



## wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2021 – 04:49 PM EDT

PDB ID : 7RF6  
Title : RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 Angstrom resolution  
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2021-07-13  
Resolution : 2.01 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.

---

The following versions of software and data (see [references](#) ①) 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	:	2.23.2
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)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2



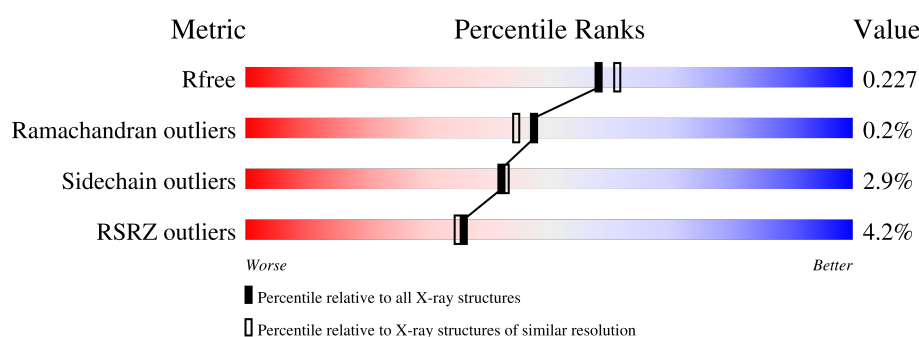
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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.



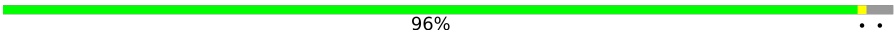
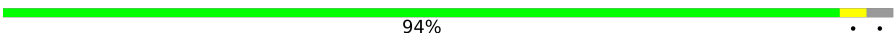

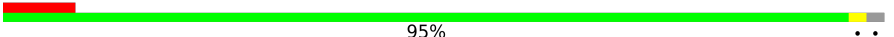






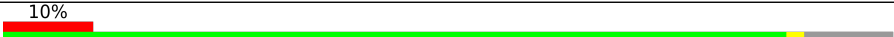


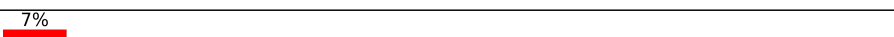
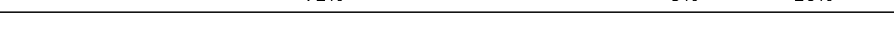
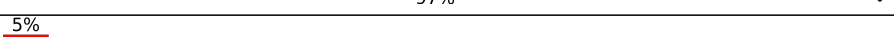



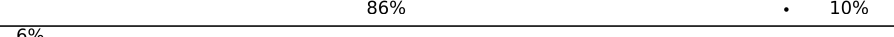





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>96%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	a	344	<div> <div>94%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
2	B	510	<div> <div>2%</div> <div>97%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
2	b	510	<div> <div>4%</div> <div>97%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
3	C	461	<div> <div>94%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
3	c	461	<div> <div>2%</div> <div>96%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	R	41	
14	r	41	
15	T	32	
15	t	32	
16	U	134	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
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
24	CLA	A	604	X	-	-	-
24	CLA	A	605	X	-	-	-
24	CLA	A	608	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	604	X	-	-	-
24	CLA	a	606	X	-	-	-
24	CLA	a	612	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106128 atoms, of which 52762 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	66	0
			6098	2030	2985	513	551	19			
1	a	334	Total	C	H	N	O	S	0	66	0
			6086	2027	2976	513	551	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7814	2610	3836	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	14	0
			6941	2302	3432	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7086	2343	3503	602	624	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	2	0
			5368	1809	2637	446	464	12			
4	d	341	Total	C	H	N	O	S	0	3	0
			5380	1813	2643	446	466	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0
			620	202	316	48	53	1		
11	l	36	Total	C	H	N	O		0	0
			600	197	304	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0
			525	171	269	37	47	1		
12	m	32	Total	C	H	N	O	S	0	0
			518	168	267	36	46	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1
			3700	1168	1830	313	385	4		0
13	o	244	Total	C	H	N	O	S	0	0
			3720	1170	1846	317	383	4		0

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	28	Total	C	H	N	O		0	0
			459	151	238	38	32			
14	r	28	Total	C	H	N	O		0	0
			459	151	238	38	32			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
15	t	30	Total	C	H	N	O	S	0	0
			512	180	256	36	38	2		

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

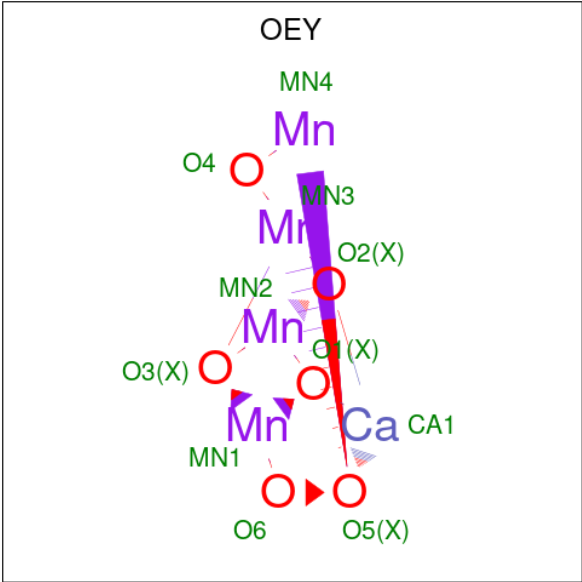
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total 413	C 128	H 217	N 35	O 30	S 3	0	0	0
19	y	30	Total 459	C 144	H 241	N 35	O 36	S 3	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

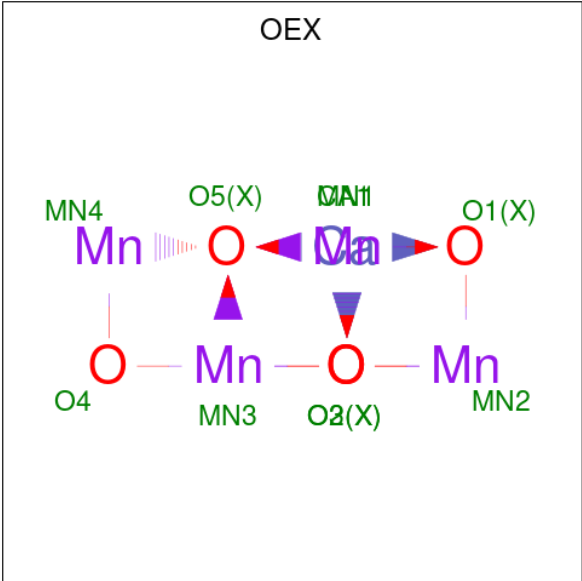
- Molecule 21 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
21	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

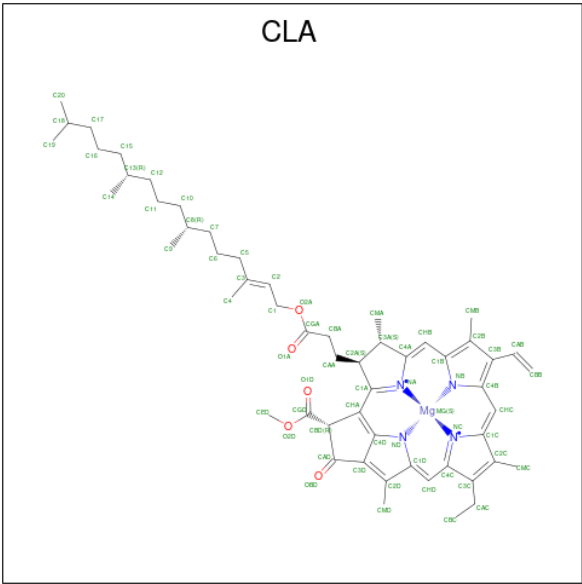
Continued from previous page...

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

- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 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
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

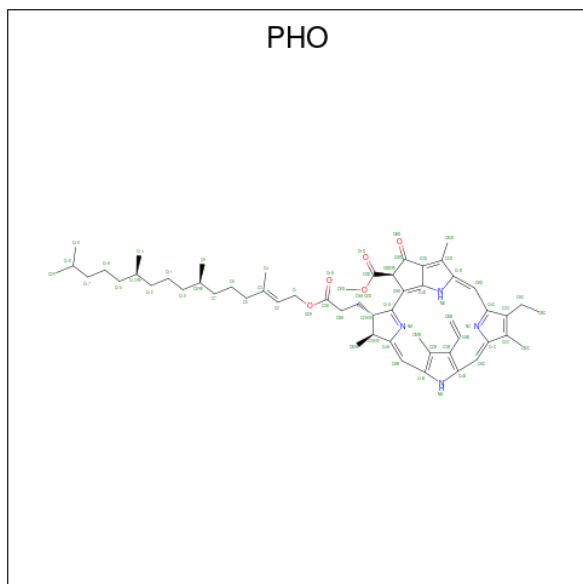
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total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

*Continued on next page...*

Continued from previous page...

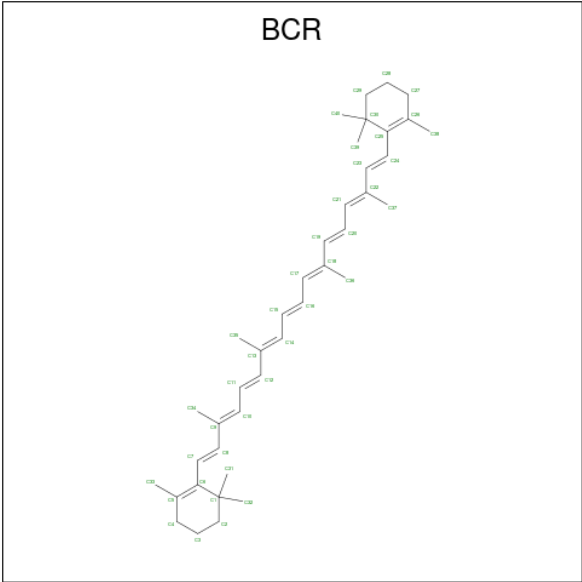
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



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

Continued on next page...

*Continued from previous page...*

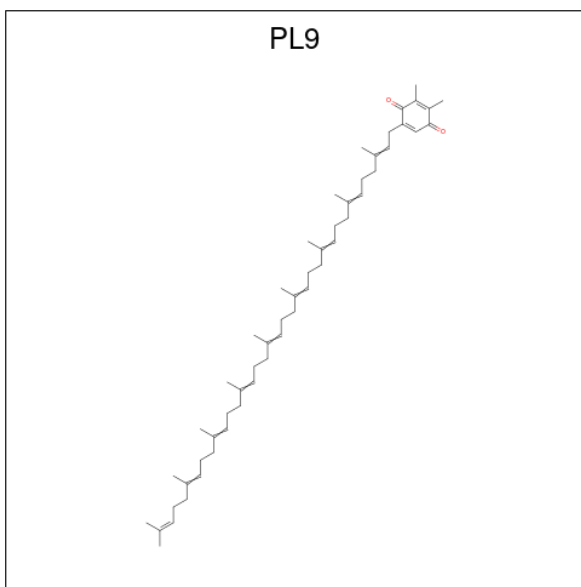
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	t	1	Total	C	H	0	0
			96	40	56		
26	x	1	Total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

- Molecule 27 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

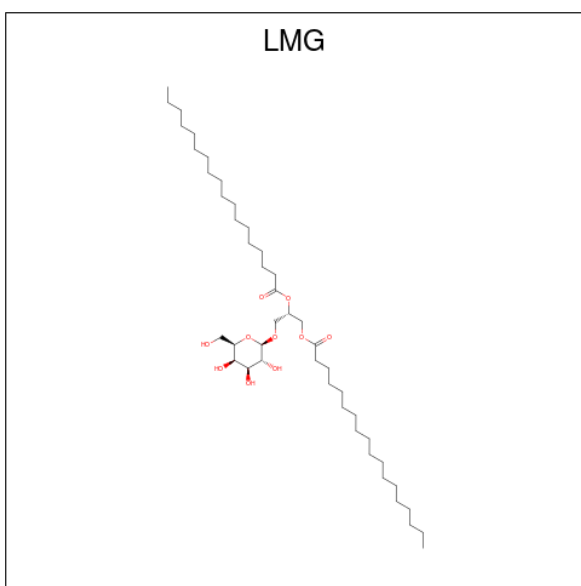
- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).





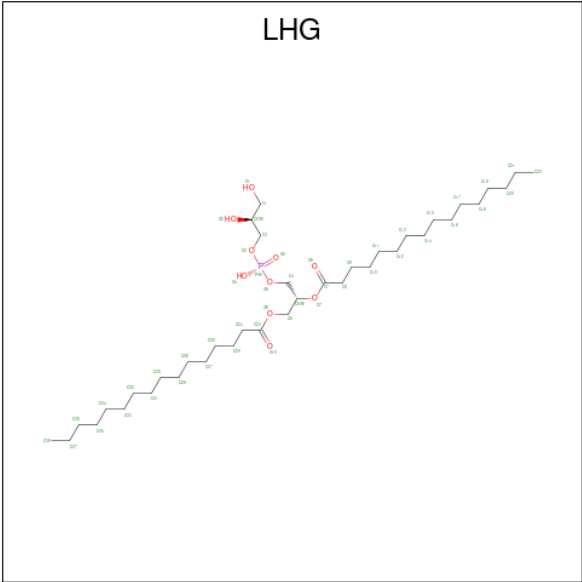
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			135	53	80	2		
28	D	1	Total	C	H	O	0	0
			135	53	80	2		
28	a	1	Total	C	H	O	0	0
			135	53	80	2		
28	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



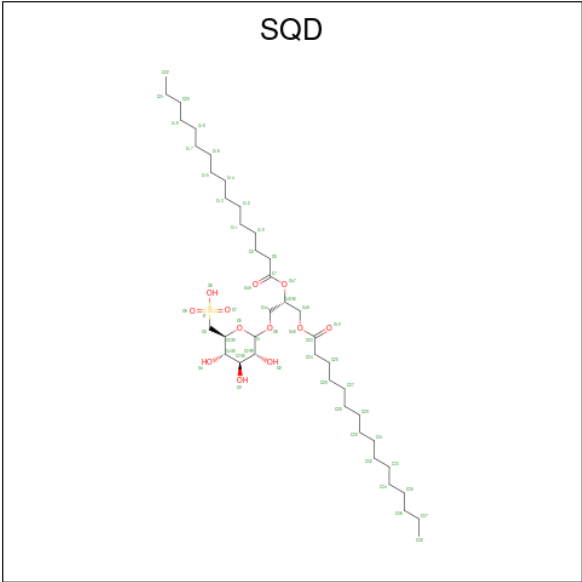
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			114	38	66	10		
29	C	1	Total	C	H	O	0	0
			114	38	66	10		
29	D	1	Total	C	H	O	0	0
			123	41	72	10		
29	D	1	Total	C	H	O	0	0
			78	27	45	6		
29	D	1	Total	C	H	O	0	0
			68	24	40	4		
29	M	1	Total	C	H	O	0	0
			123	41	72	10		
29	a	1	Total	C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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



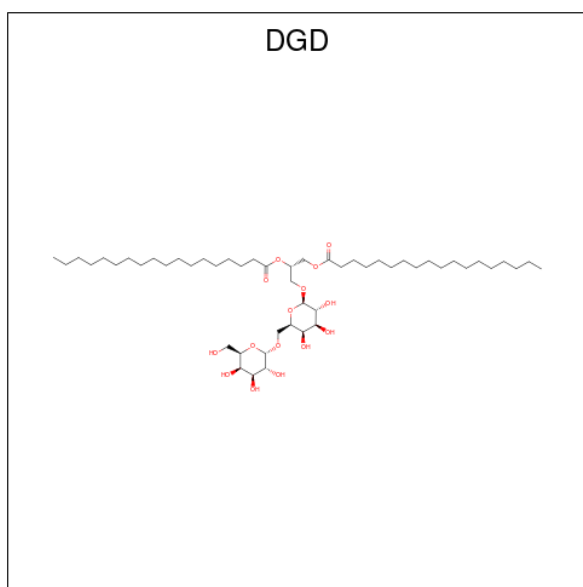
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



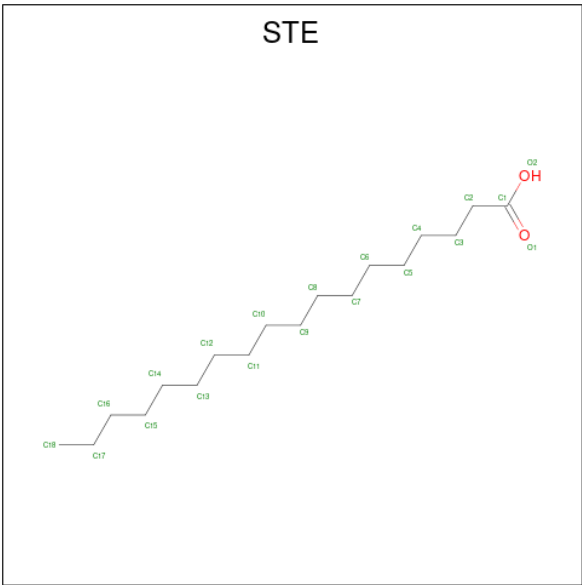
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
31	A	1	Total	C	H	O		0	0
			104	35	65	4			
31	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
31	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
31	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
31	a	1	Total	C	H	O		0	0
			92	31	56	5			
31	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
31	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	H	O	0	0
			162	51	96	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	C	1	Total	C	H	O	0	0
			144	47	82	15		
32	H	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	c	1	Total	C	H	O	0	0
			144	47	82	15		
32	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 33 is STEARIC ACID (three-letter code: STE) (formula: C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>).



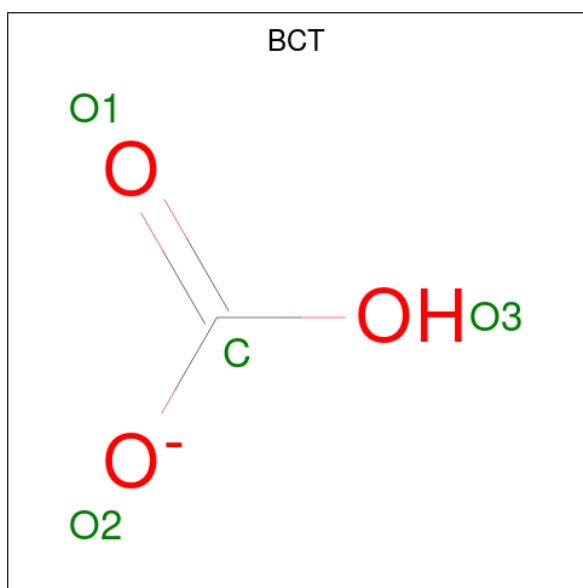
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			43	15	26	2		
33	B	1	Total	C	H	O	0	0
			34	12	20	2		
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H		0	0
			47	16	31			
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H		0	0
			47	16	31			
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	D	1	Total	C	H	O	0	0
			55	18	35	2		
33	E	1	Total	C	H	O	0	0
			28	10	16	2		
33	H	1	Total	C	H		0	0
			53	18	35			
33	I	1	Total	C	H		0	0
			41	15	26			
33	J	1	Total	C	H	O	0	0
			28	10	16	2		
33	M	1	Total	C	H	O	0	0
			37	13	22	2		

Continued on next page...

*Continued from previous page...*

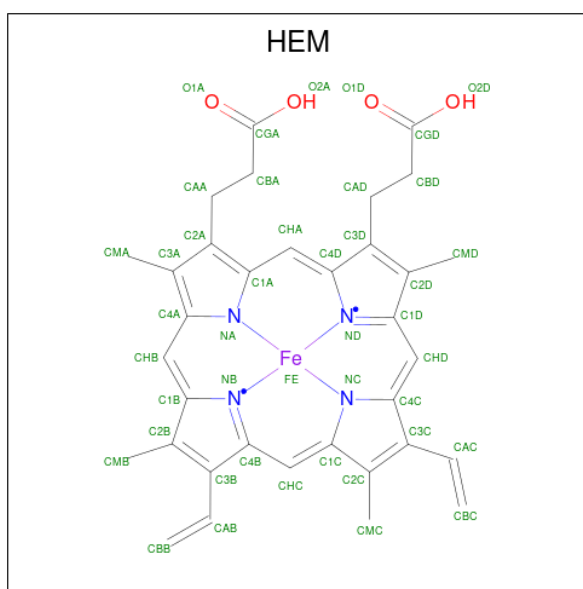
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	M	1	Total	C	H	0	0
			26	10	16		
33	T	1	Total	C	H	0	0
			47	16	31		
33	T	1	Total	C	H	0	0
			44	15	29		
33	Z	1	Total	C	H	0	0
			20	8	12		
33	a	1	Total	C	H	0	0
			26	10	16		
33	a	1	Total	C	H	O	0
			28	10	16	2	0
33	a	1	Total	C	H	0	0
			41	15	26		
33	b	1	Total	C	H	O	0
			55	18	35	2	0
33	b	1	Total	C	H	O	0
			40	14	24	2	0
33	b	1	Total	C	H	O	0
			55	18	35	2	0
33	b	1	Total	C	H	0	0
			26	10	16		
33	b	1	Total	C	H	0	0
			41	14	27		
33	c	1	Total	C	H	O	0
			55	18	35	2	0
33	d	1	Total	C	H	O	0
			43	15	26	2	0
33	d	1	Total	C	H	O	0
			55	18	35	2	0
33	j	1	Total	C	H	O	0
			28	10	16	2	0
33	k	1	Total	C	H	O	0
			28	10	16	2	0
33	l	1	Total	C	H	0	0
			53	18	35		
33	m	1	Total	C	H	O	0
			28	10	16	2	0
33	t	1	Total	C	H	O	0
			46	16	28	2	0
33	x	1	Total	C	H	O	0
			55	18	35	2	0

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

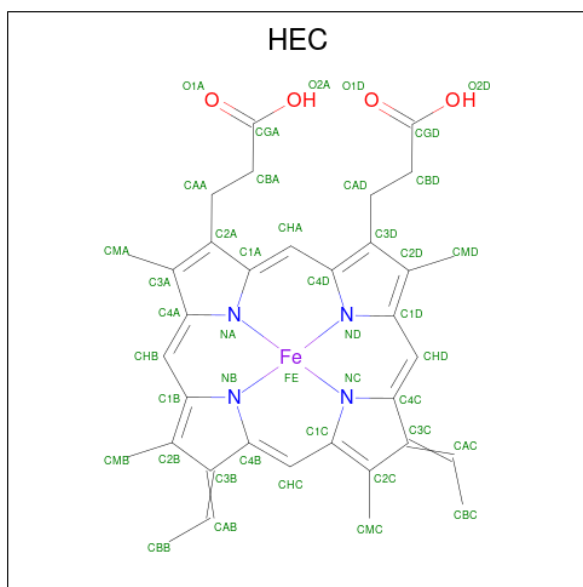
- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).





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

- Molecule 36 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	149	Total	O	0	0
			149	149		
37	B	200	Total	O	0	0
			200	200		
37	C	166	Total	O	0	0
			166	166		
37	D	124	Total	O	0	0
			124	124		
37	E	24	Total	O	0	0
			24	24		
37	F	10	Total	O	0	0
			10	10		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	28	Total O 28 28	0	0
37	I	6	Total O 6 6	0	0
37	J	13	Total O 13 13	0	0
37	K	4	Total O 4 4	0	0
37	L	12	Total O 12 12	0	0
37	M	8	Total O 8 8	0	0
37	O	96	Total O 96 96	0	0
37	R	5	Total O 5 5	0	0
37	T	12	Total O 12 12	0	0
37	U	47	Total O 47 47	0	0
37	V	78	Total O 78 78	0	0
37	X	11	Total O 11 11	0	0
37	Y	2	Total O 2 2	0	0
37	Z	7	Total O 7 7	0	0
37	a	131	Total O 131 131	0	0
37	b	207	Total O 207 207	0	0
37	c	162	Total O 162 162	0	0
37	d	123	Total O 123 123	0	0
37	e	29	Total O 29 29	0	0
37	f	7	Total O 7 7	0	0
37	h	22	Total O 22 22	0	0

*Continued on next page...*

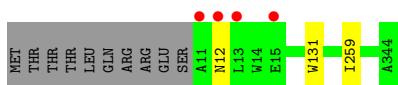
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	7	Total 7	O 7	0	0
37	j	8	Total 8	O 8	0	0
37	k	11	Total 11	O 11	0	0
37	l	8	Total 8	O 8	0	0
37	m	9	Total 9	O 9	0	0
37	o	104	Total 104	O 104	0	0
37	r	5	Total 5	O 5	0	0
37	t	9	Total 9	O 9	0	0
37	u	68	Total 68	O 68	0	0
37	v	59	Total 59	O 59	0	0
37	x	8	Total 8	O 8	0	0
37	y	3	Total 3	O 3	0	0
37	z	7	Total 7	O 7	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1



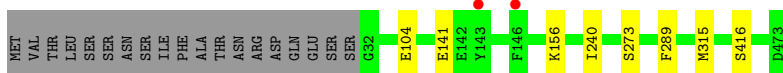
- Molecule 2: Photosystem II CP47 reaction center protein



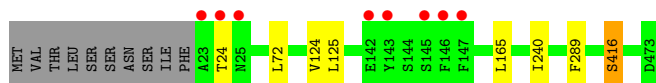
- Molecule 2: Photosystem II CP47 reaction center protein



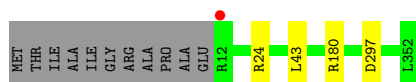
- Molecule 3: Photosystem II CP43 reaction center protein



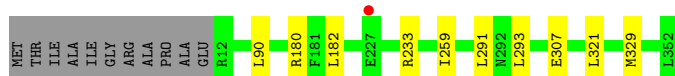
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



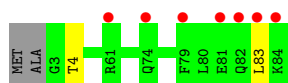
- Molecule 4: Photosystem II D2 protein



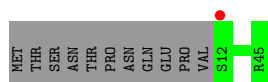
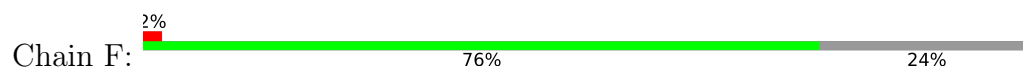
- Molecule 5: Cytochrome b559 subunit alpha



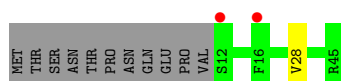
- Molecule 5: Cytochrome b559 subunit alpha



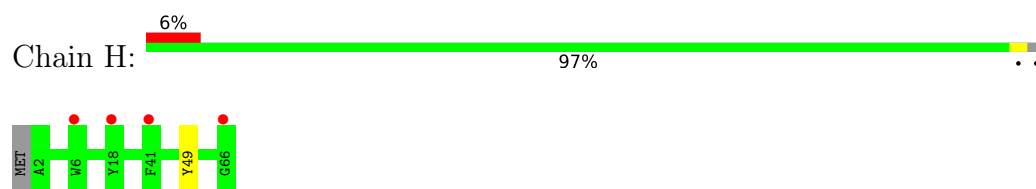
- Molecule 6: Cytochrome b559 subunit beta



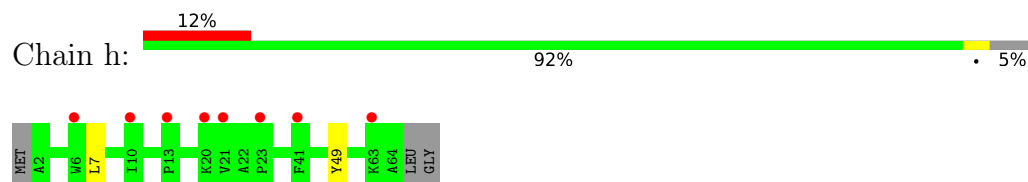
- Molecule 6: Cytochrome b559 subunit beta



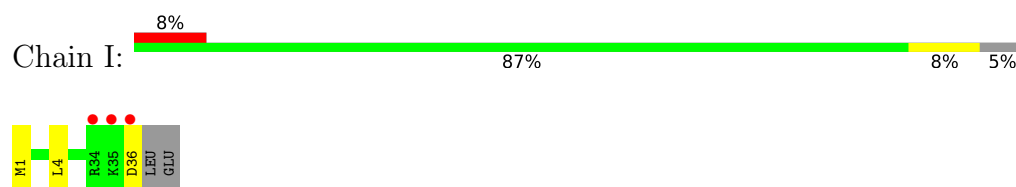
- Molecule 7: Photosystem II reaction center protein H



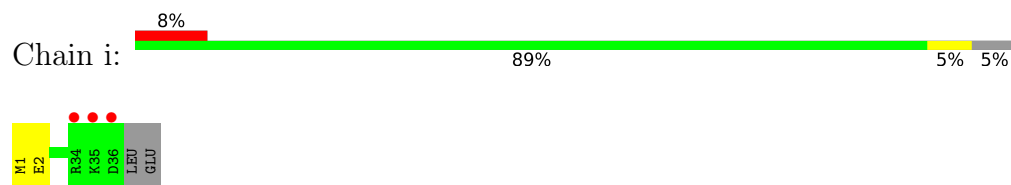
- Molecule 7: Photosystem II reaction center protein H



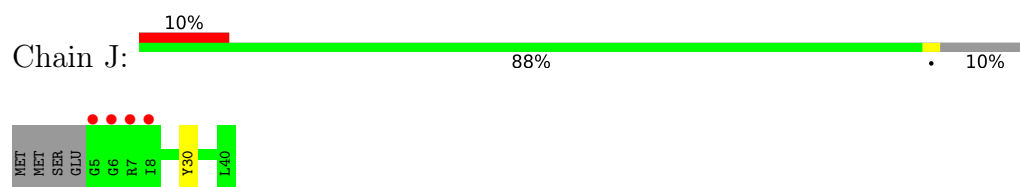
- Molecule 8: Photosystem II reaction center protein I



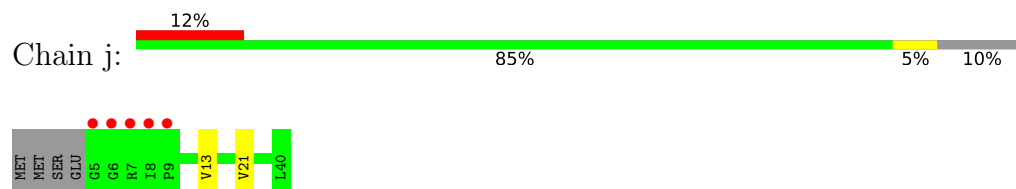
- Molecule 8: Photosystem II reaction center protein I



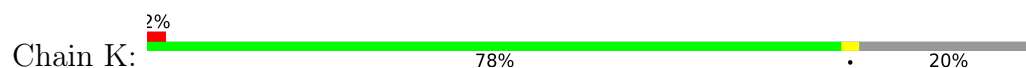
- Molecule 9: Photosystem II reaction center protein J

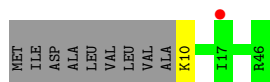


- Molecule 9: Photosystem II reaction center protein J

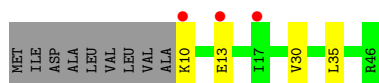


- Molecule 10: Photosystem II reaction center protein K





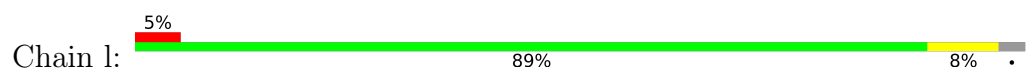
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



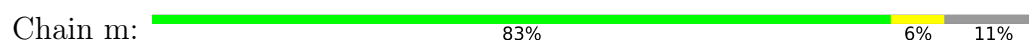
- Molecule 11: Photosystem II reaction center protein L



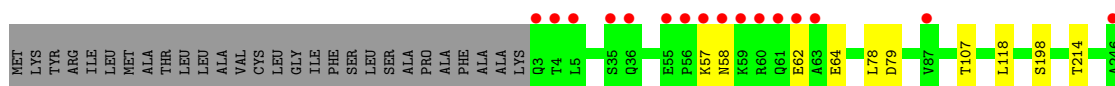
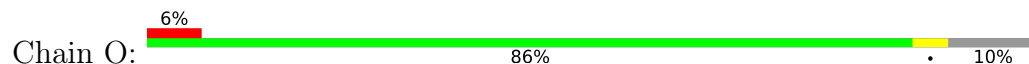
- Molecule 12: Photosystem II reaction center protein M



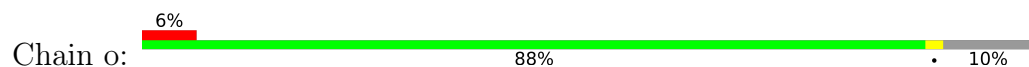
- Molecule 12: Photosystem II reaction center protein M

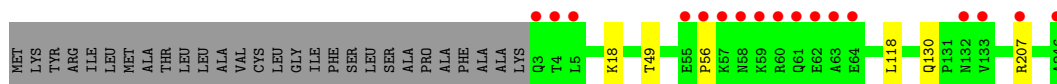


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

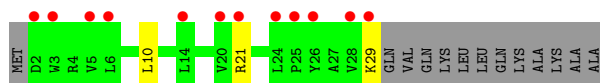


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

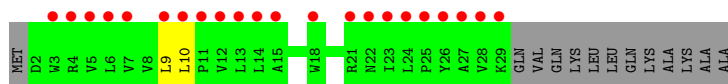




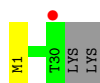
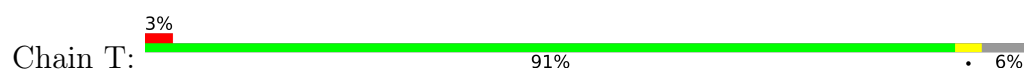
• Molecule 14: Photosystem II protein Y



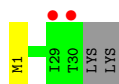
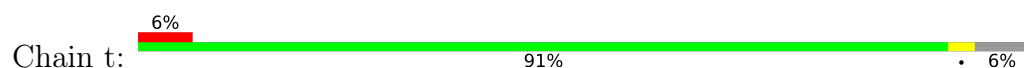
• Molecule 14: Photosystem II protein Y



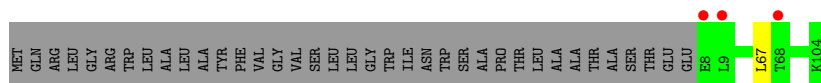
• Molecule 15: Photosystem II reaction center protein T



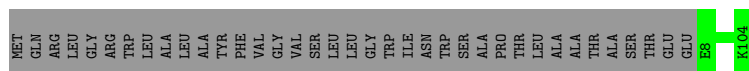
• Molecule 15: Photosystem II reaction center protein T



• Molecule 16: Photosystem II 12 kDa extrinsic protein




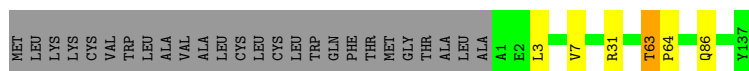
• Molecule 16: Photosystem II 12 kDa extrinsic protein




• Molecule 17: Cytochrome c-550

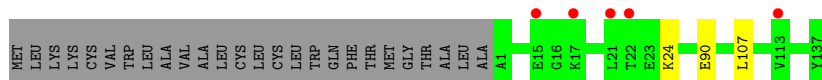


Chain V:  80% 16%




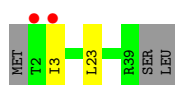
• Molecule 17: Cytochrome c-550

Chain v:  82% 16%



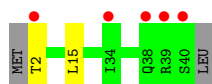
• Molecule 18: Photosystem II reaction center X protein

Chain X:  88% 5% 7%



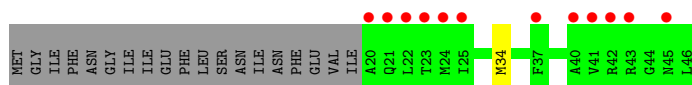
• Molecule 18: Photosystem II reaction center X protein

Chain x:  90% 5% 5%



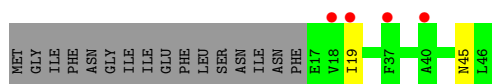
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:  57% 26% 17%




• Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:  61% 9% 30%

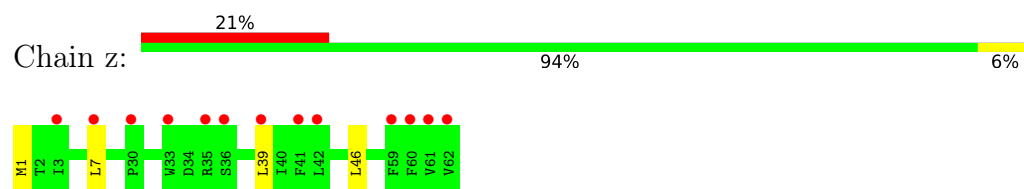


• Molecule 20: Photosystem II reaction center protein Z

Chain Z:  90% 10% 26%



- 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, $\alpha$ , $\beta$ , $\gamma$	117.04Å 221.92Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.59 – 2.01 33.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.59-2.01) 86.7 (33.59-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.180 , 0.227 0.180 , 0.227	Depositor DCC
$R_{free}$ test set	4767 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	106128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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 [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.58	0/3227	0.64	1/4397 (0.0%)
1	a	0.57	0/3224	0.65	3/4393 (0.1%)
2	B	0.61	0/4161	0.67	0/5669
2	b	0.58	0/4118	0.66	0/5611
3	C	0.58	0/3647	0.65	0/4965
3	c	0.55	0/3719	0.65	0/5061
4	D	0.63	0/2825	0.67	1/3847 (0.0%)
4	d	0.59	0/2834	0.68	0/3859
5	E	0.54	0/688	0.62	0/940
5	e	0.48	0/683	0.61	0/932
6	F	0.50	0/284	0.60	0/387
6	f	0.50	0/284	0.61	0/387
7	H	0.63	0/523	0.66	0/713
7	h	0.57	0/511	0.67	0/697
8	I	0.58	0/293	0.64	0/396
8	i	0.63	0/293	0.65	0/396
9	J	0.44	0/263	0.62	0/356
9	j	0.48	0/263	0.62	0/356
10	K	0.45	0/303	0.60	0/416
10	k	0.47	0/303	0.59	0/416
11	L	0.57	0/311	0.65	0/422
11	l	0.60	0/303	0.68	0/412
12	M	0.60	0/249	0.63	0/341
12	m	0.65	0/244	0.68	0/334
13	O	0.57	0/1904	0.70	1/2585 (0.0%)
13	o	0.58	0/1905	0.71	0/2583
14	R	0.41	0/227	0.54	0/313
14	r	0.36	0/227	0.54	0/313
15	T	0.69	0/257	0.64	0/349
15	t	0.71	0/255	0.61	0/346
16	U	0.53	0/785	0.66	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	u	0.57	0/785	0.67	0/1064
17	V	0.55	0/1085	0.68	1/1473 (0.1%)
17	v	0.53	0/1085	0.63	0/1473
18	X	0.47	0/284	0.57	0/384
18	x	0.43	0/289	0.53	0/391
19	Y	0.42	0/197	0.60	0/264
19	y	0.39	0/219	0.55	0/294
20	Z	0.43	0/490	0.54	0/669
20	z	0.37	0/488	0.48	0/666
All	All	0.57	0/44035	0.65	7/59934 (0.0%)

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

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

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	63	THR	C-N-CD	-6.37	106.59	120.60
1	a	42	LEU	CA-CB-CG	5.69	128.39	115.30
1	a	131	TRP	CA-CB-CG	-5.25	103.73	113.70
4	D	297	ASP	CB-CG-OD1	5.15	122.94	118.30
13	O	79	ASP	CB-CG-OD1	5.15	122.93	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

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

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

## 5.3 Torsion angles ⓘ

### 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	397/344 (115%)	392 (99%)	4 (1%)	1 (0%)	41	37
1	a	397/344 (115%)	390 (98%)	6 (2%)	1 (0%)	41	37
2	B	508/510 (100%)	498 (98%)	10 (2%)	0	100	100
2	b	503/510 (99%)	494 (98%)	9 (2%)	0	100	100
3	C	454/461 (98%)	442 (97%)	11 (2%)	1 (0%)	47	44
3	c	463/461 (100%)	448 (97%)	14 (3%)	1 (0%)	47	44
4	D	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	230 (95%)	11 (4%)	2 (1%)	19	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	234 (97%)	7 (3%)	1 (0%)	34	30
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	16
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
All	All	5387/5700 (94%)	5245 (97%)	134 (2%)	8 (0%)	47	49

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	58	ASN
13	O	62	GLU

### 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	324/280 (116%)	323 (100%)	1 (0%)	92	95

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	323/280 (115%)	313 (97%)	10 (3%)	40	40
2	B	408/407 (100%)	400 (98%)	8 (2%)	55	58
2	b	402/407 (99%)	393 (98%)	9 (2%)	52	55
3	C	356/362 (98%)	349 (98%)	7 (2%)	55	58
3	c	364/362 (101%)	356 (98%)	8 (2%)	52	55
4	D	277/283 (98%)	274 (99%)	3 (1%)	73	78
4	d	278/283 (98%)	268 (96%)	10 (4%)	35	34
5	E	72/73 (99%)	67 (93%)	5 (7%)	15	11
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	44
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	34
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	61
7	h	53/55 (96%)	51 (96%)	2 (4%)	33	31
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	13
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	40
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	27
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	7
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	37
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	43
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	34
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	10
13	O	206/228 (90%)	199 (97%)	7 (3%)	37	36
13	o	207/228 (91%)	202 (98%)	5 (2%)	49	51
14	R	22/33 (67%)	19 (86%)	3 (14%)	3	2
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	5
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	83 (99%)	1 (1%)	71	76
16	u	84/112 (75%)	84 (100%)	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	117/138 (85%)	113 (97%)	4 (3%)	37	36
17	v	117/138 (85%)	114 (97%)	3 (3%)	46	48
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	12
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	12
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22	18
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	5
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	47 (92%)	4 (8%)	12	8
All	All	4451/4654 (96%)	4324 (97%)	127 (3%)	42	43

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	159[A]	LEU
13	o	49	THR
2	b	492	GLU
13	o	18	LYS
17	v	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	378	ASN
5	e	60	GLN
18	x	33	GLN
5	e	82	GLN
17	V	86	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	FME	M	1	12	8,9,10	0.98	0	7,9,11	0.90	0
15	FME	t	1	15	8,9,10	1.45	1 (12%)	7,9,11	0.71	0
8	FME	i	1	8	8,9,10	1.03	1 (12%)	7,9,11	0.78	0
8	FME	I	1	8	8,9,10	0.97	1 (12%)	7,9,11	0.78	0
12	FME	m	1	12	8,9,10	0.93	0	7,9,11	0.74	0
15	FME	T	1	15	8,9,10	0.96	0	7,9,11	1.41	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	1/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.48	1.41	1.46
8	i	1	FME	CA-N	-2.16	1.43	1.46
8	I	1	FME	CA-N	-2.02	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	O1-CN-N	-2.37	119.02	125.27

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
15	T	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 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	$\# Z  > 2$
31	SQD	B	623	-	53,54,54	0.98	3 (5%)	62,65,65	2.00	15 (24%)
24	CLA	A	605	37	56,73,73	1.53	3 (5%)	55,113,113	1.83	12 (21%)
26	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.24	6 (10%)
26	BCR	T	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
26	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.29	8 (14%)
24	CLA	C	510	-	56,73,73	1.58	8 (14%)	55,113,113	1.88	11 (20%)
29	LMG	a	618	-	55,55,55	1.06	5 (9%)	63,63,63	1.45	5 (7%)
24	CLA	C	511	3	56,73,73	1.79	6 (10%)	55,113,113	1.66	10 (18%)
24	CLA	B	602	-	56,73,73	1.76	7 (12%)	55,113,113	1.62	11 (20%)
24	CLA	c	512	-	56,73,73	1.41	5 (8%)	55,113,113	1.60	11 (20%)
24	CLA	B	609	-	56,73,73	1.68	7 (12%)	55,113,113	1.61	9 (16%)
32	DGD	c	518	-	63,63,67	1.09	6 (9%)	77,77,81	1.43	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	LHG	l	101	-	48,48,48	0.85	1 (2%)	51,54,54	1.27	8 (15%)
24	CLA	C	508	-	56,73,73	1.70	7 (12%)	55,113,113	1.86	12 (21%)
33	STE	B	624	-	10,13,19	0.42	0	9,13,19	0.80	0
30	LHG	E	101	-	48,48,48	0.88	2 (4%)	51,54,54	1.26	5 (9%)
24	CLA	B	606	-	56,73,73	1.74	8 (14%)	55,113,113	1.65	10 (18%)
33	STE	B	627	-	8,11,19	0.47	0	7,11,19	0.62	0
26	BCR	A	609	-	41,41,41	1.21	5 (12%)	56,56,56	1.43	7 (12%)
24	CLA	a	604	-	56,73,73	1.58	4 (7%)	55,113,113	1.59	6 (10%)
26	BCR	b	618	-	41,41,41	1.23	4 (9%)	56,56,56	1.20	5 (8%)
24	CLA	c	511	3	56,73,73	1.86	8 (14%)	55,113,113	1.63	9 (16%)
24	CLA	b	608	-	56,73,73	1.70	8 (14%)	55,113,113	1.55	10 (18%)
29	LMG	c	522	-	49,49,55	0.87	1 (2%)	57,57,63	1.30	6 (10%)
26	BCR	c	515	-	41,41,41	1.21	3 (7%)	56,56,56	1.35	7 (12%)
34	BCT	a	610	23	0,3,3	-	-	0,3,3	-	-
33	STE	b	625	-	16,19,19	0.40	0	15,19,19	0.98	1 (6%)
31	SQD	A	617	-	38,38,54	0.96	3 (7%)	40,40,65	1.51	4 (10%)
24	CLA	b	616	-	51,68,73	1.59	12 (23%)	49,107,113	1.85	10 (20%)
33	STE	C	522	-	8,11,19	0.36	0	7,11,19	1.04	1 (14%)
24	CLA	b	613	-	56,73,73	1.58	6 (10%)	55,113,113	1.67	13 (23%)
24	CLA	b	614	-	56,73,73	1.54	7 (12%)	55,113,113	1.88	13 (23%)
22	OEX	A	602[A]	1,37,3	0,15,15	-	-	-	-	-
24	CLA	d	403	-	56,73,73	1.77	9 (16%)	55,113,113	1.82	11 (20%)
30	LHG	d	409	-	38,38,48	0.91	1 (2%)	41,44,54	1.17	2 (4%)
31	SQD	a	613	-	53,54,54	1.07	5 (9%)	62,65,65	1.89	11 (17%)
24	CLA	C	509	-	56,73,73	1.43	7 (12%)	55,113,113	1.92	10 (18%)
21	OXY	a	601[B]	1,37,3	0,16,16	-	-	-	-	-
26	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.03	3 (5%)
24	CLA	b	611	-	56,73,73	1.54	7 (12%)	55,113,113	1.54	8 (14%)
33	STE	x	102	-	16,19,19	0.39	0	15,19,19	0.75	0
33	STE	a	616	-	8,11,19	0.52	0	7,11,19	0.55	0
26	BCR	b	617	-	41,41,41	1.09	3 (7%)	56,56,56	1.38	8 (14%)
24	CLA	c	507	37	56,73,73	1.44	5 (8%)	55,113,113	1.72	11 (20%)
24	CLA	B	611	-	56,73,73	1.58	8 (14%)	55,113,113	2.10	17 (30%)
29	LMG	D	409	-	31,31,55	0.95	2 (6%)	33,33,63	1.10	1 (3%)
33	STE	d	412	-	16,19,19	0.30	0	15,19,19	1.03	0
24	CLA	b	604	-	56,73,73	1.49	6 (10%)	55,113,113	1.75	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	t	101	-	41,41,41	1.13	4 (9%)	56,56,56	1.37	7 (12%)
24	CLA	b	601	37	56,73,73	1.63	6 (10%)	55,113,113	1.70	7 (12%)
24	CLA	A	608	-	45,62,73	1.64	6 (13%)	41,99,113	1.74	11 (26%)
24	CLA	b	612	-	56,73,73	1.62	6 (10%)	55,113,113	1.76	10 (18%)
32	DGD	C	518	-	63,63,67	1.10	5 (7%)	77,77,81	1.34	7 (9%)
26	BCR	C	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.35	9 (16%)
29	LMG	D	410	-	20,26,55	0.36	0	18,26,63	1.18	0
33	STE	M	102	-	11,14,19	0.28	0	10,14,19	1.05	0
33	STE	t	102	-	14,17,19	0.32	0	13,17,19	1.02	0
26	BCR	K	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.18	2 (3%)
30	LHG	B	622	-	48,48,48	0.89	3 (6%)	51,54,54	1.32	8 (15%)
31	SQD	f	101	-	40,41,54	1.13	4 (10%)	49,52,65	2.01	12 (24%)
32	DGD	H	102	-	63,63,67	1.35	13 (20%)	77,77,81	1.38	8 (10%)
32	DGD	C	517	-	63,63,67	1.18	6 (9%)	77,77,81	1.37	9 (11%)
33	STE	D	411	-	16,19,19	0.24	0	15,19,19	1.01	0
24	CLA	c	505	-	56,73,73	1.58	5 (8%)	55,113,113	1.72	9 (16%)
24	CLA	b	610	37	56,73,73	1.46	8 (14%)	55,113,113	1.72	14 (25%)
30	LHG	d	407	-	48,48,48	0.86	3 (6%)	51,54,54	1.44	7 (13%)
24	CLA	a	606	-	56,73,73	1.71	8 (14%)	55,113,113	1.60	11 (20%)
30	LHG	A	615	-	46,46,48	1.12	4 (8%)	49,52,54	1.36	5 (10%)
33	STE	b	626	-	9,9,19	0.44	0	8,8,19	0.63	0
33	STE	j	101	-	8,11,19	0.48	0	7,11,19	0.68	0
24	CLA	b	602	-	56,73,73	1.40	8 (14%)	55,113,113	2.04	13 (23%)
29	LMG	M	101	-	51,51,55	1.06	4 (7%)	59,59,63	1.50	7 (11%)
33	STE	m	101	-	8,11,19	0.38	0	7,11,19	0.84	0
32	DGD	c	517	-	63,63,67	1.22	8 (12%)	77,77,81	1.40	15 (19%)
33	STE	Z	101	-	7,7,19	0.45	0	6,6,19	0.46	0
33	STE	c	520	-	16,19,19	0.31	0	15,19,19	0.85	0
24	CLA	B	603	-	56,73,73	1.65	8 (14%)	55,113,113	1.92	14 (25%)
24	CLA	b	615	-	56,73,73	1.75	7 (12%)	55,113,113	1.92	11 (20%)
24	CLA	B	614	-	56,73,73	1.67	9 (16%)	55,113,113	1.63	12 (21%)
24	CLA	c	509	-	56,73,73	1.54	2 (3%)	55,113,113	1.88	10 (18%)
28	PL9	a	611	-	55,55,55	1.09	6 (10%)	68,69,69	1.70	16 (23%)
32	DGD	A	618	-	67,67,67	1.21	7 (10%)	81,81,81	1.39	9 (11%)
30	LHG	D	408	-	48,48,48	1.10	4 (8%)	51,54,54	1.25	5 (9%)
24	CLA	b	606	-	56,73,73	1.86	6 (10%)	55,113,113	2.07	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	605	-	56,73,73	1.26	5 (8%)	55,113,113	1.50	10 (18%)
26	BCR	B	619	-	41,41,41	1.23	4 (9%)	56,56,56	1.27	5 (8%)
32	DGD	c	516	-	63,63,67	1.16	8 (12%)	77,77,81	1.38	10 (12%)
24	CLA	c	510	-	56,73,73	1.96	8 (14%)	55,113,113	1.88	11 (20%)
33	STE	T	102	-	15,15,19	0.39	0	14,14,19	0.83	0
26	BCR	c	514	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	9 (16%)
26	BCR	B	617	-	41,41,41	1.10	3 (7%)	56,56,56	1.32	8 (14%)
35	HEM	F	101	6,5	27,50,50	1.89	4 (14%)	17,82,82	2.37	9 (52%)
24	CLA	C	504	37	50,67,73	1.44	5 (10%)	47,105,113	1.64	8 (17%)
32	DGD	C	516	-	63,63,67	1.28	9 (14%)	77,77,81	1.40	9 (11%)
24	CLA	B	607	37	56,73,73	1.31	8 (14%)	55,113,113	1.52	5 (9%)
33	STE	a	615	-	9,9,19	0.53	0	8,8,19	0.47	0
24	CLA	D	403	-	56,73,73	1.60	7 (12%)	55,113,113	1.67	11 (20%)
24	CLA	c	502	-	56,73,73	1.54	6 (10%)	55,113,113	1.63	8 (14%)
26	BCR	k	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	4 (7%)
24	CLA	B	604	-	56,73,73	1.29	5 (8%)	55,113,113	1.82	12 (21%)
24	CLA	C	502	-	56,73,73	1.72	7 (12%)	55,113,113	1.53	7 (12%)
25	PHO	A	607	-	67,69,69	1.22	6 (8%)	85,99,99	1.14	8 (9%)
25	PHO	d	402	-	67,69,69	1.28	9 (13%)	85,99,99	1.06	6 (7%)
24	CLA	b	609	-	56,73,73	1.70	6 (10%)	55,113,113	2.07	15 (27%)
33	STE	B	620	-	13,16,19	0.36	0	12,16,19	1.09	0
33	STE	H	103	-	17,17,19	0.48	0	16,16,19	0.69	0
24	CLA	b	607	37	56,73,73	1.43	8 (14%)	55,113,113	1.50	10 (18%)
26	BCR	x	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	6 (10%)
29	LMG	c	519	-	37,37,55	1.24	6 (16%)	45,45,63	1.33	6 (13%)
21	OEY	A	601[B]	1,37,3	0,16,16	-	-	-	-	-
29	LMG	A	614	-	48,48,55	1.03	4 (8%)	56,56,63	1.41	6 (10%)
24	CLA	B	608	-	56,73,73	1.46	7 (12%)	55,113,113	1.51	11 (20%)
24	CLA	C	503	-	56,73,73	1.65	6 (10%)	55,113,113	2.03	11 (20%)
29	LMG	D	406	-	51,51,55	0.96	4 (7%)	59,59,63	1.27	4 (6%)
24	CLA	D	402	-	56,73,73	1.43	6 (10%)	55,113,113	1.72	13 (23%)
30	LHG	d	408	-	48,48,48	0.83	2 (4%)	51,54,54	1.20	4 (7%)
31	SQD	D	407	-	35,36,54	1.02	3 (8%)	42,45,65	2.16	10 (23%)
33	STE	T	103	-	14,14,19	0.43	0	13,13,19	0.78	0
36	HEC	v	201	17	26,50,50	2.42	3 (11%)	18,82,82	1.88	6 (33%)
36	HEC	V	201	17	26,50,50	2.09	4 (15%)	18,82,82	2.04	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	DGD	h	101	-	63,63,67	1.18	6 (9%)	77,77,81	1.37	11 (14%)
24	CLA	B	616	-	51,68,73	1.79	9 (17%)	49,107,113	2.08	8 (16%)
25	PHO	A	606	-	67,69,69	1.11	6 (8%)	85,99,99	1.10	5 (5%)
24	CLA	B	615	-	56,73,73	1.74	7 (12%)	55,113,113	1.46	6 (10%)
24	CLA	C	507	37	56,73,73	1.51	7 (12%)	55,113,113	1.79	13 (23%)
33	STE	a	617	-	14,14,19	0.41	0	13,13,19	0.80	0
34	BCT	D	401	23	0,3,3	-	-	0,3,3	-	-
35	HEM	e	101	6,5	27,50,50	1.95	5 (18%)	17,82,82	2.16	5 (29%)
26	BCR	C	515	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	6 (10%)
25	PHO	a	605	-	67,69,69	1.17	9 (13%)	85,99,99	1.10	5 (5%)
26	BCR	B	618	-	41,41,41	1.19	3 (7%)	56,56,56	1.15	4 (7%)
33	STE	d	411	-	13,16,19	0.30	0	12,16,19	1.18	0
24	CLA	d	404	-	56,73,73	1.67	9 (16%)	55,113,113	1.53	9 (16%)
28	PL9	A	612	-	55,55,55	1.13	5 (9%)	68,69,69	1.62	11 (16%)
24	CLA	A	604	-	56,73,73	1.56	5 (8%)	55,113,113	1.56	11 (20%)
33	STE	J	101	-	8,11,19	0.33	0	7,11,19	0.99	0
31	SQD	a	614	-	35,35,54	1.02	2 (5%)	37,37,65	1.51	6 (16%)
33	STE	C	521	-	15,15,19	0.35	0	14,14,19	0.86	0
24	CLA	c	504	37	51,68,73	1.65	7 (13%)	49,107,113	1.57	10 (20%)
33	STE	I	101	-	14,14,19	0.43	0	13,13,19	0.64	0
33	STE	b	624	-	12,15,19	0.39	0	11,15,19	0.72	0
24	CLA	a	612	37	56,73,73	1.79	6 (10%)	55,113,113	1.92	9 (16%)
24	CLA	A	613	37	56,73,73	1.61	8 (14%)	55,113,113	1.71	10 (18%)
33	STE	k	103	-	8,11,19	0.46	0	7,11,19	0.72	0
29	LMG	b	621	-	51,51,55	0.94	3 (5%)	59,59,63	1.48	10 (16%)
29	LMG	b	623	-	55,55,55	0.88	3 (5%)	63,63,63	1.40	8 (12%)
24	CLA	C	506	-	56,73,73	1.55	9 (16%)	55,113,113	1.51	8 (14%)
31	SQD	A	616	-	51,52,54	1.11	6 (11%)	60,63,65	2.14	11 (18%)
24	CLA	B	613	-	56,73,73	1.64	6 (10%)	55,113,113	1.40	8 (14%)
29	LMG	C	519	-	48,48,55	0.89	3 (6%)	56,56,63	1.37	8 (14%)
24	CLA	c	506	-	56,73,73	1.51	11 (19%)	55,113,113	1.79	11 (20%)
24	CLA	c	508	-	55,72,73	1.61	7 (12%)	53,111,113	1.76	10 (18%)
22	OEX	a	602[A]	1,37,3	0,15,15	-	-	-	-	-
26	BCR	Y	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.15	5 (8%)
30	LHG	e	102	-	41,41,48	0.88	2 (4%)	44,47,54	1.31	5 (11%)
24	CLA	B	601	37	56,73,73	1.64	7 (12%)	55,113,113	1.61	9 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LMG	d	410	-	44,44,55	1.02	3 (6%)	52,52,63	1.26	6 (11%)
33	STE	B	625	-	8,11,19	0.37	0	7,11,19	0.93	0
33	STE	b	627	-	13,13,19	0.46	0	12,12,19	0.53	0
24	CLA	B	612	-	56,73,73	1.48	3 (5%)	55,113,113	1.92	11 (20%)
24	CLA	C	512	-	56,73,73	1.40	8 (14%)	55,113,113	1.76	11 (20%)
24	CLA	b	603	-	56,73,73	1.85	8 (14%)	55,113,113	1.77	11 (20%)
33	STE	E	102	-	8,11,19	0.44	0	7,11,19	0.59	0
28	PL9	D	405	-	55,55,55	1.52	9 (16%)	68,69,69	1.71	17 (25%)
30	LHG	B	621	-	48,48,48	0.82	1 (2%)	51,54,54	1.17	5 (9%)
31	SQD	b	620	-	48,49,54	1.00	4 (8%)	57,60,65	1.92	14 (24%)
24	CLA	b	605	-	56,73,73	1.33	7 (12%)	55,113,113	1.79	13 (23%)
33	STE	M	103	-	9,9,19	0.39	0	8,8,19	0.87	0
26	BCR	d	405	-	41,41,41	1.12	3 (7%)	56,56,56	1.23	6 (10%)
33	STE	l	102	-	17,17,19	0.36	0	16,16,19	0.89	0
24	CLA	B	610	37	56,73,73	1.65	9 (16%)	55,113,113	1.75	11 (20%)
24	CLA	d	401	37	56,73,73	1.63	9 (16%)	55,113,113	1.50	9 (16%)
29	LMG	c	521	-	48,48,55	1.09	6 (12%)	56,56,63	1.27	3 (5%)
33	STE	B	626	-	15,15,19	0.44	0	14,14,19	0.67	0
28	PL9	d	406	-	55,55,55	1.50	7 (12%)	68,69,69	1.78	16 (23%)
24	CLA	c	513	-	56,73,73	1.53	7 (12%)	55,113,113	1.59	8 (14%)
26	BCR	D	404	-	41,41,41	1.18	2 (4%)	56,56,56	1.19	4 (7%)
33	STE	b	622	-	16,19,19	0.34	0	15,19,19	0.83	0
24	CLA	C	505	-	56,73,73	1.62	4 (7%)	55,113,113	1.88	9 (16%)
24	CLA	C	501	-	56,73,73	1.78	8 (14%)	55,113,113	1.83	9 (16%)
24	CLA	C	513	-	56,73,73	1.42	7 (12%)	55,113,113	1.77	9 (16%)
26	BCR	a	607	-	41,41,41	1.05	4 (9%)	56,56,56	1.22	5 (8%)
24	CLA	c	503	-	56,73,73	1.59	8 (14%)	55,113,113	1.57	9 (16%)
33	STE	C	520	-	8,11,19	0.52	0	7,11,19	0.51	0
24	CLA	c	501	-	56,73,73	1.41	5 (8%)	55,113,113	1.78	10 (18%)

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
31	SQD	B	623	-	-	22/49/69/69	0/1/1/1

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	605	37	1/1/20/20	14/37/115/115	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
26	BCR	H	101	-	-	4/29/63/63	0/2/2/2
24	CLA	C	510	-	1/1/20/20	10/37/115/115	-
29	LMG	a	618	-	-	30/50/70/70	0/1/1/1
24	CLA	C	511	3	1/1/20/20	5/37/115/115	-
24	CLA	B	602	-	1/1/20/20	6/37/115/115	-
24	CLA	c	512	-	1/1/20/20	19/37/115/115	-
24	CLA	B	609	-	-	5/37/115/115	-
32	DGD	c	518	-	-	12/51/91/95	0/2/2/2
30	LHG	l	101	-	-	15/53/53/53	-
24	CLA	C	508	-	-	9/37/115/115	-
33	STE	B	624	-	-	3/9/11/17	-
30	LHG	E	101	-	-	22/53/53/53	-
24	CLA	B	606	-	1/1/20/20	12/37/115/115	-
33	STE	B	627	-	-	5/7/9/17	-
26	BCR	A	609	-	-	8/29/63/63	0/2/2/2
24	CLA	a	604	-	1/1/20/20	5/37/115/115	-
26	BCR	b	618	-	-	4/29/63/63	0/2/2/2
24	CLA	c	511	3	1/1/20/20	11/37/115/115	-
24	CLA	b	608	-	-	1/37/115/115	-
29	LMG	c	522	-	-	20/44/64/70	0/1/1/1
26	BCR	c	515	-	-	3/29/63/63	0/2/2/2
33	STE	b	625	-	-	10/15/17/17	-
24	CLA	b	616	-	1/1/19/20	8/31/109/115	-
33	STE	C	522	-	-	3/7/9/17	-
24	CLA	b	613	-	1/1/20/20	8/37/115/115	-
24	CLA	b	614	-	1/1/20/20	15/37/115/115	-
24	CLA	d	403	-	1/1/20/20	5/37/115/115	-
30	LHG	d	409	-	-	14/43/43/53	-
31	SQD	a	613	-	-	21/49/69/69	0/1/1/1
24	CLA	C	509	-	1/1/20/20	15/37/115/115	-
26	BCR	k	101	-	-	12/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	611	-	1/1/20/20	5/37/115/115	-
33	STE	x	102	-	-	6/15/17/17	-
33	STE	a	616	-	-	3/7/9/17	-
26	BCR	b	617	-	-	6/29/63/63	0/2/2/2
24	CLA	c	507	37	1/1/20/20	12/37/115/115	-
24	CLA	B	611	-	1/1/20/20	7/37/115/115	-
29	LMG	D	409	-	-	16/33/33/70	-
33	STE	d	412	-	-	11/15/17/17	-
24	CLA	b	604	-	1/1/20/20	8/37/115/115	-
26	BCR	t	101	-	-	6/29/63/63	0/2/2/2
24	CLA	b	601	37	1/1/20/20	14/37/115/115	-
24	CLA	A	608	-	1/1/17/20	2/24/102/115	-
24	CLA	b	612	-	1/1/20/20	7/37/115/115	-
32	DGD	C	518	-	-	18/51/91/95	0/2/2/2
26	BCR	C	514	-	-	8/29/63/63	0/2/2/2
29	LMG	D	410	-	-	10/18/22/70	-
33	STE	M	102	-	-	3/10/12/17	-
33	STE	t	102	-	-	7/13/15/17	-
26	BCR	K	101	-	-	8/29/63/63	0/2/2/2
30	LHG	B	622	-	-	16/53/53/53	-
31	SQD	f	101	-	-	12/36/56/69	0/1/1/1
32	DGD	H	102	-	-	19/51/91/95	0/2/2/2
32	DGD	C	517	-	-	24/51/91/95	0/2/2/2
33	STE	D	411	-	-	11/15/17/17	-
24	CLA	c	505	-	1/1/20/20	11/37/115/115	-
24	CLA	b	610	37	1/1/20/20	3/37/115/115	-
30	LHG	d	407	-	-	21/53/53/53	-
24	CLA	a	606	-	1/1/20/20	9/37/115/115	-
30	LHG	A	615	-	-	20/51/51/53	-
33	STE	b	626	-	-	5/7/7/17	-
33	STE	j	101	-	-	4/7/9/17	-
24	CLA	b	602	-	-	5/37/115/115	-
29	LMG	M	101	-	-	23/46/66/70	0/1/1/1
33	STE	m	101	-	-	3/7/9/17	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	DGD	c	517	-	-	19/51/91/95	0/2/2/2
33	STE	Z	101	-	-	2/5/5/17	-
33	STE	c	520	-	-	8/15/17/17	-
24	CLA	B	603	-	1/1/20/20	7/37/115/115	-
24	CLA	b	615	-	1/1/20/20	8/37/115/115	-
24	CLA	B	614	-	1/1/20/20	17/37/115/115	-
24	CLA	c	509	-	1/1/20/20	12/37/115/115	-
28	PL9	a	611	-	-	23/53/73/73	0/1/1/1
32	DGD	A	618	-	-	26/55/95/95	0/2/2/2
30	LHG	D	408	-	-	23/53/53/53	-
24	CLA	b	606	-	1/1/20/20	12/37/115/115	-
24	CLA	B	605	-	1/1/20/20	8/37/115/115	-
26	BCR	B	619	-	-	5/29/63/63	0/2/2/2
32	DGD	c	516	-	-	28/51/91/95	0/2/2/2
24	CLA	c	510	-	1/1/20/20	10/37/115/115	-
33	STE	T	102	-	-	8/13/13/17	-
26	BCR	c	514	-	-	10/29/63/63	0/2/2/2
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
35	HEM	F	101	6,5	-	0/6/54/54	-
24	CLA	C	504	37	1/1/18/20	6/30/108/115	-
32	DGD	C	516	-	-	18/51/91/95	0/2/2/2
24	CLA	B	607	37	1/1/20/20	5/37/115/115	-
33	STE	a	615	-	-	4/7/7/17	-
24	CLA	D	403	-	-	10/37/115/115	-
24	CLA	c	502	-	-	4/37/115/115	-
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
24	CLA	B	604	-	1/1/20/20	12/37/115/115	-
24	CLA	C	502	-	-	8/37/115/115	-
25	PHO	A	607	-	-	1/53/103/103	0/5/6/6
25	PHO	d	402	-	-	1/53/103/103	0/5/6/6
24	CLA	b	609	-	-	11/37/115/115	-
33	STE	B	620	-	-	6/12/14/17	-
33	STE	H	103	-	-	9/15/15/17	-
24	CLA	b	607	37	1/1/20/20	13/37/115/115	-
26	BCR	x	101	-	-	7/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	c	519	-	-	11/31/51/70	0/1/1/1
29	LMG	A	614	-	-	21/43/63/70	0/1/1/1
24	CLA	C	503	-	1/1/20/20	5/37/115/115	-
24	CLA	B	608	-	-	2/37/115/115	-
29	LMG	D	406	-	-	14/46/66/70	0/1/1/1
24	CLA	D	402	-	1/1/20/20	6/37/115/115	-
30	LHG	d	408	-	-	18/53/53/53	-
31	SQD	D	407	-	-	15/28/48/69	0/1/1/1
33	STE	T	103	-	-	11/12/12/17	-
36	HEC	v	201	17	-	0/6/54/54	-
36	HEC	V	201	17	-	0/6/54/54	-
32	DGD	h	101	-	-	15/51/91/95	0/2/2/2
24	CLA	B	616	-	1/1/19/20	8/31/109/115	-
25	PHO	A	606	-	-	3/53/103/103	0/5/6/6
24	CLA	B	615	-	1/1/20/20	11/37/115/115	-
24	CLA	C	507	37	1/1/20/20	10/37/115/115	-
33	STE	a	617	-	-	8/12/12/17	-
35	HEM	e	101	6,5	-	0/6/54/54	-
26	BCR	C	515	-	-	3/29/63/63	0/2/2/2
25	PHO	a	605	-	-	2/53/103/103	0/5/6/6
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
33	STE	d	411	-	-	7/12/14/17	-
24	CLA	d	404	-	1/1/20/20	11/37/115/115	-
28	PL9	A	612	-	-	23/53/73/73	0/1/1/1
24	CLA	A	604	-	1/1/20/20	4/37/115/115	-
33	STE	J	101	-	-	5/7/9/17	-
31	SQD	a	614	-	-	18/37/37/69	-
33	STE	C	521	-	-	7/13/13/17	-
24	CLA	c	504	37	1/1/19/20	8/31/109/115	-
33	STE	I	101	-	-	4/12/12/17	-
33	STE	b	624	-	-	8/11/13/17	-
24	CLA	a	612	37	1/1/20/20	5/37/115/115	-
24	CLA	A	613	37	-	6/37/115/115	-
33	STE	k	103	-	-	4/7/9/17	-
29	LMG	b	621	-	-	24/46/66/70	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	b	623	-	-	27/50/70/70	0/1/1/1
24	CLA	C	506	-	1/1/20/20	11/37/115/115	-
31	SQD	A	616	-	-	15/47/67/69	0/1/1/1
24	CLA	B	613	-	1/1/20/20	14/37/115/115	-
29	LMG	C	519	-	-	17/43/63/70	0/1/1/1
24	CLA	c	506	-	1/1/20/20	14/37/115/115	-
24	CLA	c	508	-	-	9/36/114/115	-
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
30	LHG	e	102	-	-	27/46/46/53	-
24	CLA	B	601	37	1/1/20/20	15/37/115/115	-
29	LMG	d	410	-	-	11/39/59/70	0/1/1/1
33	STE	B	625	-	-	4/7/9/17	-
33	STE	b	627	-	-	6/11/11/17	-
24	CLA	B	612	-	1/1/20/20	8/37/115/115	-
24	CLA	C	512	-	1/1/20/20	12/37/115/115	-
24	CLA	b	603	-	1/1/20/20	9/37/115/115	-
33	STE	E	102	-	-	4/7/9/17	-
28	PL9	D	405	-	-	12/53/73/73	0/1/1/1
30	LHG	B	621	-	-	25/53/53/53	-
31	SQD	b	620	-	-	19/44/64/69	0/1/1/1
24	CLA	b	605	-	1/1/20/20	6/37/115/115	-
33	STE	M	103	-	-	1/7/7/17	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
33	STE	l	102	-	-	9/15/15/17	-
24	CLA	B	610	37	1/1/20/20	6/37/115/115	-
24	CLA	d	401	37	-	12/37/115/115	-
29	LMG	c	521	-	-	23/43/63/70	0/1/1/1
33	STE	B	626	-	-	8/13/13/17	-
28	PL9	d	406	-	-	11/53/73/73	0/1/1/1
24	CLA	c	513	-	1/1/20/20	7/37/115/115	-
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
33	STE	b	622	-	-	9/15/17/17	-
24	CLA	C	505	-	1/1/20/20	10/37/115/115	-
24	CLA	C	501	-	1/1/20/20	3/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	513	-	1/1/20/20	6/37/115/115	-
26	BCR	a	607	-	-	1/29/63/63	0/2/2/2
24	CLA	c	503	-	1/1/20/20	8/37/115/115	-
33	STE	C	520	-	-	6/7/9/17	-
24	CLA	c	501	-	1/1/20/20	2/37/115/115	-

The worst 5 of 783 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	MG-NA	9.48	2.28	2.06
24	d	403	CLA	C4B-NB	9.31	1.43	1.35
24	c	504	CLA	C4B-NB	8.70	1.43	1.35
24	b	603	CLA	C4B-NB	8.65	1.42	1.35
24	B	612	CLA	C4B-NB	8.34	1.42	1.35

The worst 5 of 1270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C4A-NA-C1A	10.06	111.23	106.71
24	b	615	CLA	C4A-NA-C1A	9.37	110.92	106.71
24	B	611	CLA	C4A-NA-C1A	9.23	110.86	106.71
31	a	613	SQD	O6-C1-C2	8.97	122.30	108.30
31	A	616	SQD	O7-S-C6	8.91	117.53	106.94

5 of 58 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	604	CLA	ND
24	A	605	CLA	ND
24	A	608	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND

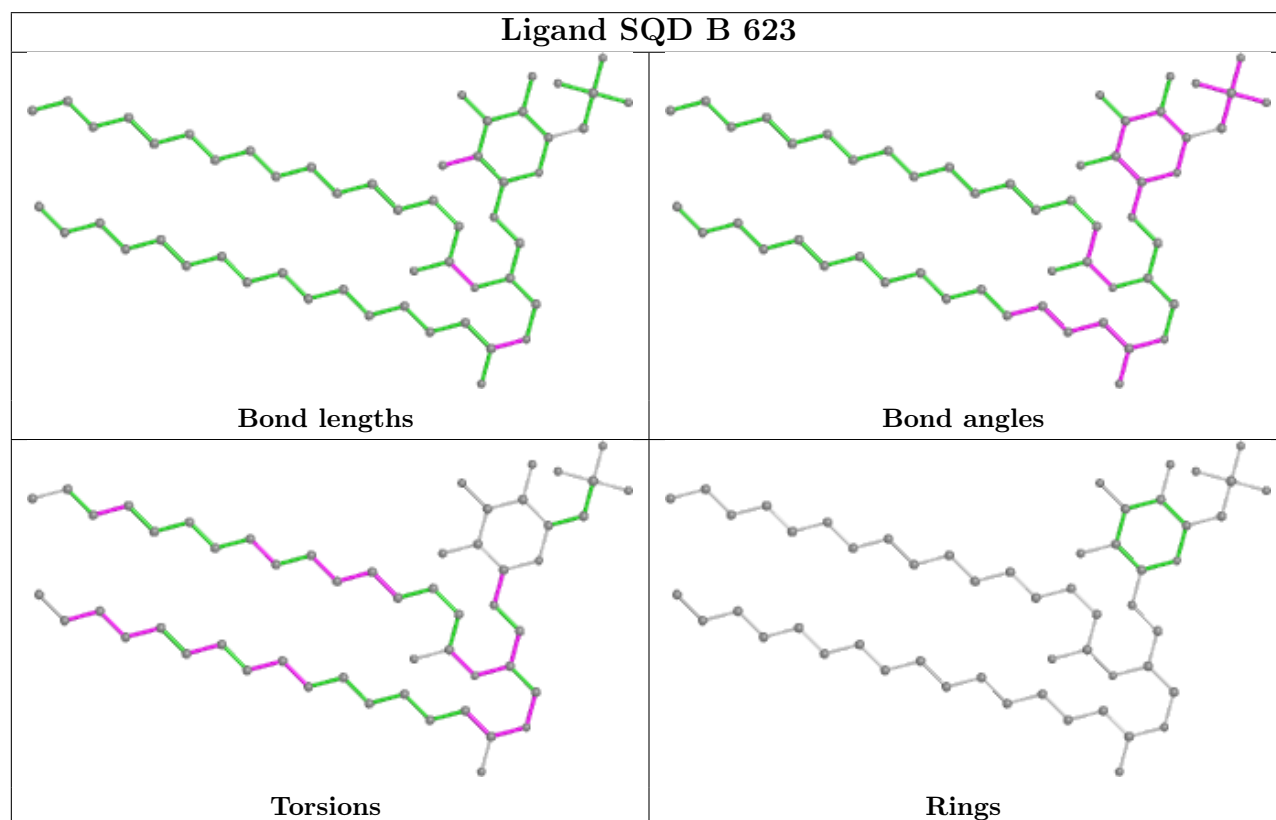
5 of 1767 torsion outliers are listed below:

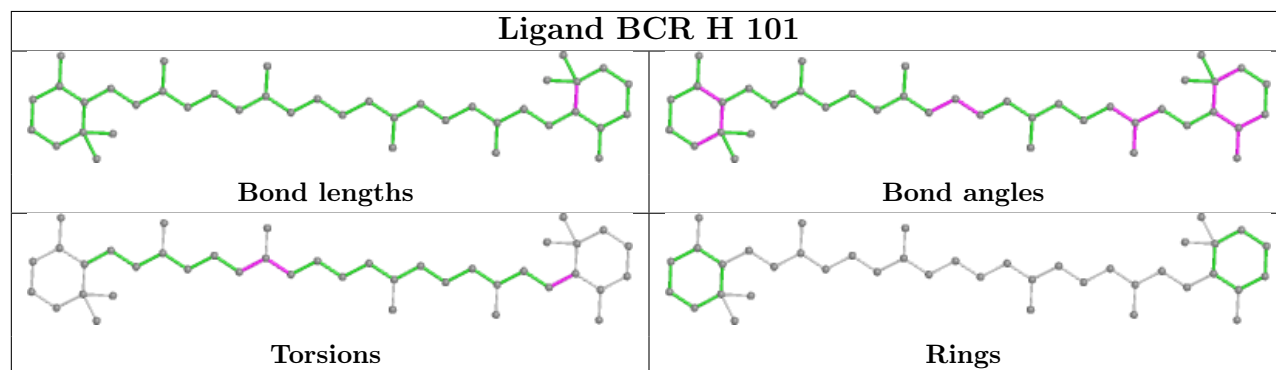
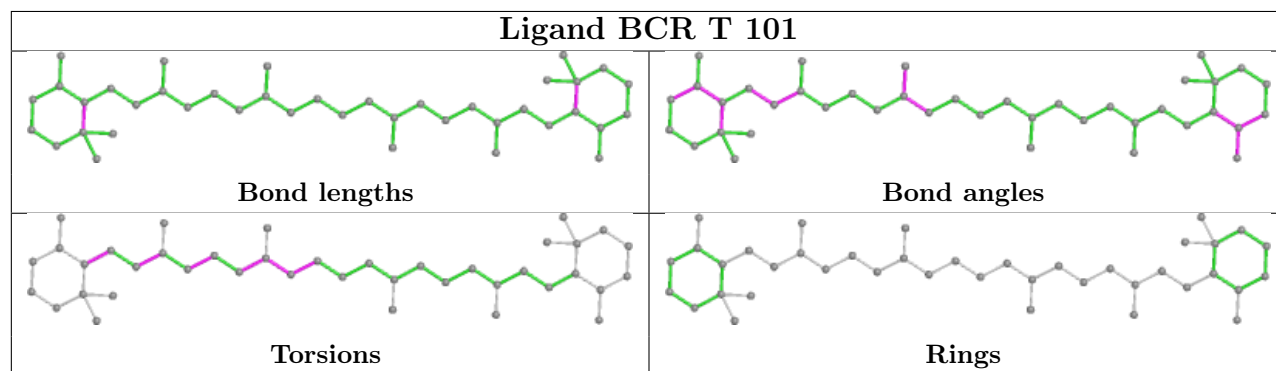
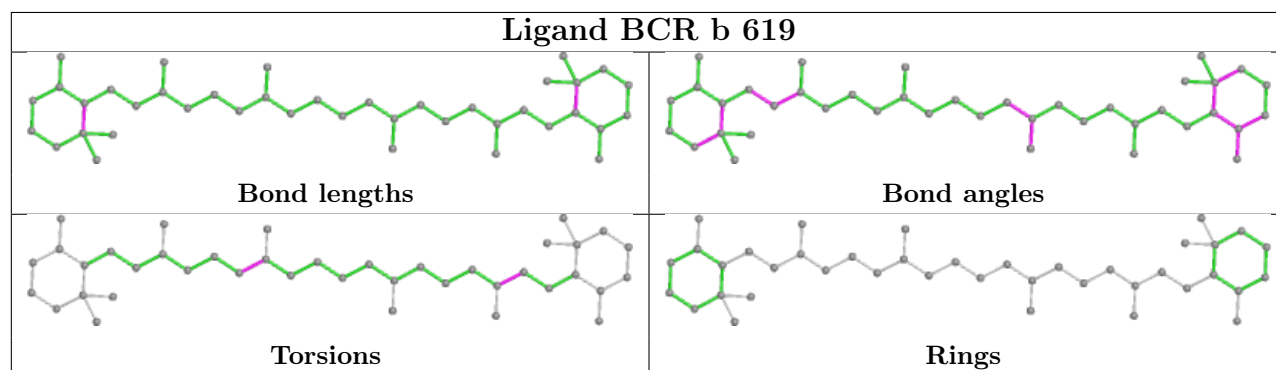
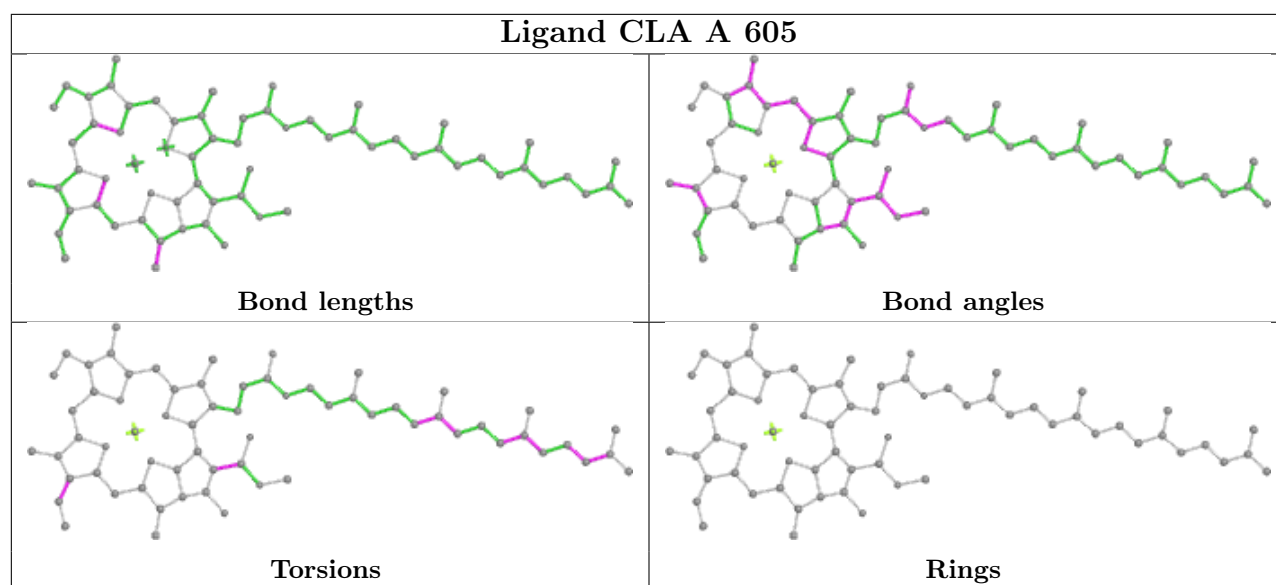
Mol	Chain	Res	Type	Atoms
24	A	608	CLA	C2-C3-C5-C6
24	A	608	CLA	C4-C3-C5-C6
24	A	613	CLA	CHA-CBD-CGD-O2D
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	601	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

No monomer is involved in short contacts.

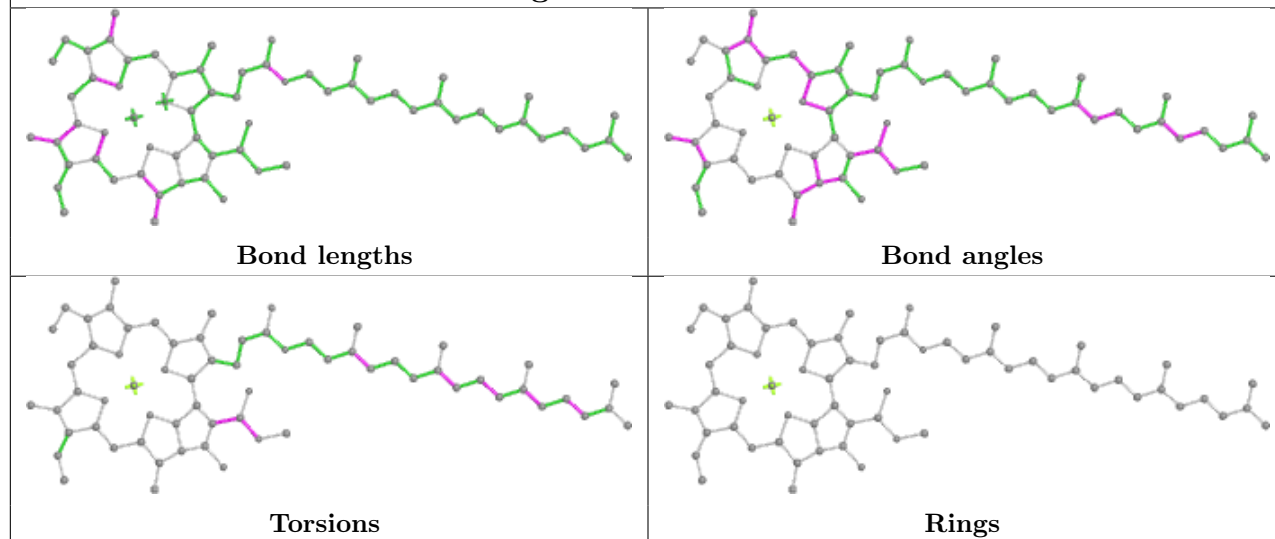
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



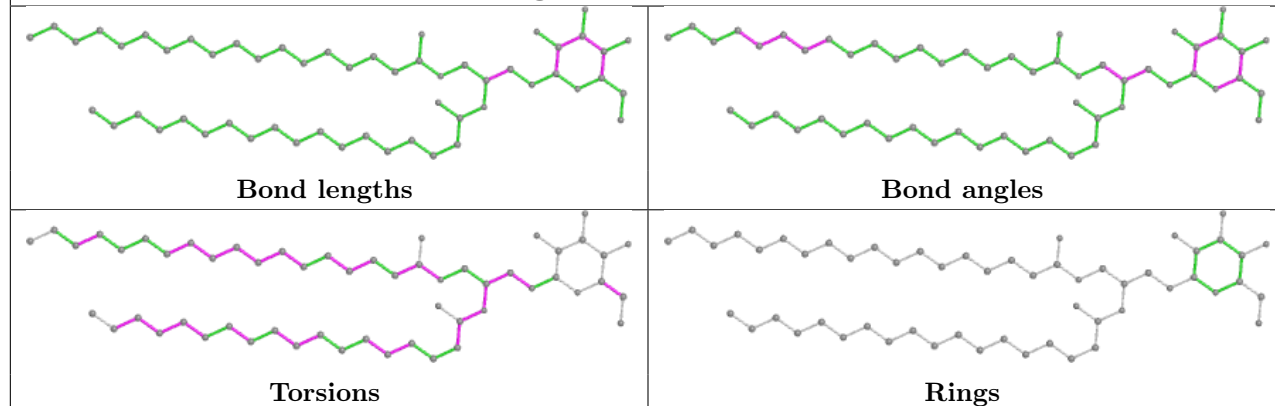




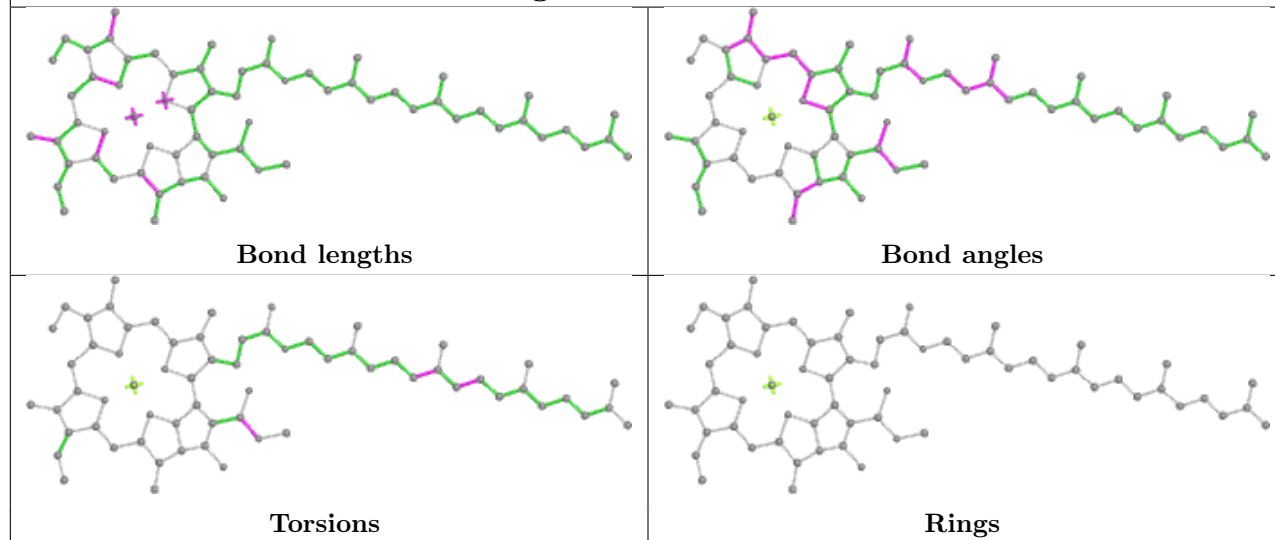
## Ligand CLA C 510

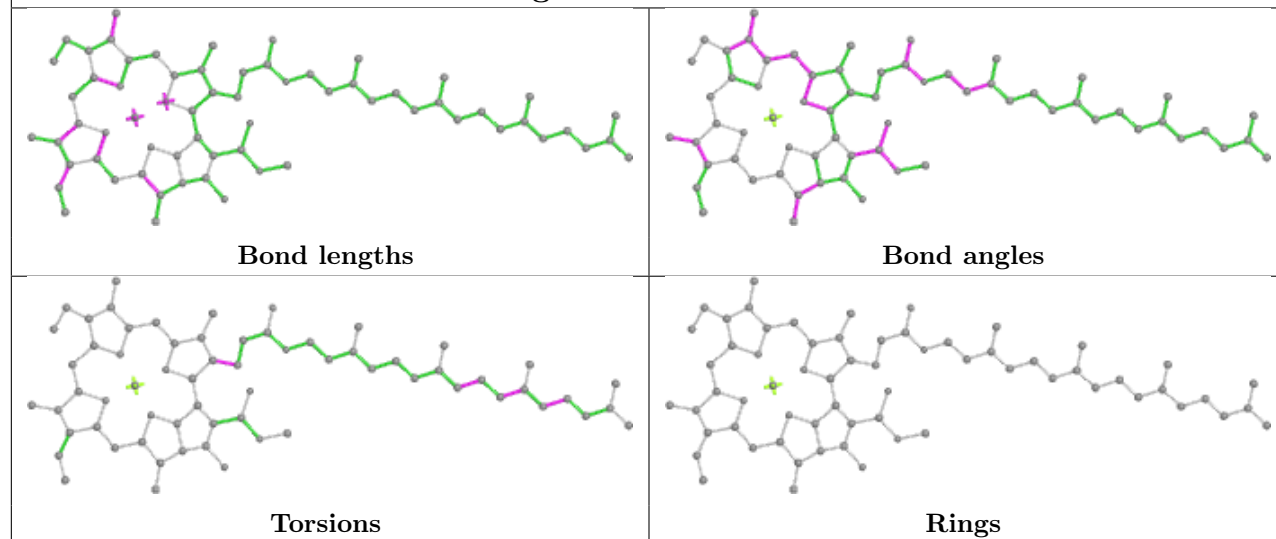
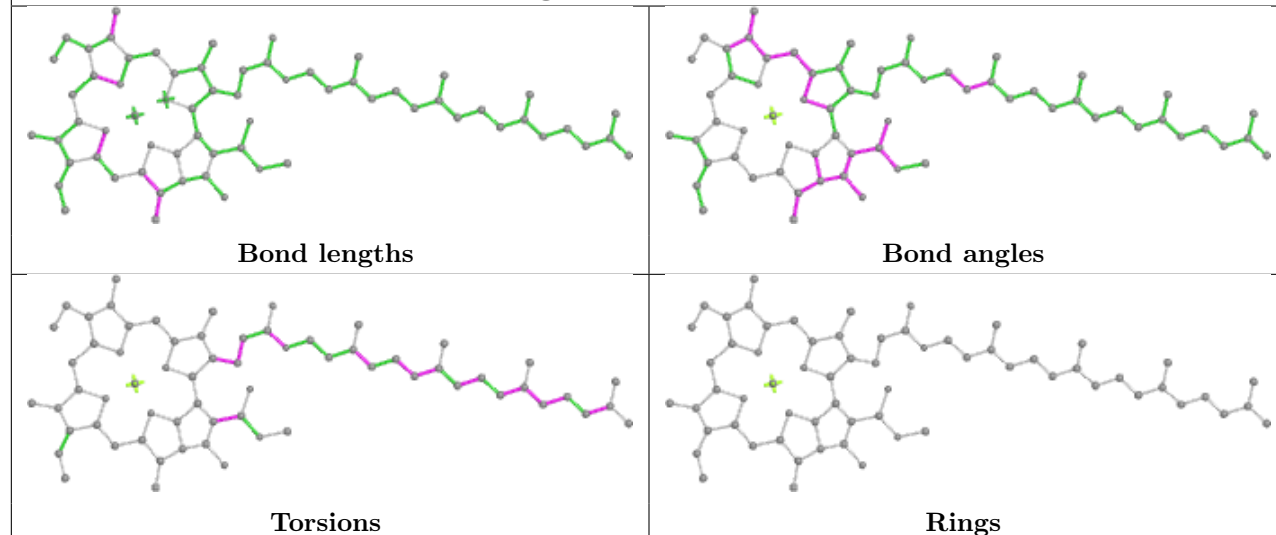
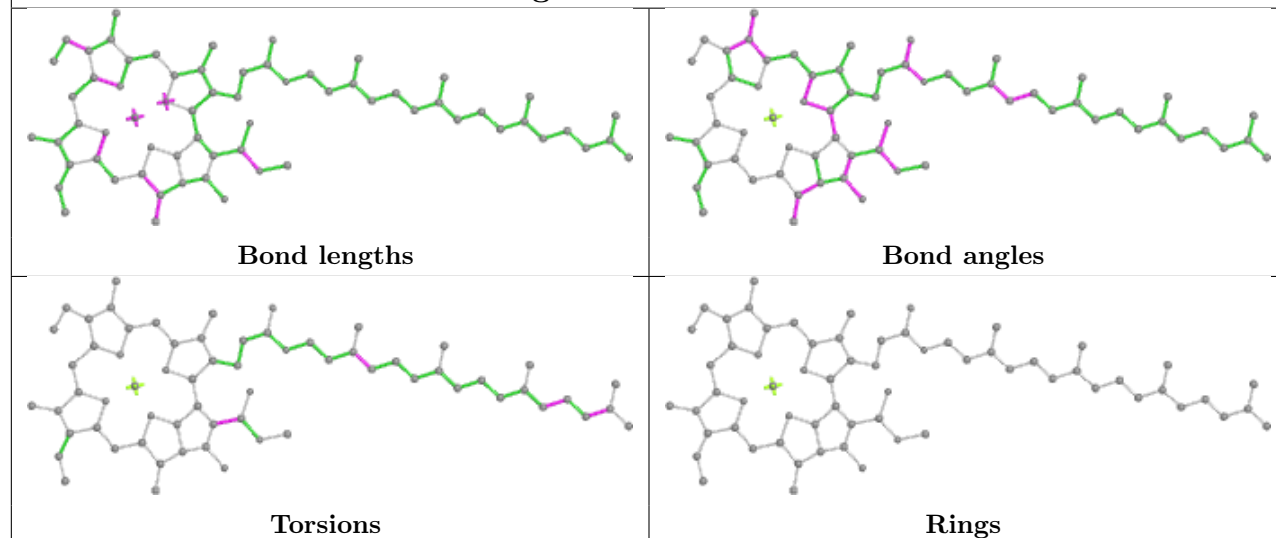


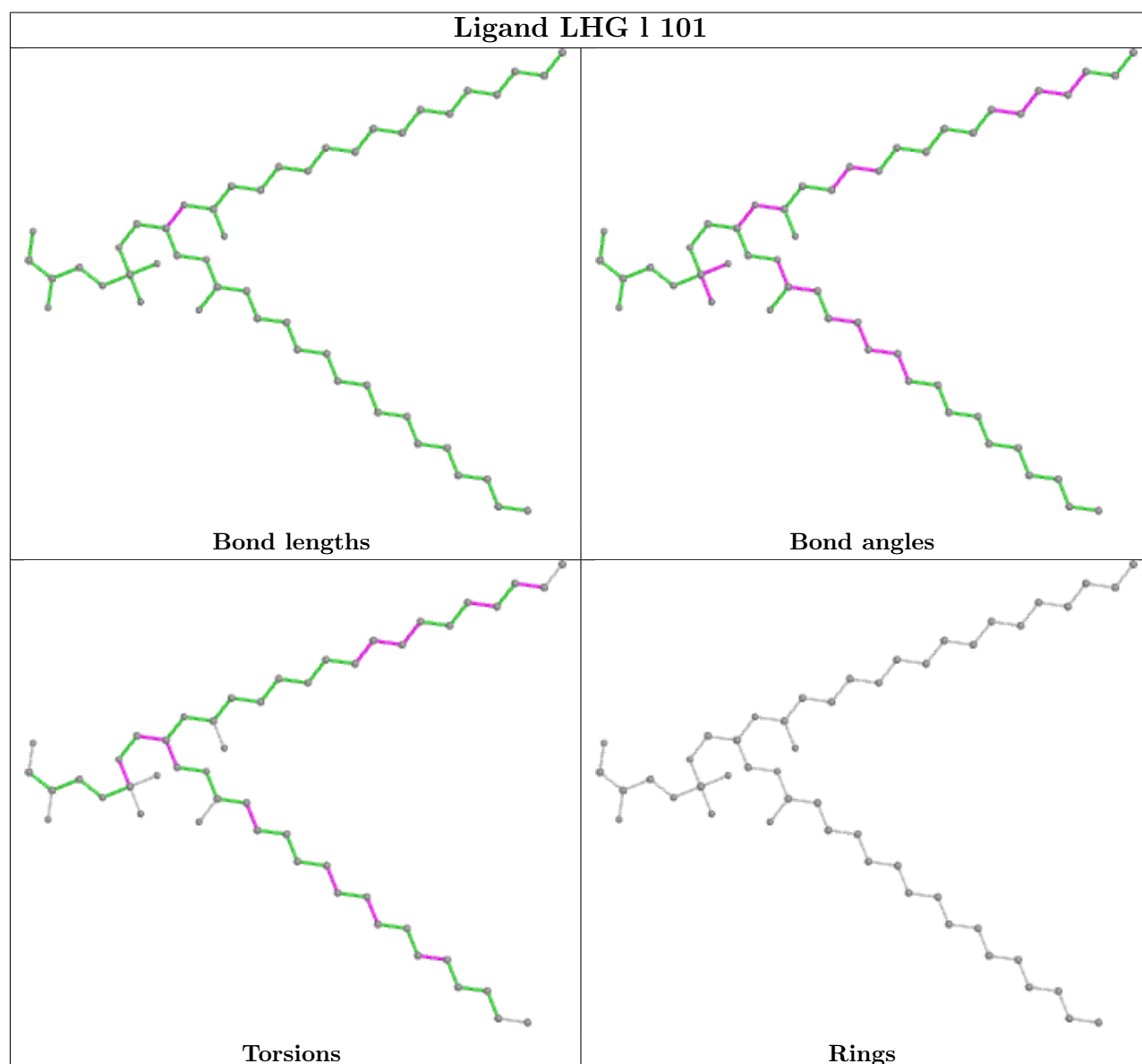
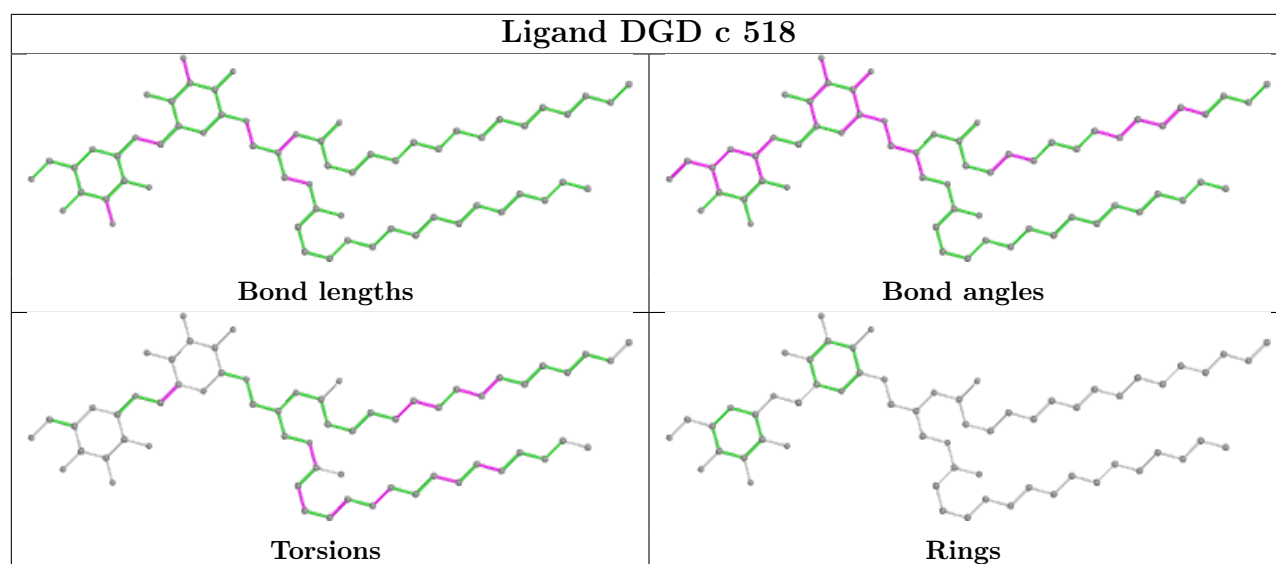
## Ligand LMG a 618

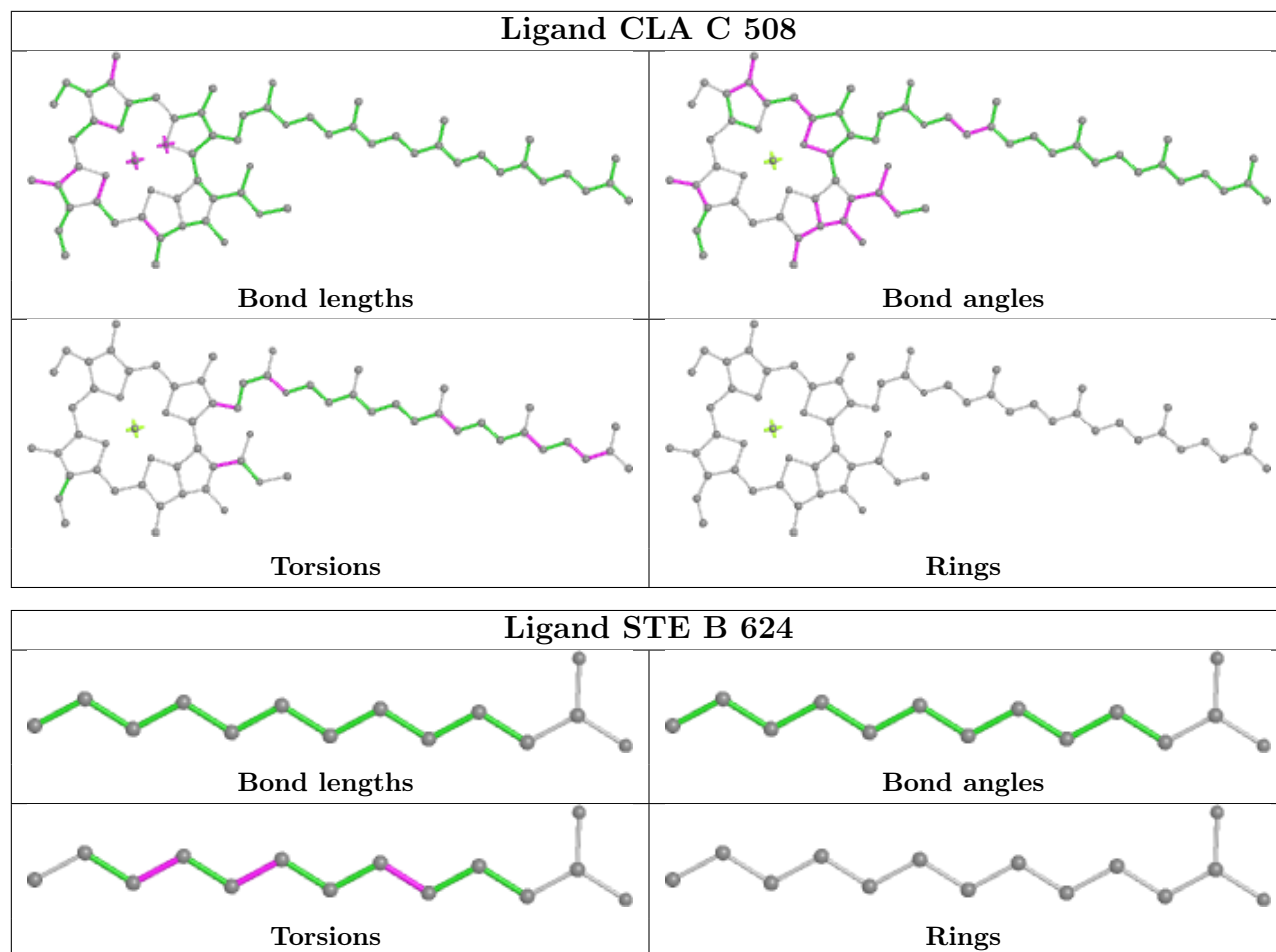


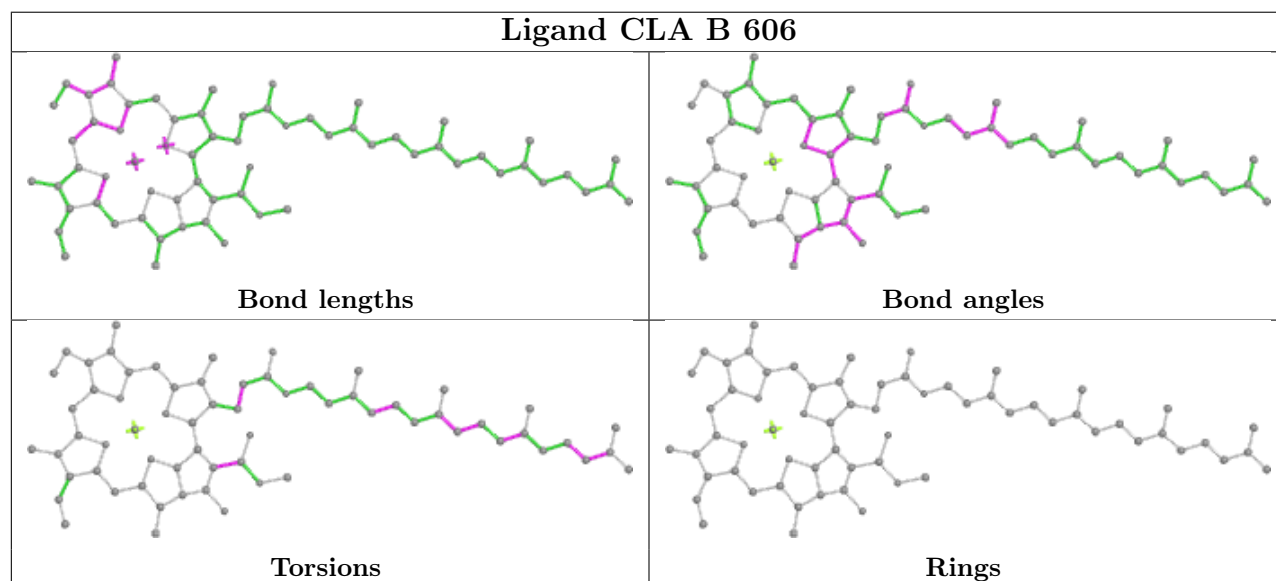
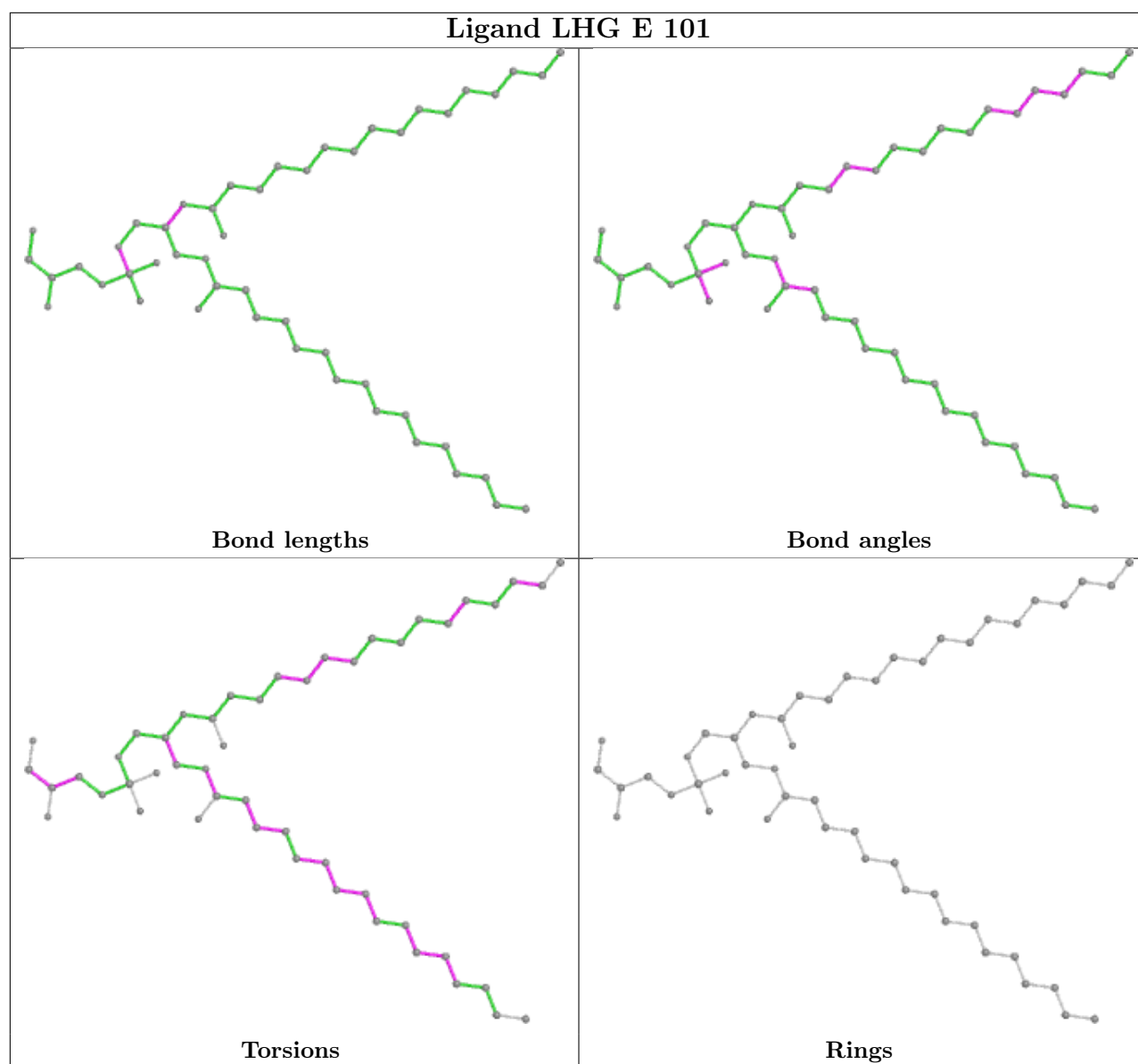
## Ligand CLA C 511

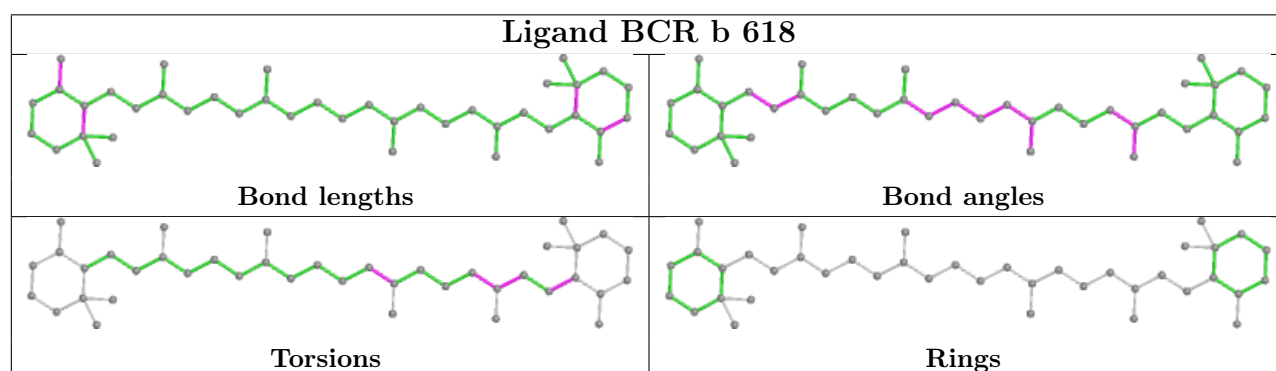
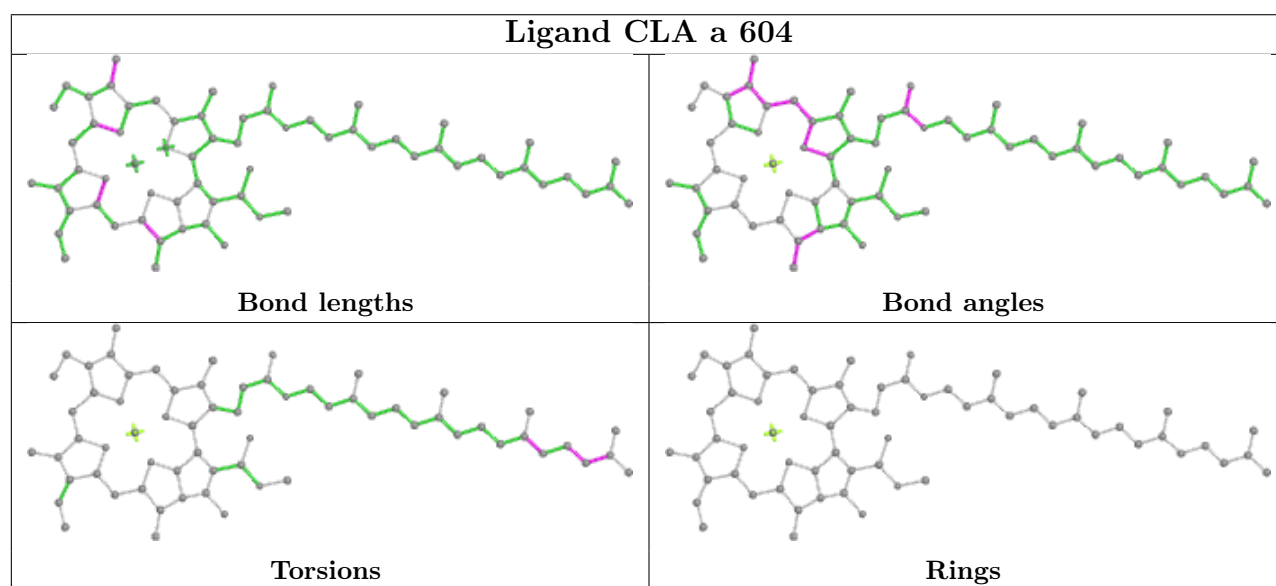
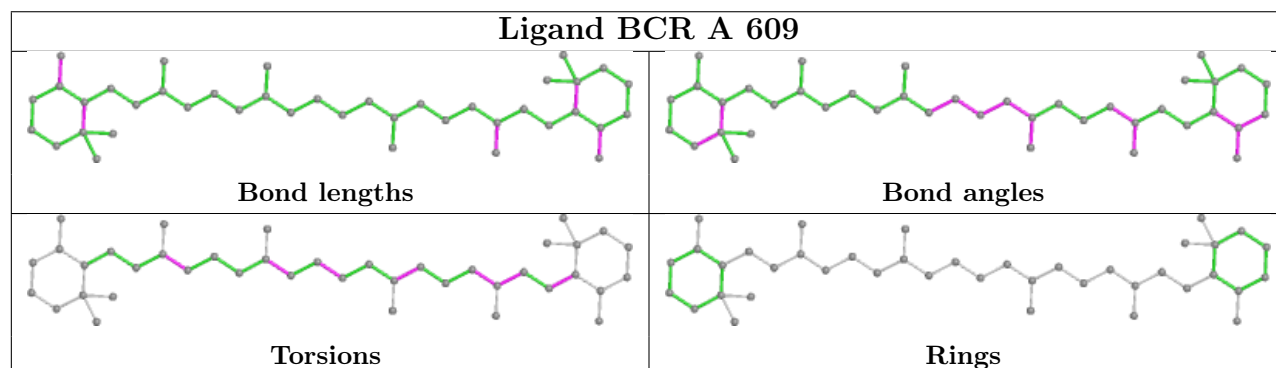
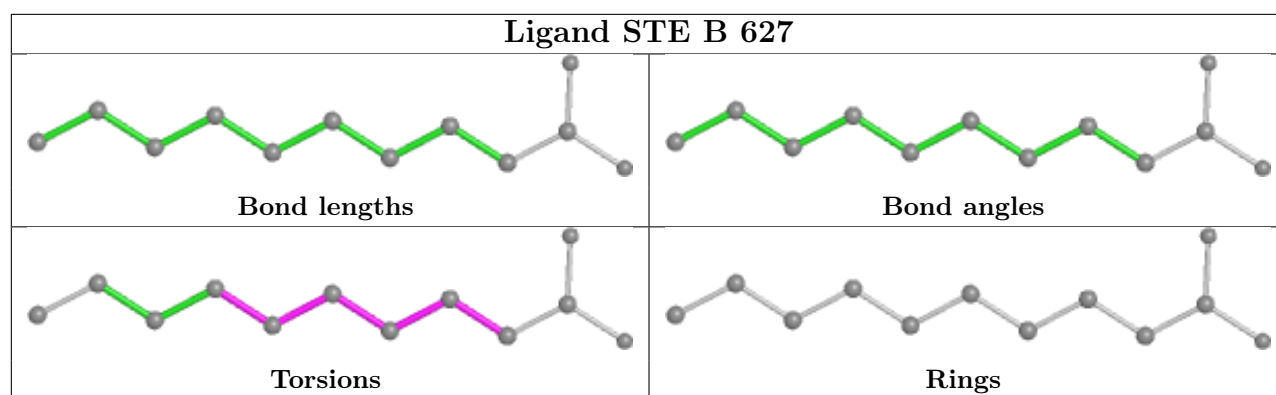


**Ligand CLA B 602****Ligand CLA c 512****Ligand CLA B 609**

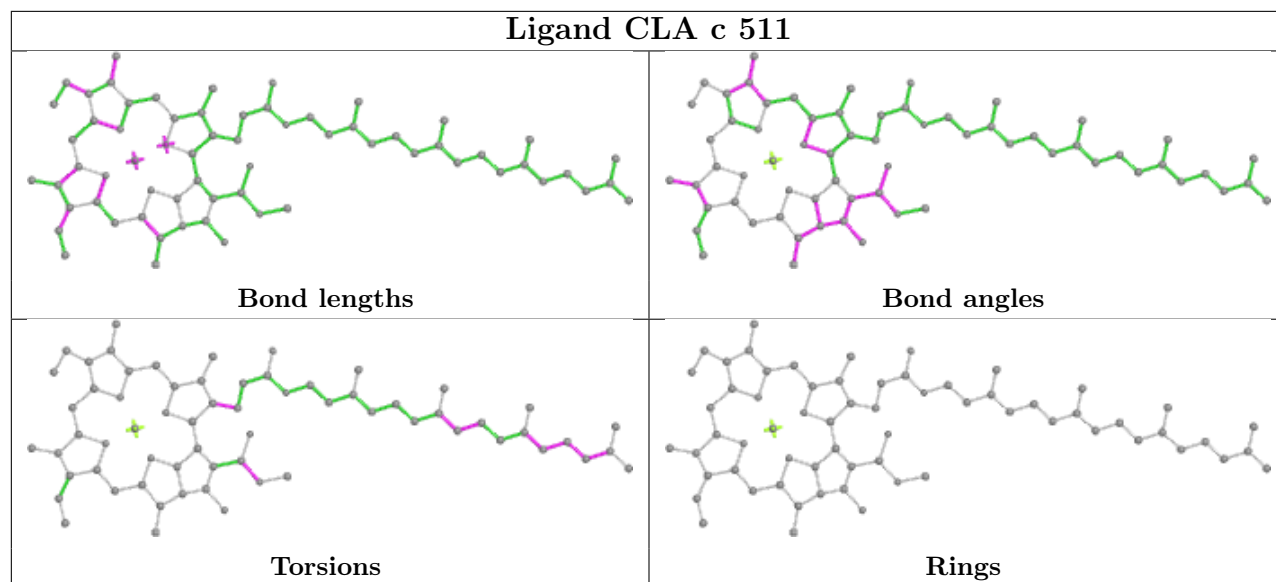




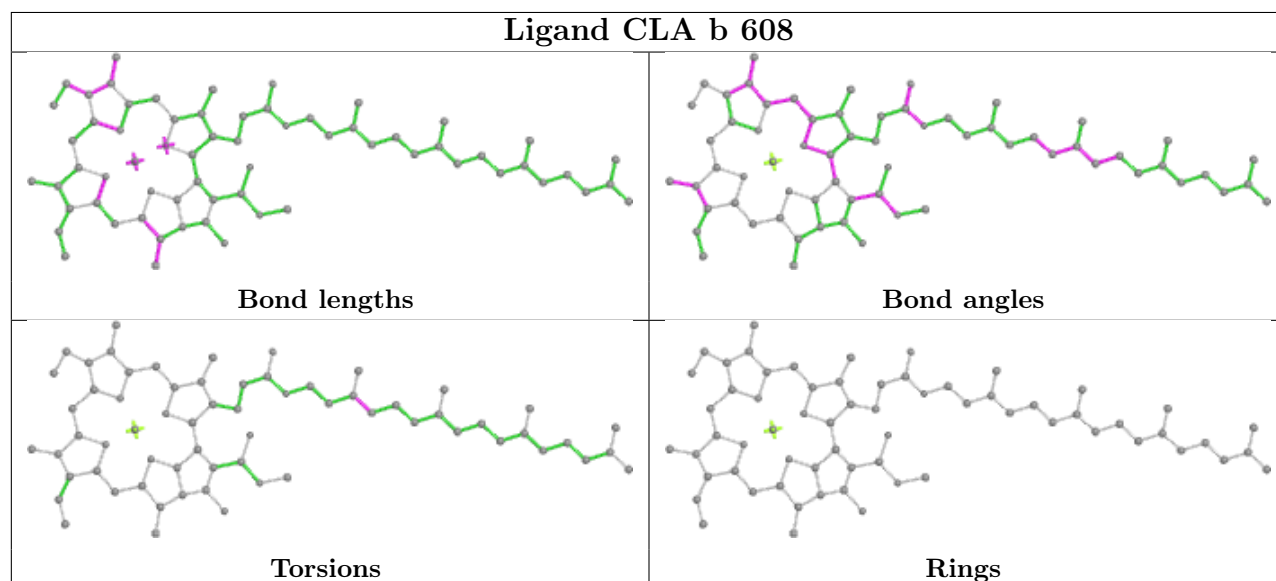




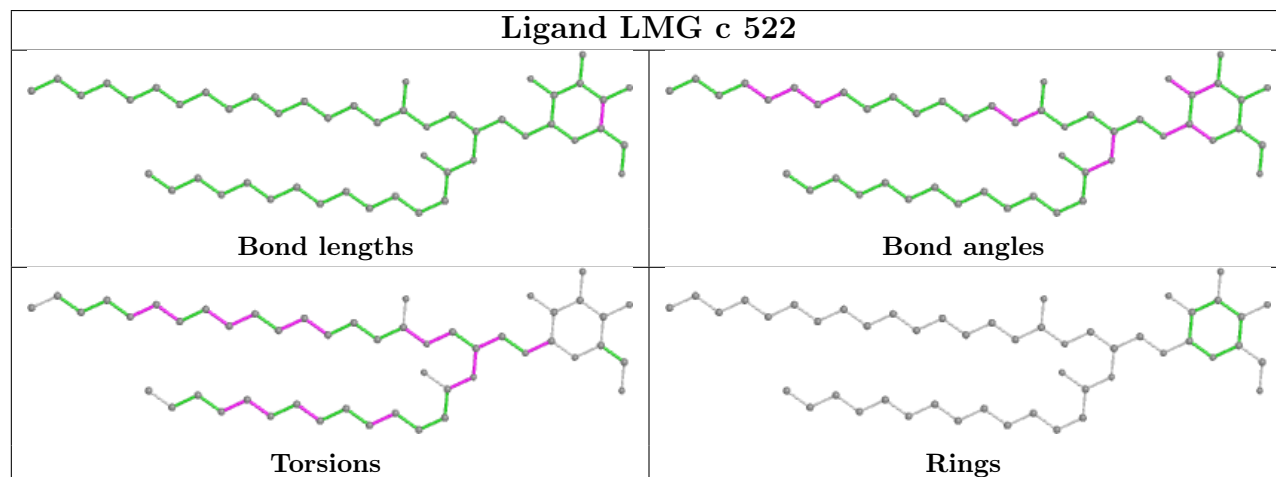
## Ligand CLA c 511

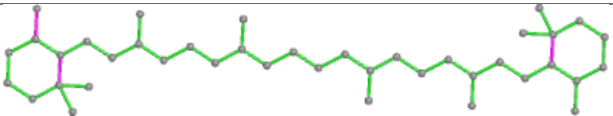
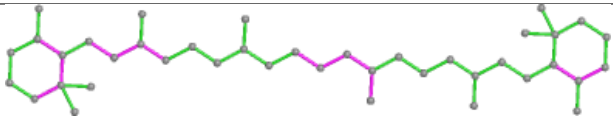
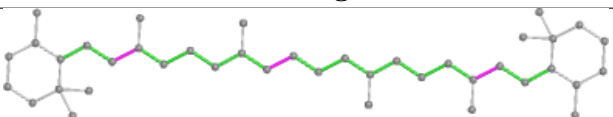
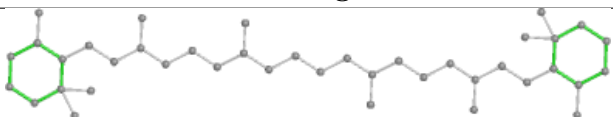



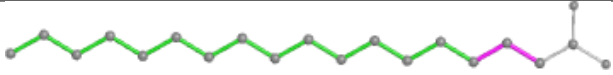
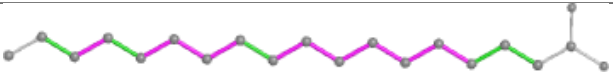
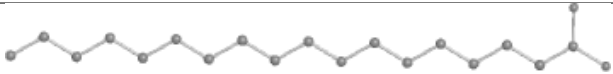
## Ligand CLA b 608

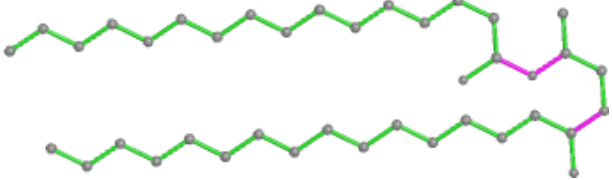
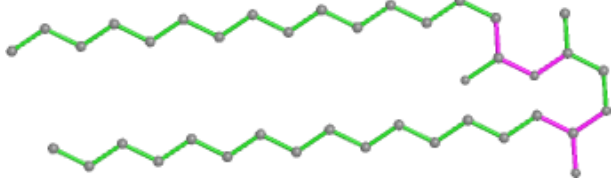
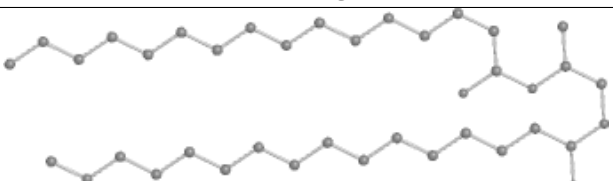
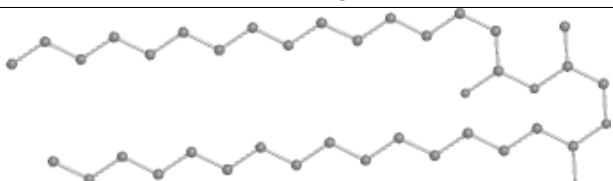


## Ligand LMG c 522



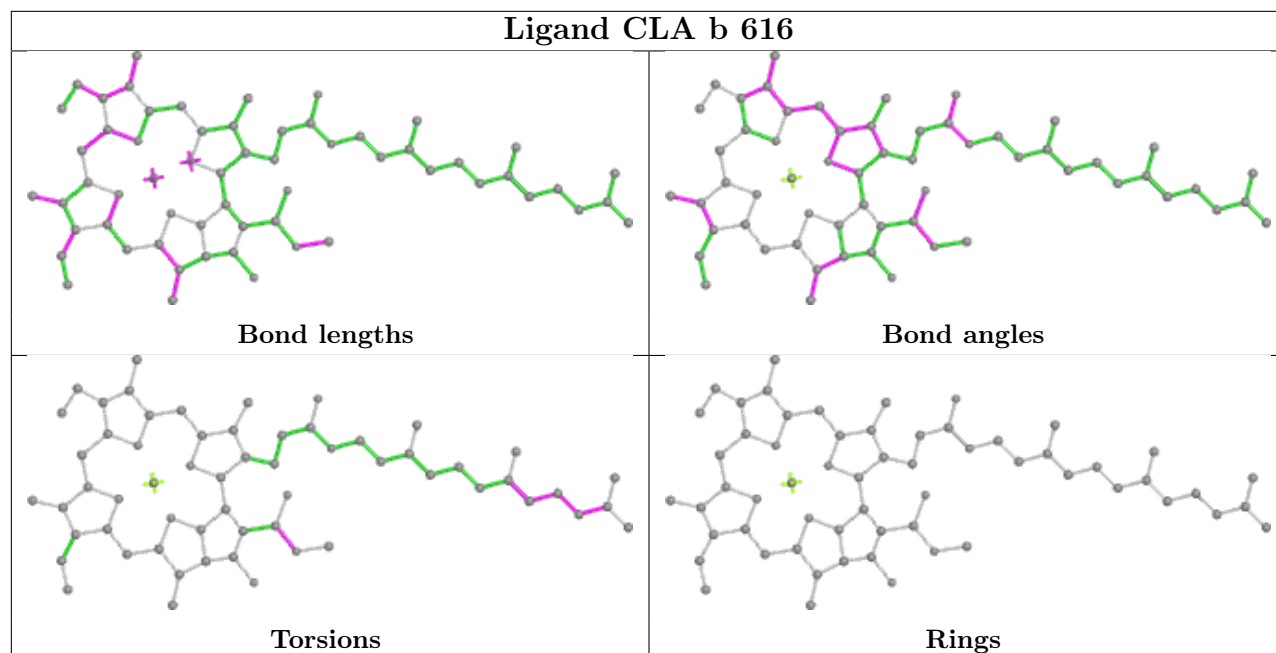
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

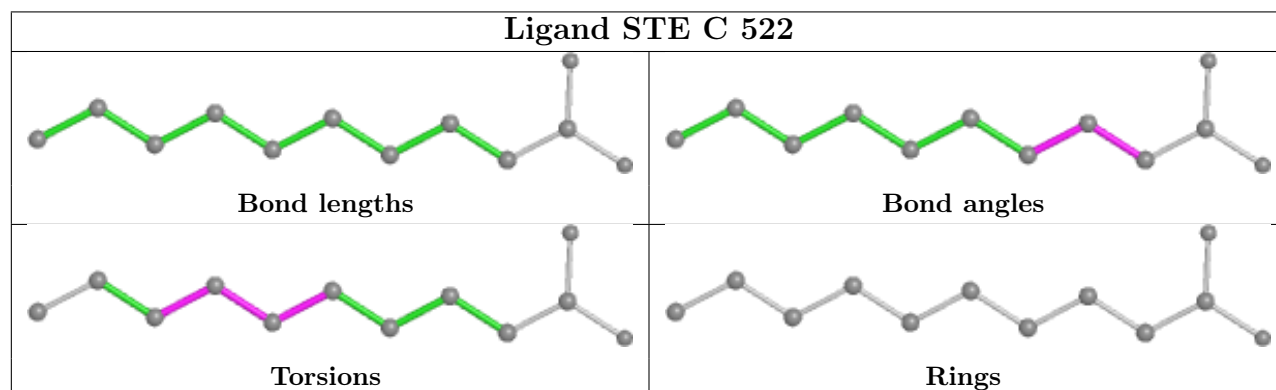
Ligand SQD A 617	
	
Bond lengths	Bond angles
	
Torsions	Rings



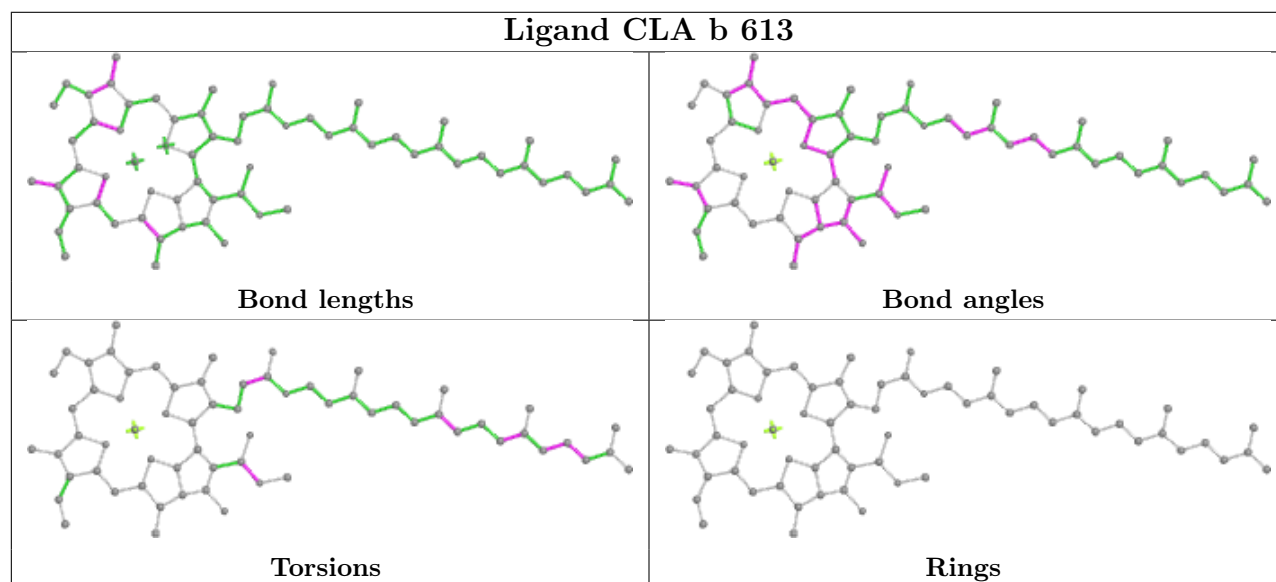
## Ligand CLA b 616

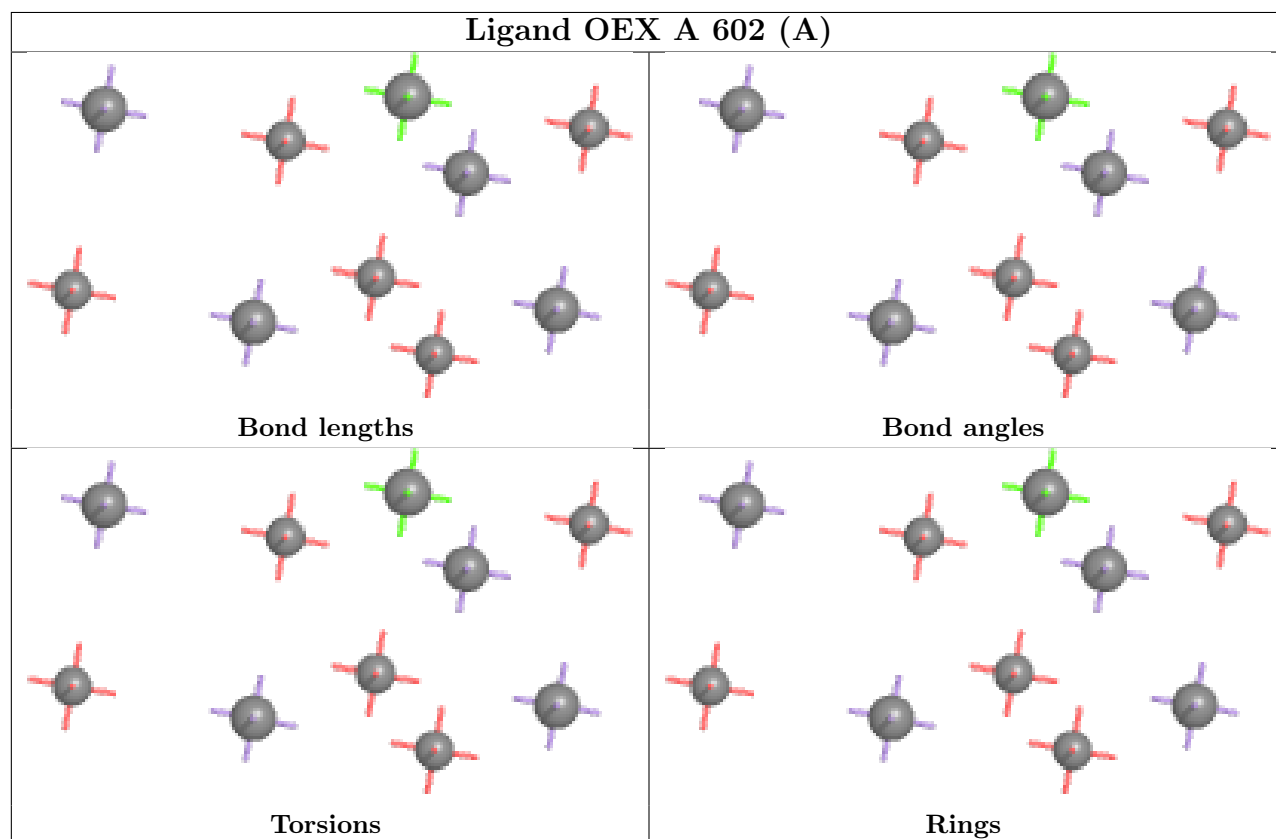
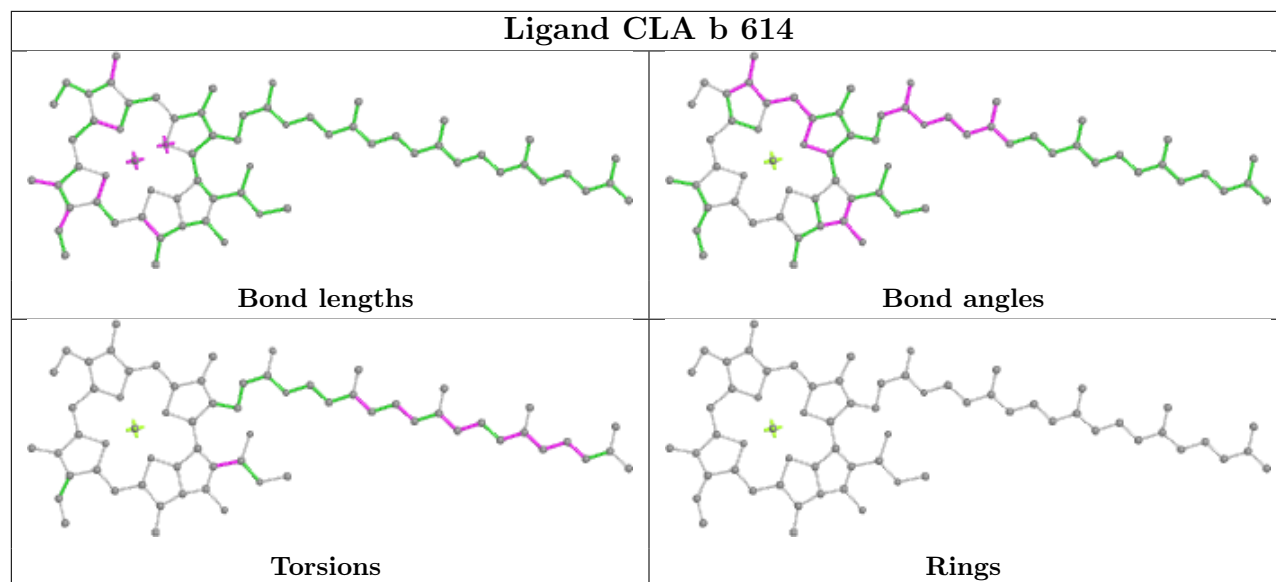


## Ligand STE C 522

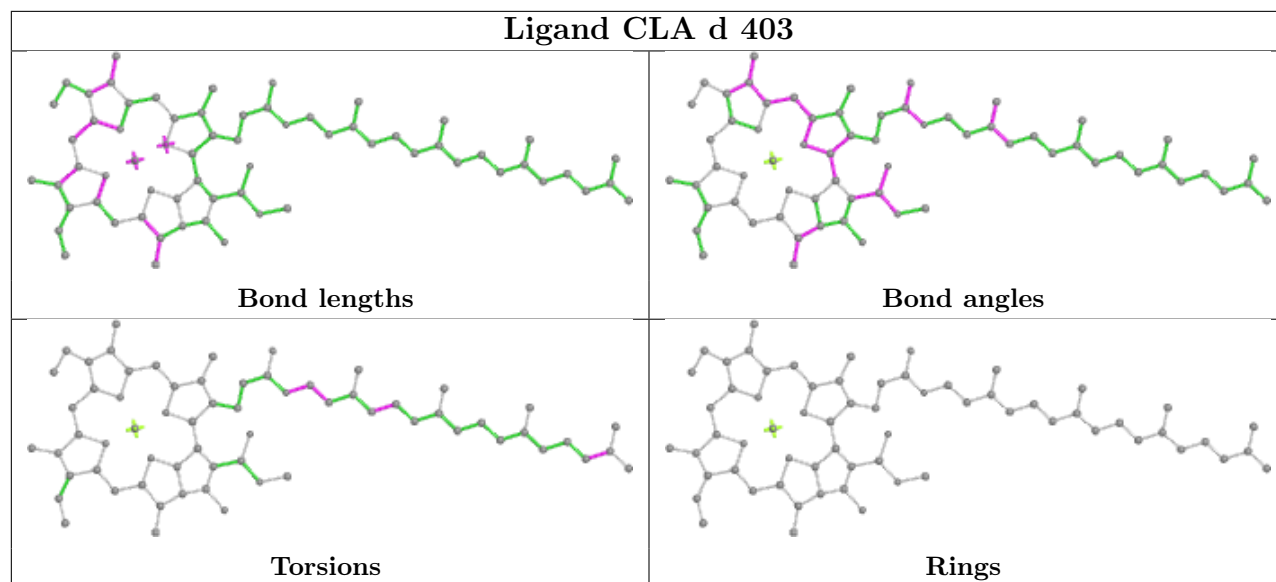


## Ligand CLA b 613

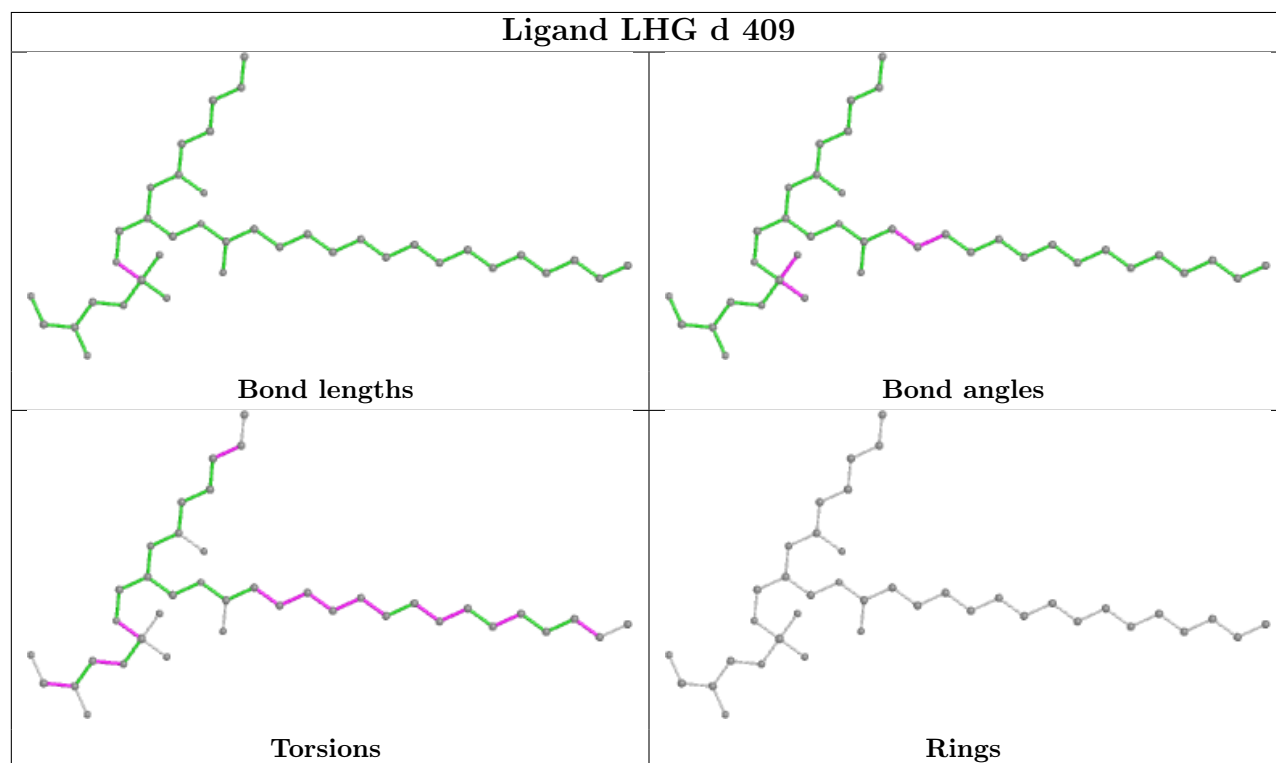


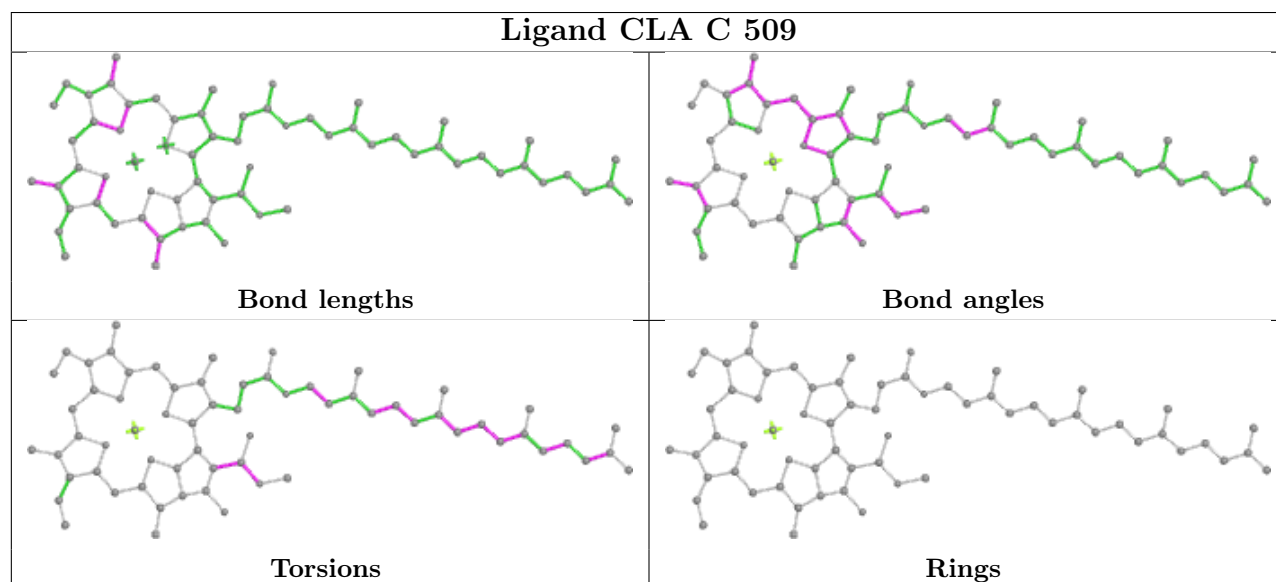
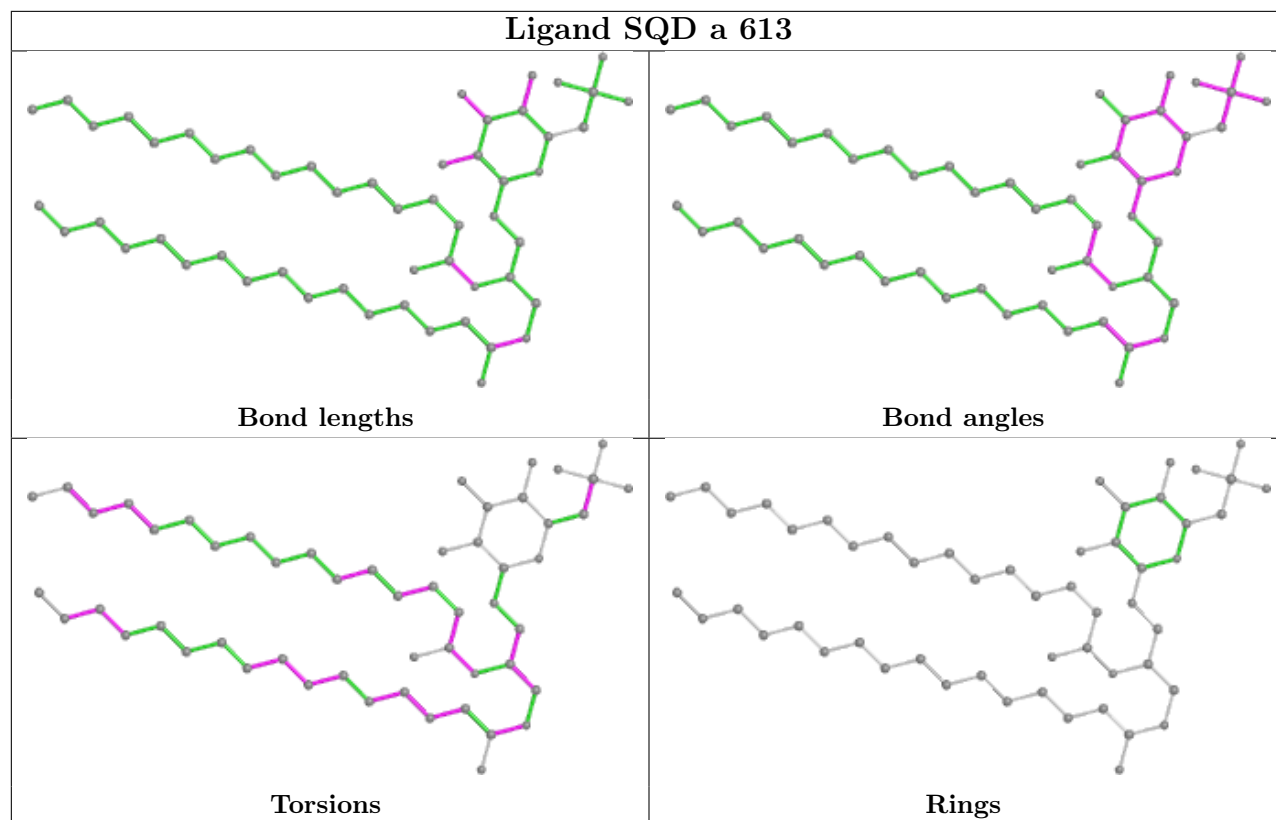


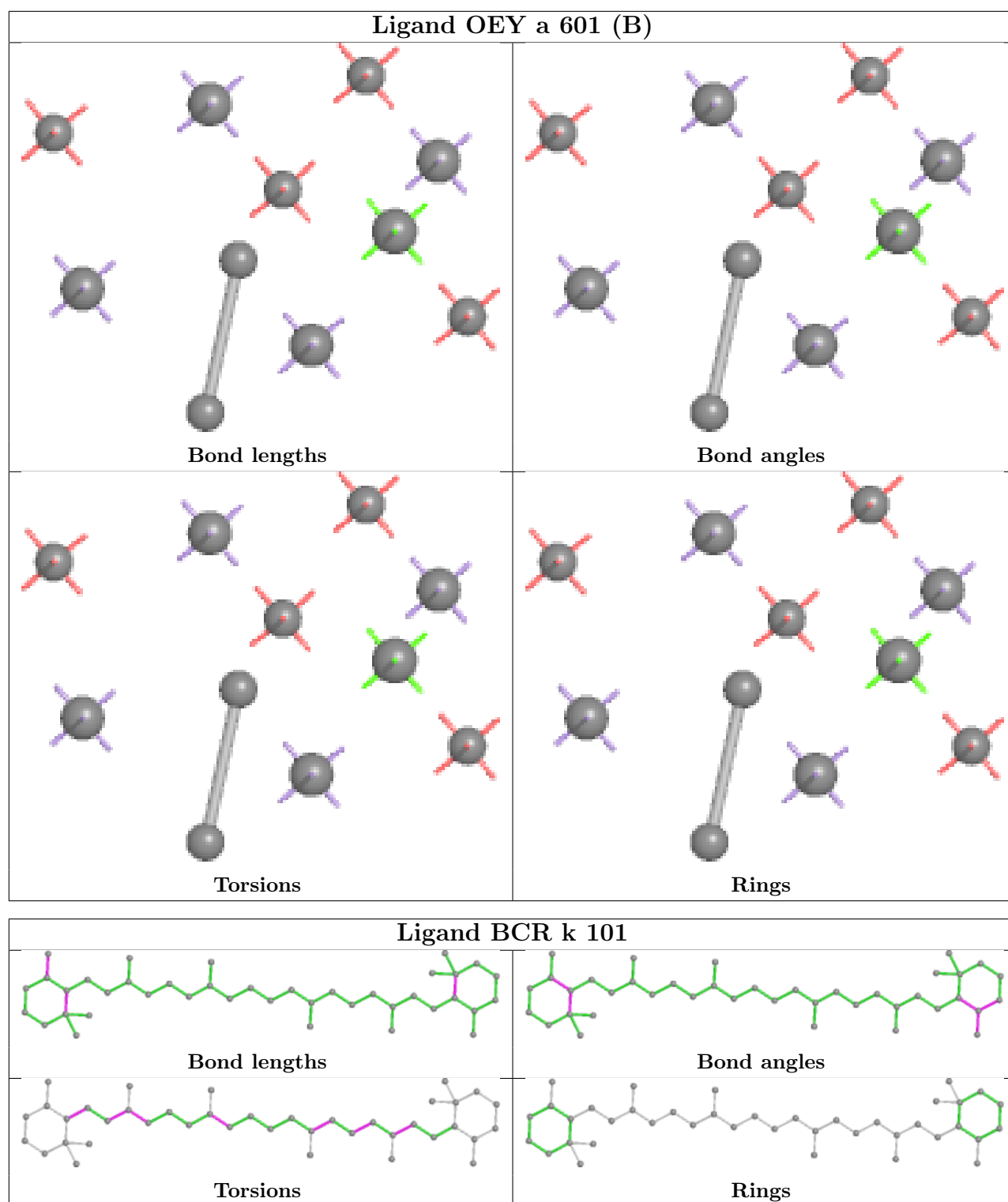
## Ligand CLA d 403

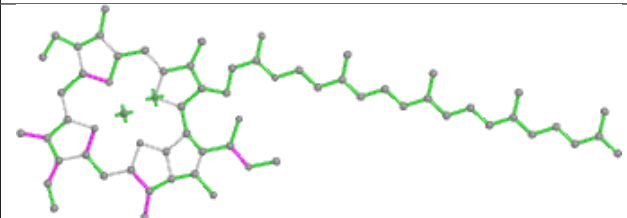
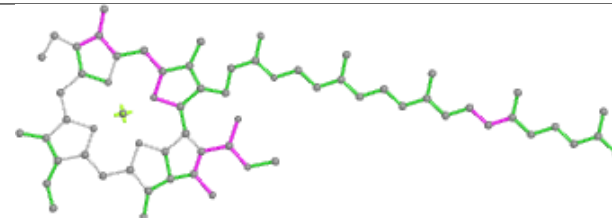
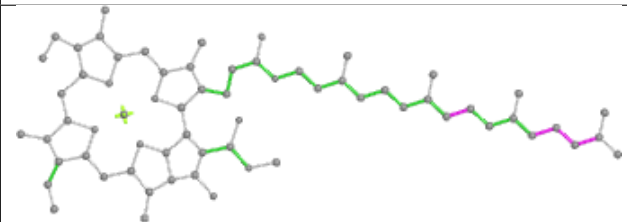
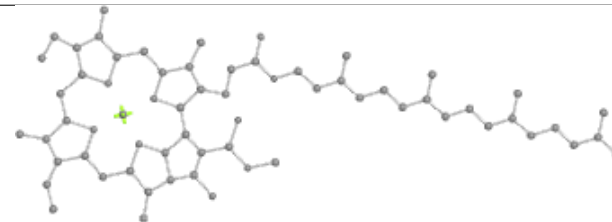


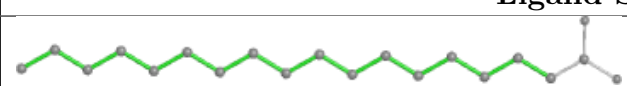
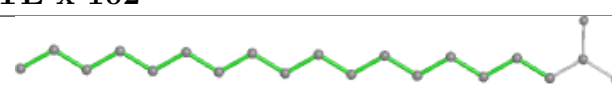
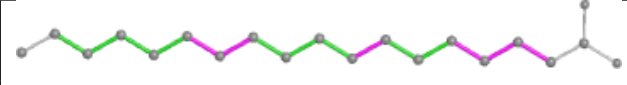
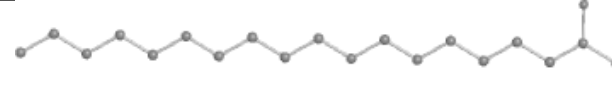
## Ligand LHG d 409

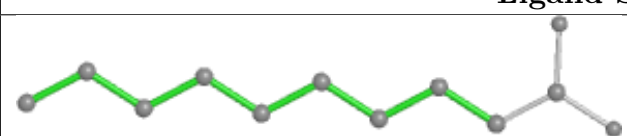
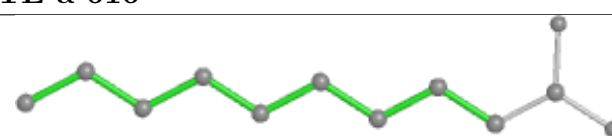
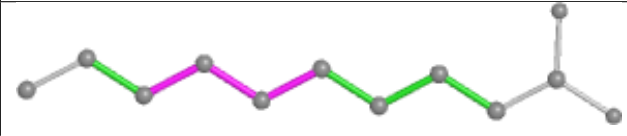
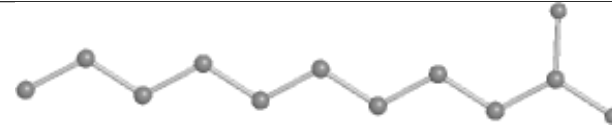


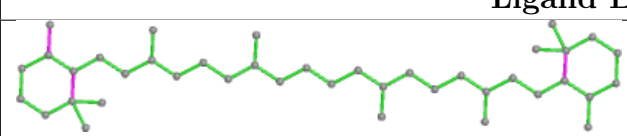
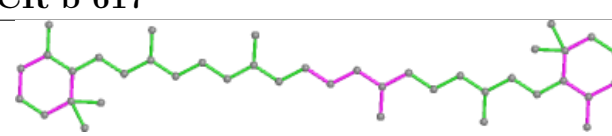
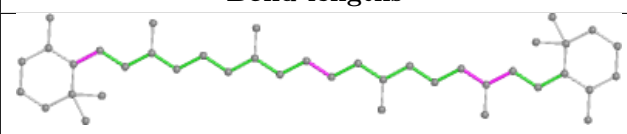
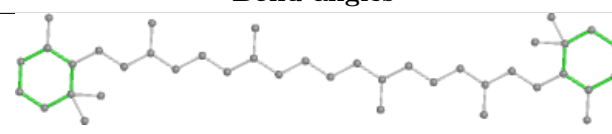




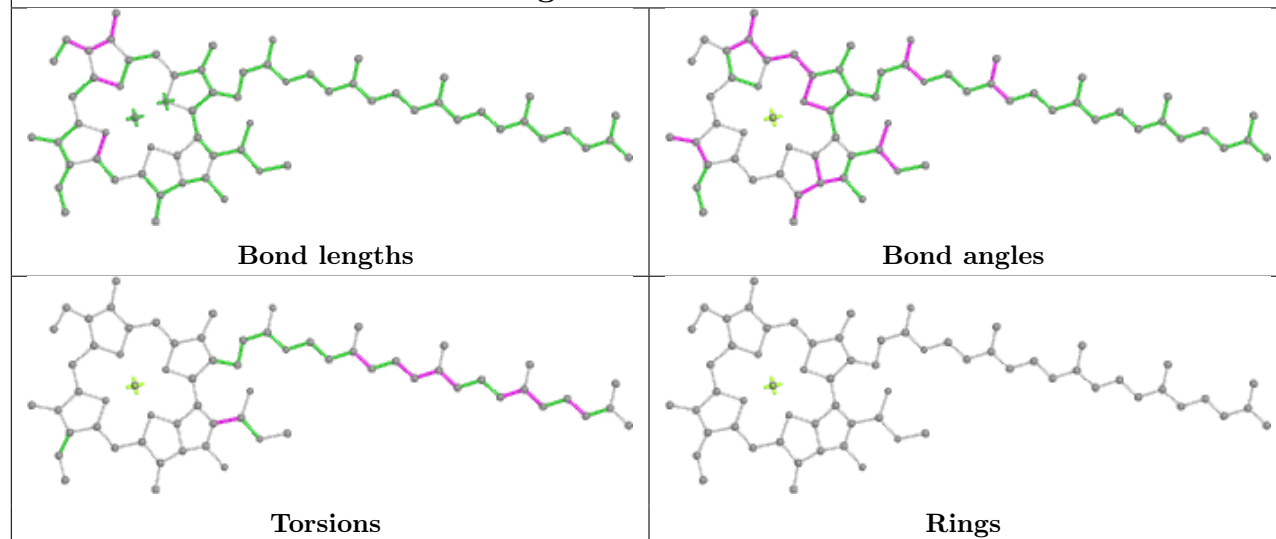
Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE x 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

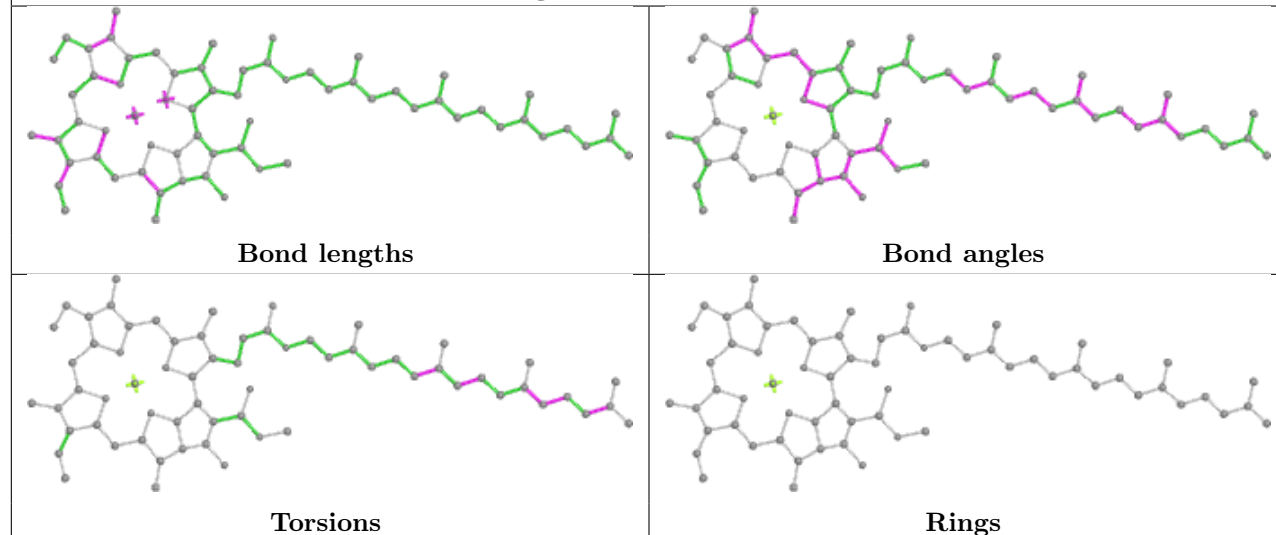
Ligand STE a 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

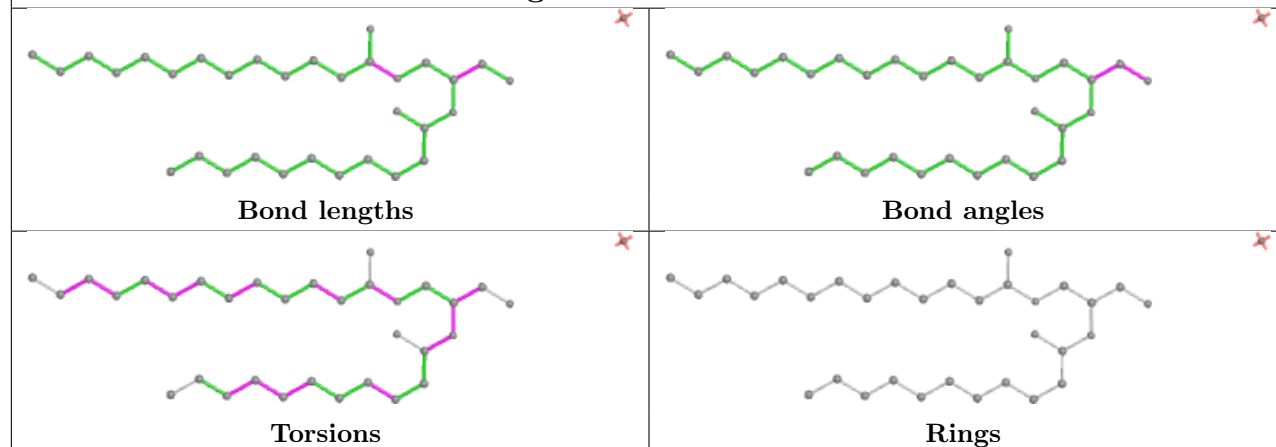
## Ligand CLA c 507

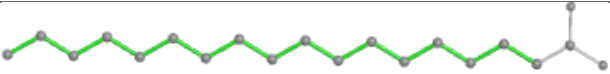
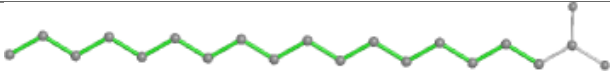


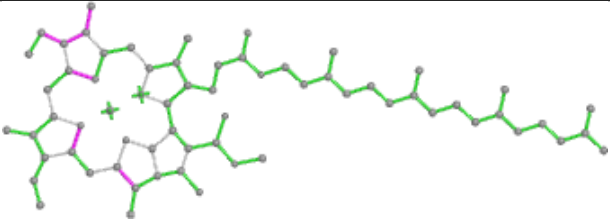
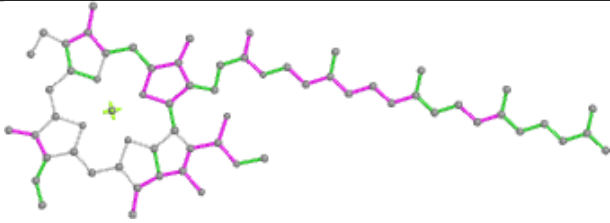
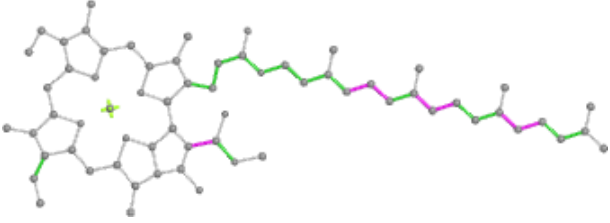
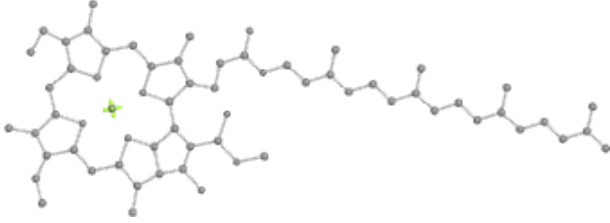
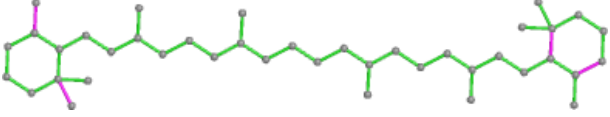
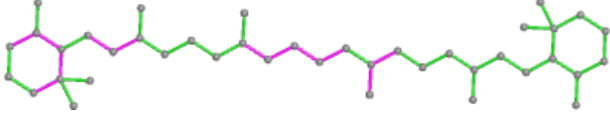
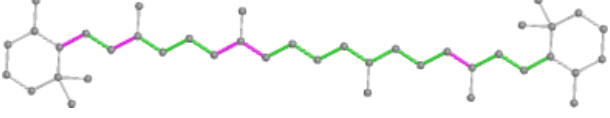
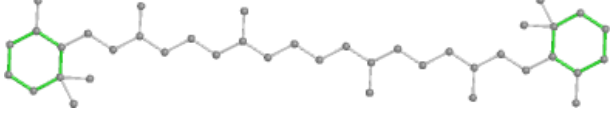


## Ligand CLA B 611



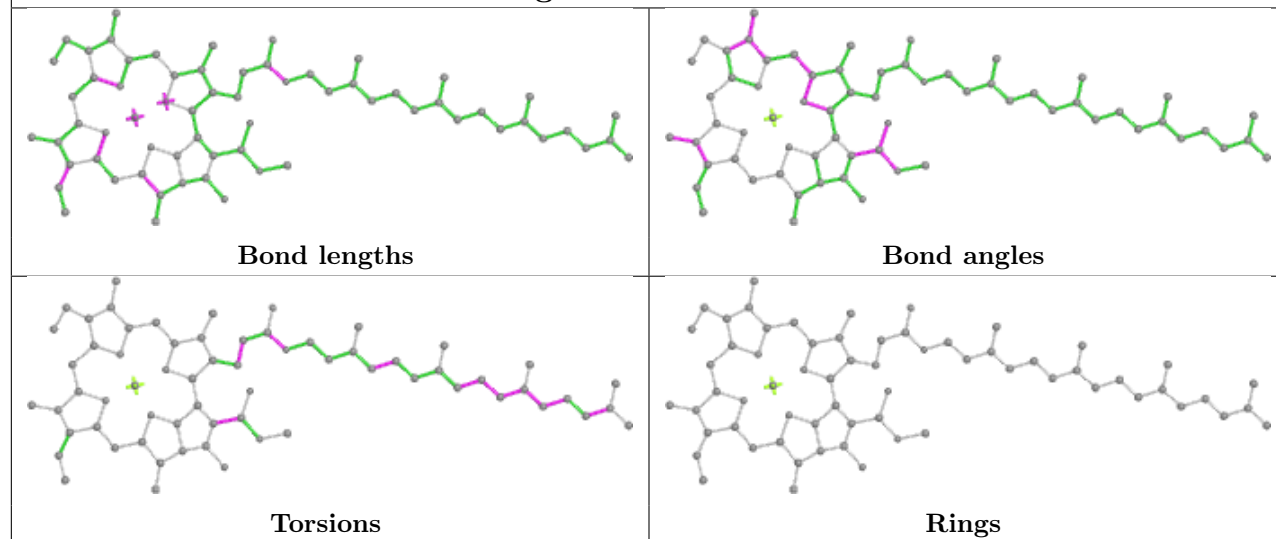
## Ligand LMG D 409



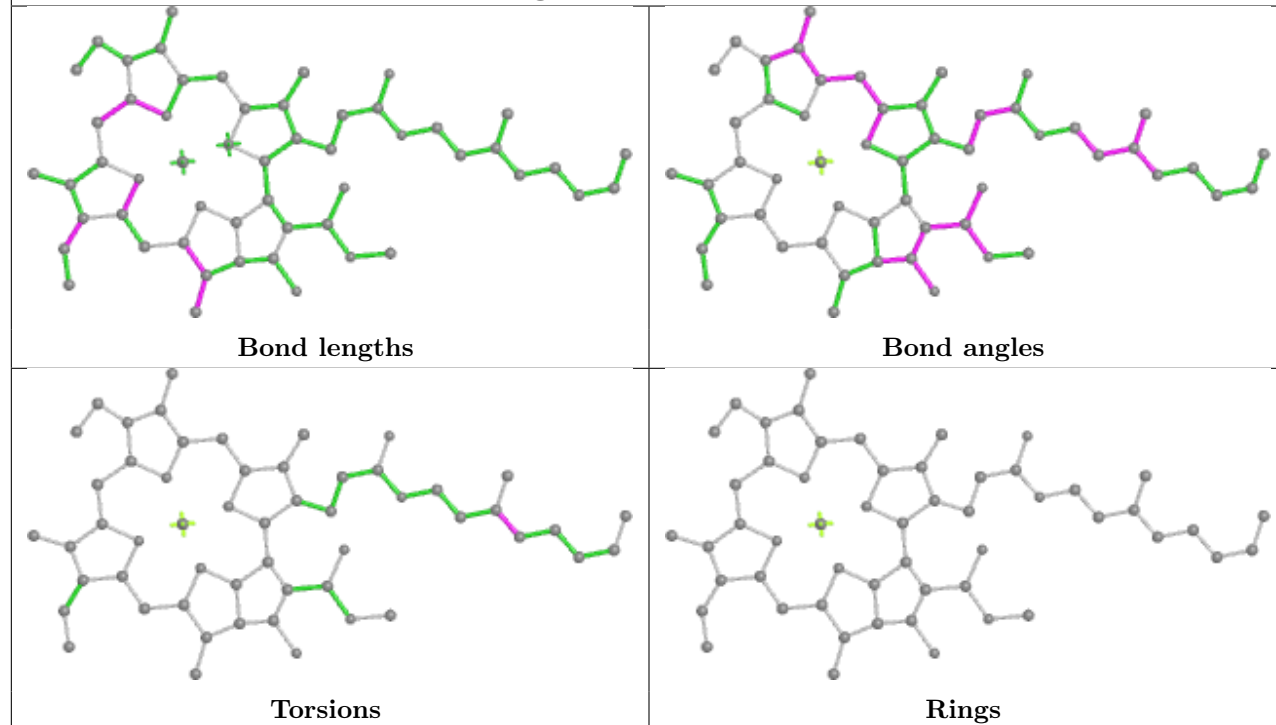
Ligand STE d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



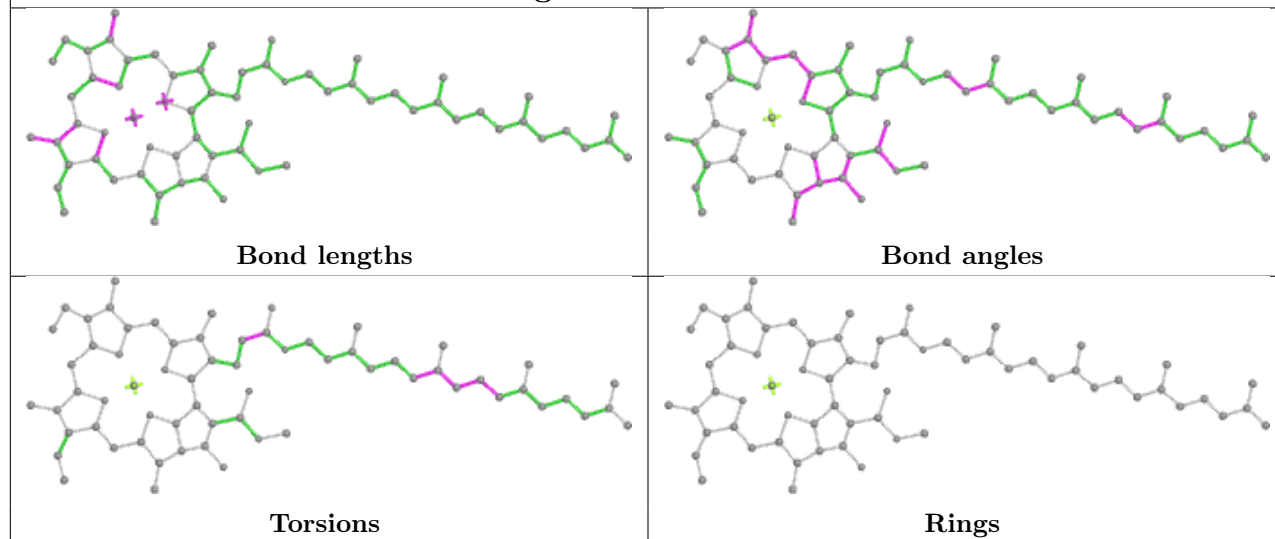
## Ligand CLA b 601



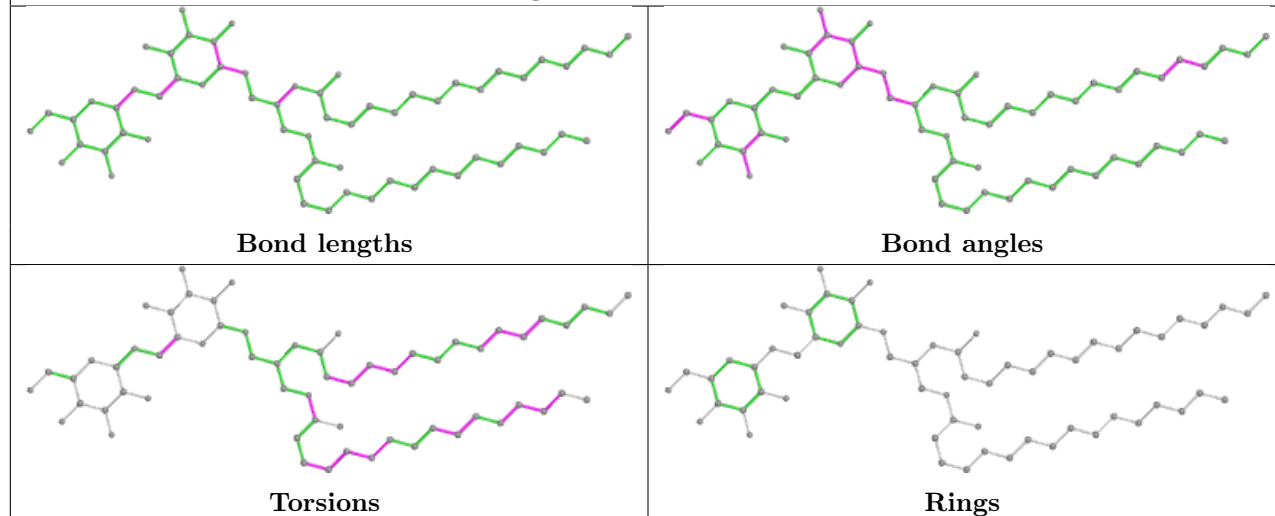
## Ligand CLA A 608



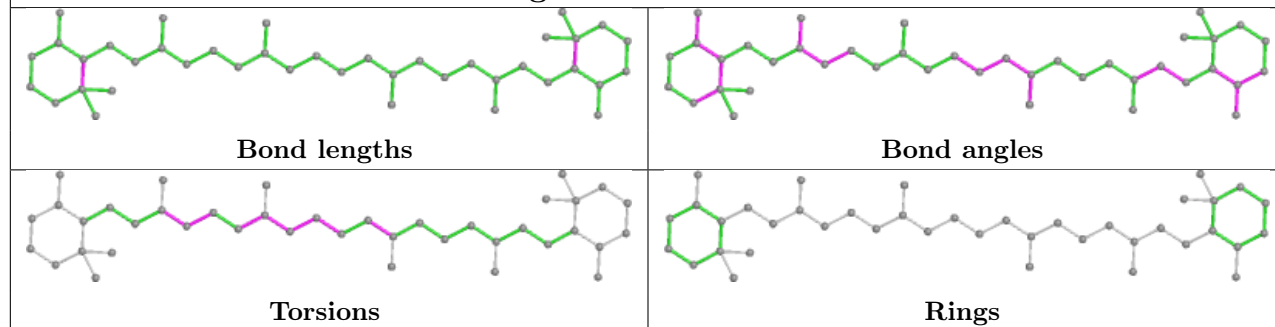
## Ligand CLA b 612

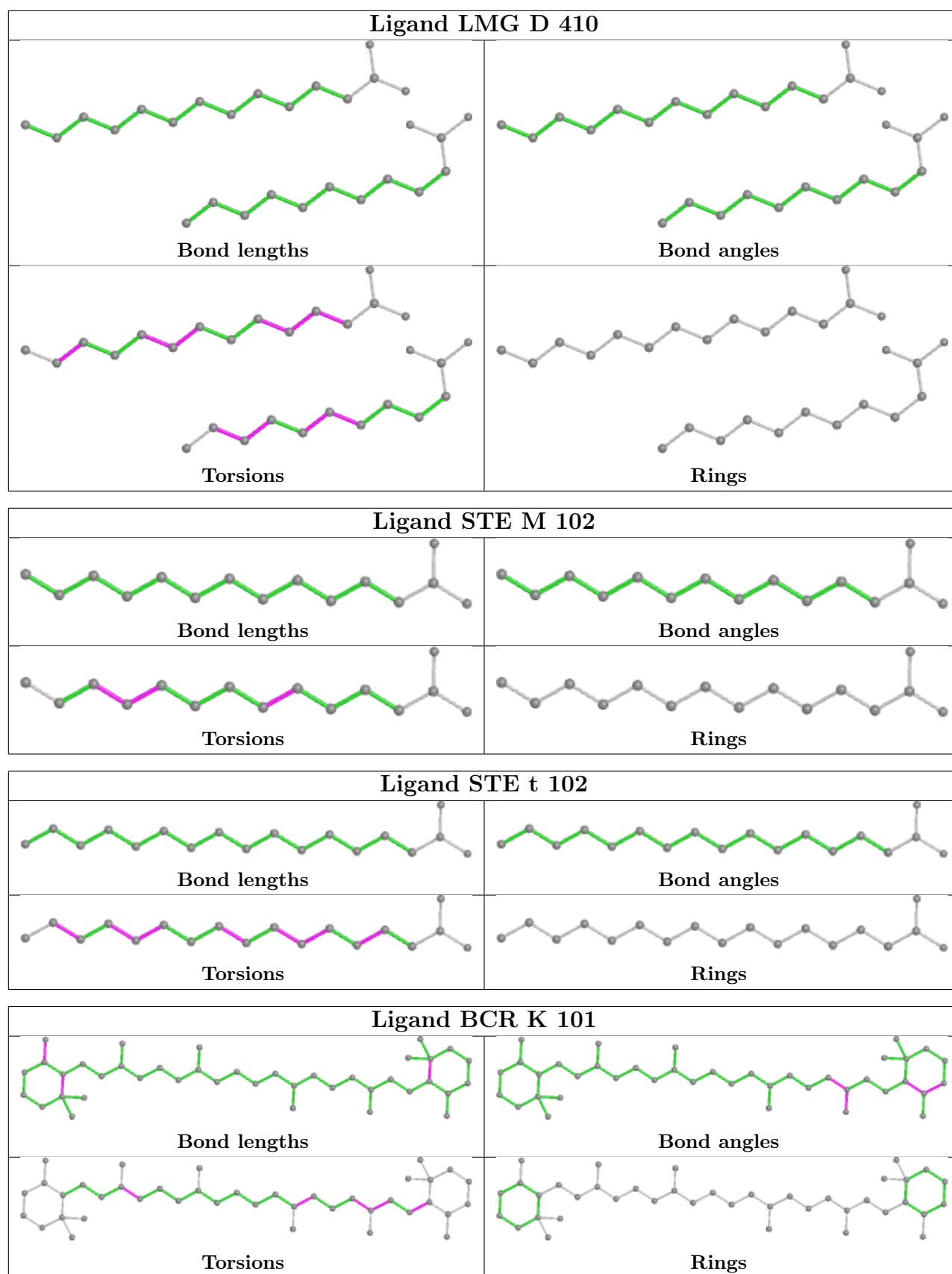


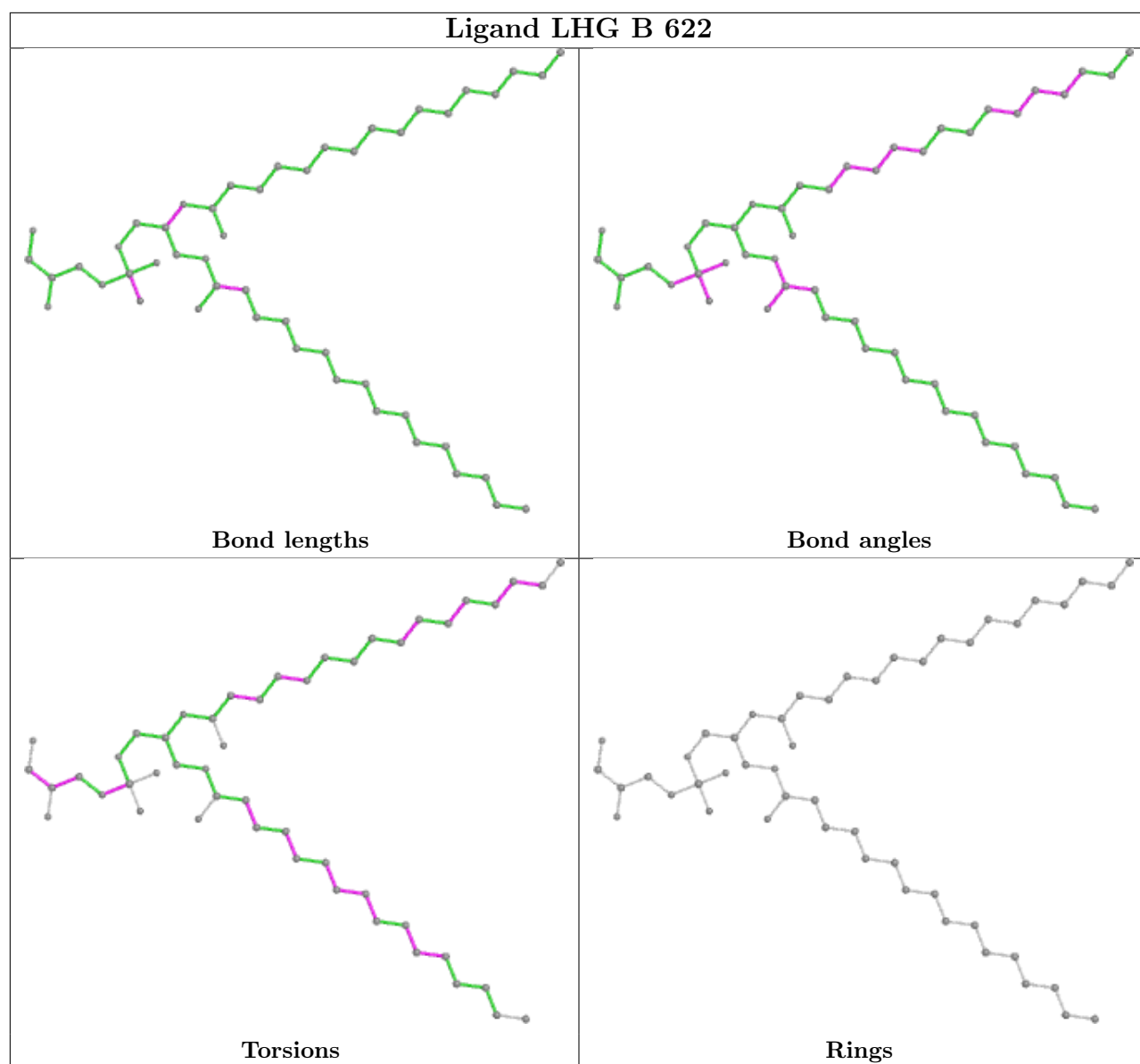
## Ligand DGD C 518

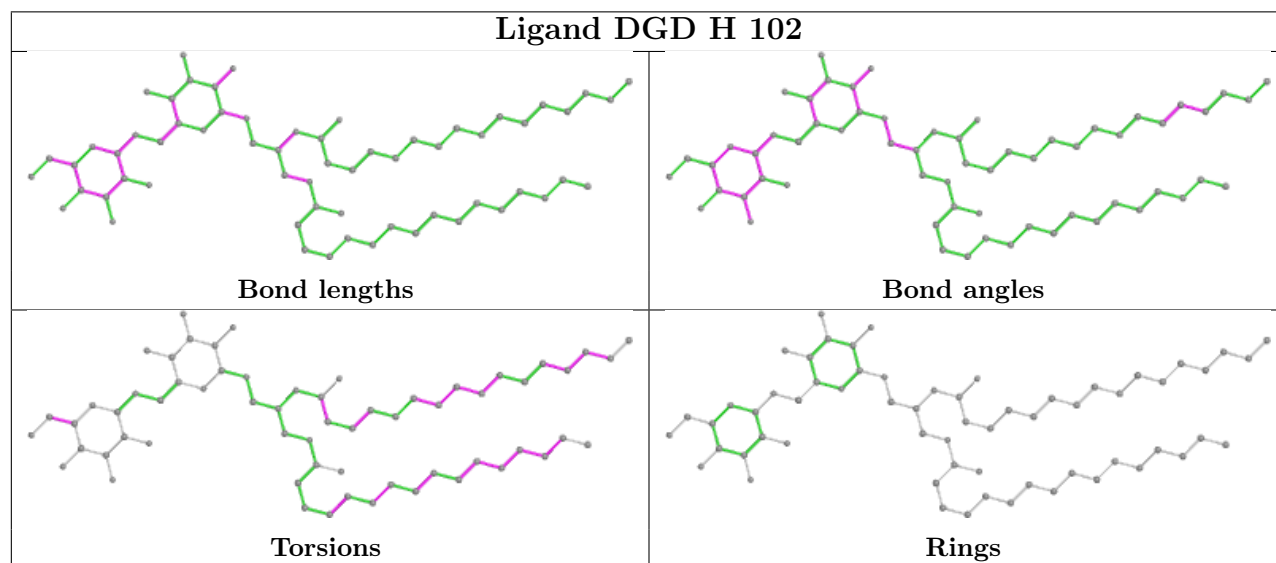
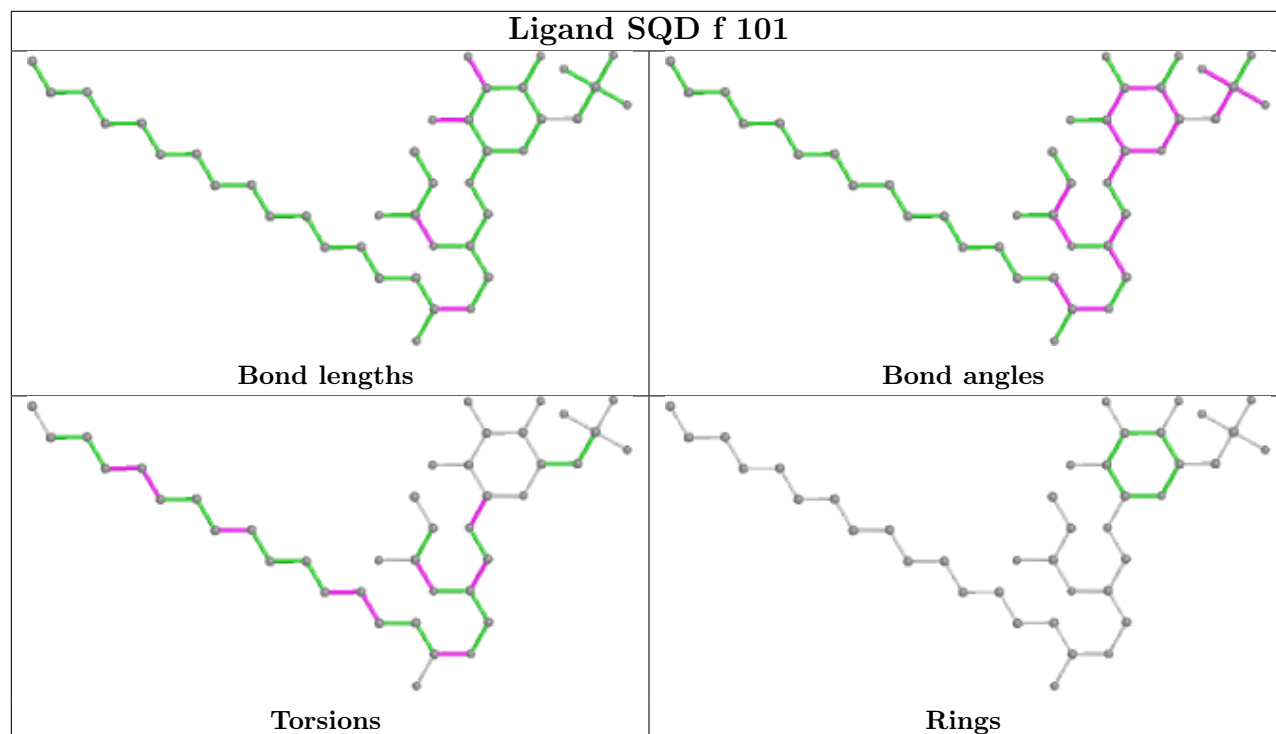


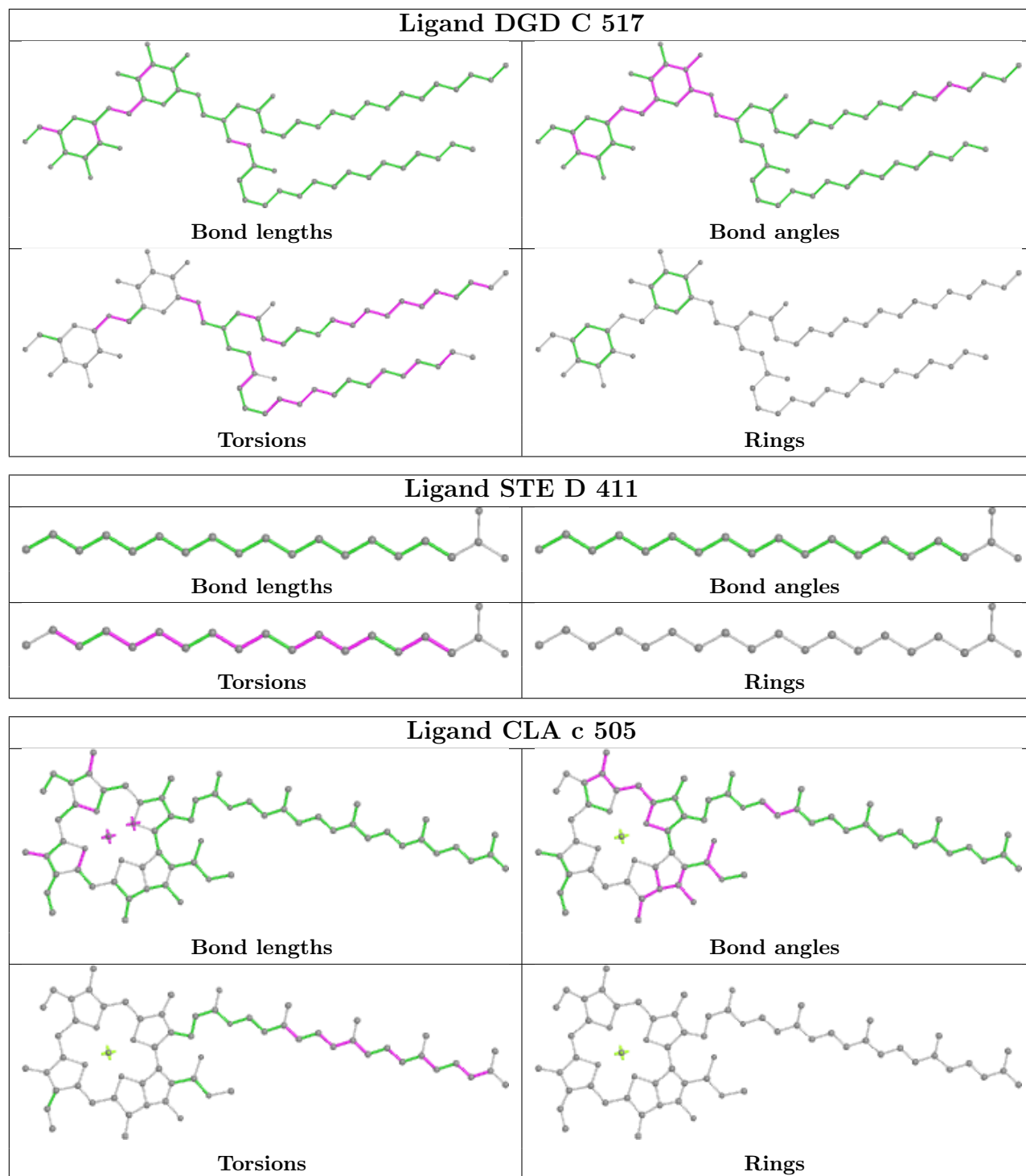
## Ligand BCR C 514



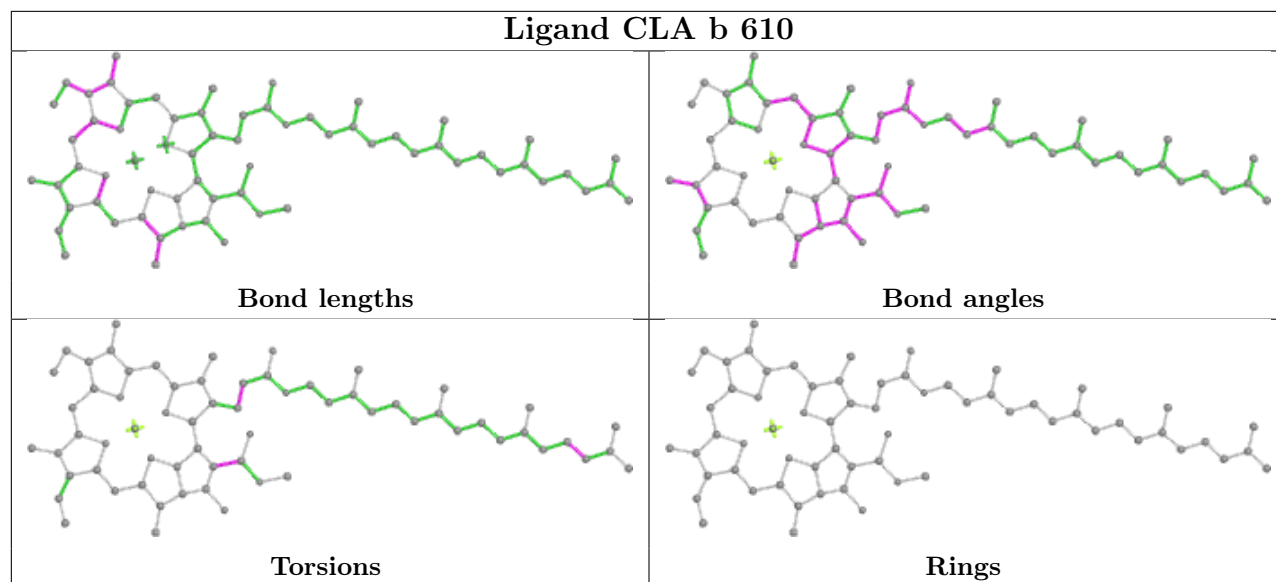




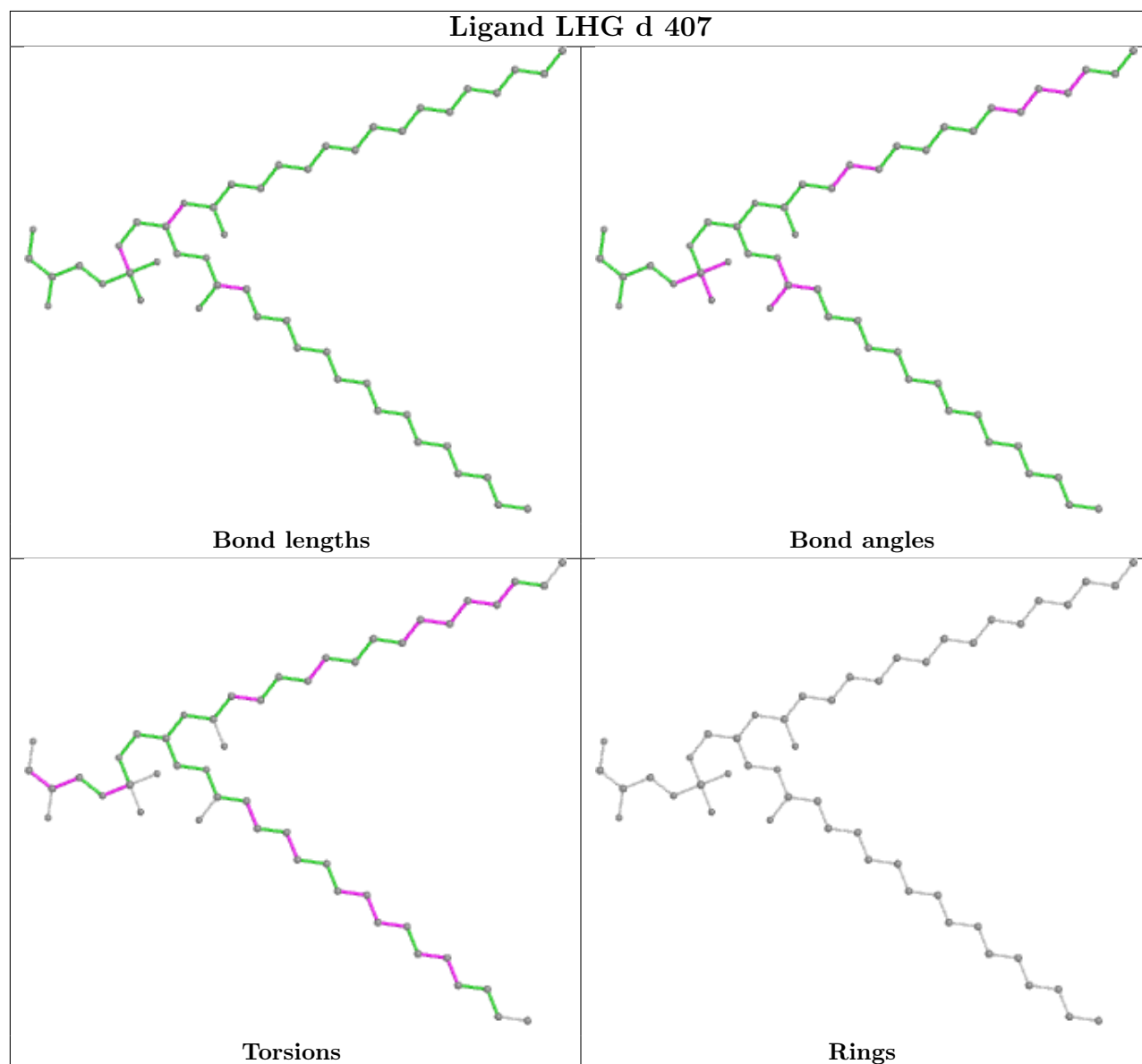




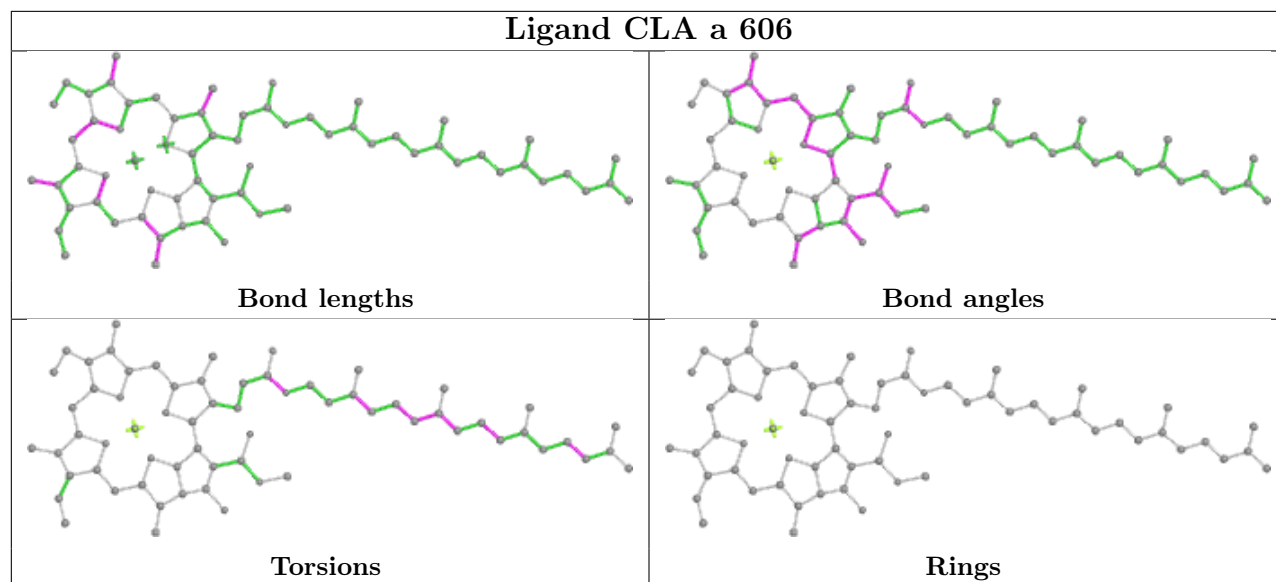
## Ligand CLA b 610



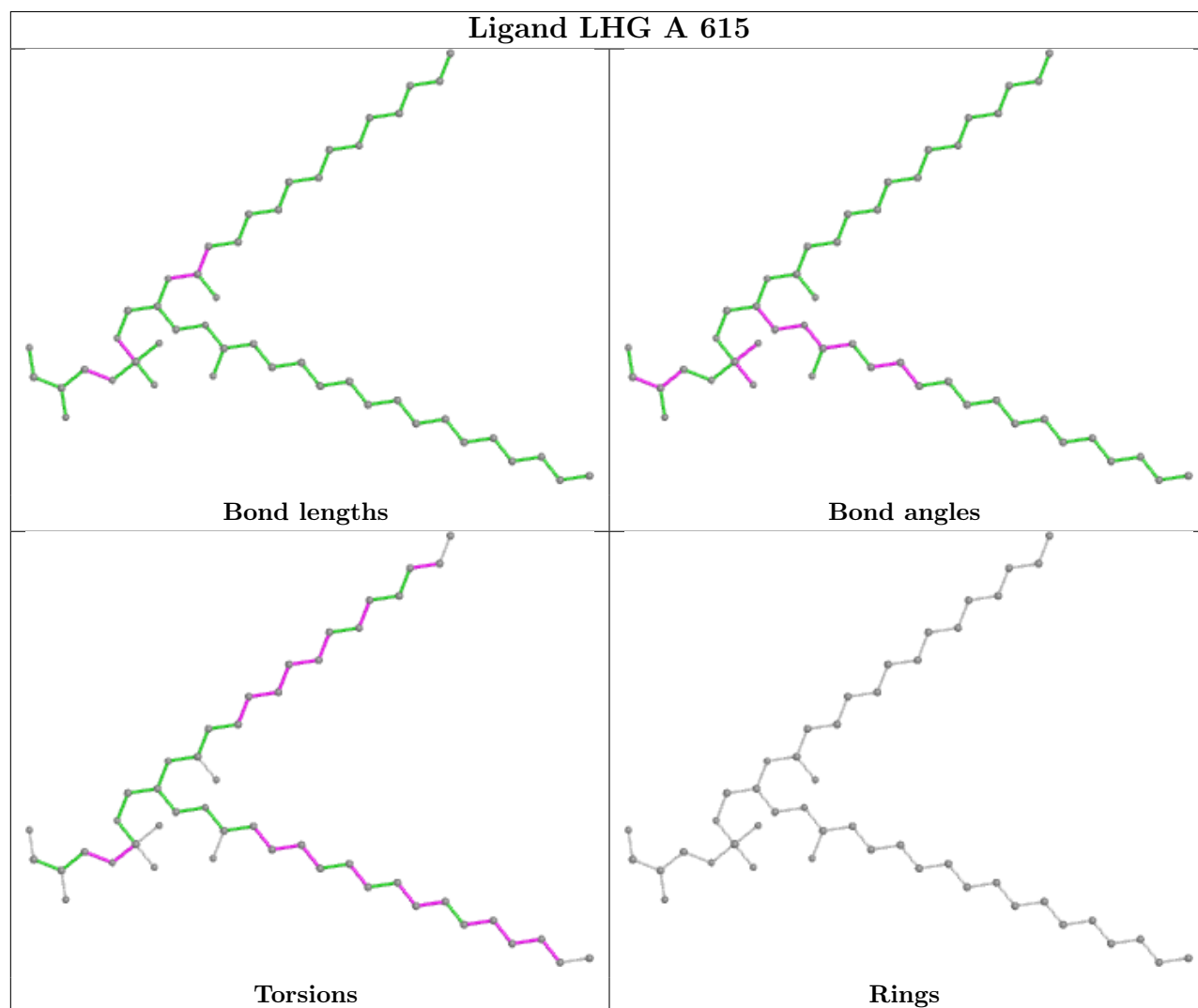
## Ligand LHG d 407



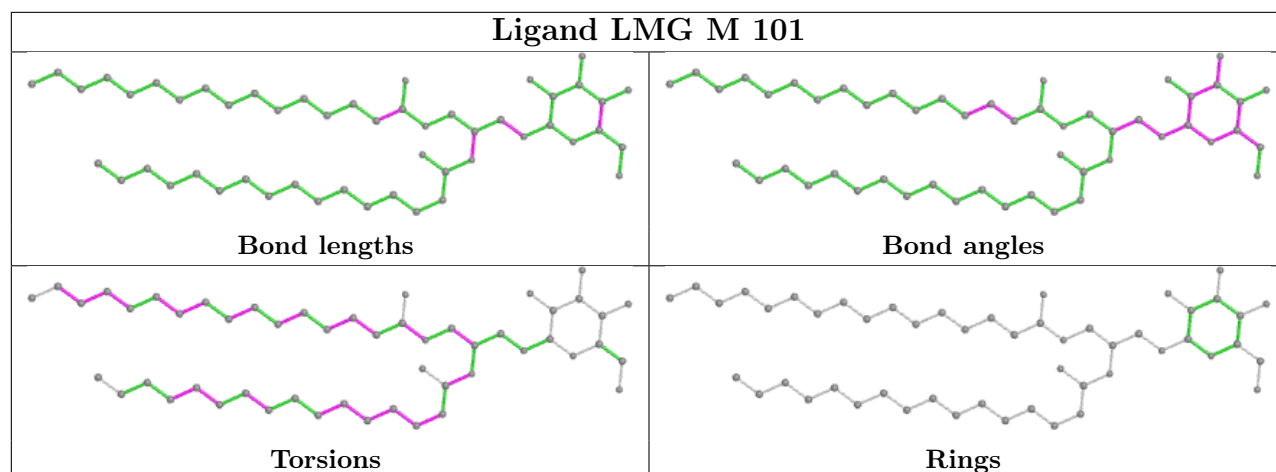
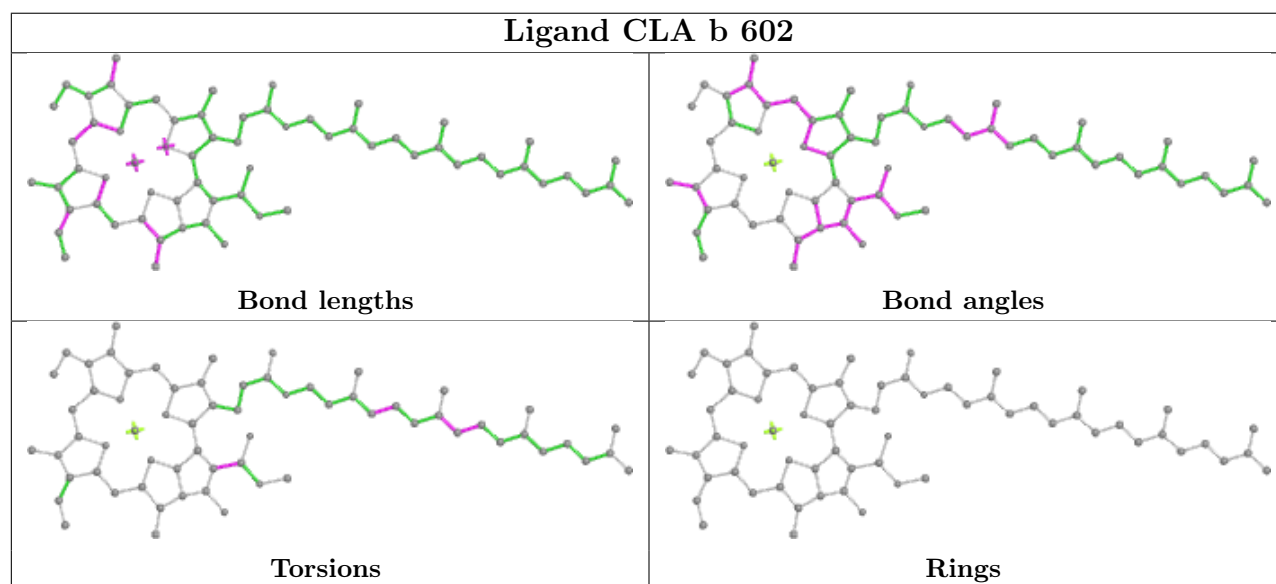
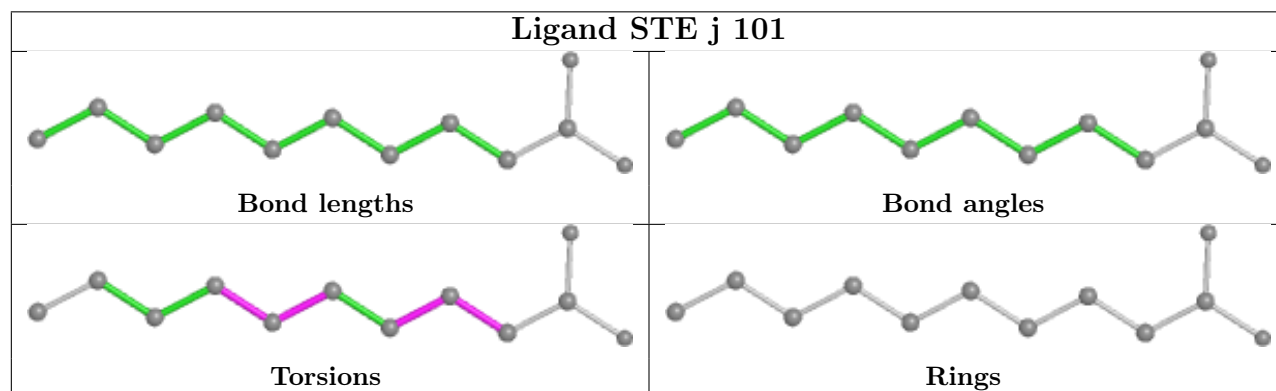
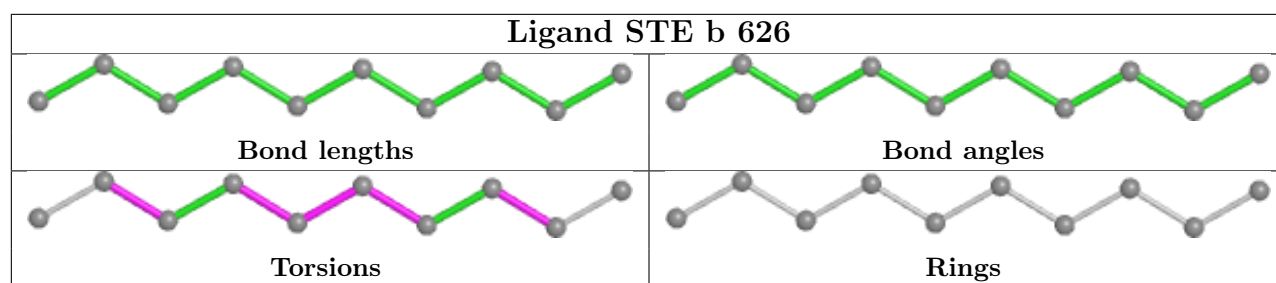
## Ligand CLA a 606

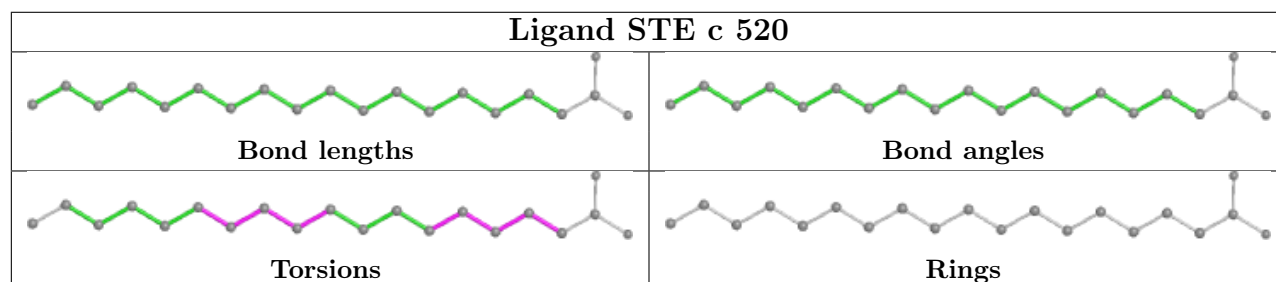
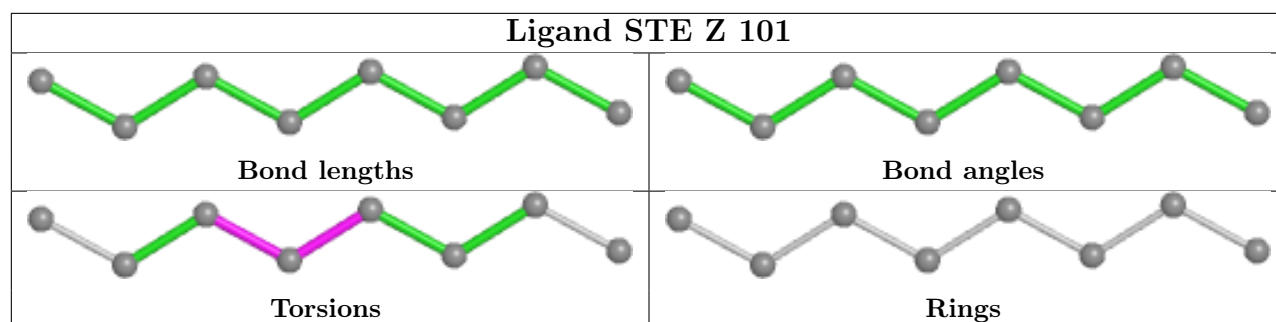
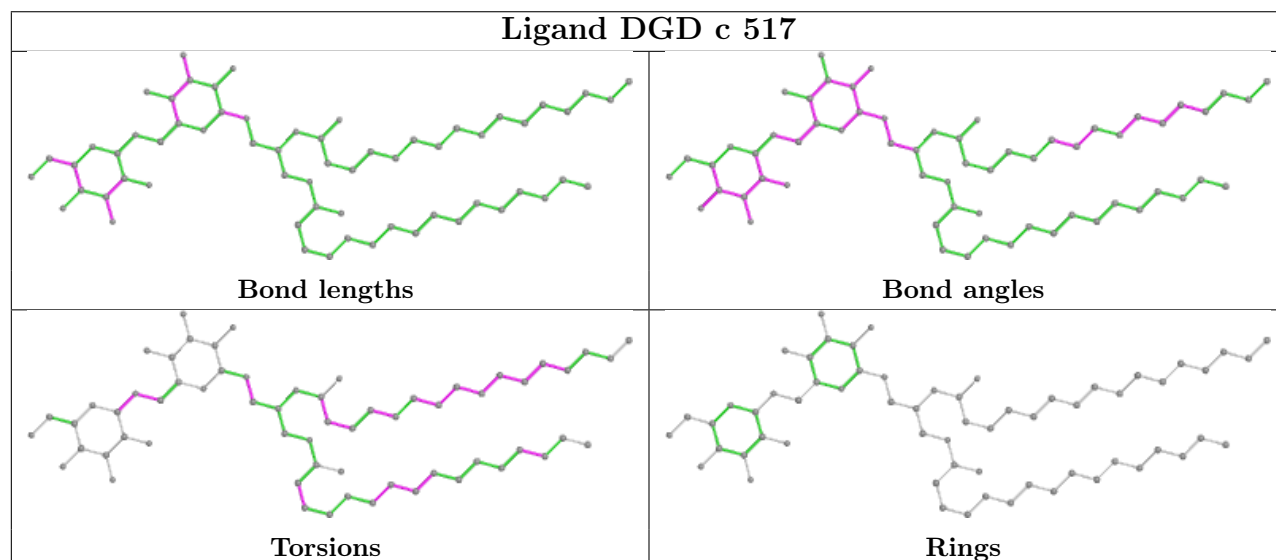
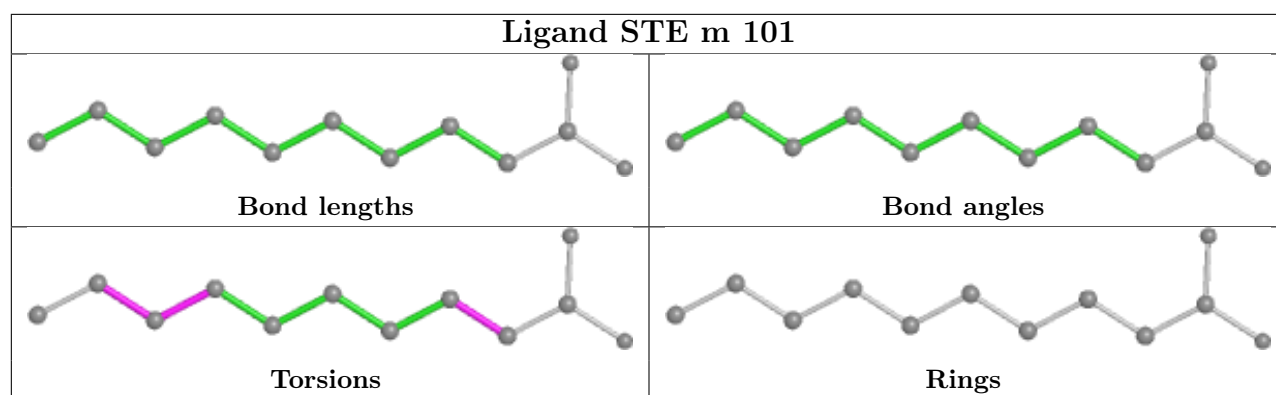


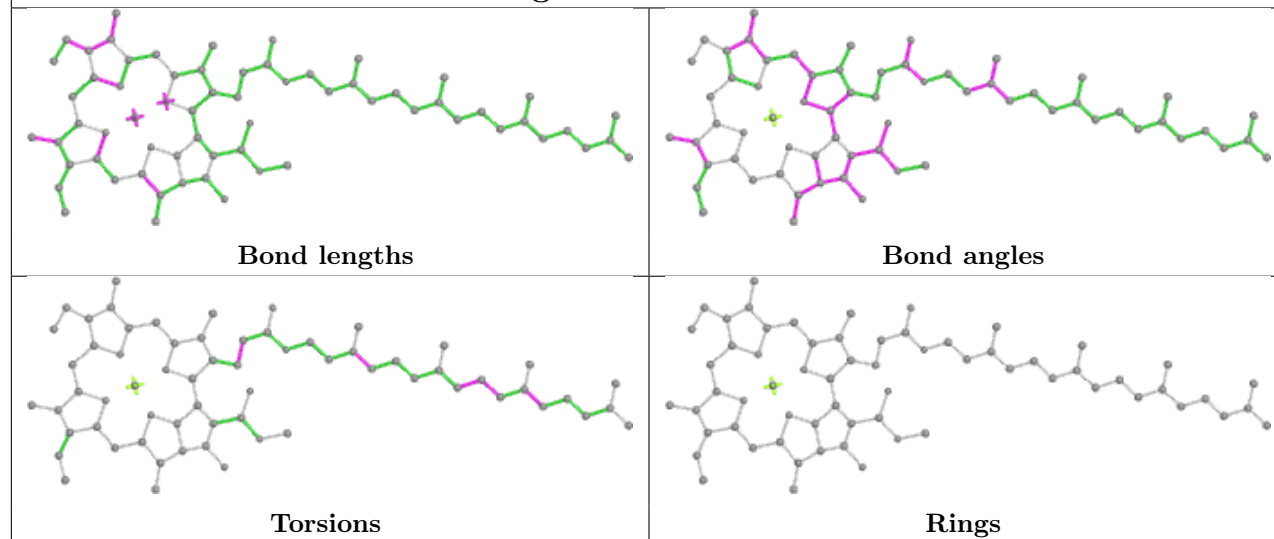
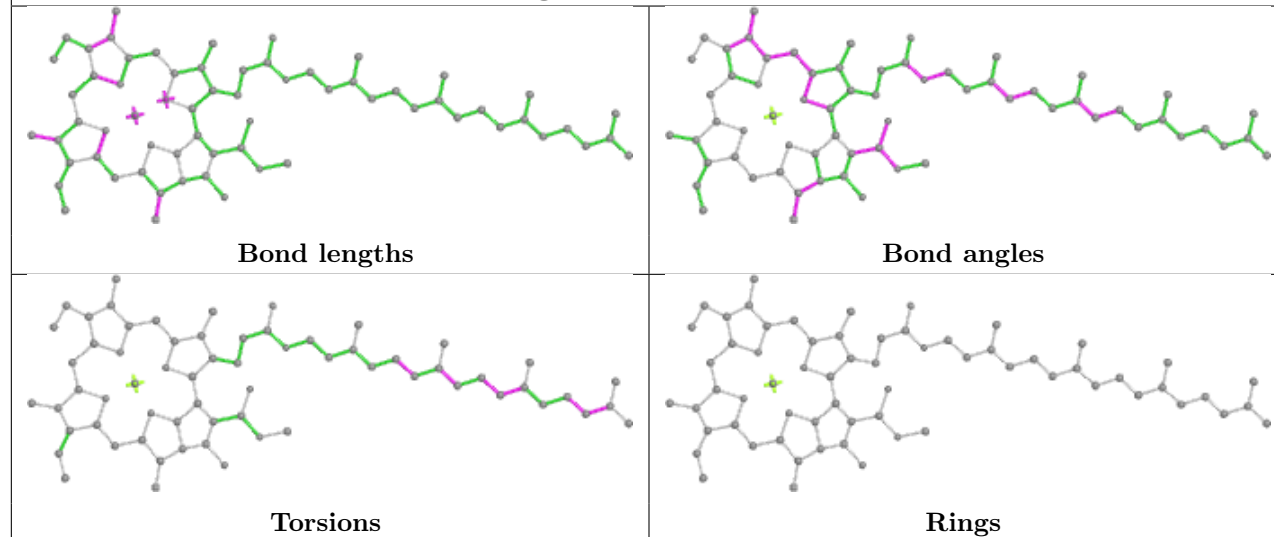
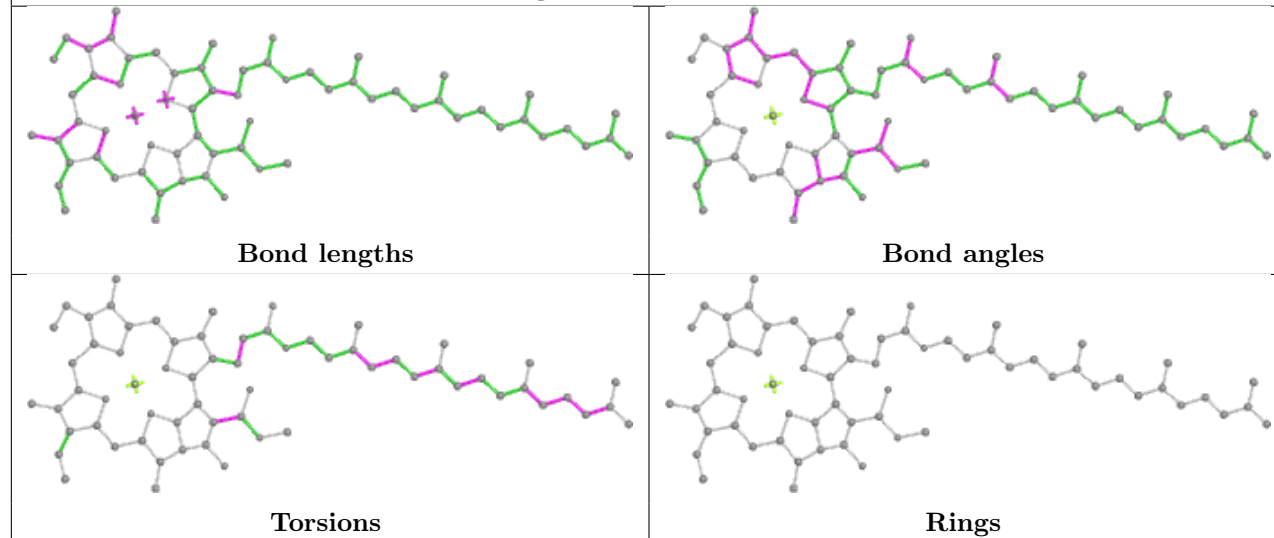
## Ligand LHG A 615

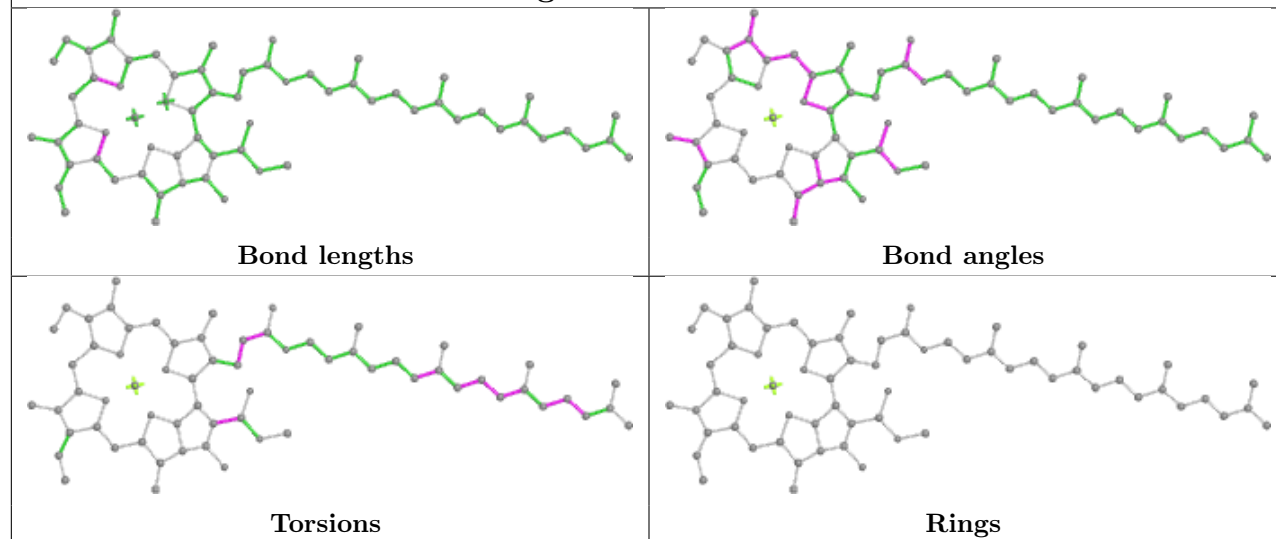
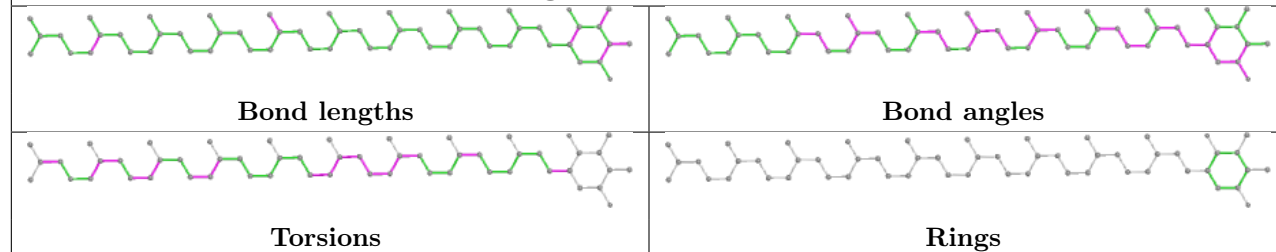
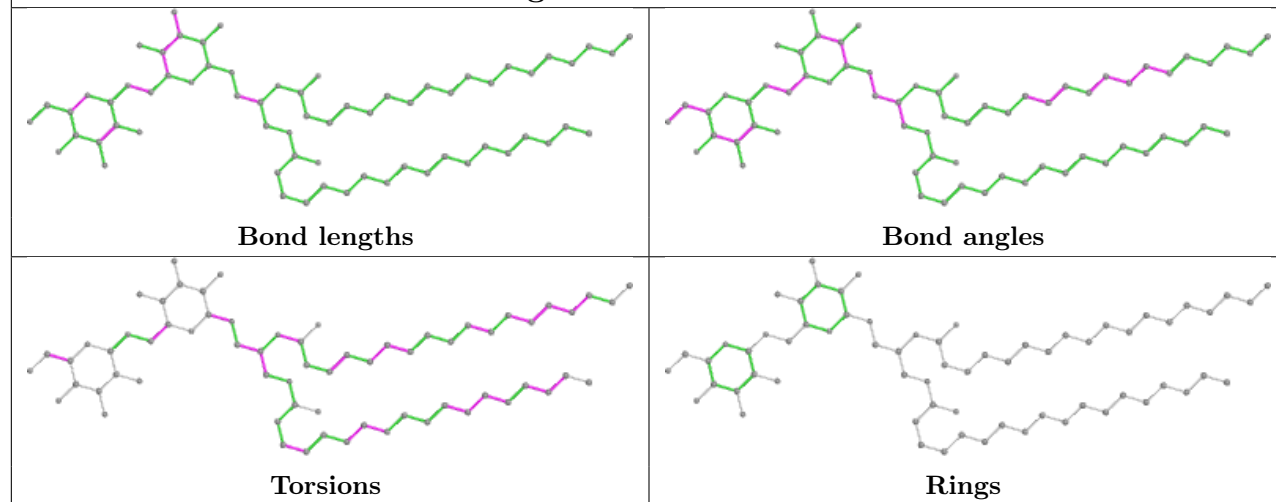


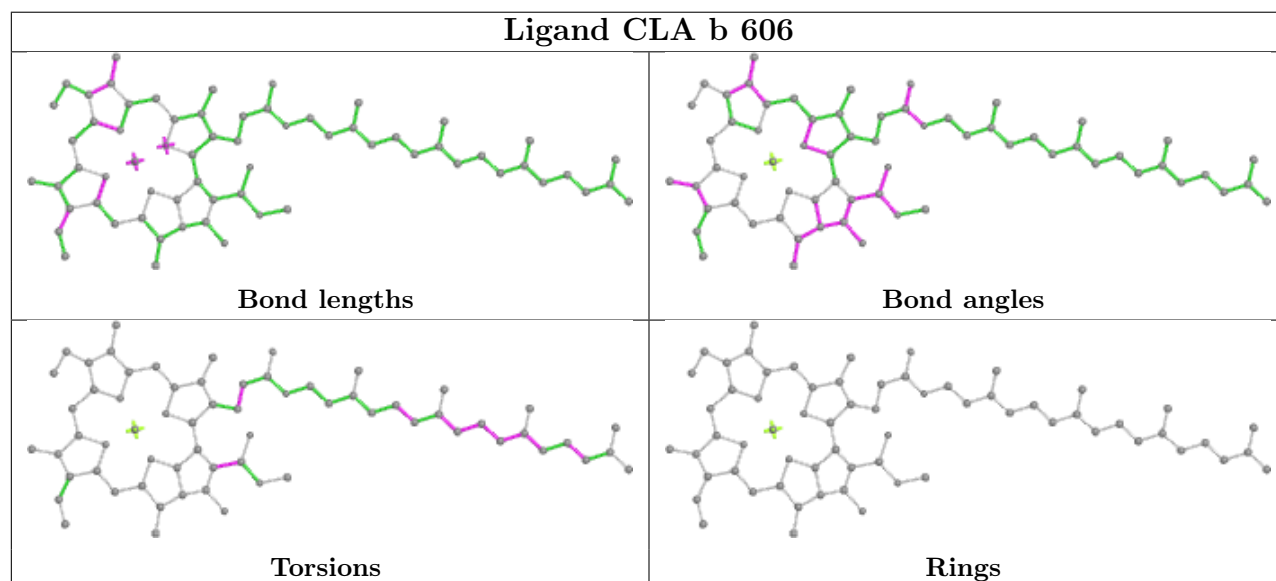
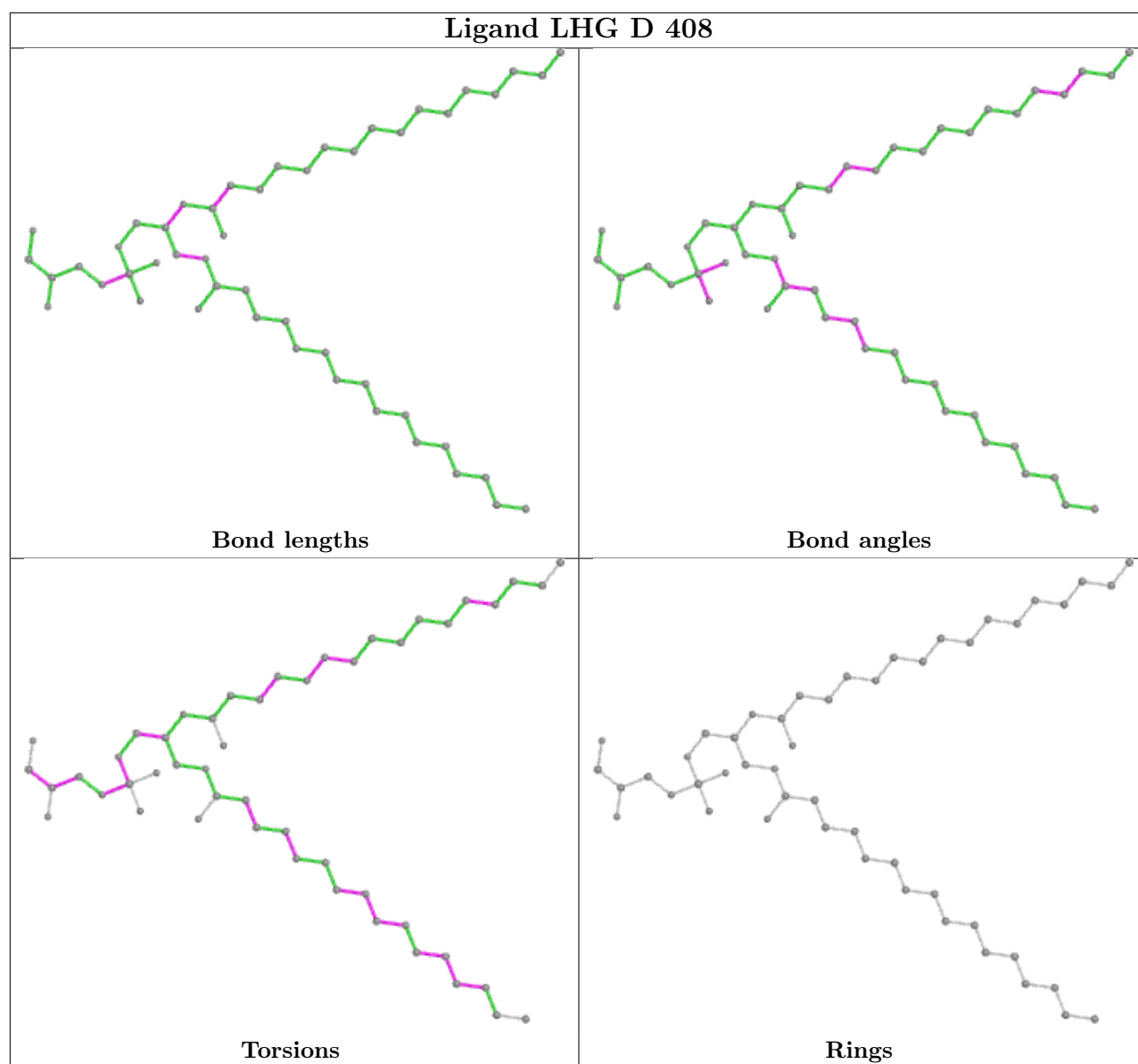


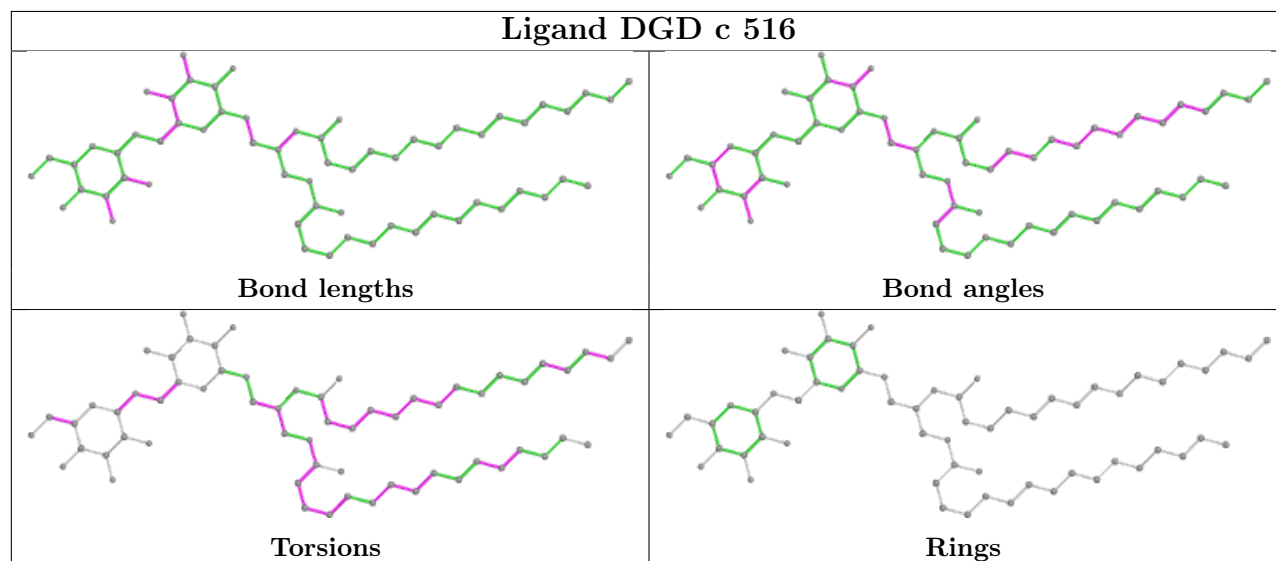
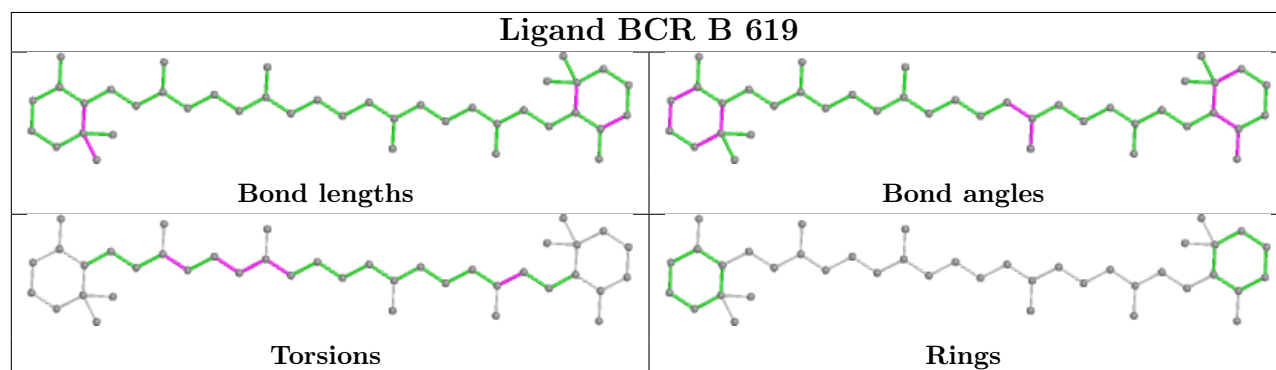
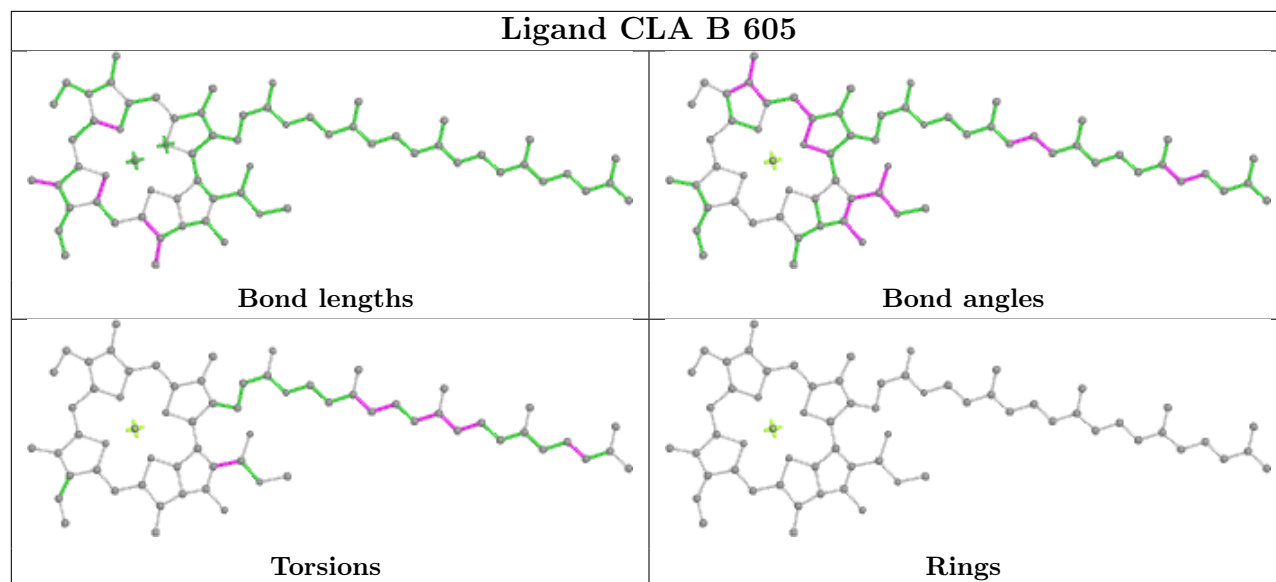




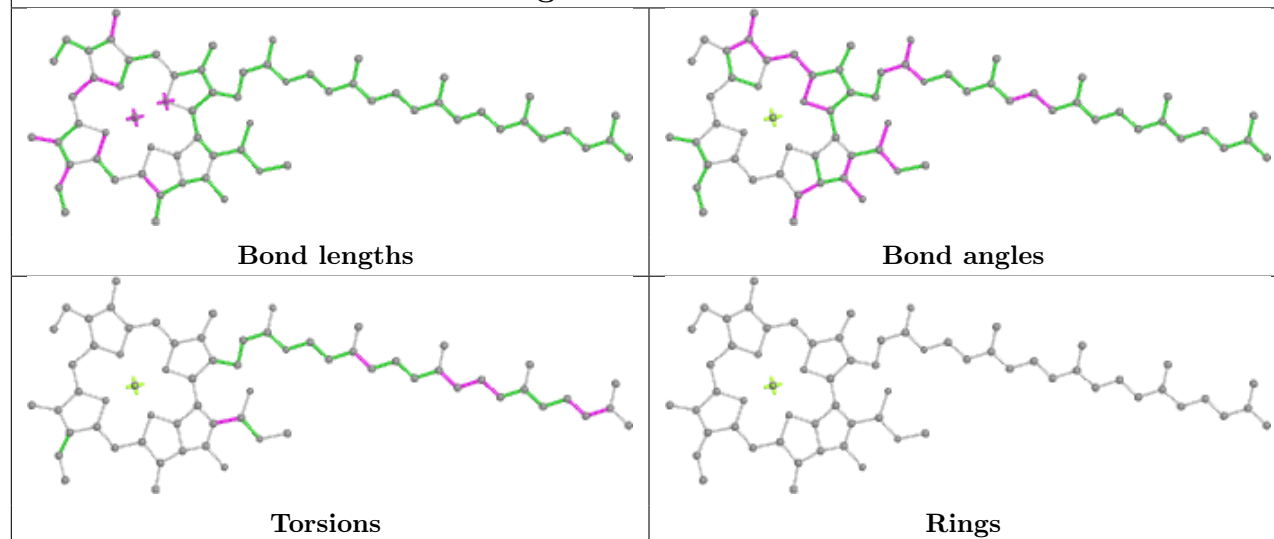
**Ligand CLA B 603****Ligand CLA b 615****Ligand CLA B 614**

**Ligand CLA c 509****Ligand PL9 a 611****Ligand DGD A 618**

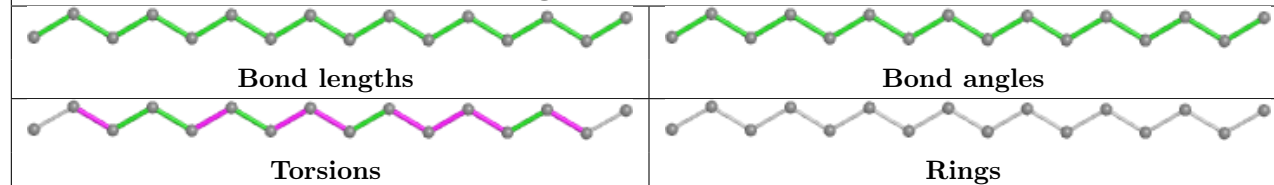




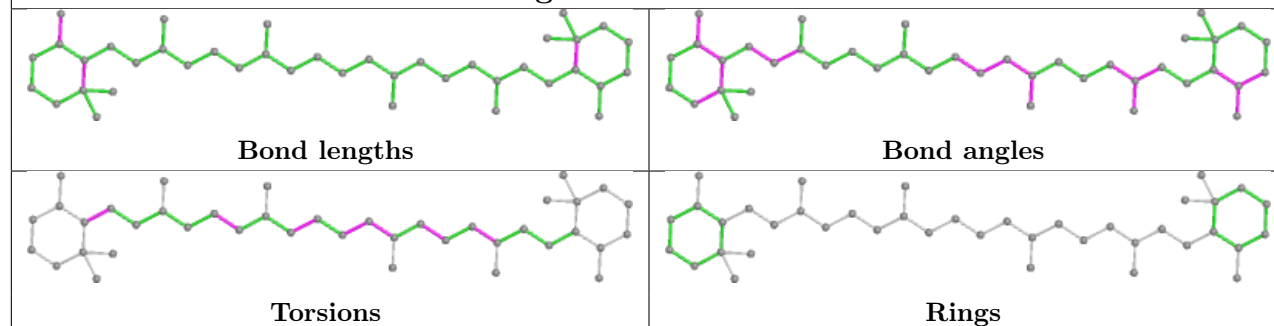
## Ligand CLA c 510



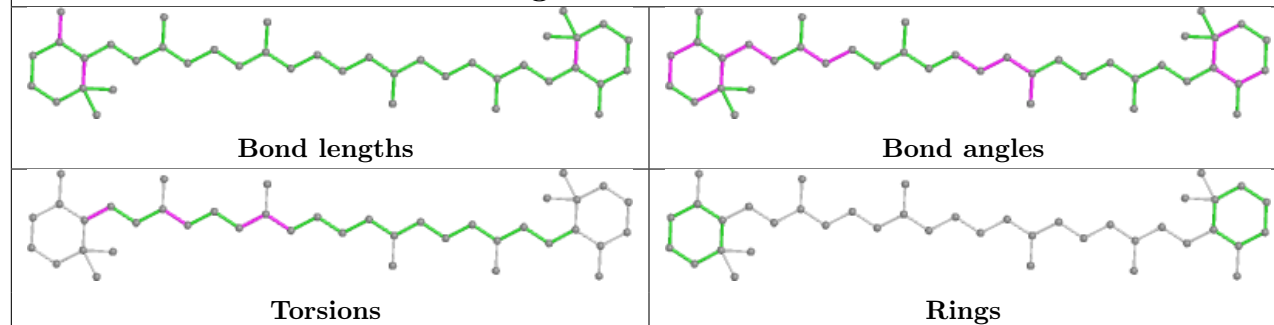
## Ligand STE T 102

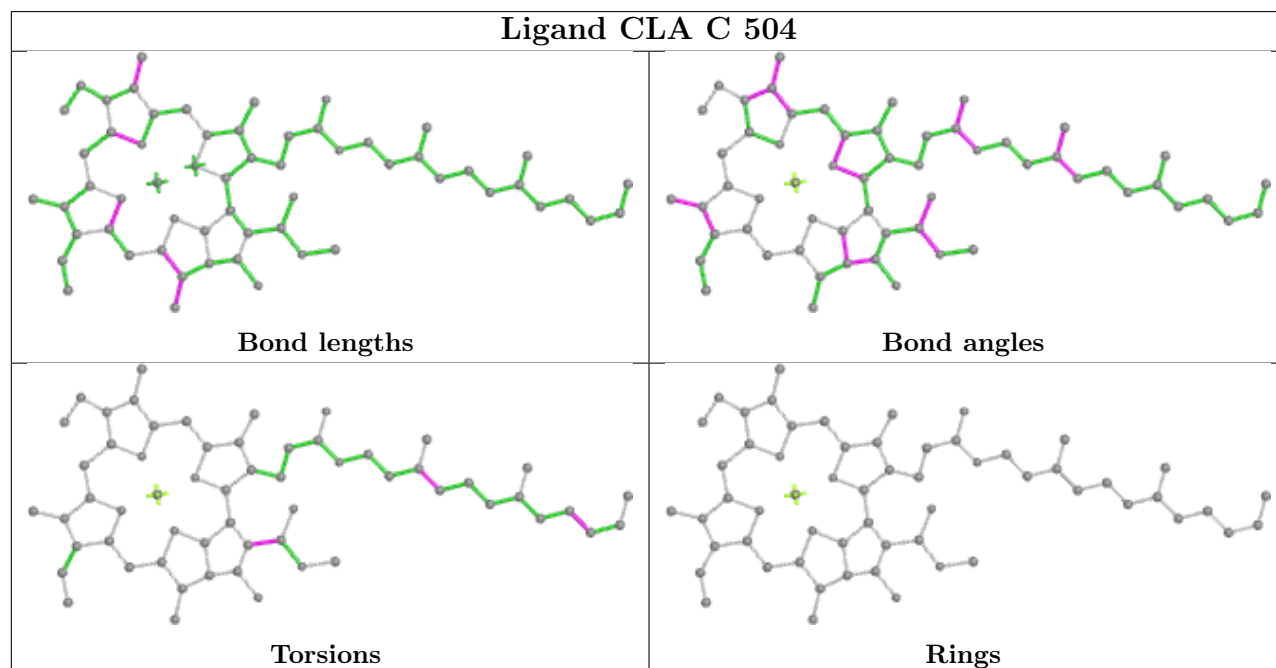
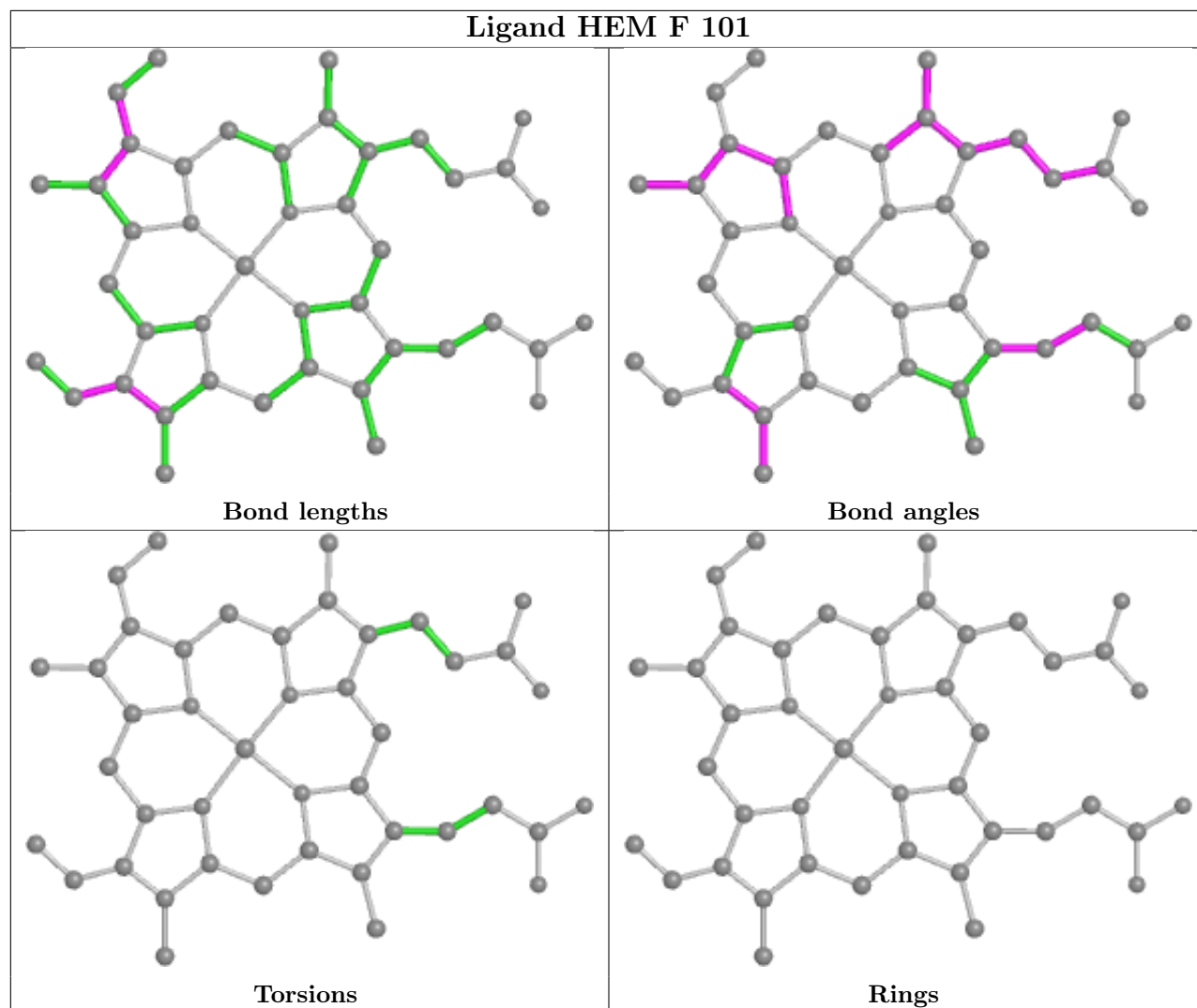


## Ligand BCR c 514

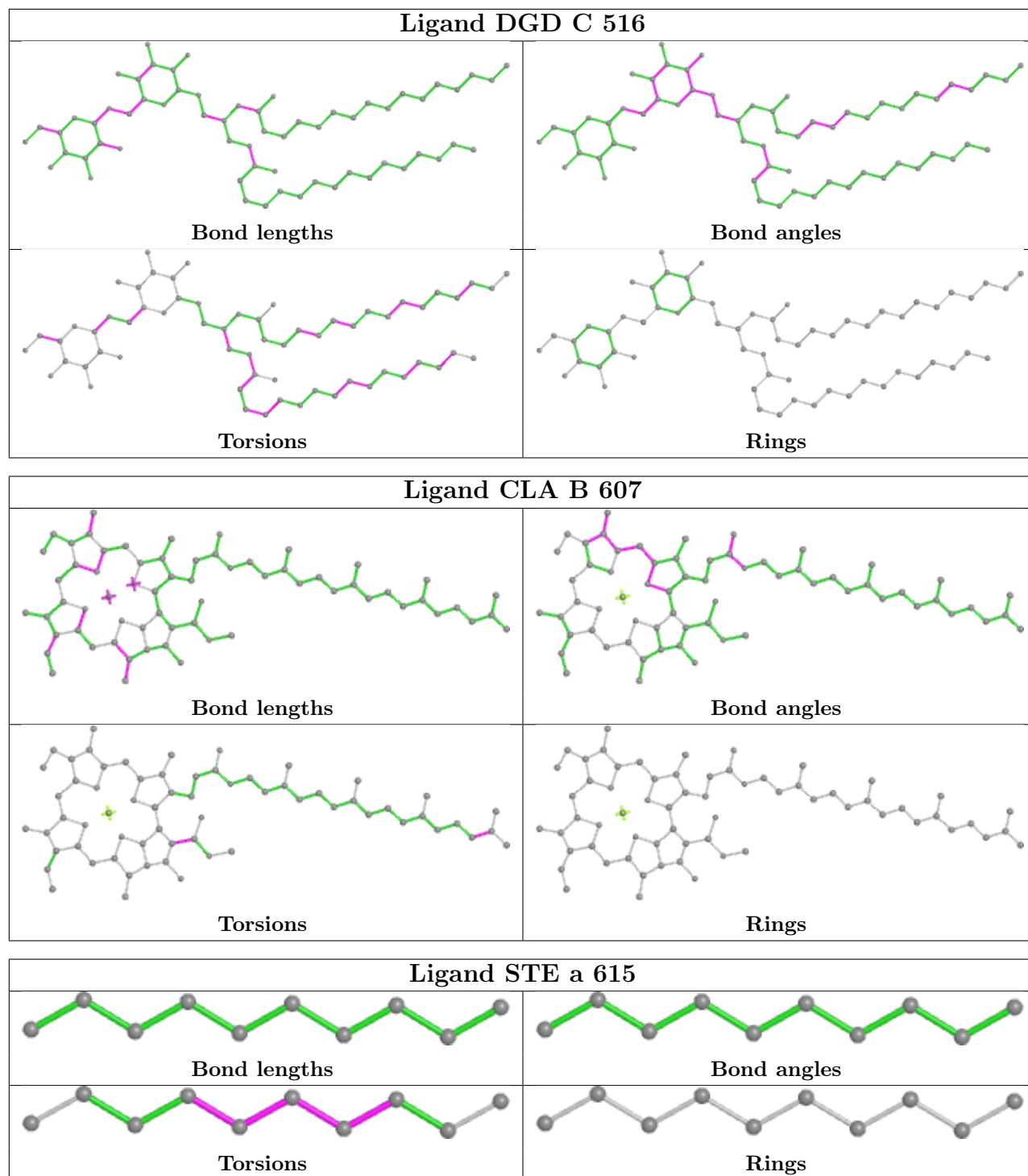


## Ligand BCR B 617

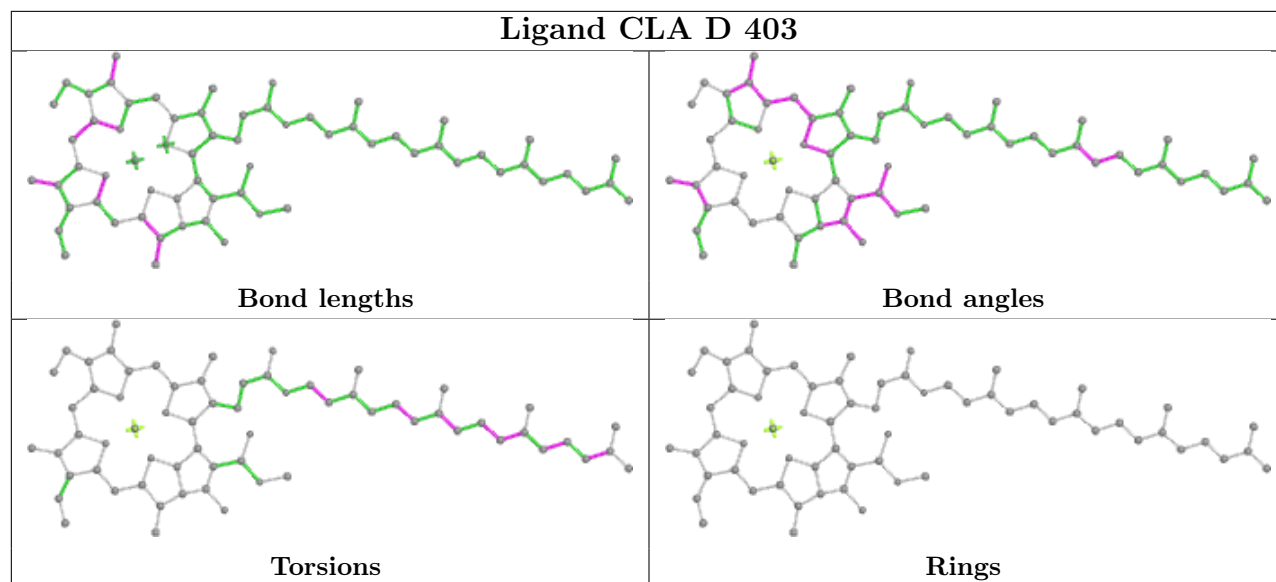




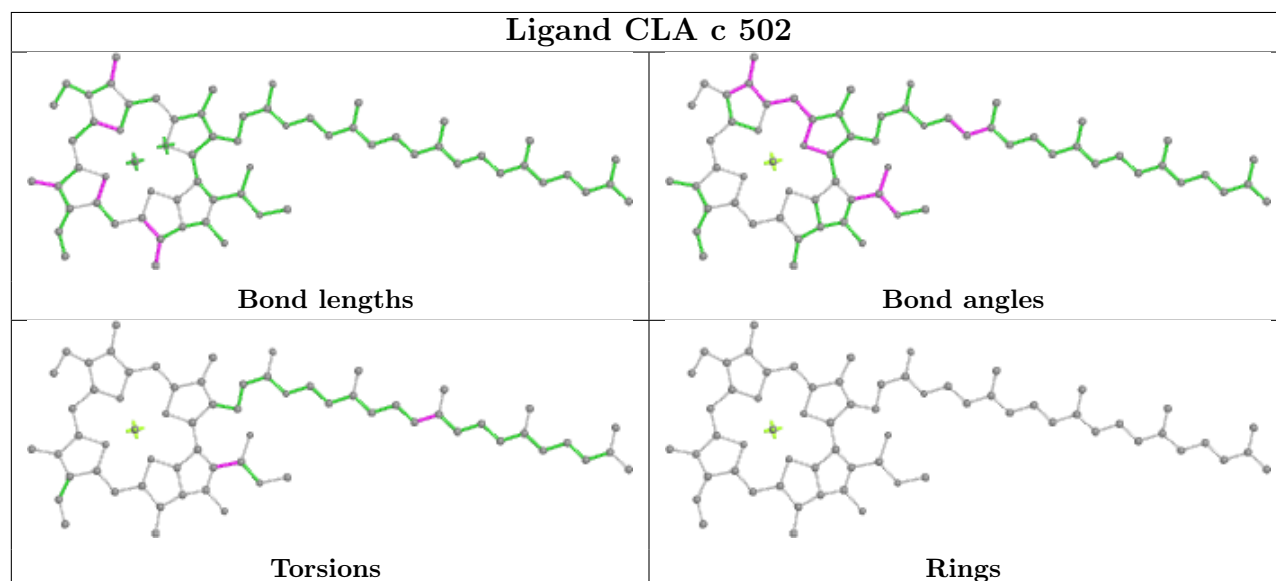




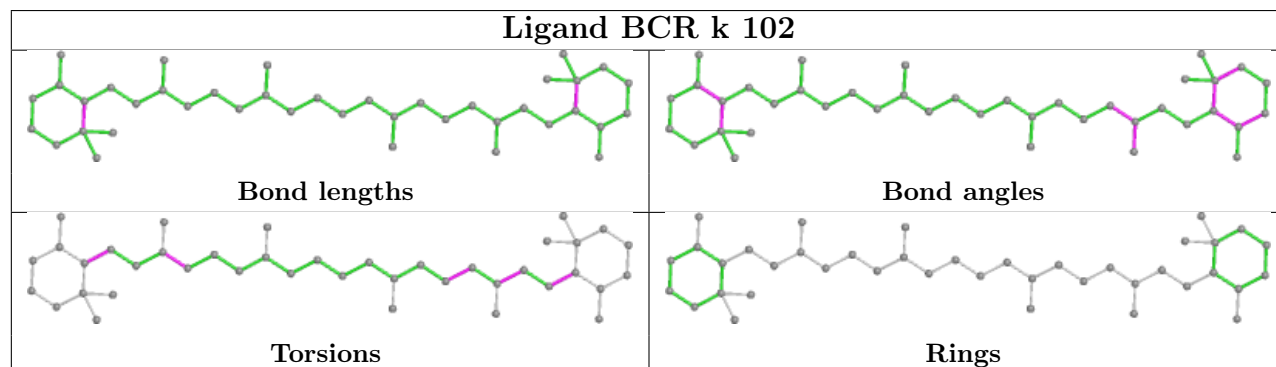
## Ligand CLA D 403



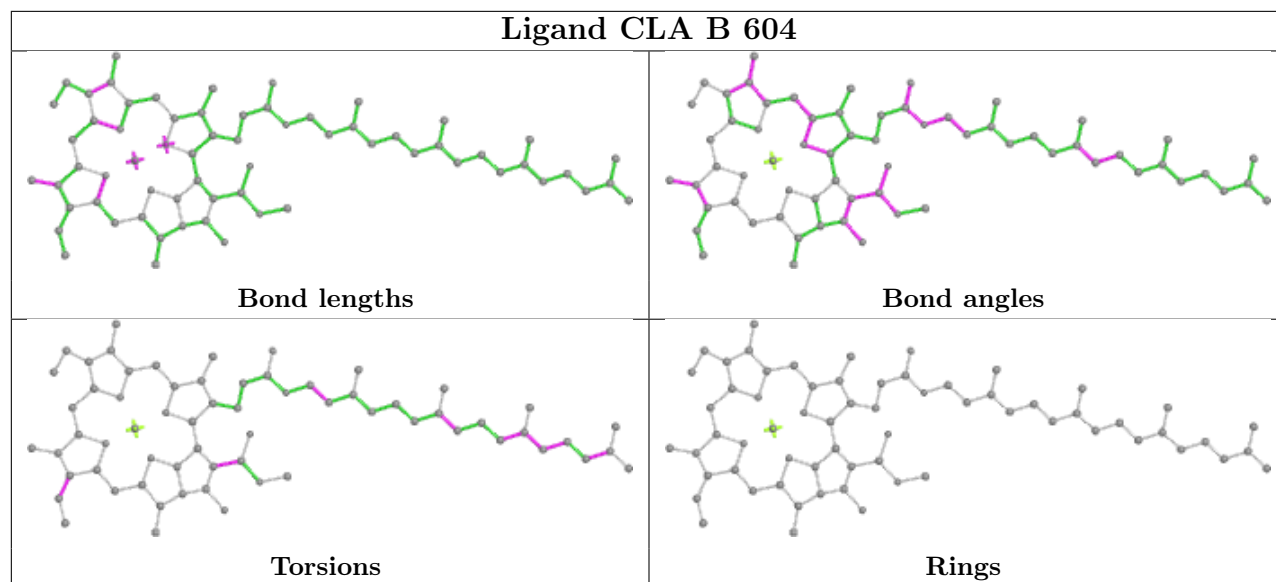
## Ligand CLA c 502



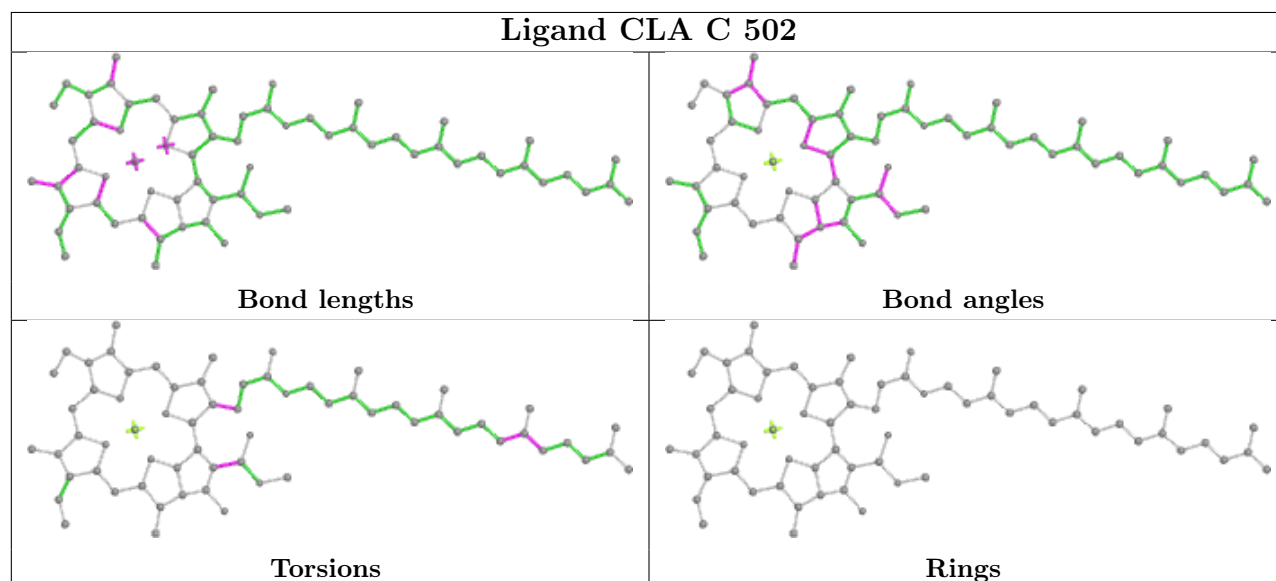
## Ligand BCR k 102



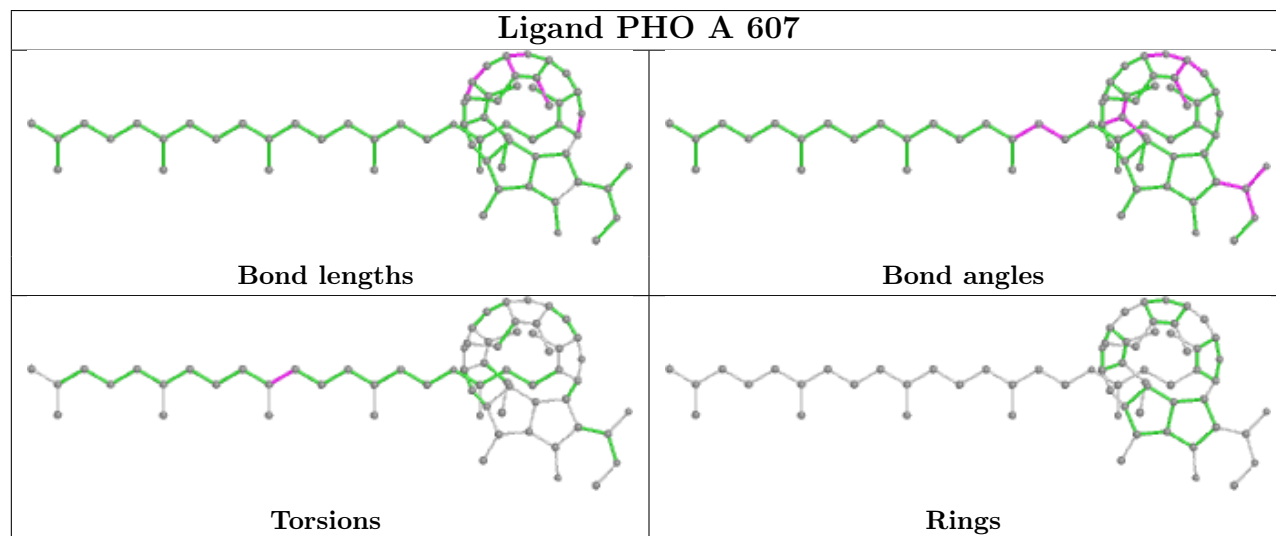
## Ligand CLA B 604

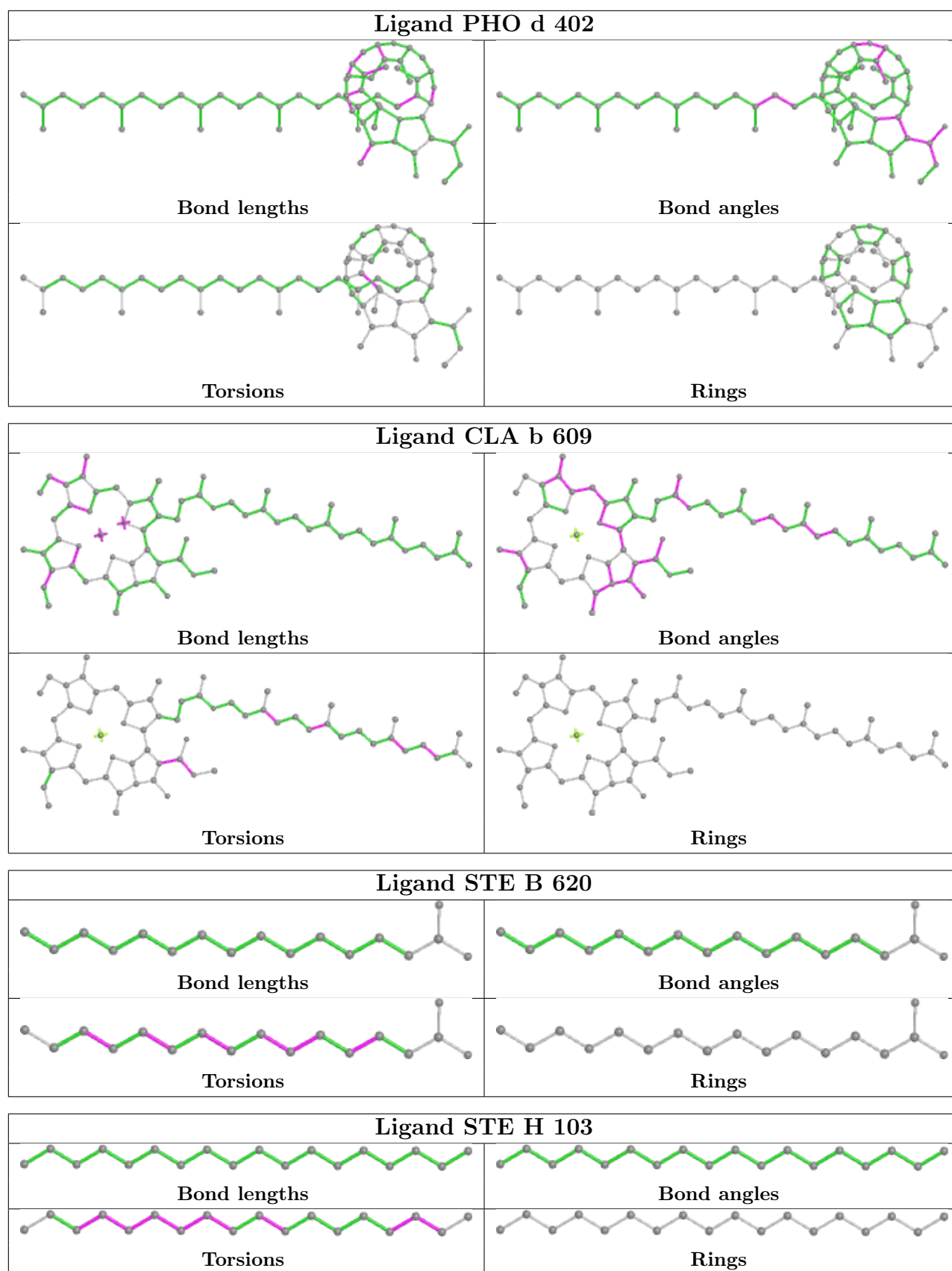


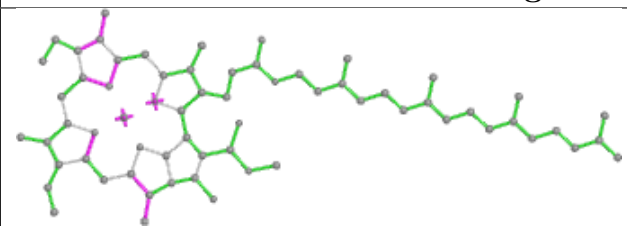
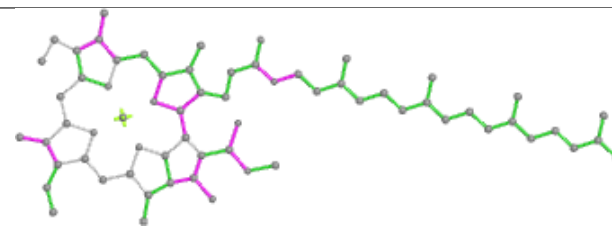
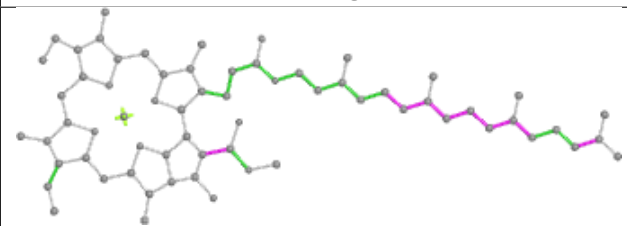
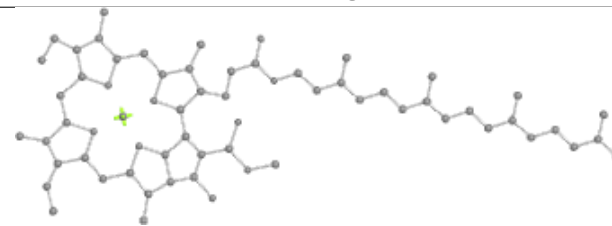
## Ligand CLA C 502

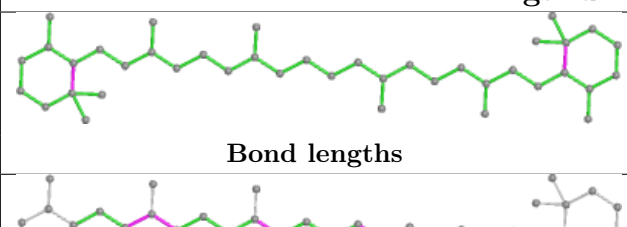
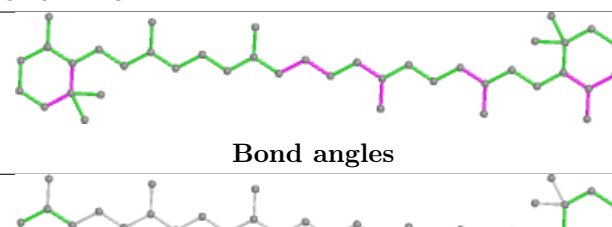
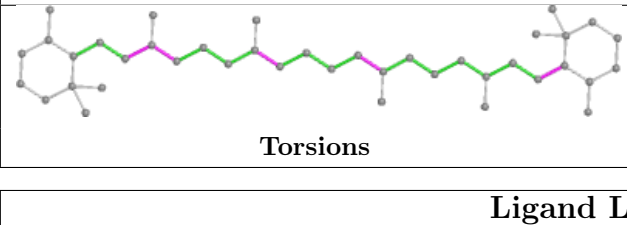
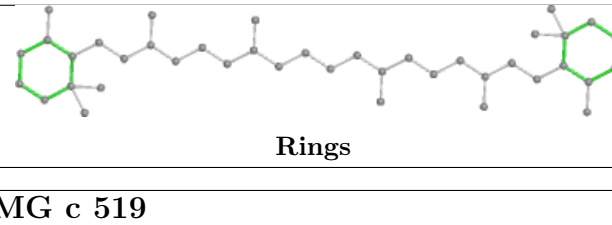


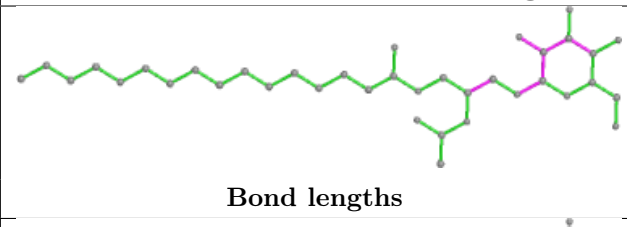
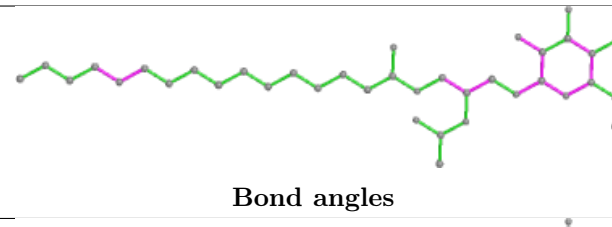
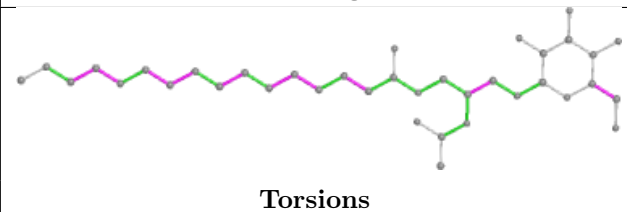

## Ligand PHO A 607

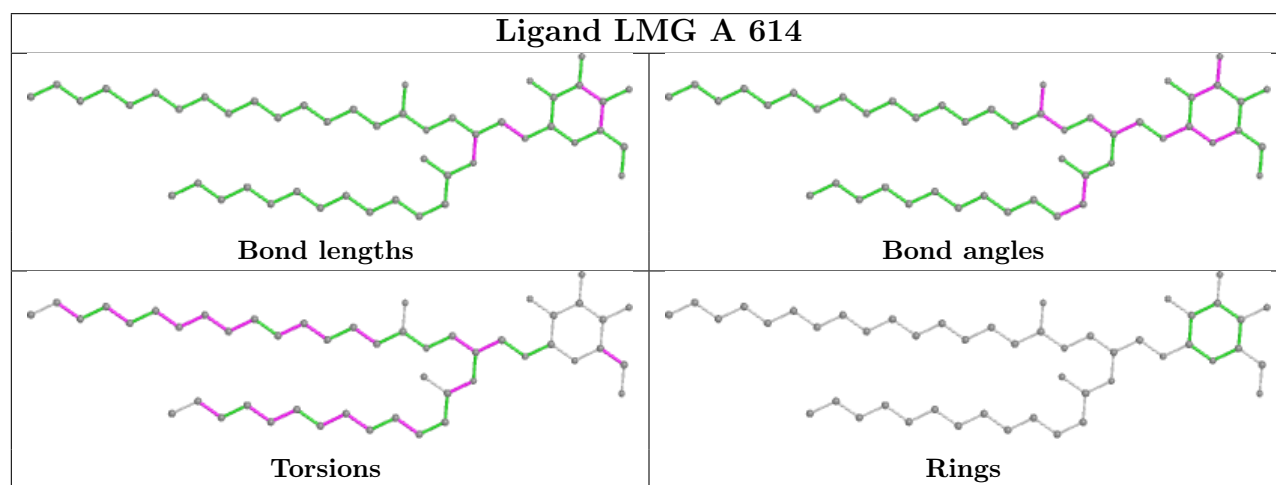
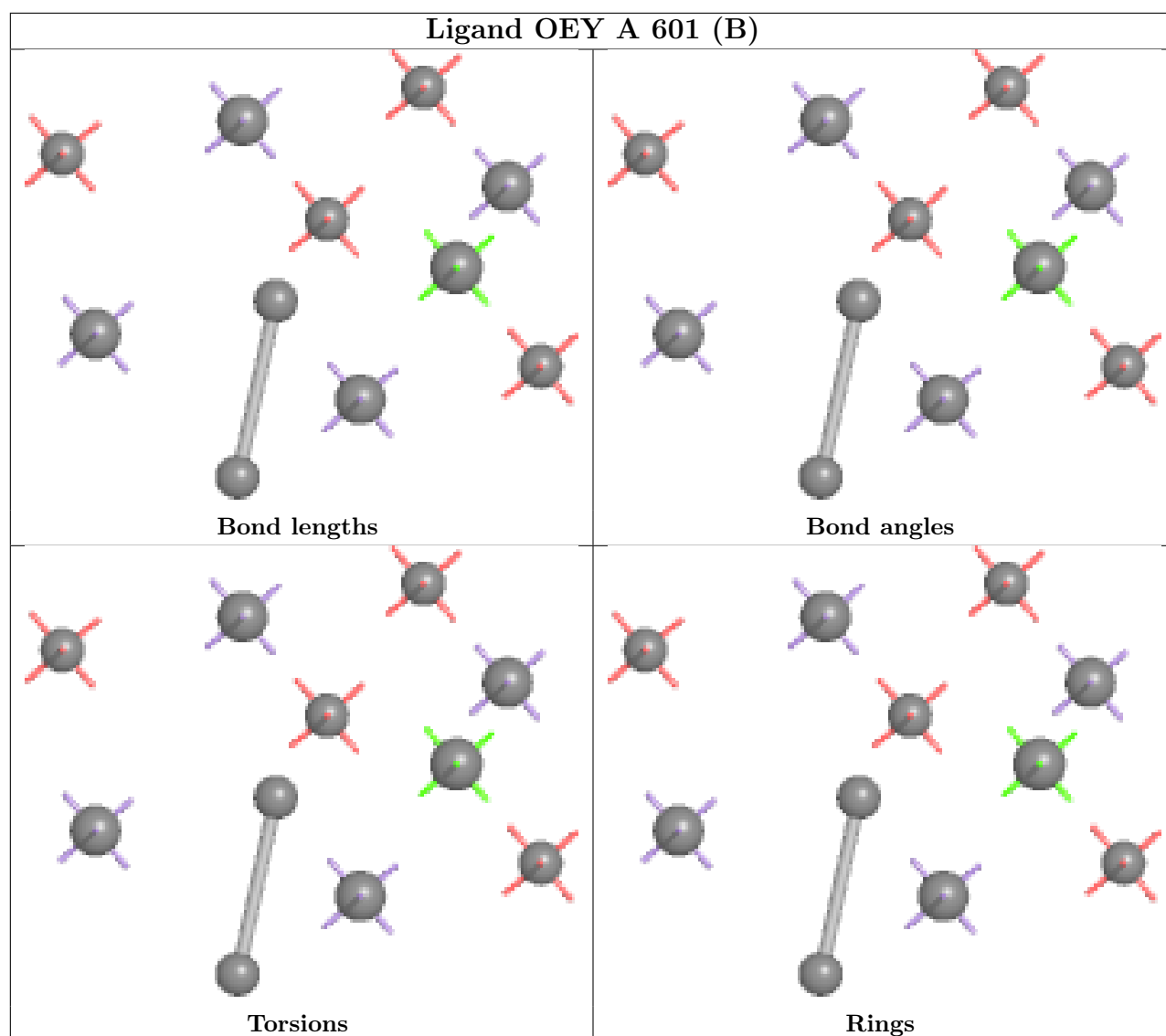


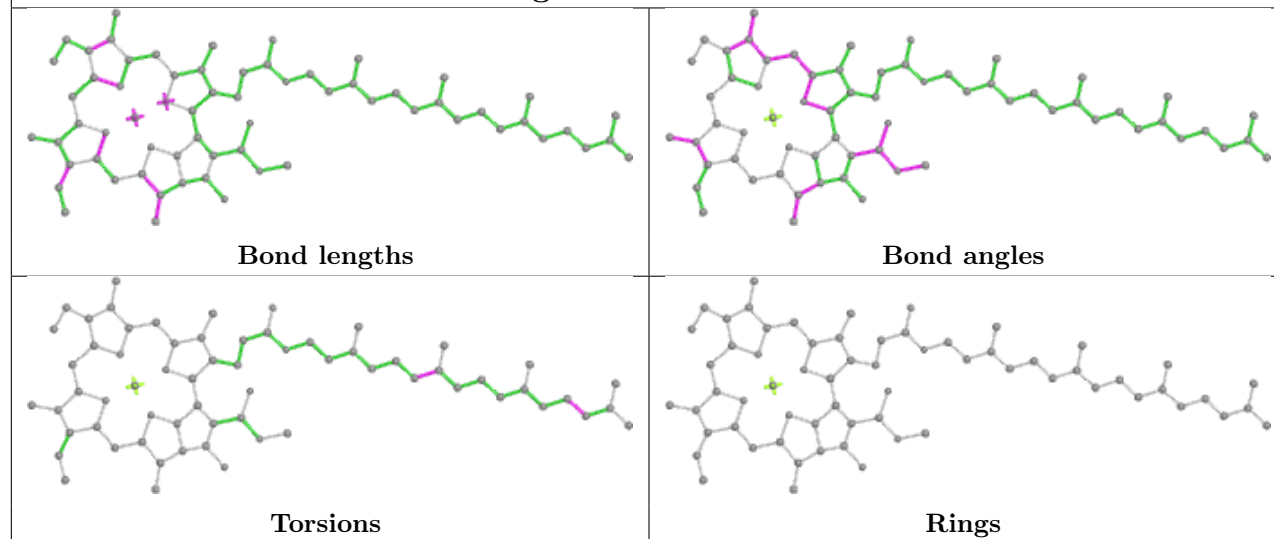
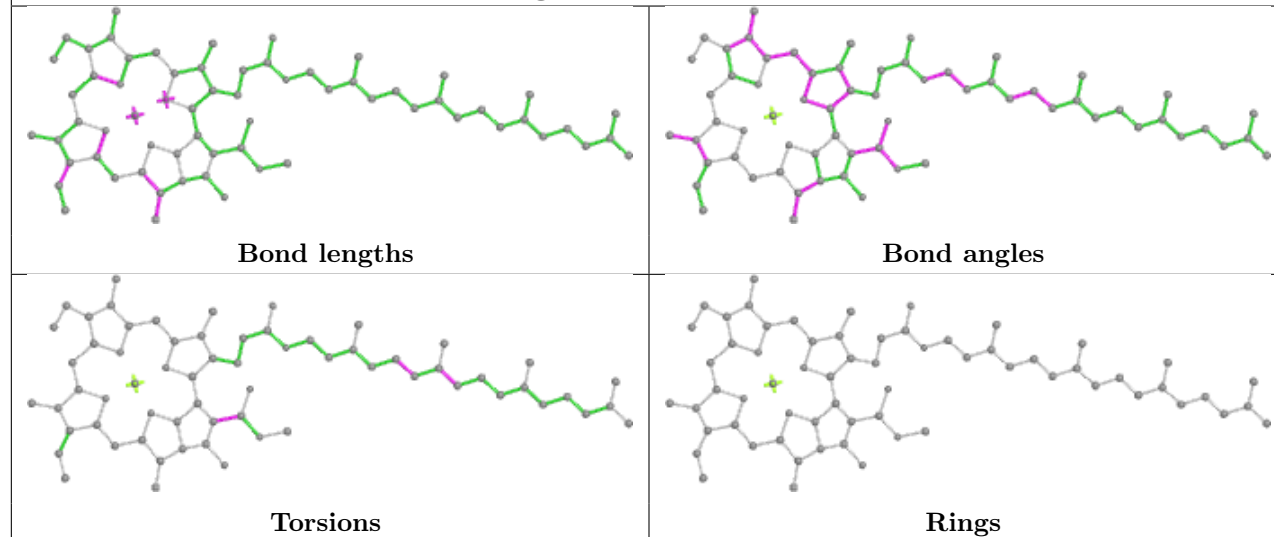
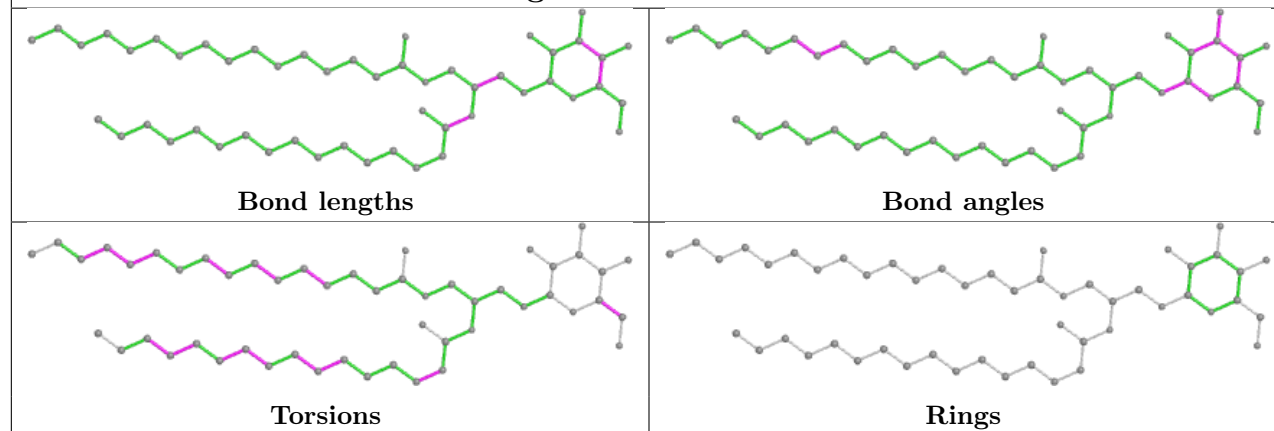


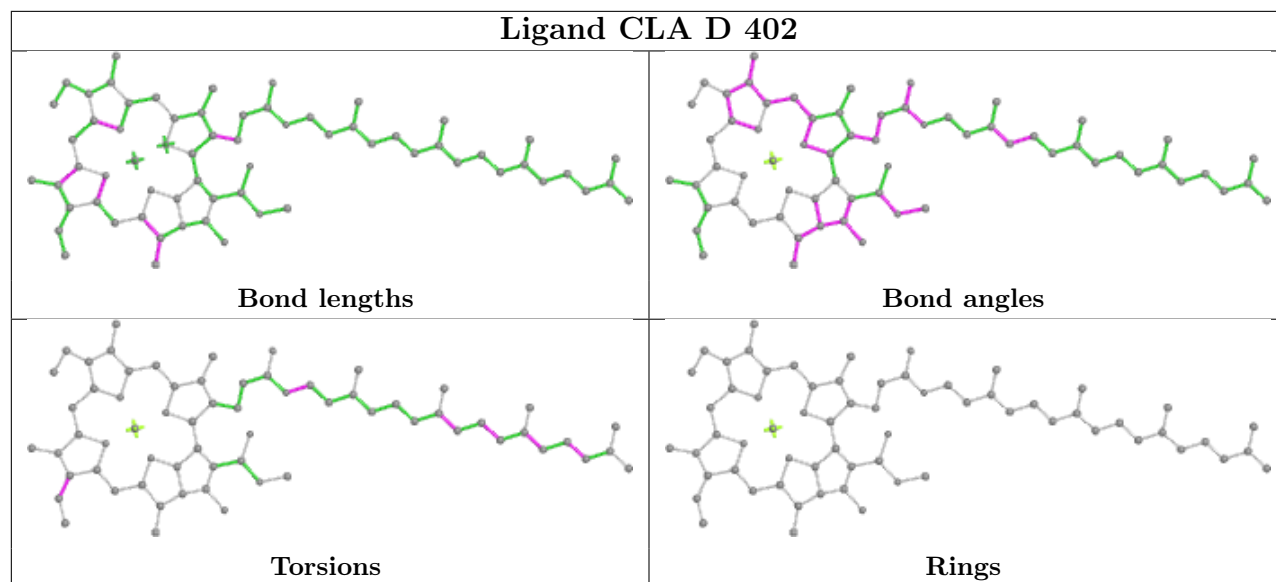
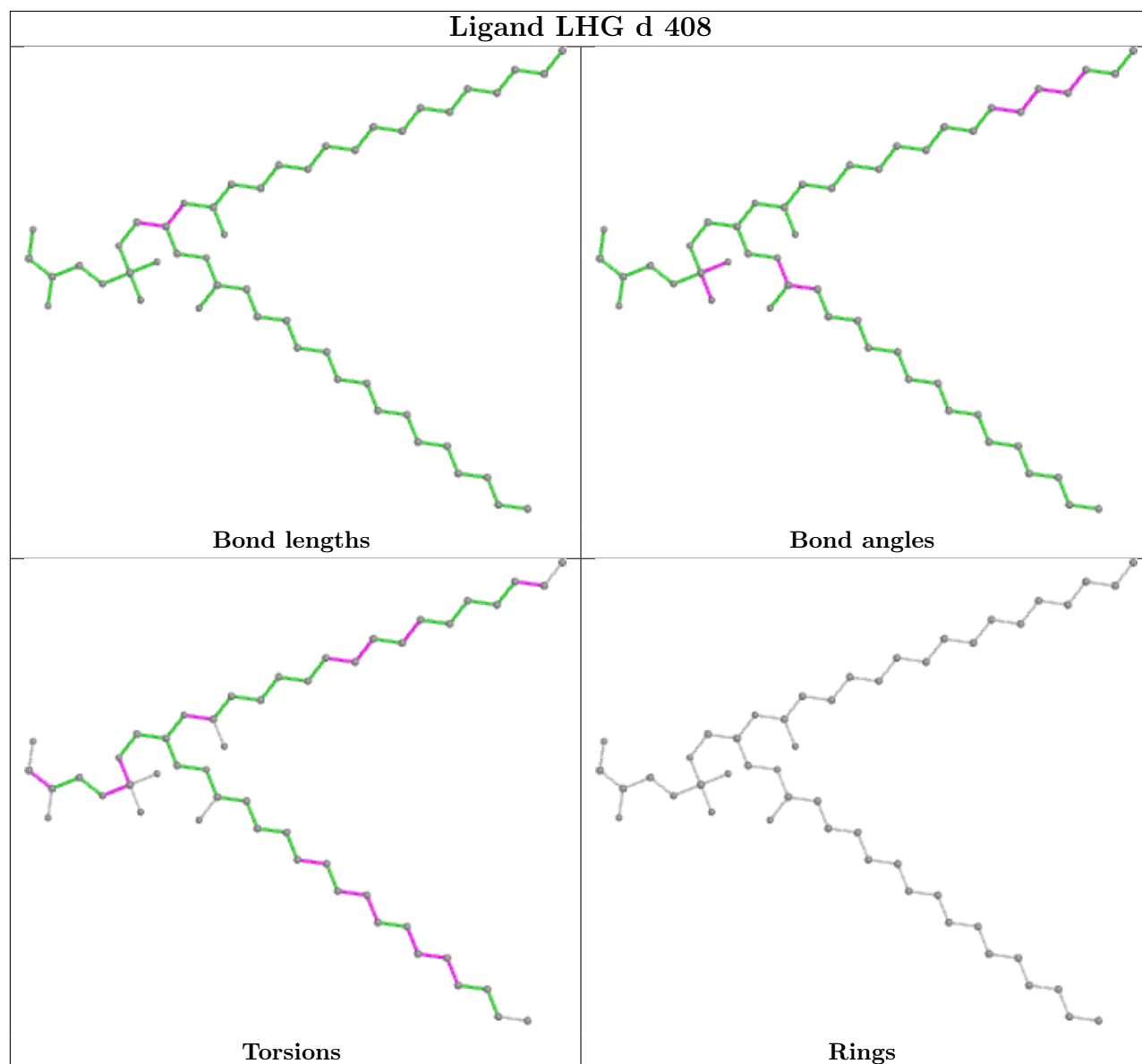
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

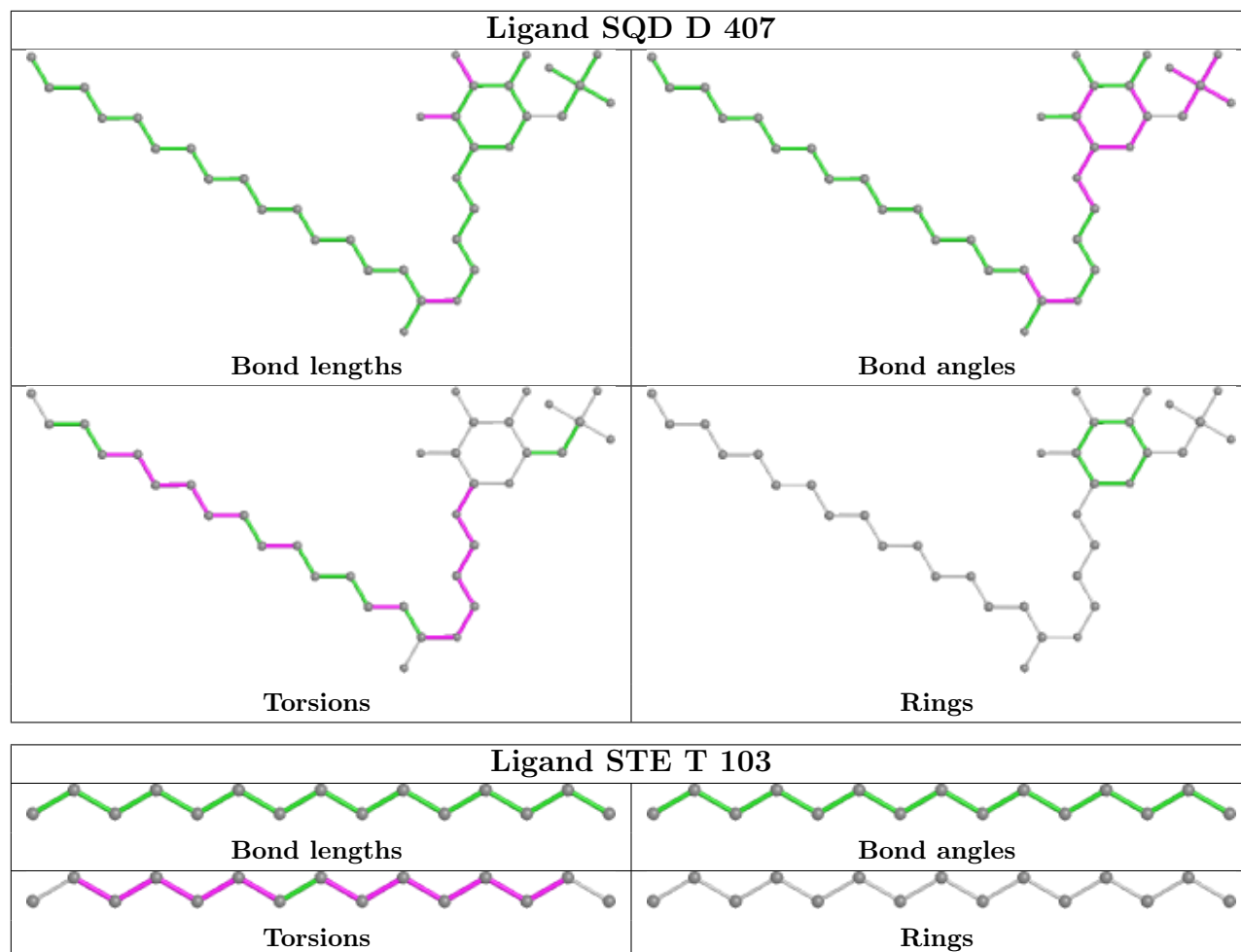
Ligand LMG c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings



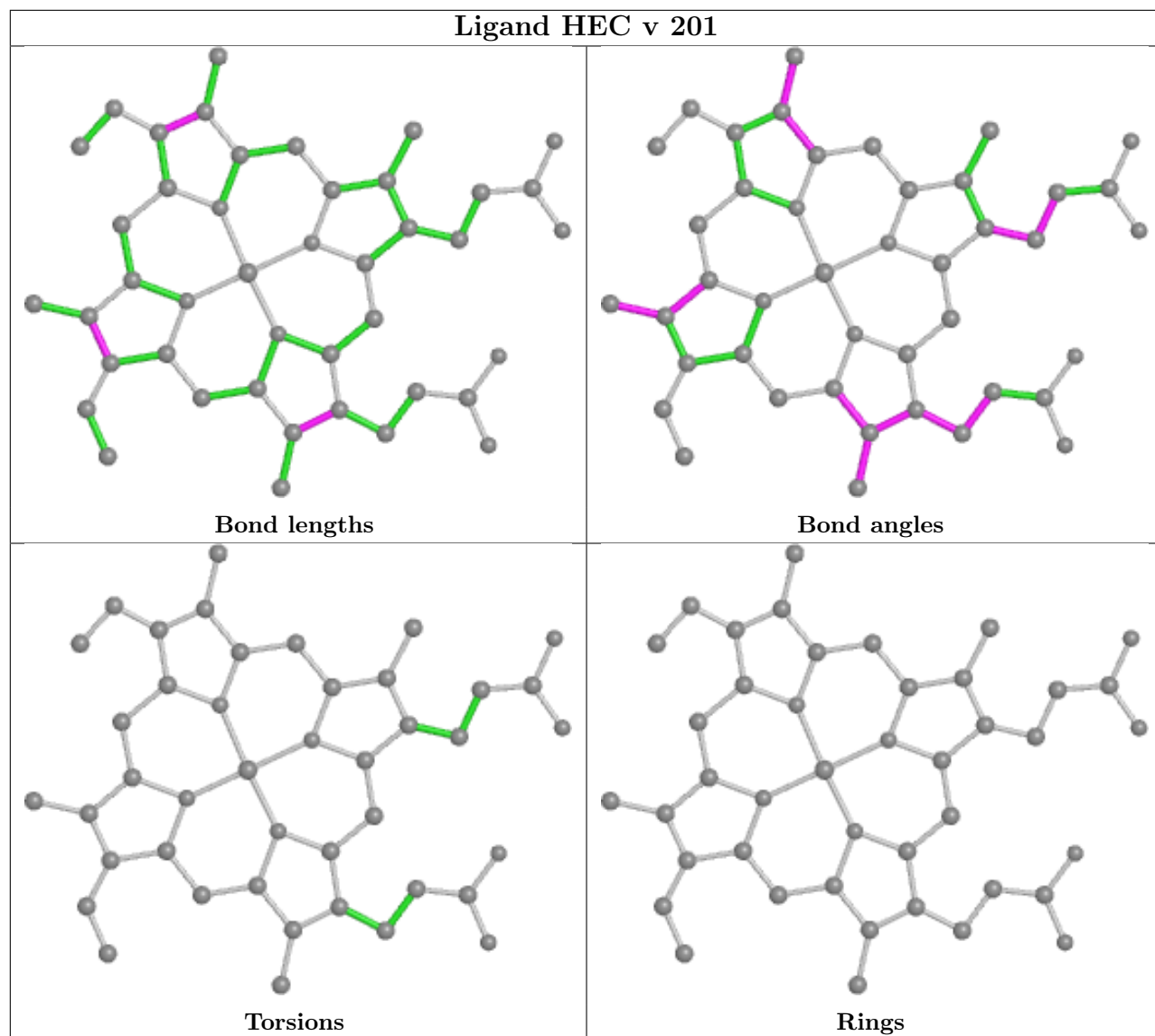
**Ligand CLA B 608****Ligand CLA C 503****Ligand LMG D 406**

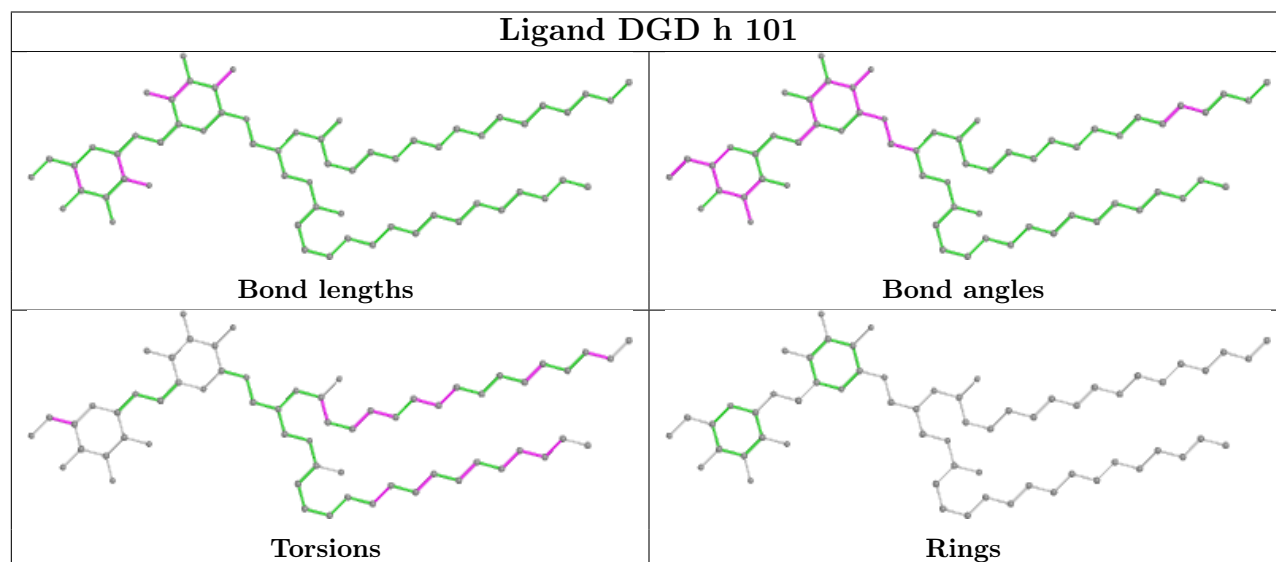
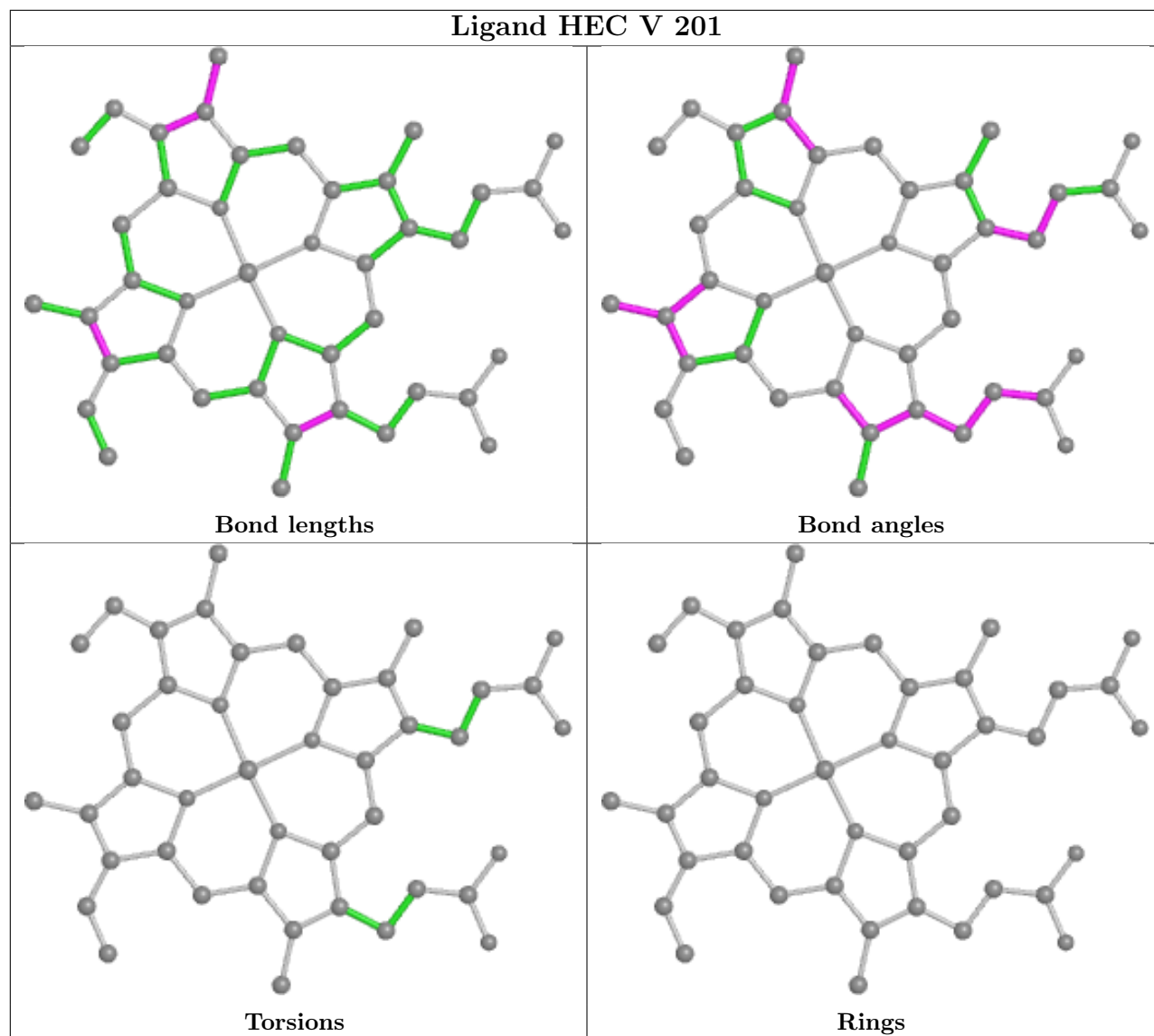
**Ligand CLA D 402****Ligand LHG d 408**

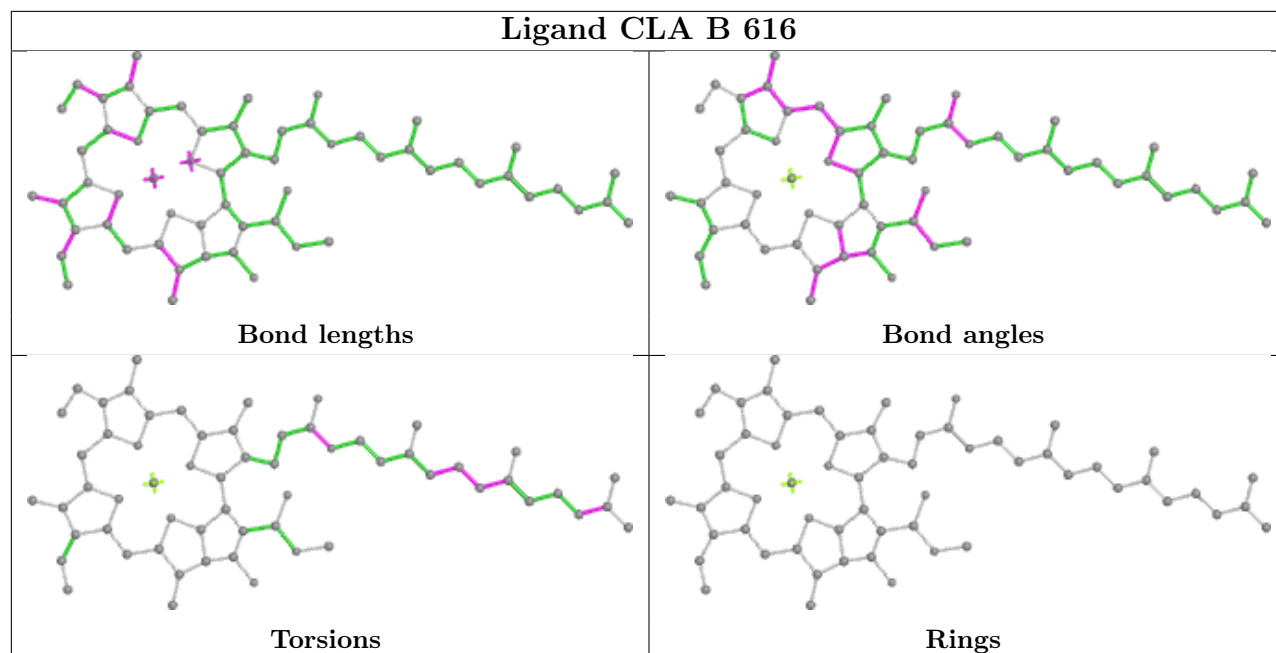
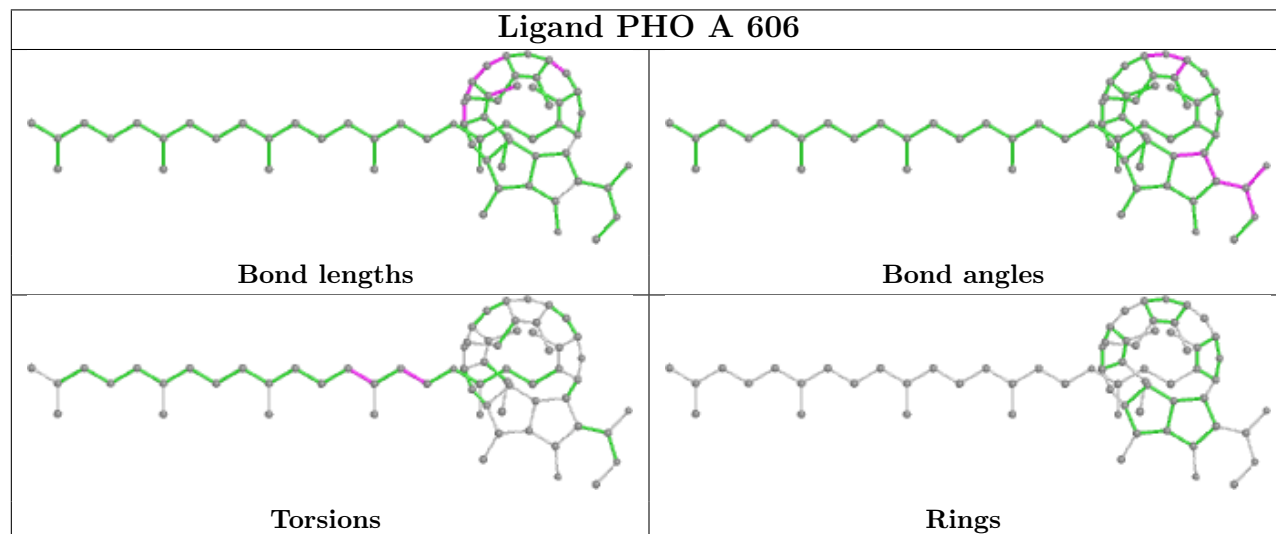
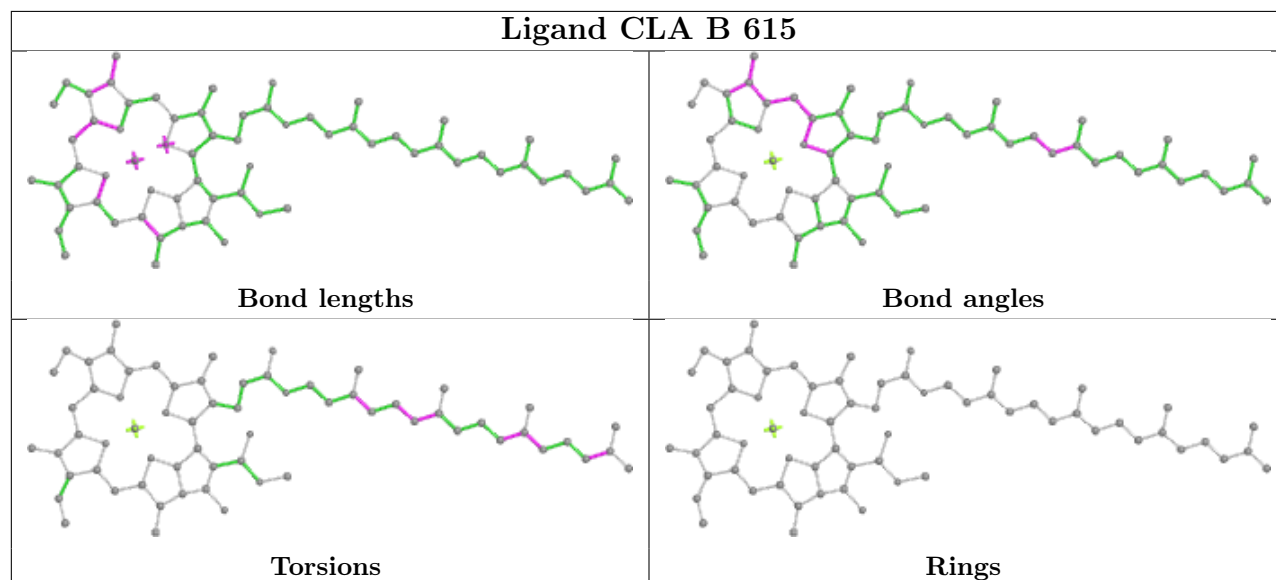


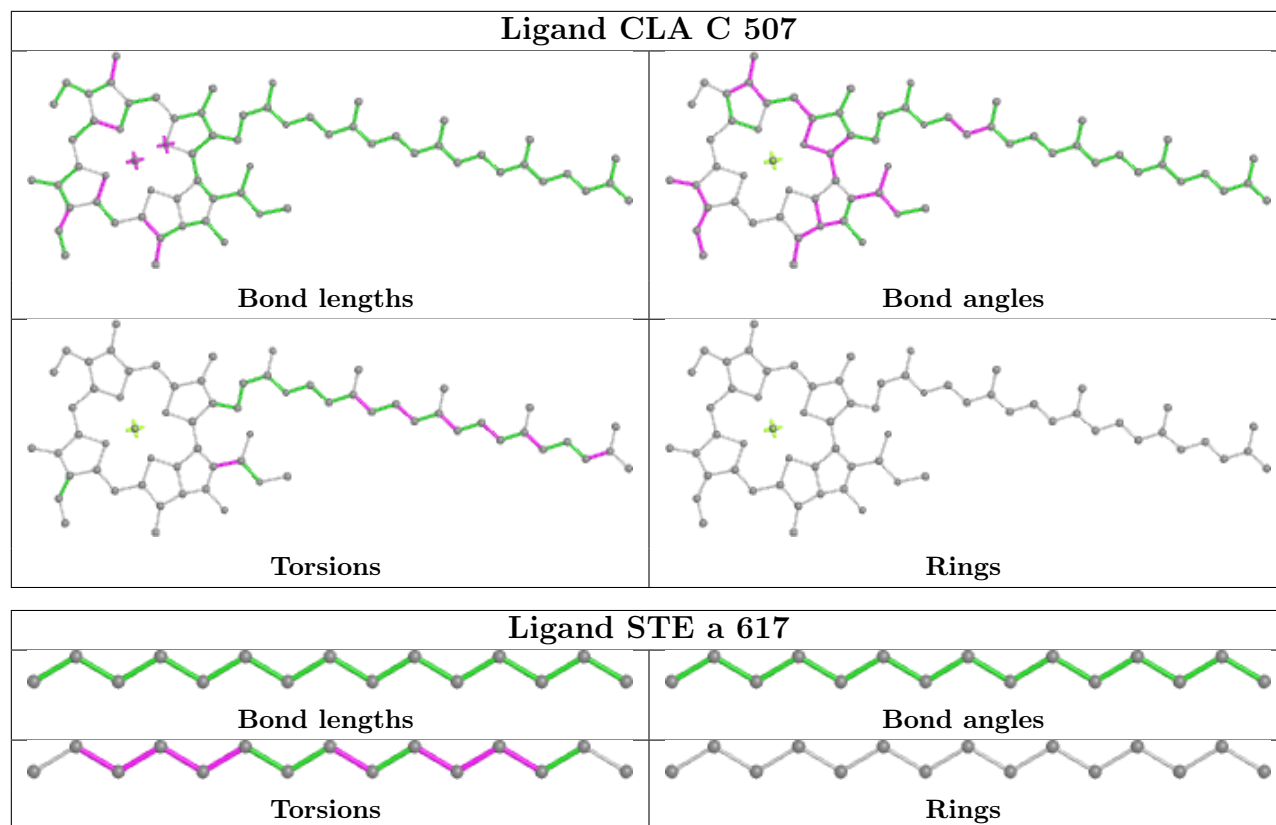


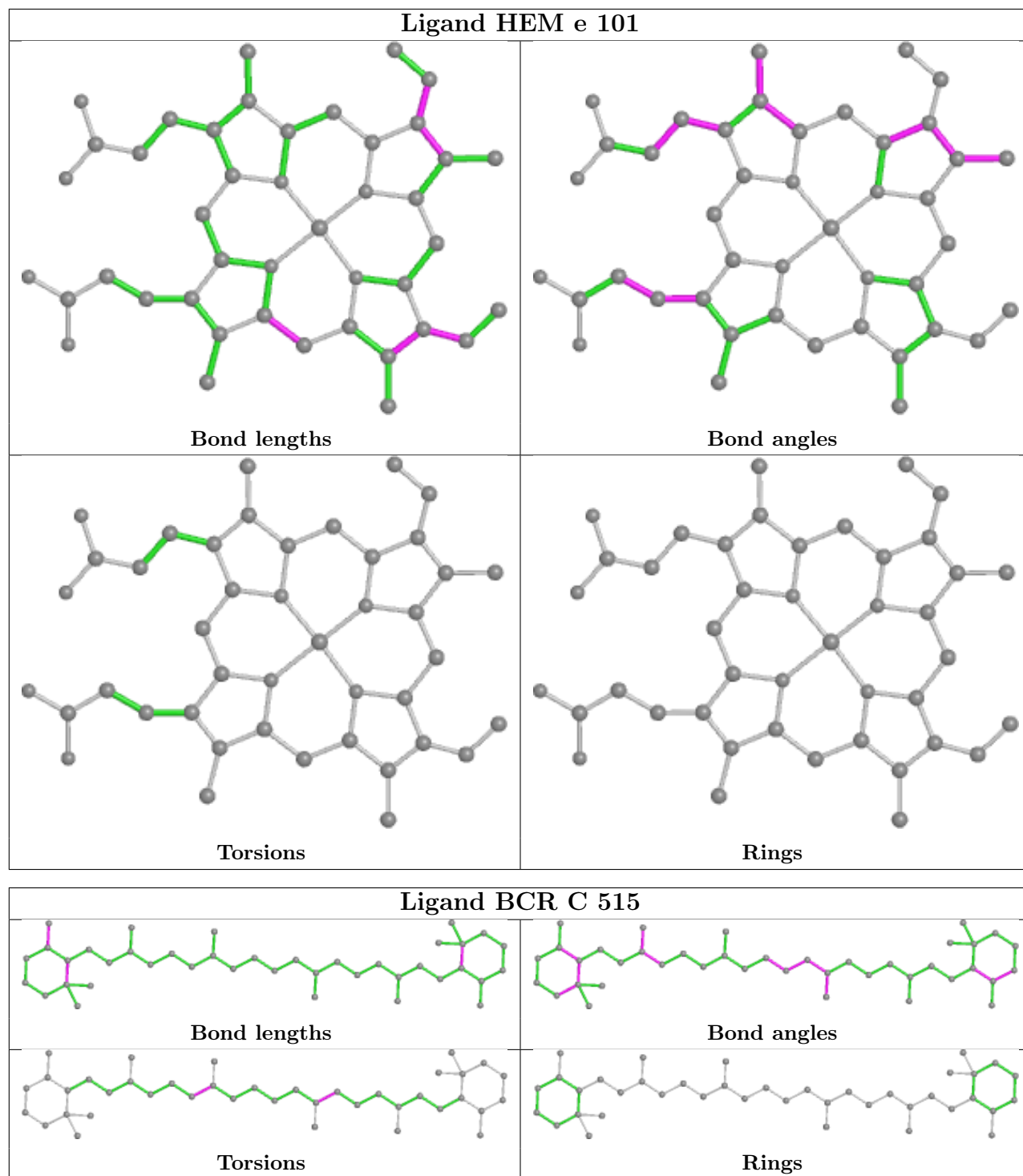
## Ligand HEC v 201

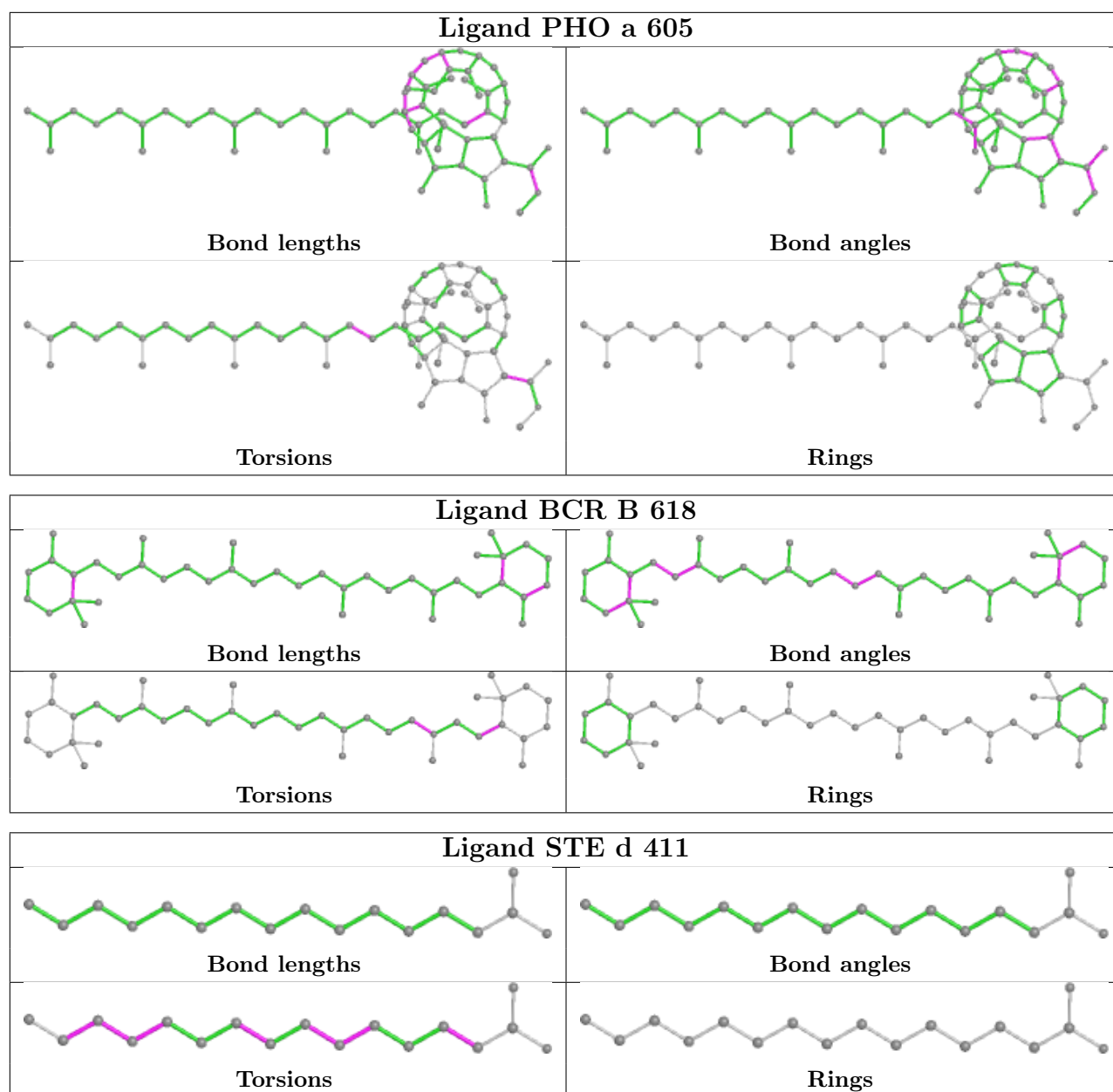


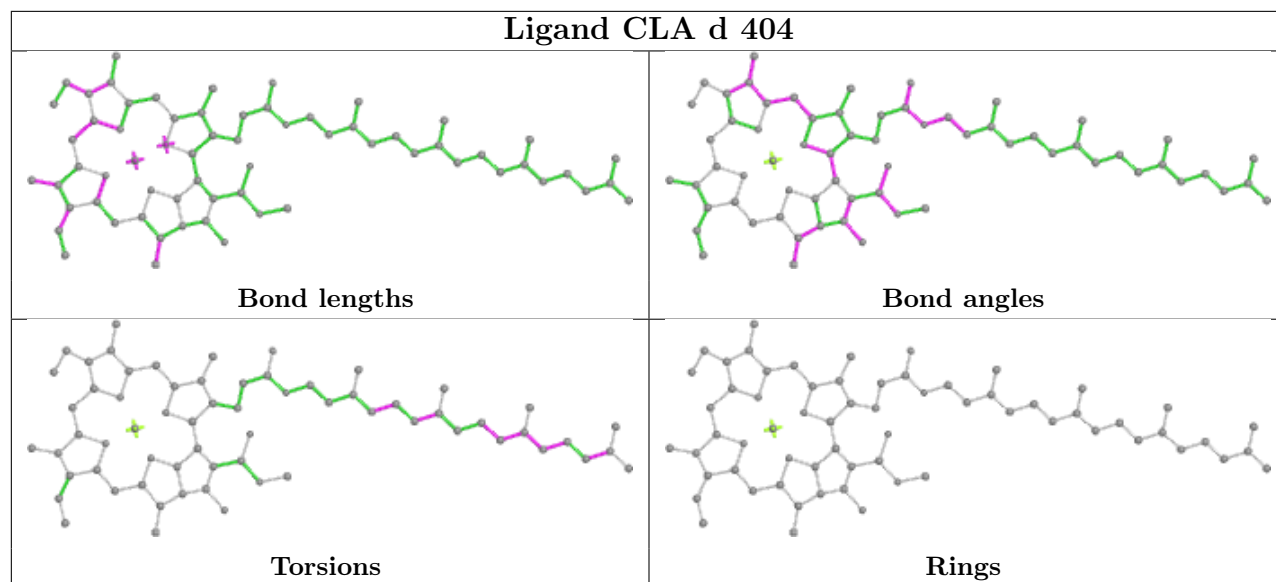
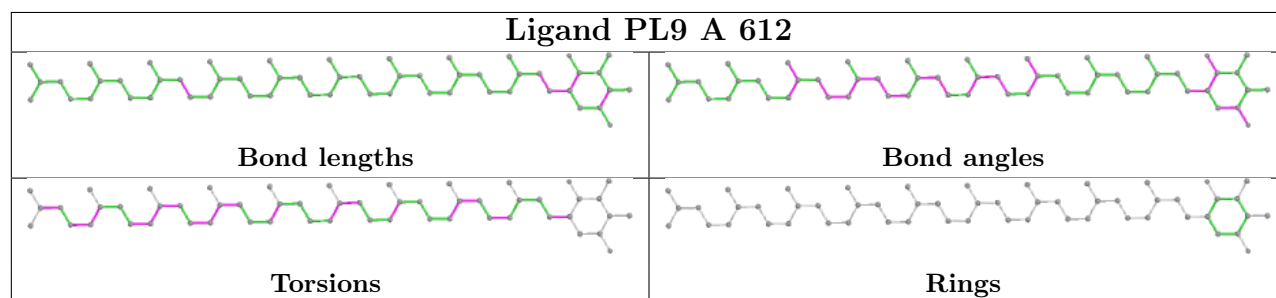
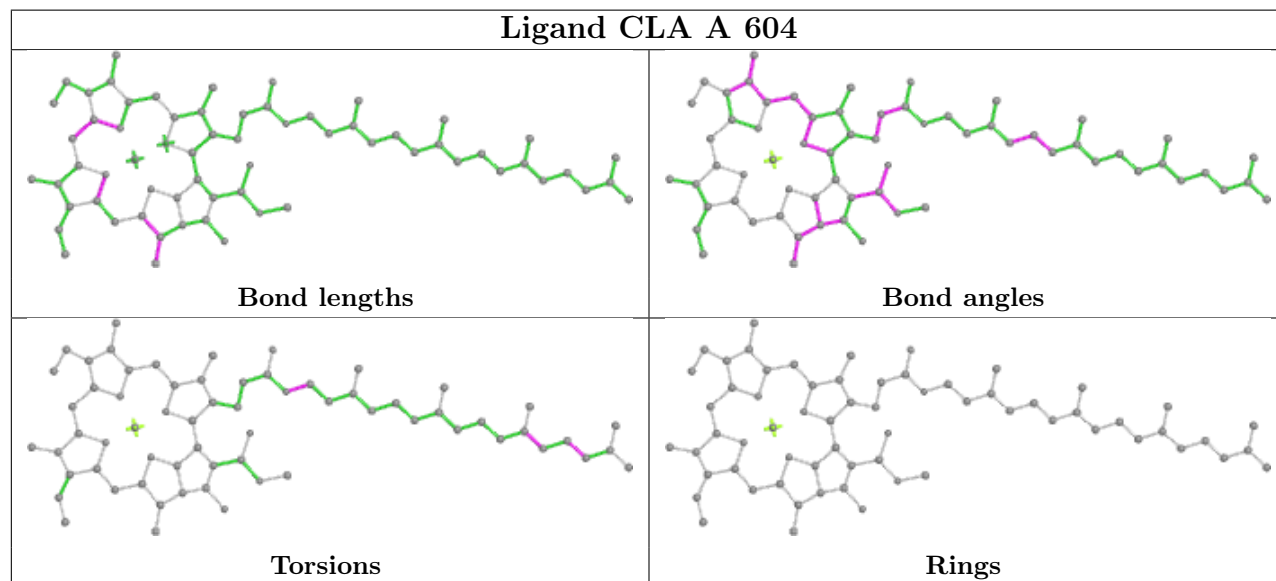


**Ligand CLA B 616****Ligand PHO A 606****Ligand CLA B 615**

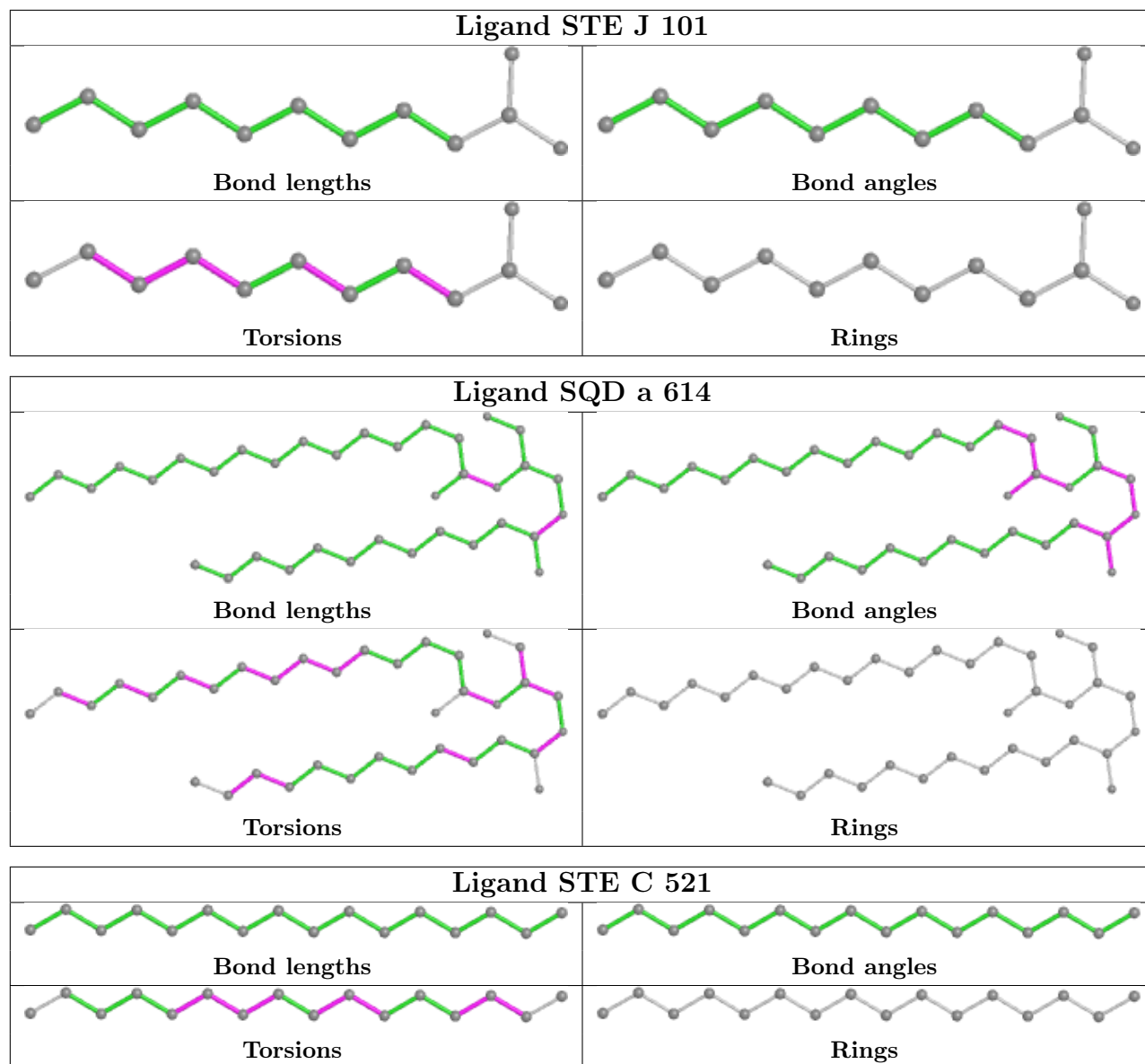


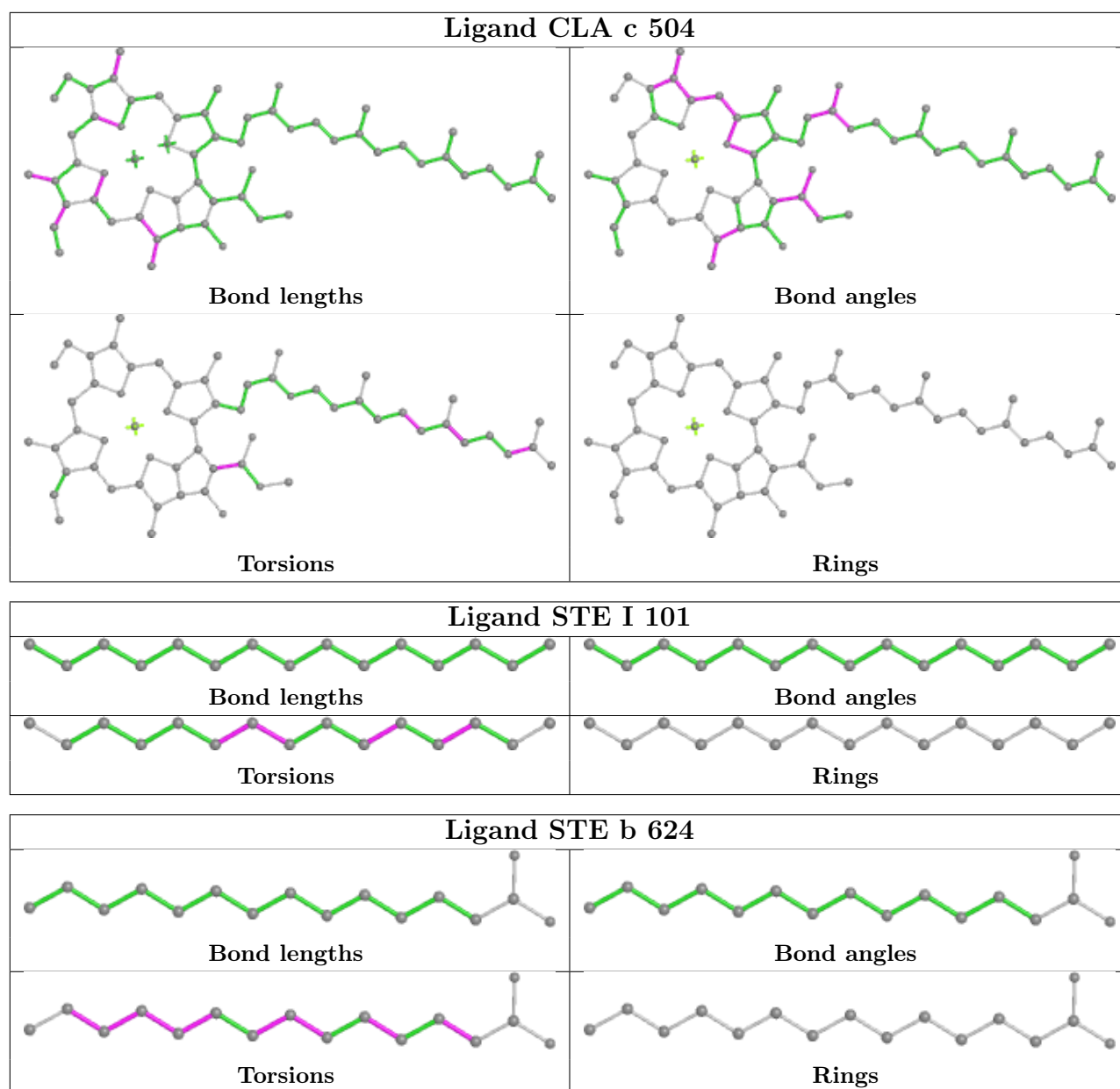




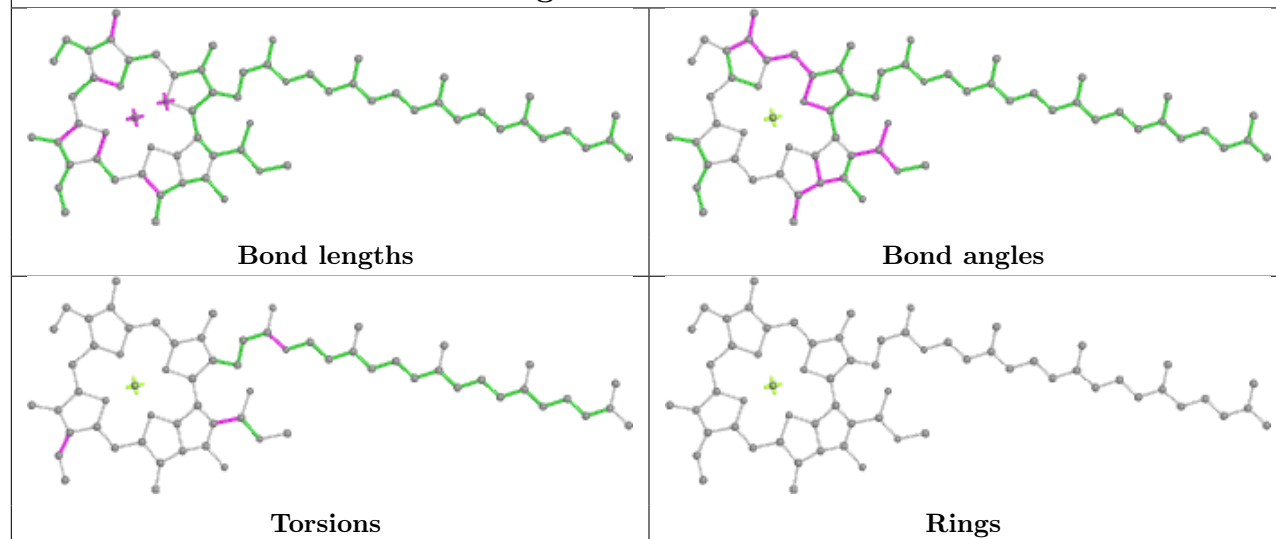
**Ligand CLA d 404****Ligand PL9 A 612****Ligand CLA A 604**



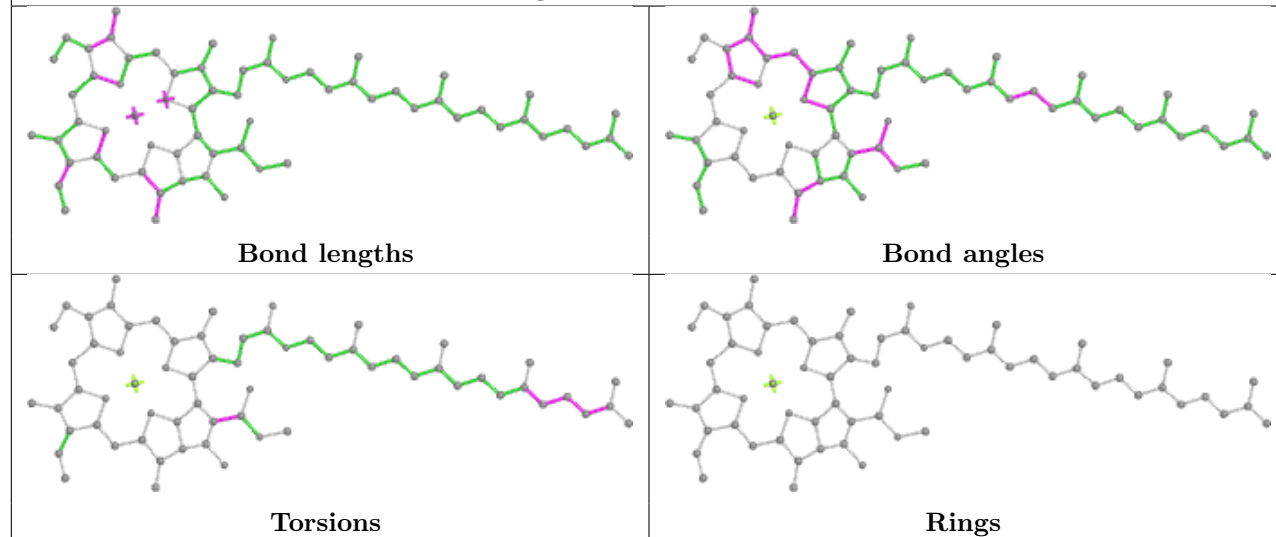




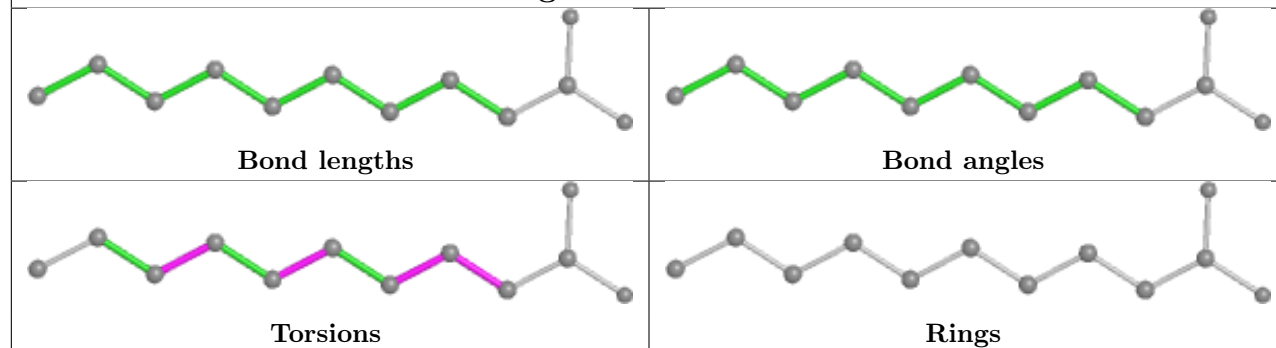
## Ligand CLA a 612

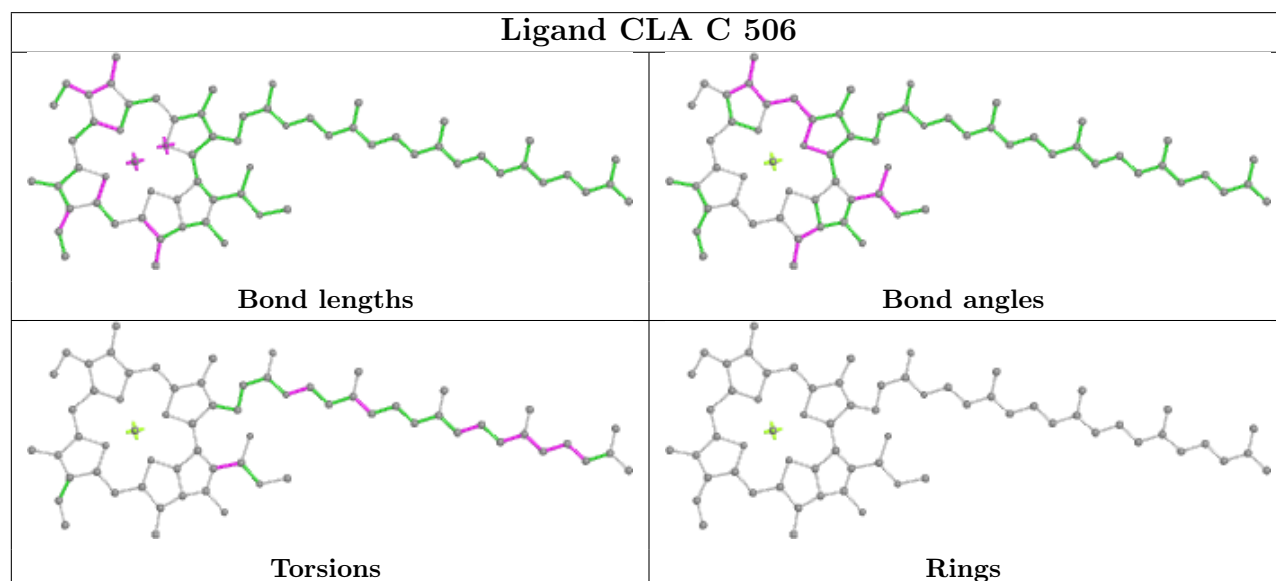
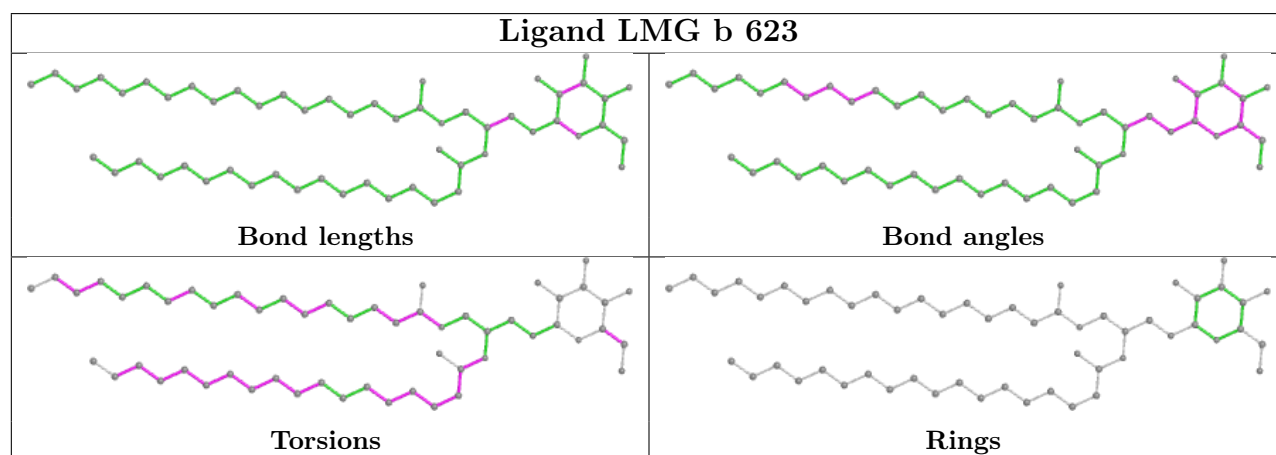
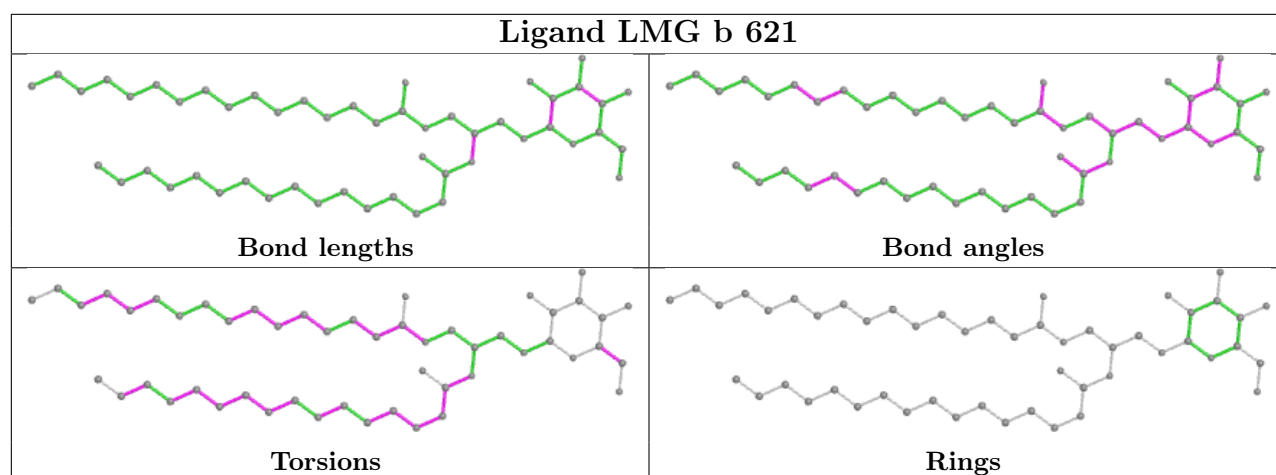


## Ligand CLA A 613

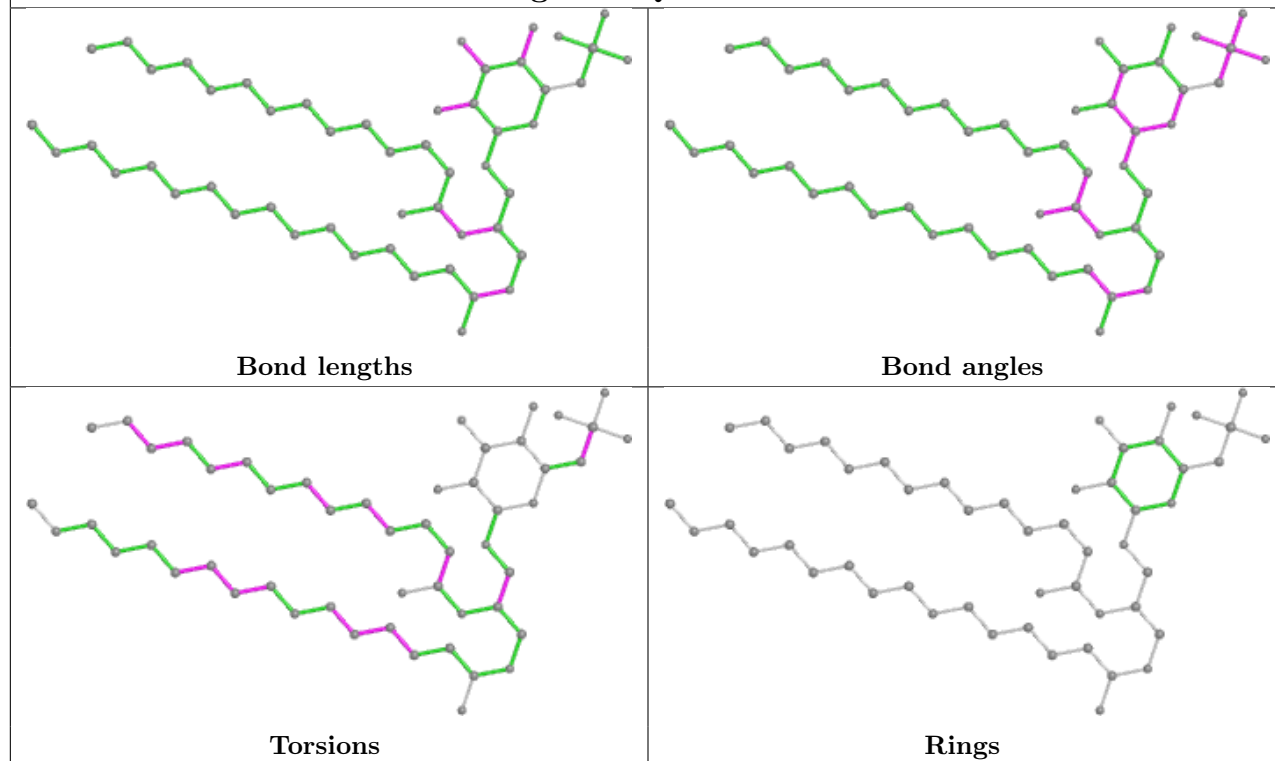


## Ligand STE k 103

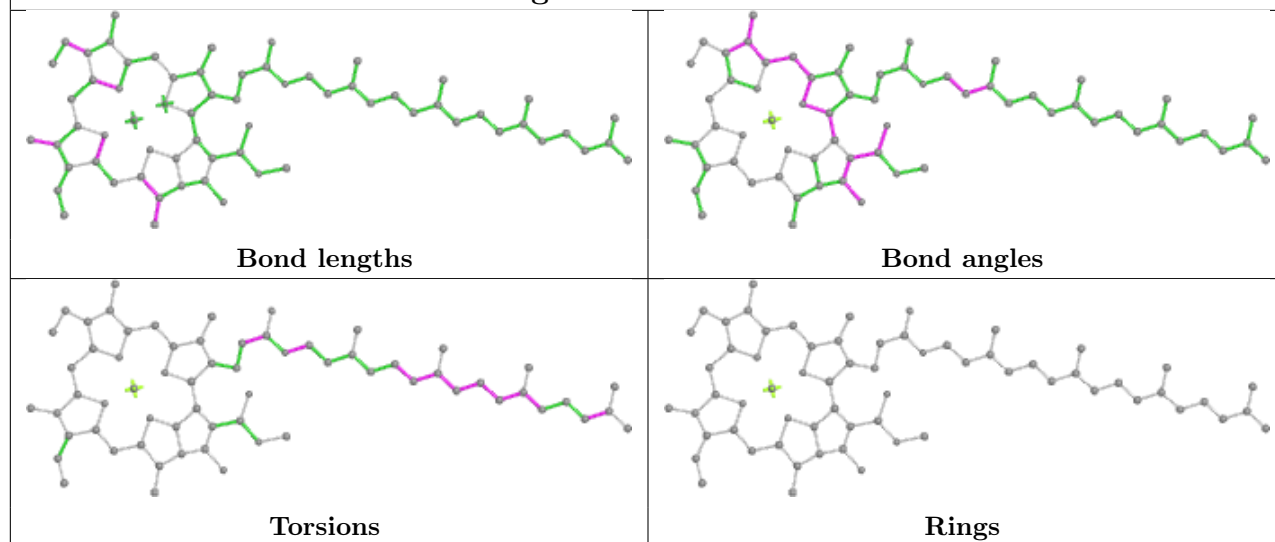


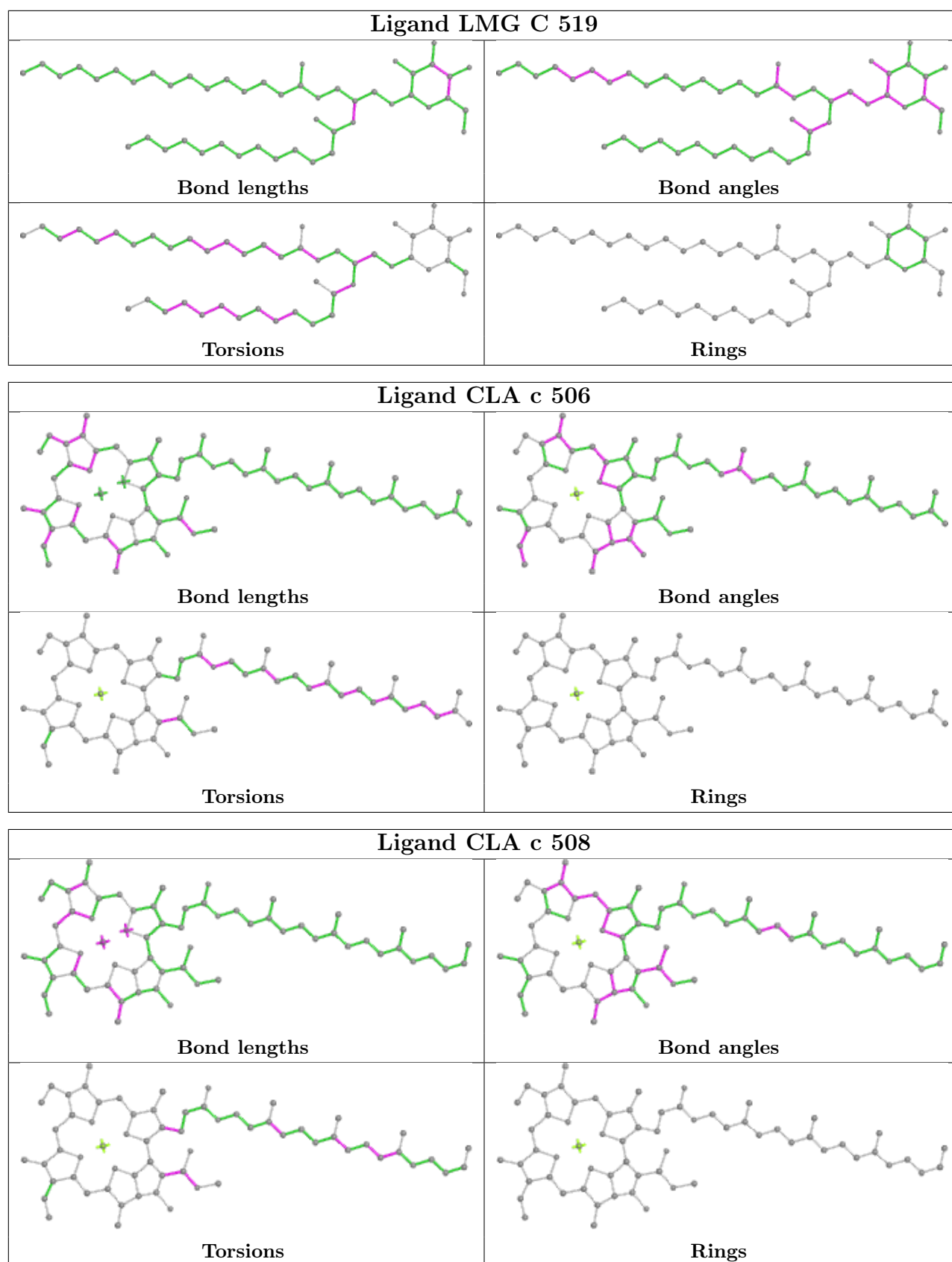


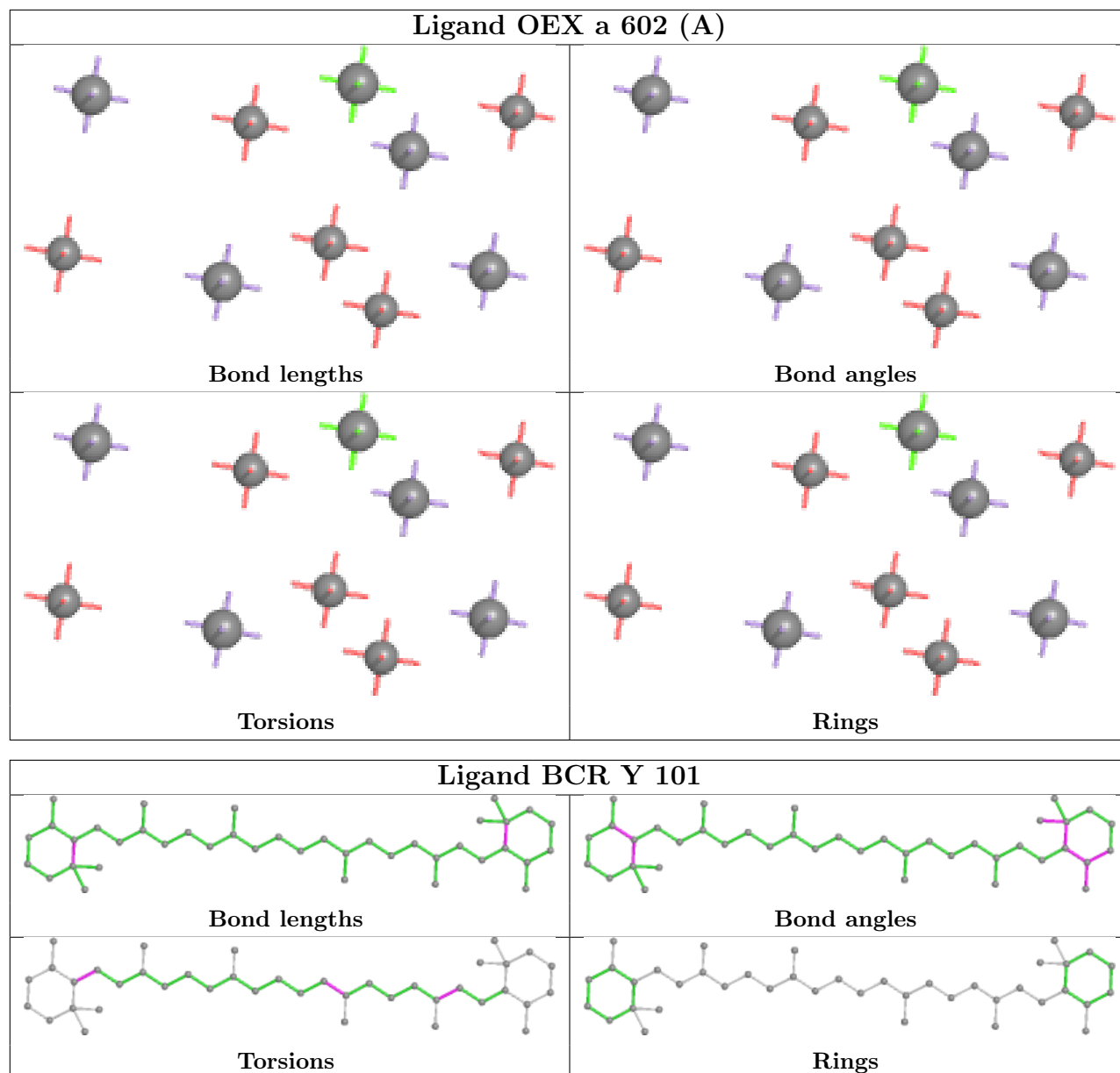
## Ligand SQD A 616

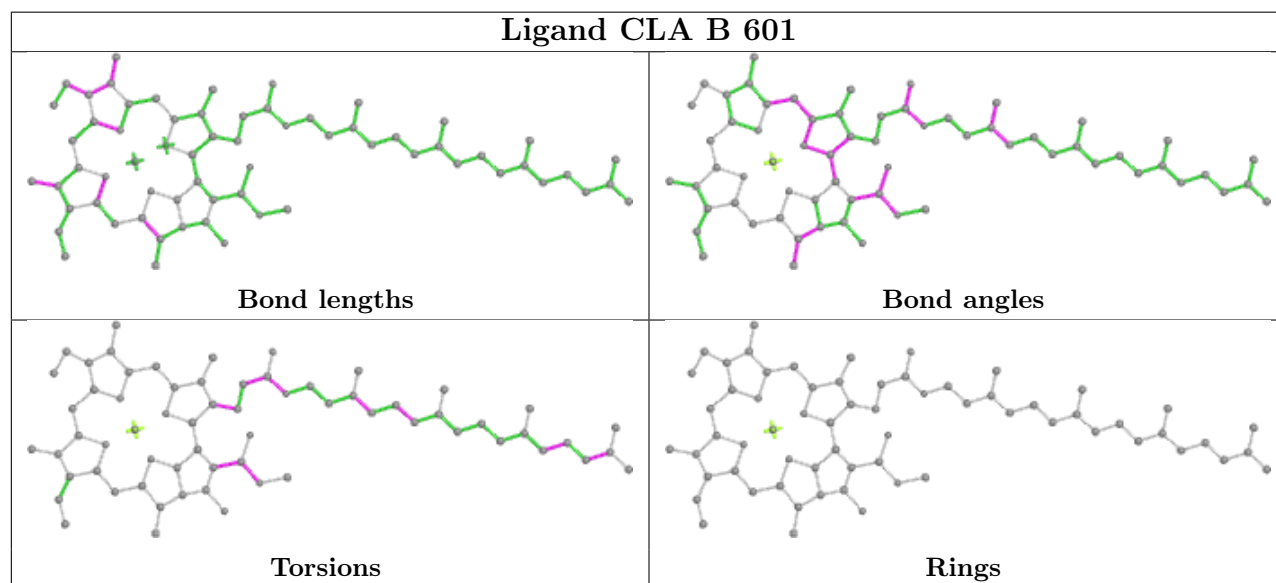
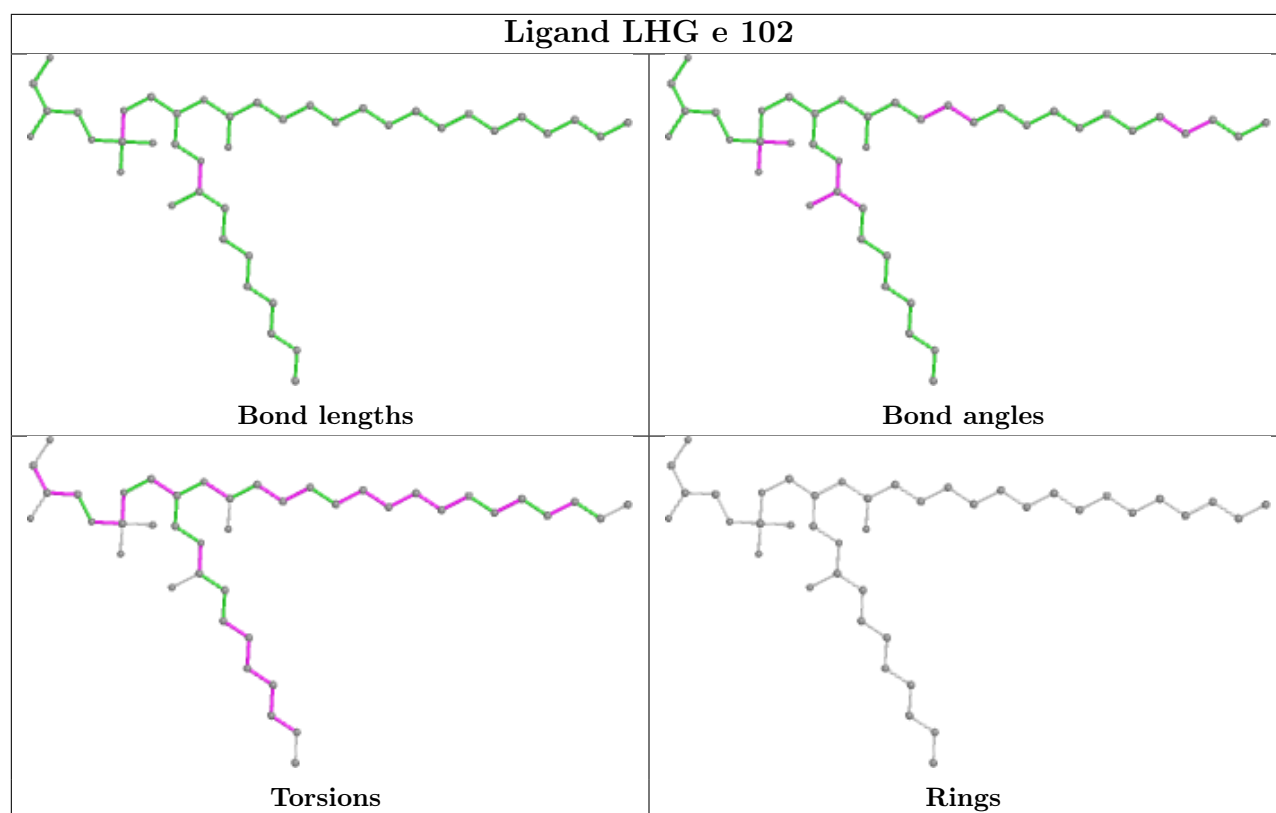


## Ligand CLA B 613

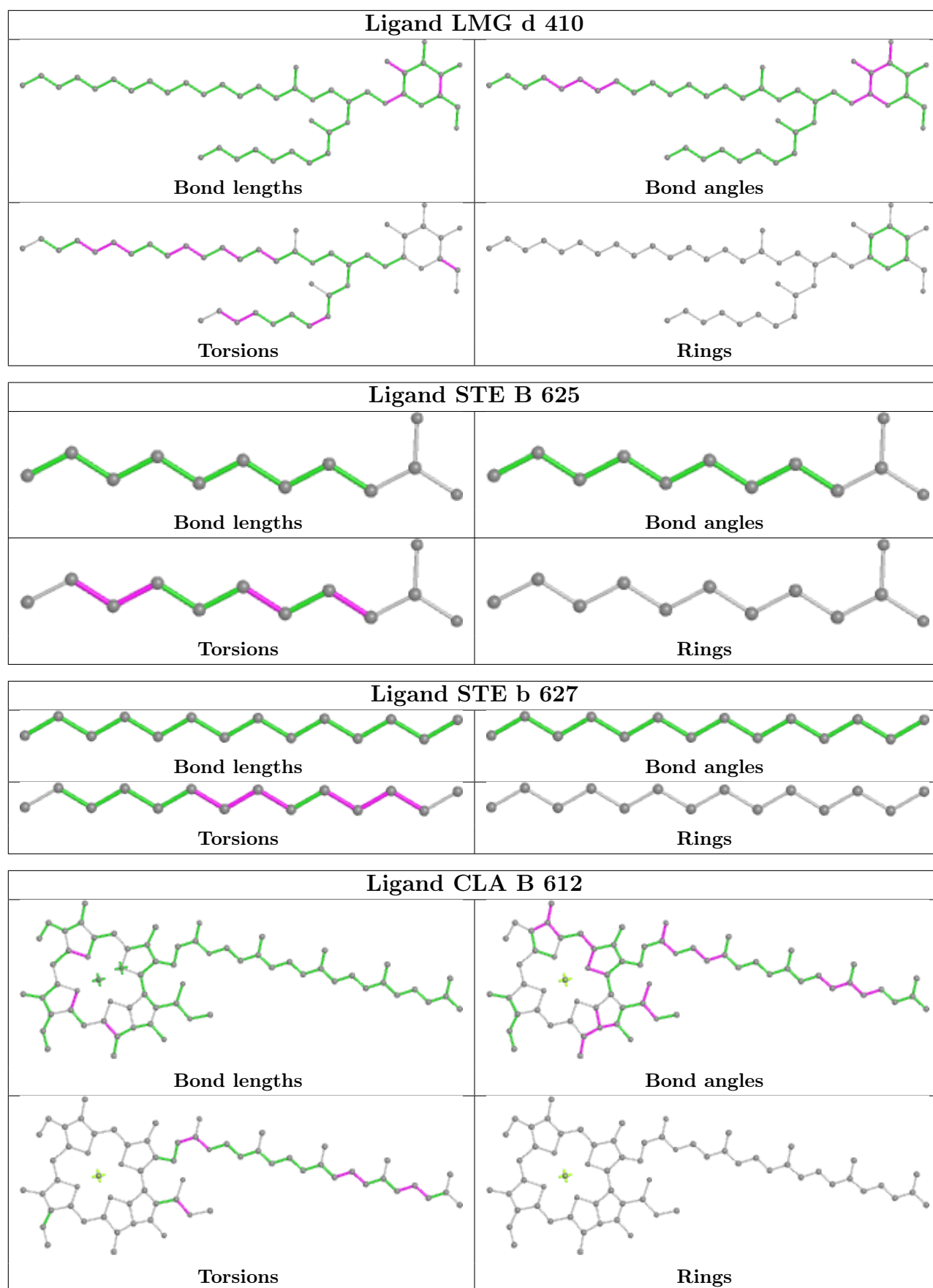


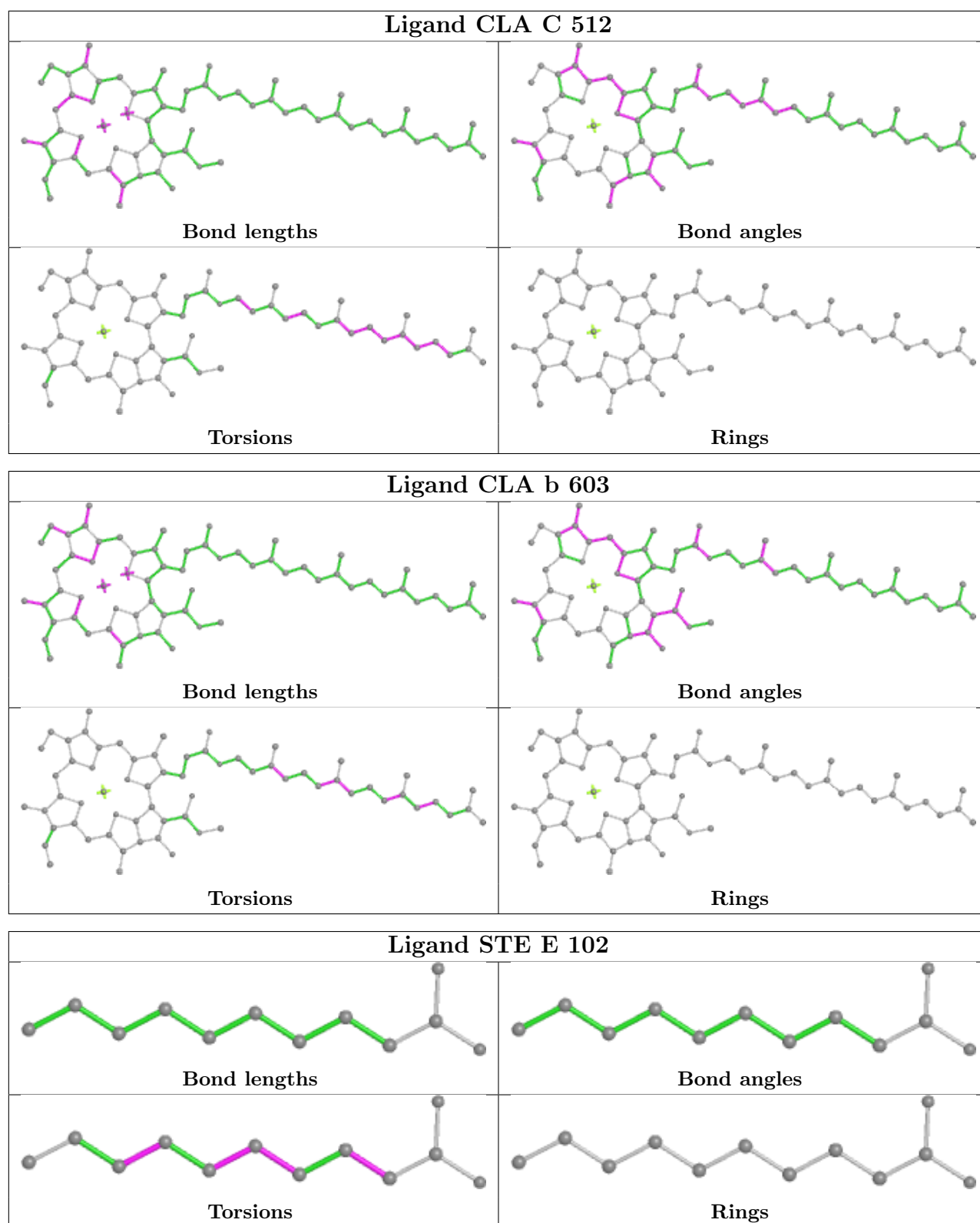


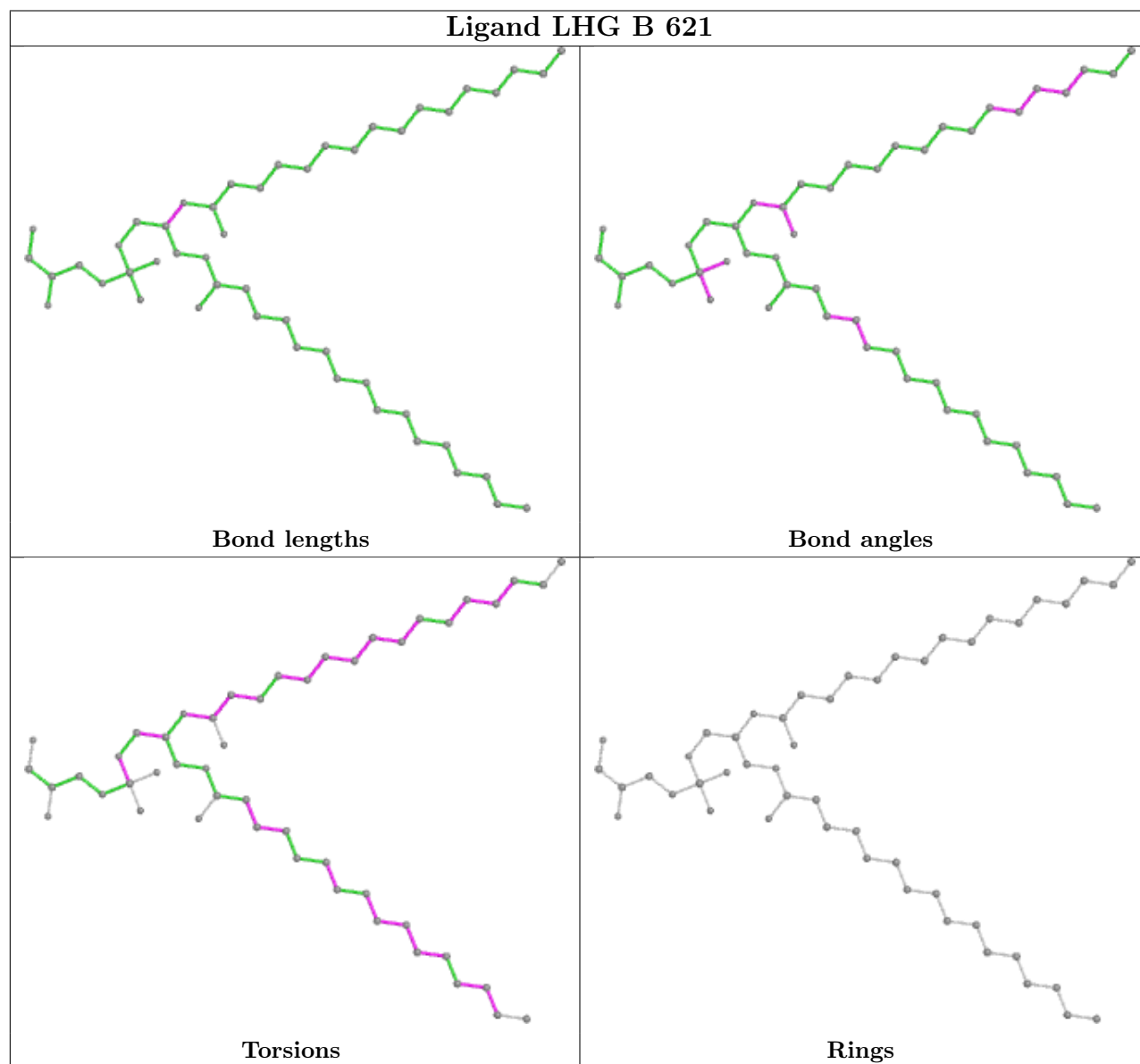
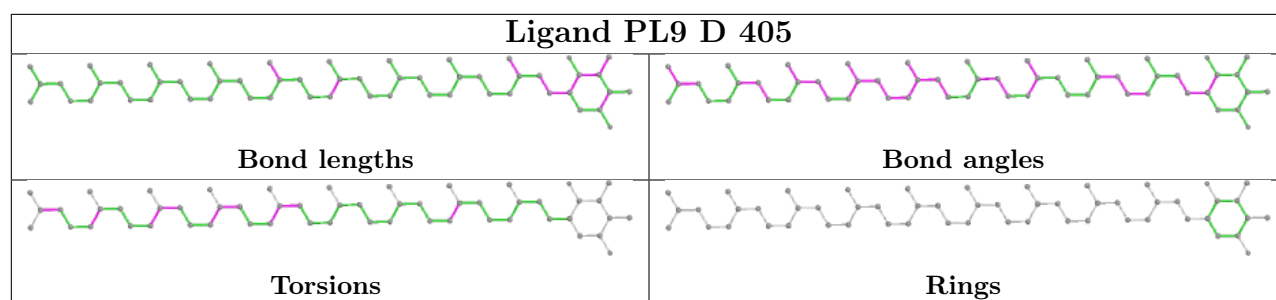


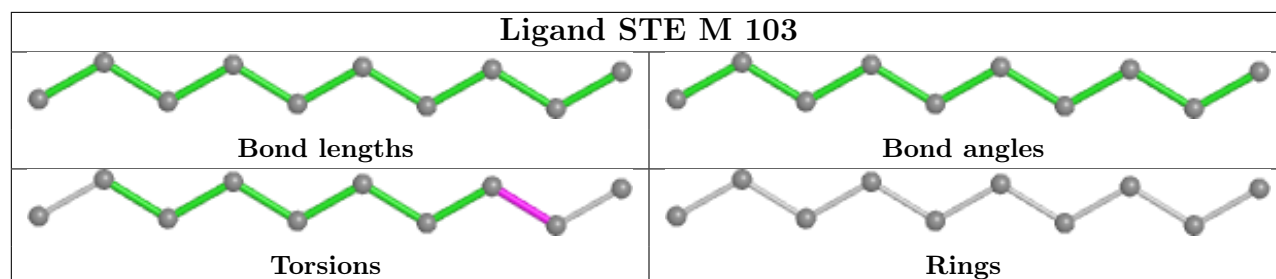
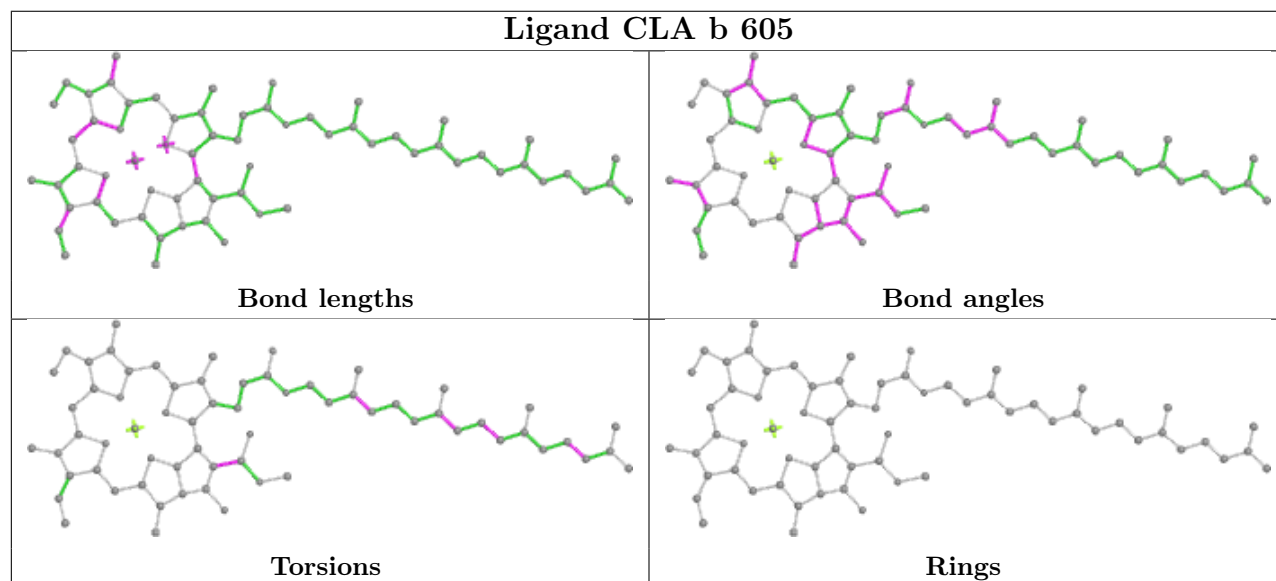
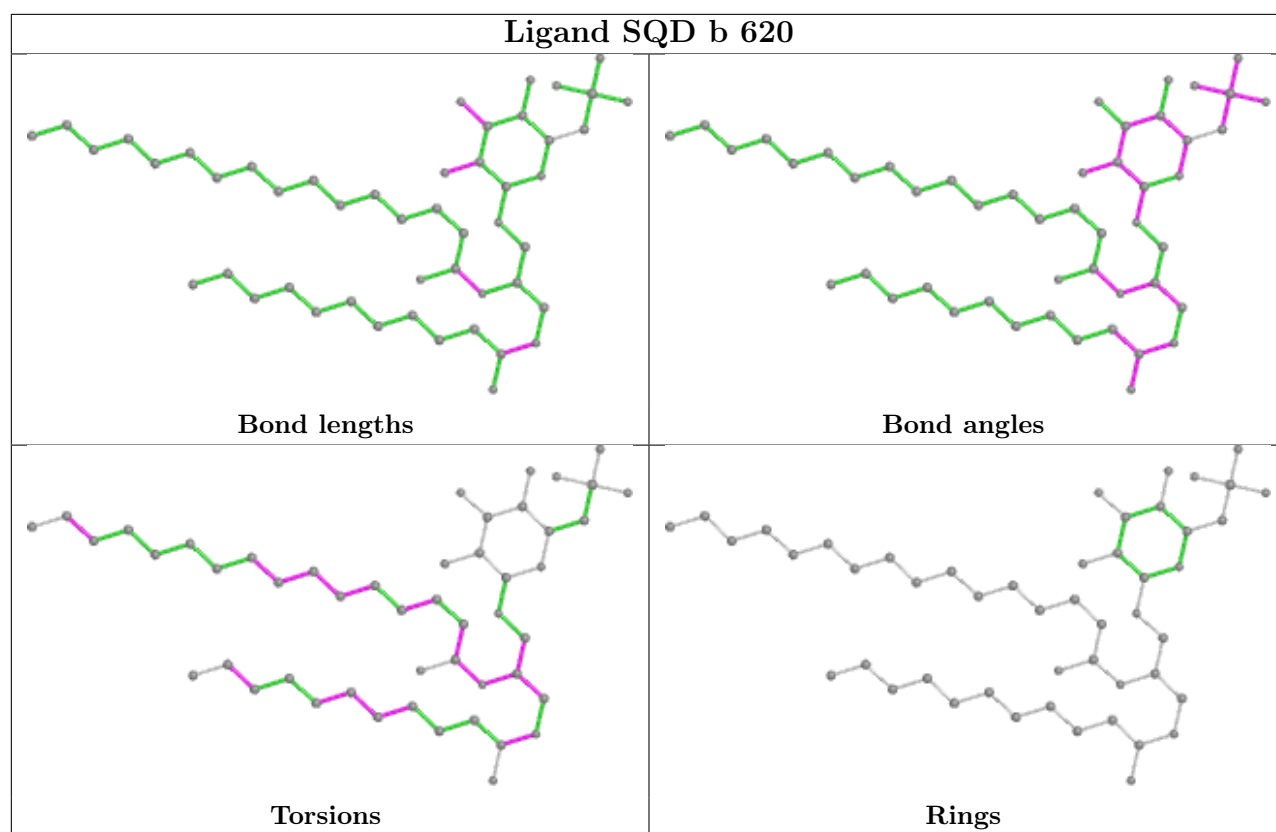


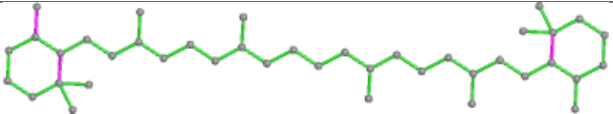
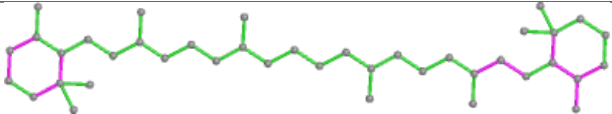
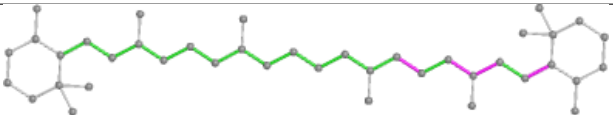
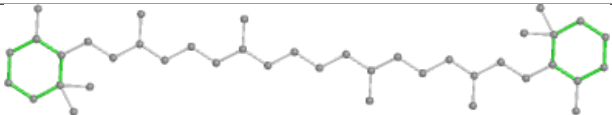








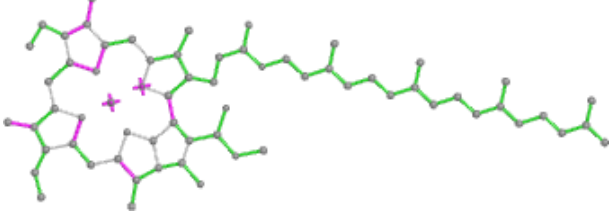
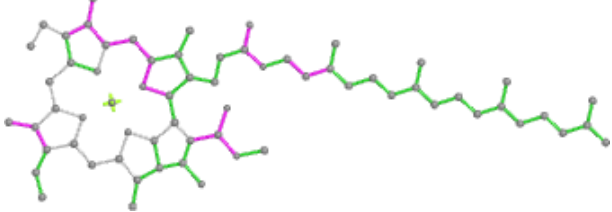
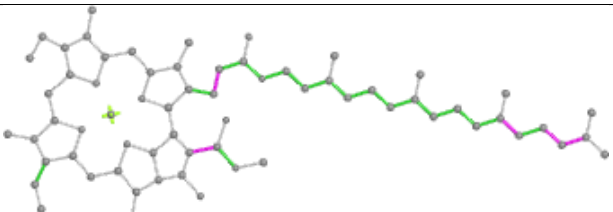
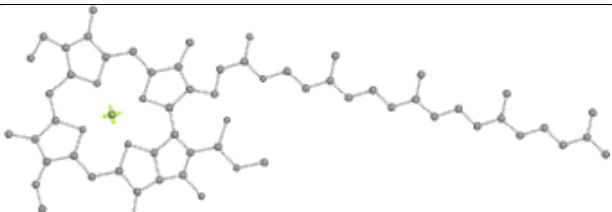


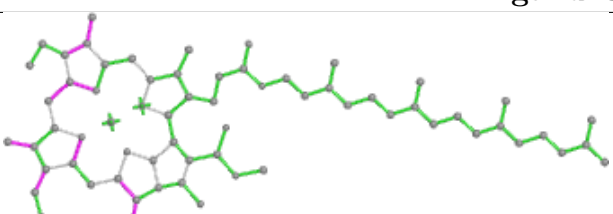
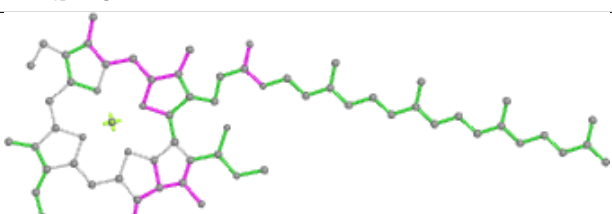
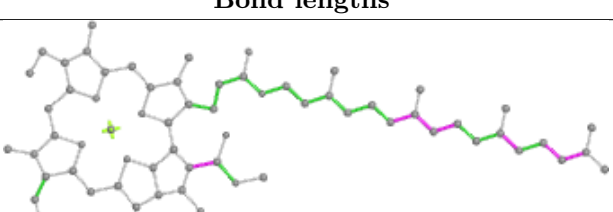
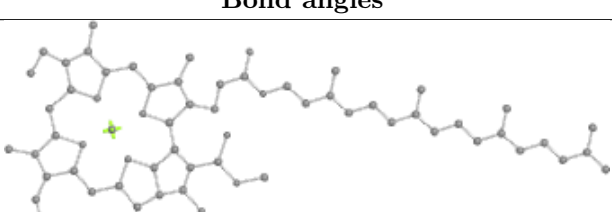


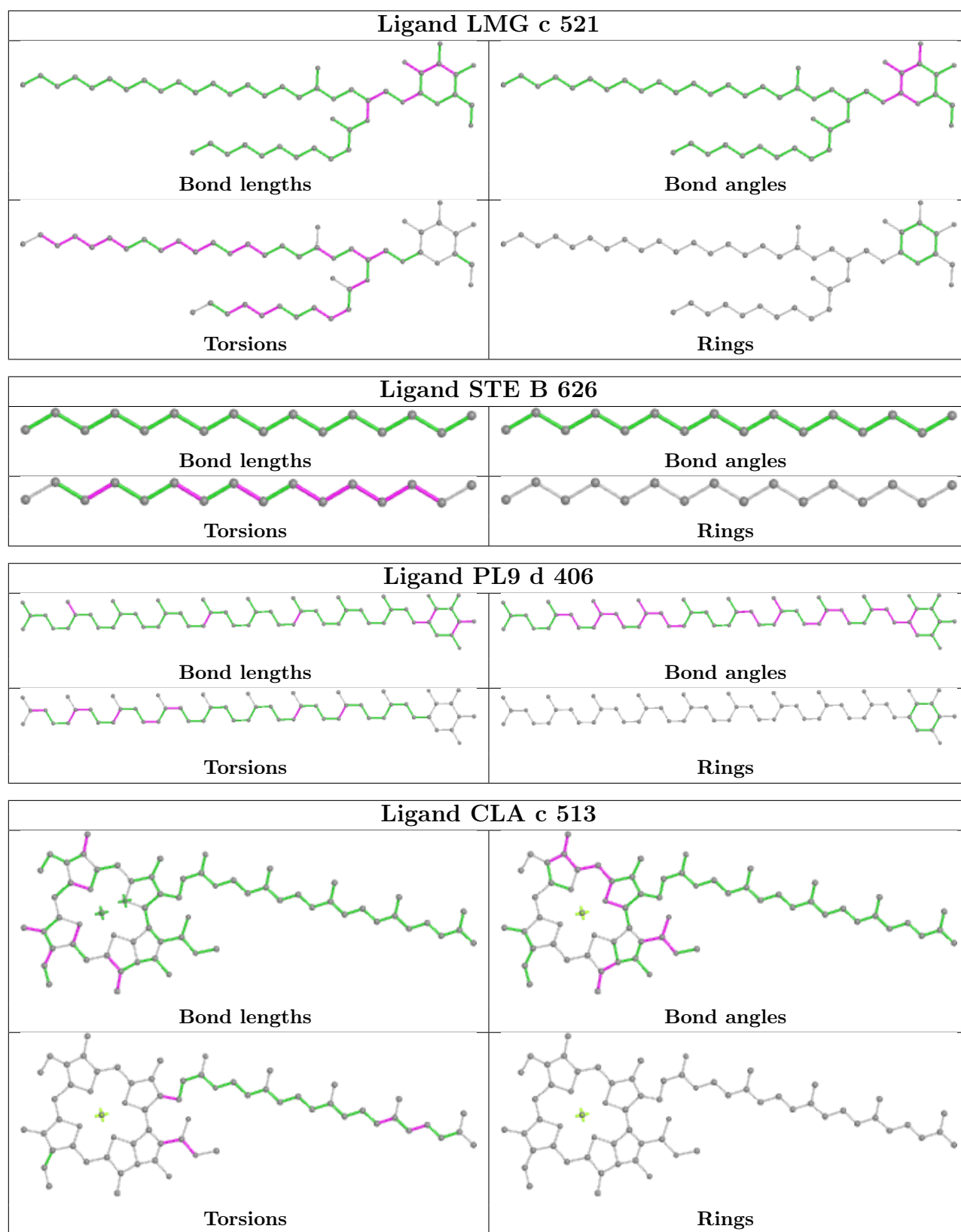


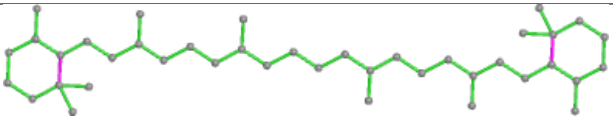
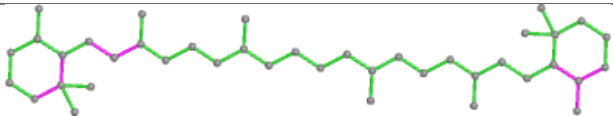
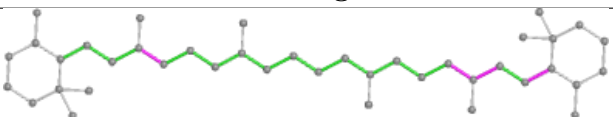
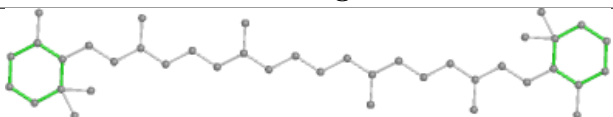
Ligand BCR d 405	
	Bond lengths
	Bond angles
	Torsions
	Rings


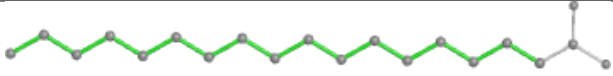
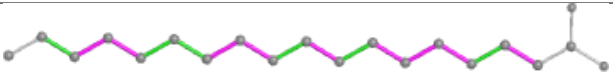
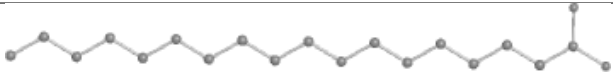
Ligand STE l 102	
	Bond lengths
	Bond angles
	Torsions
	Rings

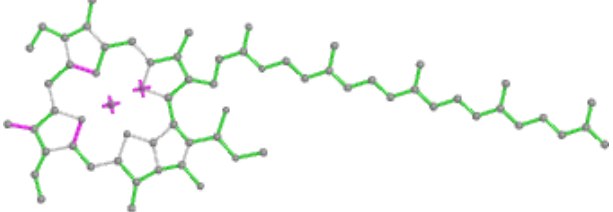
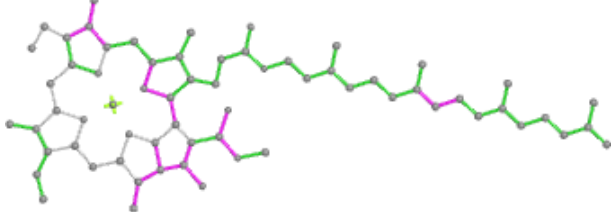
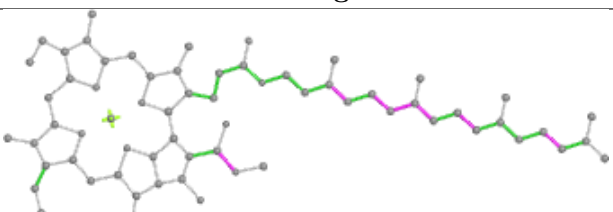
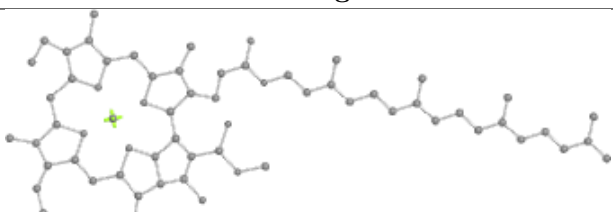
Ligand CLA B 610	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand CLA d 401	
	Bond lengths
	Bond angles
	Torsions
	Rings

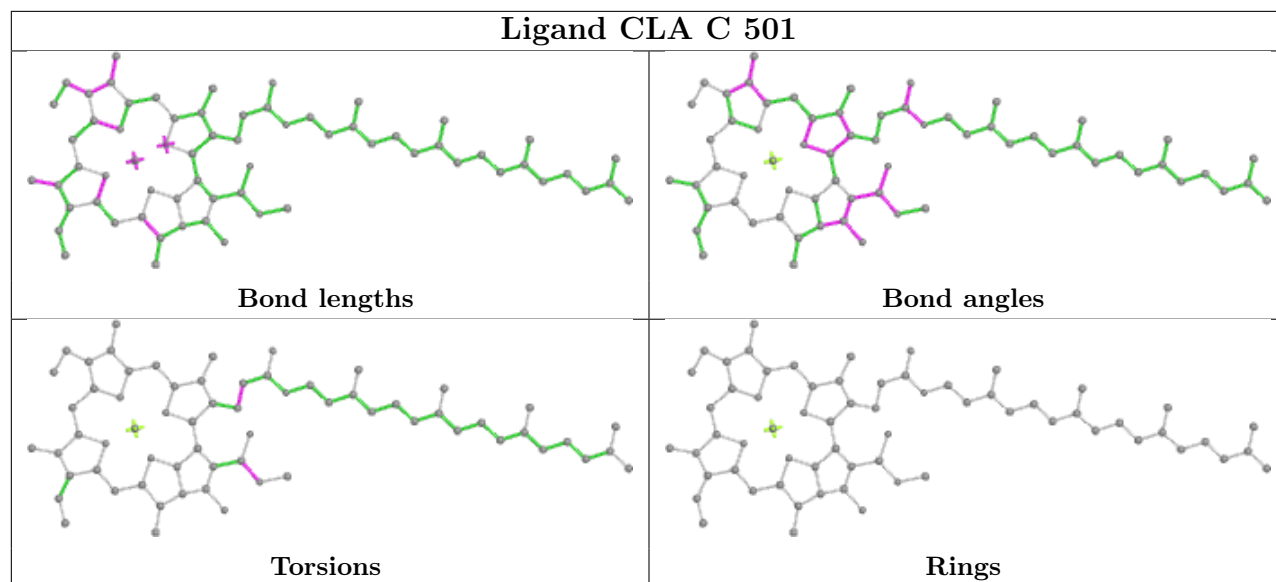


Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

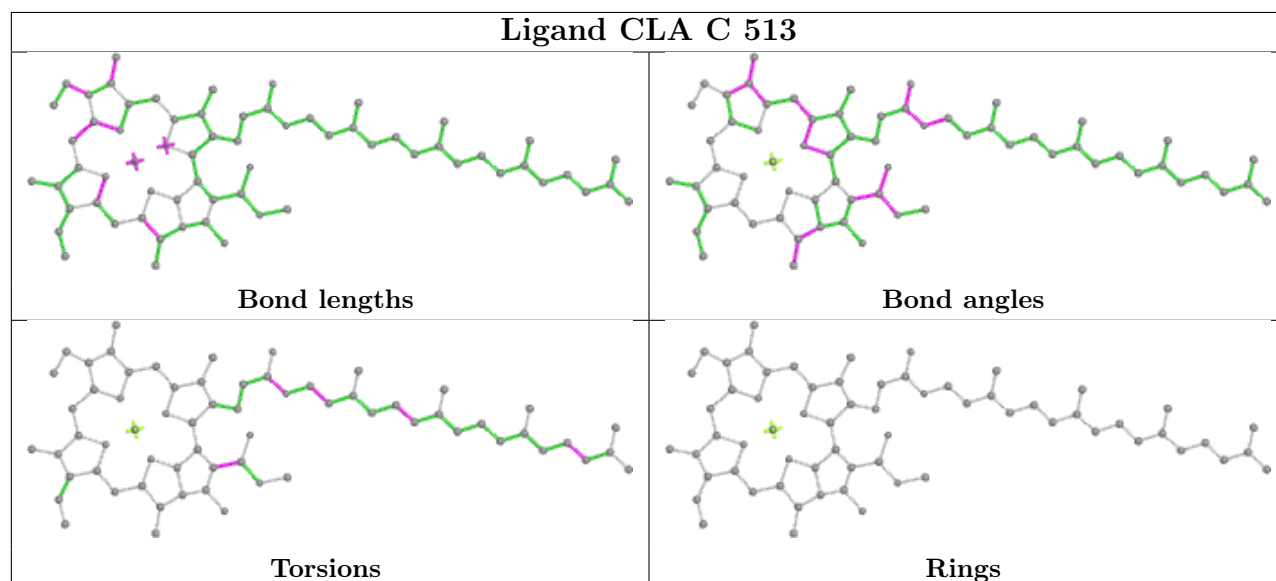
Ligand STE b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

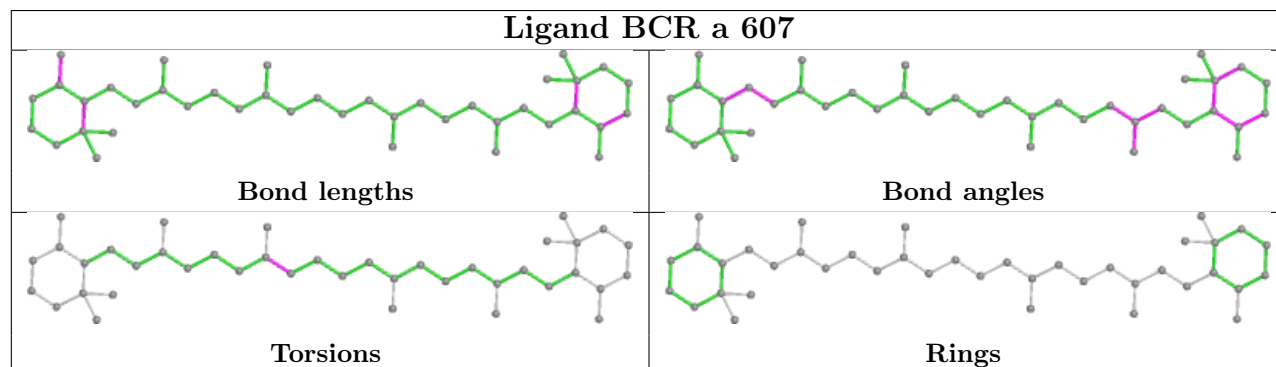
## Ligand CLA C 501



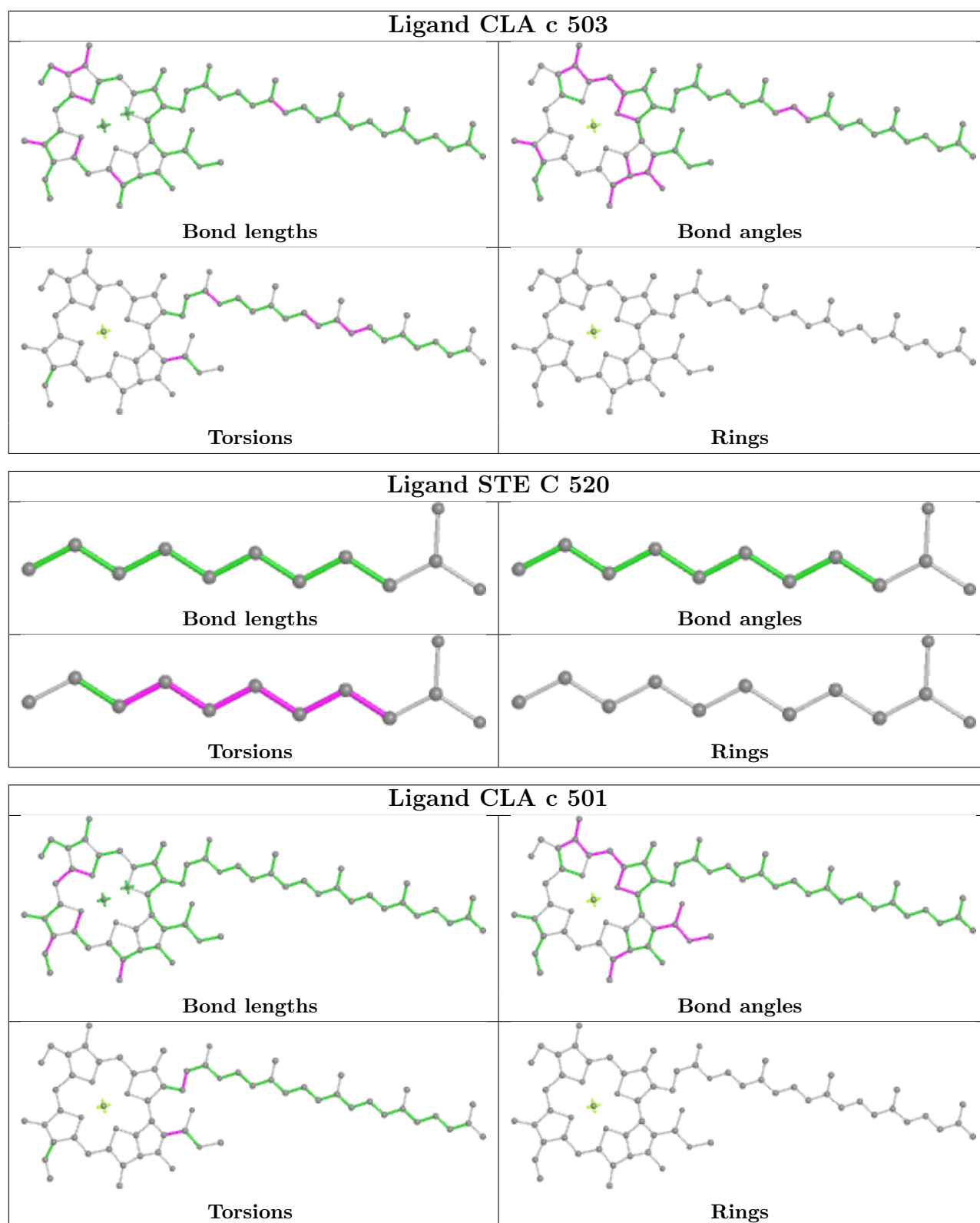
## Ligand CLA C 513



## Ligand BCR a 607







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/344 (97%)	-0.30	4 (1%) 79 78	19, 27, 44, 77	0
1	a	334/344 (97%)	-0.31	1 (0%) 94 93	22, 29, 52, 77	0
2	B	505/510 (99%)	-0.27	9 (1%) 68 66	22, 31, 57, 80	0
2	b	505/510 (99%)	-0.08	18 (3%) 42 42	22, 34, 65, 97	0
3	C	442/461 (95%)	-0.18	2 (0%) 91 90	23, 33, 48, 70	0
3	c	451/461 (97%)	-0.10	8 (1%) 68 66	24, 37, 56, 94	0
4	D	341/352 (96%)	-0.30	1 (0%) 94 93	21, 28, 43, 74	0
4	d	341/352 (96%)	-0.20	1 (0%) 94 93	22, 31, 52, 73	0
5	E	82/84 (97%)	0.09	3 (3%) 41 41	32, 47, 63, 80	0
5	e	82/84 (97%)	0.36	7 (8%) 10 10	37, 54, 70, 81	0
6	F	34/45 (75%)	-0.29	1 (2%) 51 50	33, 39, 56, 78	0
6	f	34/45 (75%)	-0.12	2 (5%) 22 21	38, 44, 68, 84	0
7	H	65/66 (98%)	0.07	4 (6%) 20 19	30, 37, 52, 67	0
7	h	63/66 (95%)	0.43	8 (12%) 3 3	36, 46, 58, 64	0
8	I	35/38 (92%)	-0.13	3 (8%) 10 9	28, 36, 65, 77	0
8	i	35/38 (92%)	0.06	3 (8%) 10 9	29, 37, 68, 85	0
9	J	36/40 (90%)	0.11	4 (11%) 5 4	31, 46, 67, 81	0
9	j	36/40 (90%)	0.21	5 (13%) 2 2	36, 50, 86, 95	0
10	K	37/46 (80%)	0.15	1 (2%) 54 53	37, 48, 65, 73	0
10	k	37/46 (80%)	0.19	3 (8%) 12 11	44, 50, 64, 76	0
11	L	37/37 (100%)	-0.31	0 100 100	23, 28, 54, 63	0
11	l	36/37 (97%)	-0.10	2 (5%) 24 23	25, 28, 66, 83	0
12	M	32/36 (88%)	0.10	0 100 100	25, 32, 54, 65	0
12	m	31/36 (86%)	-0.04	0 100 100	24, 33, 47, 61	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	0.12	16 (6%) 18 17	24, 40, 76, 127	0
13	o	244/272 (89%)	-0.02	17 (6%) 16 15	25, 38, 74, 121	0
14	R	28/41 (68%)	1.68	12 (42%) 0 0	56, 63, 77, 81	0
14	r	28/41 (68%)	3.52	22 (78%) 0 0	65, 80, 95, 99	0
15	T	29/32 (90%)	-0.27	1 (3%) 45 44	25, 29, 54, 68	0
15	t	29/32 (90%)	-0.19	2 (6%) 16 16	25, 29, 70, 80	0
16	U	97/134 (72%)	-0.12	3 (3%) 49 48	29, 39, 65, 82	0
16	u	97/134 (72%)	-0.28	0 100 100	28, 37, 52, 81	0
17	V	137/163 (84%)	-0.35	0 100 100	28, 37, 51, 73	0
17	v	137/163 (84%)	-0.04	5 (3%) 42 42	31, 44, 62, 82	0
18	X	38/41 (92%)	0.26	2 (5%) 26 25	34, 45, 62, 70	0
18	x	39/41 (95%)	0.53	5 (12%) 3 3	44, 52, 79, 92	0
19	Y	27/46 (58%)	1.54	12 (44%) 0 0	49, 63, 90, 93	0
19	y	30/46 (65%)	0.66	4 (13%) 3 2	55, 66, 81, 89	0
20	Z	62/62 (100%)	1.05	16 (25%) 0 0	50, 62, 105, 118	0
20	z	62/62 (100%)	0.97	13 (20%) 1 0	54, 67, 103, 108	0
All	All	5293/5700 (92%)	-0.06	220 (4%) 36 35	19, 35, 67, 127	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.0
2	b	495	PHE	8.0
13	O	56	PRO	7.1
14	r	6	LEU	6.8
14	r	13	LEU	6.5

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

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
12	FME	M	1	10/11	0.94	0.13	37,48,67,75	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	FME	t	1	10/11	0.94	0.10	31,44,66,66	0
8	FME	I	1	10/11	0.95	0.19	35,46,65,66	0
8	FME	i	1	10/11	0.96	0.16	33,48,59,64	0
12	FME	m	1	10/11	0.96	0.14	34,42,59,71	0
15	FME	T	1	10/11	0.96	0.08	28,45,61,61	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
33	STE	E	102	12/20	0.68	0.29	56,72,77,83	0
33	STE	H	103	18/20	0.71	0.30	49,67,78,81	0
33	STE	a	616	12/20	0.75	0.26	45,61,68,71	0
33	STE	B	627	12/20	0.76	0.35	47,60,73,74	0
33	STE	k	103	12/20	0.77	0.21	49,67,78,80	0
33	STE	b	625	20/20	0.78	0.23	47,62,72,76	0
29	LMG	c	521	48/55	0.78	0.26	50,71,93,96	0
33	STE	a	615	10/20	0.79	0.23	40,60,68,69	0
33	STE	a	617	15/20	0.79	0.20	38,57,69,77	0
33	STE	b	626	10/20	0.81	0.23	42,54,62,63	0
31	SQD	a	614	36/54	0.81	0.19	33,61,81,83	0
33	STE	m	101	12/20	0.81	0.20	45,61,75,76	0
33	STE	d	412	20/20	0.82	0.20	41,65,84,85	0
33	STE	j	101	12/20	0.82	0.16	45,58,67,70	0
29	LMG	a	618	55/55	0.82	0.17	38,58,72,83	0
32	DGD	A	618	66/66	0.82	0.18	43,61,74,82	0
29	LMG	c	522	49/55	0.83	0.18	37,56,81,96	0
24	CLA	b	601	65/65	0.83	0.18	47,65,83,96	0
26	BCR	H	101	40/40	0.83	0.15	30,46,59,63	0
33	STE	b	624	16/20	0.84	0.15	45,61,70,73	0
28	PL9	A	612	55/55	0.84	0.24	33,62,82,85	0
30	LHG	e	102	42/49	0.84	0.26	52,77,103,111	0
33	STE	b	627	14/20	0.84	0.23	50,65,77,78	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	SQD	A	617	39/54	0.84	0.19	40,59,87,92	0
29	LMG	b	623	55/55	0.84	0.29	51,68,87,91	0
29	LMG	D	409	33/55	0.84	0.20	37,56,77,84	0
33	STE	B	620	17/20	0.84	0.22	36,51,64,65	0
30	LHG	E	101	49/49	0.85	0.21	46,71,102,108	0
29	LMG	A	614	48/55	0.85	0.16	37,55,74,84	0
33	STE	B	626	16/20	0.85	0.27	45,58,70,74	0
24	CLA	C	512	65/65	0.85	0.17	33,51,81,86	0
33	STE	C	522	12/20	0.85	0.14	39,49,57,58	0
33	STE	l	102	18/20	0.85	0.16	36,49,76,78	0
24	CLA	B	601	65/65	0.85	0.16	32,58,84,95	0
28	PL9	a	611	55/55	0.86	0.19	32,65,80,88	0
24	CLA	c	513	65/65	0.86	0.21	44,65,100,105	0
24	CLA	C	513	65/65	0.86	0.19	41,62,84,92	0
26	BCR	d	405	40/40	0.86	0.14	37,52,87,93	0
26	BCR	x	101	40/40	0.86	0.15	37,52,71,75	0
24	CLA	c	512	65/65	0.86	0.17	41,56,88,94	0
33	STE	I	101	15/20	0.87	0.17	40,55,75,80	0
33	STE	B	624	14/20	0.87	0.14	36,51,61,63	0
31	SQD	B	623	54/54	0.87	0.16	39,57,81,90	0
26	BCR	Y	101	40/40	0.87	0.13	32,50,62,69	0
33	STE	c	520	20/20	0.87	0.21	36,55,71,76	0
33	STE	J	101	12/20	0.88	0.14	45,55,63,65	0
33	STE	M	103	10/20	0.88	0.16	33,43,52,58	0
33	STE	T	103	15/20	0.88	0.20	43,55,68,71	0
33	STE	Z	101	8/20	0.88	0.16	41,57,64,64	0
33	STE	D	411	20/20	0.88	0.19	35,49,68,72	0
26	BCR	C	514	40/40	0.88	0.15	38,55,68,71	0
26	BCR	k	101	40/40	0.88	0.14	39,56,68,69	0
33	STE	b	622	20/20	0.88	0.22	38,53,67,67	0
31	SQD	f	101	41/54	0.88	0.20	54,77,98,101	0
33	STE	t	102	18/20	0.88	0.15	42,55,72,77	0
33	STE	T	102	16/20	0.89	0.17	30,48,62,65	0
33	STE	C	521	16/20	0.89	0.12	37,51,64,71	0
29	LMG	C	519	48/55	0.89	0.18	39,67,85,89	0
33	STE	x	102	20/20	0.89	0.22	38,55,68,71	0
29	LMG	b	621	51/55	0.90	0.13	35,51,70,76	0
26	BCR	D	404	40/40	0.90	0.14	28,43,79,87	0
33	STE	d	411	17/20	0.90	0.14	41,52,64,65	0
29	LMG	c	519	37/55	0.90	0.15	44,63,80,85	0
24	CLA	D	403	65/65	0.90	0.14	22,42,105,112	0
29	LMG	D	406	51/55	0.90	0.19	26,52,75,84	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	d	404	65/65	0.90	0.16	28,47,81,87	0
29	LMG	D	410	28/55	0.90	0.16	36,50,61,63	0
24	CLA	a	606	65/65	0.90	0.14	19,36,78,84	0
33	STE	C	520	12/20	0.90	0.12	44,56,64,64	0
29	LMG	M	101	51/55	0.91	0.14	31,47,64,73	0
26	BCR	k	102	40/40	0.91	0.19	39,51,63,68	0
24	CLA	c	508	64/65	0.91	0.16	29,43,83,98	0
26	BCR	c	514	40/40	0.91	0.15	46,59,68,70	0
31	SQD	b	620	49/54	0.91	0.15	38,54,87,97	0
33	STE	B	625	12/20	0.92	0.10	37,51,59,66	0
24	CLA	C	502	65/65	0.92	0.14	25,39,52,59	0
26	BCR	B	618	40/40	0.92	0.10	23,38,49,49	0
26	BCR	B	619	40/40	0.92	0.12	25,41,54,62	0
24	CLA	b	615	65/65	0.92	0.14	26,39,57,63	0
32	DGD	c	518	62/66	0.92	0.15	25,49,80,86	0
24	CLA	c	502	65/65	0.92	0.14	29,40,55,62	0
31	SQD	D	407	36/54	0.92	0.17	41,65,80,82	0
32	DGD	c	517	62/66	0.93	0.13	31,51,87,90	0
24	CLA	c	510	65/65	0.93	0.15	28,45,58,71	0
24	CLA	C	506	65/65	0.93	0.12	26,42,78,84	0
24	CLA	C	511	65/65	0.93	0.12	30,48,65,70	0
24	CLA	b	602	65/65	0.93	0.15	27,41,57,62	0
29	LMG	d	410	44/55	0.93	0.14	33,51,79,86	0
24	CLA	b	606	65/65	0.93	0.13	25,39,70,73	0
24	CLA	b	609	65/65	0.93	0.15	29,43,62,68	0
24	CLA	B	615	65/65	0.93	0.12	22,36,59,63	0
24	CLA	b	616	60/65	0.93	0.14	26,41,81,83	0
24	CLA	B	616	60/65	0.93	0.14	23,37,88,95	0
31	SQD	a	613	54/54	0.93	0.17	38,60,79,84	0
24	CLA	c	506	65/65	0.93	0.12	31,48,89,90	0
26	BCR	b	619	40/40	0.93	0.12	26,47,61,69	0
24	CLA	c	507	65/65	0.93	0.14	26,43,58,64	0
24	CLA	B	604	65/65	0.93	0.13	21,32,68,71	0
32	DGD	C	517	62/66	0.93	0.13	27,47,92,108	0
32	DGD	H	102	62/66	0.93	0.11	25,43,55,60	0
24	CLA	d	401	65/65	0.94	0.14	24,37,86,90	0
28	PL9	D	405	55/55	0.94	0.11	19,31,46,47	0
24	CLA	C	505	65/65	0.94	0.15	23,39,65,81	0
33	STE	M	102	15/20	0.94	0.11	36,47,59,62	0
24	CLA	B	614	65/65	0.94	0.16	20,35,70,80	0
24	CLA	c	503	65/65	0.94	0.15	28,42,53,61	0
24	CLA	c	504	60/65	0.94	0.12	31,43,78,85	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	C	515	40/40	0.94	0.12	27,40,50,61	0
32	DGD	C	516	62/66	0.94	0.12	21,40,77,80	0
24	CLA	c	505	65/65	0.94	0.18	25,38,66,72	0
32	DGD	C	518	62/66	0.94	0.13	24,46,75,85	0
24	CLA	C	507	65/65	0.94	0.14	25,38,53,57	0
26	BCR	T	101	40/40	0.94	0.10	25,37,50,52	0
24	CLA	C	510	65/65	0.94	0.14	26,41,61,62	0
32	DGD	h	101	62/66	0.94	0.11	31,45,57,64	0
26	BCR	b	617	40/40	0.94	0.12	29,40,51,54	0
26	BCR	b	618	40/40	0.94	0.10	26,39,51,54	0
24	CLA	B	602	65/65	0.94	0.15	23,35,54,61	0
24	CLA	c	509	65/65	0.94	0.18	32,46,61,69	0
24	CLA	b	608	65/65	0.94	0.15	25,42,61,66	0
30	LHG	A	615	47/49	0.94	0.13	27,48,77,88	0
24	CLA	c	511	65/65	0.94	0.13	33,50,70,75	0
24	CLA	B	606	65/65	0.94	0.11	23,34,65,71	0
31	SQD	A	616	52/54	0.94	0.16	34,54,90,95	0
24	CLA	B	610	65/65	0.94	0.15	20,32,42,45	0
24	CLA	A	605	65/65	0.95	0.13	23,33,83,91	0
24	CLA	A	608	54/65	0.95	0.11	17,32,67,69	0
30	LHG	d	407	49/49	0.95	0.13	34,47,70,74	0
24	CLA	b	603	65/65	0.95	0.14	23,36,60,68	0
26	BCR	c	515	40/40	0.95	0.11	27,42,58,61	0
24	CLA	b	604	65/65	0.95	0.13	19,35,79,89	0
24	CLA	b	605	65/65	0.95	0.12	21,34,49,54	0
24	CLA	C	508	65/65	0.95	0.12	26,38,98,109	0
26	BCR	t	101	40/40	0.95	0.10	27,37,50,54	0
24	CLA	b	607	65/65	0.95	0.12	20,35,62,68	0
24	CLA	C	509	65/65	0.95	0.18	26,42,60,64	0
24	CLA	B	609	65/65	0.95	0.12	24,36,58,66	0
24	CLA	b	610	65/65	0.95	0.19	22,37,50,54	0
28	PL9	d	406	55/55	0.95	0.11	20,34,42,44	0
24	CLA	b	611	65/65	0.95	0.14	22,33,52,62	0
26	BCR	B	617	40/40	0.95	0.12	26,38,56,60	0
24	CLA	b	612	65/65	0.95	0.17	21,34,47,56	0
32	DGD	c	516	62/66	0.95	0.11	21,41,67,74	0
24	CLA	b	613	65/65	0.95	0.14	17,33,66,74	0
24	CLA	b	614	65/65	0.95	0.12	24,38,68,76	0
24	CLA	C	501	65/65	0.95	0.14	21,35,48,51	0
24	CLA	B	603	65/65	0.95	0.15	20,32,61,63	0
24	CLA	c	501	65/65	0.95	0.13	28,39,51,55	0
26	BCR	K	101	40/40	0.95	0.15	34,49,65,65	0

*Continued on next page...*



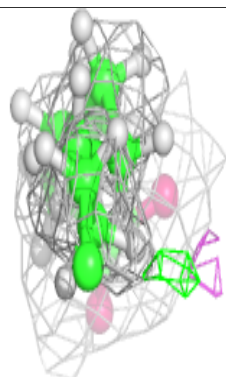
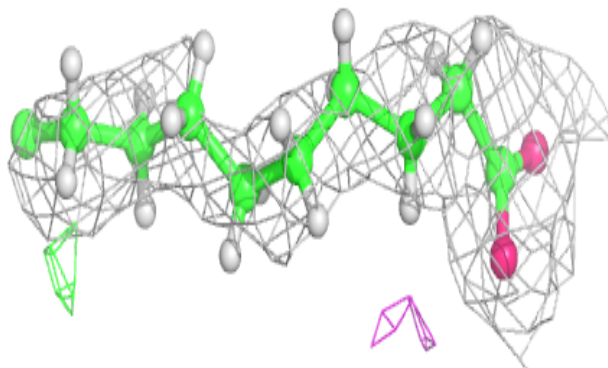
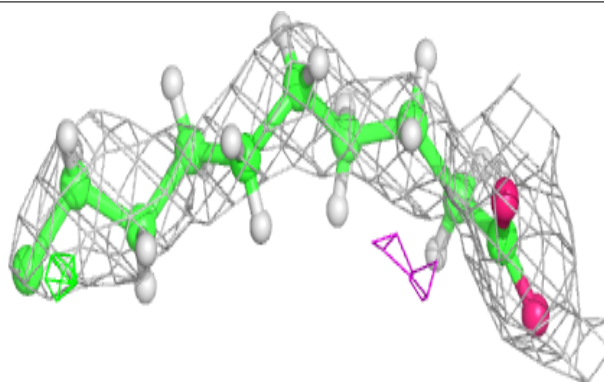
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	C	503	65/65	0.95	0.13	27,39,48,51	0
24	CLA	C	504	59/65	0.95	0.12	28,40,79,80	0
26	BCR	a	607	40/40	0.95	0.09	23,33,43,49	0
24	CLA	B	613	65/65	0.95	0.14	17,31,65,70	0
24	CLA	a	604	65/65	0.96	0.10	18,28,45,55	0
30	LHG	B	621	49/49	0.96	0.11	26,40,54,61	0
30	LHG	B	622	49/49	0.96	0.11	29,43,64,69	0
24	CLA	B	605	65/65	0.96	0.14	20,31,47,50	0
24	CLA	a	612	65/65	0.96	0.11	20,29,46,51	0
30	LHG	d	409	39/49	0.96	0.11	30,44,67,68	0
24	CLA	d	403	65/65	0.96	0.11	20,32,54,64	0
30	LHG	l	101	49/49	0.96	0.10	30,42,51,57	0
24	CLA	B	611	65/65	0.96	0.14	19,31,49,52	0
25	PHO	A	606	64/64	0.96	0.10	17,27,35,41	0
25	PHO	A	607	64/64	0.96	0.11	22,31,40,42	0
25	PHO	a	605	64/64	0.96	0.12	18,29,37,46	0
25	PHO	d	402	64/64	0.96	0.11	26,35,45,49	0
26	BCR	A	609	40/40	0.96	0.10	21,34,42,44	0
24	CLA	B	612	65/65	0.96	0.15	19,32,49,53	0
24	CLA	A	604	65/65	0.96	0.11	15,26,44,54	0
24	CLA	B	607	65/65	0.96	0.11	17,32,57,67	0
24	CLA	B	608	65/65	0.96	0.13	18,33,54,56	0
24	CLA	D	402	65/65	0.96	0.11	17,28,54,56	0
24	CLA	A	613	65/65	0.96	0.10	18,28,47,53	0
34	BCT	a	610	4/4	0.96	0.21	28,33,39,47	0
35	HEM	F	101	43/43	0.96	0.11	34,46,60,62	0
30	LHG	d	408	49/49	0.97	0.09	24,41,51,60	0
30	LHG	D	408	49/49	0.97	0.10	21,40,52,57	0
35	HEM	e	101	43/43	0.97	0.12	41,53,73,73	0
34	BCT	D	401	4/4	0.98	0.19	27,28,31,38	0
36	HEC	V	201	43/43	0.98	0.12	23,31,40,40	0
36	HEC	v	201	43/43	0.98	0.13	26,36,46,46	0
21	OEY	A	601[B]	11/11	0.99	0.13	15,20,23,26	11
27	CL	A	610	1/1	0.99	0.06	28,28,28,28	0
27	CL	A	611	1/1	0.99	0.04	27,27,27,27	0
27	CL	a	608	1/1	0.99	0.05	25,25,25,25	0
27	CL	a	609	1/1	0.99	0.03	25,25,25,25	0
21	OEY	a	601[B]	11/11	0.99	0.10	15,21,24,26	11
22	OEX	A	602[A]	10/10	0.99	0.13	29,31,35,35	10
22	OEX	a	602[A]	10/10	0.99	0.10	27,32,35,35	10
23	FE2	a	603	1/1	0.99	0.05	29,29,29,29	0
23	FE2	A	603	1/1	1.00	0.08	24,24,24,24	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.

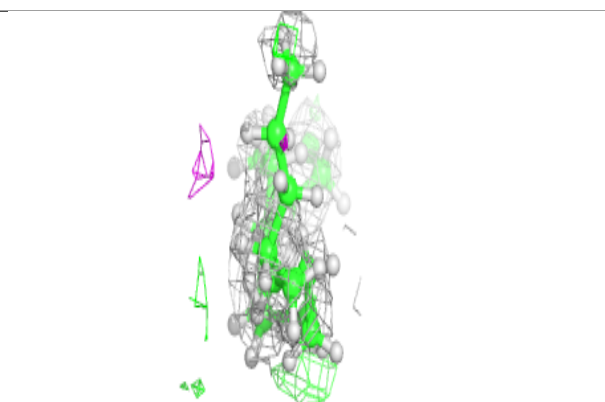
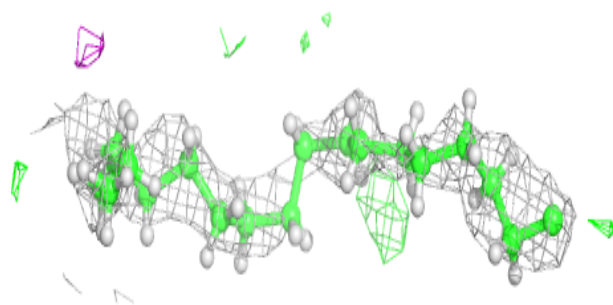
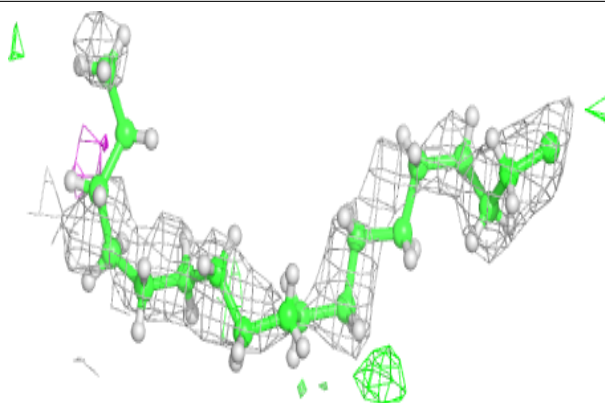
**Electron density around STE E 102:**

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

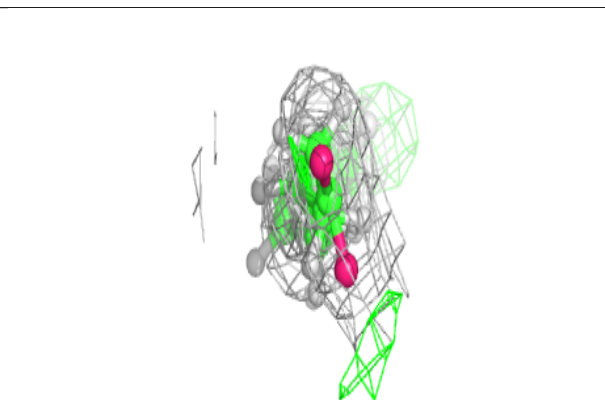
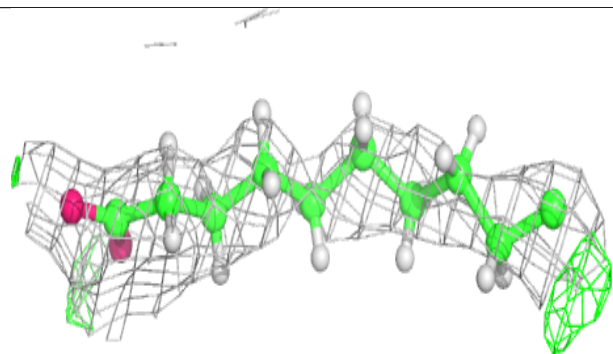
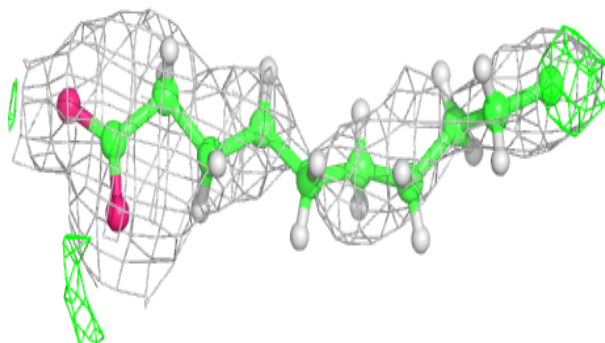


**Electron density around STE H 103:**

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

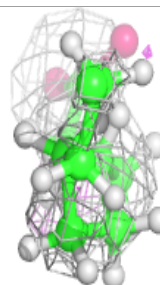
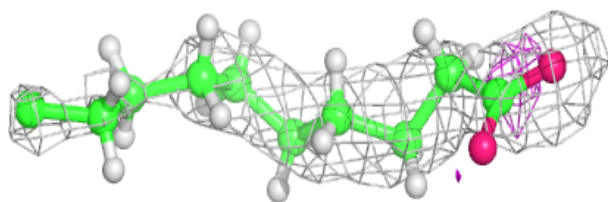
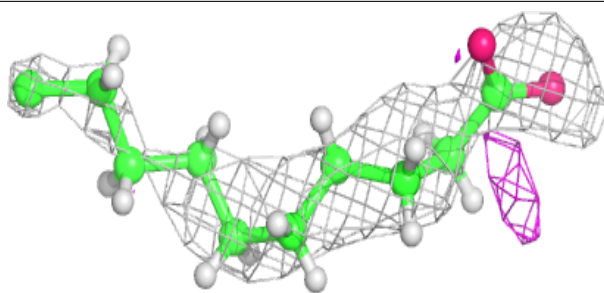
**Electron density around STE a 616:**

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

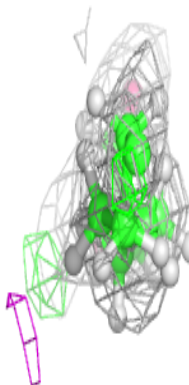
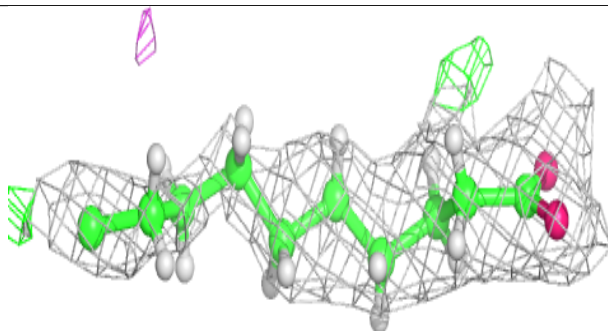
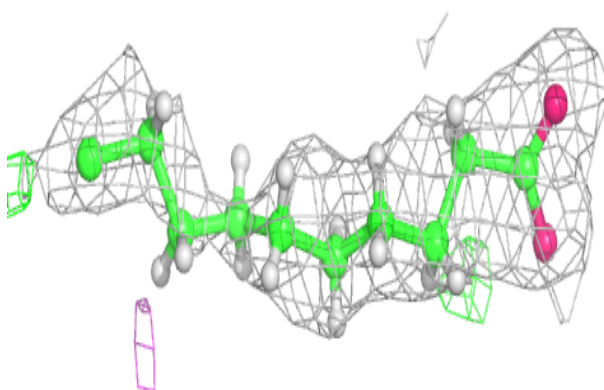


**Electron density around STE B 627:**

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

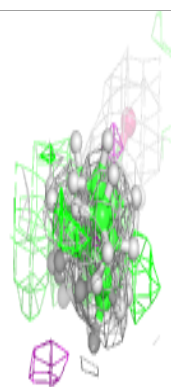
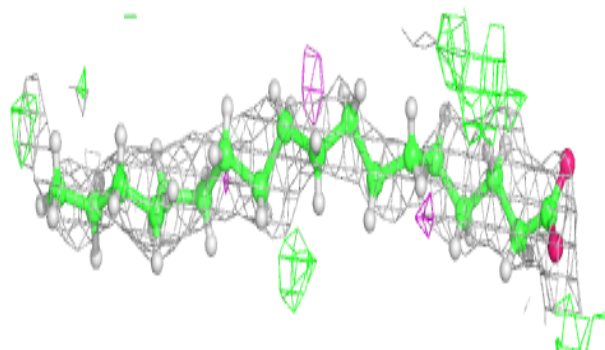
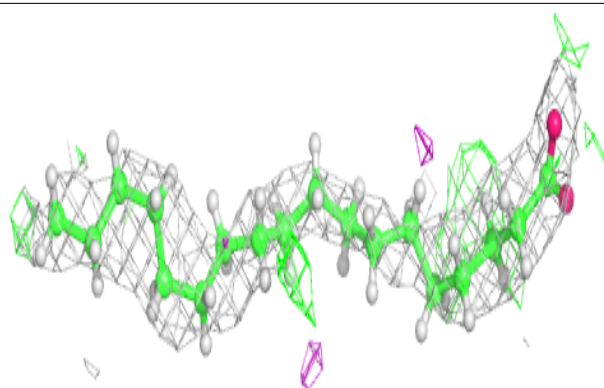
**Electron density around STE k 103:**

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

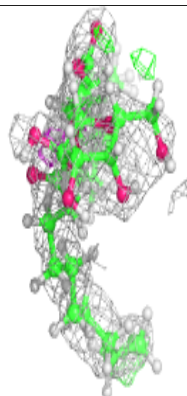
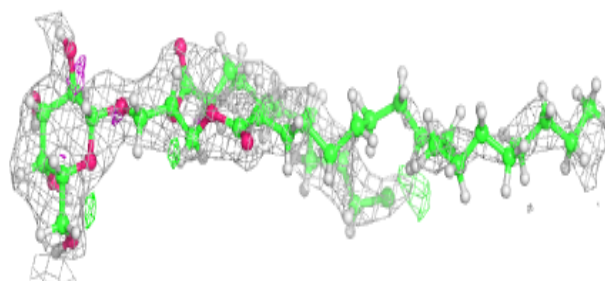
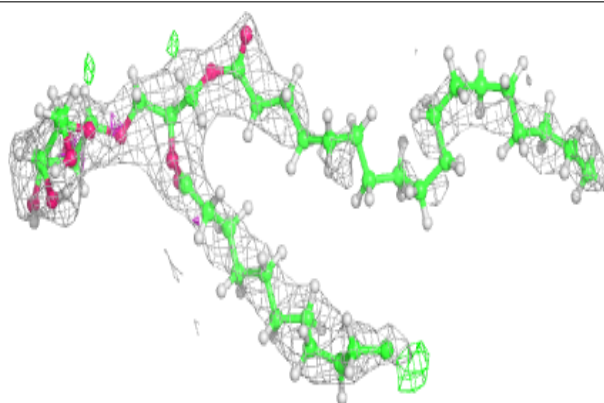


**Electron density around STE b 625:**

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

**Electron density around LMG c 521:**

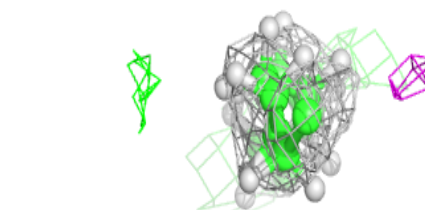
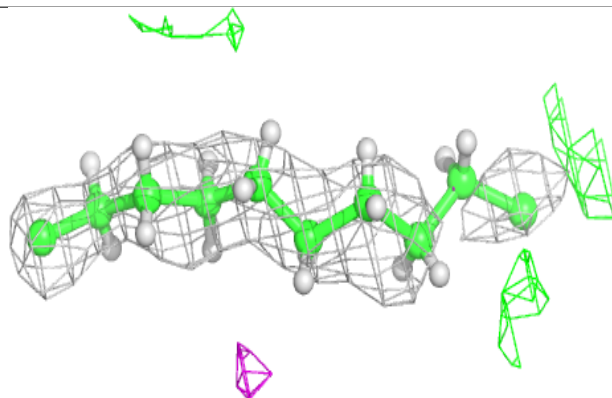
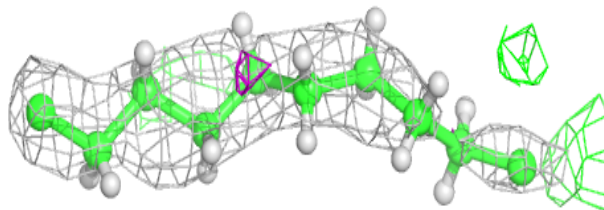
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



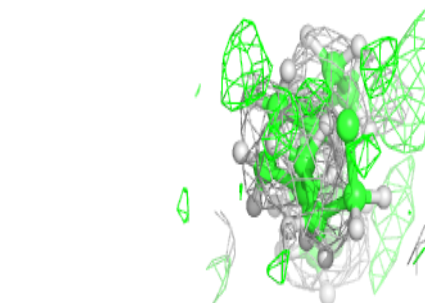
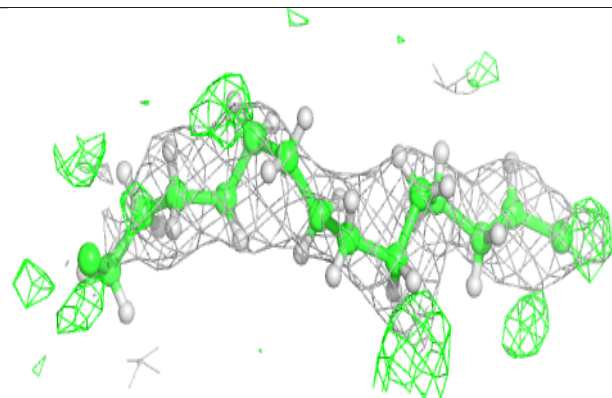
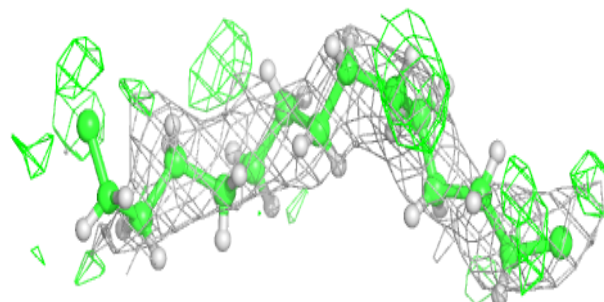


**Electron density around STE a 615:**

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

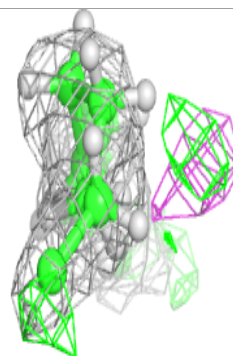
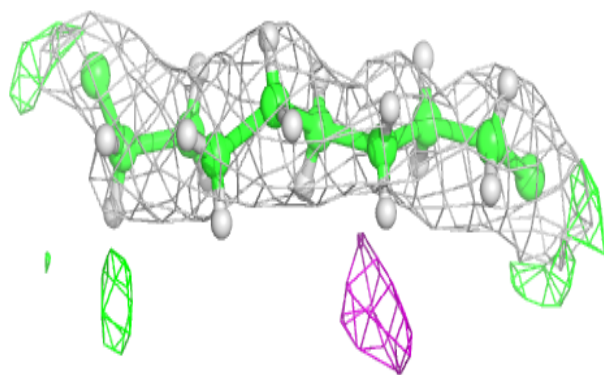
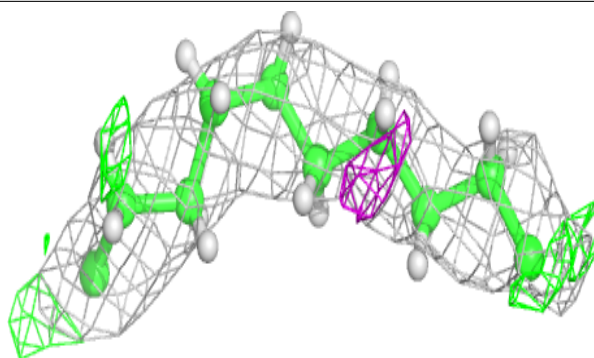
**Electron density around STE a 617:**

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



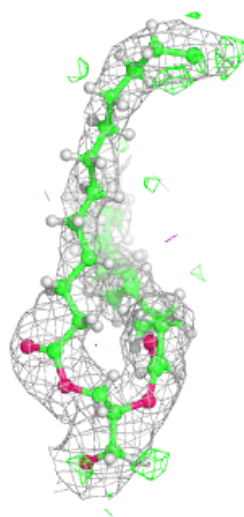
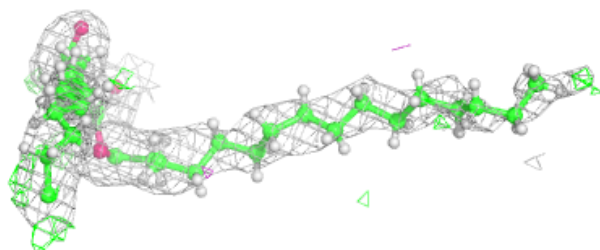
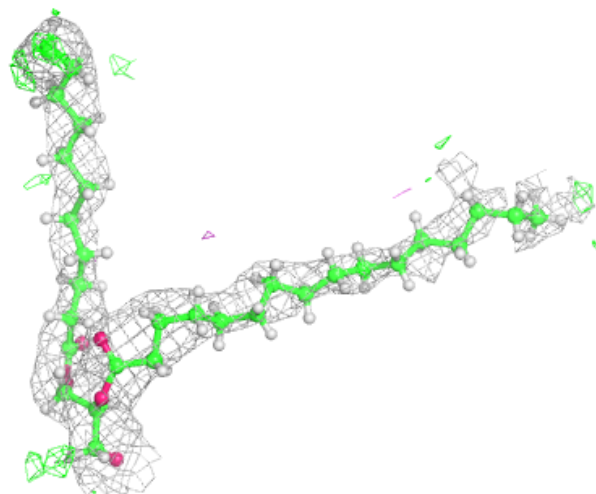
**Electron density around STE b 626:**

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



**Electron density around SQD a 614:**

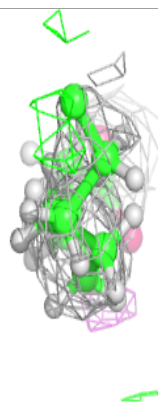
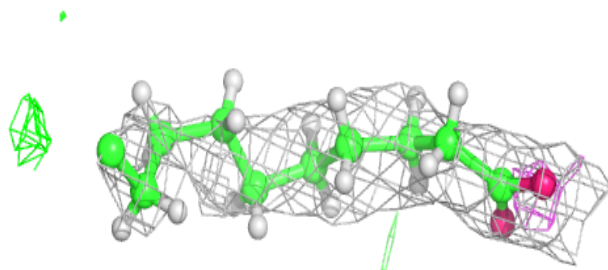
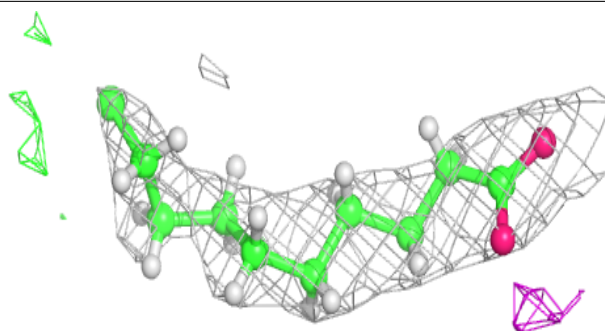
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



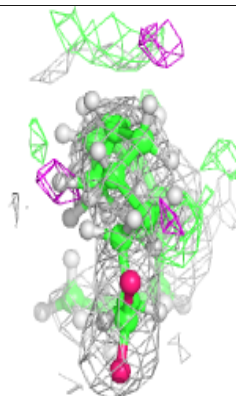
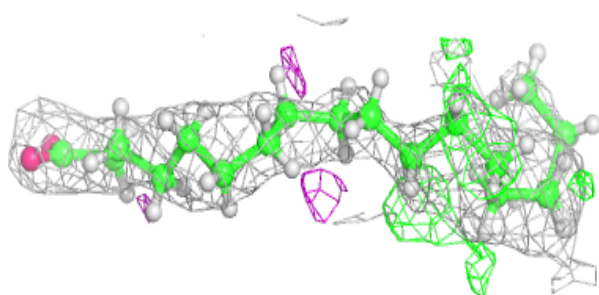
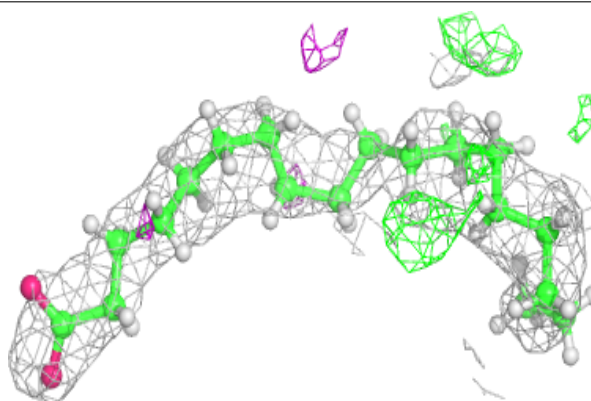


**Electron density around STE m 101:**

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

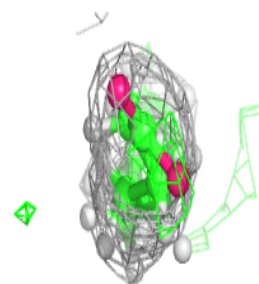
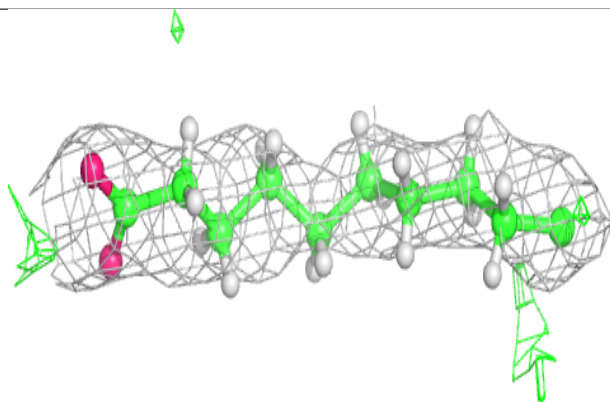
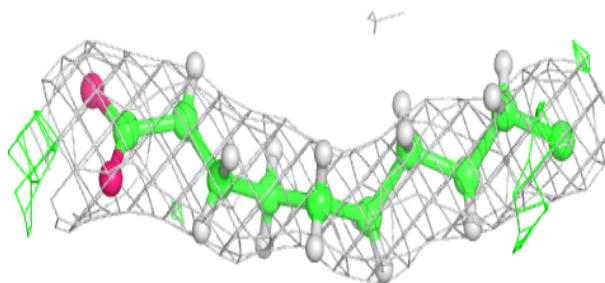
**Electron density around STE d 412:**

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

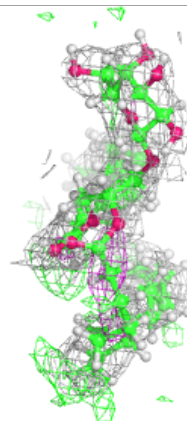
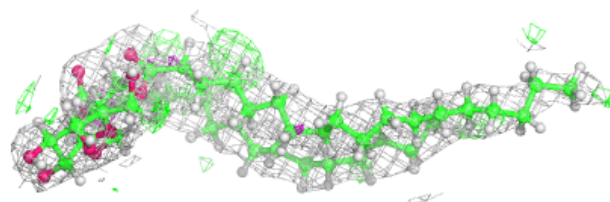
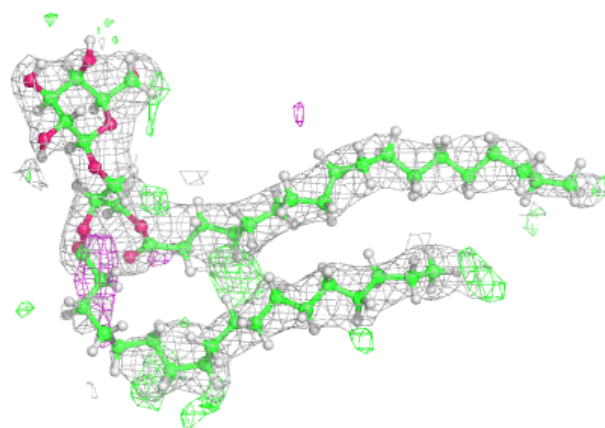


**Electron density around STE j 101:**

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

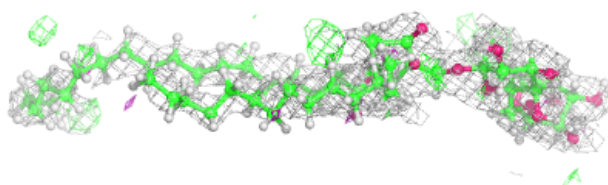
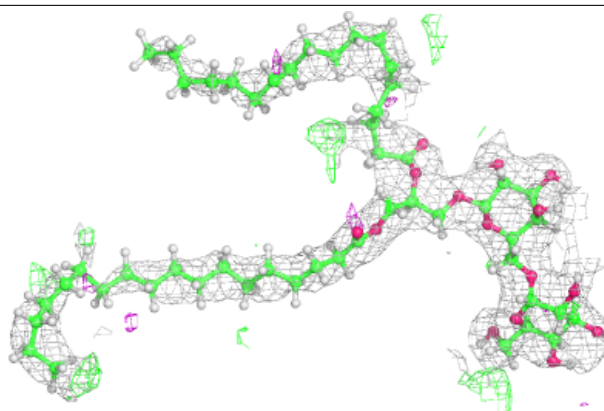
**Electron density around LMG a 618:**

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

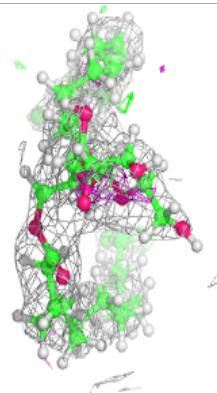
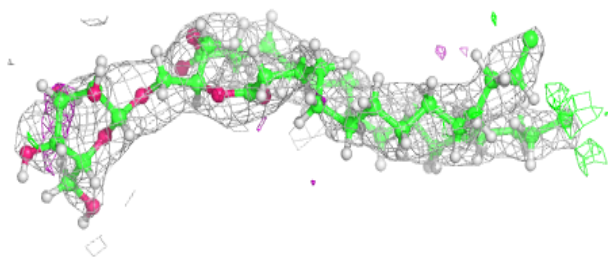
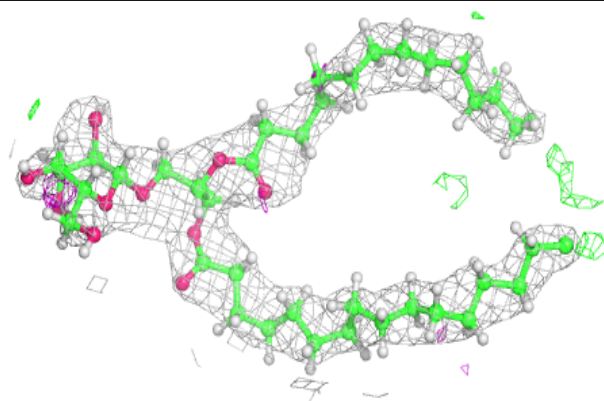


**Electron density around DGD A 618:**

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

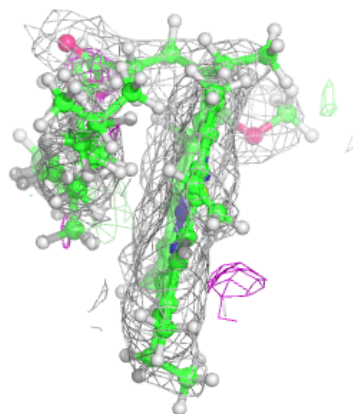
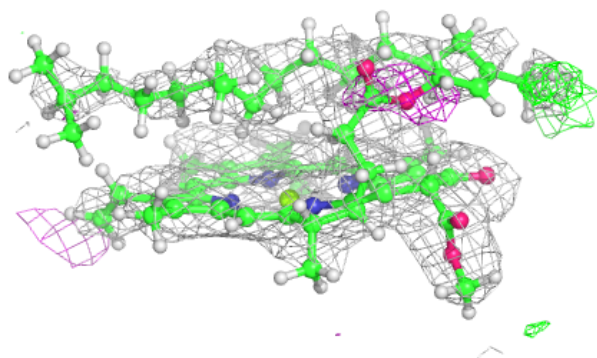
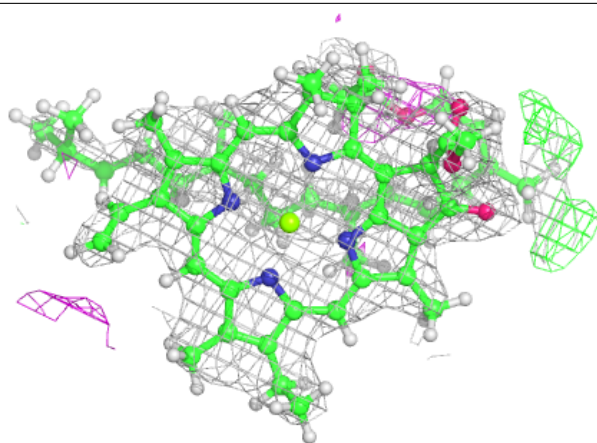
**Electron density around LMG c 522:**

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

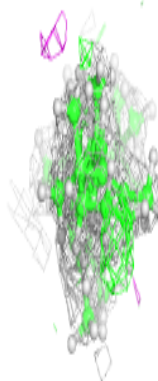
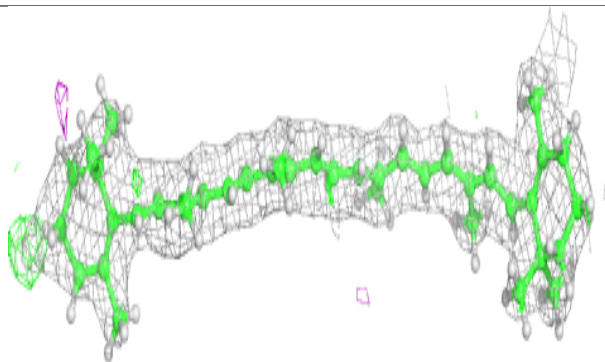
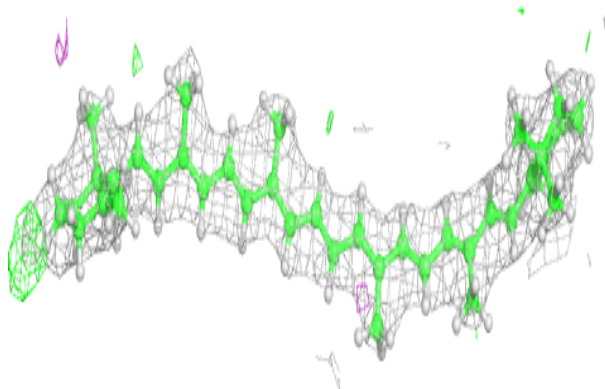


**Electron density around CLA b 601:**

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

**Electron density around BCR H 101:**

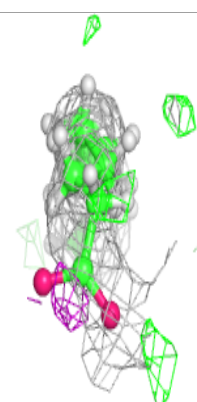
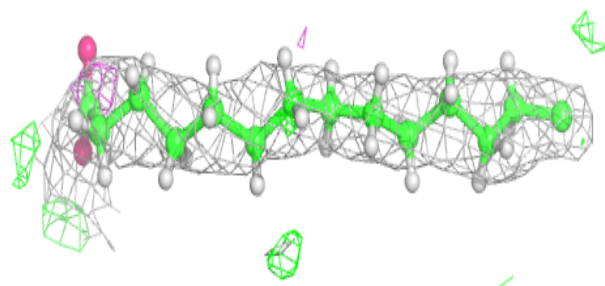
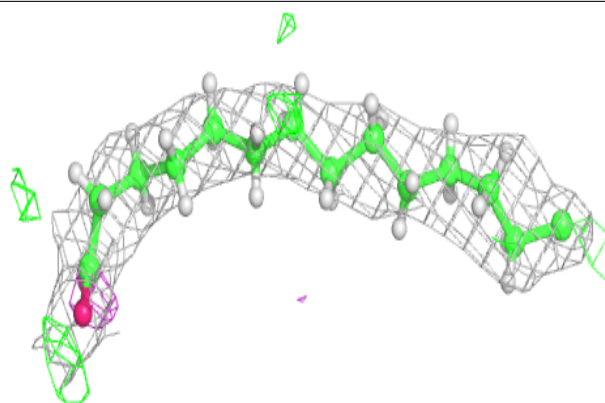
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



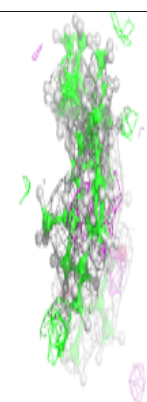
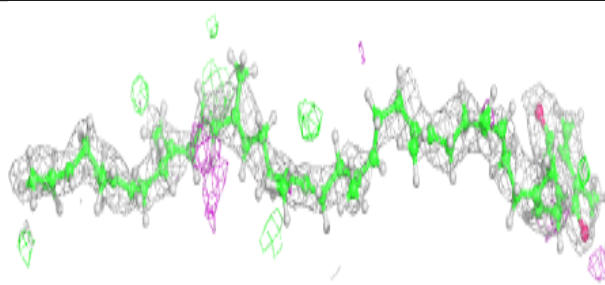
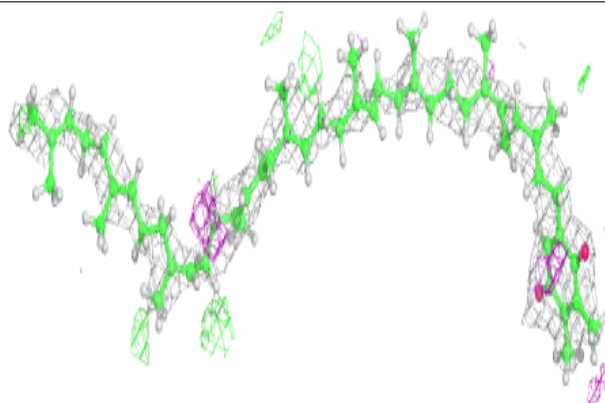


**Electron density around STE b 624:**

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

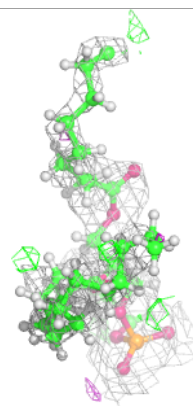
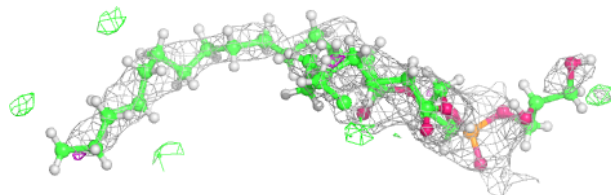
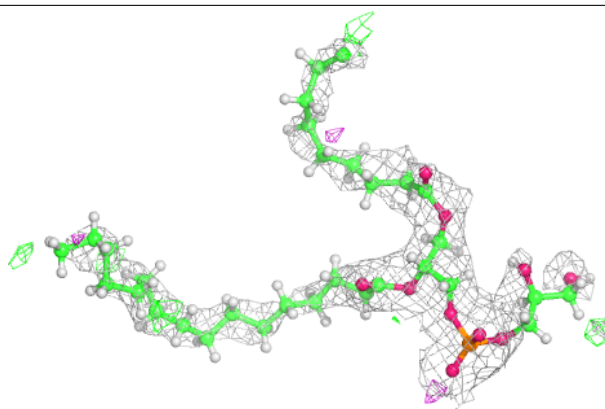
**Electron density around PL9 A 612:**

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

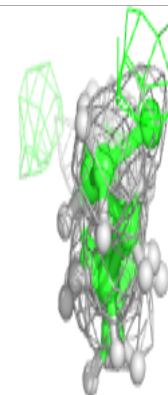
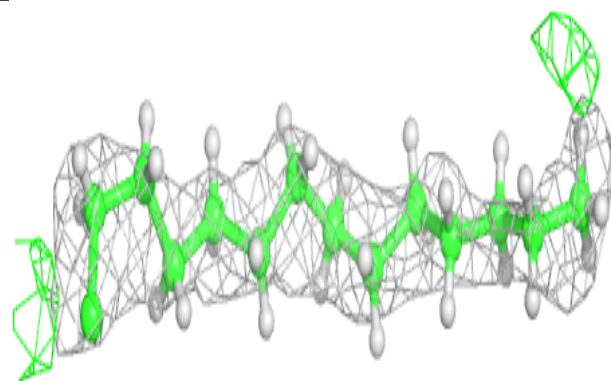
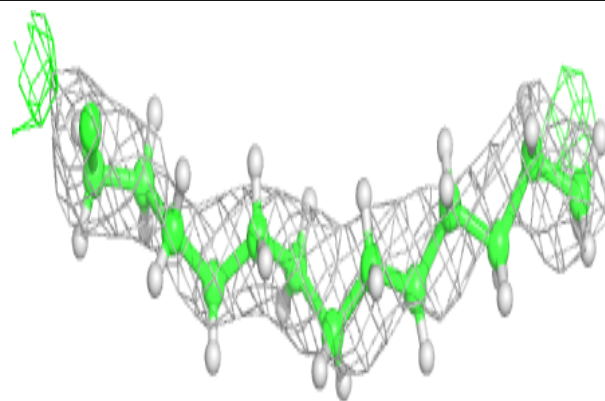


**Electron density around LHG e 102:**

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

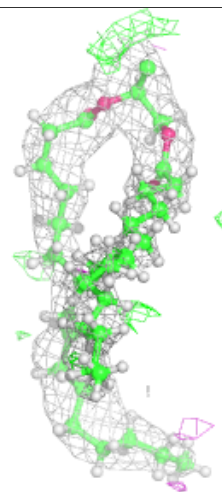
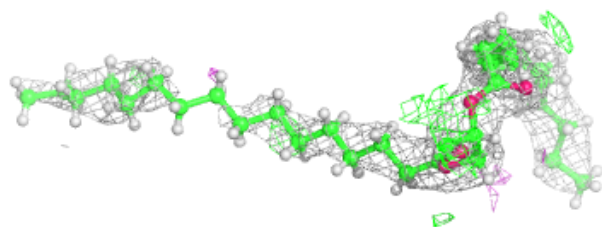
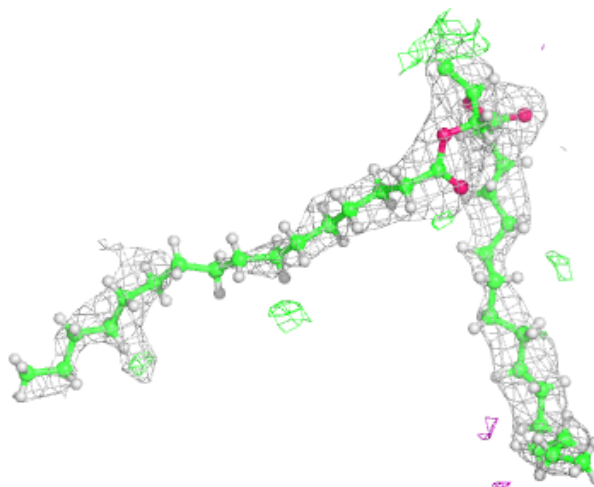
**Electron density around STE b 627:**

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



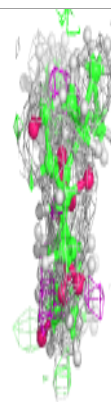
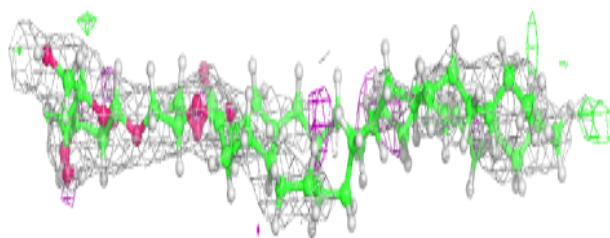
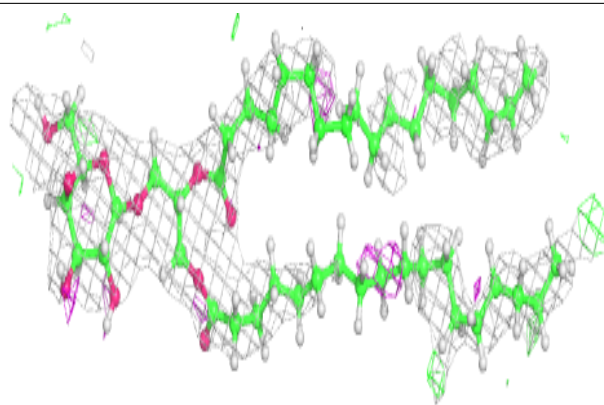
**Electron density around SQD A 617:**

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

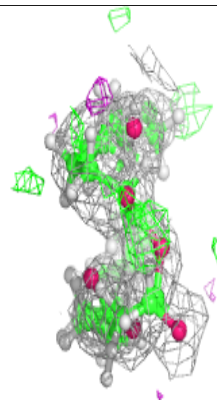
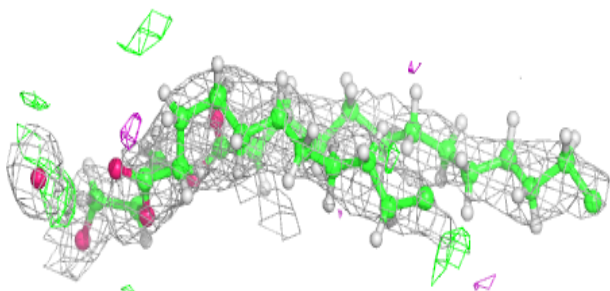
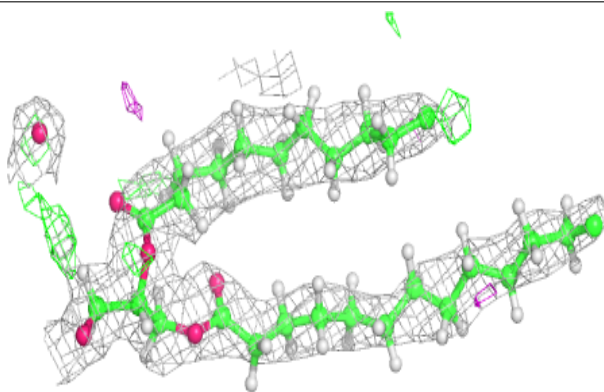


**Electron density around LMG b 623:**

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

**Electron density around LMG D 409:**

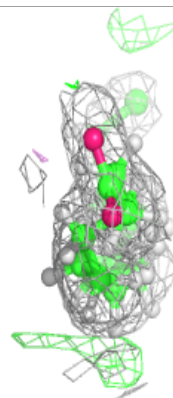
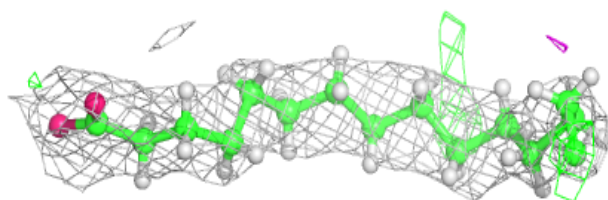
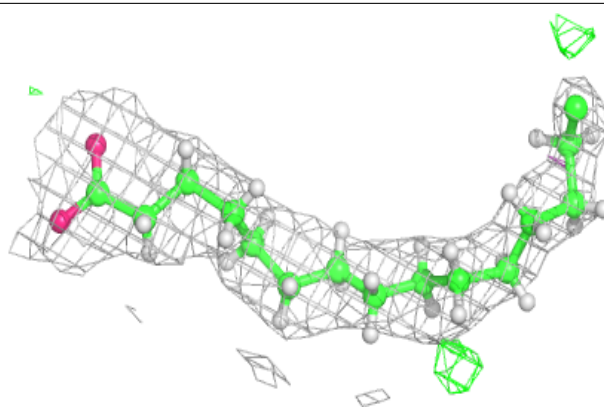
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





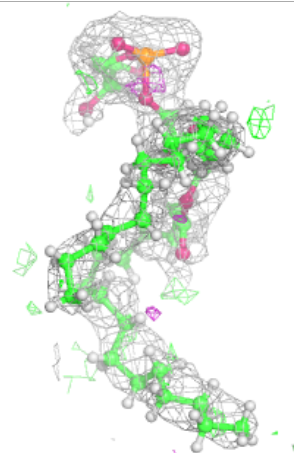
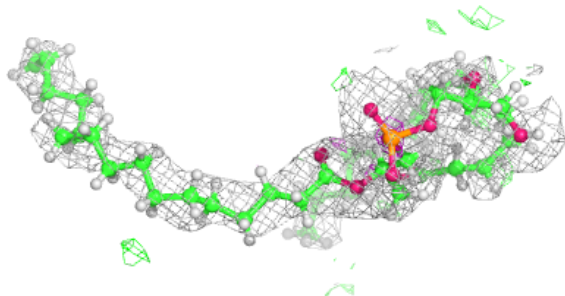
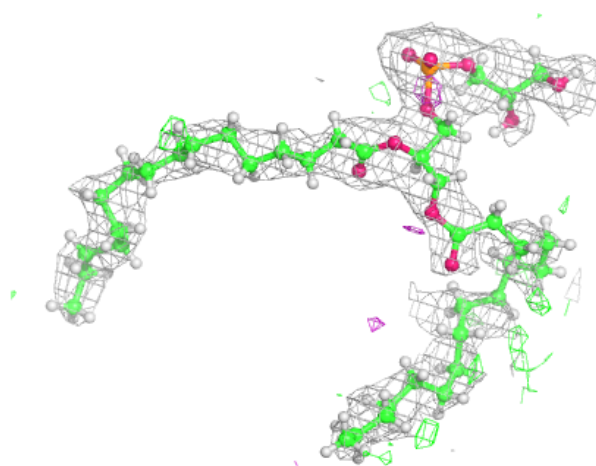
**Electron density around STE B 620:**

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



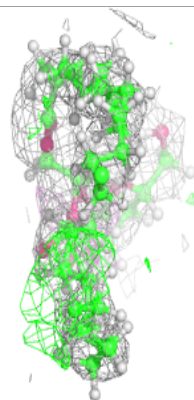
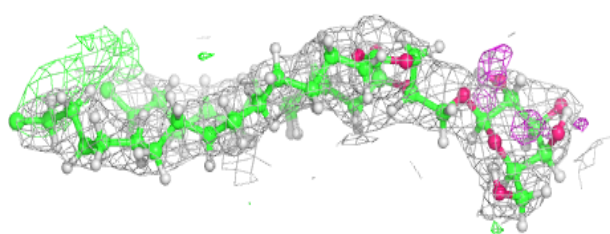
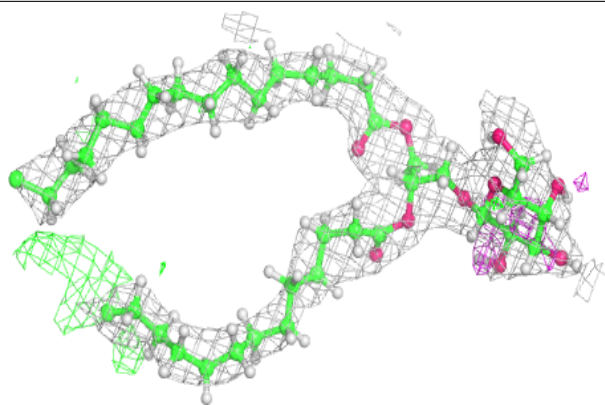
**Electron density around LHG E 101:**

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

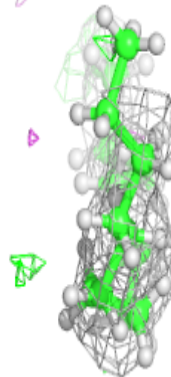
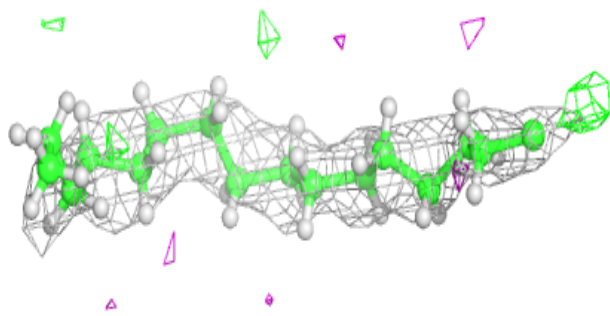
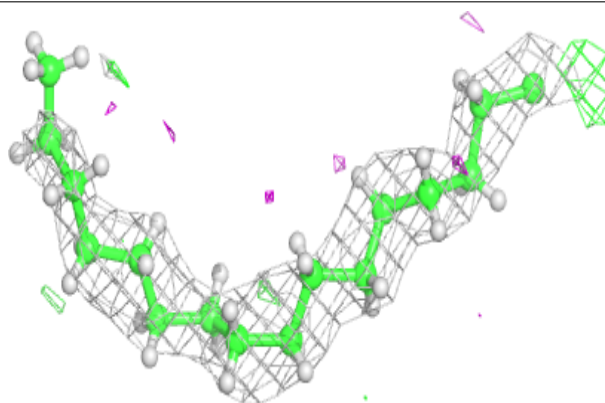


**Electron density around LMG A 614:**

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

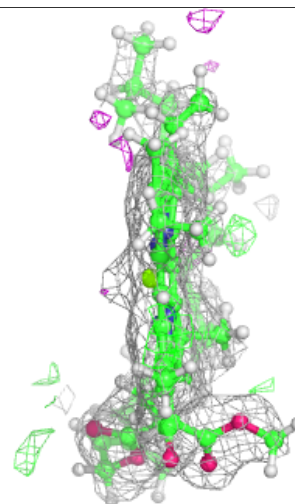
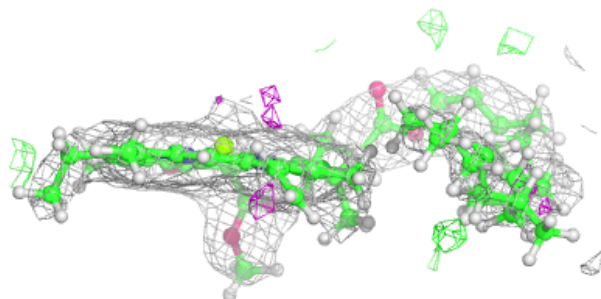
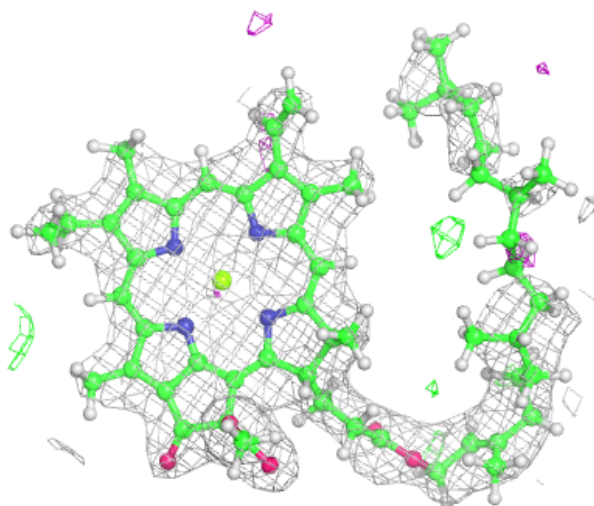
**Electron density around STE B 626:**

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



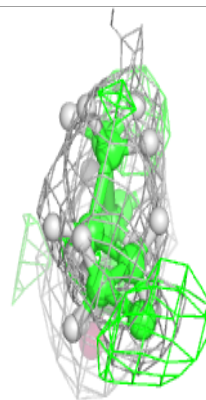
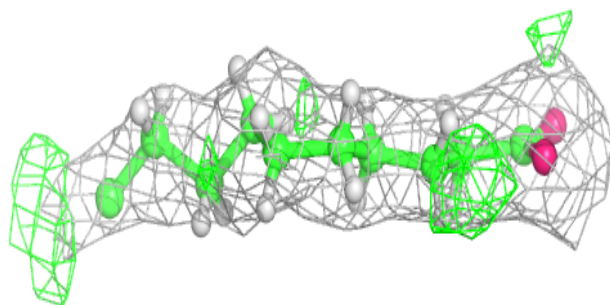
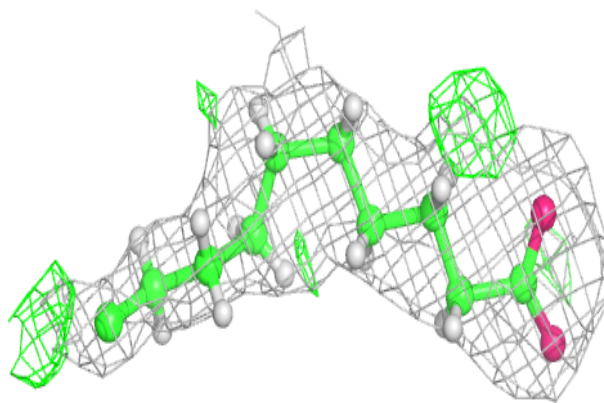
**Electron density around CLA C 512:**

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

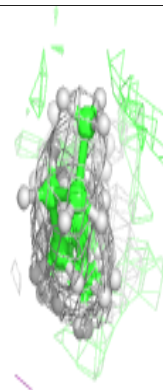
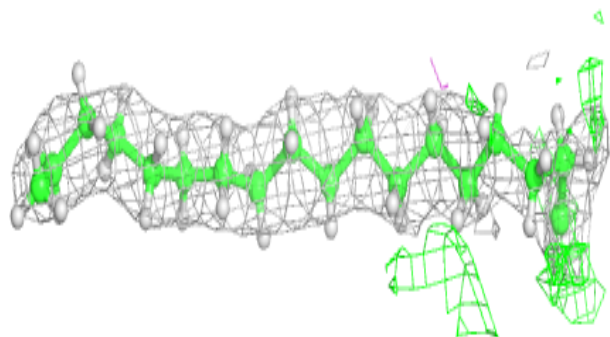
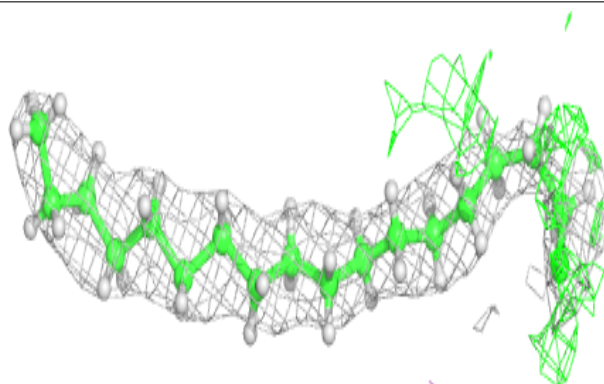


**Electron density around STE C 522:**

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

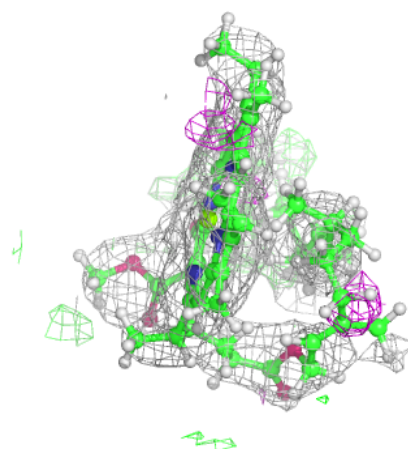
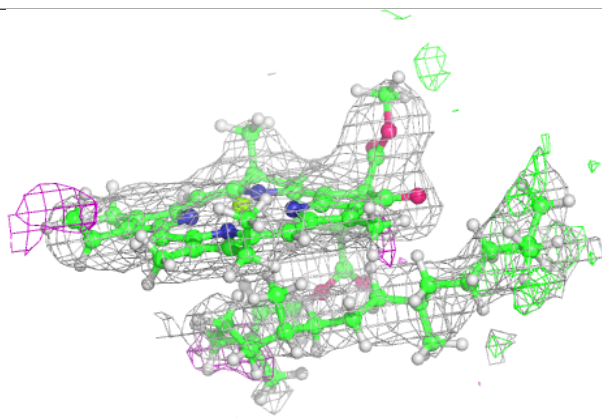
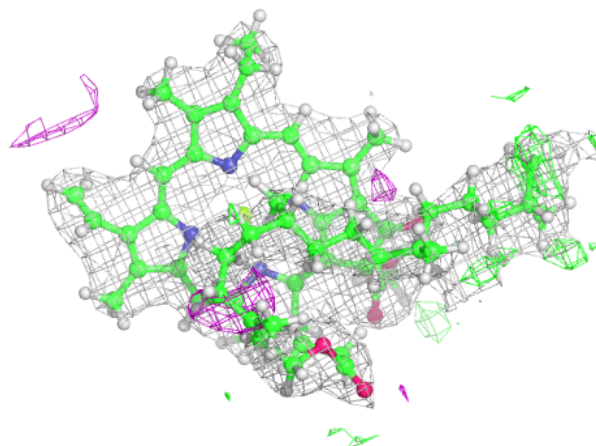
**Electron density around STE I 102:**

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



**Electron density around CLA B 601:**

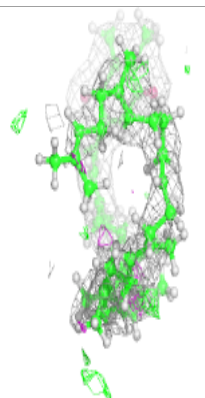
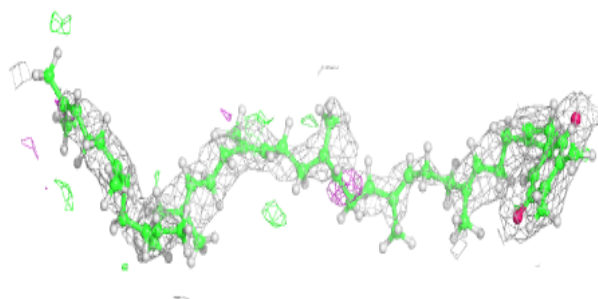
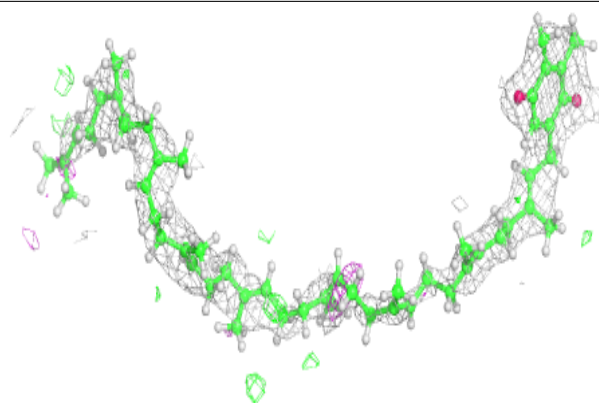
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



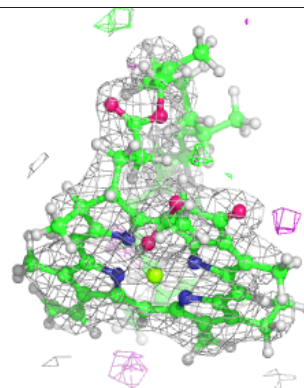
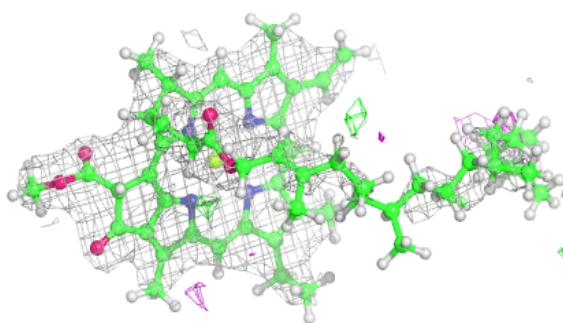
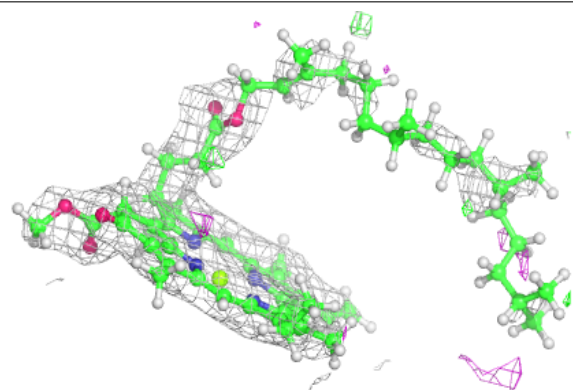


**Electron density around PL9 a 611:**

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

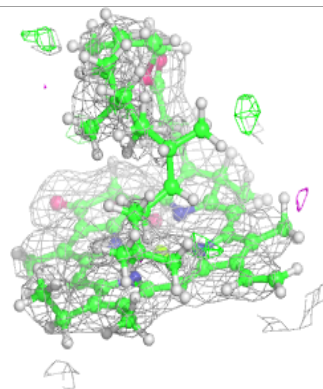
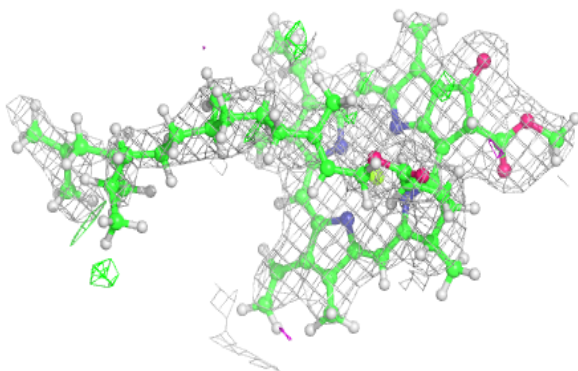
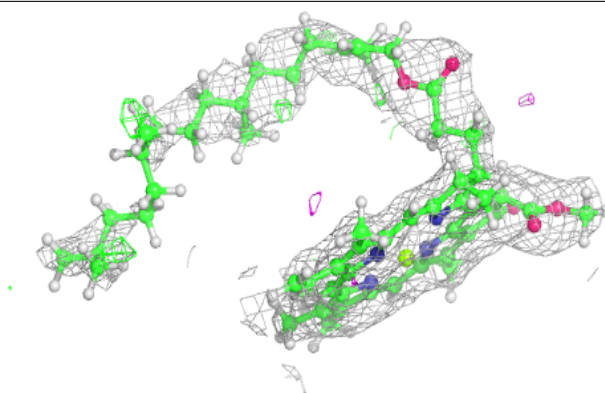
**Electron density around CLA c 513:**

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

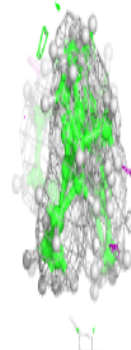
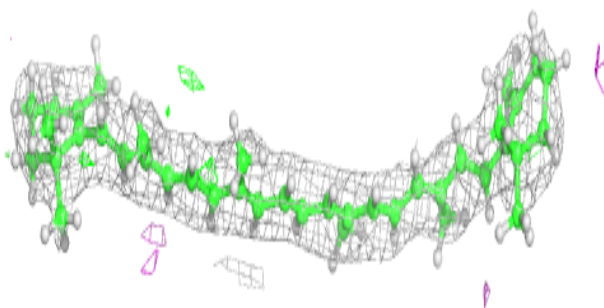
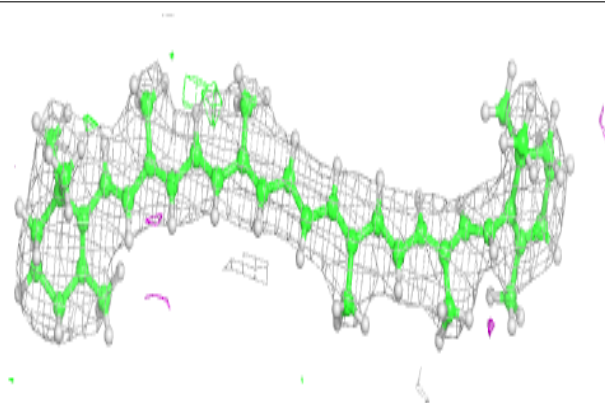


**Electron density around CLA C 513:**

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

**Electron density around BCR d 405:**

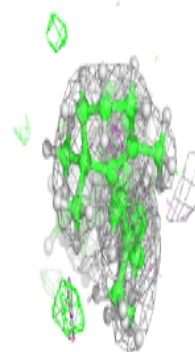
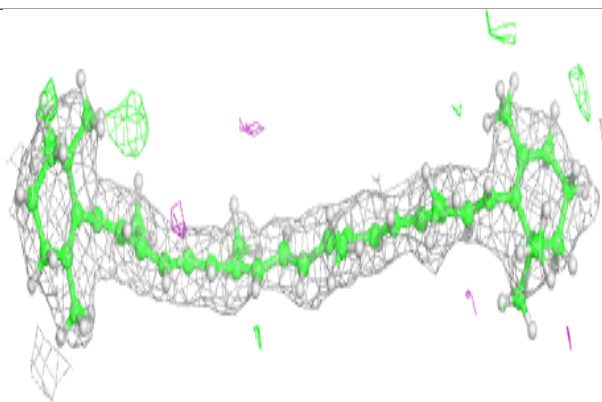
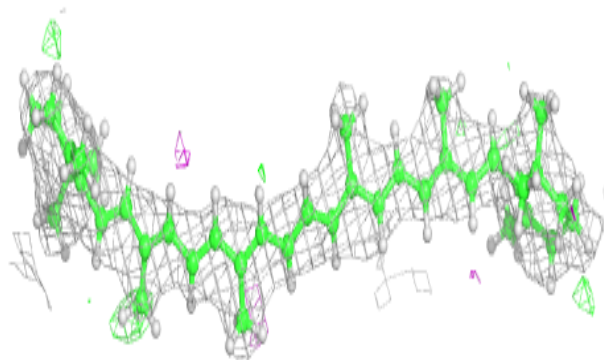
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





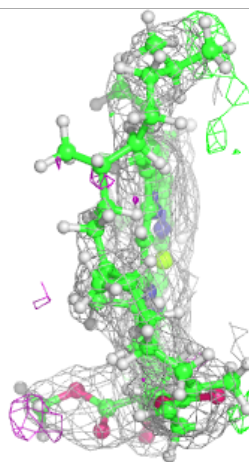
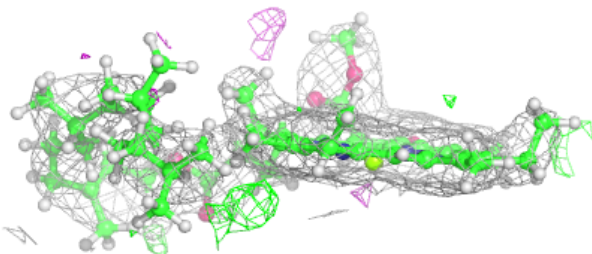
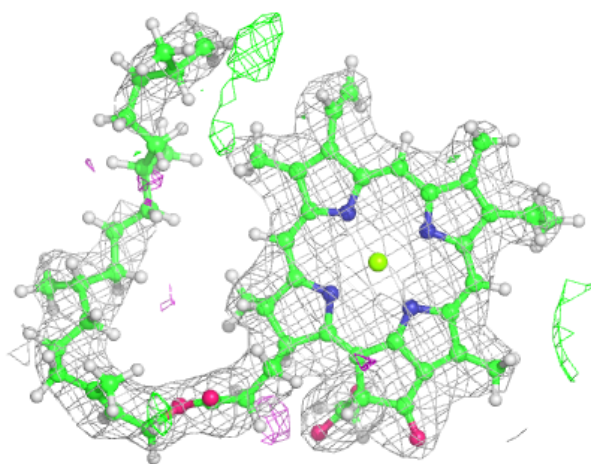
**Electron density around BCR x 101:**

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



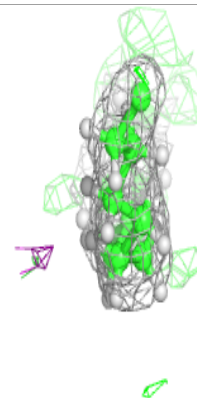
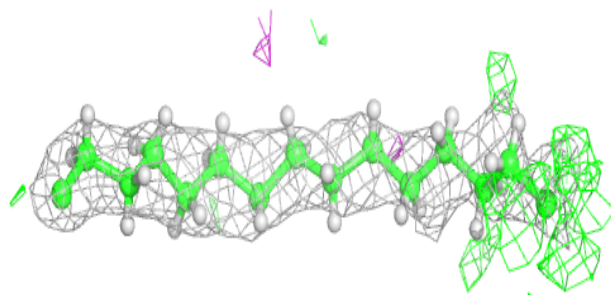
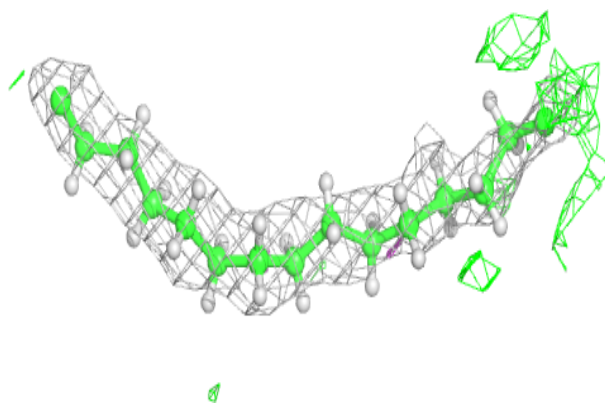
**Electron density around CLA c 512:**

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

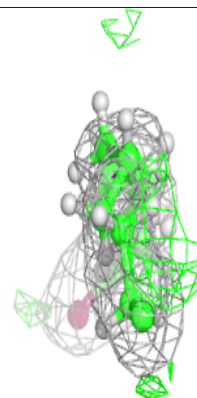
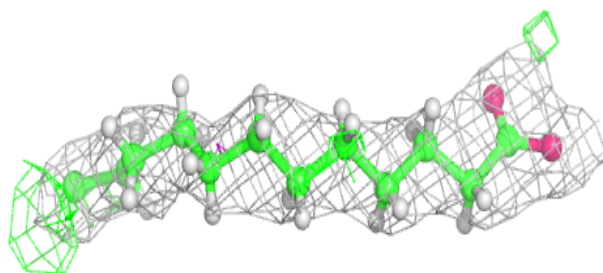
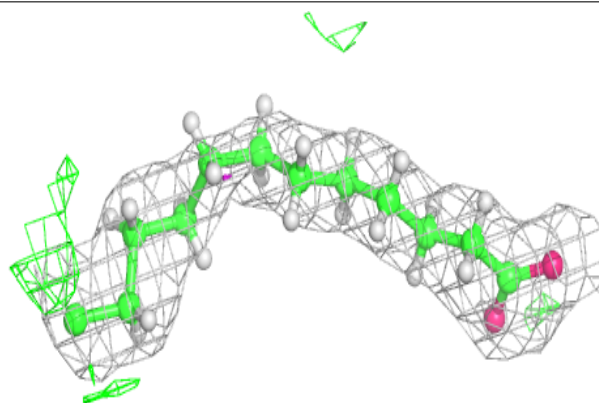


**Electron density around STE I 101:**

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

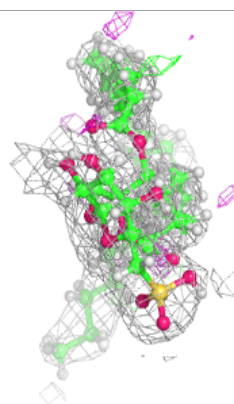
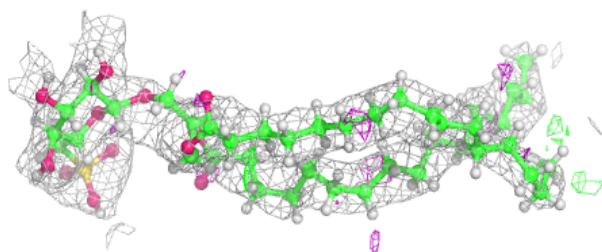
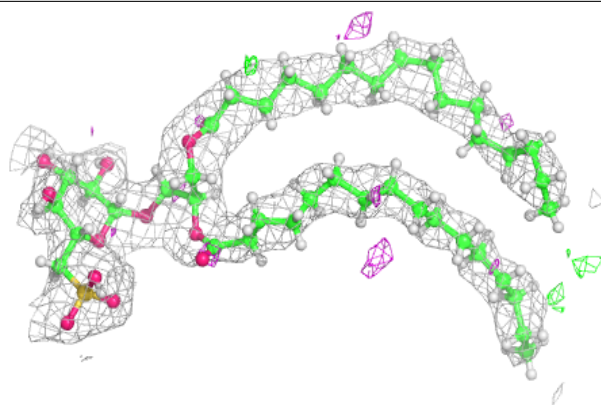
**Electron density around STE B 624:**

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

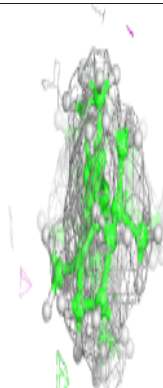
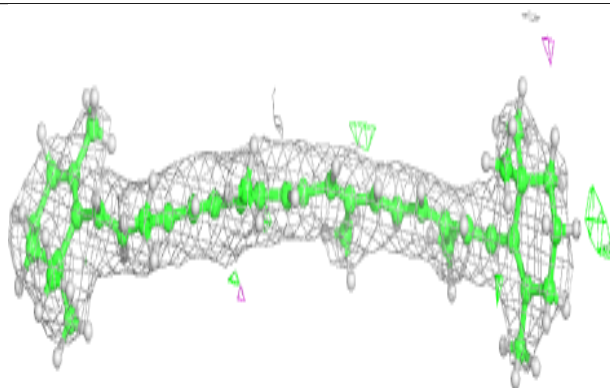
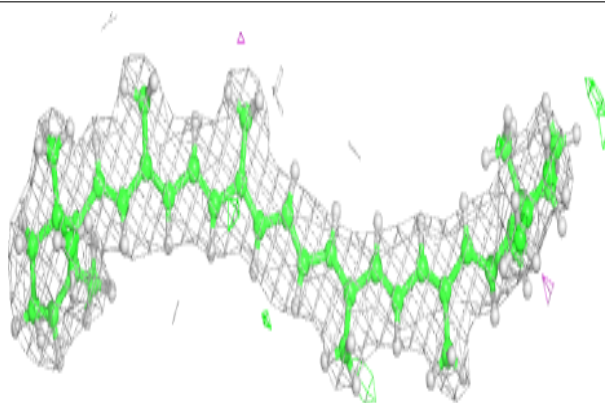


**Electron density around SQD B 623:**

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

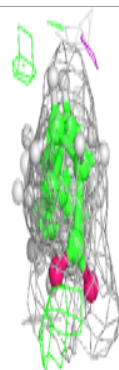
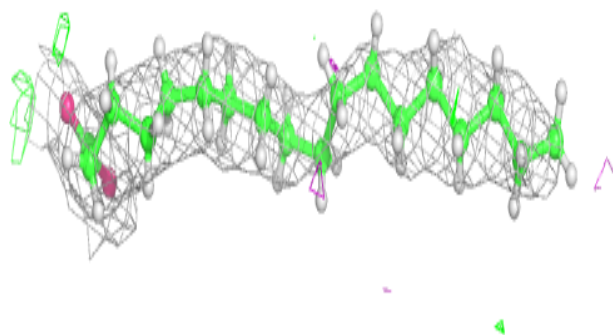
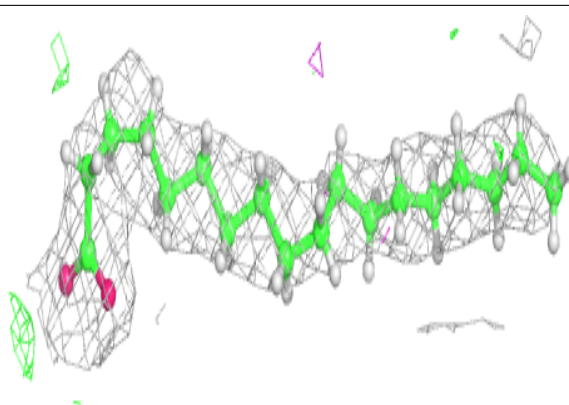
**Electron density around BCR Y 101:**

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

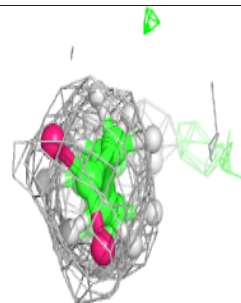
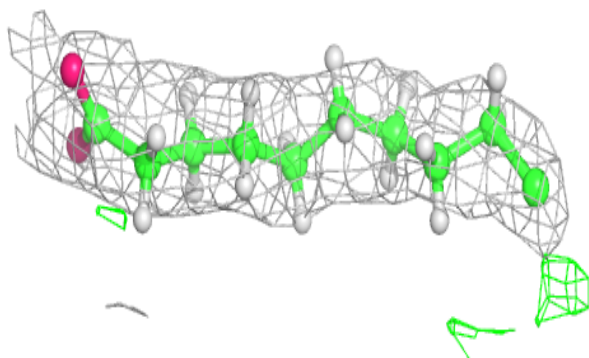
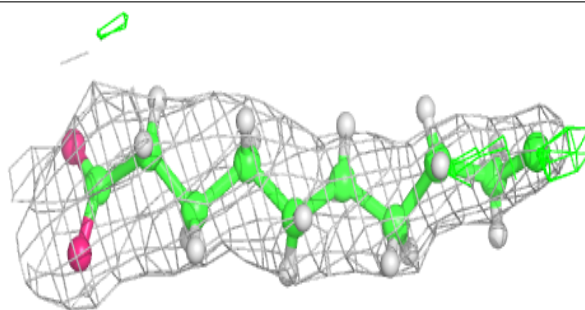


**Electron density around STE c 520:**

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

**Electron density around STE J 101:**

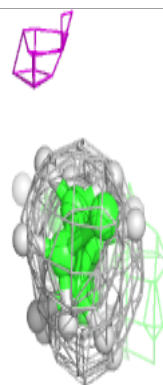
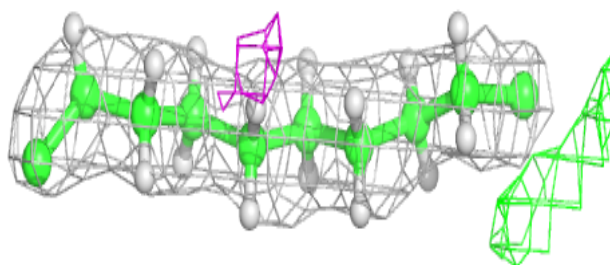
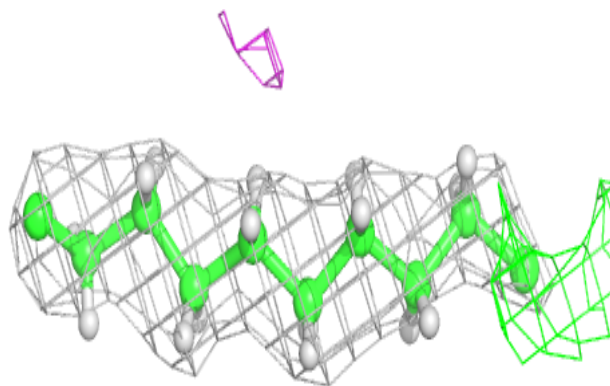
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



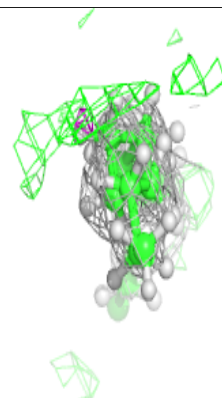
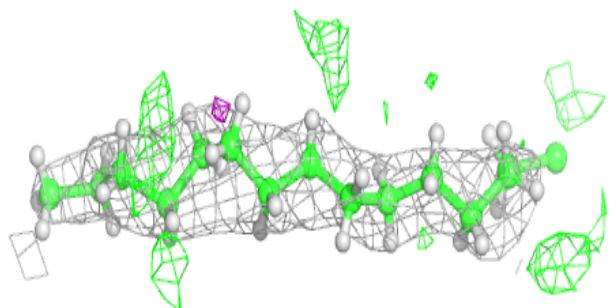
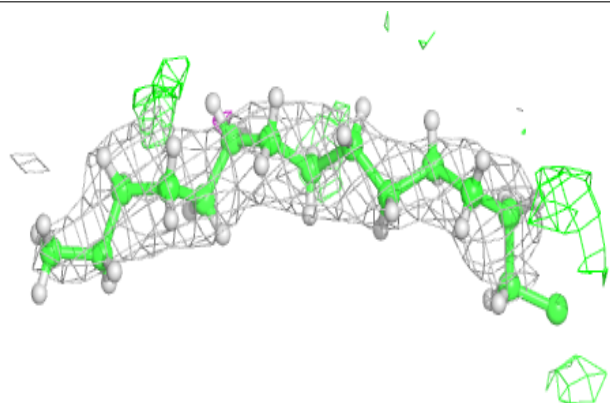


**Electron density around STE M 103:**

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

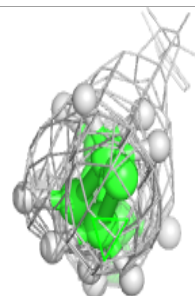
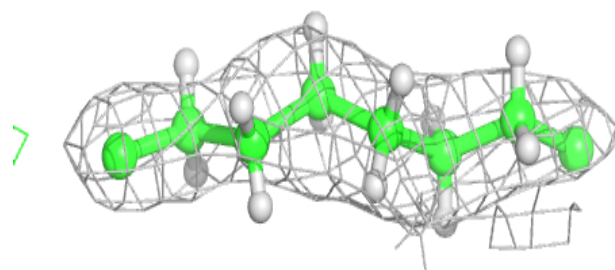
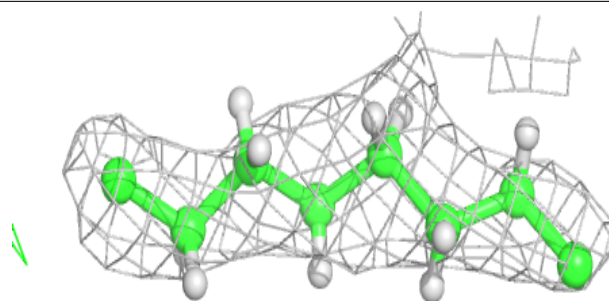
**Electron density around STE T 103:**

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

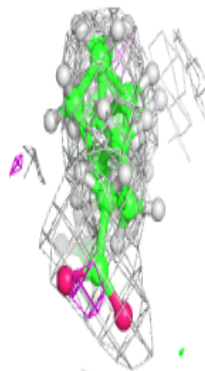
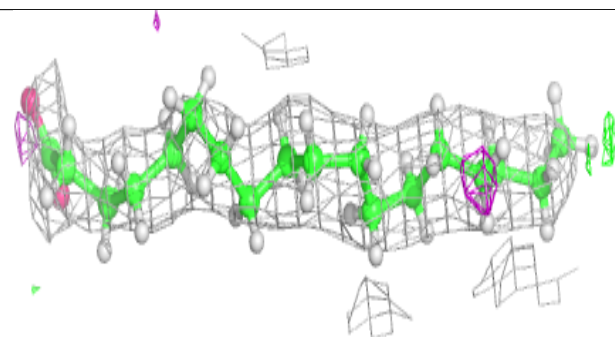
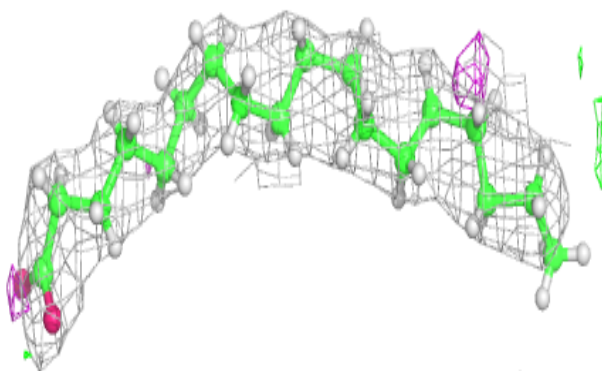


**Electron density around STE Z 101:**

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

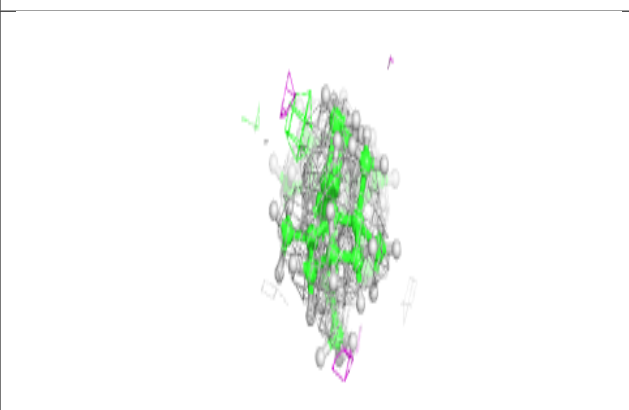
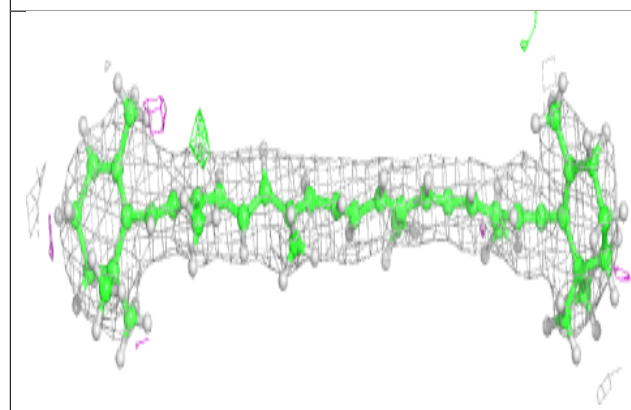
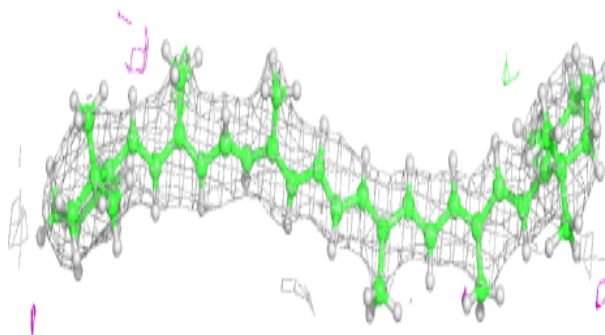
**Electron density around STE D 411:**

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

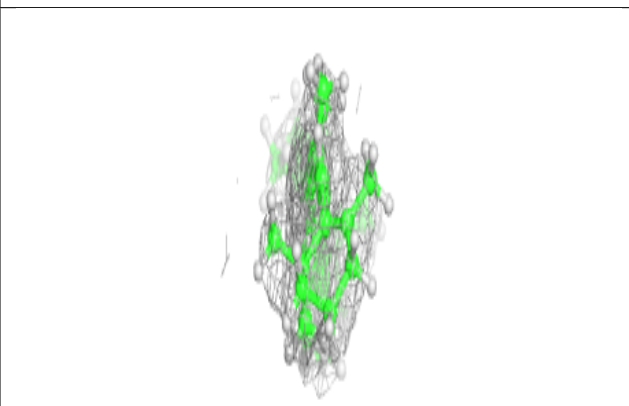
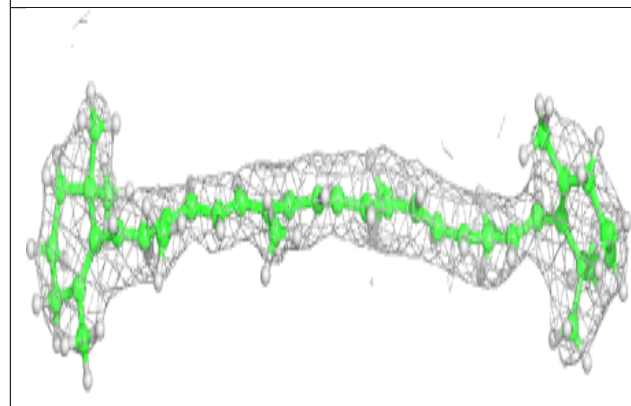
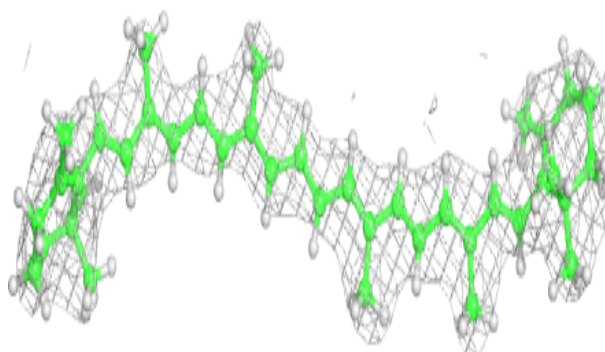


**Electron density around BCR C 514:**

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

**Electron density around BCR k 101:**

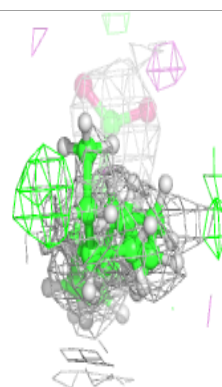
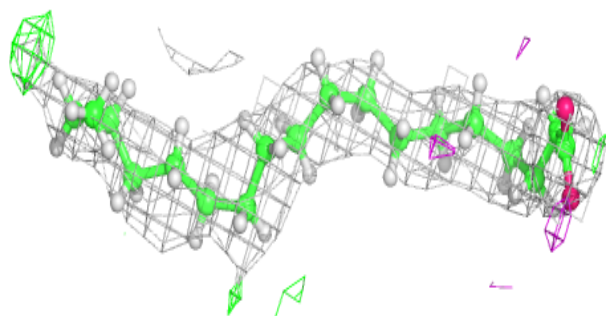
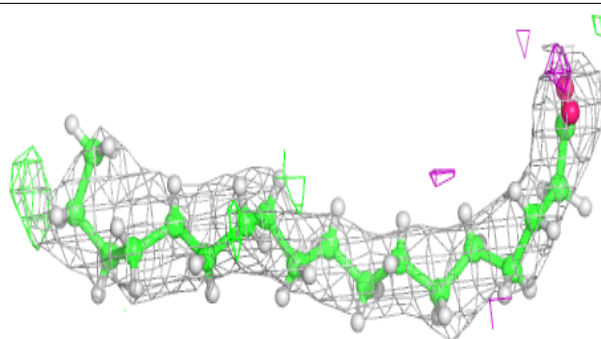
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



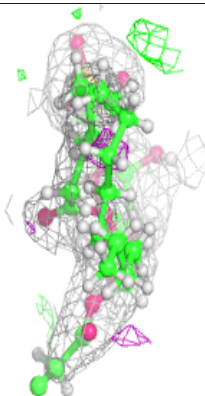
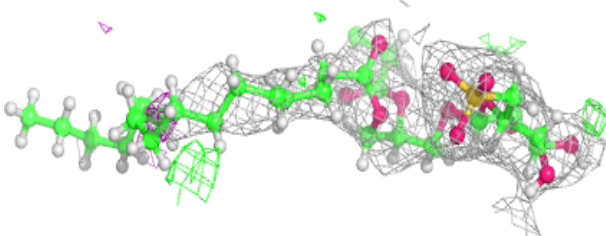
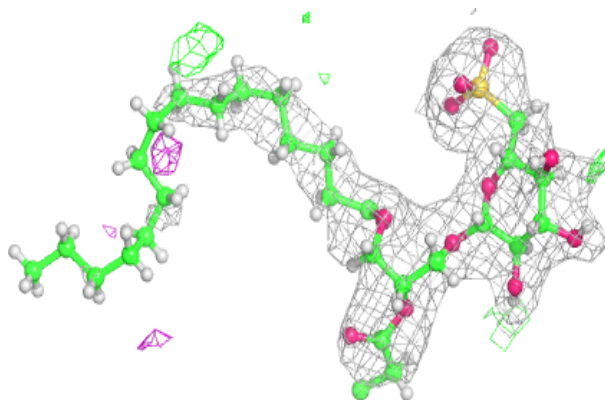


**Electron density around STE b 622:**

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

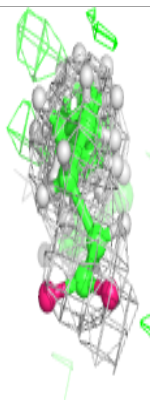
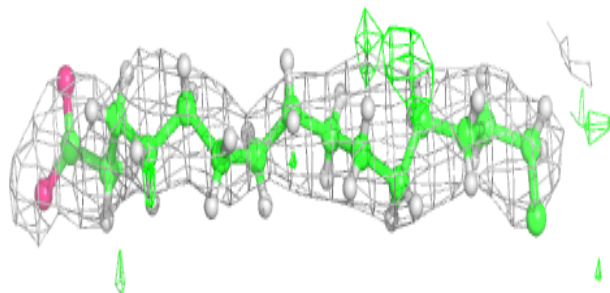
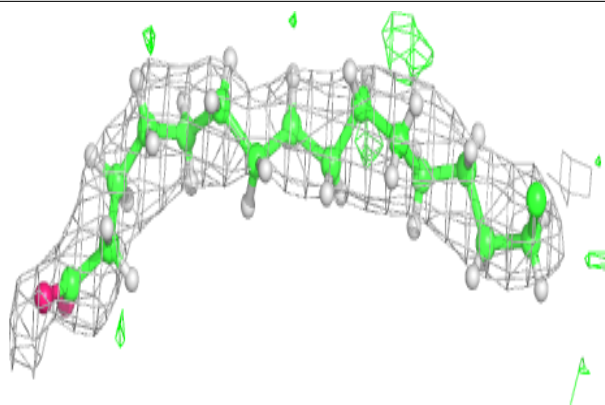
**Electron density around SQD f 101:**

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

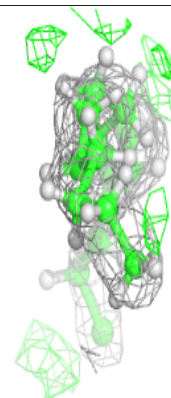
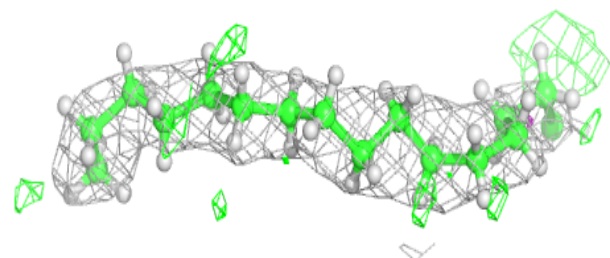
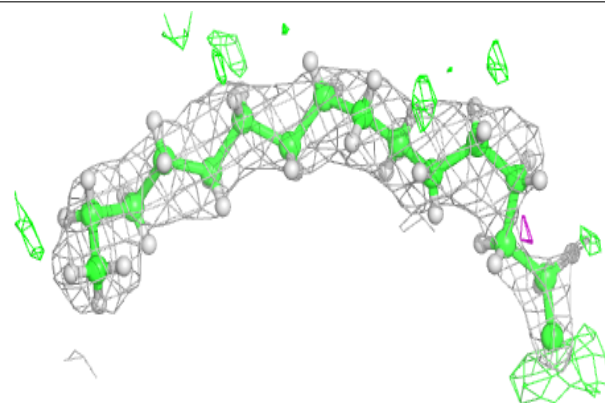


**Electron density around STE t 102:**

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

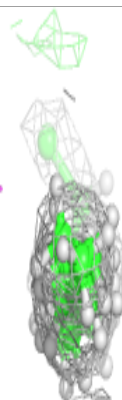
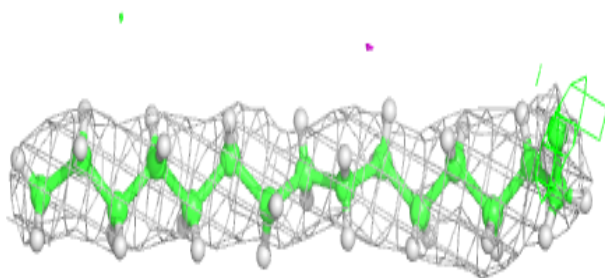
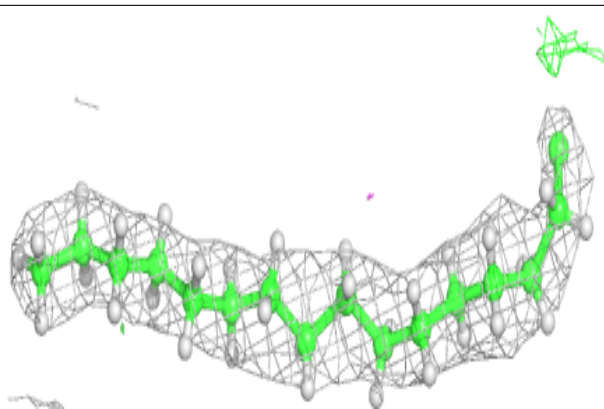
**Electron density around STE T 102:**

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



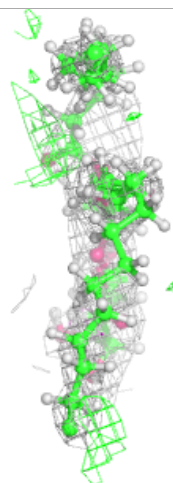
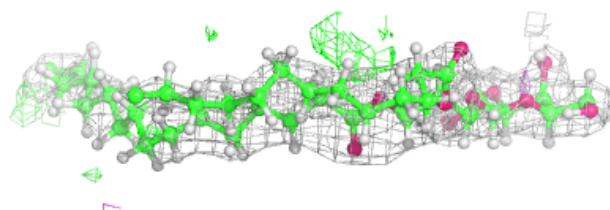
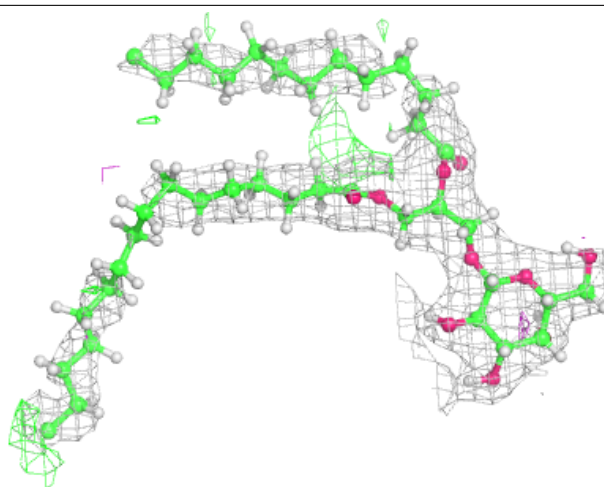
**Electron density around STE C 521:**

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



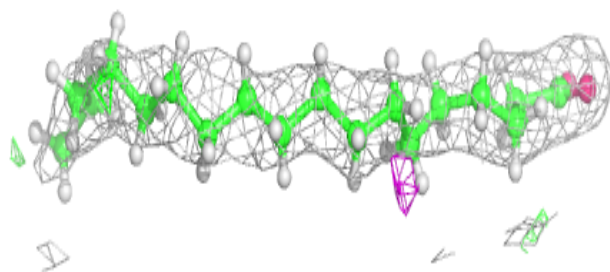
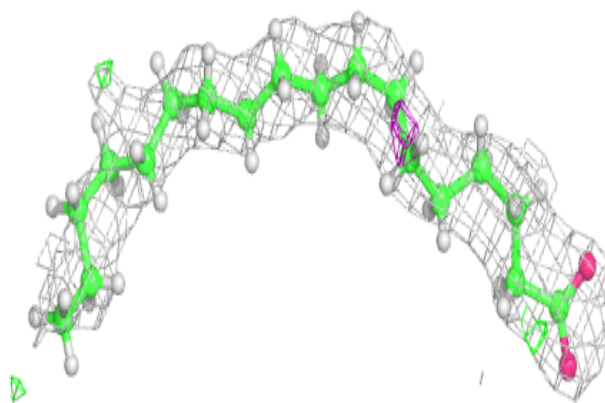
**Electron density around LMG C 519:**

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

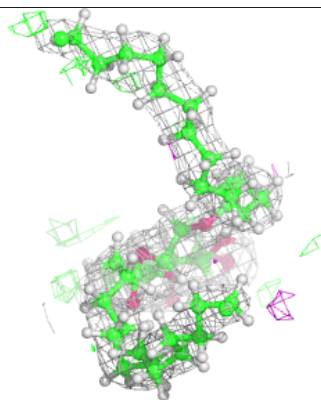
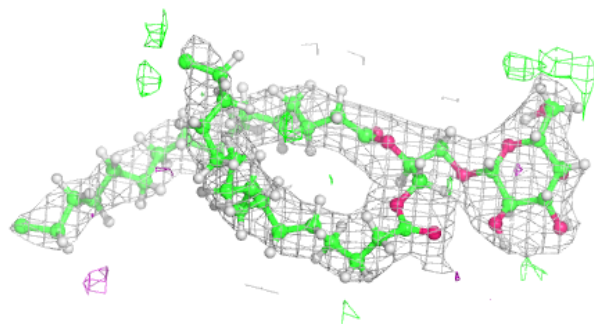
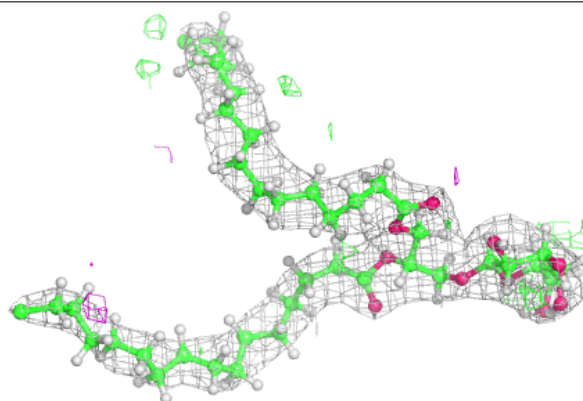


**Electron density around STE x 102:**

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

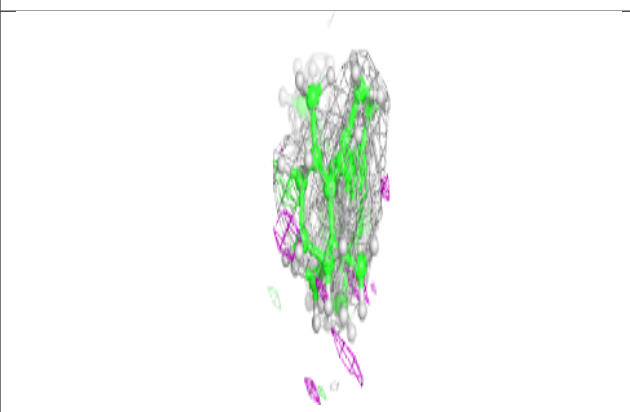
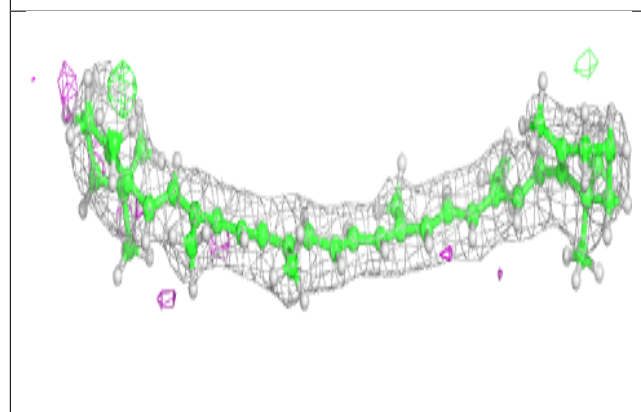
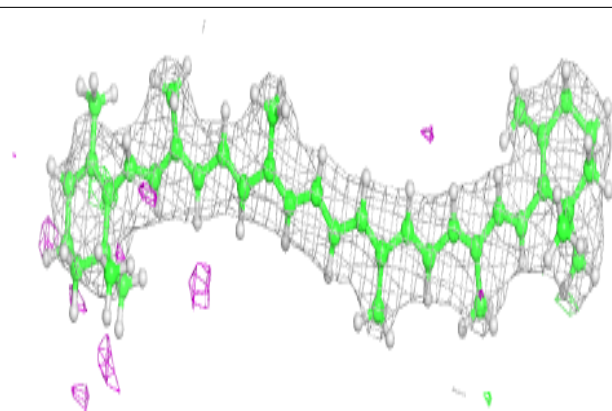
**Electron density around LMG b 621:**

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

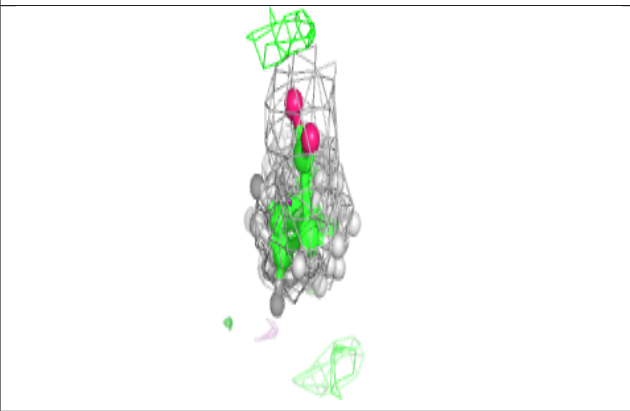
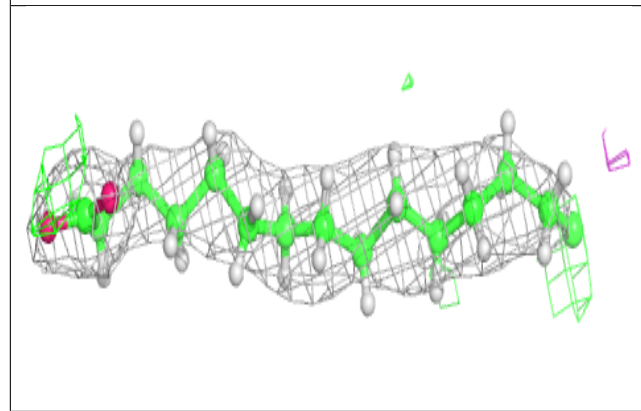
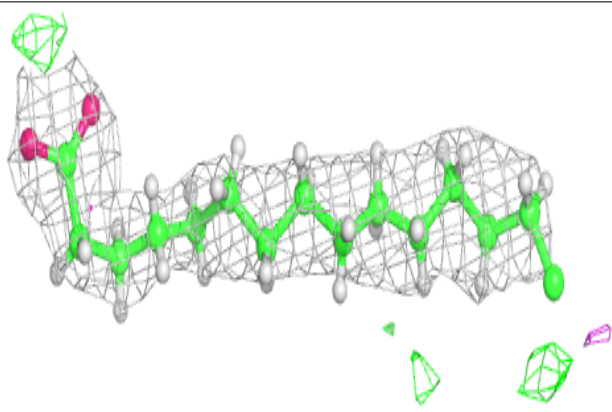


**Electron density around BCR D 404:**

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

**Electron density around STE d 411:**

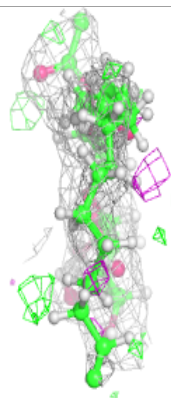
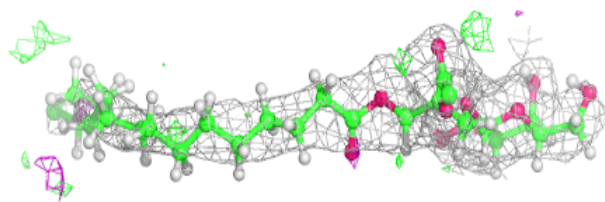
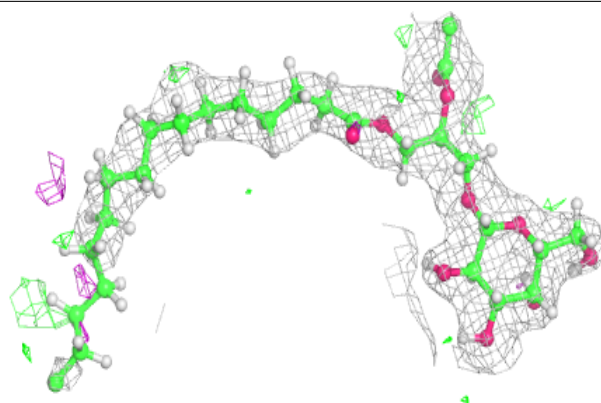
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



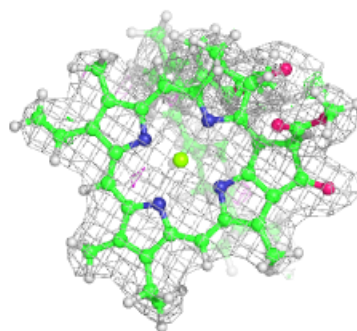
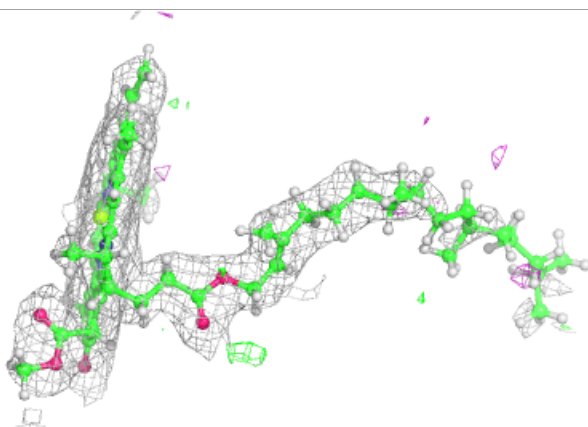
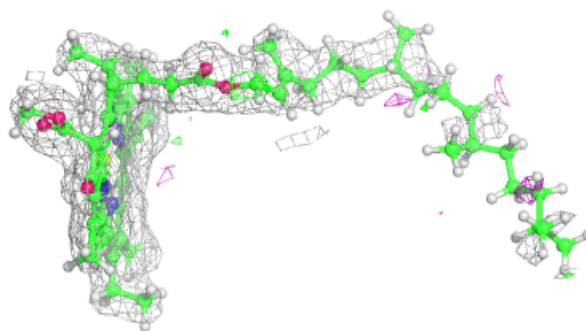


**Electron density around LMG c 519:**

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

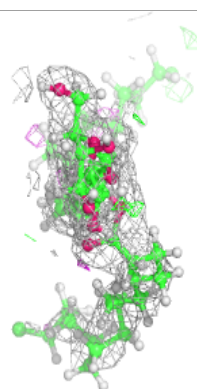
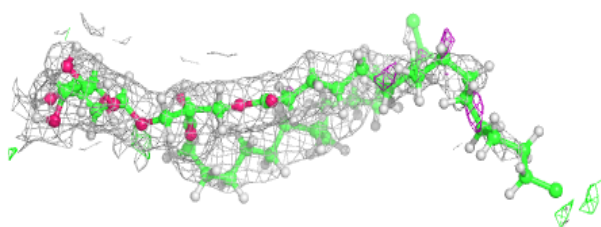
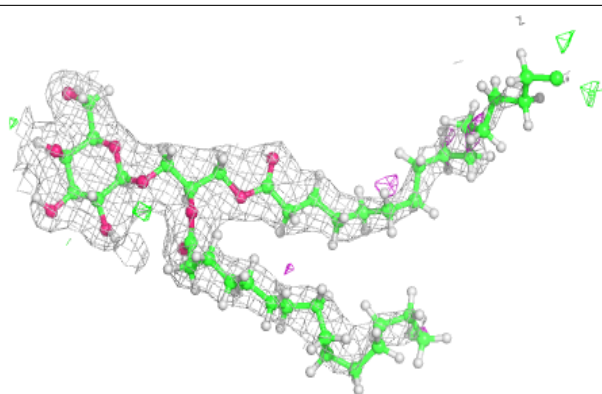
**Electron density around CLA D 403:**

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

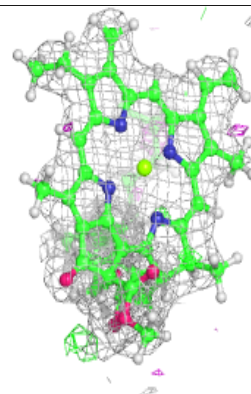
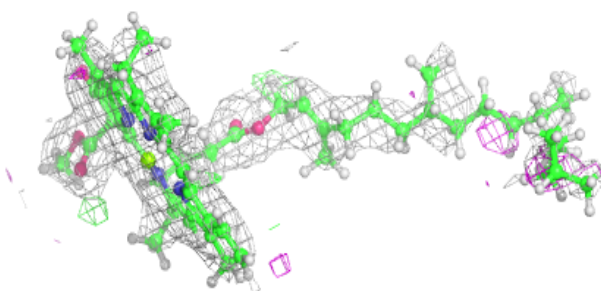
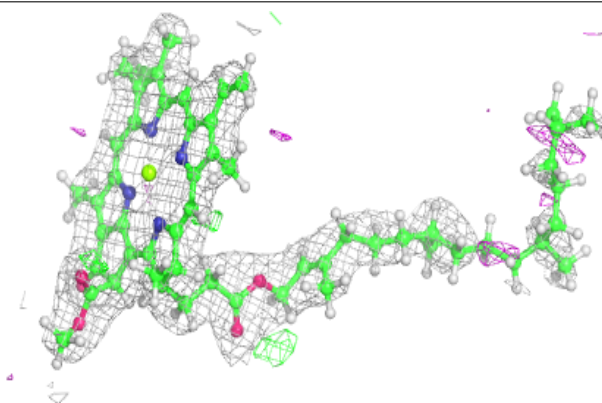


**Electron density around LMG D 406:**

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

**Electron density around CLA d 404:**

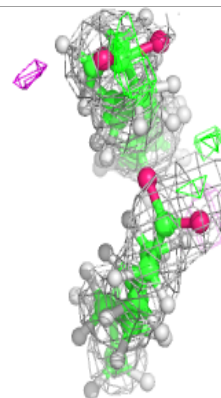
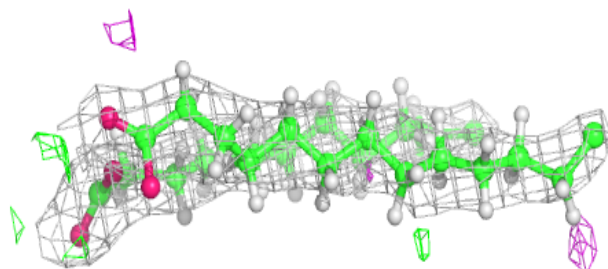
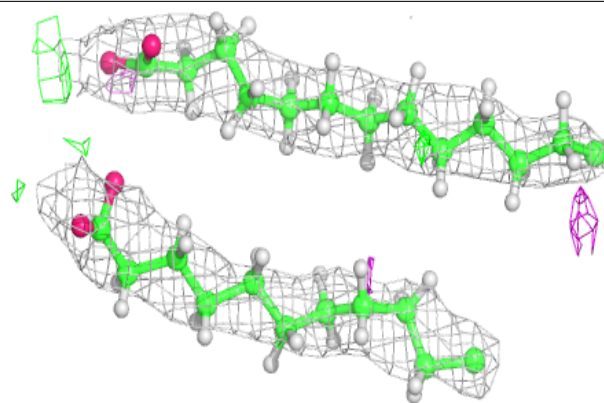
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





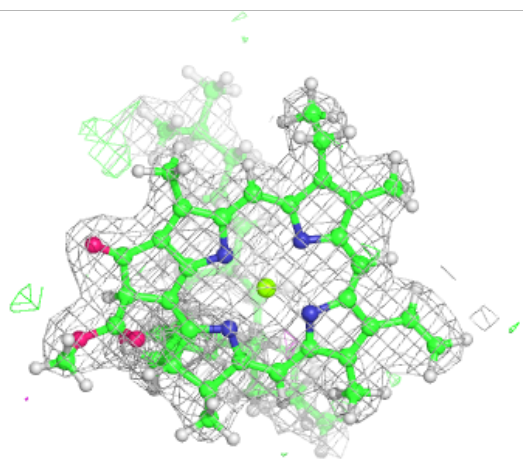
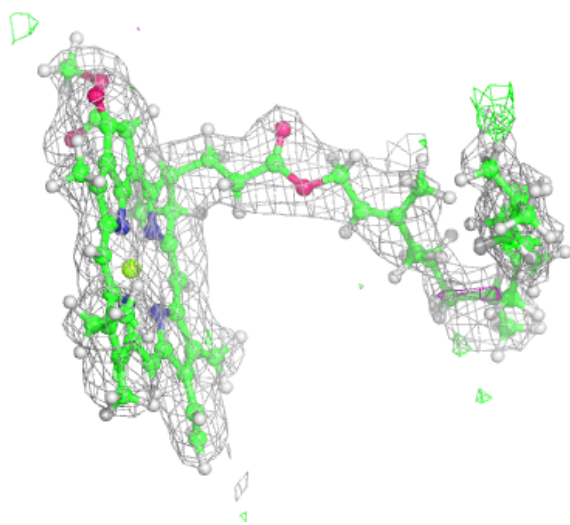
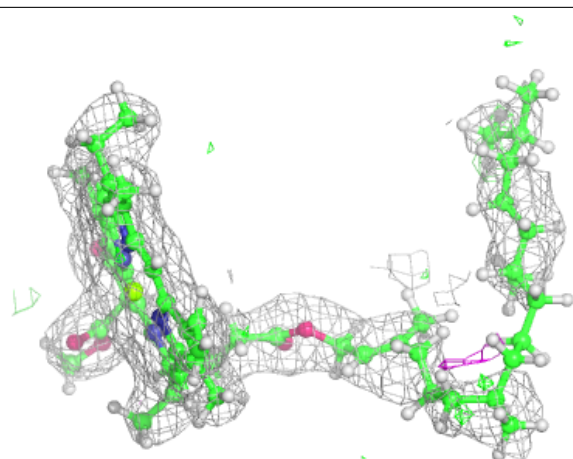
**Electron density around LMG D 410:**

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



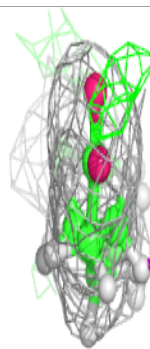
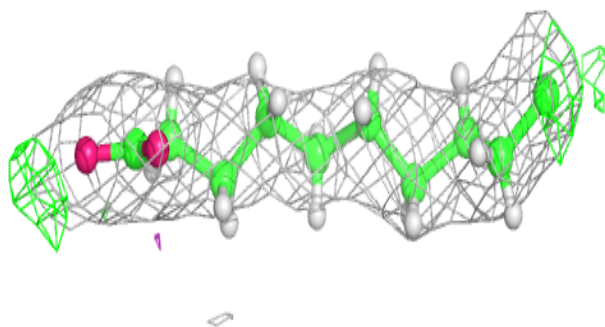
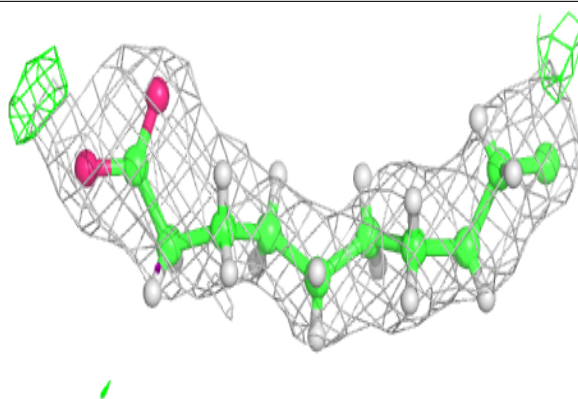
**Electron density around CLA a 606:**

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)

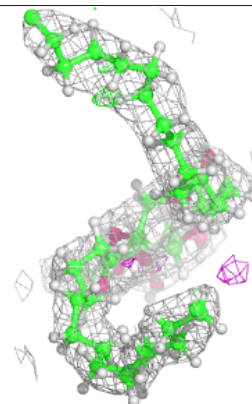
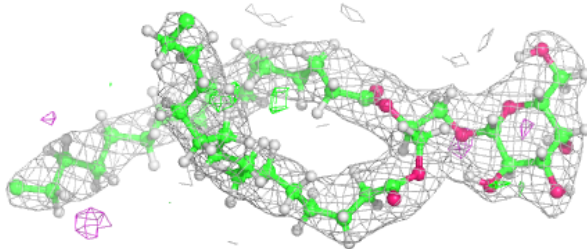
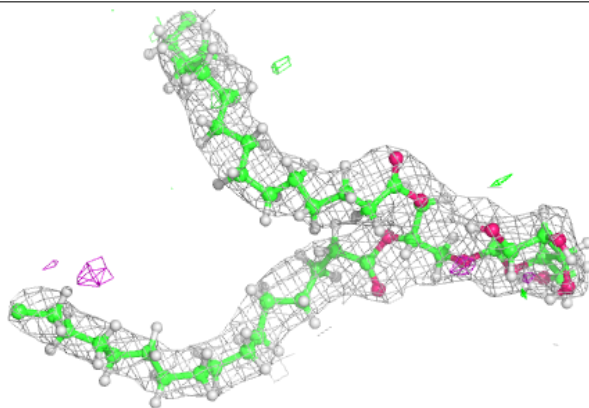


**Electron density around STE C 520:**

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

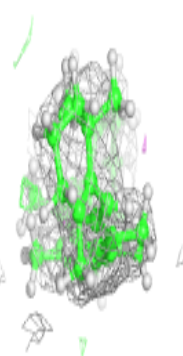
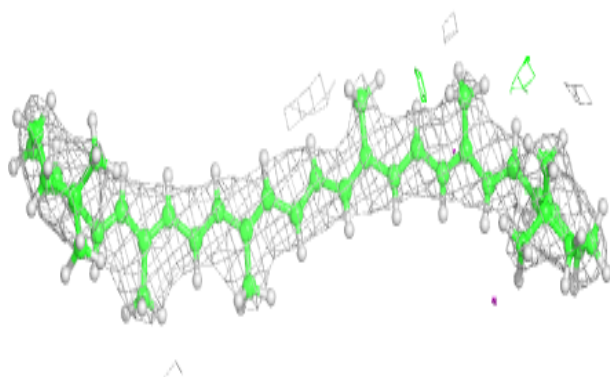
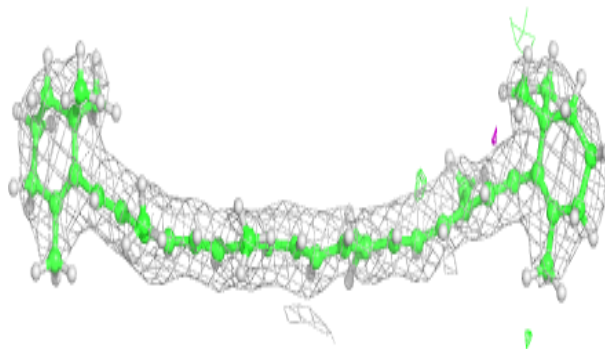
**Electron density around LMG M 101:**

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

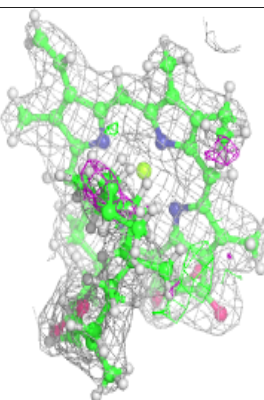
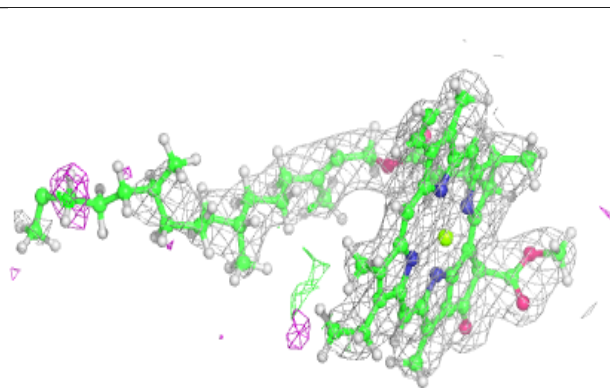
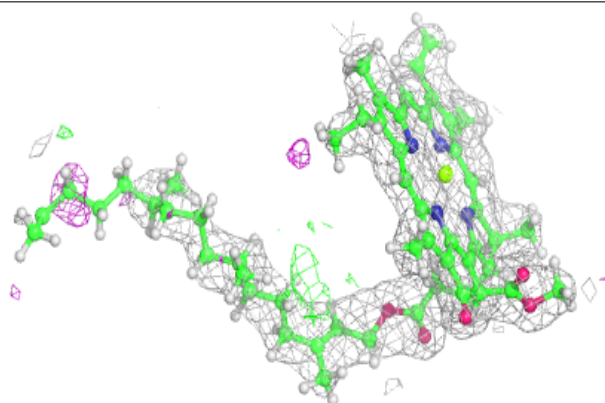


**Electron density around BCR k 102:**

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

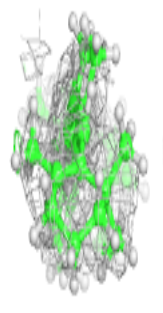
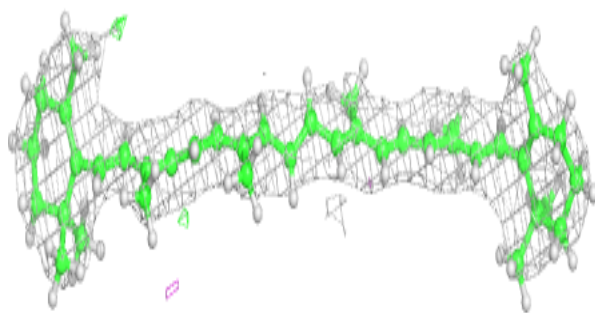
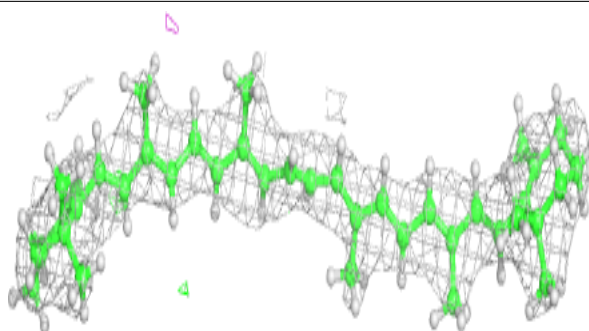
**Electron density around CLA c 508:**

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

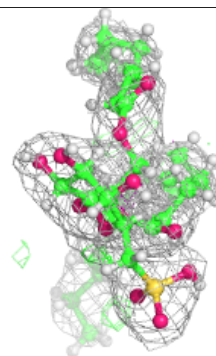
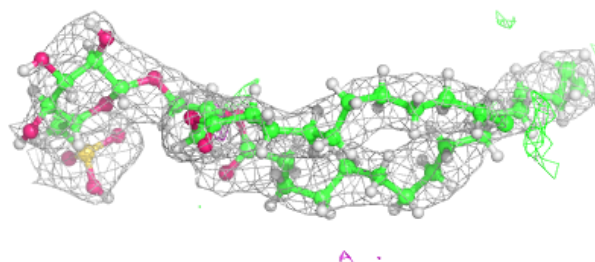
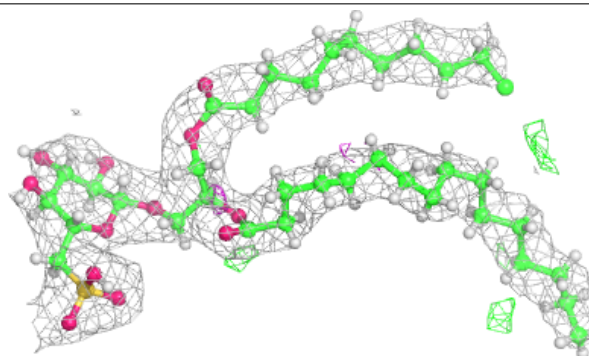


**Electron density around BCR c 514:**

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

**Electron density around SQD b 620:**

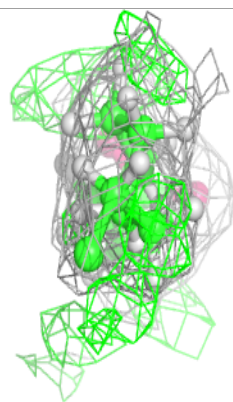
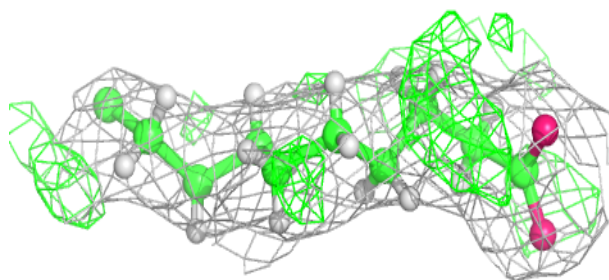
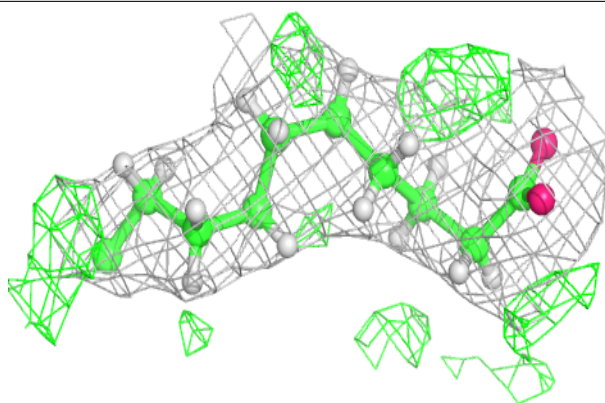
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



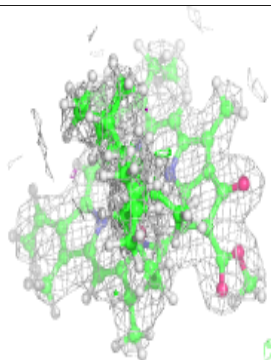
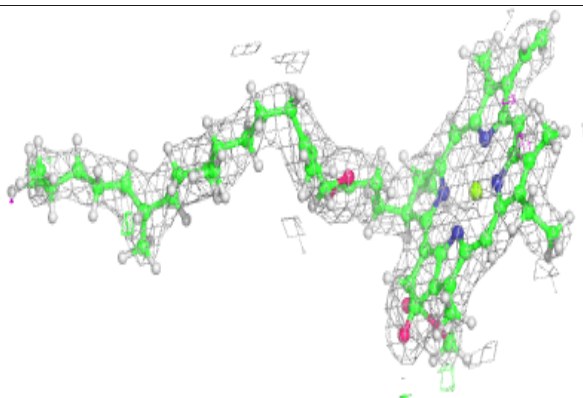
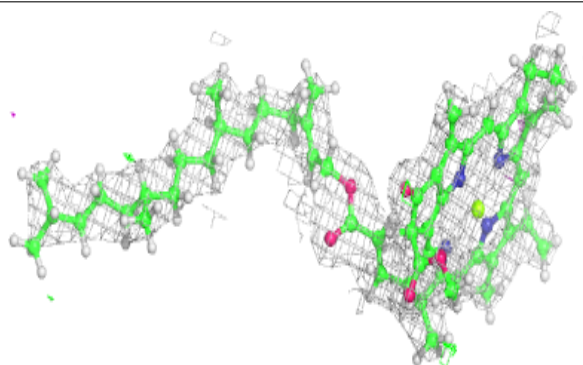


**Electron density around STE B 625:**

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

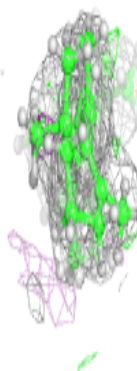
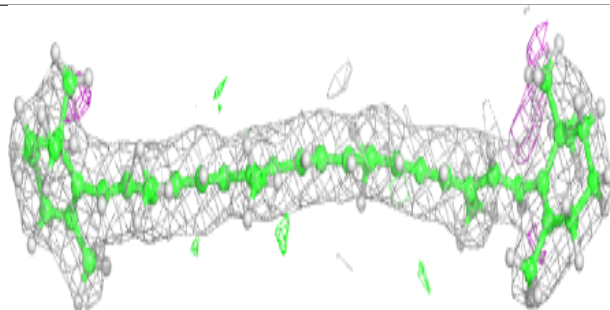
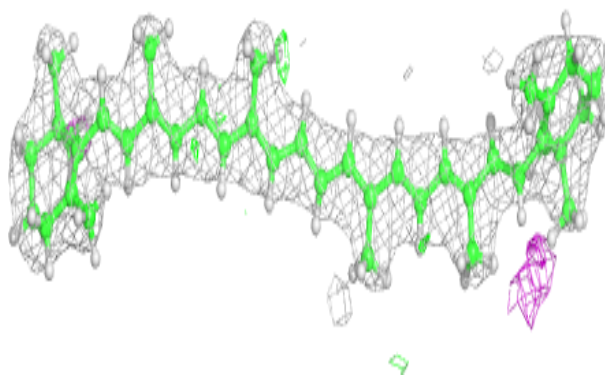
**Electron density around CLA C 502:**

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

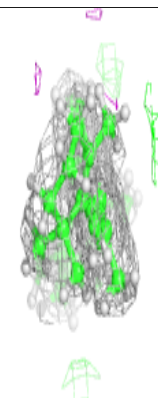
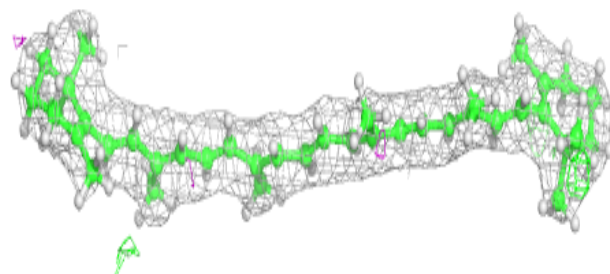
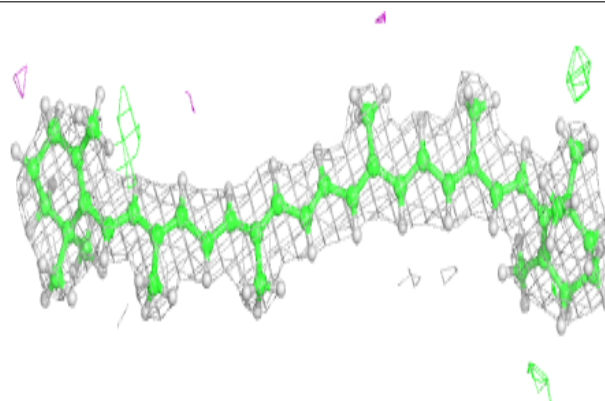


**Electron density around BCR B 618:**

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

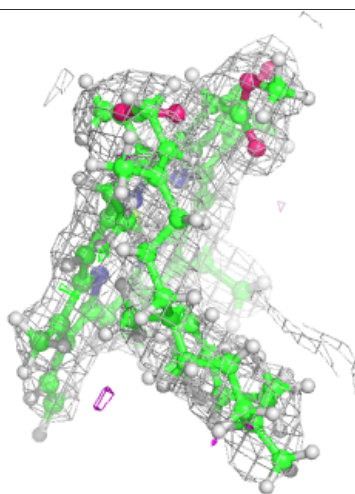
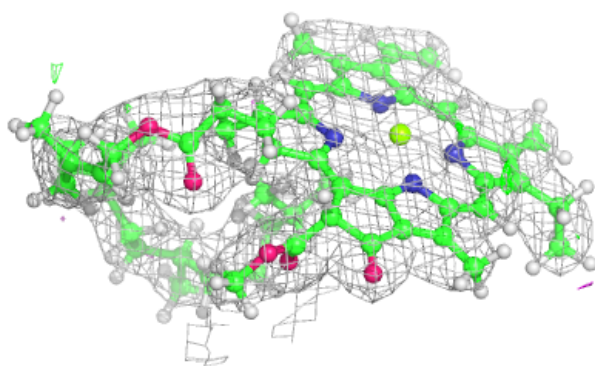
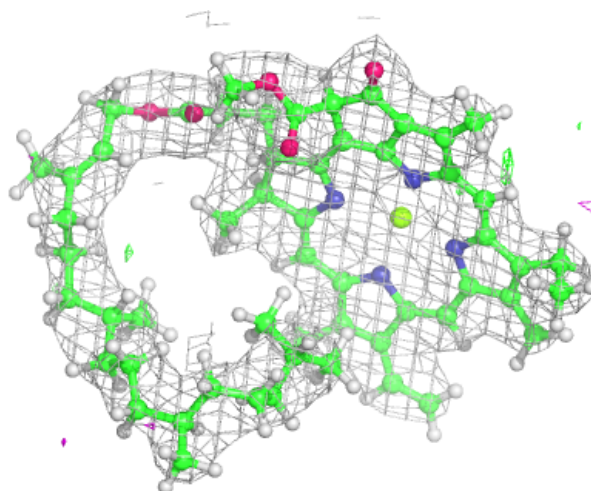
**Electron density around BCR B 619:**

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



**Electron density around CLA b 615:**

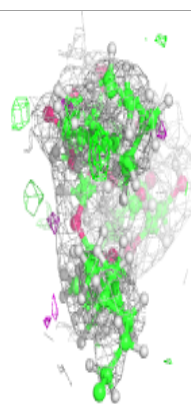
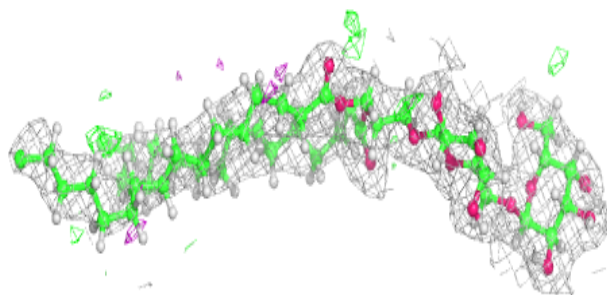
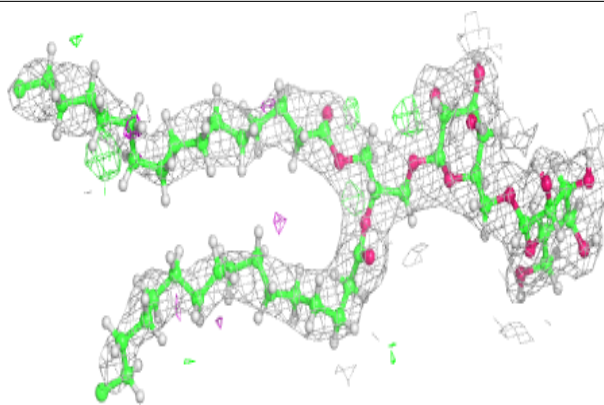
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



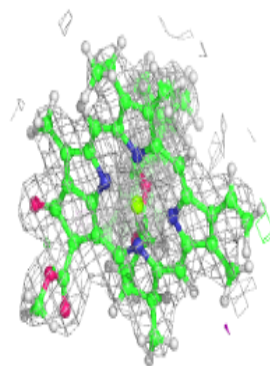
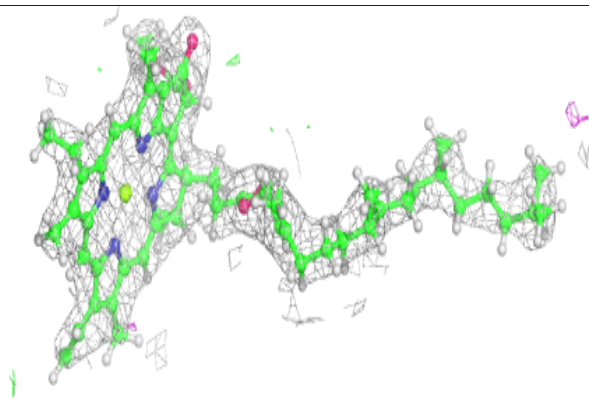
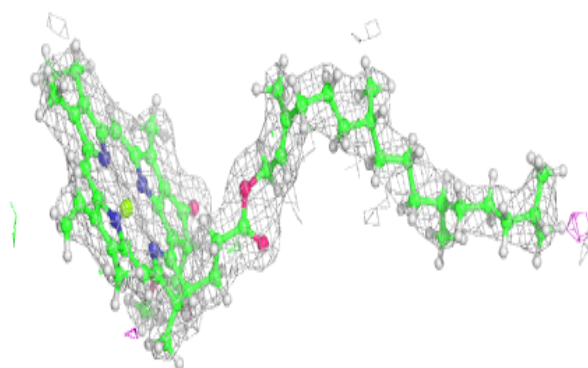


**Electron density around DGD c 518:**

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

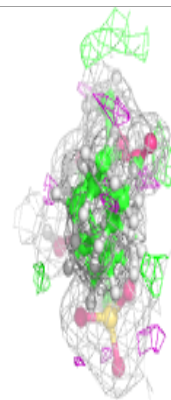
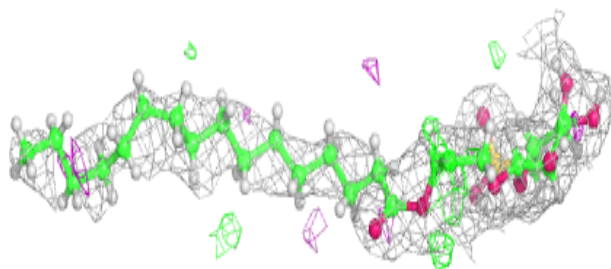
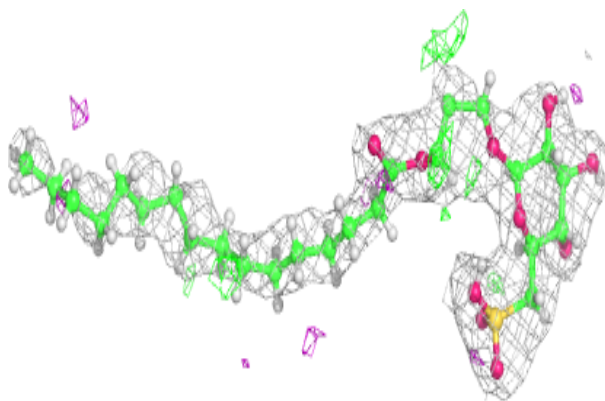
**Electron density around CLA c 502:**

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

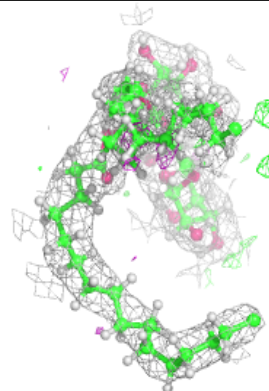
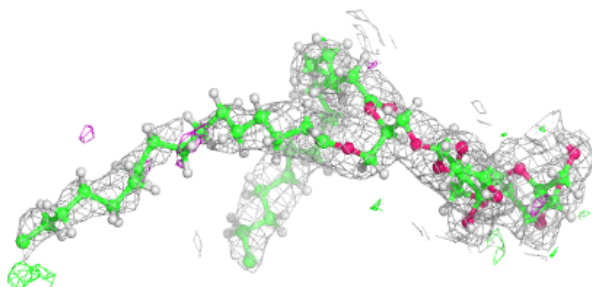
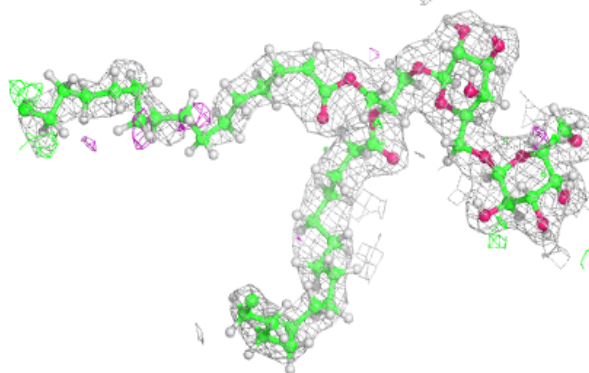


**Electron density around SQD D 407:**

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

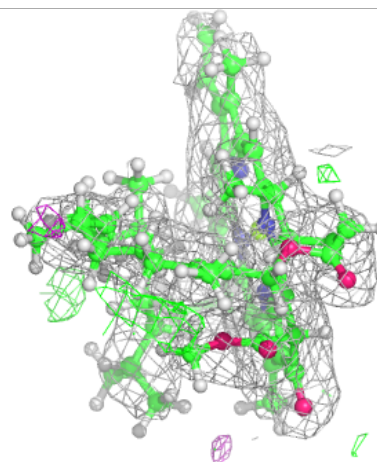
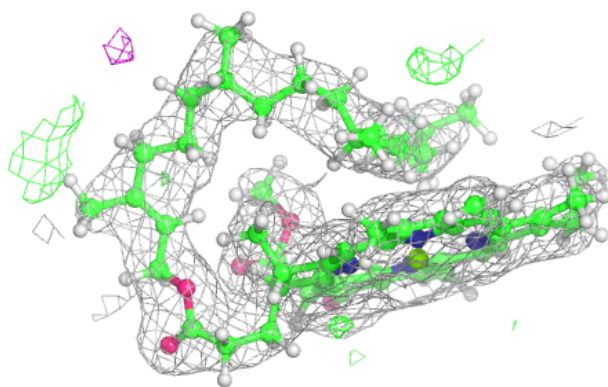
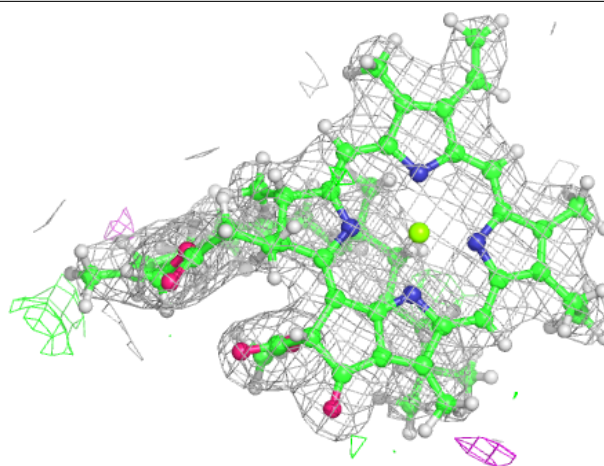
**Electron density around DGD c 517:**

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



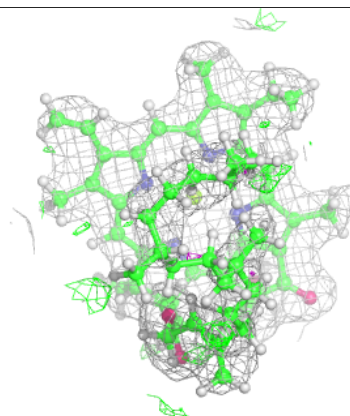
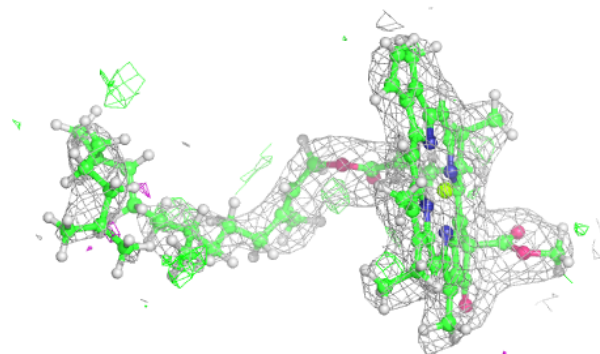
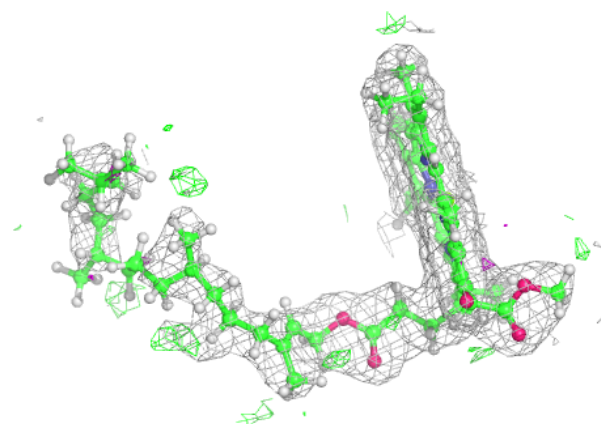
**Electron density around CLA c 510:**

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

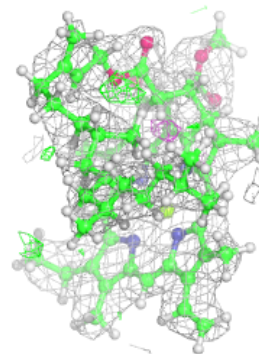
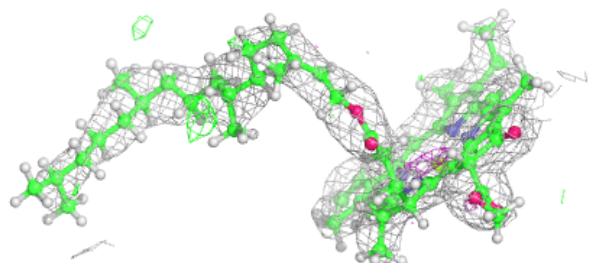
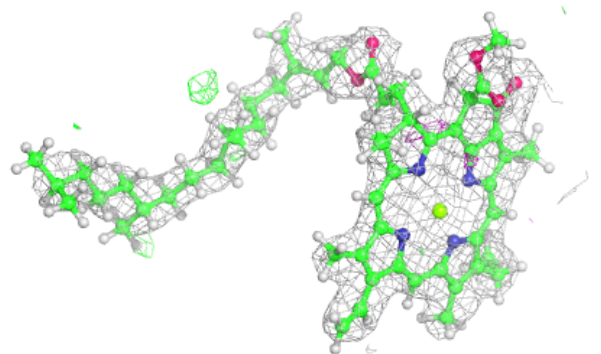


**Electron density around CLA C 506:**

$2mF_o-DF_c$  (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:**

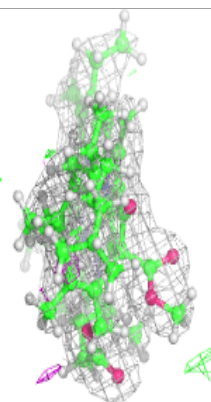
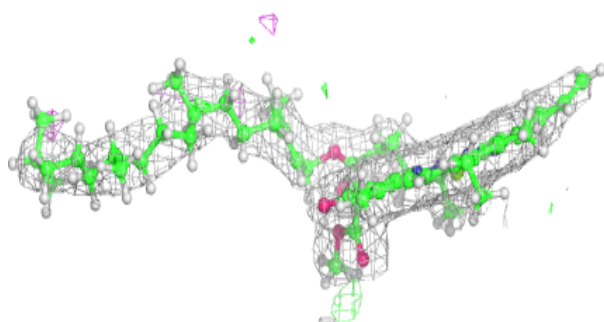
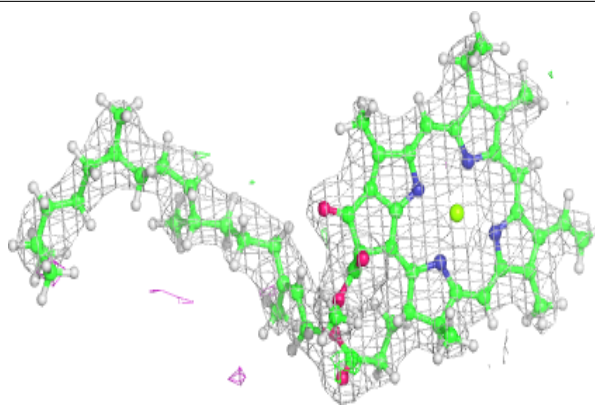
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



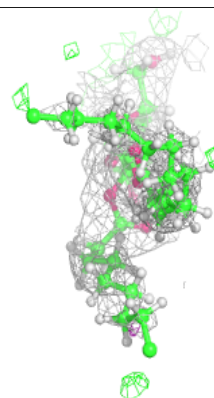
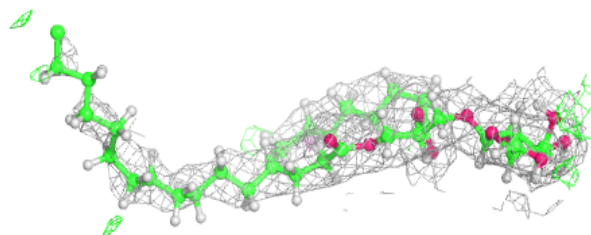
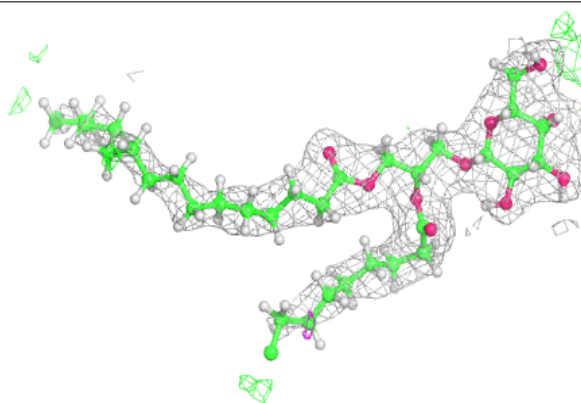


**Electron density around CLA b 602:**

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

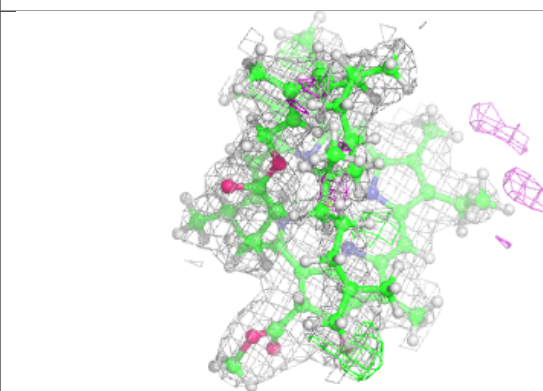
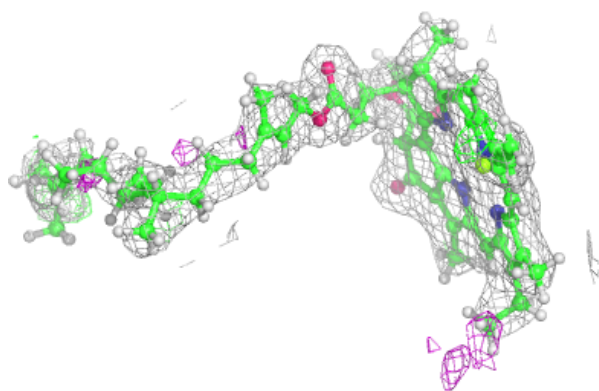
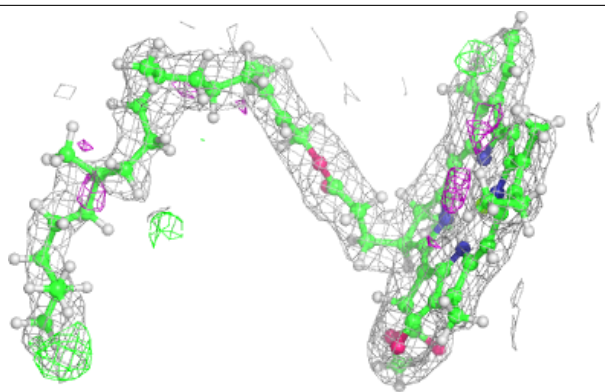
**Electron density around LMG d 410:**

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

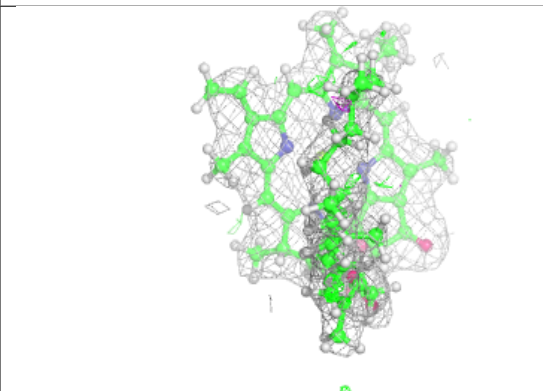
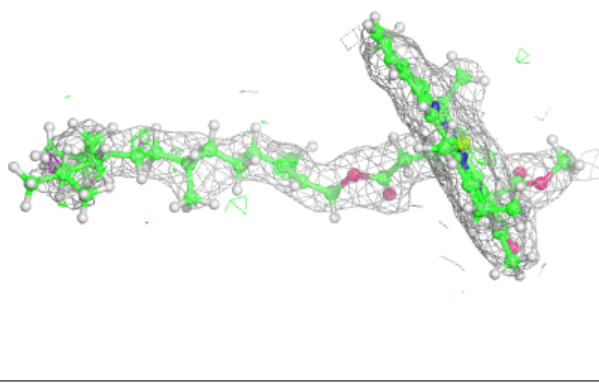
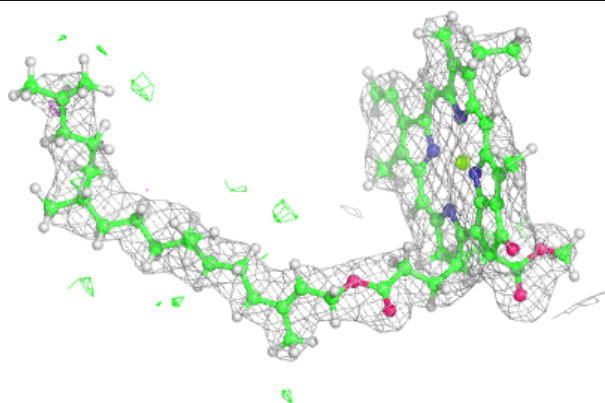


**Electron density around CLA b 606:**

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

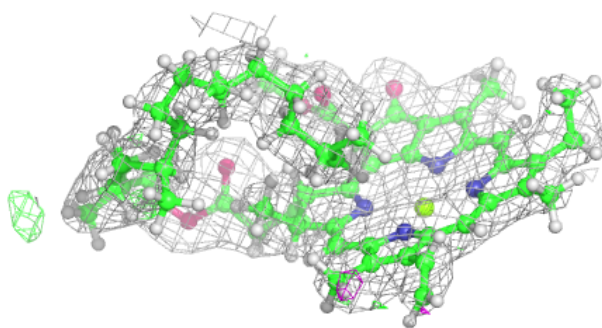
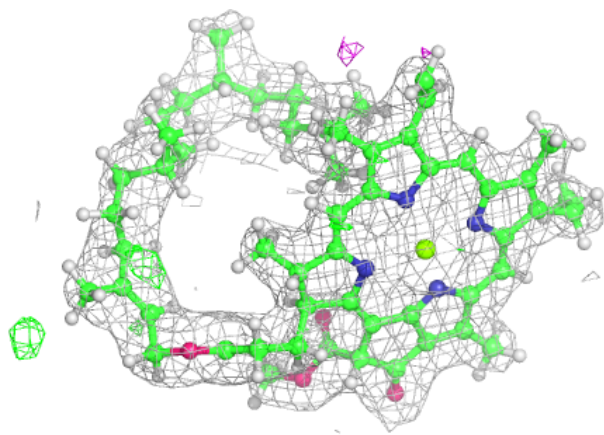
**Electron density around CLA b 609:**

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



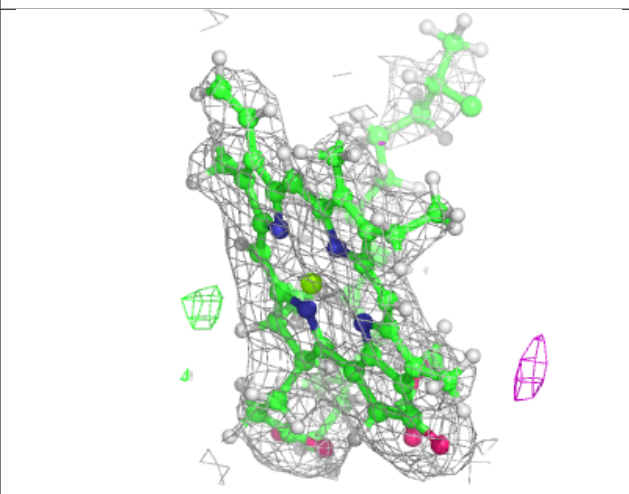
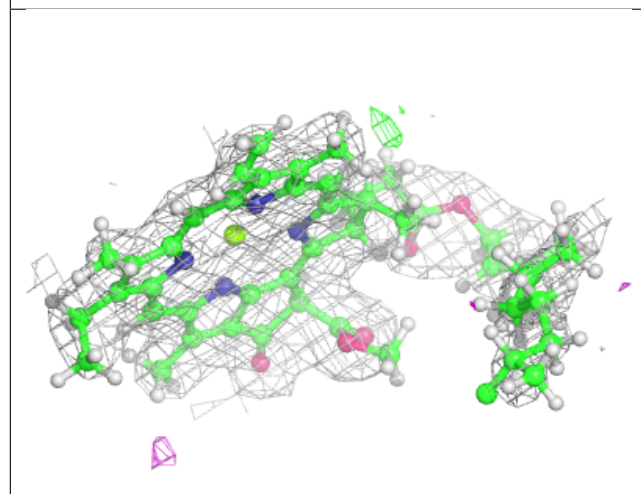
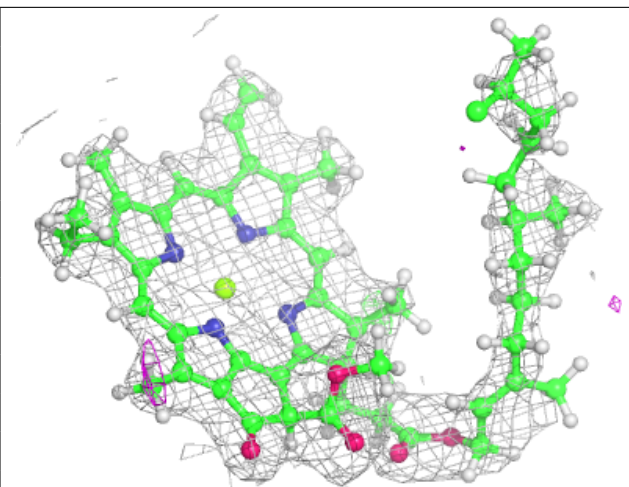
**Electron density around CLA B 615:**

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



**Electron density around CLA b 616:**

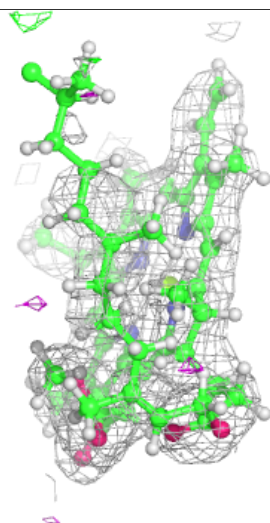
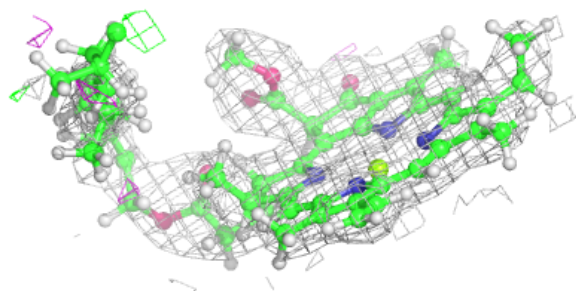
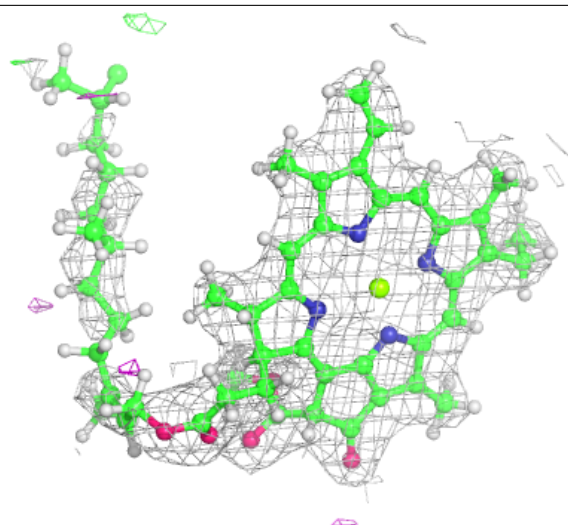
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





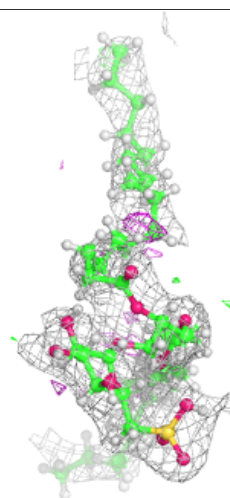
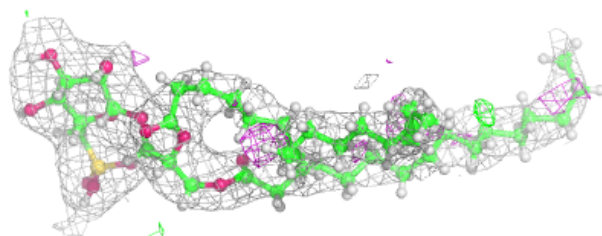
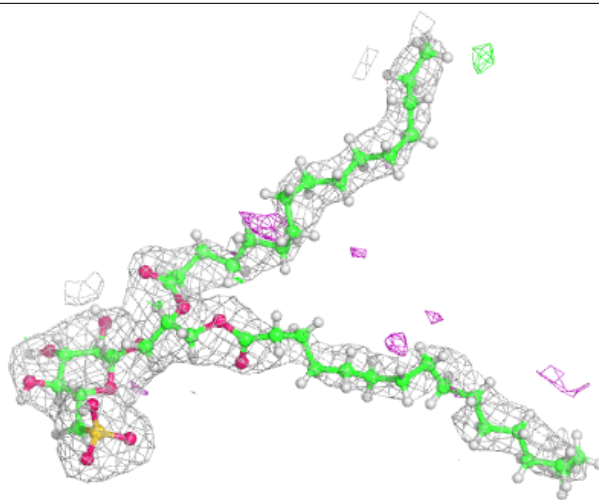
**Electron density around CLA B 616:**

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



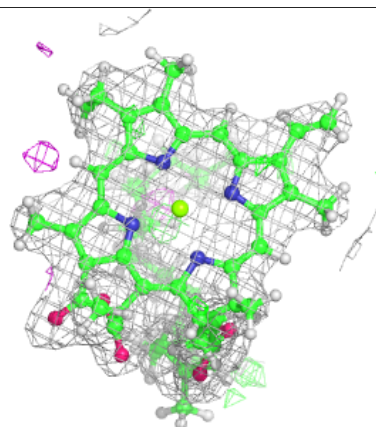
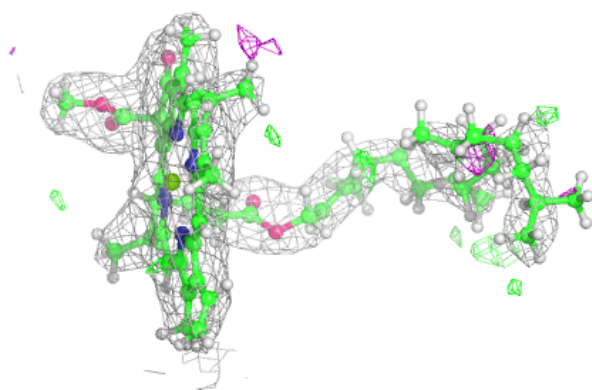
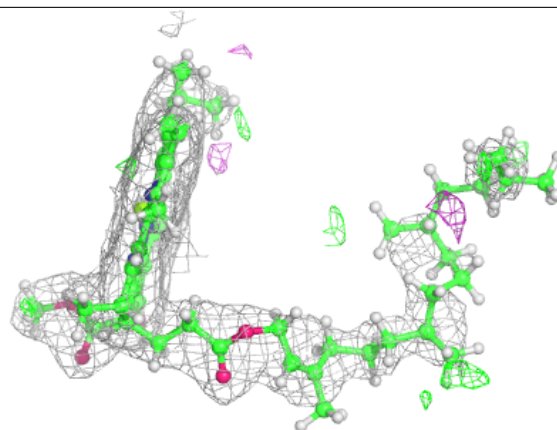
**Electron density around SQD a 613:**

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

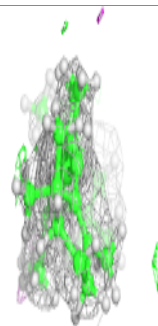
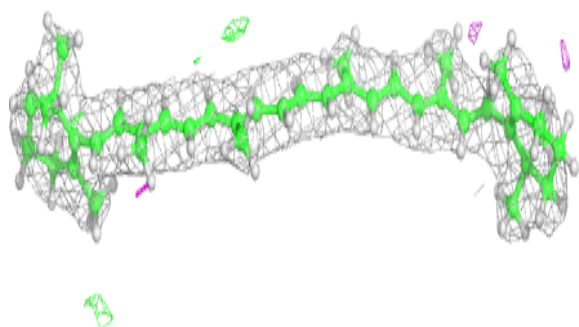
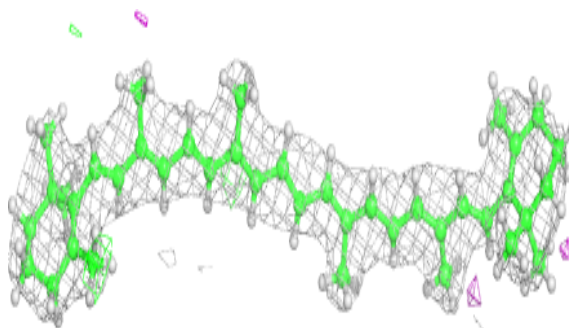


**Electron density around CLA c 506:**

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

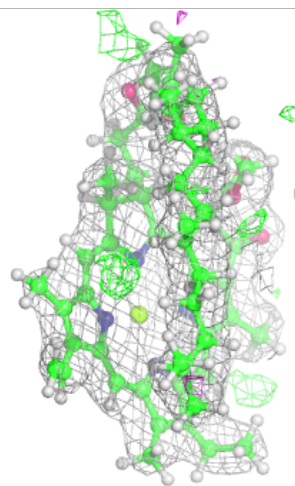
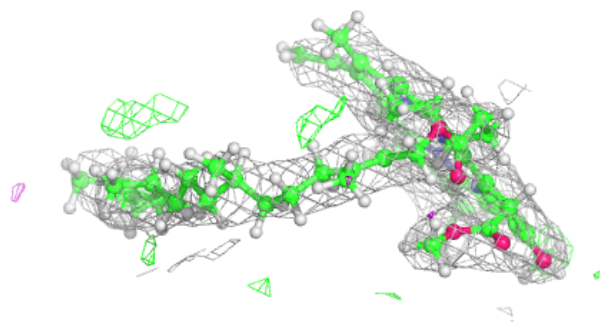
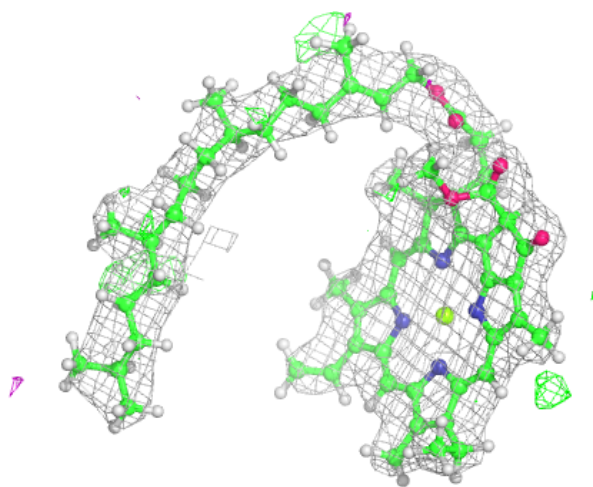
**Electron density around BCR b 619:**

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



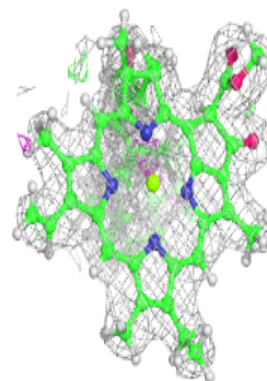
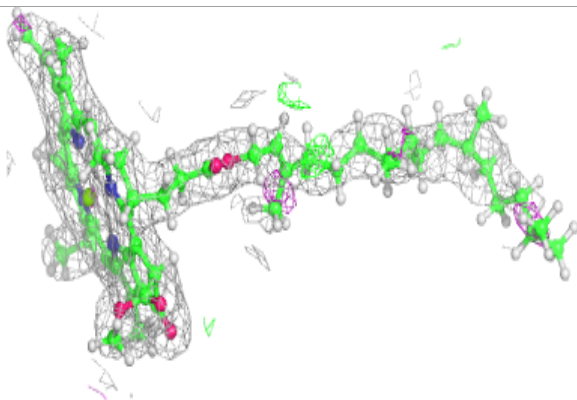
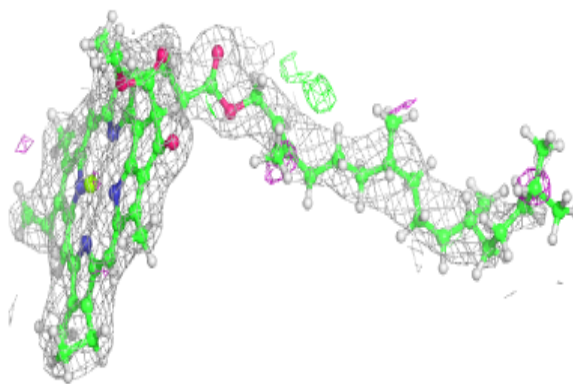
**Electron density around CLA c 507:**

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

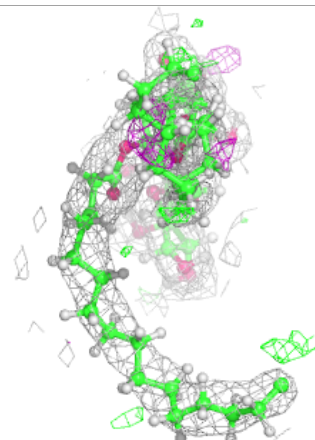
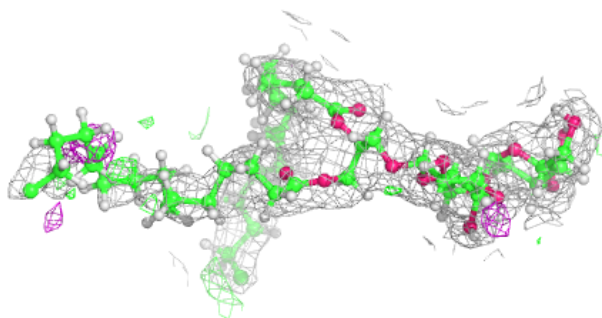
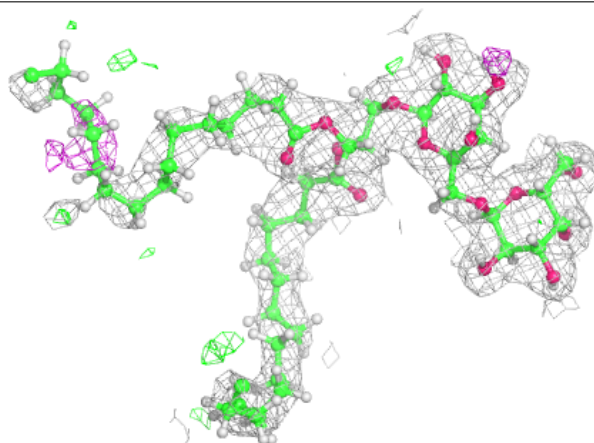


**Electron density around CLA B 604:**

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

**Electron density around DGD C 517:**

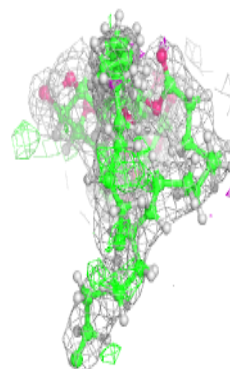
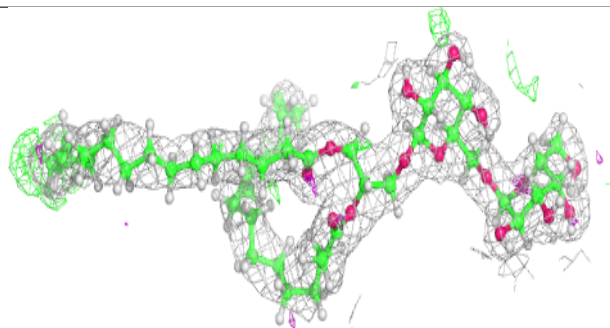
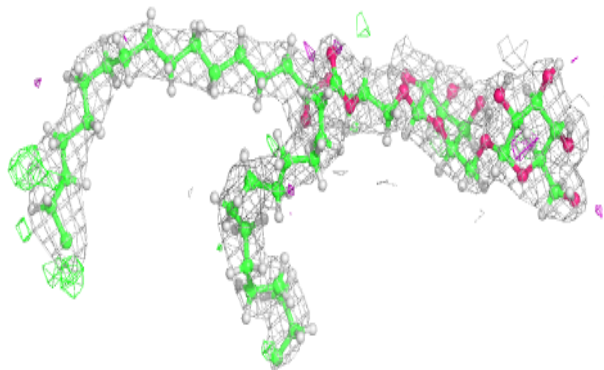
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



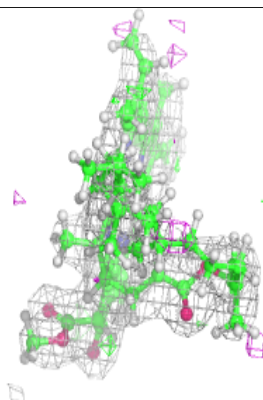
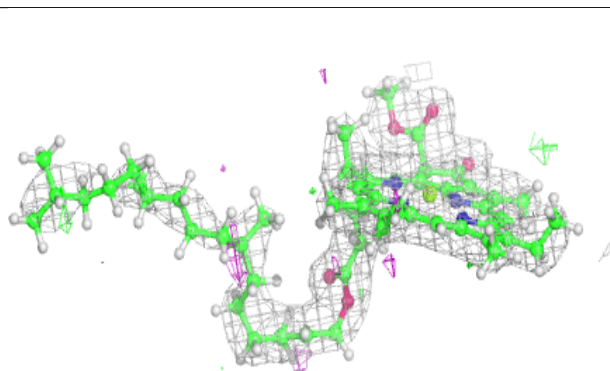
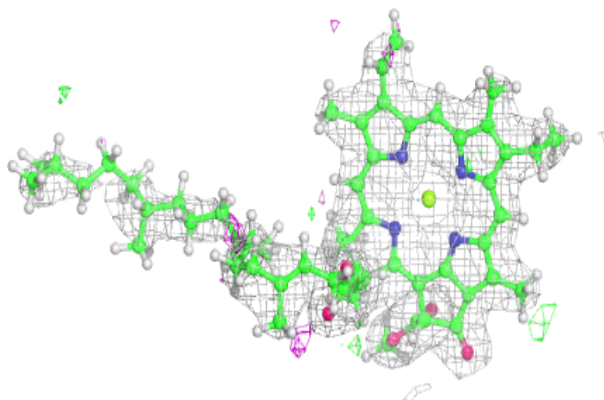


**Electron density around DGD H 102:**

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

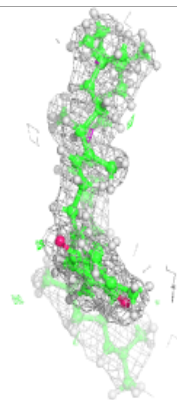
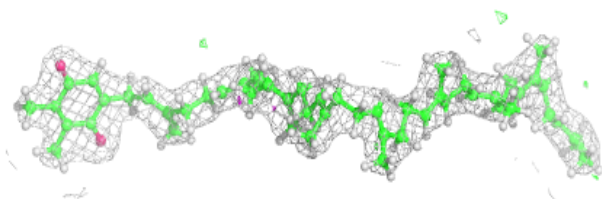
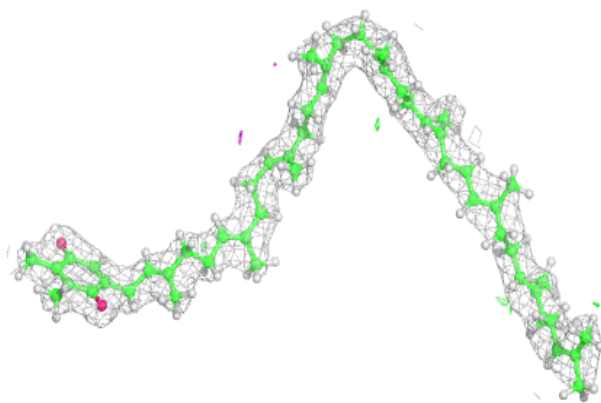
**Electron density around CLA d 401:**

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

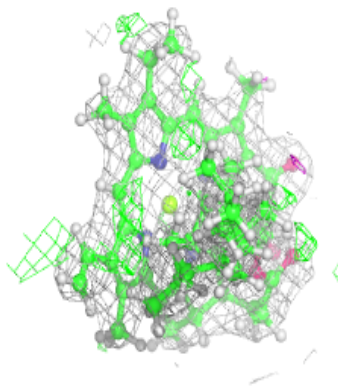
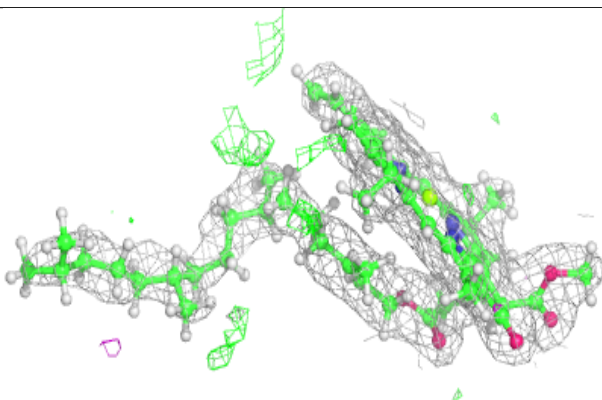
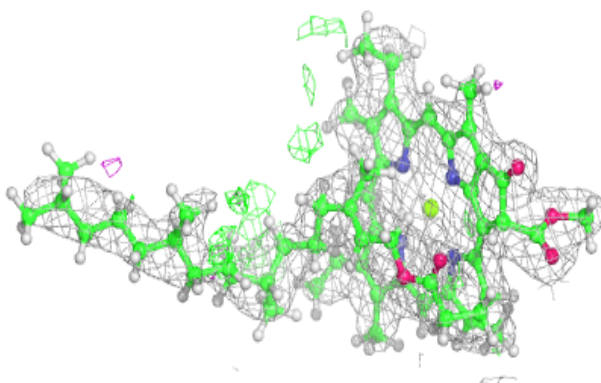


**Electron density around PL9 D 405:**

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

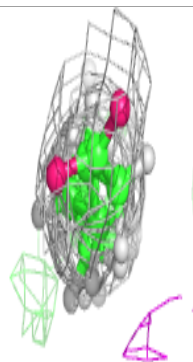
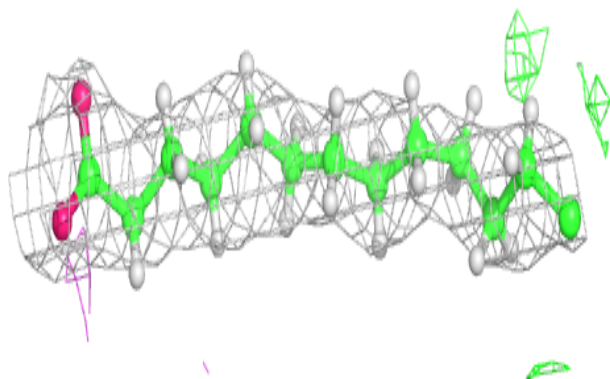
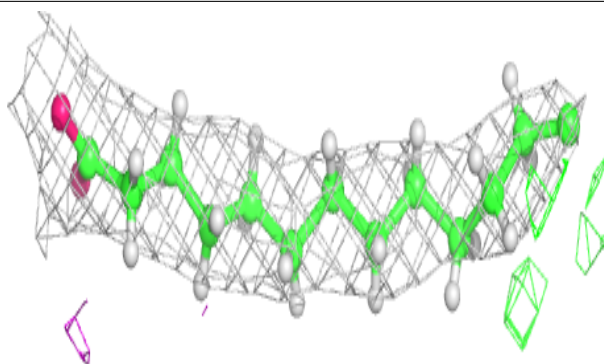
**Electron density around CLA C 505:**

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

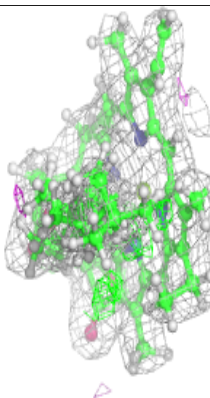
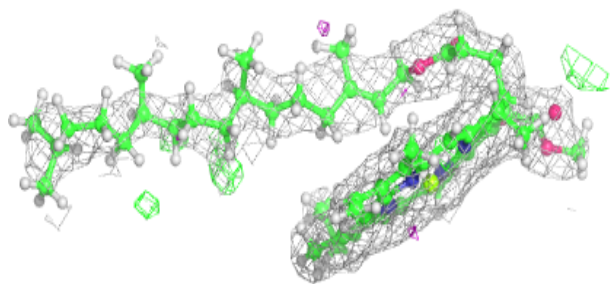
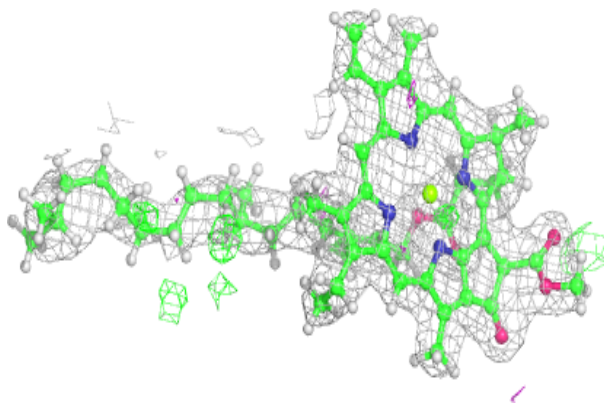


**Electron density around STE M 102:**

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

**Electron density around CLA B 614:**

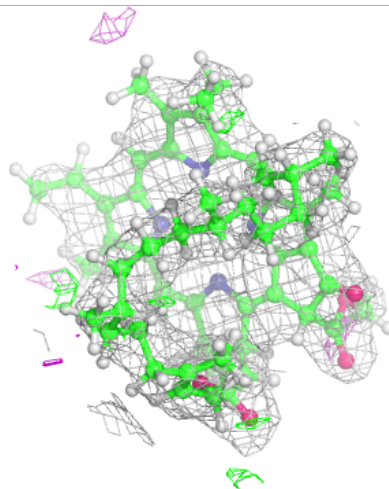
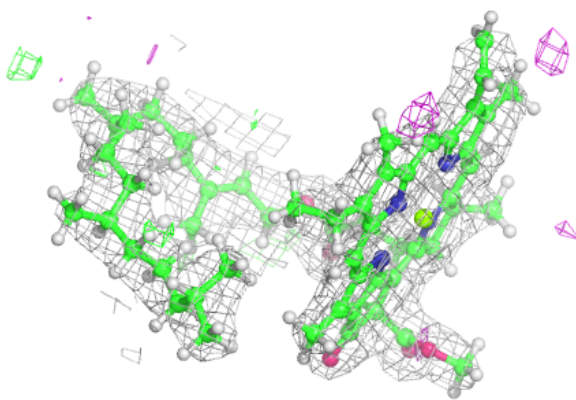
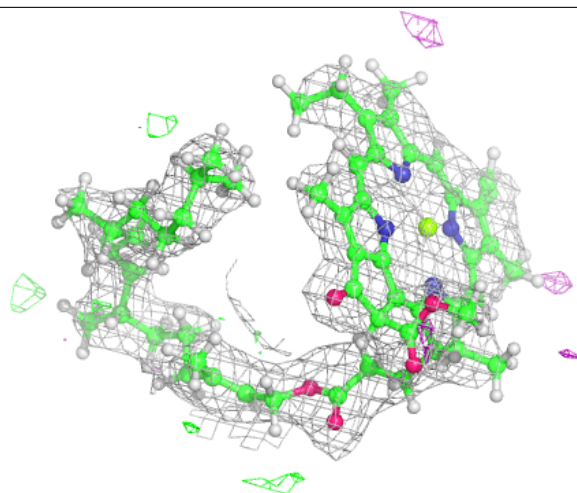
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





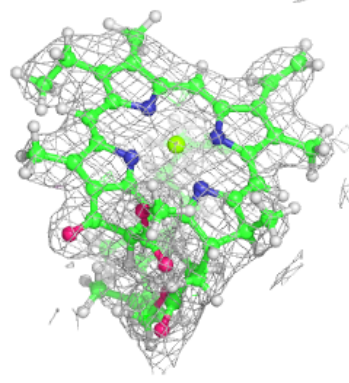
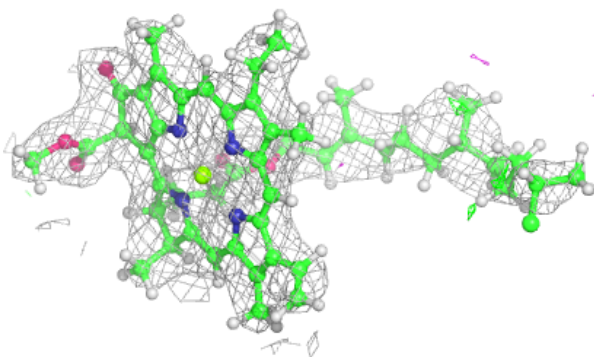
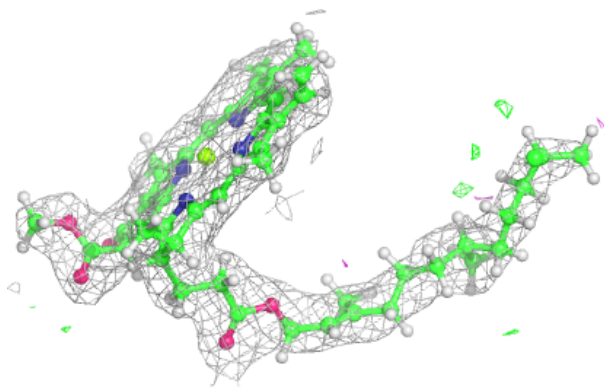
**Electron density around CLA c 503:**

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

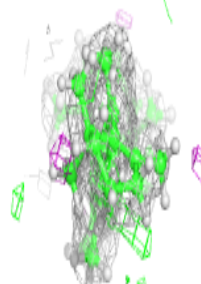
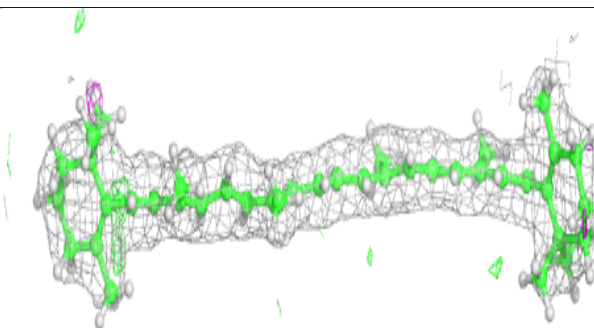
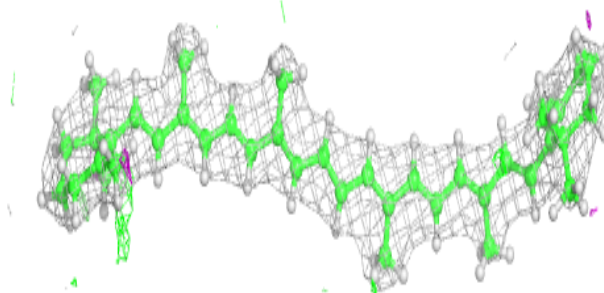


**Electron density around CLA c 504:**

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

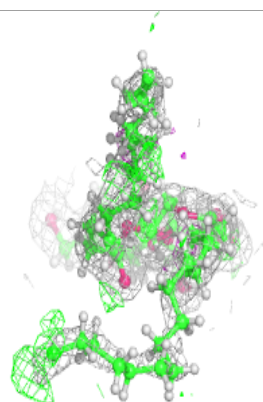
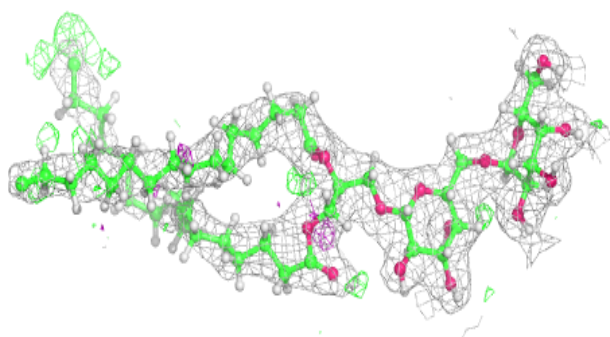
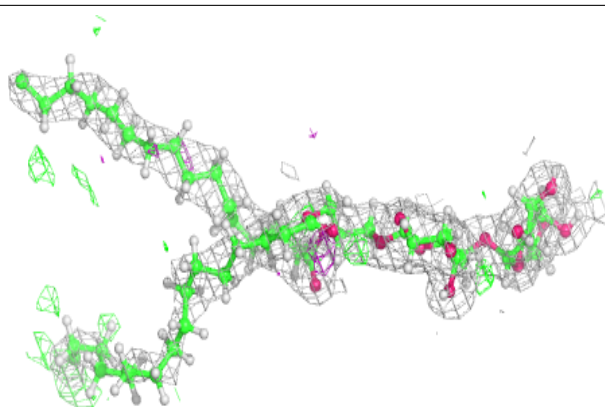
**Electron density around BCR C 515:**

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

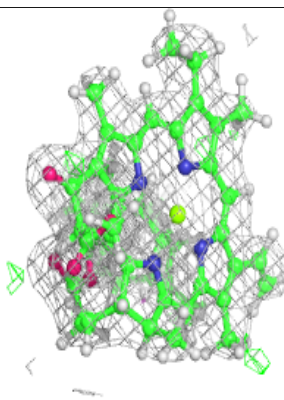
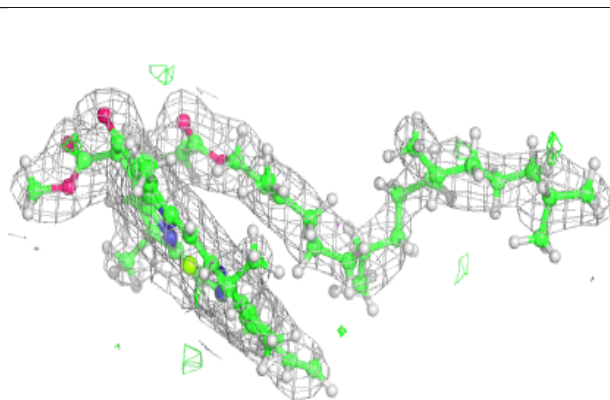
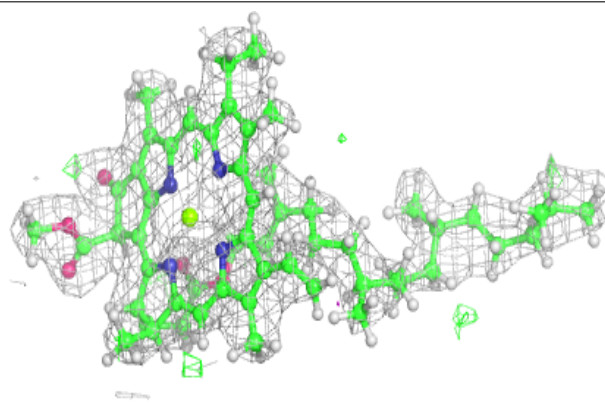


**Electron density around DGD C 516:**

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

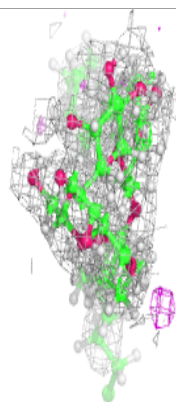
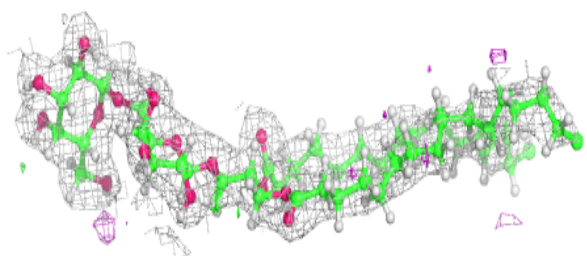
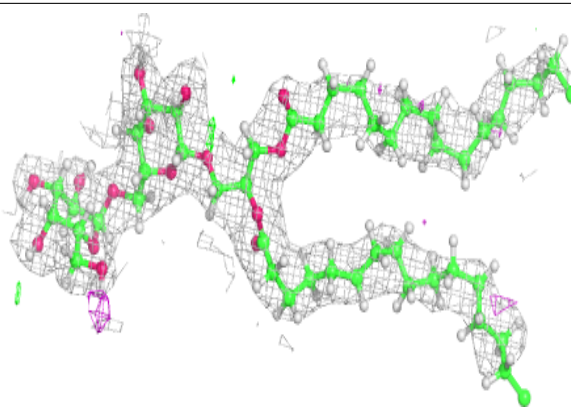
**Electron density around CLA c 505:**

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



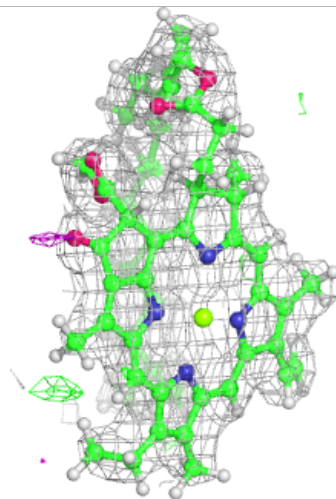
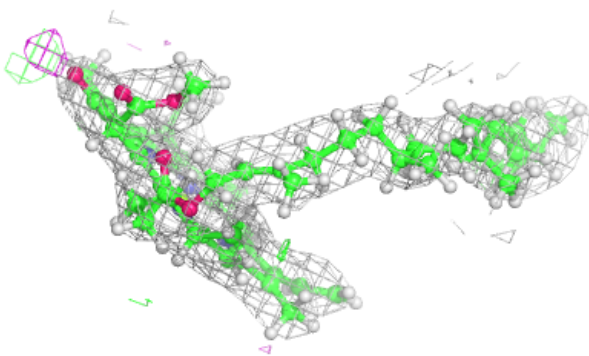
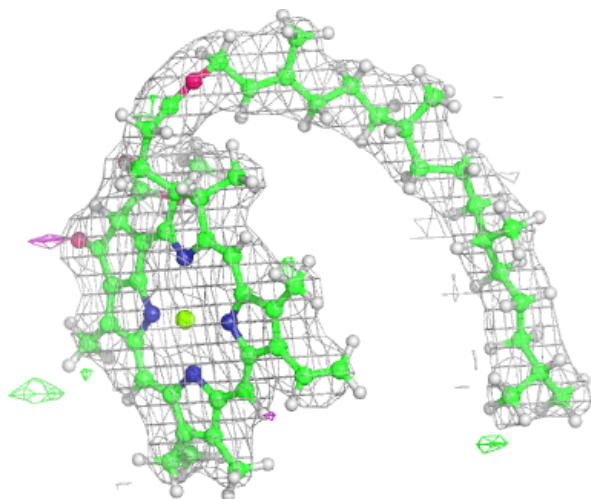
**Electron density around DGD C 518:**

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



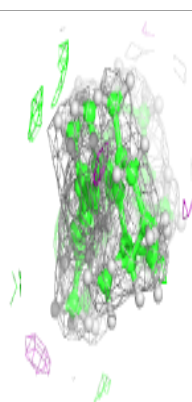
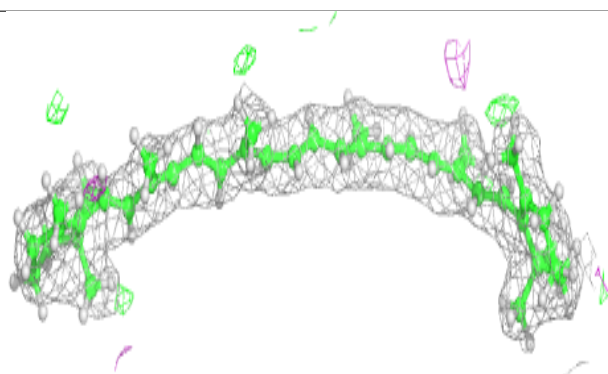
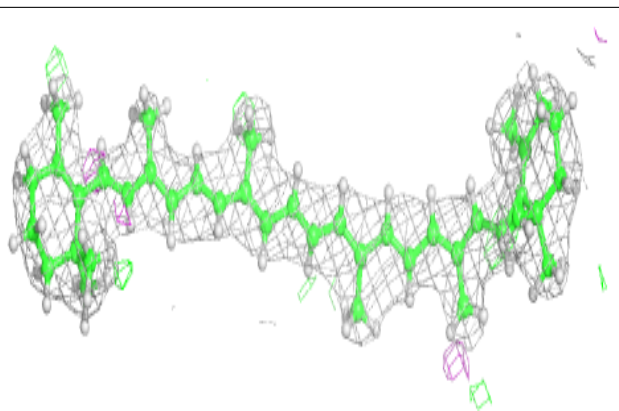
**Electron density around CLA C 507:**

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



**Electron density around BCR T 101:**

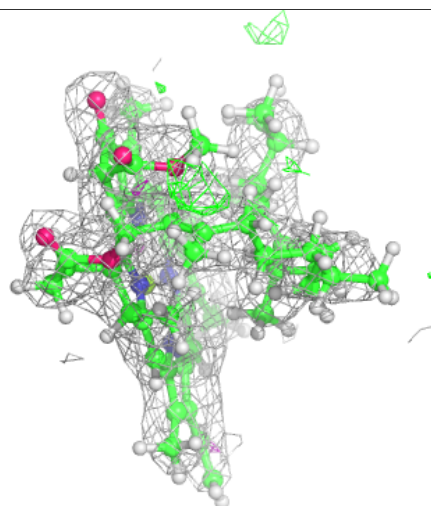
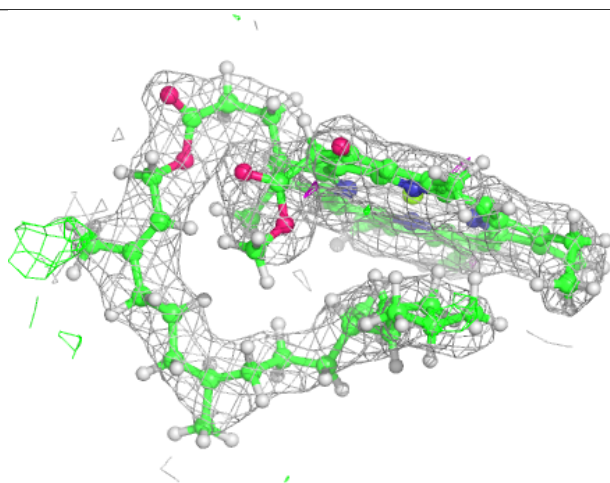
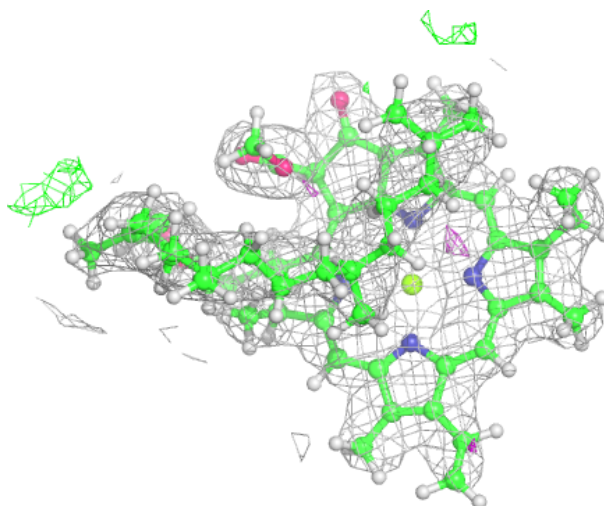
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





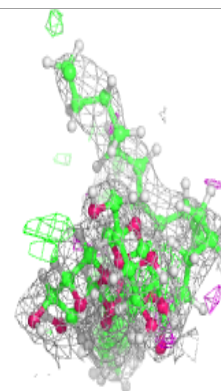
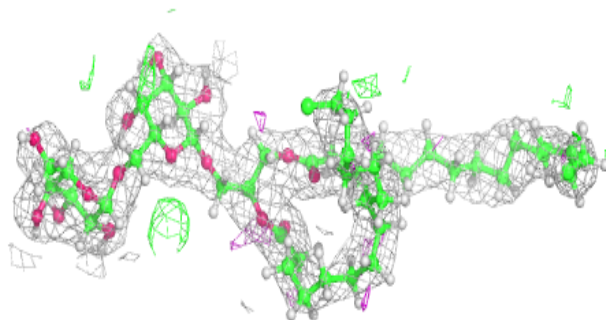
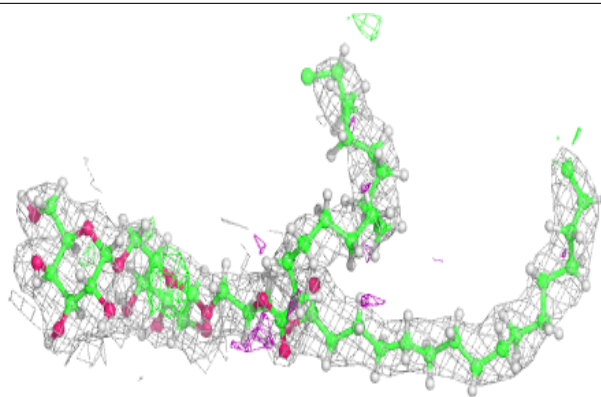
**Electron density around CLA C 510:**

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

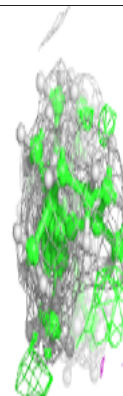
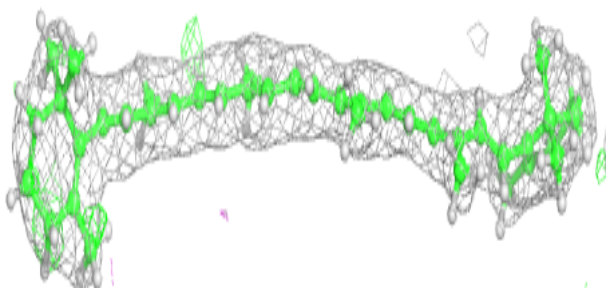
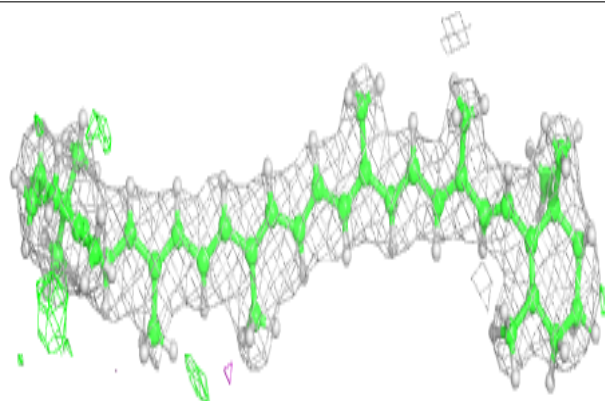


**Electron density around DGD h 101:**

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

**Electron density around BCR b 617:**

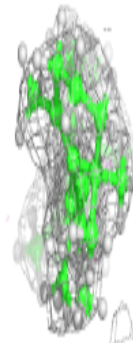
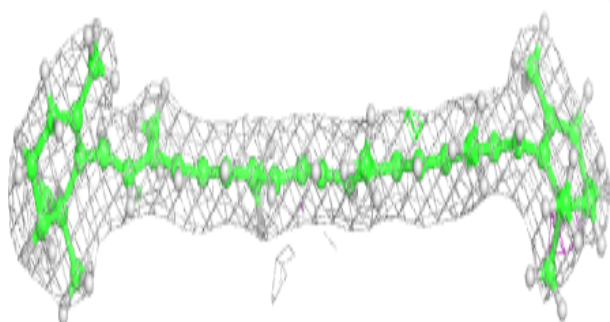
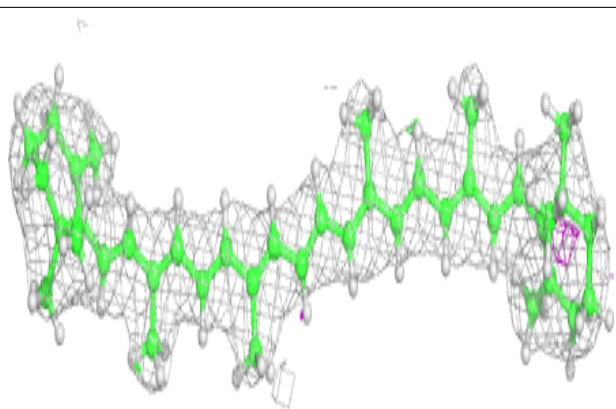
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



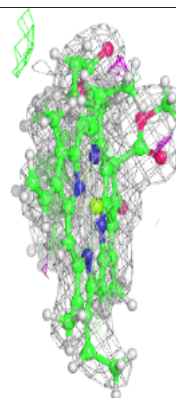
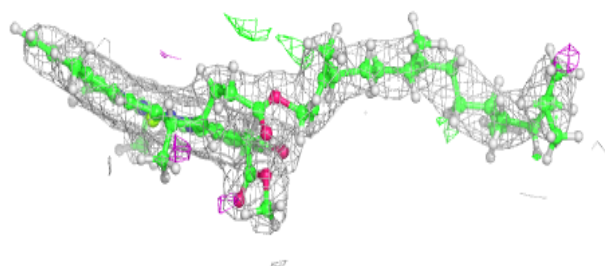
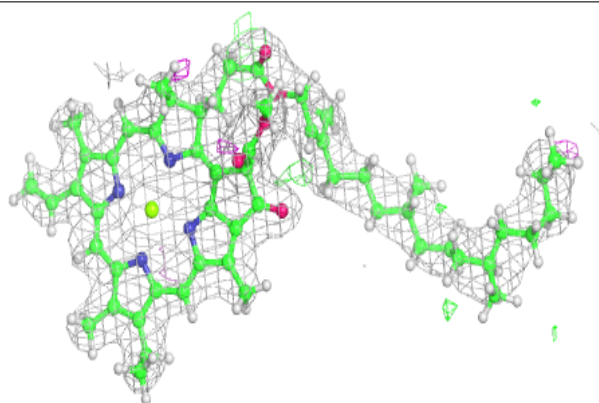


**Electron density around BCR b 618:**

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

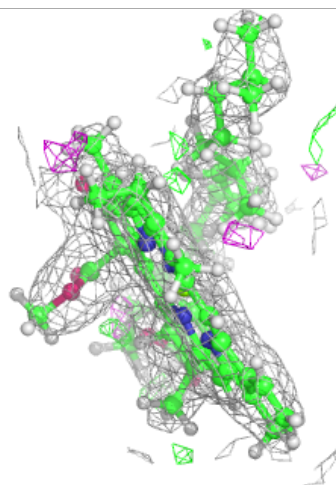
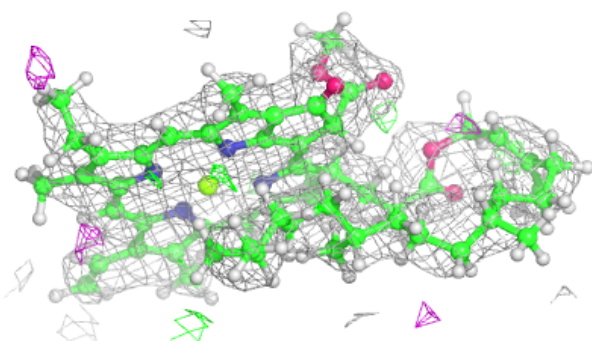
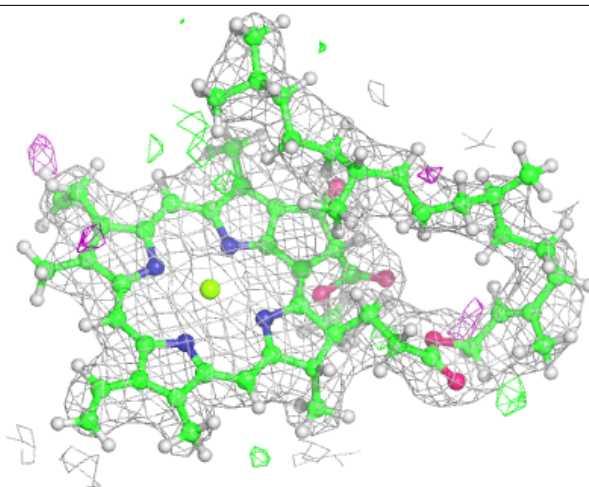
**Electron density around CLA B 602:**

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



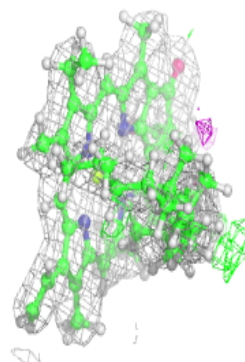
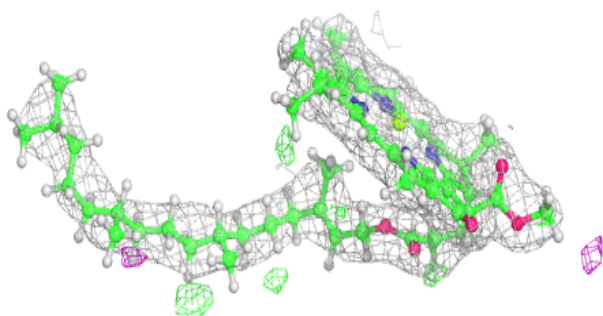
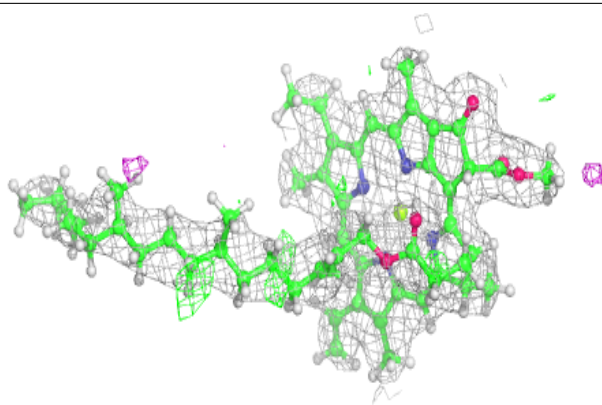
**Electron density around CLA c 509:**

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

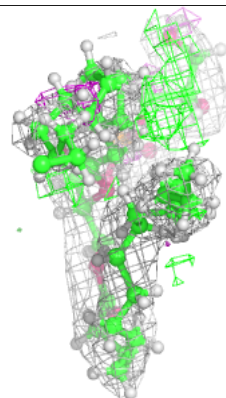
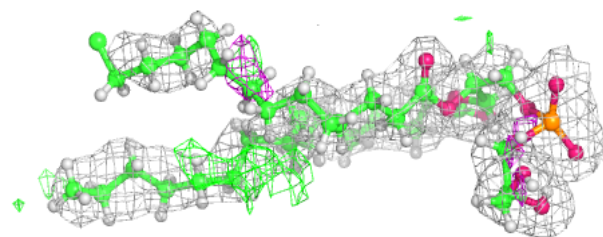
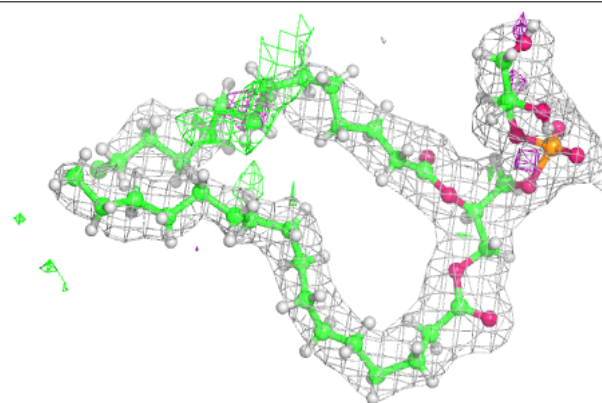


**Electron density around CLA b 608:**

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

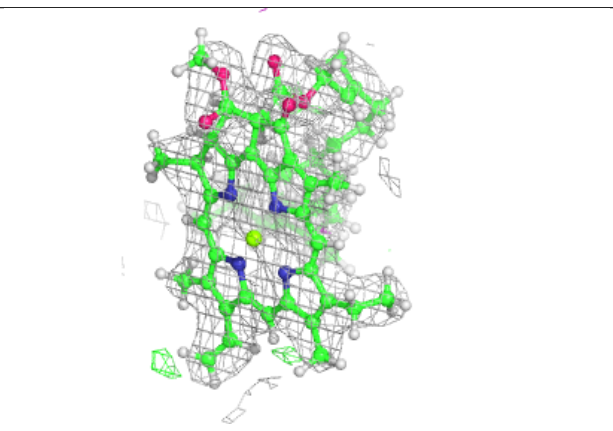
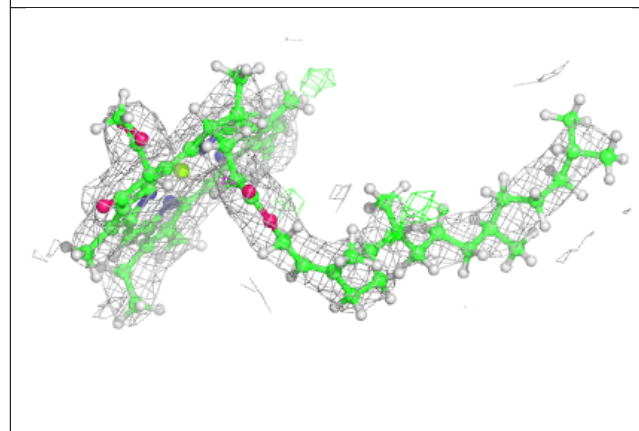
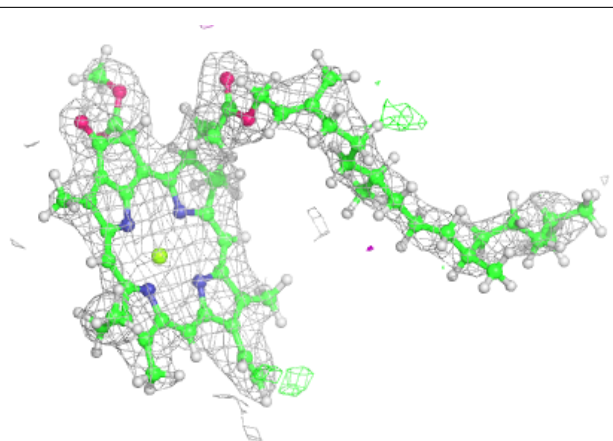
**Electron density around LHG A 615:**

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



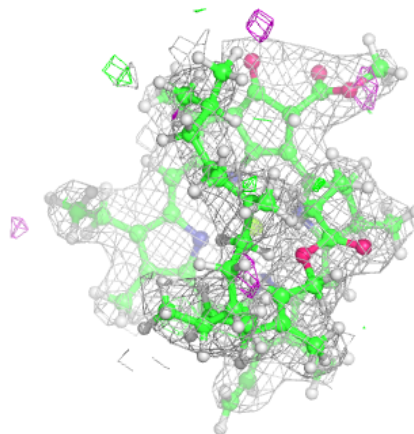
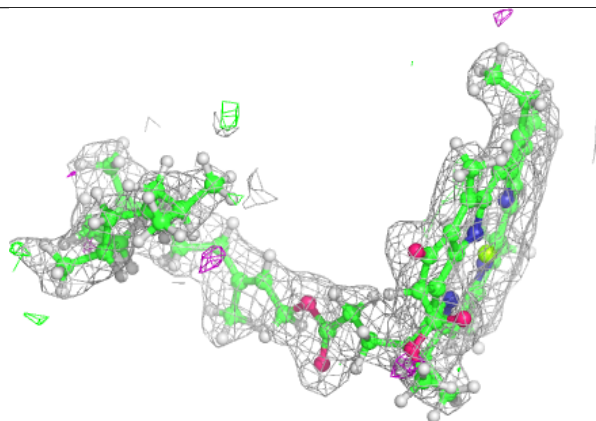
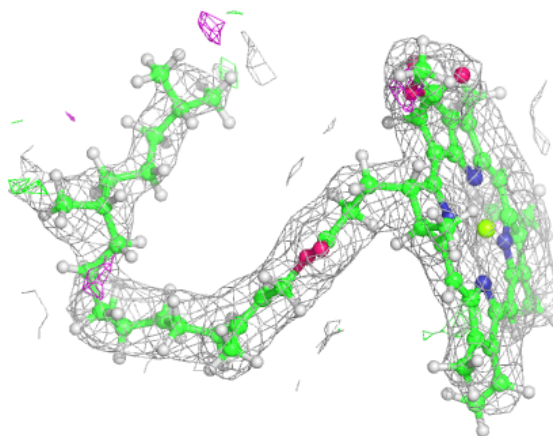
**Electron density around CLA c 511:**

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



**Electron density around CLA B 606:**

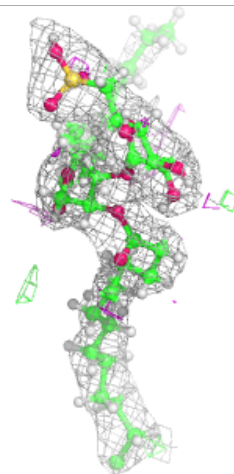
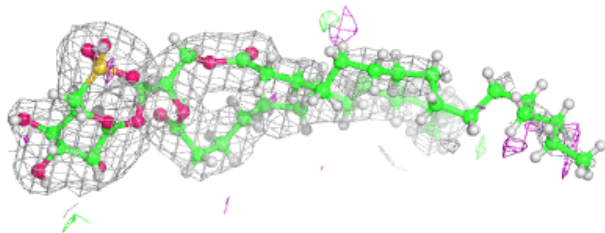
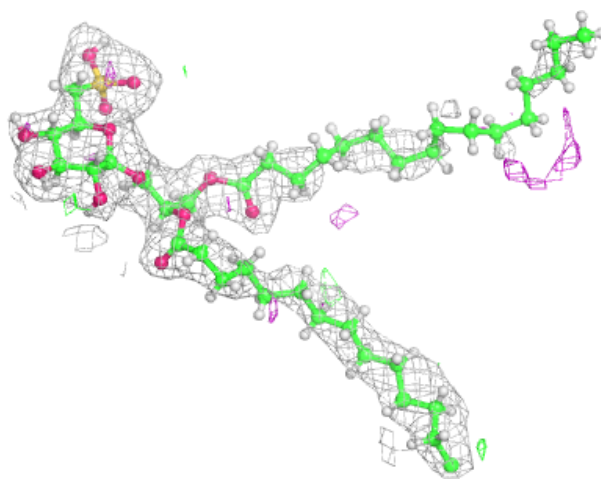
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





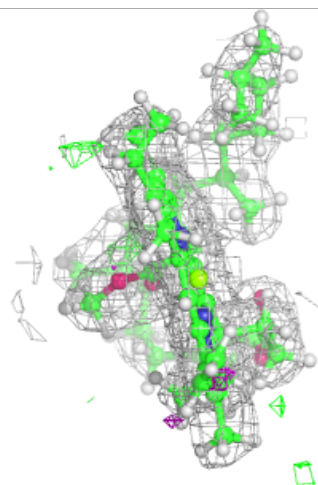
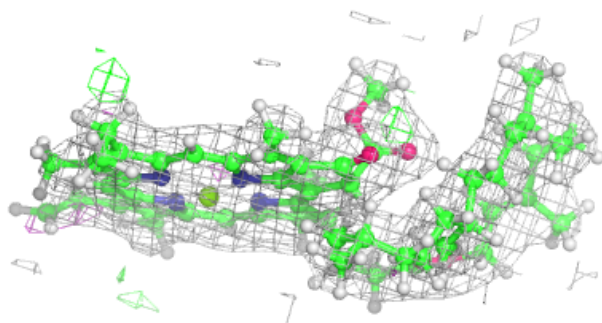
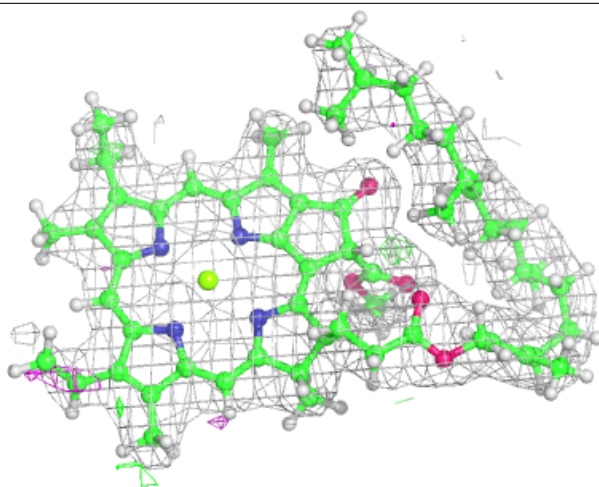
**Electron density around SQD A 616:**

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



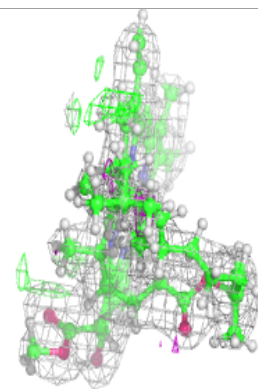
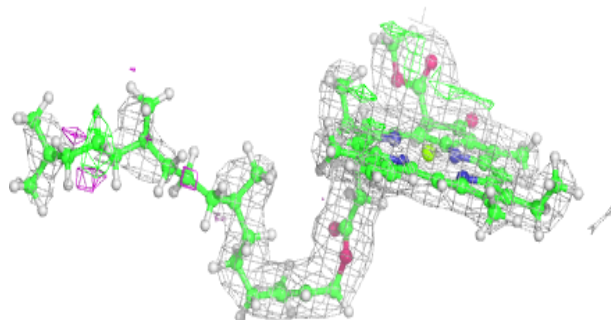
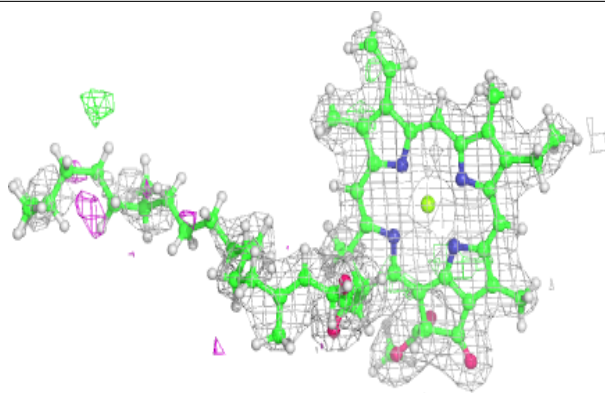
**Electron density around CLA B 610:**

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

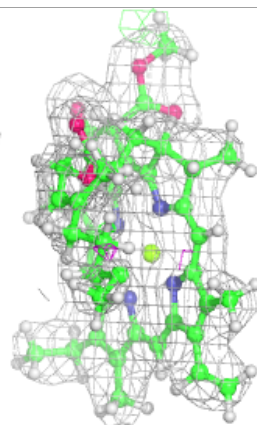
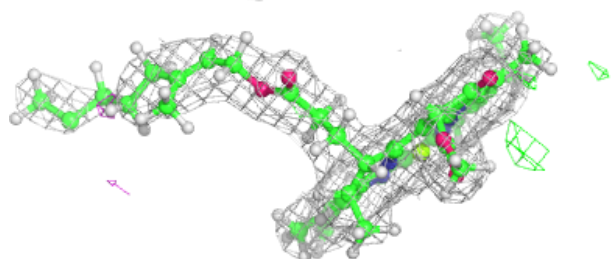
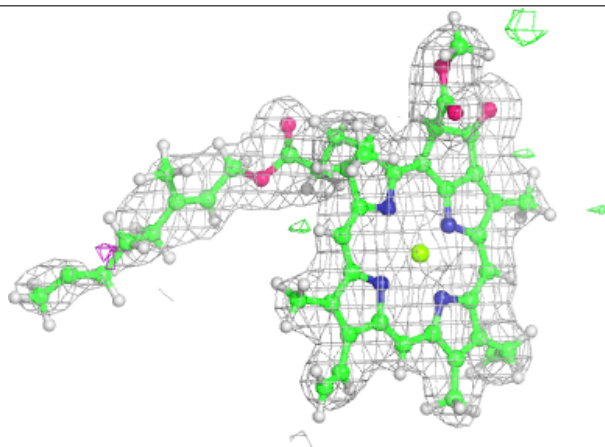


**Electron density around CLA A 605:**

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

**Electron density around CLA A 608:**

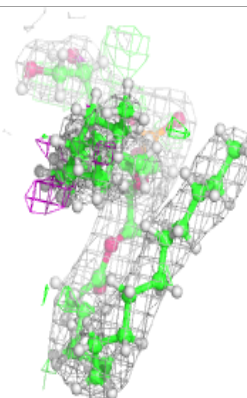
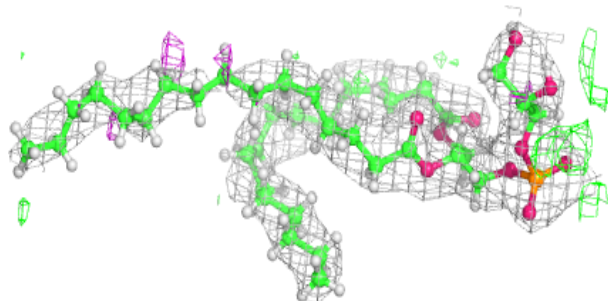
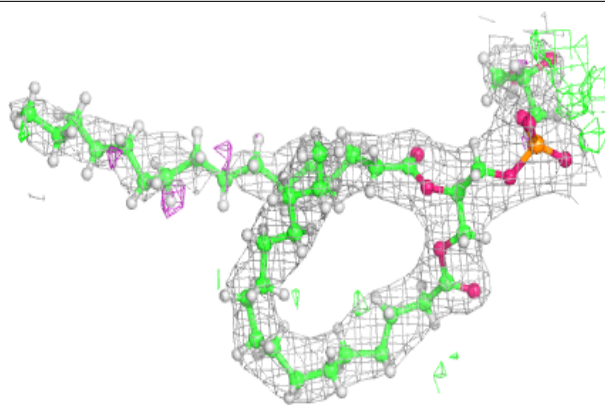
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



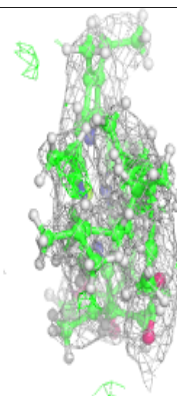
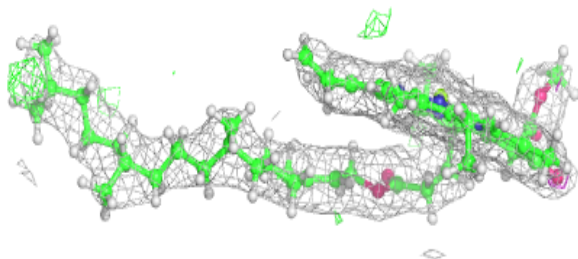
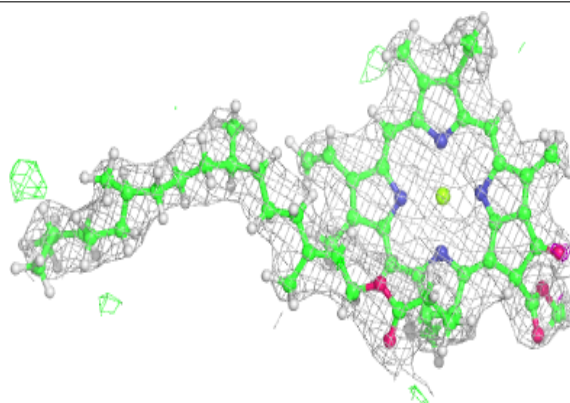


**Electron density around LHG d 407:**

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

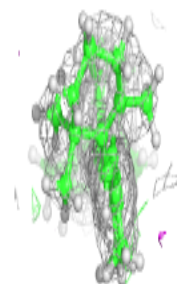
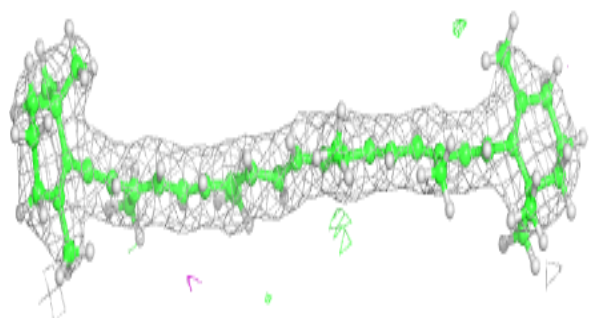
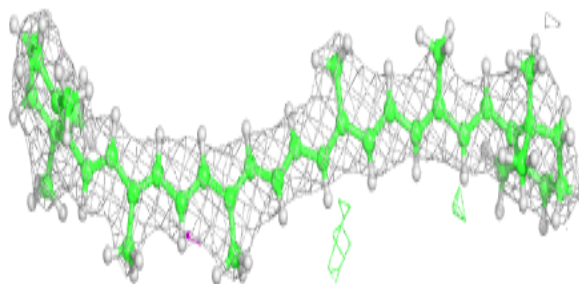
**Electron density around CLA b 603:**

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

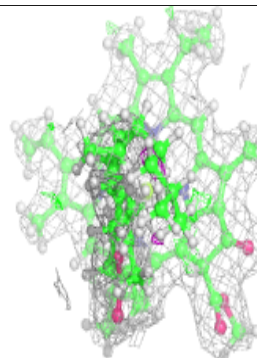
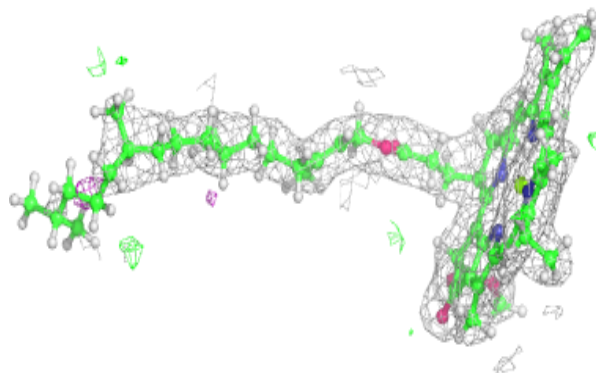
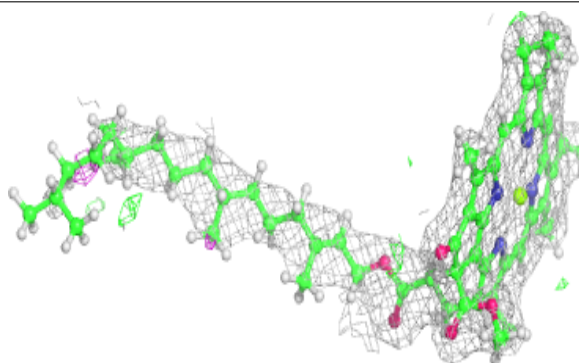


**Electron density around BCR c 515:**

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

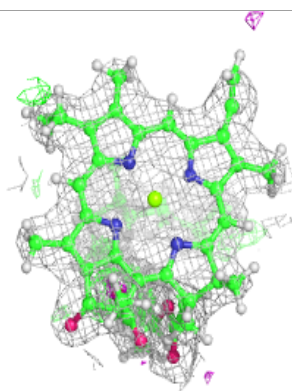
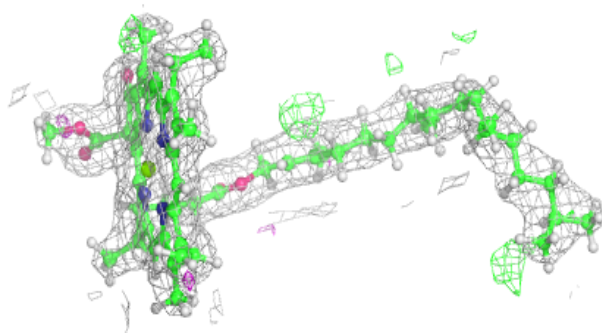
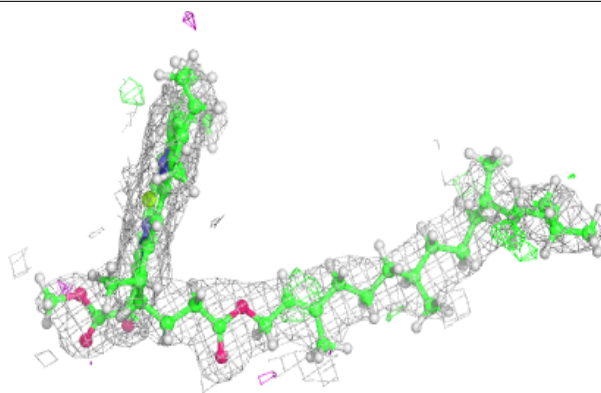
**Electron density around CLA b 604:**

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

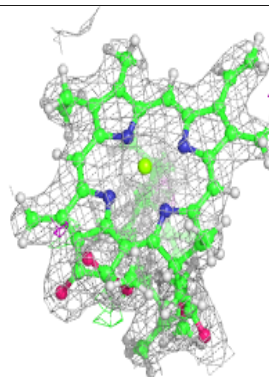
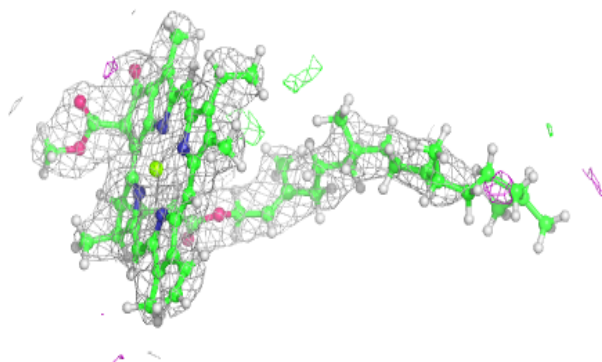
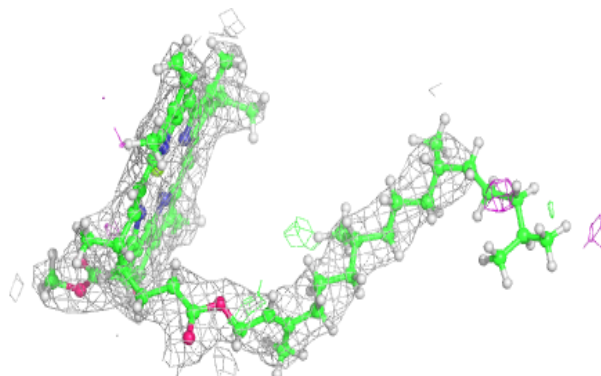


**Electron density around CLA b 605:**

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

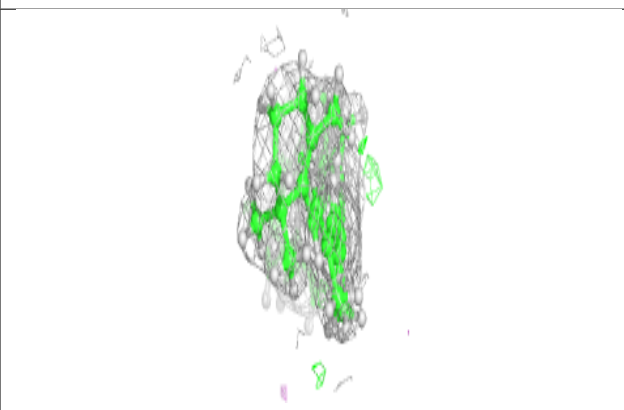
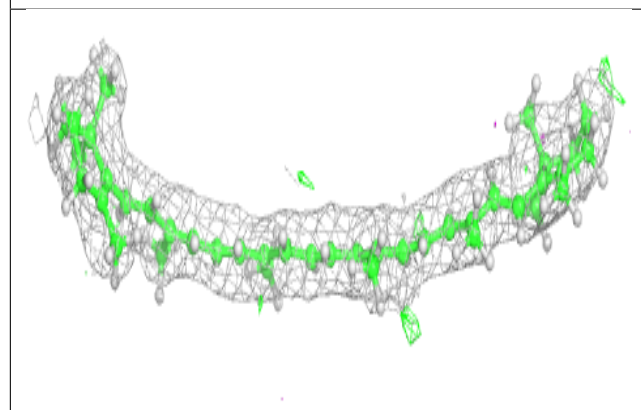
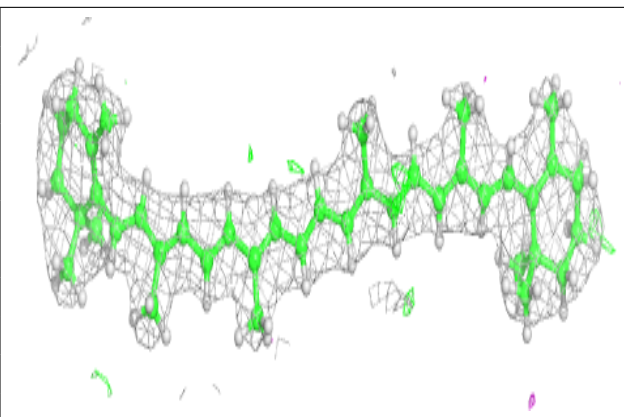
**Electron density around CLA C 508:**

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

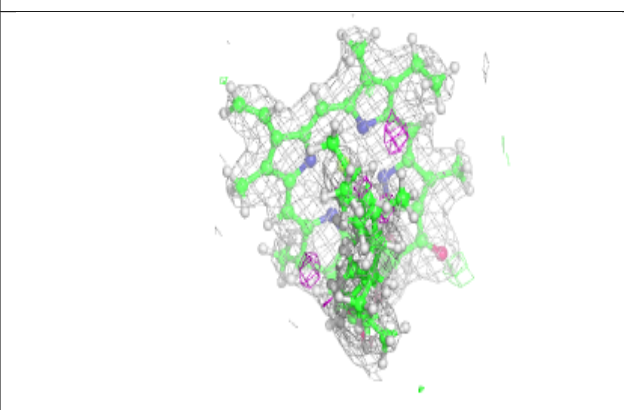
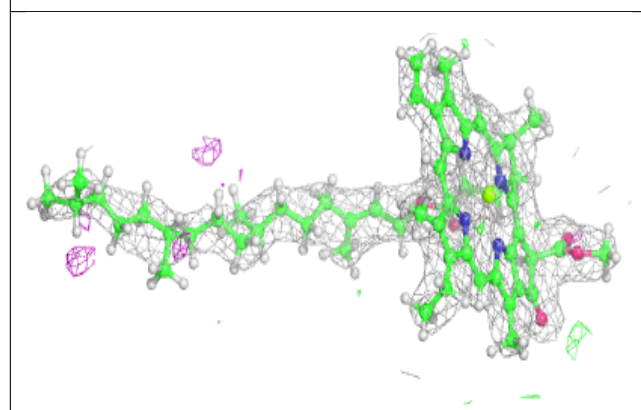
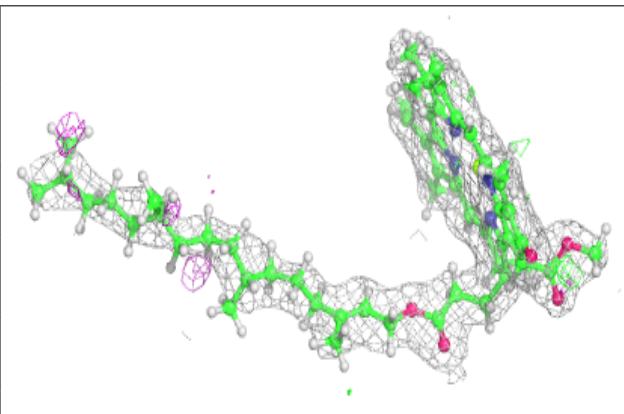


**Electron density around BCR t 101:**

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

**Electron density around CLA b 607:**

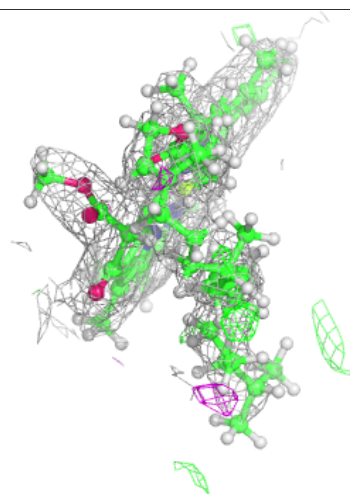
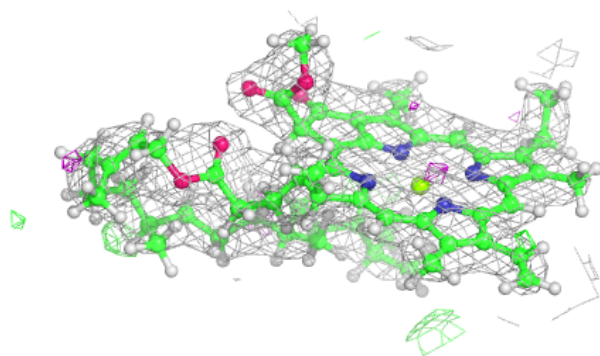
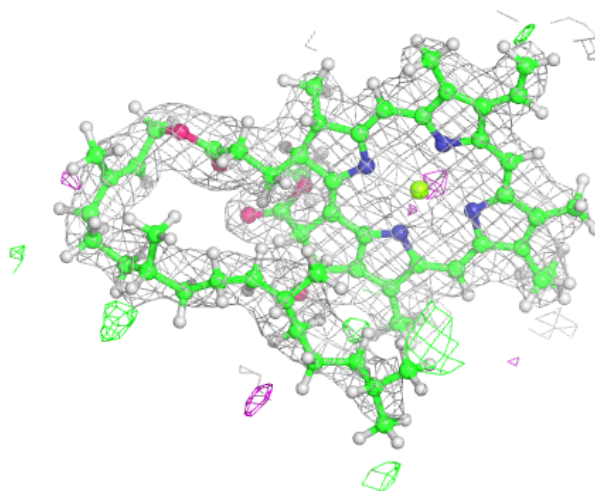
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





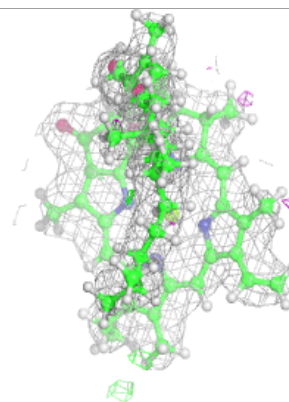
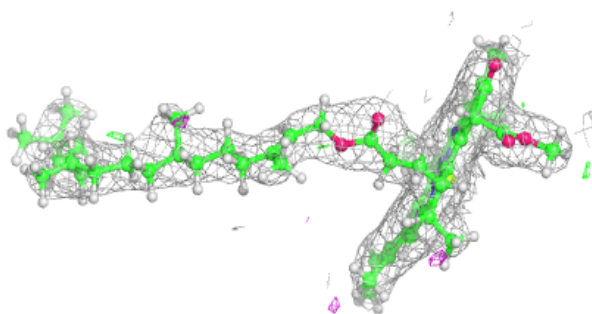
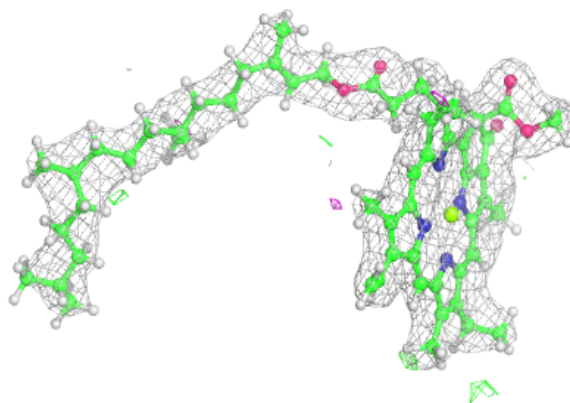
**Electron density around CLA C 509:**

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



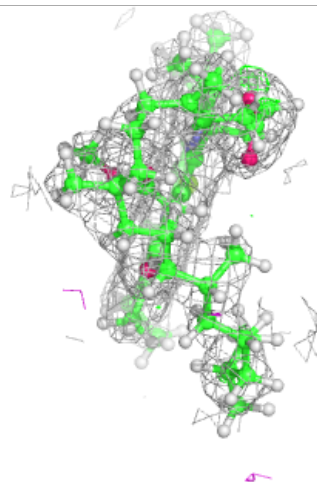
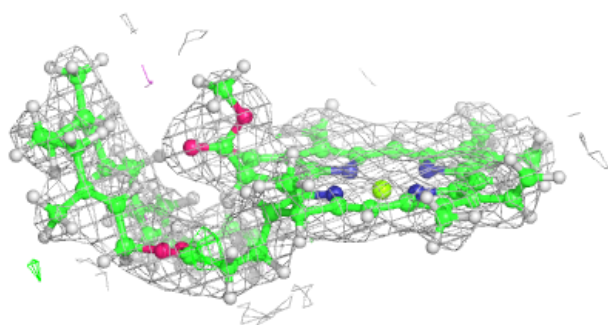
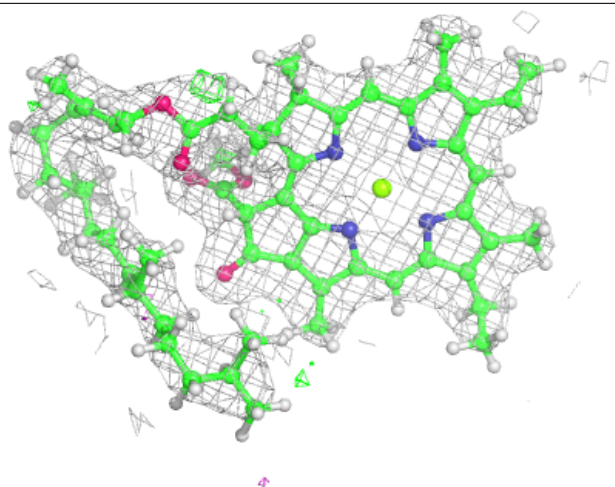
**Electron density around CLA B 609:**

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



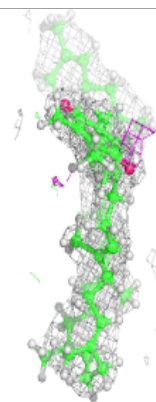
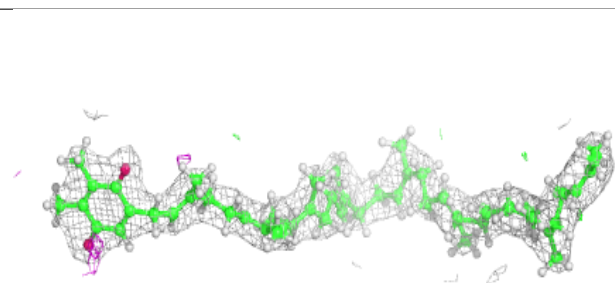
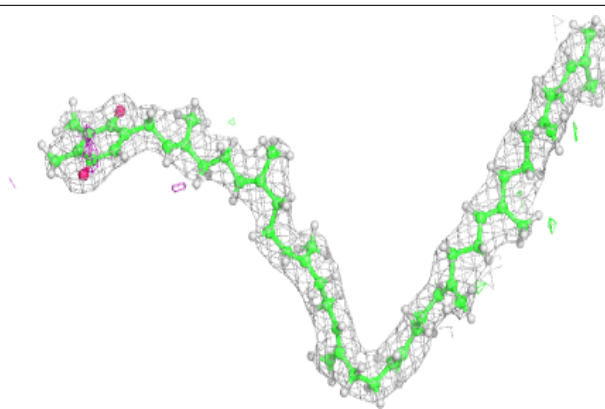
**Electron density around CLA b 610:**

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



**Electron density around PL9 d 406:**

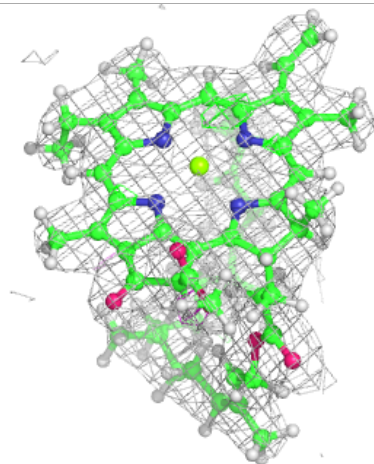
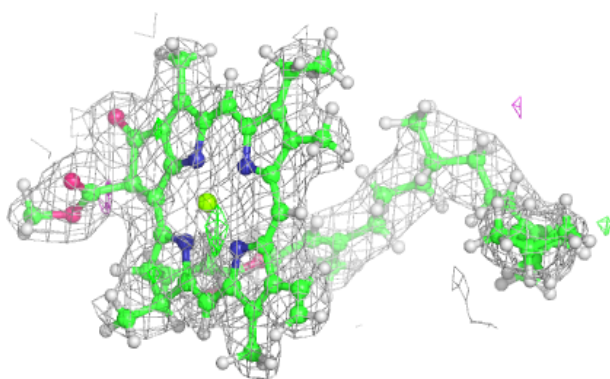
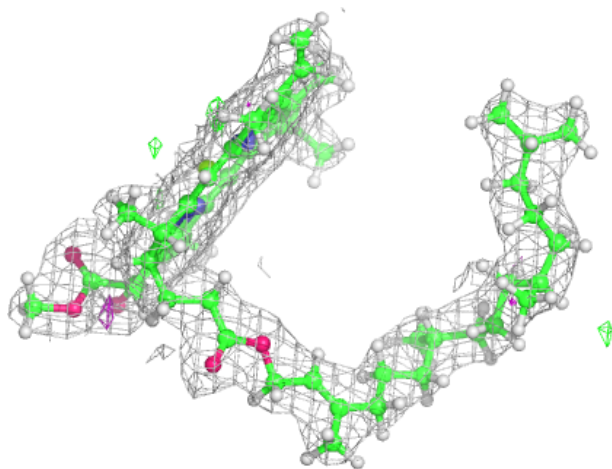
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





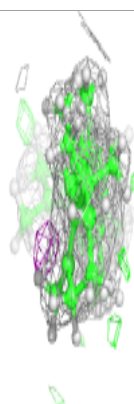
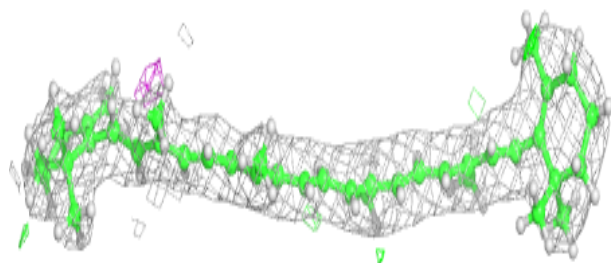
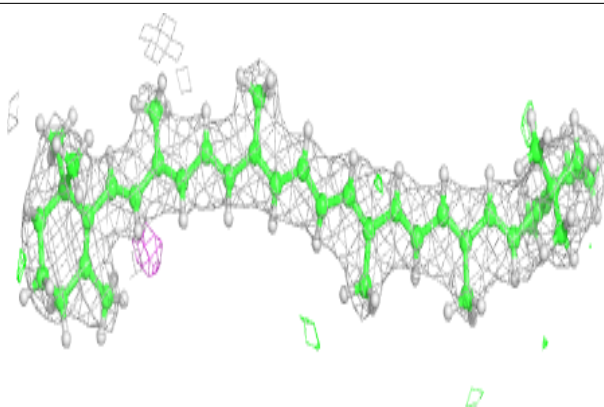
**Electron density around CLA b 611:**

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

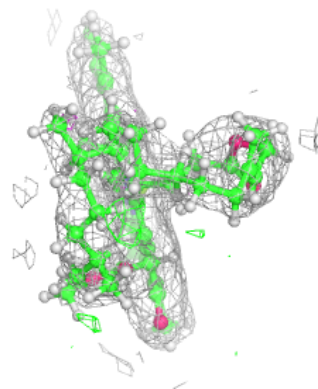
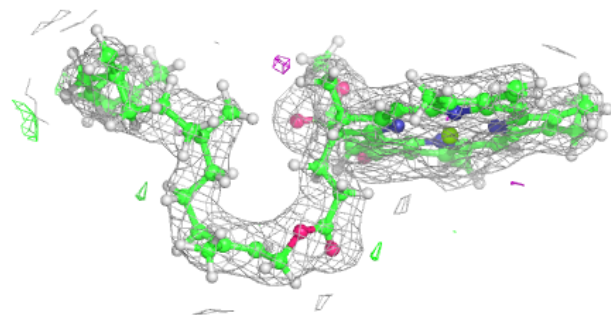
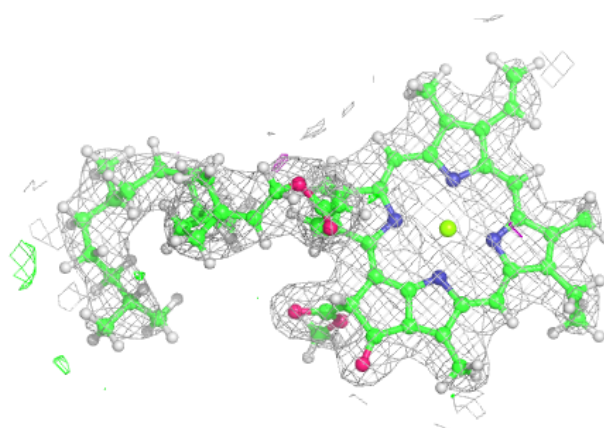


**Electron density around BCR B 617:**

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

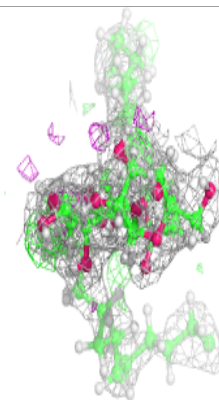
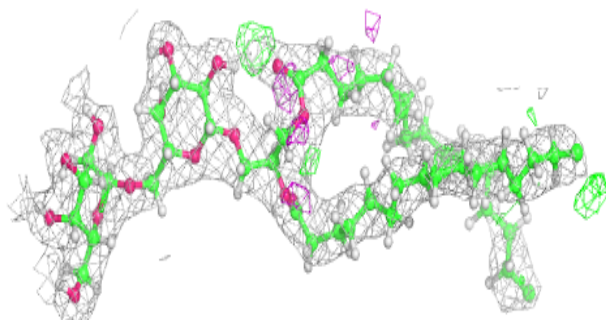
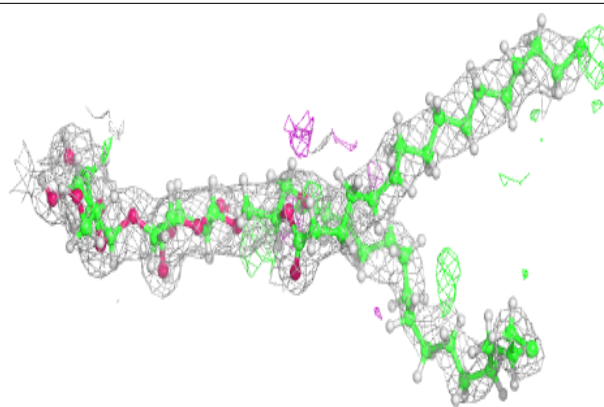
**Electron density around CLA b 612:**

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



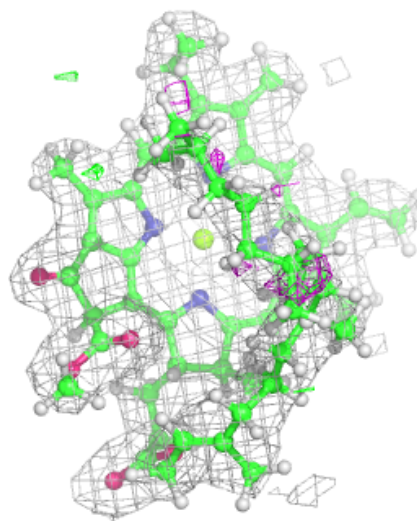
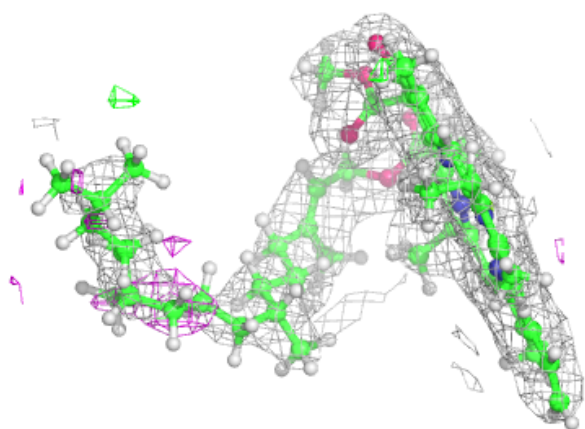
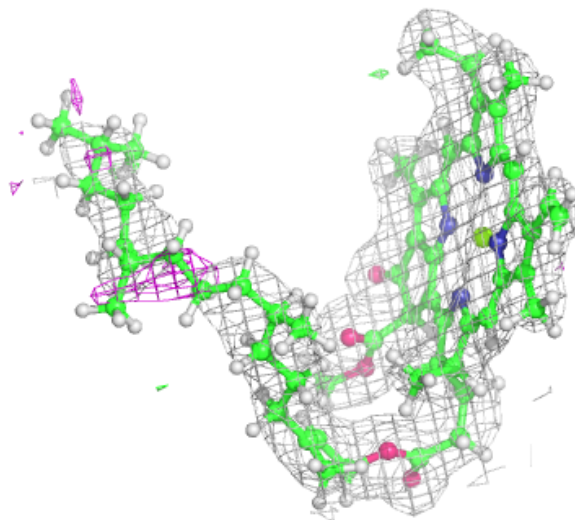
**Electron density around DGD c 516:**

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



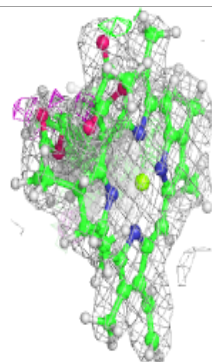
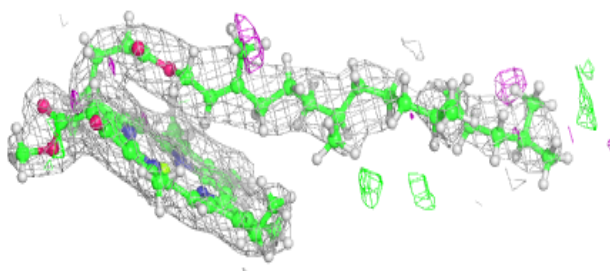
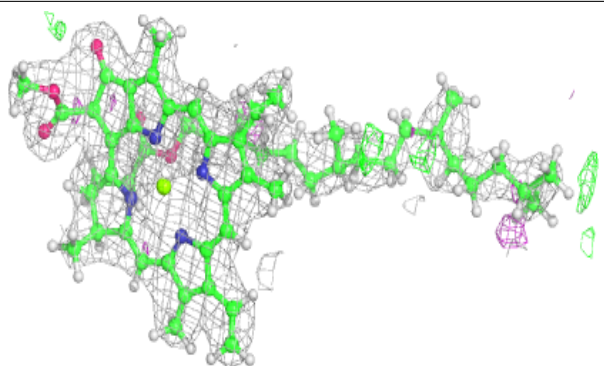
**Electron density around CLA b 613:**

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

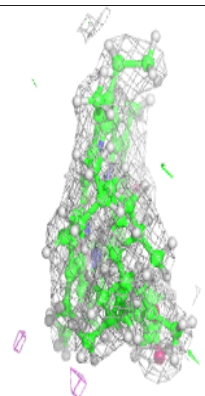
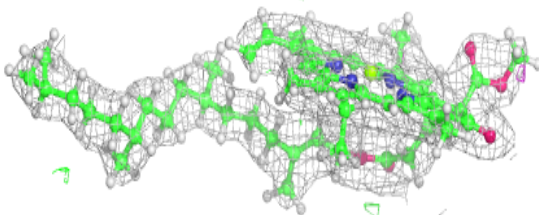
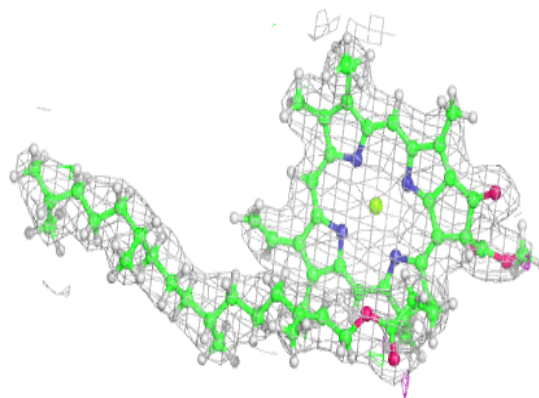


**Electron density around CLA b 614:**

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

**Electron density around CLA C 501:**

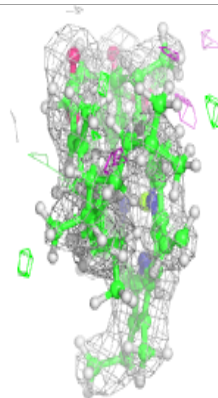
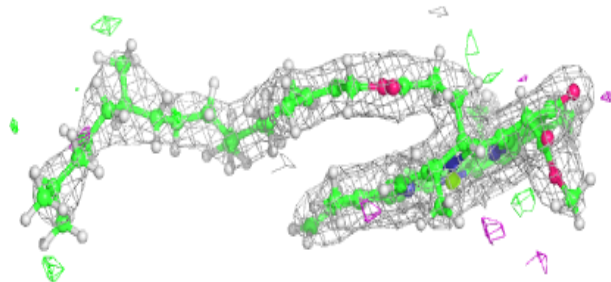
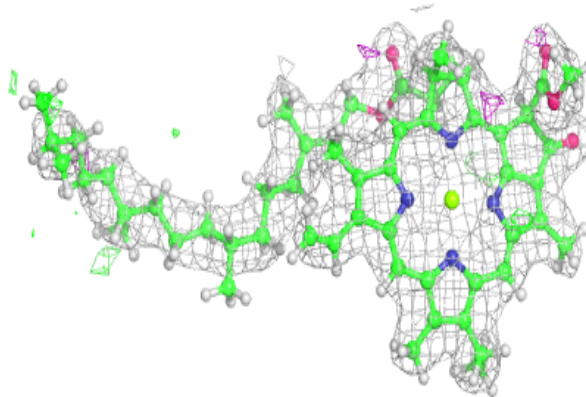
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



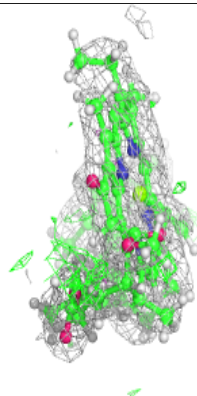
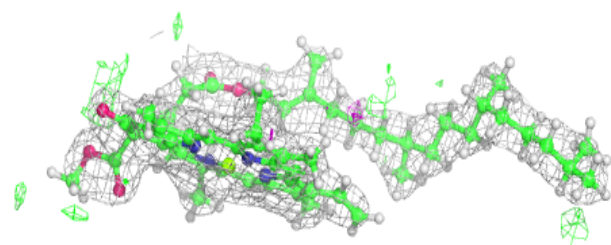
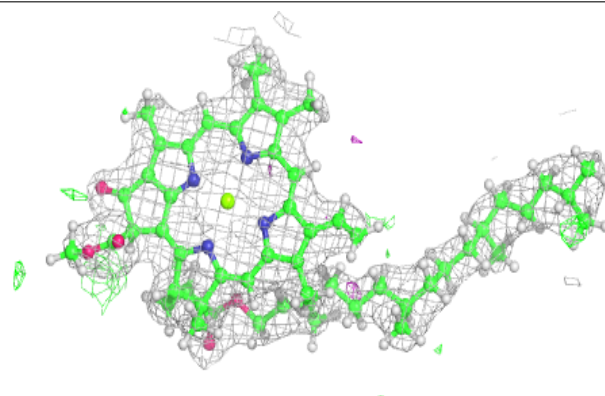


**Electron density around CLA B 603:**

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

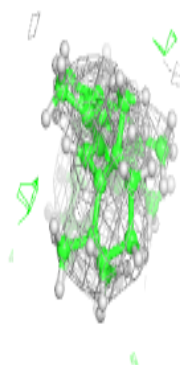
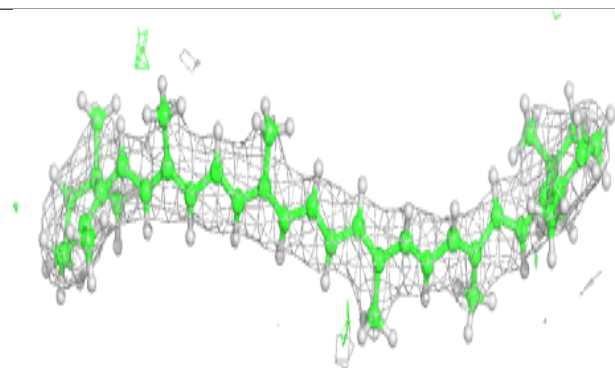
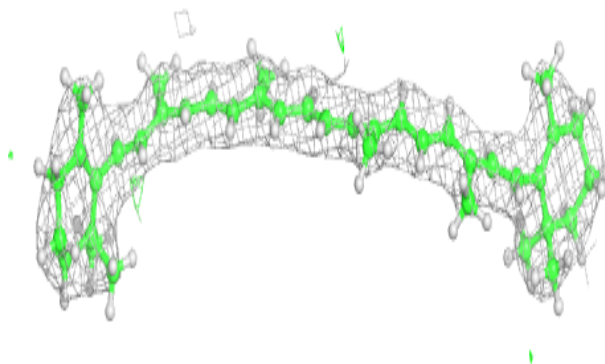
**Electron density around CLA c 501:**

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



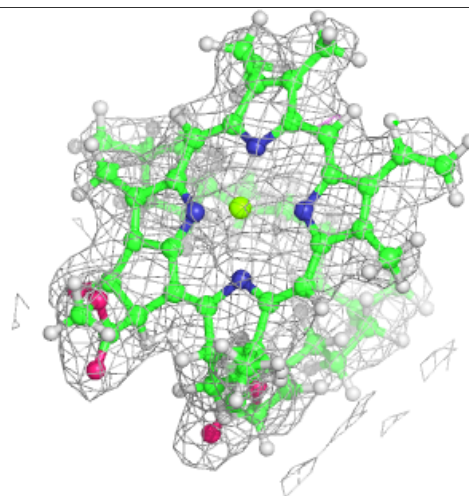
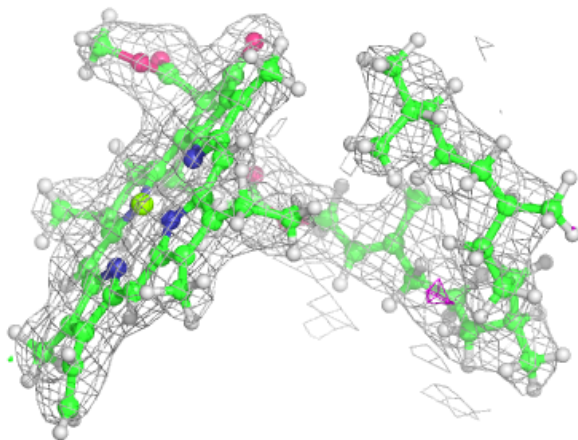
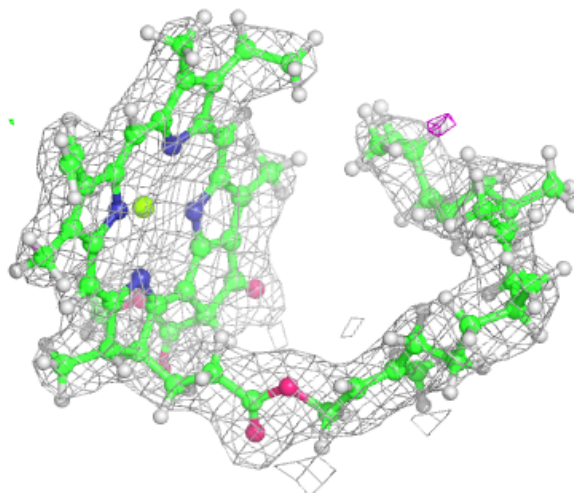
**Electron density around BCR K 101:**

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



**Electron density around CLA C 503:**

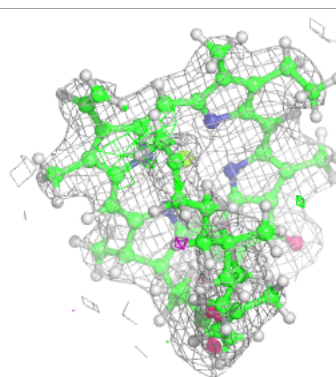
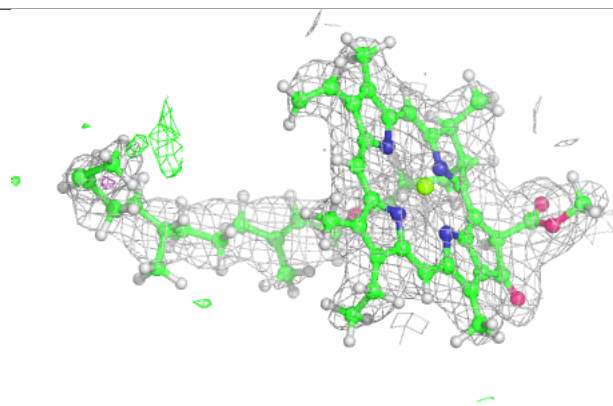
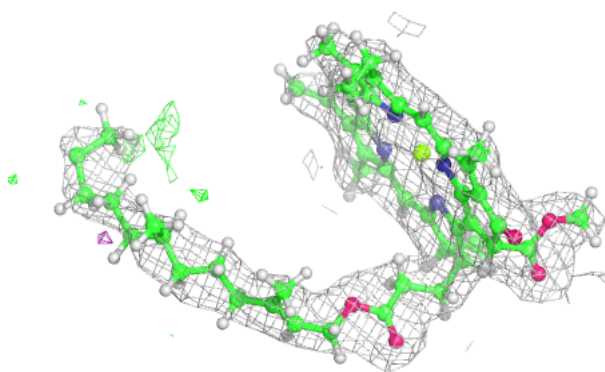
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



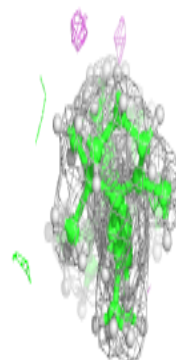
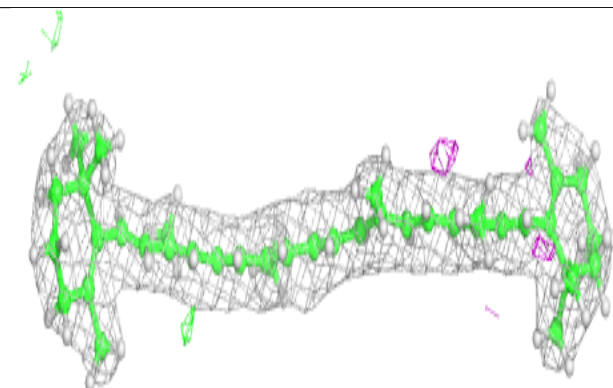
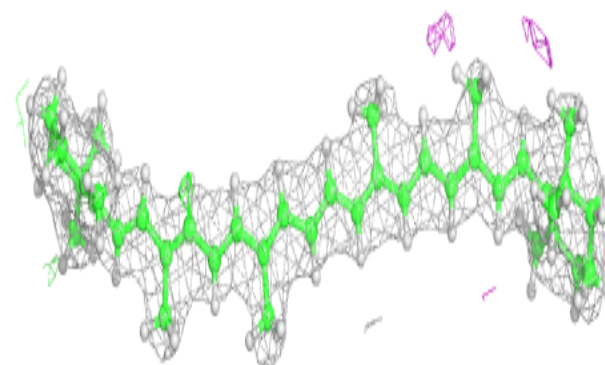


**Electron density around CLA C 504:**

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

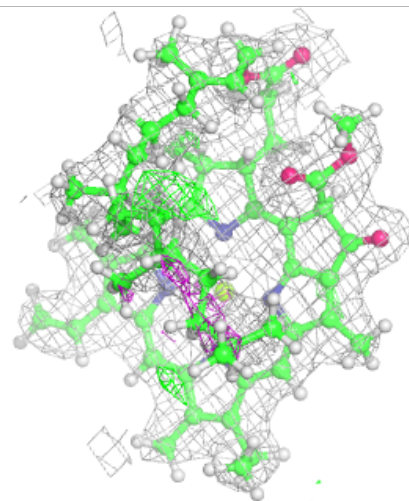
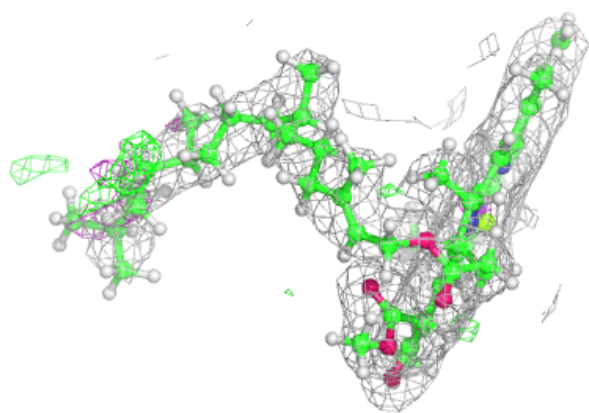
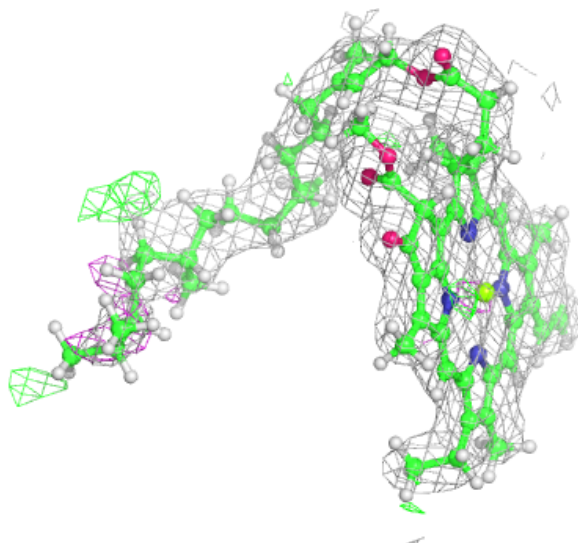
**Electron density around BCR a 607:**

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



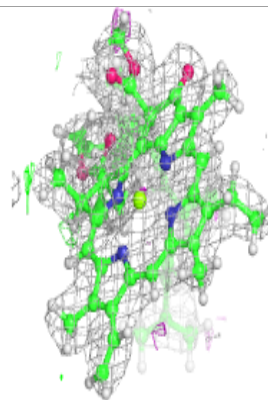
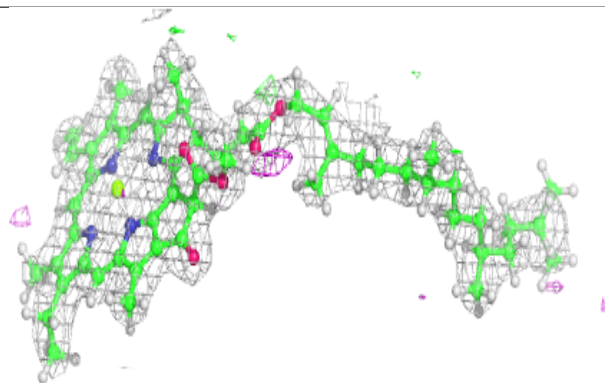
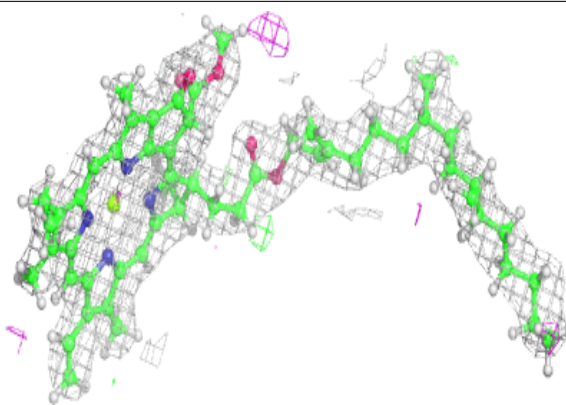
**Electron density around CLA B 613:**

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



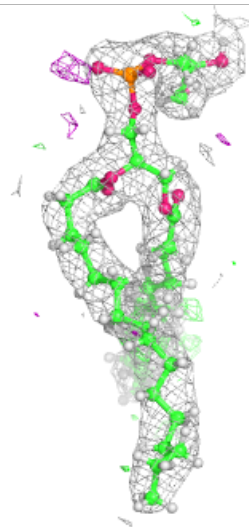
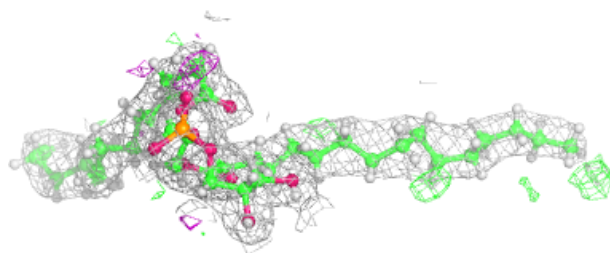
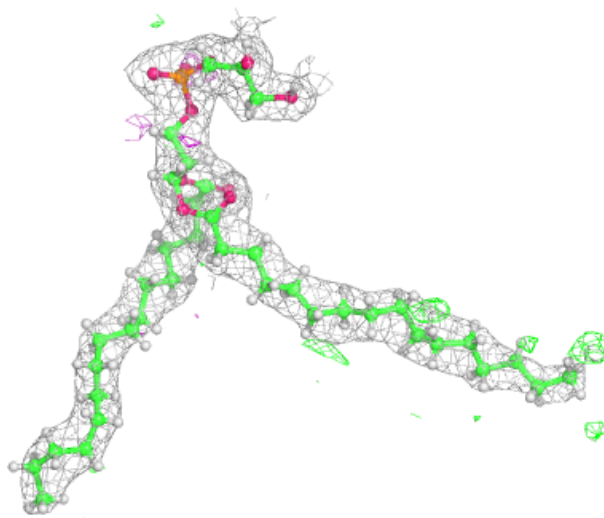
**Electron density around CLA a 604:**

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



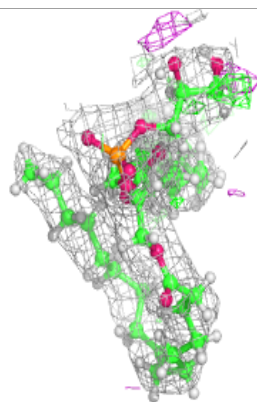
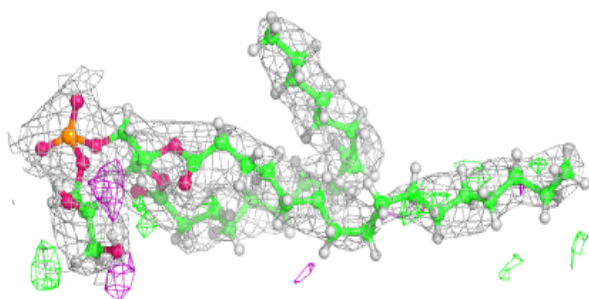
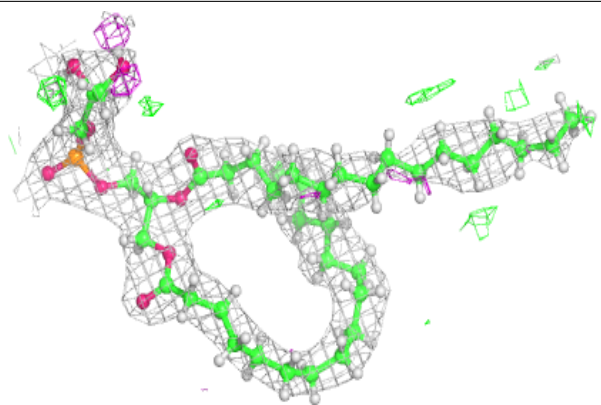
**Electron density around LHG B 621:**

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

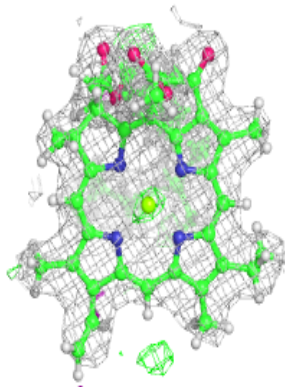
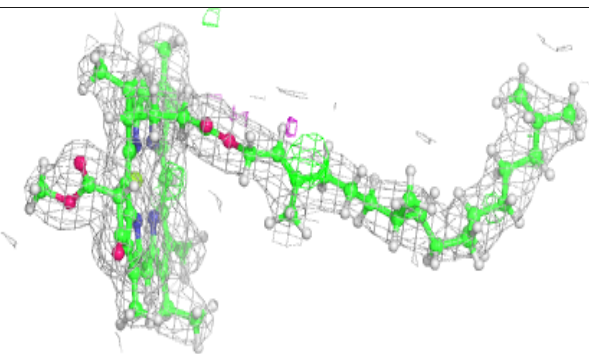
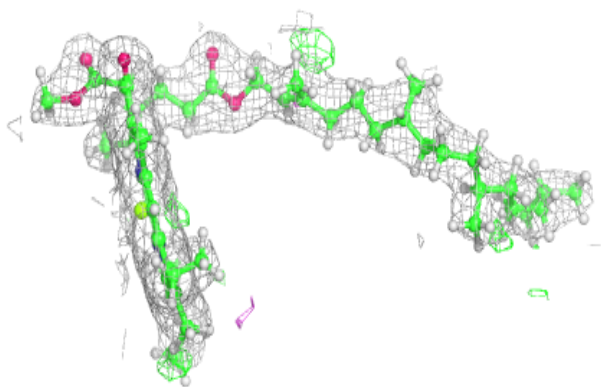


**Electron density around LHG B 622:**

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

**Electron density around CLA B 605:**

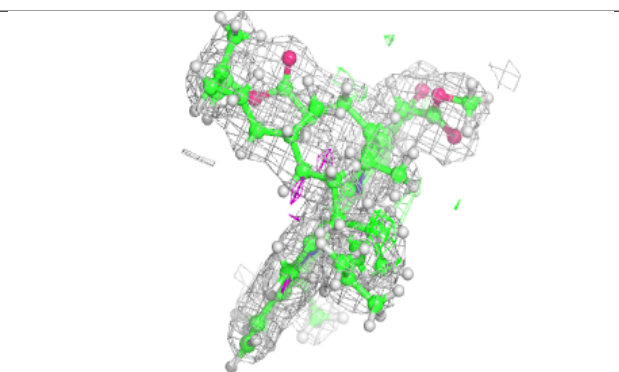
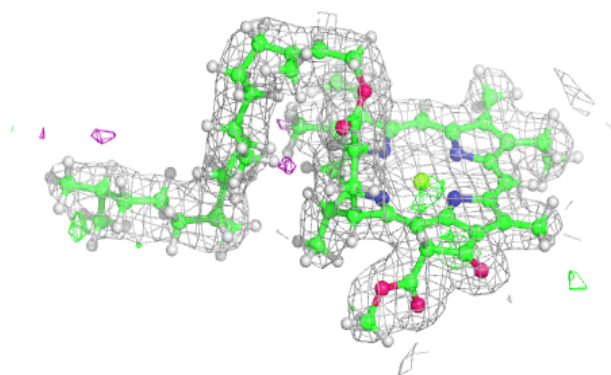
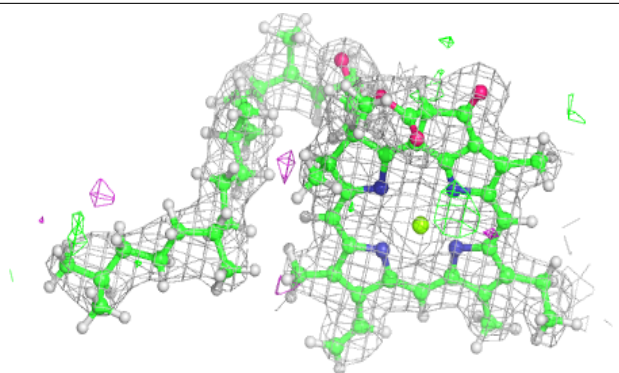
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



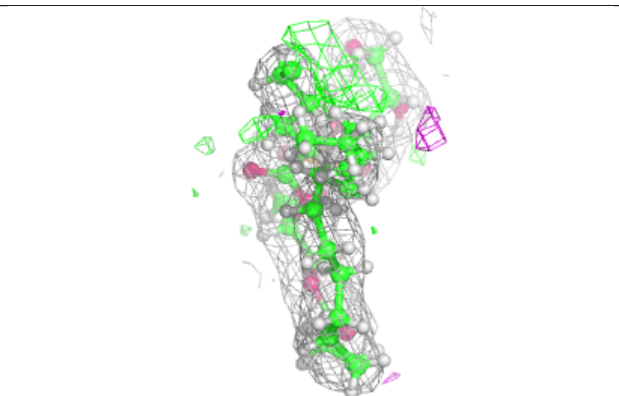
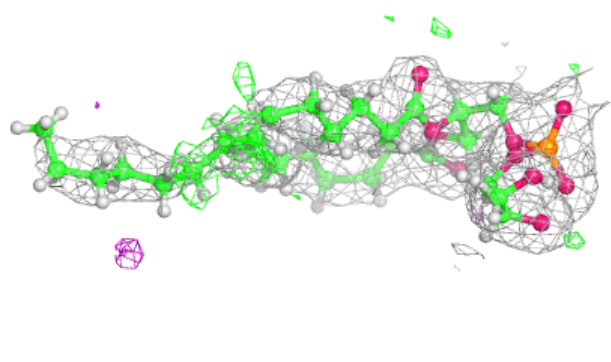
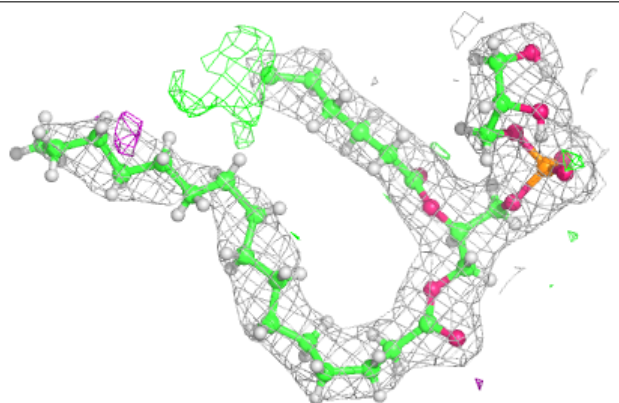


**Electron density around CLA a 612:**

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

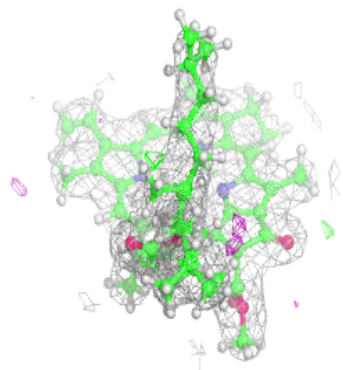
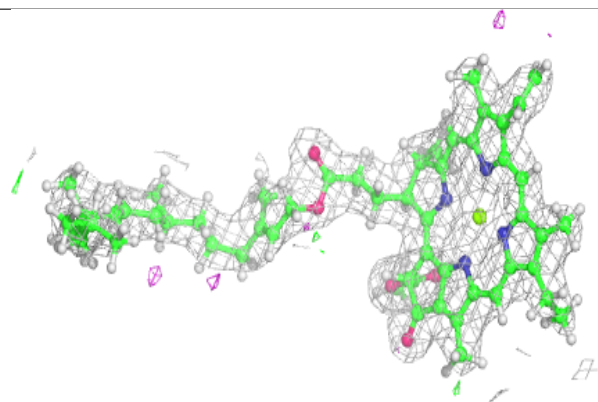
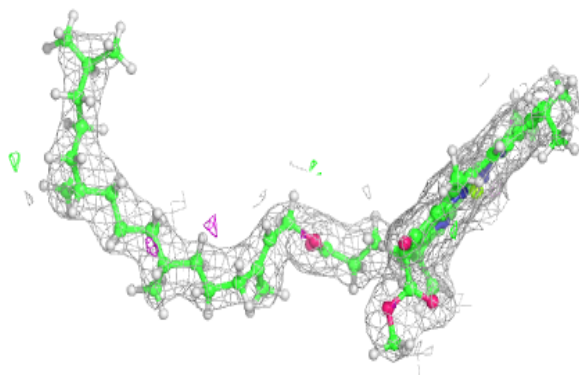
**Electron density around LHG d 409:**

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



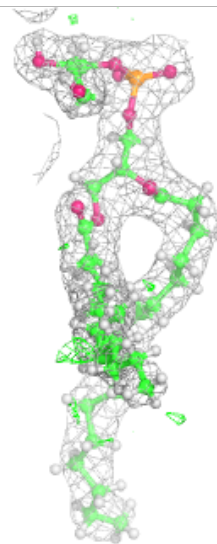
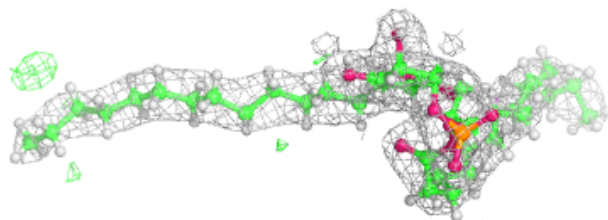
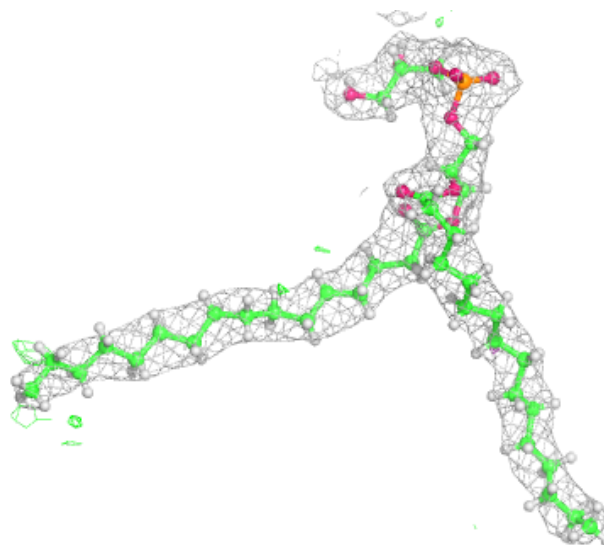
**Electron density around CLA d 403:**

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



**Electron density around LHG 1 101:**

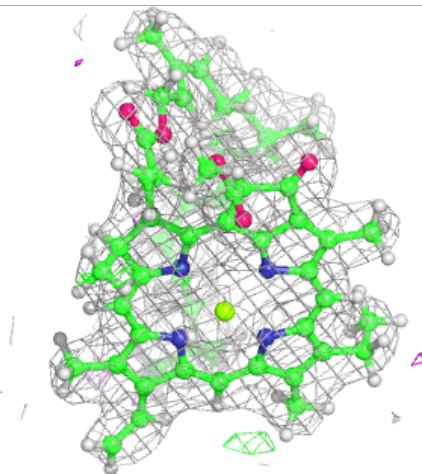
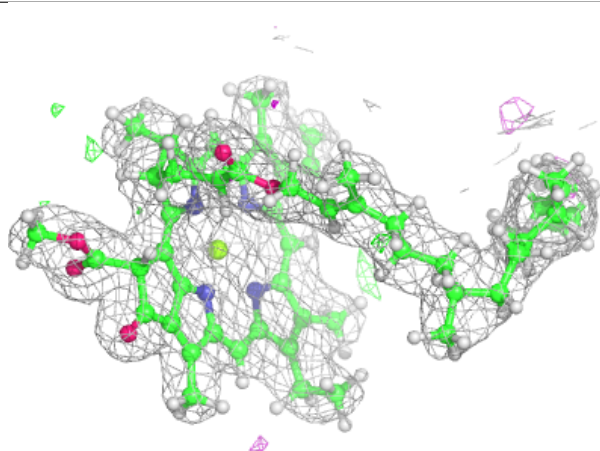
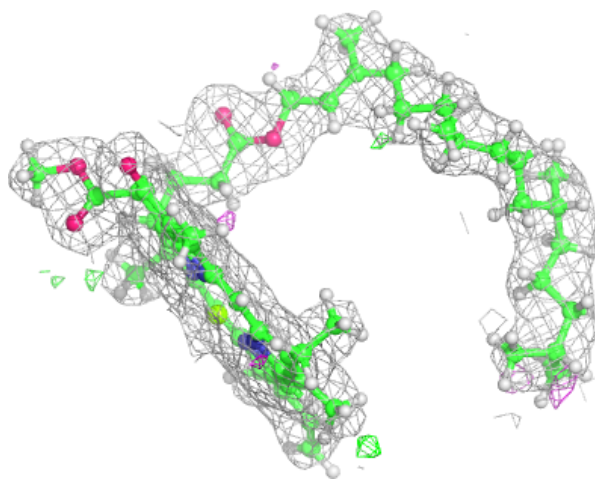
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





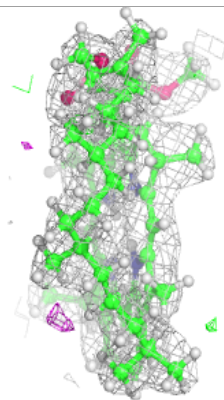
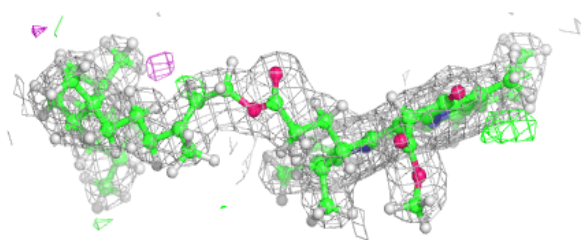
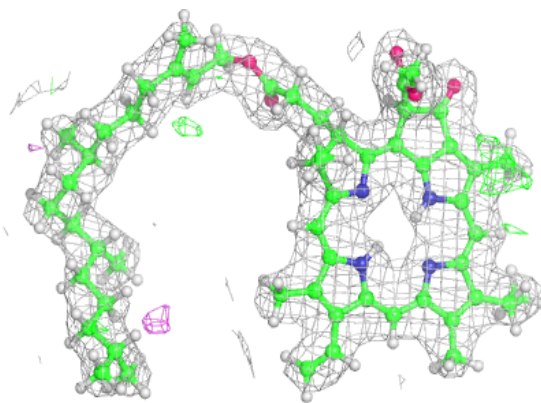
**Electron density around CLA B 611:**

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



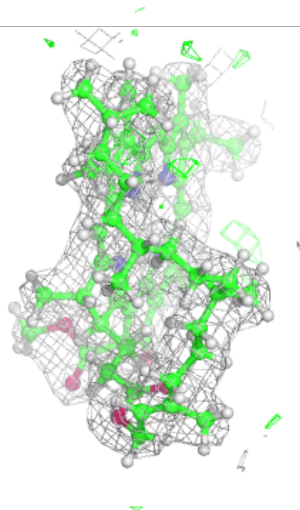
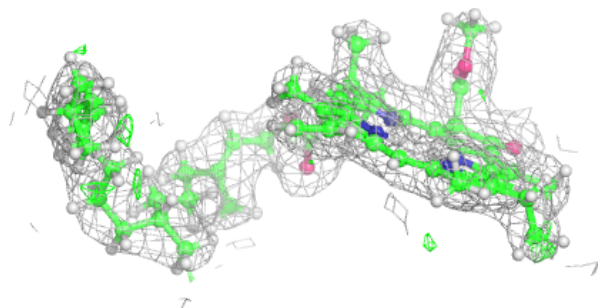
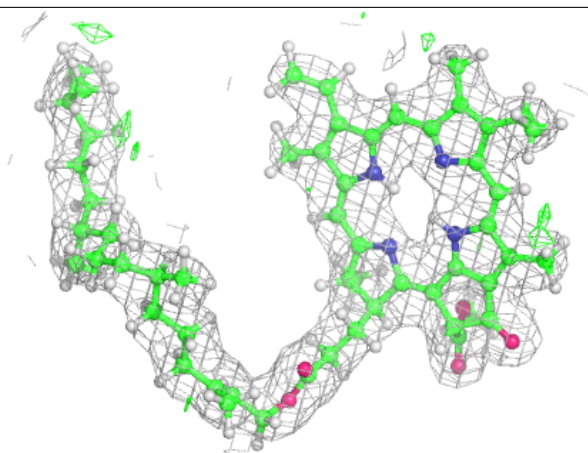
**Electron density around PHO A 606:**

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



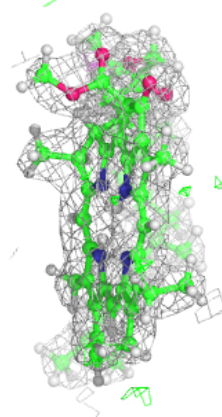
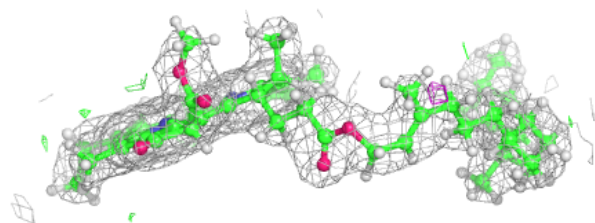
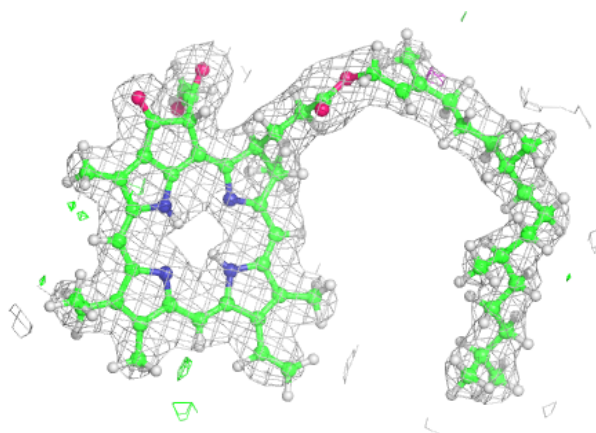
**Electron density around PHO A 607:**

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



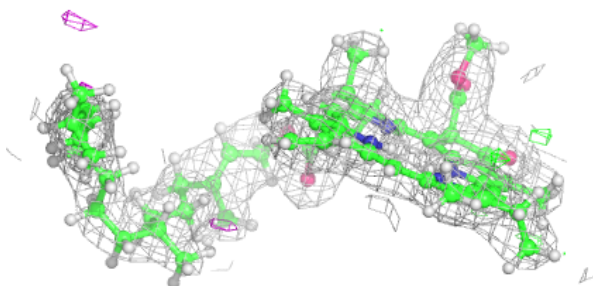
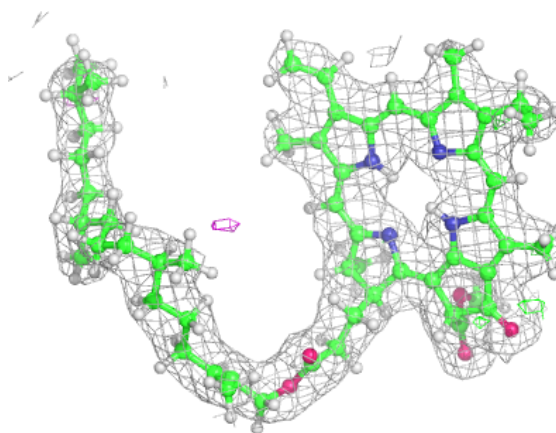
**Electron density around PHO a 605:**

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

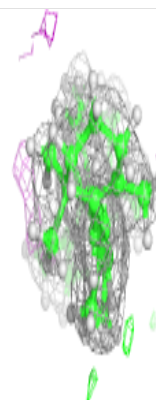
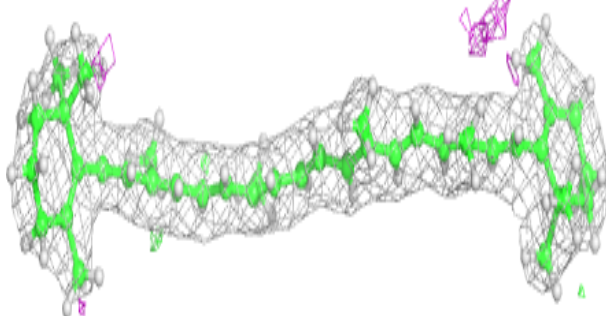
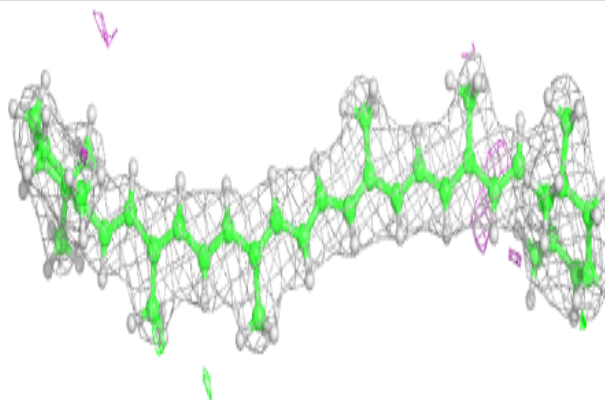


**Electron density around PHO d 402:**

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

**Electron density around BCR A 609:**

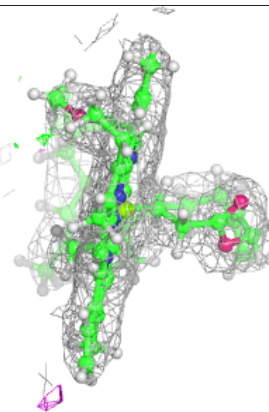
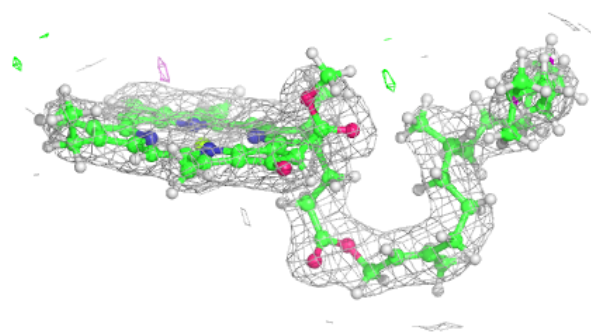
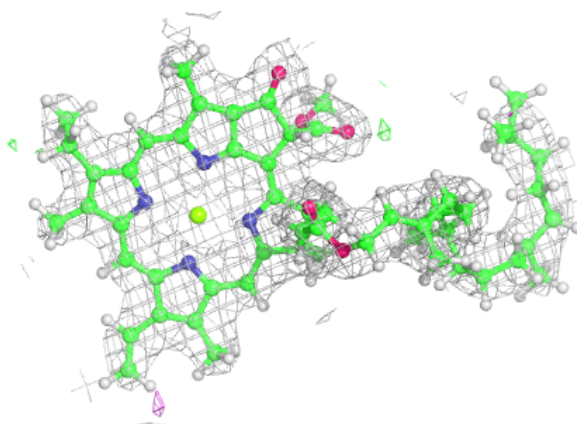
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



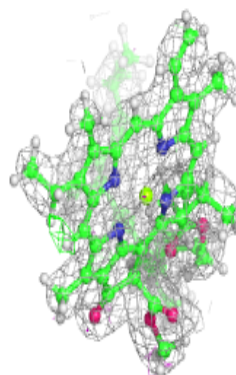
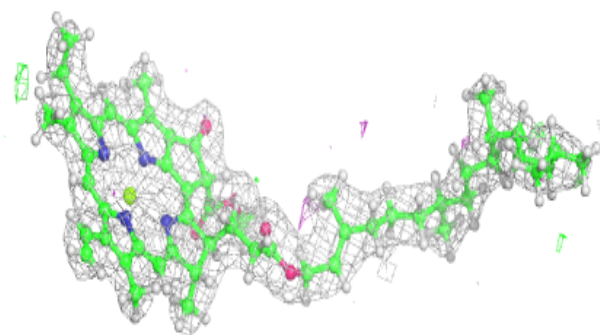
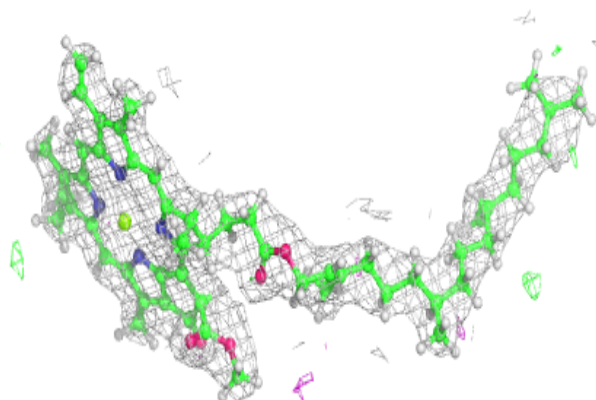


**Electron density around CLA B 612:**

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

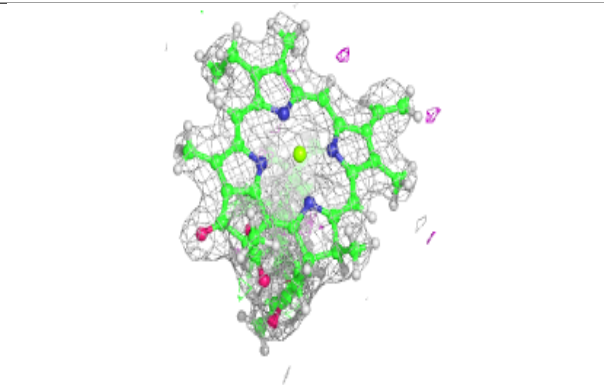
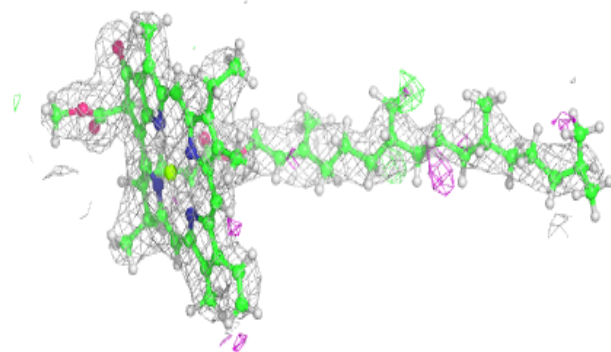
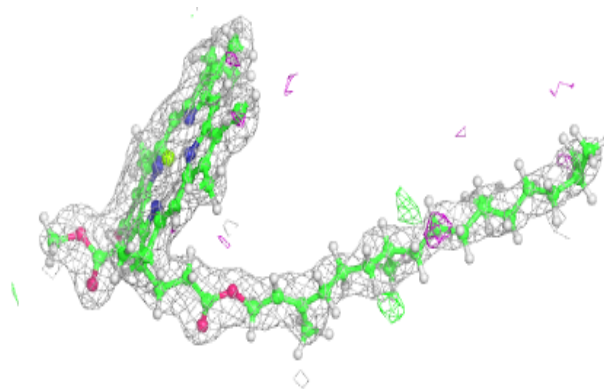
**Electron density around CLA A 604:**

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

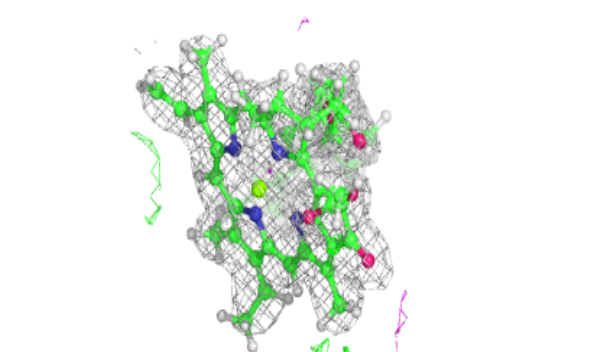
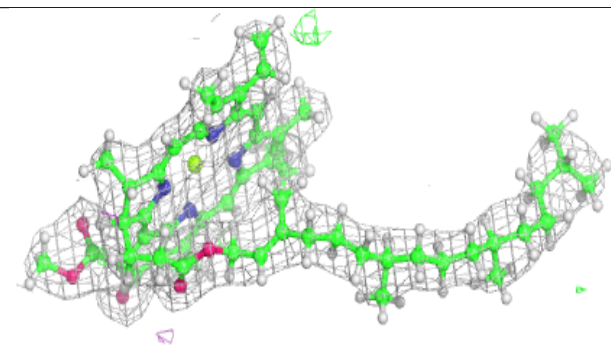
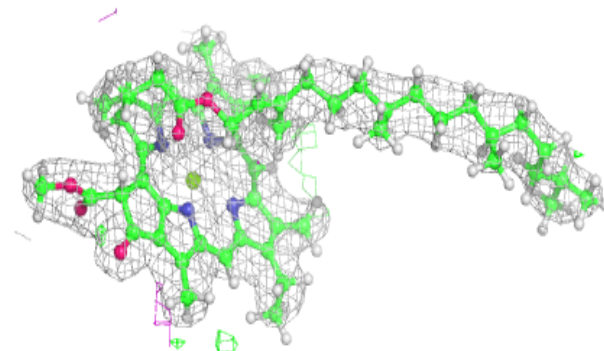


**Electron density around CLA B 607:**

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

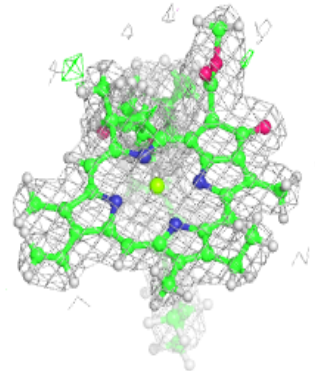
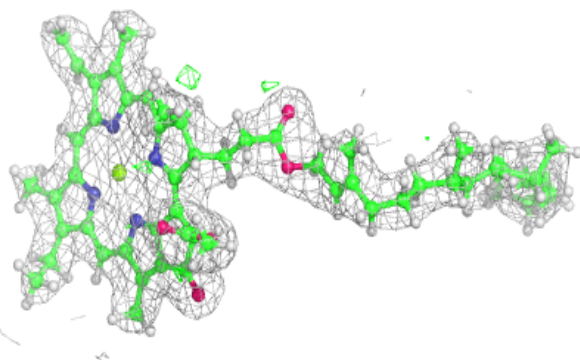
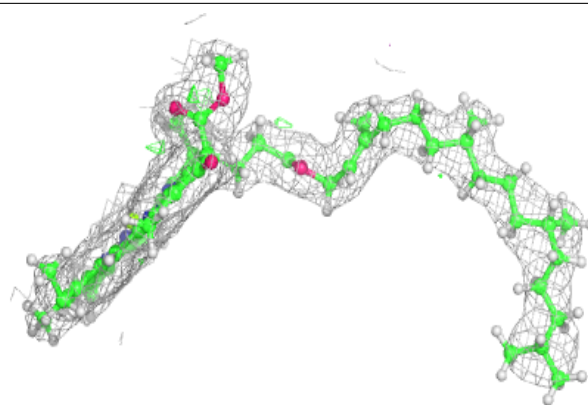
**Electron density around CLA B 608:**

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

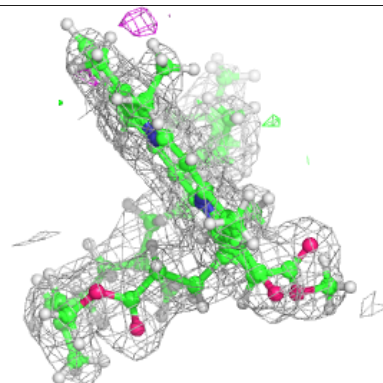
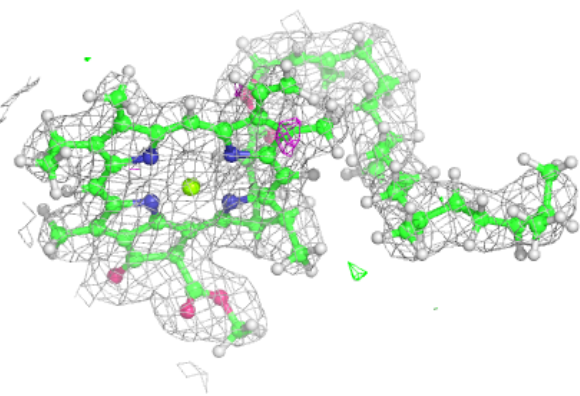
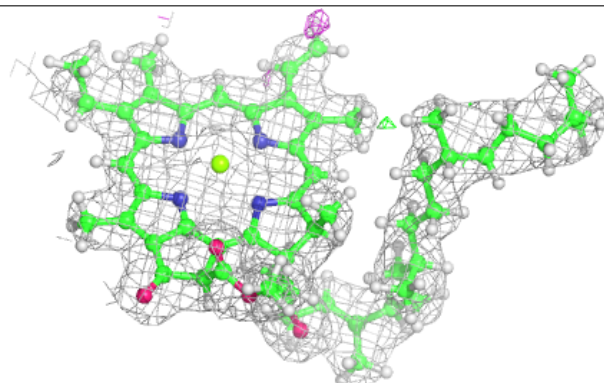


**Electron density around CLA D 402:**

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

**Electron density around CLA A 613:**

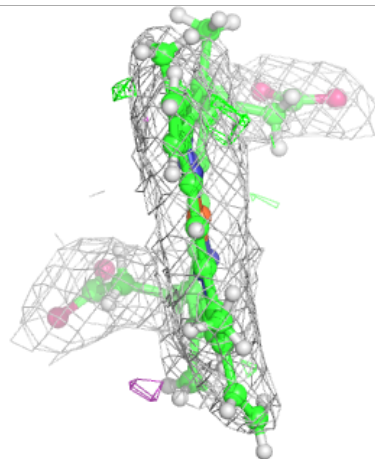
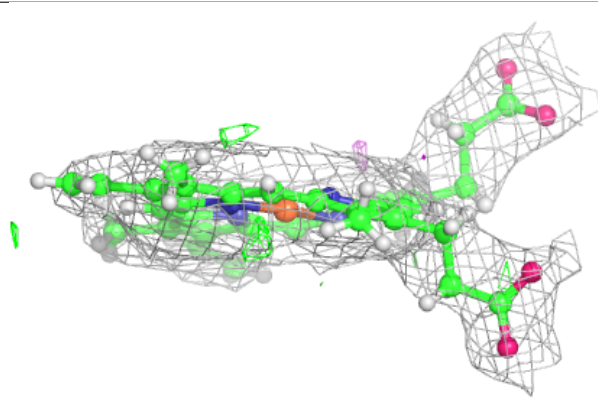
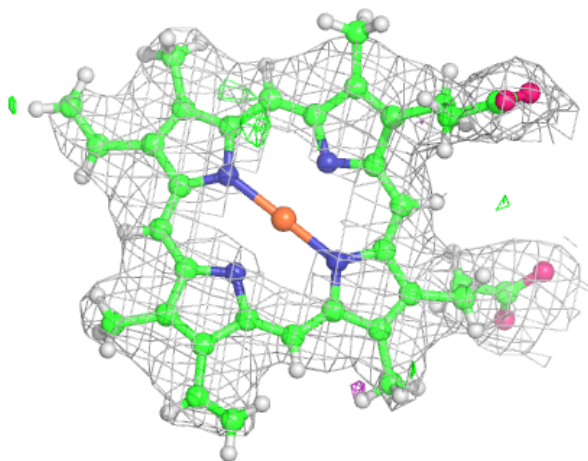
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





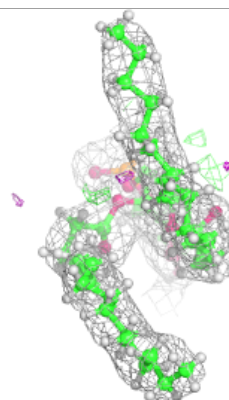
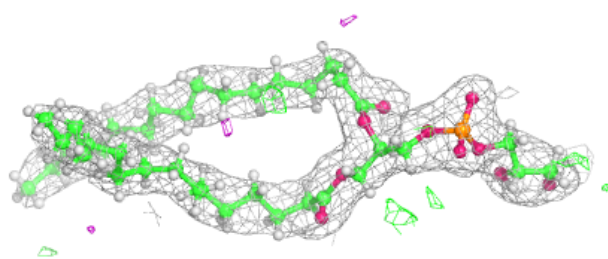
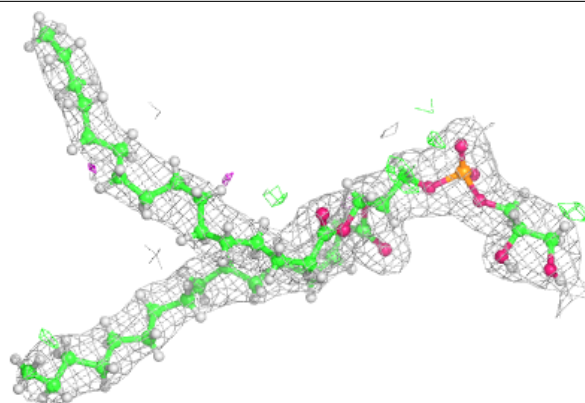
**Electron density around HEM F 101:**

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

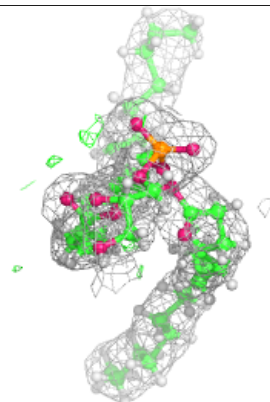
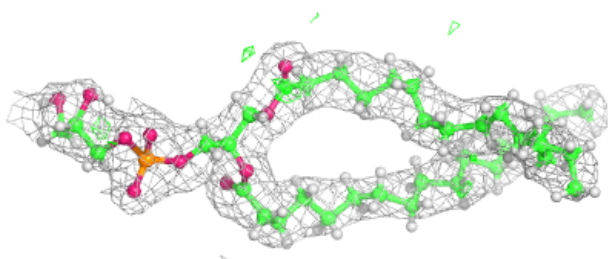
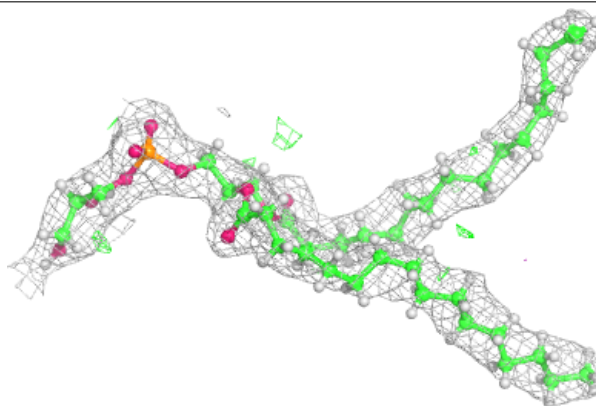


**Electron density around LHG d 408:**

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

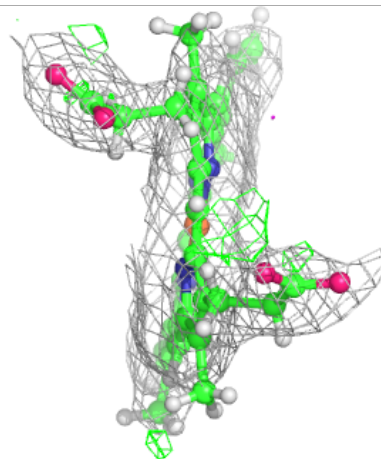
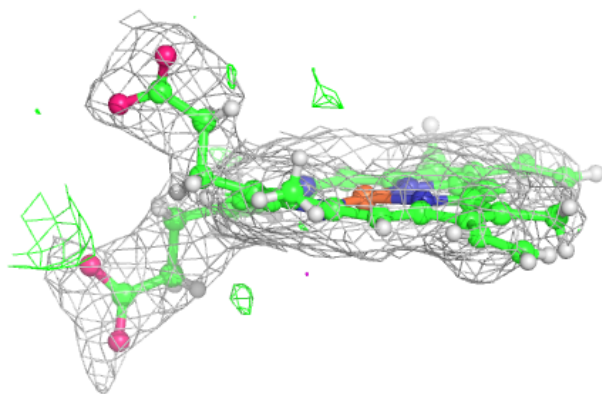
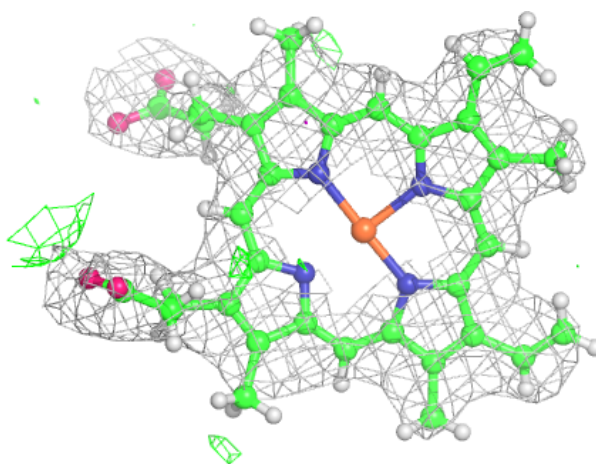
**Electron density around LHG D 408:**

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



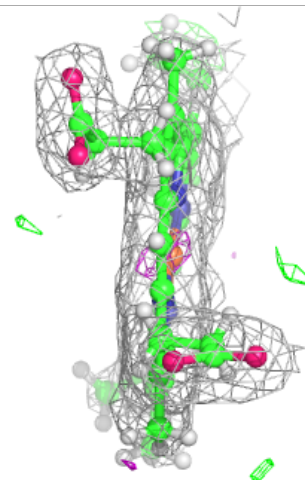
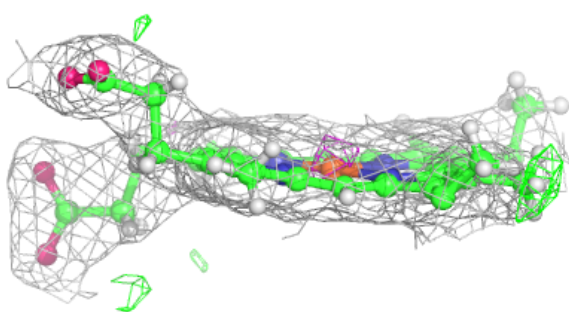
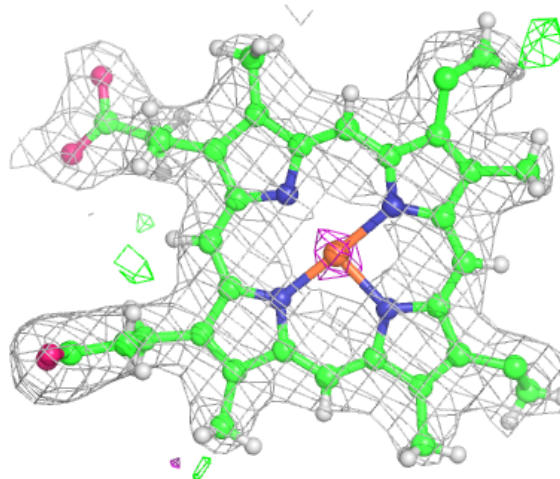
**Electron density around HEM e 101:**

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



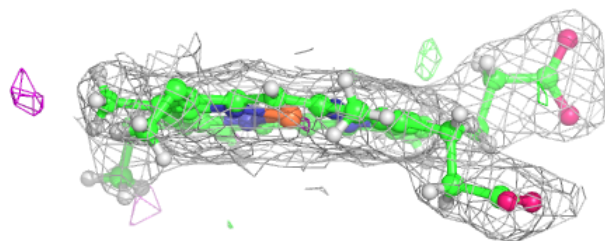
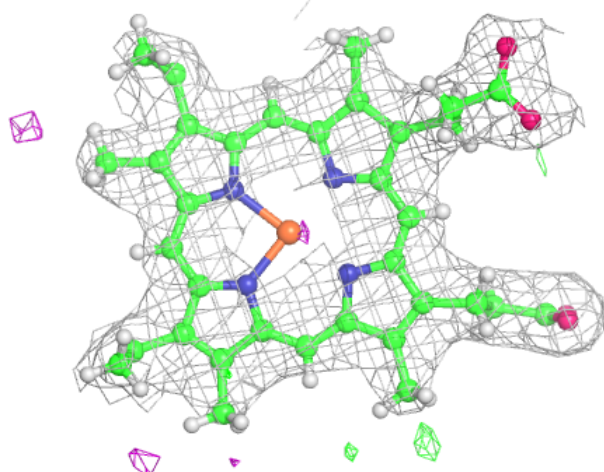
**Electron density around HEC V 201:**

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



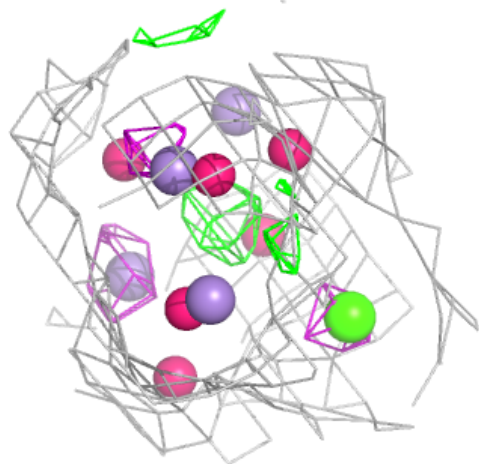
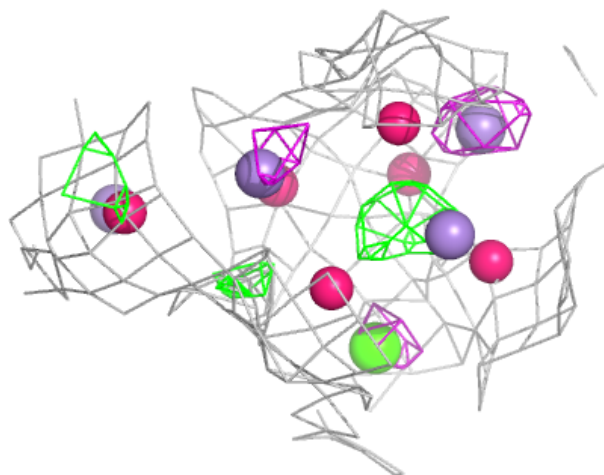
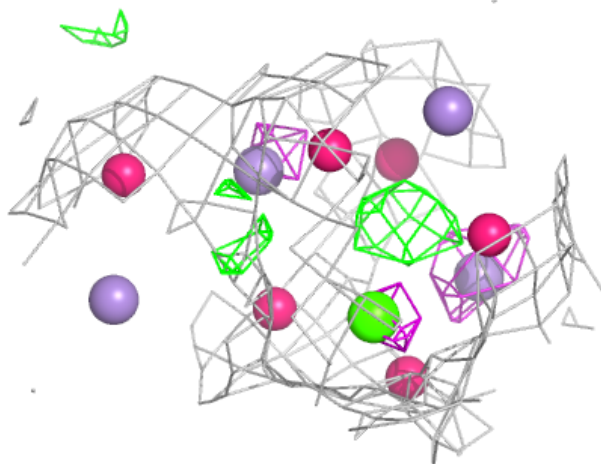
**Electron density around HEC v 201:**

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



**Electron density around OEY A 601 (B):**

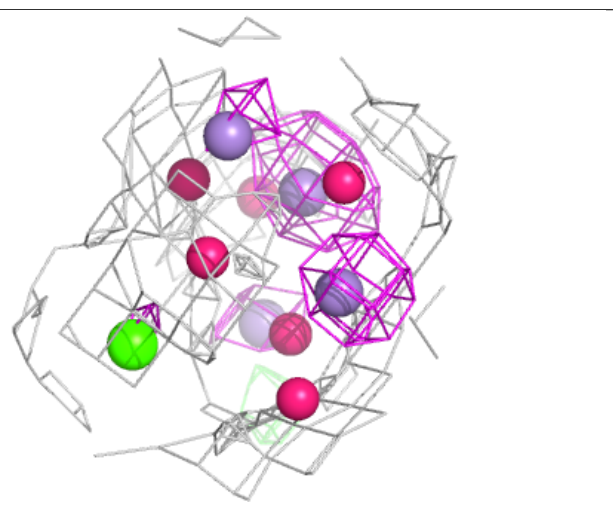
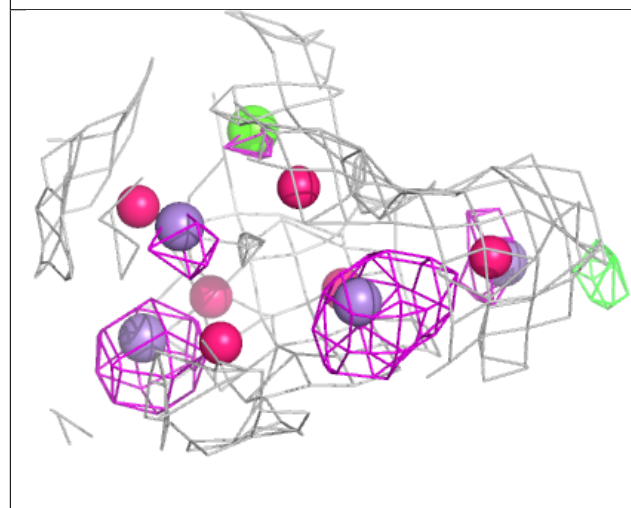
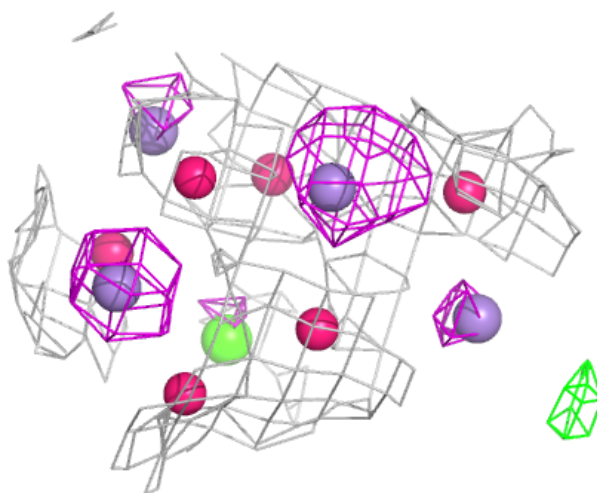
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around OEY a 601 (B):**

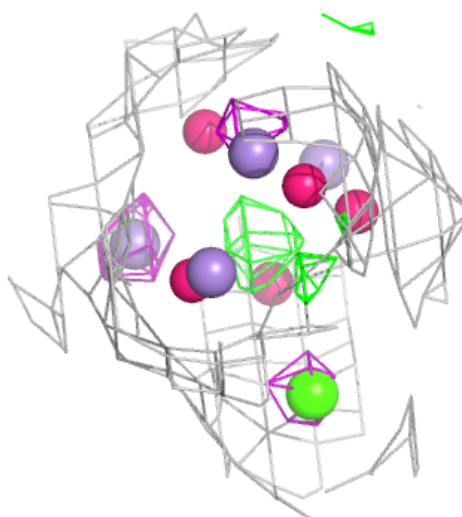
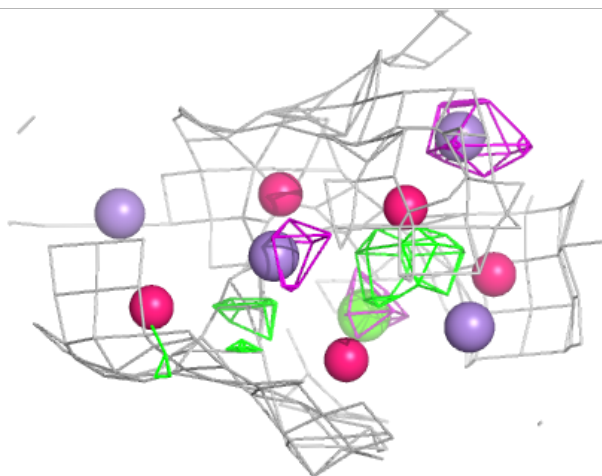
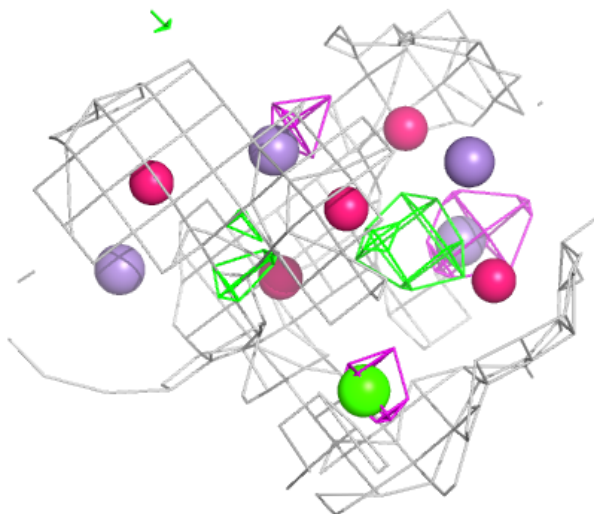
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





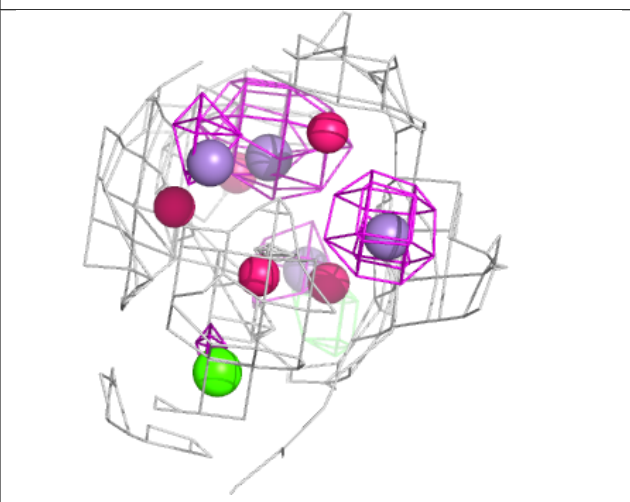
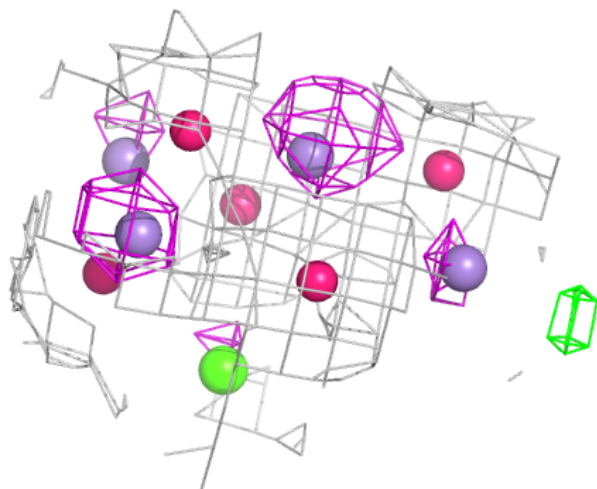
**Electron density around OEX A 602 (A):**

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



**Electron density around OEX a 602 (A):**

$2mF_o-DF_c$  (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.