



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2021 – 12:32 PM EST

PDB ID : 6DHG
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.5 Angstrom resolution
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2018-05-20
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)

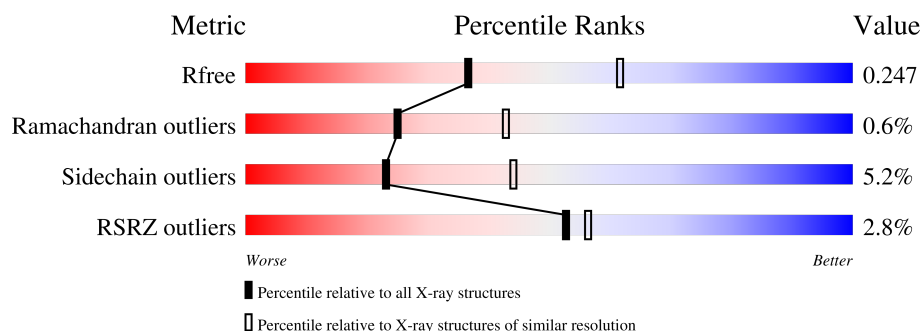
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

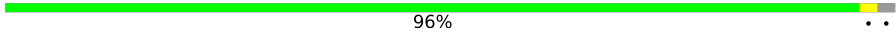
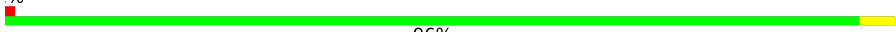
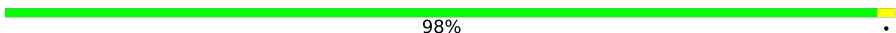




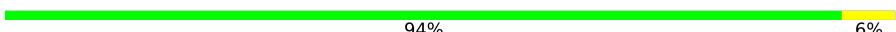





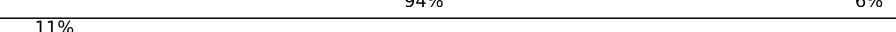



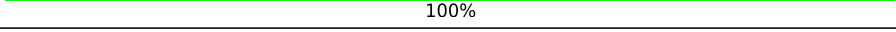







The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>
1	a	334	<div> <div></div> <div>96%</div> <div>.</div> </div>
2	B	505	<div> <div>%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
2	b	505	<div> <div>2%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>

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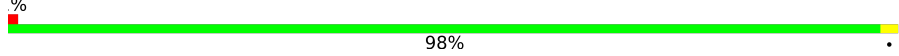
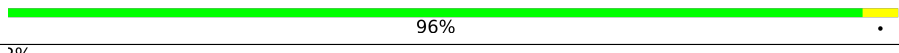


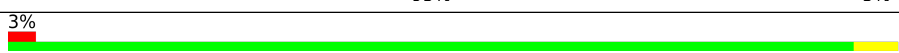
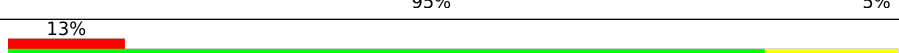


Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.17.1

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Mol	Chain	Length	Quality of chain
3	C	451	 96%
3	c	451	 96%
4	D	341	 98%
4	d	341	 98%
5	E	82	 88% 11%
5	e	82	 93% 7%
6	F	34	 100%
6	f	34	 94% 6%
7	H	65	 91% 9%
7	h	65	 91% 6%
8	I	36	 86% 14%
8	i	36	 94% 6%
9	J	36	 94% 6%
9	j	36	 94% 6%
10	K	37	 86% 14%
10	k	37	 89% 11%
11	L	37	 100%
11	l	37	 89% 5%
12	M	33	 88% 12%
12	m	33	 88% 9%
13	O	244	 90% 10%
13	o	244	 92% 7%
14	T	30	 87% 13%
14	t	30	 97%
15	U	97	 94% 6%

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Mol	Chain	Length	Quality of chain
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103658 atoms, of which 51467 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	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	0	0
			6752	2244	3335	570	590	13			
3	c	451	Total	C	H	N	O	S	0	1	0
			6901	2286	3407	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	H	N	O	S	0	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1030	338	523	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			516	172	261	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	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	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3730	1174	1850	317	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	H	N	O	0	0	0
			519	181	261	36	39			
14	t	30	Total	C	H	N	O	0	0	0
			512	180	256	36	38			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	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	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			450	144	232	35	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	H	N	O		0	0	0
			593	188	312	45	48				
18	x	38	Total	C	H	N	O		0	0	0
			593	188	312	45	48				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	R	34	Total	C	H	N	O		0	0	0
			569	184	298	47	40				
20	r	31	Total	C	H	N	O		0	0	0
			461	154	234	40	33				

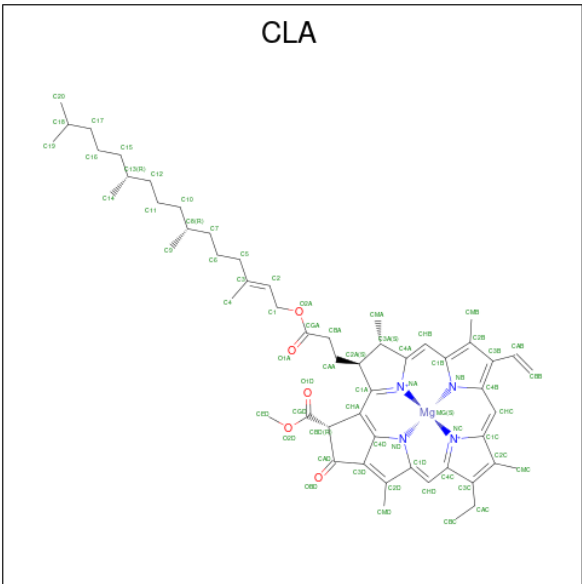
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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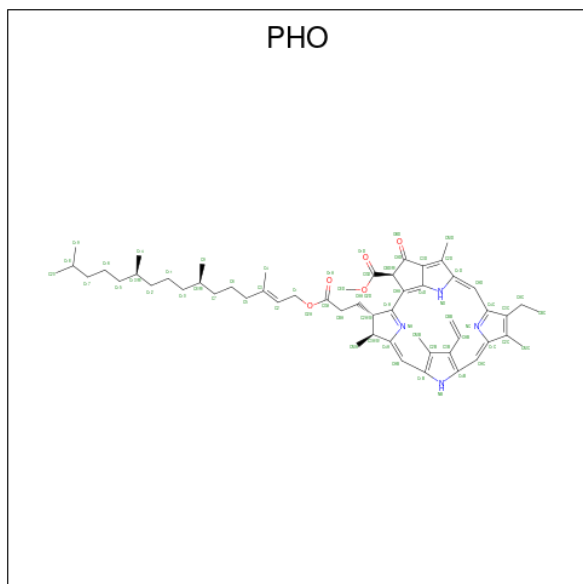
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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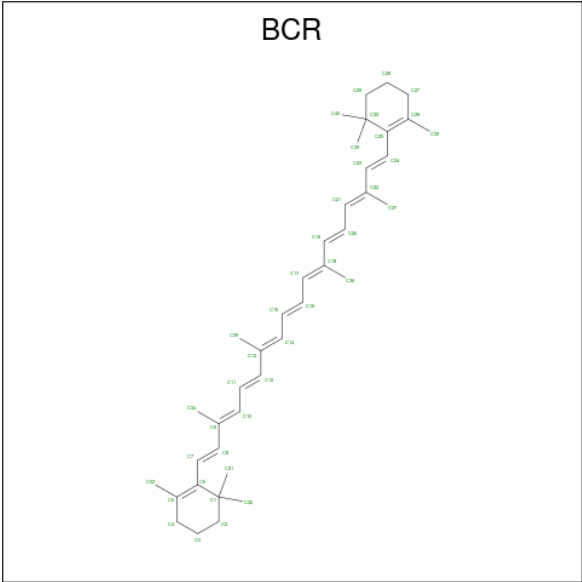
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
24	D	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
24	a	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
24	d	1	Total	C	H	N	O		0	0
			138	55	74	4	5			

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



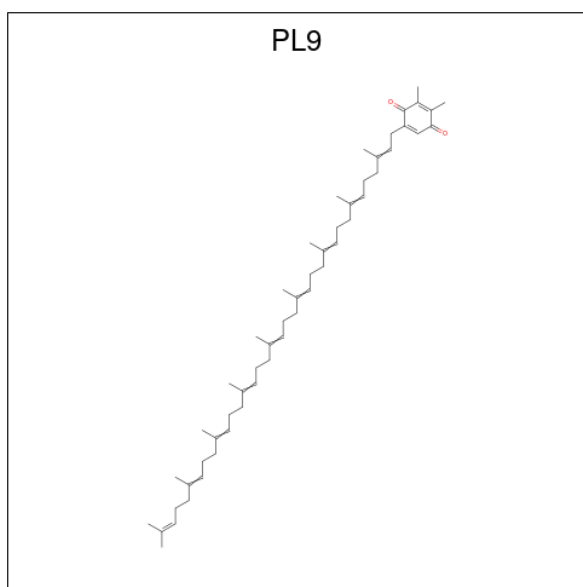
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total	C	H	0	0
			96	40	56		
25	H	1	Total	C	H	0	0
			96	40	56		
25	K	1	Total	C	H	0	0
			96	40	56		
25	T	1	Total	C	H	0	0
			96	40	56		
25	Z	1	Total	C	H	0	0
			96	40	56		
25	a	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	b	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	d	1	Total	C	H	0	0
			96	40	56		
25	k	1	Total	C	H	0	0
			96	40	56		
25	t	1	Total	C	H	0	0
			96	40	56		
25	x	1	Total	C	H	0	0
			96	40	56		

- Molecule 26 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



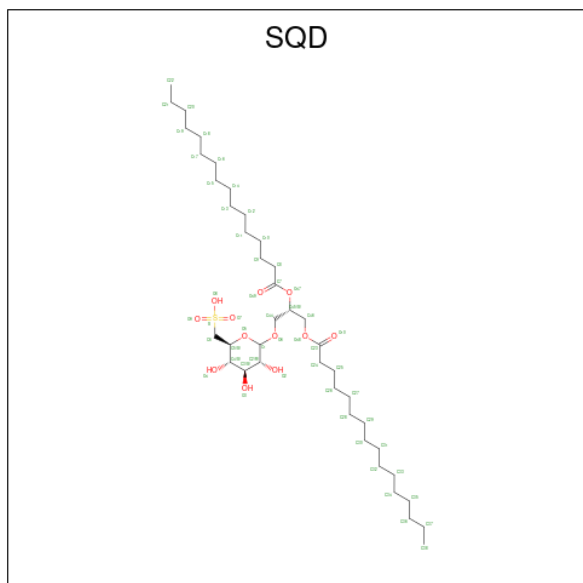
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

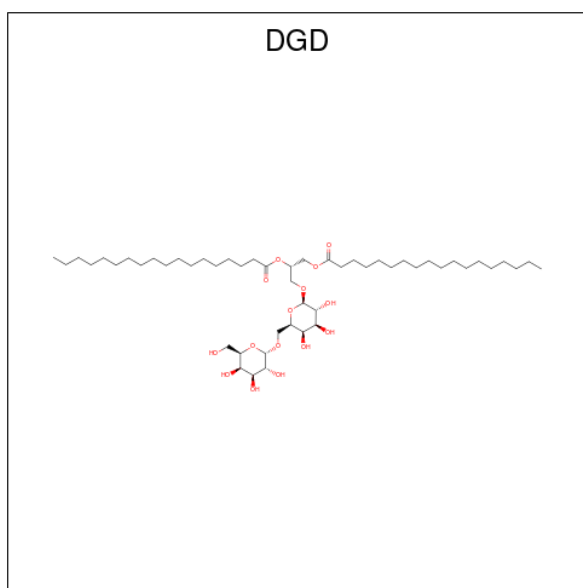
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	a	1	Total	C	H	O		0	0
			92	31	56	5			
27	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

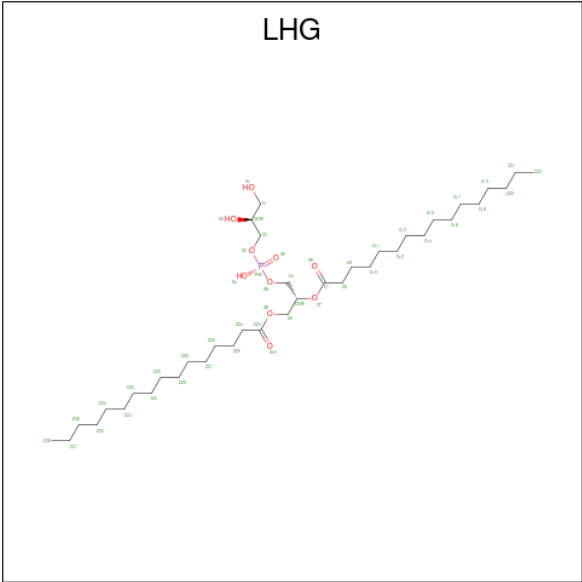
- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: $C_{51}H_{96}O_{15}$).



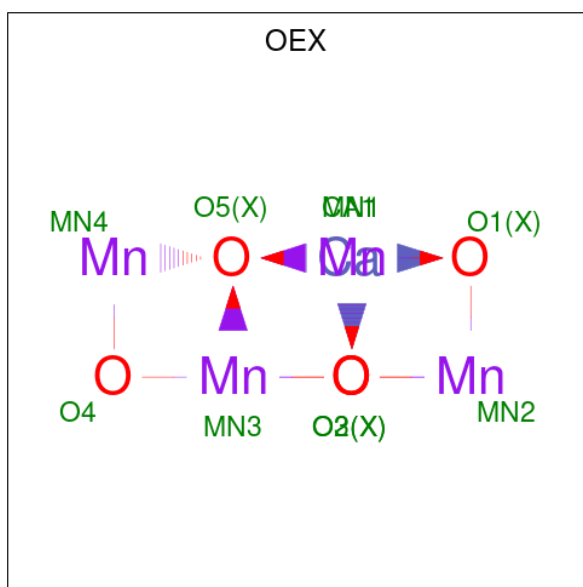
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			162	51	96	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	H	1	Total	C	H	O	0	0
			144	47	82	15		
28	a	1	Total	C	H	O	0	0
			119	39	75	5		
28	c	1	Total	C	H	O	0	0
			144	47	82	15		
28	c	1	Total	C	H	O	0	0
			144	47	82	15		
28	c	1	Total	C	H	O	0	0
			144	47	82	15		
28	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



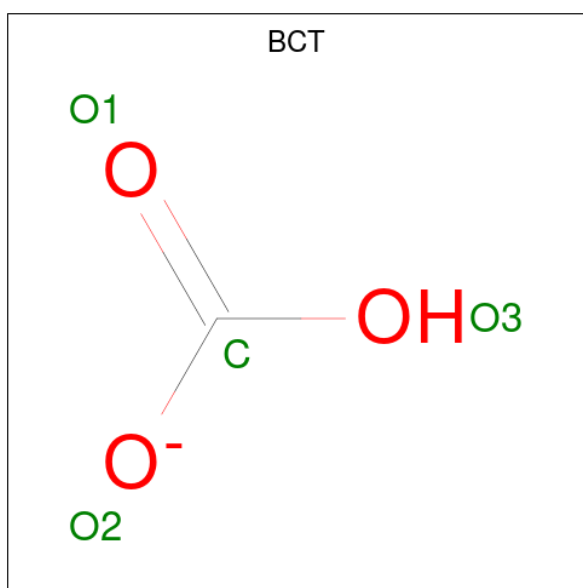
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
29	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
29	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
29	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

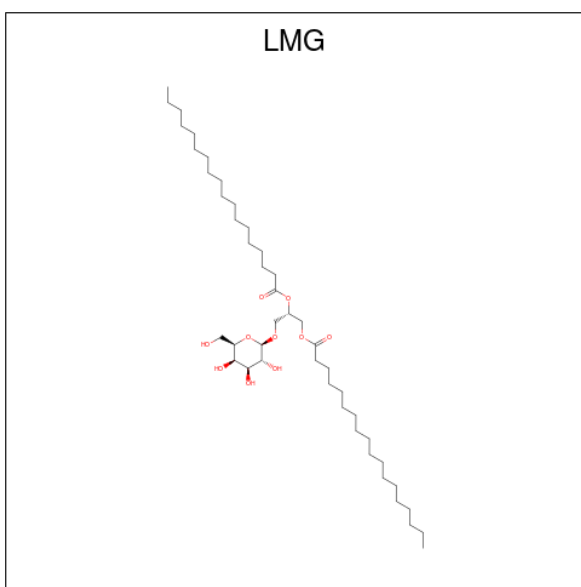


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			5	1	1	3		
31	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	6	Total	C	H	O	0	0
			226	79	137	10		
32	C	3	Total	C	H	O	0	0
			103	36	63	4		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	E	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			
32	I	1	Total	C	H		0	0
			41	15	26			
32	J	1	Total	C	H	O	0	0
			28	10	16	2		
32	M	2	Total	C	H	O	0	0
			63	23	38	2		
32	T	1	Total	C	H		0	0
			47	16	31			
32	a	1	Total	C	H	O	0	0
			28	10	16	2		
32	b	5	Total	C	H	O	0	0
			220	75	139	6		
32	c	2	Total	C	H	O	0	0
			83	28	51	4		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H		0	0
			26	10	16			
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

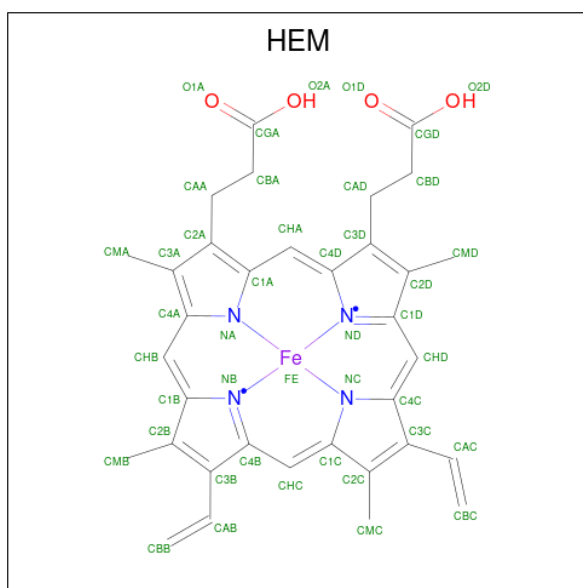
- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			123	41	72	10		
33	D	1	Total	C	H	O	0	0
			78	27	45	6		
33	D	1	Total	C	H	O	0	0
			68	24	40	4		
33	M	1	Total	C	H	O	0	0
			123	41	72	10		
33	b	1	Total	C	H	O	0	0
			141	45	86	10		
33	c	1	Total	C	H	O	0	0
			81	27	44	10		
33	c	1	Total	C	H	O	0	0
			117	38	69	10		
33	c	1	Total	C	H	O	0	0
			117	39	68	10		
33	d	1	Total	C	H	O	0	0
			57	21	34	2		
33	d	1	Total	C	H	O	0	0
			102	34	58	10		
33	m	1	Total	C	H	O	0	0
			123	41	72	10		

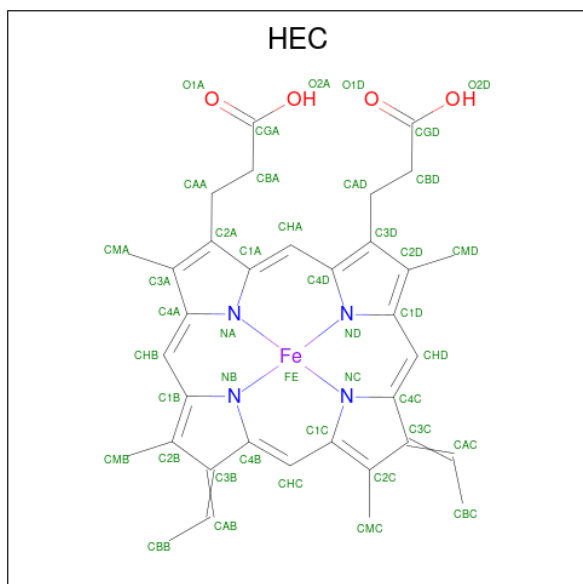
- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	E	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
34	e	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	136	Total	O	0	0
			136	136		
36	B	216	Total	O	0	0
			216	216		
36	C	192	Total	O	0	0
			192	192		
36	D	138	Total	O	0	0
			138	138		
36	E	30	Total	O	0	0
			30	30		
36	F	10	Total	O	0	0
			10	10		
36	H	25	Total	O	0	0
			25	25		
36	I	16	Total	O	0	0
			16	16		
36	J	13	Total	O	0	0
			13	13		
36	L	7	Total	O	0	0
			7	7		
36	M	7	Total	O	0	0
			7	7		
36	O	128	Total	O	0	0
			128	128		
36	T	11	Total	O	0	0
			11	11		
36	U	47	Total	O	0	0
			47	47		
36	V	73	Total	O	0	0
			73	73		
36	Y	6	Total	O	0	0
			6	6		
36	X	8	Total	O	0	0
			8	8		
36	Z	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	R	4	Total 4	O 4	0	0
36	a	119	Total 119	O 119	0	0
36	b	190	Total 190	O 190	0	0
36	c	162	Total 162	O 162	0	0
36	d	120	Total 120	O 120	0	0
36	e	22	Total 22	O 22	0	0
36	f	4	Total 4	O 4	0	0
36	h	19	Total 19	O 19	0	0
36	i	10	Total 10	O 10	0	0
36	j	8	Total 8	O 8	0	0
36	k	5	Total 5	O 5	0	0
36	l	11	Total 11	O 11	0	0
36	m	5	Total 5	O 5	0	0
36	o	113	Total 113	O 113	0	0
36	t	11	Total 11	O 11	0	0
36	u	54	Total 54	O 54	0	0
36	v	64	Total 64	O 64	0	0
36	y	4	Total 4	O 4	0	0
36	x	13	Total 13	O 13	0	0
36	z	1	Total 1	O 1	0	0
36	r	5	Total 5	O 5	0	0

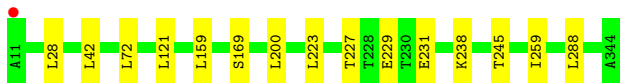
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

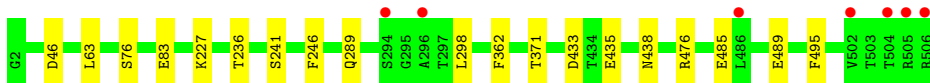
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1



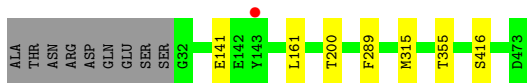
- Molecule 2: Photosystem II CP47 reaction center protein



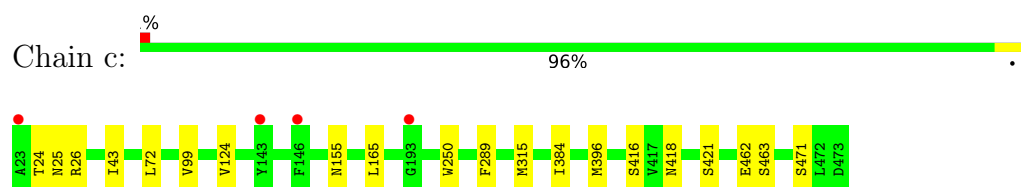
- Molecule 2: Photosystem II CP47 reaction center protein



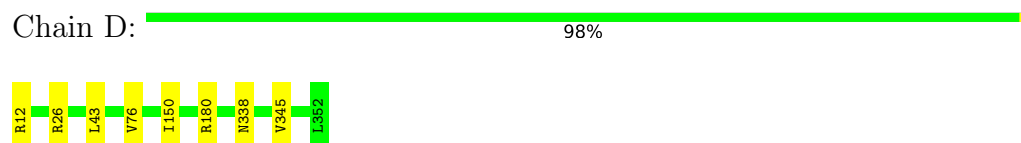
- Molecule 3: Photosystem II CP43 reaction center protein



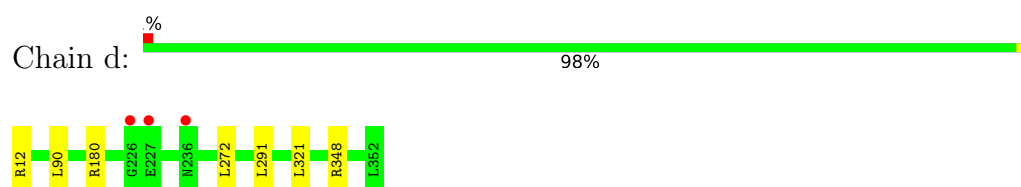
- Molecule 3: Photosystem II CP43 reaction center protein



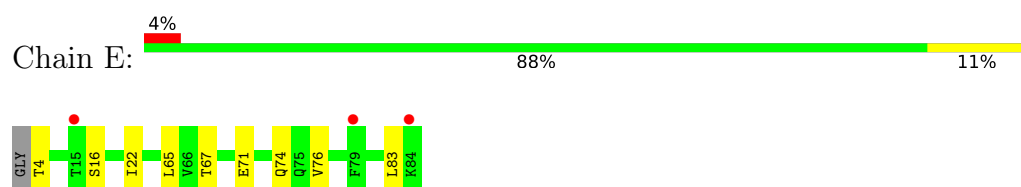
- Molecule 4: Photosystem II D2 protein



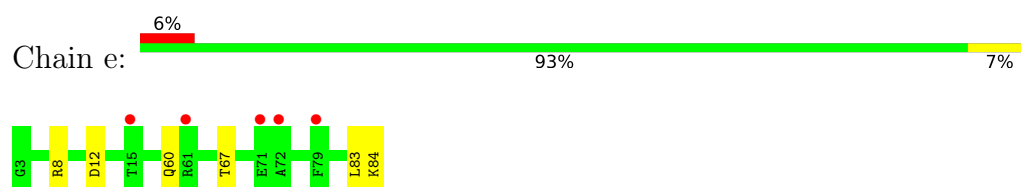
- Molecule 4: Photosystem II D2 protein



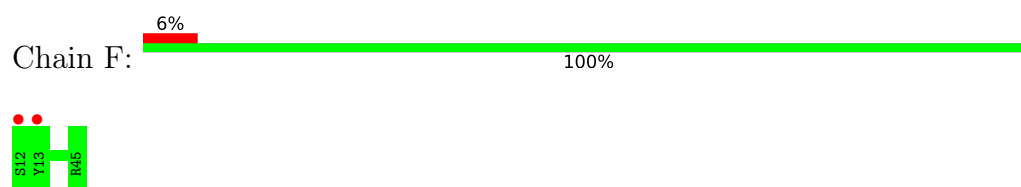
- Molecule 5: Cytochrome b559 subunit alpha



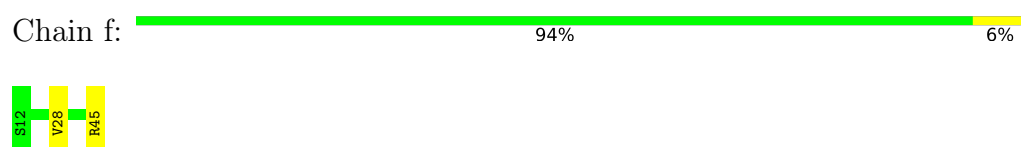
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta




- Molecule 7: Photosystem II reaction center protein H

Chain H:  91% 9%




- Molecule 7: Photosystem II reaction center protein H

Chain h:  3% 91% 6%



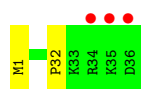
- Molecule 8: Photosystem II reaction center protein I

Chain I:  86% 14%



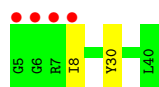
- Molecule 8: Photosystem II reaction center protein I

Chain i:  8% 94% 6%




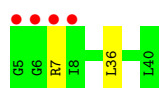
- Molecule 9: Photosystem II reaction center protein J

Chain J:  11% 94% 6%




- Molecule 9: Photosystem II reaction center protein J

Chain j:  11% 94% 6%

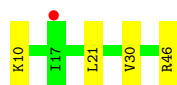
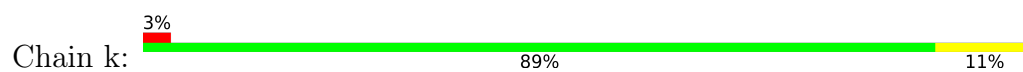


- Molecule 10: Photosystem II reaction center protein K

Chain K:  86% 14%



- Molecule 10: Photosystem II reaction center protein K

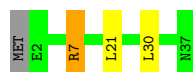
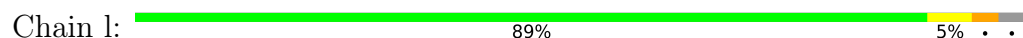


- Molecule 11: Photosystem II reaction center protein L

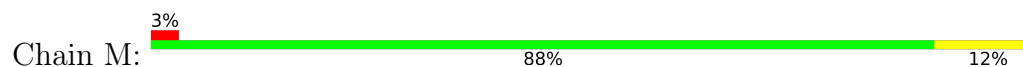


There are no outlier residues recorded for this chain.

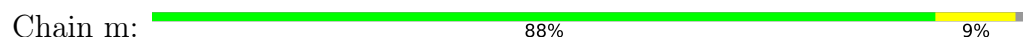
- Molecule 11: Photosystem II reaction center protein L



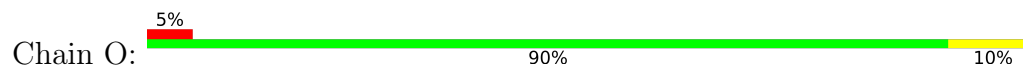
- Molecule 12: Photosystem II reaction center protein M



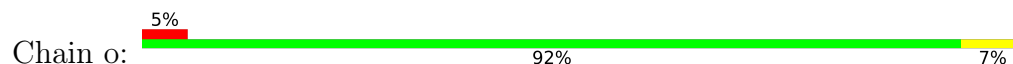
- Molecule 12: Photosystem II reaction center protein M



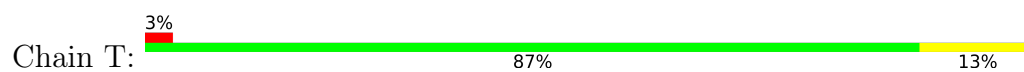
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



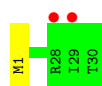
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



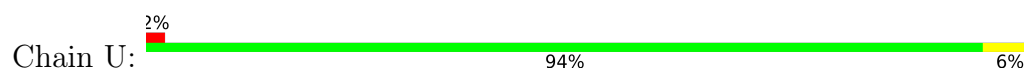
- Molecule 14: Photosystem II reaction center protein T



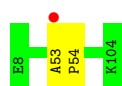
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



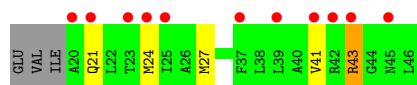
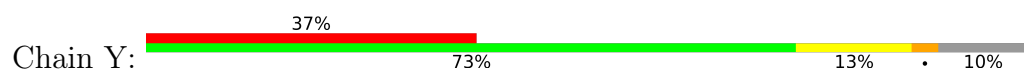
- Molecule 16: Cytochrome c-550



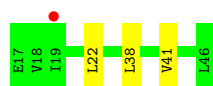
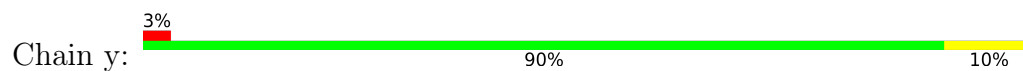
- Molecule 16: Cytochrome c-550



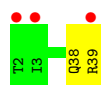
- Molecule 17: Photosystem II reaction center protein Ycf12



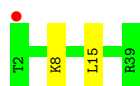
- Molecule 17: Photosystem II reaction center protein Ycf12



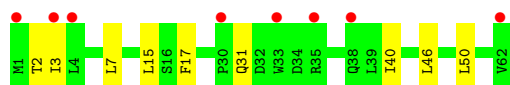
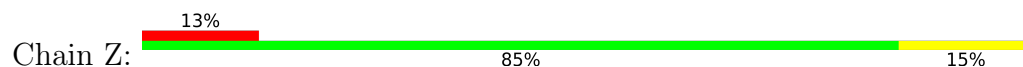
- Molecule 18: Photosystem II reaction center X protein



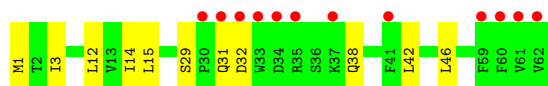
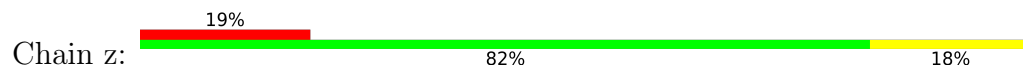
- Molecule 18: Photosystem II reaction center X protein



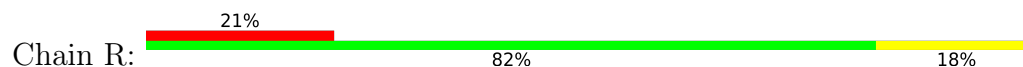
- Molecule 19: Photosystem II reaction center protein Z



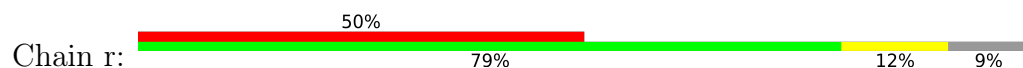
- Molecule 19: Photosystem II reaction center protein Z

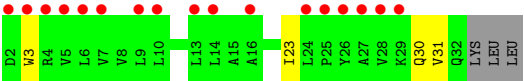


- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.55Å 222.69Å 309.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.78 – 2.50 30.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.78-2.50) 87.6 (30.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.167 , 0.246 0.167 , 0.247	Depositor DCC
R_{free} test set	2481 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103658	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: DGD, CL, LMG, PHO, PL9, CLA, OEX, LHG, SQD, BCT, FME, UNL, HEM, HEC, FE2, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.72	1/2707 (0.0%)	0.73	1/3692 (0.0%)
1	a	0.68	0/2704	0.71	1/3688 (0.0%)
2	B	0.68	0/4160	0.71	2/5668 (0.0%)
2	b	0.63	0/4118	0.69	0/5611
3	C	0.64	0/3530	0.68	0/4807
3	c	0.59	0/3610	0.67	0/4914
4	D	0.69	0/2812	0.70	0/3832
4	d	0.63	0/2821	0.69	1/3844 (0.0%)
5	E	0.57	0/684	0.66	0/935
5	e	0.56	0/683	0.63	0/932
6	F	0.57	0/284	0.59	0/387
6	f	0.54	0/284	0.58	0/387
7	H	0.68	1/520 (0.2%)	0.72	0/709
7	h	0.62	0/511	0.74	0/697
8	I	0.67	0/293	0.75	0/396
8	i	0.76	0/293	0.74	0/396
9	J	0.54	0/263	0.70	0/356
9	j	0.54	0/261	0.64	0/353
10	K	0.50	0/314	0.65	0/427
10	k	0.51	0/303	0.72	0/416
11	L	0.69	0/311	0.74	0/422
11	l	0.62	0/303	0.71	0/412
12	M	0.70	0/249	0.71	0/341
12	m	0.75	0/244	0.67	0/334
13	O	0.62	0/1914	0.77	2/2596 (0.1%)
13	o	0.60	0/1905	0.76	3/2583 (0.1%)
14	T	0.79	1/257 (0.4%)	0.77	0/349
14	t	0.71	0/255	0.64	0/346
15	U	0.62	0/785	0.70	0/1064
15	u	0.65	0/785	0.75	0/1064
16	V	0.58	0/1085	0.69	0/1473
16	v	0.62	0/1085	0.69	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.47	0/197	0.69	0/264
17	y	0.39	0/219	0.57	0/294
18	X	0.61	0/284	0.70	0/384
18	x	0.40	0/284	0.62	0/384
19	Z	0.53	0/490	0.64	0/669
19	z	0.48	0/488	0.56	0/666
20	R	0.39	0/277	0.57	0/380
20	r	0.39	0/233	0.55	0/323
All	All	0.64	3/42805 (0.0%)	0.70	10/58268 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	Y	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	6	TYR	CD2-CE2	-5.58	1.30	1.39
1	A	135	TYR	CD1-CE1	-5.56	1.31	1.39
7	H	41	PHE	CB-CG	-5.18	1.42	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	7.76	125.28	118.30
13	O	158	ASP	CB-CG-OD1	6.08	123.78	118.30
4	d	348	ARG	NE-CZ-NH2	-5.81	117.39	120.30
13	o	102	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	183	MET	CA-CB-CG	5.64	122.88	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	Y	21	GLN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	332/334 (99%)	322 (97%)	9 (3%)	1 (0%)	41	61
1	a	332/334 (99%)	320 (96%)	11 (3%)	1 (0%)	41	61
2	B	508/505 (101%)	488 (96%)	19 (4%)	1 (0%)	47	68
2	b	503/505 (100%)	480 (95%)	20 (4%)	3 (1%)	25	43
3	C	440/451 (98%)	420 (96%)	19 (4%)	1 (0%)	47	68
3	c	450/451 (100%)	433 (96%)	15 (3%)	2 (0%)	34	54
4	D	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	41	61
4	d	340/341 (100%)	323 (95%)	17 (5%)	0	100	100
5	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	j	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
10	K	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4	6
10	k	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	33 (97%)	0	1 (3%)	4	6
12	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	m	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
13	O	243/244 (100%)	225 (93%)	14 (6%)	4 (2%)	9	17
13	o	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	13	24
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
15	u	95/97 (98%)	91 (96%)	3 (3%)	1 (1%)	14	26
16	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	v	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
17	Y	25/30 (83%)	18 (72%)	5 (20%)	2 (8%)	1	1
17	y	28/30 (93%)	23 (82%)	4 (14%)	1 (4%)	3	4
18	X	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	7
18	x	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	47 (78%)	11 (18%)	2 (3%)	4	5
20	R	32/34 (94%)	30 (94%)	1 (3%)	1 (3%)	4	5
20	r	29/34 (85%)	24 (83%)	3 (10%)	2 (7%)	1	1
All	All	5235/5326 (98%)	4963 (95%)	243 (5%)	29 (1%)	25	43

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	62	GLU
17	Y	41	VAL
3	c	416	SER

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	270/270 (100%)	262 (97%)	8 (3%)	41	68
1	a	269/270 (100%)	256 (95%)	13 (5%)	25	48
2	B	407/403 (101%)	391 (96%)	16 (4%)	32	57
2	b	402/403 (100%)	388 (96%)	14 (4%)	36	62
3	C	344/352 (98%)	338 (98%)	6 (2%)	60	82
3	c	353/352 (100%)	335 (95%)	18 (5%)	24	45
4	D	276/276 (100%)	269 (98%)	7 (2%)	47	73
4	d	277/276 (100%)	271 (98%)	6 (2%)	52	77
5	E	72/72 (100%)	62 (86%)	10 (14%)	3	6
5	e	71/72 (99%)	65 (92%)	6 (8%)	10	21
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	28/28 (100%)	26 (93%)	2 (7%)	14	28
7	H	53/54 (98%)	48 (91%)	5 (9%)	8	17
7	h	53/54 (98%)	49 (92%)	4 (8%)	13	26
8	I	32/32 (100%)	28 (88%)	4 (12%)	4	8
8	i	32/32 (100%)	31 (97%)	1 (3%)	40	67
9	J	24/24 (100%)	22 (92%)	2 (8%)	11	22
9	j	23/24 (96%)	21 (91%)	2 (9%)	10	20
10	K	31/30 (103%)	26 (84%)	5 (16%)	2	4
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	7
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	19
12	M	28/29 (97%)	25 (89%)	3 (11%)	6	13
12	m	28/29 (97%)	26 (93%)	2 (7%)	14	28
13	O	208/207 (100%)	189 (91%)	19 (9%)	9	18
13	o	207/207 (100%)	192 (93%)	15 (7%)	14	28
14	T	26/26 (100%)	24 (92%)	2 (8%)	13	25
14	t	25/26 (96%)	25 (100%)	0	100	100
15	U	84/84 (100%)	78 (93%)	6 (7%)	14	28
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	117/117 (100%)	112 (96%)	5 (4%)	29	53
16	v	117/117 (100%)	111 (95%)	6 (5%)	24	45
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2	4
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	18
18	X	31/31 (100%)	30 (97%)	1 (3%)	39	65
18	x	31/31 (100%)	29 (94%)	2 (6%)	17	33
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	3
19	z	51/52 (98%)	42 (82%)	9 (18%)	2	3
20	R	28/29 (97%)	23 (82%)	5 (18%)	2	3
20	r	19/29 (66%)	17 (90%)	2 (10%)	7	13
All	All	4321/4348 (99%)	4093 (95%)	228 (5%)	23	43

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	R	13	LEU
19	z	31	GLN
3	c	24	THR
19	z	12	LEU
13	o	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	58	ASN
5	e	74	GLN
2	b	281	GLN
3	c	28	GLN
2	b	179	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
14	FME	t	1	14	8,9,10	1.07	1 (12%)	7,9,11	1.04	0
12	FME	M	1	12	8,9,10	1.14	1 (12%)	7,9,11	1.08	0
8	FME	i	1	8	8,9,10	1.25	1 (12%)	7,9,11	1.06	0
8	FME	I	1	8	8,9,10	1.09	1 (12%)	7,9,11	1.33	1 (14%)
12	FME	m	1	12	8,9,10	1.06	1 (12%)	7,9,11	0.66	0
14	FME	T	1	14	8,9,10	0.96	1 (12%)	7,9,11	1.55	1 (14%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.68	1.42	1.46
14	t	1	FME	CA-N	-2.51	1.42	1.46
14	T	1	FME	CA-N	-2.47	1.42	1.46
12	m	1	FME	CA-N	-2.40	1.42	1.46
8	I	1	FME	CA-N	-2.33	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-2.37	119.17	122.82
14	T	1	FME	CA-N-CN	-2.36	119.19	122.82

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 149 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
23	CLA	c	510	-	59,73,73	1.34	6 (10%)	67,113,113	1.74	13 (19%)
23	CLA	a	405	-	59,73,73	1.53	8 (13%)	67,113,113	1.55	11 (16%)
33	LMG	C	519	-	48,48,55	1.03	6 (12%)	56,56,63	1.32	6 (10%)
23	CLA	d	402	36	59,73,73	1.63	8 (13%)	67,113,113	1.98	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	513	-	59,73,73	1.42	8 (13%)	67,113,113	1.33	11 (16%)
28	DGD	C	518	-	63,63,67	1.11	7 (11%)	77,77,81	1.42	11 (14%)
23	CLA	b	606	-	59,73,73	1.47	8 (13%)	67,113,113	1.90	19 (28%)
29	LHG	A	413	-	48,48,48	0.86	2 (4%)	51,54,54	1.52	9 (17%)
27	SQD	F	101	-	35,36,54	0.93	1 (2%)	42,45,65	1.95	10 (23%)
23	CLA	C	510	-	59,73,73	1.38	6 (10%)	67,113,113	1.53	9 (13%)
25	BCR	D	405	-	41,41,41	1.08	3 (7%)	56,56,56	1.18	5 (8%)
29	LHG	E	101	-	48,48,48	0.91	3 (6%)	51,54,54	1.21	3 (5%)
23	CLA	b	609	-	59,73,73	1.41	7 (11%)	67,113,113	1.51	15 (22%)
27	SQD	b	601	-	48,49,54	1.01	2 (4%)	57,60,65	2.23	17 (29%)
23	CLA	C	514	-	59,73,73	1.47	9 (15%)	67,113,113	1.73	13 (19%)
23	CLA	b	617	-	54,68,73	1.55	9 (16%)	61,107,113	1.73	11 (18%)
23	CLA	D	404	-	59,73,73	1.39	9 (15%)	67,113,113	1.40	10 (14%)
23	CLA	A	404	-	59,73,73	1.58	9 (15%)	67,113,113	1.46	8 (11%)
23	CLA	c	505	-	59,73,73	1.61	6 (10%)	67,113,113	1.42	10 (14%)
23	CLA	c	511	3	59,73,73	1.79	6 (10%)	67,113,113	1.56	10 (14%)
23	CLA	c	506	-	59,73,73	1.41	10 (16%)	67,113,113	1.63	13 (19%)
23	CLA	b	610	-	59,73,73	1.46	9 (15%)	67,113,113	1.40	11 (16%)
23	CLA	A	407	-	48,62,73	1.55	10 (20%)	53,99,113	1.94	13 (24%)
29	LHG	D	409	-	46,46,48	1.07	3 (6%)	49,52,54	1.28	5 (10%)
28	DGD	A	412	-	67,67,67	1.41	12 (17%)	81,81,81	1.37	6 (7%)
28	DGD	h	101	-	63,63,67	1.20	6 (9%)	77,77,81	1.59	17 (22%)
28	DGD	a	413	-	43,43,67	1.46	4 (9%)	45,45,81	1.22	5 (11%)
33	LMG	M	101	-	51,51,55	0.98	2 (3%)	59,59,63	1.48	9 (15%)
23	CLA	B	609	-	59,73,73	1.66	11 (18%)	67,113,113	1.71	16 (23%)
23	CLA	c	512	-	59,73,73	1.52	6 (10%)	67,113,113	1.48	11 (16%)
23	CLA	C	509	-	59,73,73	1.62	9 (15%)	67,113,113	1.79	14 (20%)
27	SQD	a	411	-	53,54,54	0.99	5 (9%)	62,65,65	1.90	9 (14%)
23	CLA	B	602	-	59,73,73	1.56	8 (13%)	67,113,113	1.36	9 (13%)
33	LMG	c	522	-	48,48,55	1.19	6 (12%)	56,56,63	1.36	5 (8%)
23	CLA	B	603	-	59,73,73	1.57	10 (16%)	67,113,113	1.70	13 (19%)
26	PL9	A	409	-	55,55,55	1.34	5 (9%)	68,69,69	1.44	8 (11%)
23	CLA	B	615	-	59,73,73	1.97	10 (16%)	67,113,113	1.48	13 (19%)
25	BCR	c	515	-	41,41,41	1.21	4 (9%)	56,56,56	1.42	12 (21%)
23	CLA	C	502	-	59,73,73	1.78	7 (11%)	67,113,113	1.97	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	b	622	-	55,55,55	1.06	4 (7%)	63,63,63	1.56	5 (7%)
23	CLA	B	614	-	59,73,73	1.60	9 (15%)	67,113,113	1.83	12 (17%)
23	CLA	b	613	-	59,73,73	1.19	8 (13%)	67,113,113	1.97	16 (23%)
23	CLA	b	611	36	59,73,73	1.41	9 (15%)	67,113,113	1.42	13 (19%)
29	LHG	l	101	-	48,48,48	0.79	2 (4%)	51,54,54	1.16	3 (5%)
29	LHG	d	407	-	48,48,48	0.81	0	51,54,54	1.31	5 (9%)
23	CLA	C	506	-	59,73,73	1.40	6 (10%)	67,113,113	1.69	14 (20%)
23	CLA	c	503	-	59,73,73	1.83	9 (15%)	67,113,113	1.48	9 (13%)
23	CLA	A	405	36	59,73,73	1.55	7 (11%)	67,113,113	1.63	11 (16%)
28	DGD	C	516	-	63,63,67	1.38	7 (11%)	77,77,81	1.33	10 (12%)
33	LMG	c	524	-	49,49,55	1.16	4 (8%)	57,57,63	1.29	4 (7%)
28	DGD	C	517	-	63,63,67	1.24	10 (15%)	77,77,81	1.56	12 (15%)
33	LMG	d	410	-	18,21,55	0.83	0	16,20,63	0.79	0
25	BCR	a	409	-	41,41,41	1.11	3 (7%)	56,56,56	1.33	6 (10%)
29	LHG	e	101	-	41,41,48	0.87	3 (7%)	44,47,54	1.37	6 (13%)
23	CLA	C	503	-	59,73,73	1.33	7 (11%)	67,113,113	1.57	10 (14%)
23	CLA	B	612	-	59,73,73	1.21	5 (8%)	67,113,113	1.75	15 (22%)
33	LMG	d	411	-	44,44,55	1.21	4 (9%)	52,52,63	1.49	6 (11%)
28	DGD	H	102	-	63,63,67	1.34	13 (20%)	77,77,81	1.50	12 (15%)
23	CLA	c	507	36	59,73,73	1.44	9 (15%)	67,113,113	1.66	13 (19%)
25	BCR	c	521	-	41,41,41	0.97	2 (4%)	56,56,56	1.18	5 (8%)
23	CLA	B	610	36	59,73,73	1.52	8 (13%)	67,113,113	1.65	10 (14%)
23	CLA	a	406	36	59,73,73	1.33	8 (13%)	67,113,113	1.95	16 (23%)
25	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	7 (12%)
31	BCT	a	404	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	B	604	-	59,73,73	1.65	8 (13%)	67,113,113	1.57	9 (13%)
23	CLA	B	611	-	59,73,73	1.54	9 (15%)	67,113,113	1.56	11 (16%)
27	SQD	A	410	-	51,52,54	1.10	6 (11%)	60,63,65	2.10	12 (20%)
33	LMG	c	519	-	37,37,55	1.13	4 (10%)	45,45,63	1.30	6 (13%)
23	CLA	D	402	36	59,73,73	1.30	7 (11%)	67,113,113	1.27	9 (13%)
25	BCR	t	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.44	13 (23%)
29	LHG	d	408	-	48,48,48	0.68	0	51,54,54	1.20	4 (7%)
27	SQD	B	621	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	15 (24%)
23	CLA	b	614	-	59,73,73	1.44	8 (13%)	67,113,113	1.75	14 (20%)
25	BCR	b	619	-	41,41,41	1.29	2 (4%)	56,56,56	1.31	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	604	-	59,73,73	1.54	9 (15%)	67,113,113	1.61	11 (16%)
24	PHO	D	401	-	67,69,69	1.28	9 (13%)	85,99,99	1.19	8 (9%)
23	CLA	b	608	36	59,73,73	1.31	8 (13%)	67,113,113	1.43	11 (16%)
23	CLA	C	511	-	59,73,73	1.46	8 (13%)	67,113,113	1.56	8 (11%)
23	CLA	B	616	-	54,68,73	1.60	9 (16%)	61,107,113	1.64	12 (19%)
25	BCR	T	101	-	41,41,41	1.19	4 (9%)	56,56,56	1.45	9 (16%)
23	CLA	a	408	-	59,73,73	1.72	9 (15%)	67,113,113	1.46	13 (19%)
30	OEX	A	414	1,3,36	0,15,15	0.00	-	-		
25	BCR	b	618	-	41,41,41	1.16	3 (7%)	56,56,56	1.28	6 (10%)
23	CLA	C	507	-	59,73,73	1.56	9 (15%)	67,113,113	1.59	16 (23%)
34	HEM	e	102	6,5	27,50,50	1.84	4 (14%)	17,82,82	2.26	5 (29%)
26	PL9	a	410	-	55,55,55	1.27	5 (9%)	68,69,69	1.55	16 (23%)
25	BCR	B	618	-	41,41,41	1.37	4 (9%)	56,56,56	1.44	7 (12%)
23	CLA	d	403	-	59,73,73	1.42	8 (13%)	67,113,113	1.32	7 (10%)
25	BCR	d	405	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	8 (14%)
31	BCT	A	415	21	0,3,3	0.00	-	0,3,3	0.00	-
29	LHG	D	408	-	48,48,48	1.04	3 (6%)	51,54,54	1.26	6 (11%)
25	BCR	Z	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.43	10 (17%)
24	PHO	d	401	-	67,69,69	1.27	9 (13%)	85,99,99	1.22	9 (10%)
23	CLA	c	508	-	58,72,73	1.34	8 (13%)	65,111,113	1.41	11 (16%)
25	BCR	A	408	-	41,41,41	1.18	3 (7%)	56,56,56	1.51	10 (17%)
24	PHO	a	407	-	67,69,69	1.16	7 (10%)	85,99,99	1.08	5 (5%)
23	CLA	B	608	-	59,73,73	1.33	10 (16%)	67,113,113	1.40	11 (16%)
23	CLA	b	602	36	59,73,73	1.82	10 (16%)	67,113,113	1.51	14 (20%)
33	LMG	D	407	-	51,51,55	1.01	5 (9%)	59,59,63	1.20	3 (5%)
29	LHG	L	101	-	48,48,48	0.93	4 (8%)	51,54,54	1.08	2 (3%)
23	CLA	C	513	-	59,73,73	1.48	9 (15%)	67,113,113	1.51	14 (20%)
35	HEC	v	201	16	26,50,50	2.66	4 (15%)	18,82,82	1.44	3 (16%)
30	OEX	a	415	1,3,36	0,15,15	0.00	-	-		
23	CLA	C	508	36	59,73,73	1.58	10 (16%)	67,113,113	1.39	9 (13%)
23	CLA	b	615	-	59,73,73	1.53	7 (11%)	67,113,113	1.65	15 (22%)
25	BCR	C	515	-	41,41,41	1.26	5 (12%)	56,56,56	1.33	8 (14%)
26	PL9	D	406	-	55,55,55	1.58	9 (16%)	68,69,69	1.65	14 (20%)
33	LMG	C	501	-	48,48,55	1.17	6 (12%)	56,56,63	1.37	10 (17%)
24	PHO	A	406	-	67,69,69	1.28	10 (14%)	85,99,99	1.04	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	607	36	59,73,73	1.30	10 (16%)	67,113,113	1.36	9 (13%)
23	CLA	c	502	-	59,73,73	1.33	5 (8%)	67,113,113	1.69	12 (17%)
28	DGD	c	516	-	63,63,67	1.19	5 (7%)	77,77,81	1.55	15 (19%)
33	LMG	m	101	-	51,51,55	0.96	4 (7%)	59,59,63	1.55	8 (13%)
23	CLA	B	605	-	59,73,73	1.64	9 (15%)	67,113,113	1.50	15 (22%)
23	CLA	c	501	-	59,73,73	1.54	7 (11%)	67,113,113	2.13	11 (16%)
23	CLA	c	504	36	54,68,73	1.61	7 (12%)	61,107,113	1.55	7 (11%)
25	BCR	x	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.40	11 (19%)
25	BCR	H	101	-	41,41,41	1.26	3 (7%)	56,56,56	1.34	7 (12%)
33	LMG	D	411	-	20,26,55	0.53	0	18,26,63	1.14	0
28	DGD	c	518	-	63,63,67	1.27	9 (14%)	77,77,81	1.53	12 (15%)
25	BCR	B	617	-	41,41,41	1.28	4 (9%)	56,56,56	1.39	9 (16%)
23	CLA	B	613	-	59,73,73	1.49	9 (15%)	67,113,113	1.81	16 (23%)
23	CLA	b	612	-	59,73,73	1.54	10 (16%)	67,113,113	1.45	15 (22%)
35	HEC	V	201	16	26,50,50	2.60	6 (23%)	18,82,82	1.75	3 (16%)
23	CLA	b	607	-	59,73,73	1.52	8 (13%)	67,113,113	1.56	14 (20%)
27	SQD	A	411	-	38,38,54	1.09	4 (10%)	40,40,65	1.47	4 (10%)
28	DGD	c	517	-	63,63,67	1.19	6 (9%)	77,77,81	1.34	8 (10%)
34	HEM	E	103	6,5	27,50,50	1.91	5 (18%)	17,82,82	1.98	6 (35%)
23	CLA	C	505	36	53,67,73	1.51	8 (15%)	59,105,113	1.45	10 (16%)
25	BCR	c	514	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	8 (14%)
23	CLA	d	404	-	59,73,73	1.60	8 (13%)	67,113,113	1.55	10 (14%)
33	LMG	D	410	-	31,31,55	1.15	3 (9%)	33,33,63	1.11	2 (6%)
25	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.13	3 (5%)
23	CLA	B	606	-	59,73,73	1.63	10 (16%)	67,113,113	1.83	15 (22%)
25	BCR	b	620	-	41,41,41	1.07	3 (7%)	56,56,56	1.29	8 (14%)
23	CLA	b	616	-	59,73,73	2.17	7 (11%)	67,113,113	1.63	11 (16%)
23	CLA	b	605	-	59,73,73	1.25	5 (8%)	67,113,113	1.97	17 (25%)
27	SQD	a	412	-	35,35,54	1.06	2 (5%)	37,37,65	1.44	5 (13%)
23	CLA	B	601	36	59,73,73	1.80	9 (15%)	67,113,113	1.39	10 (14%)
23	CLA	b	603	-	59,73,73	1.59	10 (16%)	67,113,113	1.62	14 (20%)
23	CLA	C	512	3	59,73,73	1.83	7 (11%)	67,113,113	1.65	10 (14%)
29	LHG	d	409	-	38,38,48	0.86	2 (5%)	41,44,54	1.11	3 (7%)
25	BCR	B	619	-	41,41,41	1.18	4 (9%)	56,56,56	1.25	7 (12%)
25	BCR	C	520	-	41,41,41	1.03	3 (7%)	56,56,56	1.36	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	f	101	-	40,41,54	1.12	5 (12%)	49,52,65	1.80	13 (26%)
23	CLA	C	504	-	59,73,73	1.77	8 (13%)	67,113,113	1.97	19 (28%)
23	CLA	c	509	-	59,73,73	1.50	6 (10%)	67,113,113	1.97	12 (17%)
23	CLA	D	403	-	59,73,73	1.28	7 (11%)	67,113,113	1.67	9 (13%)
26	PL9	d	406	-	55,55,55	1.36	7 (12%)	68,69,69	1.79	19 (27%)

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
23	CLA	c	510	-	3/3/25/25	15/37/135/135	-
23	CLA	a	405	-	2/2/25/25	6/37/135/135	-
33	LMG	C	519	-	-	16/43/63/70	0/1/1/1
23	CLA	d	402	36	3/3/25/25	4/37/135/135	-
23	CLA	c	513	-	3/3/25/25	10/37/135/135	-
28	DGD	C	518	-	-	15/51/91/95	0/2/2/2
23	CLA	b	606	-	3/3/25/25	8/37/135/135	-
29	LHG	A	413	-	-	15/53/53/53	-
27	SQD	F	101	-	-	13/28/48/69	0/1/1/1
23	CLA	C	510	-	3/3/25/25	9/37/135/135	-
25	BCR	D	405	-	-	3/29/63/63	0/2/2/2
29	LHG	E	101	-	-	27/53/53/53	-
23	CLA	b	609	-	2/2/25/25	6/37/135/135	-
27	SQD	b	601	-	-	21/44/64/69	0/1/1/1
23	CLA	C	514	-	3/3/25/25	13/37/135/135	-
23	CLA	b	617	-	3/3/24/25	6/31/129/135	-
23	CLA	D	404	-	2/2/25/25	12/37/135/135	-
23	CLA	A	404	-	3/3/25/25	4/37/135/135	-
23	CLA	c	505	-	2/2/25/25	10/37/135/135	-
23	CLA	c	511	3	3/3/25/25	10/37/135/135	-
23	CLA	c	506	-	2/2/25/25	17/37/135/135	-
23	CLA	b	610	-	2/2/25/25	13/37/135/135	-
23	CLA	A	407	-	3/3/22/25	6/24/122/135	-
29	LHG	D	409	-	-	23/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	A	412	-	-	28/55/95/95	0/2/2/2
28	DGD	h	101	-	-	17/51/91/95	0/2/2/2
28	DGD	a	413	-	-	21/45/45/95	-
33	LMG	M	101	-	-	19/46/66/70	0/1/1/1
23	CLA	B	609	-	2/2/25/25	6/37/135/135	-
23	CLA	c	512	-	3/3/25/25	23/37/135/135	-
23	CLA	C	509	-	3/3/25/25	6/37/135/135	-
27	SQD	a	411	-	-	22/49/69/69	0/1/1/1
23	CLA	B	602	-	3/3/25/25	7/37/135/135	-
33	LMG	c	522	-	-	21/43/63/70	0/1/1/1
23	CLA	B	603	-	3/3/25/25	11/37/135/135	-
26	PL9	A	409	-	-	19/53/73/73	0/1/1/1
23	CLA	B	615	-	3/3/25/25	7/37/135/135	-
25	BCR	c	515	-	-	5/29/63/63	0/2/2/2
23	CLA	C	502	-	3/3/25/25	4/37/135/135	-
33	LMG	b	622	-	-	20/50/70/70	0/1/1/1
23	CLA	B	614	-	3/3/25/25	13/37/135/135	-
23	CLA	b	613	-	3/3/25/25	11/37/135/135	-
23	CLA	b	611	36	3/3/25/25	1/37/135/135	-
29	LHG	l	101	-	-	16/53/53/53	-
29	LHG	d	407	-	-	21/53/53/53	-
23	CLA	C	506	-	3/3/25/25	13/37/135/135	-
23	CLA	c	503	-	3/3/25/25	9/37/135/135	-
23	CLA	A	405	36	3/3/25/25	4/37/135/135	-
28	DGD	C	516	-	-	24/51/91/95	0/2/2/2
33	LMG	c	524	-	-	16/44/64/70	0/1/1/1
28	DGD	C	517	-	-	20/51/91/95	0/2/2/2
33	LMG	d	410	-	-	13/15/17/70	-
25	BCR	a	409	-	-	2/29/63/63	0/2/2/2
29	LHG	e	101	-	-	30/46/46/53	-
23	CLA	C	503	-	3/3/25/25	12/37/135/135	-
23	CLA	B	612	-	3/3/25/25	19/37/135/135	-
33	LMG	d	411	-	-	8/39/59/70	0/1/1/1
28	DGD	H	102	-	-	16/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	507	36	3/3/25/25	10/37/135/135	-
25	BCR	c	521	-	-	7/29/63/63	0/2/2/2
23	CLA	B	610	36	3/3/25/25	10/37/135/135	-
23	CLA	a	406	36	3/3/25/25	12/37/135/135	-
25	BCR	K	101	-	-	13/29/63/63	0/2/2/2
23	CLA	B	604	-	2/2/25/25	13/37/135/135	-
23	CLA	B	611	-	3/3/25/25	6/37/135/135	-
27	SQD	A	410	-	-	18/47/67/69	0/1/1/1
33	LMG	c	519	-	-	12/31/51/70	0/1/1/1
23	CLA	D	402	36	2/2/25/25	5/37/135/135	-
25	BCR	t	101	-	-	7/29/63/63	0/2/2/2
29	LHG	d	408	-	-	19/53/53/53	-
27	SQD	B	621	-	-	23/49/69/69	0/1/1/1
23	CLA	b	614	-	3/3/25/25	10/37/135/135	-
25	BCR	b	619	-	-	13/29/63/63	0/2/2/2
23	CLA	b	604	-	3/3/25/25	10/37/135/135	-
24	PHO	D	401	-	-	2/53/103/103	0/5/6/6
23	CLA	b	608	36	3/3/25/25	15/37/135/135	-
23	CLA	C	511	-	3/3/25/25	14/37/135/135	-
23	CLA	B	616	-	3/3/24/25	8/31/129/135	-
25	BCR	T	101	-	-	2/29/63/63	0/2/2/2
23	CLA	a	408	-	3/3/25/25	8/37/135/135	-
25	BCR	b	618	-	-	5/29/63/63	0/2/2/2
23	CLA	C	507	-	1/1/25/25	19/37/135/135	-
34	HEM	e	102	6,5	-	0/6/54/54	-
26	PL9	a	410	-	-	20/53/73/73	0/1/1/1
25	BCR	B	618	-	-	3/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/25/25	8/37/135/135	-
25	BCR	d	405	-	-	13/29/63/63	0/2/2/2
29	LHG	D	408	-	-	26/53/53/53	-
25	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
24	PHO	d	401	-	-	4/53/103/103	0/5/6/6
23	CLA	c	508	-	1/1/24/25	15/36/134/135	-
25	BCR	A	408	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	407	-	-	6/53/103/103	0/5/6/6
23	CLA	B	608	-	2/2/25/25	0/37/135/135	-
23	CLA	b	602	36	2/2/25/25	16/37/135/135	-
33	LMG	D	407	-	-	18/46/66/70	0/1/1/1
29	LHG	L	101	-	-	23/53/53/53	-
23	CLA	C	513	-	3/3/25/25	11/37/135/135	-
35	HEC	v	201	16	-	0/6/54/54	-
23	CLA	C	508	36	3/3/25/25	7/37/135/135	-
23	CLA	b	615	-	3/3/25/25	15/37/135/135	-
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
26	PL9	D	406	-	-	11/53/73/73	0/1/1/1
33	LMG	C	501	-	-	21/43/63/70	0/1/1/1
24	PHO	A	406	-	-	9/53/103/103	0/5/6/6
23	CLA	B	607	36	3/3/25/25	9/37/135/135	-
23	CLA	c	502	-	2/2/25/25	8/37/135/135	-
28	DGD	c	516	-	-	23/51/91/95	0/2/2/2
33	LMG	m	101	-	-	21/46/66/70	0/1/1/1
23	CLA	B	605	-	3/3/25/25	12/37/135/135	-
23	CLA	c	501	-	3/3/25/25	6/37/135/135	-
23	CLA	c	504	36	3/3/24/25	9/31/129/135	-
25	BCR	x	102	-	-	11/29/63/63	0/2/2/2
25	BCR	H	101	-	-	10/29/63/63	0/2/2/2
33	LMG	D	411	-	-	11/18/22/70	-
28	DGD	c	518	-	-	22/51/91/95	0/2/2/2
25	BCR	B	617	-	-	11/29/63/63	0/2/2/2
23	CLA	B	613	-	3/3/25/25	6/37/135/135	-
23	CLA	b	612	-	3/3/25/25	14/37/135/135	-
35	HEC	V	201	16	-	0/6/54/54	-
23	CLA	b	607	-	3/3/25/25	11/37/135/135	-
27	SQD	A	411	-	-	14/39/39/69	-
28	DGD	c	517	-	-	19/51/91/95	0/2/2/2
34	HEM	E	103	6,5	-	0/6/54/54	-
23	CLA	C	505	36	3/3/23/25	8/30/128/135	-
25	BCR	c	514	-	-	15/29/63/63	0/2/2/2
23	CLA	d	404	-	3/3/25/25	7/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	D	410	-	-	17/33/33/70	-
25	BCR	k	101	-	-	13/29/63/63	0/2/2/2
23	CLA	B	606	-	3/3/25/25	13/37/135/135	-
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
23	CLA	b	616	-	3/3/25/25	8/37/135/135	-
23	CLA	b	605	-	3/3/25/25	11/37/135/135	-
27	SQD	a	412	-	-	19/37/37/69	-
23	CLA	B	601	36	3/3/25/25	12/37/135/135	-
23	CLA	b	603	-	3/3/25/25	10/37/135/135	-
23	CLA	C	512	3	3/3/25/25	7/37/135/135	-
29	LHG	d	409	-	-	11/43/43/53	-
25	BCR	B	619	-	-	5/29/63/63	0/2/2/2
25	BCR	C	520	-	-	11/29/63/63	0/2/2/2
27	SQD	f	101	-	-	16/36/56/69	0/1/1/1
23	CLA	C	504	-	1/1/25/25	7/37/135/135	-
23	CLA	c	509	-	3/3/25/25	15/37/135/135	-
23	CLA	D	403	-	1/1/25/25	10/37/135/135	-
26	PL9	d	406	-	-	18/53/73/73	0/1/1/1

The worst 5 of 892 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	MG-NA	11.51	2.33	2.06
23	B	615	CLA	C4B-NB	9.83	1.44	1.35
23	c	503	CLA	C4B-NB	9.41	1.43	1.35
23	C	512	CLA	MG-NA	8.81	2.27	2.06
35	v	201	HEC	C3B-C2B	-8.55	1.31	1.40

The worst 5 of 1425 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C4A-NA-C1A	11.10	111.69	106.71
23	c	501	CLA	C4A-NA-C1A	10.59	111.47	106.71
23	C	502	CLA	C4A-NA-C1A	10.55	111.45	106.71
23	d	402	CLA	C4A-NA-C1A	10.41	111.38	106.71
27	A	410	SQD	O6-C1-C2	10.12	124.11	108.30

5 of 188 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	NC
23	A	404	CLA	NA
23	A	404	CLA	ND
23	A	405	CLA	NC
23	A	405	CLA	NA

5 of 1732 torsion outliers are listed below:

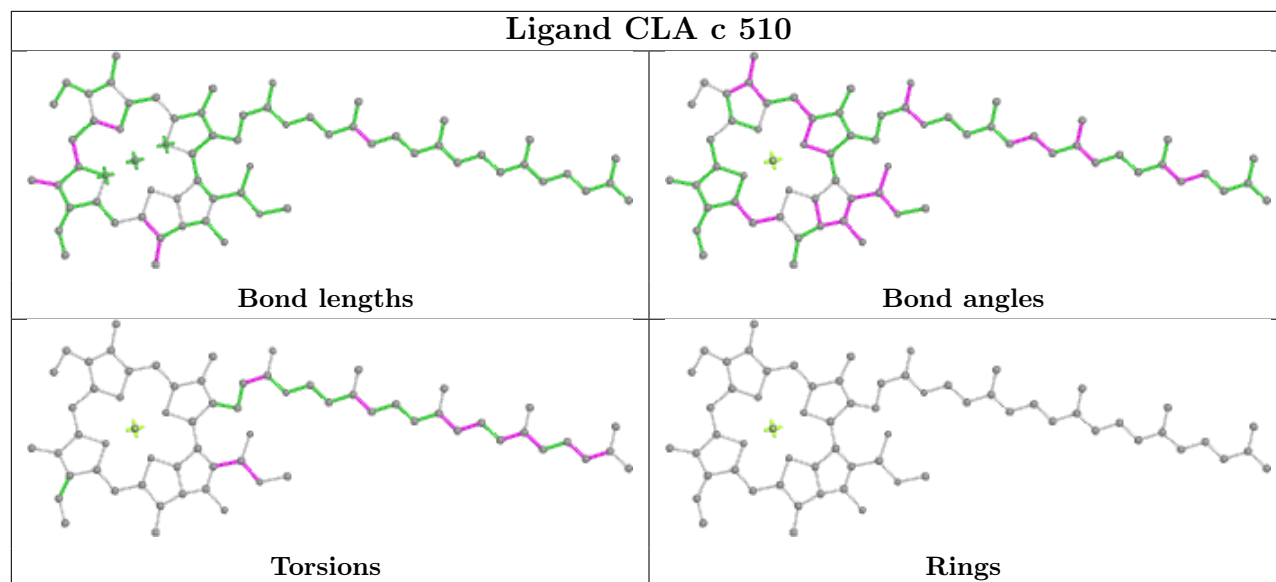
Mol	Chain	Res	Type	Atoms
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	A	407	CLA	C2-C3-C5-C6
23	A	407	CLA	C4-C3-C5-C6
23	B	601	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

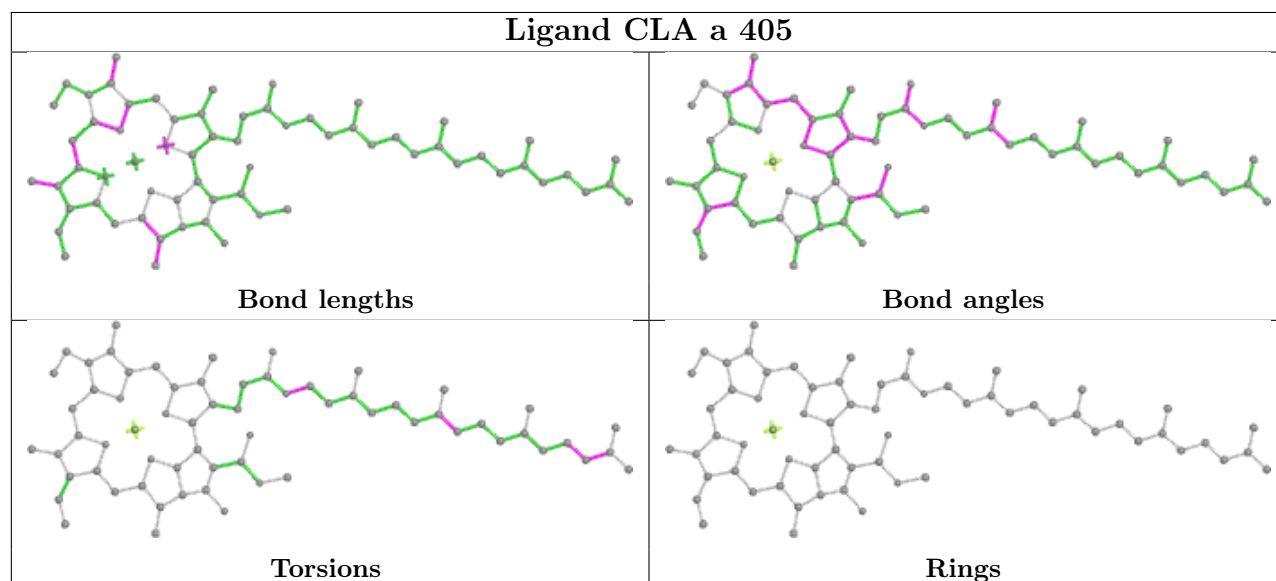
No monomer is involved in short contacts.

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

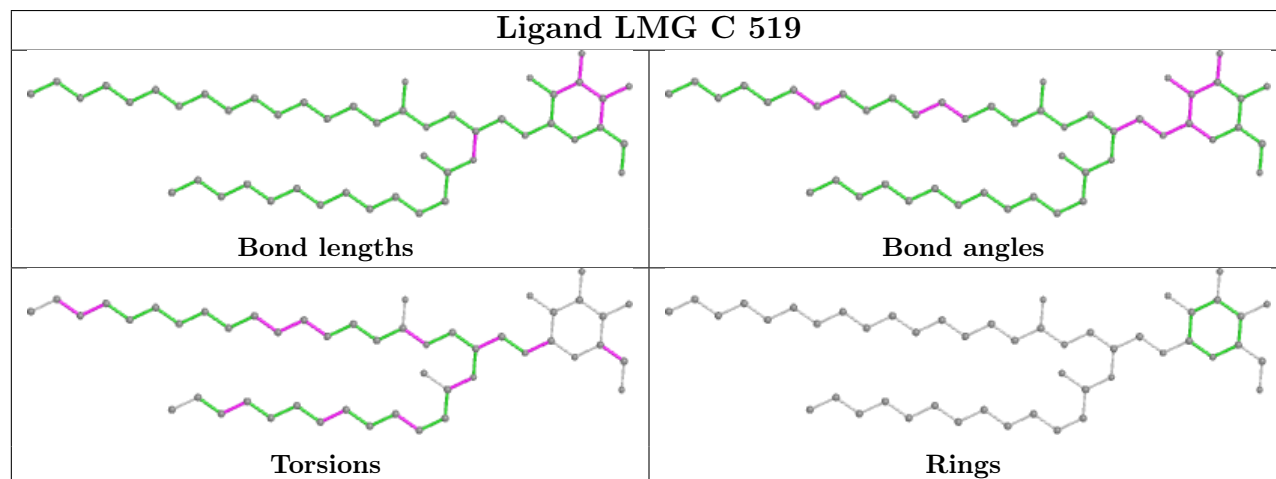
Ligand CLA c 510



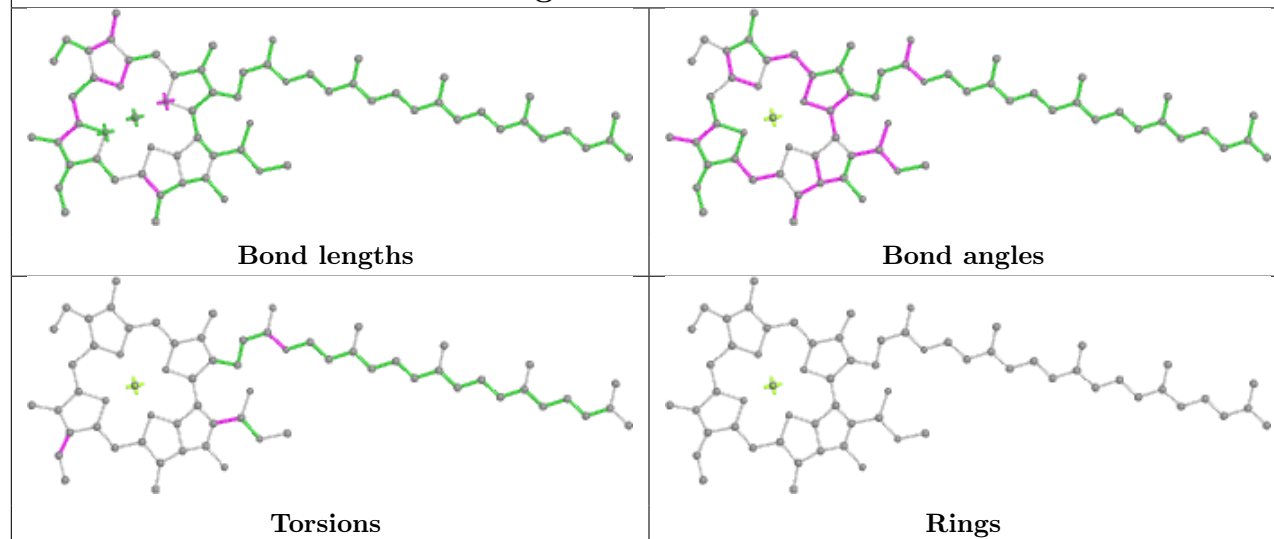
Ligand CLA a 405



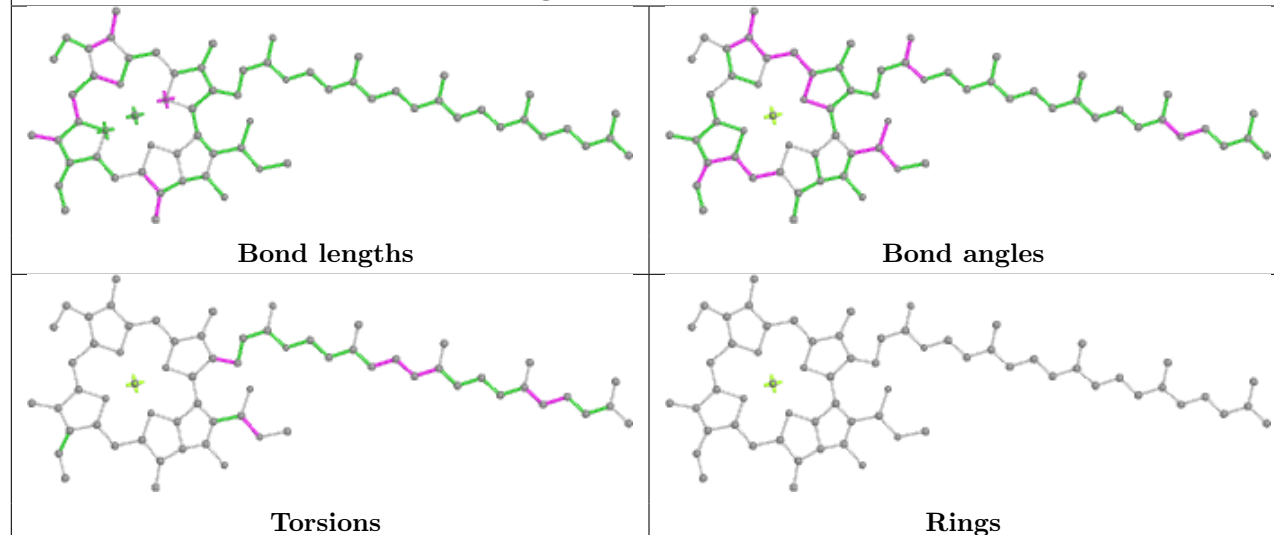
Ligand LMG C 519



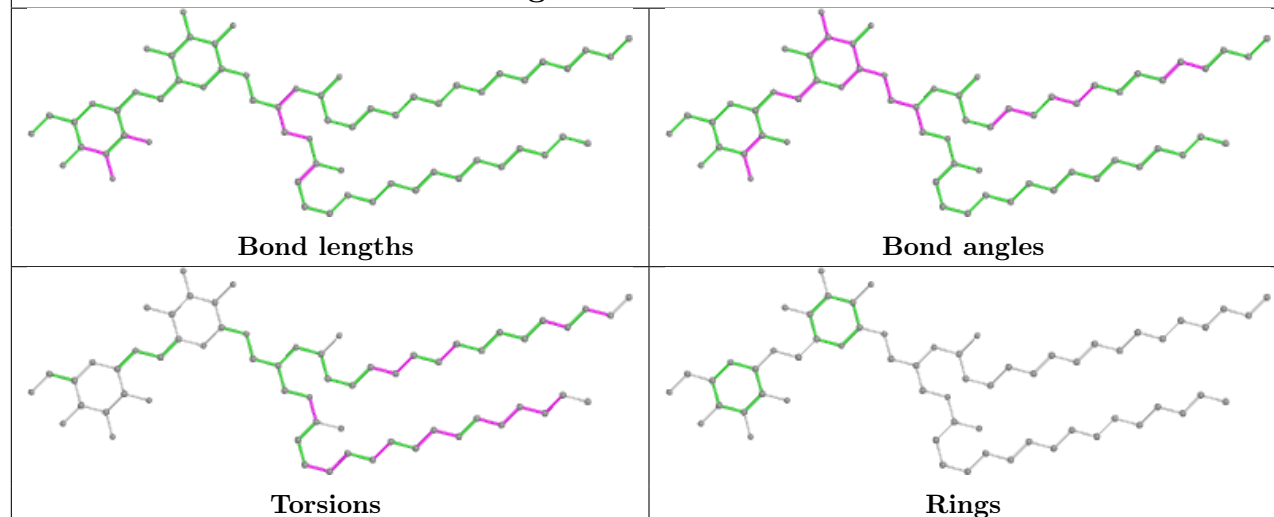
Ligand CLA d 402



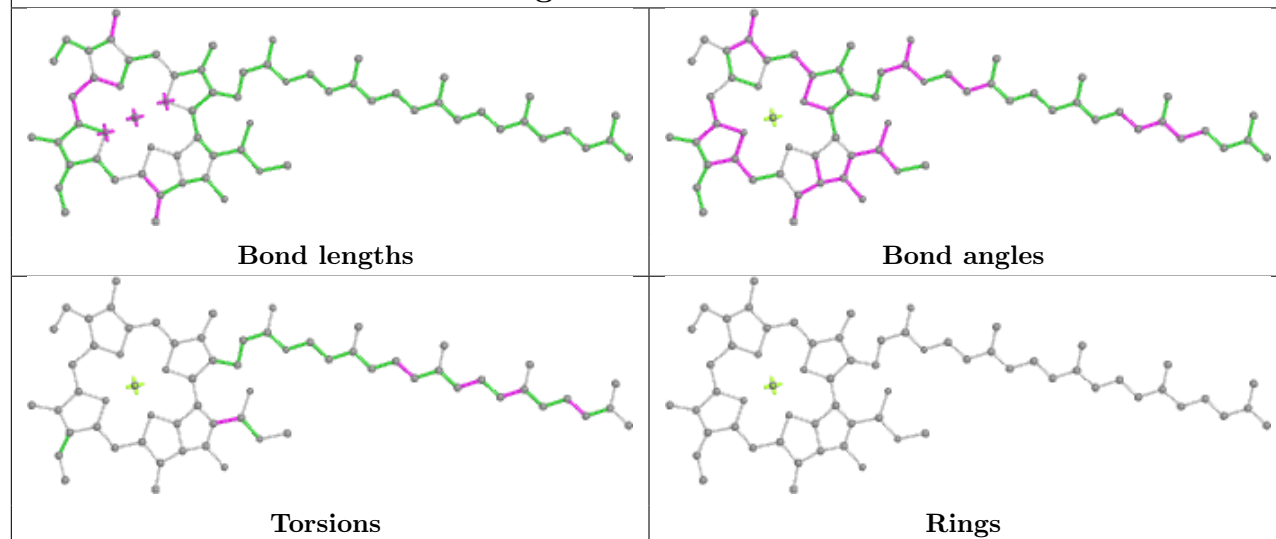
Ligand CLA c 513



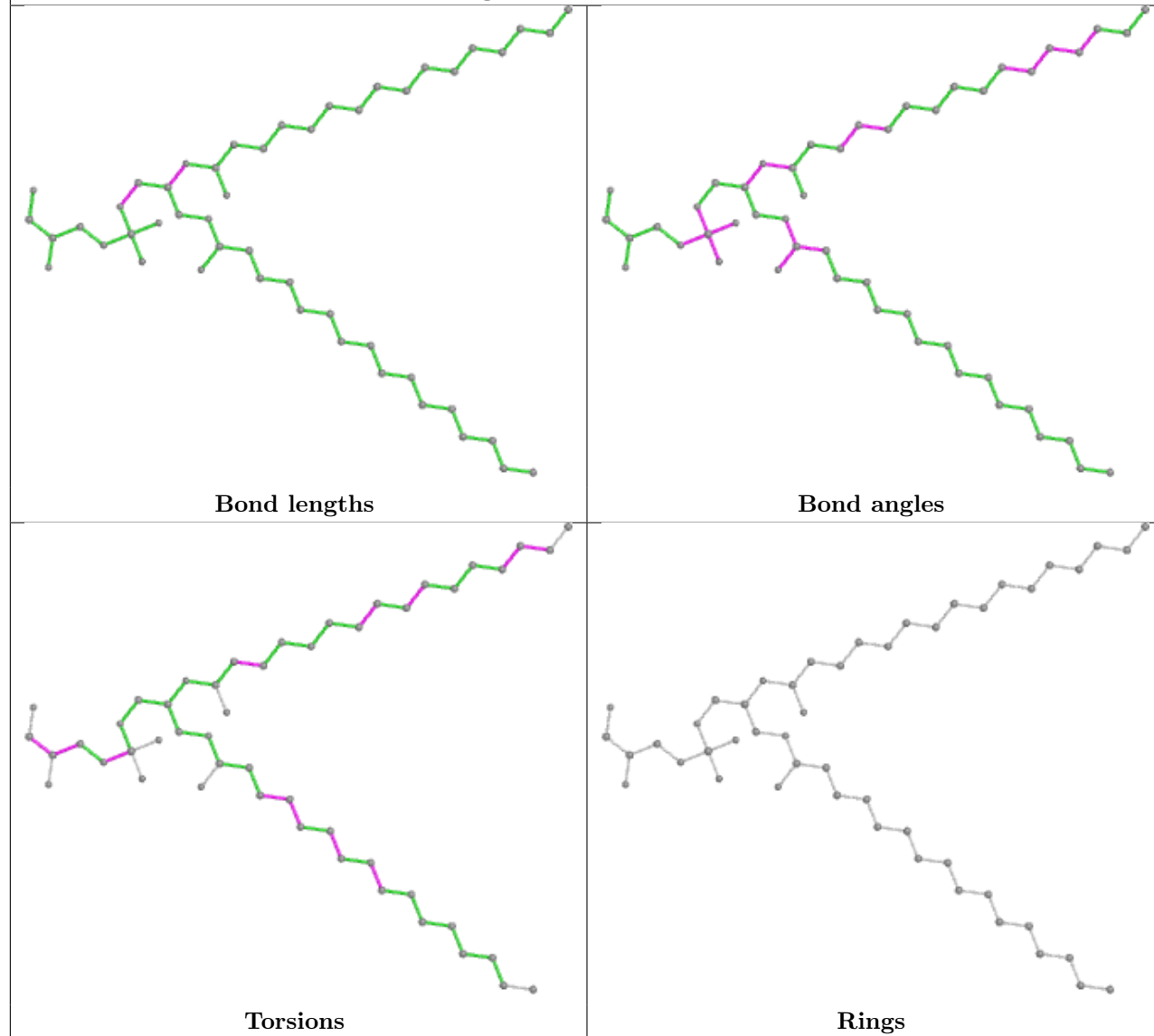
Ligand DGD C 518

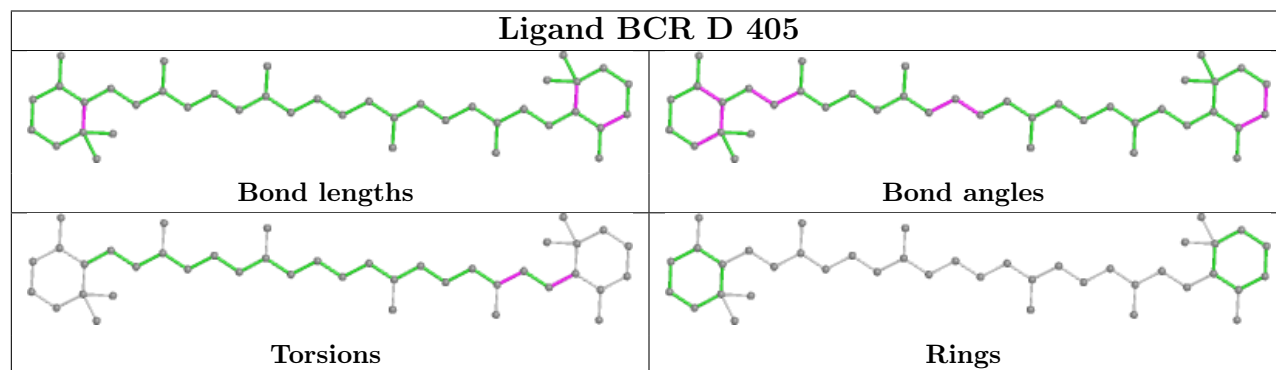
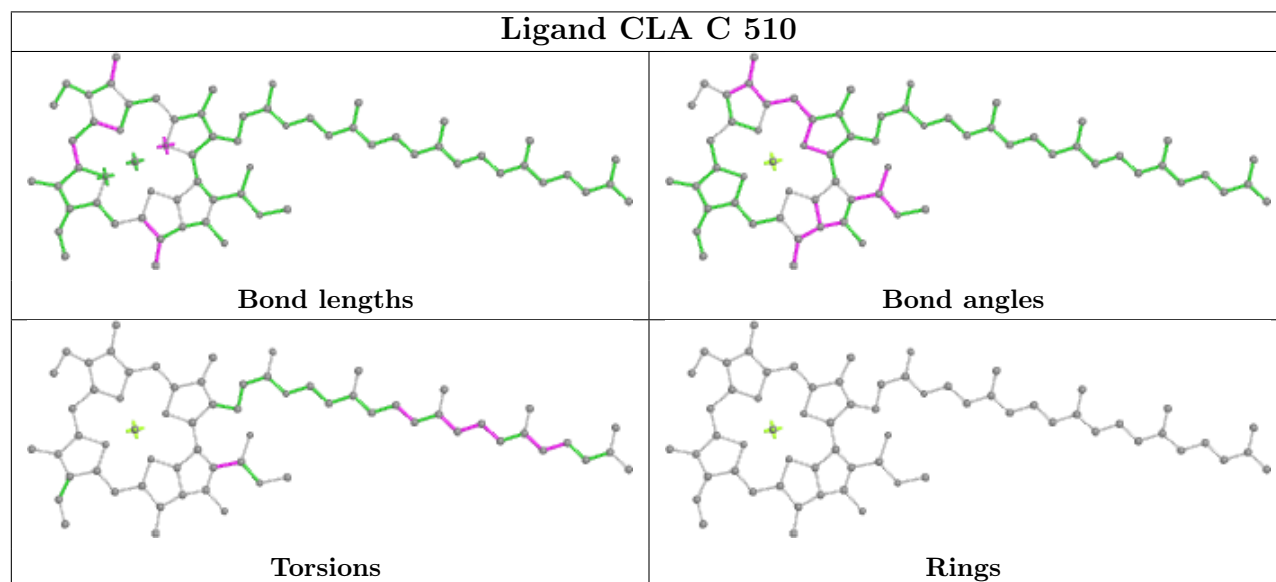
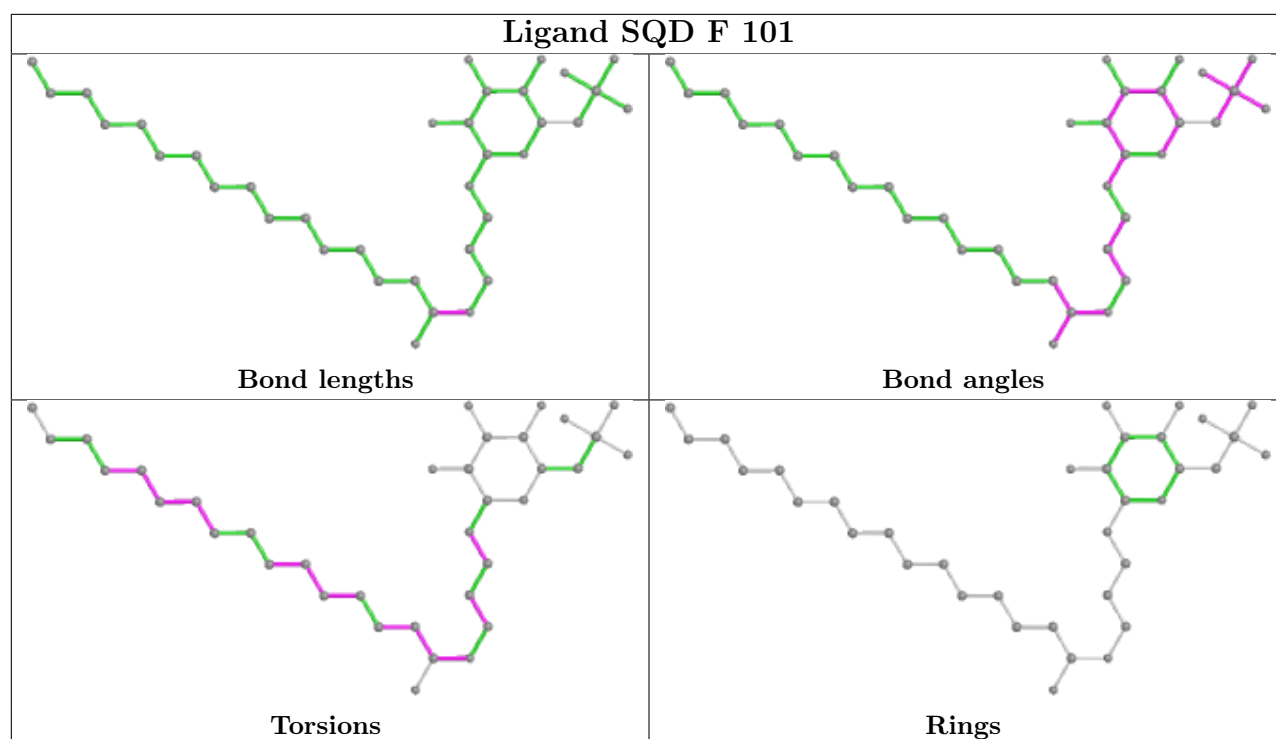


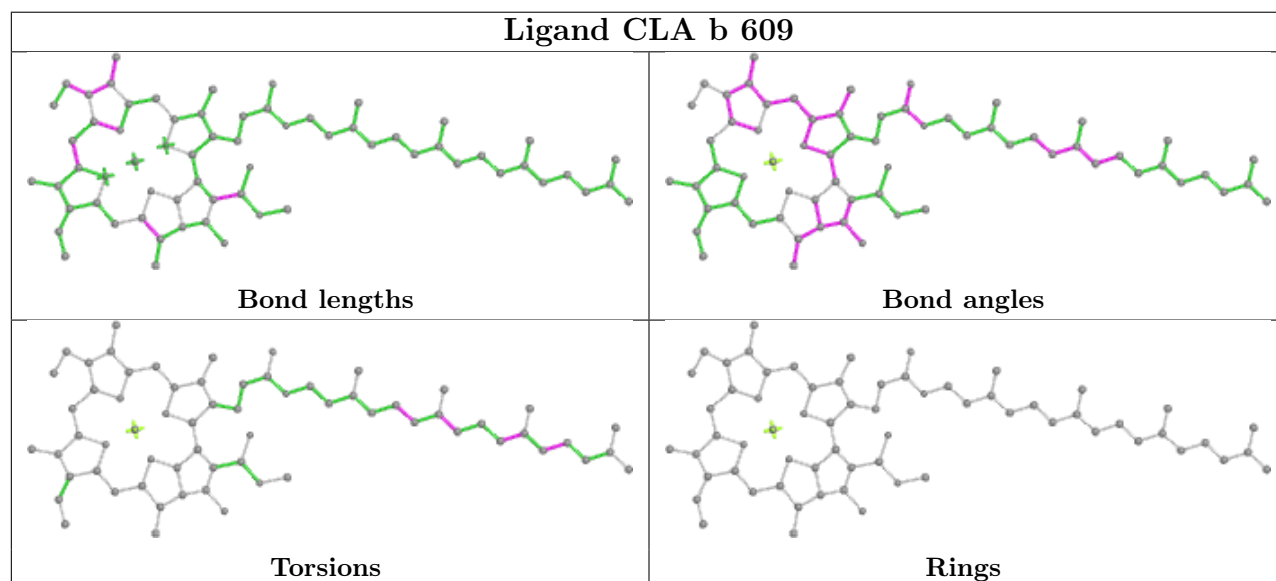
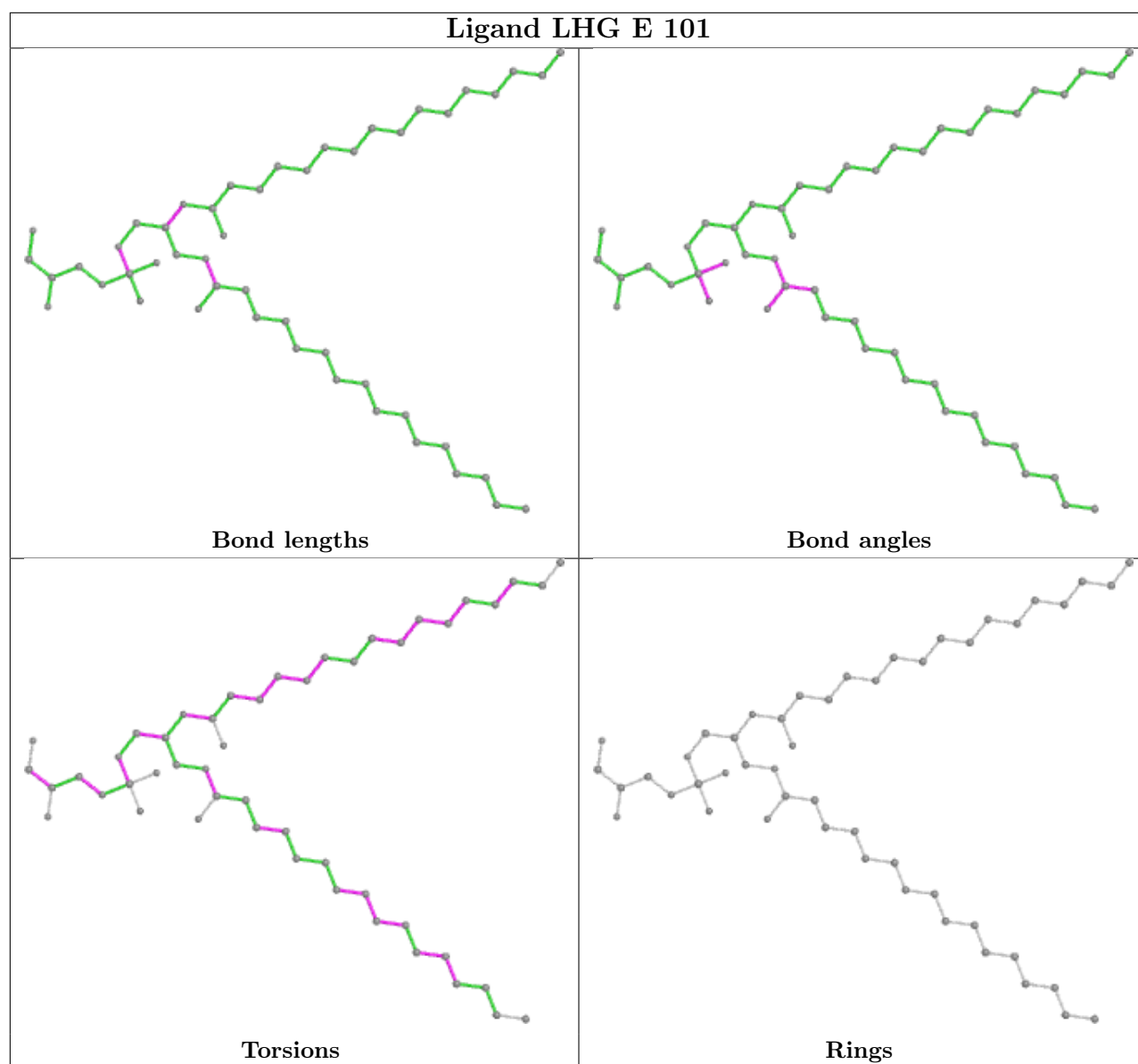
Ligand CLA b 606

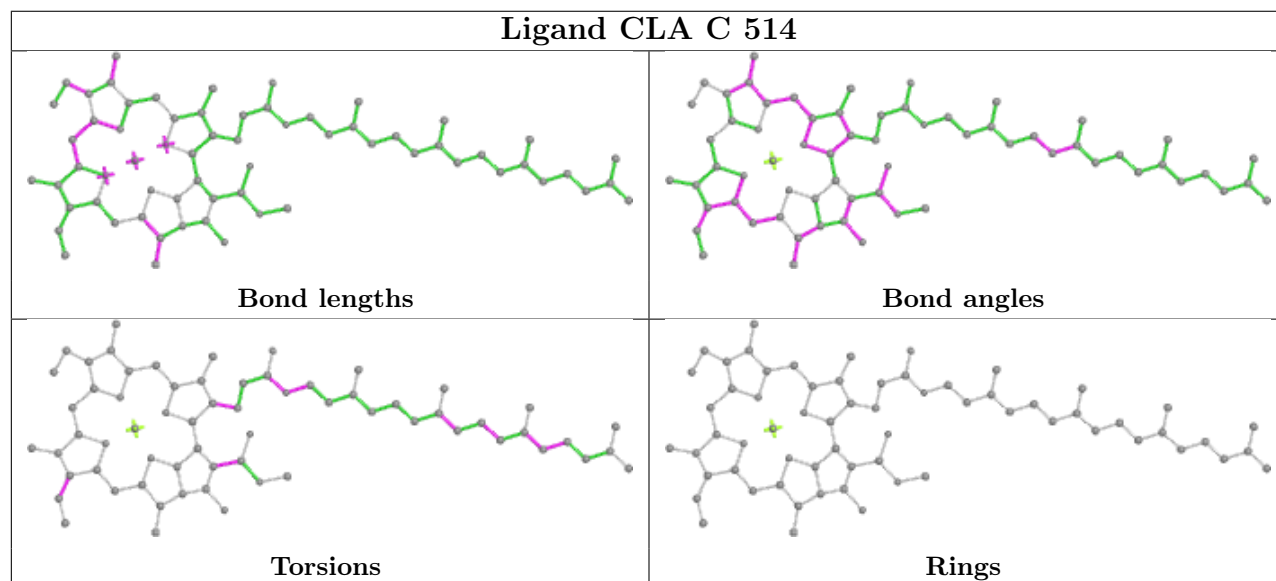
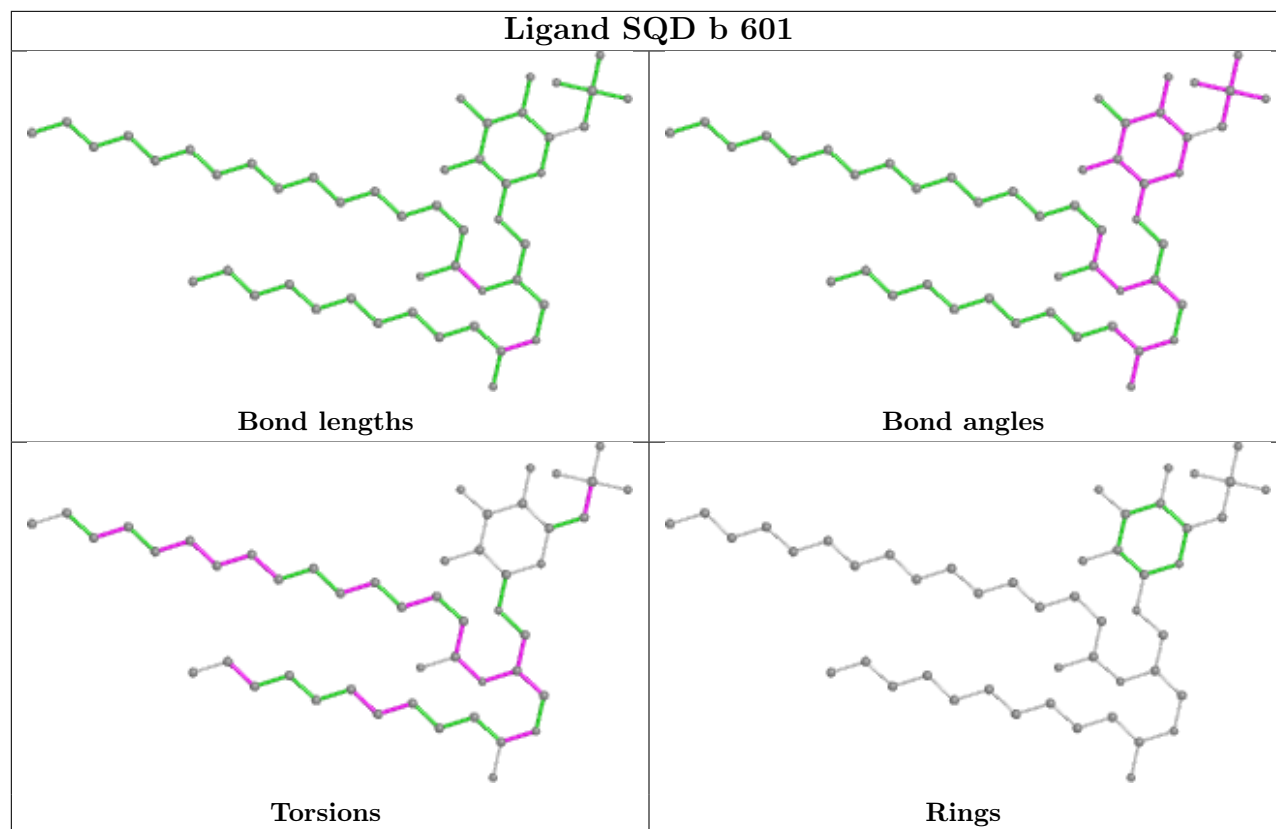


Ligand LHG A 413

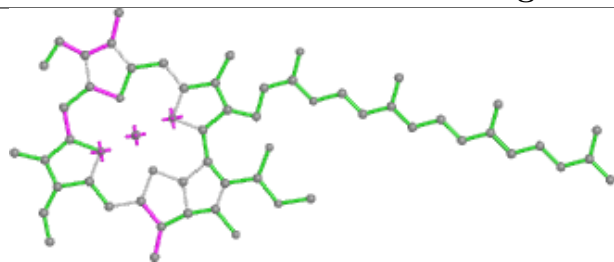




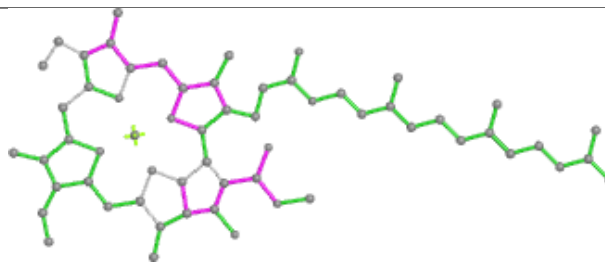




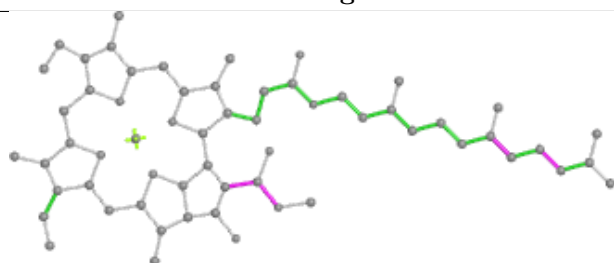
Ligand CLA b 617



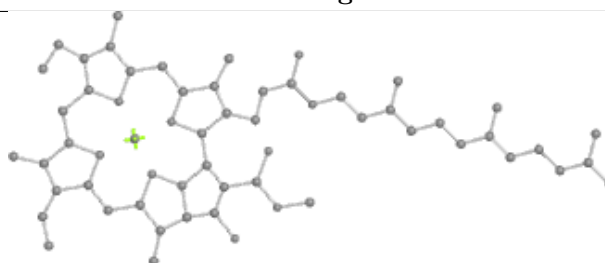
Bond lengths



Bond angles

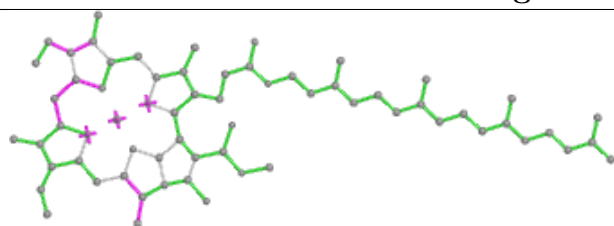


Torsions

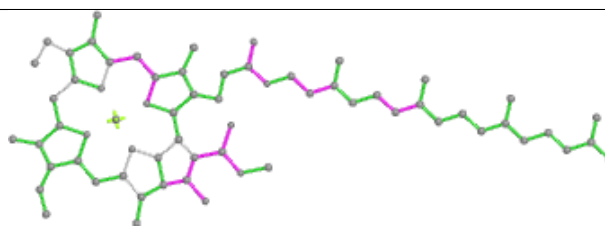


Rings

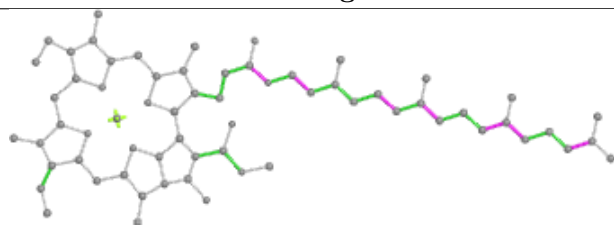
Ligand CLA D 404



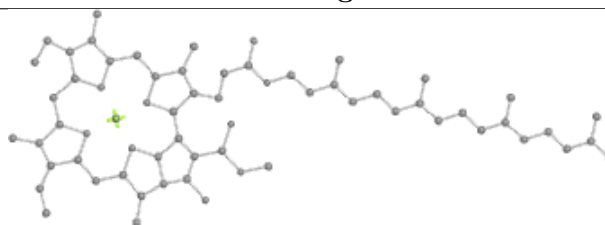
Bond lengths



Bond angles

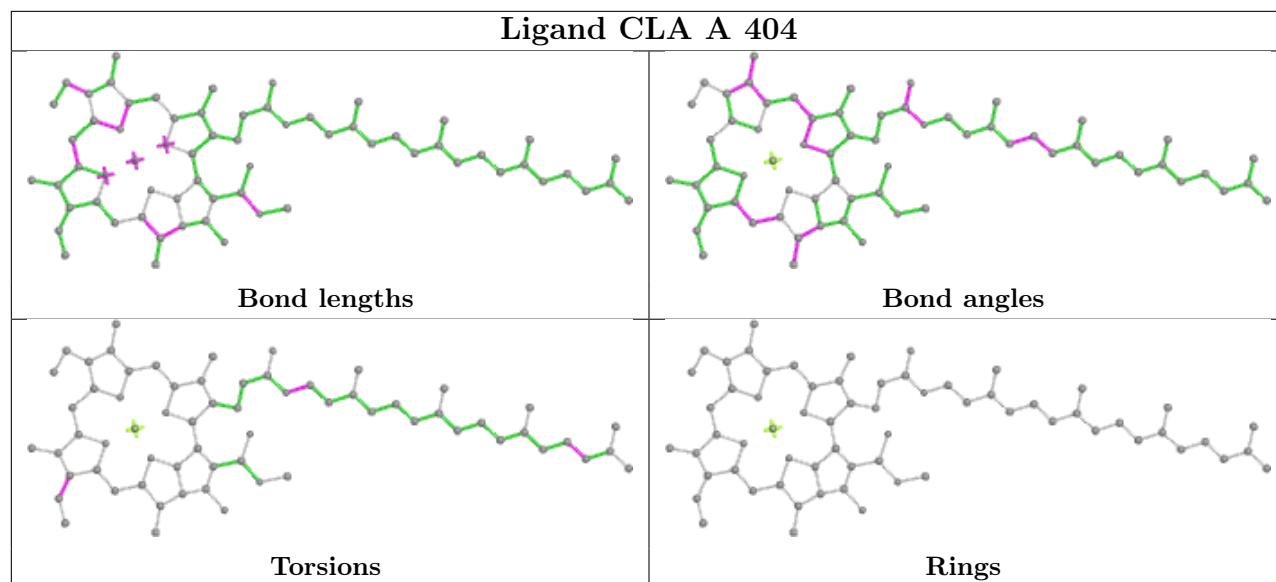


Torsions

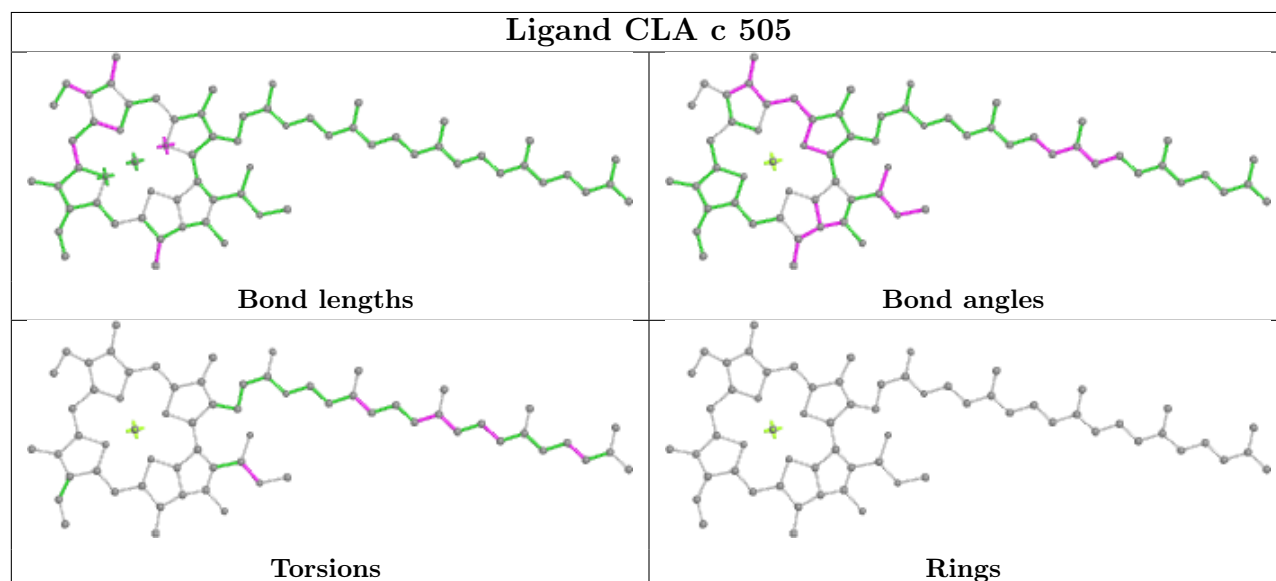


Rings

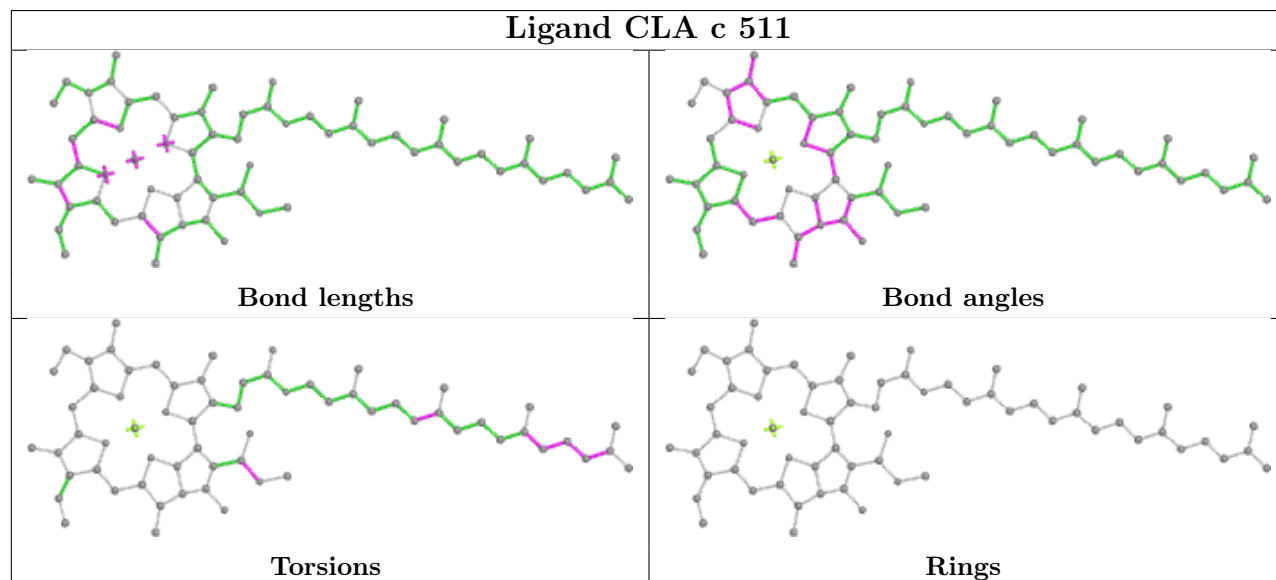
Ligand CLA A 404

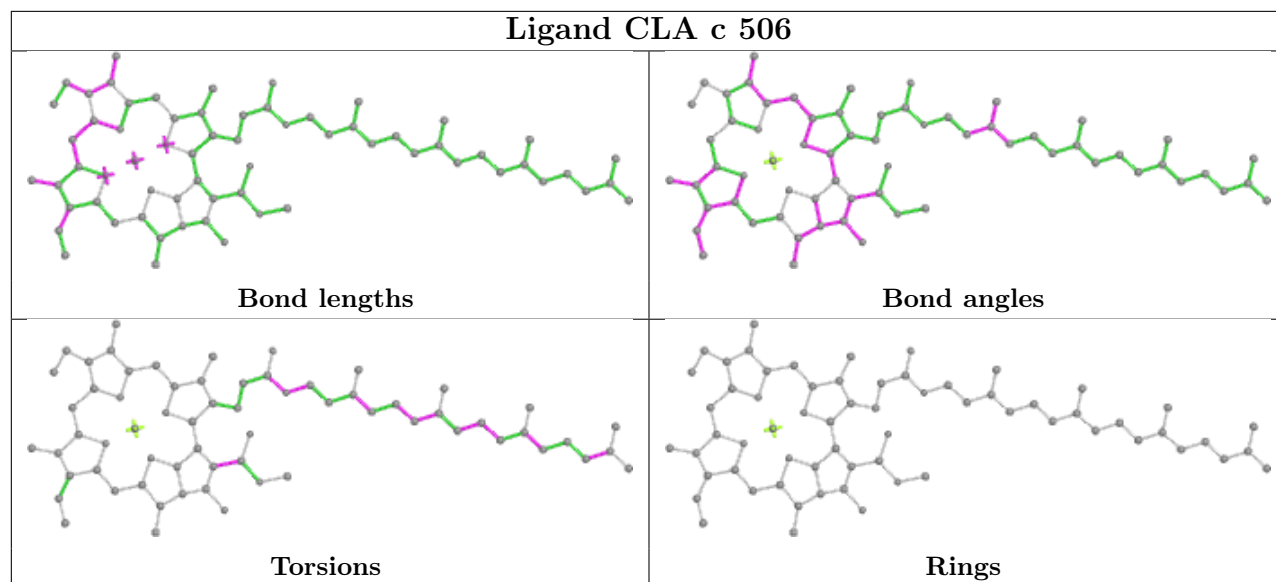
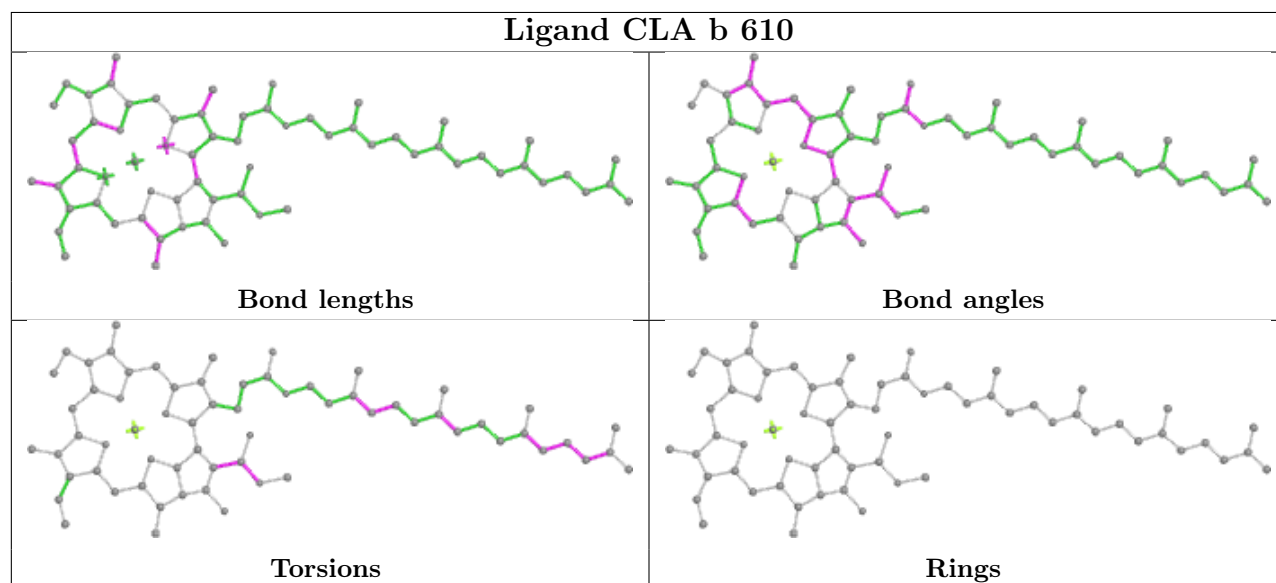


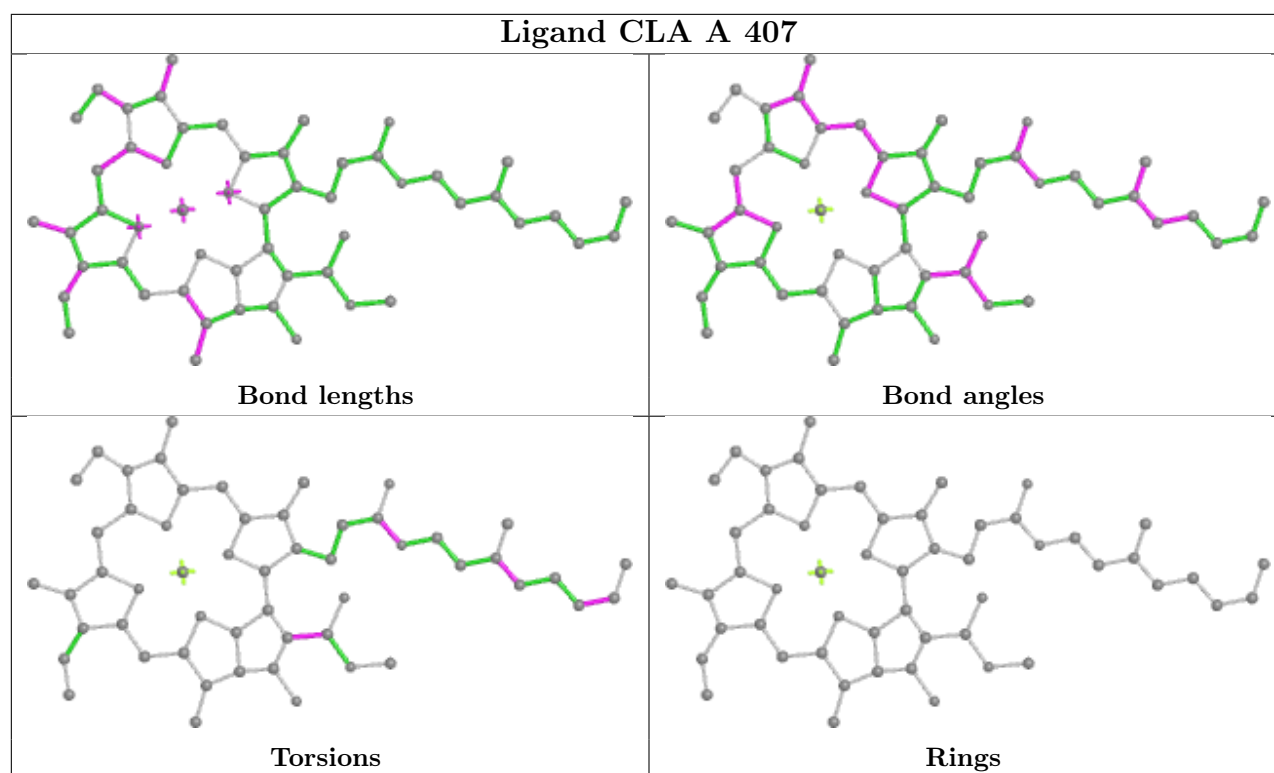
Ligand CLA c 505

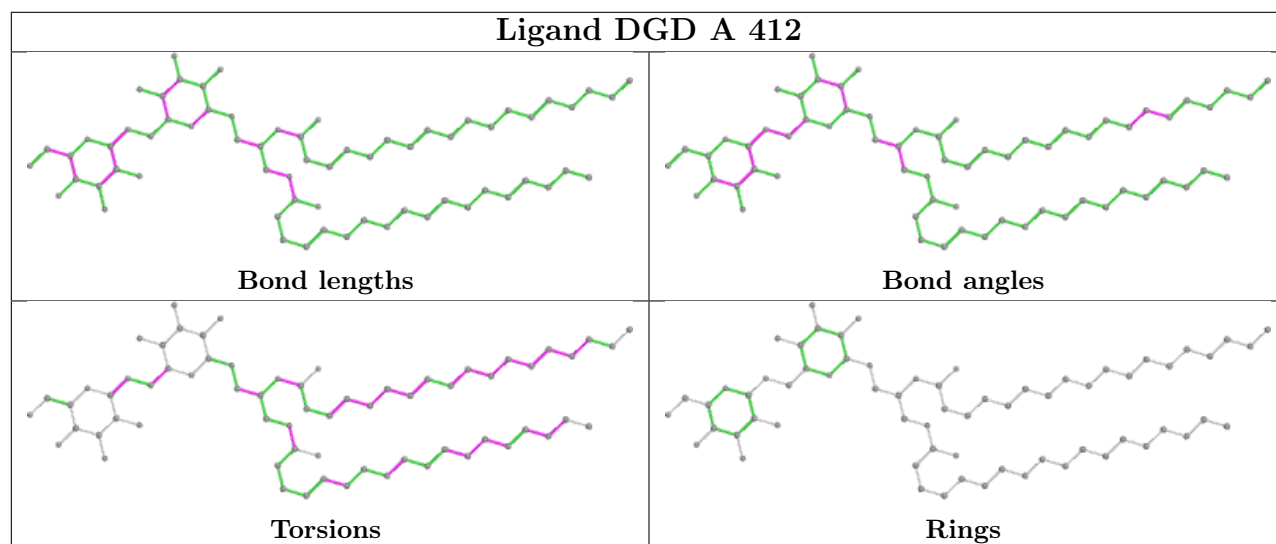
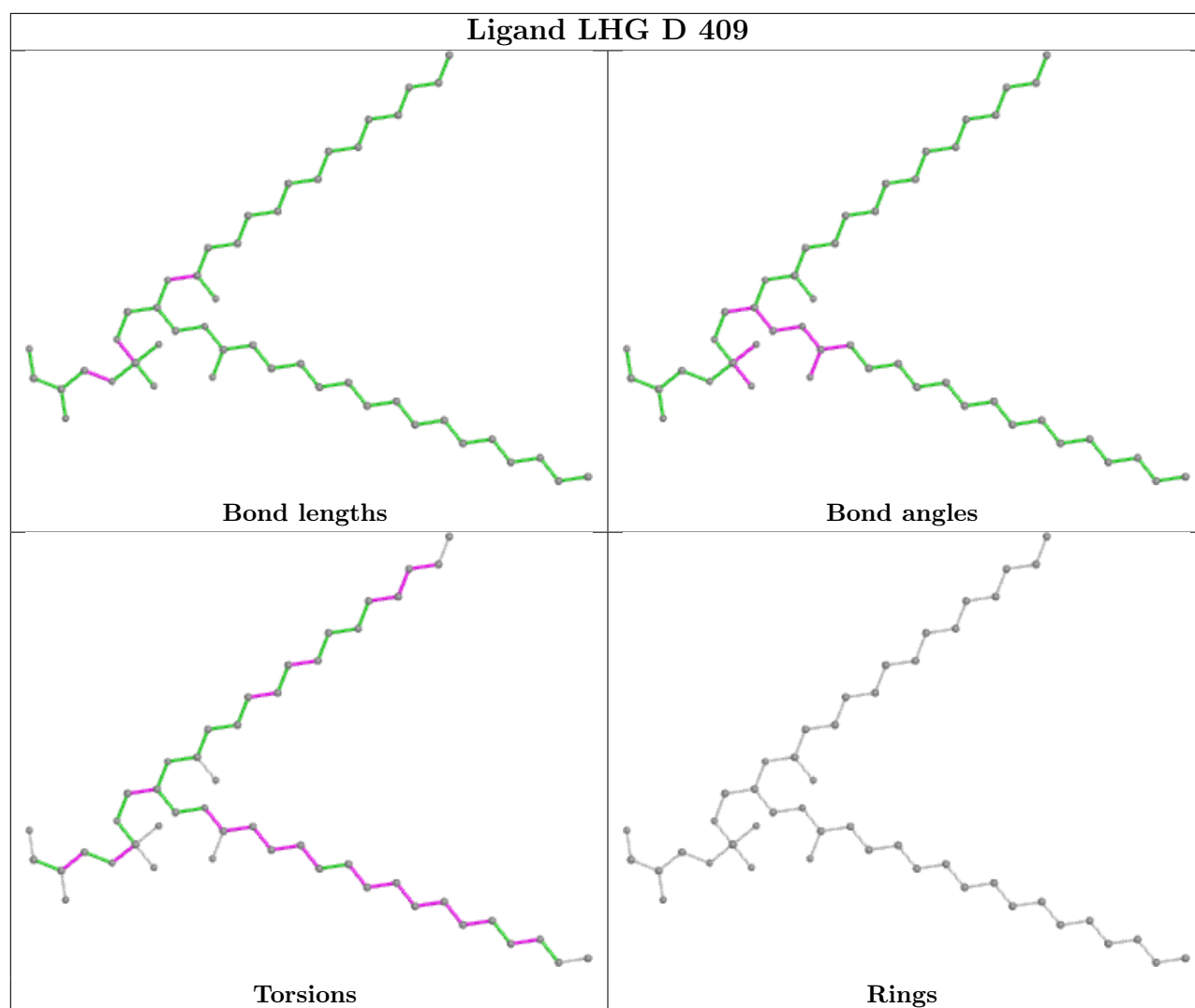


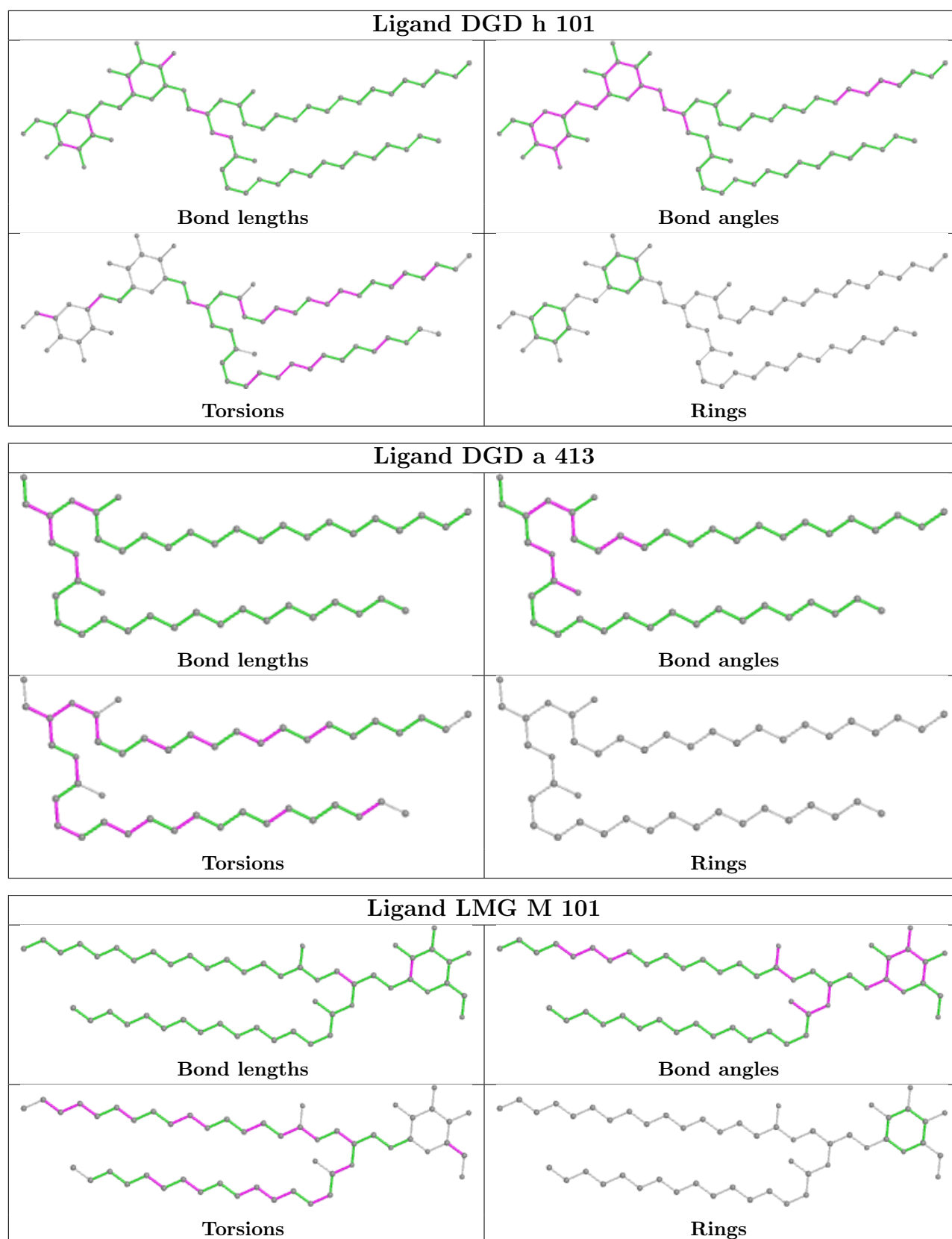
Ligand CLA c 511

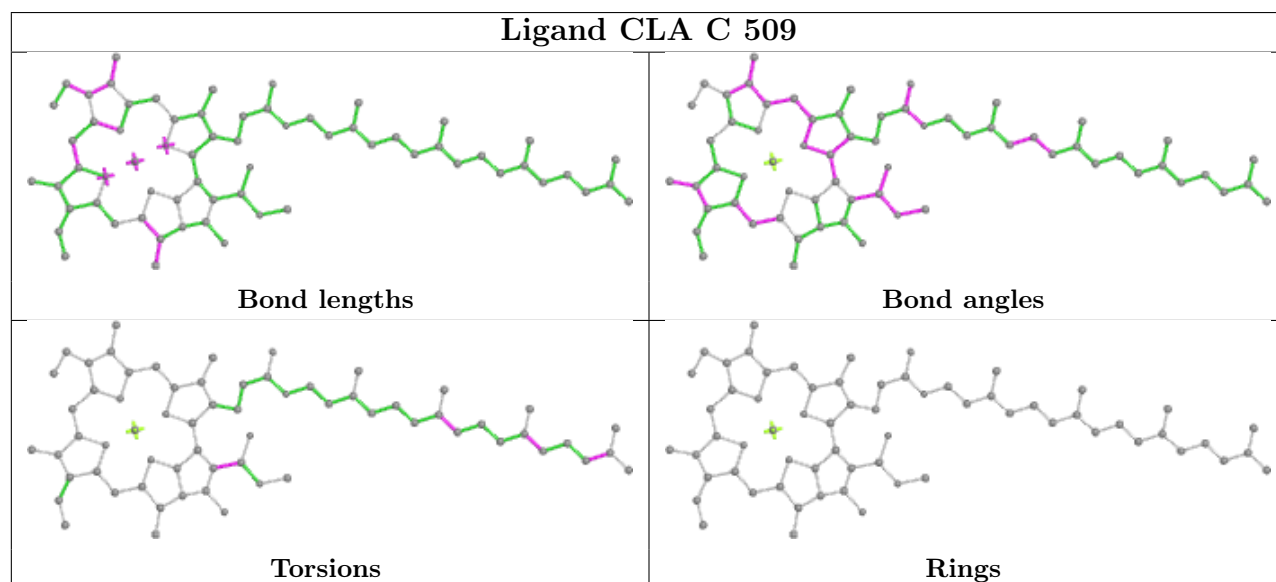
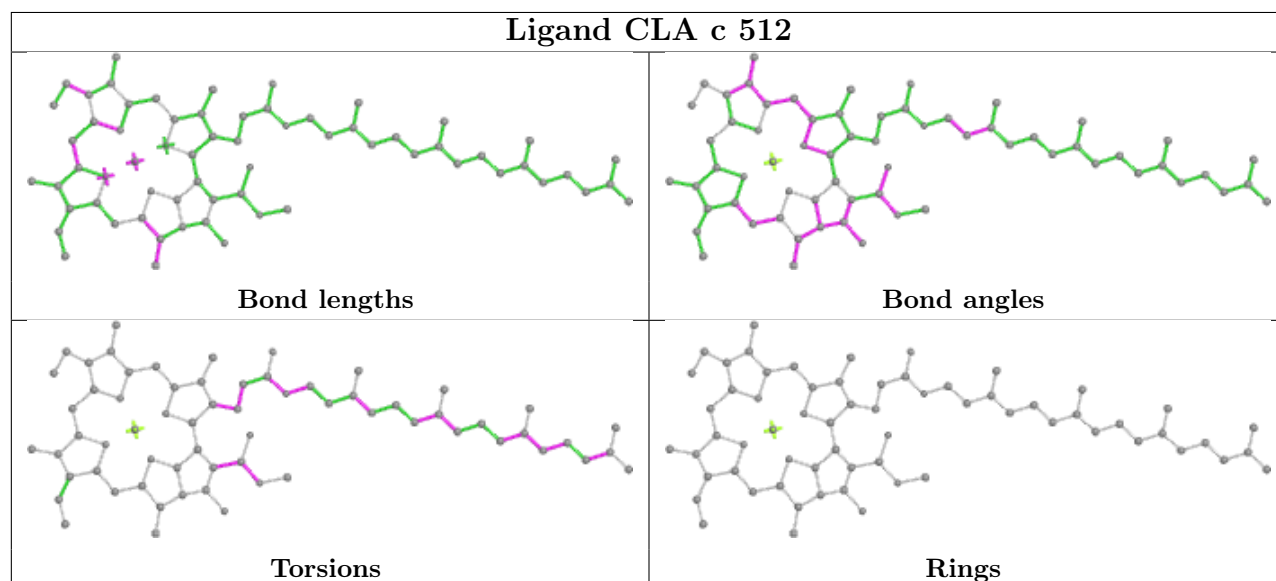
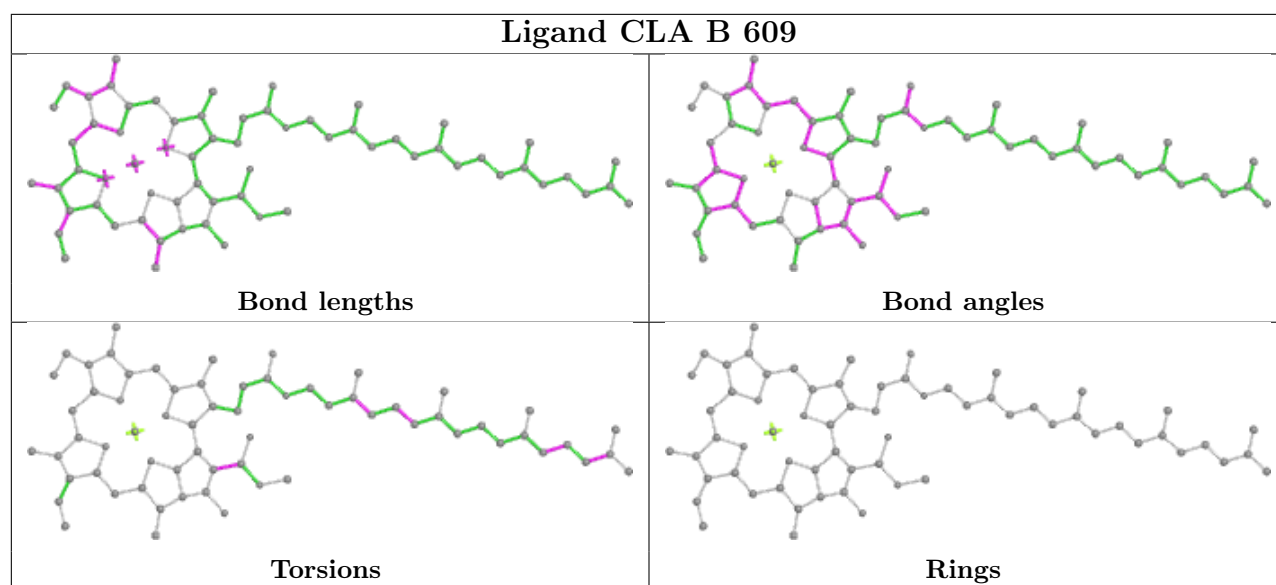


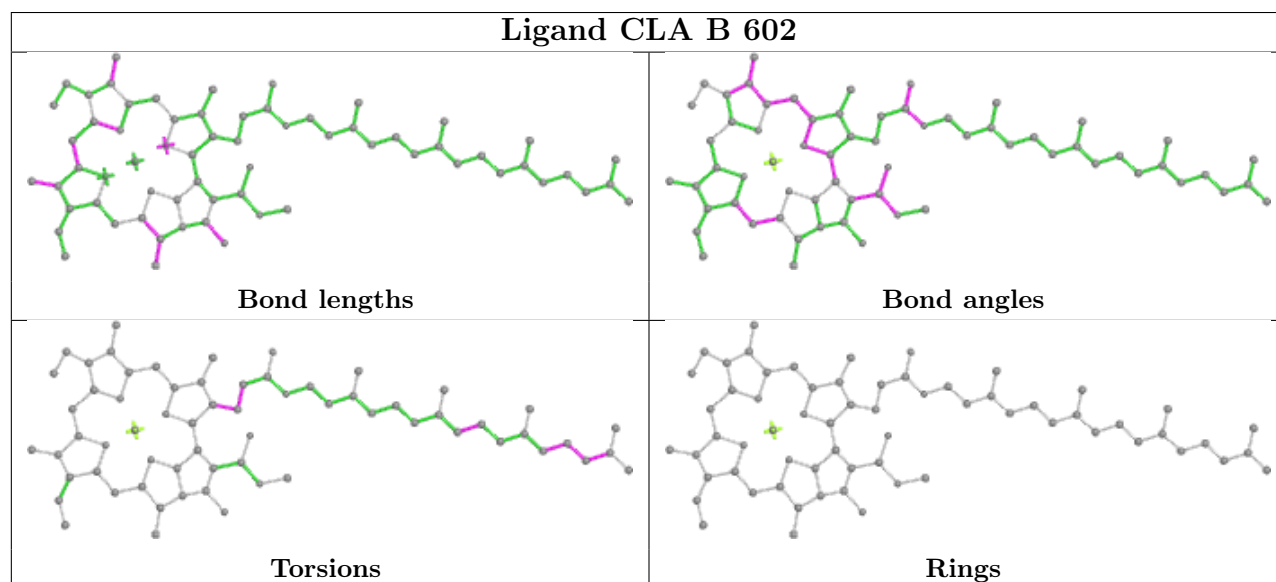
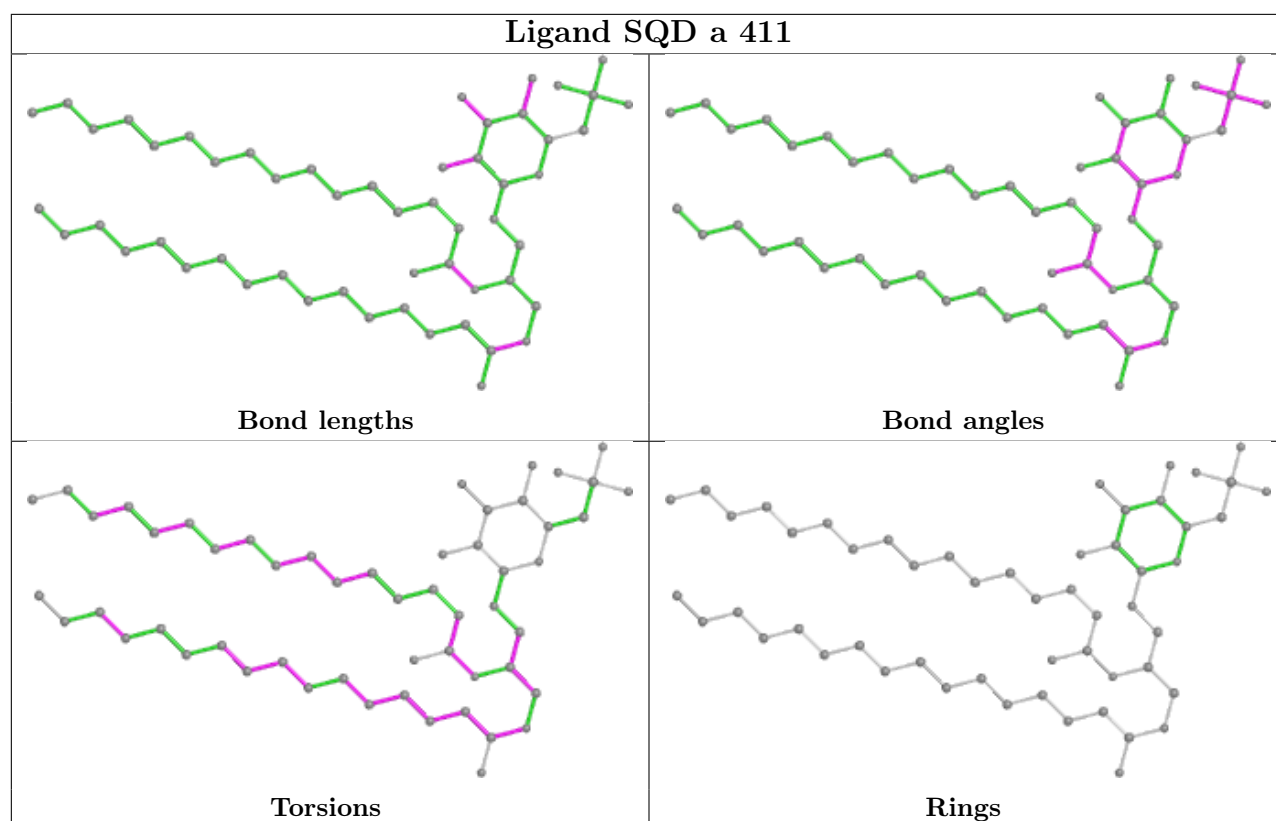
Ligand CLA c 506**Ligand CLA b 610**

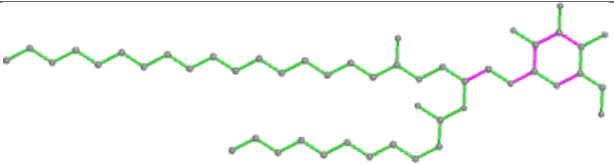
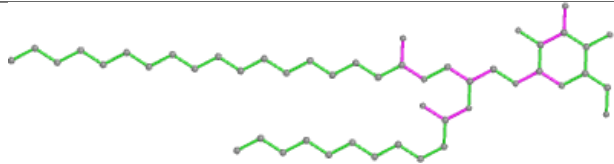
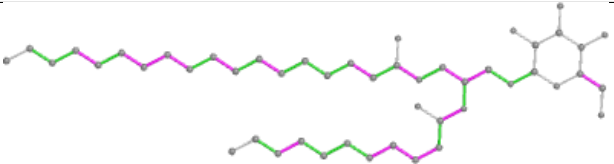

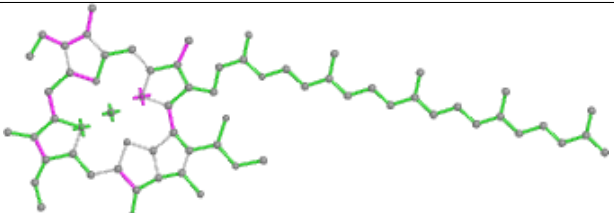
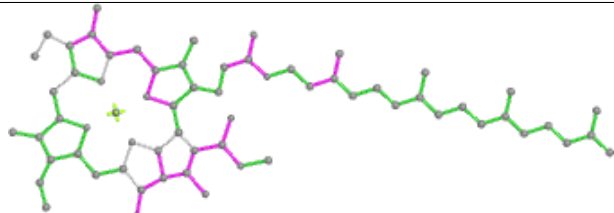
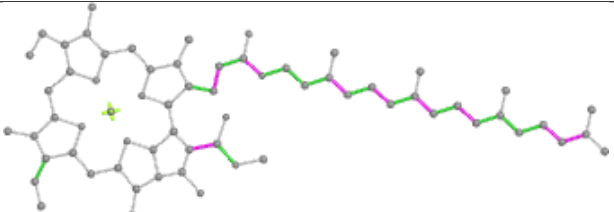
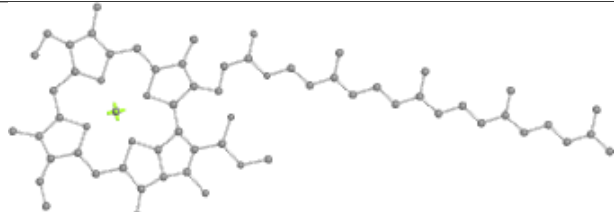
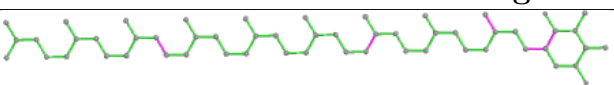
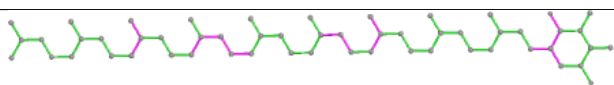
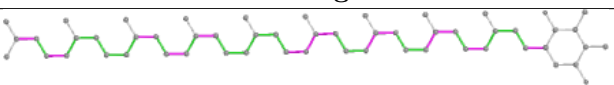
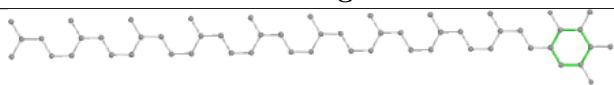


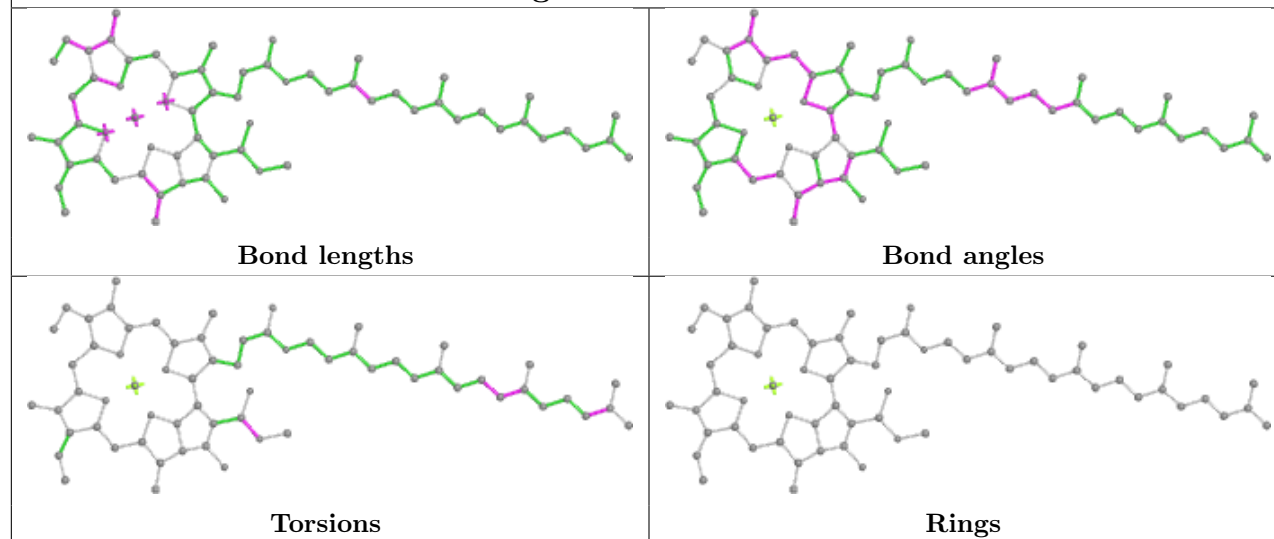
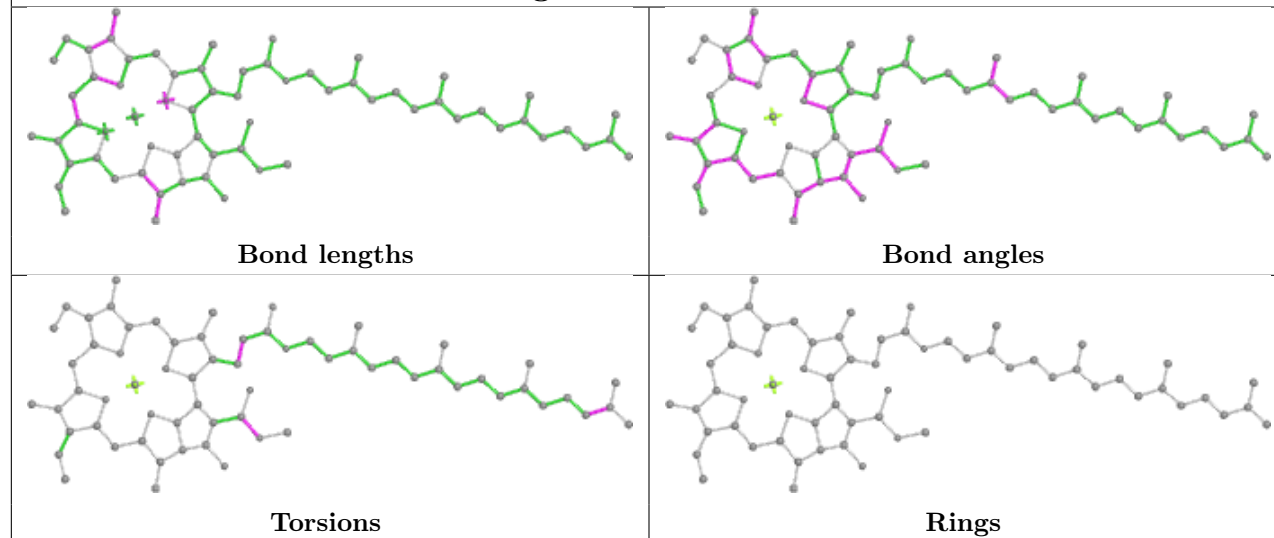


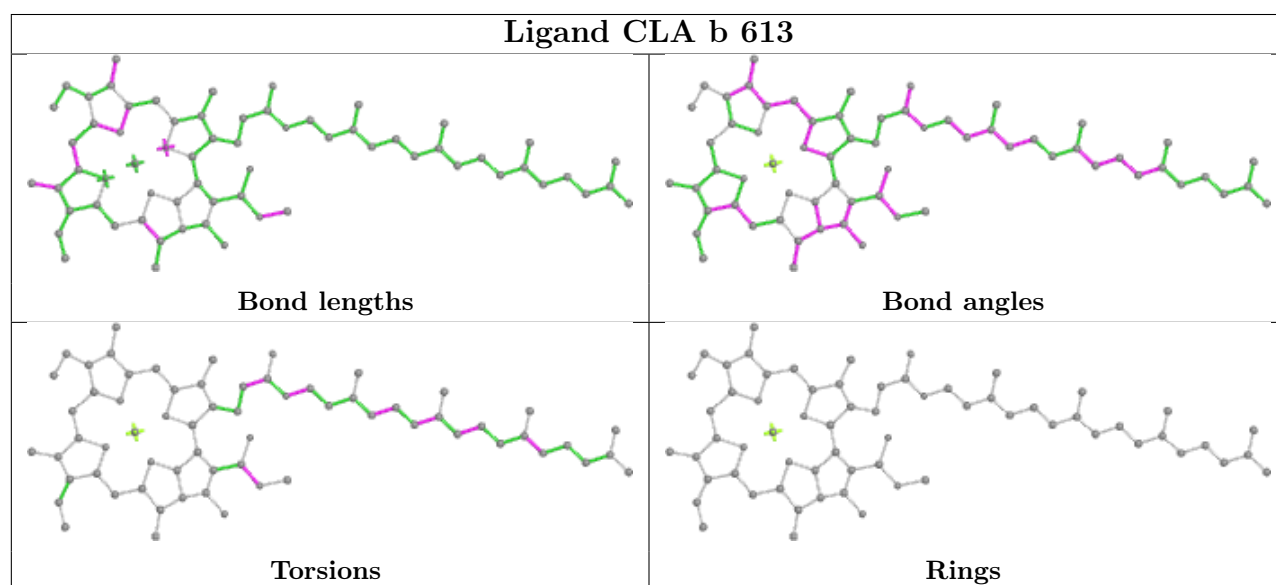
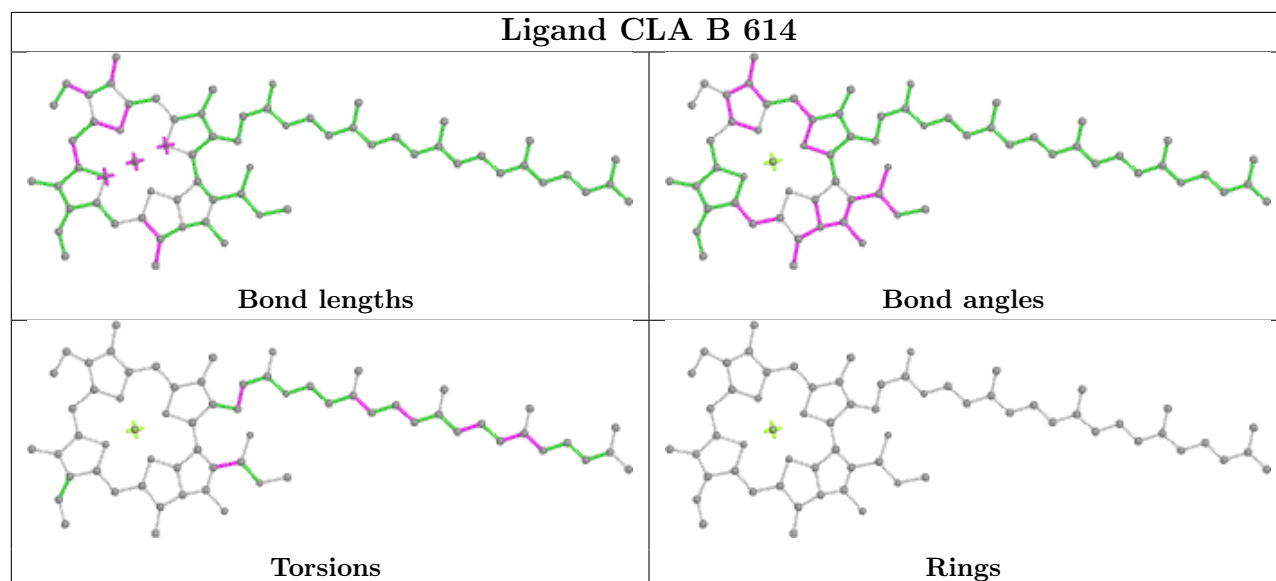
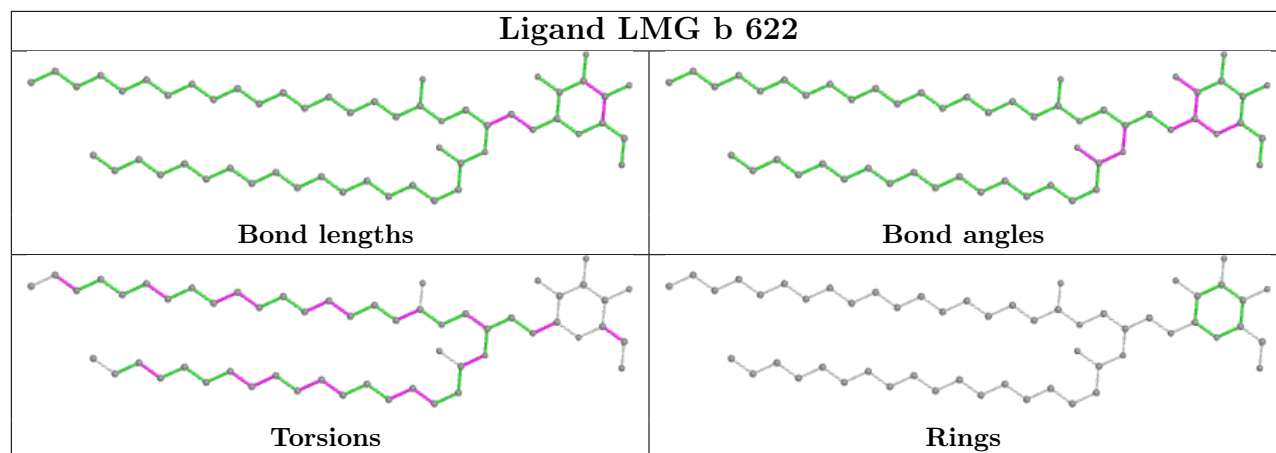




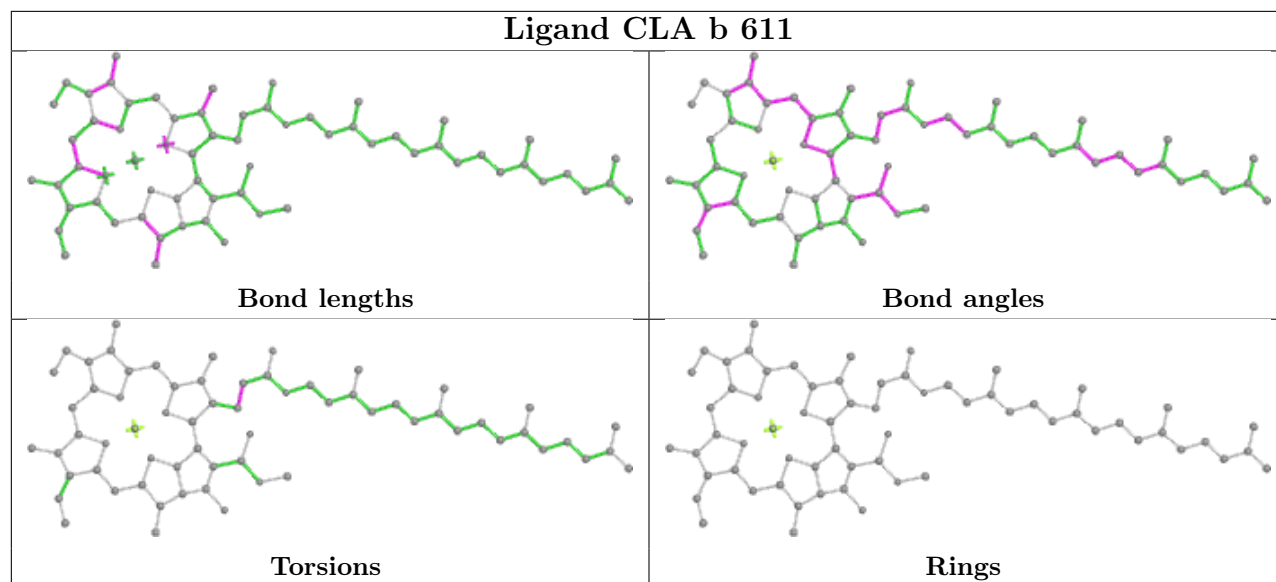


Ligand LMG c 522	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA B 603	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 A 409	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

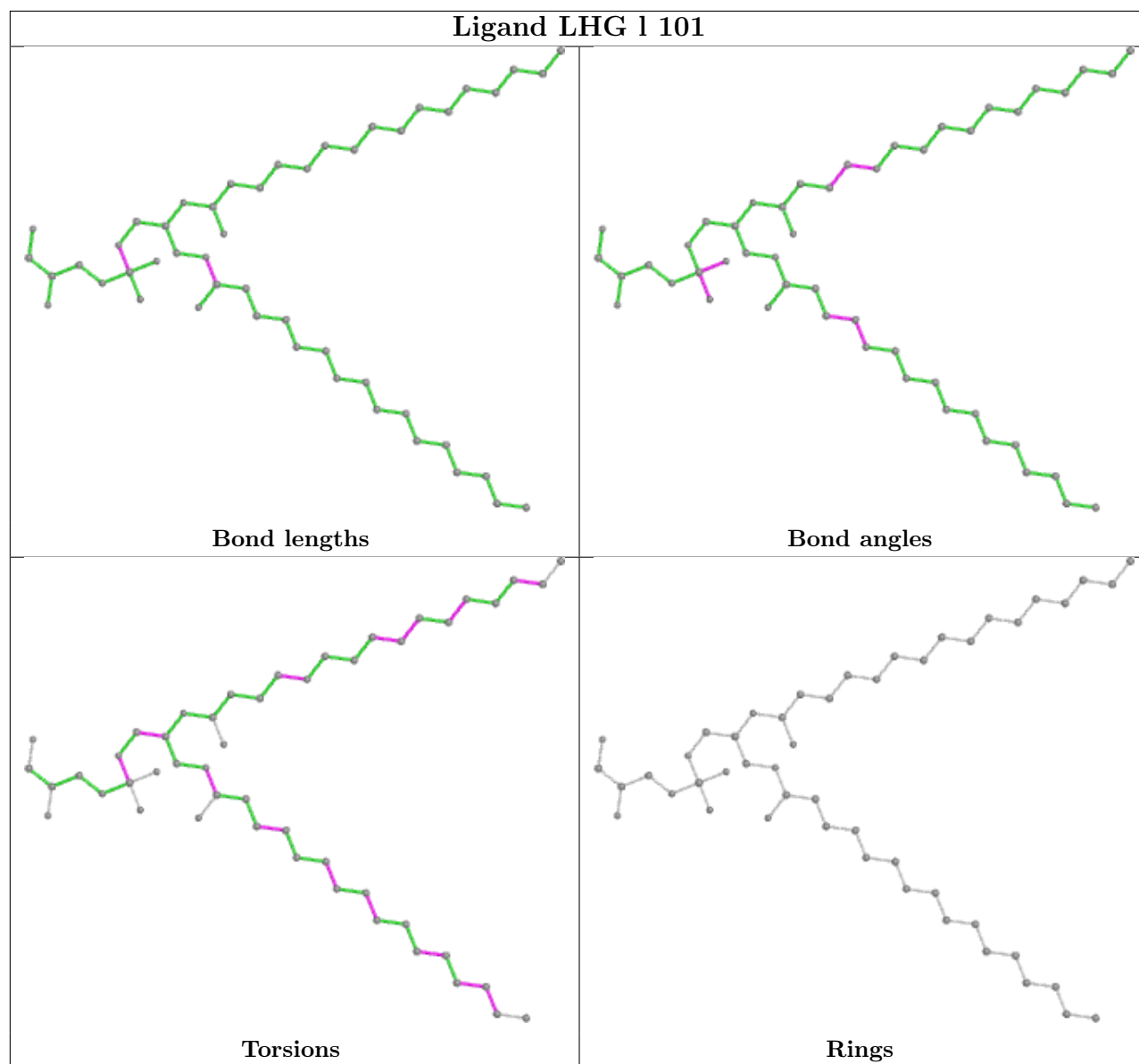
Ligand CLA B 615**Ligand BCR c 515****Ligand CLA C 502**

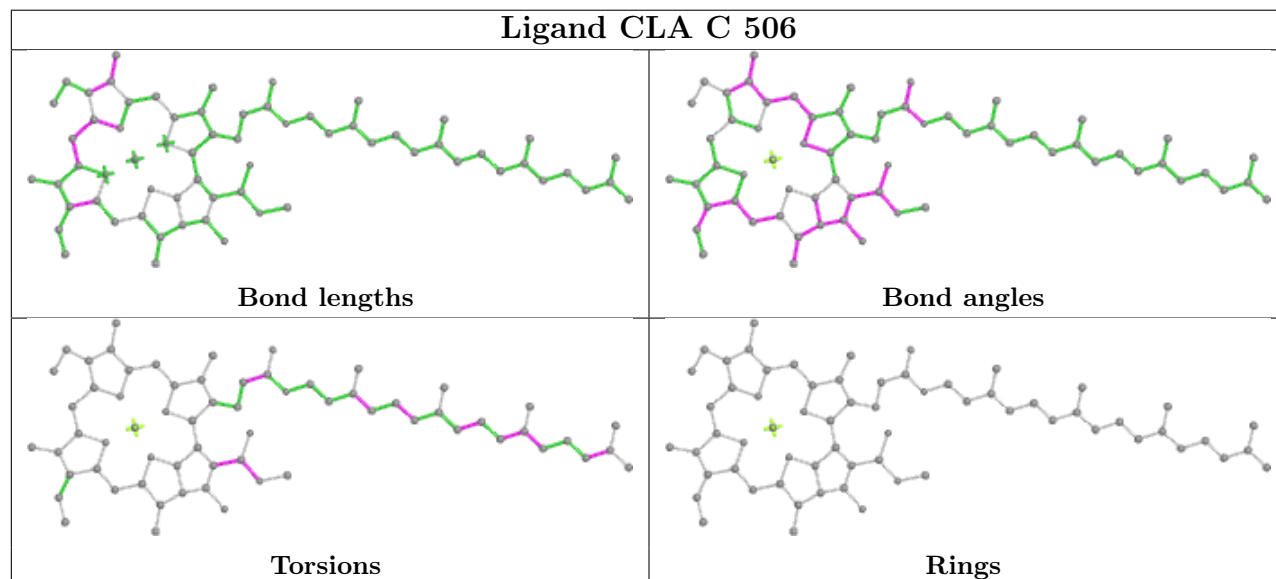
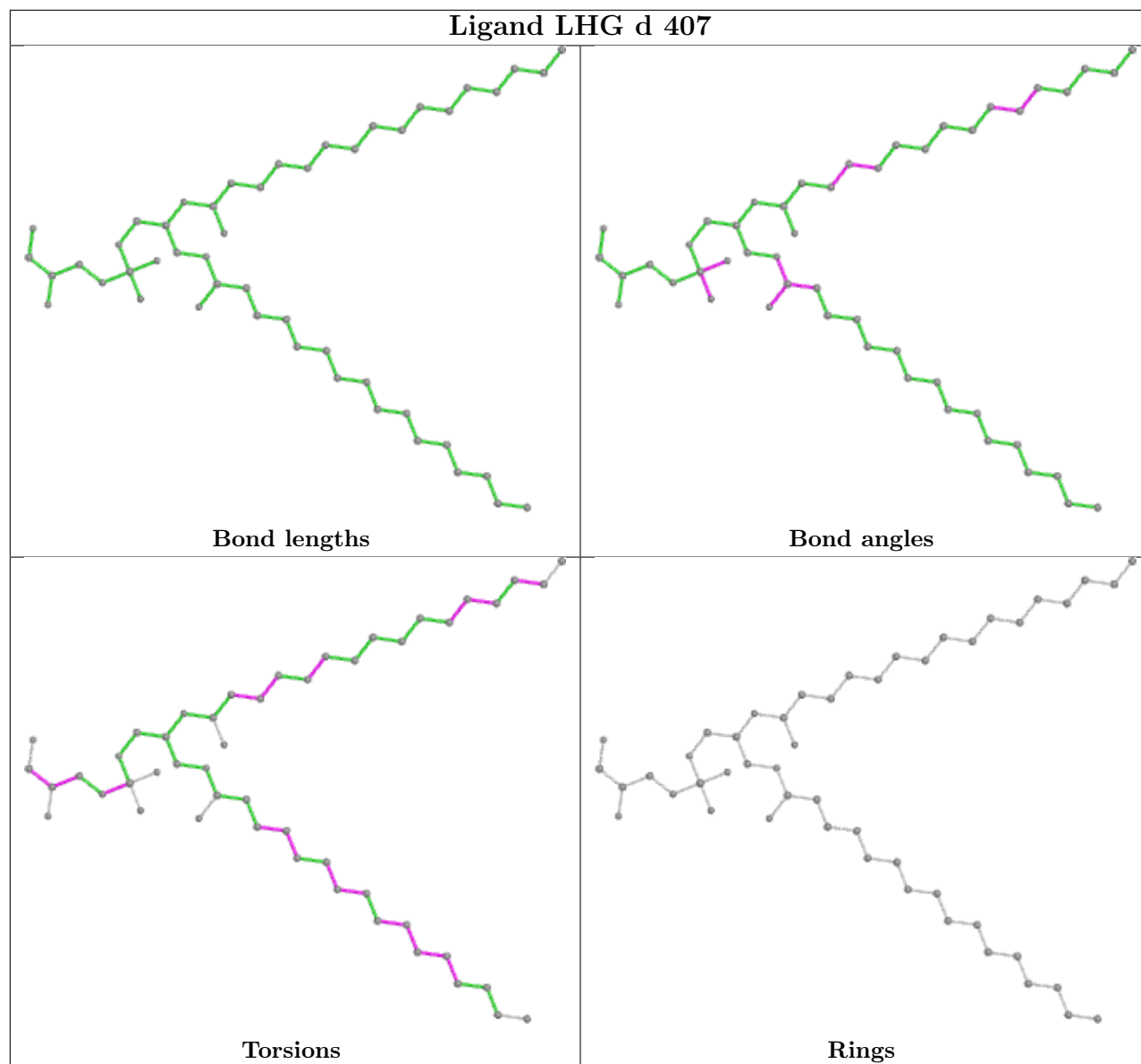


Ligand CLA b 611

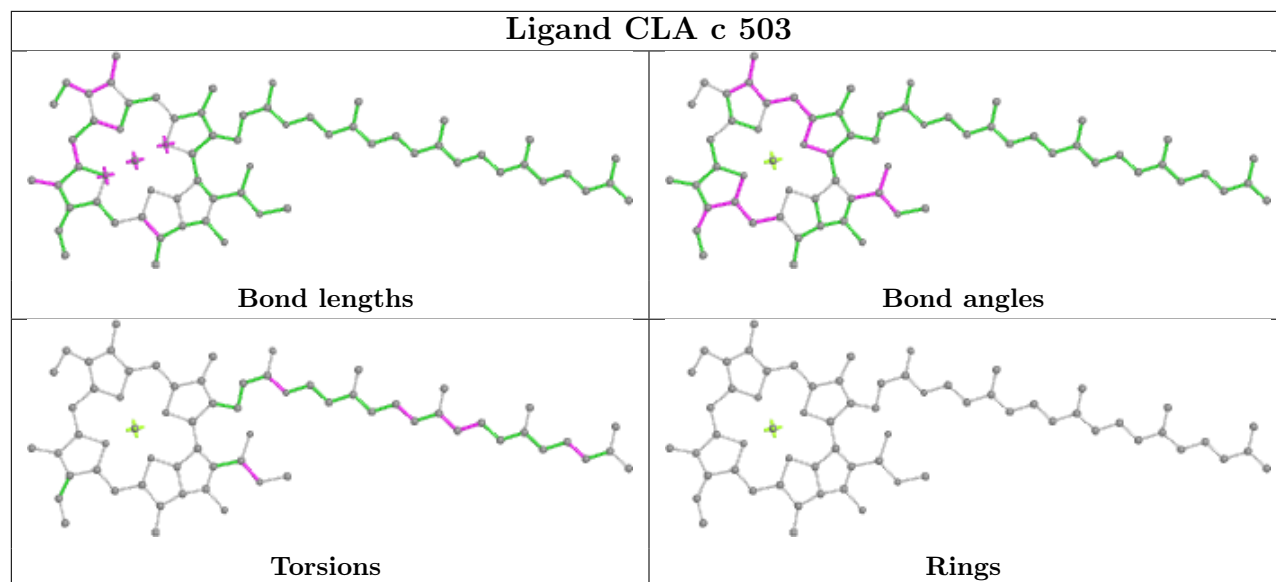


Ligand LHG l 101

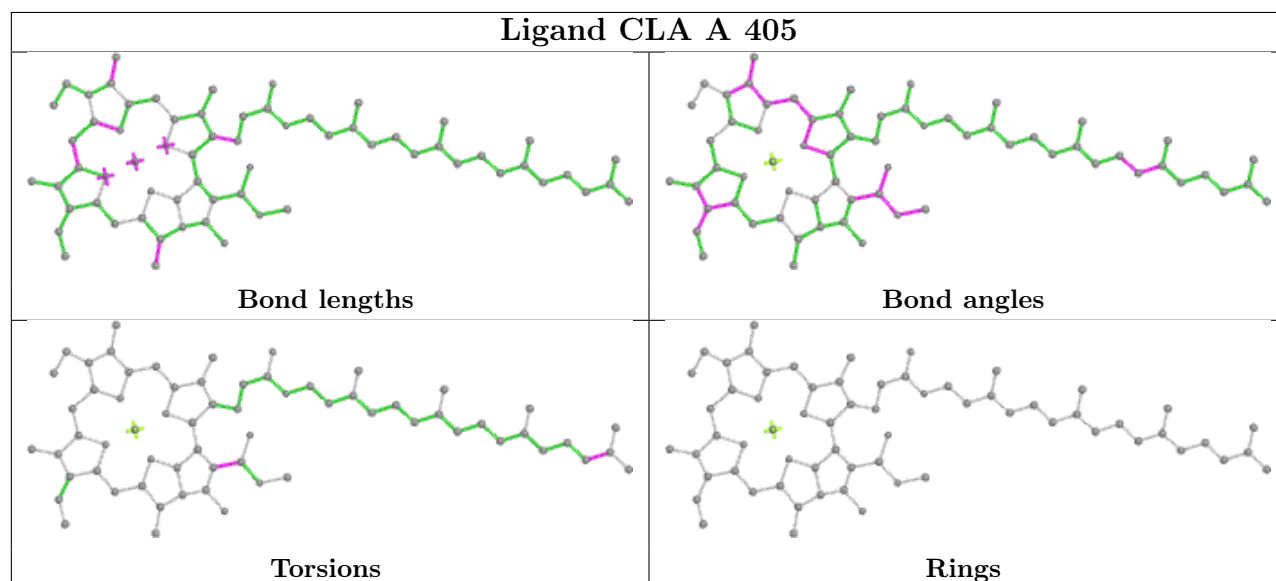




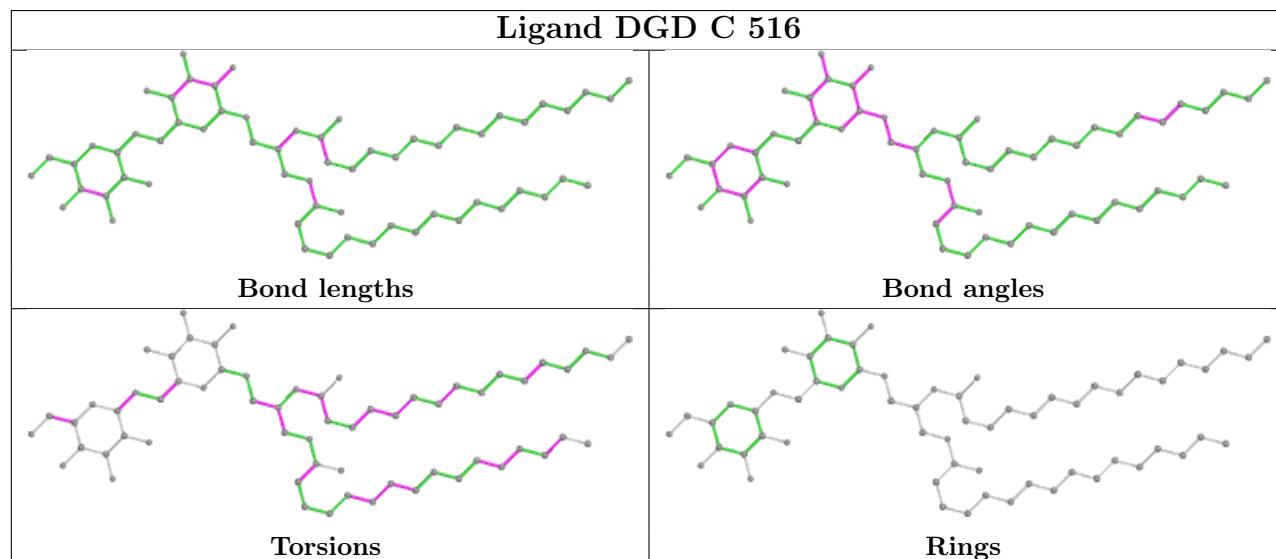
Ligand CLA c 503

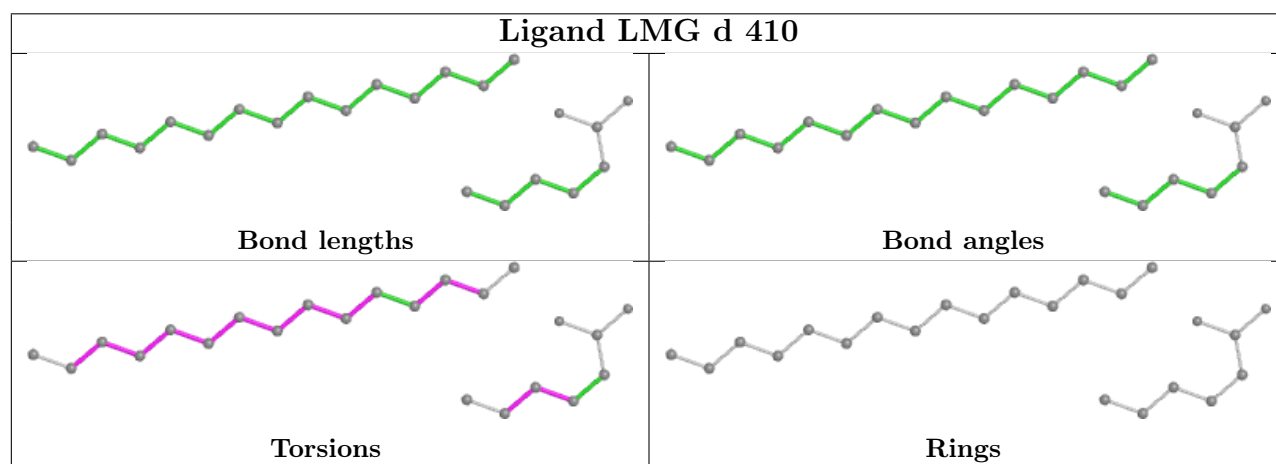
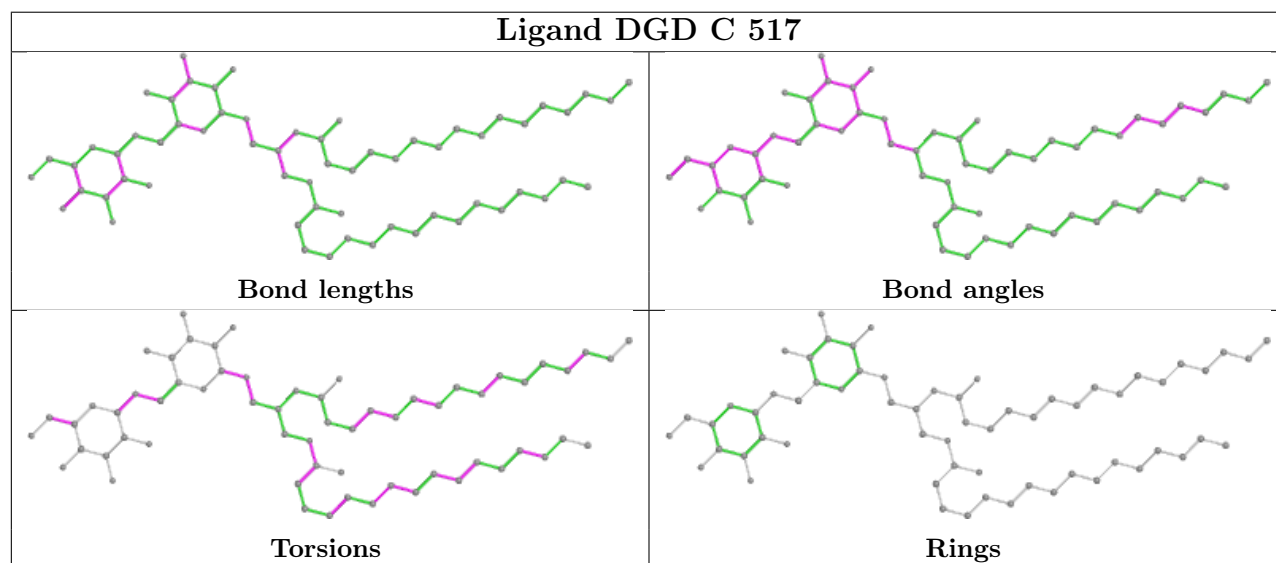
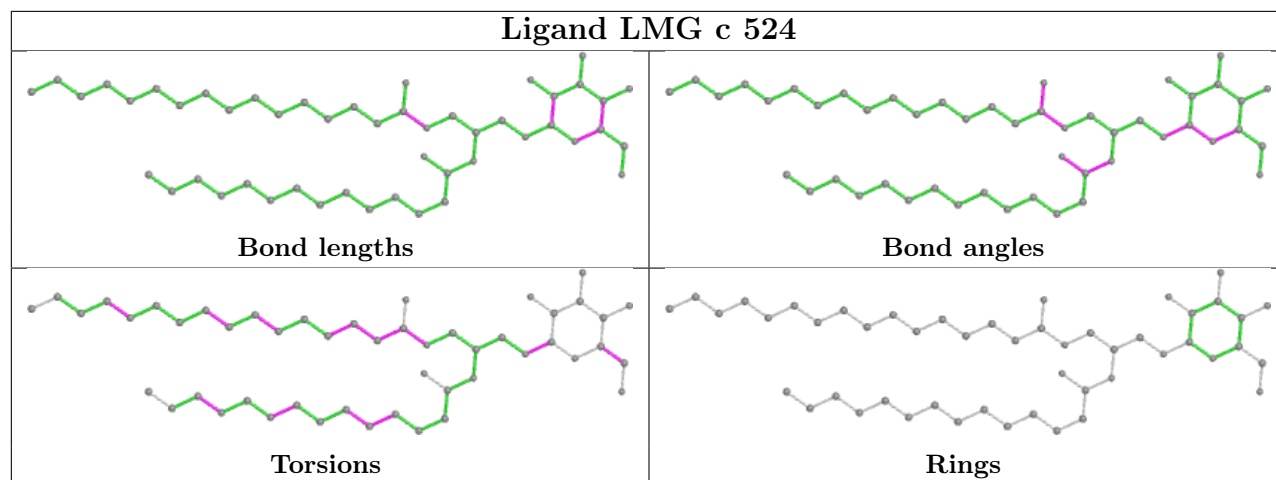


Ligand CLA A 405

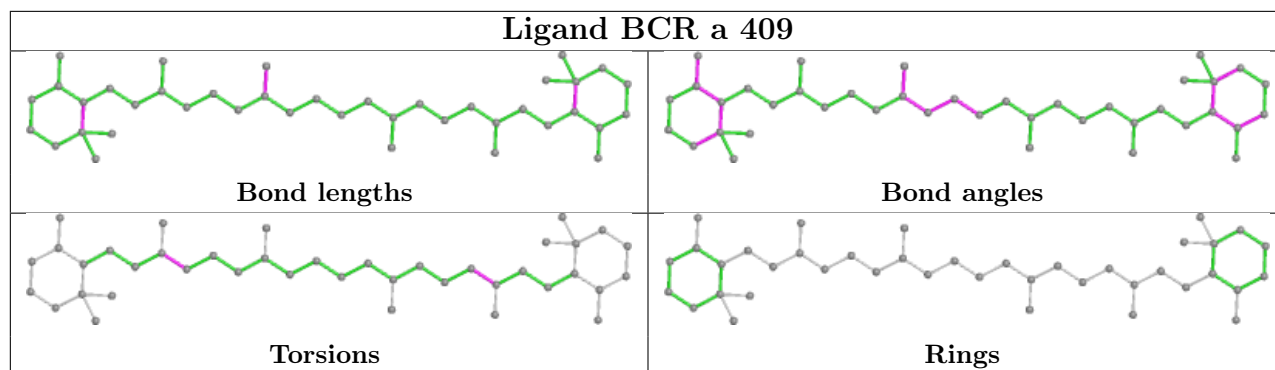


Ligand DGD C 516

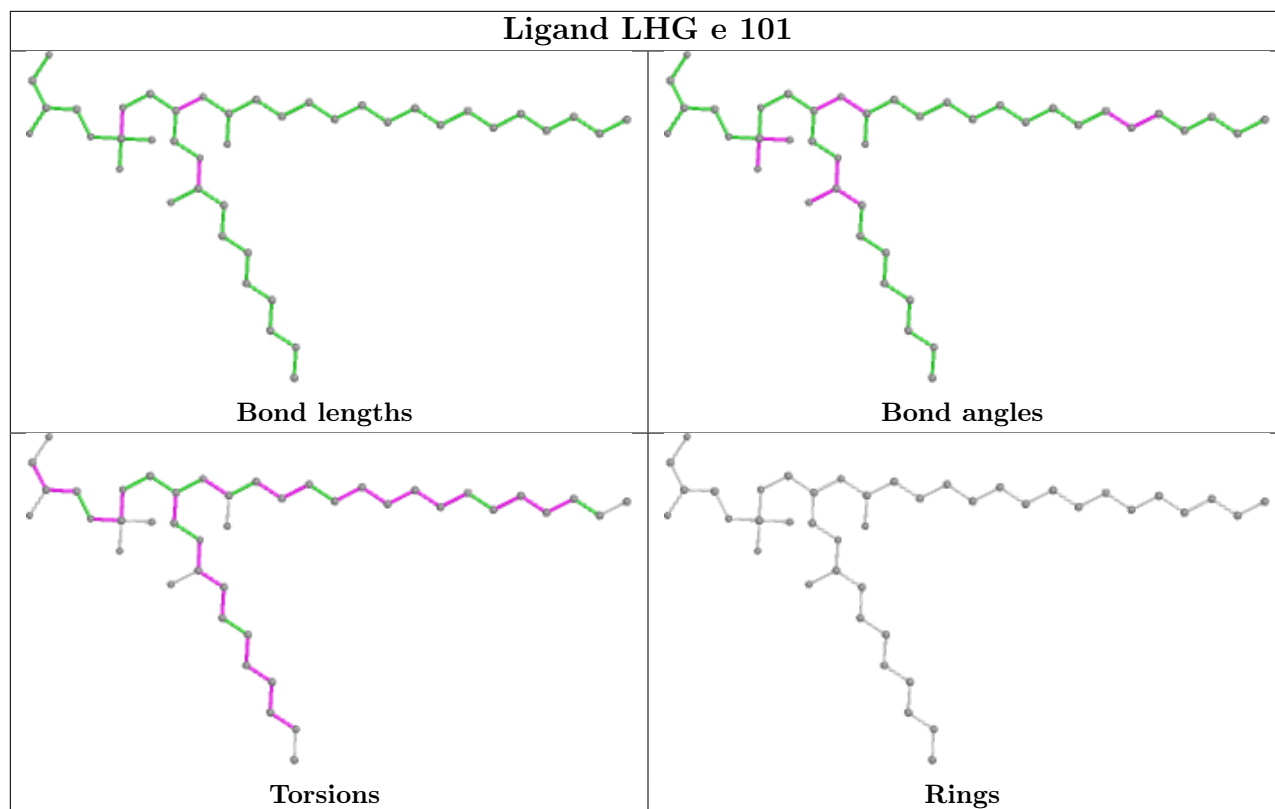




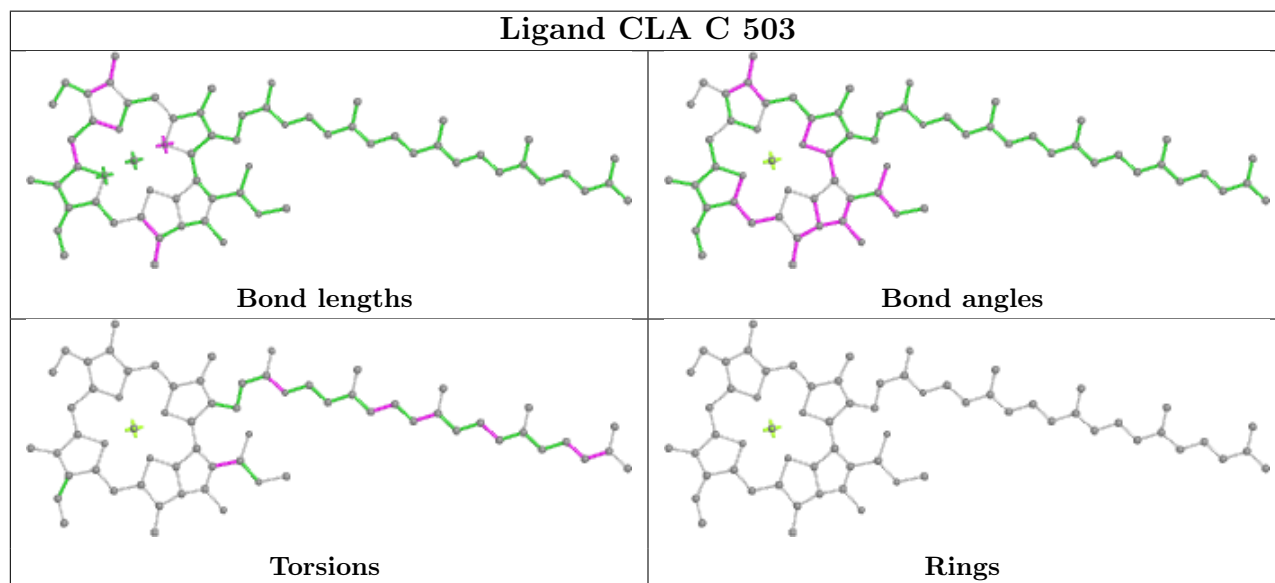
Ligand BCR a 409



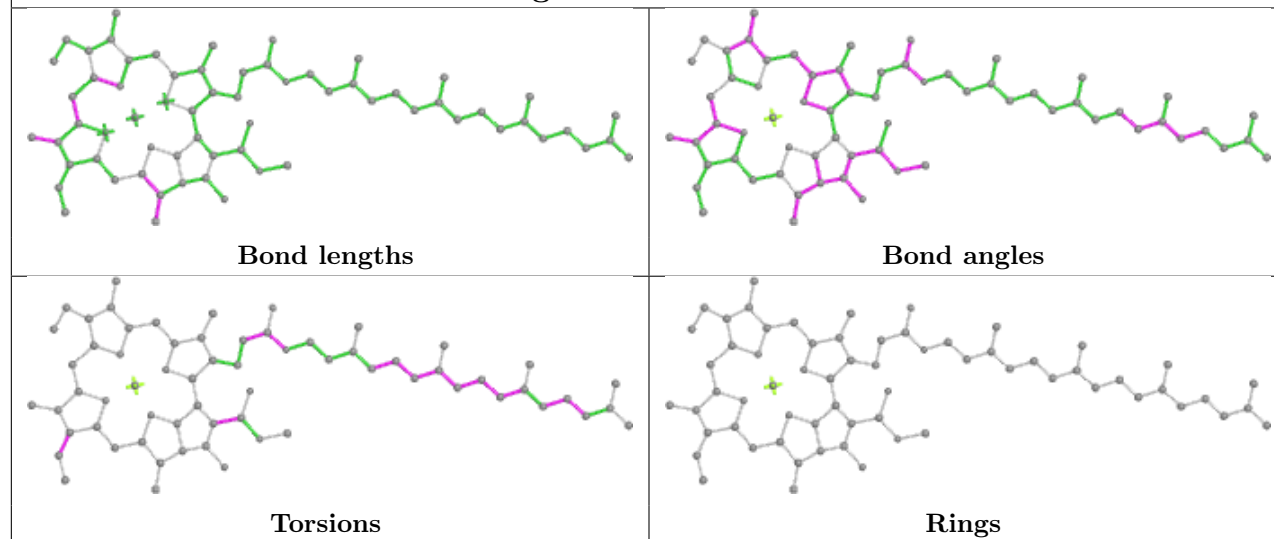
Ligand LHG e 101



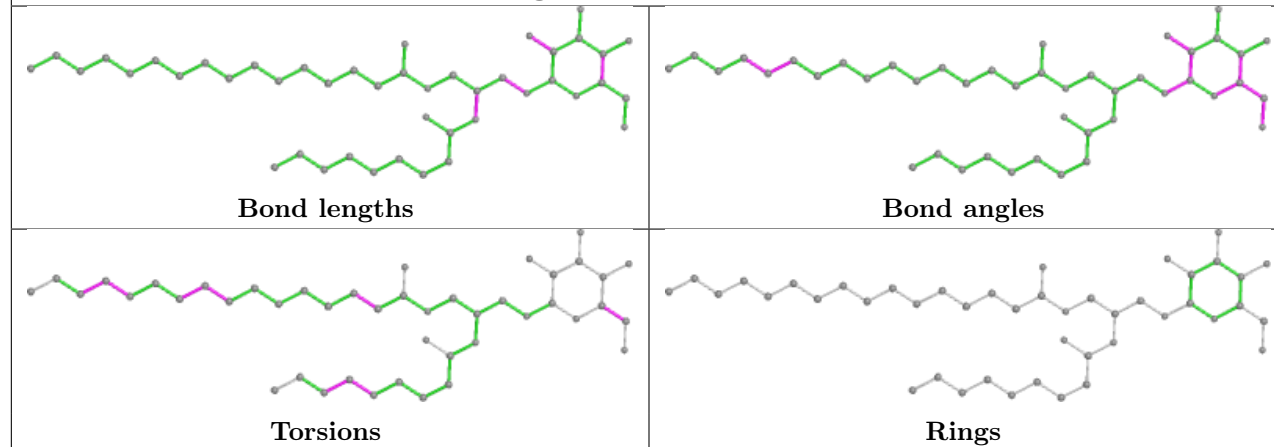
Ligand CLA C 503



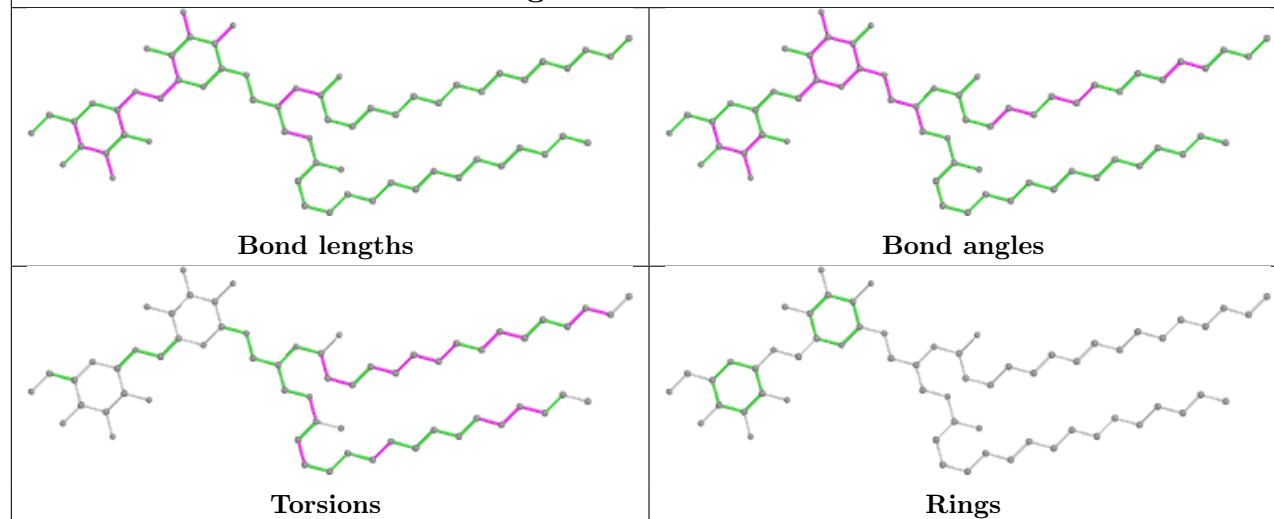
Ligand CLA B 612



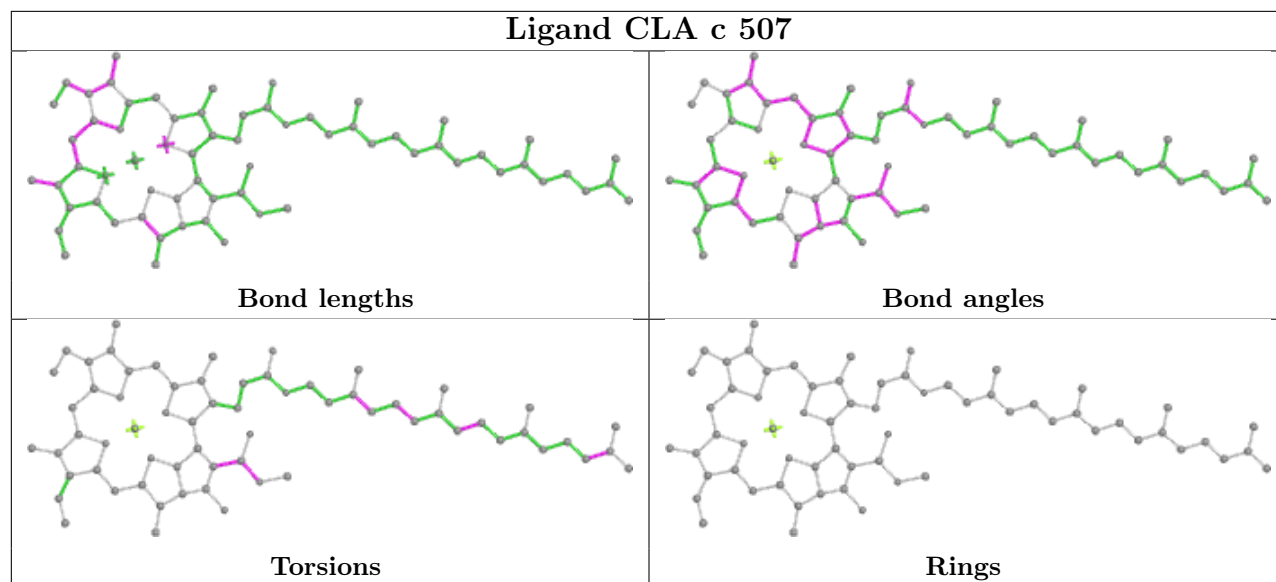
Ligand LMG d 411



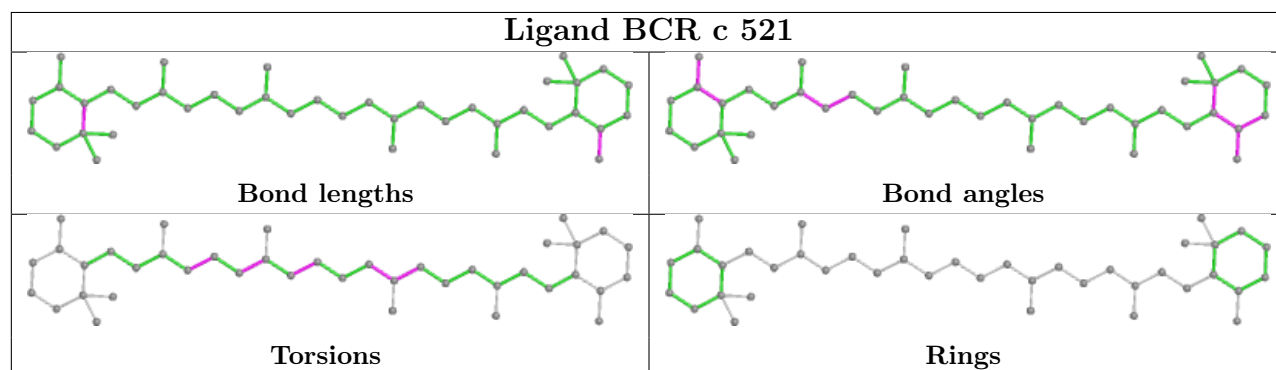
Ligand DGD H 102



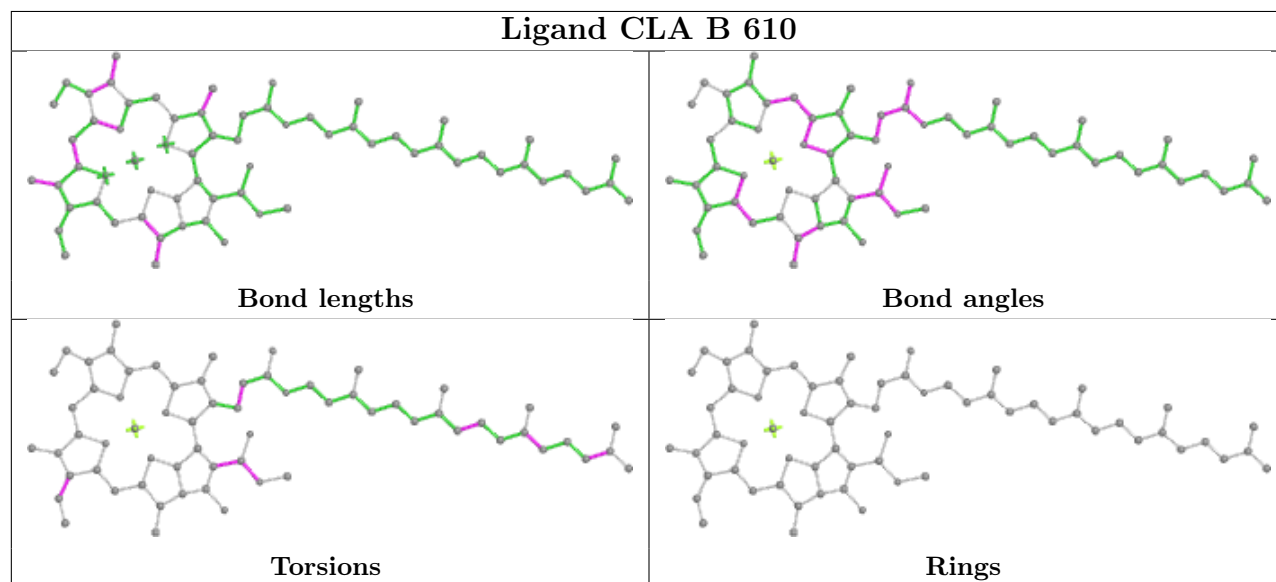
Ligand CLA c 507

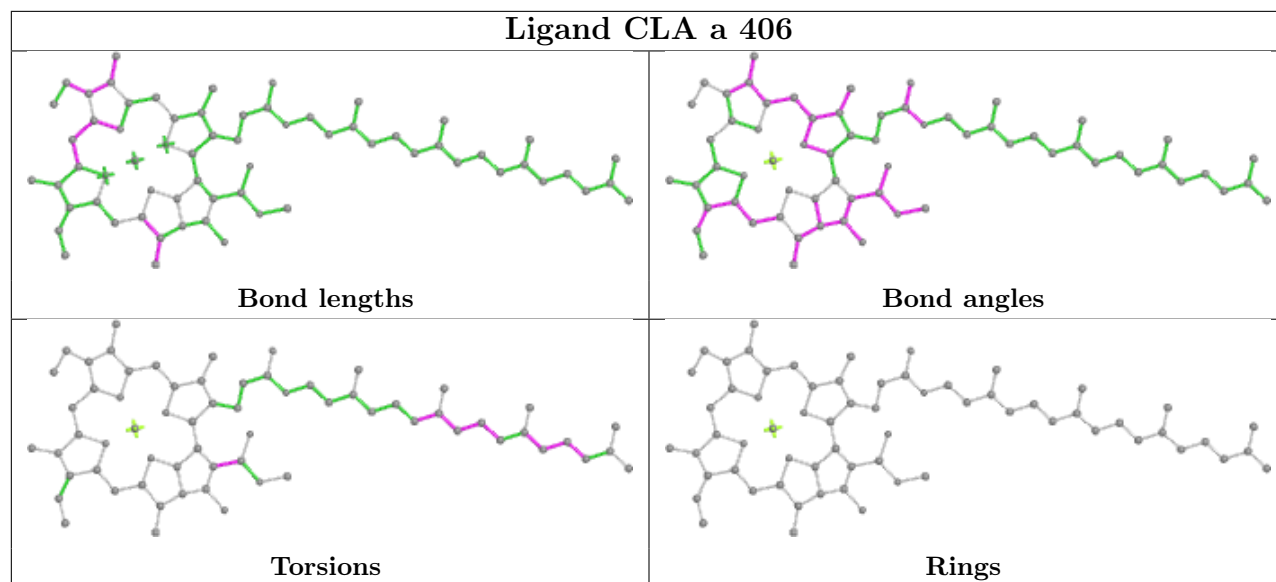
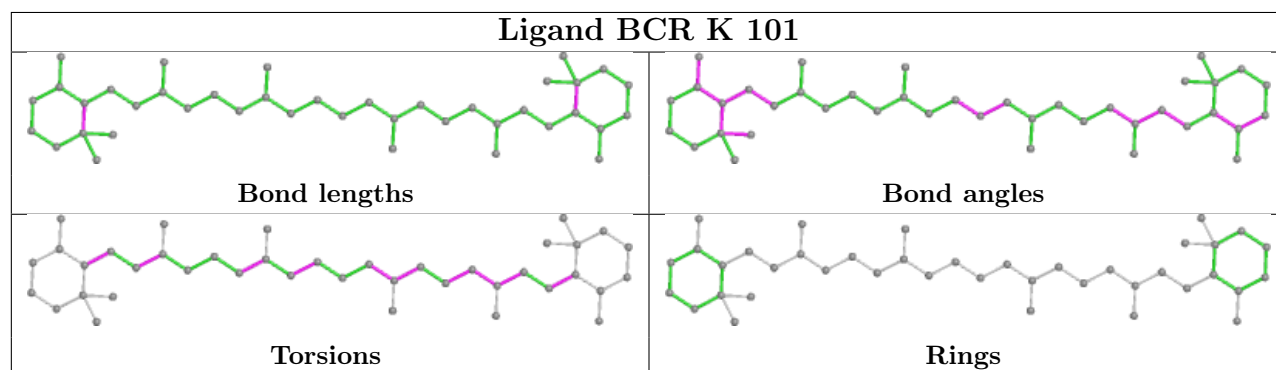
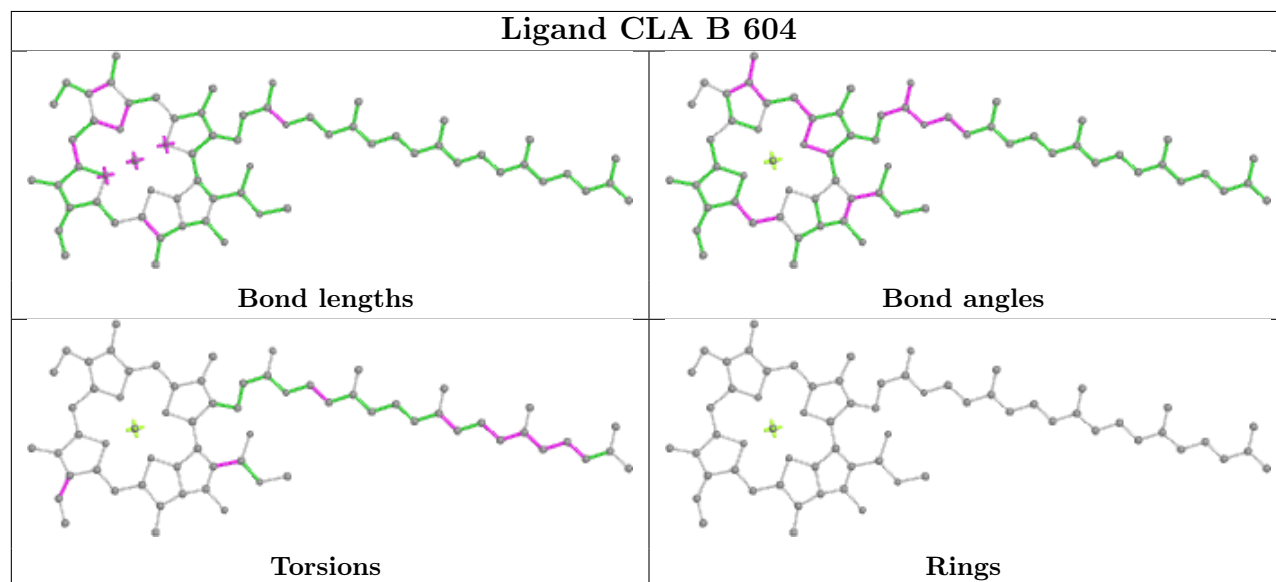


Ligand BCR c 521

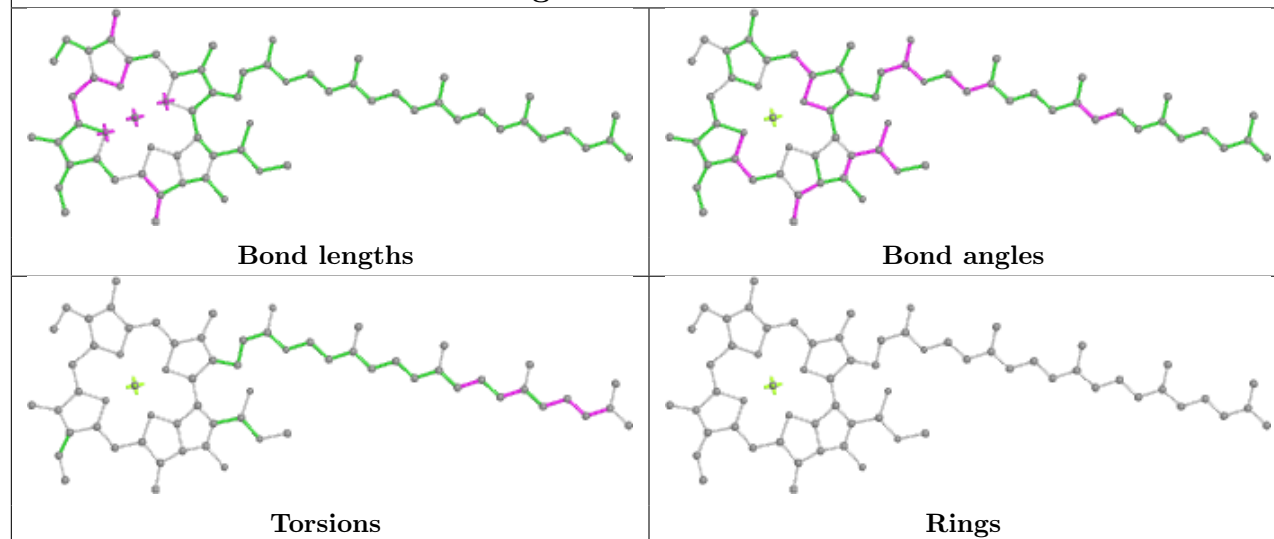


Ligand CLA B 610

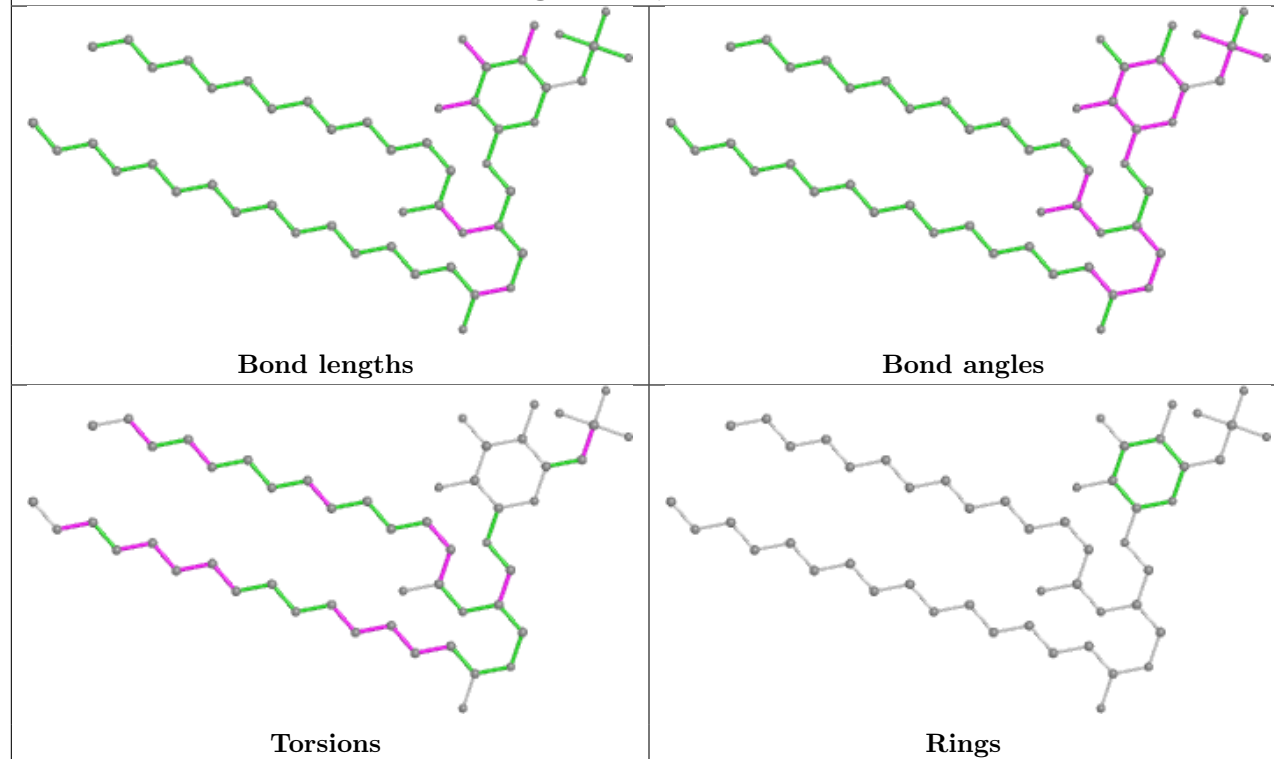


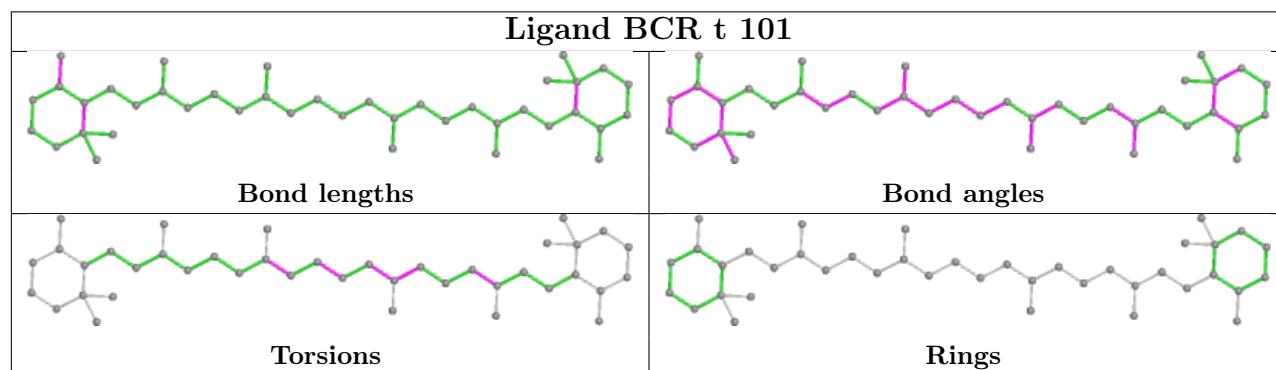
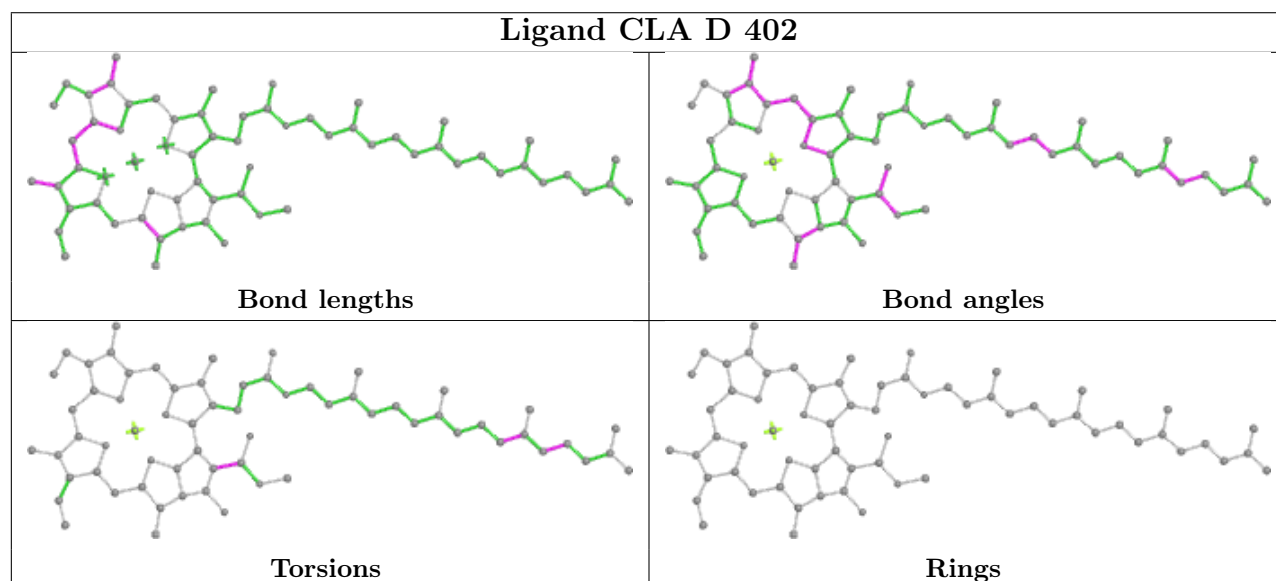
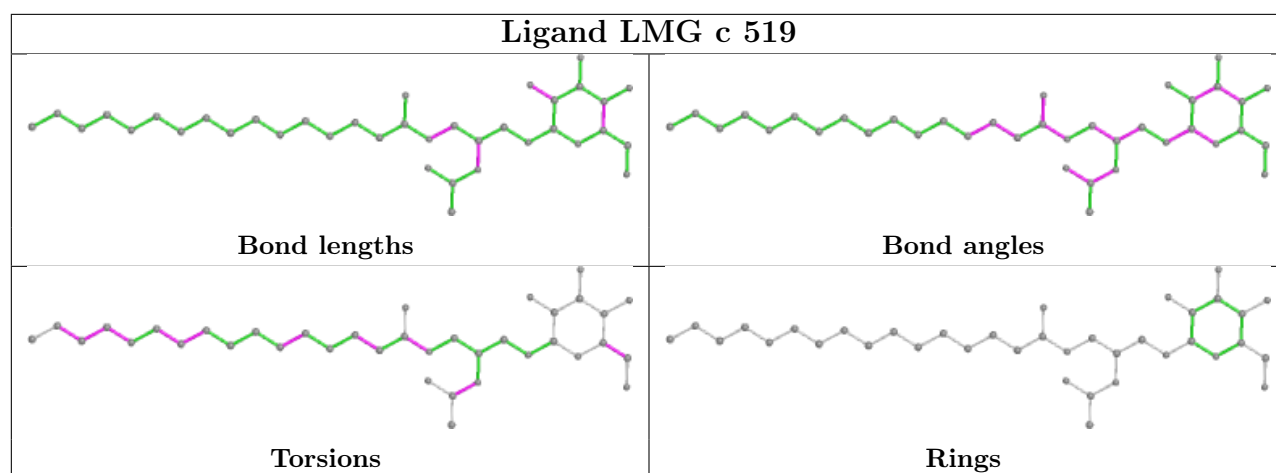
Ligand CLA a 406**Ligand BCR K 101****Ligand CLA B 604**

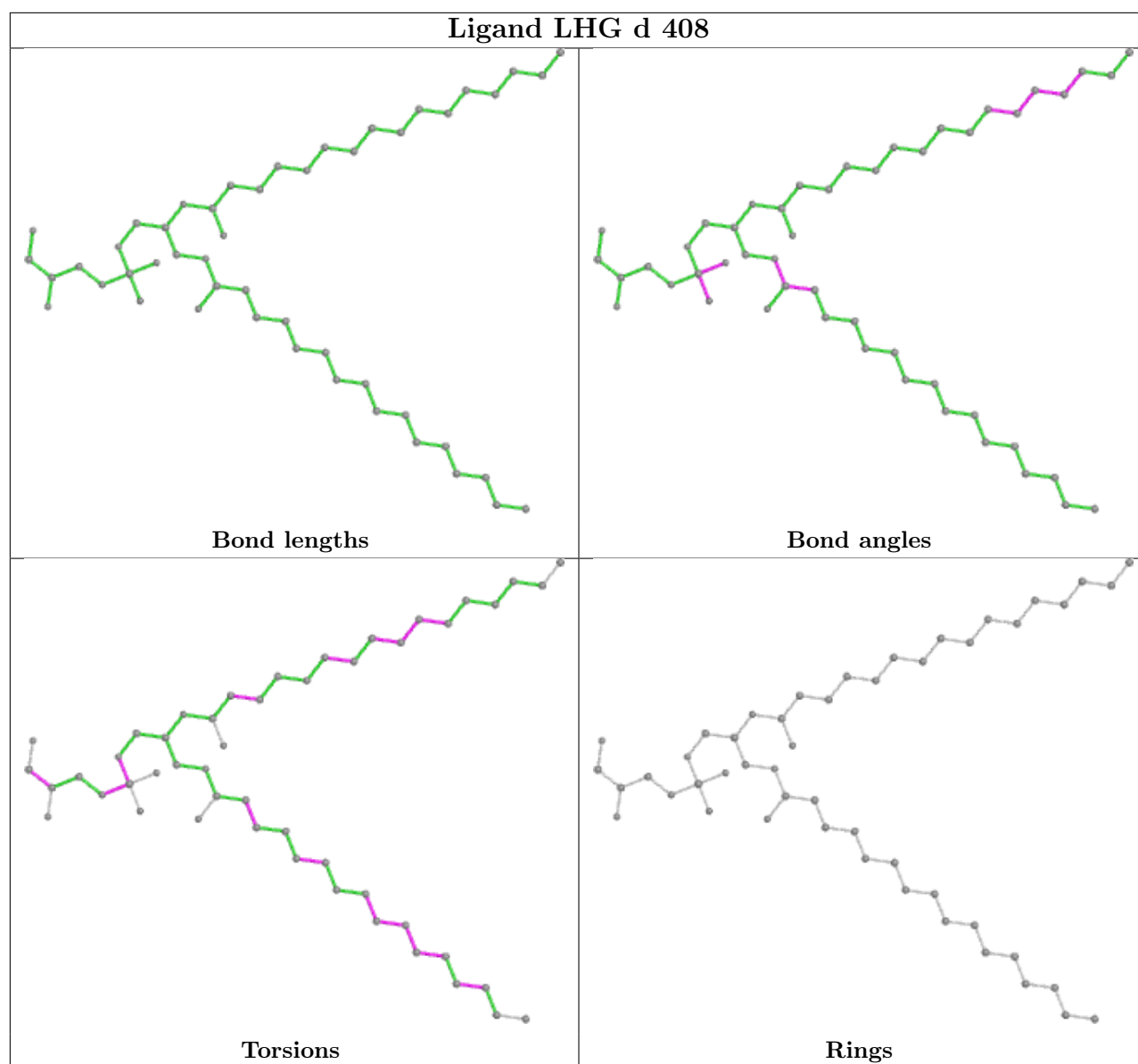
Ligand CLA B 611

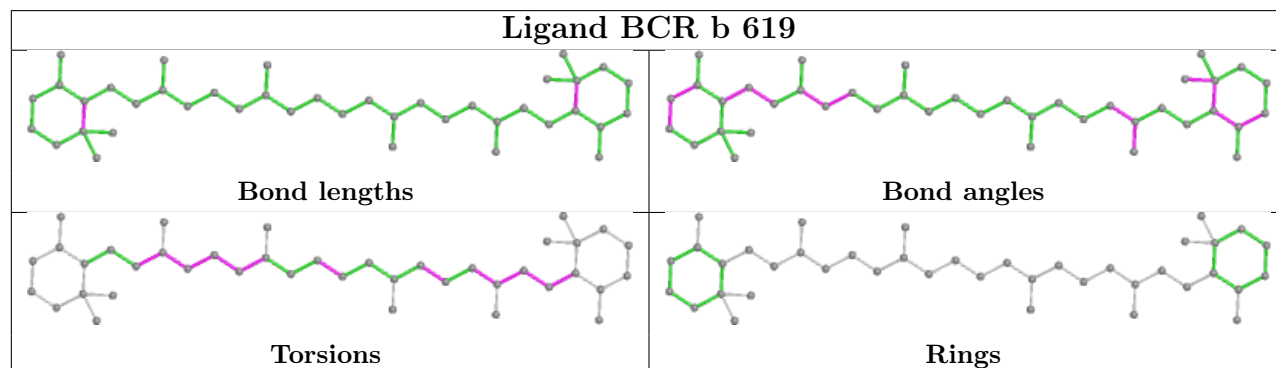
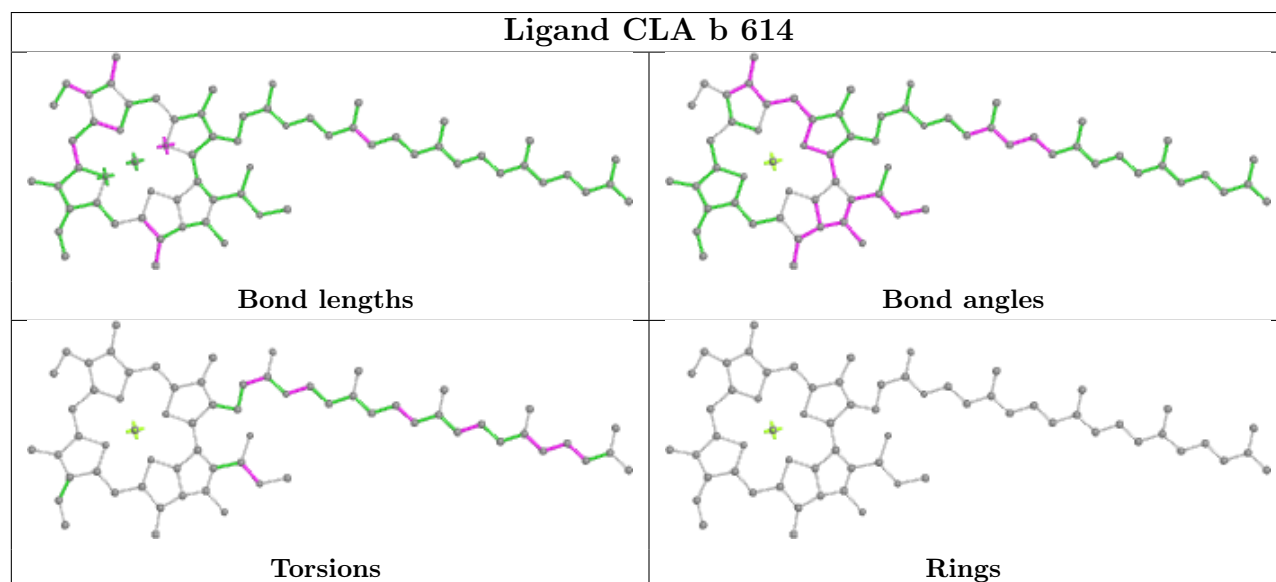
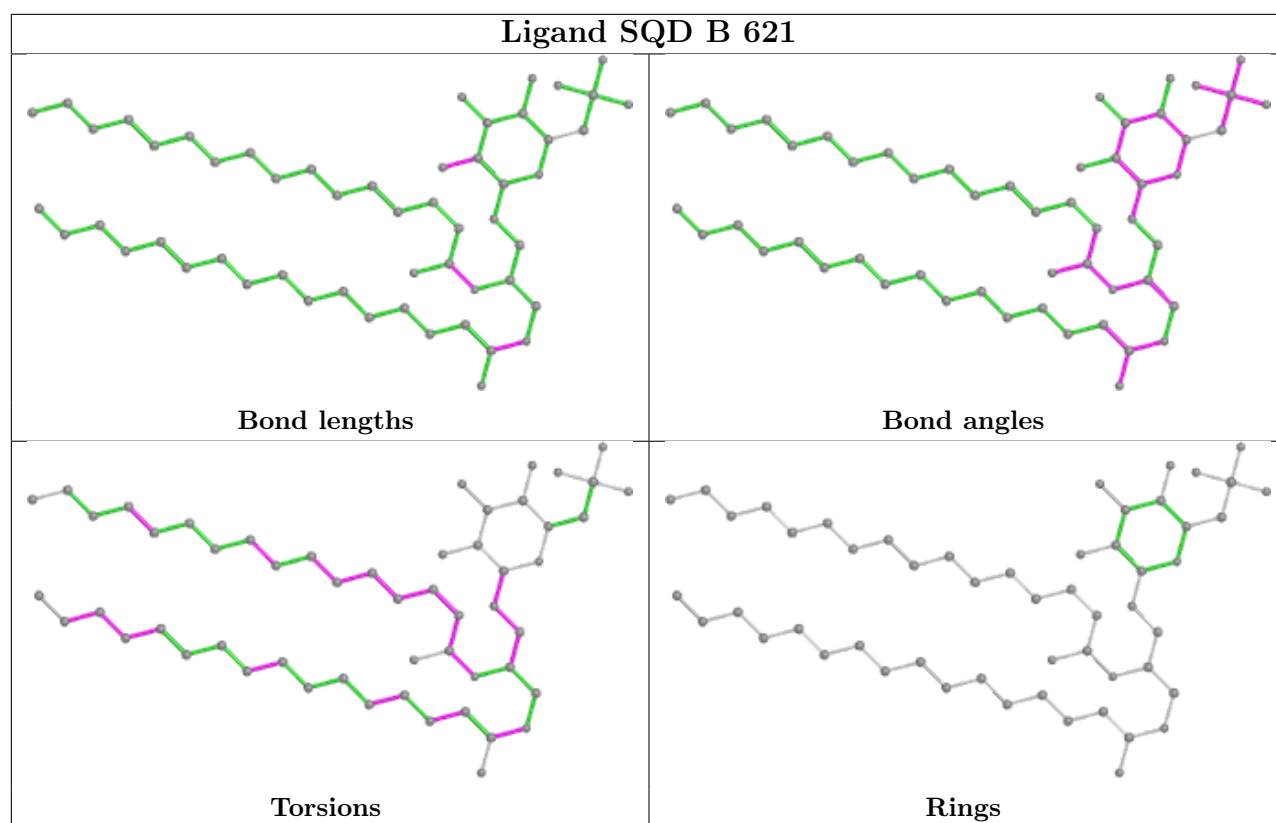


Ligand SQD A 410

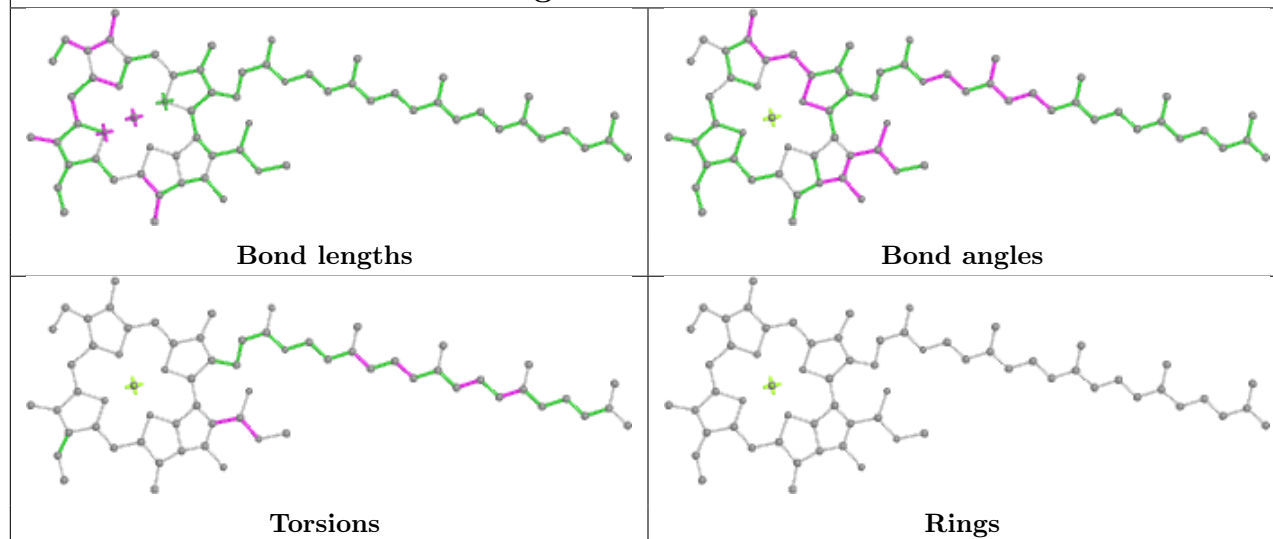




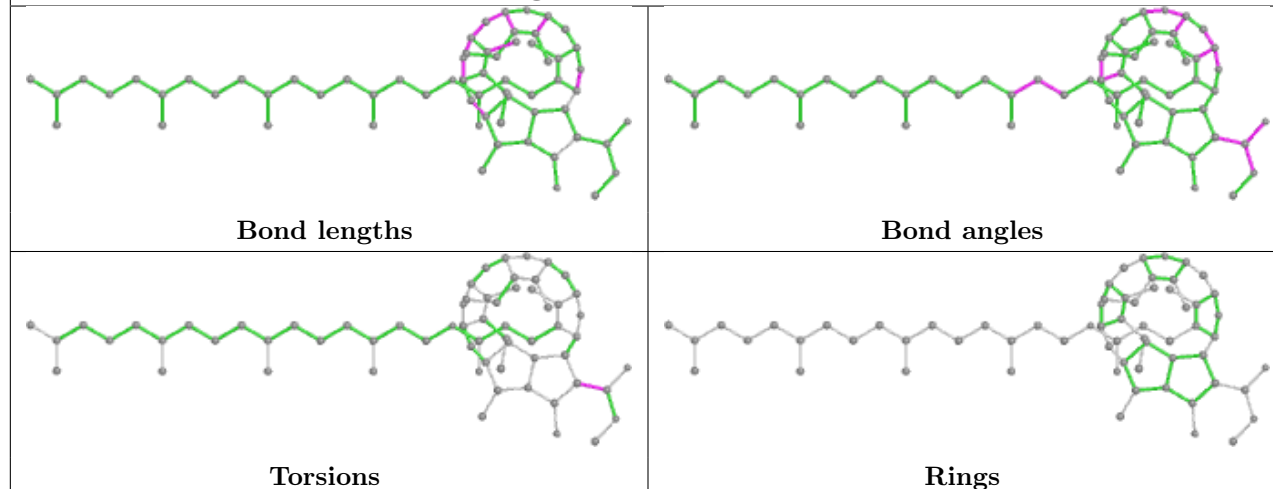




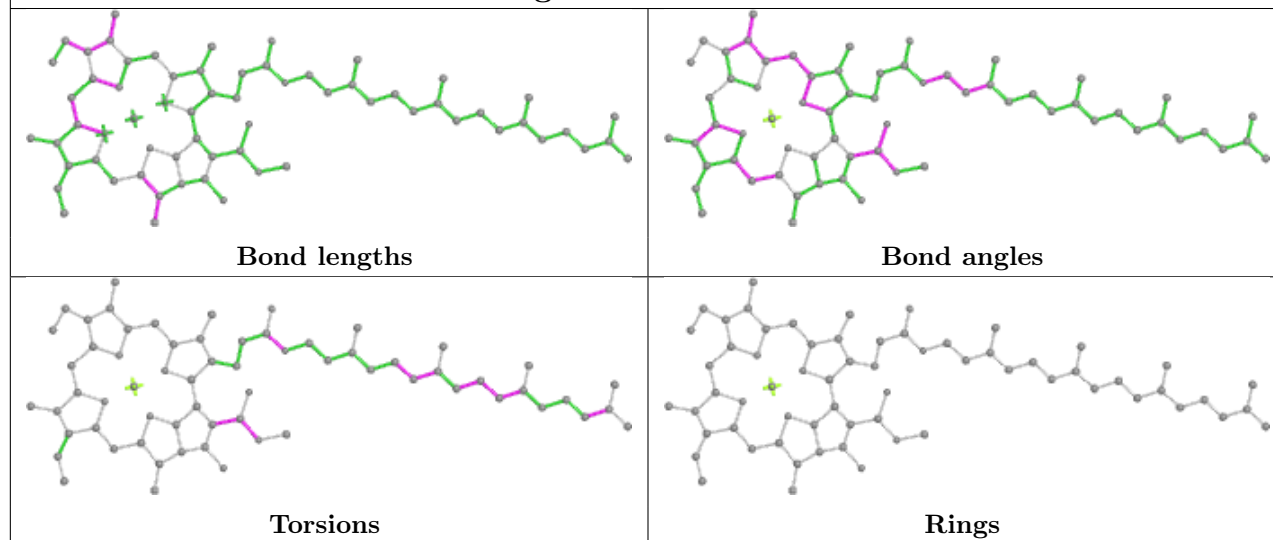
Ligand CLA b 604



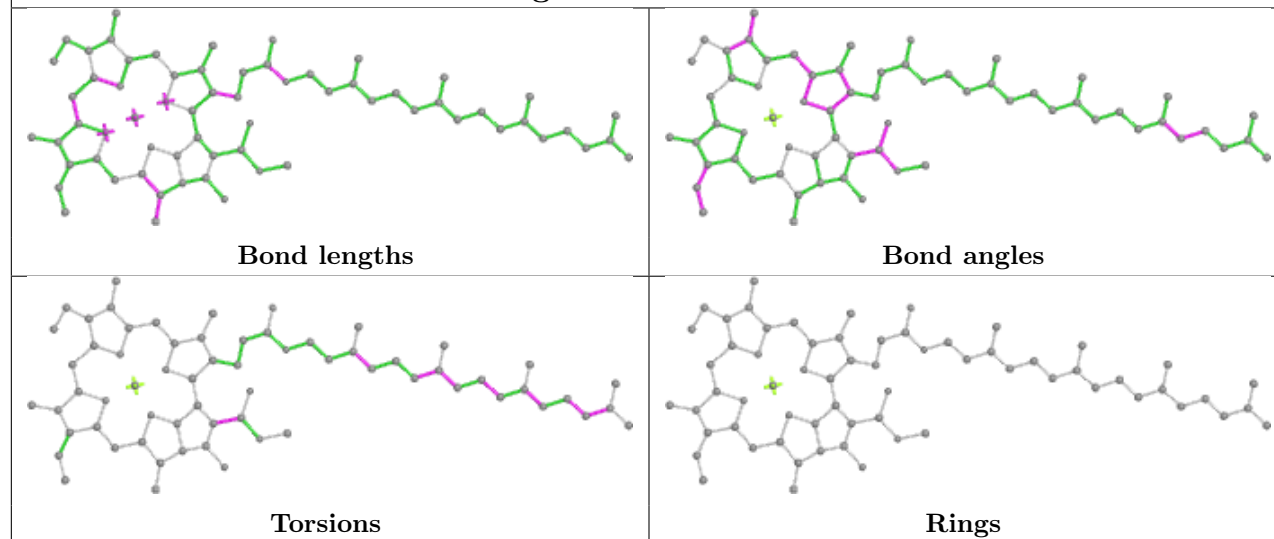
Ligand PHO D 401



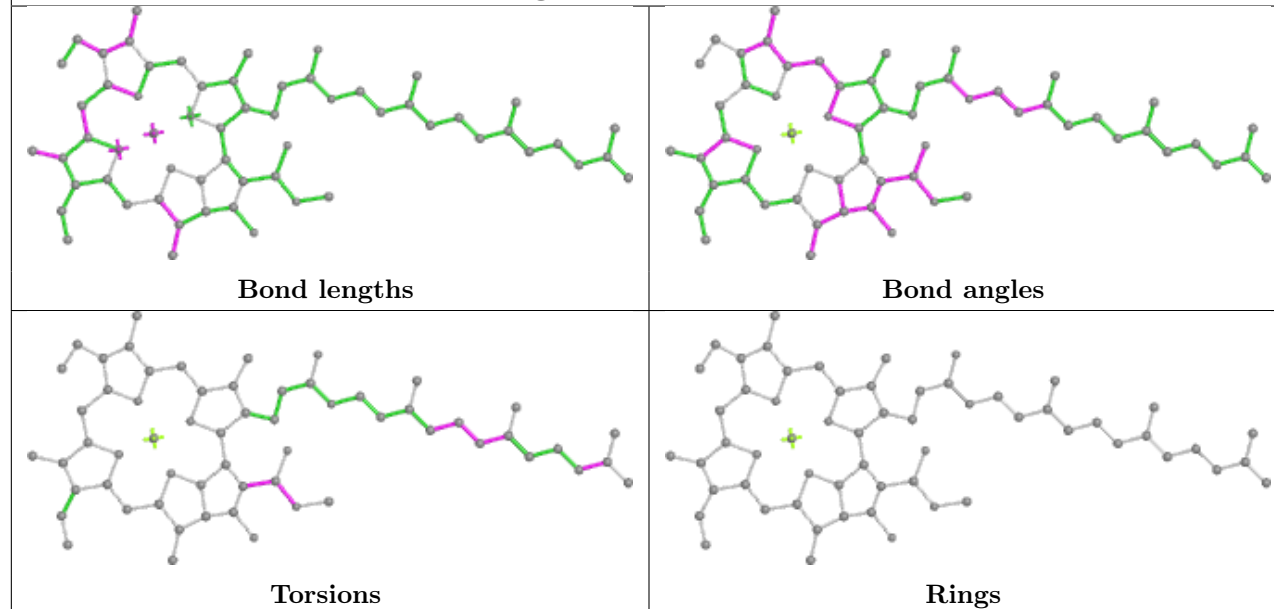
Ligand CLA b 608



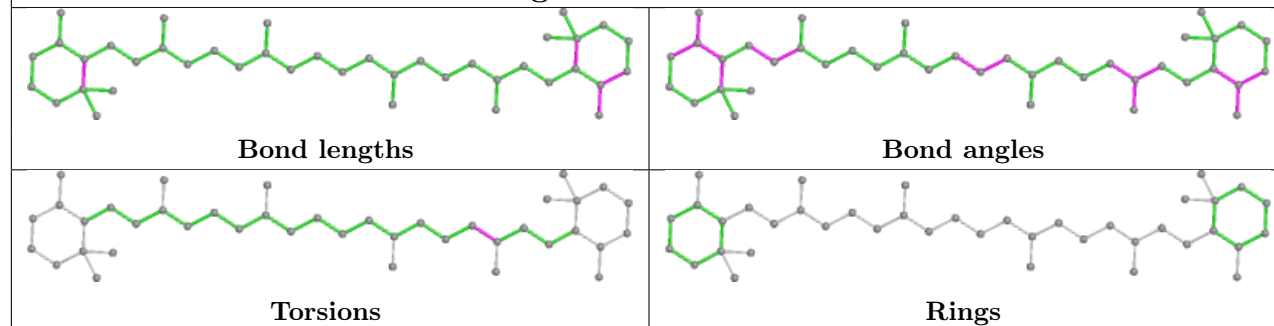
Ligand CLA C 511



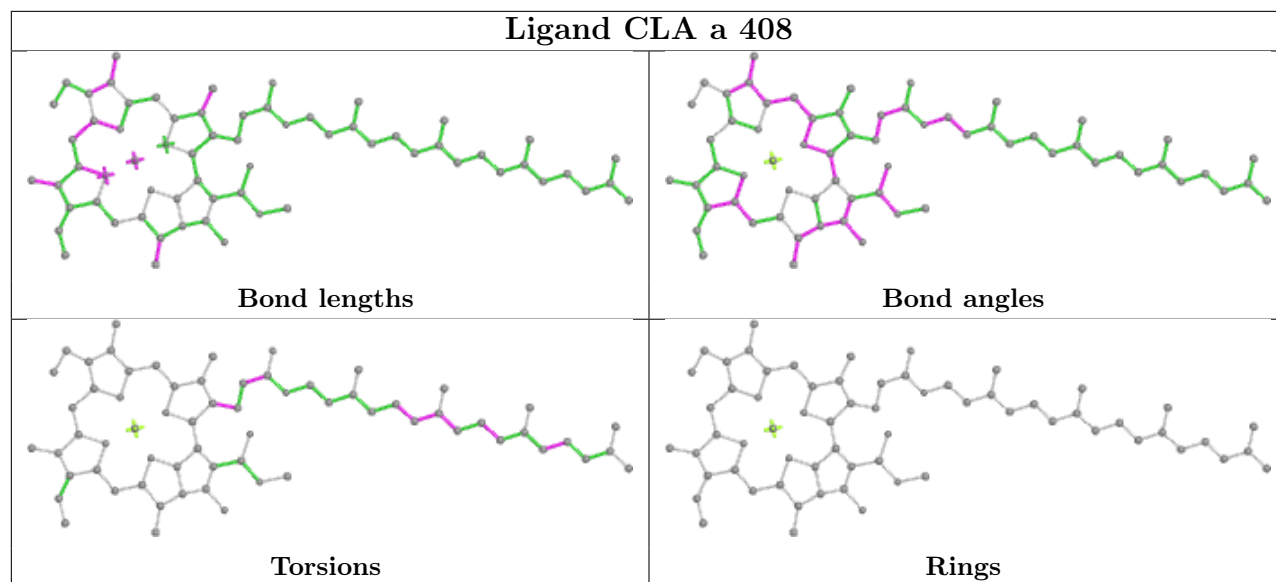
Ligand CLA B 616



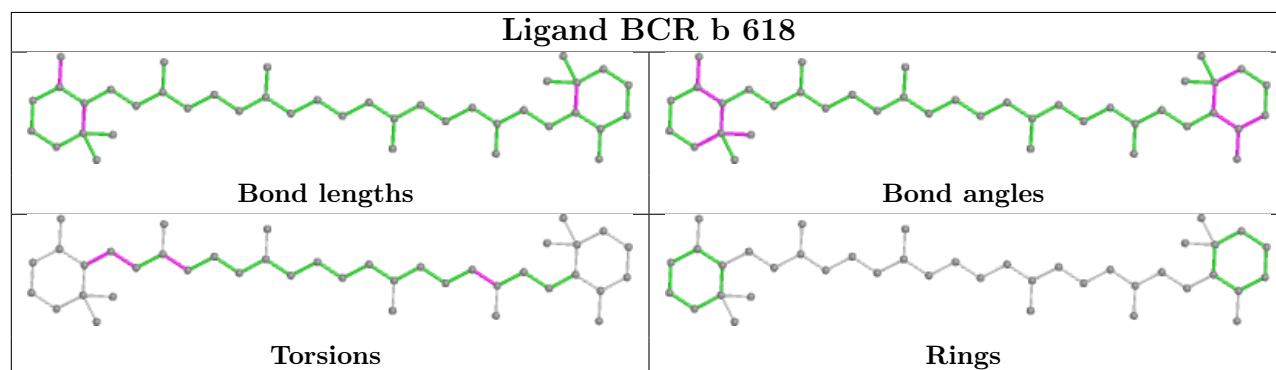
Ligand BCR T 101



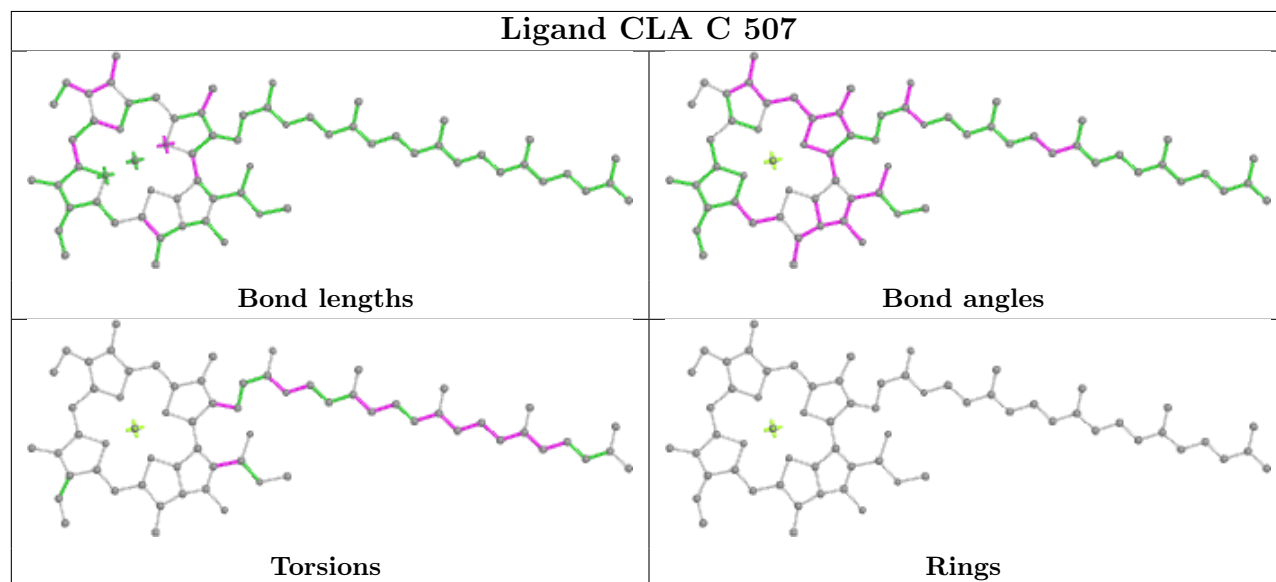
Ligand CLA a 408

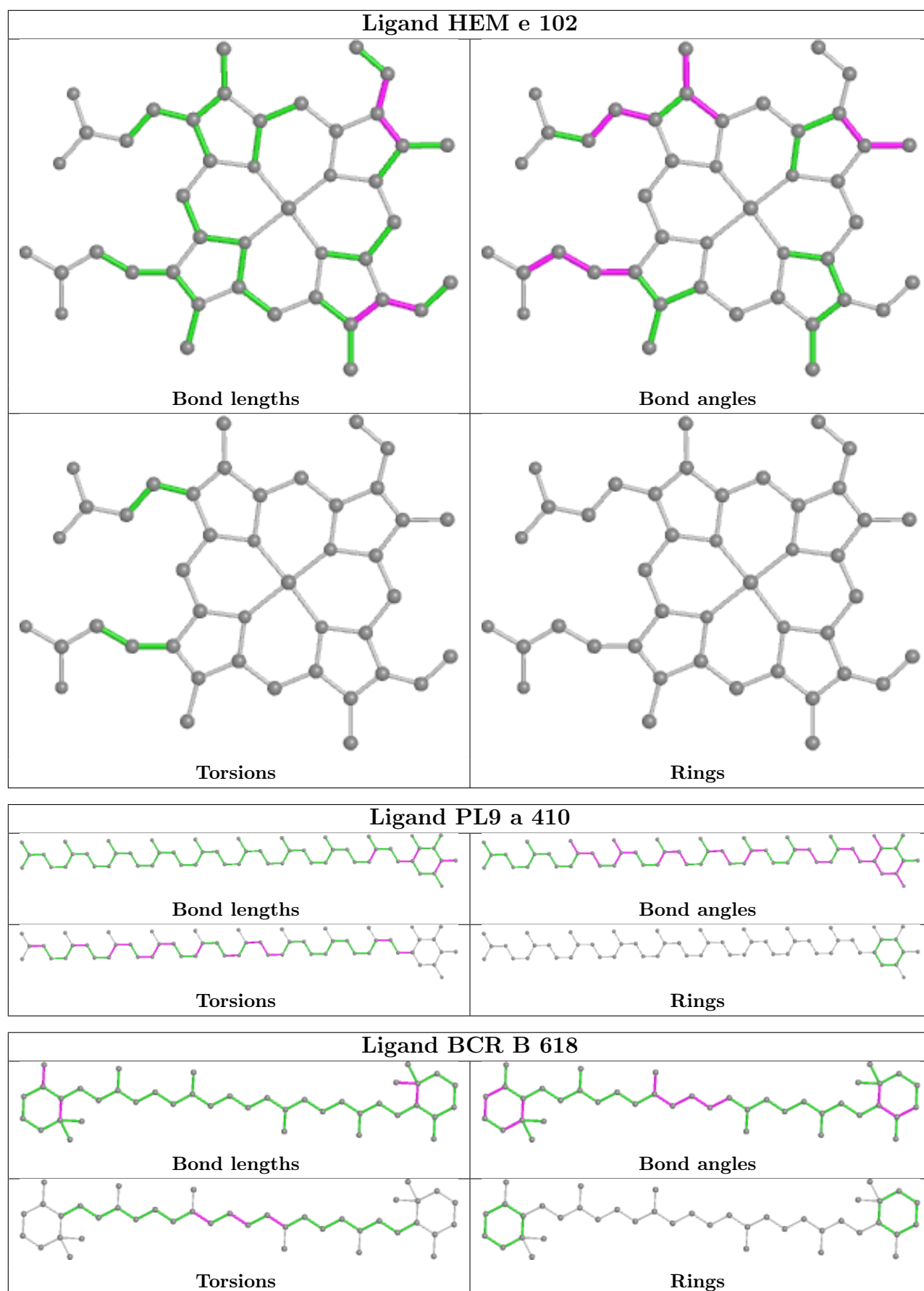


Ligand BCR b 618

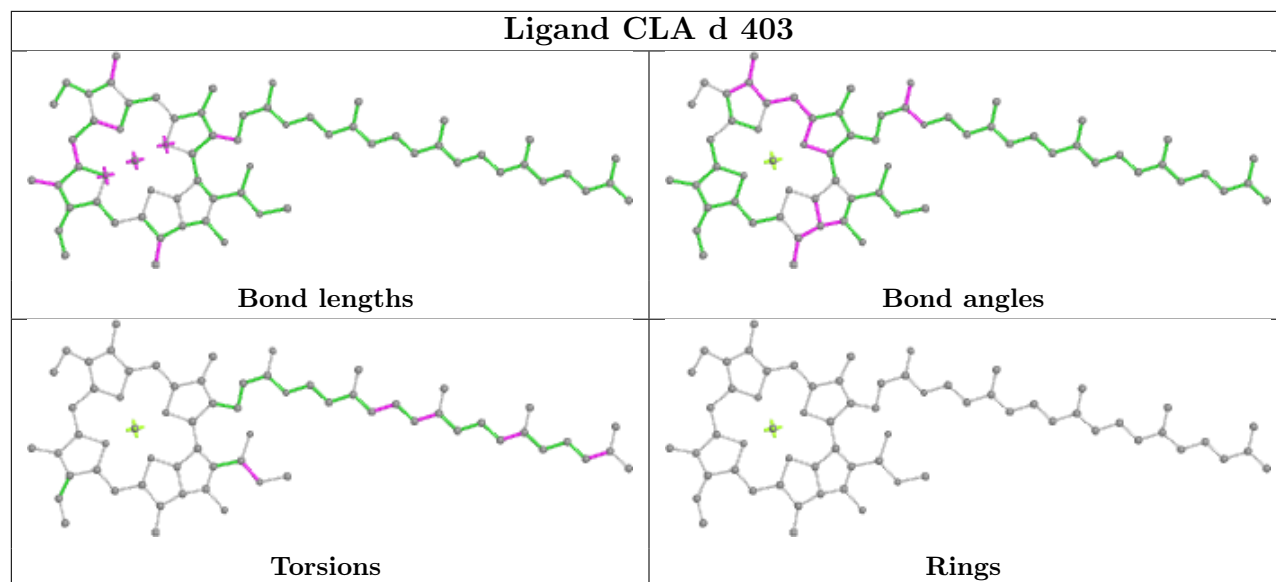


Ligand CLA C 507

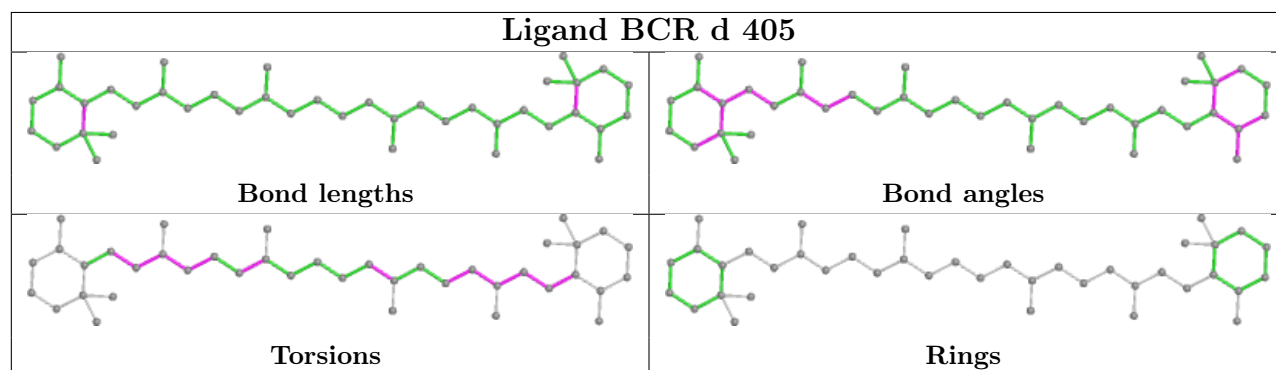


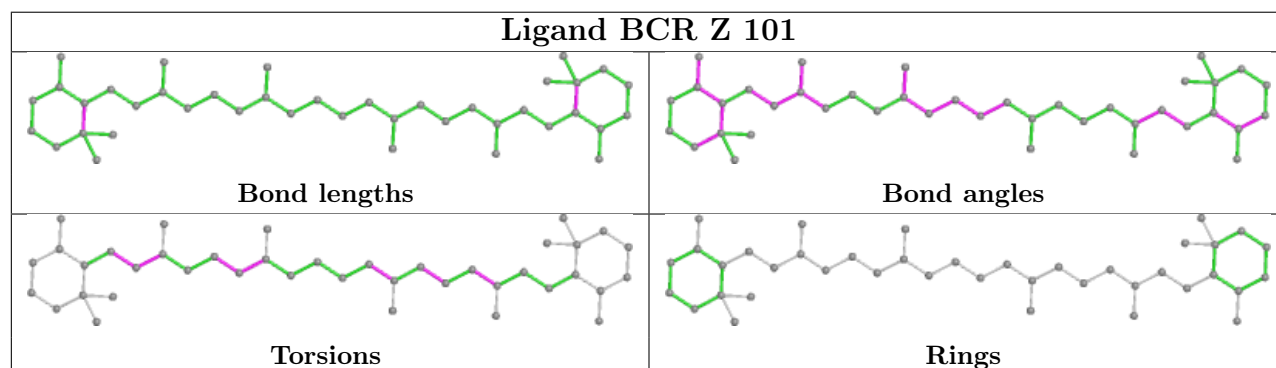
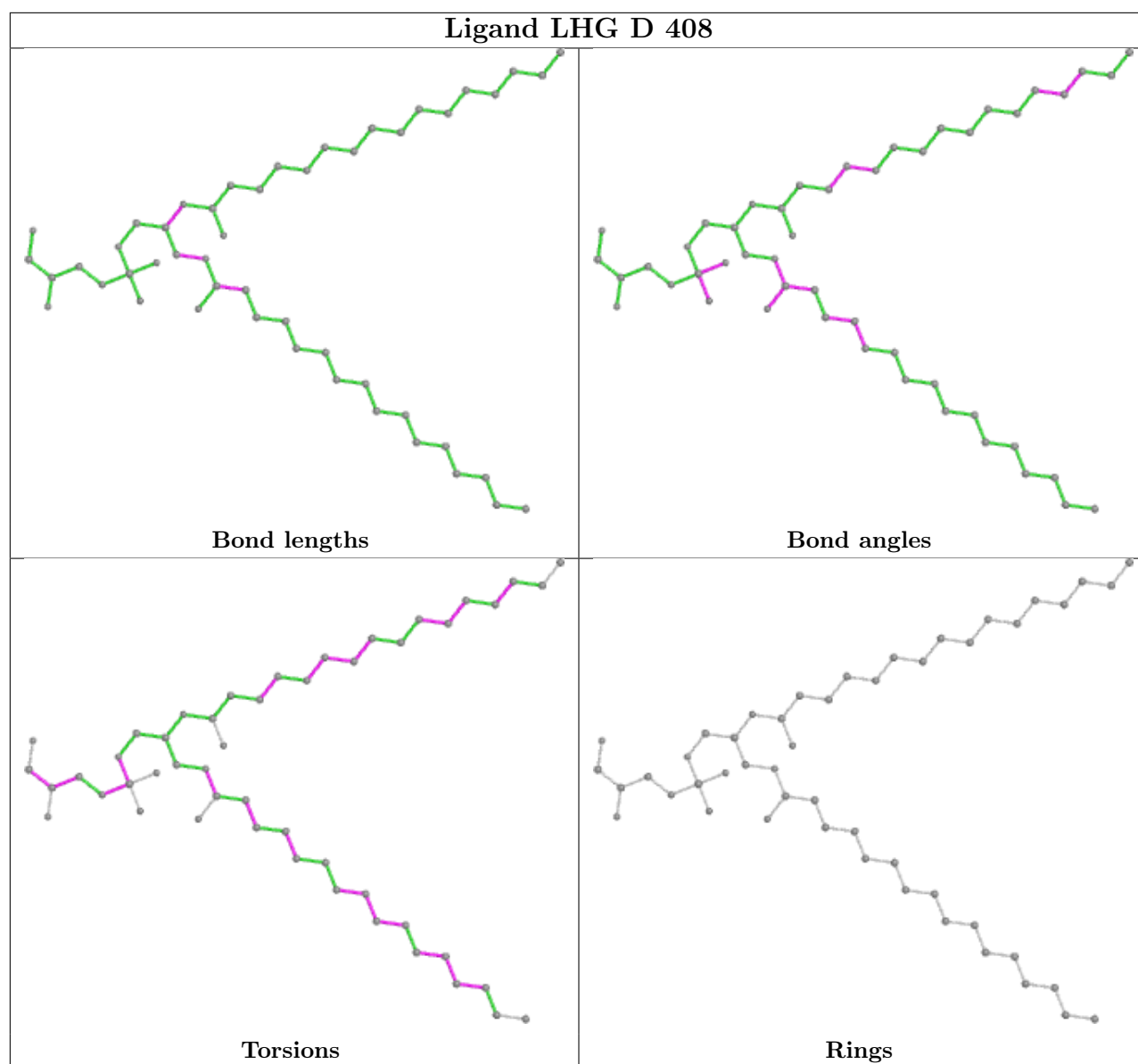


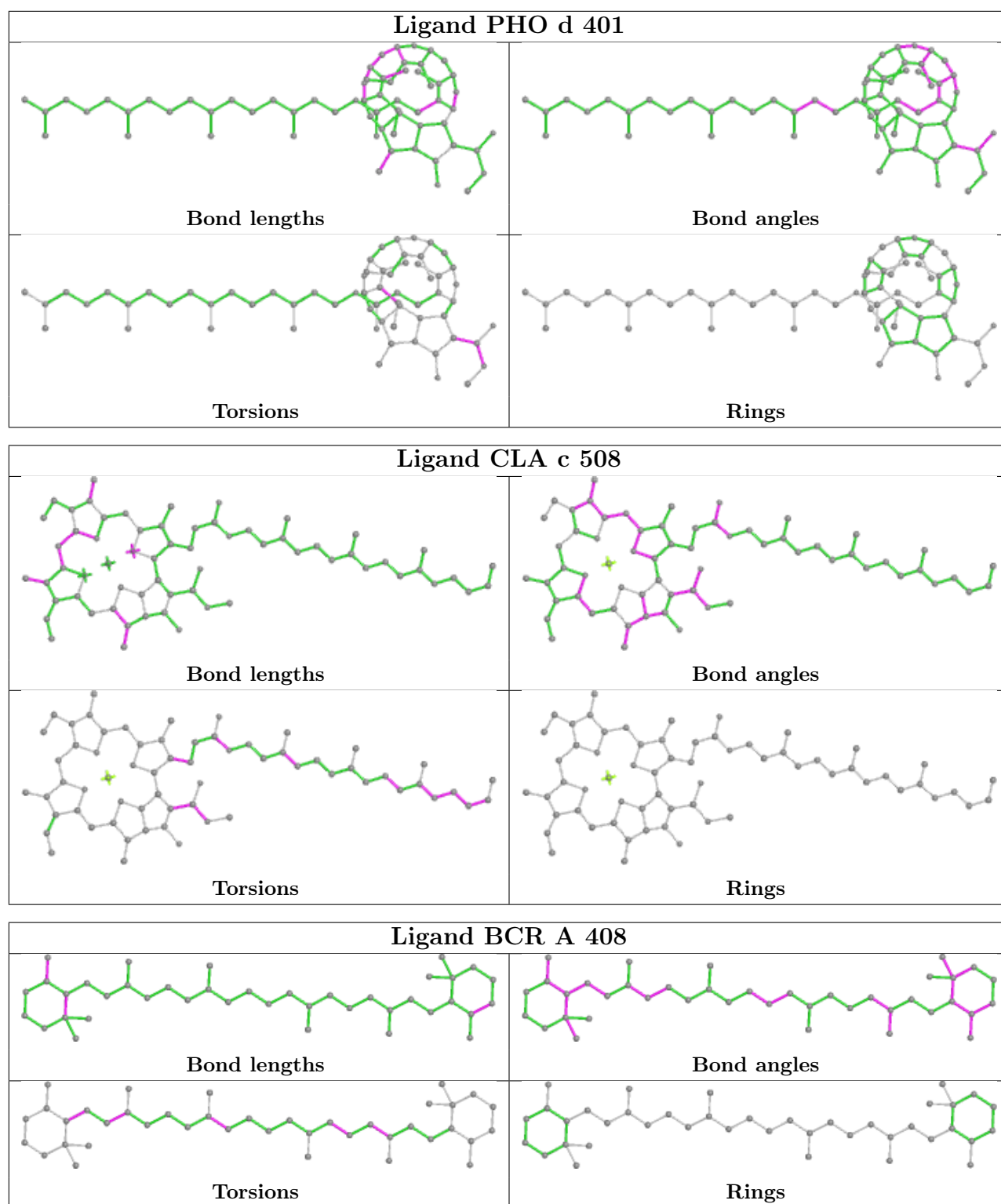
Ligand CLA d 403

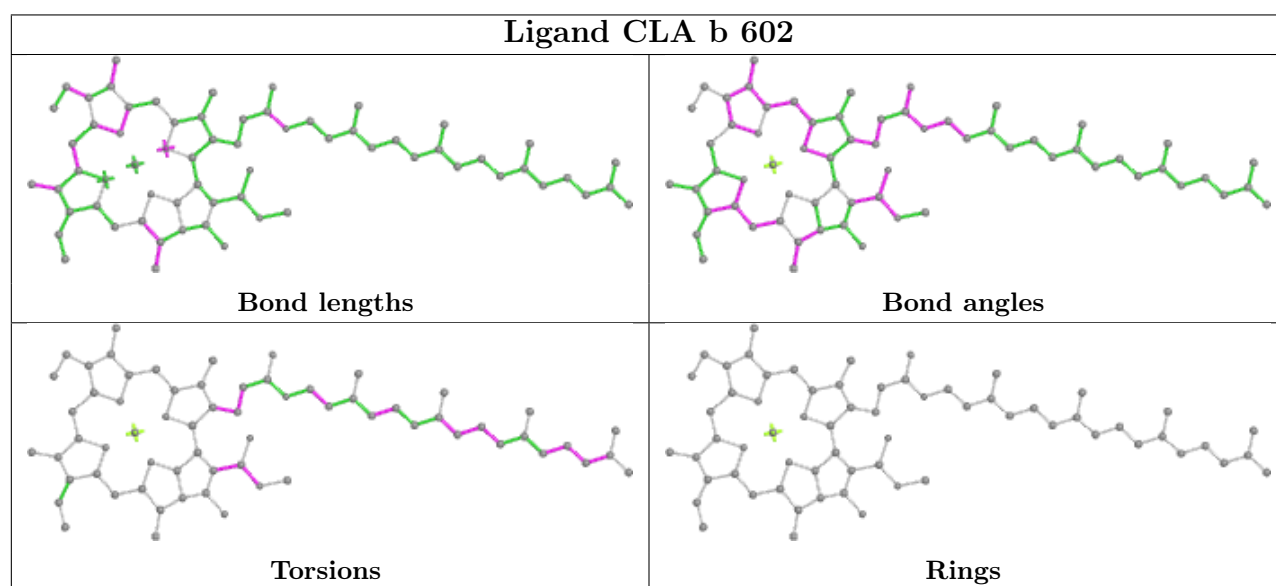
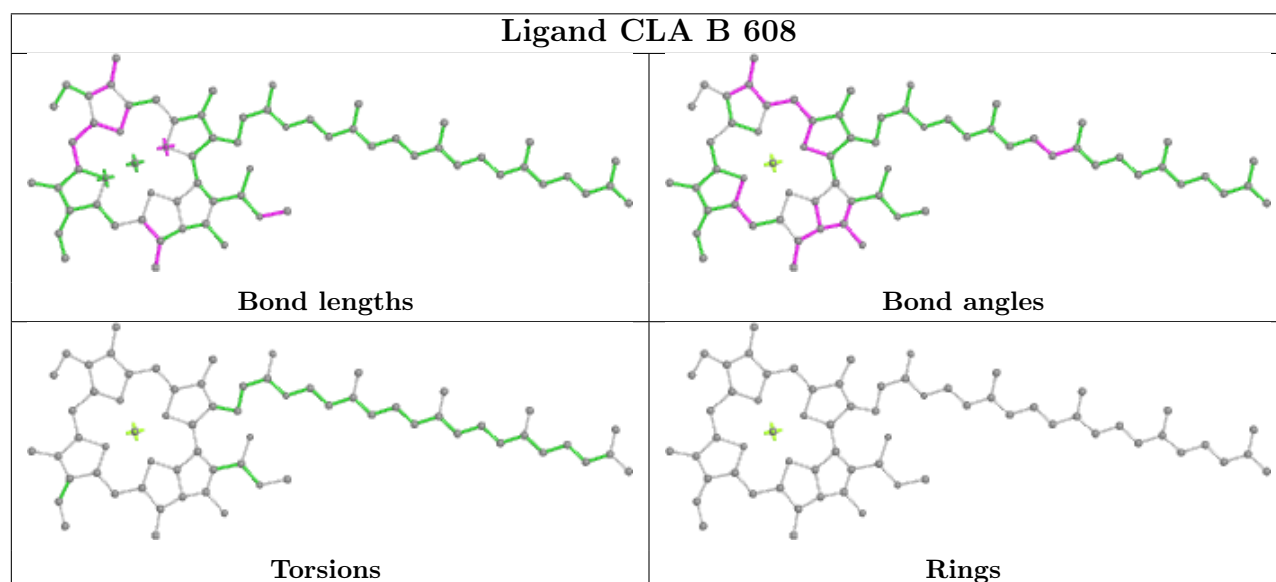
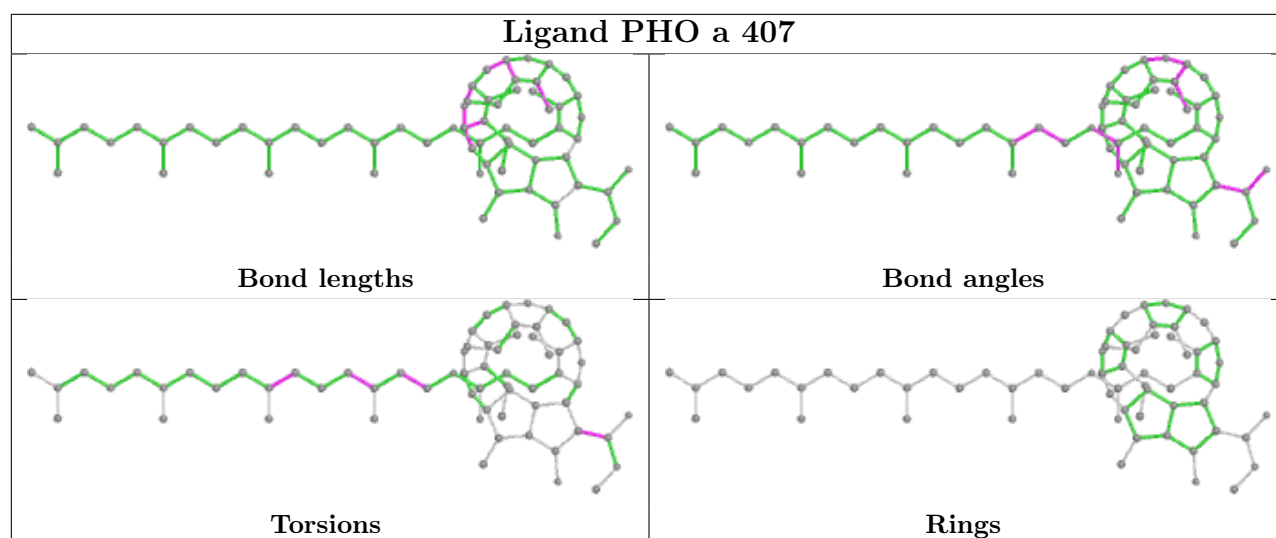


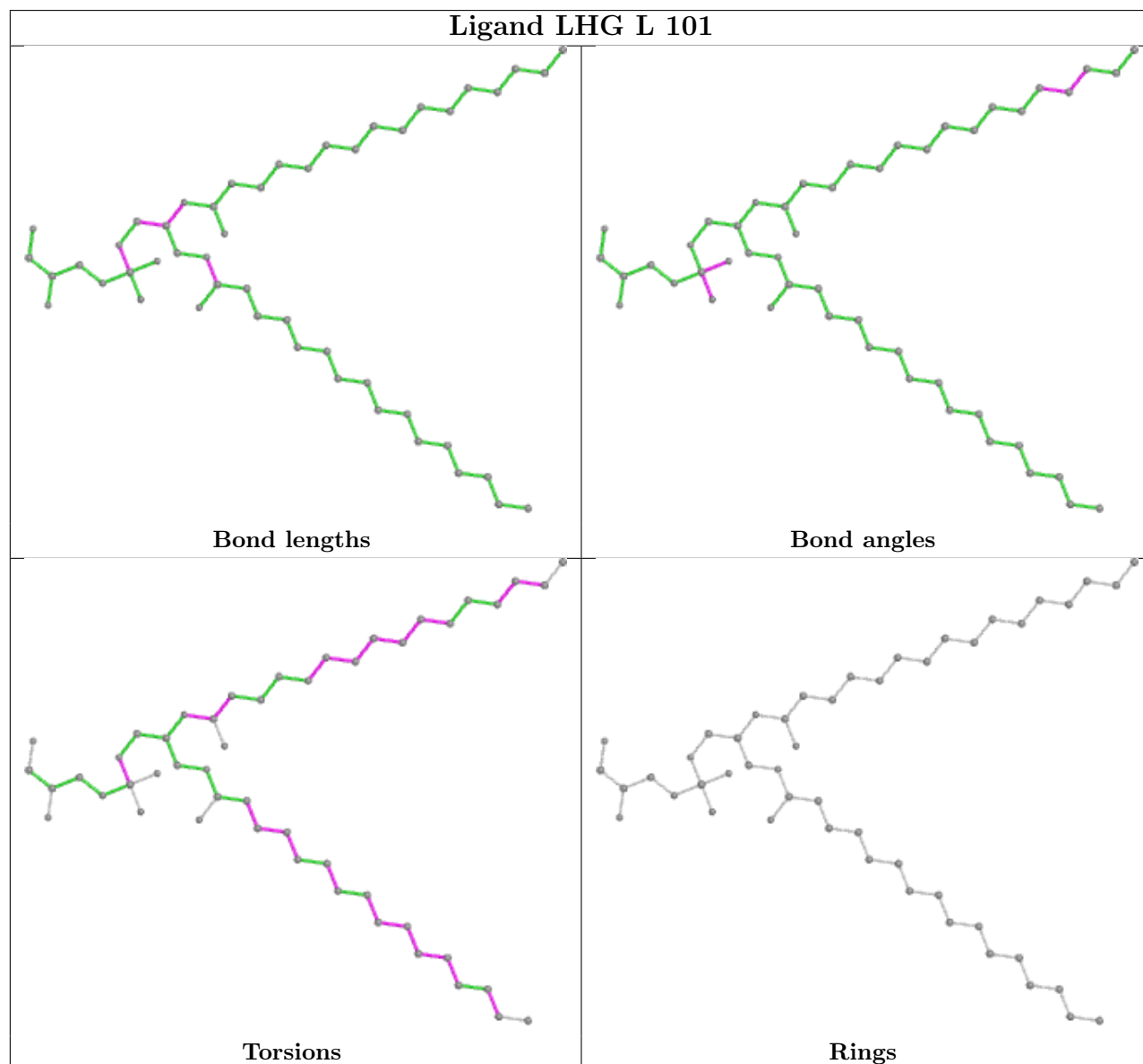
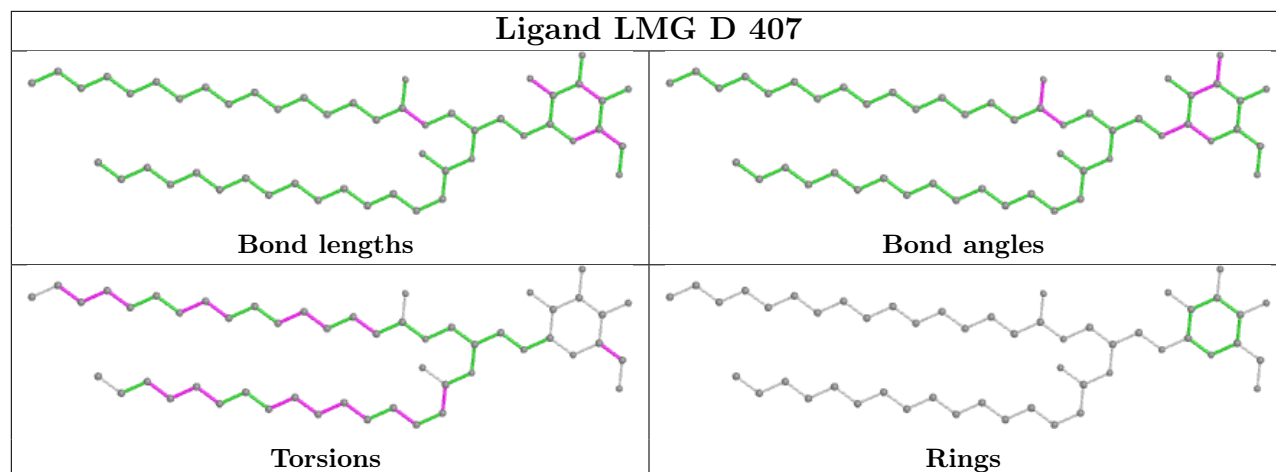
Ligand BCR d 405



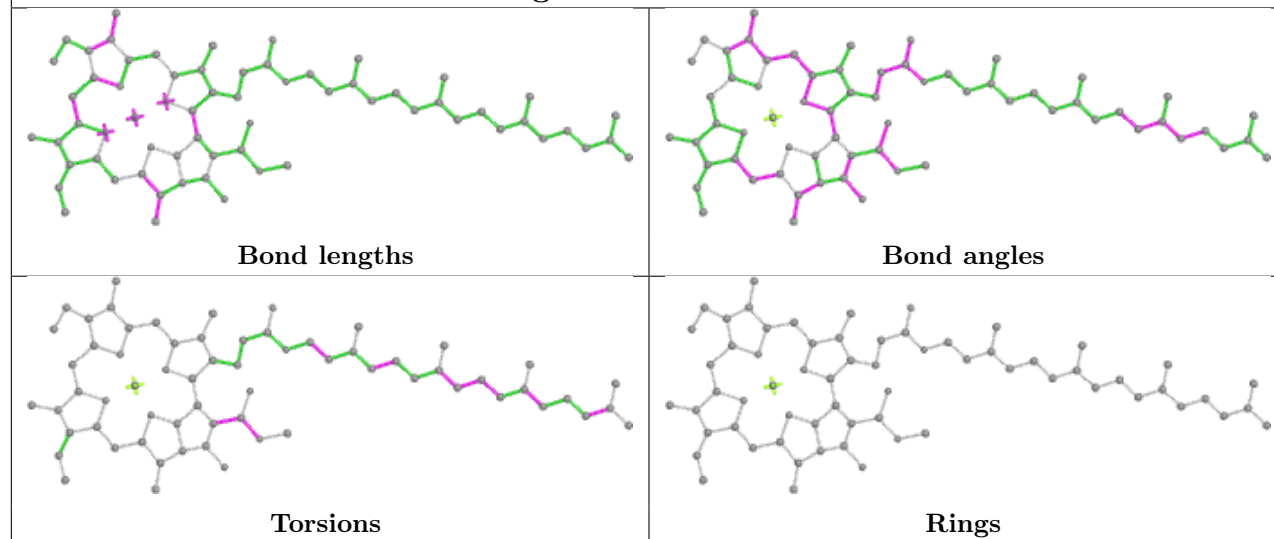




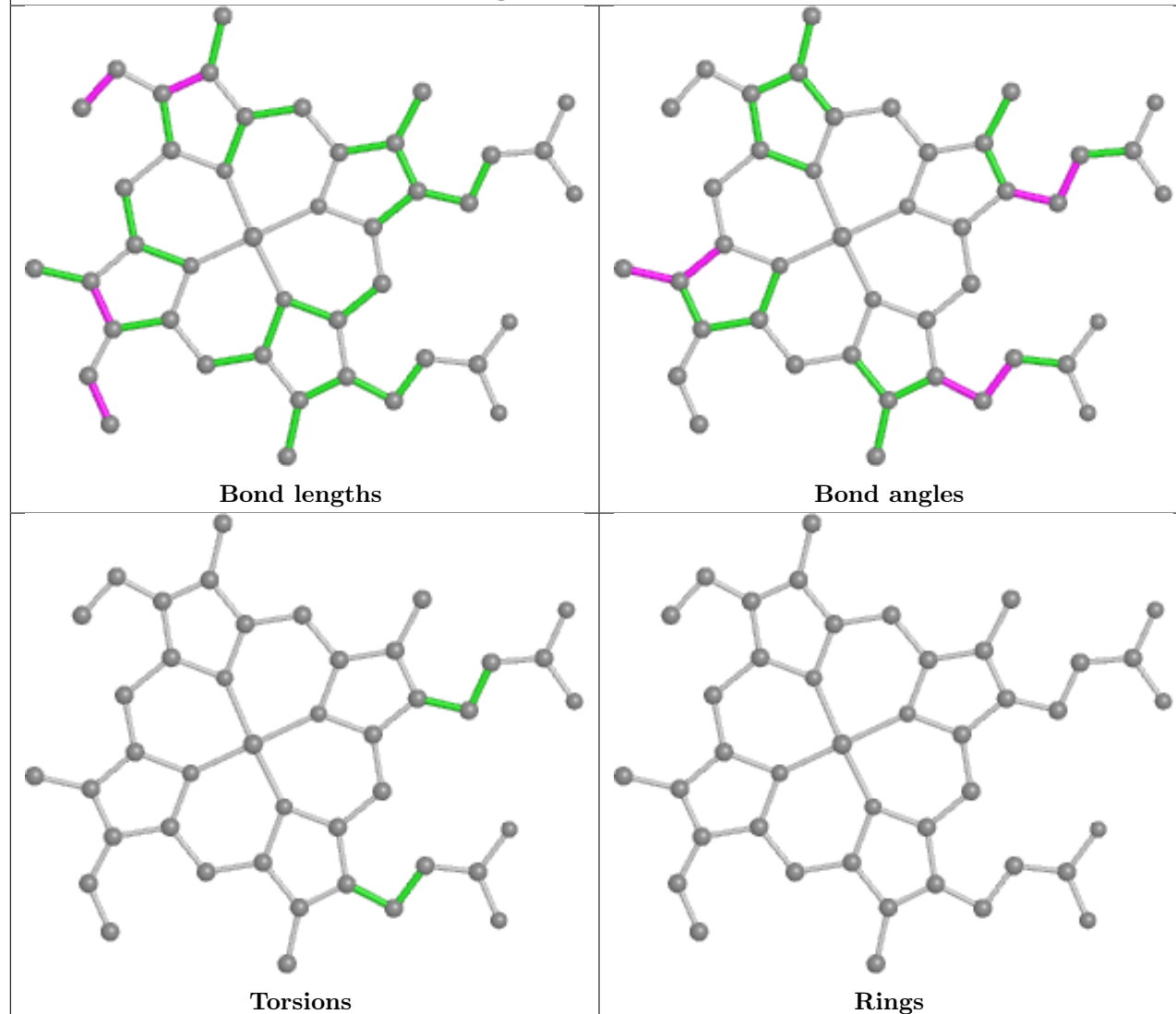




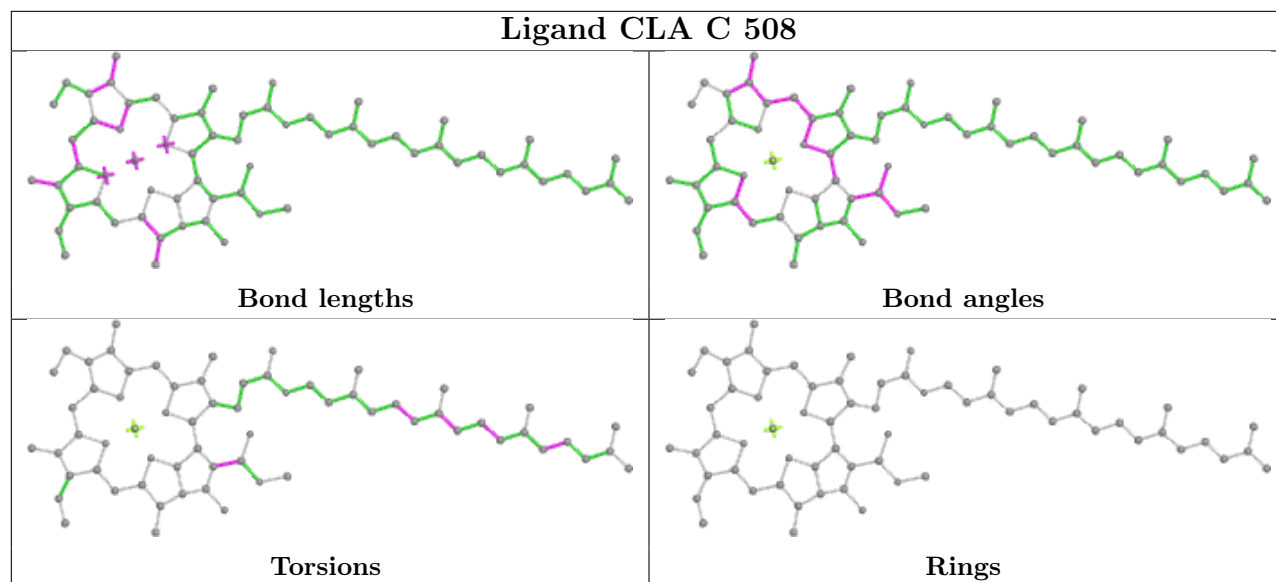
Ligand CLA C 513



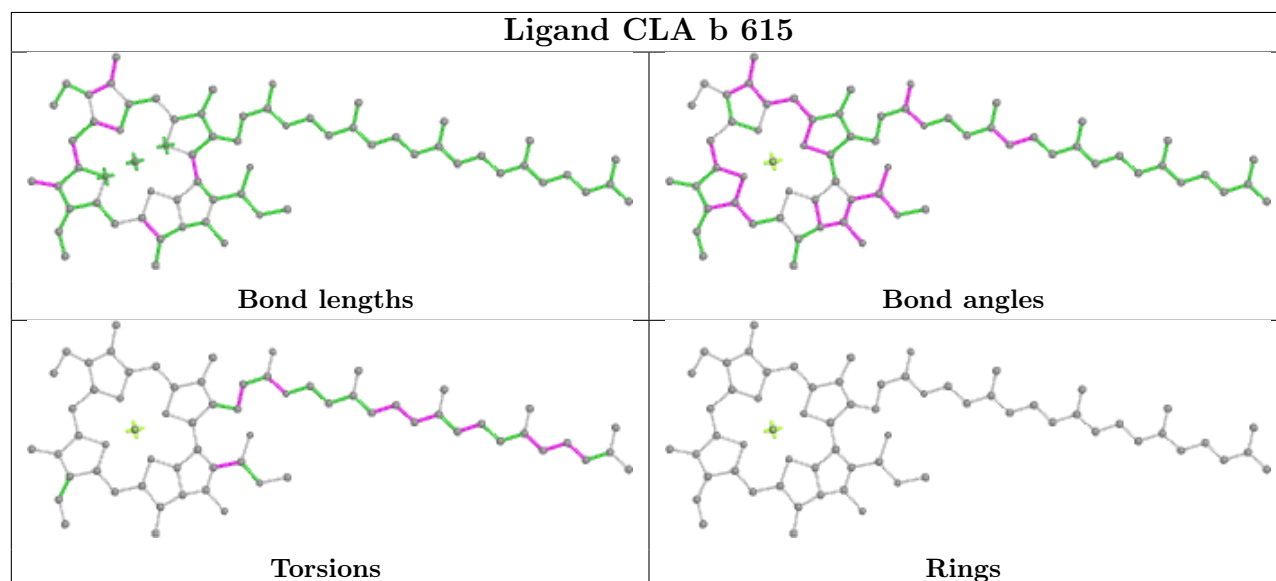
Ligand HEC v 201



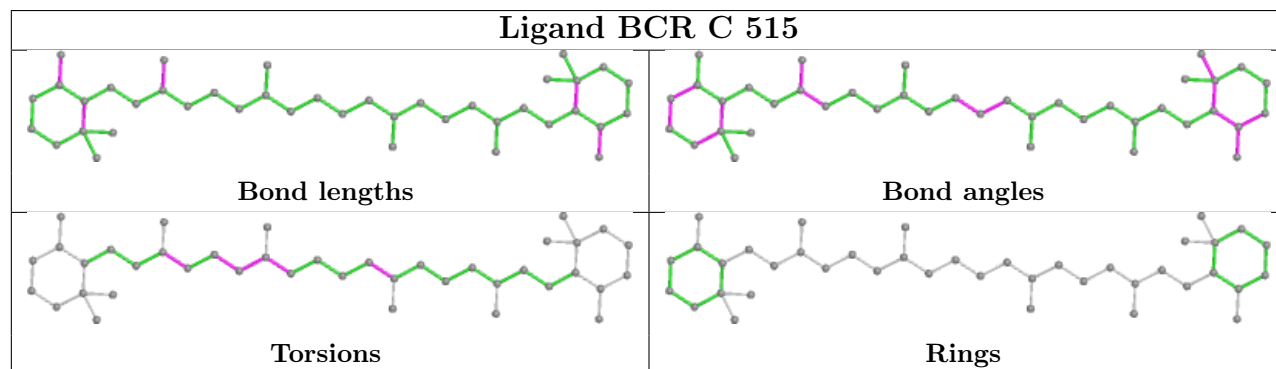
Ligand CLA C 508

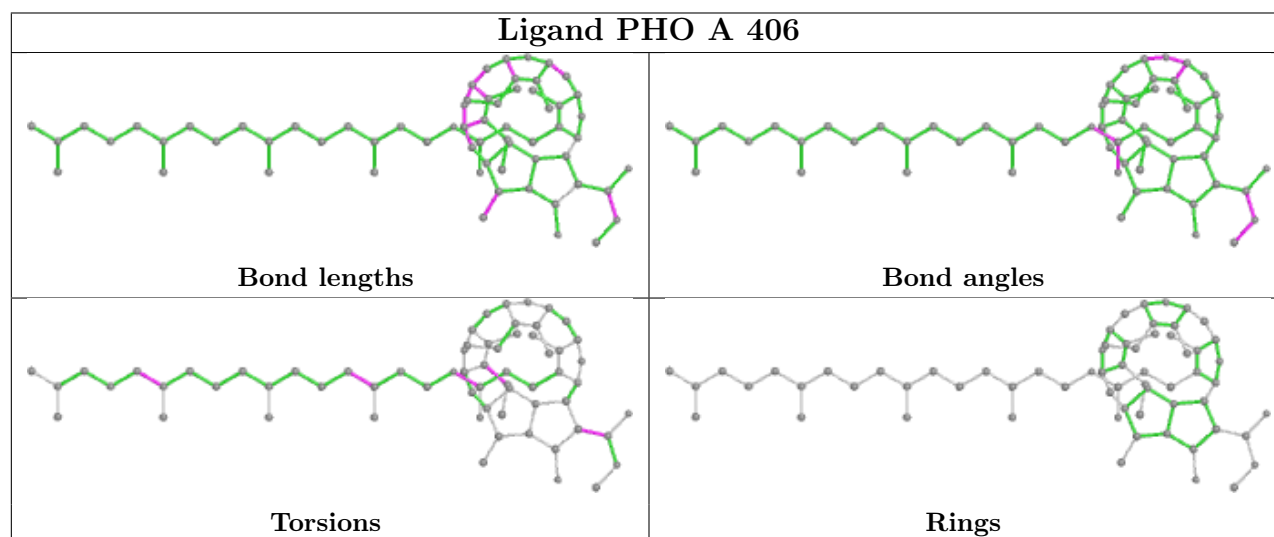
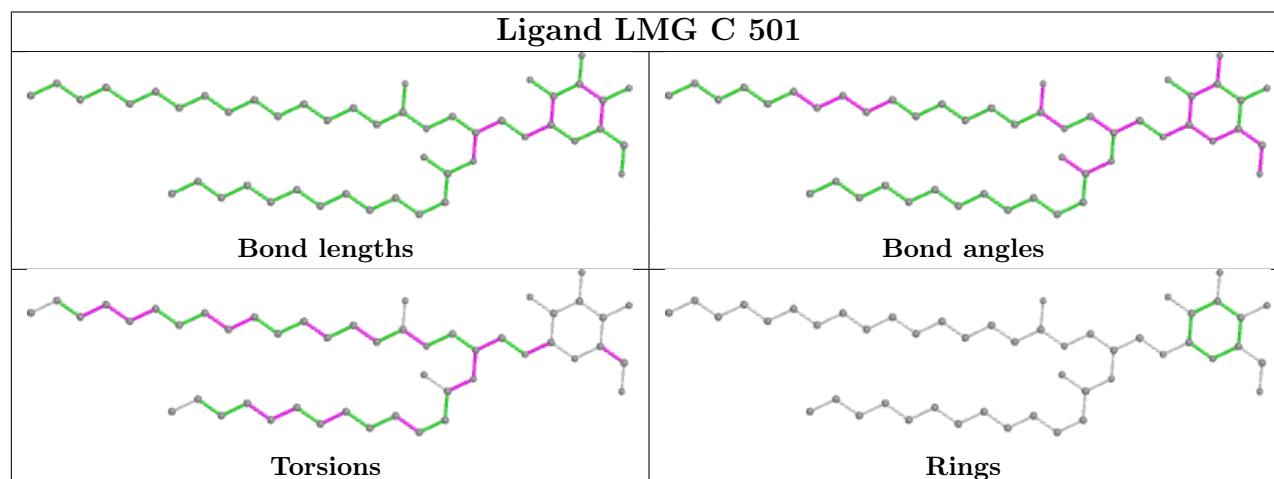
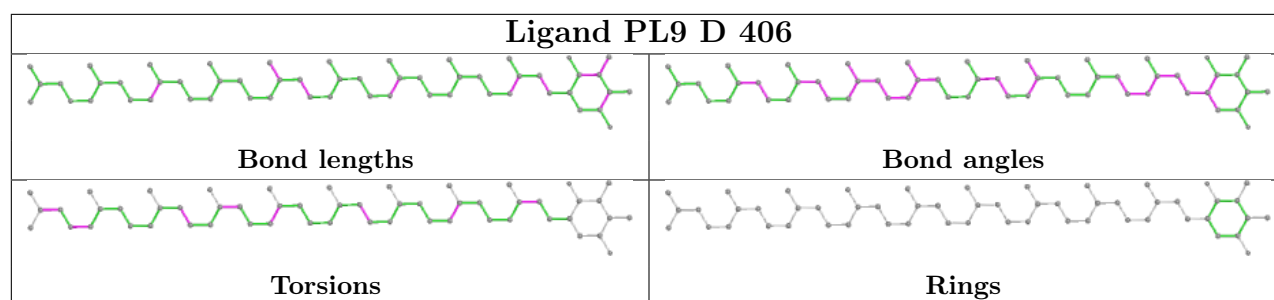


Ligand CLA b 615

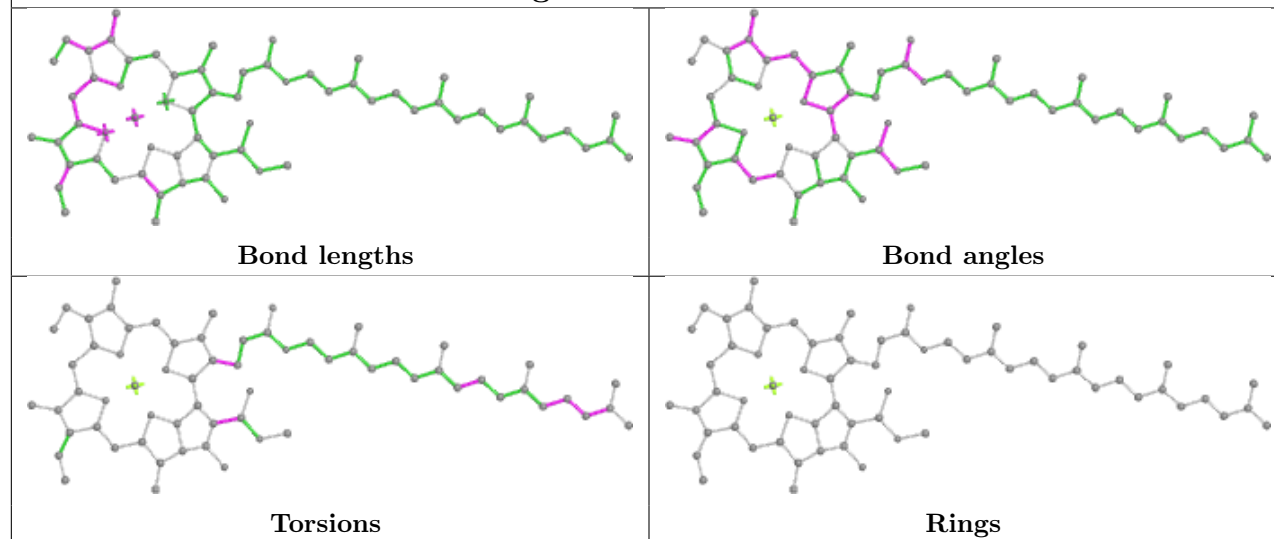


Ligand BCR C 515

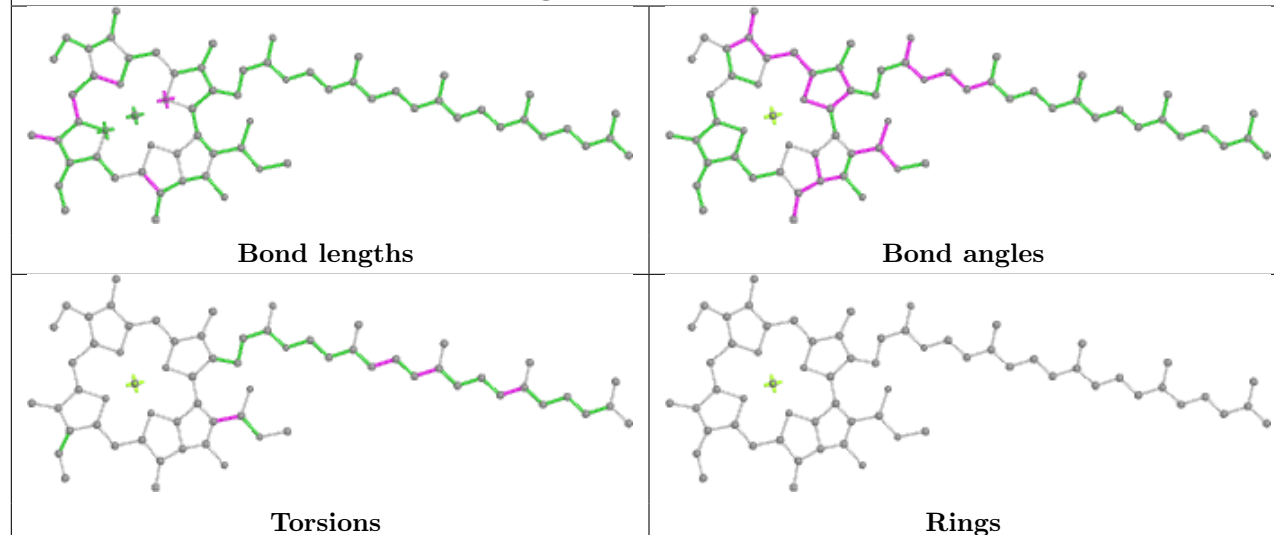




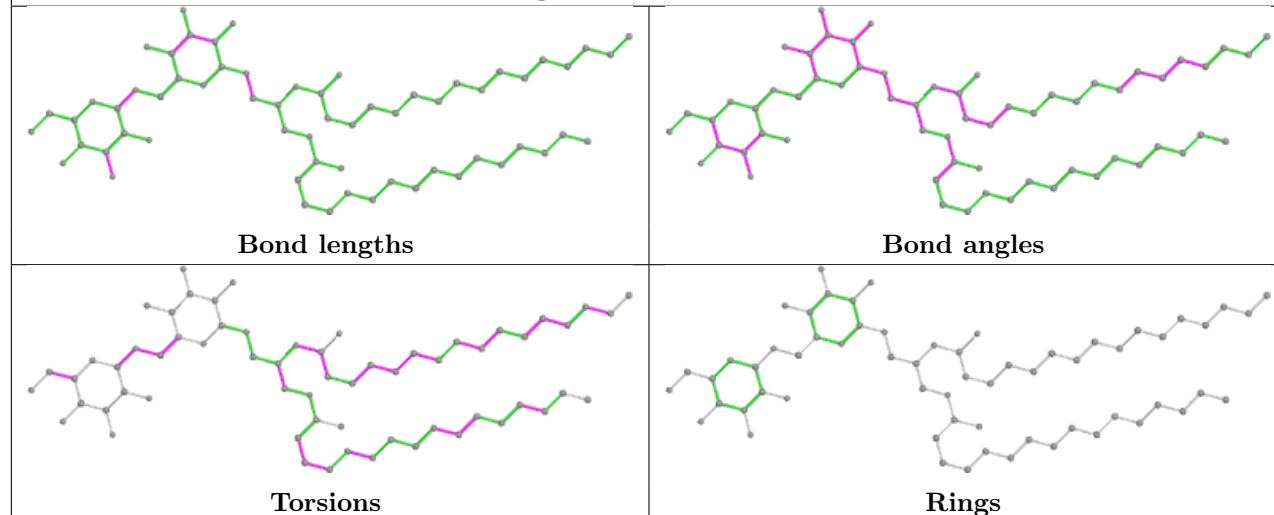
Ligand CLA B 607

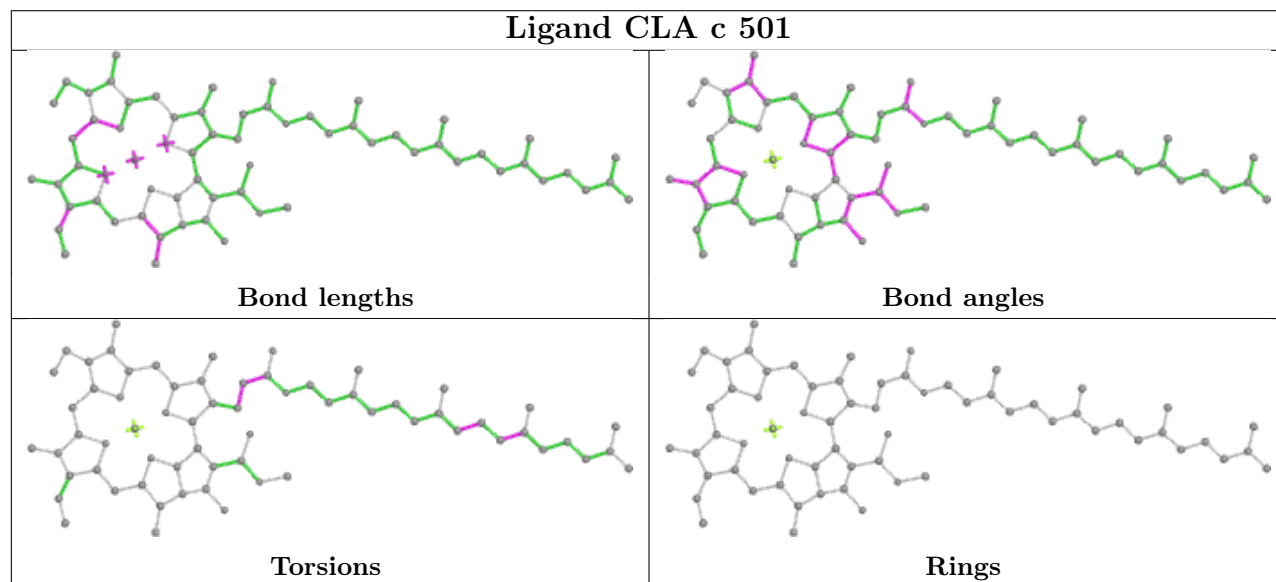
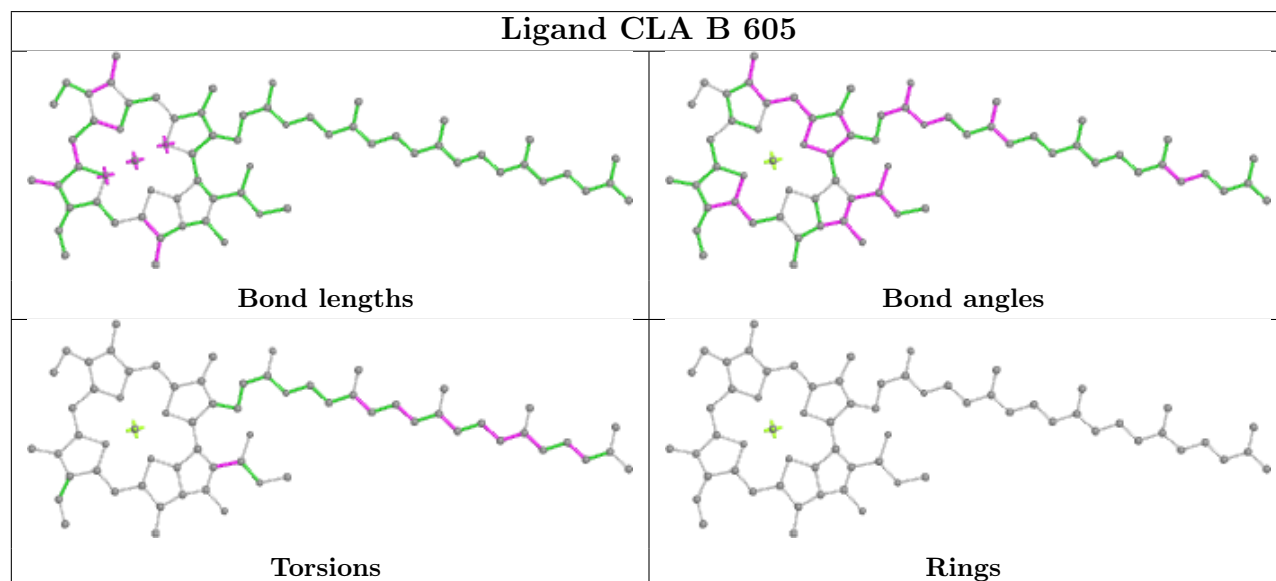
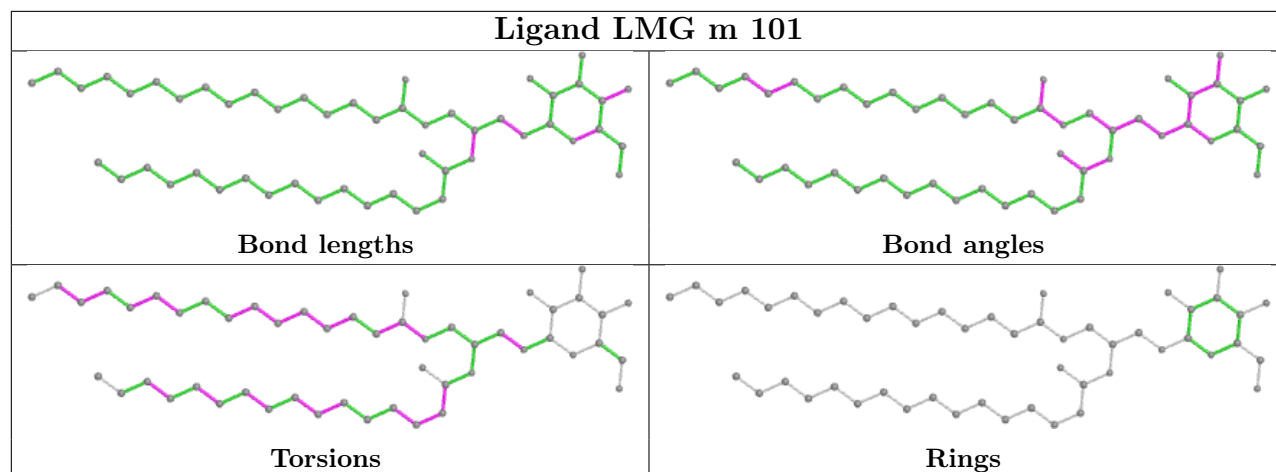


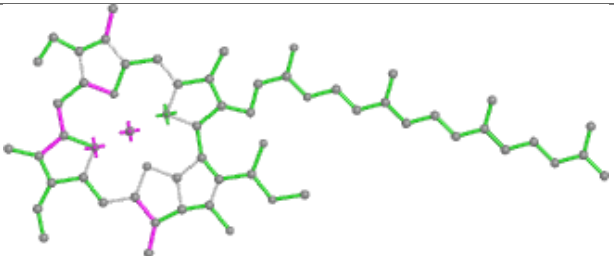
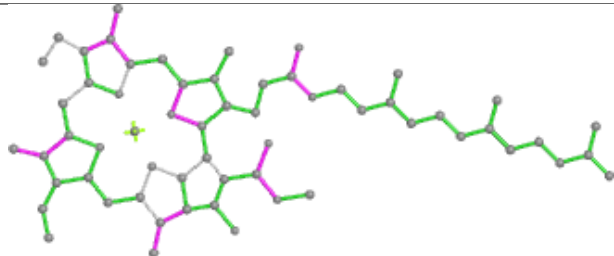
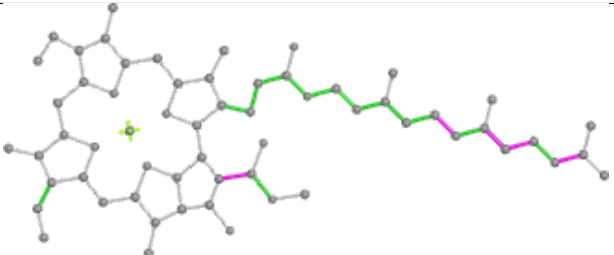
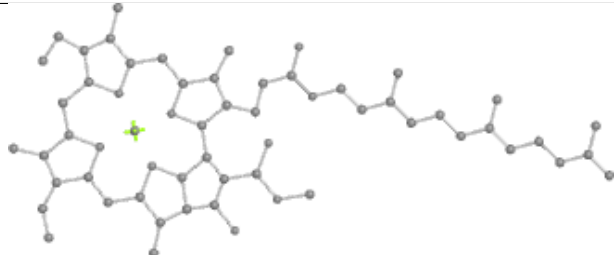
Ligand CLA c 502

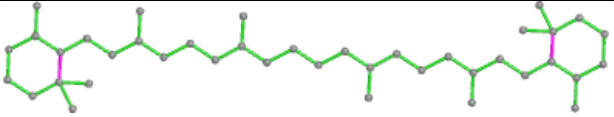
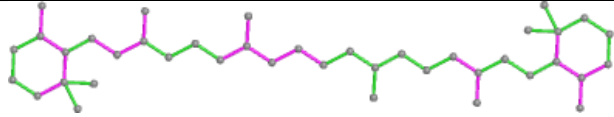
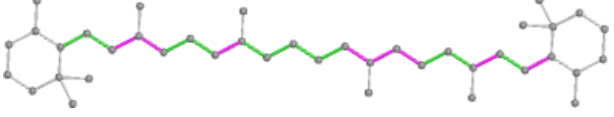
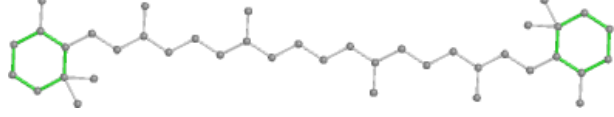


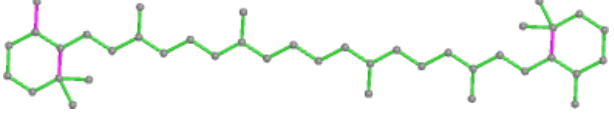
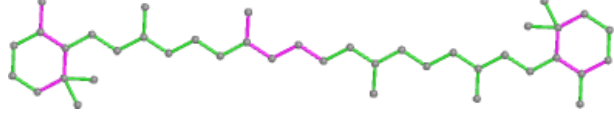
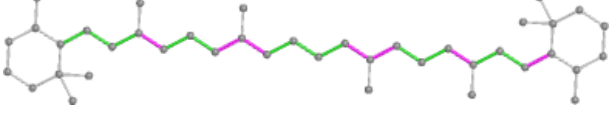
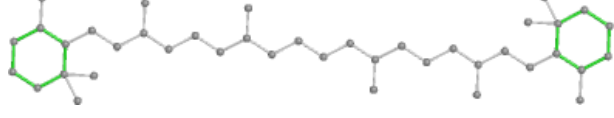
Ligand DGD c 516

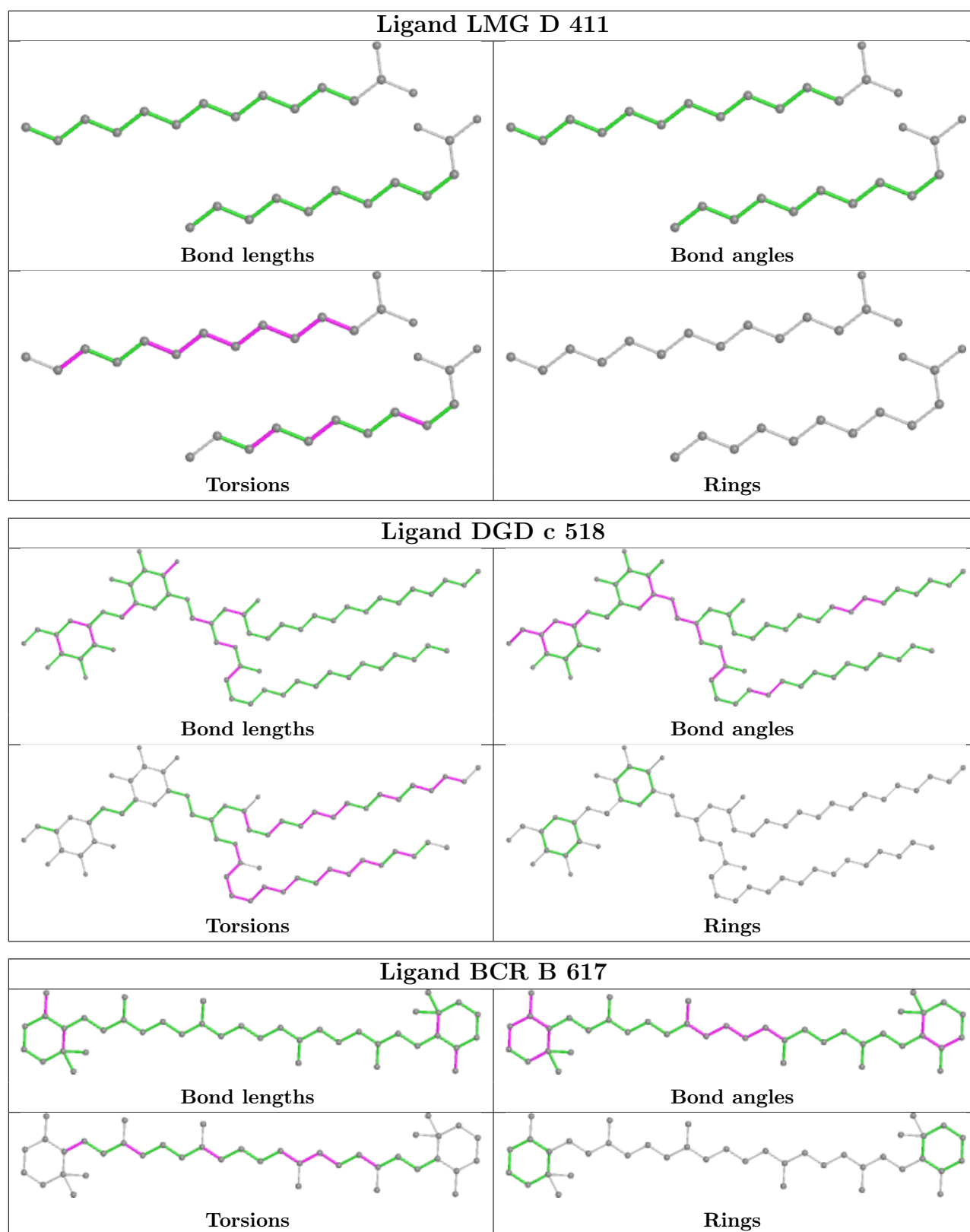


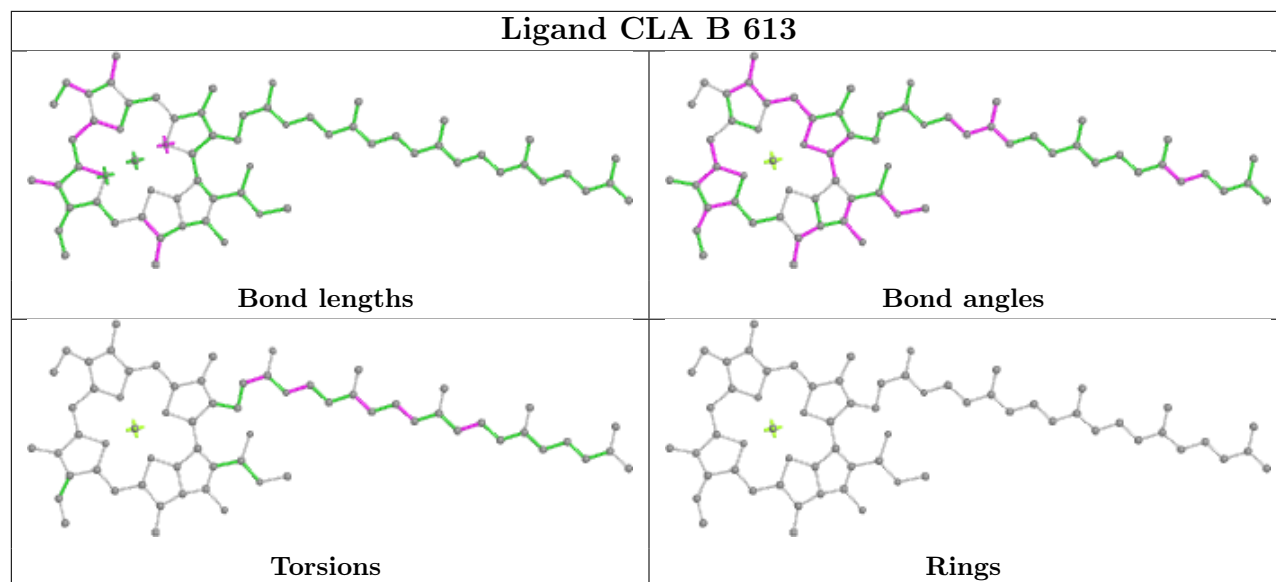
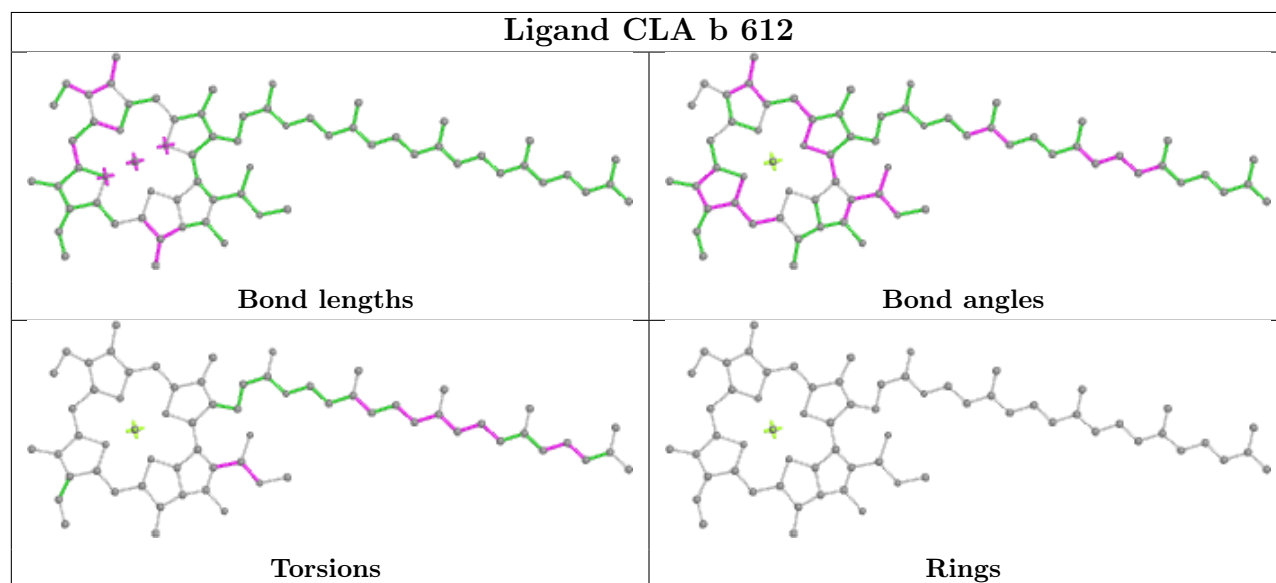


Ligand CLA c 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

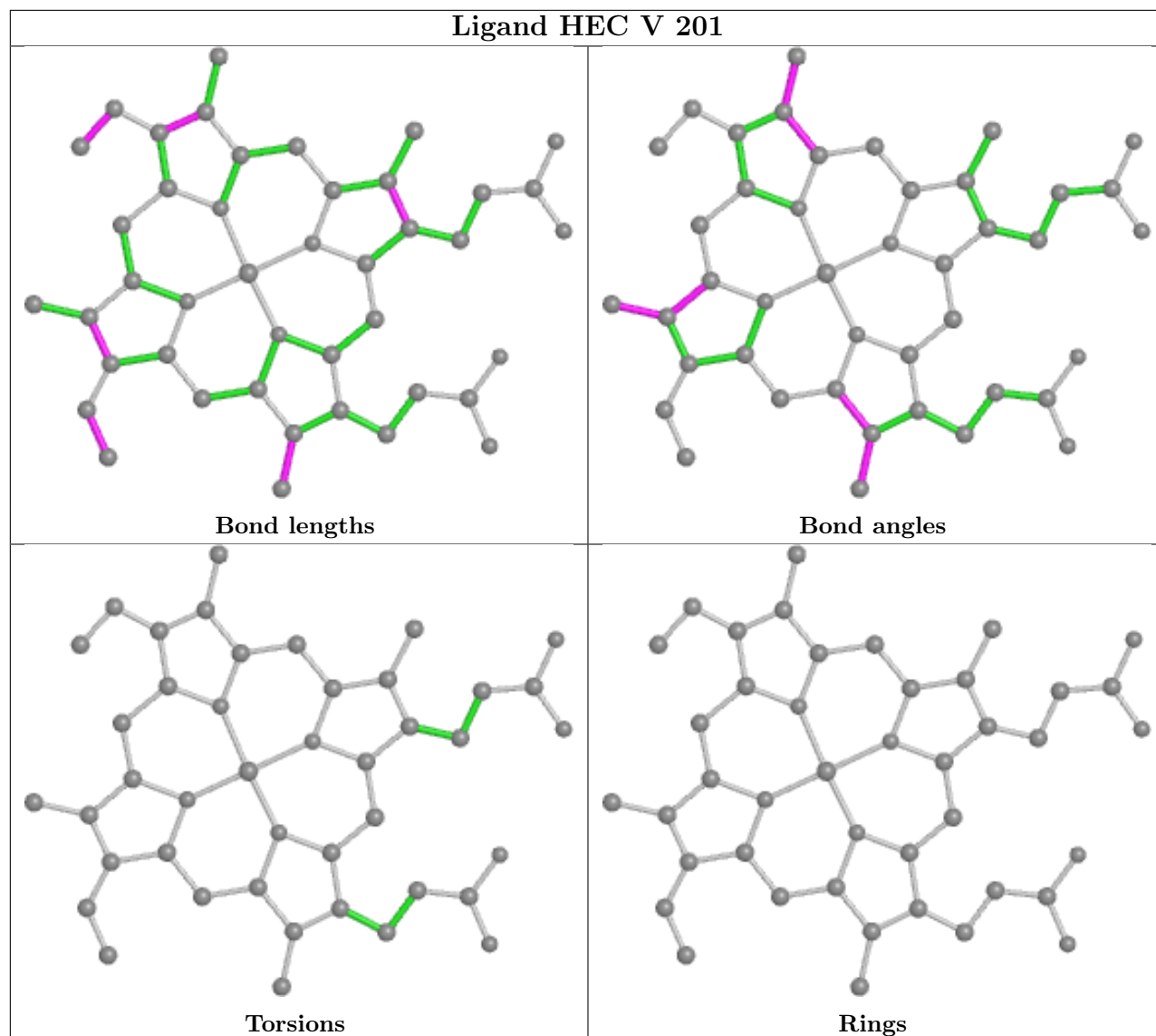
Ligand BCR x 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

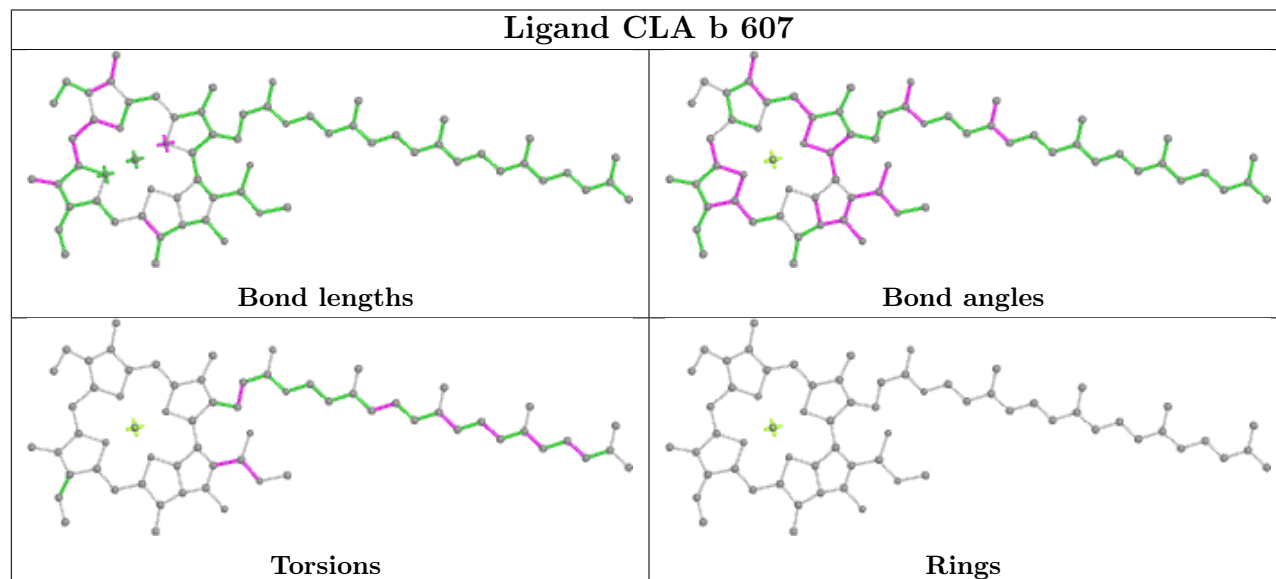


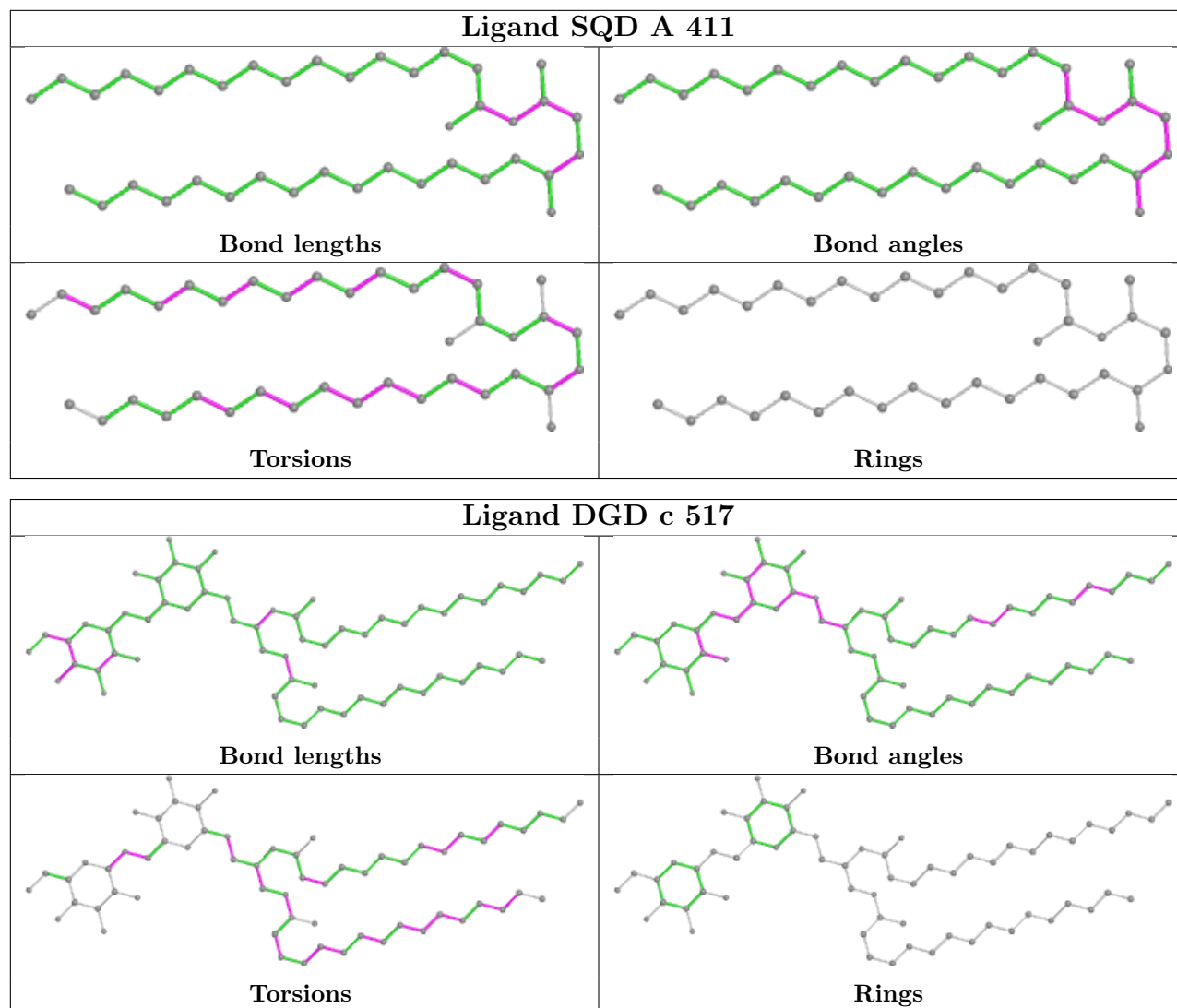
Ligand CLA B 613**Ligand CLA b 612**

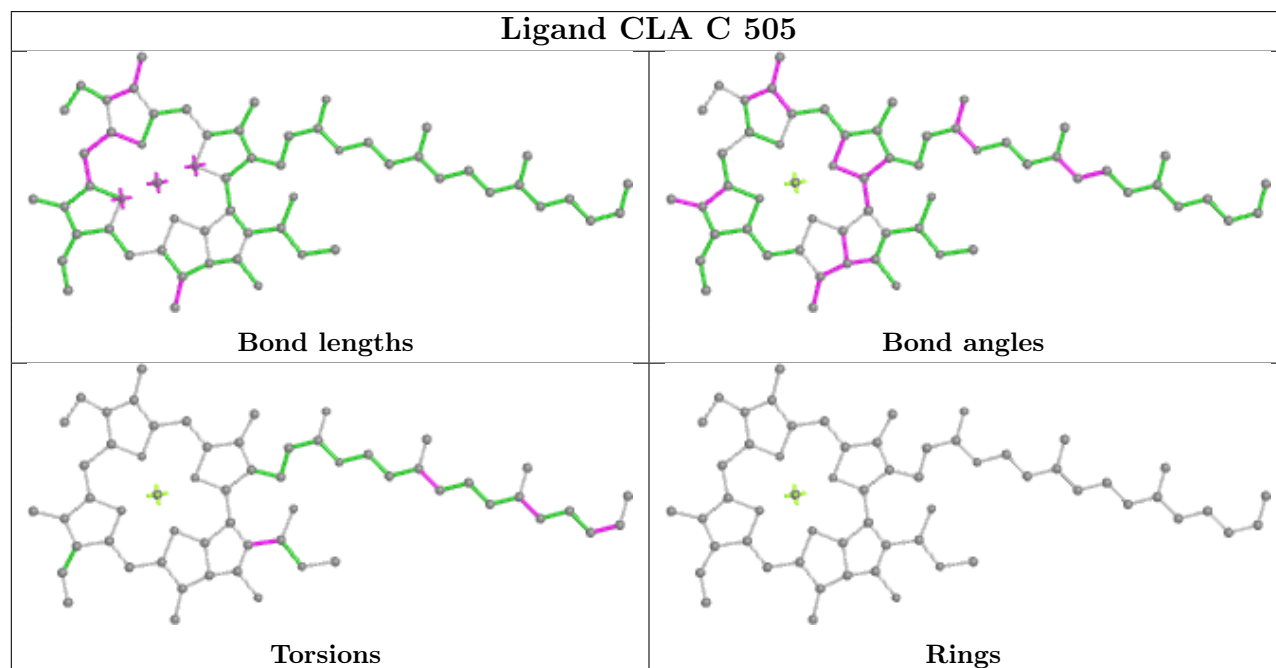
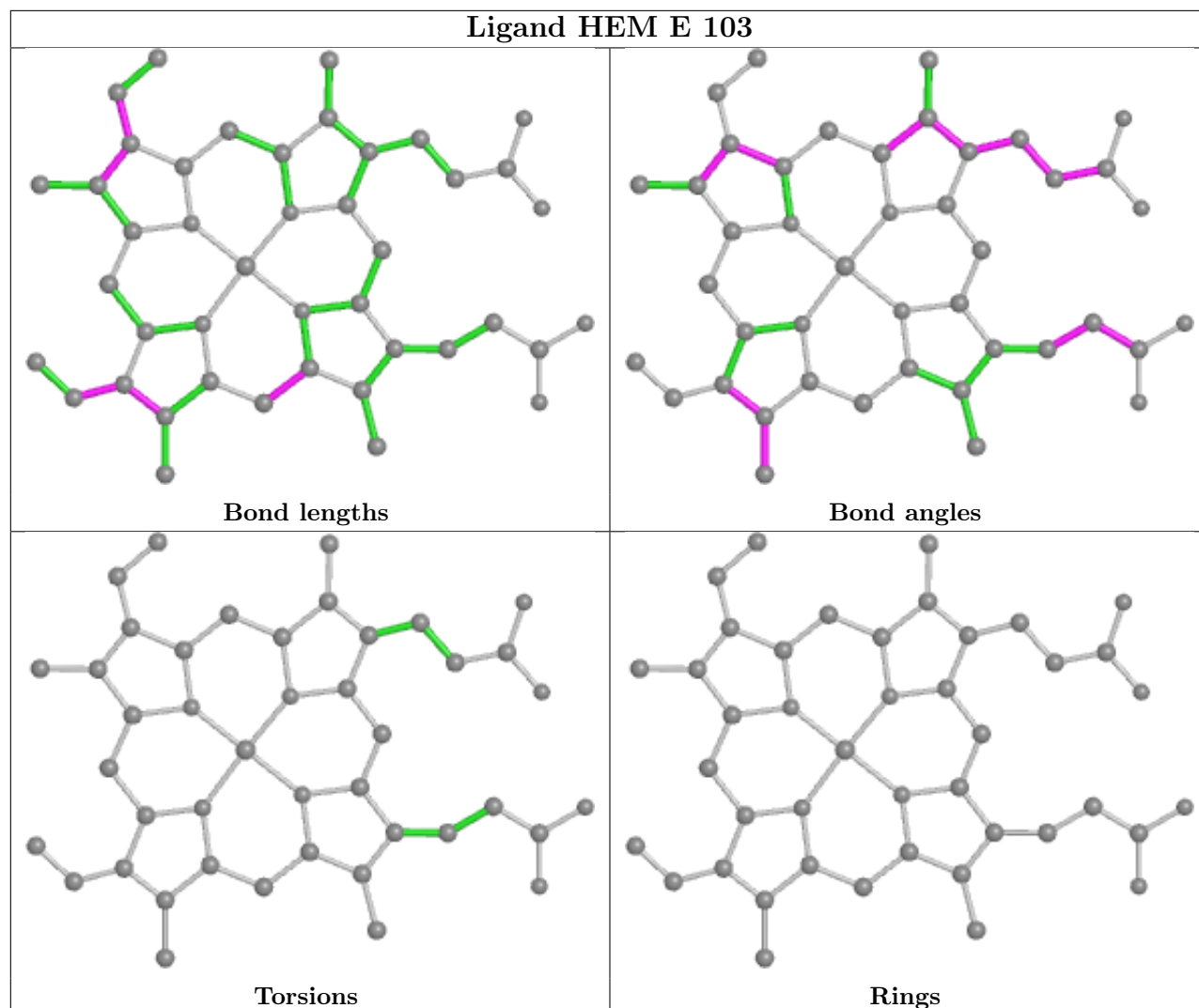
Ligand HEC V 201



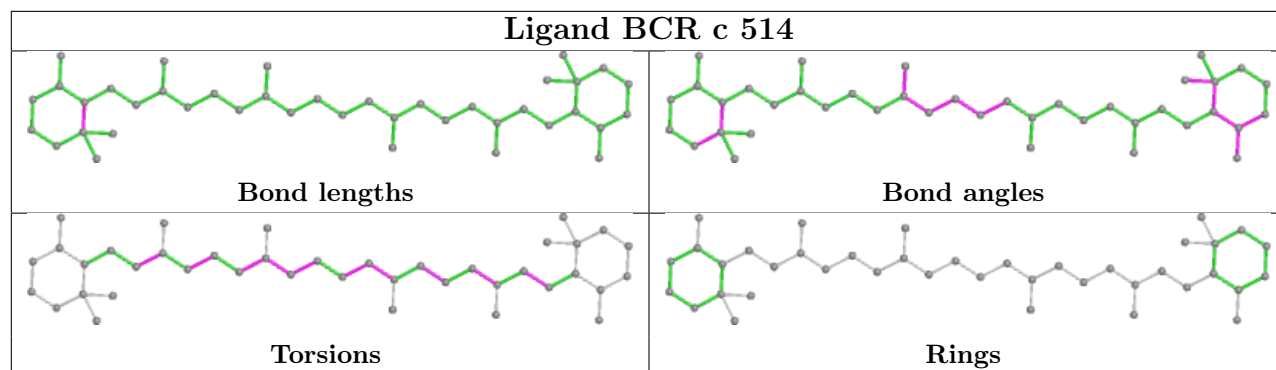
Ligand CLA b 607



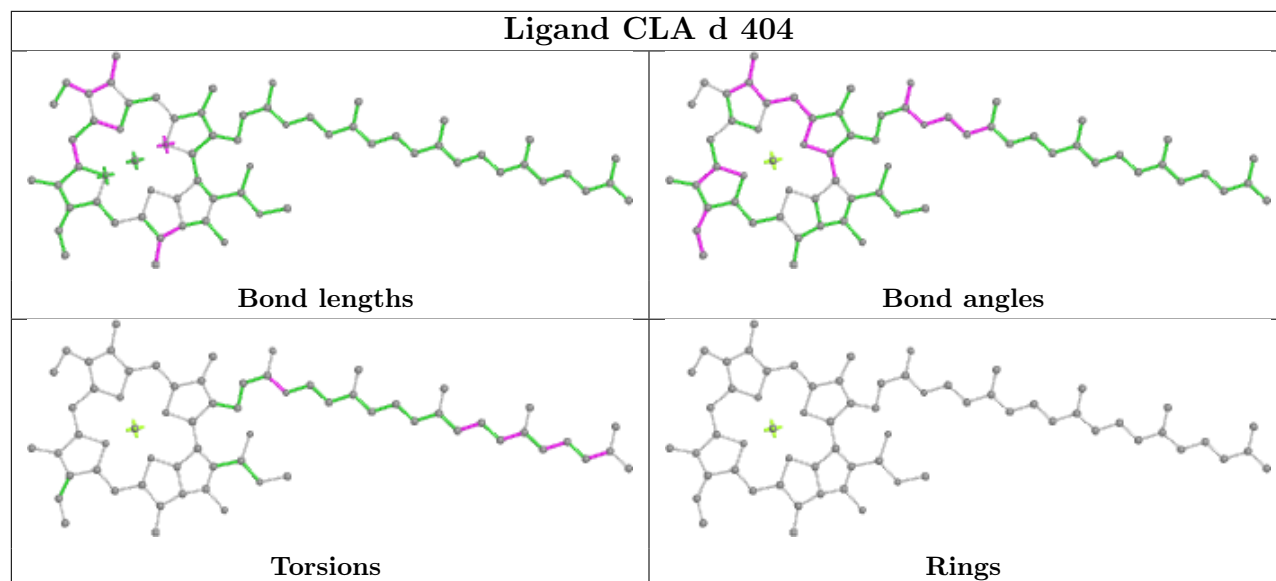




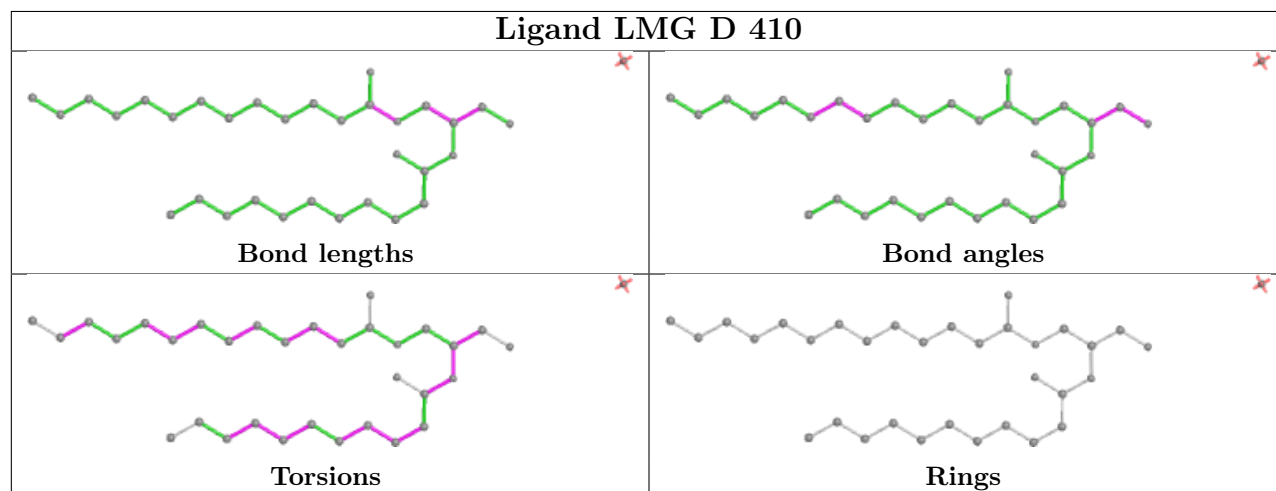
Ligand BCR c 514

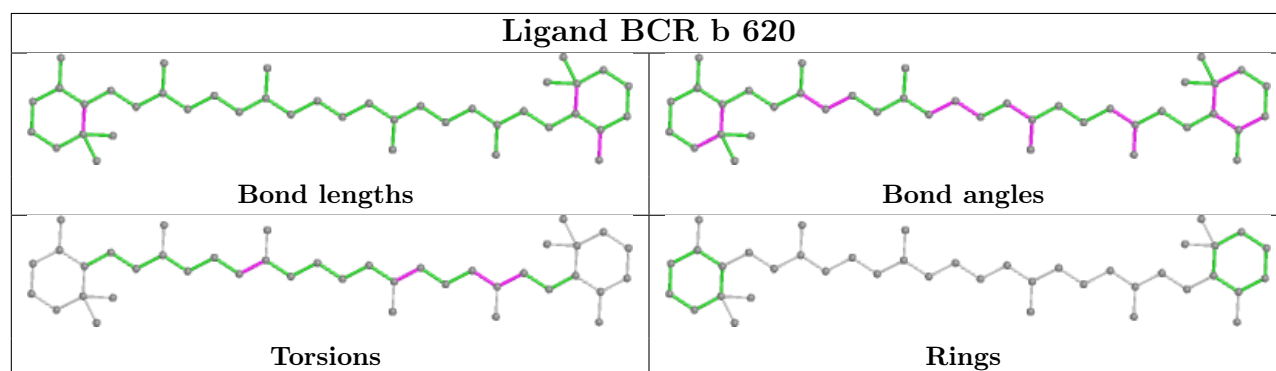
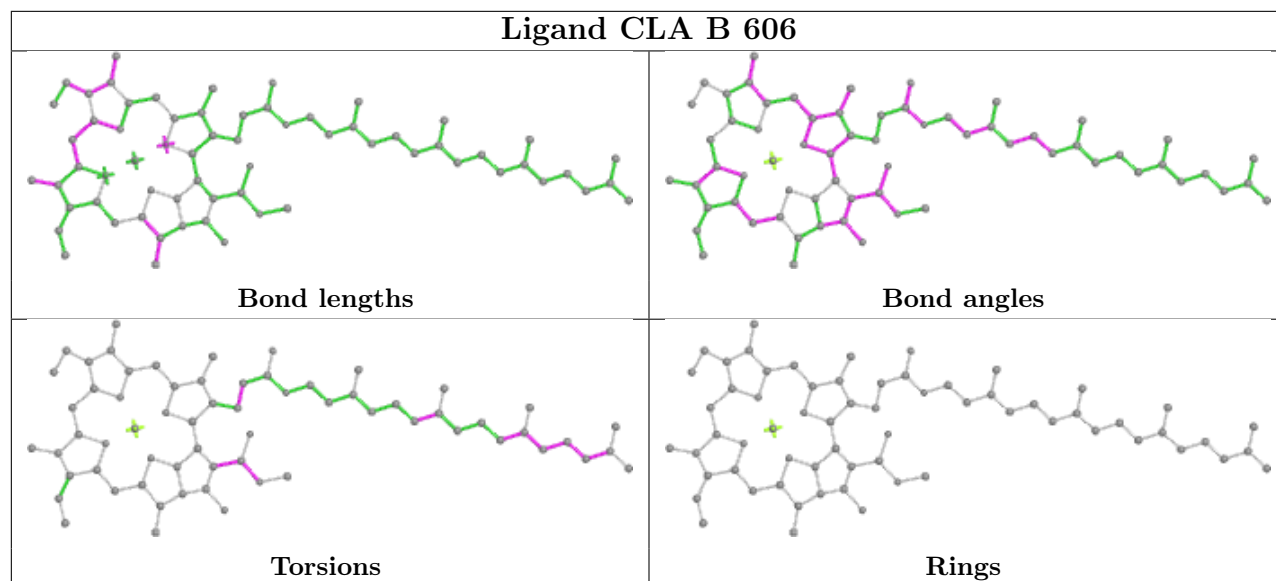
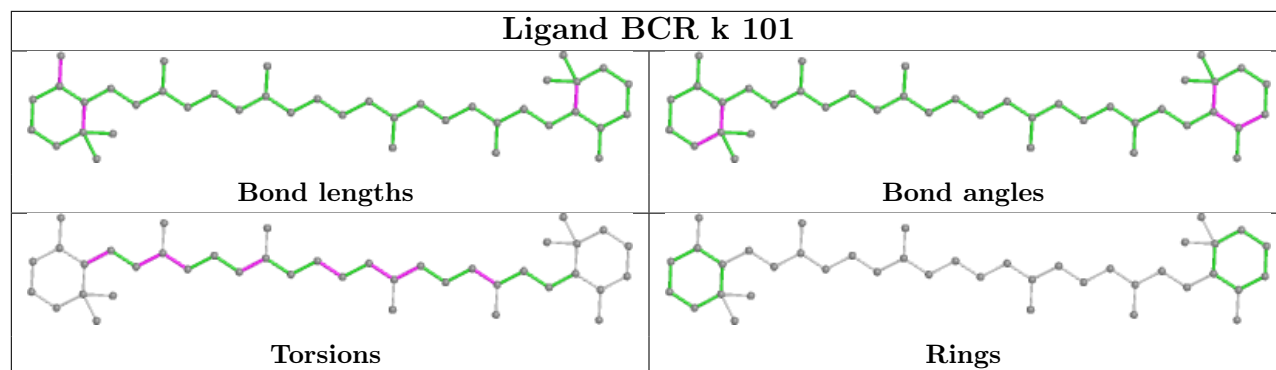


Ligand CLA d 404

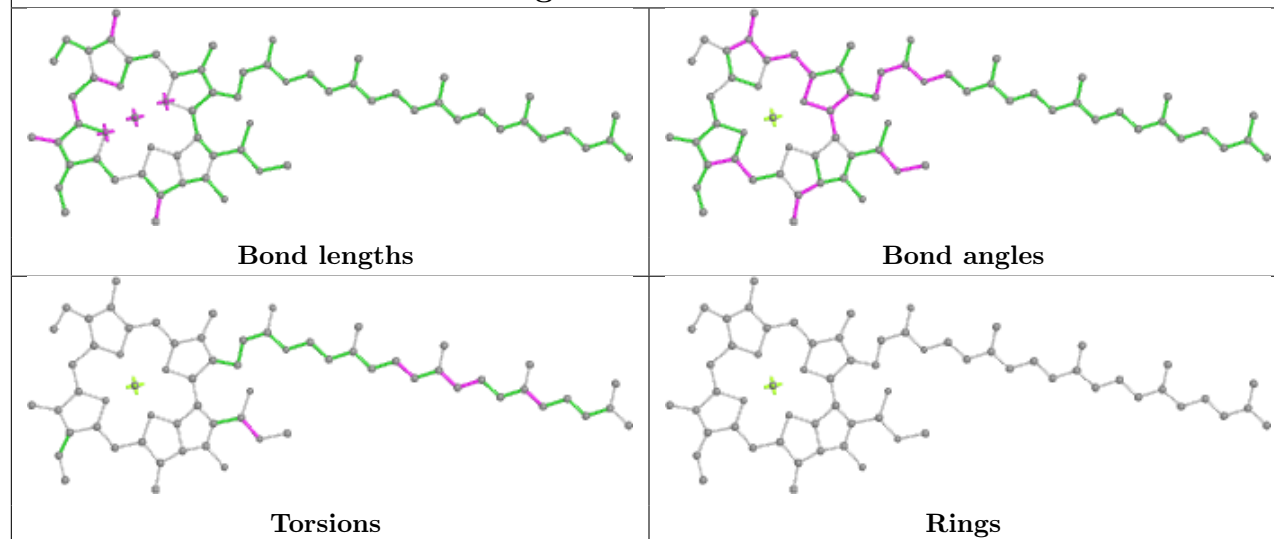


Ligand LMG D 410

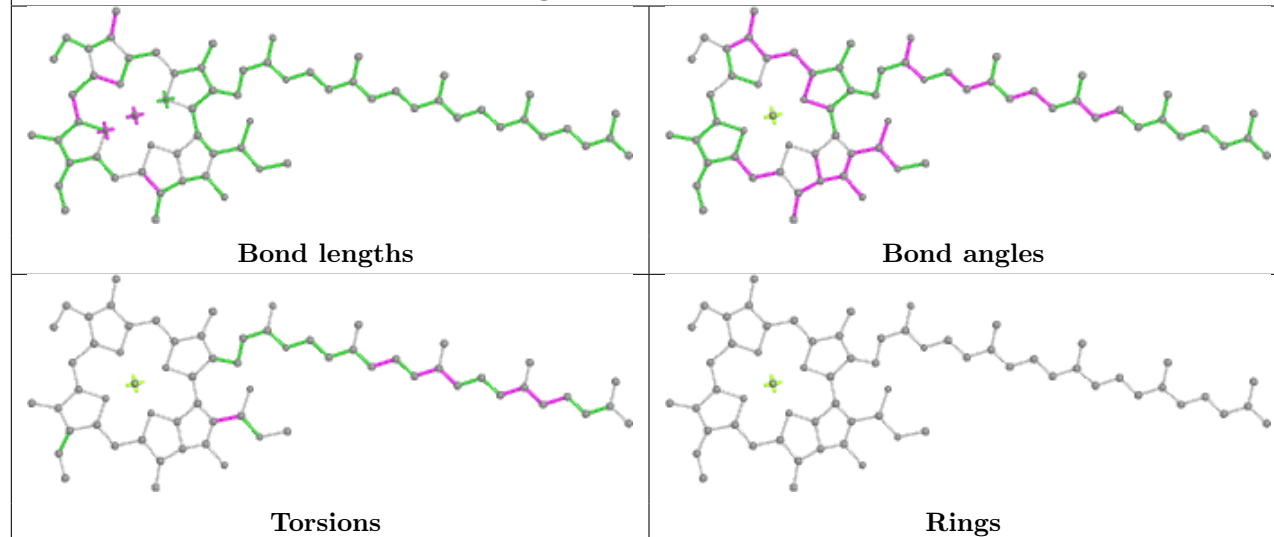




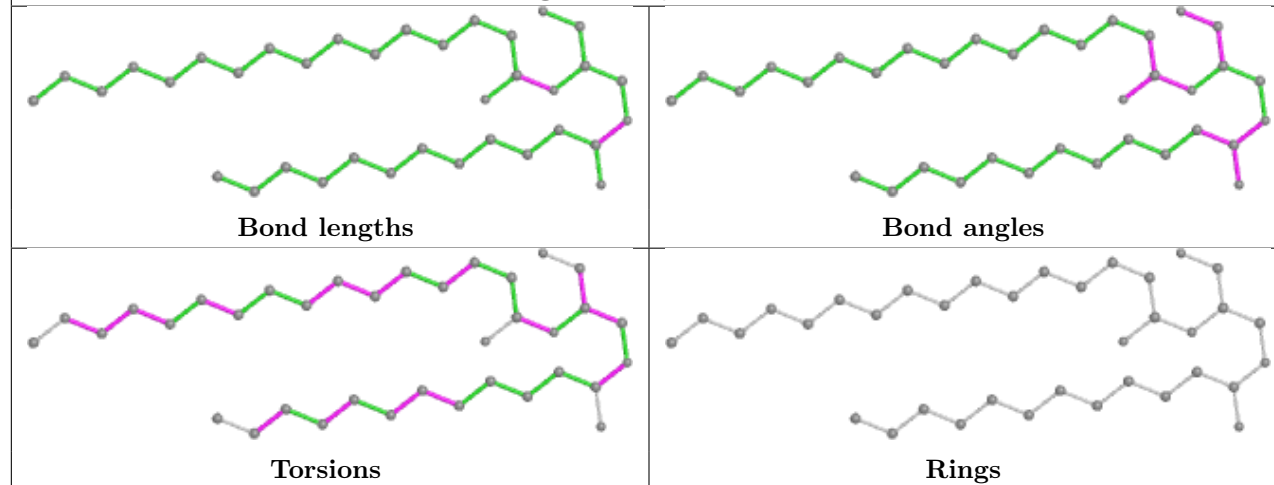
Ligand CLA b 616



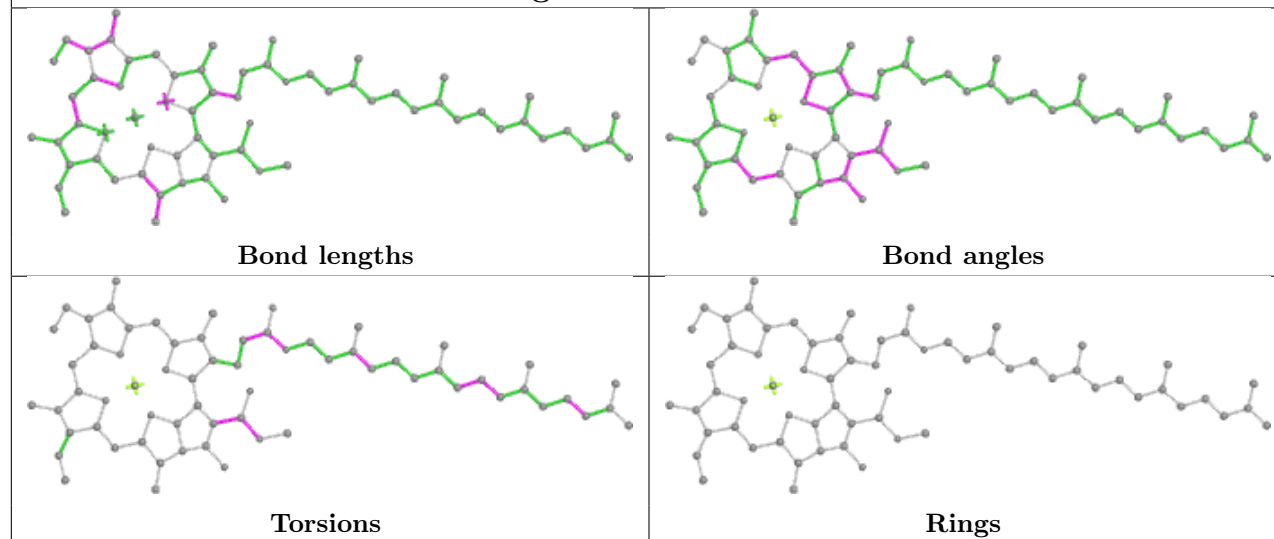
Ligand CLA b 605



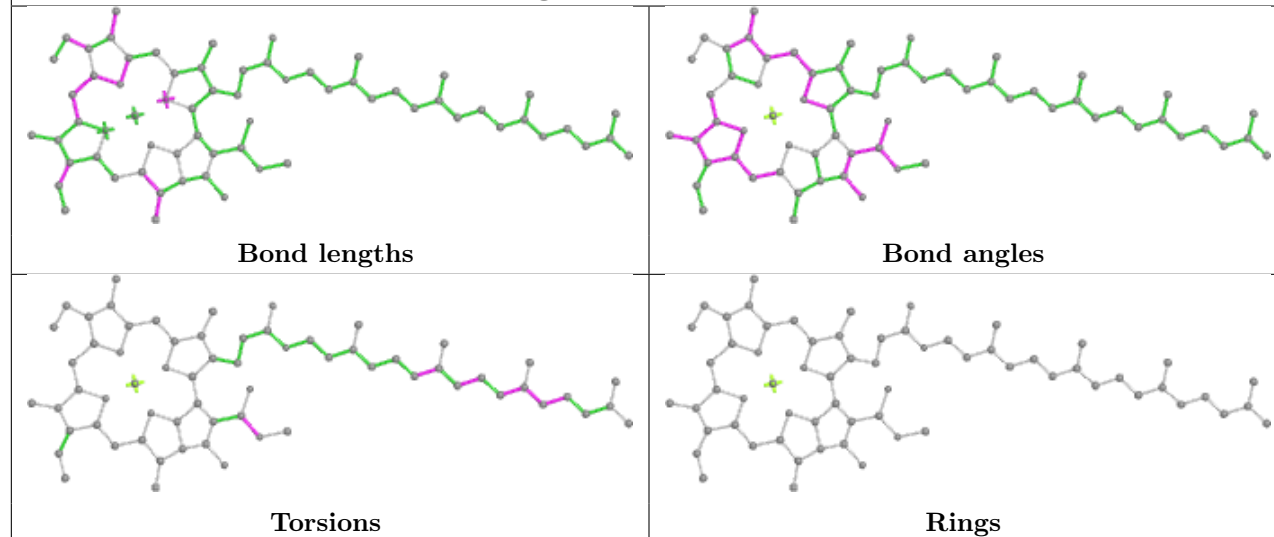
Ligand SQD a 412



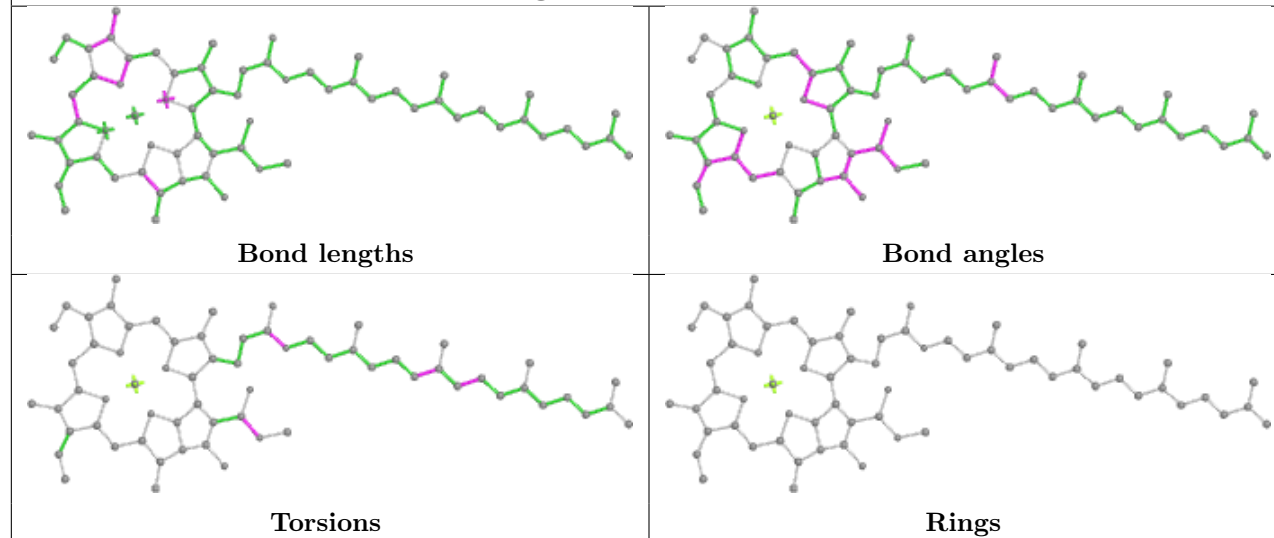
Ligand CLA B 601

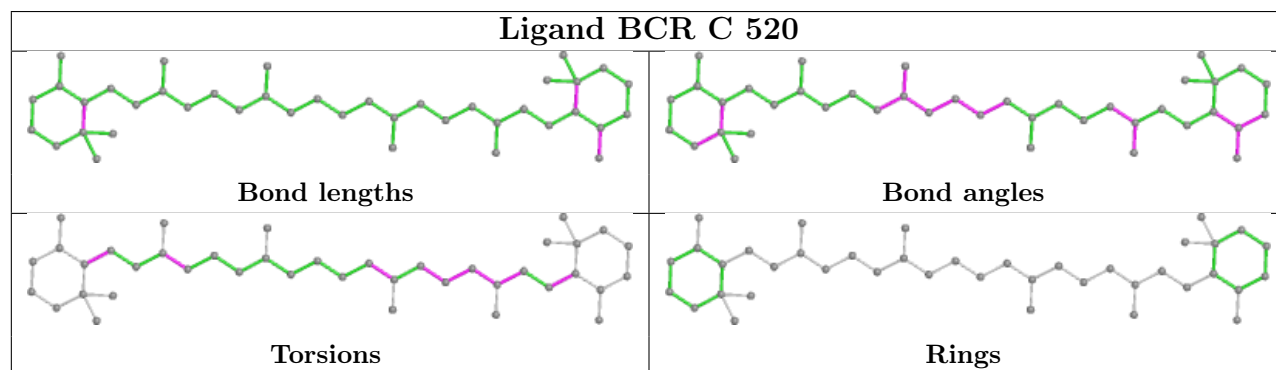
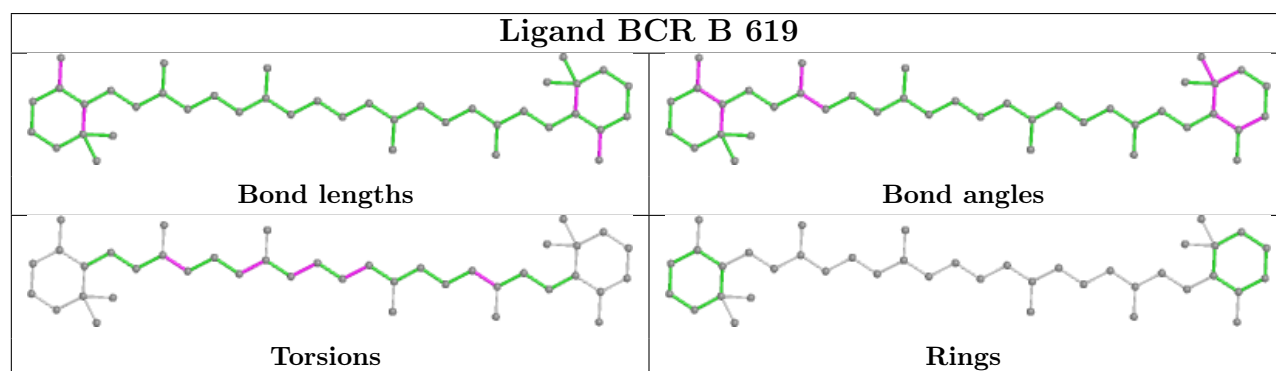
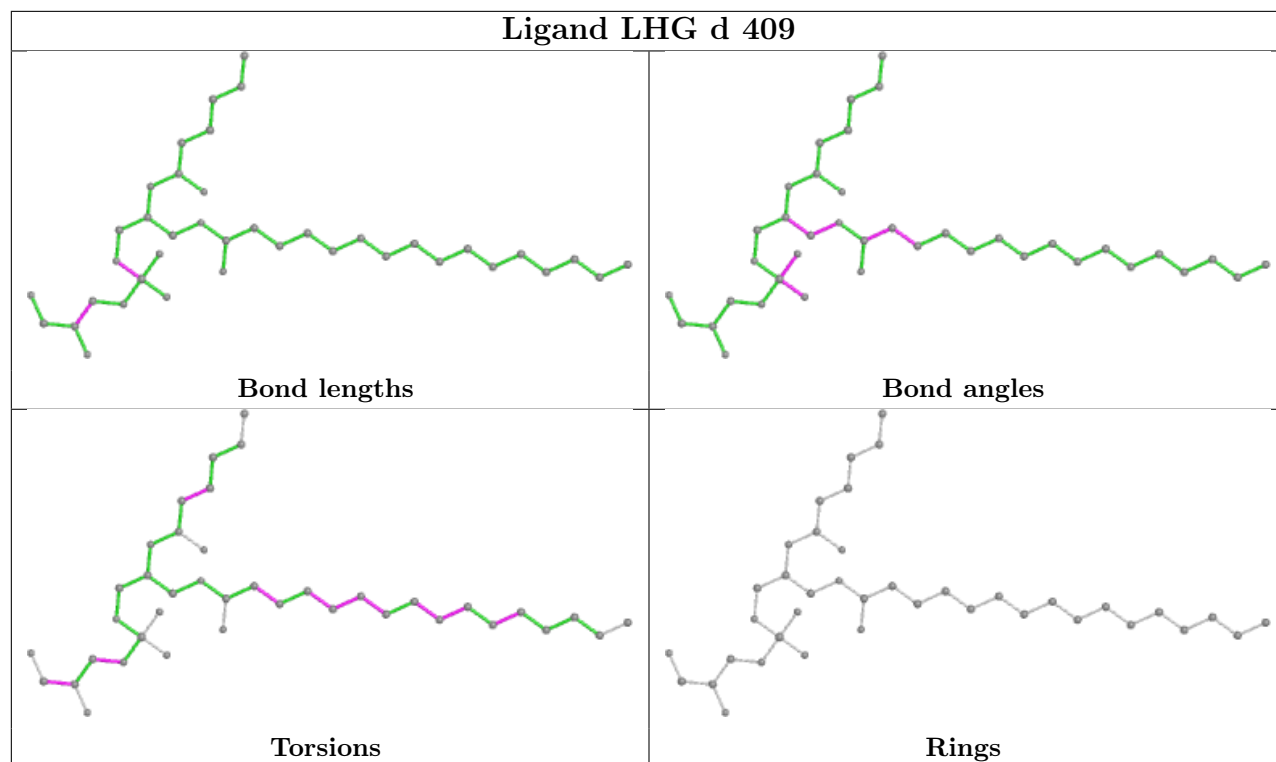


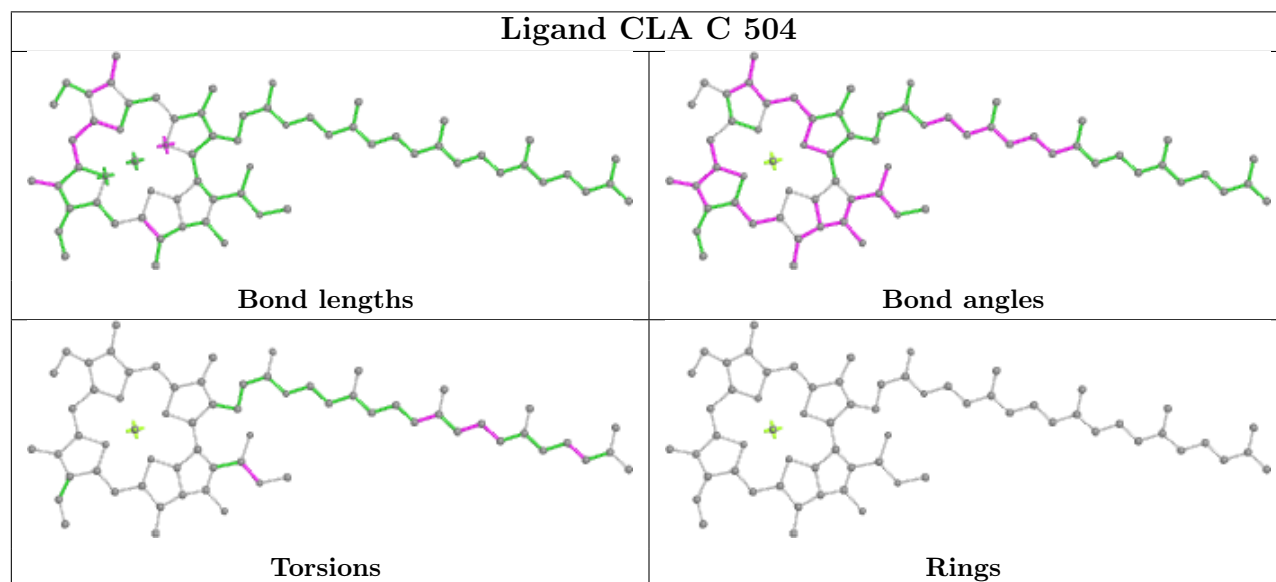
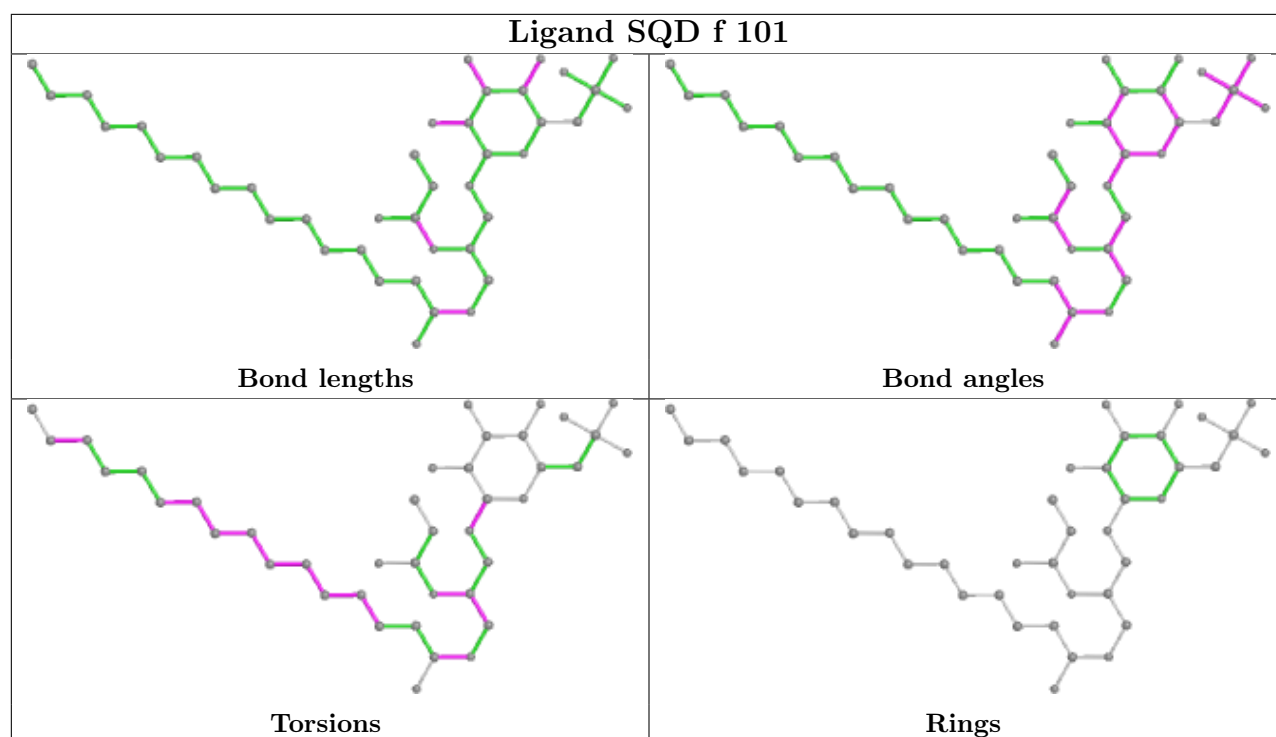
Ligand CLA b 603

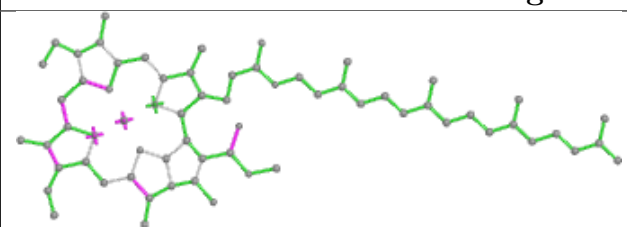
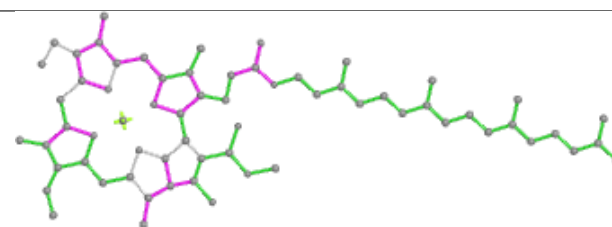
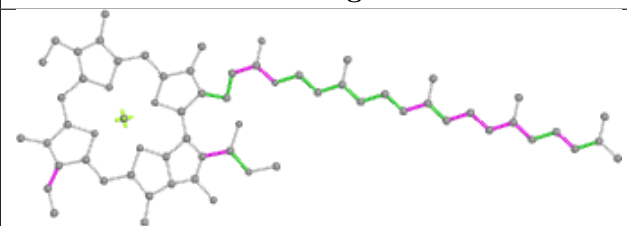
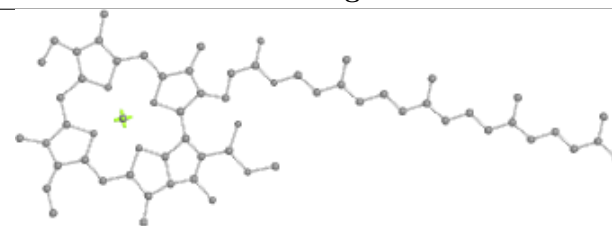


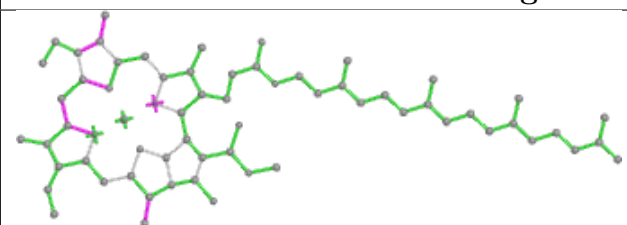
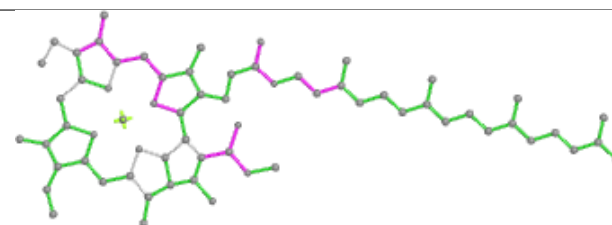
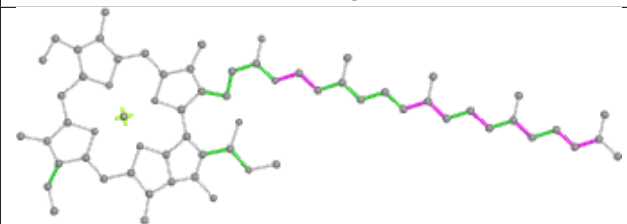
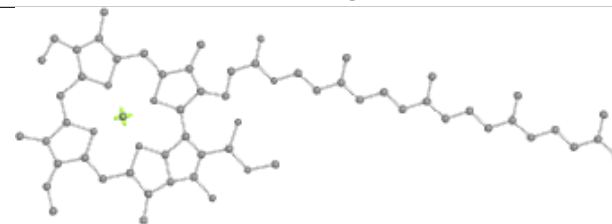
Ligand CLA C 512

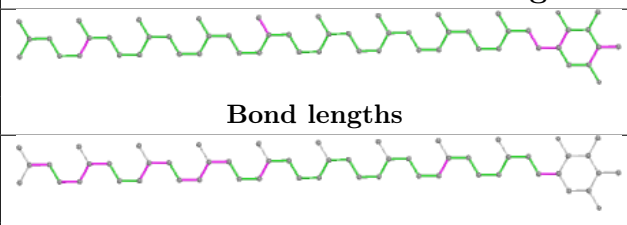
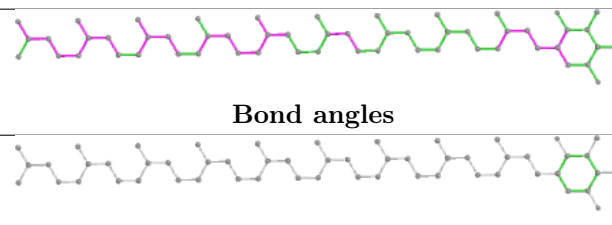
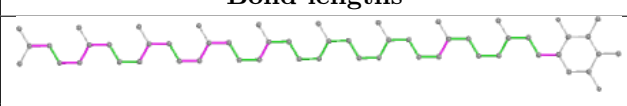
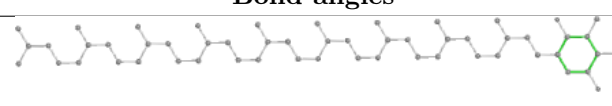






Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA D 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.63	3 (0%) 84 86	27, 35, 53, 81	0
1	a	334/334 (100%)	-0.59	1 (0%) 94 94	26, 36, 63, 84	0
2	B	505/505 (100%)	-0.51	7 (1%) 75 77	27, 39, 67, 107	0
2	b	505/505 (100%)	-0.41	12 (2%) 59 62	27, 42, 78, 104	0
3	C	442/451 (98%)	-0.47	1 (0%) 95 95	29, 42, 59, 81	0
3	c	451/451 (100%)	-0.42	4 (0%) 84 86	31, 46, 68, 109	0
4	D	341/341 (100%)	-0.50	0 100 100	27, 36, 53, 90	0
4	d	341/341 (100%)	-0.46	3 (0%) 84 86	28, 40, 62, 92	0
5	E	81/82 (98%)	-0.11	3 (3%) 41 45	39, 56, 74, 91	0
5	e	82/82 (100%)	0.23	5 (6%) 21 22	44, 63, 85, 94	0
6	F	34/34 (100%)	-0.58	2 (5%) 22 23	42, 48, 69, 86	0
6	f	34/34 (100%)	-0.46	0 100 100	49, 54, 83, 98	0
7	H	65/65 (100%)	-0.17	0 100 100	37, 45, 66, 87	0
7	h	63/65 (96%)	-0.12	2 (3%) 47 51	43, 54, 69, 78	0
8	I	35/36 (97%)	-0.49	0 100 100	32, 43, 73, 80	0
8	i	35/36 (97%)	-0.21	3 (8%) 10 10	33, 46, 83, 90	0
9	J	36/36 (100%)	0.19	4 (11%) 5 5	43, 54, 80, 104	0
9	j	36/36 (100%)	0.06	4 (11%) 5 5	42, 58, 93, 101	0
10	K	37/37 (100%)	-0.26	0 100 100	46, 60, 75, 77	0
10	k	37/37 (100%)	-0.05	1 (2%) 54 58	59, 67, 76, 82	0
11	L	37/37 (100%)	-0.46	0 100 100	29, 36, 75, 75	0
11	l	36/37 (97%)	-0.43	0 100 100	29, 37, 72, 83	0
12	M	32/33 (96%)	-0.36	1 (3%) 49 52	32, 38, 69, 75	0
12	m	31/33 (93%)	-0.42	0 100 100	32, 38, 57, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.13	12 (4%) 29 31	28, 48, 85, 150	0
13	o	244/244 (100%)	-0.26	12 (4%) 29 31	29, 46, 88, 133	0
14	T	29/30 (96%)	-0.77	1 (3%) 45 48	29, 37, 67, 74	0
14	t	29/30 (96%)	-0.60	2 (6%) 16 17	31, 37, 89, 92	0
15	U	97/97 (100%)	-0.34	2 (2%) 63 66	36, 49, 77, 103	0
15	u	97/97 (100%)	-0.50	1 (1%) 82 84	36, 46, 64, 91	0
16	V	137/137 (100%)	-0.63	0 100 100	34, 46, 62, 92	0
16	v	137/137 (100%)	-0.36	3 (2%) 62 65	36, 53, 76, 99	0
17	Y	27/30 (90%)	1.63	11 (40%) 0 0	57, 79, 114, 120	0
17	y	30/30 (100%)	0.39	1 (3%) 46 50	64, 78, 94, 111	0
18	X	38/38 (100%)	-0.13	3 (7%) 12 12	42, 53, 78, 83	0
18	x	38/38 (100%)	0.14	1 (2%) 56 59	52, 63, 87, 96	0
19	Z	62/62 (100%)	0.40	8 (12%) 3 3	55, 69, 115, 123	0
19	z	62/62 (100%)	0.77	12 (19%) 1 1	62, 79, 121, 127	0
20	R	34/34 (100%)	1.39	7 (20%) 1 0	66, 75, 95, 103	0
20	r	31/34 (91%)	2.19	17 (54%) 0 0	79, 93, 106, 110	0
All	All	5300/5326 (99%)	-0.35	149 (2%) 53 56	26, 44, 80, 150	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	20	ALA	8.4
13	O	60	ARG	7.9
19	z	33	TRP	7.2
13	o	3	GLN	7.0
13	O	3	GLN	6.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.96	0.16	41,55,69,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	FME	T	1	10/11	0.96	0.14	33,58,80,90	0
8	FME	i	1	10/11	0.96	0.18	39,54,68,78	0
12	FME	m	1	10/11	0.96	0.16	37,54,75,81	0
8	FME	I	1	10/11	0.97	0.14	48,61,72,83	0
14	FME	t	1	10/11	0.97	0.10	36,55,82,88	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	UNL	H	103	53/-	0.74	0.32	44,89,115,116	0
32	UNL	c	523	28/-	0.75	0.22	55,80,93,95	0
32	UNL	a	414	28/-	0.78	0.29	44,66,82,84	0
32	UNL	x	101	55/-	0.78	0.31	43,71,92,94	0
33	LMG	c	522	48/55	0.80	0.26	42,89,123,138	0
28	DGD	A	412	66/66	0.82	0.23	41,75,100,124	0
32	UNL	E	102	28/-	0.82	0.32	66,88,97,103	0
32	UNL	c	520	55/-	0.82	0.23	48,72,94,101	0
33	LMG	d	410	23/55	0.82	0.27	43,73,104,105	0
32	UNL	B	624	46/-	0.83	0.20	55,68,83,87	0
33	LMG	b	622	55/55	0.84	0.27	48,80,99,104	0
32	UNL	b	621	55/-	0.84	0.23	42,68,96,118	0
32	UNL	B	625	28/-	0.84	0.41	47,67,91,99	0
28	DGD	a	413	44/66	0.85	0.18	36,62,86,88	0
29	LHG	E	101	49/49	0.85	0.23	54,88,118,126	0
33	LMG	D	410	33/55	0.85	0.20	34,61,107,111	0
29	LHG	e	101	42/49	0.85	0.30	68,92,115,158	0
27	SQD	a	412	36/54	0.85	0.19	40,72,101,113	0
23	CLA	c	512	65/65	0.85	0.19	45,68,99,114	0
32	UNL	b	623	40/-	0.86	0.21	52,68,91,100	0
32	UNL	b	625	55/-	0.86	0.19	50,73,87,98	0
32	UNL	b	626	26/-	0.86	0.28	52,65,76,78	0
23	CLA	b	602	65/65	0.86	0.21	55,76,104,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	UNL	B	626	47/-	0.86	0.34	54,73,88,96	0
25	BCR	x	102	40/40	0.87	0.16	40,62,84,87	0
26	PL9	A	409	55/55	0.87	0.26	35,70,101,113	0
32	UNL	C	522	28/-	0.87	0.18	41,61,81,83	0
26	PL9	a	410	55/55	0.87	0.23	42,77,101,112	0
32	UNL	t	102	26/-	0.87	0.25	56,75,87,88	0
32	UNL	j	101	28/-	0.88	0.16	53,67,81,85	0
23	CLA	C	514	65/65	0.88	0.22	48,77,110,115	0
25	BCR	H	101	40/40	0.88	0.15	35,51,65,69	0
25	BCR	K	101	40/40	0.88	0.16	38,60,75,91	0
25	BCR	k	101	40/40	0.88	0.17	45,71,86,89	0
32	UNL	B	620	43/-	0.88	0.15	41,59,81,83	0
27	SQD	b	601	49/54	0.88	0.17	47,68,101,117	0
27	SQD	f	101	41/54	0.89	0.22	58,91,129,142	0
32	UNL	m	102	28/-	0.89	0.18	38,58,78,78	0
23	CLA	c	513	65/65	0.89	0.23	47,74,109,113	0
32	UNL	D	412	55/-	0.89	0.26	35,65,88,94	0
23	CLA	B	616	60/65	0.90	0.17	24,45,91,96	0
32	UNL	b	624	44/-	0.90	0.20	48,68,88,89	0
33	LMG	C	501	48/55	0.90	0.17	40,67,86,111	0
33	LMG	C	519	48/55	0.90	0.20	53,85,105,121	0
32	UNL	d	412	43/-	0.90	0.20	50,62,78,83	0
33	LMG	D	411	28/55	0.90	0.18	34,58,76,80	0
23	CLA	D	404	65/65	0.90	0.17	26,47,133,138	0
32	UNL	l	102	53/-	0.90	0.19	36,55,96,102	0
32	UNL	C	521	28/-	0.90	0.14	35,50,62,67	0
32	UNL	T	102	47/-	0.91	0.21	34,52,79,81	0
27	SQD	A	411	39/54	0.91	0.23	43,73,96,111	0
27	SQD	B	621	54/54	0.91	0.16	43,67,104,121	0
27	SQD	F	101	36/54	0.91	0.16	48,76,102,107	0
23	CLA	B	601	65/65	0.91	0.16	36,65,116,139	0
23	CLA	C	513	65/65	0.91	0.17	35,62,112,146	0
32	UNL	B	622	34/-	0.91	0.16	38,55,71,72	0
23	CLA	a	408	65/65	0.91	0.16	22,41,107,114	0
32	UNL	I	101	41/-	0.91	0.14	42,62,95,99	0
33	LMG	c	519	37/55	0.91	0.18	45,74,99,105	0
32	UNL	J	101	28/-	0.91	0.23	48,62,74,75	0
33	LMG	c	524	49/55	0.91	0.15	31,60,96,125	0
32	UNL	M	103	26/-	0.91	0.20	36,54,72,72	0
23	CLA	c	508	64/65	0.92	0.15	32,54,97,122	0
25	BCR	d	405	40/40	0.92	0.16	39,59,110,121	0
33	LMG	D	407	51/55	0.92	0.18	34,64,86,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	DGD	c	517	62/66	0.92	0.15	37,62,94,112	0
23	CLA	d	404	65/65	0.92	0.16	31,56,111,137	0
25	BCR	C	515	40/40	0.92	0.15	24,46,60,75	0
32	UNL	C	523	47/-	0.92	0.15	47,60,78,78	0
25	BCR	D	405	40/40	0.92	0.15	34,50,95,115	0
23	CLA	b	617	60/65	0.92	0.14	33,50,94,105	0
32	UNL	B	623	28/-	0.92	0.12	36,52,70,76	0
23	CLA	c	511	65/65	0.93	0.17	45,66,85,88	0
27	SQD	a	411	54/54	0.93	0.16	45,75,97,102	0
28	DGD	c	518	62/66	0.93	0.15	30,63,82,92	0
23	CLA	c	502	65/65	0.93	0.15	36,52,71,82	0
33	LMG	M	101	51/55	0.93	0.13	33,54,75,89	0
23	CLA	c	503	65/65	0.93	0.19	33,54,68,71	0
23	CLA	c	507	65/65	0.93	0.15	35,51,66,69	0
23	CLA	C	503	65/65	0.93	0.14	37,51,67,80	0
28	DGD	C	516	62/66	0.93	0.15	27,44,87,103	0
28	DGD	C	517	62/66	0.93	0.14	40,62,111,122	0
33	LMG	d	411	44/55	0.93	0.14	41,63,94,112	0
33	LMG	m	101	51/55	0.93	0.14	37,60,85,98	0
25	BCR	T	101	40/40	0.94	0.13	30,50,64,70	0
25	BCR	Z	101	40/40	0.94	0.17	41,63,81,84	0
25	BCR	b	618	40/40	0.94	0.13	31,50,67,67	0
28	DGD	h	101	62/66	0.94	0.13	35,55,69,73	0
25	BCR	b	620	40/40	0.94	0.14	34,58,75,80	0
29	LHG	d	407	49/49	0.94	0.16	38,59,98,112	0
29	LHG	d	409	39/49	0.94	0.14	35,56,75,81	0
25	BCR	c	514	40/40	0.94	0.21	44,65,80,80	0
25	BCR	c	521	40/40	0.94	0.18	39,61,68,74	0
23	CLA	b	605	65/65	0.94	0.16	25,42,84,98	0
23	CLA	b	607	65/65	0.94	0.12	30,48,78,87	0
23	CLA	c	509	65/65	0.94	0.22	37,56,73,83	0
23	CLA	c	510	65/65	0.94	0.16	39,57,78,89	0
23	CLA	b	615	65/65	0.94	0.17	24,46,85,89	0
23	CLA	b	616	65/65	0.94	0.14	33,48,69,80	0
23	CLA	C	506	65/65	0.94	0.19	27,46,69,79	0
23	CLA	B	606	65/65	0.94	0.13	26,43,85,94	0
25	BCR	B	618	40/40	0.94	0.12	29,45,68,69	0
25	BCR	B	619	40/40	0.94	0.12	33,49,66,84	0
23	CLA	B	615	65/65	0.94	0.15	27,46,70,81	0
25	BCR	C	520	40/40	0.94	0.18	42,60,75,79	0
23	CLA	c	504	60/65	0.94	0.14	36,54,83,87	0
32	UNL	M	102	37/-	0.94	0.13	37,51,63,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	505	65/65	0.94	0.17	31,48,70,79	0
23	CLA	c	506	65/65	0.94	0.16	35,60,114,126	0
28	DGD	H	102	62/66	0.94	0.13	32,52,68,76	0
26	PL9	D	406	55/55	0.95	0.13	22,38,49,55	0
23	CLA	C	512	65/65	0.95	0.14	37,58,76,83	0
29	LHG	D	409	47/49	0.95	0.14	36,56,90,108	0
27	SQD	A	410	52/54	0.95	0.15	37,68,94,102	0
23	CLA	A	405	65/65	0.95	0.13	23,41,104,122	0
23	CLA	B	604	65/65	0.95	0.14	25,41,92,98	0
23	CLA	c	501	65/65	0.95	0.15	30,46,58,67	0
23	CLA	A	407	54/65	0.95	0.14	25,38,83,85	0
25	BCR	b	619	40/40	0.95	0.11	33,46,58,62	0
23	CLA	a	406	65/65	0.95	0.14	31,48,99,114	0
25	BCR	B	617	40/40	0.95	0.13	32,48,61,67	0
25	BCR	c	515	40/40	0.95	0.15	32,52,66,80	0
23	CLA	B	613	65/65	0.95	0.14	24,36,71,82	0
23	CLA	C	507	65/65	0.95	0.14	27,49,103,114	0
23	CLA	C	508	65/65	0.95	0.15	29,44,66,71	0
23	CLA	C	511	65/65	0.95	0.13	35,55,81,86	0
23	CLA	b	614	65/65	0.95	0.15	23,41,92,97	0
28	DGD	C	518	62/66	0.96	0.12	32,58,86,104	0
23	CLA	C	509	65/65	0.96	0.12	28,51,114,130	0
23	CLA	b	606	65/65	0.96	0.14	27,43,57,61	0
28	DGD	c	516	62/66	0.96	0.12	25,46,78,94	0
23	CLA	C	510	65/65	0.96	0.14	35,51,71,72	0
23	CLA	b	608	65/65	0.96	0.12	23,42,73,81	0
23	CLA	b	610	65/65	0.96	0.12	27,48,67,93	0
29	LHG	A	413	49/49	0.96	0.13	31,53,82,87	0
23	CLA	b	613	65/65	0.96	0.16	24,40,56,65	0
23	CLA	d	402	65/65	0.96	0.12	26,39,50,54	0
23	CLA	d	403	65/65	0.96	0.12	24,41,75,83	0
25	BCR	t	101	40/40	0.96	0.10	31,45,57,65	0
23	CLA	B	605	65/65	0.96	0.17	23,39,55,60	0
29	LHG	l	101	49/49	0.96	0.12	38,51,63,81	0
24	PHO	A	406	64/64	0.96	0.12	20,35,49,55	0
24	PHO	a	407	64/64	0.96	0.14	24,36,48,50	0
25	BCR	A	408	40/40	0.96	0.10	25,37,50,51	0
26	PL9	d	406	55/55	0.96	0.13	27,41,49,54	0
23	CLA	B	603	65/65	0.96	0.15	26,42,69,76	0
23	CLA	B	609	65/65	0.96	0.12	23,42,59,66	0
23	CLA	C	504	65/65	0.96	0.12	30,50,63,68	0
23	CLA	D	403	65/65	0.96	0.11	22,37,58,68	0

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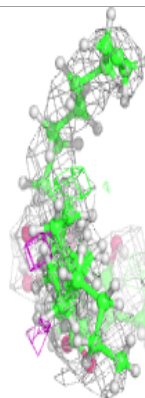
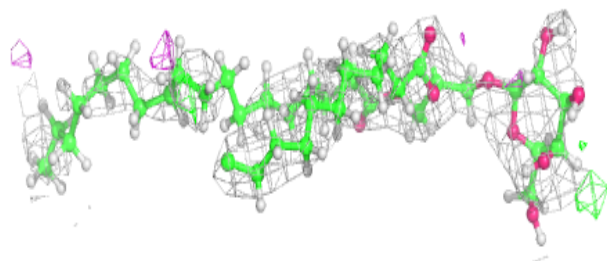
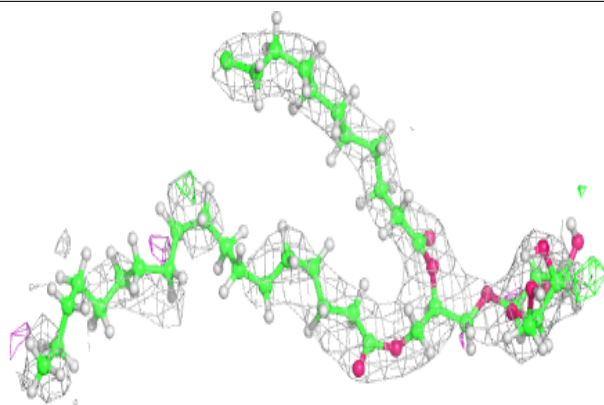
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	C	505	59/65	0.96	0.14	30,52,92,107	0
23	CLA	B	610	65/65	0.96	0.16	25,39,55,62	0
23	CLA	B	602	65/65	0.96	0.15	28,44,72,77	0
23	CLA	B	614	65/65	0.96	0.14	25,46,93,105	0
23	CLA	b	603	65/65	0.96	0.16	28,50,75,82	0
23	CLA	b	604	65/65	0.96	0.15	28,44,70,74	0
25	BCR	a	409	40/40	0.96	0.11	25,42,57,63	0
34	HEM	E	103	43/43	0.96	0.14	39,53,69,76	0
23	CLA	b	609	65/65	0.97	0.12	27,48,72,79	0
23	CLA	B	607	65/65	0.97	0.12	18,41,77,85	0
23	CLA	b	611	65/65	0.97	0.13	26,41,59,70	0
23	CLA	b	612	65/65	0.97	0.11	26,38,58,62	0
23	CLA	D	402	65/65	0.97	0.12	22,35,54,60	0
23	CLA	B	611	65/65	0.97	0.12	20,34,47,48	0
29	LHG	D	408	49/49	0.97	0.11	30,46,62,65	0
24	PHO	D	401	64/64	0.97	0.10	26,37,47,51	0
23	CLA	B	612	65/65	0.97	0.16	23,38,55,59	0
29	LHG	L	101	49/49	0.97	0.13	31,46,63,69	0
24	PHO	d	401	64/64	0.97	0.11	32,45,59,68	0
29	LHG	d	408	49/49	0.97	0.12	27,48,66,67	0
23	CLA	a	405	65/65	0.97	0.12	25,37,55,65	0
23	CLA	C	502	65/65	0.97	0.12	25,43,59,68	0
23	CLA	A	404	65/65	0.97	0.12	19,33,54,68	0
34	HEM	e	102	43/43	0.97	0.12	46,63,79,83	0
23	CLA	B	608	65/65	0.98	0.11	24,40,58,65	0
31	BCT	a	404	4/4	0.98	0.23	27,36,48,58	0
35	HEC	V	201	43/43	0.98	0.11	28,38,50,51	0
35	HEC	v	201	43/43	0.98	0.15	37,45,57,61	0
21	FE2	A	401	1/1	0.99	0.09	32,32,32,32	0
21	FE2	a	401	1/1	0.99	0.07	39,39,39,39	0
22	CL	A	402	1/1	0.99	0.06	36,36,36,36	0
22	CL	A	403	1/1	0.99	0.09	36,36,36,36	0
30	OEX	A	414	10/10	0.99	0.11	31,36,39,42	0
30	OEX	a	415	10/10	0.99	0.11	29,33,38,39	0
31	BCT	A	415	4/4	0.99	0.24	32,35,39,42	0
22	CL	a	402	1/1	1.00	0.08	34,34,34,34	0
22	CL	a	403	1/1	1.00	0.03	32,32,32,32	0

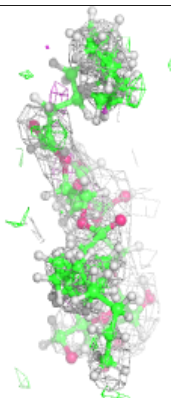
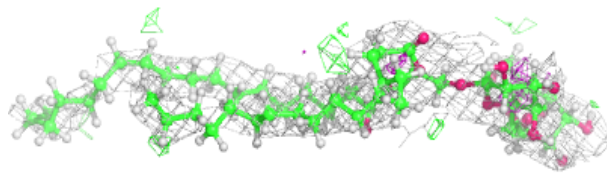
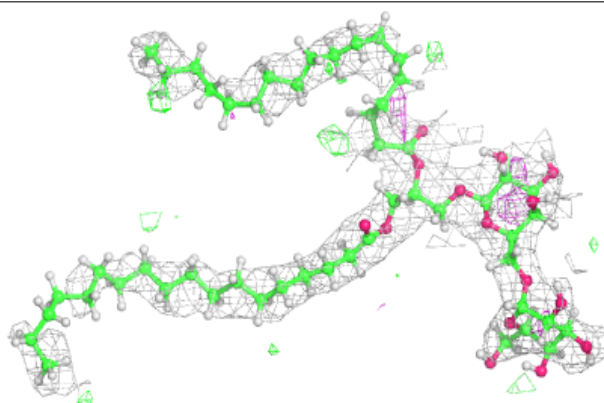
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMG c 522:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

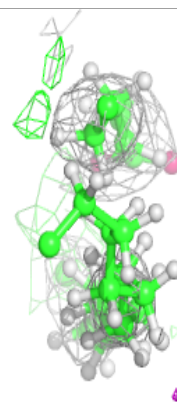
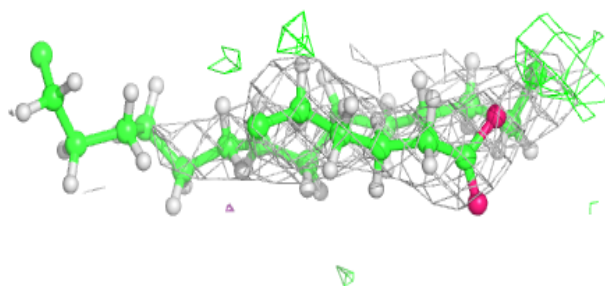
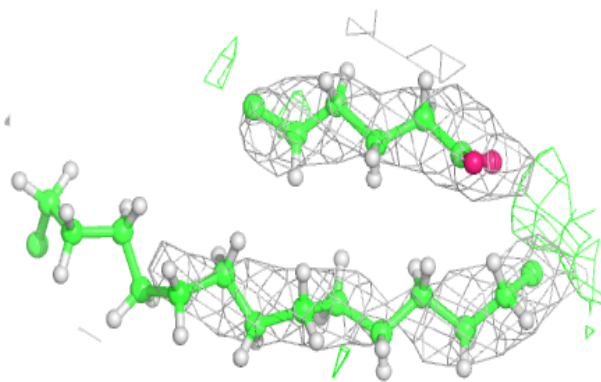
**Electron density around DGD A 412:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

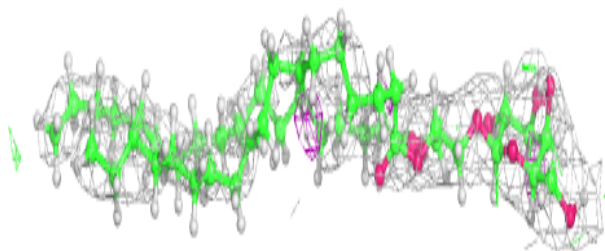
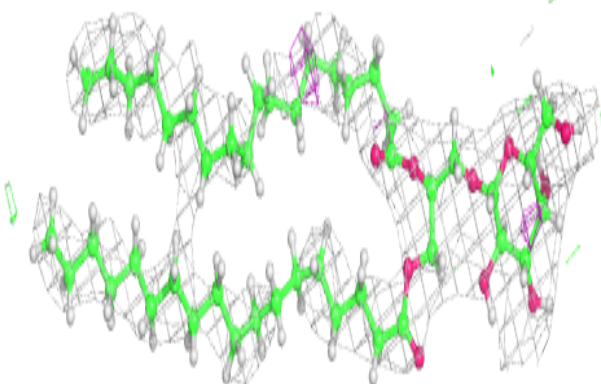


Electron density around LMG d 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

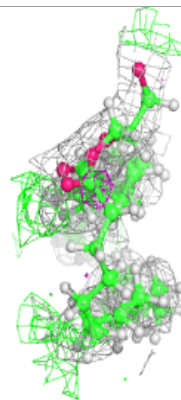
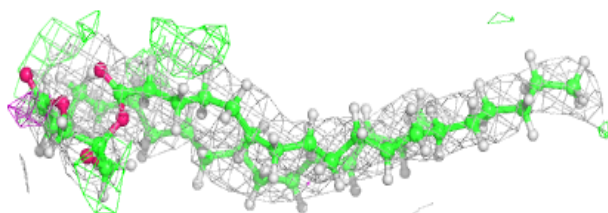
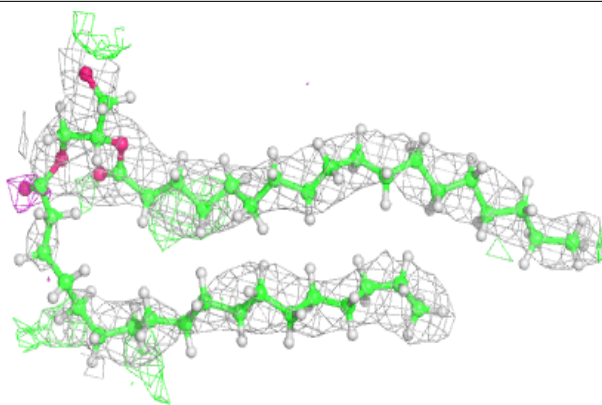
**Electron density around LMG b 622:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



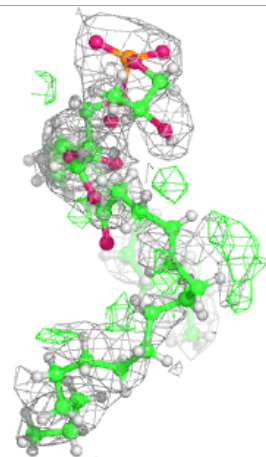
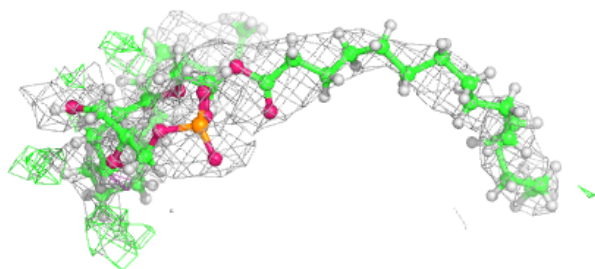
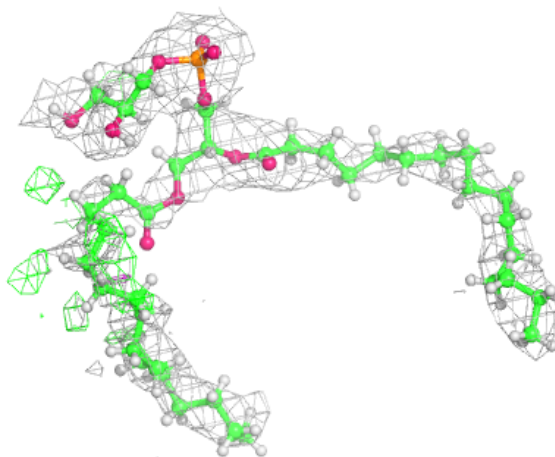
Electron density around DGD a 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



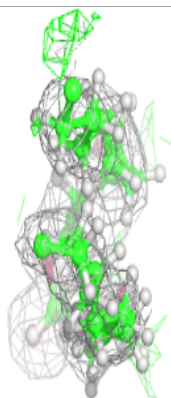
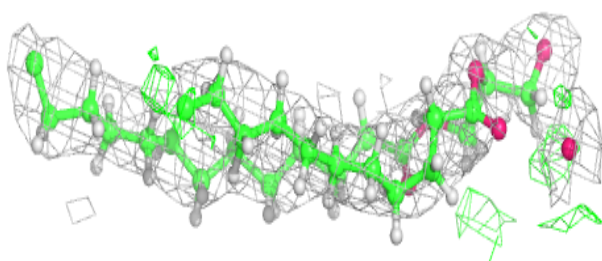
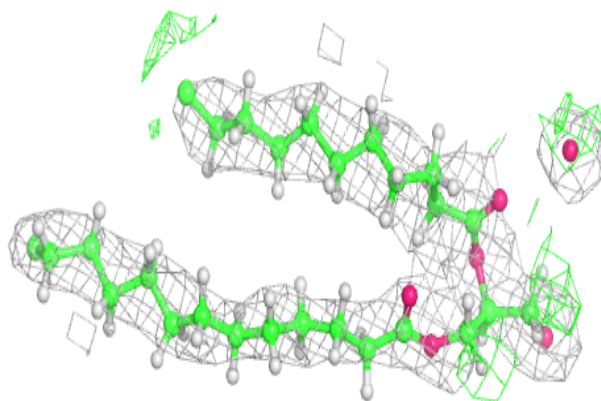
Electron density around LHG E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

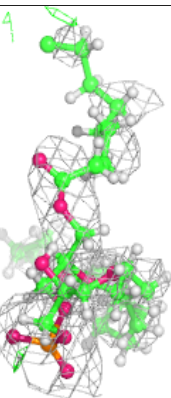
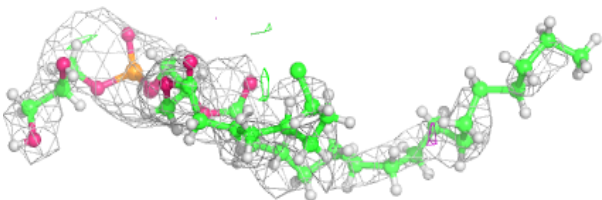
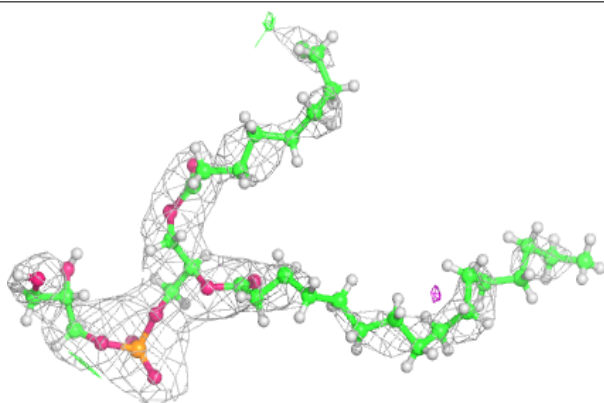


Electron density around LMG D 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

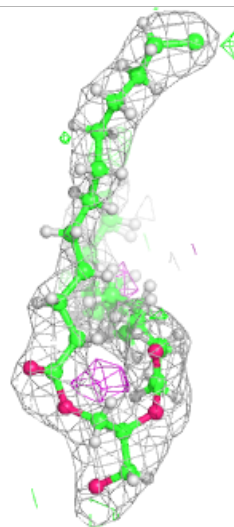
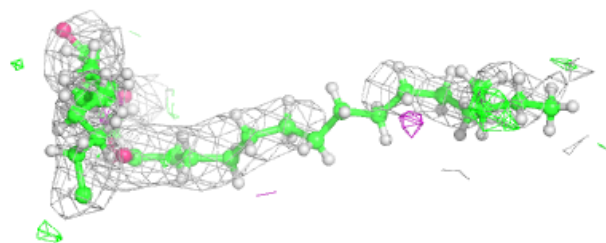
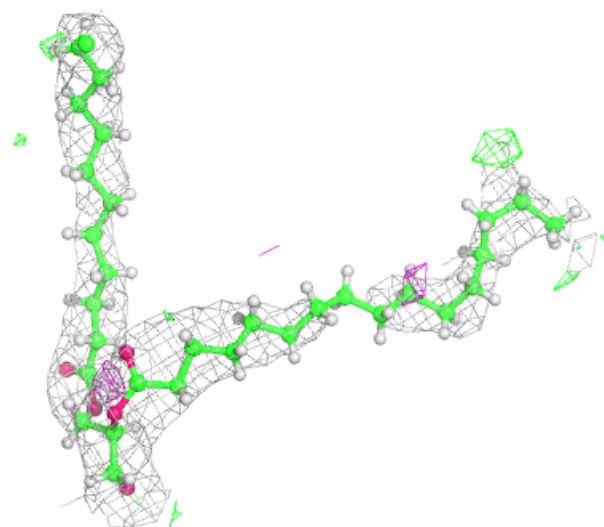
**Electron density around LHG e 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



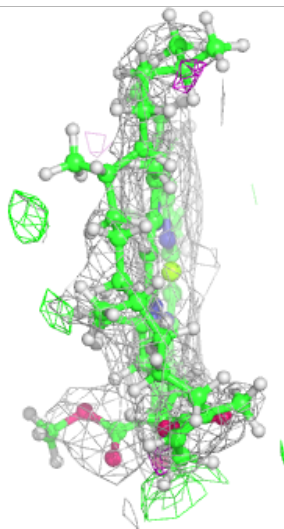
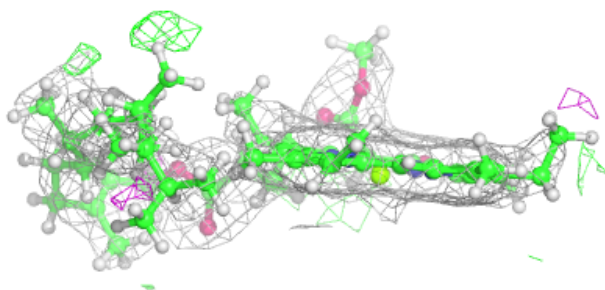
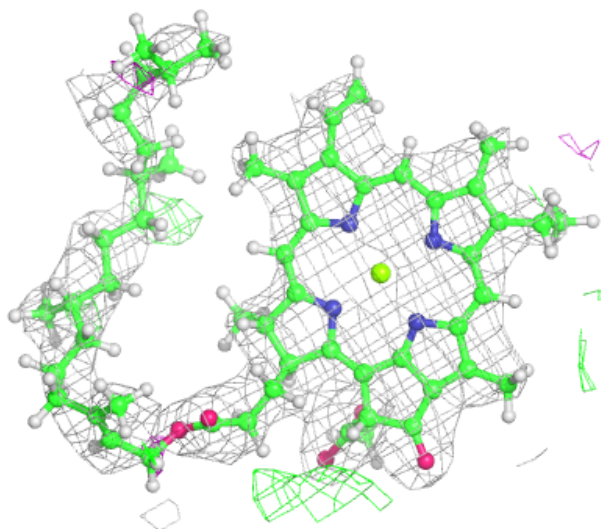
Electron density around SQD a 412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



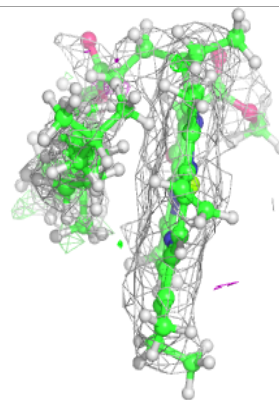
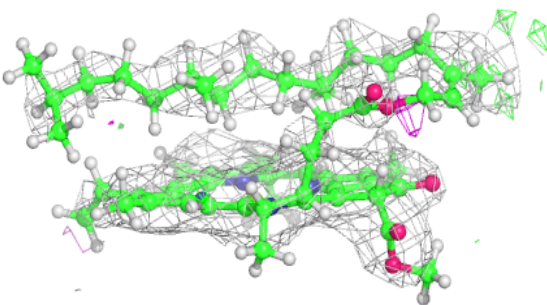
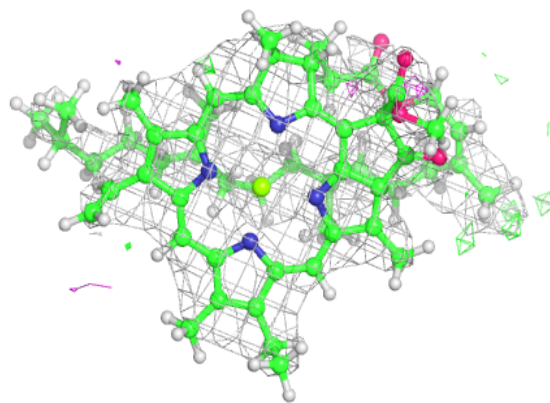
Electron density around CLA c 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

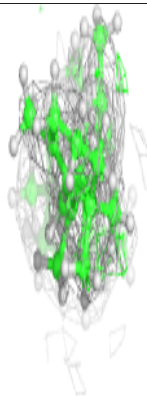
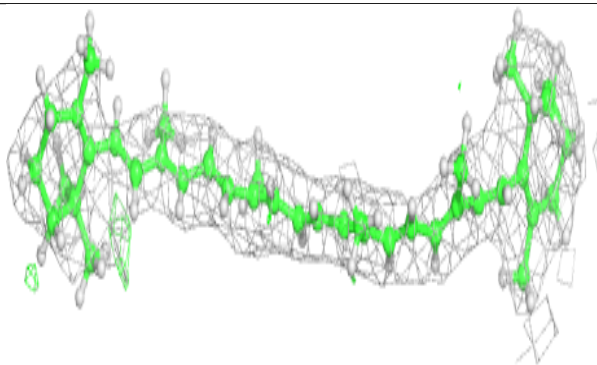
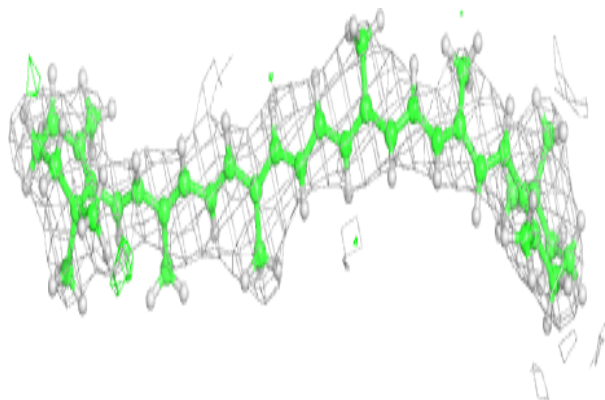


Electron density around CLA b 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

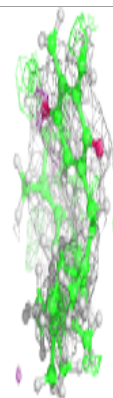
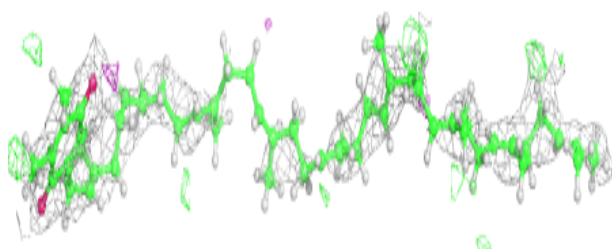
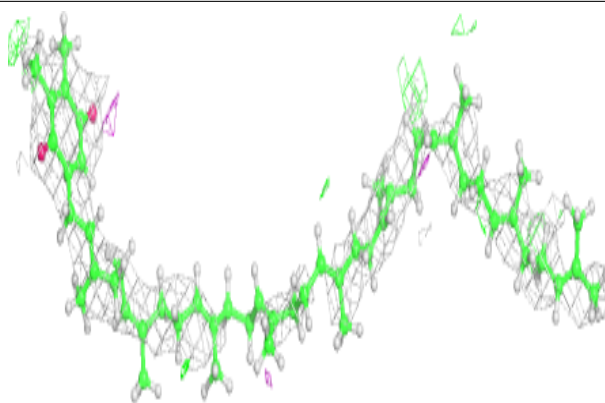
**Electron density around BCR x 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

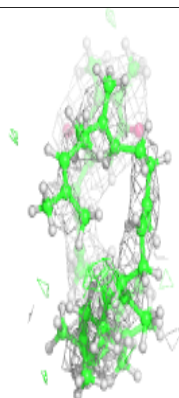
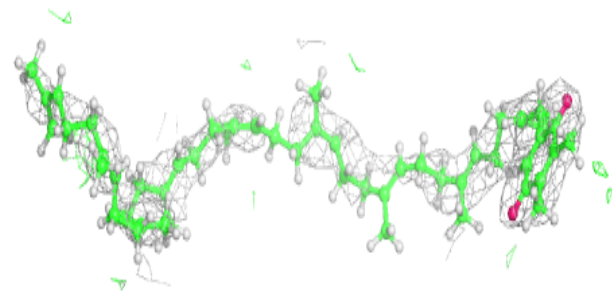
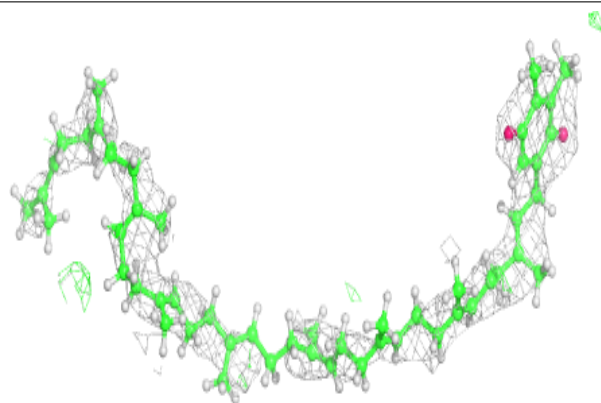


Electron density around PL9 A 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

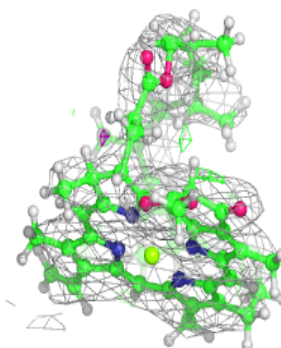
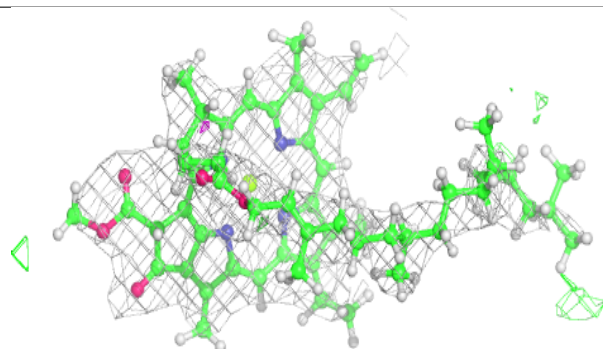
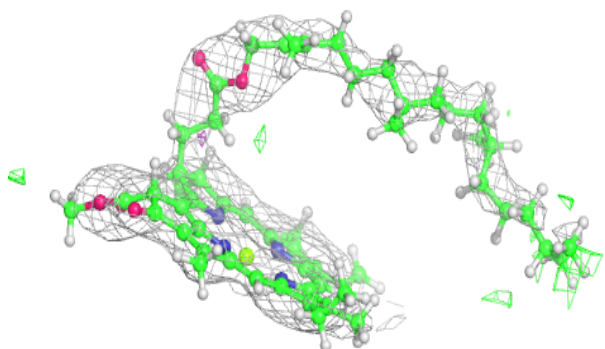
**Electron density around PL9 a 410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

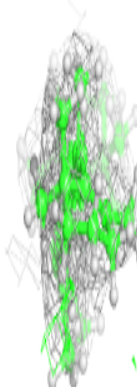
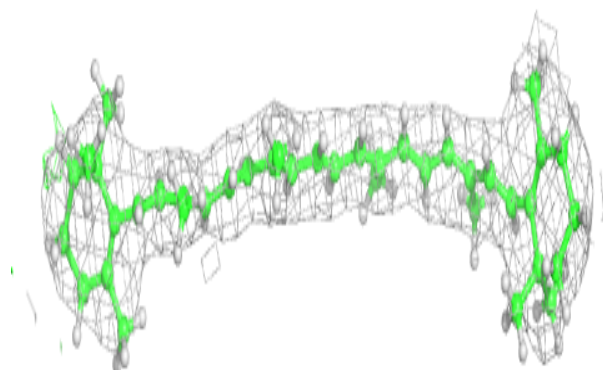
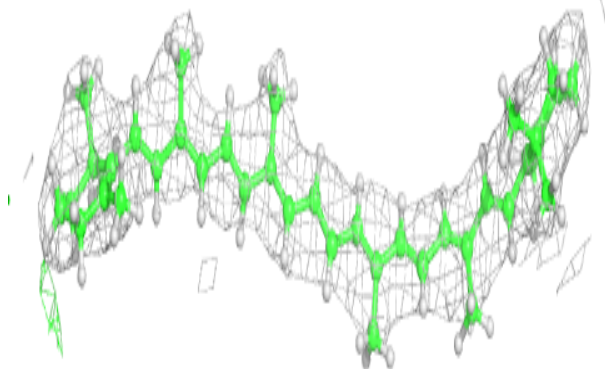


Electron density around CLA C 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

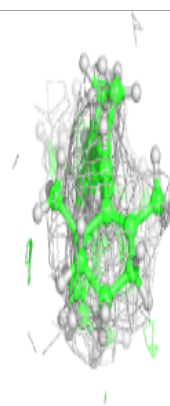
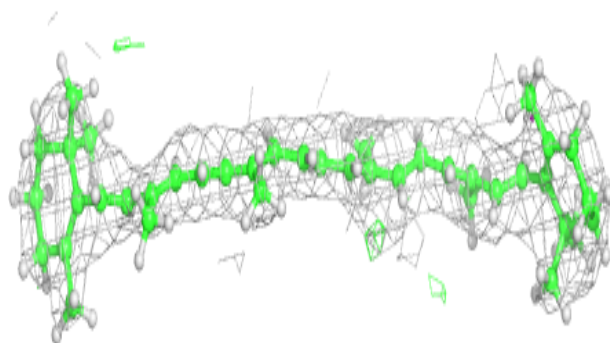
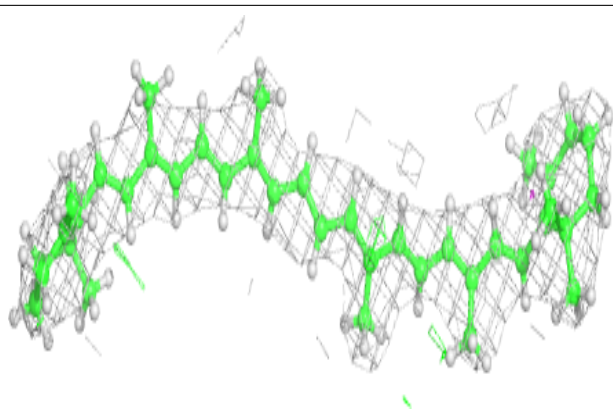
**Electron density around BCR H 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

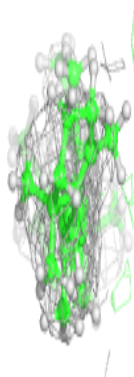
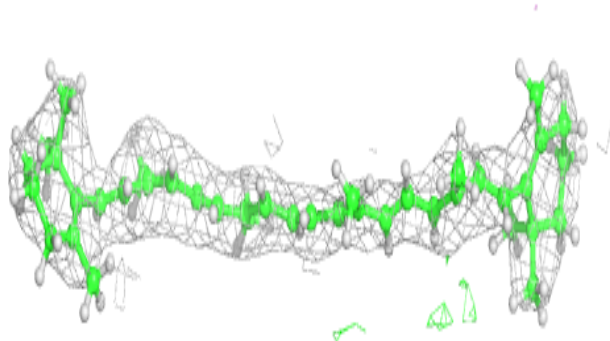
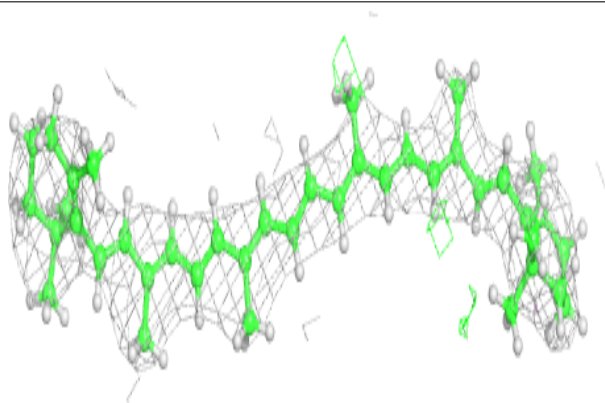


Electron density around BCR K 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

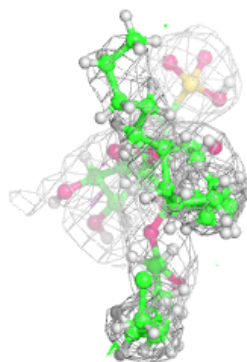
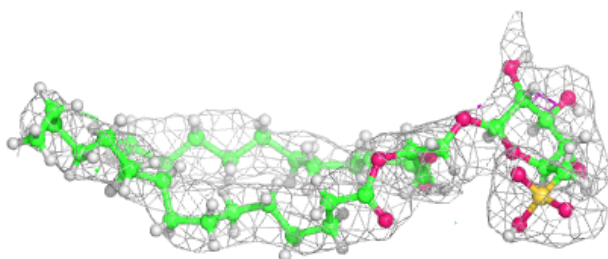
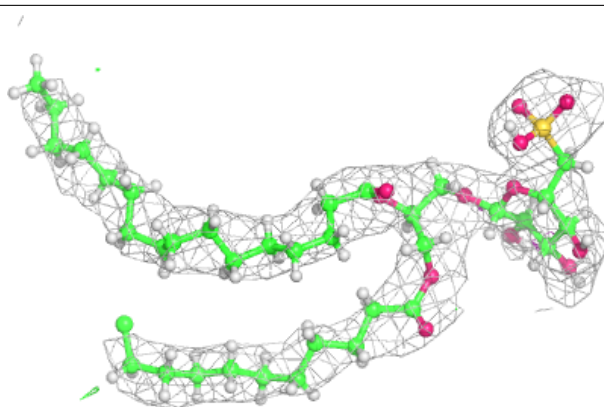
**Electron density around BCR k 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

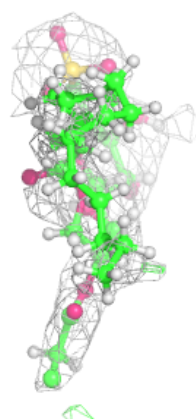
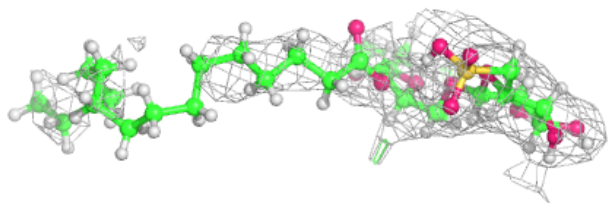
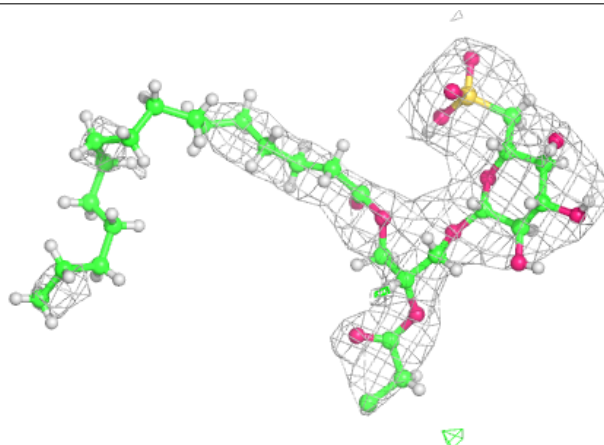


Electron density around SQD b 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

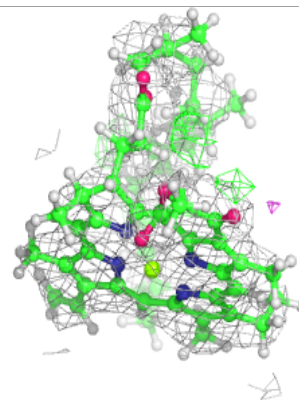
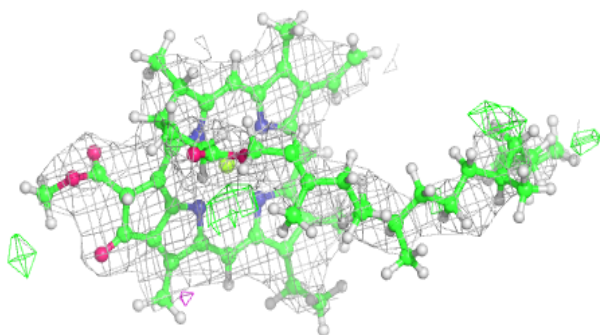
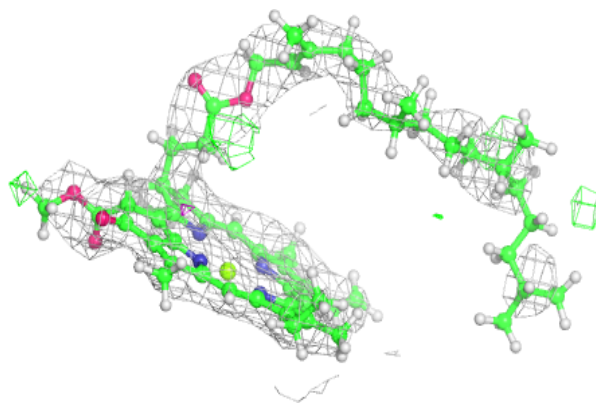
**Electron density around SQD f 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



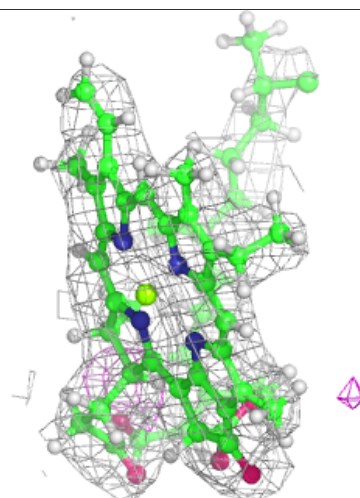
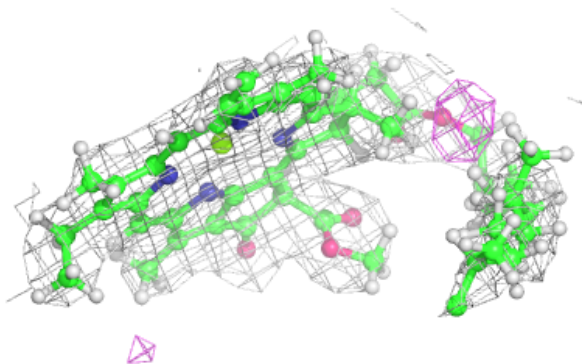
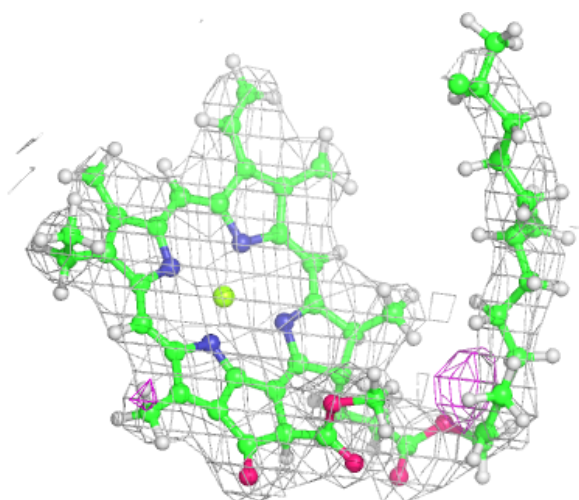
Electron density around CLA c 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



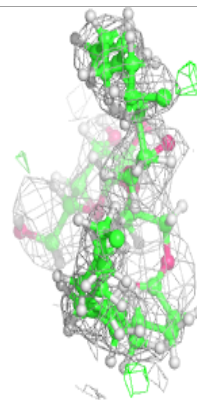
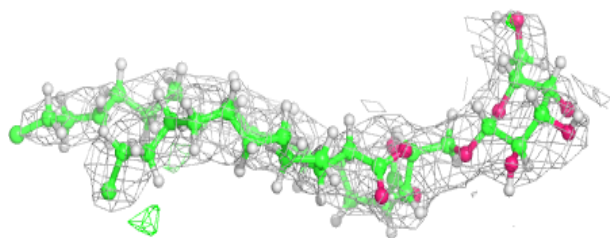
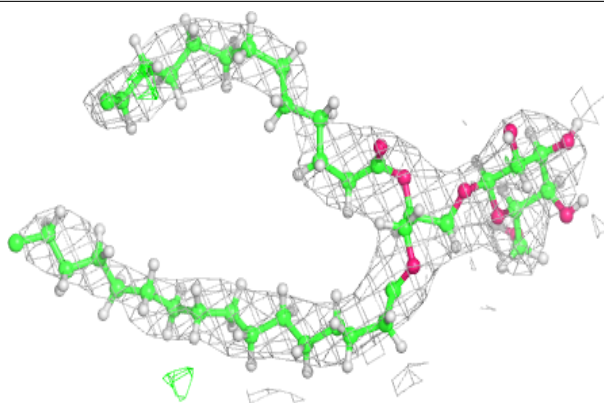
Electron density around CLA B 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



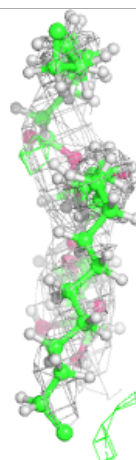
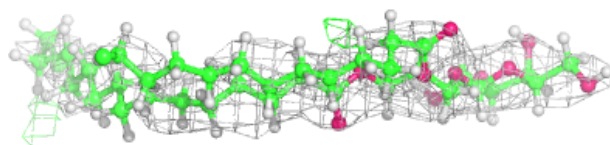
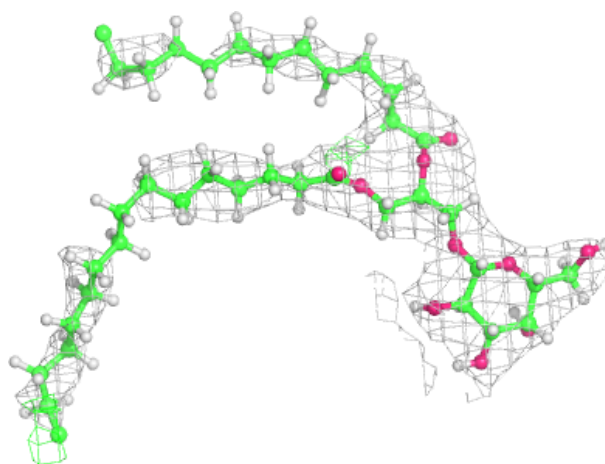
Electron density around LMG C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



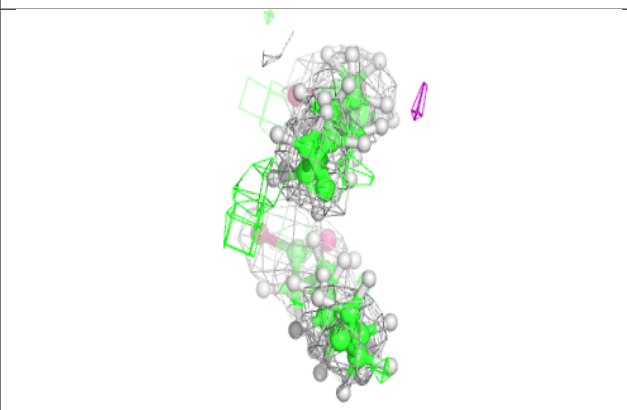
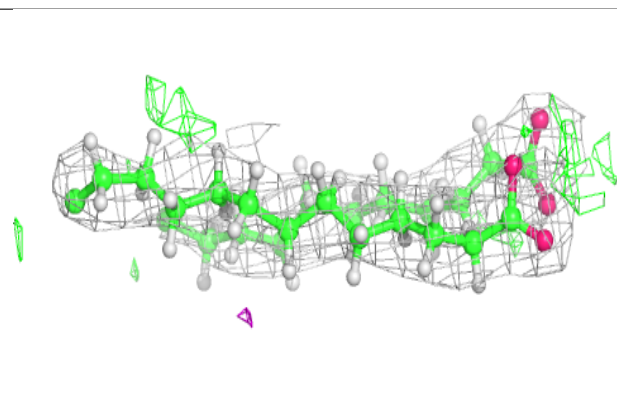
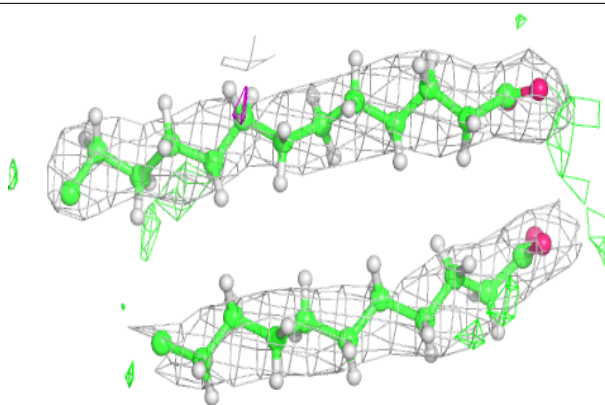
Electron density around LMG C 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

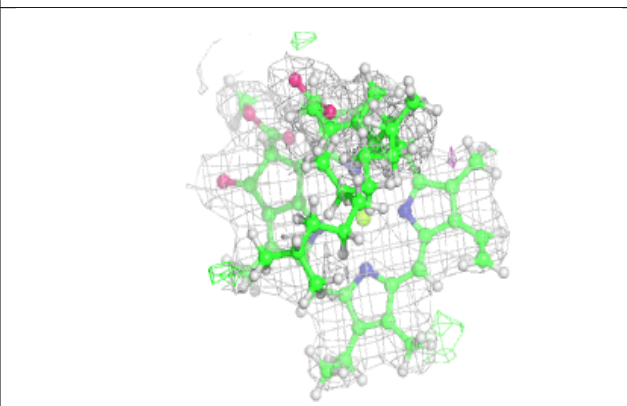
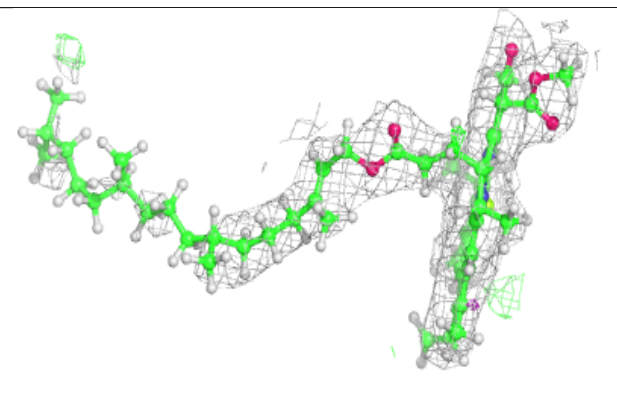
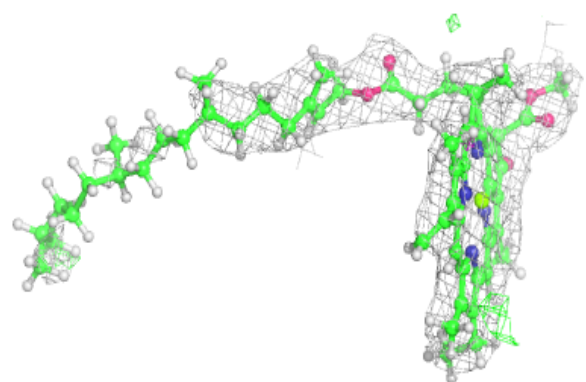


Electron density around LMG D 411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

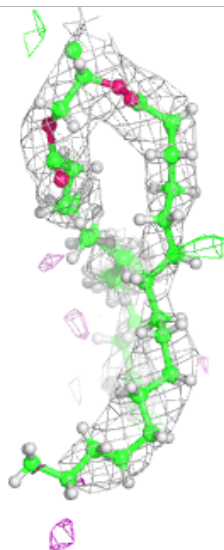
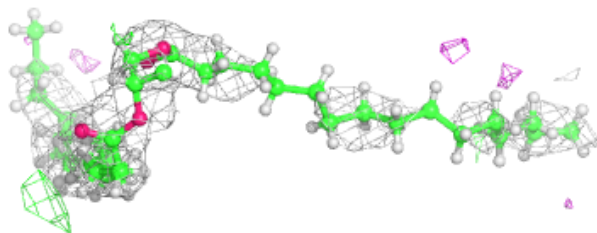
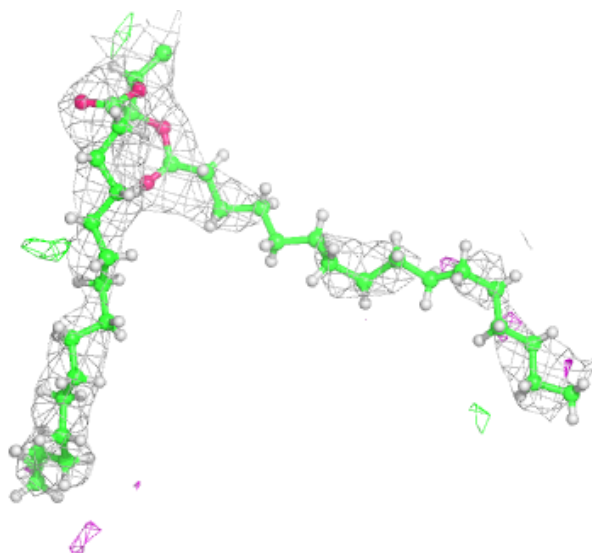
**Electron density around CLA D 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



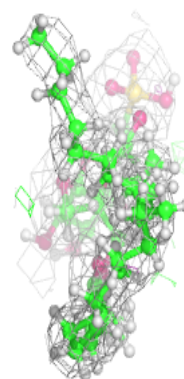
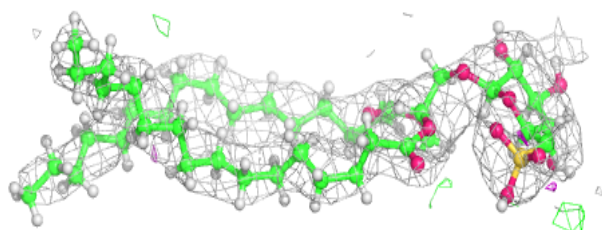
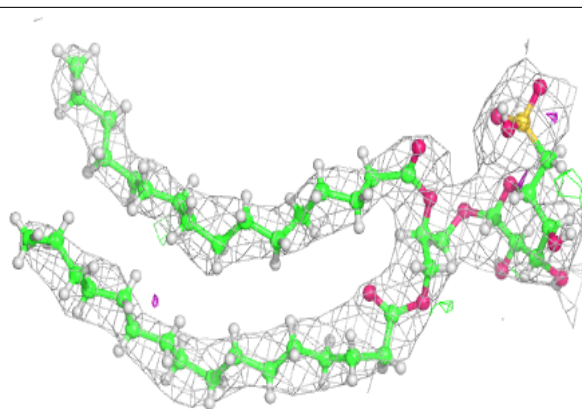
Electron density around SQD A 411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

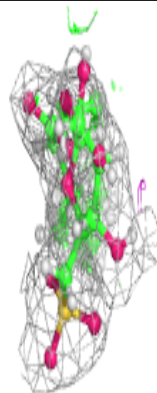
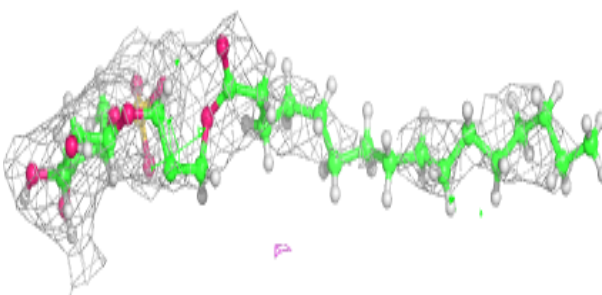
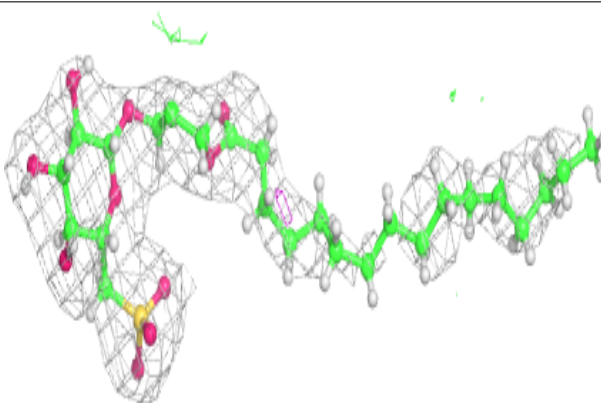


Electron density around SQD B 621:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

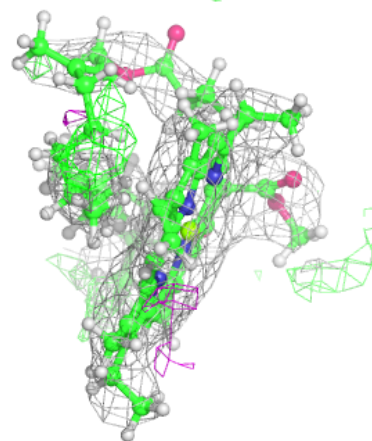
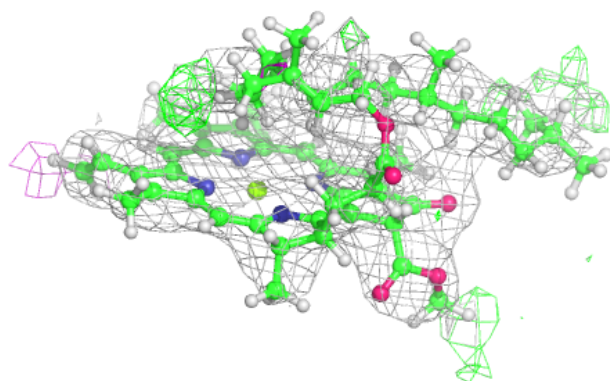
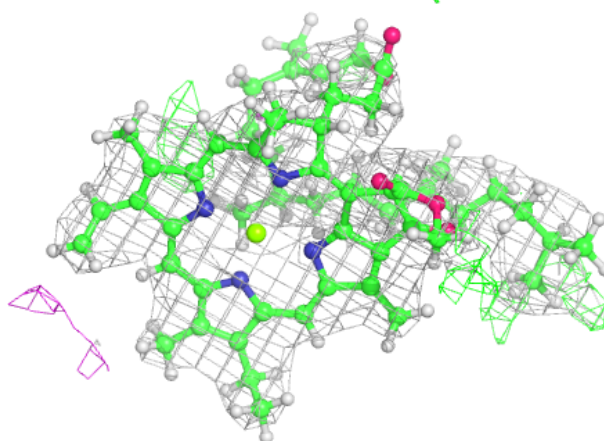
**Electron density around SQD F 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



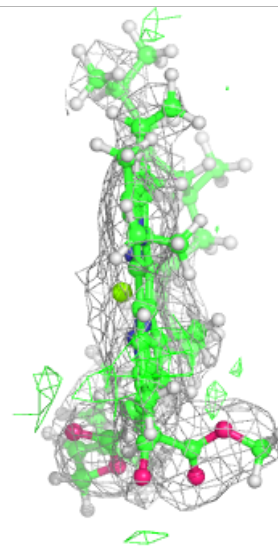
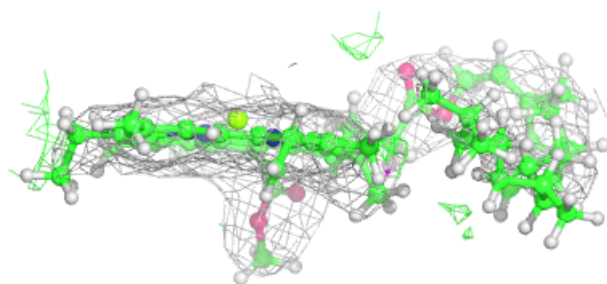
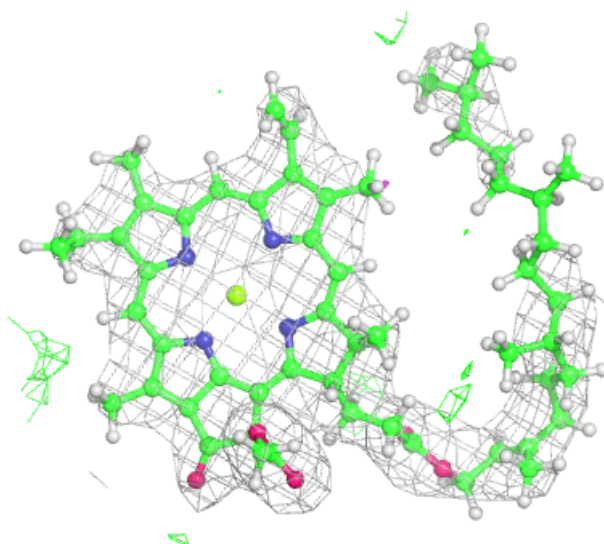
Electron density around CLA B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



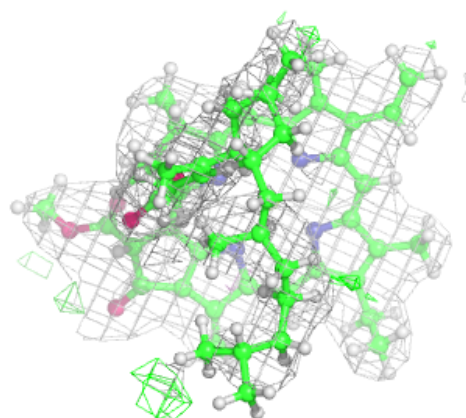
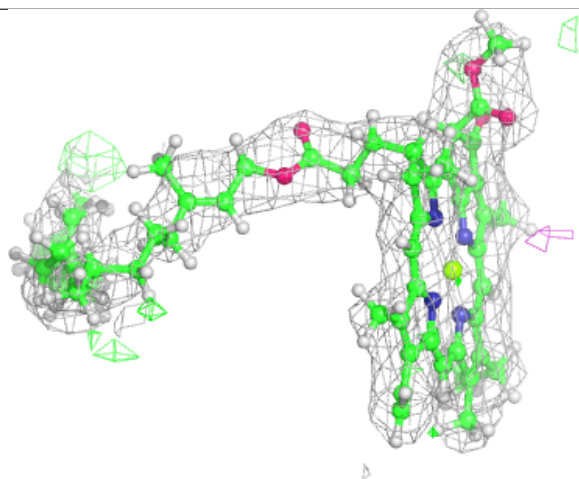
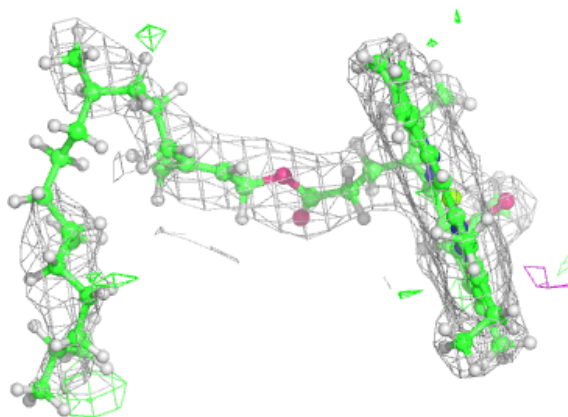
Electron density around CLA C 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



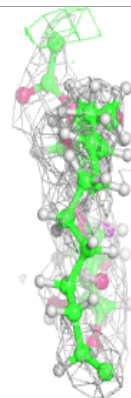
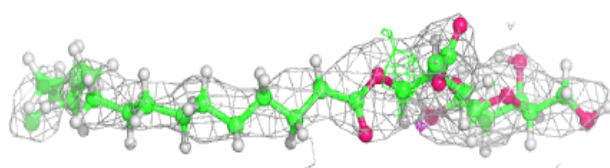
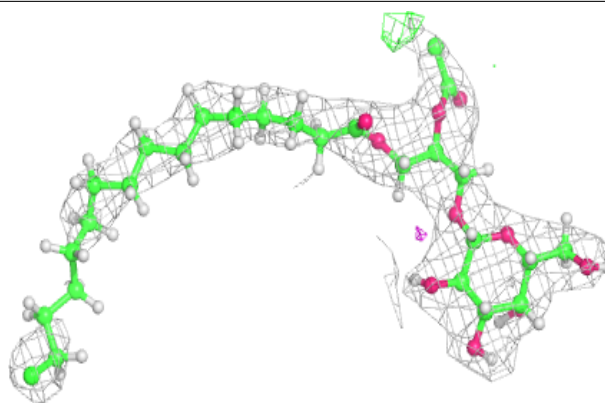
Electron density around CLA a 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

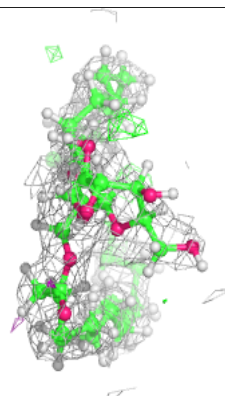
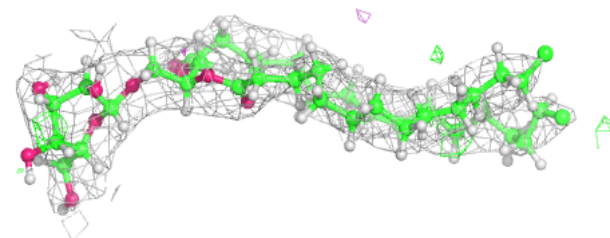
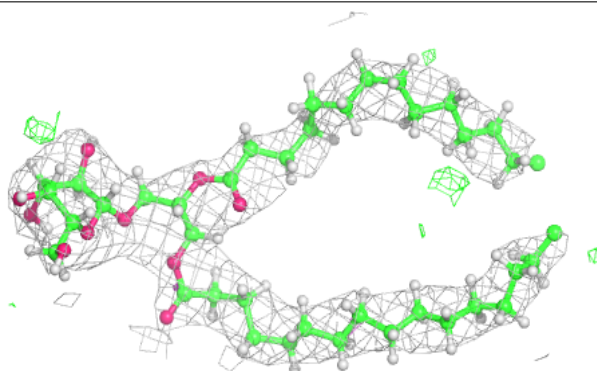


Electron density around LMG c 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

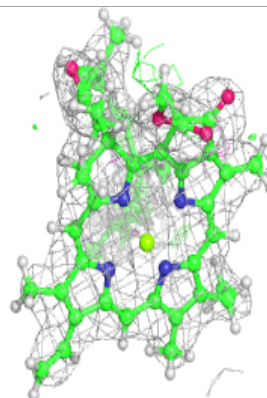
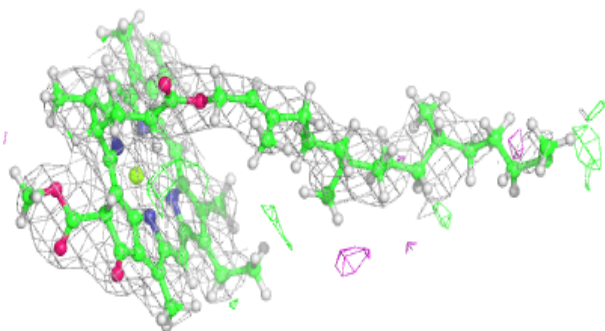
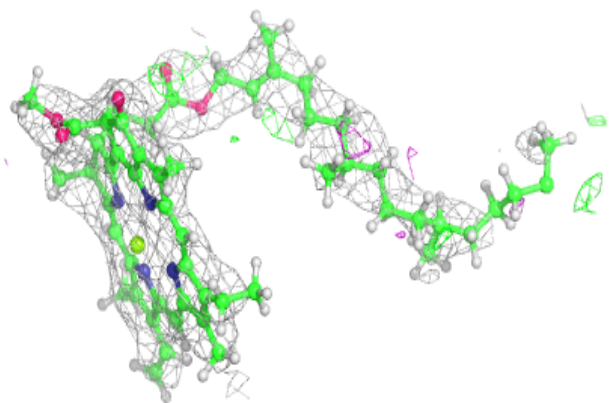
**Electron density around LMG c 524:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

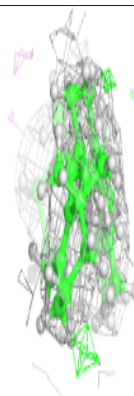
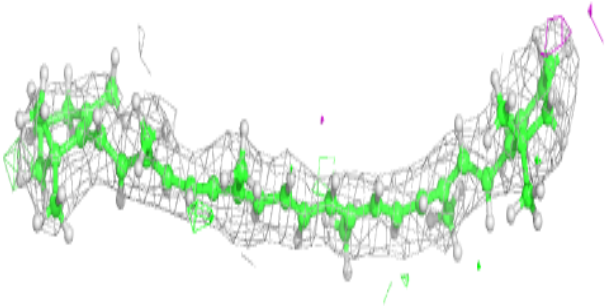
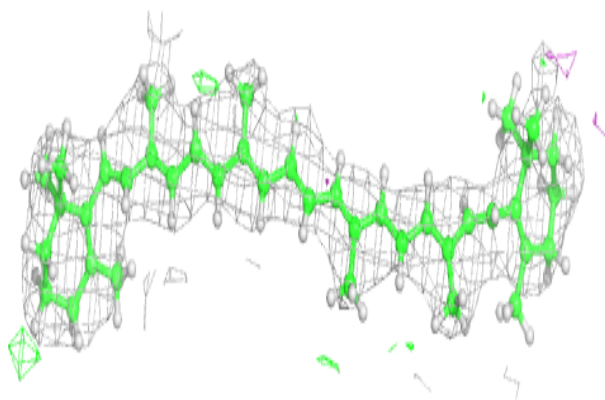


Electron density around CLA c 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

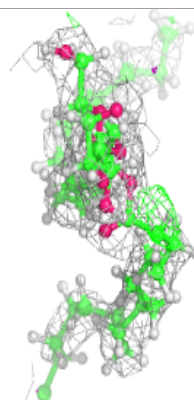
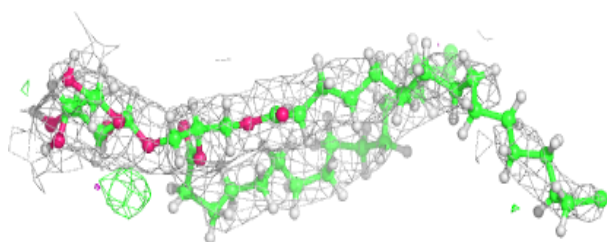
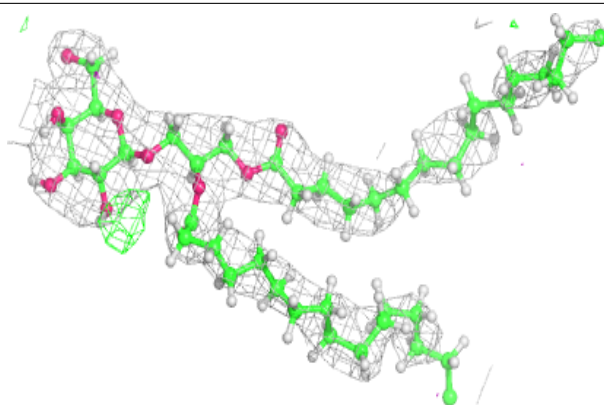
**Electron density around BCR d 405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

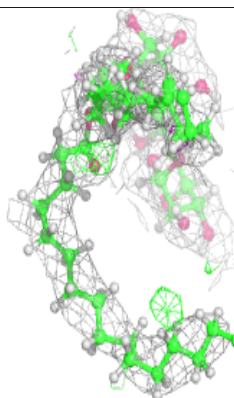
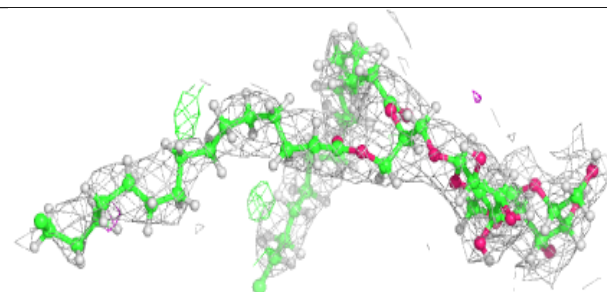
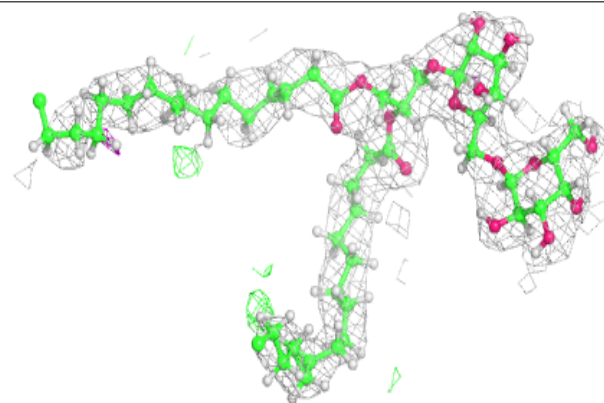


Electron density around LMG D 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

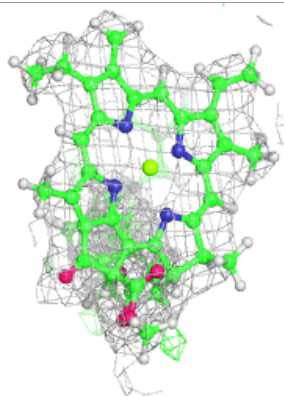
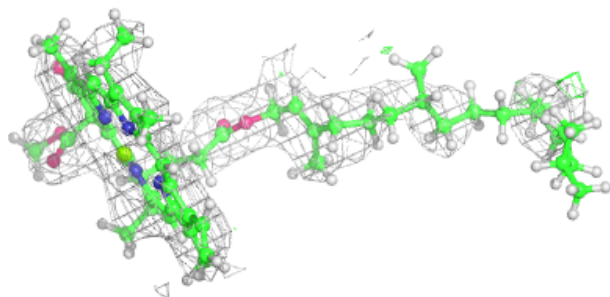
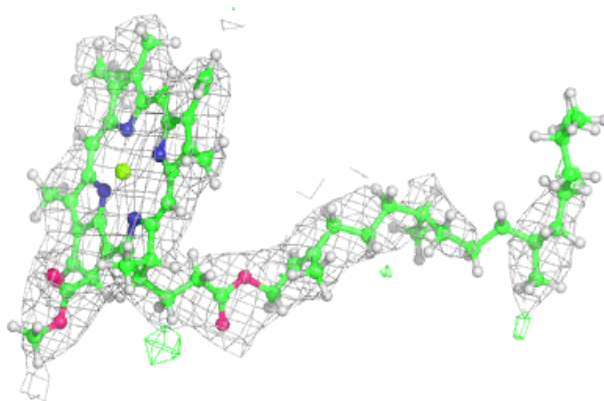
**Electron density around DGD c 517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

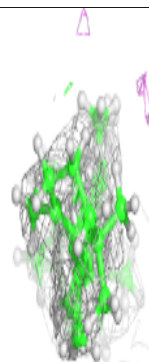
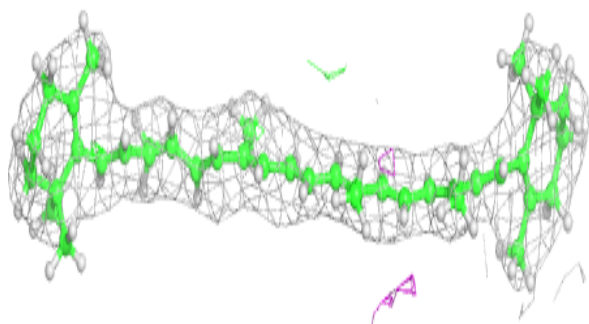
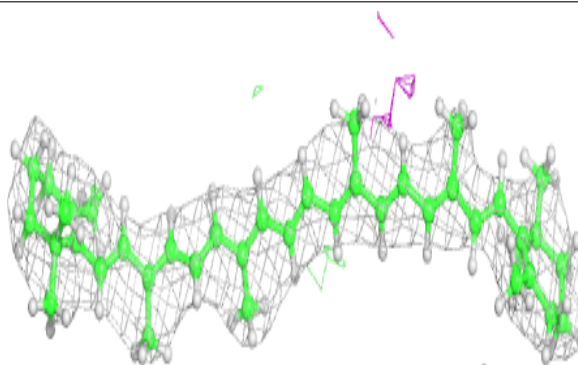


Electron density around CLA d 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

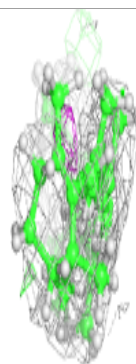
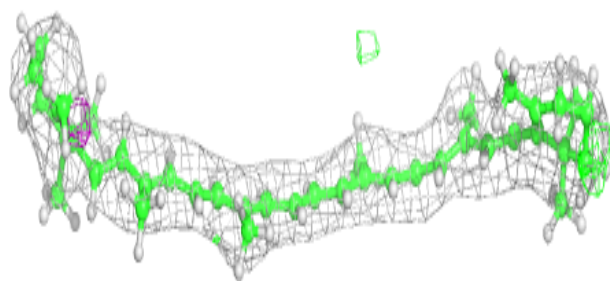
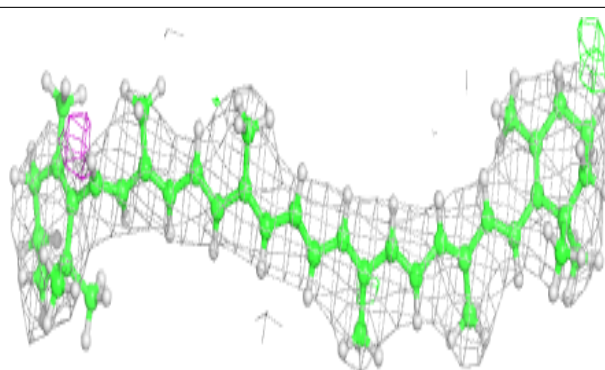
**Electron density around BCR C 515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



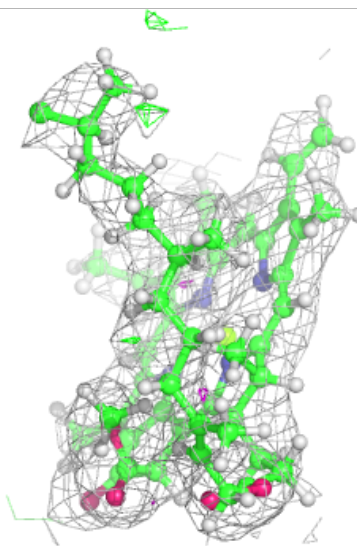
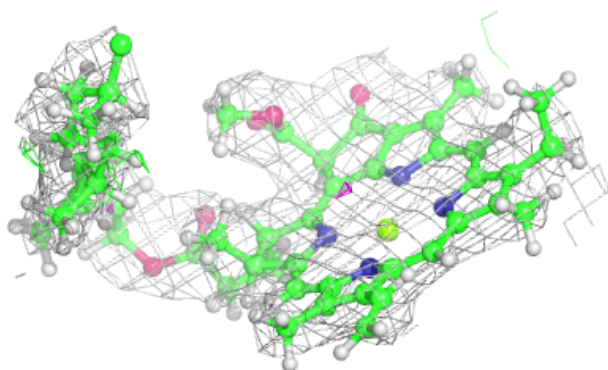
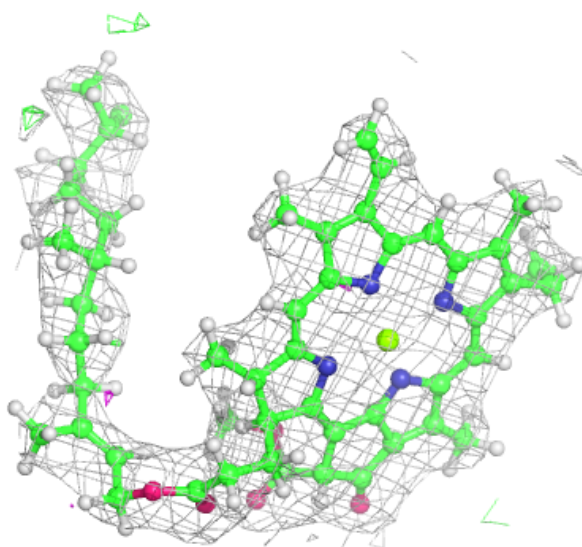
Electron density around BCR D 405:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



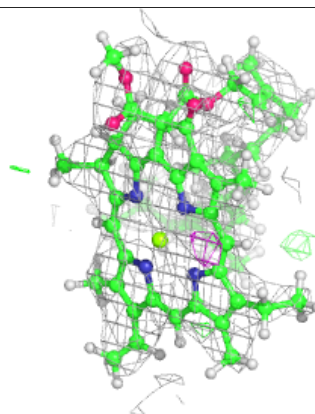
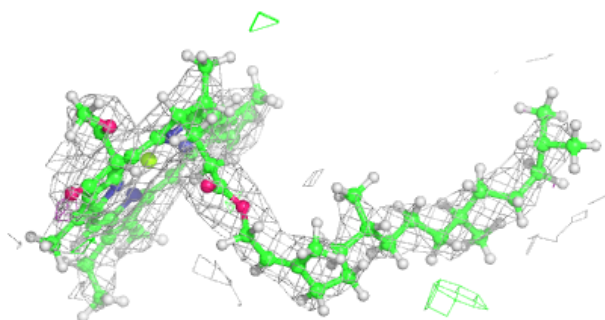
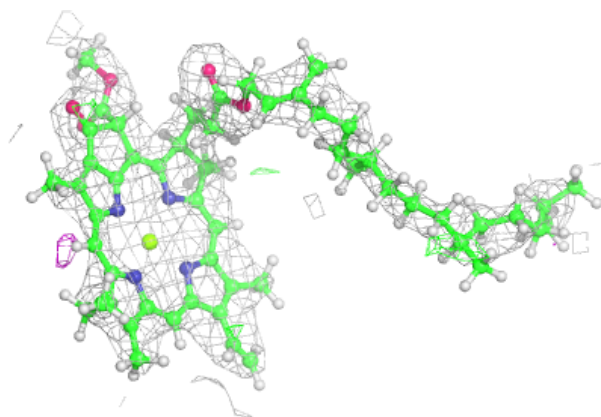
Electron density around CLA b 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



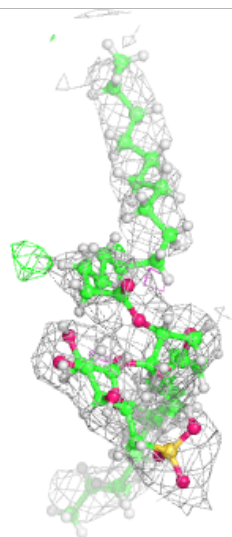
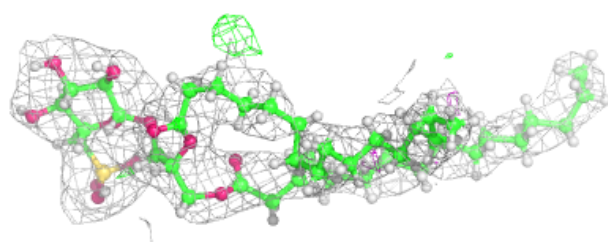
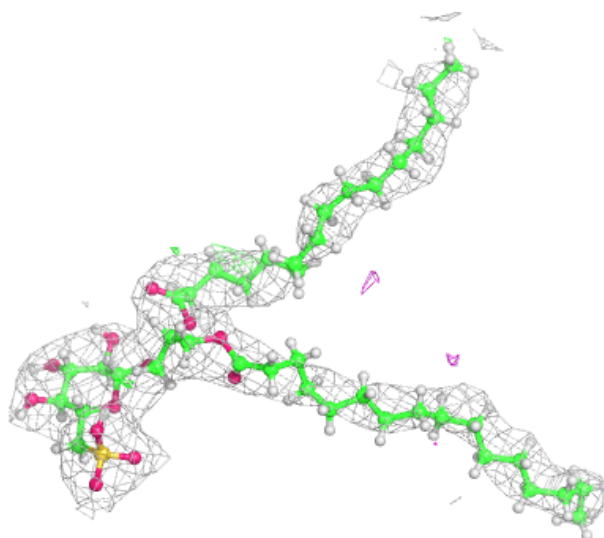
Electron density around CLA c 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



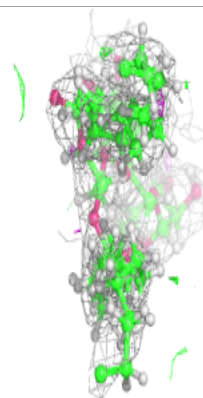
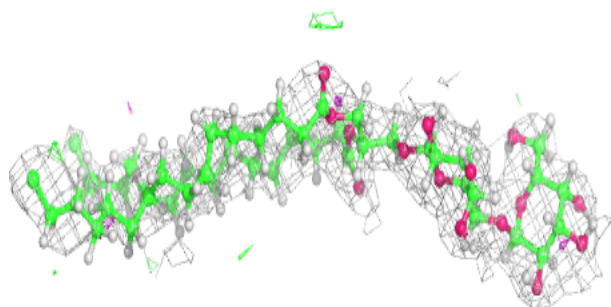
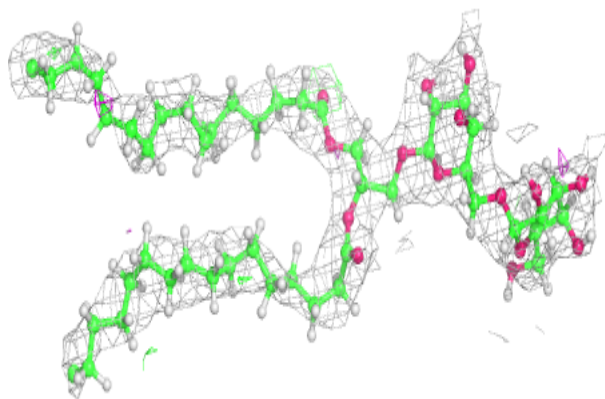
Electron density around SQD a 411:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

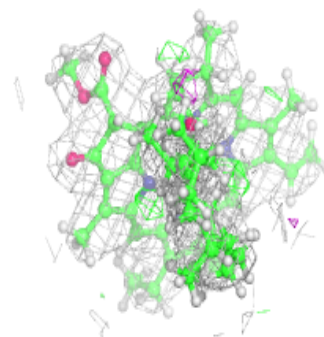
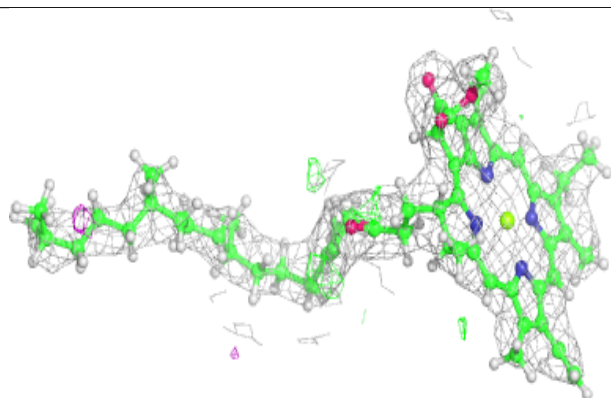
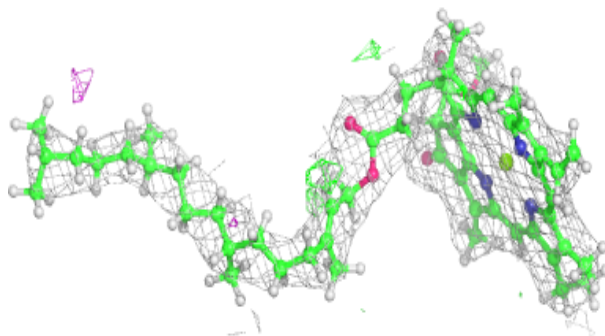


Electron density around DGD c 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

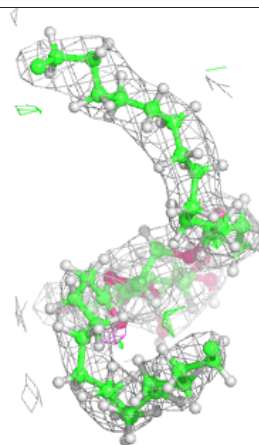
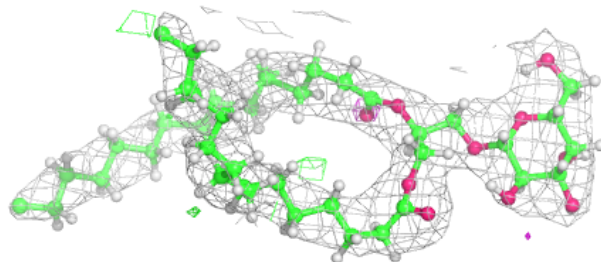
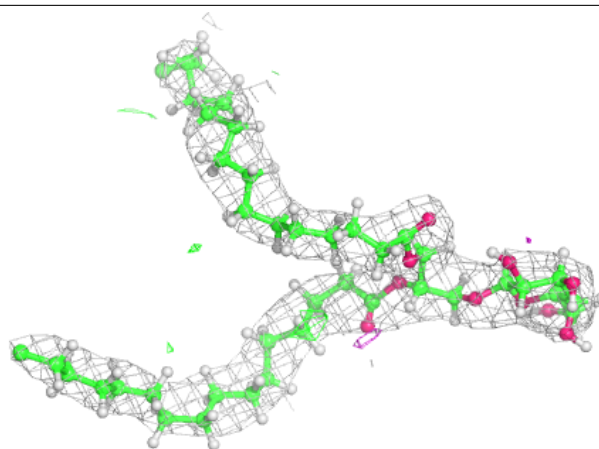
**Electron density around CLA c 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



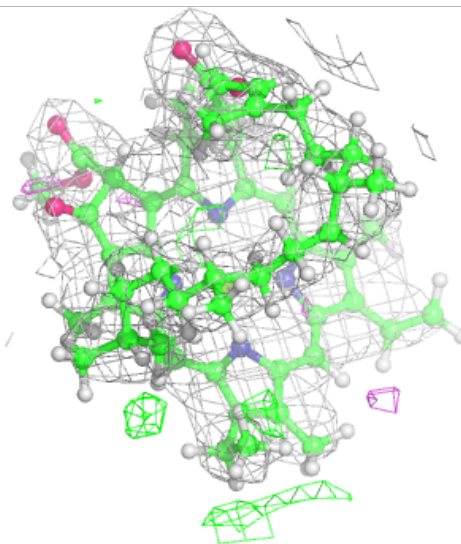
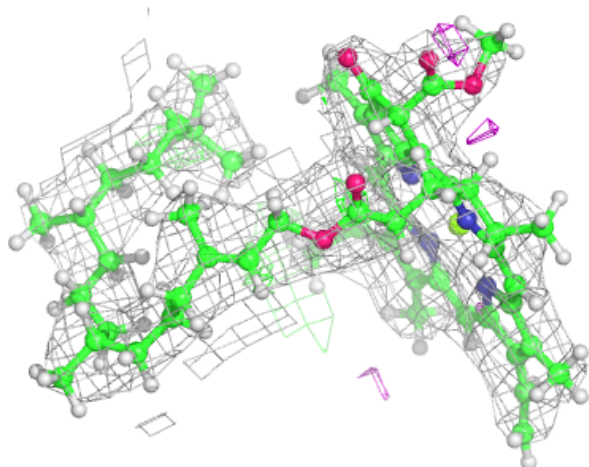
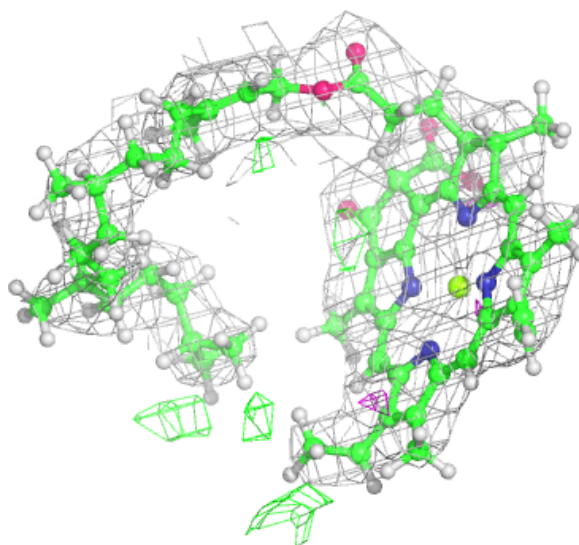
Electron density around LMG M 101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



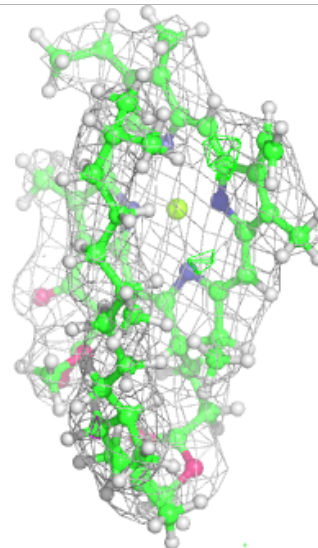
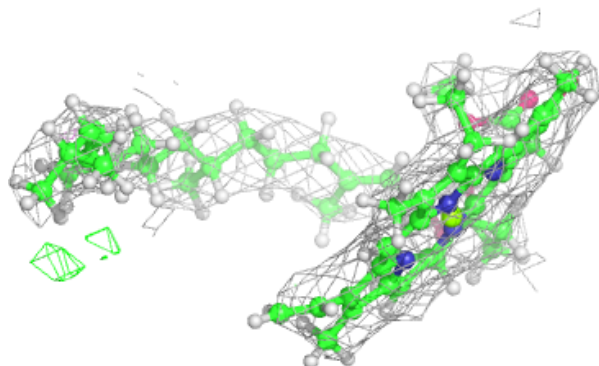
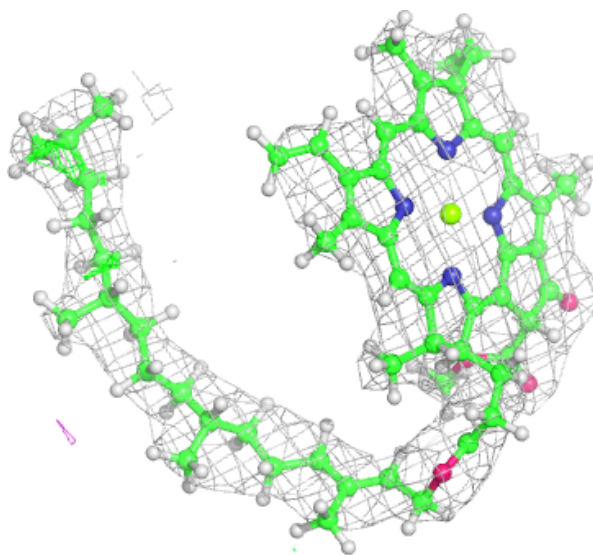
Electron density around CLA c 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



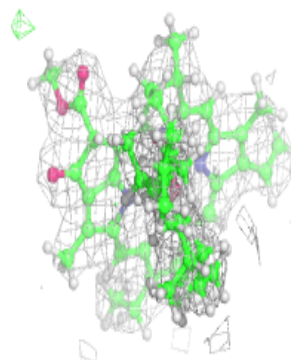
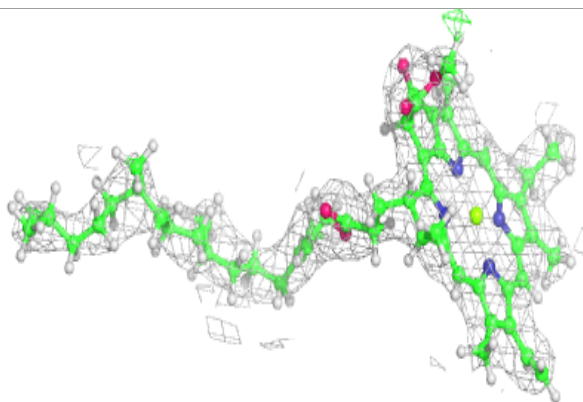
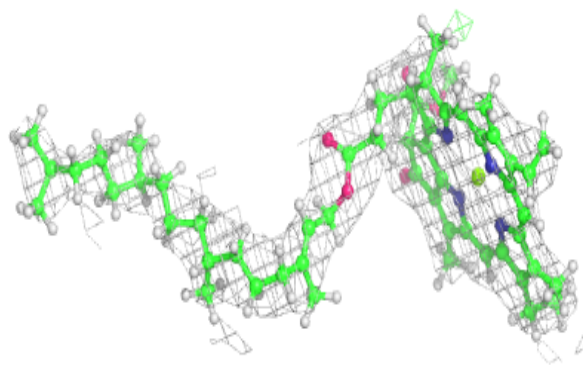
Electron density around CLA c 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

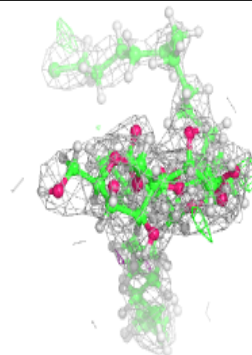
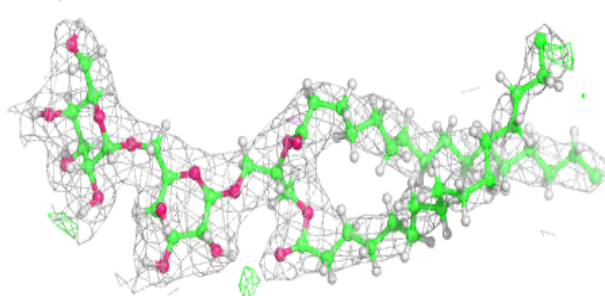
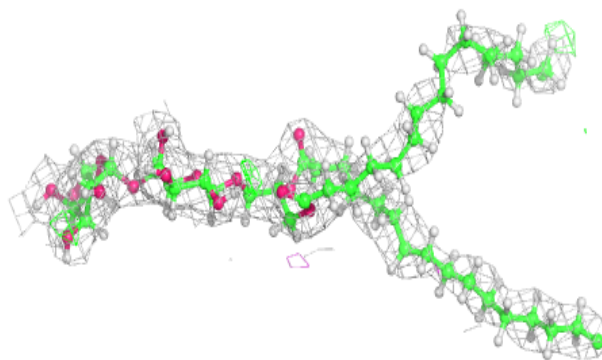


Electron density around CLA C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

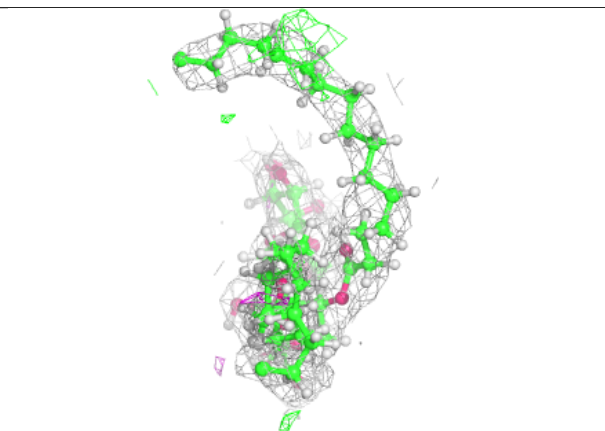
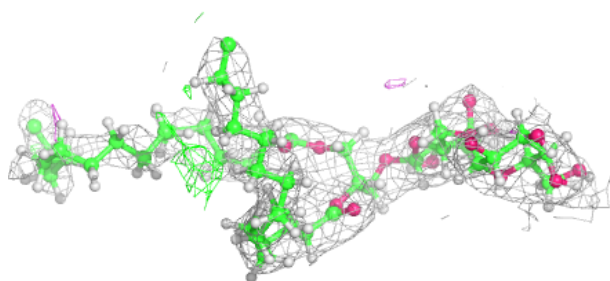
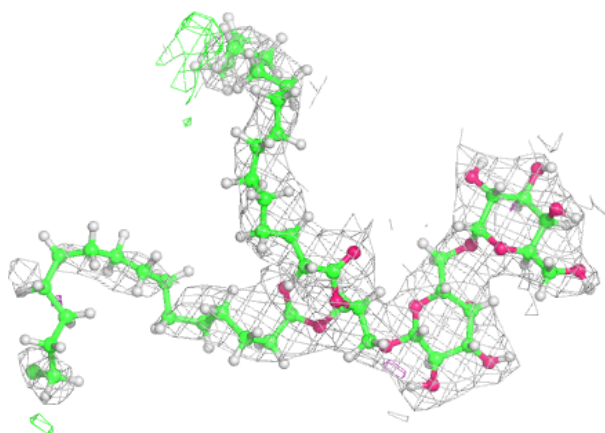
**Electron density around DGD C 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

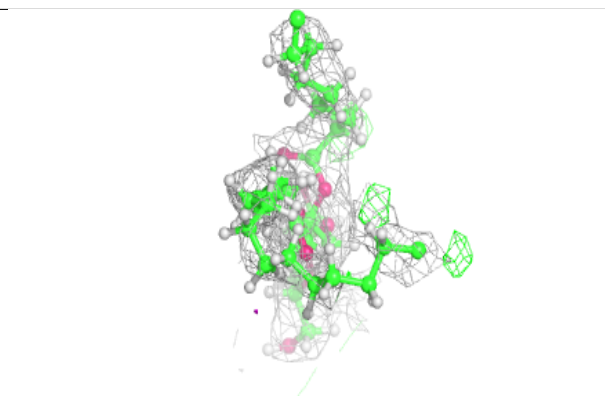
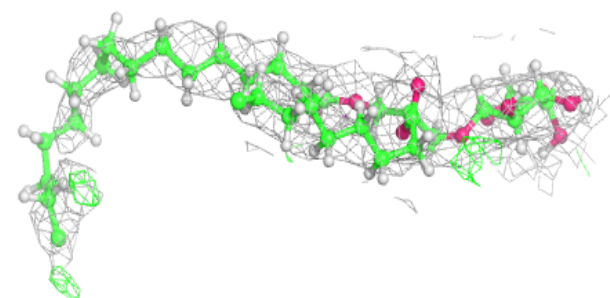
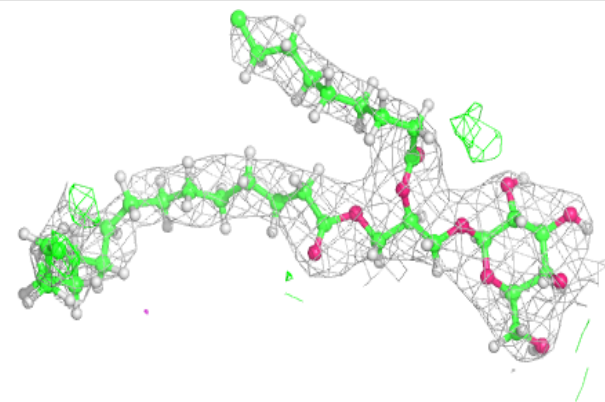


Electron density around DGD C 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

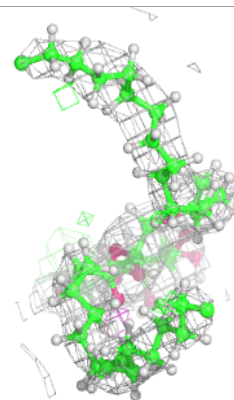
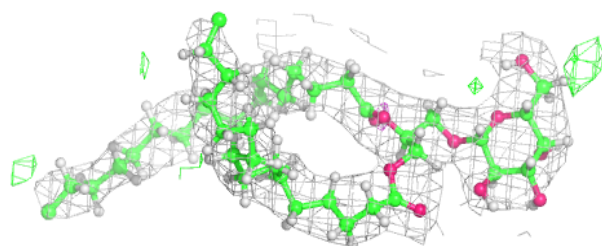
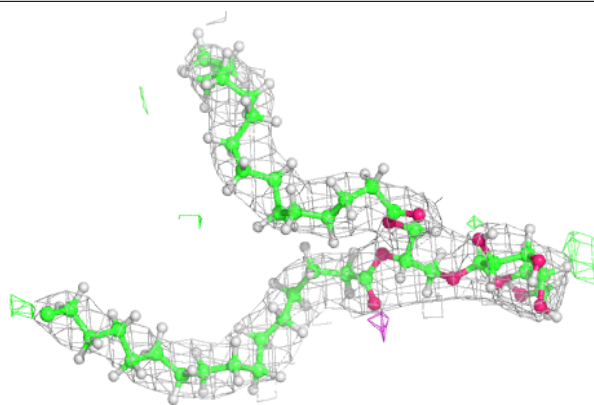
**Electron density around LMG d 411:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

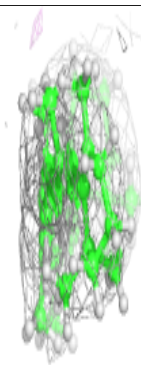
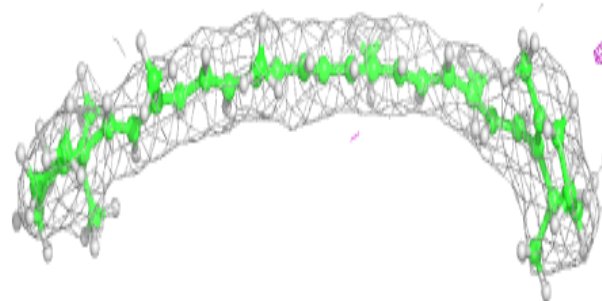
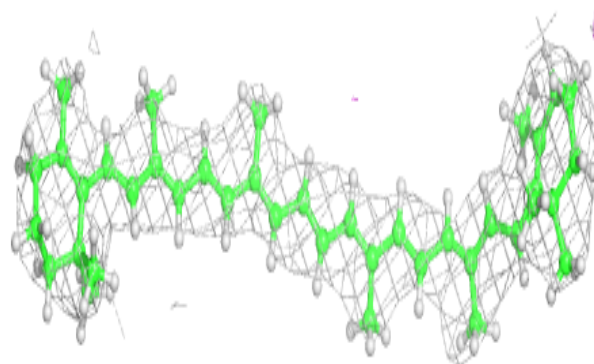


Electron density around LMG m 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

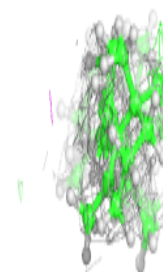
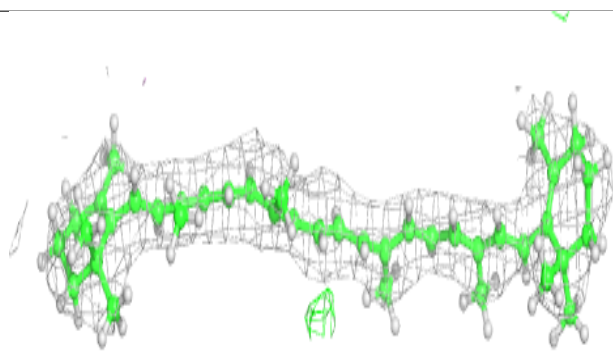
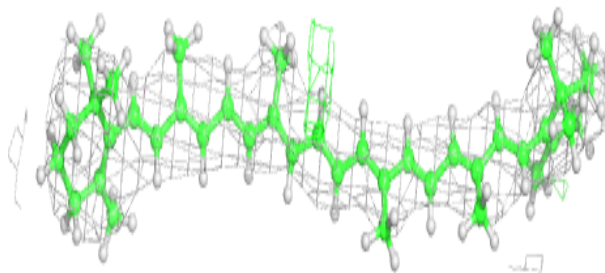
**Electron density around BCR T 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

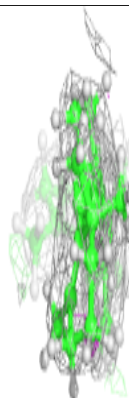
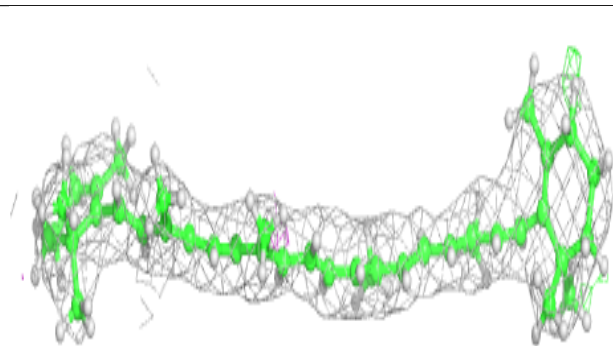
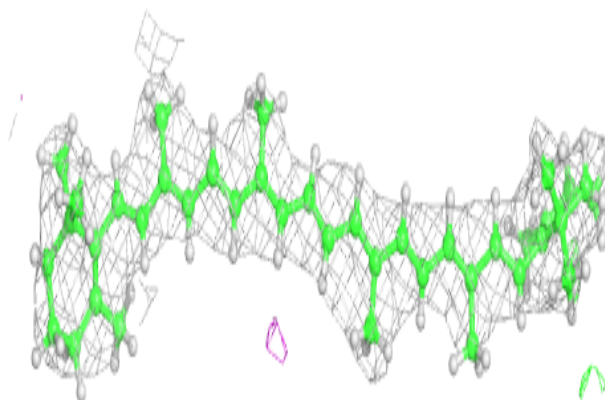


Electron density around BCR Z 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

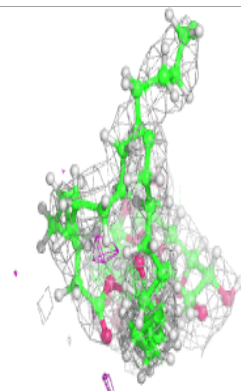
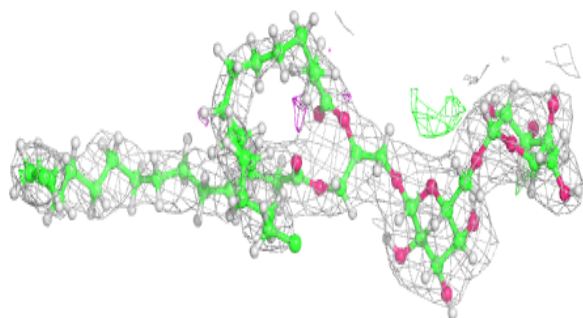
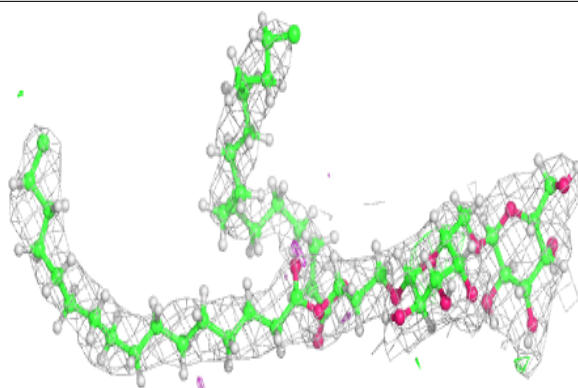
**Electron density around BCR b 618:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

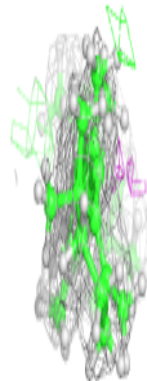
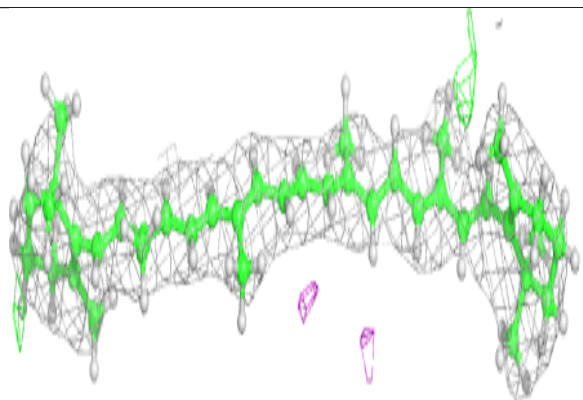
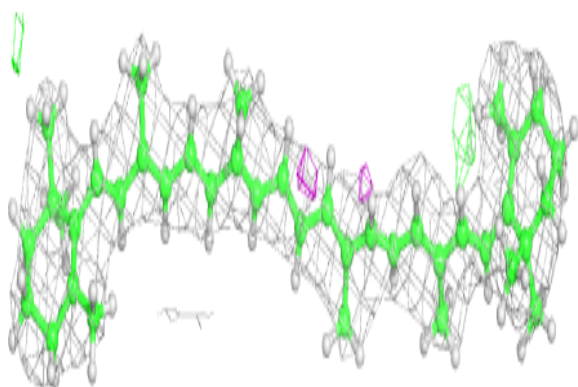


Electron density around DGD h 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

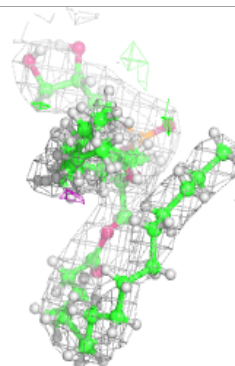
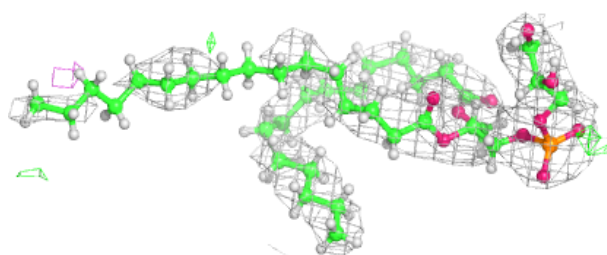
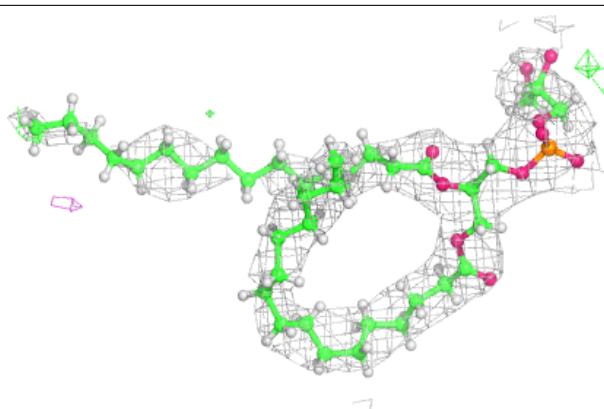
**Electron density around BCR b 620:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

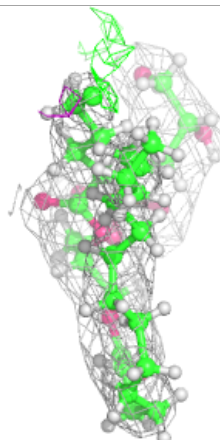
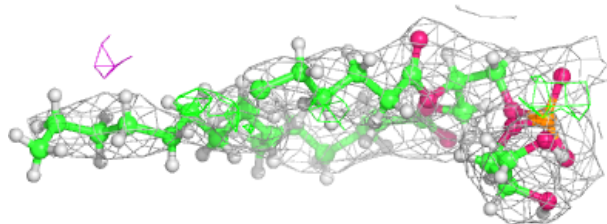
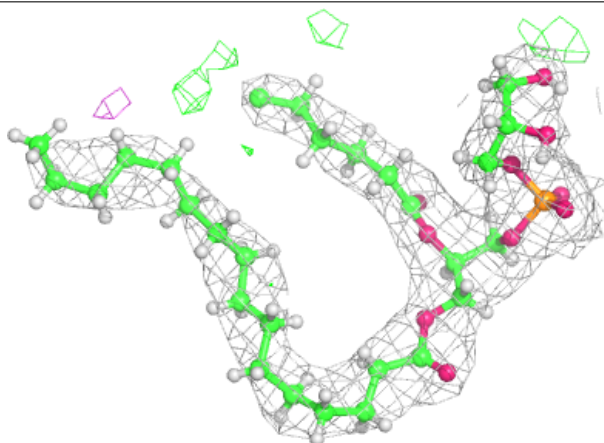


Electron density around LHG d 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

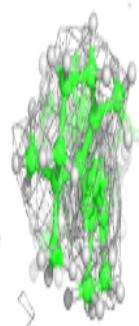
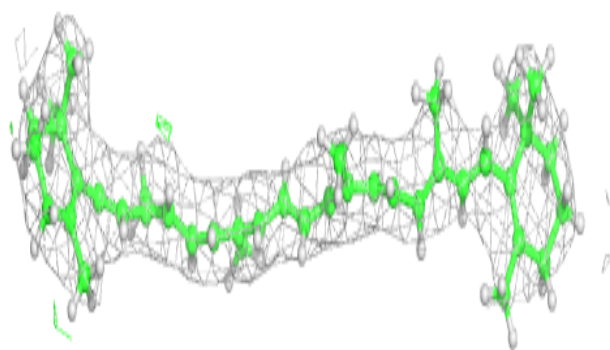
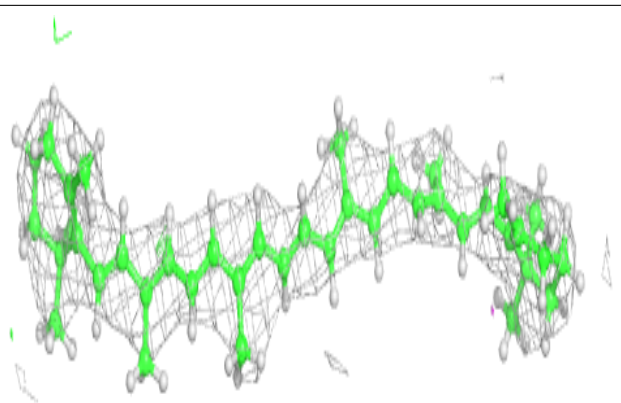
**Electron density around LHG d 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

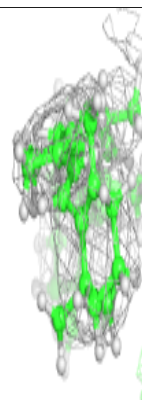
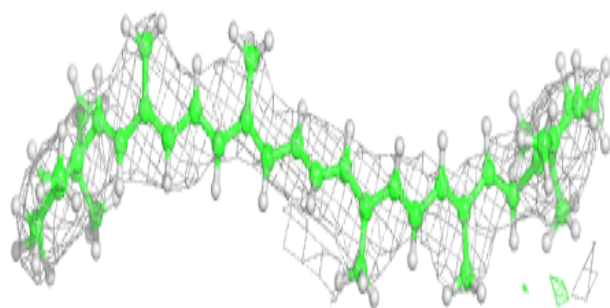
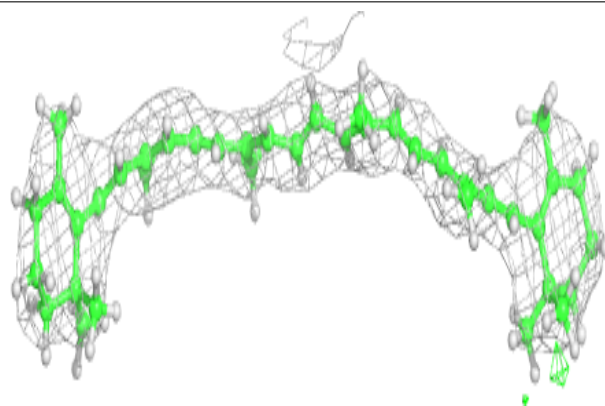


Electron density around BCR c 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

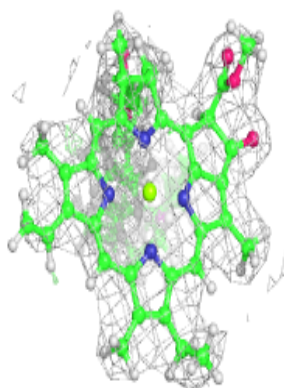
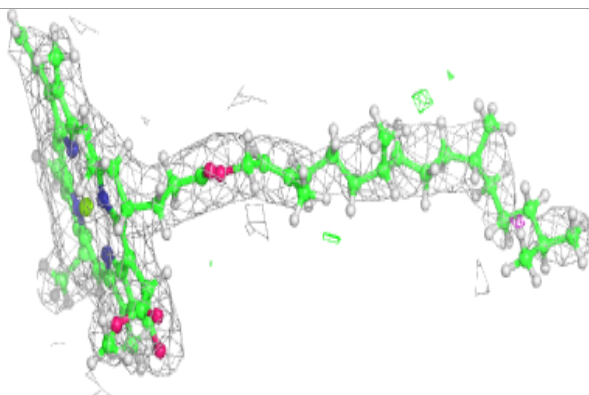
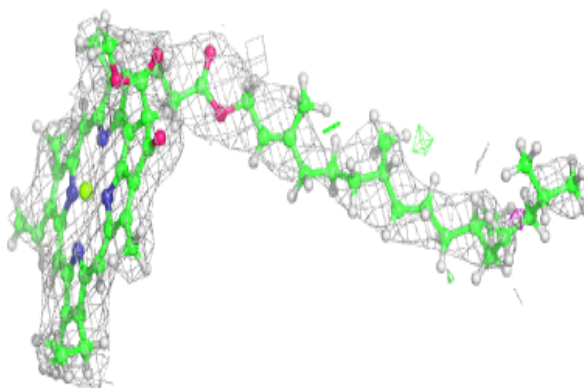
**Electron density around BCR c 521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

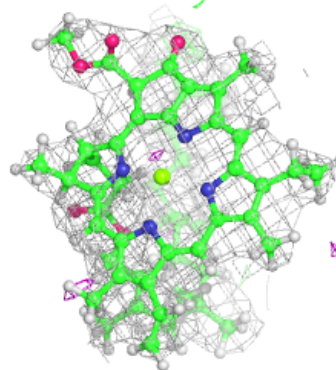
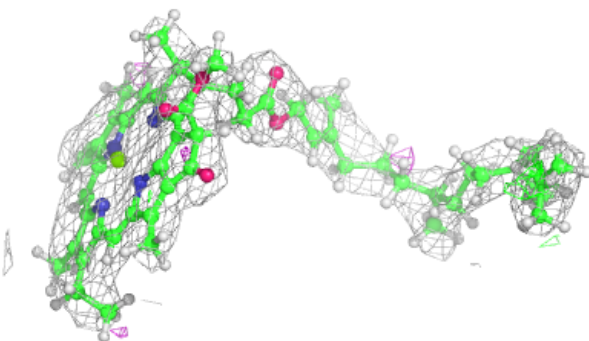
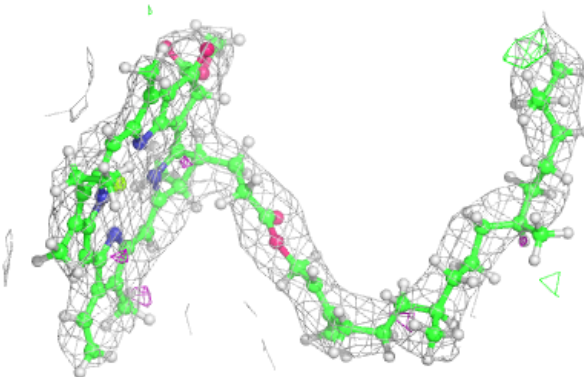


Electron density around CLA b 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

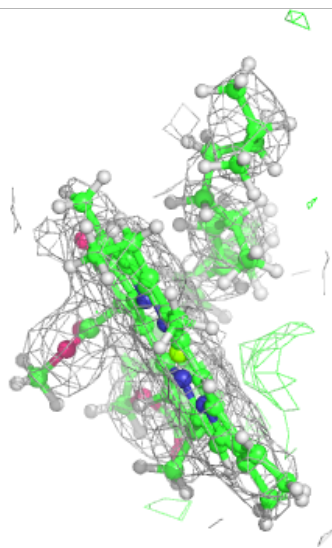
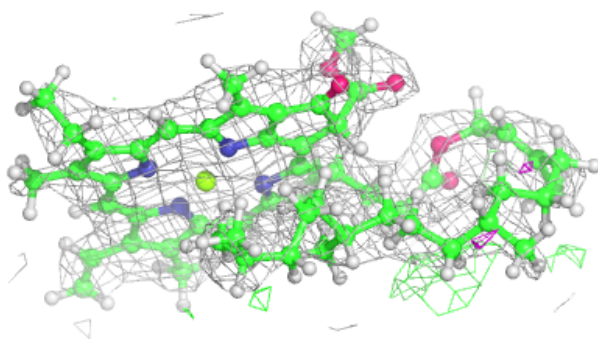
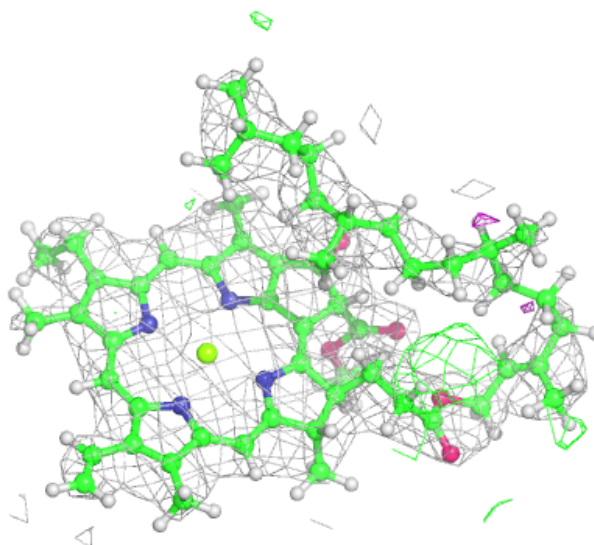
**Electron density around CLA b 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



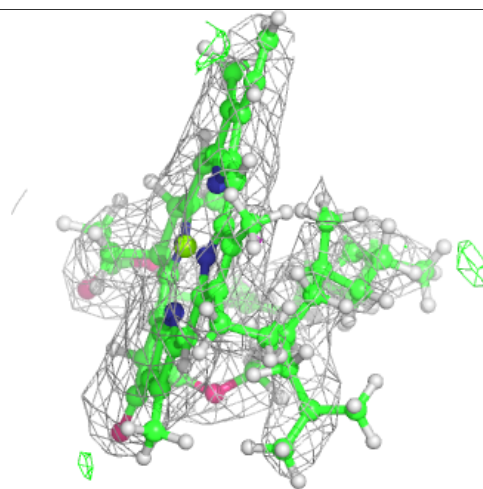
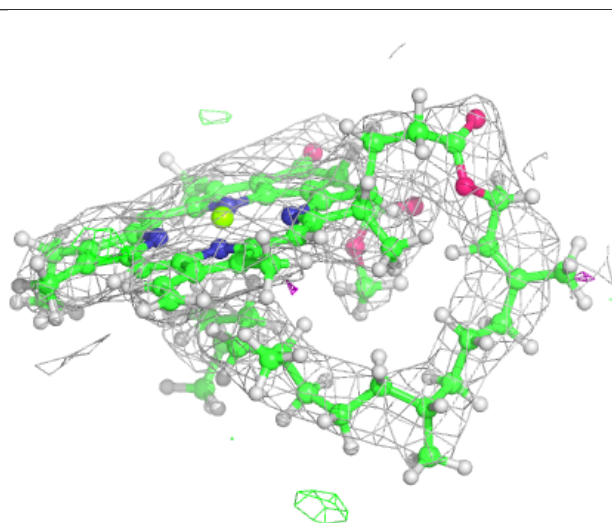
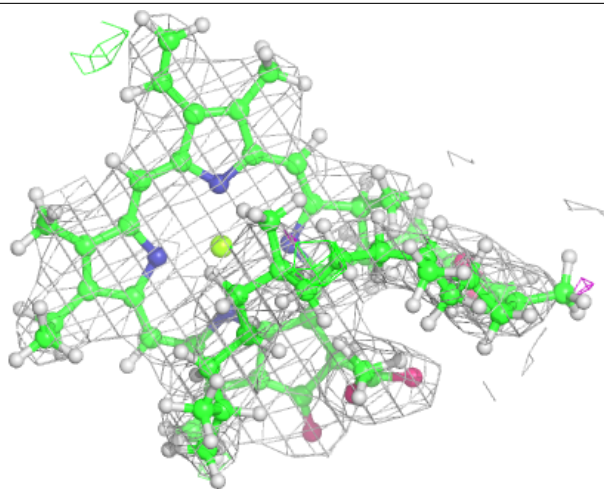
Electron density around CLA c 509:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



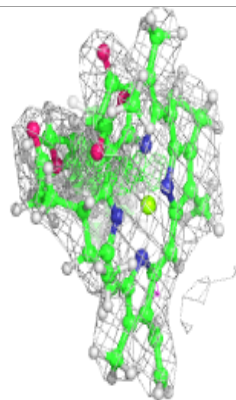
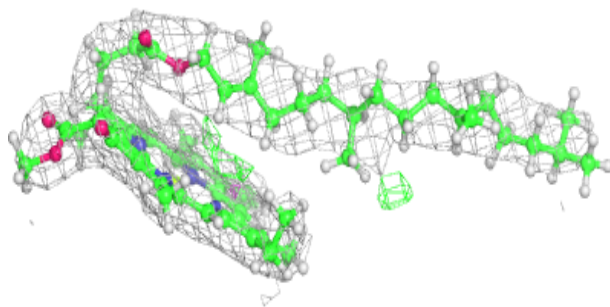
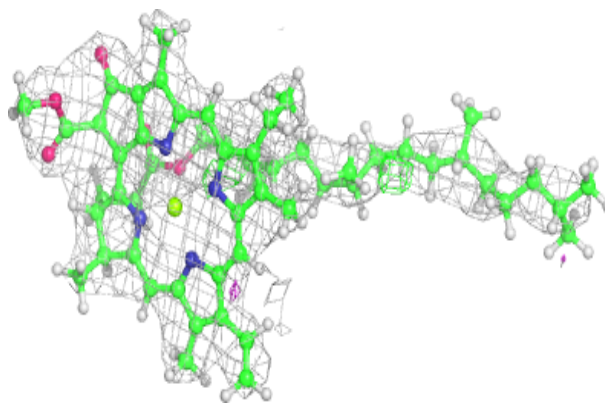
Electron density around CLA c 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



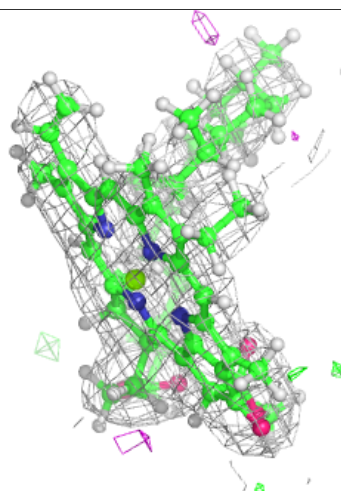
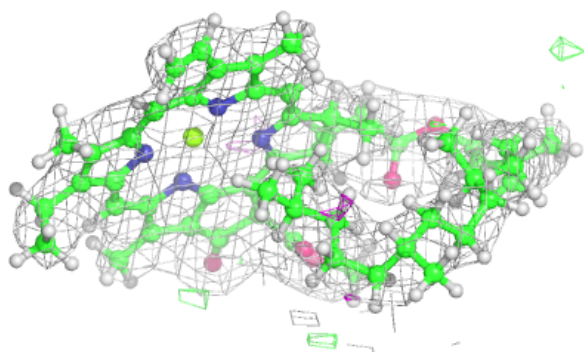
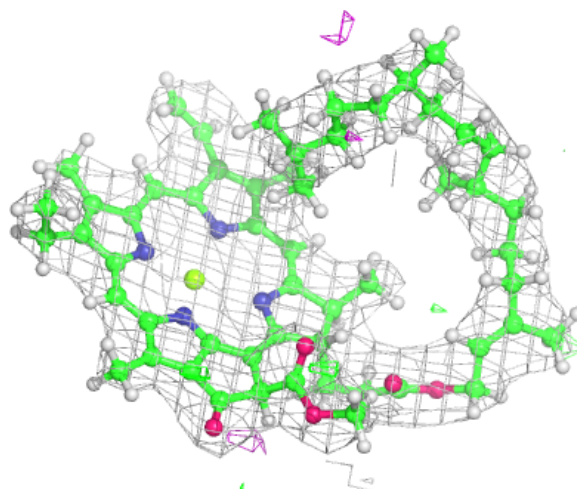
Electron density around CLA b 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



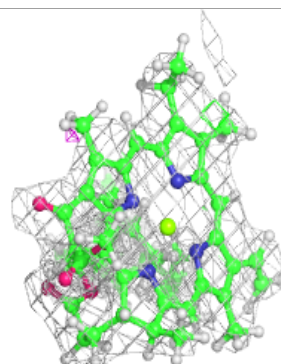
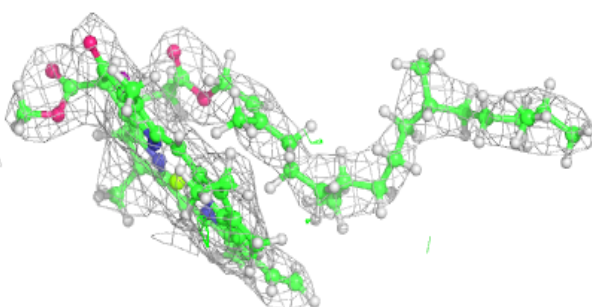
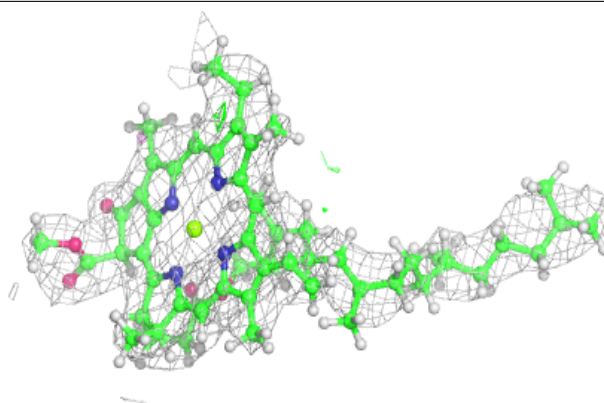
Electron density around CLA b 616:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

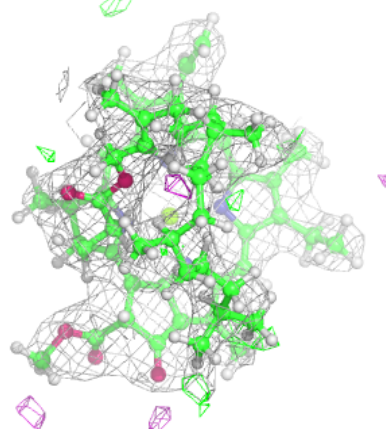
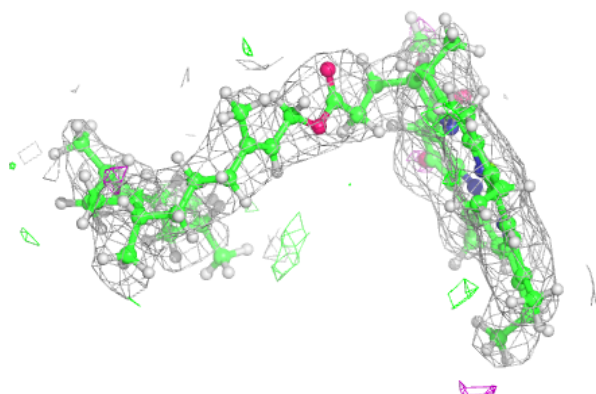
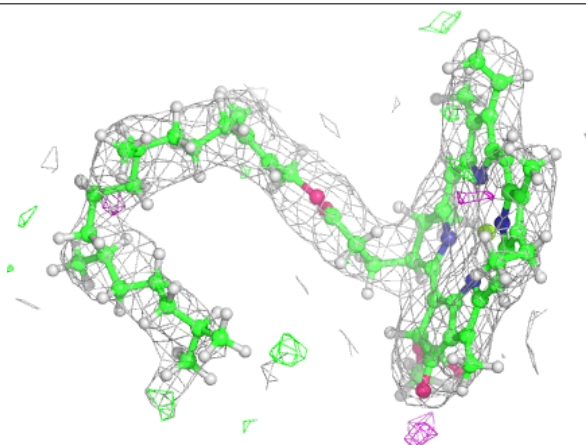


Electron density around CLA C 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

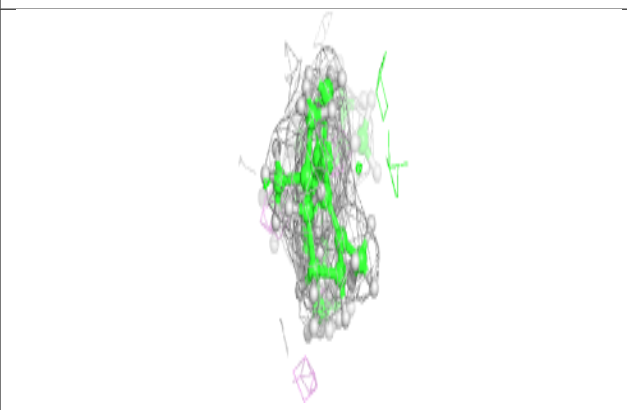
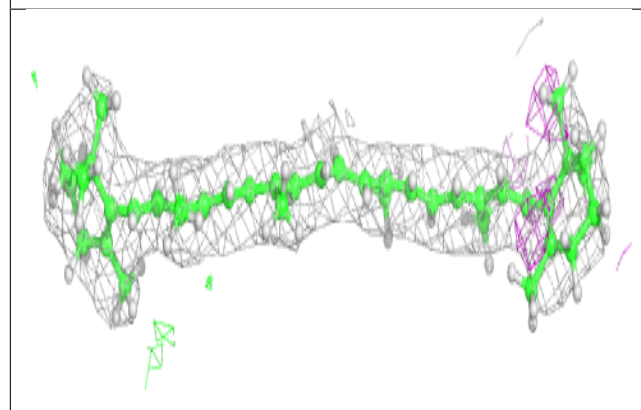
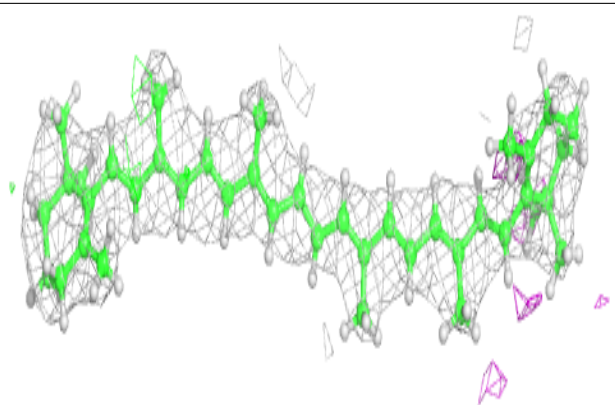
**Electron density around CLA B 606:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

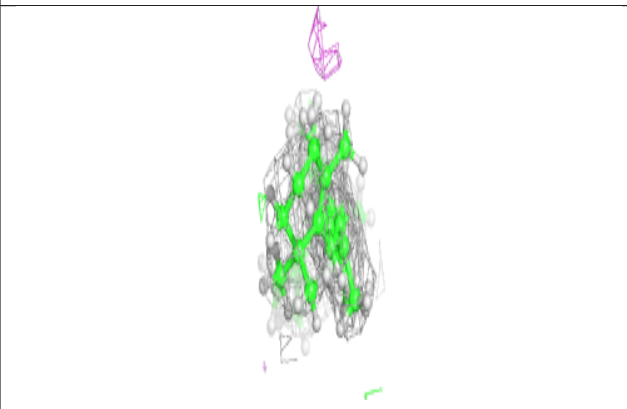
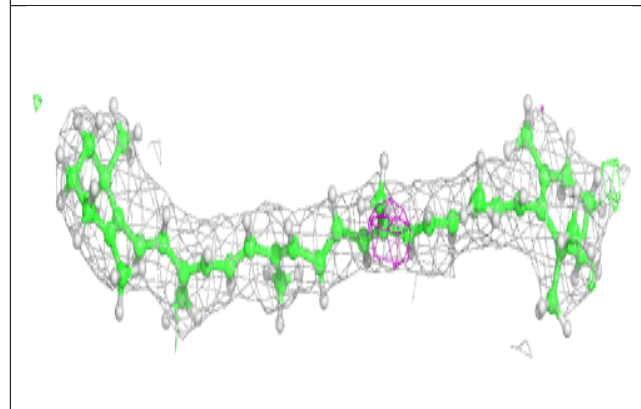
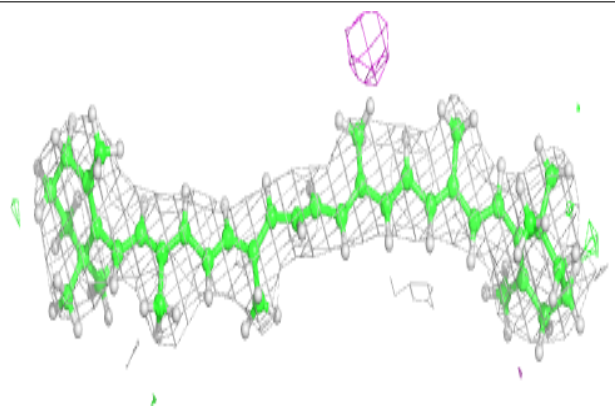


Electron density around BCR B 618:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

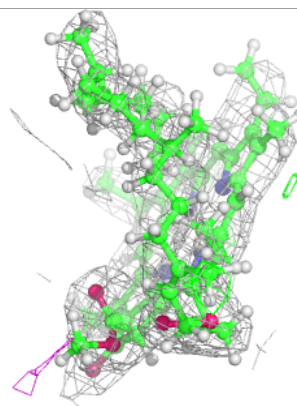
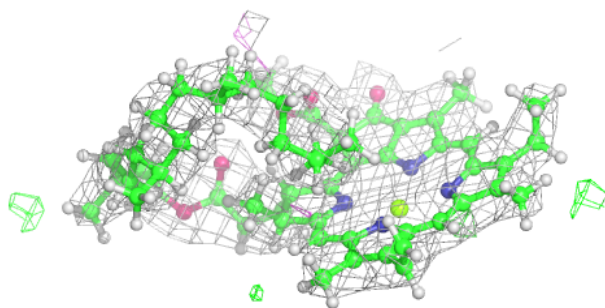
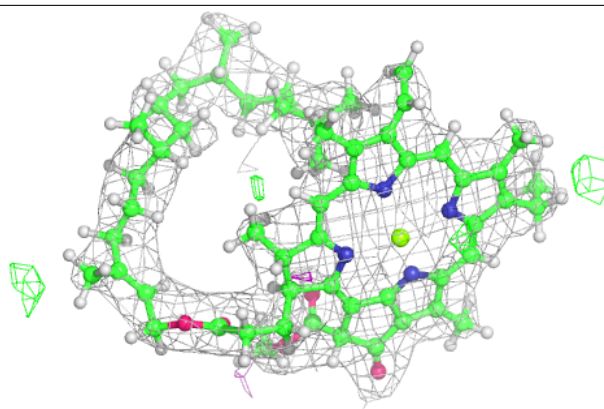
**Electron density around BCR B 619:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

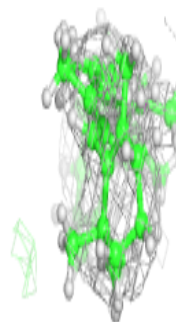
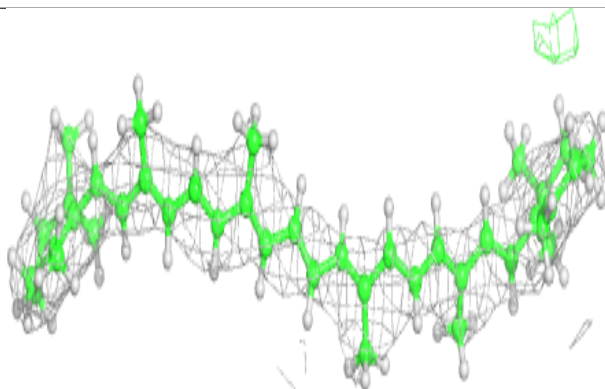
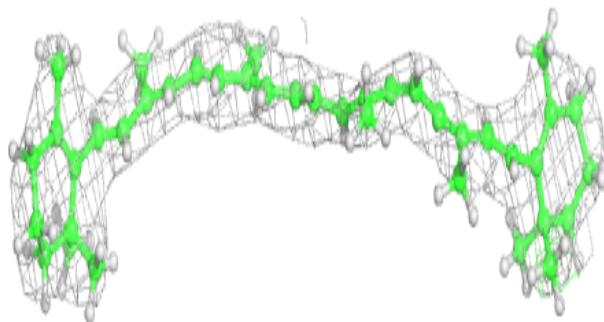


Electron density around CLA B 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

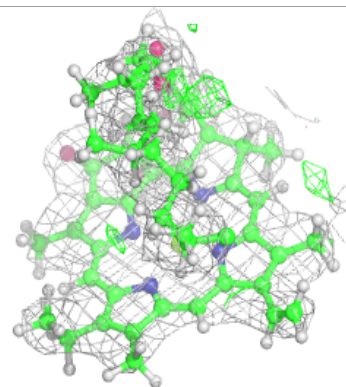
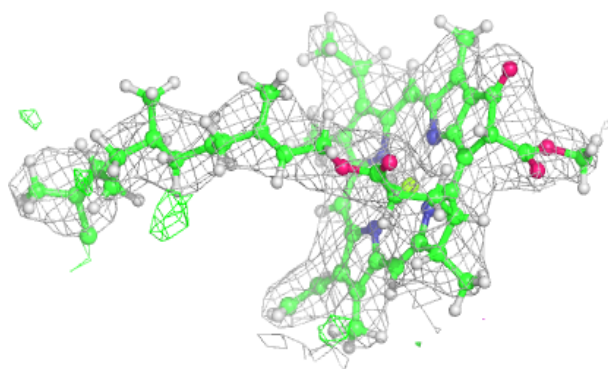
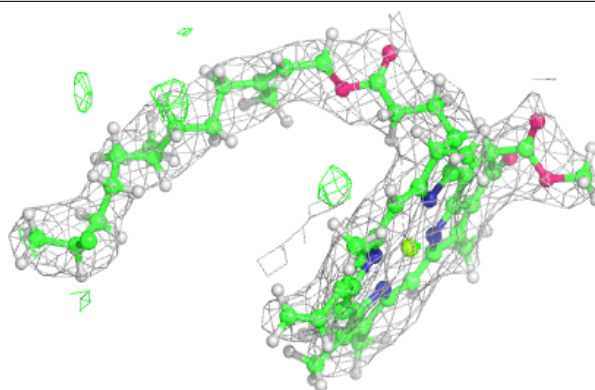
**Electron density around BCR C 520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

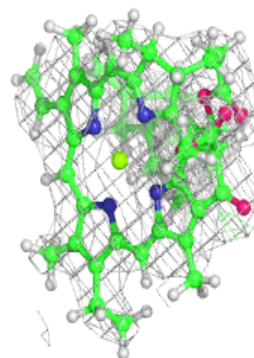
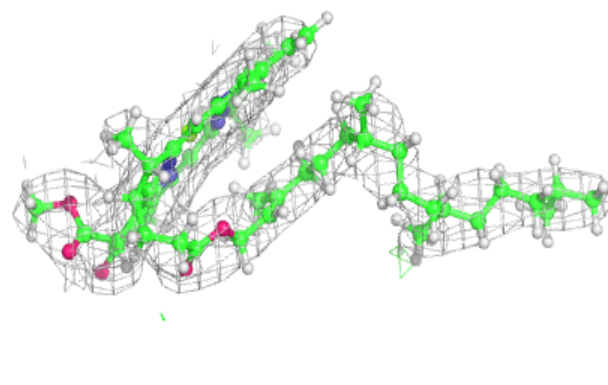
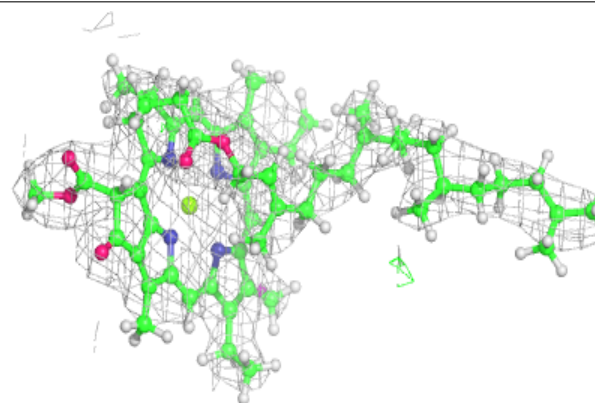


Electron density around CLA c 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

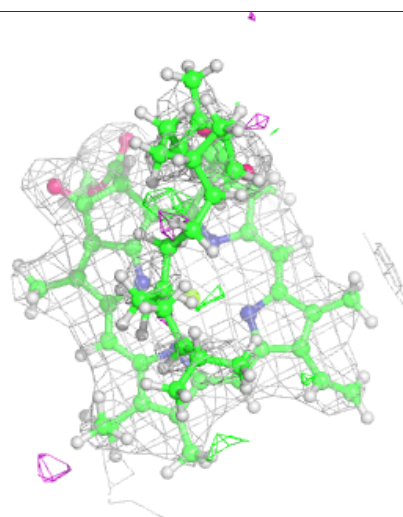
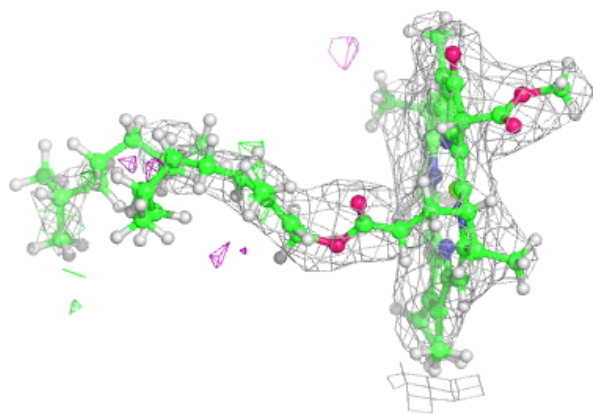
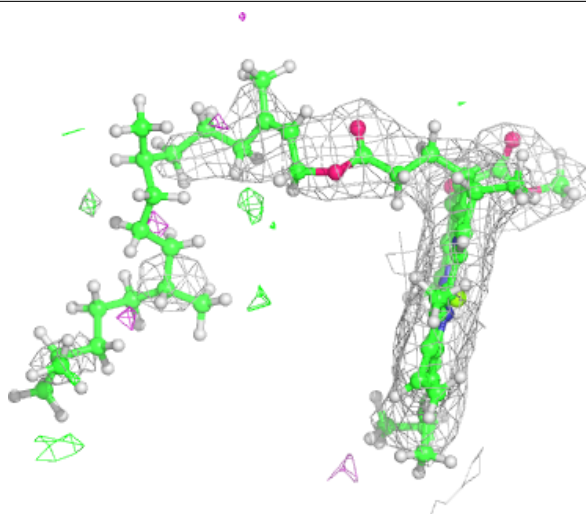
**Electron density around CLA c 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



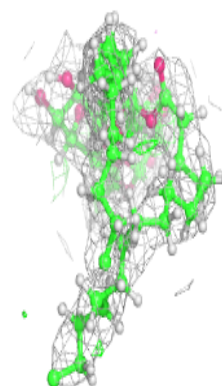
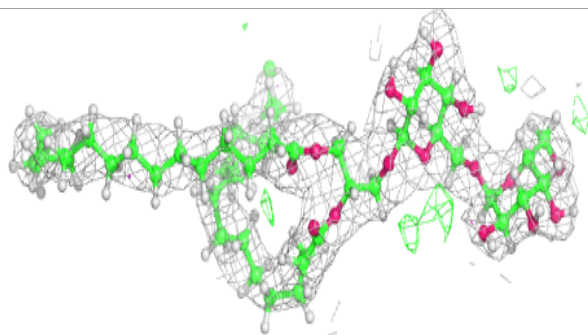
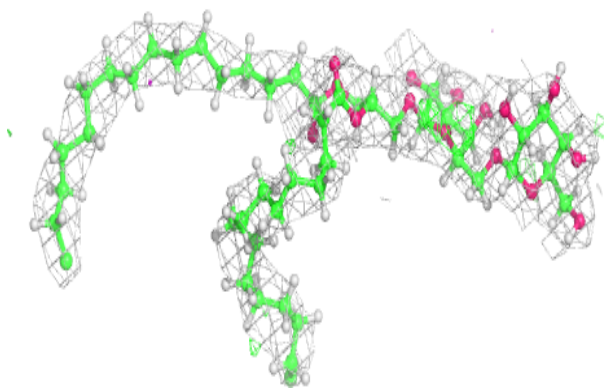
Electron density around CLA c 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

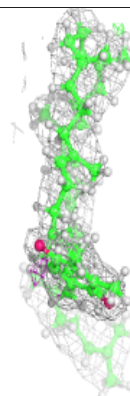
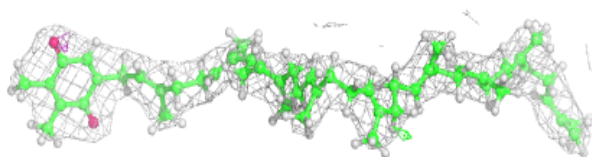
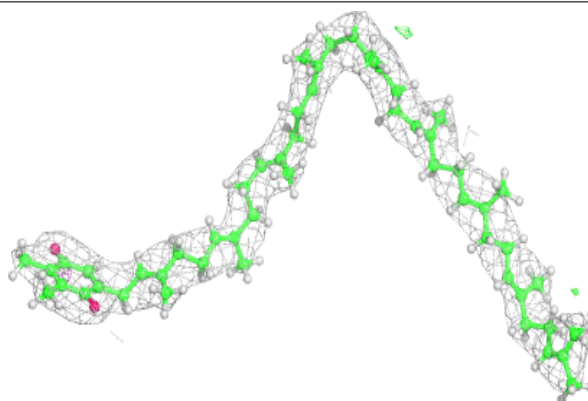


Electron density around DGD H 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

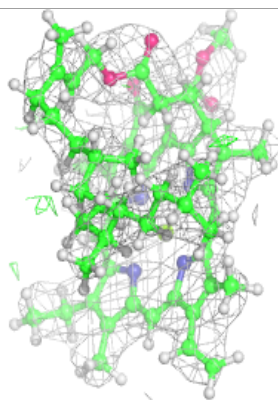
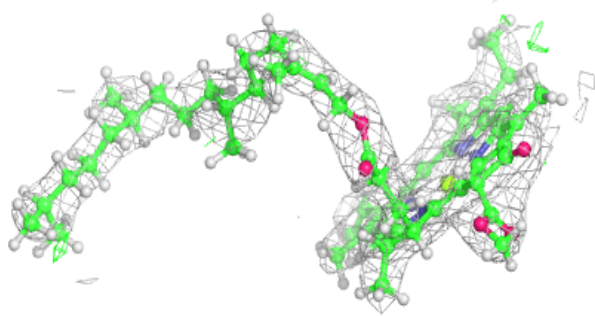
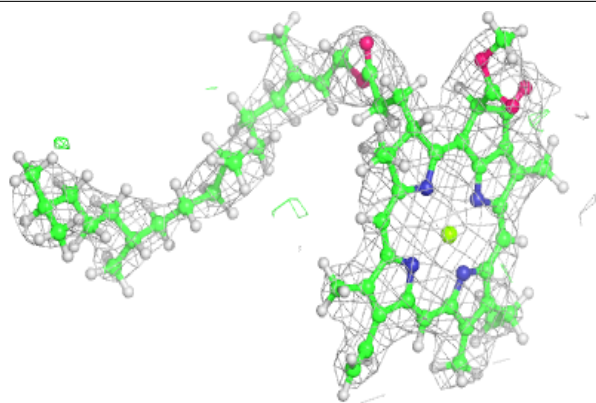
**Electron density around PL9 D 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

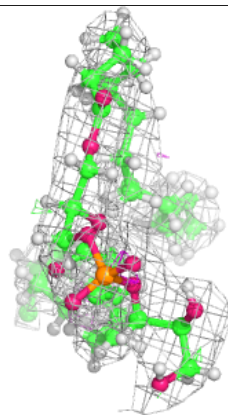
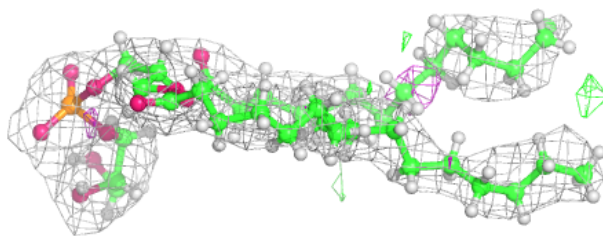
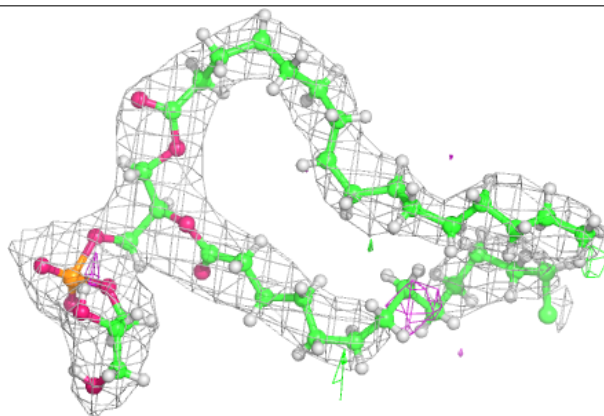


Electron density around CLA C 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

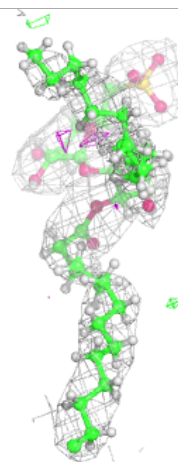
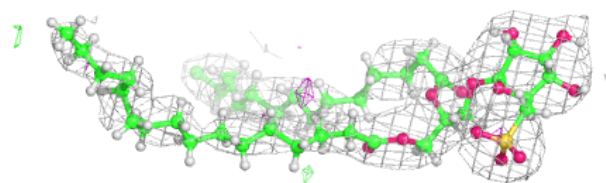
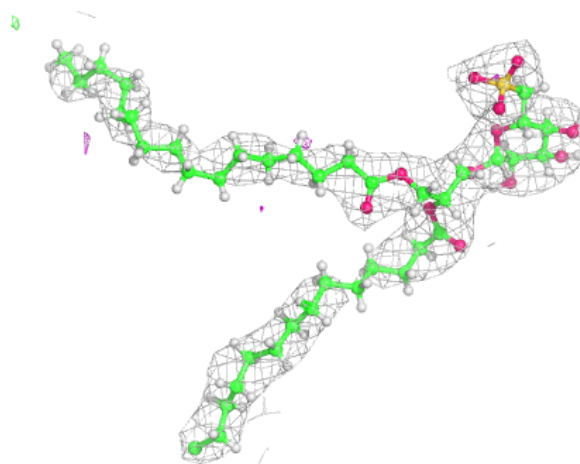
**Electron density around LHG D 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



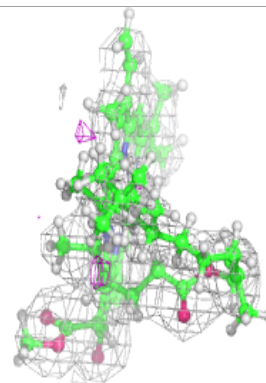
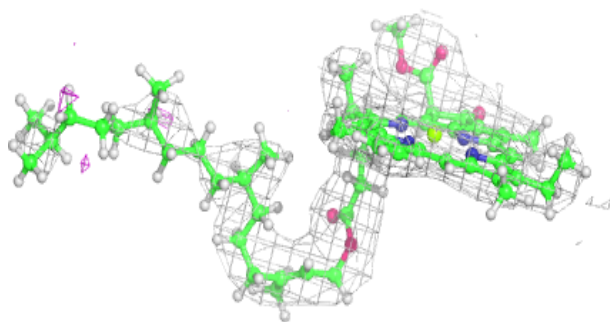
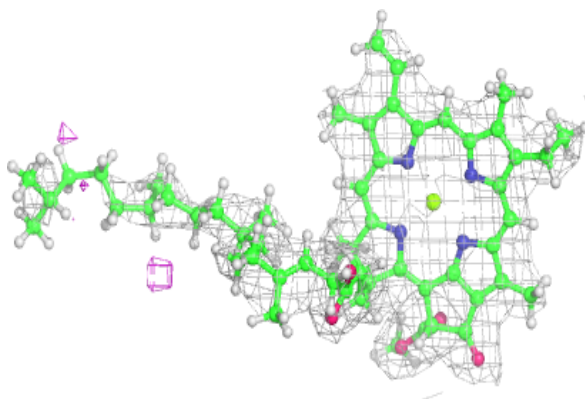
Electron density around SQD A 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

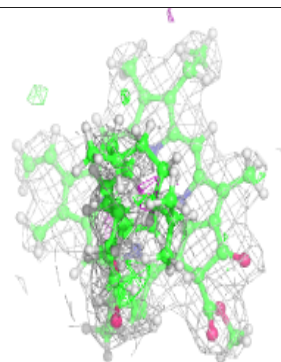
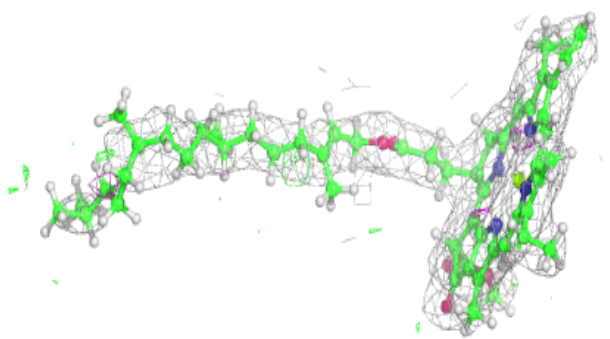
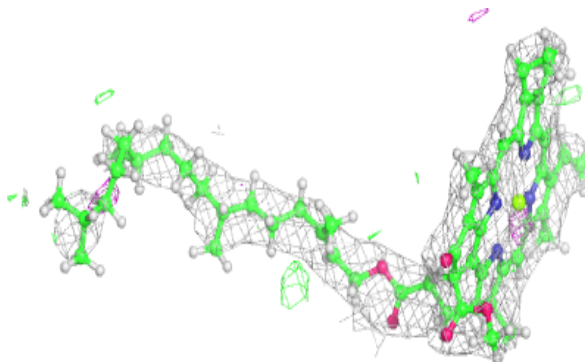


Electron density around CLA A 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

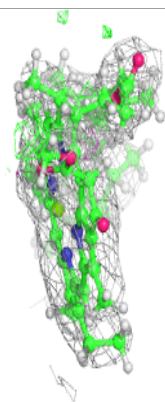
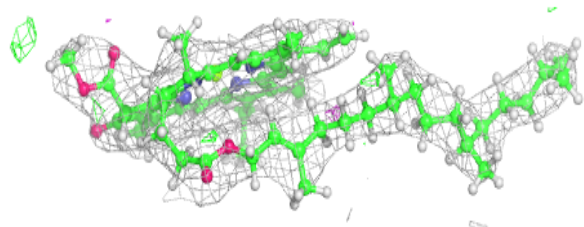
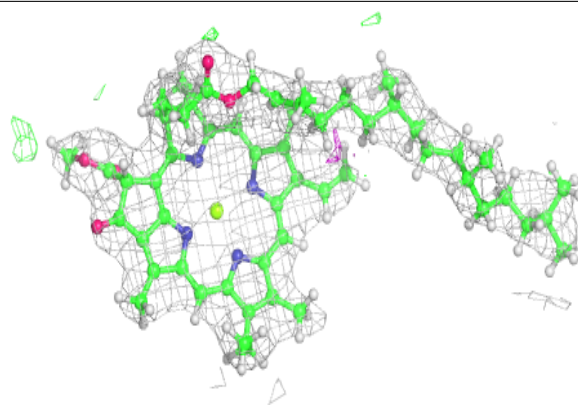
**Electron density around CLA B 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



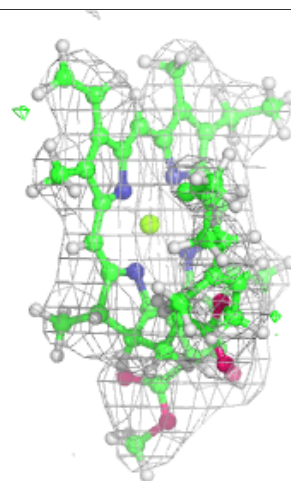
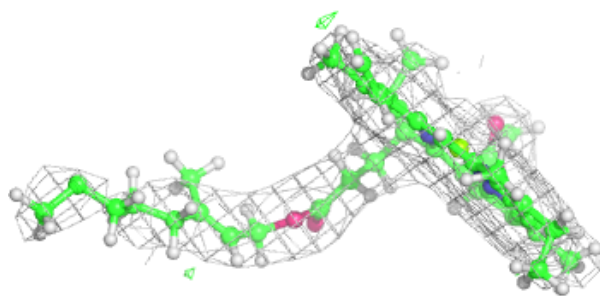
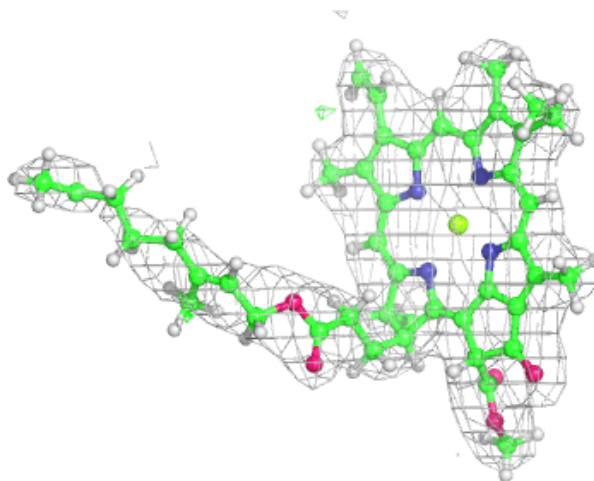
Electron density around CLA c 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



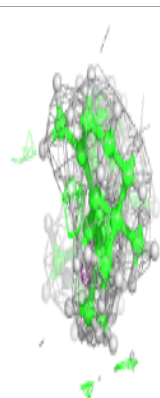
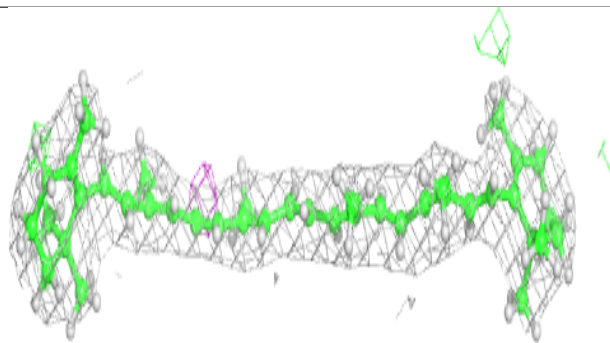
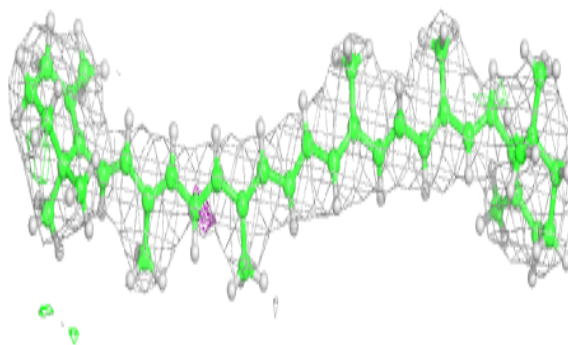
Electron density around CLA A 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

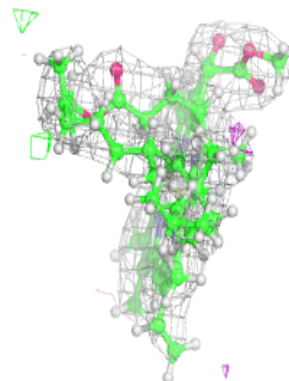
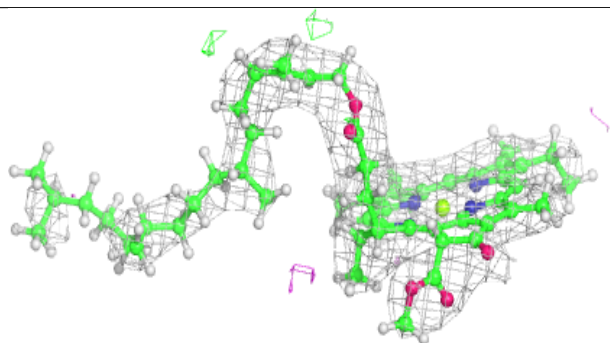
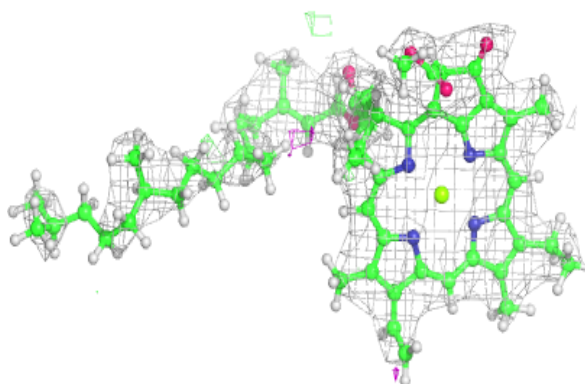


Electron density around BCR b 619:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

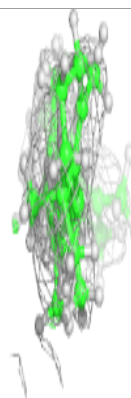
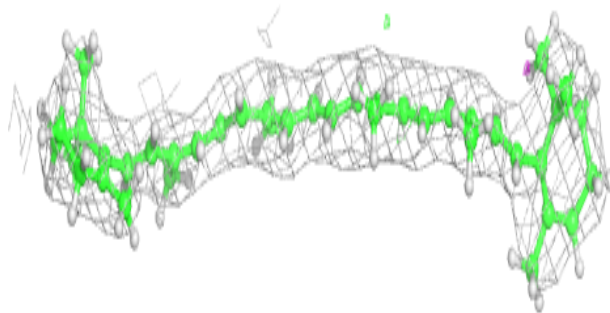
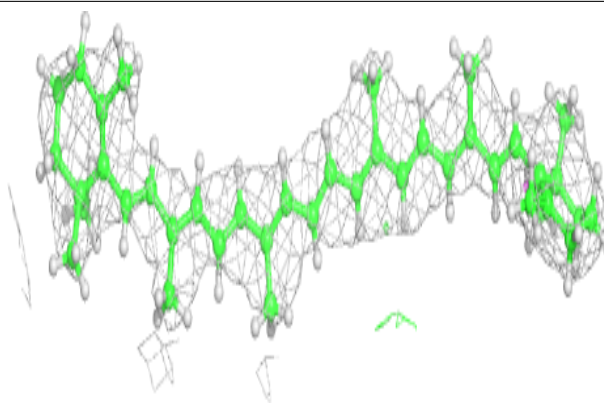
**Electron density around CLA a 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

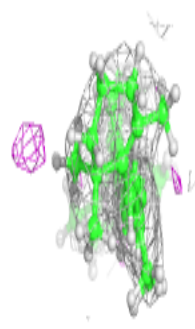
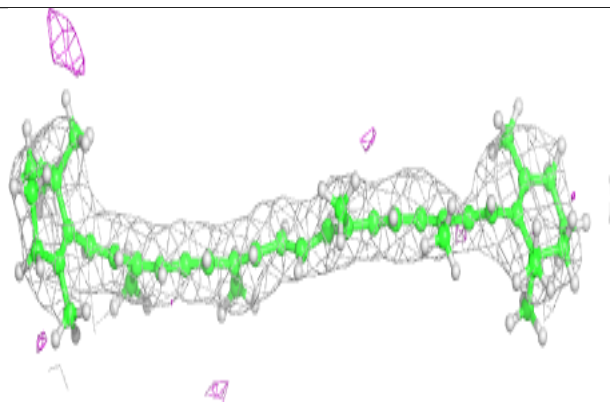
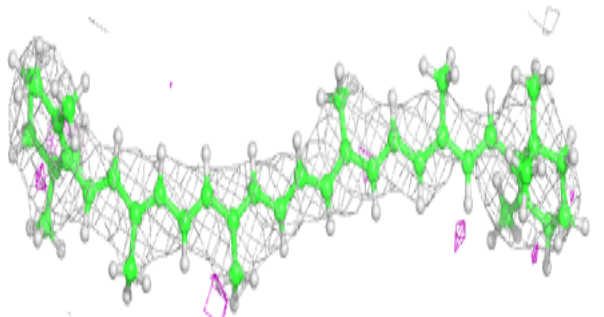


Electron density around BCR B 617:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

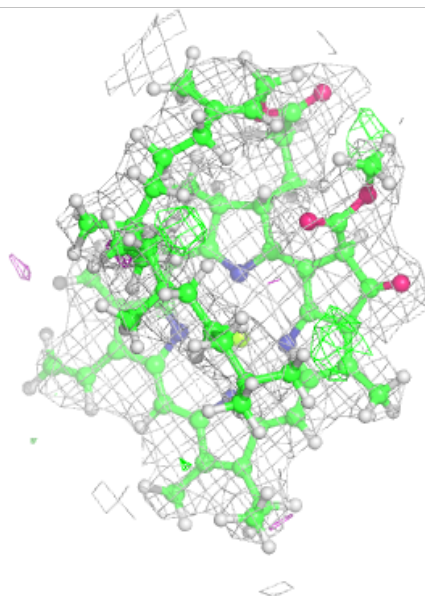
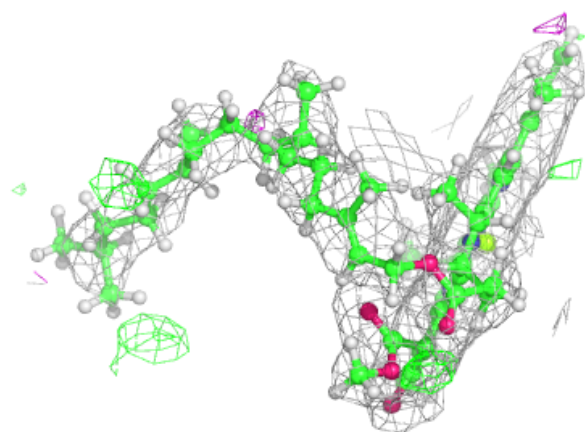
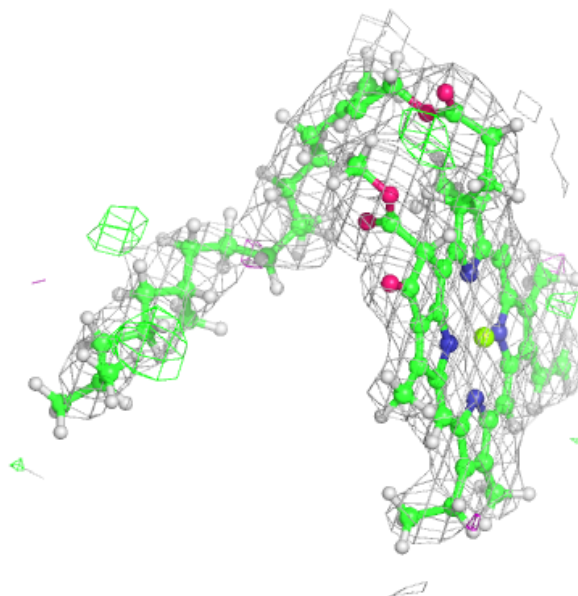
**Electron density around BCR c 515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



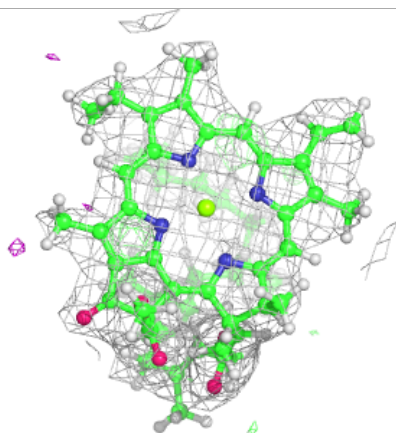
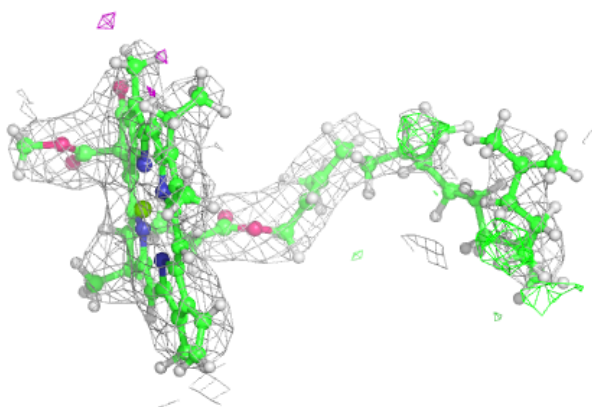
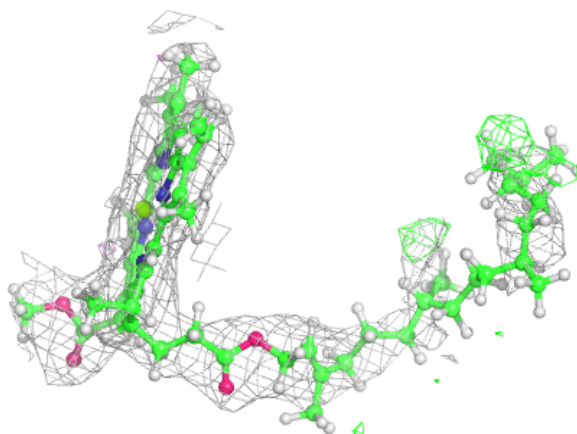
Electron density around CLA B 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



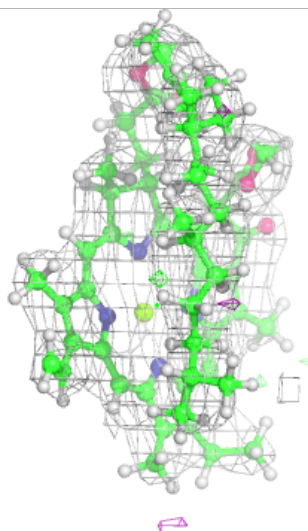
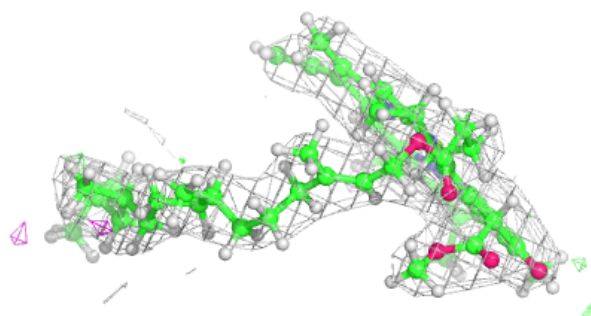
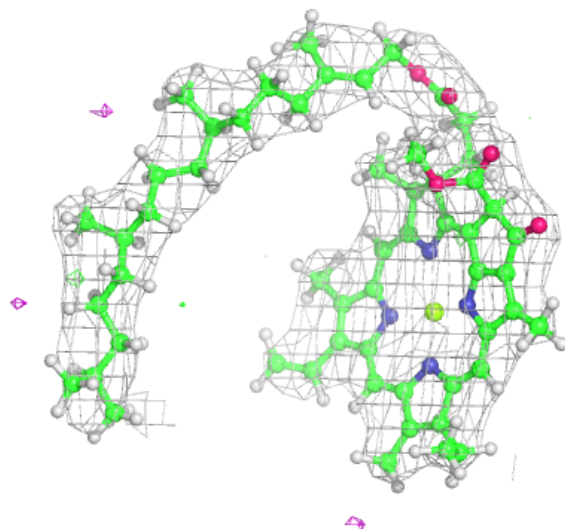
Electron density around CLA C 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



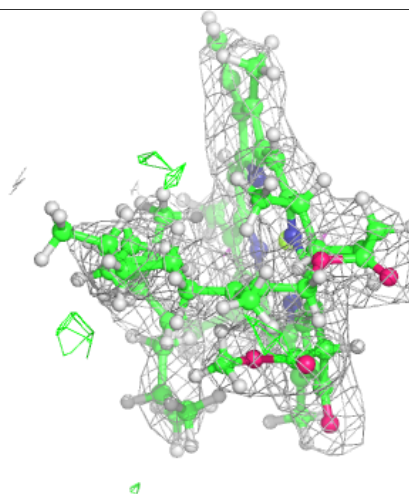
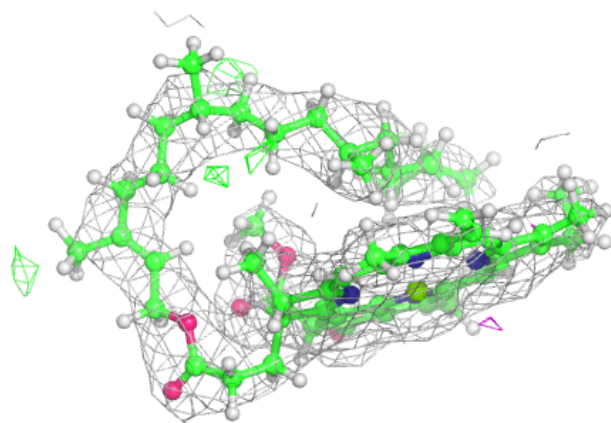
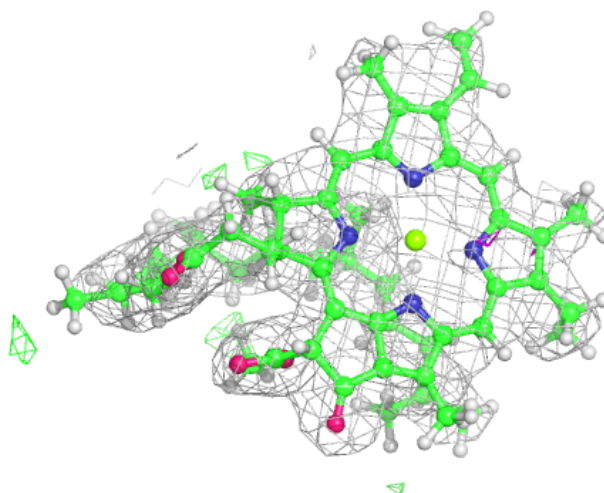
Electron density around CLA C 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



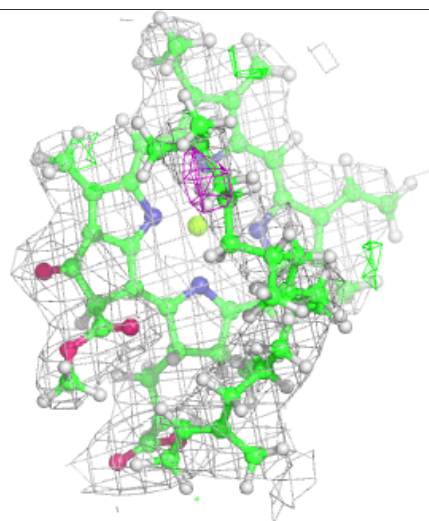
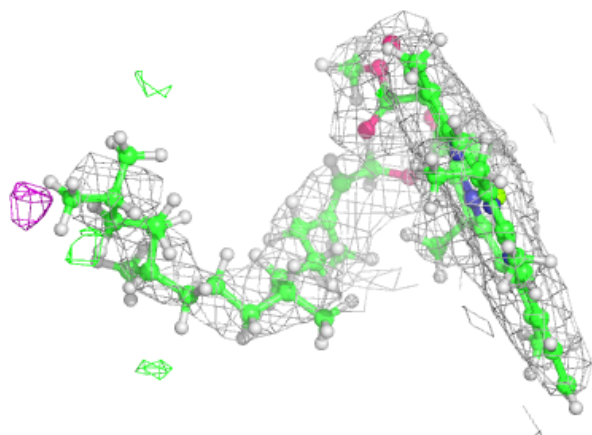
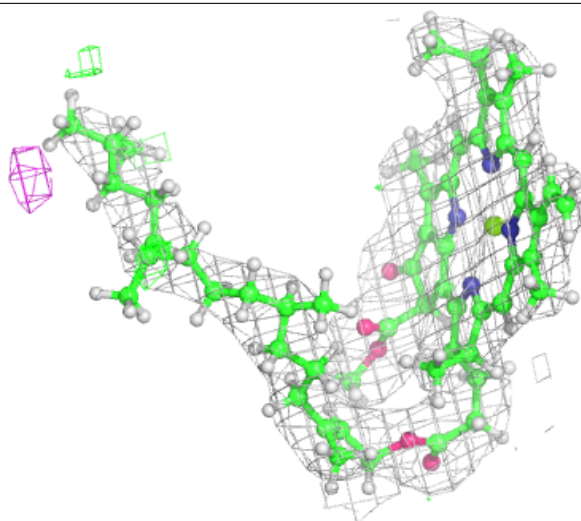
Electron density around CLA C 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



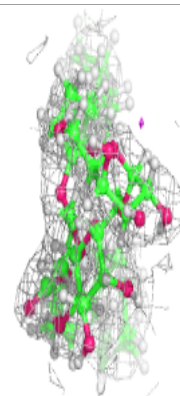
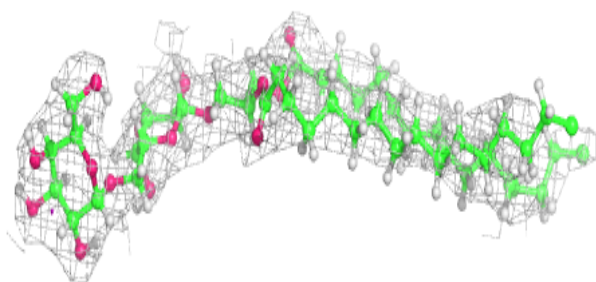
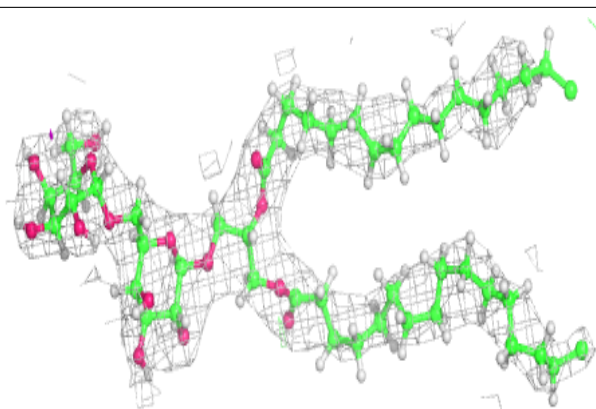
Electron density around CLA b 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

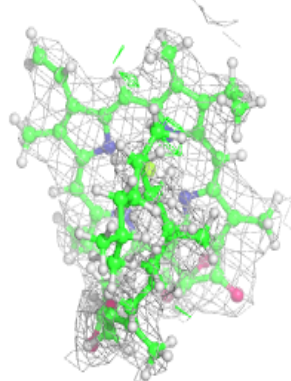
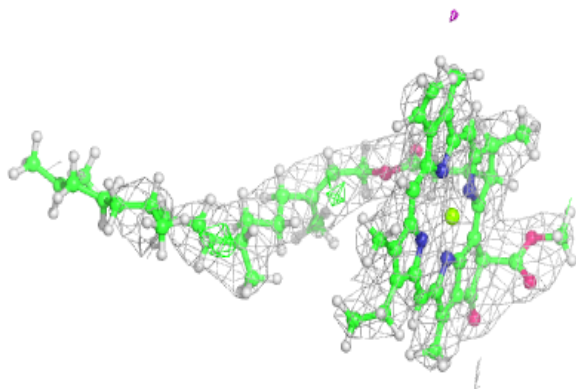
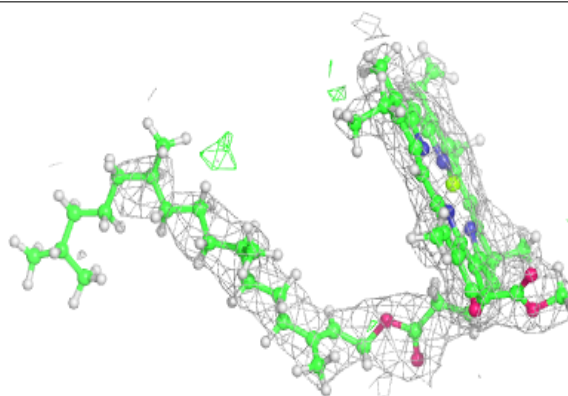


Electron density around DGD C 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

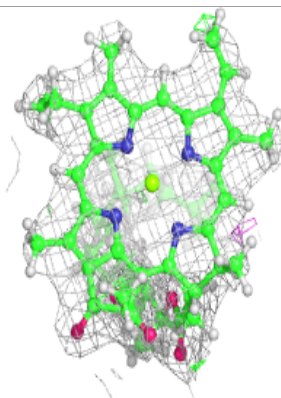
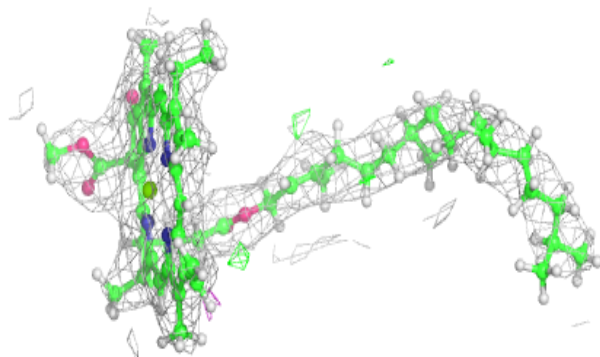
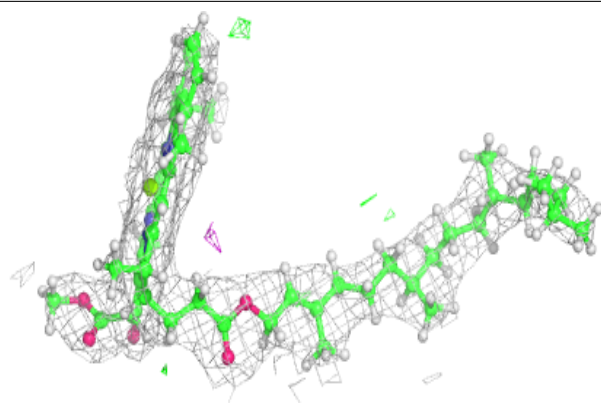
**Electron density around CLA C 509:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

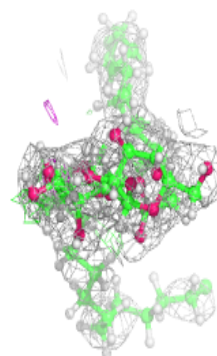
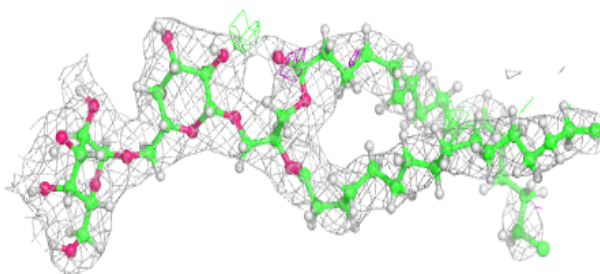
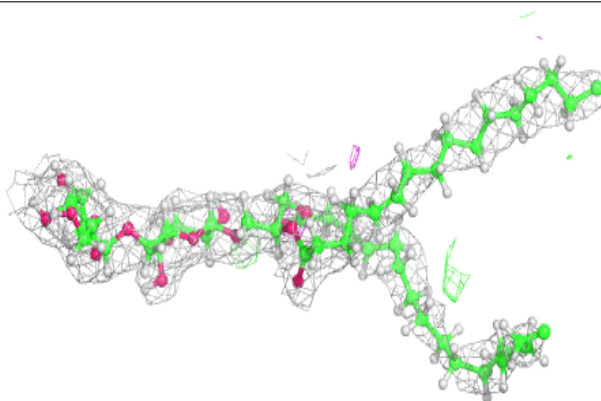


Electron density around CLA b 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

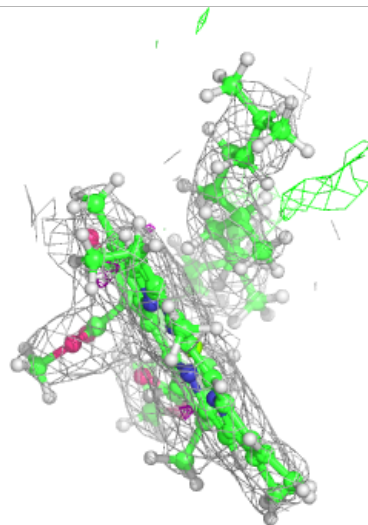
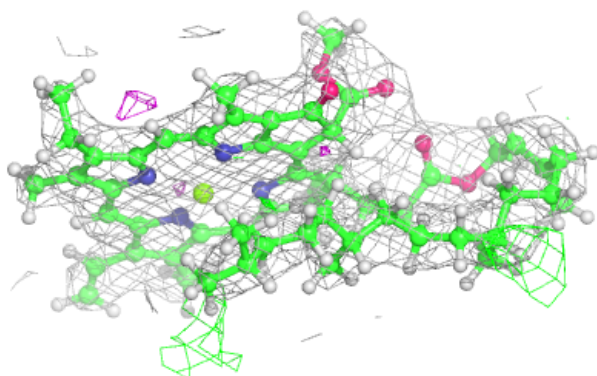
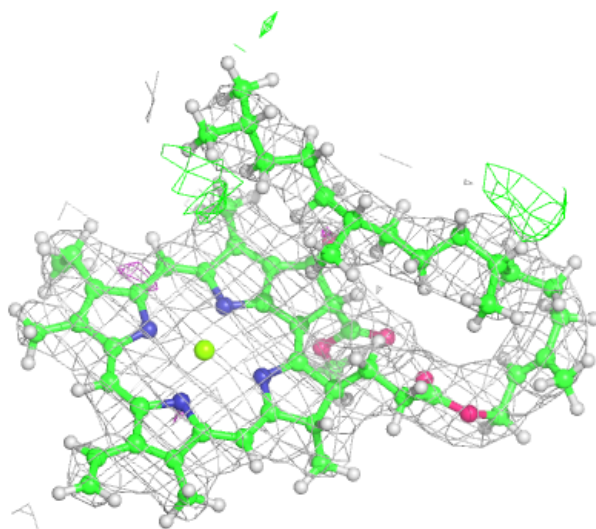
**Electron density around DGD c 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



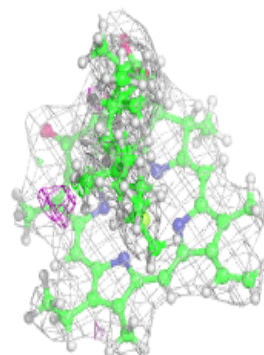
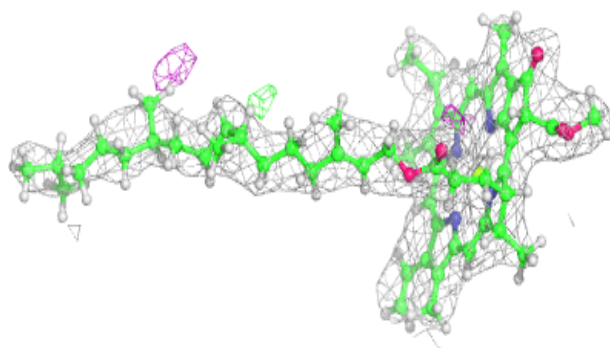
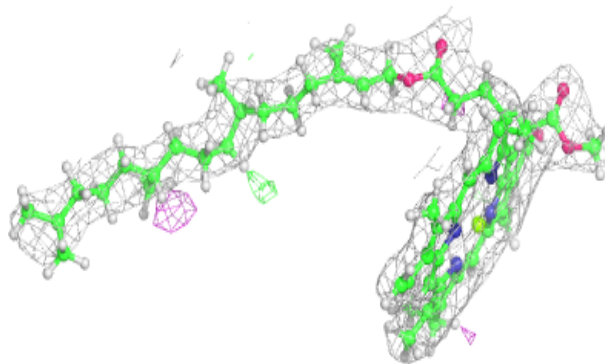
Electron density around CLA C 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

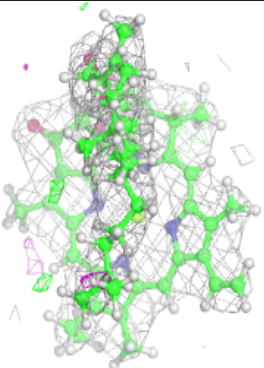
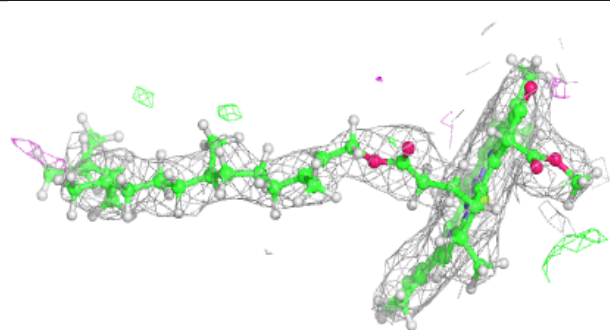
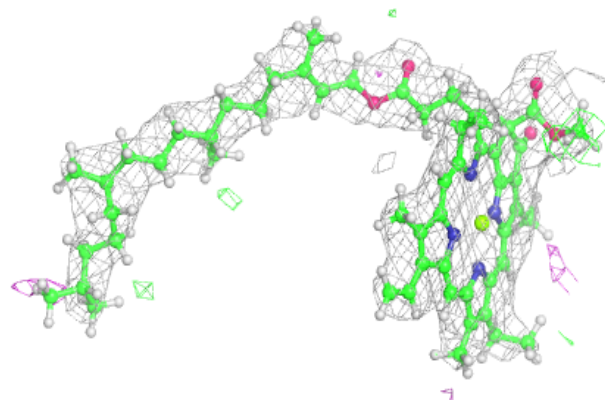


Electron density around CLA b 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

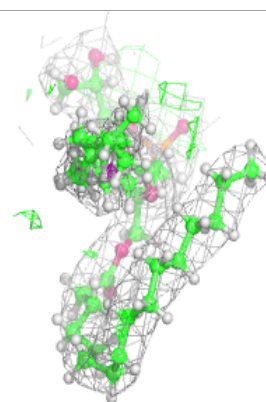
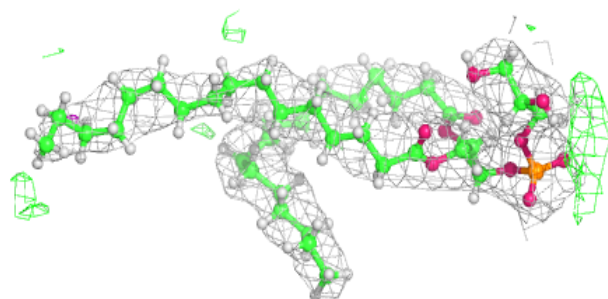
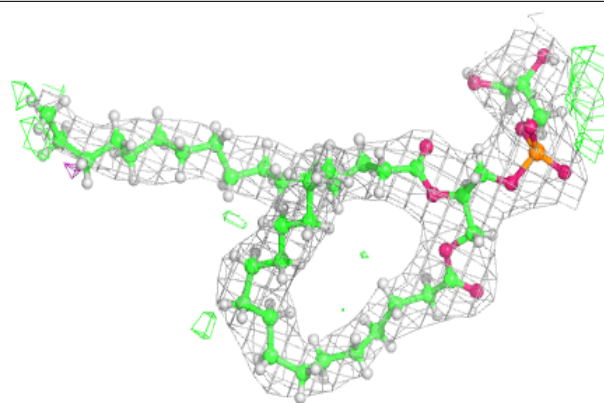
**Electron density around CLA b 610:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

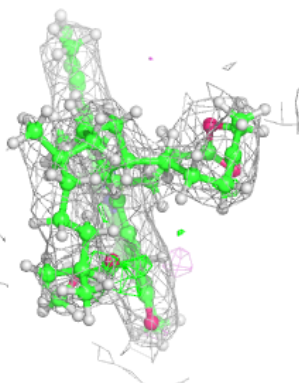
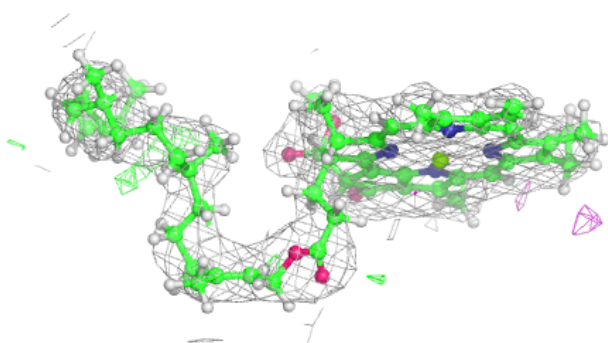
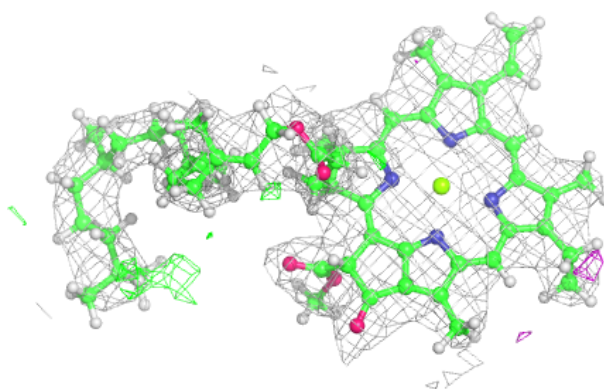


Electron density around LHG A 413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

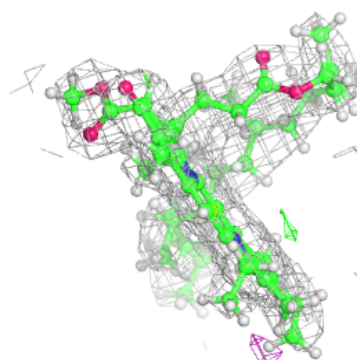
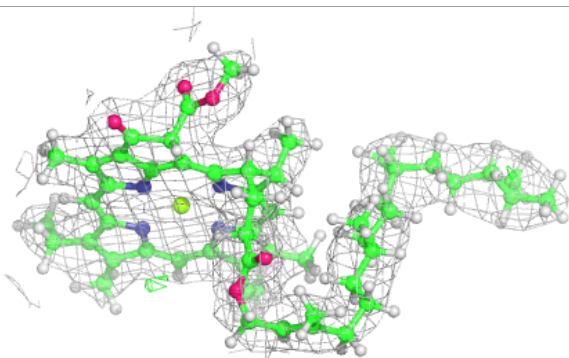
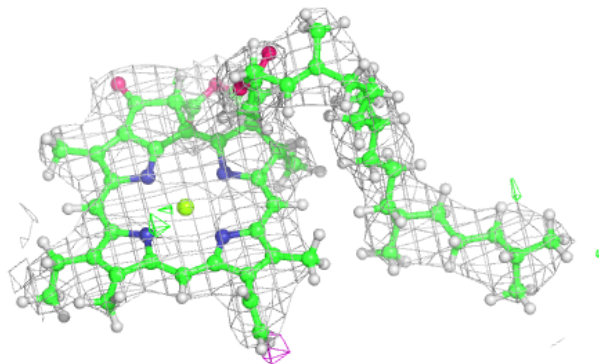
**Electron density around CLA b 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

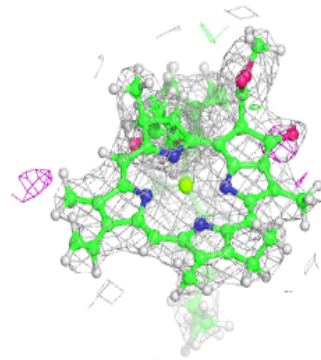
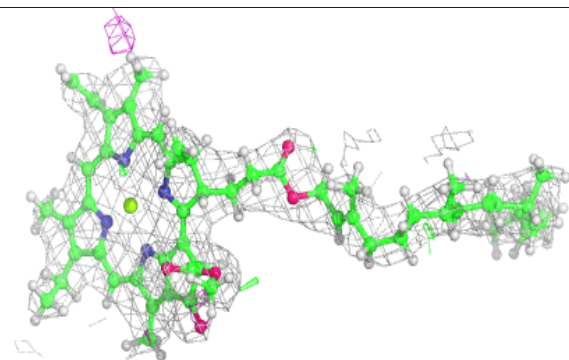
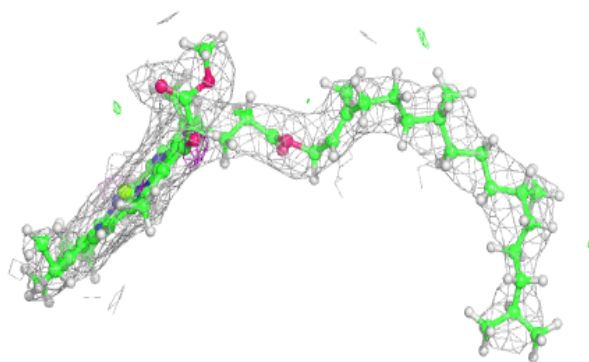


Electron density around CLA d 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

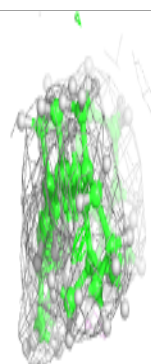
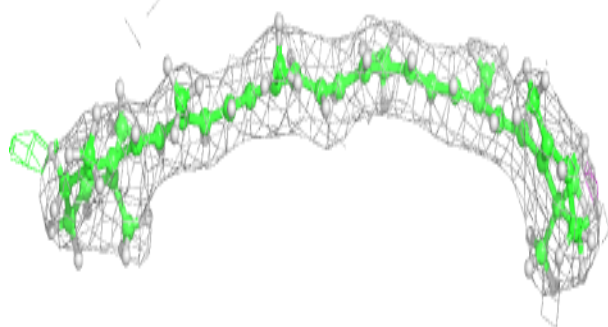
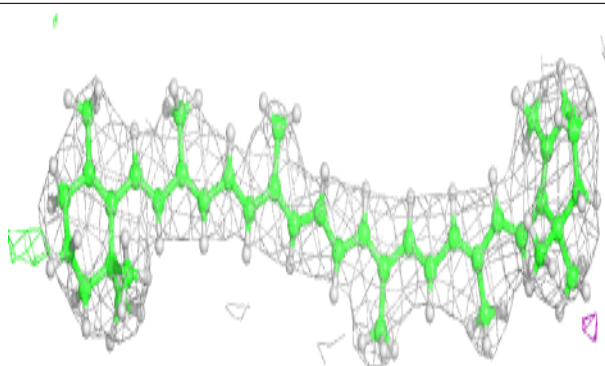
**Electron density around CLA d 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

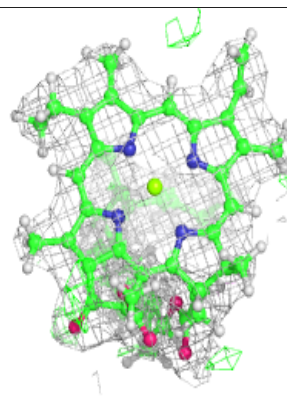
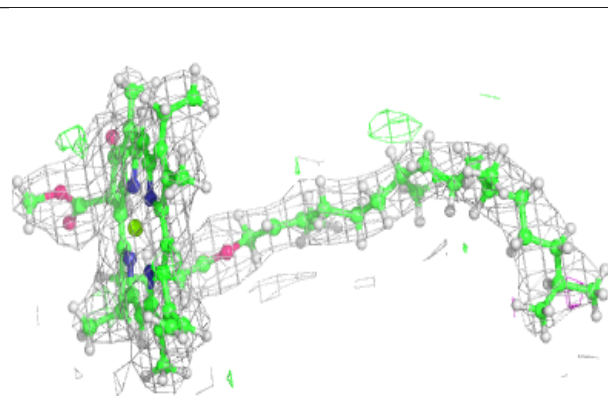
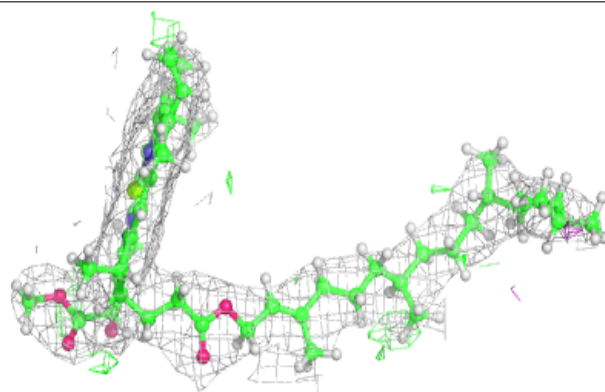


Electron density around BCR t 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

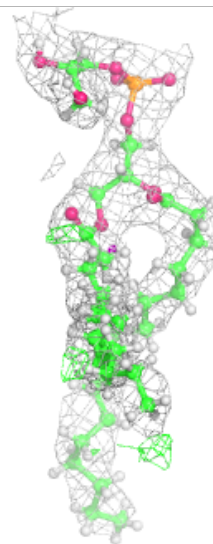
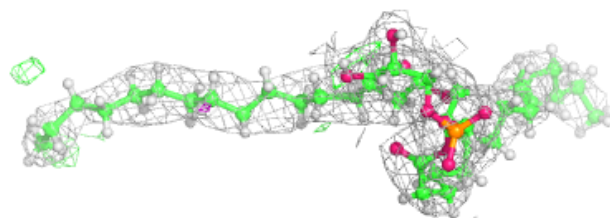
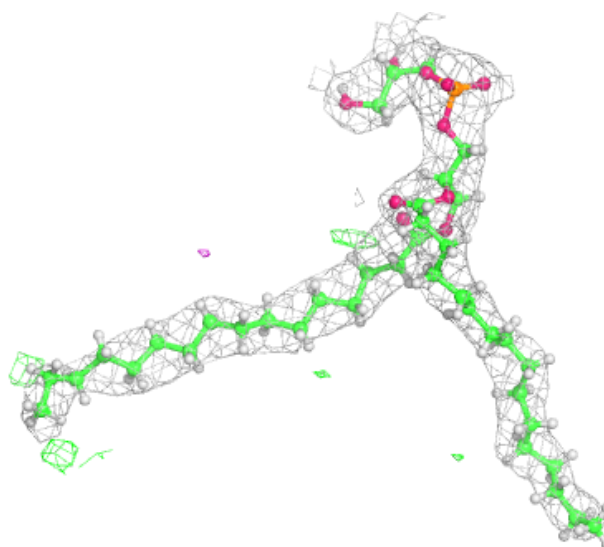
**Electron density around CLA B 605:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



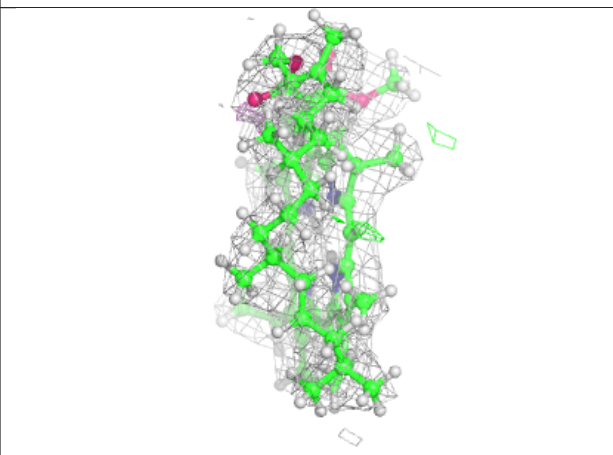
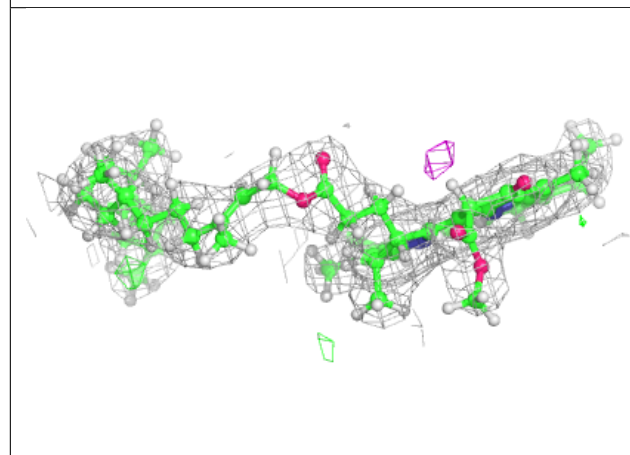
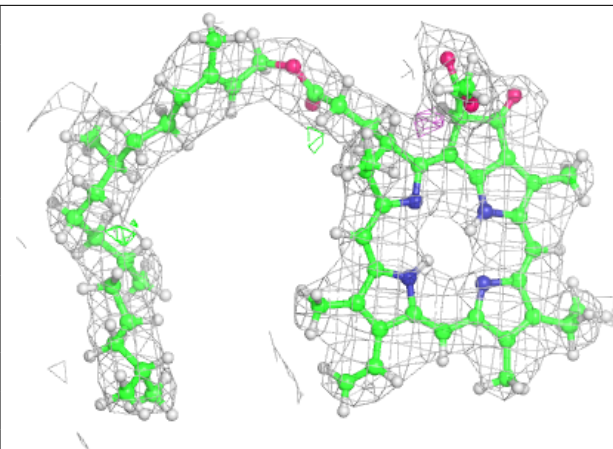
Electron density around LHG 1 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



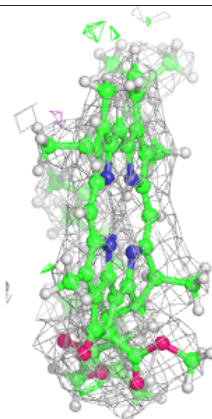
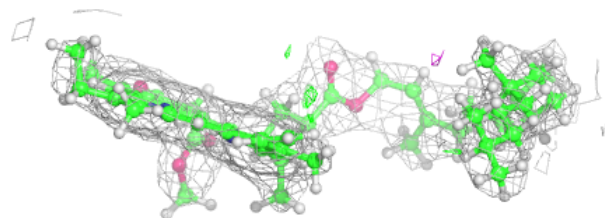
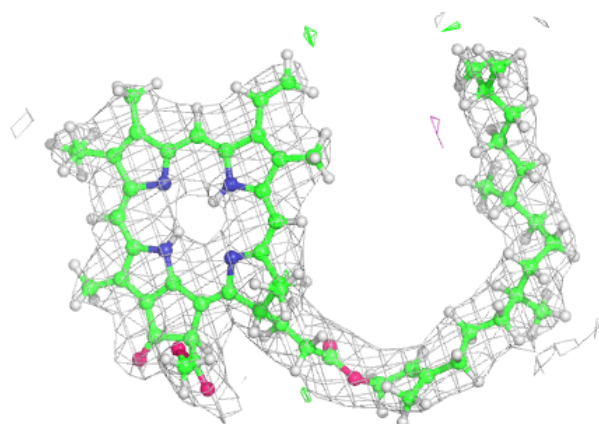
Electron density around PHO A 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

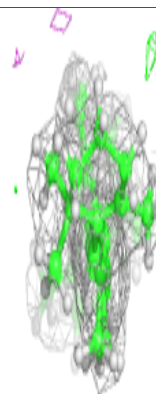
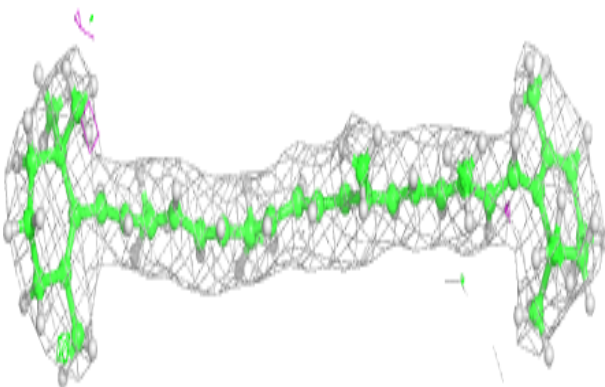
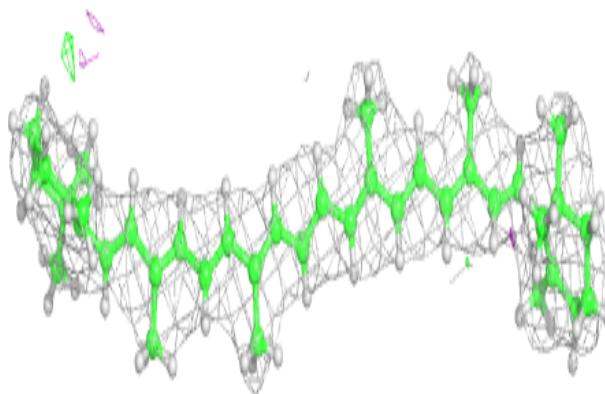


Electron density around PHO a 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

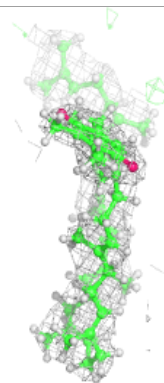
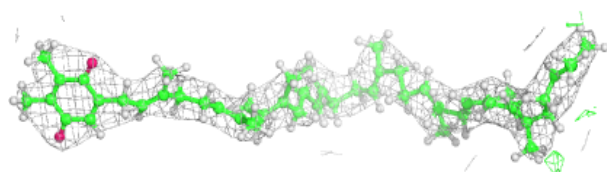
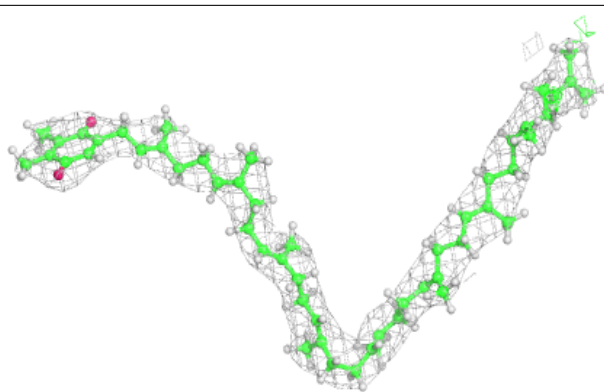
**Electron density around BCR A 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

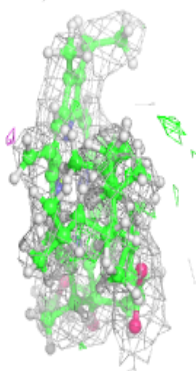
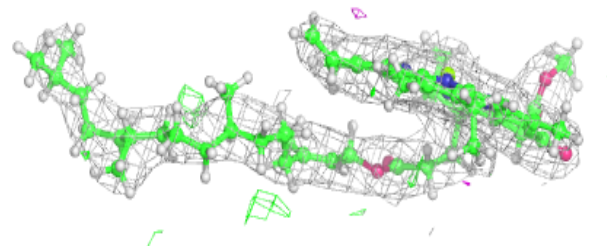
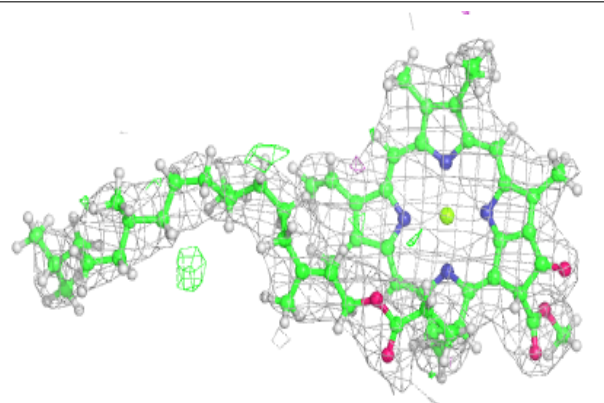


Electron density around PL9 d 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

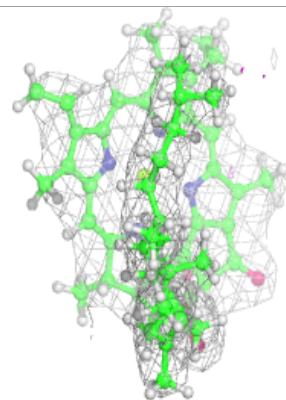
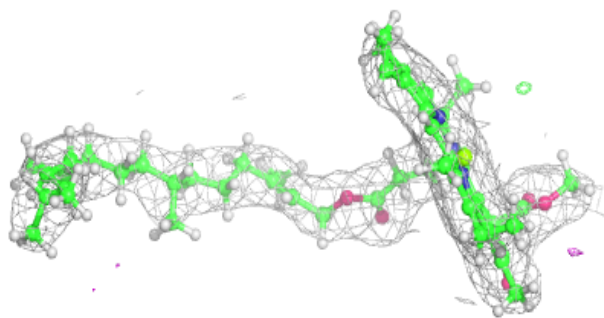
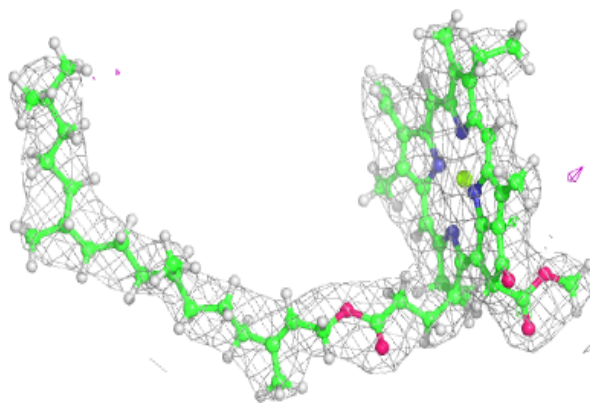
**Electron density around CLA B 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



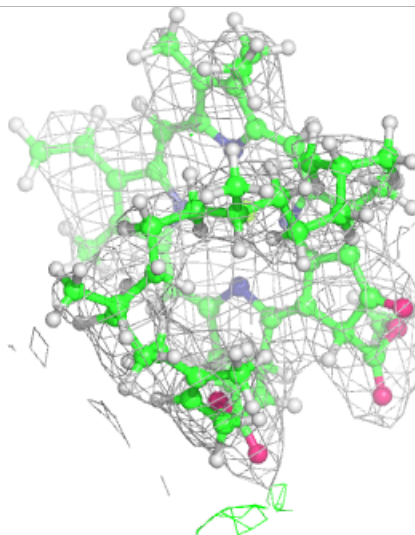
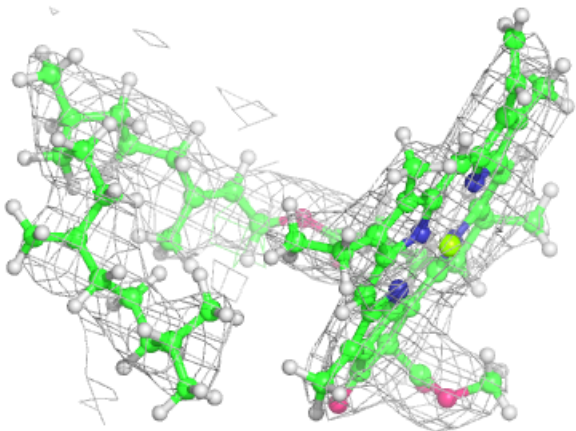
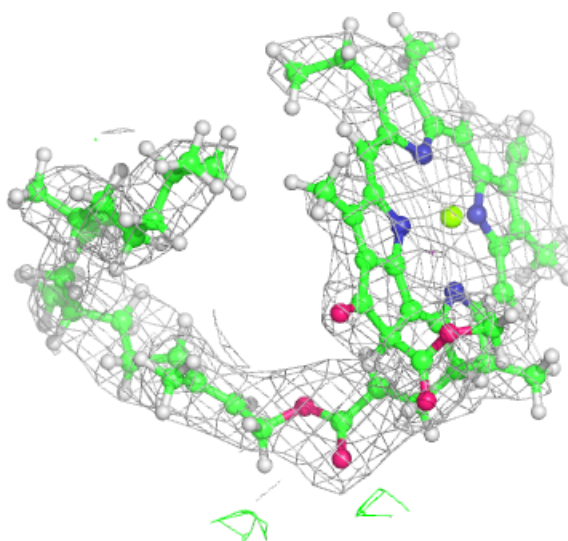
Electron density around CLA B 609:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



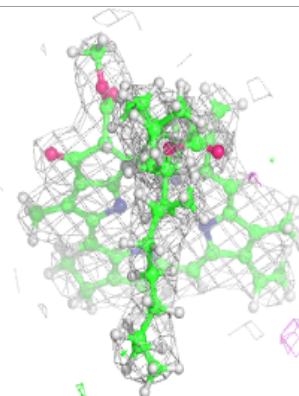
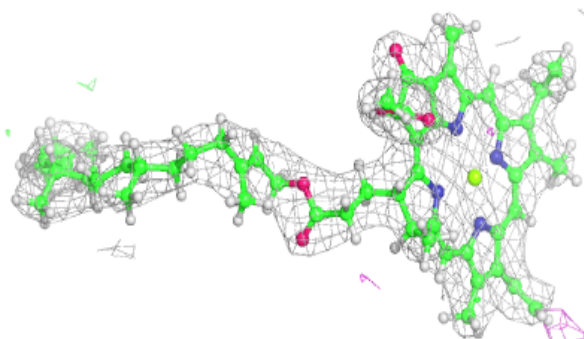
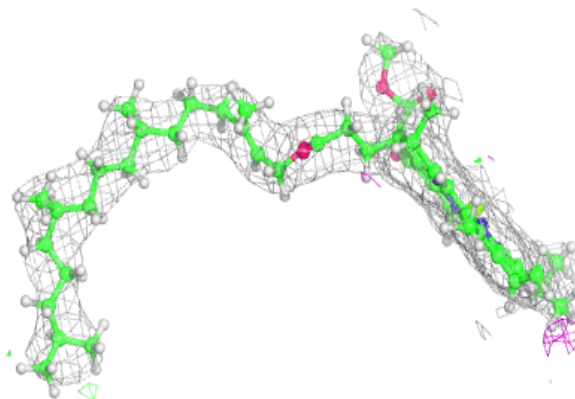
Electron density around CLA C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

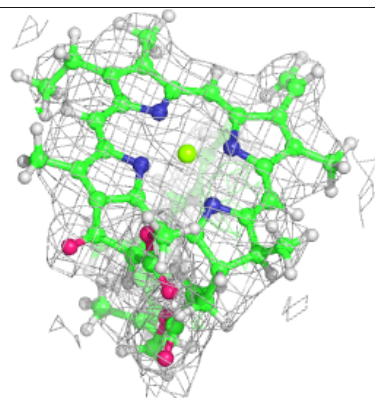
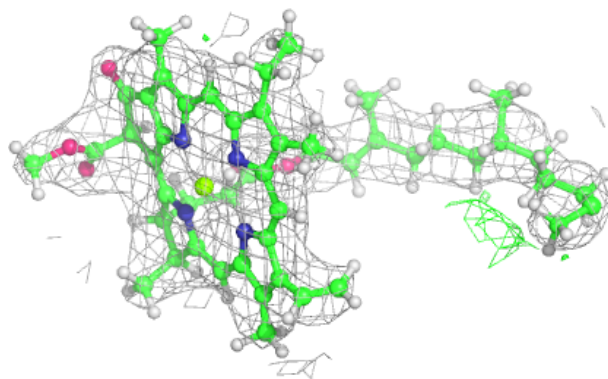
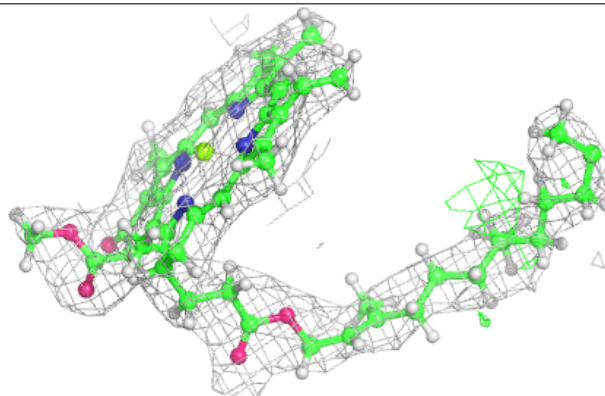


Electron density around CLA D 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

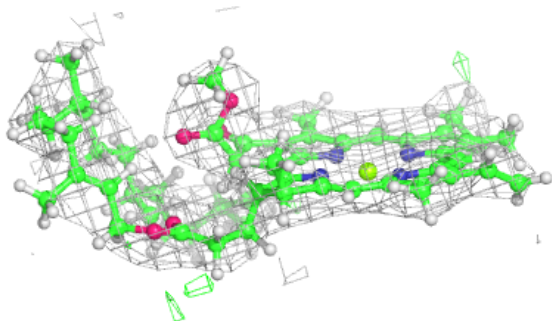
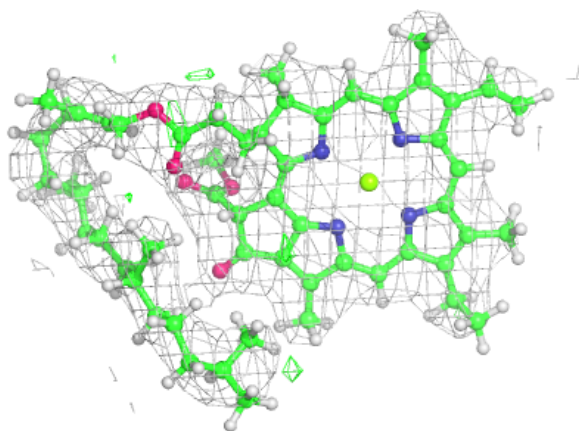
**Electron density around CLA C 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

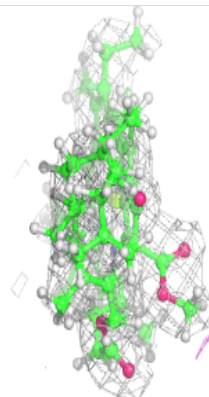
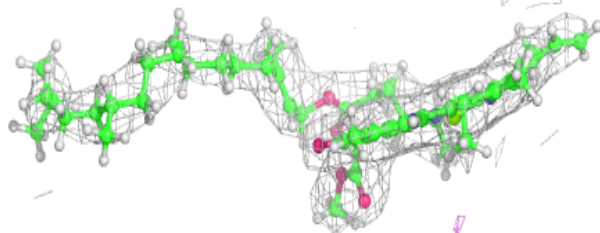
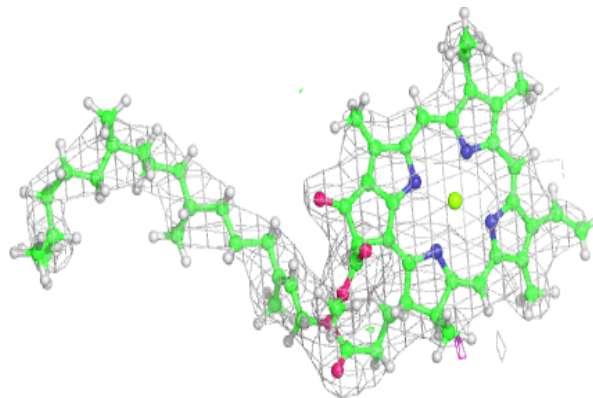


Electron density around CLA B 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

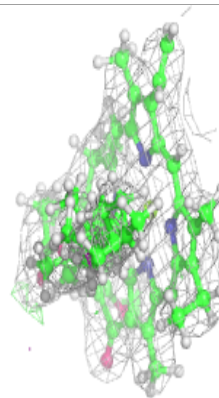
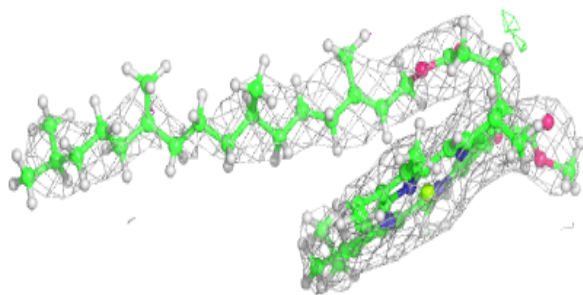
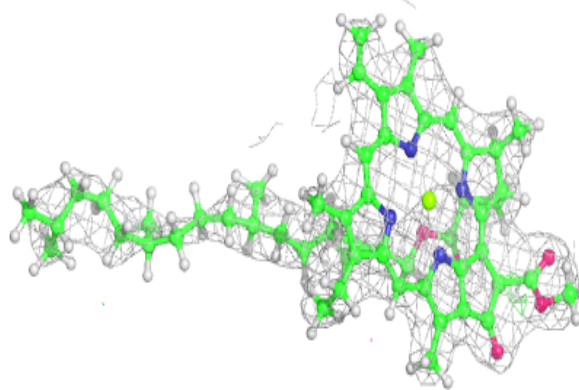
**Electron density around CLA B 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

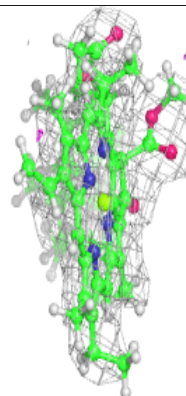
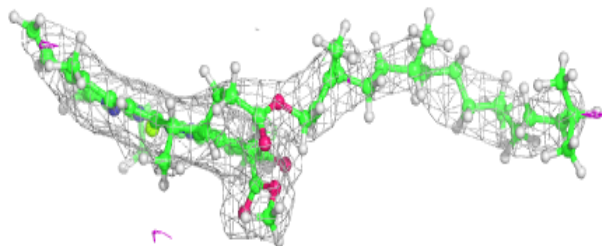
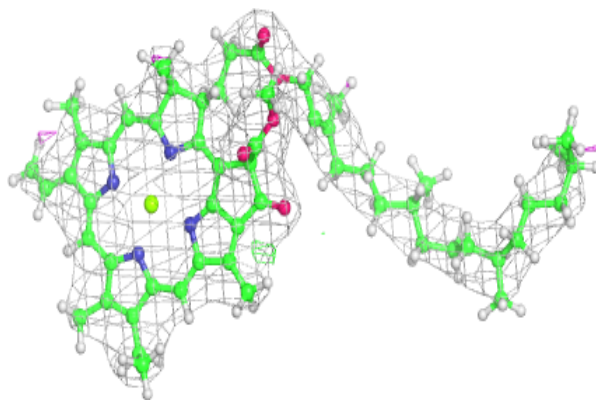


Electron density around CLA B 614:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

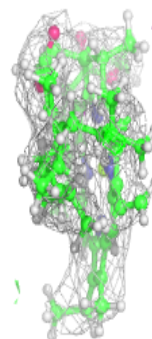
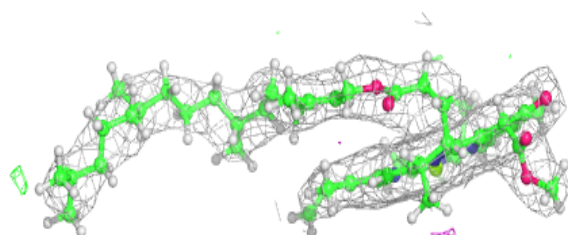
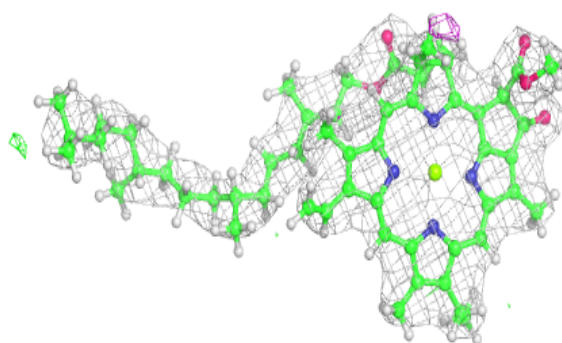
**Electron density around CLA b 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

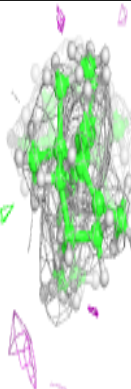
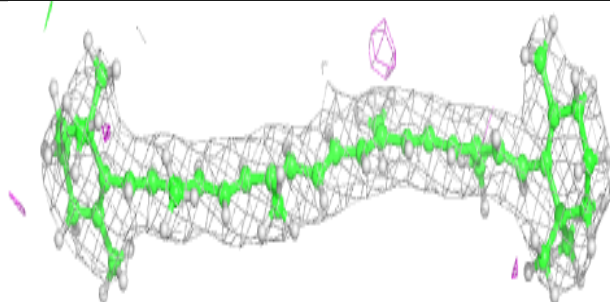
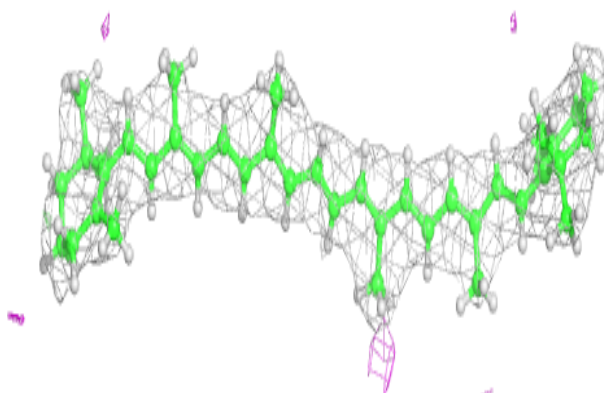


Electron density around CLA b 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

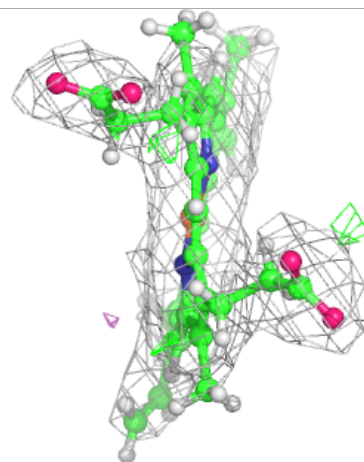
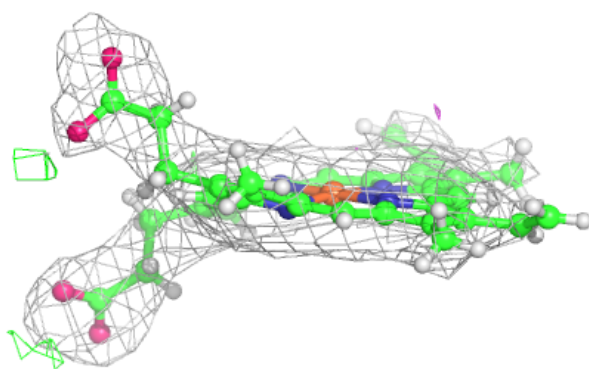
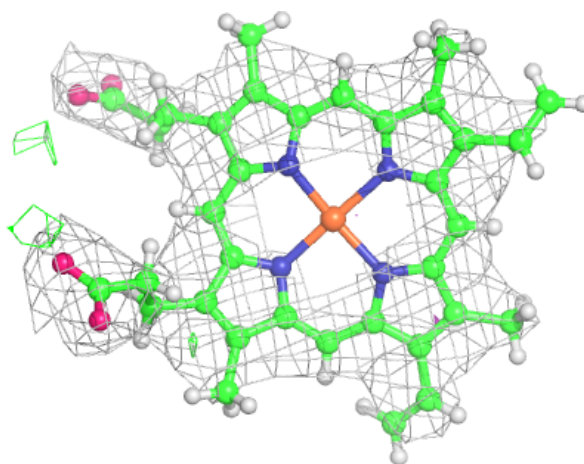
**Electron density around BCR a 409:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



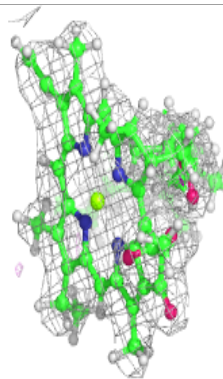
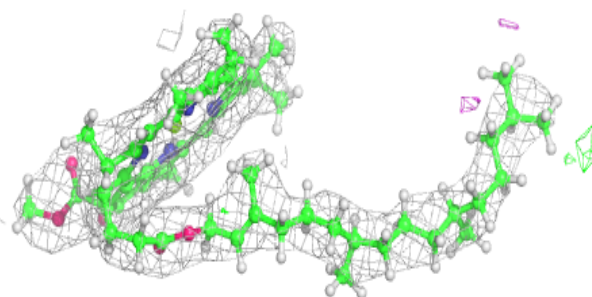
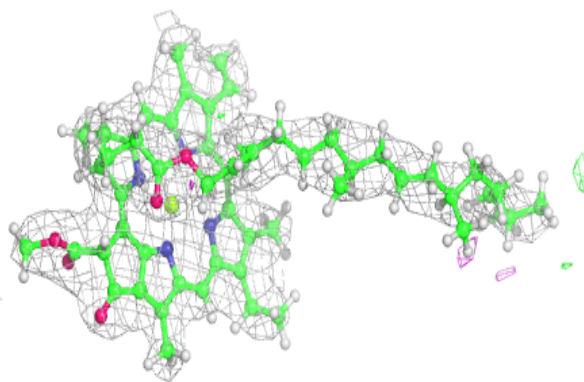
Electron density around HEM E 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

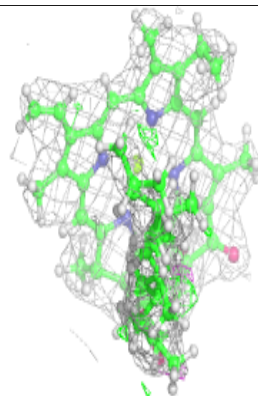
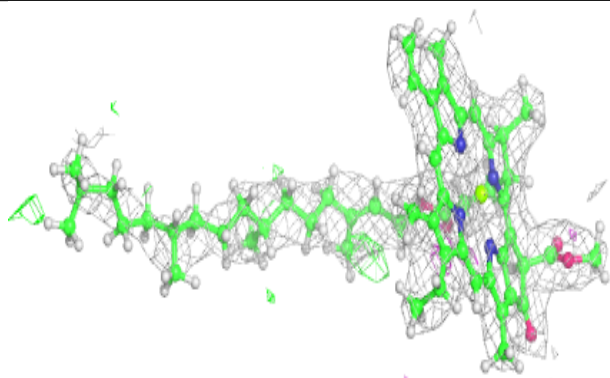
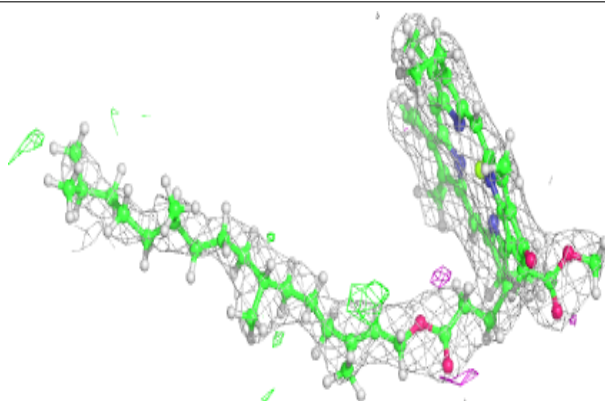


Electron density around CLA b 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

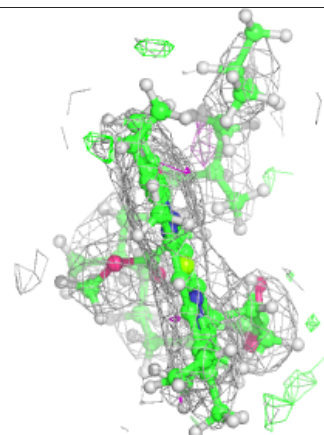
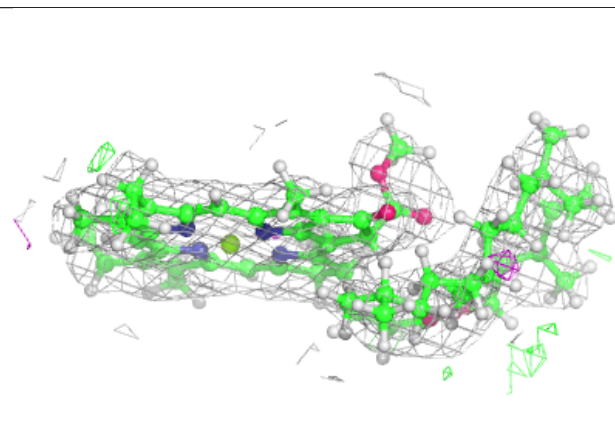
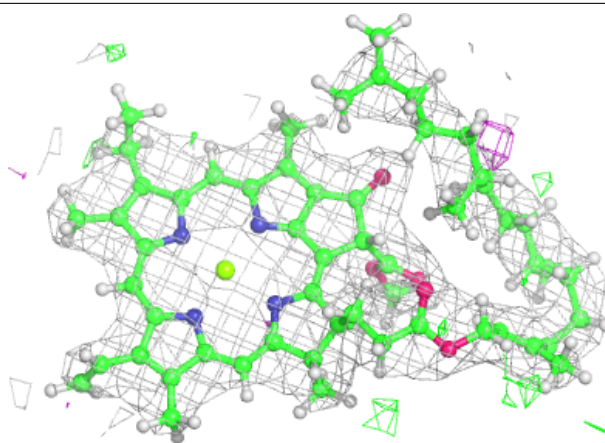
**Electron density around CLA B 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



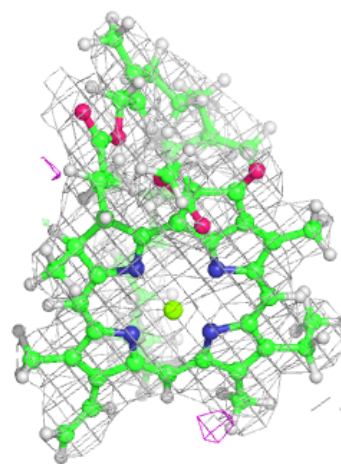
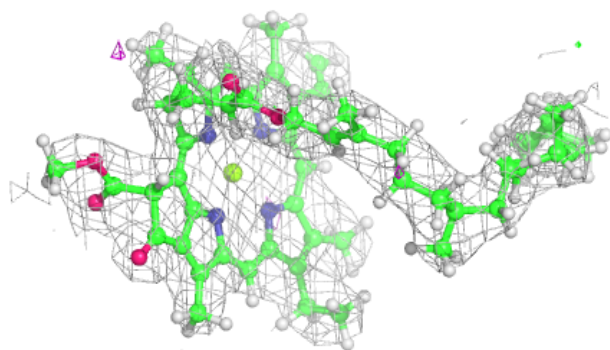
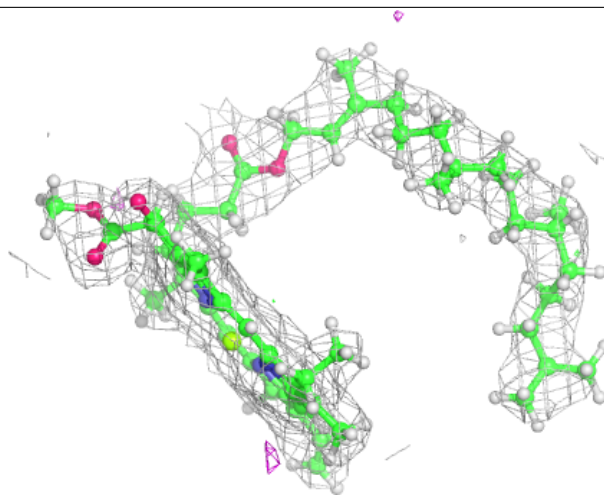
Electron density around CLA b 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



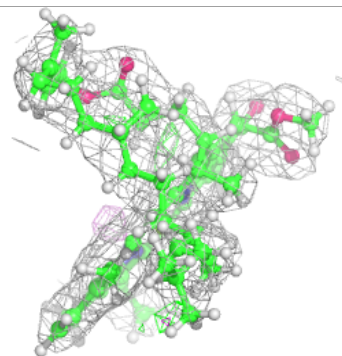
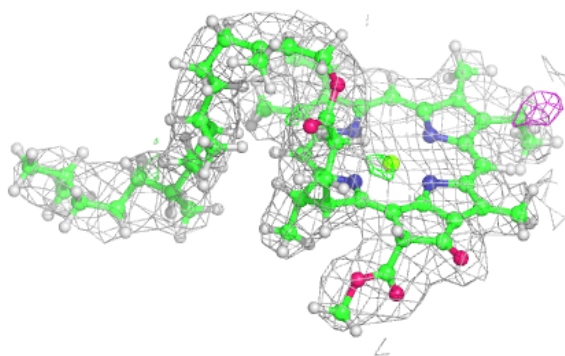
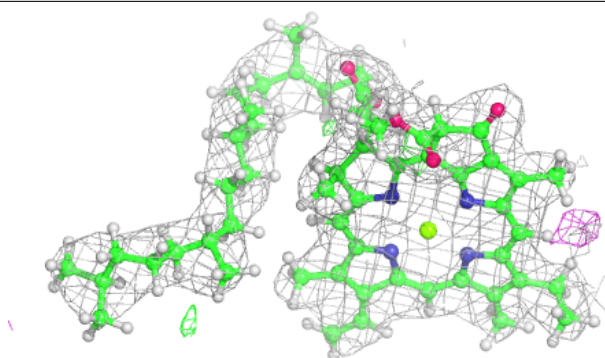
Electron density around CLA b 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

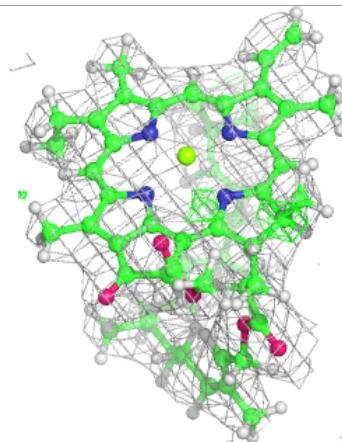
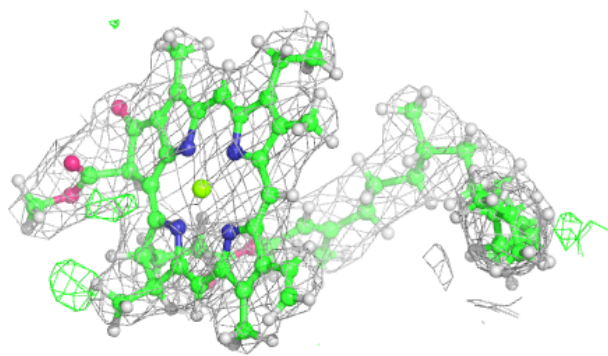
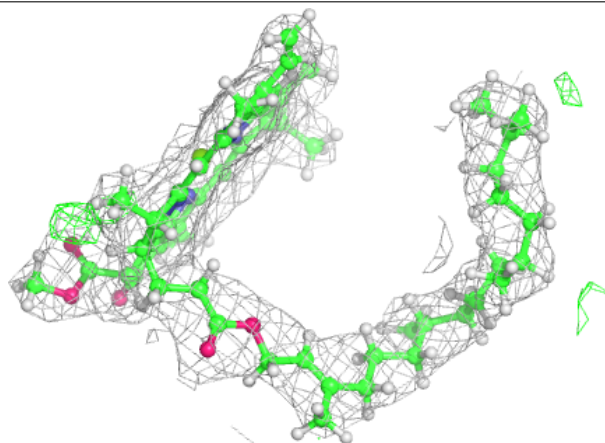


Electron density around CLA D 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

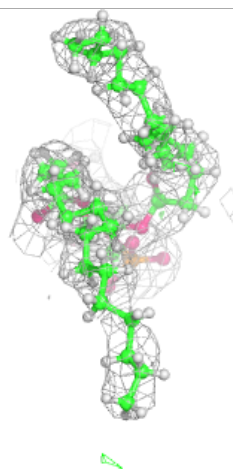
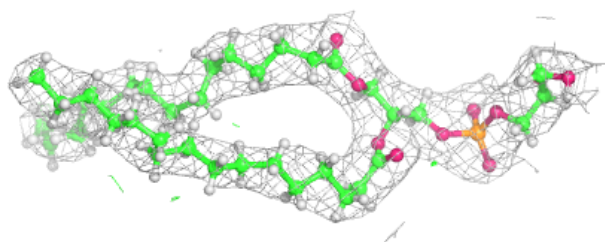
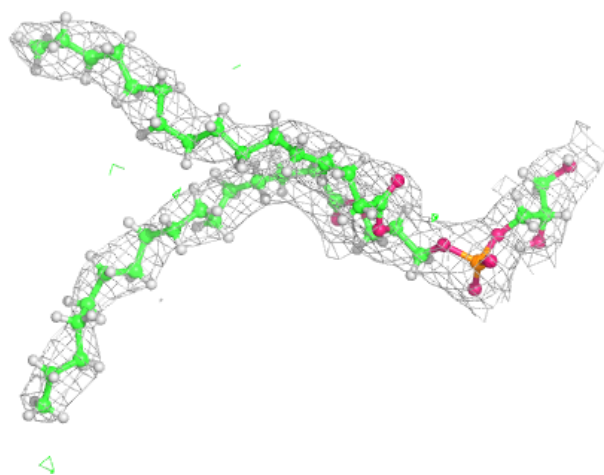
**Electron density around CLA B 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



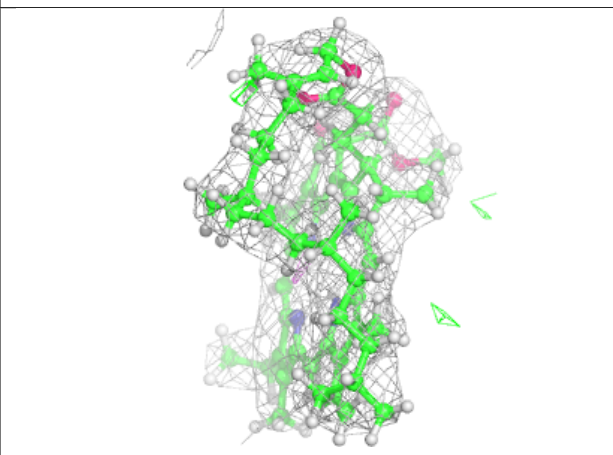
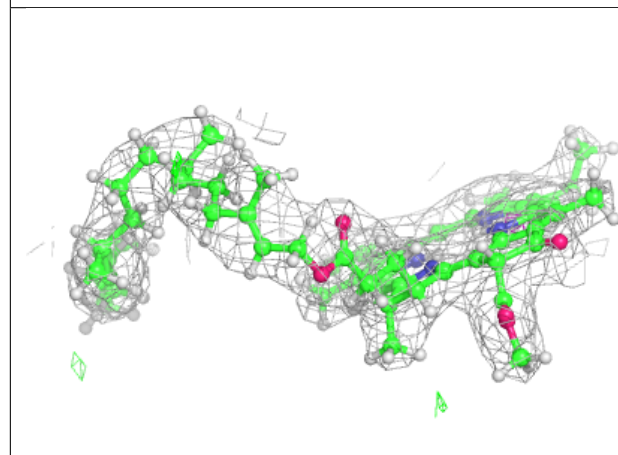
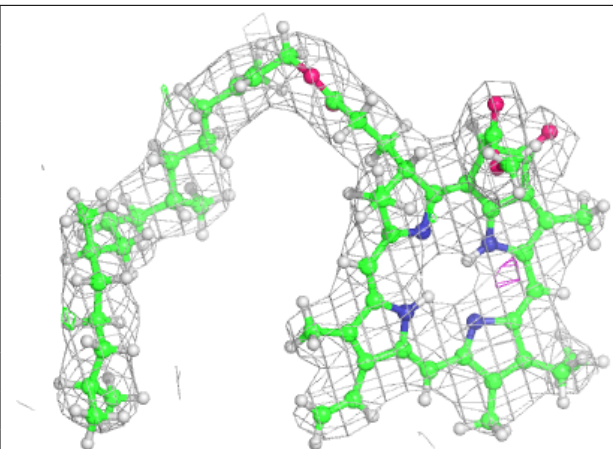
Electron density around LHG D 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

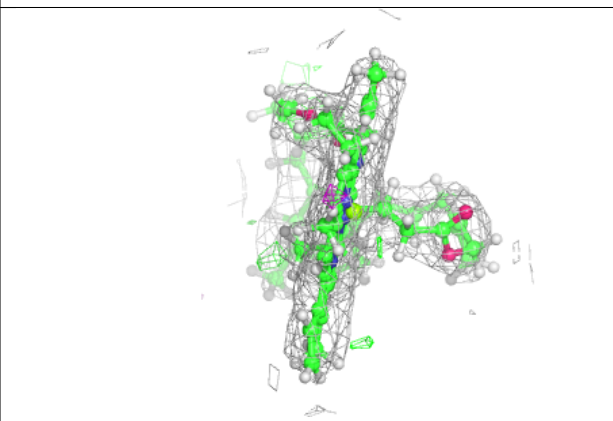
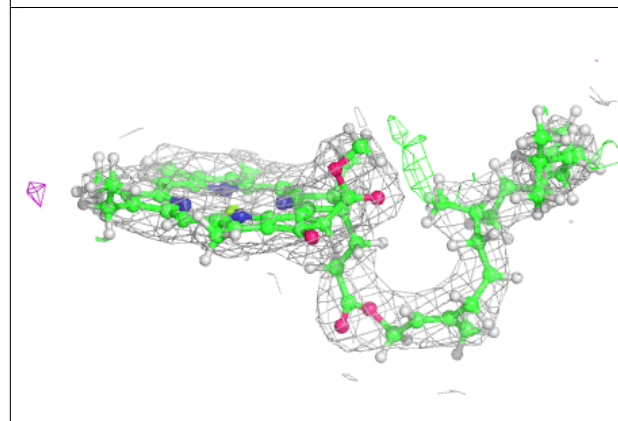
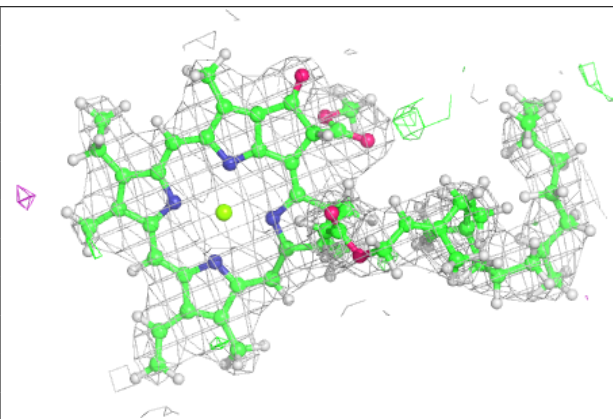


Electron density around PHO D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

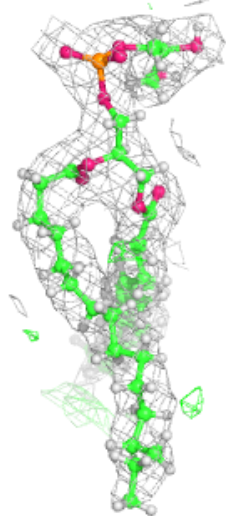
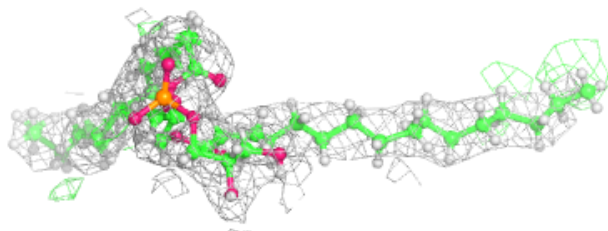
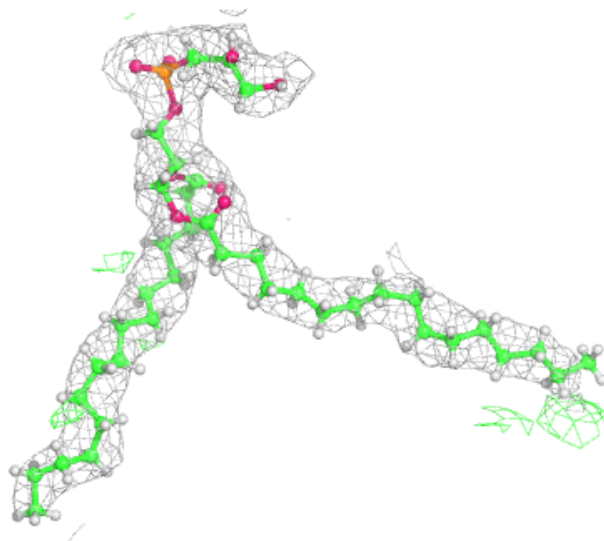
**Electron density around CLA B 612:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



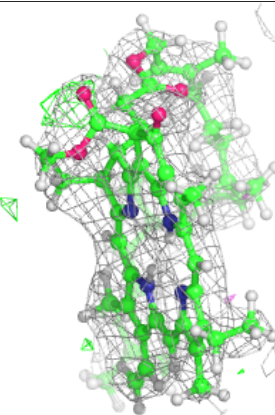
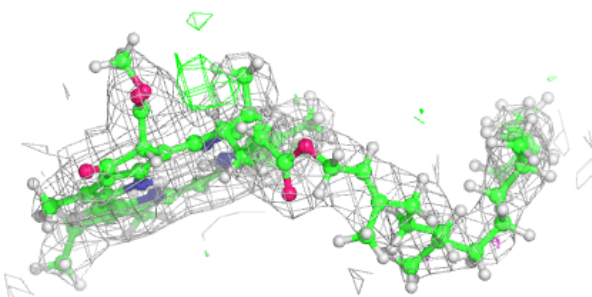
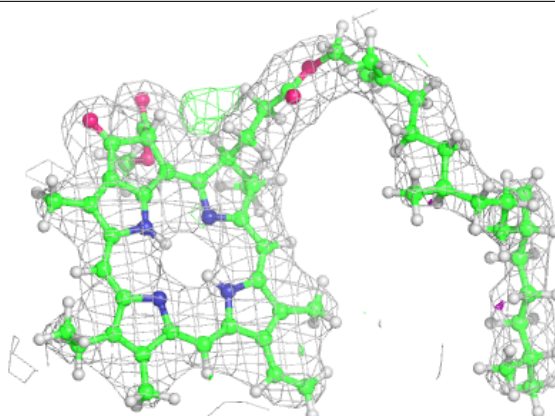
Electron density around LHG L 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

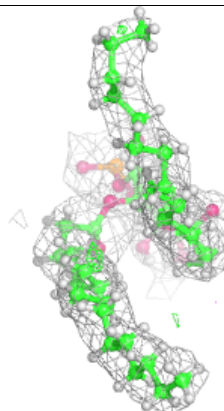
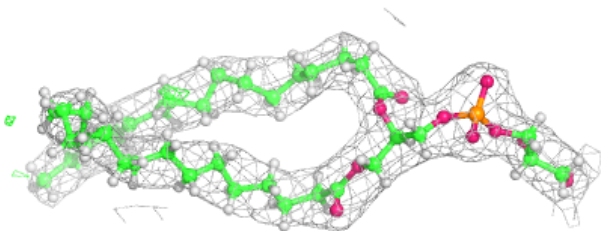
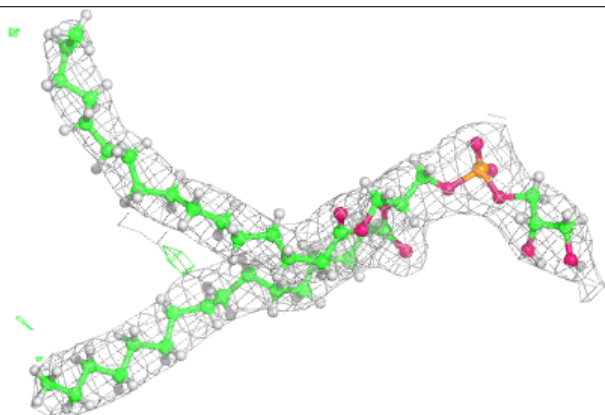


Electron density around PHO d 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

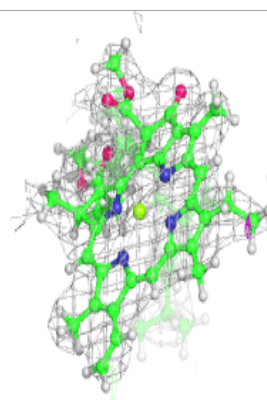
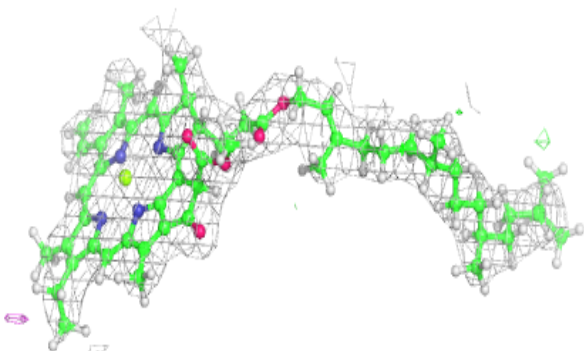
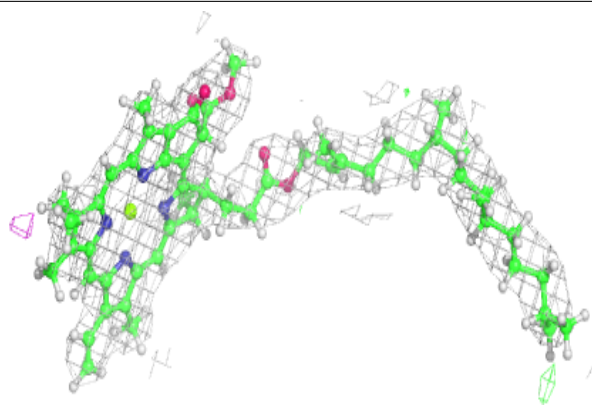
**Electron density around LHG d 408:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

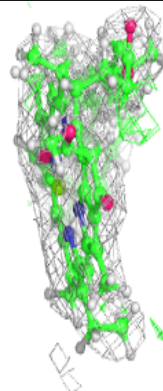
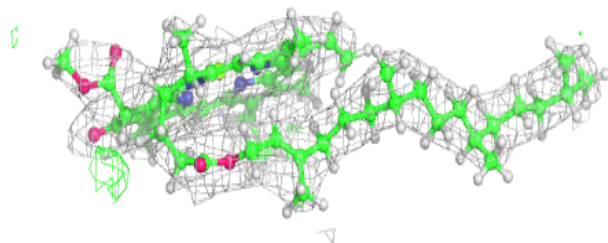
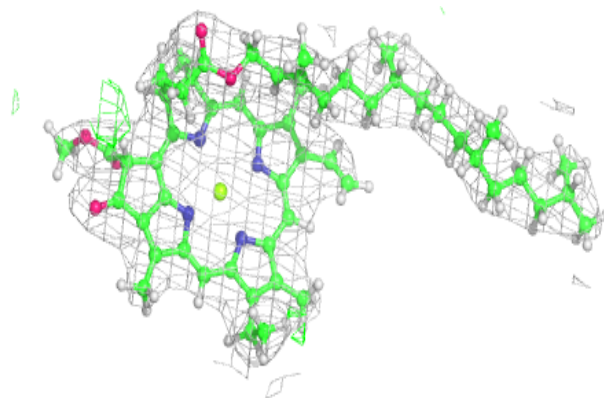


Electron density around CLA a 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

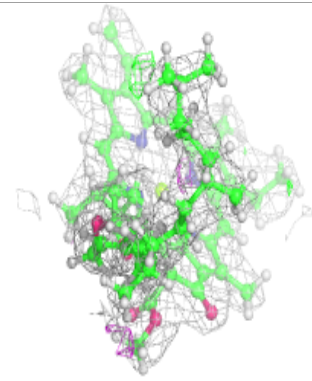
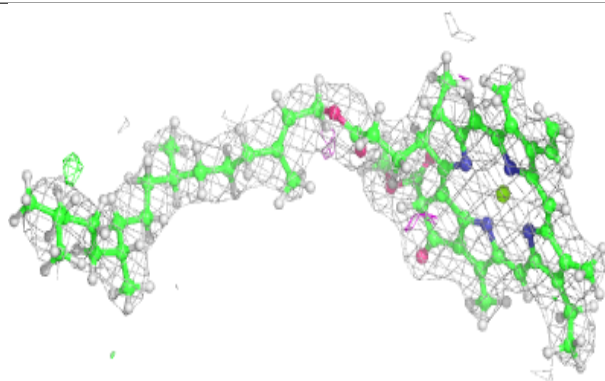
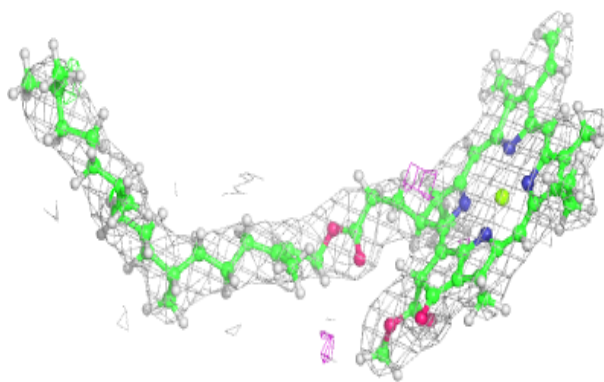
**Electron density around CLA C 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

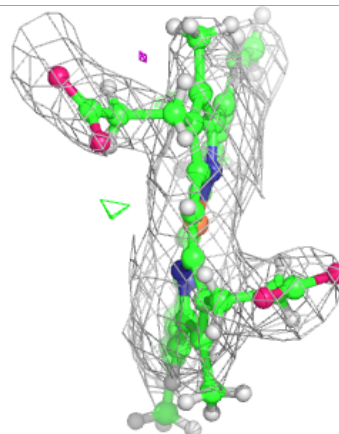
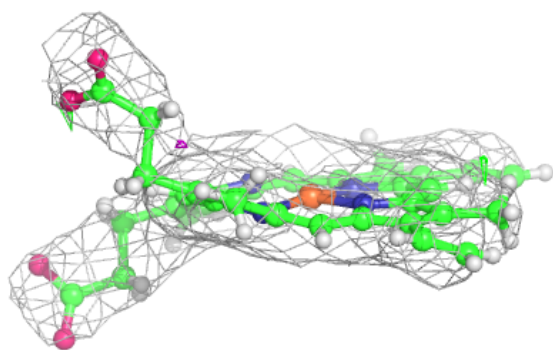
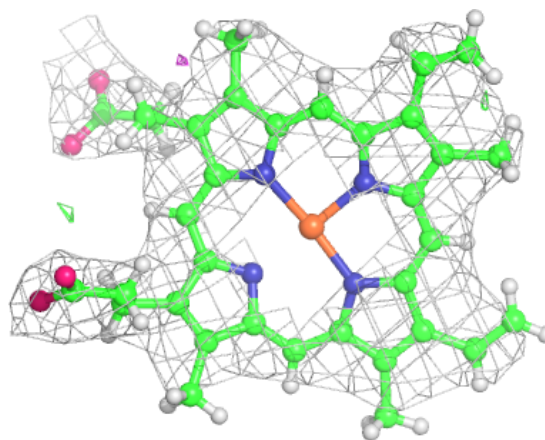


Electron density around CLA A 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

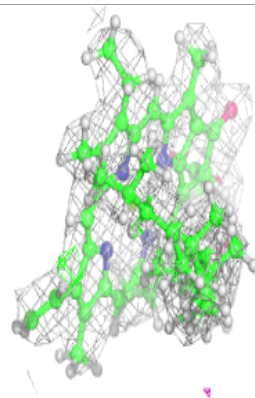
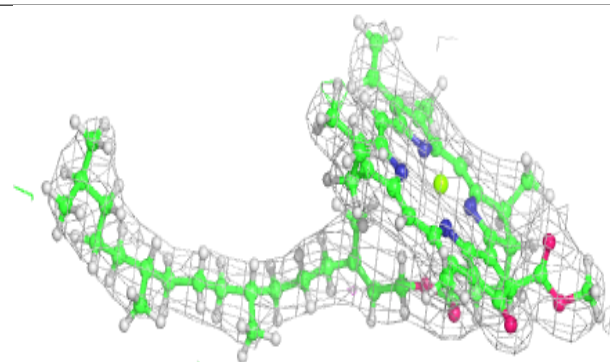
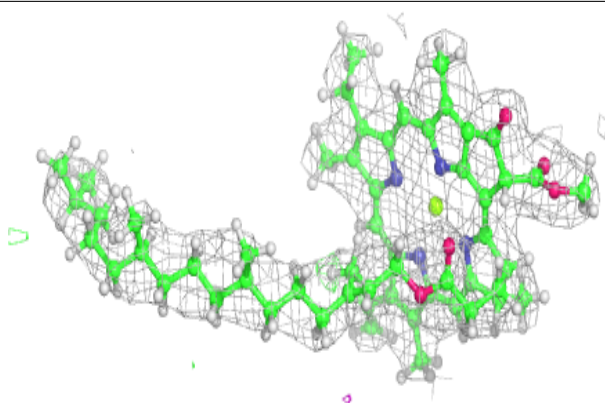
**Electron density around HEM e 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



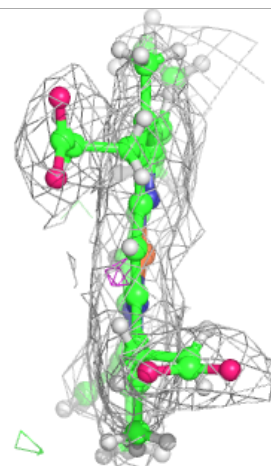
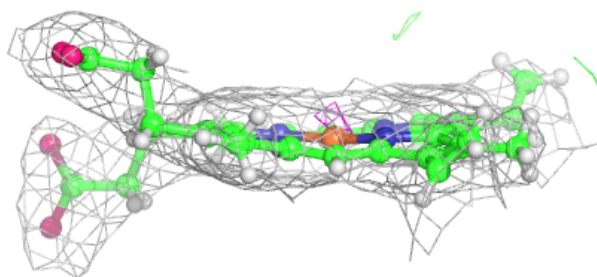
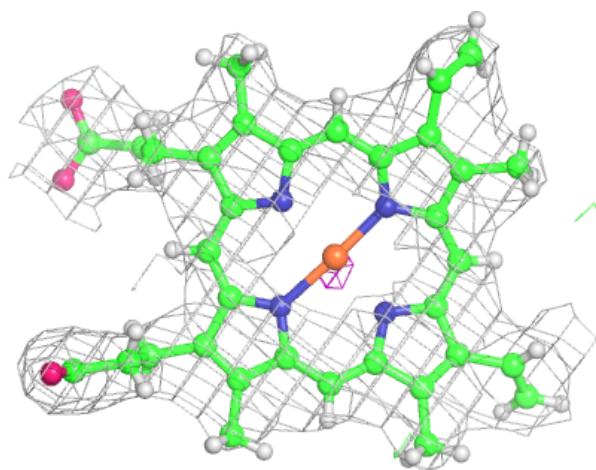
Electron density around CLA B 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



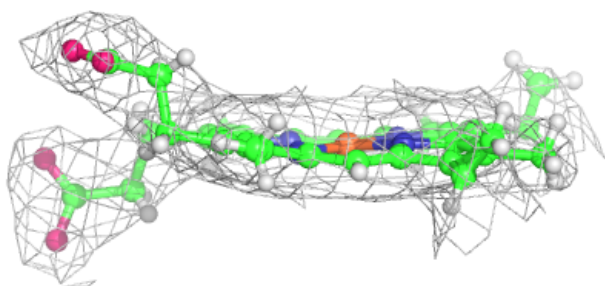
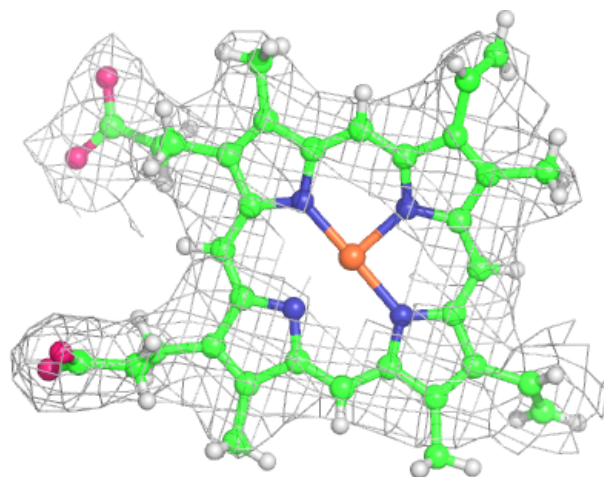
Electron density around HEC V 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC v 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.