



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 09:54 pm BST

PDB ID : 4TNK  
Title : RT XFEL structure of Photosystem II 250 microsec after the third illumination at 5.2 Å resolution  
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.  
Deposited on : 2014-06-04  
Resolution : 5.20 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](mailto: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.

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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 : 2.11  
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)

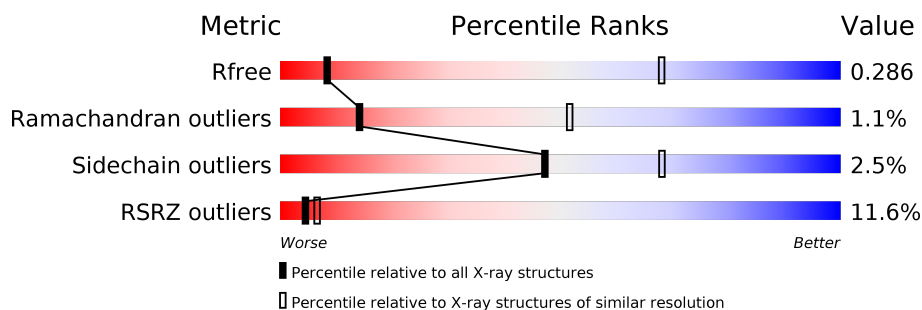
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.20 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	1167 (6.60-3.80)
Ramachandran outliers	138981	1173 (6.60-3.80)
Sidechain outliers	138945	1148 (6.60-3.80)
RSRZ outliers	127900	1008 (6.64-3.74)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>12%</div> <div>95%</div> <div>..</div> </div>
1	a	344	<div> <div>18%</div> <div>95%</div> <div>..</div> </div>
2	B	510	<div> <div>8%</div> <div>94%</div> <div>..</div> </div>
2	b	510	<div> <div>15%</div> <div>94%</div> <div>..</div> </div>
3	C	461	<div> <div>10%</div> <div>94%</div> <div>..</div> </div>

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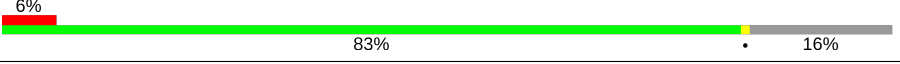


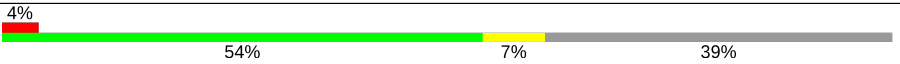
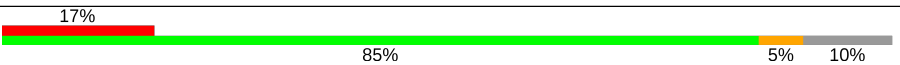

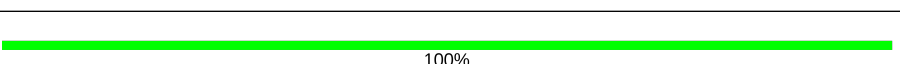
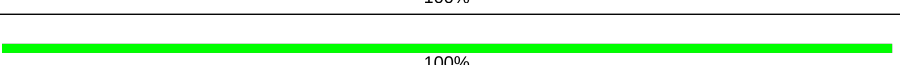
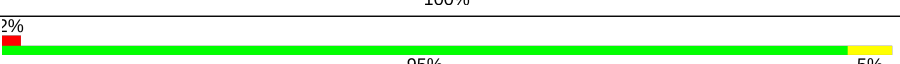
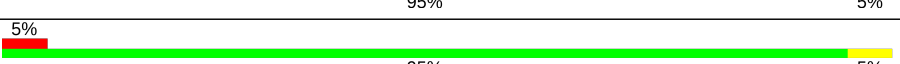
Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.11

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Mol	Chain	Length	Quality of chain
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	

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Mol	Chain	Length	Quality of chain
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	406	X	-	-	X
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	X
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	X
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	X
22	CLA	C	512	X	-	-	X
22	CLA	C	519	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	403	X	-	-	X
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	X
22	CLA	a	406	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	X
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	X
22	CLA	b	620	X	-	-	X
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	X
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	405	X	-	-	X
22	CLA	d	406	X	-	-	-
23	PHO	d	401	-	-	-	X
24	PL9	A	407	-	-	-	X
24	PL9	D	405	-	-	-	X
24	PL9	J	101	-	-	-	X
24	PL9	a	407	-	-	-	X
24	PL9	d	407	-	-	-	X
24	PL9	j	101	-	-	-	X
25	BCR	A	408	-	-	-	X
25	BCR	B	616	-	-	-	X
25	BCR	B	619	-	-	-	X
25	BCR	C	513	-	-	-	X
25	BCR	C	520	-	-	-	X
25	BCR	F	102	-	-	-	X
25	BCR	H	102	-	-	-	X
25	BCR	b	624	-	-	-	X
25	BCR	c	513	-	-	-	X
25	BCR	c	514	-	-	-	X
25	BCR	c	521	-	-	-	X
25	BCR	g	101	-	-	-	X
25	BCR	i	101	-	-	-	X
25	BCR	x	101	-	-	-	X
26	DGD	A	409	-	-	-	X
26	DGD	B	626	-	-	-	X
26	DGD	C	516	-	-	-	X
26	DGD	D	407	-	-	-	X
26	DGD	a	408	-	-	-	X
26	DGD	b	601	-	-	-	X
26	DGD	d	410	-	-	-	X
28	CL	A	411	-	-	-	X
30	SQD	B	622	-	-	-	X
30	SQD	B	627	-	-	-	X
30	SQD	b	602	-	-	-	X
30	SQD	d	403	-	-	-	X
31	LMG	C	517	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	b	627	-	-	-	X
31	LMG	c	518	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	102	-	-	-	X
31	LMG	m	101	-	-	-	X
32	LMT	B	623	-	-	-	X
32	LMT	B	624	-	-	-	X
32	LMT	B	628	-	-	-	X
32	LMT	D	408	-	-	-	X
32	LMT	I	102	-	-	-	X
32	LMT	M	102	-	-	-	X
32	LMT	b	603	-	-	-	X
32	LMT	b	628	-	-	-	X
32	LMT	b	629	-	-	-	X
32	LMT	d	411	-	-	-	X
32	LMT	i	103	-	-	-	X
35	CA	K	102	-	-	-	X
35	CA	O	301	-	-	-	X
35	CA	o	301	-	-	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	x	37	Total	C	N	O		0	0	0
			270	182	41	47				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	G	28	Total	C	N	O		0	0	0
			140	84	28	28				

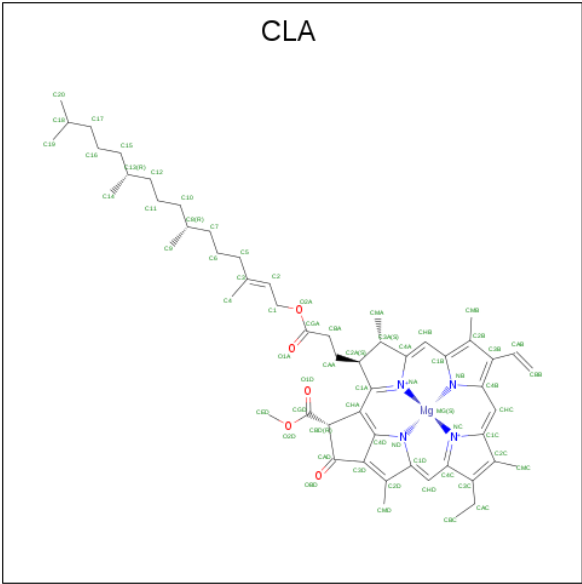
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- 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 CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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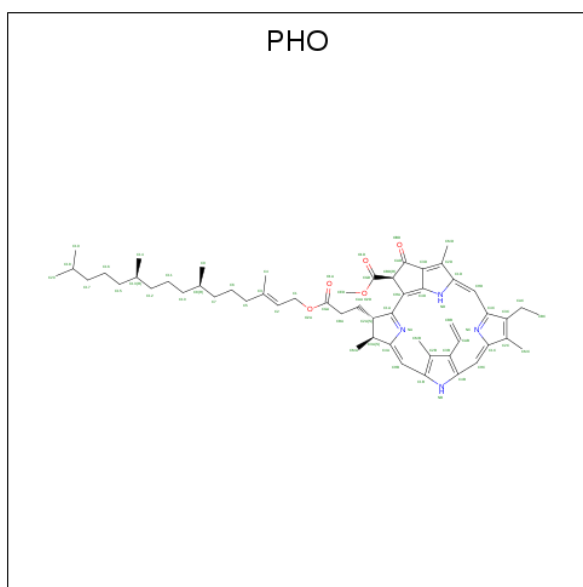
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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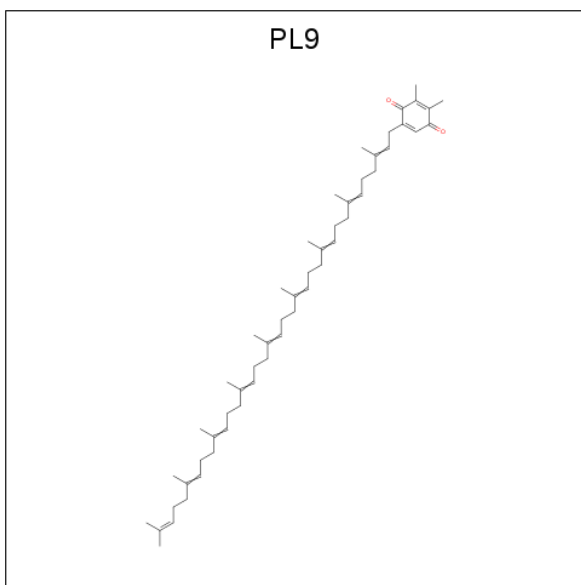
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



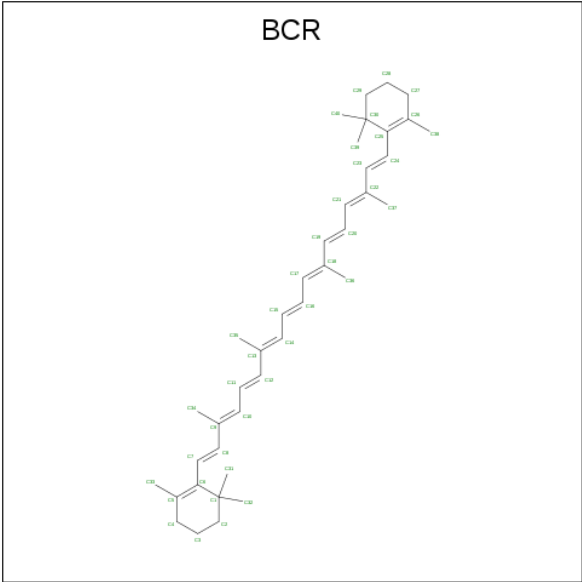
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			45	43	2		
24	D	1	Total	C	O	0	0
			55	53	2		
24	J	1	Total	C	O	0	0
			35	33	2		
24	a	1	Total	C	O	0	0
			45	43	2		
24	d	1	Total	C	O	0	0
			55	53	2		
24	j	1	Total	C	O	0	0
			35	33	2		

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



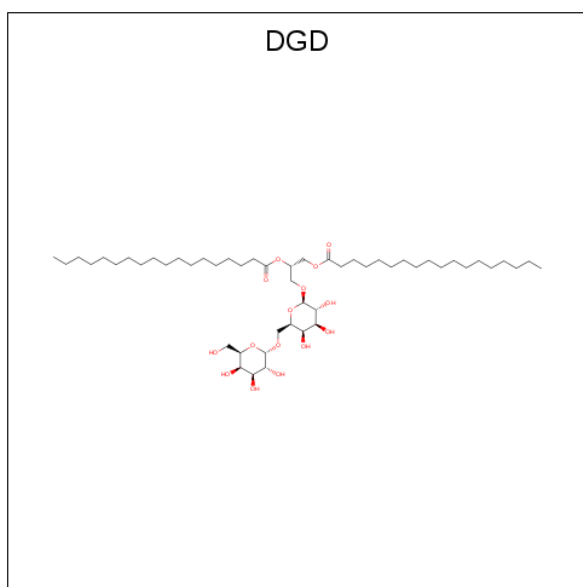
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	f	1	Total C 40 40	0	0
25	i	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	g	1	Total C 40 40	0	0
25	x	1	Total C 40 40	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 56 41 15	0	0

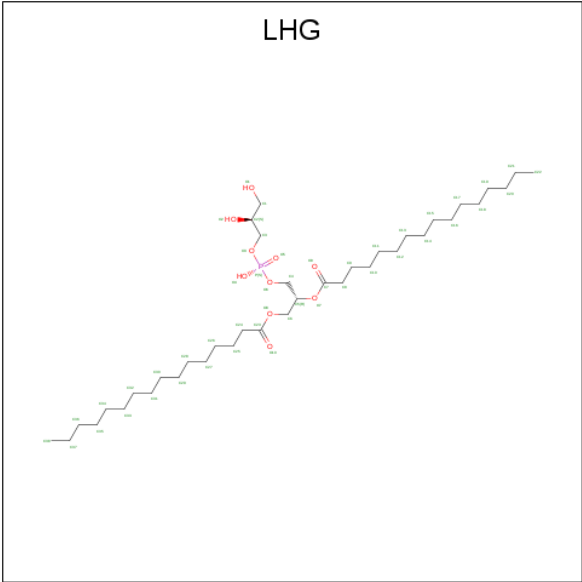
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			58	43	15		
26	B	1	Total	C	O	0	0
			52	37	15		
26	C	1	Total	C	O	0	0
			53	38	15		
26	C	1	Total	C	O	0	0
			62	47	15		
26	C	1	Total	C	O	0	0
			66	51	15		
26	D	1	Total	C	O	0	0
			63	48	15		
26	a	1	Total	C	O	0	0
			56	41	15		
26	b	1	Total	C	O	0	0
			52	37	15		
26	b	1	Total	C	O	0	0
			58	43	15		
26	c	1	Total	C	O	0	0
			53	38	15		
26	c	1	Total	C	O	0	0
			62	47	15		
26	c	1	Total	C	O	0	0
			66	51	15		
26	d	1	Total	C	O	0	0
			63	48	15		

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



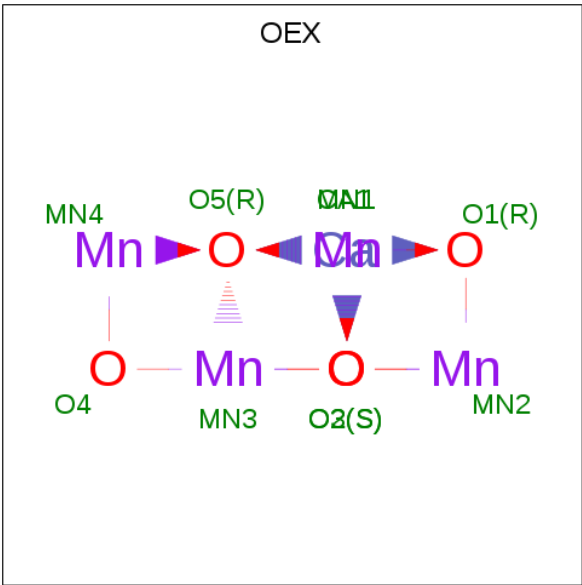


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			39	28	10	1		
27	C	1	Total	C	O	P	0	0
			37	26	10	1		
27	a	1	Total	C	O	P	0	0
			39	28	10	1		
27	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

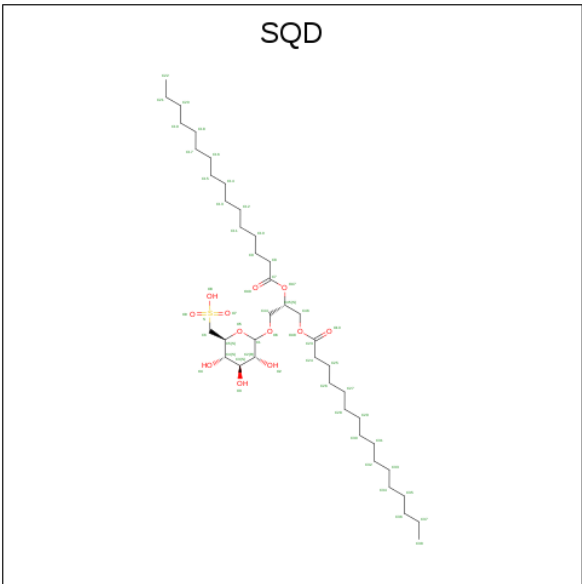
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn<sub>4</sub>O<sub>5</sub>).



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

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



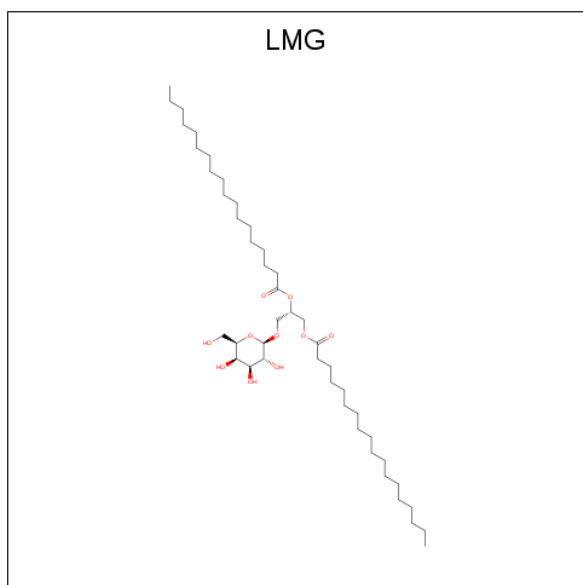
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



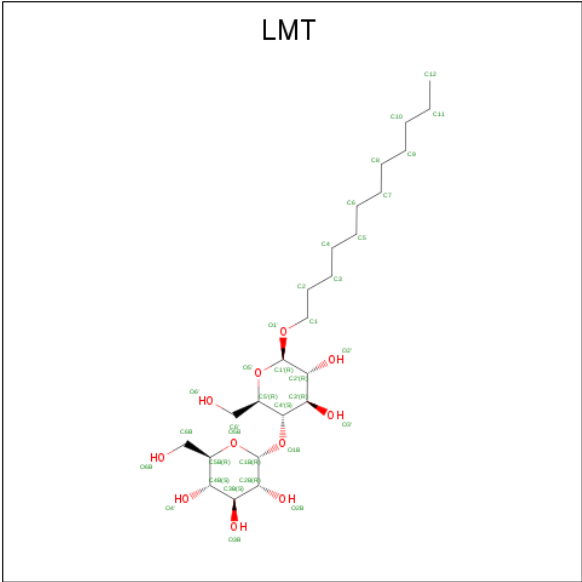
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			49	39	10		
31	B	1	Total	C	O	0	0
			49	39	10		

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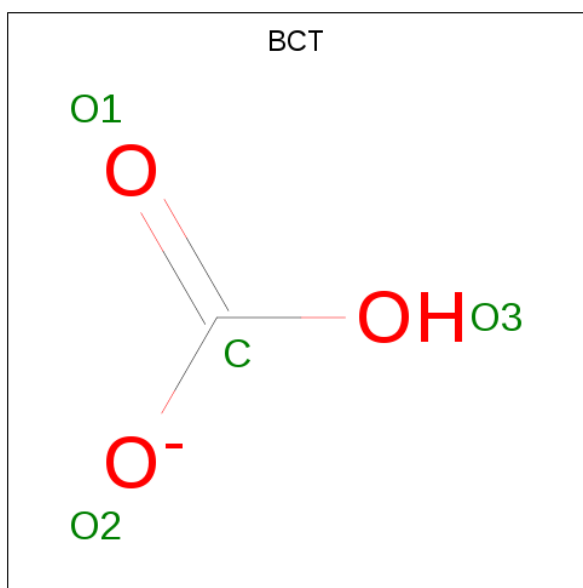
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			45	35	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			46	36	10		
31	E	1	Total	C	O	0	0
			44	34	10		
31	I	1	Total	C	O	0	0
			43	33	10		
31	L	1	Total	C	O	0	0
			51	41	10		
31	M	1	Total	C	O	0	0
			42	32	10		
31	a	1	Total	C	O	0	0
			42	32	10		
31	b	1	Total	C	O	0	0
			49	39	10		
31	b	1	Total	C	O	0	0
			42	32	10		
31	c	1	Total	C	O	0	0
			45	35	10		
31	c	1	Total	C	O	0	0
			48	38	10		
31	d	1	Total	C	O	0	0
			49	39	10		
31	d	1	Total	C	O	0	0
			48	38	10		
31	d	1	Total	C	O	0	0
			46	36	10		
31	e	1	Total	C	O	0	0
			44	34	10		
31	i	1	Total	C	O	0	0
			43	33	10		
31	l	1	Total	C	O	0	0
			51	41	10		
31	m	1	Total	C	O	0	0
			42	32	10		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



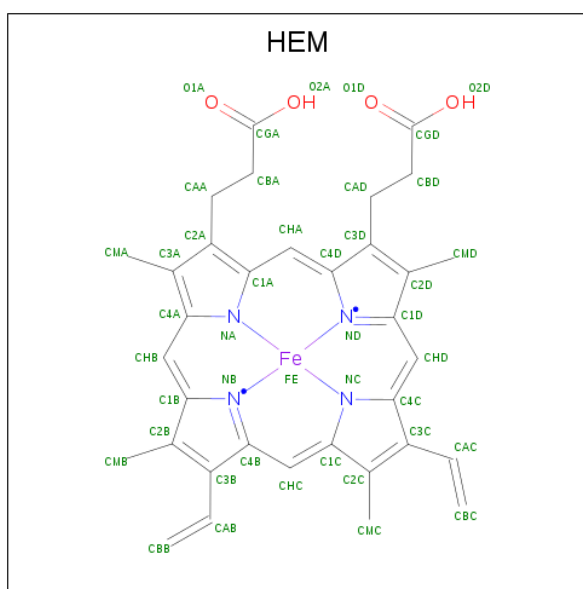
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			31	20	11		
32	I	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	d	1	Total	C	O	0	0
			31	20	11		
32	i	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			4	1	3		
33	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



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

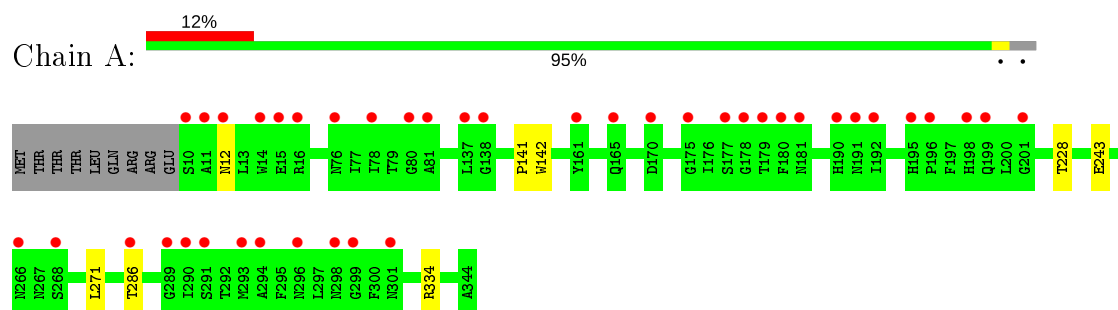
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total 1	Ca 1	0	0
35	O	1	Total 1	Ca 1	0	0
35	K	1	Total 1	Ca 1	0	0
35	k	1	Total 1	Ca 1	0	0

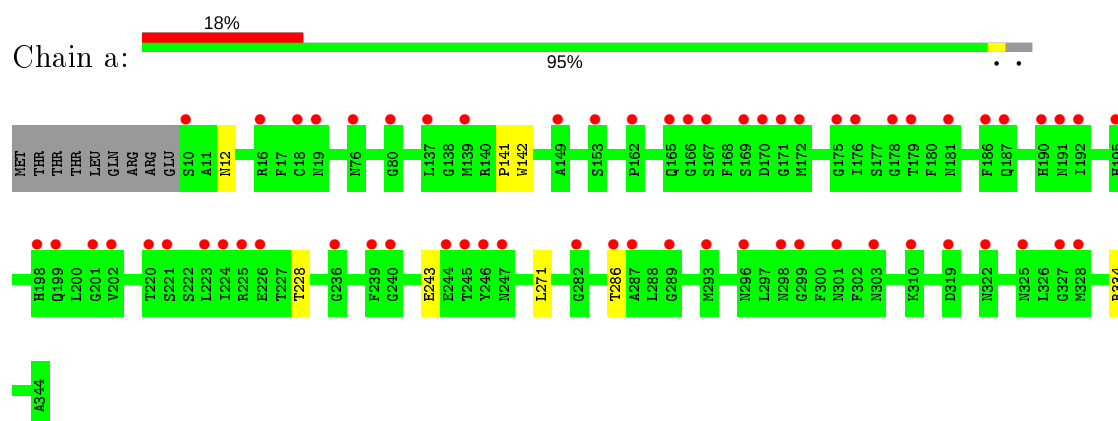
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

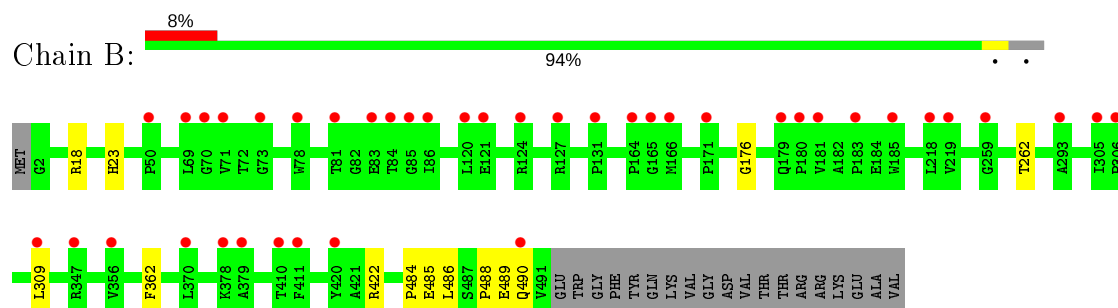
- Molecule 1: Photosystem Q(B) protein 1



- Molecule 1: Photosystem Q(B) protein 1

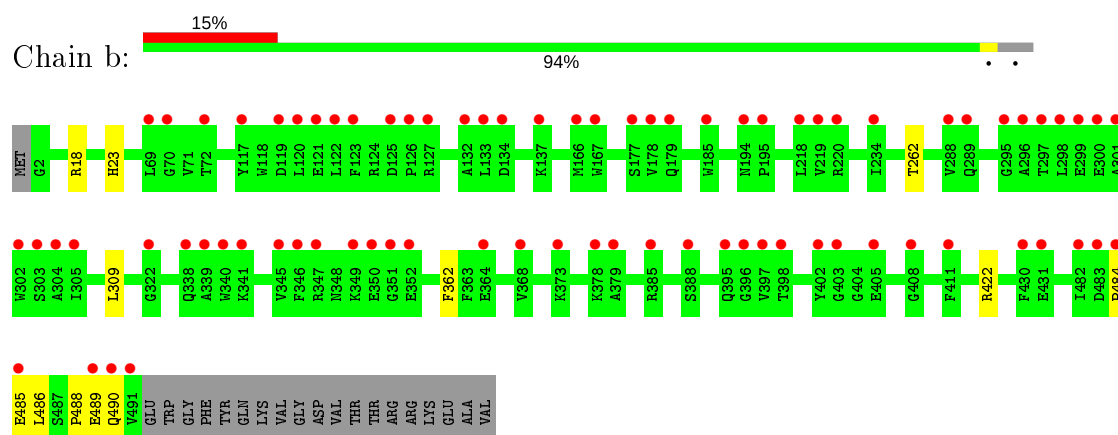


- Molecule 2: Photosystem II core light harvesting protein

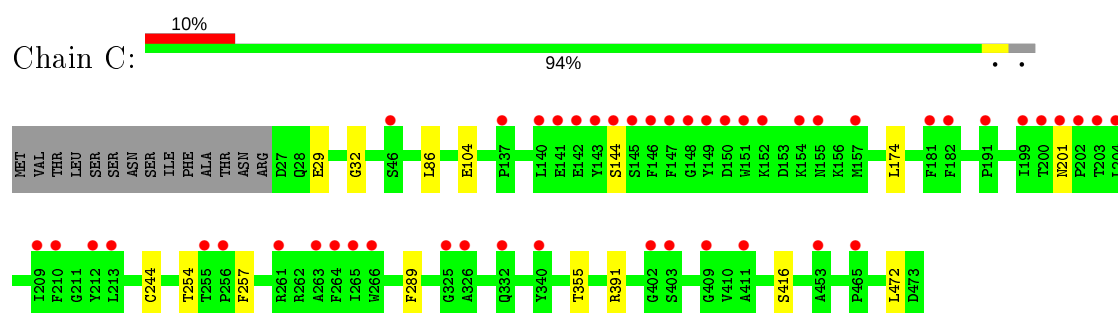


- Molecule 2: Photosystem II core light harvesting protein

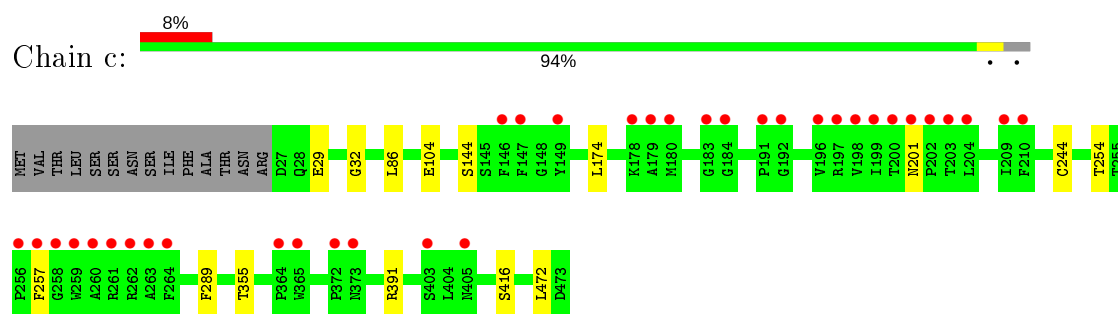




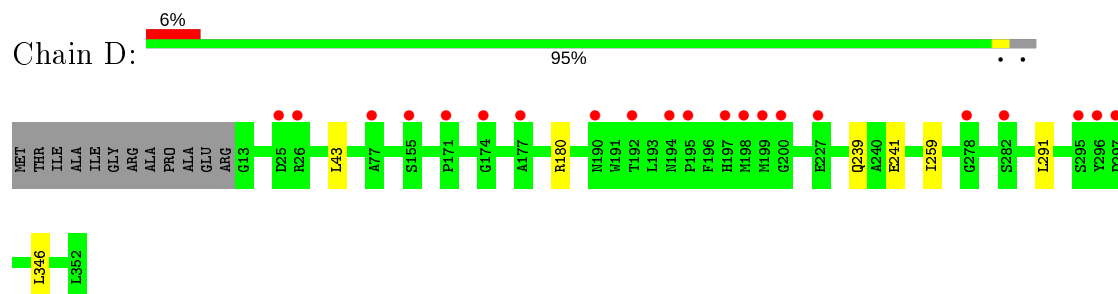
• Molecule 3: Photosystem II CP43 protein



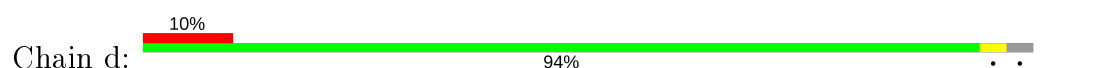
• Molecule 3: Photosystem II CP43 protein

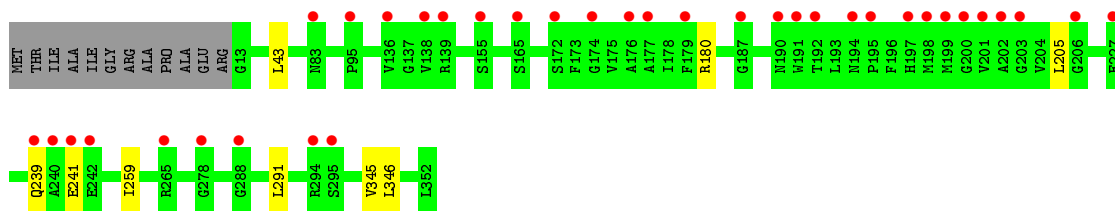


• Molecule 4: Photosystem II D2 protein

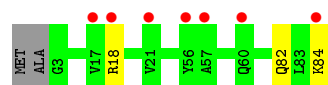


• Molecule 4: Photosystem II D2 protein

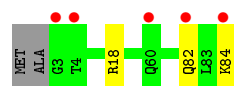




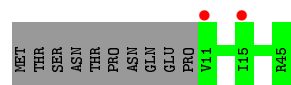
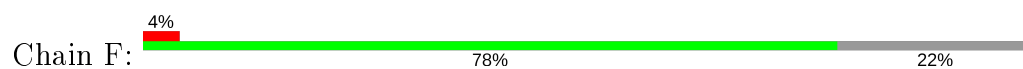
• Molecule 5: Cytochrome b559 subunit alpha



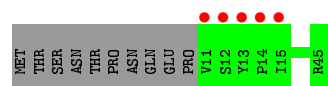
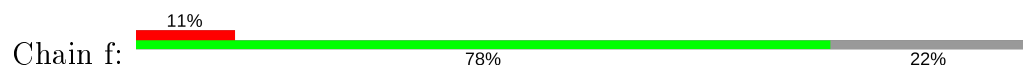
• Molecule 5: Cytochrome b559 subunit alpha



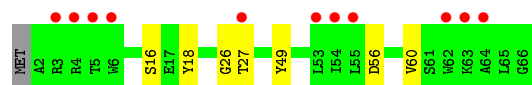
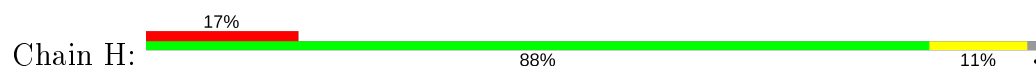
• Molecule 6: Cytochrome b559 subunit beta



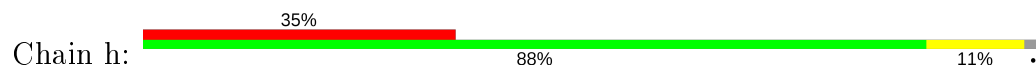
• Molecule 6: Cytochrome b559 subunit beta

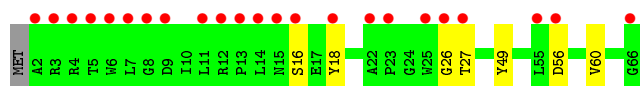


• Molecule 7: Photosystem II reaction center protein H

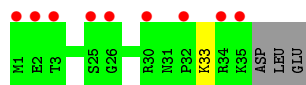
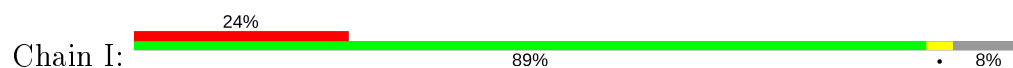


• Molecule 7: Photosystem II reaction center protein H

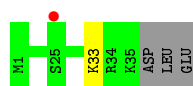
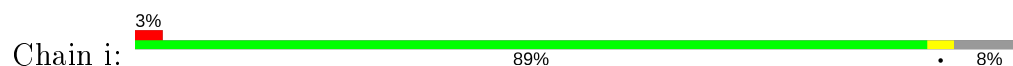




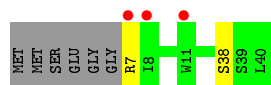
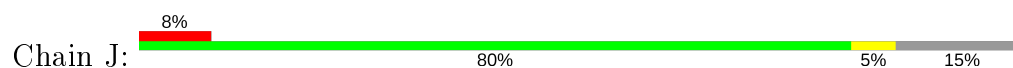
- Molecule 8: Photosystem II reaction center protein I



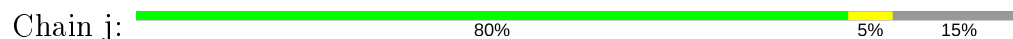
- Molecule 8: Photosystem II reaction center protein I



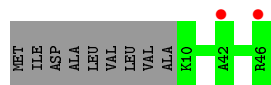
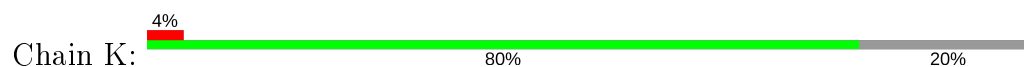
- Molecule 9: Photosystem II reaction center protein J



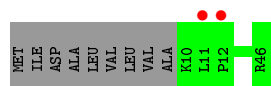
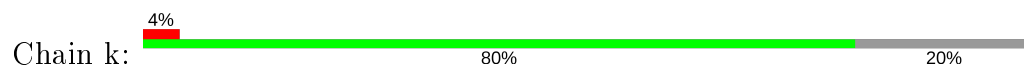
- Molecule 9: Photosystem II reaction center protein J



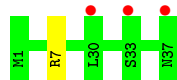
- Molecule 10: Photosystem II reaction center protein K



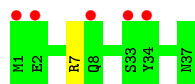
- Molecule 10: Photosystem II reaction center protein K



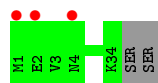
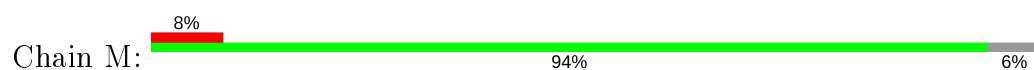
- Molecule 11: Photosystem II reaction center protein L



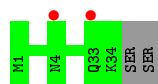
- Molecule 11: Photosystem II reaction center protein L



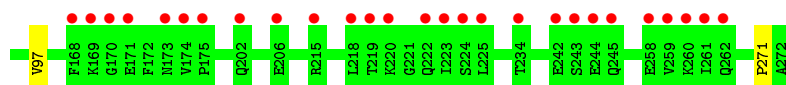
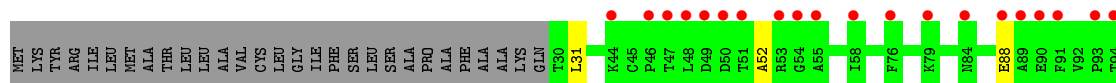
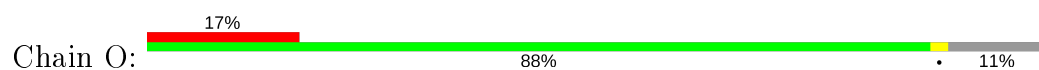
- Molecule 12: Photosystem II reaction center protein M



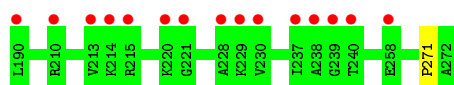
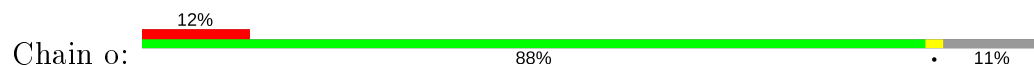
- Molecule 12: Photosystem II reaction center protein M



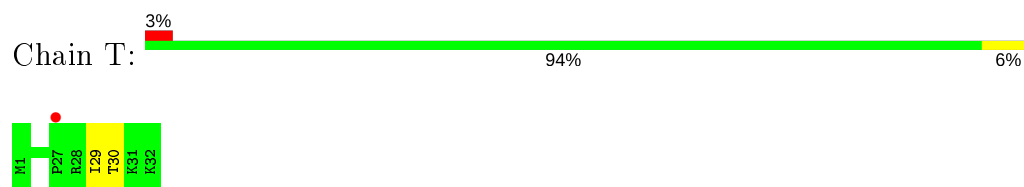
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



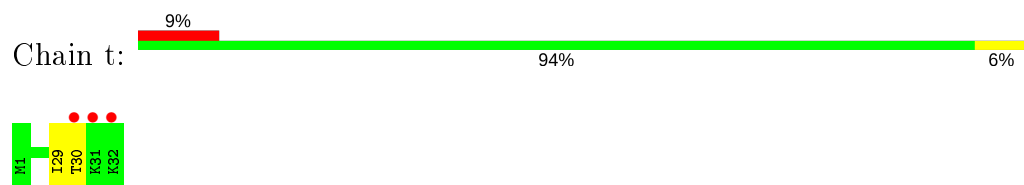
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



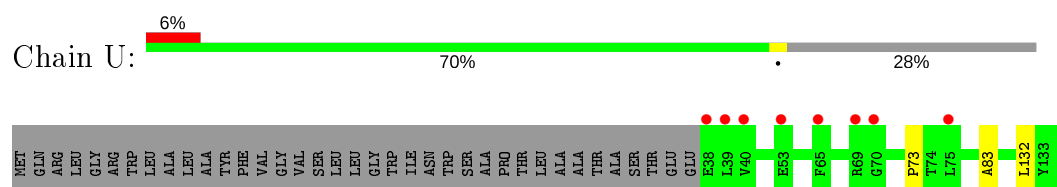
- Molecule 14: Photosystem II reaction center protein T



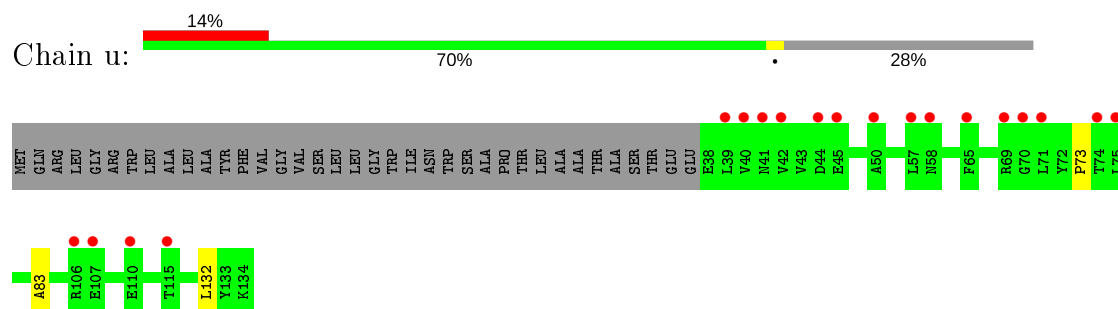
- Molecule 14: Photosystem II reaction center protein T



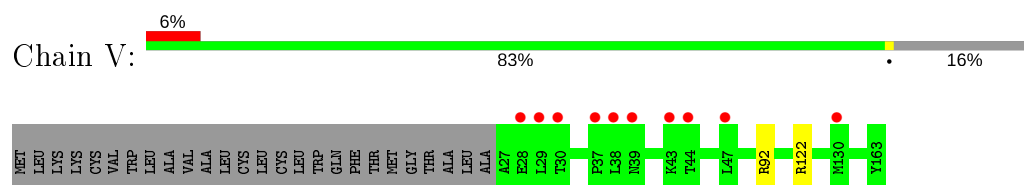
- Molecule 15: Photosystem II 12 kDa extrinsic protein



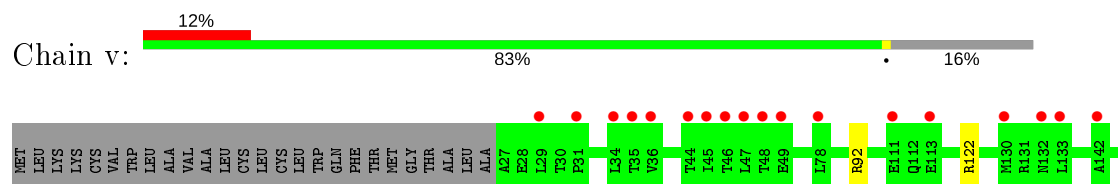
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

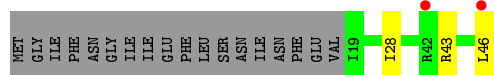


- Molecule 16: Cytochrome c-550

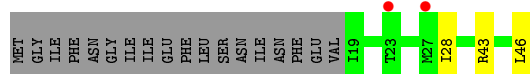




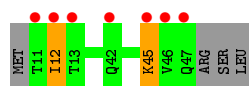
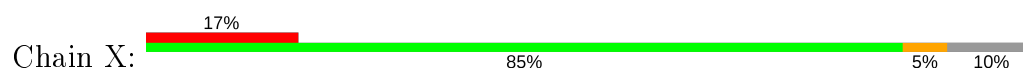
- Molecule 17: Photosystem II reaction center protein Ycf12



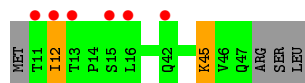
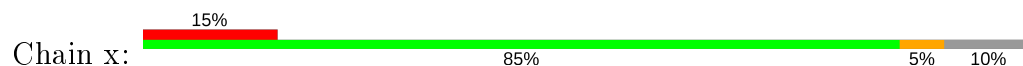
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Y



There are no outlier residues recorded for this chain.

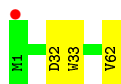
- Molecule 19: Photosystem II reaction center protein Y



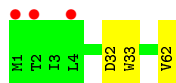
There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z





- Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.62Å 229.30Å 306.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.41 – 5.20 68.41 – 5.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (68.41-5.20) 97.9 (68.41-5.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, $R_{free}$	0.271 , 0.289 0.275 , 0.286	Depositor DCC
$R_{free}$ test set	1753 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	176.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 157.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LHG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, BCT, HEM, SQD, BCR, LMG

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	0.25	0/2713	0.42	0/3700
1	a	0.24	0/2713	0.42	0/3700
2	B	0.24	0/3986	0.41	0/5433
2	b	0.24	0/3986	0.41	0/5433
3	C	0.23	0/3556	0.42	0/4842
3	c	0.23	0/3556	0.42	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.44	0/933
5	e	0.23	0/685	0.43	0/933
6	F	0.23	0/291	0.40	0/397
6	f	0.23	0/291	0.41	0/397
7	H	0.24	0/520	0.46	0/709
7	h	0.23	0/520	0.46	0/709
8	I	0.25	0/293	0.44	0/395
8	i	0.26	0/293	0.44	0/395
9	J	0.21	0/255	0.41	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.27	0/303	0.49	0/416
10	k	0.27	0/303	0.49	0/416
11	L	0.23	0/311	0.40	0/422
11	l	0.22	0/311	0.40	0/422
12	M	0.24	0/270	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.23	0/1876	0.44	0/2548
13	o	0.23	0/1876	0.44	0/2548
14	T	0.25	0/284	0.41	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.23	0/785	0.43	0/1064
15	u	0.23	0/785	0.44	0/1064
16	V	0.22	0/1081	0.42	0/1468
16	v	0.22	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	g	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.27	0/273	0.44	0/370
18	x	0.26	0/273	0.45	0/370
20	Z	0.25	0/490	0.45	0/669
20	z	0.24	0/490	0.45	0/669
All	All	0.24	0/41950	0.42	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	13	50
1	a	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	13	50
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	19	59
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	25	65
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
4	D	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	41	76
4	d	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	22
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	22
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	30
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	30
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	207 (86%)	31 (13%)	3 (1%)	13	50
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	13	50
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	29
14	t	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	4	29
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	37
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	37
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	26
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	26
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	19
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	19
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	42
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	42
All	All	5138/5618 (92%)	4677 (91%)	406 (8%)	55 (1%)	14	51

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	267 (98%)	4 (2%)	65	80
1	a	271/280 (97%)	267 (98%)	4 (2%)	65	80
2	B	390/407 (96%)	381 (98%)	9 (2%)	50	70
2	b	390/407 (96%)	381 (98%)	9 (2%)	50	70
3	C	347/362 (96%)	336 (97%)	11 (3%)	39	61
3	c	347/362 (96%)	336 (97%)	11 (3%)	39	61
4	D	275/283 (97%)	269 (98%)	6 (2%)	52	71
4	d	275/283 (97%)	267 (97%)	8 (3%)	42	64
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	65
5	e	72/73 (99%)	70 (97%)	2 (3%)	43	65
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	13	39
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	39
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	62
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	62
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	54
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	54
10	K	30/37 (81%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	64
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	76	86
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	86
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	60
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	60
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	84
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	84
16	V	116/138 (84%)	114 (98%)	2 (2%)	60	78
16	v	116/138 (84%)	114 (98%)	2 (2%)	60	78
17	g	20/37 (54%)	18 (90%)	2 (10%)	7	27
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	27
18	X	30/34 (88%)	28 (93%)	2 (7%)	16	42
18	x	30/34 (88%)	28 (93%)	2 (7%)	16	42
20	Z	52/52 (100%)	50 (96%)	2 (4%)	33	57
20	z	52/52 (100%)	50 (96%)	2 (4%)	33	57
All	All	4244/4594 (92%)	4140 (98%)	104 (2%)	47	68

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	X	12	ILE
2	b	309	LEU
16	v	92	ARG
18	X	45	LYS
1	a	243	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	117	HIS

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Mol	Chain	Res	Type
4	d	117	HIS
4	D	332	GLN
1	A	266	ASN
1	a	241	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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
26	DGD	a	408	-	57,57,67	0.97	0	71,71,81	1.39	8 (11%)
22	CLA	C	508	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	8 (11%)
32	LMT	M	103	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	C	501	-	59,73,73	1.43	4 (6%)	67,113,113	1.48	8 (11%)
29	OEX	a	411	1,3	0,15,15	0.00	-	-		
22	CLA	c	512	-	59,73,73	1.45	5 (8%)	67,113,113	1.47	8 (11%)
22	CLA	c	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	7 (10%)
32	LMT	I	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.05	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	DGD	b	601	-	53,53,67	1.05	4 (7%)	67,67,81	1.32	7 (10%)
26	DGD	C	516	-	67,67,67	0.88	0	81,81,81	1.43	10 (12%)
22	CLA	b	605	-	59,73,73	1.46	5 (8%)	67,113,113	1.48	8 (11%)
22	CLA	C	519	-	59,73,73	1.40	5 (8%)	67,113,113	1.45	8 (11%)
22	CLA	B	602	-	59,73,73	1.39	5 (8%)	67,113,113	1.46	9 (13%)
25	BCR	j	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.54	13 (23%)
25	BCR	H	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	6 (10%)
32	LMT	d	411	-	32,32,36	1.18	5 (15%)	43,43,47	1.02	2 (4%)
32	LMT	B	629	-	36,36,36	1.15	6 (16%)	47,47,47	1.03	1 (2%)
32	LMT	B	623	-	36,36,36	1.13	5 (13%)	47,47,47	1.01	1 (2%)
22	CLA	c	503	-	59,73,73	1.44	5 (8%)	67,113,113	1.52	8 (11%)
22	CLA	B	604	-	59,73,73	1.43	5 (8%)	67,113,113	1.52	7 (10%)
22	CLA	A	403	-	59,73,73	1.43	5 (8%)	67,113,113	1.50	8 (11%)
22	CLA	b	608	-	59,73,73	1.41	5 (8%)	67,113,113	1.54	10 (14%)
27	LHG	c	519	-	36,36,48	0.75	2 (5%)	39,42,54	1.27	4 (10%)
22	CLA	b	609	-	59,73,73	1.42	5 (8%)	67,113,113	1.50	8 (11%)
22	CLA	b	612	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	7 (10%)
32	LMT	b	603	-	36,36,36	1.13	5 (13%)	47,47,47	0.98	1 (2%)
22	CLA	a	406	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	7 (10%)
25	BCR	b	624	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	9 (16%)
30	SQD	B	627	-	46,47,54	1.01	3 (6%)	55,58,65	1.81	10 (18%)
26	DGD	B	626	-	53,53,67	1.06	3 (5%)	67,67,81	1.31	7 (10%)
26	DGD	D	407	-	64,64,67	0.98	4 (6%)	78,78,81	1.33	8 (10%)
22	CLA	c	510	3	59,73,73	1.44	4 (6%)	67,113,113	1.48	9 (13%)
22	CLA	B	608	-	59,73,73	1.46	5 (8%)	67,113,113	1.46	8 (11%)
22	CLA	B	613	-	59,73,73	1.38	5 (8%)	67,113,113	1.50	8 (11%)
31	LMG	I	101	-	43,43,55	0.85	1 (2%)	51,51,63	1.25	5 (9%)
22	CLA	b	615	-	59,73,73	1.48	5 (8%)	67,113,113	1.59	11 (16%)
31	LMG	c	522	-	48,48,55	0.78	0	56,56,63	1.29	5 (8%)
24	PL9	D	405	-	55,55,55	1.16	3 (5%)	68,69,69	1.54	13 (19%)
25	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	8 (14%)
22	CLA	C	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	9 (13%)
25	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	8 (14%)
26	DGD	c	516	-	63,63,67	0.93	2 (3%)	77,77,81	1.44	11 (14%)
22	CLA	C	507	-	59,73,73	1.44	5 (8%)	67,113,113	1.55	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	SQD	b	602	-	46,47,54	1.02	4 (8%)	55,58,65	1.83	10 (18%)
22	CLA	C	504	-	59,73,73	1.40	5 (8%)	67,113,113	1.56	10 (14%)
25	BCR	y	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.25	7 (12%)
24	PL9	j	101	-	35,35,55	1.11	2 (5%)	44,45,69	1.59	8 (18%)
22	CLA	b	607	-	59,73,73	1.40	5 (8%)	67,113,113	1.42	8 (11%)
22	CLA	c	506	-	59,73,73	1.41	5 (8%)	67,113,113	1.47	8 (11%)
31	LMG	D	409	-	46,46,55	0.79	1 (2%)	54,54,63	1.32	4 (7%)
22	CLA	c	504	-	59,73,73	1.42	5 (8%)	67,113,113	1.53	9 (13%)
22	CLA	c	508	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	8 (11%)
32	LMT	B	624	-	36,36,36	1.11	4 (11%)	47,47,47	1.01	2 (4%)
25	BCR	C	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	8 (14%)
24	PL9	d	407	-	55,55,55	1.10	5 (9%)	68,69,69	1.54	13 (19%)
22	CLA	b	614	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	9 (13%)
23	PHO	d	402	-	67,69,69	1.27	8 (11%)	85,99,99	1.01	5 (5%)
22	CLA	b	613	-	59,73,73	1.45	5 (8%)	67,113,113	1.43	8 (11%)
22	CLA	B	606	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	9 (13%)
25	BCR	f	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	7 (12%)
30	SQD	A	413	-	50,51,54	0.96	3 (6%)	59,62,65	1.78	10 (16%)
22	CLA	B	611	-	59,73,73	1.40	5 (8%)	67,113,113	1.53	8 (11%)
23	PHO	A	405	-	67,69,69	1.25	8 (11%)	85,99,99	1.00	5 (5%)
22	CLA	A	404	-	59,73,73	1.40	5 (8%)	67,113,113	1.47	7 (10%)
22	CLA	B	614	-	59,73,73	1.45	5 (8%)	67,113,113	1.50	9 (13%)
22	CLA	B	601	-	59,73,73	1.46	5 (8%)	67,113,113	1.47	8 (11%)
22	CLA	c	511	-	59,73,73	1.43	5 (8%)	67,113,113	1.49	8 (11%)
22	CLA	b	610	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	8 (11%)
31	LMG	d	408	-	49,49,55	0.77	0	57,57,63	1.34	7 (12%)
25	BCR	b	622	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	10 (17%)
25	BCR	A	408	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
31	LMG	C	521	-	48,48,55	0.77	0	56,56,63	1.30	5 (8%)
25	BCR	g	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.31	8 (14%)
31	LMG	E	101	-	44,44,55	0.76	0	52,52,63	1.29	3 (5%)
32	LMT	D	408	-	32,32,36	1.18	5 (15%)	43,43,47	1.02	2 (4%)
30	SQD	a	412	-	50,51,54	0.96	3 (6%)	59,62,65	1.76	11 (18%)
22	CLA	a	404	-	59,73,73	1.40	5 (8%)	67,113,113	1.47	8 (11%)
22	CLA	D	404	-	59,73,73	1.43	4 (6%)	67,113,113	1.48	8 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	SQD	B	622	-	42,43,54	1.05	3 (7%)	51,54,65	1.81	11 (21%)
26	DGD	C	514	-	54,54,67	0.98	2 (3%)	68,68,81	1.26	5 (7%)
31	LMG	b	627	-	42,42,55	0.87	1 (2%)	50,50,63	1.23	4 (8%)
22	CLA	b	617	-	59,73,73	1.41	5 (8%)	67,113,113	1.50	9 (13%)
31	LMG	d	412	-	46,46,55	0.80	1 (2%)	54,54,63	1.29	6 (11%)
22	CLA	b	616	-	59,73,73	1.42	5 (8%)	67,113,113	1.49	8 (11%)
22	CLA	d	406	-	59,73,73	1.45	5 (8%)	67,113,113	1.49	8 (11%)
27	LHG	a	409	-	38,38,48	0.68	1 (2%)	41,44,54	1.21	3 (7%)
22	CLA	A	402	-	59,73,73	1.45	5 (8%)	67,113,113	1.43	8 (11%)
25	BCR	b	621	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	7 (12%)
22	CLA	a	403	-	59,73,73	1.46	5 (8%)	67,113,113	1.47	9 (13%)
22	CLA	B	615	-	59,73,73	1.43	6 (10%)	67,113,113	1.48	7 (10%)
31	LMG	B	625	-	49,49,55	0.77	0	57,57,63	1.33	6 (10%)
22	CLA	C	511	-	59,73,73	1.43	5 (8%)	67,113,113	1.52	8 (11%)
22	CLA	C	512	-	59,73,73	1.43	4 (6%)	67,113,113	1.51	10 (14%)
34	HEM	V	201	16	27,50,50	2.20	6 (22%)	17,82,82	1.46	2 (11%)
22	CLA	c	507	-	59,73,73	1.44	5 (8%)	67,113,113	1.56	10 (14%)
25	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
27	LHG	A	410	-	38,38,48	0.70	1 (2%)	41,44,54	1.20	3 (7%)
31	LMG	D	406	-	48,48,55	0.78	0	56,56,63	1.39	4 (7%)
22	CLA	b	620	-	59,73,73	1.43	6 (10%)	67,113,113	1.44	8 (11%)
26	DGD	B	620	-	59,59,67	0.94	0	73,73,81	1.34	7 (9%)
30	SQD	a	401	-	53,54,54	0.95	3 (5%)	62,65,65	1.58	10 (16%)
22	CLA	b	618	-	59,73,73	1.40	4 (6%)	67,113,113	1.48	9 (13%)
31	LMG	L	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.35	5 (8%)
26	DGD	c	515	-	54,54,67	0.97	1 (1%)	68,68,81	1.29	5 (7%)
22	CLA	d	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.44	8 (11%)
24	PL9	A	407	-	45,45,55	1.00	4 (8%)	56,57,69	1.56	9 (16%)
26	DGD	b	625	-	59,59,67	0.92	0	73,73,81	1.36	7 (9%)
22	CLA	C	510	3	59,73,73	1.42	4 (6%)	67,113,113	1.54	8 (11%)
25	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.61	13 (23%)
31	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.29	6 (11%)
23	PHO	d	401	-	67,69,69	1.23	8 (11%)	85,99,99	1.02	6 (7%)
30	SQD	F	103	-	44,45,54	1.04	3 (6%)	53,56,65	1.70	11 (20%)
22	CLA	B	603	-	59,73,73	1.43	5 (8%)	67,113,113	1.54	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	HEM	f	101	5,6	27,50,50	2.14	5 (18%)	17,82,82	1.51	4 (23%)
30	SQD	d	403	-	42,43,54	1.04	3 (7%)	51,54,65	1.77	11 (21%)
32	LMT	b	629	-	36,36,36	1.11	5 (13%)	47,47,47	1.03	2 (4%)
25	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	9 (16%)
31	LMG	l	101	-	51,51,55	0.74	1 (1%)	59,59,63	1.33	6 (10%)
29	OEX	A	412	1,3	0,15,15	0.00	-	-		
32	LMT	b	628	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	1 (2%)
33	BCT	D	402	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	609	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	8 (11%)
30	SQD	A	414	-	53,54,54	0.95	3 (5%)	62,65,65	1.57	9 (14%)
31	LMG	a	402	-	42,42,55	0.88	2 (4%)	50,50,63	1.23	3 (6%)
31	LMG	C	517	-	45,45,55	0.77	0	53,53,63	1.30	6 (11%)
26	DGD	c	517	-	67,67,67	0.90	2 (2%)	81,81,81	1.40	9 (11%)
22	CLA	b	619	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	9 (13%)
30	SQD	f	103	-	44,45,54	1.02	3 (6%)	53,56,65	1.70	11 (20%)
25	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	8 (14%)
22	CLA	c	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.52	7 (10%)
34	HEM	v	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.41	2 (11%)
25	BCR	b	623	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	10 (17%)
32	LMT	M	102	-	36,36,36	1.15	6 (16%)	47,47,47	1.02	2 (4%)
32	LMT	B	628	-	36,36,36	1.13	5 (13%)	47,47,47	1.01	1 (2%)
22	CLA	B	610	-	59,73,73	1.48	6 (10%)	67,113,113	1.60	10 (14%)
26	DGD	d	410	-	64,64,67	0.95	2 (3%)	78,78,81	1.36	9 (11%)
25	BCR	C	520	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	9 (16%)
31	LMG	d	409	-	48,48,55	0.78	0	56,56,63	1.40	5 (8%)
31	LMG	i	102	-	43,43,55	0.84	1 (2%)	51,51,63	1.25	3 (5%)
25	BCR	x	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	3 (5%)
22	CLA	B	607	-	59,73,73	1.41	5 (8%)	67,113,113	1.47	7 (10%)
22	CLA	C	503	-	59,73,73	1.42	5 (8%)	67,113,113	1.52	8 (11%)
32	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.04	1 (2%)
25	BCR	i	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
31	LMG	m	101	-	42,42,55	0.87	2 (4%)	50,50,63	1.23	4 (8%)
31	LMG	e	101	-	44,44,55	0.77	0	52,52,63	1.28	3 (5%)
22	CLA	b	606	-	59,73,73	1.40	5 (8%)	67,113,113	1.46	7 (10%)
22	CLA	c	501	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	b	611	-	59,73,73	1.44	5 (8%)	67,113,113	1.41	8 (11%)
31	LMG	B	621	-	49,49,55	0.79	1 (2%)	57,57,63	1.31	7 (12%)
24	PL9	J	101	-	35,35,55	1.05	2 (5%)	44,45,69	1.62	7 (15%)
22	CLA	H	101	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	7 (10%)
22	CLA	C	505	-	59,73,73	1.43	5 (8%)	67,113,113	1.49	7 (10%)
22	CLA	B	605	-	59,73,73	1.40	5 (8%)	67,113,113	1.53	8 (11%)
22	CLA	c	520	-	59,73,73	1.43	5 (8%)	67,113,113	1.49	9 (13%)
32	LMT	i	103	-	36,36,36	1.10	5 (13%)	47,47,47	1.02	2 (4%)
22	CLA	D	403	-	59,73,73	1.41	5 (8%)	67,113,113	1.44	8 (11%)
33	BCT	d	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	C	509	-	59,73,73	1.45	5 (8%)	67,113,113	1.42	7 (10%)
25	BCR	B	616	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	8 (14%)
24	PL9	a	407	-	45,45,55	1.04	3 (6%)	56,57,69	1.59	9 (16%)
23	PHO	D	401	-	67,69,69	1.26	9 (13%)	85,99,99	1.00	5 (5%)
26	DGD	C	515	-	63,63,67	0.93	1 (1%)	77,77,81	1.42	12 (15%)
22	CLA	B	612	-	59,73,73	1.38	5 (8%)	67,113,113	1.51	8 (11%)
25	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.40	9 (16%)
25	BCR	F	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	7 (12%)
22	CLA	A	406	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	7 (10%)
34	HEM	F	101	5,6	27,50,50	2.17	5 (18%)	17,82,82	1.44	3 (17%)
22	CLA	a	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.45	9 (13%)
31	LMG	b	626	-	49,49,55	0.80	1 (2%)	57,57,63	1.33	8 (14%)
22	CLA	c	509	-	59,73,73	1.47	5 (8%)	67,113,113	1.46	9 (13%)
27	LHG	C	518	-	36,36,48	0.71	0	39,42,54	1.28	4 (10%)
22	CLA	C	506	-	59,73,73	1.40	5 (8%)	67,113,113	1.49	8 (11%)
26	DGD	A	409	-	57,57,67	0.96	1 (1%)	71,71,81	1.43	7 (9%)
31	LMG	M	101	-	42,42,55	0.87	0	50,50,63	1.23	4 (8%)
25	BCR	B	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	8 (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
26	DGD	a	408	-	-	14/45/85/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	E	101	-	-	16/39/59/70	0/1/1/1
22	CLA	C	508	-	3/3/20/25	15/37/135/135	-
32	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	C	501	-	3/3/20/25	13/37/135/135	-
25	BCR	C	513	-	-	5/29/63/63	0/2/2/2
22	CLA	c	502	-	3/3/20/25	10/37/135/135	-
32	LMT	I	102	-	-	3/21/61/61	0/2/2/2
26	DGD	b	601	-	-	18/41/81/95	0/2/2/2
26	DGD	C	516	-	-	23/55/95/95	0/2/2/2
22	CLA	b	605	-	3/3/20/25	16/37/135/135	-
22	CLA	C	519	-	3/3/20/25	12/37/135/135	-
22	CLA	B	602	-	3/3/20/25	14/37/135/135	-
25	BCR	j	102	-	-	7/29/63/63	0/2/2/2
25	BCR	H	102	-	-	9/29/63/63	0/2/2/2
32	LMT	d	411	-	-	1/17/57/61	0/2/2/2
32	LMT	B	629	-	-	4/21/61/61	0/2/2/2
32	LMT	B	623	-	-	2/21/61/61	0/2/2/2
23	PHO	d	402	-	-	13/53/103/103	0/5/6/6
22	CLA	B	604	-	3/3/20/25	15/37/135/135	-
22	CLA	A	403	-	3/3/20/25	14/37/135/135	-
22	CLA	b	608	-	3/3/20/25	5/37/135/135	-
22	CLA	H	101	-	3/3/20/25	19/37/135/135	-
22	CLA	b	609	-	3/3/20/25	15/37/135/135	-
22	CLA	b	612	-	3/3/20/25	13/37/135/135	-
32	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	a	406	-	3/3/20/25	8/37/135/135	-
25	BCR	b	624	-	-	5/29/63/63	0/2/2/2
30	SQD	B	627	-	-	16/42/62/69	0/1/1/1
26	DGD	B	626	-	-	18/41/81/95	0/2/2/2
26	DGD	D	407	-	-	36/52/92/95	0/2/2/2
22	CLA	c	510	3	3/3/20/25	15/37/135/135	-
22	CLA	B	608	-	3/3/20/25	11/37/135/135	-
22	CLA	B	613	-	3/3/20/25	17/37/135/135	-
31	LMG	I	101	-	-	19/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	615	-	3/3/20/25	11/37/135/135	-
31	LMG	c	522	-	-	19/43/63/70	0/1/1/1
24	PL9	D	405	-	-	12/53/73/73	0/1/1/1
22	CLA	b	607	-	3/3/20/25	13/37/135/135	-
22	CLA	C	502	-	3/3/20/25	11/37/135/135	-
25	BCR	c	521	-	-	6/29/63/63	0/2/2/2
26	DGD	c	516	-	-	21/51/91/95	0/2/2/2
22	CLA	C	507	-	3/3/20/25	14/37/135/135	-
30	SQD	b	602	-	-	14/42/62/69	0/1/1/1
22	CLA	C	504	-	3/3/20/25	18/37/135/135	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
24	PL9	j	101	-	-	8/29/49/73	0/1/1/1
25	BCR	B	619	-	-	5/29/63/63	0/2/2/2
22	CLA	c	506	-	3/3/20/25	13/37/135/135	-
31	LMG	D	409	-	-	15/41/61/70	0/1/1/1
22	CLA	c	504	-	3/3/20/25	19/37/135/135	-
22	CLA	c	508	-	3/3/20/25	16/37/135/135	-
32	LMT	B	624	-	-	3/21/61/61	0/2/2/2
22	CLA	c	512	-	3/3/20/25	18/37/135/135	-
24	PL9	d	407	-	-	11/53/73/73	0/1/1/1
22	CLA	b	614	-	3/3/20/25	18/37/135/135	-
22	CLA	c	503	-	3/3/20/25	17/37/135/135	-
22	CLA	b	613	-	3/3/20/25	11/37/135/135	-
22	CLA	B	606	-	3/3/20/25	8/37/135/135	-
25	BCR	f	102	-	-	6/29/63/63	0/2/2/2
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
22	CLA	B	611	-	3/3/20/25	13/37/135/135	-
23	PHO	A	405	-	-	13/53/103/103	0/5/6/6
22	CLA	A	404	-	3/3/20/25	10/37/135/135	-
22	CLA	B	614	-	3/3/20/25	9/37/135/135	-
22	CLA	B	601	-	3/3/20/25	15/37/135/135	-
22	CLA	c	511	-	3/3/20/25	18/37/135/135	-
22	CLA	b	610	-	3/3/20/25	12/37/135/135	-
31	LMG	d	408	-	-	25/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	622	-	-	7/29/63/63	0/2/2/2
25	BCR	A	408	-	-	4/29/63/63	0/2/2/2
31	LMG	C	521	-	-	20/43/63/70	0/1/1/1
25	BCR	g	101	-	-	5/29/63/63	0/2/2/2
26	DGD	B	620	-	-	18/47/87/95	0/2/2/2
32	LMT	D	408	-	-	2/17/57/61	0/2/2/2
30	SQD	a	412	-	-	21/46/66/69	0/1/1/1
22	CLA	a	404	-	3/3/20/25	15/37/135/135	-
22	CLA	D	404	-	2/2/20/25	6/37/135/135	-
30	SQD	B	622	-	-	14/38/58/69	0/1/1/1
26	DGD	C	514	-	-	19/42/82/95	0/2/2/2
31	LMG	b	627	-	-	15/37/57/70	0/1/1/1
22	CLA	b	617	-	3/3/20/25	15/37/135/135	-
31	LMG	d	412	-	-	14/41/61/70	0/1/1/1
22	CLA	b	616	-	3/3/20/25	12/37/135/135	-
22	CLA	d	406	-	2/2/20/25	6/37/135/135	-
27	LHG	a	409	-	-	11/43/43/53	-
22	CLA	A	402	-	3/3/20/25	8/37/135/135	-
25	BCR	b	621	-	-	2/29/63/63	0/2/2/2
23	PHO	D	401	-	-	10/53/103/103	0/5/6/6
22	CLA	B	615	-	3/3/20/25	18/37/135/135	-
31	LMG	B	625	-	-	24/44/64/70	0/1/1/1
22	CLA	C	512	-	3/3/20/25	20/37/135/135	-
34	HEM	V	201	16	-	2/6/54/54	-
22	CLA	c	507	-	3/3/20/25	14/37/135/135	-
25	BCR	K	101	-	-	5/29/63/63	0/2/2/2
27	LHG	A	410	-	-	12/43/43/53	-
31	LMG	D	406	-	-	21/43/63/70	0/1/1/1
22	CLA	b	620	-	3/3/20/25	19/37/135/135	-
22	CLA	A	406	-	3/3/20/25	8/37/135/135	-
30	SQD	a	401	-	-	15/49/69/69	0/1/1/1
22	CLA	b	618	-	3/3/20/25	16/37/135/135	-
31	LMG	L	101	-	-	26/46/66/70	0/1/1/1
26	DGD	c	515	-	-	19/42/82/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	405	-	3/3/20/25	12/37/135/135	-
24	PL9	A	407	-	-	18/41/61/73	0/1/1/1
26	DGD	b	625	-	-	18/47/87/95	0/2/2/2
22	CLA	C	510	3	3/3/20/25	17/37/135/135	-
25	BCR	J	102	-	-	6/29/63/63	0/2/2/2
31	LMG	c	518	-	-	22/40/60/70	0/1/1/1
23	PHO	d	401	-	-	12/53/103/103	0/5/6/6
30	SQD	F	103	-	-	11/40/60/69	0/1/1/1
22	CLA	B	603	-	3/3/20/25	9/37/135/135	-
34	HEM	f	101	5,6	-	0/6/54/54	-
30	SQD	d	403	-	-	16/38/58/69	0/1/1/1
32	LMT	b	629	-	-	3/21/61/61	0/2/2/2
22	CLA	C	505	-	3/3/20/25	17/37/135/135	-
31	LMG	l	101	-	-	27/46/66/70	0/1/1/1
32	LMT	b	628	-	-	3/21/61/61	0/2/2/2
27	LHG	c	519	-	-	17/41/41/53	-
22	CLA	B	609	-	3/3/20/25	18/37/135/135	-
30	SQD	A	414	-	-	14/49/69/69	0/1/1/1
31	LMG	a	402	-	-	16/37/57/70	0/1/1/1
31	LMG	C	517	-	-	22/40/60/70	0/1/1/1
26	DGD	c	517	-	-	22/55/95/95	0/2/2/2
22	CLA	b	619	-	3/3/20/25	10/37/135/135	-
30	SQD	f	103	-	-	10/40/60/69	0/1/1/1
25	BCR	c	514	-	-	5/29/63/63	0/2/2/2
22	CLA	c	505	-	3/3/20/25	17/37/135/135	-
34	HEM	v	201	16	-	2/6/54/54	-
25	BCR	b	623	-	-	4/29/63/63	0/2/2/2
32	LMT	M	102	-	-	0/21/61/61	0/2/2/2
32	LMT	B	628	-	-	2/21/61/61	0/2/2/2
22	CLA	B	610	-	3/3/20/25	10/37/135/135	-
26	DGD	d	410	-	-	36/52/92/95	0/2/2/2
25	BCR	C	520	-	-	6/29/63/63	0/2/2/2
31	LMG	d	409	-	-	21/43/63/70	0/1/1/1
31	LMG	i	102	-	-	18/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	B	607	-	3/3/20/25	12/37/135/135	-
22	CLA	C	503	-	3/3/20/25	15/37/135/135	-
32	LMT	b	604	-	-	5/21/61/61	0/2/2/2
25	BCR	i	101	-	-	4/29/63/63	0/2/2/2
31	LMG	m	101	-	-	17/37/57/70	0/1/1/1
31	LMG	e	101	-	-	20/39/59/70	0/1/1/1
22	CLA	b	606	-	3/3/20/25	20/37/135/135	-
22	CLA	c	501	-	3/3/20/25	13/37/135/135	-
22	CLA	b	611	-	3/3/20/25	8/37/135/135	-
31	LMG	B	621	-	-	15/44/64/70	0/1/1/1
24	PL9	J	101	-	-	9/29/49/73	0/1/1/1
22	CLA	C	511	-	3/3/20/25	18/37/135/135	-
22	CLA	B	605	-	3/3/20/25	16/37/135/135	-
22	CLA	c	520	-	3/3/20/25	10/37/135/135	-
32	LMT	i	103	-	-	4/21/61/61	0/2/2/2
22	CLA	D	403	-	3/3/20/25	13/37/135/135	-
25	BCR	c	513	-	-	5/29/63/63	0/2/2/2
22	CLA	C	509	-	3/3/20/25	13/37/135/135	-
25	BCR	B	616	-	-	3/29/63/63	0/2/2/2
24	PL9	a	407	-	-	18/41/61/73	0/1/1/1
22	CLA	a	403	-	3/3/20/25	8/37/135/135	-
26	DGD	C	515	-	-	20/51/91/95	0/2/2/2
22	CLA	B	612	-	3/3/20/25	15/37/135/135	-
25	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	BCR	F	102	-	-	6/29/63/63	0/2/2/2
34	HEM	F	101	5,6	-	0/6/54/54	-
22	CLA	a	405	-	3/3/20/25	8/37/135/135	-
31	LMG	b	626	-	-	14/44/64/70	0/1/1/1
22	CLA	c	509	-	3/3/20/25	16/37/135/135	-
27	LHG	C	518	-	-	14/41/41/53	-
22	CLA	C	506	-	3/3/20/25	12/37/135/135	-
26	DGD	A	409	-	-	16/45/85/95	0/2/2/2
31	LMG	M	101	-	-	18/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	617	-	-	8/29/63/63	0/2/2/2

The worst 5 of 612 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	C4B-NB	7.98	1.42	1.35
22	A	402	CLA	C4B-NB	7.84	1.42	1.35
22	a	403	CLA	C4B-NB	7.83	1.42	1.35
22	B	601	CLA	C4B-NB	7.82	1.42	1.35
22	b	605	CLA	C4B-NB	7.81	1.42	1.35

The worst 5 of 1228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.60	110.12	106.71
22	B	611	CLA	C4A-NA-C1A	7.55	110.10	106.71
22	B	605	CLA	C4A-NA-C1A	7.39	110.03	106.71
22	b	608	CLA	C4A-NA-C1A	7.34	110.01	106.71
22	C	501	CLA	C4A-NA-C1A	7.23	109.96	106.71

5 of 208 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	ND

5 of 2157 torsion outliers are listed below:

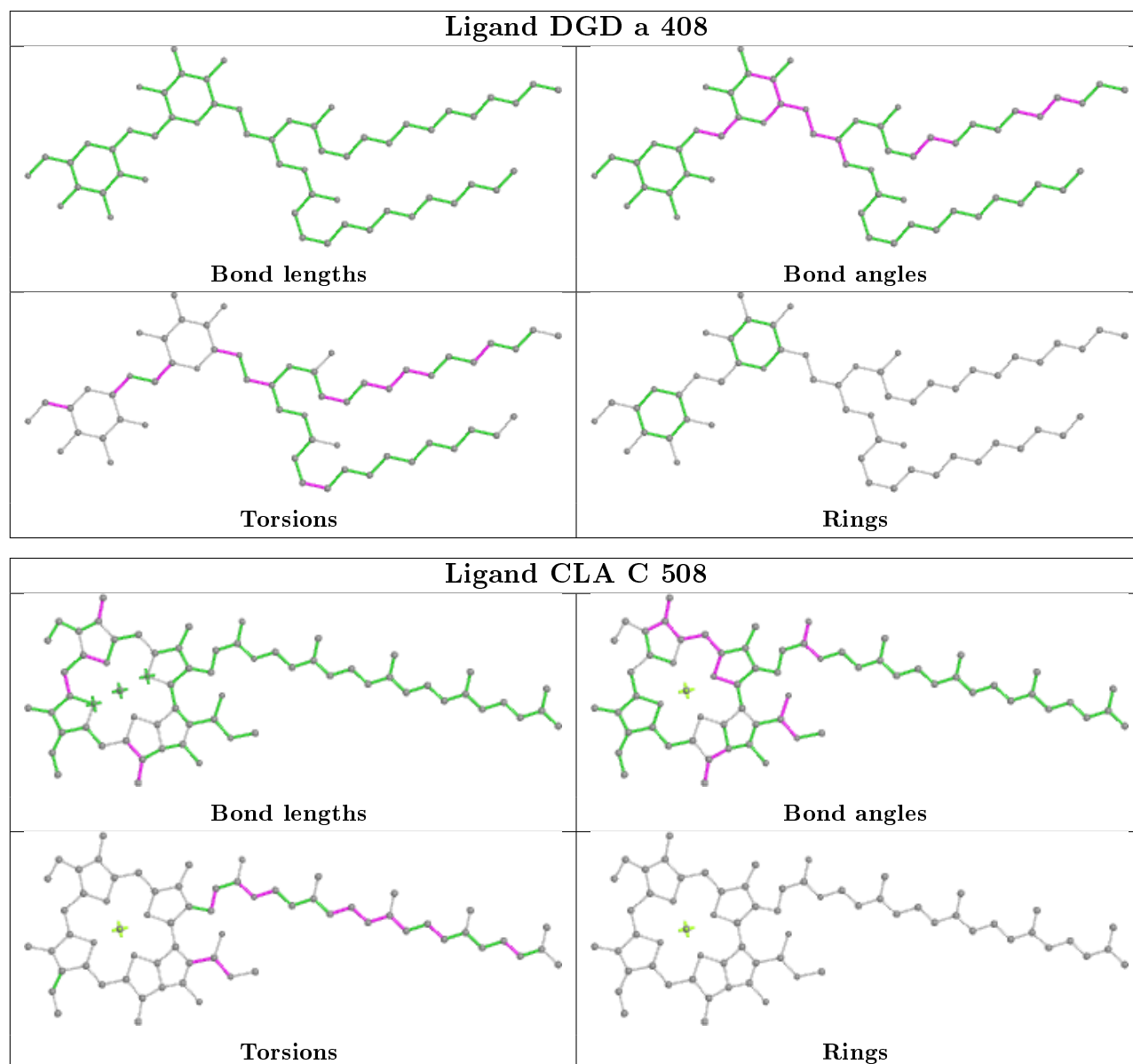
Mol	Chain	Res	Type	Atoms
26	a	408	DGD	C2D-C1D-O3G-C3G
31	E	101	LMG	C2-C1-O1-C7
31	E	101	LMG	O6-C1-O1-C7
26	b	601	DGD	O1B-C1B-O2G-C2G
26	b	601	DGD	O2G-C2G-C3G-O3G

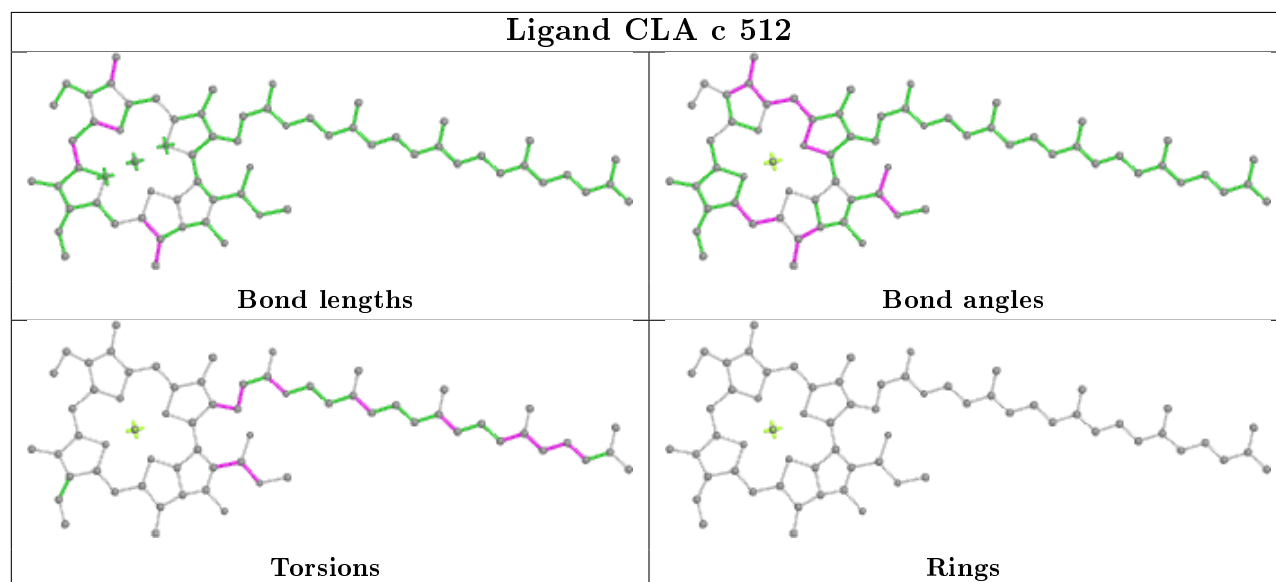
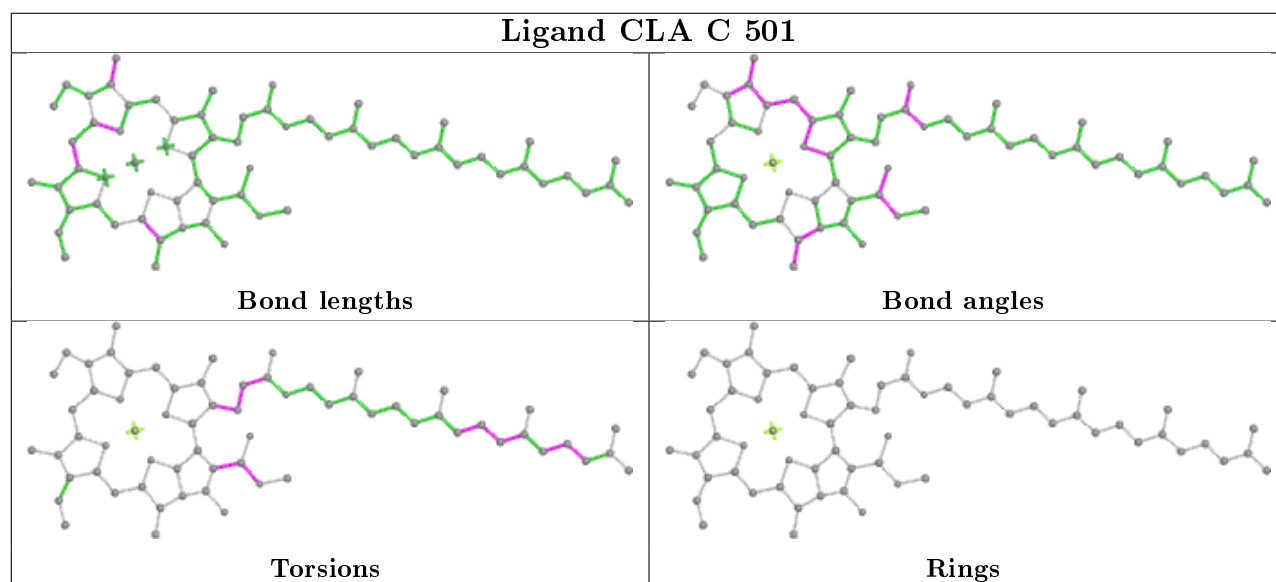
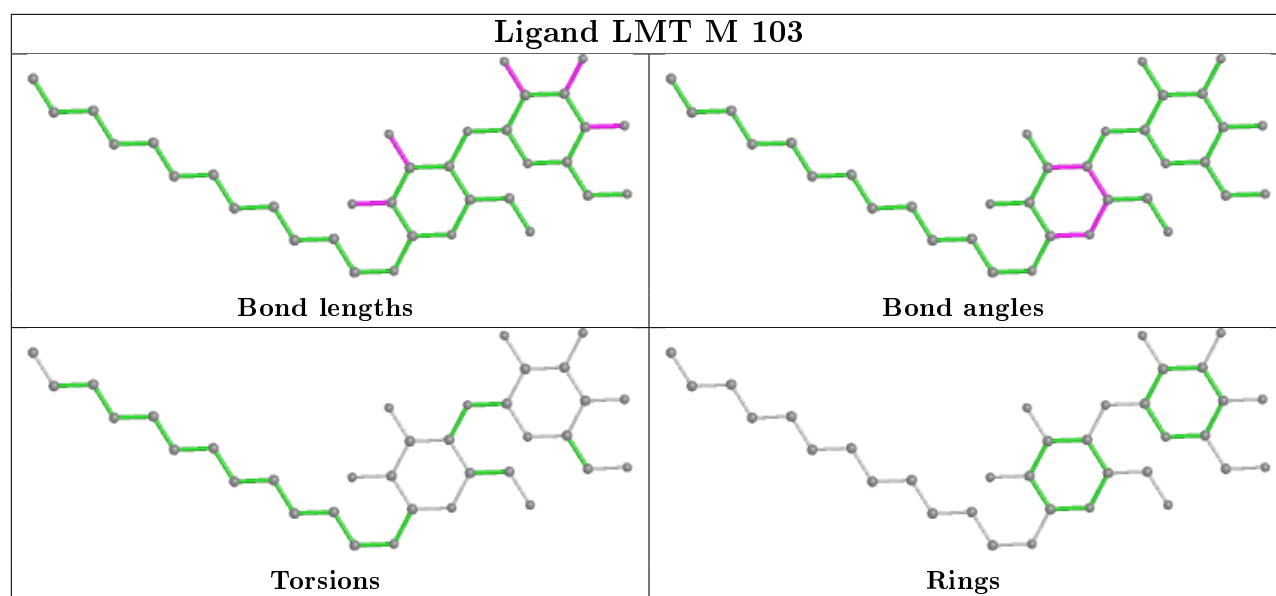
There are no ring outliers.

No monomer is involved in short contacts.

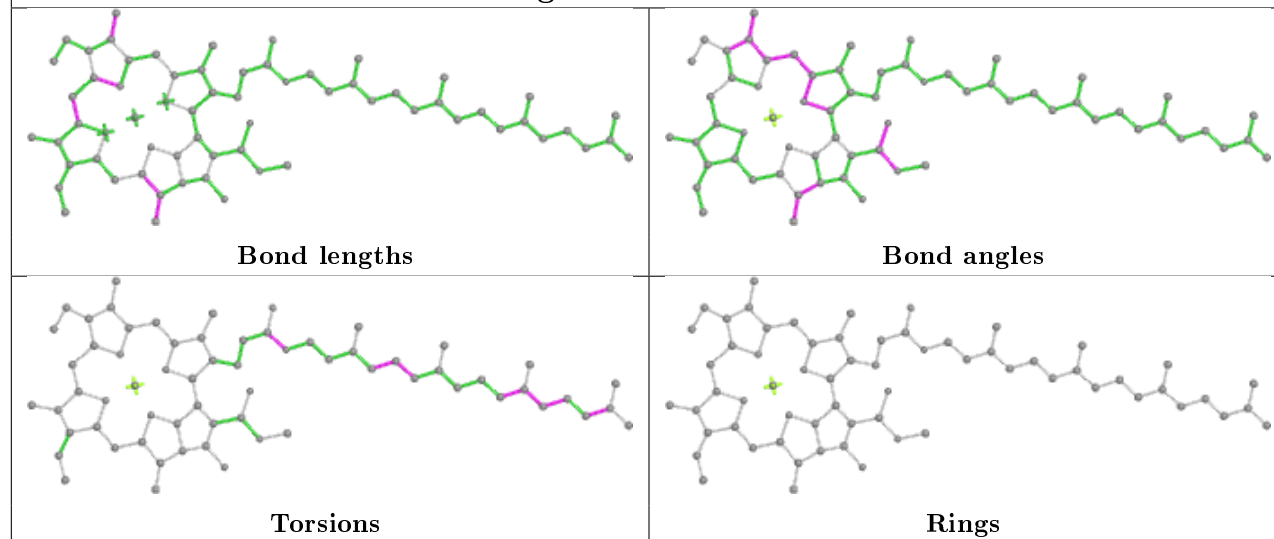
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

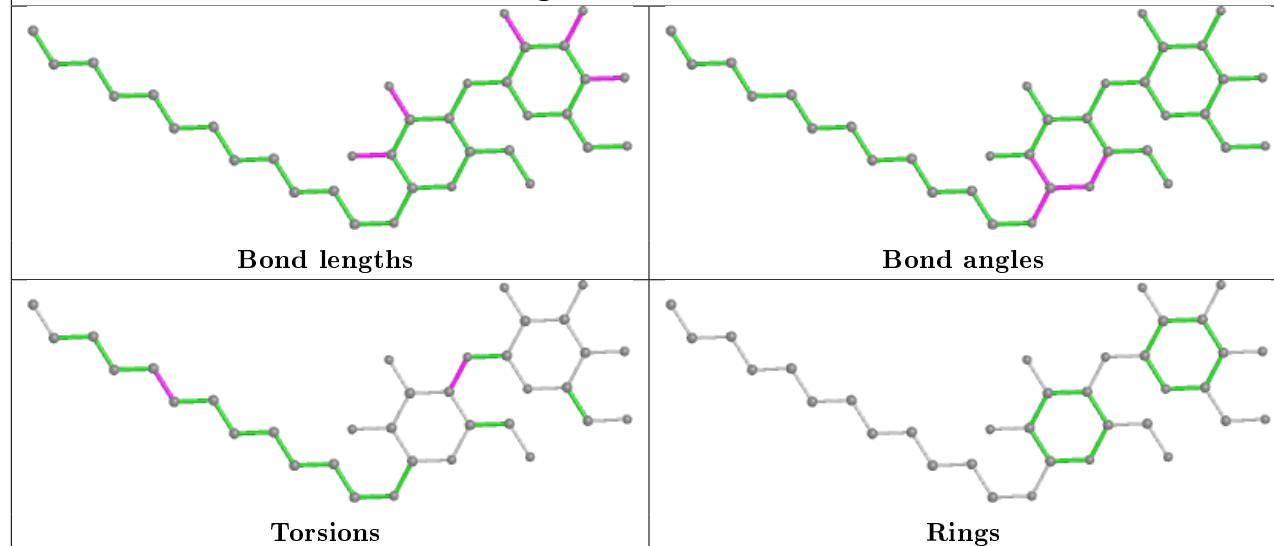




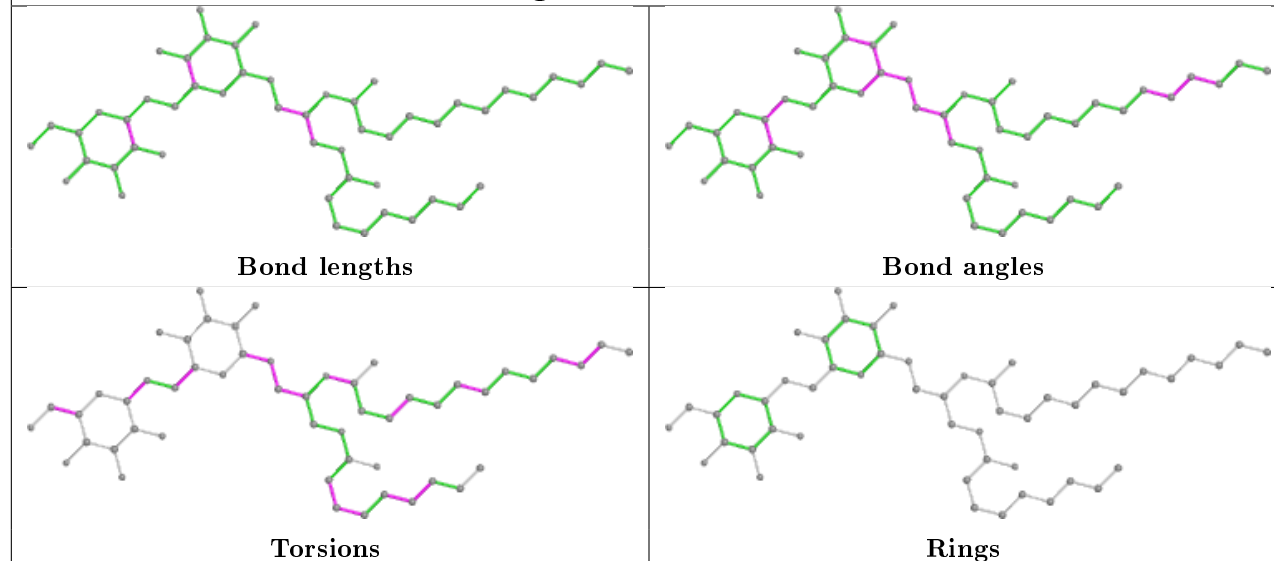
## Ligand CLA c 502

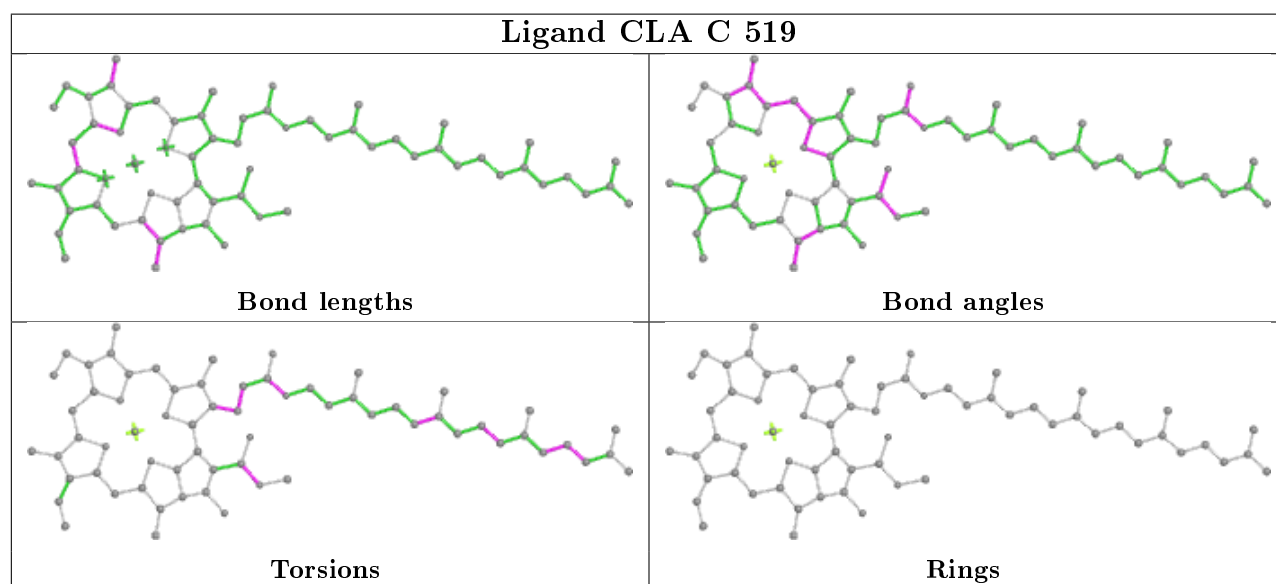
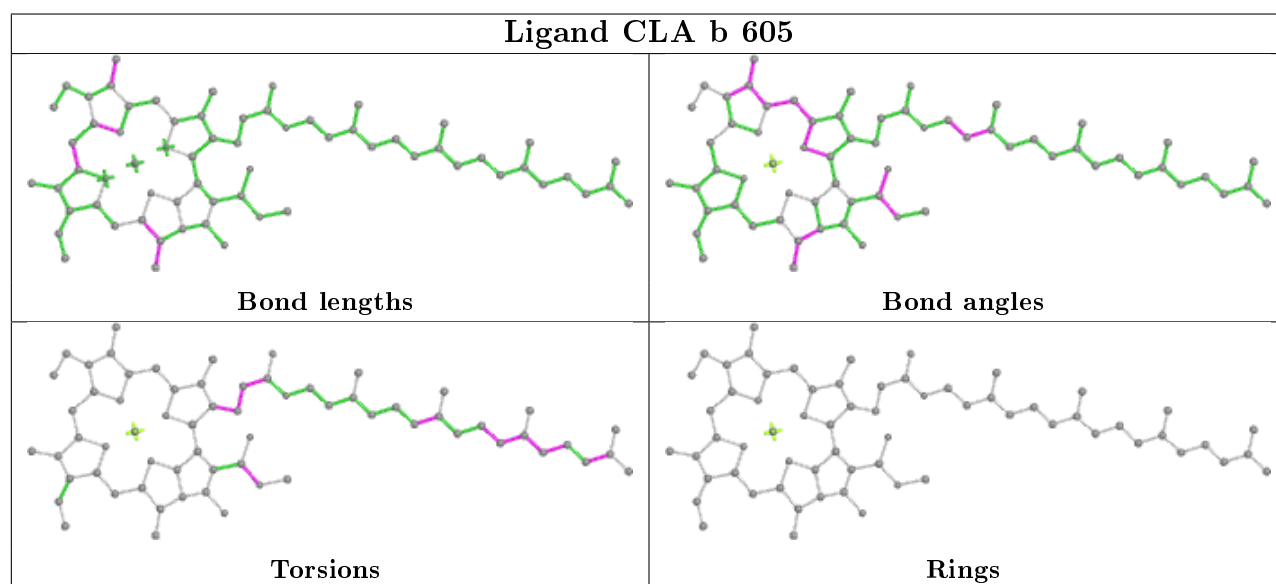
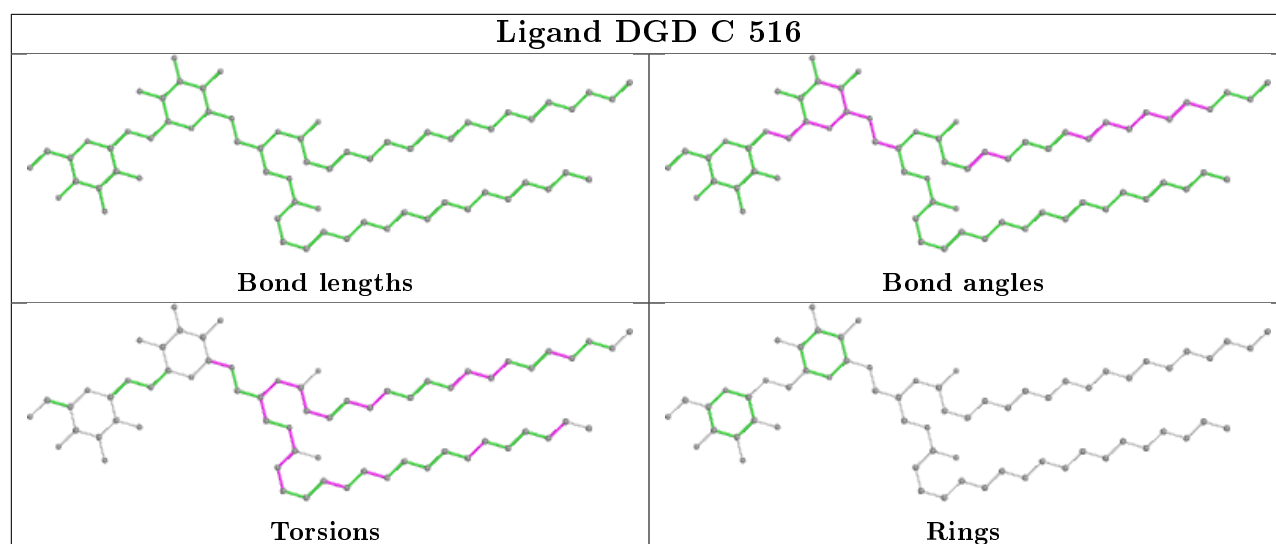


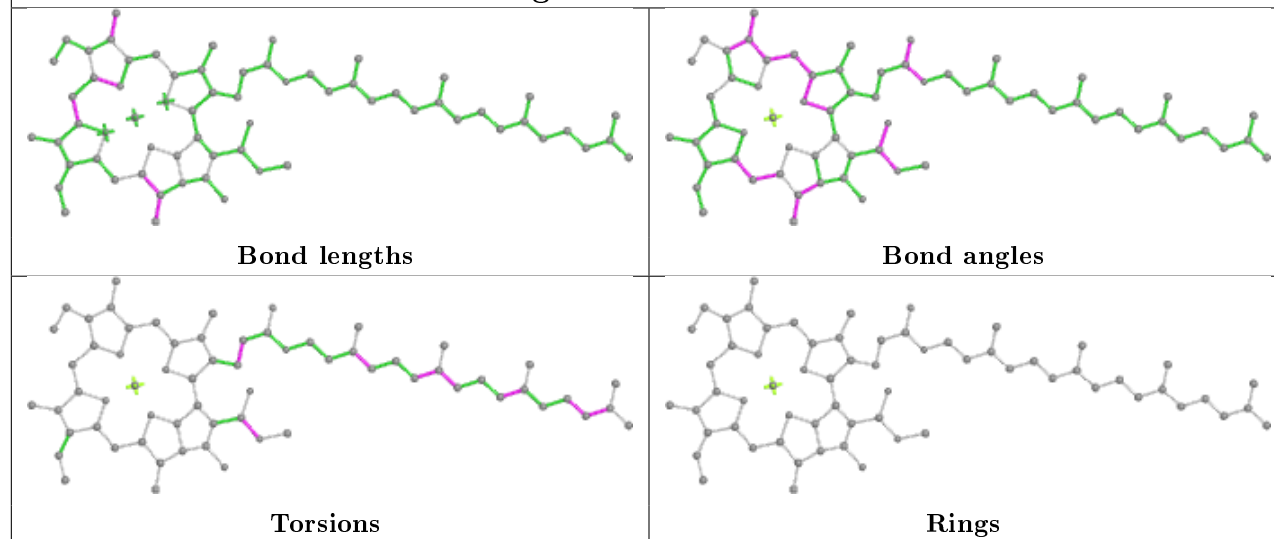
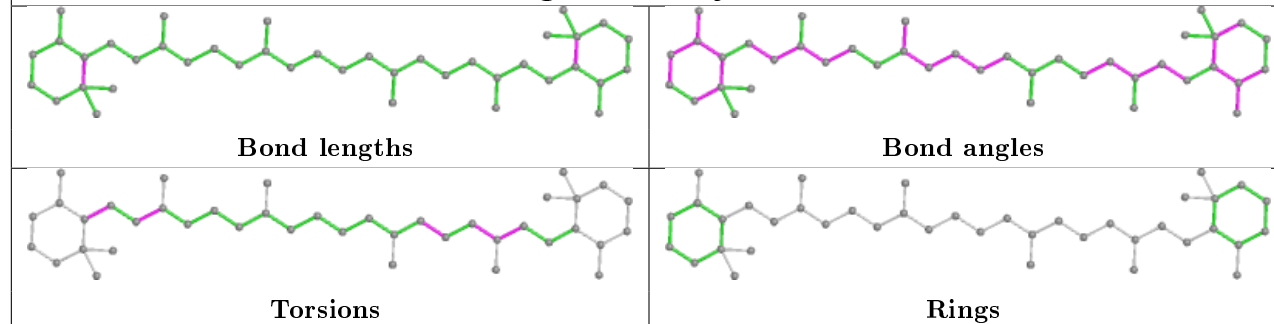
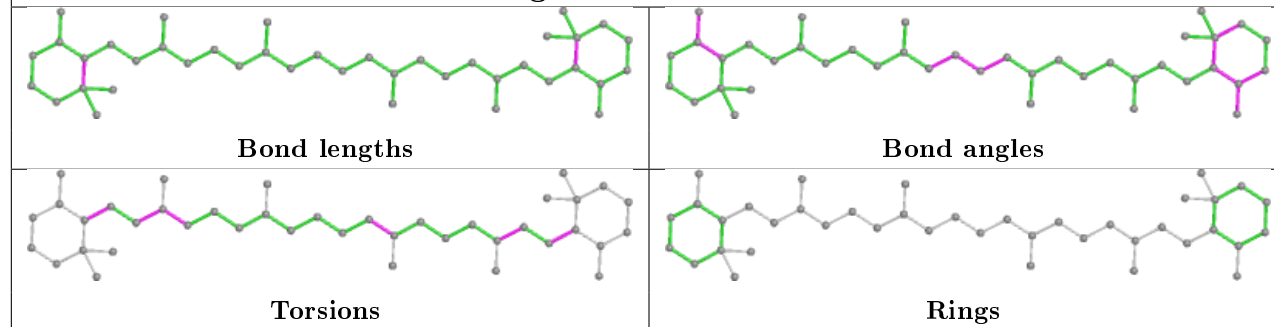
## Ligand LMT I 102



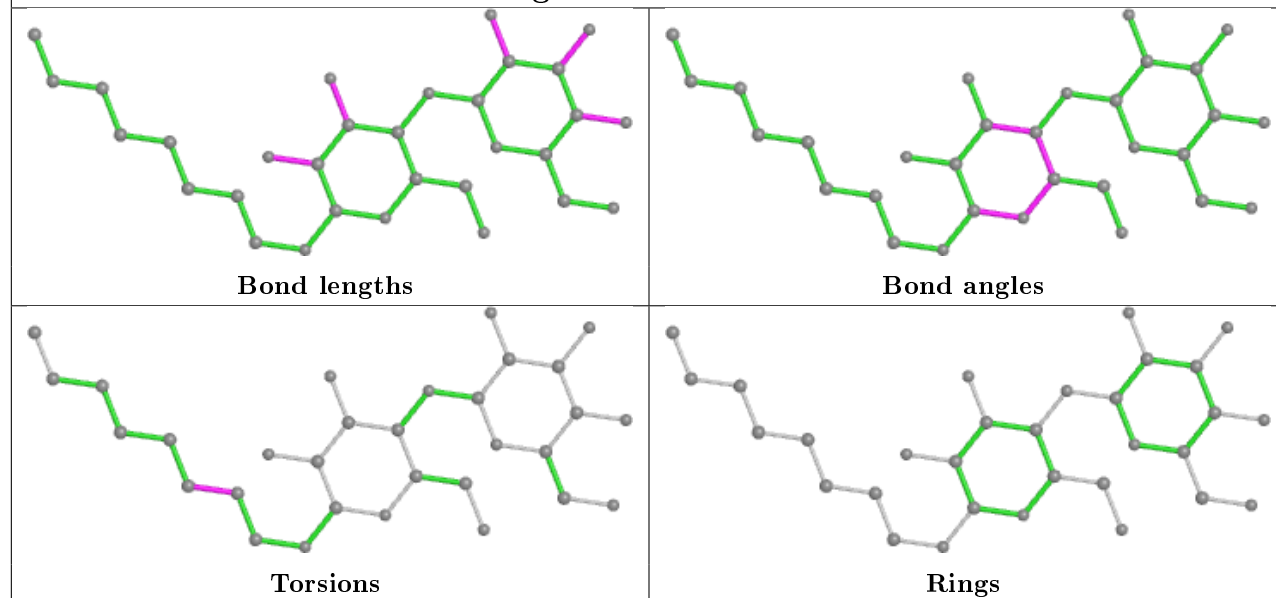
## Ligand DGD b 601



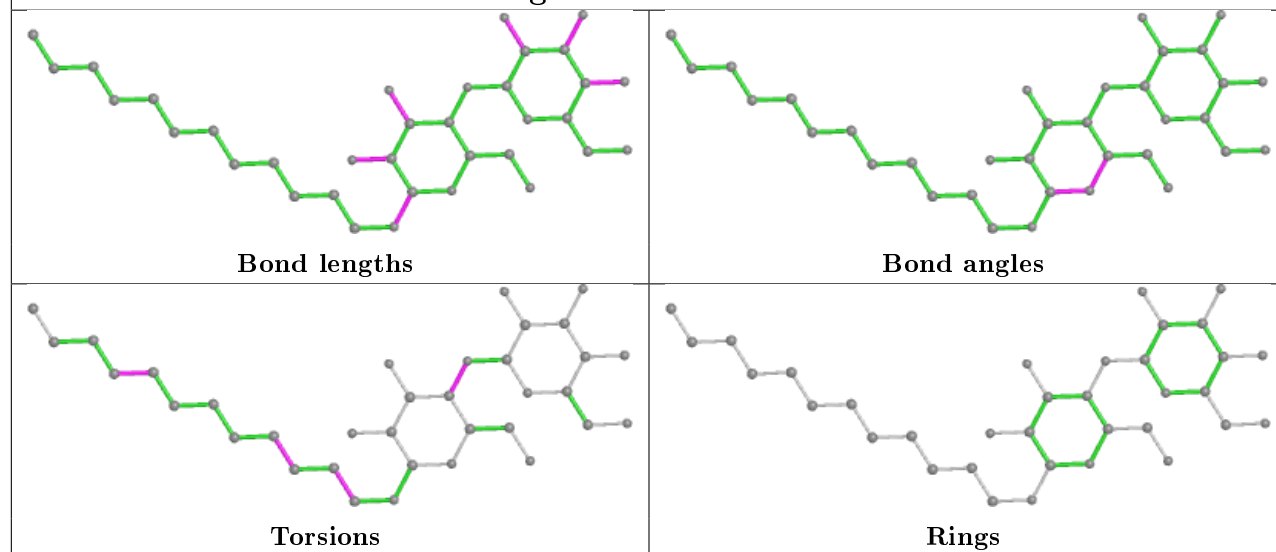


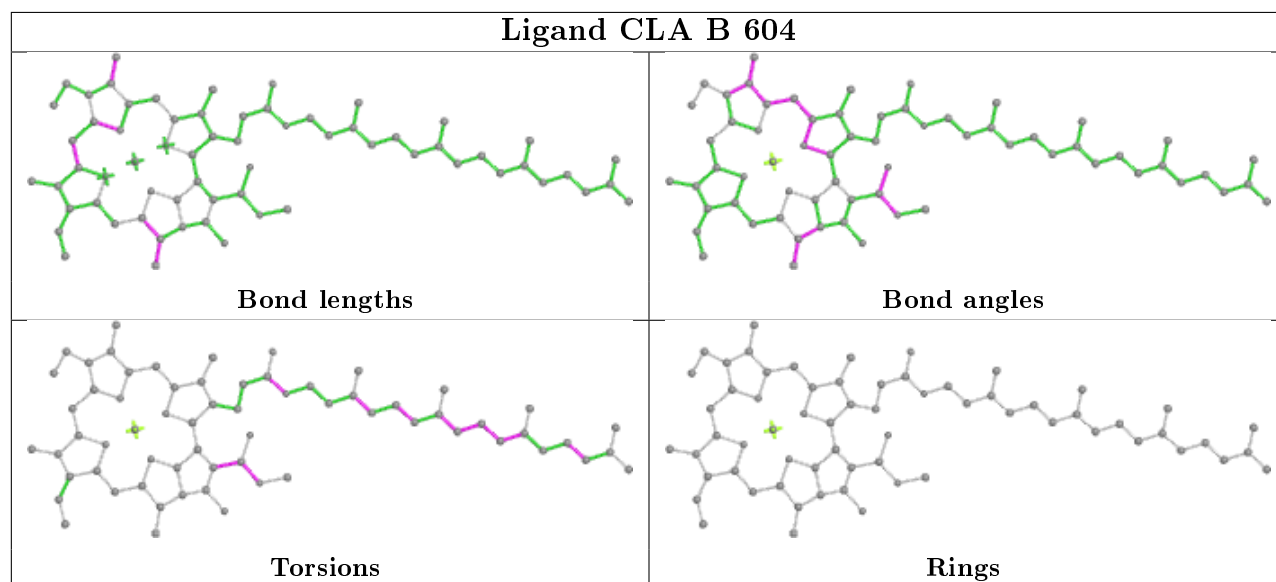
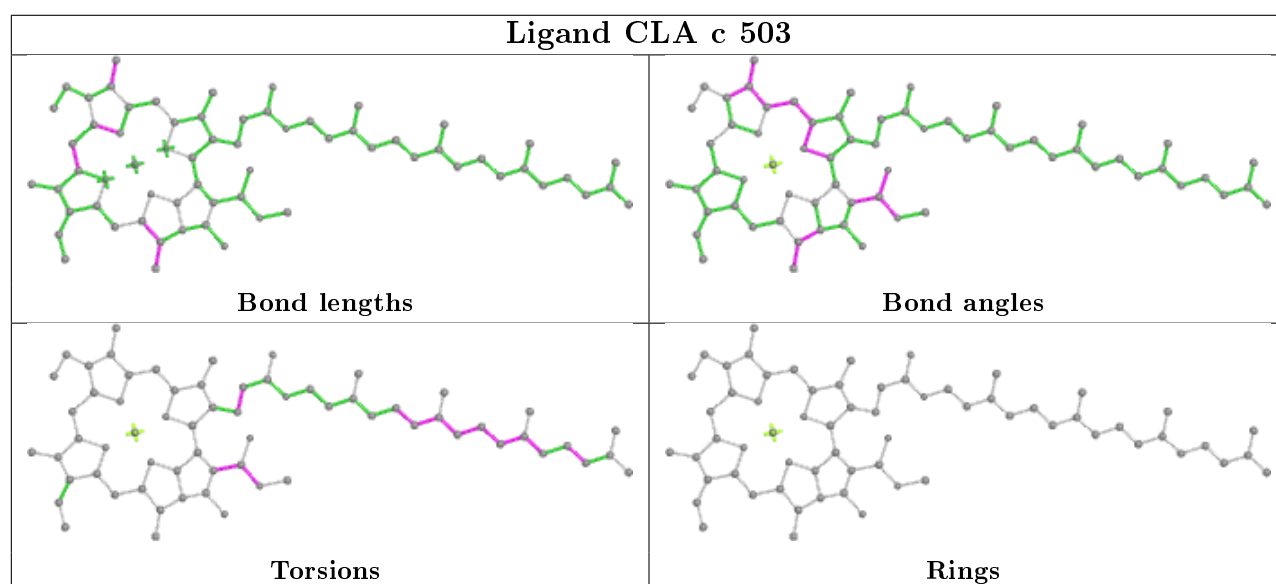
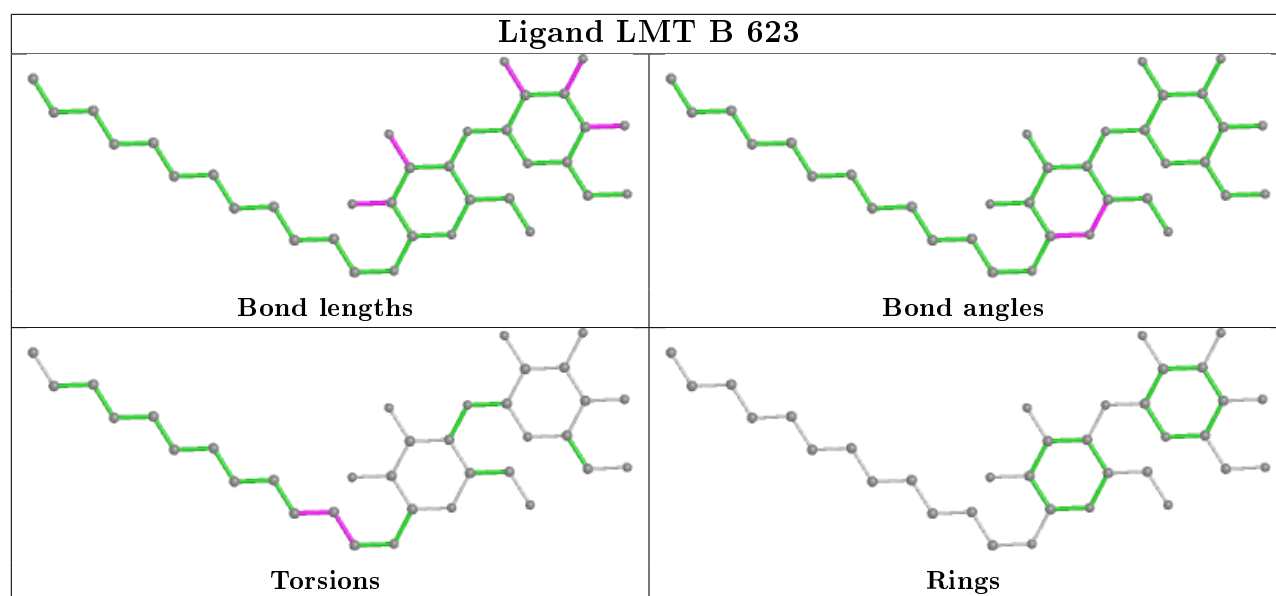
**Ligand CLA B 602****Ligand BCR j 102****Ligand BCR H 102**

## Ligand LMT d 411

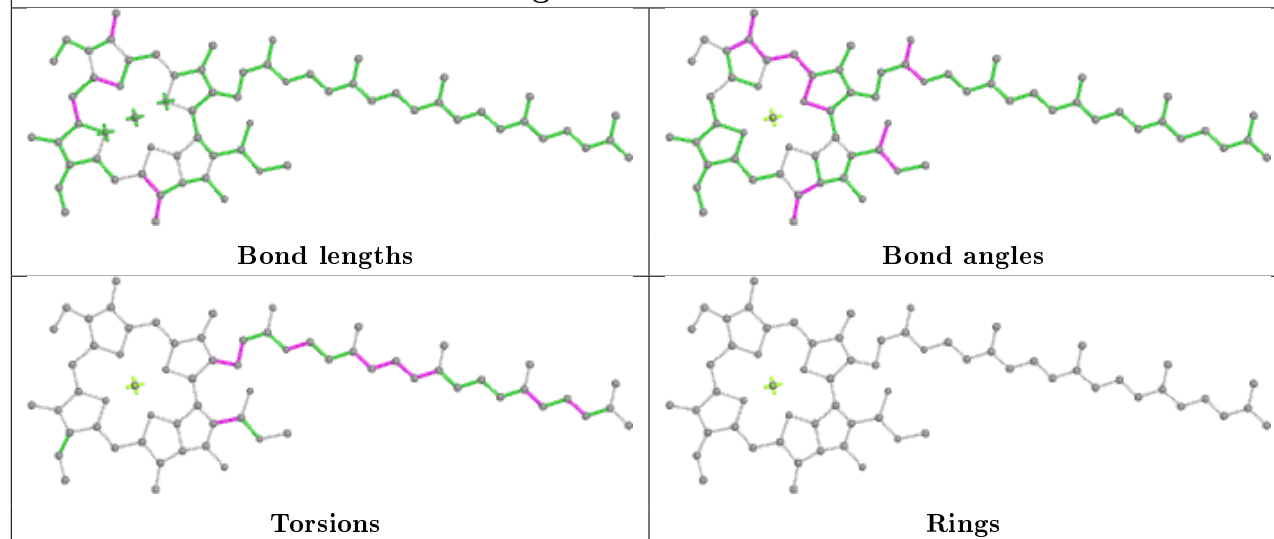
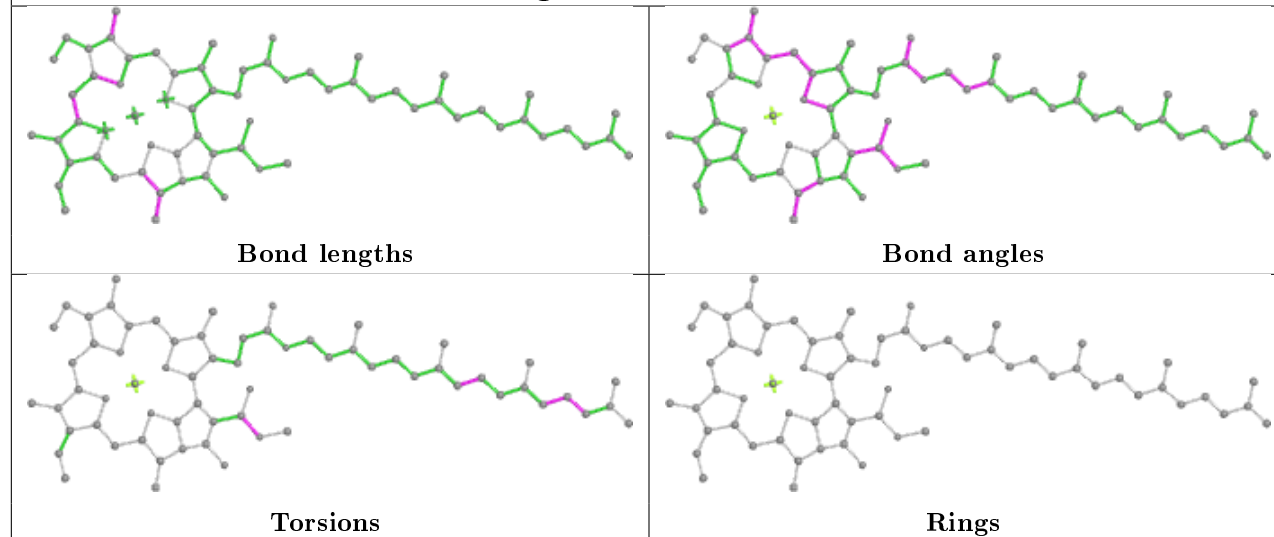


## Ligand LMT B 629

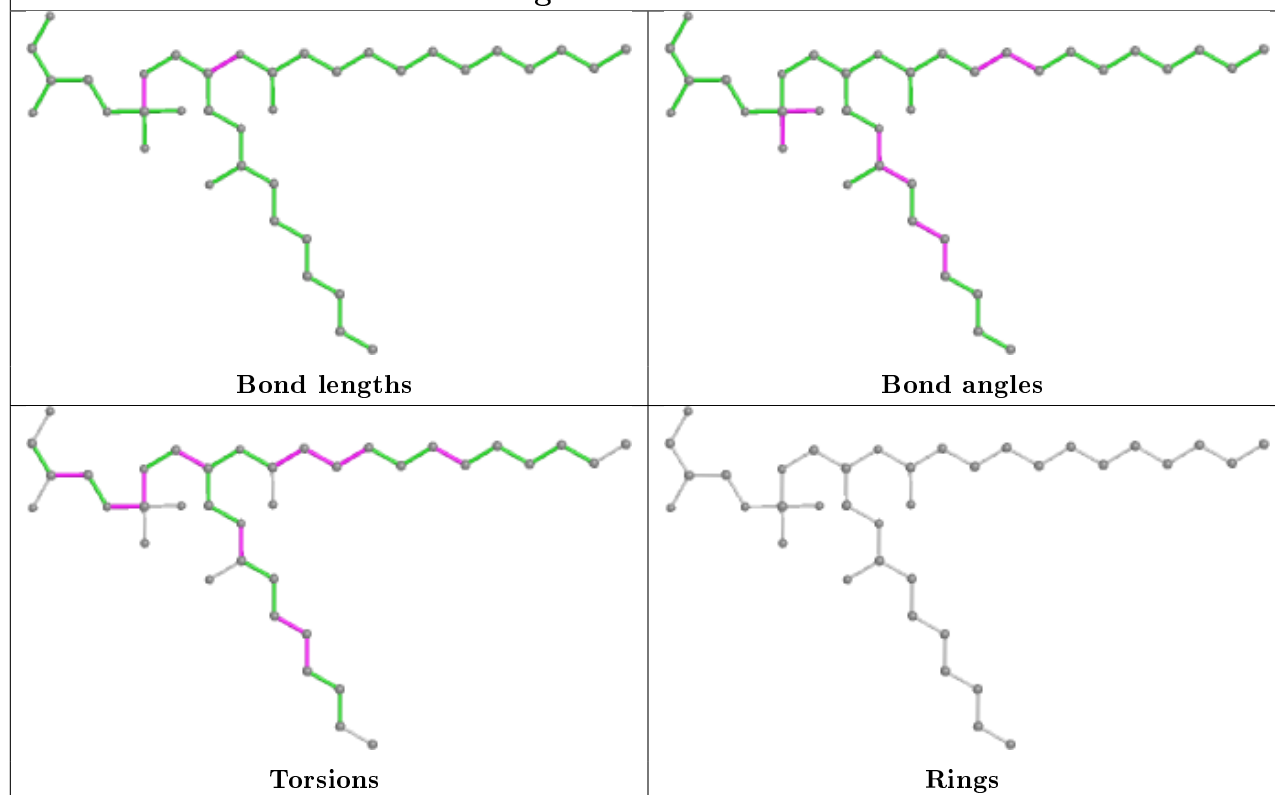




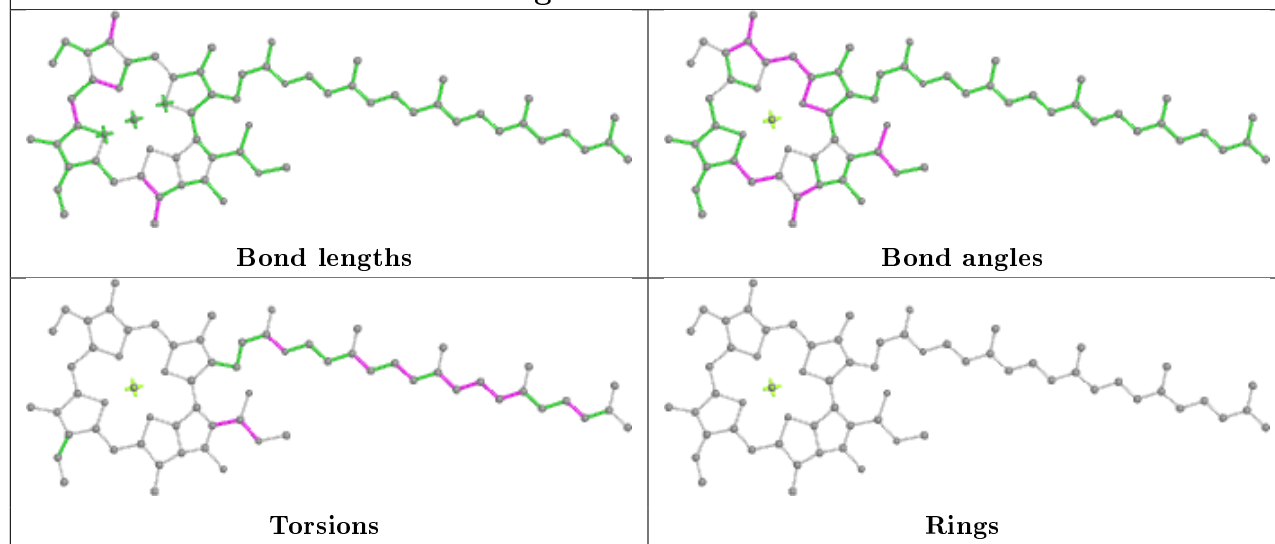


**Ligand CLA A 403****Ligand CLA b 608**

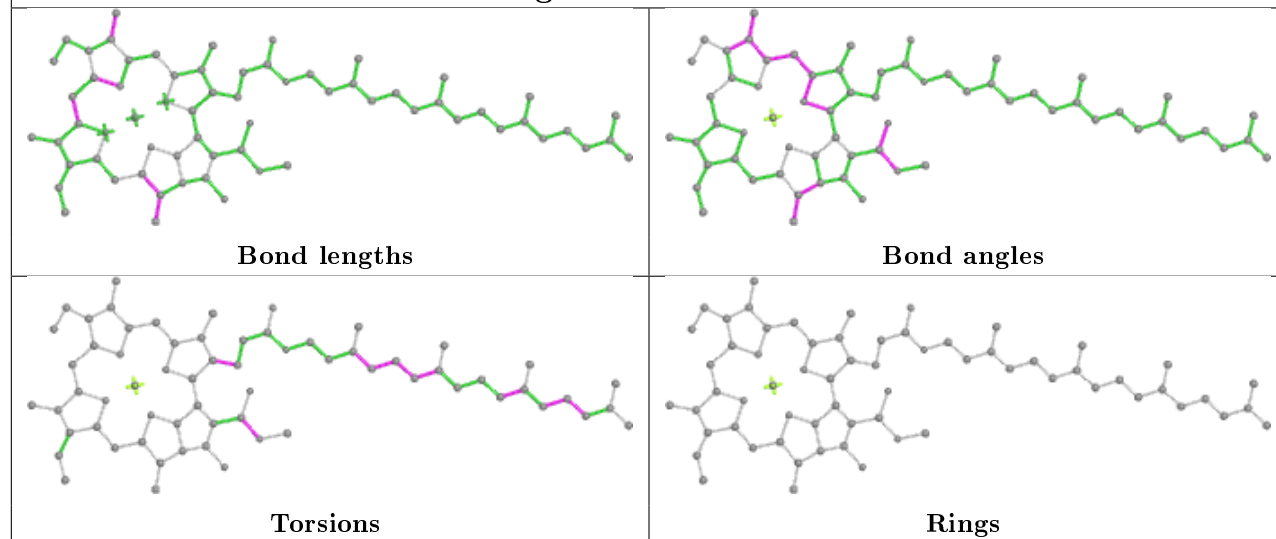
## Ligand LHG c 519



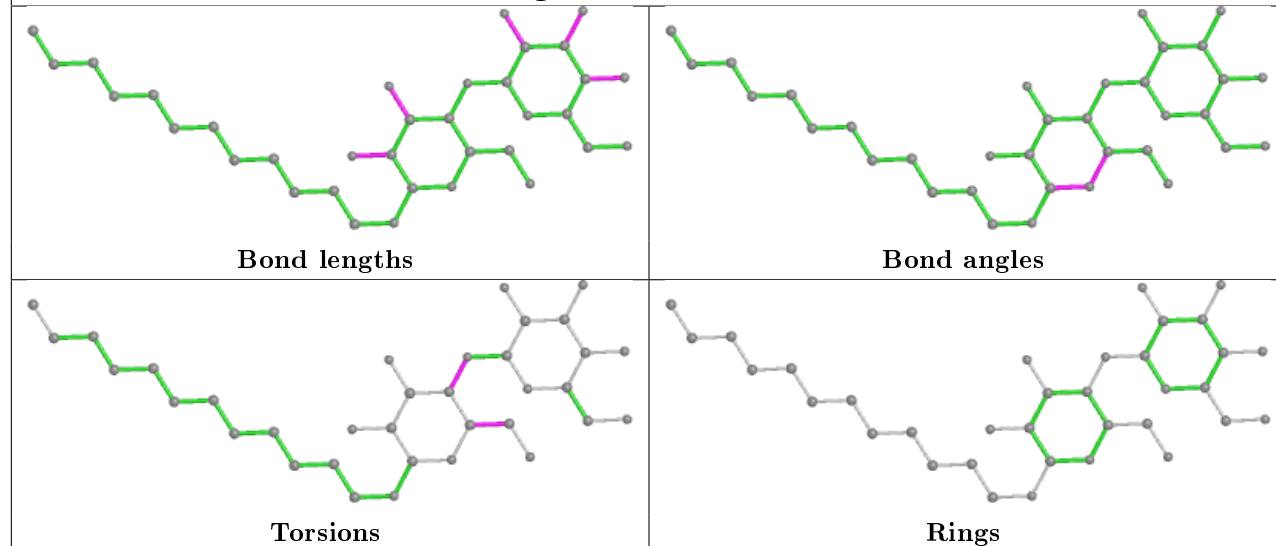
## Ligand CLA b 609



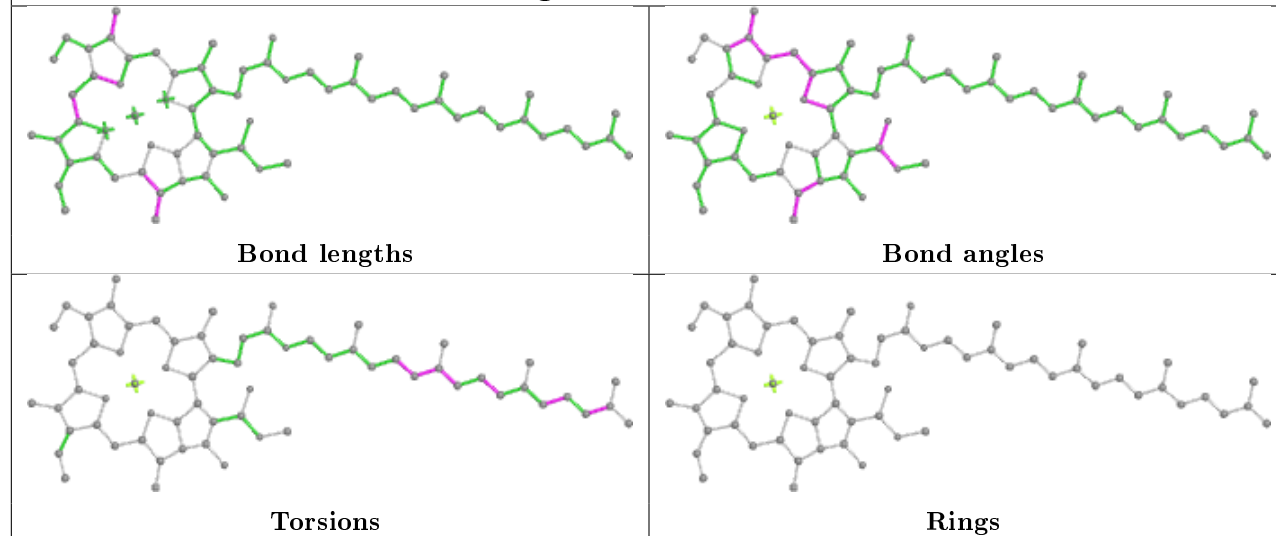
## Ligand CLA b 612

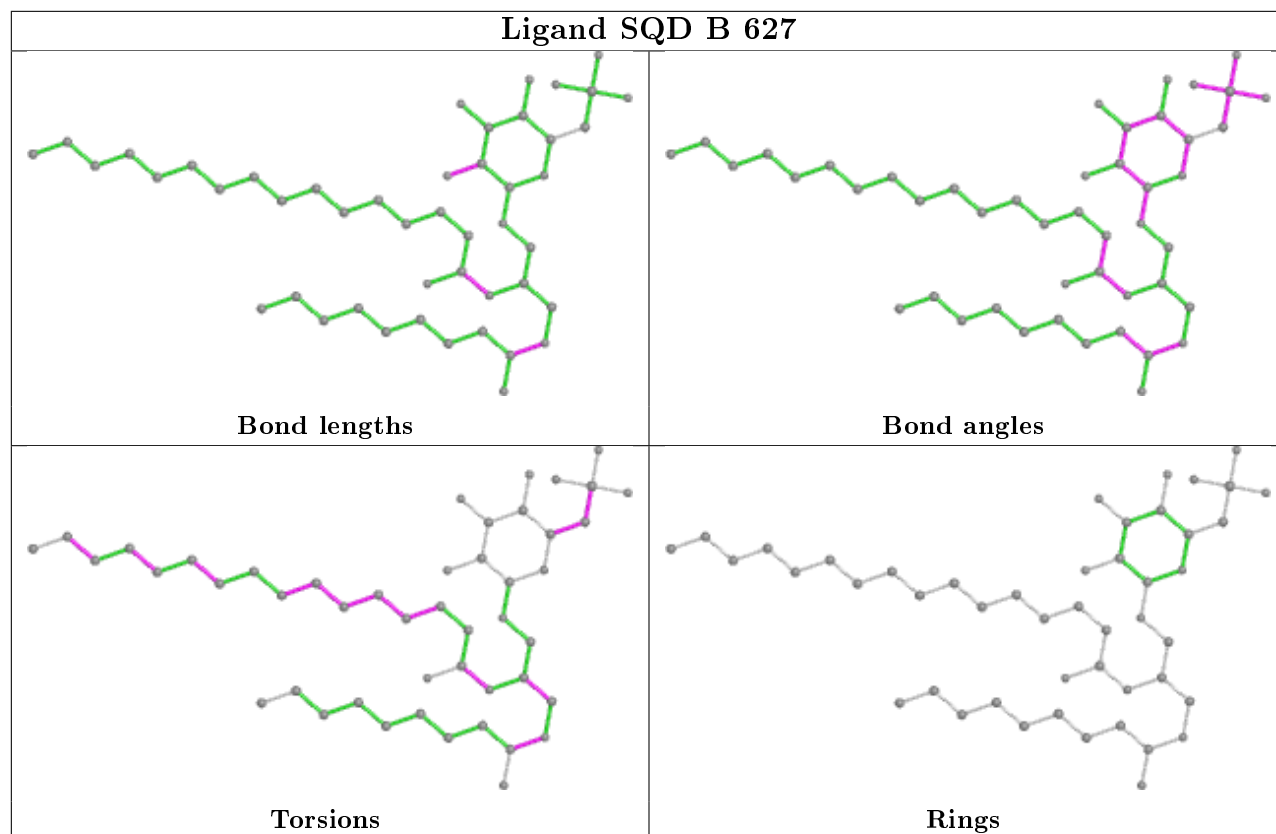
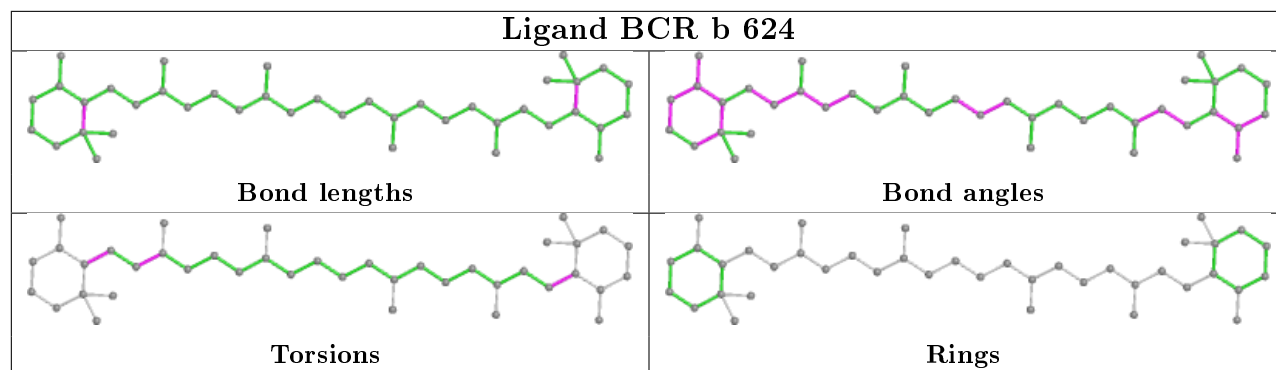


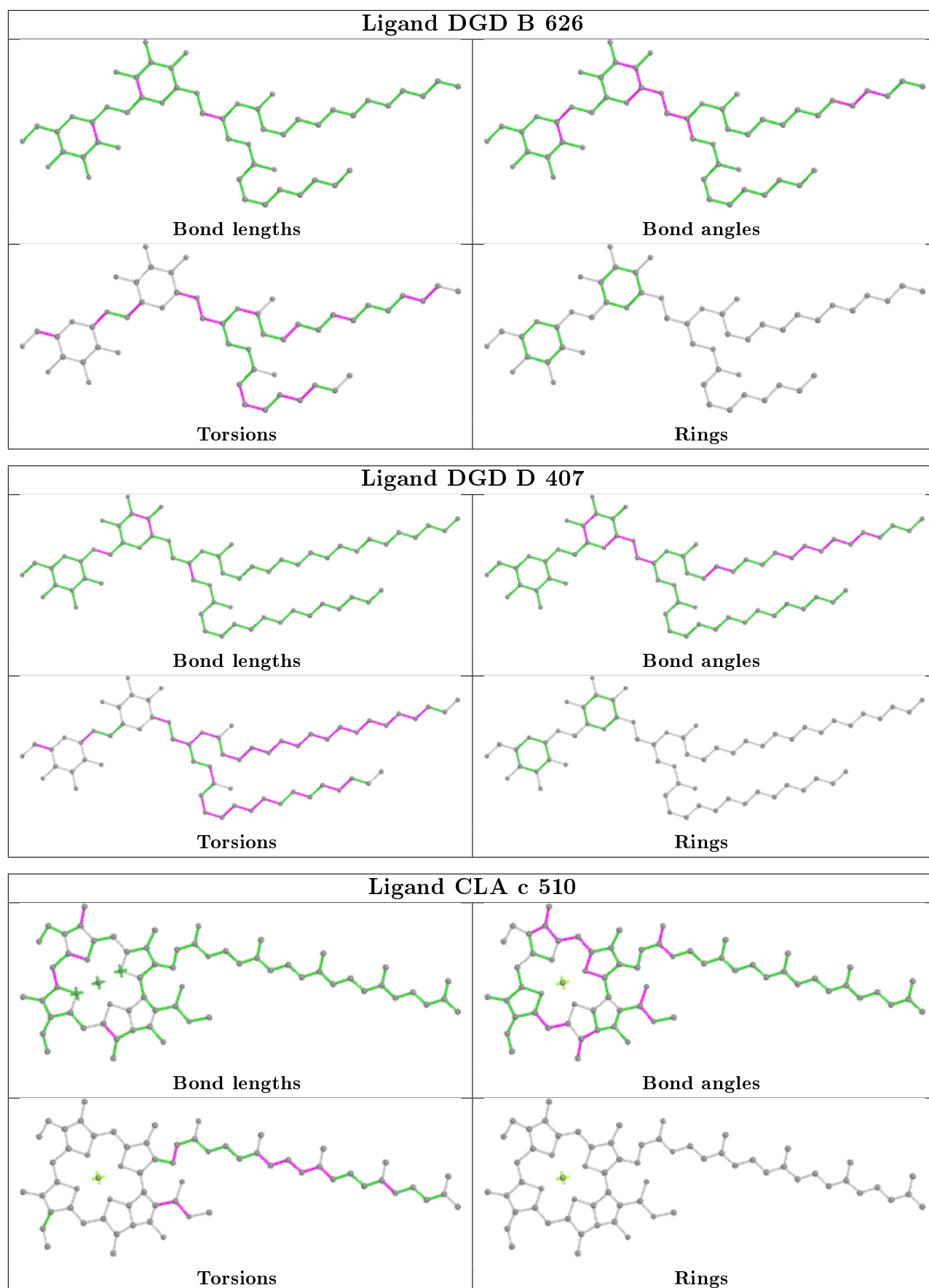
## Ligand LMT b 603

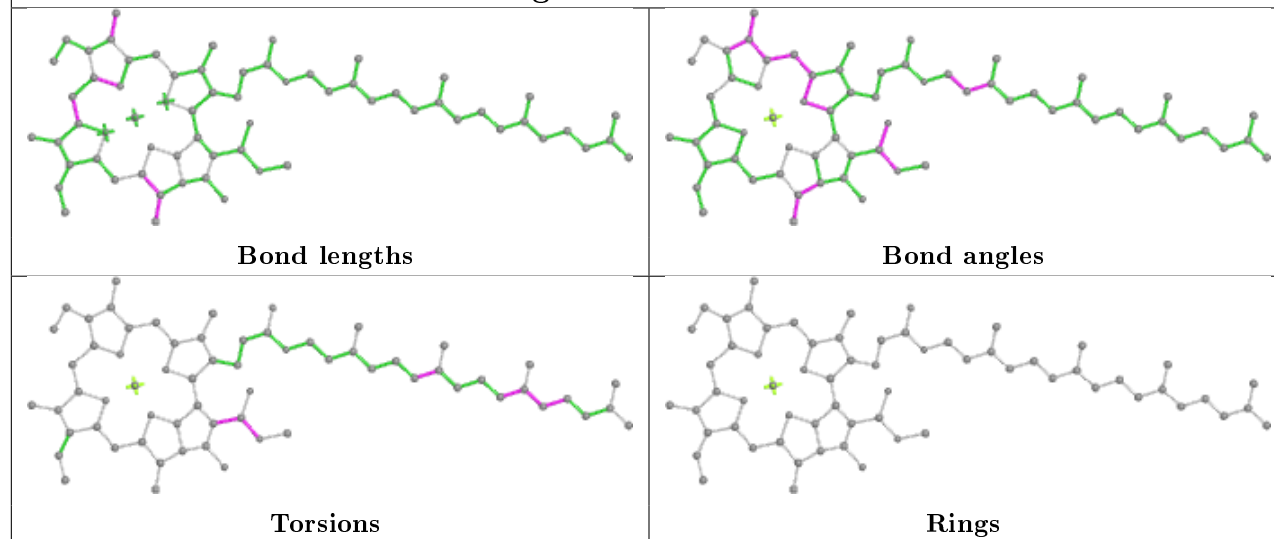
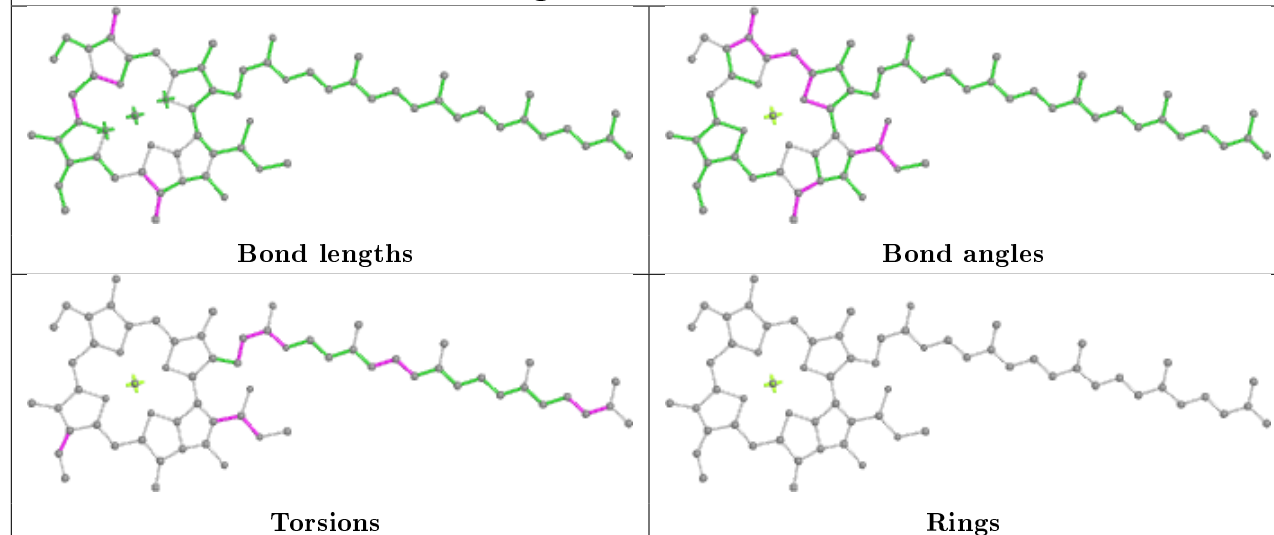
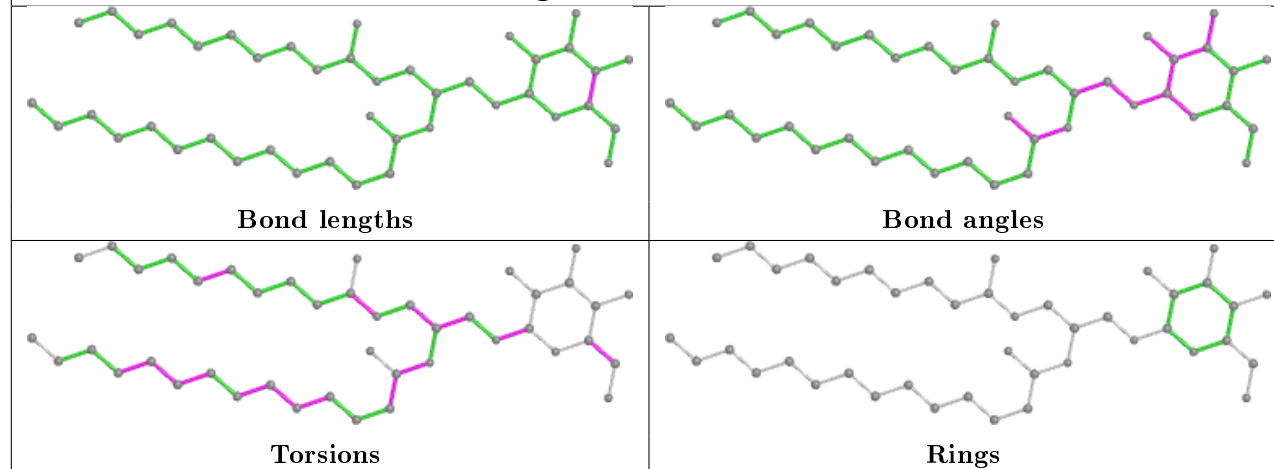


## Ligand CLA a 406

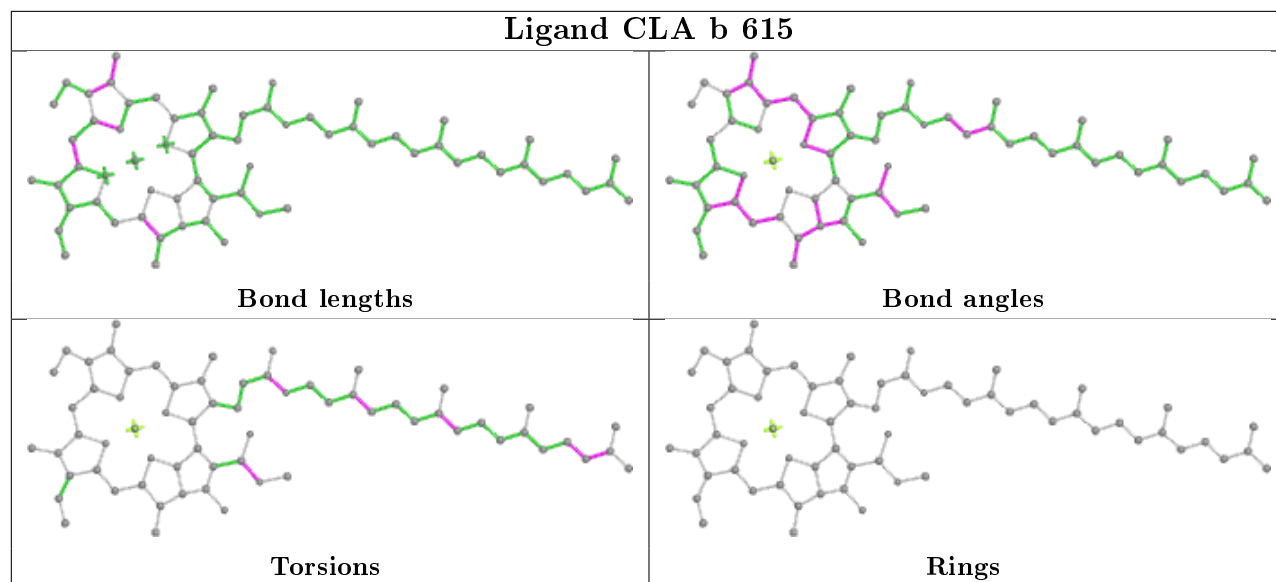




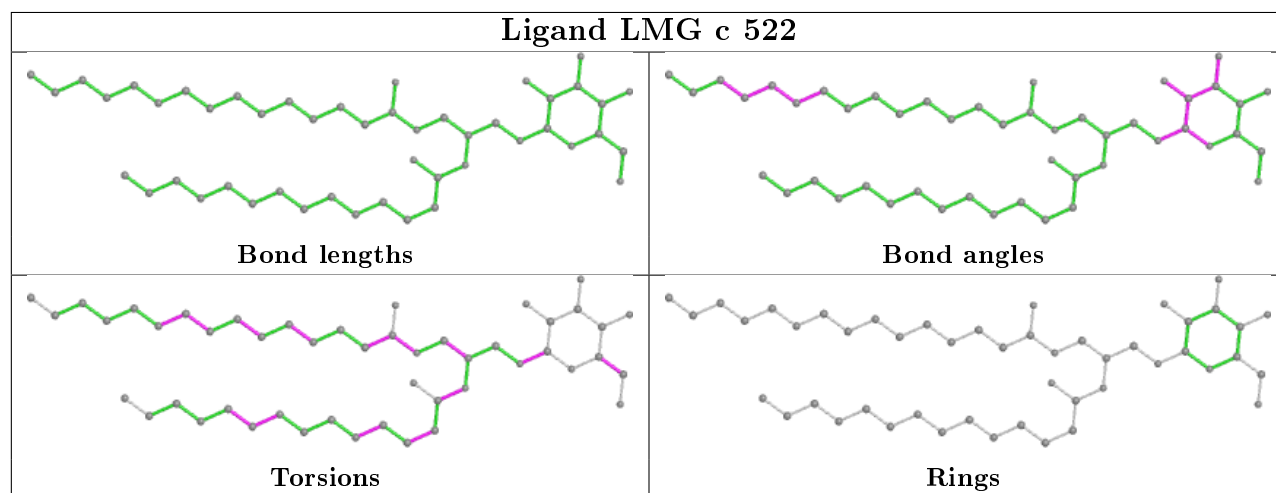


**Ligand CLA B 608****Ligand CLA B 613****Ligand LMG I 101**

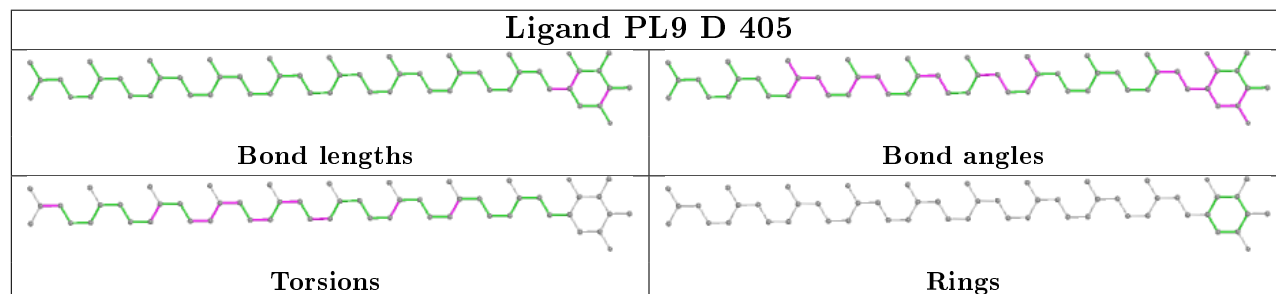
## Ligand CLA b 615



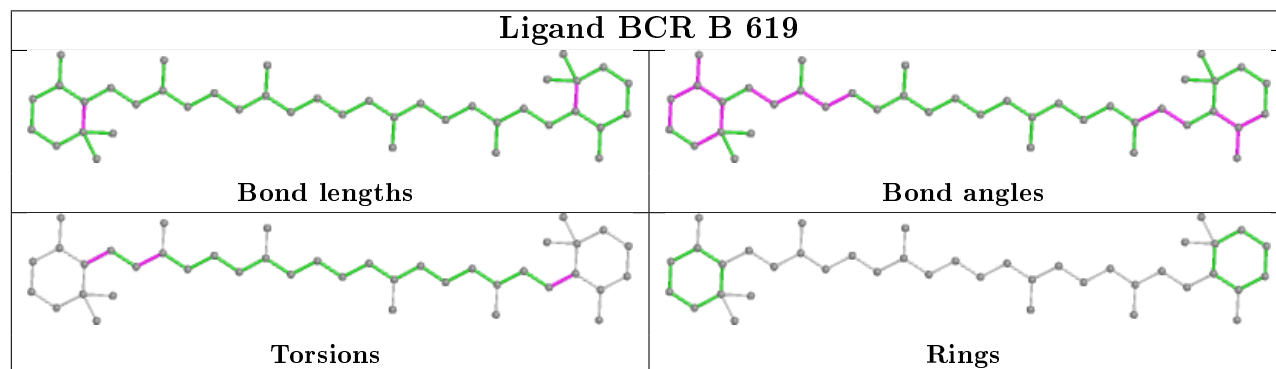
## Ligand LMG c 522

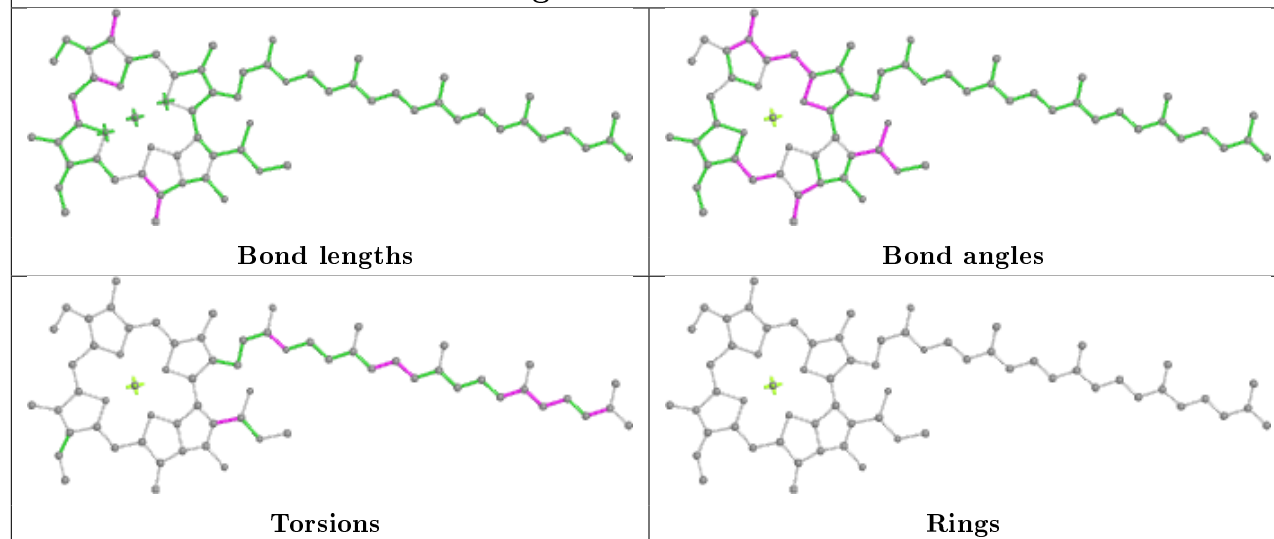
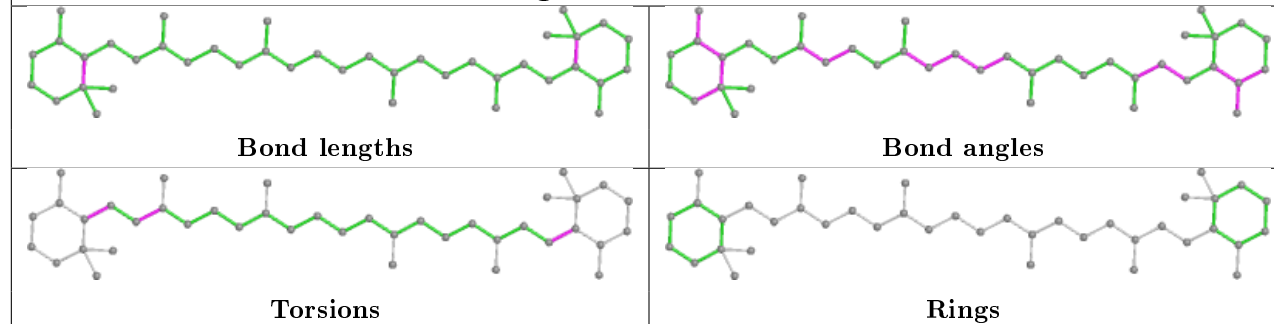
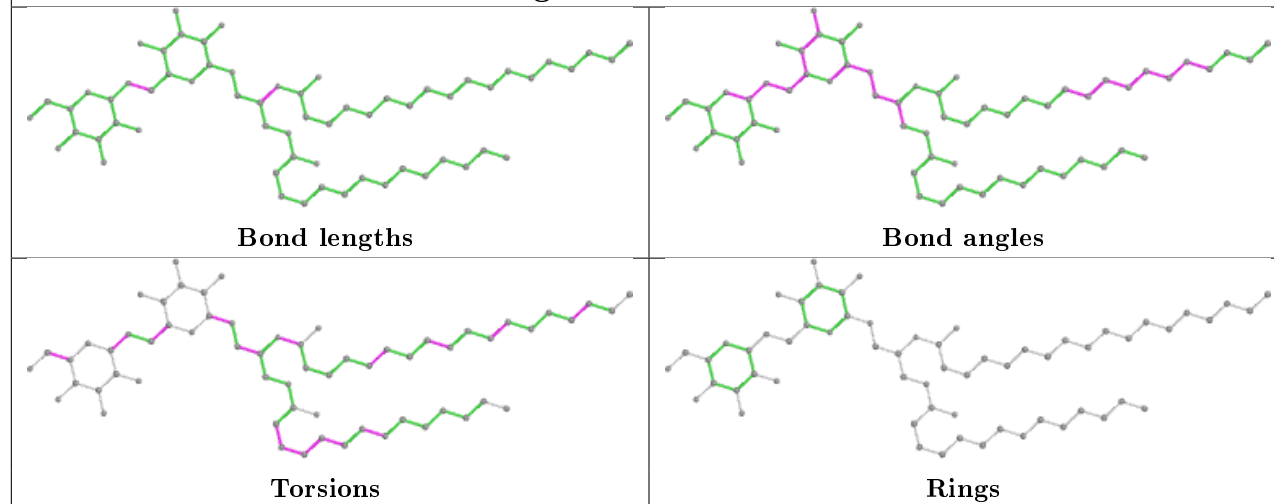


## Ligand PL9 D 405



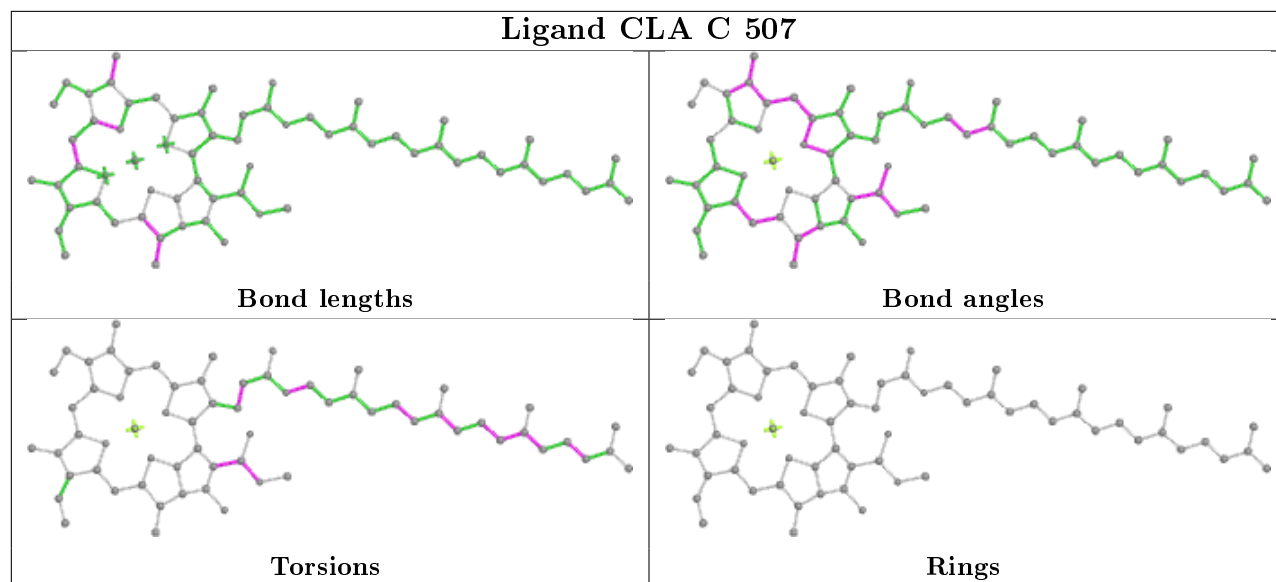
## Ligand BCR B 619



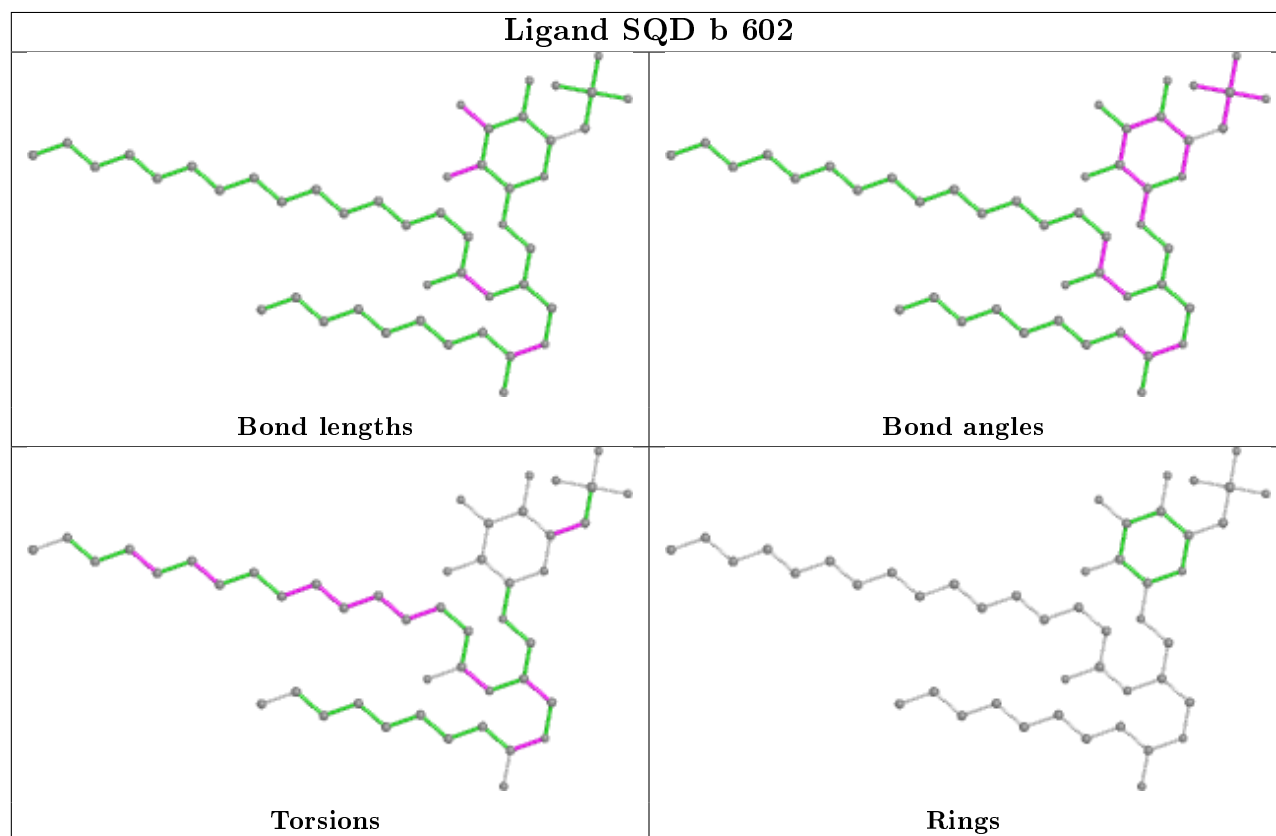
**Ligand CLA C 502****Ligand BCR c 521****Ligand DGD c 516**

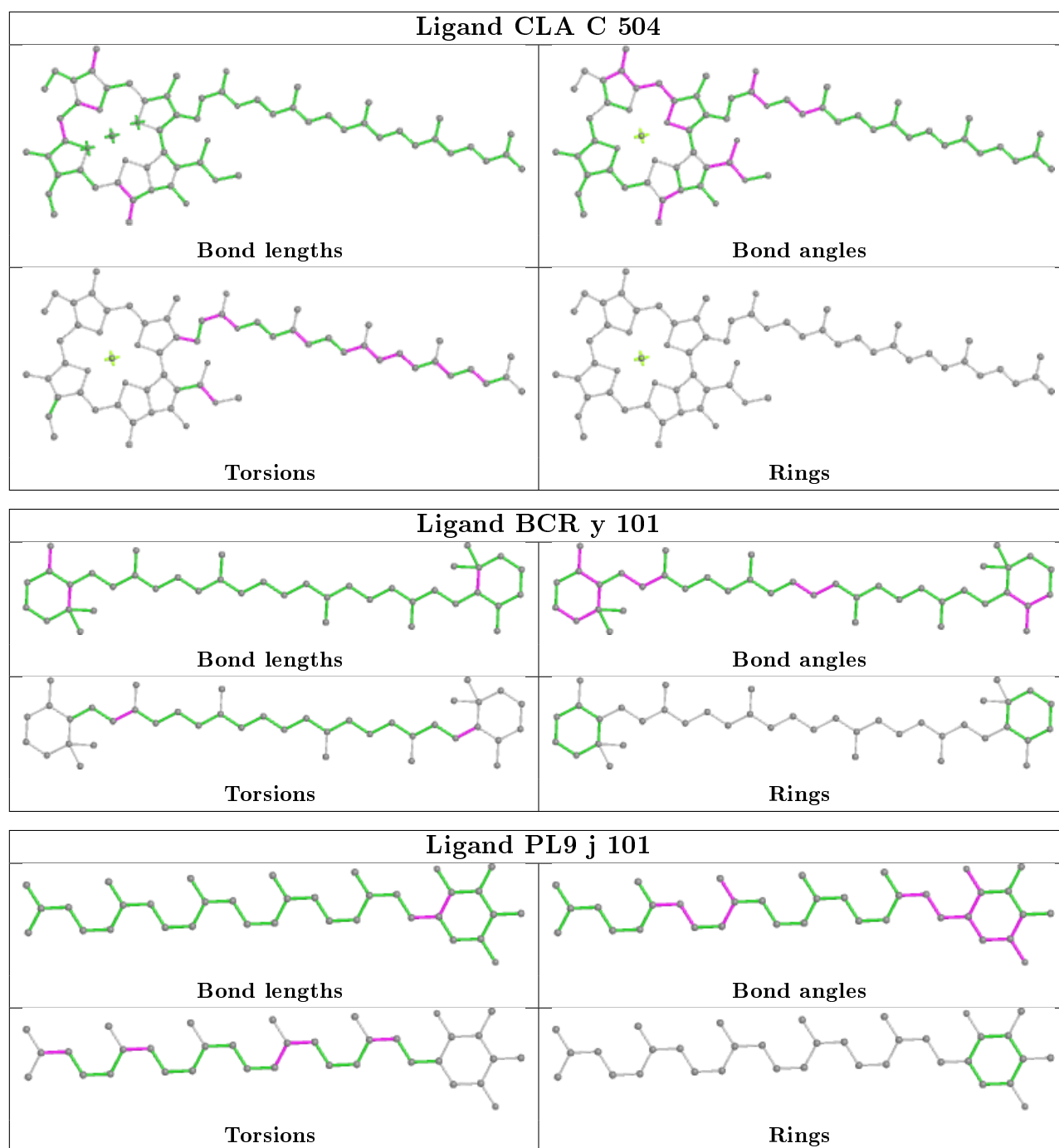


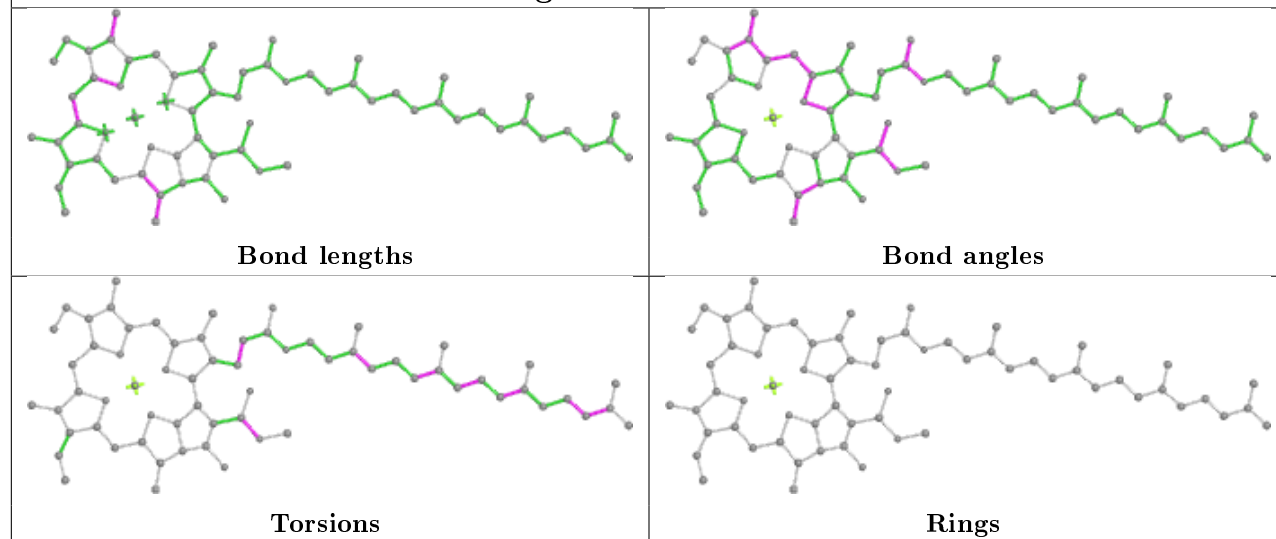
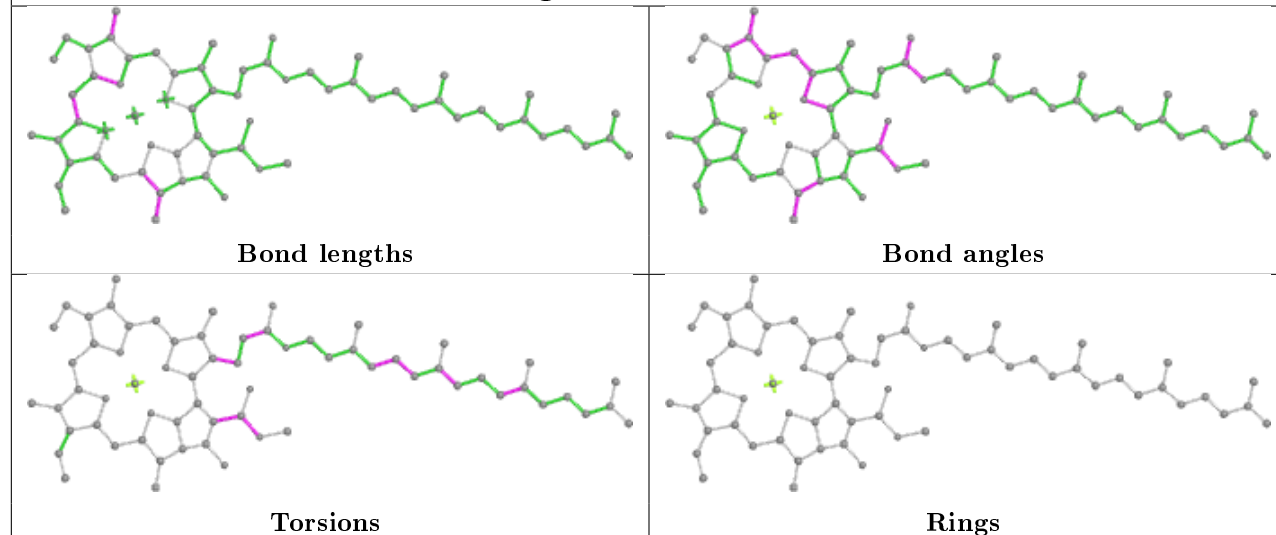
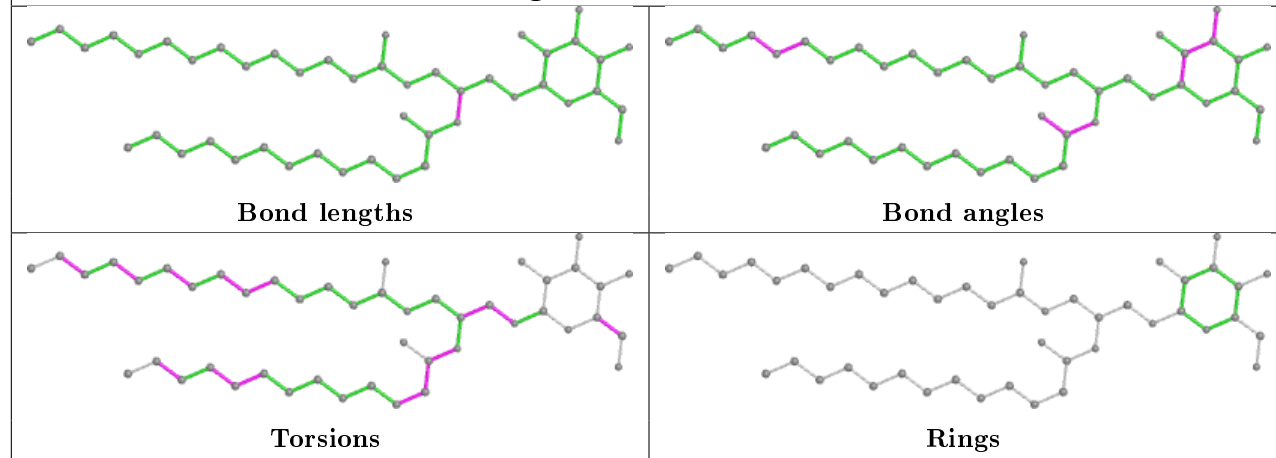
## Ligand CLA C 507



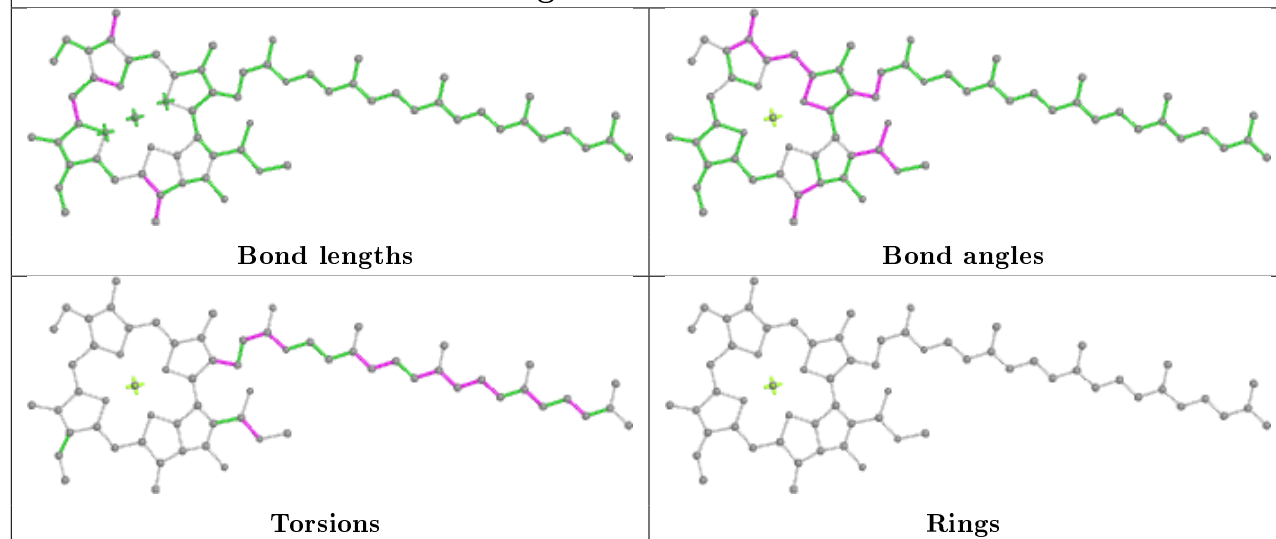
## Ligand SQD b 602



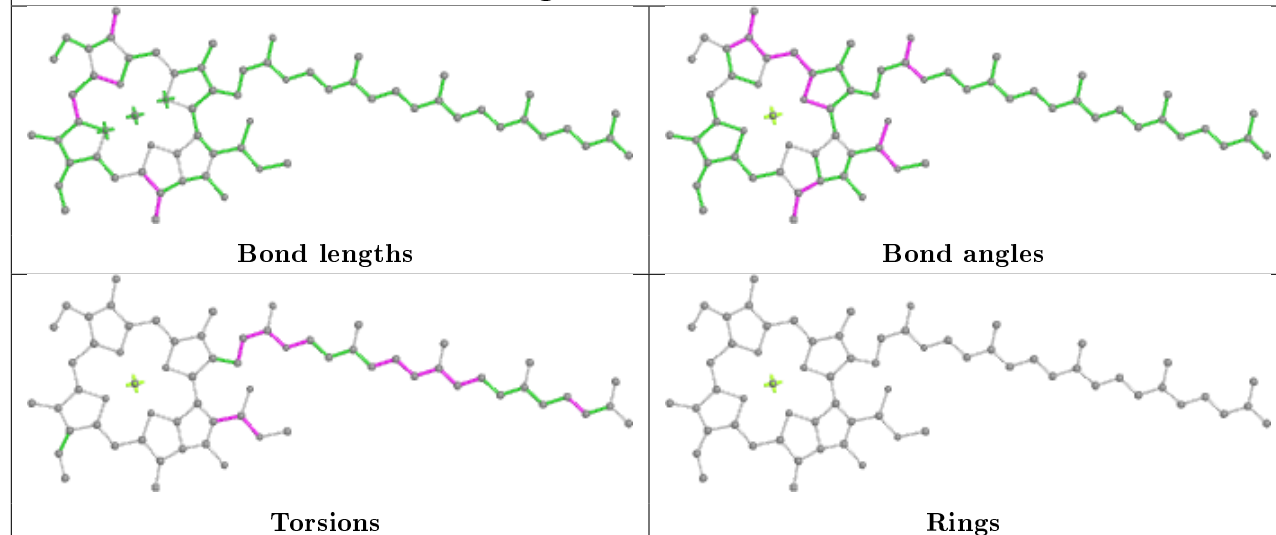


**Ligand CLA b 607****Ligand CLA c 506****Ligand LMG D 409**

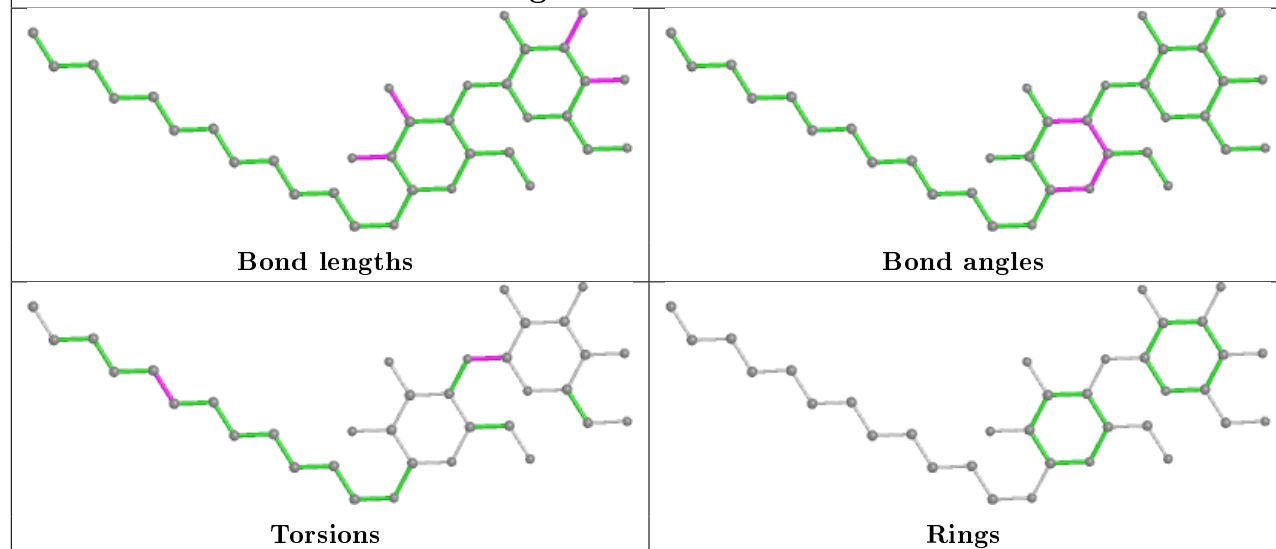
## Ligand CLA c 504

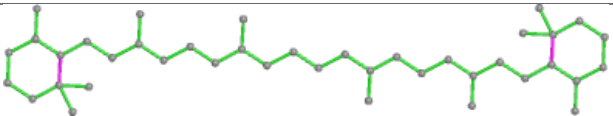
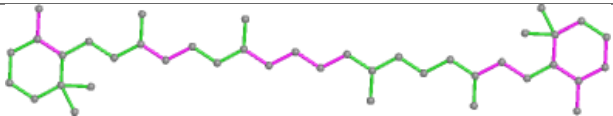
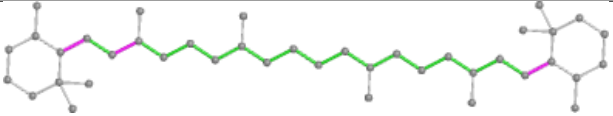
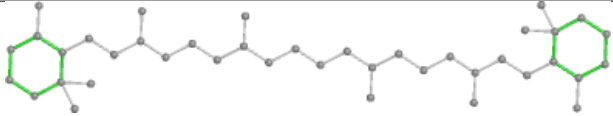


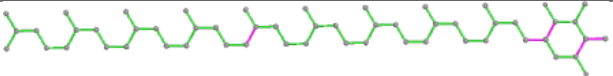
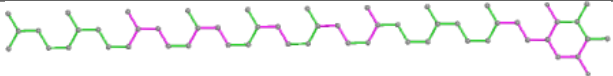
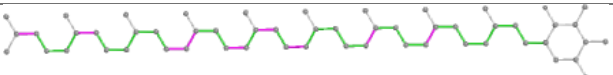
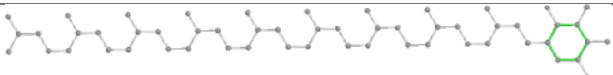
## Ligand CLA c 508

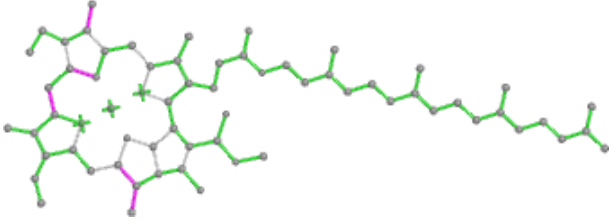
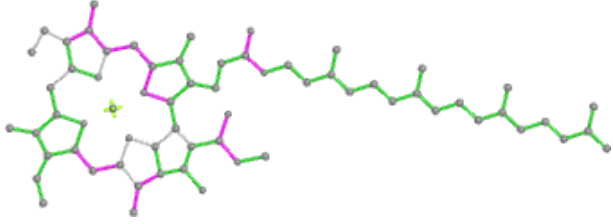
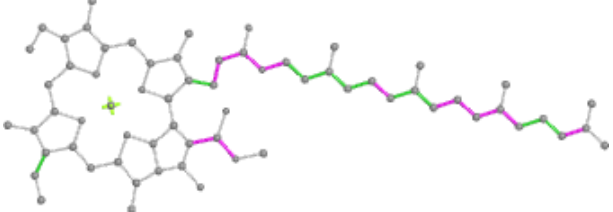
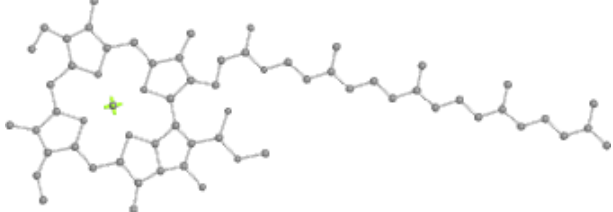


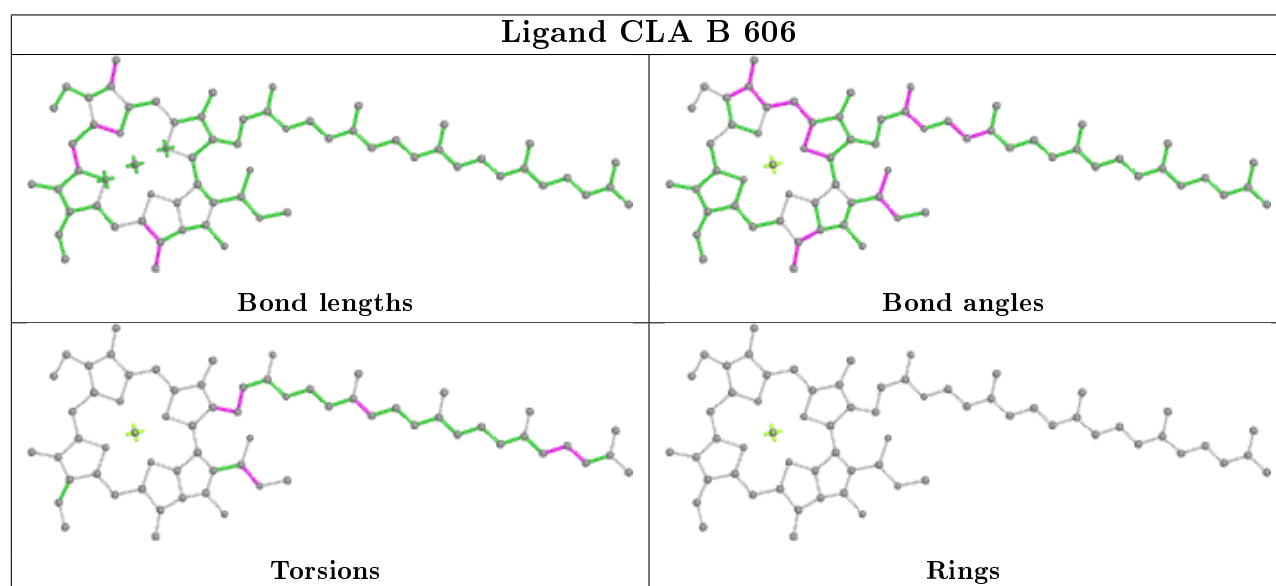
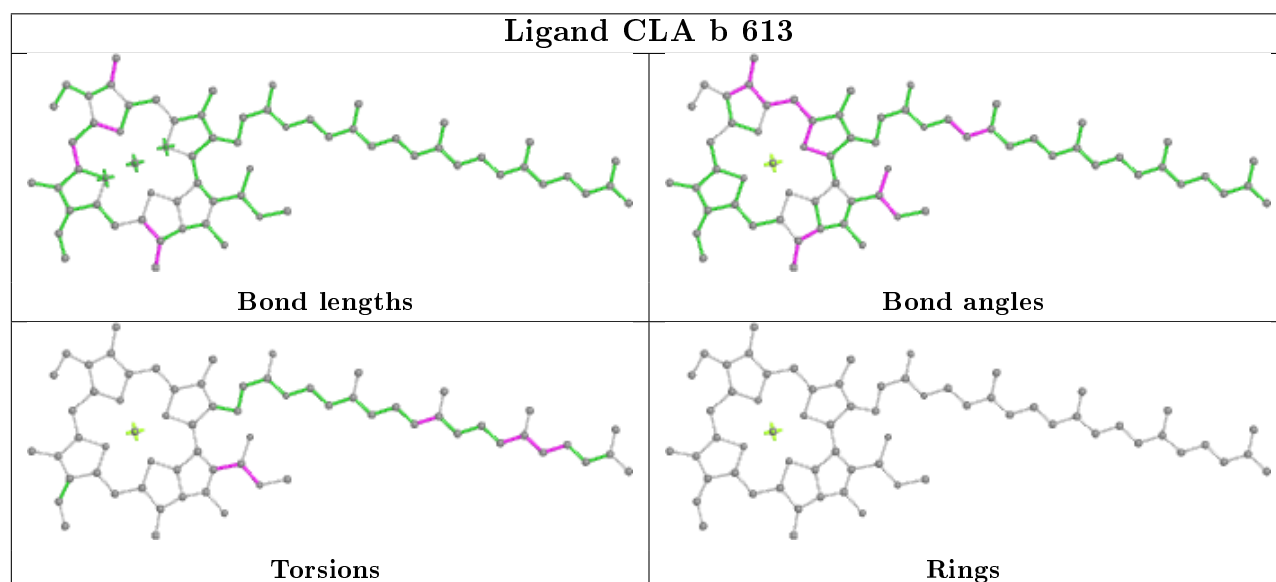
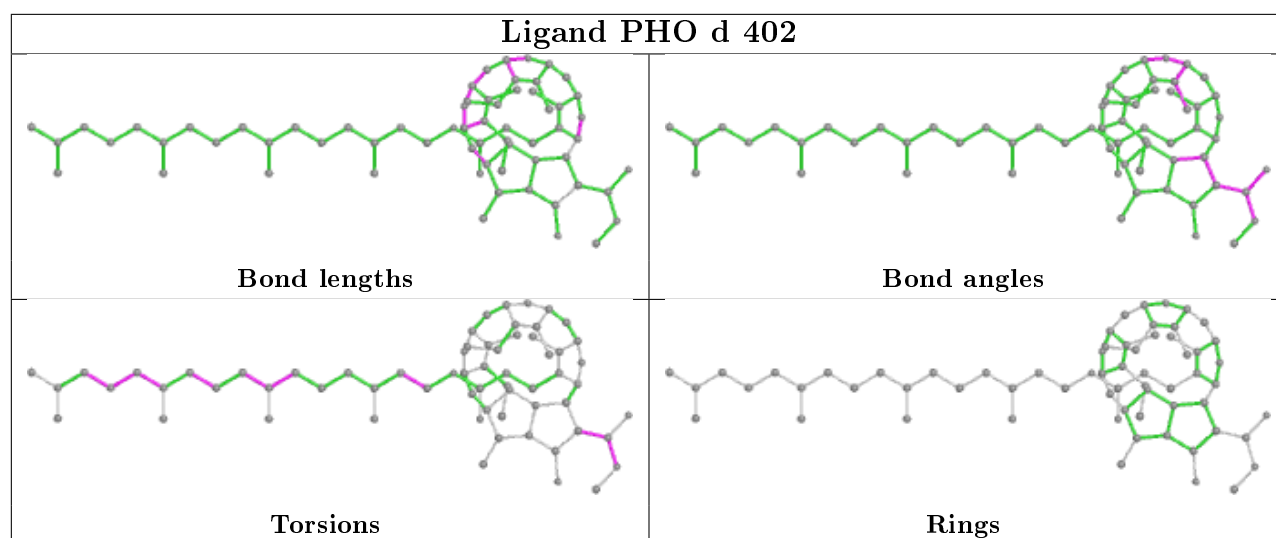
## Ligand LMT B 624

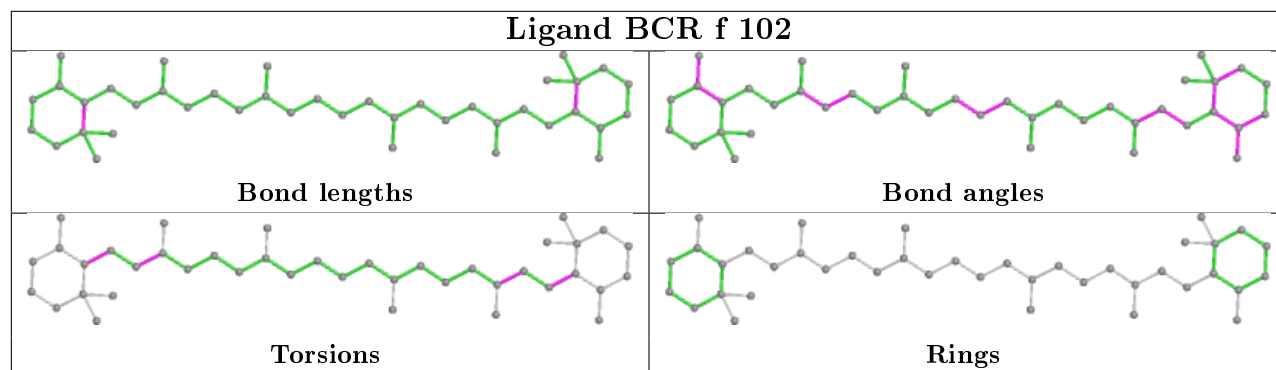
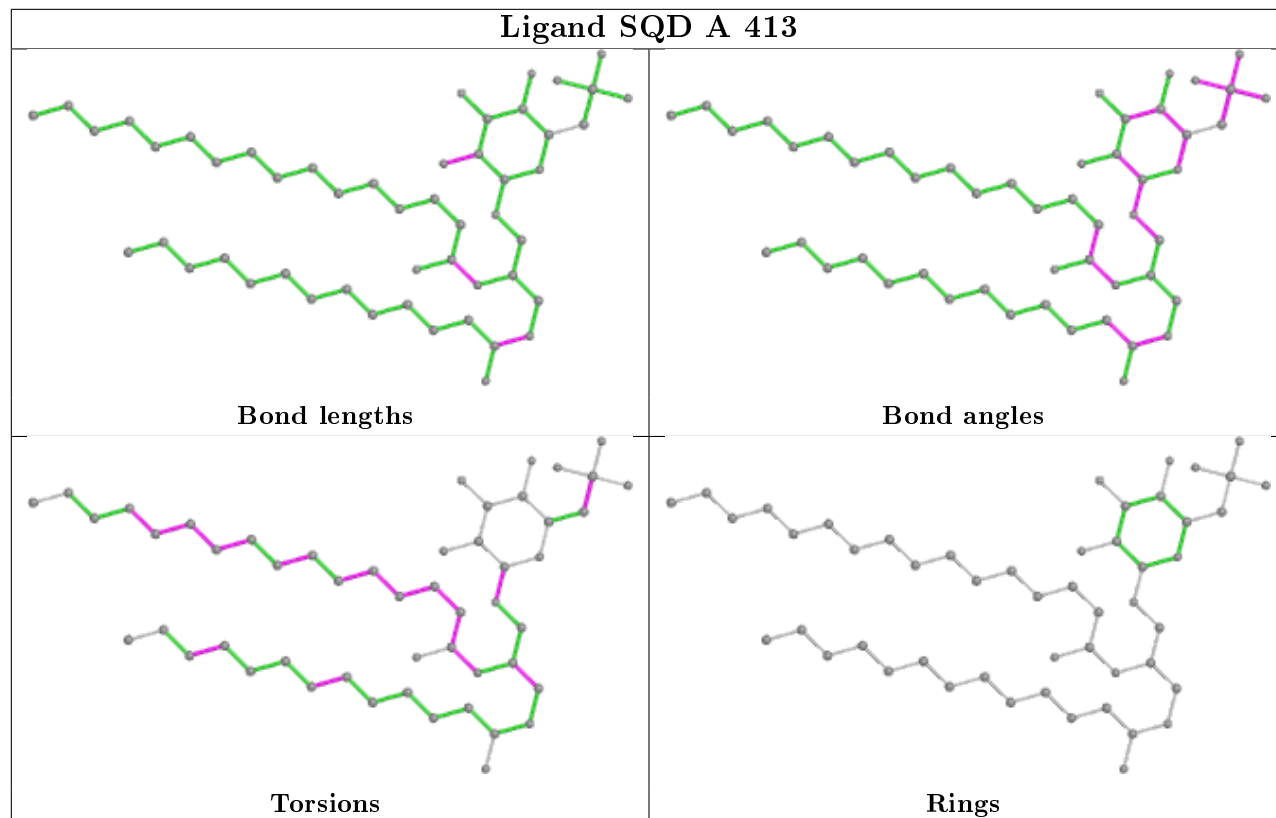
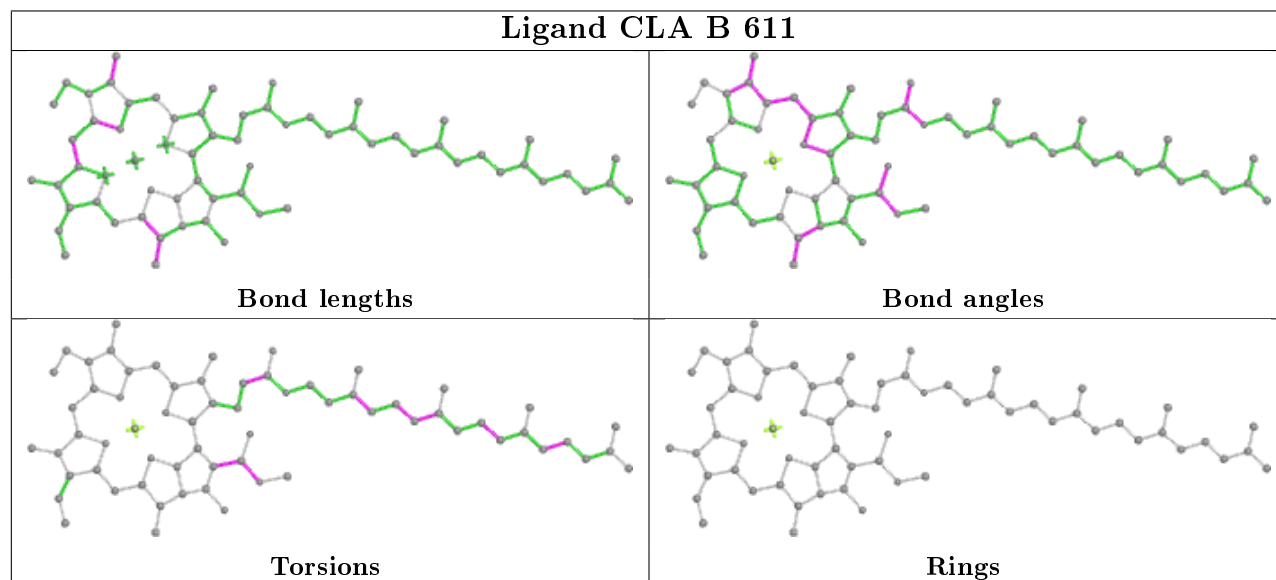


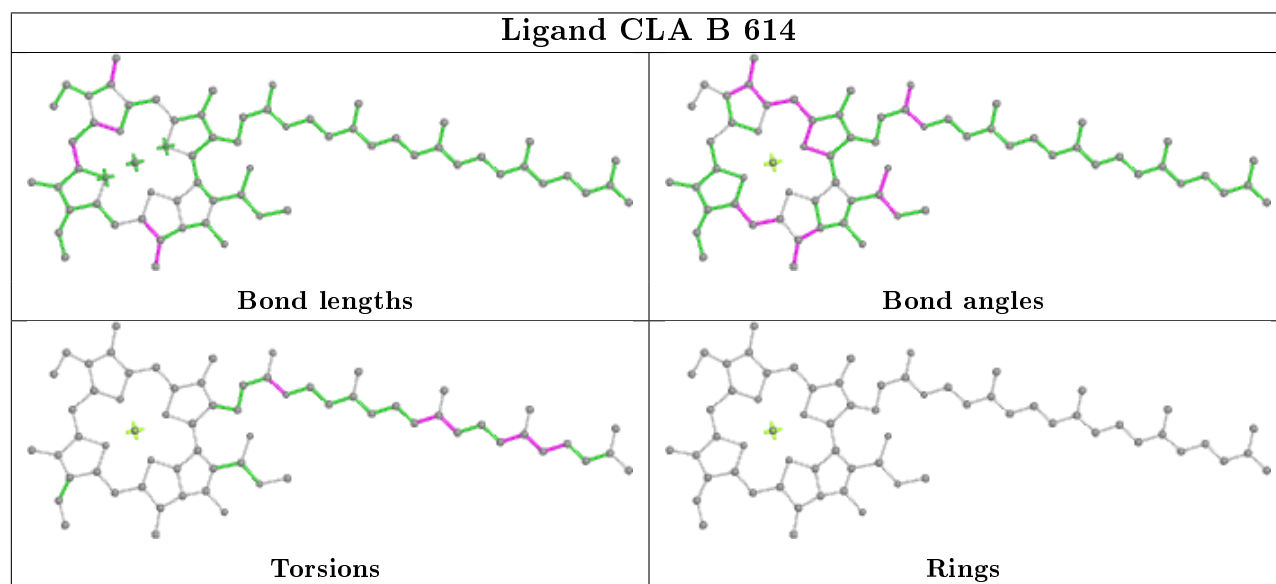
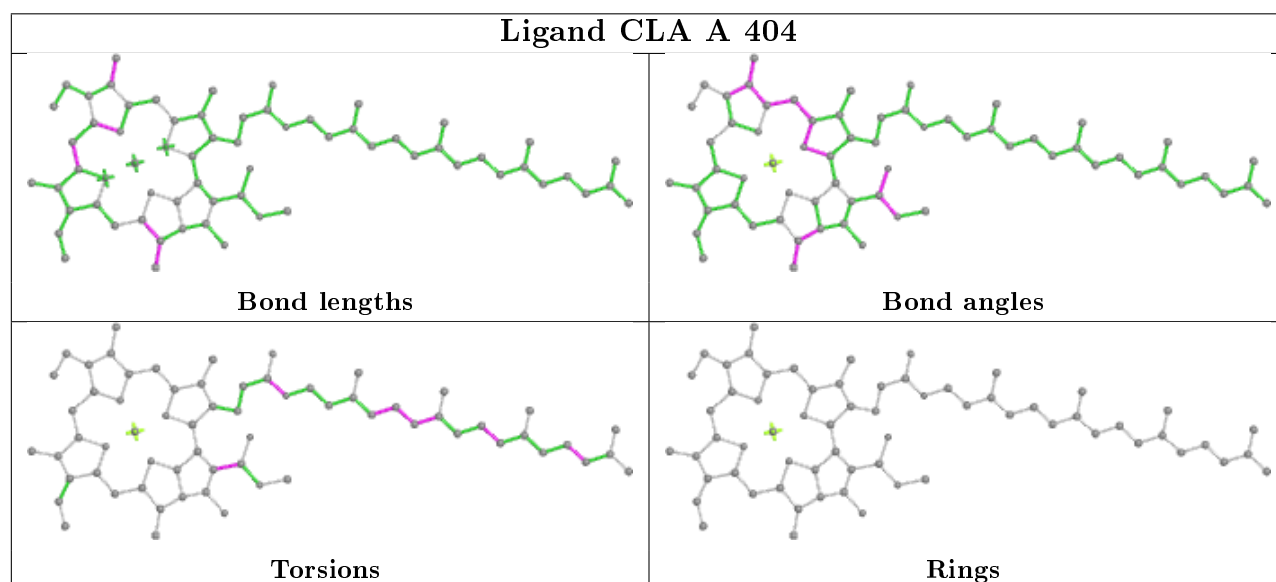
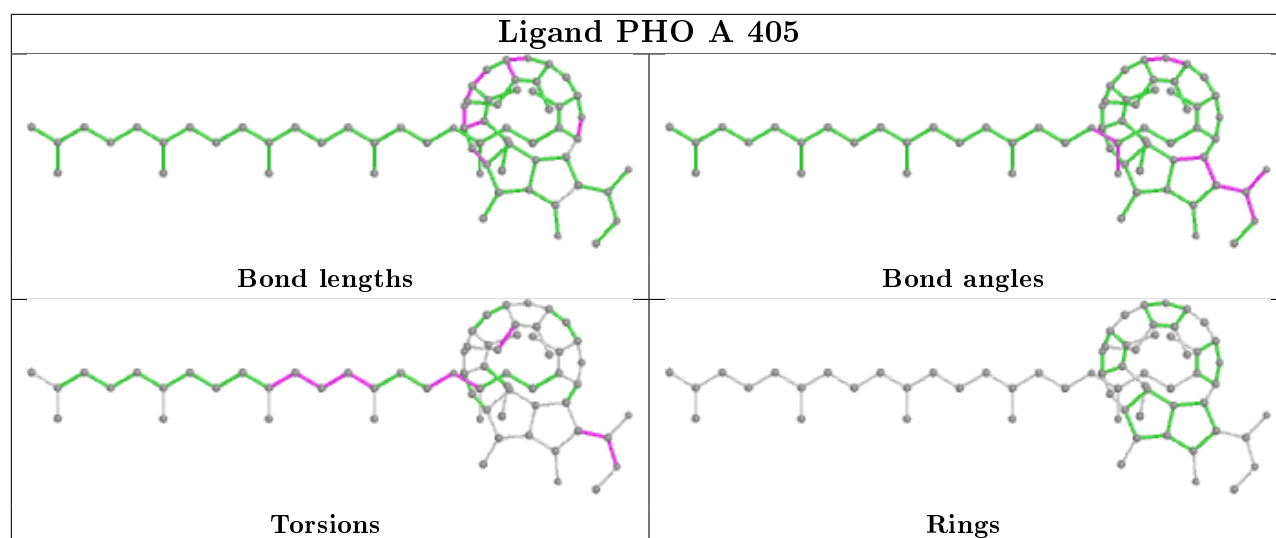
Ligand BCR C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

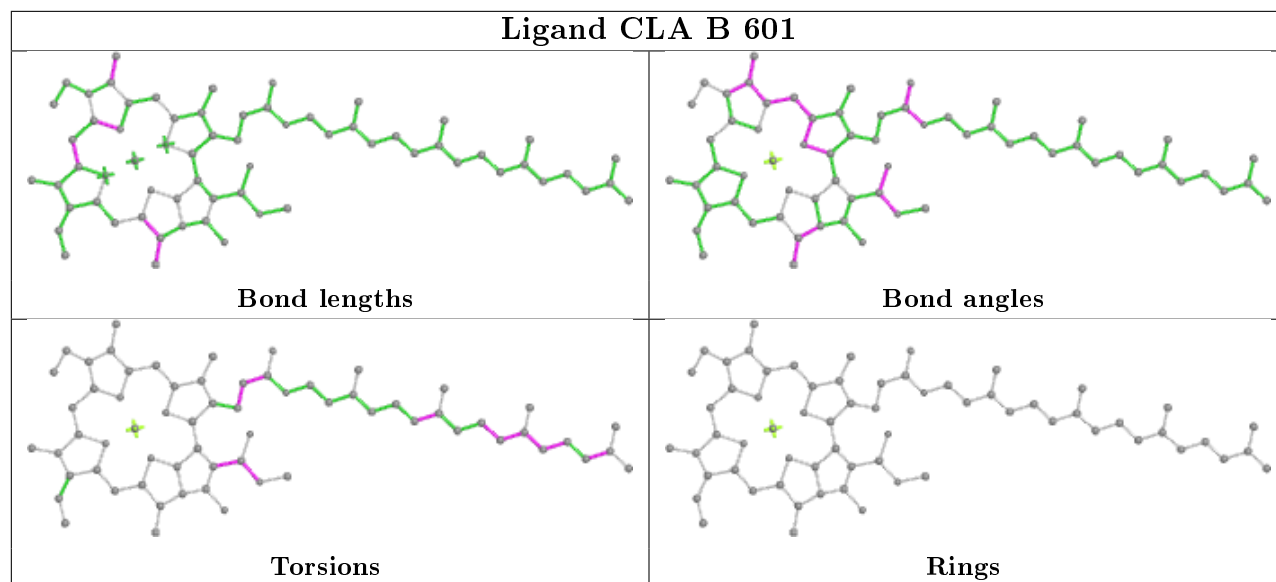


**Ligand BCR f 102****Ligand SQD A 413****Ligand CLA B 611**

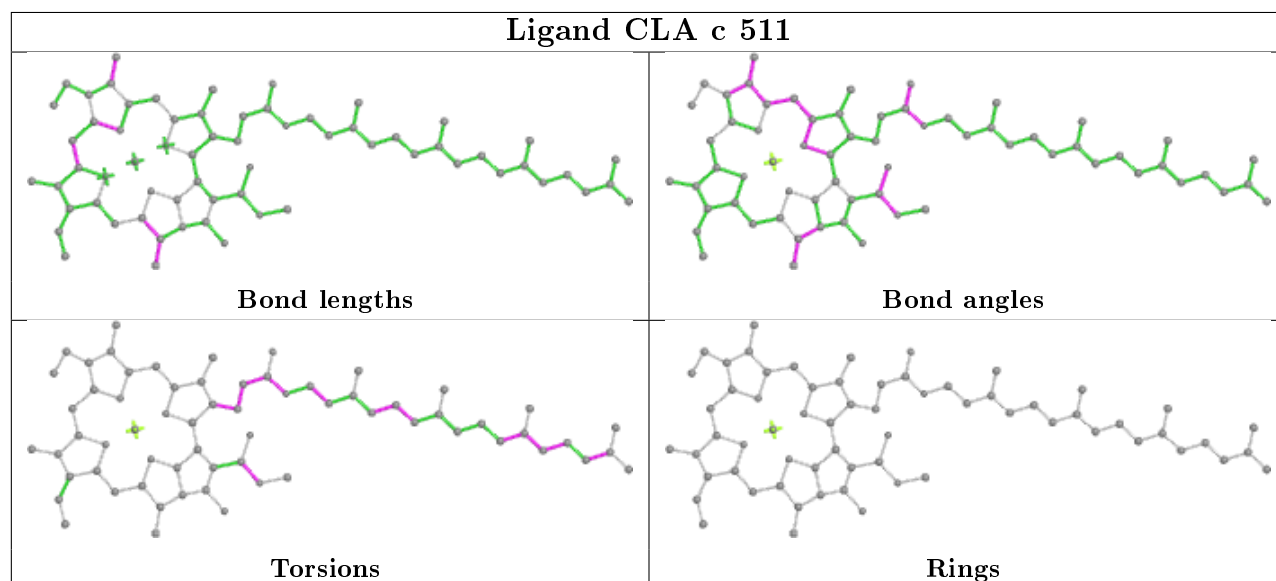




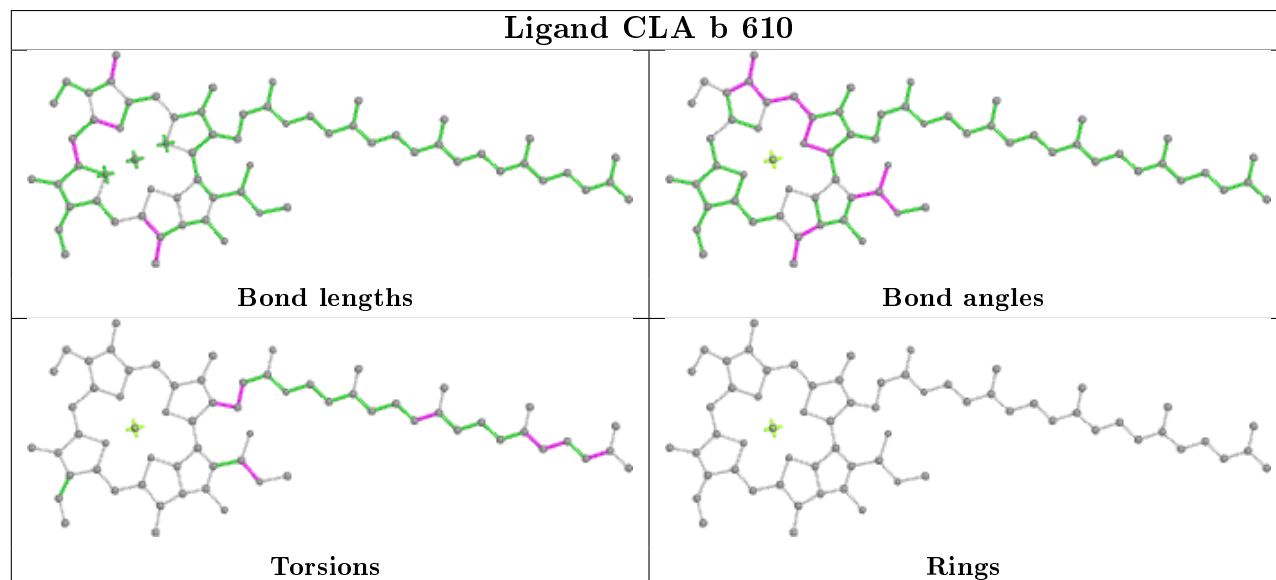
## Ligand CLA B 601

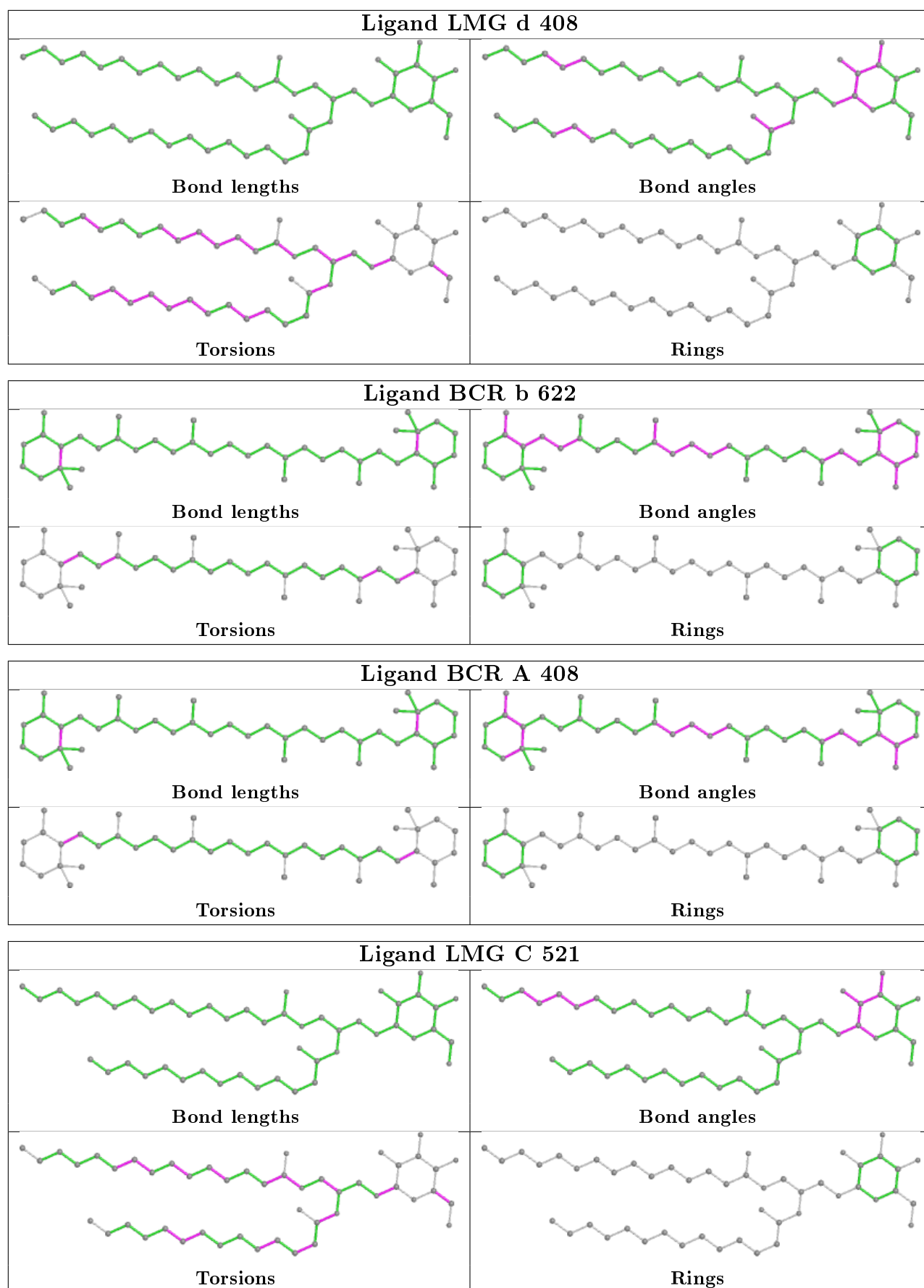


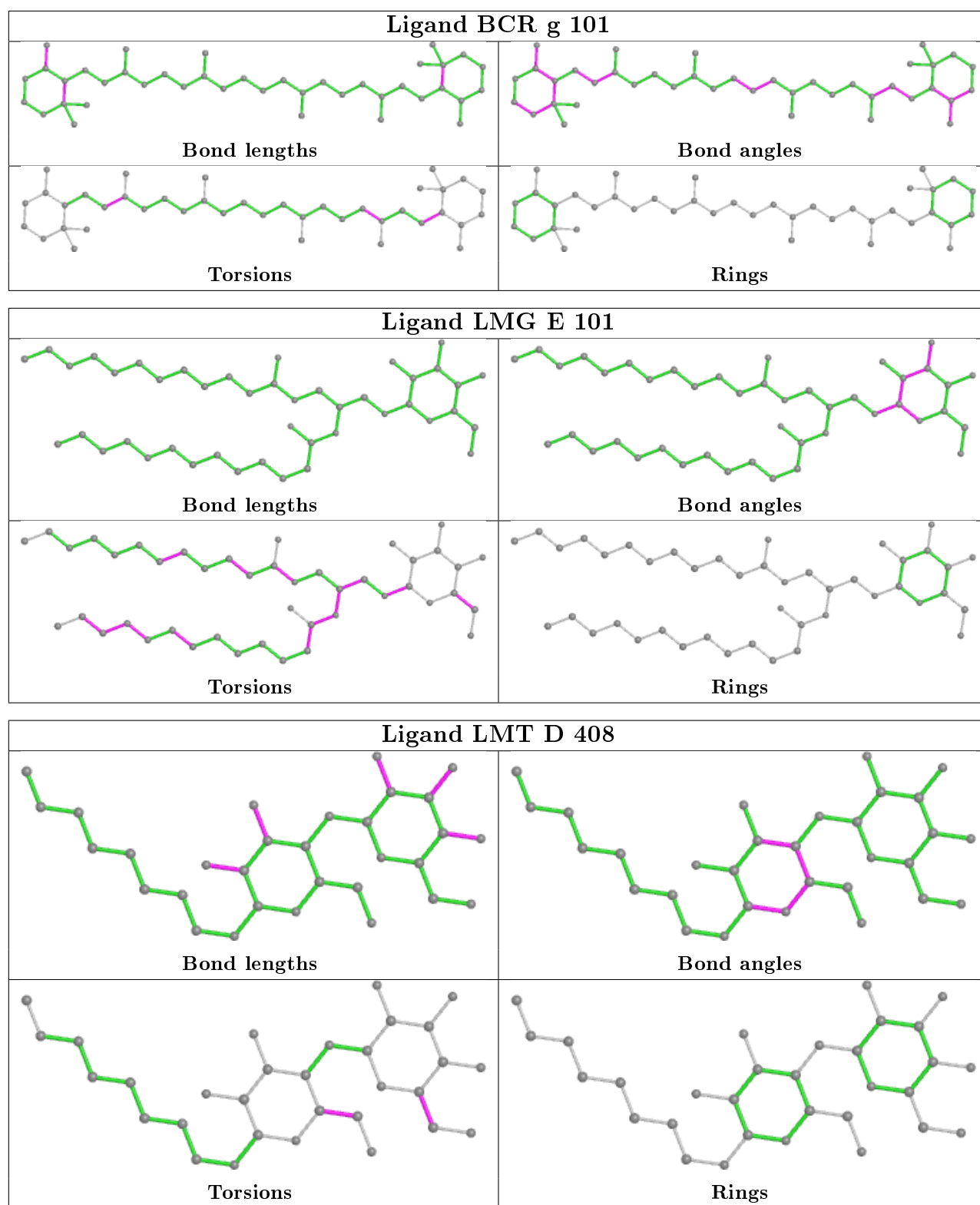
## Ligand CLA c 511



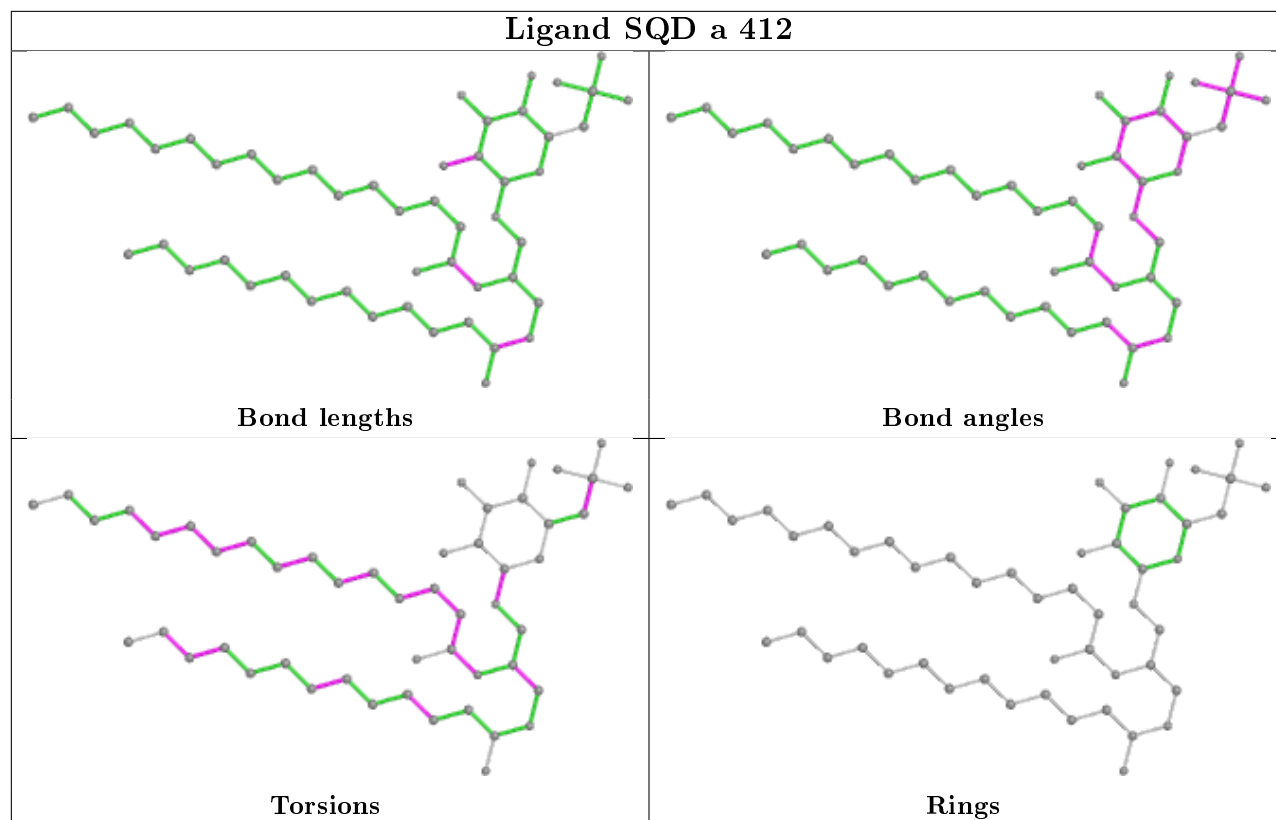
## Ligand CLA b 610



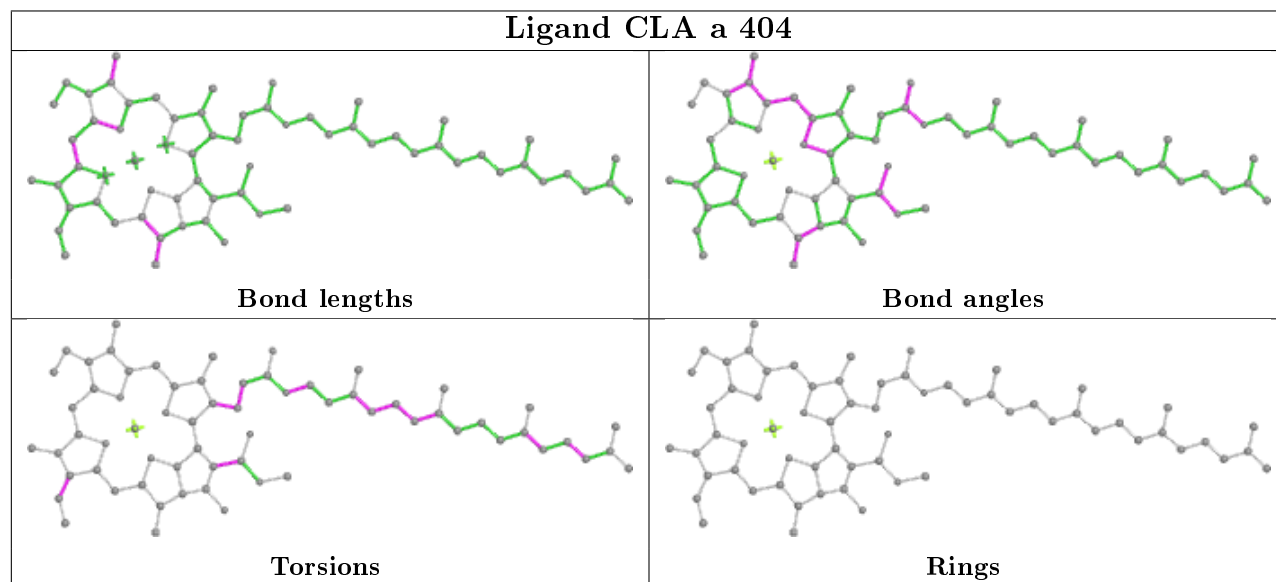


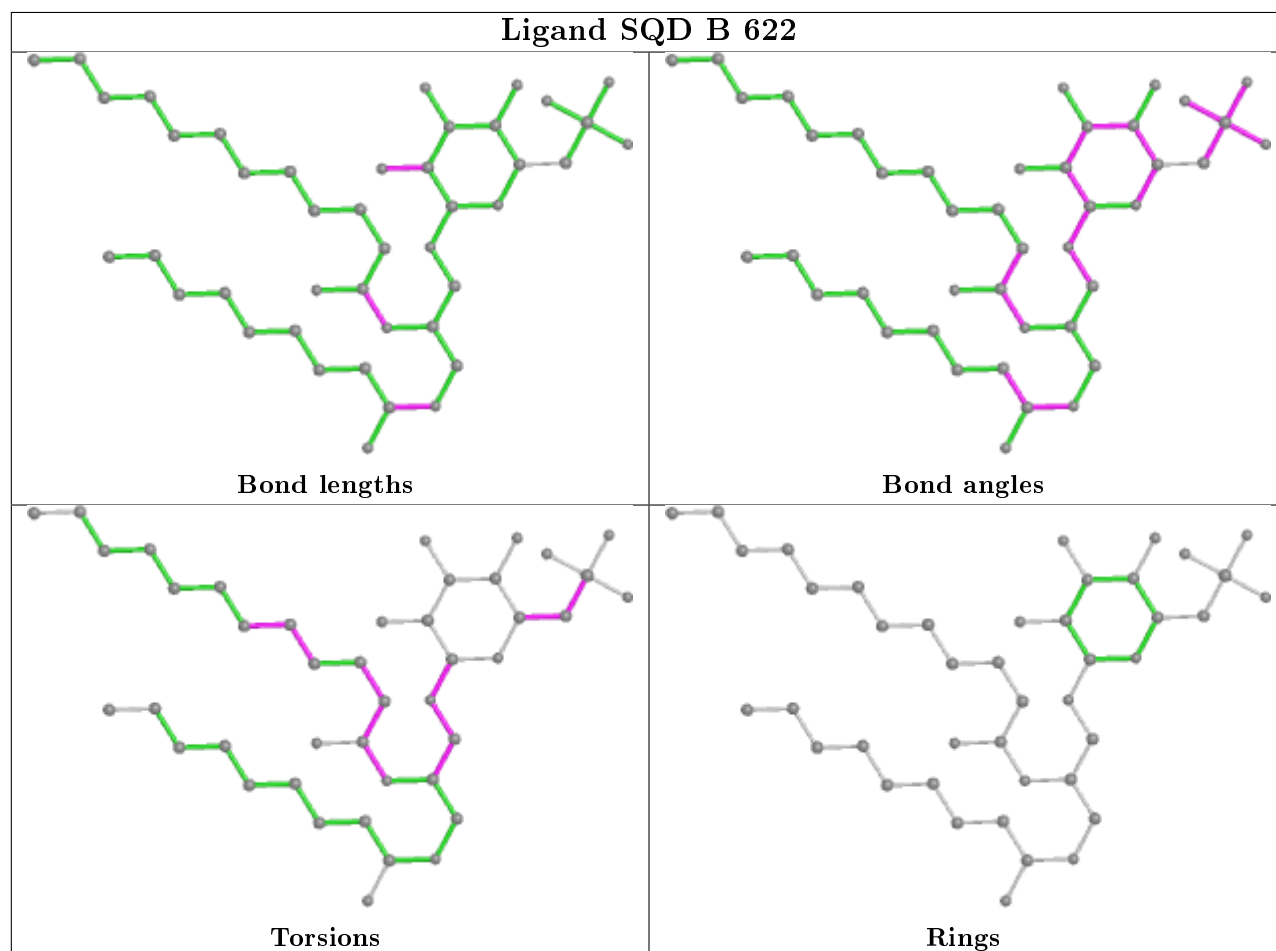
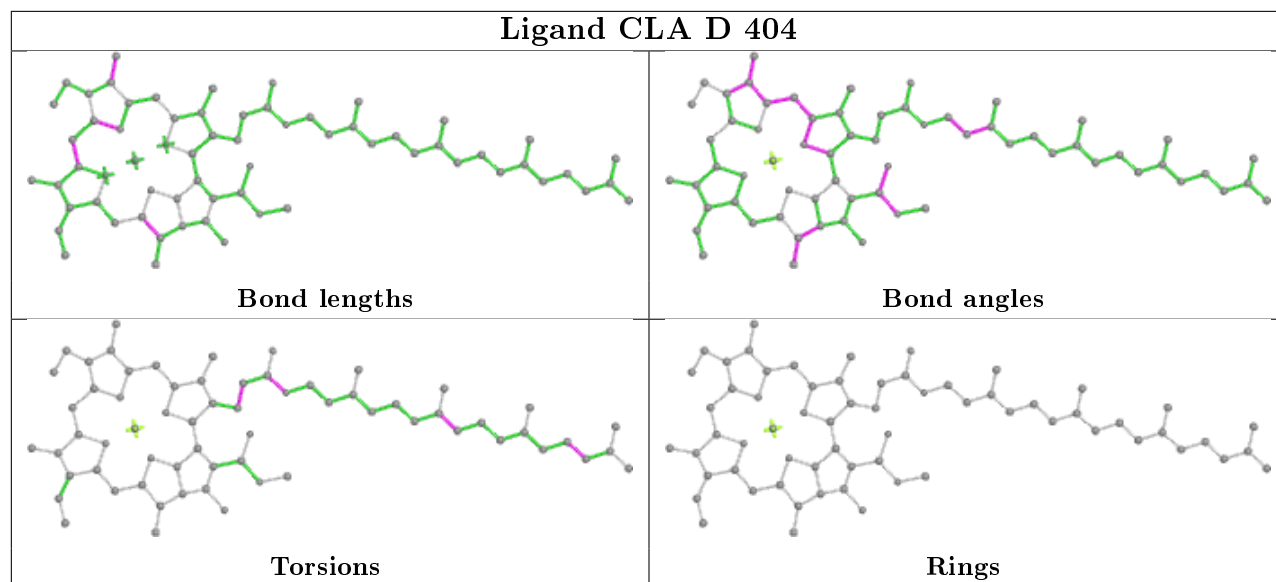


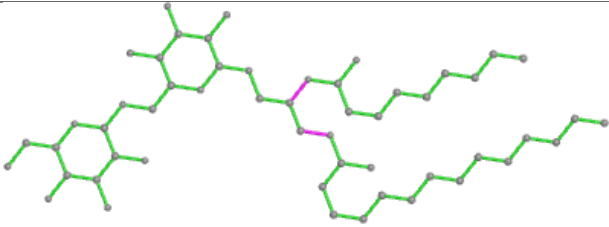
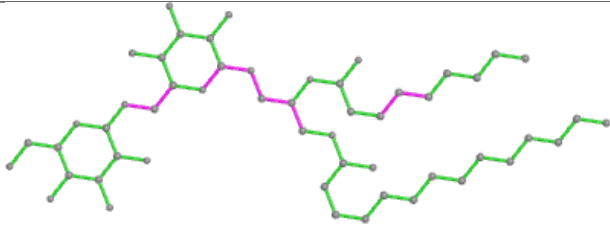
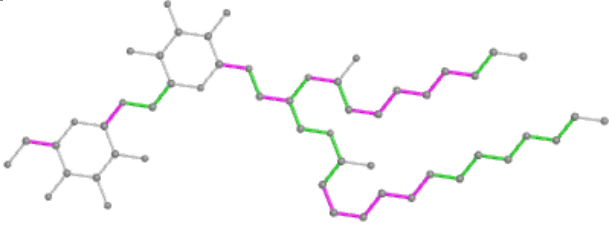
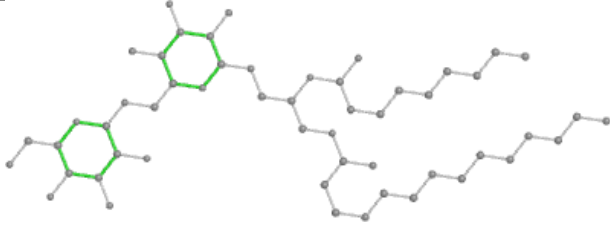
## Ligand SQD a 412

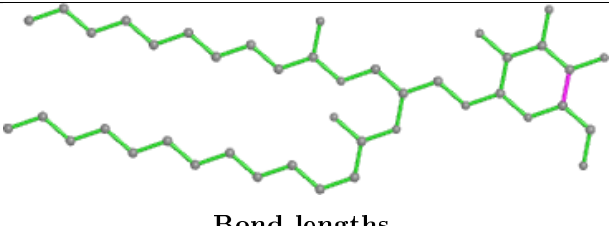
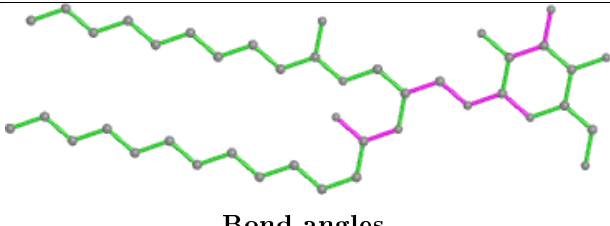
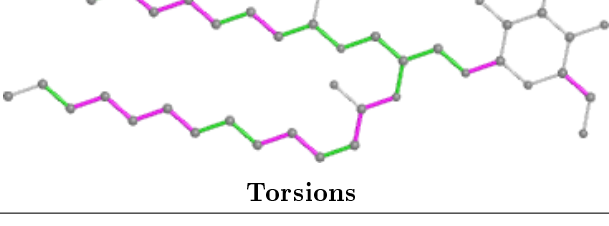
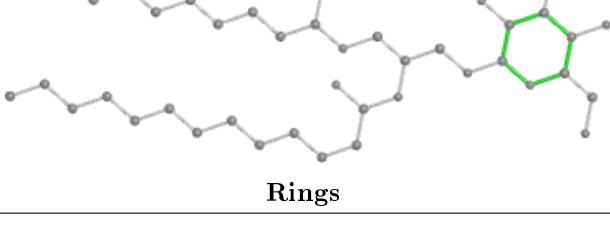


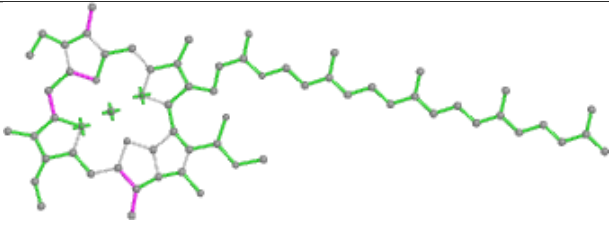
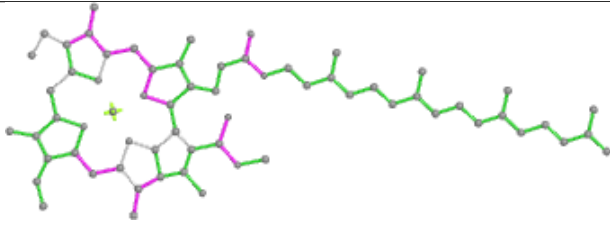
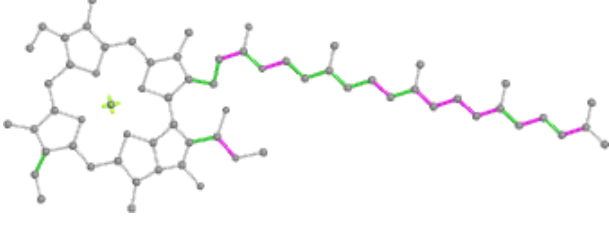
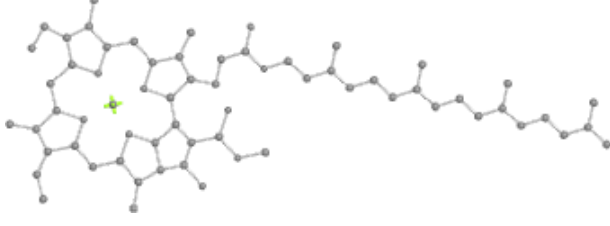
## Ligand CLA a 404

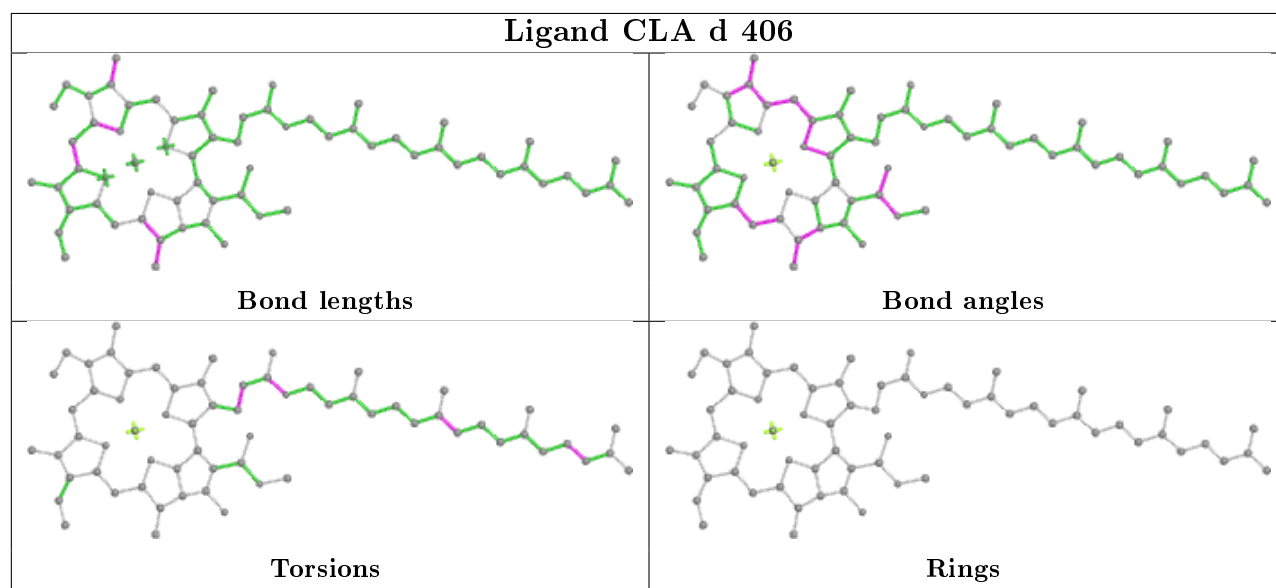
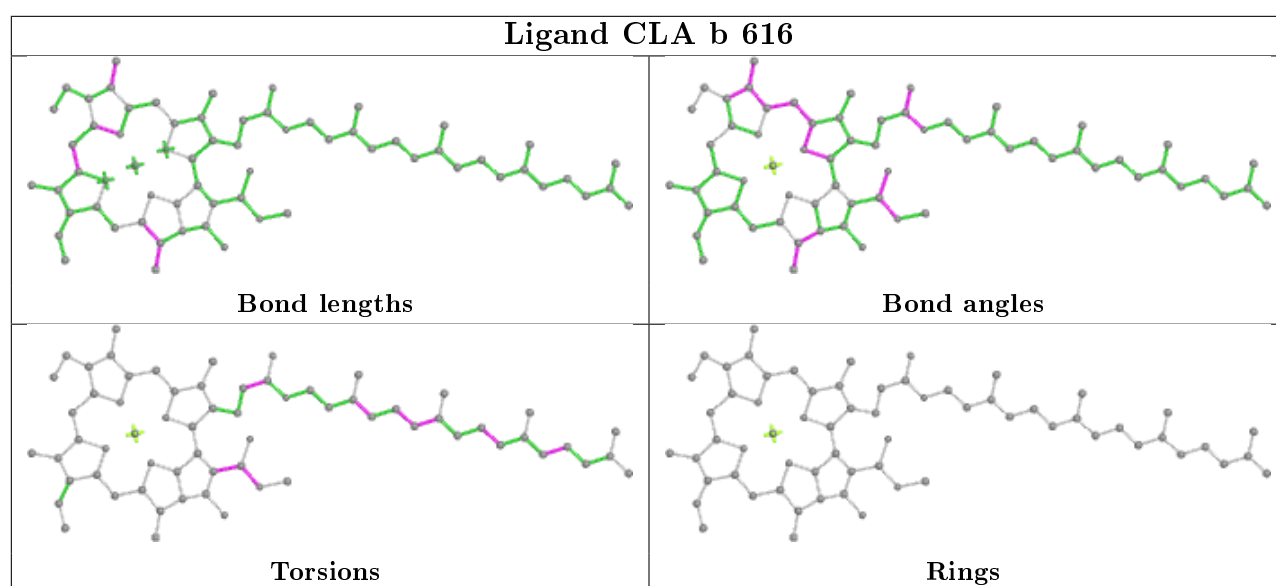
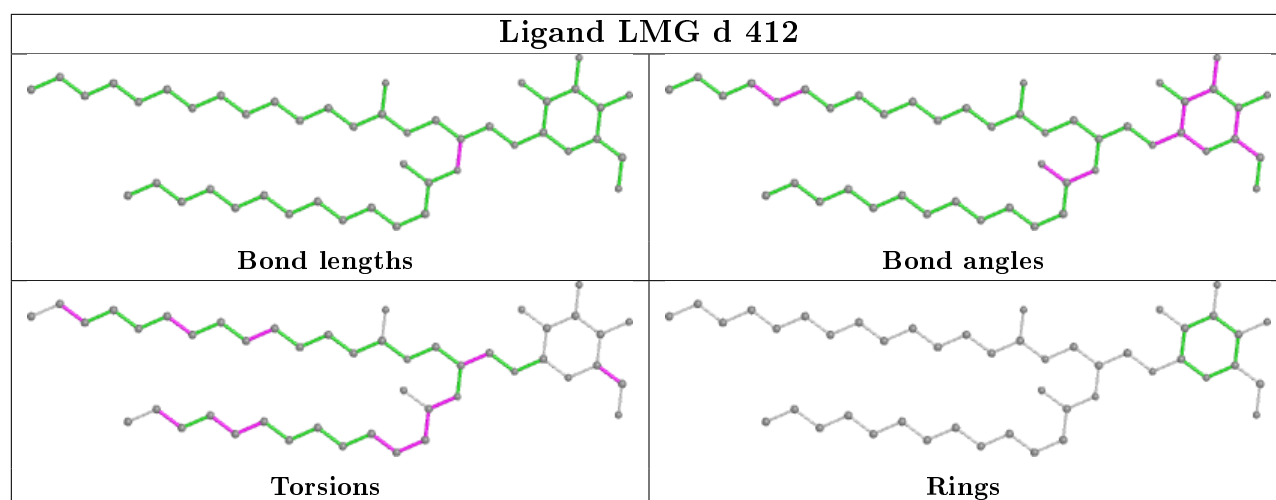


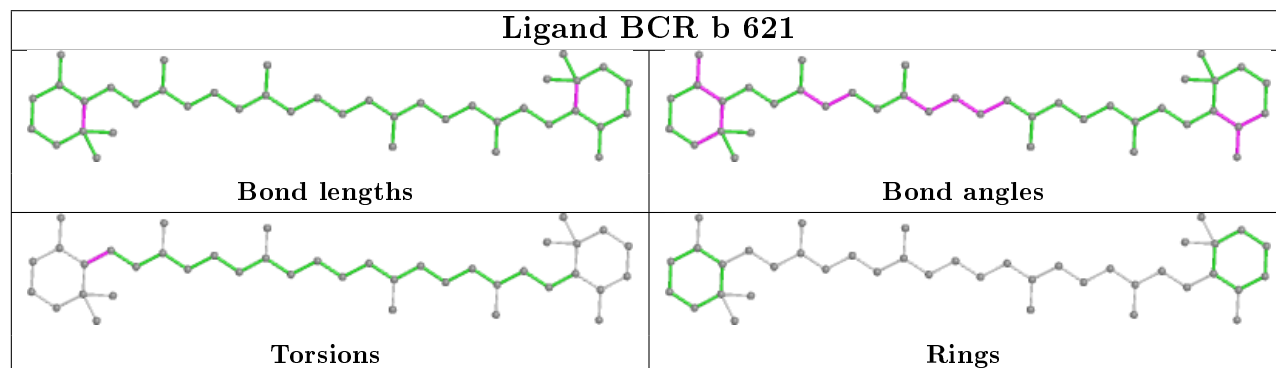
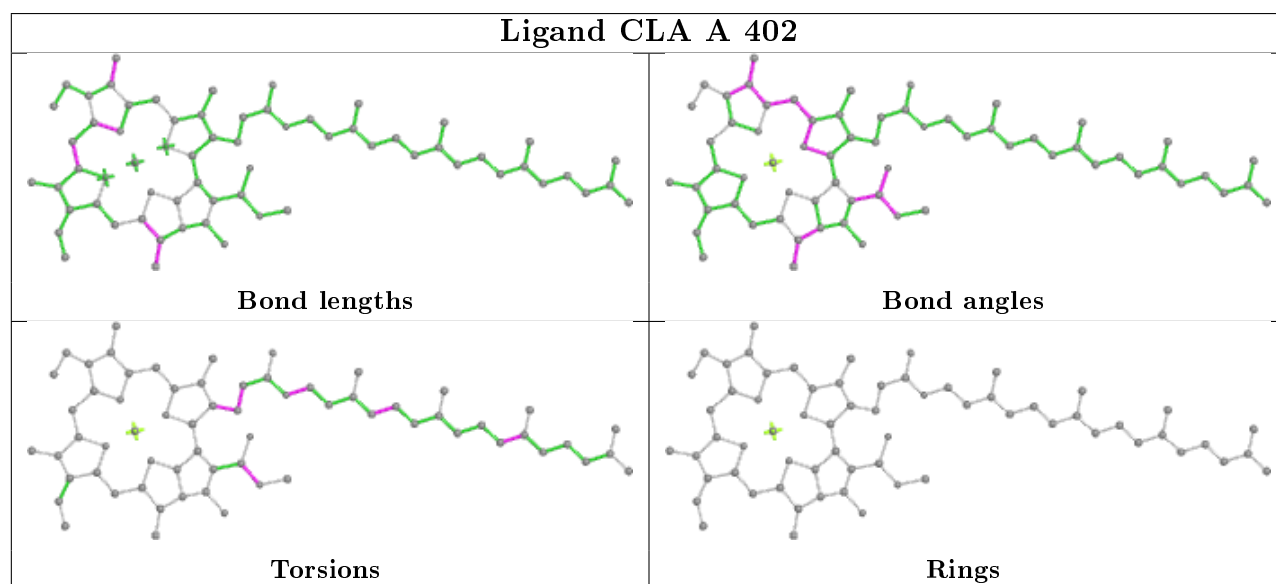
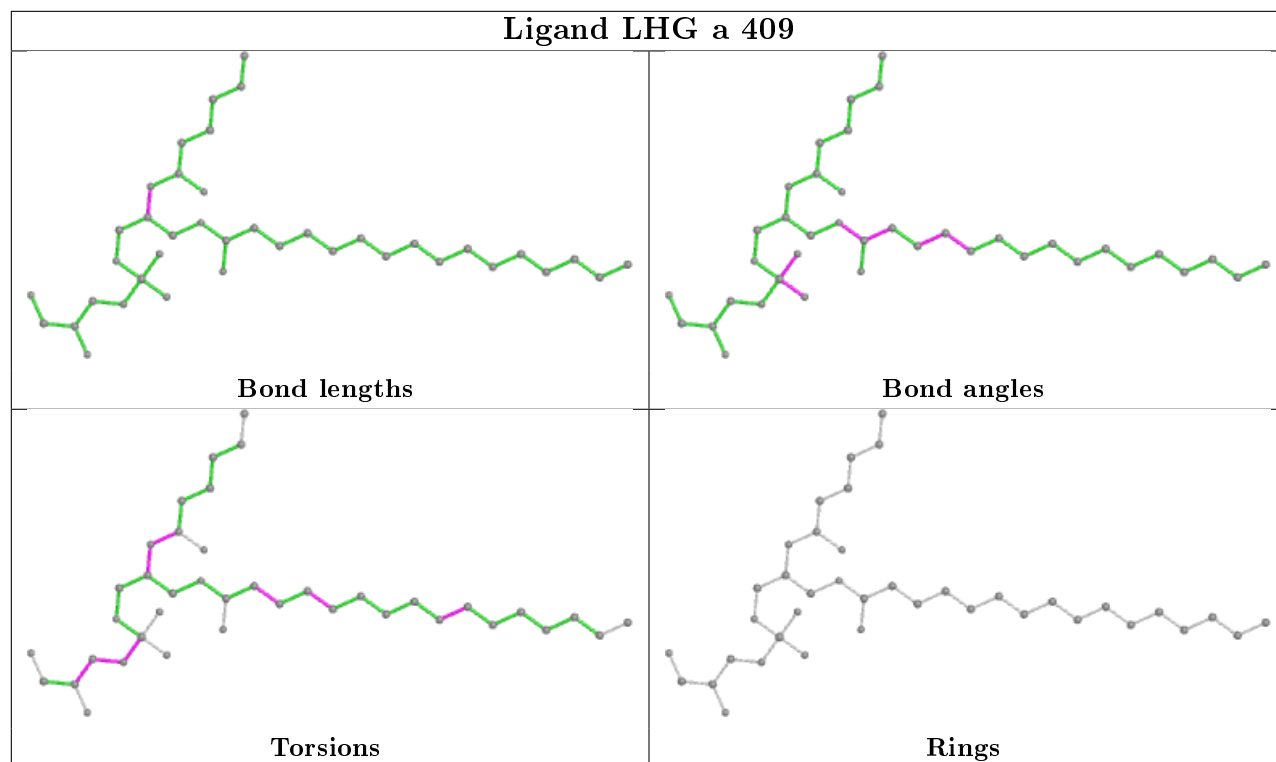


Ligand DGD C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

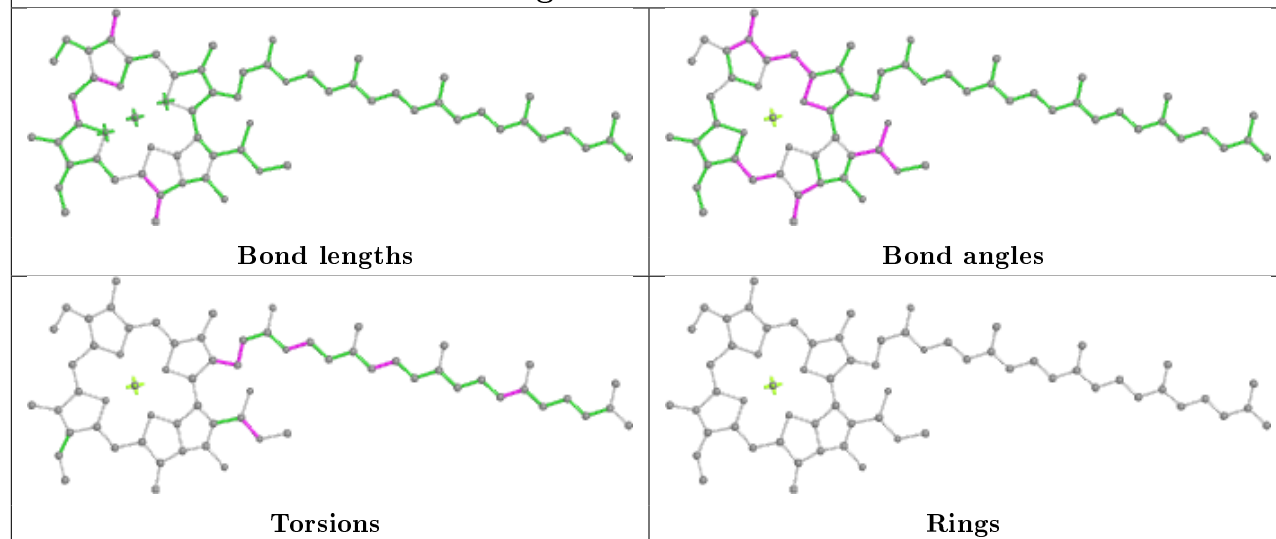
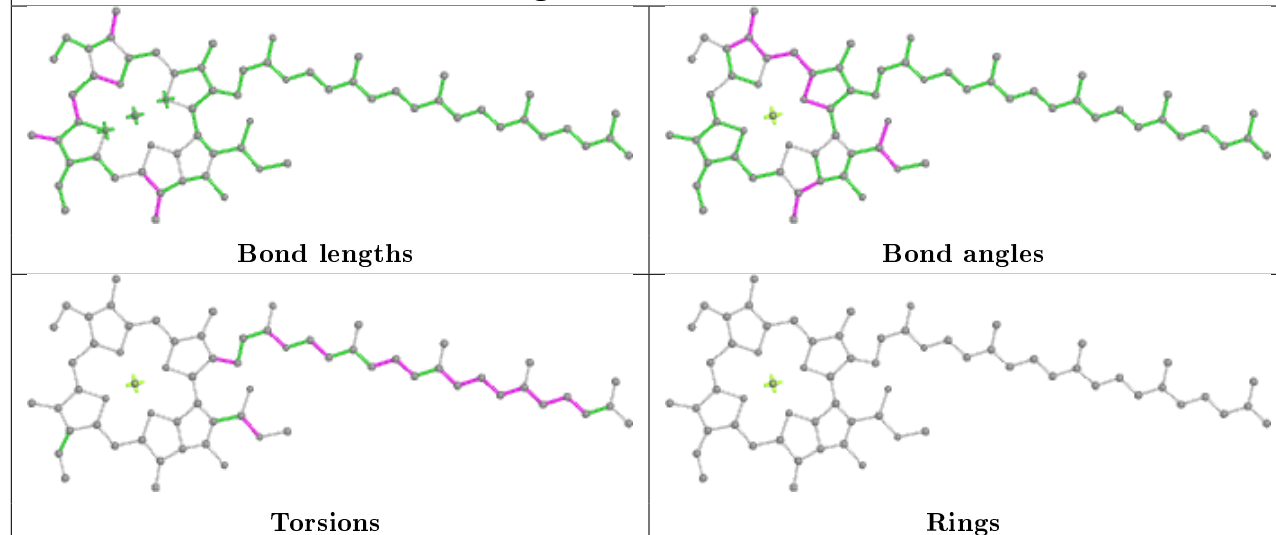
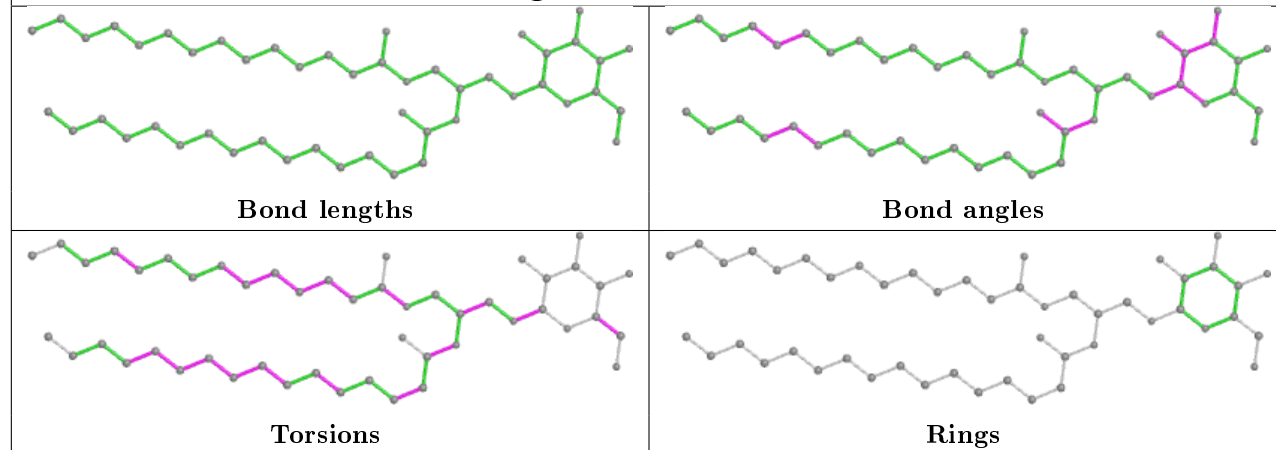
Ligand LMG b 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

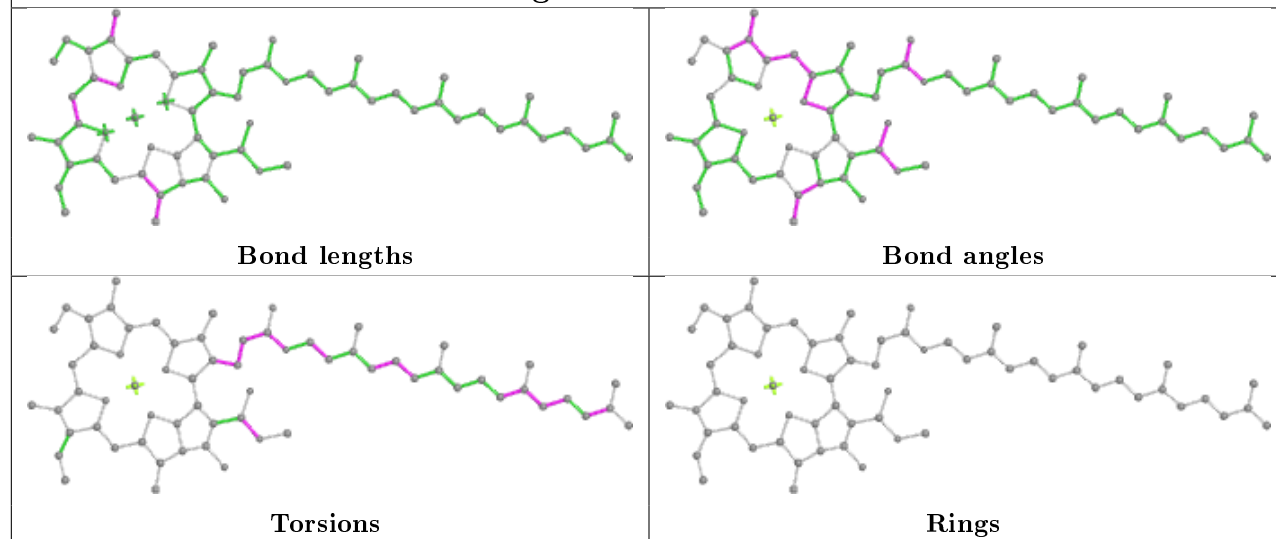
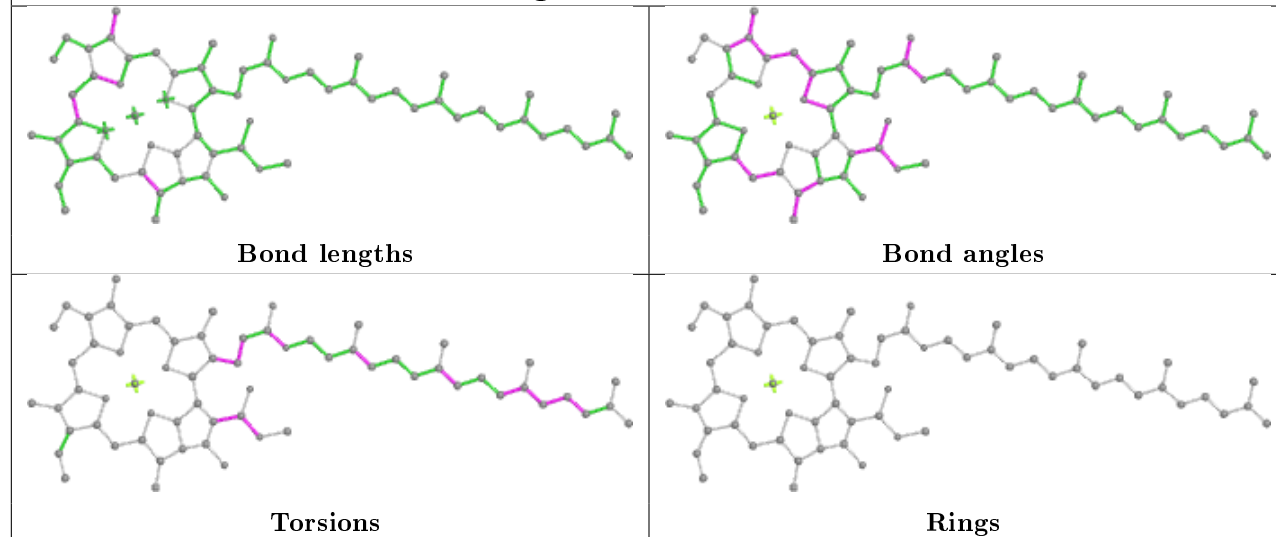
Ligand CLA b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings



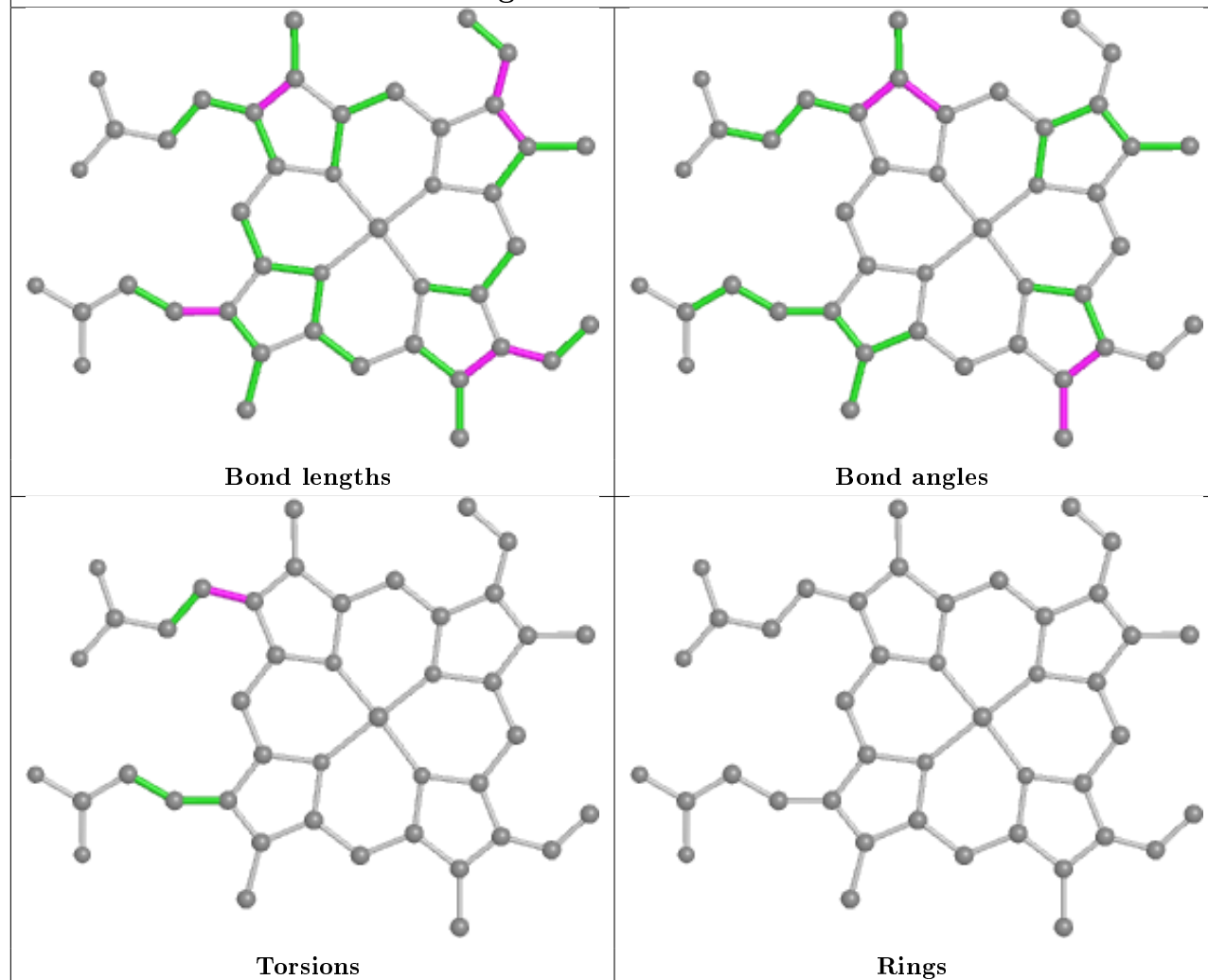




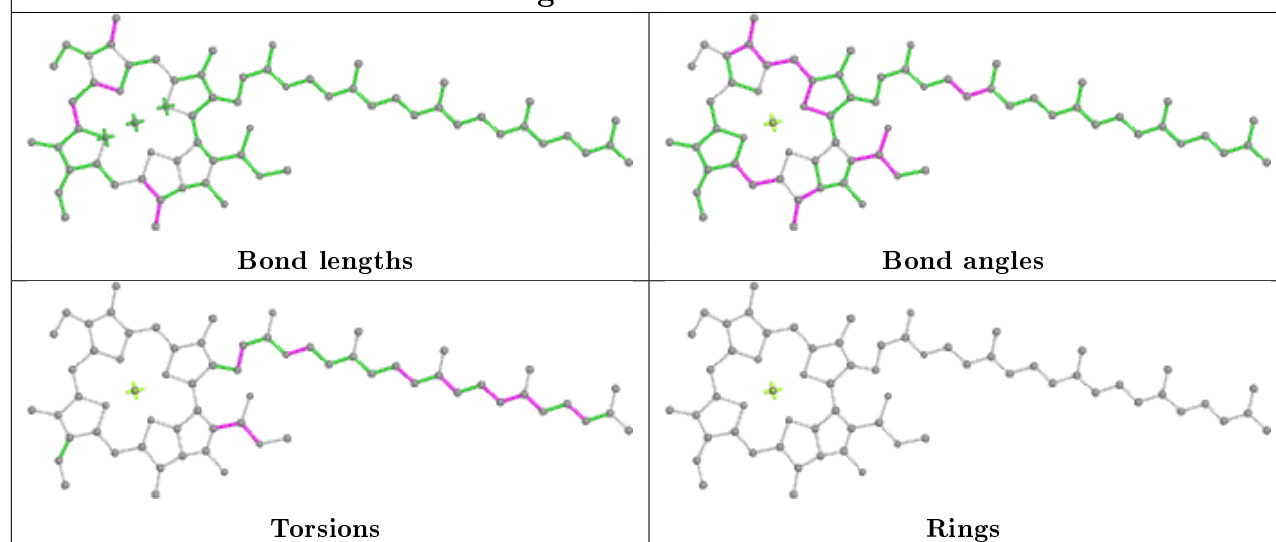
**Ligand CLA a 403****Ligand CLA B 615****Ligand LMG B 625**

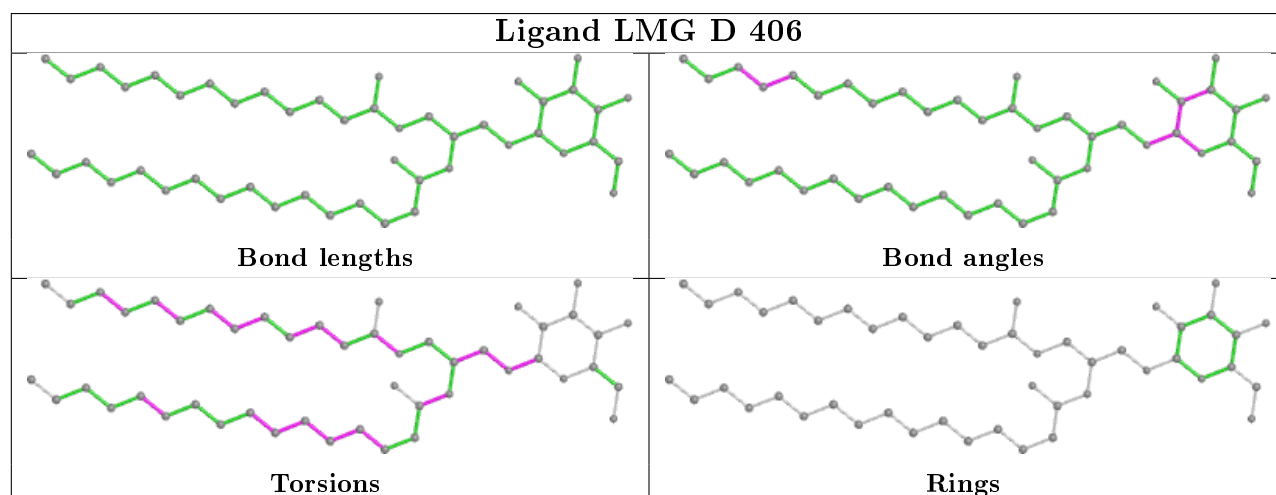
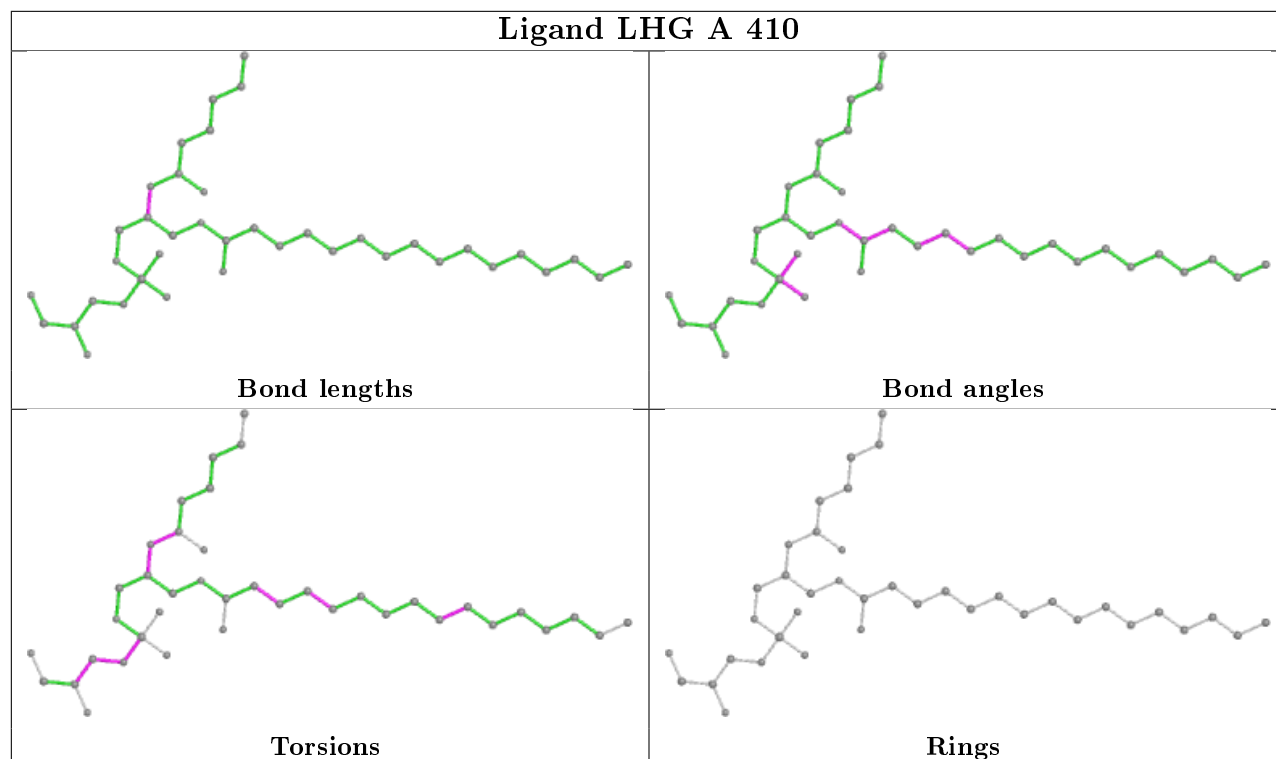
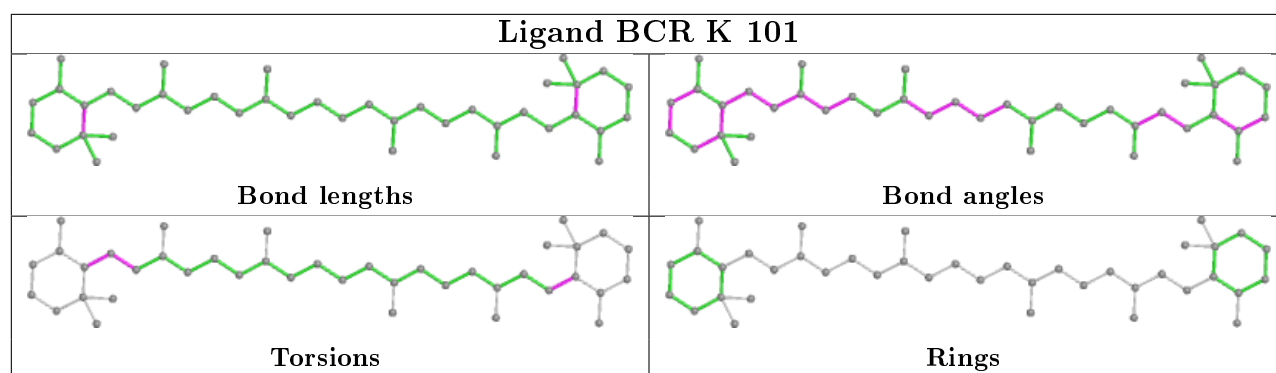
**Ligand CLA C 511****Ligand CLA C 512**

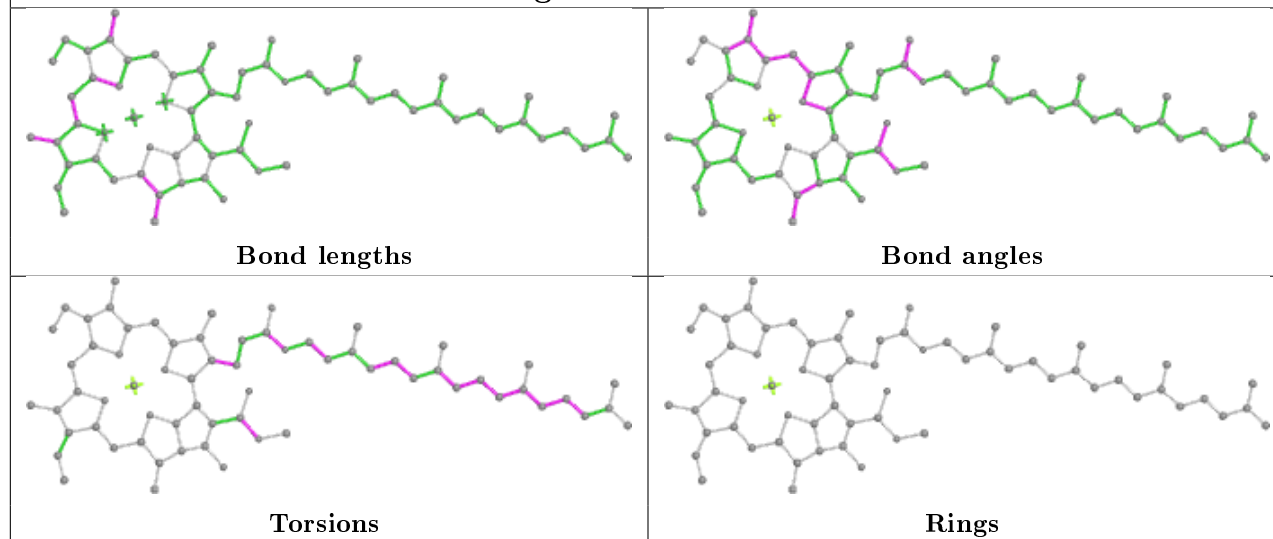
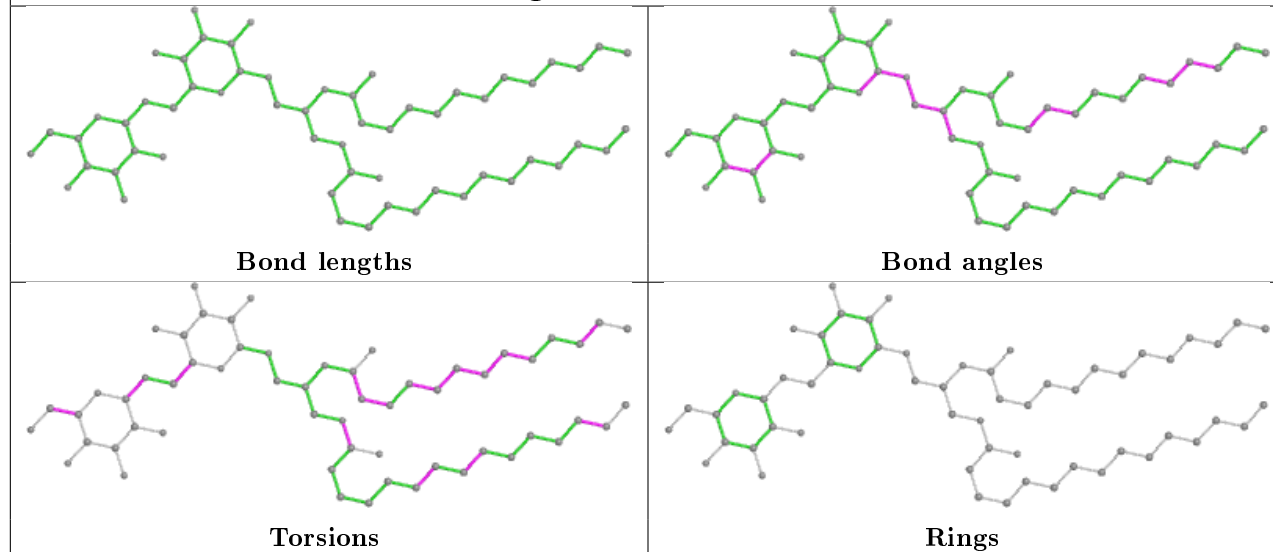
## Ligand HEM V 201

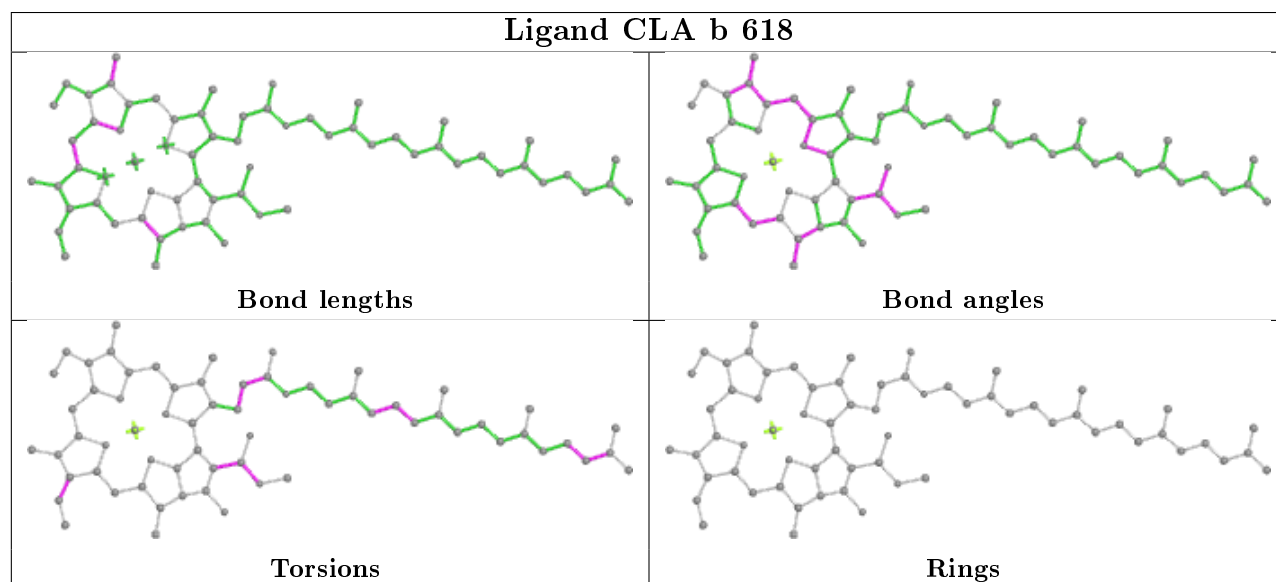
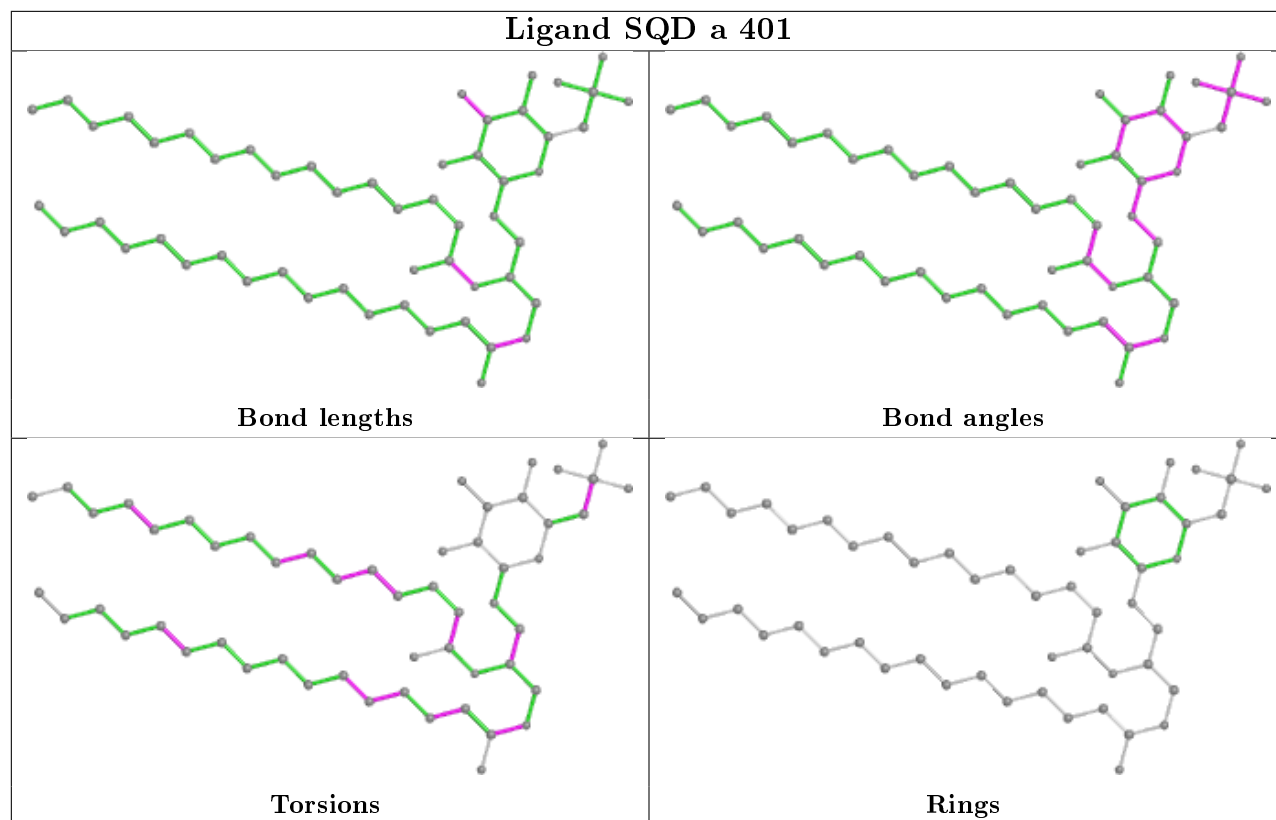


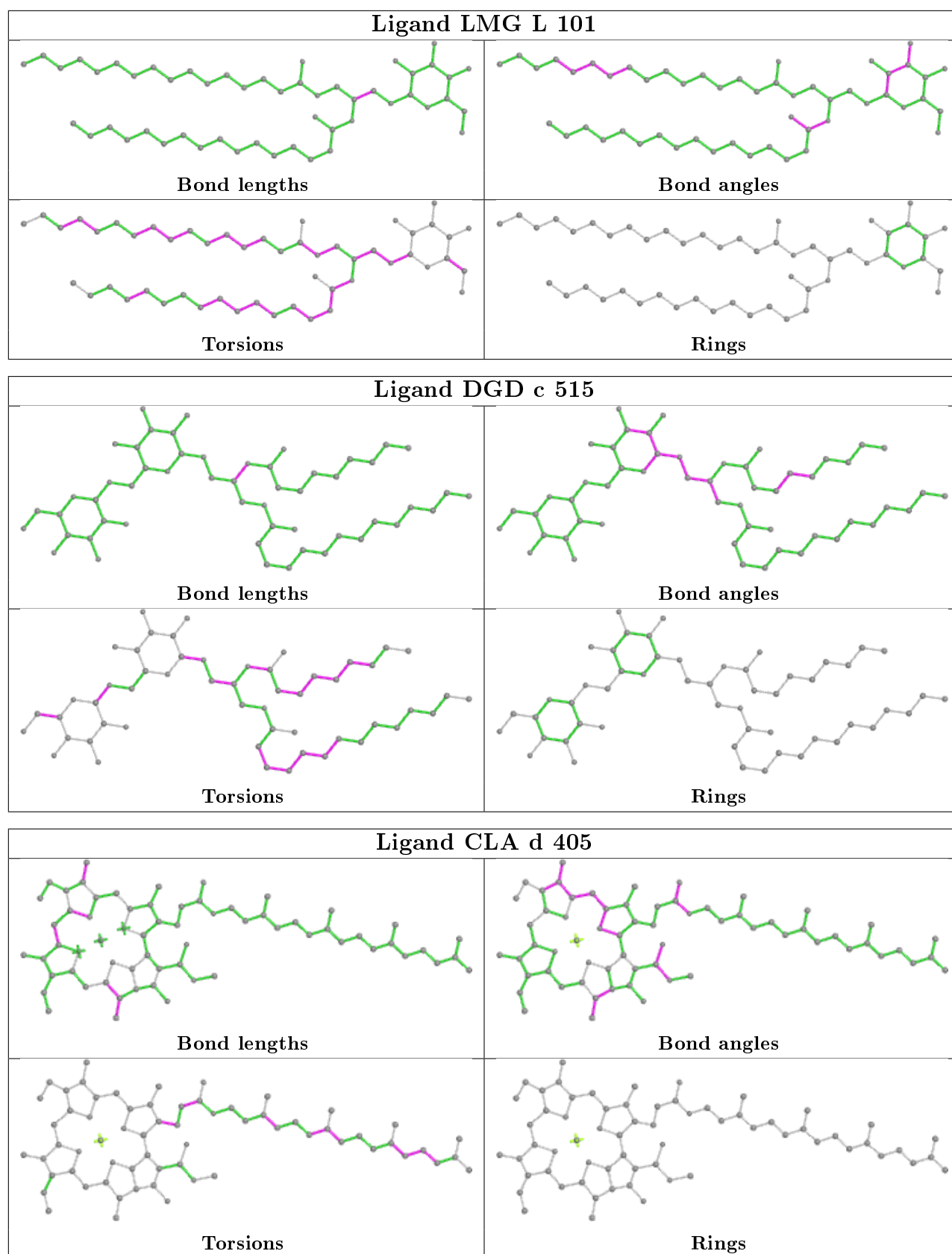
## Ligand CLA c 507

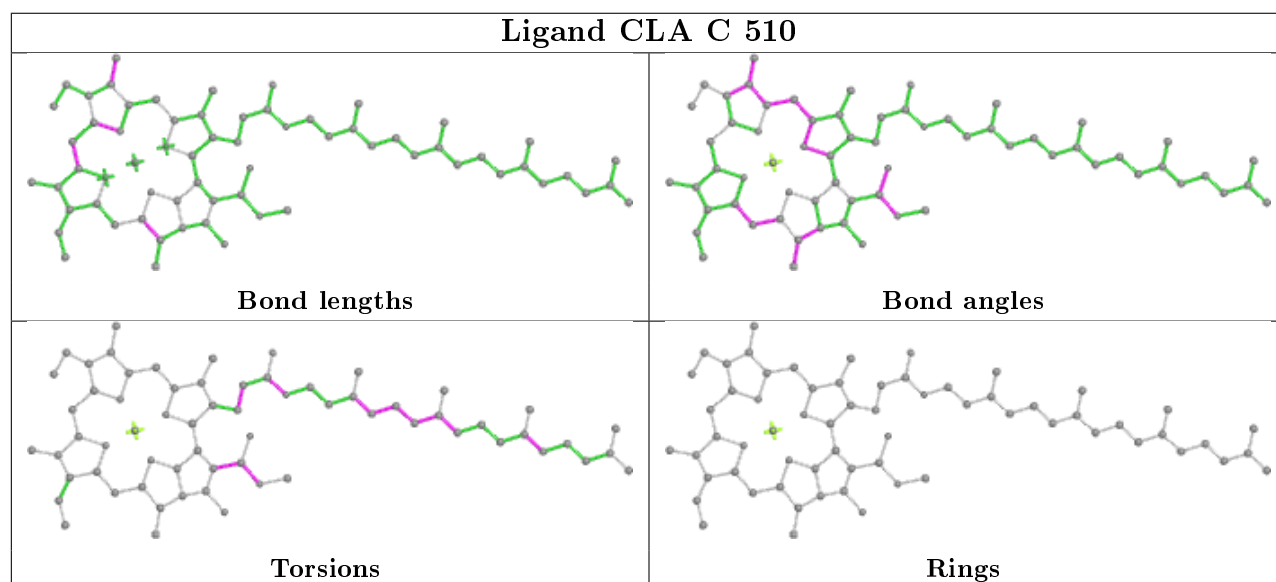
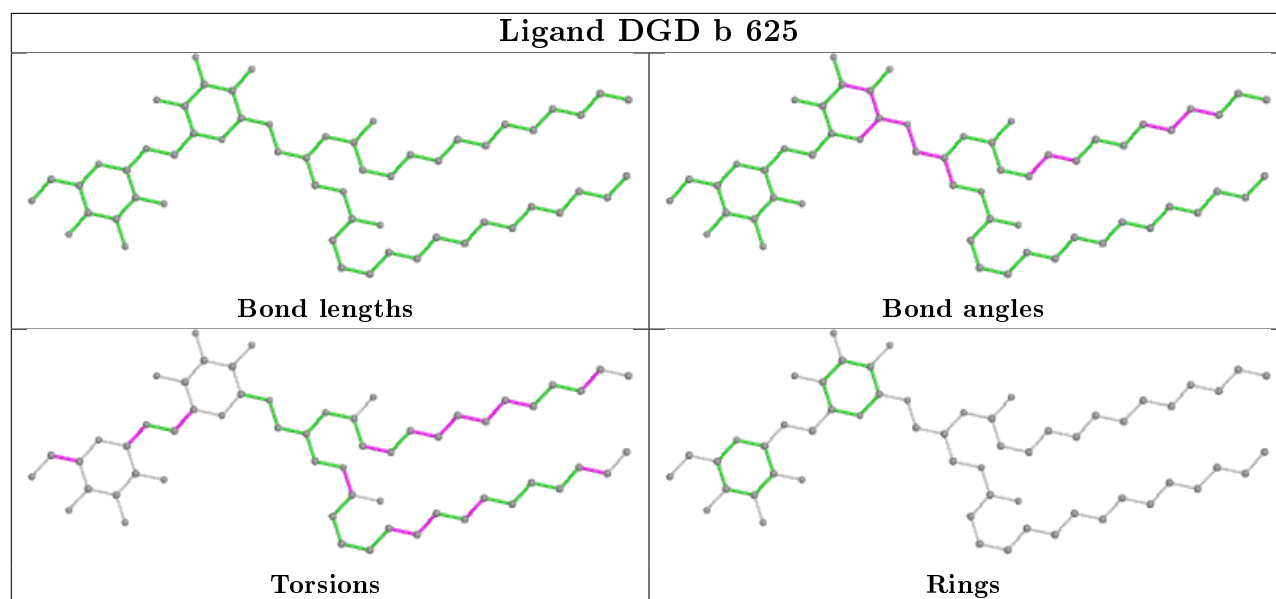
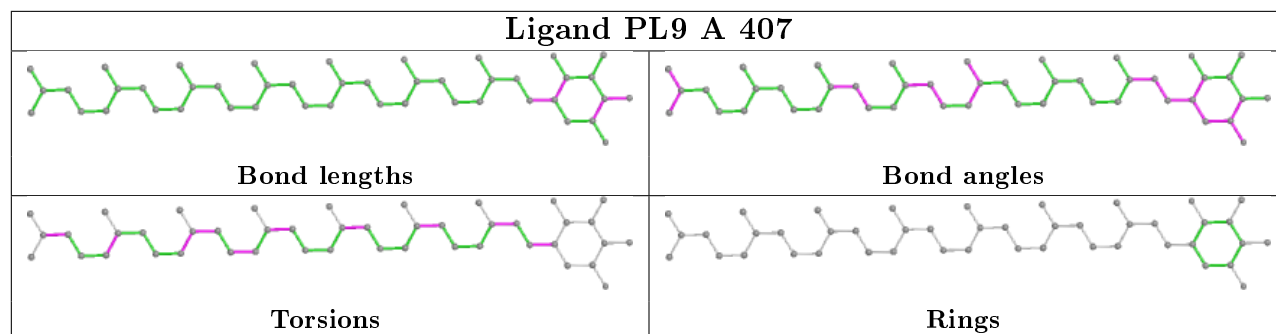




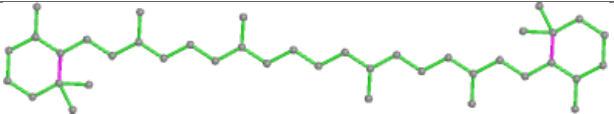
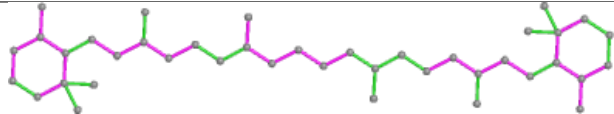
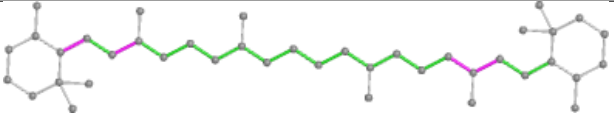
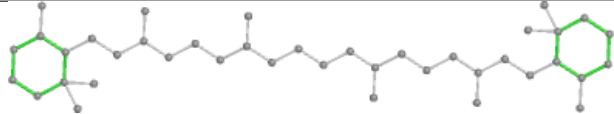
**Ligand CLA b 620****Ligand DGD B 620**

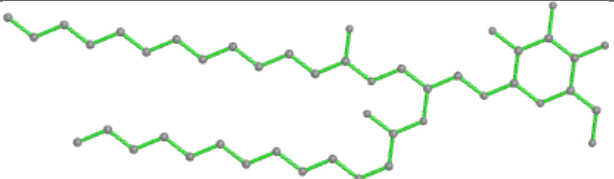
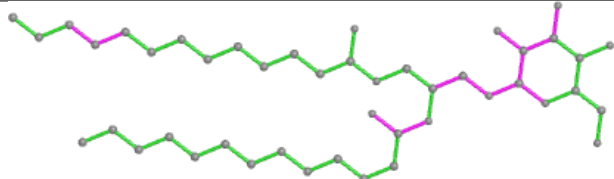
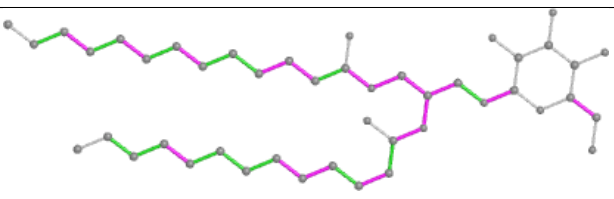
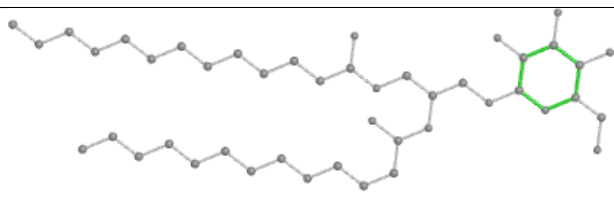


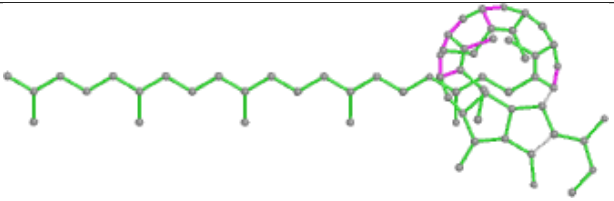
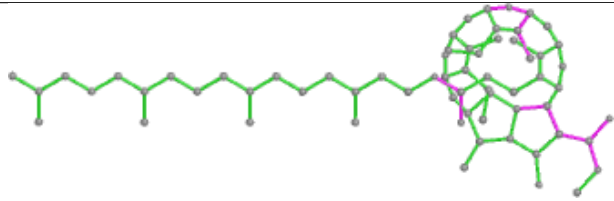
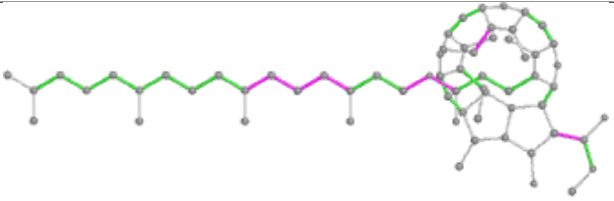
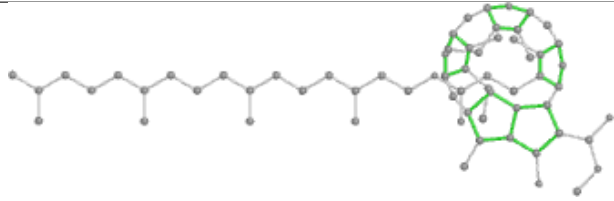




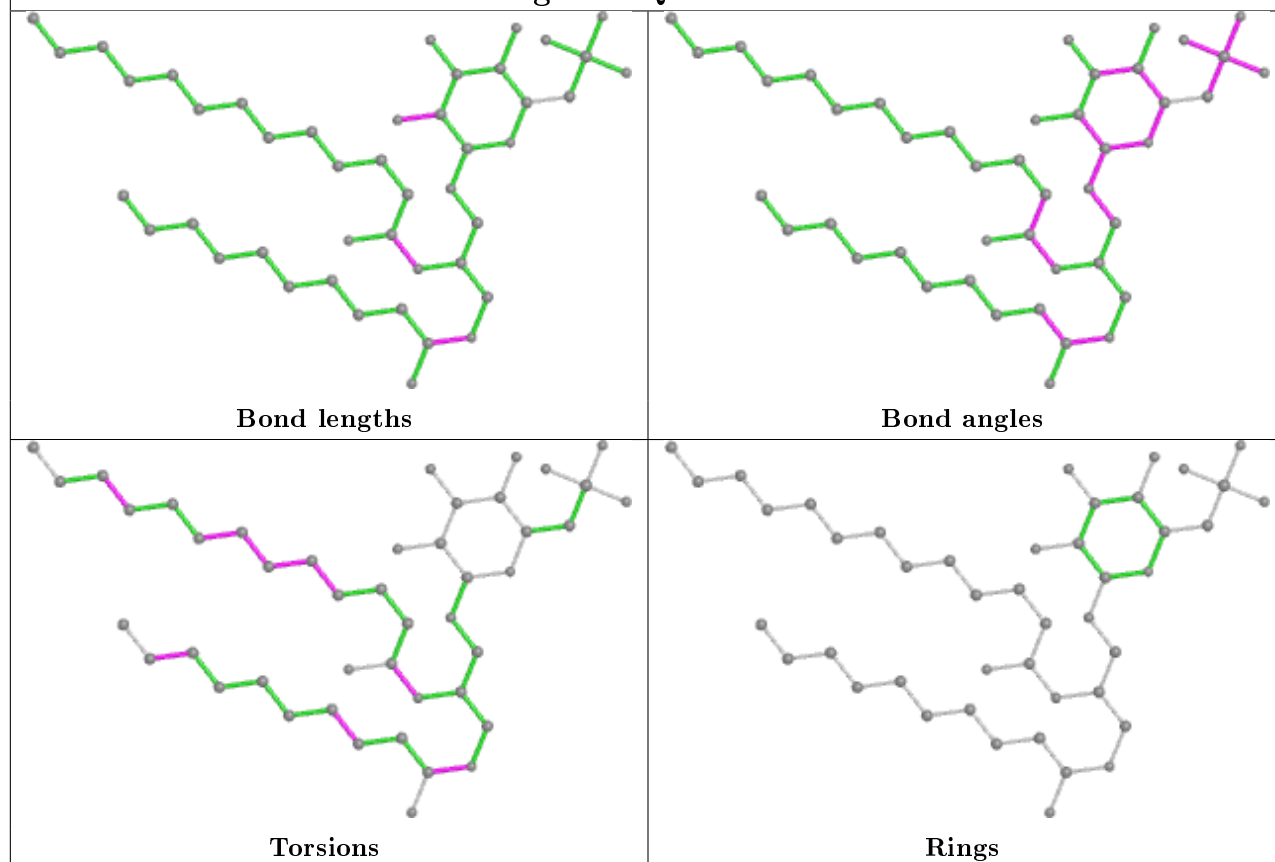


Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

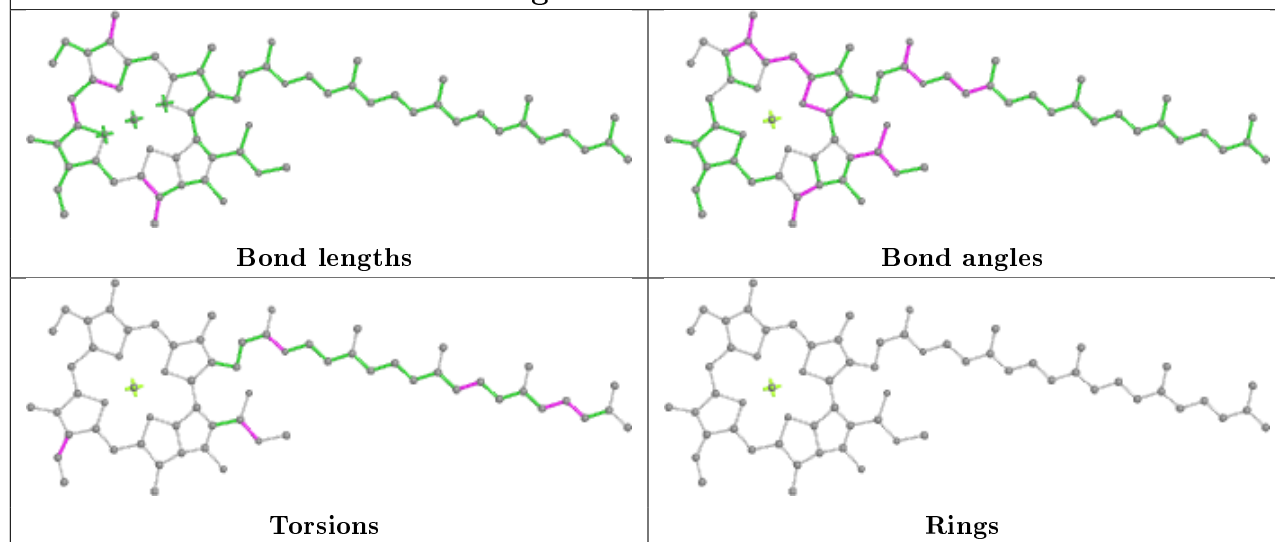
Ligand LMG c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

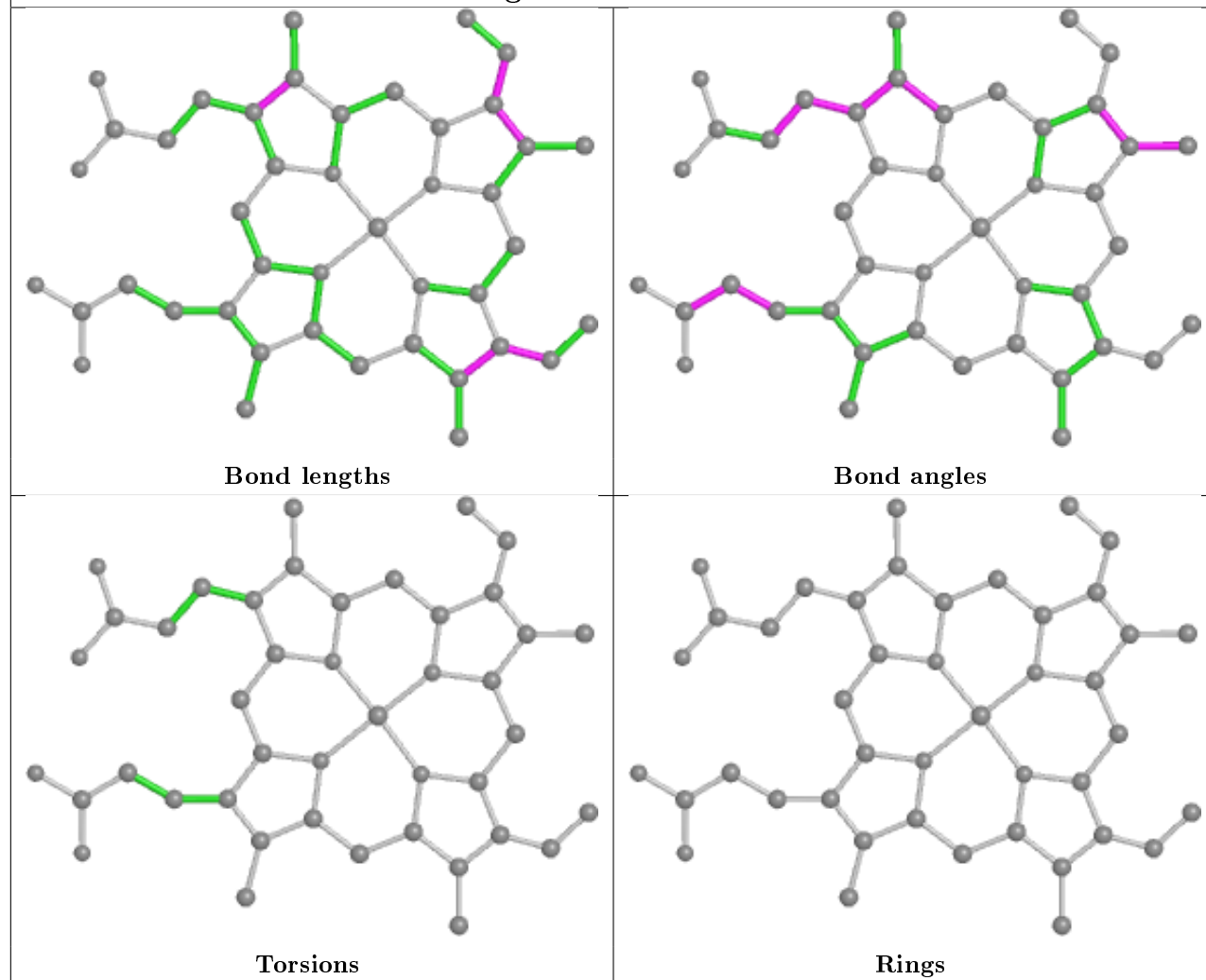
## Ligand SQD F 103

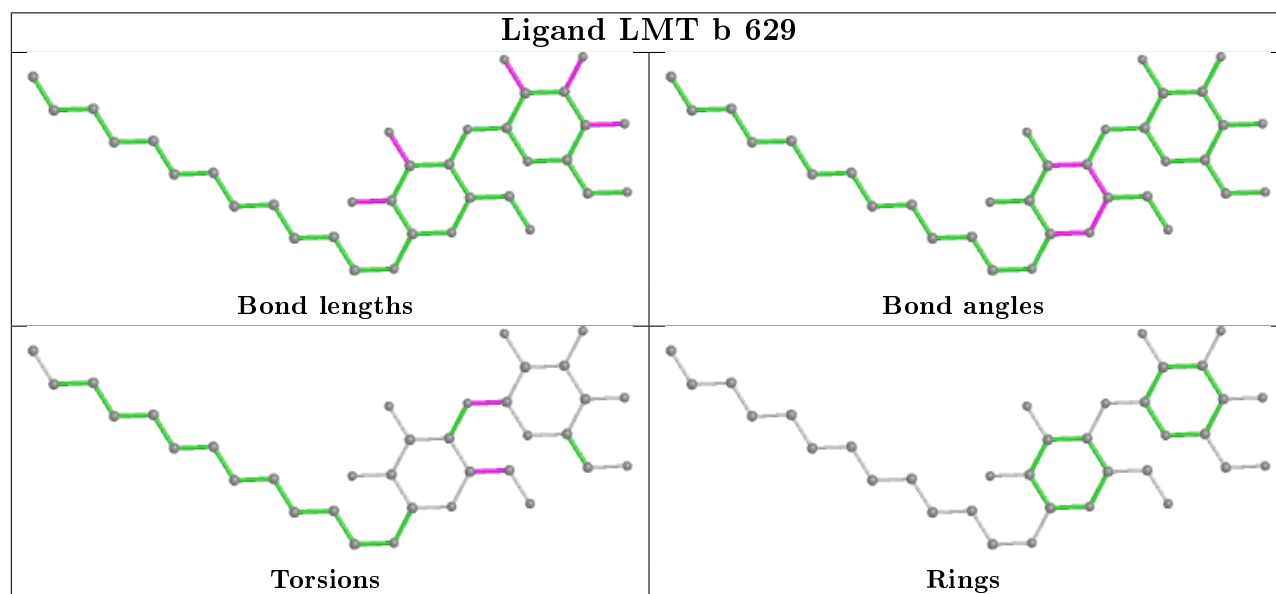
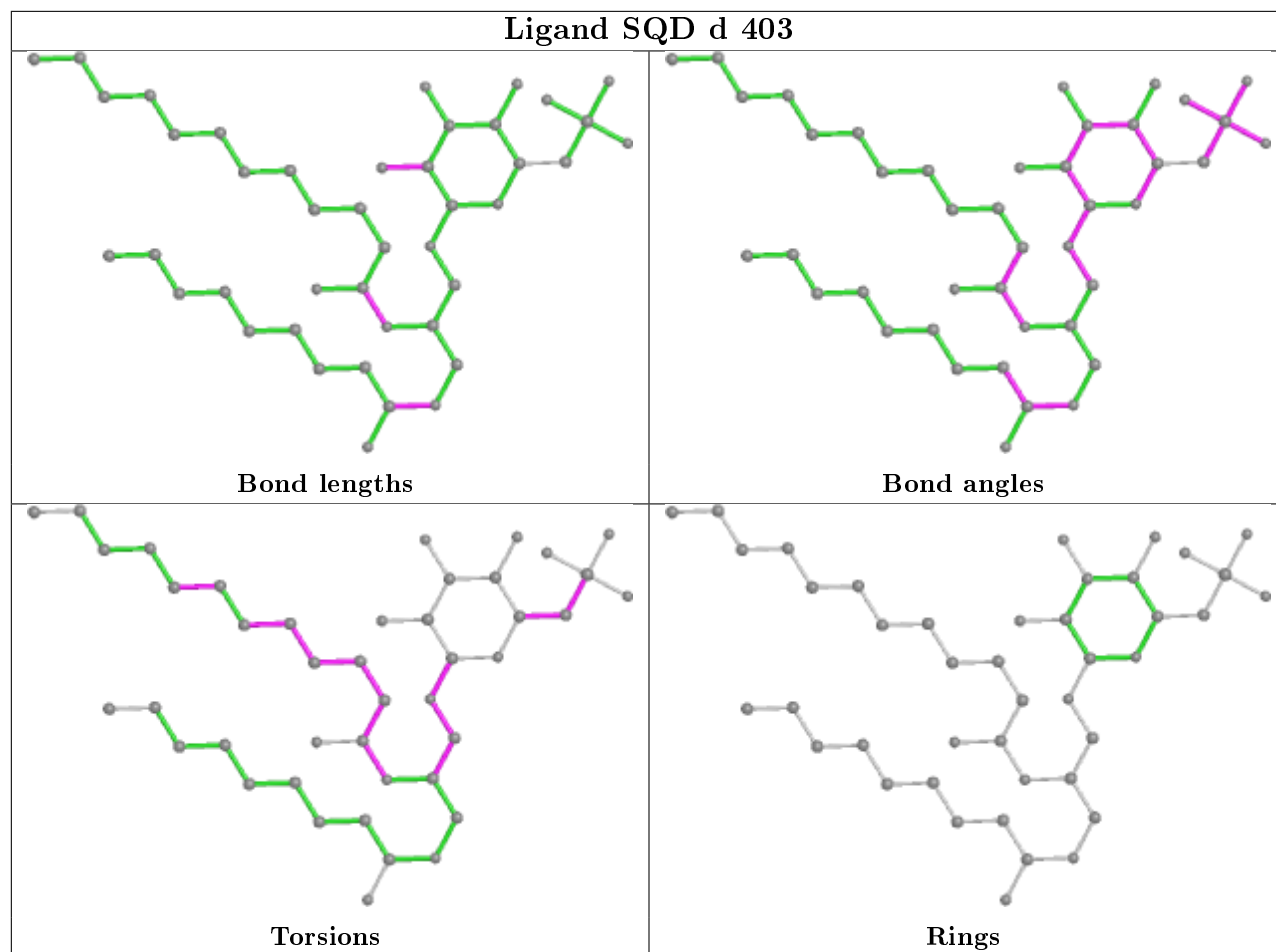


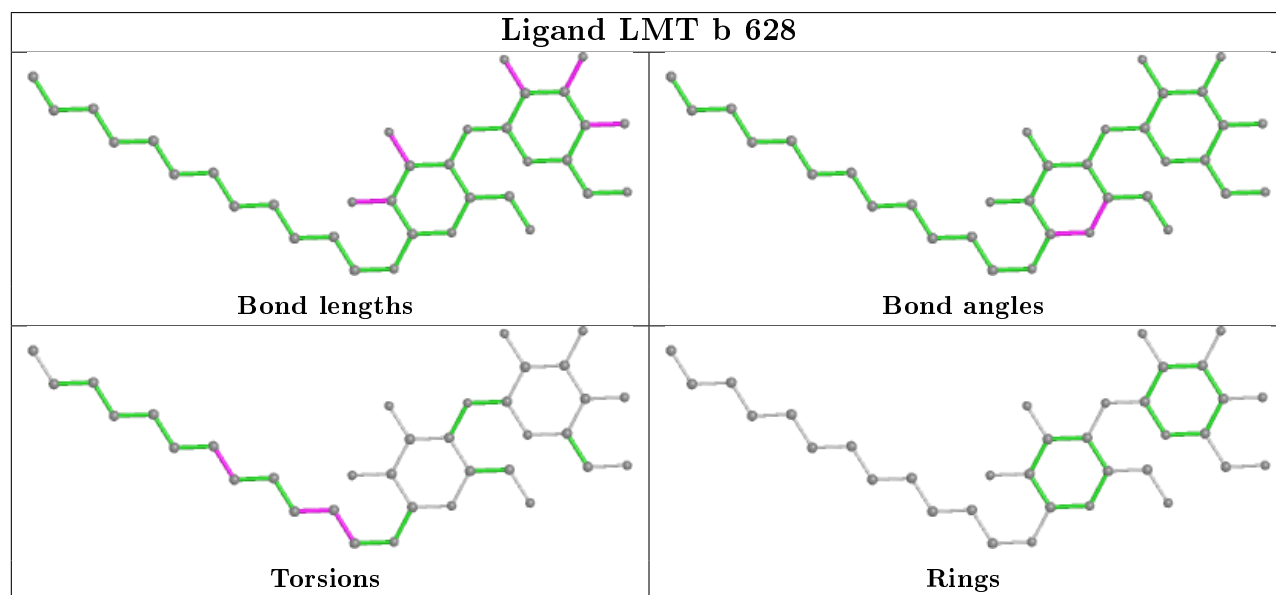
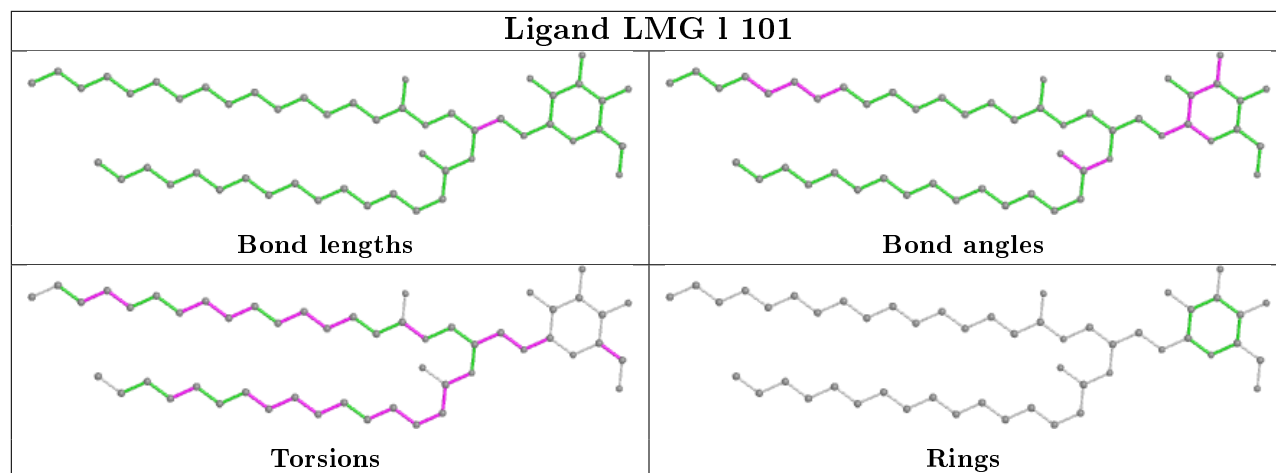
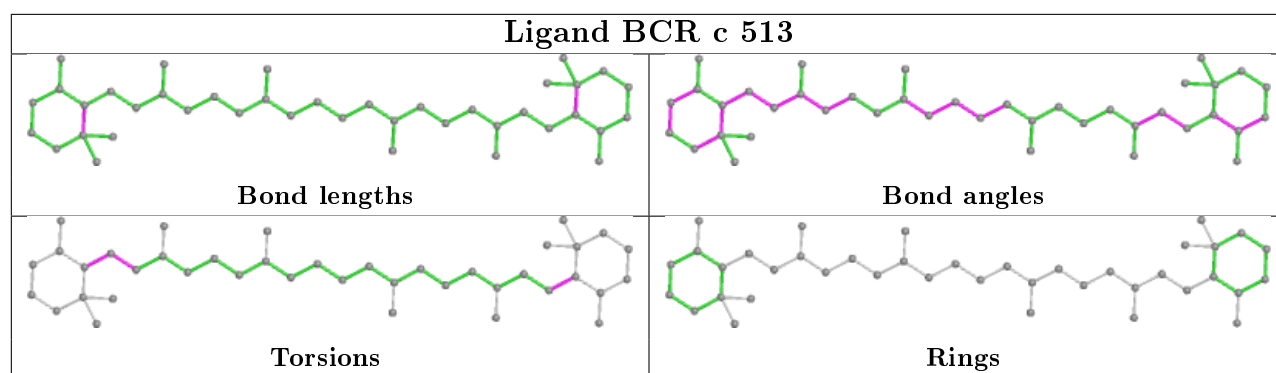
## Ligand CLA B 603



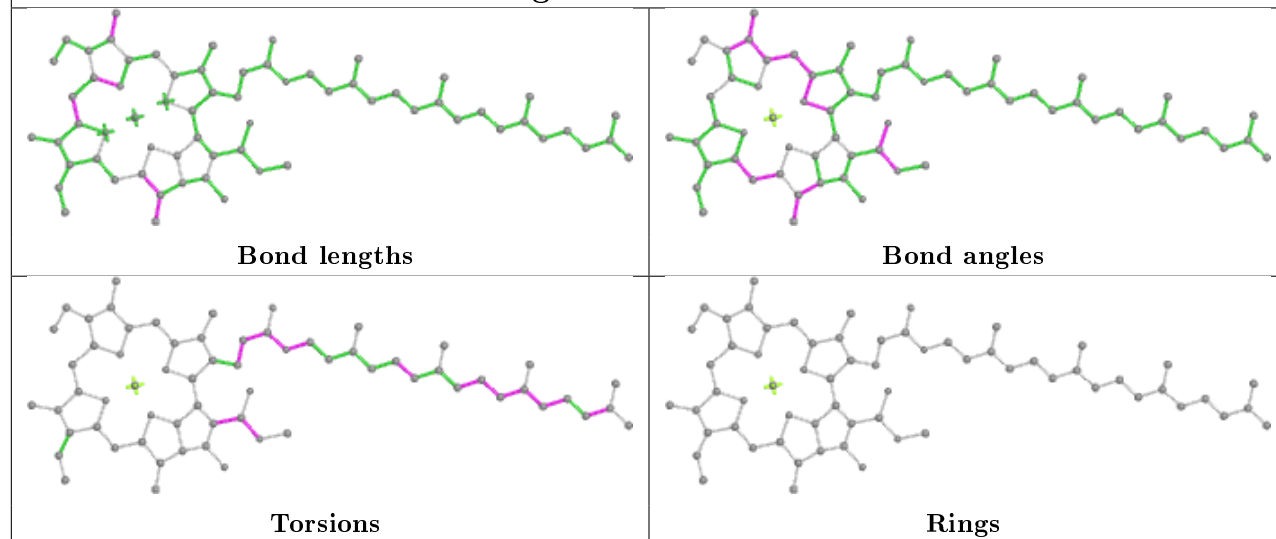
## Ligand HEM f 101



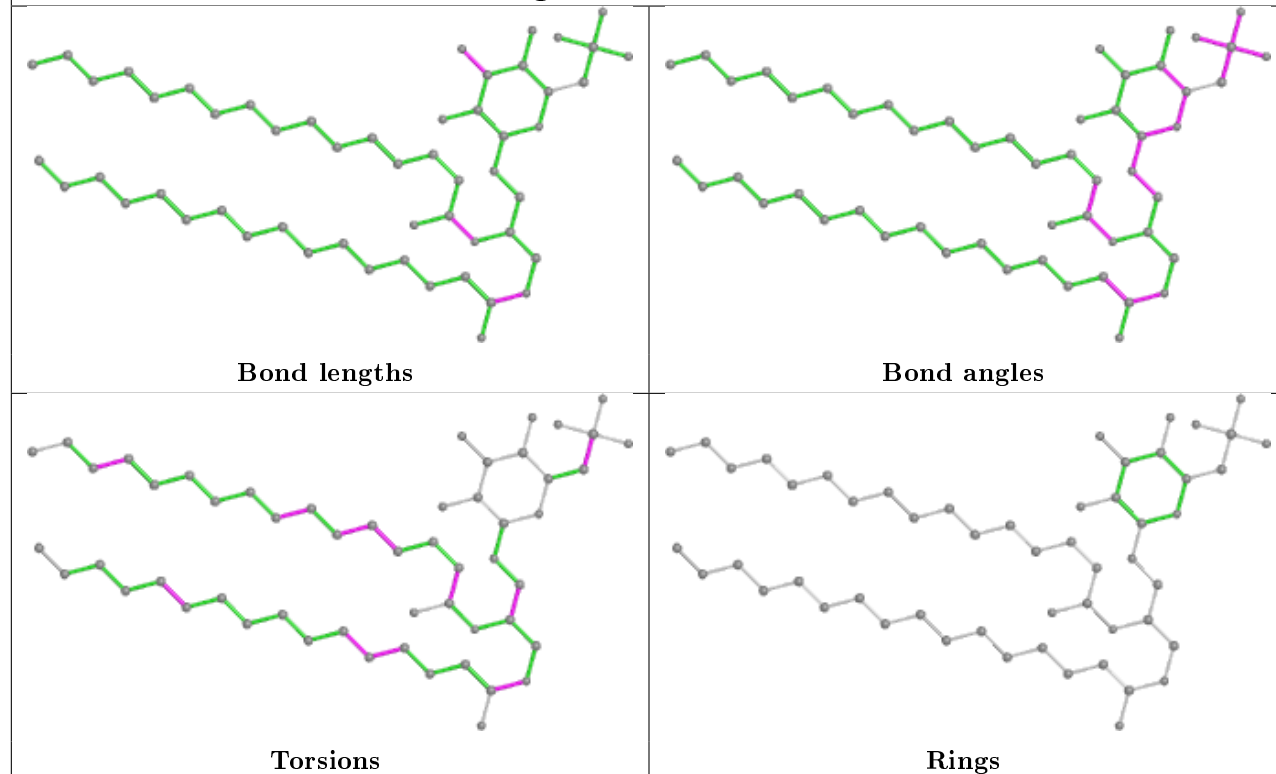


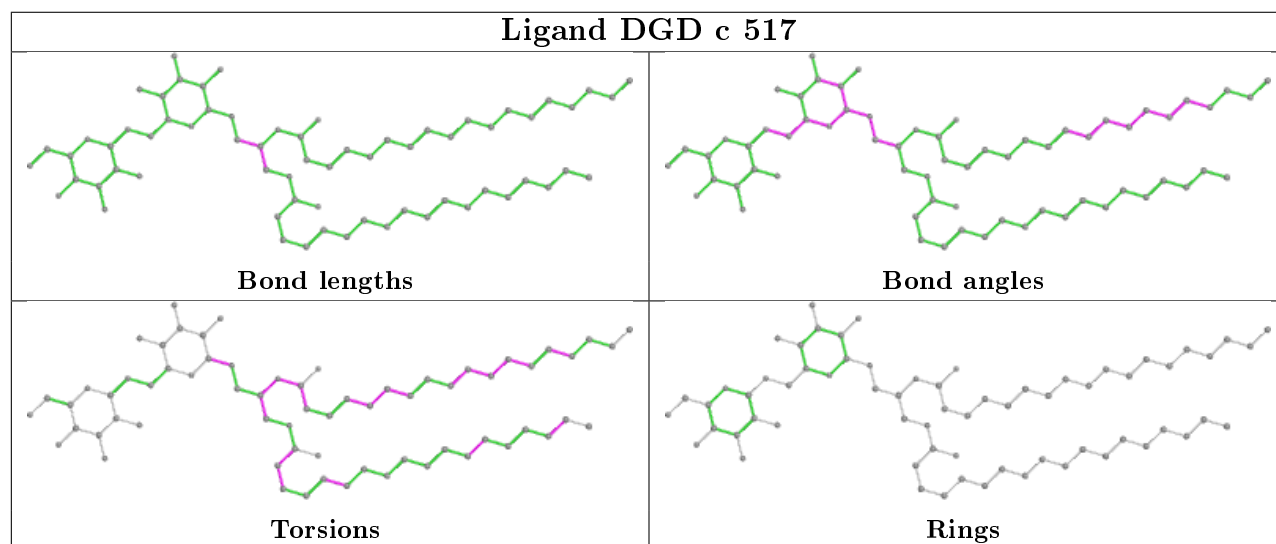
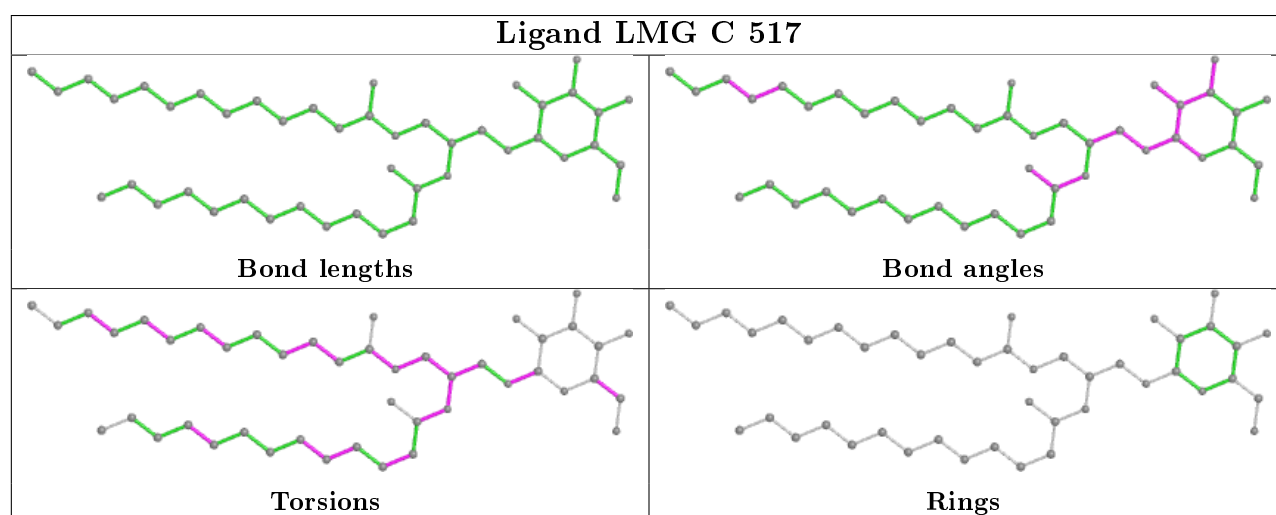
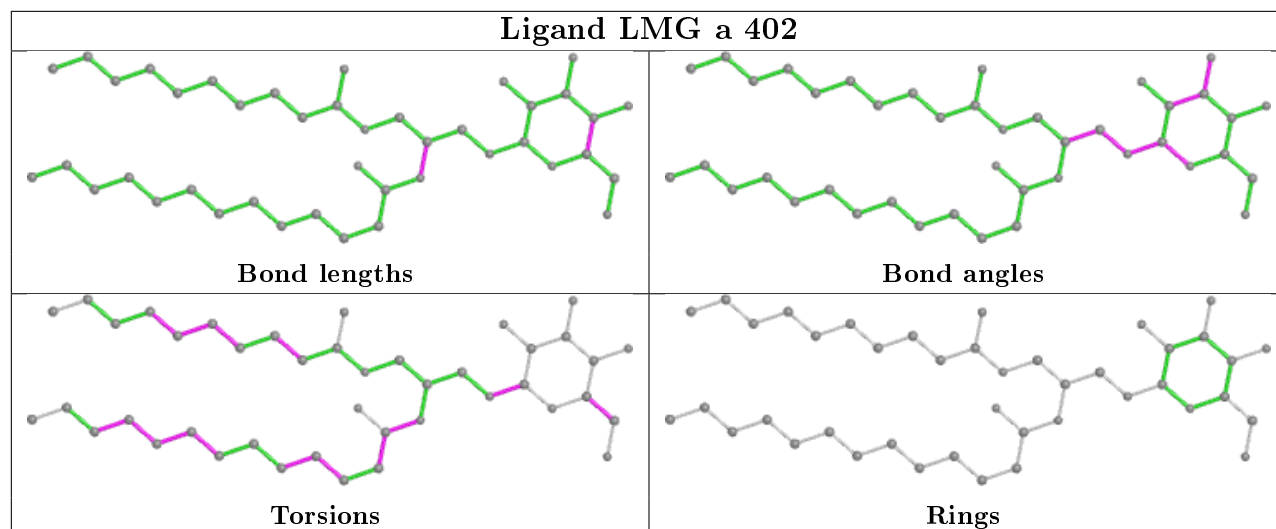


## Ligand CLA B 609

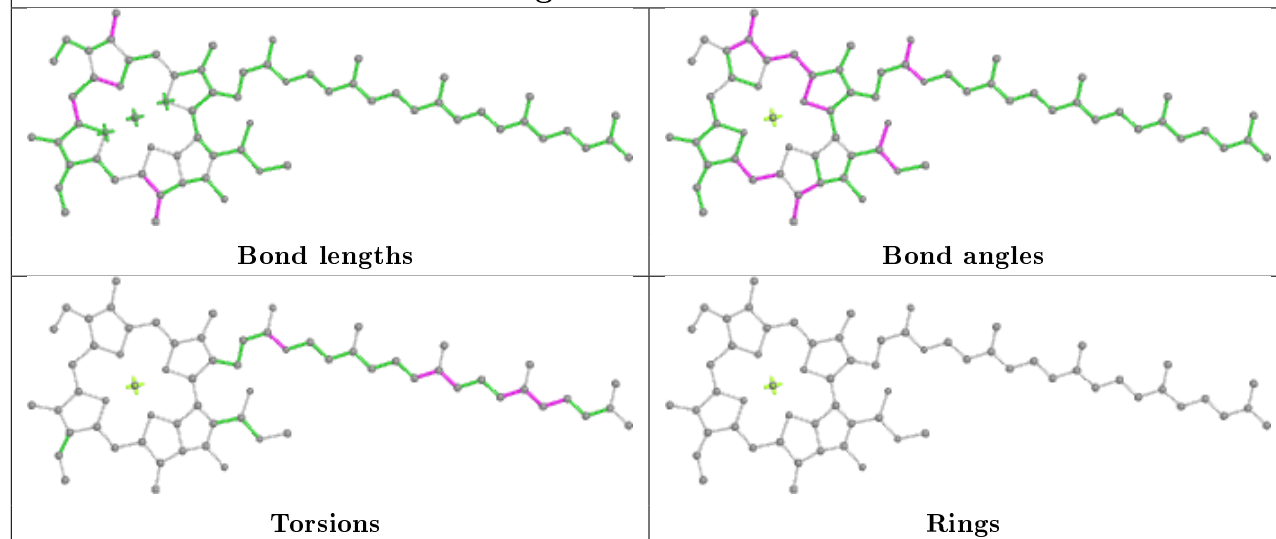


## Ligand SQD A 414

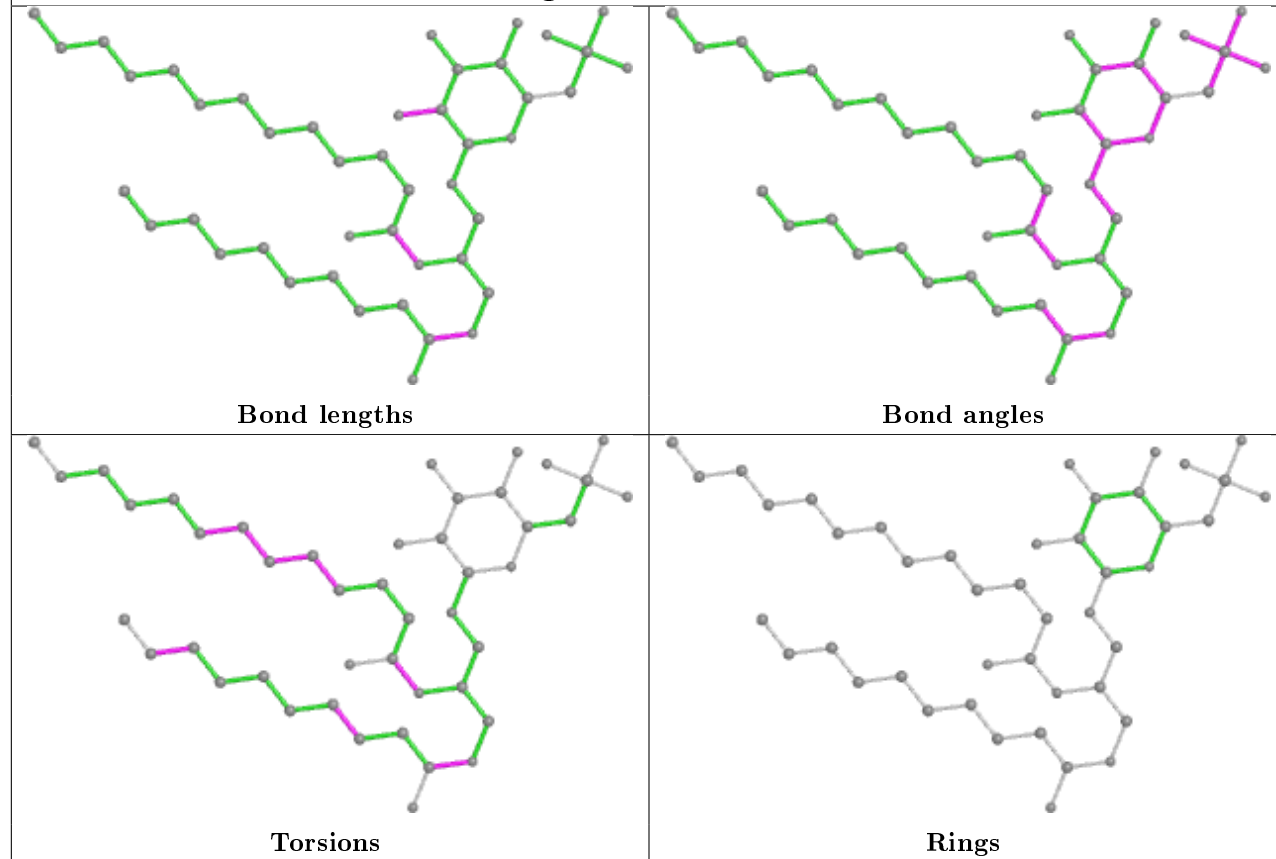




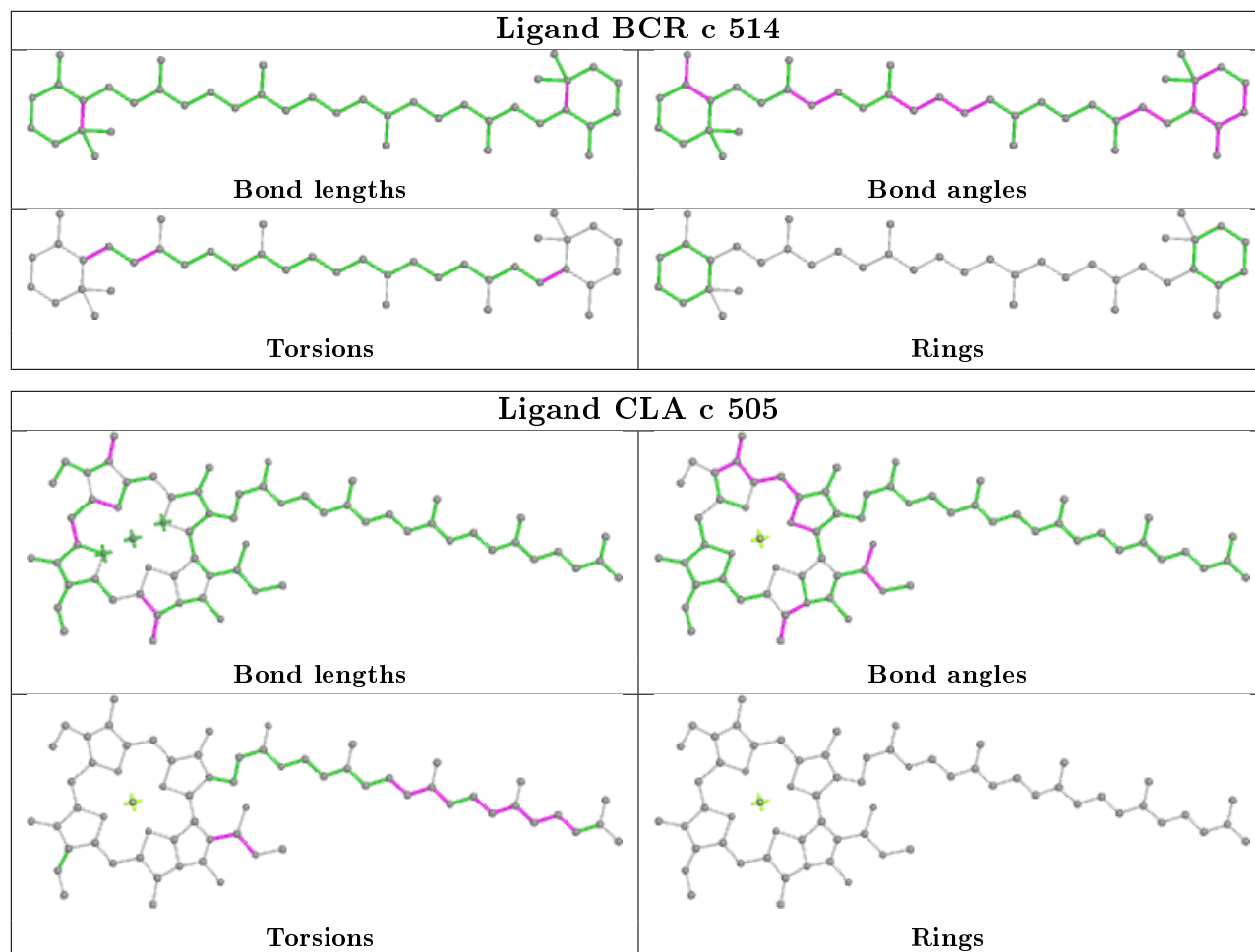
## Ligand CLA b 619



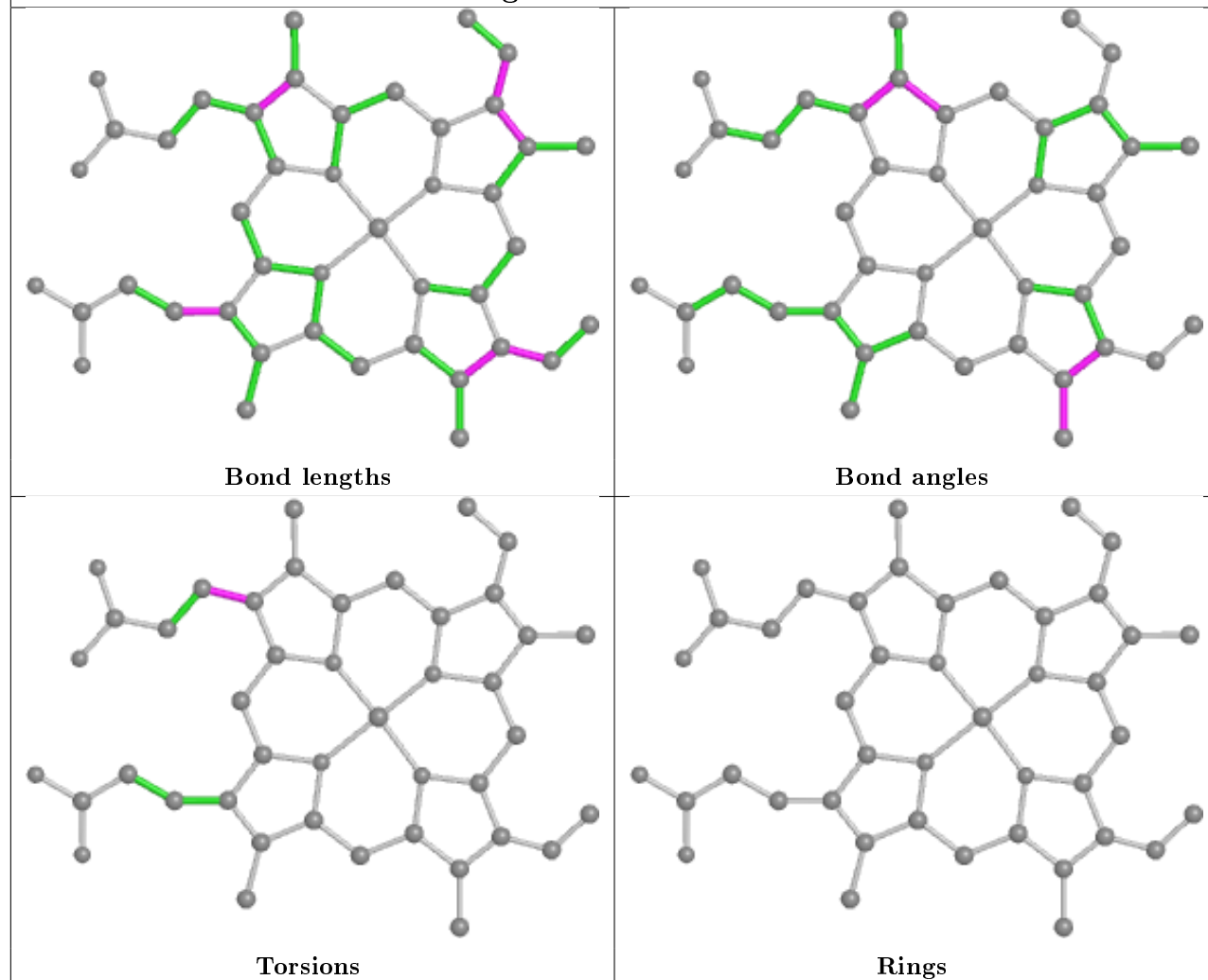
## Ligand SQD f 103



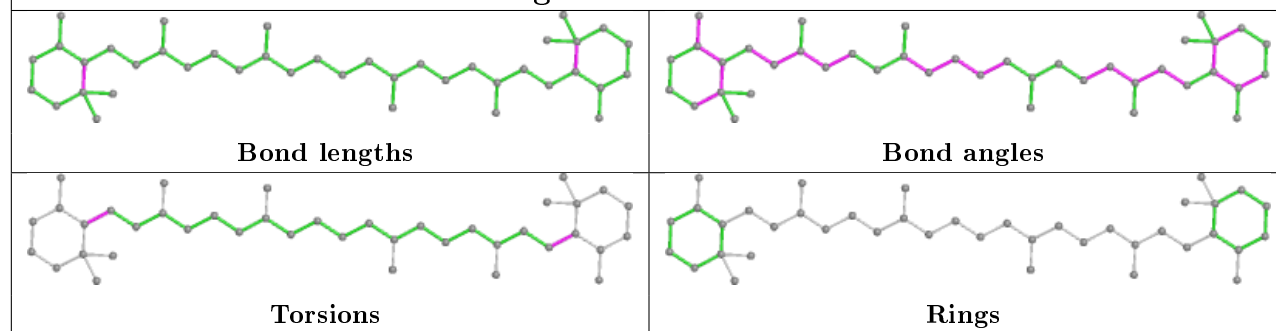


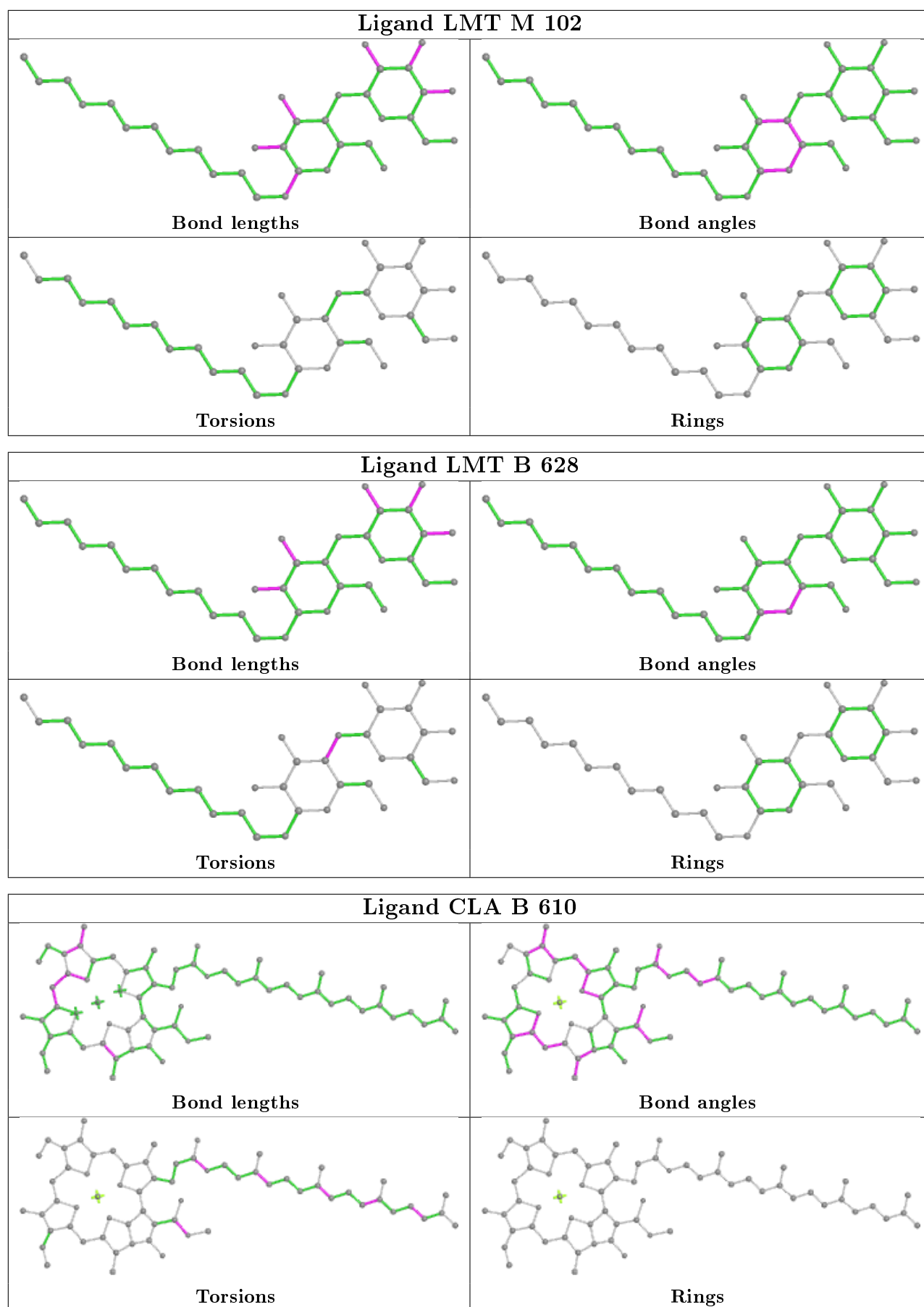


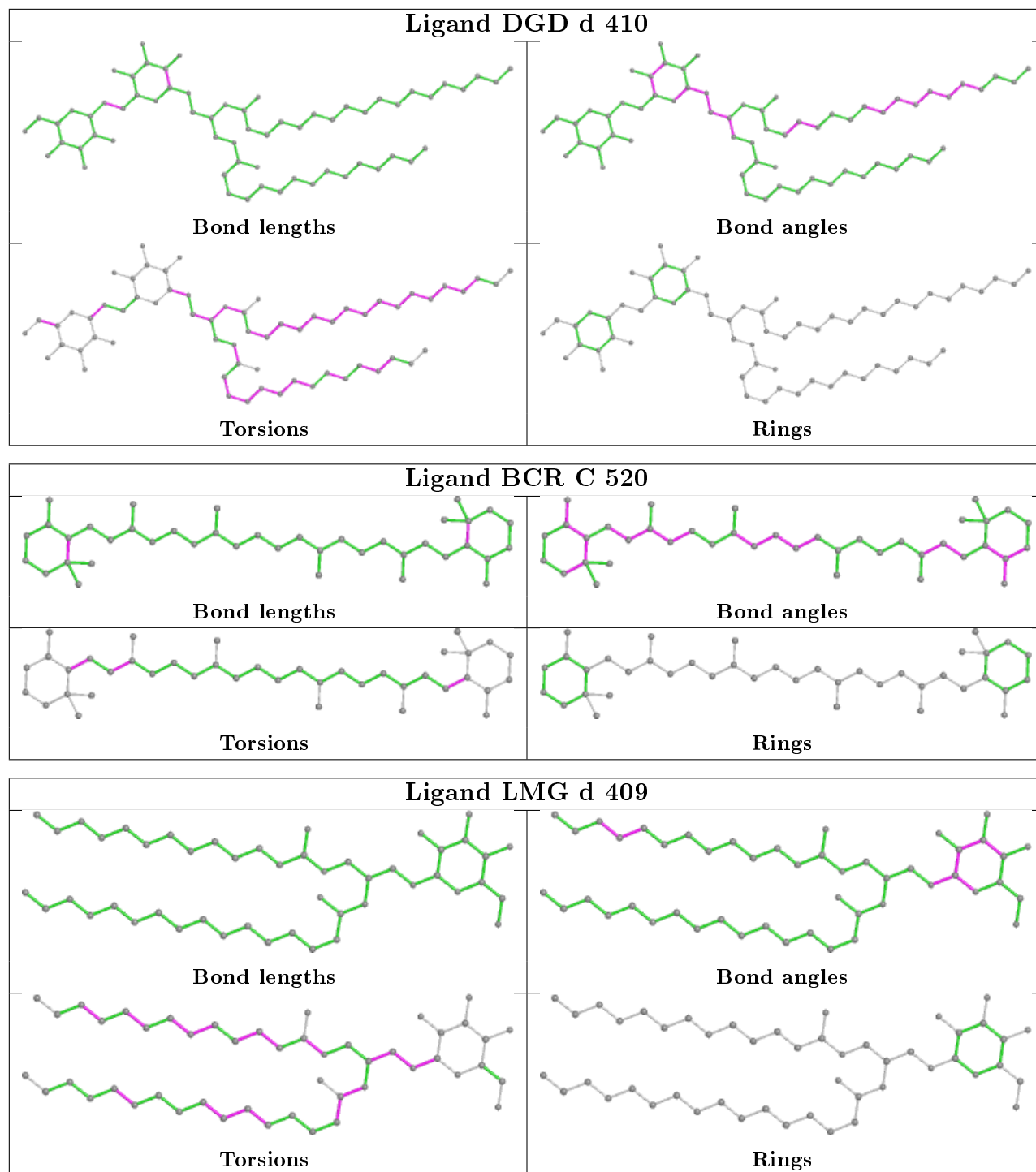
## Ligand HEM v 201



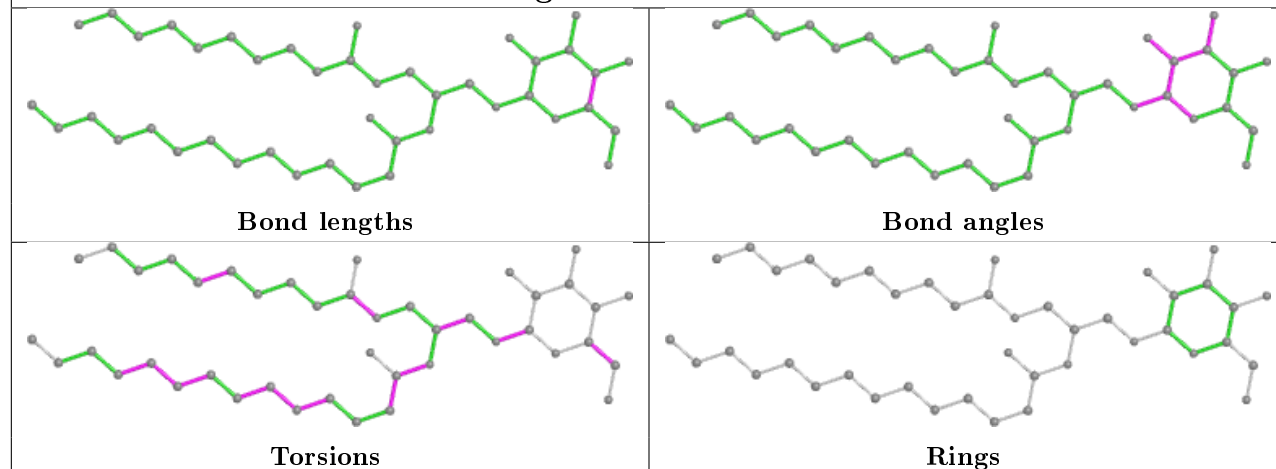
## Ligand BCR b 623



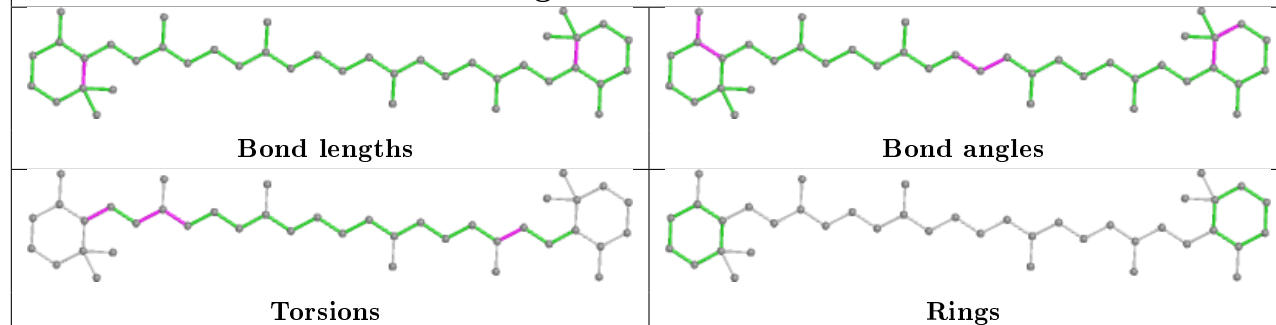




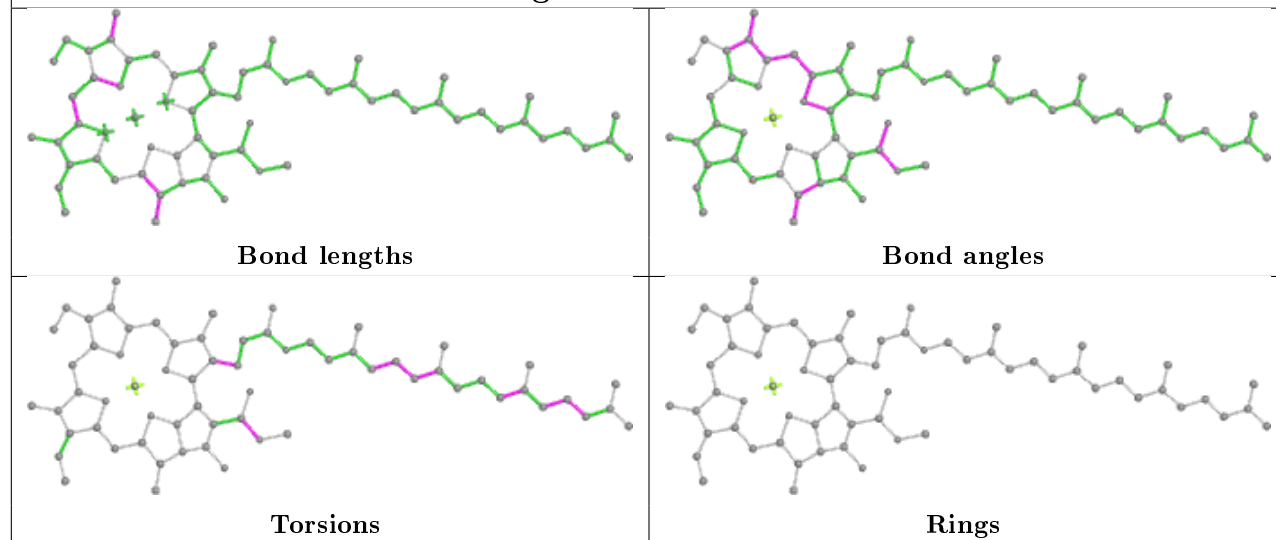
## Ligand LMG i 102

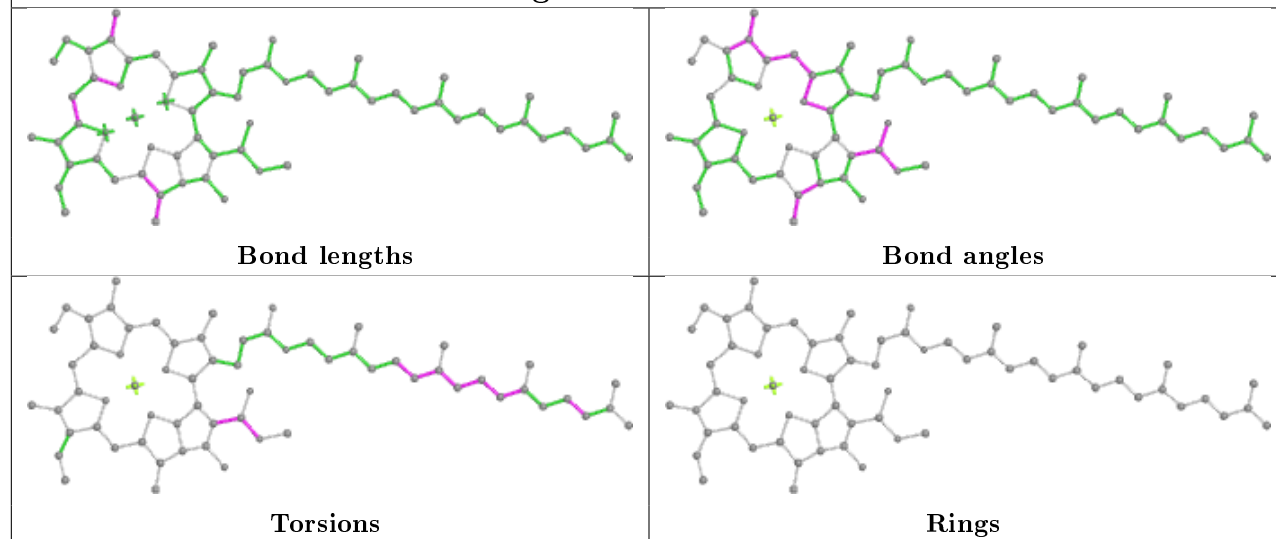
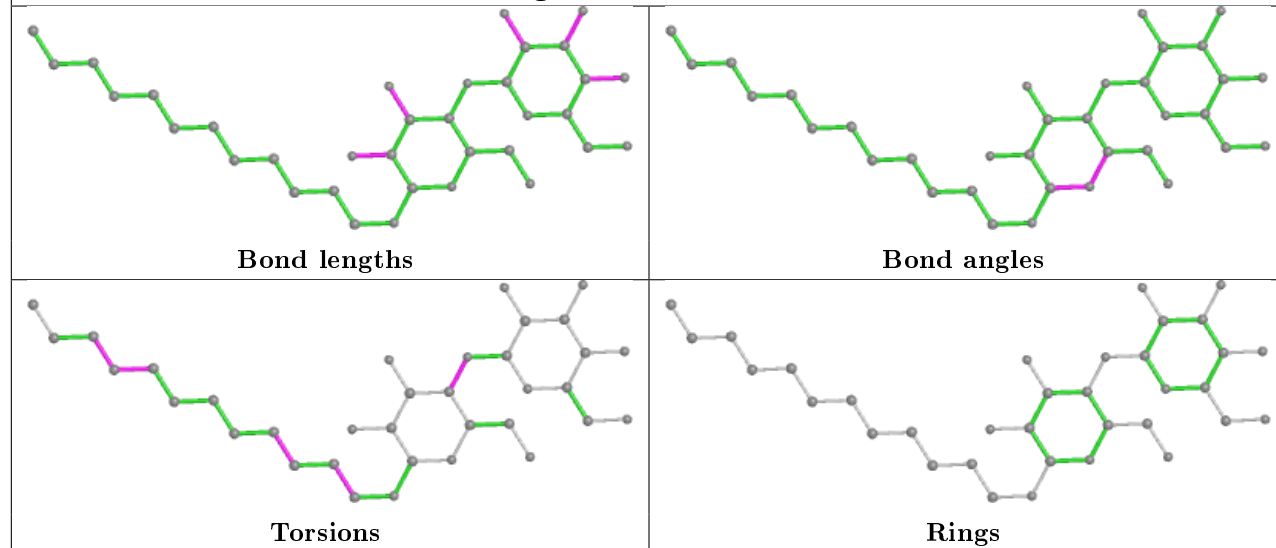
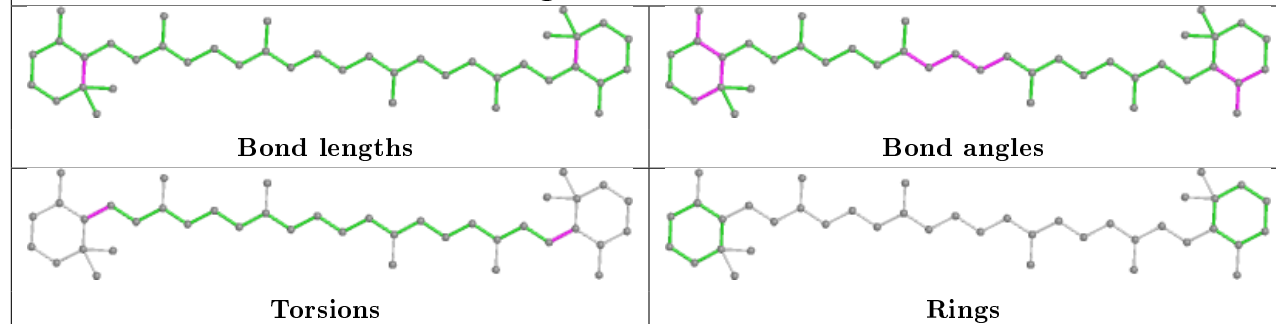


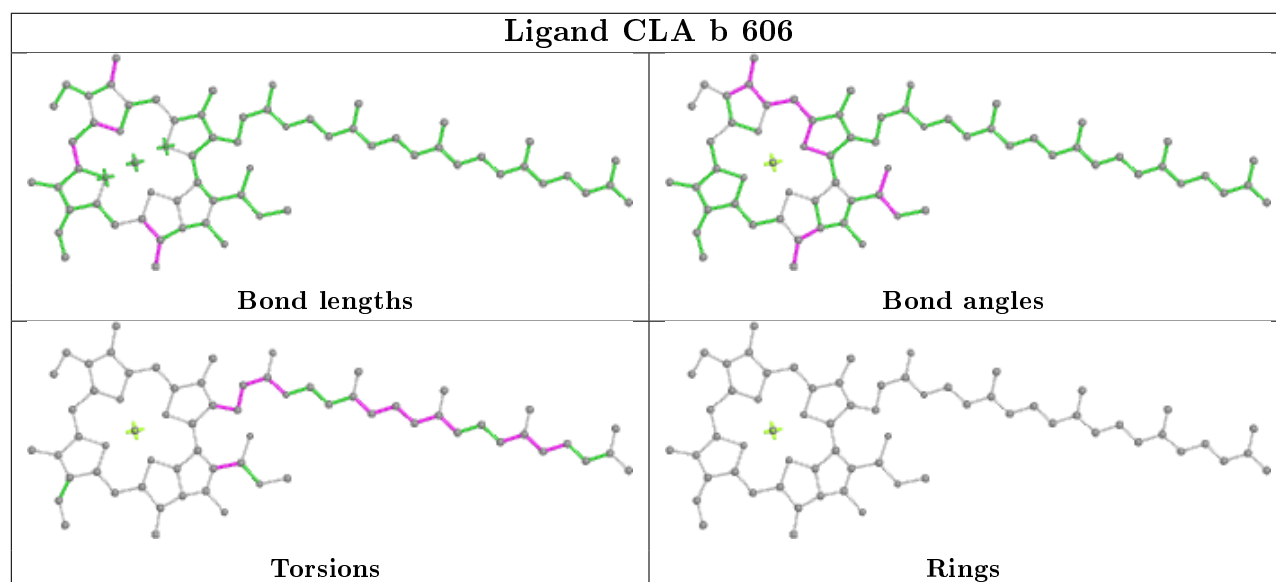
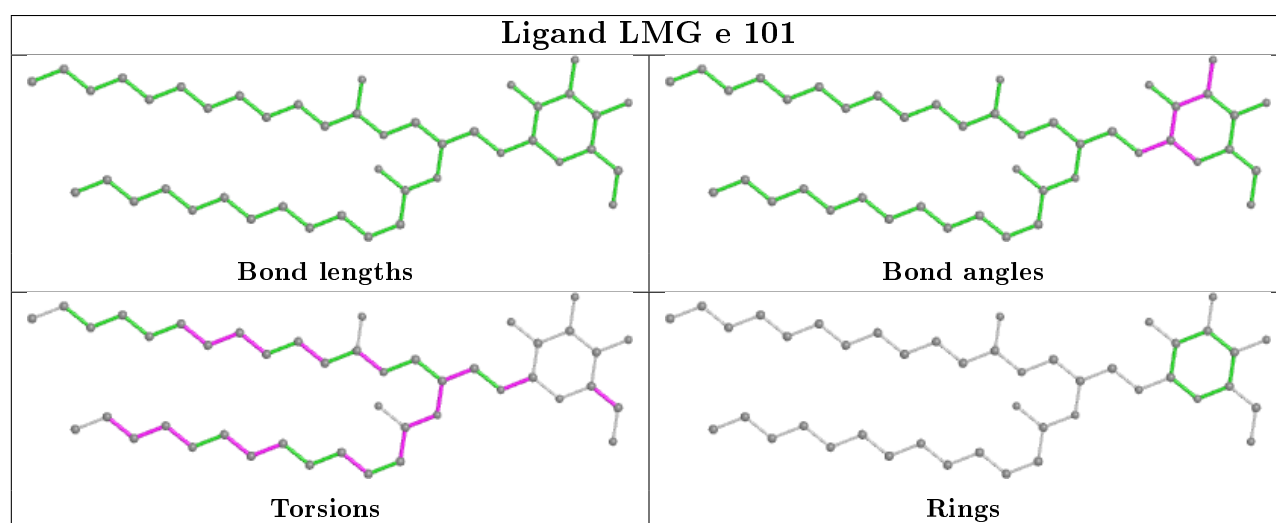
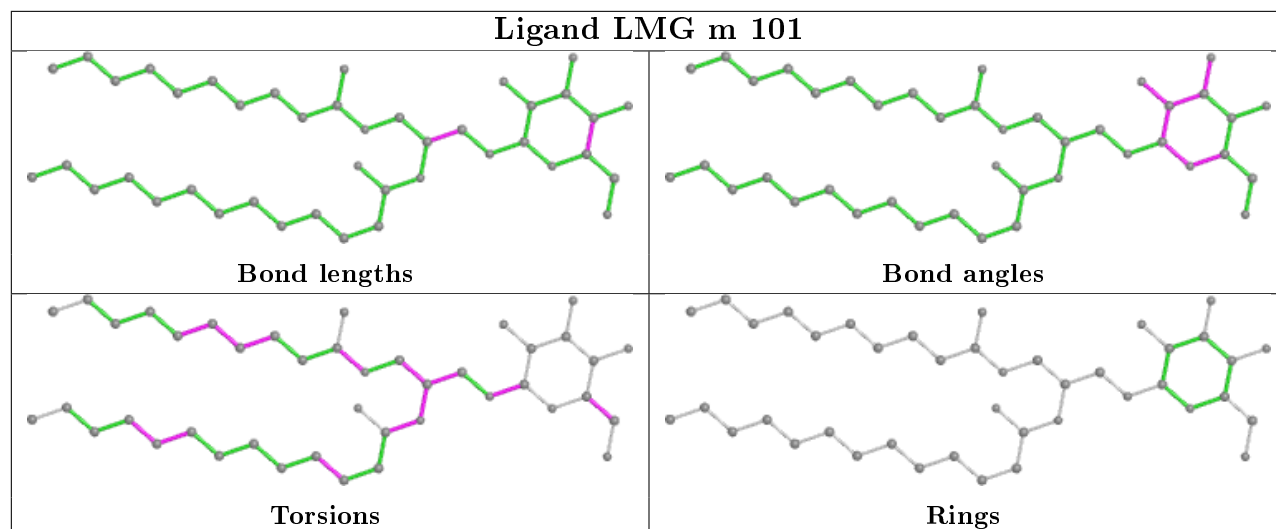
## Ligand BCR x 101

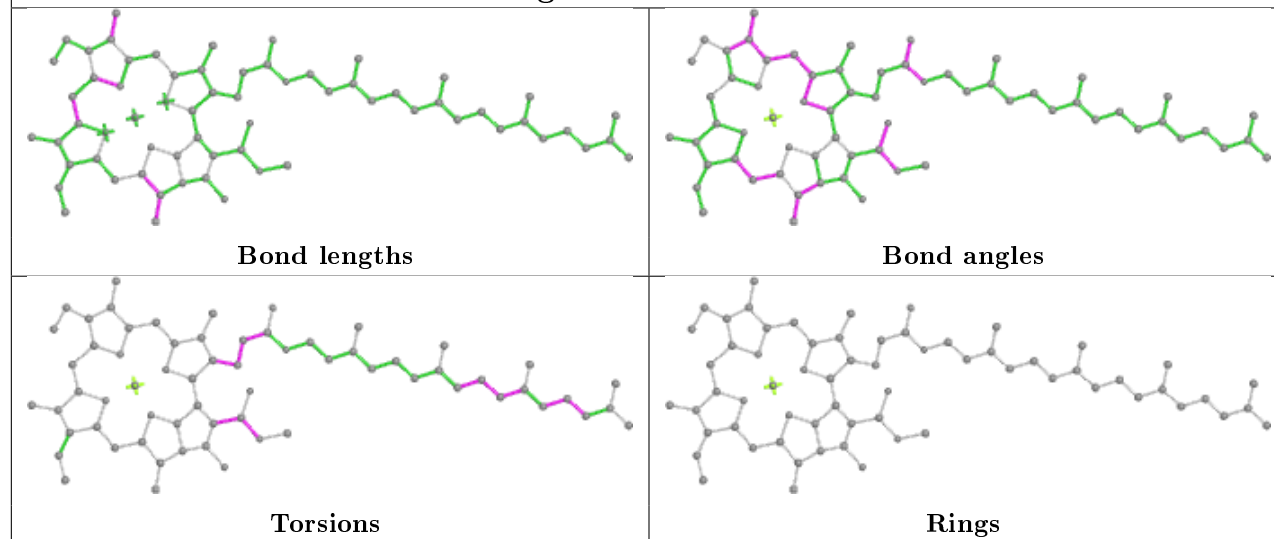
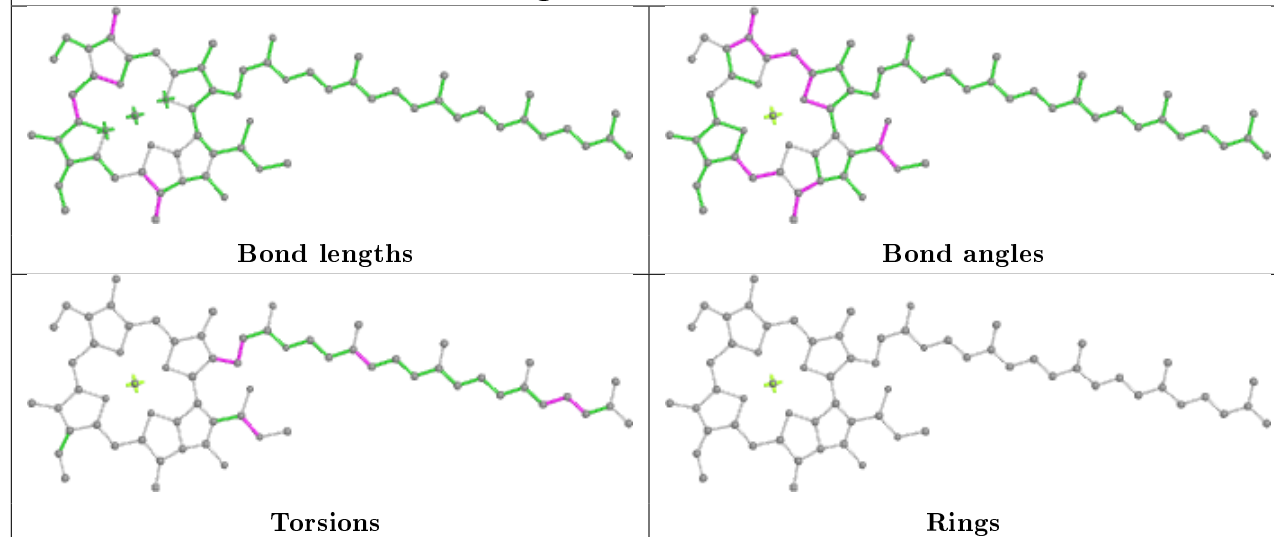
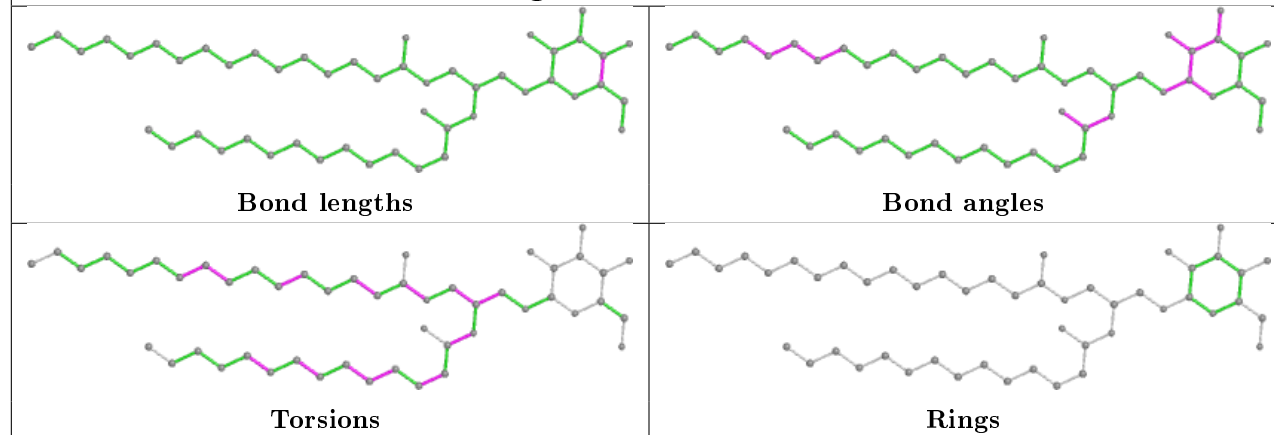


## Ligand CLA B 607

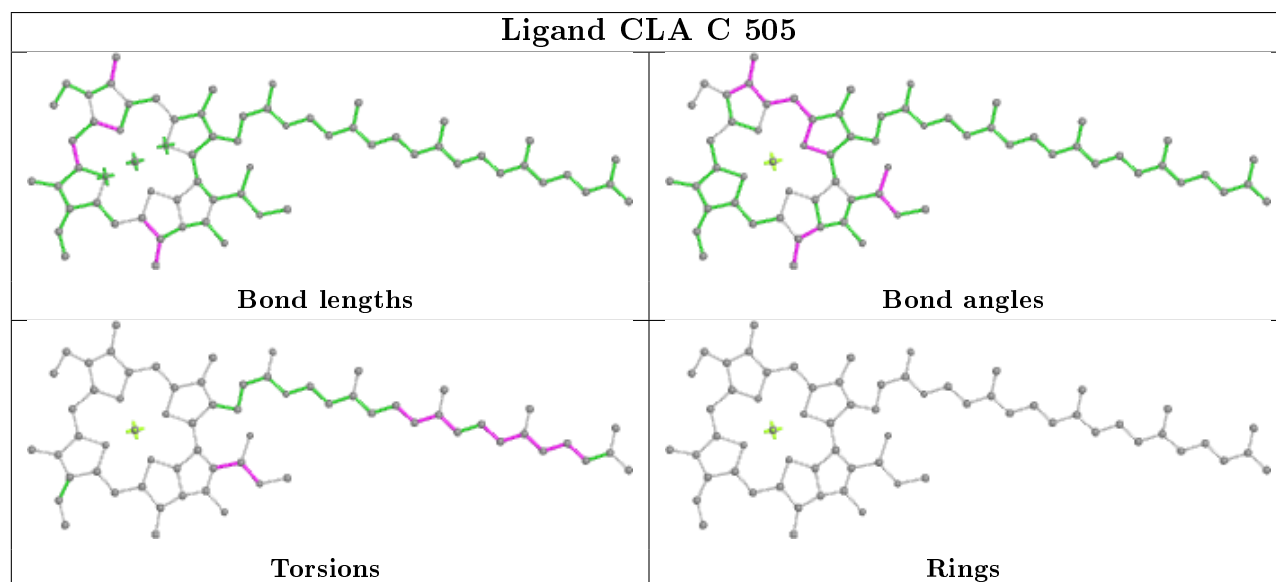
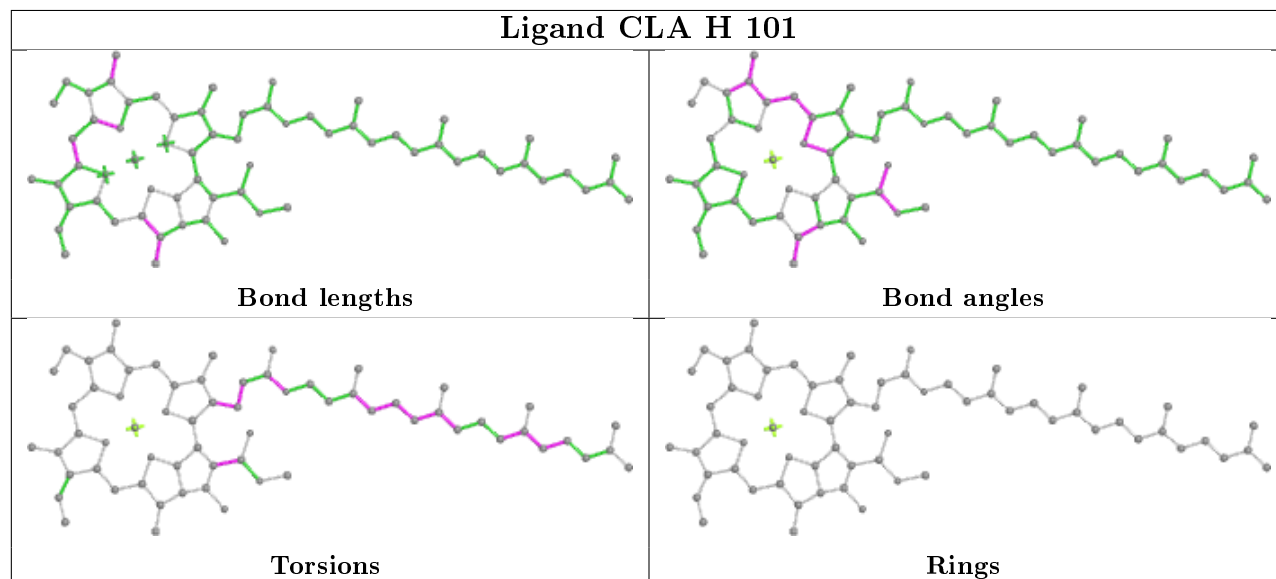
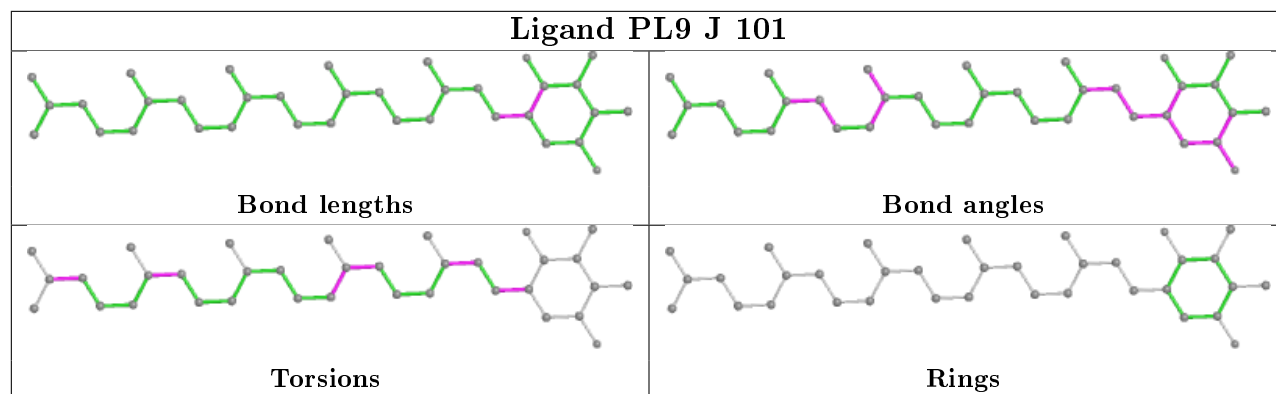


**Ligand CLA C 503****Ligand LMT b 604****Ligand BCR i 101**

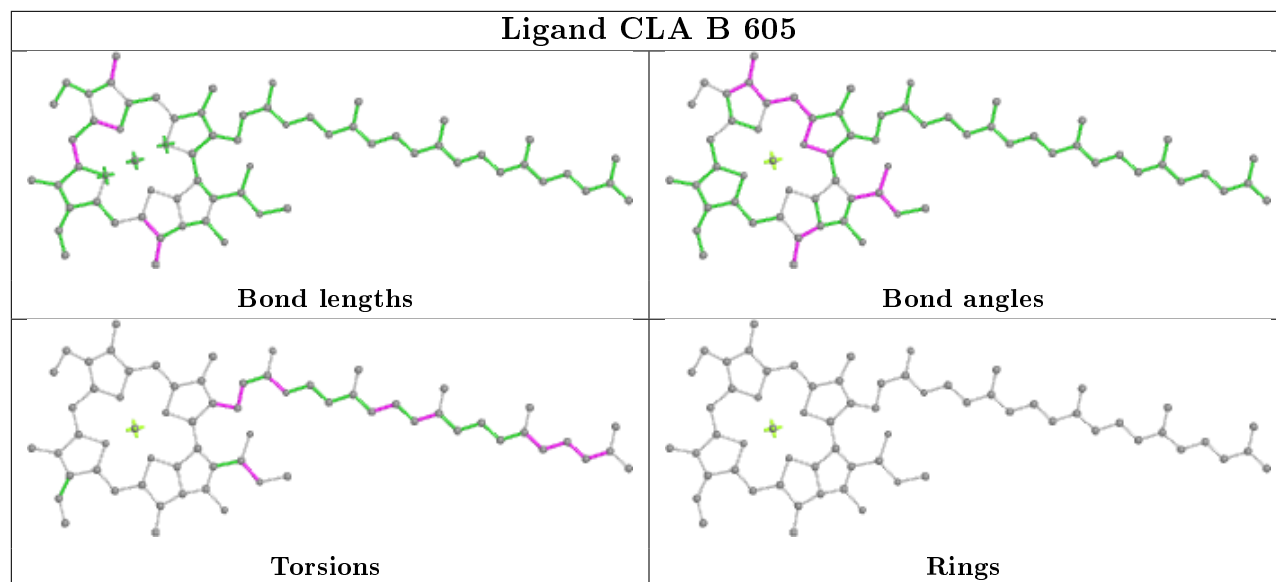


**Ligand CLA c 501****Ligand CLA b 611****Ligand LMG B 621**

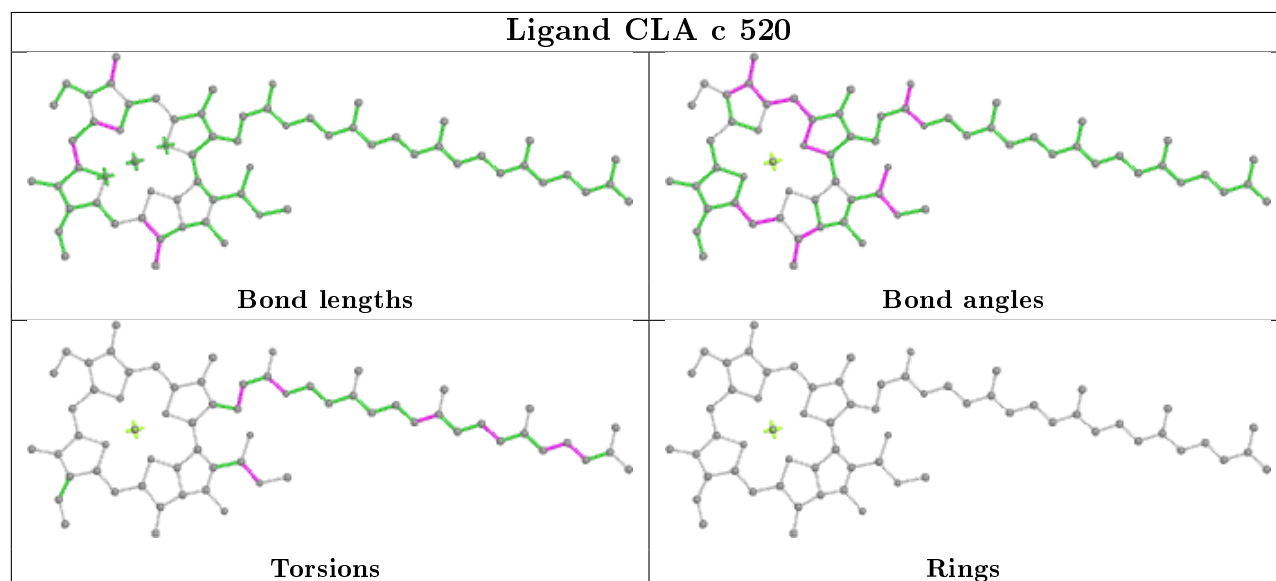




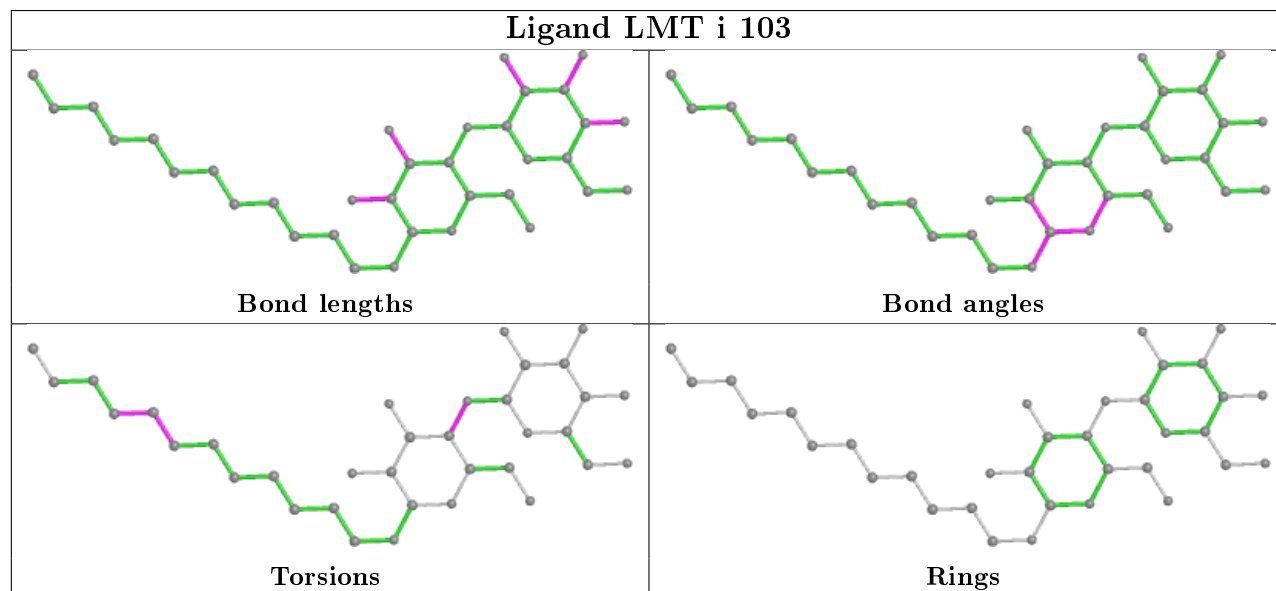
## Ligand CLA B 605

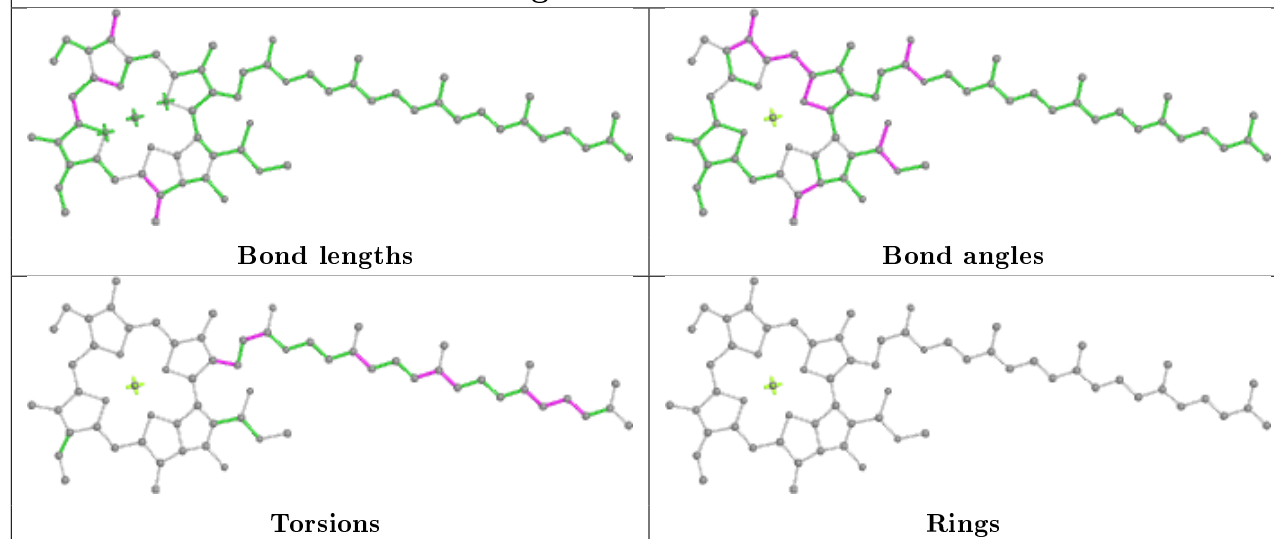
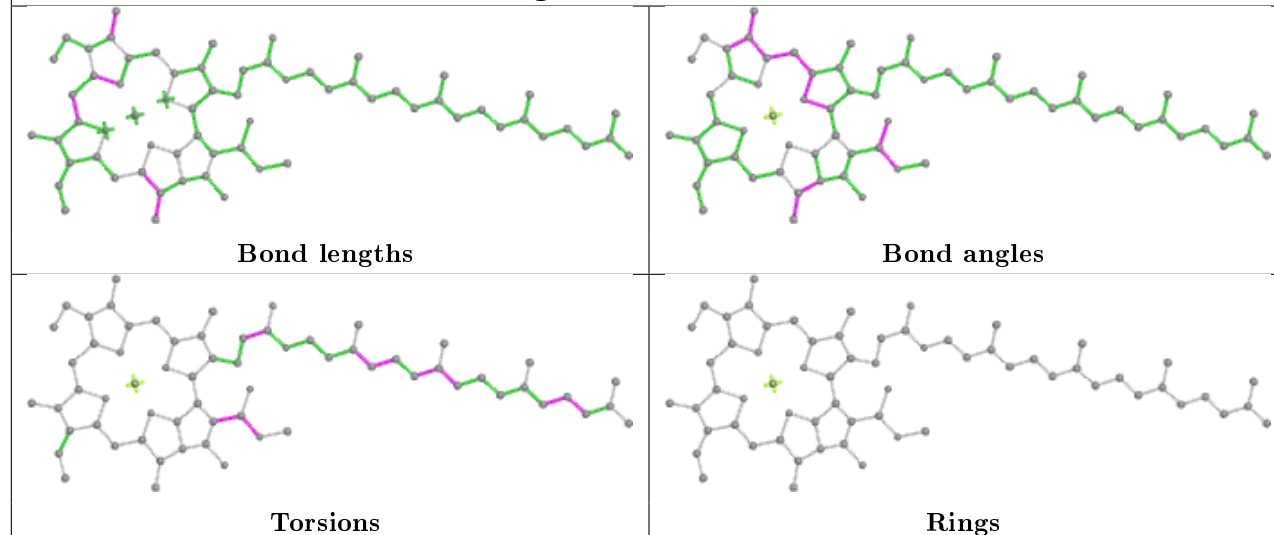
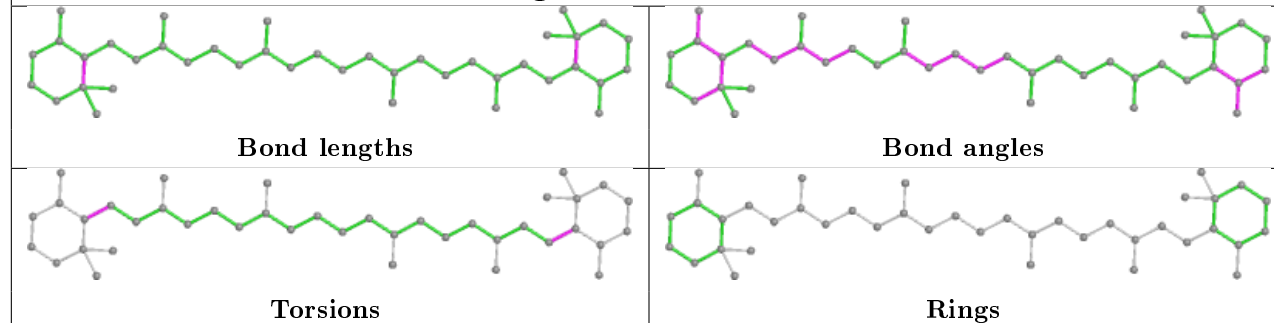


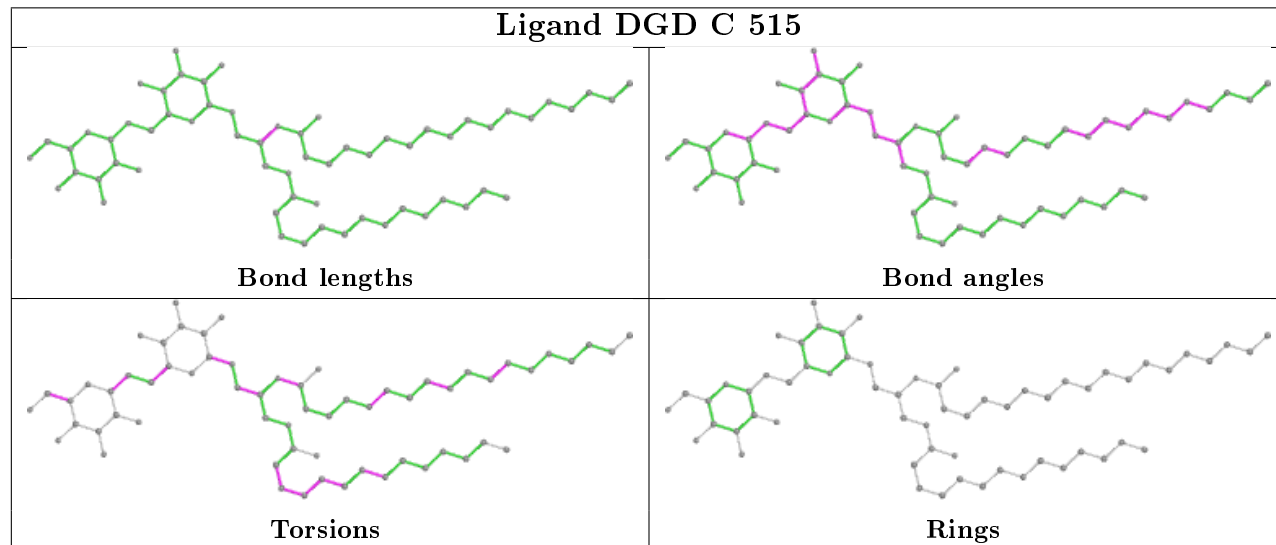
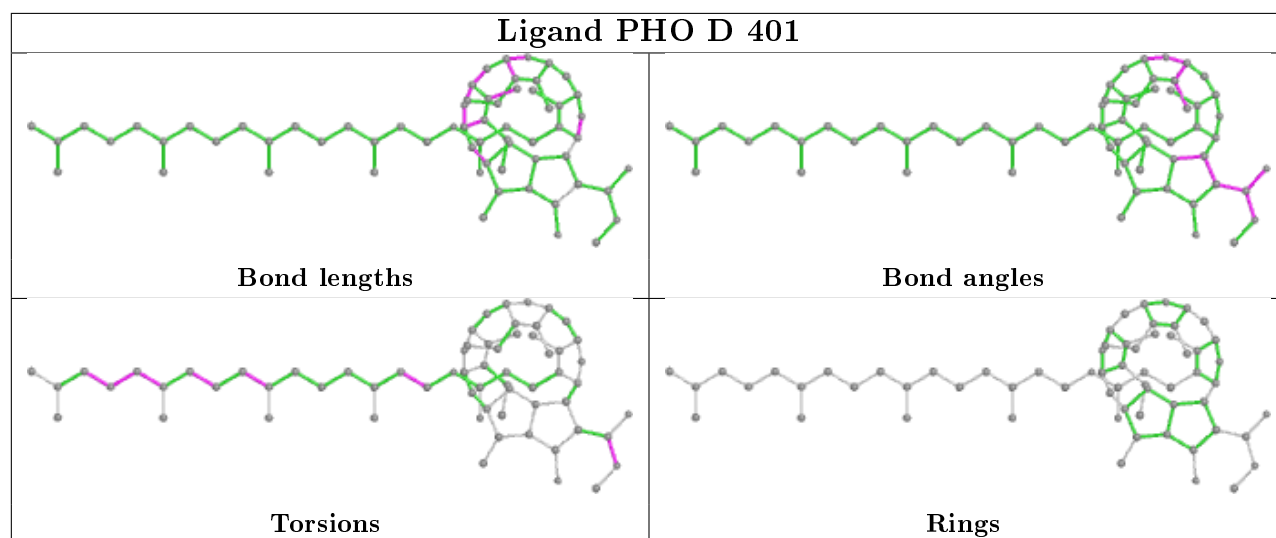
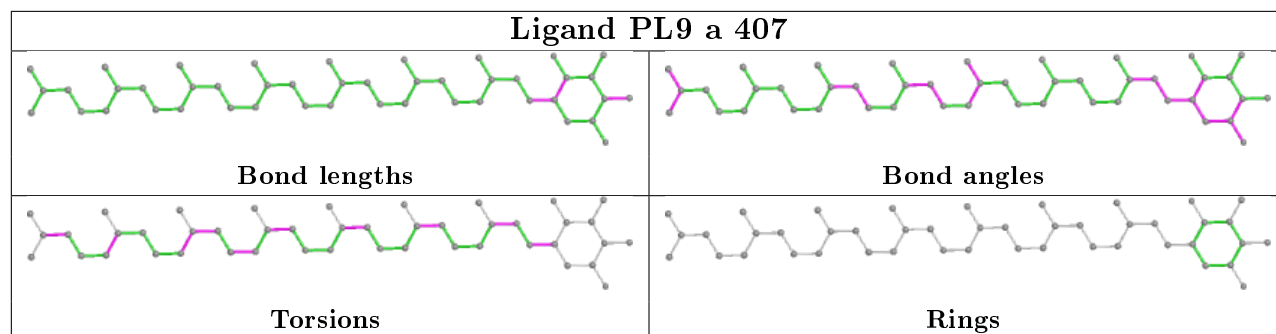
## Ligand CLA c 520

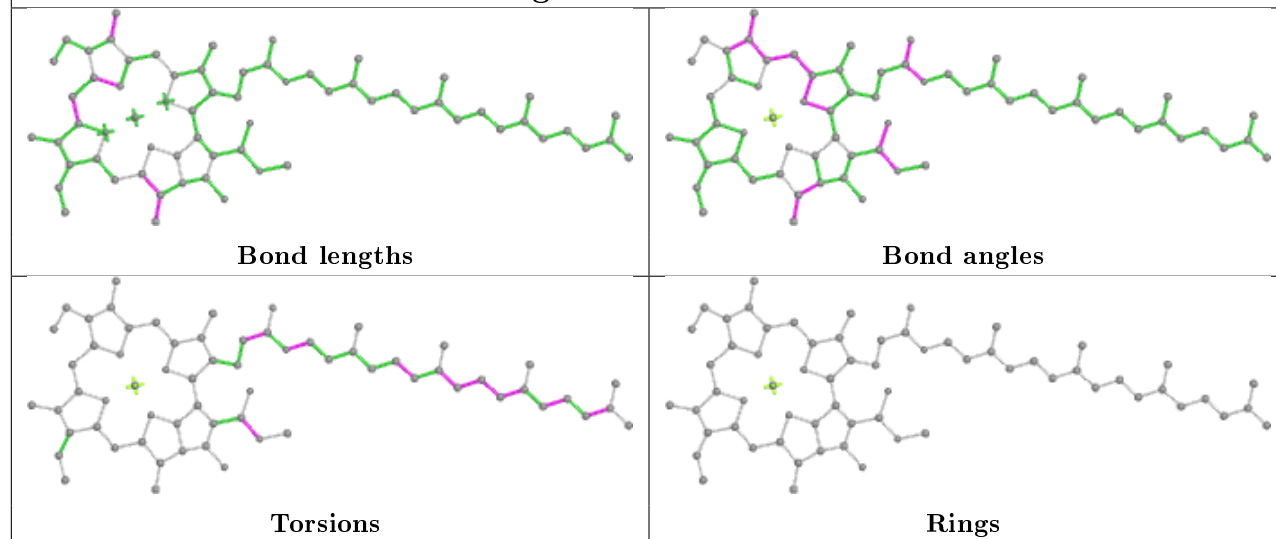
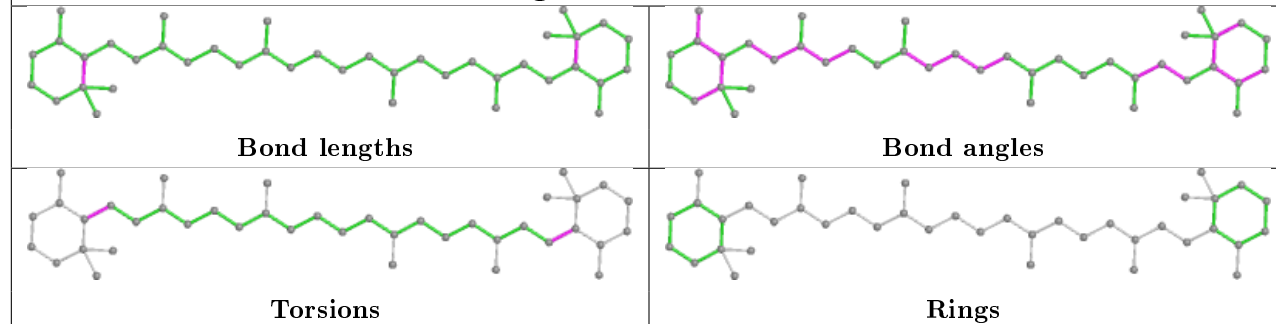
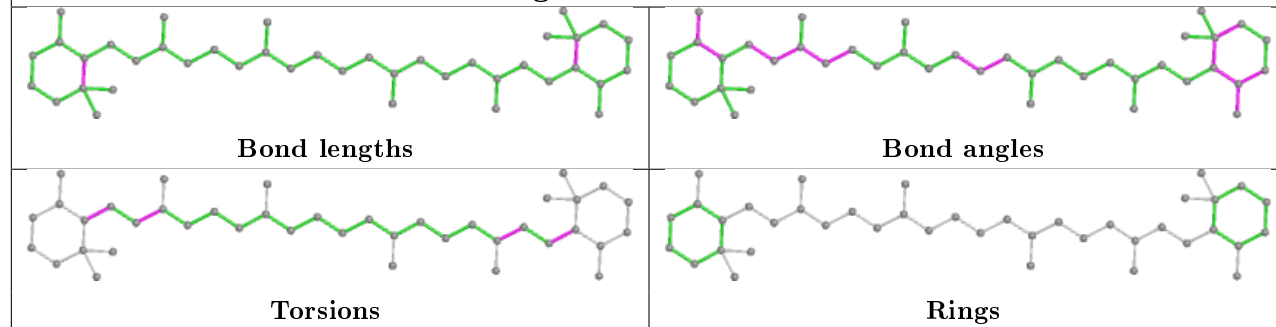


## Ligand LMT i 103

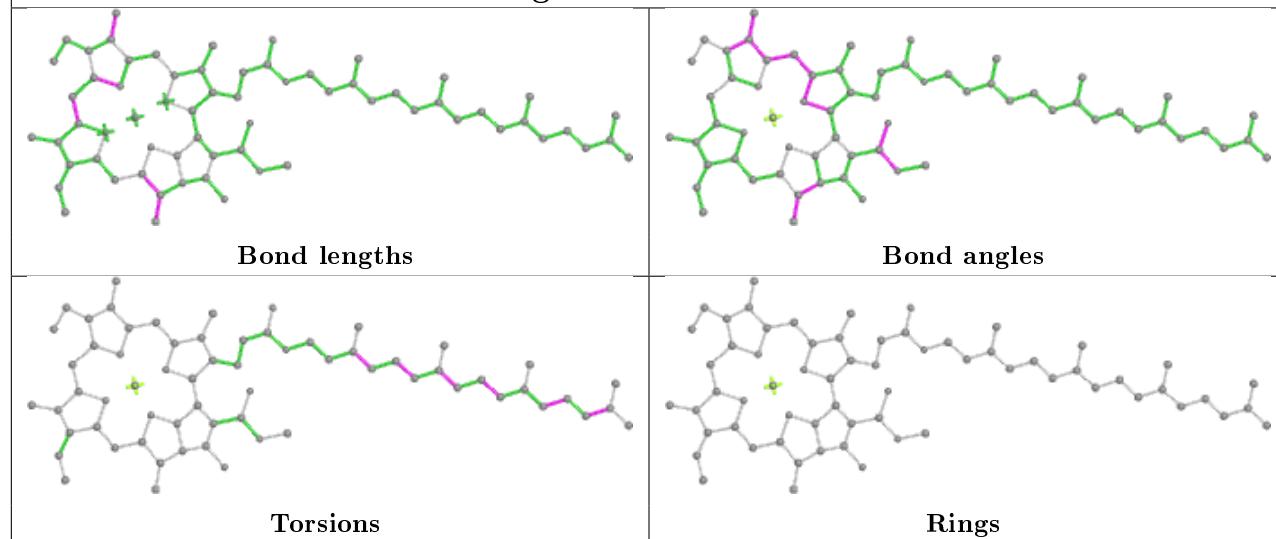


**Ligand CLA D 403****Ligand CLA C 509****Ligand BCR B 616**

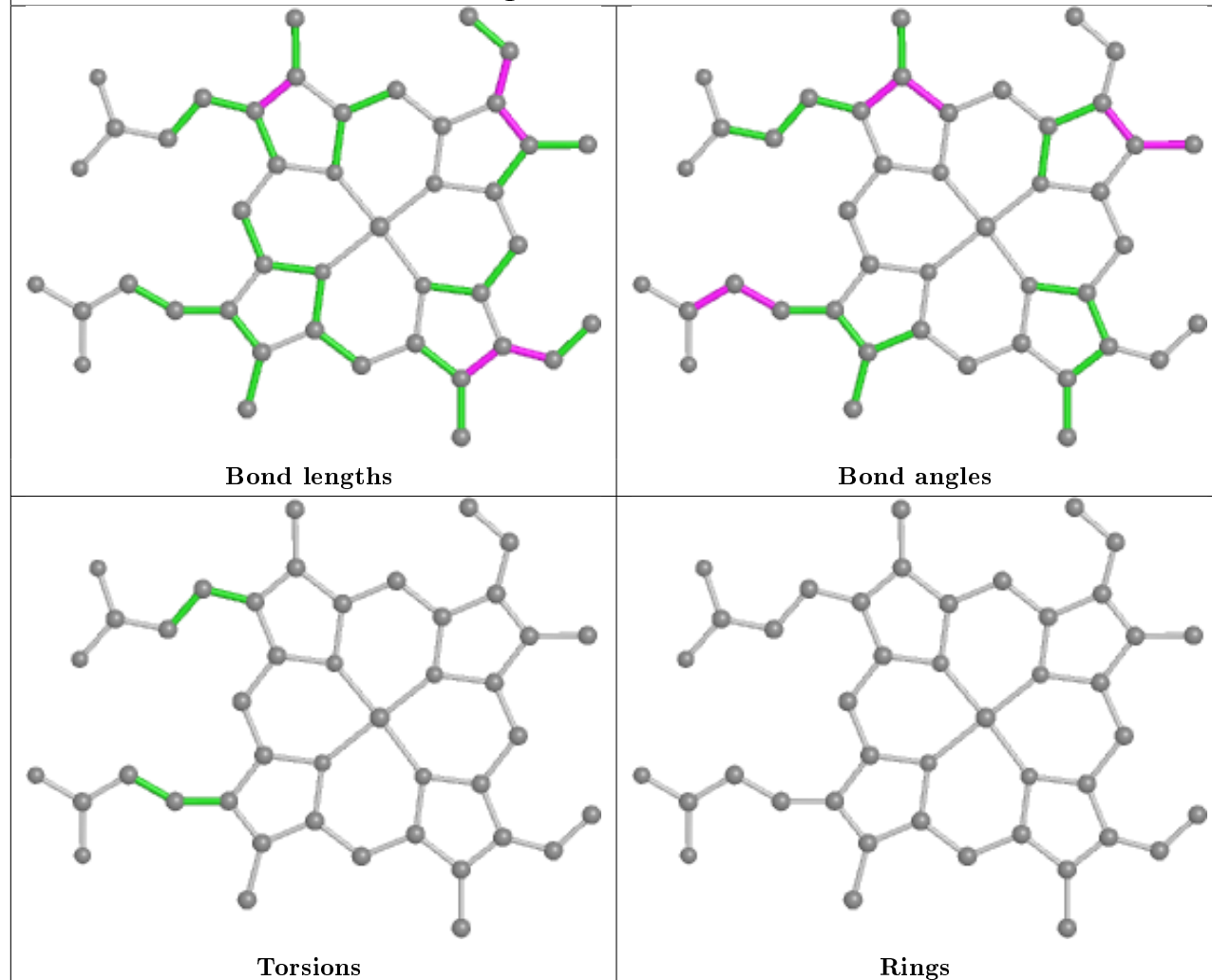


**Ligand CLA B 612****Ligand BCR B 618****Ligand BCR F 102**

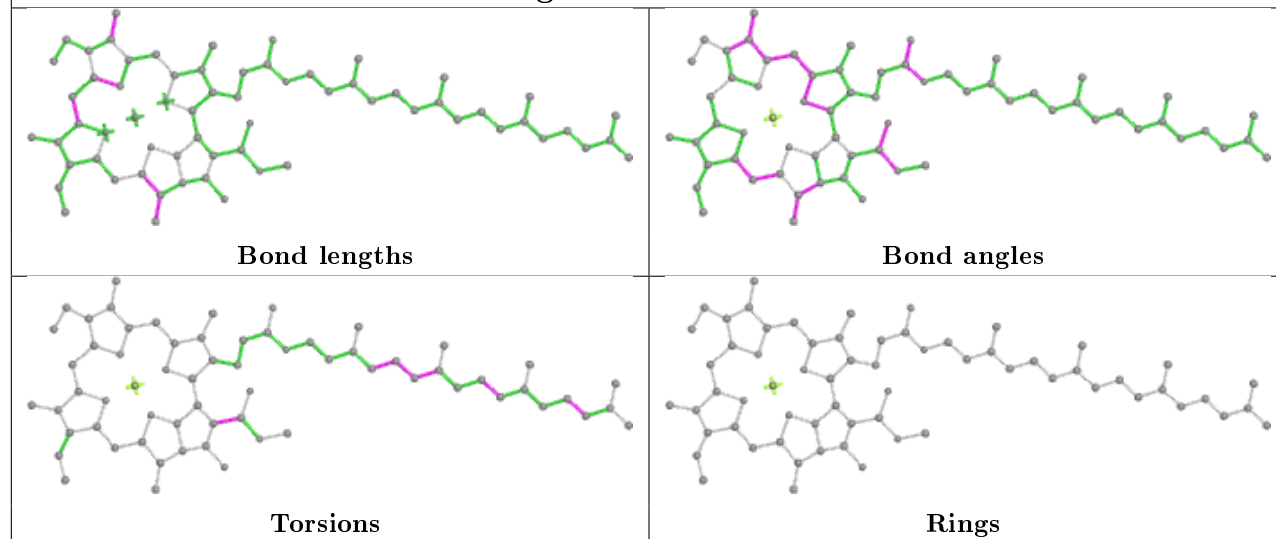
## Ligand CLA A 406



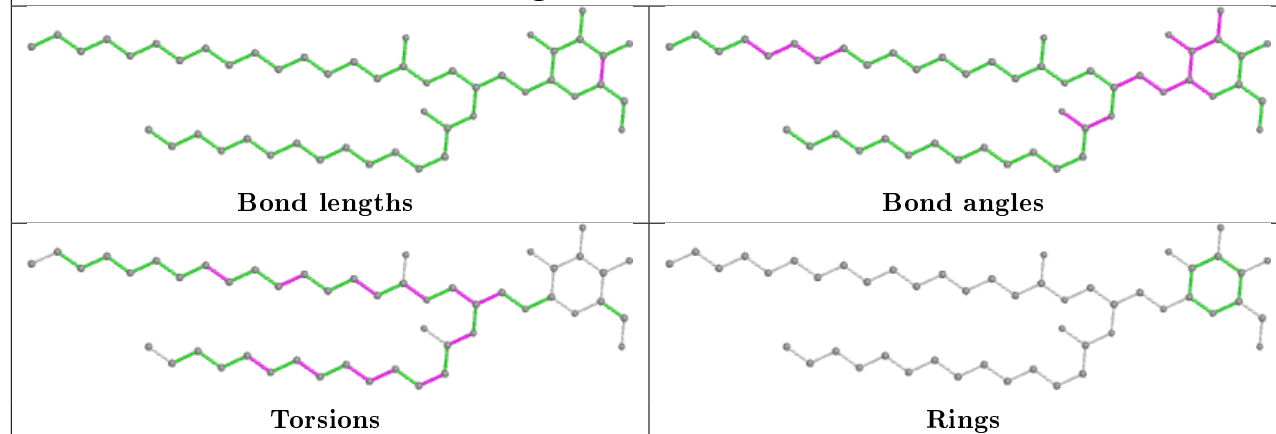
## Ligand HEM F 101



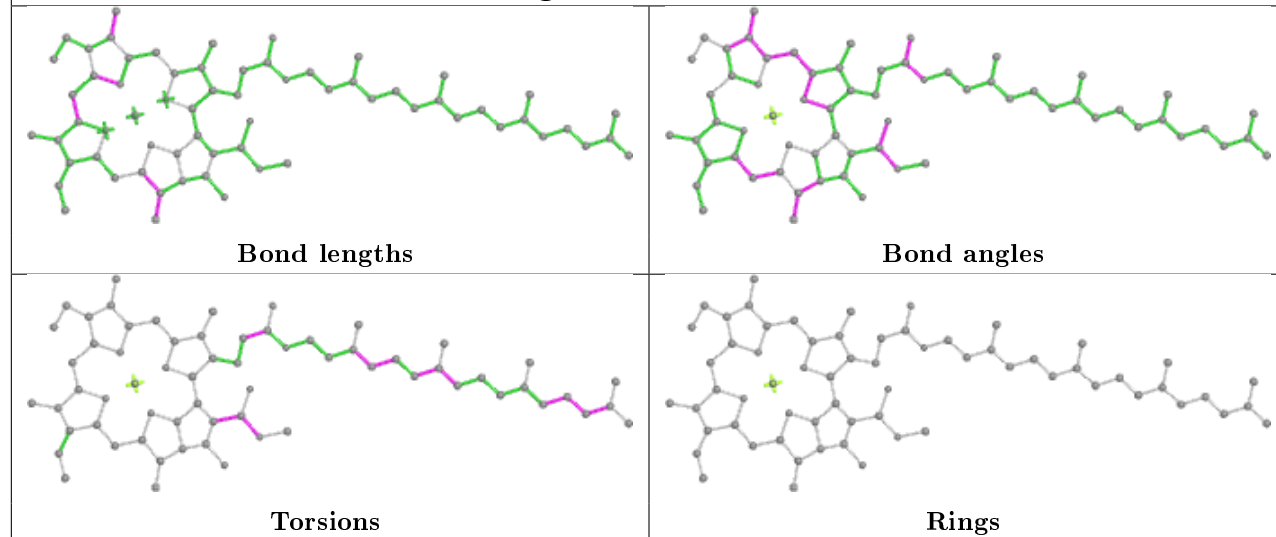
## Ligand CLA a 405

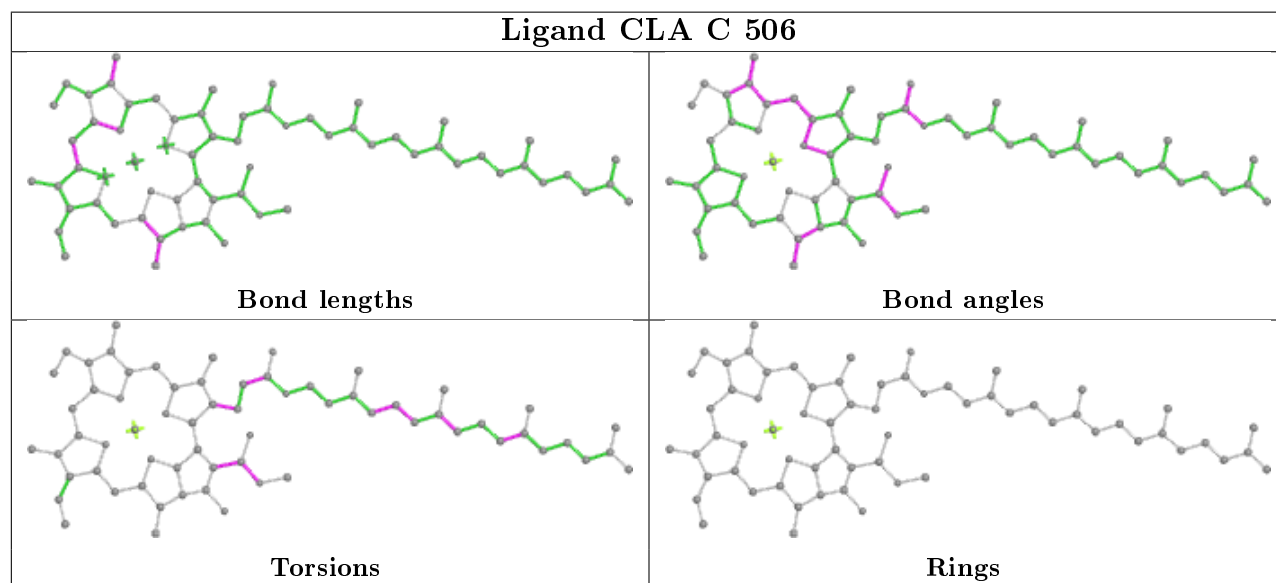
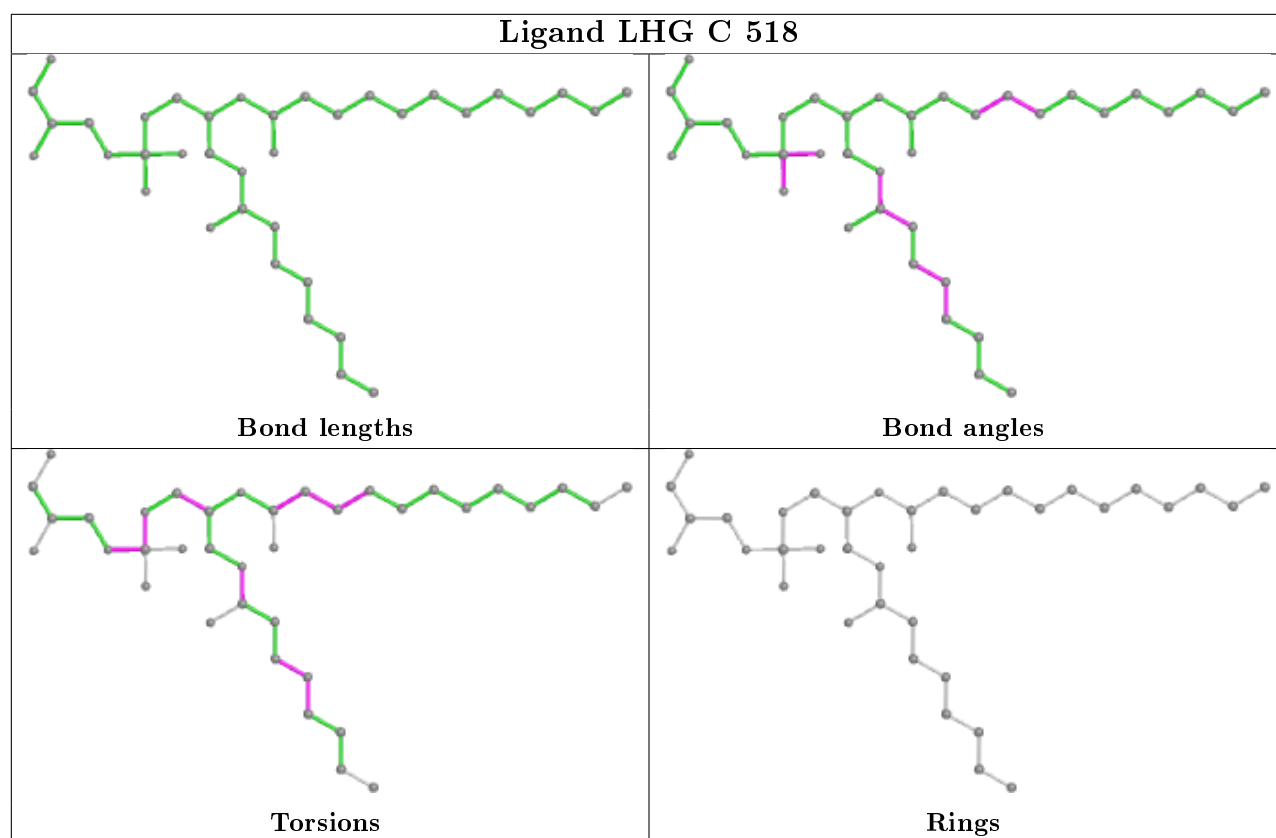


## Ligand LMG b 626

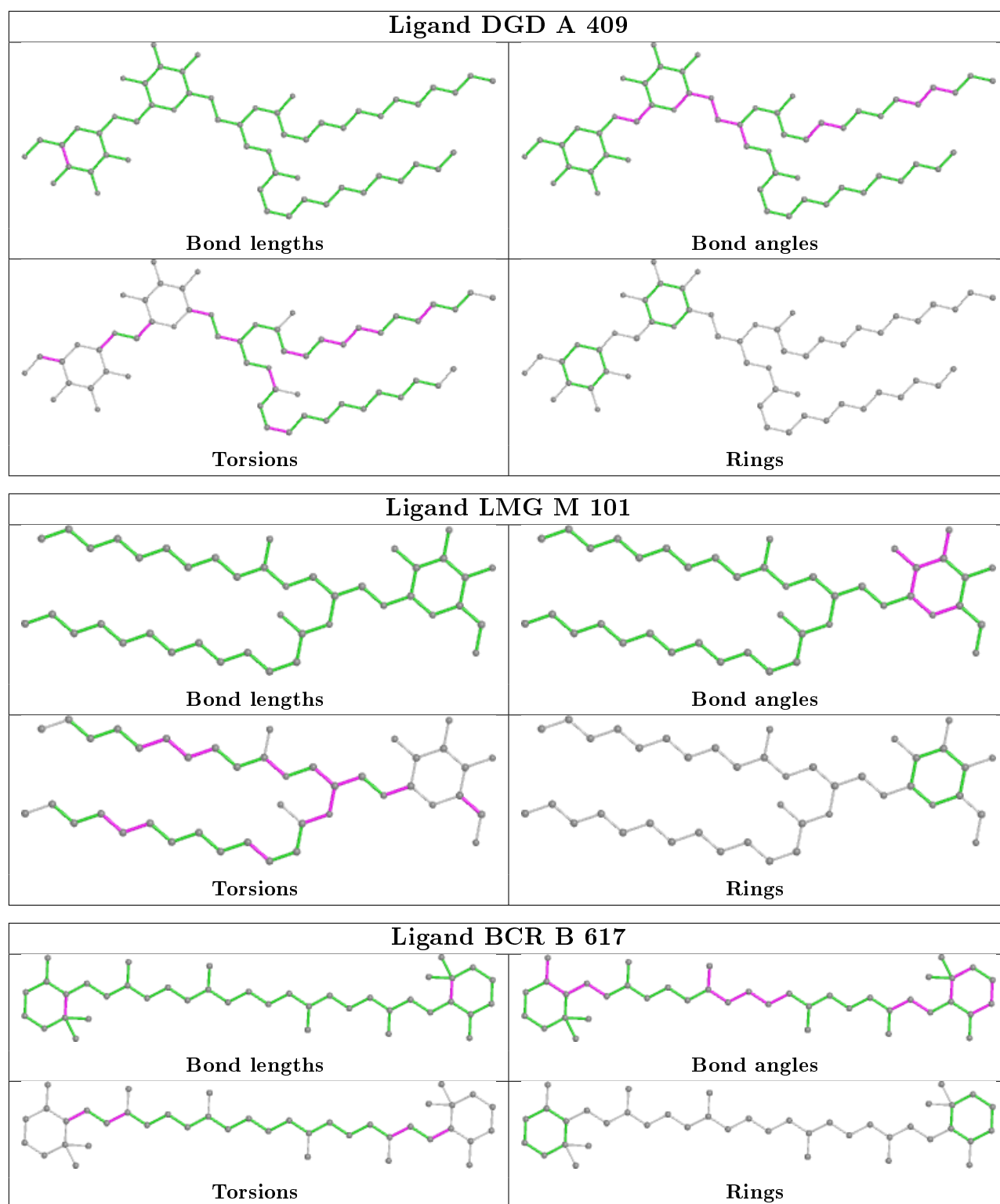


## Ligand CLA c 509









## 5.7 Other polymers ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/344 (97%)	0.68	41 (12%) 4 6	206, 208, 208, 209	0
1	a	335/344 (97%)	0.84	62 (18%) 1 2	206, 208, 209, 209	0
2	B	490/510 (96%)	0.43	41 (8%) 11 11	206, 207, 209, 210	0
2	b	490/510 (96%)	0.67	78 (15%) 1 3	206, 208, 209, 210	0
3	C	447/461 (96%)	0.54	48 (10%) 6 7	206, 208, 209, 209	0
3	c	447/461 (96%)	0.40	36 (8%) 12 11	205, 208, 209, 210	0
4	D	340/352 (96%)	0.34	21 (6%) 20 17	205, 207, 208, 210	0
4	d	340/352 (96%)	0.55	36 (10%) 6 7	206, 208, 209, 209	0
5	E	82/84 (97%)	0.65	7 (8%) 10 10	206, 208, 209, 209	0
5	e	82/84 (97%)	0.38	5 (6%) 21 18	207, 208, 209, 209	0
6	F	35/45 (77%)	0.08	2 (5%) 23 21	207, 207, 208, 209	0
6	f	35/45 (77%)	0.11	5 (14%) 2 4	207, 208, 209, 209	0
7	H	65/66 (98%)	0.74	11 (16%) 1 3	206, 208, 209, 209	0
7	h	65/66 (98%)	1.18	23 (35%) 0 1	207, 208, 209, 209	0
8	I	35/38 (92%)	1.08	9 (25%) 0 1	207, 208, 209, 209	0
8	i	35/38 (92%)	0.33	1 (2%) 51 41	206, 207, 209, 210	0
9	J	34/40 (85%)	0.46	3 (8%) 10 10	207, 208, 208, 209	0
9	j	34/40 (85%)	-0.36	0 100 100	206, 208, 209, 209	0
10	K	37/46 (80%)	0.12	2 (5%) 25 23	207, 208, 209, 209	0
10	k	37/46 (80%)	0.18	2 (5%) 25 23	207, 208, 209, 209	0
11	L	37/37 (100%)	0.68	3 (8%) 12 11	207, 208, 209, 209	0
11	l	37/37 (100%)	0.52	5 (13%) 3 4	206, 208, 209, 210	0
12	M	34/36 (94%)	0.56	3 (8%) 10 10	206, 207, 208, 209	0
12	m	34/36 (94%)	0.31	2 (5%) 22 19	207, 207, 208, 209	0

*Continued on next page...*

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	0.96	47 (19%) 1 2	205, 208, 209, 210	0
13	o	243/272 (89%)	0.91	32 (13%) 3 5	206, 208, 209, 210	0
14	T	32/32 (100%)	0.40	1 (3%) 49 39	206, 208, 208, 209	0
14	t	32/32 (100%)	0.67	3 (9%) 8 9	206, 207, 209, 209	0
15	U	97/134 (72%)	0.97	8 (8%) 11 11	206, 207, 208, 209	0
15	u	97/134 (72%)	1.15	19 (19%) 1 2	206, 207, 208, 209	0
16	V	137/163 (84%)	0.39	10 (7%) 15 13	206, 207, 208, 209	0
16	v	137/163 (84%)	0.76	19 (13%) 2 4	206, 208, 209, 209	0
17	g	28/46 (60%)	0.17	2 (7%) 16 14	207, 208, 209, 209	0
17	y	28/46 (60%)	0.40	2 (7%) 16 14	206, 208, 209, 209	0
18	X	37/41 (90%)	0.68	7 (18%) 1 2	206, 208, 209, 210	0
18	x	37/41 (90%)	0.87	6 (16%) 1 3	207, 208, 208, 209	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.24	1 (1%) 72 62	206, 207, 208, 209	0
20	z	62/62 (100%)	0.57	3 (4%) 30 26	207, 208, 209, 210	0
All	All	5214/5674 (91%)	0.60	606 (11%) 4 6	205, 208, 209, 210	0

The worst 5 of 606 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	84	LYS	9.2
1	A	190	HIS	6.9
3	c	202	PRO	6.7
2	B	84	THR	6.6
1	a	299	GLY	6.4

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	PL9	J	101	35/55	0.19	0.59	206,207,210,210	0
32	LMT	I	102	35/35	0.26	1.23	206,208,210,210	0
24	PL9	j	101	35/55	0.30	0.49	205,208,209,210	0
32	LMT	i	103	35/35	0.30	1.35	206,209,210,210	0
35	CA	O	301	1/1	0.31	0.46	208,208,208,208	0
35	CA	K	102	1/1	0.44	0.74	210,210,210,210	0
24	PL9	d	407	55/55	0.48	0.54	205,207,208,208	0
31	LMG	I	101	43/55	0.49	1.17	205,208,210,211	0
31	LMG	b	627	42/55	0.49	0.56	204,207,211,211	0
31	LMG	C	517	45/55	0.50	1.11	206,207,209,210	0
22	CLA	c	502	65/65	0.51	0.70	206,207,208,209	0
25	BCR	F	102	40/40	0.53	0.56	205,207,208,208	0
31	LMG	e	101	44/55	0.55	0.55	205,208,209,211	0
22	CLA	b	605	65/65	0.56	1.38	206,208,210,210	0
26	DGD	a	408	56/66	0.56	0.50	206,208,210,211	0
26	DGD	A	409	56/66	0.56	0.58	206,208,210,211	0
25	BCR	b	624	40/40	0.57	1.02	205,206,207,208	0
21	FE2	a	413	1/1	0.57	0.23	206,206,206,206	0
32	LMT	d	411	31/35	0.57	0.80	206,209,210,211	0
25	BCR	J	102	40/40	0.60	0.36	205,207,209,209	0
28	CL	A	411	1/1	0.60	0.80	204,204,204,204	0
35	CA	o	301	1/1	0.61	0.65	209,209,209,209	0
25	BCR	H	102	40/40	0.61	1.22	206,207,209,210	0
22	CLA	B	601	65/65	0.62	0.70	205,208,209,209	0
23	PHO	d	401	64/64	0.62	0.51	206,207,208,208	0
25	BCR	C	513	40/40	0.62	1.11	205,207,208,208	0
26	DGD	d	410	63/66	0.62	0.79	206,208,210,211	0
21	FE2	A	401	1/1	0.62	0.17	209,209,209,209	0
24	PL9	A	407	45/55	0.62	0.46	206,207,208,210	0
24	PL9	D	405	55/55	0.63	0.43	205,207,208,208	0
31	LMG	i	102	43/55	0.64	0.83	205,207,209,210	0
24	PL9	a	407	45/55	0.64	0.44	205,207,208,209	0
26	DGD	C	516	66/66	0.64	0.43	205,207,208,208	0
22	CLA	C	502	65/65	0.64	0.58	206,207,208,208	0
25	BCR	c	514	40/40	0.65	1.27	206,208,208,209	0
32	LMT	b	629	35/35	0.65	0.93	206,208,209,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	LMT	b	628	35/35	0.65	0.55	206,208,210,210	0
22	CLA	b	620	65/65	0.66	1.17	206,208,209,210	0
32	LMT	D	408	31/35	0.66	0.73	207,208,210,210	0
30	SQD	B	627	47/54	0.67	0.68	206,208,210,212	0
25	BCR	f	102	40/40	0.67	0.39	206,207,208,209	0
31	LMG	a	402	42/55	0.68	0.42	204,207,209,210	0
22	CLA	C	512	65/65	0.69	0.92	205,207,209,211	0
31	LMG	m	101	42/55	0.69	0.51	205,207,209,210	0
32	LMT	M	102	35/35	0.69	0.42	205,208,209,209	0
32	LMT	B	623	35/35	0.69	0.81	206,208,210,210	0
31	LMG	C	521	48/55	0.69	0.34	206,207,208,209	0
32	LMT	b	604	35/35	0.70	0.35	207,208,210,210	0
26	DGD	D	407	63/66	0.70	0.72	206,208,209,210	0
25	BCR	B	616	40/40	0.70	0.41	205,207,208,209	0
32	LMT	b	603	35/35	0.71	0.66	206,208,210,210	0
22	CLA	c	512	65/65	0.71	0.82	206,207,209,210	0
25	BCR	x	101	40/40	0.71	0.91	206,207,209,209	0
22	CLA	C	505	65/65	0.71	0.67	206,207,209,210	0
31	LMG	E	101	44/55	0.71	0.47	204,208,209,210	0
32	LMT	B	629	35/35	0.72	0.39	206,208,209,210	0
22	CLA	a	406	65/65	0.72	0.81	206,208,208,209	0
30	SQD	d	403	43/54	0.72	0.80	205,208,209,209	0
25	BCR	c	513	40/40	0.72	0.92	206,207,208,209	0
25	BCR	j	102	40/40	0.73	0.26	206,208,209,210	0
25	BCR	g	101	40/40	0.73	0.82	205,207,208,209	0
31	LMG	c	518	45/55	0.73	0.88	206,208,209,210	0
30	SQD	b	602	47/54	0.73	0.44	205,208,209,212	0
25	BCR	B	619	40/40	0.73	1.17	205,207,208,208	0
22	CLA	C	508	65/65	0.74	0.87	205,207,208,209	0
30	SQD	B	622	43/54	0.74	0.60	205,208,209,212	0
32	LMT	B	624	35/35	0.74	0.53	206,207,211,212	0
32	LMT	B	628	35/35	0.74	0.61	206,208,210,211	0
25	BCR	B	617	40/40	0.74	0.34	205,207,208,209	0
31	LMG	c	522	48/55	0.75	0.33	205,207,209,210	0
22	CLA	B	613	65/65	0.75	0.46	206,207,208,209	0
26	DGD	B	626	52/66	0.75	0.55	206,208,210,211	0
22	CLA	b	619	65/65	0.75	0.96	206,208,209,209	0
22	CLA	a	405	65/65	0.75	0.41	205,207,209,209	0
25	BCR	b	622	40/40	0.75	0.32	205,207,208,208	0
25	BCR	A	408	40/40	0.75	0.55	206,207,208,208	0
25	BCR	C	520	40/40	0.76	1.09	206,207,209,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	b	623	40/40	0.76	0.31	205,206,207,207	0
22	CLA	c	510	65/65	0.76	0.46	206,208,209,211	0
22	CLA	d	405	65/65	0.77	0.46	205,207,208,208	0
25	BCR	i	101	40/40	0.77	0.70	206,207,208,208	0
22	CLA	C	506	65/65	0.77	0.94	206,207,208,209	0
22	CLA	C	511	65/65	0.77	1.22	206,207,208,209	0
32	LMT	M	103	35/35	0.77	0.35	206,208,209,209	0
22	CLA	b	618	65/65	0.78	0.38	206,207,209,210	0
22	CLA	a	404	65/65	0.78	0.80	204,207,208,208	0
22	CLA	A	406	65/65	0.78	0.78	206,208,209,209	0
26	DGD	b	625	58/66	0.78	0.37	206,207,208,209	0
27	LHG	c	519	37/49	0.79	0.28	204,207,210,213	0
31	LMG	d	409	48/55	0.79	0.34	206,207,209,210	0
22	CLA	c	505	65/65	0.79	0.81	205,207,208,209	0
30	SQD	a	401	54/54	0.80	0.60	205,208,210,213	0
26	DGD	b	601	52/66	0.80	0.47	204,208,209,210	0
22	CLA	b	612	65/65	0.80	0.49	205,207,209,209	0
22	CLA	b	616	65/65	0.80	0.45	206,207,208,209	0
22	CLA	a	403	65/65	0.80	0.58	205,207,208,210	0
25	BCR	c	521	40/40	0.80	1.53	206,208,209,209	0
23	PHO	A	405	64/64	0.80	0.40	205,207,208,209	0
30	SQD	A	414	54/54	0.80	0.45	205,207,209,210	0
22	CLA	B	603	65/65	0.80	0.60	205,207,208,208	0
22	CLA	c	508	65/65	0.81	0.56	205,208,209,209	0
30	SQD	f	103	45/54	0.81	0.72	205,208,210,210	0
22	CLA	A	404	65/65	0.81	0.44	204,207,208,209	0
30	SQD	F	103	45/54	0.81	0.63	205,208,209,210	0
22	CLA	b	606	65/65	0.81	0.51	205,207,209,210	0
27	LHG	C	518	37/49	0.81	0.29	205,208,210,211	0
22	CLA	b	608	65/65	0.81	0.44	205,207,208,209	0
22	CLA	b	613	65/65	0.81	0.65	205,207,208,209	0
31	LMG	M	101	42/55	0.81	0.36	205,208,209,210	0
27	LHG	a	409	39/49	0.81	0.32	206,207,209,209	0
33	BCT	d	404	4/4	0.82	0.85	206,207,208,208	0
23	PHO	d	402	64/64	0.82	0.26	206,207,209,209	0
22	CLA	B	615	65/65	0.82	0.99	206,207,209,209	0
22	CLA	c	506	65/65	0.82	0.92	206,208,209,209	0
31	LMG	D	409	46/55	0.82	0.35	205,207,208,209	0
22	CLA	C	504	65/65	0.82	0.42	205,207,208,209	0
25	BCR	y	101	40/40	0.82	0.81	206,207,208,208	0
22	CLA	C	507	65/65	0.82	0.36	206,207,208,208	0
35	CA	k	101	1/1	0.83	0.29	208,208,208,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	LMG	l	101	51/55	0.83	0.29	206,207,209,209	0
23	PHO	D	401	64/64	0.83	0.36	205,207,208,209	0
22	CLA	B	614	65/65	0.83	0.91	205,207,208,209	0
22	CLA	b	614	65/65	0.83	0.71	206,207,209,210	0
34	HEM	v	201	43/43	0.83	0.72	206,207,208,209	0
22	CLA	c	511	65/65	0.83	0.97	206,208,209,209	0
26	DGD	B	620	58/66	0.83	0.38	205,207,209,209	0
22	CLA	d	406	65/65	0.83	0.66	206,207,209,209	0
22	CLA	C	509	65/65	0.83	0.37	205,207,208,208	0
30	SQD	A	413	51/54	0.84	0.26	204,207,209,209	0
22	CLA	c	504	65/65	0.84	0.44	205,207,208,209	0
26	DGD	c	517	66/66	0.84	0.25	206,207,209,209	0
22	CLA	C	501	65/65	0.84	0.58	206,208,209,209	0
22	CLA	c	501	65/65	0.84	0.75	206,207,209,209	0
22	CLA	C	519	65/65	0.84	0.31	205,207,209,209	0
25	BCR	B	618	40/40	0.84	0.29	205,206,208,208	0
31	LMG	D	406	48/55	0.85	0.28	204,207,208,209	0
22	CLA	B	605	65/65	0.85	0.84	206,207,208,209	0
31	LMG	L	101	51/55	0.85	0.31	205,207,208,209	0
26	DGD	C	515	62/66	0.85	0.34	205,207,209,210	0
22	CLA	b	607	65/65	0.85	0.66	205,207,208,208	0
31	LMG	B	621	49/55	0.85	0.23	206,207,208,209	0
22	CLA	b	610	65/65	0.86	0.62	206,207,209,209	0
31	LMG	d	408	49/55	0.86	0.24	205,207,208,209	0
27	LHG	A	410	39/49	0.86	0.25	206,207,209,210	0
22	CLA	b	615	65/65	0.86	0.31	205,207,208,209	0
22	CLA	B	607	65/65	0.86	0.47	206,207,208,209	0
22	CLA	C	503	65/65	0.86	0.41	206,207,208,209	0
22	CLA	B	608	65/65	0.86	0.86	205,207,209,210	0
25	BCR	b	621	40/40	0.86	0.29	206,207,208,208	0
22	CLA	D	404	65/65	0.86	0.71	205,207,208,208	0
22	CLA	c	503	65/65	0.86	0.56	206,207,208,209	0
31	LMG	B	625	49/55	0.86	0.23	205,207,208,208	0
22	CLA	b	609	65/65	0.87	0.60	206,207,208,209	0
22	CLA	B	604	65/65	0.87	0.71	206,207,208,209	0
22	CLA	B	609	65/65	0.87	0.73	206,207,209,210	0
26	DGD	c	515	53/66	0.87	0.34	205,207,209,210	0
31	LMG	b	626	49/55	0.87	0.23	205,207,209,209	0
22	CLA	c	520	65/65	0.88	0.33	206,207,208,209	0
22	CLA	C	510	65/65	0.88	0.56	206,207,209,209	0
22	CLA	D	403	65/65	0.88	0.36	205,207,208,208	0
30	SQD	a	412	51/54	0.89	0.23	205,207,208,209	0

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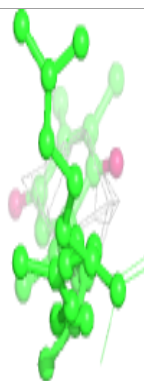
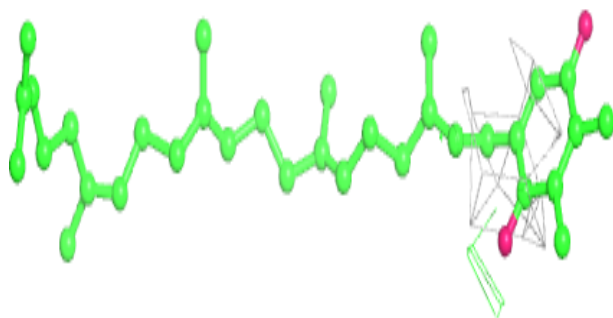
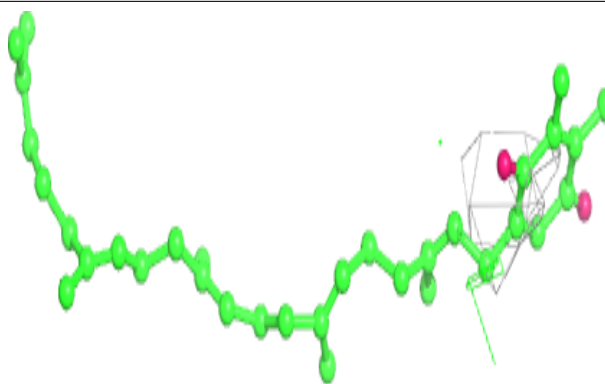
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	A	402	65/65	0.89	0.46	206,207,208,209	0
34	HEM	F	101	43/43	0.89	0.72	206,207,208,210	0
22	CLA	A	403	65/65	0.89	0.62	205,207,208,208	0
26	DGD	C	514	53/66	0.89	0.30	205,206,208,209	0
22	CLA	b	611	65/65	0.90	0.27	206,207,208,209	0
34	HEM	V	201	43/43	0.90	0.44	201,207,208,209	0
22	CLA	B	610	65/65	0.90	0.32	205,207,208,208	0
22	CLA	c	509	65/65	0.90	0.31	206,207,209,209	0
22	CLA	H	101	65/65	0.90	0.40	206,207,208,209	0
31	LMG	d	412	46/55	0.90	0.21	205,207,208,209	0
26	DGD	c	516	62/66	0.90	0.21	206,208,208,209	0
22	CLA	c	507	65/65	0.90	0.31	206,207,209,209	0
25	BCR	K	101	40/40	0.90	0.83	206,207,208,209	0
22	CLA	B	606	65/65	0.91	0.27	205,207,208,209	0
33	BCT	D	402	4/4	0.91	0.40	208,208,208,208	0
22	CLA	B	612	65/65	0.92	0.26	203,207,208,209	0
22	CLA	B	602	65/65	0.92	0.62	205,207,208,209	0
34	HEM	f	101	43/43	0.92	0.43	206,207,209,209	0
22	CLA	B	611	65/65	0.93	0.46	205,207,208,208	0
22	CLA	b	617	65/65	0.93	0.36	206,207,208,209	0
28	CL	a	410	1/1	0.94	0.40	205,205,205,205	0
29	OEX	A	412	10/10	0.94	0.50	197,202,205,206	0
29	OEX	a	411	10/10	0.97	0.54	200,204,205,206	0

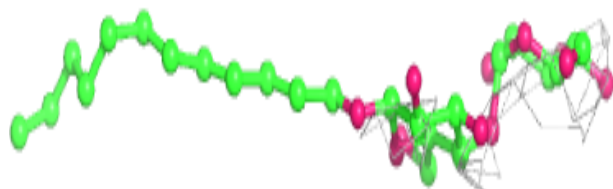
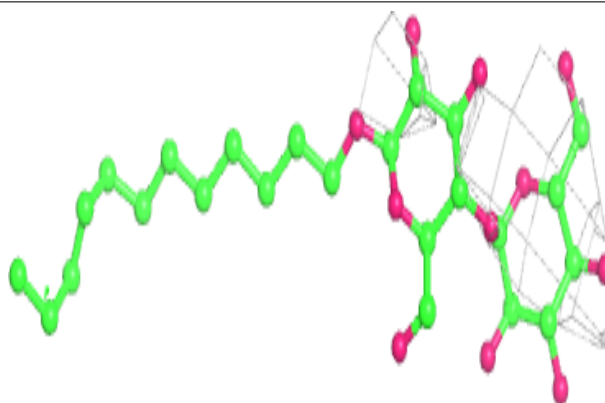
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PL9 J 101:**

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

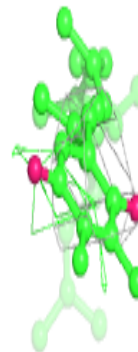
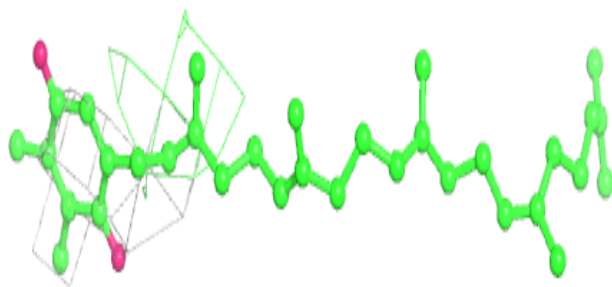
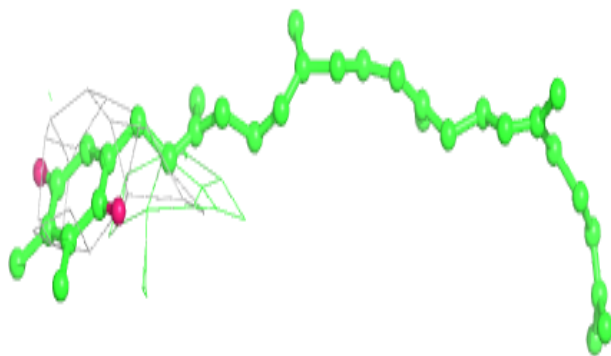
**Electron density around LMT I 102:**

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

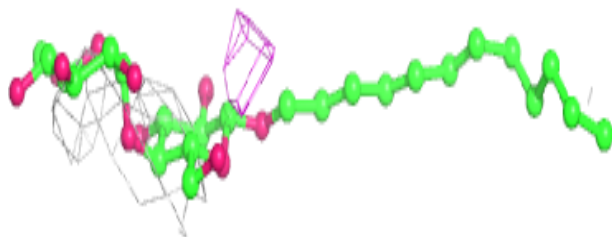
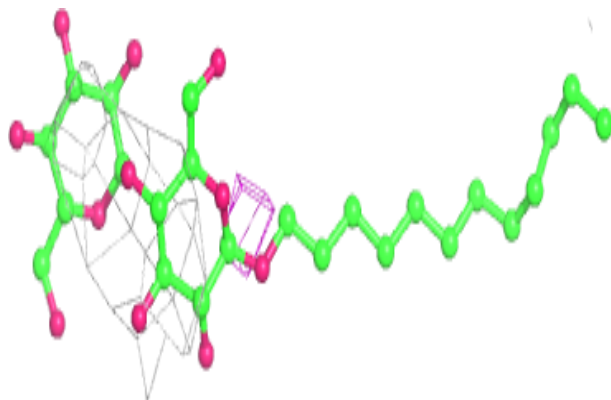


**Electron density around PL9 j 101:**

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

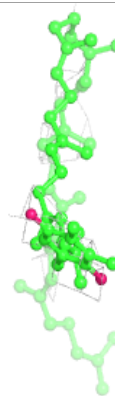
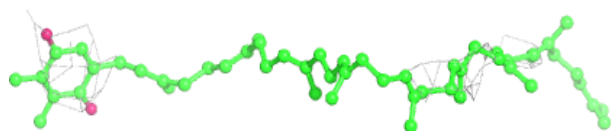
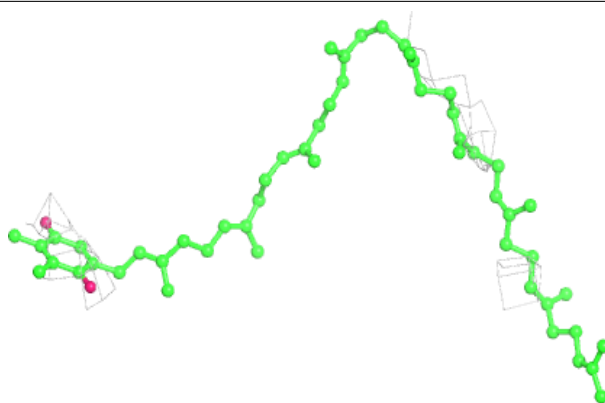
**Electron density around LMT i 103:**

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

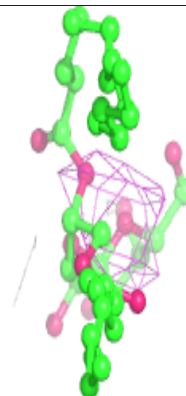
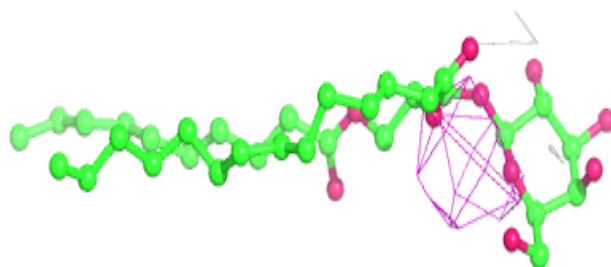
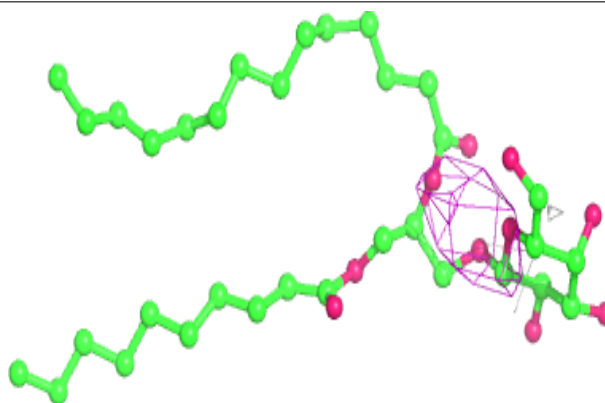


**Electron density around PL9 d 407:**

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

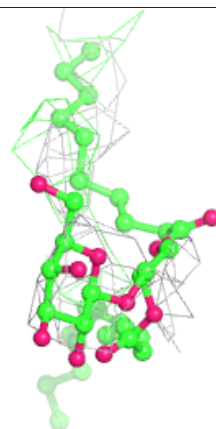
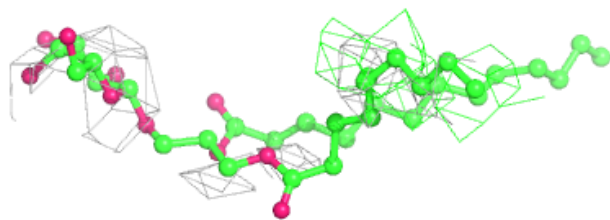
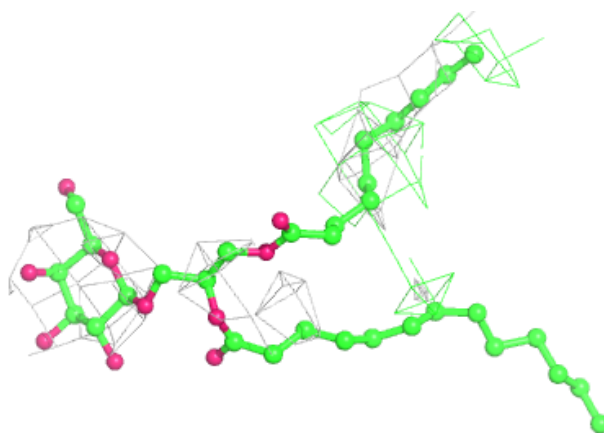
**Electron density around LMG I 101:**

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

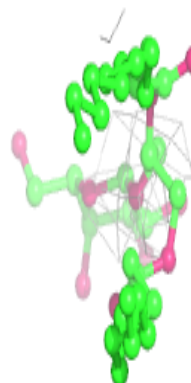
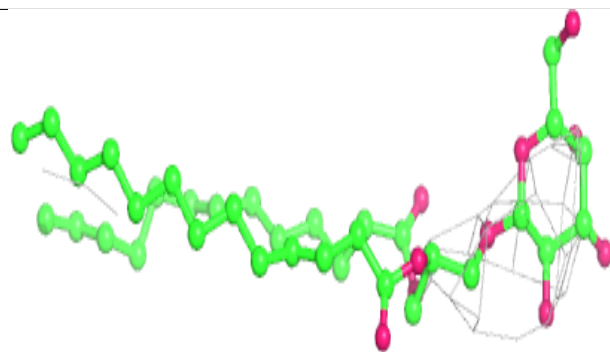
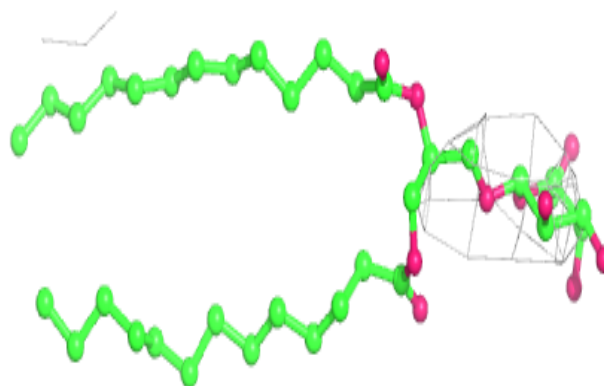


**Electron density around LMG b 627:**

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

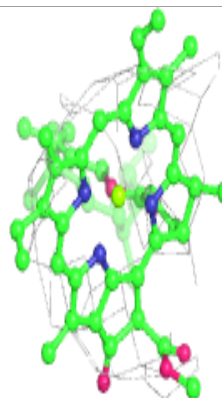
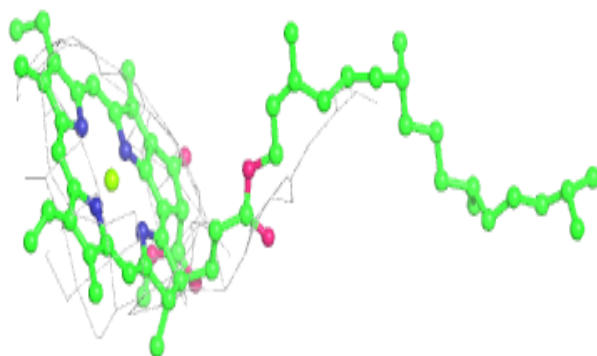
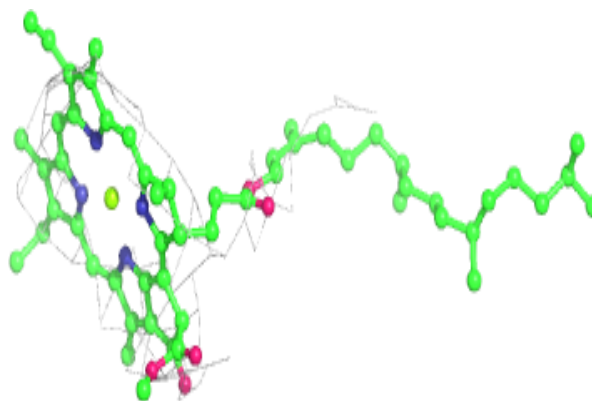
**Electron density around LMG C 517:**

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

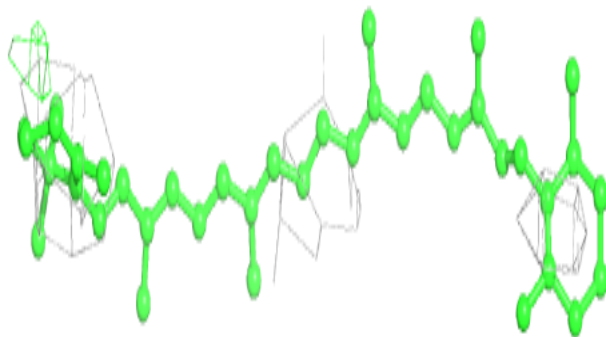
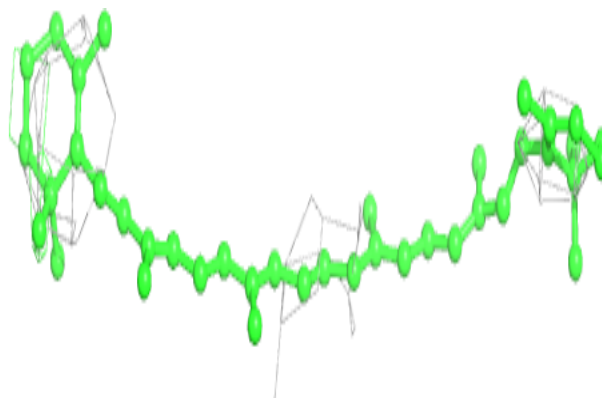


**Electron density around CLA c 502:**

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

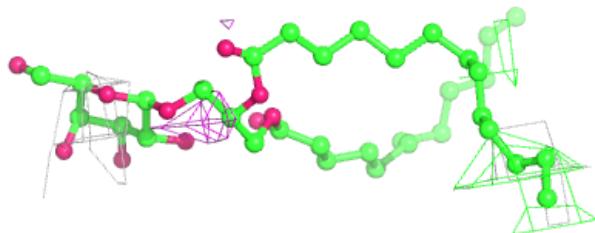
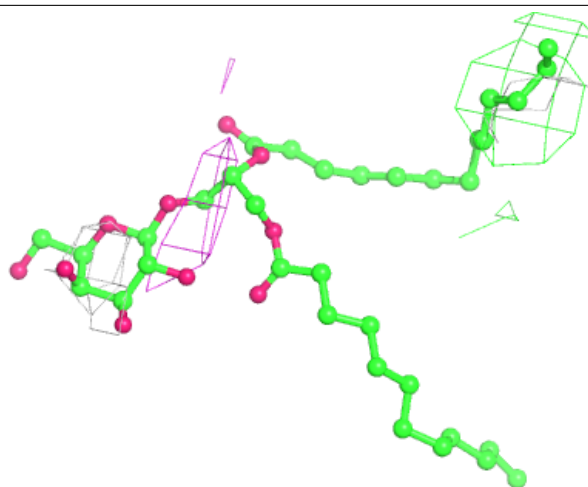
**Electron density around BCR F 102:**

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



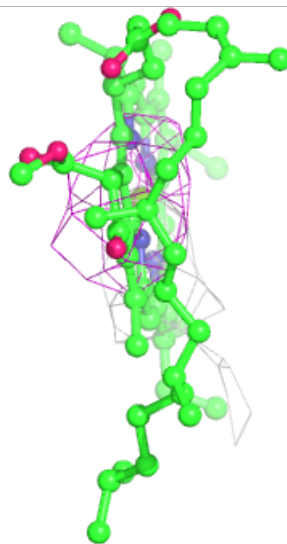
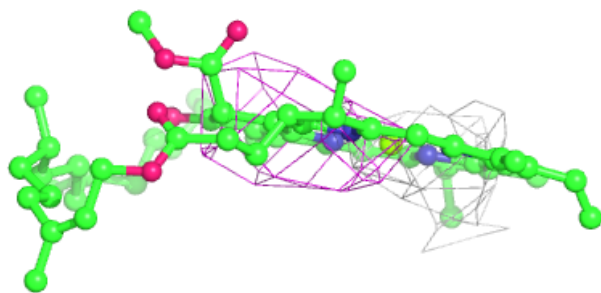
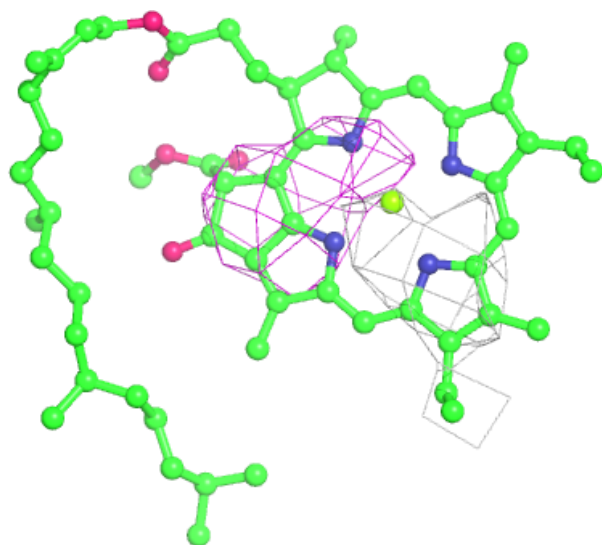
**Electron density around LMG e 101:**

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



**Electron density around CLA b 605:**

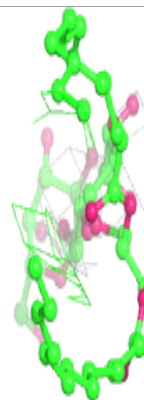
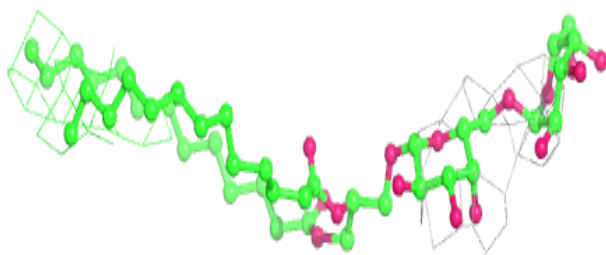
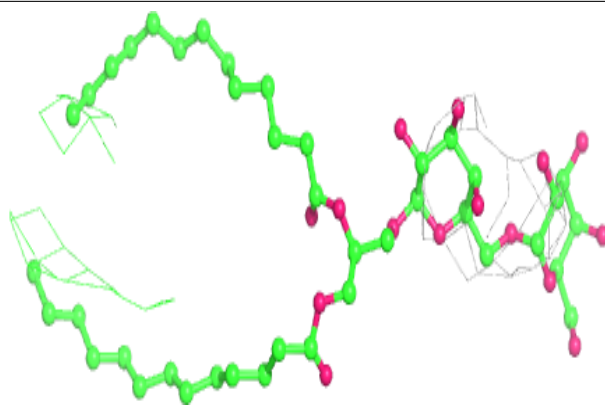
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



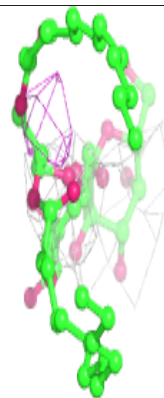
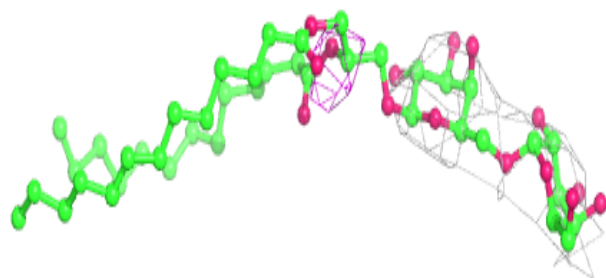
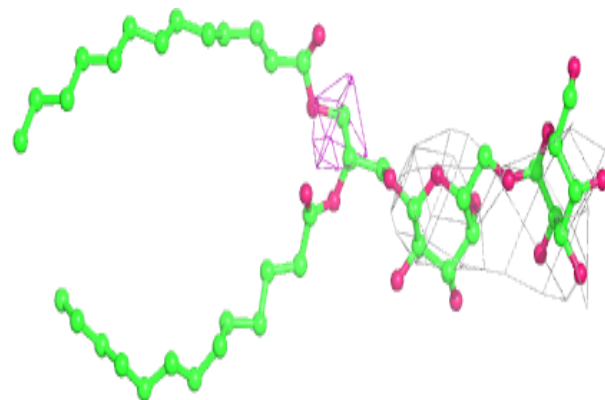


**Electron density around DGD a 408:**

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

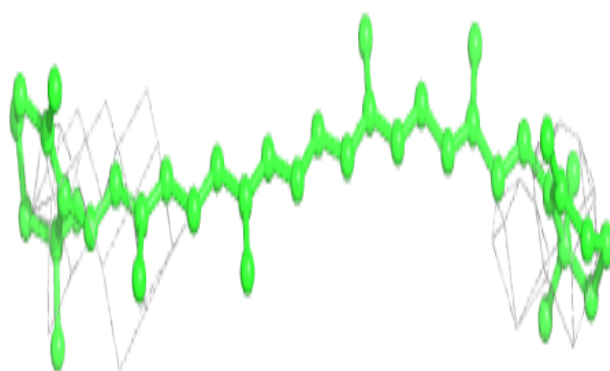
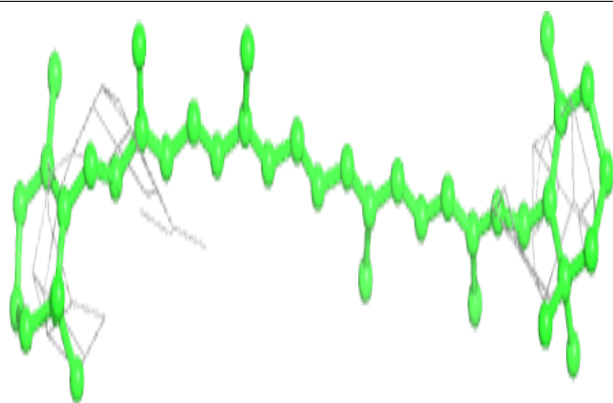
**Electron density around DGD A 409:**

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

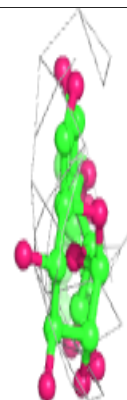
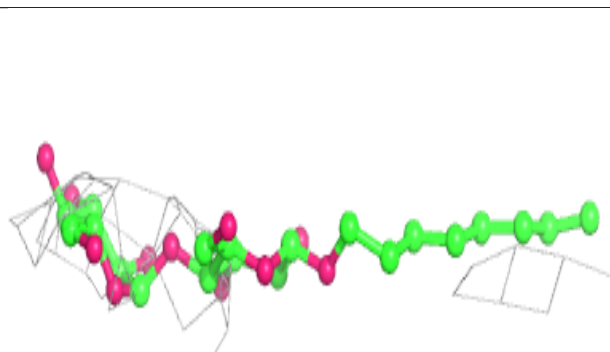
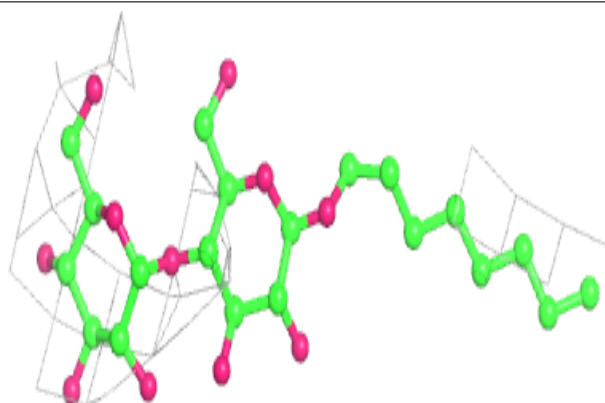


**Electron density around BCR b 624:**

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

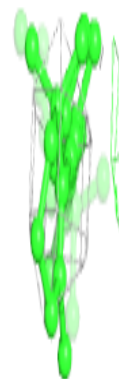
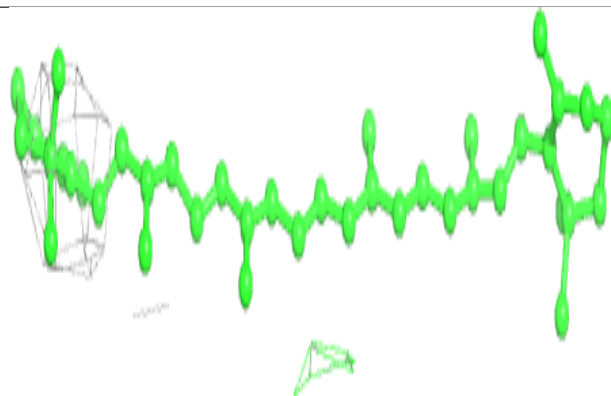
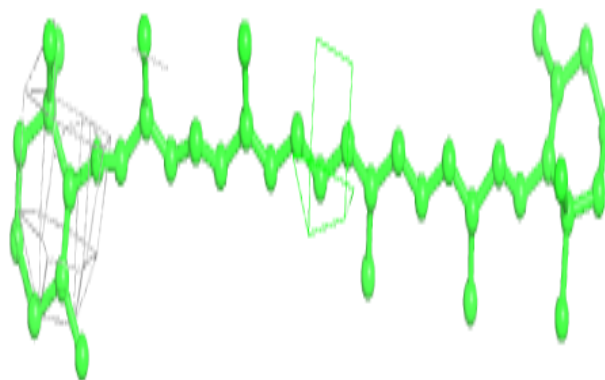
**Electron density around LMT d 411:**

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

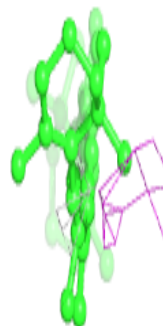
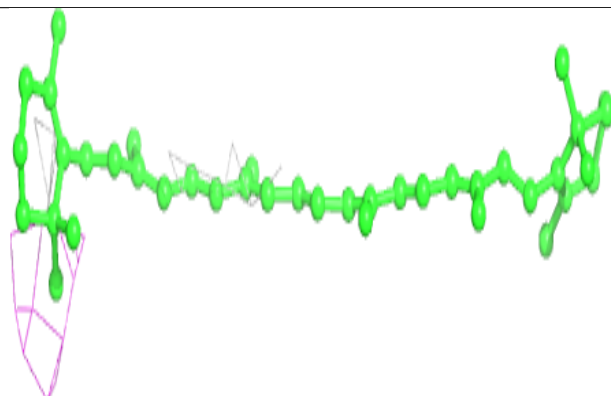
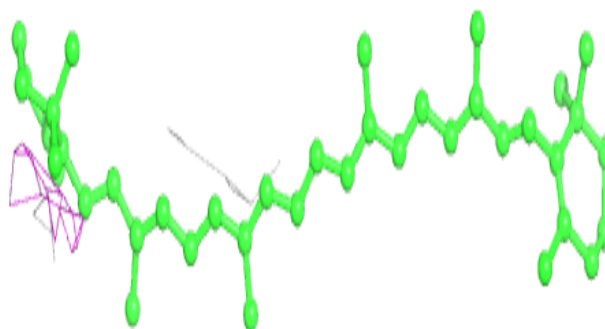


**Electron density around BCR J 102:**

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

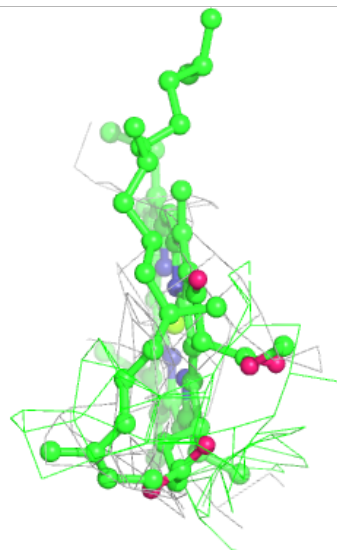
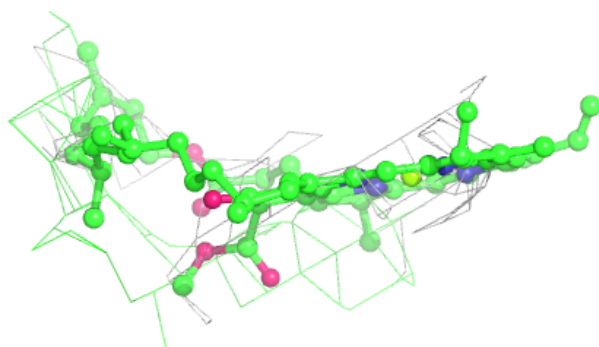
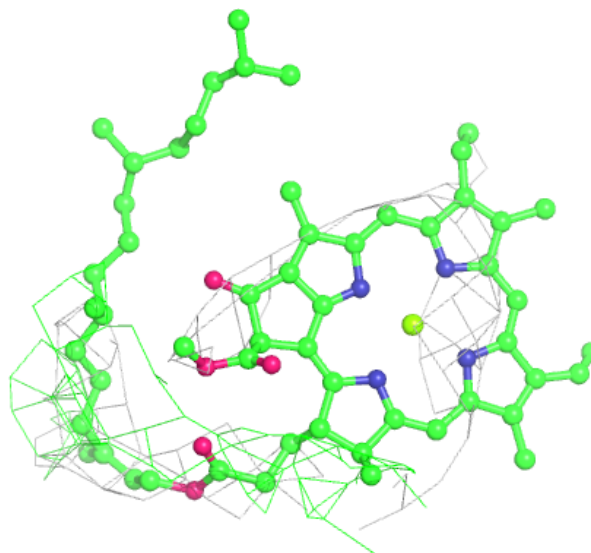
**Electron density around BCR H 102:**

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



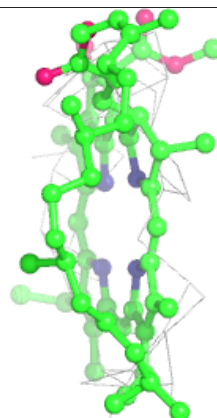
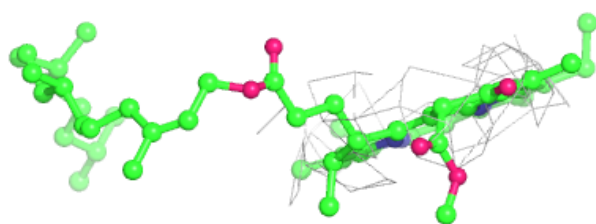
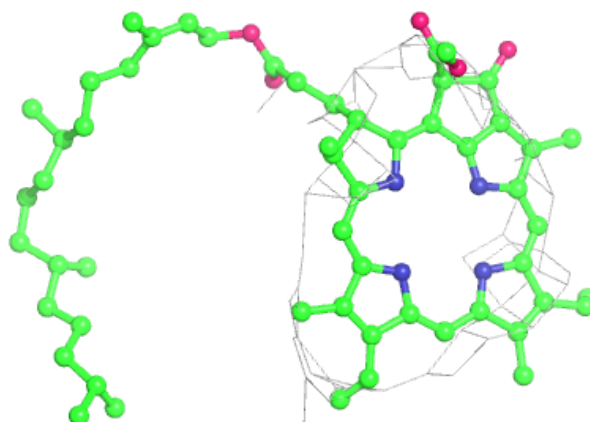
**Electron density around CLA B 601:**

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

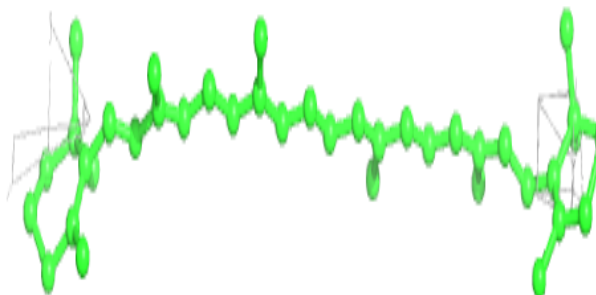
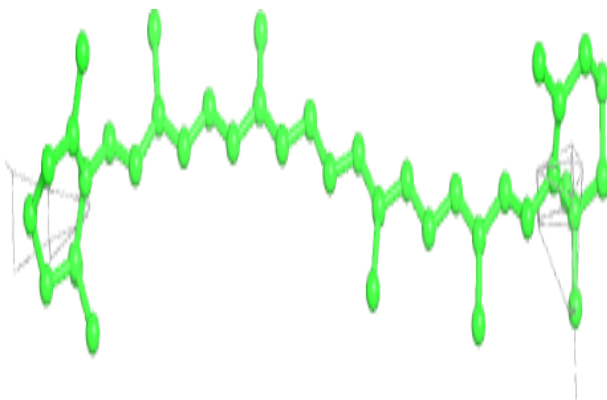


**Electron density around PHO d 401:**

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

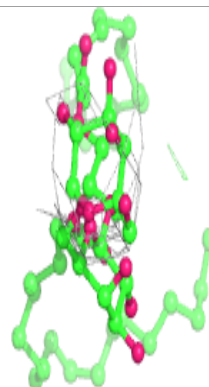
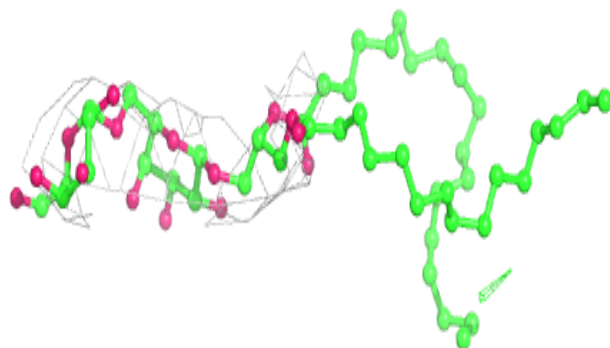
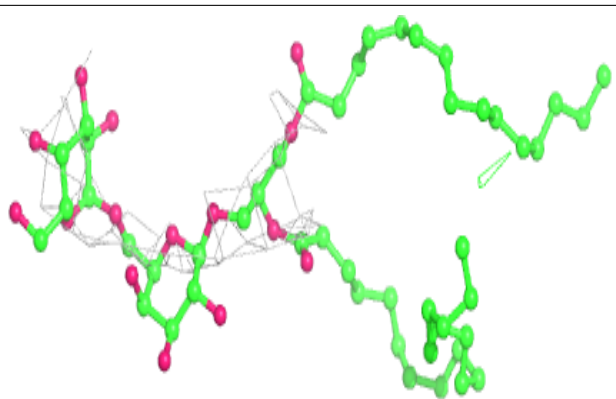
**Electron density around BCR C 513:**

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

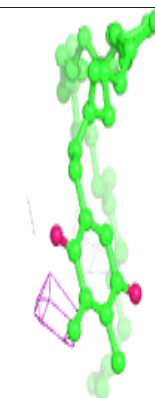
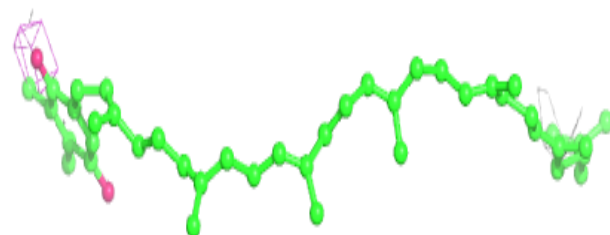
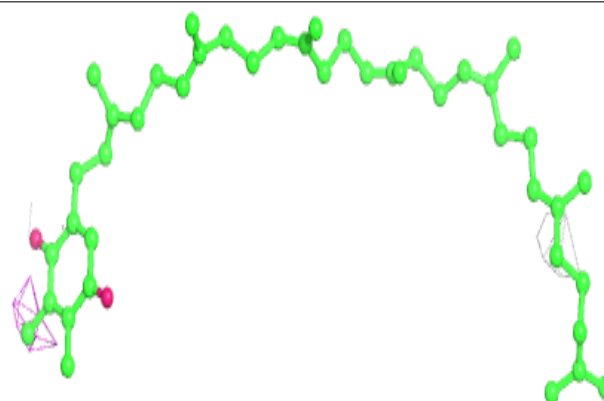


**Electron density around DGD d 410:**

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

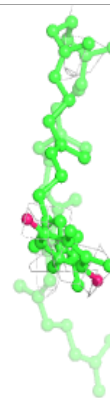
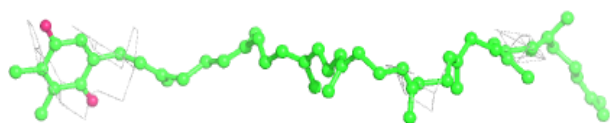
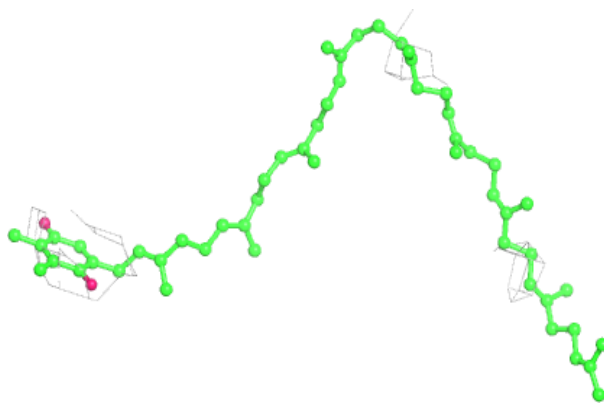
**Electron density around PL9 A 407:**

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

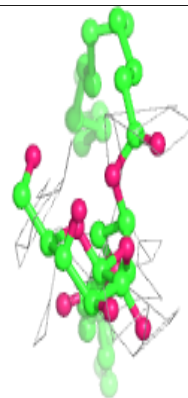
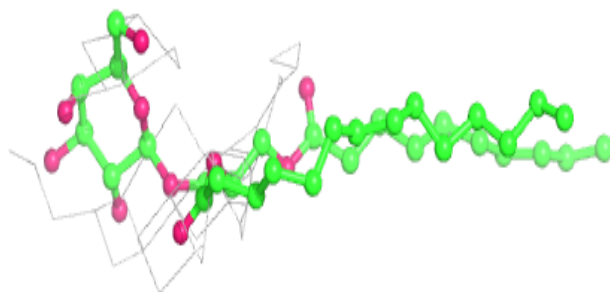
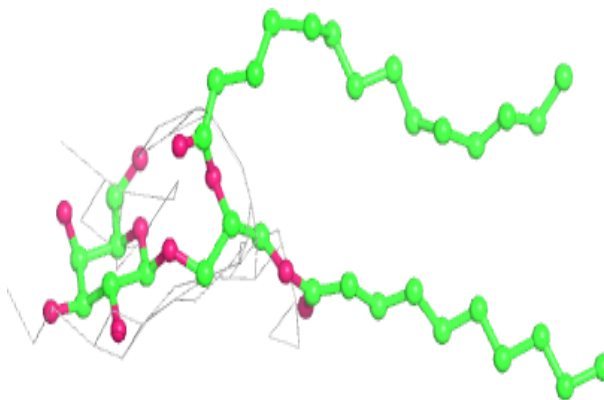


**Electron density around PL9 D 405:**

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

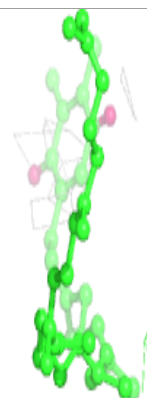
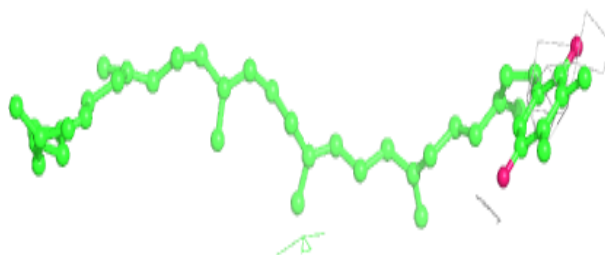
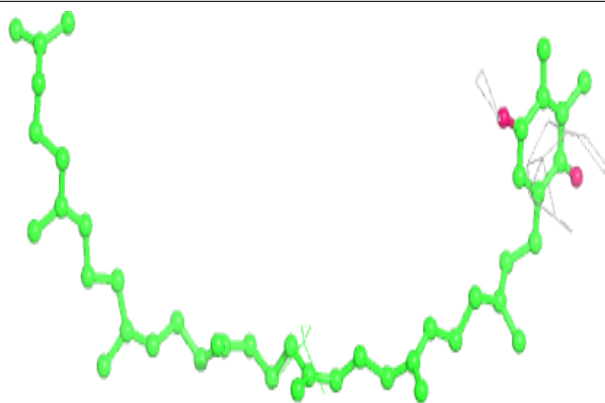
**Electron density around LMG i 102:**

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

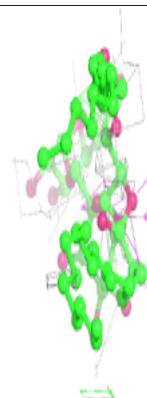
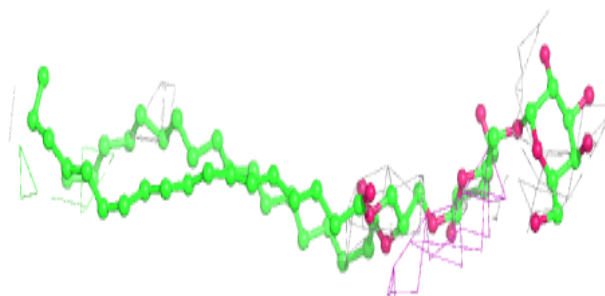
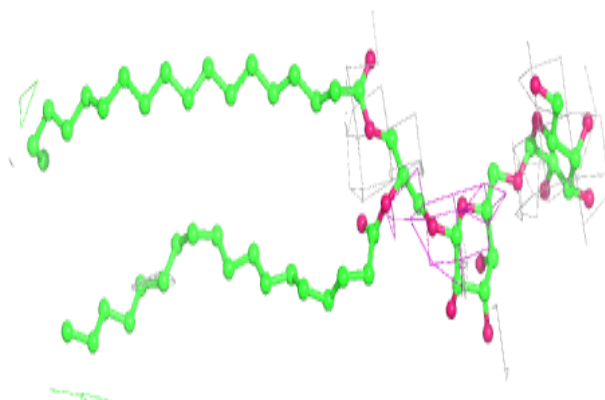


**Electron density around PL9 a 407:**

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

**Electron density around DGD C 516:**

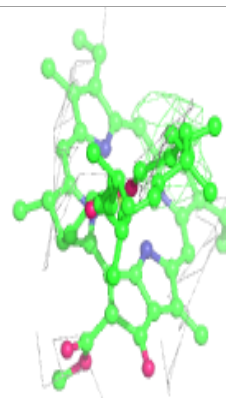
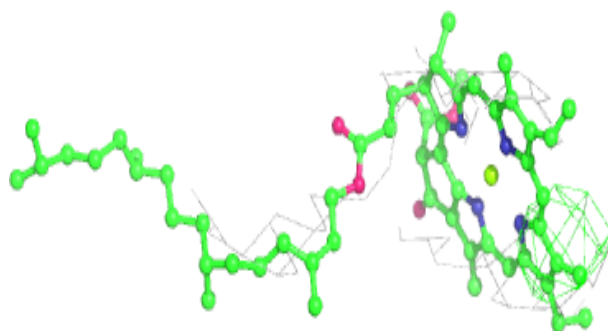
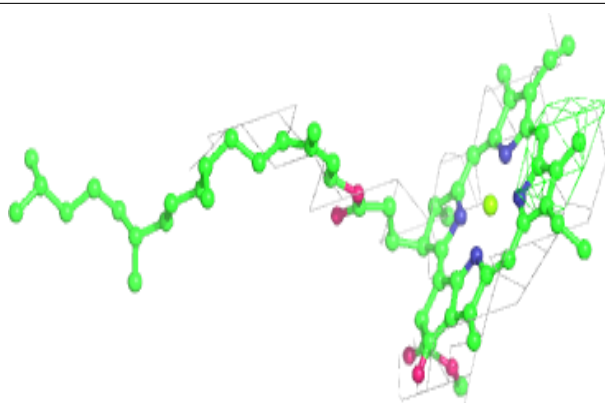
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



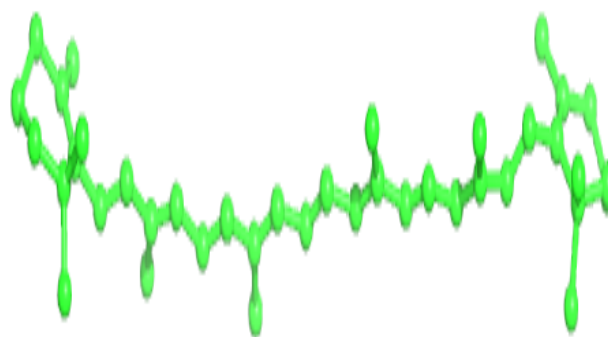
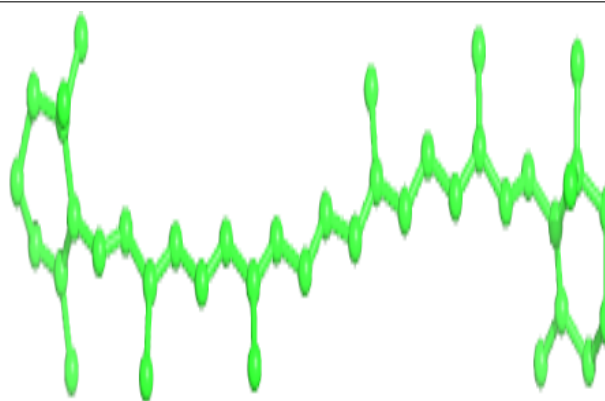


**Electron density around CLA C 502:**

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

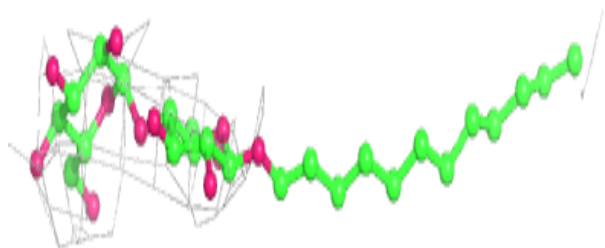
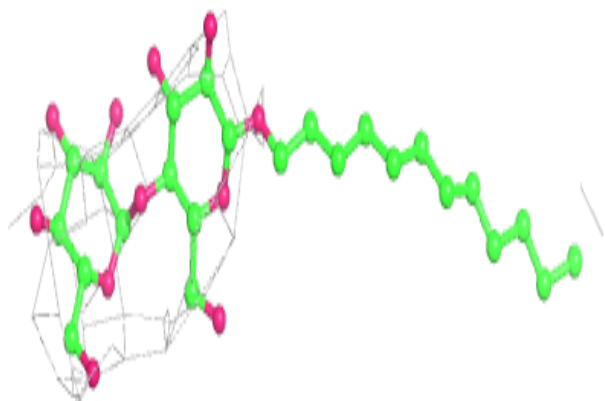
**Electron density around BCR c 514:**

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

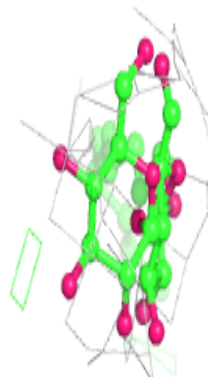
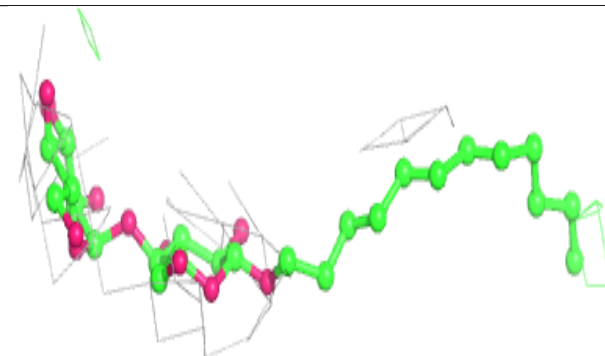
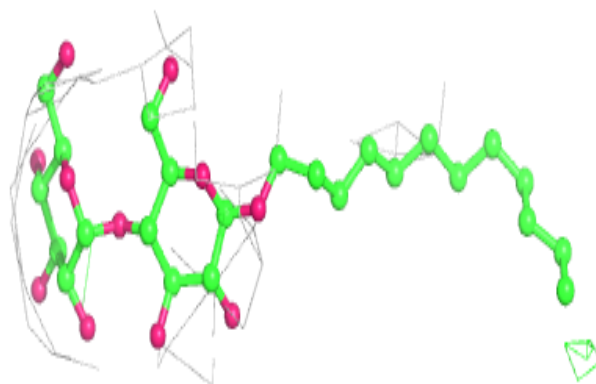


**Electron density around LMT b 629:**

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

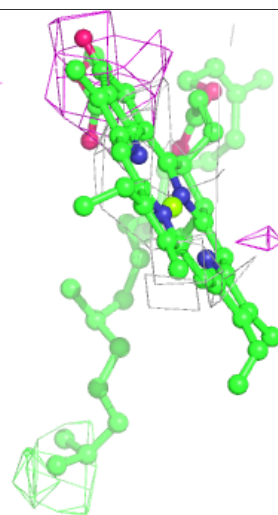
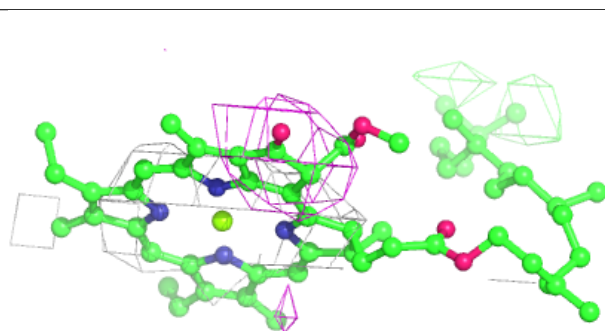
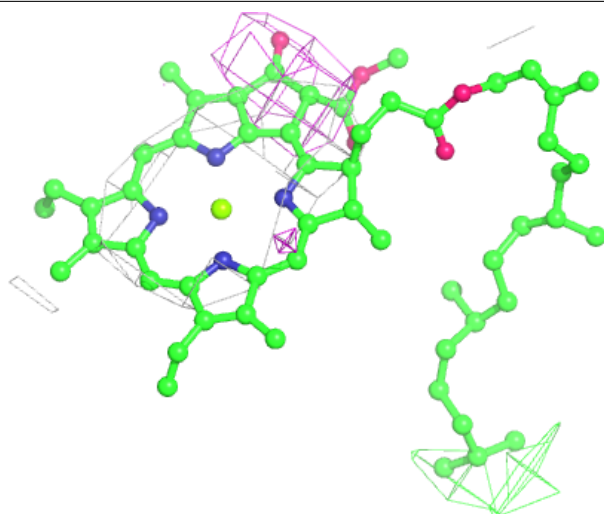
**Electron density around LMT b 628:**

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



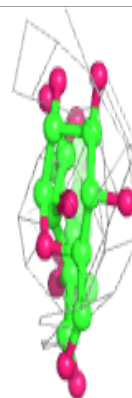
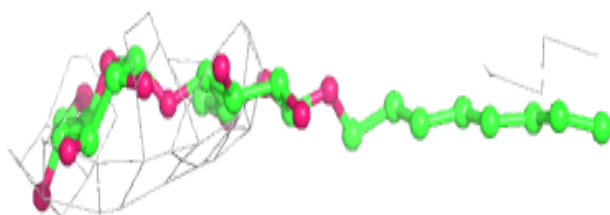
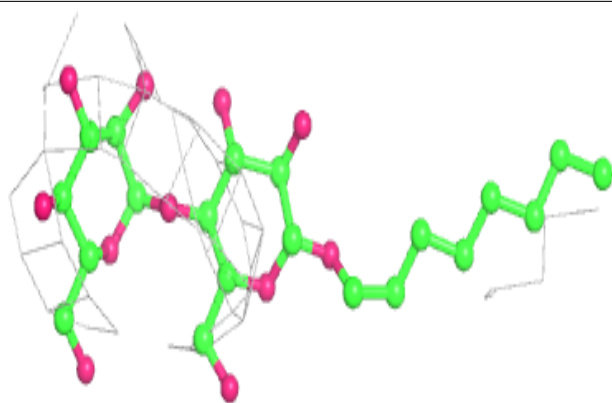
**Electron density around CLA b 620:**

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

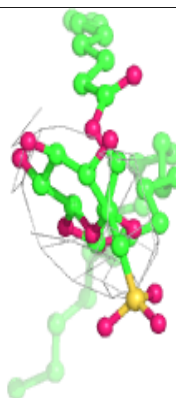
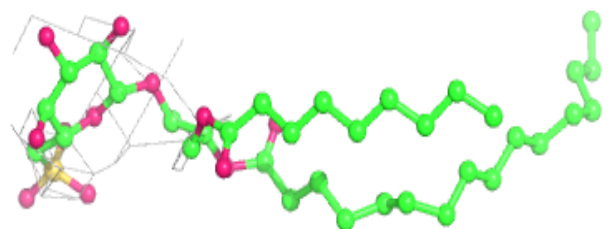
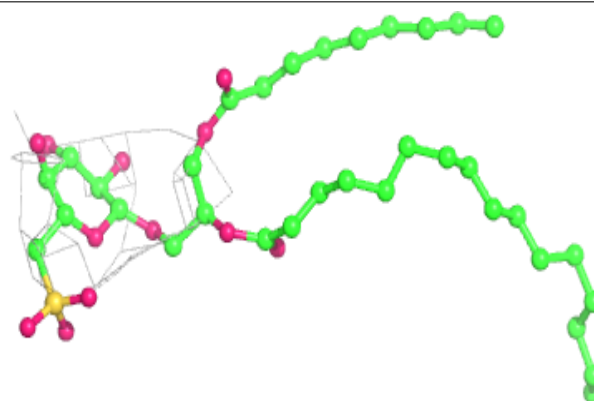


**Electron density around LMT D 408:**

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

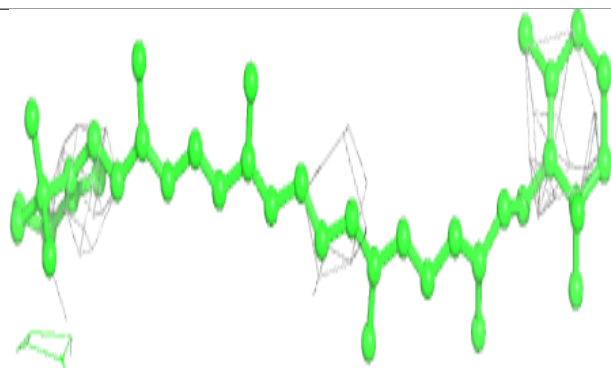
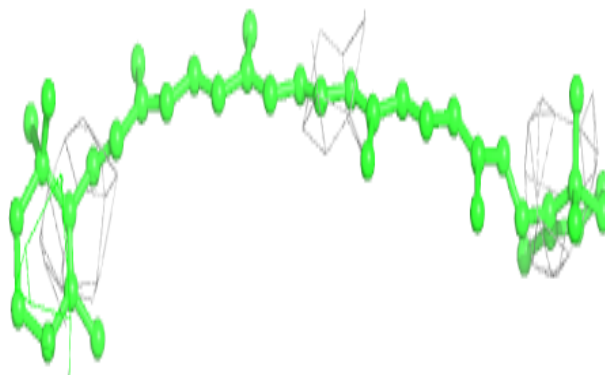
**Electron density around SQD B 627:**

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

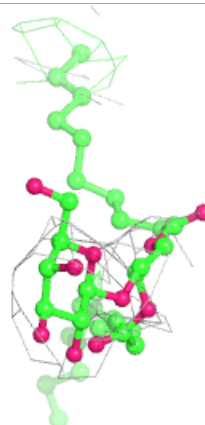
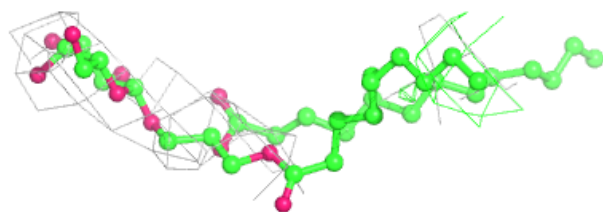
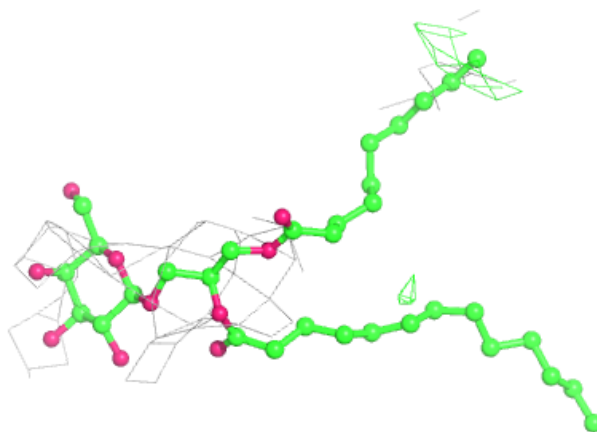


**Electron density around BCR f 102:**

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

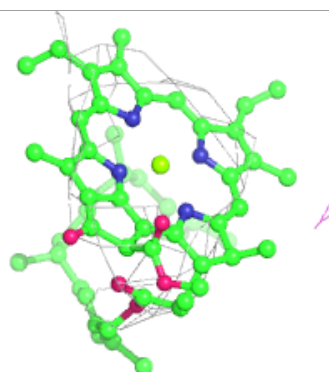
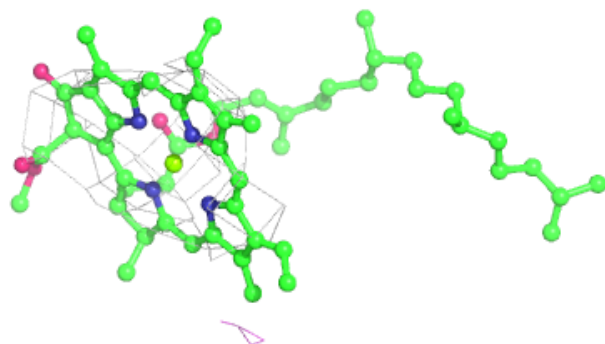
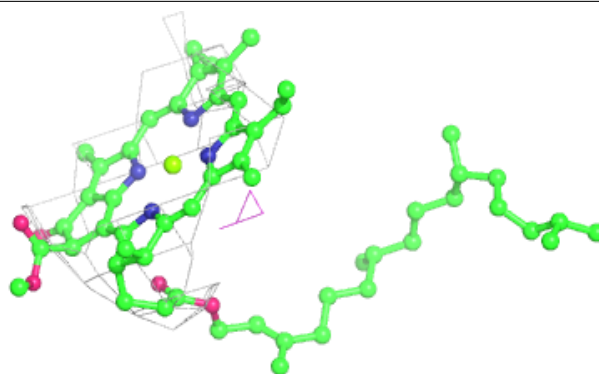
**Electron density around LMG a 402:**

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

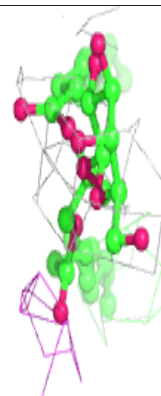
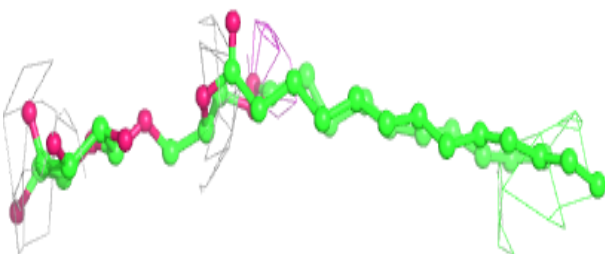
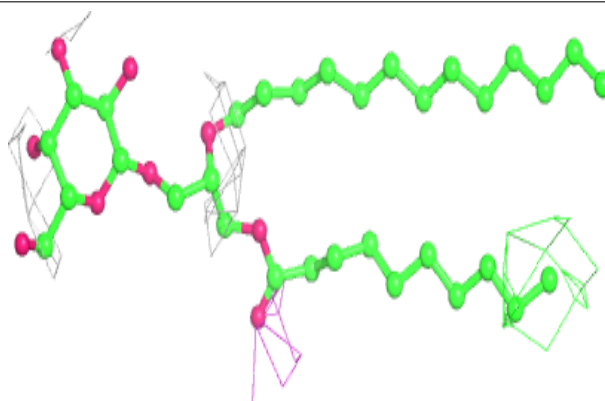


**Electron density around CLA C 512:**

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

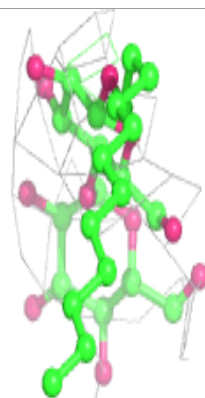
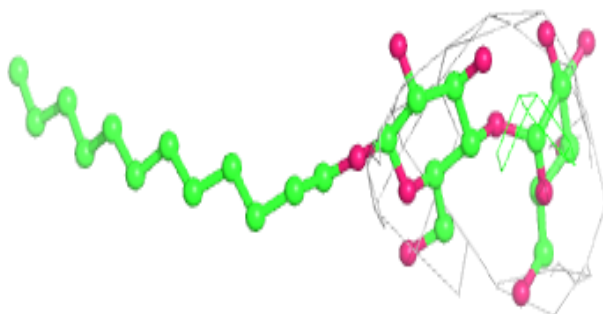
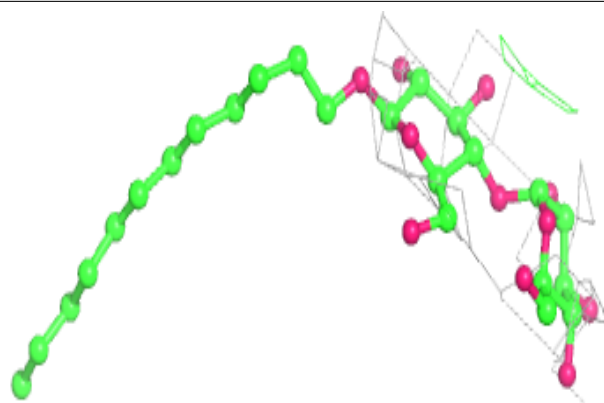
**Electron density around LMG m 101:**

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

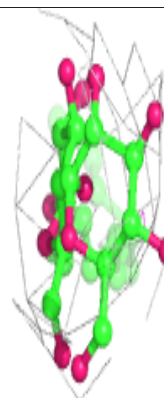
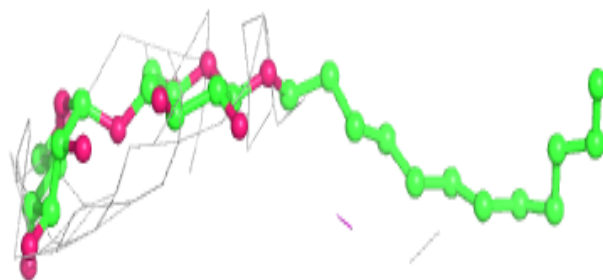
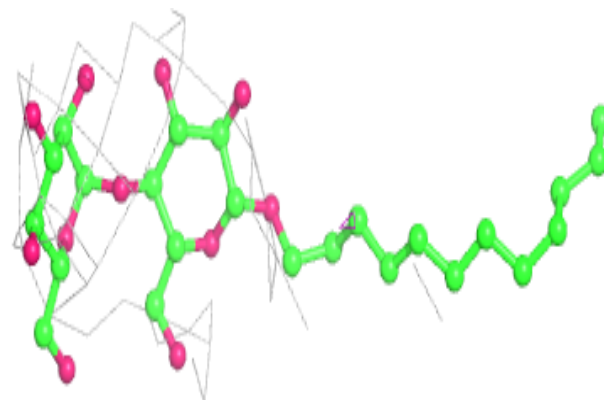


**Electron density around LMT M 102:**

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

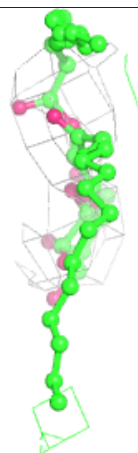
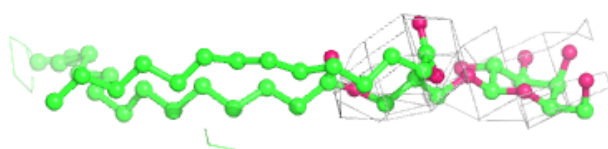
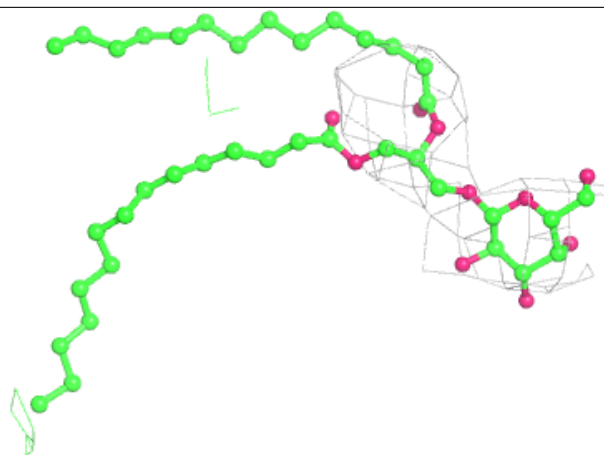
**Electron density around LMT B 623:**

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

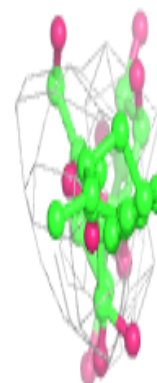
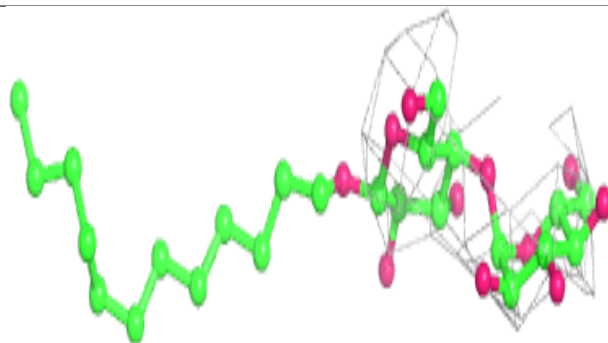
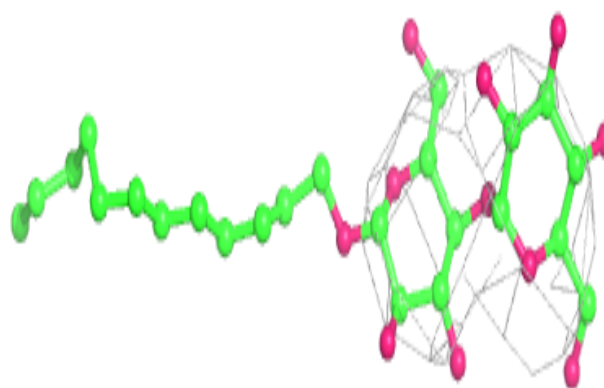


**Electron density around LMG C 521:**

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

**Electron density around LMT b 604:**

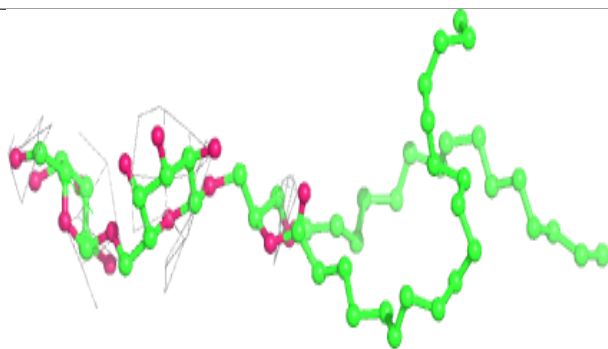
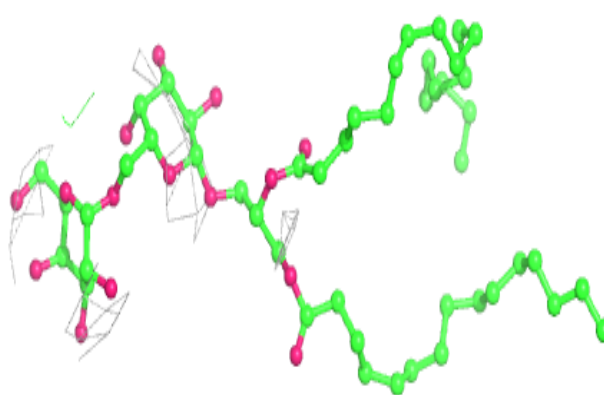
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



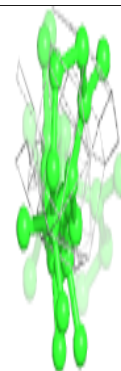
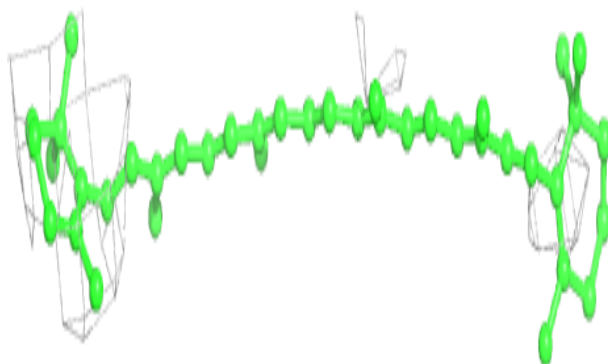
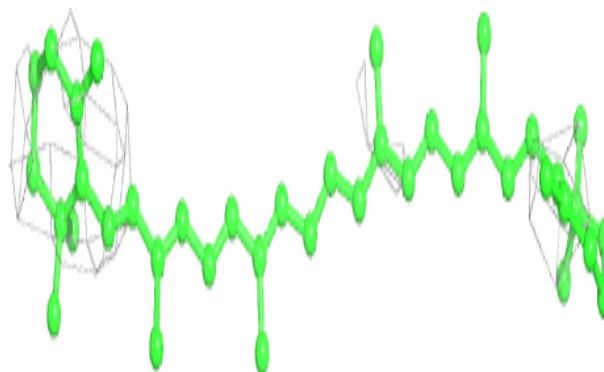


**Electron density around DGD D 407:**

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

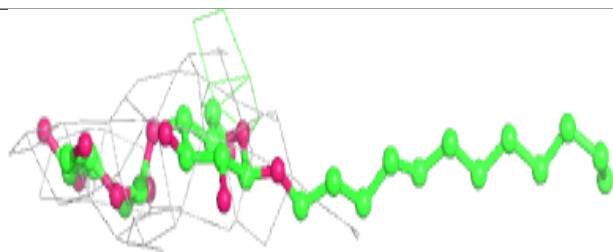
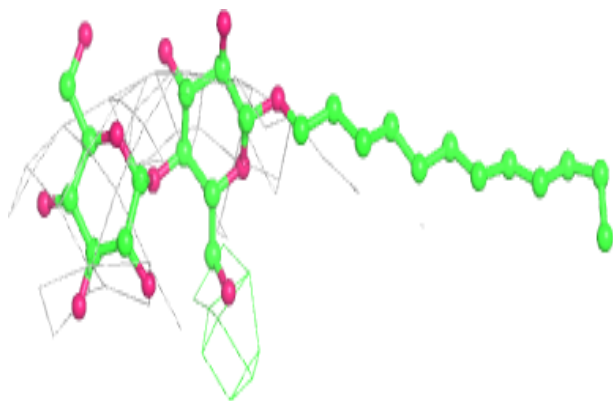
**Electron density around BCR B 616:**

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

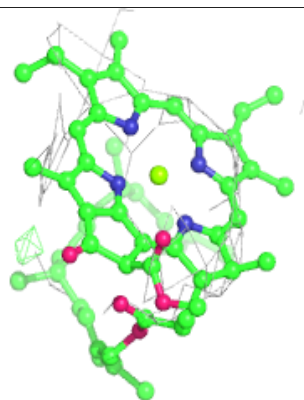
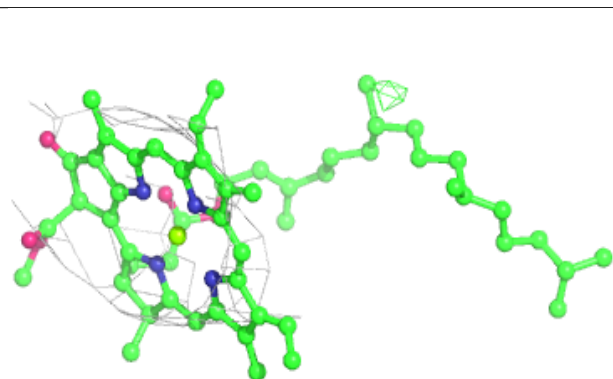
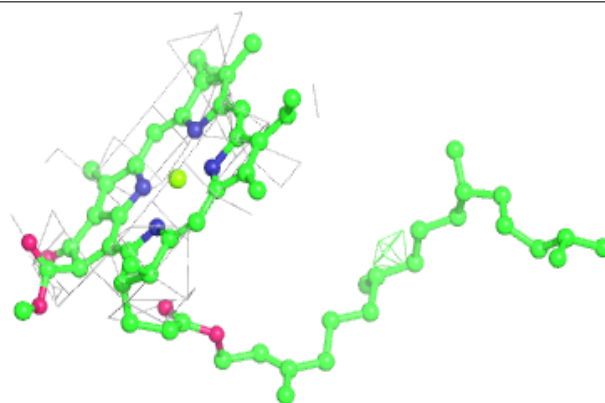


**Electron density around LMT b 603:**

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

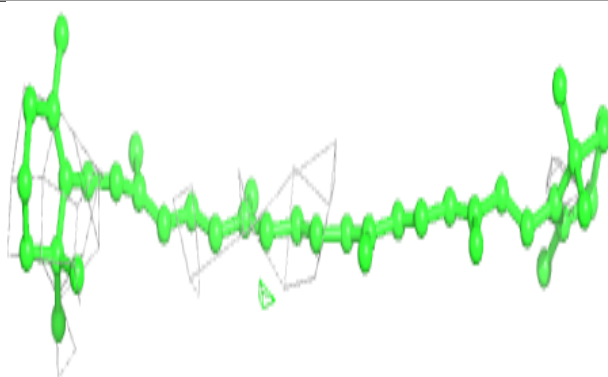
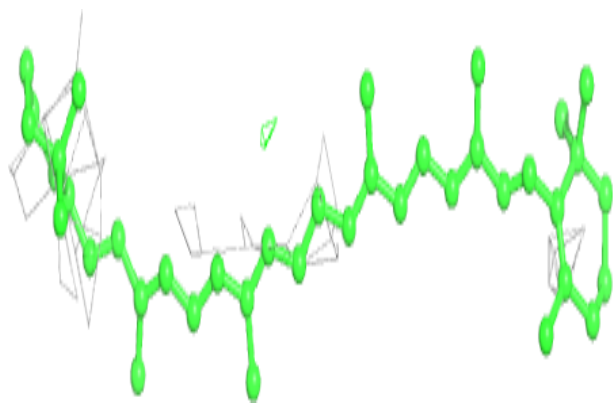
**Electron density around CLA c 512:**

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

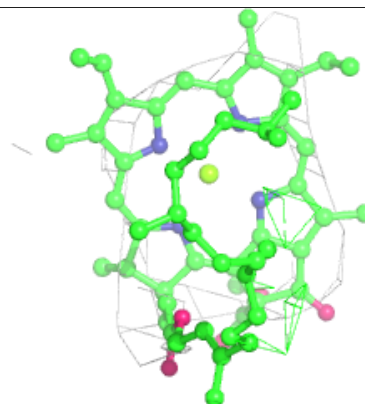
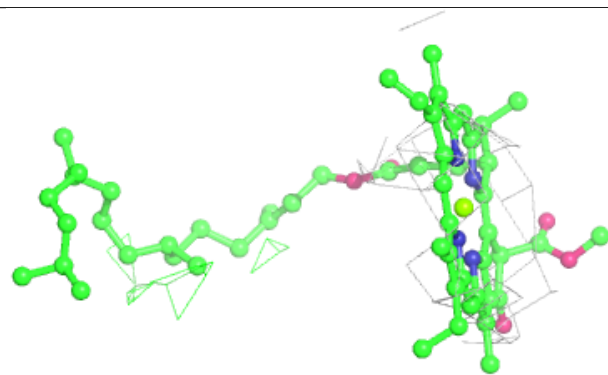
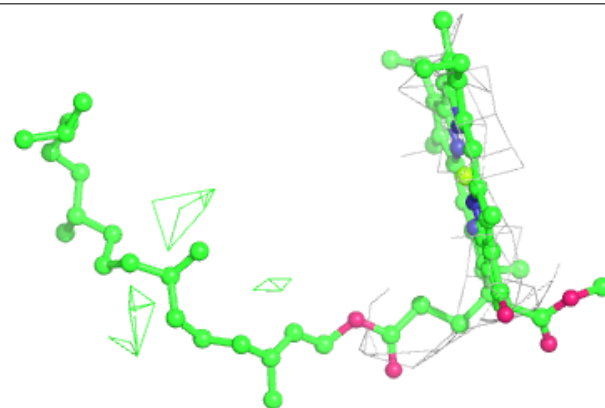


**Electron density around BCR x 101:**

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

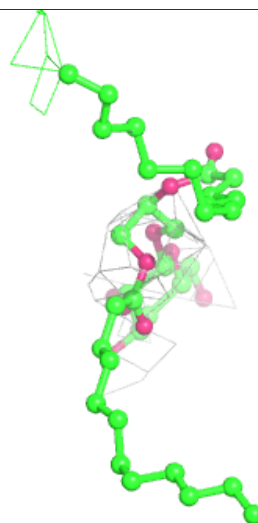
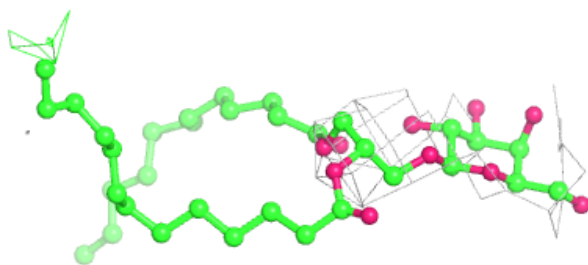
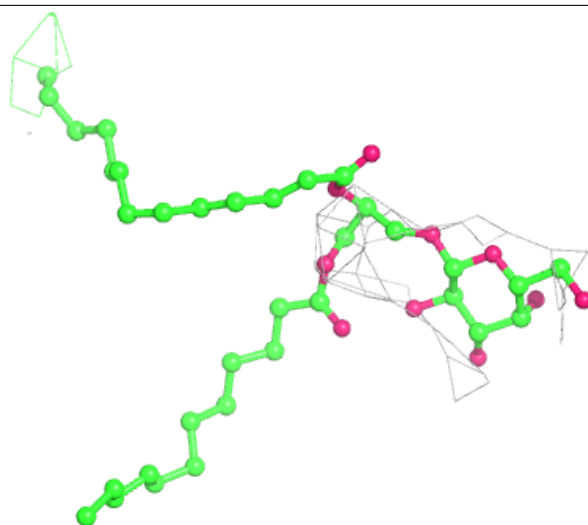
**Electron density around CLA C 505:**

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



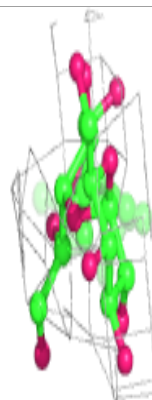
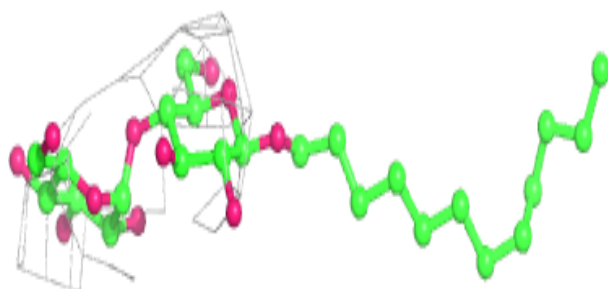
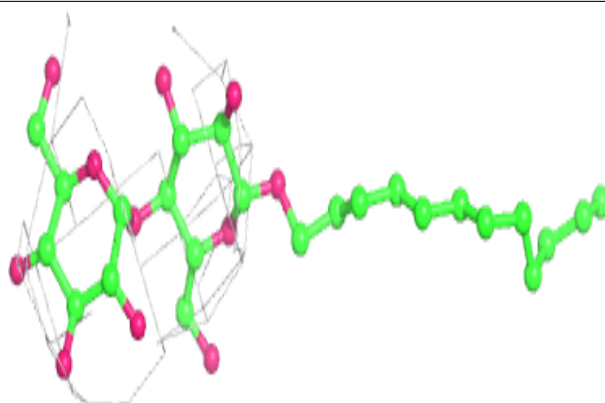
**Electron density around LMG E 101:**

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

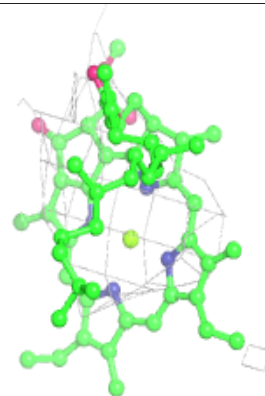
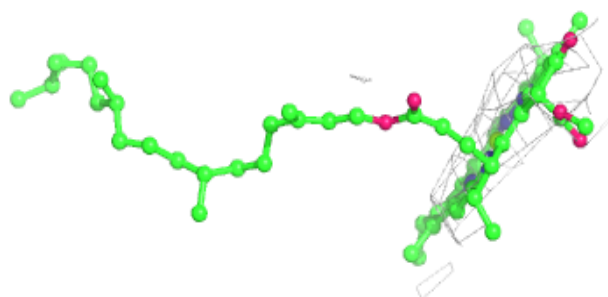
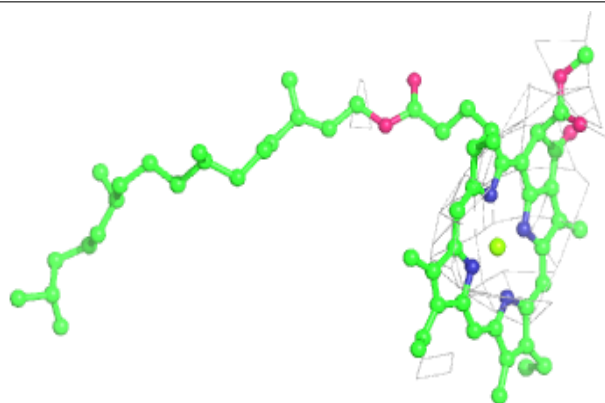


**Electron density around LMT B 629:**

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

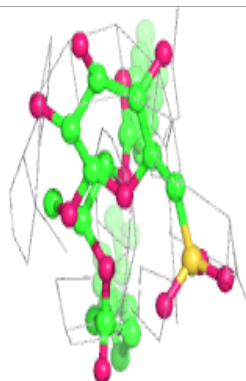
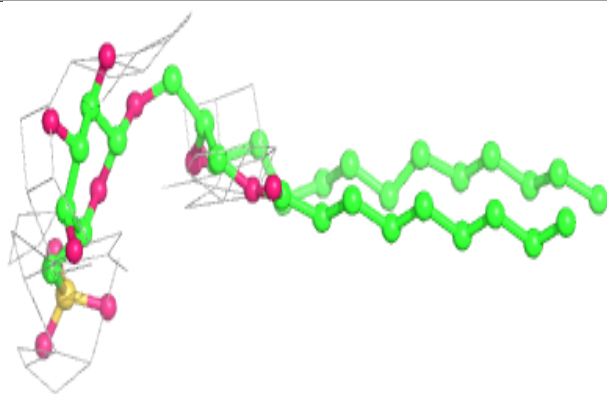
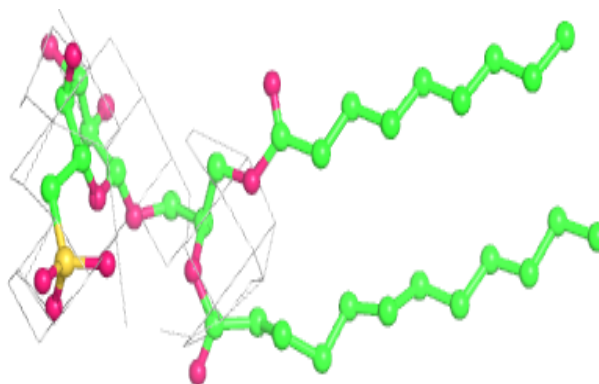
**Electron density around CLA a 406:**

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

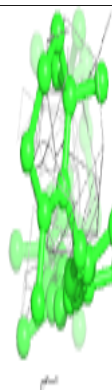
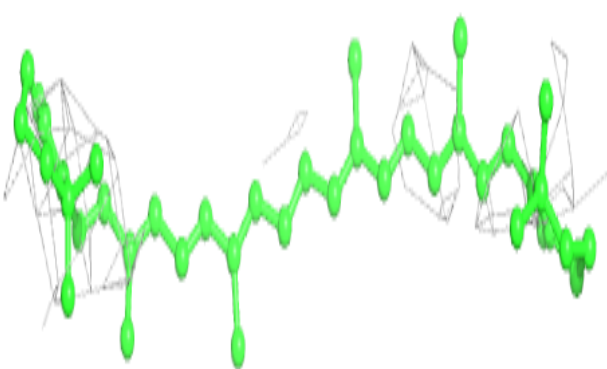
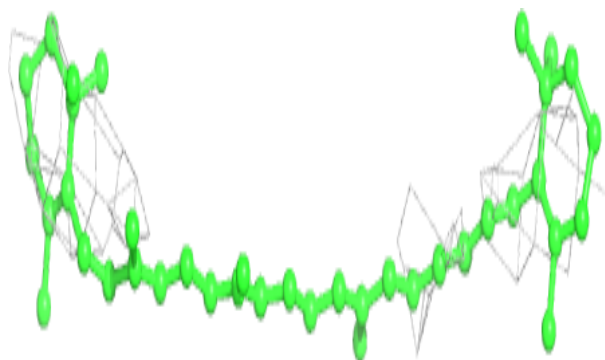


**Electron density around SQD d 403:**

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

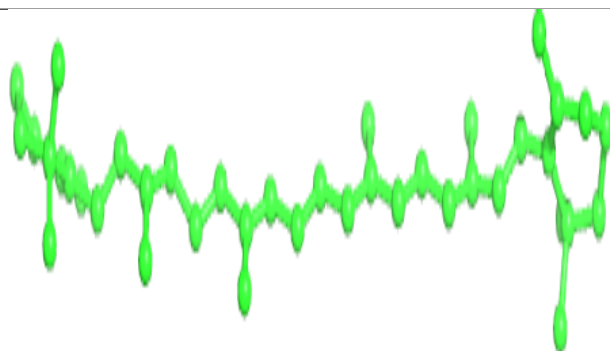
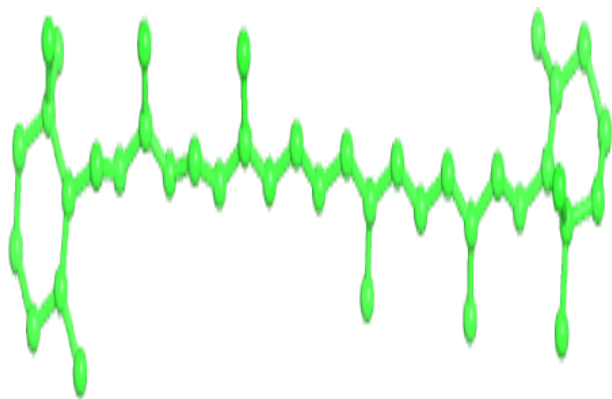
**Electron density around BCR c 513:**

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

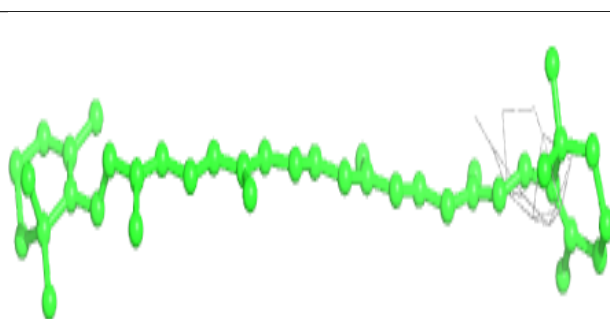
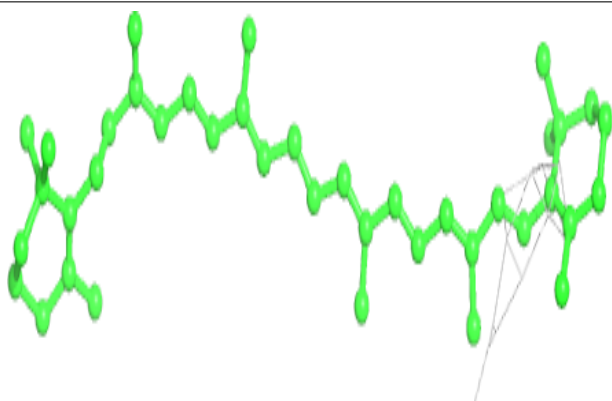


**Electron density around BCR j 102:**

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

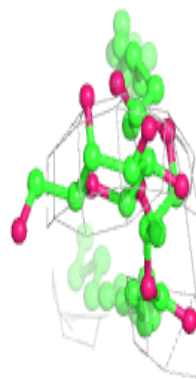
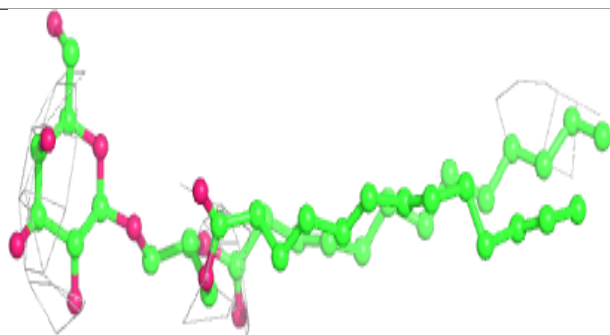
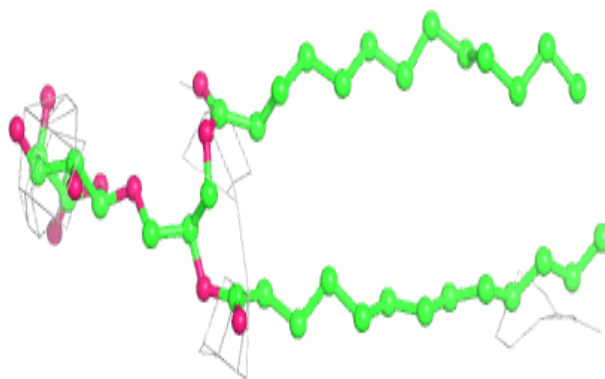
**Electron density around BCR g 101:**

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

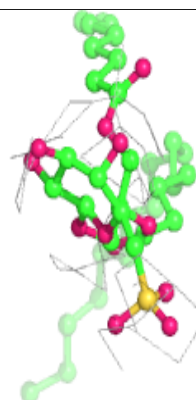
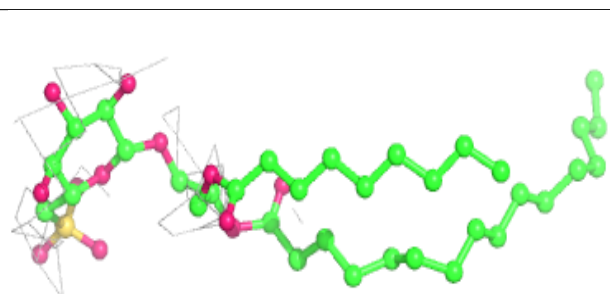
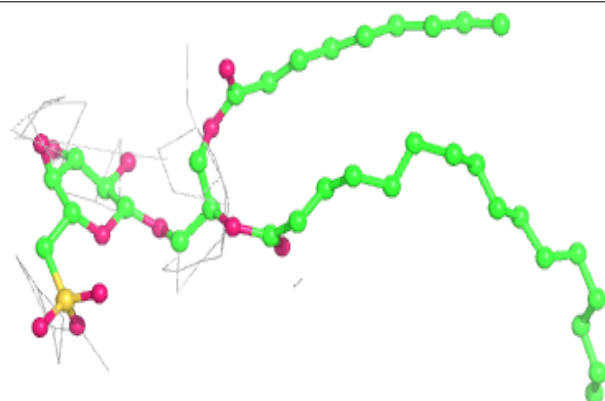


**Electron density around LMG c 518:**

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

**Electron density around SQD b 602:**

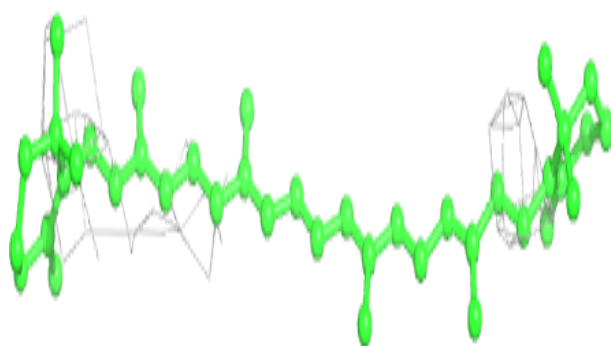
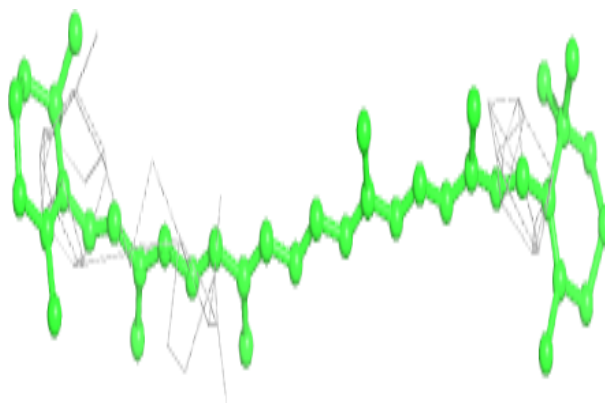
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



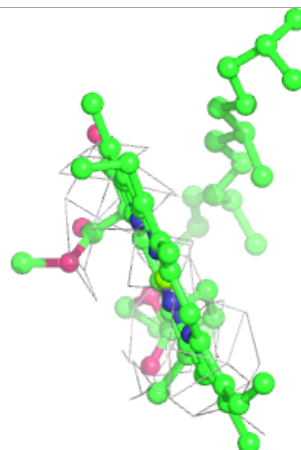
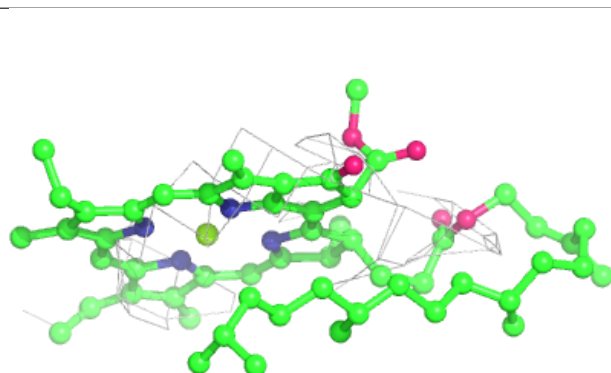
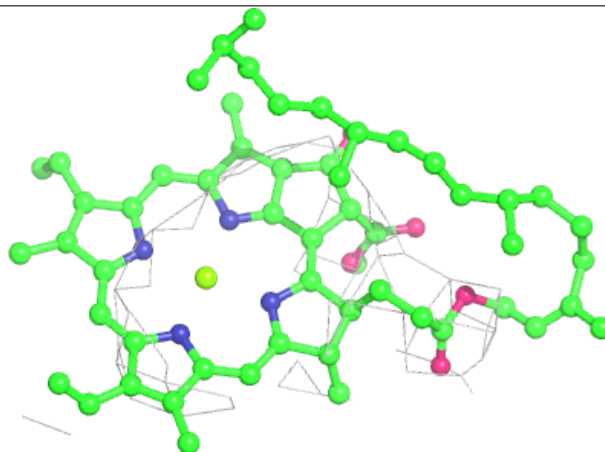


**Electron density around BCR B 619:**

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

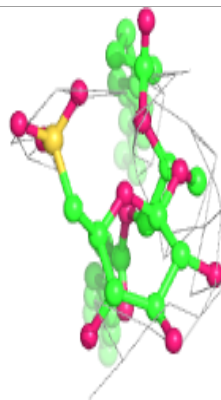
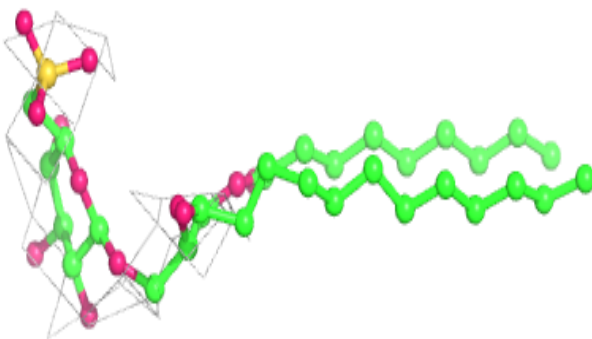
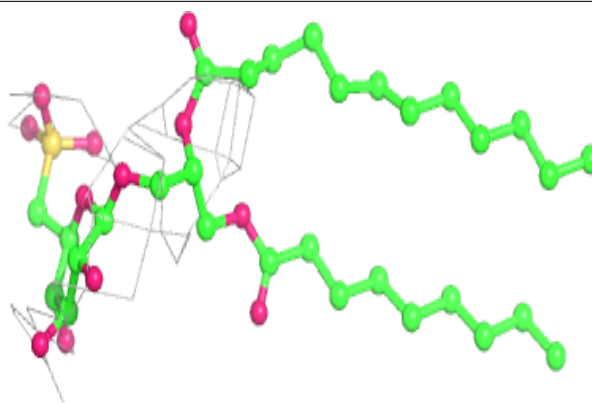
**Electron density around CLA C 508:**

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

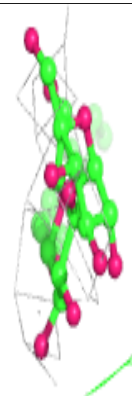
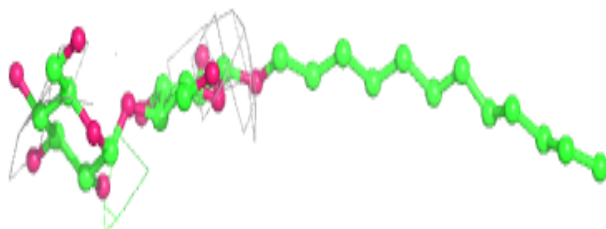
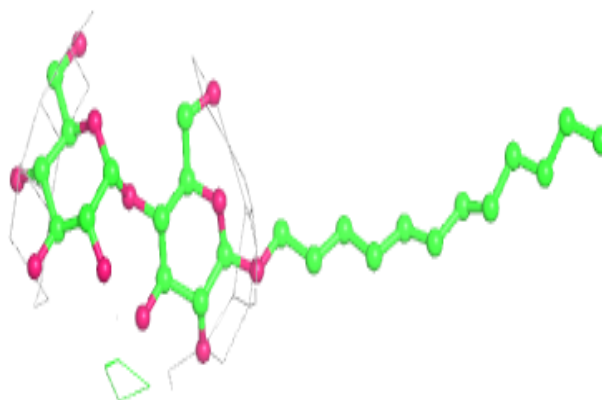


**Electron density around SQD B 622:**

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

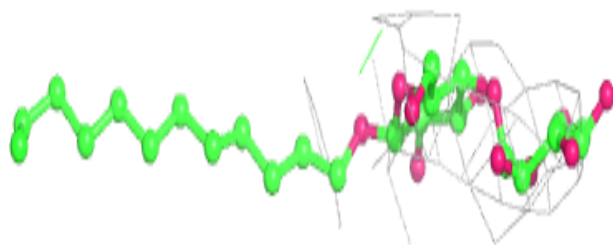
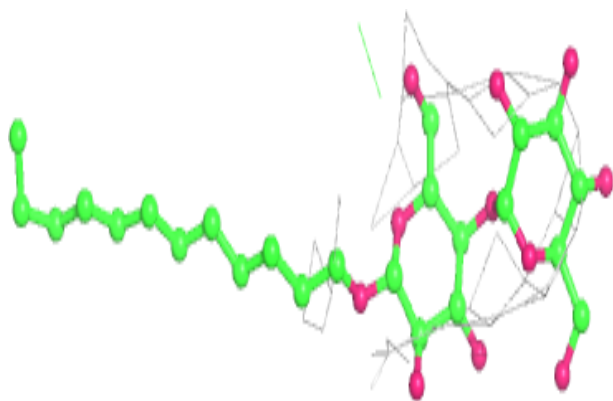
**Electron density around LMT B 624:**

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

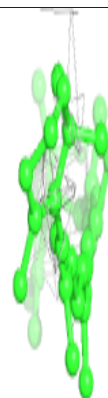
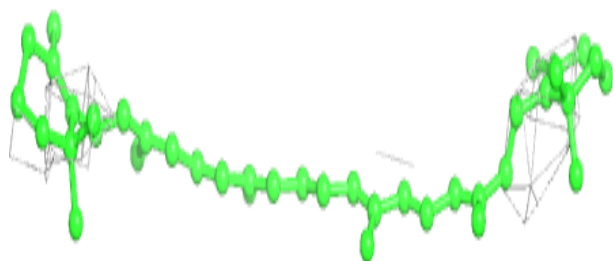
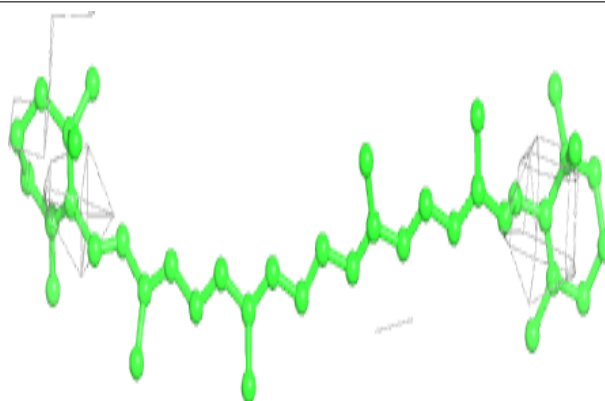


**Electron density around LMT B 628:**

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

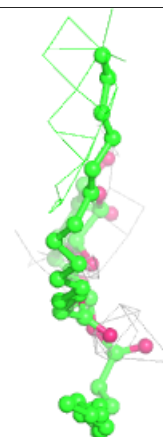
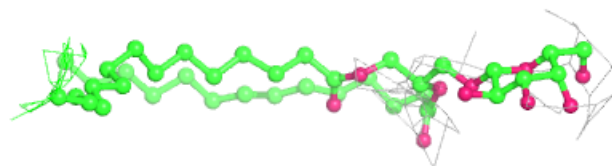
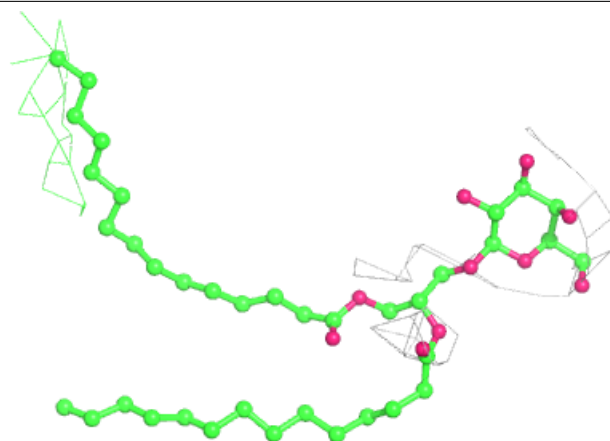
**Electron density around BCR B 617:**

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

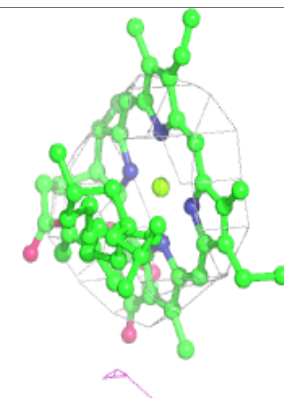
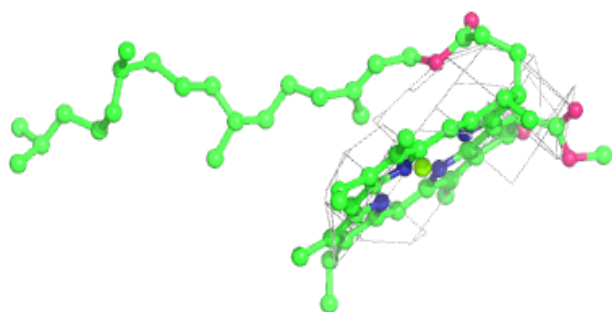
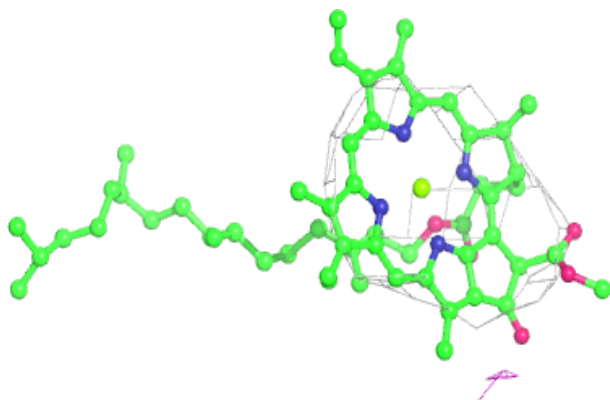


**Electron density around LMG c 522:**

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

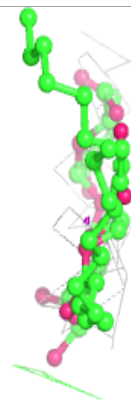
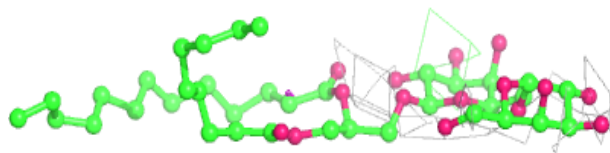
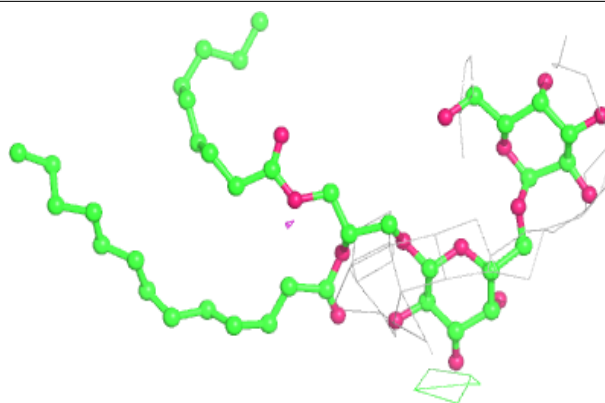
**Electron density around CLA B 613:**

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



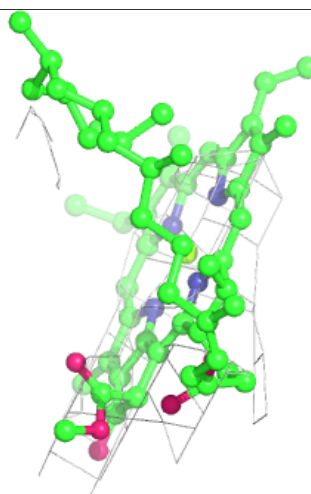
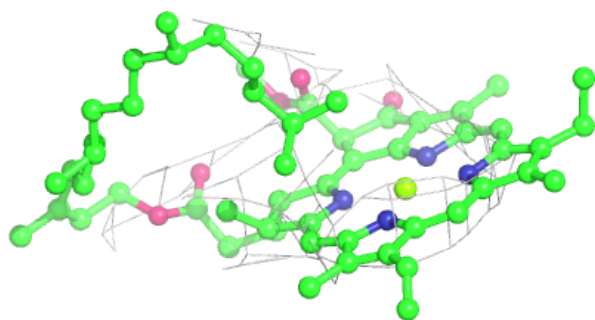
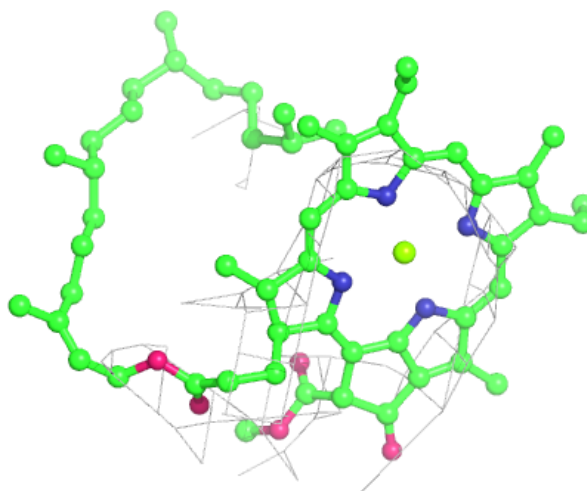
**Electron density around DGD B 626:**

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



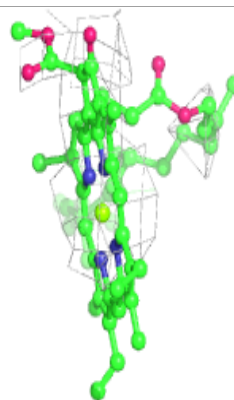
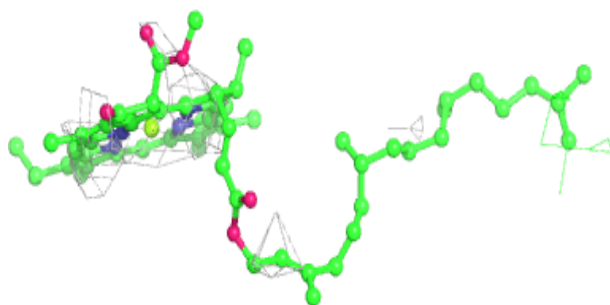
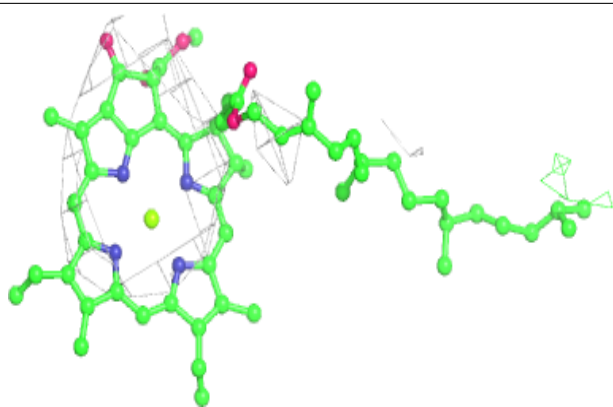
**Electron density around CLA b 619:**

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

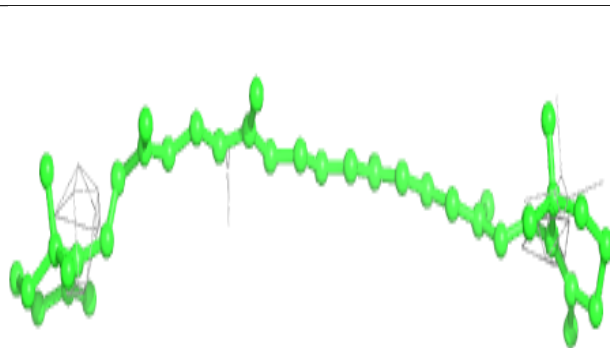
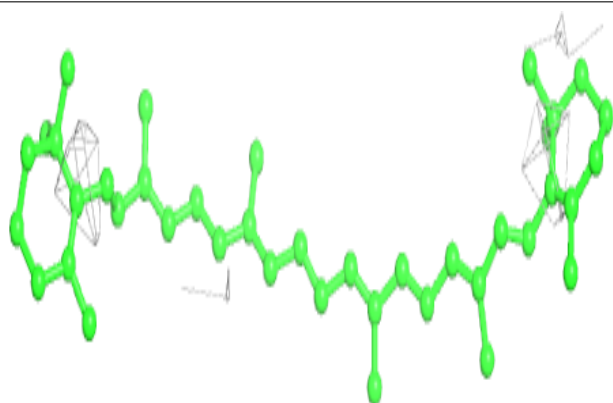


**Electron density around CLA a 405:**

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

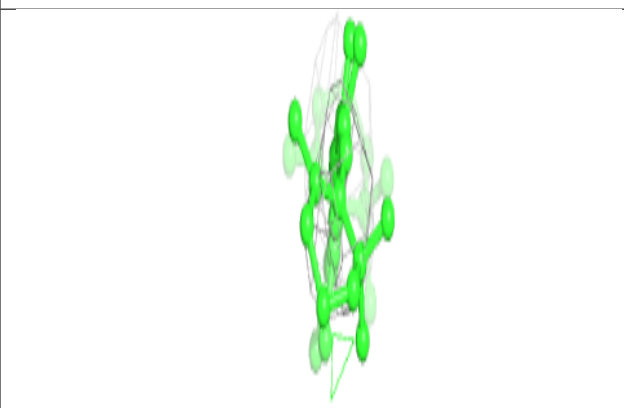
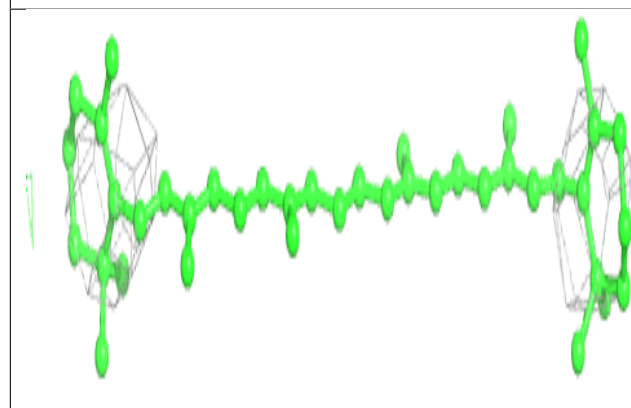
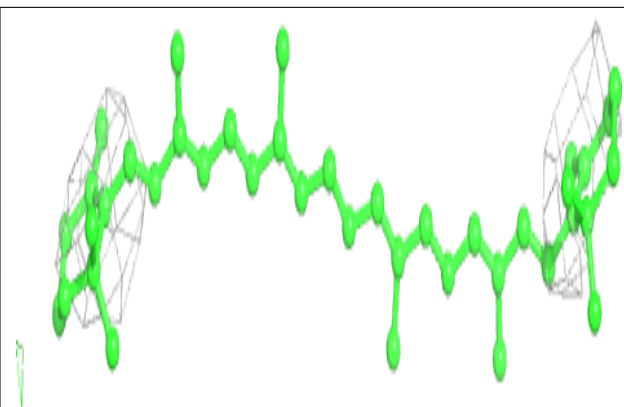
**Electron density around BCR b 622:**

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

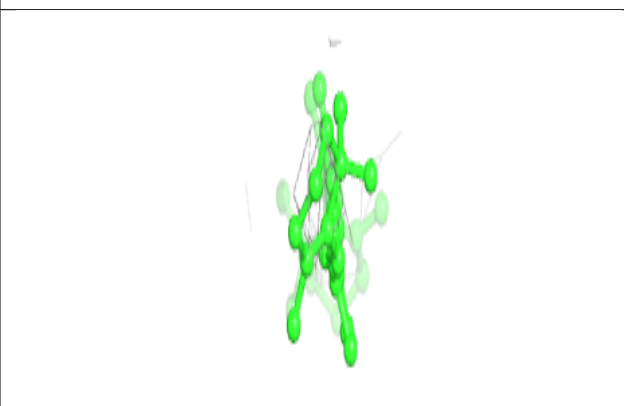
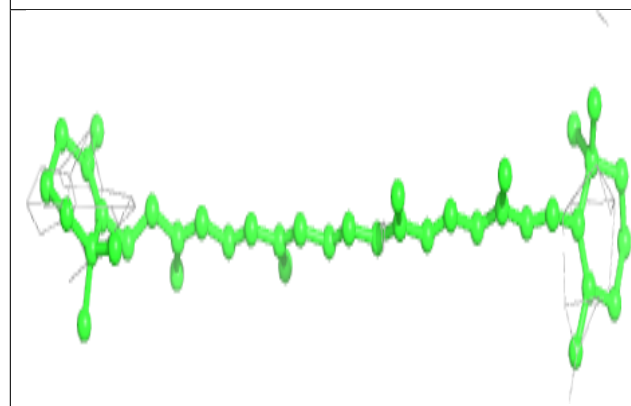
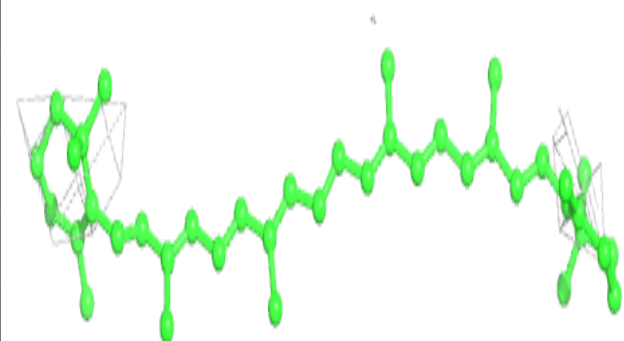


**Electron density around BCR A 408:**

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

**Electron density around BCR C 520:**

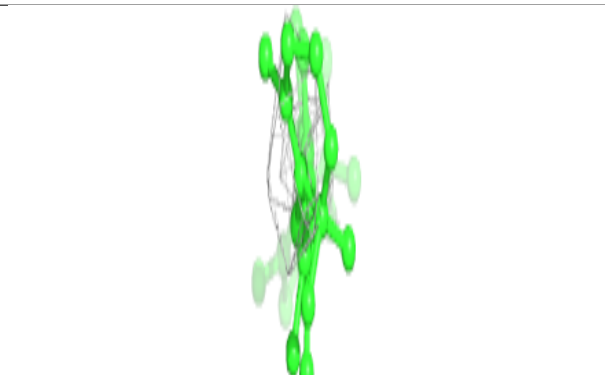
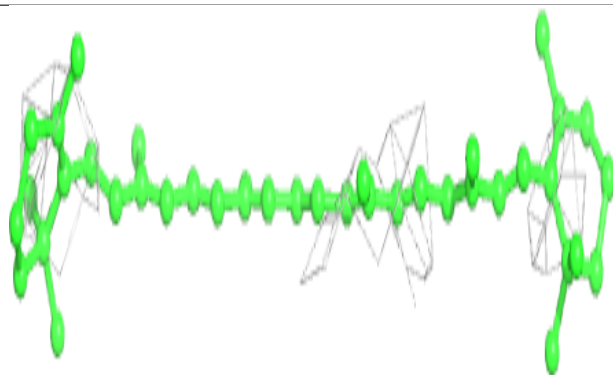
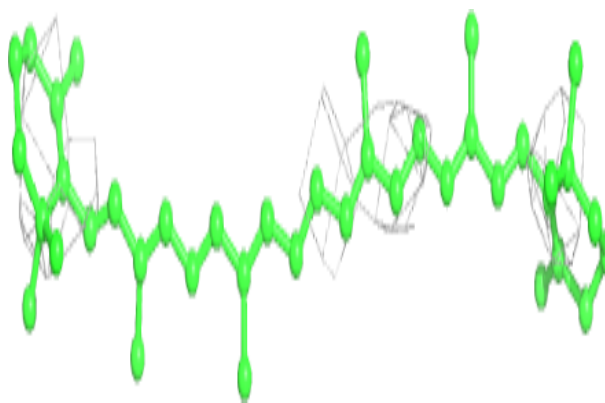
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



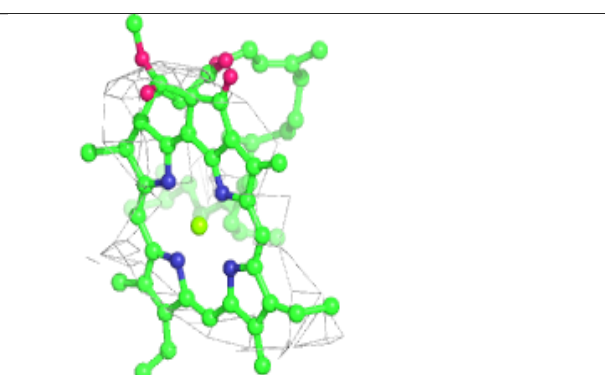
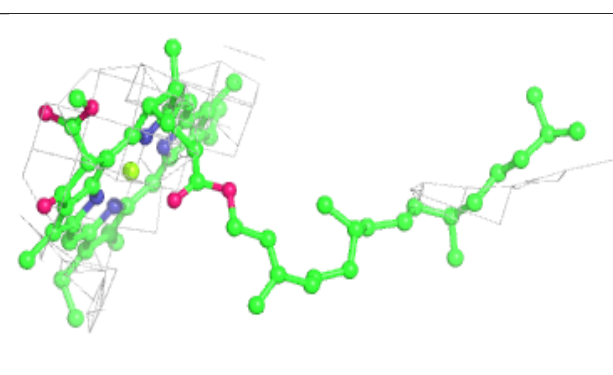
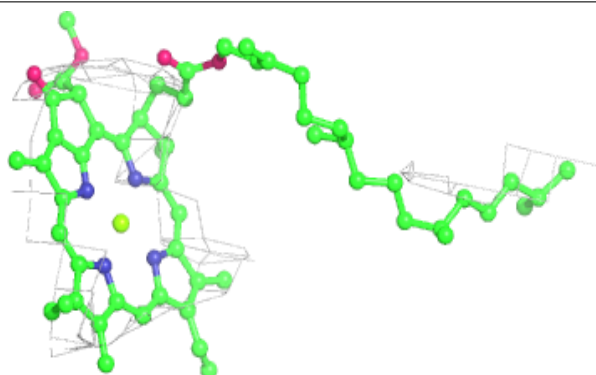


**Electron density around BCR b 623:**

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

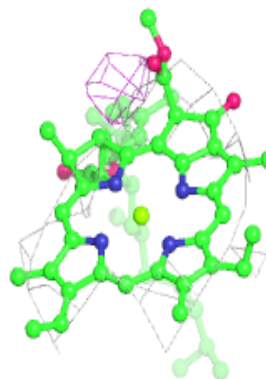
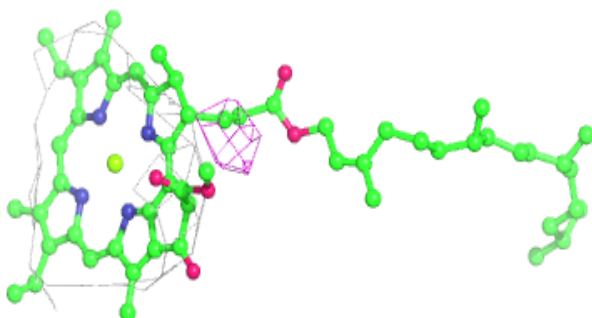
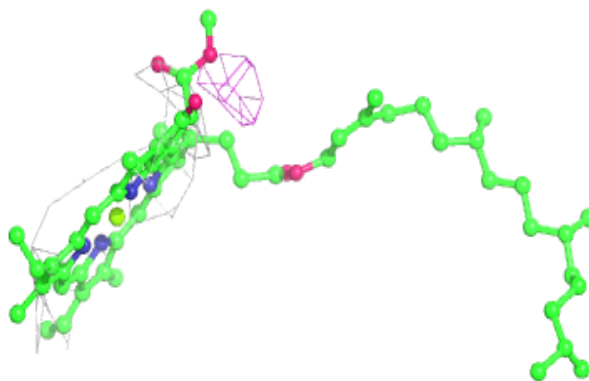
**Electron density around CLA c 510:**

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

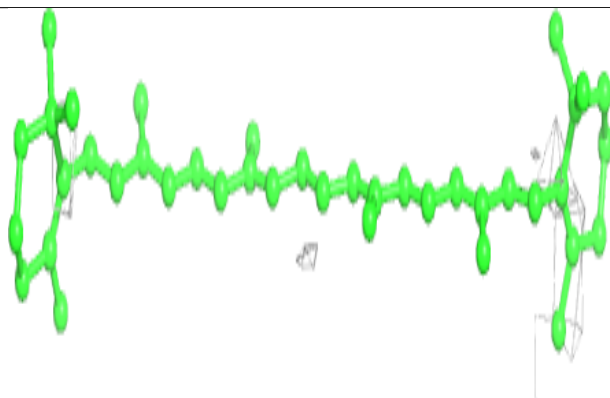
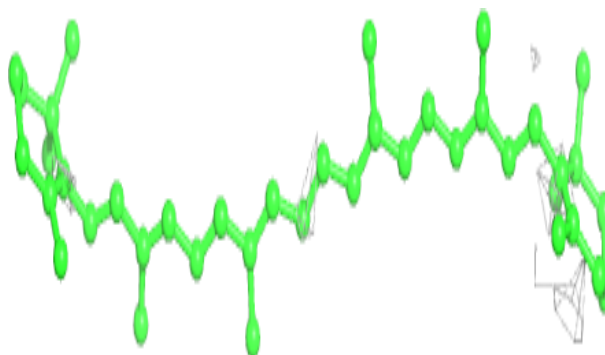


**Electron density around CLA d 405:**

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

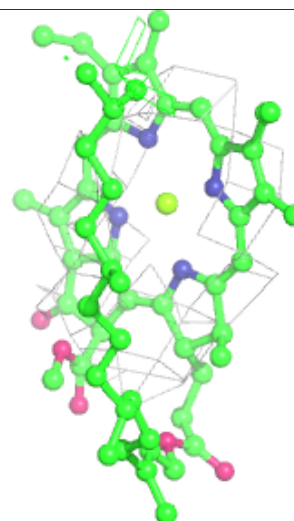
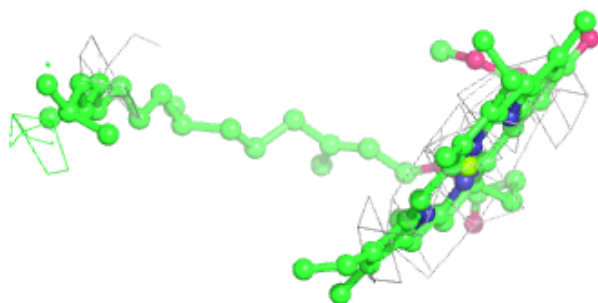
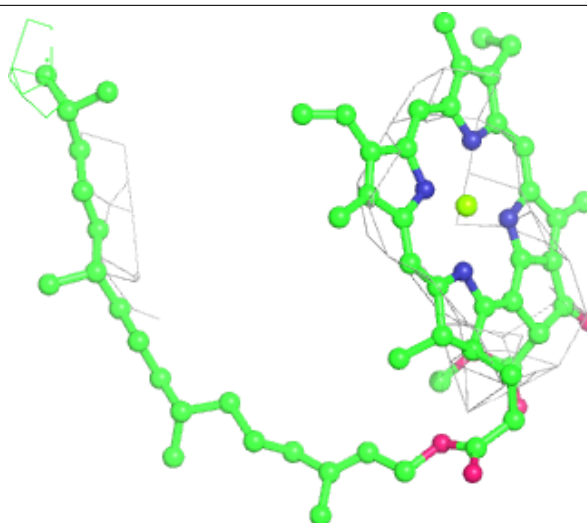
**Electron density around BCR i 101:**

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



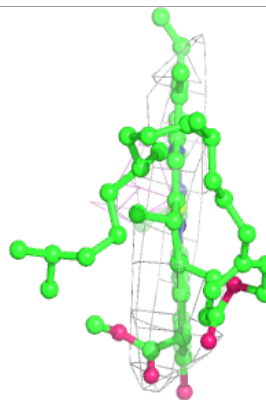
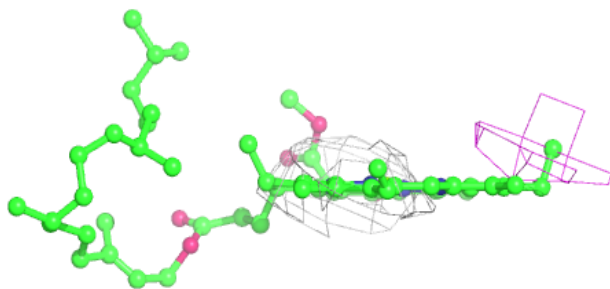
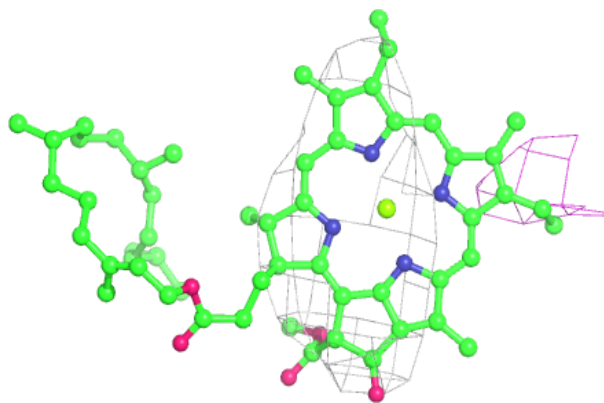
**Electron density around CLA C 506:**

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

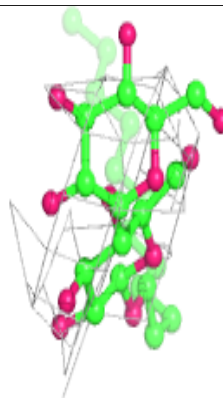
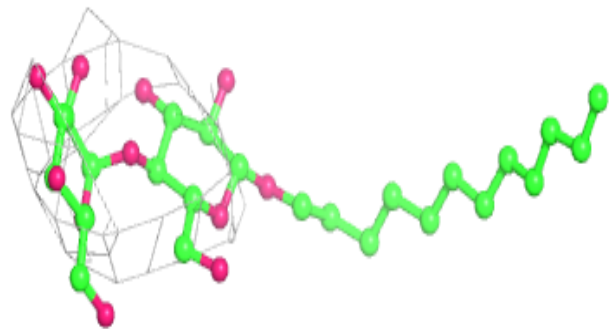
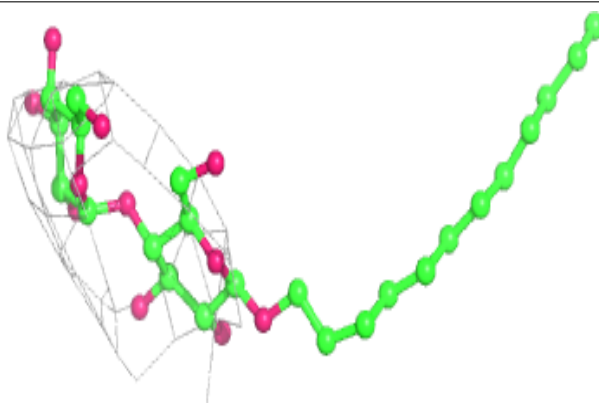


**Electron density around CLA C 511:**

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

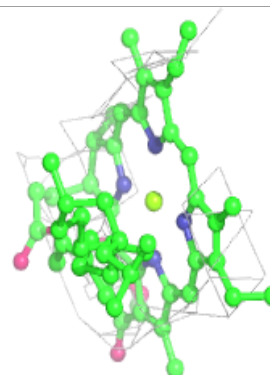
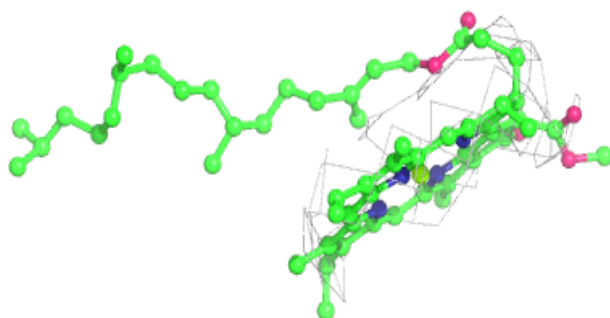
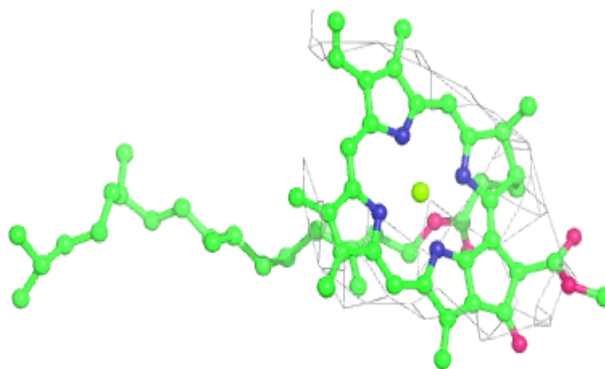
**Electron density around LMT M 103:**

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

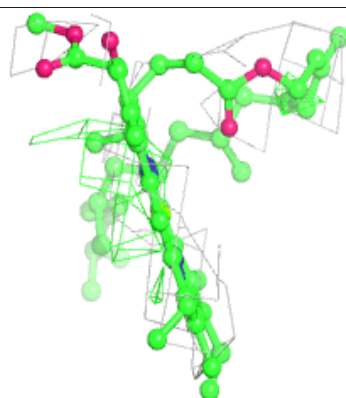
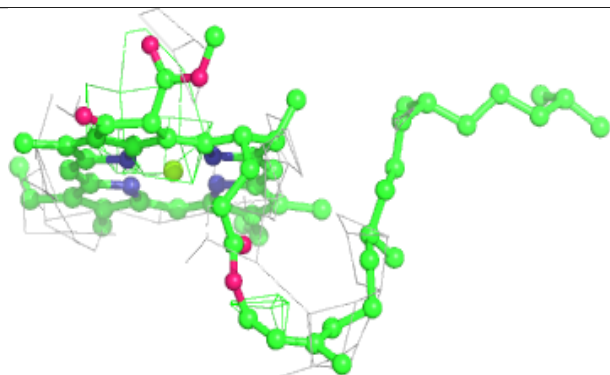
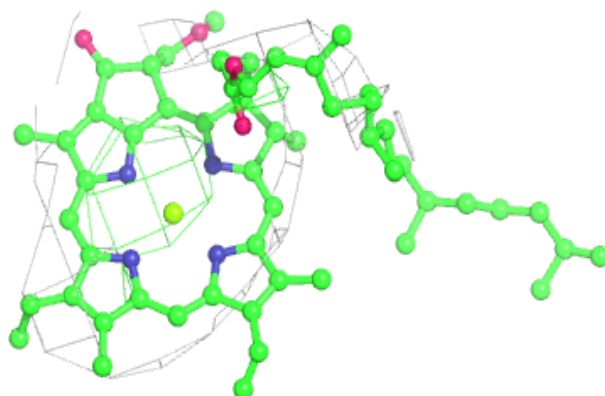


**Electron density around CLA b 618:**

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

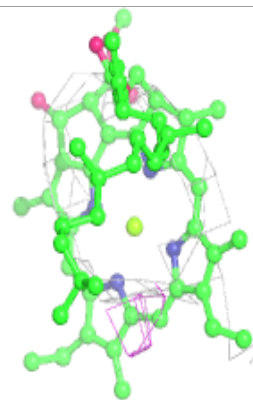
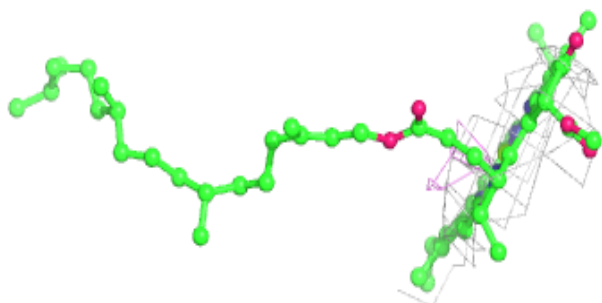
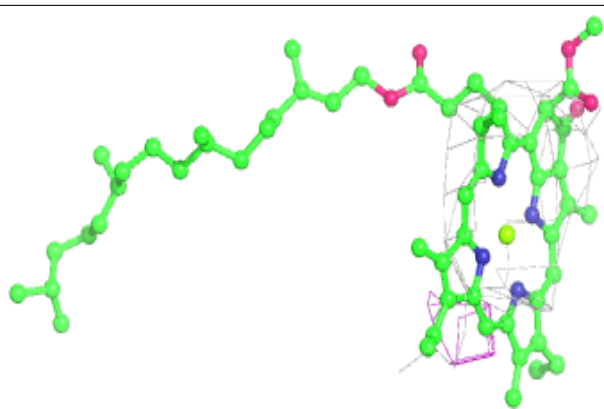
**Electron density around CLA a 404:**

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

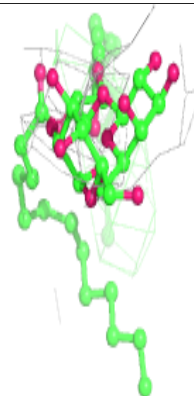
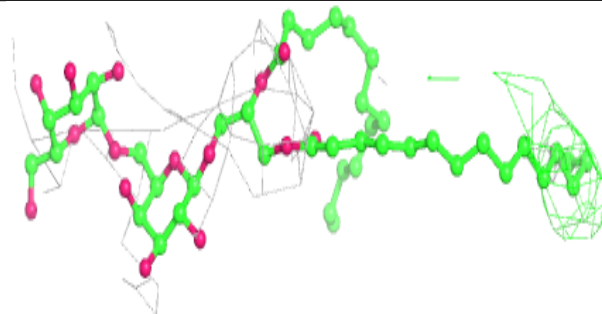
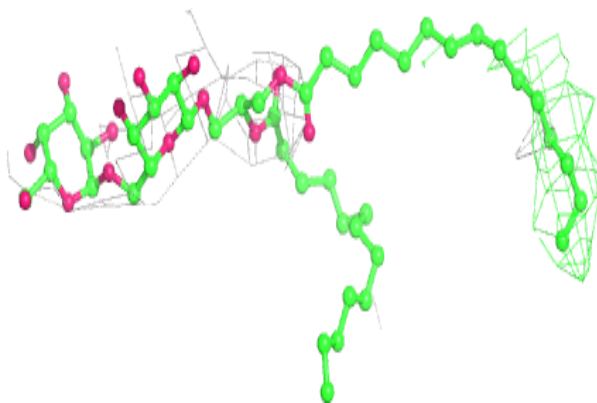


**Electron density around CLA A 406:**

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

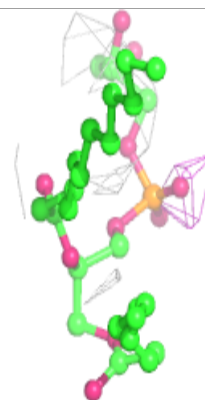
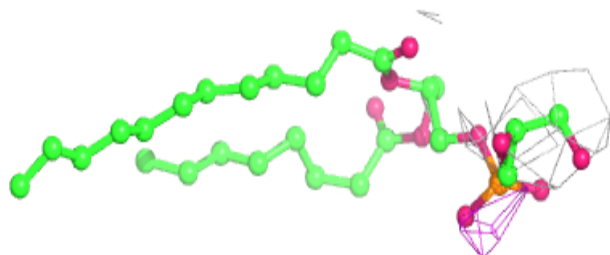
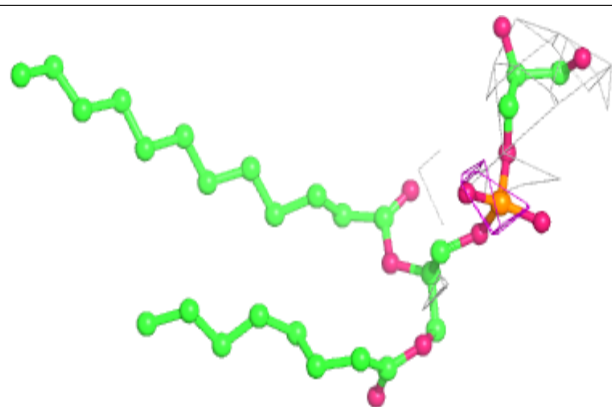
**Electron density around DGD b 625:**

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

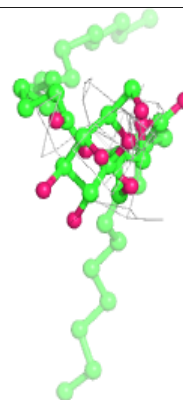
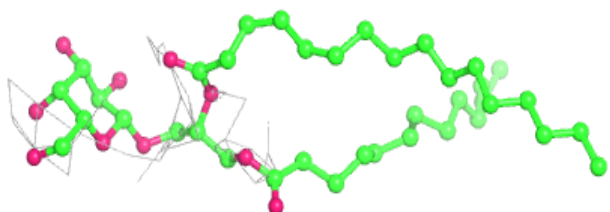
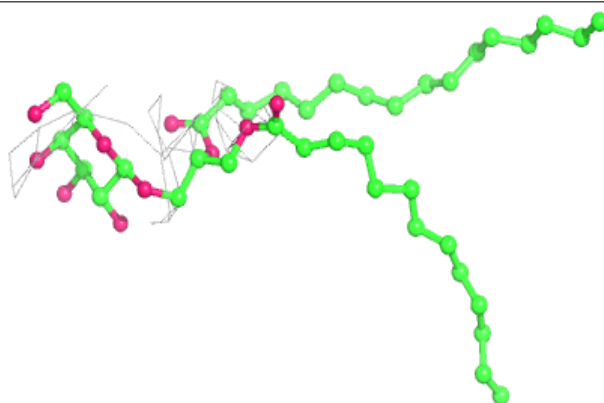


**Electron density around LHG c 519:**

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

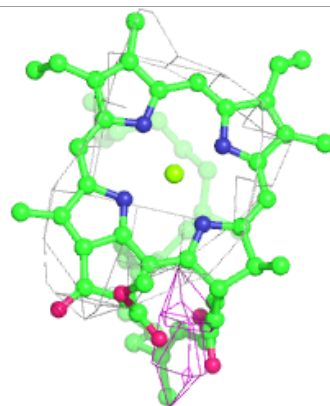
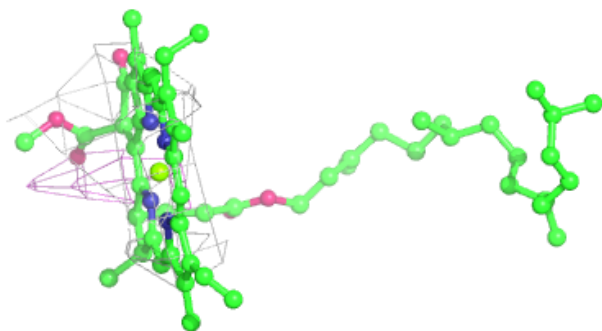
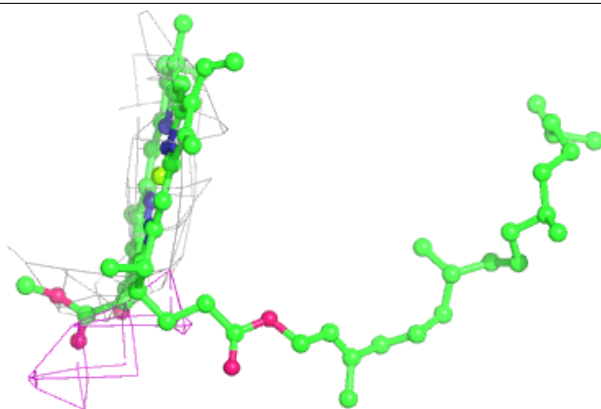
**Electron density around LMG d 409:**

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



**Electron density around CLA c 505:**

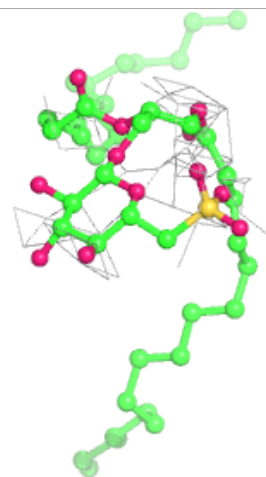
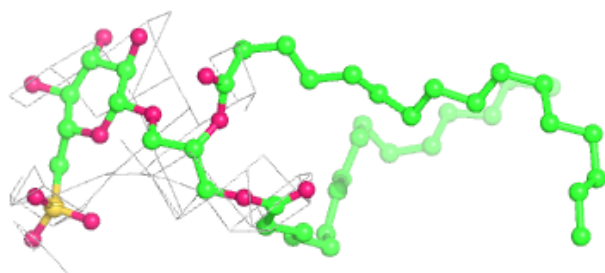
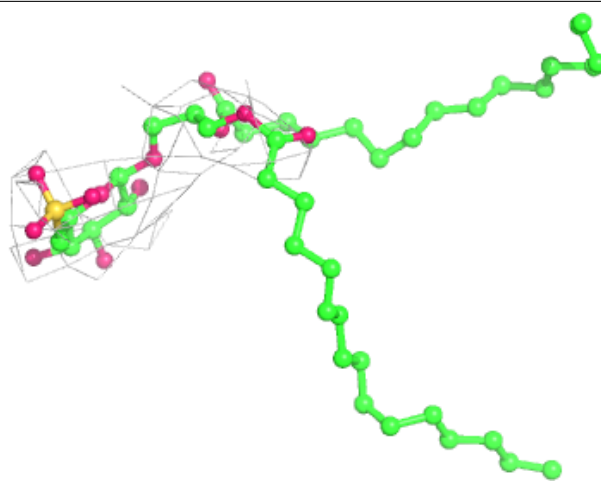
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





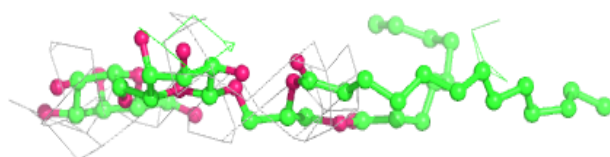
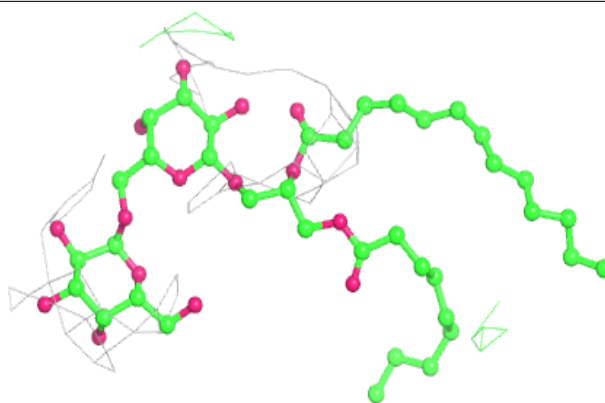
**Electron density around SQD a 401:**

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

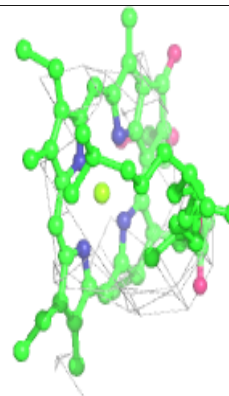
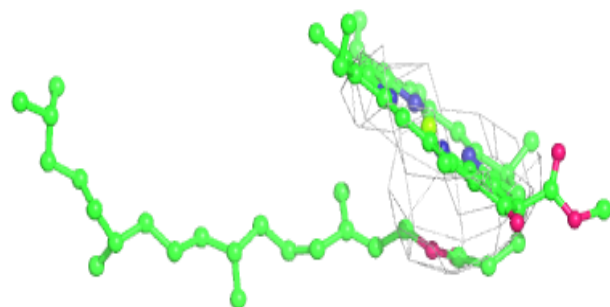
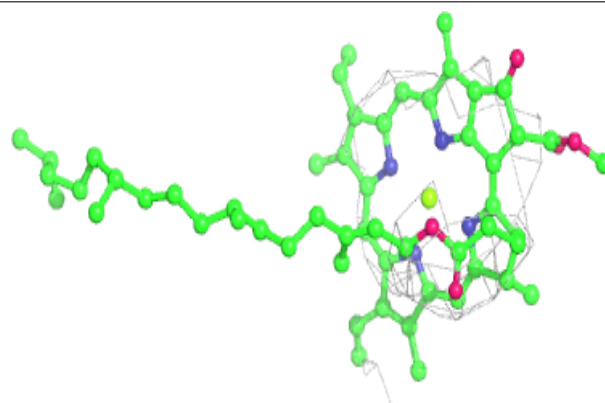


**Electron density around DGD b 601:**

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

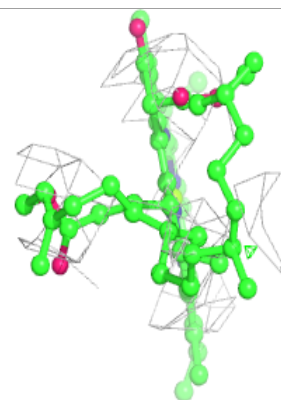
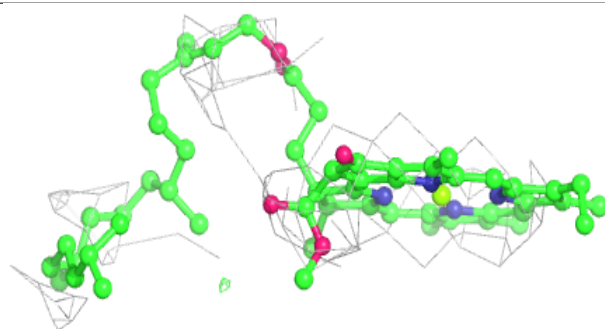
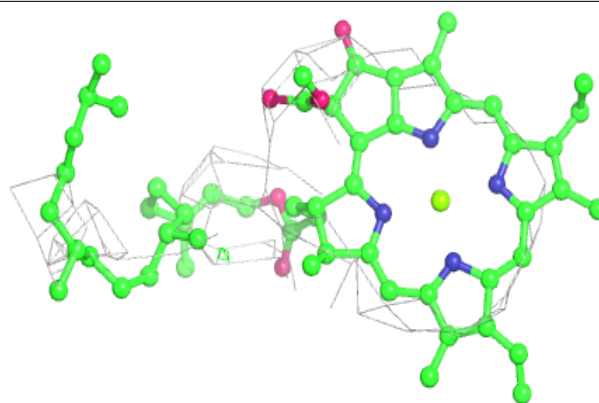
**Electron density around CLA b 612:**

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

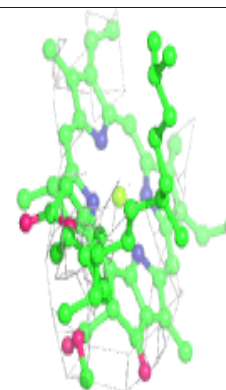
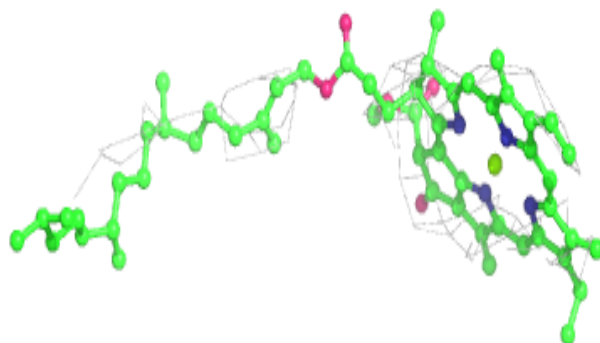
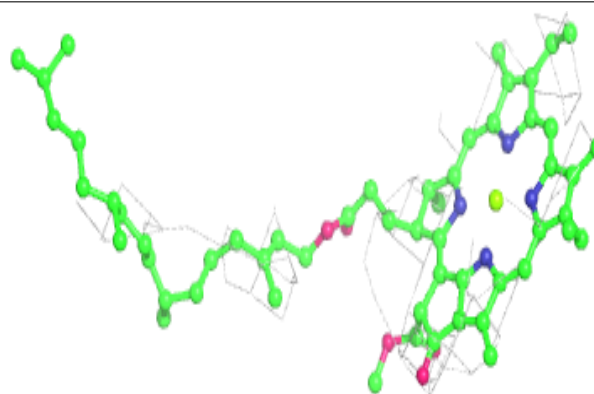


**Electron density around CLA b 616:**

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

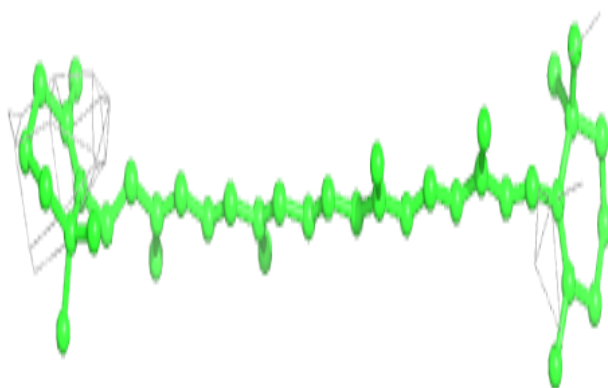
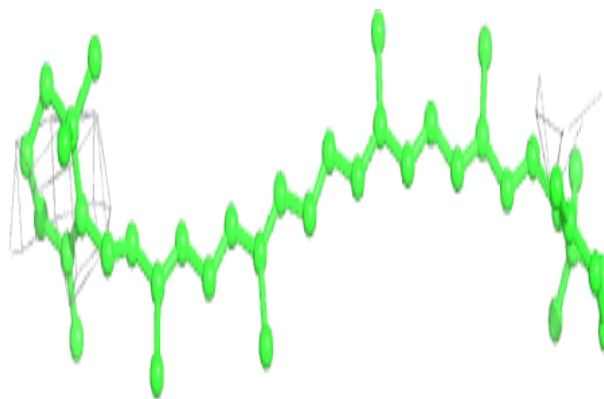
**Electron density around CLA a 403:**

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

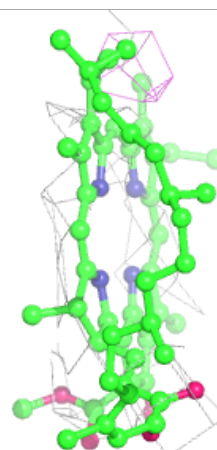
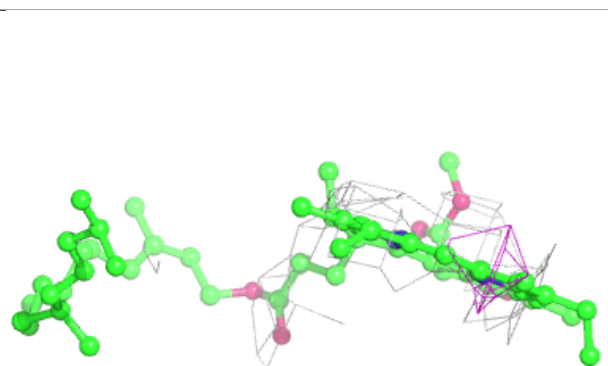
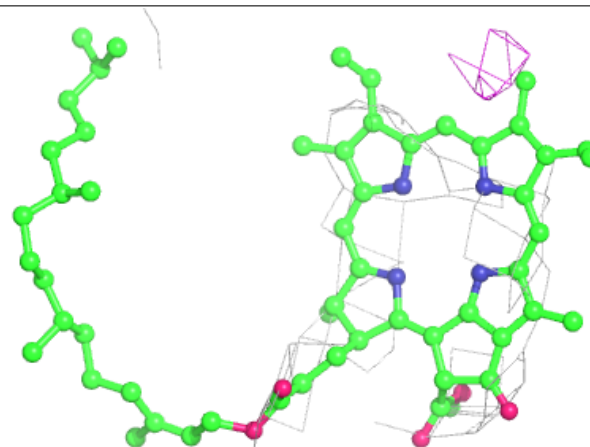


**Electron density around BCR c 521:**

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

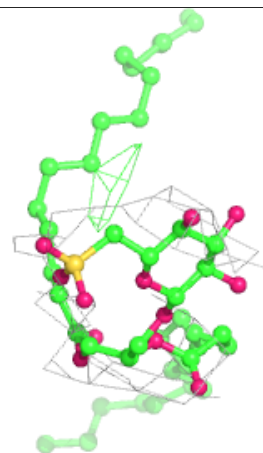
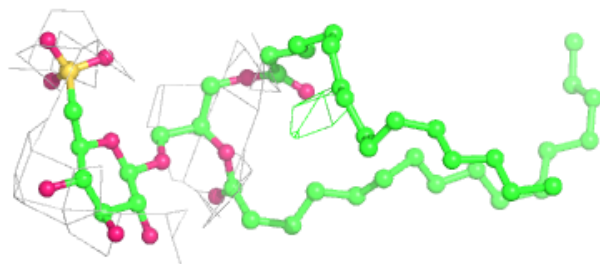
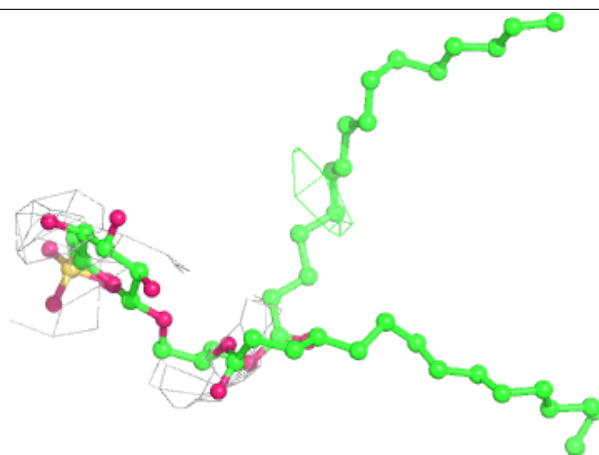
**Electron density around PHO A 405:**

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

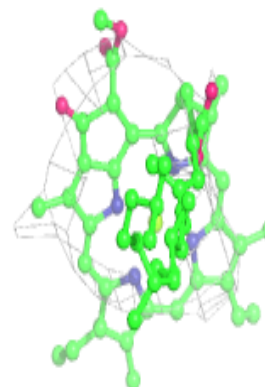
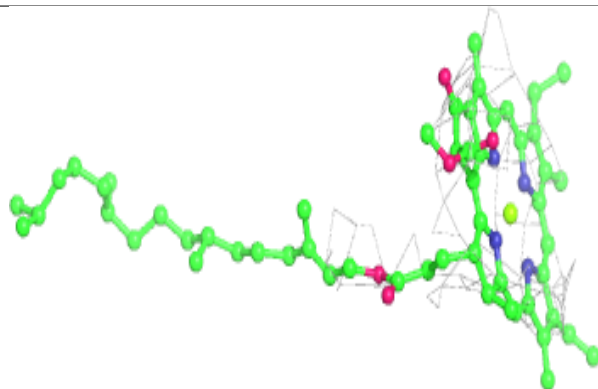
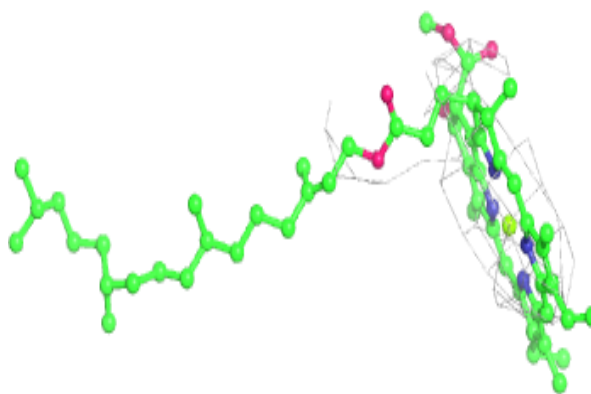


**Electron density around SQD A 414:**

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

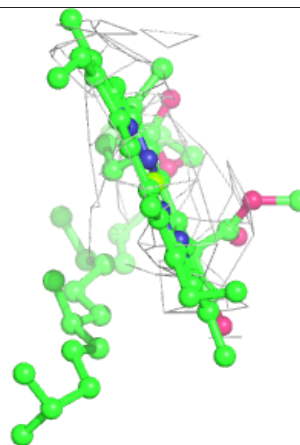
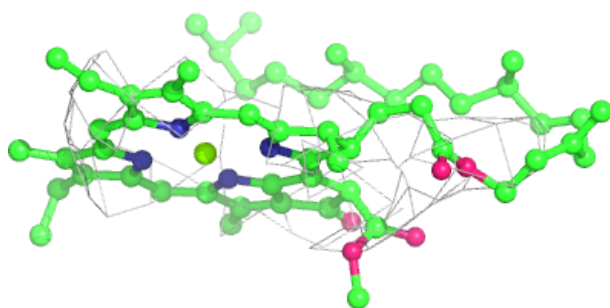
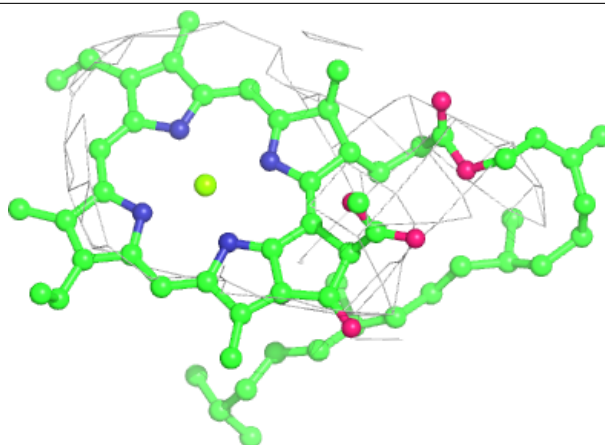
**Electron density around CLA B 603:**

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

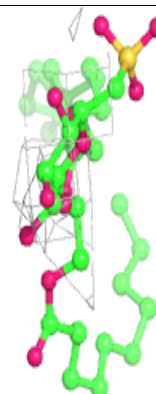
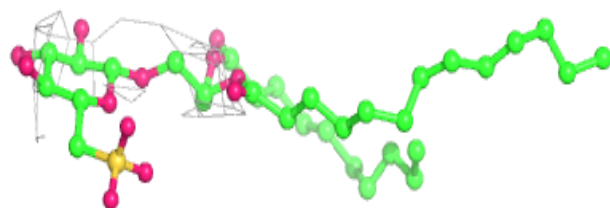
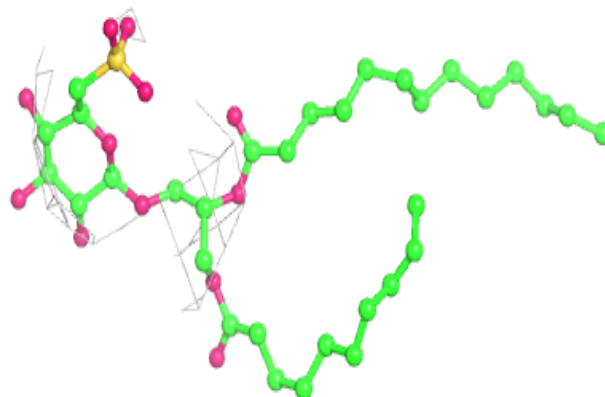


**Electron density around CLA c 508:**

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

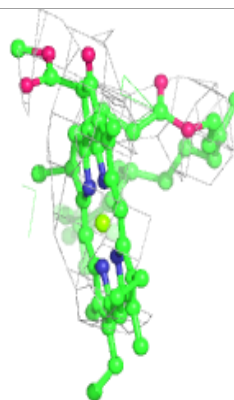
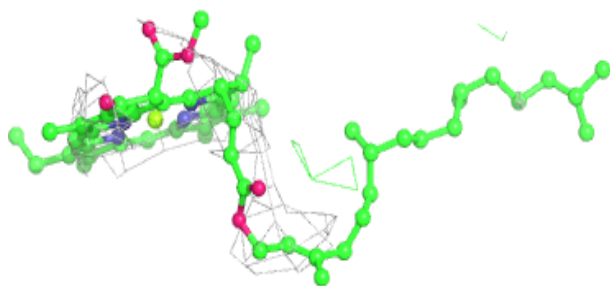
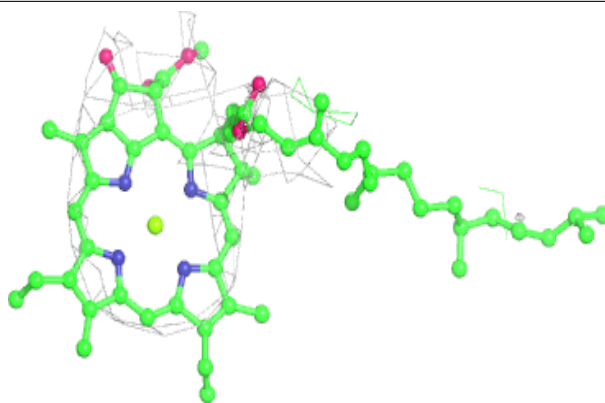
**Electron density around SQD f 103:**

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

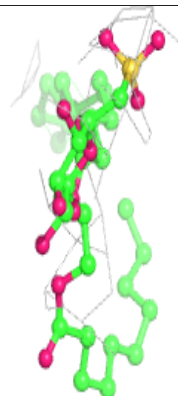
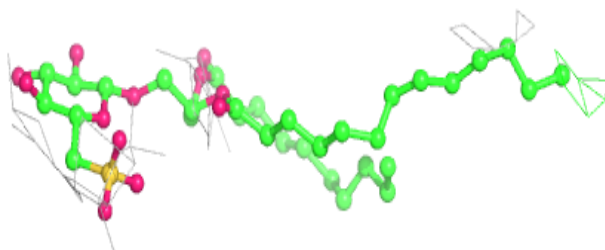
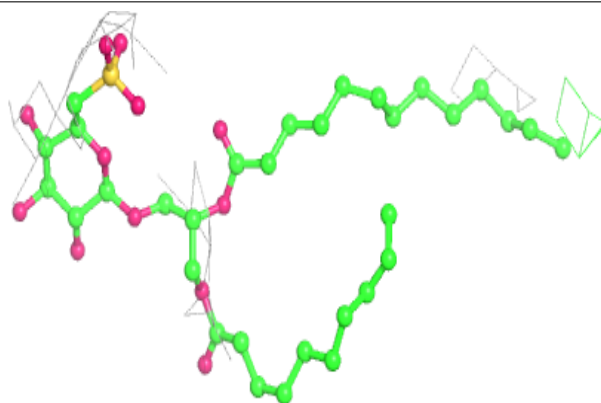


**Electron density around CLA A 404:**

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

**Electron density around SQD F 103:**

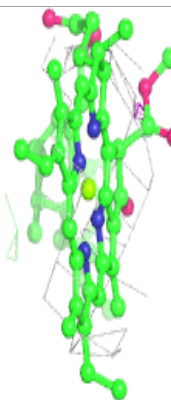
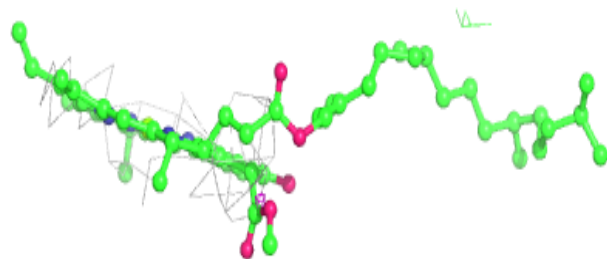
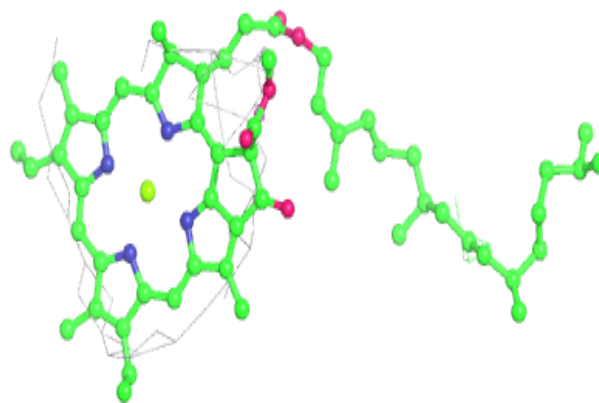
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



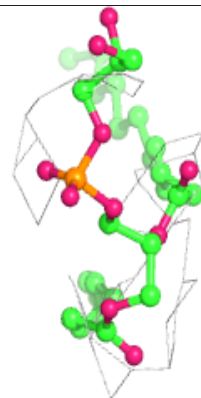
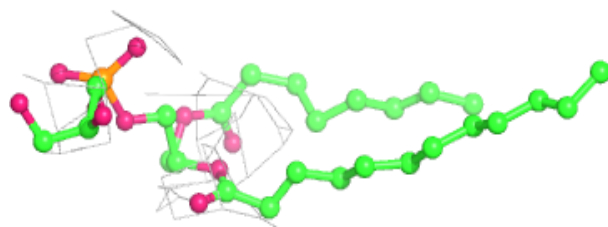
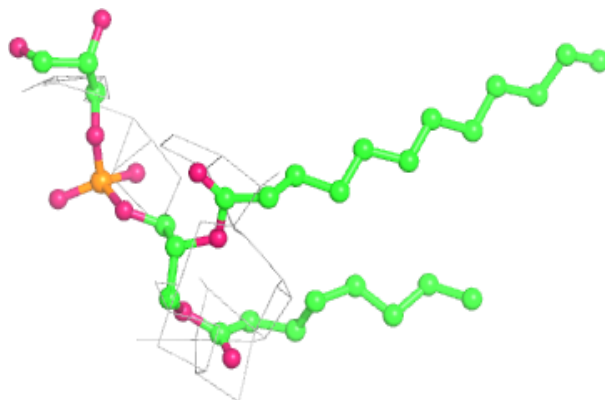


**Electron density around CLA b 606:**

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

**Electron density around LHG C 518:**

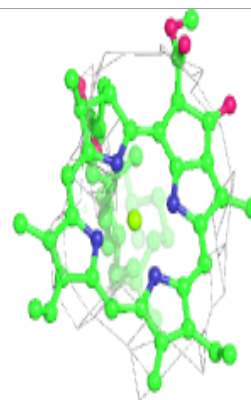
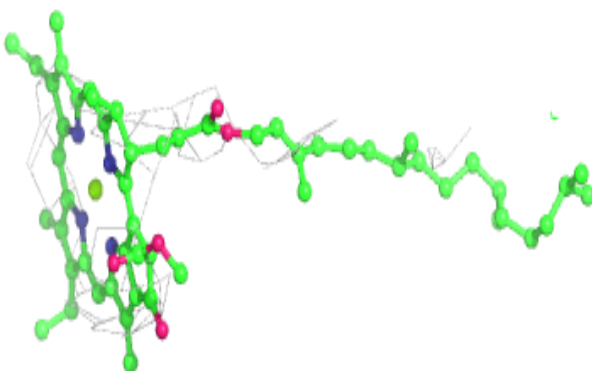
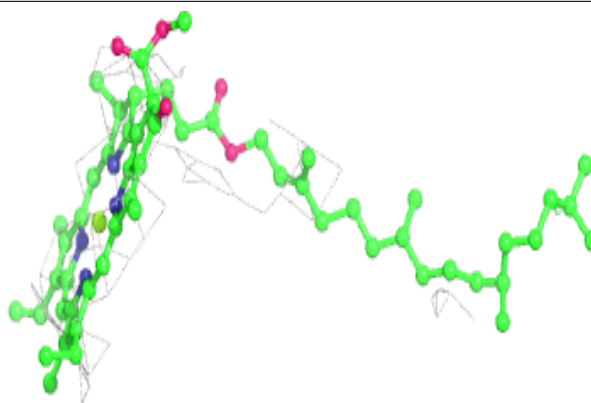
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



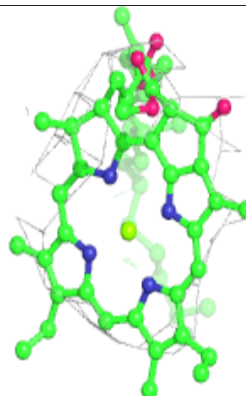
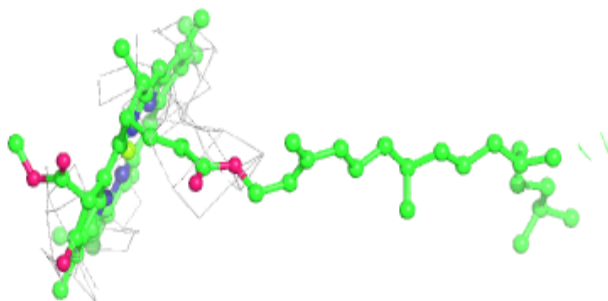
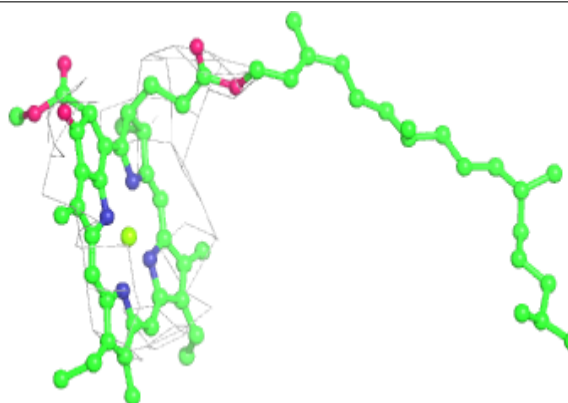


**Electron density around CLA b 608:**

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

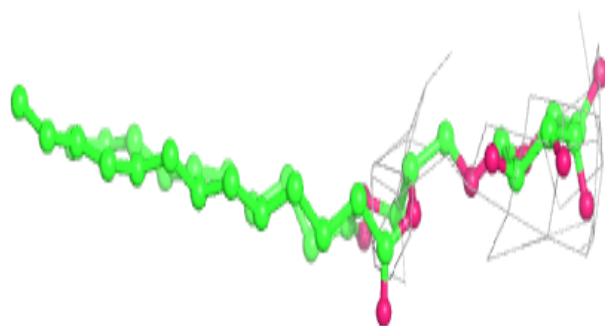
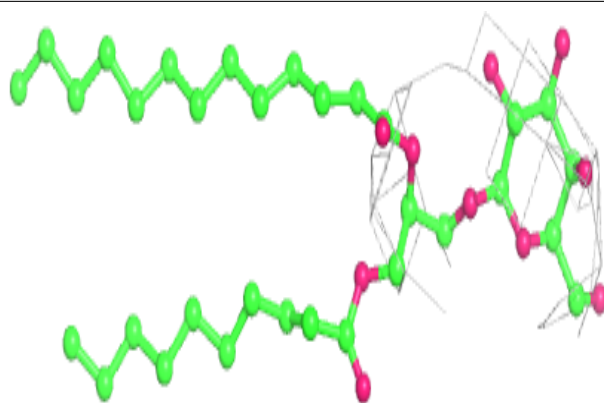
**Electron density around CLA b 613:**

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

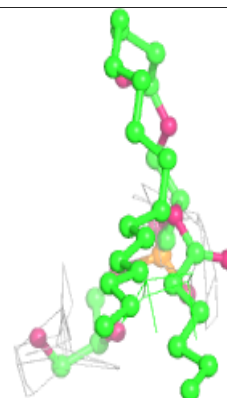
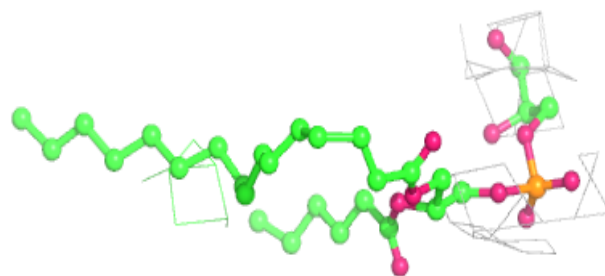
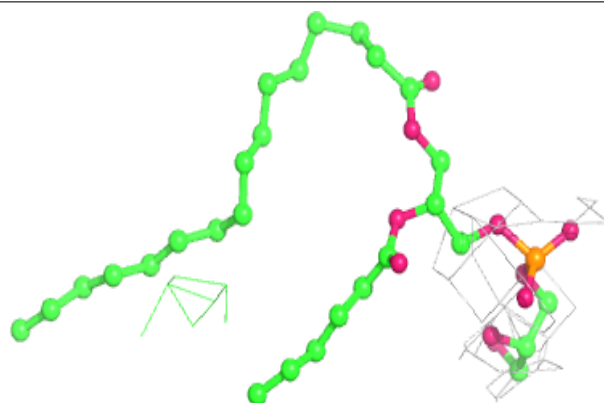


**Electron density around LMG M 101:**

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

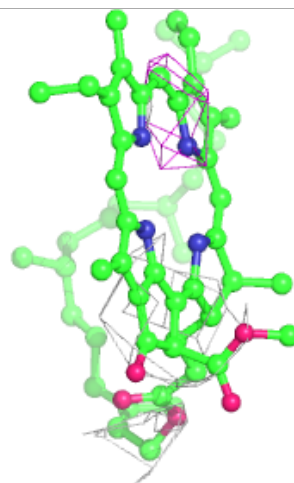
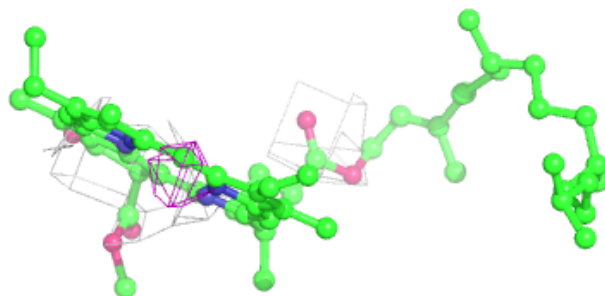
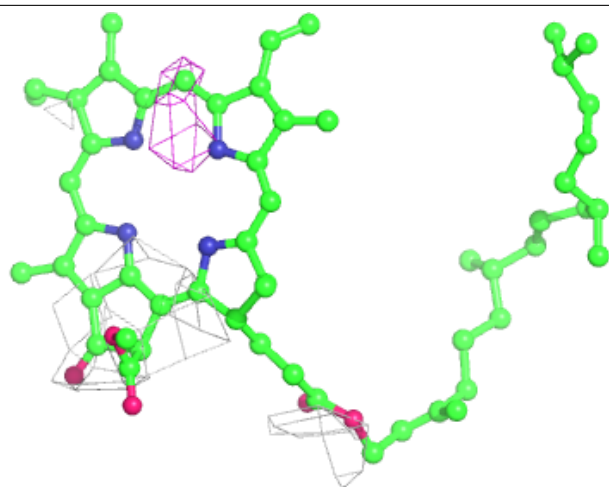
**Electron density around LHG a 409:**

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



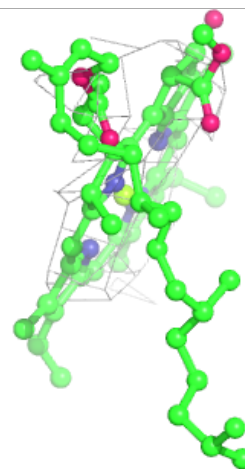
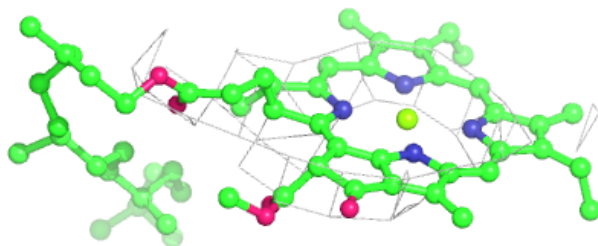
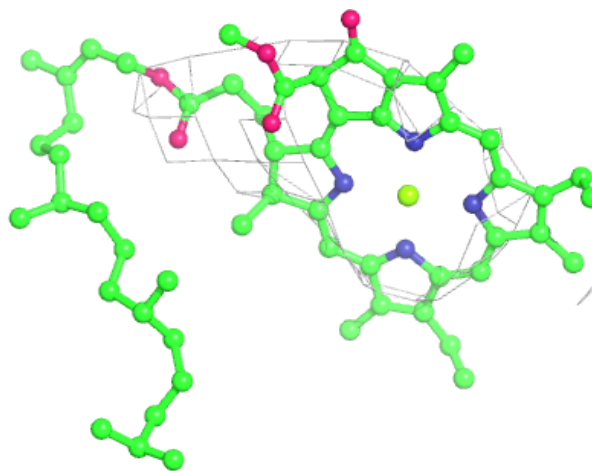
**Electron density around PHO d 402:**

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



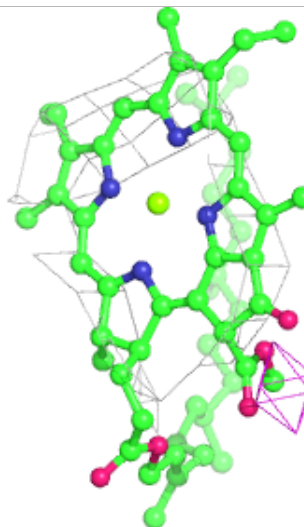
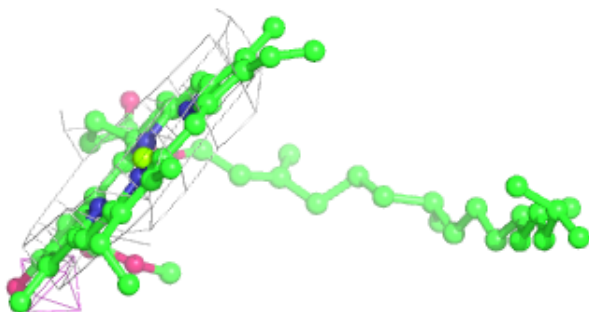
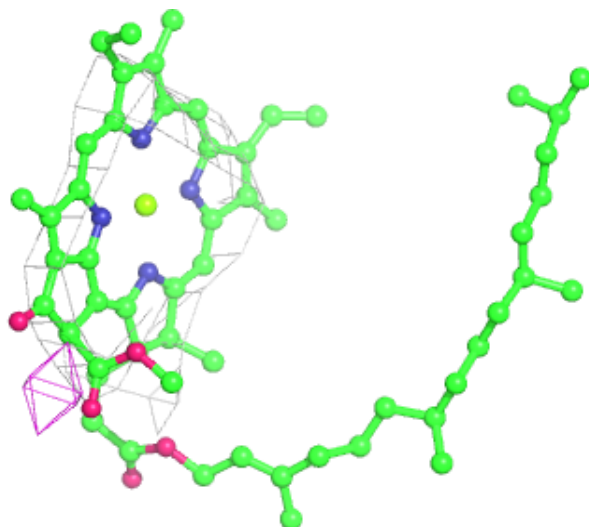
**Electron density around CLA B 615:**

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



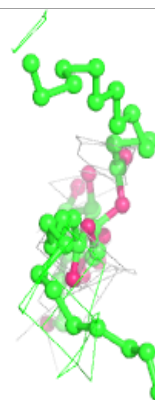
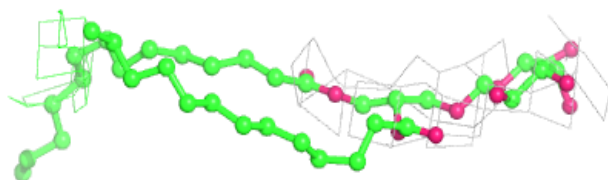
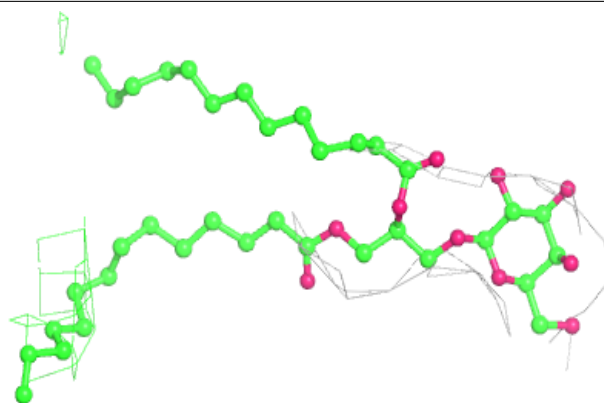
**Electron density around CLA c 506:**

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

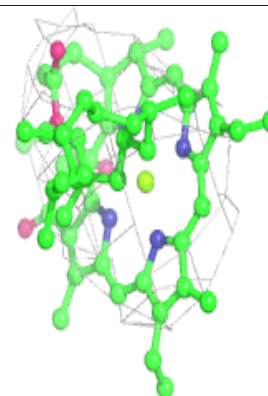
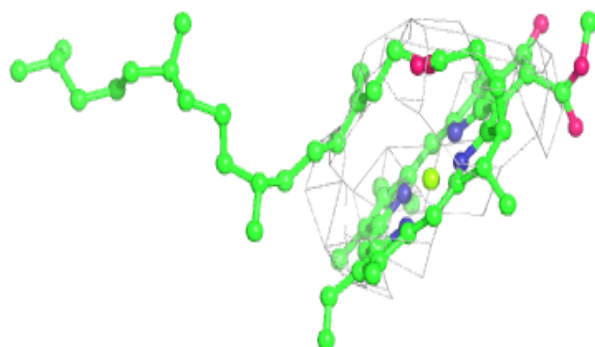
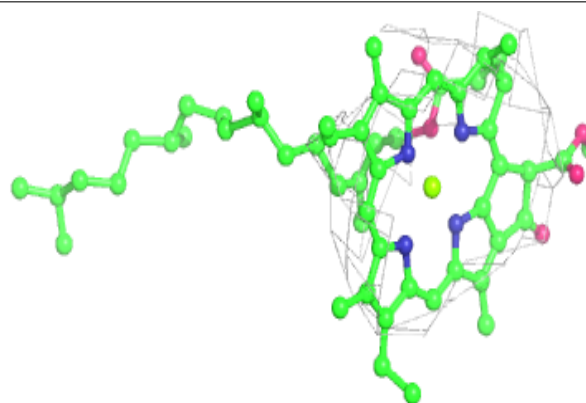


**Electron density around LMG D 409:**

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

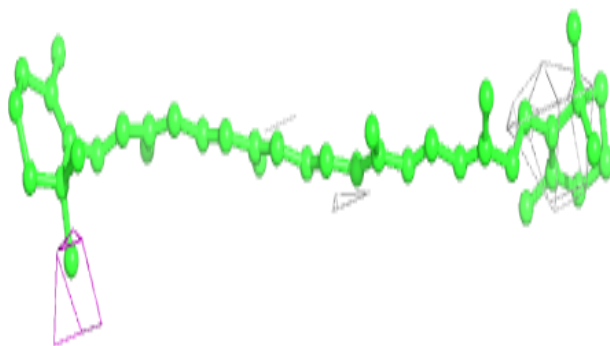
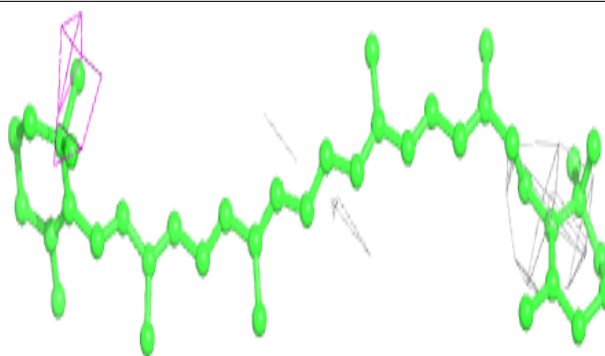
**Electron density around CLA C 504:**

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

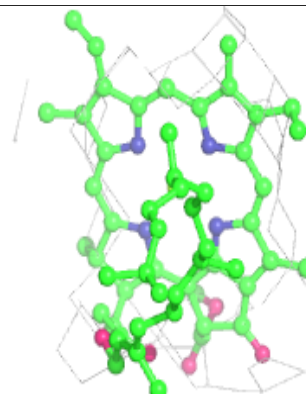
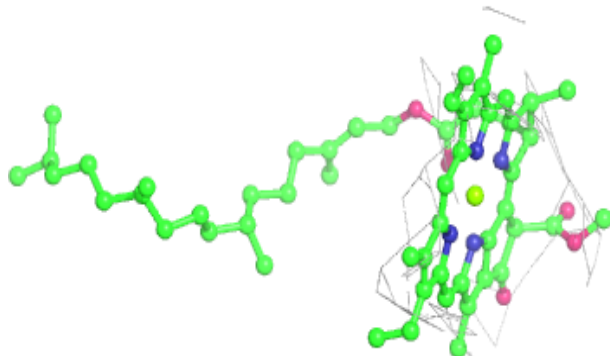
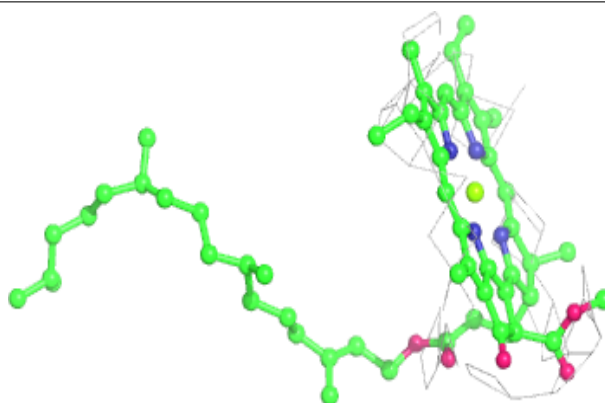


**Electron density around BCR y 101:**

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

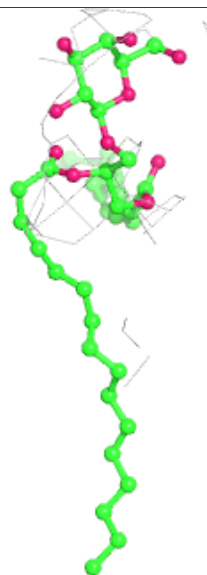
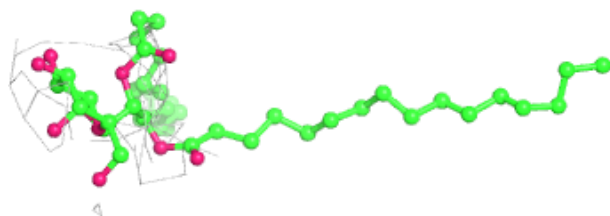
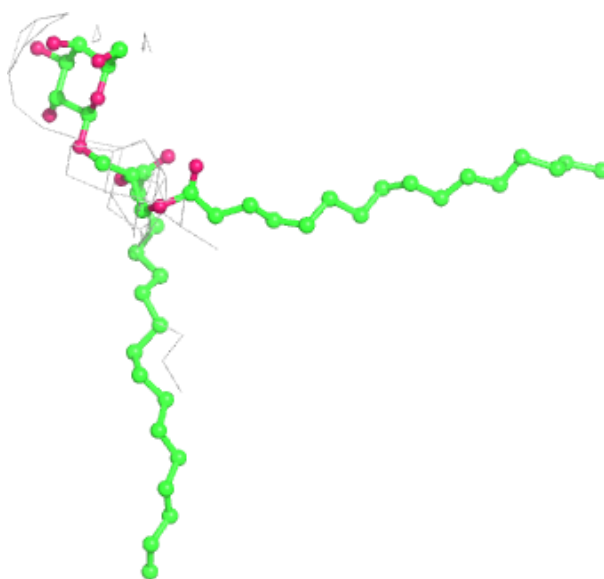
**Electron density around CLA C 507:**

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



**Electron density around LMG 1 101:**

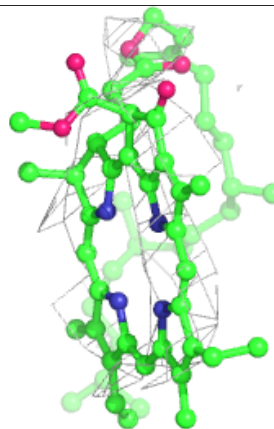
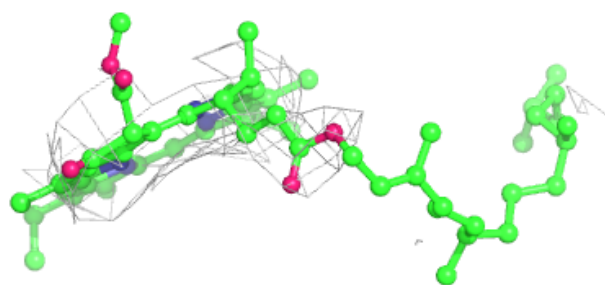
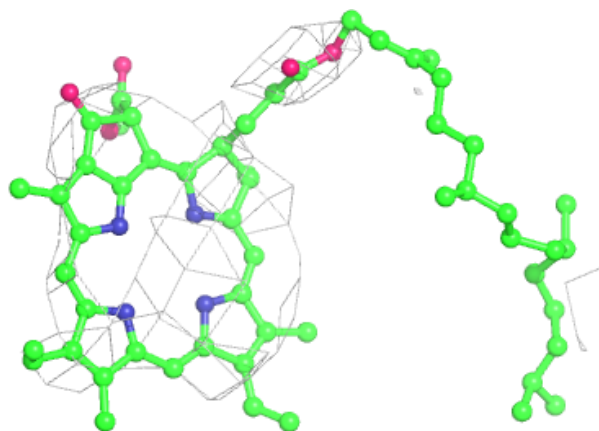
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





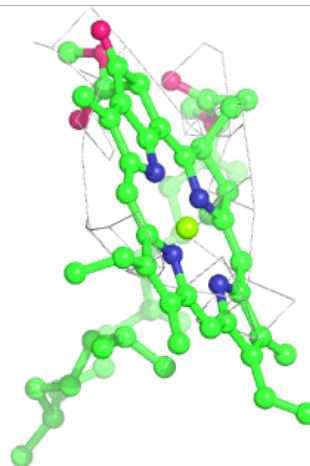
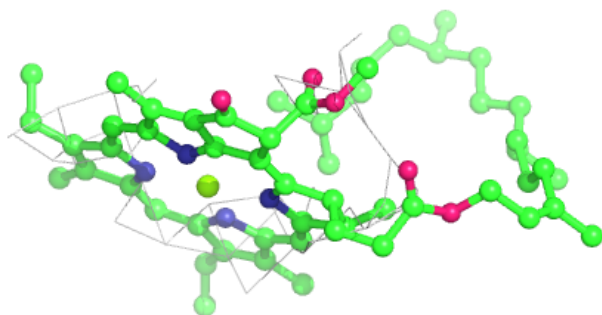
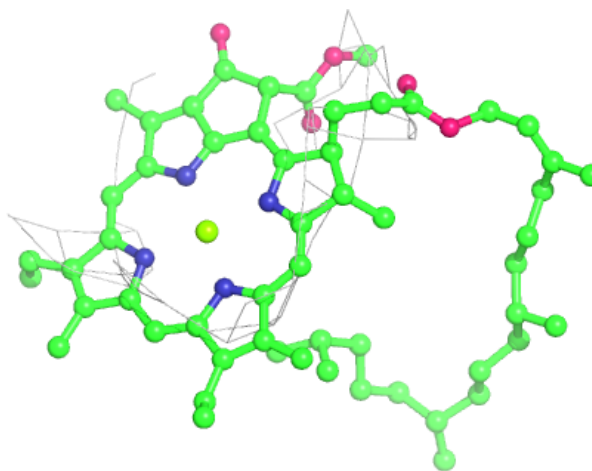
**Electron density around PHO D 401:**

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



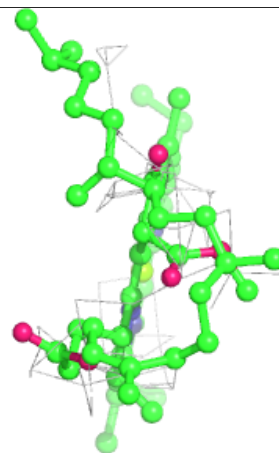
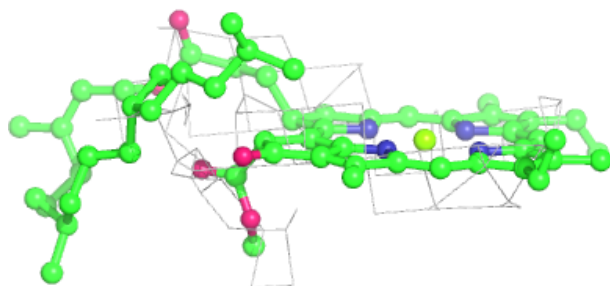
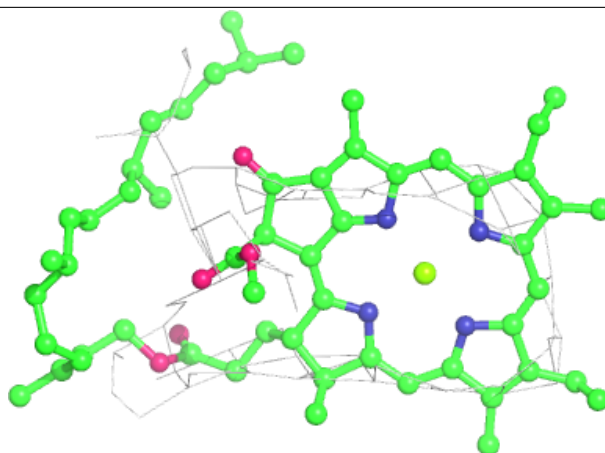
**Electron density around CLA B 614:**

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



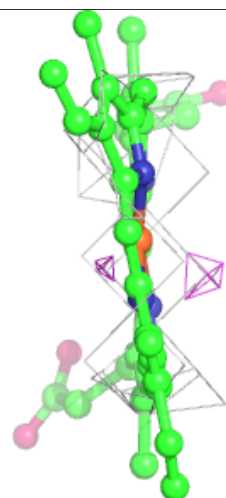
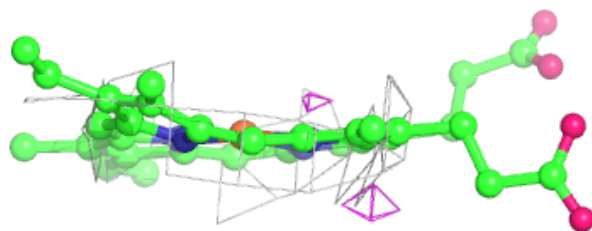
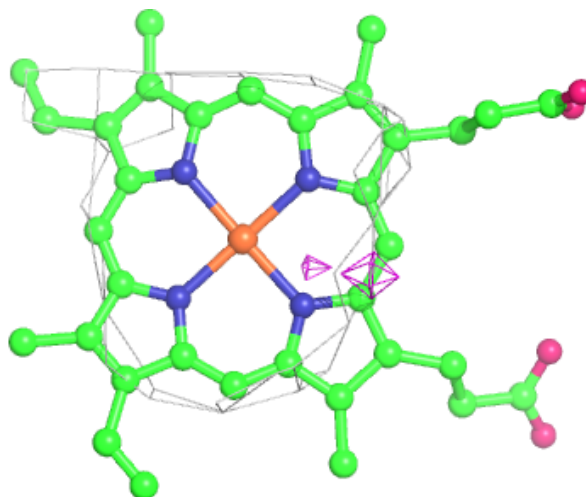
**Electron density around CLA b 614:**

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



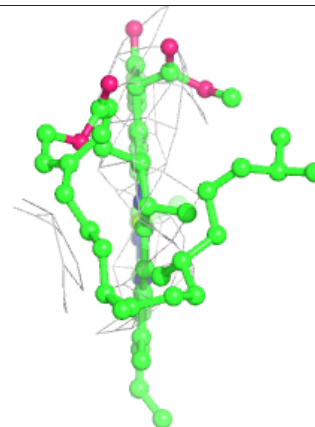
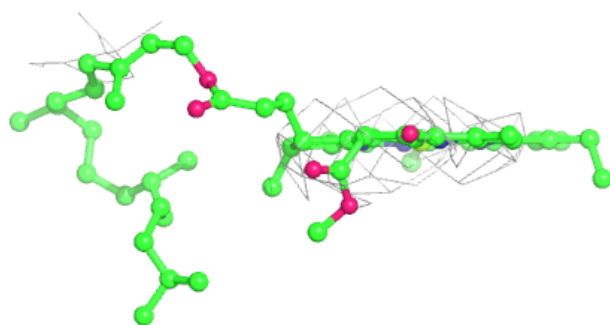
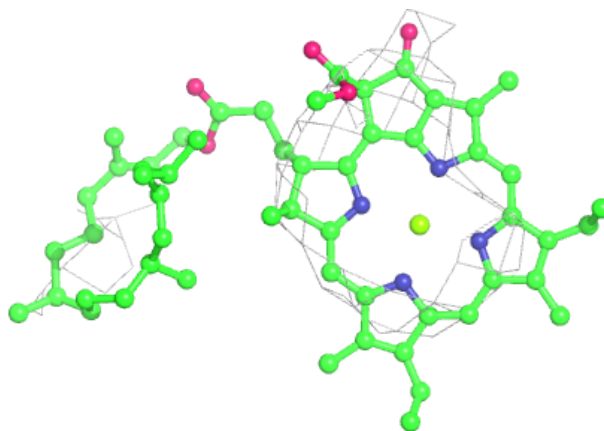
**Electron density around HEM v 201:**

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

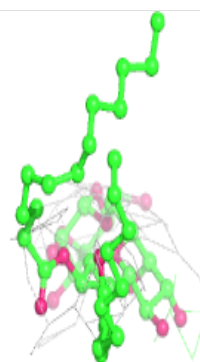
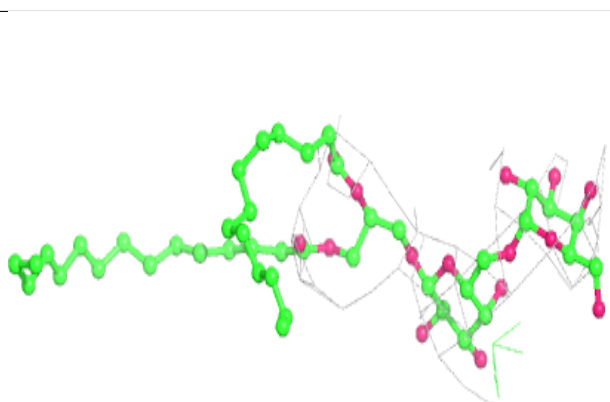
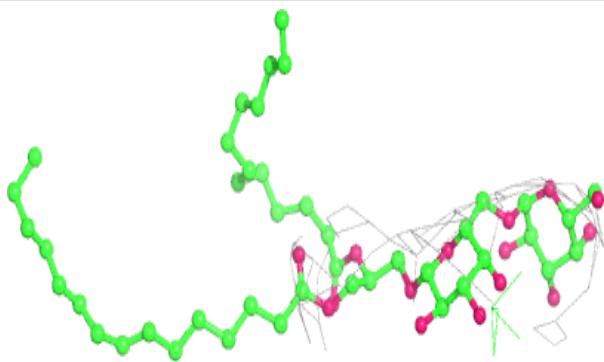


**Electron density around CLA c 511:**

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

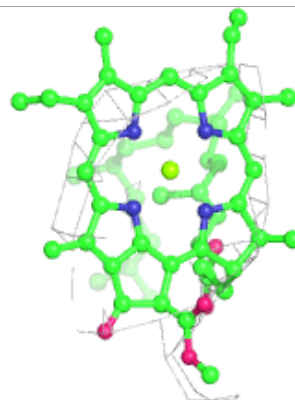
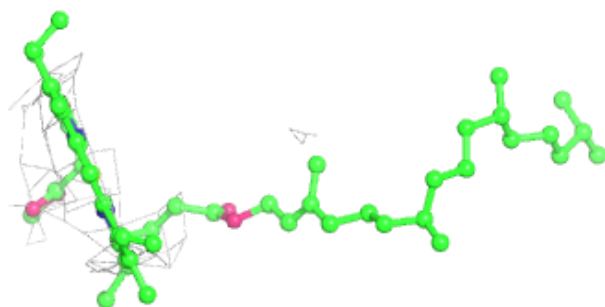
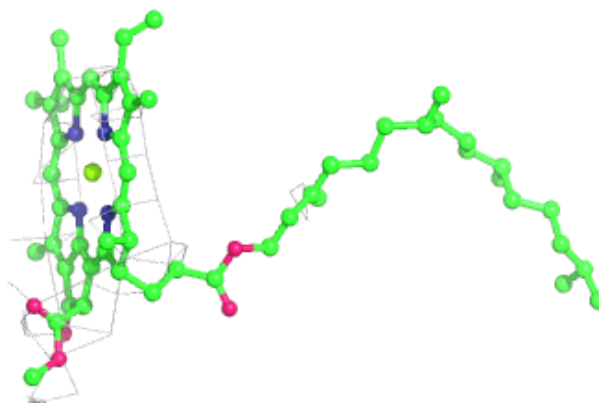
**Electron density around DGD B 620:**

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



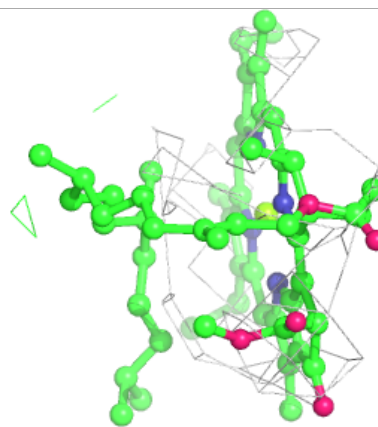
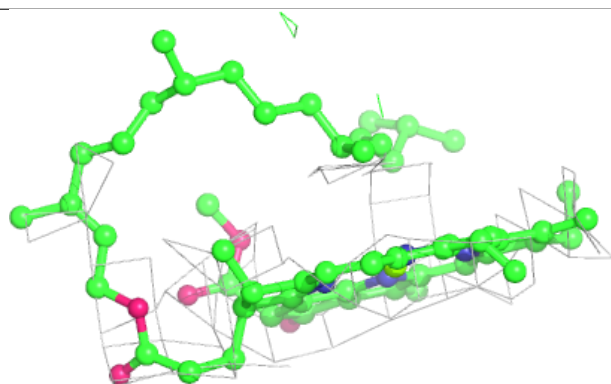
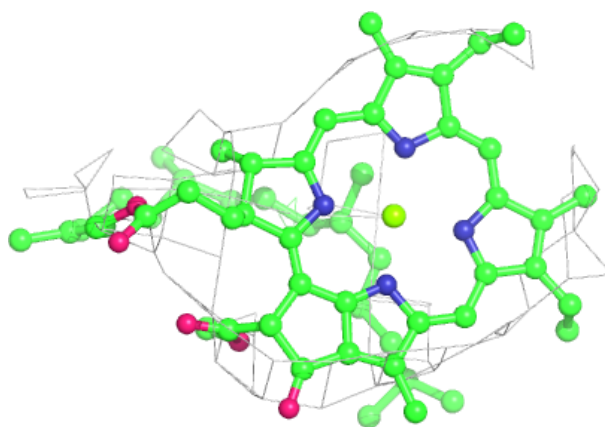
**Electron density around CLA d 406:**

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



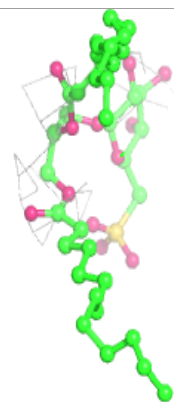
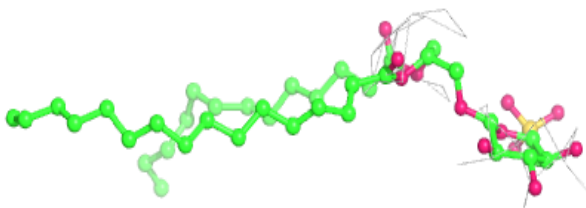
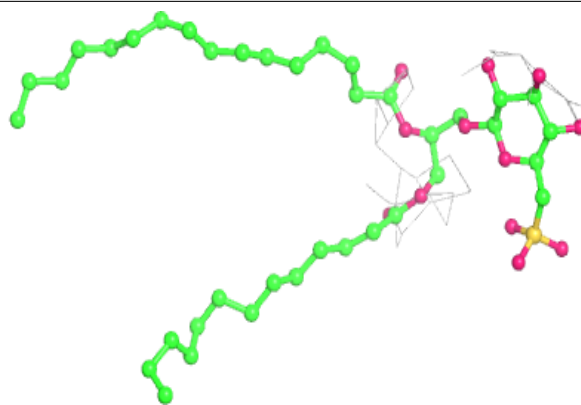
**Electron density around CLA C 509:**

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

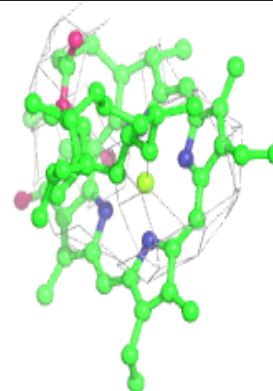
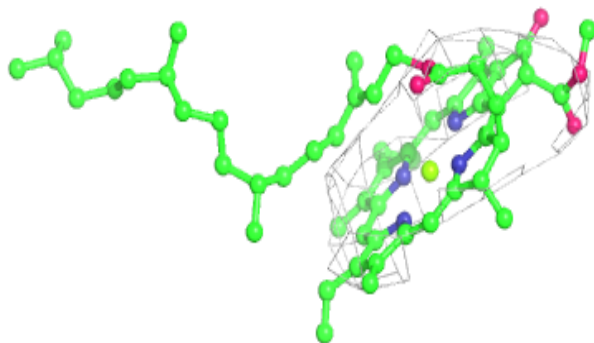
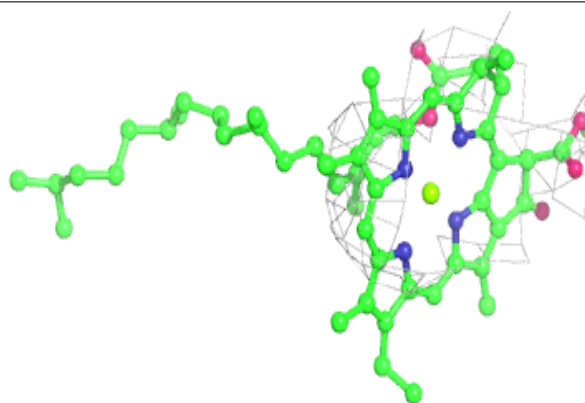


**Electron density around SQD A 413:**

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

**Electron density around CLA c 504:**

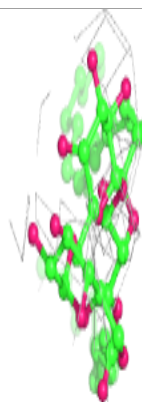
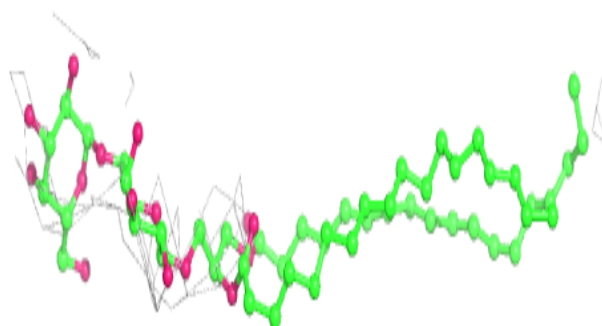
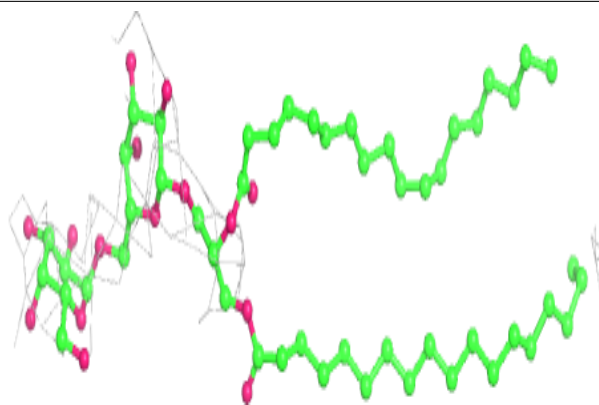
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



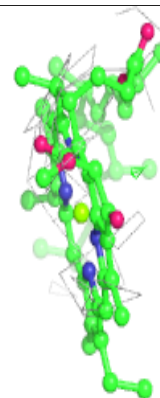
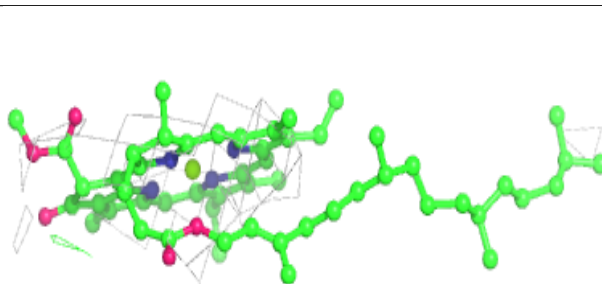
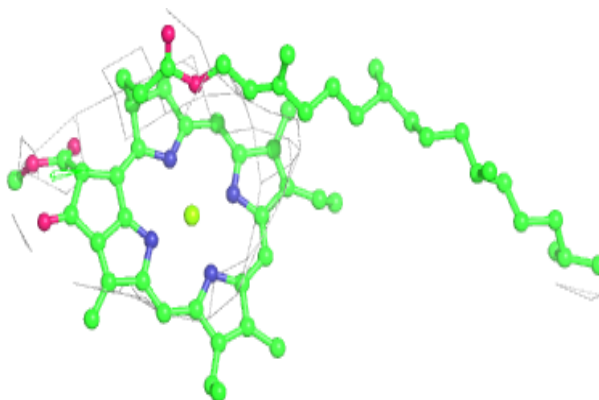


**Electron density around DGD c 517:**

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

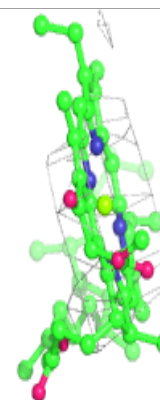
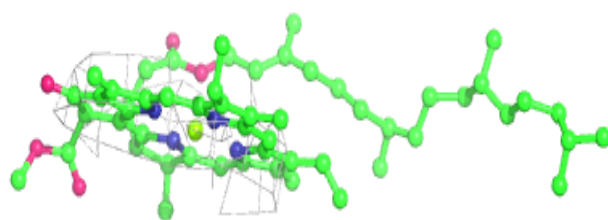
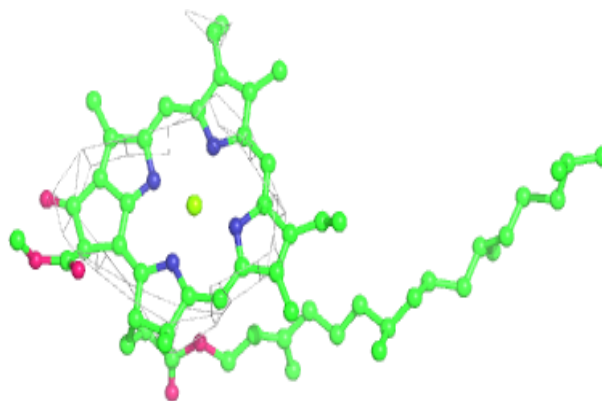
**Electron density around CLA C 501:**

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

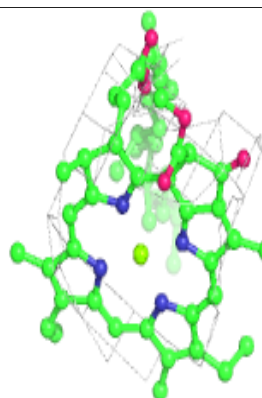
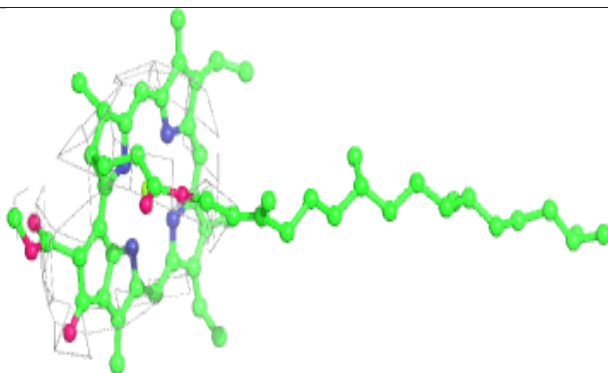
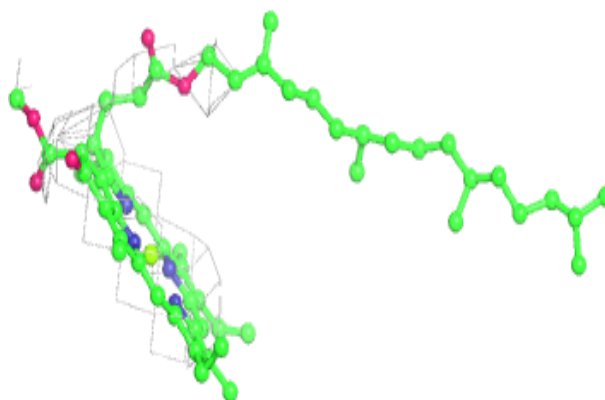


**Electron density around CLA c 501:**

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

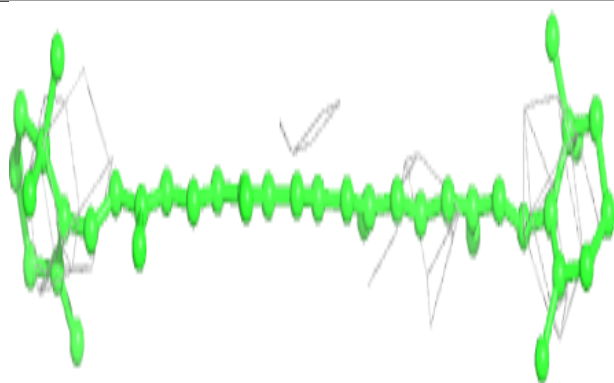
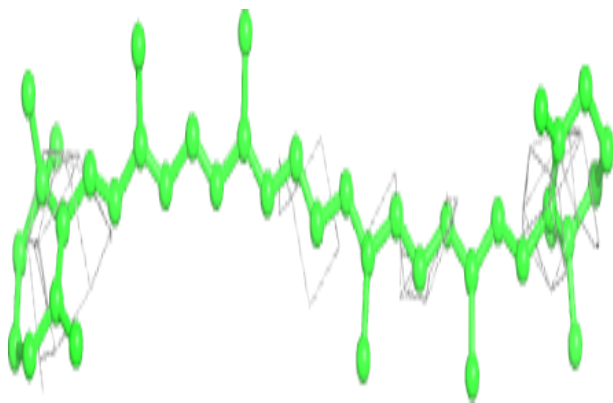
**Electron density around CLA C 519:**

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

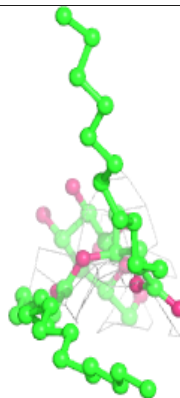
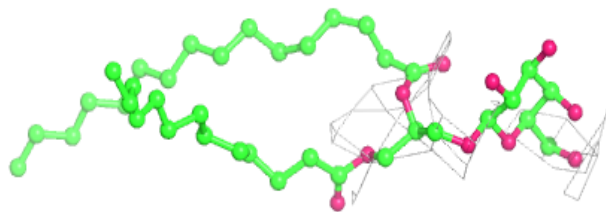
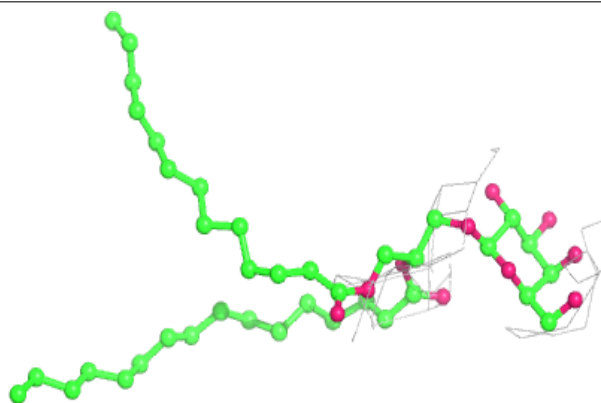


**Electron density around BCR B 618:**

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

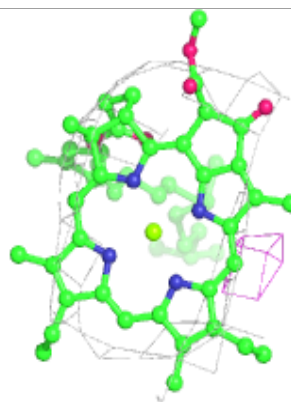
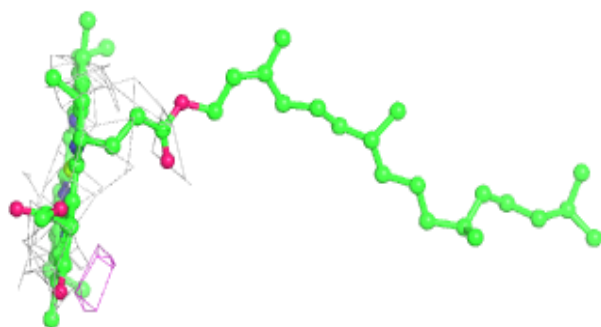
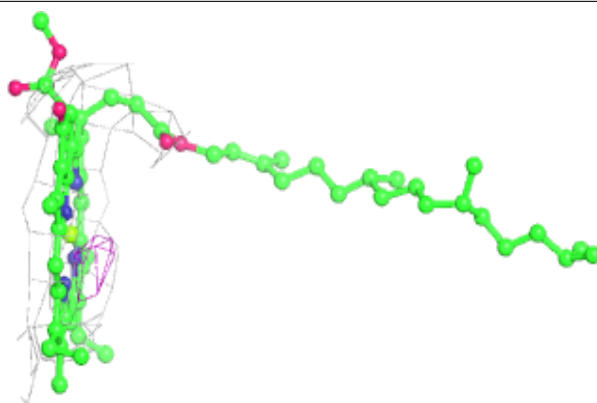
**Electron density around LMG D 406:**

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



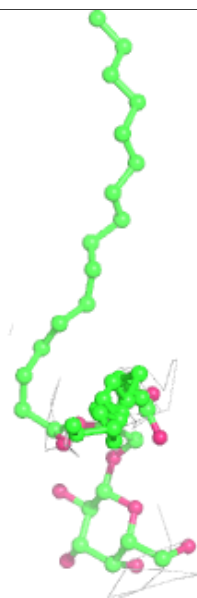
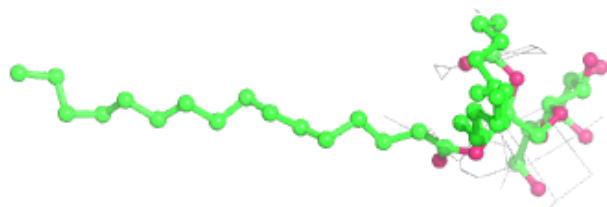
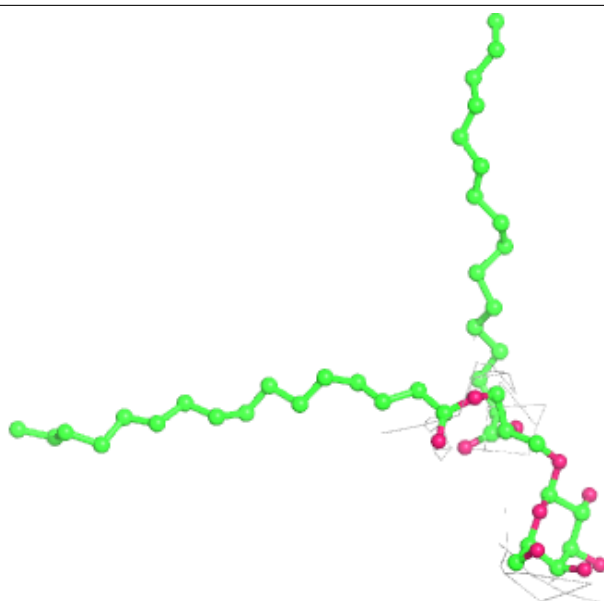
**Electron density around CLA B 605:**

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



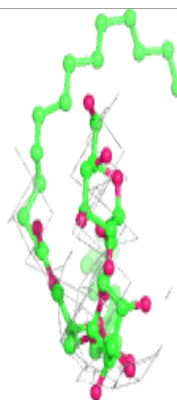
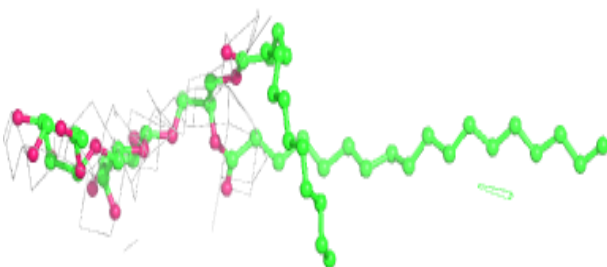
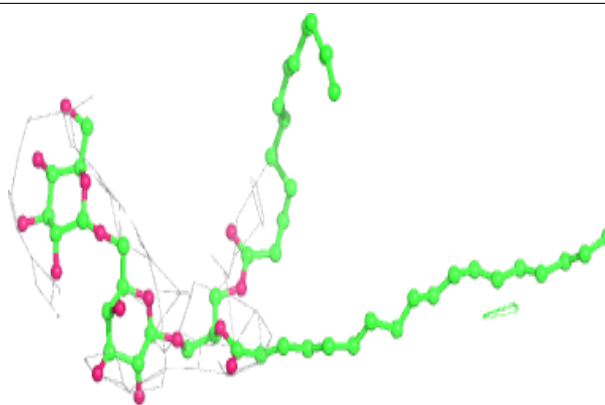
**Electron density around LMG L 101:**

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

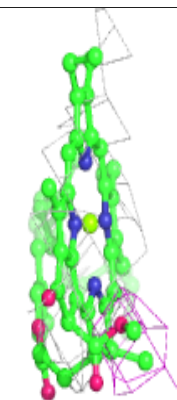
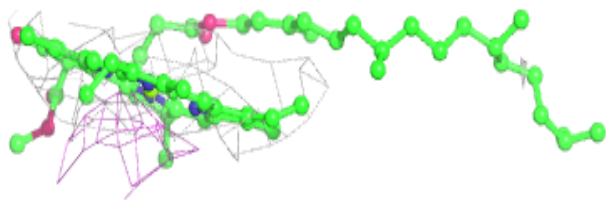
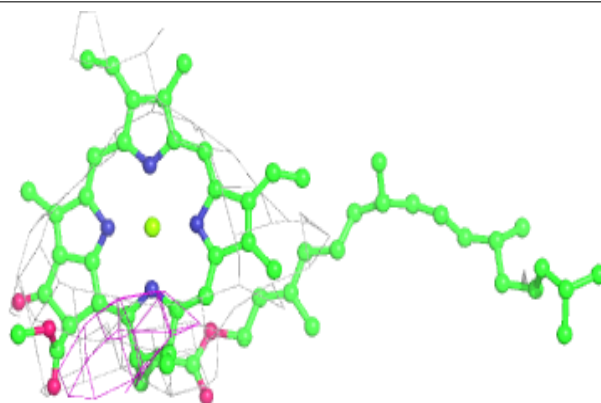


**Electron density around DGD C 515:**

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

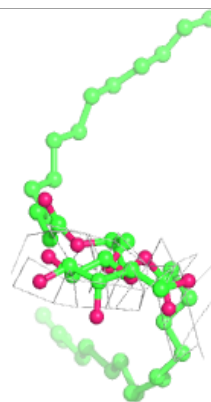
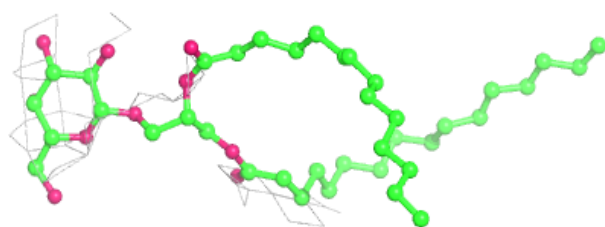
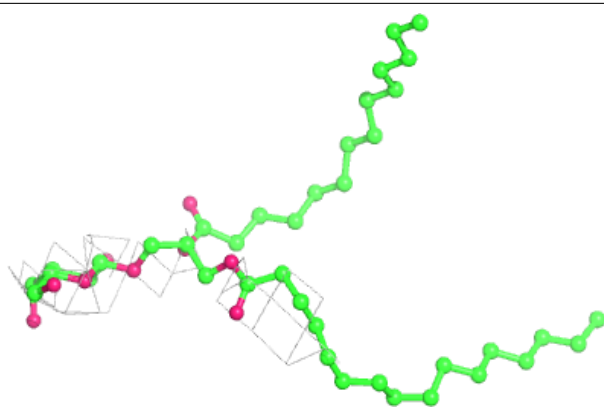
**Electron density around CLA b 607:**

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

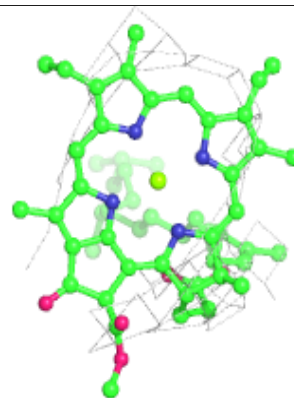
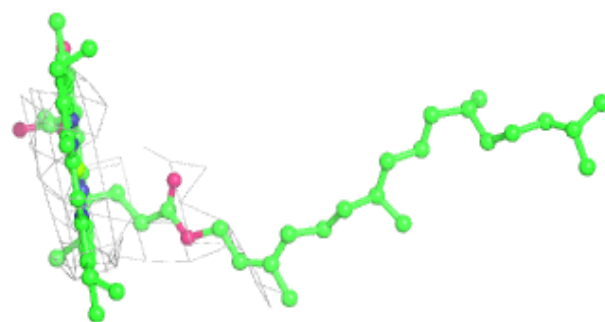
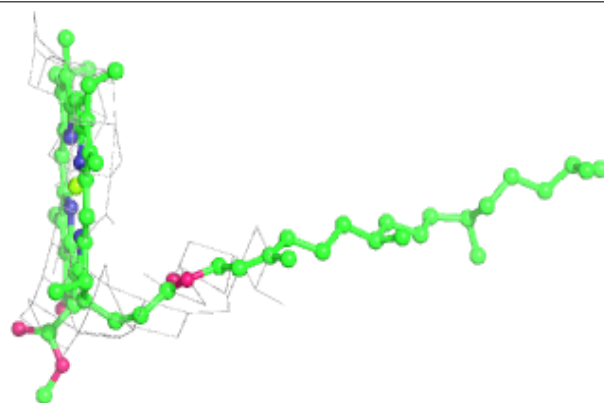


**Electron density around LMG B 621:**

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

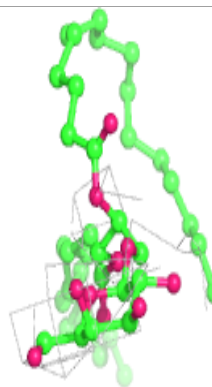
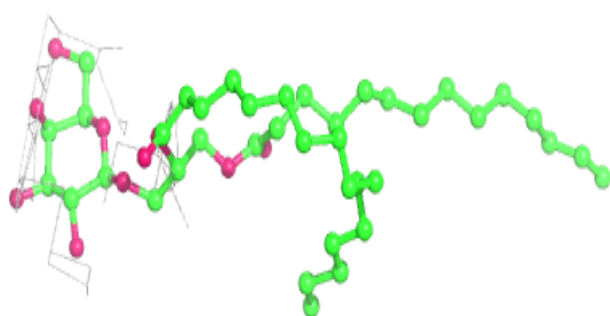
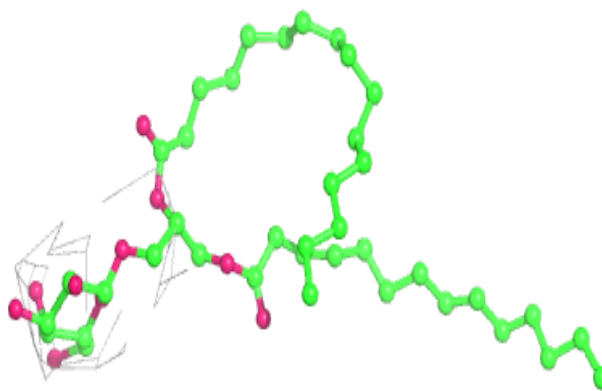
**Electron density around CLA b 610:**

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

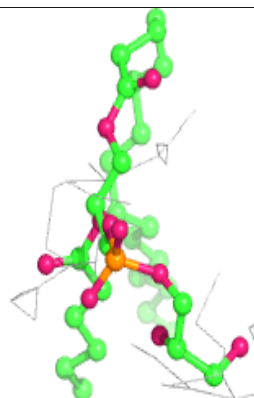
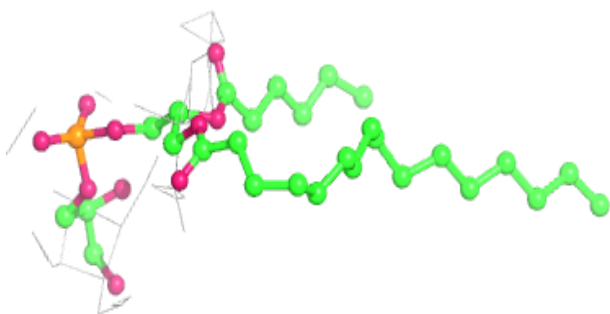
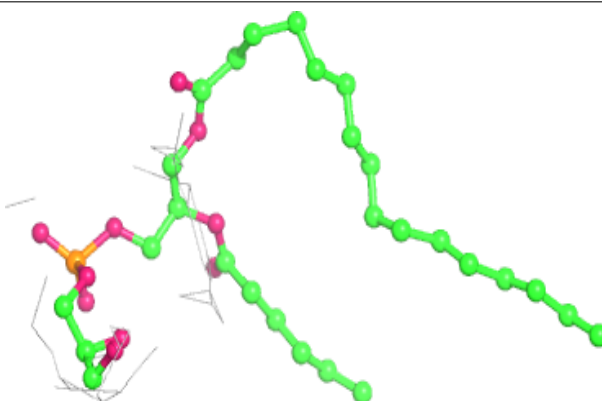


**Electron density around LMG d 408:**

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

**Electron density around LHG A 410:**

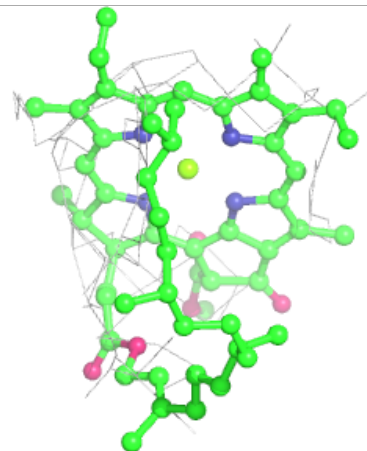
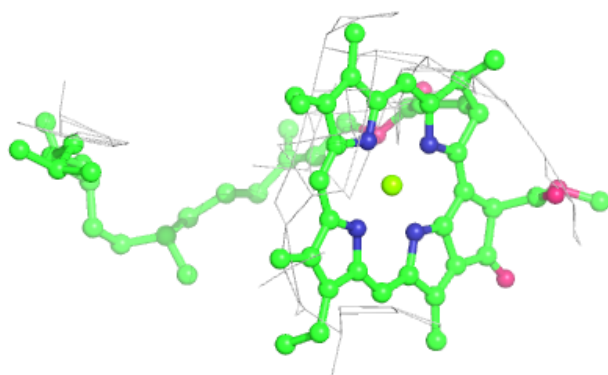
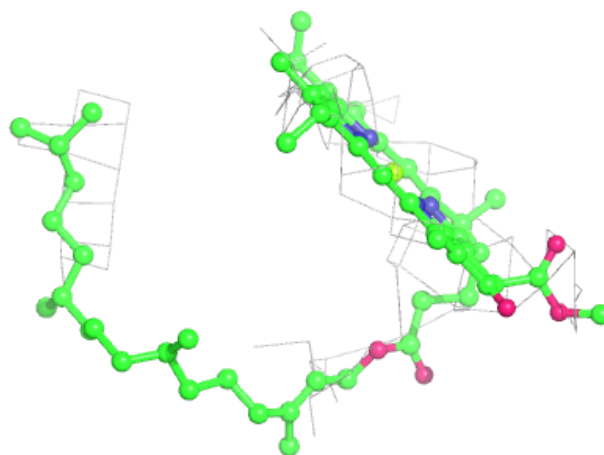
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





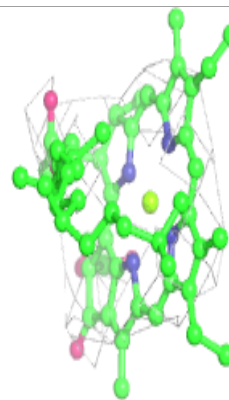
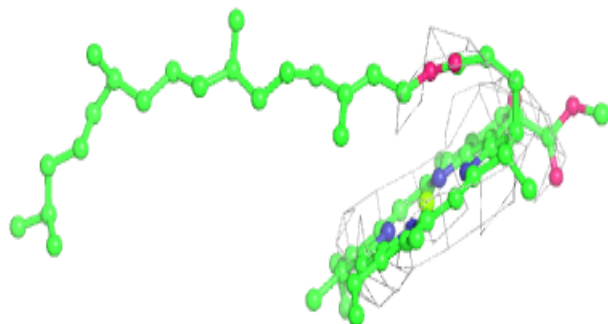
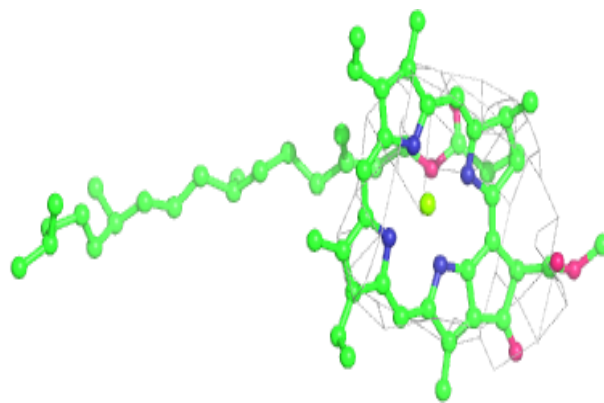
**Electron density around CLA b 615:**

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



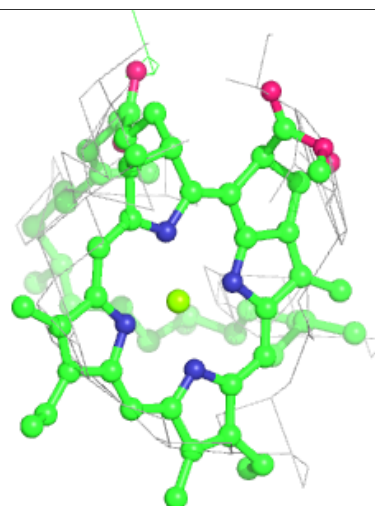
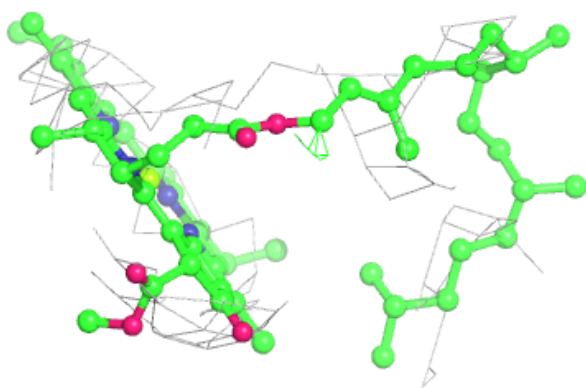
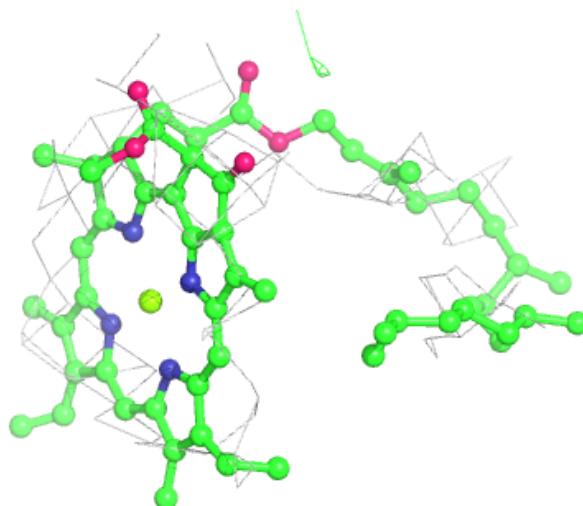
**Electron density around CLA B 607:**

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



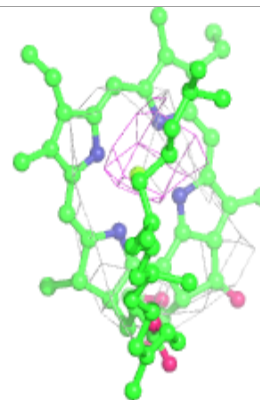
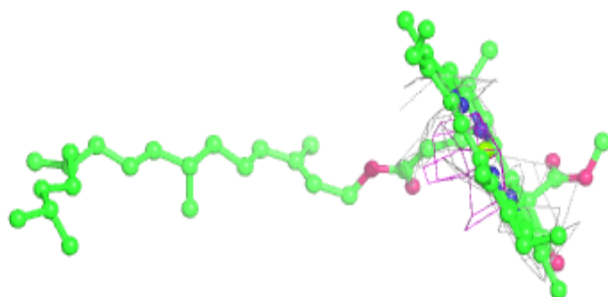
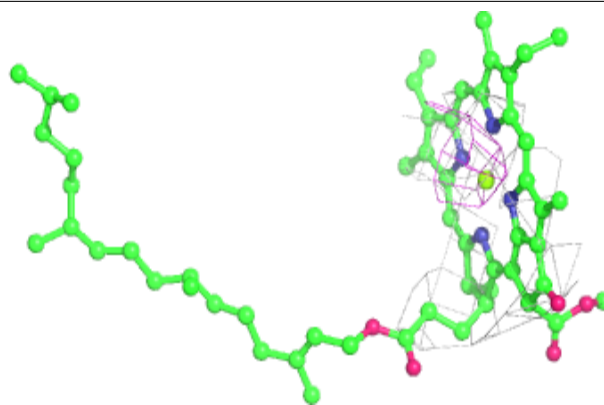
**Electron density around CLA C 503:**

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

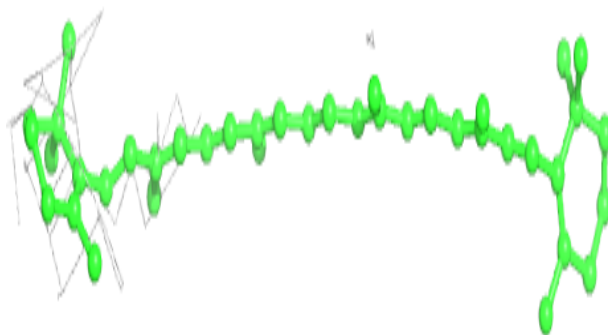
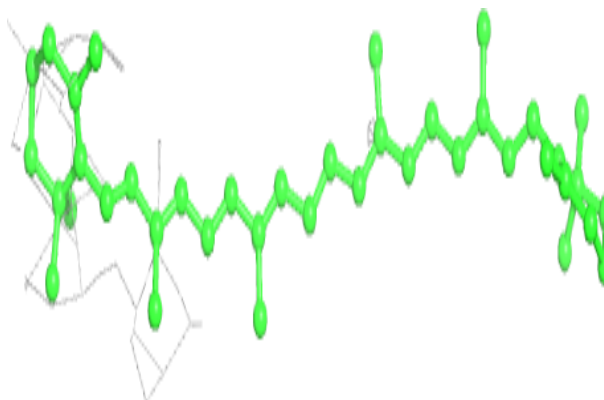


**Electron density around CLA B 608:**

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

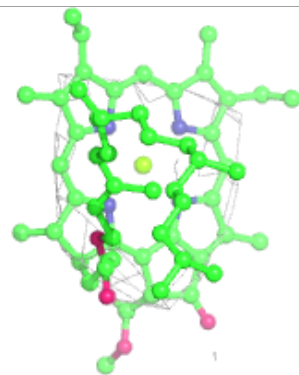
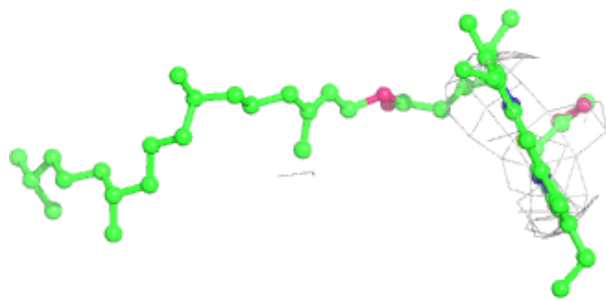
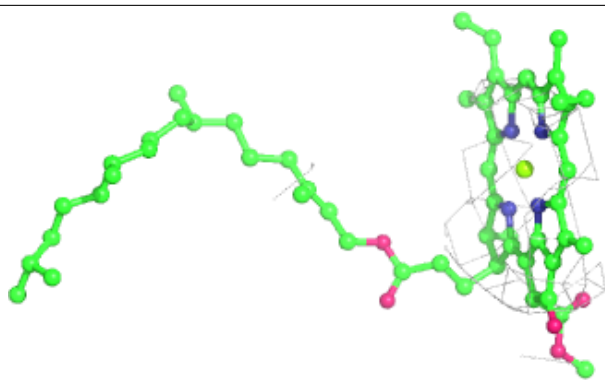
**Electron density around BCR b 621:**

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



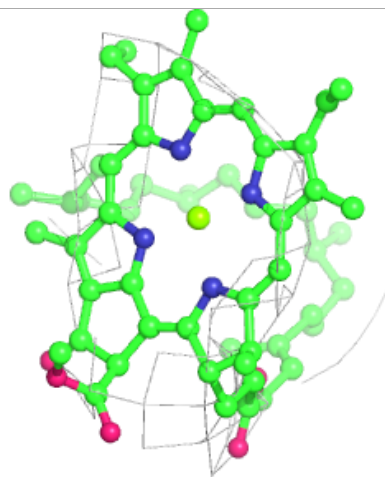
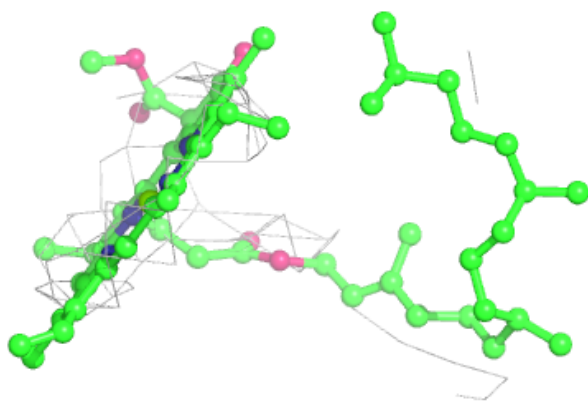
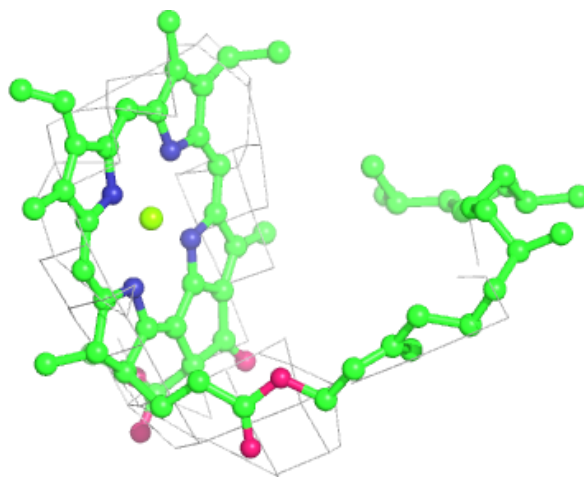
**Electron density around CLA D 404:**

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



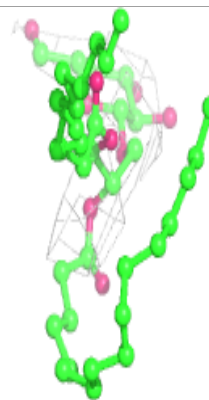
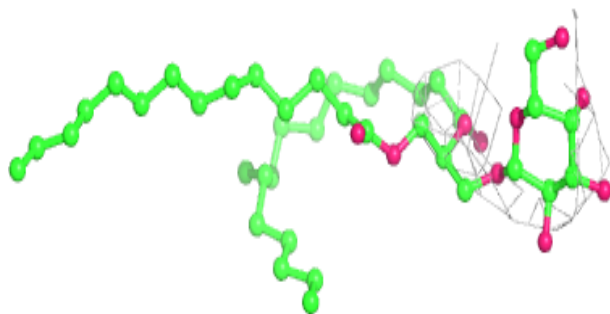
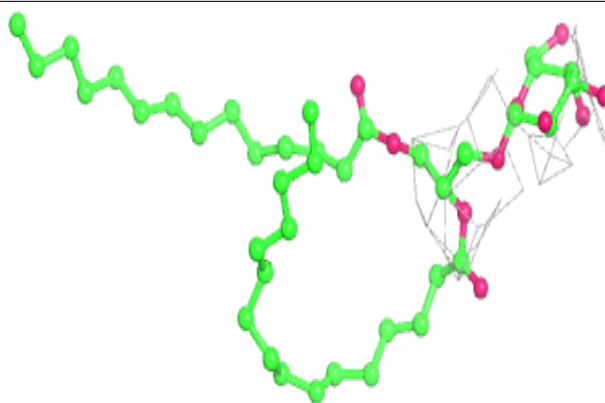
**Electron density around CLA c 503:**

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

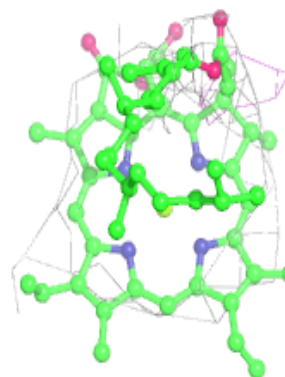
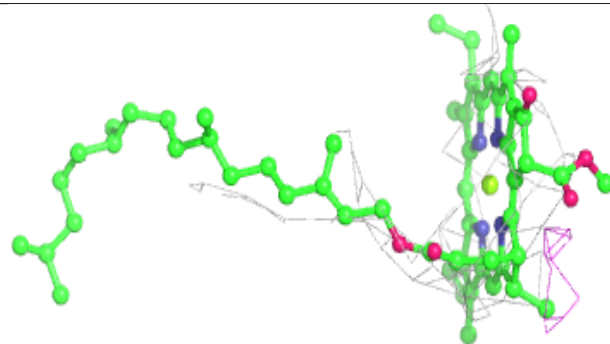
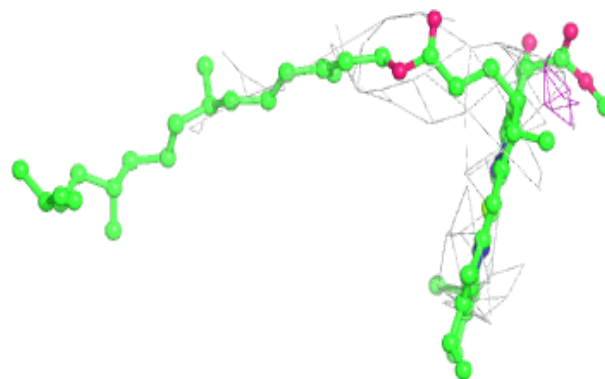


**Electron density around LMG B 625:**

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

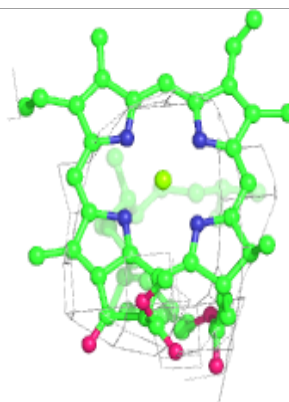
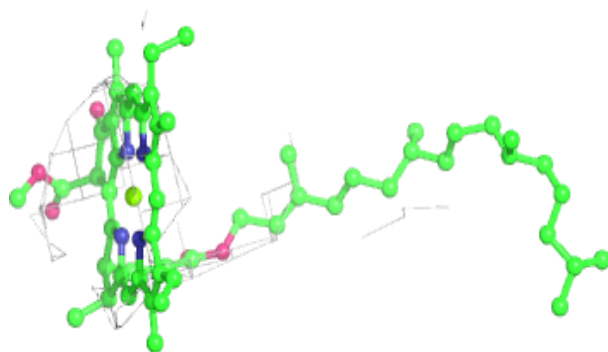
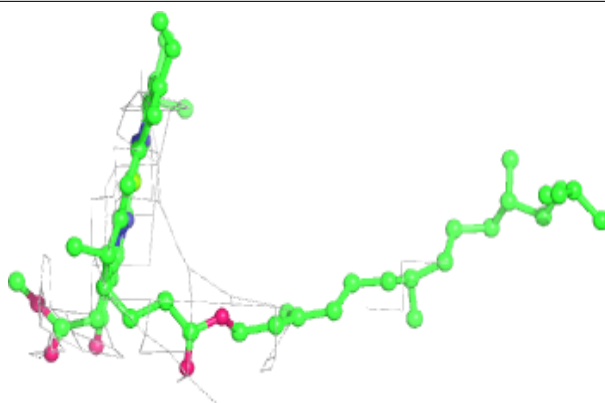
**Electron density around CLA b 609:**

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



**Electron density around CLA B 604:**

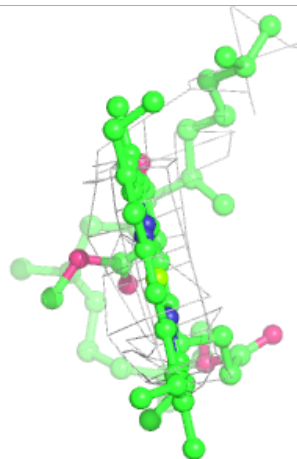
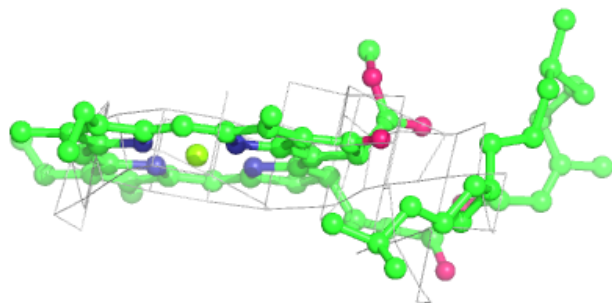
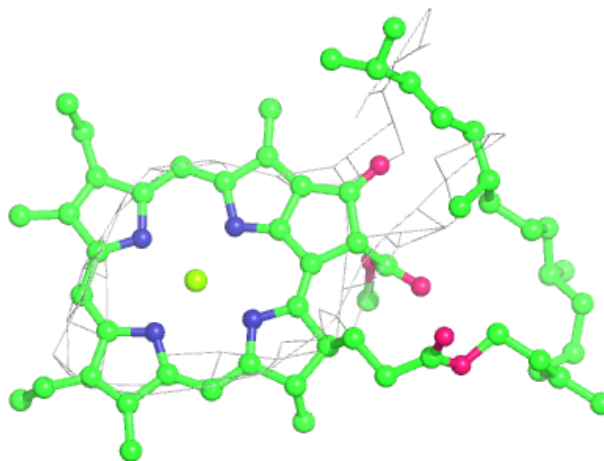
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





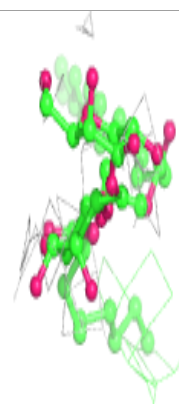
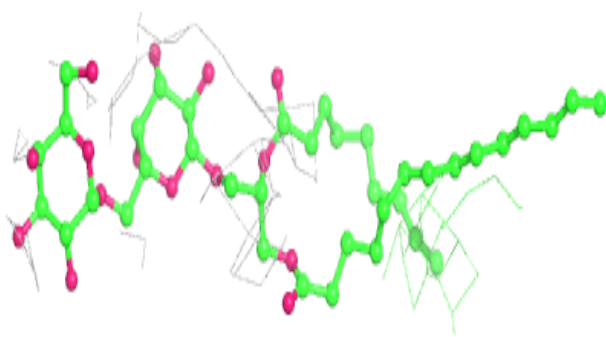
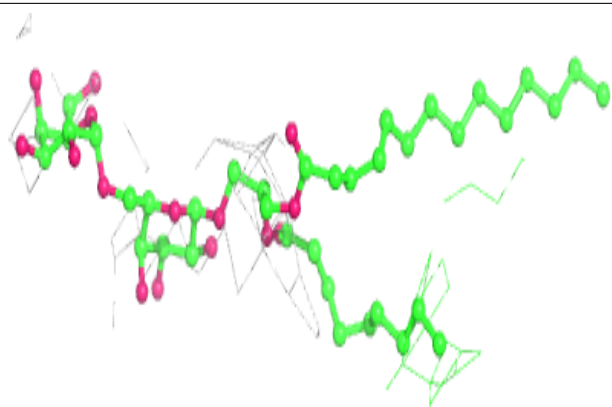
**Electron density around CLA B 609:**

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

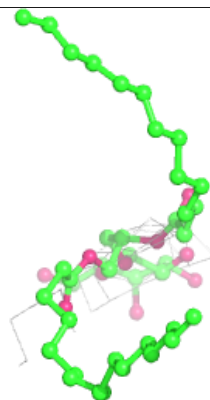
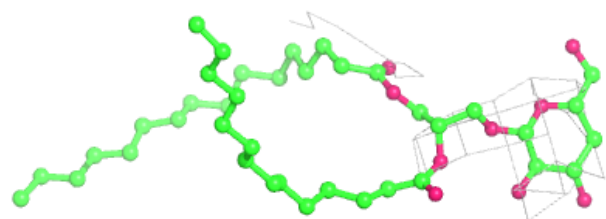
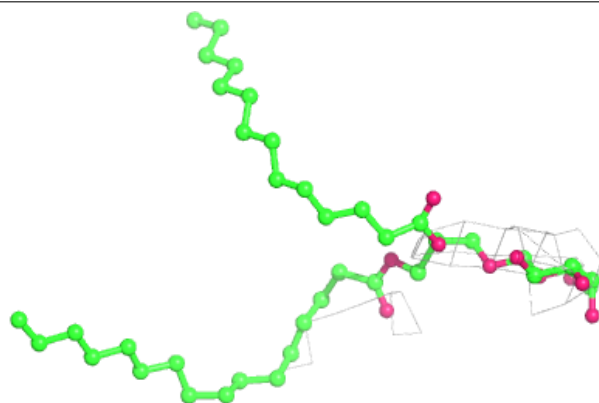


**Electron density around DGD c 515:**

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

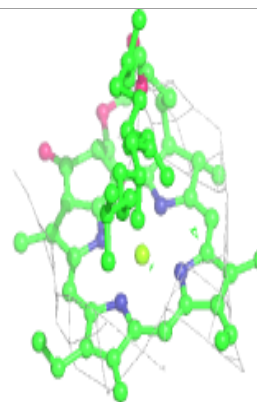
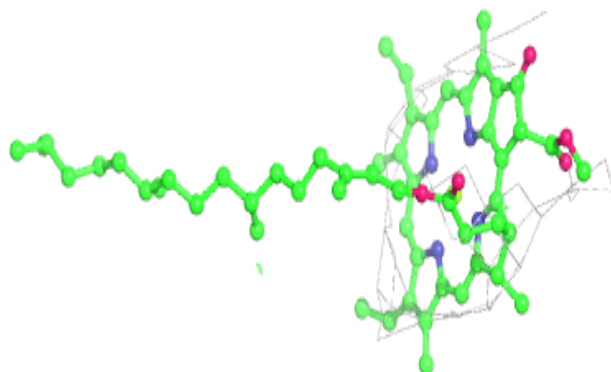
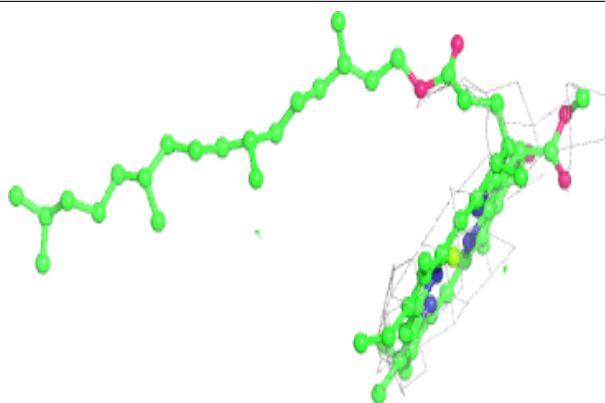
**Electron density around LMG b 626:**

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

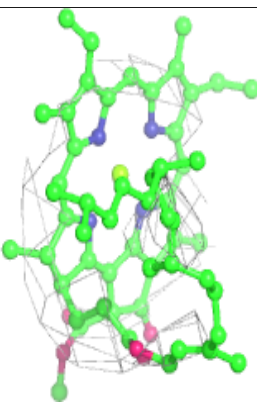
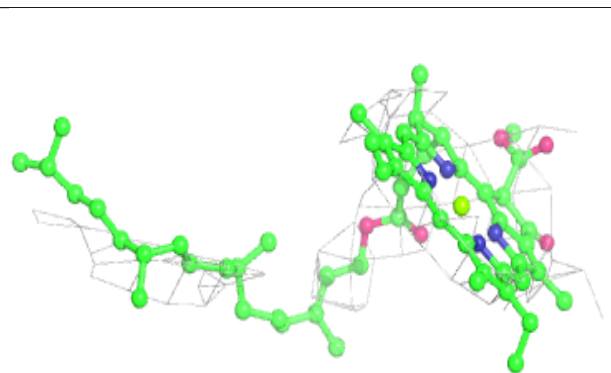
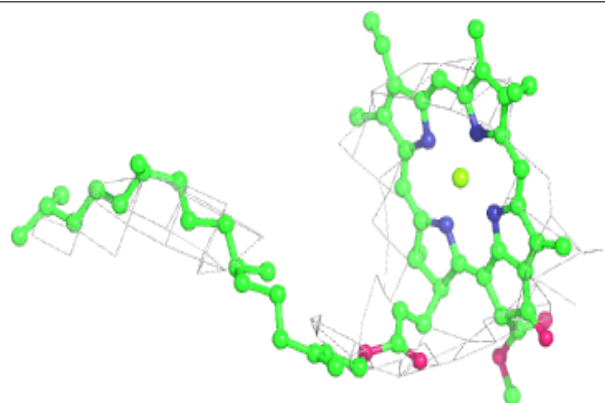


**Electron density around CLA c 520:**

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

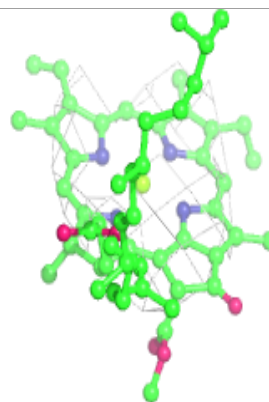
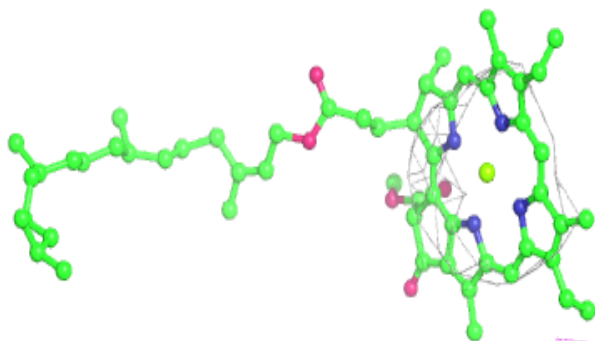
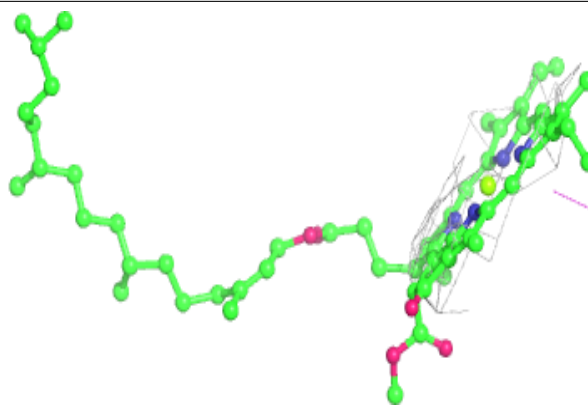
**Electron density around CLA C 510:**

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

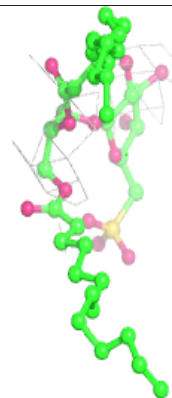
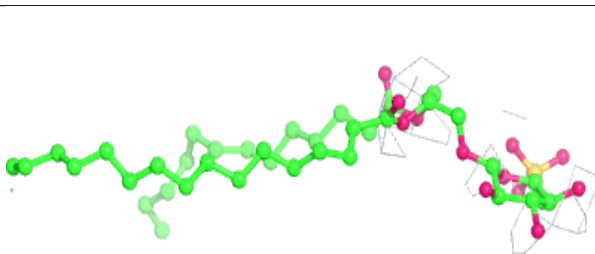
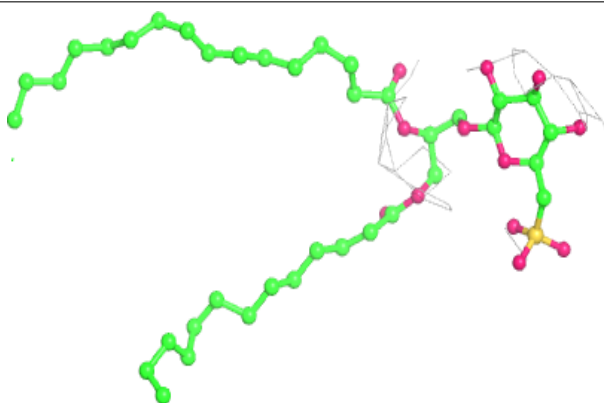


**Electron density around CLA D 403:**

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

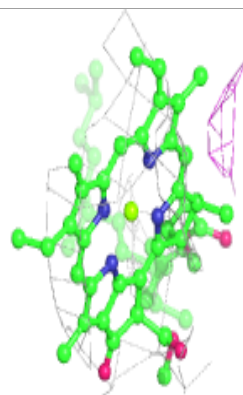
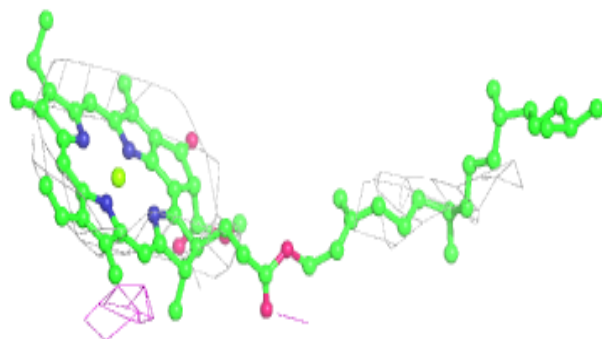
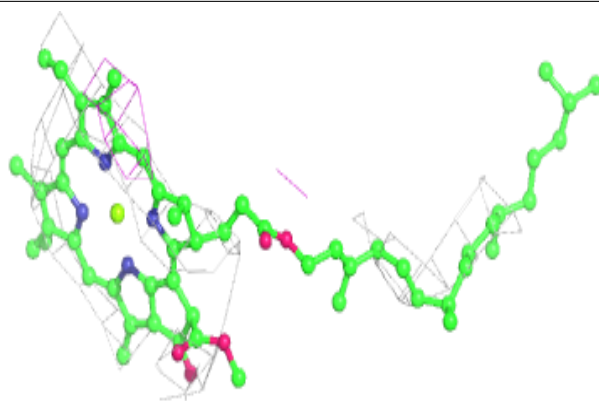
**Electron density around SQD a 412:**

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



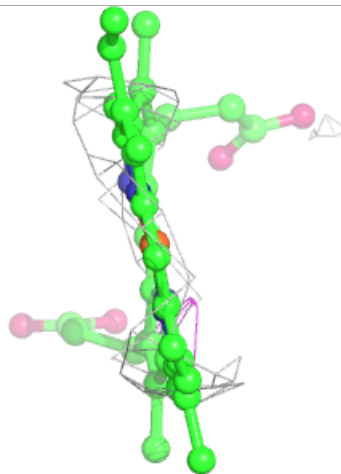
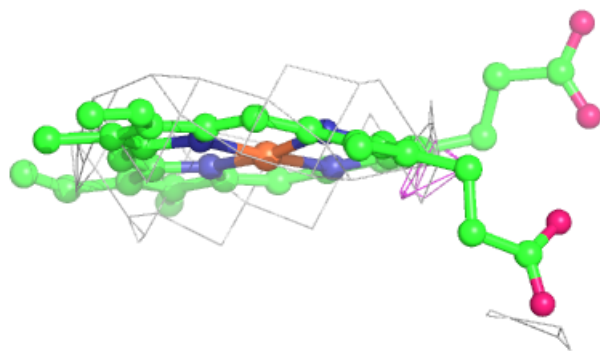
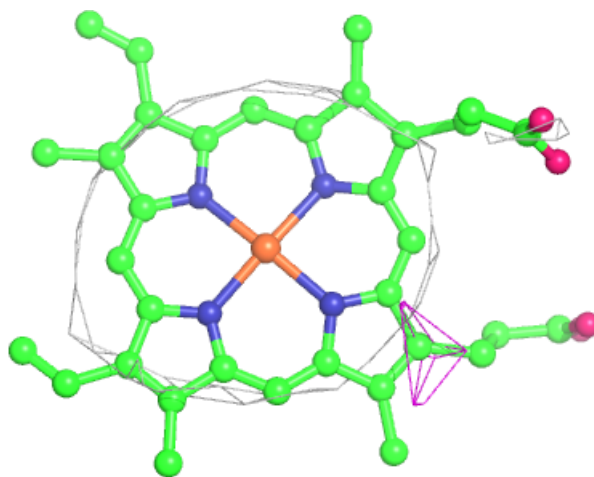
**Electron density around CLA A 402:**

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



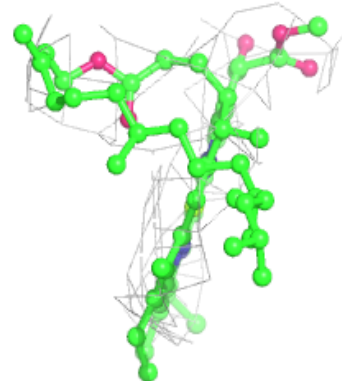
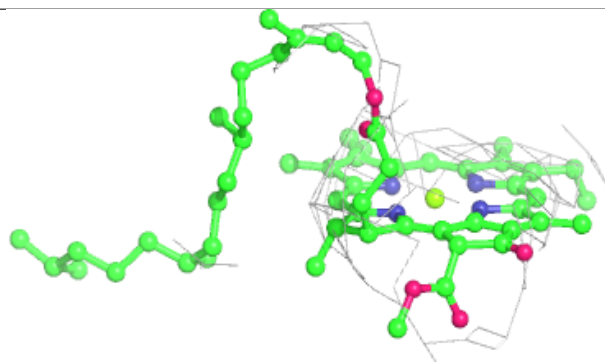
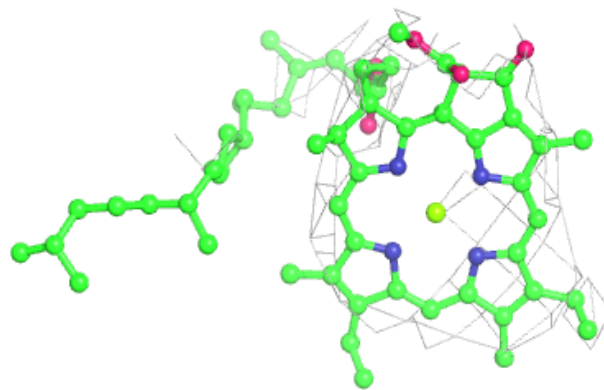
**Electron density around HEM F 101:**

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

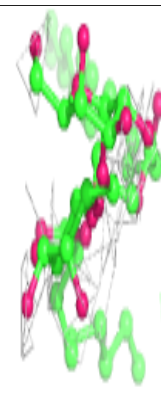
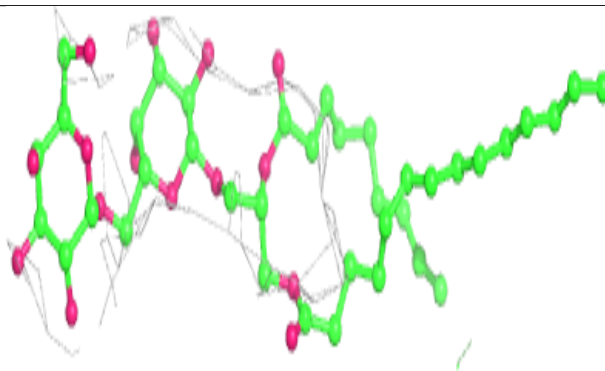
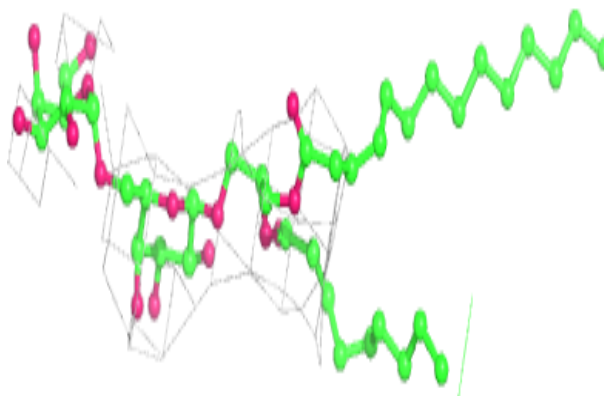


**Electron density around CLA A 403:**

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

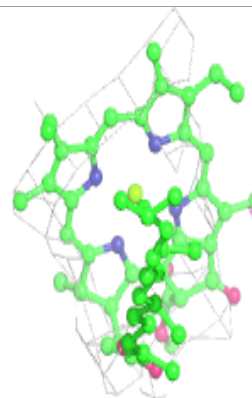
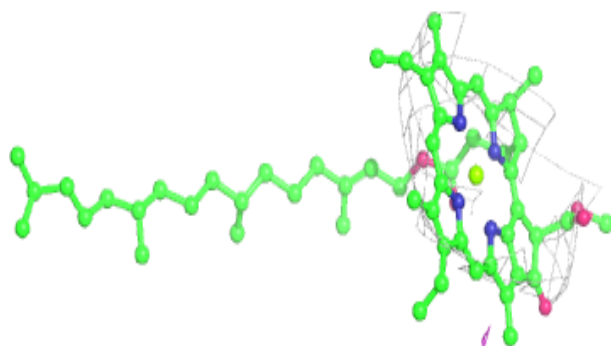
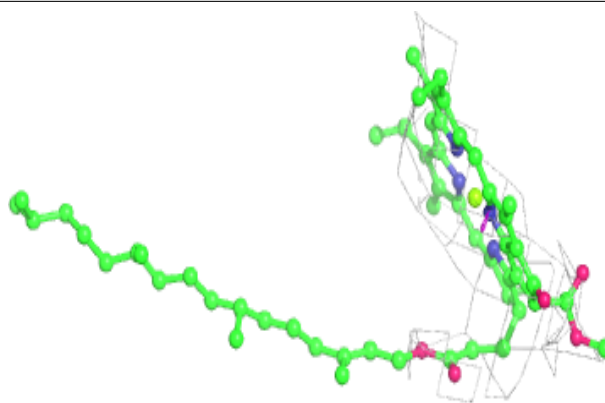
**Electron density around DGD C 514:**

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



**Electron density around CLA b 611:**

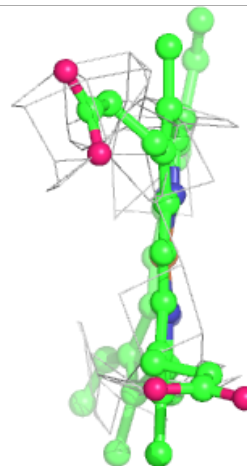
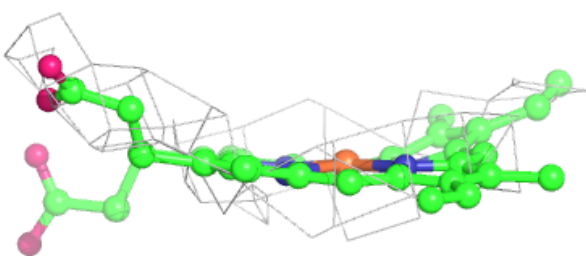
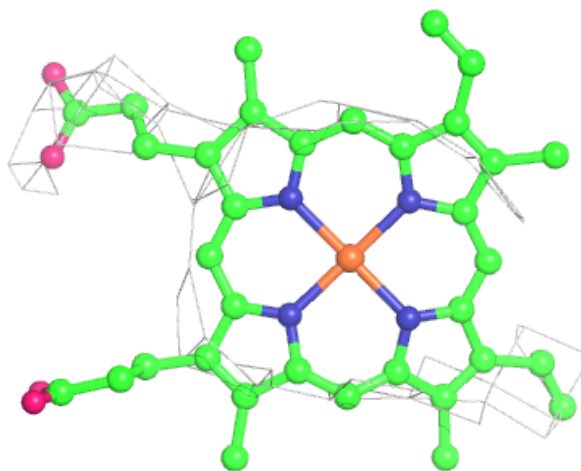
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





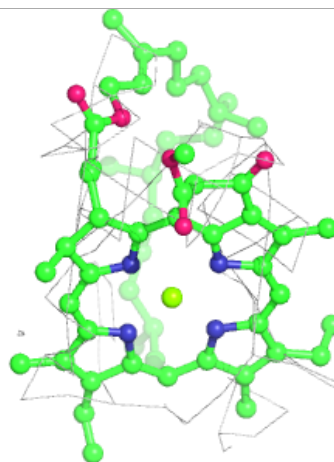
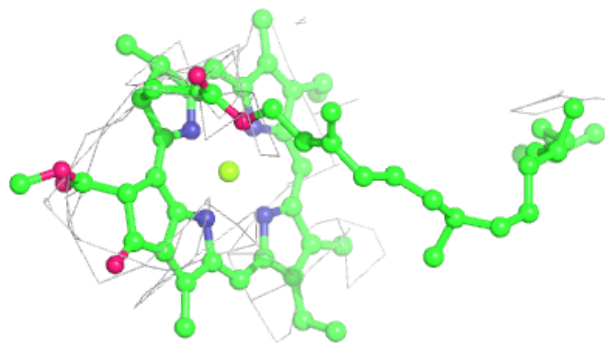
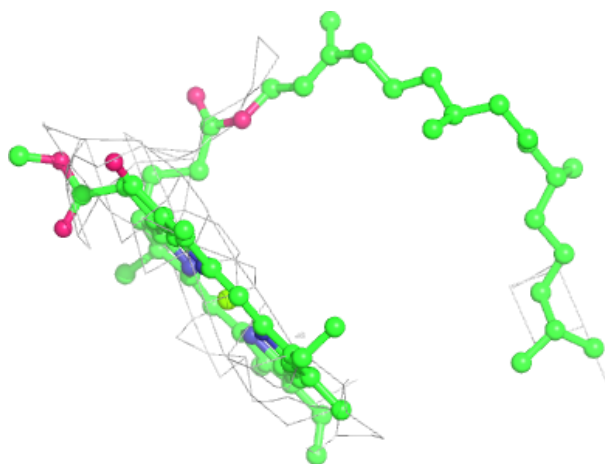
**Electron density around HEM V 201:**

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



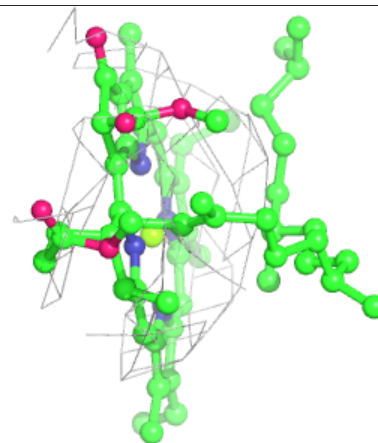
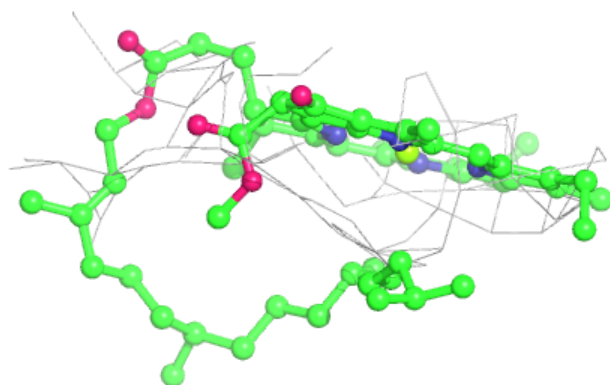
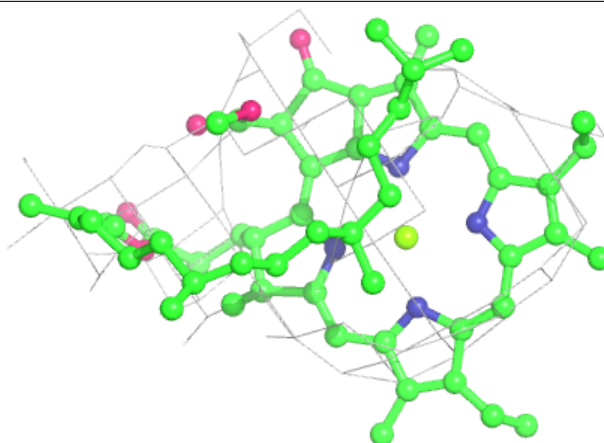
**Electron density around CLA B 610:**

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

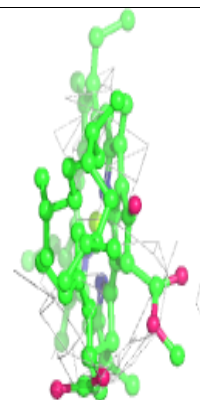
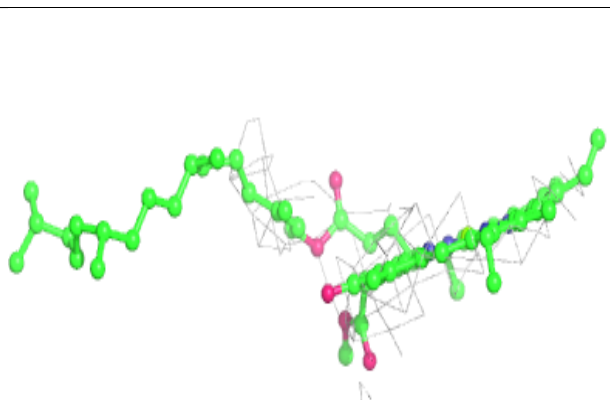
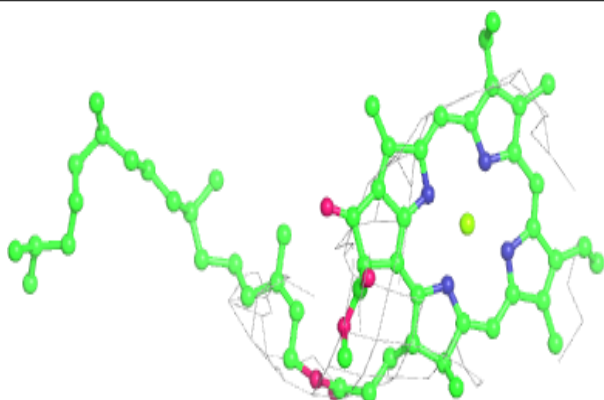


**Electron density around CLA c 509:**

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

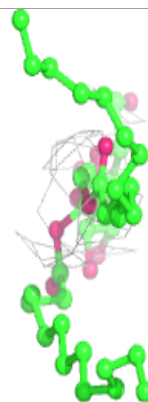
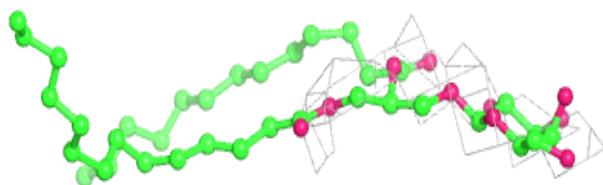
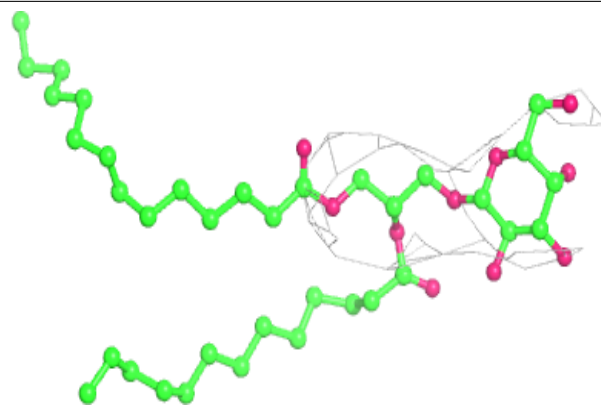
**Electron density around CLA H 101:**

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

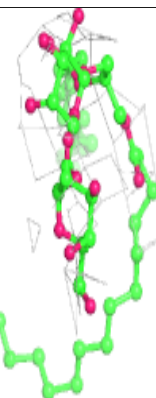
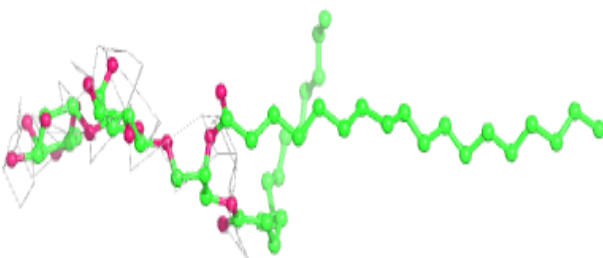
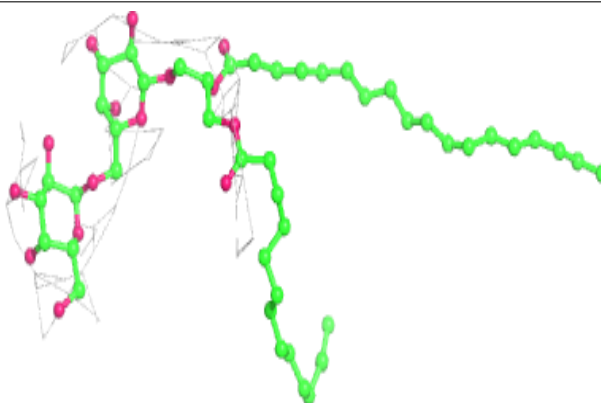


**Electron density around LMG d 412:**

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

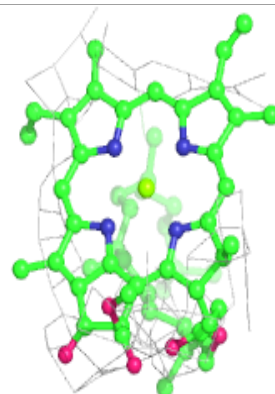
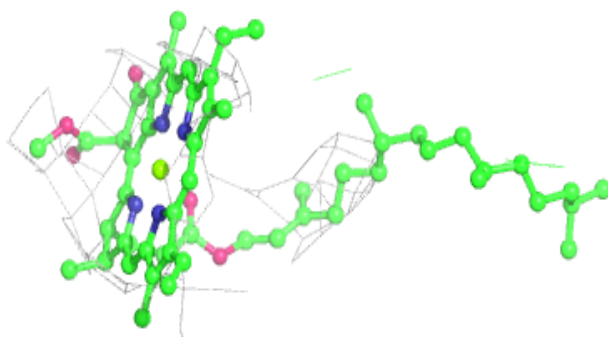
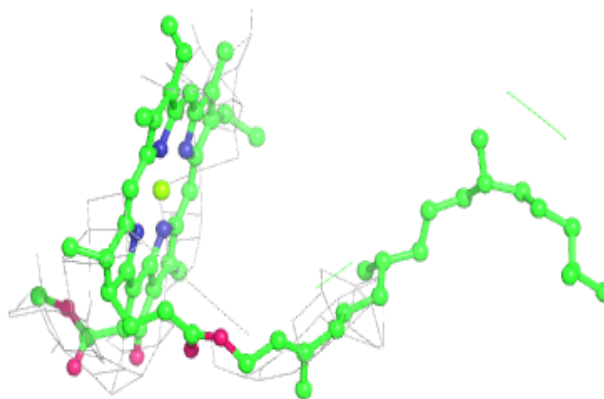
**Electron density around DGD c 516:**

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

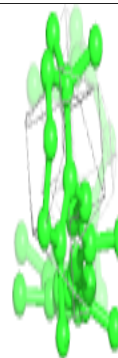
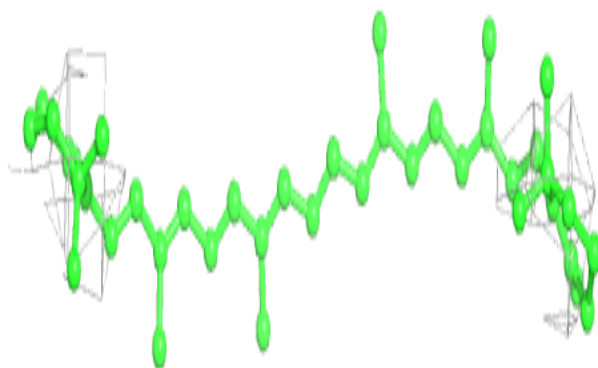
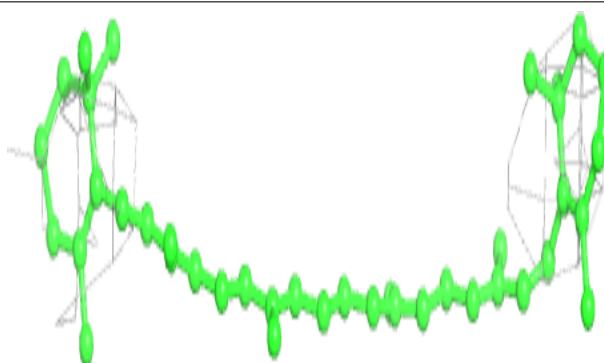


**Electron density around CLA c 507:**

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

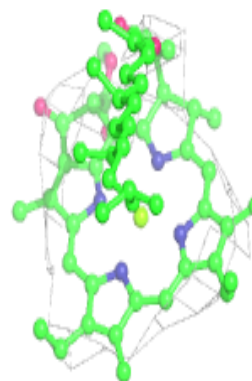
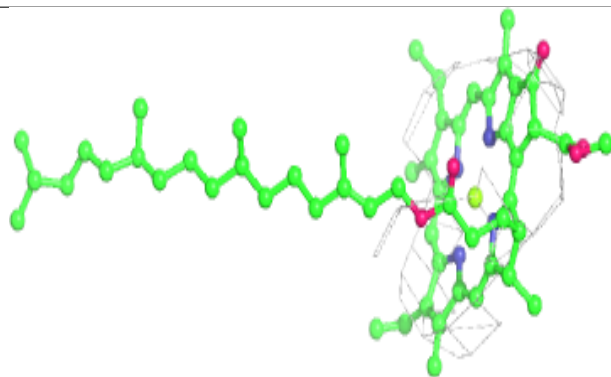
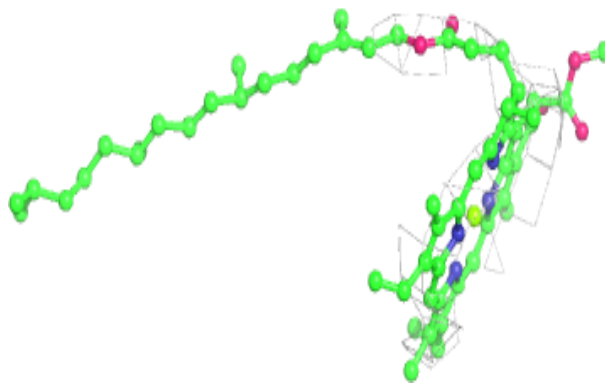
**Electron density around BCR K 101:**

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



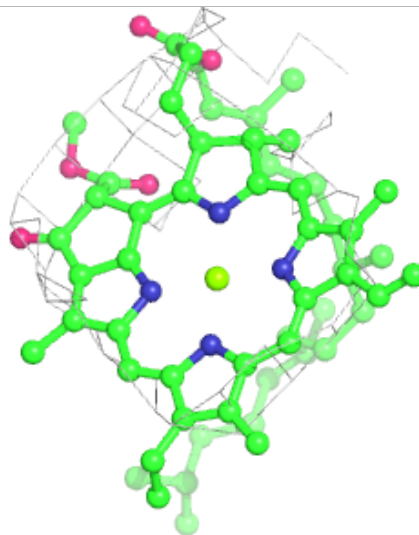
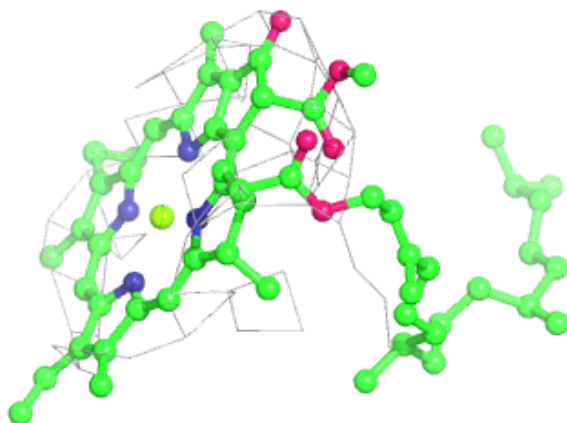
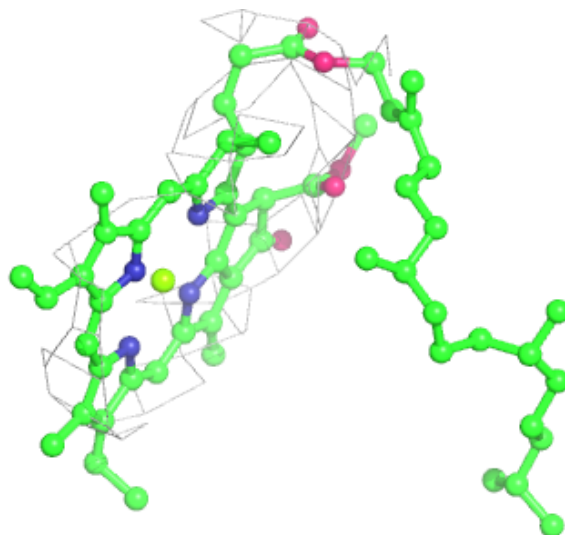
**Electron density around CLA B 606:**

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



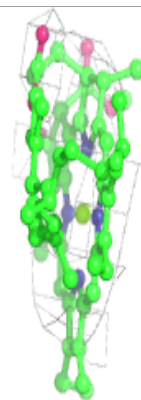
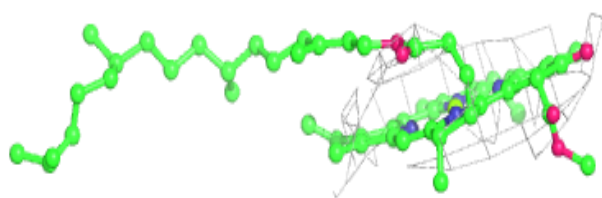
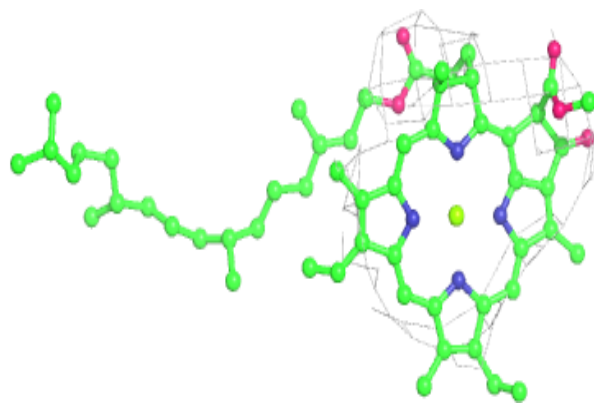
**Electron density around CLA B 612:**

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



**Electron density around CLA B 602:**

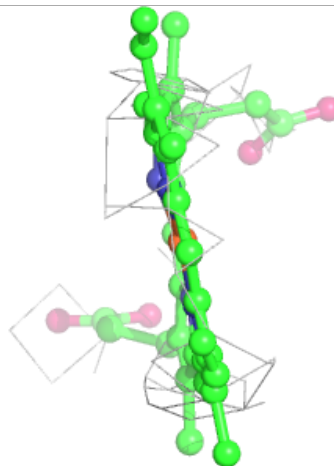
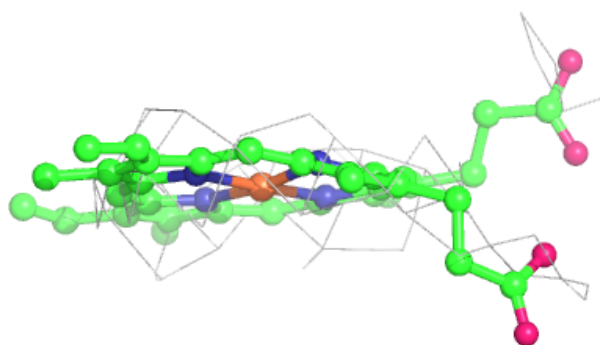
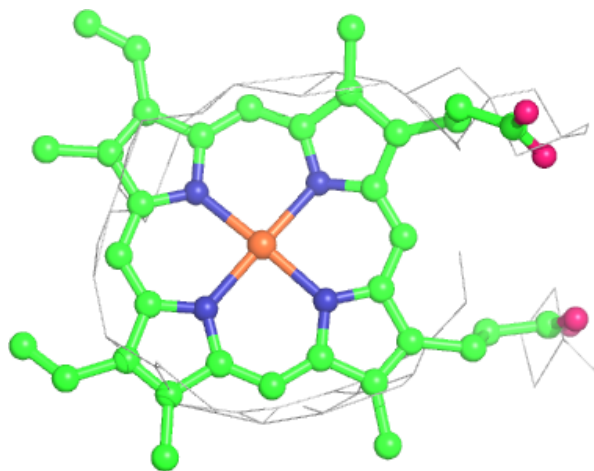
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





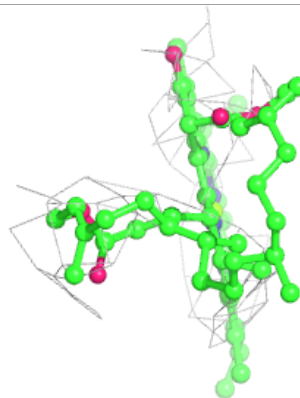
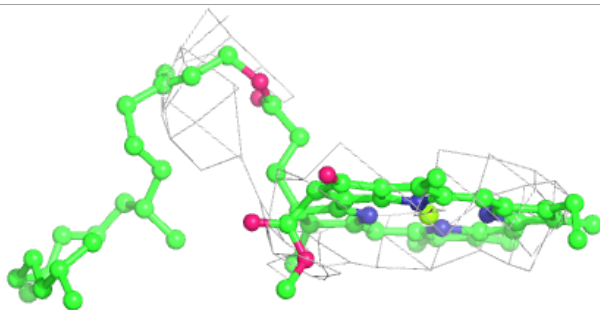
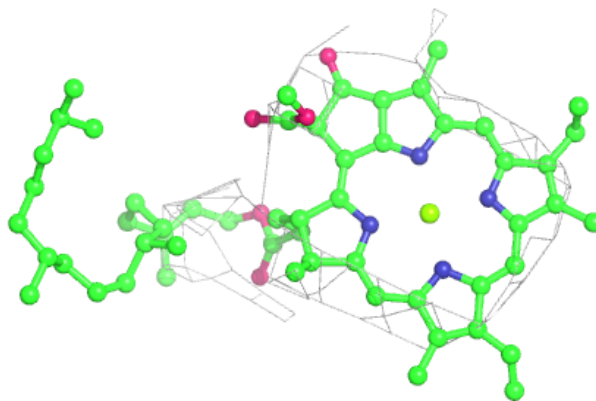
**Electron density around HEM f 101:**

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



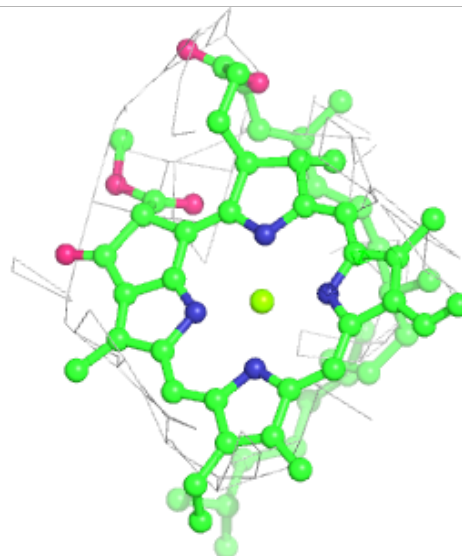
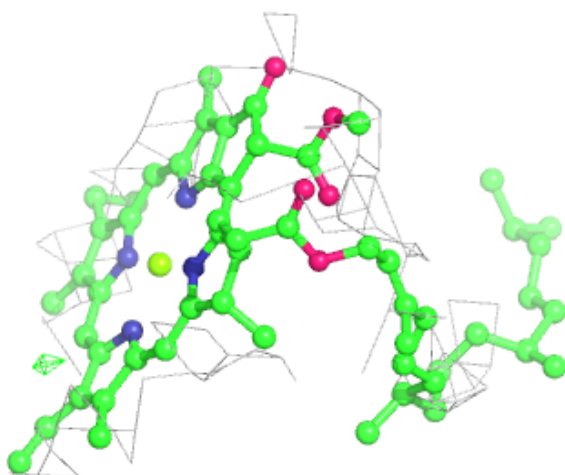
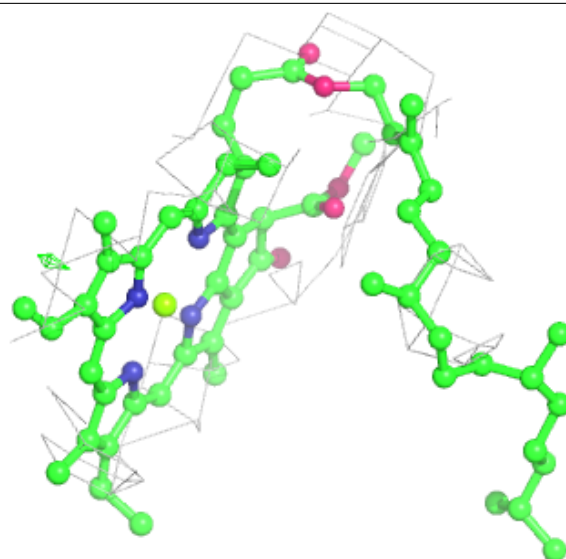
**Electron density around CLA B 611:**

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



**Electron density around CLA b 617:**

$2mF_o-DF_c$  (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.