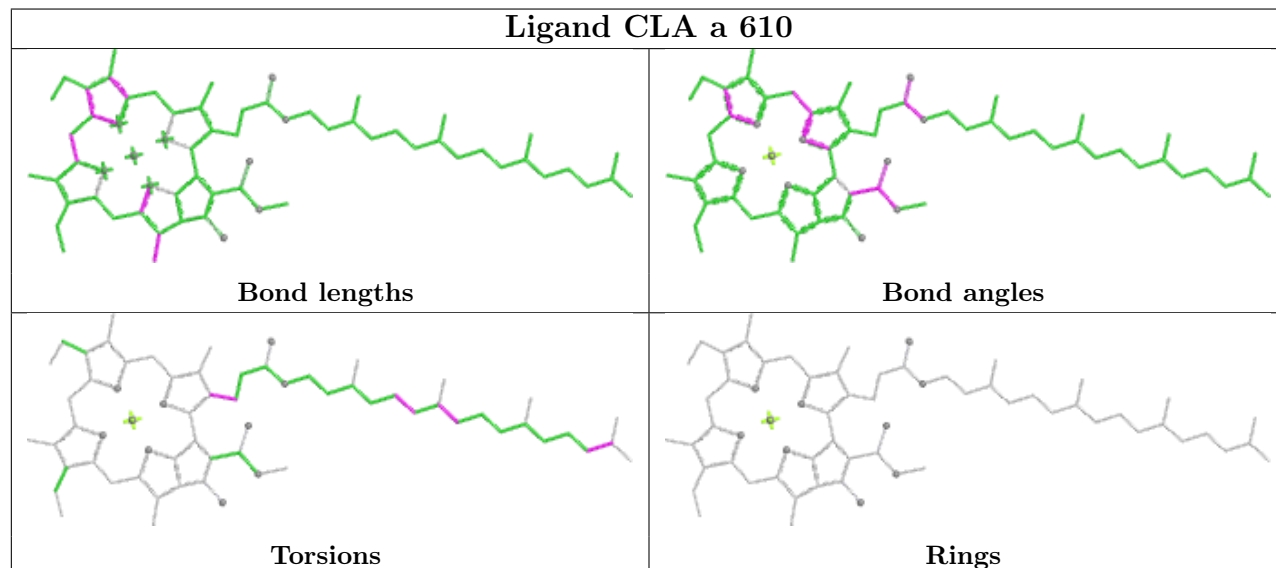
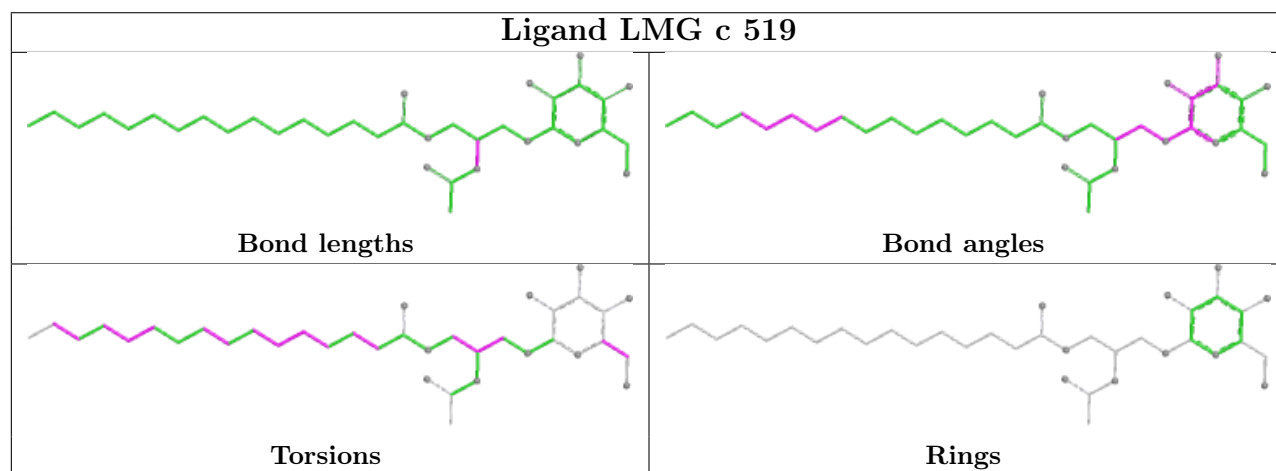


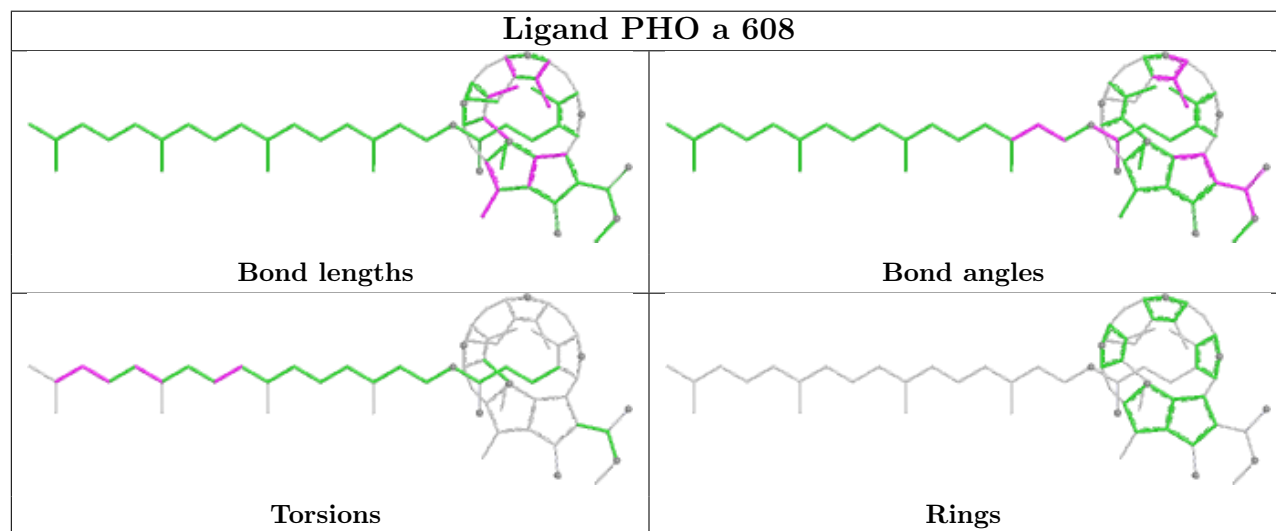
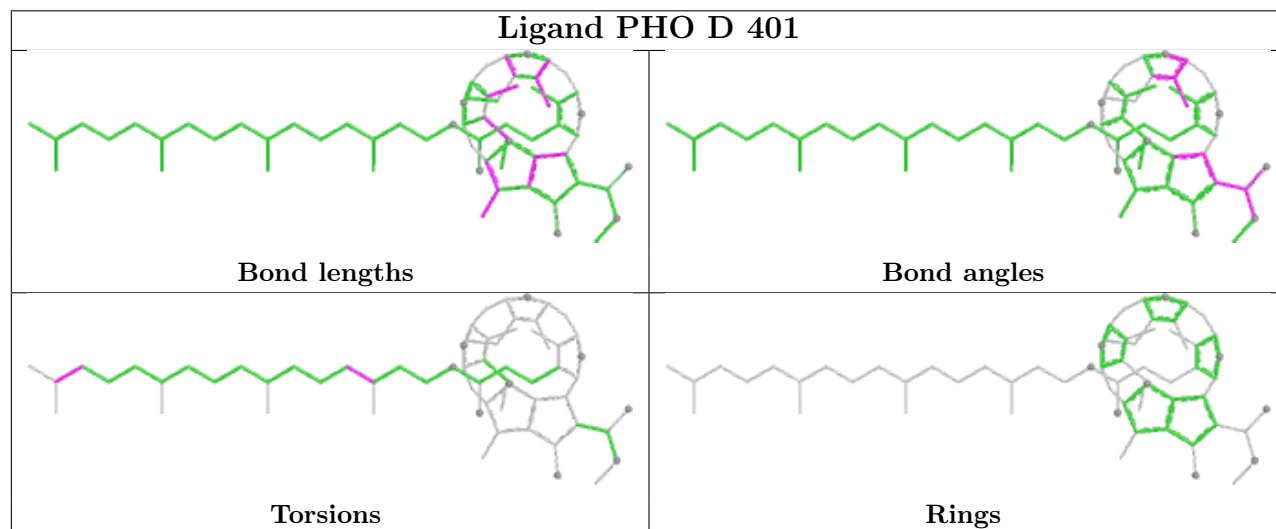
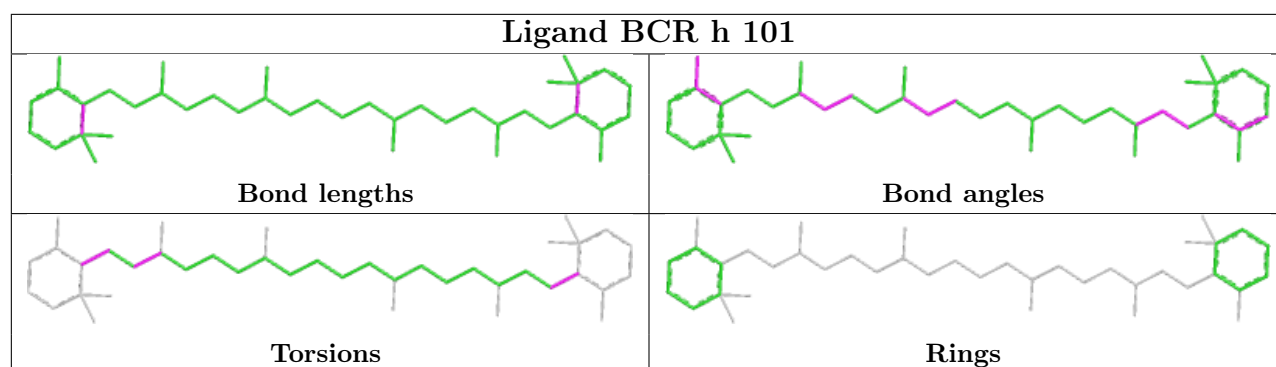
Ligand LMG B 620

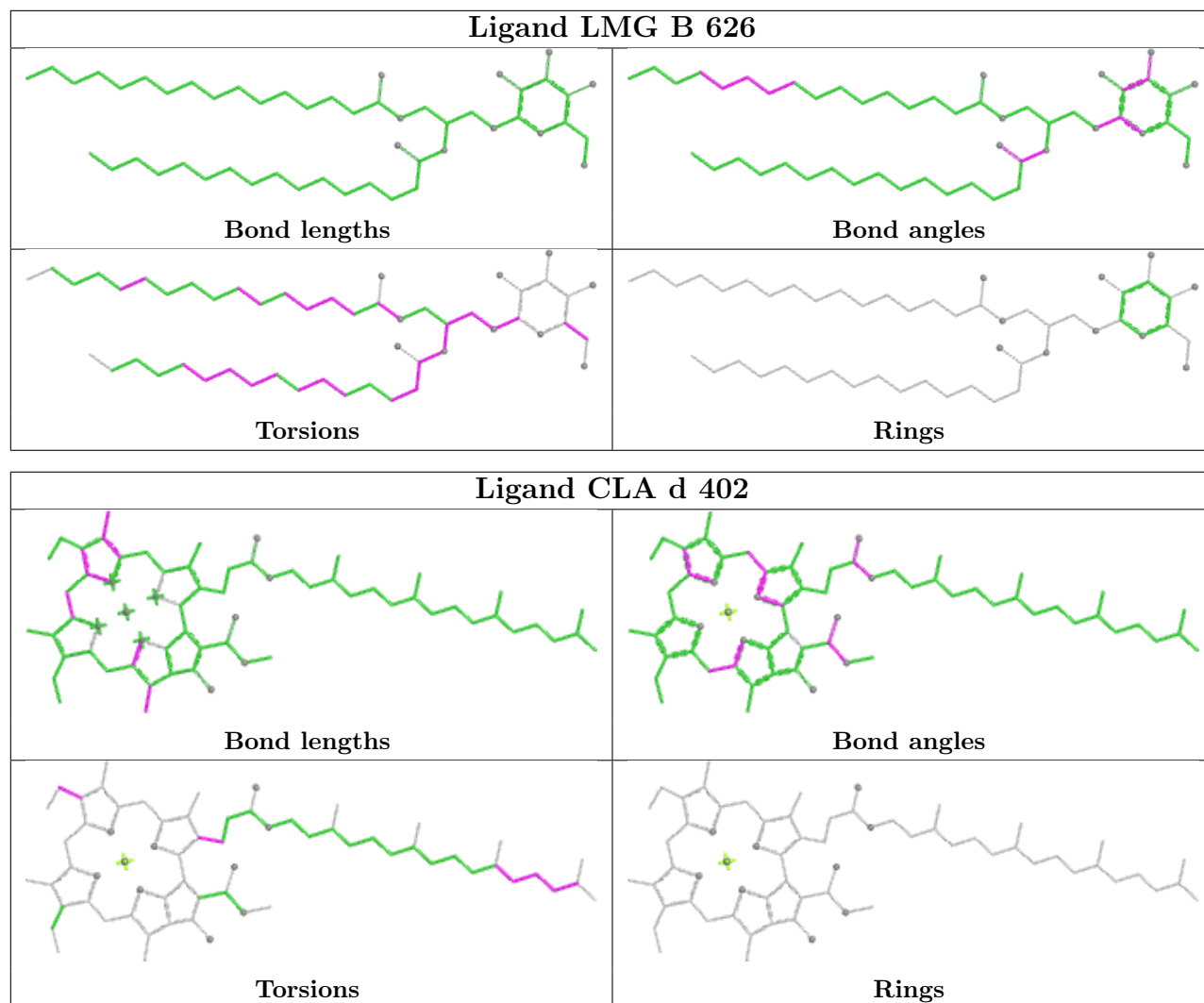


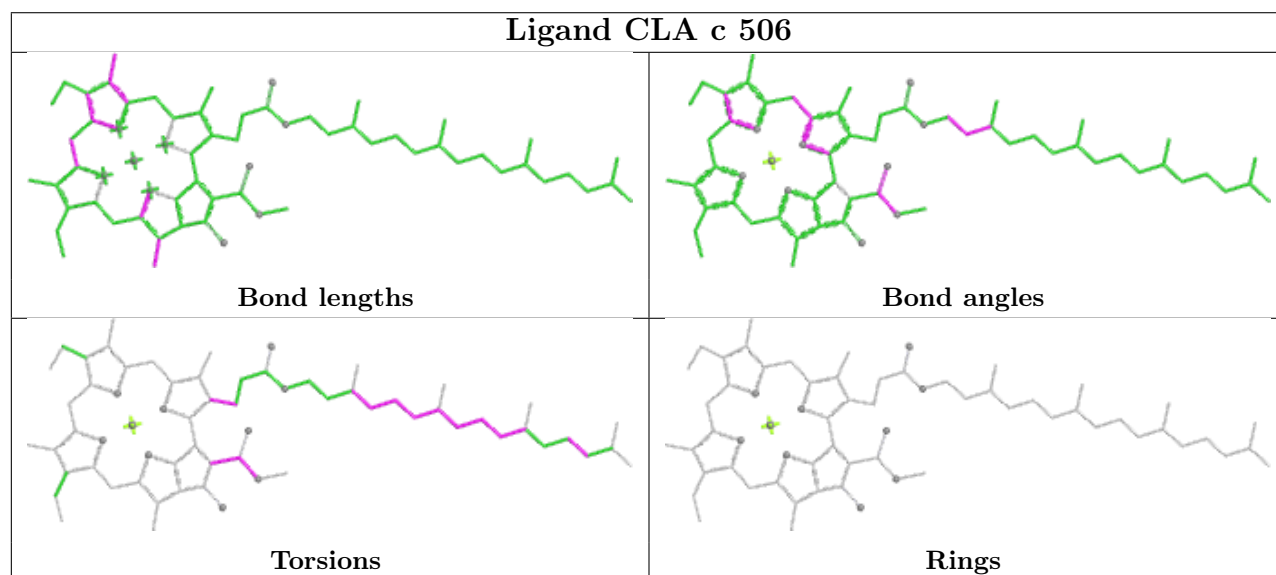
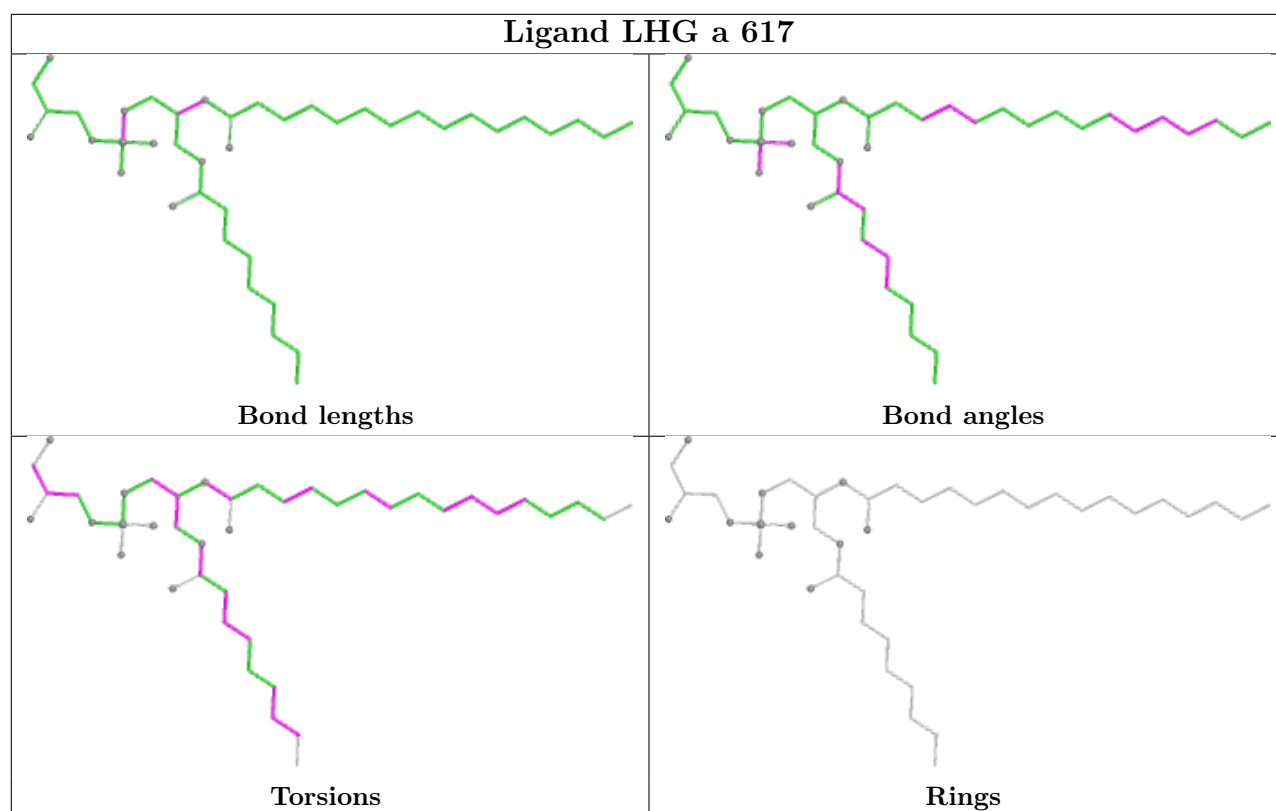
Ligand CLA B 604

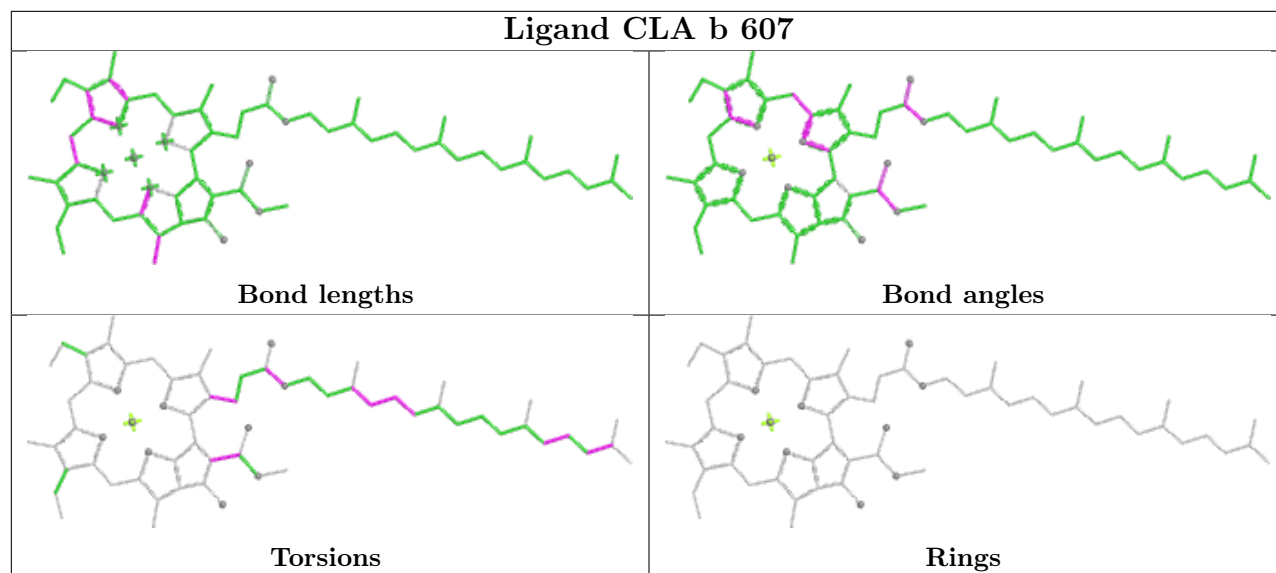
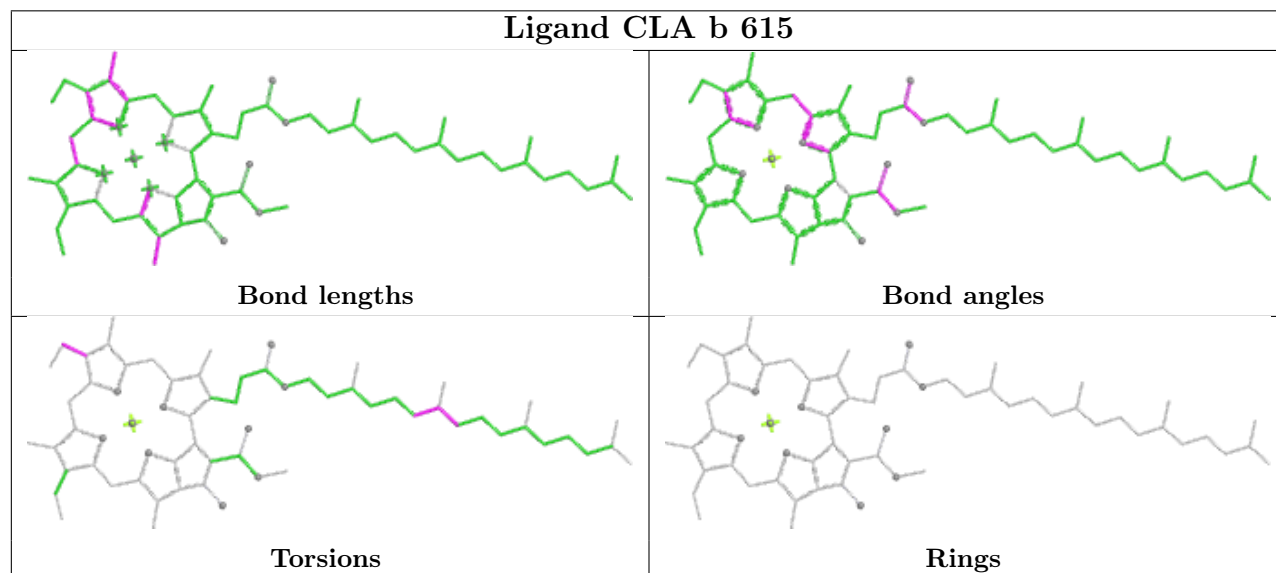
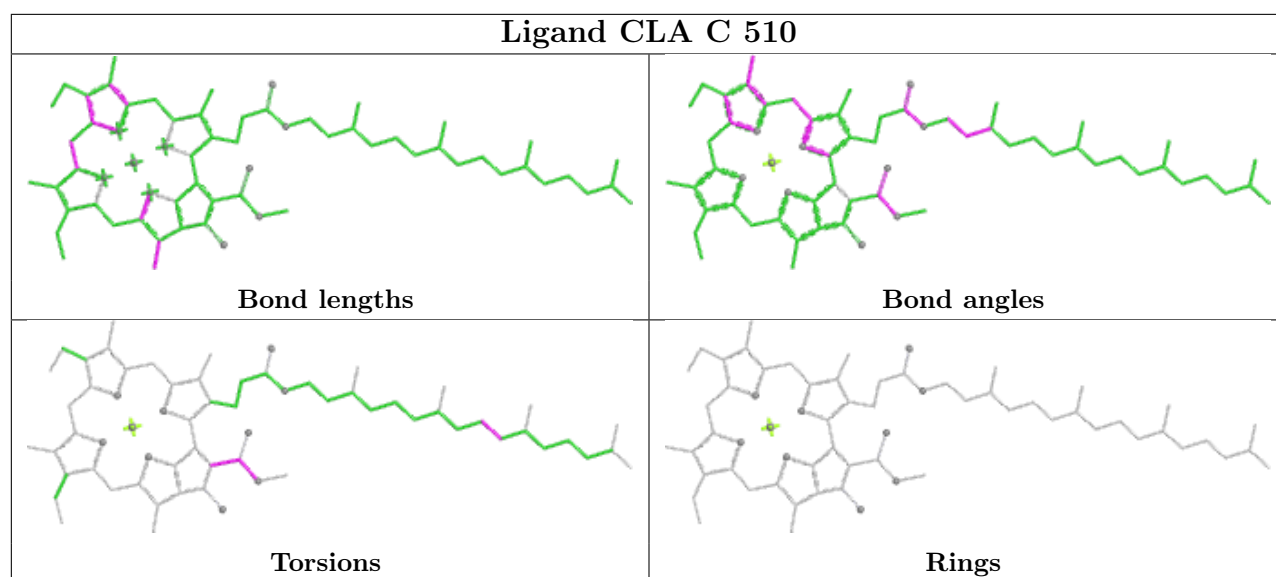


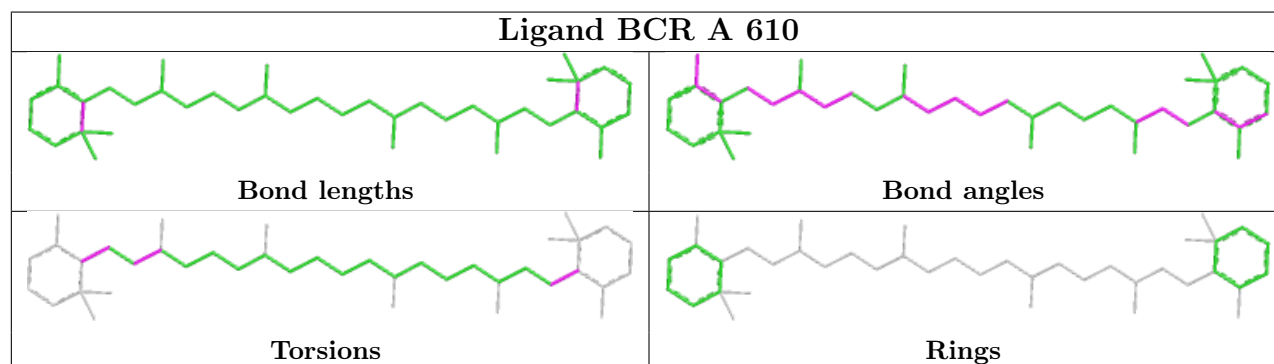
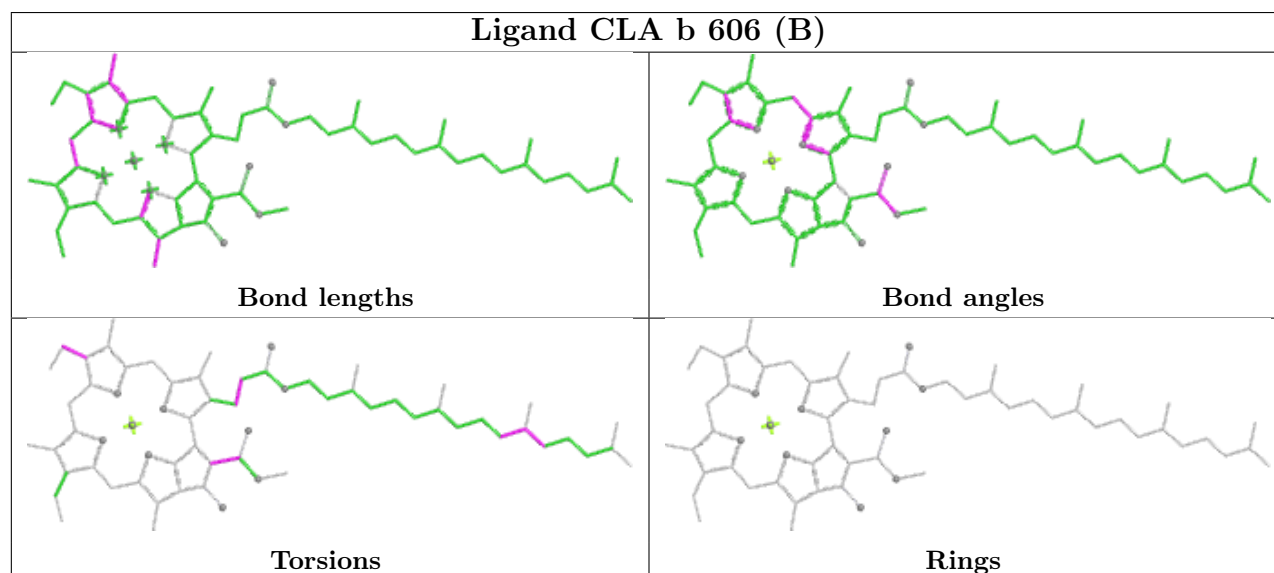
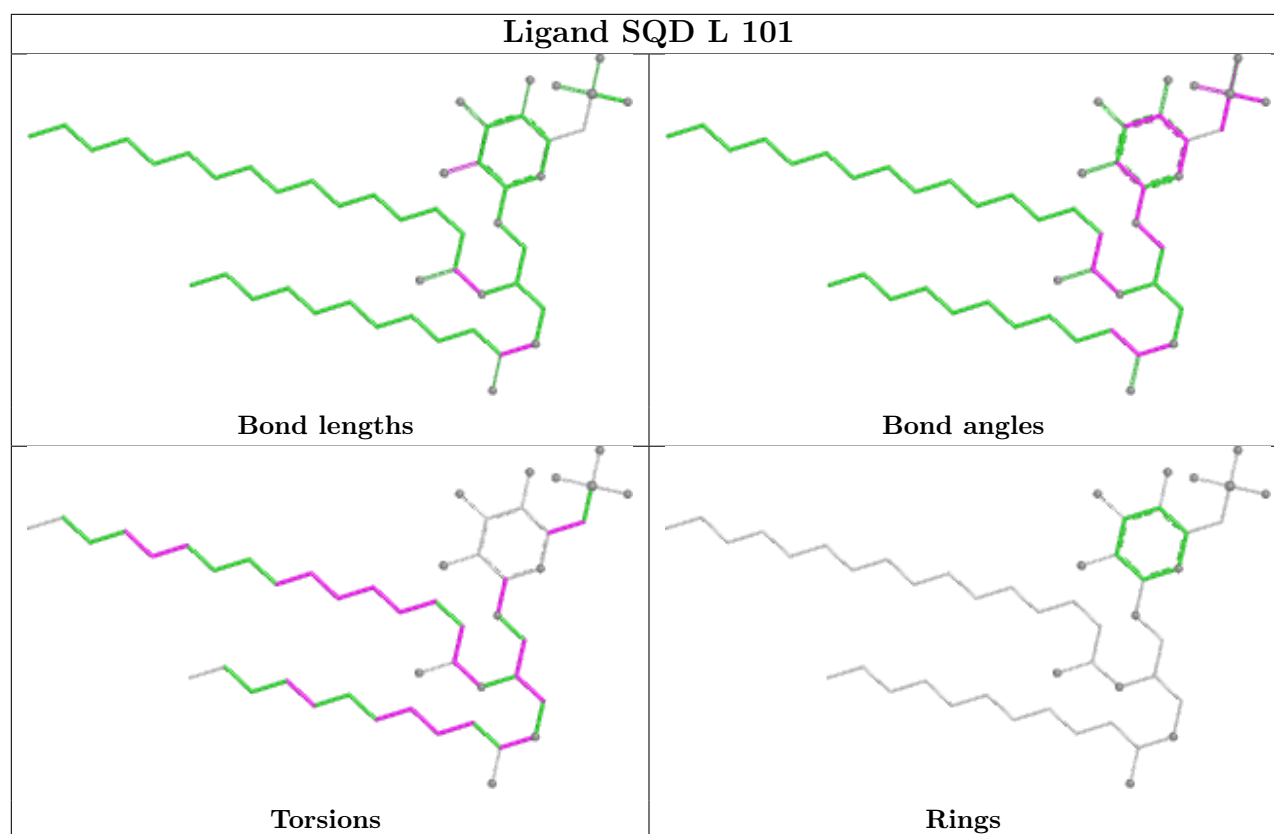
Ligand CLA B 601**Ligand CLA a 610****Ligand LMG c 519**

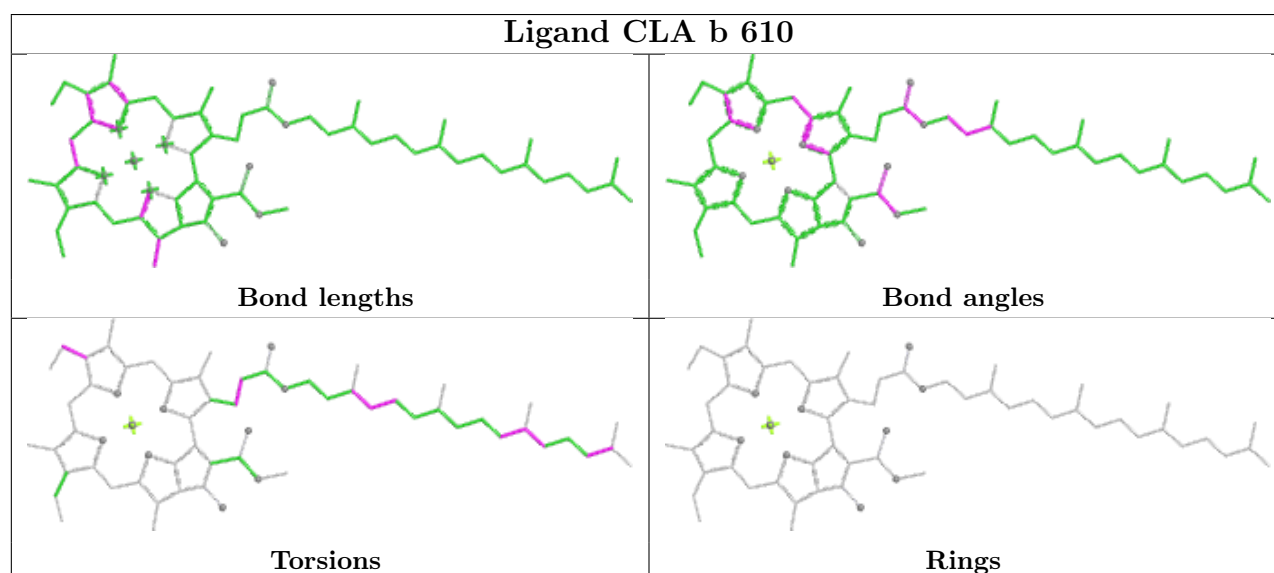
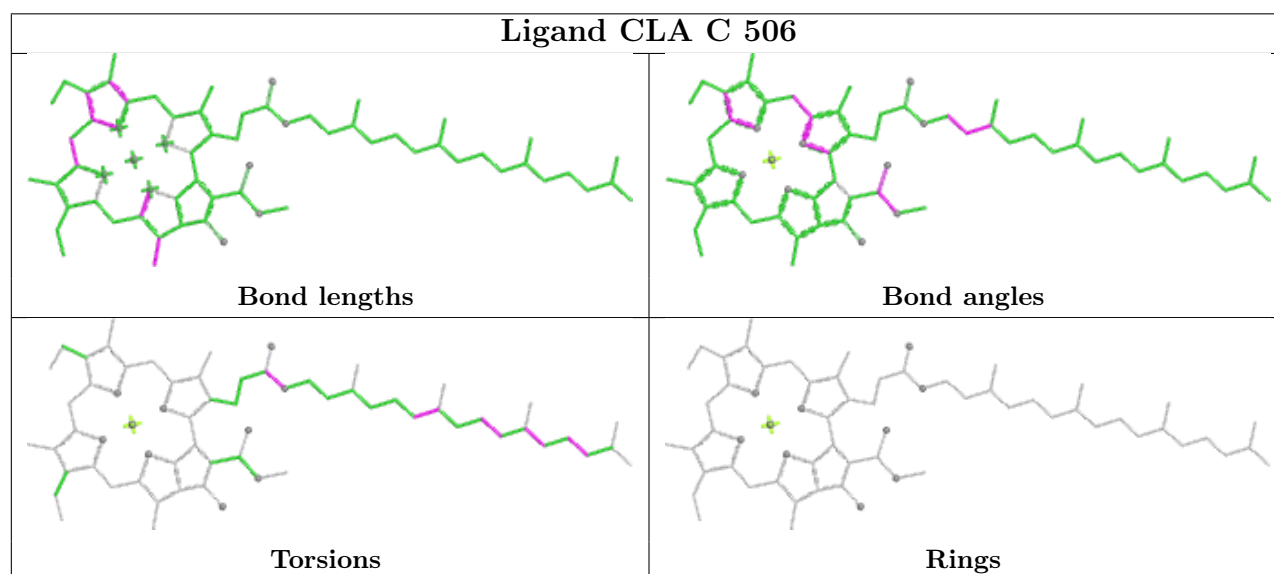
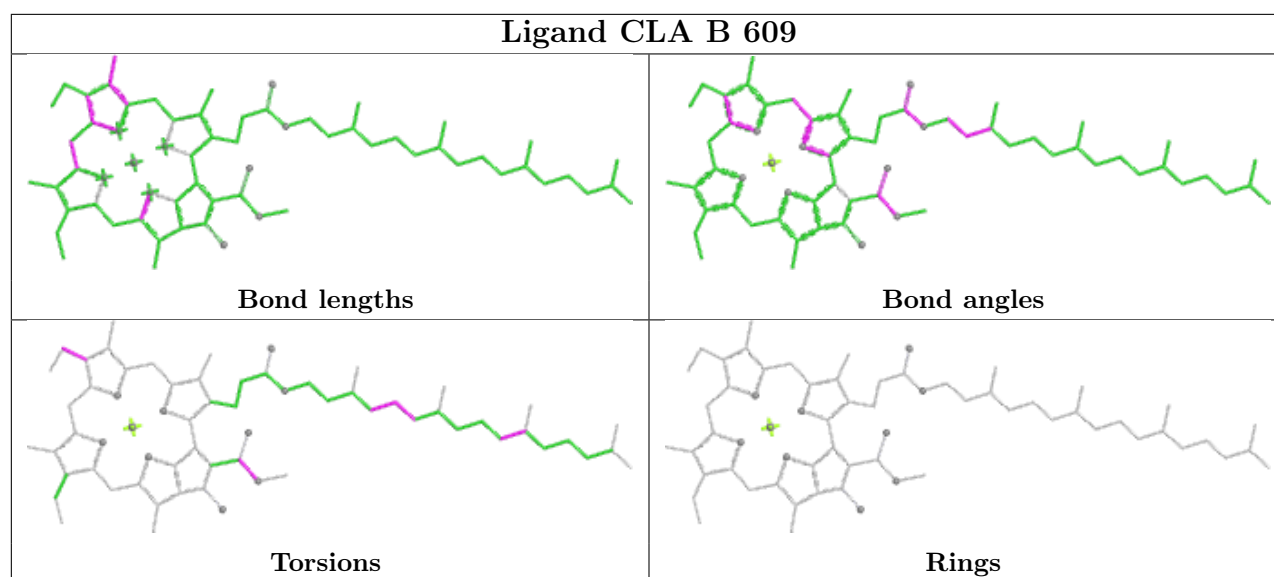


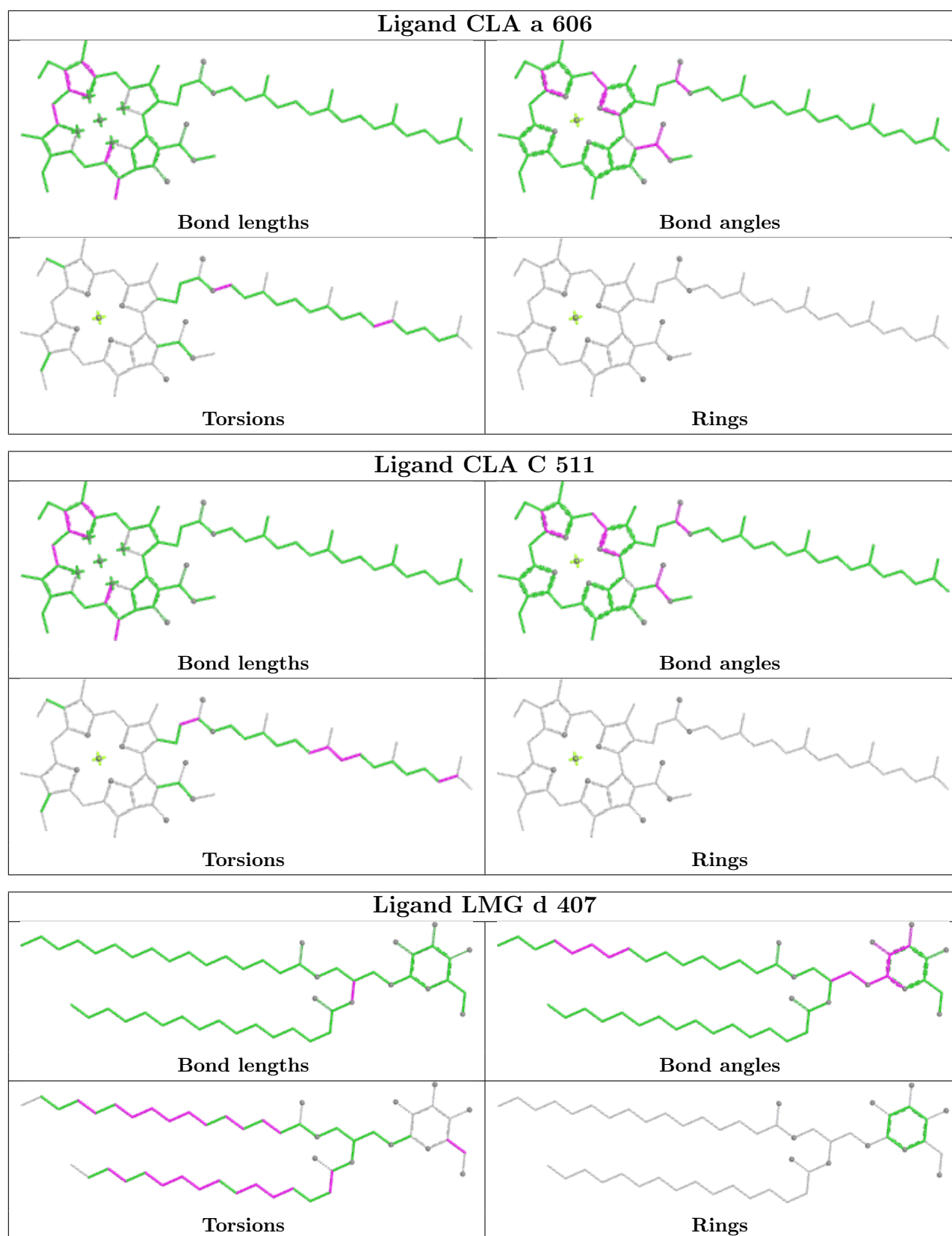


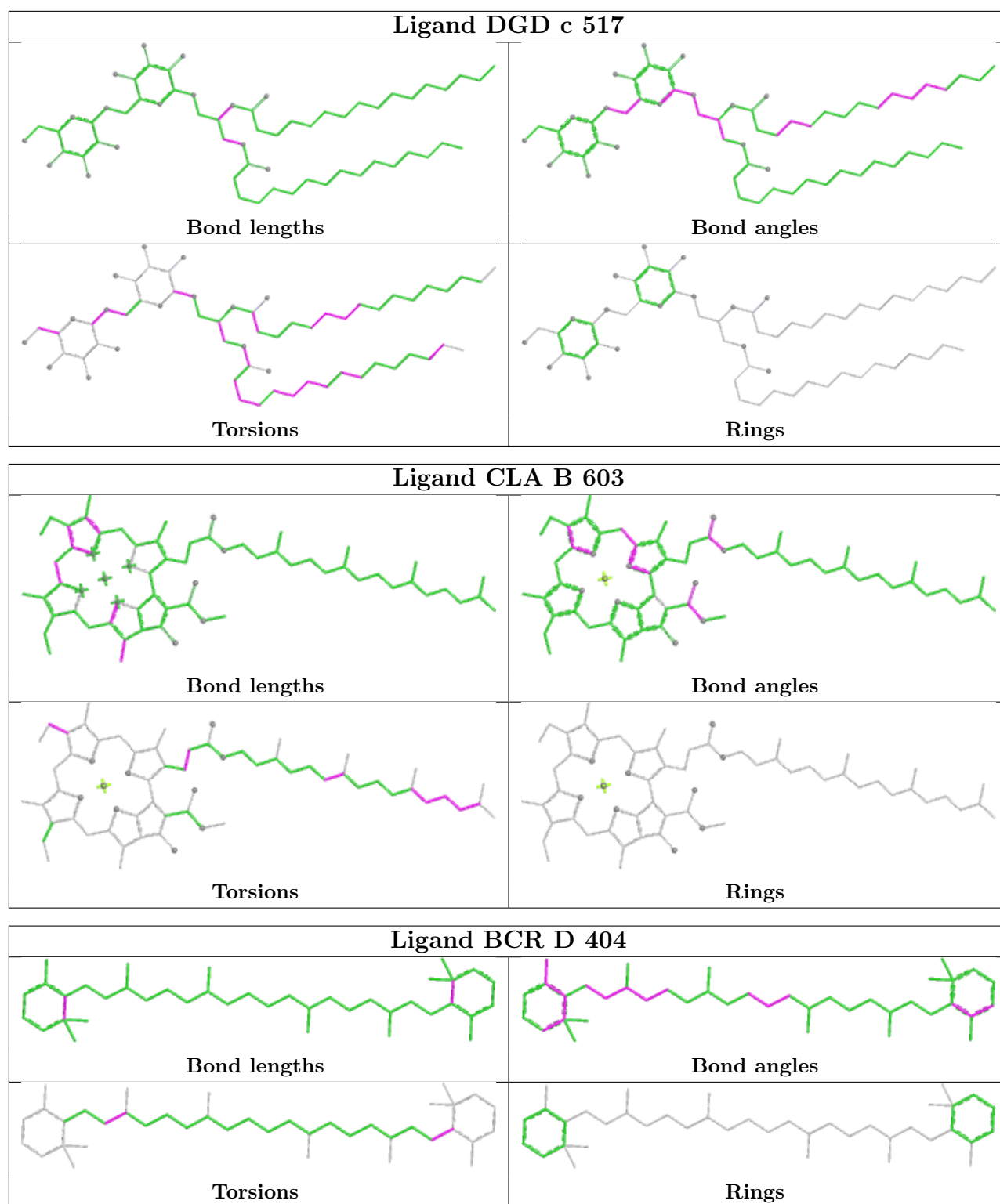


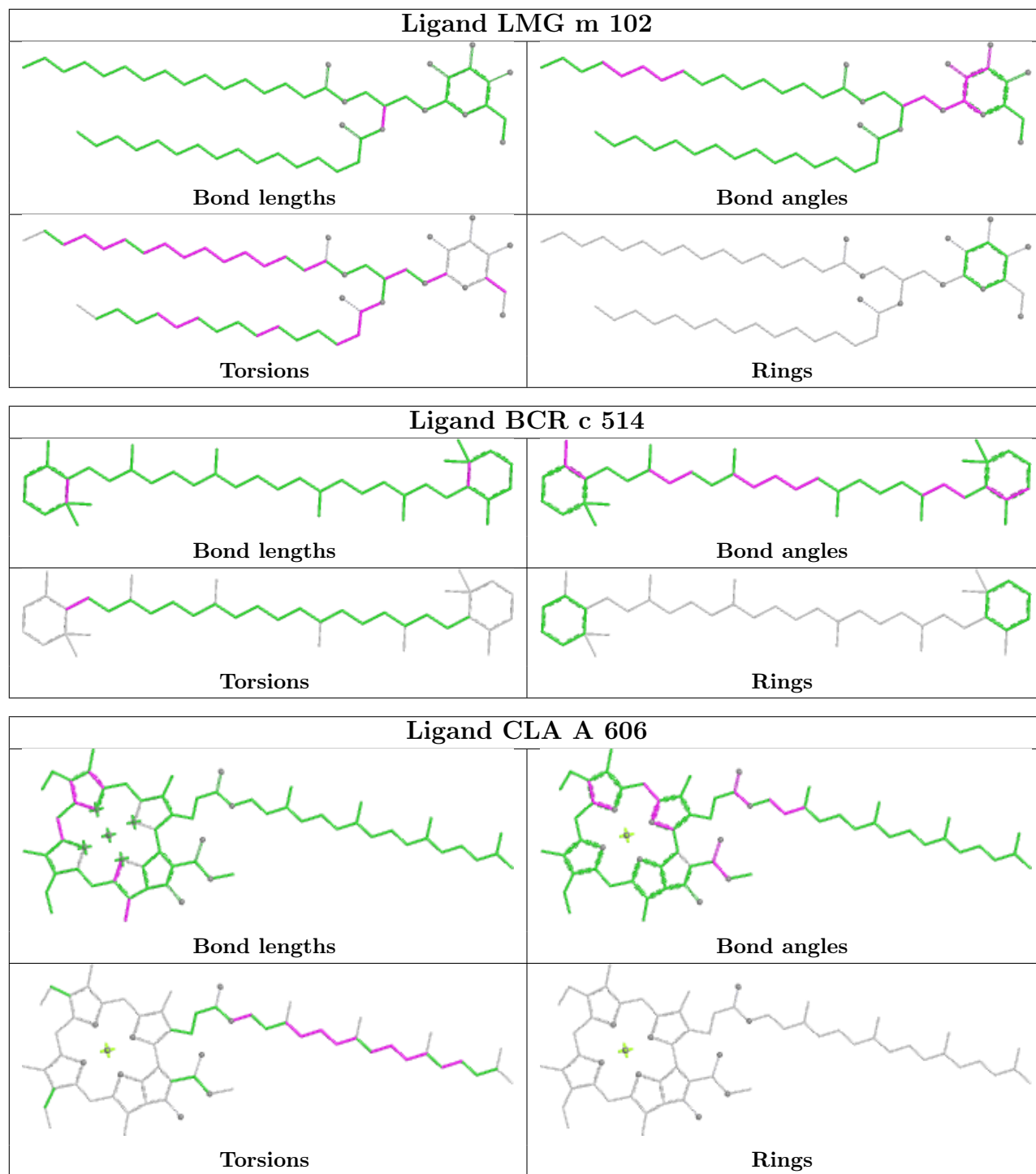


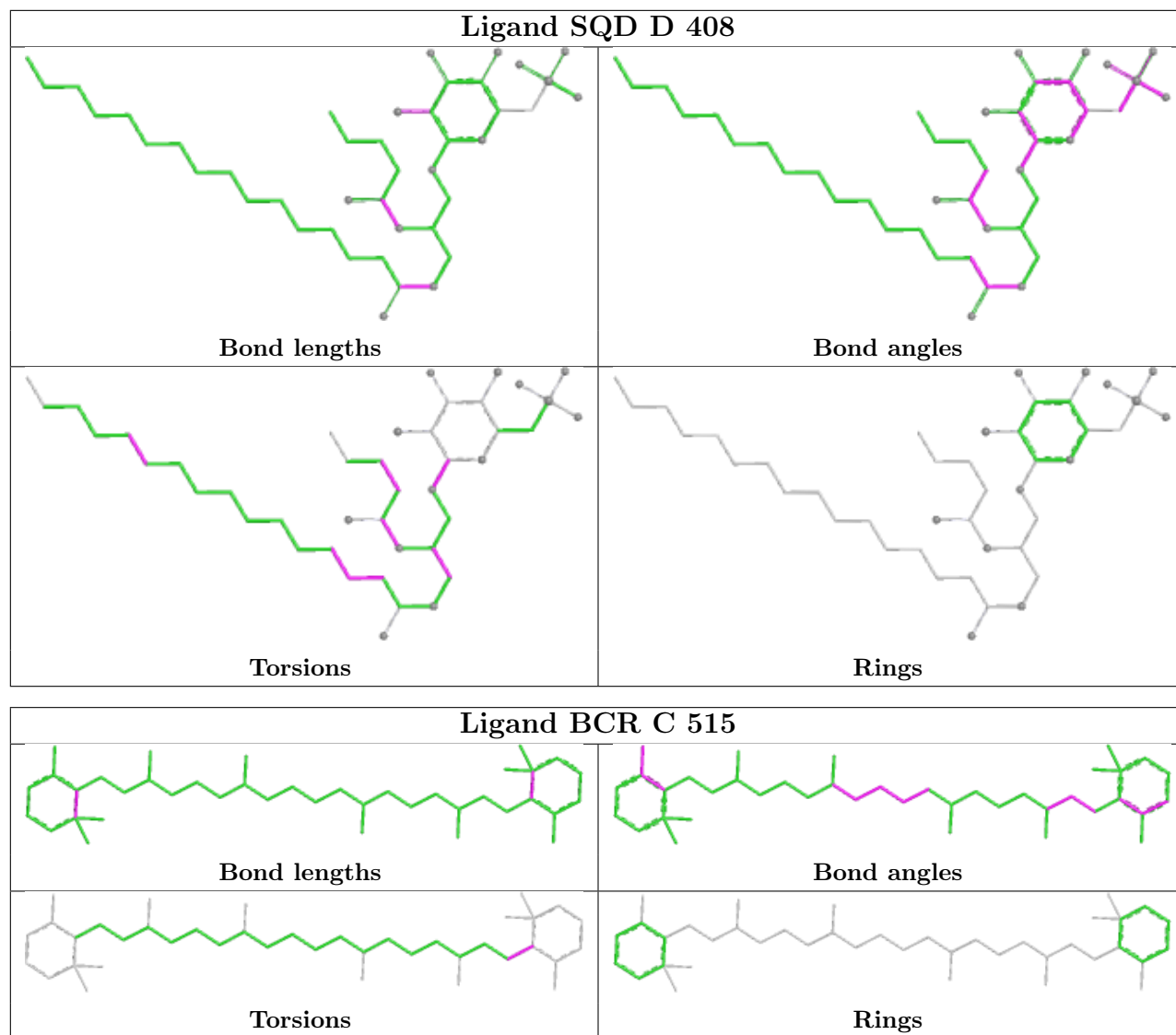


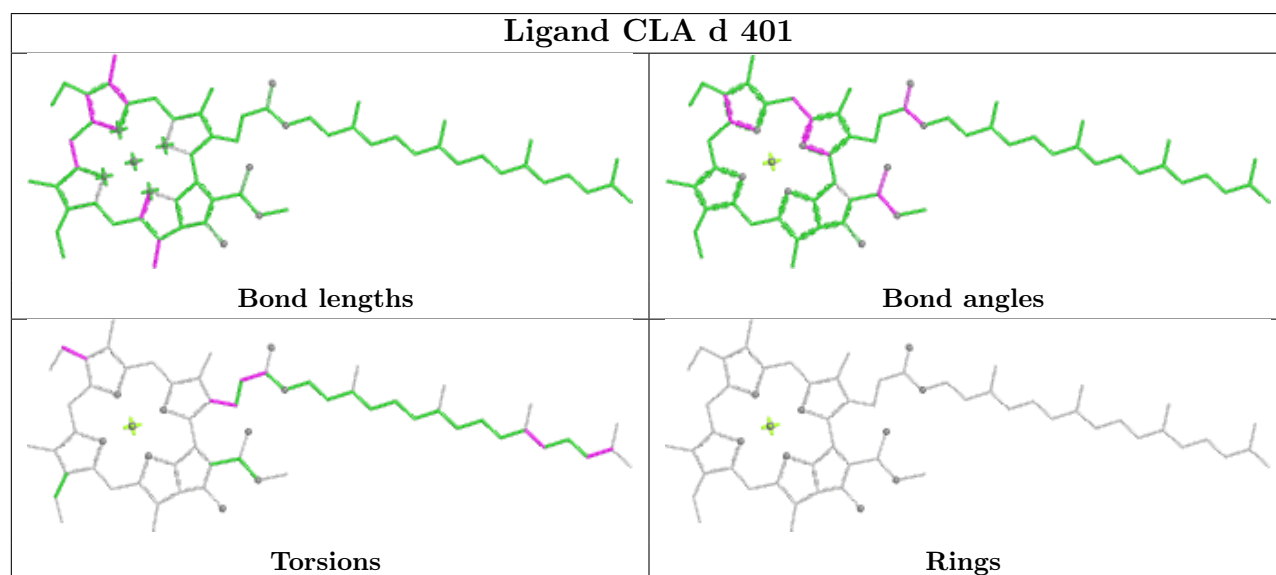
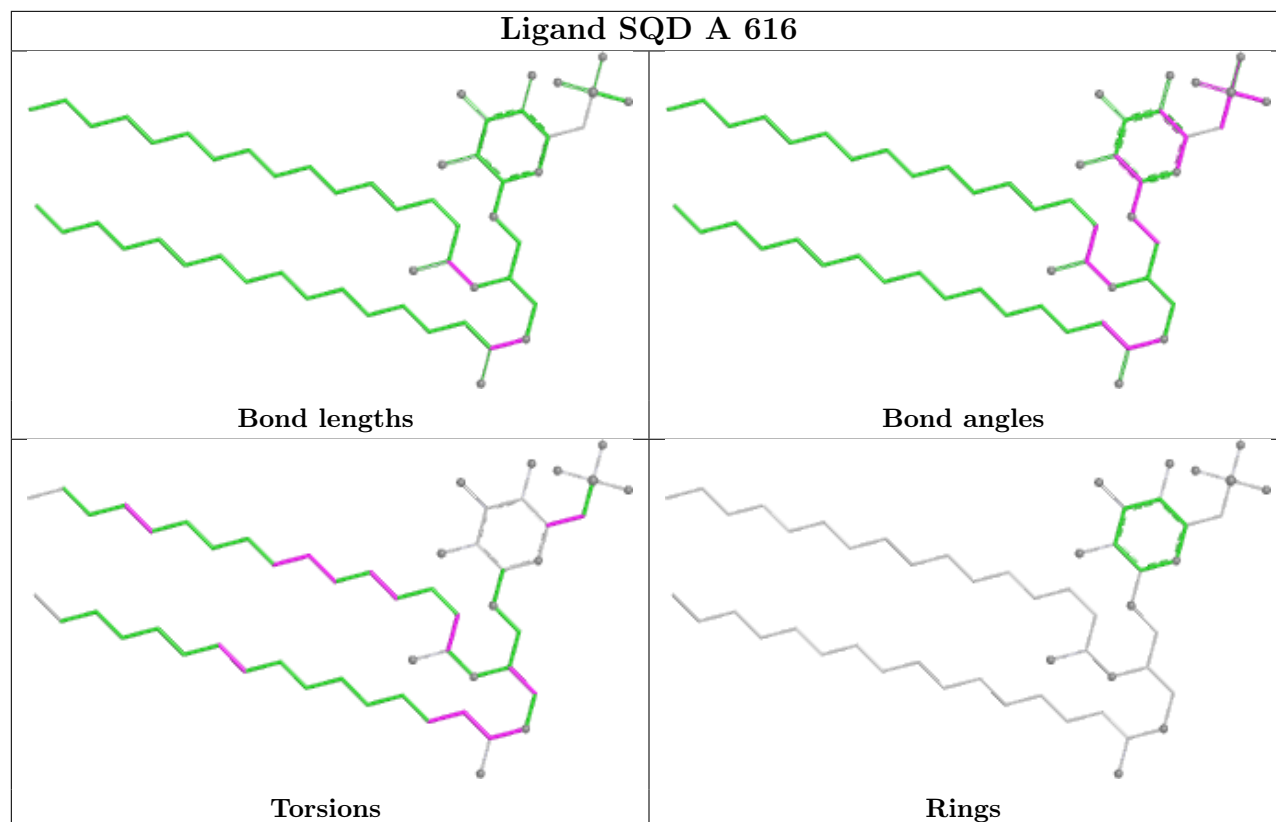


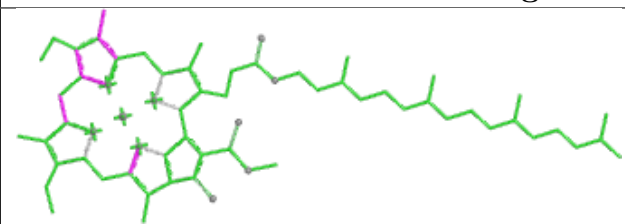
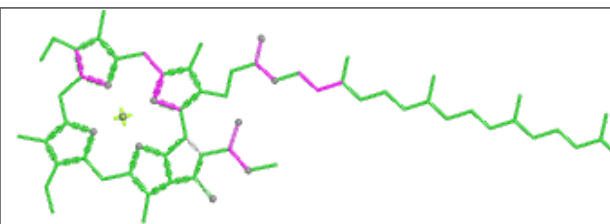
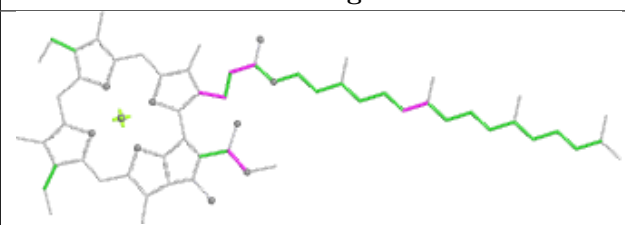
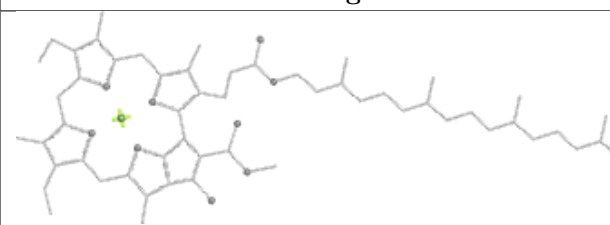


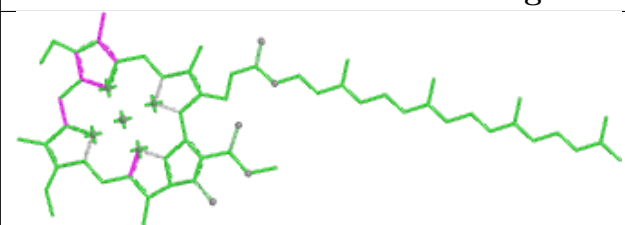
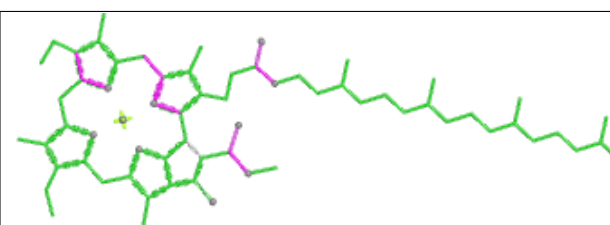
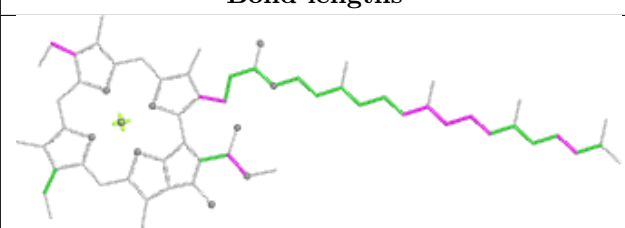
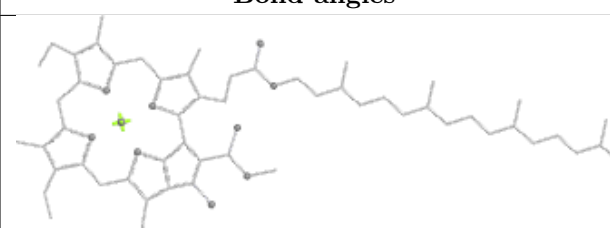


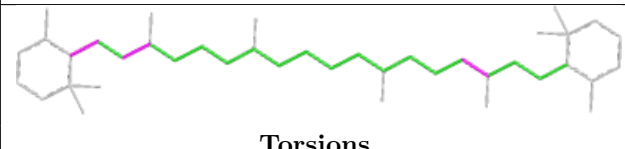
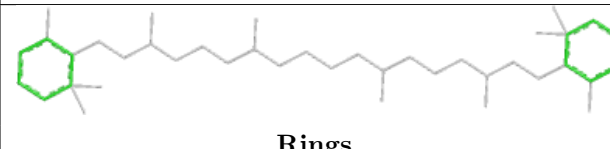


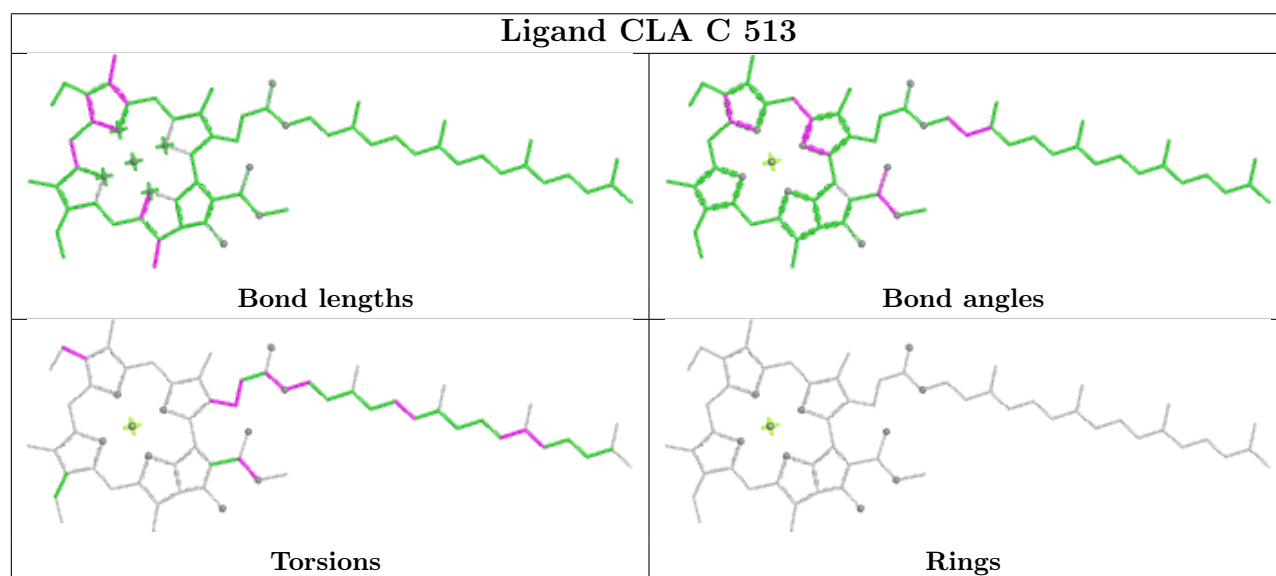
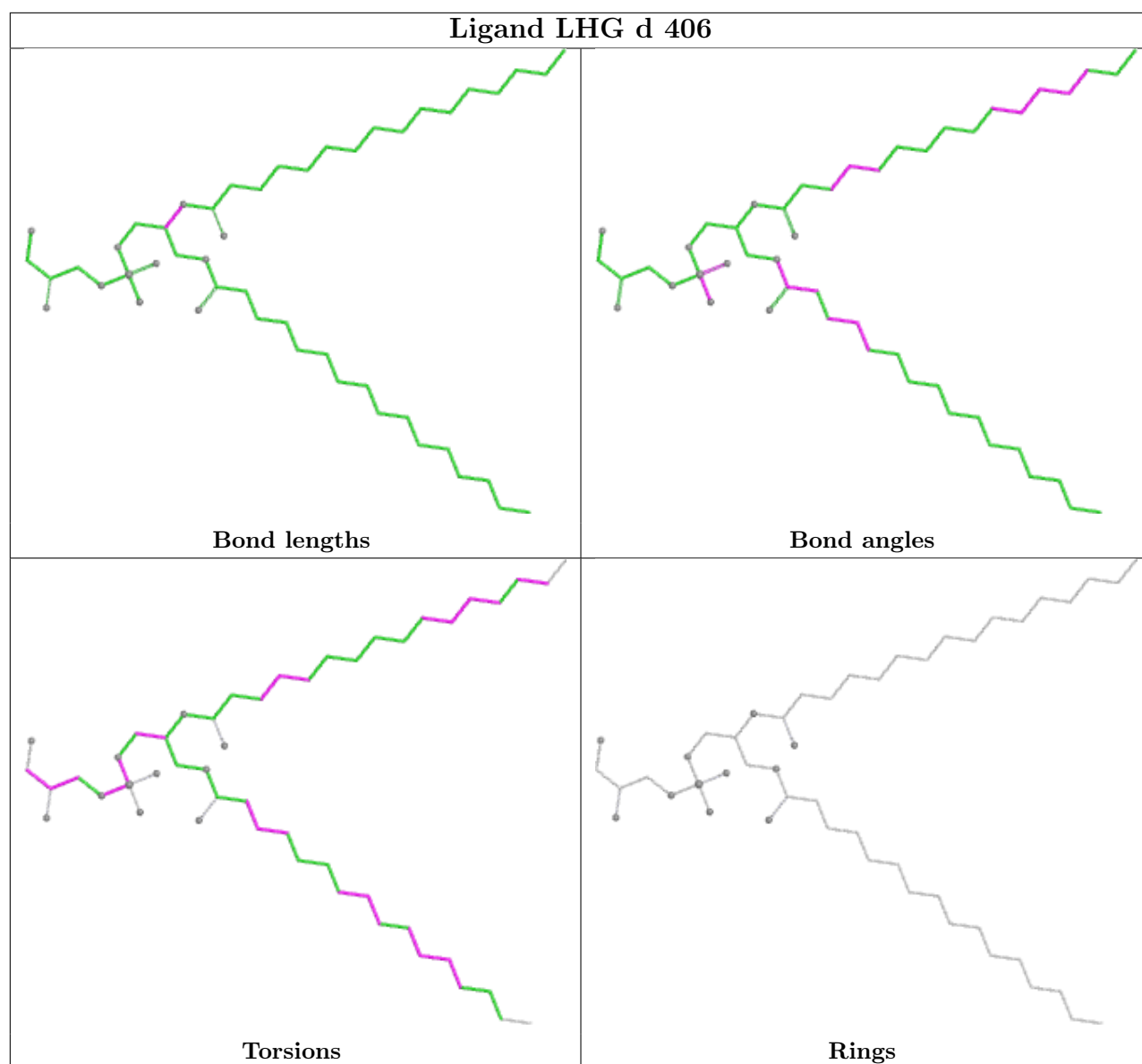


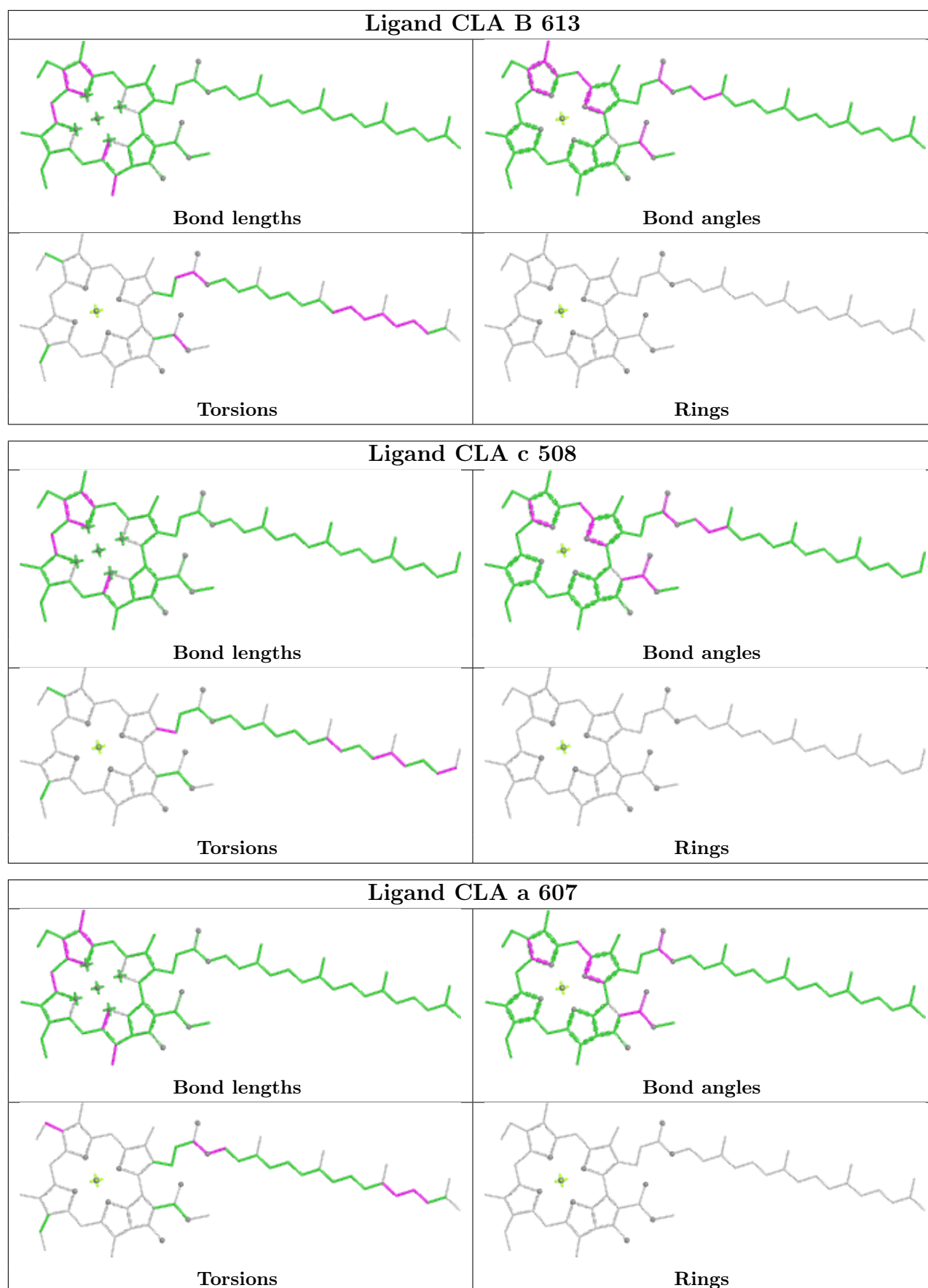


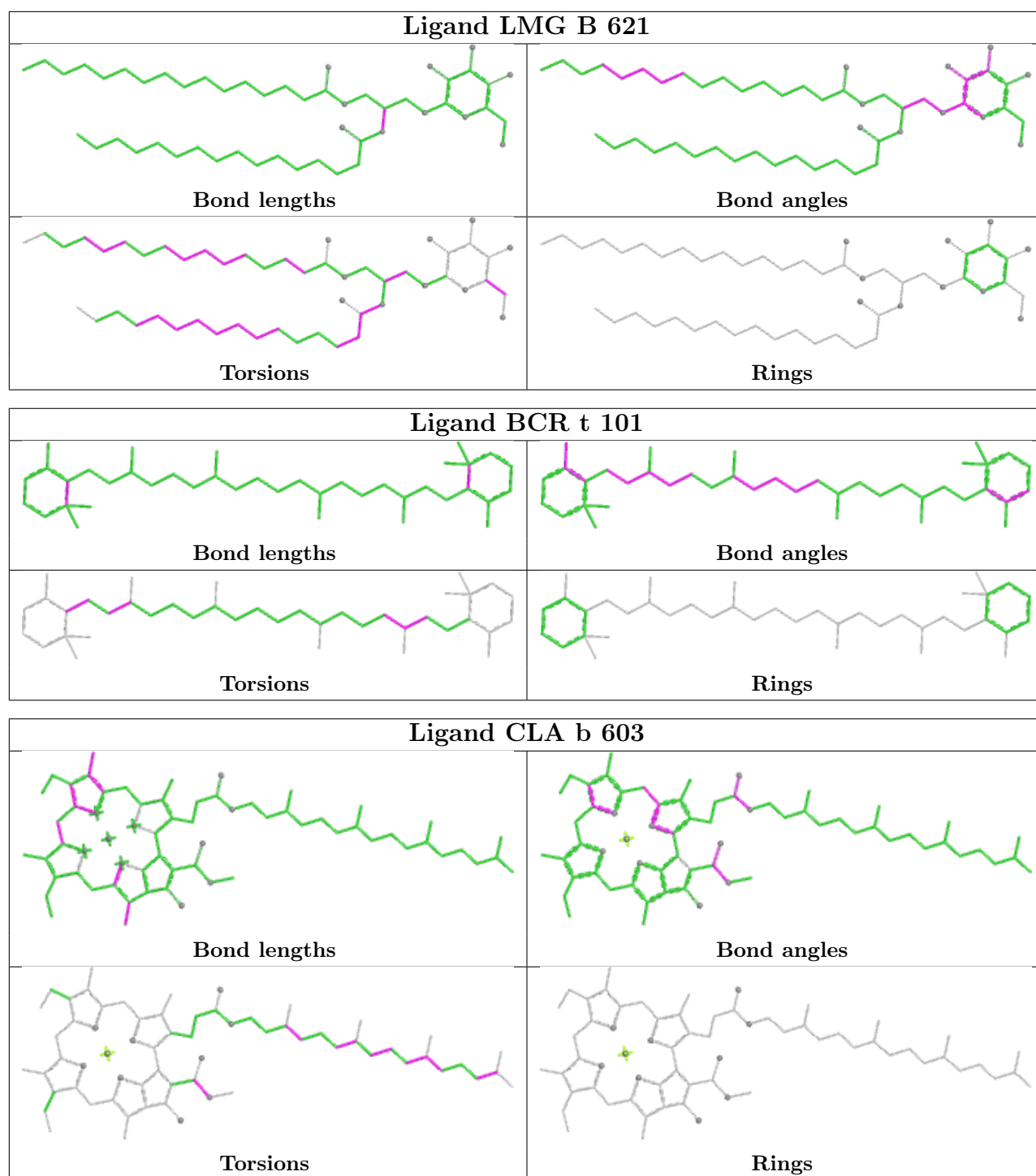
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

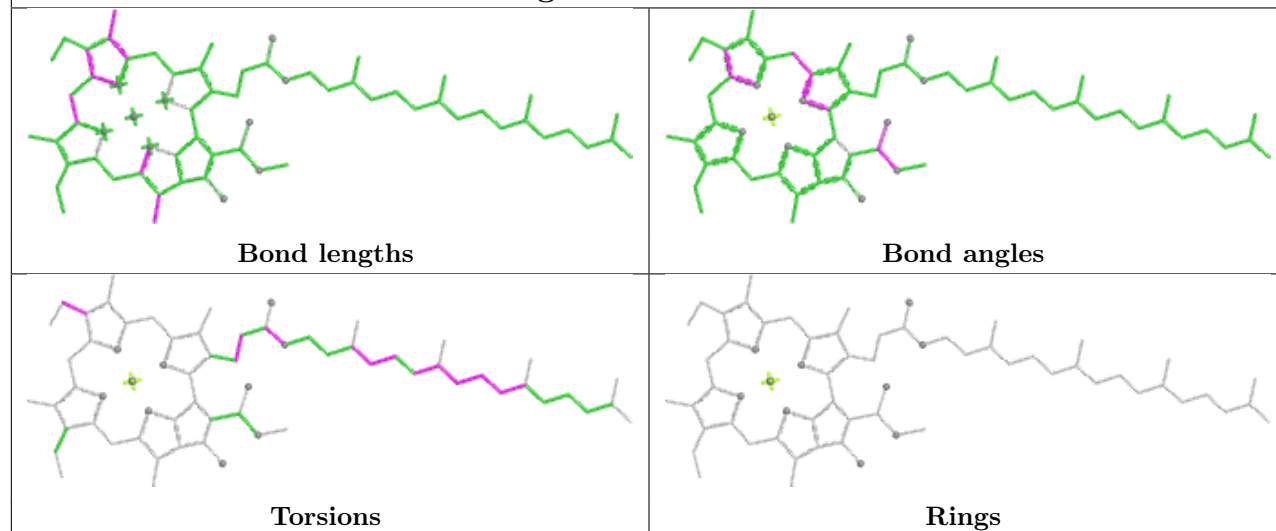
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



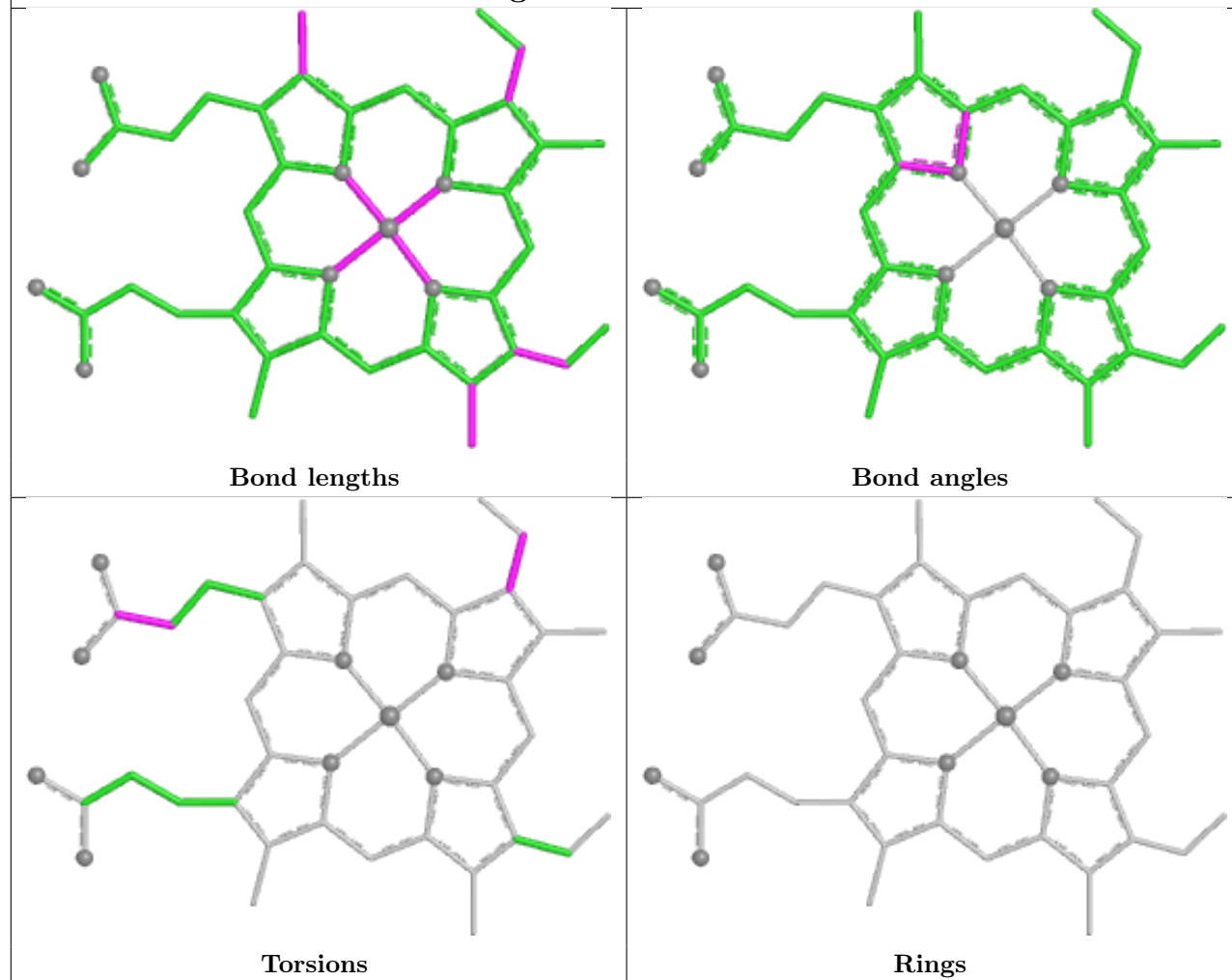


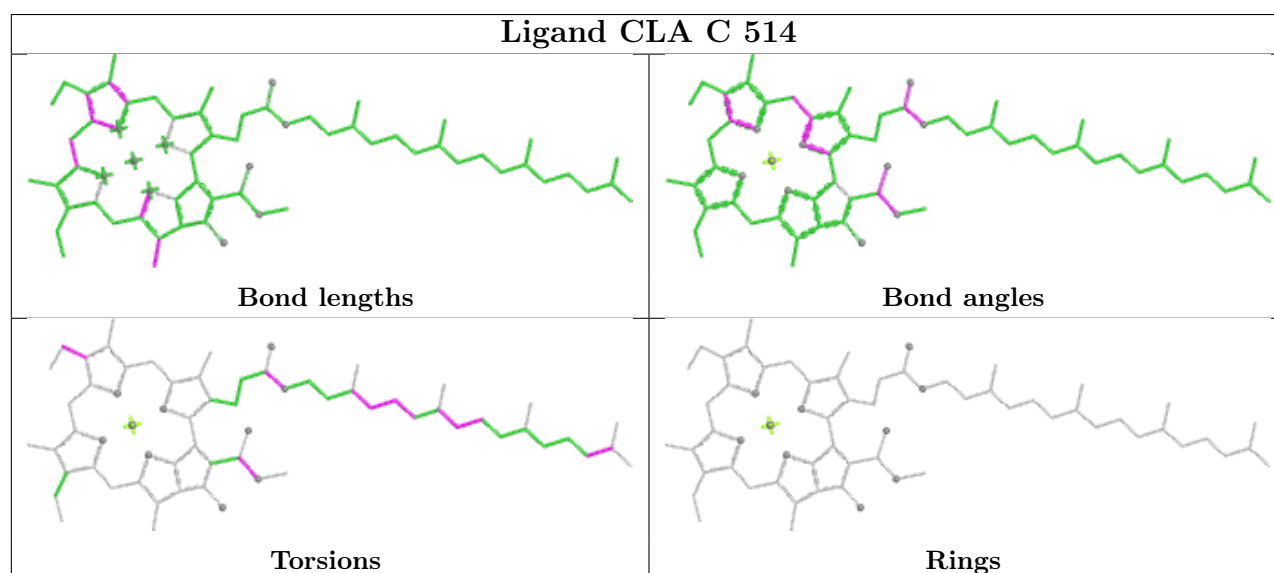
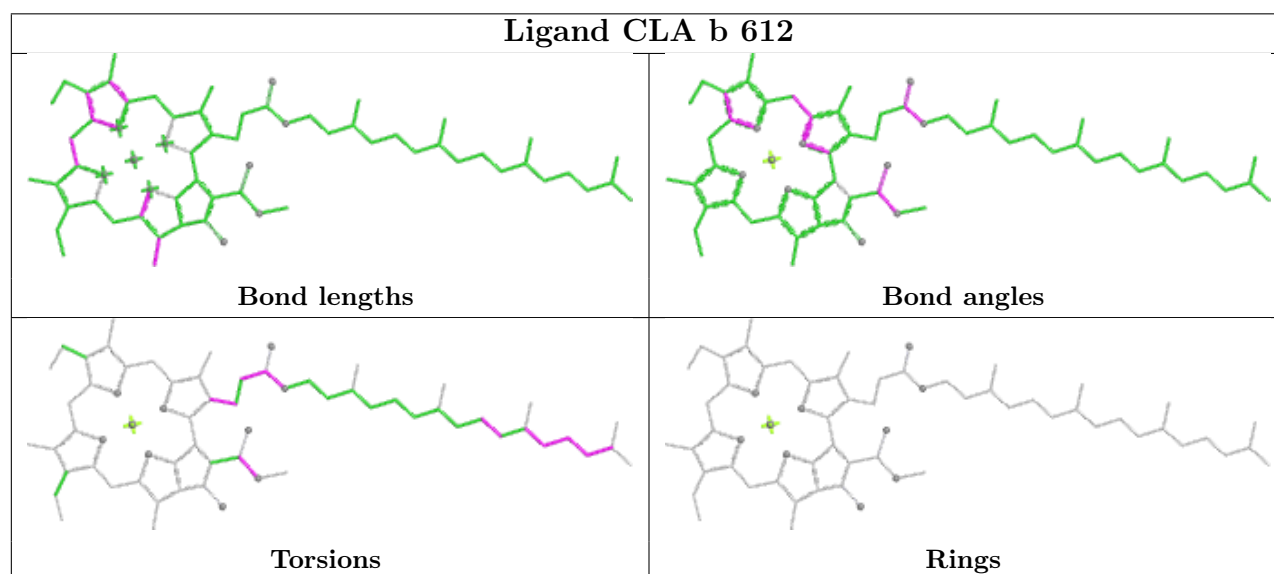
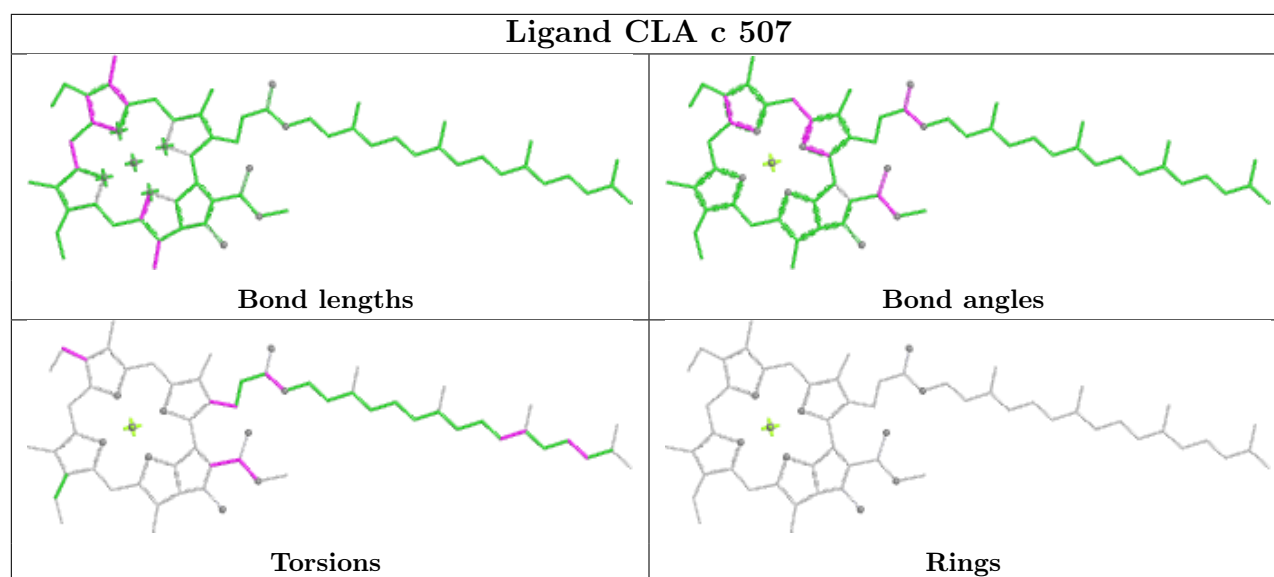


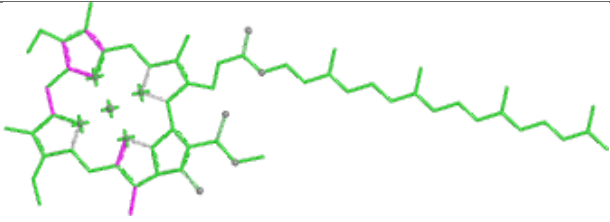
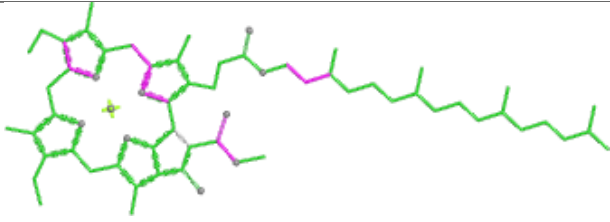
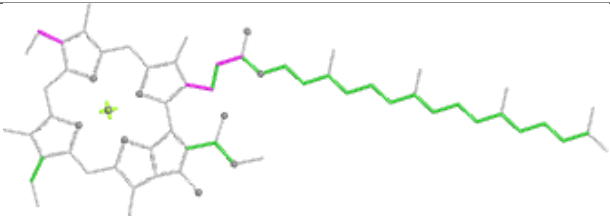
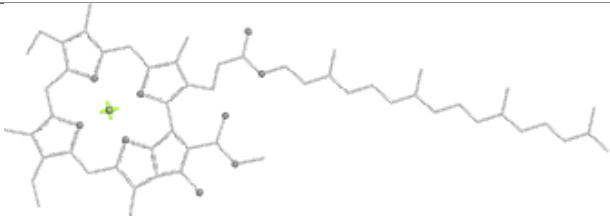
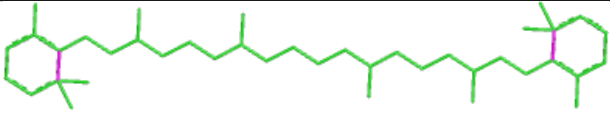
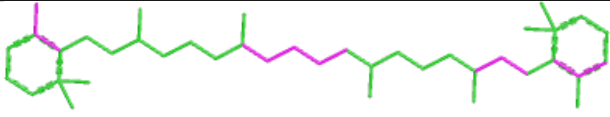
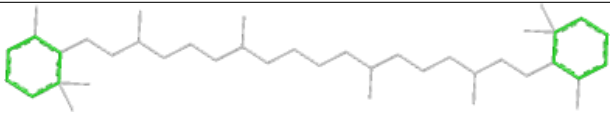
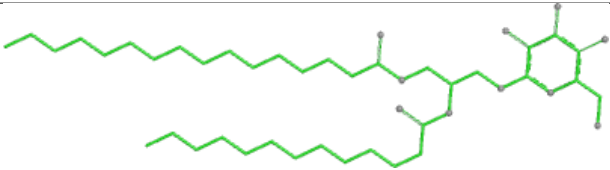
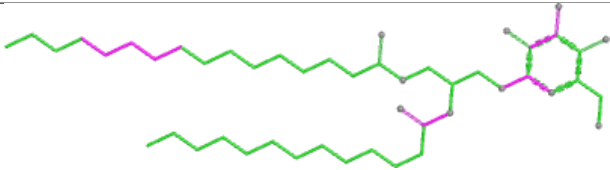
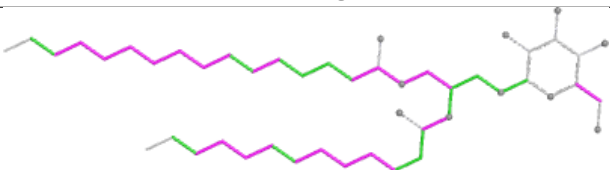
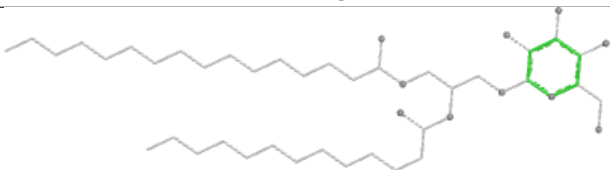
Ligand CLA c 505



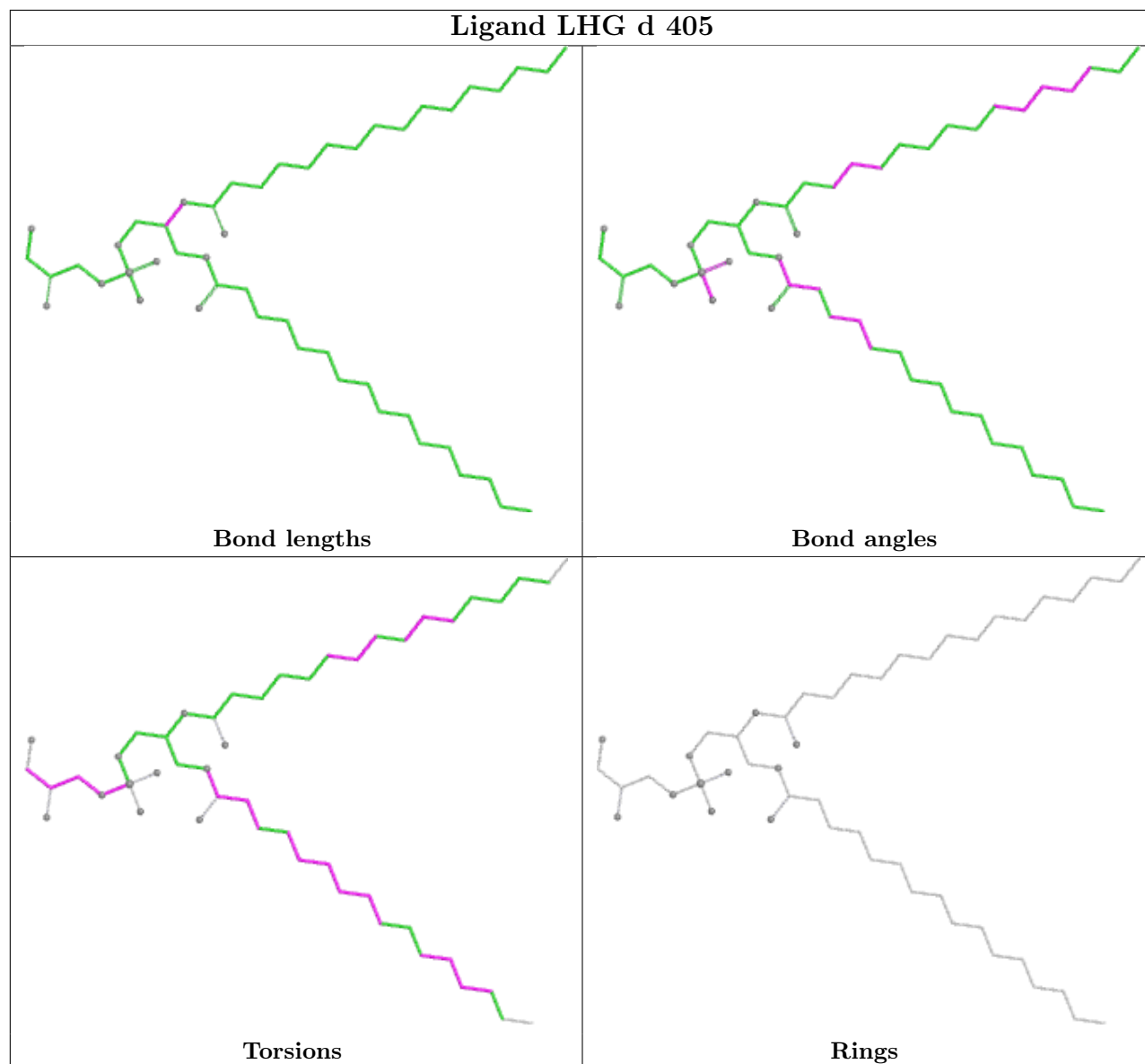
Ligand HEM E 101



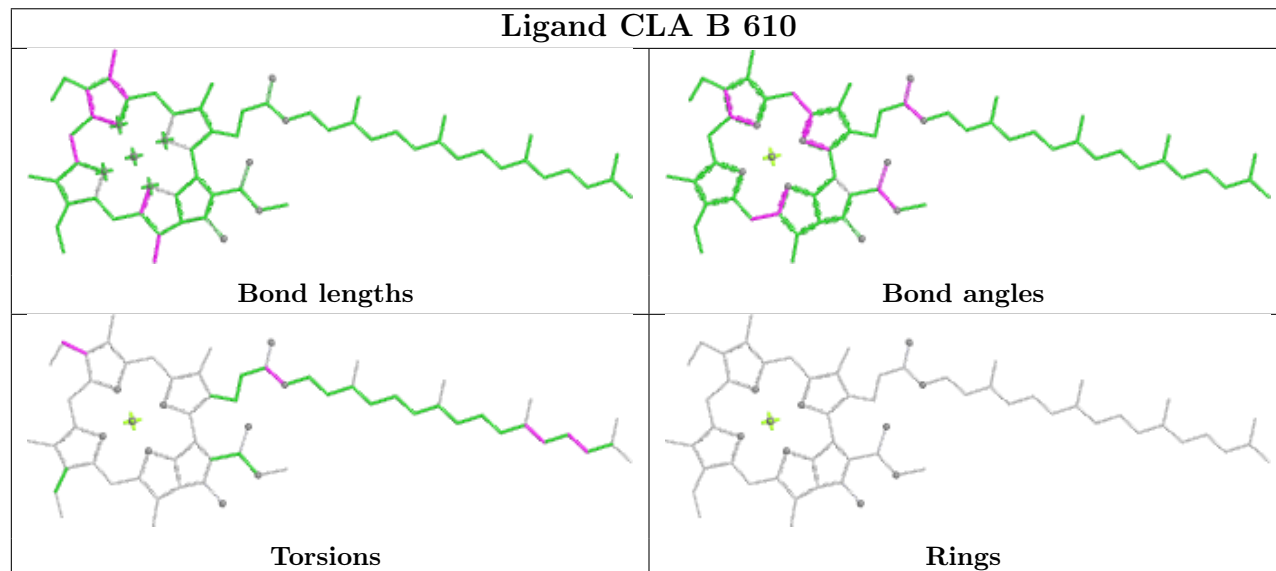


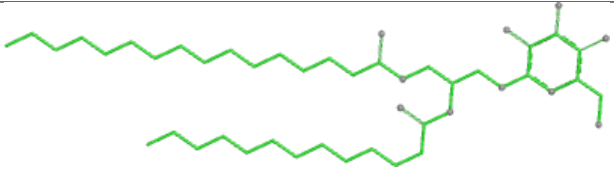
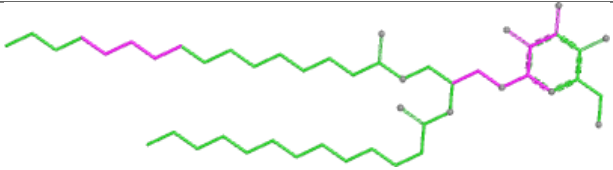
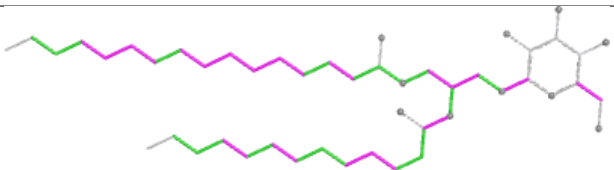
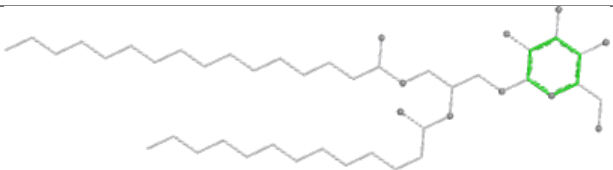
Ligand CLA D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 522	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

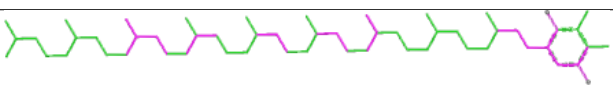
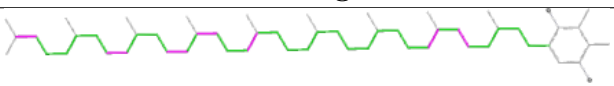
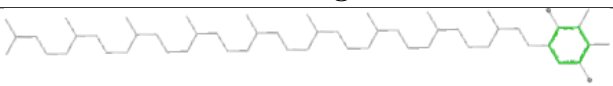
Ligand LHG d 405

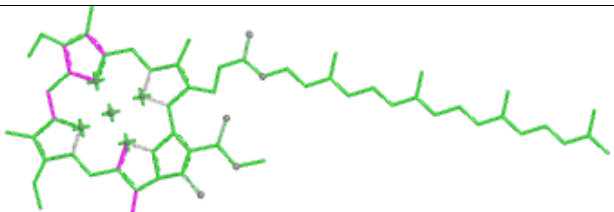
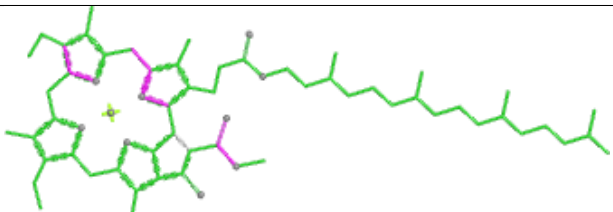
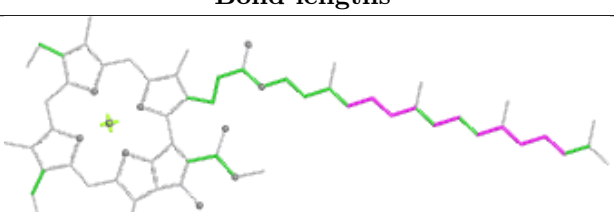
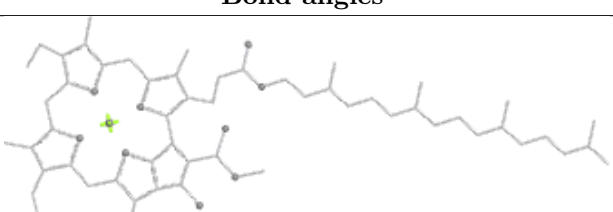


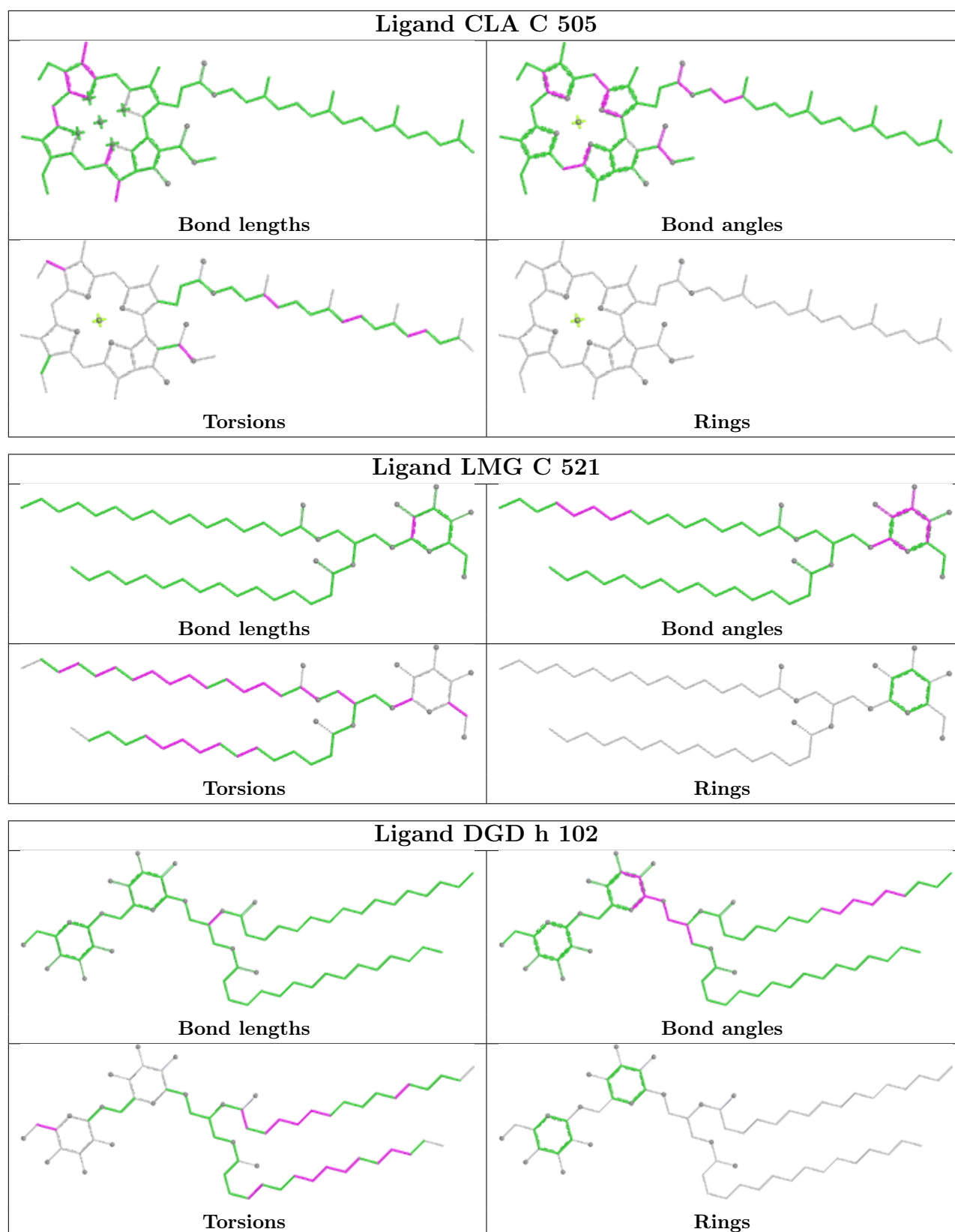
Ligand CLA B 610

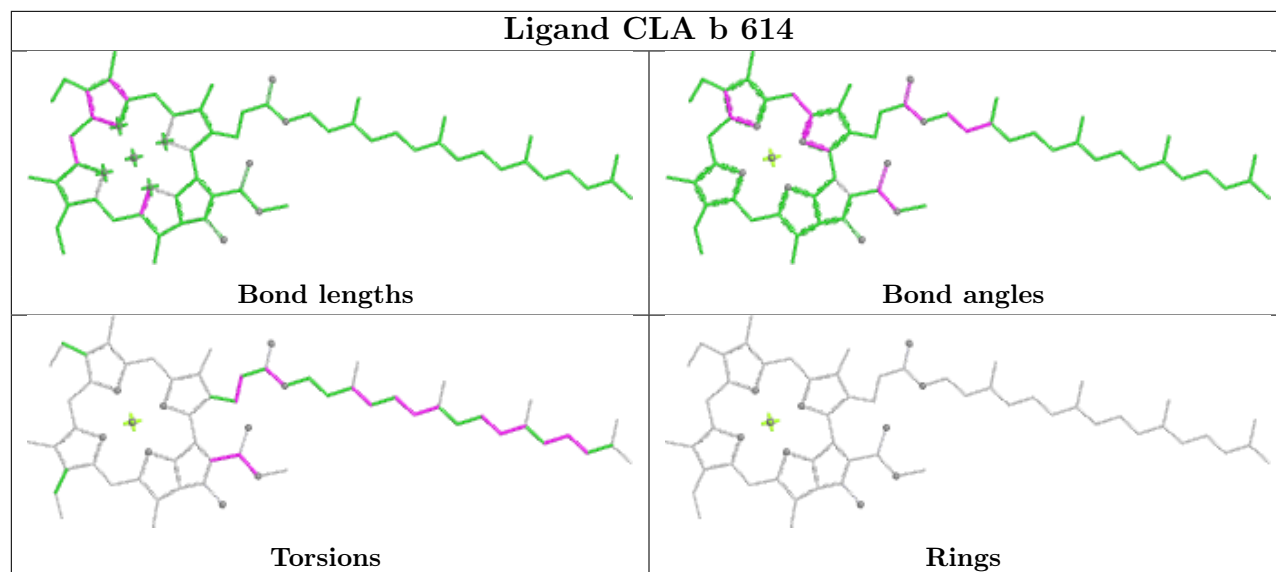
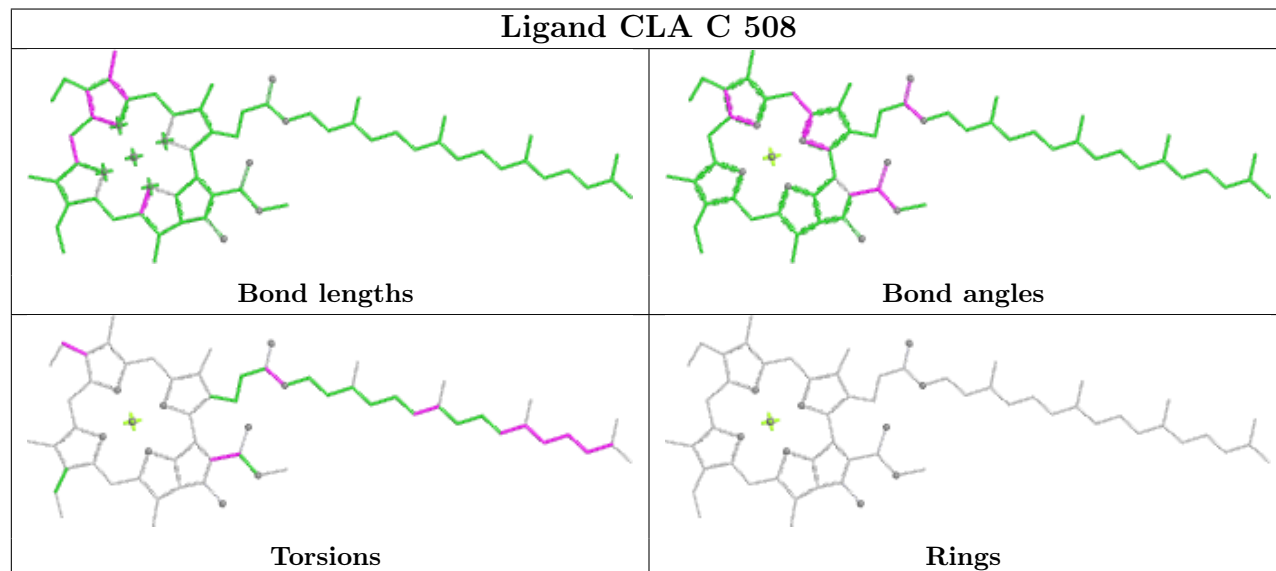
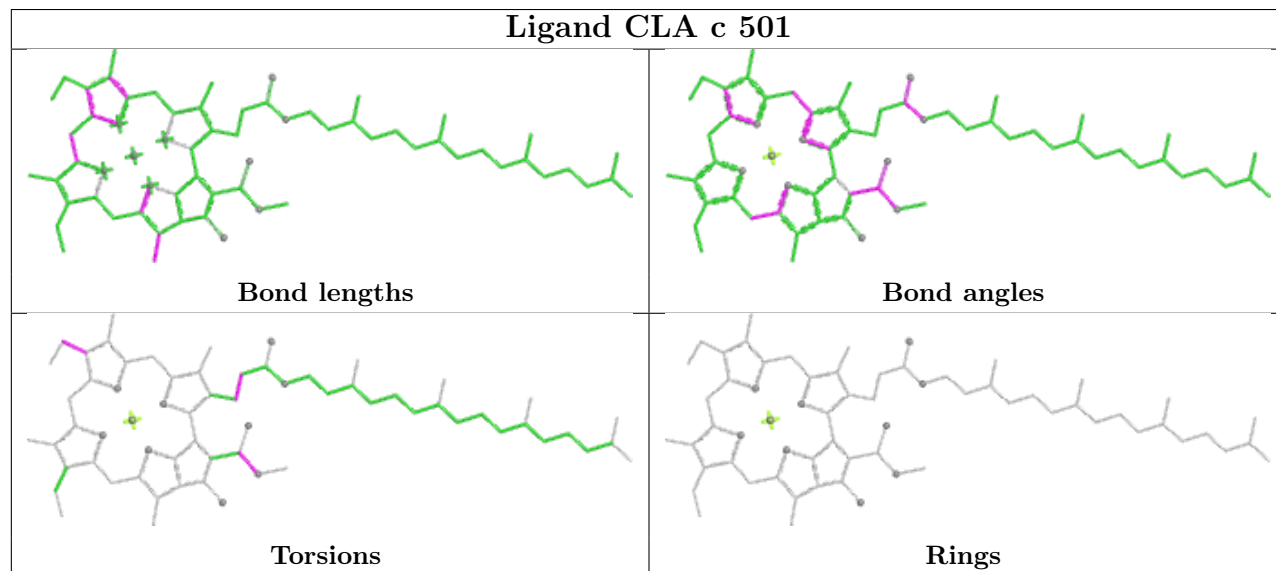


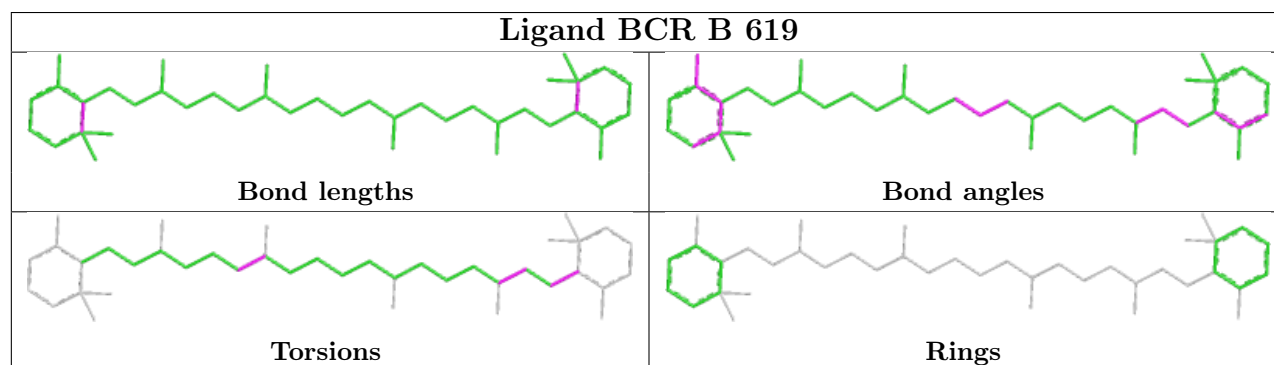
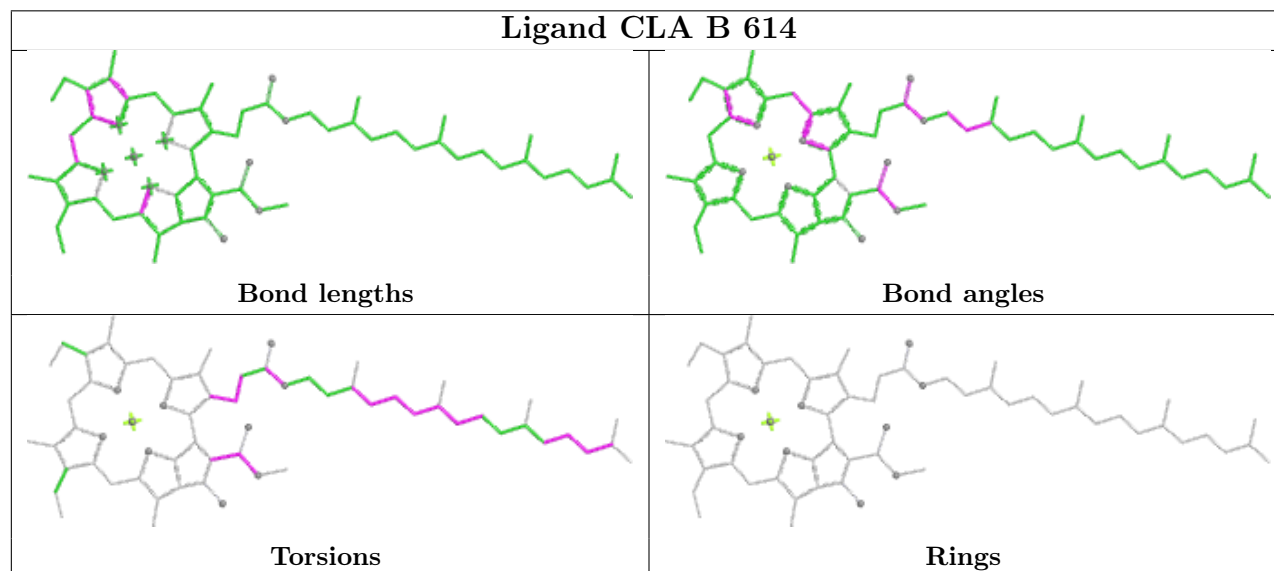
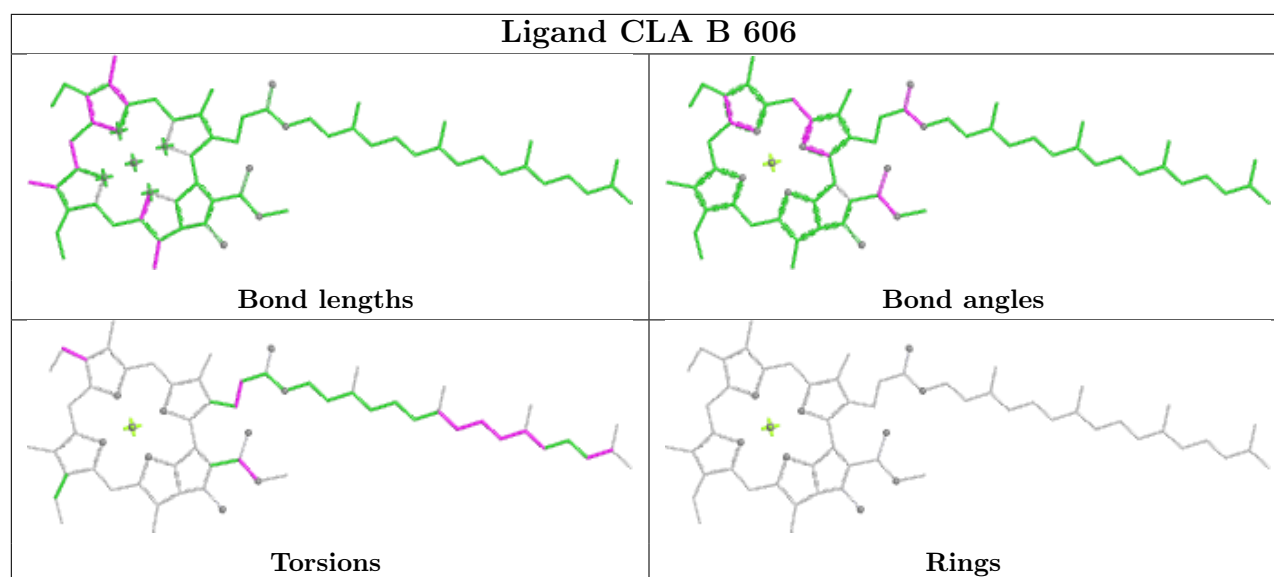
Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

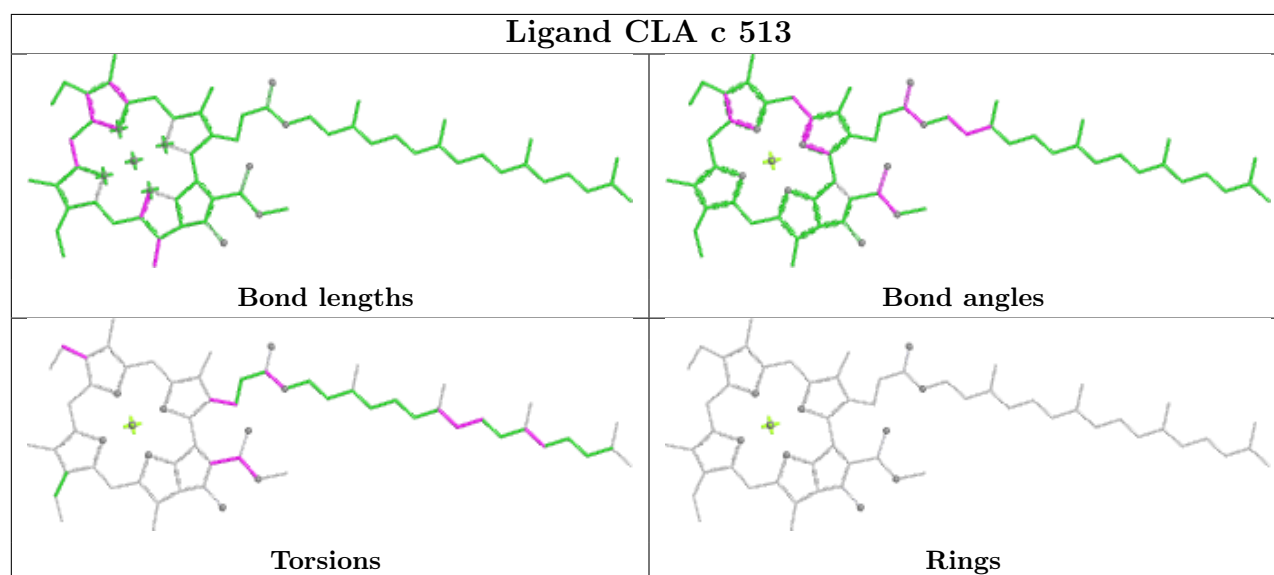
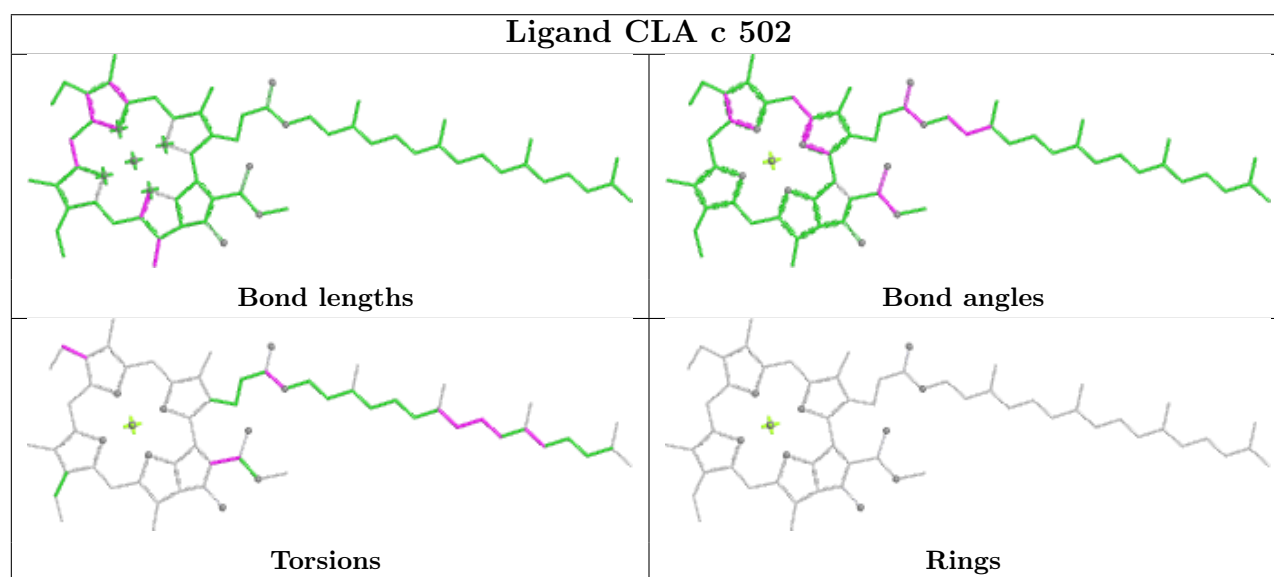
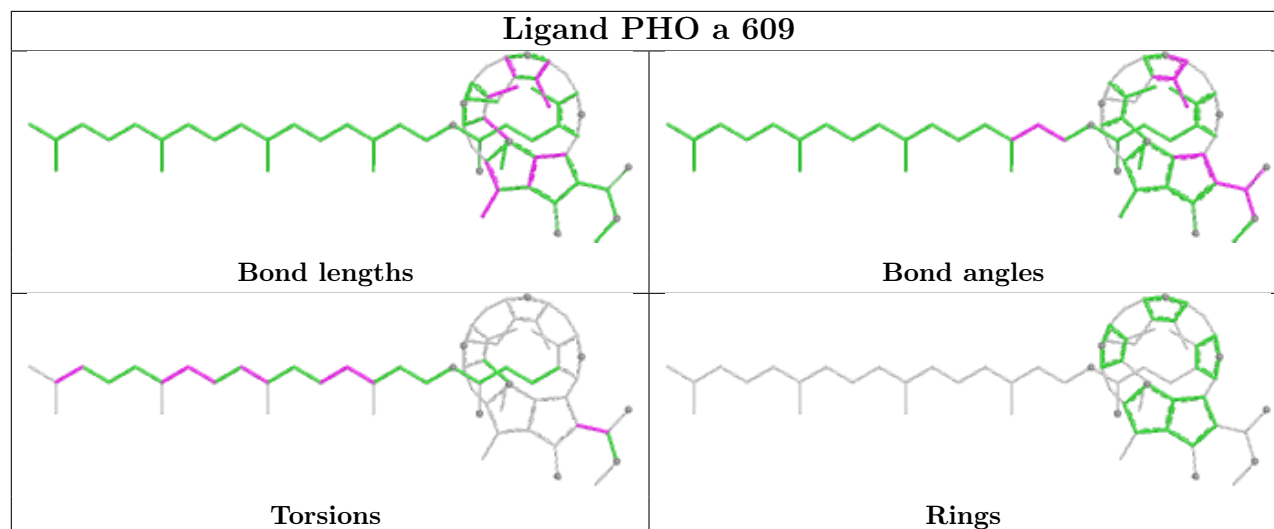
Ligand PL9 d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

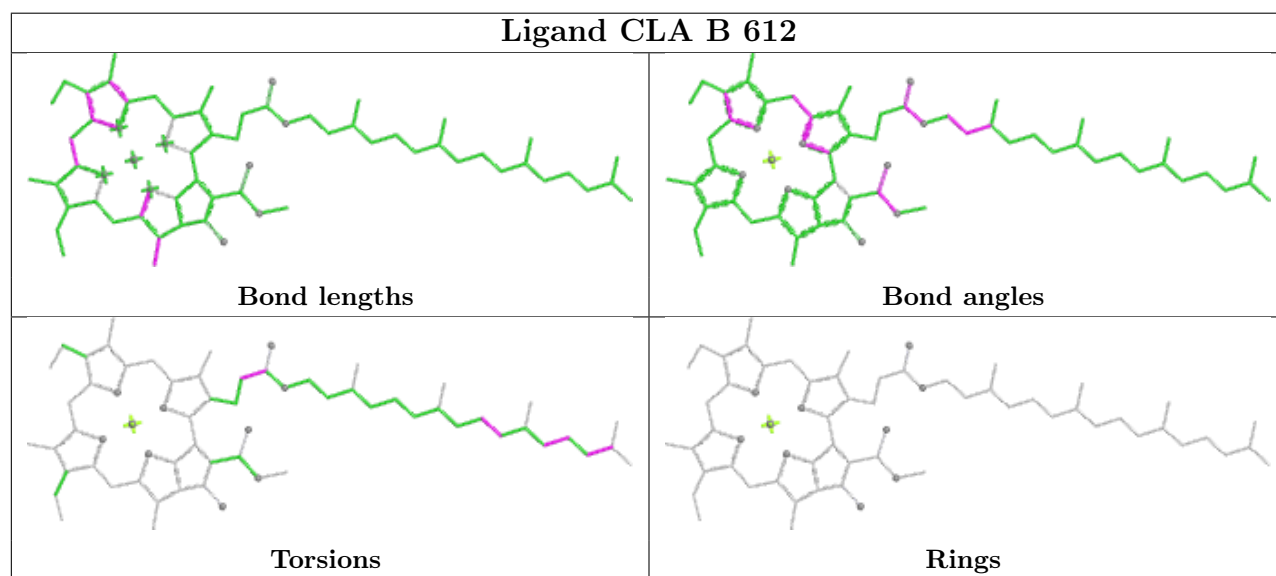
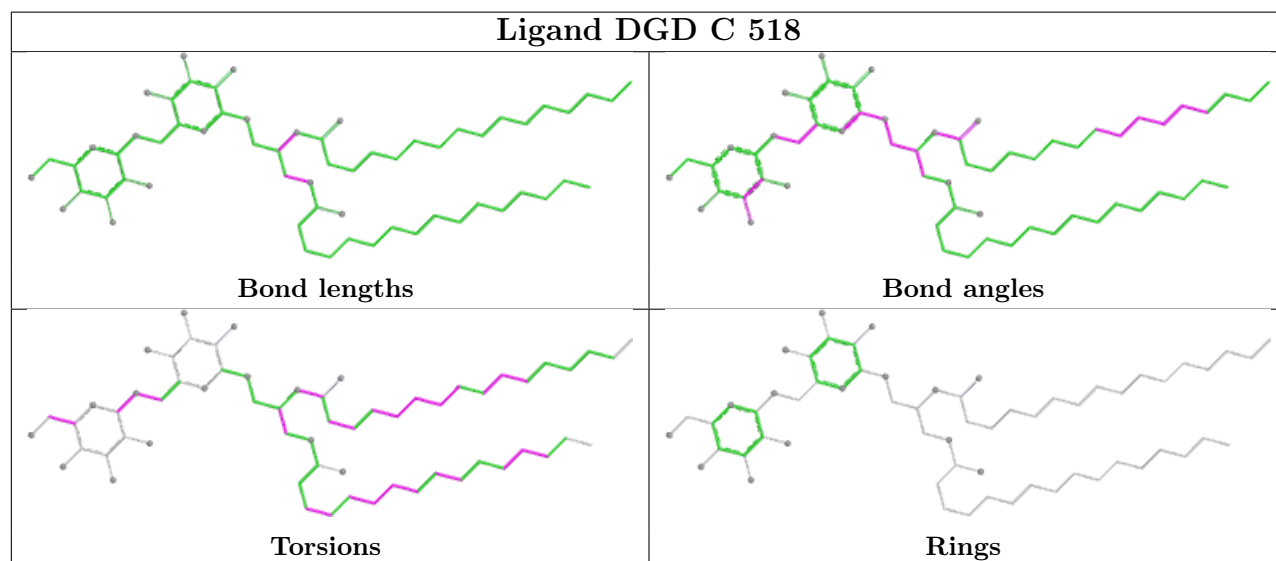
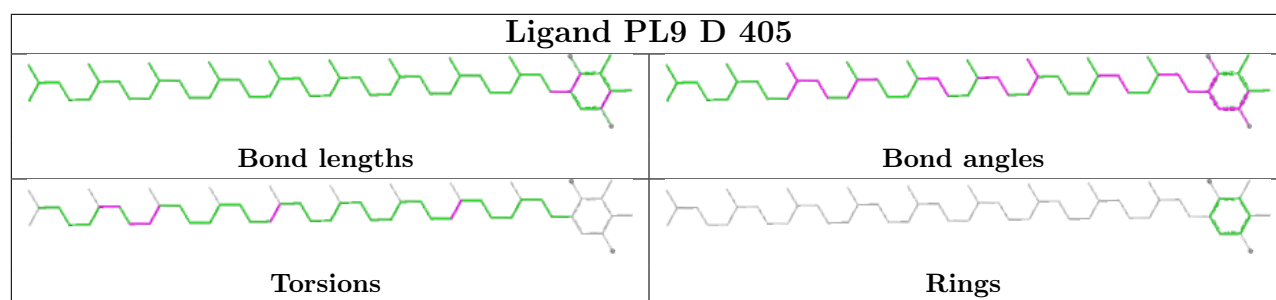
Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

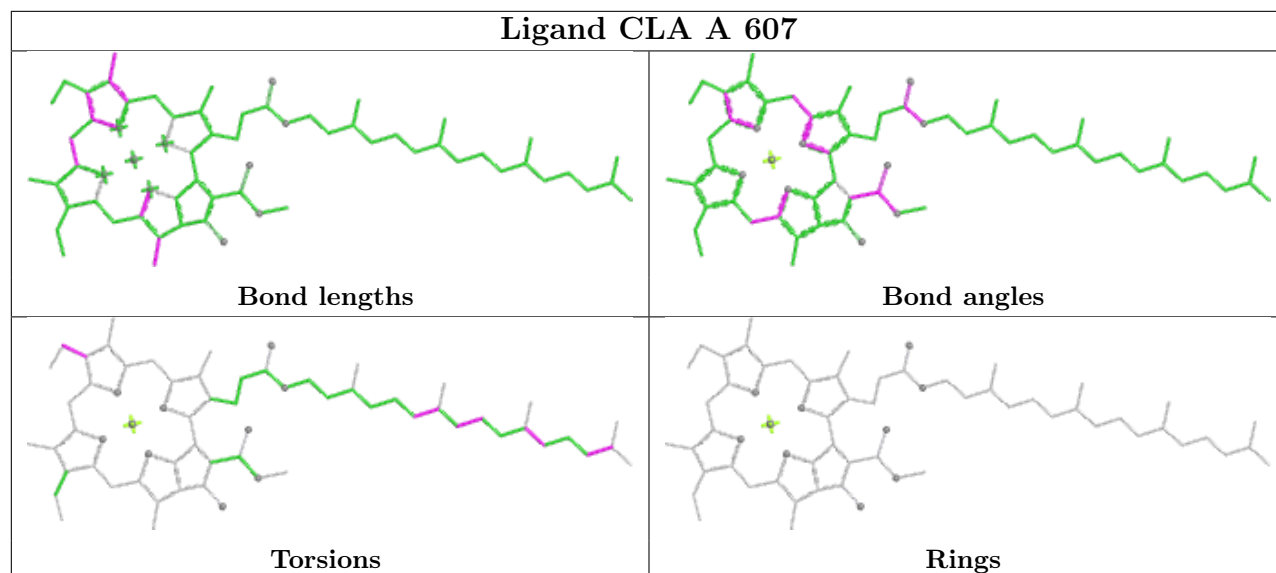
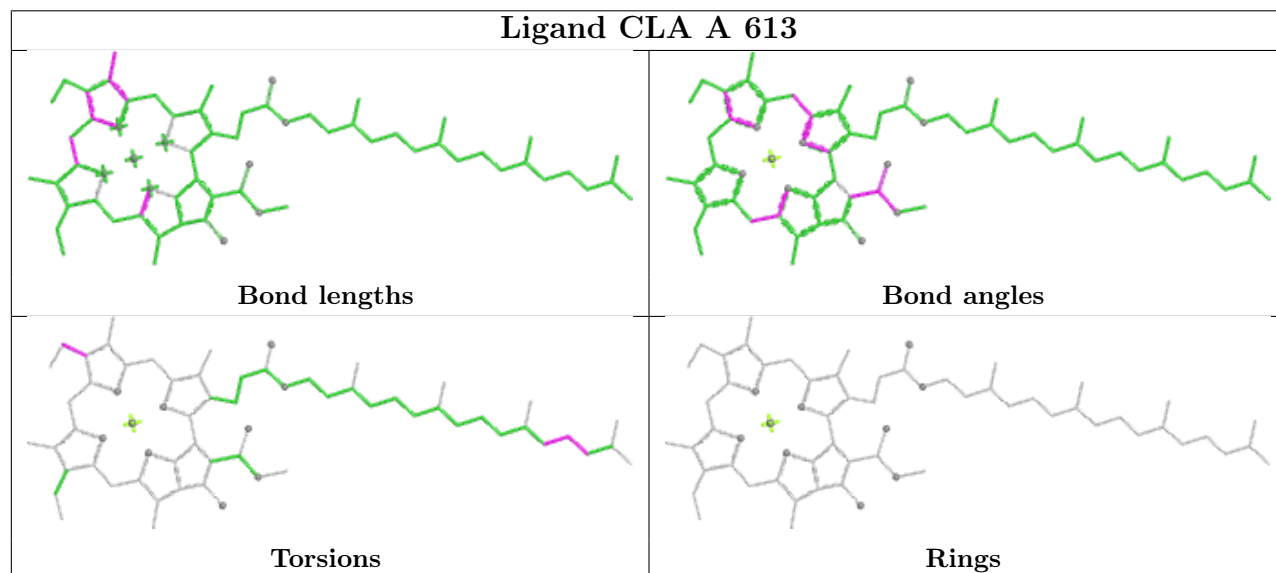
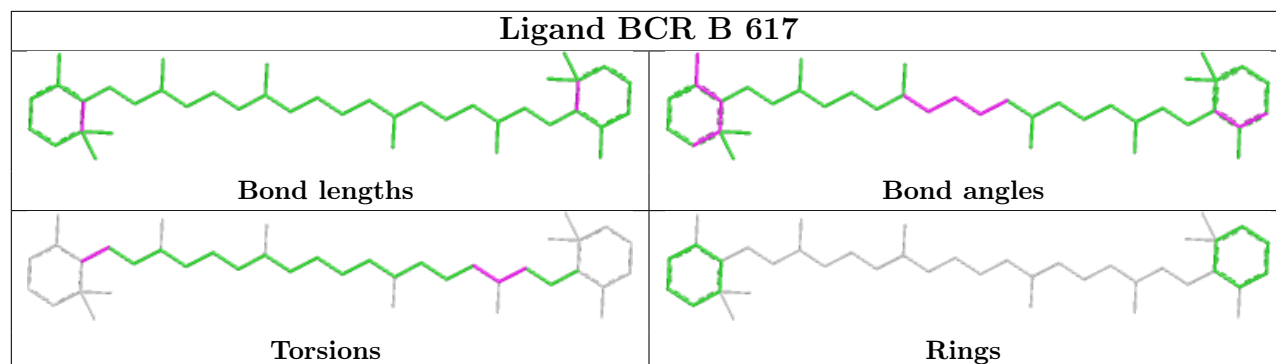


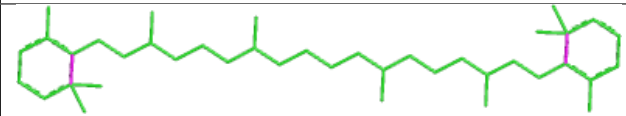
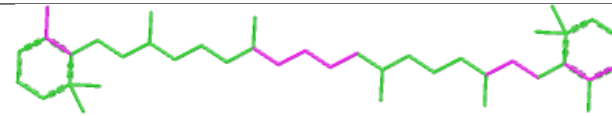
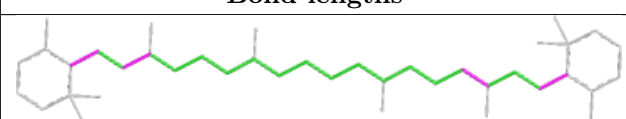
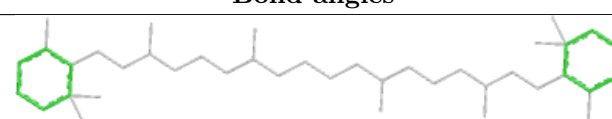
Ligand CLA b 614**Ligand CLA C 508****Ligand CLA c 501**

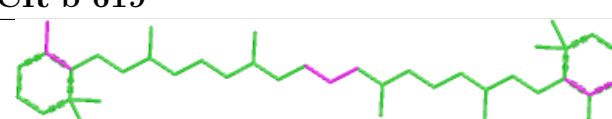
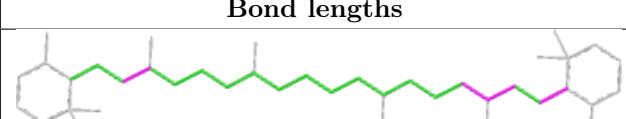
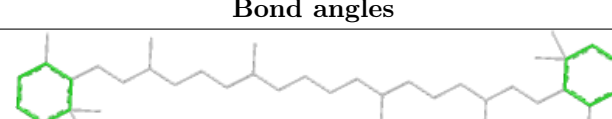


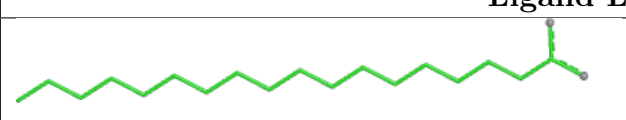
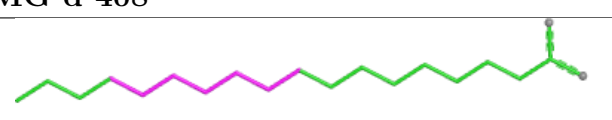
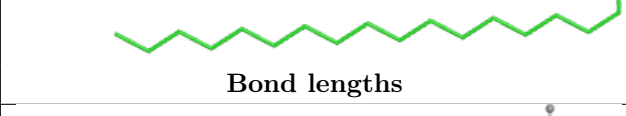
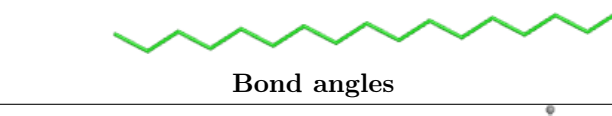


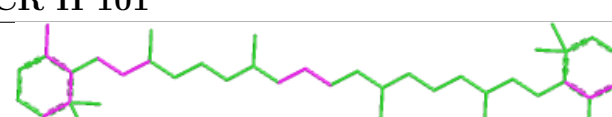
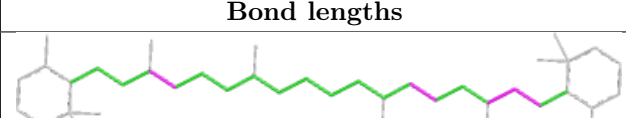
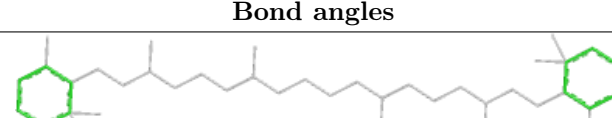


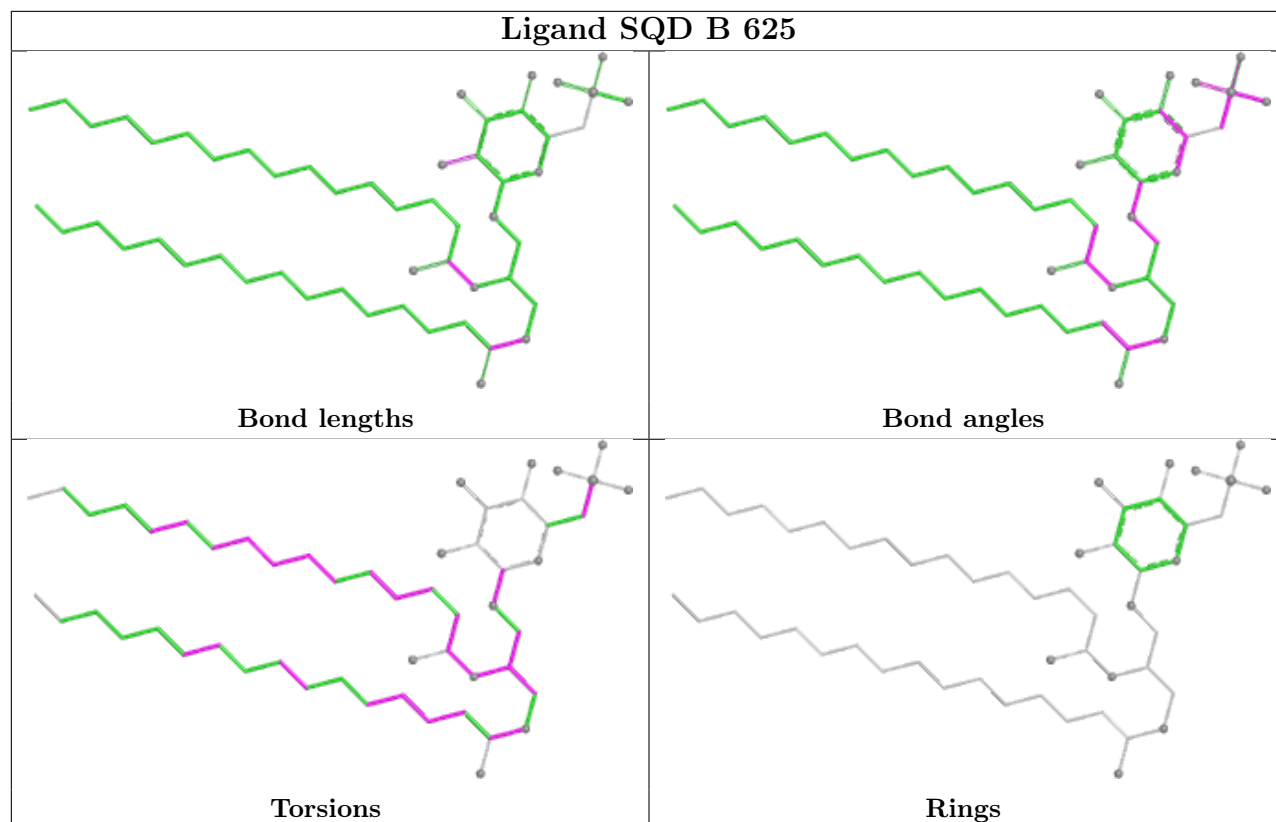


Ligand BCR c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG d 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 101	
	
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 Fit of model and data

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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