



## wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 4, 2021 – 10:46 AM EDT

PDB ID : 7RF4  
Title : RT XFEL structure of Photosystem II 50 microseconds after the second illumination at 2.27 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 : 2.27 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references](#) 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

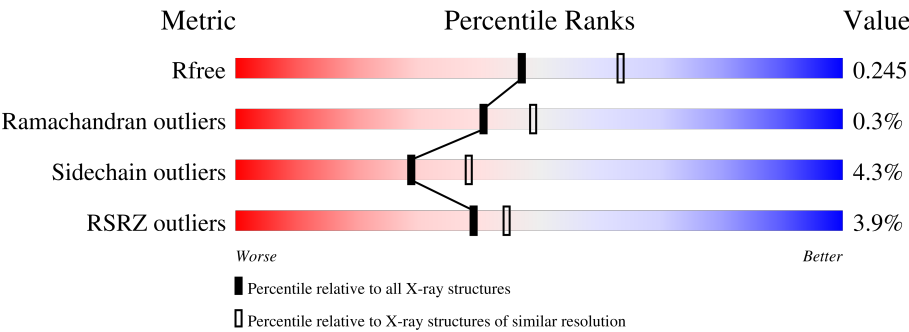


# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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.



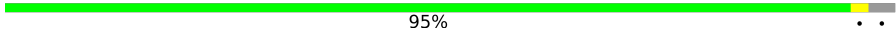
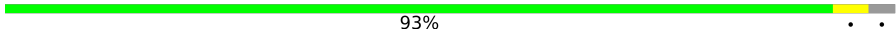
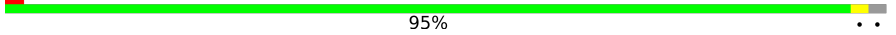
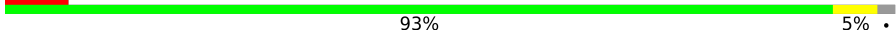


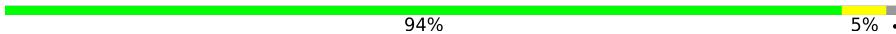







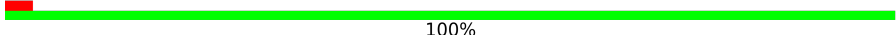










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	6980 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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

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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	

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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
22	CLA	A	402	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 103252 atoms, of which 51649 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5141	1717	2519	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			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	2	0
			6781	2249	3355	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	444	463	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- 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			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

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

- 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	0
			459	151	238	38	32			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	28	Total	C	H	N	O	0	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		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- 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
			2137	675	1073	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2137	675	1073	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	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

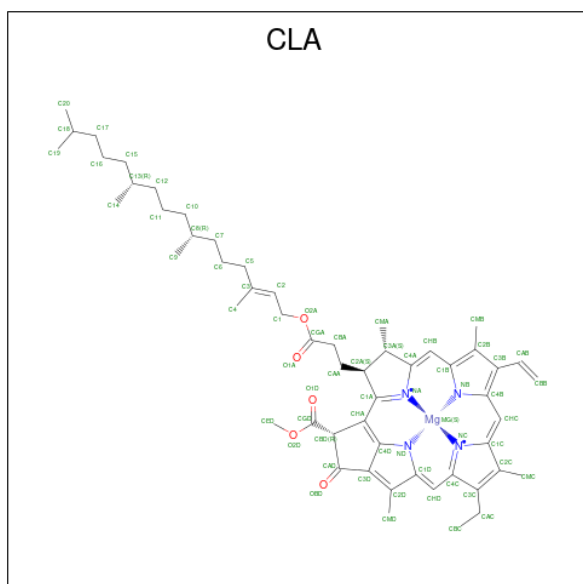
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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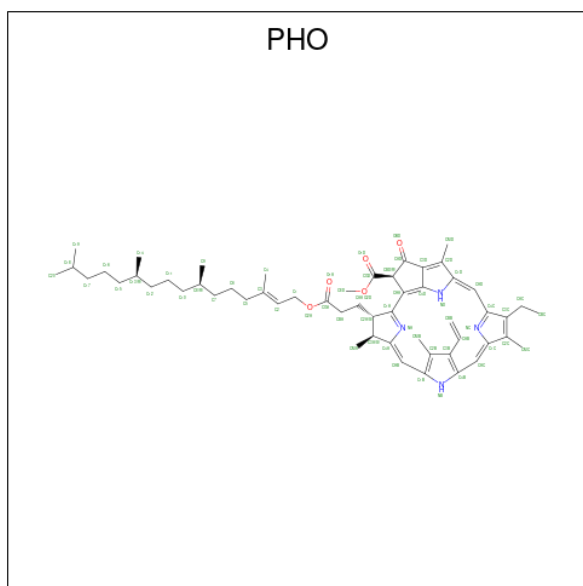
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).

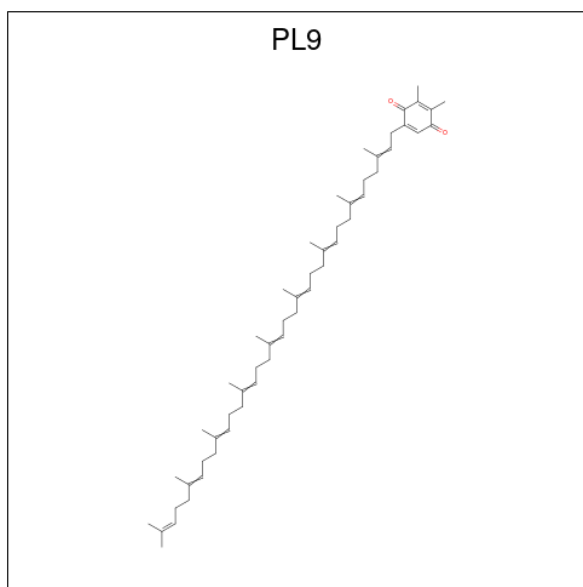


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

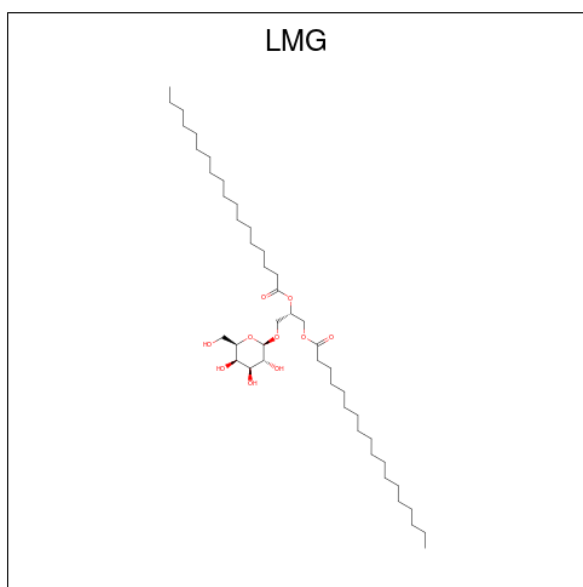
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



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

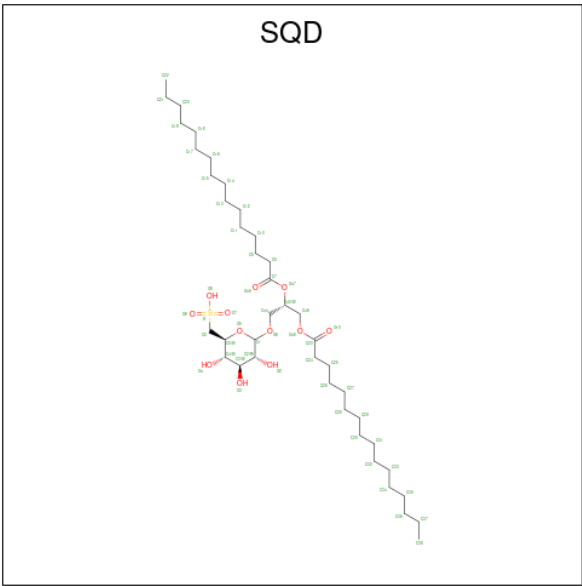
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

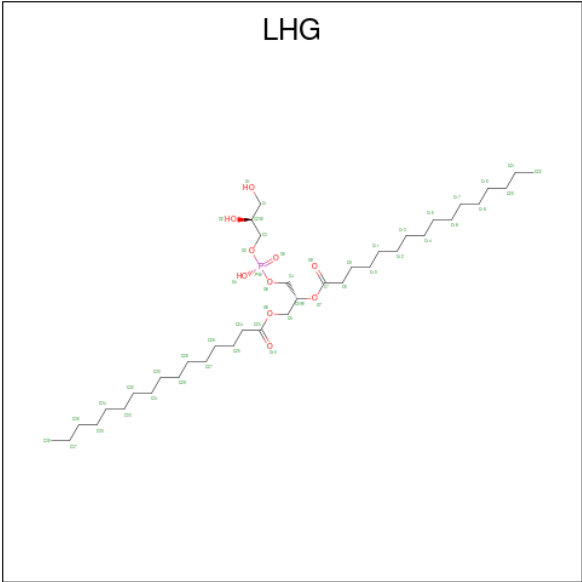
L]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
27	t	1	Total	C	H	O		0	0
			92	31	56	5			

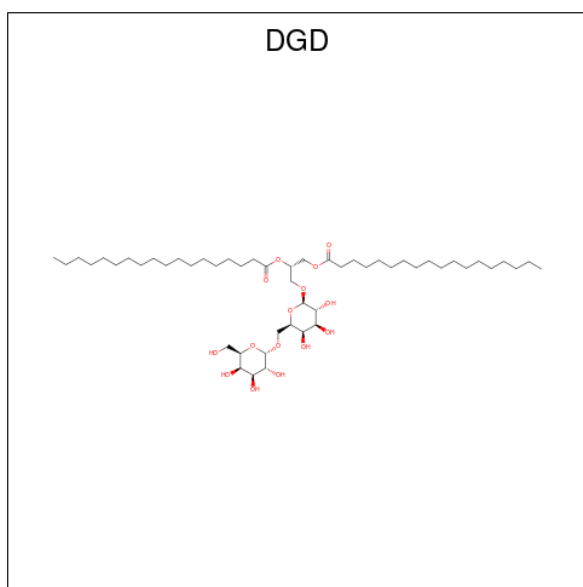
- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).





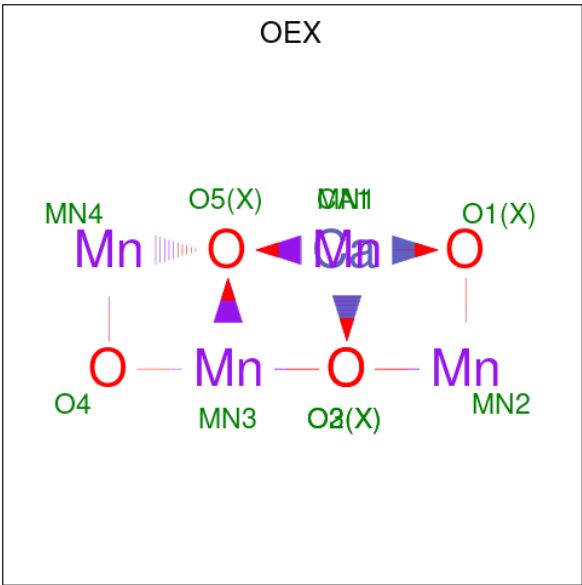
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	a	1	Total	C	H	O	P	0	0
			123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

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



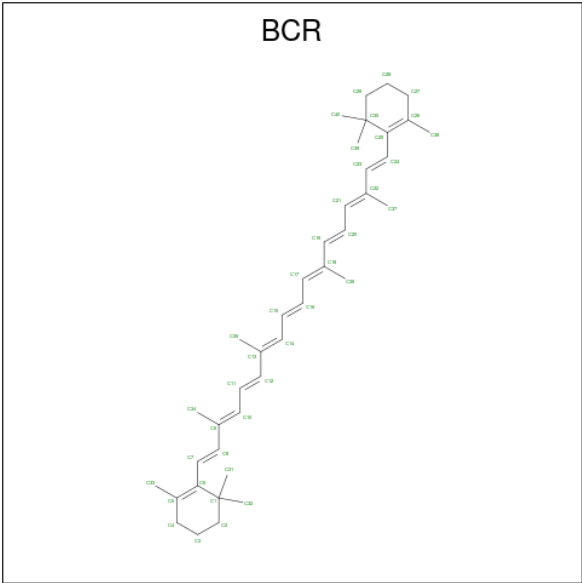
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 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
30	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



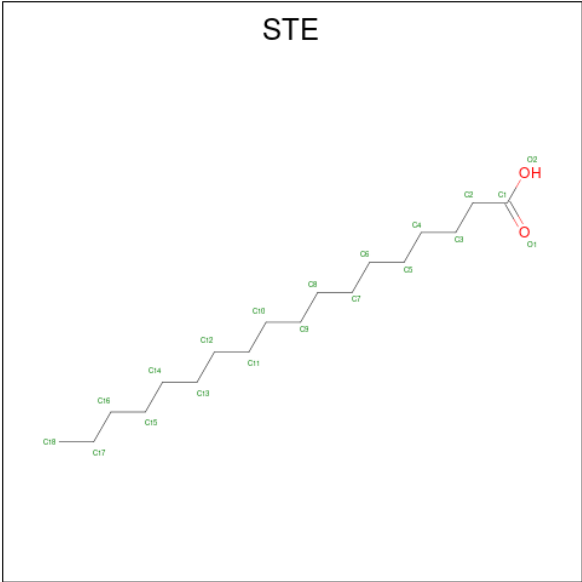
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	B	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	C	1	Total	C	H	0	0
			96	40	56		
31	D	1	Total	C	H	0	0
			96	40	56		
31	H	1	Total	C	H	0	0
			96	40	56		
31	I	1	Total	C	H	0	0
			96	40	56		
31	K	1	Total	C	H	0	0
			96	40	56		
31	K	1	Total	C	H	0	0
			96	40	56		
31	T	1	Total	C	H	0	0
			96	40	56		
31	Z	1	Total	C	H	0	0
			96	40	56		
31	a	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	c	1	Total	C	H	0	0
			96	40	56		
31	c	1	Total	C	H	0	0
			96	40	56		
31	d	1	Total	C	H	0	0
			96	40	56		
31	k	1	Total	C	H	0	0
			96	40	56		
31	k	1	Total	C	H	0	0
			96	40	56		
31	t	1	Total	C	H	0	0
			96	40	56		
31	x	1	Total	C	H	0	0
			96	40	56		

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>).



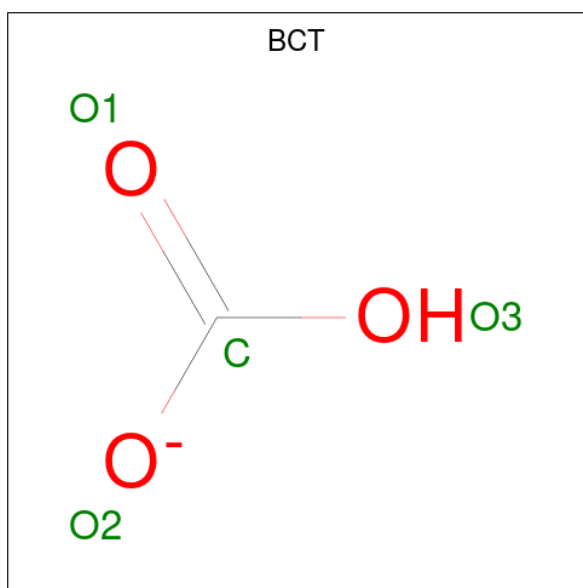
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H		0	0
			47	16	31			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			
32	I	1	Total	C	H		0	0
			41	15	26			
32	J	1	Total	C	H	O	0	0
			28	10	16	2		
32	L	1	Total	C	H	O	0	0
			28	10	16	2		
32	M	1	Total	C	H	O	0	0
			37	13	22	2		
32	M	1	Total	C	H		0	0
			26	10	16			

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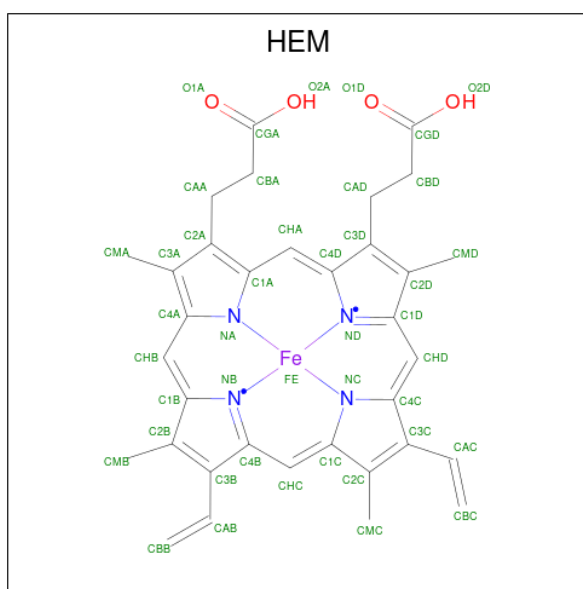
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	R	1	Total C H O 28 10 16 2	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	a	1	Total C H 41 15 26	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H 44 15 29	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	b	1	Total C H 41 14 27	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	d	1	Total C H O 55 18 35 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	t	1	Total C H 26 10 16	0	0
32	x	1	Total C H O 55 18 35 2	0	0

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



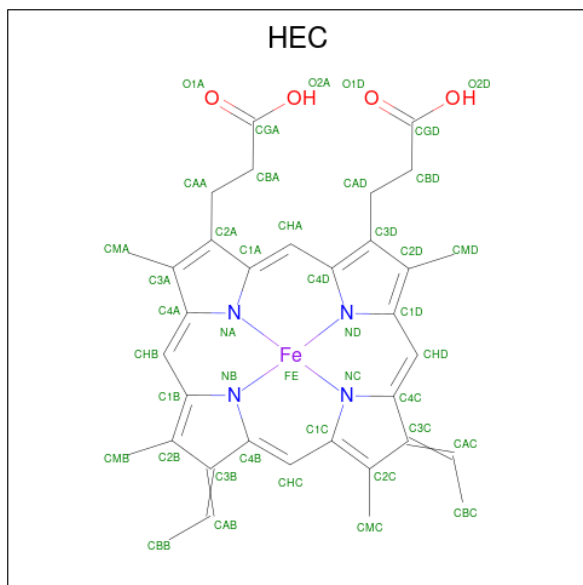
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	V	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	V	1	Total	Na	0	0
			1	1		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	125	Total	O	0	0
			125	125		
37	B	135	Total	O	0	0
			135	135		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	C	119	Total 119	O 119	0	0
37	D	103	Total 103	O 103	0	0
37	E	20	Total 20	O 20	0	0
37	F	5	Total 5	O 5	0	0
37	H	22	Total 22	O 22	0	0
37	I	12	Total 12	O 12	0	0
37	J	11	Total 11	O 11	0	0
37	K	6	Total 6	O 6	0	0
37	L	9	Total 9	O 9	0	0
37	M	6	Total 6	O 6	0	0
37	O	68	Total 68	O 68	0	0
37	R	8	Total 8	O 8	0	0
37	T	7	Total 7	O 7	0	0
37	U	30	Total 30	O 30	0	0
37	V	49	Total 49	O 49	0	0
37	X	9	Total 9	O 9	0	0
37	Y	3	Total 3	O 3	0	0
37	Z	6	Total 6	O 6	0	0
37	a	99	Total 99	O 99	0	0
37	b	114	Total 114	O 114	0	0
37	c	120	Total 120	O 120	0	0

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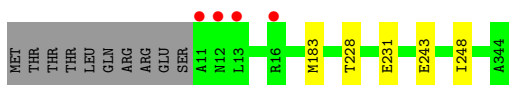
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	d	88	Total 88	O 88	0	0
37	e	18	Total 18	O 18	0	0
37	f	5	Total 5	O 5	0	0
37	h	22	Total 22	O 22	0	0
37	i	8	Total 8	O 8	0	0
37	j	9	Total 9	O 9	0	0
37	k	2	Total 2	O 2	0	0
37	l	11	Total 11	O 11	0	0
37	m	2	Total 2	O 2	0	0
37	o	70	Total 70	O 70	0	0
37	t	11	Total 11	O 11	0	0
37	u	35	Total 35	O 35	0	0
37	v	32	Total 32	O 32	0	0
37	x	7	Total 7	O 7	0	0
37	y	6	Total 6	O 6	0	0
37	z	11	Total 11	O 11	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.

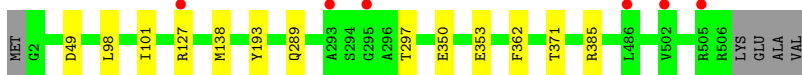
- Molecule 1: Photosystem II protein D1 1



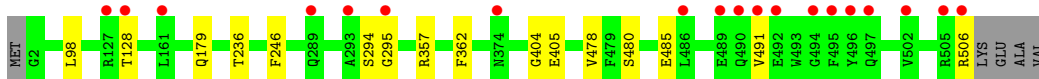
- Molecule 1: Photosystem II protein D1 1



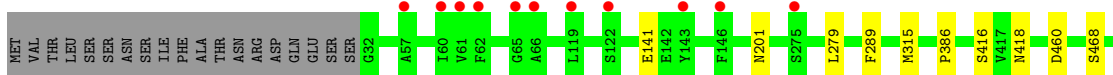
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



D473

- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  2% 95%

MET VAL THR LEU ALA SER SER ASN SER ILE PHE A23 T24 T25 R26 E29 A57 L72 A123 V124 L125 Y143 S144 S145 F146 F147 L166 T200 T255 R262 L279 F289 K316 T355 S416 D473

- Molecule 4: Photosystem II D2 protein

Chain D:  95%

MET THR ILE ALA ILE ILE ARG ALA PRO ALA ALA GLU R12 R180 Q224 E227 T238 Y296 M329 D333 V345 L352

- Molecule 4: Photosystem II D2 protein

Chain d:  93%

MET THR ILE ALA ILE ILE ARG ALA PRO ALA ALA GLU R12 L90 R180 F181 L182 E227 S230 R233 T259 L291 N292 L293 D297 E307 L321 L352

- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  2% 95%


MET ALA G3 I22 R61 F79 R84

- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  7% 93% 5%


MET ALA G3 T4 Q60 R61 L65 E71 Q74 Q75 F79 Q82 L83 K84

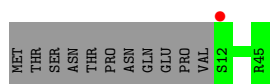
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  2% 73% 24%

MET THR SER ASN THR PRO ASN GLN PRO VAL S12 R45

- Molecule 6: Cytochrome b559 subunit beta

Chain f:  2% 76% 24%



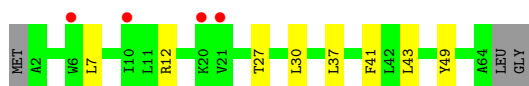
- Molecule 7: Photosystem II reaction center protein H

Chain H: 94% 5%



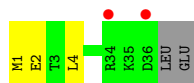
- Molecule 7: Photosystem II reaction center protein H

Chain h: 6% 83% 12% 5%



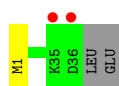
- Molecule 8: Photosystem II reaction center protein I

Chain I: 5% 87% 8% 5%



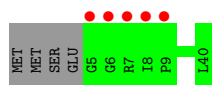
- Molecule 8: Photosystem II reaction center protein I

Chain i: 5% 92% 5%



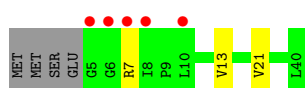
- Molecule 9: Photosystem II reaction center protein J

Chain J: 12% 90% 10%

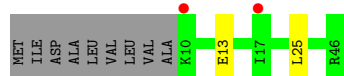
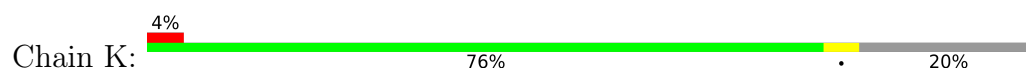


- Molecule 9: Photosystem II reaction center protein J

Chain j: 12% 82% 8% 10%



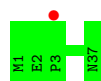
- Molecule 10: Photosystem II reaction center protein K



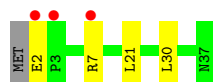
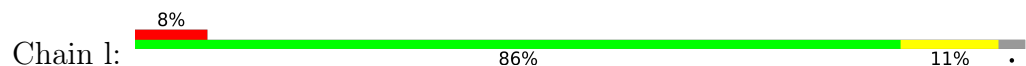
- Molecule 10: Photosystem II reaction center protein K



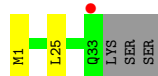
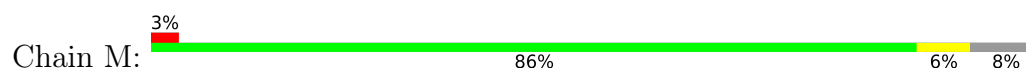
- Molecule 11: Photosystem II reaction center protein L



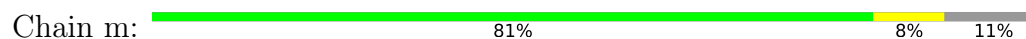
- Molecule 11: Photosystem II reaction center protein L



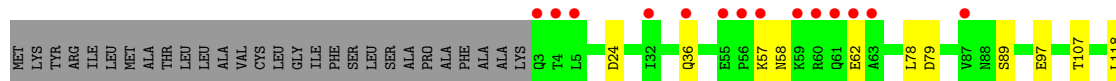
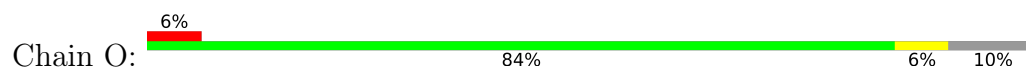
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

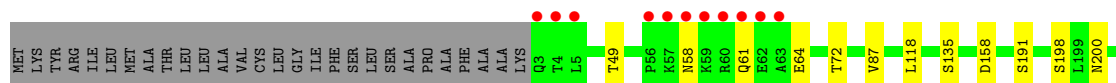
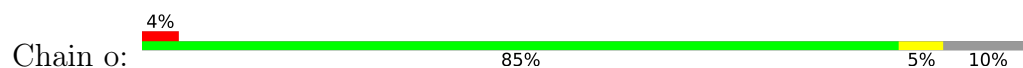


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

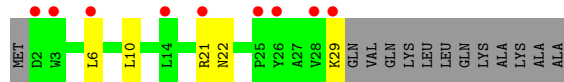




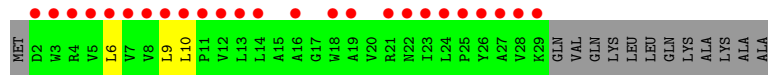
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



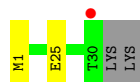
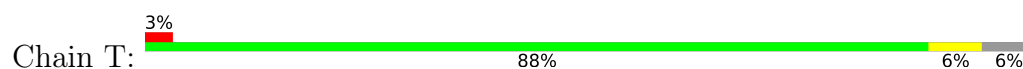
- Molecule 14: Photosystem II protein Y



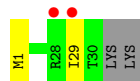
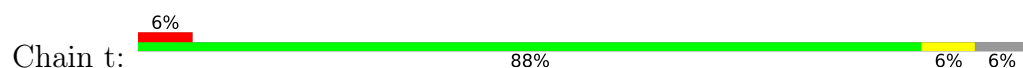
- Molecule 14: Photosystem II protein Y



- Molecule 15: Photosystem II reaction center protein T

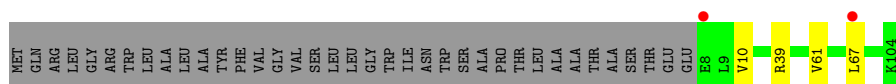


- Molecule 15: Photosystem II reaction center protein T

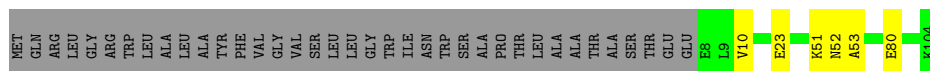


- Molecule 16: Photosystem II 12 kDa extrinsic protein

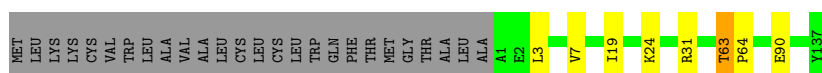
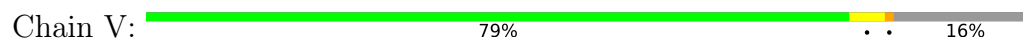




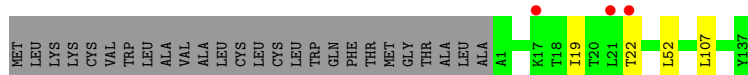
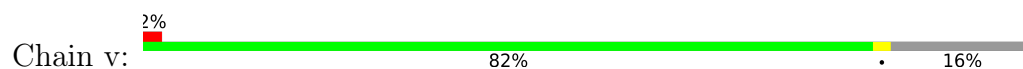
- Molecule 16: Photosystem II 12 kDa extrinsic protein



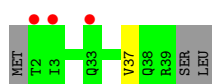
- Molecule 17: Cytochrome c-550



- Molecule 17: Cytochrome c-550



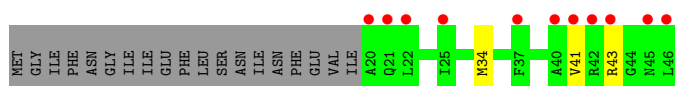
- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein

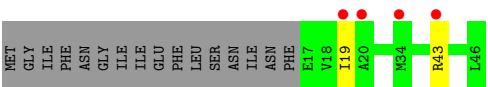


- Molecule 19: Photosystem II reaction center protein Ycf12

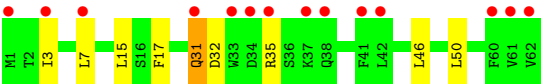
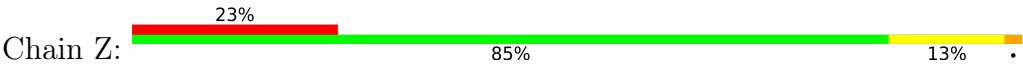


- Molecule 19: Photosystem II reaction center protein Ycf12

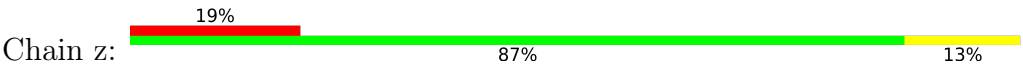




● Molecule 20: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.07Å 222.05Å 308.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.27 33.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.45-2.27) 84.3 (33.45-2.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.182 , 0.244 0.182 , 0.245	Depositor DCC
$R_{free}$ test set	3275 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.8	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	0.95	EDS
Total number of atoms	103252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, CL, OEX, DGD, FE2, STE, PL9, LHG, HEM, SQD, FME, BCT, HEC, PHO, CLA, NA, 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	0.66	0/2707	0.70	1/3692 (0.0%)
1	a	0.66	0/2704	0.68	0/3688
2	B	0.66	1/4161 (0.0%)	0.68	1/5669 (0.0%)
2	b	0.64	0/4118	0.68	0/5611
3	C	0.62	1/3547 (0.0%)	0.68	1/4830 (0.0%)
3	c	0.58	0/3619	0.68	0/4926
4	D	0.68	1/2812 (0.0%)	0.70	2/3832 (0.1%)
4	d	0.64	0/2821	0.70	1/3844 (0.0%)
5	E	0.59	0/688	0.59	0/940
5	e	0.54	0/683	0.62	0/932
6	F	0.49	0/284	0.63	0/387
6	f	0.47	0/284	0.64	0/387
7	H	0.65	0/523	0.65	0/713
7	h	0.59	0/511	0.69	0/697
8	I	0.63	0/293	0.72	0/396
8	i	0.64	0/293	0.66	0/396
9	J	0.56	0/263	0.64	0/356
9	j	0.52	0/263	0.63	0/356
10	K	0.56	0/303	0.61	0/416
10	k	0.47	0/303	0.62	0/416
11	L	0.61	0/311	0.68	0/422
11	l	0.68	0/303	0.68	0/412
12	M	0.62	0/249	0.60	0/341
12	m	0.68	0/244	0.70	0/334
13	O	0.60	0/1904	0.75	1/2585 (0.0%)
13	o	0.63	0/1905	0.77	1/2583 (0.0%)
14	R	0.42	0/227	0.61	0/313
14	r	0.38	0/227	0.52	0/313
15	T	0.82	0/257	0.76	0/349
15	t	0.68	0/255	0.64	0/346
16	U	0.57	0/785	0.70	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	u	0.64	0/785	0.74	0/1064
17	V	0.59	0/1085	0.70	1/1473 (0.1%)
17	v	0.54	0/1085	0.67	0/1473
18	X	0.56	0/284	0.67	0/384
18	x	0.49	0/289	0.63	0/391
19	Y	0.44	0/197	0.62	0/264
19	y	0.36	0/219	0.54	0/294
20	Z	0.47	0/490	0.55	0/669
20	z	0.43	0/488	0.53	0/666
All	All	0.62	3/42769 (0.0%)	0.68	9/58224 (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
16	u	0	1
17	V	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	468	SER	C-N	-6.11	1.20	1.34
2	B	193	TYR	CD2-CE2	-5.45	1.31	1.39
4	D	296	TYR	CE1-CZ	-5.44	1.31	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	183	MET	CA-CB-CG	6.10	123.68	113.30
4	D	333	ASP	CB-CG-OD2	-5.80	113.08	118.30
4	d	297	ASP	CB-CG-OD1	5.76	123.48	118.30
3	C	460	ASP	CB-CG-OD1	5.72	123.45	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
16	u	52	ASN	Peptide

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	325 (98%)	7 (2%)	0	100	100
1	a	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	487 (97%)	13 (3%)	3 (1%)	25	29
3	C	442/461 (96%)	424 (96%)	17 (4%)	1 (0%)	47	57
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	47	57
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	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%)	61 (97%)	1 (2%)	1 (2%)	9	8
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	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%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	12 (5%)	3 (1%)	13	12
13	o	242/272 (89%)	228 (94%)	13 (5%)	1 (0%)	34	40
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%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	14	14
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	25
17	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	3	1
20	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	2
20	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	9	7
All	All	5231/5700 (92%)	5049 (96%)	165 (3%)	17 (0%)	41	49

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
20	Z	31	GLN
3	c	416	SER
16	u	53	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	266 (98%)	4 (2%)	65	77
1	a	269/280 (96%)	258 (96%)	11 (4%)	30	41
2	B	408/407 (100%)	397 (97%)	11 (3%)	44	59
2	b	402/407 (99%)	389 (97%)	13 (3%)	39	52
3	C	346/362 (96%)	339 (98%)	7 (2%)	55	70
3	c	354/362 (98%)	341 (96%)	13 (4%)	34	45
4	D	276/283 (98%)	271 (98%)	5 (2%)	59	72
4	d	277/283 (98%)	264 (95%)	13 (5%)	26	34
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	39
5	e	71/73 (97%)	67 (94%)	4 (6%)	21	27
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	47
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	45
7	h	53/55 (96%)	45 (85%)	8 (15%)	3	2
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	22
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	4
10	K	30/37 (81%)	28 (93%)	2 (7%)	16	19
10	k	30/37 (81%)	24 (80%)	6 (20%)	1	1
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	5
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	47
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	17
13	O	206/228 (90%)	195 (95%)	11 (5%)	22	29
13	o	207/228 (91%)	196 (95%)	11 (5%)	22	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	22/33 (67%)	17 (77%)	5 (23%)	1	0
14	r	22/33 (67%)	19 (86%)	3 (14%)	3	3
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	44
15	t	25/28 (89%)	24 (96%)	1 (4%)	31	42
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	34
16	u	84/112 (75%)	80 (95%)	4 (5%)	25	34
17	V	117/138 (85%)	111 (95%)	6 (5%)	24	31
17	v	117/138 (85%)	113 (97%)	4 (3%)	37	49
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	52
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	21
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	7
19	y	22/37 (60%)	21 (96%)	1 (4%)	27	36
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2	2
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	3
All	All	4321/4654 (93%)	4135 (96%)	186 (4%)	29	38

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	180	ARG
10	k	17	ILE
4	d	230	SER
7	h	7	LEU
11	l	30	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	234	ASN
20	z	31	GLN
13	o	61	GLN
13	O	88	ASN
1	a	181	ASN



### 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	$\# Z  > 2$
8	FME	I	1	8	8,9,10	1.10	1 (12%)	7,9,11	0.80	0
12	FME	m	1	12	8,9,10	1.03	0	7,9,11	1.37	1 (14%)
12	FME	M	1	12	8,9,10	1.03	1 (12%)	7,9,11	0.98	0
8	FME	i	1	8	8,9,10	1.09	1 (12%)	7,9,11	1.13	0
15	FME	T	1	15	8,9,10	0.96	0	7,9,11	1.11	1 (14%)
15	FME	t	1	15	8,9,10	1.46	1 (12%)	7,9,11	1.22	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
8	FME	I	1	8	-	4/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
15	FME	T	1	15	-	4/7/9/11	-
15	FME	t	1	15	-	3/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.80	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.13	1.43	1.46
8	I	1	FME	CA-N	-2.01	1.43	1.46
8	i	1	FME	CA-N	-2.01	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	2.98	127.41	122.82
15	t	1	FME	CA-N-CN	-2.26	119.35	122.82
15	T	1	FME	CG-CB-CA	2.21	119.09	112.95

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	N-CA-CB-CG
15	T	1	FME	N-CA-CB-CG
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 190 ligands modelled in this entry, 7 are monoatomic - leaving 183 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
22	CLA	b	608	-	56,73,73	1.56	9 (16%)	55,113,113	1.49	10 (18%)
31	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.39	9 (16%)
27	SQD	B	622	-	53,54,54	1.01	3 (5%)	62,65,65	1.98	13 (20%)
22	CLA	C	506	-	56,73,73	1.53	10 (17%)	55,113,113	1.61	12 (21%)
32	STE	c	520	-	16,19,19	0.40	0	15,19,19	0.71	0
28	LHG	D	410	-	48,48,48	0.92	3 (6%)	51,54,54	1.22	6 (11%)
31	BCR	c	515	-	41,41,41	1.17	4 (9%)	56,56,56	1.32	8 (14%)
32	STE	l	102	-	17,17,19	0.42	0	16,16,19	0.82	0
32	STE	j	101	-	8,11,19	0.44	0	7,11,19	0.68	0
22	CLA	B	614	-	56,73,73	1.74	7 (12%)	55,113,113	1.55	12 (21%)
32	STE	R	101	-	8,11,19	0.39	0	7,11,19	0.72	0
22	CLA	B	604	-	56,73,73	1.44	6 (10%)	55,113,113	2.17	17 (30%)
33	BCT	a	408	21	0,3,3	-	-	0,3,3	-	-
25	PL9	A	408	-	55,55,55	1.79	4 (7%)	68,69,69	1.57	15 (22%)
27	SQD	t	102	-	35,35,54	1.10	2 (5%)	37,37,65	1.36	4 (10%)
33	BCT	D	402	21	0,3,3	-	-	0,3,3	-	-
22	CLA	B	605	-	56,73,73	1.39	6 (10%)	55,113,113	1.54	10 (18%)
22	CLA	C	501	-	56,73,73	1.61	8 (14%)	55,113,113	1.72	9 (16%)
22	CLA	b	607	37	56,73,73	1.51	12 (21%)	55,113,113	1.51	7 (12%)
22	CLA	b	614	-	56,73,73	1.54	8 (14%)	55,113,113	1.68	11 (20%)
32	STE	b	621	-	16,19,19	0.41	0	15,19,19	0.87	0
22	CLA	B	616	-	51,68,73	1.67	8 (15%)	49,107,113	1.82	10 (20%)
32	STE	b	627	-	13,13,19	0.45	0	12,12,19	0.55	0
31	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.16	6 (10%)
22	CLA	B	607	37	56,73,73	1.63	10 (17%)	55,113,113	1.61	8 (14%)
31	BCR	B	619	-	41,41,41	1.23	3 (7%)	56,56,56	1.50	12 (21%)
32	STE	b	623	-	12,15,19	0.43	0	11,15,19	0.76	0
32	STE	a	413	-	14,14,19	0.46	0	13,13,19	0.70	0
31	BCR	k	102	-	41,41,41	1.14	3 (7%)	56,56,56	1.22	5 (8%)
26	LMG	M	101	-	51,51,55	1.04	4 (7%)	59,59,63	1.39	9 (15%)
28	LHG	l	101	-	48,48,48	0.80	2 (4%)	51,54,54	1.12	3 (5%)
22	CLA	d	403	-	56,73,73	1.62	11 (19%)	55,113,113	1.44	7 (12%)
31	BCR	C	514	-	41,41,41	1.24	2 (4%)	56,56,56	1.35	8 (14%)
26	LMG	b	622	-	55,55,55	1.14	7 (12%)	63,63,63	1.37	7 (11%)
32	STE	X	101	-	16,19,19	0.28	0	15,19,19	1.14	0
27	SQD	D	409	-	35,36,54	1.03	3 (8%)	42,45,65	2.04	10 (23%)
28	LHG	D	413	-	48,48,48	0.98	3 (6%)	51,54,54	1.35	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	OEX	A	414	3,37,1	0,15,15	-	-	-		
32	STE	d	412	-	16,19,19	0.37	0	15,19,19	0.81	0
22	CLA	c	510	-	56,73,73	1.55	8 (14%)	55,113,113	1.59	9 (16%)
31	BCR	b	617	-	41,41,41	1.12	3 (7%)	56,56,56	1.28	6 (10%)
22	CLA	b	616	-	51,68,73	1.60	9 (17%)	49,107,113	1.97	12 (24%)
25	PL9	d	407	-	55,55,55	1.53	10 (18%)	68,69,69	1.59	16 (23%)
22	CLA	B	601	37	56,73,73	1.80	8 (14%)	55,113,113	1.57	8 (14%)
26	LMG	d	410	-	44,44,55	1.25	5 (11%)	52,52,63	1.28	5 (9%)
32	STE	t	103	-	10,13,19	0.51	0	9,13,19	0.67	0
22	CLA	B	603	-	56,73,73	1.49	9 (16%)	55,113,113	1.84	16 (29%)
29	DGD	A	413	-	67,67,67	1.24	8 (11%)	81,81,81	1.37	11 (13%)
28	LHG	d	408	-	48,48,48	0.70	1 (2%)	51,54,54	1.18	4 (7%)
22	CLA	d	405	-	56,73,73	1.79	9 (16%)	55,113,113	1.57	7 (12%)
22	CLA	d	401	37	56,73,73	1.68	6 (10%)	55,113,113	1.37	10 (18%)
32	STE	M	103	-	9,9,19	0.61	0	8,8,19	0.46	0
22	CLA	b	610	37	56,73,73	1.51	11 (19%)	55,113,113	1.58	10 (18%)
22	CLA	C	502	-	56,73,73	1.68	7 (12%)	55,113,113	1.70	12 (21%)
22	CLA	D	405	-	56,73,73	1.62	7 (12%)	55,113,113	1.50	10 (18%)
32	STE	b	624	-	14,14,19	0.34	0	13,13,19	1.00	0
30	OEX	a	414	3,37,1	0,15,15	-	-	-		
22	CLA	B	609	-	56,73,73	1.48	7 (12%)	55,113,113	1.70	13 (23%)
22	CLA	b	615	-	56,73,73	1.88	8 (14%)	55,113,113	1.61	10 (18%)
22	CLA	c	509	-	56,73,73	1.39	6 (10%)	55,113,113	1.78	12 (21%)
26	LMG	D	408	-	51,51,55	0.88	1 (1%)	59,59,63	1.27	3 (5%)
27	SQD	A	410	-	51,52,54	1.09	4 (7%)	60,63,65	2.09	14 (23%)
22	CLA	A	405	-	45,62,73	1.79	8 (17%)	41,99,113	1.89	11 (26%)
22	CLA	b	606	-	56,73,73	1.90	11 (19%)	55,113,113	1.84	7 (12%)
27	SQD	f	102	-	40,41,54	1.14	4 (10%)	49,52,65	1.91	11 (22%)
32	STE	d	411	-	13,16,19	0.38	0	12,16,19	0.88	0
28	LHG	e	101	-	41,41,48	1.03	3 (7%)	44,47,54	1.29	4 (9%)
34	HEM	f	101	6,5	27,50,50	1.98	5 (18%)	17,82,82	2.12	6 (35%)
27	SQD	A	412	-	38,38,54	1.06	3 (7%)	40,40,65	1.42	4 (10%)
22	CLA	b	612	-	56,73,73	1.59	9 (16%)	55,113,113	1.91	12 (21%)
22	CLA	A	402	-	56,73,73	1.83	6 (10%)	55,113,113	1.70	11 (20%)
22	CLA	c	513	-	56,73,73	1.57	7 (12%)	55,113,113	1.44	9 (16%)
22	CLA	b	611	-	56,73,73	1.70	9 (16%)	55,113,113	1.68	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LMG	Y	101	-	48,48,55	1.07	7 (14%)	56,56,63	1.24	6 (10%)
26	LMG	c	522	-	49,49,55	1.20	5 (10%)	57,57,63	1.42	7 (12%)
32	STE	B	623	-	8,11,19	0.42	0	7,11,19	0.80	0
22	CLA	c	504	37	51,68,73	1.62	5 (9%)	49,107,113	1.69	12 (24%)
32	STE	x	102	-	16,19,19	0.47	0	15,19,19	0.63	0
34	HEM	F	101	6,5	27,50,50	1.98	5 (18%)	17,82,82	2.26	6 (35%)
22	CLA	C	510	-	56,73,73	1.62	8 (14%)	55,113,113	1.87	7 (12%)
29	DGD	c	516	-	63,63,67	1.29	8 (12%)	77,77,81	1.45	13 (16%)
22	CLA	c	508	-	55,72,73	1.61	7 (12%)	53,111,113	1.38	8 (15%)
35	HEC	v	201	17	26,50,50	2.40	5 (19%)	18,82,82	2.53	6 (33%)
31	BCR	K	102	-	41,41,41	1.11	3 (7%)	56,56,56	1.22	5 (8%)
22	CLA	c	507	37	56,73,73	1.66	11 (19%)	55,113,113	1.78	17 (30%)
22	CLA	b	601	37	56,73,73	1.70	9 (16%)	55,113,113	1.66	10 (18%)
26	LMG	A	409	-	48,48,55	1.17	3 (6%)	56,56,63	1.43	9 (16%)
32	STE	L	103	-	8,11,19	0.45	0	7,11,19	0.75	0
22	CLA	b	604	-	56,73,73	1.52	6 (10%)	55,113,113	1.92	16 (29%)
25	PL9	a	409	-	55,55,55	1.02	3 (5%)	68,69,69	1.66	16 (23%)
22	CLA	C	504	37	50,67,73	1.78	9 (18%)	47,105,113	1.57	9 (19%)
22	CLA	C	511	3	56,73,73	1.61	9 (16%)	55,113,113	1.75	9 (16%)
32	STE	H	103	-	17,17,19	0.44	0	16,16,19	0.68	0
35	HEC	V	201	17	26,50,50	2.13	3 (11%)	18,82,82	2.41	6 (33%)
26	LMG	D	412	-	31,31,55	1.02	3 (9%)	33,33,63	1.16	4 (12%)
22	CLA	b	602	-	56,73,73	1.68	10 (17%)	55,113,113	1.78	13 (23%)
22	CLA	c	506	-	56,73,73	1.75	8 (14%)	55,113,113	1.52	6 (10%)
26	LMG	B	626	-	55,55,55	1.21	6 (10%)	63,63,63	1.31	5 (7%)
31	BCR	b	618	-	41,41,41	1.52	3 (7%)	56,56,56	1.30	7 (12%)
22	CLA	B	611	-	56,73,73	1.55	9 (16%)	55,113,113	2.02	12 (21%)
25	PL9	D	407	-	55,55,55	1.43	8 (14%)	68,69,69	1.60	15 (22%)
28	LHG	L	102	-	48,48,48	0.81	2 (4%)	51,54,54	1.16	4 (7%)
29	DGD	h	101	-	63,63,67	1.09	4 (6%)	77,77,81	1.41	14 (18%)
22	CLA	B	613	-	56,73,73	1.65	7 (12%)	55,113,113	1.64	12 (21%)
32	STE	c	523	-	8,11,19	0.40	0	7,11,19	0.77	0
32	STE	b	620	-	15,15,19	0.44	0	14,14,19	0.80	0
22	CLA	c	505	-	56,73,73	1.55	5 (8%)	55,113,113	1.61	10 (18%)
22	CLA	C	509	-	56,73,73	1.50	7 (12%)	55,113,113	1.79	12 (21%)
22	CLA	B	606	-	56,73,73	2.00	9 (16%)	55,113,113	1.44	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LHG	a	410	-	48,48,48	0.89	1 (2%)	51,54,54	1.27	6 (11%)
26	LMG	c	519	-	37,37,55	1.43	7 (18%)	45,45,63	1.36	5 (11%)
26	LMG	B	621	-	20,26,55	0.64	0	18,26,63	1.09	1 (5%)
22	CLA	B	610	37	56,73,73	1.59	9 (16%)	55,113,113	1.77	12 (21%)
28	LHG	A	411	-	48,48,48	0.86	3 (6%)	51,54,54	1.23	6 (11%)
29	DGD	c	517	-	63,63,67	1.07	6 (9%)	77,77,81	1.55	13 (16%)
28	LHG	d	409	-	38,38,48	0.91	2 (5%)	41,44,54	1.21	5 (12%)
22	CLA	D	403	-	56,73,73	1.54	6 (10%)	55,113,113	1.51	10 (18%)
22	CLA	b	613	-	56,73,73	1.62	8 (14%)	55,113,113	1.91	13 (23%)
31	BCR	I	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.40	9 (16%)
22	CLA	B	615	-	56,73,73	1.65	11 (19%)	55,113,113	1.59	9 (16%)
22	CLA	d	404	37	56,73,73	1.79	7 (12%)	55,113,113	1.74	10 (18%)
31	BCR	t	101	-	41,41,41	1.20	4 (9%)	56,56,56	1.36	8 (14%)
32	STE	C	520	-	8,11,19	0.35	0	7,11,19	1.19	0
32	STE	a	412	-	8,11,19	0.47	0	7,11,19	0.68	0
29	DGD	C	515	-	63,63,67	1.34	10 (15%)	77,77,81	1.36	11 (14%)
32	STE	B	620	-	13,16,19	0.36	0	12,16,19	0.95	0
31	BCR	d	406	-	41,41,41	1.17	2 (4%)	56,56,56	1.33	8 (14%)
22	CLA	D	404	37	56,73,73	1.75	9 (16%)	55,113,113	1.66	11 (20%)
26	LMG	c	521	-	48,48,55	1.08	4 (8%)	56,56,63	1.34	7 (12%)
22	CLA	b	609	-	56,73,73	1.68	8 (14%)	55,113,113	1.71	11 (20%)
32	STE	B	627	-	8,11,19	0.42	0	7,11,19	0.72	0
29	DGD	C	516	-	63,63,67	1.23	9 (14%)	77,77,81	1.49	16 (20%)
31	BCR	D	406	-	41,41,41	1.20	2 (4%)	56,56,56	1.18	6 (10%)
22	CLA	b	603	-	56,73,73	1.83	10 (17%)	55,113,113	2.08	14 (25%)
29	DGD	H	102	-	63,63,67	1.33	8 (12%)	77,77,81	1.54	12 (15%)
22	CLA	C	507	37	56,73,73	1.47	9 (16%)	55,113,113	1.87	11 (20%)
32	STE	b	625	-	16,19,19	0.50	0	15,19,19	0.70	0
22	CLA	C	512	-	56,73,73	1.51	7 (12%)	55,113,113	1.69	10 (18%)
31	BCR	x	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.41	9 (16%)
22	CLA	A	403	37	56,73,73	2.09	8 (14%)	55,113,113	1.55	10 (18%)
22	CLA	B	612	-	56,73,73	1.34	6 (10%)	55,113,113	1.86	10 (18%)
31	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.06	3 (5%)
22	CLA	B	602	-	56,73,73	1.77	9 (16%)	55,113,113	1.68	14 (25%)
23	PHO	d	402	-	67,69,69	1.29	7 (10%)	85,99,99	1.23	11 (12%)
31	BCR	T	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.28	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	BCR	b	619	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	8 (14%)
32	STE	C	519	-	15,15,19	0.49	0	14,14,19	0.67	0
31	BCR	B	617	-	41,41,41	1.16	3 (7%)	56,56,56	1.40	7 (12%)
31	BCR	B	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.34	5 (8%)
22	CLA	C	503	-	56,73,73	1.63	8 (14%)	55,113,113	1.99	12 (21%)
22	CLA	C	508	-	56,73,73	1.57	8 (14%)	55,113,113	1.58	8 (14%)
31	BCR	K	101	-	41,41,41	1.24	3 (7%)	56,56,56	1.21	5 (8%)
22	CLA	b	605	-	56,73,73	1.60	8 (14%)	55,113,113	1.75	12 (21%)
22	CLA	c	502	-	56,73,73	1.63	9 (16%)	55,113,113	1.73	11 (20%)
27	SQD	a	411	-	53,54,54	1.05	4 (7%)	62,65,65	1.72	11 (17%)
27	SQD	L	101	-	48,49,54	0.97	3 (6%)	57,60,65	2.20	16 (28%)
32	STE	M	102	-	11,14,19	0.46	0	10,14,19	0.79	0
32	STE	B	625	-	15,15,19	0.47	0	14,14,19	0.84	0
22	CLA	a	404	-	56,73,73	1.23	7 (12%)	55,113,113	1.50	11 (20%)
29	DGD	C	517	-	63,63,67	1.18	8 (12%)	77,77,81	1.56	12 (15%)
22	CLA	c	503	-	56,73,73	1.58	8 (14%)	55,113,113	1.50	8 (14%)
32	STE	B	624	-	14,17,19	0.36	0	13,17,19	0.94	0
22	CLA	a	402	-	56,73,73	1.70	7 (12%)	55,113,113	1.83	11 (20%)
31	BCR	a	405	-	41,41,41	1.21	4 (9%)	56,56,56	1.44	8 (14%)
22	CLA	B	608	-	56,73,73	1.73	10 (17%)	55,113,113	1.43	10 (18%)
22	CLA	c	511	3	56,73,73	1.75	5 (8%)	55,113,113	1.83	7 (12%)
22	CLA	C	513	-	56,73,73	1.70	8 (14%)	55,113,113	1.69	11 (20%)
32	STE	t	104	-	9,9,19	0.54	0	8,8,19	0.45	0
32	STE	b	626	-	9,9,19	0.49	0	8,8,19	0.50	0
23	PHO	A	404	-	67,69,69	1.30	10 (14%)	85,99,99	1.24	8 (9%)
23	PHO	a	403	-	67,69,69	1.23	8 (11%)	85,99,99	1.12	5 (5%)
32	STE	I	102	-	14,14,19	0.51	0	13,13,19	0.51	0
32	STE	J	101	-	8,11,19	0.31	0	7,11,19	1.01	0
22	CLA	c	501	-	56,73,73	1.62	8 (14%)	55,113,113	1.95	12 (21%)
29	DGD	c	518	-	63,63,67	1.23	9 (14%)	77,77,81	1.40	11 (14%)
31	BCR	Z	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.34	5 (8%)
28	LHG	D	411	-	46,46,48	1.00	3 (6%)	49,52,54	1.20	3 (6%)
23	PHO	D	401	-	67,69,69	1.27	7 (10%)	85,99,99	1.10	4 (4%)
32	STE	Z	102	-	7,7,19	0.49	0	6,6,19	0.29	0
22	CLA	c	512	-	56,73,73	1.76	7 (12%)	55,113,113	1.60	13 (23%)
22	CLA	C	505	-	56,73,73	1.58	6 (10%)	55,113,113	1.68	11 (20%)
32	STE	C	518	-	8,11,19	0.50	0	7,11,19	0.72	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LMG	m	101	-	51,51,55	1.30	6 (11%)	59,59,63	1.39	8 (13%)

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
22	CLA	b	608	-	1/1/20/20	6/37/115/115	-
31	BCR	c	514	-	-	8/29/63/63	0/2/2/2
27	SQD	B	622	-	-	25/49/69/69	0/1/1/1
22	CLA	C	506	-	1/1/20/20	21/37/115/115	-
32	STE	c	520	-	-	7/15/17/17	-
28	LHG	D	410	-	-	25/53/53/53	-
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2
32	STE	l	102	-	-	7/15/15/17	-
32	STE	j	101	-	-	2/7/9/17	-
22	CLA	B	614	-	1/1/20/20	21/37/115/115	-
32	STE	R	101	-	-	4/7/9/17	-
22	CLA	B	604	-	1/1/20/20	16/37/115/115	-
25	PL9	A	408	-	-	19/53/73/73	0/1/1/1
27	SQD	t	102	-	-	14/37/37/69	-
22	CLA	B	605	-	1/1/20/20	14/37/115/115	-
22	CLA	C	501	-	1/1/20/20	2/37/115/115	-
22	CLA	b	607	37	1/1/20/20	16/37/115/115	-
22	CLA	b	614	-	1/1/20/20	19/37/115/115	-
32	STE	b	621	-	-	8/15/17/17	-
22	CLA	B	616	-	1/1/19/20	10/31/109/115	-
32	STE	b	627	-	-	7/11/11/17	-
31	BCR	H	101	-	-	10/29/63/63	0/2/2/2
22	CLA	B	607	37	1/1/20/20	13/37/115/115	-
31	BCR	B	619	-	-	6/29/63/63	0/2/2/2
32	STE	b	623	-	-	9/11/13/17	-
32	STE	a	413	-	-	8/12/12/17	-
31	BCR	k	102	-	-	4/29/63/63	0/2/2/2
26	LMG	M	101	-	-	20/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	l	101	-	-	17/53/53/53	-
22	CLA	d	403	-	1/1/20/20	10/37/115/115	-
31	BCR	C	514	-	-	7/29/63/63	0/2/2/2
26	LMG	b	622	-	-	30/50/70/70	0/1/1/1
32	STE	X	101	-	-	11/15/17/17	-
27	SQD	D	409	-	-	13/28/48/69	0/1/1/1
28	LHG	D	413	-	-	20/53/53/53	-
32	STE	d	412	-	-	7/15/17/17	-
22	CLA	c	510	-	1/1/20/20	16/37/115/115	-
31	BCR	b	617	-	-	9/29/63/63	0/2/2/2
22	CLA	b	616	-	1/1/19/20	10/31/109/115	-
25	PL9	d	407	-	-	16/53/73/73	0/1/1/1
22	CLA	B	601	37	1/1/20/20	16/37/115/115	-
26	LMG	d	410	-	-	10/39/59/70	0/1/1/1
32	STE	t	103	-	-	4/9/11/17	-
22	CLA	B	603	-	1/1/20/20	14/37/115/115	-
29	DGD	A	413	-	-	32/55/95/95	0/2/2/2
28	LHG	d	408	-	-	26/53/53/53	-
22	CLA	d	405	-	1/1/20/20	12/37/115/115	-
22	CLA	d	401	37	-	14/37/115/115	-
32	STE	M	103	-	-	2/7/7/17	-
22	CLA	b	610	37	1/1/20/20	7/37/115/115	-
22	CLA	C	502	-	1/1/20/20	10/37/115/115	-
22	CLA	D	405	-	-	13/37/115/115	-
32	STE	b	624	-	-	7/12/12/17	-
22	CLA	B	609	-	-	8/37/115/115	-
22	CLA	b	615	-	1/1/20/20	11/37/115/115	-
22	CLA	c	509	-	1/1/20/20	9/37/115/115	-
26	LMG	D	408	-	-	15/46/66/70	0/1/1/1
27	SQD	A	410	-	-	20/47/67/69	0/1/1/1
22	CLA	A	405	-	1/1/17/20	5/24/102/115	-
22	CLA	b	606	-	1/1/20/20	5/37/115/115	-
27	SQD	f	102	-	-	14/36/56/69	0/1/1/1
32	STE	d	411	-	-	6/12/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	e	101	-	-	24/46/46/53	-
34	HEM	f	101	6,5	-	0/6/54/54	-
27	SQD	A	412	-	-	19/39/39/69	-
22	CLA	b	612	-	1/1/20/20	5/37/115/115	-
22	CLA	A	402	-	1/1/20/20	7/37/115/115	-
22	CLA	c	513	-	1/1/20/20	10/37/115/115	-
22	CLA	b	611	-	-	10/37/115/115	-
26	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
26	LMG	c	522	-	-	25/44/64/70	0/1/1/1
32	STE	B	623	-	-	4/7/9/17	-
22	CLA	c	504	37	1/1/19/20	9/31/109/115	-
32	STE	x	102	-	-	11/15/17/17	-
34	HEM	F	101	6,5	-	0/6/54/54	-
22	CLA	C	510	-	1/1/20/20	12/37/115/115	-
29	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	c	508	-	-	12/36/114/115	-
35	HEC	v	201	17	-	0/6/54/54	-
31	BCR	K	102	-	-	9/29/63/63	0/2/2/2
22	CLA	c	507	37	1/1/20/20	11/37/115/115	-
22	CLA	b	601	37	1/1/20/20	23/37/115/115	-
26	LMG	A	409	-	-	18/43/63/70	0/1/1/1
32	STE	L	103	-	-	5/7/9/17	-
22	CLA	b	604	-	1/1/20/20	11/37/115/115	-
25	PL9	a	409	-	-	28/53/73/73	0/1/1/1
22	CLA	C	504	37	1/1/18/20	8/30/108/115	-
22	CLA	C	511	3	1/1/20/20	6/37/115/115	-
32	STE	H	103	-	-	8/15/15/17	-
35	HEC	V	201	17	-	0/6/54/54	-
26	LMG	D	412	-	-	19/33/33/70	-
22	CLA	b	602	-	1/1/20/20	12/37/115/115	-
22	CLA	c	506	-	1/1/20/20	14/37/115/115	-
26	LMG	B	626	-	-	35/50/70/70	0/1/1/1
31	BCR	b	618	-	-	2/29/63/63	0/2/2/2
22	CLA	B	611	-	-	6/37/115/115	-
25	PL9	D	407	-	-	13/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	L	102	-	-	23/53/53/53	-
29	DGD	h	101	-	-	17/51/91/95	0/2/2/2
22	CLA	B	613	-	1/1/20/20	11/37/115/115	-
32	STE	c	523	-	-	5/7/9/17	-
32	STE	b	620	-	-	7/13/13/17	-
22	CLA	c	505	-	1/1/20/20	10/37/115/115	-
22	CLA	C	509	-	1/1/20/20	15/37/115/115	-
22	CLA	B	606	-	1/1/20/20	10/37/115/115	-
28	LHG	a	410	-	-	22/53/53/53	-
26	LMG	c	519	-	-	12/31/51/70	0/1/1/1
26	LMG	B	621	-	-	10/18/22/70	-
22	CLA	B	610	37	1/1/20/20	10/37/115/115	-
28	LHG	A	411	-	-	23/53/53/53	-
29	DGD	c	517	-	-	21/51/91/95	0/2/2/2
28	LHG	d	409	-	-	11/43/43/53	-
22	CLA	D	403	-	1/1/20/20	6/37/115/115	-
22	CLA	b	613	-	1/1/20/20	11/37/115/115	-
31	BCR	I	101	-	-	5/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/20/20	6/37/115/115	-
22	CLA	d	404	37	1/1/20/20	6/37/115/115	-
31	BCR	t	101	-	-	13/29/63/63	0/2/2/2
32	STE	C	520	-	-	2/7/9/17	-
32	STE	a	412	-	-	4/7/9/17	-
29	DGD	C	515	-	-	24/51/91/95	0/2/2/2
32	STE	B	620	-	-	5/12/14/17	-
31	BCR	d	406	-	-	9/29/63/63	0/2/2/2
22	CLA	D	404	37	1/1/20/20	9/37/115/115	-
26	LMG	c	521	-	-	22/43/63/70	0/1/1/1
22	CLA	b	609	-	1/1/20/20	13/37/115/115	-
32	STE	B	627	-	-	4/7/9/17	-
29	DGD	C	516	-	-	26/51/91/95	0/2/2/2
31	BCR	D	406	-	-	7/29/63/63	0/2/2/2
22	CLA	b	603	-	1/1/20/20	8/37/115/115	-
29	DGD	H	102	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	507	37	1/1/20/20	7/37/115/115	-
32	STE	b	625	-	-	7/15/17/17	-
22	CLA	C	512	-	1/1/20/20	14/37/115/115	-
31	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	A	403	37	-	12/37/115/115	-
22	CLA	B	612	-	1/1/20/20	10/37/115/115	-
31	BCR	k	101	-	-	12/29/63/63	0/2/2/2
22	CLA	B	602	-	1/1/20/20	10/37/115/115	-
23	PHO	d	402	-	-	9/53/103/103	0/5/6/6
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
31	BCR	b	619	-	-	7/29/63/63	0/2/2/2
32	STE	C	519	-	-	5/13/13/17	-
31	BCR	B	617	-	-	9/29/63/63	0/2/2/2
31	BCR	B	618	-	-	10/29/63/63	0/2/2/2
22	CLA	C	503	-	1/1/20/20	9/37/115/115	-
22	CLA	C	508	-	-	10/37/115/115	-
31	BCR	K	101	-	-	12/29/63/63	0/2/2/2
22	CLA	b	605	-	1/1/20/20	15/37/115/115	-
22	CLA	c	502	-	-	12/37/115/115	-
27	SQD	a	411	-	-	23/49/69/69	0/1/1/1
27	SQD	L	101	-	-	29/44/64/69	0/1/1/1
32	STE	M	102	-	-	4/10/12/17	-
32	STE	B	625	-	-	7/13/13/17	-
22	CLA	a	404	-	1/1/20/20	8/37/115/115	-
29	DGD	C	517	-	-	13/51/91/95	0/2/2/2
22	CLA	c	503	-	1/1/20/20	9/37/115/115	-
32	STE	B	624	-	-	11/13/15/17	-
22	CLA	a	402	-	-	2/37/115/115	-
31	BCR	a	405	-	-	3/29/63/63	0/2/2/2
22	CLA	B	608	-	1/1/20/20	11/37/115/115	-
22	CLA	c	511	3	1/1/20/20	14/37/115/115	-
22	CLA	C	513	-	1/1/20/20	9/37/115/115	-
32	STE	t	104	-	-	3/7/7/17	-
32	STE	b	626	-	-	4/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	A	404	-	-	7/53/103/103	0/5/6/6
23	PHO	a	403	-	-	6/53/103/103	0/5/6/6
32	STE	I	102	-	-	4/12/12/17	-
32	STE	J	101	-	-	6/7/9/17	-
22	CLA	c	501	-	1/1/20/20	10/37/115/115	-
29	DGD	c	518	-	-	17/51/91/95	0/2/2/2
31	BCR	Z	101	-	-	13/29/63/63	0/2/2/2
28	LHG	D	411	-	-	19/51/51/53	-
23	PHO	D	401	-	-	3/53/103/103	0/5/6/6
32	STE	Z	102	-	-	4/5/5/17	-
22	CLA	c	512	-	1/1/20/20	20/37/115/115	-
22	CLA	C	505	-	1/1/20/20	9/37/115/115	-
32	STE	C	518	-	-	2/7/9/17	-
26	LMG	m	101	-	-	24/46/66/70	0/1/1/1

The worst 5 of 879 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	403	CLA	C4B-NB	10.45	1.44	1.35
22	B	606	CLA	MG-NA	9.77	2.29	2.06
25	A	408	PL9	C7-C3	-9.72	1.41	1.51
22	B	614	CLA	C4B-NB	9.21	1.43	1.35
22	A	402	CLA	C4B-NB	9.03	1.43	1.35

The worst 5 of 1336 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	9.61	111.03	106.71
22	c	511	CLA	C4A-NA-C1A	9.46	110.96	106.71
27	L	101	SQD	O6-C1-C2	9.05	122.43	108.30
22	C	511	CLA	C4A-NA-C1A	8.63	110.59	106.71
22	C	510	CLA	C4A-NA-C1A	8.48	110.52	106.71

5 of 60 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	405	CLA	ND
22	B	601	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	602	CLA	ND
22	B	603	CLA	ND

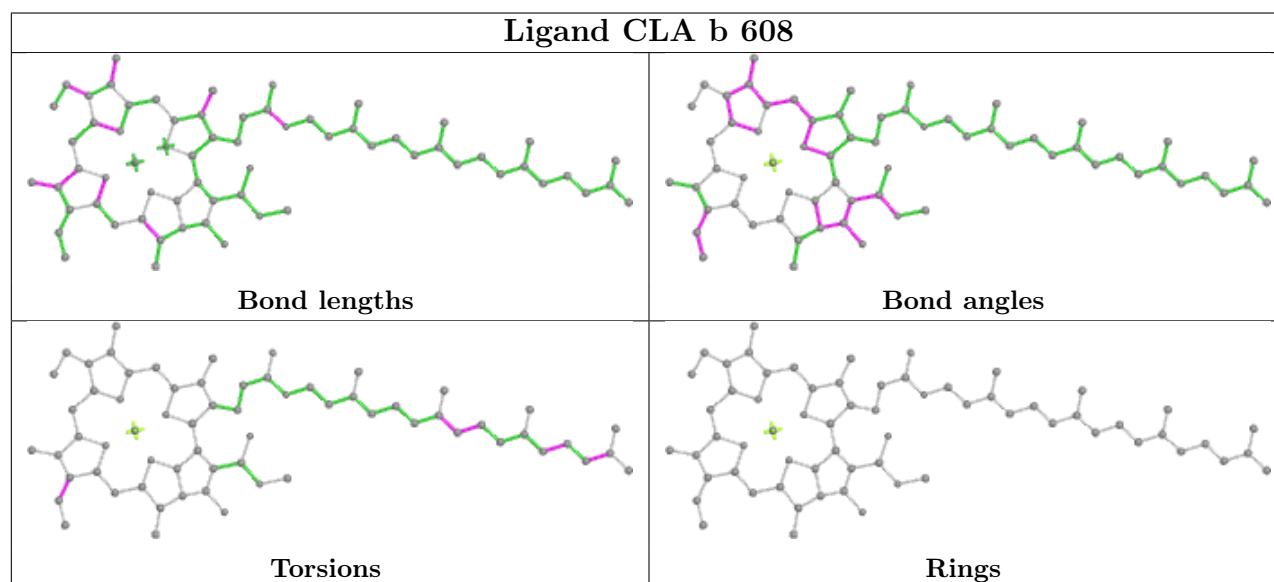
5 of 2059 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C2C-C3C-CAC-CBC
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	C4-C3-C5-C6
22	B	612	CLA	CHA-CBD-CGD-O1D

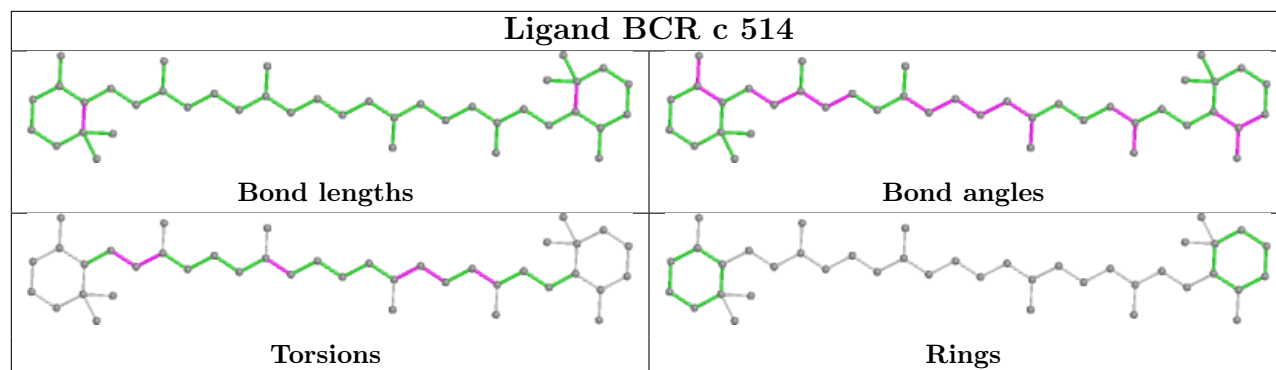
There are no ring outliers.

No monomer is involved in short contacts.

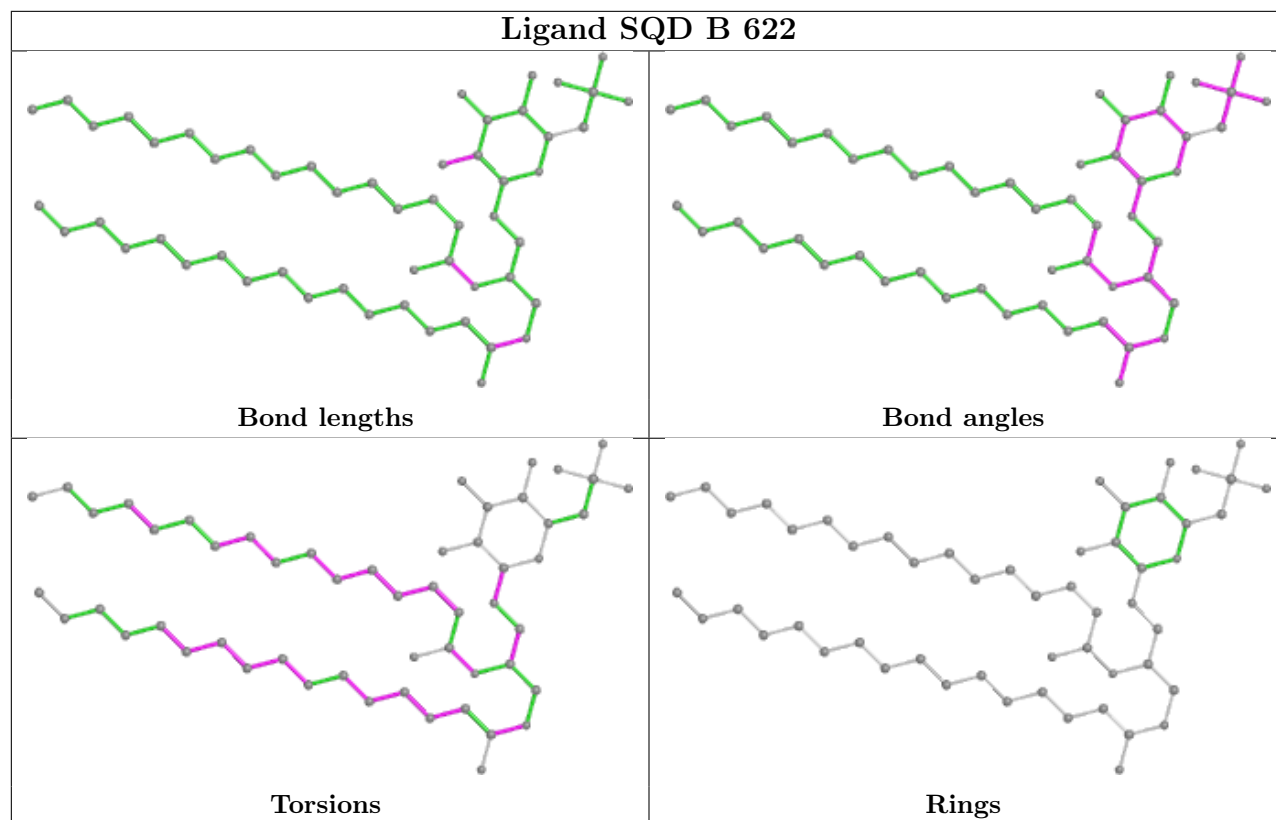
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



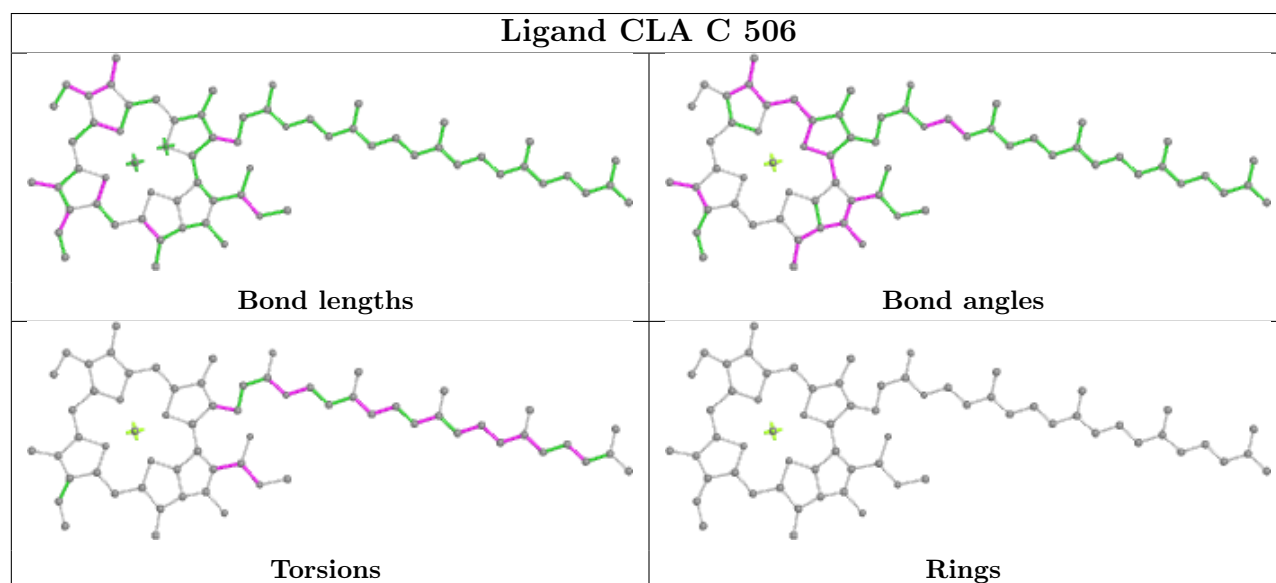
## Ligand BCR c 514

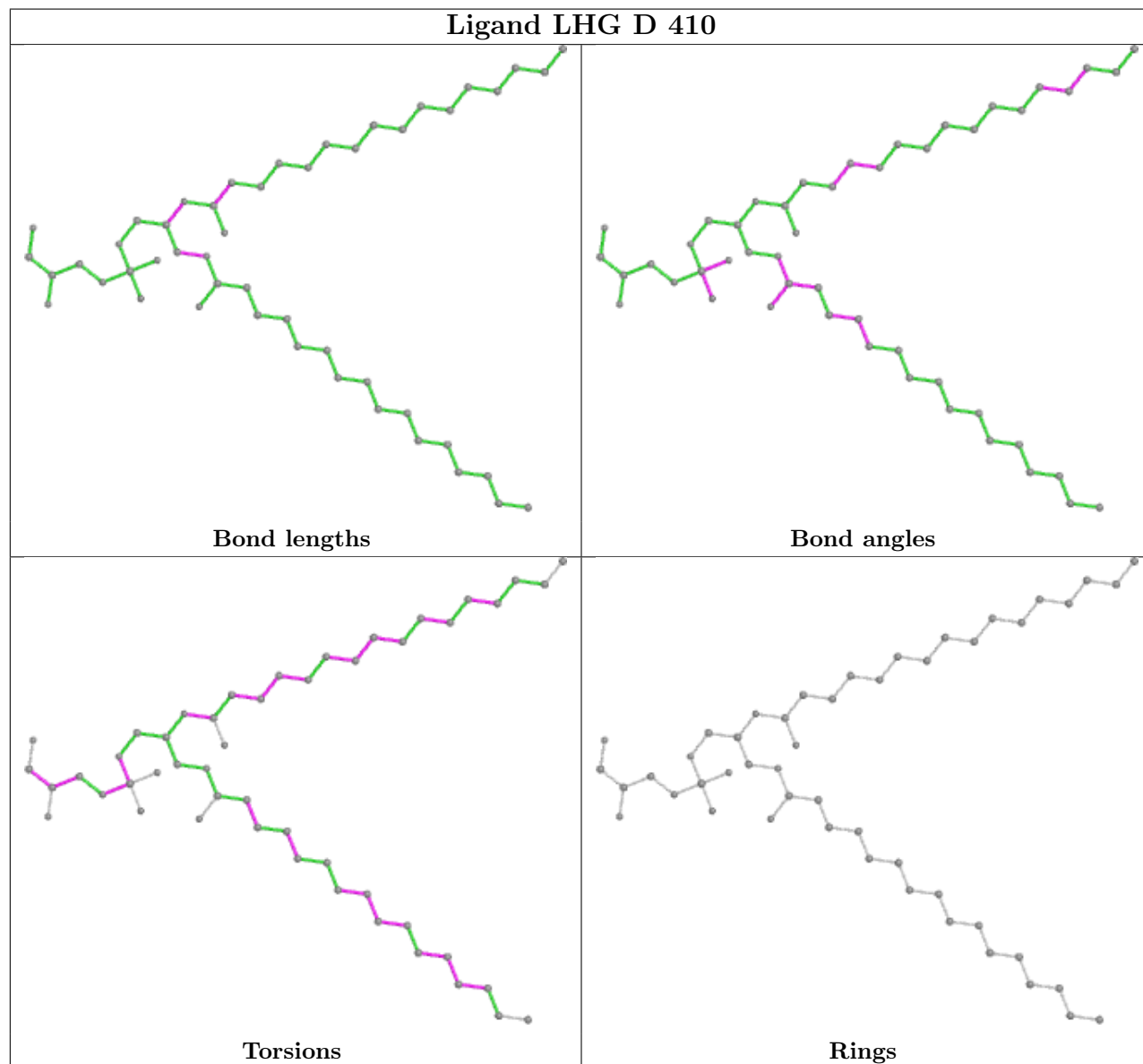
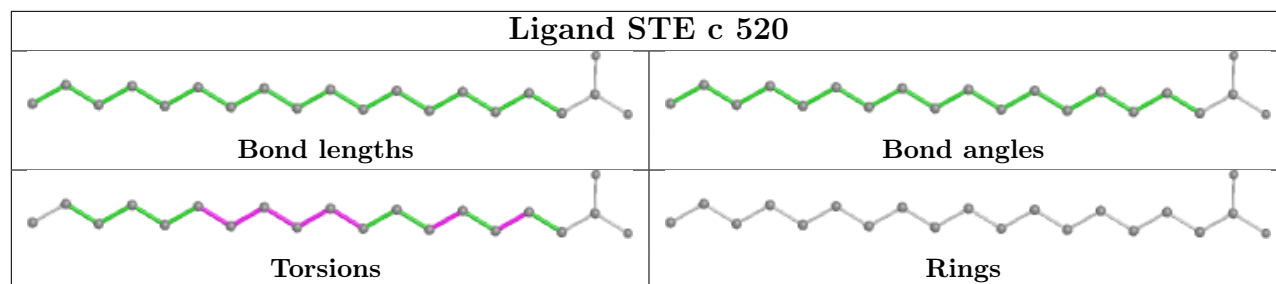


## Ligand SQD B 622

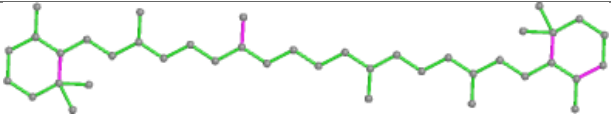
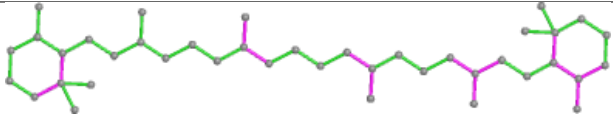
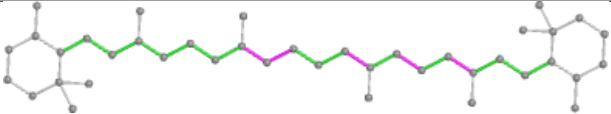
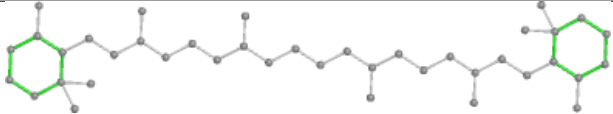






## Ligand CLA C 506

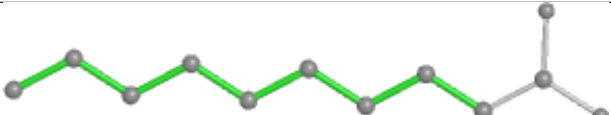
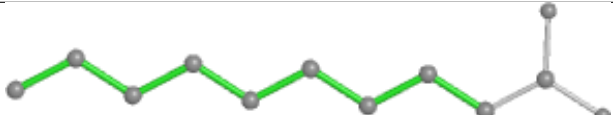
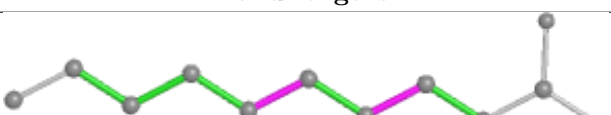
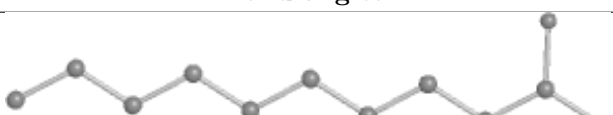


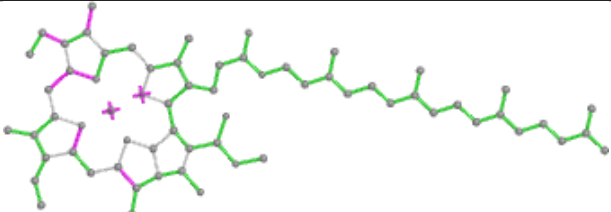
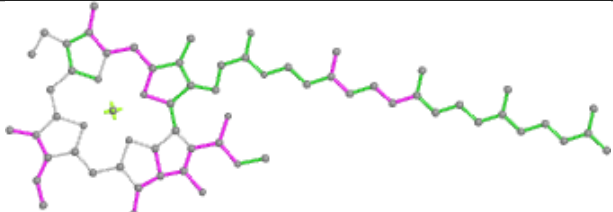
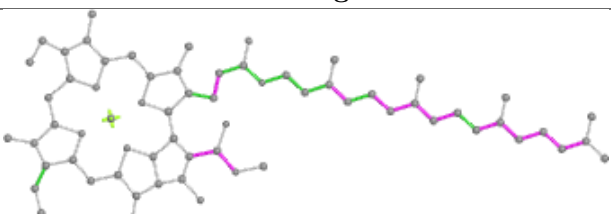
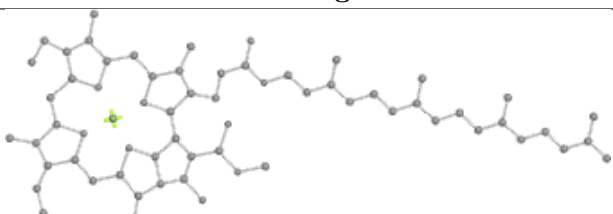


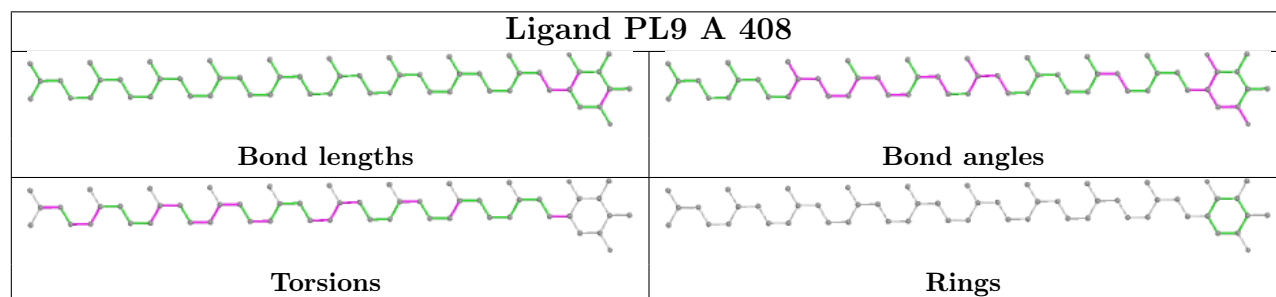
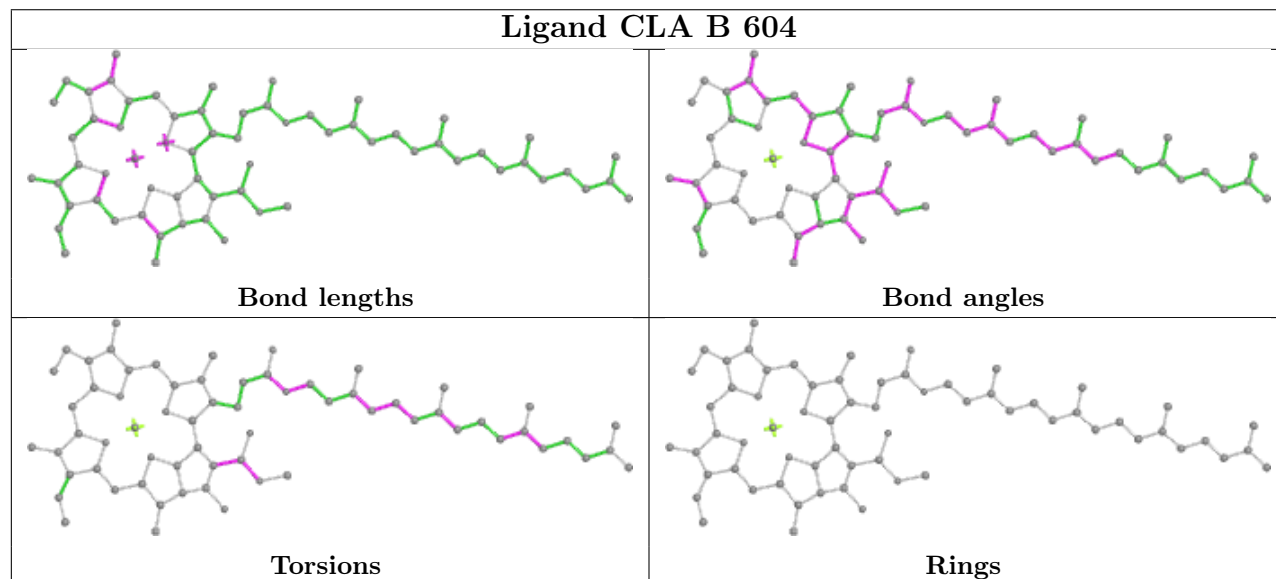
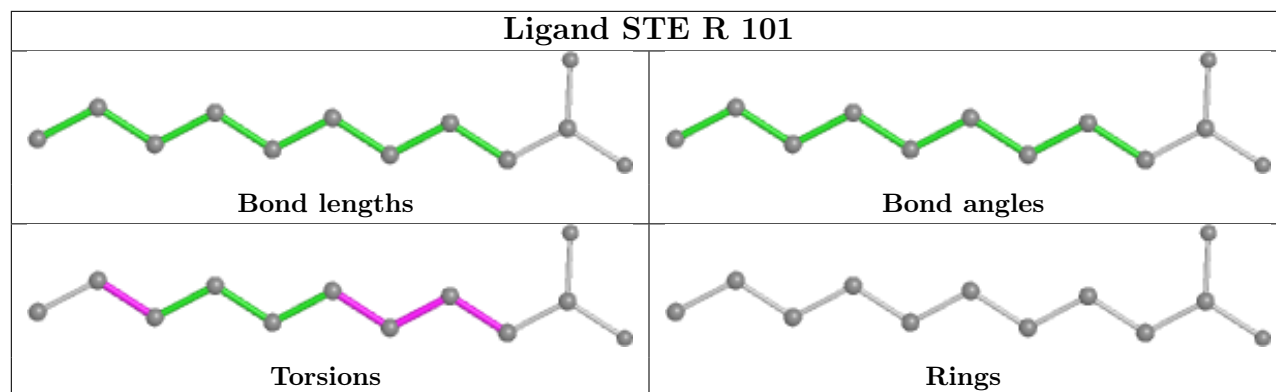


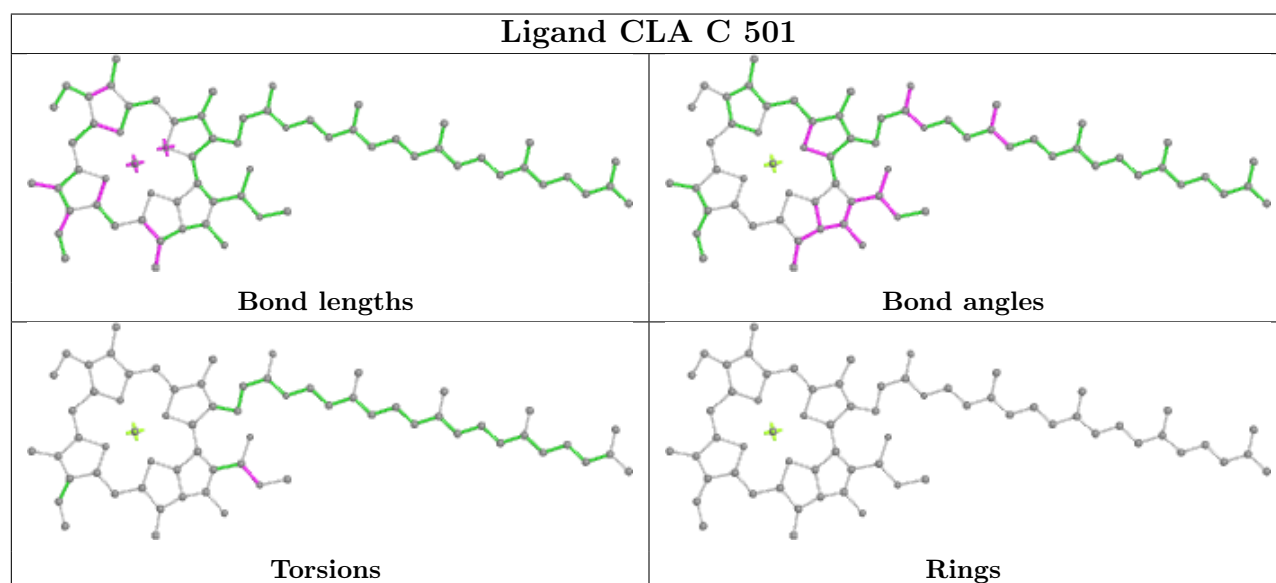
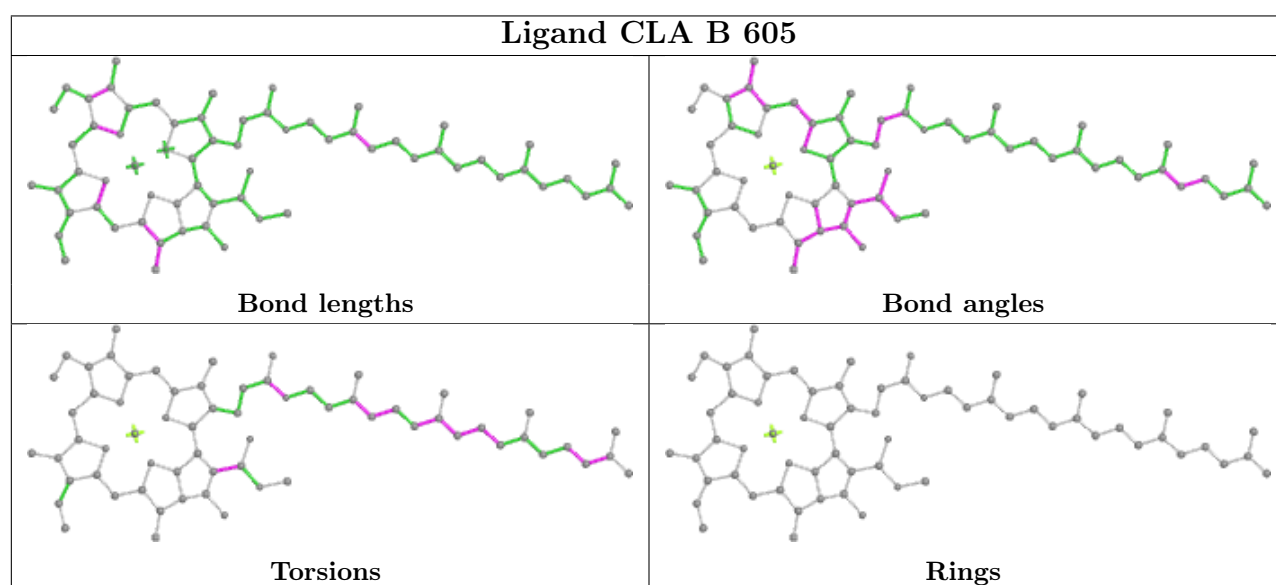
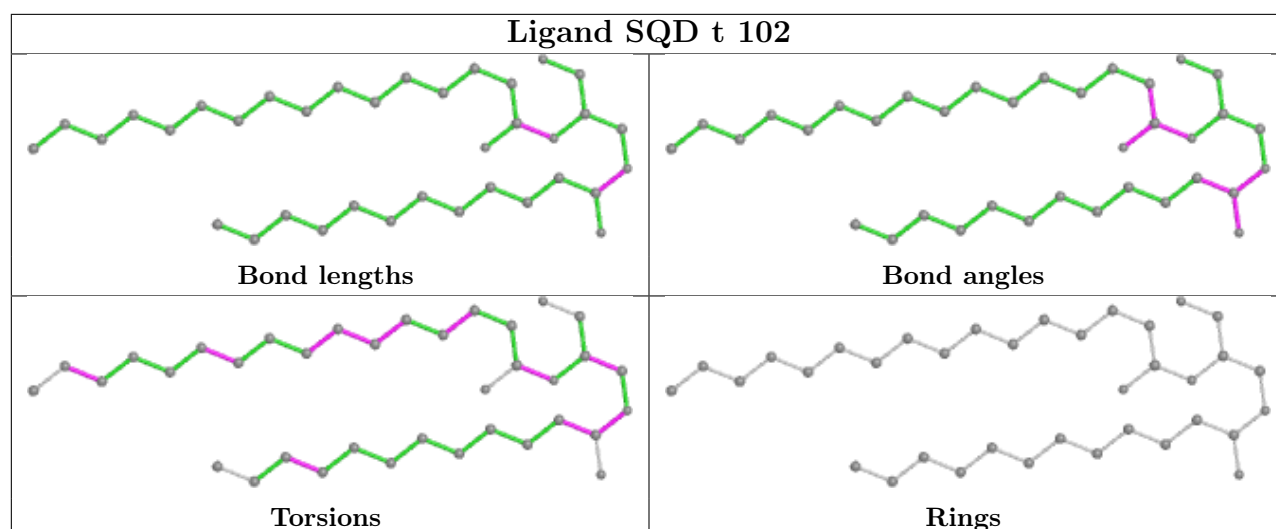
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE l 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

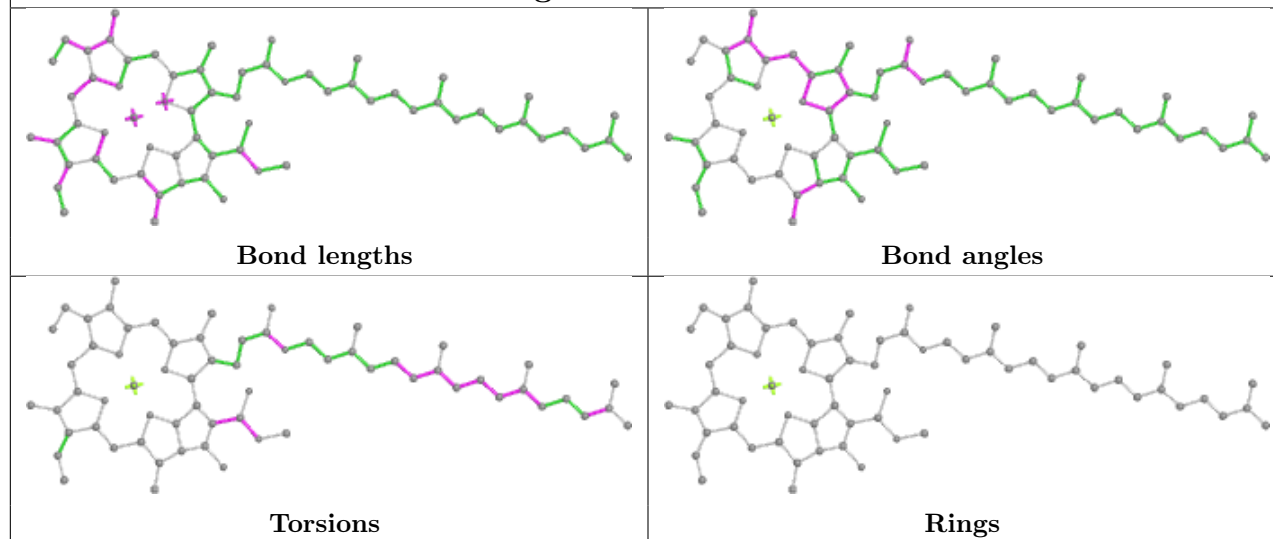
Ligand STE j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

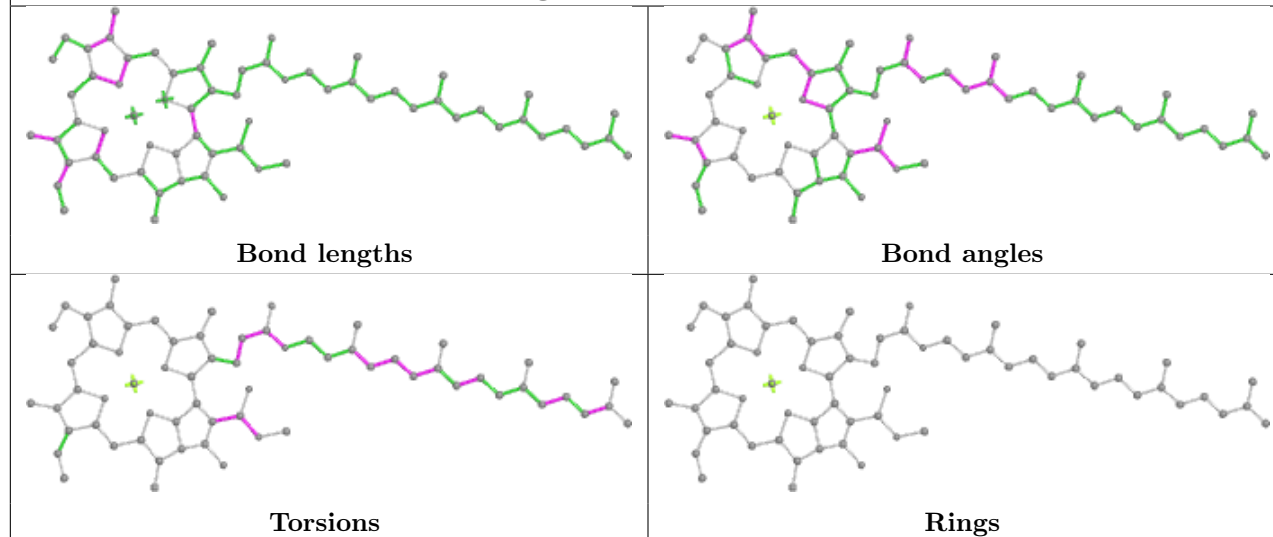




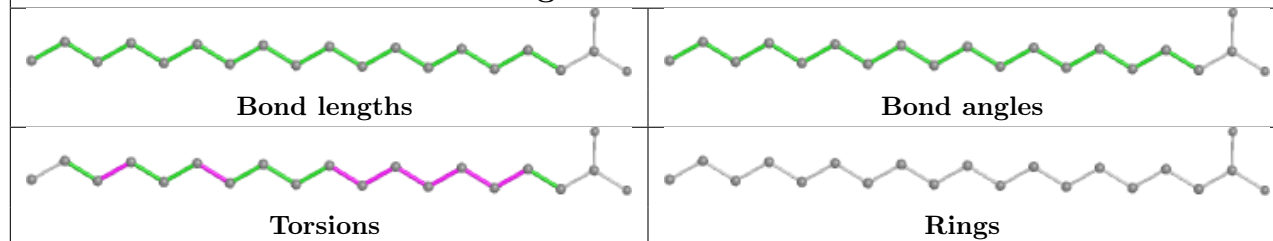
## Ligand CLA b 607

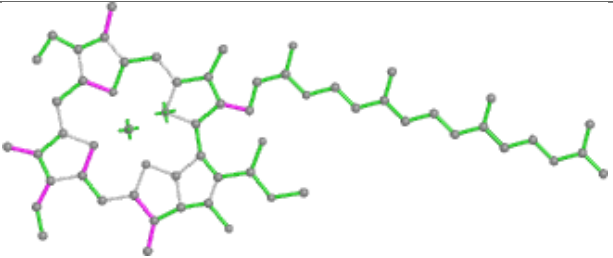
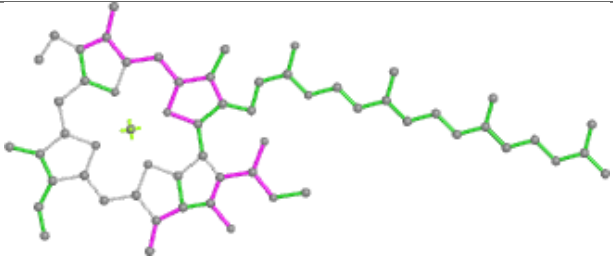
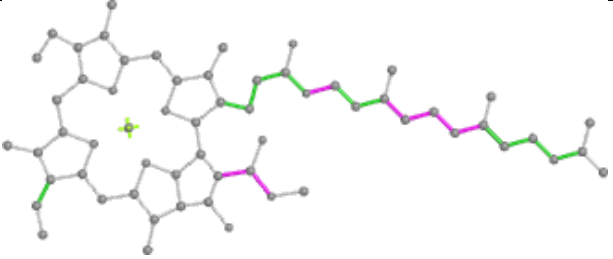
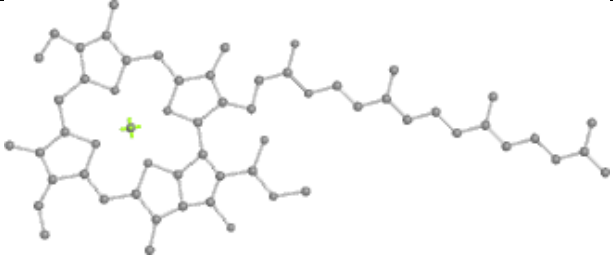




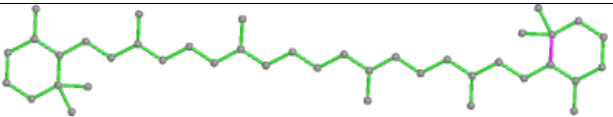
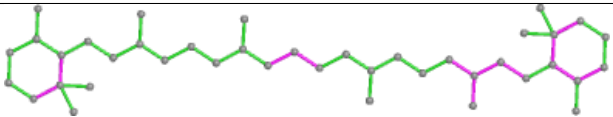
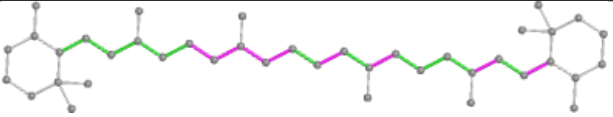
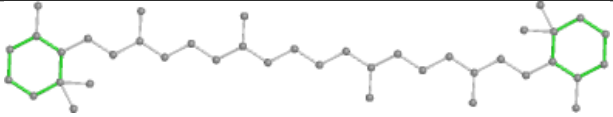


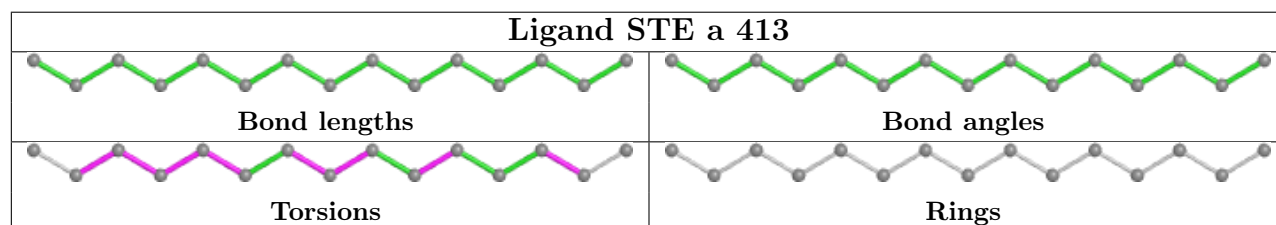
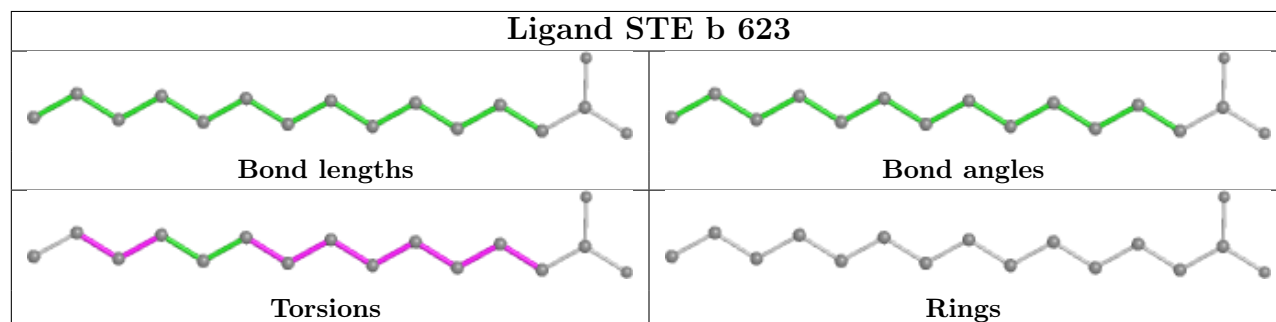
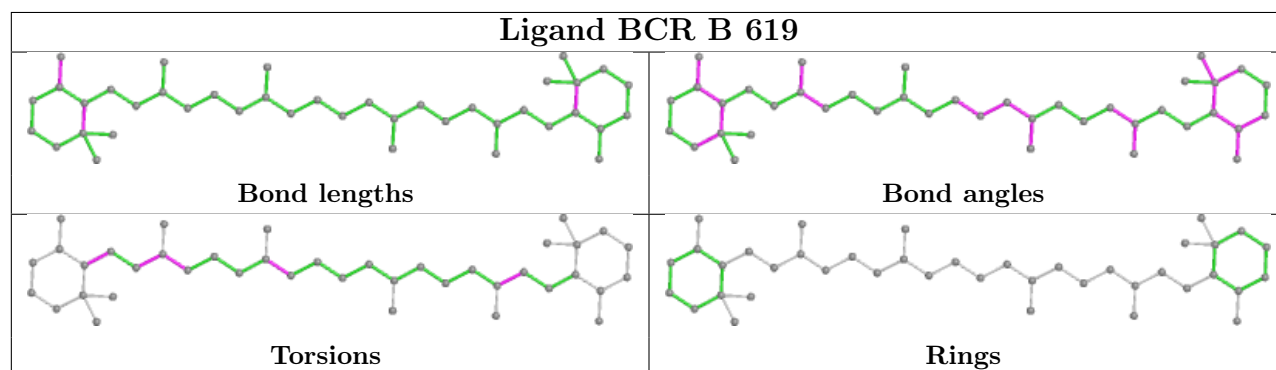
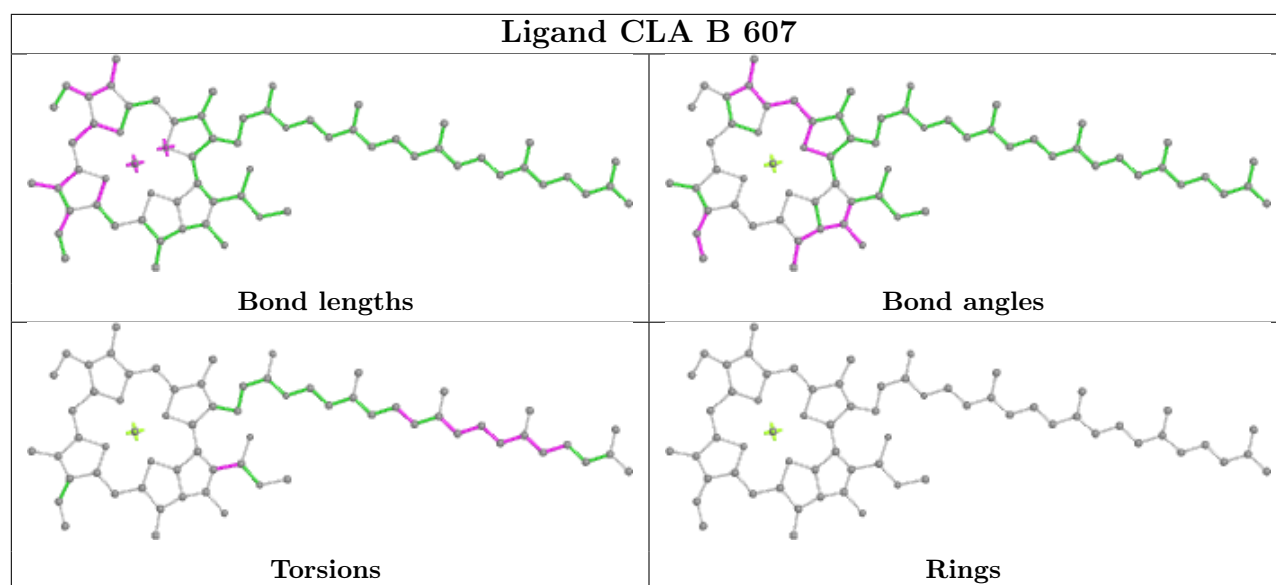
## Ligand CLA b 614

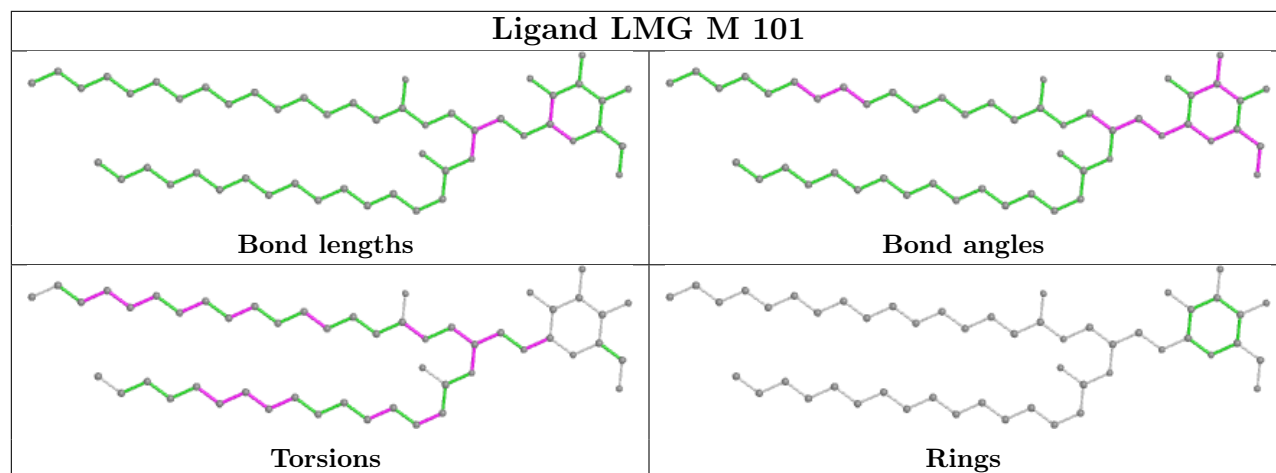
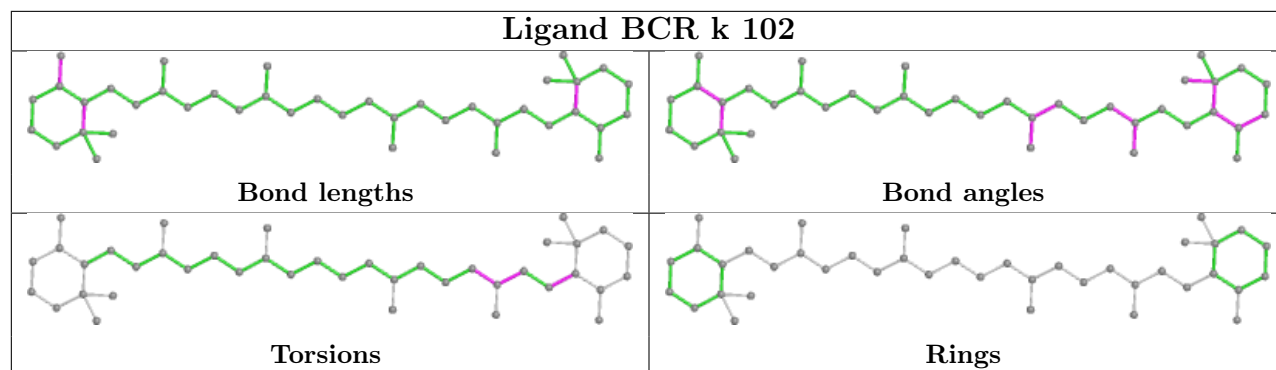


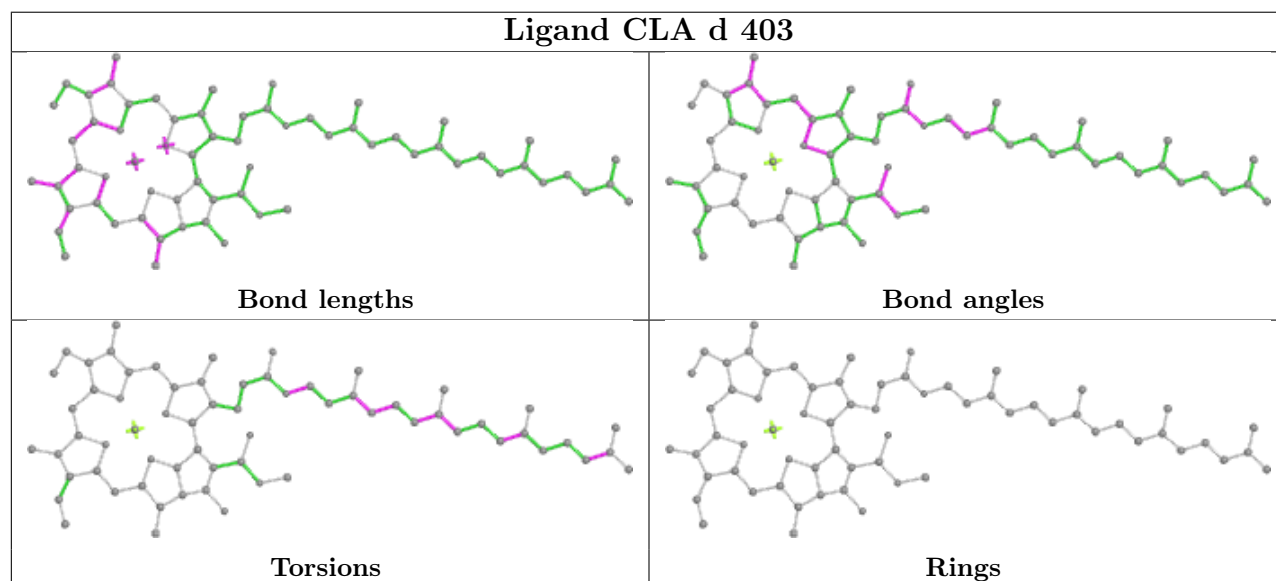
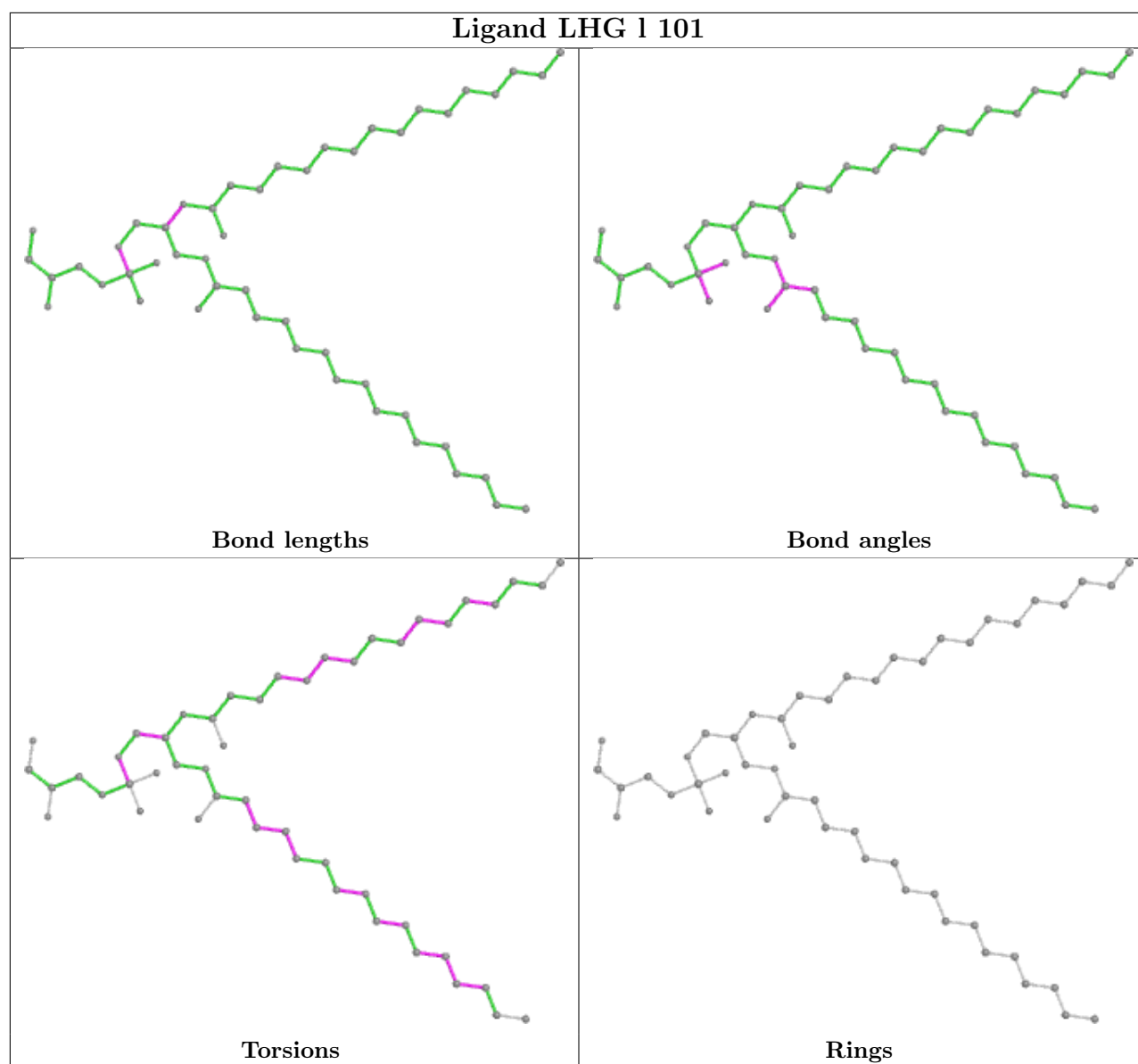
## Ligand STE b 621



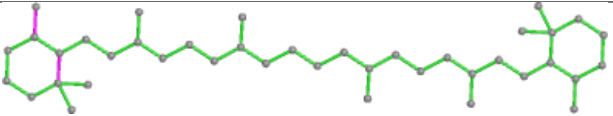
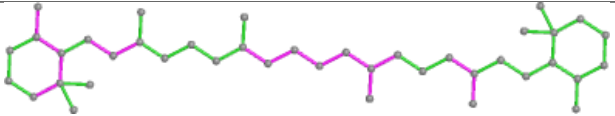
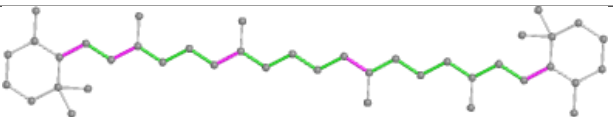
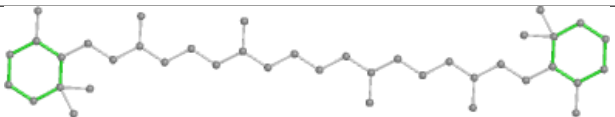
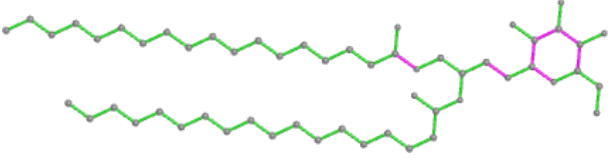
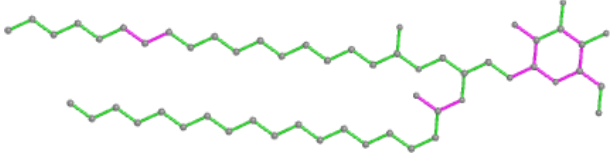
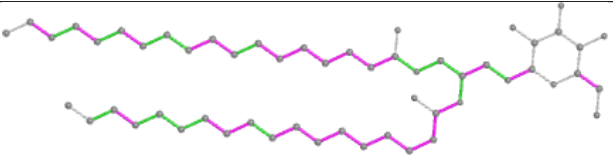
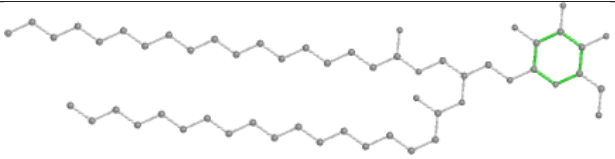


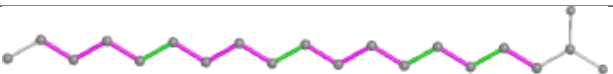
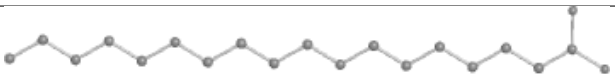
Ligand CLA B 616	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE b 627	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR H 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

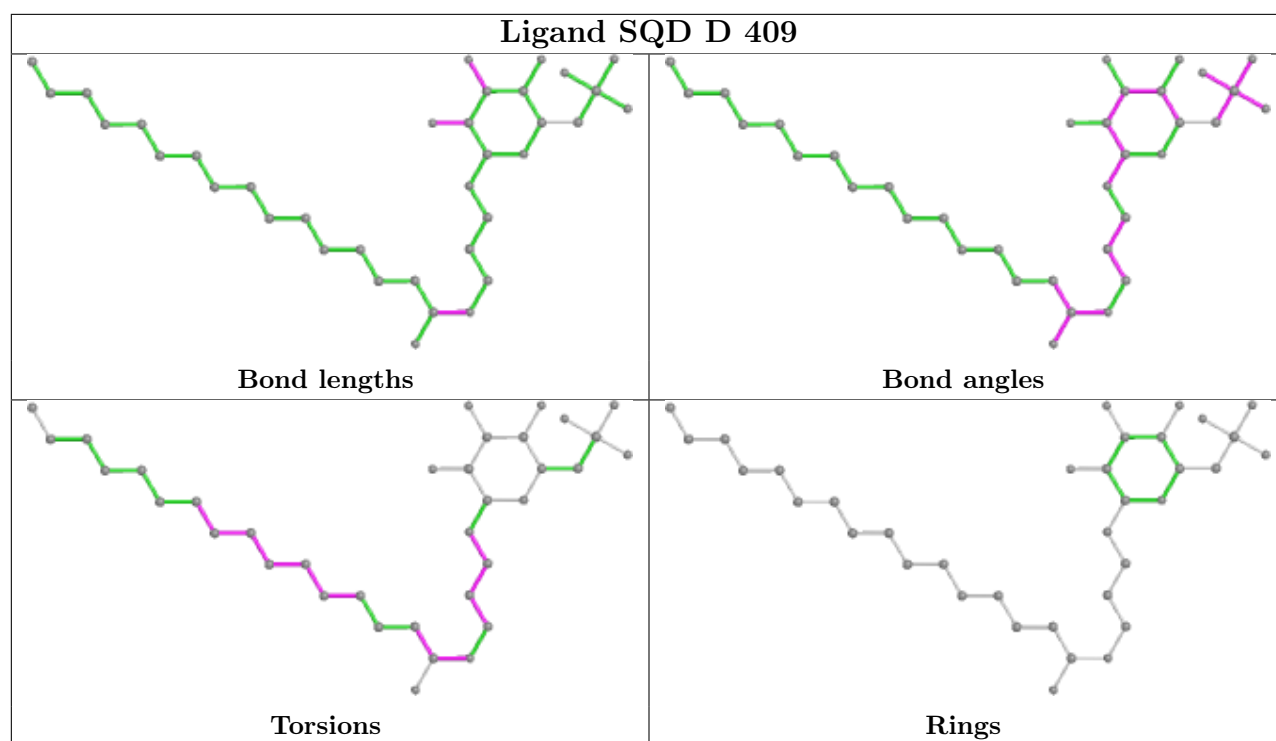


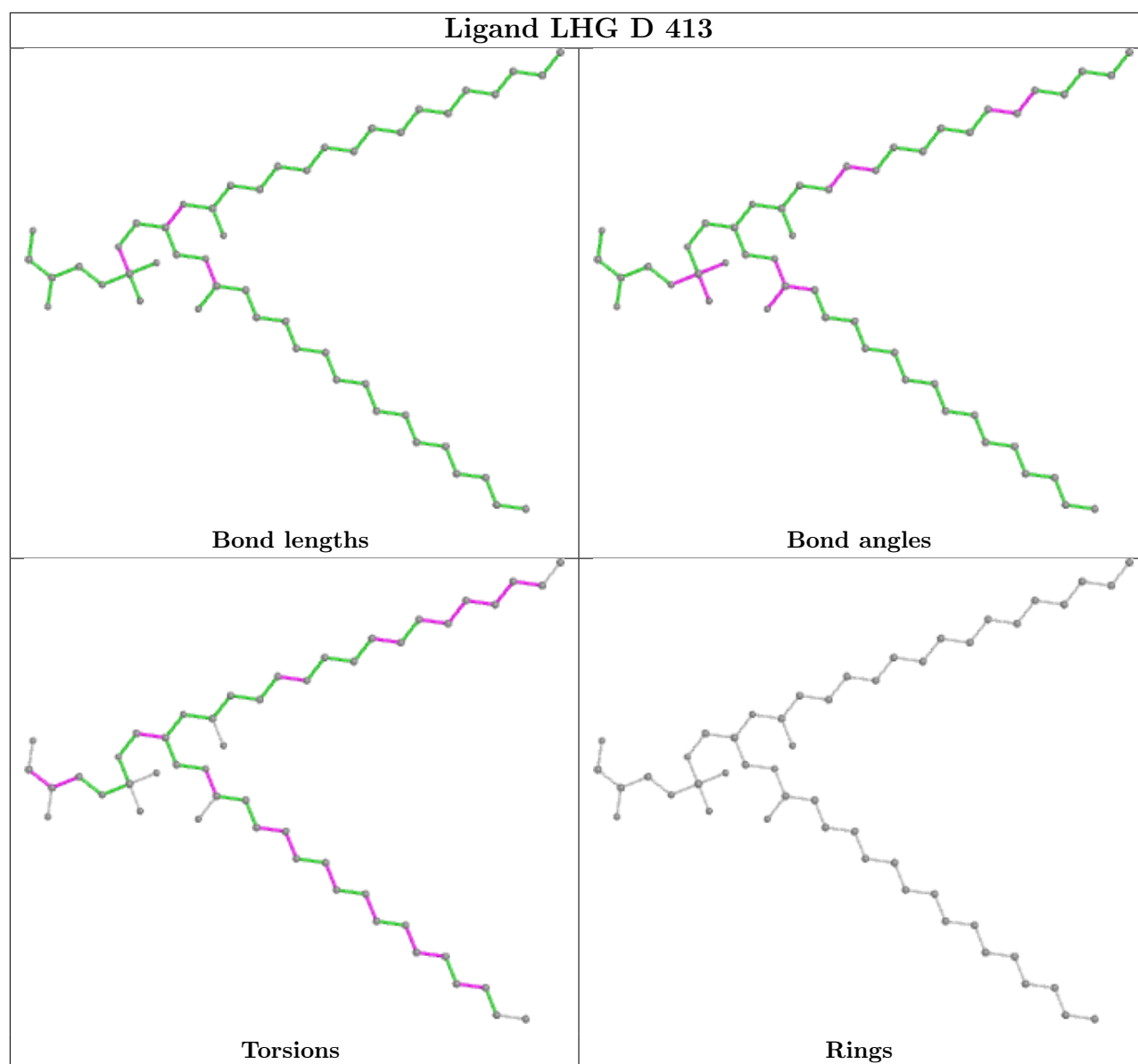


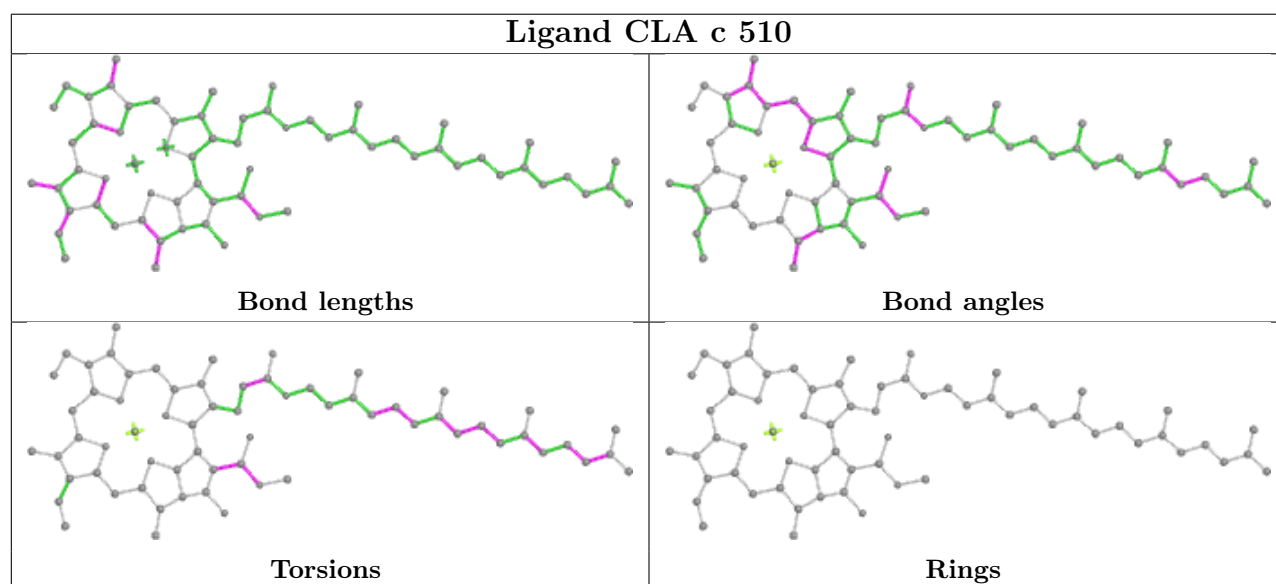
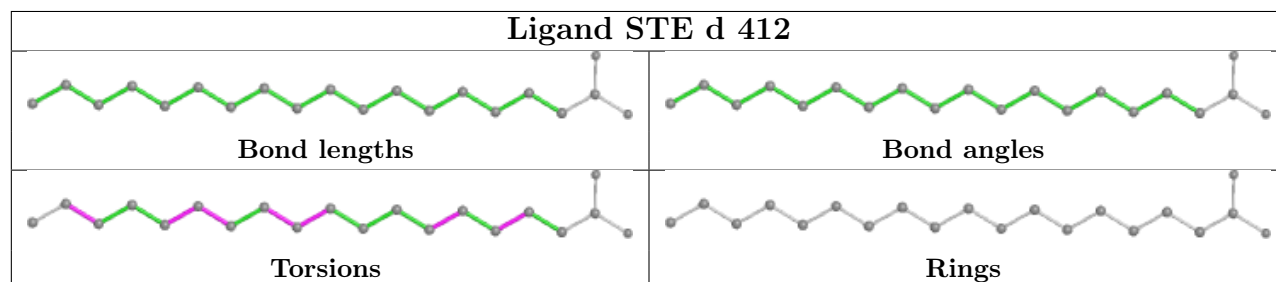
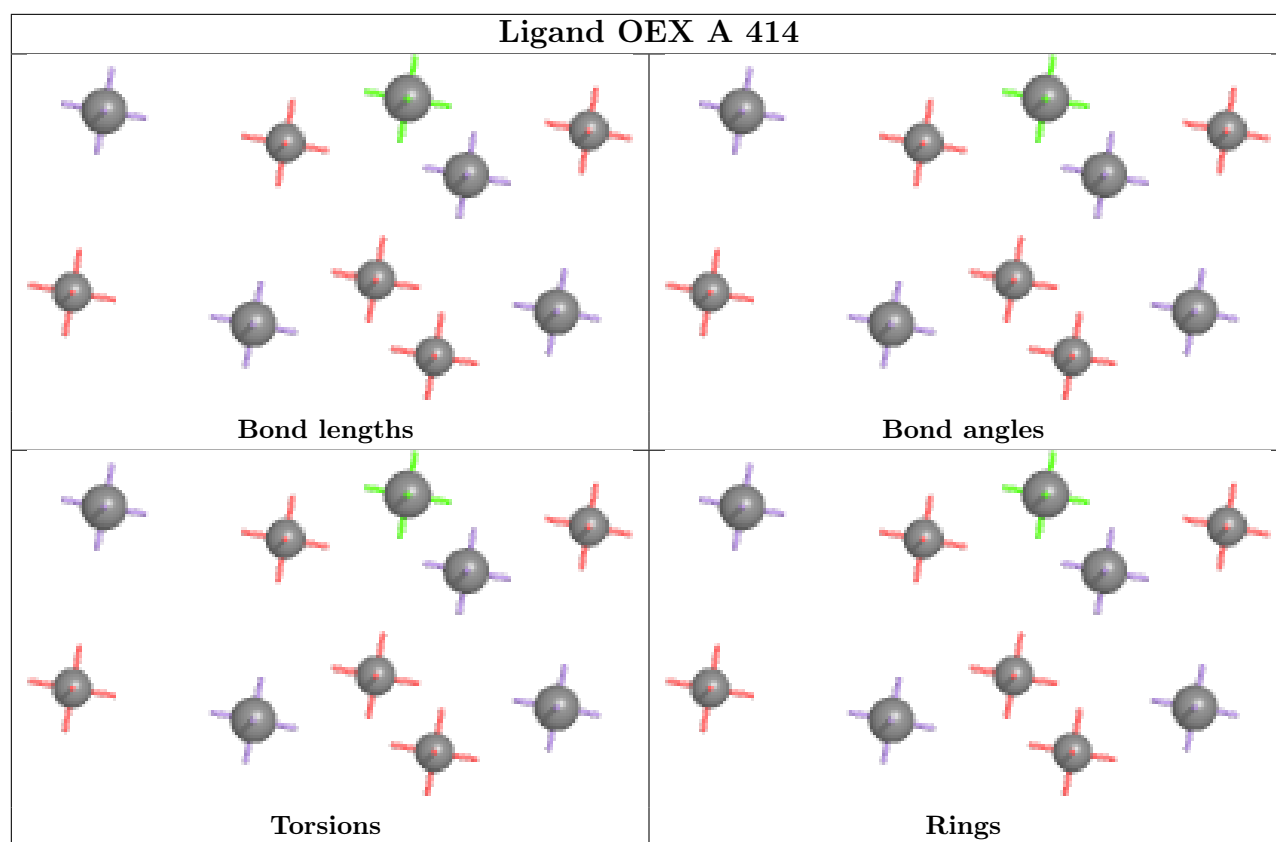




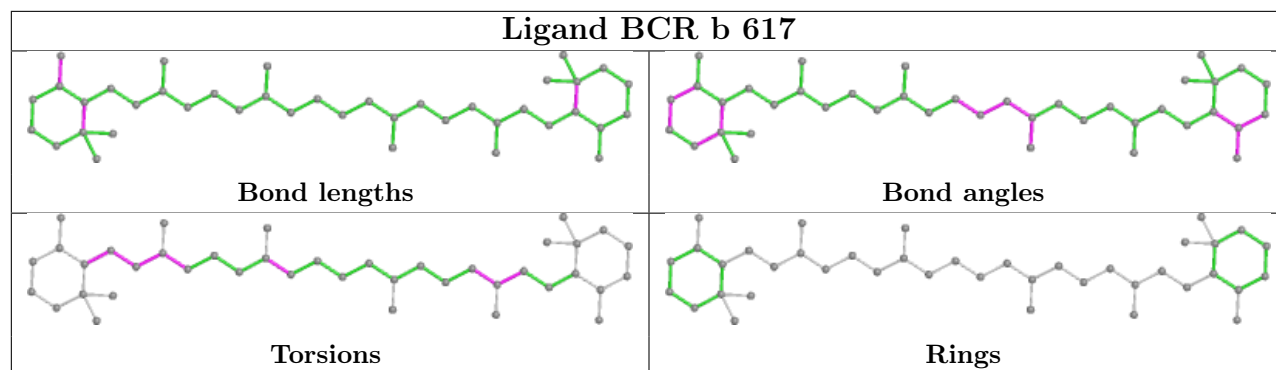
Ligand BCR C 514	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG b 622	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE X 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



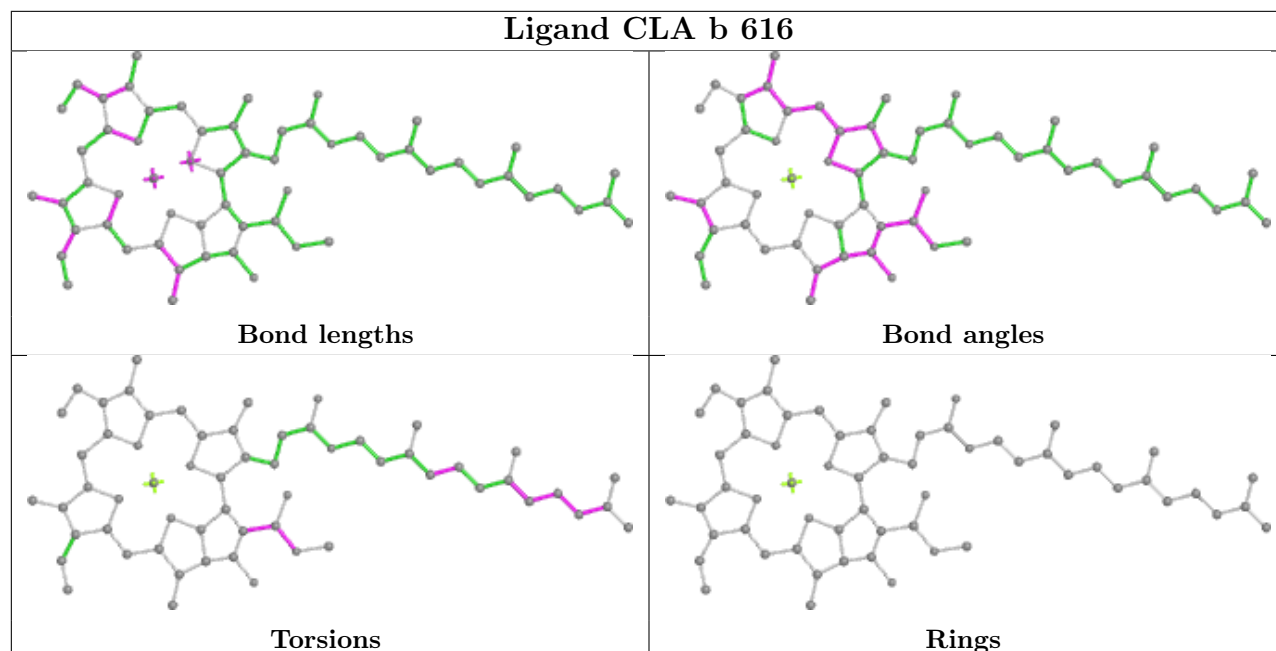




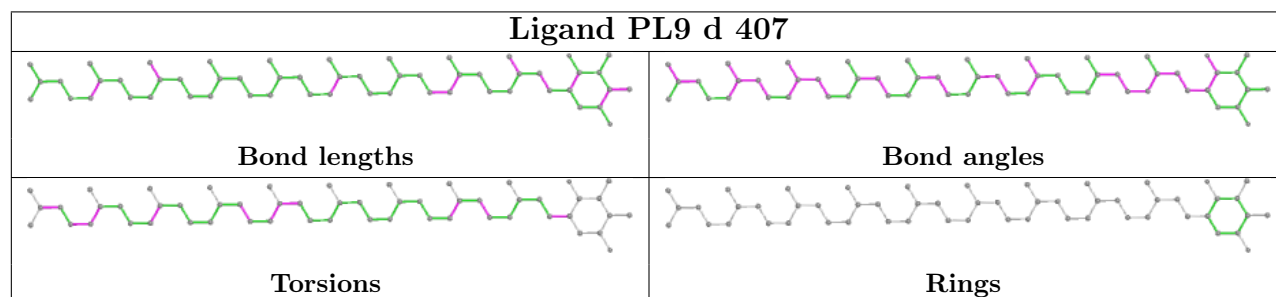
## Ligand BCR b 617



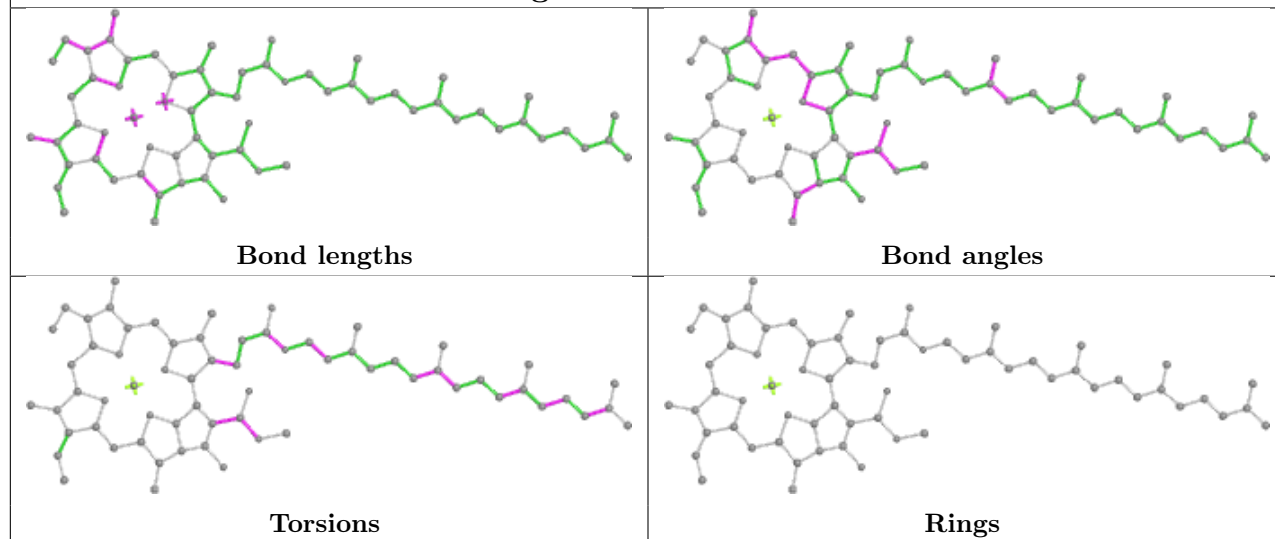
## Ligand CLA b 616



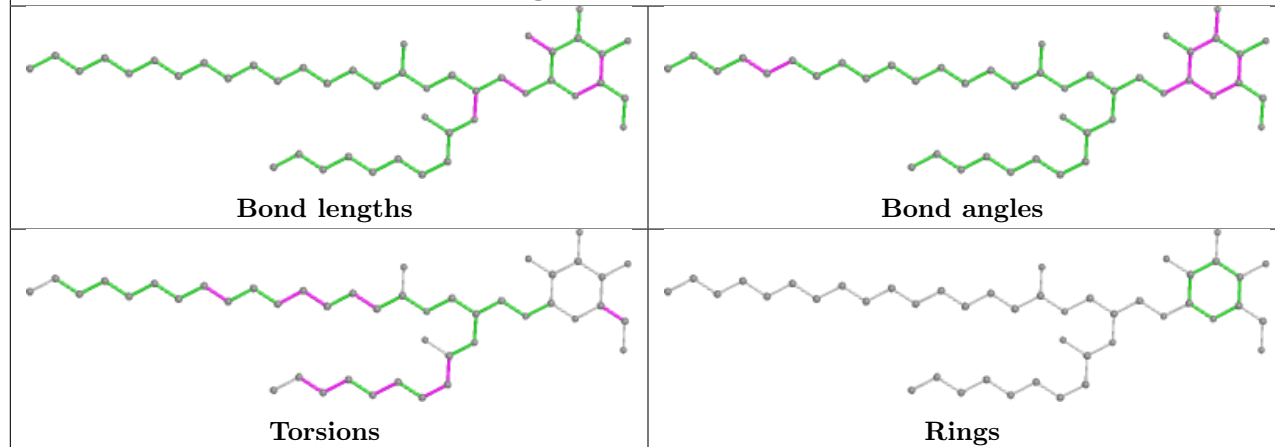
## Ligand PL9 d 407



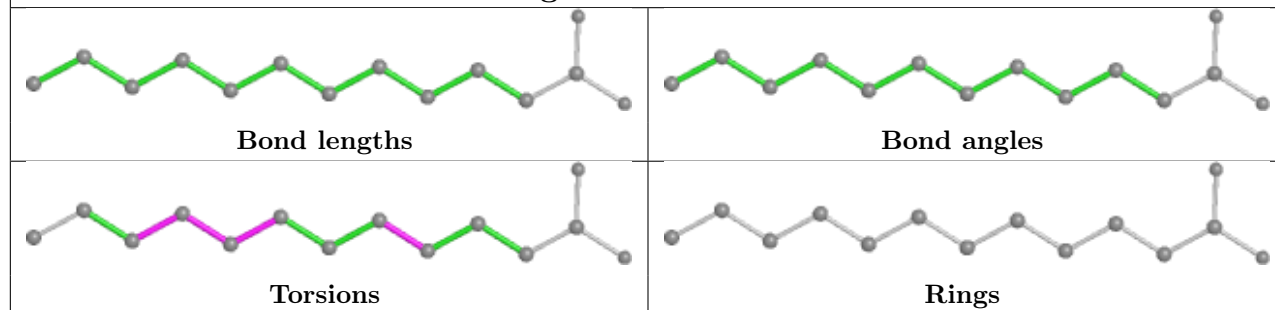
## Ligand CLA B 601

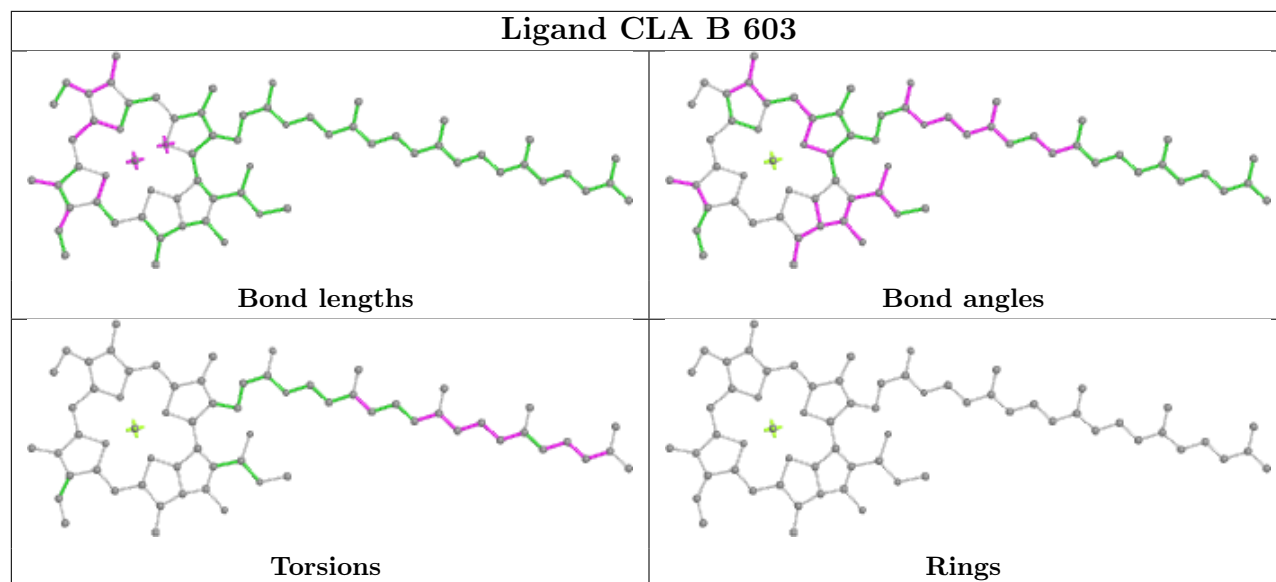
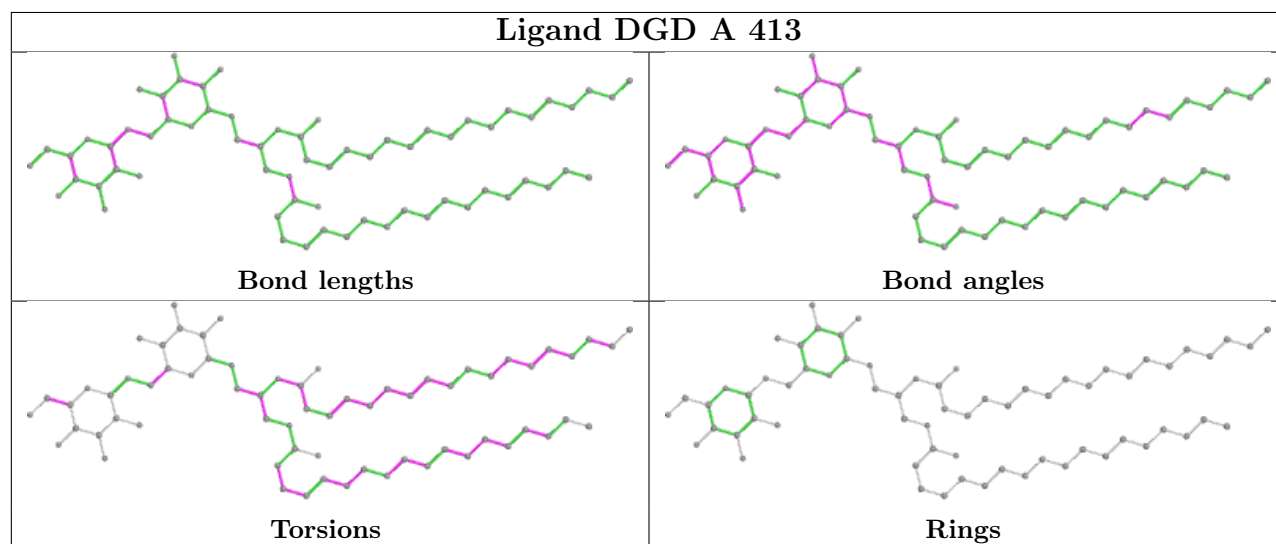


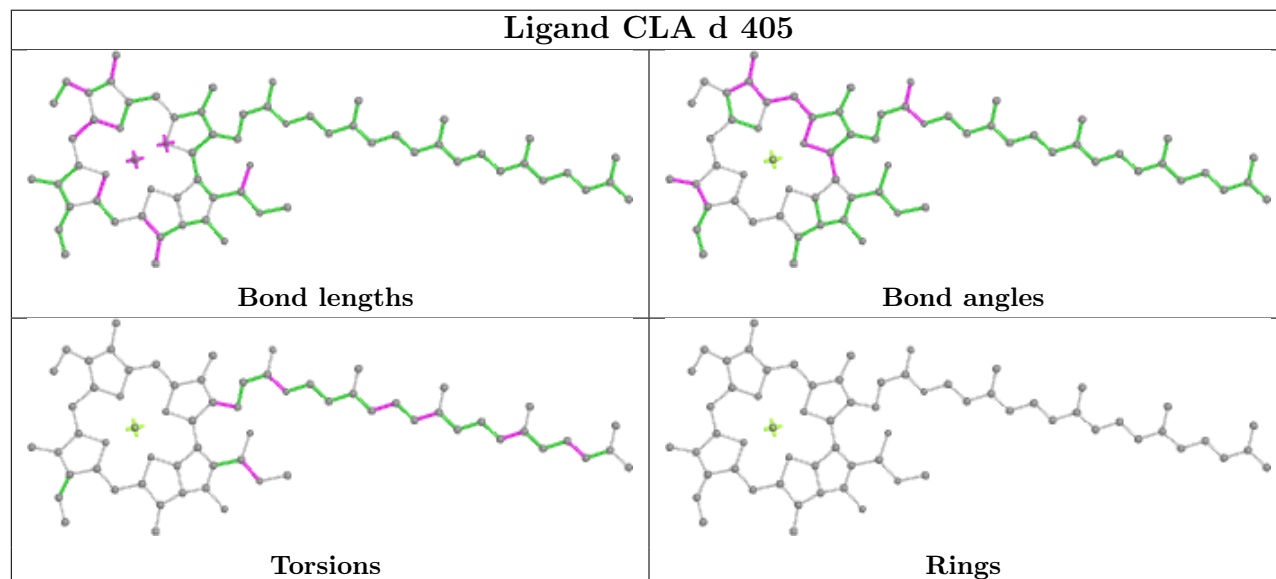
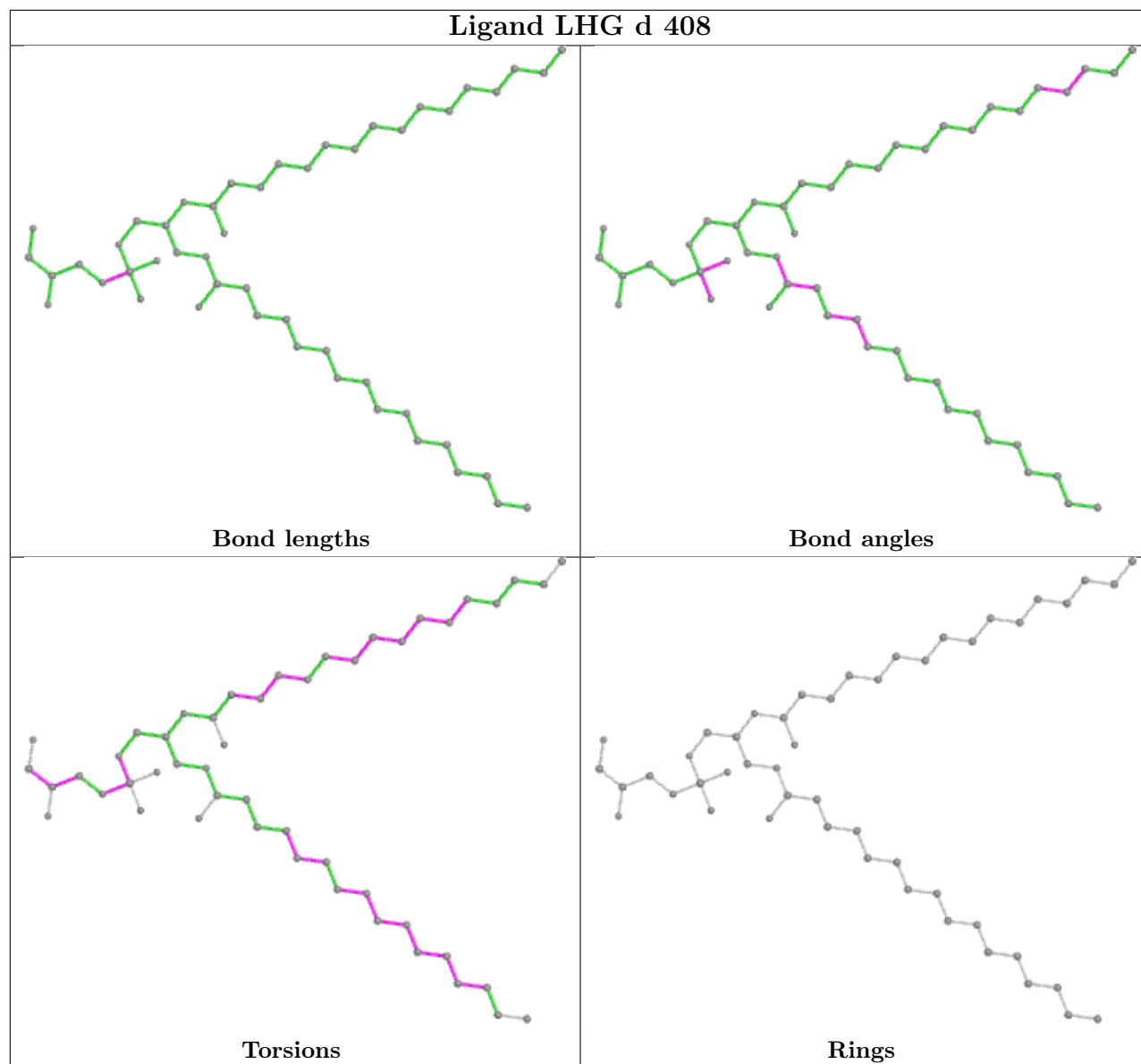
## Ligand LMG d 410



## Ligand STE t 103

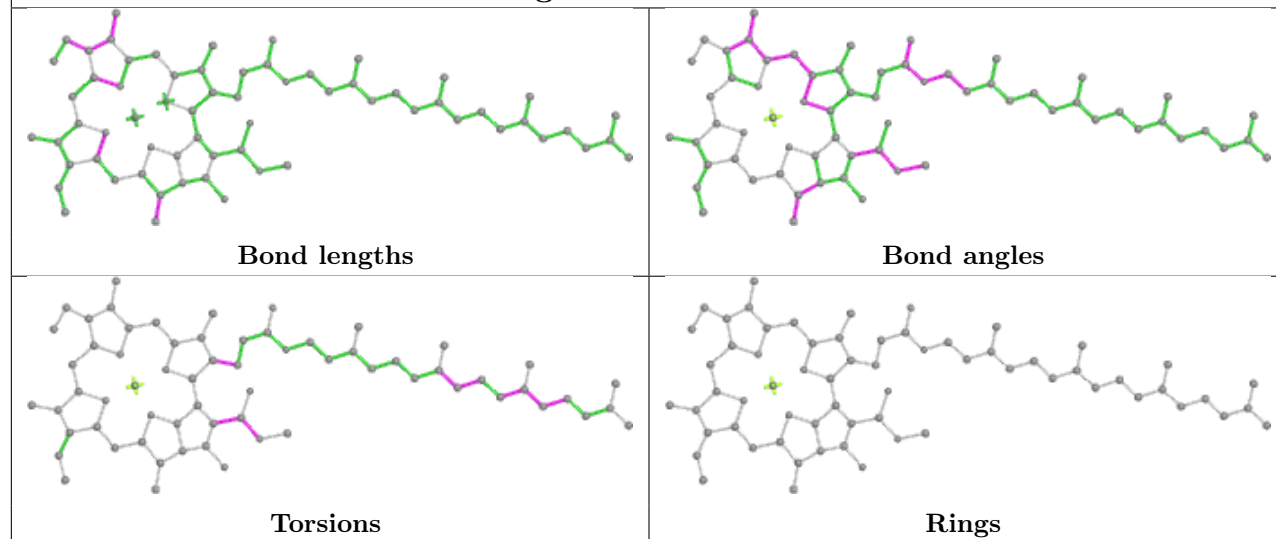


**Ligand CLA B 603****Ligand DGD A 413**

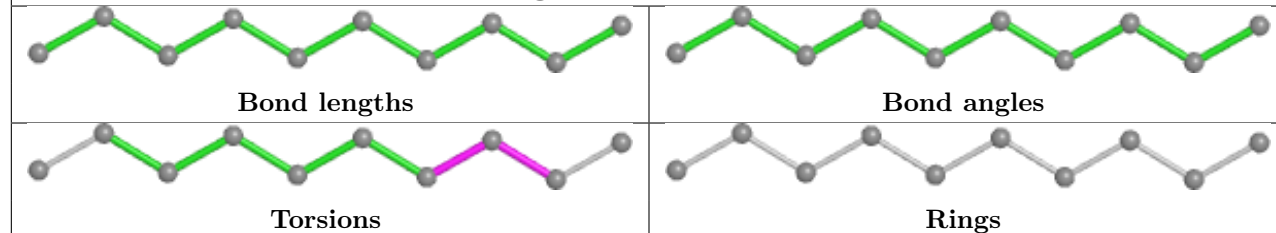




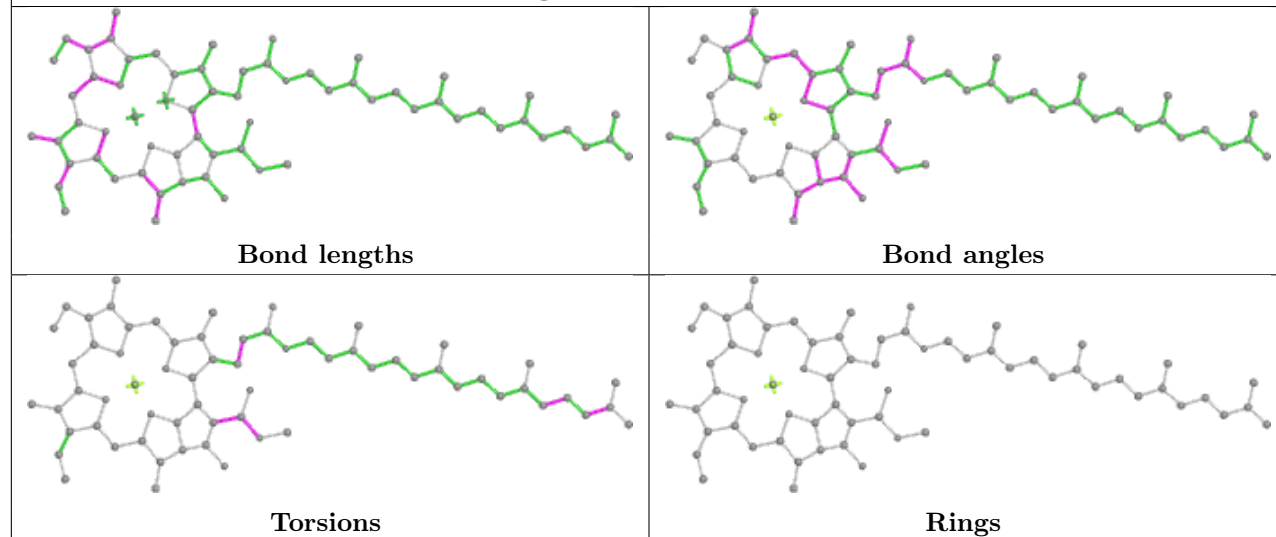
## Ligand CLA d 401

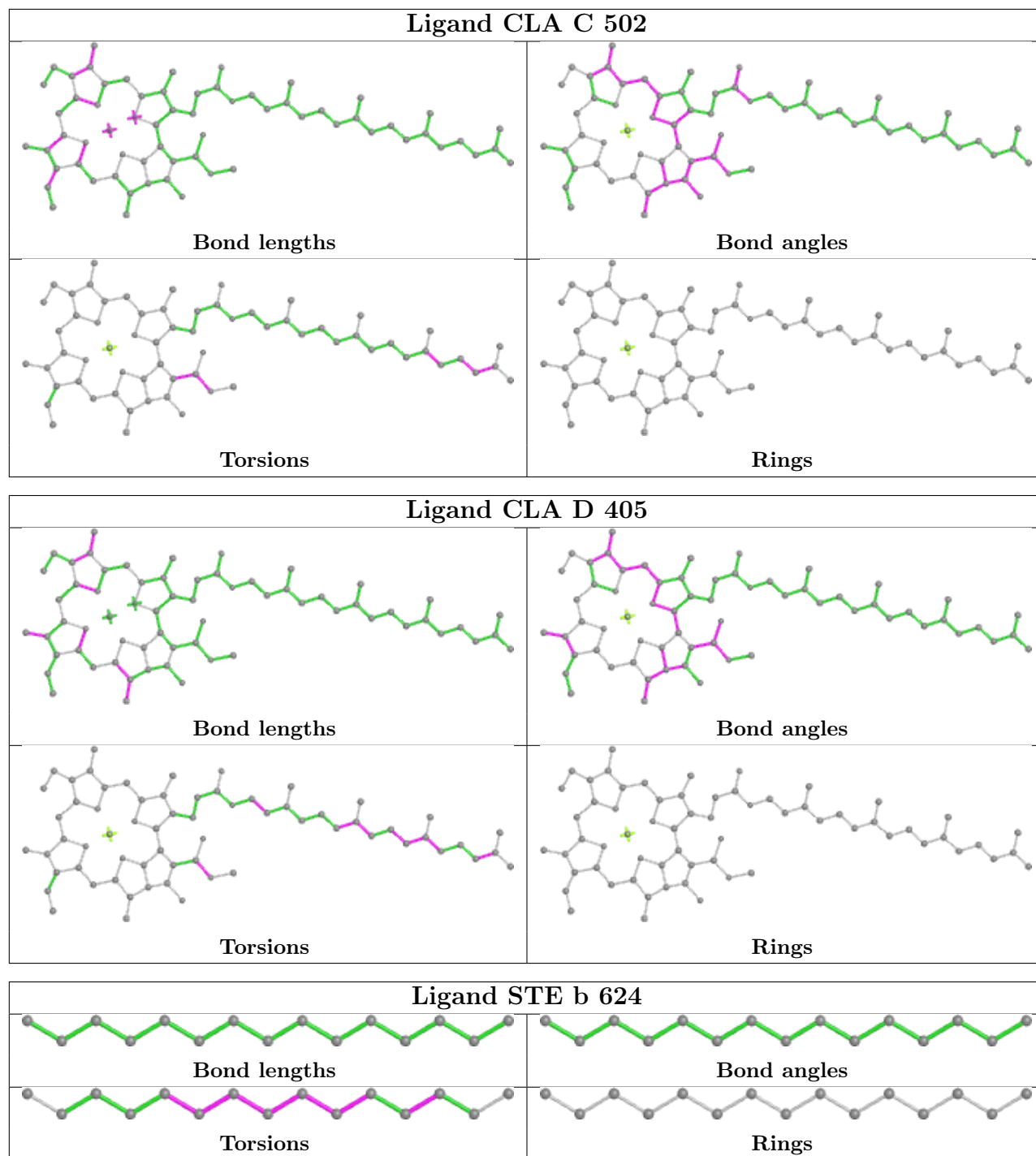


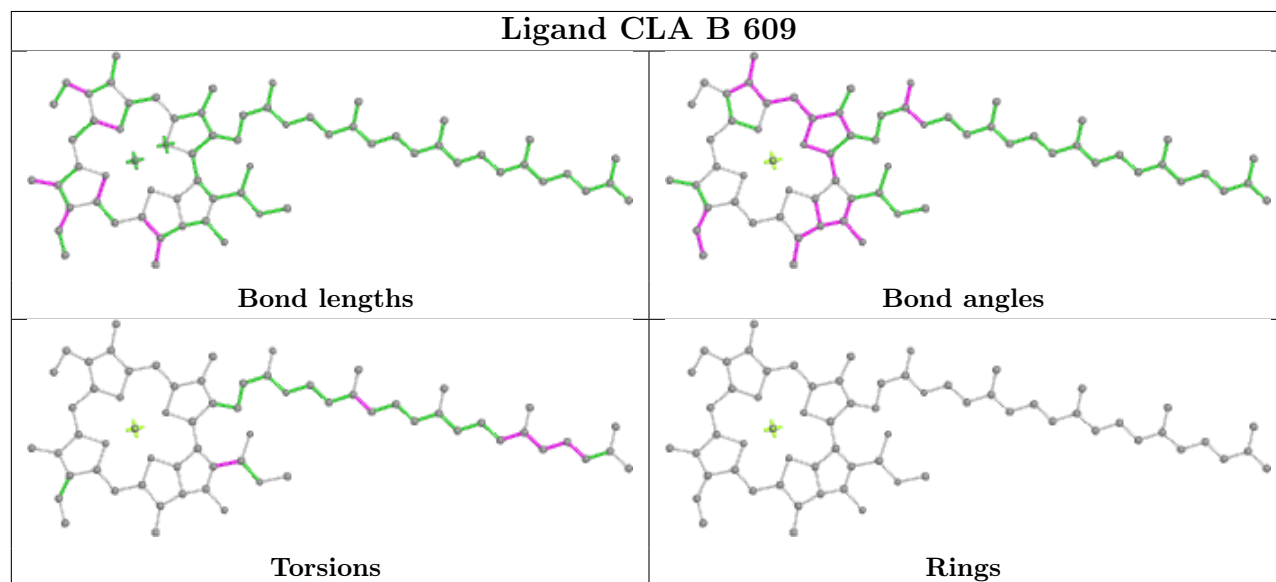
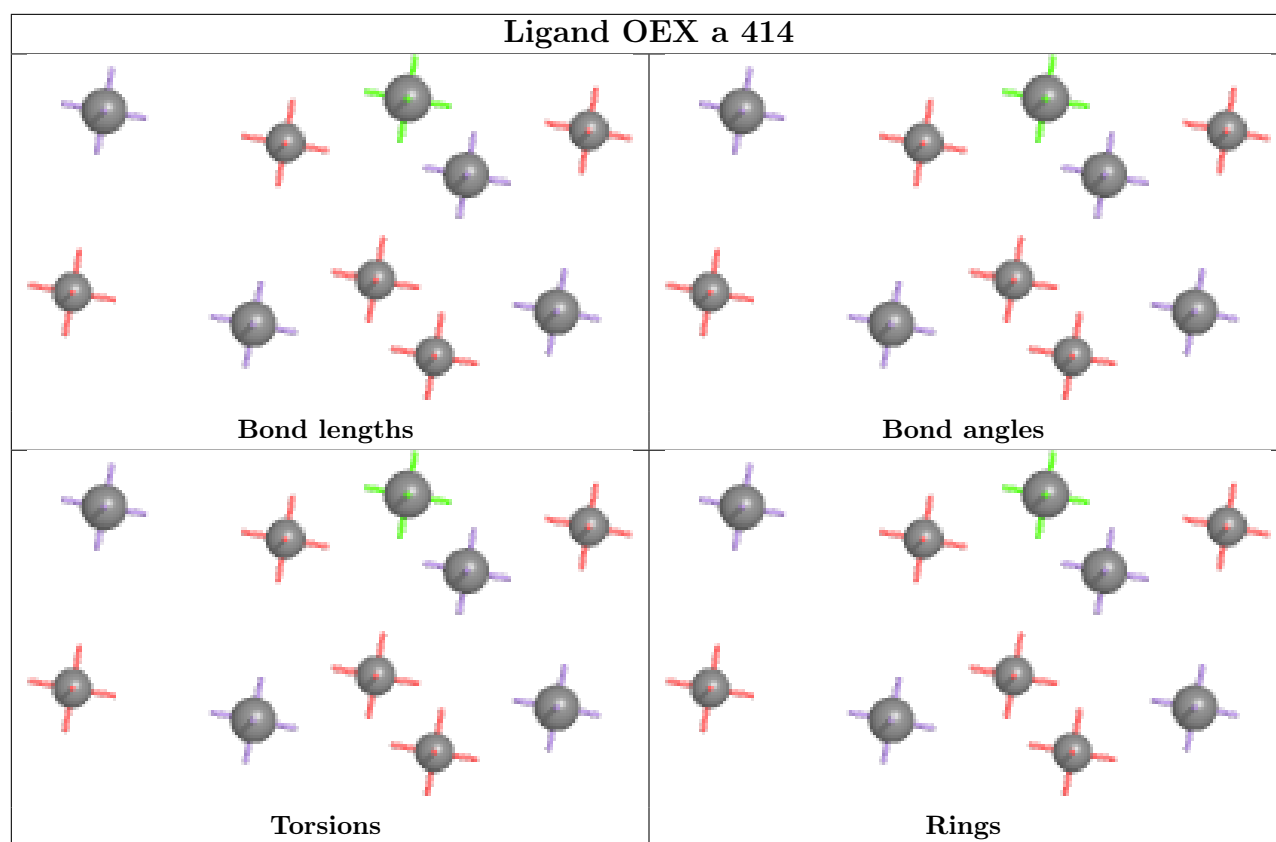
## Ligand STE M 103

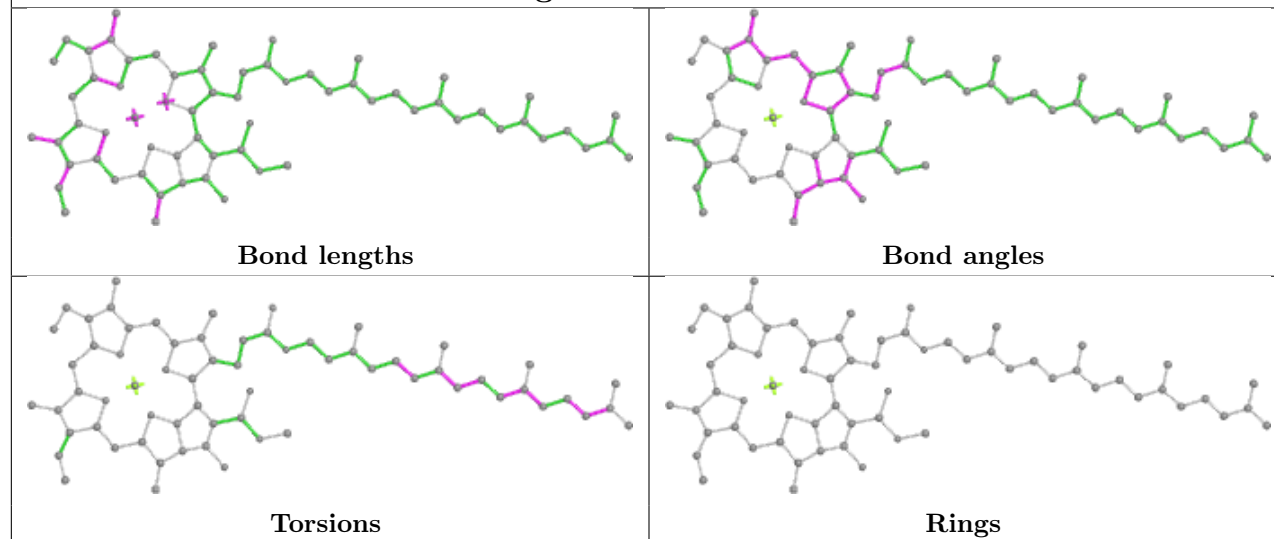
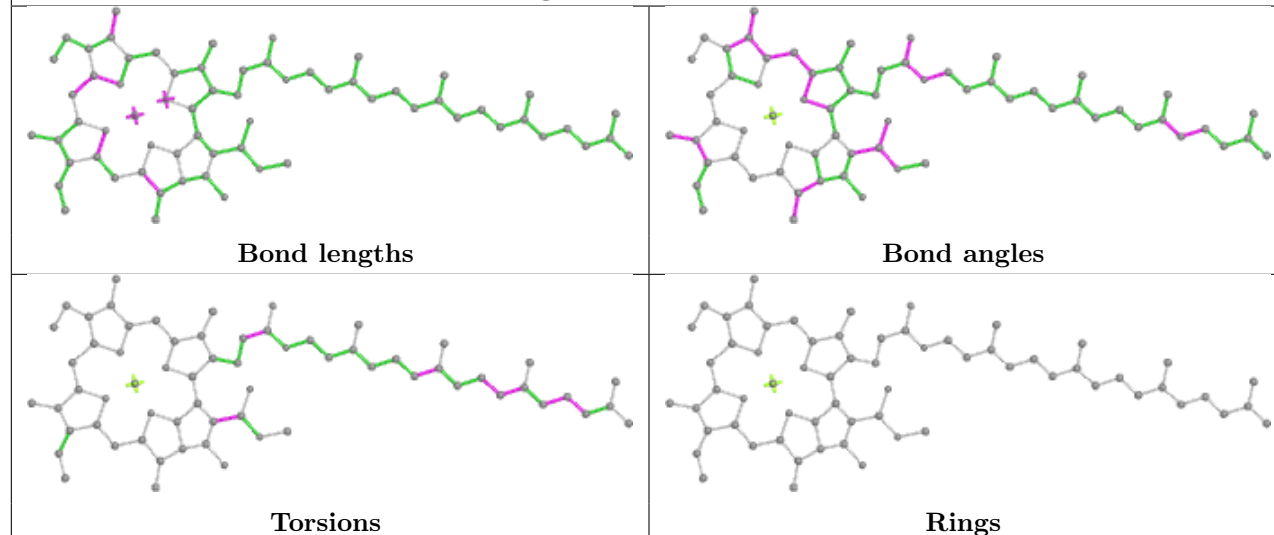
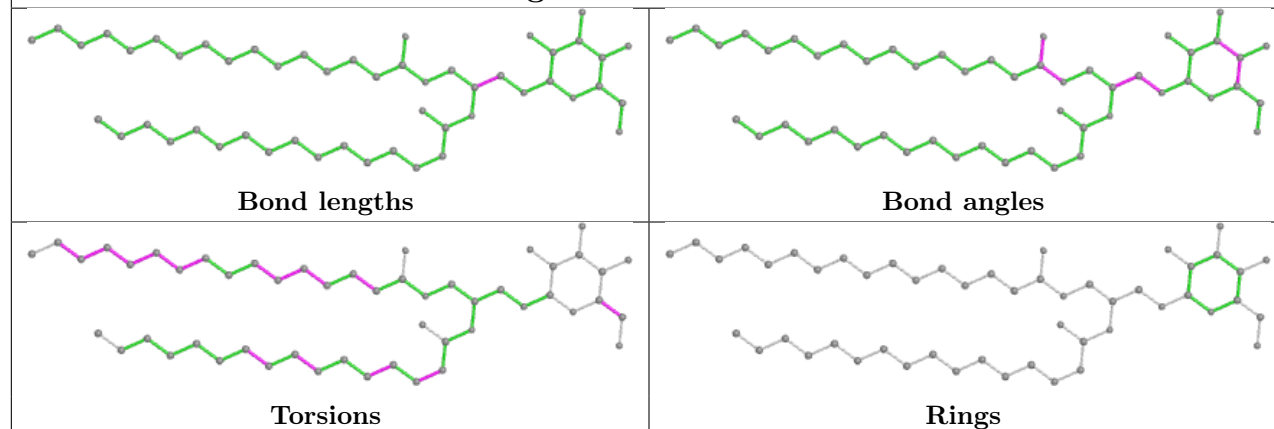


## Ligand CLA b 610

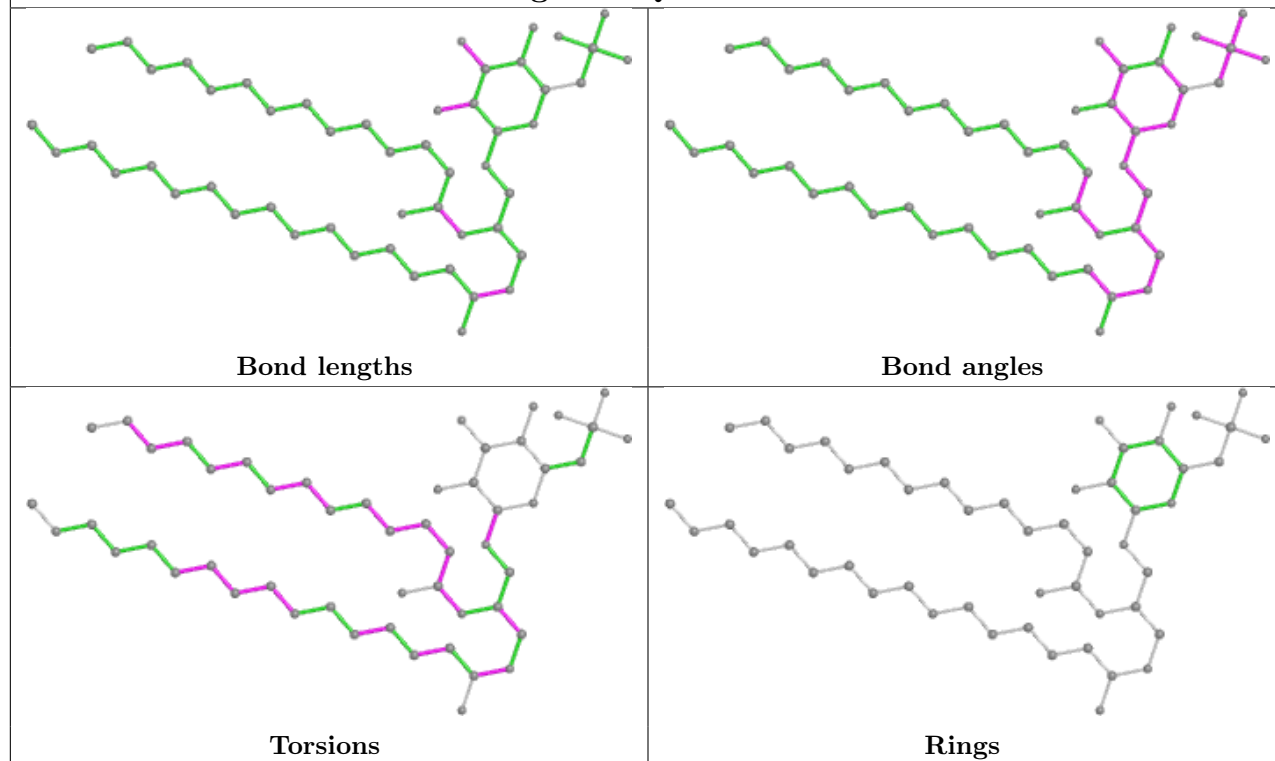




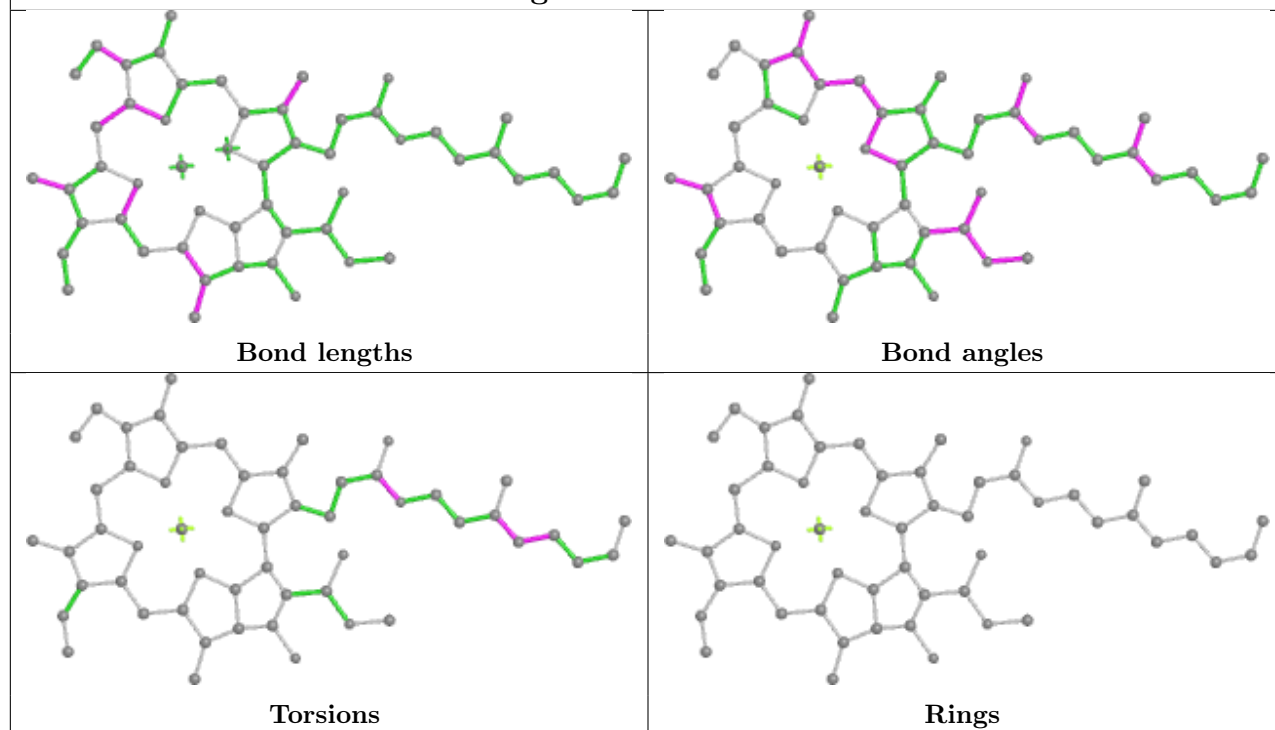


**Ligand CLA b 615****Ligand CLA c 509****Ligand LMG D 408**

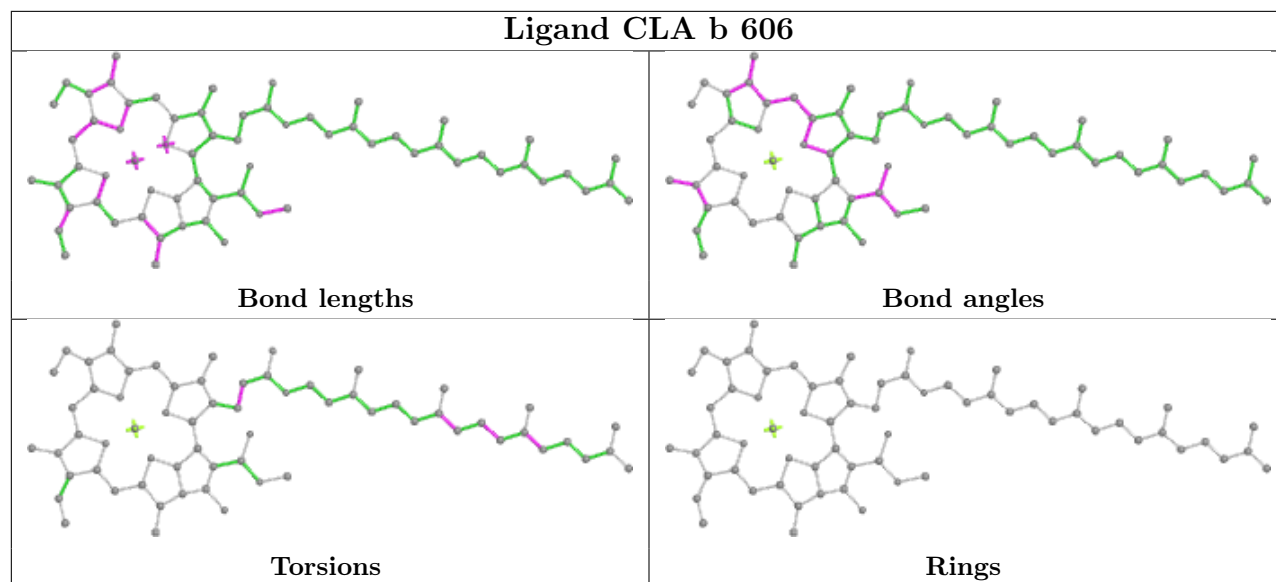
## Ligand SQD A 410



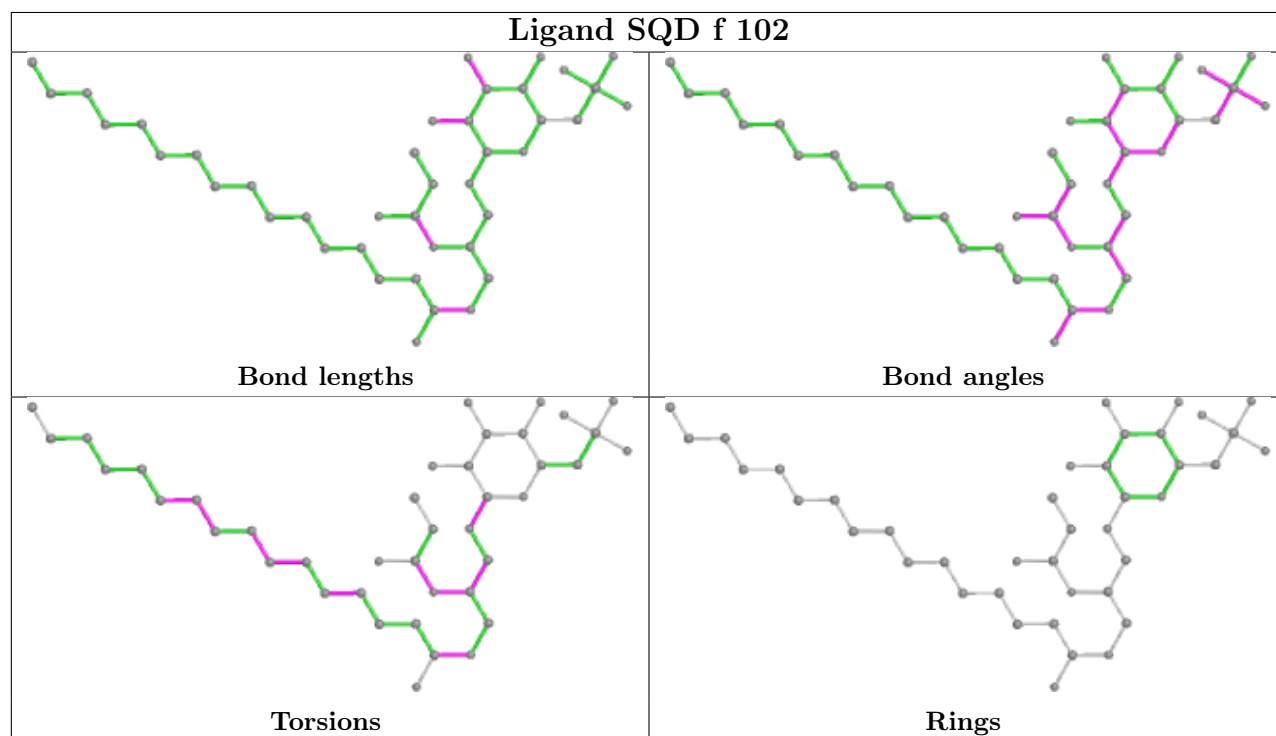
## Ligand CLA A 405



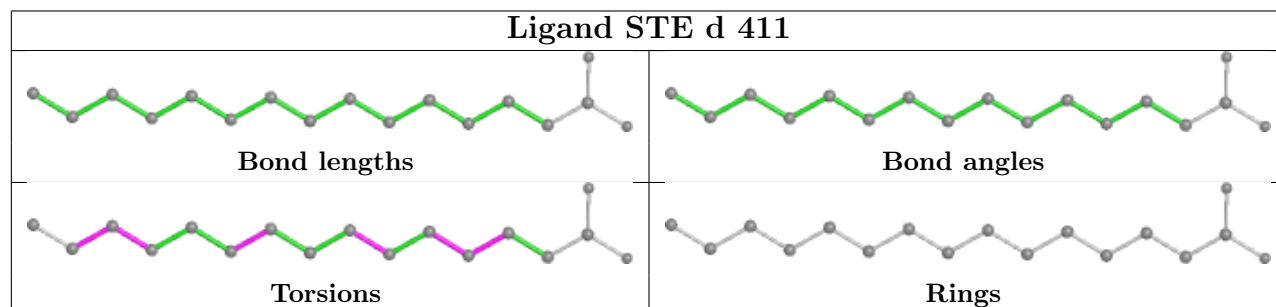
## Ligand CLA b 606

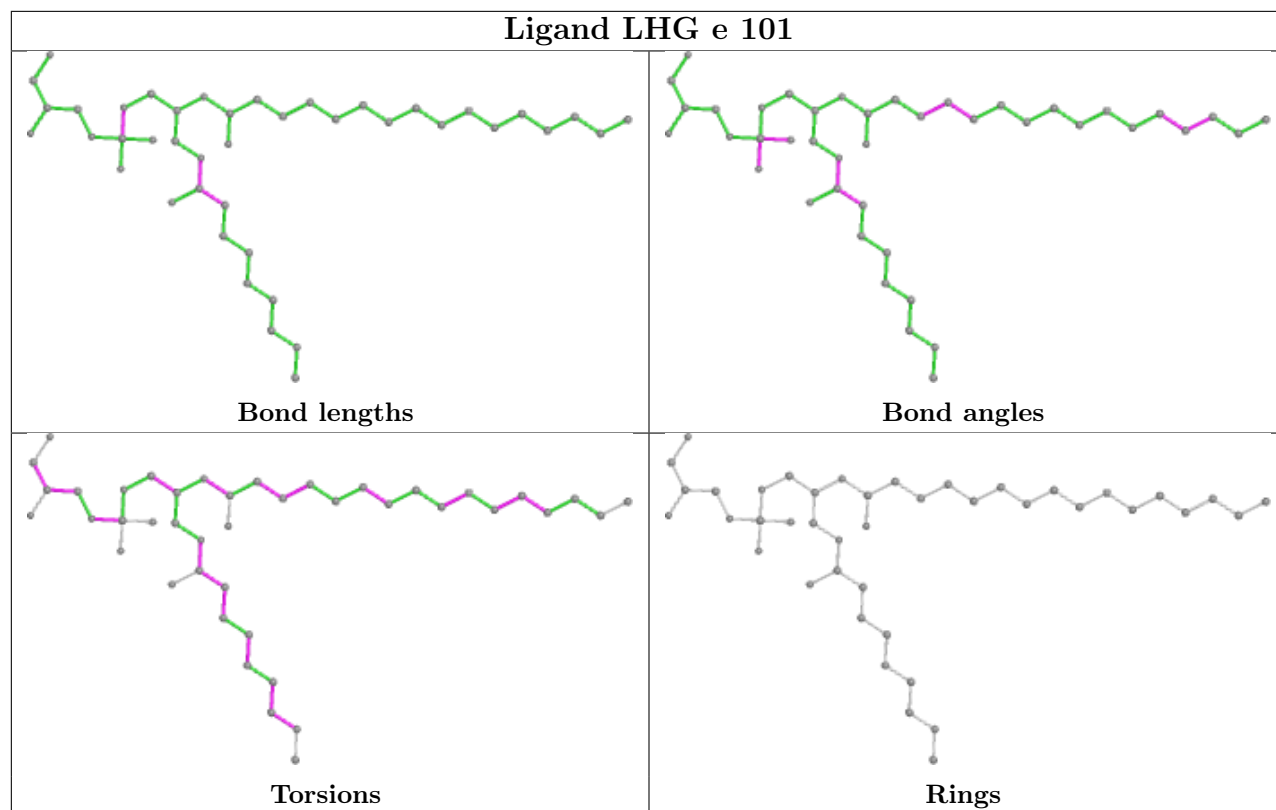


## Ligand SQD f 102

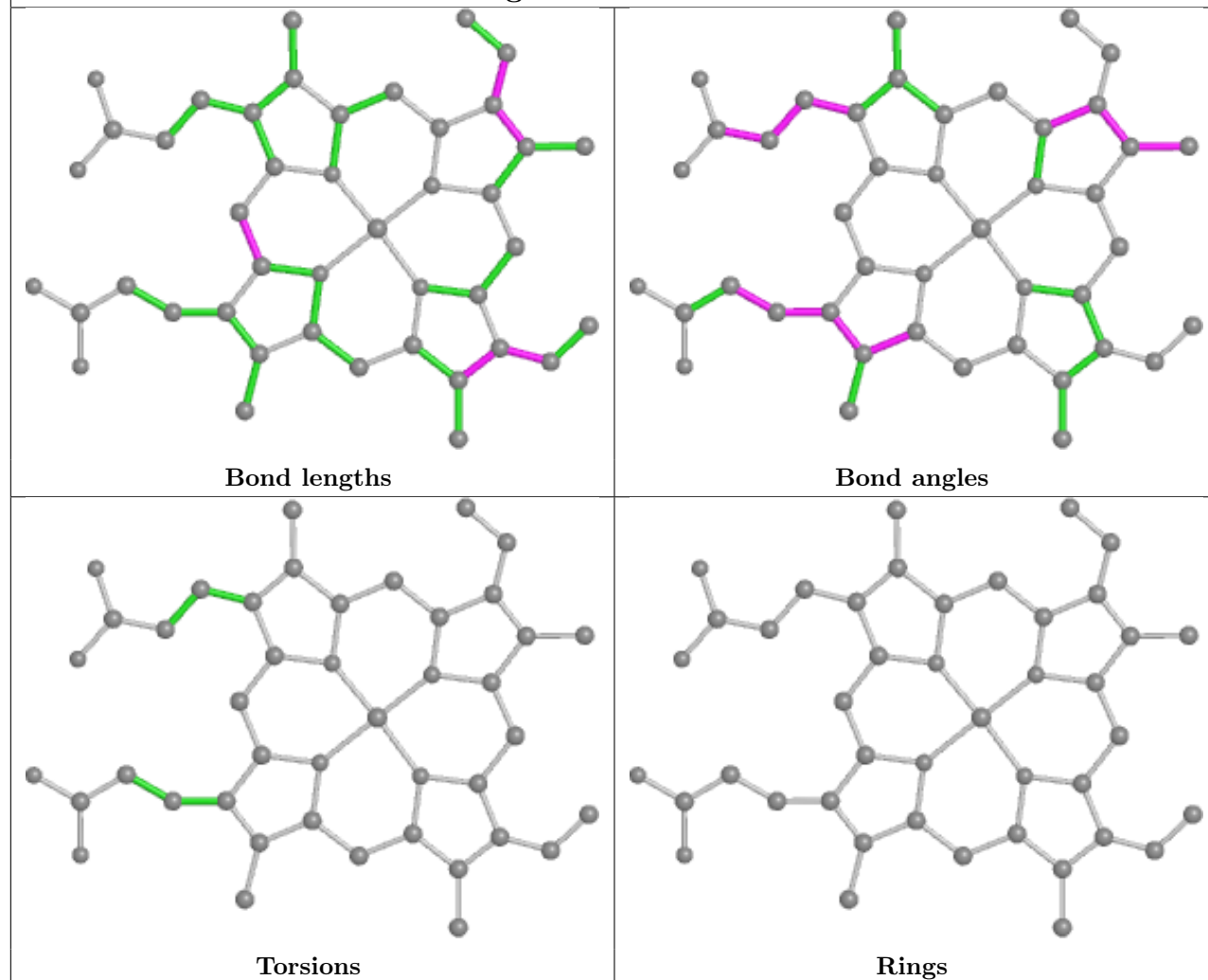


## Ligand STE d 411

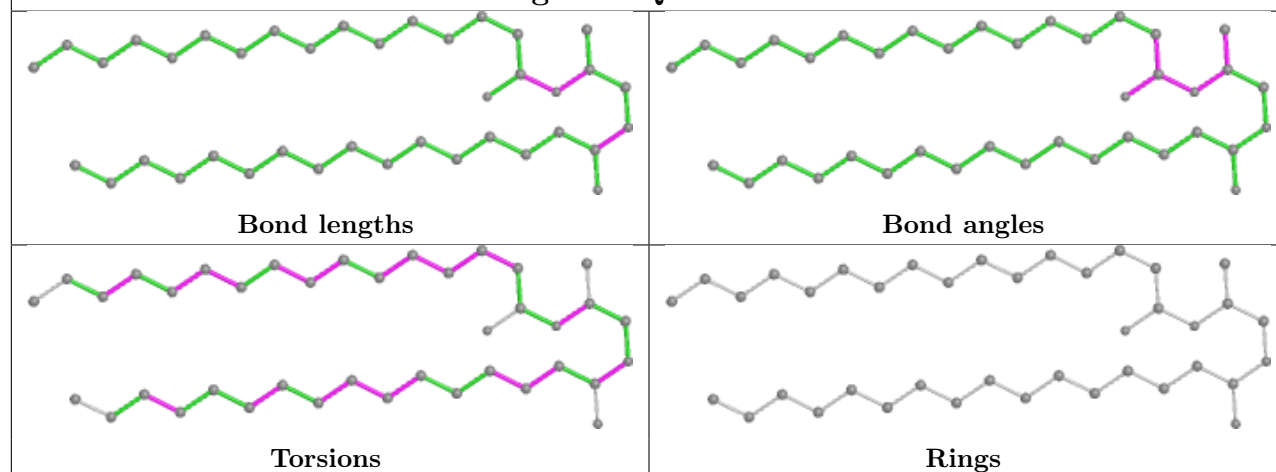




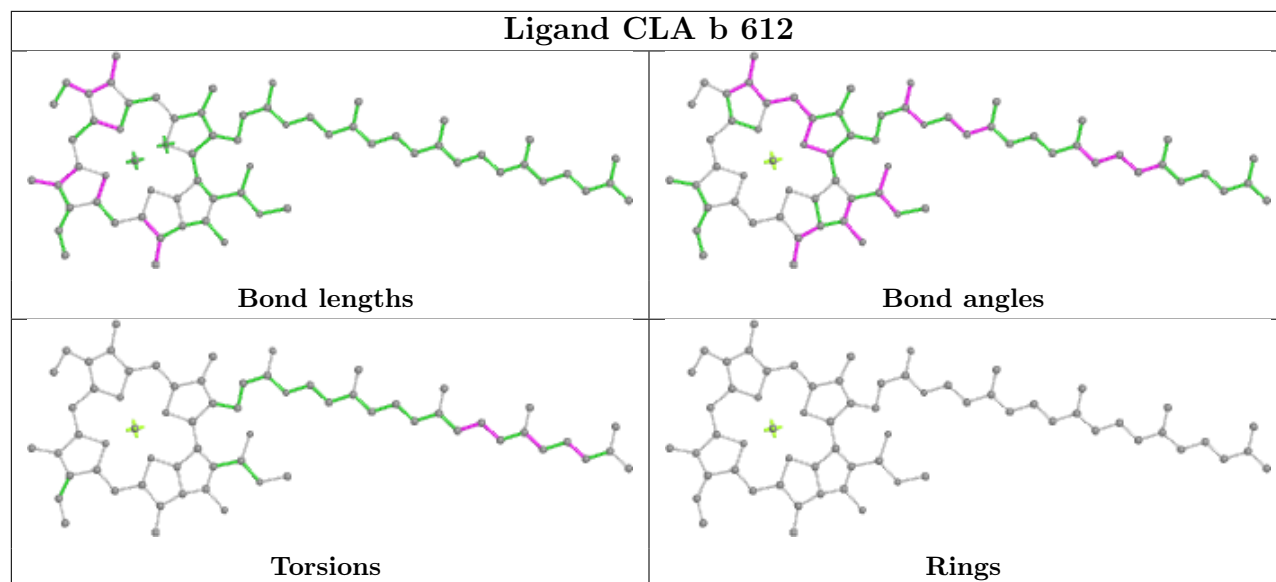
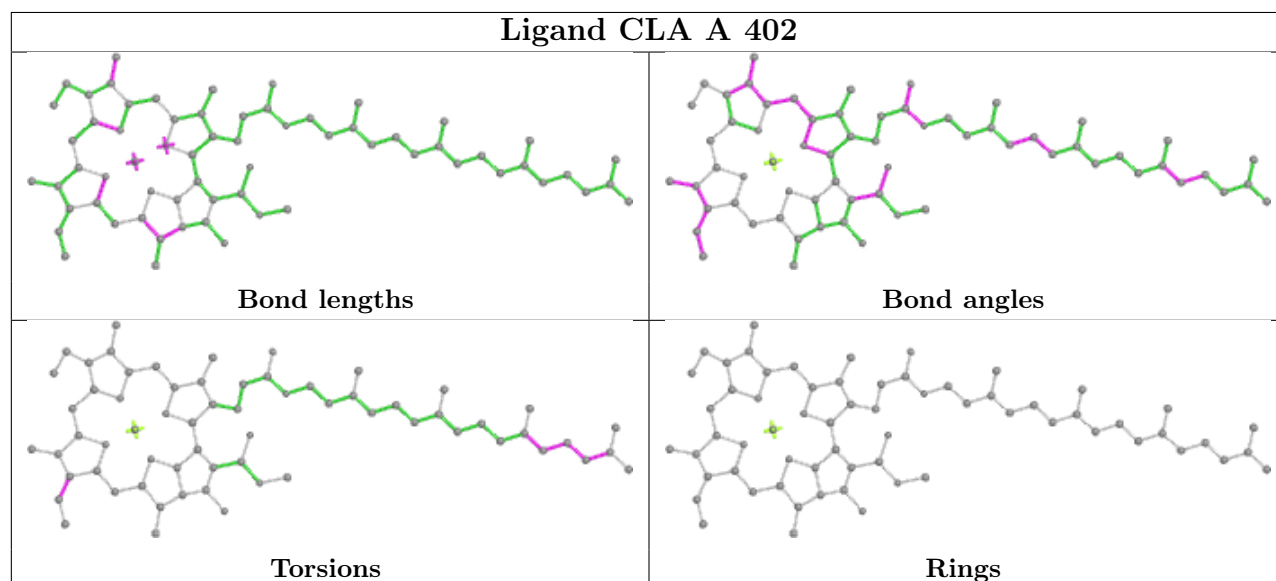
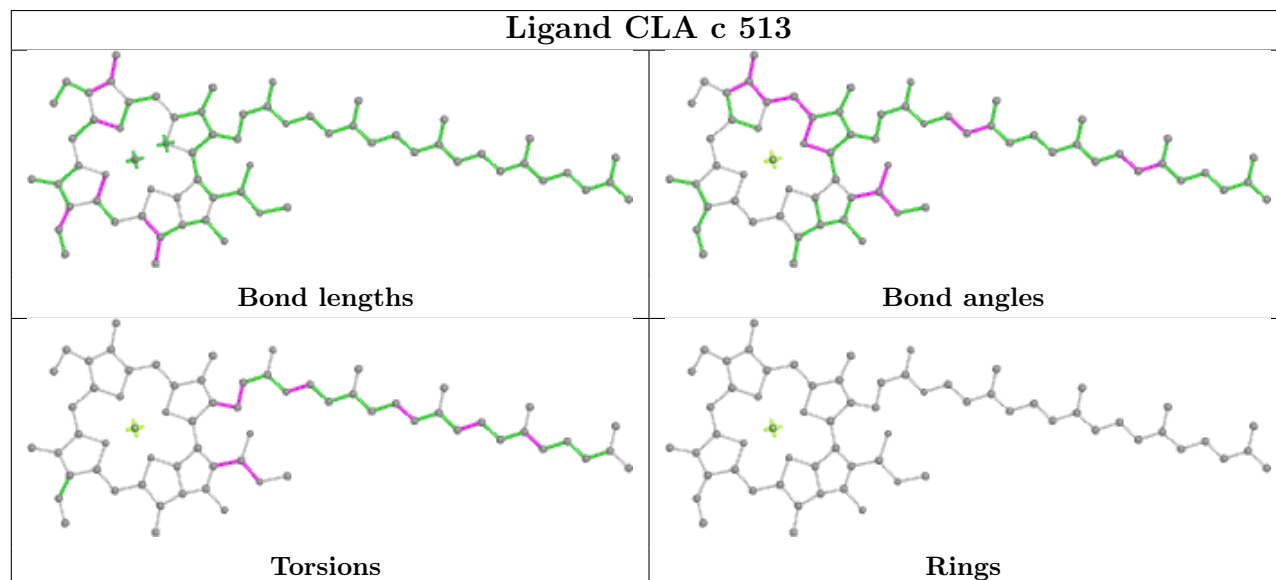
## Ligand HEM f 101



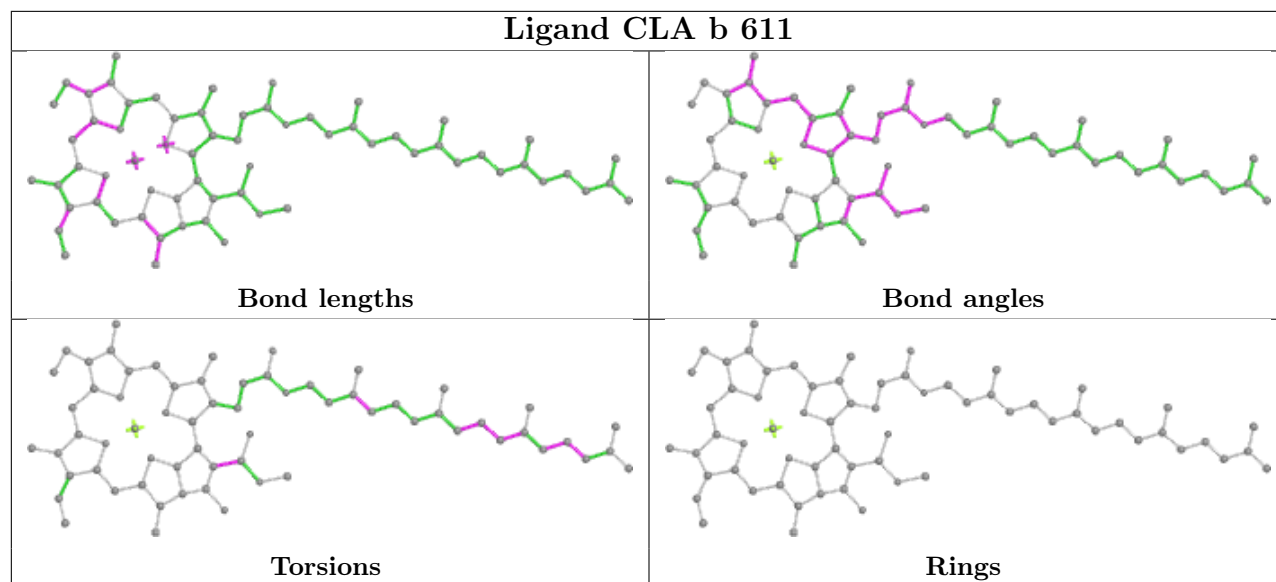
## Ligand SQD A 412



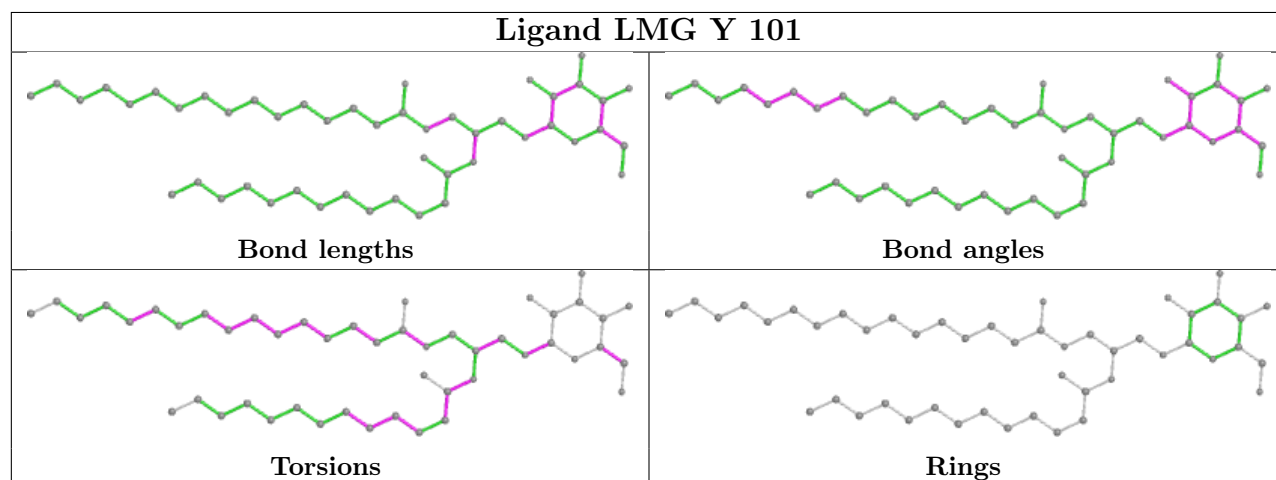


**Ligand CLA b 612****Ligand CLA A 402****Ligand CLA c 513**

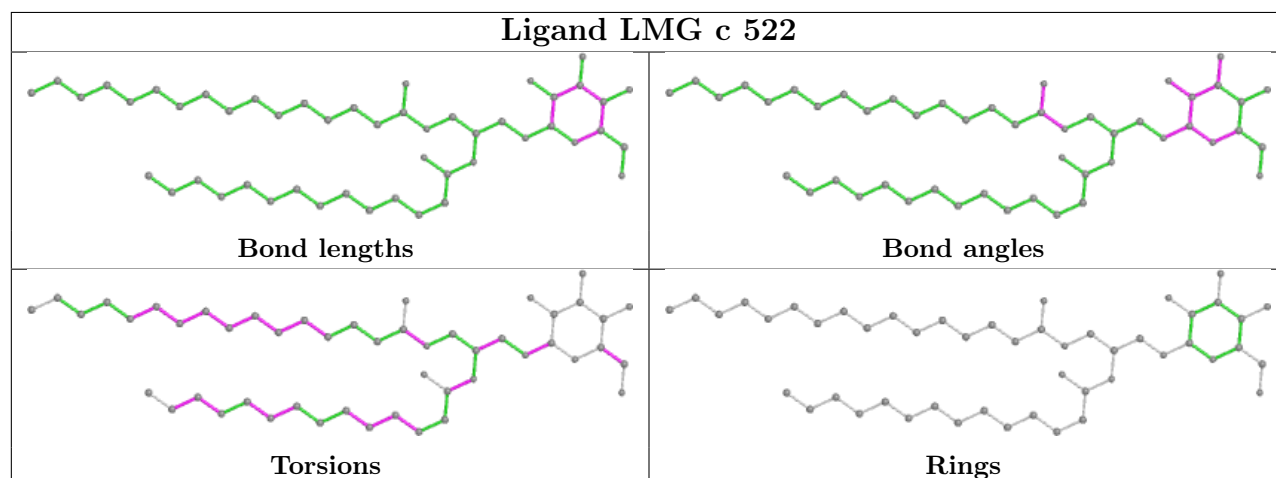
## Ligand CLA b 611

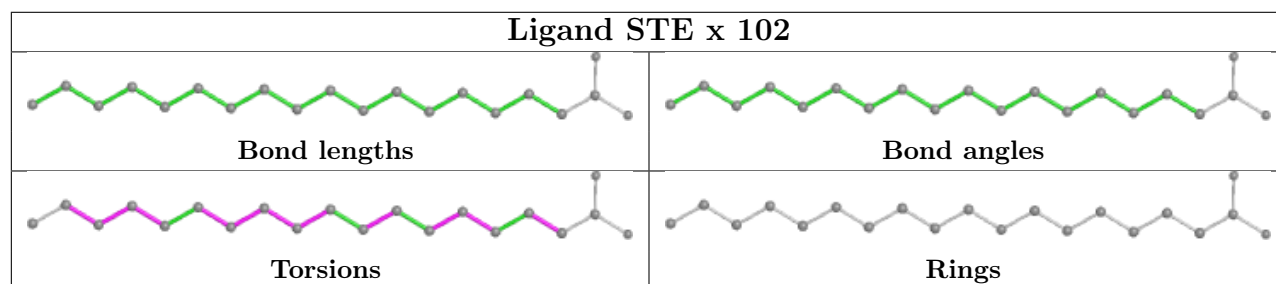
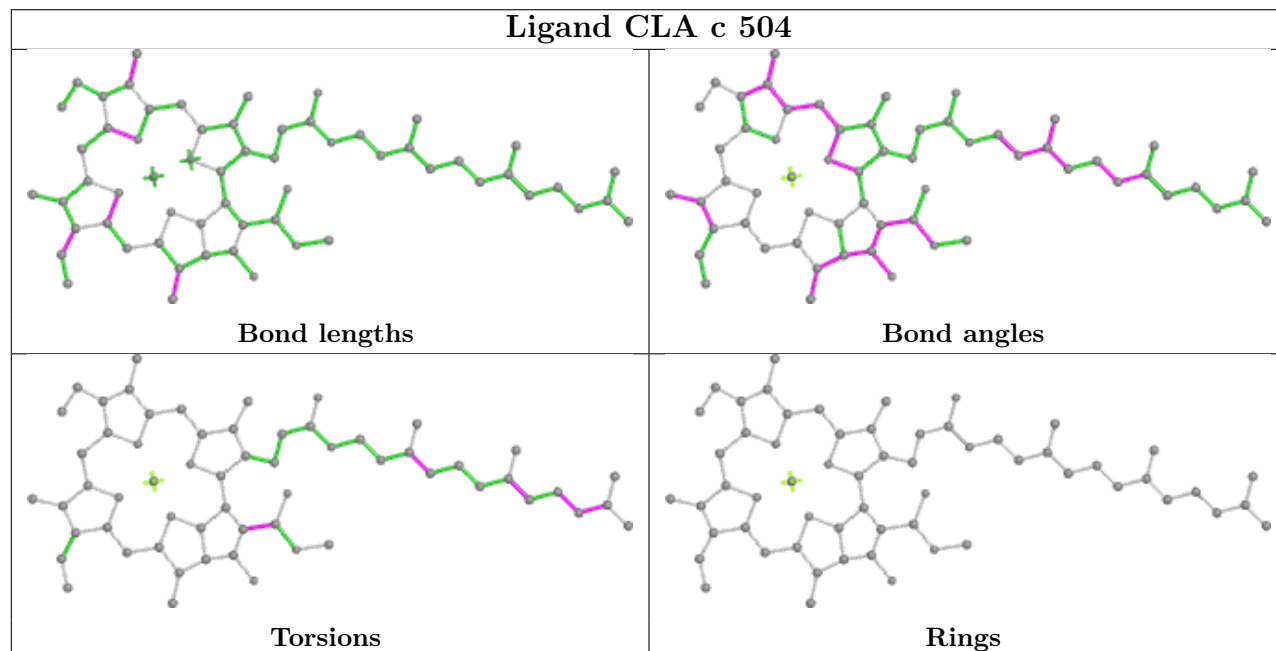
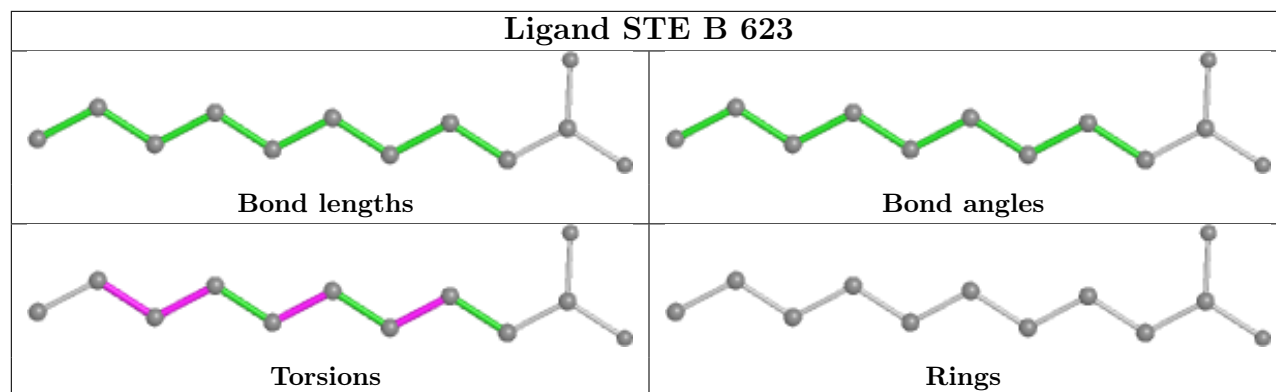


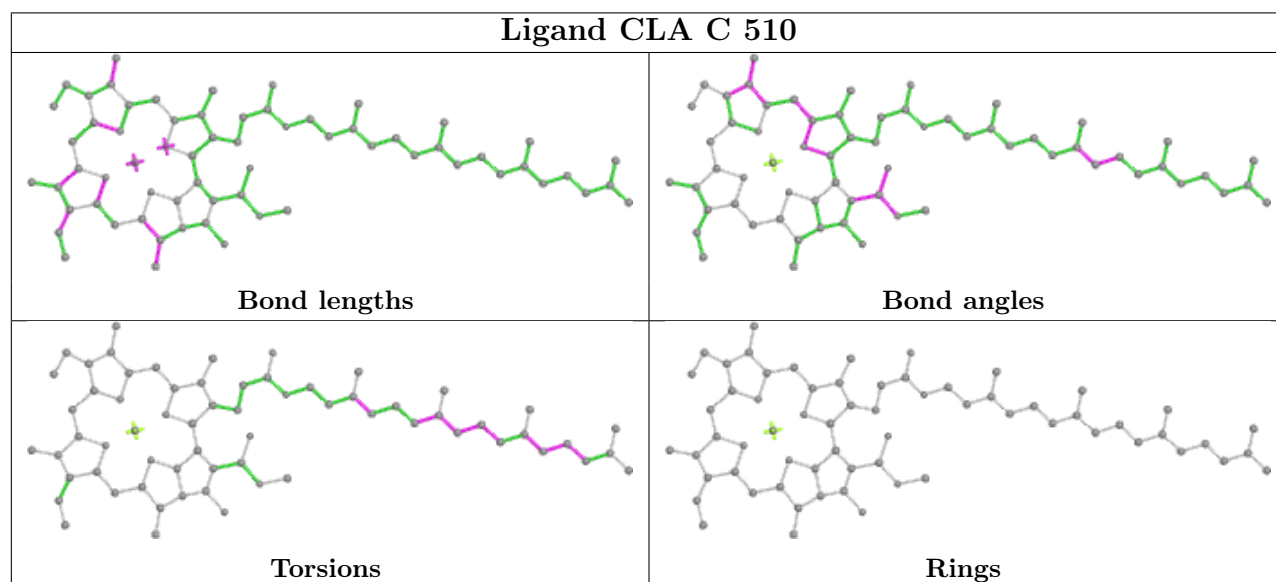
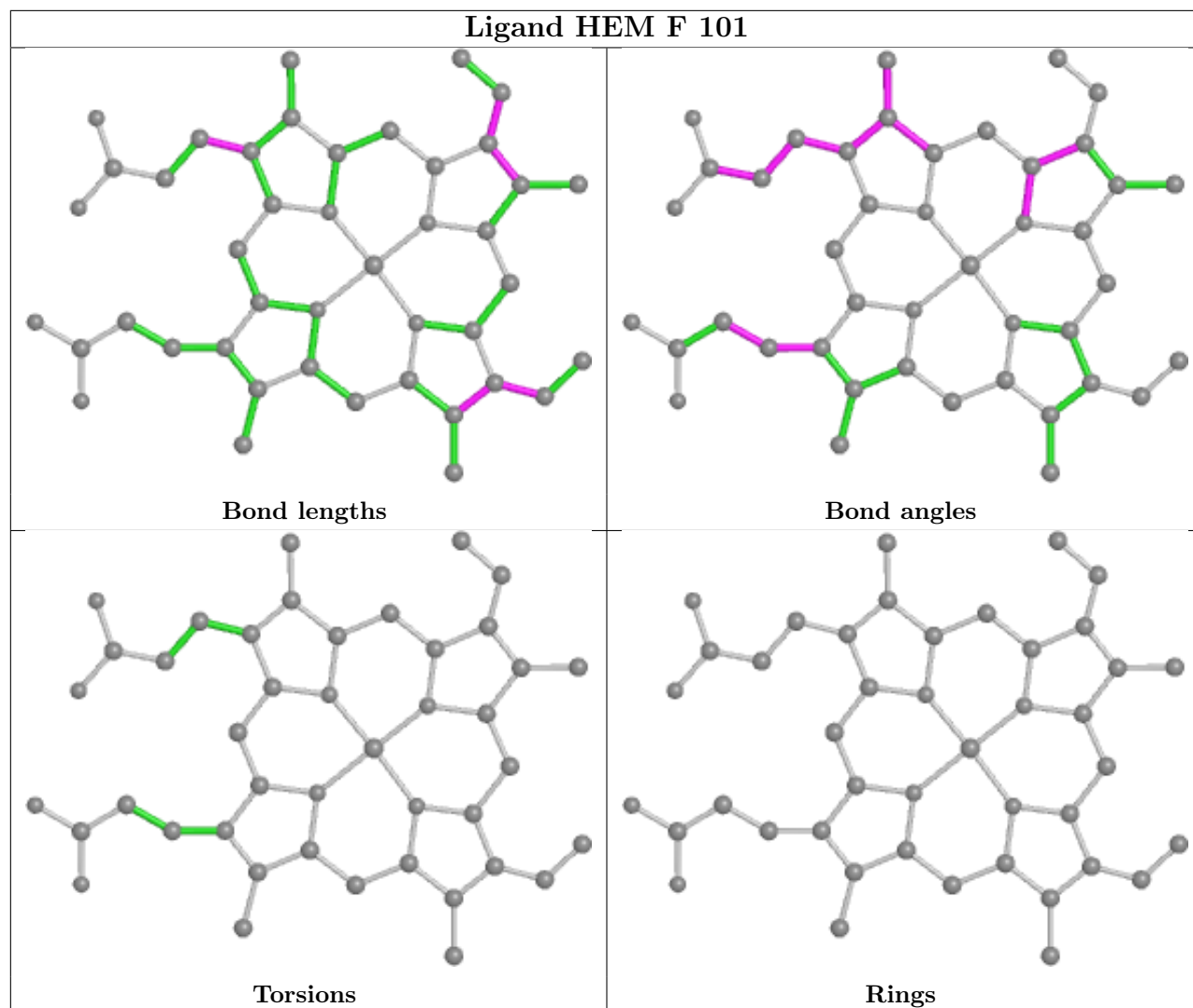
## Ligand LMG Y 101

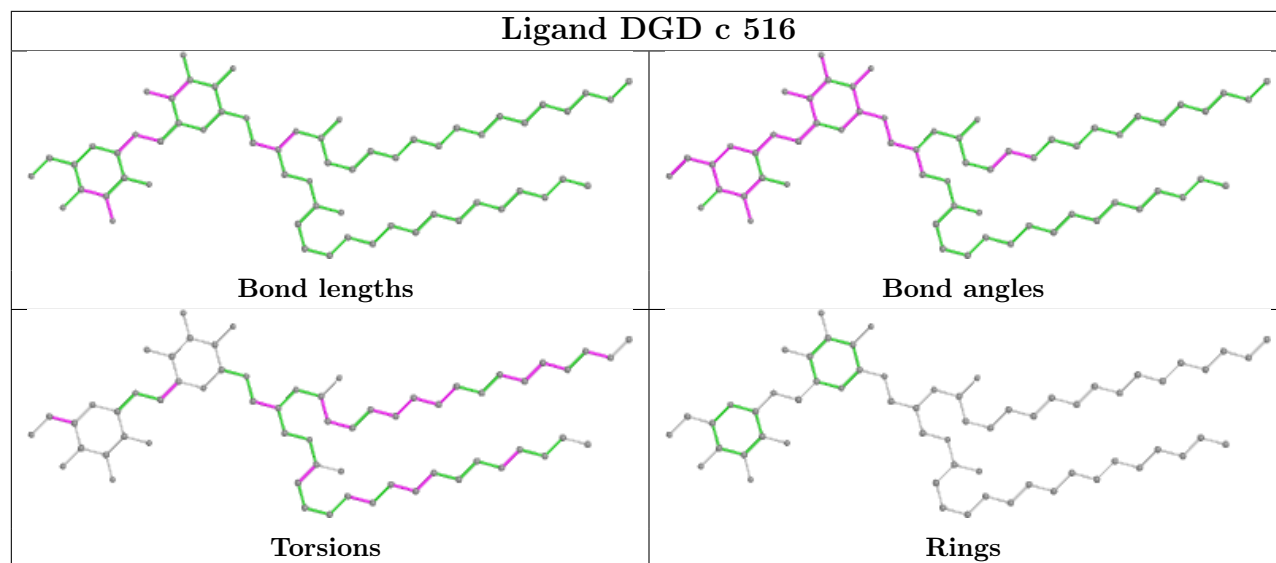
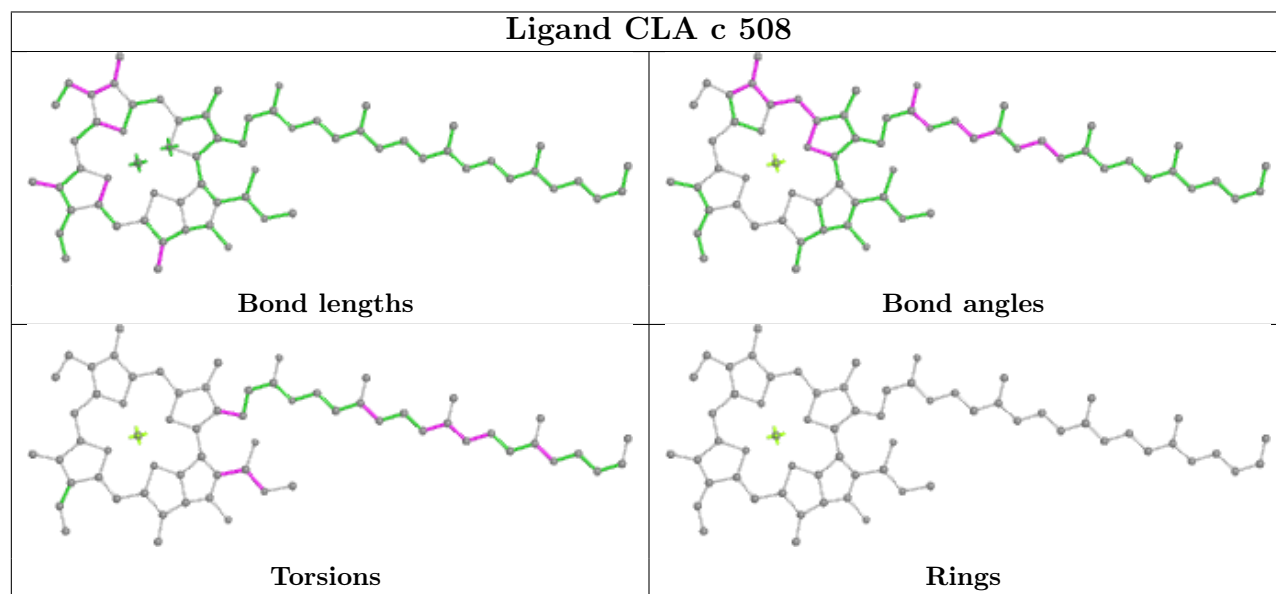


## Ligand LMG c 522

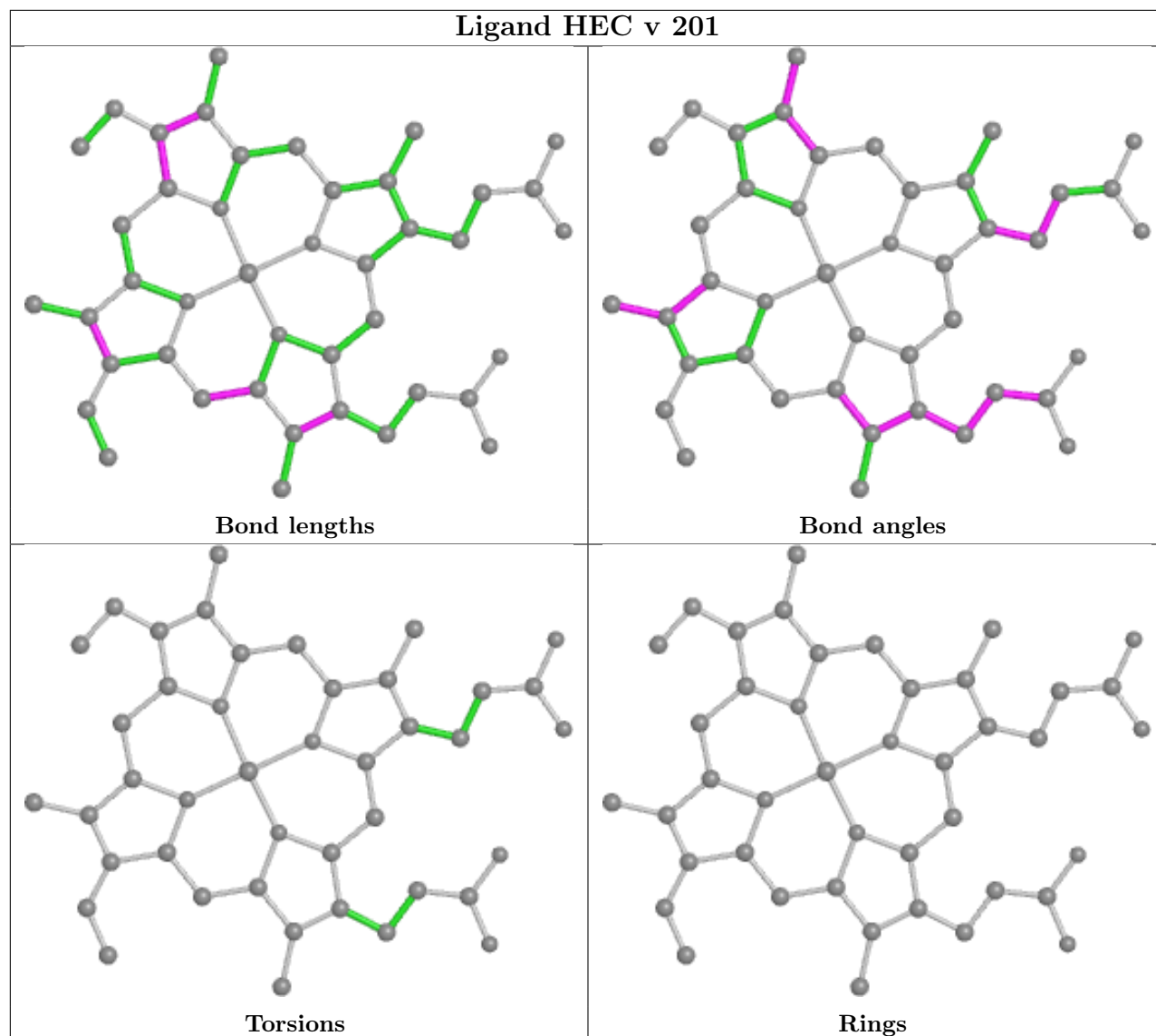




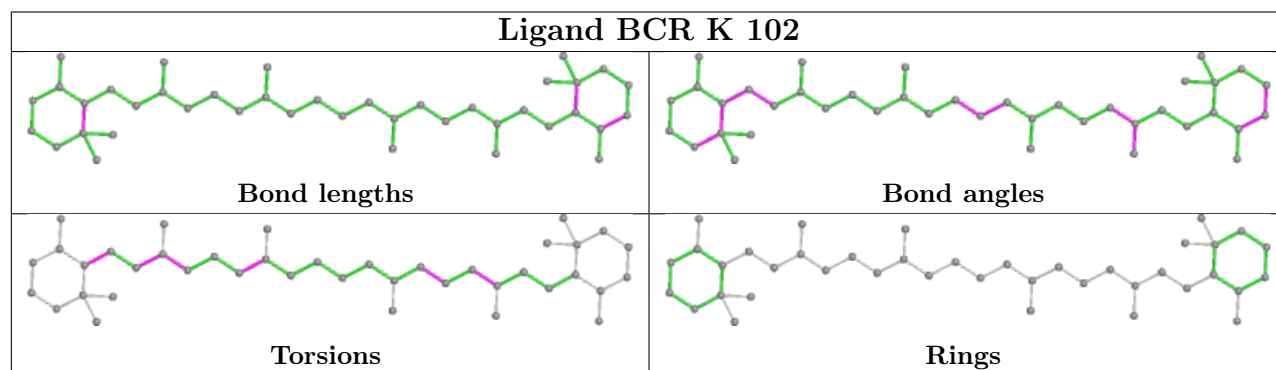


**Ligand DGD c 516****Ligand CLA c 508**

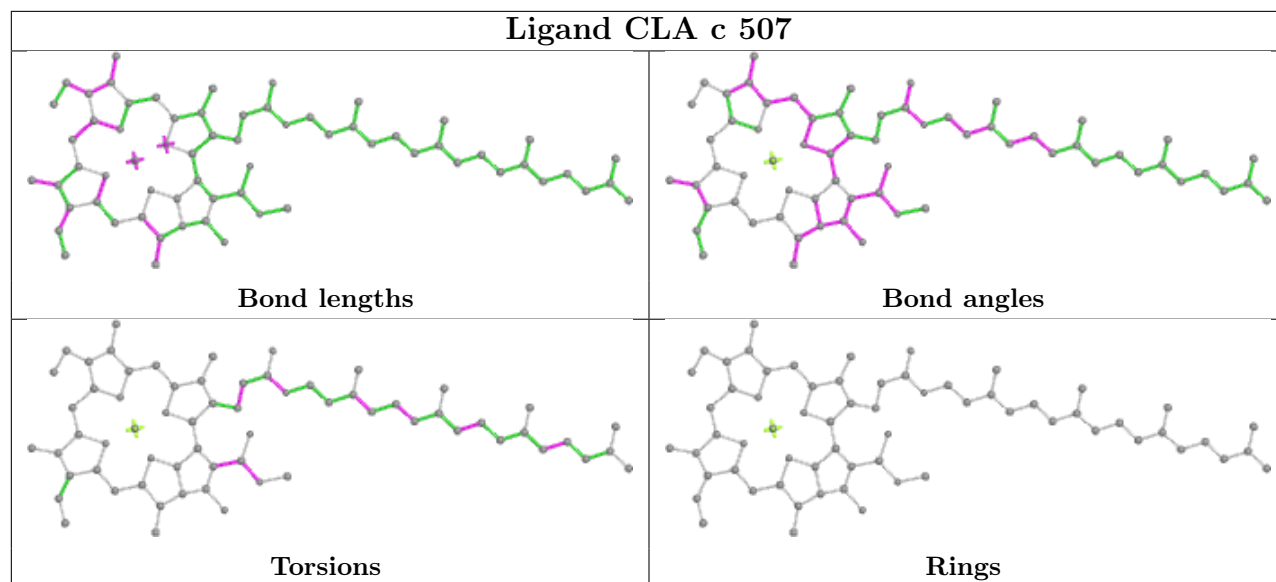
## Ligand HEC v 201



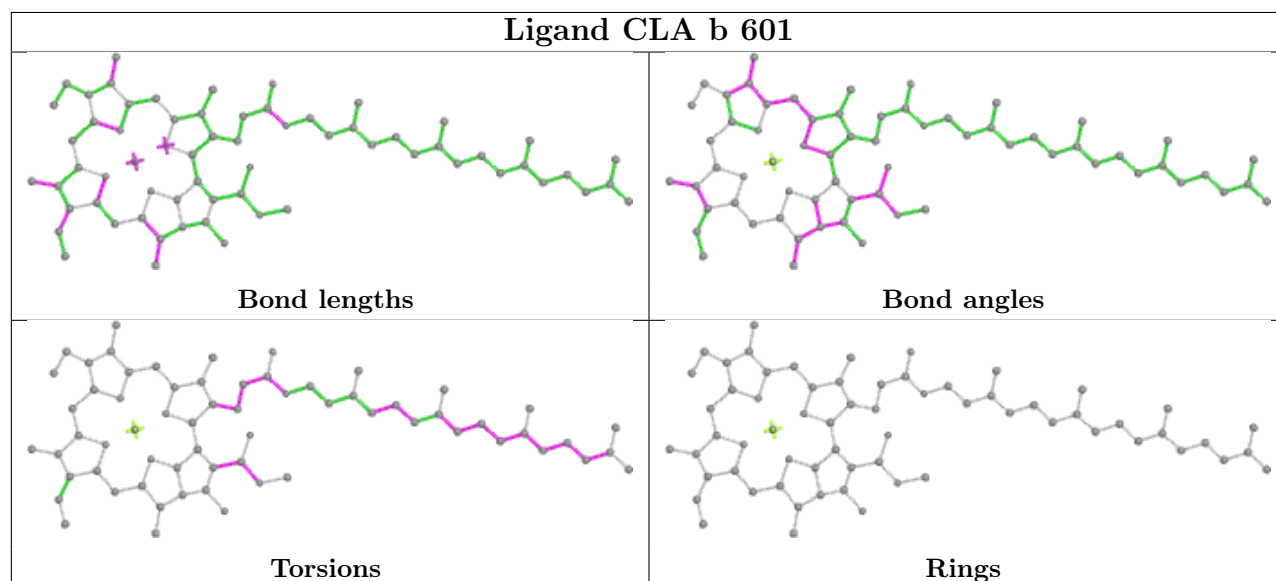
## Ligand BCR K 102



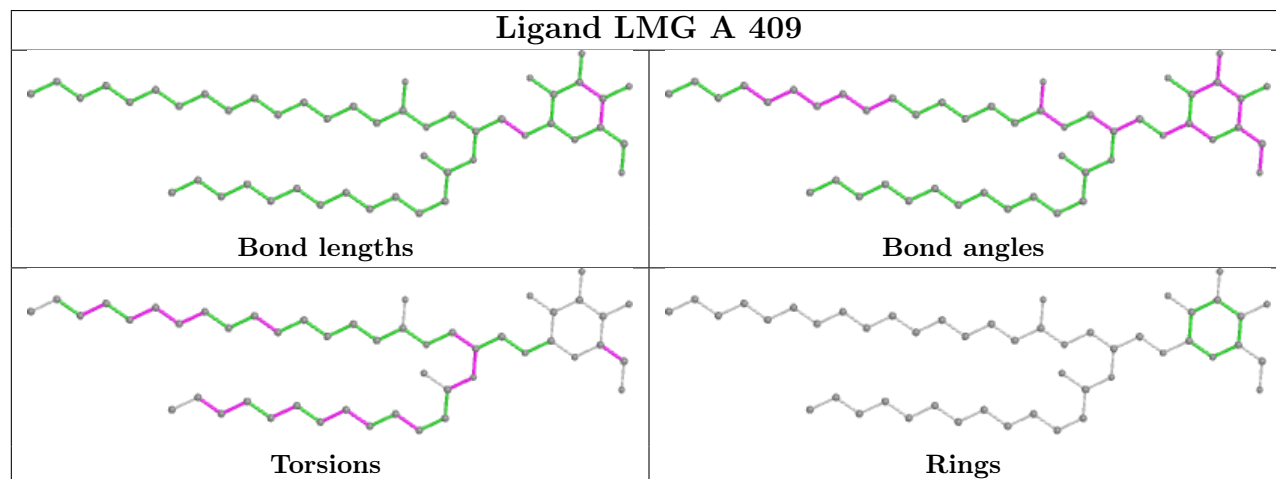
## Ligand CLA c 507

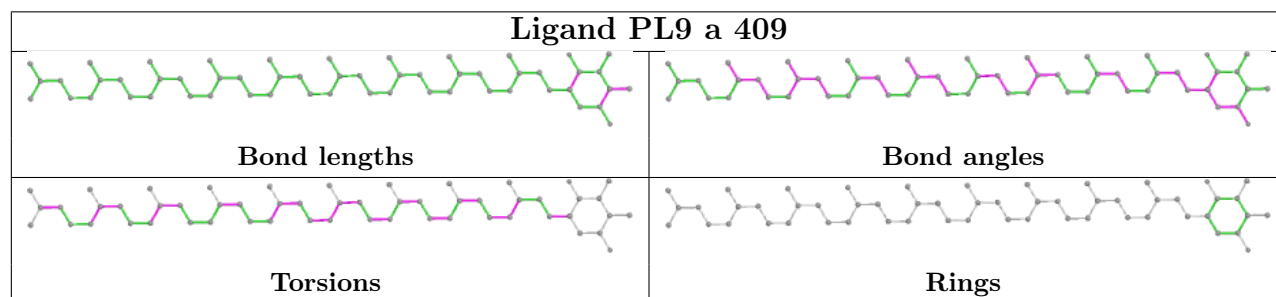
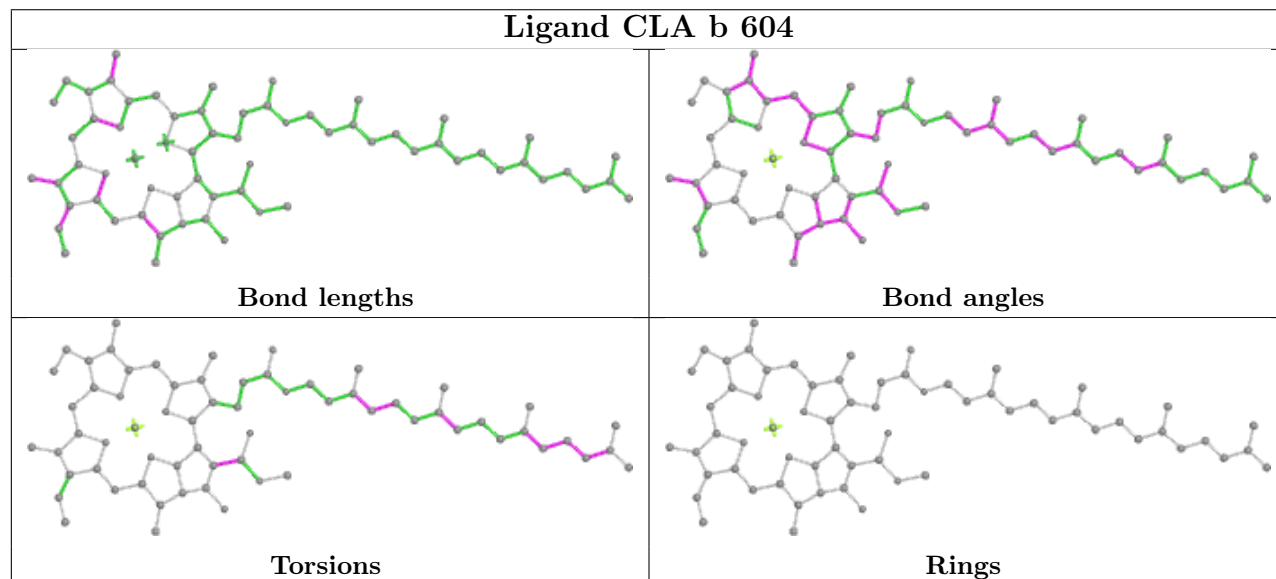
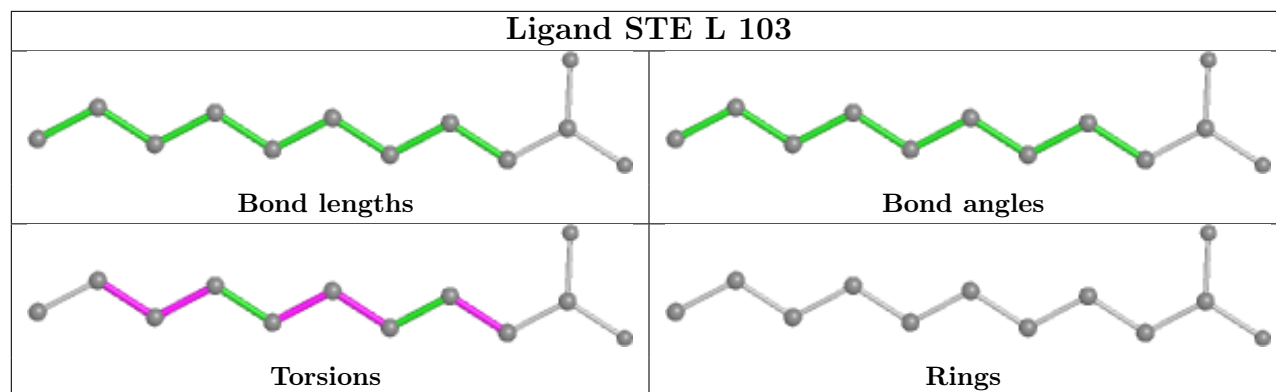


## Ligand CLA b 601

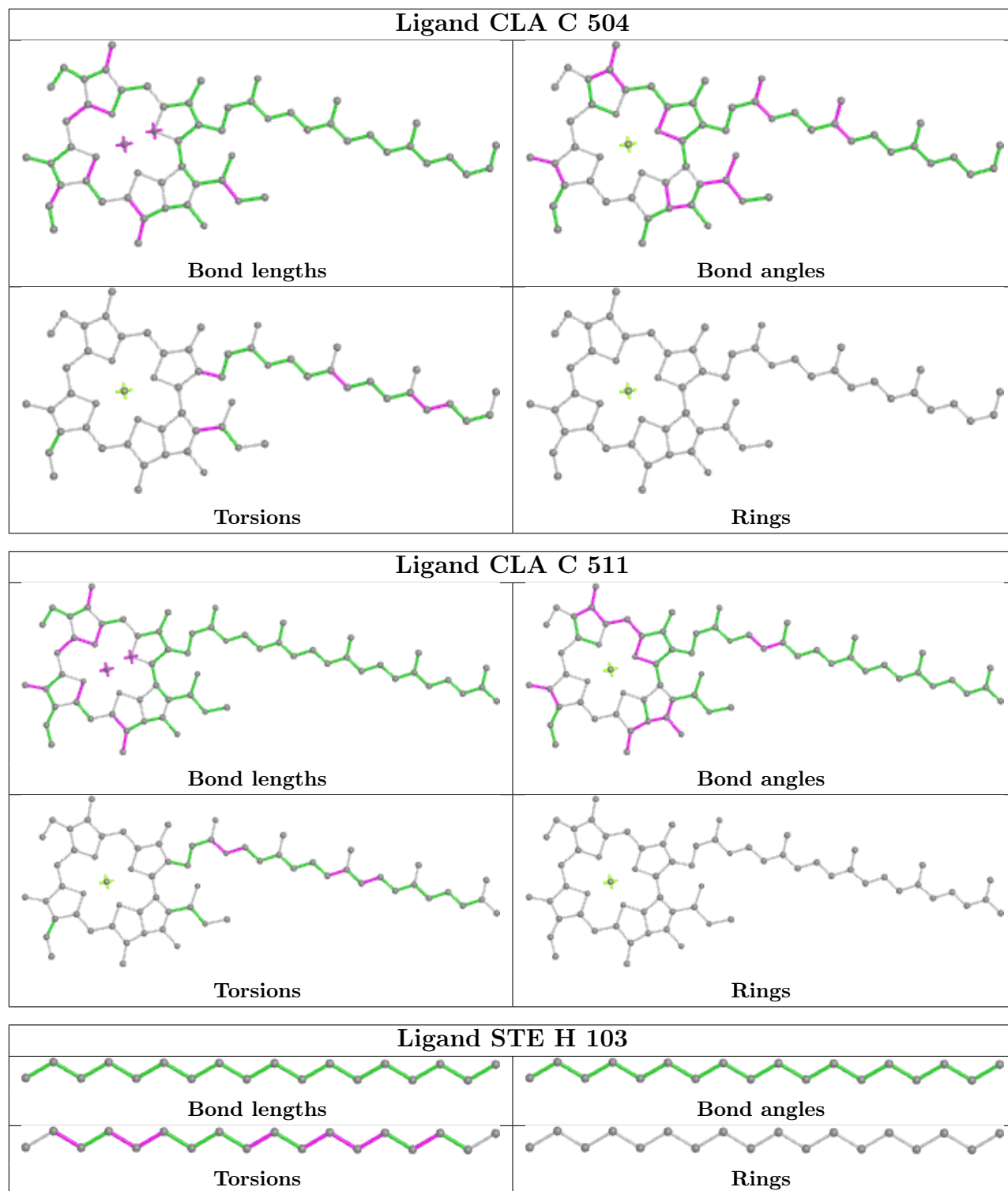


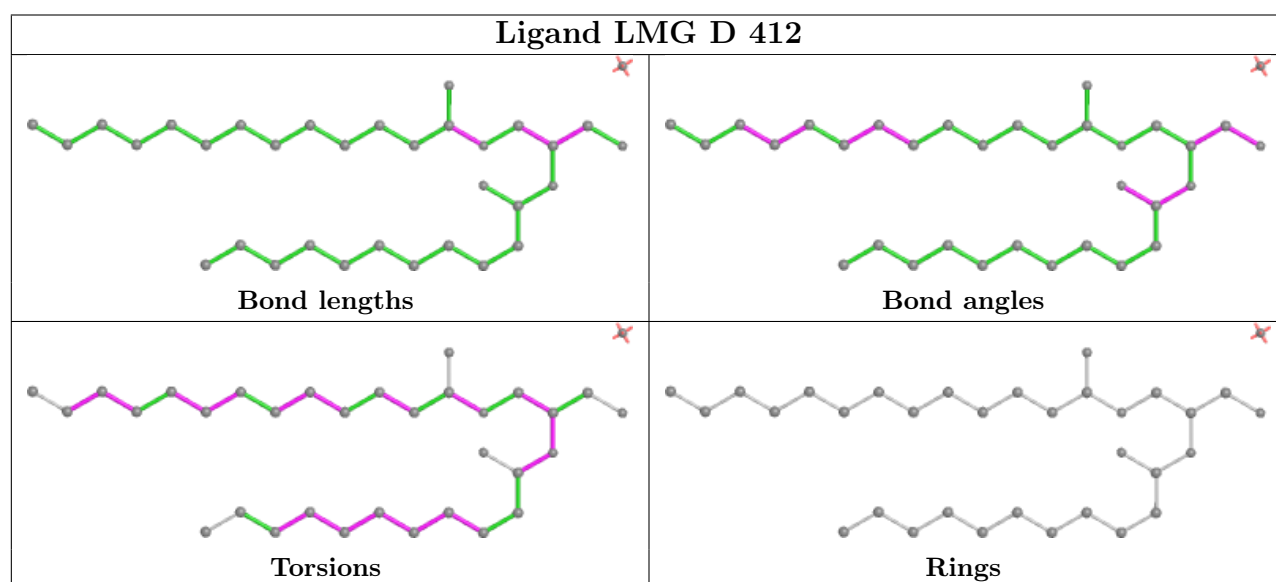
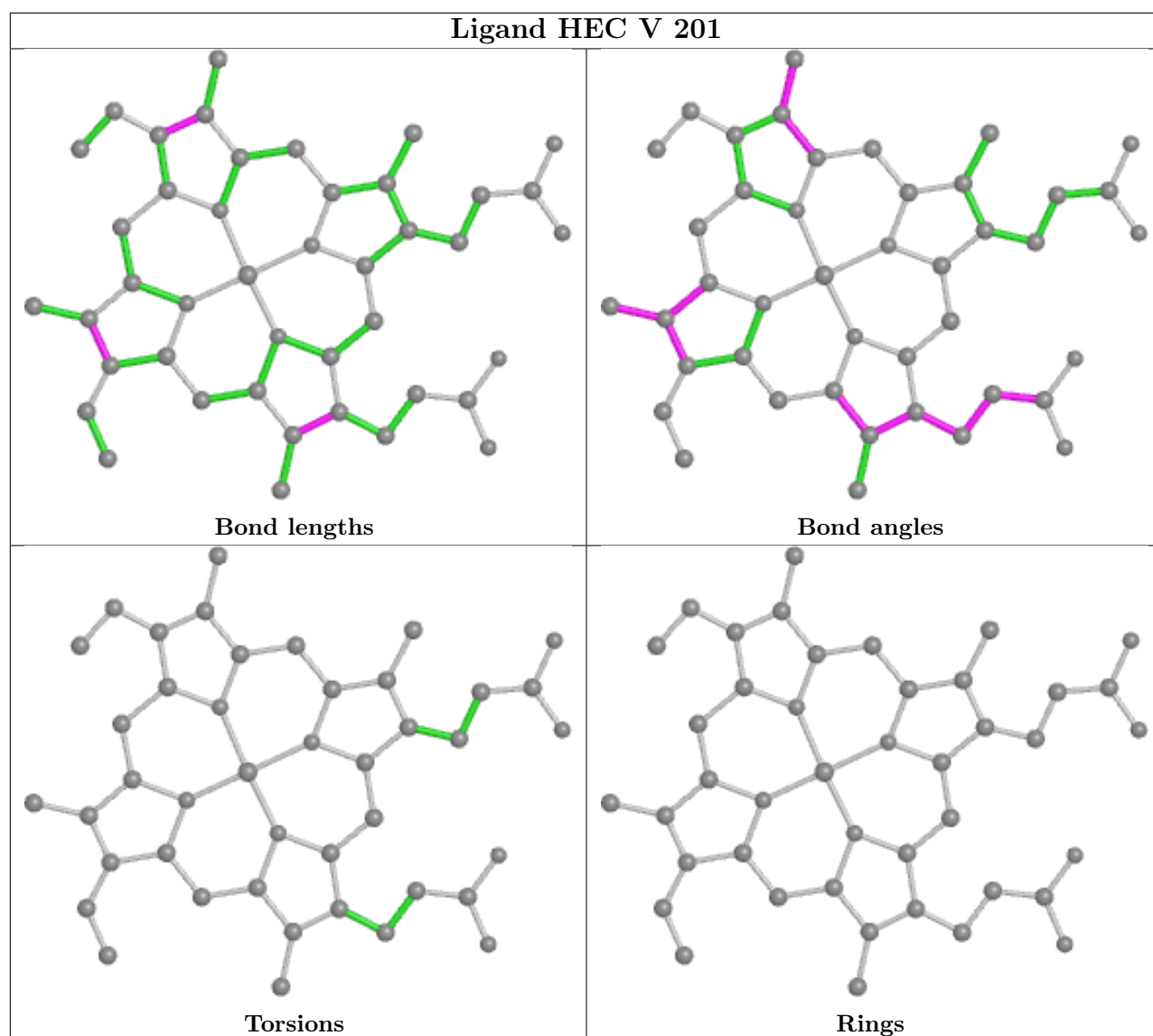
## Ligand LMG A 409



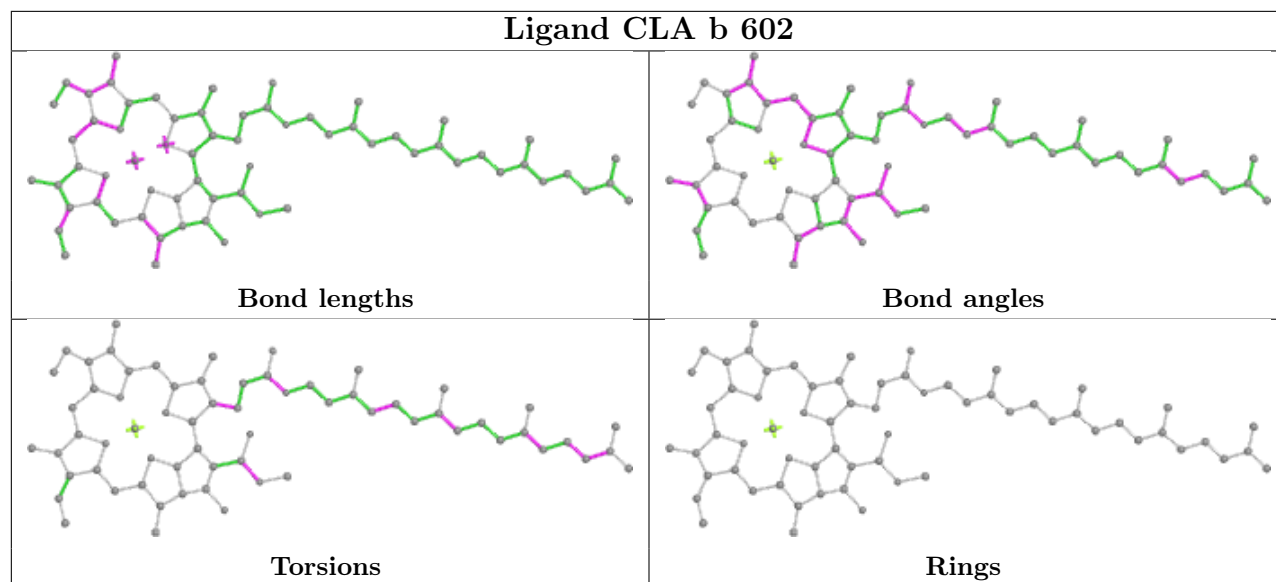




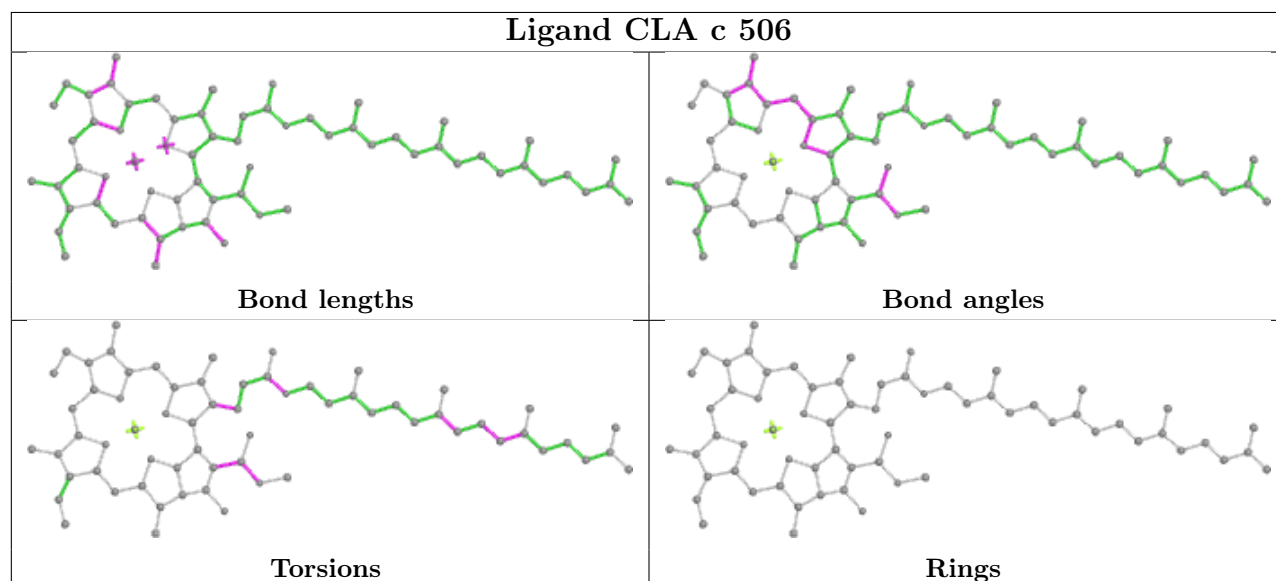




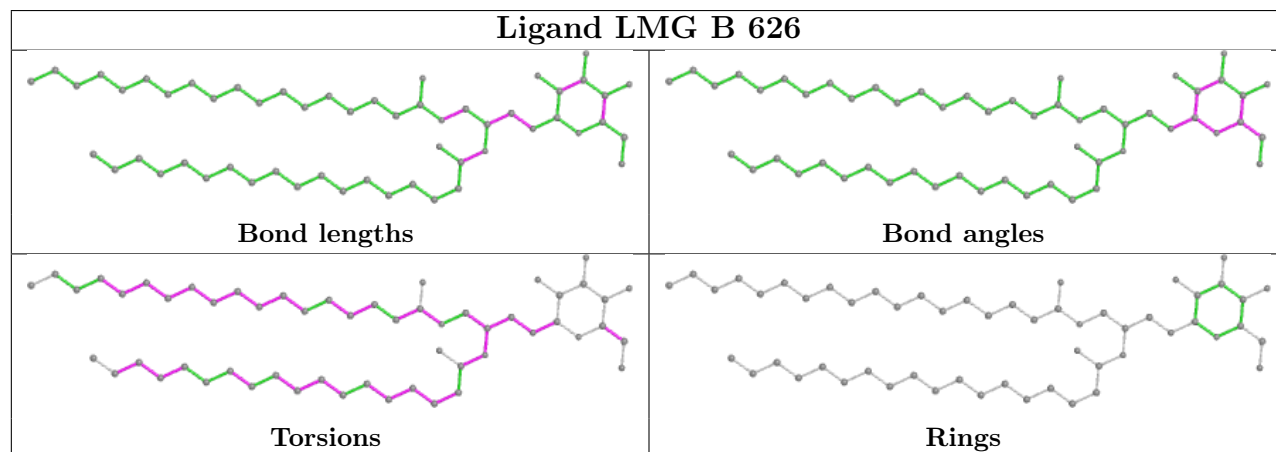
## Ligand CLA b 602

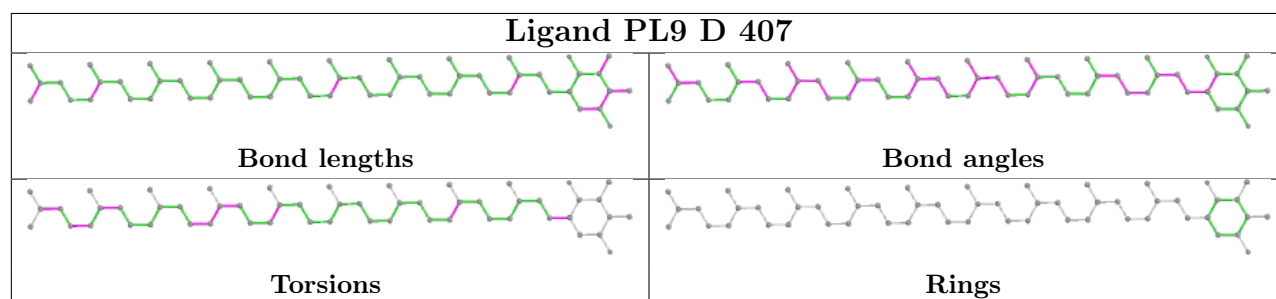
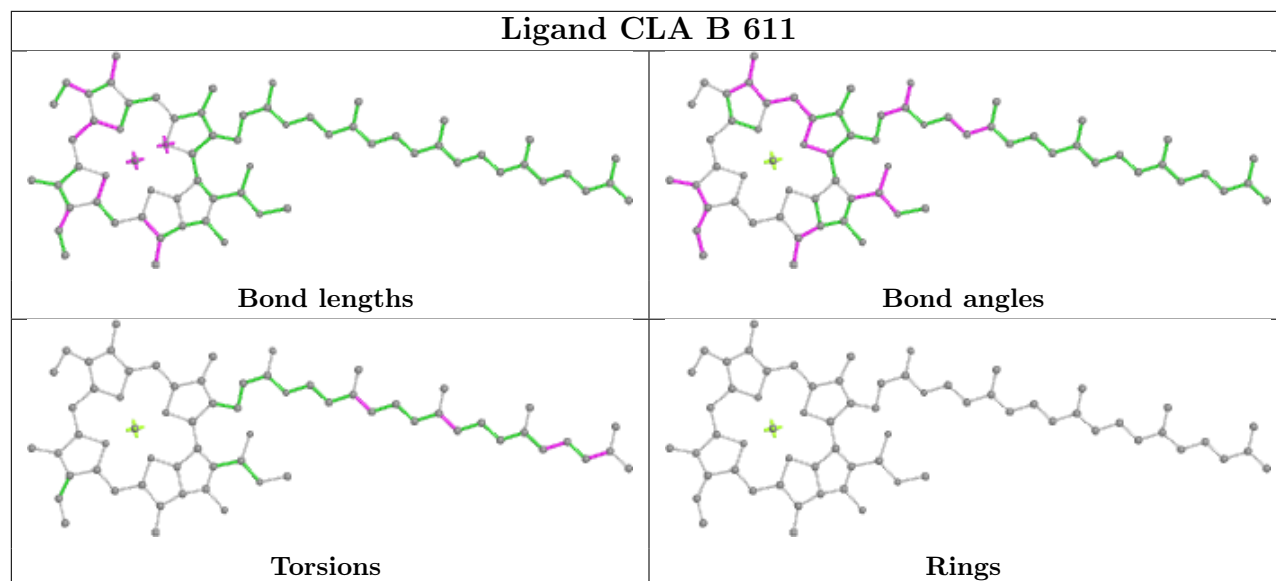
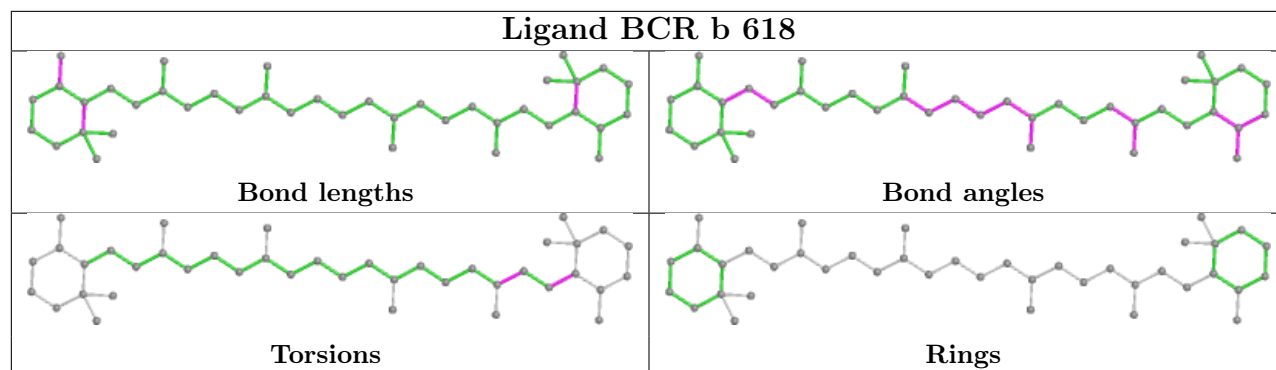


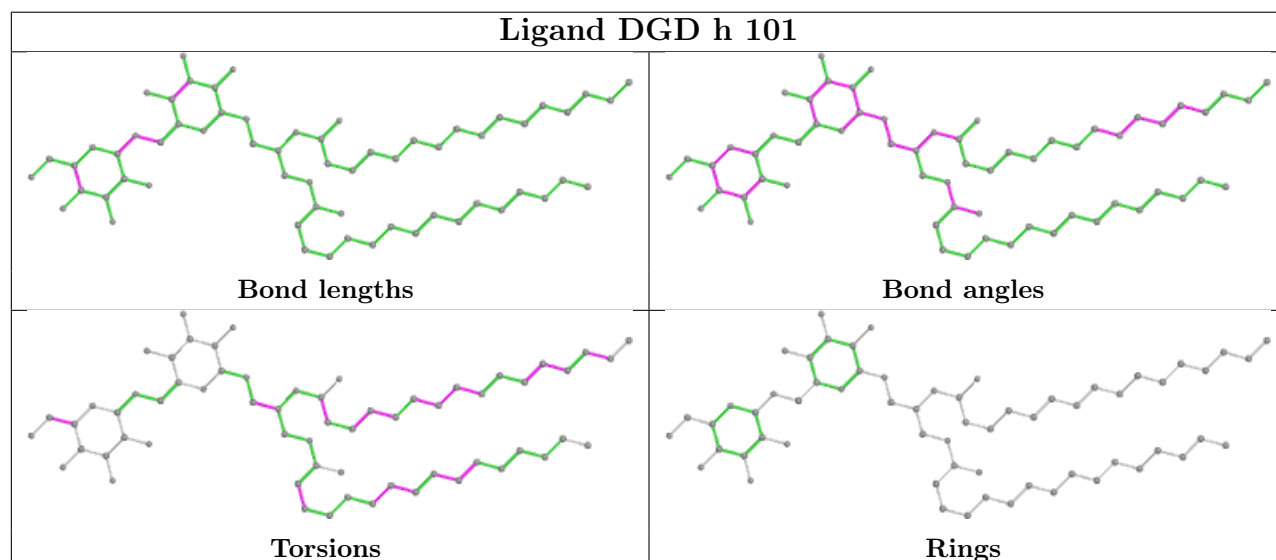
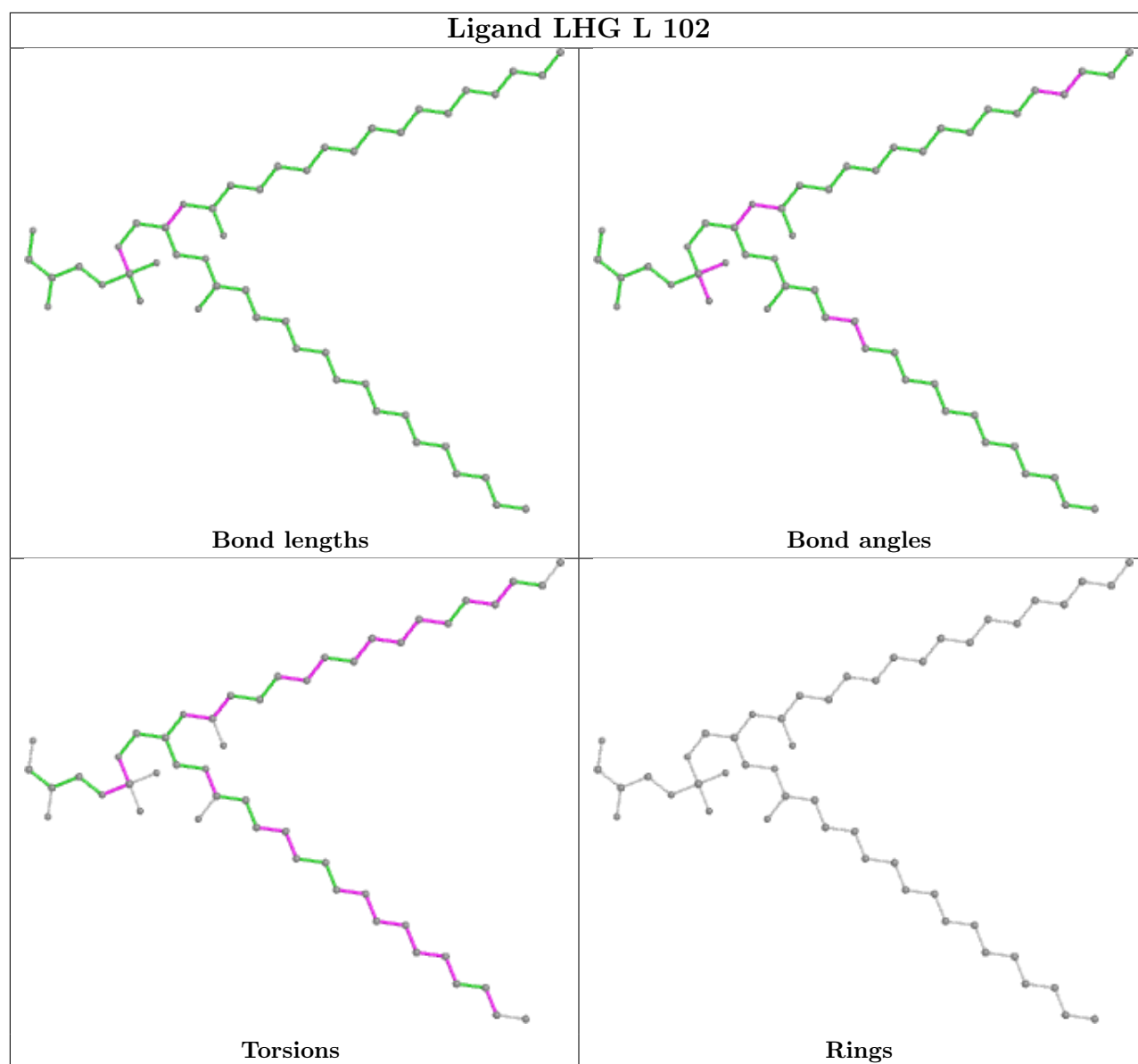
## Ligand CLA c 506

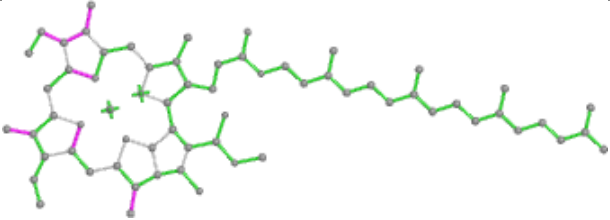
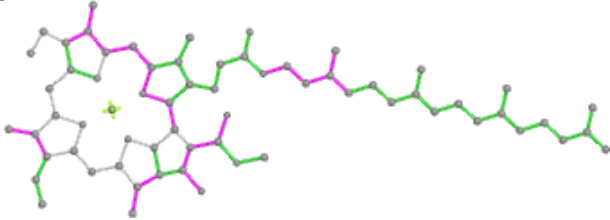
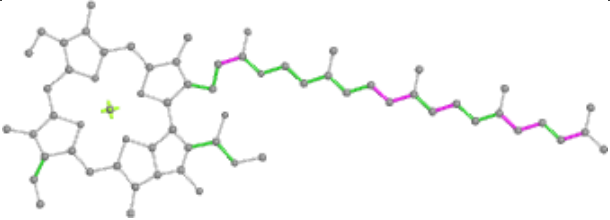
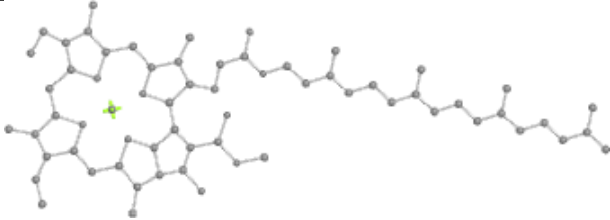
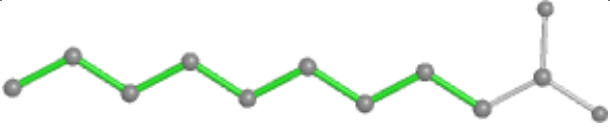
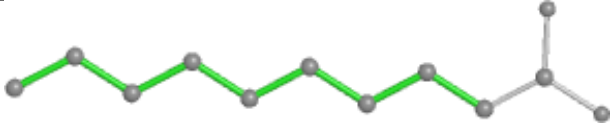
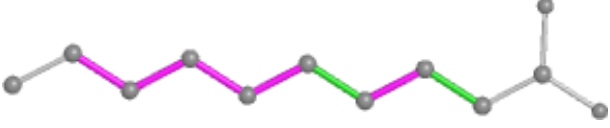
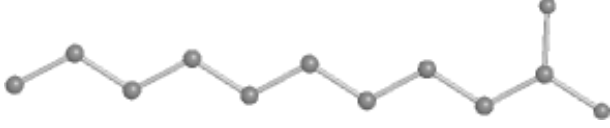






## Ligand LMG B 626

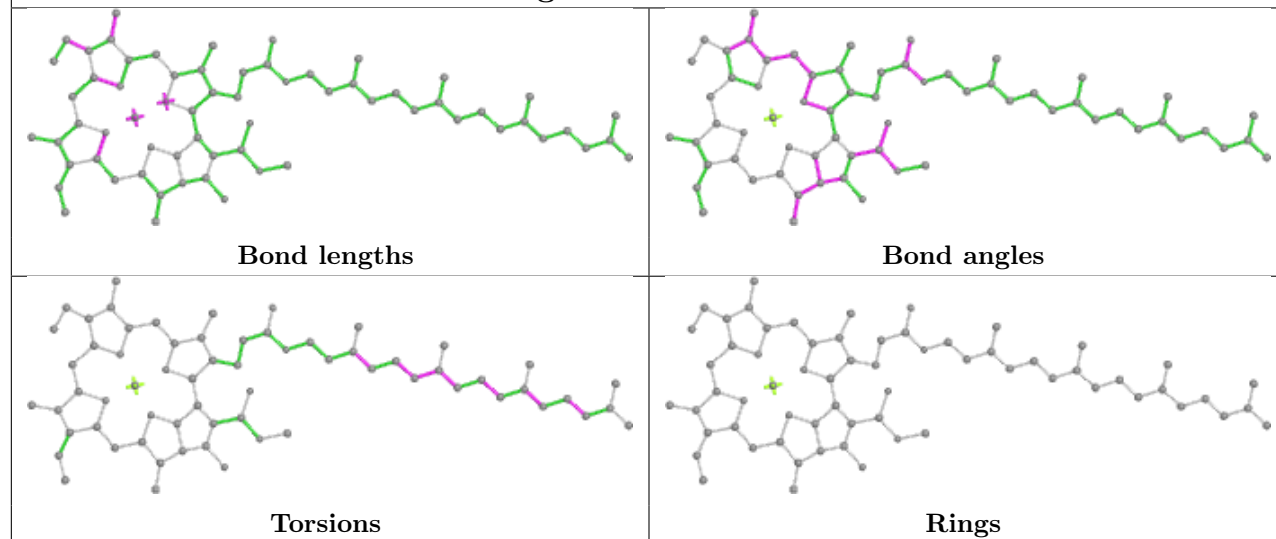




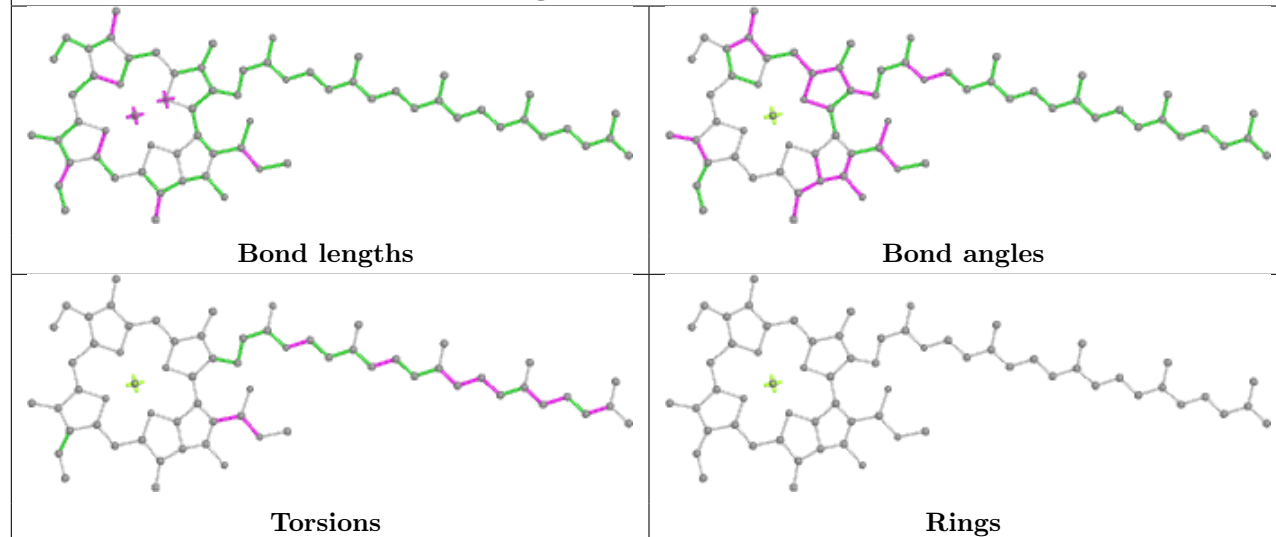


Ligand CLA B 613	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE c 523	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE b 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

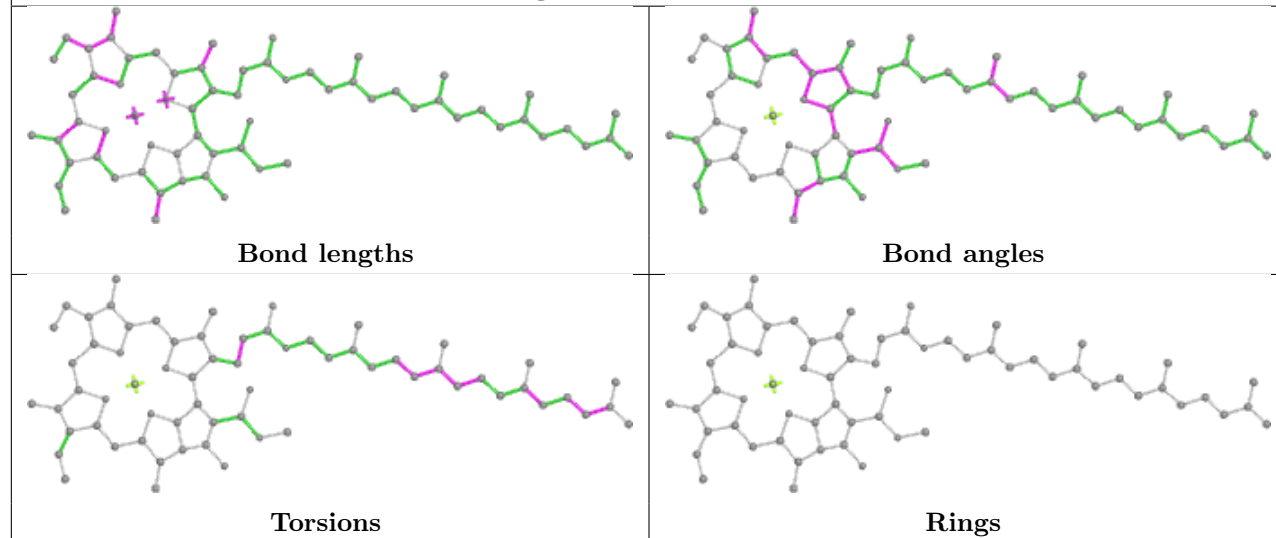
## Ligand CLA c 505

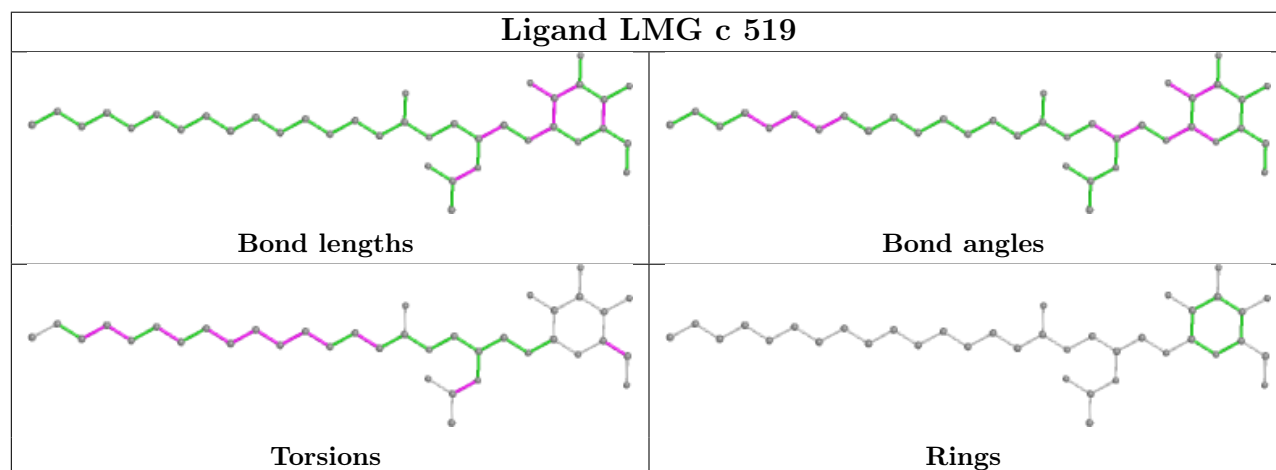
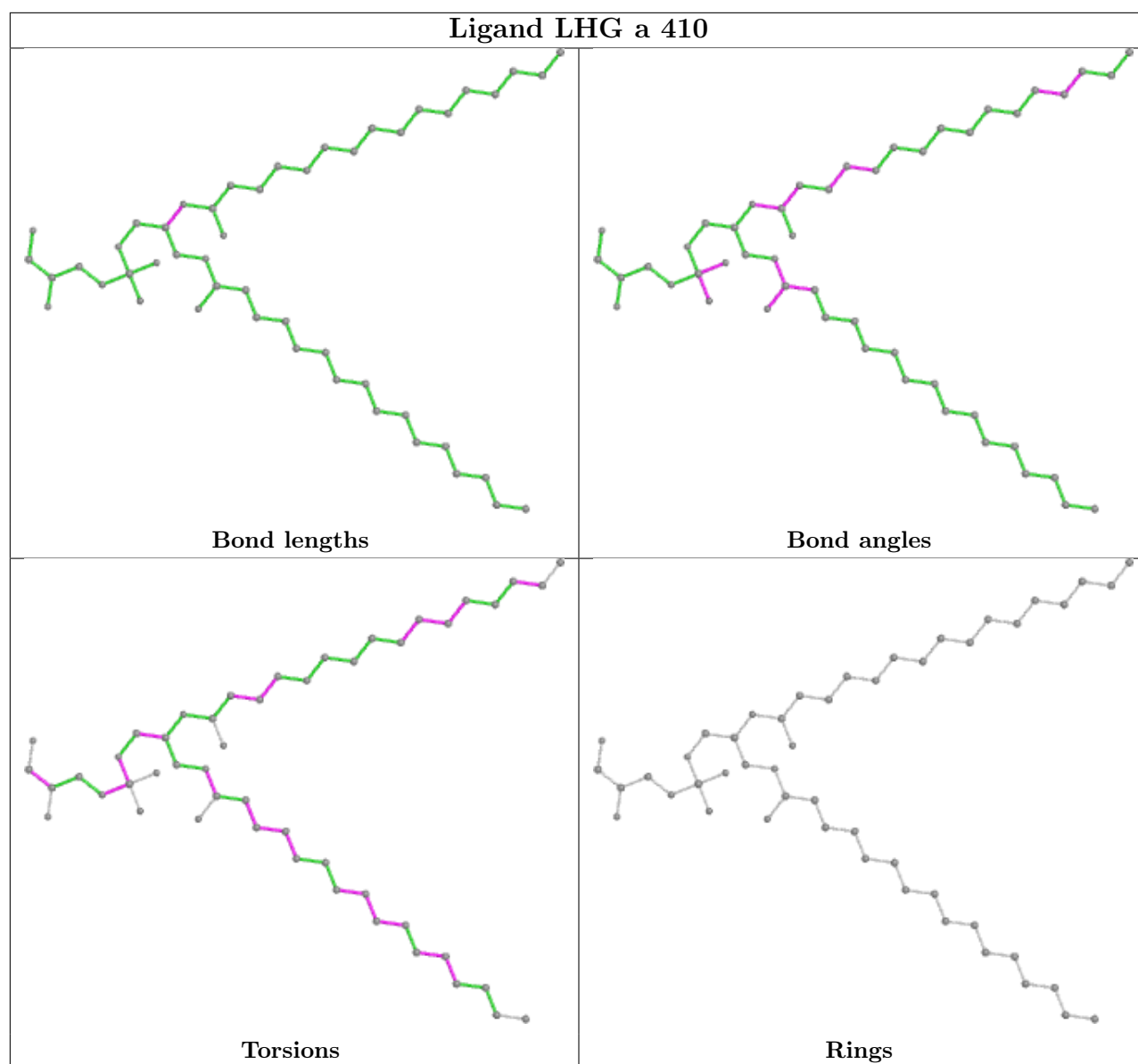


## Ligand CLA C 509

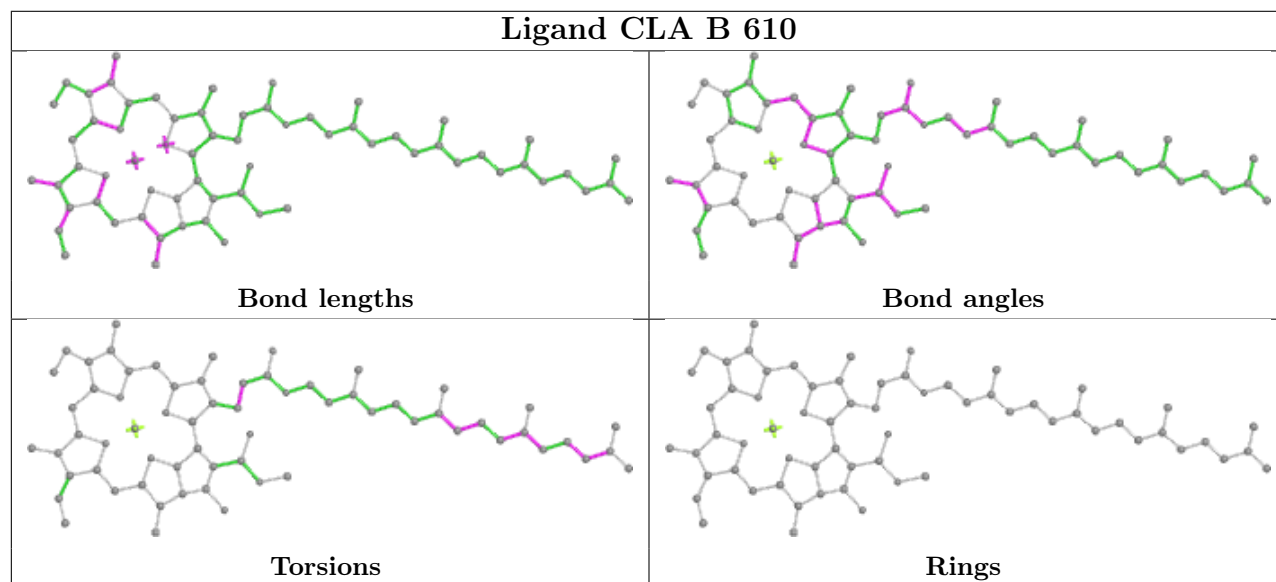
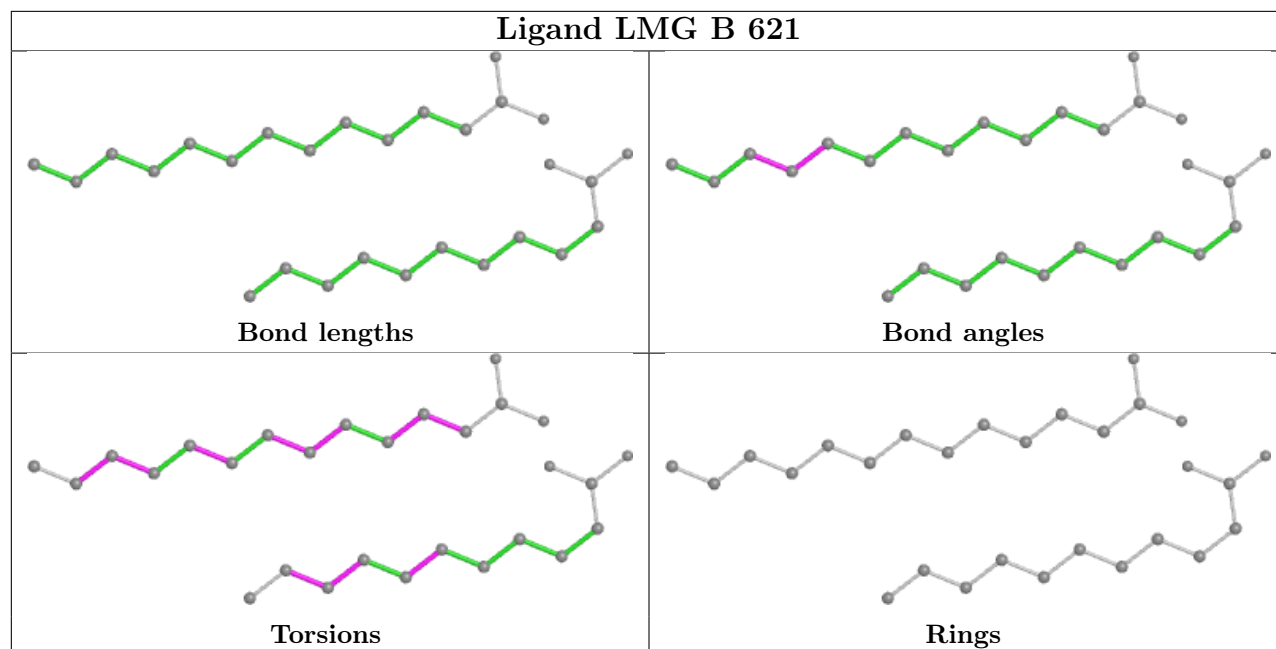


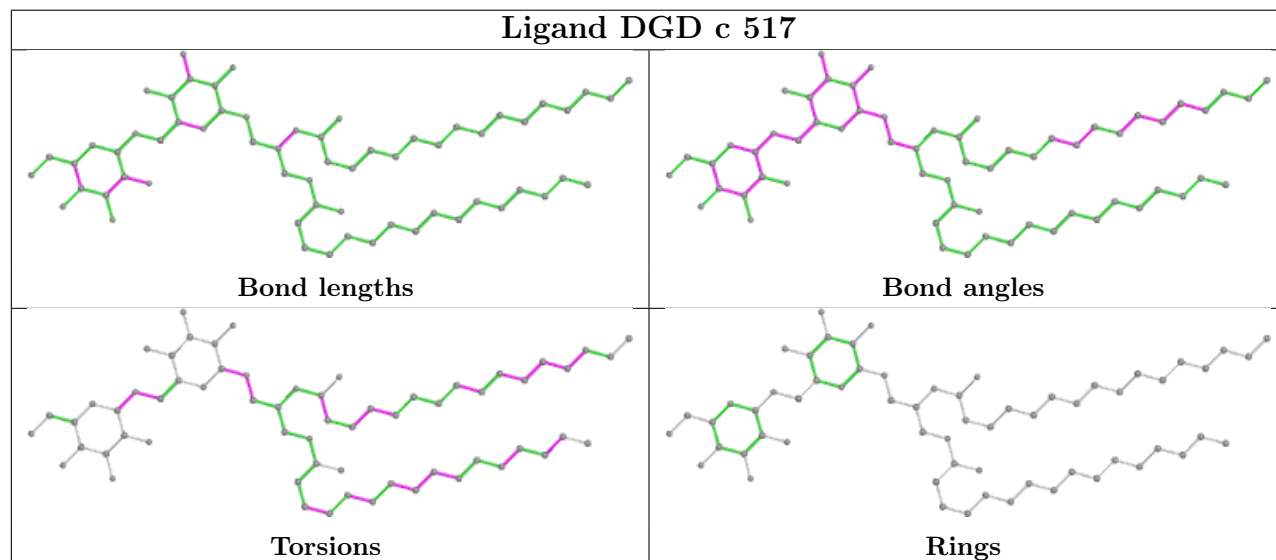
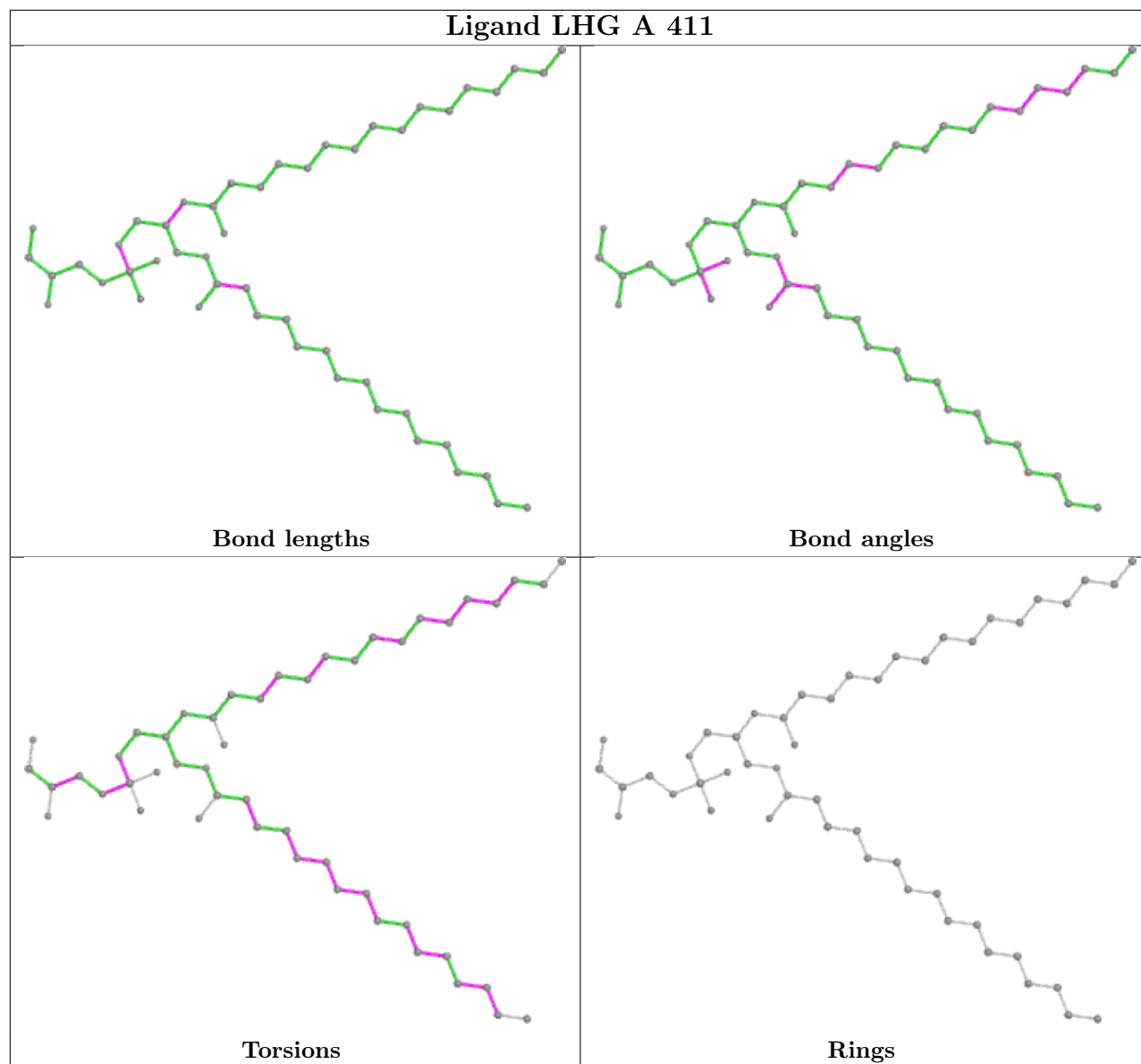
## Ligand CLA B 606

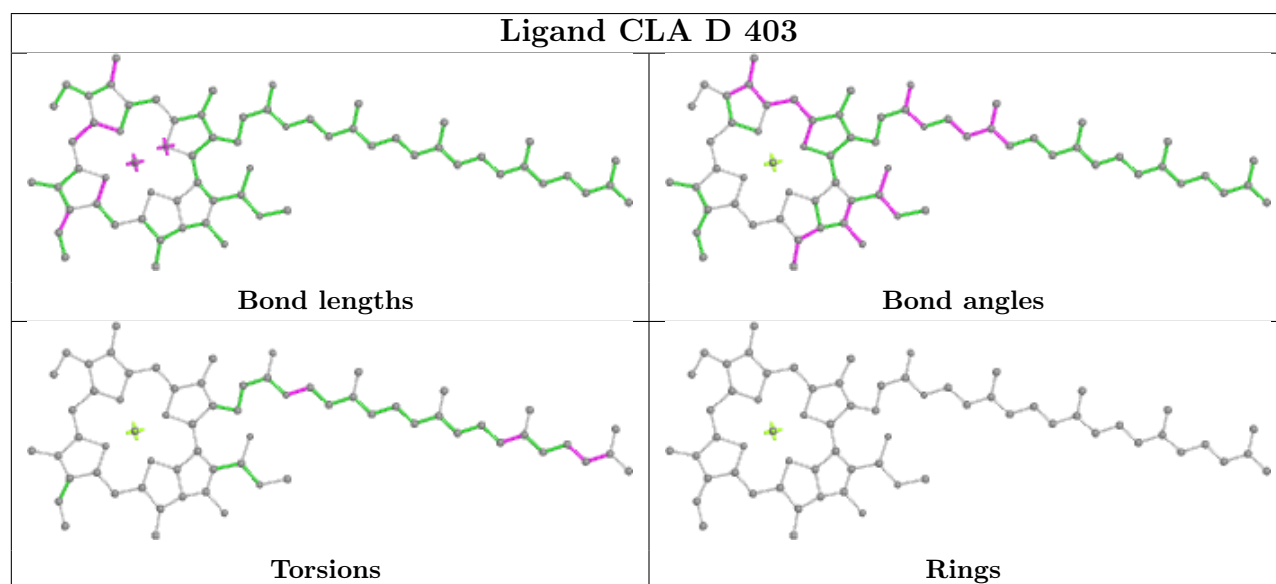
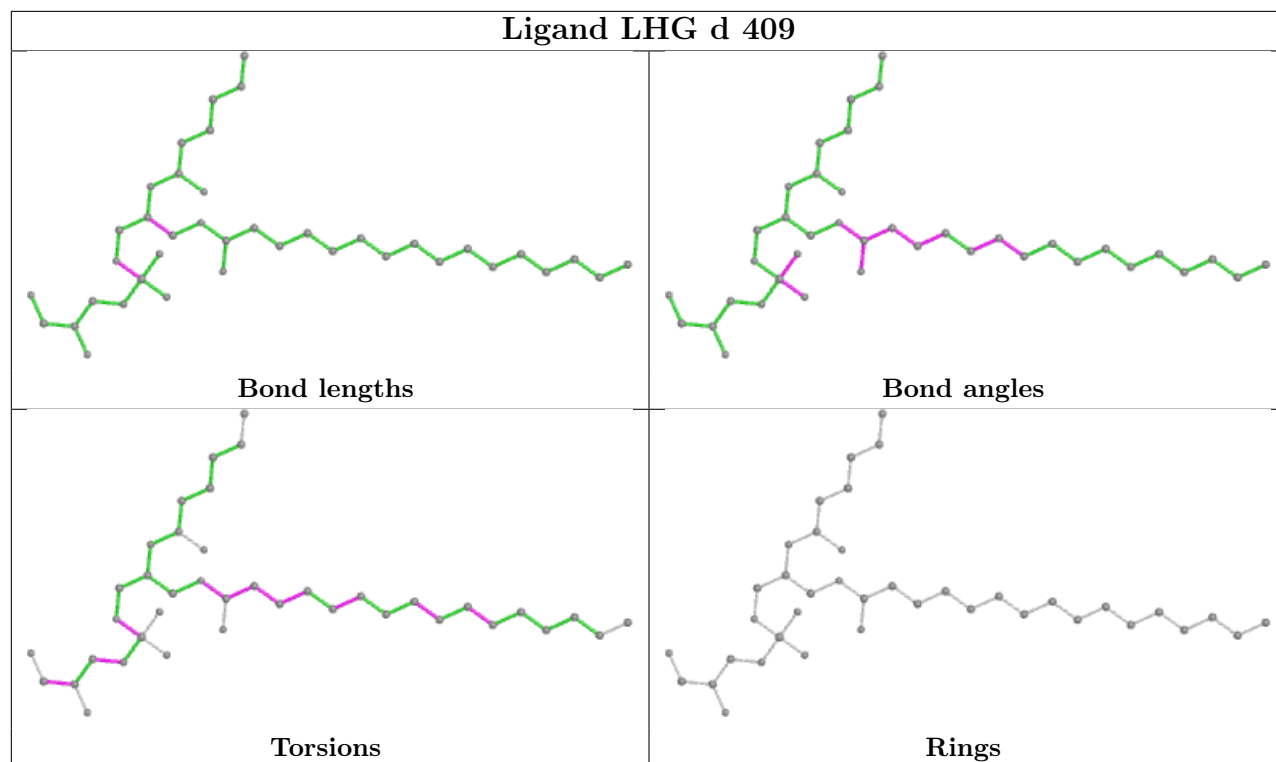


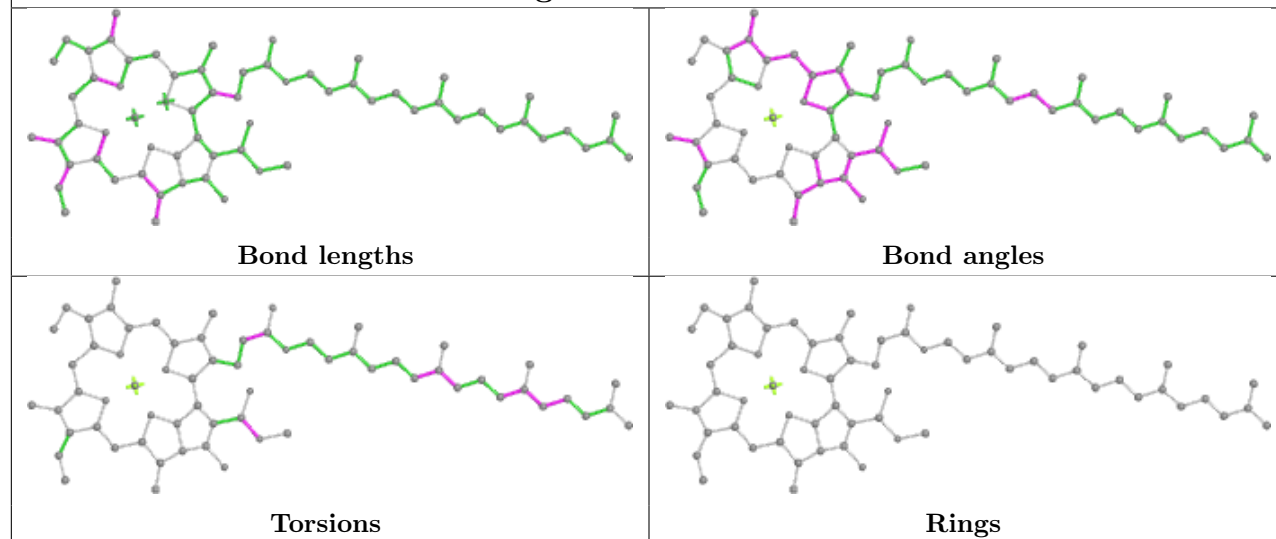
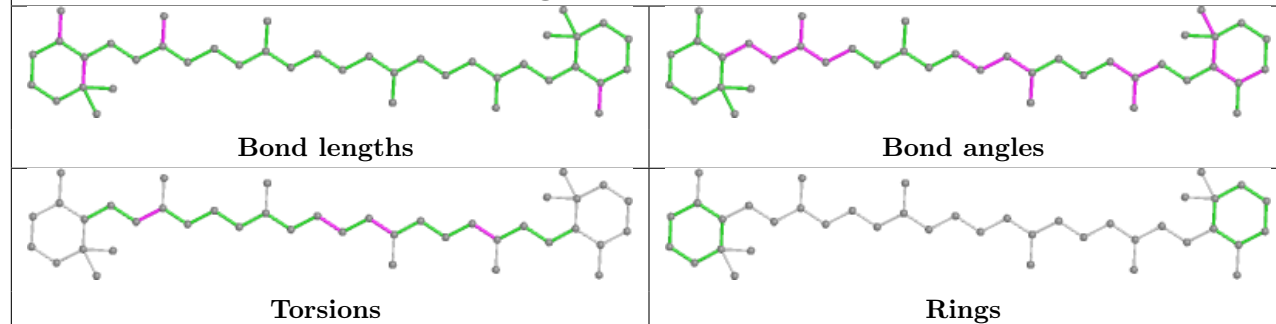
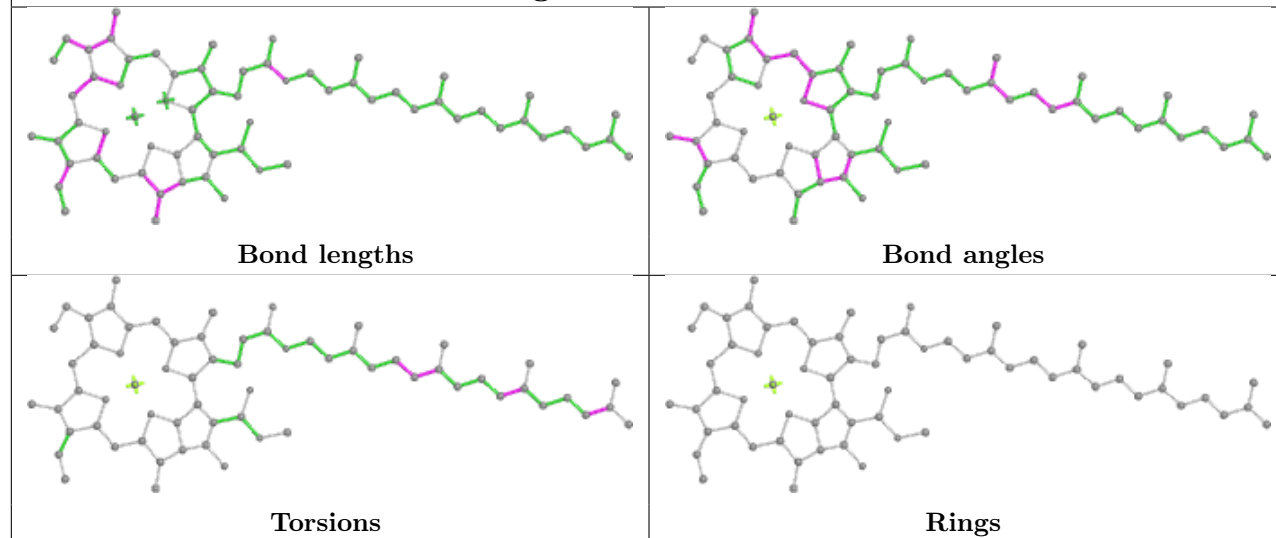


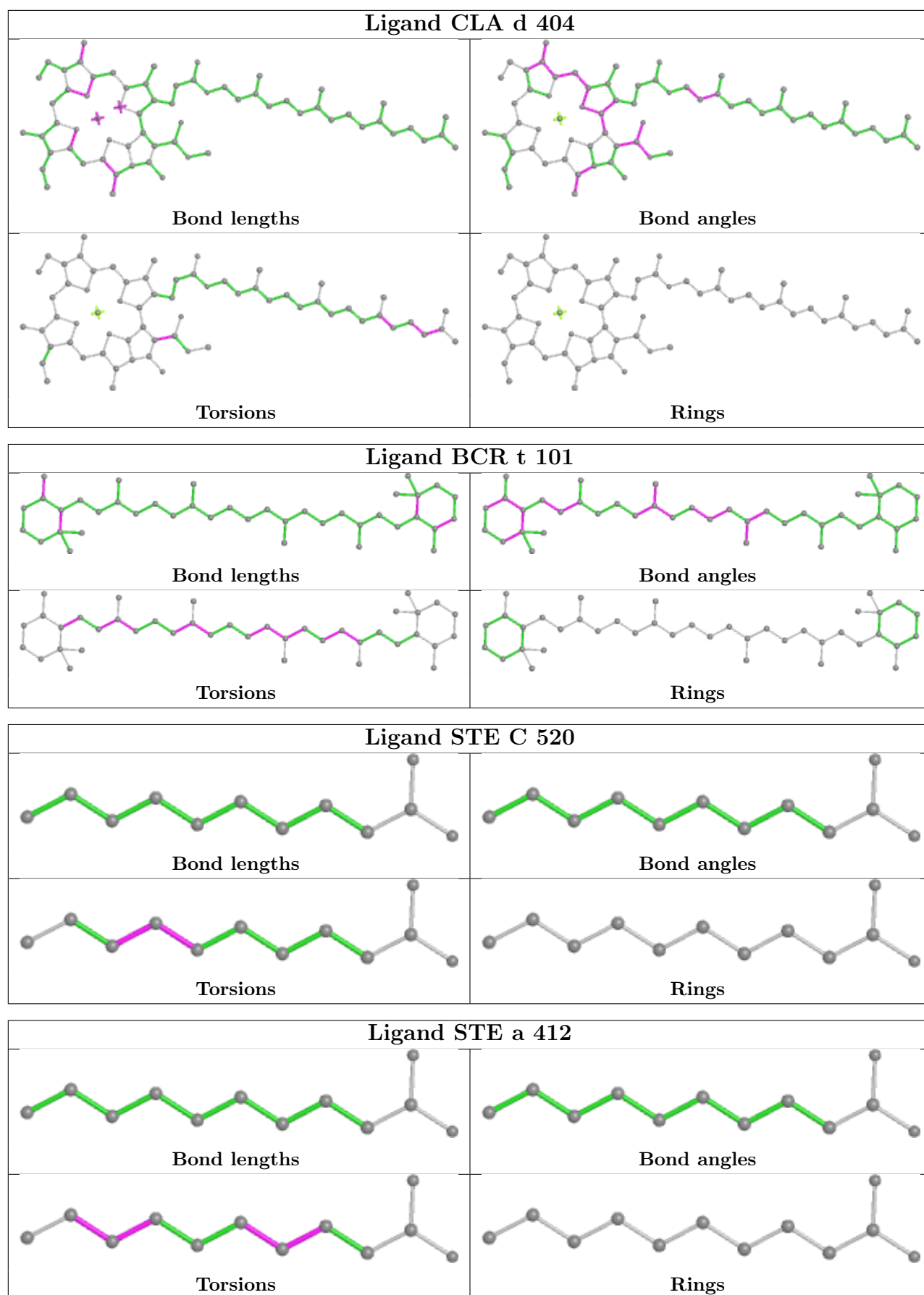


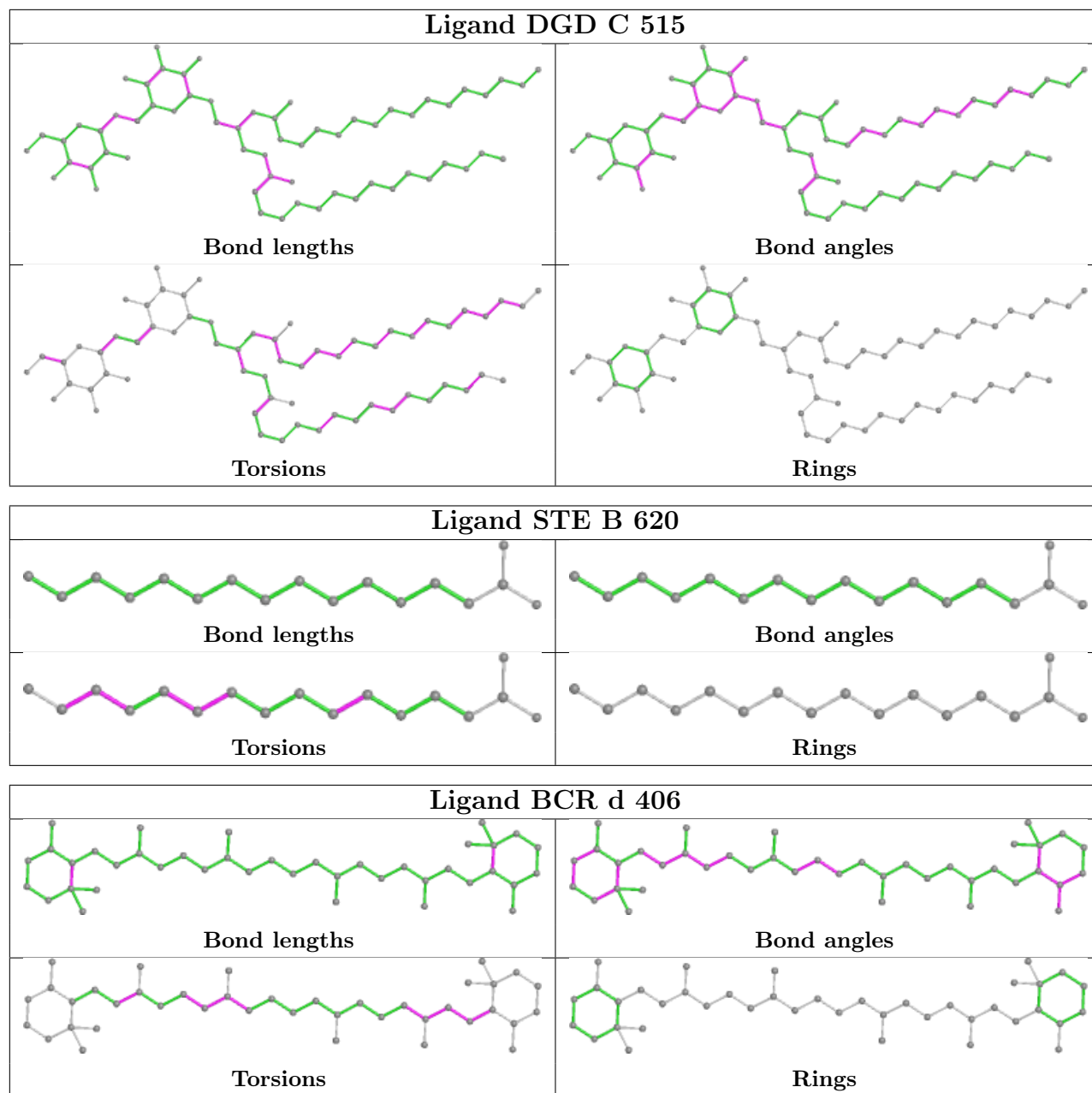




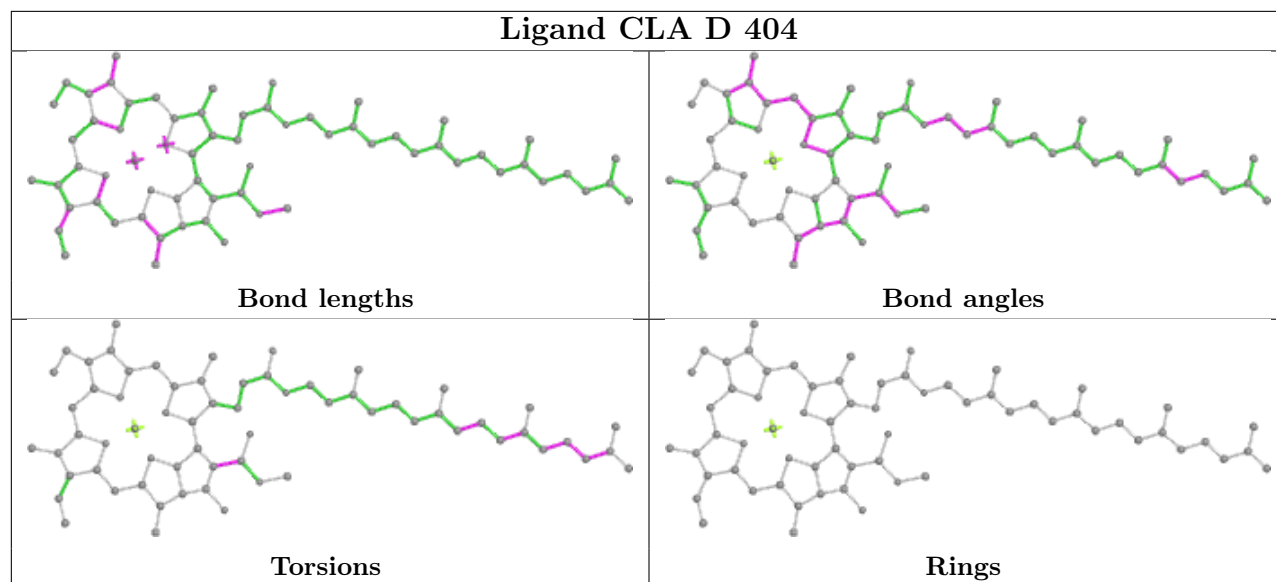


**Ligand CLA b 613****Ligand BCR I 101****Ligand CLA B 615**

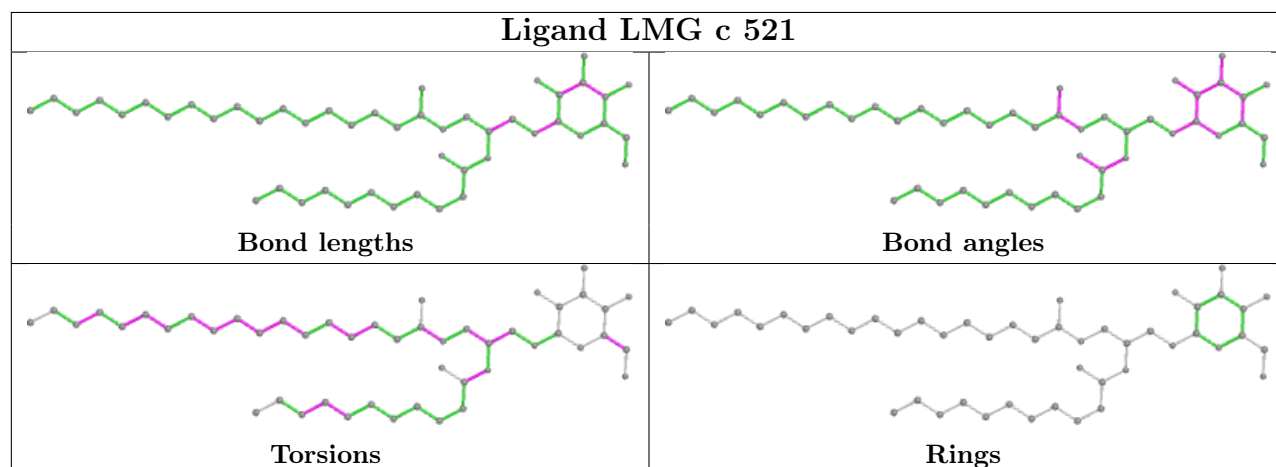




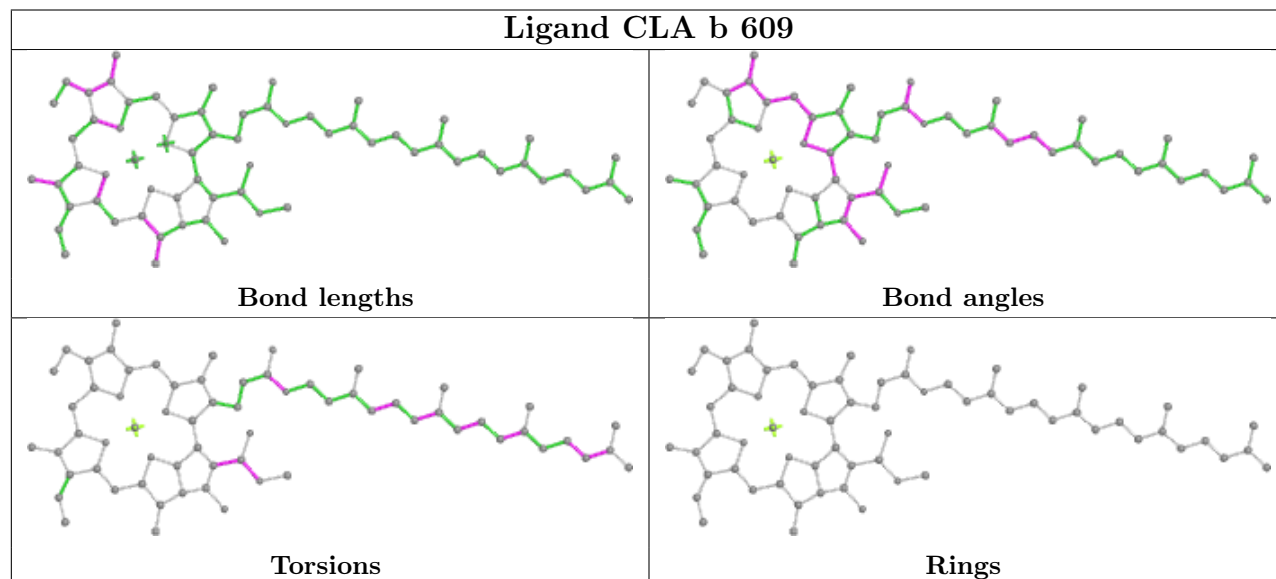
## Ligand CLA D 404

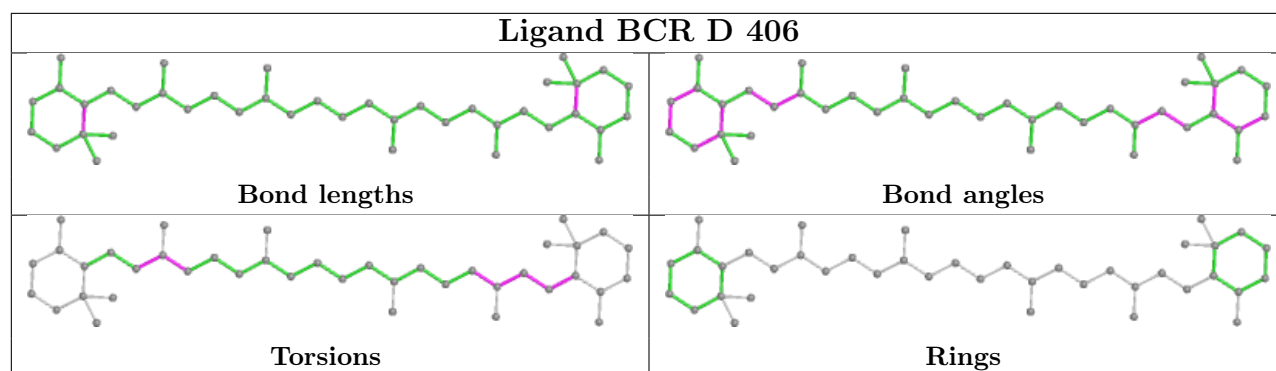
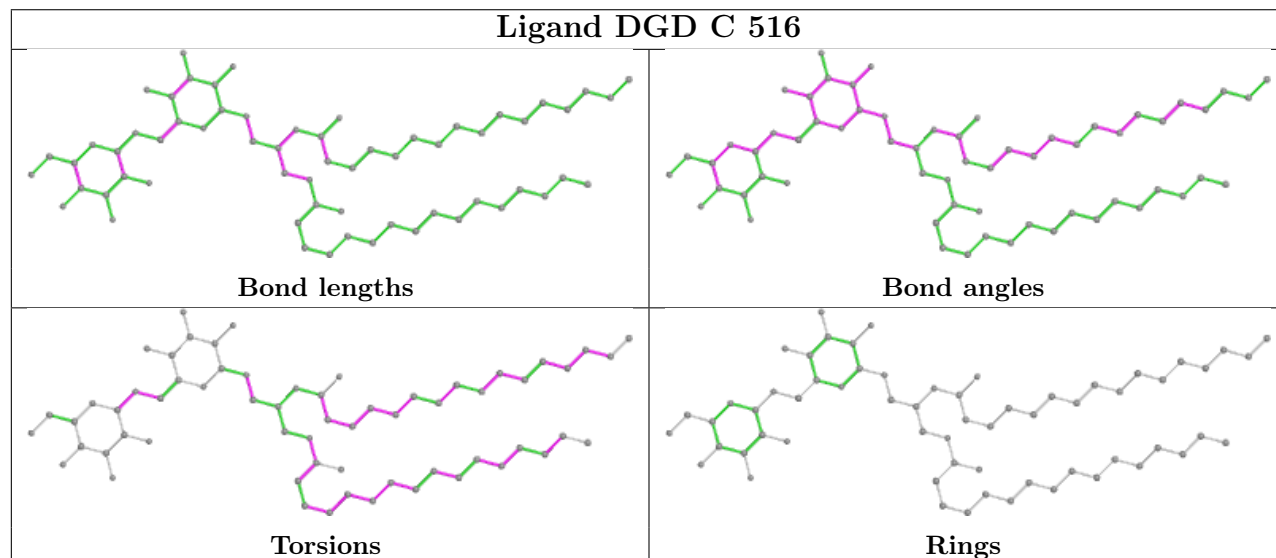
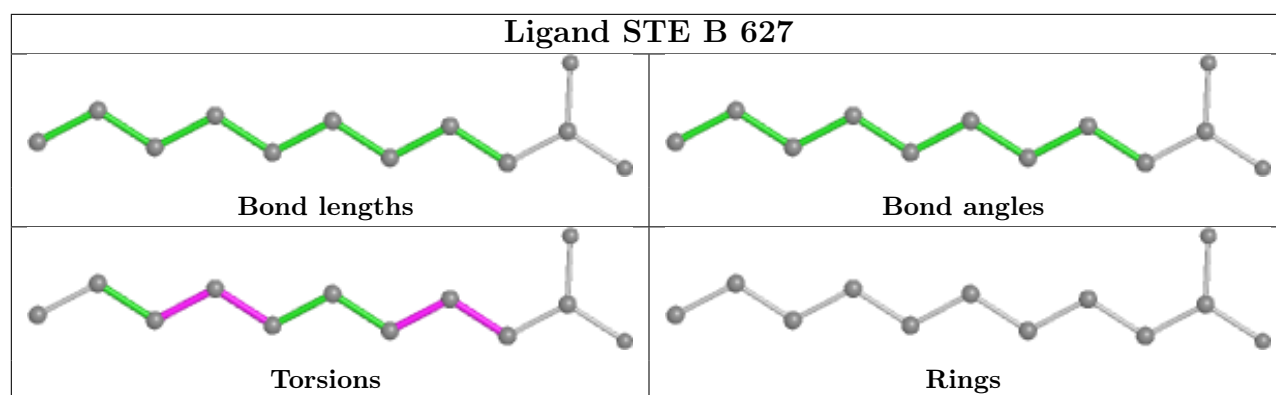


## Ligand LMG c 521



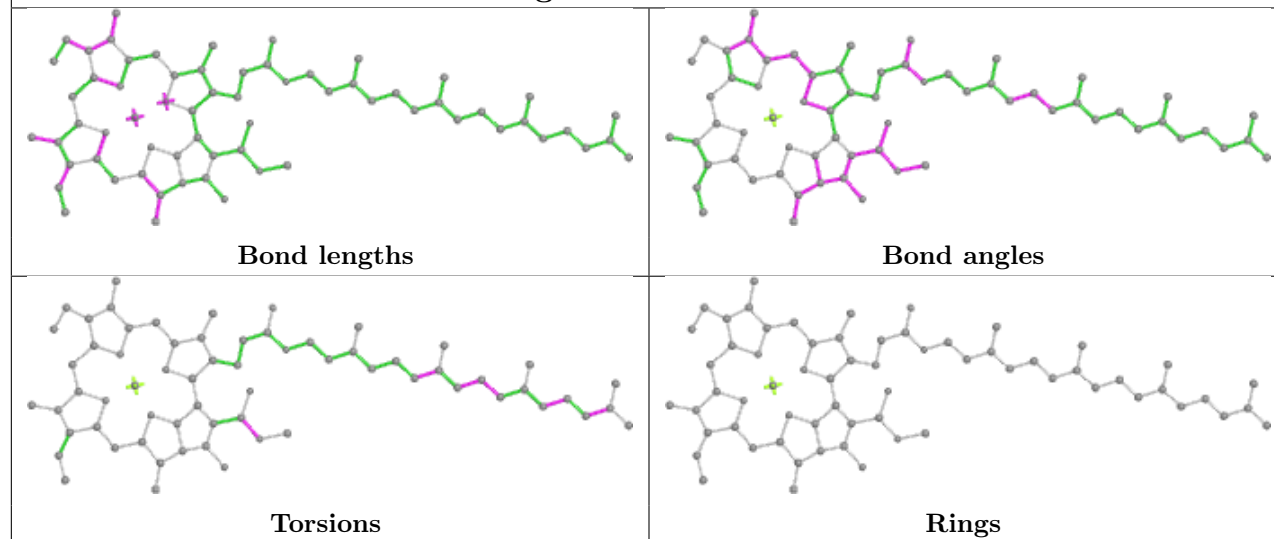
## Ligand CLA b 609



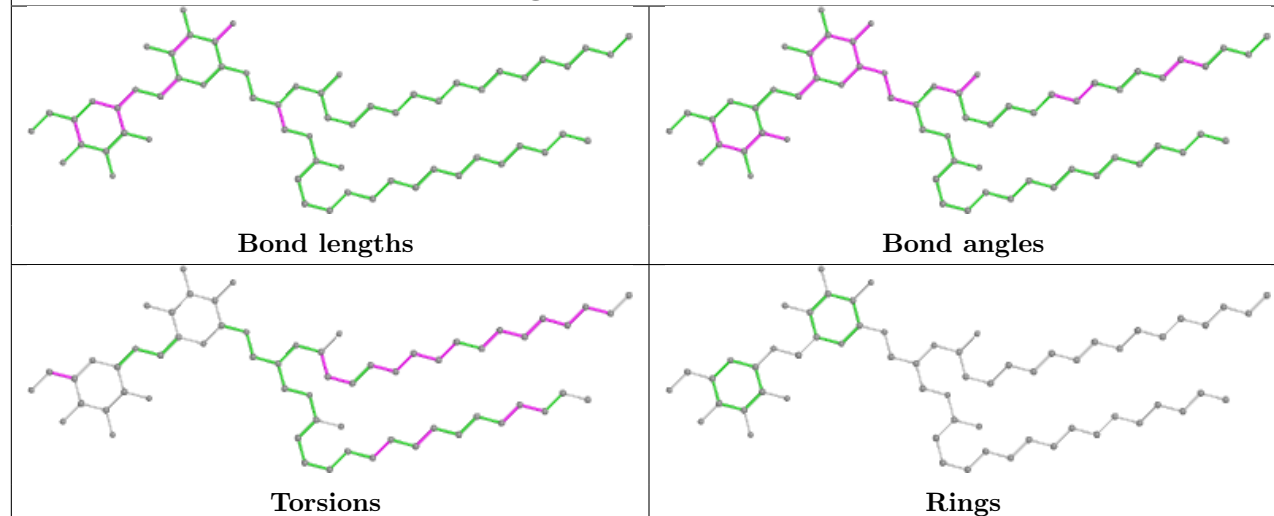




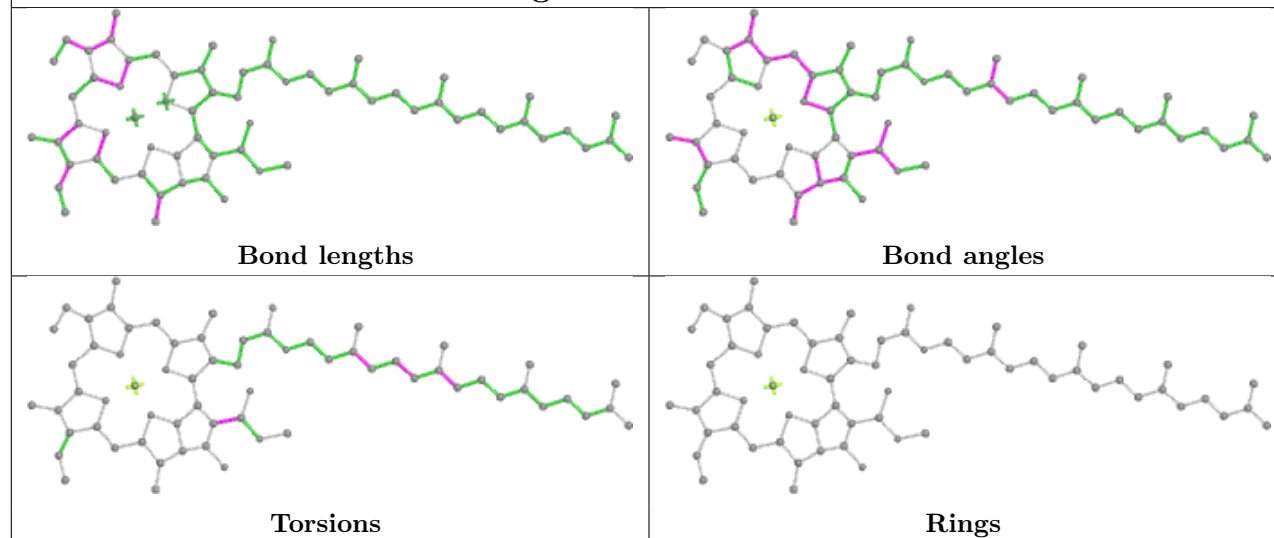
## Ligand CLA b 603

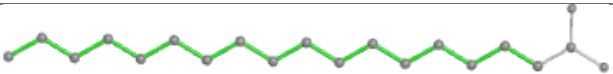
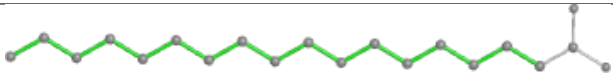
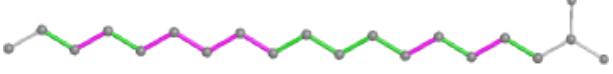
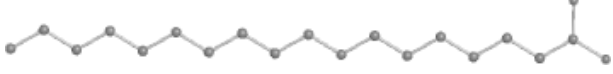


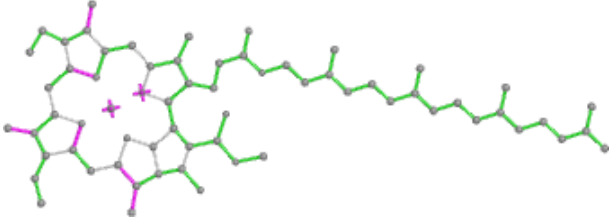
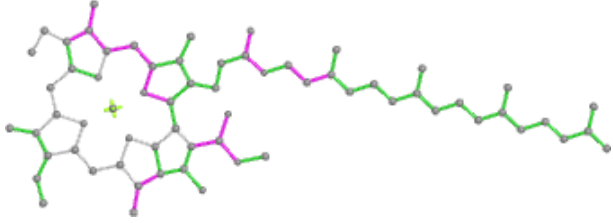
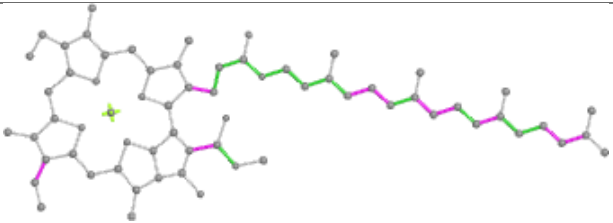
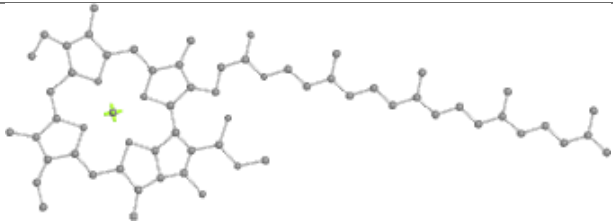
## Ligand DGD H 102

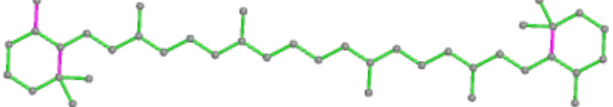
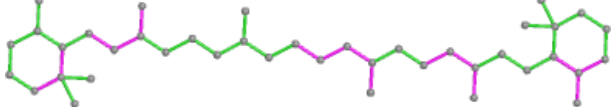
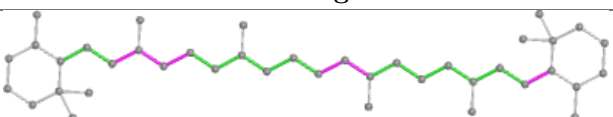
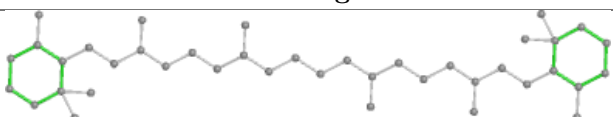


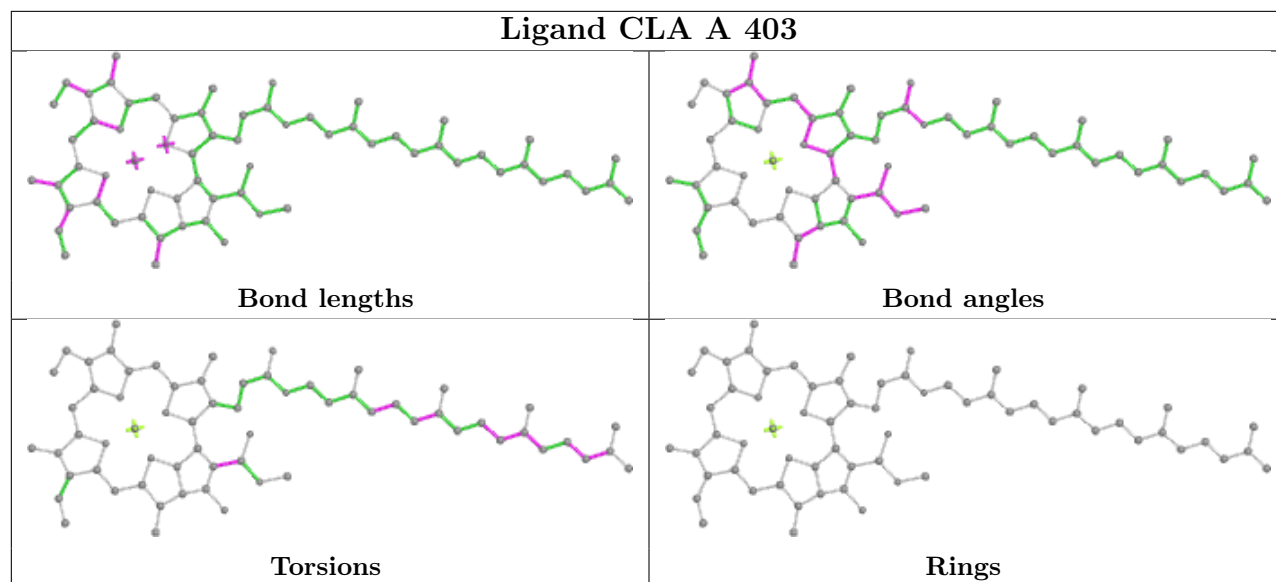
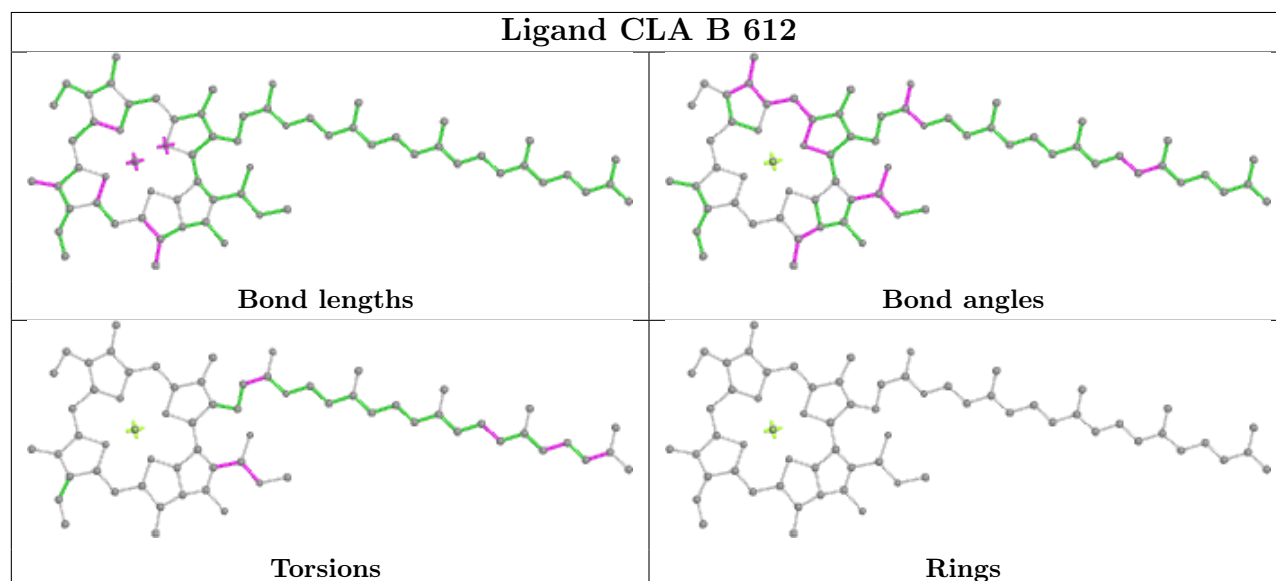
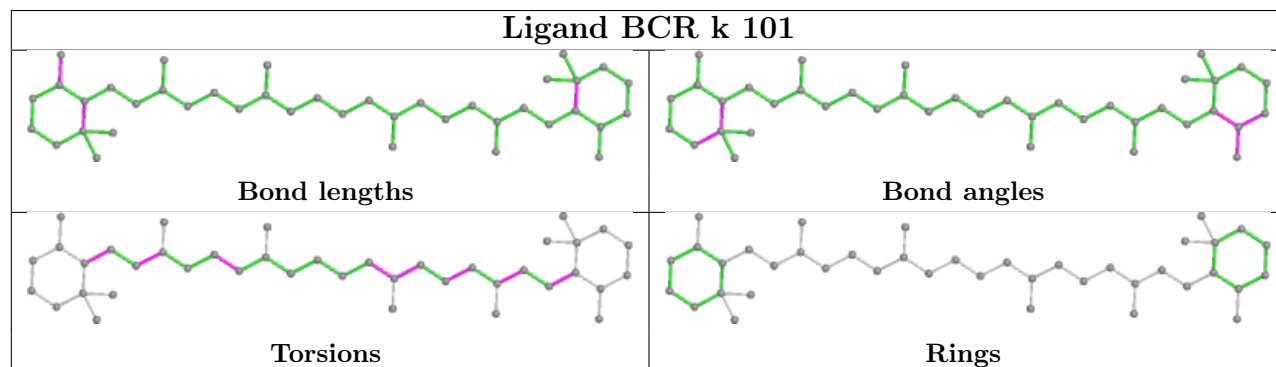
## Ligand CLA C 507

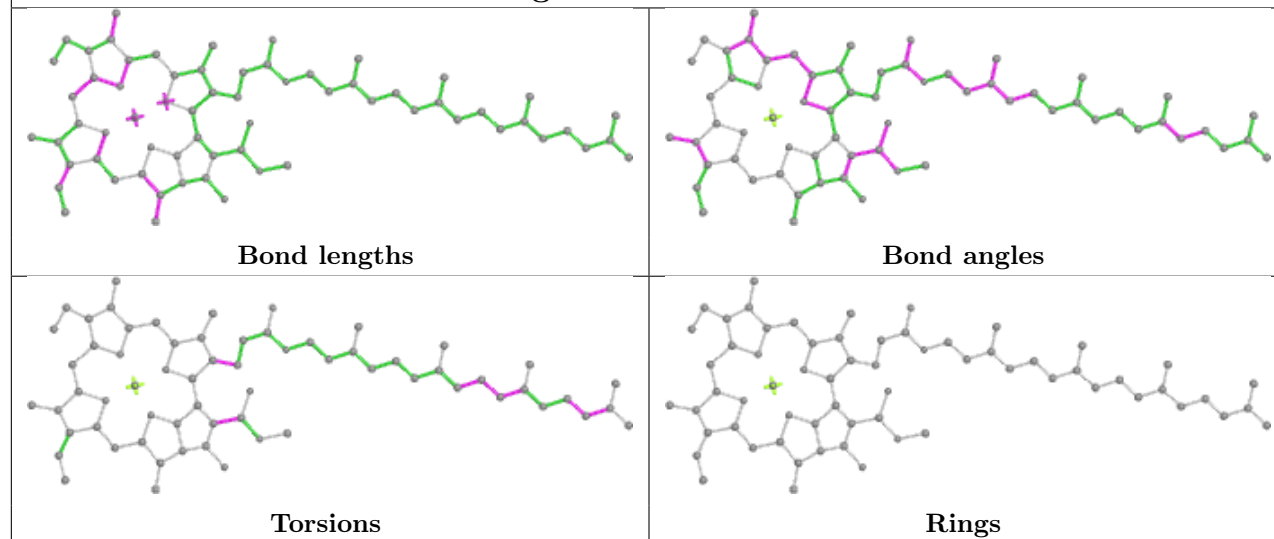
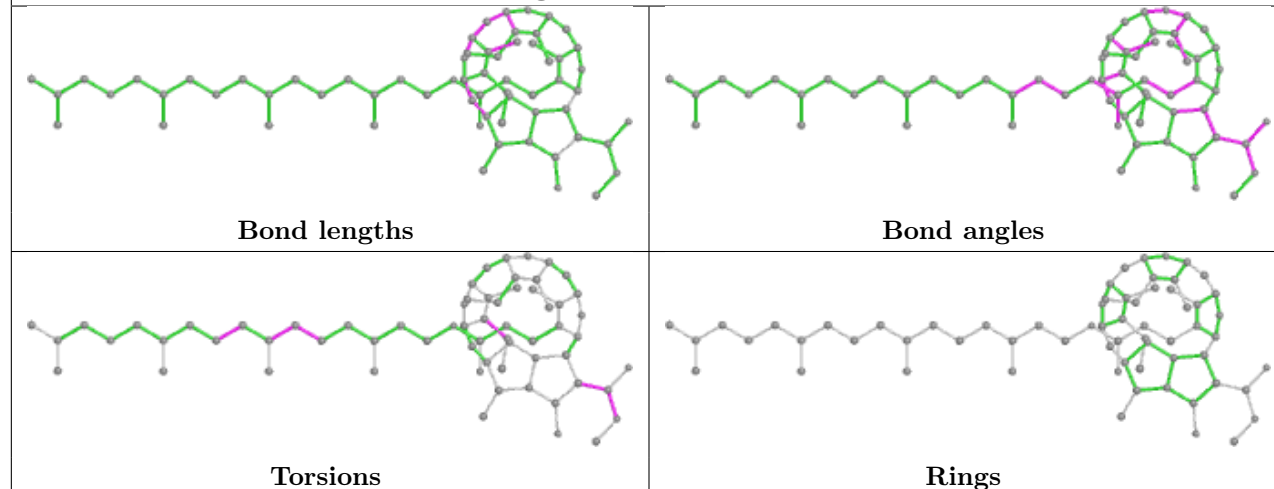
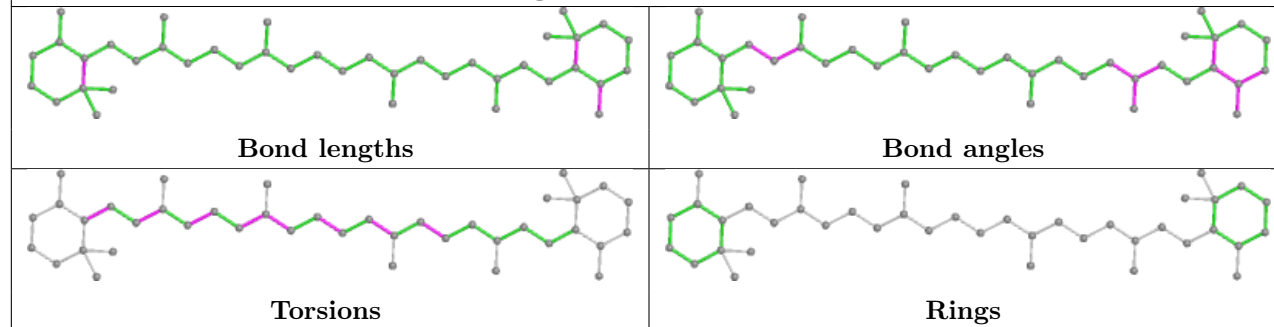


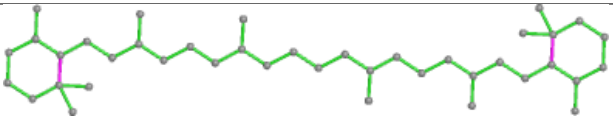
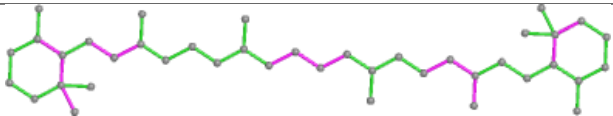
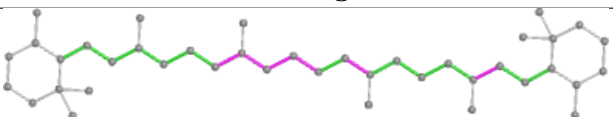
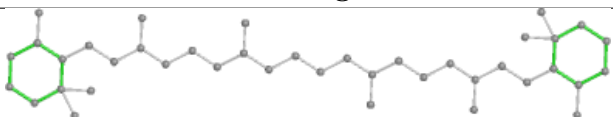
Ligand STE b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings




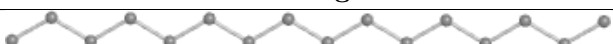
Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

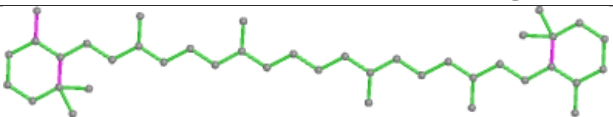
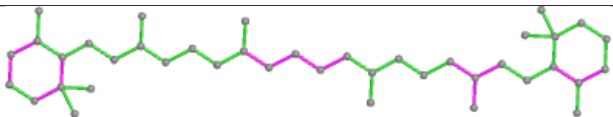
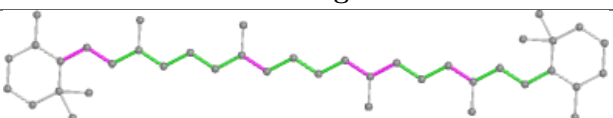
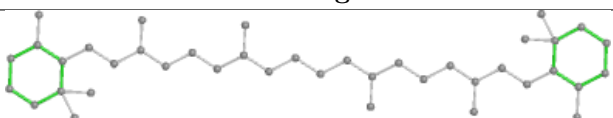
Ligand BCR x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

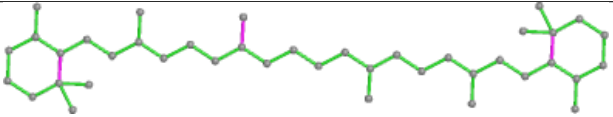
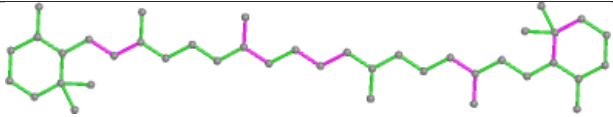
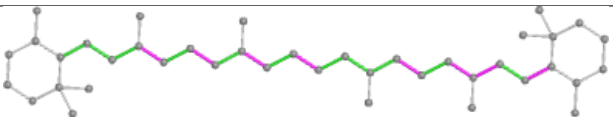
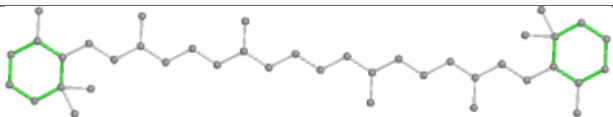
**Ligand CLA A 403****Ligand CLA B 612****Ligand BCR k 101**

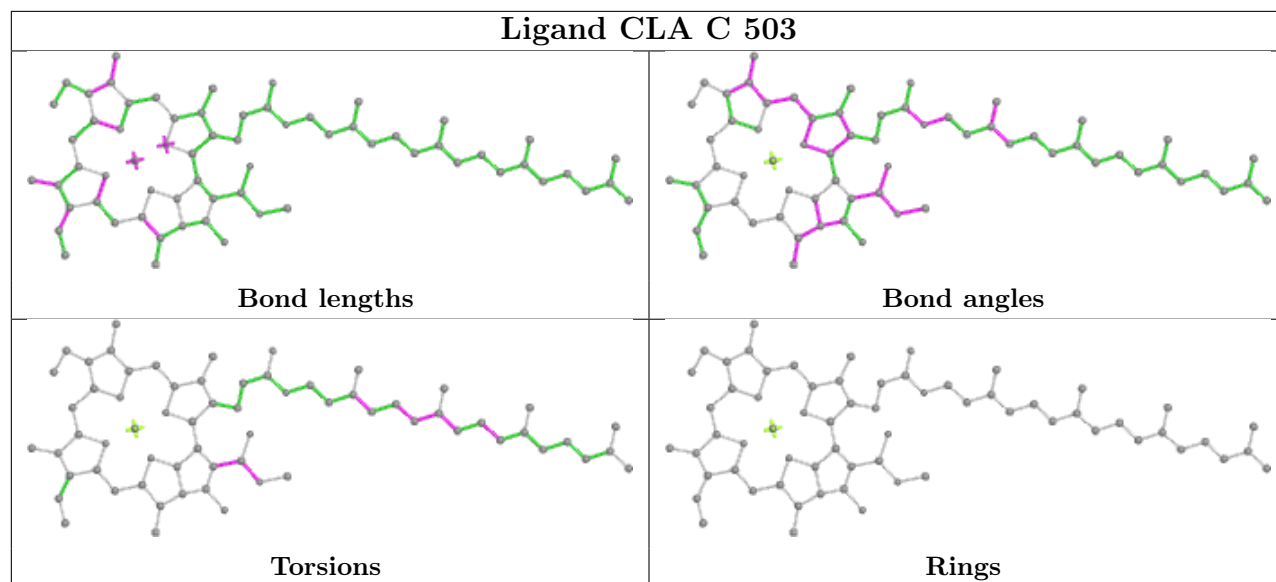
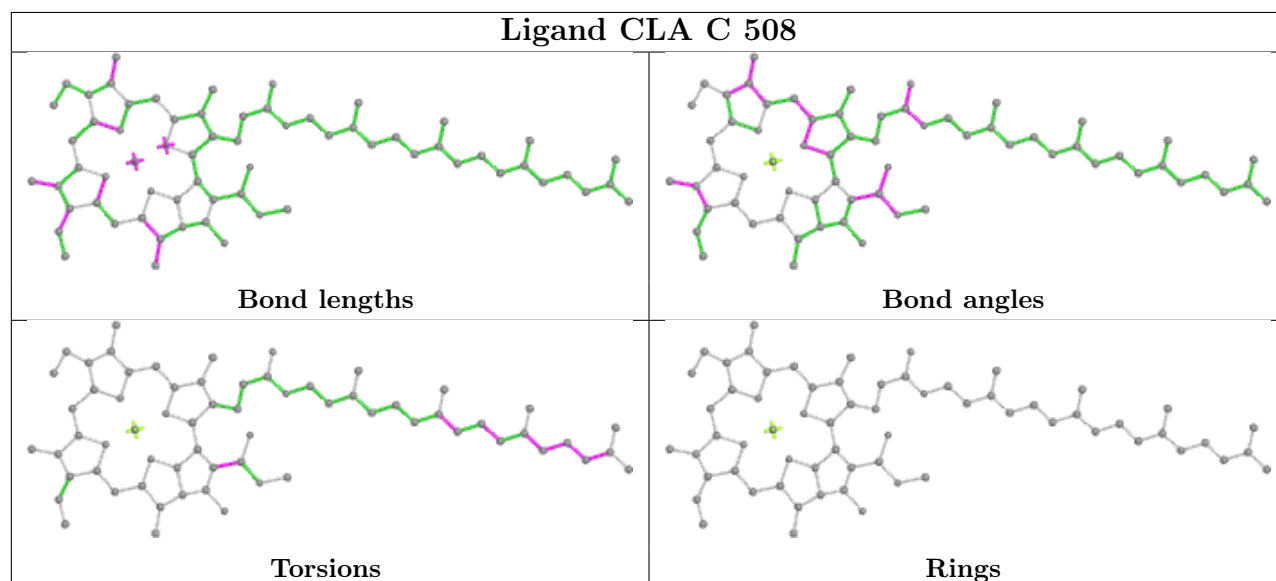
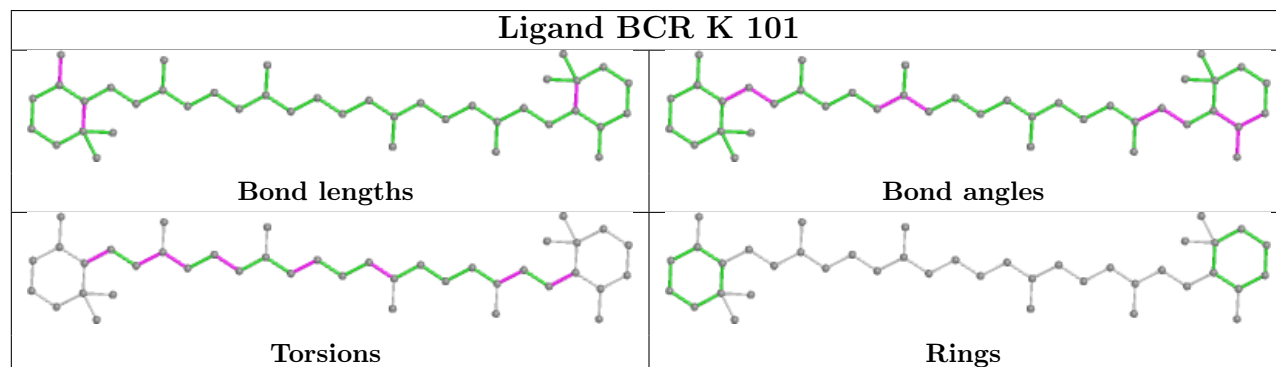
**Ligand CLA B 602****Ligand PHO d 402****Ligand BCR T 101**

Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

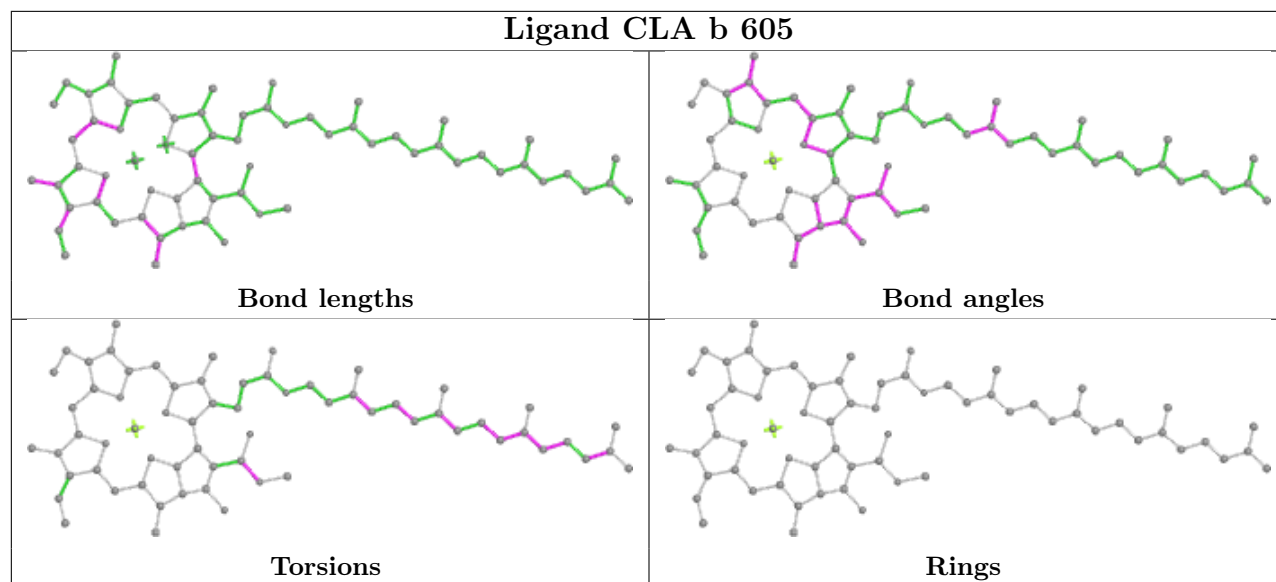
Ligand STE C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

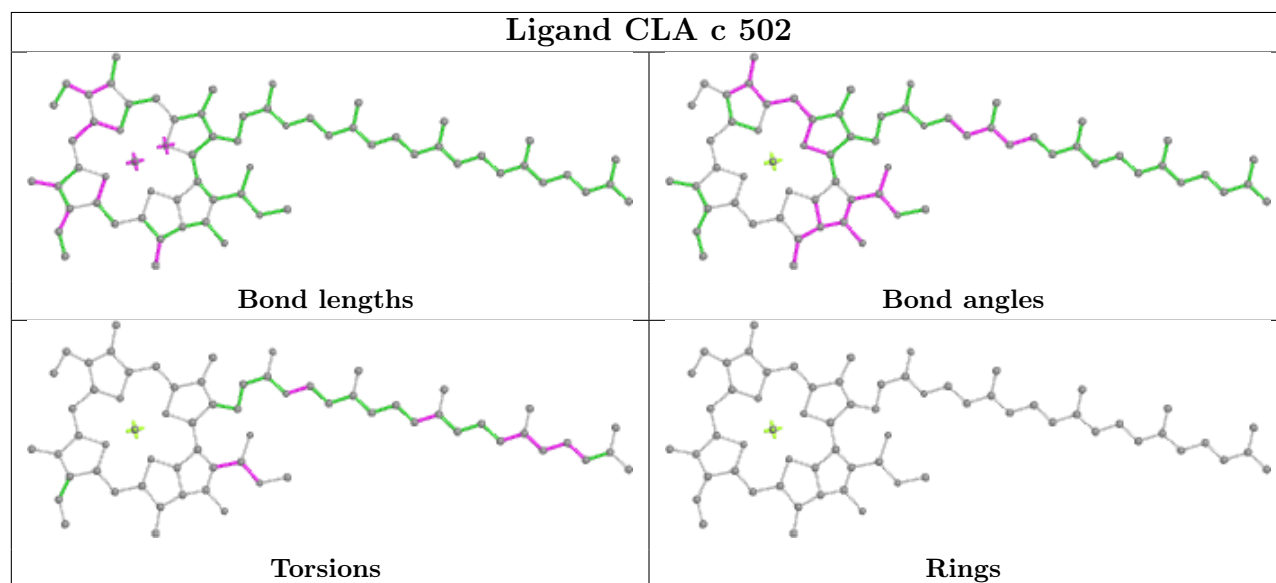
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

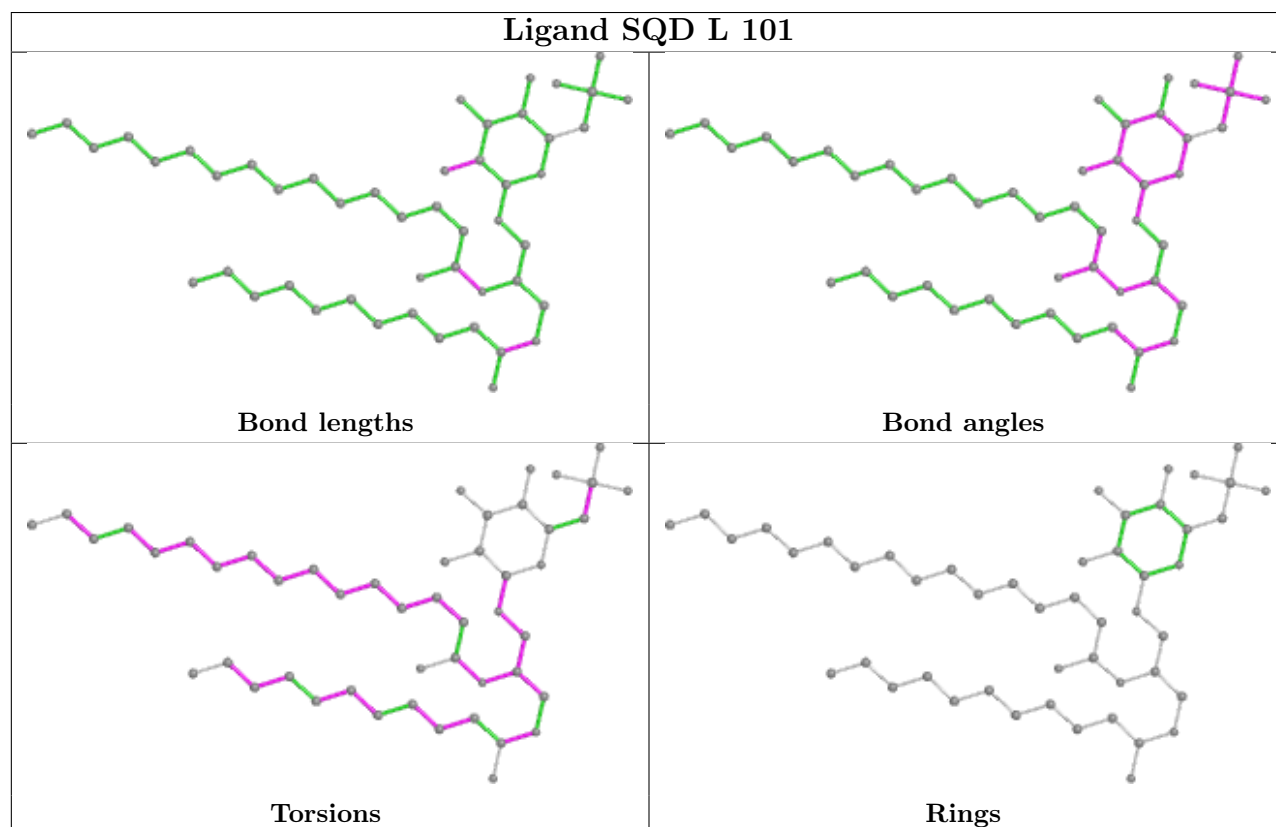
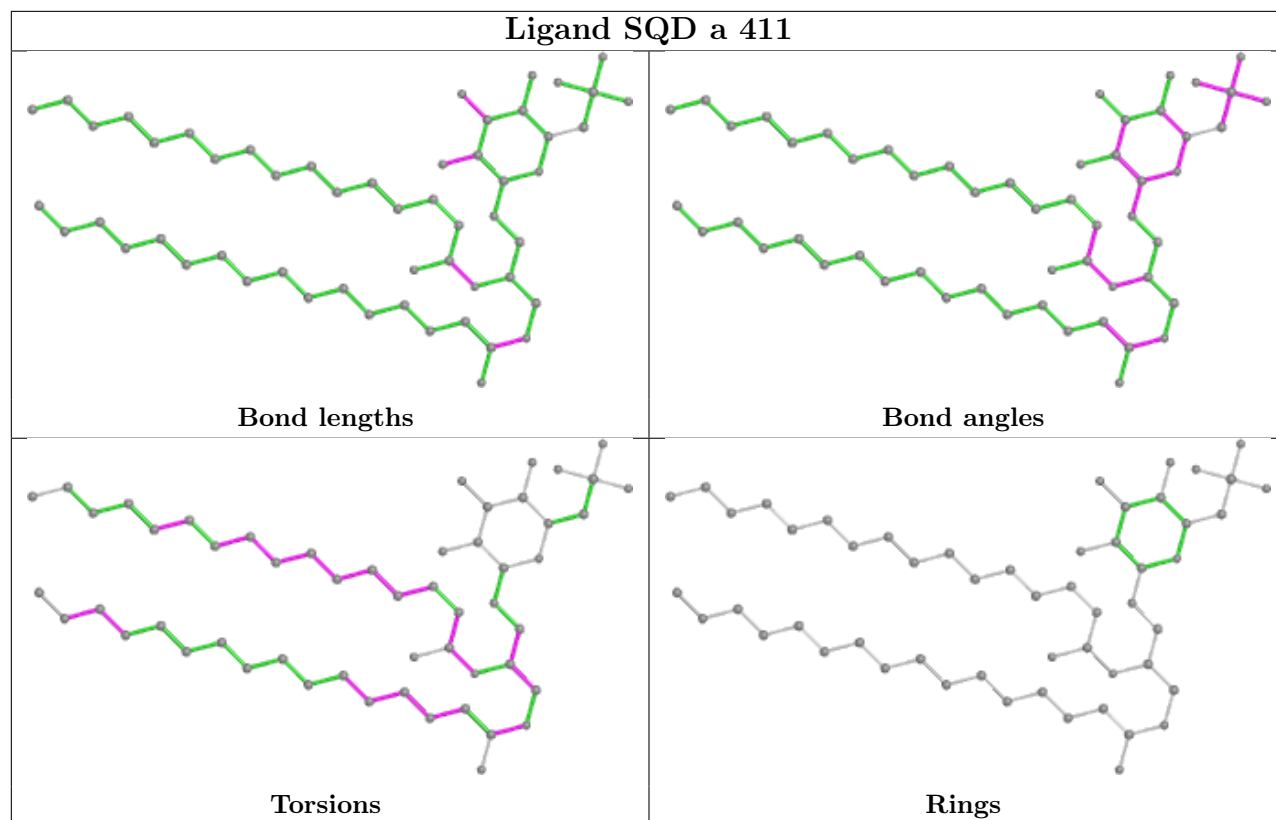
**Ligand CLA C 503****Ligand CLA C 508****Ligand BCR K 101**

## Ligand CLA b 605

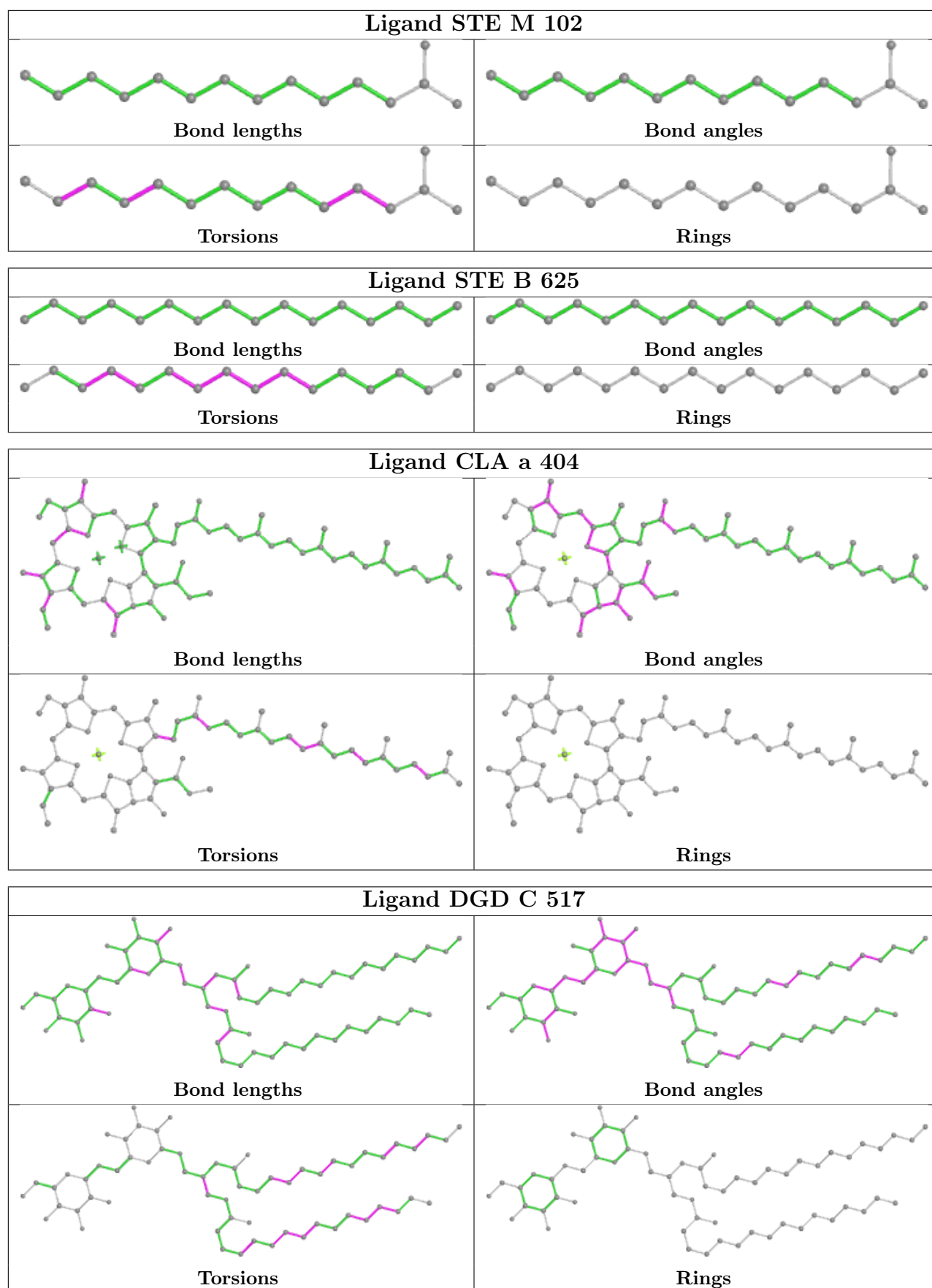


## Ligand CLA c 502

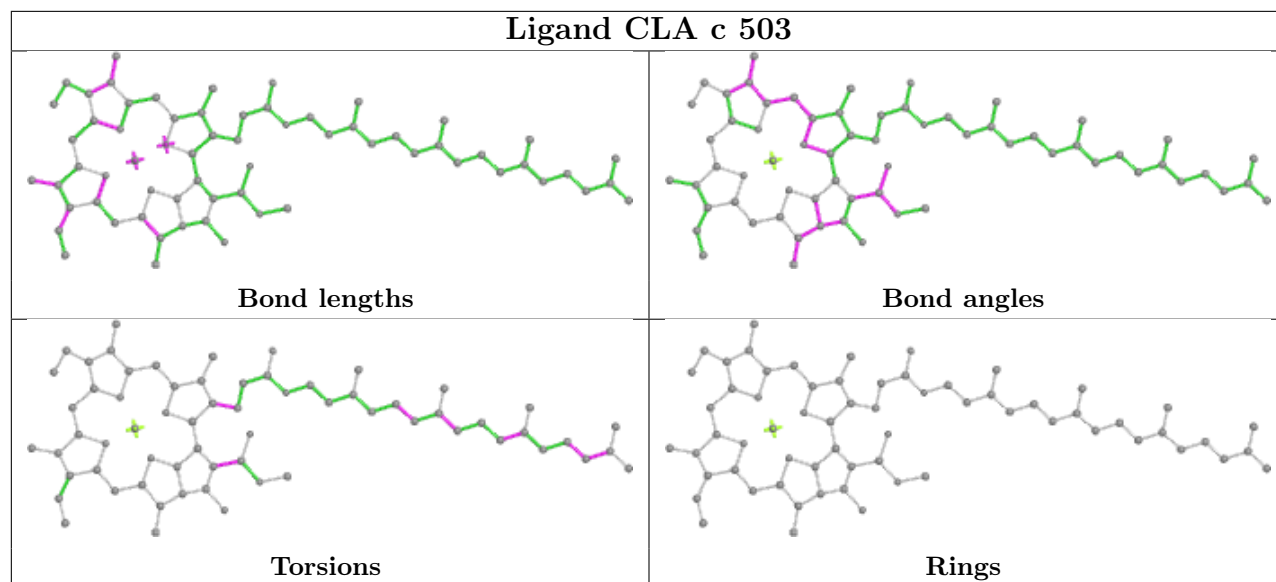




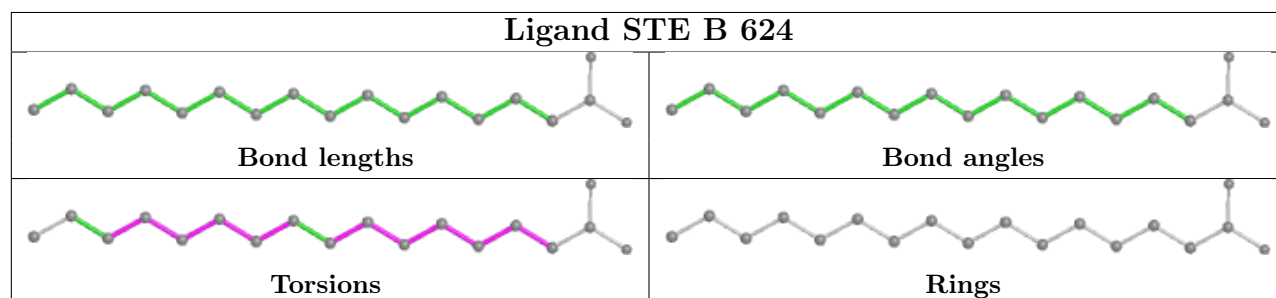




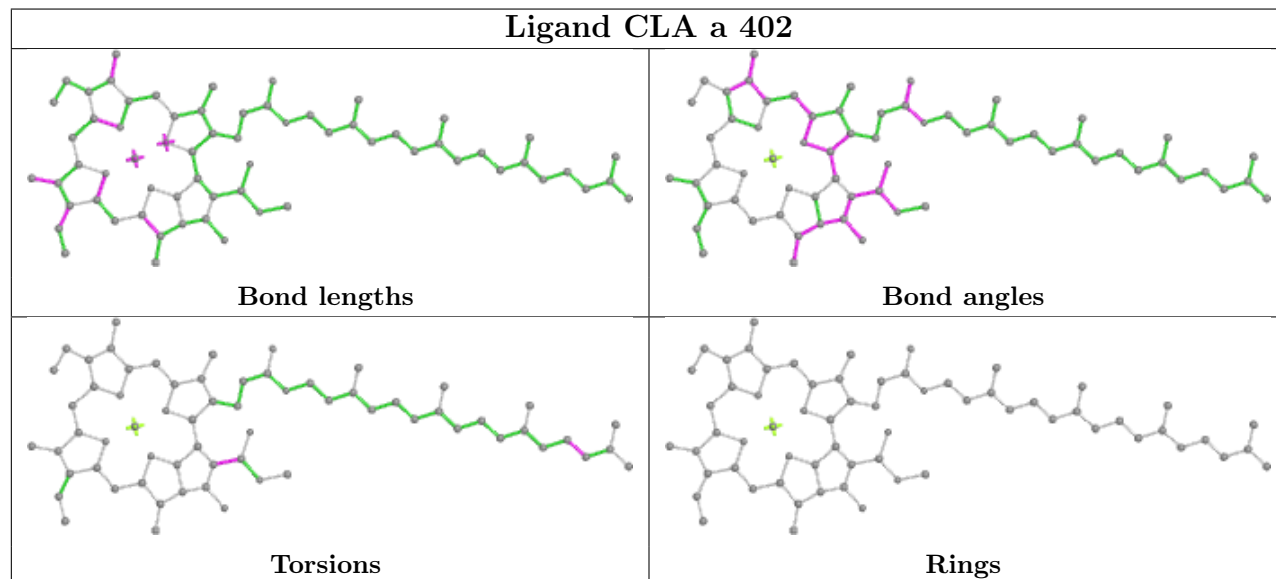
## Ligand CLA c 503

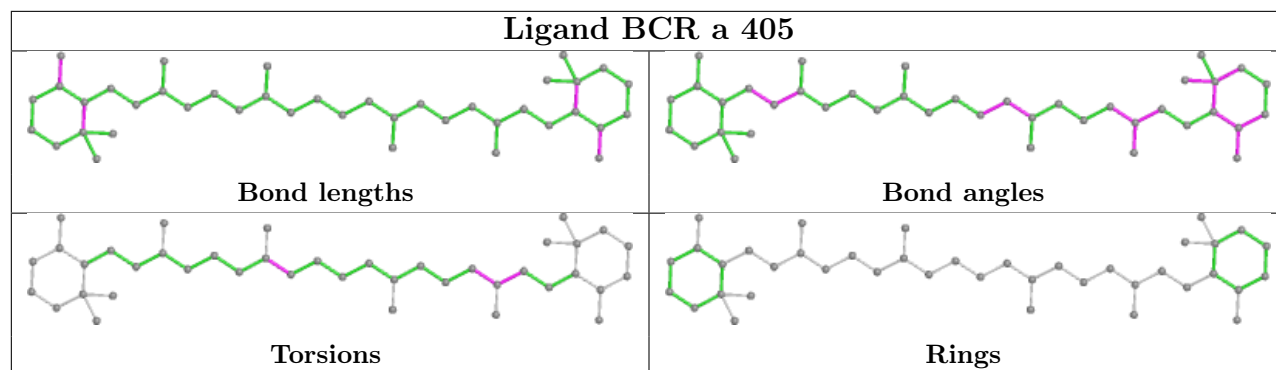
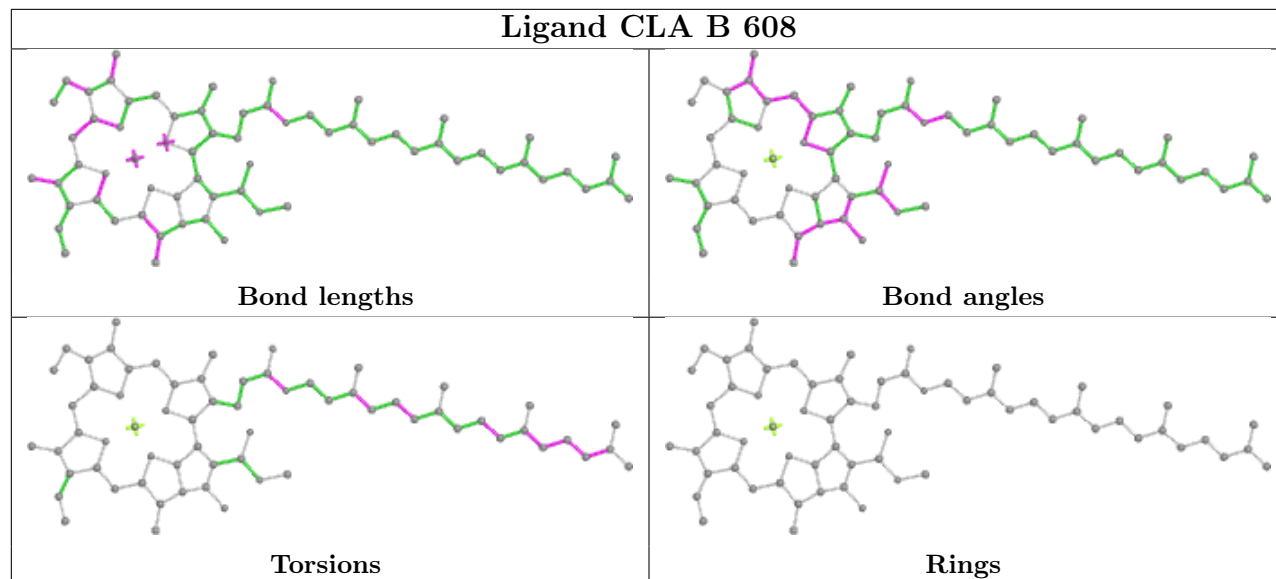
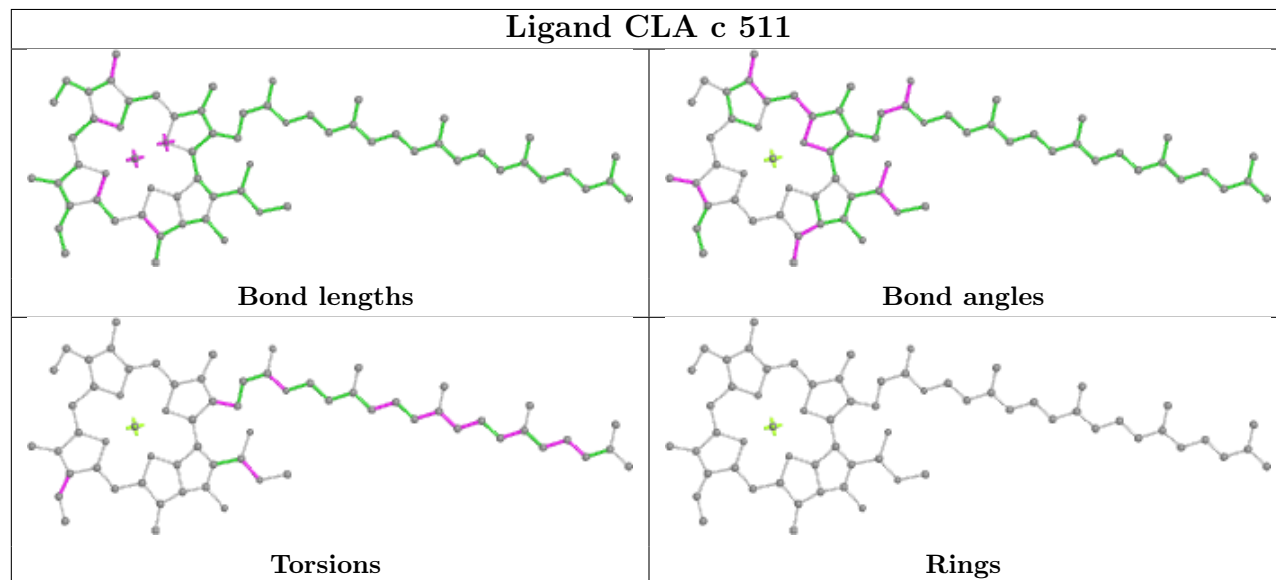


## Ligand STE B 624

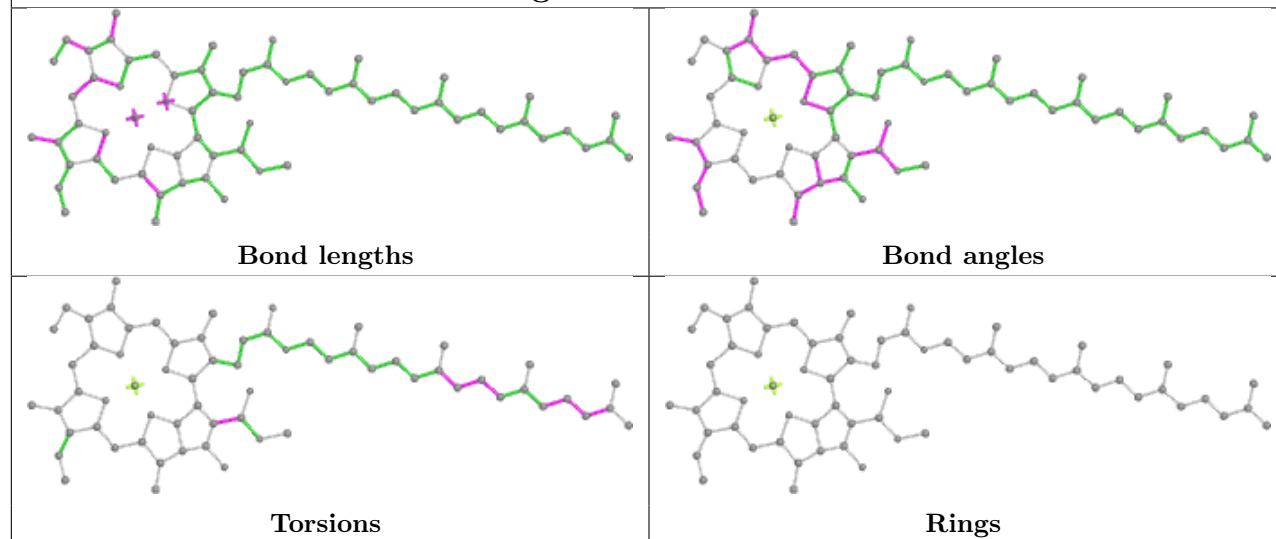


## Ligand CLA a 402

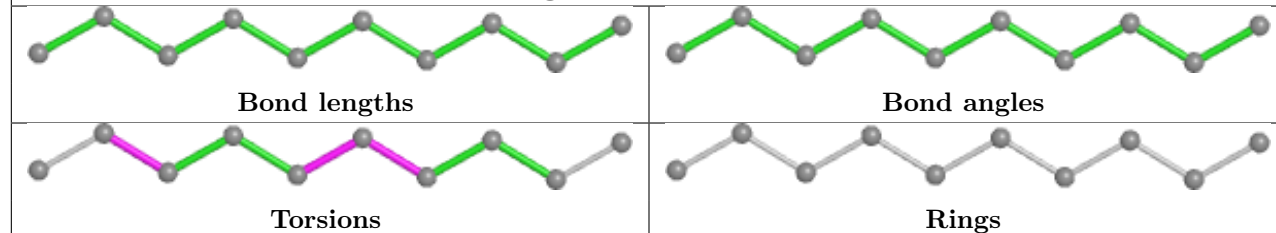


**Ligand BCR a 405****Ligand CLA B 608****Ligand CLA c 511**

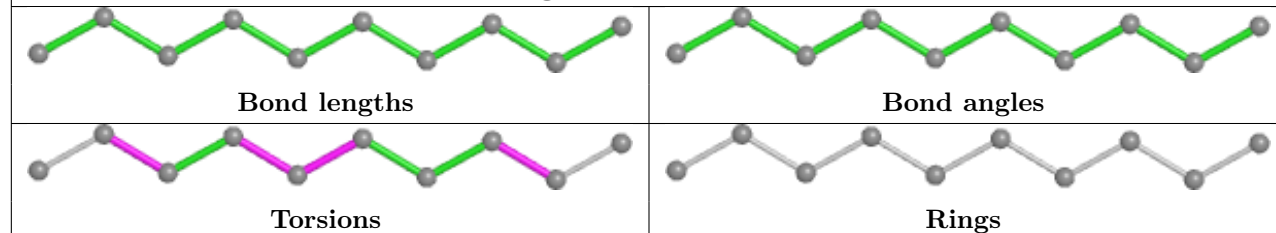
## Ligand CLA C 513



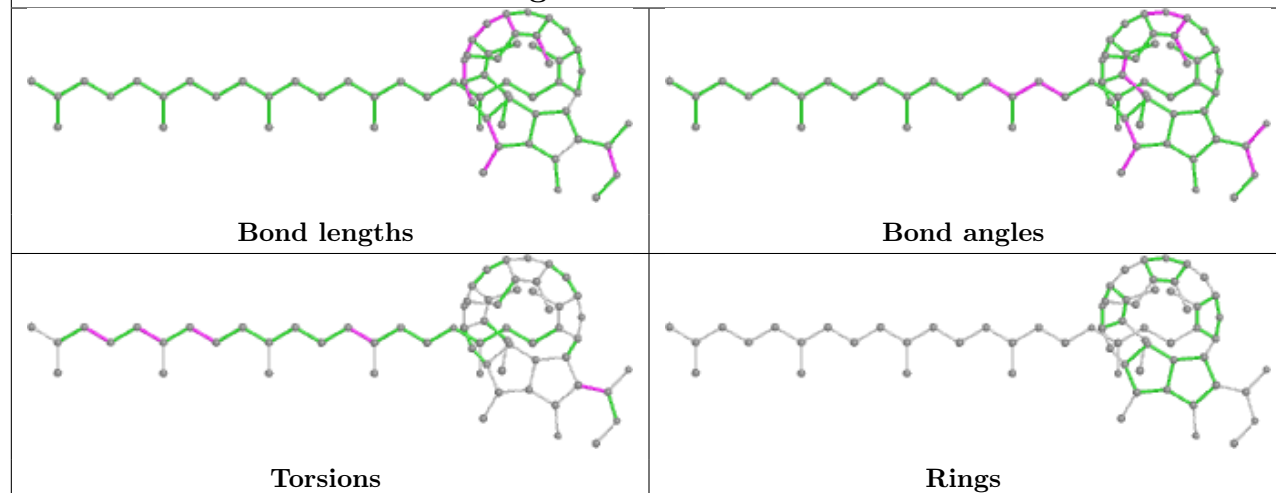
## Ligand STE t 104

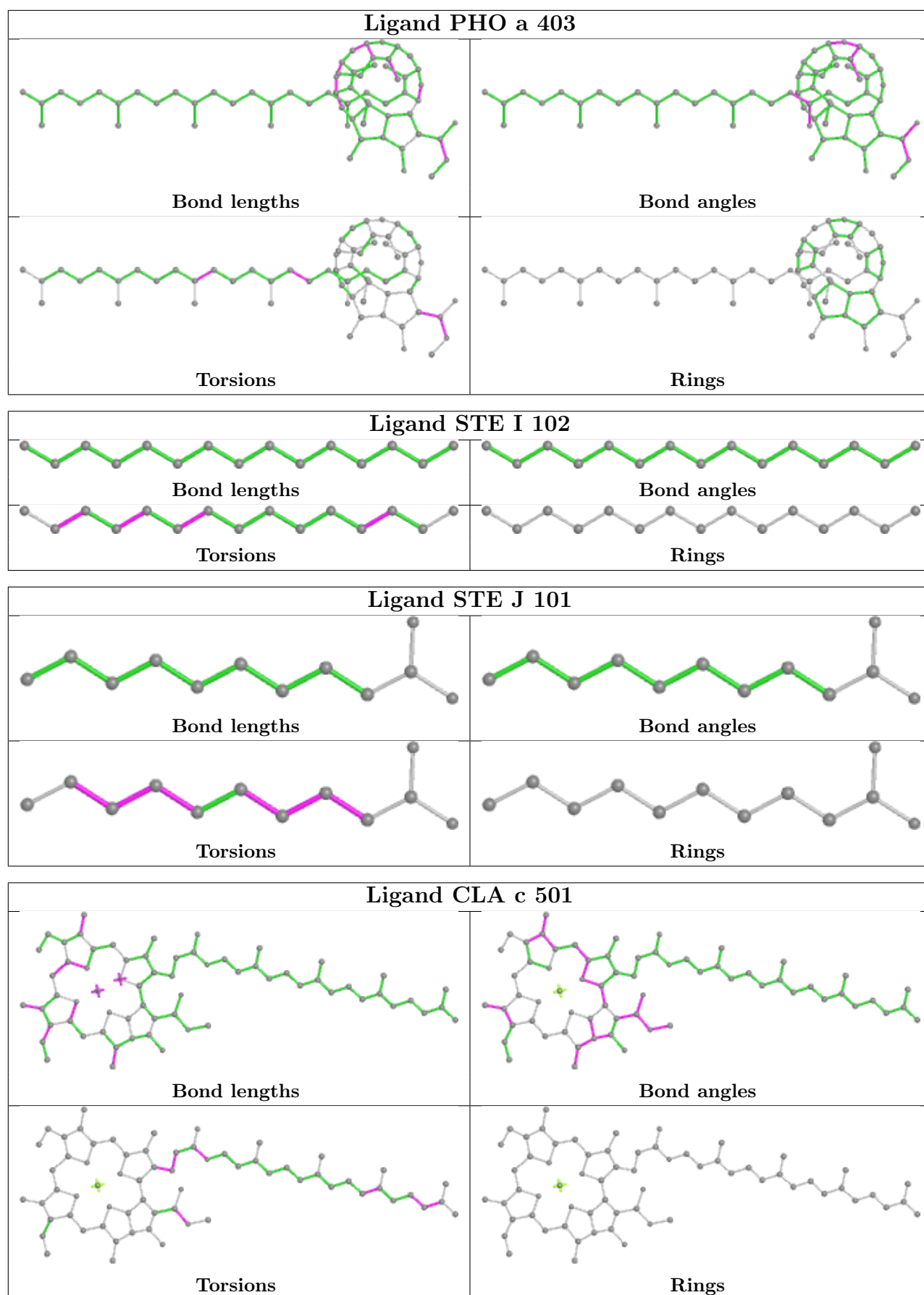


## Ligand STE b 626

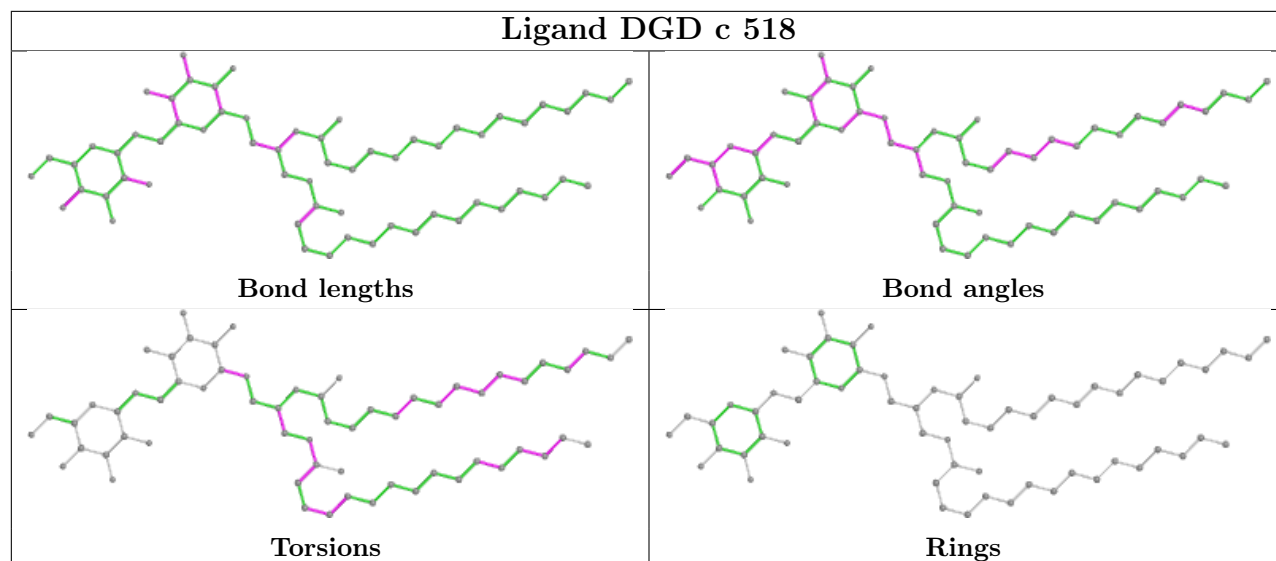


## Ligand PHO A 404

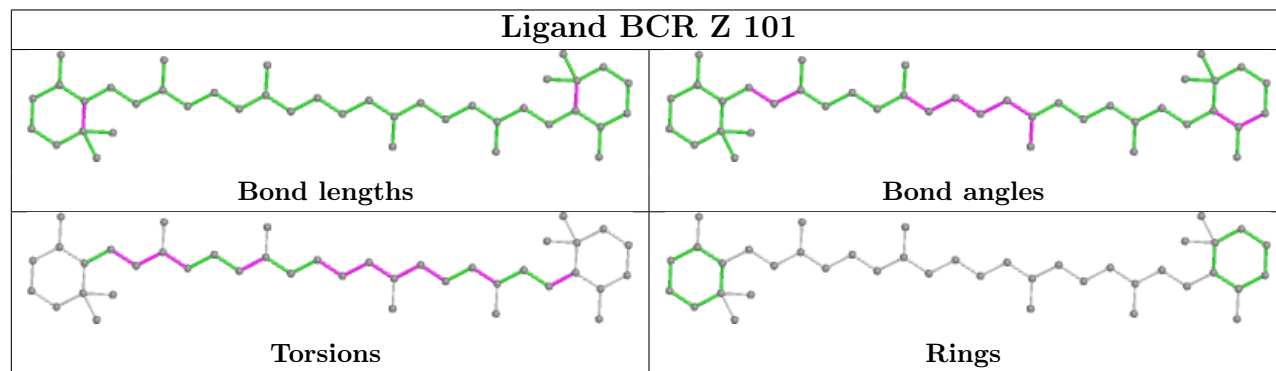


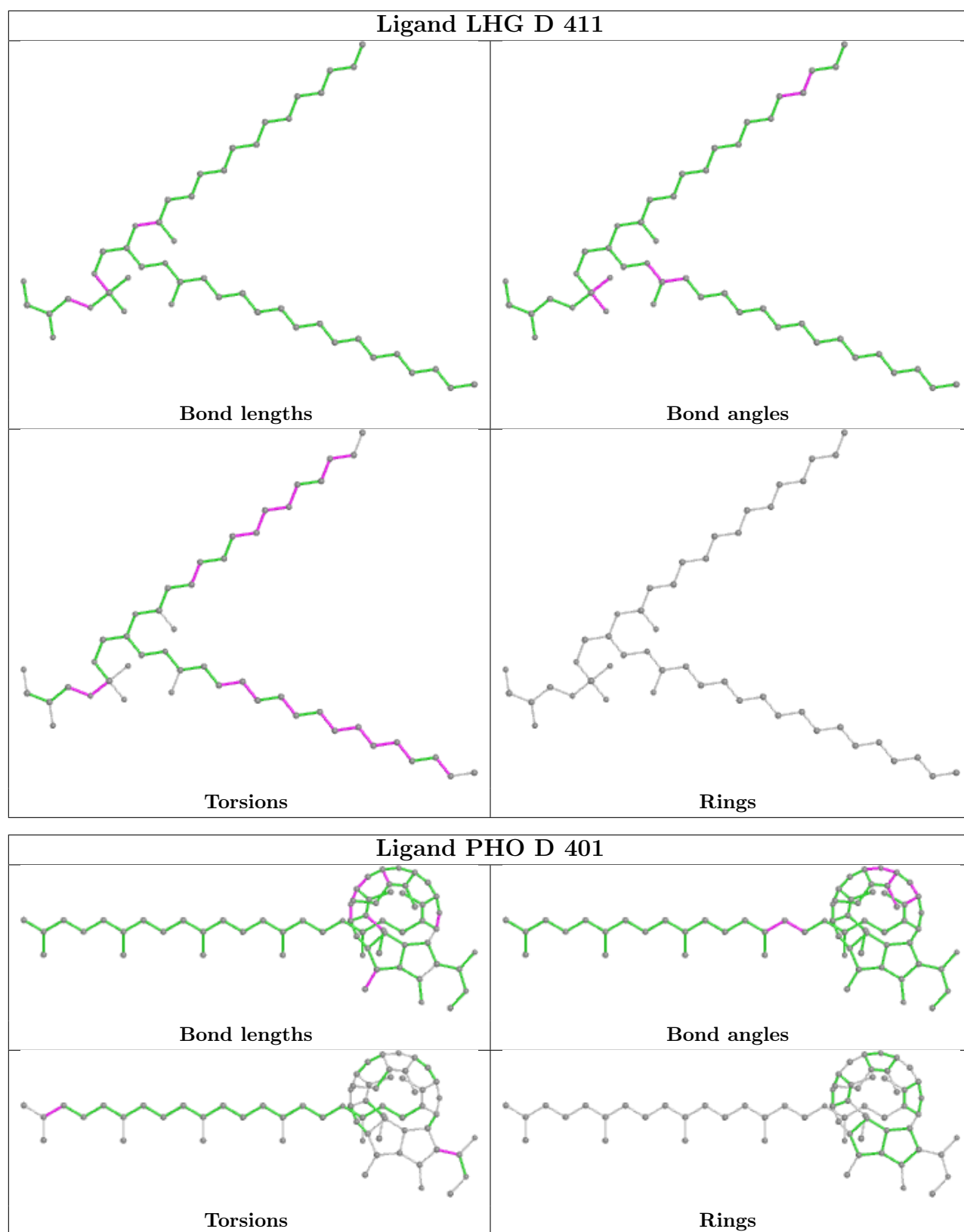


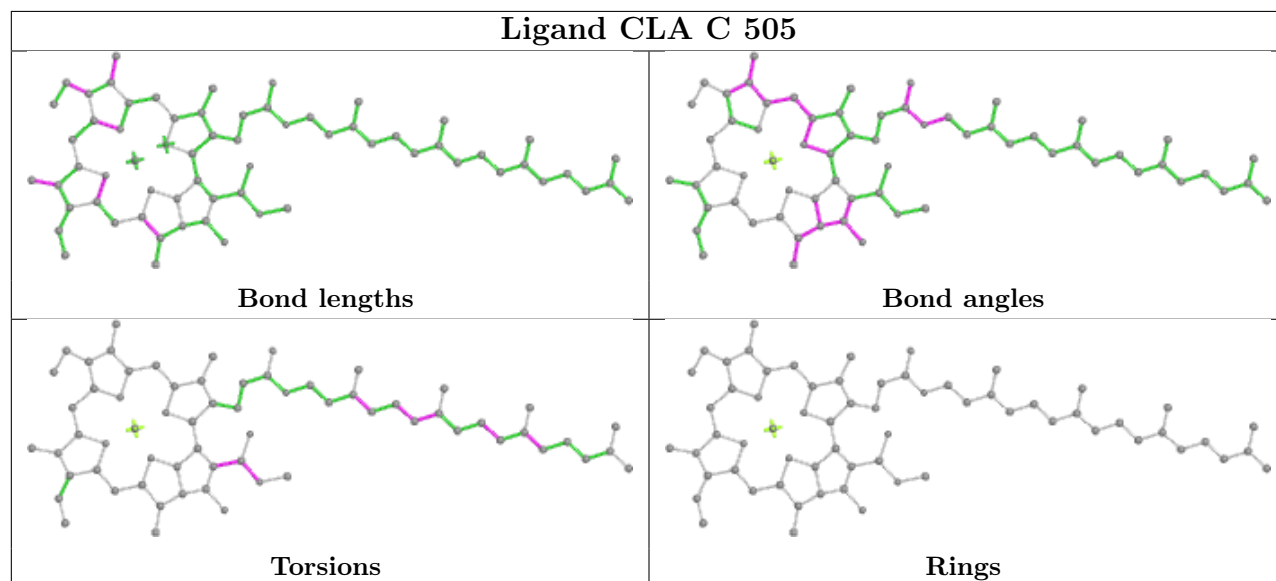
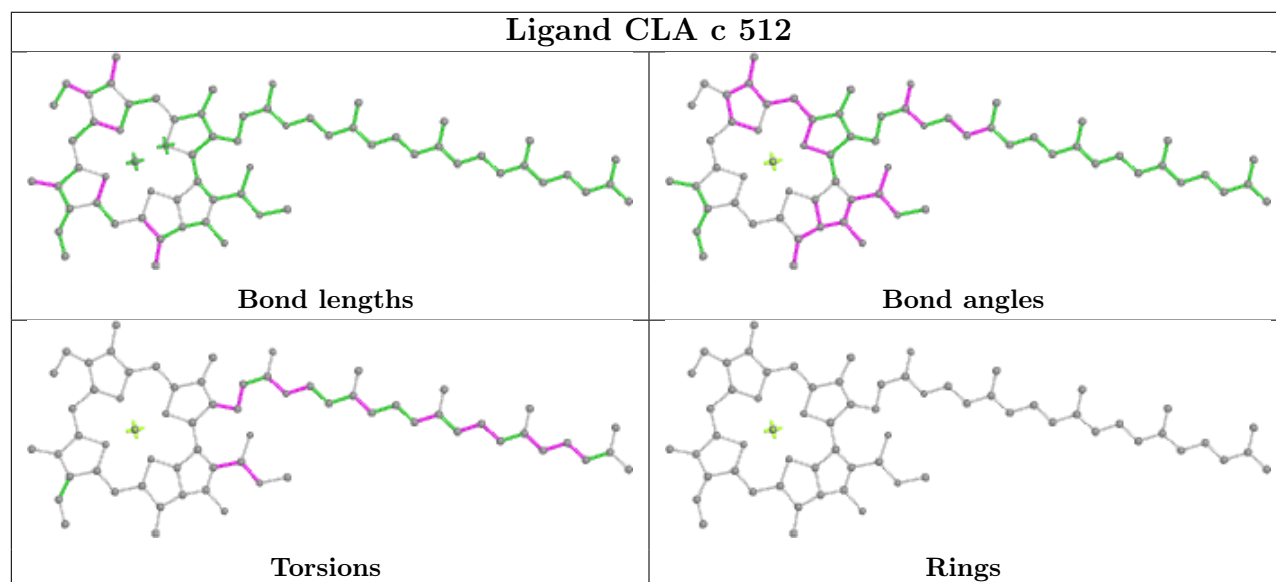
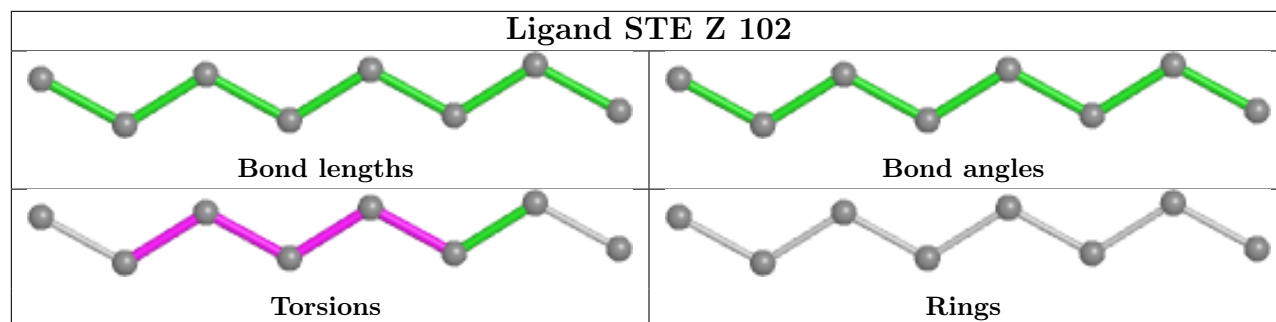
## Ligand DGD c 518



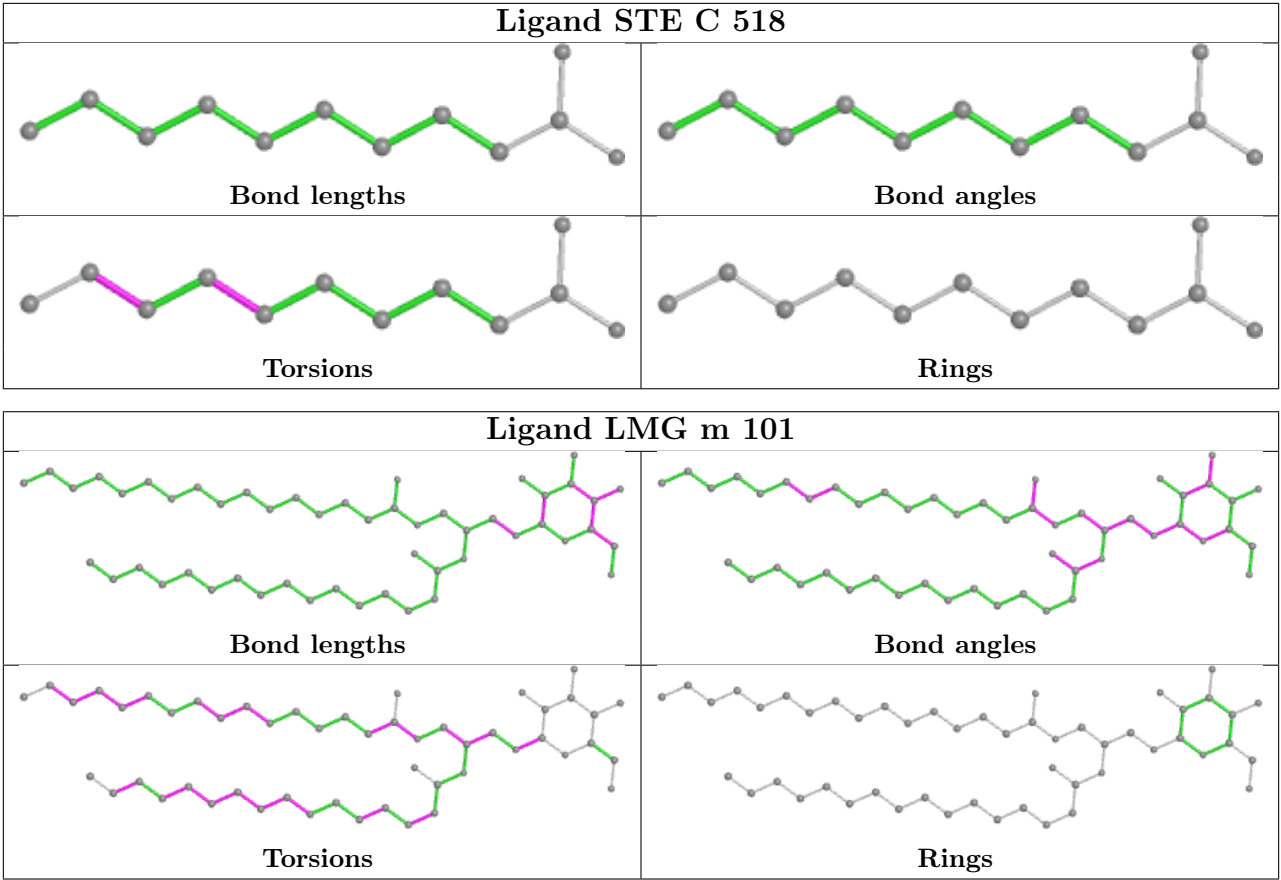
## Ligand BCR Z 101











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.20

## 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%)	-0.37	4 (1%) 79 82	26, 34, 52, 83	0
1	a	334/344 (97%)	-0.40	1 (0%) 94 95	28, 36, 61, 81	0
2	B	505/510 (99%)	-0.34	6 (1%) 79 82	27, 38, 66, 87	0
2	b	505/510 (99%)	-0.18	19 (3%) 40 45	30, 41, 72, 102	0
3	C	442/461 (95%)	-0.25	11 (2%) 57 63	28, 41, 58, 80	0
3	c	451/461 (97%)	-0.16	10 (2%) 62 68	29, 45, 65, 98	0
4	D	341/352 (96%)	-0.35	1 (0%) 94 95	27, 35, 53, 78	0
4	d	341/352 (96%)	-0.24	1 (0%) 94 95	26, 39, 62, 85	0
5	E	82/84 (97%)	-0.09	2 (2%) 59 65	37, 56, 73, 84	0
5	e	82/84 (97%)	0.27	6 (7%) 15 18	43, 66, 80, 90	0
6	F	34/45 (75%)	-0.44	1 (2%) 51 57	39, 48, 65, 82	0
6	f	34/45 (75%)	-0.26	1 (2%) 51 57	46, 54, 81, 96	0
7	H	65/66 (98%)	-0.09	0 100 100	36, 45, 61, 69	0
7	h	63/66 (95%)	0.18	4 (6%) 20 24	45, 55, 67, 72	0
8	I	35/38 (92%)	-0.23	2 (5%) 23 28	37, 44, 67, 81	0
8	i	35/38 (92%)	-0.15	2 (5%) 23 28	34, 45, 72, 87	0
9	J	36/40 (90%)	-0.04	5 (13%) 2 3	39, 56, 82, 89	0
9	j	36/40 (90%)	0.21	5 (13%) 2 3	44, 59, 93, 103	0
10	K	37/46 (80%)	0.12	2 (5%) 25 31	45, 55, 70, 75	0
10	k	37/46 (80%)	-0.06	2 (5%) 25 31	53, 60, 77, 83	0
11	L	37/37 (100%)	-0.40	1 (2%) 54 60	29, 35, 64, 73	0
11	l	36/37 (97%)	-0.25	3 (8%) 11 14	31, 36, 73, 85	0
12	M	32/36 (88%)	0.03	1 (3%) 49 54	34, 39, 65, 74	0
12	m	31/36 (86%)	-0.04	0 100 100	32, 38, 57, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.02	15 (6%) 21 26	32, 47, 85, 122	0
13	o	244/272 (89%)	-0.18	12 (4%) 29 35	28, 45, 81, 127	0
14	R	28/41 (68%)	1.58	9 (32%) 0 0	65, 72, 90, 91	0
14	r	28/41 (68%)	3.58	25 (89%) 0 0	83, 99, 117, 127	0
15	T	29/32 (90%)	-0.43	1 (3%) 45 50	30, 36, 61, 81	0
15	t	29/32 (90%)	-0.36	2 (6%) 16 21	33, 37, 78, 89	0
16	U	97/134 (72%)	-0.20	2 (2%) 63 69	33, 49, 76, 95	0
16	u	97/134 (72%)	-0.39	0 100 100	37, 45, 60, 80	0
17	V	137/163 (84%)	-0.52	0 100 100	31, 46, 58, 78	0
17	v	137/163 (84%)	-0.19	3 (2%) 62 68	37, 52, 74, 86	0
18	X	38/41 (92%)	0.18	3 (7%) 12 16	44, 53, 73, 78	0
18	x	39/41 (95%)	0.28	5 (12%) 3 4	53, 62, 90, 101	0
19	Y	27/46 (58%)	1.27	11 (40%) 0 0	58, 77, 95, 102	0
19	y	30/46 (65%)	0.49	4 (13%) 3 4	67, 80, 90, 100	0
20	Z	62/62 (100%)	0.69	14 (22%) 0 1	59, 73, 113, 122	0
20	z	62/62 (100%)	0.84	12 (19%) 1 1	63, 78, 114, 121	0
All	All	5293/5700 (92%)	-0.16	208 (3%) 39 44	26, 43, 77, 127	0

The worst 5 of 208 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.3
20	Z	62	VAL	7.7
14	r	9	LEU	6.9
14	r	28	VAL	6.6
1	A	13	LEU	6.3

## 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
15	FME	t	1	10/11	0.92	0.11	34,54,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	FME	T	1	10/11	0.93	0.13	31,58,77,77	0
8	FME	I	1	10/11	0.95	0.19	46,58,68,81	0
12	FME	m	1	10/11	0.96	0.12	44,53,72,80	0
12	FME	M	1	10/11	0.97	0.12	45,56,70,76	0
8	FME	i	1	10/11	0.97	0.16	42,55,68,74	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
32	STE	a	412	12/20	0.72	0.36	47,74,84,88	0
32	STE	b	625	20/20	0.76	0.28	42,67,89,95	0
32	STE	x	102	20/20	0.76	0.25	50,66,80,86	0
32	STE	B	624	18/20	0.78	0.22	52,72,90,94	0
32	STE	c	520	20/20	0.79	0.26	42,64,85,89	0
32	STE	B	625	16/20	0.79	0.29	40,64,82,85	0
31	BCR	H	101	40/40	0.81	0.17	35,52,66,74	0
26	LMG	c	521	48/55	0.81	0.23	34,77,102,106	0
28	LHG	e	101	42/49	0.81	0.27	62,89,116,133	0
32	STE	R	101	12/20	0.81	0.31	60,82,101,105	0
32	STE	M	103	10/20	0.82	0.19	40,56,67,71	0
32	STE	B	620	17/20	0.83	0.21	37,60,76,76	0
28	LHG	A	411	49/49	0.83	0.23	45,84,111,116	0
26	LMG	D	412	33/55	0.83	0.20	32,62,92,94	0
32	STE	I	102	15/20	0.83	0.16	42,58,80,82	0
22	CLA	b	601	65/65	0.83	0.19	48,73,101,104	0
22	CLA	c	512	65/65	0.84	0.17	42,63,90,104	0
32	STE	a	413	15/20	0.84	0.20	36,63,77,86	0
32	STE	b	621	20/20	0.84	0.25	42,60,79,84	0
32	STE	J	101	12/20	0.84	0.16	49,65,72,74	0
26	LMG	B	626	55/55	0.84	0.18	40,64,84,98	0
32	STE	B	627	12/20	0.84	0.45	42,68,79,82	0
26	LMG	b	622	55/55	0.85	0.27	49,78,102,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	C	512	65/65	0.85	0.19	39,61,93,102	0
32	STE	b	623	16/20	0.85	0.17	53,73,83,90	0
32	STE	b	624	15/20	0.85	0.20	50,66,87,92	0
27	SQD	A	412	39/54	0.85	0.20	45,66,96,103	0
32	STE	b	627	14/20	0.85	0.36	54,77,98,104	0
31	BCR	x	101	40/40	0.85	0.16	37,58,76,80	0
32	STE	H	103	18/20	0.85	0.34	52,77,88,89	0
32	STE	L	103	12/20	0.86	0.20	48,66,88,88	0
25	PL9	a	409	55/55	0.86	0.23	41,72,95,100	0
32	STE	C	518	12/20	0.86	0.17	39,57,68,69	0
22	CLA	c	513	65/65	0.86	0.21	47,77,104,108	0
29	DGD	A	413	66/66	0.86	0.15	47,64,83,89	0
32	STE	l	102	18/20	0.86	0.17	38,52,75,78	0
27	SQD	t	102	36/54	0.86	0.18	31,66,91,95	0
22	CLA	B	601	65/65	0.87	0.17	40,70,93,104	0
32	STE	C	519	16/20	0.87	0.15	47,62,75,75	0
25	PL9	A	408	55/55	0.87	0.23	32,67,92,100	0
27	SQD	L	101	49/54	0.87	0.16	40,66,100,105	0
32	STE	c	523	12/20	0.87	0.24	55,74,88,90	0
32	STE	d	412	20/20	0.87	0.18	40,68,83,90	0
22	CLA	C	513	65/65	0.87	0.21	41,63,99,108	0
31	BCR	K	101	40/40	0.87	0.15	40,57,75,78	0
32	STE	b	620	16/20	0.88	0.22	40,55,81,91	0
26	LMG	c	519	37/55	0.89	0.18	45,69,89,99	0
22	CLA	c	502	65/65	0.89	0.18	32,48,68,72	0
26	LMG	c	522	49/55	0.89	0.16	28,62,92,100	0
26	LMG	m	101	51/55	0.89	0.15	39,58,78,87	0
22	CLA	c	508	64/65	0.89	0.17	37,55,93,115	0
32	STE	b	626	10/20	0.89	0.33	49,60,69,71	0
31	BCR	k	101	40/40	0.89	0.14	46,68,84,90	0
31	BCR	k	102	40/40	0.89	0.21	46,63,76,78	0
27	SQD	B	622	54/54	0.89	0.18	38,65,89,98	0
26	LMG	Y	101	48/55	0.89	0.19	52,75,93,102	0
27	SQD	f	102	41/54	0.89	0.20	62,87,107,118	0
22	CLA	a	404	65/65	0.89	0.15	24,44,87,96	0
31	BCR	d	406	40/40	0.90	0.14	35,61,97,109	0
32	STE	B	623	12/20	0.90	0.11	38,60,72,73	0
22	CLA	D	405	65/65	0.90	0.15	26,50,128,138	0
32	STE	X	101	20/20	0.90	0.18	39,56,75,81	0
26	LMG	A	409	48/55	0.90	0.16	34,63,79,96	0
32	STE	t	104	10/20	0.90	0.26	43,60,72,77	0
26	LMG	B	621	28/55	0.90	0.16	36,52,67,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	LMG	d	410	44/55	0.91	0.16	41,61,89,106	0
32	STE	C	520	12/20	0.91	0.12	36,47,59,66	0
26	LMG	M	101	51/55	0.91	0.13	36,54,76,86	0
32	STE	j	101	12/20	0.91	0.13	50,64,71,72	0
26	LMG	D	408	51/55	0.91	0.20	32,65,89,99	0
22	CLA	d	405	65/65	0.91	0.16	32,54,94,107	0
31	BCR	c	514	40/40	0.91	0.16	45,67,82,87	0
22	CLA	C	507	65/65	0.92	0.15	26,46,66,68	0
32	STE	Z	102	8/20	0.92	0.13	43,65,79,79	0
29	DGD	c	518	62/66	0.92	0.17	35,62,87,98	0
31	BCR	C	514	40/40	0.92	0.14	29,46,59,77	0
27	SQD	a	411	54/54	0.92	0.16	47,69,98,106	0
22	CLA	b	616	60/65	0.92	0.16	31,49,92,99	0
22	CLA	C	508	65/65	0.92	0.13	30,49,107,117	0
22	CLA	c	506	65/65	0.92	0.14	35,57,100,103	0
22	CLA	B	616	60/65	0.92	0.16	23,43,89,97	0
22	CLA	b	609	65/65	0.93	0.14	31,52,71,79	0
31	BCR	B	619	40/40	0.93	0.12	29,49,73,84	0
22	CLA	b	615	65/65	0.93	0.14	27,46,66,74	0
27	SQD	D	409	36/54	0.93	0.17	51,77,96,105	0
22	CLA	B	606	65/65	0.93	0.13	30,45,78,92	0
31	BCR	Z	101	40/40	0.93	0.13	42,64,78,82	0
22	CLA	C	502	65/65	0.93	0.14	28,47,68,78	0
22	CLA	B	615	65/65	0.93	0.14	27,42,67,84	0
22	CLA	b	602	65/65	0.93	0.17	33,47,65,71	0
32	STE	M	102	15/20	0.93	0.12	38,53,63,66	0
32	STE	d	411	17/20	0.93	0.13	48,63,70,78	0
22	CLA	c	509	65/65	0.93	0.20	30,53,72,80	0
22	CLA	c	510	65/65	0.93	0.15	35,50,66,84	0
22	CLA	c	511	65/65	0.93	0.16	43,63,80,86	0
32	STE	t	103	14/20	0.93	0.15	43,57,69,70	0
29	DGD	C	516	62/66	0.93	0.14	31,54,103,124	0
29	DGD	c	517	62/66	0.93	0.14	38,60,95,104	0
36	NA	V	202	1/1	0.93	0.18	60,60,60,60	0
22	CLA	B	602	65/65	0.94	0.17	26,43,63,67	0
29	DGD	C	517	62/66	0.94	0.13	31,53,79,87	0
29	DGD	H	102	62/66	0.94	0.12	33,51,66,72	0
22	CLA	C	509	65/65	0.94	0.18	30,50,68,77	0
22	CLA	b	604	65/65	0.94	0.14	26,44,80,95	0
29	DGD	h	101	62/66	0.94	0.14	34,52,67,70	0
31	BCR	B	617	40/40	0.94	0.12	30,45,64,65	0
31	BCR	B	618	40/40	0.94	0.10	29,45,60,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	b	606	65/65	0.94	0.12	28,46,80,92	0
22	CLA	C	511	65/65	0.94	0.14	32,59,76,80	0
31	BCR	D	406	40/40	0.94	0.11	34,51,88,99	0
22	CLA	b	613	65/65	0.94	0.17	23,41,82,97	0
22	CLA	d	401	65/65	0.94	0.15	28,47,105,111	0
31	BCR	K	102	40/40	0.94	0.16	39,58,71,71	0
27	SQD	A	410	52/54	0.94	0.16	37,66,96,101	0
31	BCR	a	405	40/40	0.94	0.11	24,39,58,59	0
31	BCR	b	617	40/40	0.94	0.13	32,48,65,66	0
31	BCR	b	619	40/40	0.94	0.13	30,55,81,85	0
22	CLA	b	614	65/65	0.94	0.15	25,43,80,87	0
31	BCR	c	515	40/40	0.94	0.14	33,53,70,76	0
22	CLA	B	614	65/65	0.94	0.17	26,46,80,96	0
25	PL9	D	407	55/55	0.94	0.12	26,39,54,62	0
22	CLA	C	505	65/65	0.94	0.16	26,47,73,76	0
22	CLA	C	506	65/65	0.94	0.13	30,50,89,98	0
22	CLA	c	503	65/65	0.94	0.16	34,49,61,67	0
22	CLA	c	504	60/65	0.94	0.12	35,51,84,100	0
22	CLA	c	505	65/65	0.94	0.17	31,46,72,76	0
22	CLA	B	604	65/65	0.94	0.14	25,40,87,96	0
22	CLA	c	507	65/65	0.94	0.14	31,50,65,78	0
29	DGD	C	515	62/66	0.94	0.13	27,47,83,98	0
22	CLA	b	610	65/65	0.95	0.18	28,43,58,68	0
22	CLA	b	611	65/65	0.95	0.14	24,41,57,66	0
22	CLA	b	612	65/65	0.95	0.17	27,41,52,54	0
22	CLA	d	403	65/65	0.95	0.14	23,41,64,74	0
22	CLA	d	404	65/65	0.95	0.13	22,37,52,55	0
22	CLA	C	503	65/65	0.95	0.14	31,47,57,61	0
31	BCR	T	101	40/40	0.95	0.10	32,46,58,65	0
23	PHO	a	403	64/64	0.95	0.14	23,36,44,47	0
22	CLA	C	504	59/65	0.95	0.13	32,48,87,92	0
22	CLA	D	403	65/65	0.95	0.12	22,36,54,66	0
31	BCR	b	618	40/40	0.95	0.10	29,44,60,62	0
22	CLA	D	404	65/65	0.95	0.12	23,35,56,65	0
25	PL9	d	407	55/55	0.95	0.11	24,40,53,63	0
28	LHG	a	410	49/49	0.95	0.14	39,57,79,91	0
28	LHG	d	409	39/49	0.95	0.12	32,52,69,75	0
22	CLA	c	501	65/65	0.95	0.14	32,49,65,71	0
22	CLA	B	613	65/65	0.95	0.16	22,40,73,81	0
22	CLA	B	603	65/65	0.95	0.16	23,39,62,68	0
22	CLA	A	403	65/65	0.95	0.15	25,41,95,103	0
22	CLA	A	405	54/65	0.95	0.12	22,39,70,82	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	C	501	65/65	0.95	0.12	26,42,59,65	0
29	DGD	c	516	62/66	0.95	0.11	30,47,80,87	0
22	CLA	b	605	65/65	0.95	0.14	25,38,56,62	0
22	CLA	C	510	65/65	0.95	0.14	29,48,65,73	0
22	CLA	b	607	65/65	0.95	0.13	24,41,81,86	0
22	CLA	b	608	65/65	0.95	0.15	31,48,71,77	0
22	CLA	B	609	65/65	0.95	0.12	28,43,61,65	0
23	PHO	A	404	64/64	0.96	0.12	17,35,45,49	0
23	PHO	D	401	64/64	0.96	0.13	26,40,50,54	0
22	CLA	B	611	65/65	0.96	0.15	20,36,53,58	0
23	PHO	d	402	64/64	0.96	0.12	28,43,55,68	0
22	CLA	b	603	65/65	0.96	0.15	24,42,74,90	0
22	CLA	B	612	65/65	0.96	0.15	23,36,50,60	0
22	CLA	A	402	65/65	0.96	0.12	20,33,48,57	0
22	CLA	B	608	65/65	0.96	0.13	27,43,64,69	0
28	LHG	D	410	49/49	0.96	0.11	31,46,59,66	0
28	LHG	D	411	47/49	0.96	0.12	28,53,83,89	0
28	LHG	D	413	49/49	0.96	0.13	32,47,74,88	0
22	CLA	a	402	65/65	0.96	0.12	23,36,50,58	0
22	CLA	B	605	65/65	0.96	0.15	21,38,53,60	0
31	BCR	t	101	40/40	0.96	0.10	27,44,59,62	0
22	CLA	B	610	65/65	0.96	0.14	24,38,49,60	0
28	LHG	l	101	49/49	0.96	0.12	34,49,63,70	0
33	BCT	a	408	4/4	0.96	0.16	34,44,53,64	0
34	HEM	F	101	43/43	0.96	0.12	36,54,73,75	0
34	HEM	f	101	43/43	0.96	0.14	43,64,91,99	0
31	BCR	I	101	40/40	0.96	0.09	27,40,50,54	0
28	LHG	L	102	49/49	0.97	0.10	30,45,63,73	0
24	CL	A	407	1/1	0.97	0.08	37,37,37,37	0
28	LHG	d	408	49/49	0.97	0.11	29,47,61,72	0
35	HEC	V	201	43/43	0.97	0.13	24,39,48,49	0
35	HEC	v	201	43/43	0.97	0.13	29,44,55,61	0
22	CLA	B	607	65/65	0.97	0.12	19,40,81,87	0
30	OEX	A	414	10/10	0.98	0.15	27,36,39,39	0
33	BCT	D	402	4/4	0.98	0.17	28,35,45,54	0
24	CL	a	407	1/1	0.99	0.05	34,34,34,34	0
30	OEX	a	414	10/10	0.99	0.14	29,35,39,44	0
21	FE2	a	401	1/1	0.99	0.07	36,36,36,36	0
24	CL	A	406	1/1	0.99	0.08	36,36,36,36	0
21	FE2	A	401	1/1	0.99	0.11	31,31,31,31	0
24	CL	a	406	1/1	0.99	0.06	33,33,33,33	0

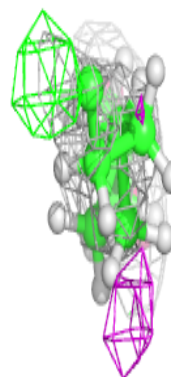
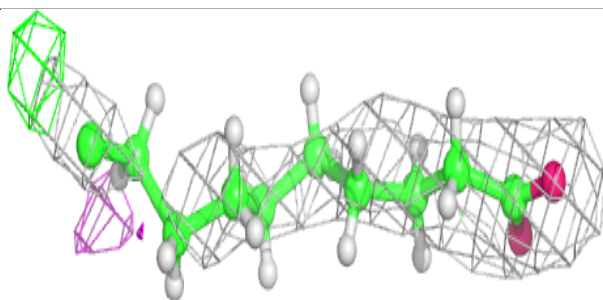
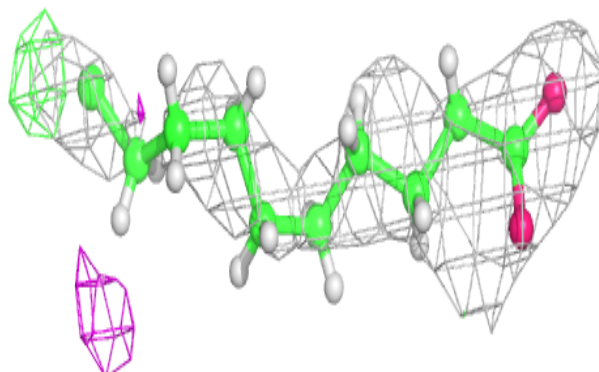
The following is a graphical depiction of the model fit to experimental electron density of all



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.

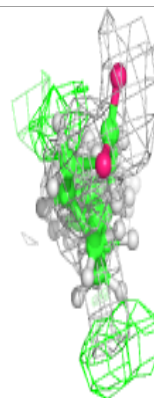
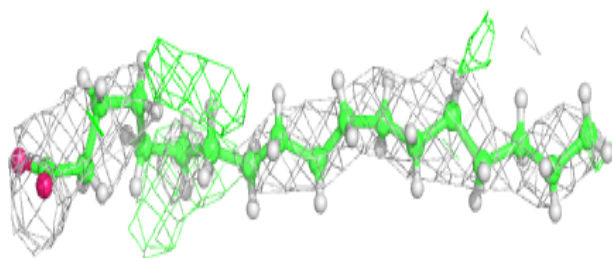
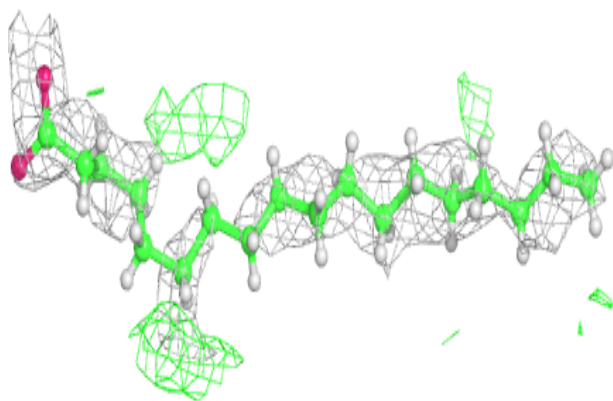
**Electron density around STE a 412:**

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

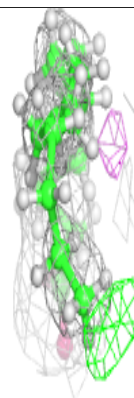
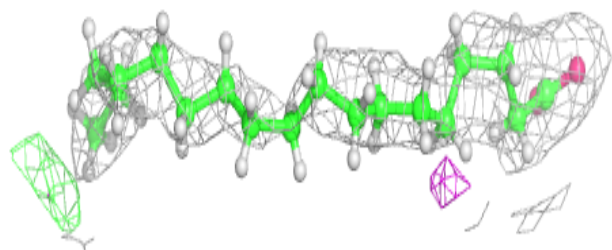
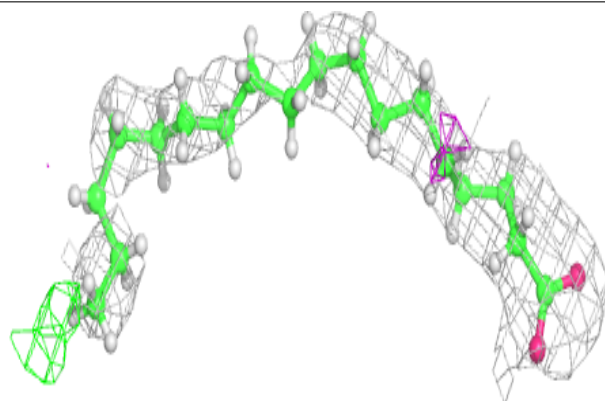


**Electron density around STE b 625:**

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

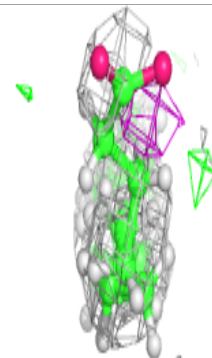
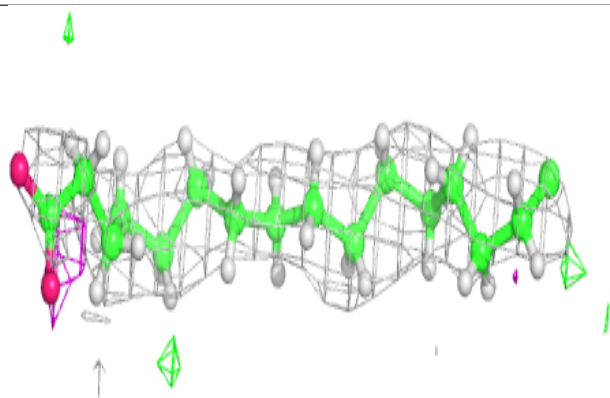
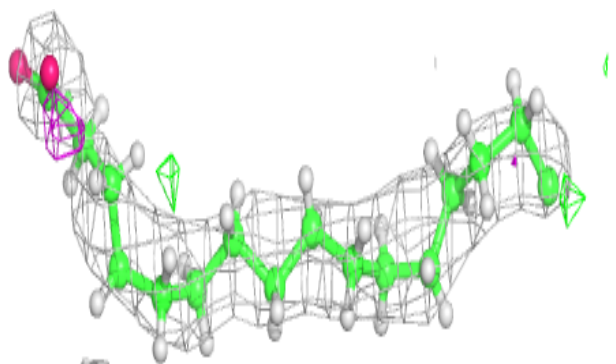
**Electron density around STE x 102:**

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

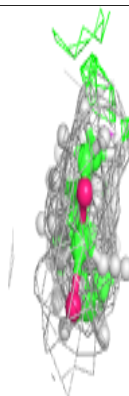
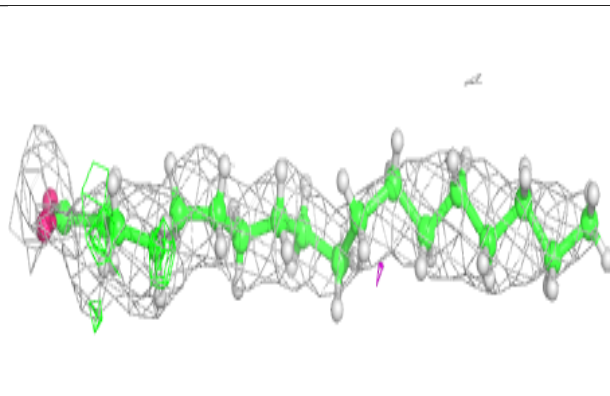
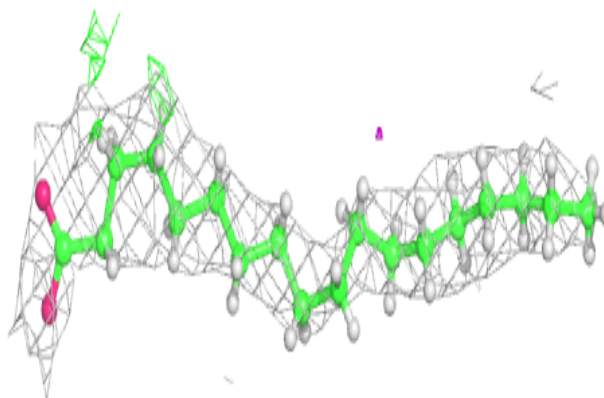


**Electron density around STE B 624:**

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

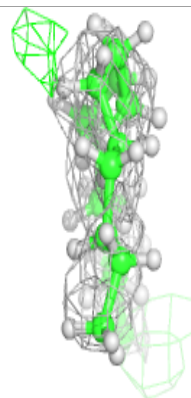
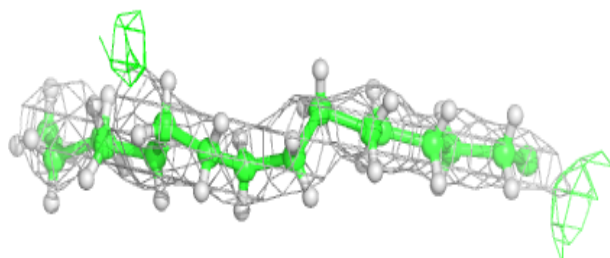
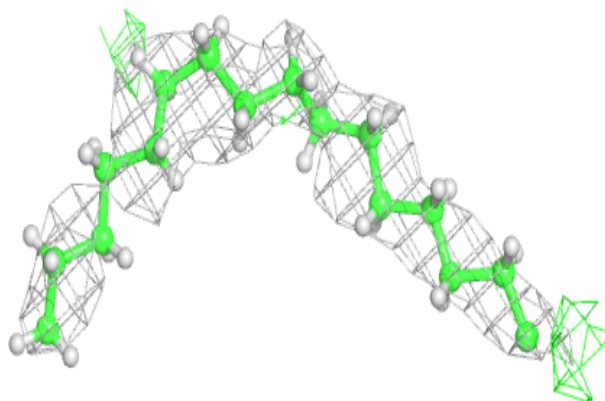
**Electron density around STE c 520:**

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

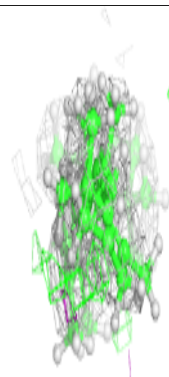
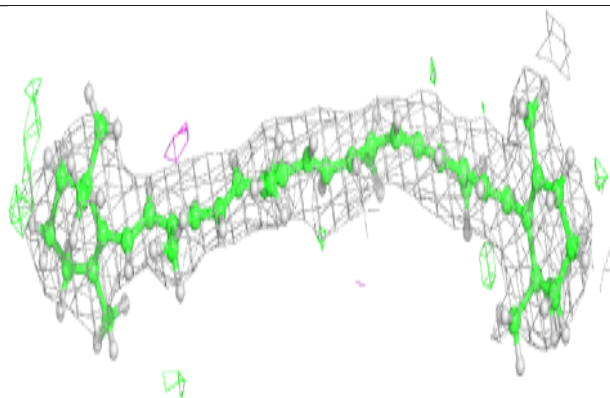
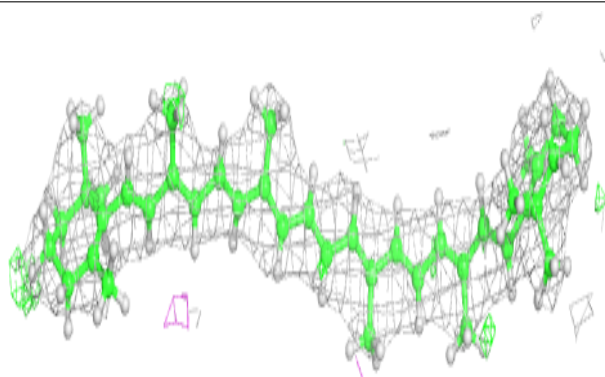


**Electron density around STE B 625:**

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

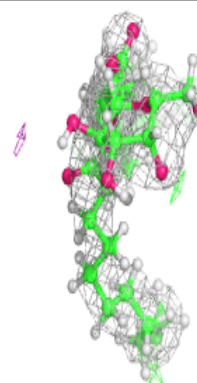
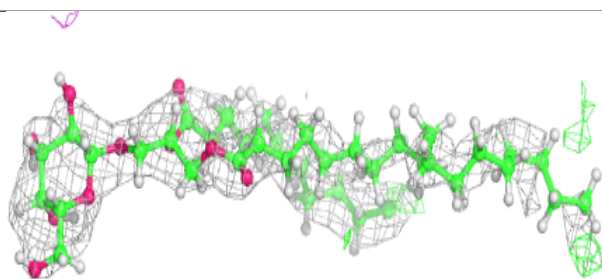
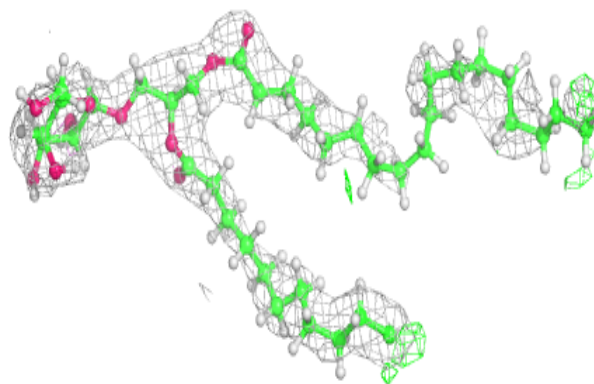
**Electron density around BCR H 101:**

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

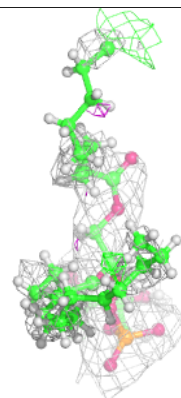
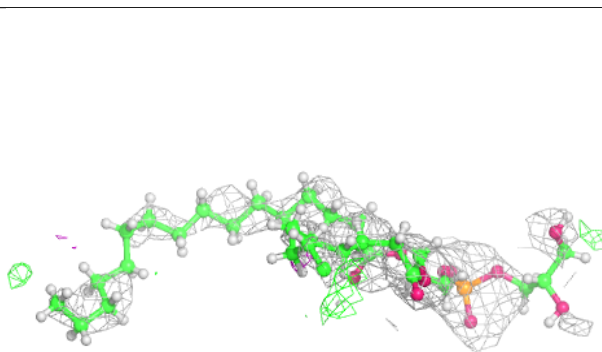
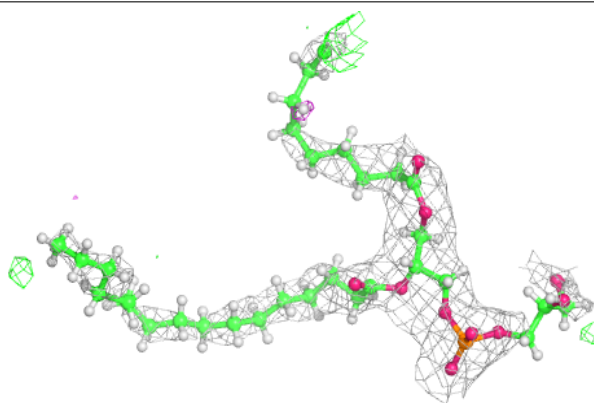


**Electron density around LMG c 521:**

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

**Electron density around LHG e 101:**

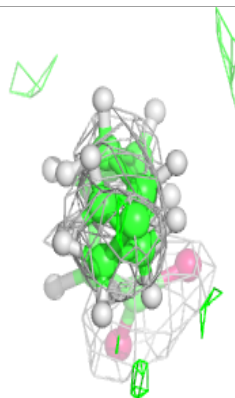
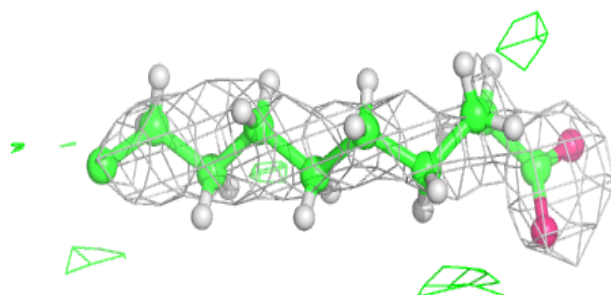
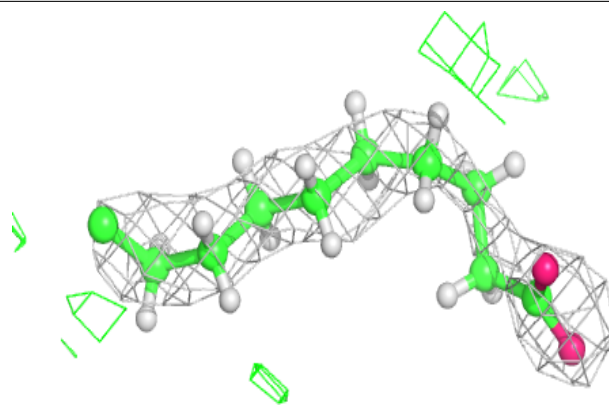
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



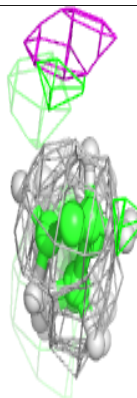
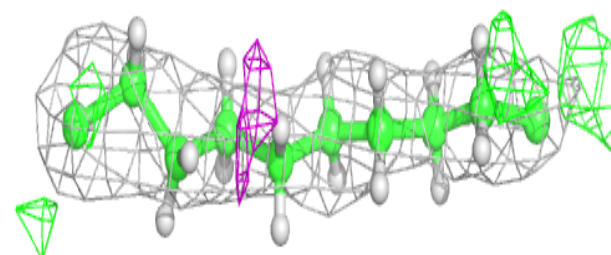
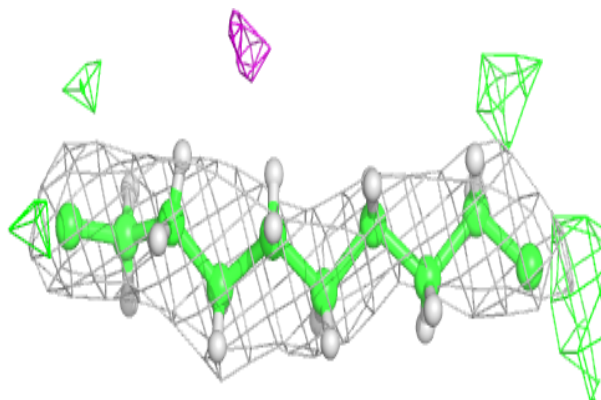


**Electron density around STE R 101:**

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

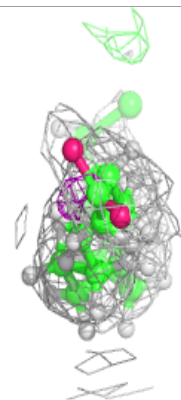
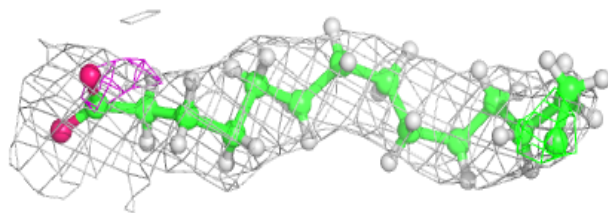
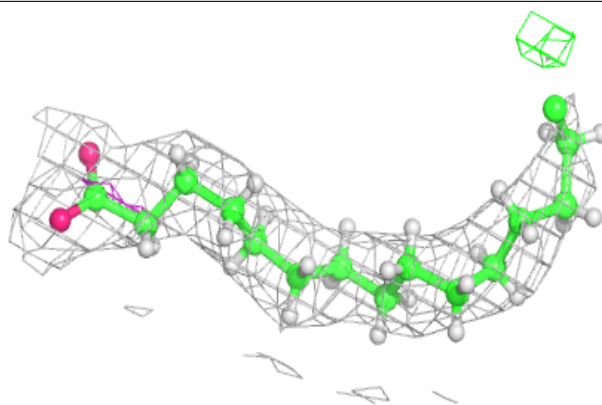
**Electron density around STE M 103:**

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



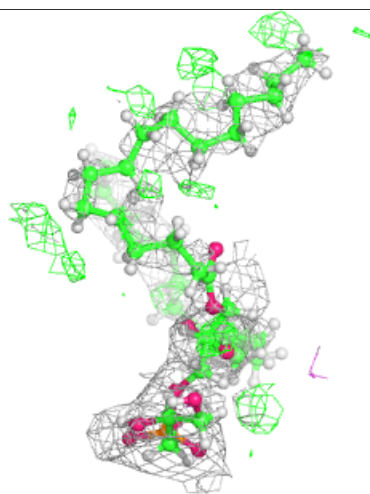
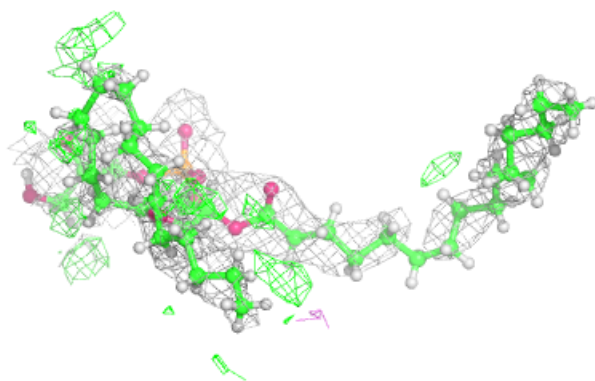
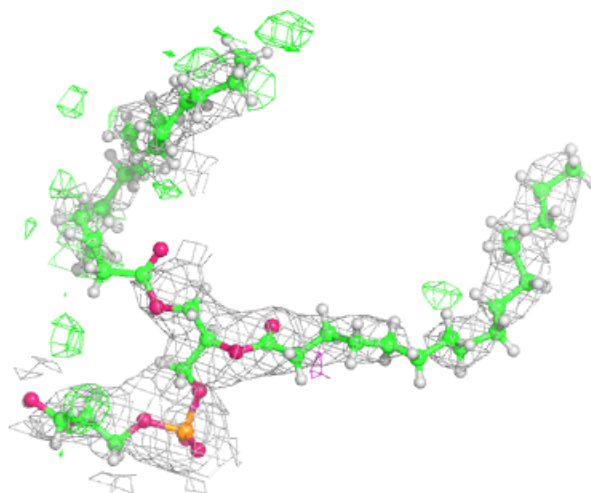
**Electron density around STE B 620:**

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



**Electron density around LHG A 411:**

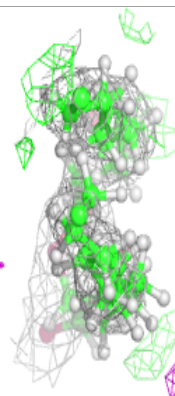
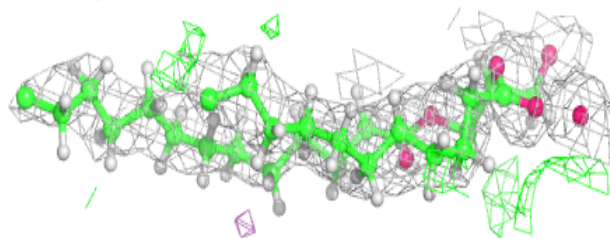
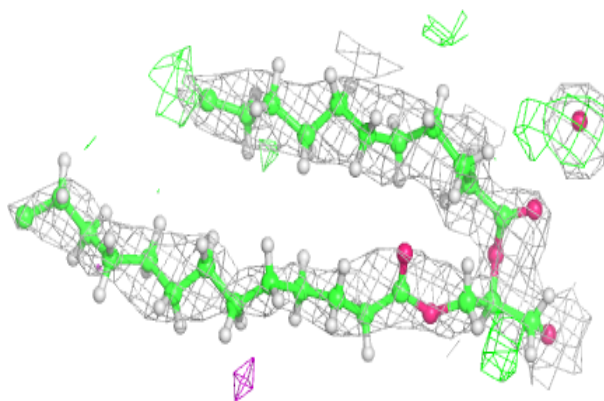
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



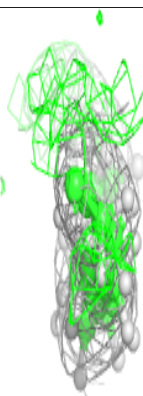
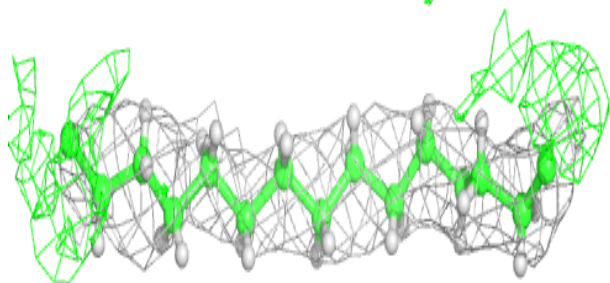
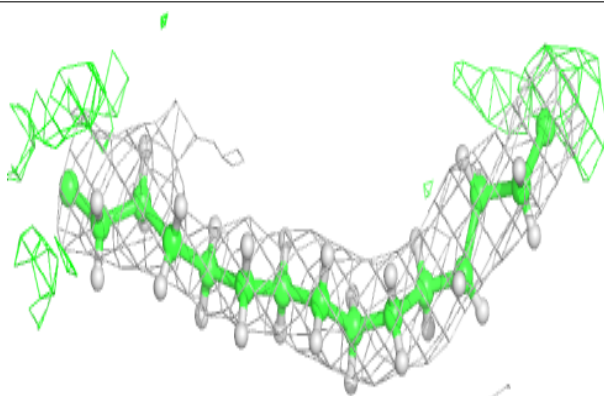


**Electron density around LMG D 412:**

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

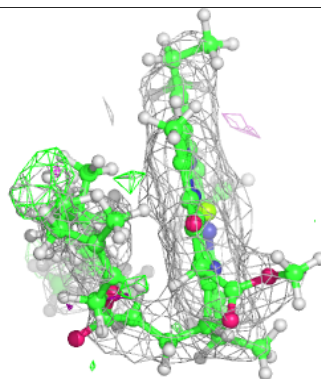
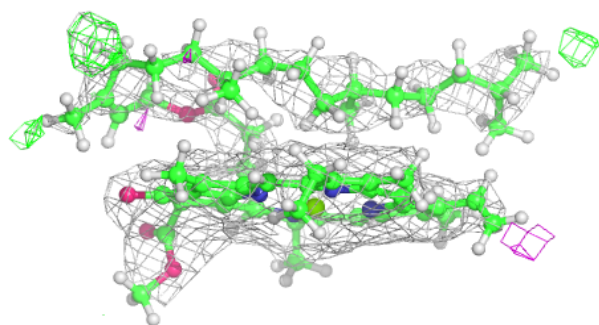
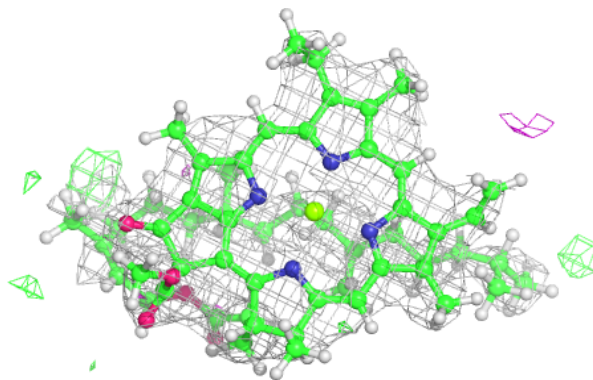
**Electron density around STE I 102:**

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



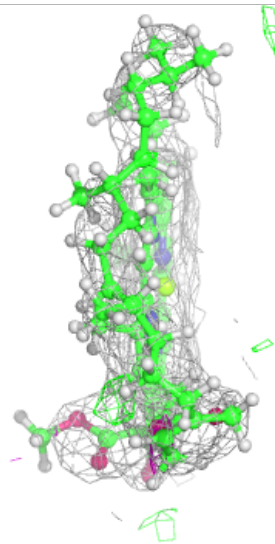
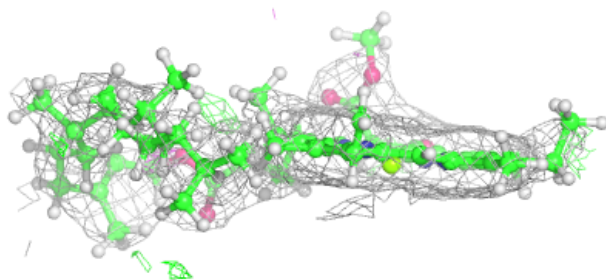
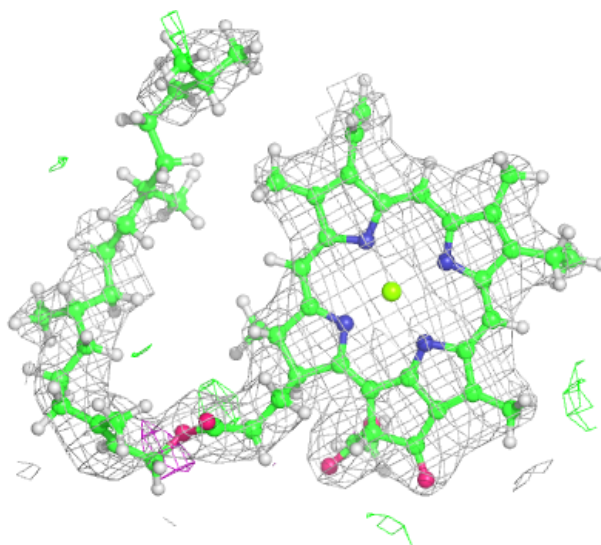
**Electron density around CLA b 601:**

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



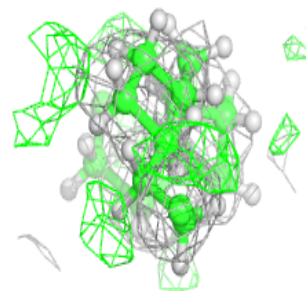
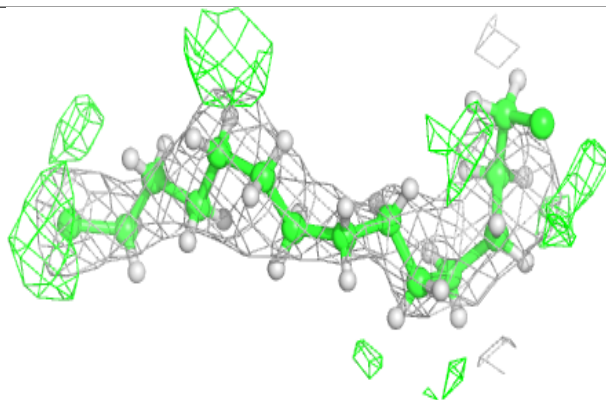
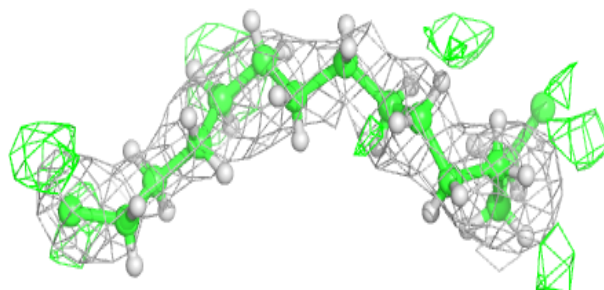
**Electron density around CLA c 512:**

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

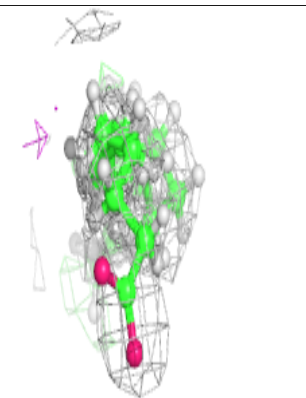
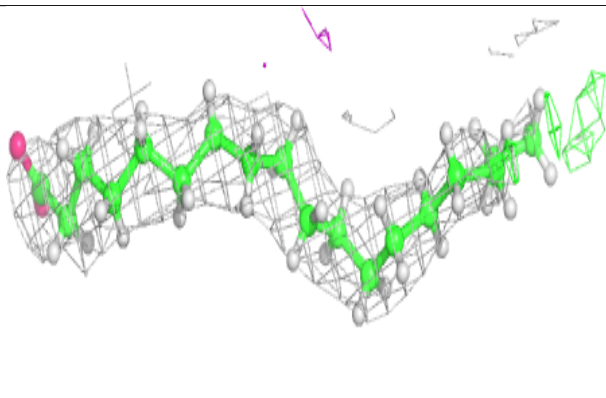
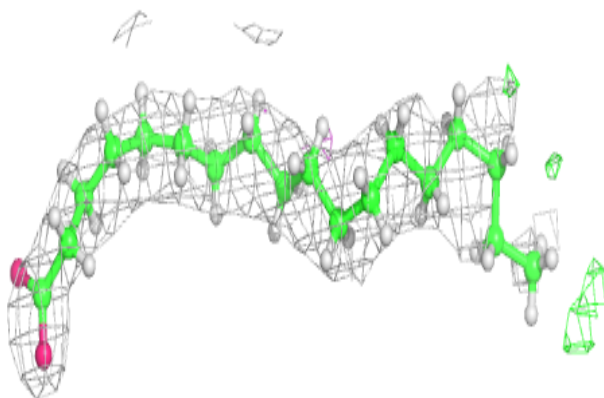


**Electron density around STE a 413:**

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

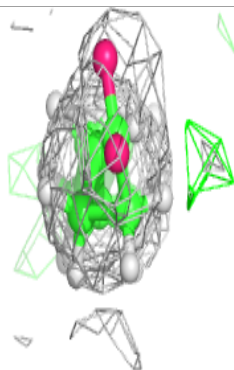
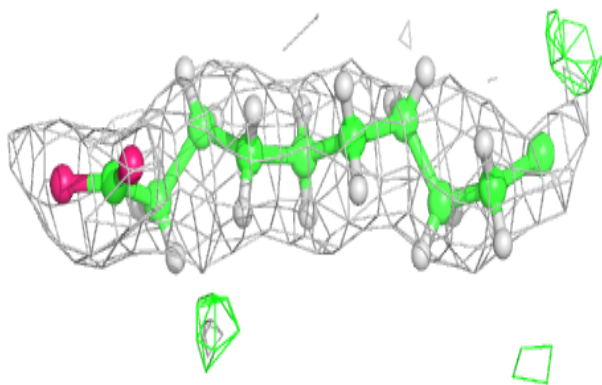
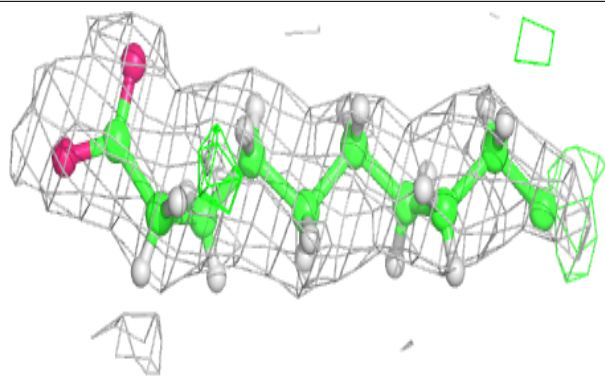
**Electron density around STE b 621:**

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

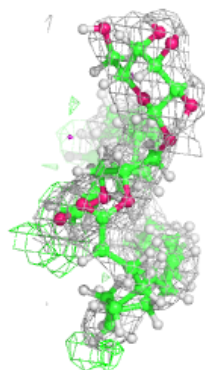
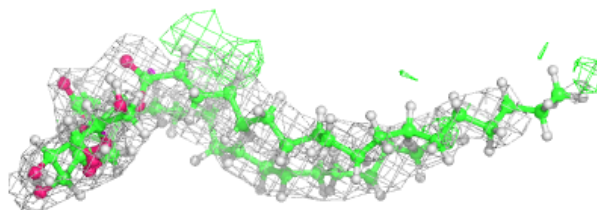
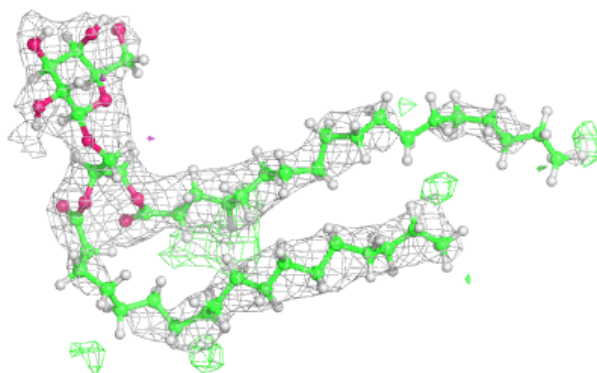


**Electron density around STE J 101:**

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

**Electron density around LMG B 626:**

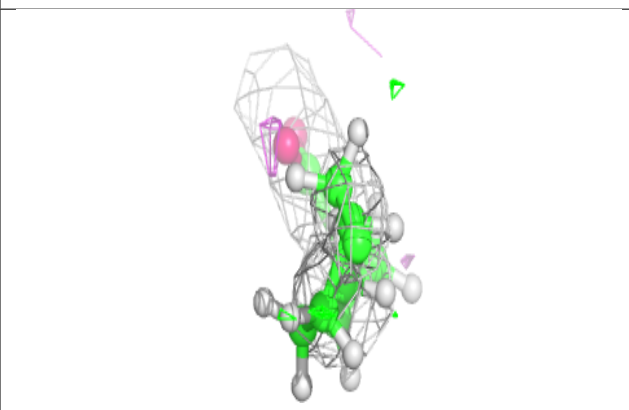
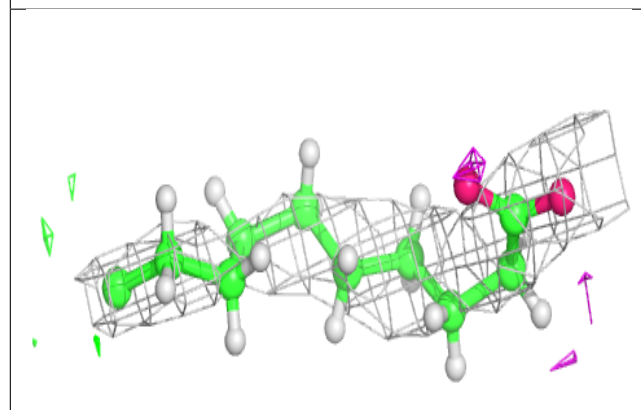
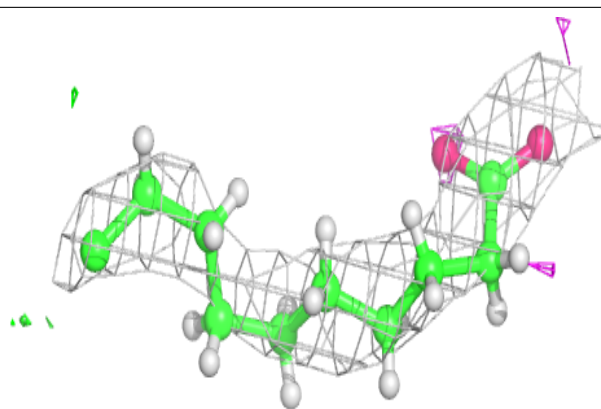
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



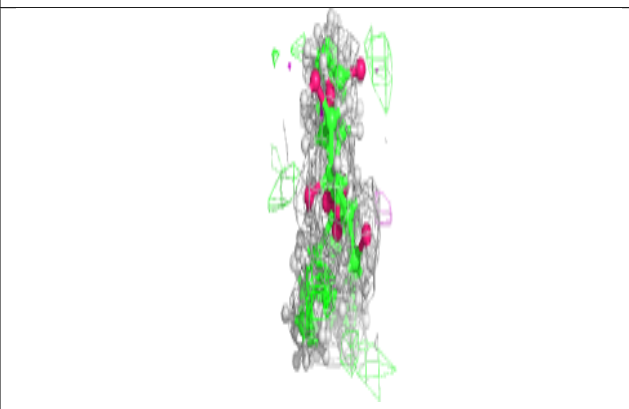
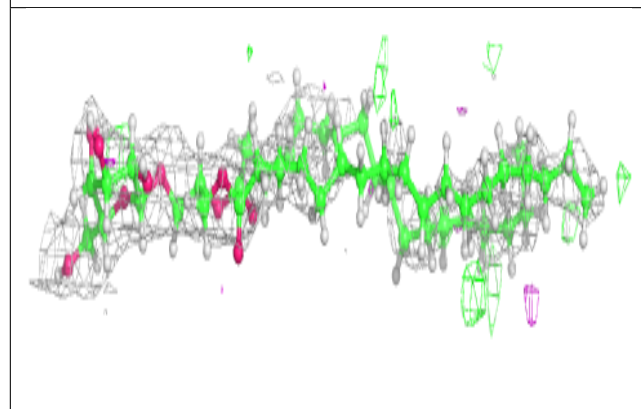
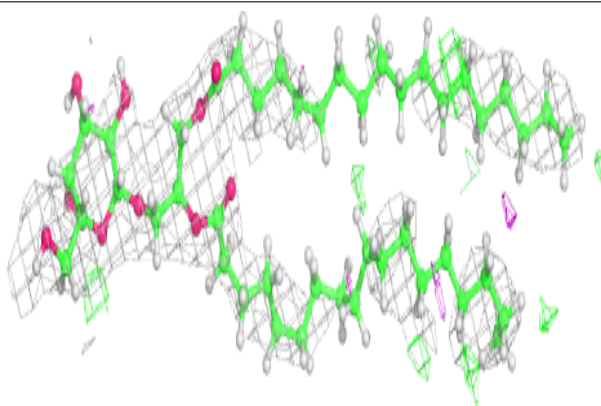


**Electron density around STE B 627:**

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

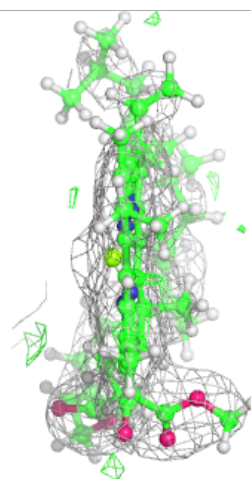
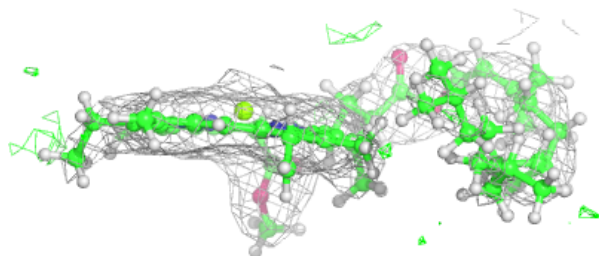
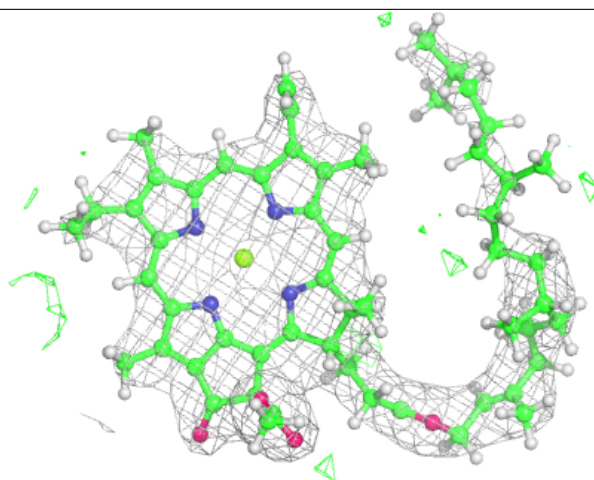
**Electron density around LMG b 622:**

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



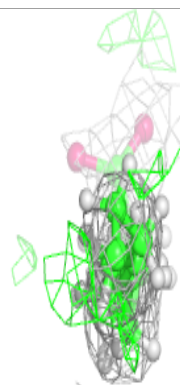
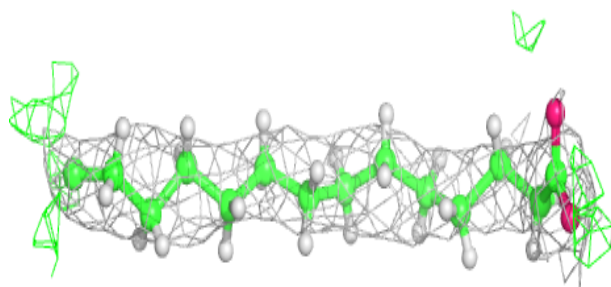
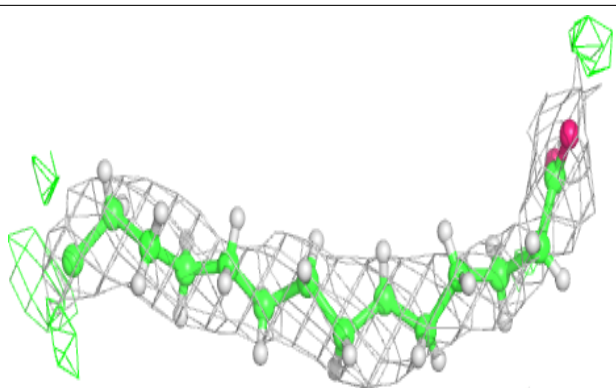
**Electron density around CLA C 512:**

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

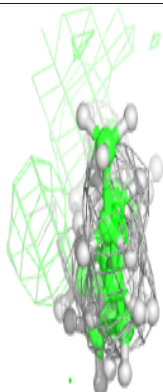
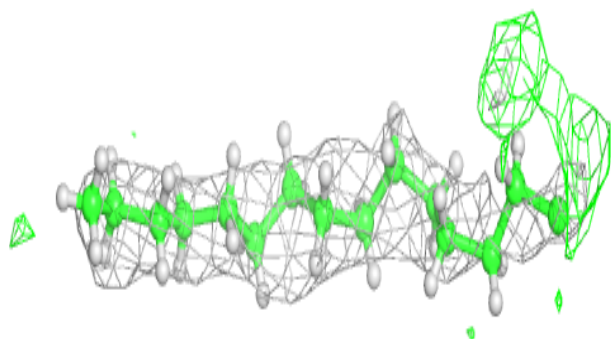
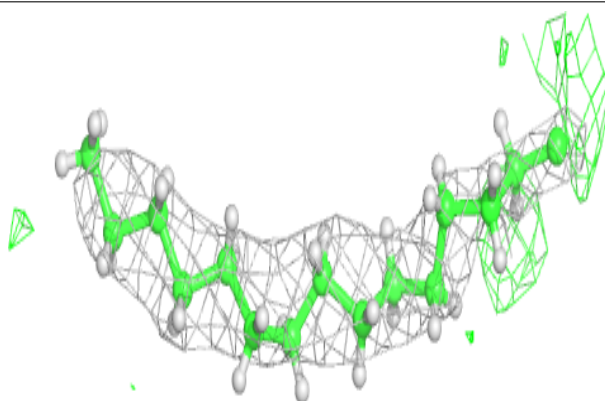


**Electron density around STE b 623:**

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

**Electron density around STE b 624:**

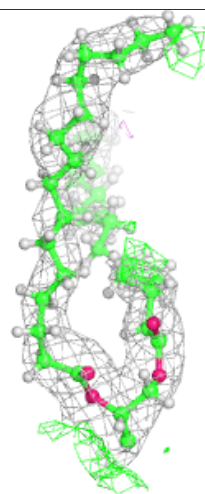
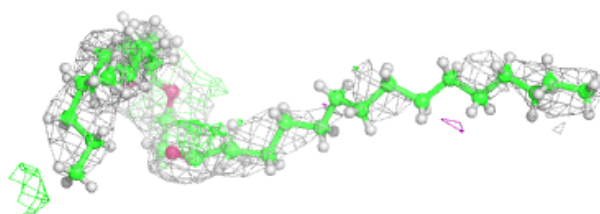
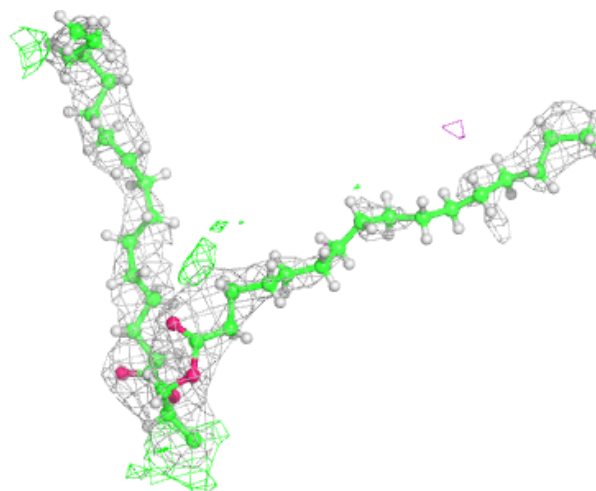
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





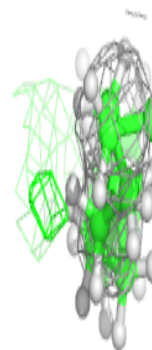
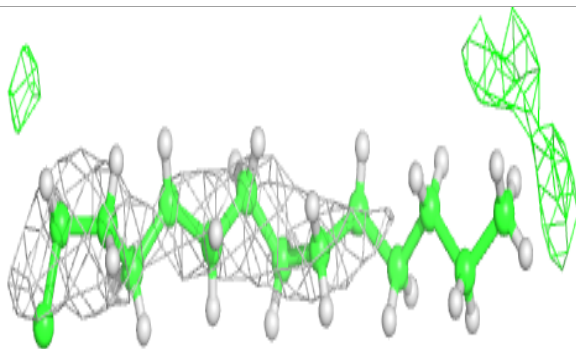
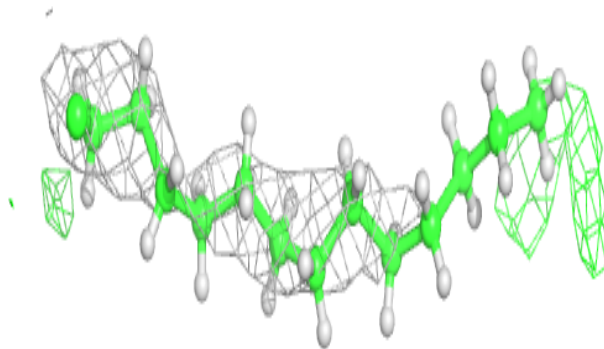
**Electron density around SQD A 412:**

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

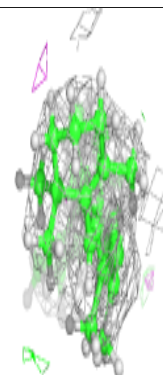
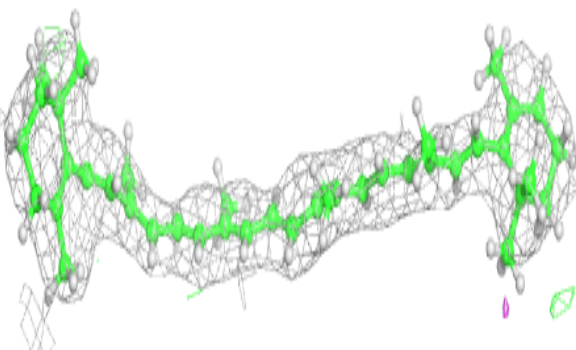
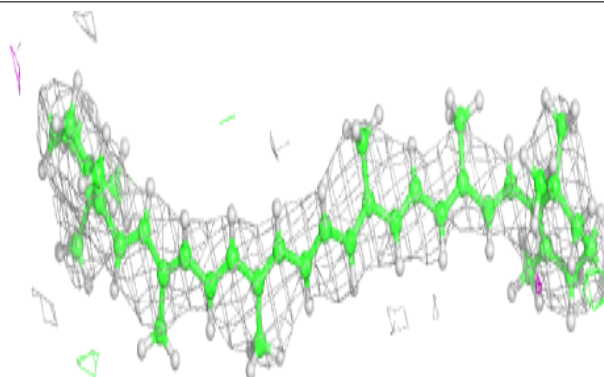


**Electron density around STE b 627:**

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

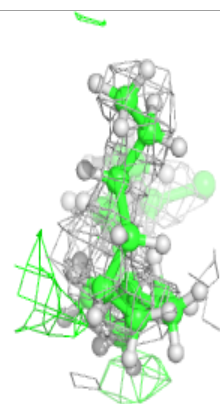
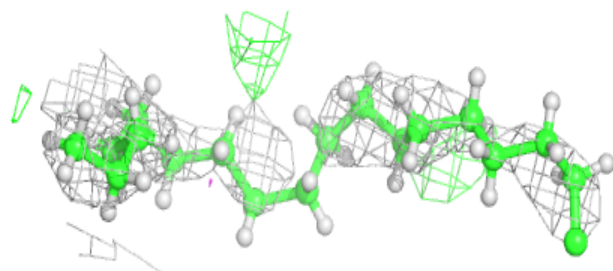
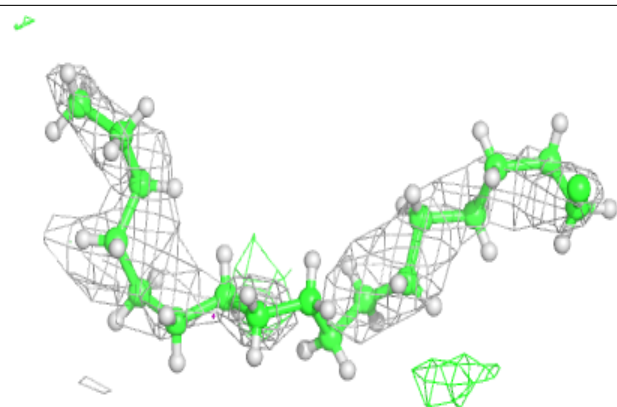
**Electron density around BCR x 101:**

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

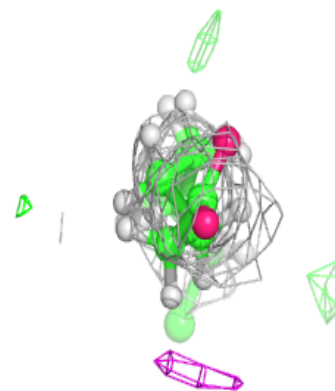
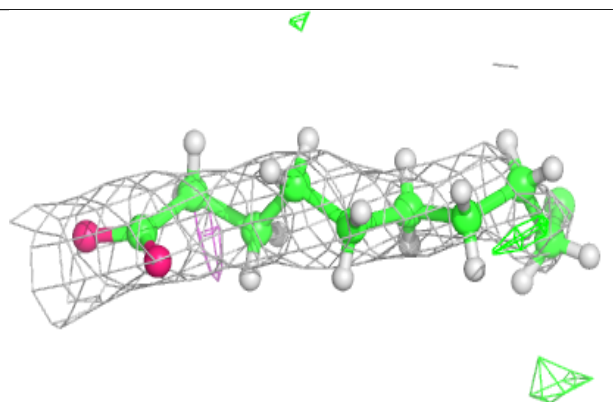
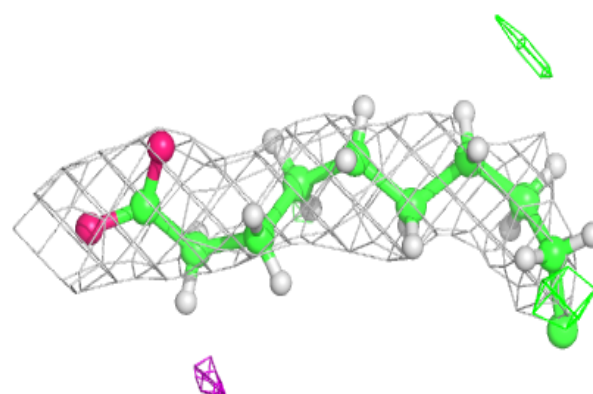


**Electron density around STE H 103:**

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

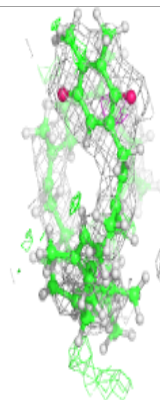
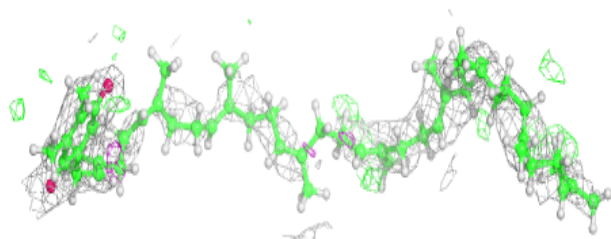
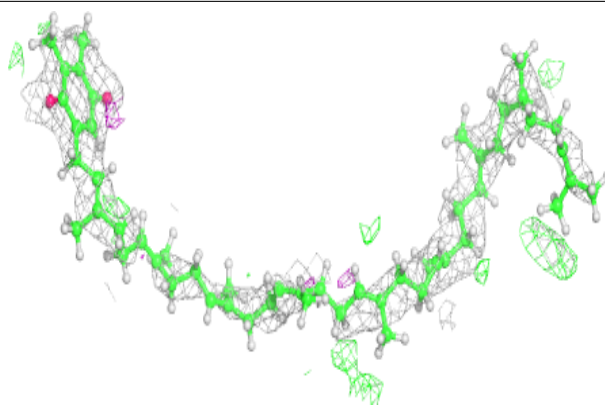
**Electron density around STE L 103:**

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

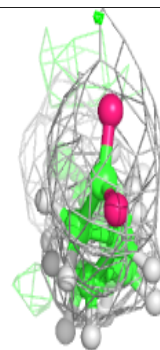
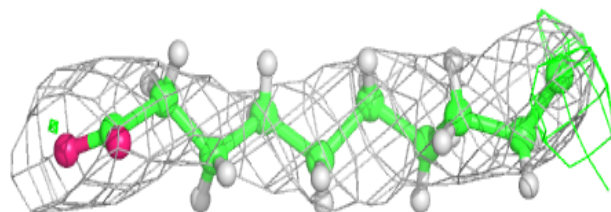
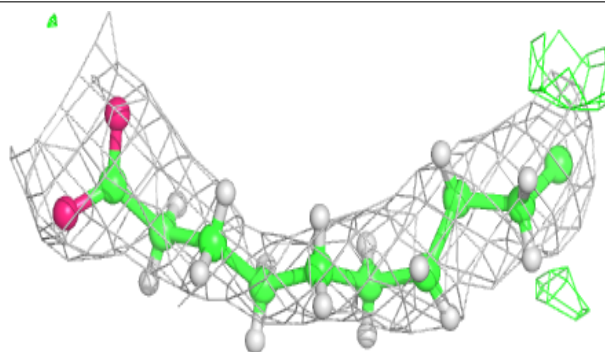


**Electron density around PL9 a 409:**

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

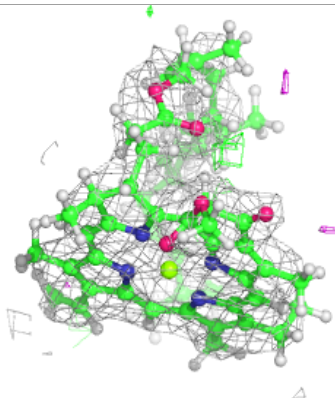
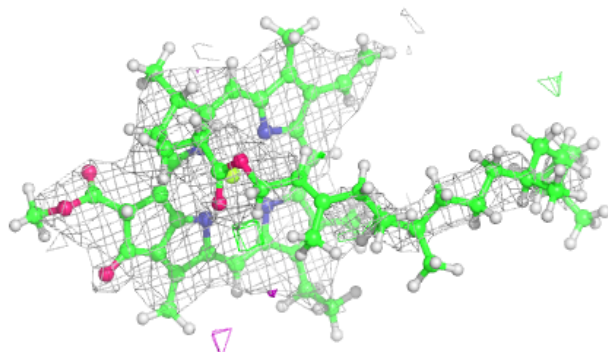
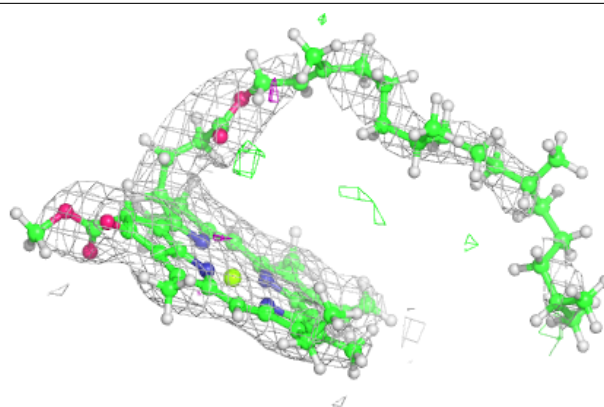
**Electron density around STE C 518:**

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

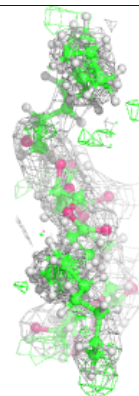
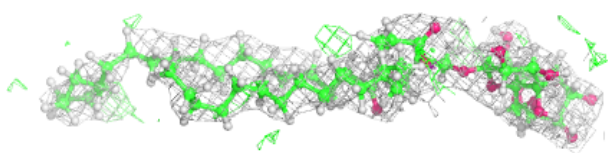
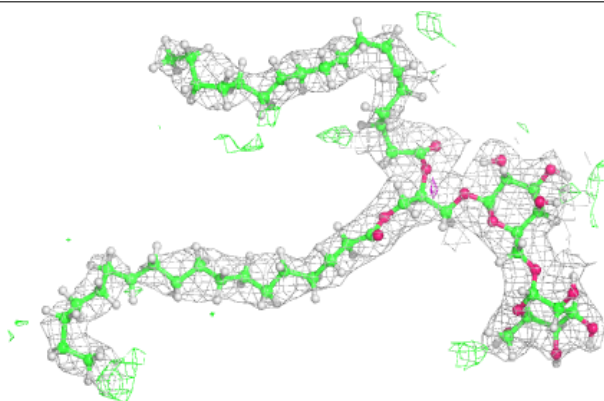


**Electron density around CLA c 513:**

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

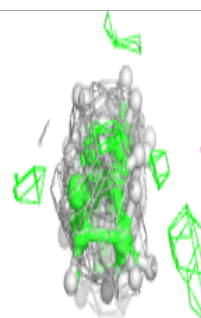
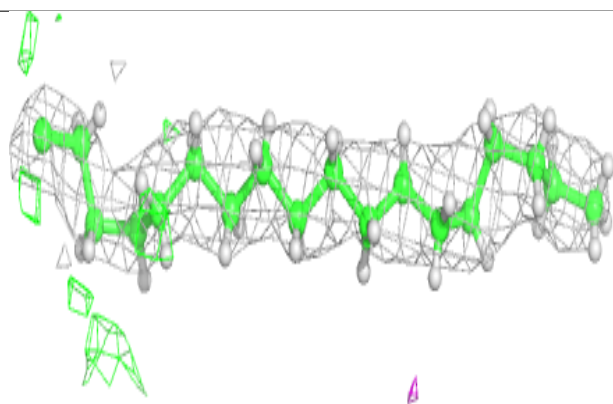
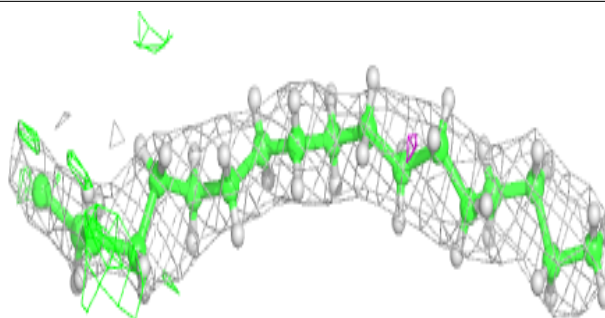
**Electron density around DGD A 413:**

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



**Electron density around STE 1 102:**

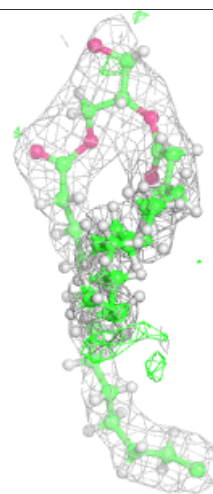
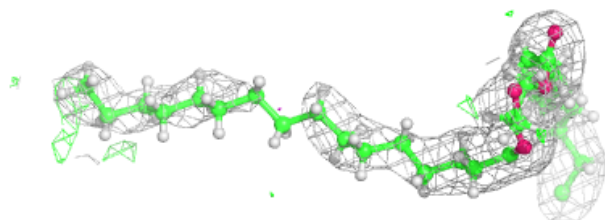
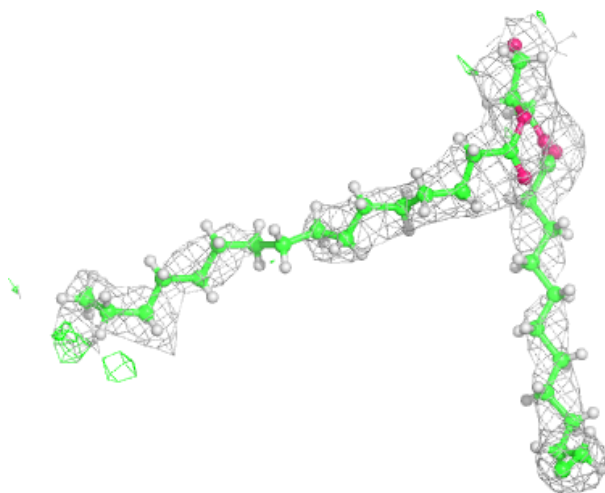
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





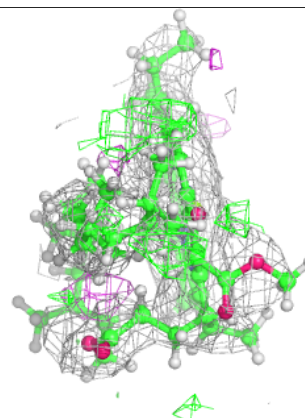
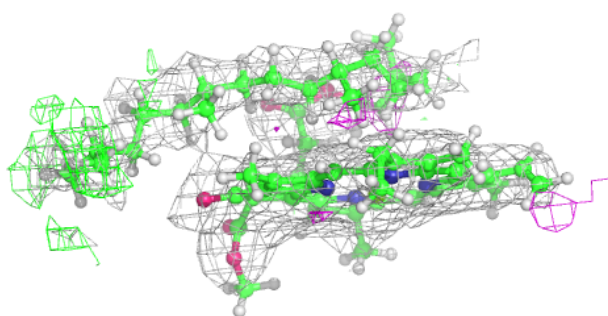
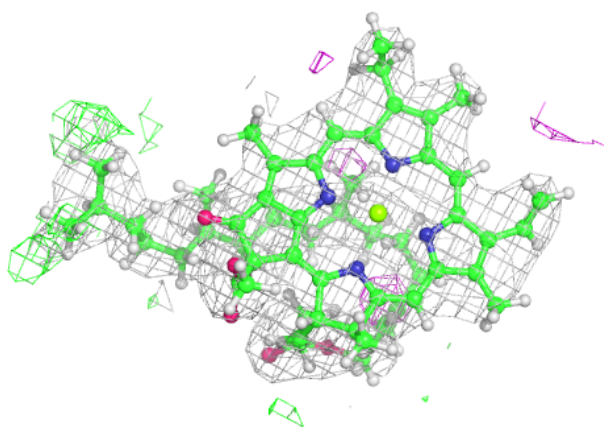
**Electron density around SQD t 102:**

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

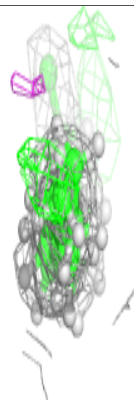
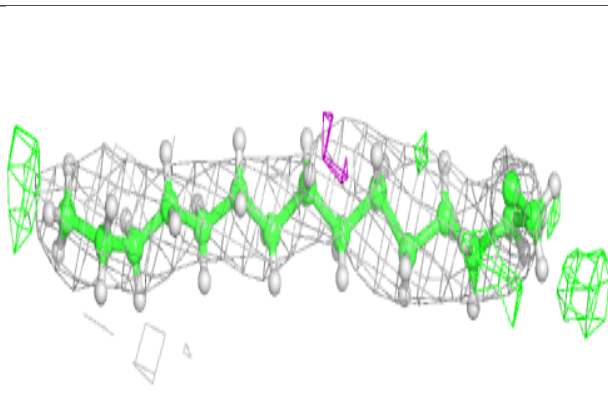
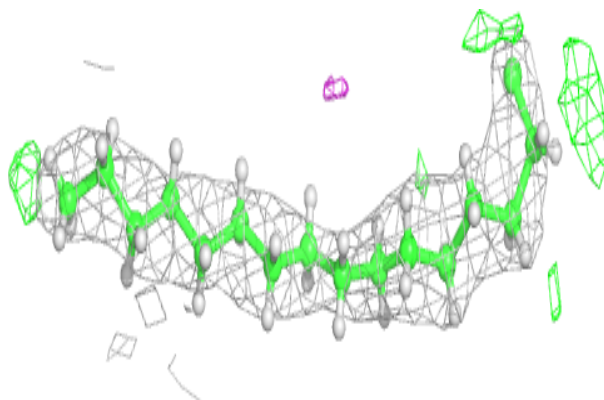


**Electron density around CLA B 601:**

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

**Electron density around STE C 519:**

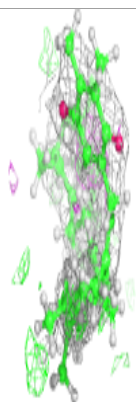
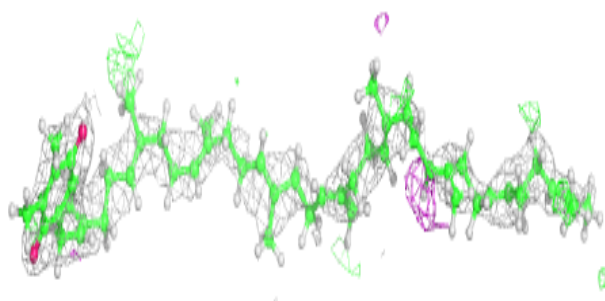
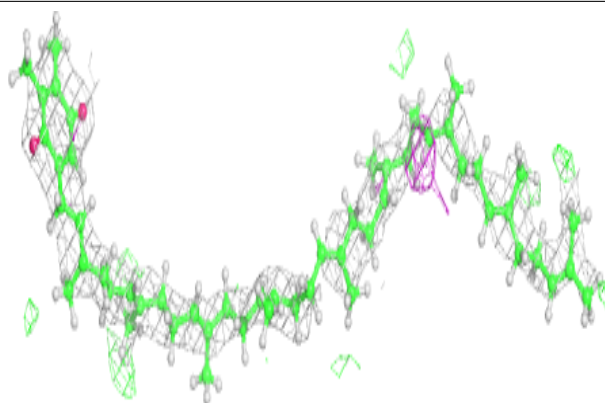
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



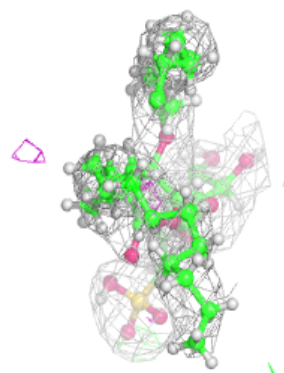
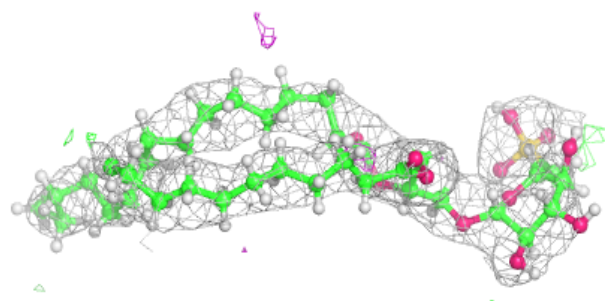
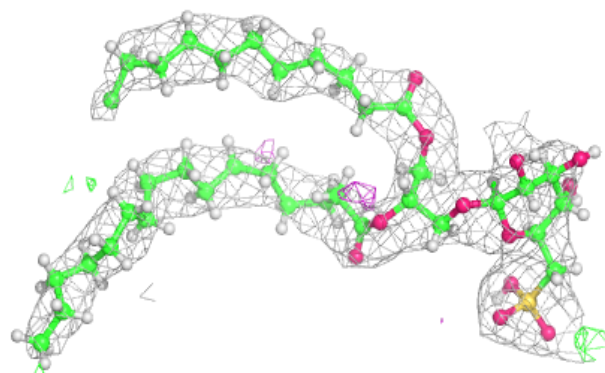


**Electron density around PL9 A 408:**

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

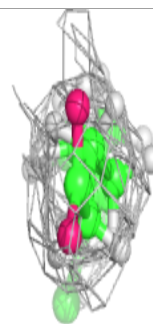
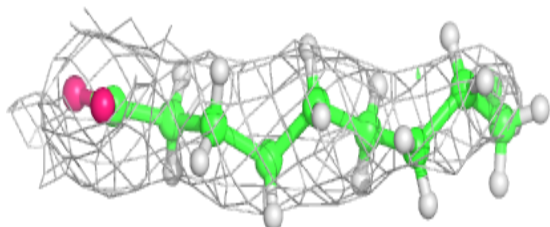
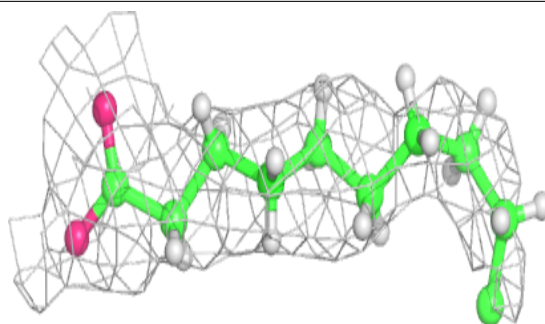
**Electron density around SQD L 101:**

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

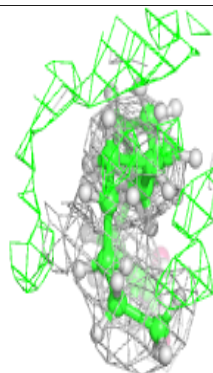
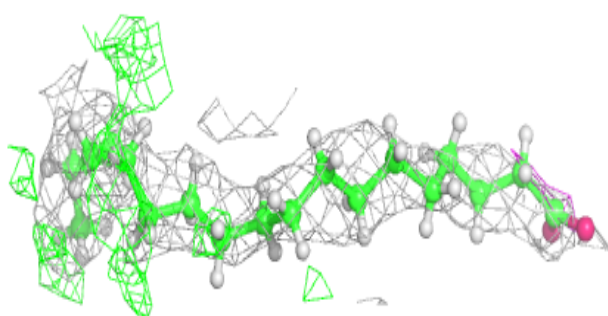
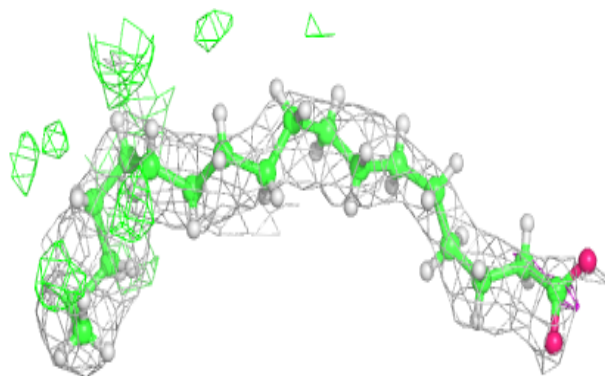


**Electron density around STE c 523:**

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

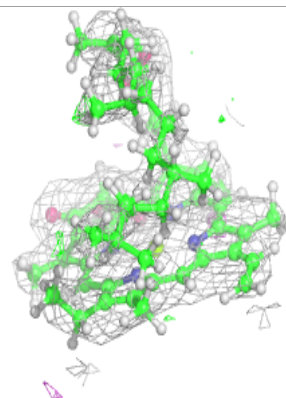
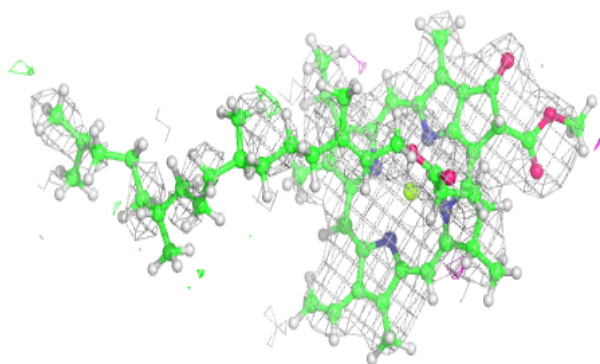
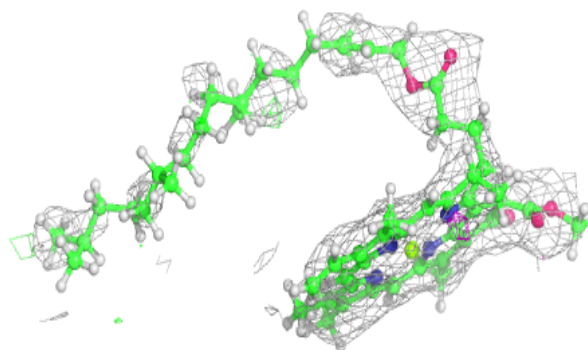
**Electron density around STE d 412:**

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

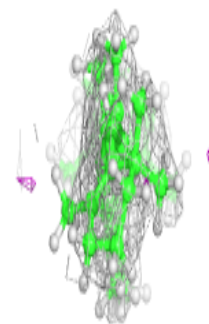
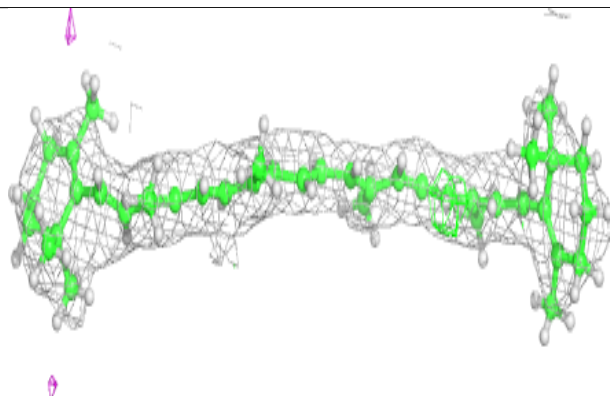
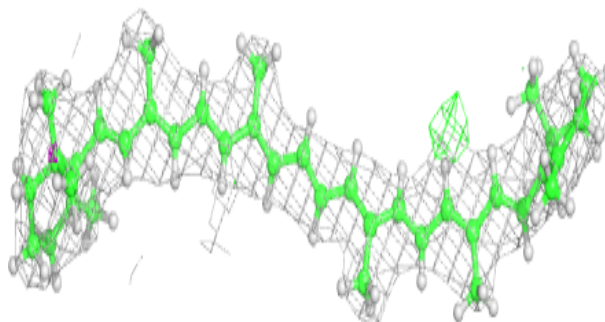


**Electron density around CLA C 513:**

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

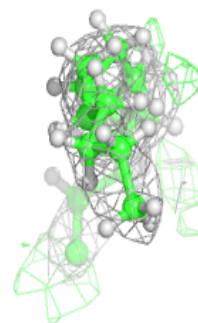
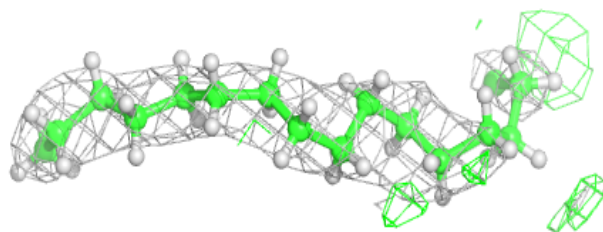
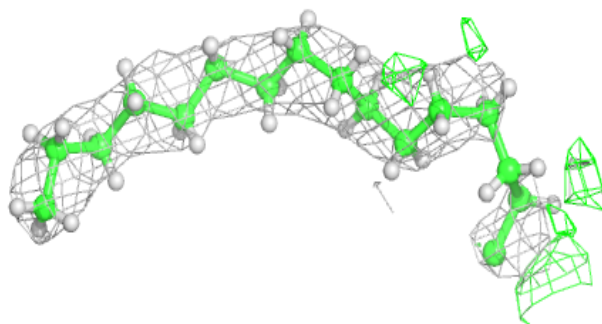
**Electron density around BCR K 101:**

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

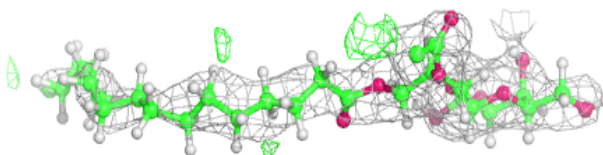
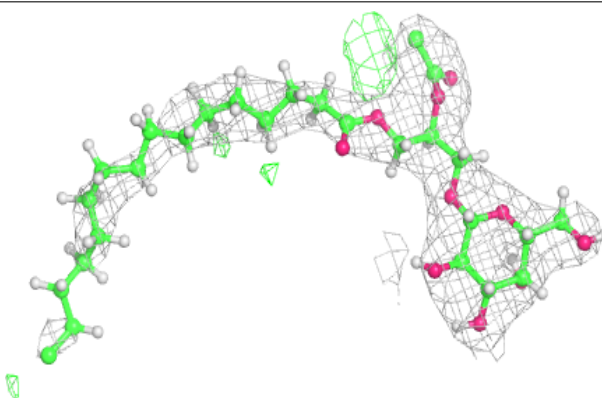


**Electron density around STE b 620:**

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

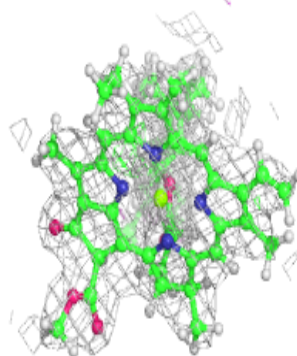
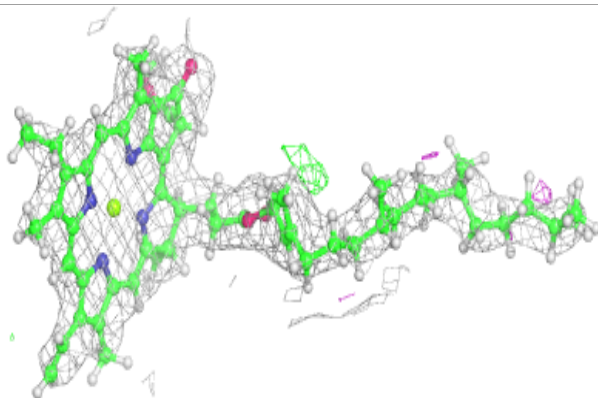
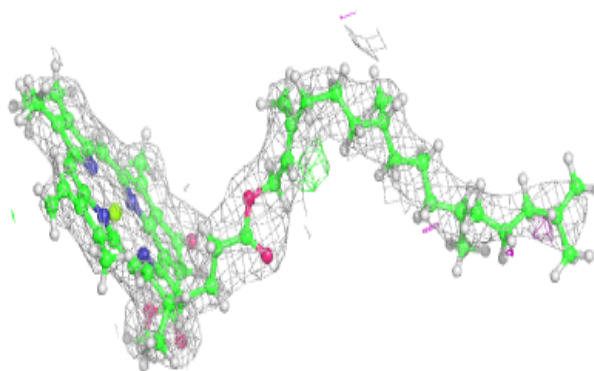
**Electron density around LMG c 519:**

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

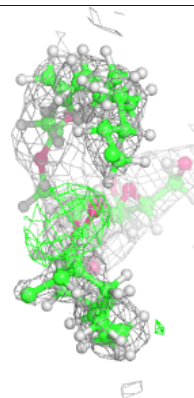
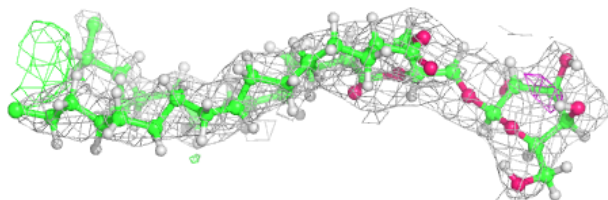
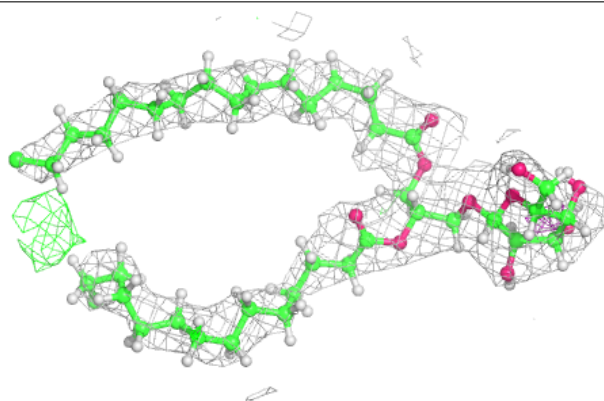


**Electron density around CLA c 502:**

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

**Electron density around LMG c 522:**

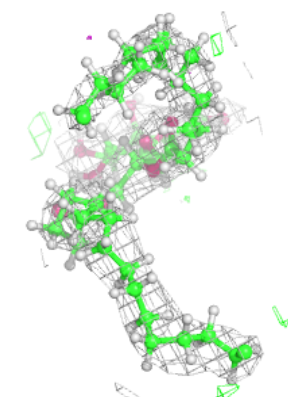
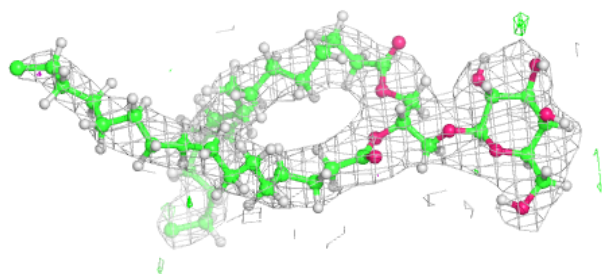
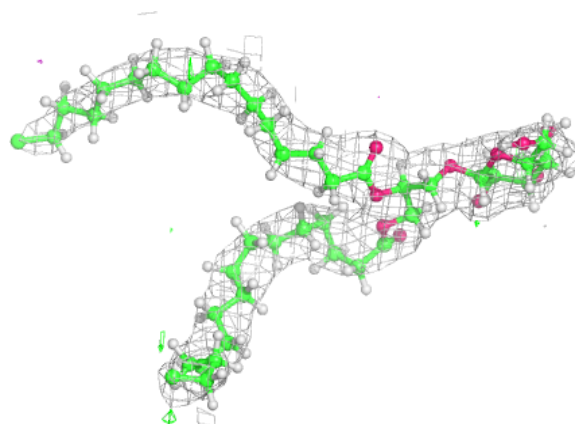
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



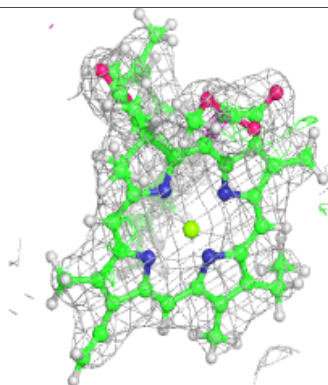
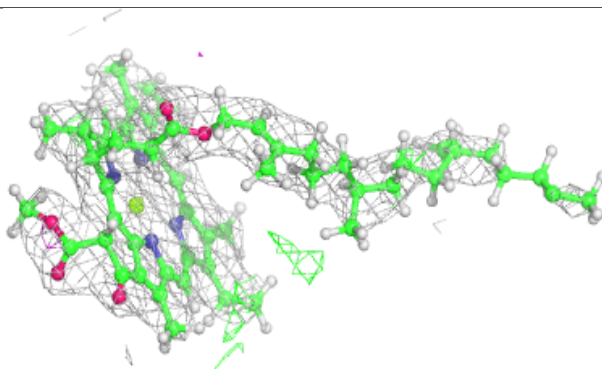
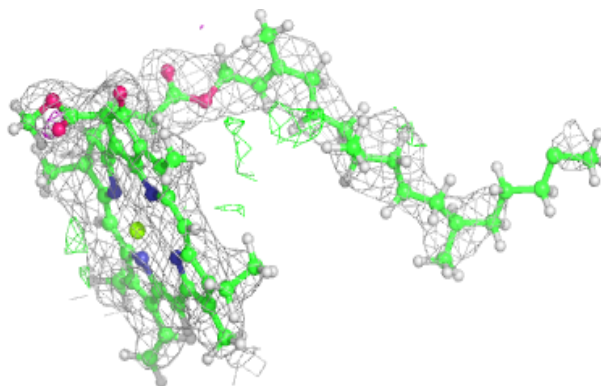


**Electron density around LMG m 101:**

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

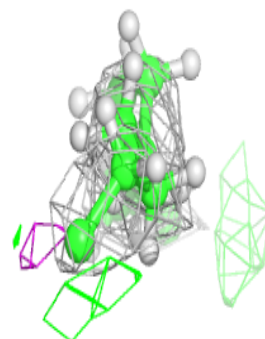
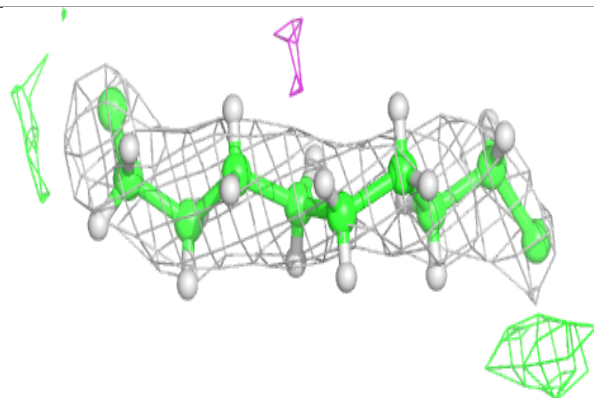
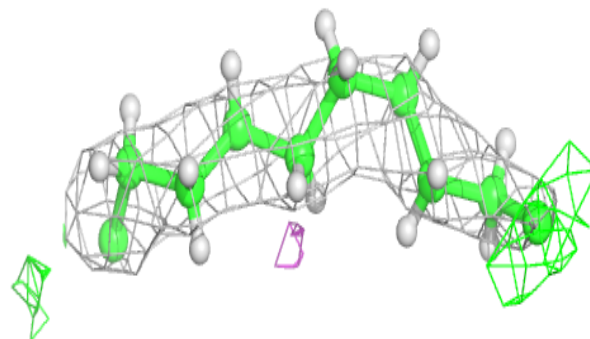
**Electron density around CLA c 508:**

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

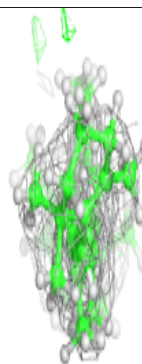
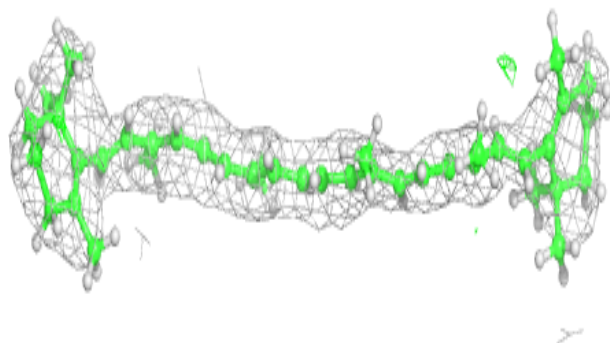
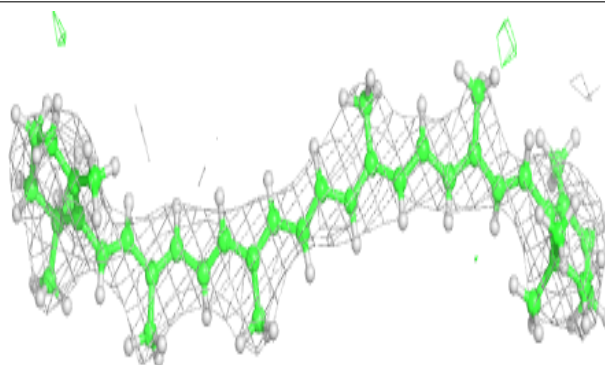


**Electron density around STE b 626:**

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

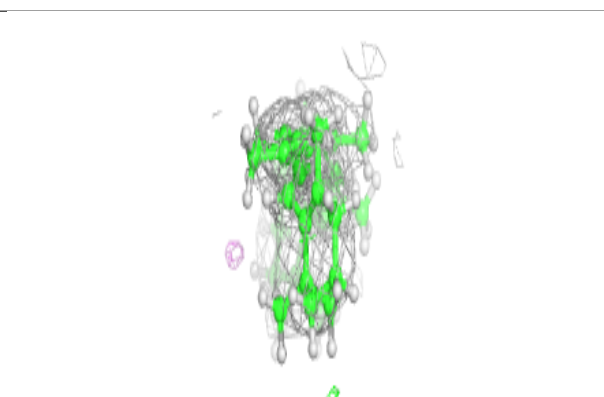
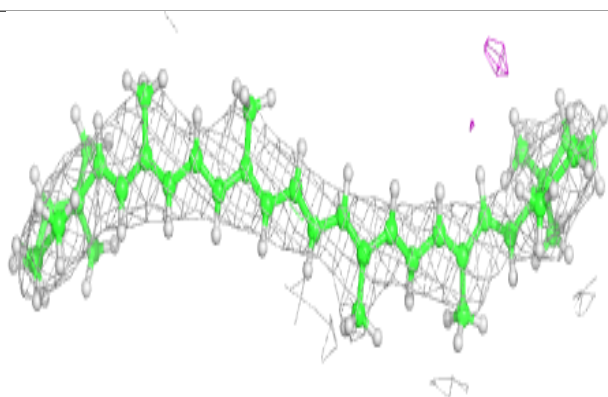
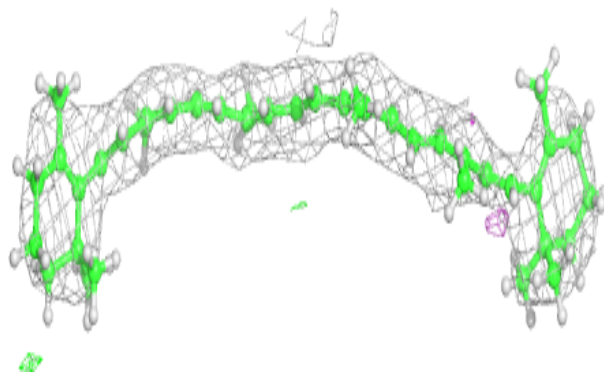
**Electron density around BCR k 101:**

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

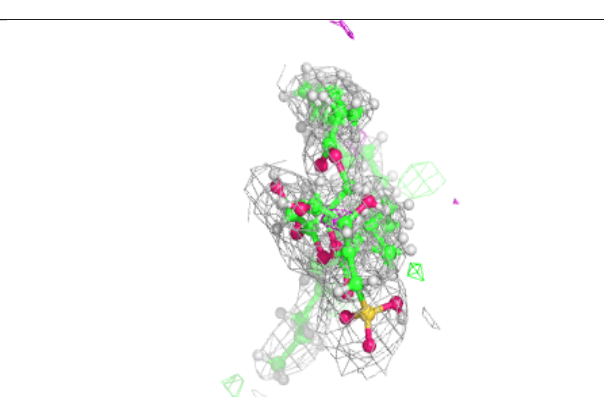
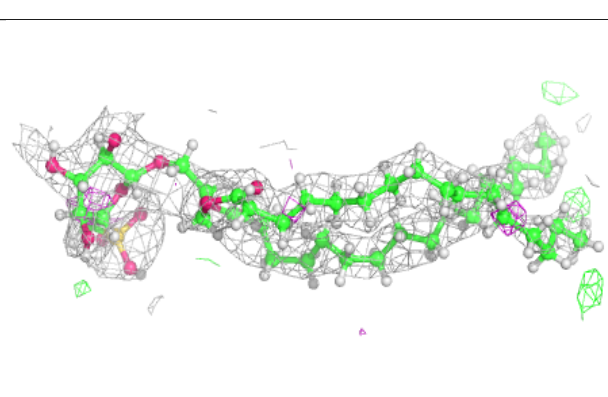
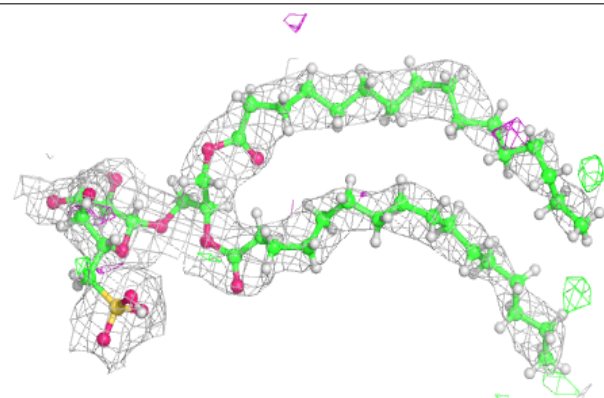


**Electron density around BCR k 102:**

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

**Electron density around SQD B 622:**

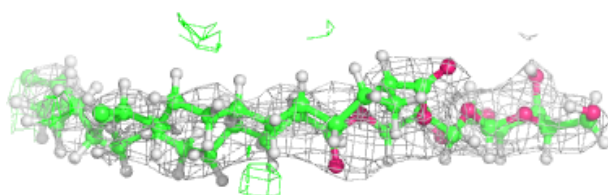
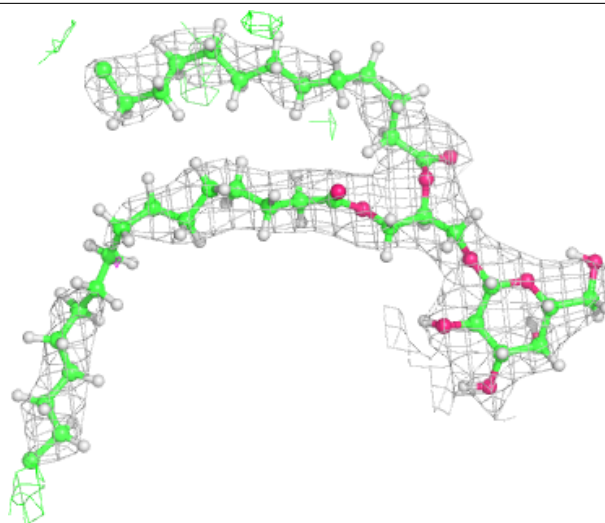
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





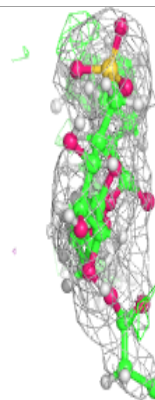
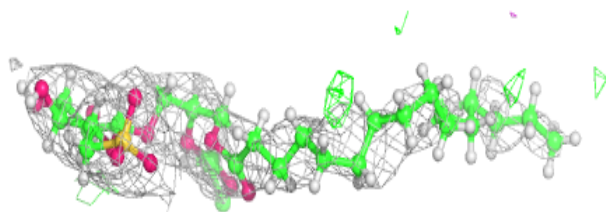
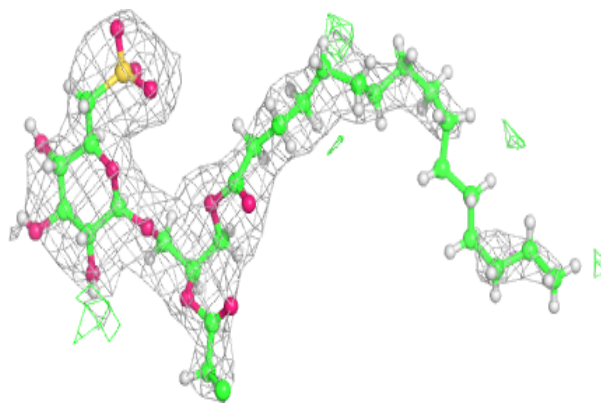
**Electron density around LMG Y 101:**

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



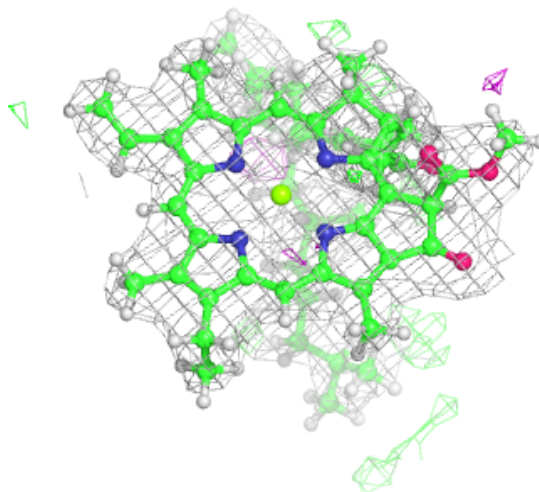
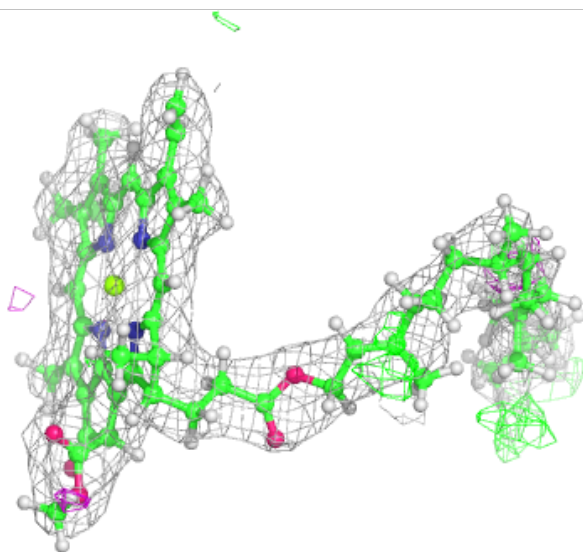
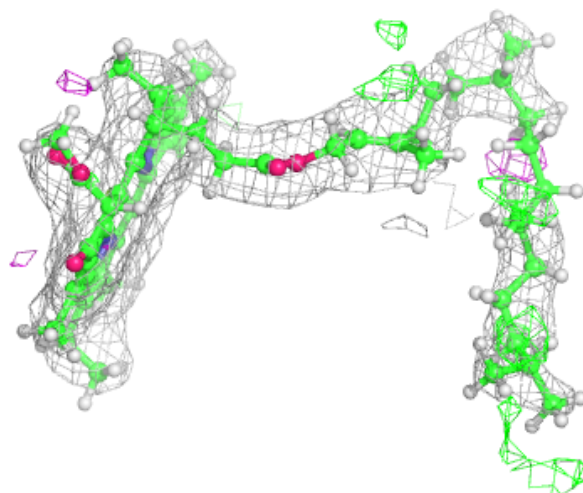
**Electron density around SQD f 102:**

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



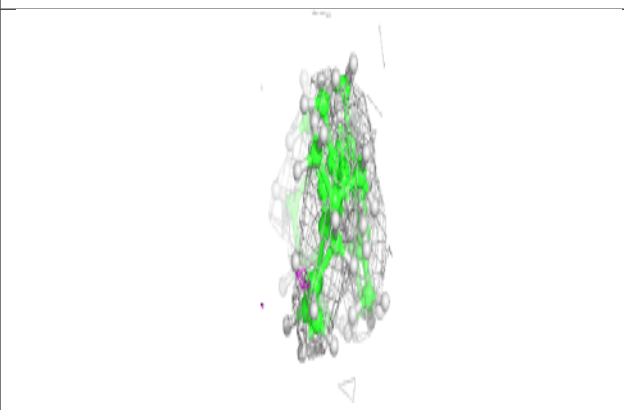
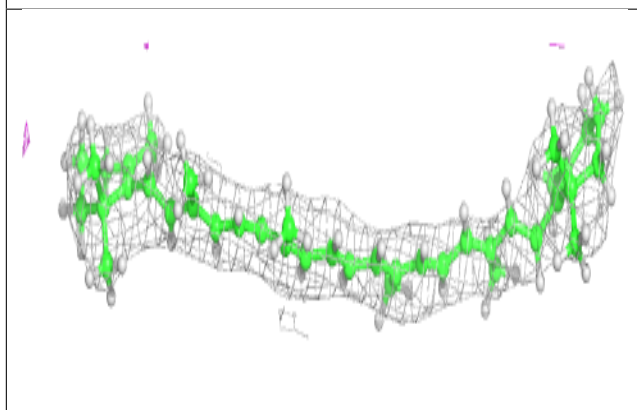
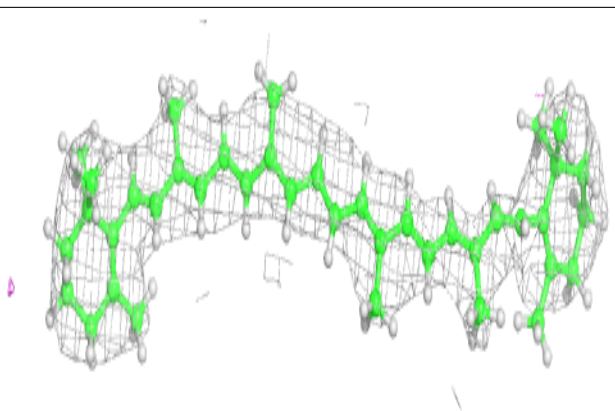
**Electron density around CLA a 404:**

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

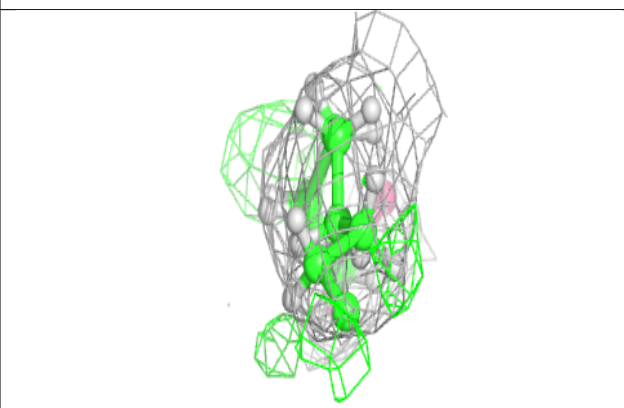
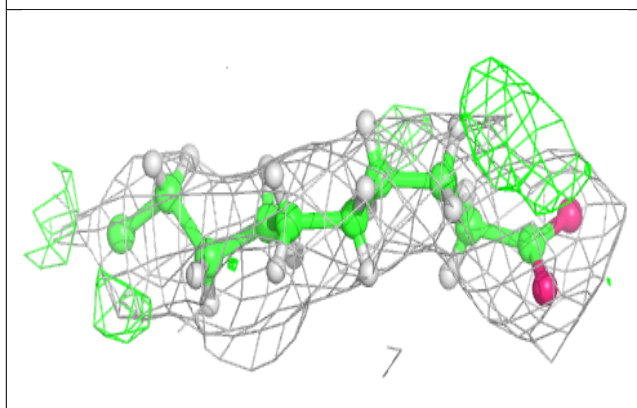
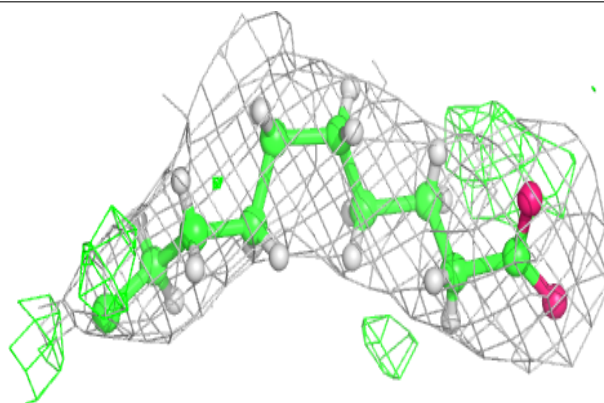


**Electron density around BCR d 406:**

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

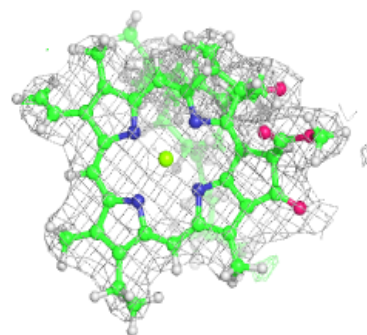
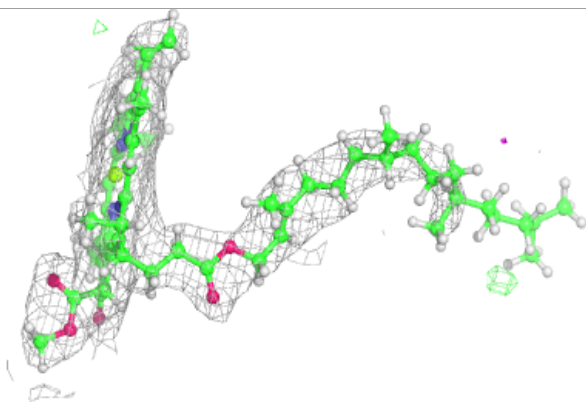
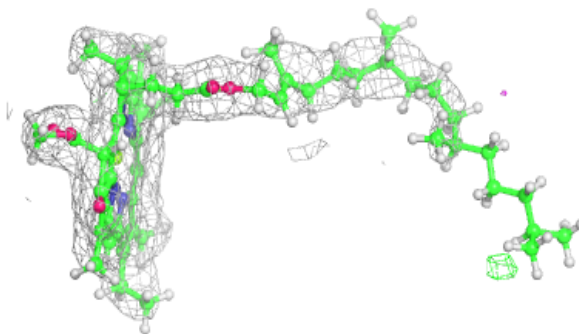
**Electron density around STE B 623:**

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

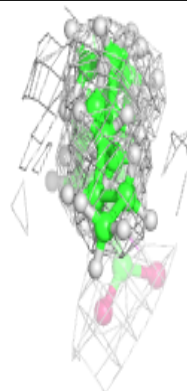
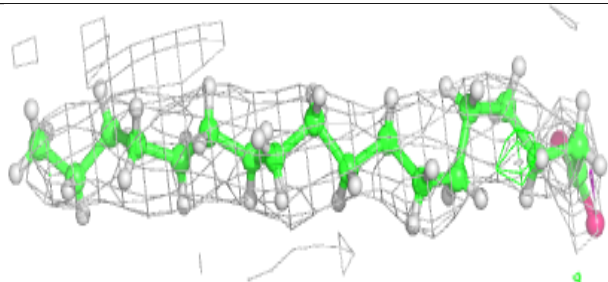
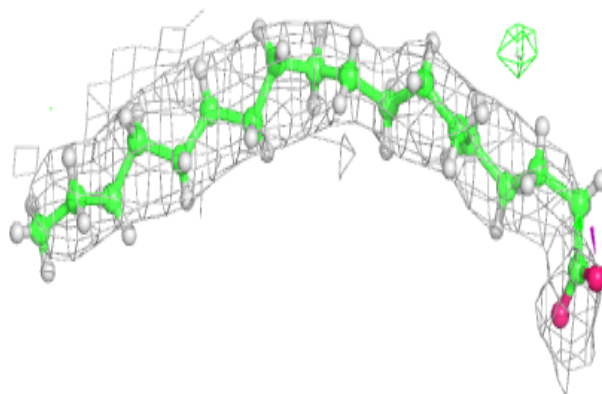


**Electron density around CLA D 405:**

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

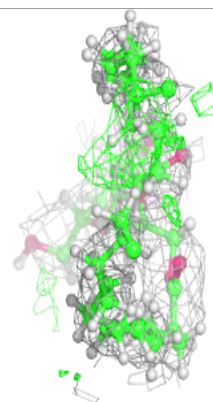
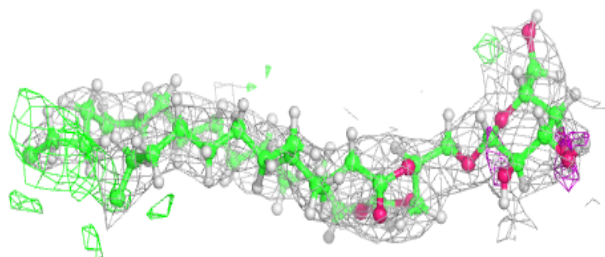
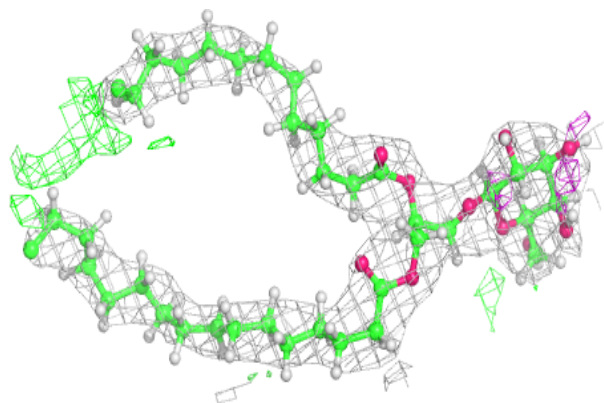
**Electron density around STE X 101:**

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

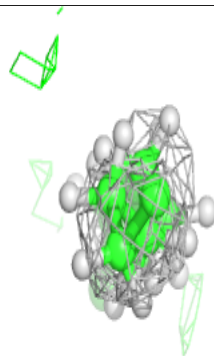
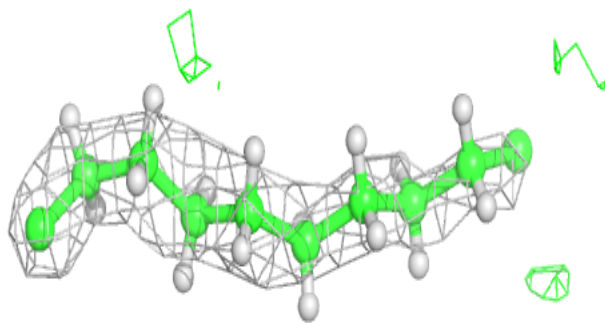
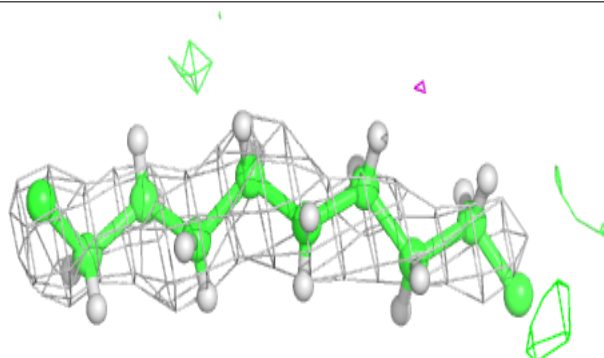


**Electron density around LMG A 409:**

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

**Electron density around STE t 104:**

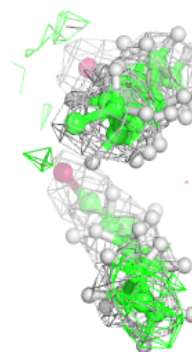
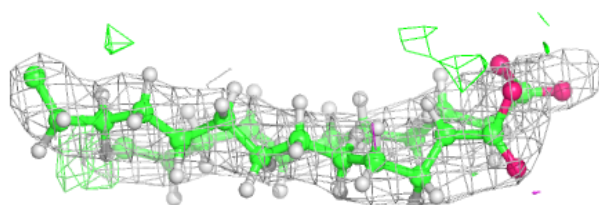
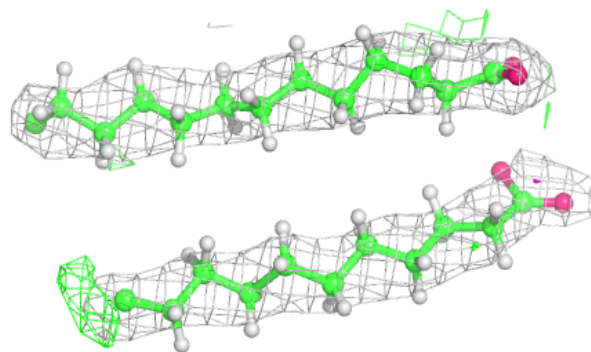
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



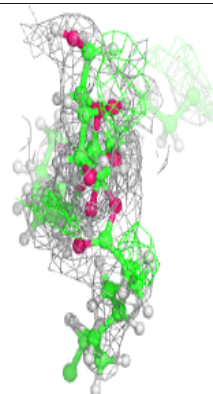
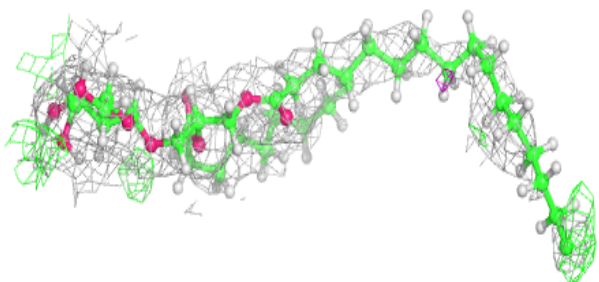
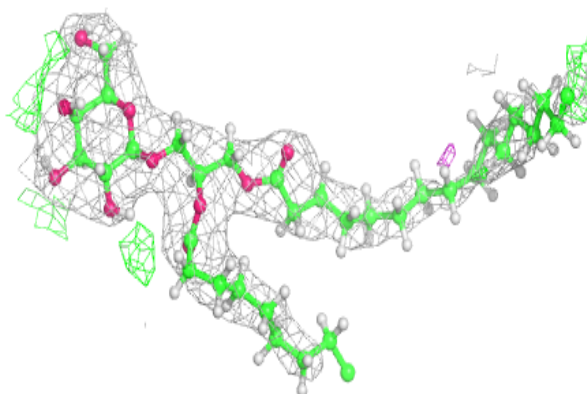


**Electron density around LMG B 621:**

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

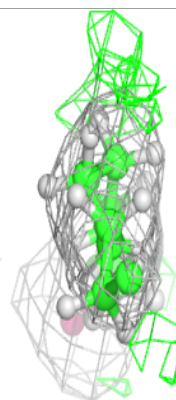
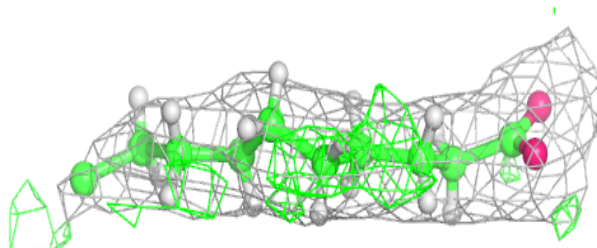
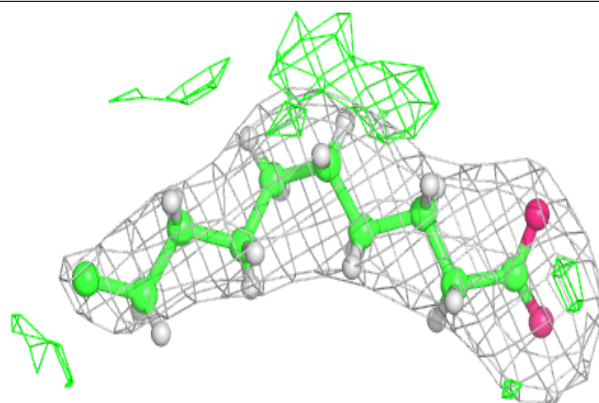
**Electron density around LMG d 410:**

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

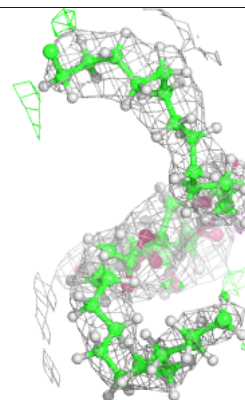
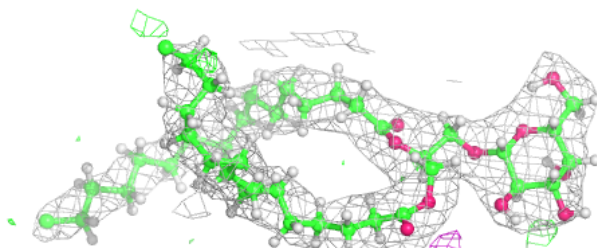
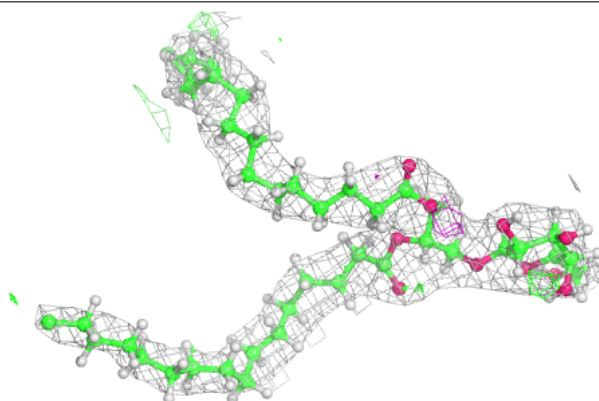


**Electron density around STE C 520:**

$2mF_o-DF_c$  (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:**

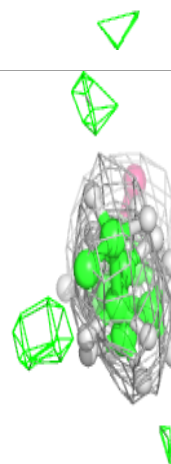
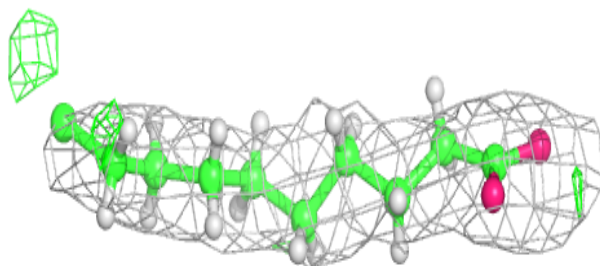
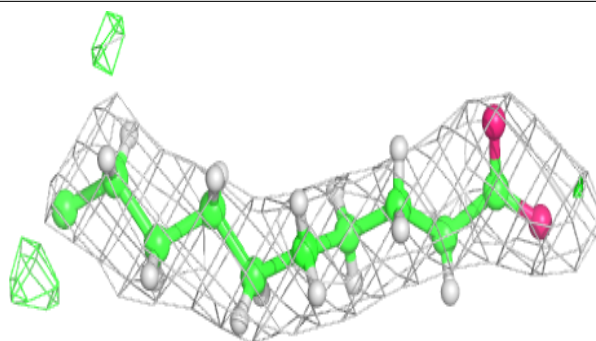
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



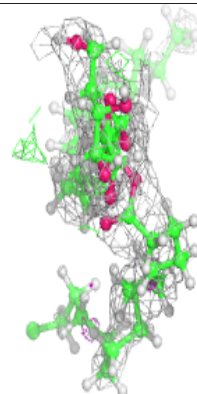
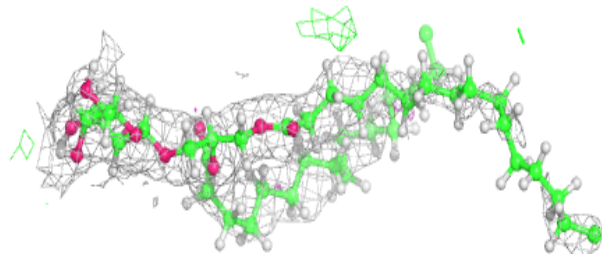
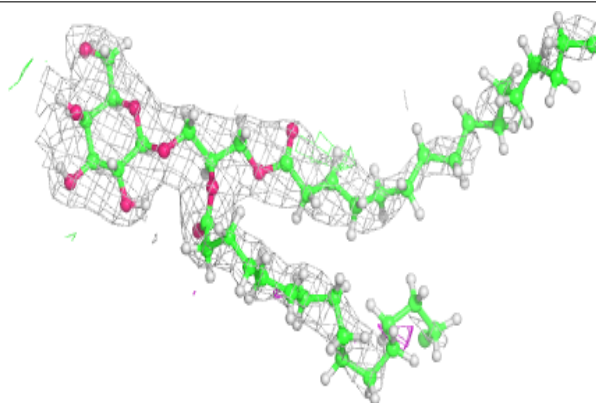


**Electron density around STE j 101:**

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

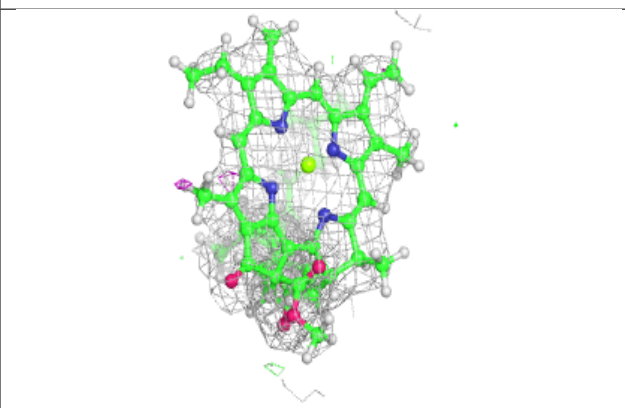
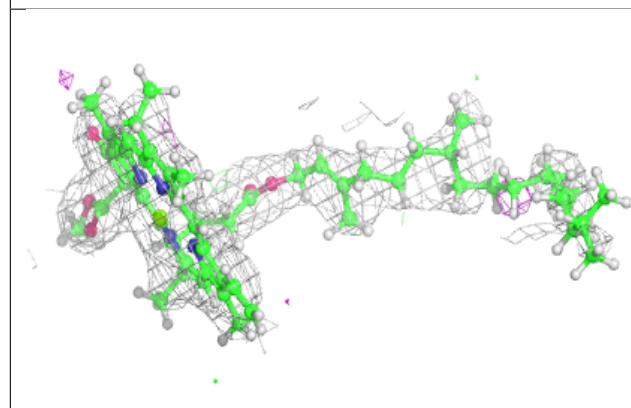
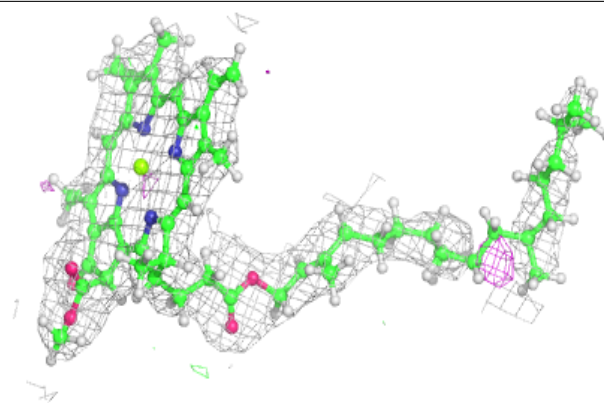
**Electron density around LMG D 408:**

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

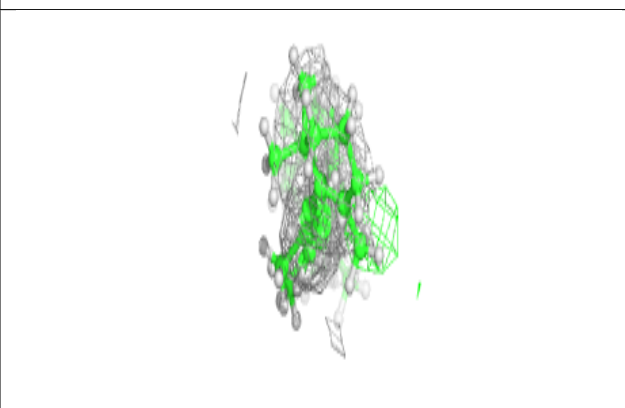
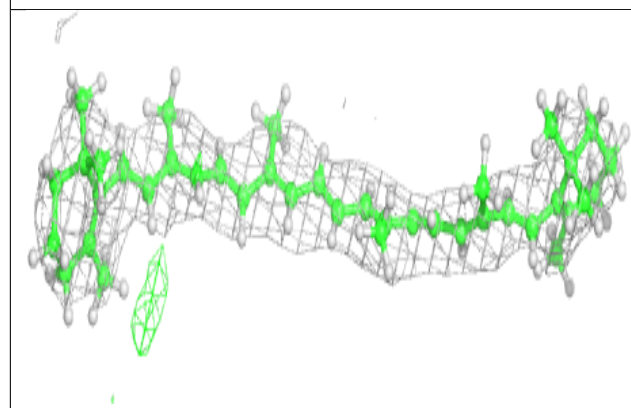
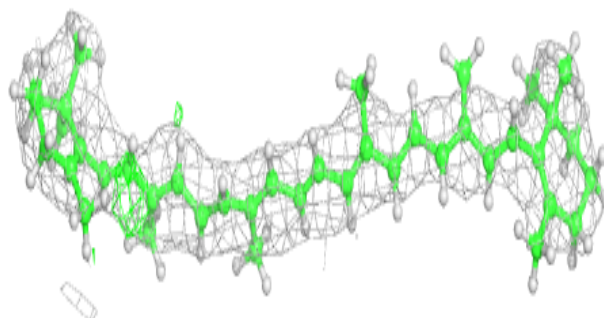


**Electron density around CLA d 405:**

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

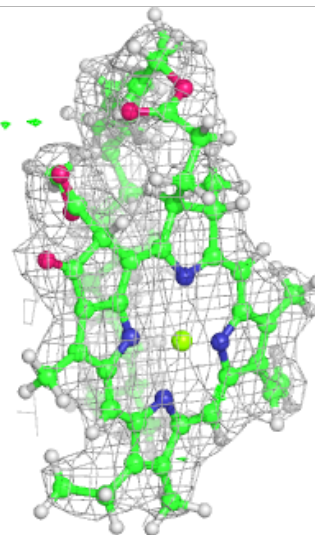
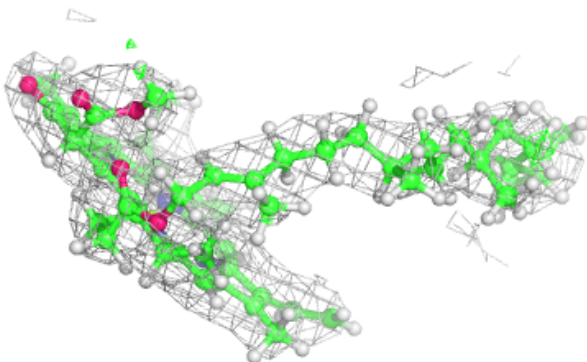
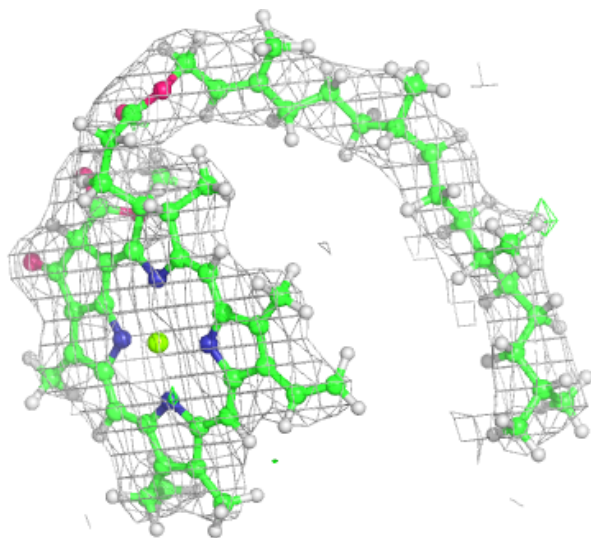
**Electron density around BCR c 514:**

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



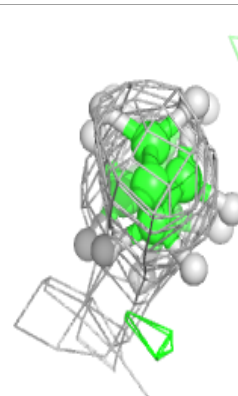
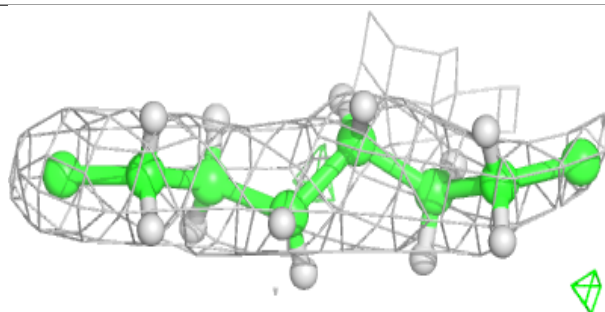
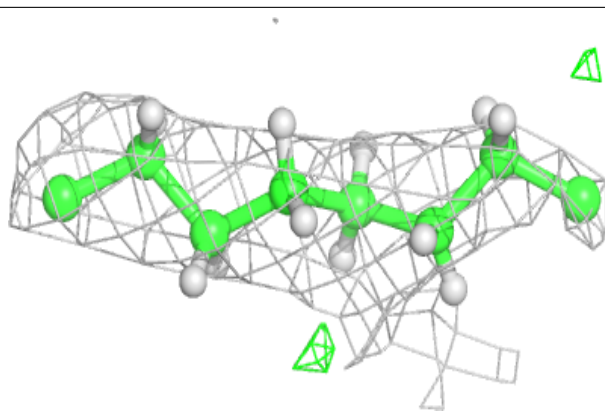
**Electron density around CLA C 507:**

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

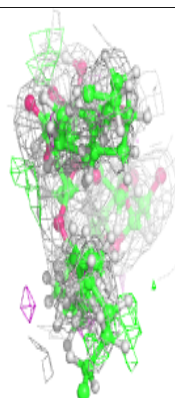
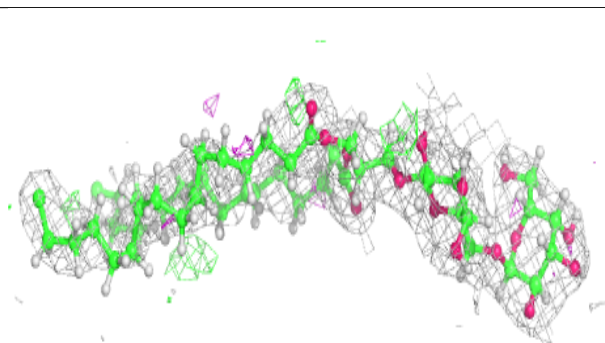
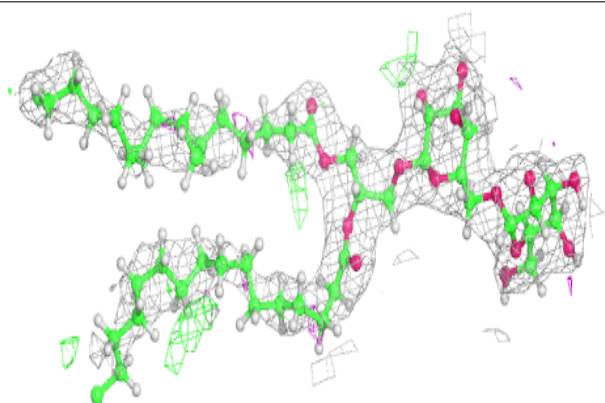


**Electron density around STE Z 102:**

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

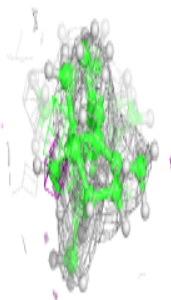
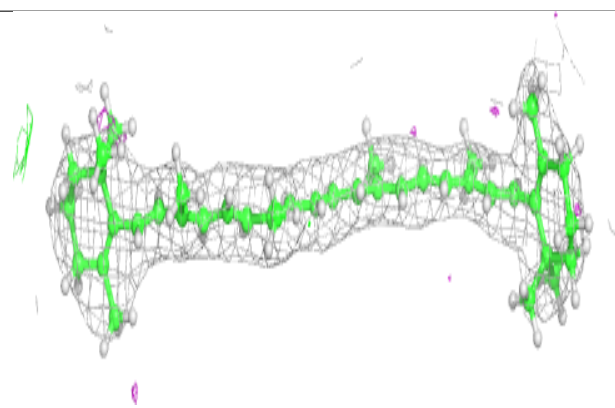
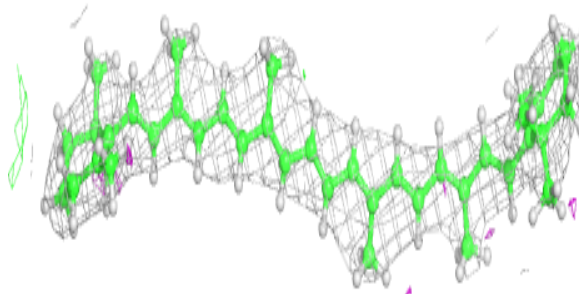
**Electron density around DGD c 518:**

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



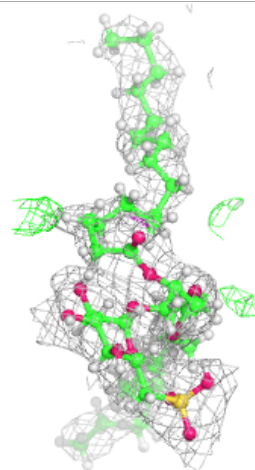
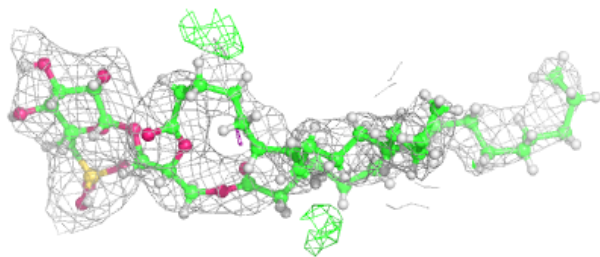
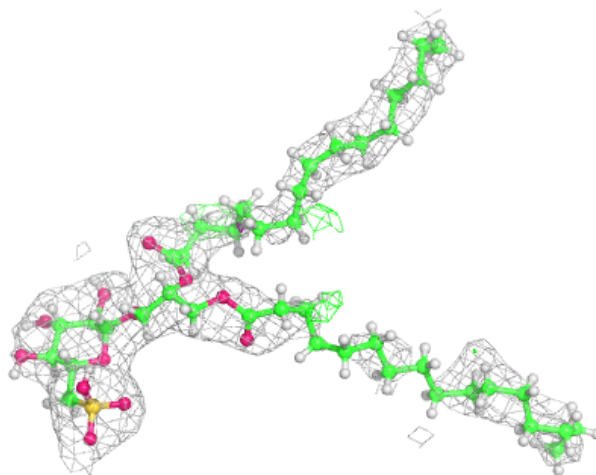
**Electron density around BCR C 514:**

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



**Electron density around SQD a 411:**

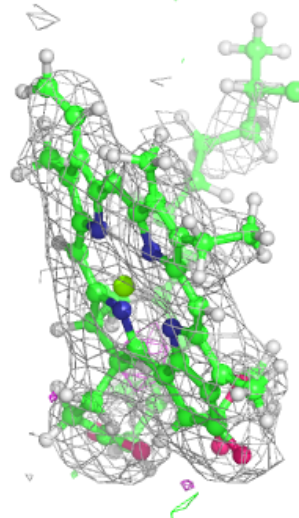
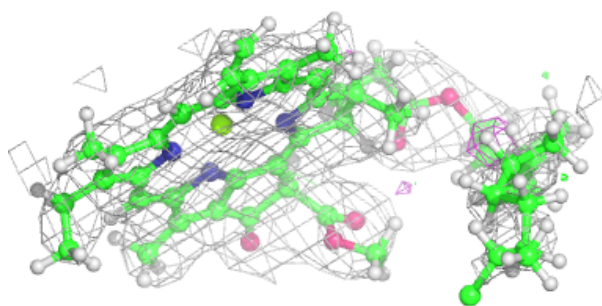
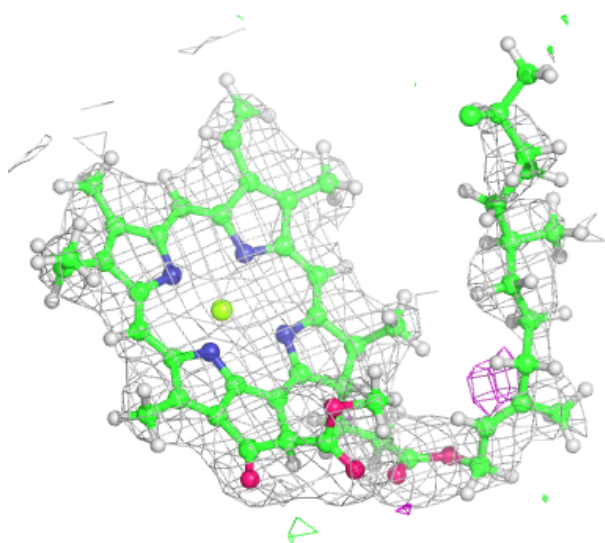
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





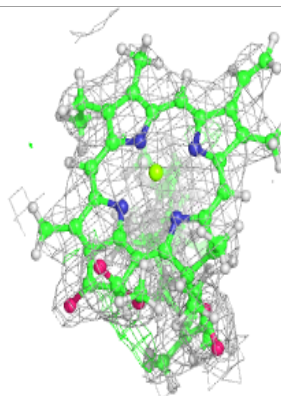
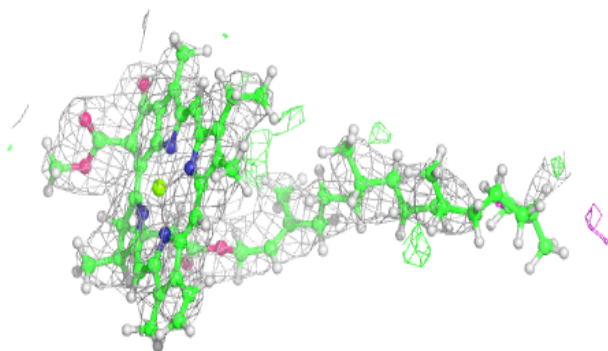
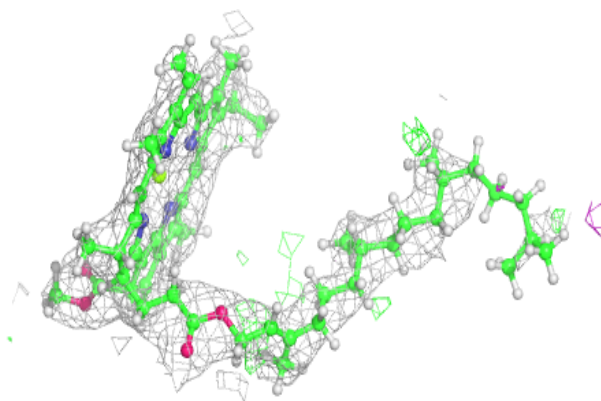
**Electron density around CLA b 616:**

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



**Electron density around CLA C 508:**

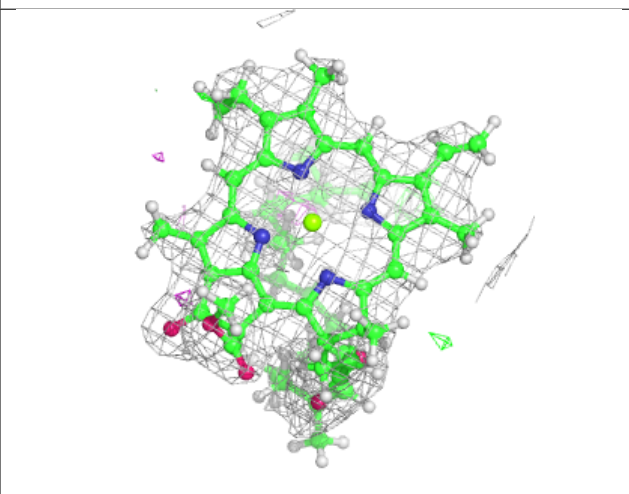
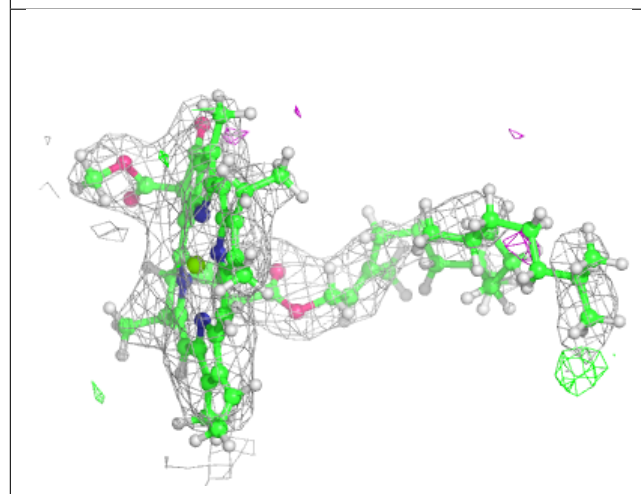
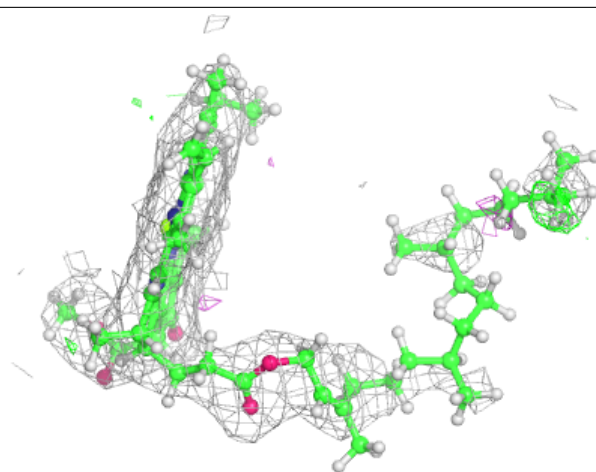
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





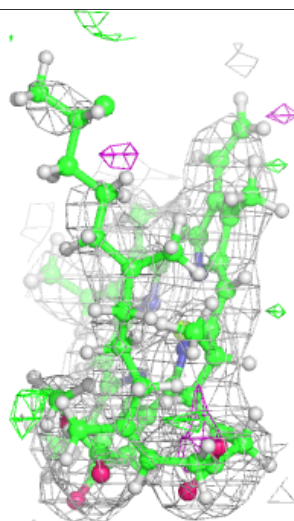
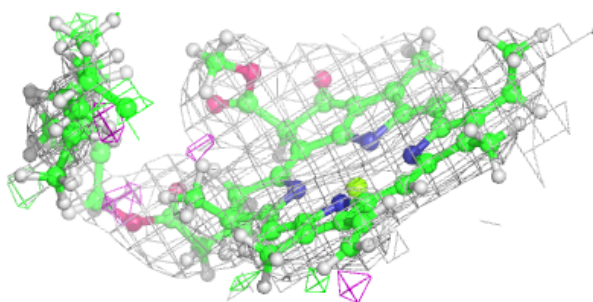
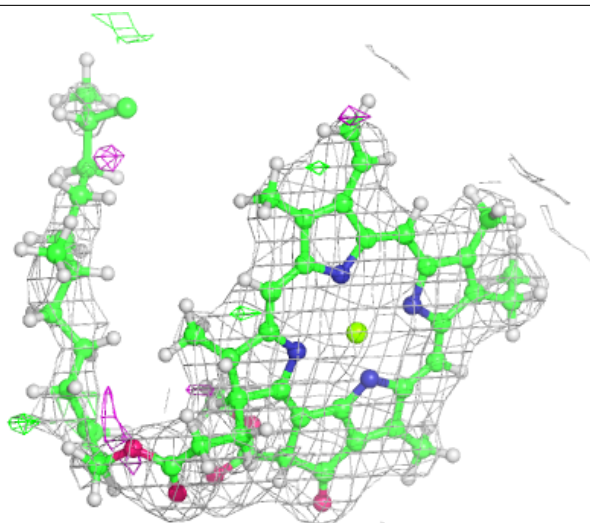
**Electron density around CLA c 506:**

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



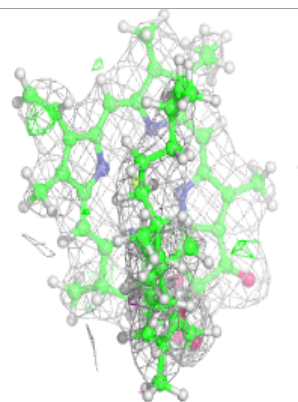
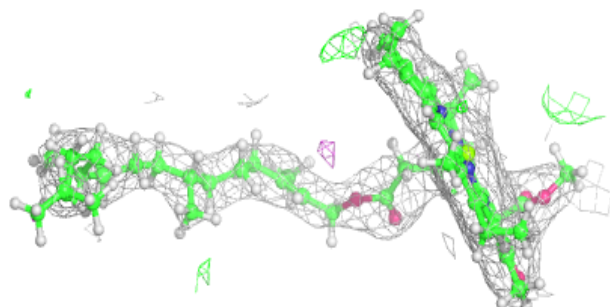
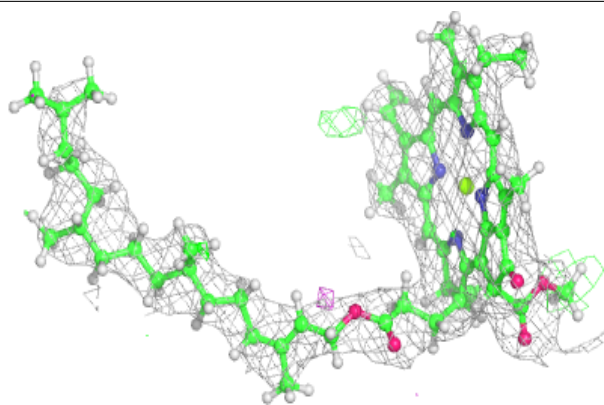
**Electron density around CLA B 616:**

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

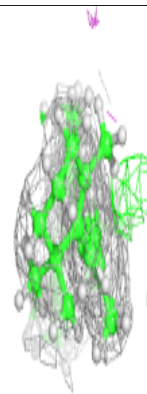
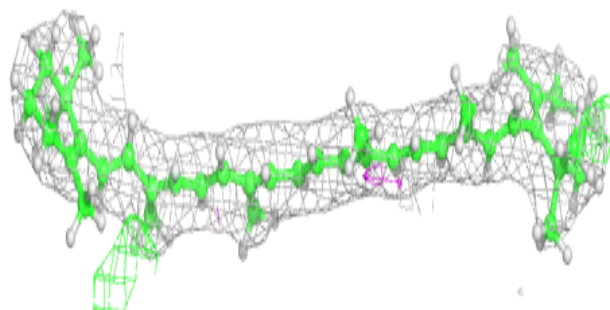
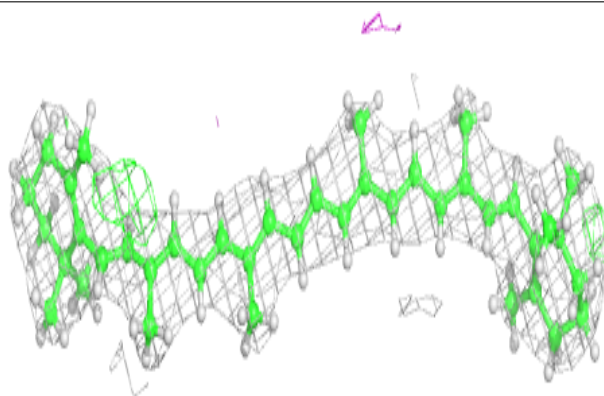


**Electron density around CLA b 609:**

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

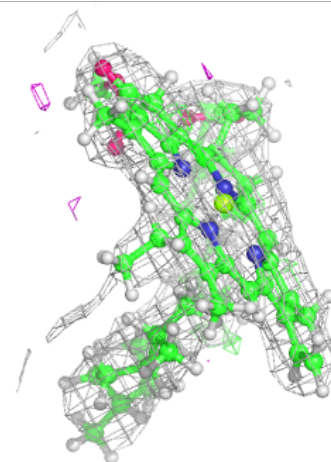
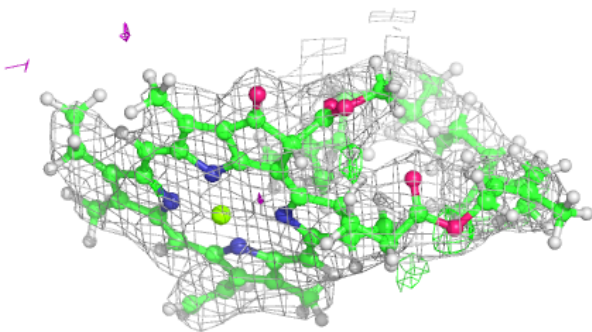
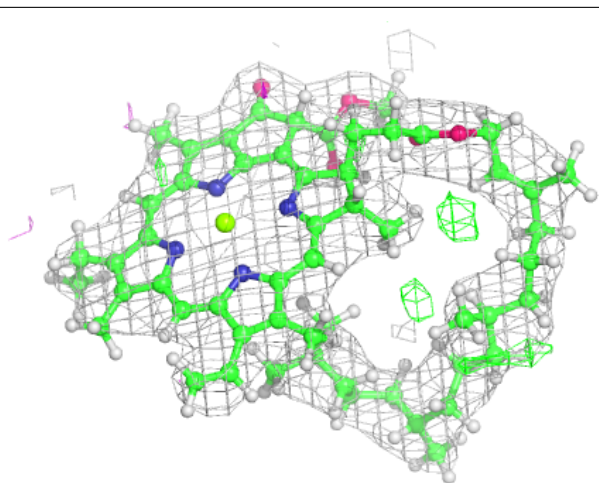
**Electron density around BCR B 619:**

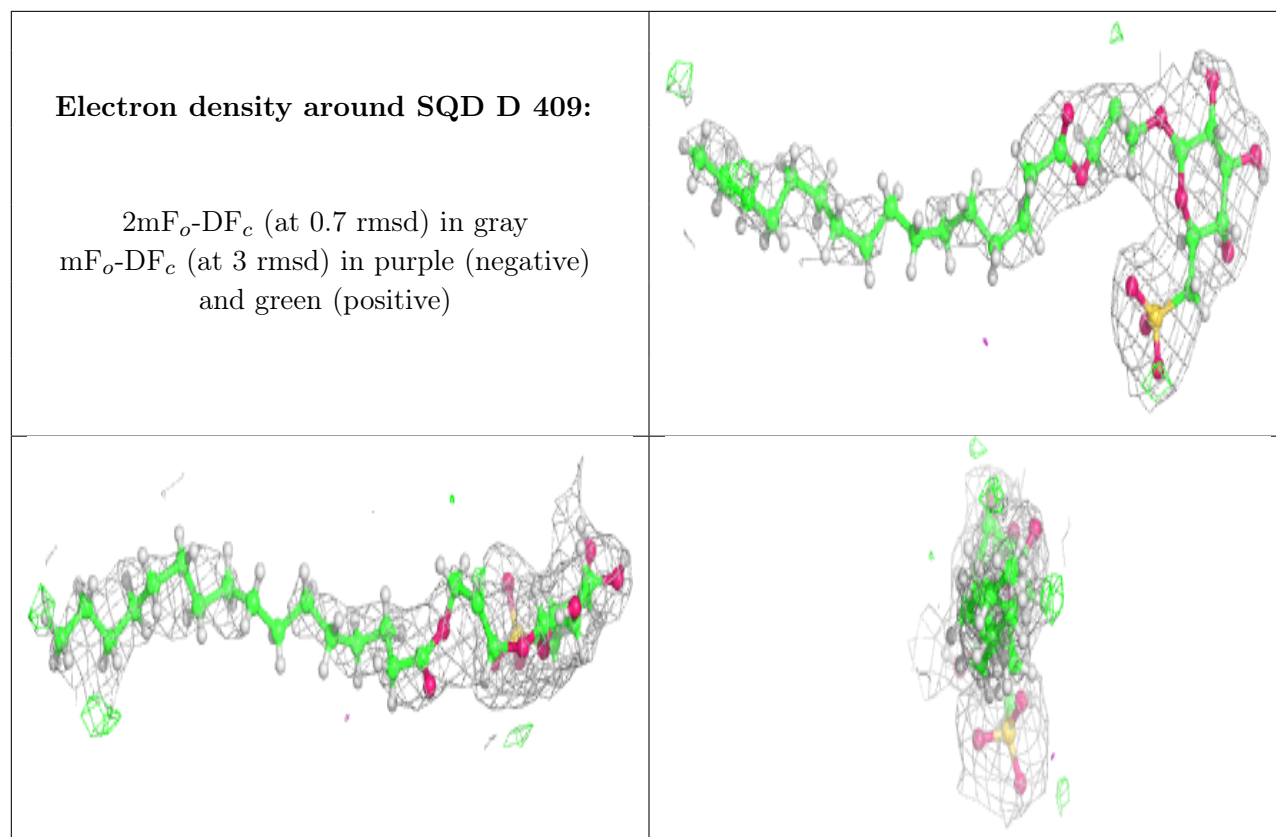
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA b 615:**

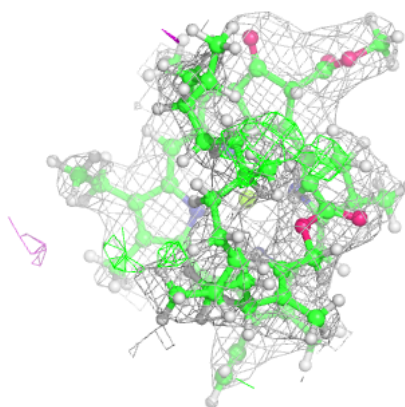
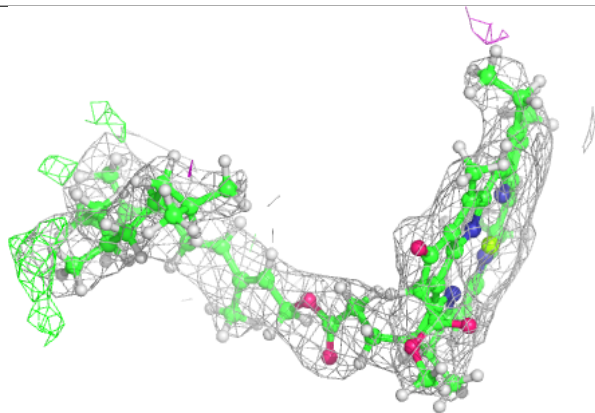
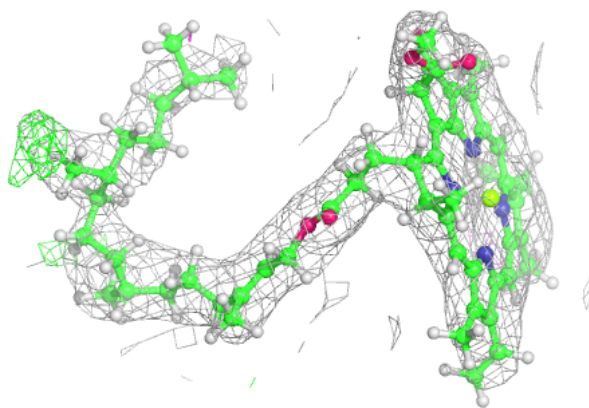
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA B 606:**

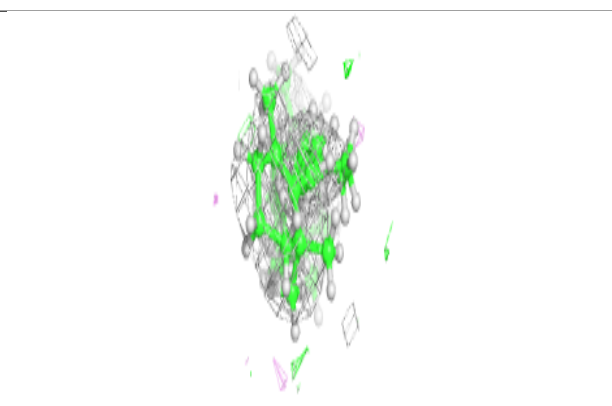
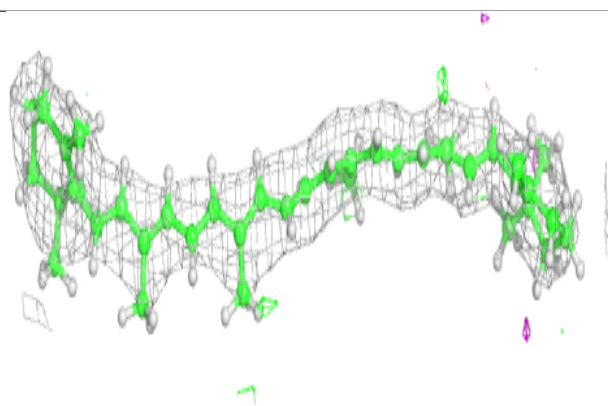
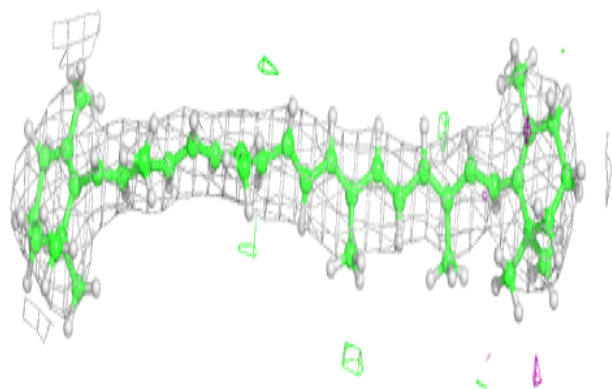
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



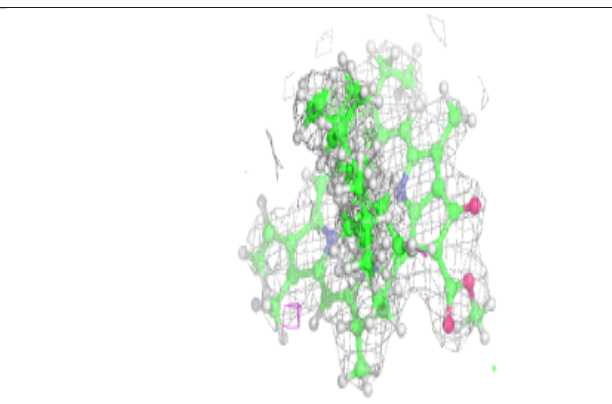
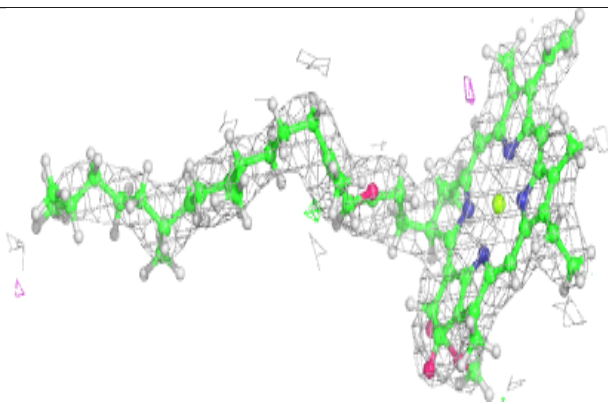
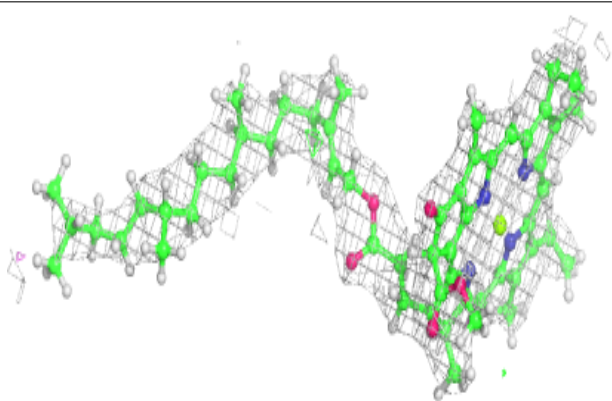


**Electron density around BCR Z 101:**

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

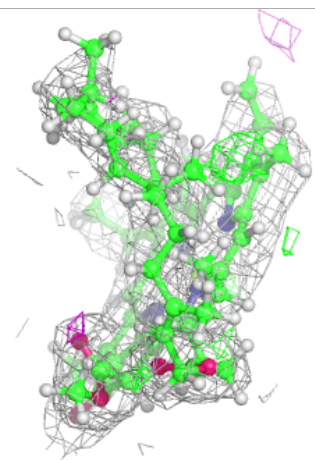
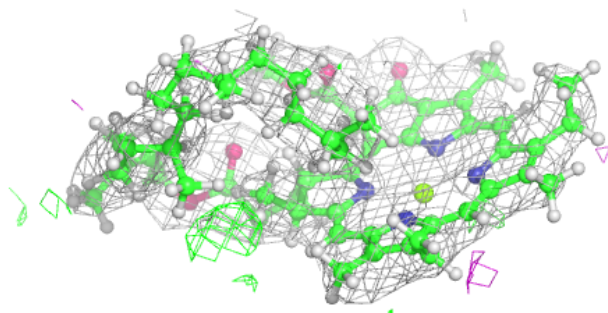
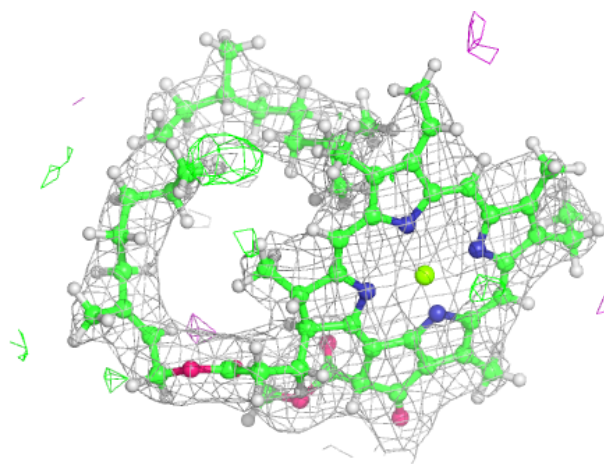
**Electron density around CLA C 502:**

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



**Electron density around CLA B 615:**

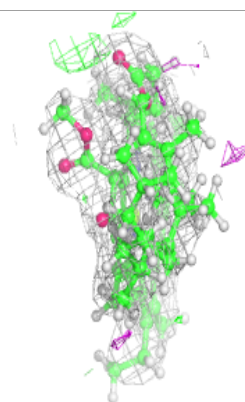
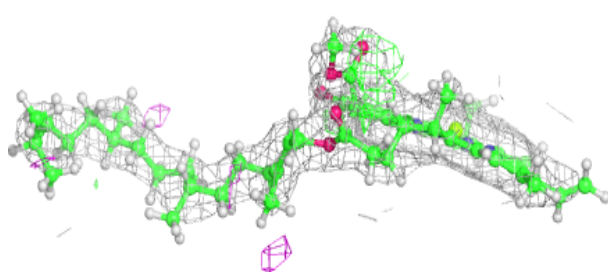
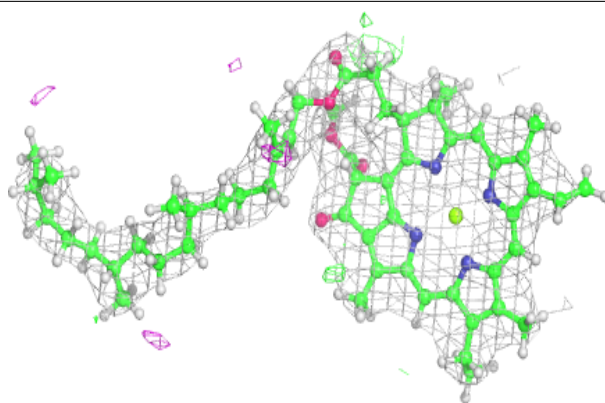
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



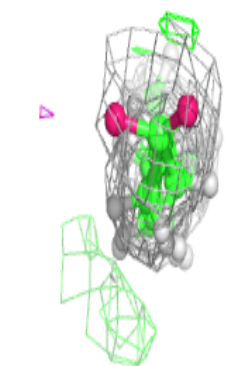
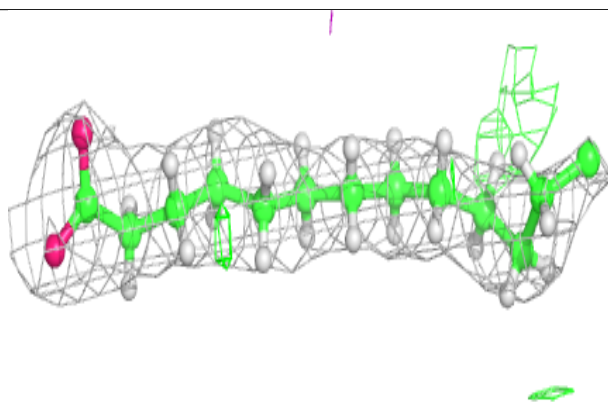
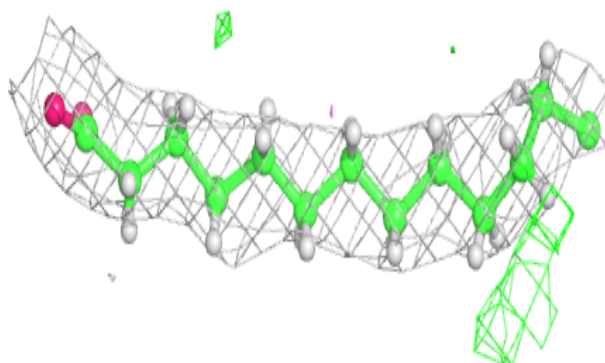


**Electron density around CLA b 602:**

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

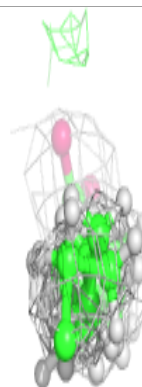
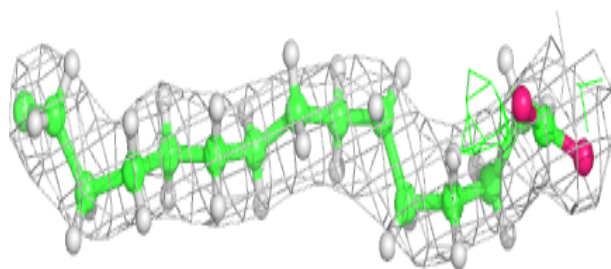
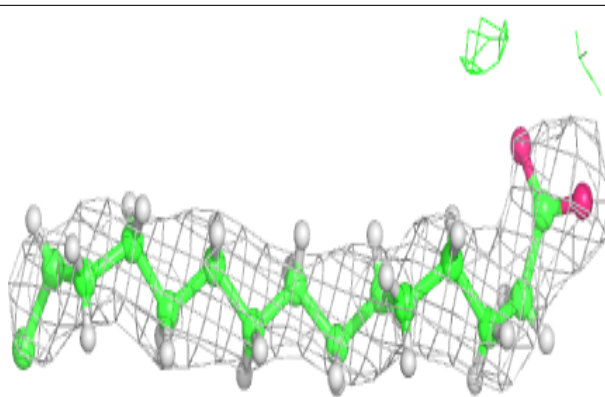
**Electron density around STE M 102:**

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



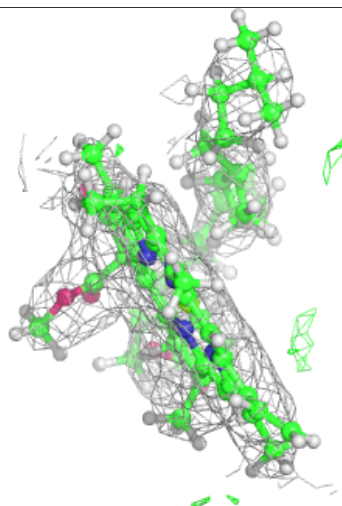
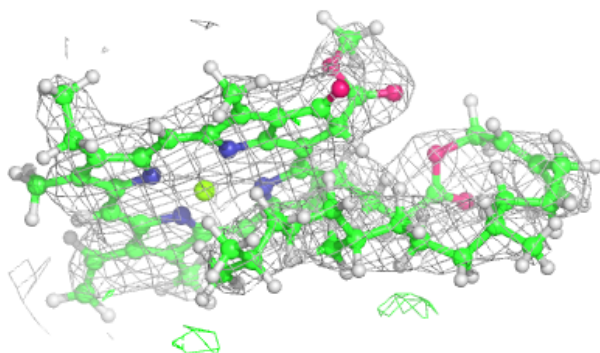
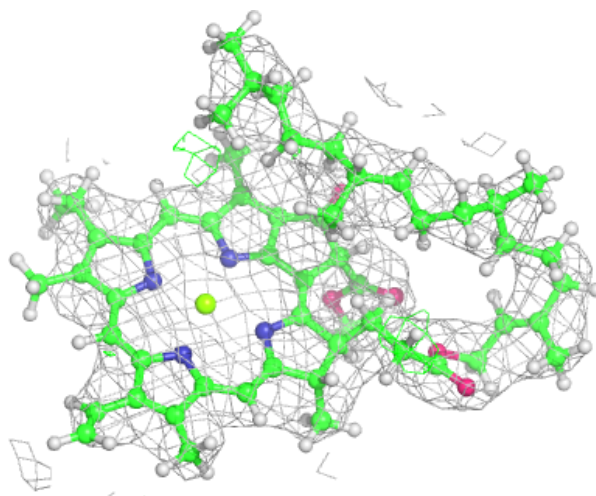
**Electron density around STE d 411:**

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



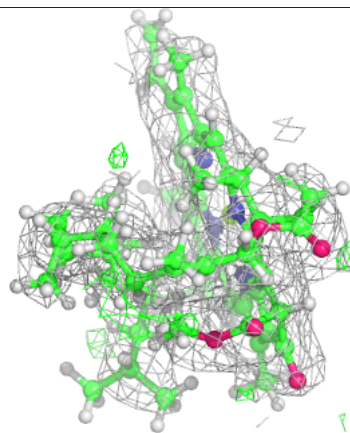
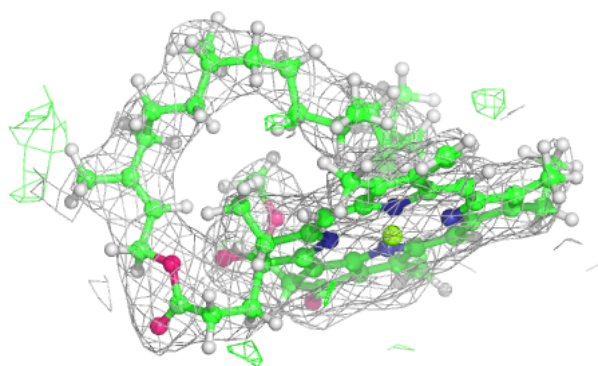
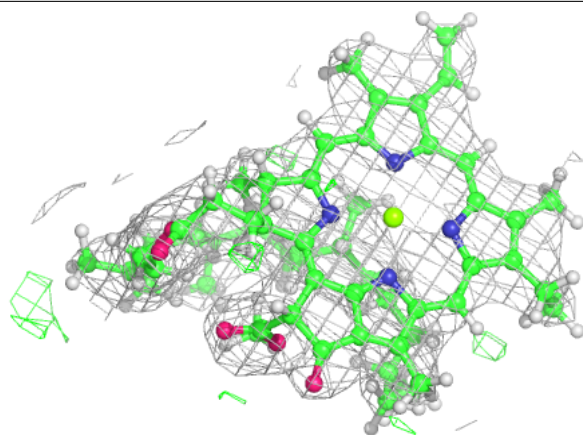
**Electron density around CLA c 509:**

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

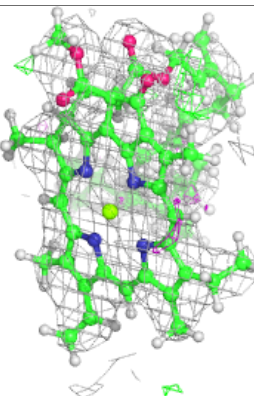
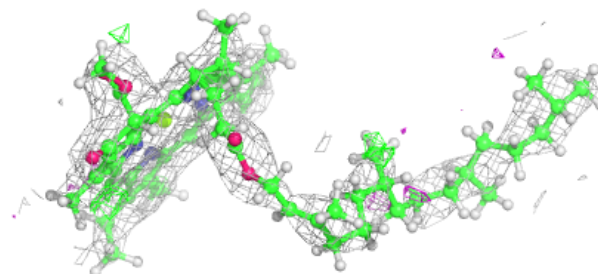
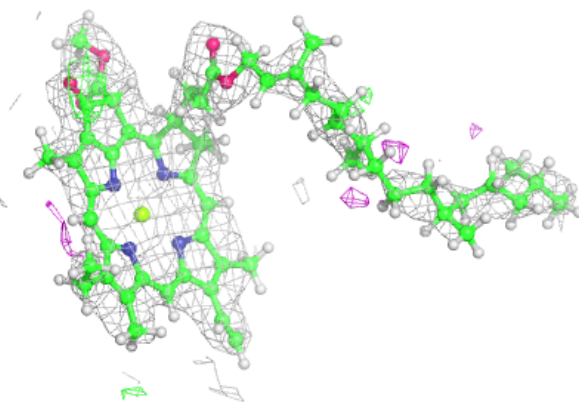


**Electron density around CLA c 510:**

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

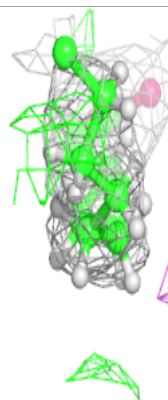
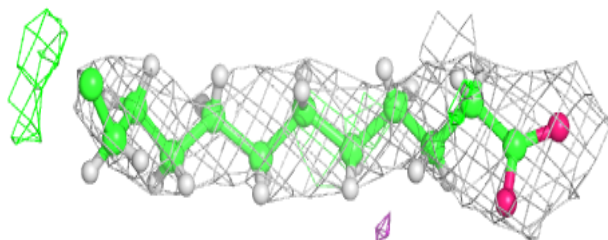
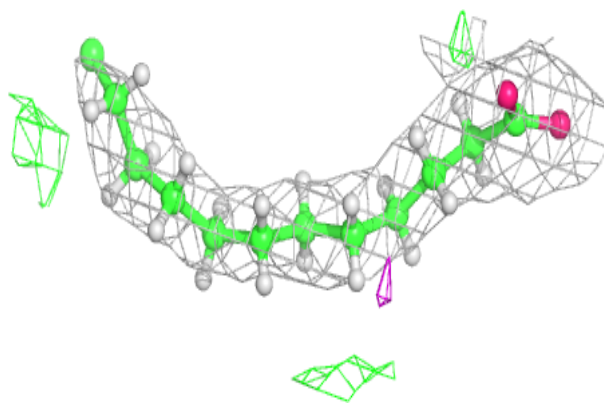
**Electron density around CLA c 511:**

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



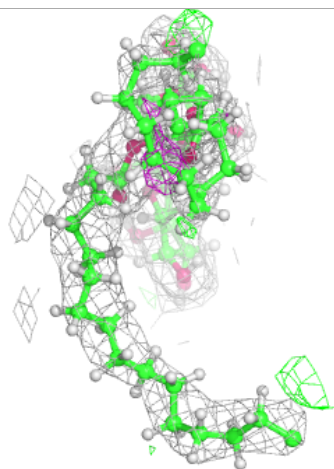
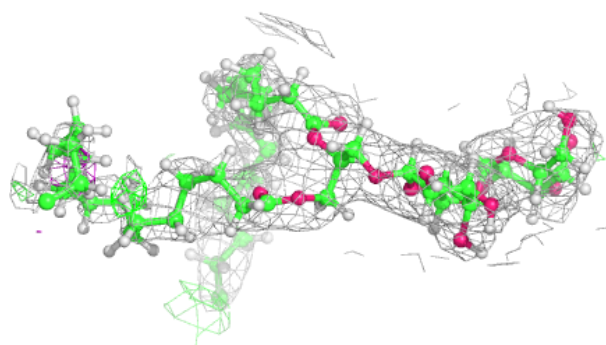
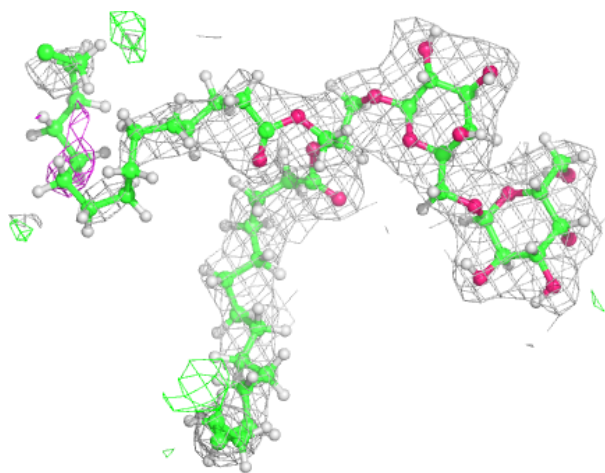
**Electron density around STE t 103:**

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



**Electron density around DGD C 516:**

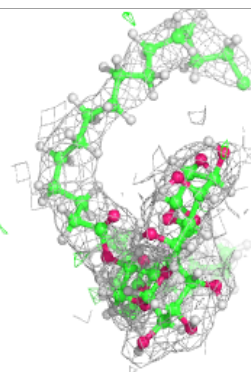
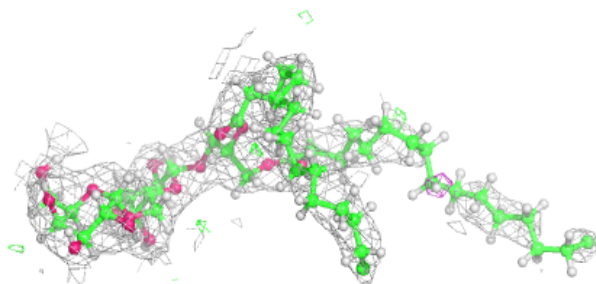
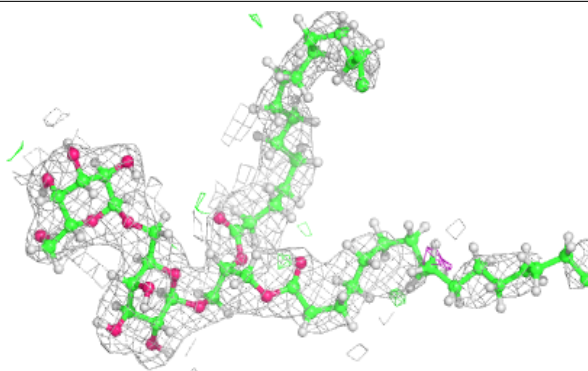
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



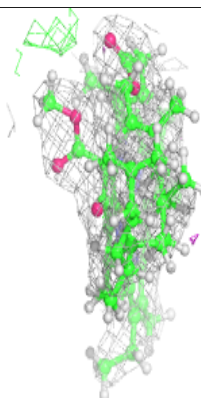
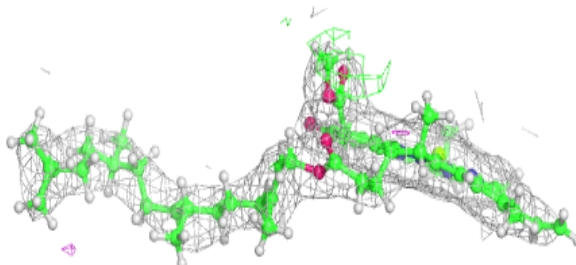
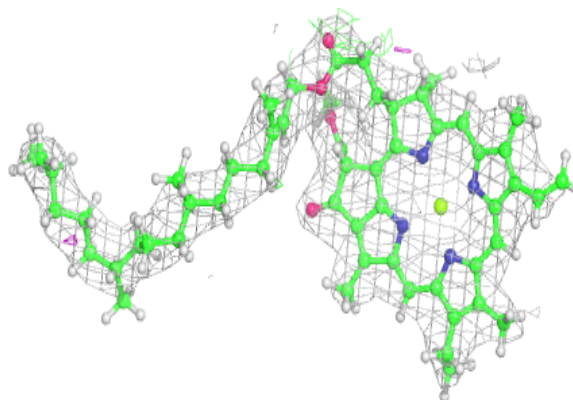


**Electron density around DGD c 517:**

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

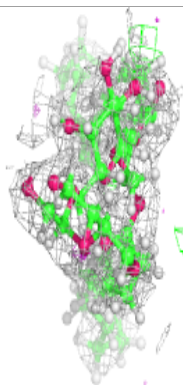
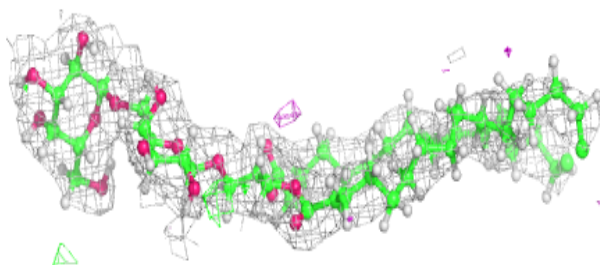
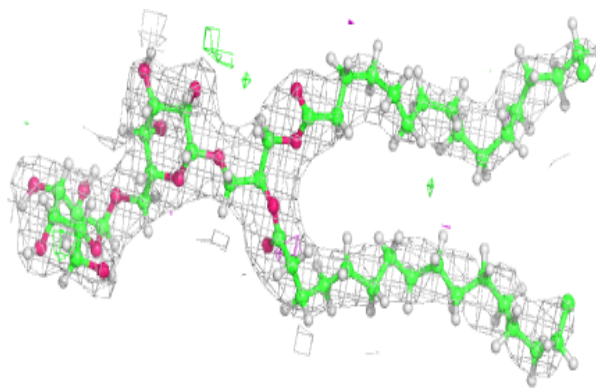
**Electron density around CLA B 602:**

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

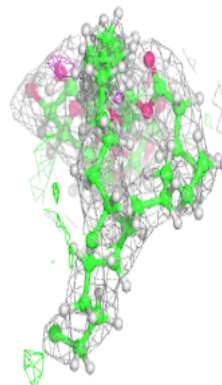
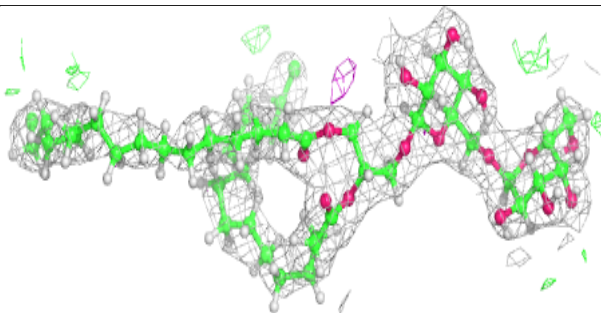
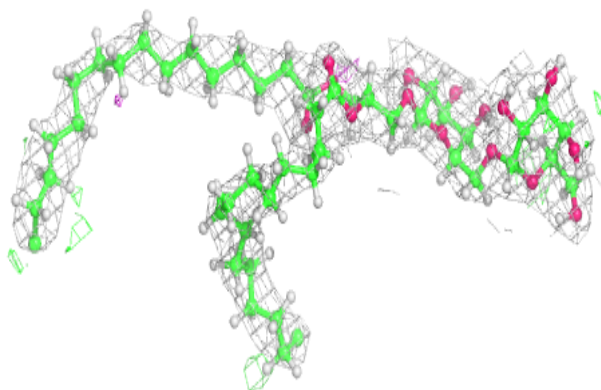


**Electron density around DGD C 517:**

$2mF_o-DF_c$  (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:**

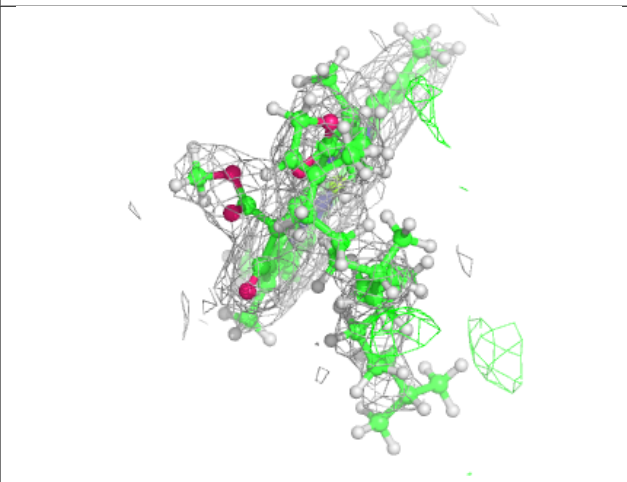
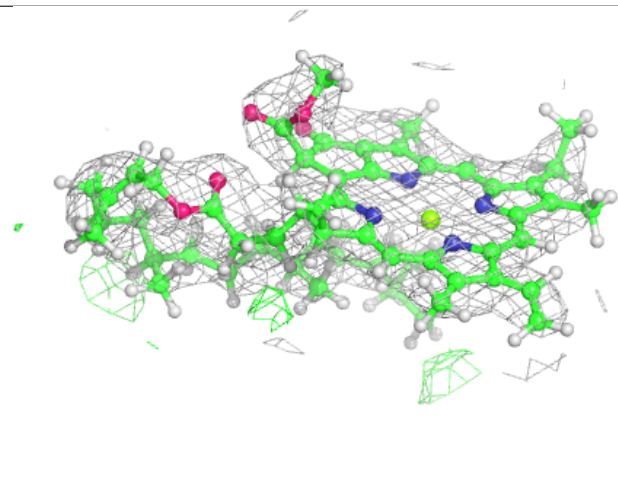
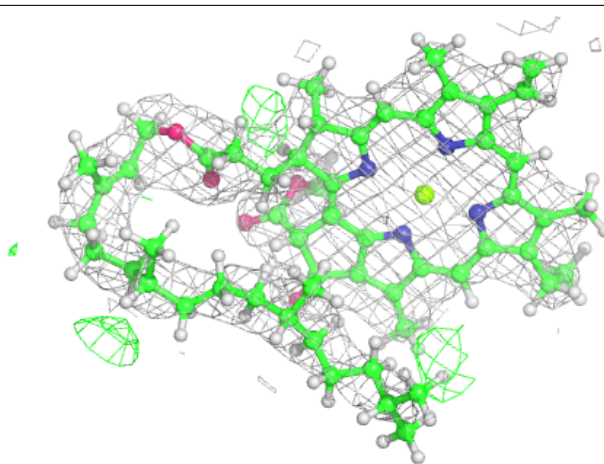
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





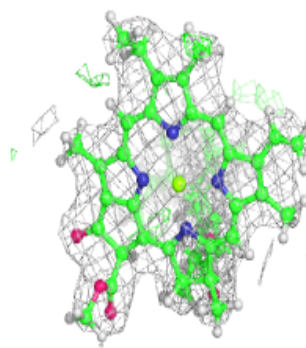
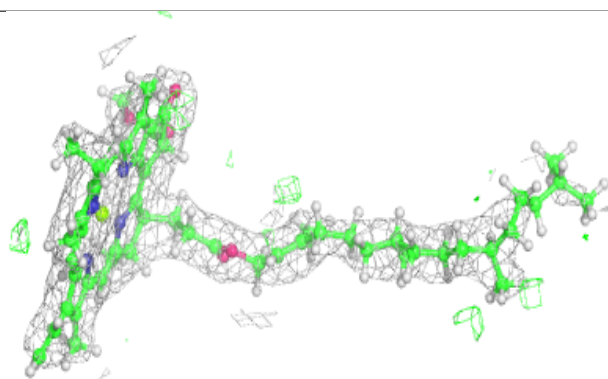
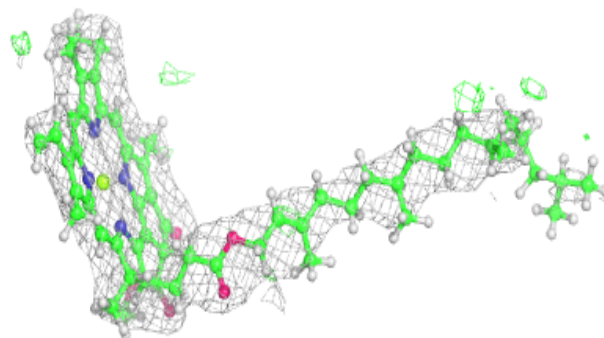
**Electron density around CLA C 509:**

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

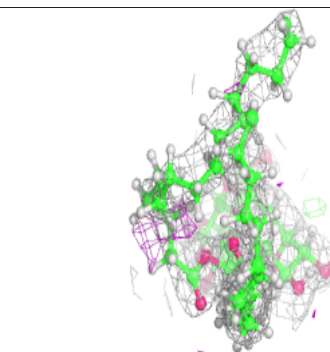
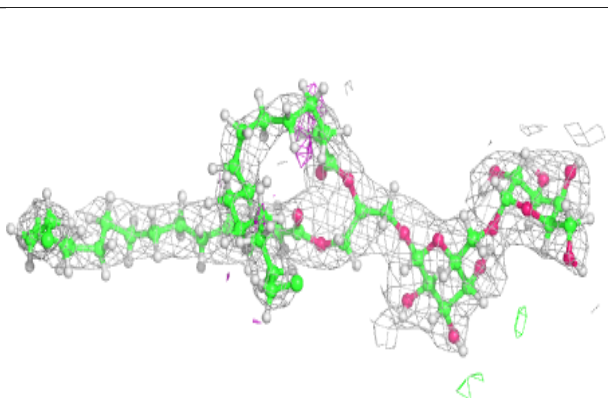
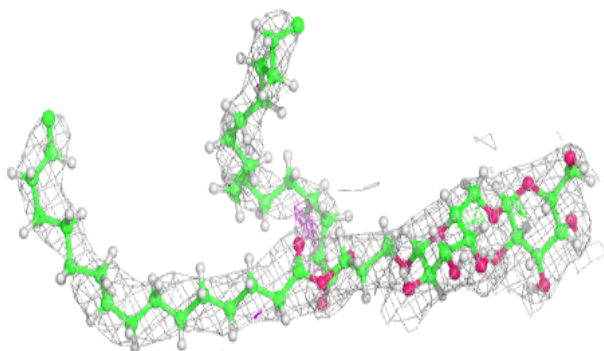


**Electron density around CLA b 604:**

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

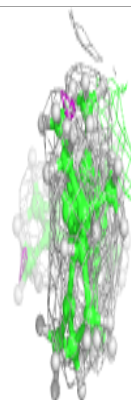
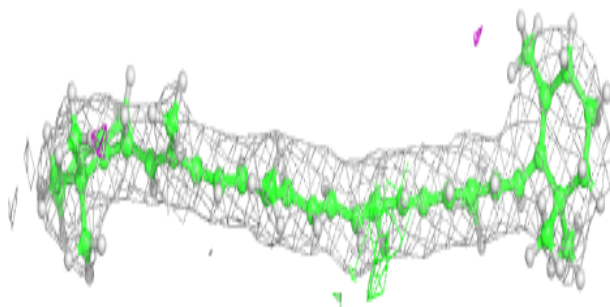
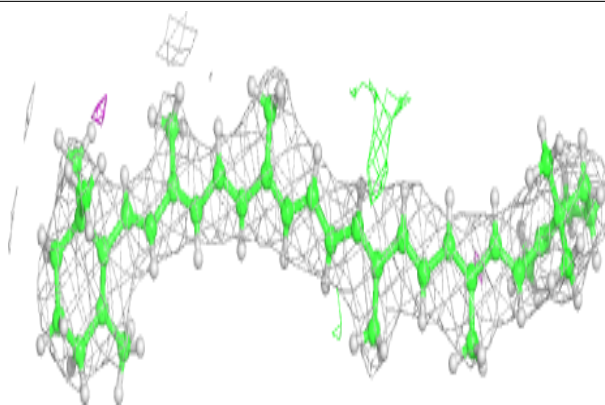
**Electron density around DGD h 101:**

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

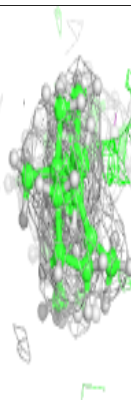
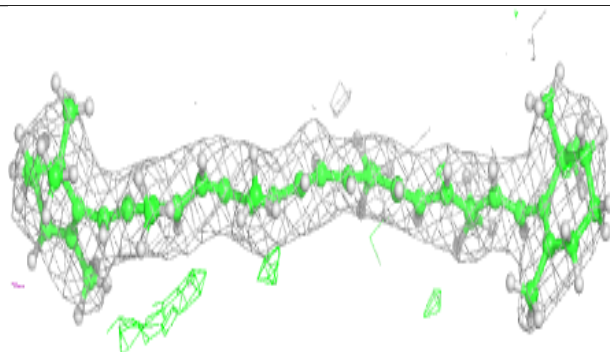
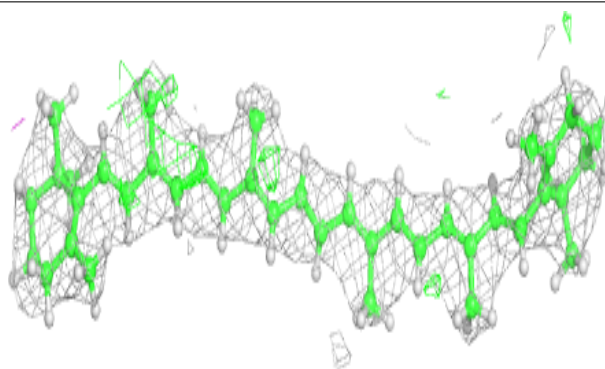


**Electron density around BCR B 617:**

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

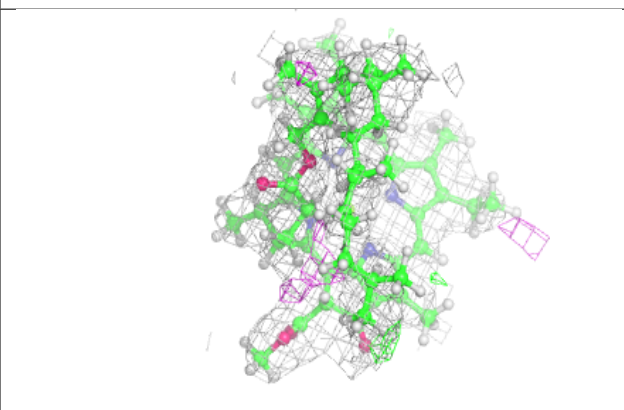
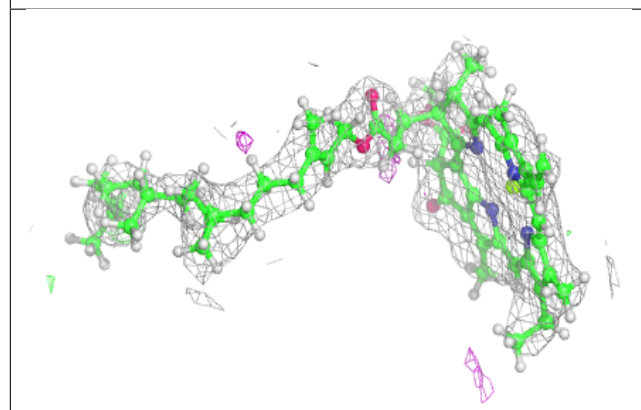
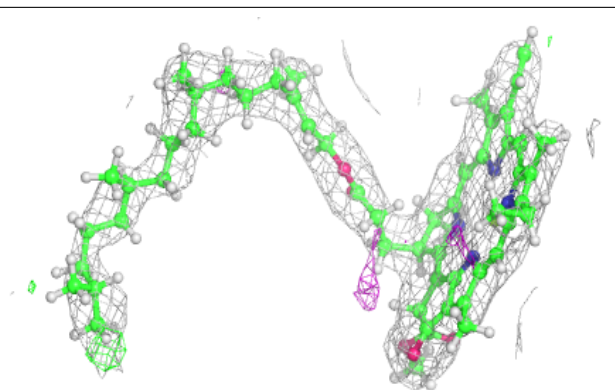
**Electron density around BCR B 618:**

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

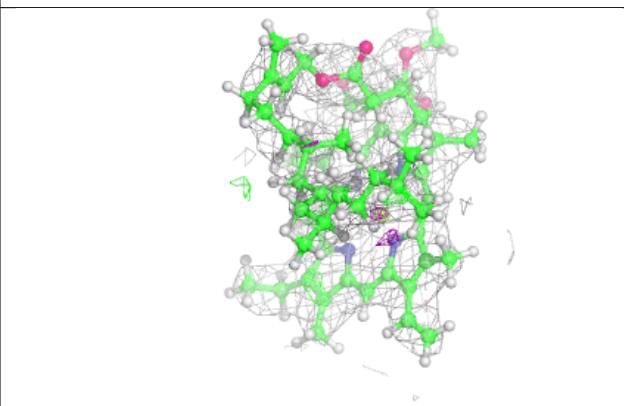
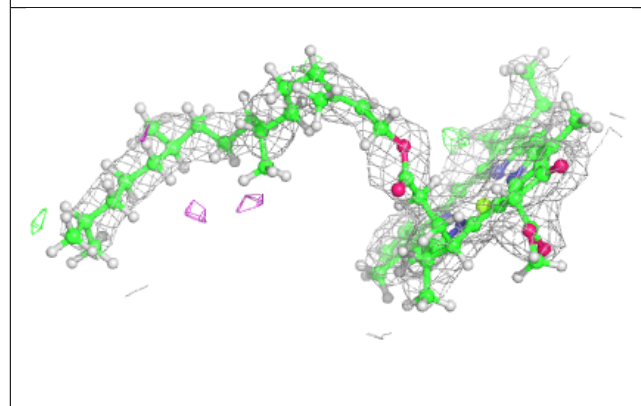
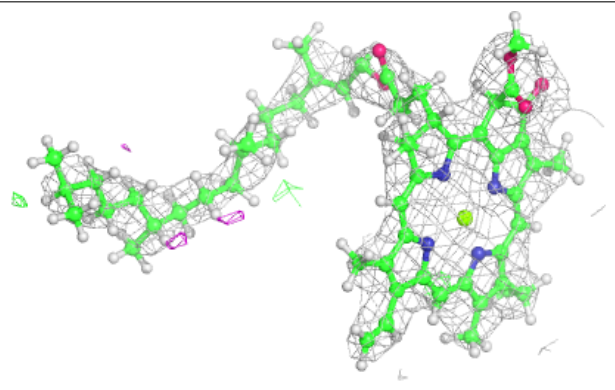


**Electron density around CLA b 606:**

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

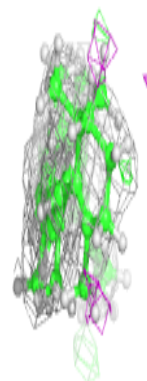
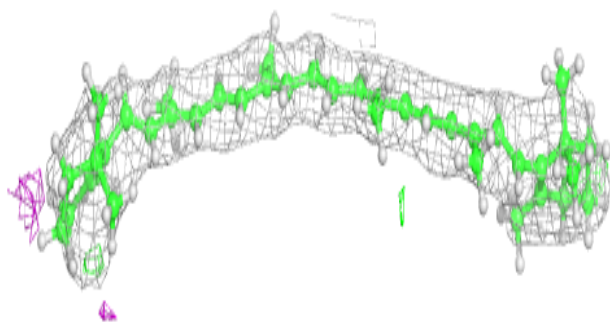
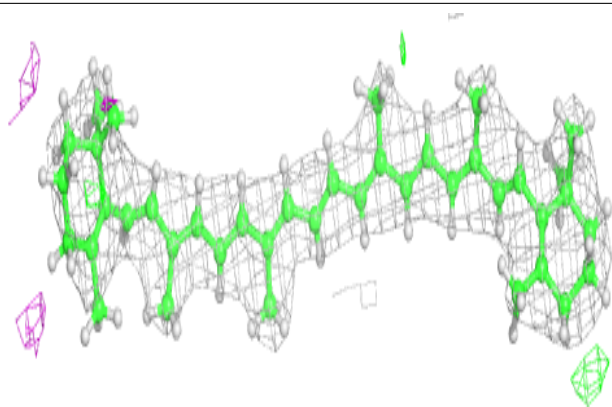
**Electron density around CLA C 511:**

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



**Electron density around BCR D 406:**

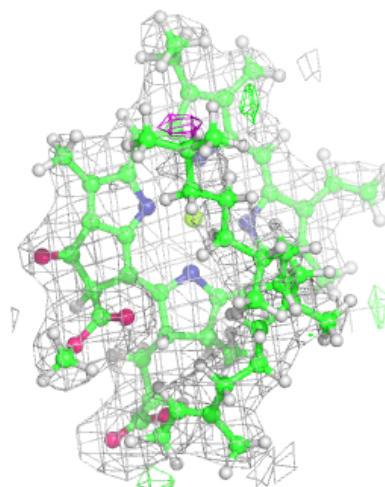
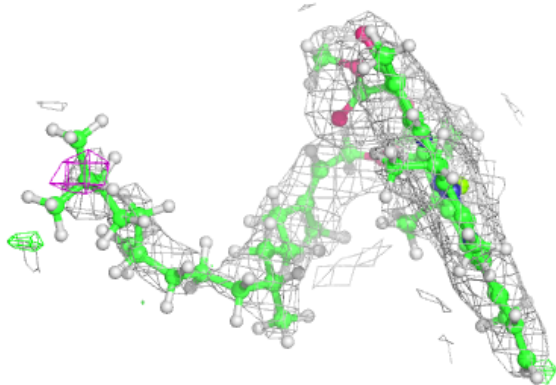
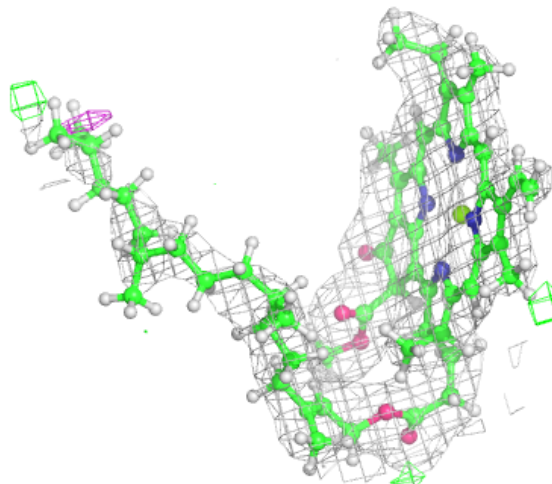
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





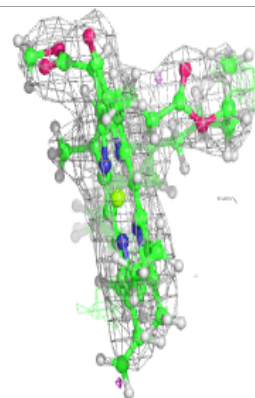
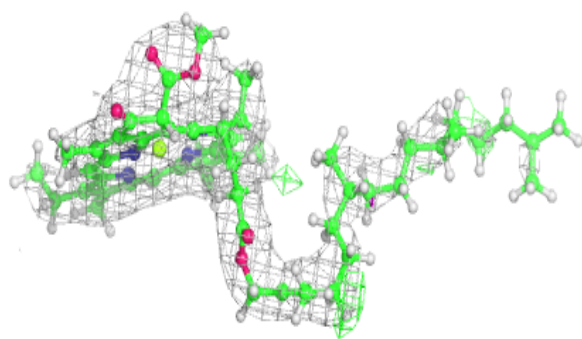
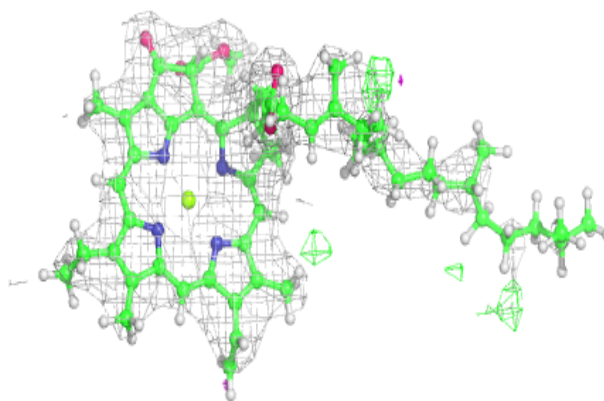
**Electron density around CLA b 613:**

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)

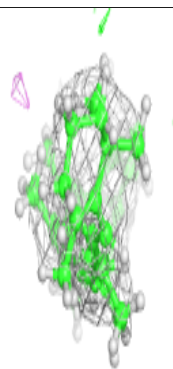
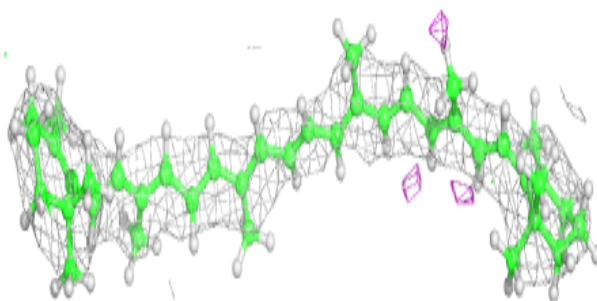
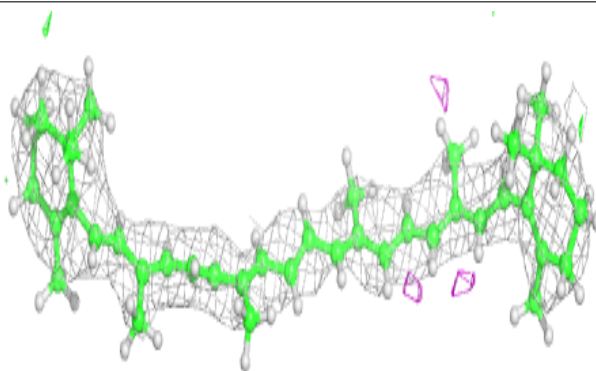


**Electron density around CLA d 401:**

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

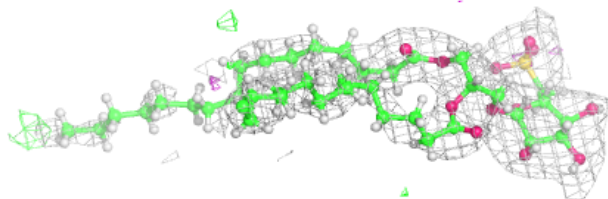
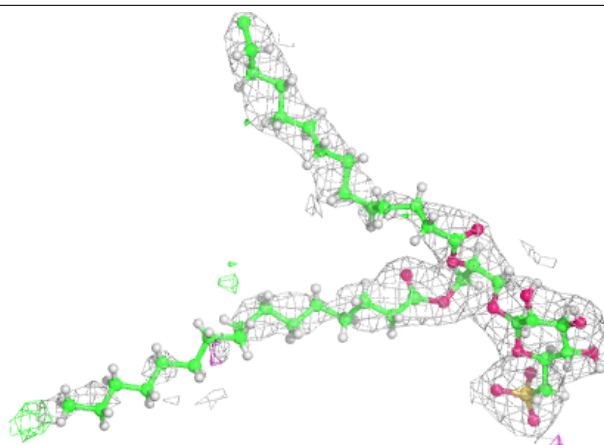
**Electron density around BCR K 102:**

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

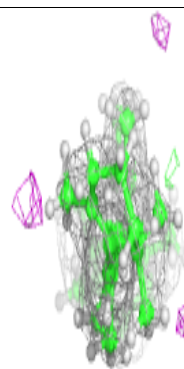
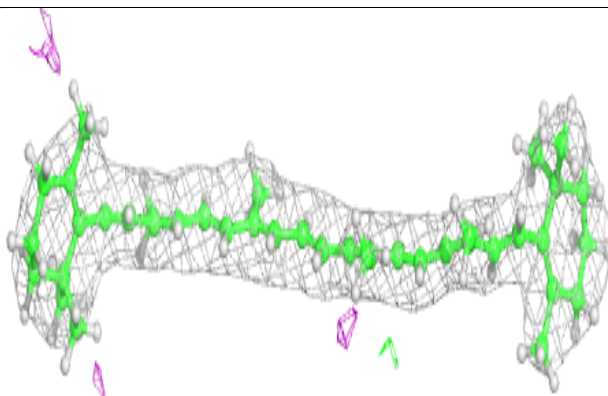
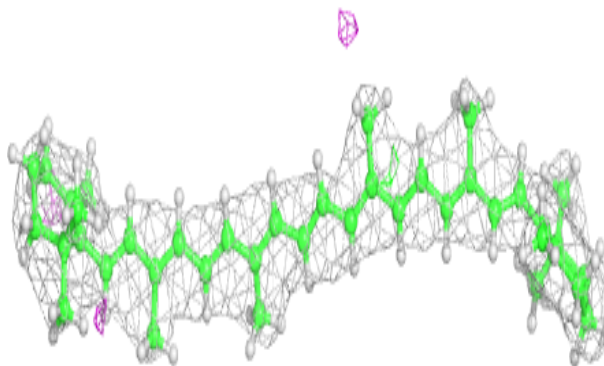


**Electron density around SQD A 410:**

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

**Electron density around BCR a 405:**

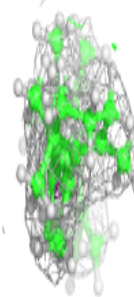
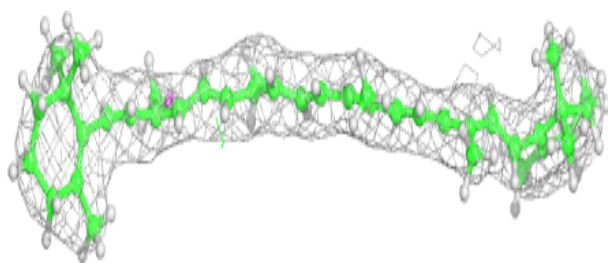
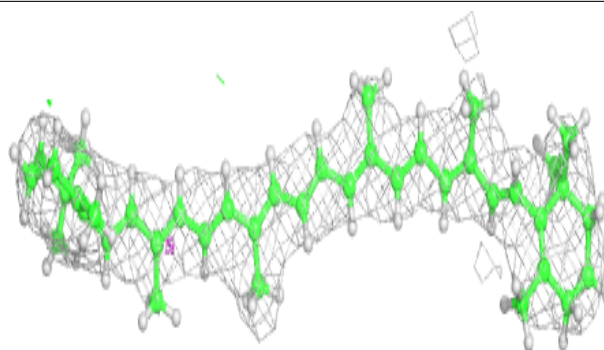
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



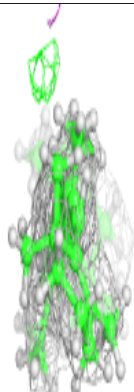
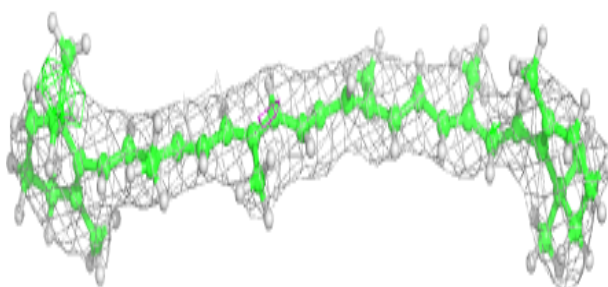
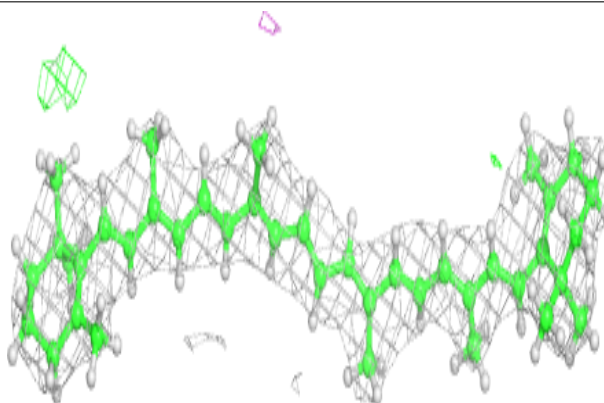


**Electron density around BCR b 617:**

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

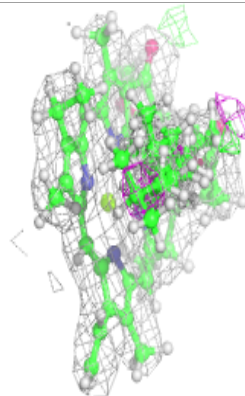
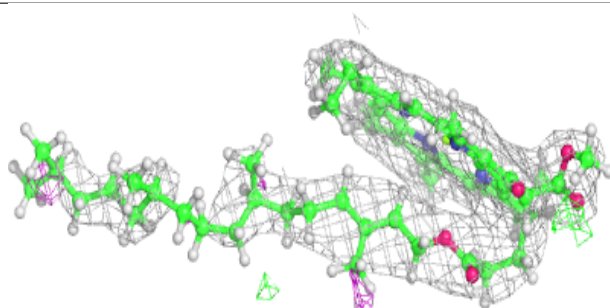
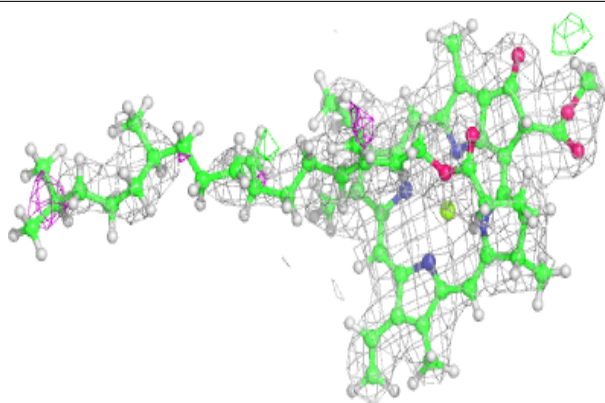
**Electron density around BCR b 619:**

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

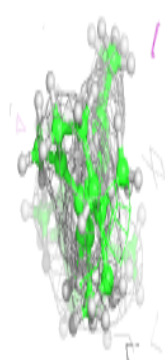
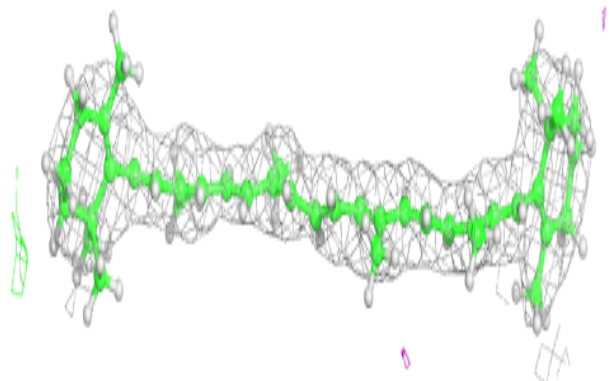
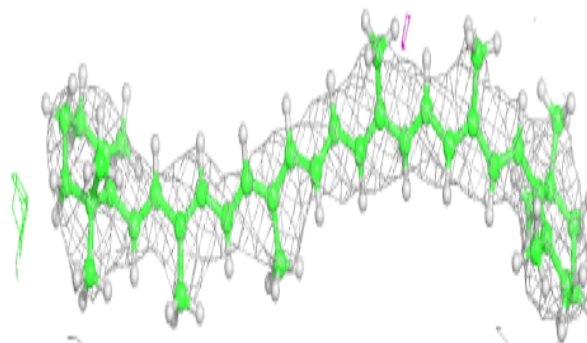


**Electron density around CLA b 614:**

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

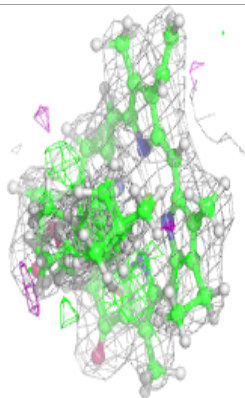
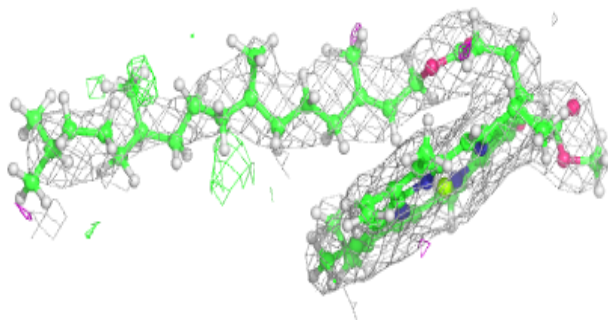
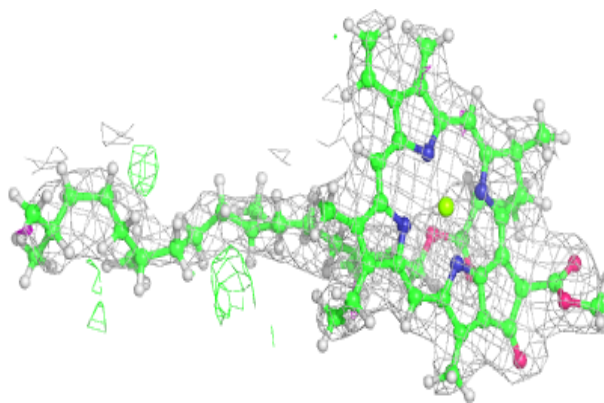
**Electron density around BCR c 515:**

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

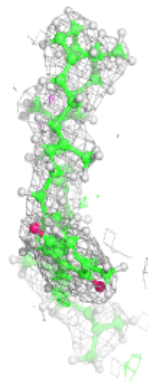
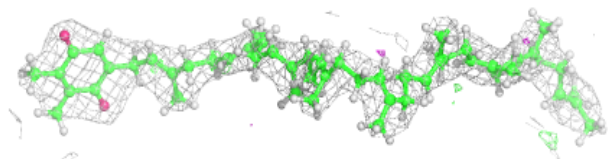
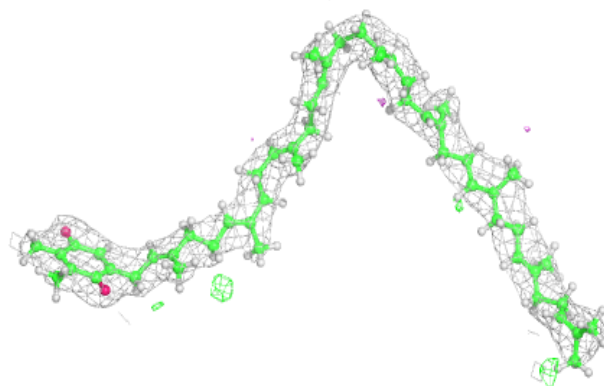


**Electron density around CLA B 614:**

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

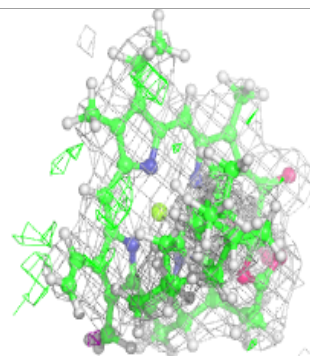
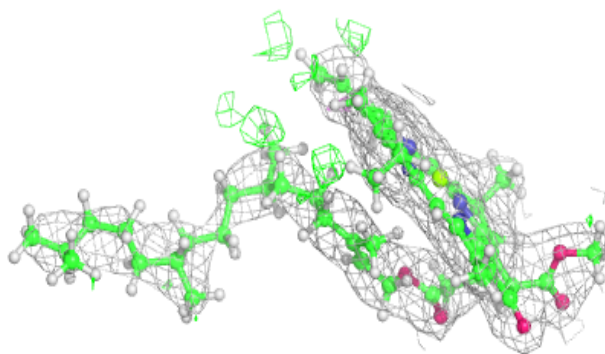
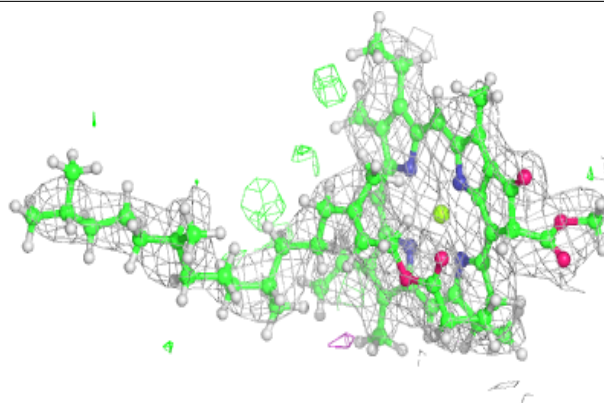
**Electron density around PL9 D 407:**

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

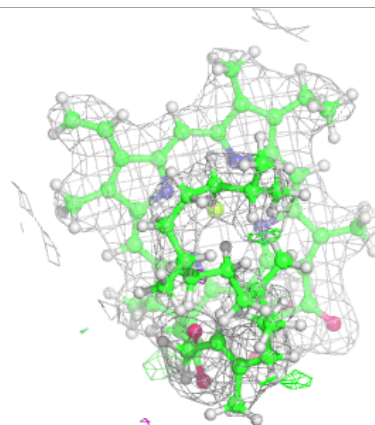
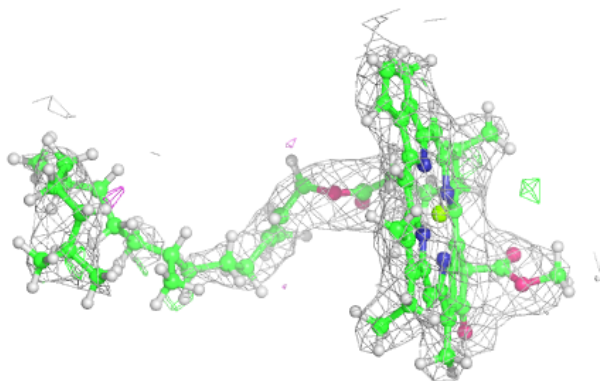
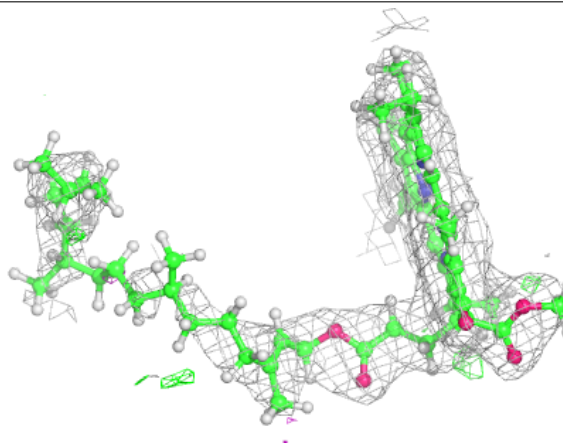


**Electron density around CLA C 505:**

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

**Electron density around CLA C 506:**

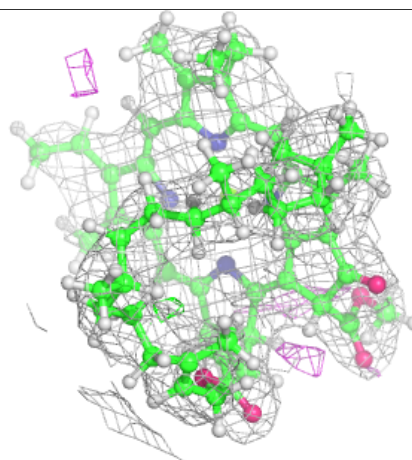
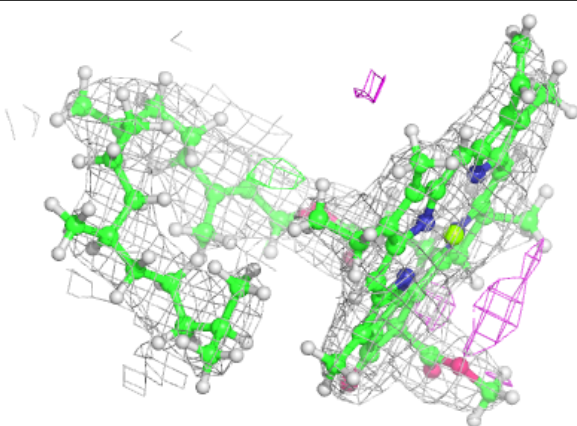
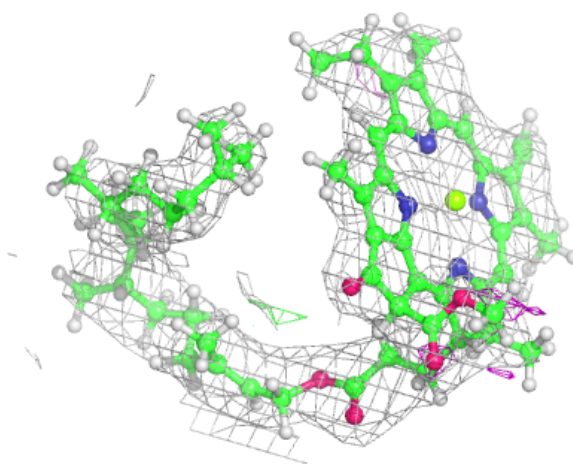
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





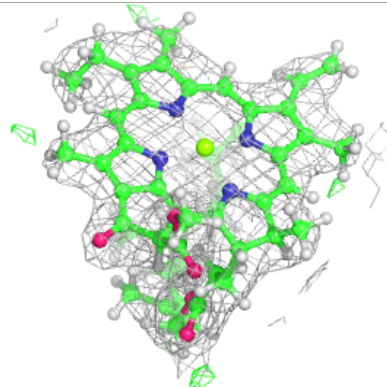
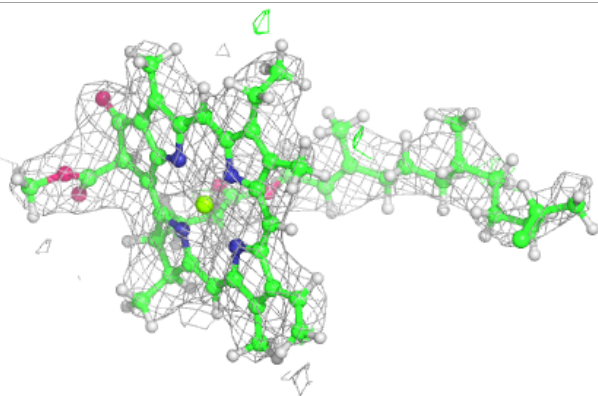
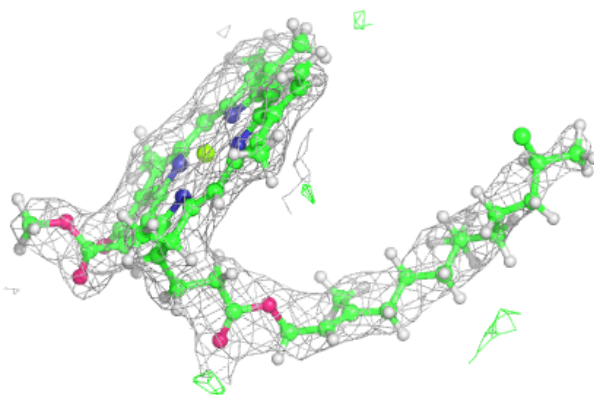
**Electron density around CLA c 503:**

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

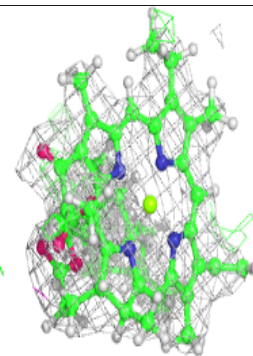
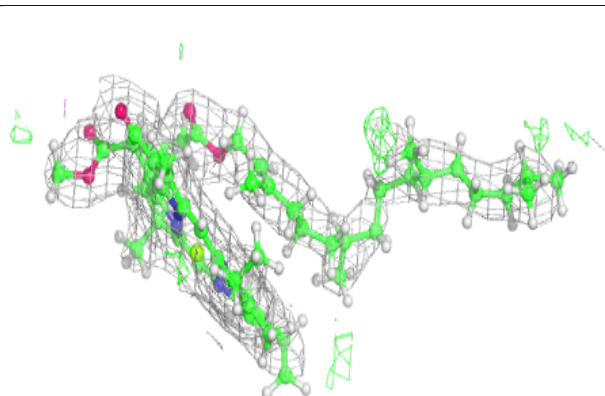
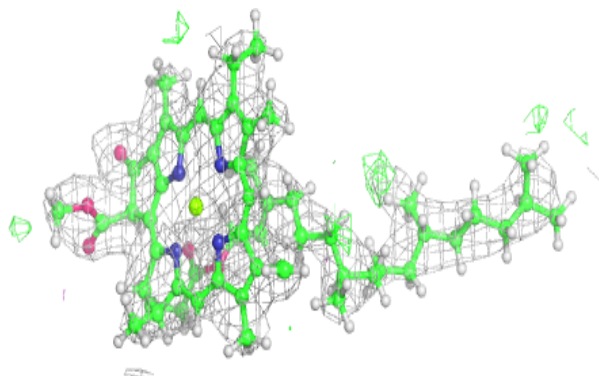


**Electron density around CLA c 504:**

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

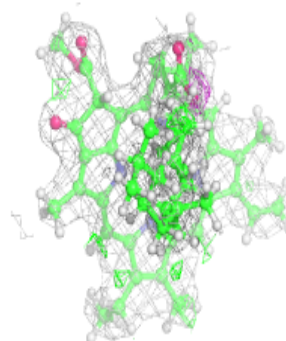
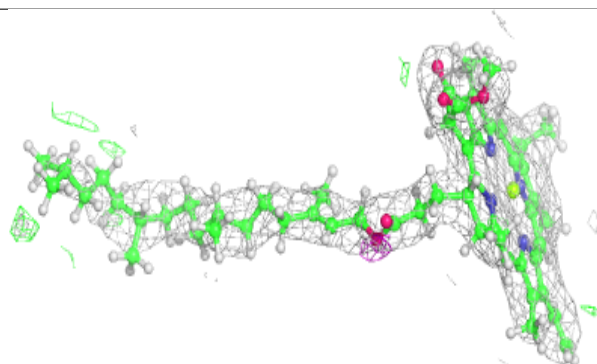
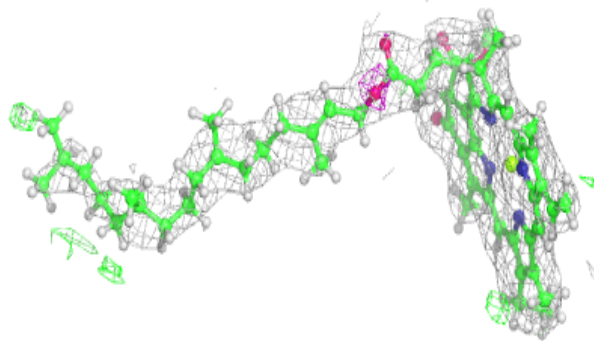
**Electron density around CLA c 505:**

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



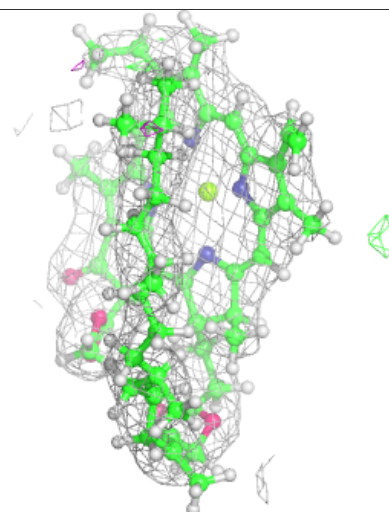
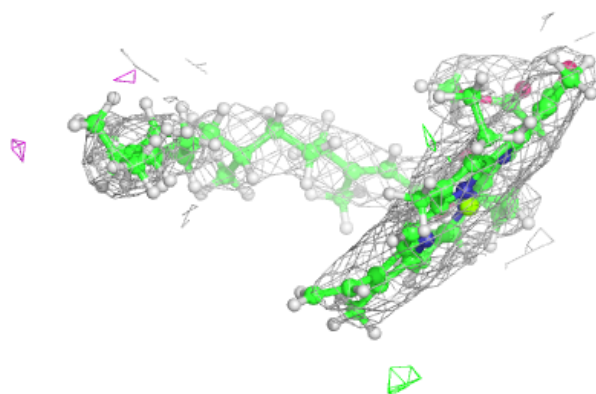
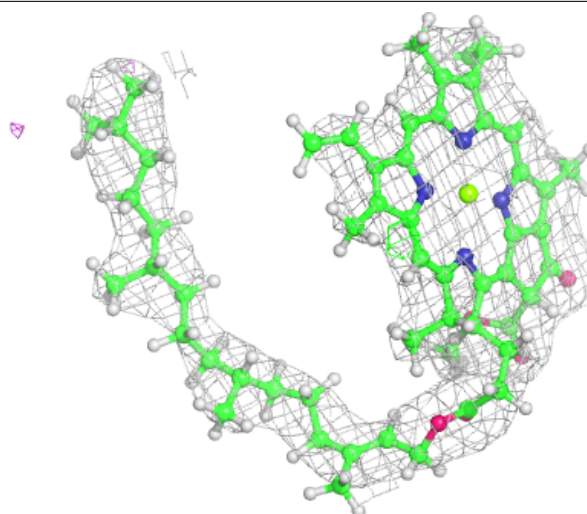
**Electron density around CLA B 604:**

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



**Electron density around CLA c 507:**

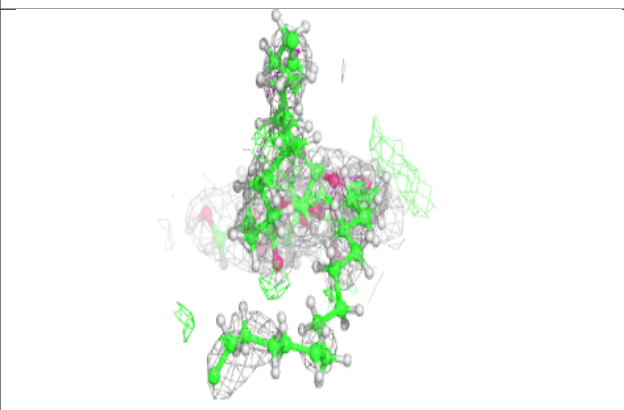
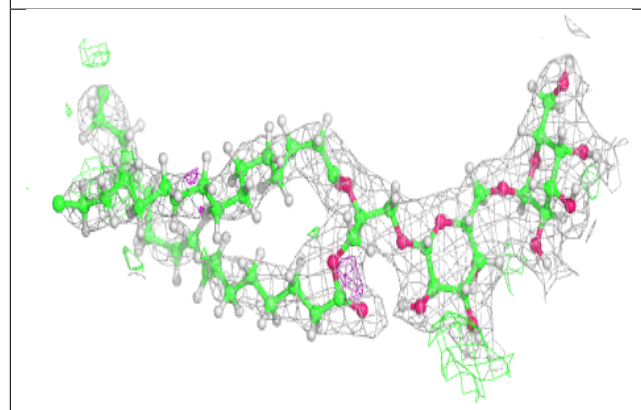
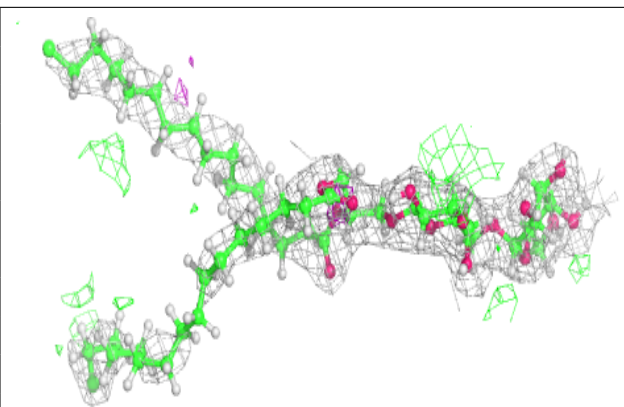
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



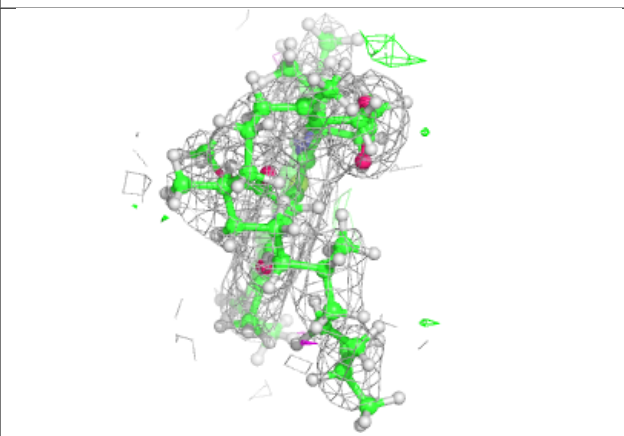
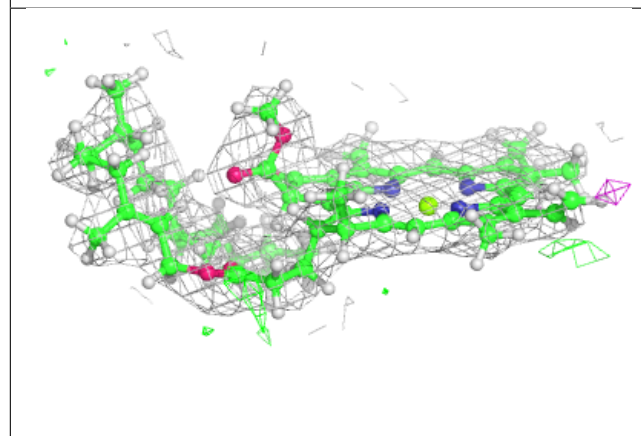
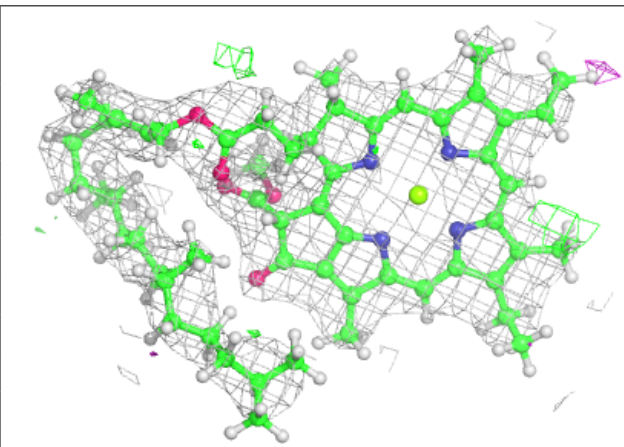


**Electron density around DGD C 515:**

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

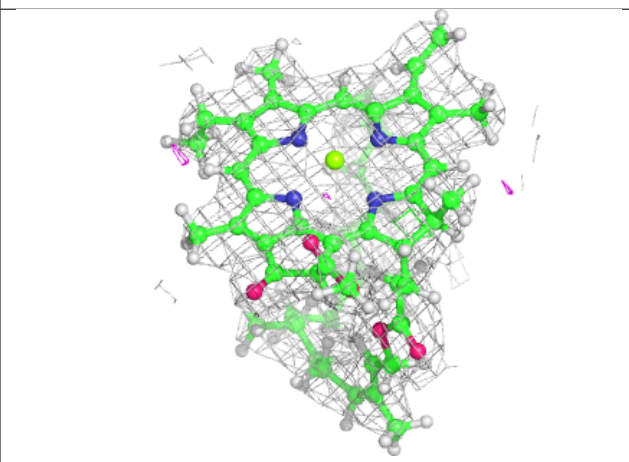
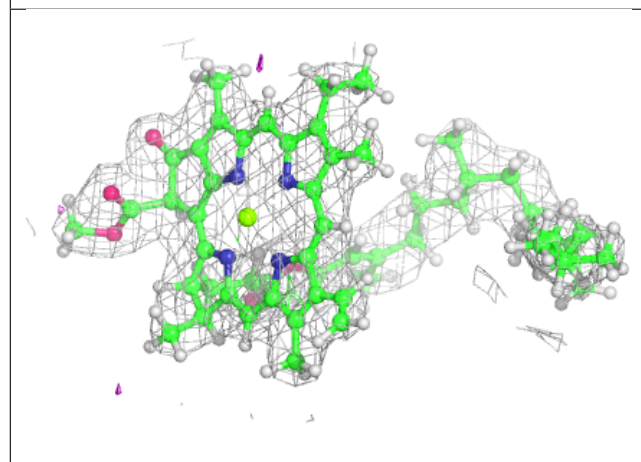
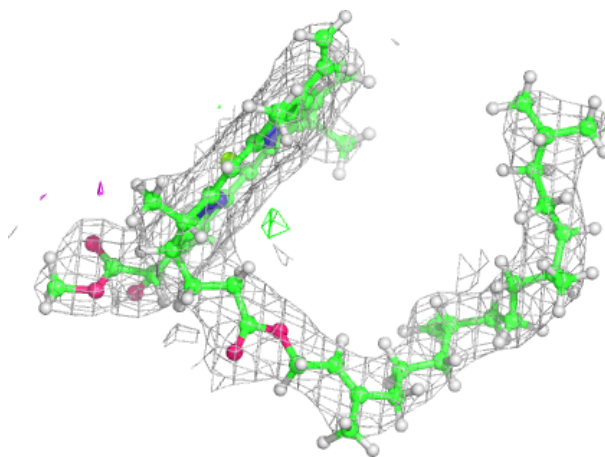
**Electron density around CLA b 610:**

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



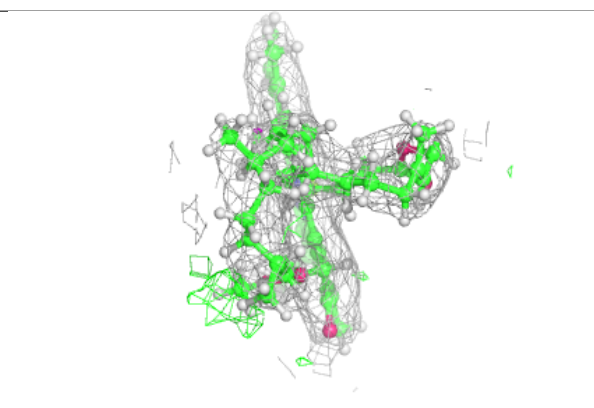
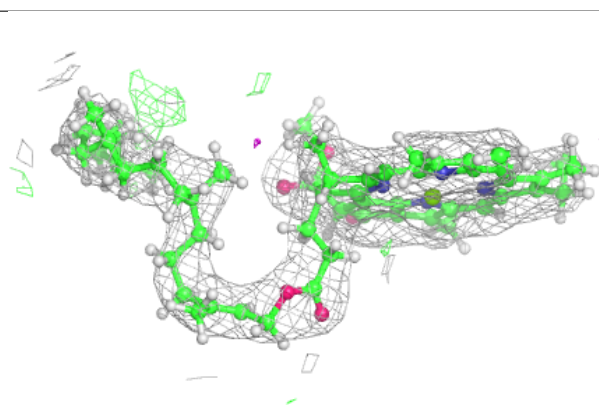
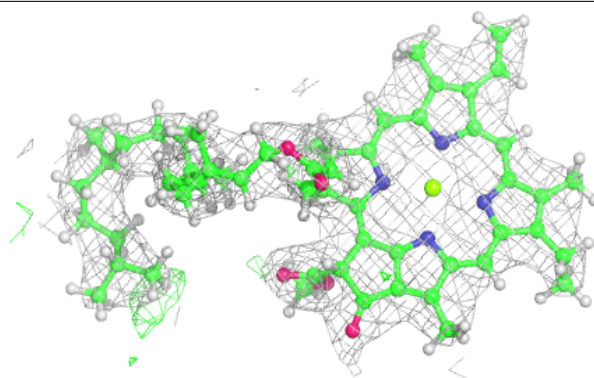
**Electron density around CLA b 611:**

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

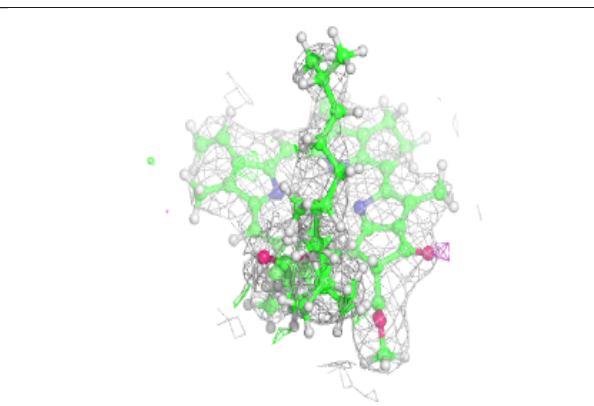
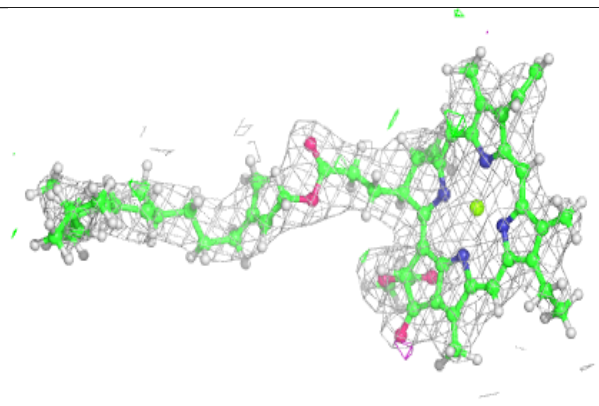
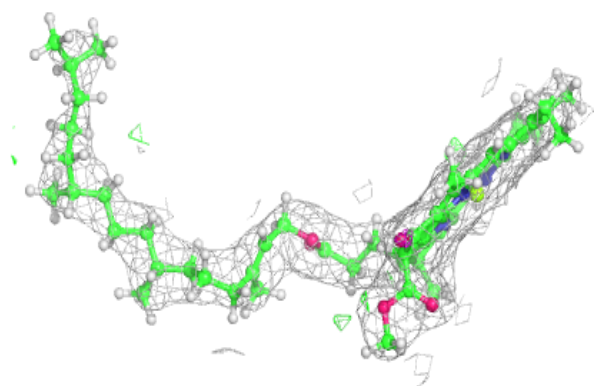


**Electron density around CLA b 612:**

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

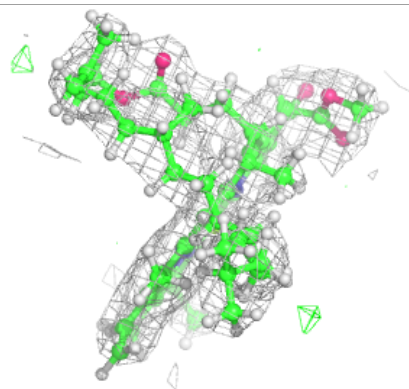
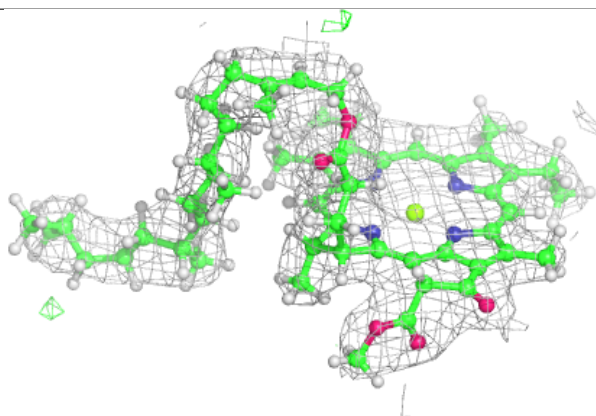
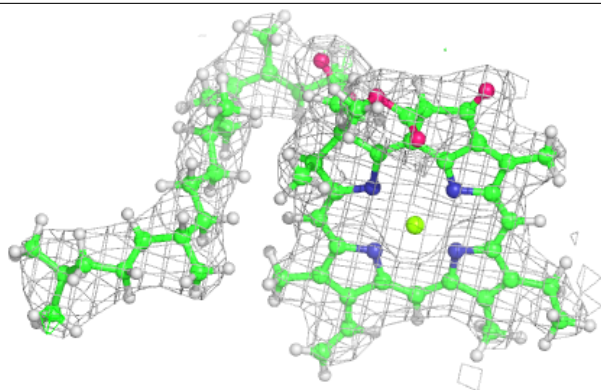
**Electron density around CLA d 403:**

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



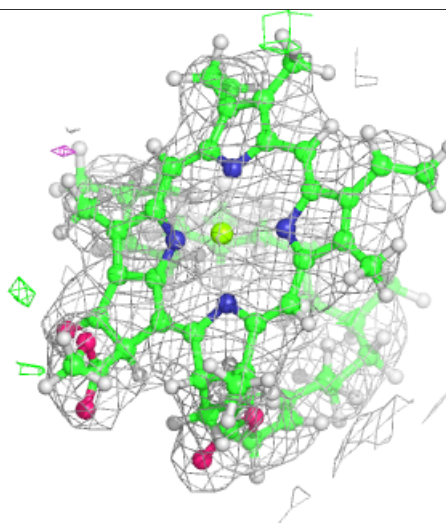
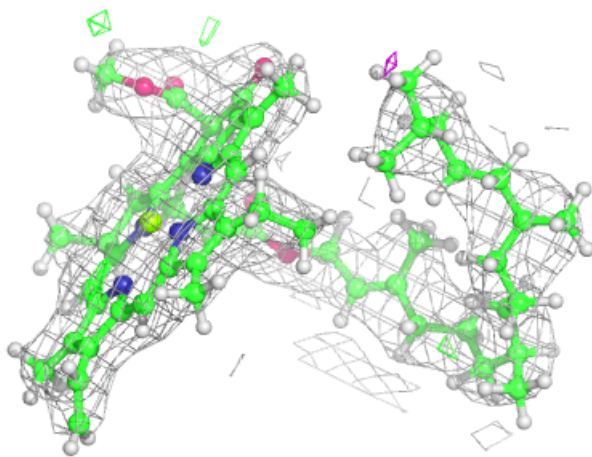
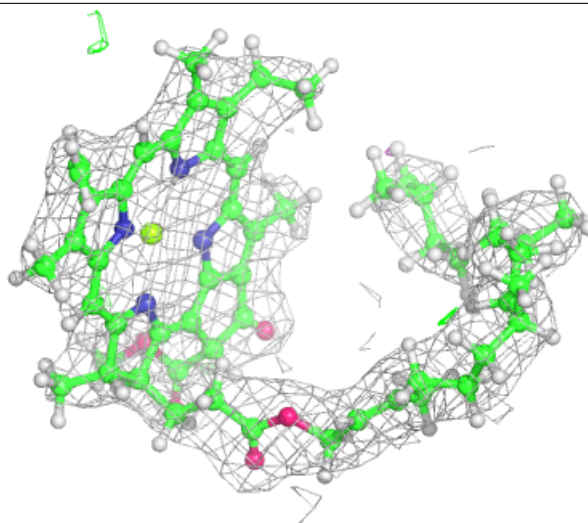
**Electron density around CLA d 404:**

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



**Electron density around CLA C 503:**

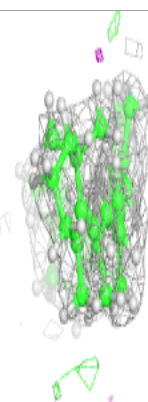
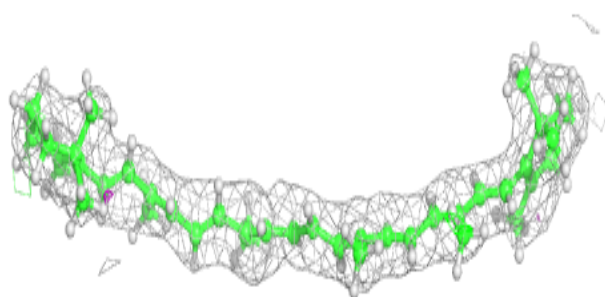
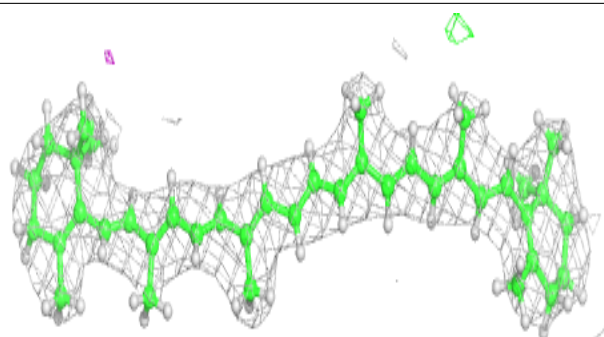
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



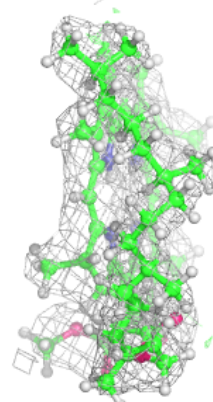
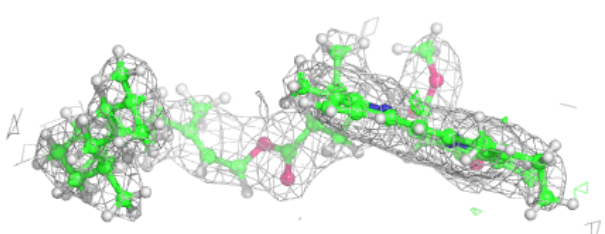
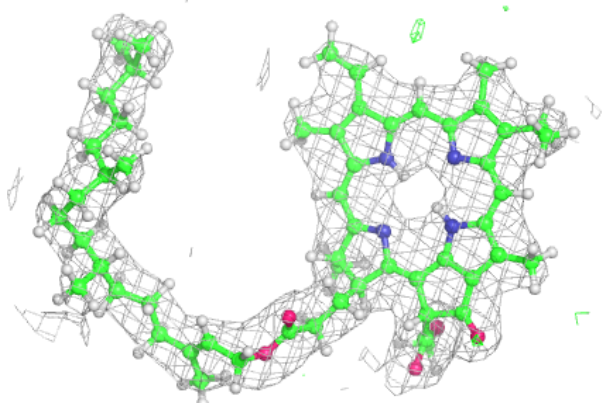


**Electron density around BCR T 101:**

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

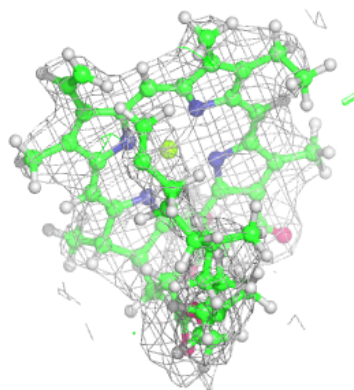
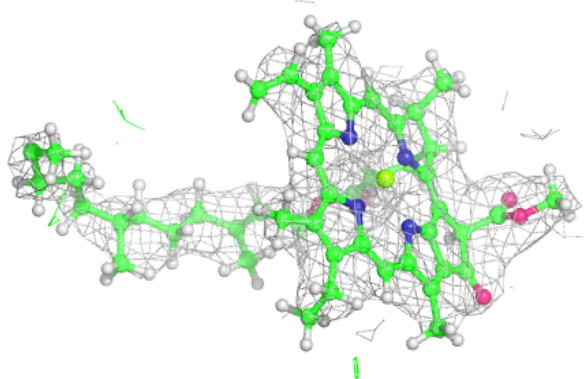
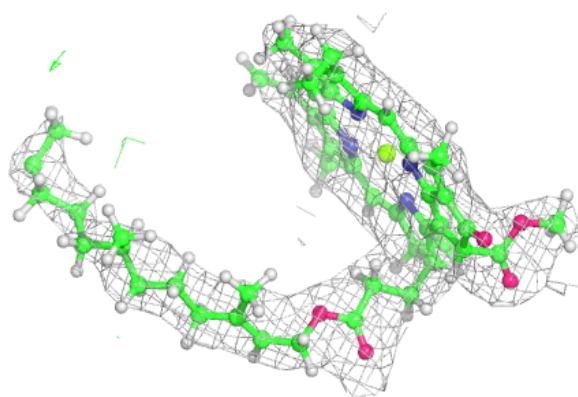
**Electron density around PHO a 403:**

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

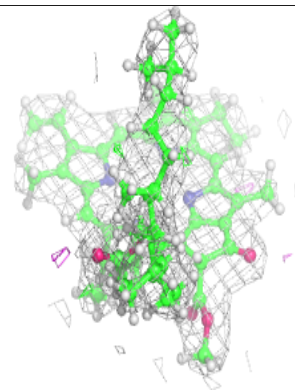
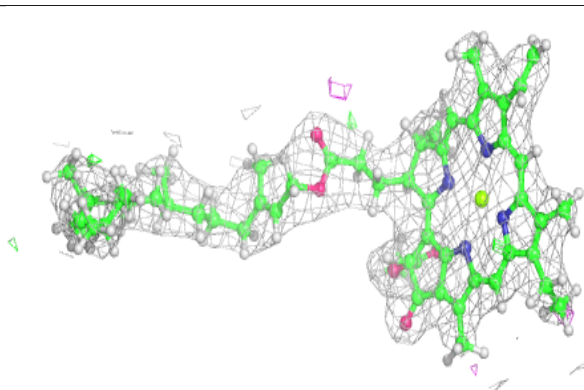
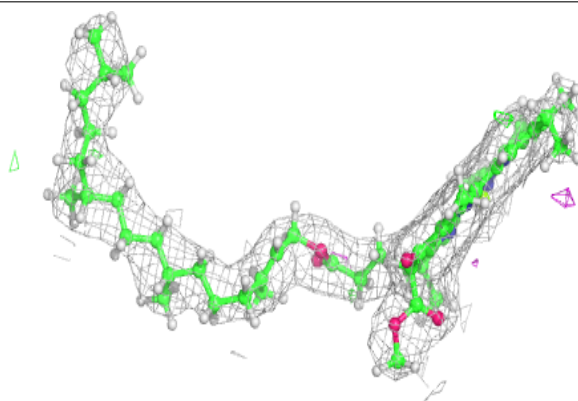


**Electron density around CLA C 504:**

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

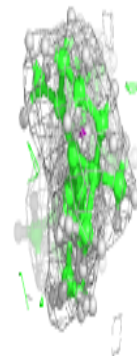
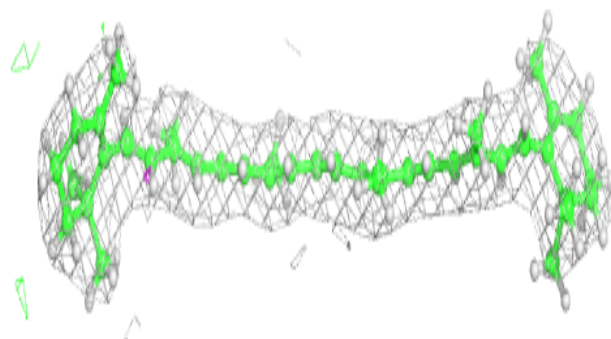
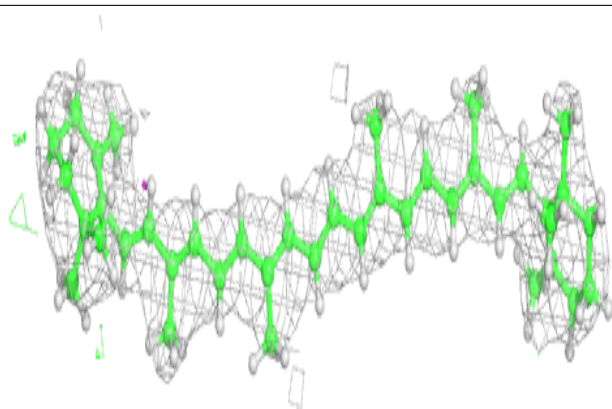
**Electron density around CLA D 403:**

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

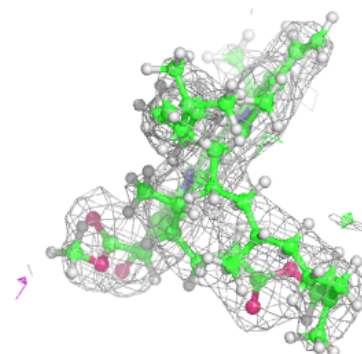
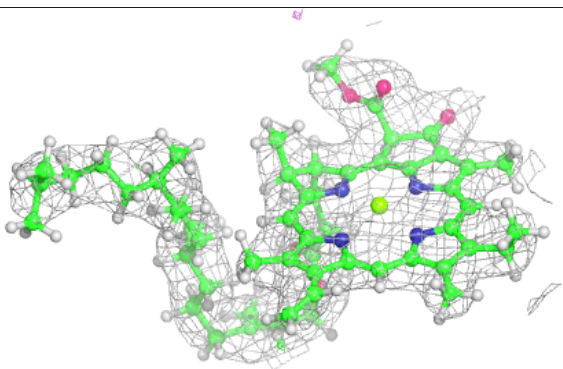
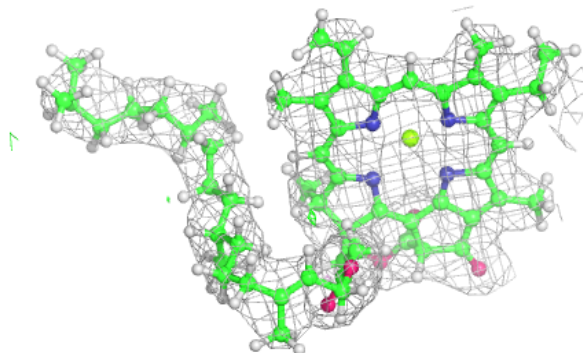


**Electron density around BCR b 618:**

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

**Electron density around CLA D 404:**

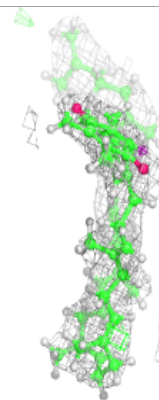
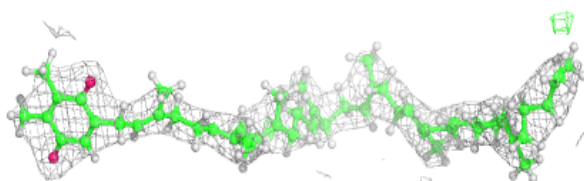
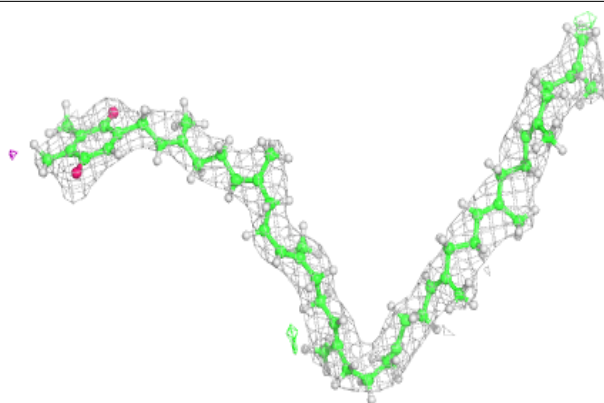
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



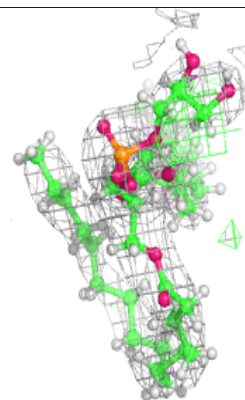
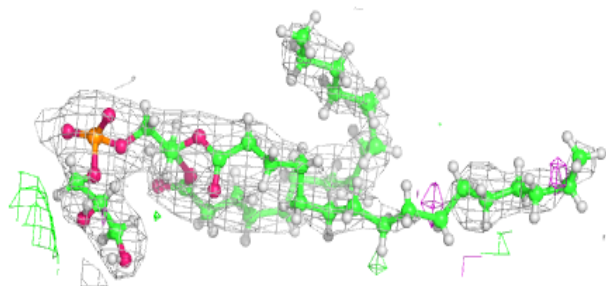
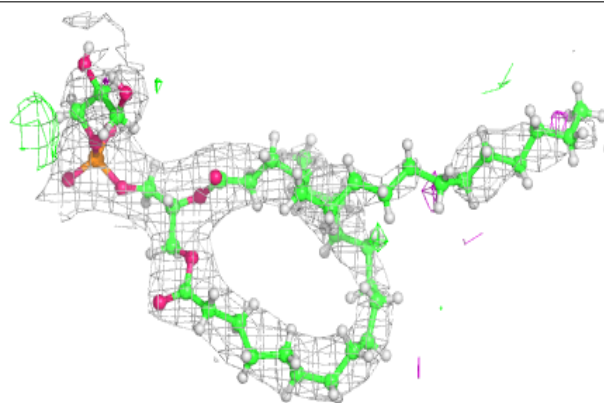


**Electron density around PL9 d 407:**

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

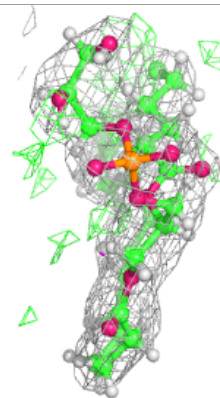
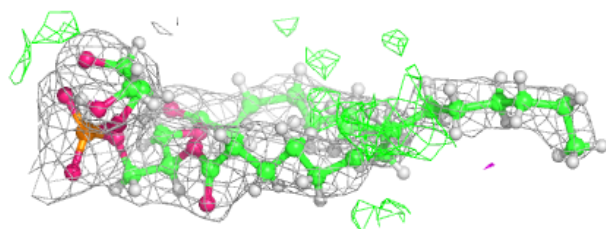
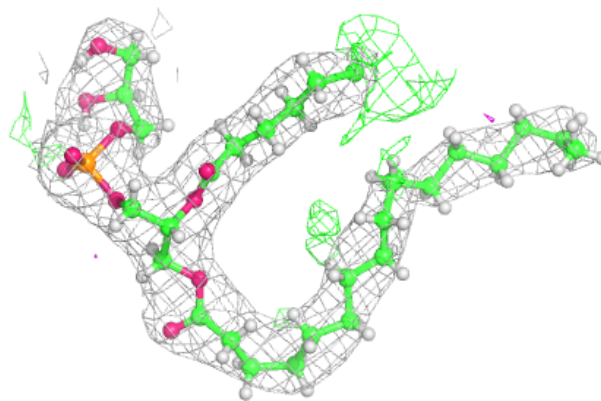
**Electron density around LHG a 410:**

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

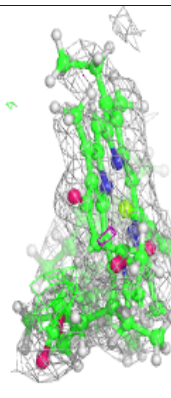
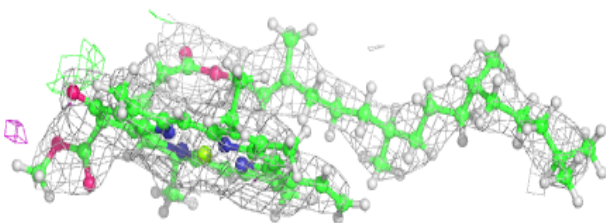
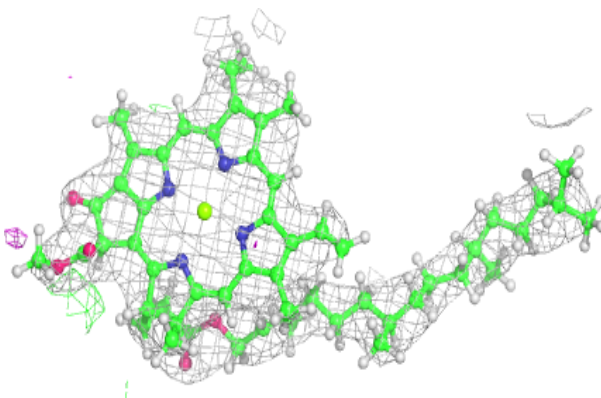


**Electron density around LHG d 409:**

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

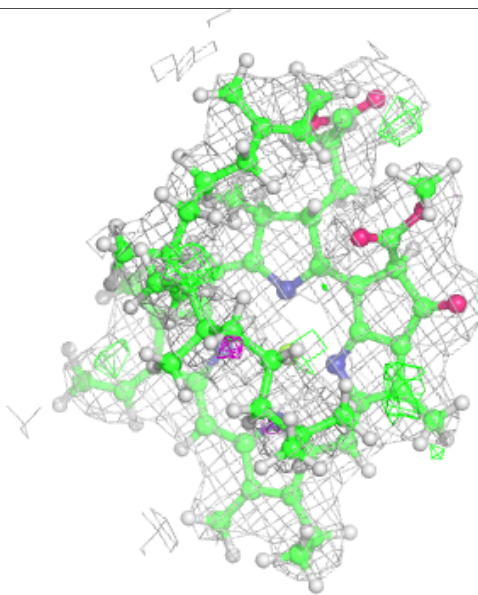
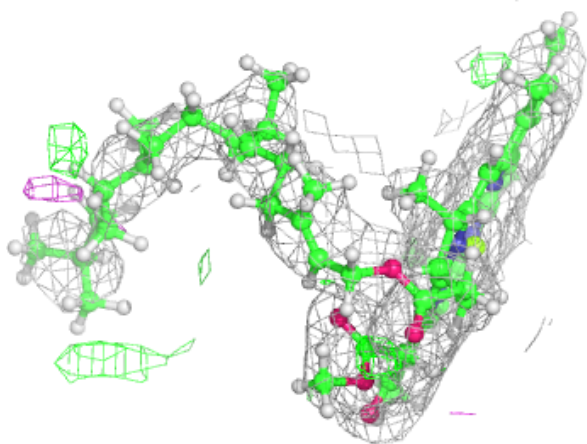
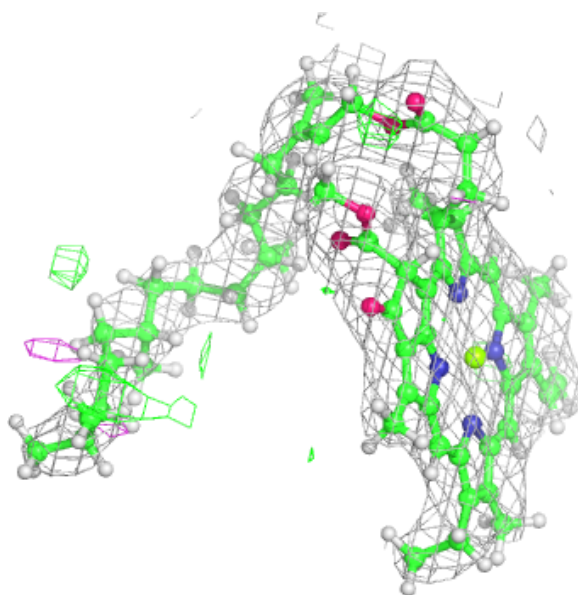
**Electron density around CLA c 501:**

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



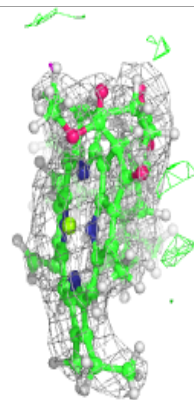
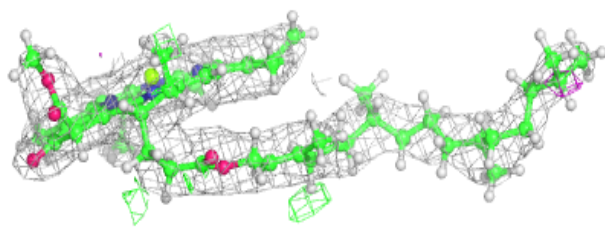
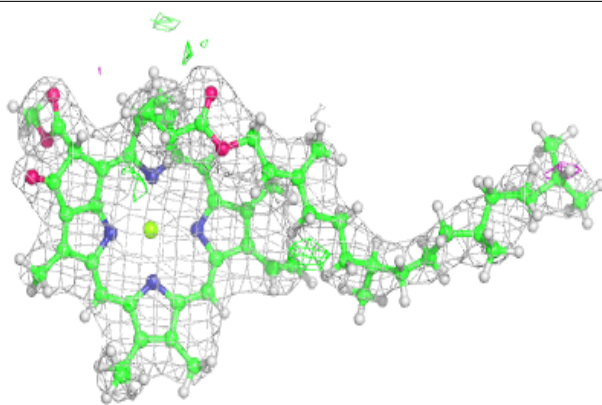
**Electron density around CLA B 613:**

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

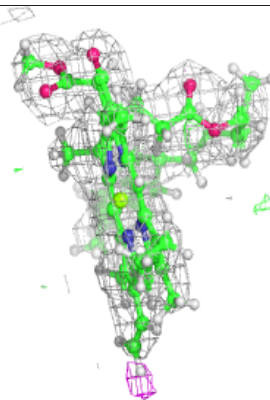
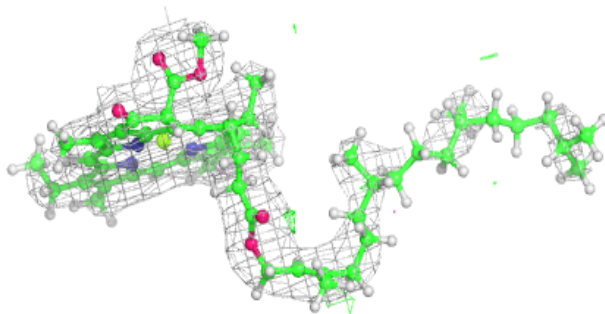
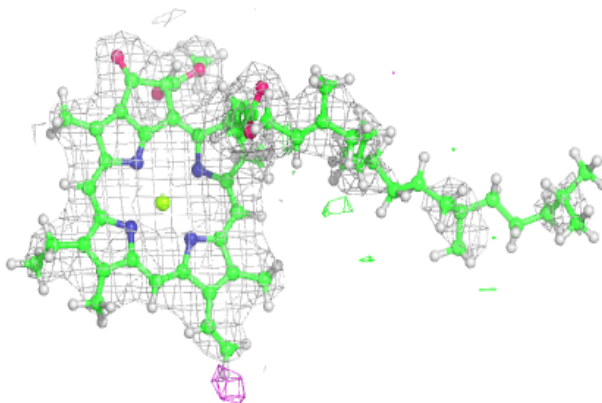


**Electron density around CLA B 603:**

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

**Electron density around CLA A 403:**

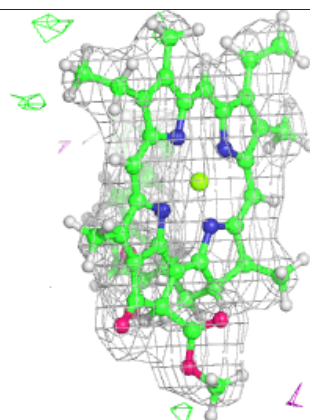
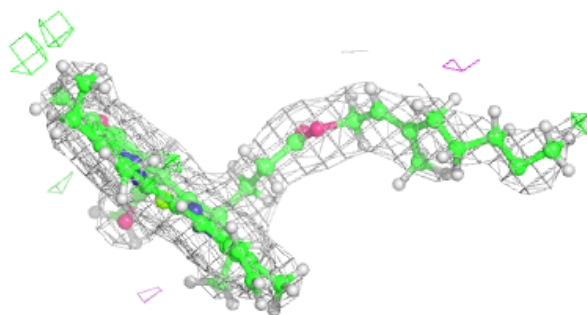
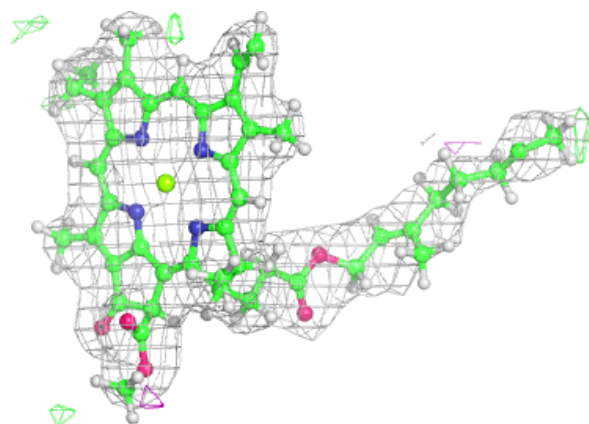
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



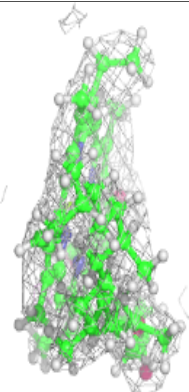
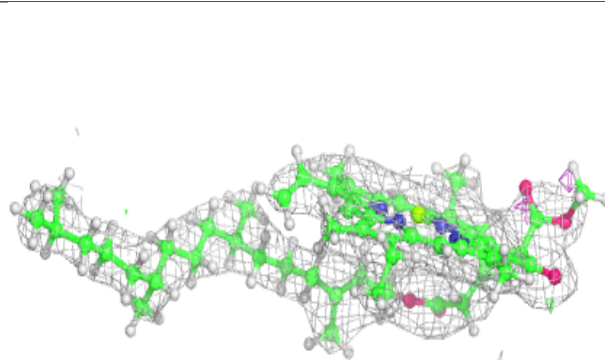
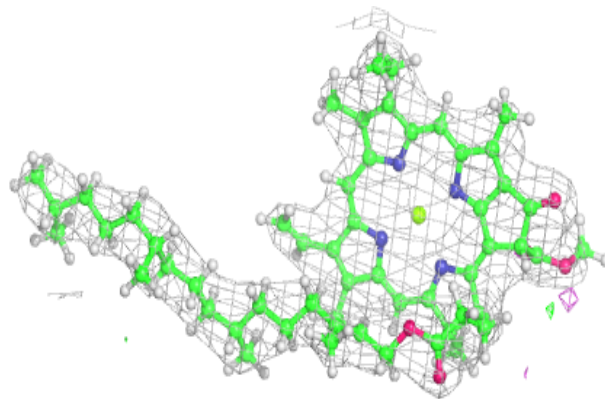


**Electron density around CLA A 405:**

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

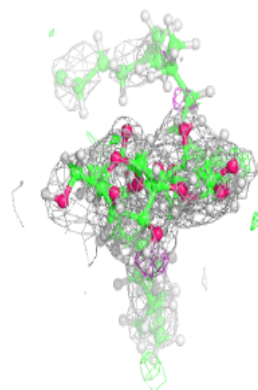
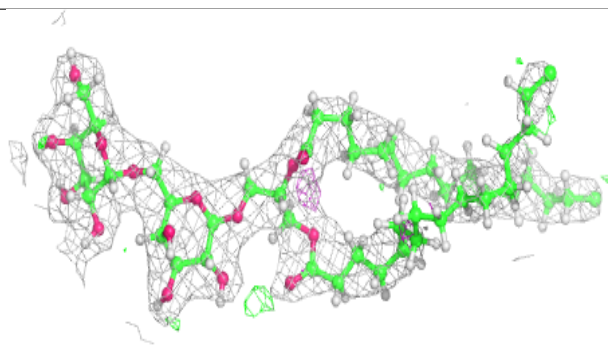
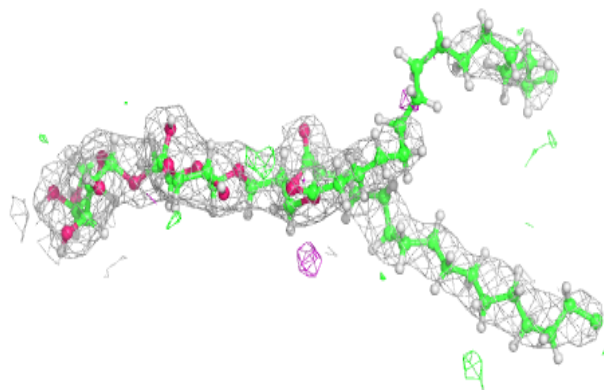
**Electron density around CLA C 501:**

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

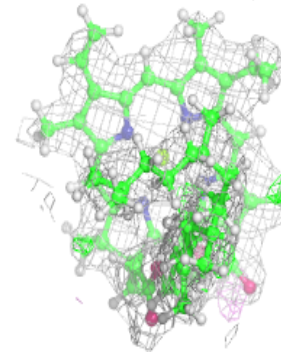
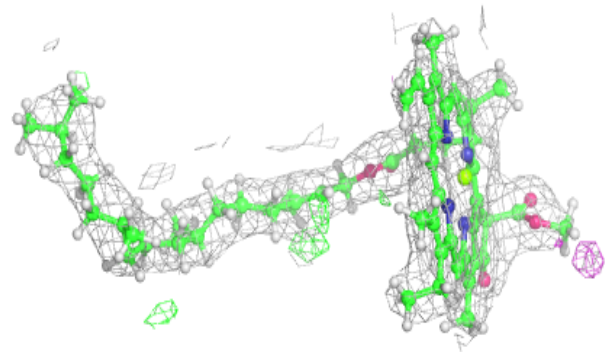
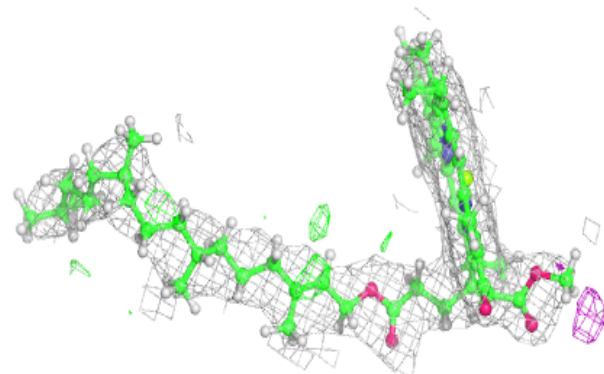


**Electron density around DGD c 516:**

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

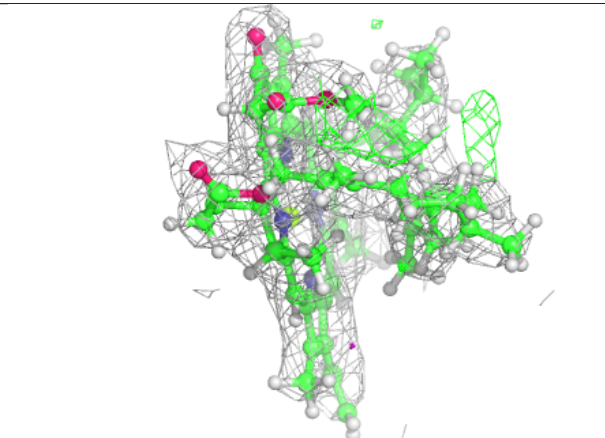
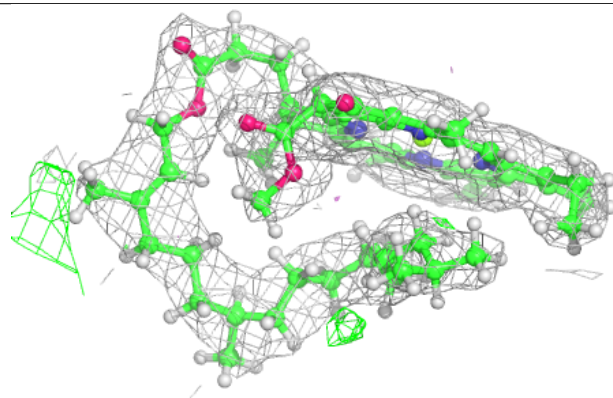
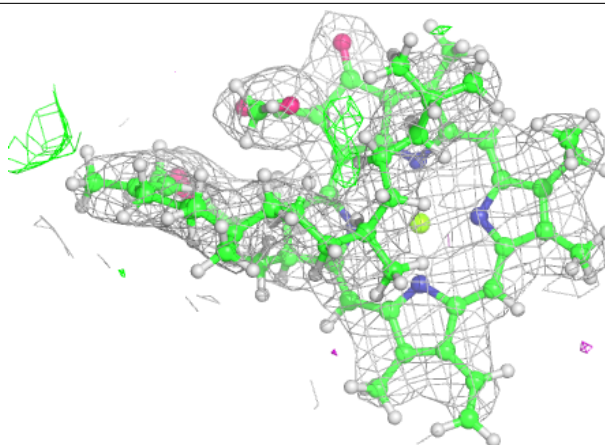
**Electron density around CLA b 605:**

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

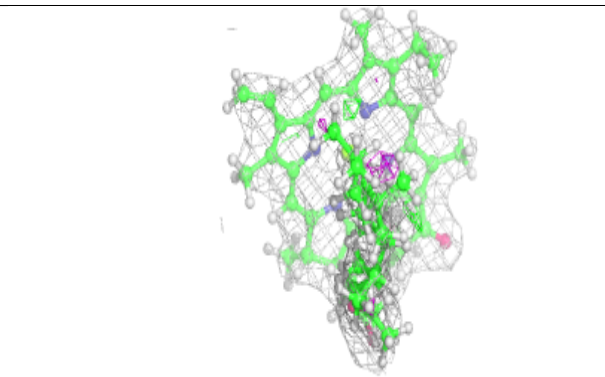
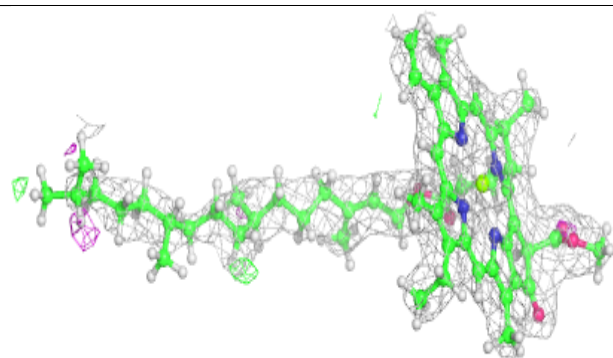
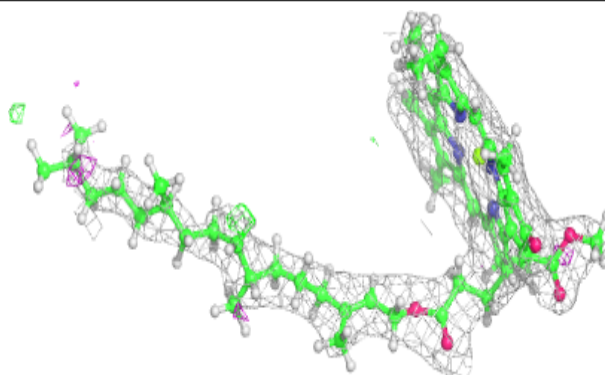


**Electron density around CLA C 510:**

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

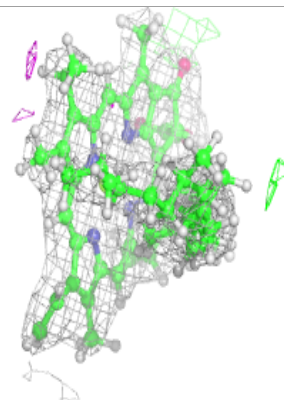
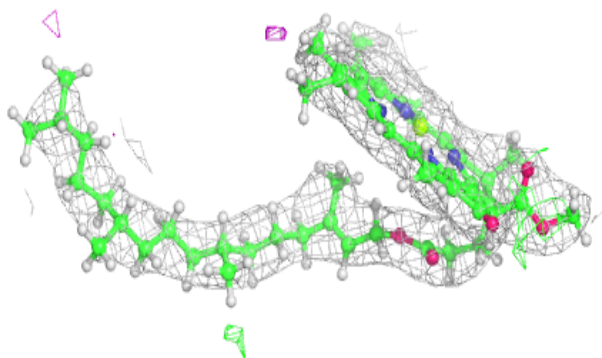
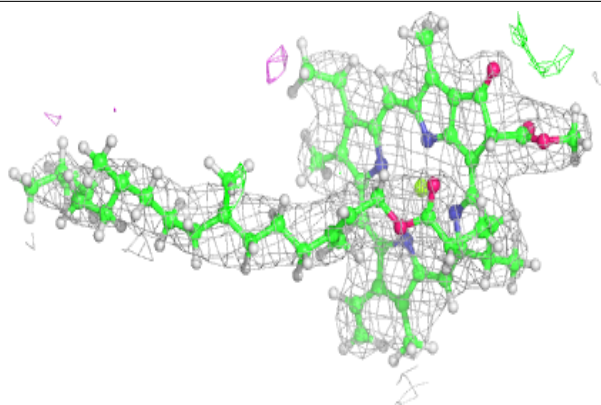
**Electron density around CLA b 607:**

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

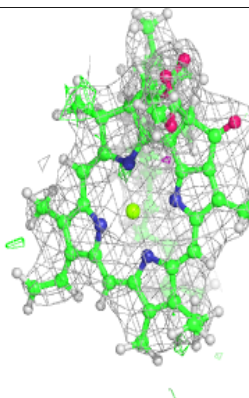
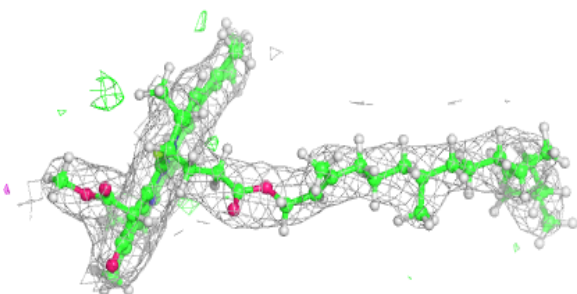
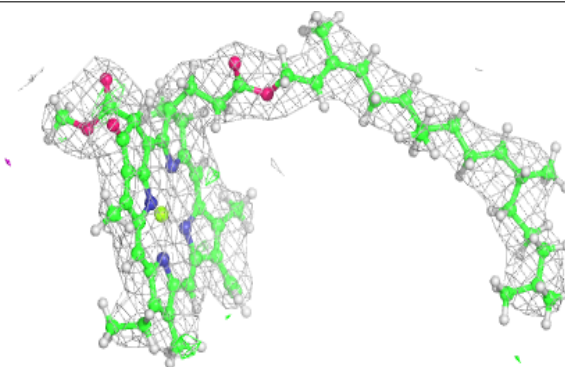


**Electron density around CLA b 608:**

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

**Electron density around CLA B 609:**

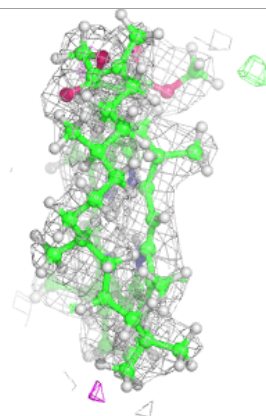
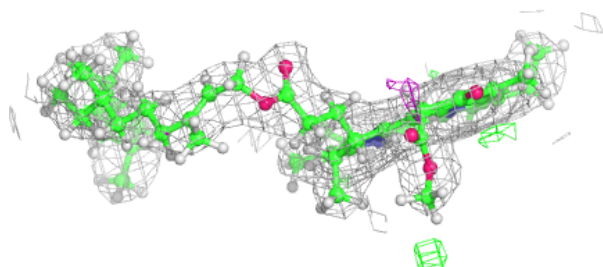
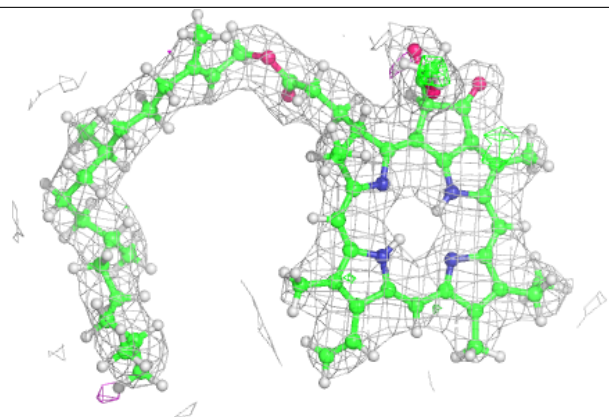
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



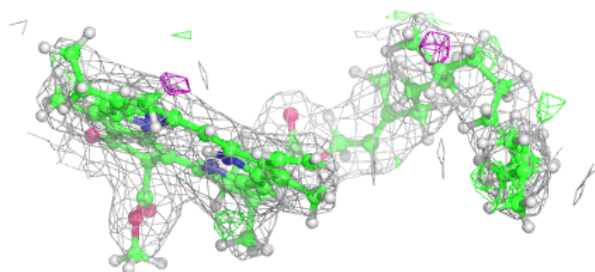
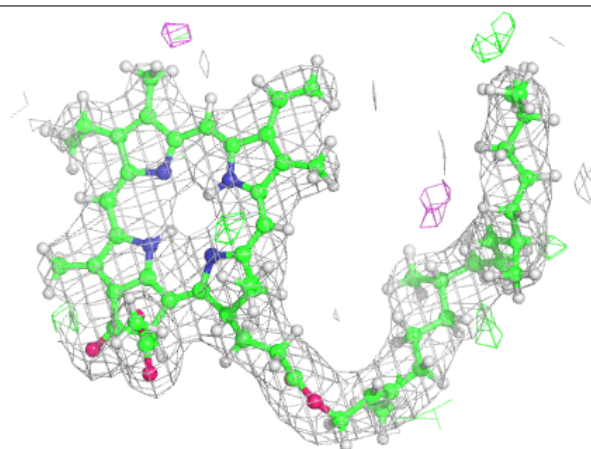


**Electron density around PHO A 404:**

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

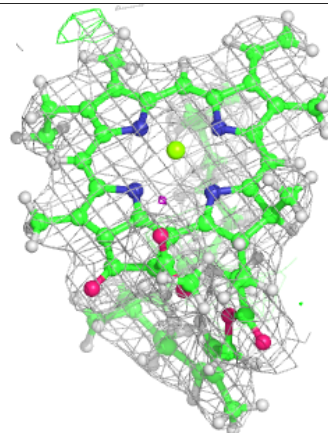
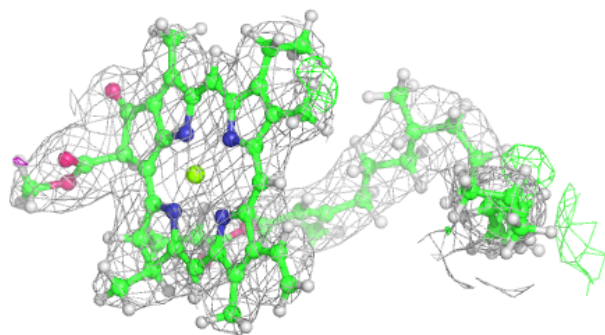
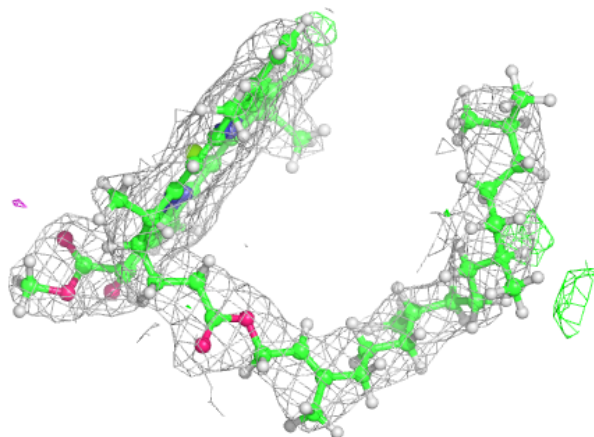
**Electron density around PHO D 401:**

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



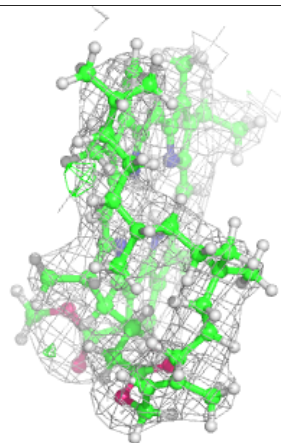
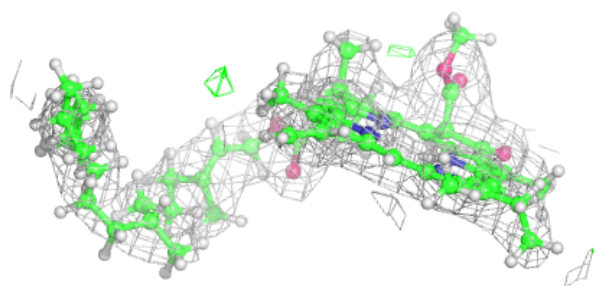
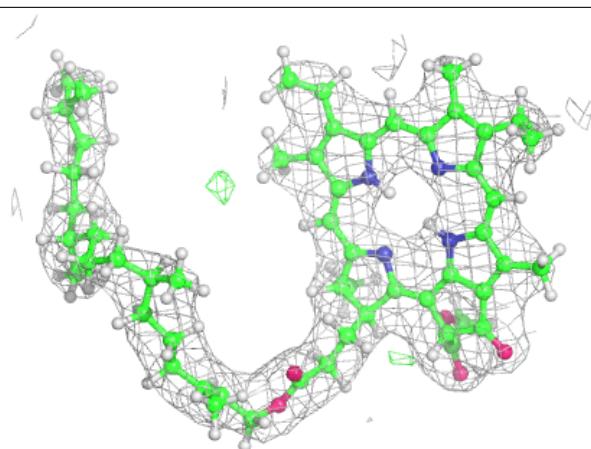
**Electron density around CLA B 611:**

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

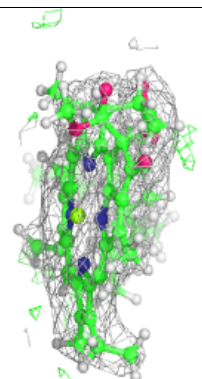
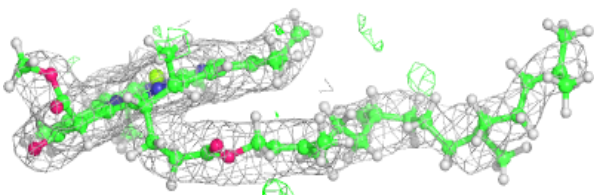
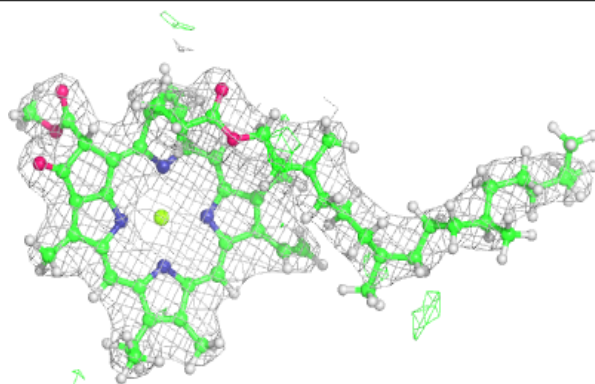


**Electron density around PHO d 402:**

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

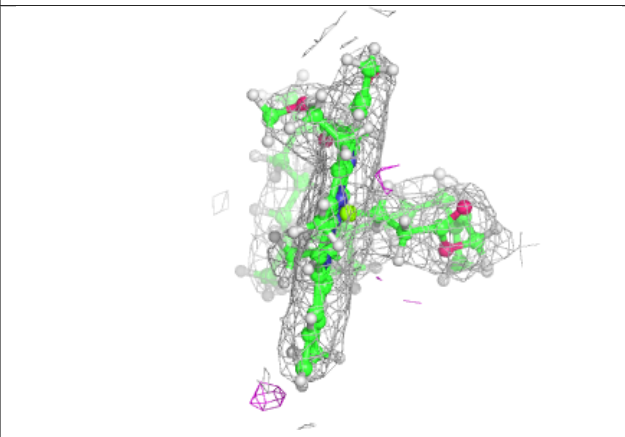
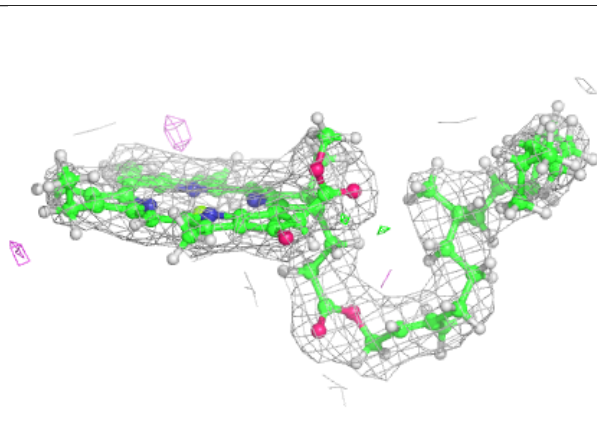
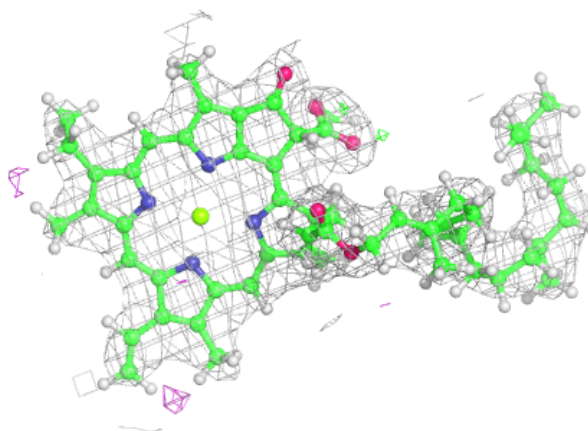
**Electron density around CLA b 603:**

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

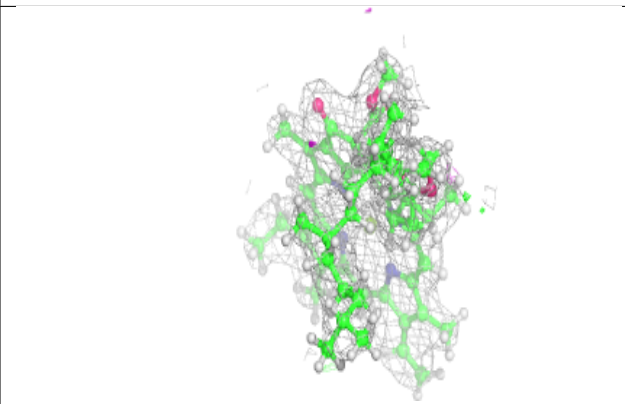
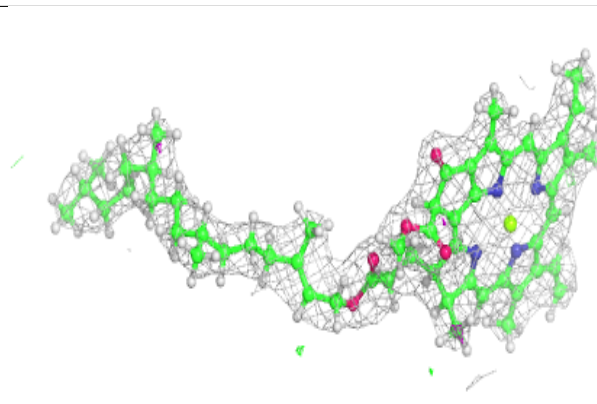
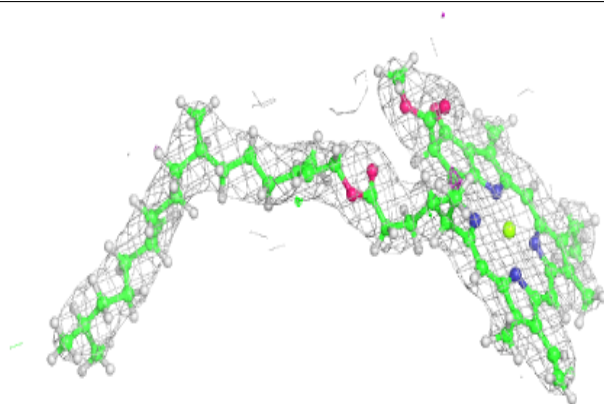


**Electron density around CLA B 612:**

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

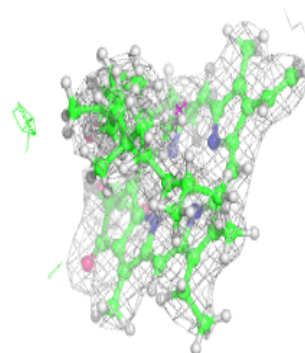
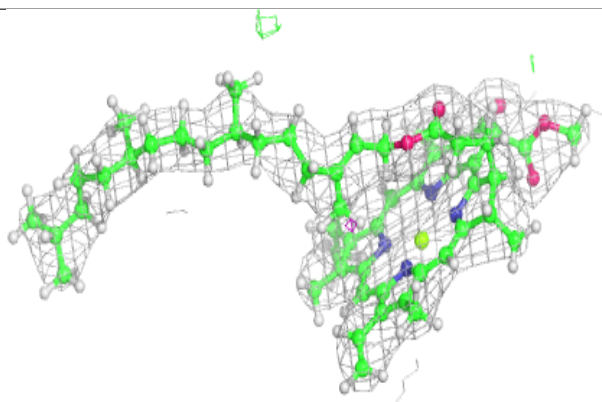
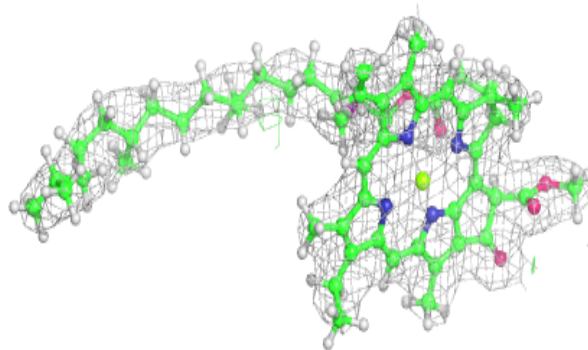
**Electron density around CLA A 402:**

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



**Electron density around CLA B 608:**

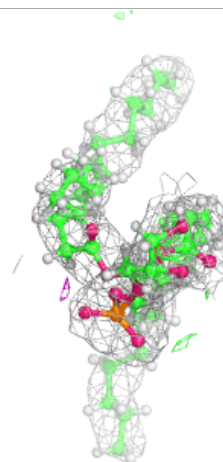
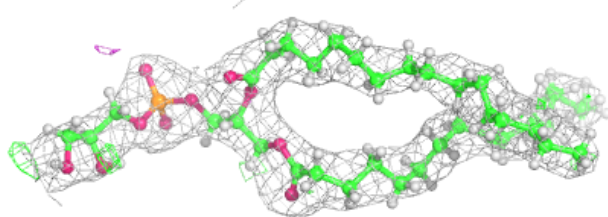
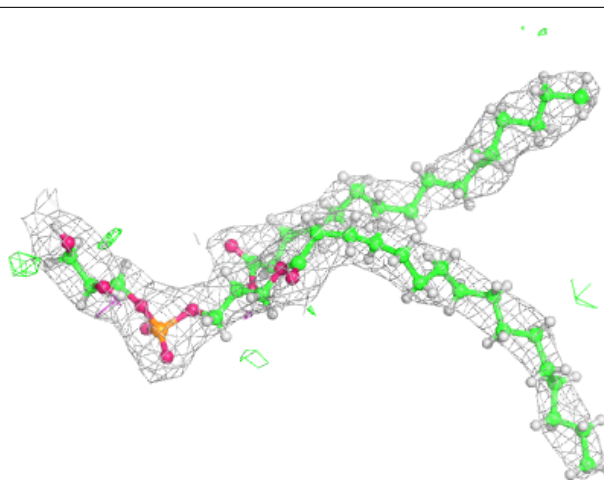
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





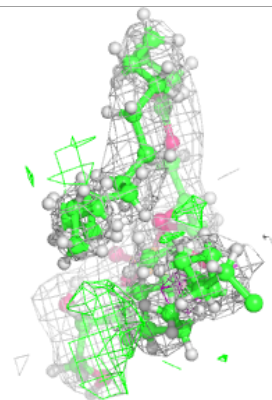
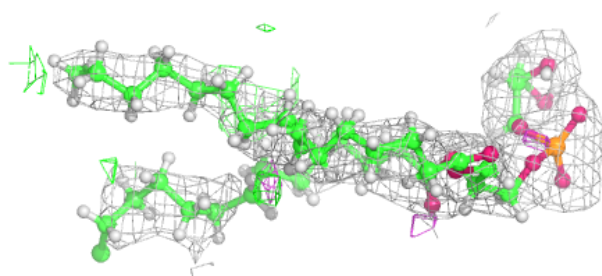
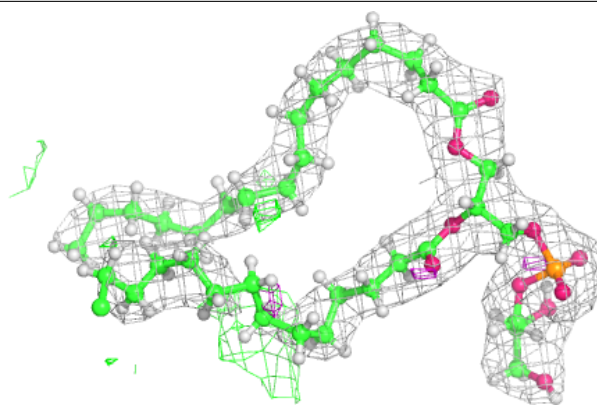
**Electron density around LHG D 410:**

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

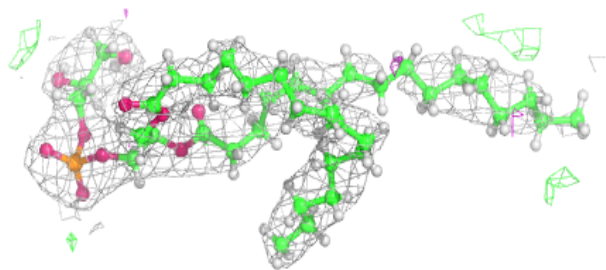
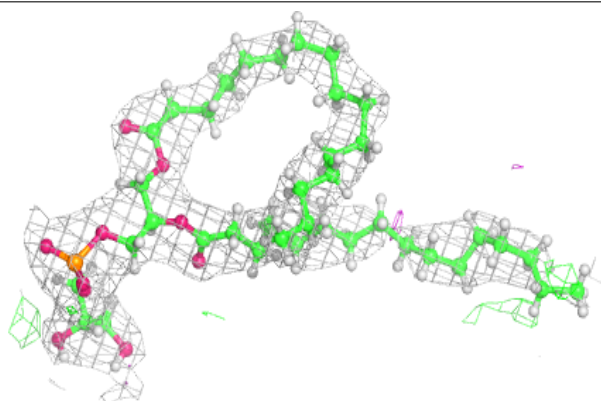


**Electron density around LHG D 411:**

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

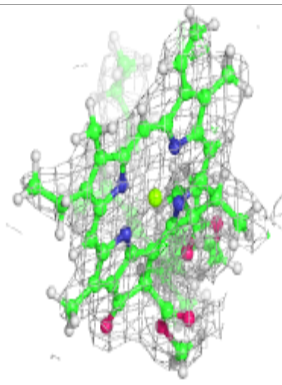
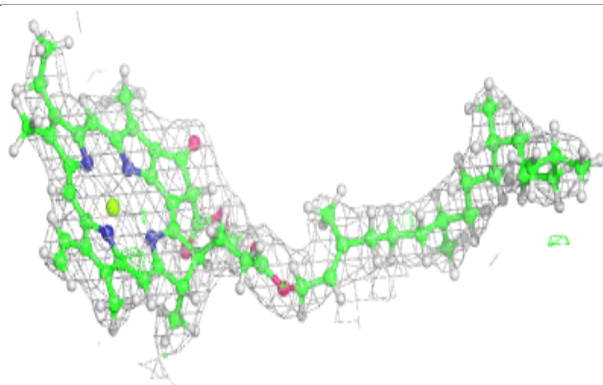
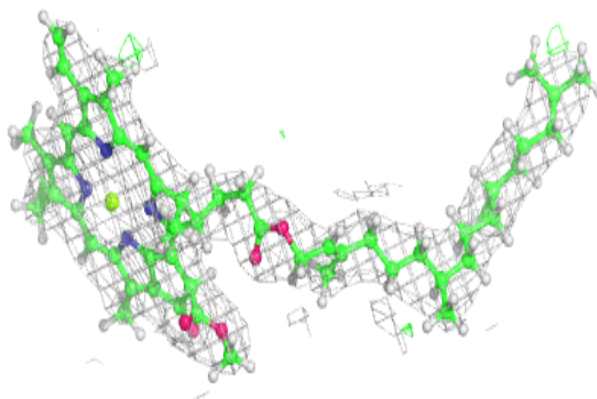
**Electron density around LHG D 413:**

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

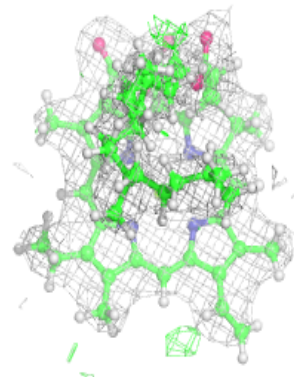
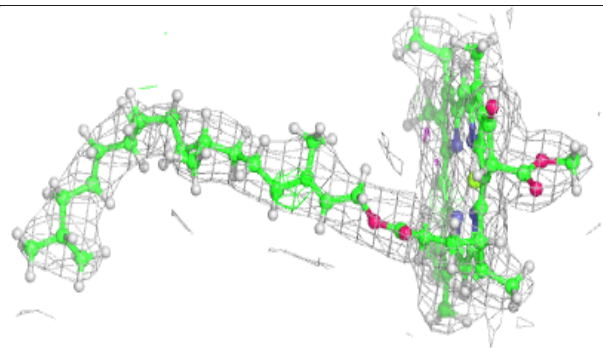
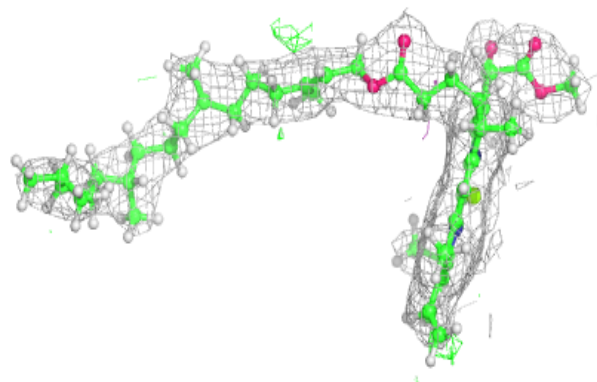


**Electron density around CLA a 402:**

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

**Electron density around CLA B 605:**

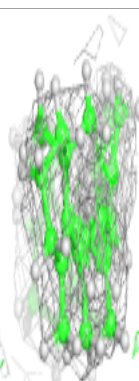
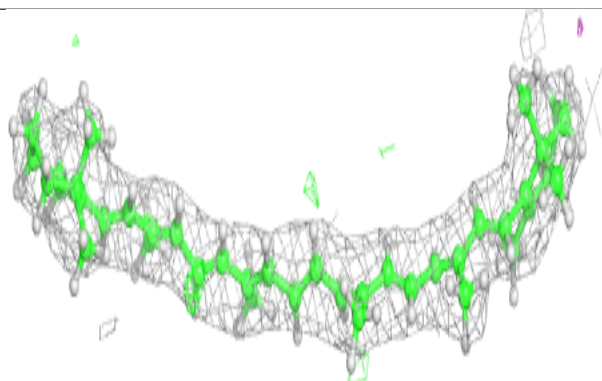
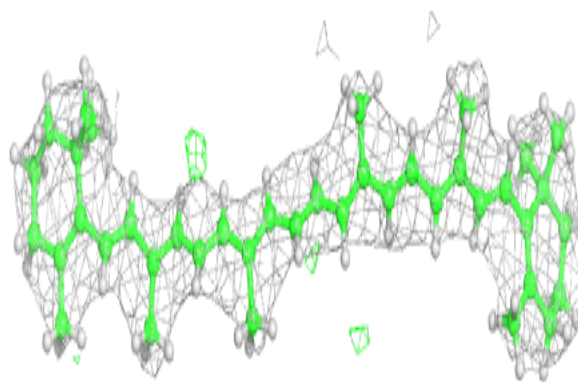
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



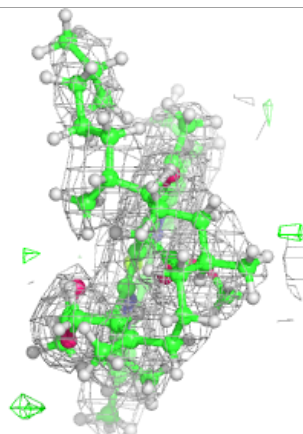
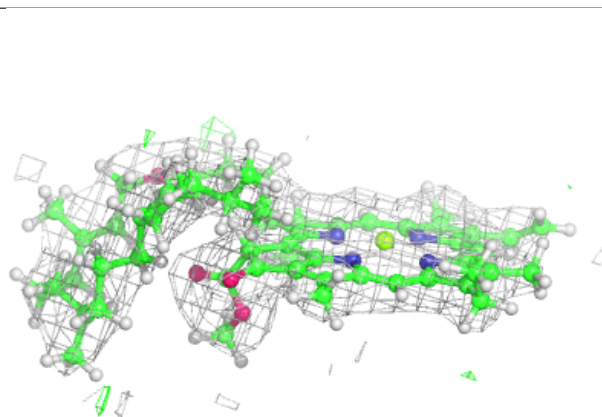
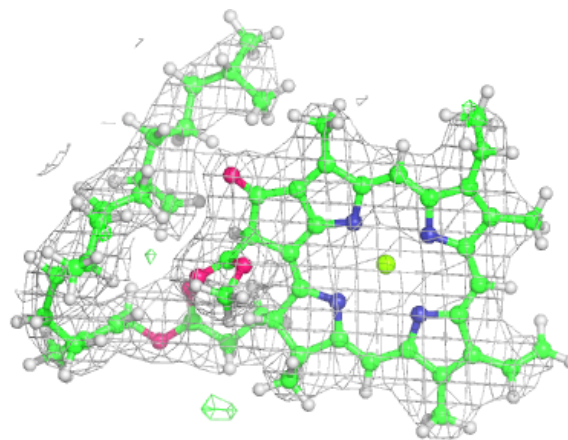


**Electron density around BCR t 101:**

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

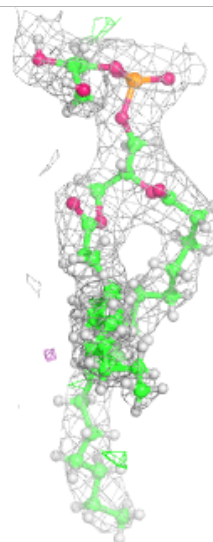
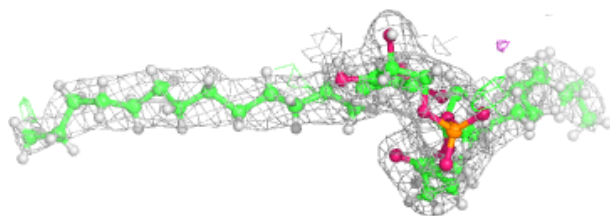
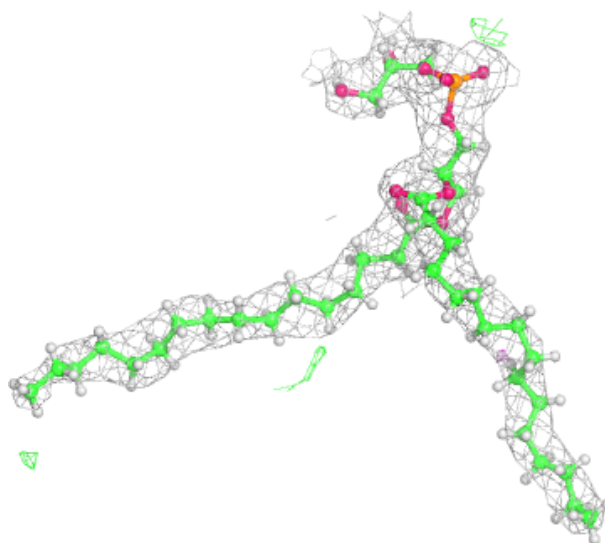
**Electron density around CLA B 610:**

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



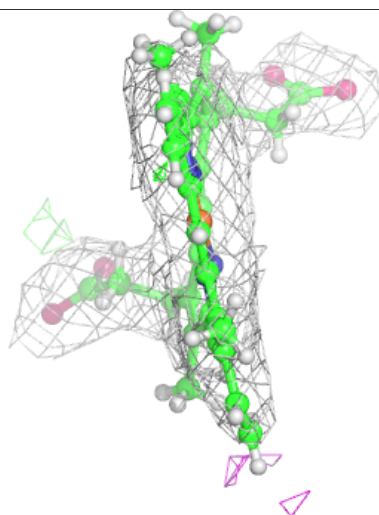
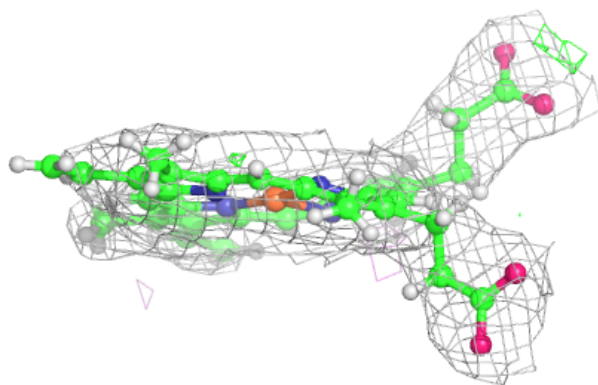
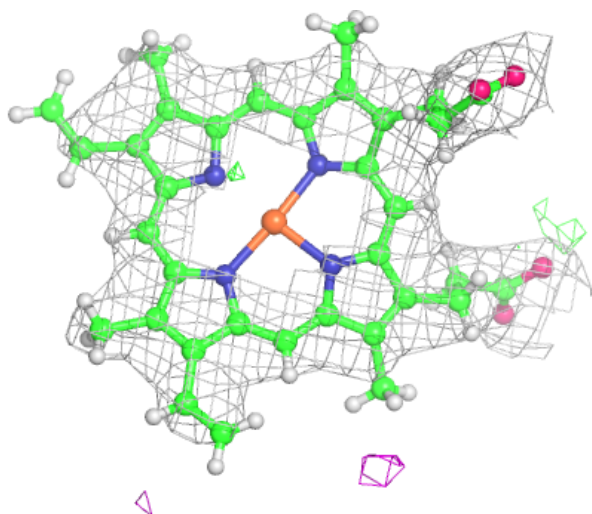
**Electron density around LHG 1 101:**

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



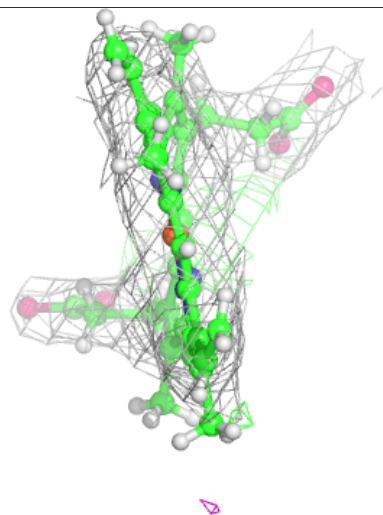
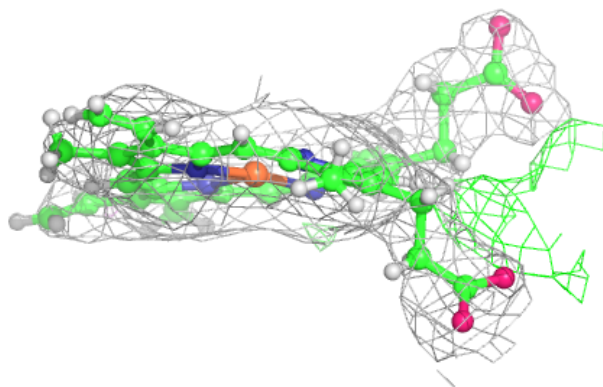
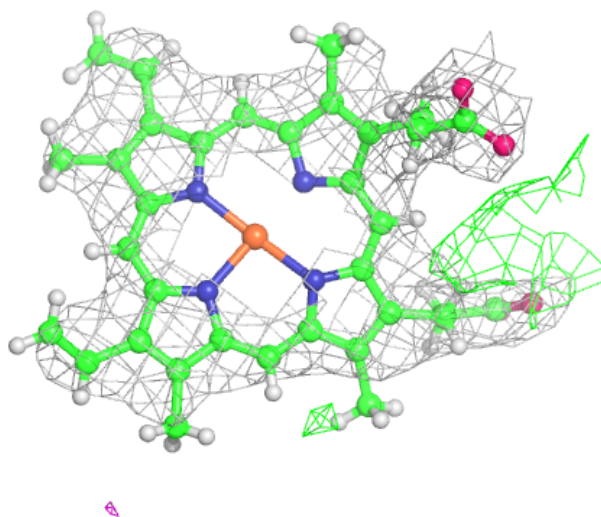
**Electron density around HEM F 101:**

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



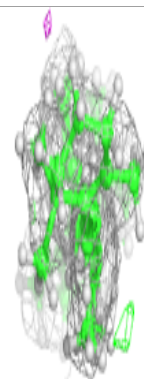
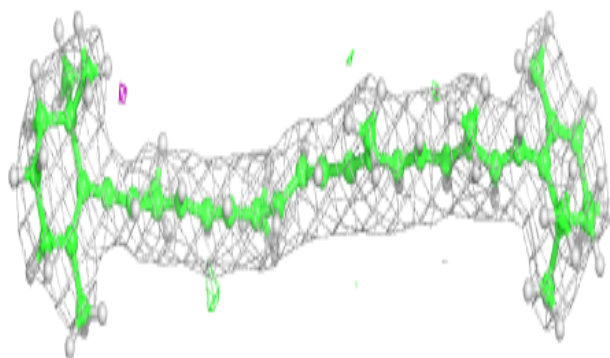
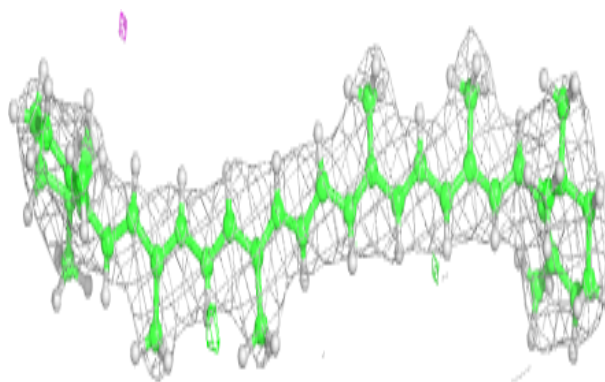
**Electron density around HEM f 101:**

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



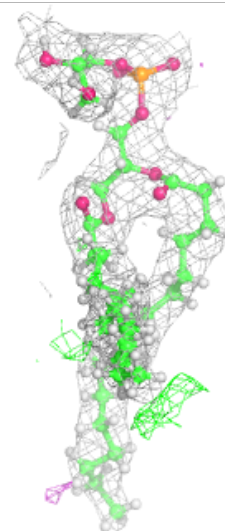
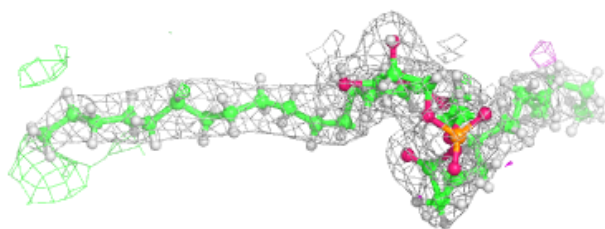
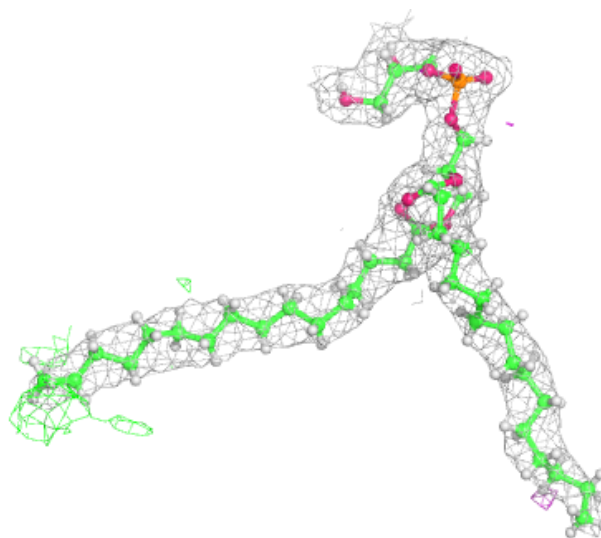
**Electron density around BCR I 101:**

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



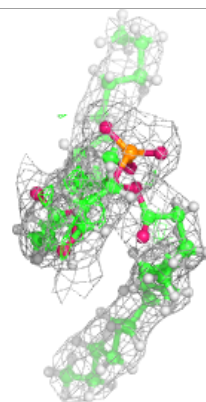
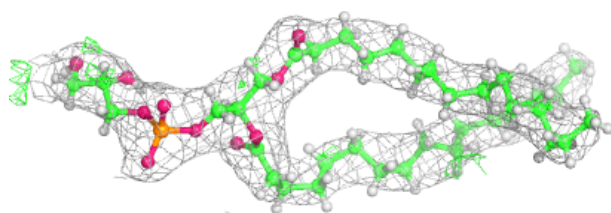
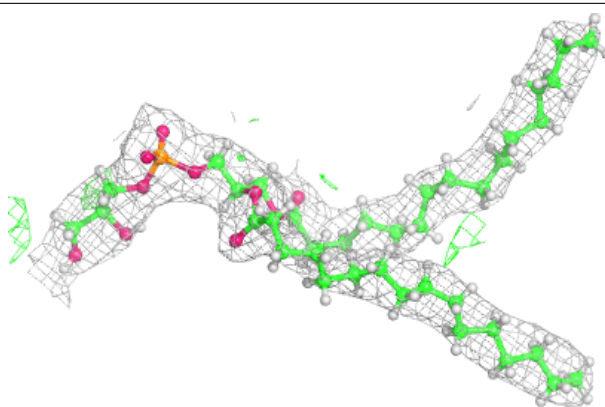
**Electron density around LHG L 102:**

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



**Electron density around LHG d 408:**

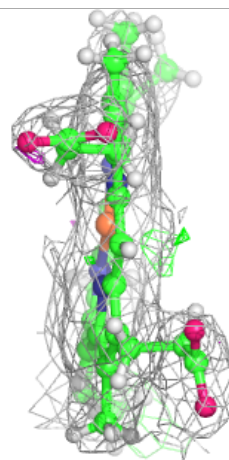
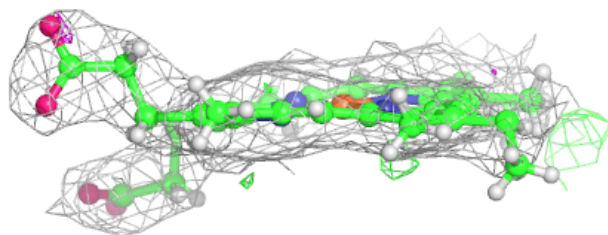
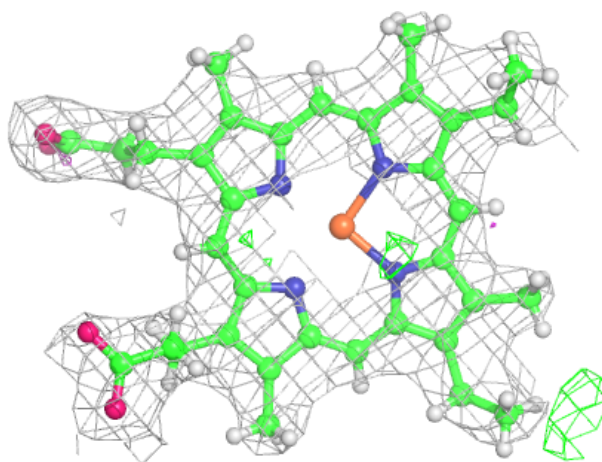
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





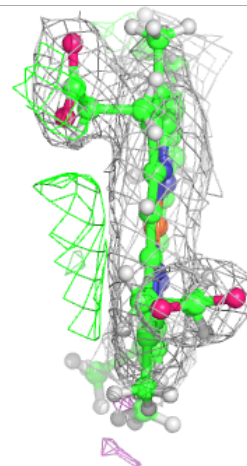
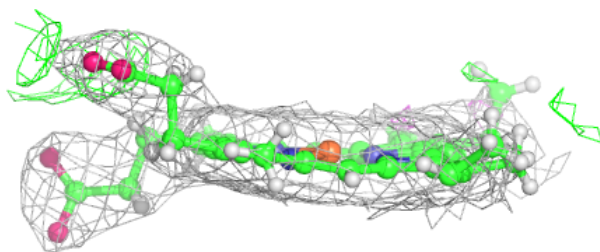
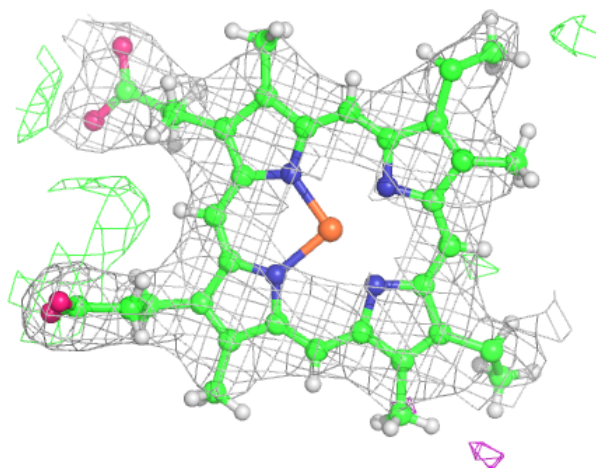
**Electron density around HEC V 201:**

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



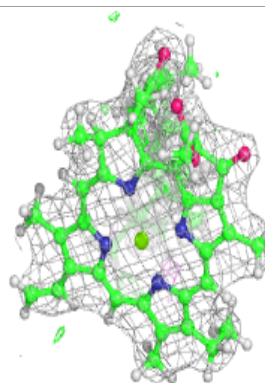
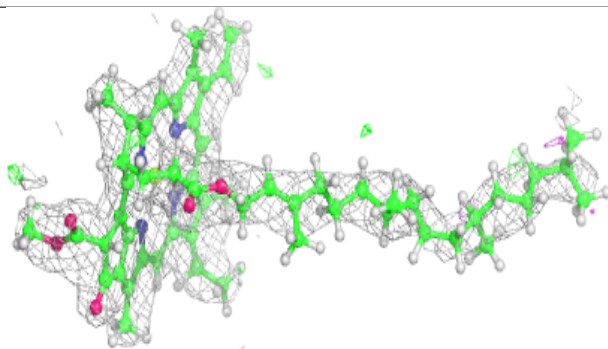
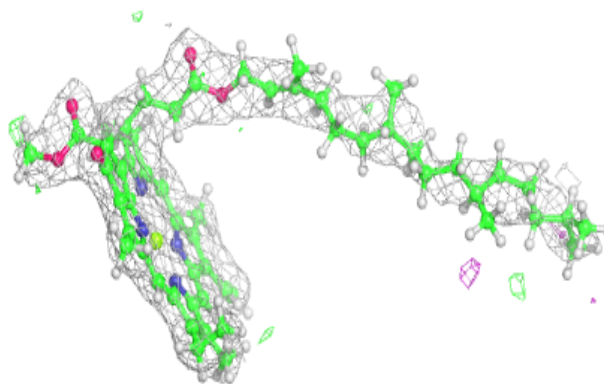
**Electron density around HEC v 201:**

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



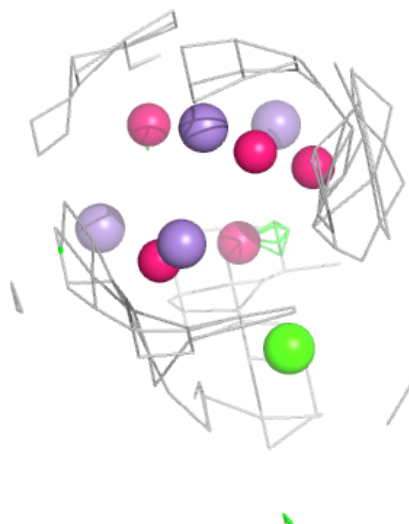
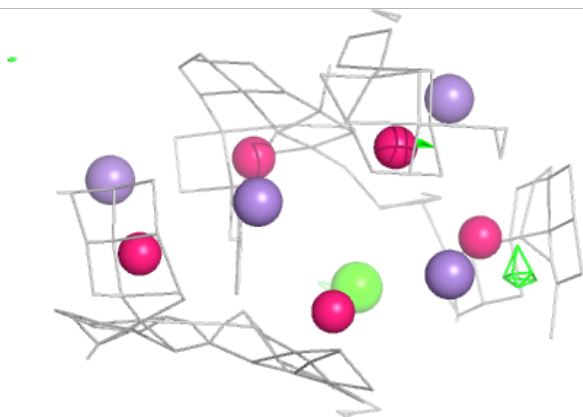
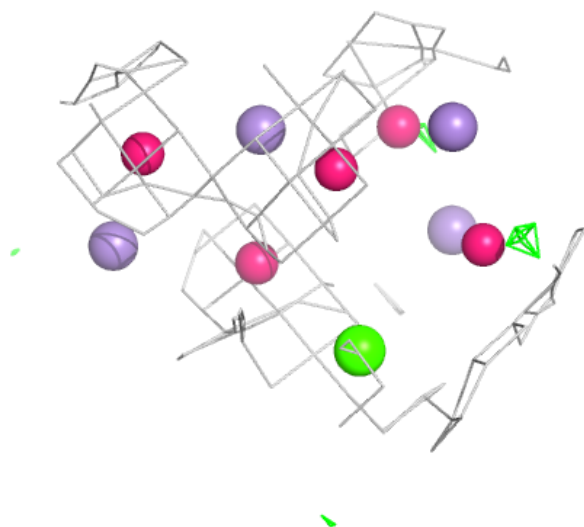
**Electron density around CLA B 607:**

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



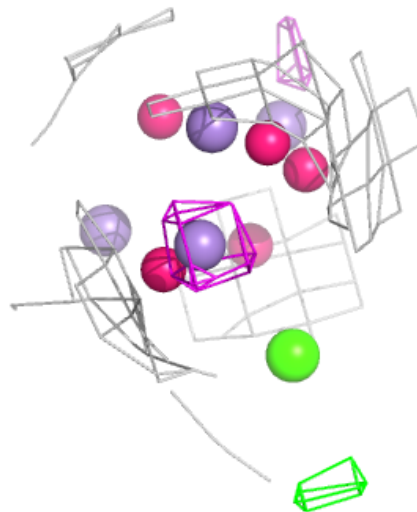
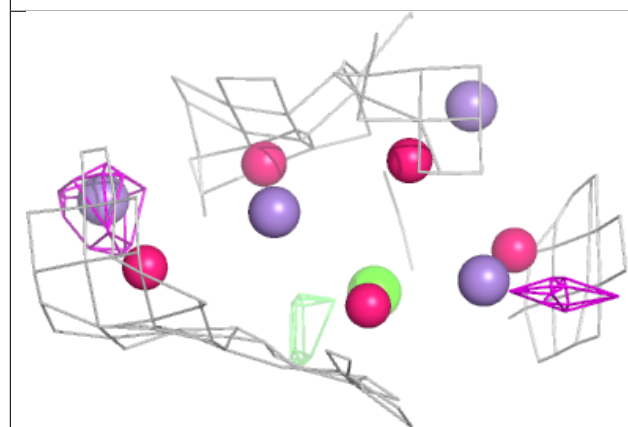
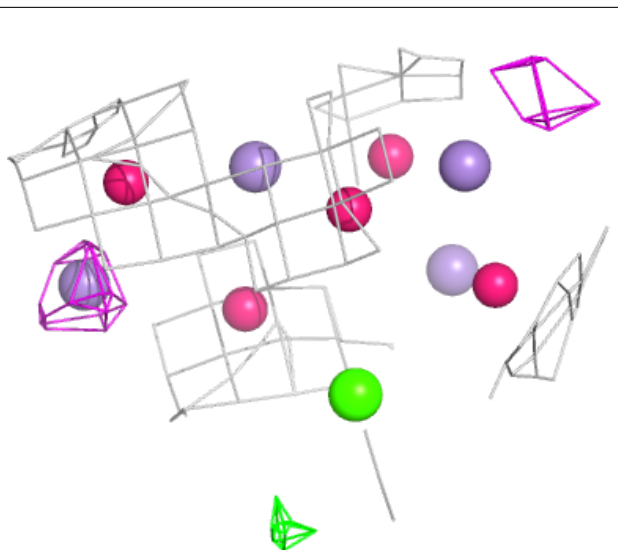
**Electron density around OEX A 414:**

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



**Electron density around OEX a 414:**

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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.