



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 10:45 PM EDT

PDB ID : 5WS6  
Title : Native XFEL structure of Photosystem II (preflash two-flash dataset)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2016-12-05  
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

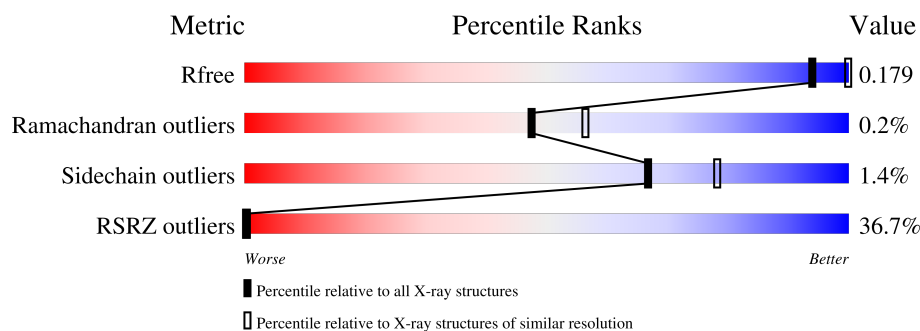
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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>22%</div> <div>97%</div> </div>
1	a	344	<div> <div>32%</div> <div>97%</div> </div>
2	B	505	<div> <div>30%</div> <div>99%</div> </div>
2	b	505	<div> <div>33%</div> <div>98%</div> </div>
3	C	455	<div> <div>36%</div> <div>98%</div> </div>
3	c	455	<div> <div>42%</div> <div>98%</div> </div>
4	D	342	<div> <div>26%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	X	40	<div> <div>55%</div> <div>95%</div> <div>5%</div> </div>
17	x	40	<div> <div>62%</div> <div>95%</div> <div>5%</div> </div>
18	Y	30	<div> <div>80%</div> <div>93%</div> <div>• •</div> </div>
18	y	30	<div> <div>80%</div> <div>93%</div> <div>• •</div> </div>
19	Z	62	<div> <div>82%</div> <div>95%</div> <div>5%</div> </div>
19	z	62	<div> <div>89%</div> <div>94%</div> <div>6%</div> </div>
20	R	34	<div> <div>100%</div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	404	X	-	-	-
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	350	X	-	-	-
24	CLA	a	403	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	X
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
27	SQD	A	411	-	-	-	X
27	SQD	A	413	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	SQD	B	620	-	-	-	X
27	SQD	a	411	-	-	-	X
27	SQD	b	620	-	-	-	X
27	SQD	f	101	-	-	-	X
28	GOL	V	202	-	-	-	X
28	GOL	v	202	-	-	-	X
31	PL9	a	414[A]	-	-	-	X
31	PL9	a	414[B]	-	-	-	X
32	UNL	A	417	-	-	-	X
32	UNL	B	629	-	-	-	X
32	UNL	D	409	-	-	-	X
32	UNL	K	101	-	-	-	X
32	UNL	a	415	-	-	-	X
32	UNL	d	409	-	-	-	X
32	UNL	d	410	-	-	-	X
32	UNL	i	101	-	-	-	X
32	UNL	j	102	-	-	-	X
32	UNL	m	101	-	-	-	X
33	LMG	A	418	-	-	-	X
33	LMG	B	621	-	-	-	X
33	LMG	C	520	-	-	-	X
33	LMG	C	521	-	-	-	X
33	LMG	Z	101	-	-	-	X
33	LMG	a	417	-	-	-	X
33	LMG	c	522	-	-	-	X
33	LMG	z	101	-	-	-	X
34	LMT	A	359	-	-	-	X
34	LMT	B	622	-	-	-	X
34	LMT	B	630	-	-	-	X
34	LMT	E	102	-	-	-	X
34	LMT	I	101	-	-	-	X
34	LMT	M	101	-	-	-	X
34	LMT	a	359	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	b	622	-	-	-	X
34	LMT	b	630	-	-	-	X
34	LMT	e	101	-	-	-	X
34	LMT	m	102	-	-	-	X
35	HTG	C	523	-	-	-	X
35	HTG	D	410	-	-	-	X
35	HTG	b	623	-	-	-	X
35	HTG	b	624	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	HTG	b	625	-	-	-	X
35	HTG	c	523	-	-	-	X
35	HTG	c	526	-	-	-	X
35	HTG	h	101	-	-	-	X
36	DGD	H	102	-	-	-	X
36	DGD	h	103	-	-	-	X
38	LHG	D	357	-	-	-	X
38	LHG	D	407	-	-	-	X
38	LHG	E	101	-	-	-	X
38	LHG	a	419	-	-	-	X

## 2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 53280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	29	0
			2850	1865	467	502	16			
1	a	334	Total	C	N	O	S	0	29	0
			2852	1867	466	503	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	10	0
			3542	2315	590	624	13			
3	c	455	Total	C	N	O	S	0	10	0
			3577	2340	595	629	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2748	1819	450	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2739	1814	449	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	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	N	O	S	0	1	0
			265	178	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			



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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		

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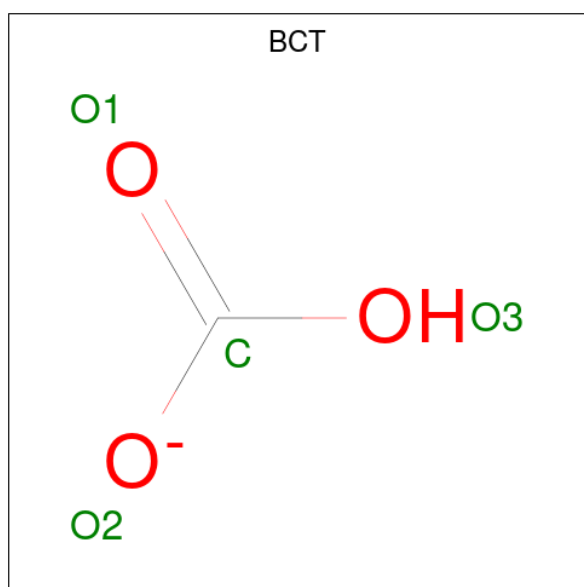
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	1
			2	2		

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

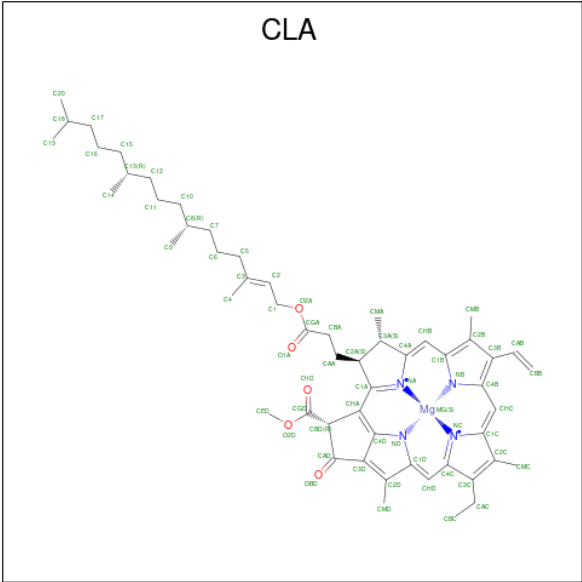
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	1
			8	2	6		
23	a	1	Total	C	O	0	1
			8	2	6		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ).



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

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

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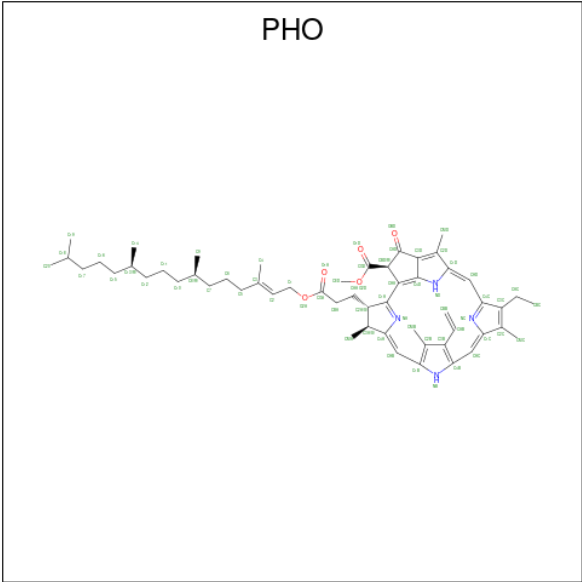
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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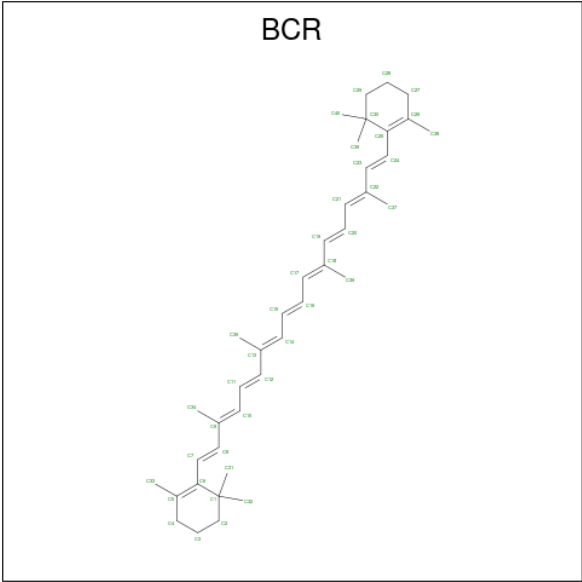
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



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

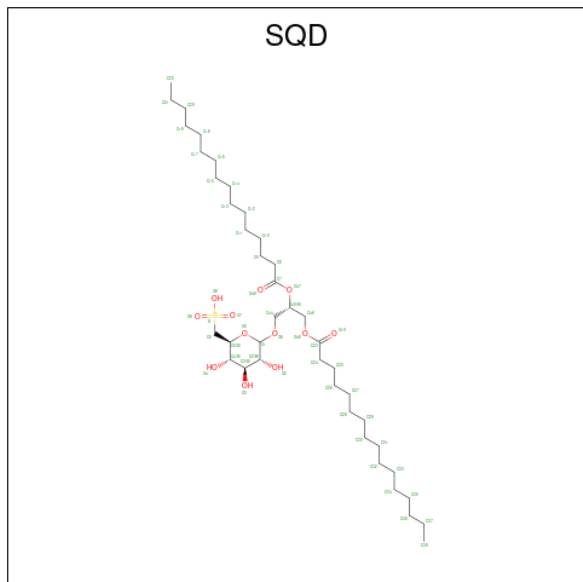
- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	1	Total C 40 40	0	0



- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



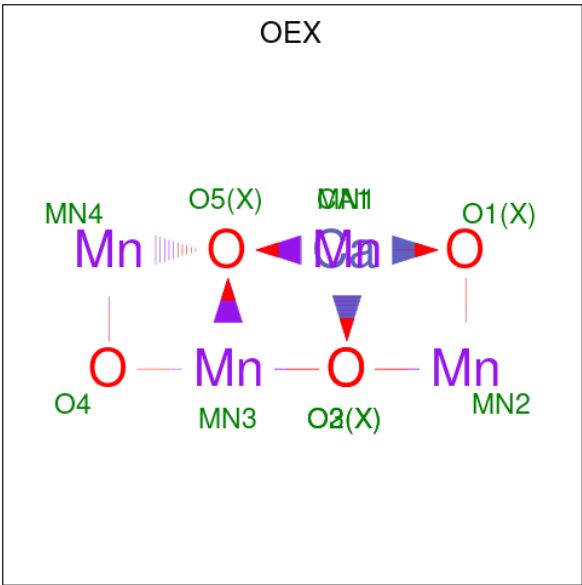
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



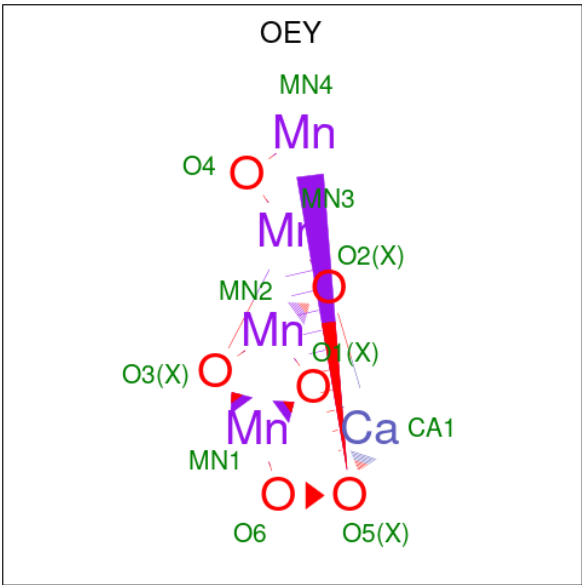
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



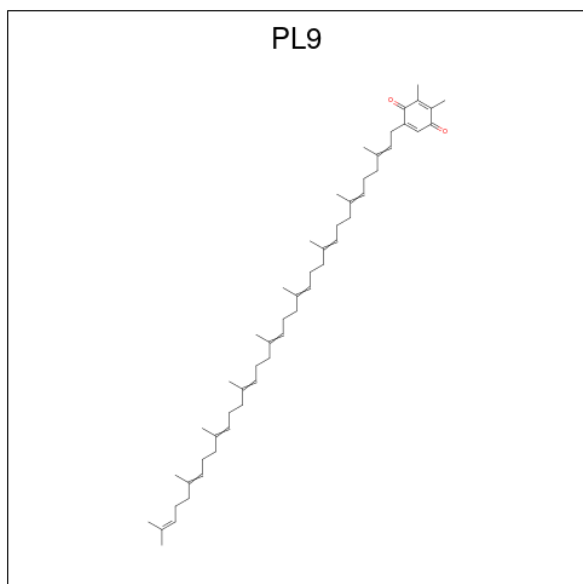
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ).



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

- Molecule 31 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
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	0
			55	53	2		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	0
			55	53	2		

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

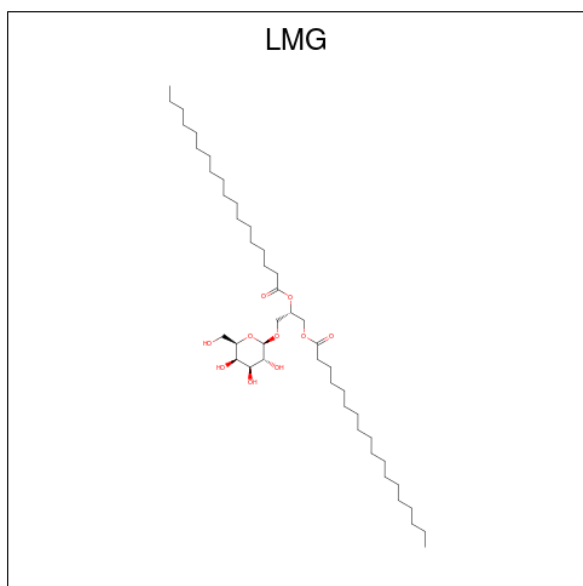
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			

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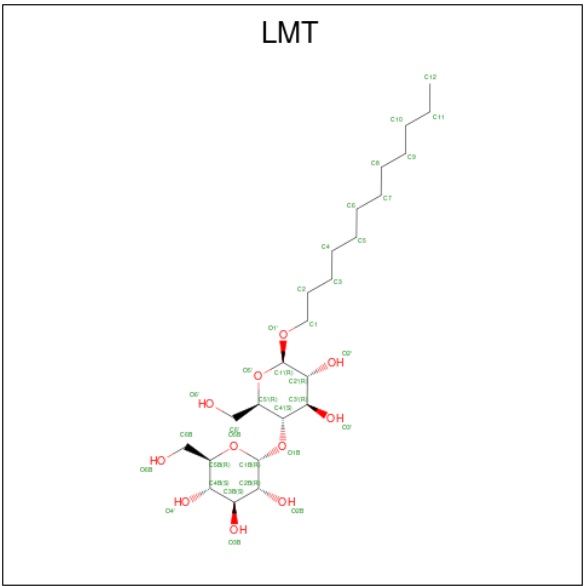
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	K	1	Total C O 34 29 5	0	0
32	M	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	2	Total C O 53 47 6	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0
32	x	1	Total C O 18 16 2	0	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



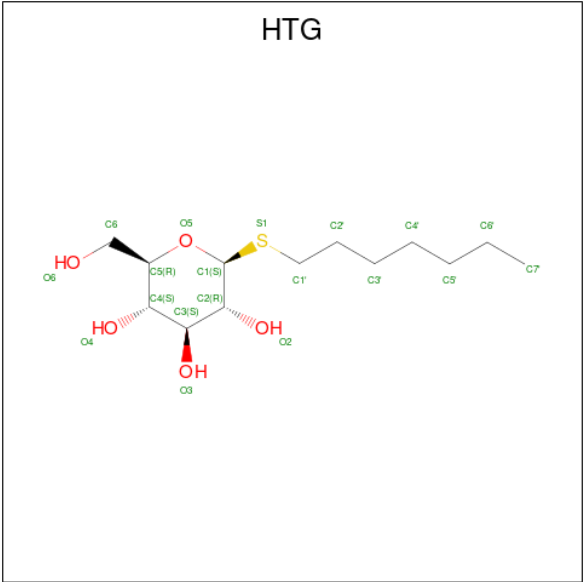
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			51	41	10		
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	1	Total C O 35 24 11	0	0
34	B	1	Total C O 35 24 11	0	0
34	B	1	Total C O 25 19 6	0	0
34	E	1	Total C O 35 24 11	0	0
34	I	1	Total C O 35 24 11	0	0
34	M	1	Total C O 35 24 11	0	0
34	M	1	Total C O 35 24 11	0	0
34	a	1	Total C O 35 24 11	0	0
34	a	1	Total C O 35 24 11	0	0
34	b	1	Total C O 25 19 6	0	0
34	b	1	Total C O 25 19 6	0	0
34	e	1	Total C O 35 24 11	0	0
34	m	1	Total C O 35 24 11	0	0
34	t	1	Total C O 26 19 7	0	0

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	V	1	Total	C	O		0	0
			11	6	5			
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		

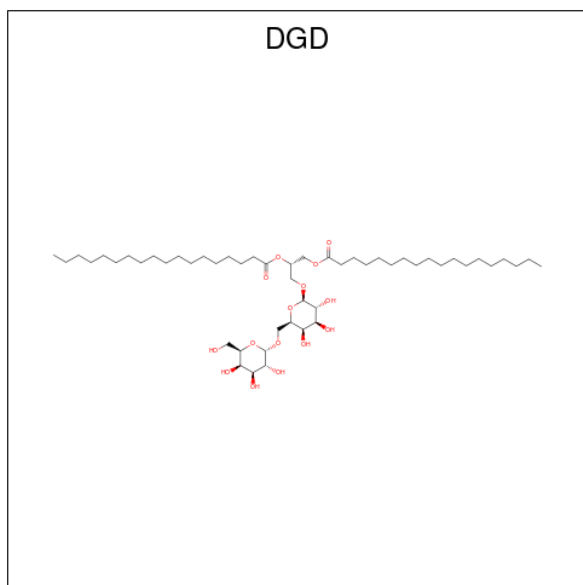
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).

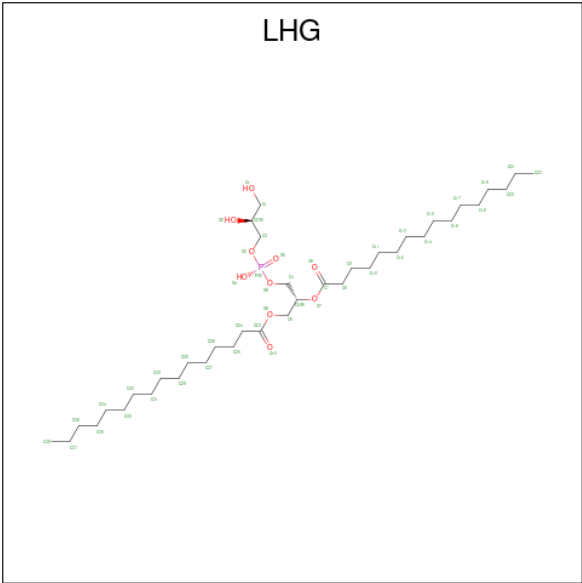


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15	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

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	C	1	Total	Ca	0	0
			1	1		
37	O	1	Total	Ca	0	0
			1	1		
37	V	1	Total	Ca	0	0
			1	1		
37	b	1	Total	Ca	0	0
			1	1		
37	c	2	Total	Ca	0	0
			2	2		
37	o	1	Total	Ca	0	0
			1	1		
37	v	1	Total	Ca	0	0
			1	1		

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



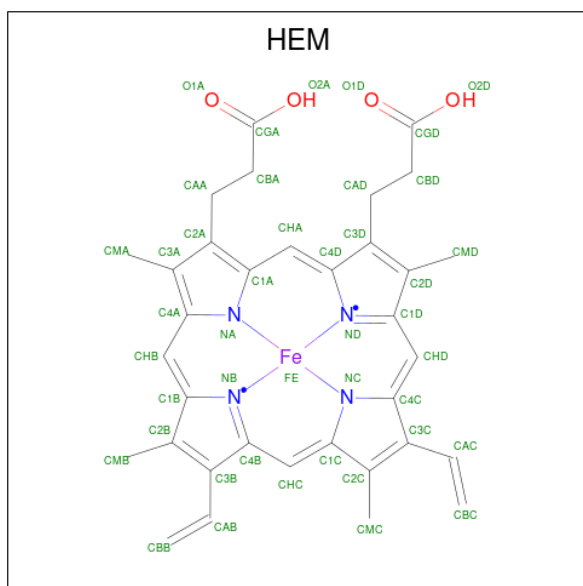
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	L	1	Total	C	O	P	0	0
			49	38	10	1		
38	a	1	Total	C	O	P	0	0
			42	31	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

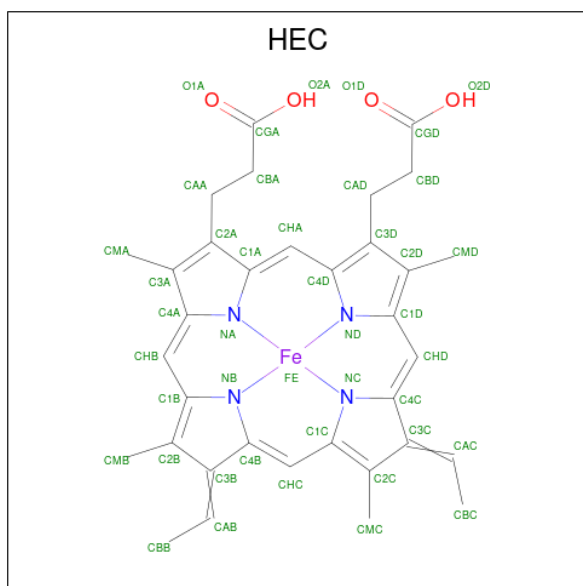
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	j	1	Total	Mg	0	0
			1	1		

- Molecule 41 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	125	Total	O	0	5
			130	130		
42	B	164	Total	O	0	0
			164	164		
42	C	147	Total	O	0	0
			147	147		
42	D	112	Total	O	0	0
			112	112		
42	E	14	Total	O	0	0
			14	14		
42	F	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	H	20	Total 20	O 20	0	0
42	I	6	Total 6	O 6	0	0
42	J	4	Total 4	O 4	0	0
42	K	7	Total 7	O 7	0	0
42	L	4	Total 4	O 4	0	0
42	M	7	Total 7	O 7	0	0
42	O	74	Total 74	O 74	0	0
42	T	8	Total 8	O 8	0	0
42	U	33	Total 33	O 33	0	0
42	V	65	Total 65	O 65	0	0
42	X	2	Total 2	O 2	0	0
42	Y	1	Total 1	O 1	0	0
42	a	128	Total 133	O 133	0	5
42	b	185	Total 185	O 185	0	0
42	c	122	Total 122	O 122	0	0
42	d	109	Total 109	O 109	0	0
42	e	7	Total 7	O 7	0	0
42	f	3	Total 3	O 3	0	0
42	h	14	Total 14	O 14	0	0
42	i	3	Total 3	O 3	0	0
42	j	2	Total 2	O 2	0	0

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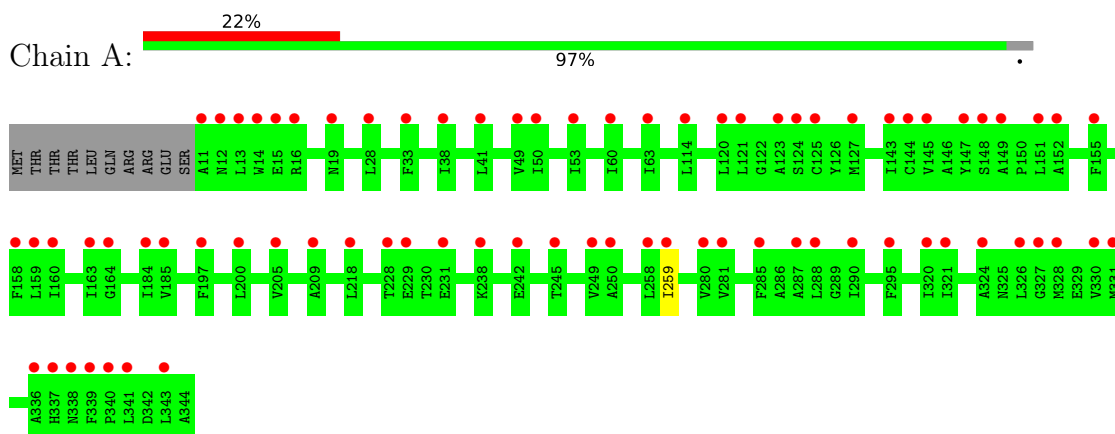
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	k	3	Total 3	O 3	0	0
42	l	6	Total 6	O 6	0	0
42	m	11	Total 11	O 11	0	0
42	o	78	Total 78	O 78	0	0
42	t	5	Total 5	O 5	0	0
42	u	47	Total 47	O 47	0	0
42	v	49	Total 49	O 49	0	0
42	x	4	Total 4	O 4	0	0
42	y	1	Total 1	O 1	0	0

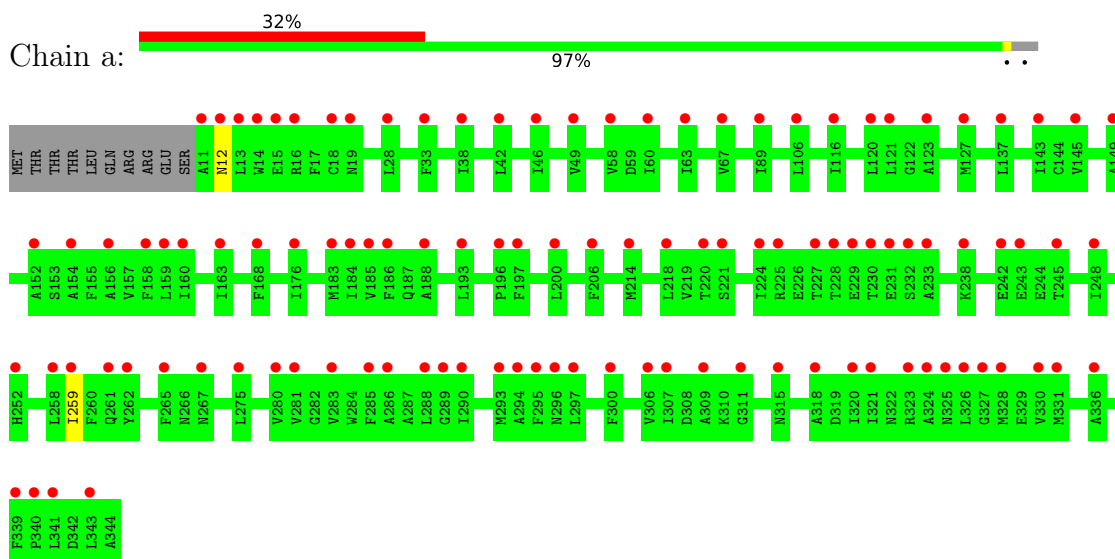
### 3 Residue-property plots [i](#)

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 D1 protein

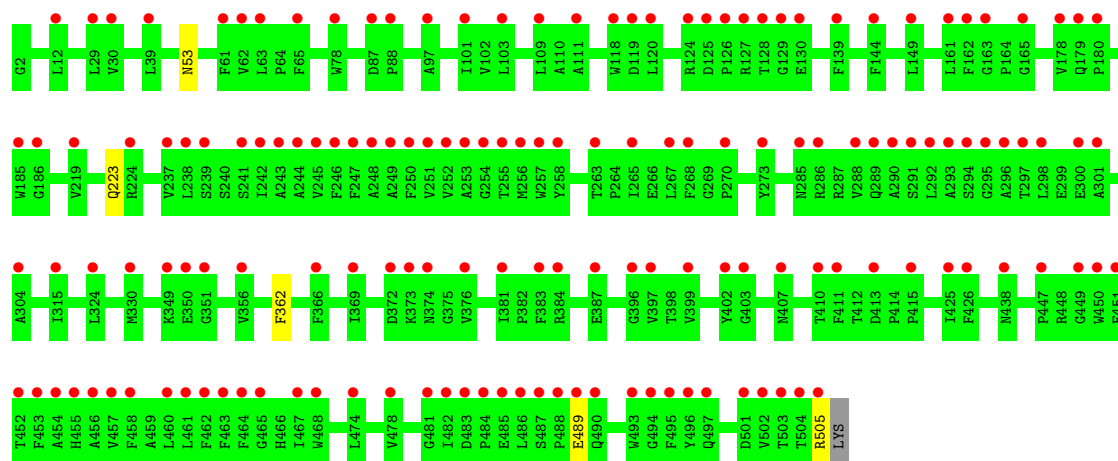


- Molecule 1: Photosystem II D1 protein

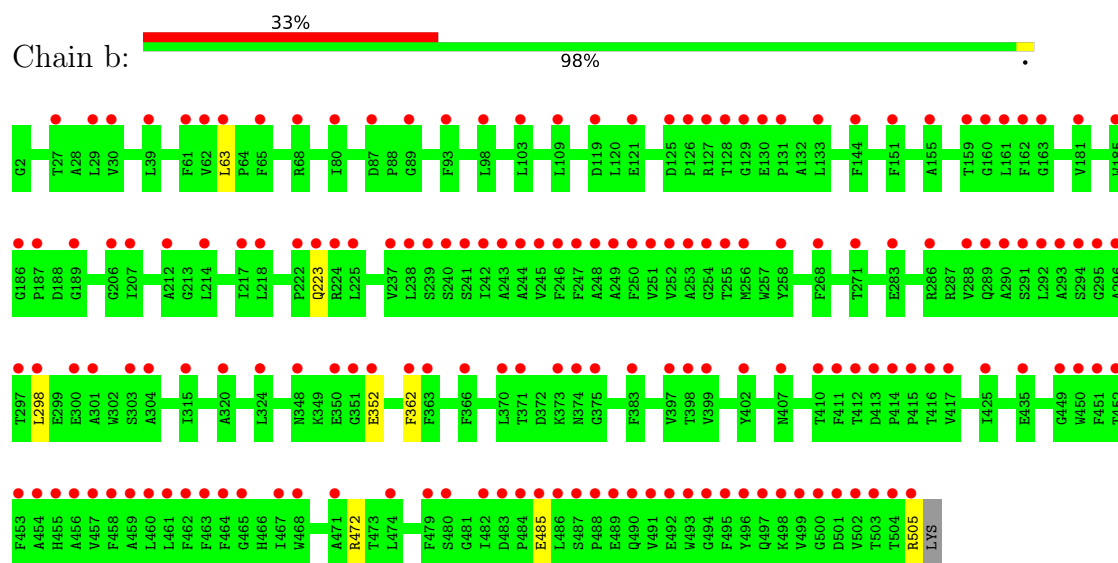


- Molecule 2: Photosystem II CP47 reaction center protein

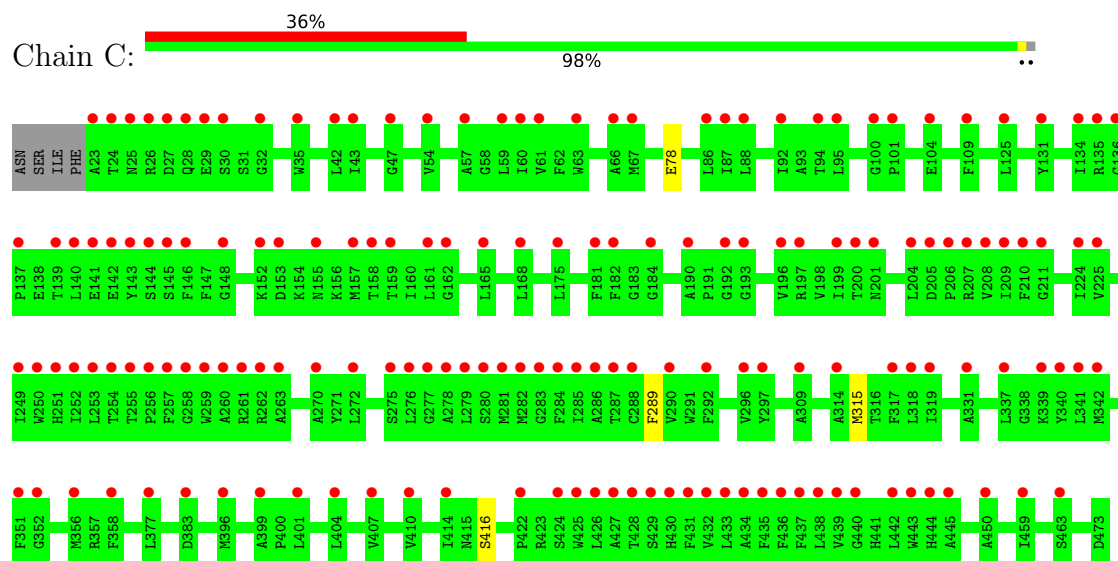




• Molecule 2: Photosystem II CP47 reaction center protein

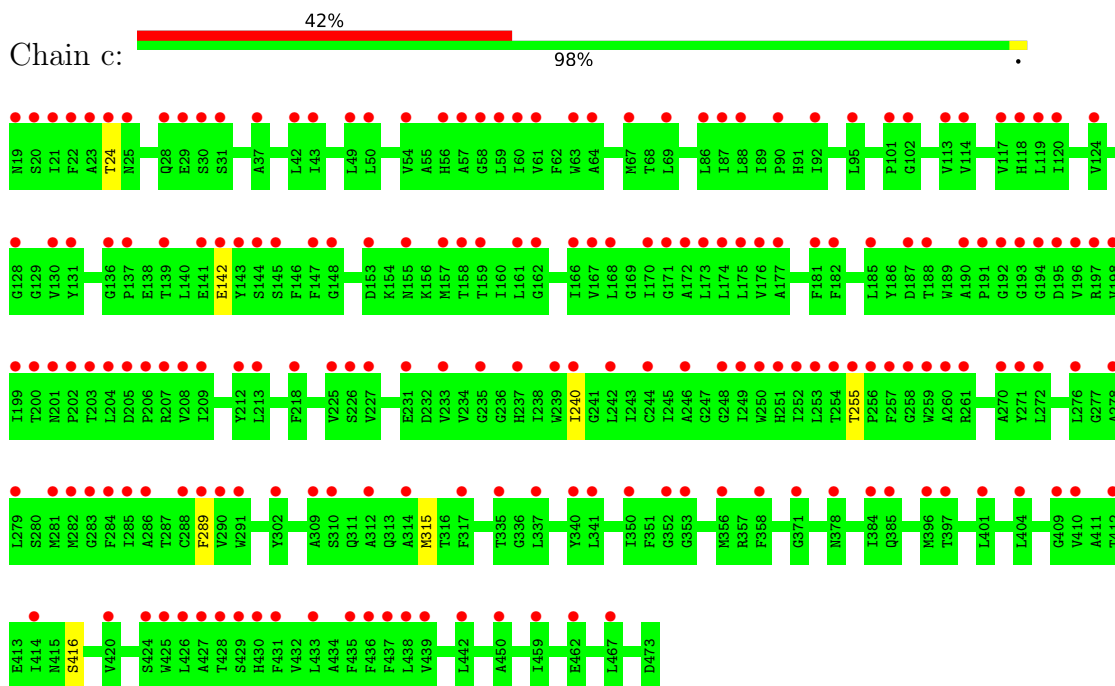


• Molecule 3: Photosystem II CP43 chlorophyll protein

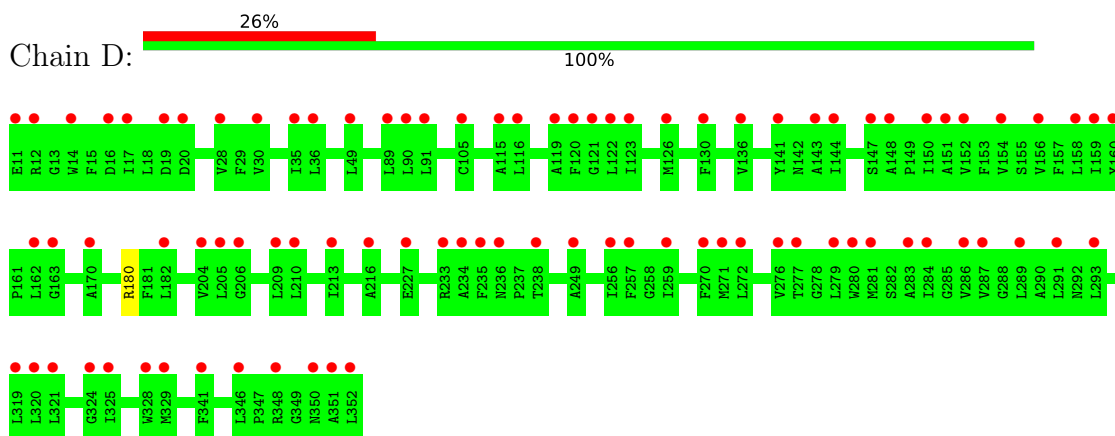




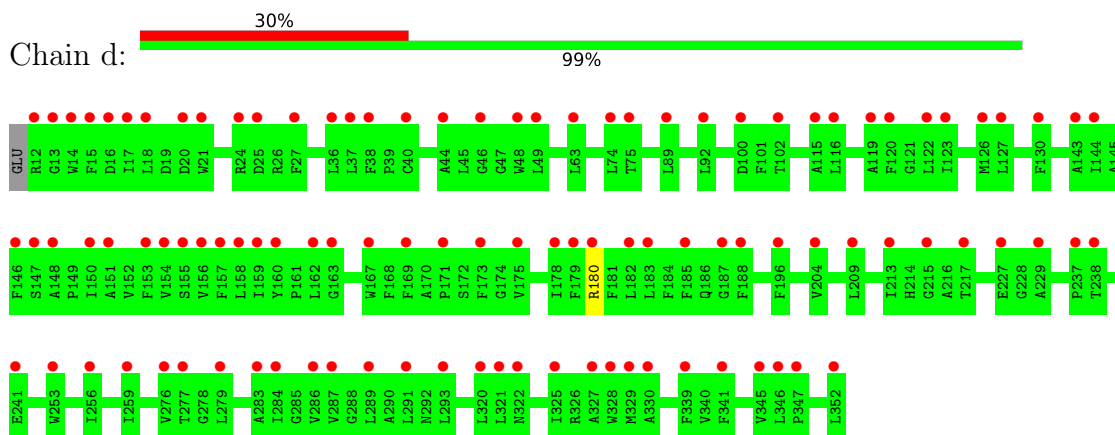
• Molecule 3: Photosystem II CP43 chlorophyll protein



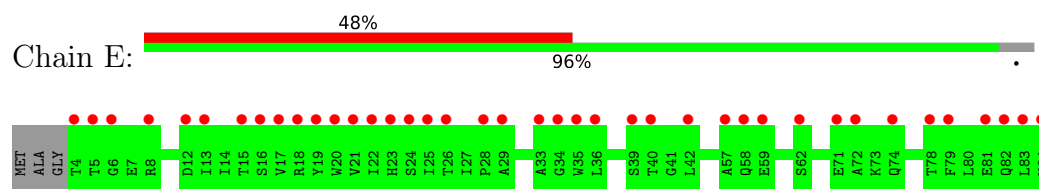
• Molecule 4: Photosystem II D2 protein



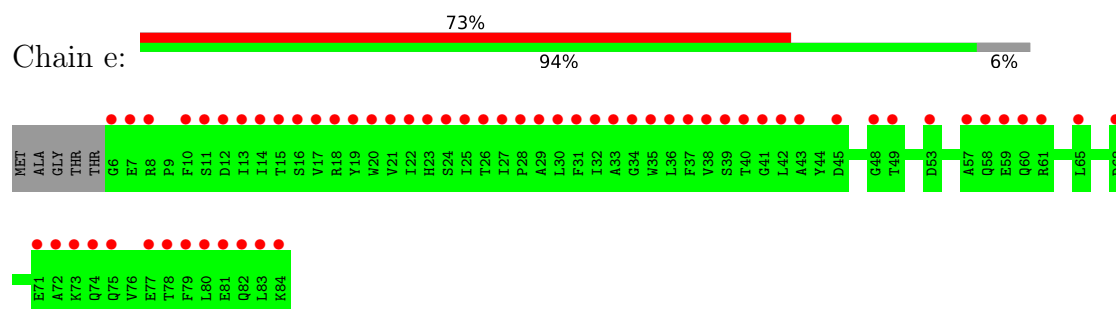
• Molecule 4: Photosystem II D2 protein



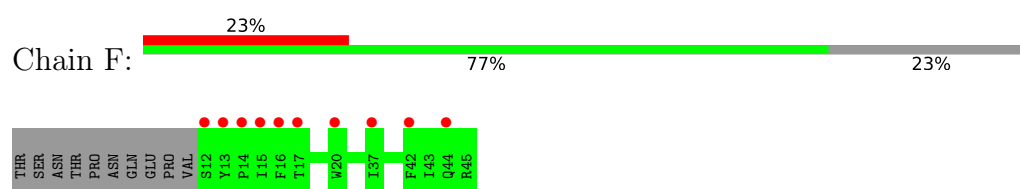
- Molecule 5: Cytochrome b559 subunit alpha



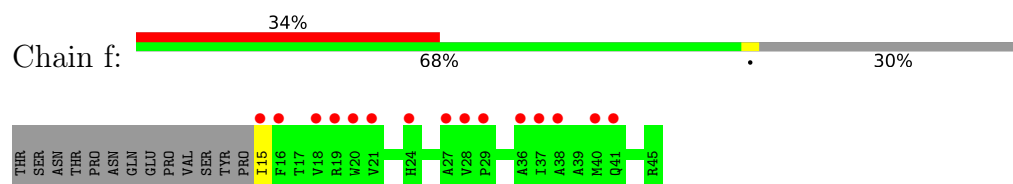
- Molecule 5: Cytochrome b559 subunit alpha



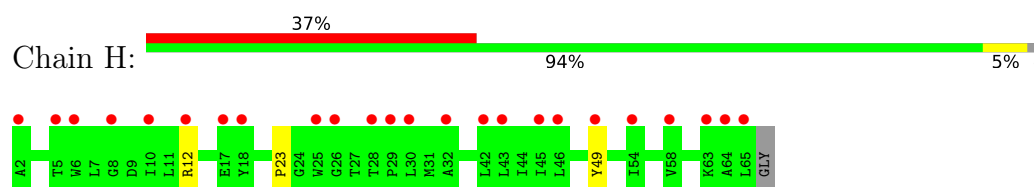
- Molecule 6: Cytochrome b559 subunit beta



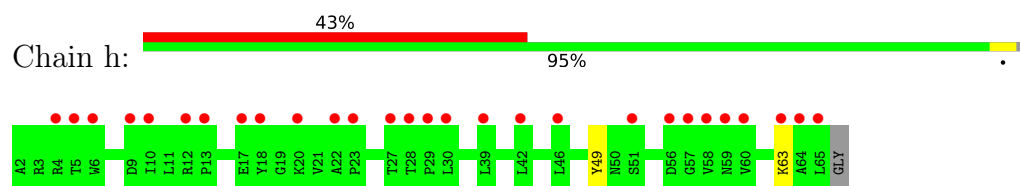
- Molecule 6: Cytochrome b559 subunit beta



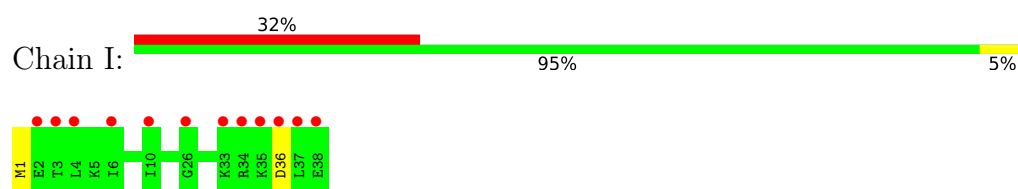
- Molecule 7: Photosystem II reaction center protein H



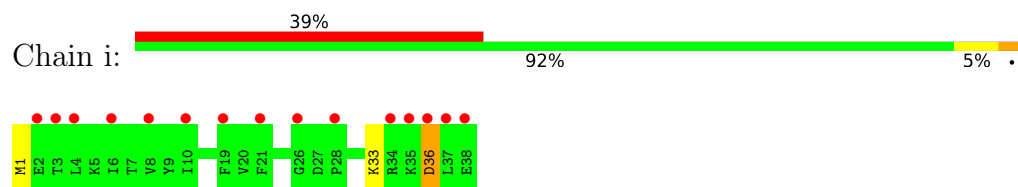
- Molecule 7: Photosystem II reaction center protein H



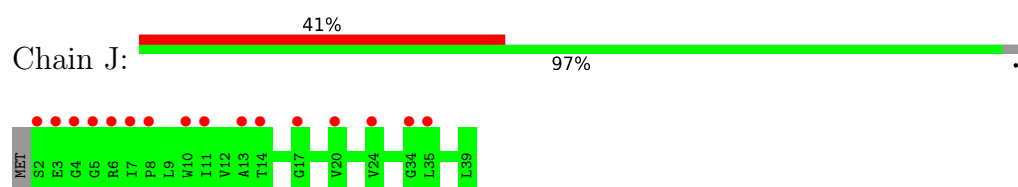
- Molecule 8: Photosystem II reaction center protein I



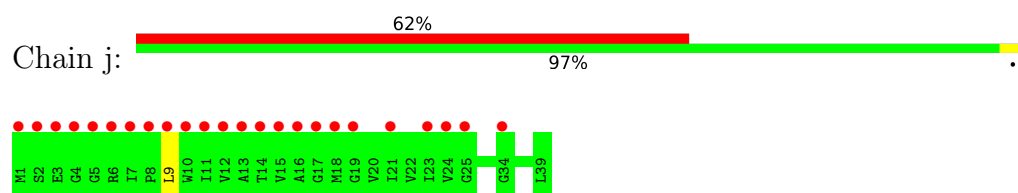
• Molecule 8: Photosystem II reaction center protein I



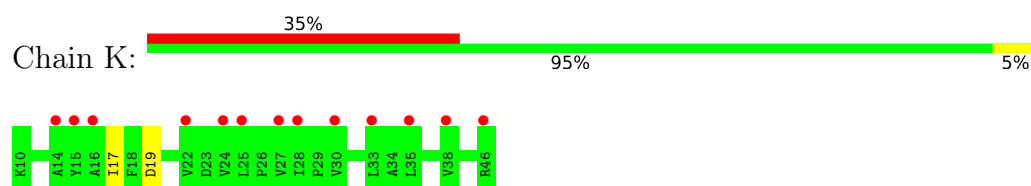
• Molecule 9: Photosystem II reaction center protein J



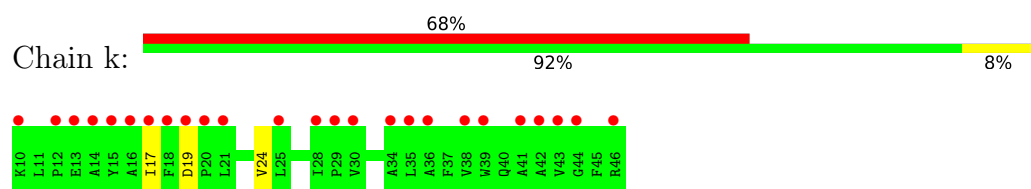
• Molecule 9: Photosystem II reaction center protein J



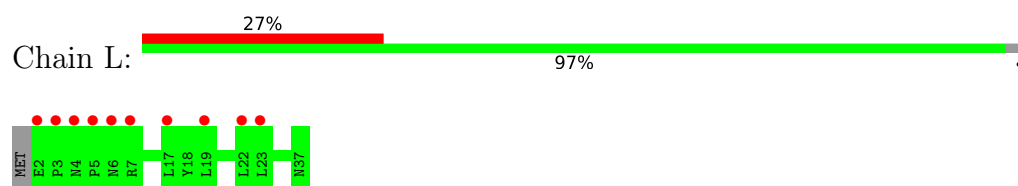
• Molecule 10: Photosystem II reaction center protein K



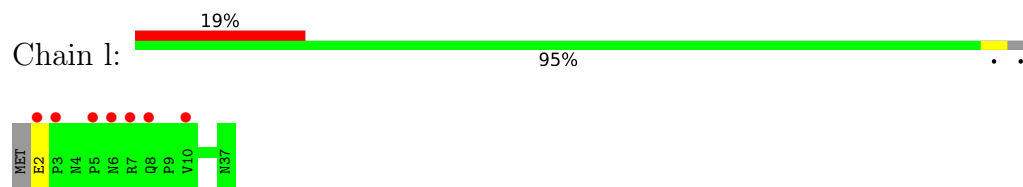
• Molecule 10: Photosystem II reaction center protein K



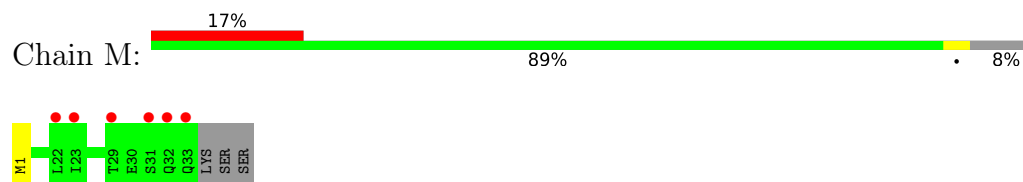
• Molecule 11: Photosystem II reaction center protein L



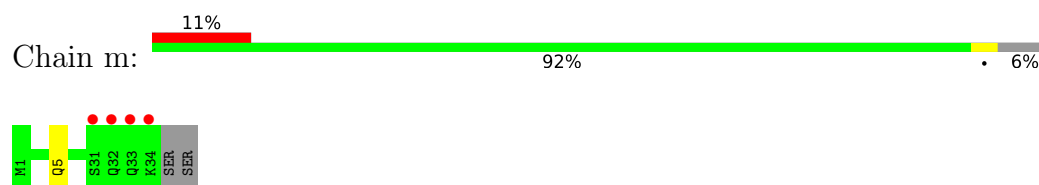
- Molecule 11: Photosystem II reaction center protein L



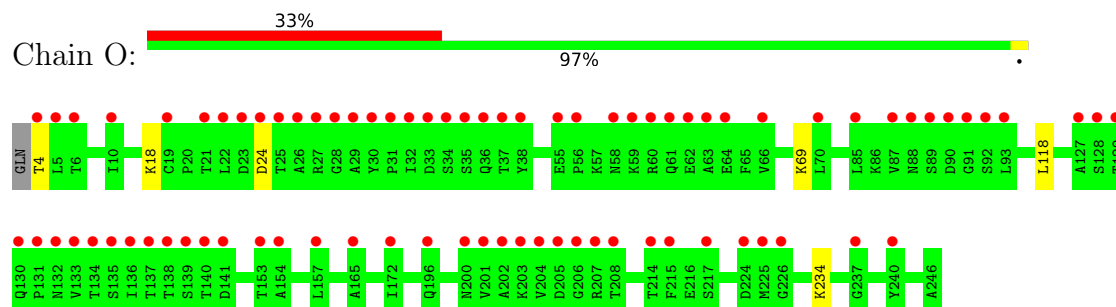
- Molecule 12: Photosystem II reaction center protein M



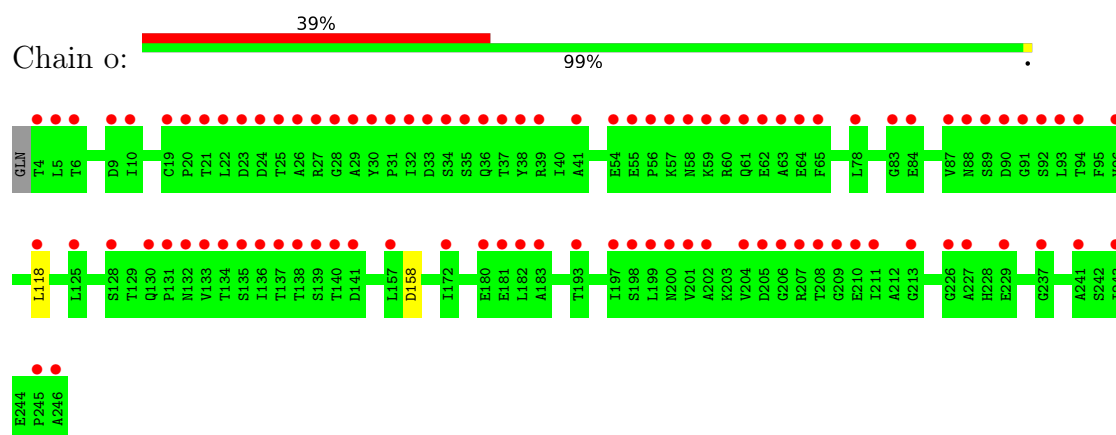
- Molecule 12: Photosystem II reaction center protein M



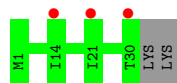
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



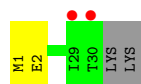
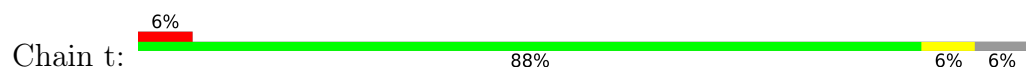
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



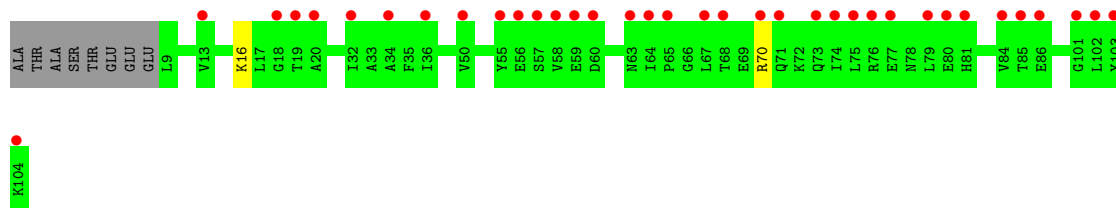
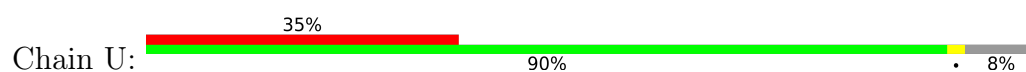
- Molecule 14: Photosystem II reaction center protein T



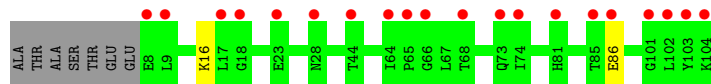
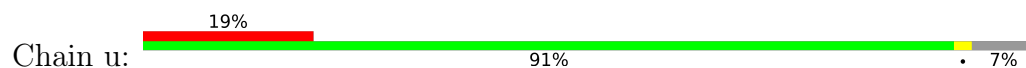
- Molecule 14: Photosystem II reaction center protein T



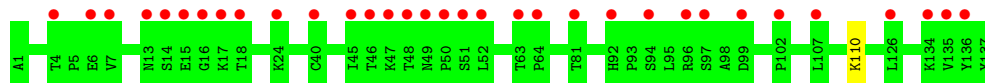
- Molecule 15: Photosystem II 12 kDa extrinsic protein



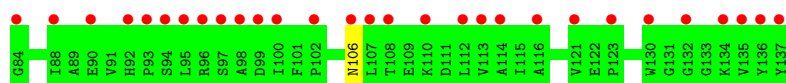
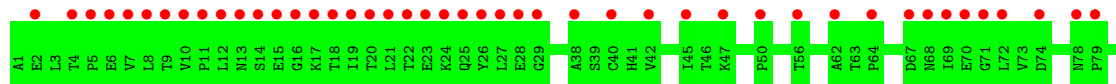
- Molecule 15: Photosystem II 12 kDa extrinsic protein



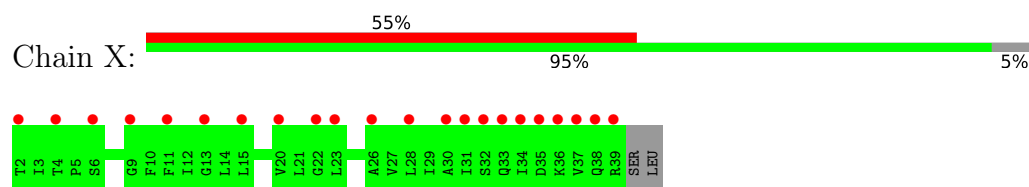
- Molecule 16: Cytochrome c-550



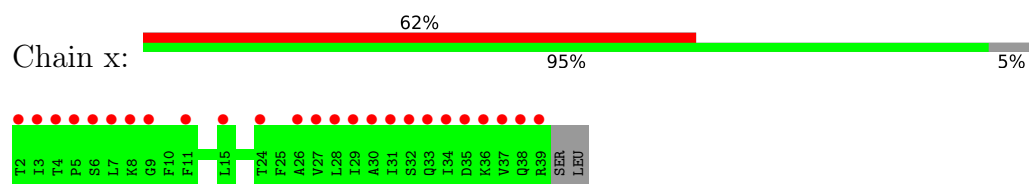
- Molecule 16: Cytochrome c-550



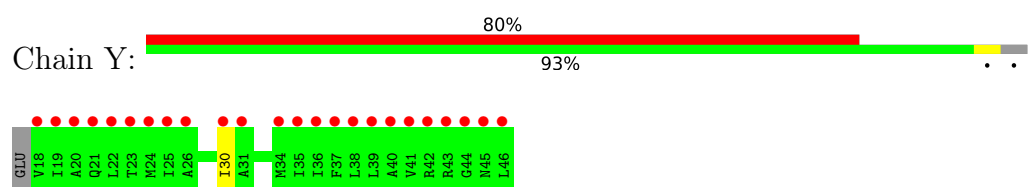
- Molecule 17: Photosystem II reaction center protein X



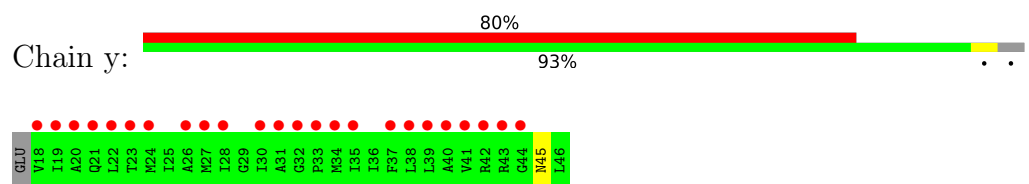
- Molecule 17: Photosystem II reaction center protein X



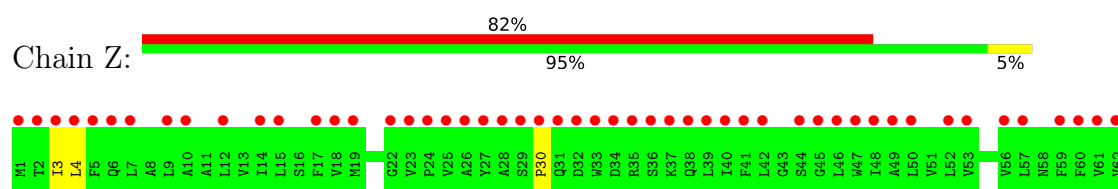
- Molecule 18: Photosystem II reaction center protein Ycf12



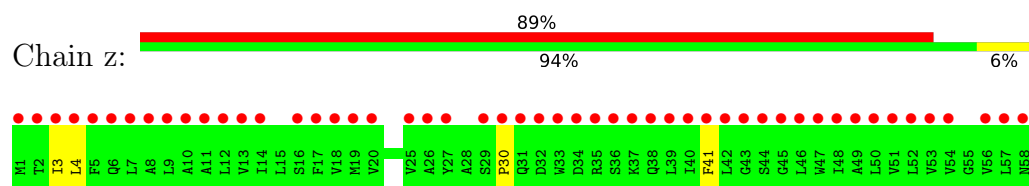
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



D2	D3	D4	D5	D6	D7	D8	D9	D10	D11	D12	D13	D14	D15	D16	D17	D18	D19	D20	D21	D22	D23	D24	D25	D26	D27	D28	D29	D30	D31	D32	D33	D34	D35
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.96Å 230.22Å 286.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 47.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 100.0 (47.05-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.129 , 0.175 0.136 , 0.179	Depositor DCC
$R_{free}$ test set	17119 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 80.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	53280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: MG, PL9, FME, LHG, BCT, BCR, OEY, CA, UNL, HEM, HEC, LMT, CLA, PHO, DGD, OEX, FE2, HTG, SQD, CL, GOL, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.50	0/2952	0.59	0/4019
1	a	0.43	0/2957	0.55	0/4027
2	B	0.43	0/4171	0.54	0/5683
2	b	0.41	0/4138	0.53	0/5640
3	C	0.42	0/3667	0.53	0/4992
3	c	0.38	0/3703	0.50	0/5041
4	D	0.46	0/2847	0.56	0/3878
4	d	0.43	0/2838	0.53	0/3866
5	E	0.36	0/687	0.50	0/936
5	e	0.35	0/667	0.47	0/908
6	F	0.42	0/284	0.50	0/387
6	f	0.38	0/257	0.53	0/349
7	H	0.37	0/530	0.57	0/723
7	h	0.33	0/519	0.50	0/708
8	I	0.37	0/311	0.48	0/419
8	i	0.34	0/311	0.49	0/419
9	J	0.34	0/278	0.46	0/376
9	j	0.32	0/283	0.46	0/383
10	K	0.37	0/303	0.51	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.43	0/311	0.47	0/423
11	l	0.41	0/311	0.49	0/423
12	M	0.45	0/261	0.61	0/357
12	m	0.42	0/262	0.59	0/357
13	O	0.39	0/1935	0.56	0/2623
13	o	0.39	0/1910	0.57	1/2589 (0.0%)
14	T	0.49	0/257	0.55	0/349
14	t	0.47	0/257	0.51	0/349
15	U	0.38	0/776	0.54	0/1052
15	u	0.37	0/785	0.54	0/1064
16	V	0.38	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.34	0/1085	0.48	0/1473
17	X	0.33	0/284	0.46	0/384
17	x	0.31	0/284	0.45	0/384
18	Y	0.29	0/216	0.44	0/289
18	y	0.30	0/216	0.47	0/289
19	Z	0.31	0/490	0.44	0/669
19	z	0.29	0/490	0.39	0/669
20	R	0.28	0/279	0.39	0/383
All	All	0.41	0/43500	0.53	1/59185 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	359/344 (104%)	355 (99%)	3 (1%)	1 (0%)	41	47
1	a	360/344 (105%)	355 (99%)	4 (1%)	1 (0%)	41	47
2	B	510/505 (101%)	506 (99%)	4 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	34	38
3	c	463/455 (102%)	449 (97%)	12 (3%)	2 (0%)	34	38
4	D	343/342 (100%)	333 (97%)	10 (3%)	0	100	100
4	d	342/342 (100%)	336 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9	8
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	2
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	7
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	7
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5316/5384 (99%)	5202 (98%)	104 (2%)	10 (0%)	47	56

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/279 (106%)	295 (100%)	0	100	100
1	a	296/279 (106%)	295 (100%)	1 (0%)	92	96
2	B	410/403 (102%)	405 (99%)	5 (1%)	71	82
2	b	406/403 (101%)	398 (98%)	8 (2%)	55	66
3	C	360/356 (101%)	357 (99%)	3 (1%)	81	89
3	c	364/356 (102%)	358 (98%)	6 (2%)	62	75
4	D	280/277 (101%)	279 (100%)	1 (0%)	91	95
4	d	279/277 (101%)	278 (100%)	1 (0%)	91	95
5	E	73/73 (100%)	73 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	31	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	55/54 (102%)	51 (93%)	4 (7%)	14	14
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	68
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	52
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	22
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	41
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	17
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	6
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	52
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	46
13	O	211/207 (102%)	205 (97%)	6 (3%)	43	53
13	o	208/207 (100%)	207 (100%)	1 (0%)	88	94
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	25 (96%)	1 (4%)	33	41
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	59
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	59
16	V	117/117 (100%)	116 (99%)	1 (1%)	78	87
16	v	117/117 (100%)	116 (99%)	1 (1%)	78	87
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	27	33
18	y	22/23 (96%)	21 (96%)	1 (4%)	27	33
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	41
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	22
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4416/4403 (100%)	4353 (99%)	63 (1%)	67	78

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	12	ASN

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Mol	Chain	Res	Type
14	t	2	GLU
2	b	485	GLU
13	o	118	LEU
18	y	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	223	GLN
3	c	201	ASN
13	o	130	GLN
2	b	331	ASN
4	d	83	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	$\# Z  > 2$
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.30	0
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.21	1 (14%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.37	0
14	FME	t	1	14	8,9,10	0.66	0	7,9,11	1.57	2 (28%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.06	1 (14%)
8	FME	i	1	8	8,9,10	0.65	0	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
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.72	117.64	124.78
14	t	1	FME	C-CA-N	2.26	113.81	109.73
12	M	1	FME	O-C-CA	-2.09	119.30	124.78
8	I	1	FME	O-C-CA	-2.05	119.39	124.78
8	i	1	FME	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	O-C-CA-CB
12	M	1	FME	O1-CN-N-CA
14	T	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 227 ligands modelled in this entry, 18 are monoatomic and 18 are unknown - leaving 191 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	HTG	b	625	-	19,19,19	1.09	2 (10%)	23,24,24	1.75	3 (13%)
24	CLA	B	614	2	65,73,73	1.96	17 (26%)	76,113,113	2.99	28 (36%)
24	CLA	c	512	3	65,73,73	2.03	16 (24%)	76,113,113	2.73	29 (38%)
34	LMT	b	630	-	25,25,36	0.52	1 (4%)	30,30,47	0.85	0
33	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.07	5 (8%)
24	CLA	B	613	2	65,73,73	2.02	16 (24%)	76,113,113	2.81	31 (40%)
31	PL9	D	405	-	55,55,55	0.67	2 (3%)	68,69,69	1.74	20 (29%)
34	LMT	B	630	-	25,25,36	0.43	0	30,30,47	0.73	1 (3%)
24	CLA	c	508	3	65,73,73	2.07	16 (24%)	76,113,113	2.67	30 (39%)
24	CLA	c	510	3	65,73,73	2.04	16 (24%)	76,113,113	2.78	26 (34%)
24	CLA	c	513	3	65,73,73	2.04	15 (23%)	76,113,113	2.80	28 (36%)
34	LMT	A	359	-	36,36,36	0.55	1 (2%)	47,47,47	0.86	0
31	PL9	A	416[A]	-	55,55,55	0.63	1 (1%)	68,69,69	2.01	23 (33%)
38	LHG	D	407	-	48,48,48	0.90	2 (4%)	51,54,54	0.99	3 (5%)
34	LMT	B	622	-	36,36,36	0.41	0	47,47,47	1.07	2 (4%)
33	LMG	Z	101	-	37,37,55	0.99	3 (8%)	45,45,63	1.48	7 (15%)
24	CLA	b	604	2	65,73,73	1.98	15 (23%)	76,113,113	2.75	26 (34%)
41	HEC	V	203	16	32,50,50	1.47	4 (12%)	24,82,82	1.51	4 (16%)
35	HTG	b	624	-	19,19,19	1.02	1 (5%)	23,24,24	1.37	1 (4%)
33	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.13	6 (10%)
33	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.18	6 (10%)
35	HTG	B	625	-	19,19,19	0.99	1 (5%)	23,24,24	1.60	3 (13%)
34	LMT	a	359	-	36,36,36	0.50	1 (2%)	47,47,47	0.90	2 (4%)
26	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.61	12 (21%)
24	CLA	C	503	3	65,73,73	2.01	15 (23%)	76,113,113	2.71	25 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.08	3 (6%)
38	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	4 (7%)
28	GOL	b	627	-	5,5,5	0.34	0	5,5,5	0.37	0
36	DGD	h	103	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	3 (3%)
28	GOL	V	202	-	5,5,5	0.37	0	5,5,5	0.35	0
24	CLA	C	506	3	65,73,73	2.00	16 (24%)	76,113,113	2.70	27 (35%)
24	CLA	b	601	42	65,73,73	2.10	16 (24%)	76,113,113	2.72	26 (34%)
24	CLA	B	608	2	65,73,73	2.00	15 (23%)	76,113,113	2.78	28 (36%)
25	PHO	a	405	-	51,69,69	1.80	9 (17%)	47,99,99	1.92	11 (23%)
26	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.54	10 (17%)
24	CLA	C	513	3	65,73,73	2.04	16 (24%)	76,113,113	2.76	27 (35%)
27	SQD	a	411	-	53,54,54	1.05	3 (5%)	62,65,65	1.25	7 (11%)
24	CLA	b	607	42	65,73,73	1.97	16 (24%)	76,113,113	2.86	27 (35%)
29	OEX	a	412[A]	42,3,1	0,15,15	-	-	-	-	-
24	CLA	C	509	3	65,73,73	2.09	17 (26%)	76,113,113	2.73	28 (36%)
38	LHG	a	419	-	41,41,48	1.03	2 (4%)	44,47,54	0.90	2 (4%)
41	HEC	v	203	16	32,50,50	1.49	4 (12%)	24,82,82	1.59	5 (20%)
33	LMG	j	101	40	51,51,55	0.88	2 (3%)	59,59,63	1.13	5 (8%)
26	BCR	c	517	-	41,41,41	1.04	1 (2%)	56,56,56	1.64	13 (23%)
24	CLA	B	607	42	65,73,73	1.96	15 (23%)	76,113,113	2.86	27 (35%)
24	CLA	c	504	3	65,73,73	1.97	17 (26%)	76,113,113	2.78	26 (34%)
26	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.57	14 (25%)
33	LMG	J	101	40	51,51,55	0.88	2 (3%)	59,59,63	0.90	3 (5%)
24	CLA	A	406	42	65,73,73	2.03	17 (26%)	76,113,113	2.78	31 (40%)
26	BCR	b	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.63	12 (21%)
24	CLA	c	503	3	65,73,73	2.05	16 (24%)	76,113,113	2.76	27 (35%)
24	CLA	C	508	42	65,73,73	2.00	16 (24%)	76,113,113	2.68	28 (36%)
34	LMT	b	622	-	25,25,36	0.46	0	30,30,47	0.70	0
35	HTG	b	628	-	19,19,19	0.91	2 (10%)	23,24,24	1.29	3 (13%)
39	HEM	E	103	5,6	41,50,50	1.31	5 (12%)	45,82,82	1.92	13 (28%)
38	LHG	l	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.10	3 (5%)
26	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	12 (21%)
34	LMT	I	101	-	36,36,36	0.48	1 (2%)	47,47,47	1.07	3 (6%)
26	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.50	8 (14%)
27	SQD	f	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.43	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	611	2	65,73,73	1.97	15 (23%)	76,113,113	2.88	29 (38%)
24	CLA	b	608	2	65,73,73	2.03	17 (26%)	76,113,113	2.78	31 (40%)
24	CLA	B	604	2	65,73,73	1.97	15 (23%)	76,113,113	2.73	28 (36%)
24	CLA	c	515	3	65,73,73	2.08	18 (27%)	76,113,113	2.78	29 (38%)
24	CLA	c	514	3	65,73,73	2.02	16 (24%)	76,113,113	2.77	30 (39%)
28	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.12	0
31	PL9	a	414[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.98	22 (32%)
24	CLA	B	601	42	65,73,73	2.06	15 (23%)	76,113,113	2.74	27 (35%)
23	BCT	A	403[B]	21	2,3,3	0.69	0	2,3,3	0.83	0
24	CLA	a	350	42	65,73,73	2.02	16 (24%)	76,113,113	2.86	26 (34%)
26	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.77	12 (21%)
36	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.16	5 (6%)
24	CLA	C	514	3	65,73,73	2.06	16 (24%)	76,113,113	2.75	26 (34%)
38	LHG	E	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.11	5 (11%)
24	CLA	B	612	2	65,73,73	1.97	18 (27%)	76,113,113	2.81	28 (36%)
28	GOL	A	412	-	5,5,5	0.40	0	5,5,5	0.35	0
34	LMT	E	102	-	36,36,36	0.47	0	47,47,47	0.82	0
24	CLA	c	506	42	65,73,73	2.06	17 (26%)	76,113,113	2.78	29 (38%)
26	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.71	15 (26%)
36	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.94	4 (5%)
24	CLA	b	610	42	65,73,73	2.08	17 (26%)	76,113,113	2.79	28 (36%)
35	HTG	c	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.35	1 (4%)
26	BCR	h	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	11 (19%)
35	HTG	B	623	-	19,19,19	0.97	1 (5%)	23,24,24	1.39	5 (21%)
23	BCT	a	420[A]	21	2,3,3	0.67	0	2,3,3	0.97	0
24	CLA	B	610	42	65,73,73	2.04	15 (23%)	76,113,113	2.78	29 (38%)
27	SQD	b	620	-	53,54,54	1.03	3 (5%)	62,65,65	1.47	9 (14%)
26	BCR	b	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.56	10 (17%)
29	OEX	A	414[A]	42,3,1	0,15,15	-	-	-	-	-
27	SQD	B	620	-	53,54,54	1.02	3 (5%)	62,65,65	1.40	8 (12%)
24	CLA	b	615	2	65,73,73	2.02	16 (24%)	76,113,113	2.77	27 (35%)
27	SQD	A	413	-	53,54,54	1.01	3 (5%)	62,65,65	1.10	6 (9%)
38	LHG	D	357	-	48,48,48	0.89	2 (4%)	51,54,54	1.20	5 (9%)
31	PL9	a	414[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.89	21 (30%)
38	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.09	5 (9%)
24	CLA	b	616	2	65,73,73	2.01	17 (26%)	76,113,113	2.80	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.83	0
24	CLA	b	602	2	65,73,73	2.06	16 (24%)	76,113,113	2.86	30 (39%)
35	HTG	c	526	-	19,19,19	1.03	2 (10%)	23,24,24	1.49	3 (13%)
24	CLA	A	409	1	65,73,73	2.01	17 (26%)	76,113,113	2.87	30 (39%)
35	HTG	B	624	-	19,19,19	0.90	1 (5%)	23,24,24	1.39	1 (4%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.19	4 (6%)
31	PL9	A	416[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.87	20 (29%)
36	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	6 (7%)
28	GOL	a	416	-	5,5,5	0.35	0	5,5,5	0.65	0
38	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	0.90	3 (5%)
30	OEY	a	413[B]	42,3,1	0,16,16	-	-	-	-	-
35	HTG	C	523	-	19,19,19	1.06	2 (10%)	23,24,24	1.82	5 (21%)
24	CLA	b	603	2	65,73,73	2.02	16 (24%)	76,113,113	2.83	26 (34%)
24	CLA	c	507	3	65,73,73	1.97	16 (24%)	76,113,113	2.64	25 (32%)
36	DGD	c	518	-	63,63,67	0.83	2 (3%)	77,77,81	1.09	4 (5%)
23	BCT	a	420[B]	21	2,3,3	0.66	0	2,3,3	0.86	0
24	CLA	b	609	2	65,73,73	2.02	17 (26%)	76,113,113	2.78	27 (35%)
24	CLA	B	603	2	65,73,73	2.00	16 (24%)	76,113,113	2.92	29 (38%)
26	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	11 (19%)
35	HTG	V	204	-	11,11,19	0.23	0	15,15,24	1.05	1 (6%)
24	CLA	b	605	2	65,73,73	1.95	18 (27%)	76,113,113	2.94	25 (32%)
24	CLA	B	609	2	65,73,73	1.99	16 (24%)	76,113,113	2.84	25 (32%)
24	CLA	B	616	2	65,73,73	2.02	16 (24%)	76,113,113	2.81	26 (34%)
24	CLA	d	402	4	65,73,73	1.97	17 (26%)	76,113,113	2.71	30 (39%)
24	CLA	C	507	3	65,73,73	2.05	18 (27%)	76,113,113	2.76	31 (40%)
24	CLA	c	505	3	65,73,73	2.01	16 (24%)	76,113,113	2.72	23 (30%)
26	BCR	A	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	11 (19%)
35	HTG	b	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.51	3 (13%)
27	SQD	A	411	-	53,54,54	0.94	3 (5%)	62,65,65	1.81	13 (20%)
24	CLA	b	614	2	65,73,73	1.96	16 (24%)	76,113,113	2.83	28 (36%)
26	BCR	b	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	16 (28%)
33	LMG	A	418	-	51,51,55	0.91	2 (3%)	59,59,63	1.21	5 (8%)
27	SQD	a	409	-	53,54,54	0.96	3 (5%)	62,65,65	1.78	13 (20%)
35	HTG	D	410	-	16,16,19	1.08	2 (12%)	20,21,24	1.36	1 (5%)
28	GOL	B	626	-	5,5,5	0.37	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	c	511	3	65,73,73	2.09	17 (26%)	76,113,113	2.74	28 (36%)
24	CLA	B	615	2	65,73,73	1.95	14 (21%)	76,113,113	2.83	28 (36%)
26	BCR	D	404	-	41,41,41	1.04	1 (2%)	56,56,56	1.84	18 (32%)
26	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.68	11 (19%)
34	LMT	M	103	-	36,36,36	0.42	0	47,47,47	0.95	2 (4%)
24	CLA	c	509	42	65,73,73	2.04	16 (24%)	76,113,113	2.78	26 (34%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
31	PL9	d	405	-	55,55,55	0.61	1 (1%)	68,69,69	1.73	19 (27%)
24	CLA	C	504	3	65,73,73	1.99	15 (23%)	76,113,113	2.78	23 (30%)
34	LMT	e	101	-	36,36,36	0.47	0	47,47,47	0.80	1 (2%)
24	CLA	b	611	2	65,73,73	1.99	16 (24%)	76,113,113	2.83	24 (31%)
24	CLA	B	605	2	65,73,73	1.98	16 (24%)	76,113,113	2.87	28 (36%)
24	CLA	C	502	3	65,73,73	2.02	17 (26%)	76,113,113	2.83	29 (38%)
35	HTG	C	522	-	19,19,19	1.00	1 (5%)	23,24,24	1.41	2 (8%)
39	HEM	e	102	5,6	41,50,50	1.28	5 (12%)	45,82,82	1.76	11 (24%)
24	CLA	d	403	4	65,73,73	2.04	16 (24%)	76,113,113	2.81	30 (39%)
28	GOL	v	202	-	5,5,5	0.37	0	5,5,5	0.29	0
24	CLA	A	404	1	65,73,73	2.05	17 (26%)	76,113,113	2.85	28 (36%)
24	CLA	B	602	2	65,73,73	2.07	16 (24%)	76,113,113	2.78	31 (40%)
34	LMT	m	102	-	36,36,36	0.42	0	47,47,47	0.87	1 (2%)
35	HTG	h	101	-	16,16,19	1.15	2 (12%)	20,21,24	1.62	2 (10%)
26	BCR	a	408	-	41,41,41	0.97	1 (2%)	56,56,56	1.56	11 (19%)
38	LHG	D	406	-	48,48,48	0.89	3 (6%)	51,54,54	0.99	3 (5%)
27	SQD	F	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.66	8 (15%)
24	CLA	A	405	42	65,73,73	2.01	16 (24%)	76,113,113	2.92	28 (36%)
36	DGD	c	520	-	63,63,67	0.82	2 (3%)	77,77,81	1.09	3 (3%)
24	CLA	B	606	2	65,73,73	1.93	16 (24%)	76,113,113	2.98	27 (35%)
26	BCR	d	404	-	41,41,41	1.14	1 (2%)	56,56,56	1.83	14 (25%)
24	CLA	a	407	1	65,73,73	2.00	17 (26%)	76,113,113	2.72	30 (39%)
28	GOL	a	410	-	5,5,5	0.36	0	5,5,5	0.35	0
28	GOL	c	502	-	5,5,5	0.41	0	5,5,5	0.31	0
26	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.75	14 (25%)
33	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.10	4 (8%)
33	LMG	b	621	-	51,51,55	0.86	2 (3%)	59,59,63	1.27	5 (8%)
25	PHO	A	407	-	51,69,69	1.82	7 (13%)	47,99,99	1.82	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	0.93	4 (5%)
24	CLA	a	403	1	65,73,73	2.05	15 (23%)	76,113,113	2.77	33 (43%)
26	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.62	12 (21%)
30	OEY	A	415[B]	42,3,1	0,16,16	-	-	-	-	-
24	CLA	C	512	3	65,73,73	2.06	17 (26%)	76,113,113	2.67	26 (34%)
23	BCT	A	403[A]	21	2,3,3	0.67	0	2,3,3	0.79	0
24	CLA	C	510	3	65,73,73	2.11	17 (26%)	76,113,113	2.78	28 (36%)
24	CLA	b	606	2	65,73,73	1.97	15 (23%)	76,113,113	2.83	30 (39%)
28	GOL	B	627	-	5,5,5	0.47	0	5,5,5	0.38	0
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.11	3 (5%)
35	HTG	B	628	-	19,19,19	0.97	2 (10%)	23,24,24	1.31	3 (13%)
36	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	0.94	4 (5%)
24	CLA	D	402	4	65,73,73	1.96	18 (27%)	76,113,113	2.88	29 (38%)
24	CLA	C	511	3	65,73,73	2.04	16 (24%)	76,113,113	2.82	29 (38%)
38	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
24	CLA	D	403	4	65,73,73	1.99	15 (23%)	76,113,113	2.81	29 (38%)
24	CLA	a	404	42	65,73,73	2.01	17 (26%)	76,113,113	2.81	28 (36%)
25	PHO	A	408	-	51,69,69	1.90	8 (15%)	47,99,99	2.02	11 (23%)
26	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.49	14 (25%)
26	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.75	14 (25%)
34	LMT	t	101	-	26,26,36	0.56	1 (3%)	31,31,47	1.14	2 (6%)
24	CLA	C	505	42	65,73,73	1.99	16 (24%)	76,113,113	2.79	32 (42%)
24	CLA	b	612	2	65,73,73	2.04	17 (26%)	76,113,113	2.67	27 (35%)
24	CLA	b	613	2	65,73,73	2.07	15 (23%)	76,113,113	2.73	27 (35%)
25	PHO	a	406	-	51,69,69	1.89	8 (15%)	47,99,99	2.07	13 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	b	625	-	-	2/10/30/30	0/1/1/1
24	CLA	B	614	2	1/1/15/20	13/37/115/115	-
24	CLA	c	512	3	1/1/15/20	8/37/115/115	-
34	LMT	b	630	-	-	9/17/37/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	c	521	-	-	8/46/66/70	0/1/1/1
24	CLA	B	613	2	1/1/15/20	6/37/115/115	-
31	PL9	D	405	-	-	15/53/73/73	0/1/1/1
34	LMT	B	630	-	-	11/17/37/61	0/1/1/2
24	CLA	c	508	3	1/1/15/20	13/37/115/115	-
24	CLA	c	510	3	1/1/15/20	4/37/115/115	-
24	CLA	c	513	3	1/1/15/20	5/37/115/115	-
34	LMT	A	359	-	-	4/21/61/61	0/2/2/2
31	PL9	A	416[A]	-	-	15/53/73/73	0/1/1/1
38	LHG	D	407	-	-	10/53/53/53	-
34	LMT	B	622	-	-	8/21/61/61	0/2/2/2
33	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
24	CLA	b	604	2	1/1/15/20	7/37/115/115	-
41	HEC	V	203	16	-	2/10/54/54	-
35	HTG	b	624	-	-	3/10/30/30	0/1/1/1
33	LMG	c	522	-	-	10/46/66/70	0/1/1/1
33	LMG	a	417	-	-	13/46/66/70	0/1/1/1
35	HTG	B	625	-	-	4/10/30/30	0/1/1/1
34	LMT	a	359	-	-	7/21/61/61	0/2/2/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	503	3	1/1/15/20	9/37/115/115	-
34	LMT	M	101	-	-	3/21/61/61	0/2/2/2
38	LHG	d	408	-	-	12/53/53/53	-
28	GOL	b	627	-	-	2/4/4/4	-
36	DGD	h	103	-	-	11/51/91/95	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-
24	CLA	C	506	3	1/1/15/20	7/37/115/115	-
24	CLA	b	601	42	1/1/15/20	16/37/115/115	-
24	CLA	B	608	2	-	4/37/115/115	-
25	PHO	a	405	-	-	2/37/103/103	0/5/6/6
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
24	CLA	C	513	3	1/1/15/20	9/37/115/115	-
27	SQD	a	411	-	-	15/49/69/69	0/1/1/1
24	CLA	b	607	42	1/1/15/20	2/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	a	419	-	-	9/46/46/53	-
24	CLA	C	509	3	1/1/15/20	4/37/115/115	-
41	HEC	v	203	16	-	2/10/54/54	-
33	LMG	j	101	40	-	9/46/66/70	0/1/1/1
26	BCR	c	517	-	-	4/29/63/63	0/2/2/2
24	CLA	B	607	42	1/1/15/20	4/37/115/115	-
24	CLA	c	504	3	1/1/15/20	7/37/115/115	-
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
33	LMG	J	101	40	-	11/46/66/70	0/1/1/1
24	CLA	A	406	42	1/1/15/20	4/37/115/115	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
24	CLA	c	503	3	1/1/15/20	4/37/115/115	-
24	CLA	C	508	42	1/1/15/20	6/37/115/115	-
34	LMT	b	622	-	-	5/17/37/61	0/1/1/2
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
39	HEM	E	103	5,6	-	5/12/54/54	-
38	LHG	l	101	-	-	16/53/53/53	-
26	BCR	K	102	-	-	2/29/63/63	0/2/2/2
34	LMT	I	101	-	-	9/21/61/61	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	SQD	f	101	-	-	13/38/58/69	0/1/1/1
24	CLA	B	611	2	1/1/15/20	3/37/115/115	-
24	CLA	c	515	3	1/1/15/20	7/37/115/115	-
24	CLA	B	604	2	1/1/15/20	11/37/115/115	-
24	CLA	b	608	2	-	2/37/115/115	-
24	CLA	c	514	3	1/1/15/20	9/37/115/115	-
28	GOL	C	525	-	-	2/4/4/4	-
31	PL9	a	414[A]	-	-	16/53/73/73	0/1/1/1
24	CLA	B	601	42	1/1/15/20	12/37/115/115	-
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
24	CLA	a	350	42	1/1/15/20	7/37/115/115	-
36	DGD	C	517	-	-	15/51/91/95	0/2/2/2
24	CLA	C	514	3	1/1/15/20	9/37/115/115	-
38	LHG	E	101	-	-	16/46/46/53	-
24	CLA	B	612	2	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	A	412	-	-	2/4/4/4	-
34	LMT	E	102	-	-	9/21/61/61	0/2/2/2
24	CLA	c	506	42	1/1/15/20	6/37/115/115	-
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
36	DGD	c	519	-	-	11/51/91/95	0/2/2/2
24	CLA	b	610	42	1/1/15/20	7/37/115/115	-
35	HTG	c	523	-	-	4/10/30/30	0/1/1/1
26	BCR	h	102	-	-	2/29/63/63	0/2/2/2
35	HTG	B	623	-	-	2/10/30/30	0/1/1/1
24	CLA	B	610	42	1/1/15/20	8/37/115/115	-
27	SQD	b	620	-	-	20/49/69/69	0/1/1/1
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	SQD	B	620	-	-	17/49/69/69	0/1/1/1
24	CLA	b	615	2	1/1/15/20	4/37/115/115	-
27	SQD	A	413	-	-	7/49/69/69	0/1/1/1
38	LHG	D	357	-	-	14/53/53/53	-
31	PL9	a	414[B]	-	-	21/53/73/73	0/1/1/1
38	LHG	d	406	-	-	8/53/53/53	-
24	CLA	b	616	2	1/1/15/20	12/37/115/115	-
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
24	CLA	b	602	2	1/1/15/20	4/37/115/115	-
35	HTG	c	526	-	-	1/10/30/30	0/1/1/1
24	CLA	A	409	1	-	10/37/115/115	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
33	LMG	C	521	-	-	10/46/66/70	0/1/1/1
31	PL9	A	416[B]	-	-	18/53/73/73	0/1/1/1
36	DGD	C	518	-	-	10/51/91/95	0/2/2/2
28	GOL	a	416	-	-	3/4/4/4	-
38	LHG	d	407	-	-	15/53/53/53	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
24	CLA	b	603	2	1/1/15/20	5/37/115/115	-
24	CLA	c	507	3	1/1/15/20	3/37/115/115	-
36	DGD	c	518	-	-	21/51/91/95	0/2/2/2
24	CLA	b	609	2	1/1/15/20	6/37/115/115	-
24	CLA	B	603	2	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
35	HTG	V	204	-	-	0/2/19/30	0/1/1/1
24	CLA	b	605	2	1/1/15/20	5/37/115/115	-
24	CLA	B	609	2	1/1/15/20	6/37/115/115	-
24	CLA	B	616	2	1/1/15/20	8/37/115/115	-
24	CLA	d	402	4	1/1/15/20	4/37/115/115	-
24	CLA	C	507	3	1/1/15/20	11/37/115/115	-
24	CLA	c	505	3	1/1/15/20	1/37/115/115	-
26	BCR	A	410	-	-	1/29/63/63	0/2/2/2
35	HTG	b	623	-	-	6/10/30/30	0/1/1/1
27	SQD	A	411	-	-	15/49/69/69	0/1/1/1
24	CLA	b	614	2	1/1/15/20	13/37/115/115	-
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
33	LMG	A	418	-	-	10/46/66/70	0/1/1/1
27	SQD	a	409	-	-	12/49/69/69	0/1/1/1
35	HTG	D	410	-	-	0/7/27/30	0/1/1/1
28	GOL	B	626	-	-	4/4/4/4	-
24	CLA	c	511	3	1/1/15/20	10/37/115/115	-
24	CLA	B	615	2	1/1/15/20	10/37/115/115	-
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
26	BCR	y	101	-	-	6/29/63/63	0/2/2/2
34	LMT	M	103	-	-	7/21/61/61	0/2/2/2
24	CLA	c	509	42	1/1/15/20	9/37/115/115	-
33	LMG	C	520	-	-	14/46/66/70	0/1/1/1
31	PL9	d	405	-	-	9/53/73/73	0/1/1/1
24	CLA	C	504	3	-	3/37/115/115	-
34	LMT	e	101	-	-	6/21/61/61	0/2/2/2
24	CLA	b	611	2	1/1/15/20	3/37/115/115	-
24	CLA	B	605	2	1/1/15/20	7/37/115/115	-
24	CLA	C	502	3	1/1/15/20	6/37/115/115	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
39	HEM	e	102	5,6	-	7/12/54/54	-
24	CLA	d	403	4	1/1/15/20	6/37/115/115	-
28	GOL	v	202	-	-	2/4/4/4	-
24	CLA	A	404	1	1/1/15/20	1/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	602	2	1/1/15/20	7/37/115/115	-
34	LMT	m	102	-	-	5/21/61/61	0/2/2/2
35	HTG	h	101	-	-	0/7/27/30	0/1/1/1
26	BCR	a	408	-	-	0/29/63/63	0/2/2/2
38	LHG	D	406	-	-	16/53/53/53	-
27	SQD	F	101	-	-	10/38/58/69	0/1/1/1
24	CLA	A	405	42	1/1/15/20	6/37/115/115	-
36	DGD	c	520	-	-	11/51/91/95	0/2/2/2
24	CLA	B	606	2	1/1/15/20	7/37/115/115	-
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
24	CLA	a	407	1	1/1/15/20	8/37/115/115	-
28	GOL	a	410	-	-	4/4/4/4	-
28	GOL	c	502	-	-	0/4/4/4	-
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
33	LMG	b	621	-	-	10/46/66/70	0/1/1/1
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
36	DGD	H	102	-	-	15/51/91/95	0/2/2/2
24	CLA	a	403	1	1/1/15/20	1/37/115/115	-
26	BCR	C	516	-	-	1/29/63/63	0/2/2/2
24	CLA	C	512	3	1/1/15/20	5/37/115/115	-
24	CLA	C	510	3	1/1/15/20	4/37/115/115	-
24	CLA	b	606	2	1/1/15/20	10/37/115/115	-
28	GOL	B	627	-	-	3/4/4/4	-
33	LMG	B	621	-	-	12/46/66/70	0/1/1/1
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
36	DGD	C	519	-	-	11/51/91/95	0/2/2/2
24	CLA	D	402	4	1/1/15/20	0/37/115/115	-
24	CLA	C	511	3	1/1/15/20	10/37/115/115	-
38	LHG	L	101	-	-	13/53/53/53	-
24	CLA	D	403	4	1/1/15/20	10/37/115/115	-
24	CLA	a	404	42	-	3/37/115/115	-
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
34	LMT	t	101	-	-	5/17/38/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	505	42	1/1/15/20	6/37/115/115	-
24	CLA	b	612	2	1/1/15/20	6/37/115/115	-
24	CLA	b	613	2	1/1/15/20	8/37/115/115	-
25	PHO	a	406	-	-	2/37/103/103	0/5/6/6

The worst 5 of 1335 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3B-C2B	6.97	1.50	1.40
24	B	613	CLA	C3B-C2B	6.61	1.49	1.40
24	B	612	CLA	C3B-C2B	6.52	1.49	1.40
25	A	408	PHO	C3B-C2B	6.46	1.49	1.40
24	A	404	CLA	C3B-C2B	6.46	1.49	1.40

The worst 5 of 2685 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	404	CLA	C1D-ND-C4D	-10.11	99.15	106.33
24	b	605	CLA	C1D-ND-C4D	-10.02	99.22	106.33
24	c	513	CLA	C1D-ND-C4D	-9.98	99.24	106.33
24	B	614	CLA	C1D-ND-C4D	-9.96	99.26	106.33
24	a	350	CLA	C1D-ND-C4D	-9.84	99.34	106.33

5 of 65 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	404	CLA	ND
24	A	405	CLA	ND
24	A	406	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND

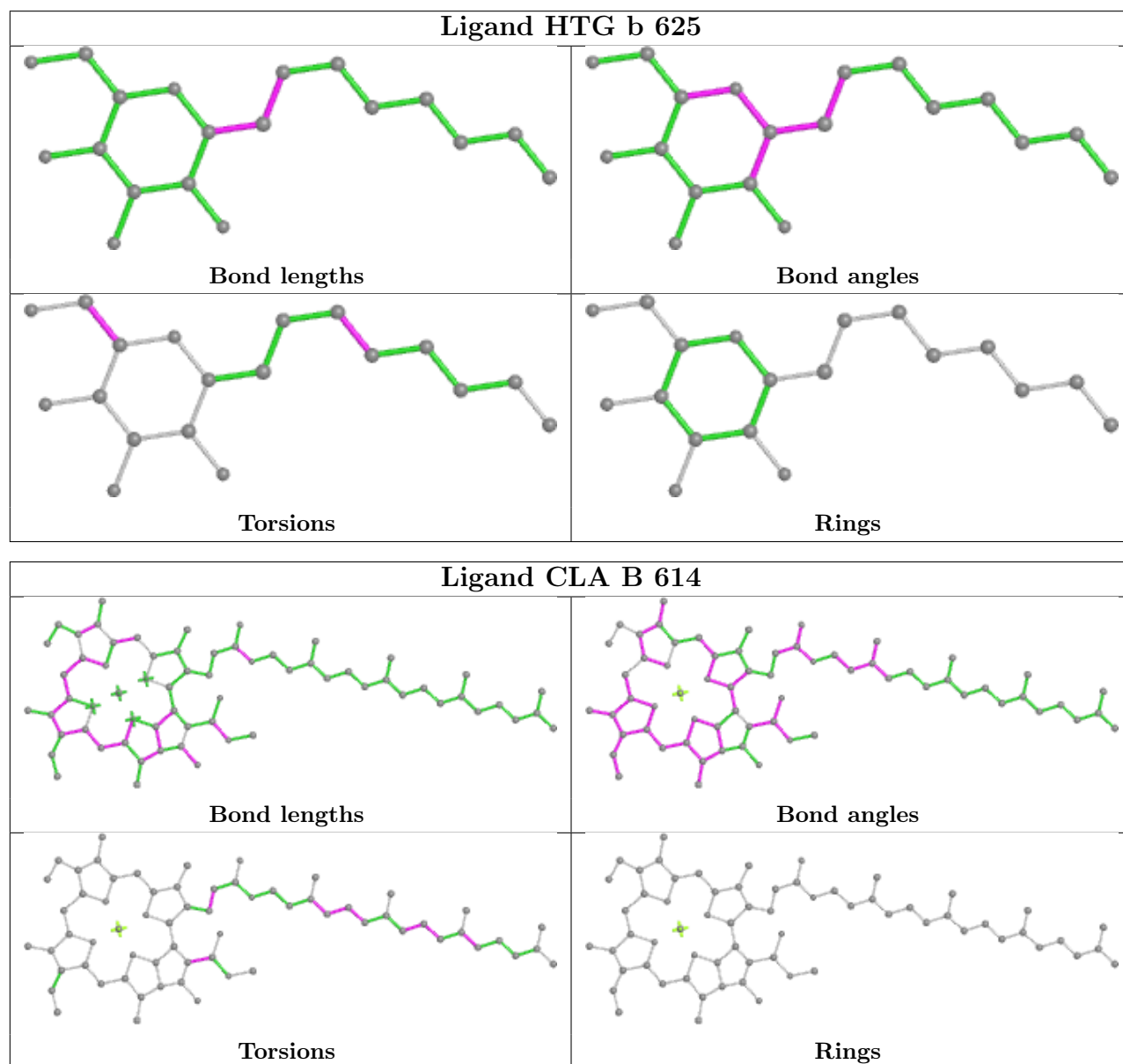
5 of 1239 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D

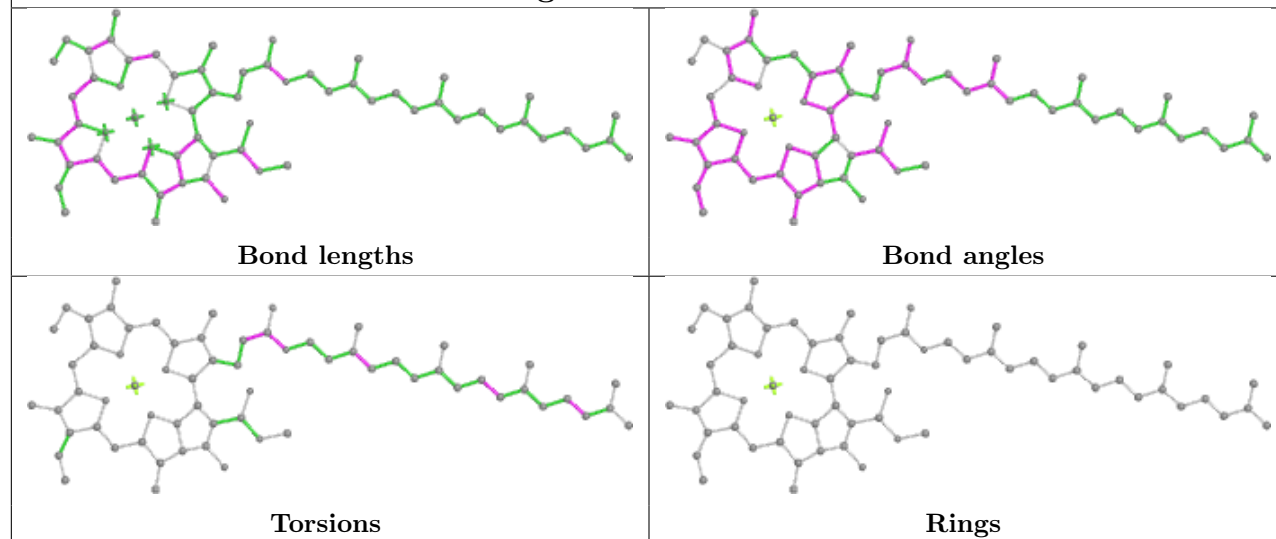
There are no ring outliers.

No monomer is involved in short contacts.

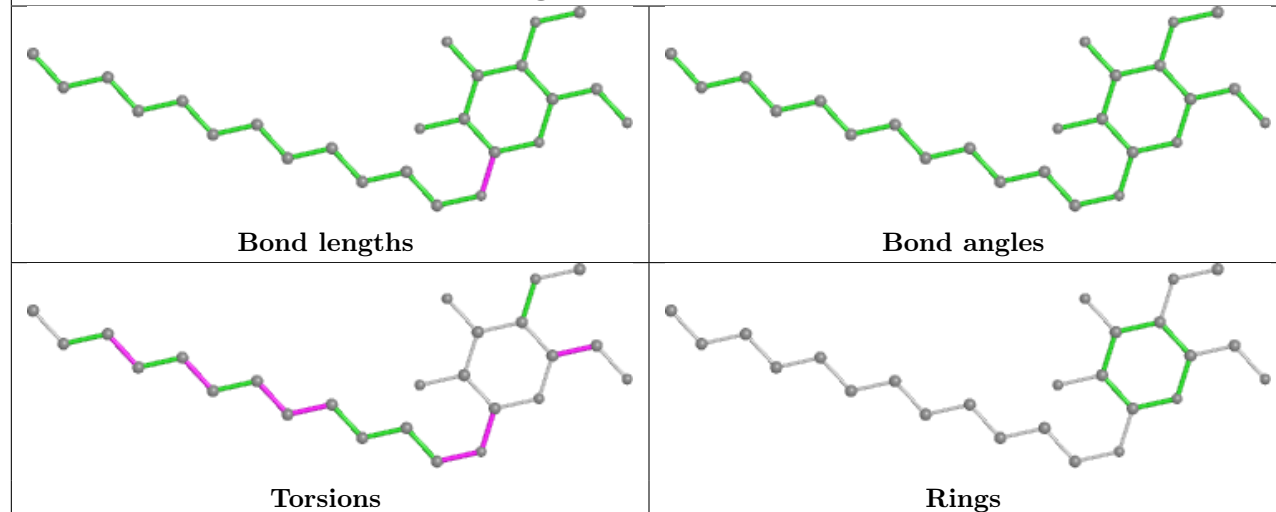
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



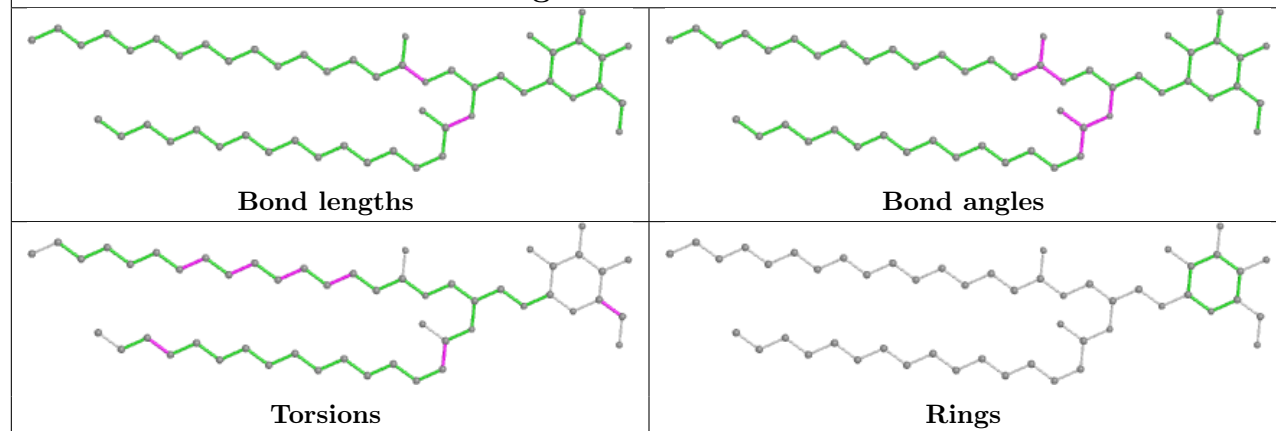
## Ligand CLA c 512

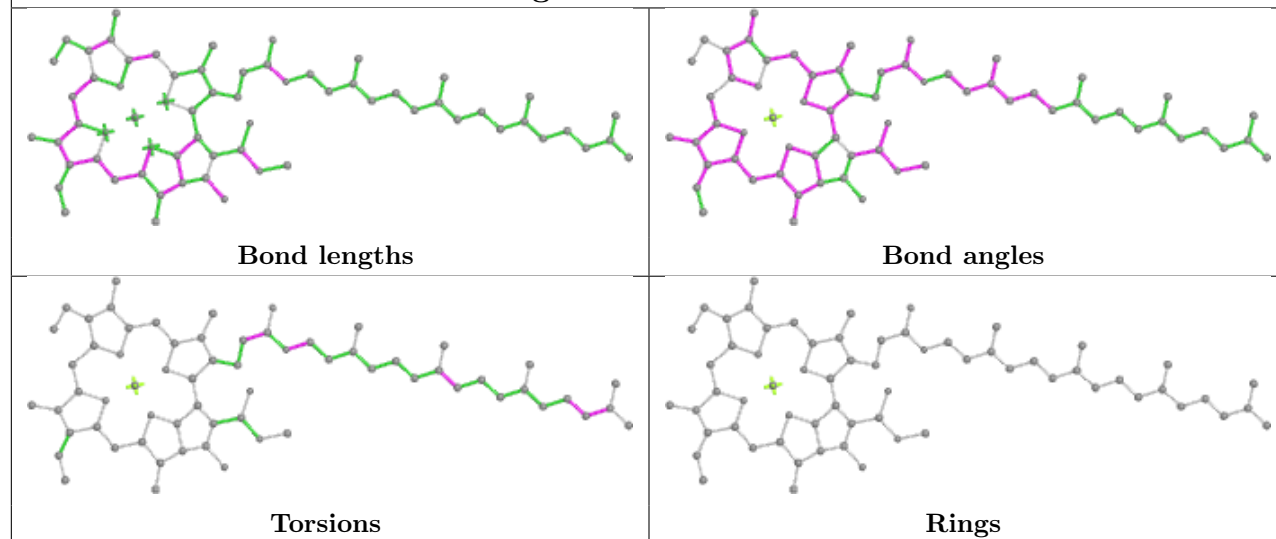
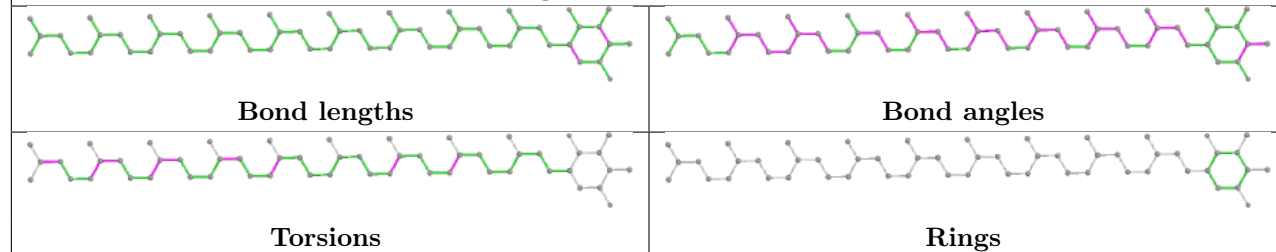
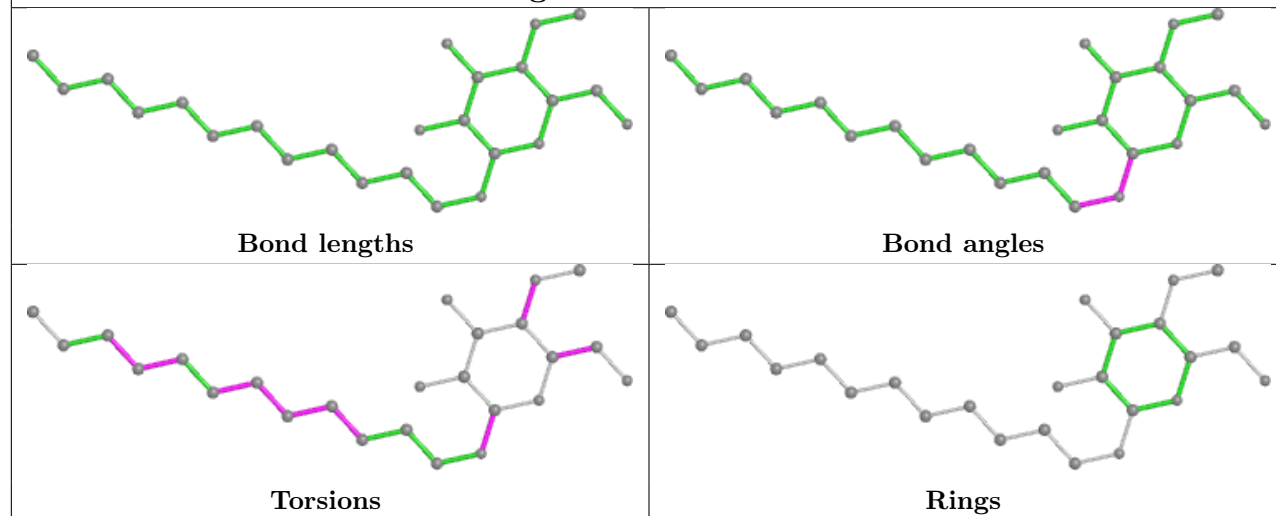


## Ligand LMT b 630

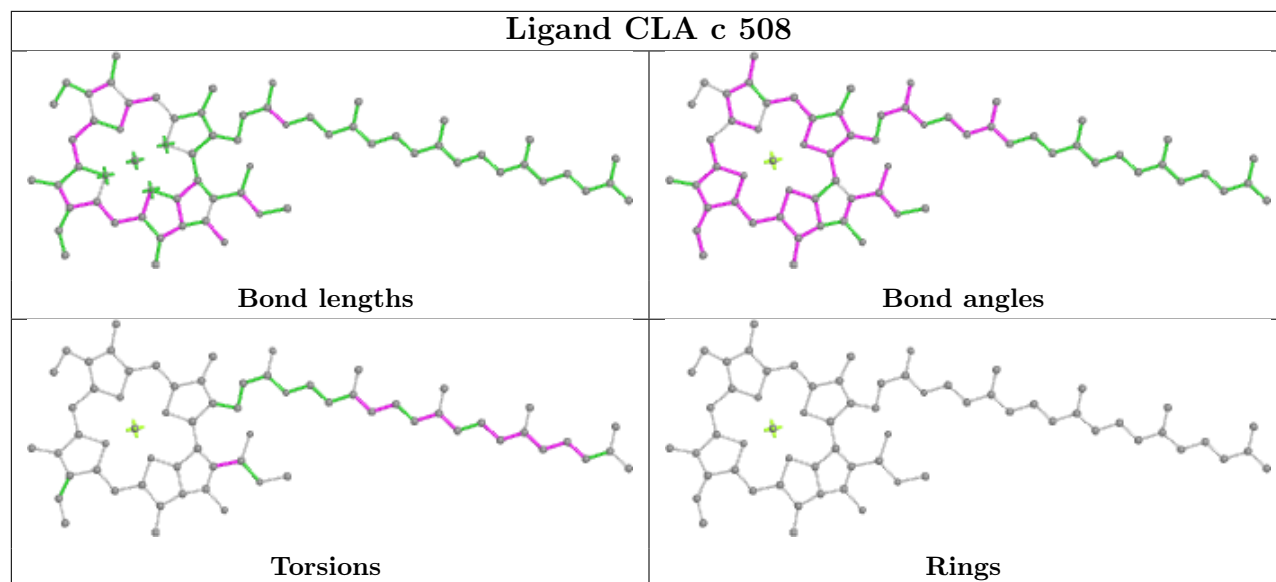


## Ligand LMG c 521

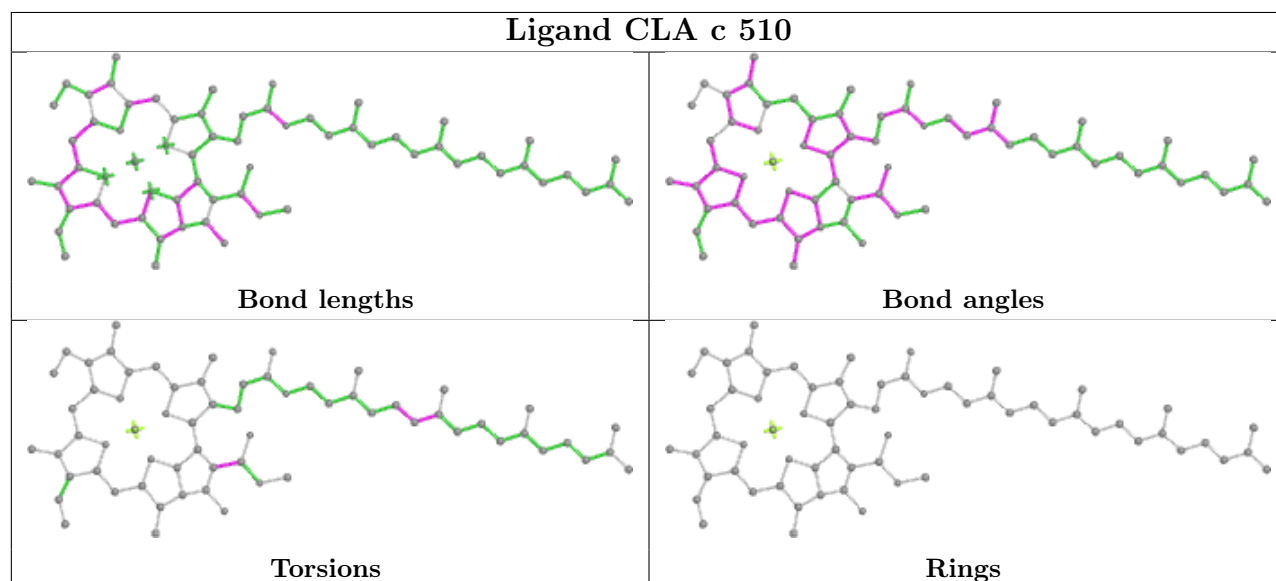


**Ligand CLA B 613****Ligand PL9 D 405****Ligand LMT B 630**

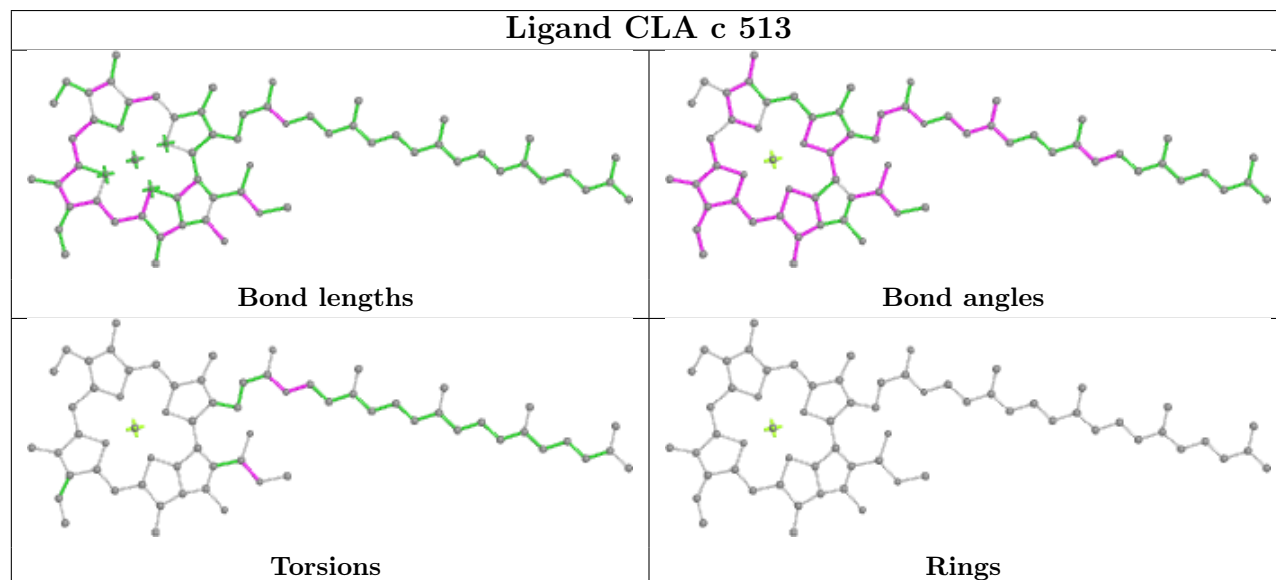
## Ligand CLA c 508

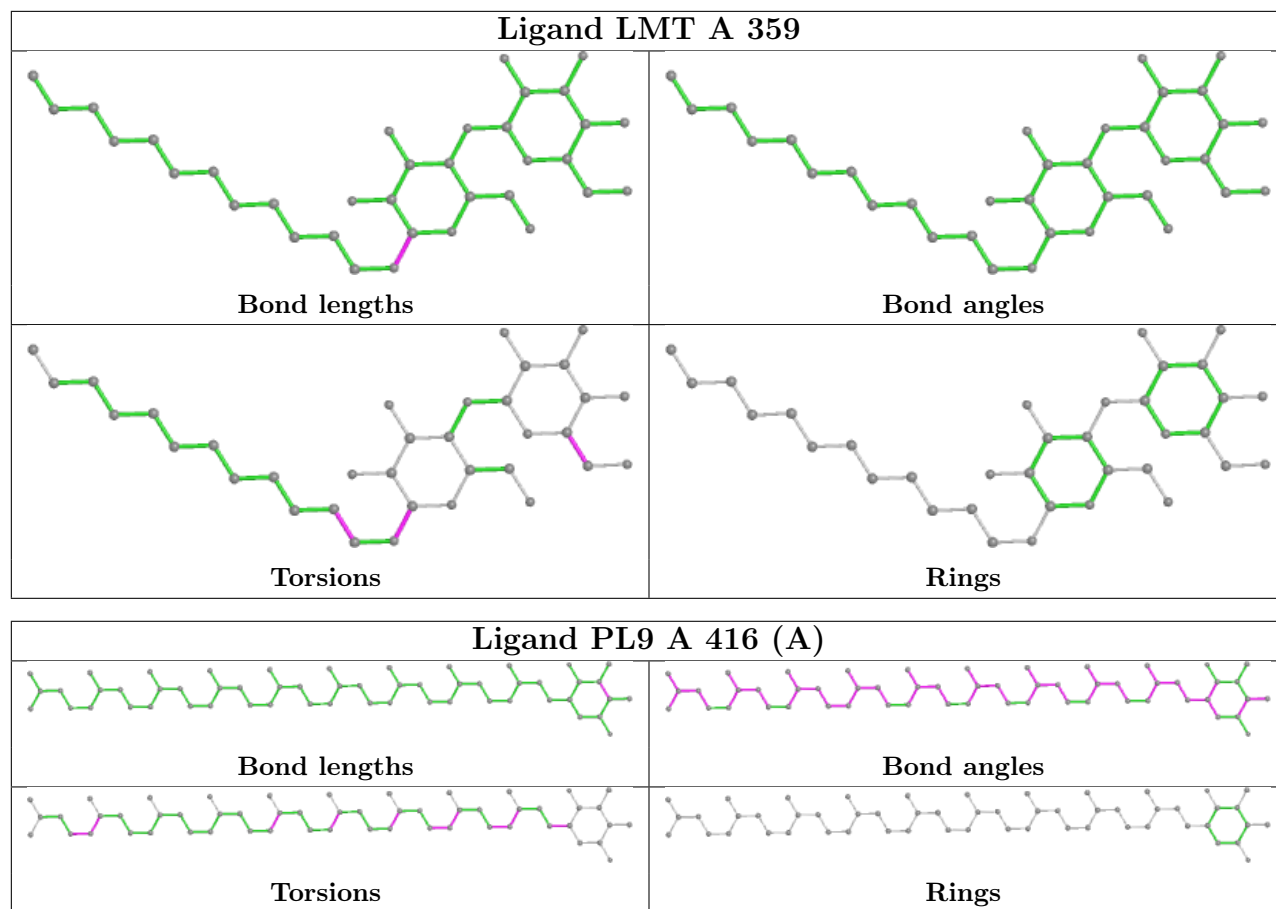


## Ligand CLA c 510

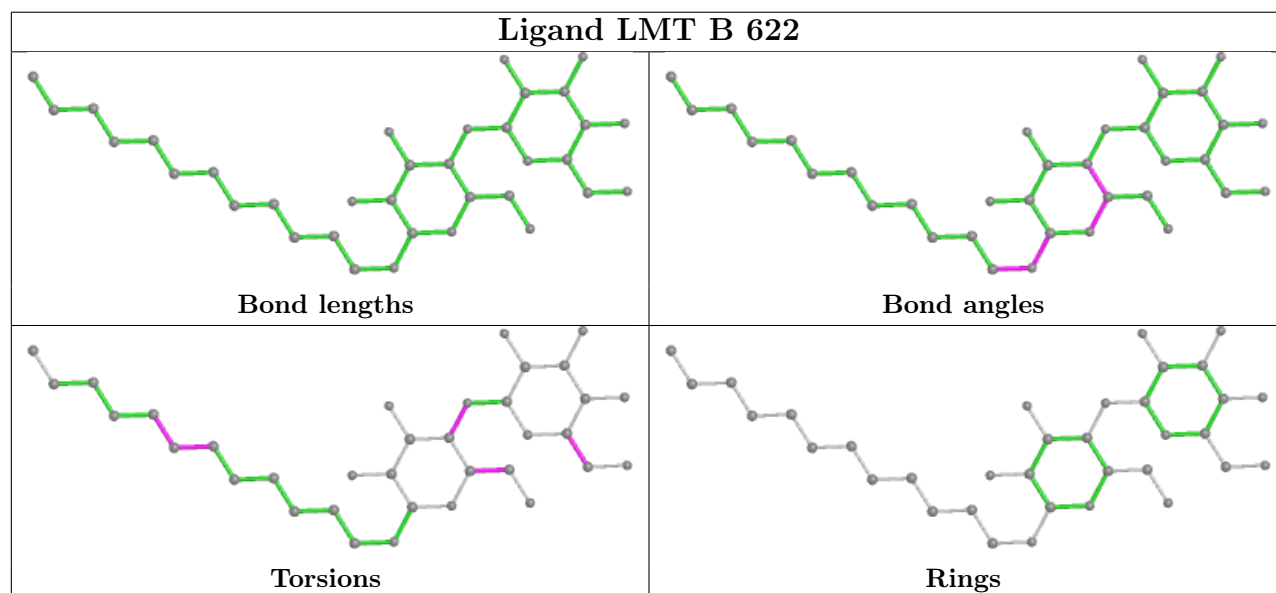
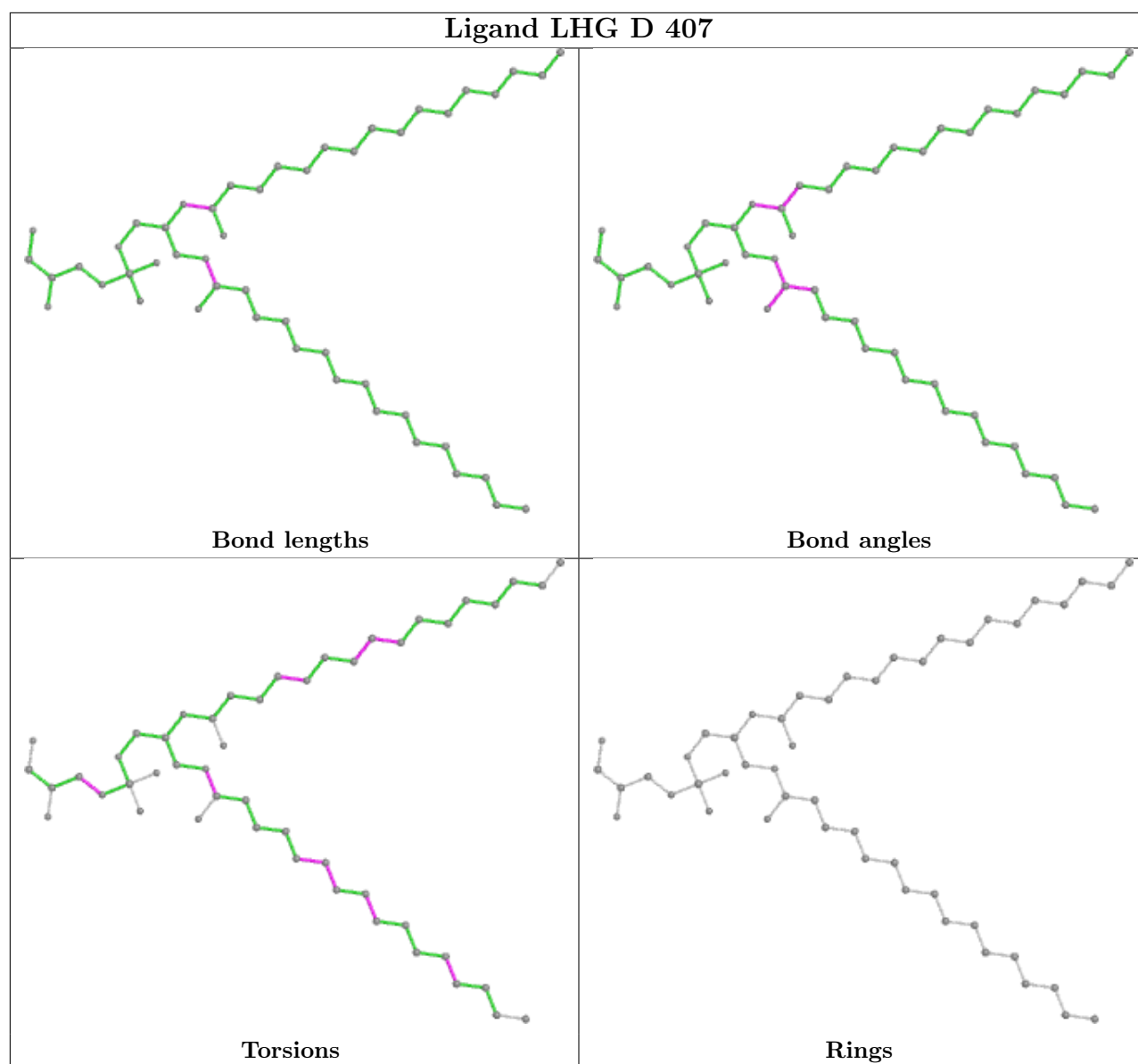


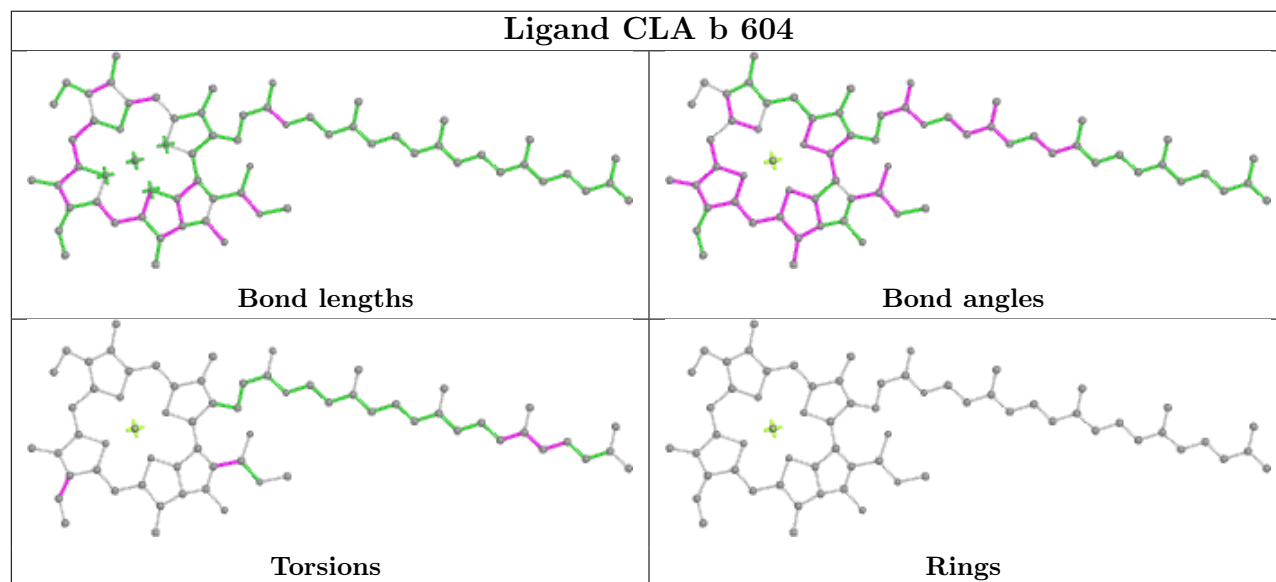
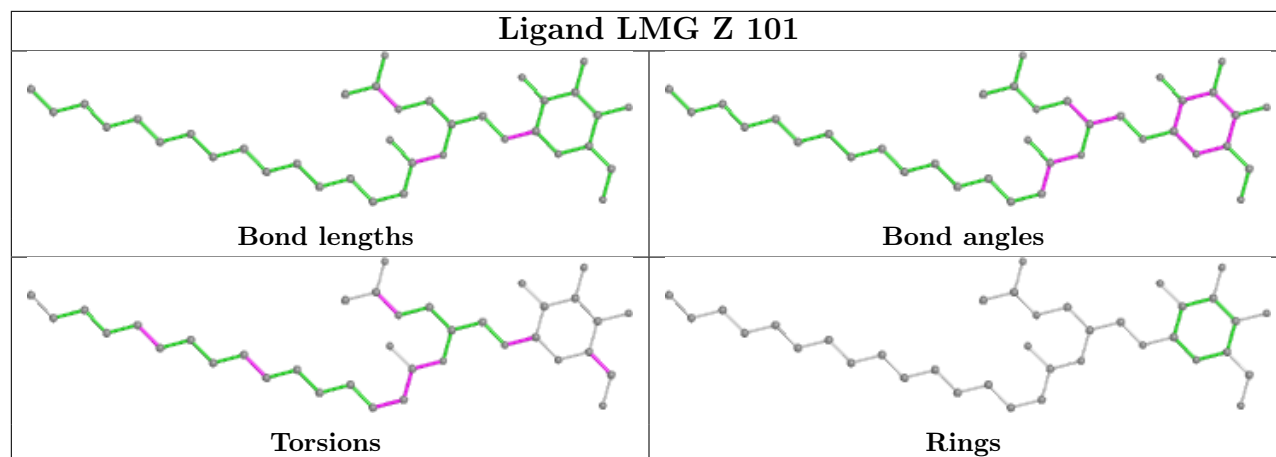
## Ligand CLA c 513



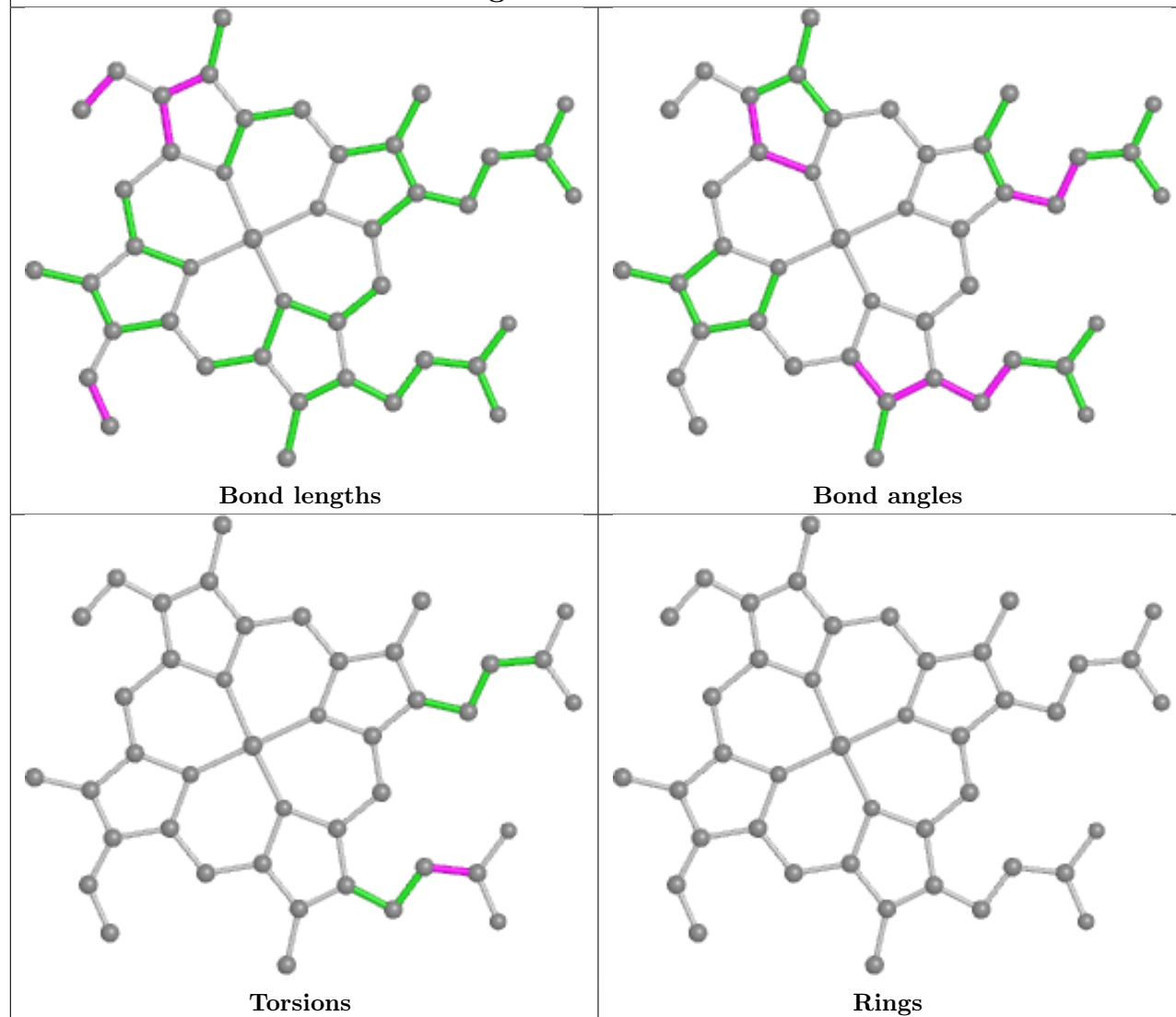




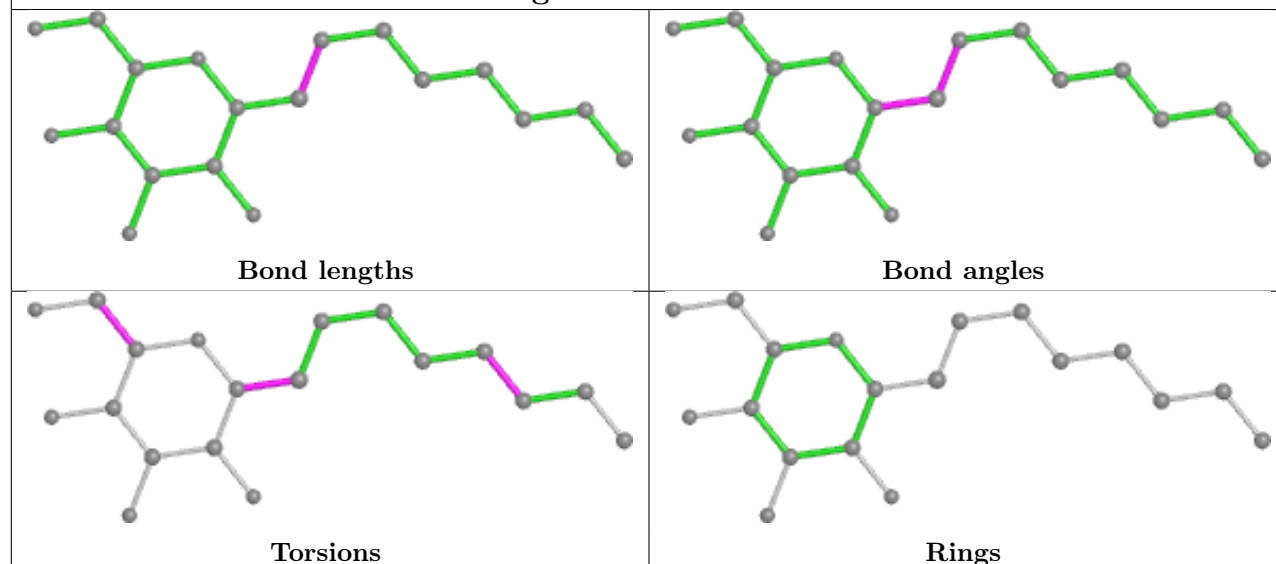




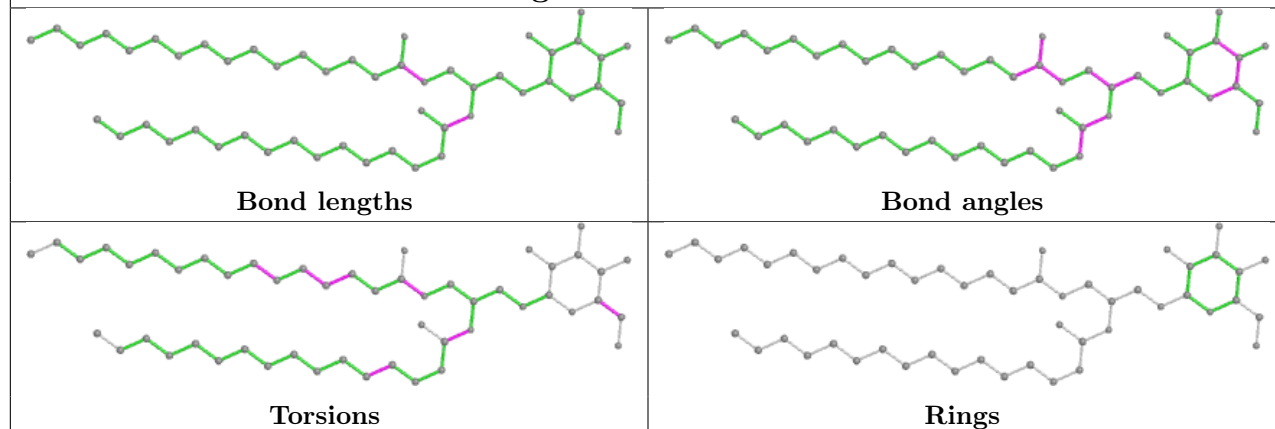
## Ligand HEC V 203



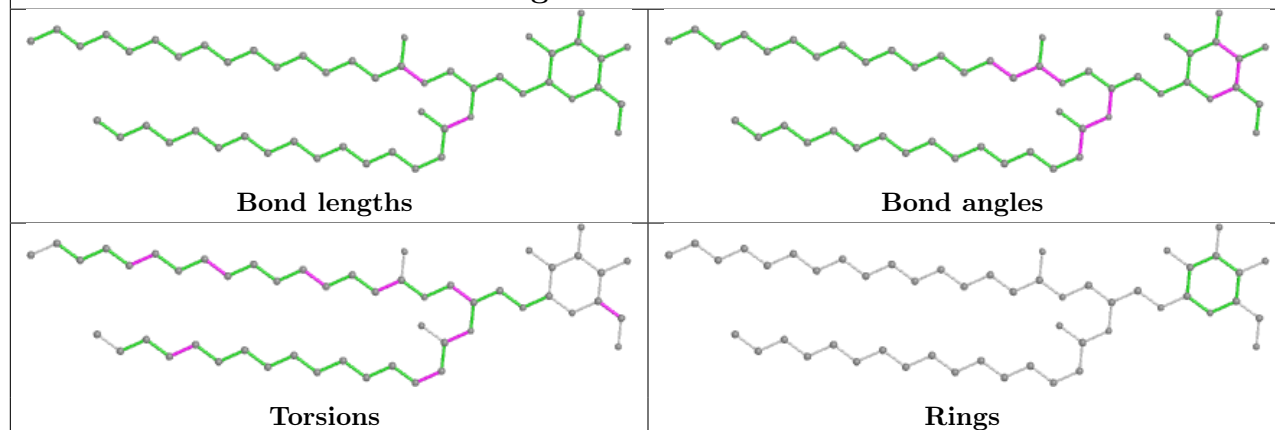
## Ligand HTG b 624



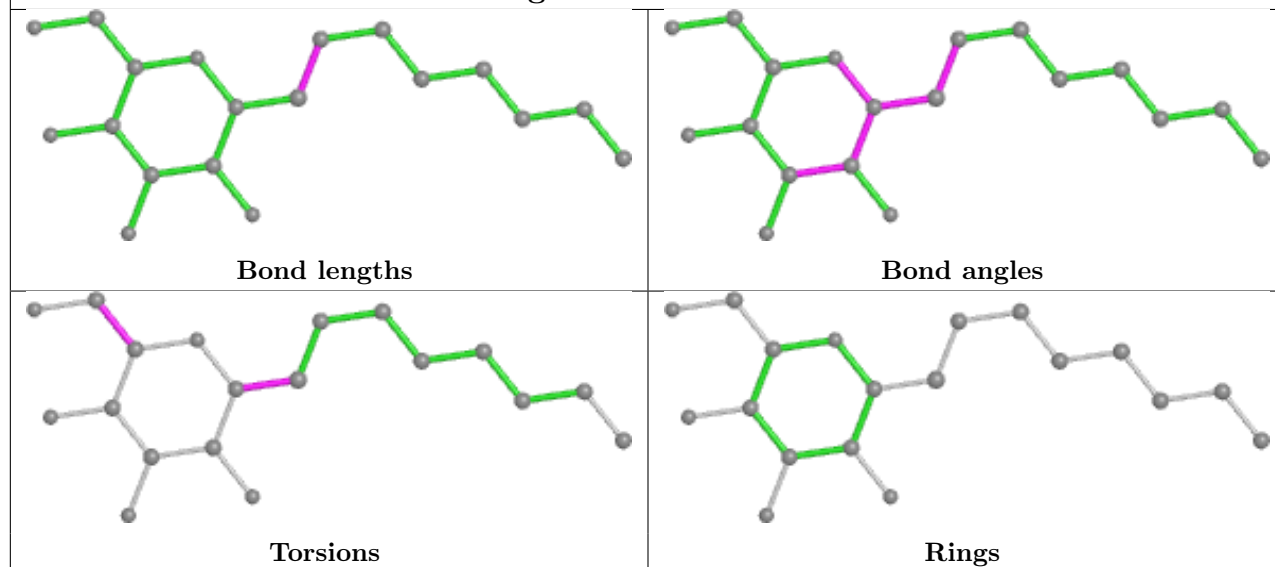
## Ligand LMG c 522

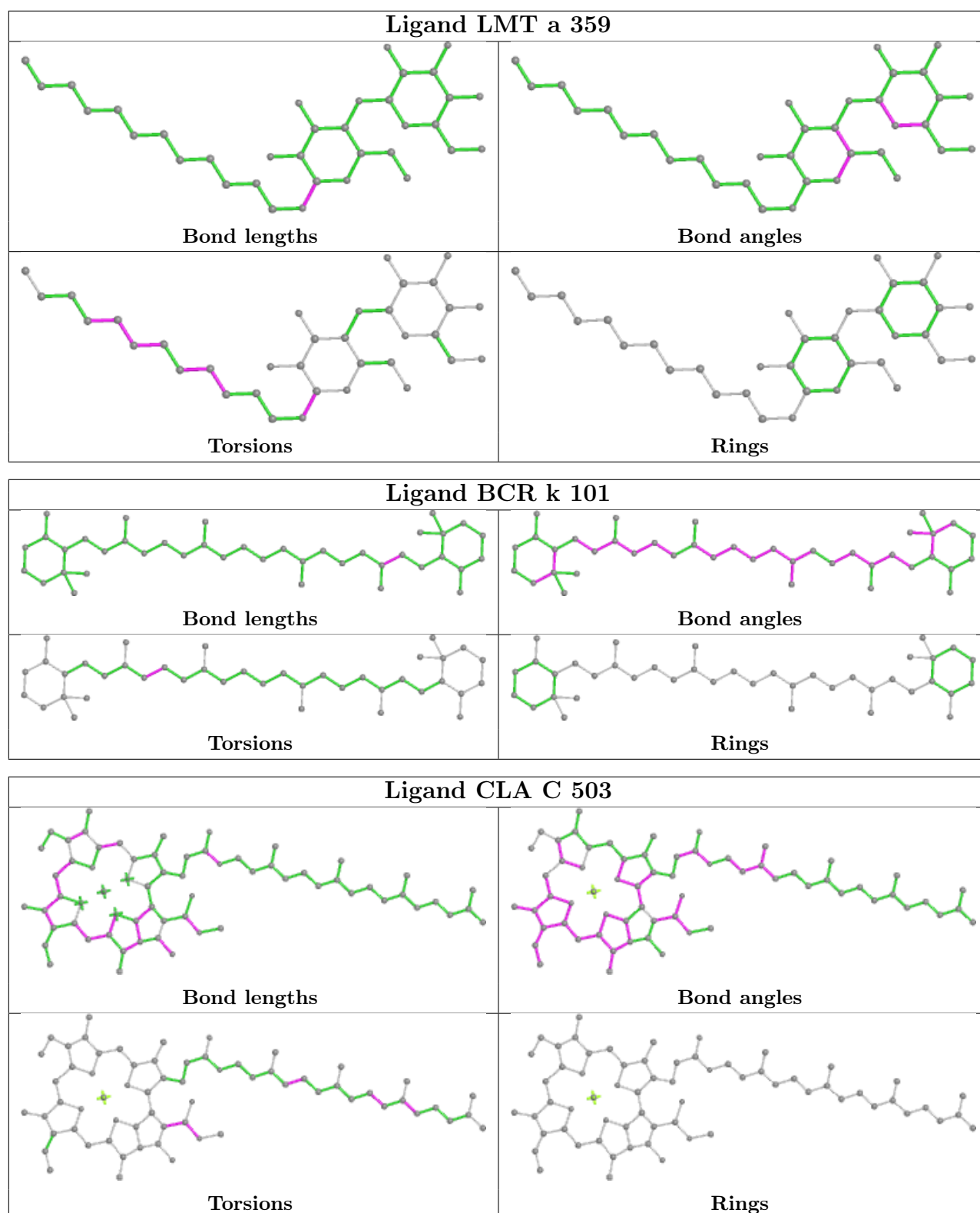


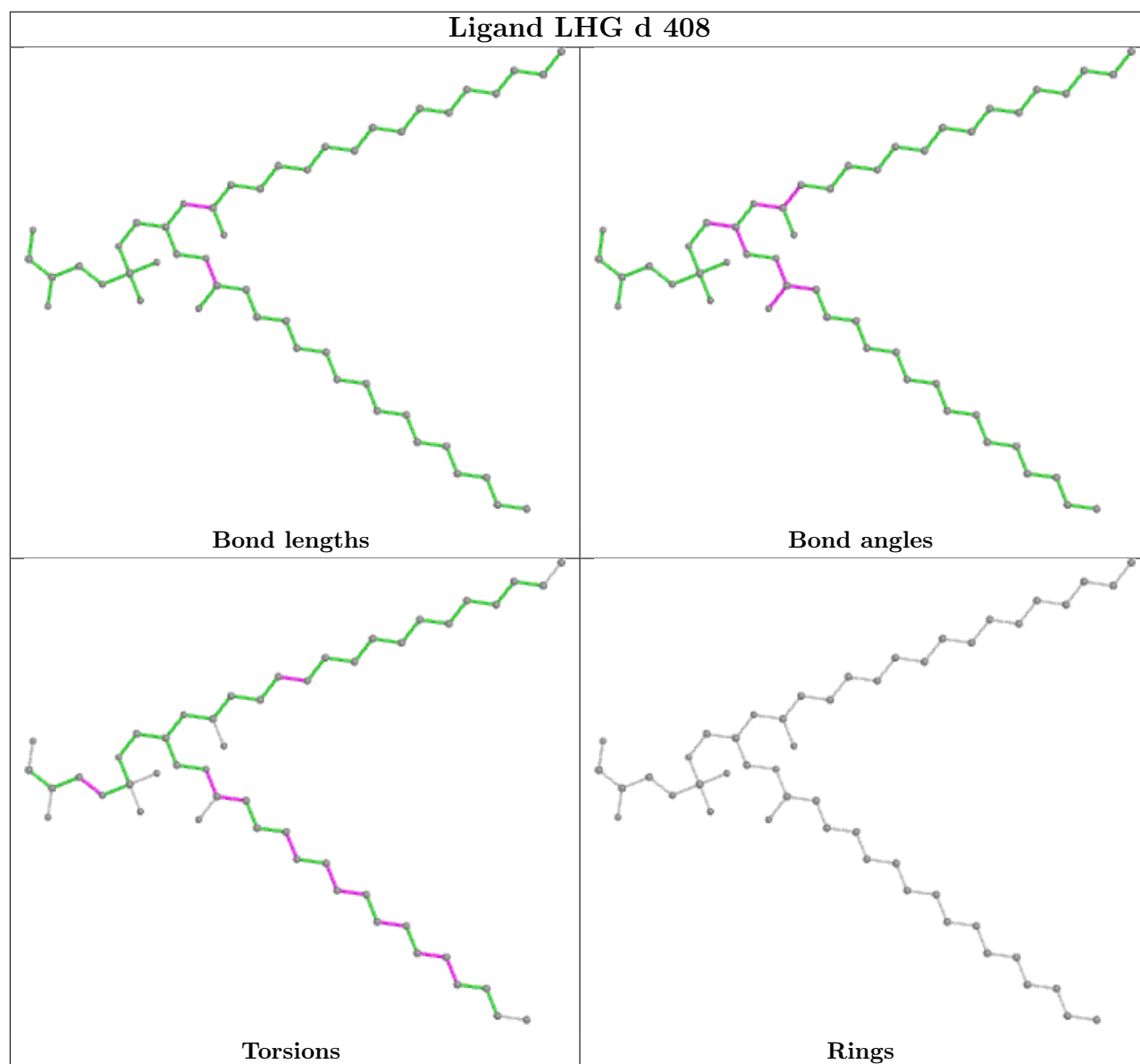
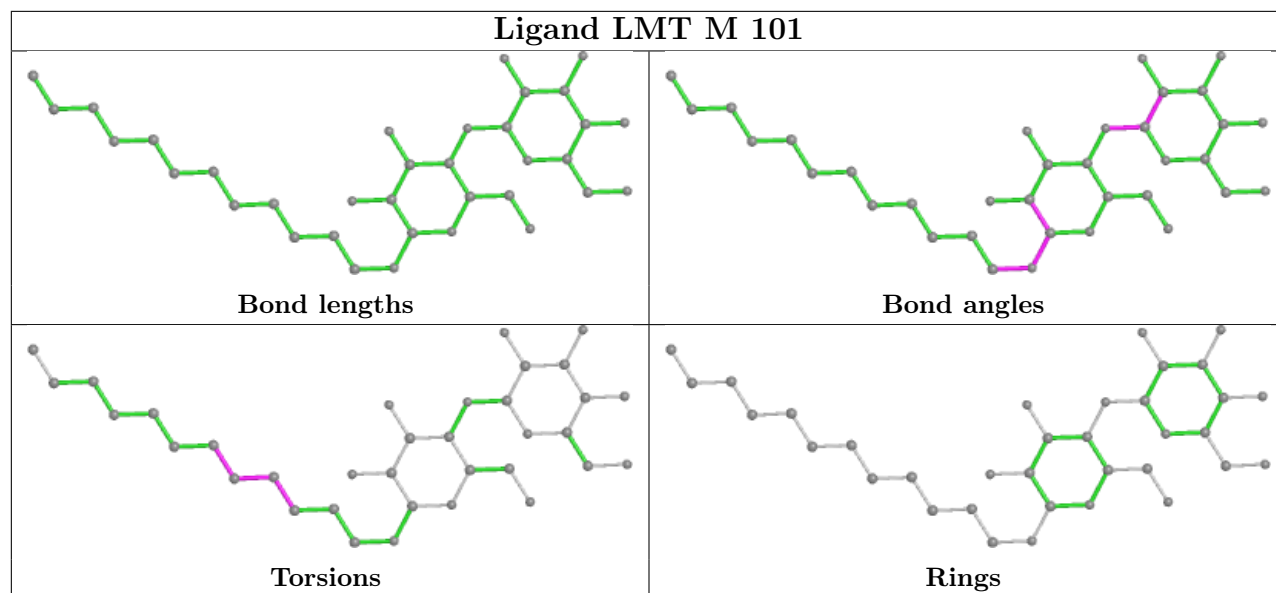
## Ligand LMG a 417

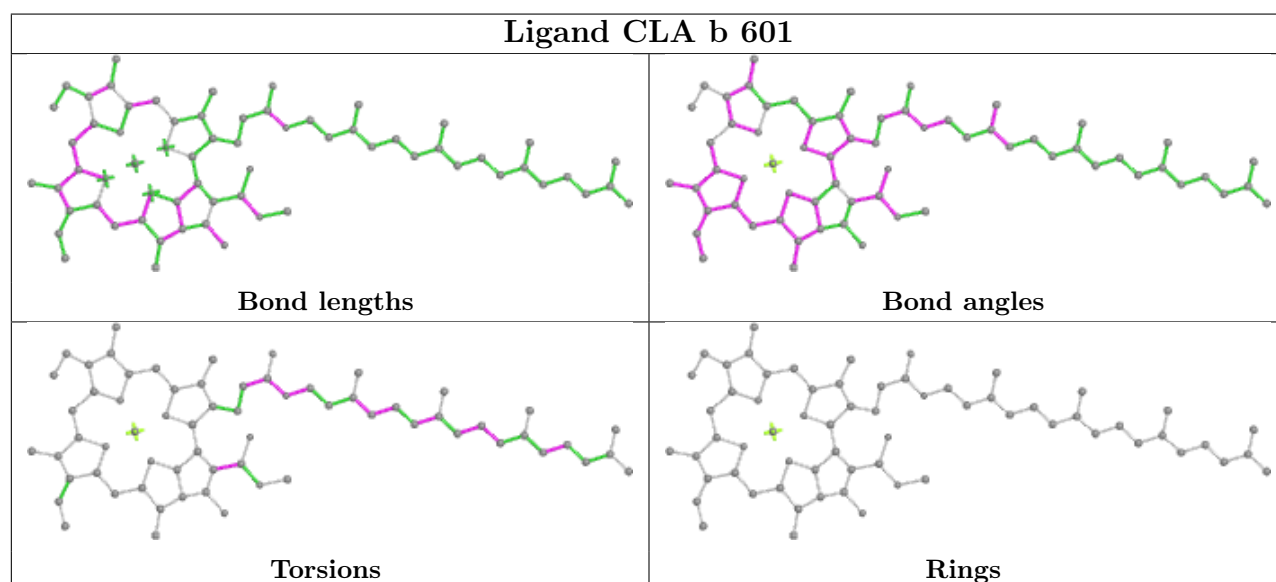
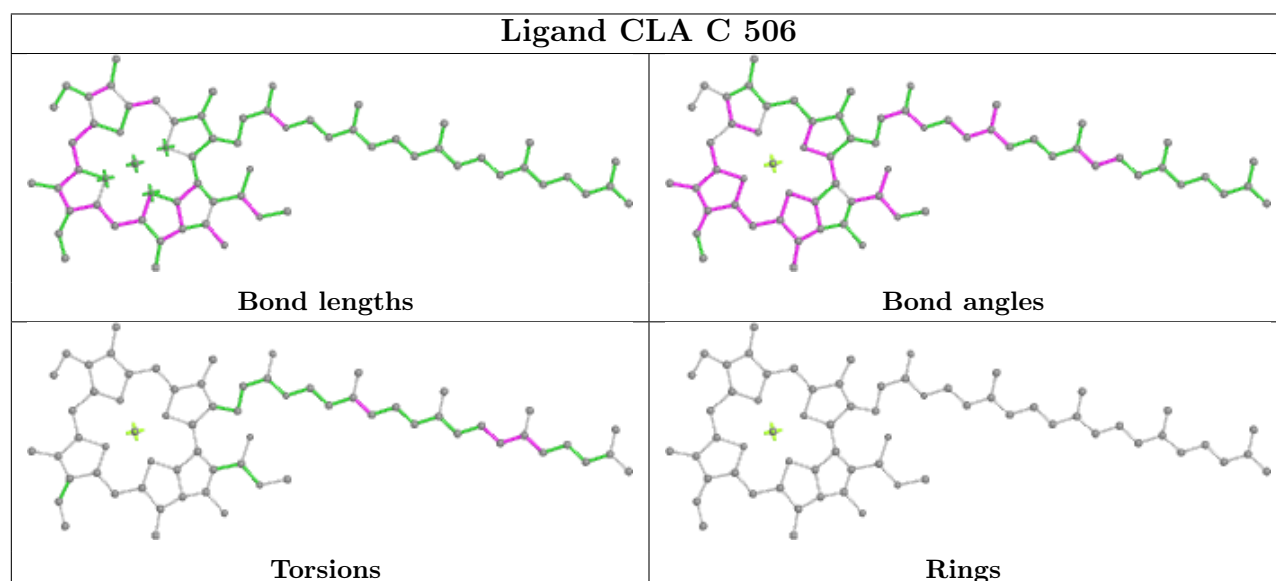
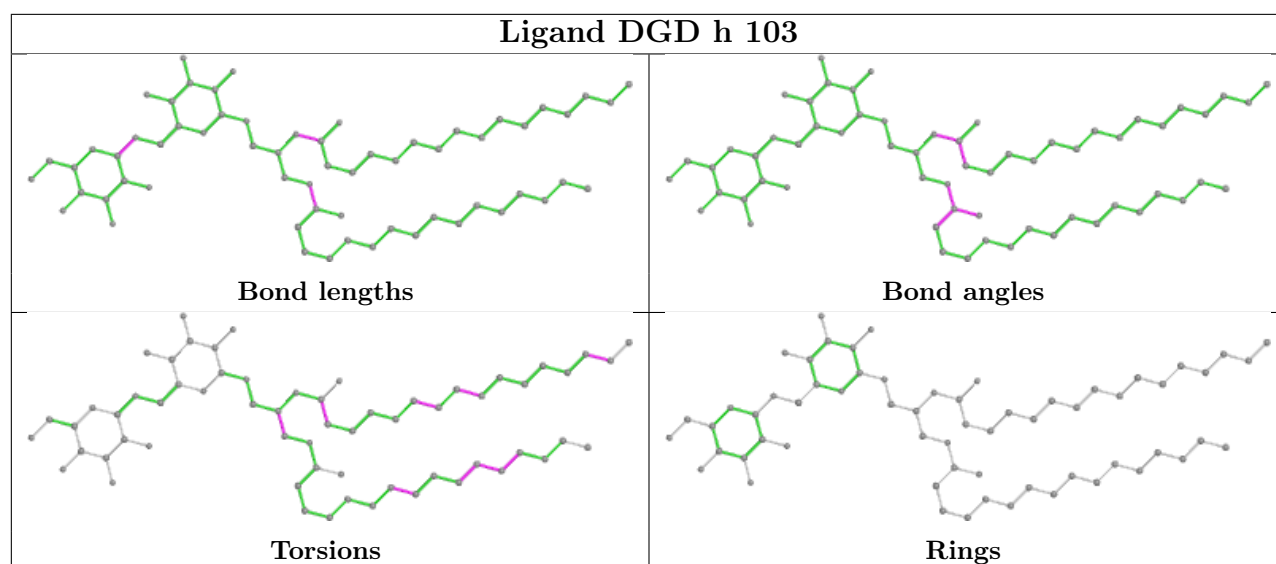


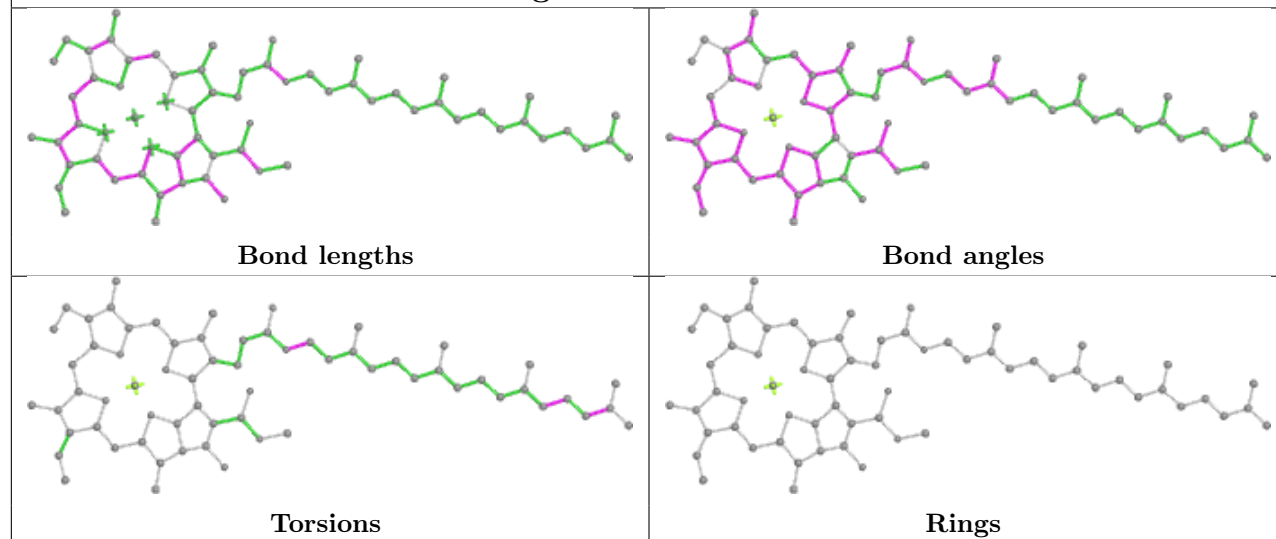
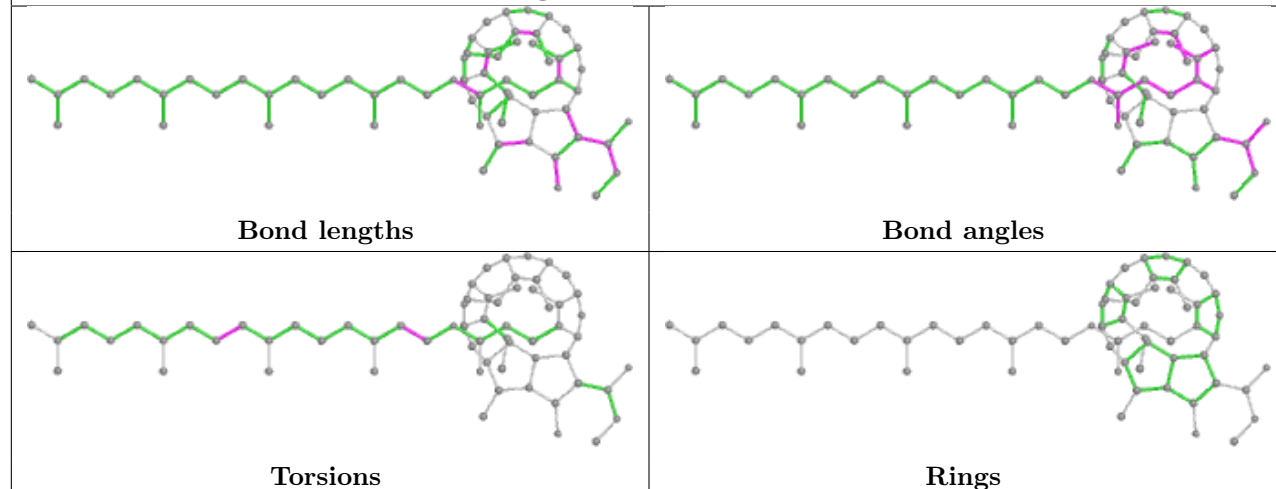
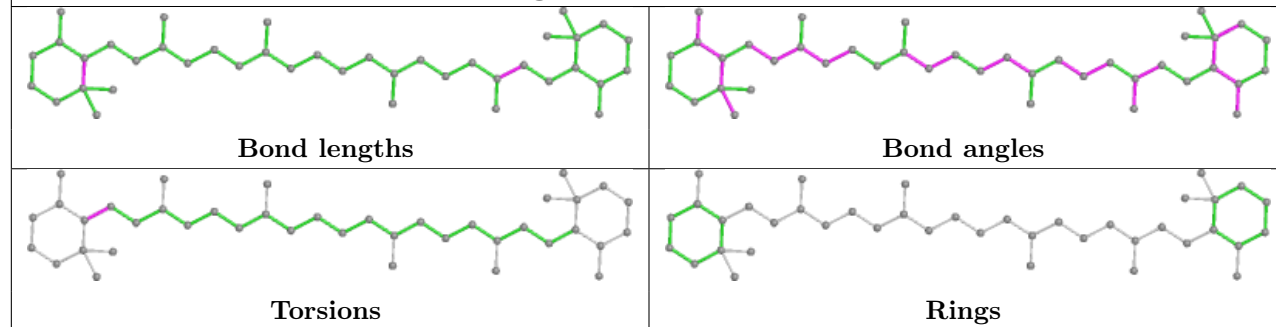
## Ligand HTG B 625



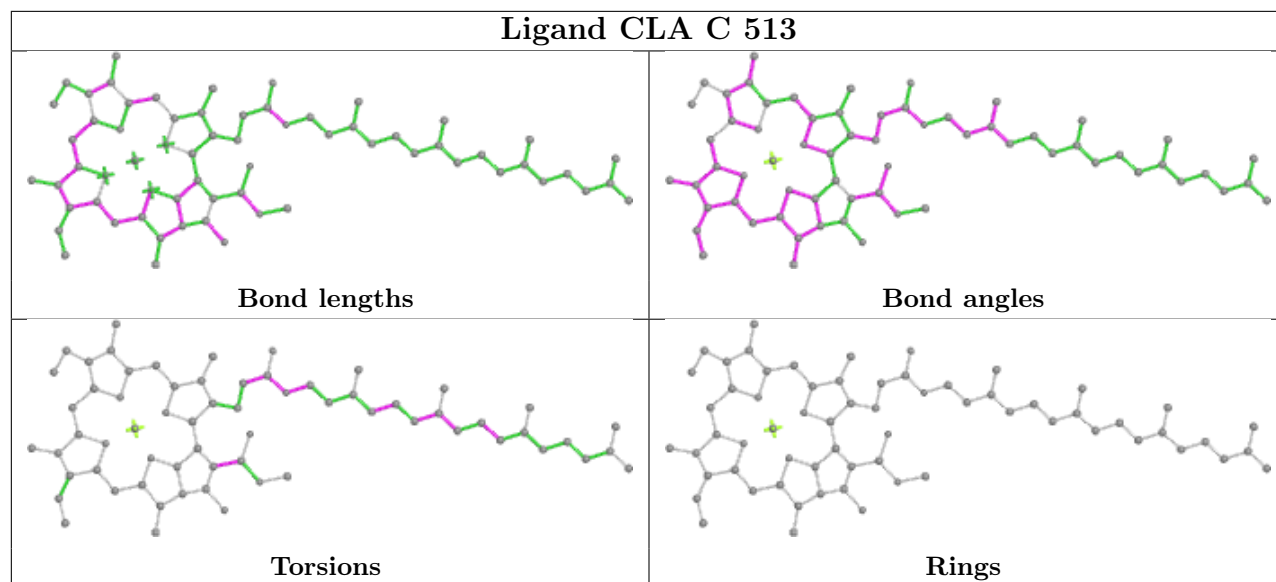
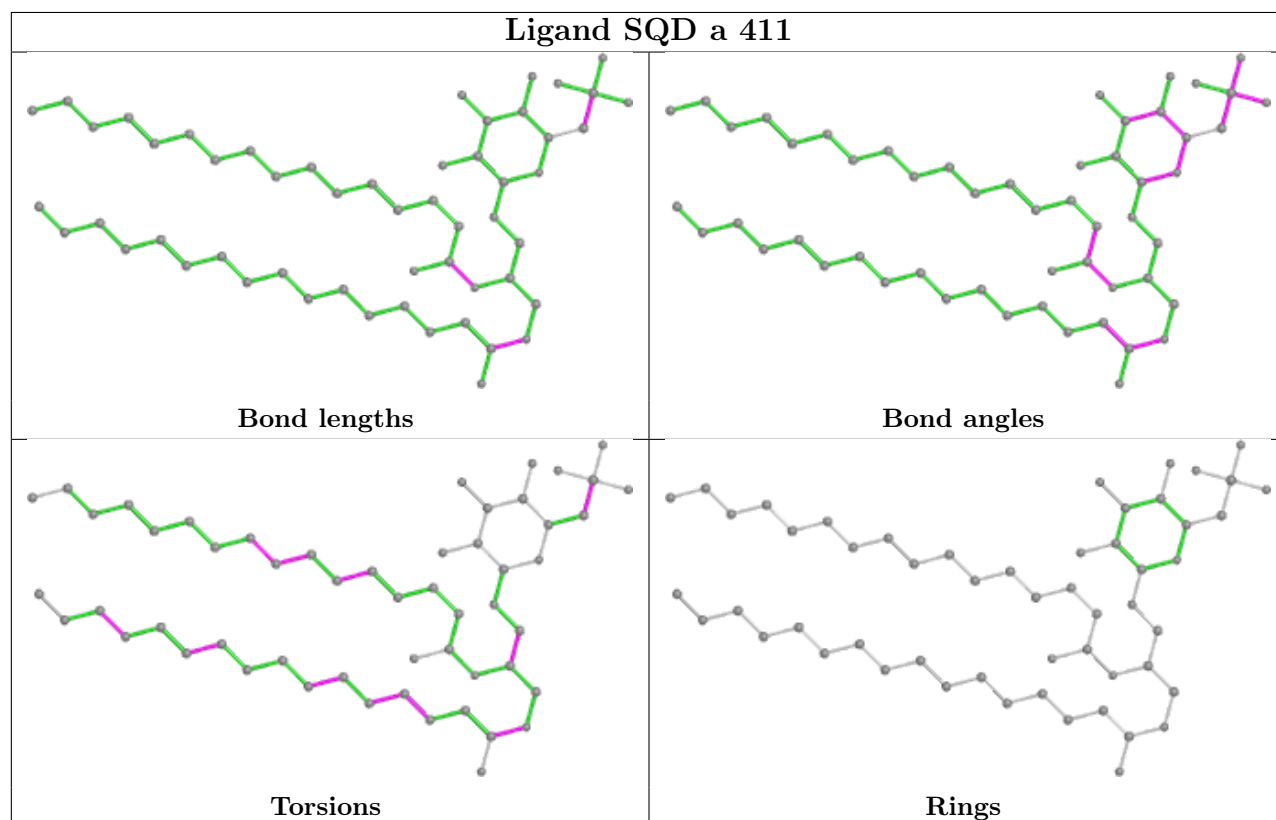




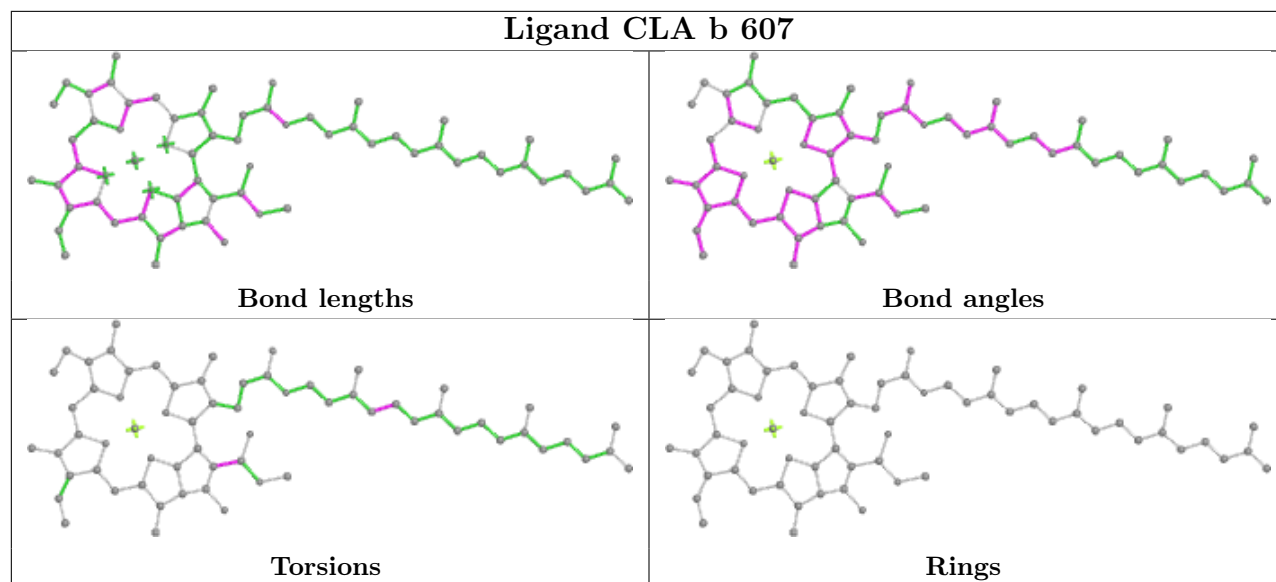


**Ligand CLA B 608****Ligand PHO a 405****Ligand BCR B 617**

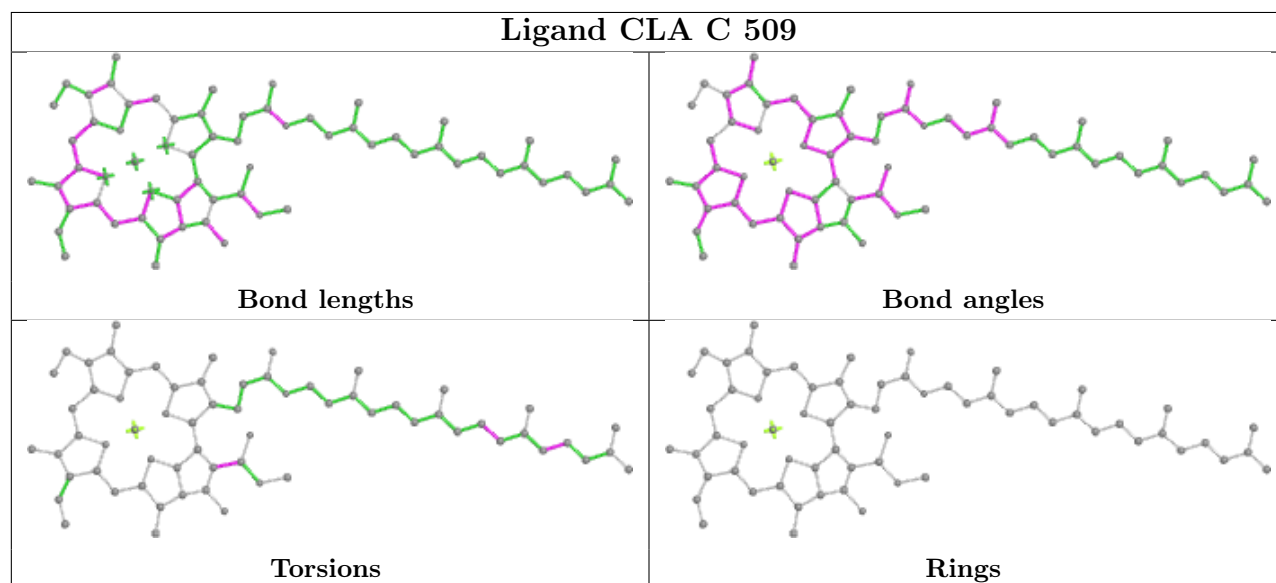


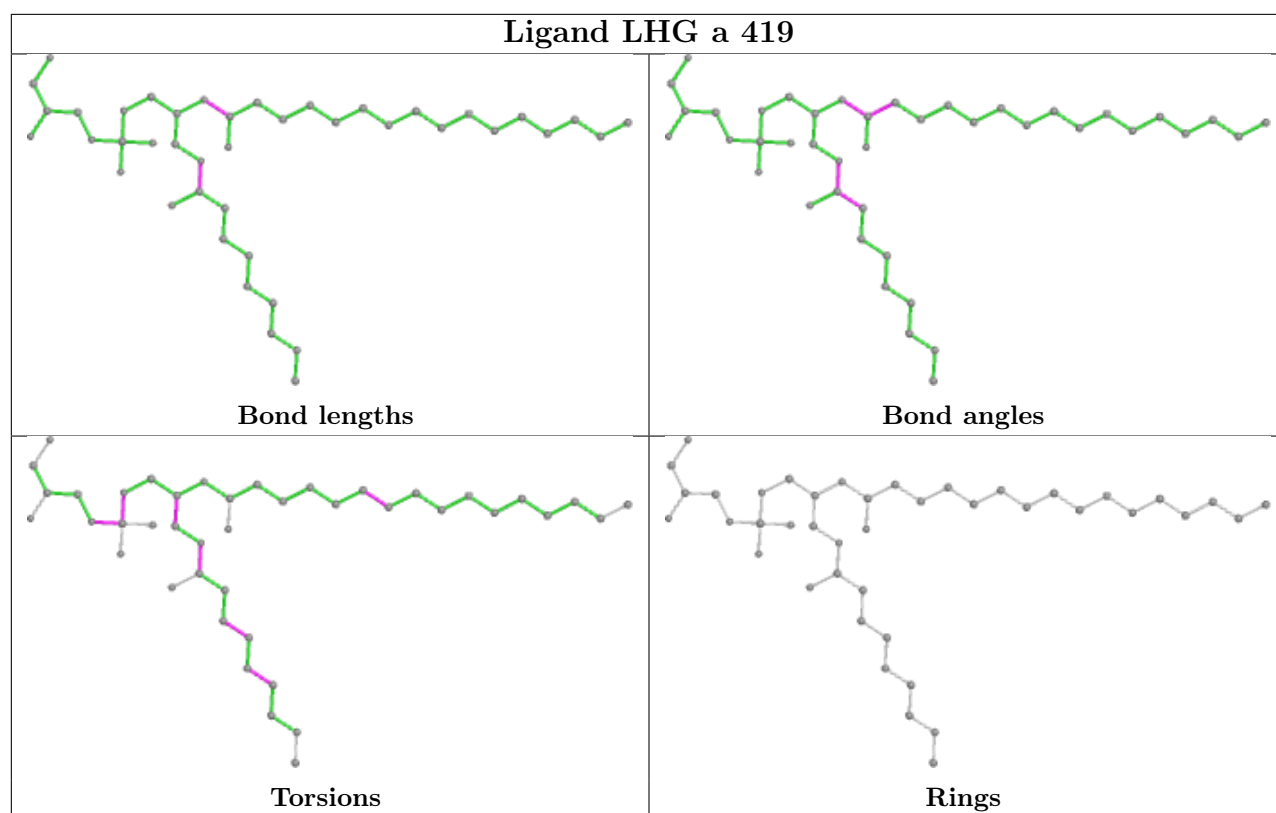
**Ligand CLA C 513****Ligand SQD a 411**

## Ligand CLA b 607

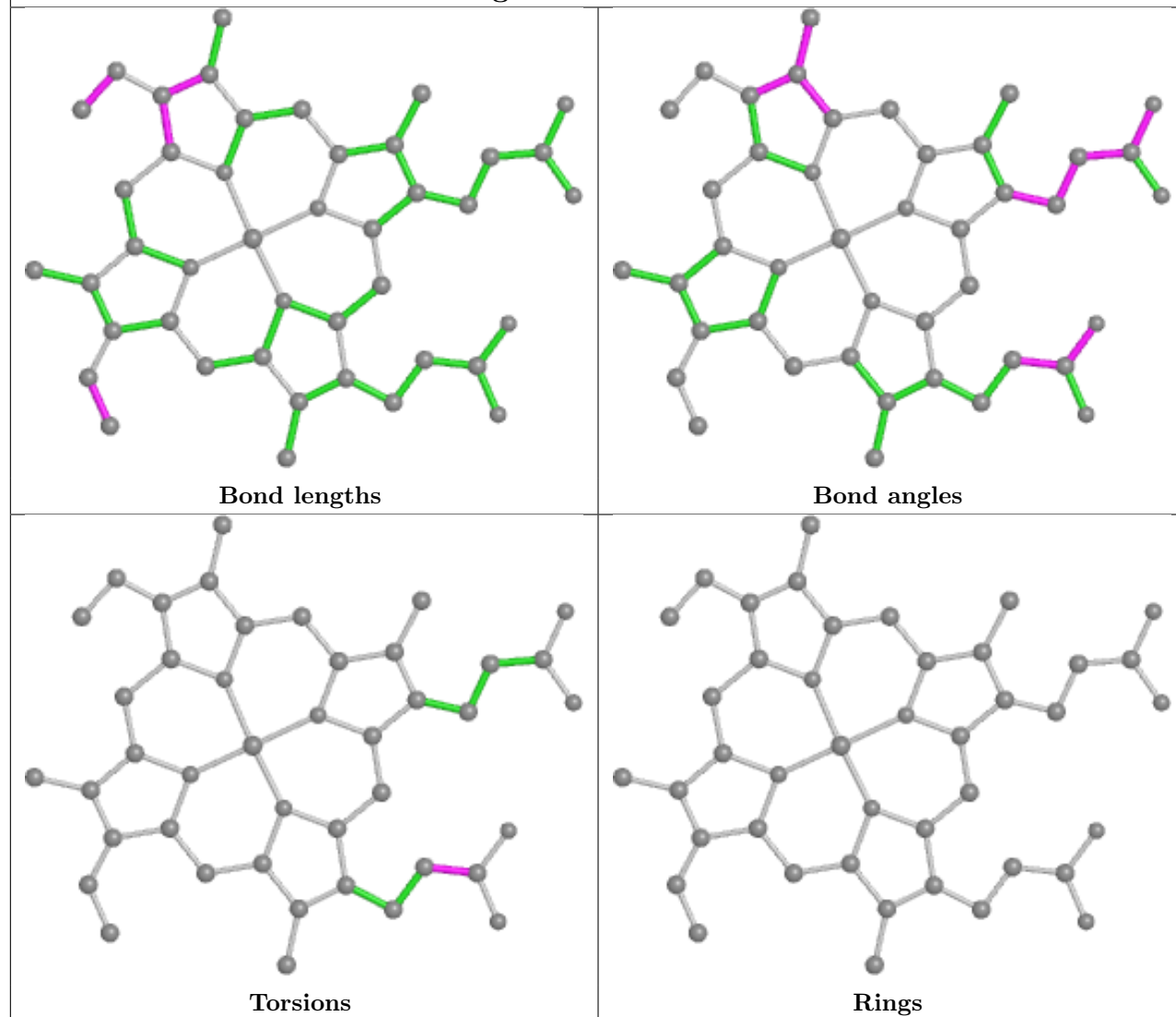


## Ligand CLA C 509

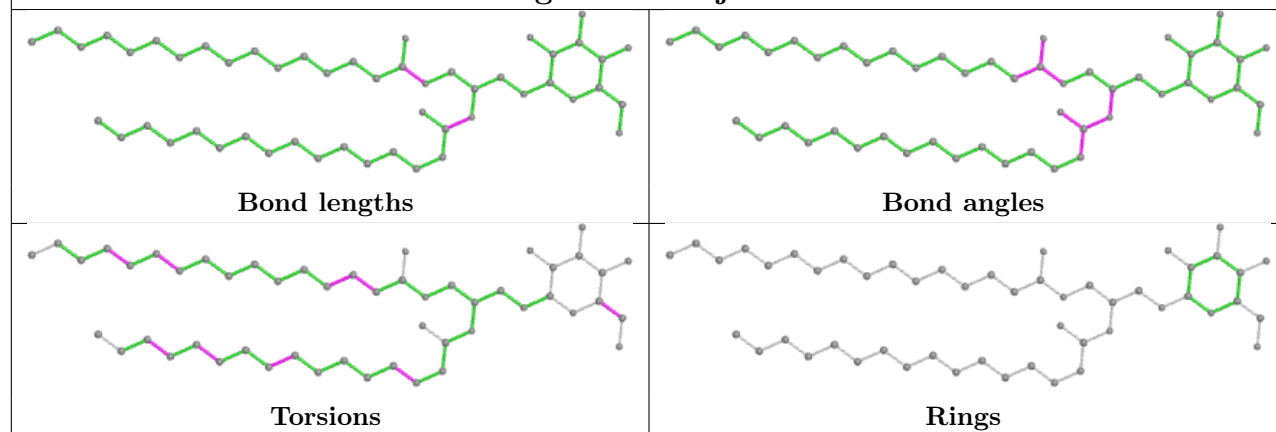


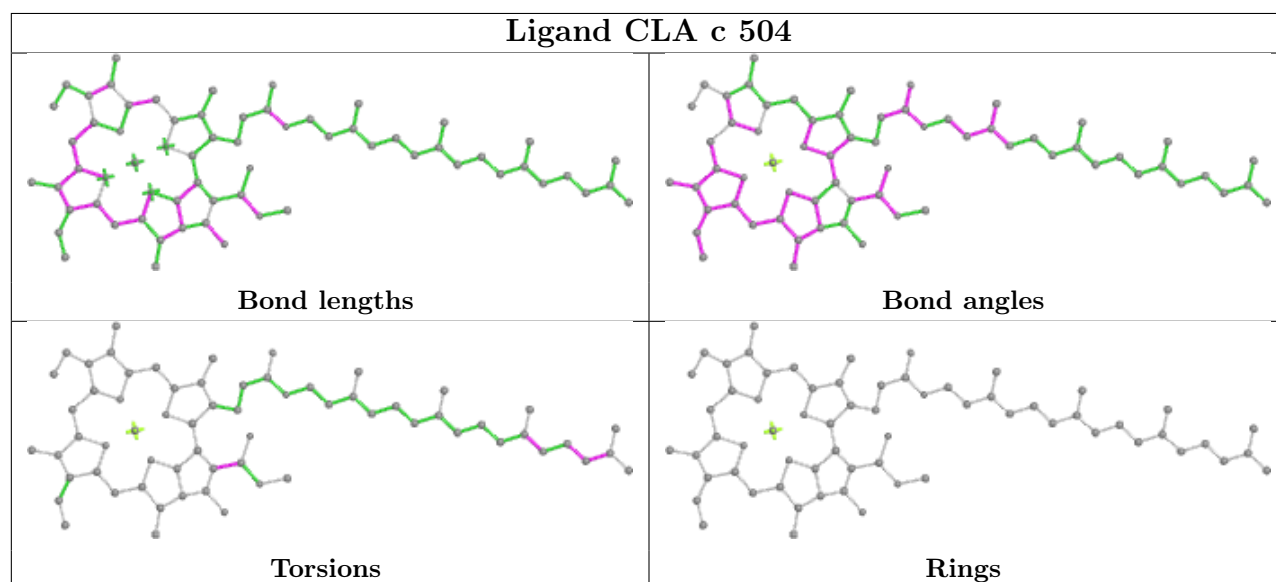
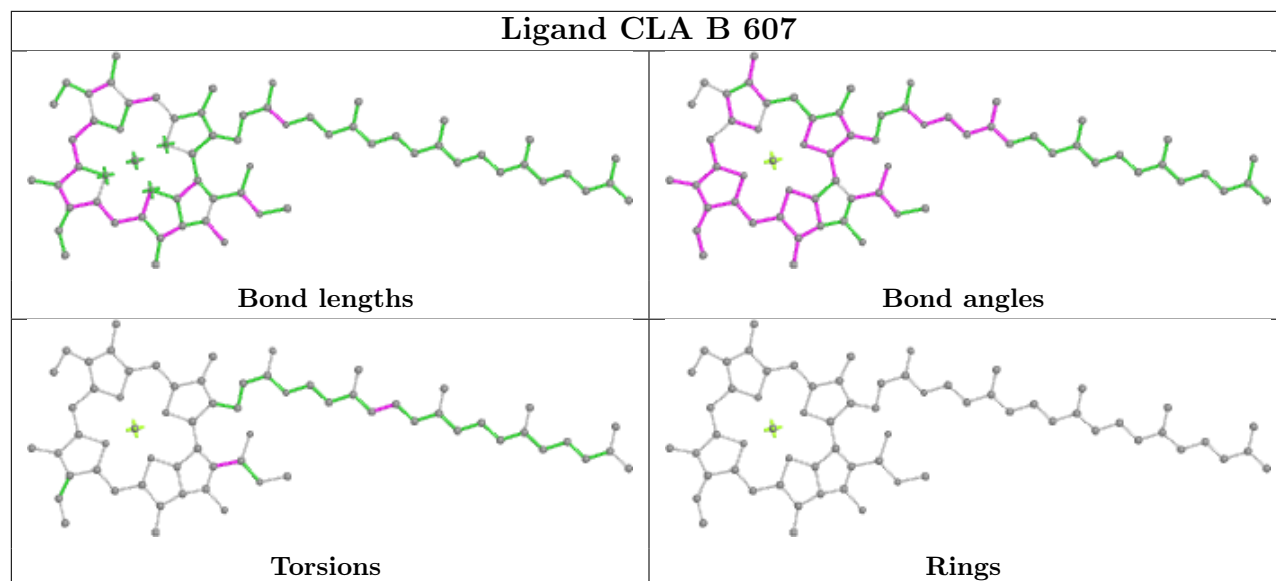
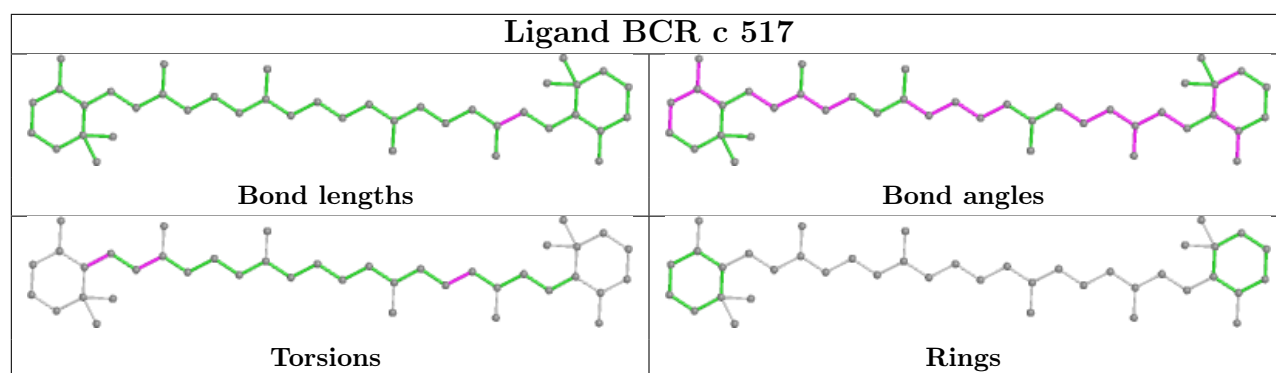


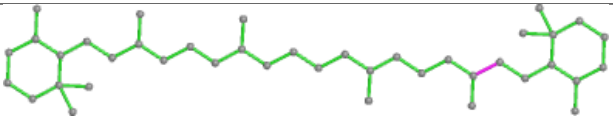
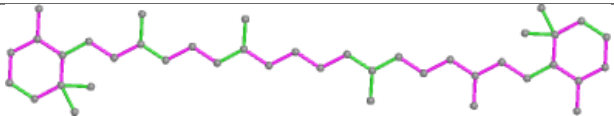
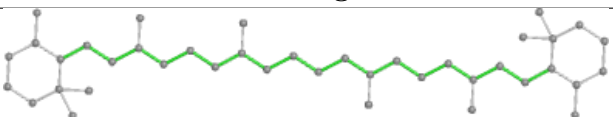
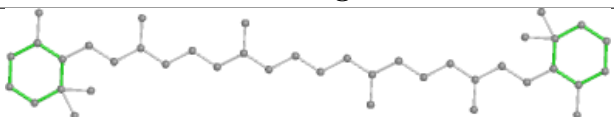
## Ligand HEC v 203

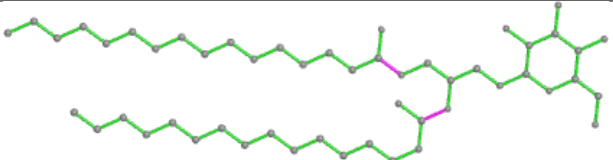
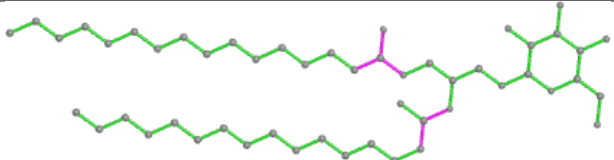
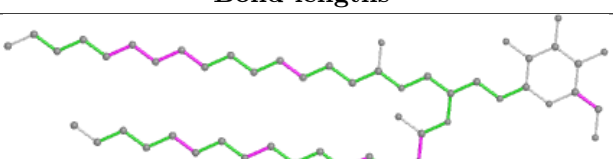
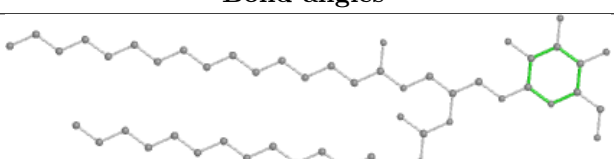


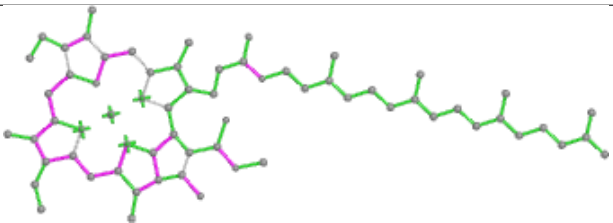
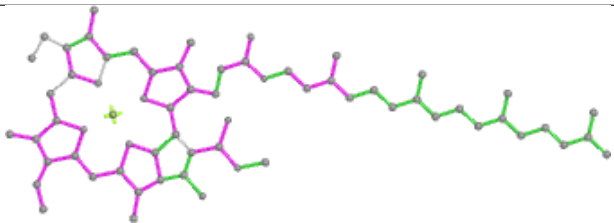
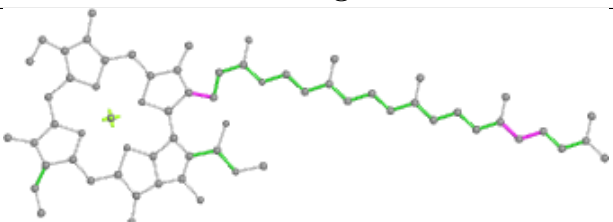
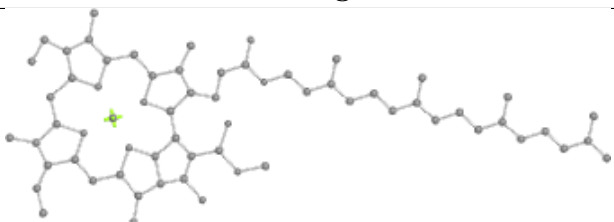
## Ligand LMG j 101

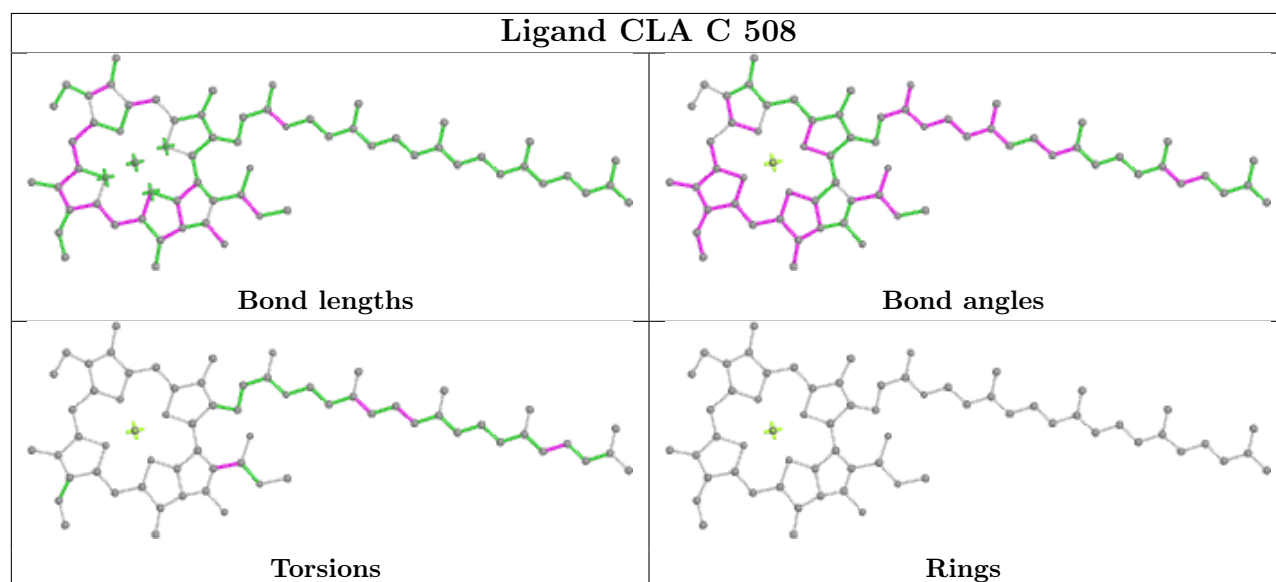
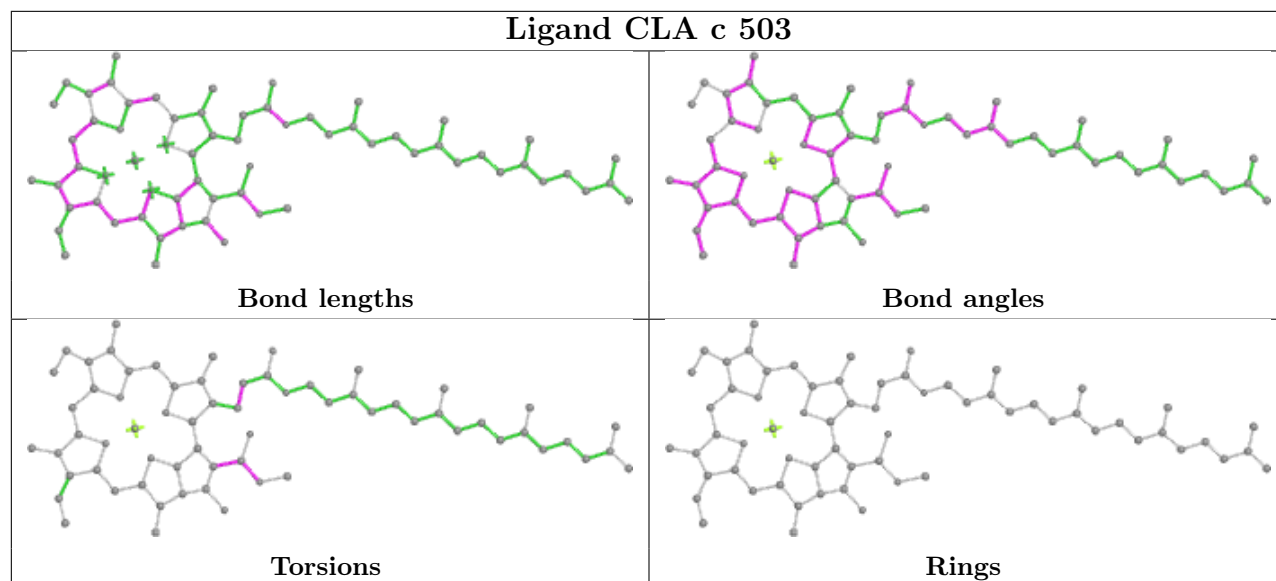
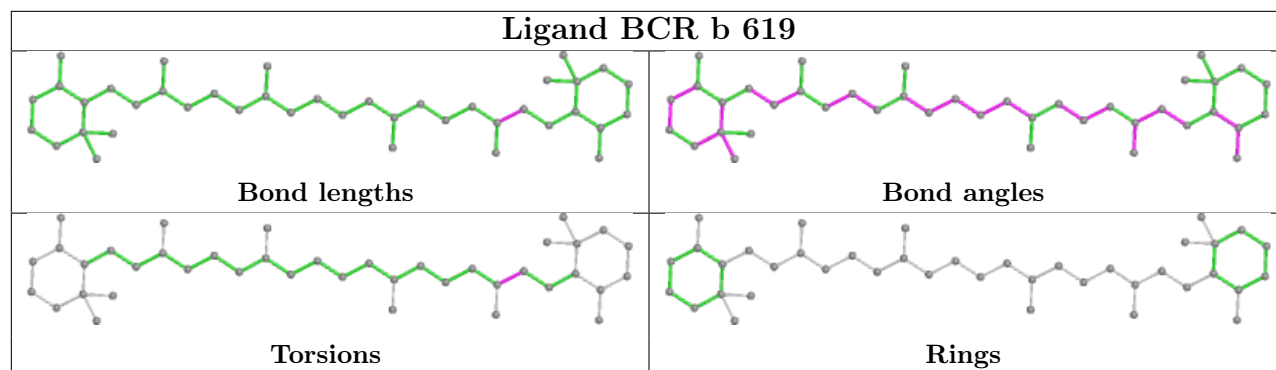


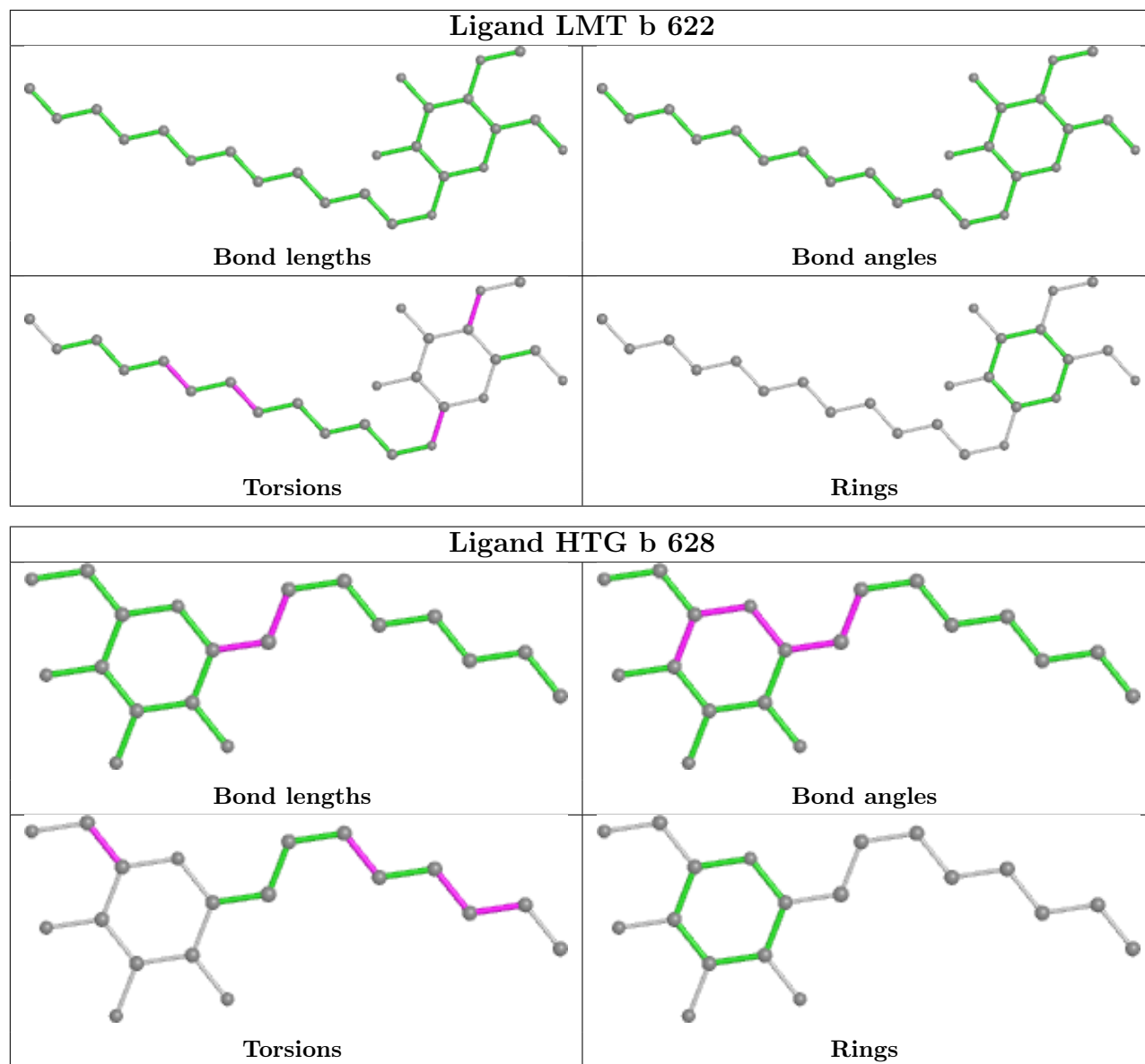


Ligand BCR B 618	
	Bond lengths
	Bond angles
	Torsions
	Rings

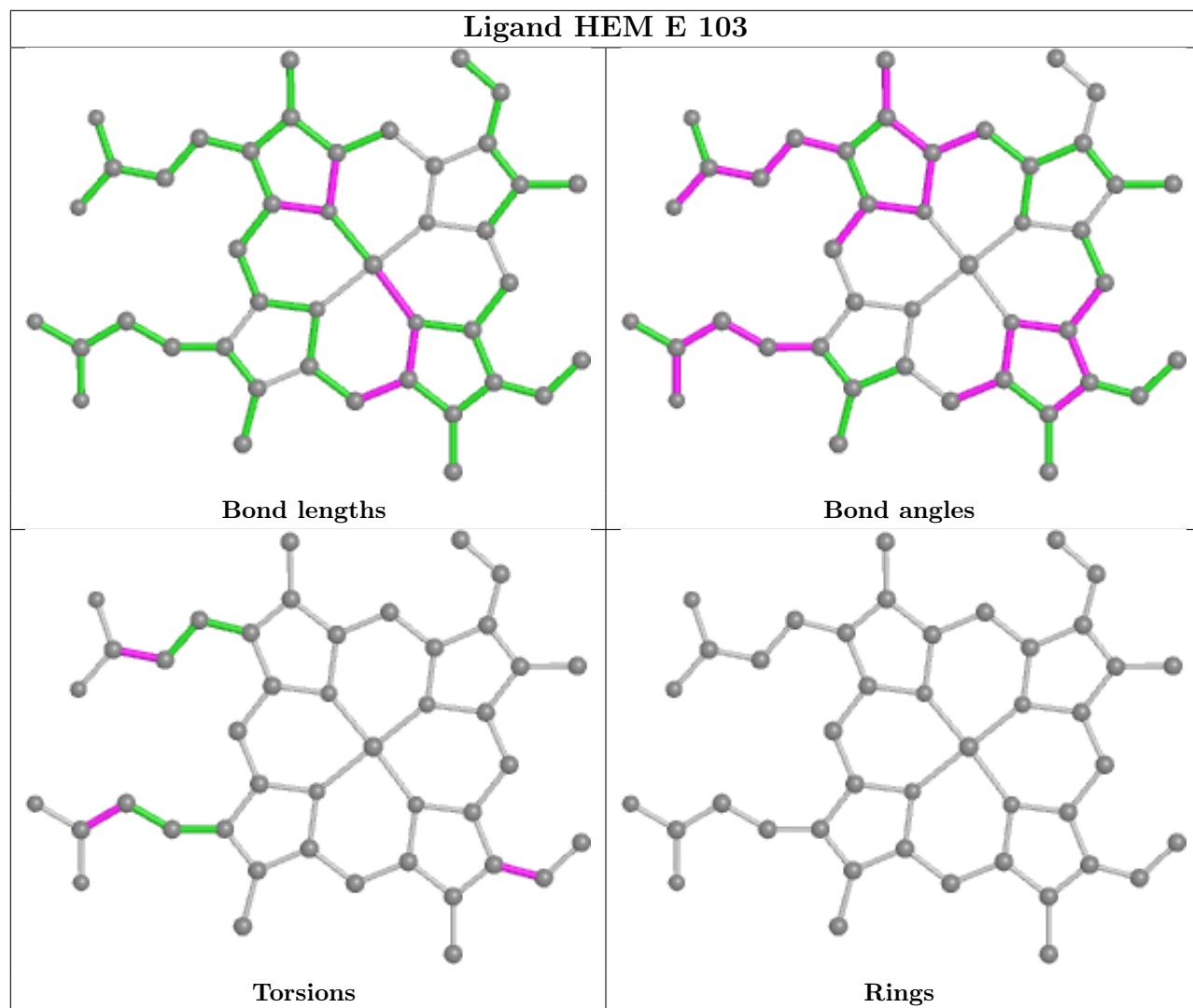
Ligand LMG J 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand CLA A 406	
	Bond lengths
	Bond angles
	Torsions
	Rings

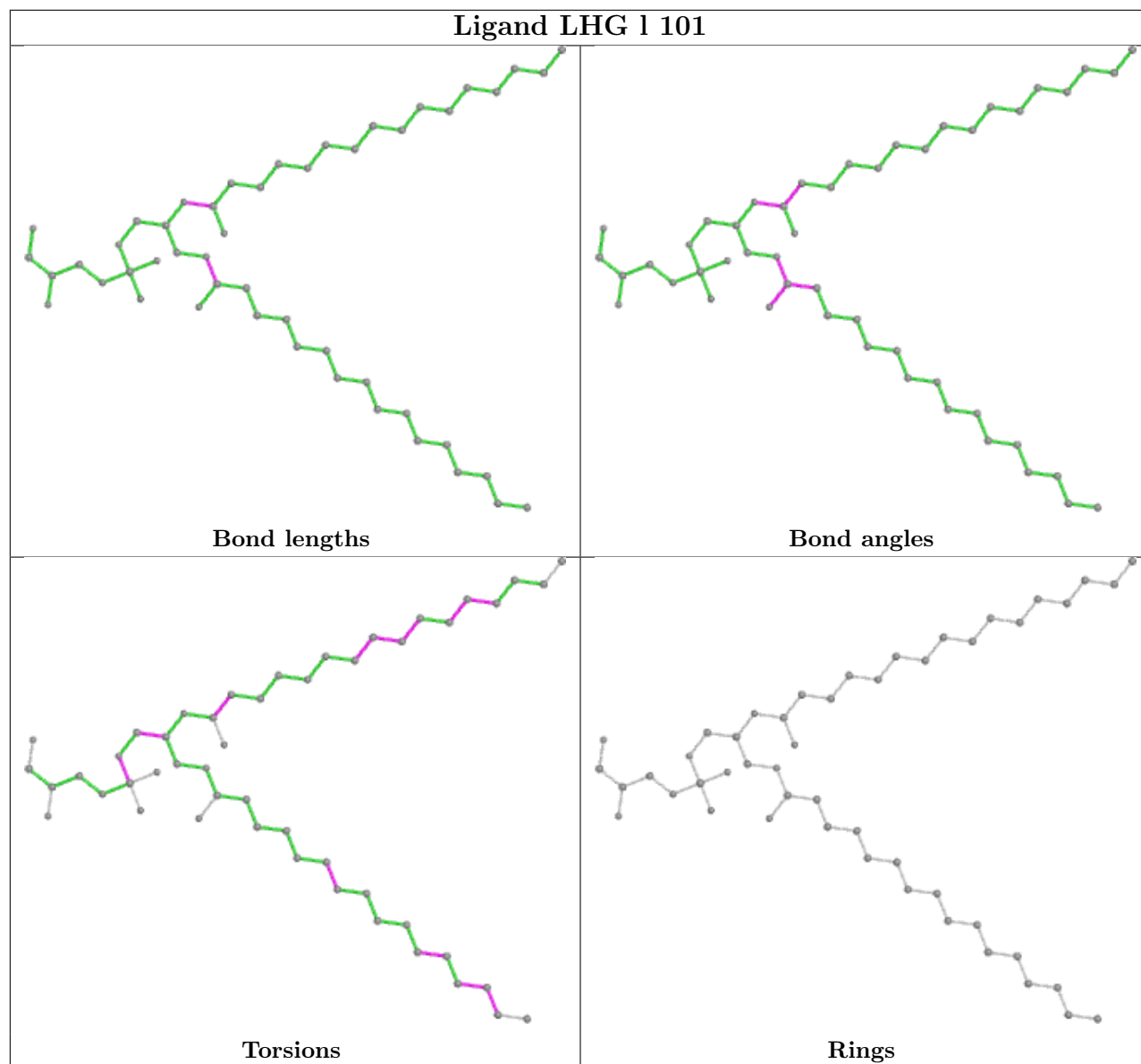




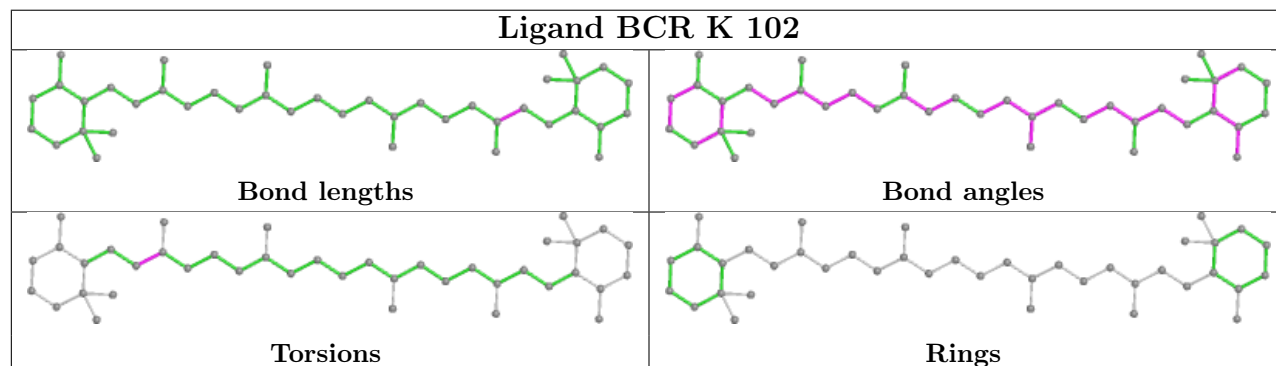


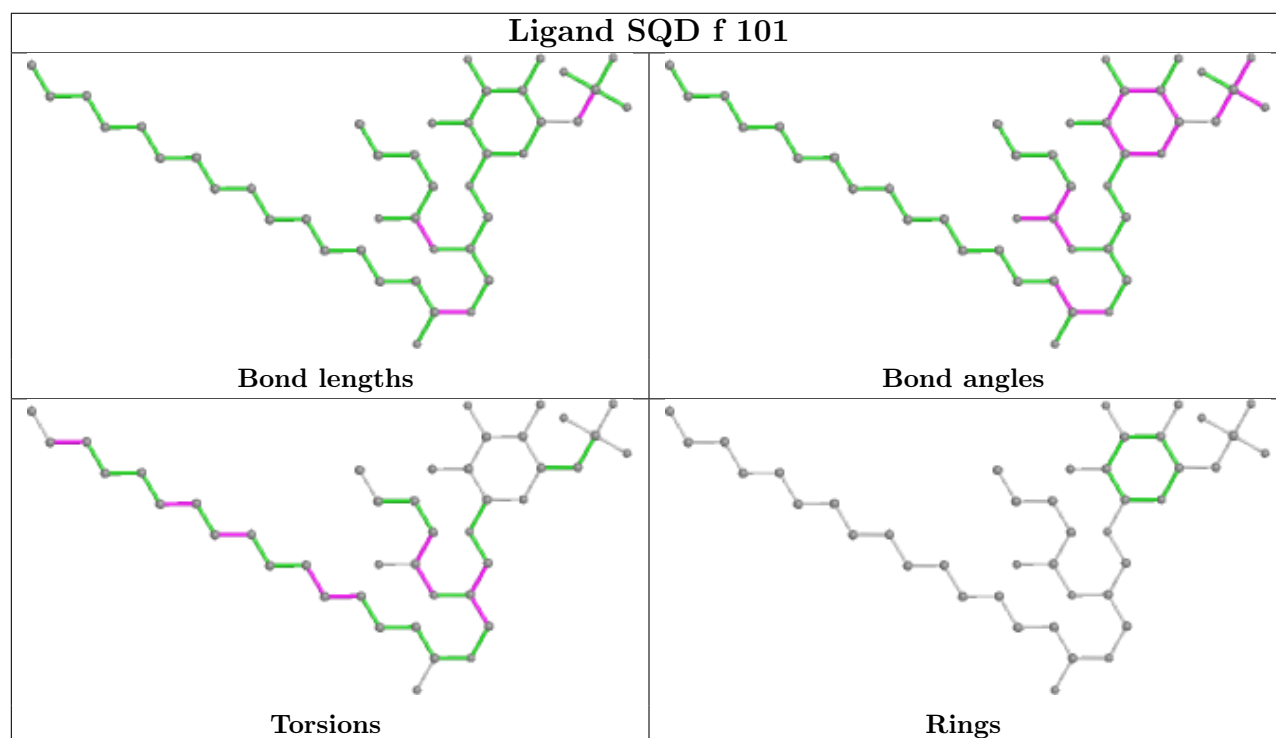
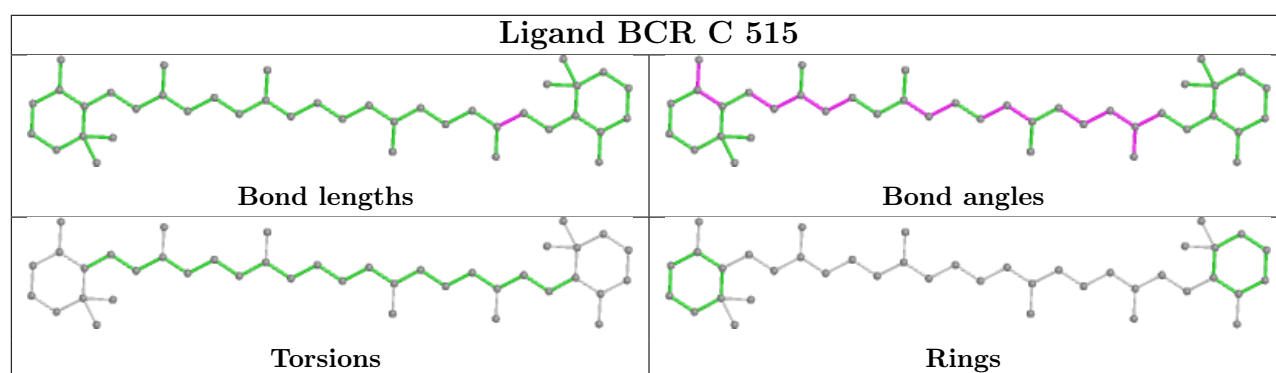
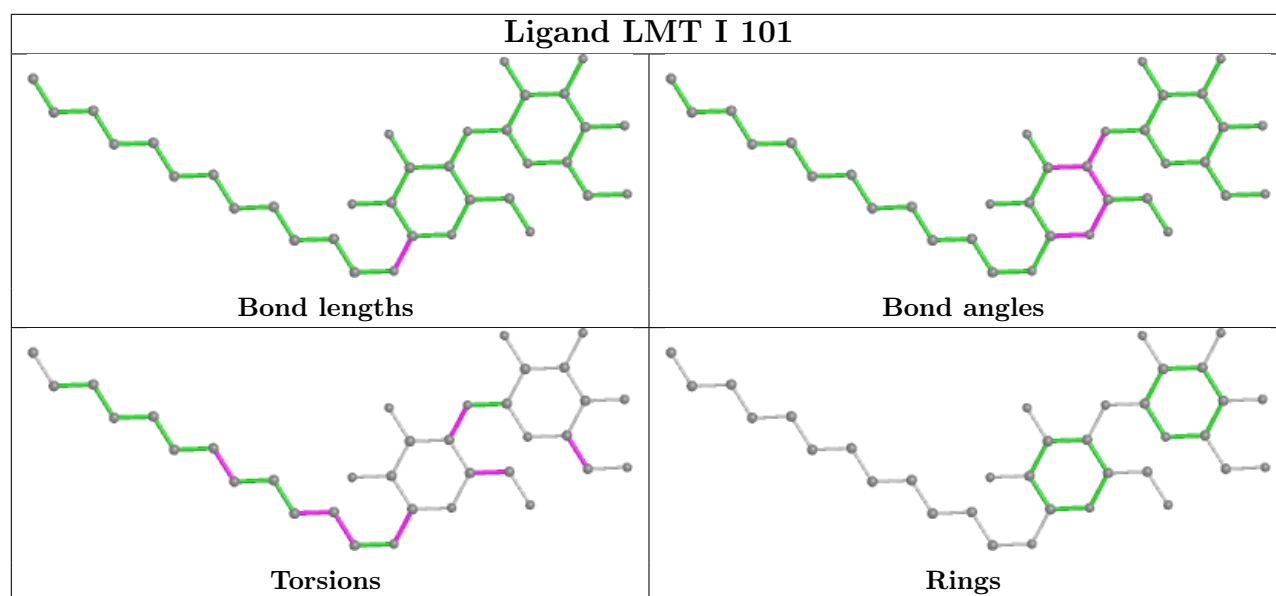


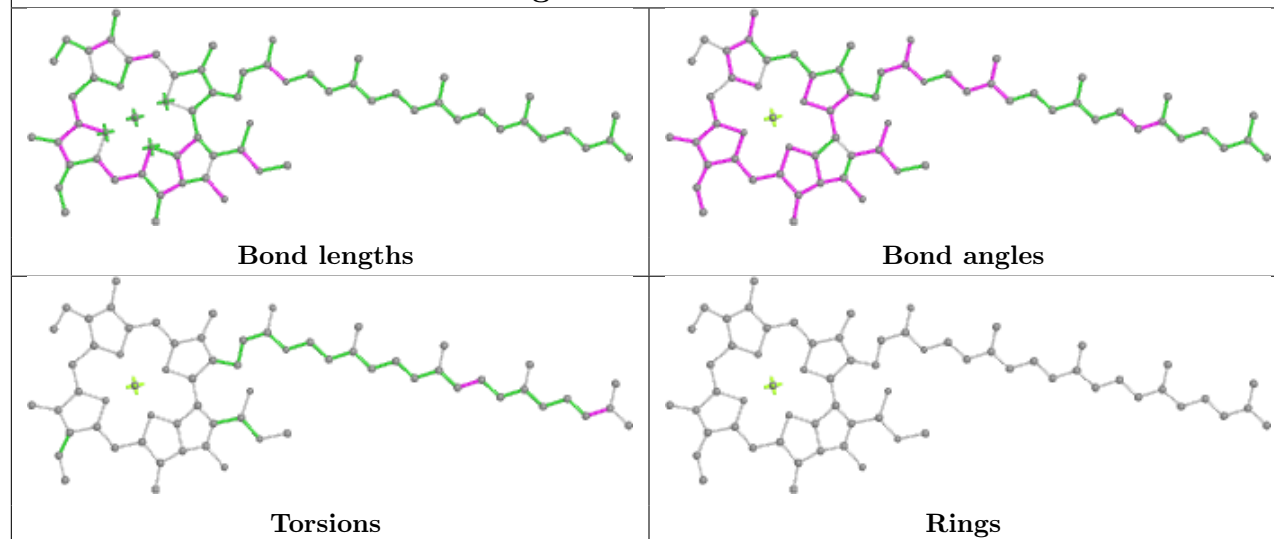
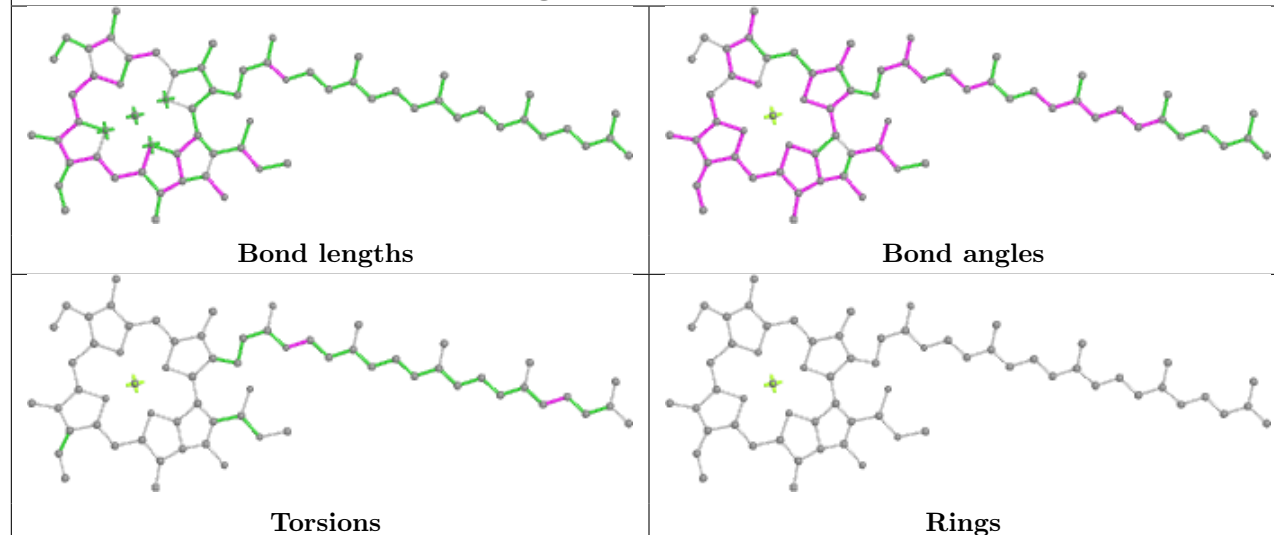
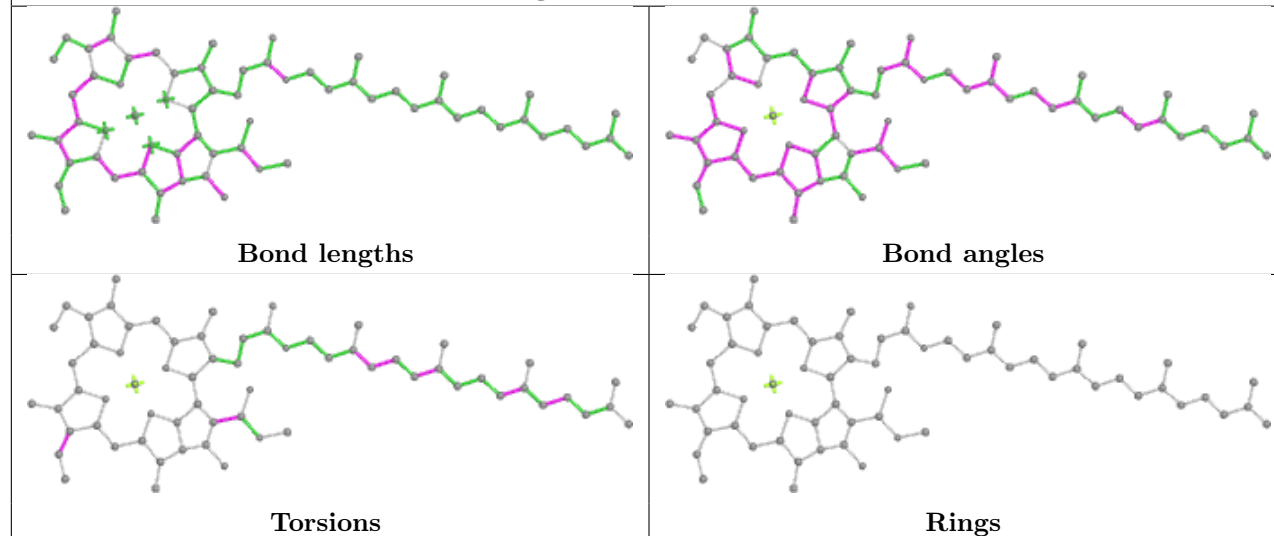
## Ligand LHG 1 101

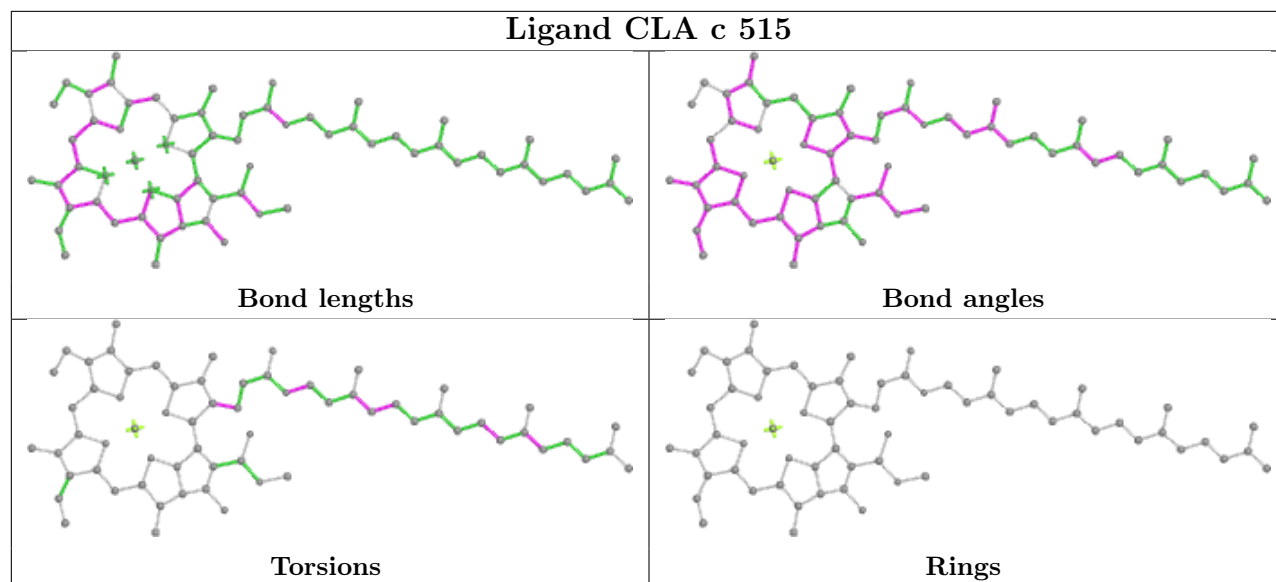
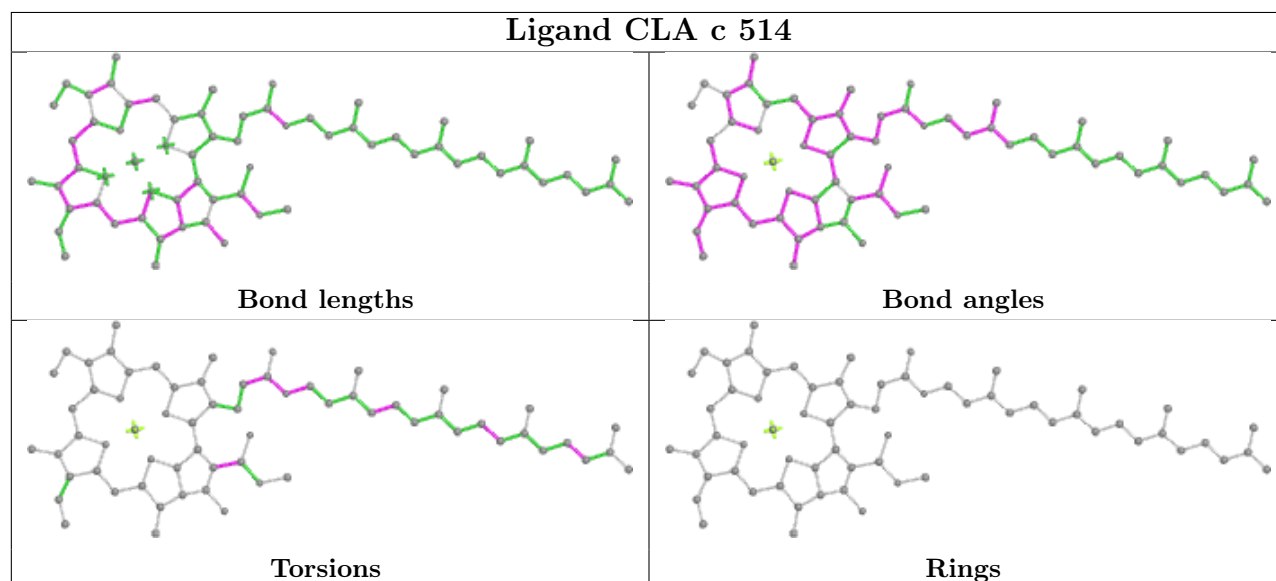
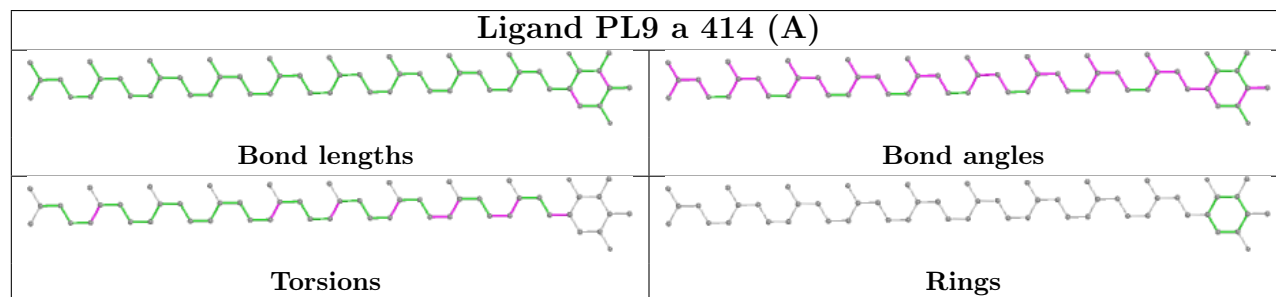


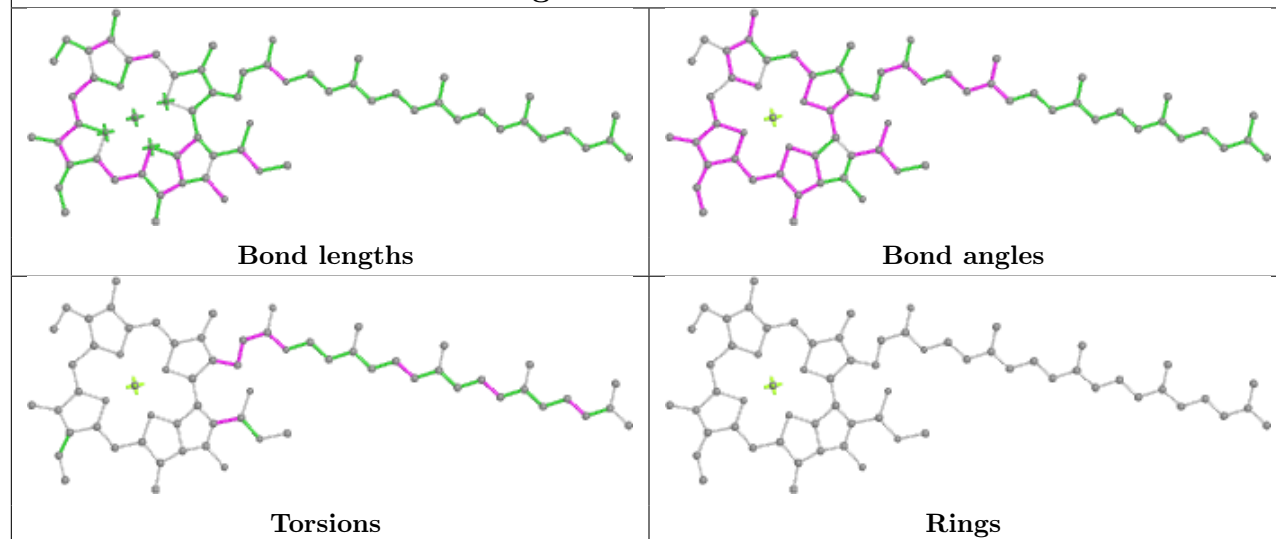
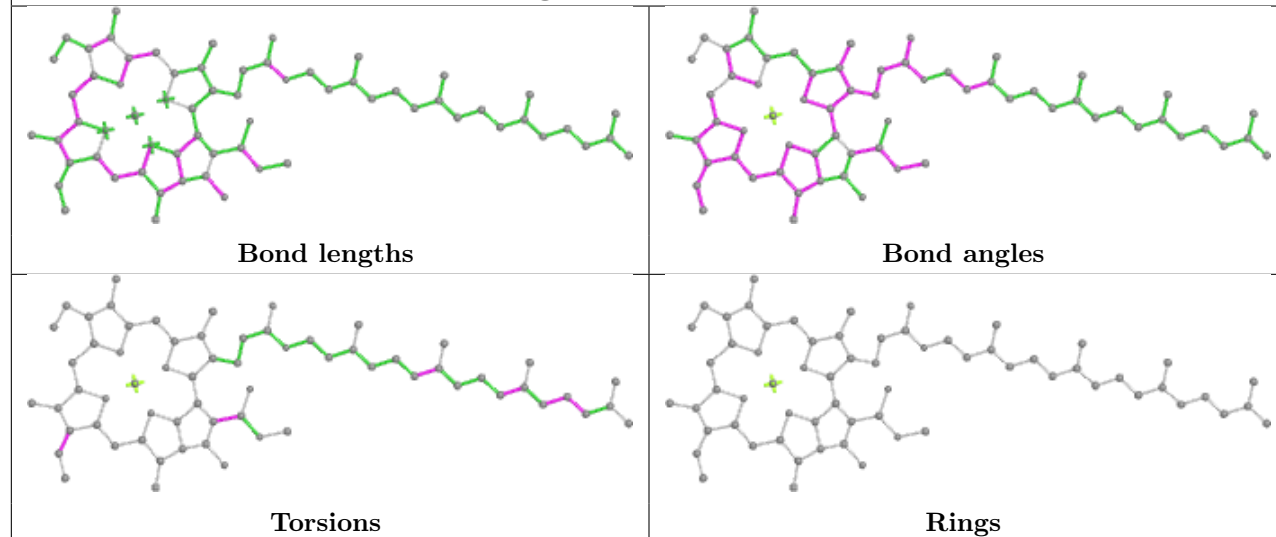
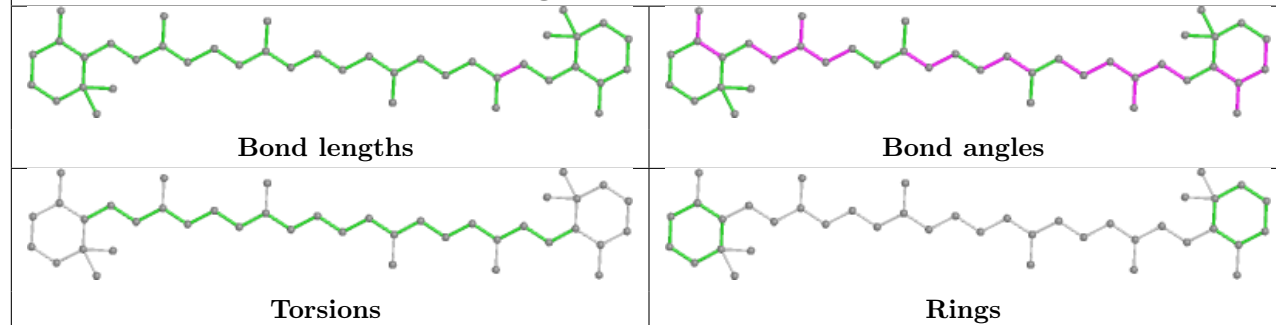
## Ligand BCR K 102

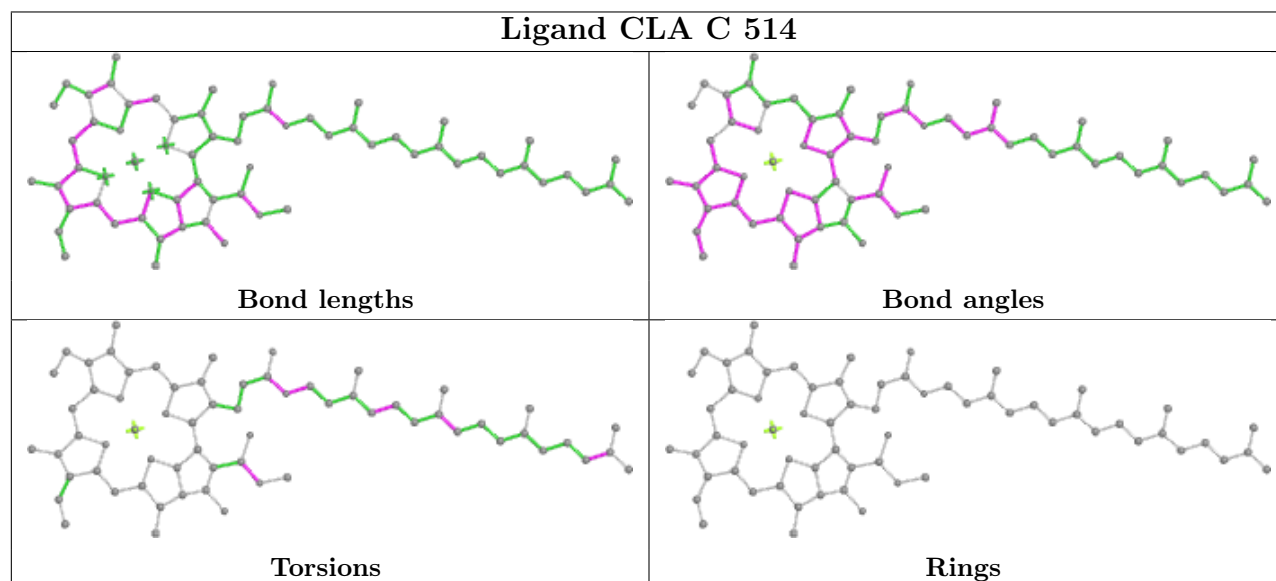
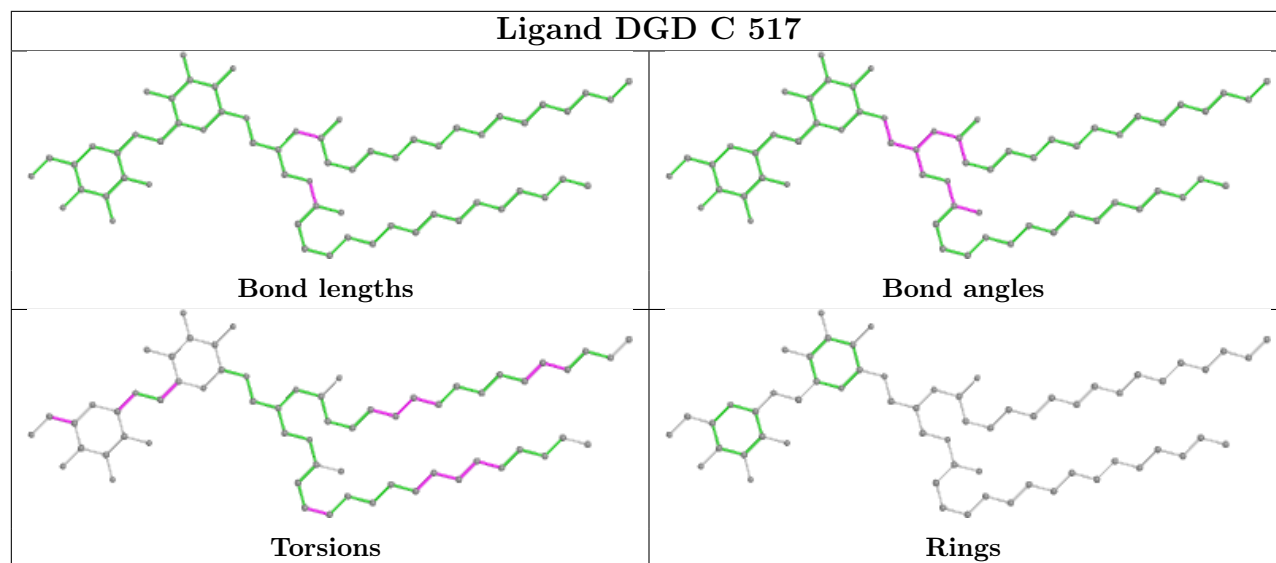


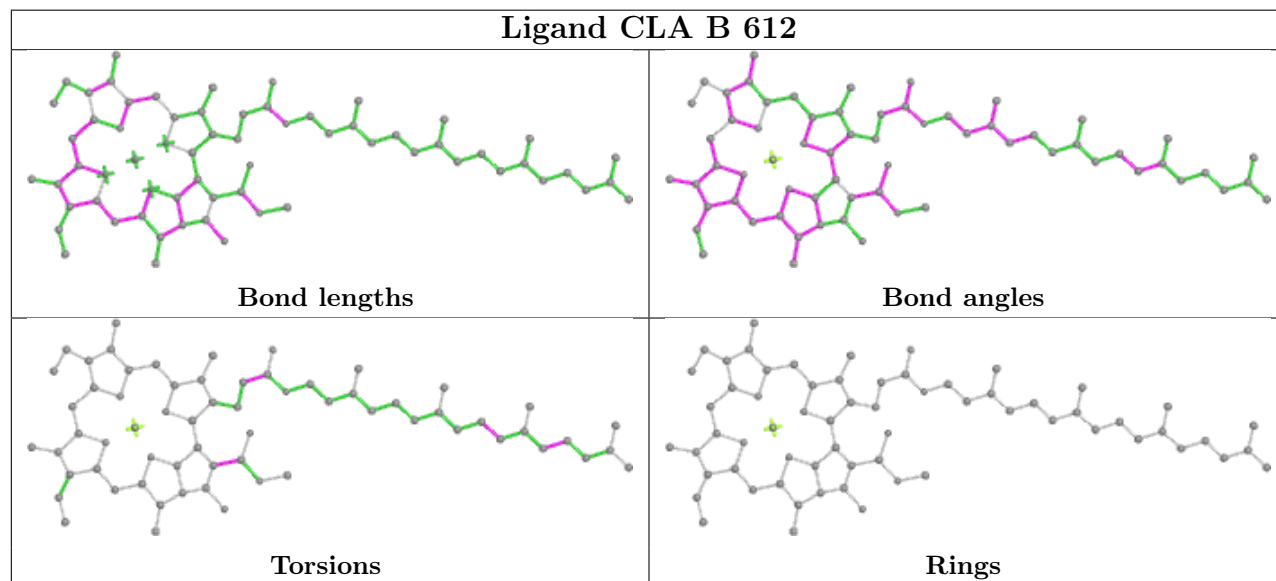
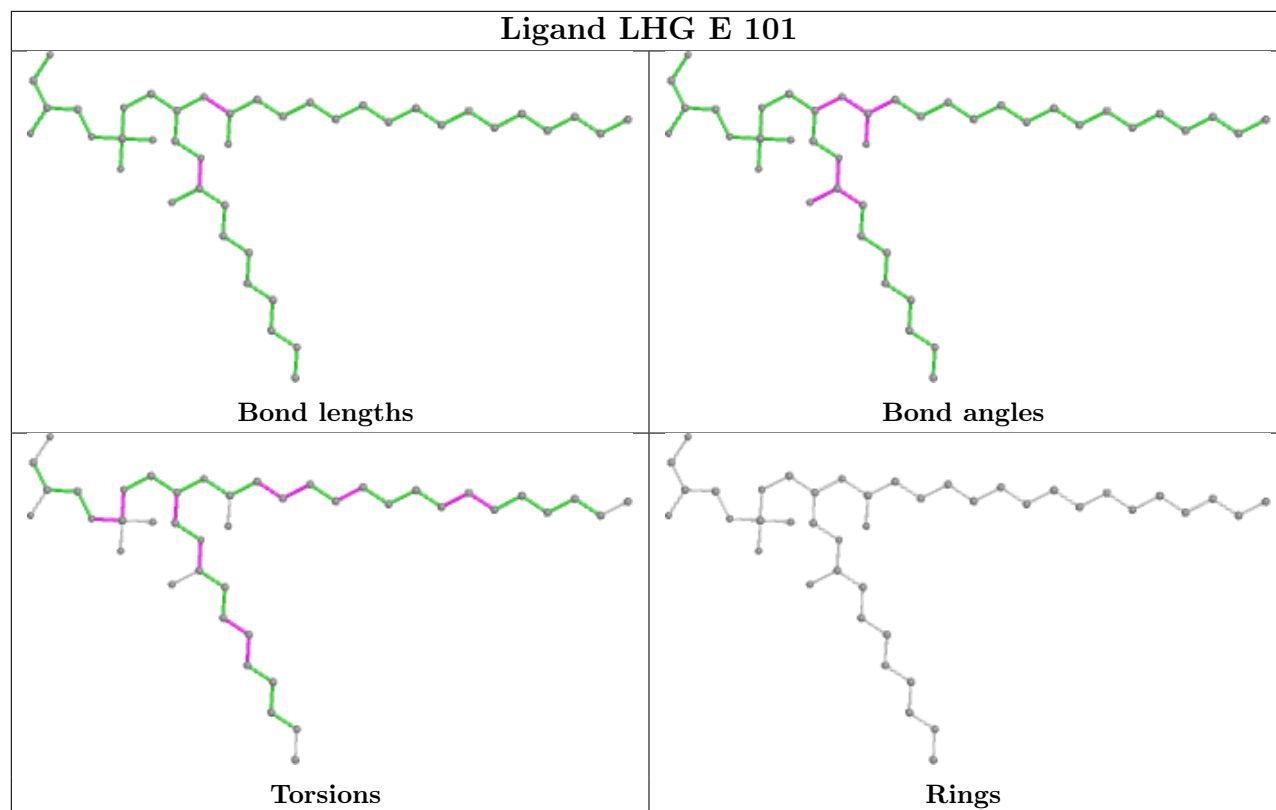


**Ligand CLA B 611****Ligand CLA b 608****Ligand CLA B 604**

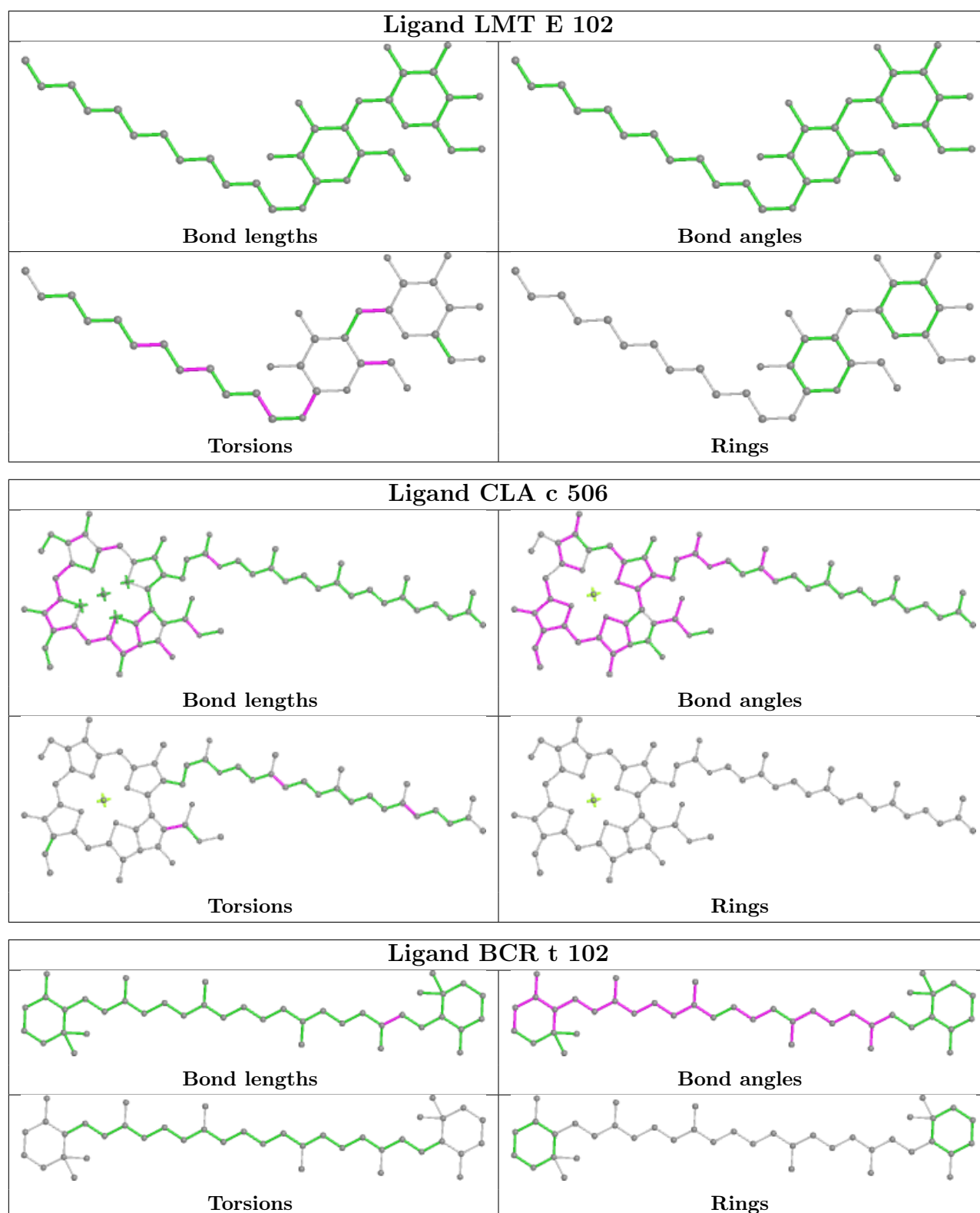
**Ligand CLA c 515****Ligand CLA c 514****Ligand PL9 a 414 (A)**

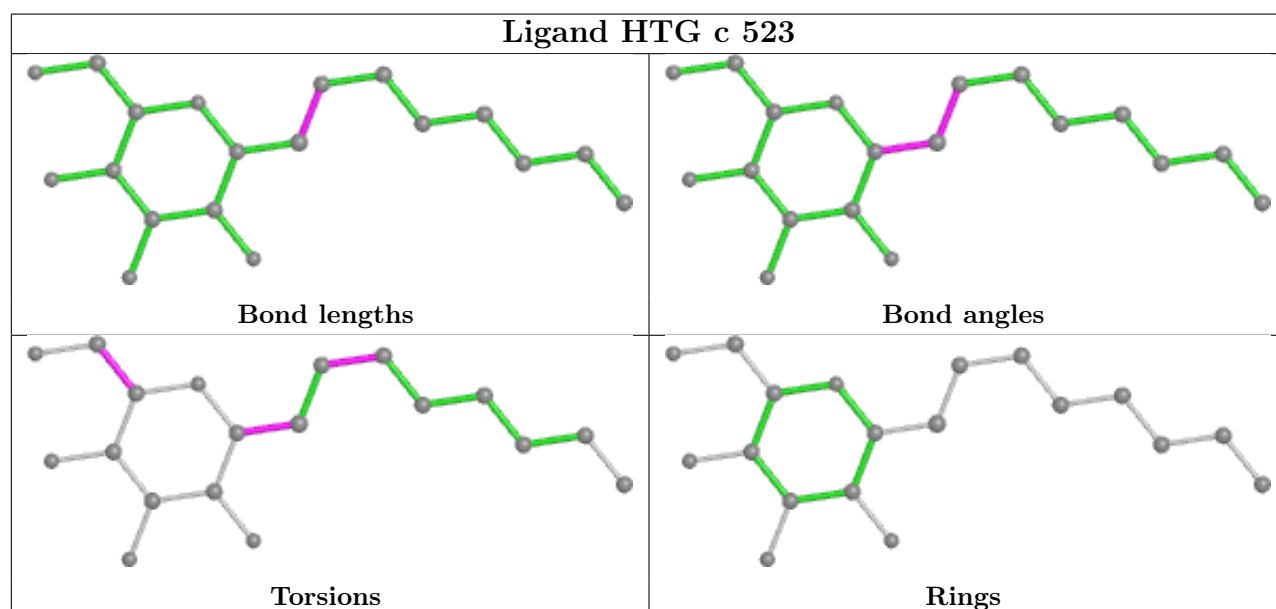
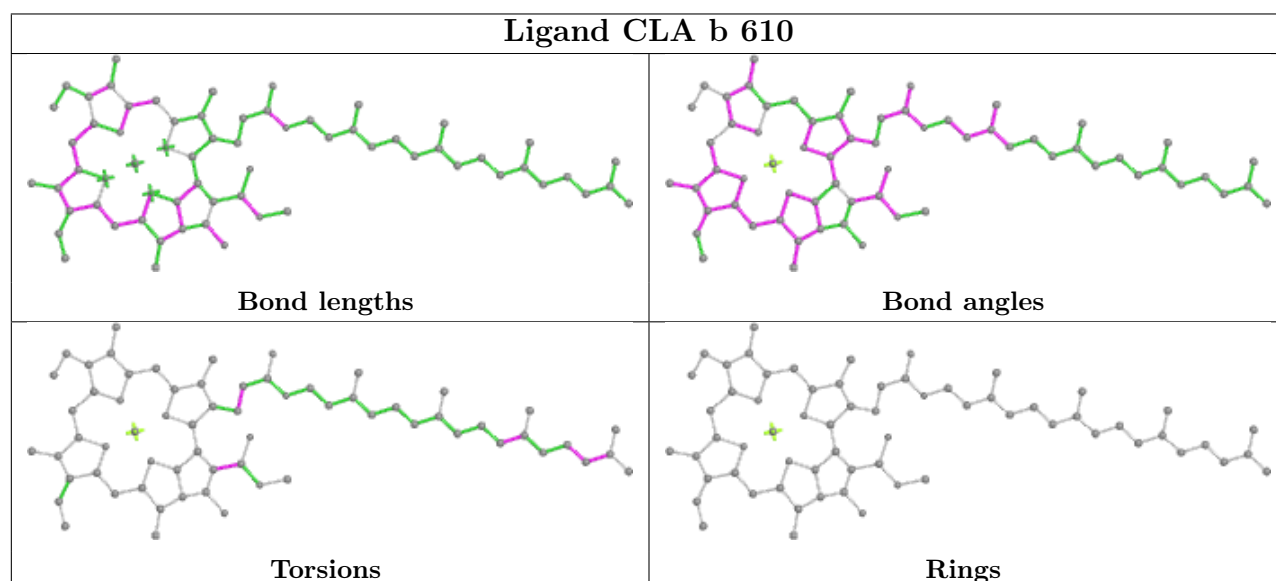
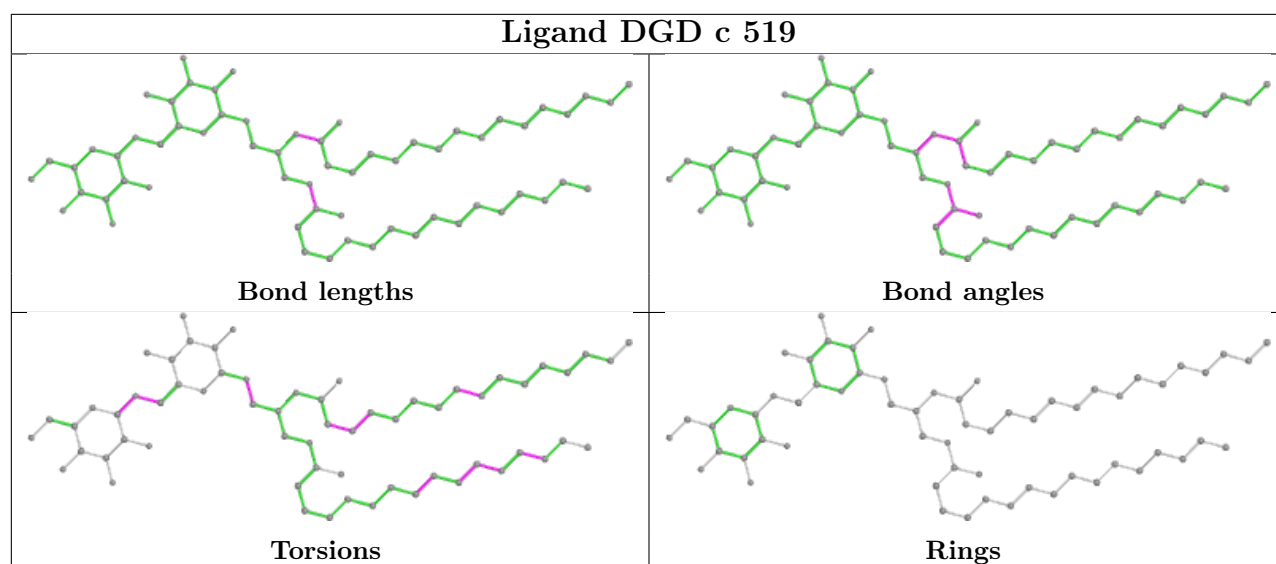
**Ligand CLA B 601****Ligand CLA a 350****Ligand BCR c 516**



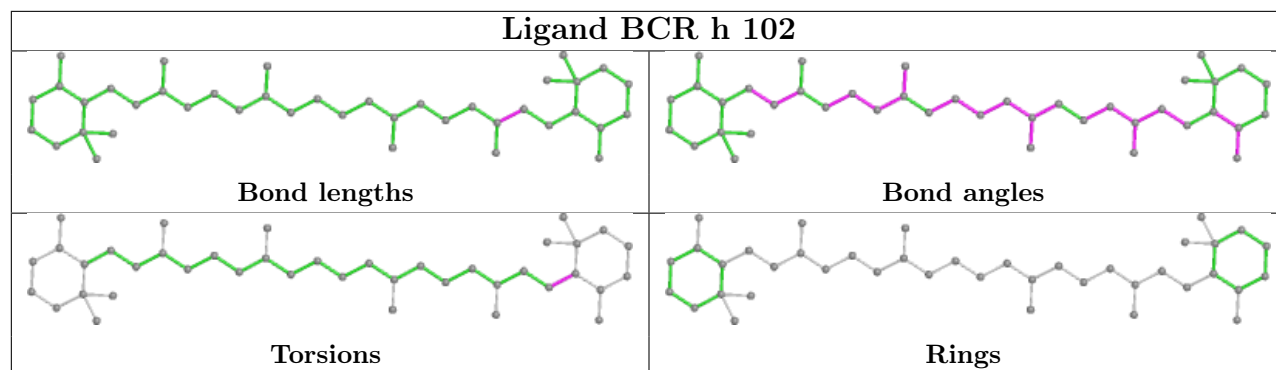




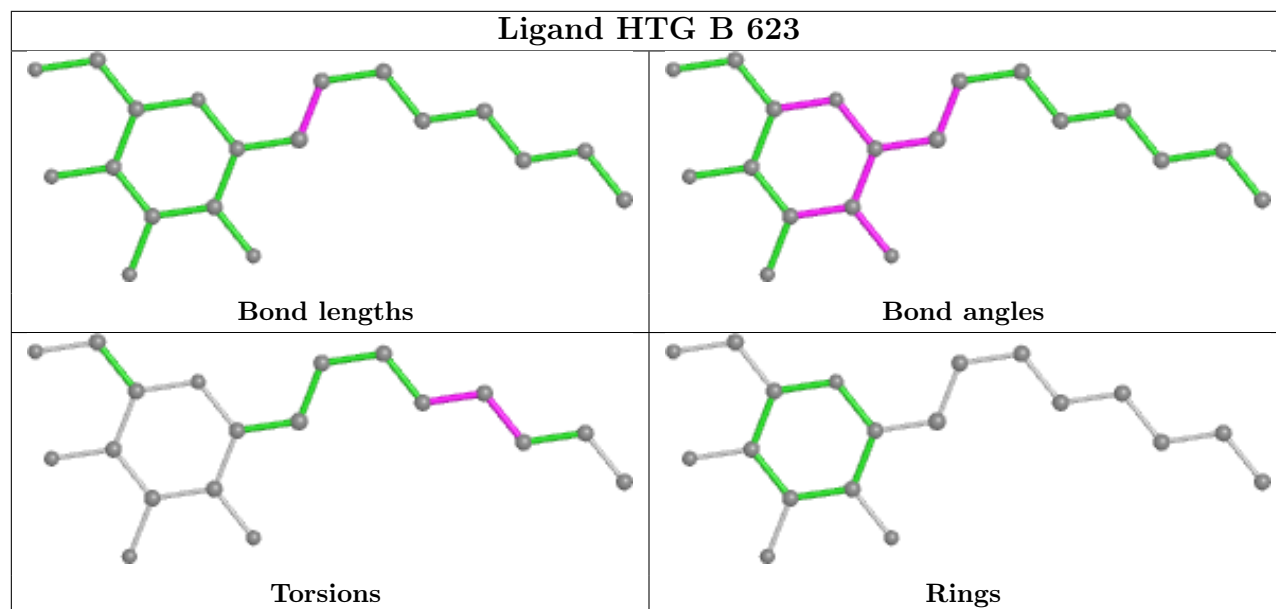




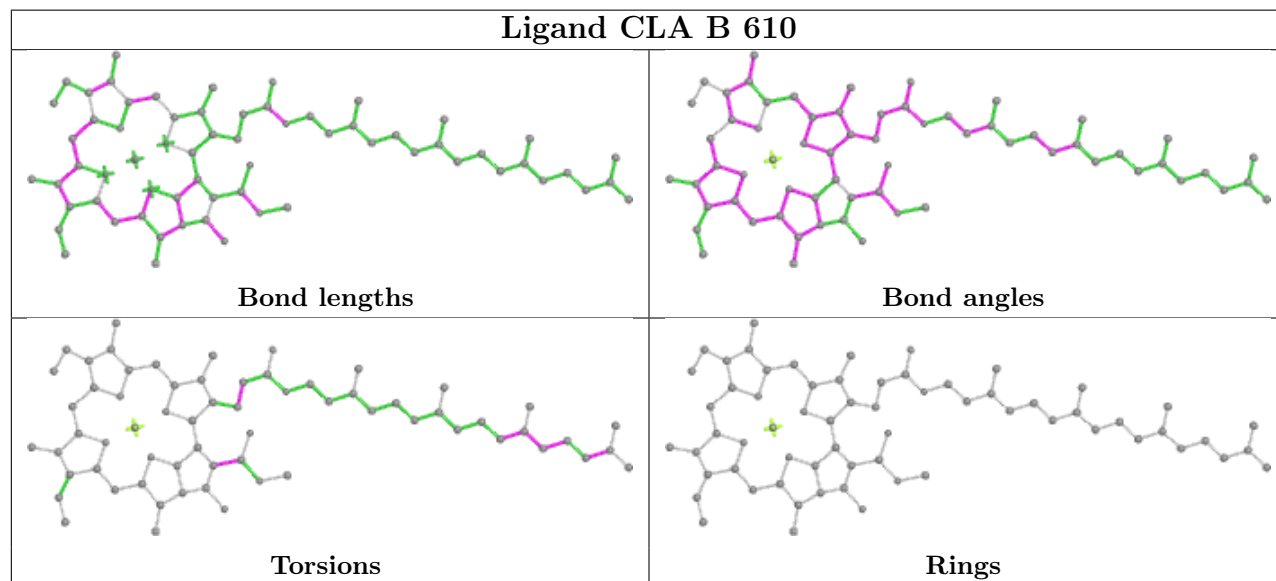
## Ligand BCR h 102

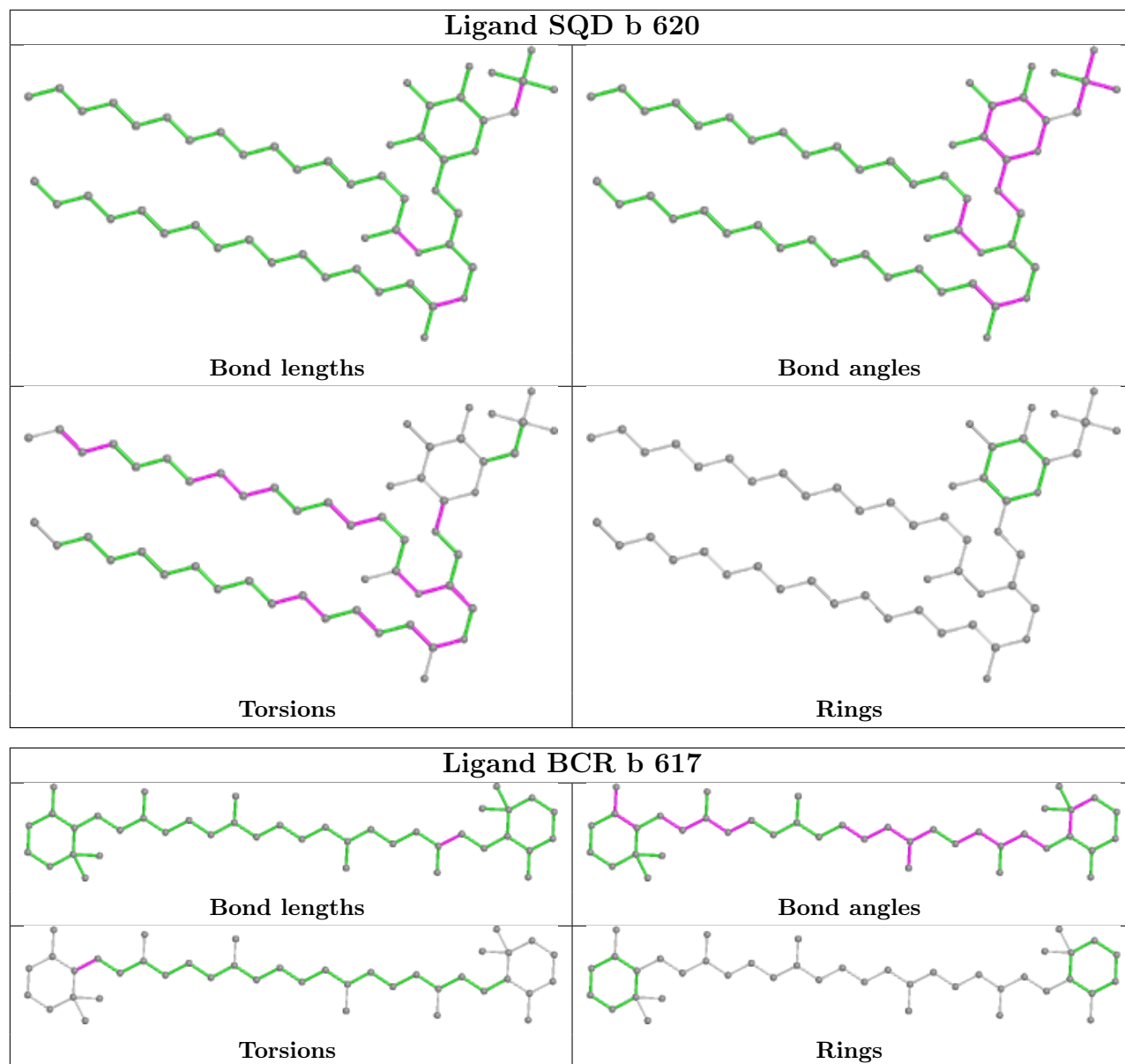


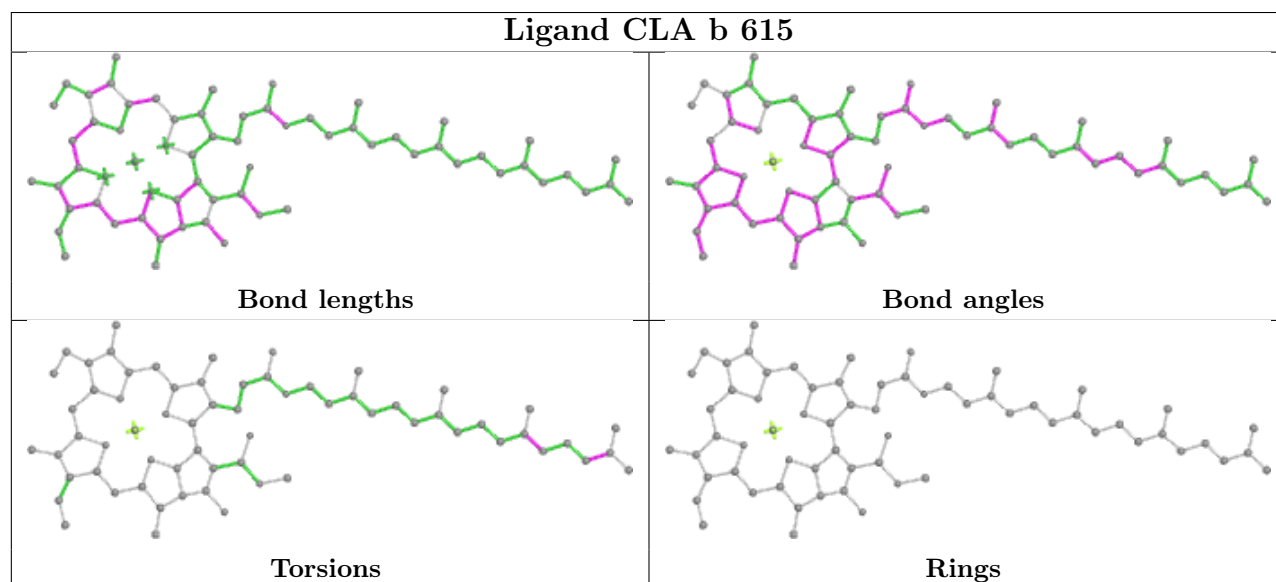
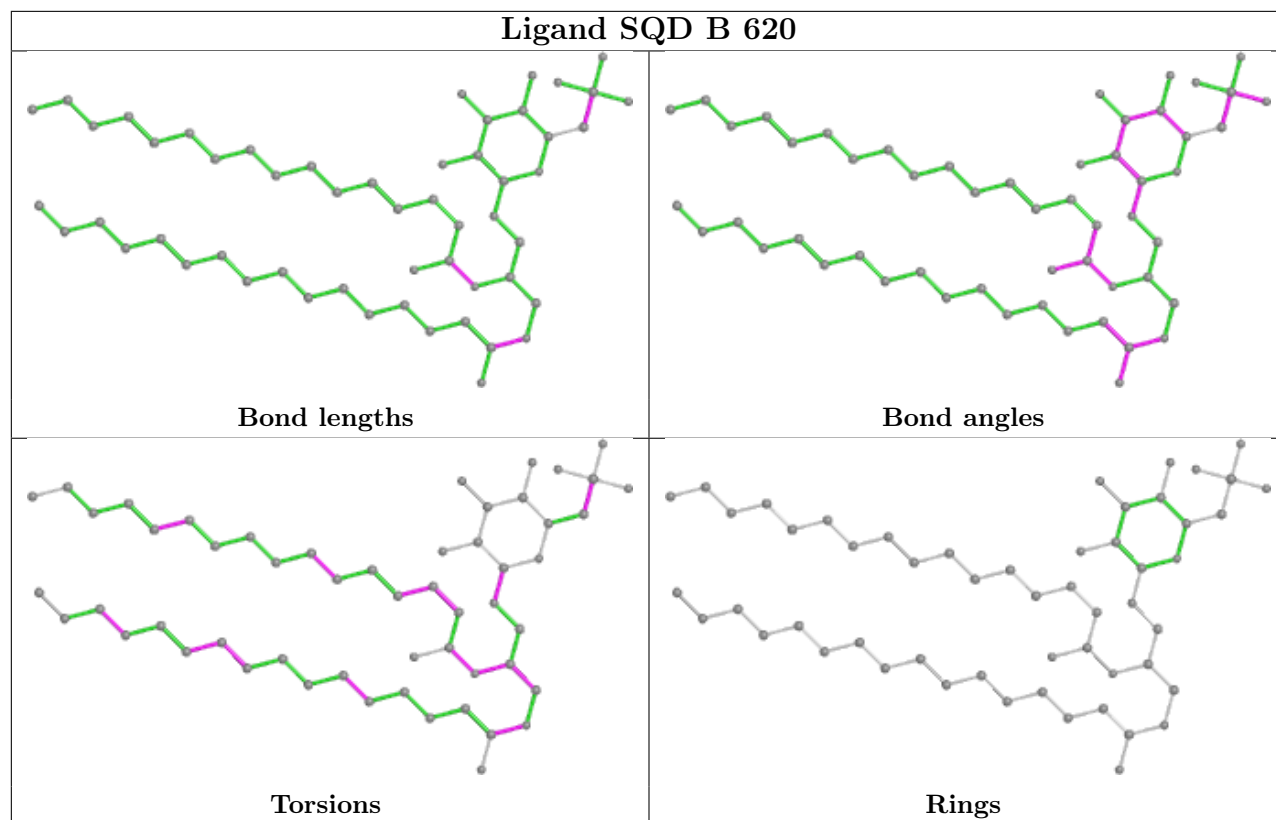
## Ligand HTG B 623

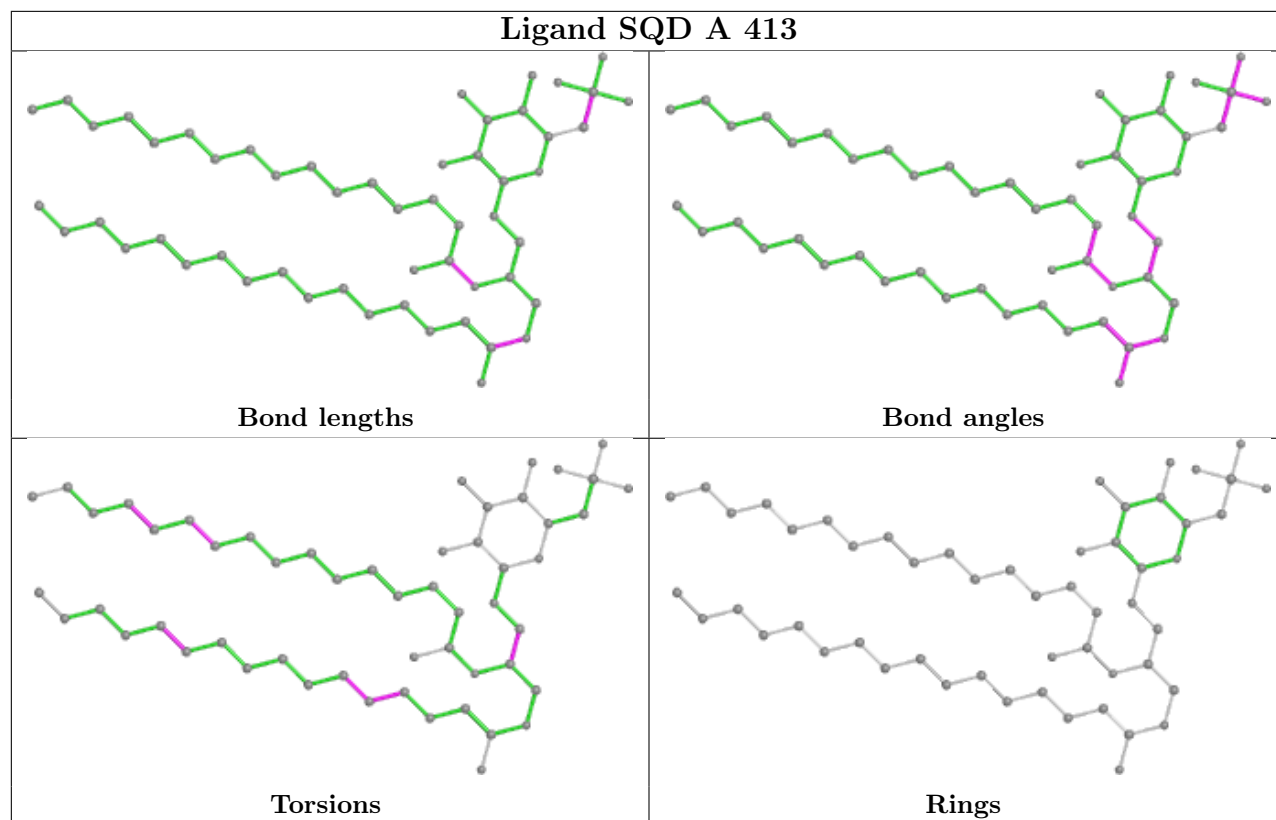


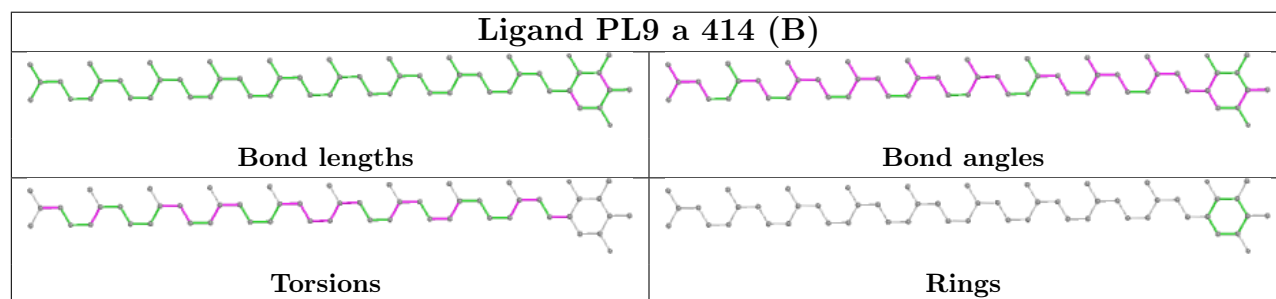
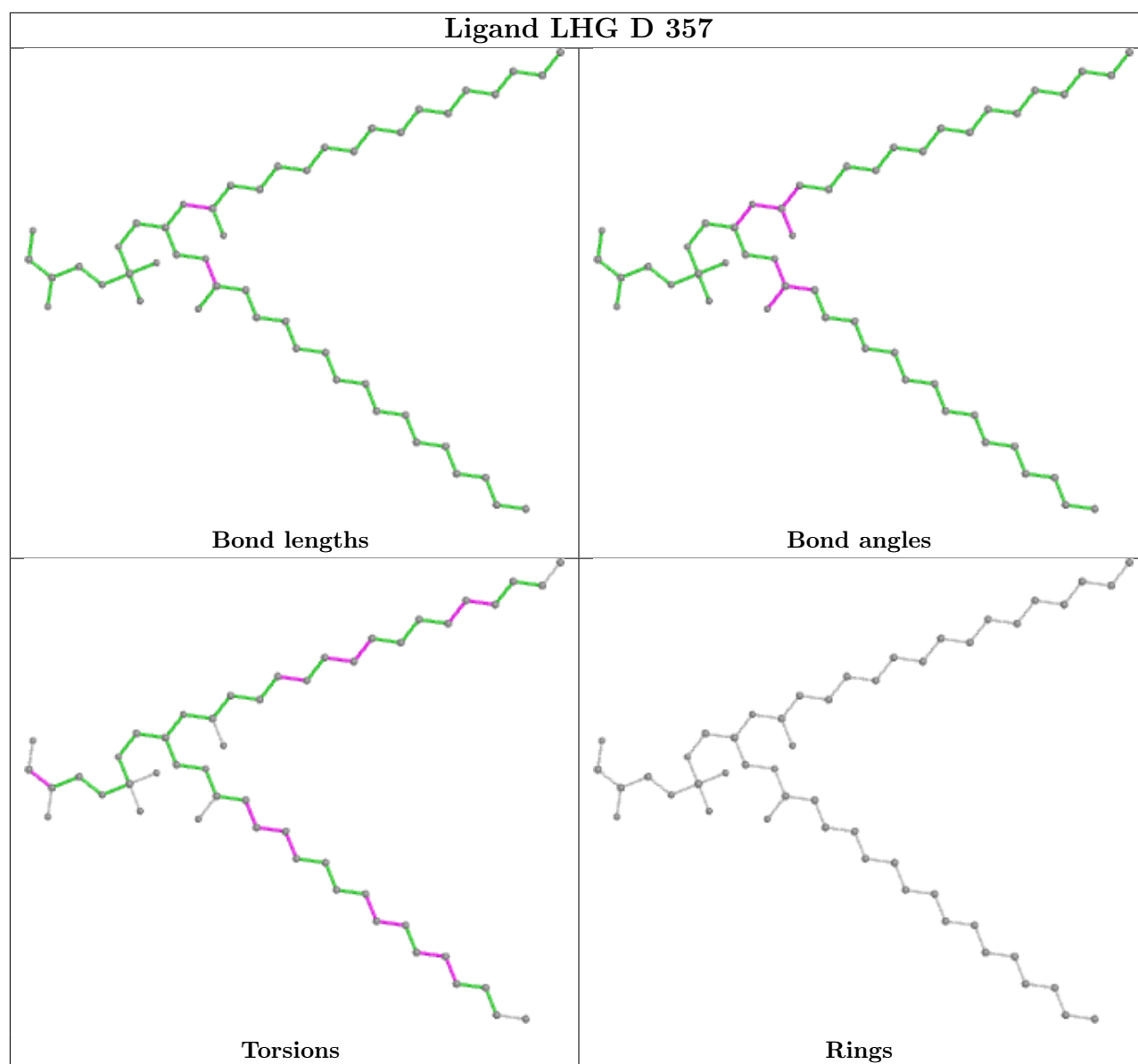
## Ligand CLA B 610

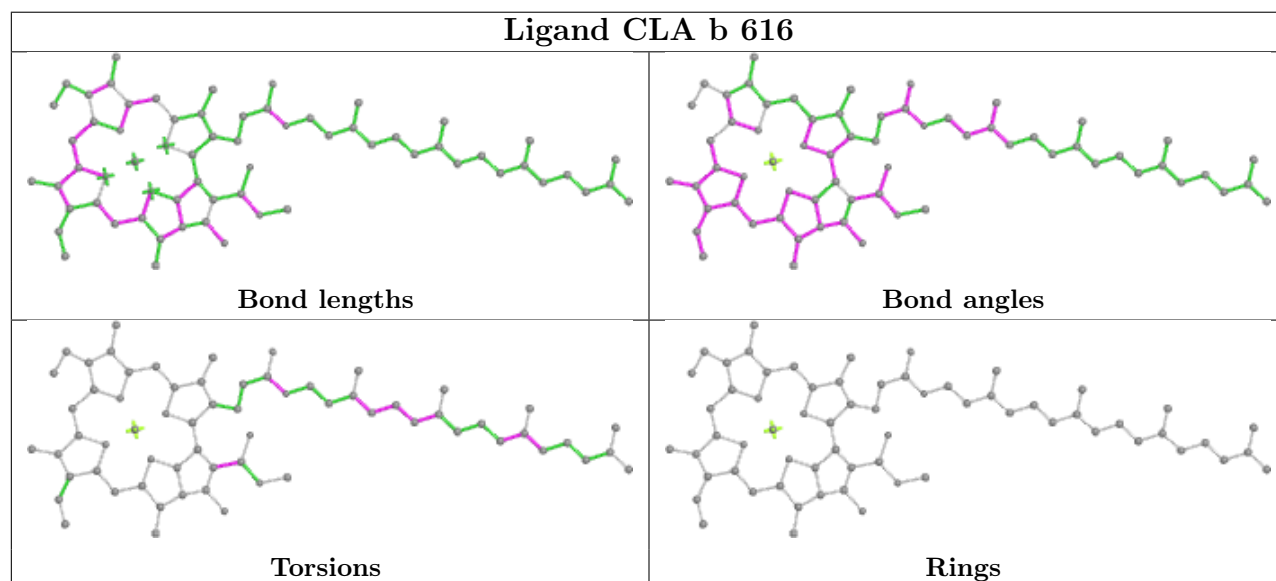
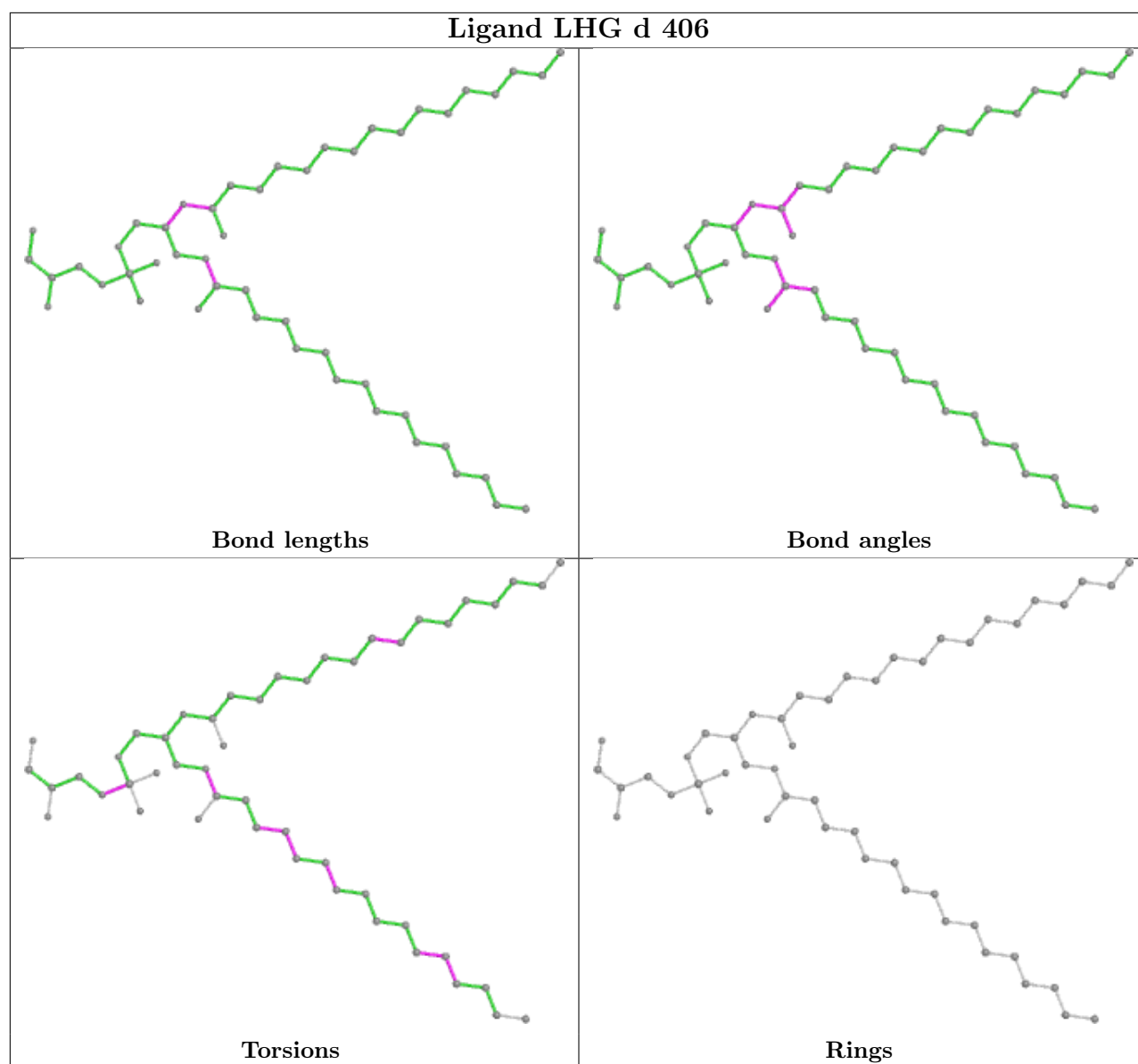




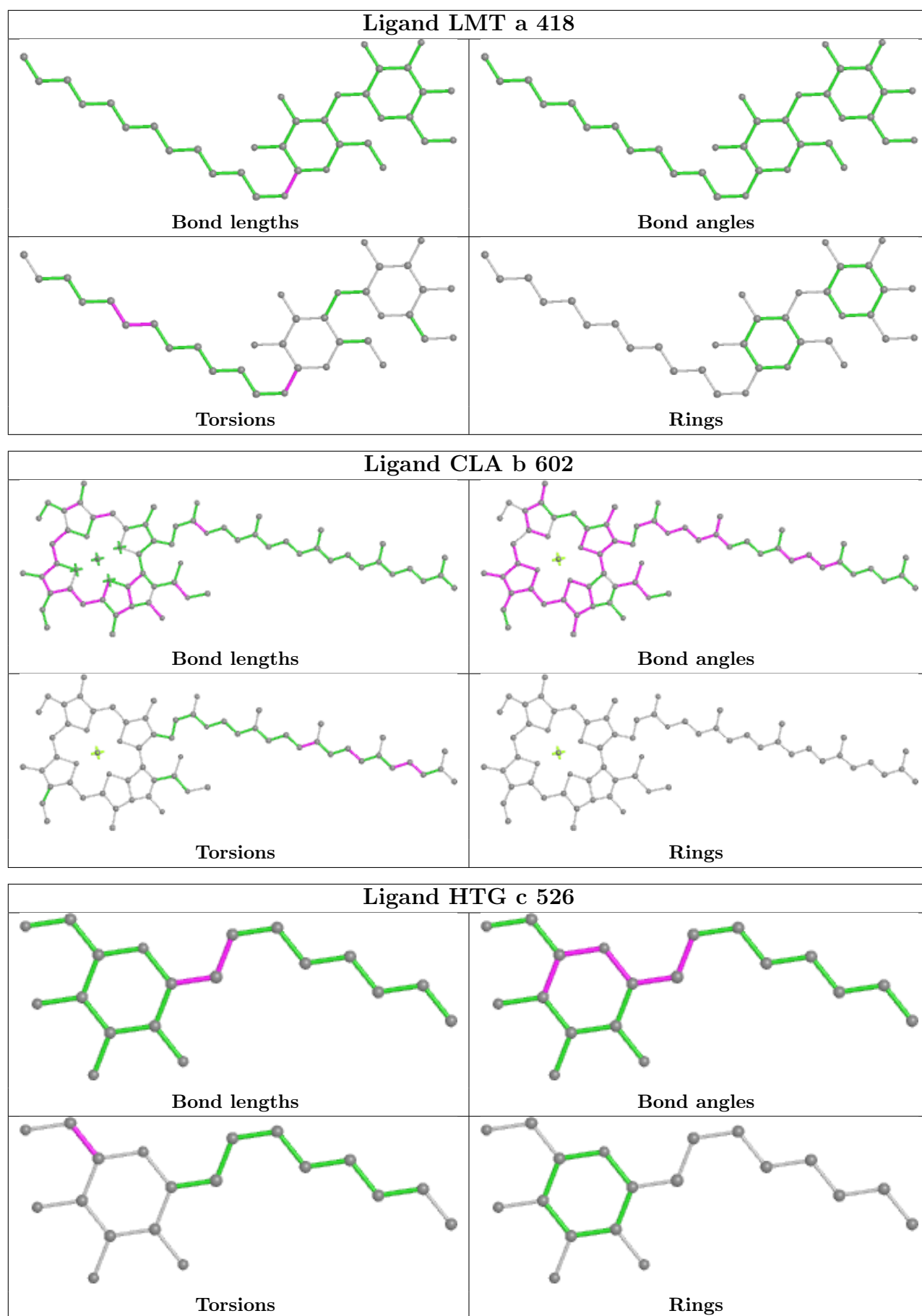




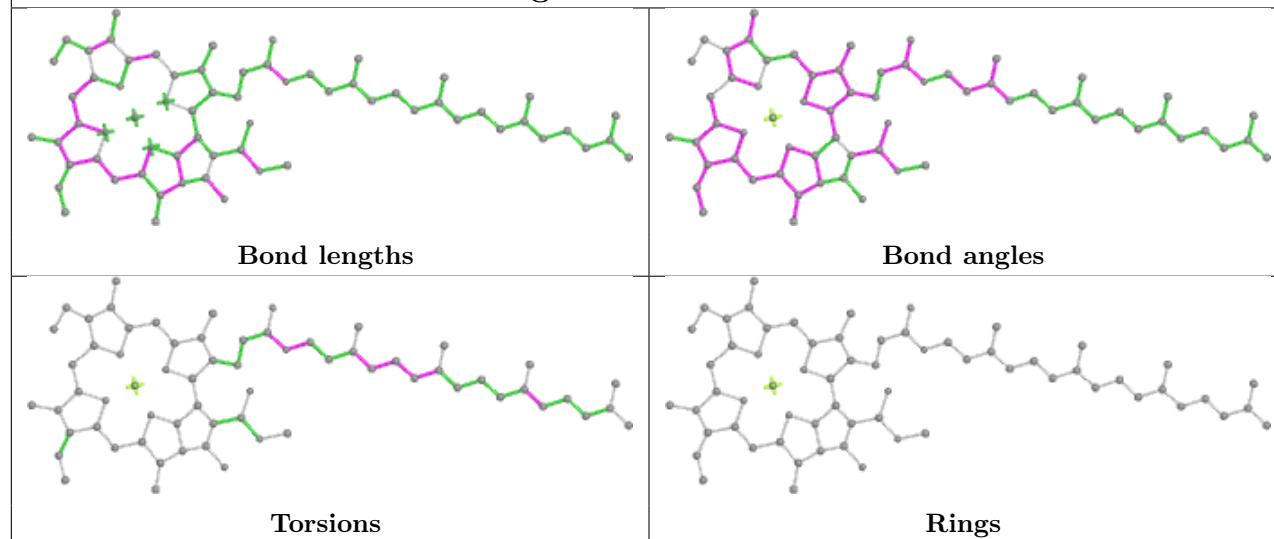




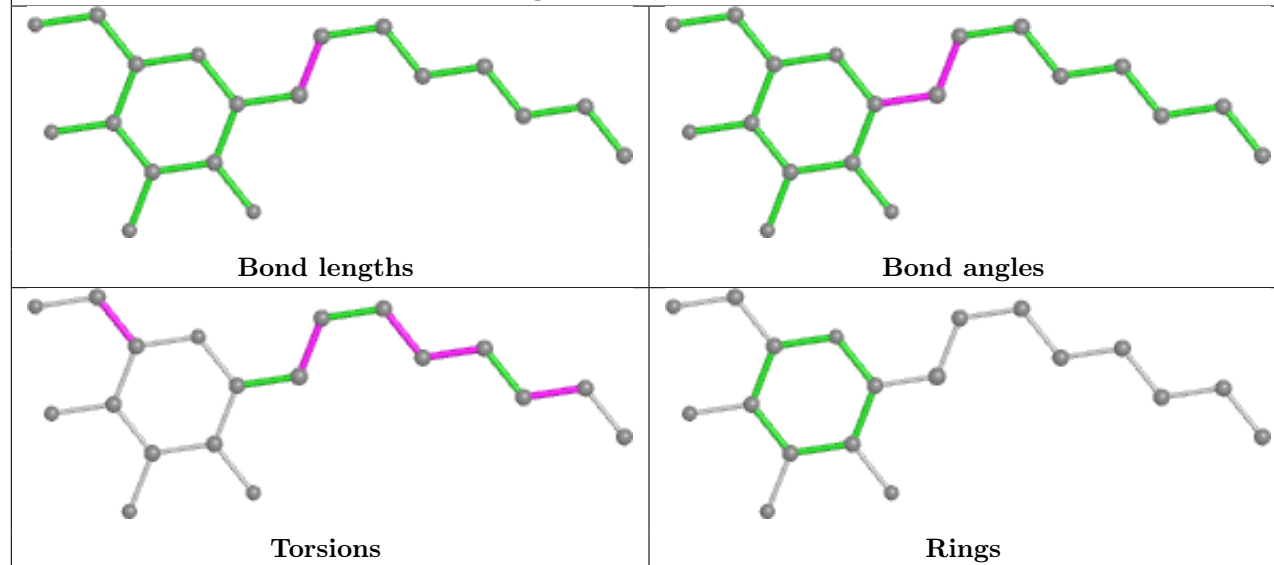




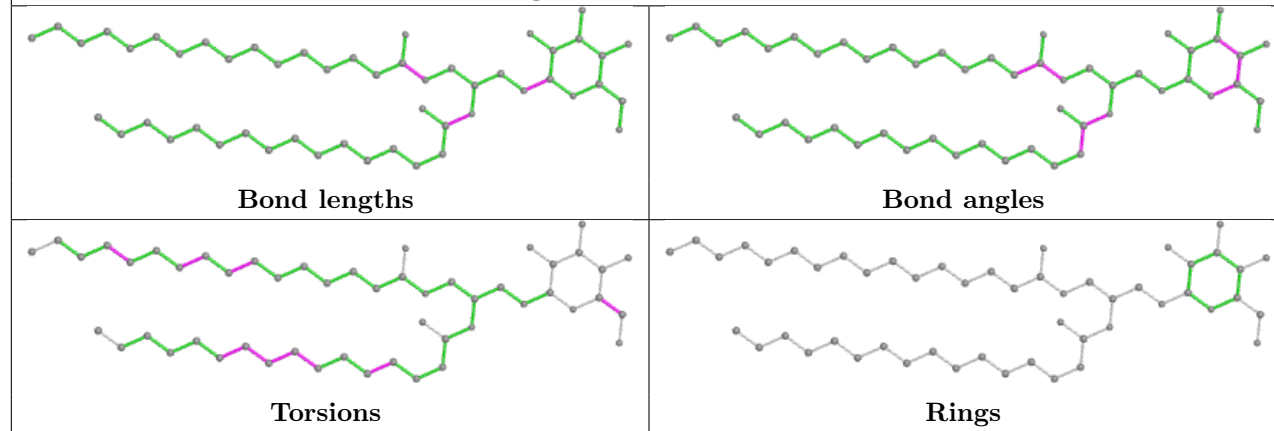
## Ligand CLA A 409

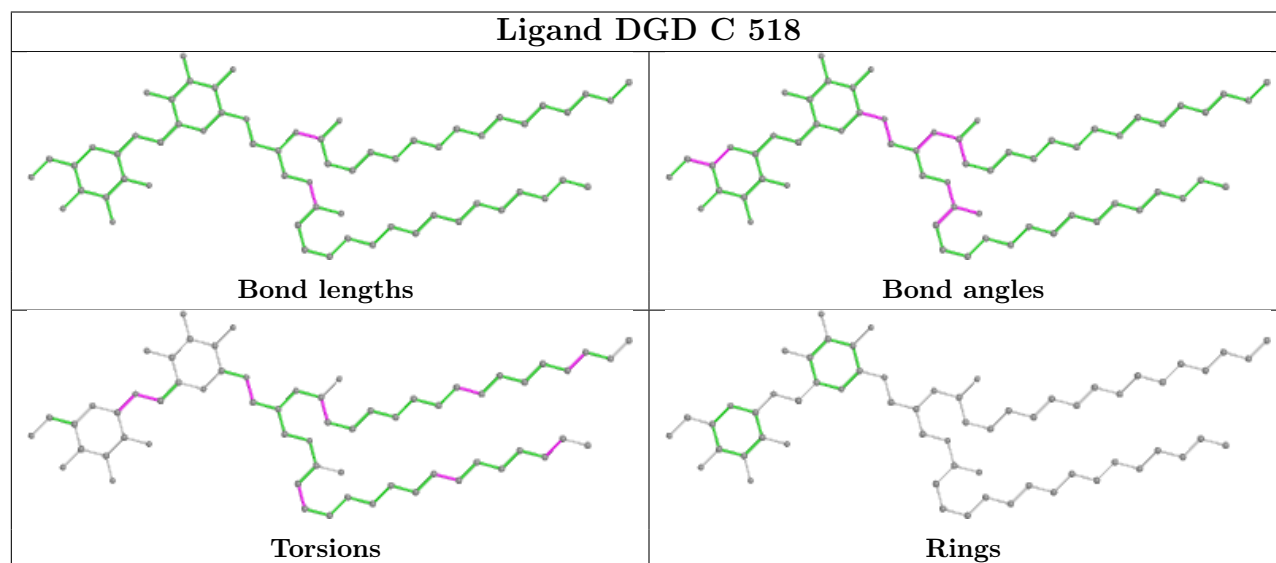
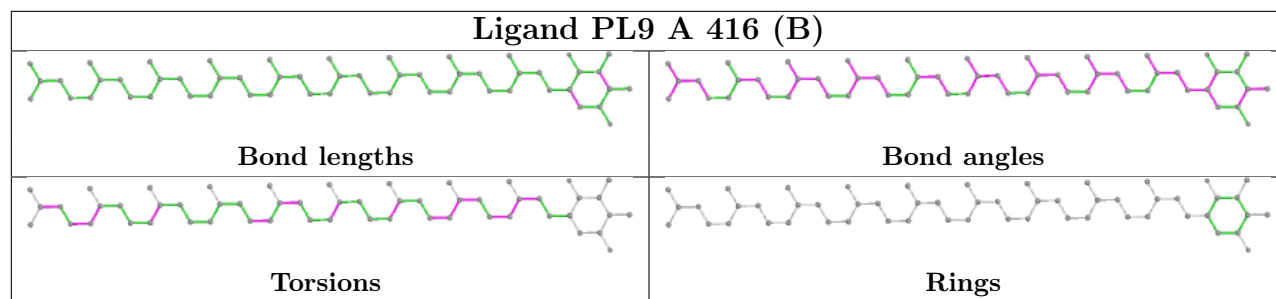


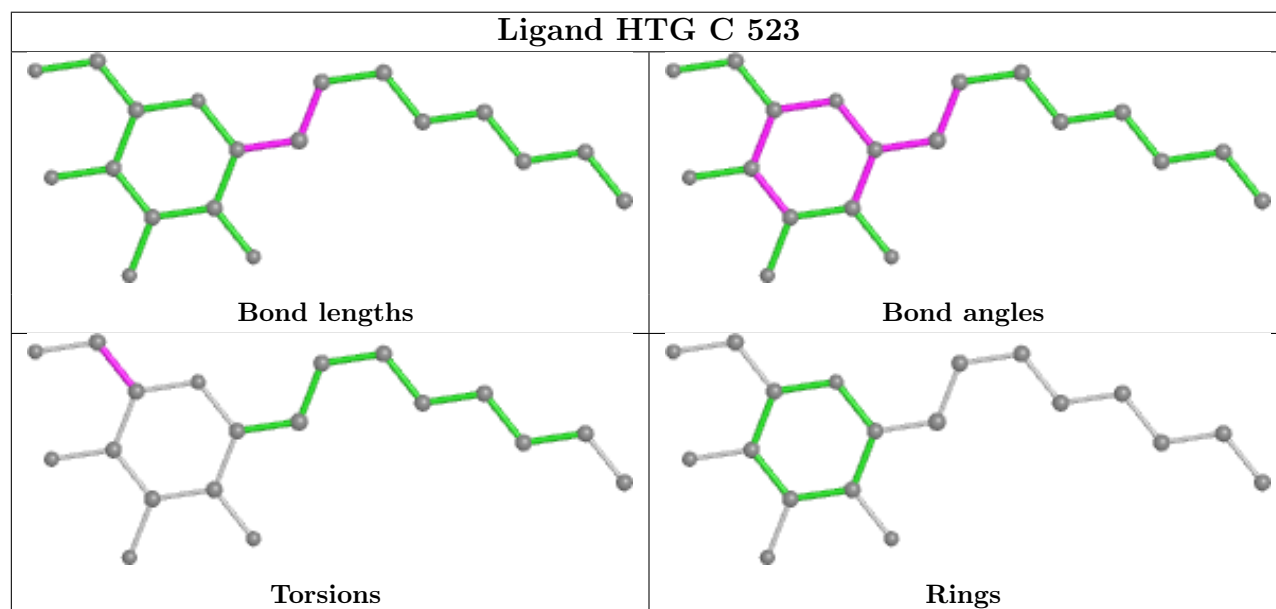
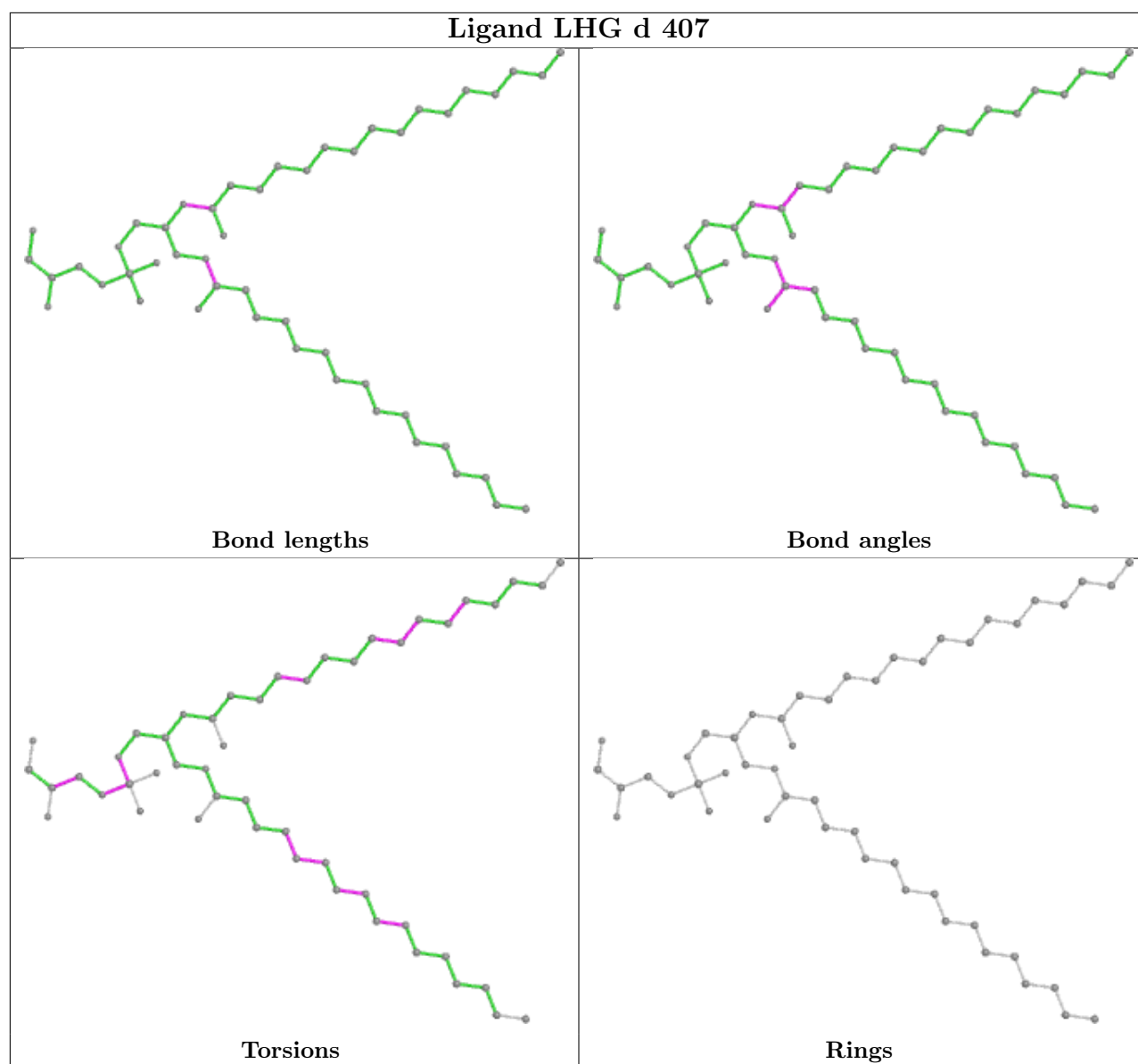
## Ligand HTG B 624



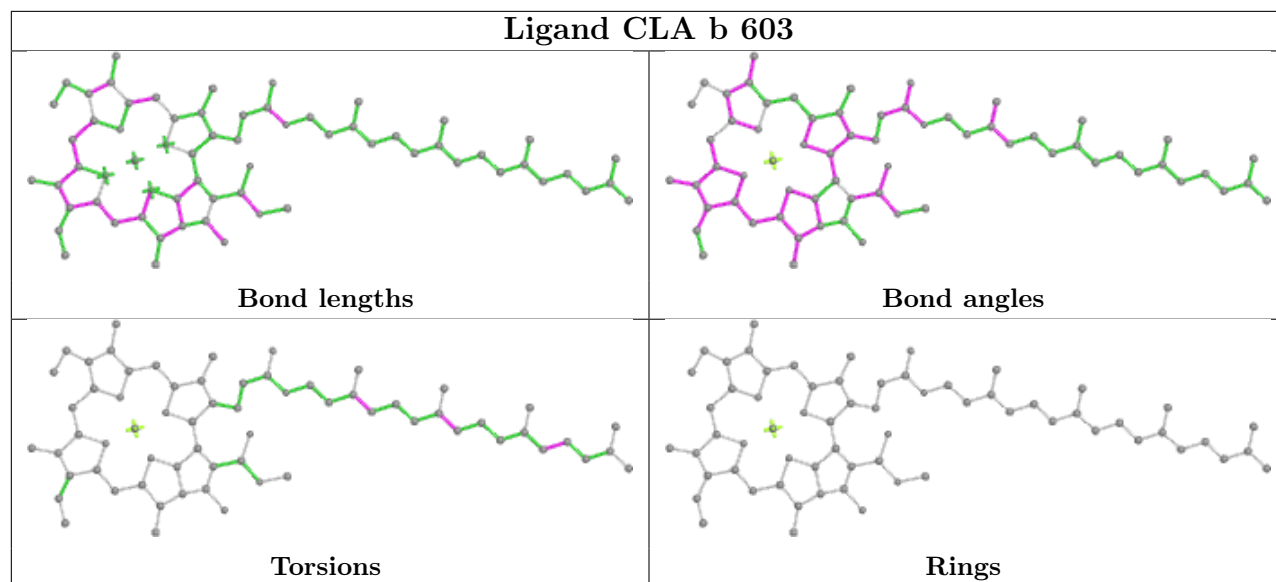
## Ligand LMG C 521



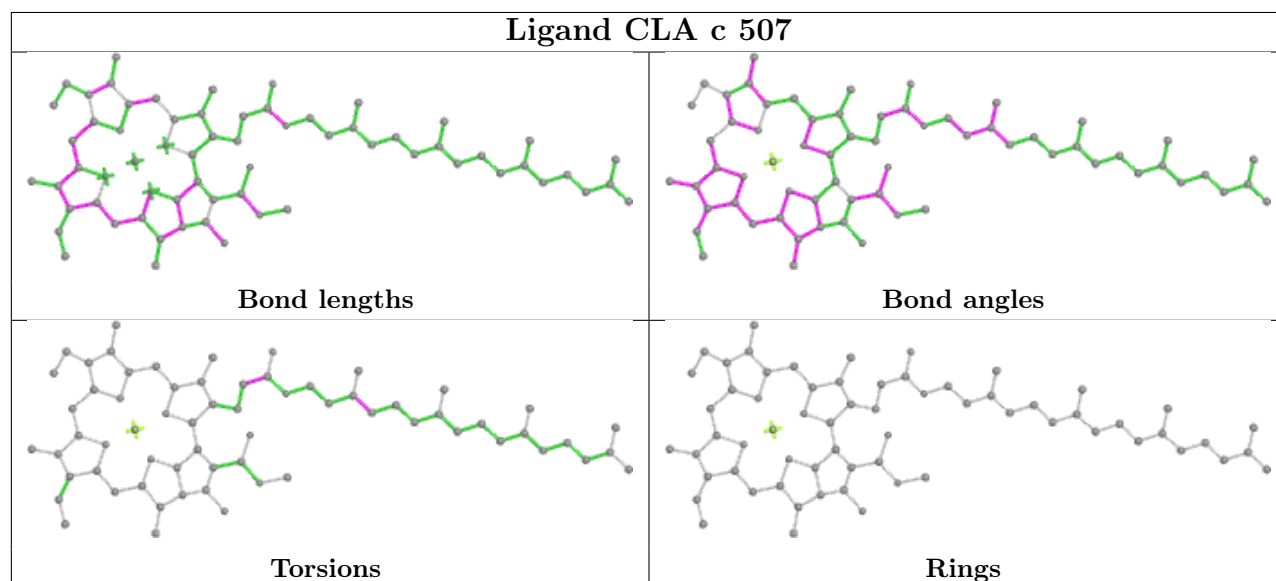




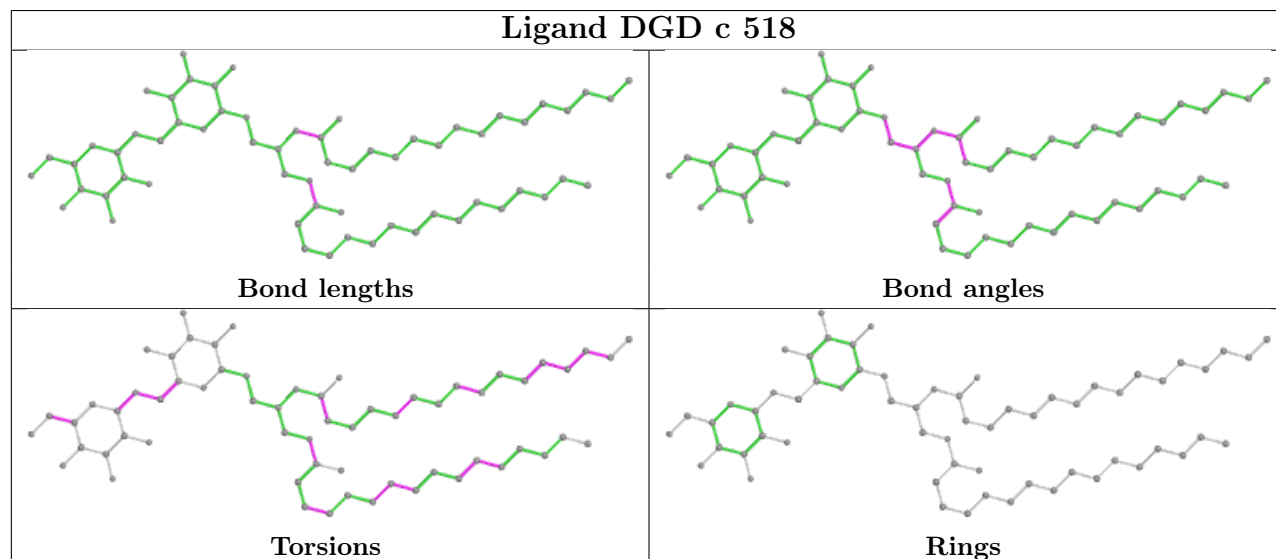
## Ligand CLA b 603



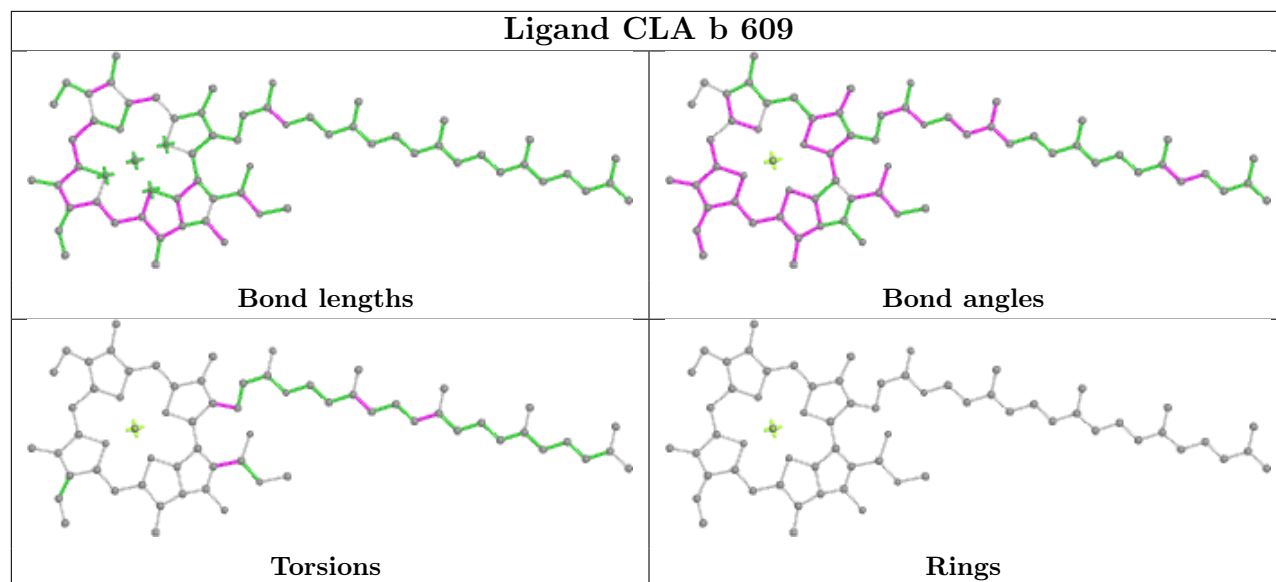
## Ligand CLA c 507



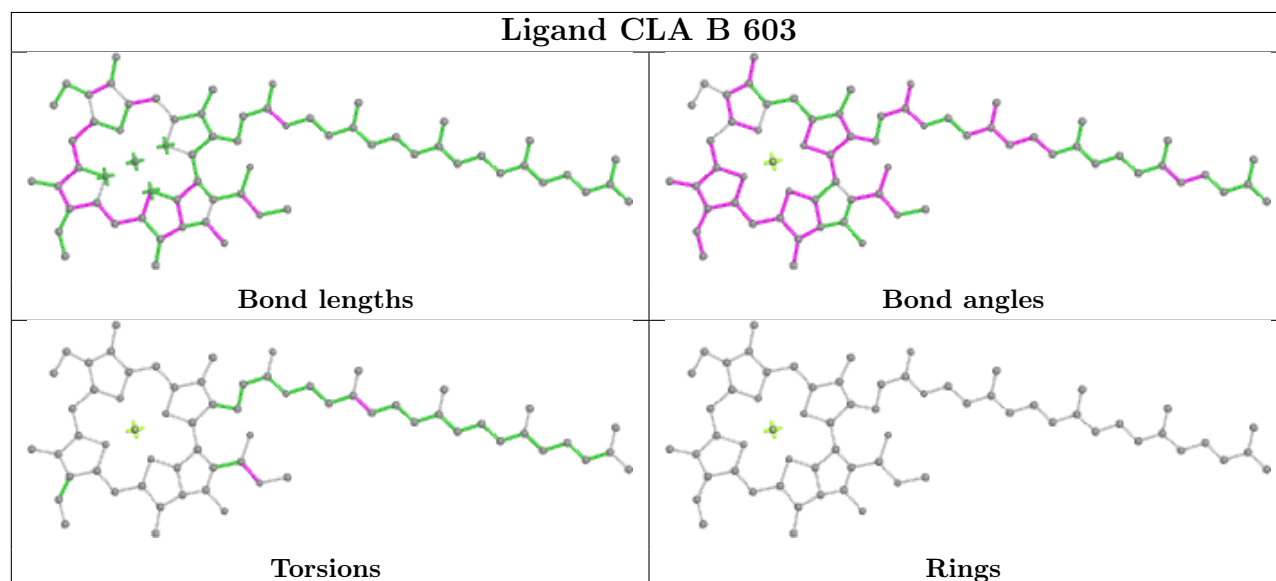
## Ligand DGD c 518



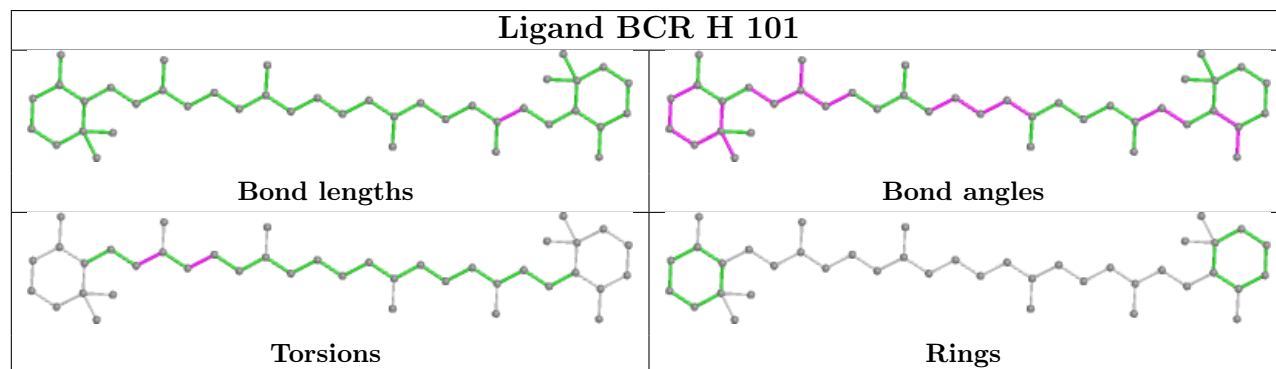
## Ligand CLA b 609

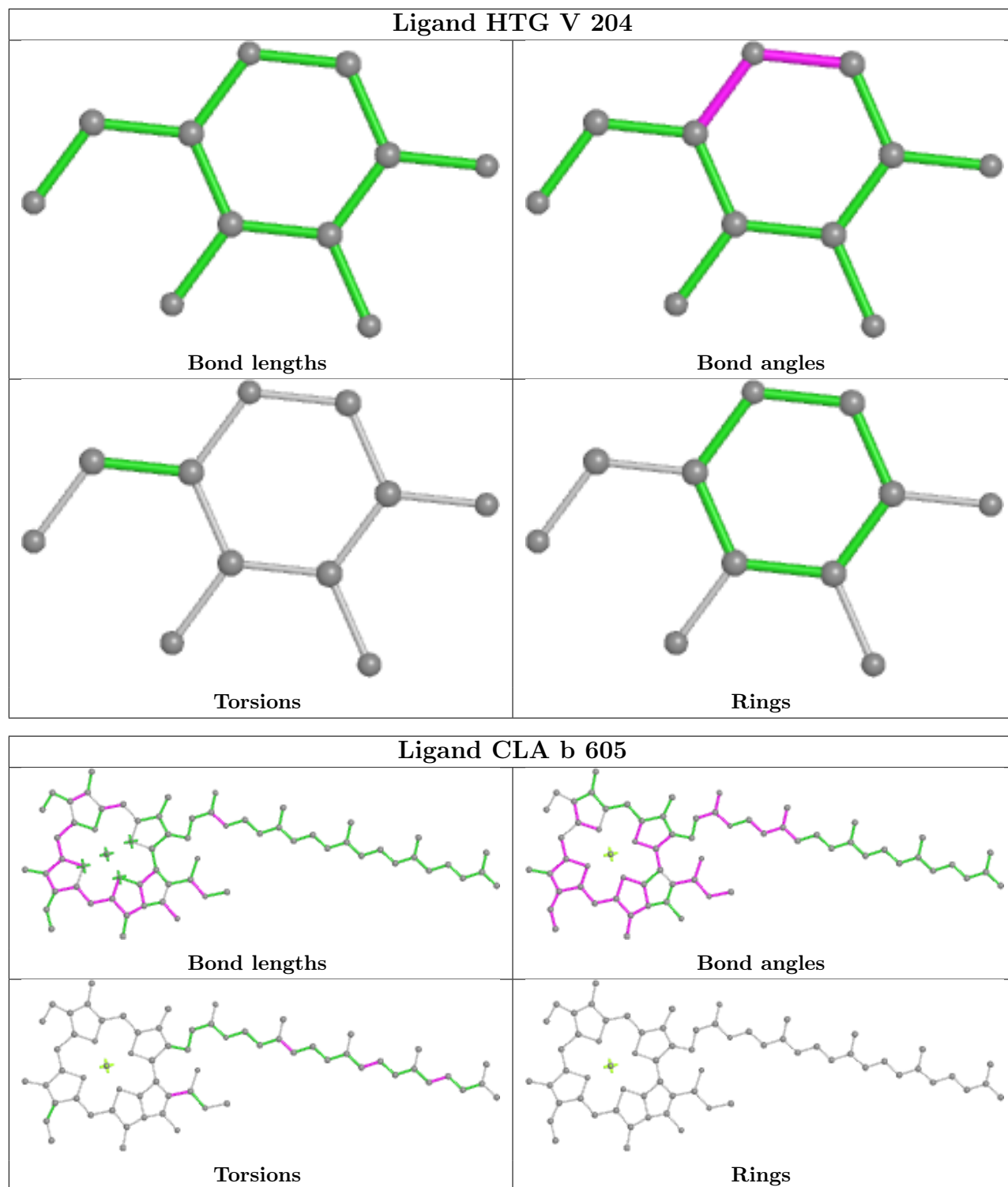


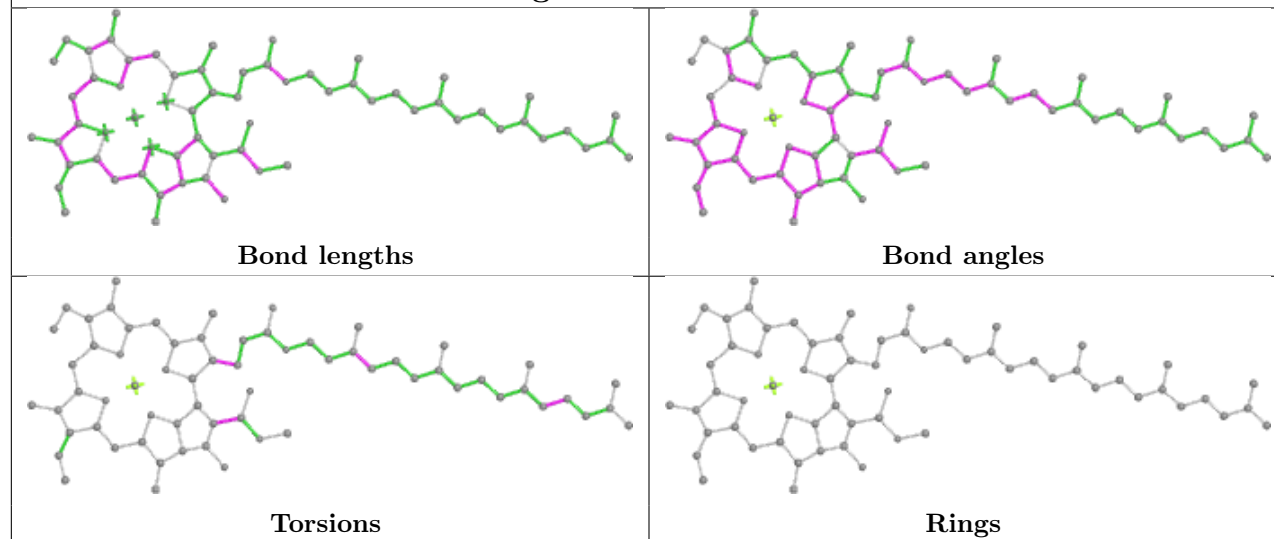
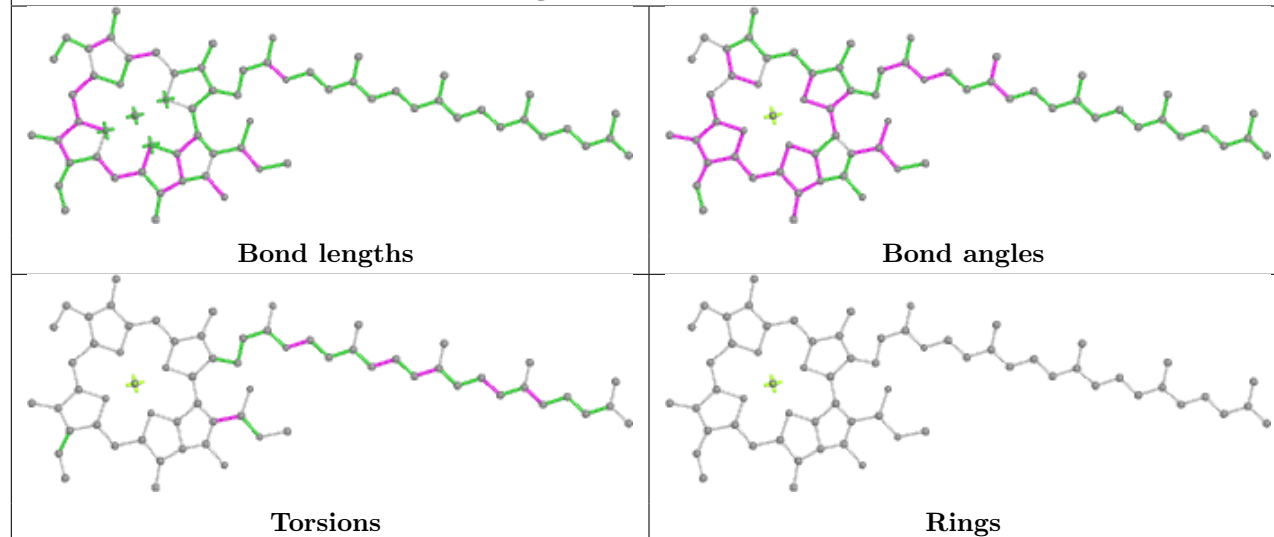
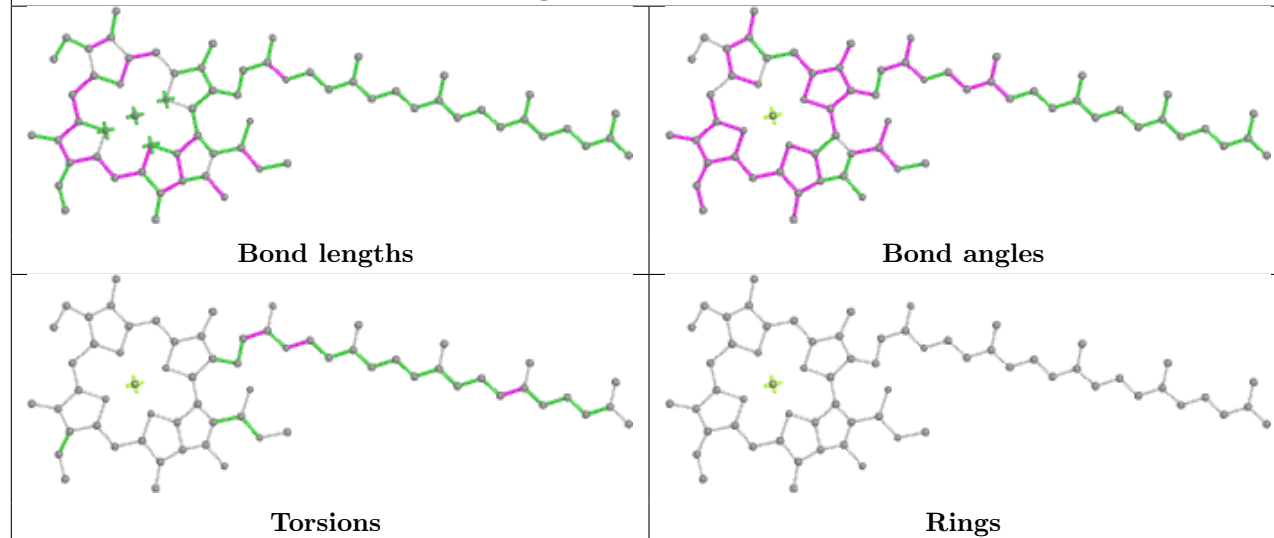
## Ligand CLA B 603



## Ligand BCR H 101

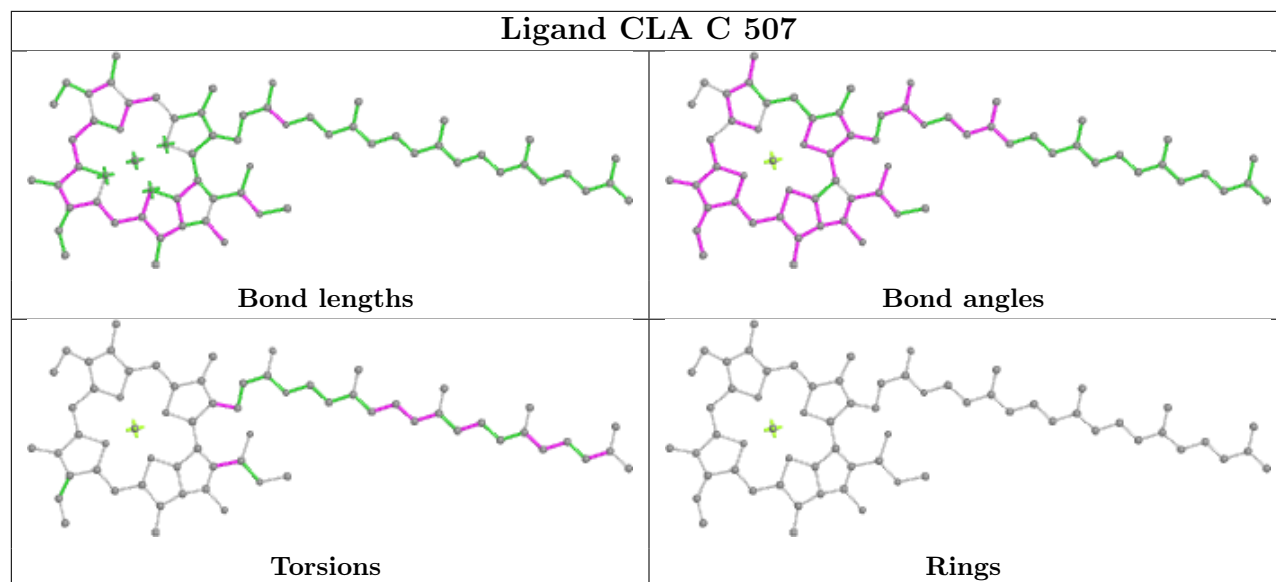




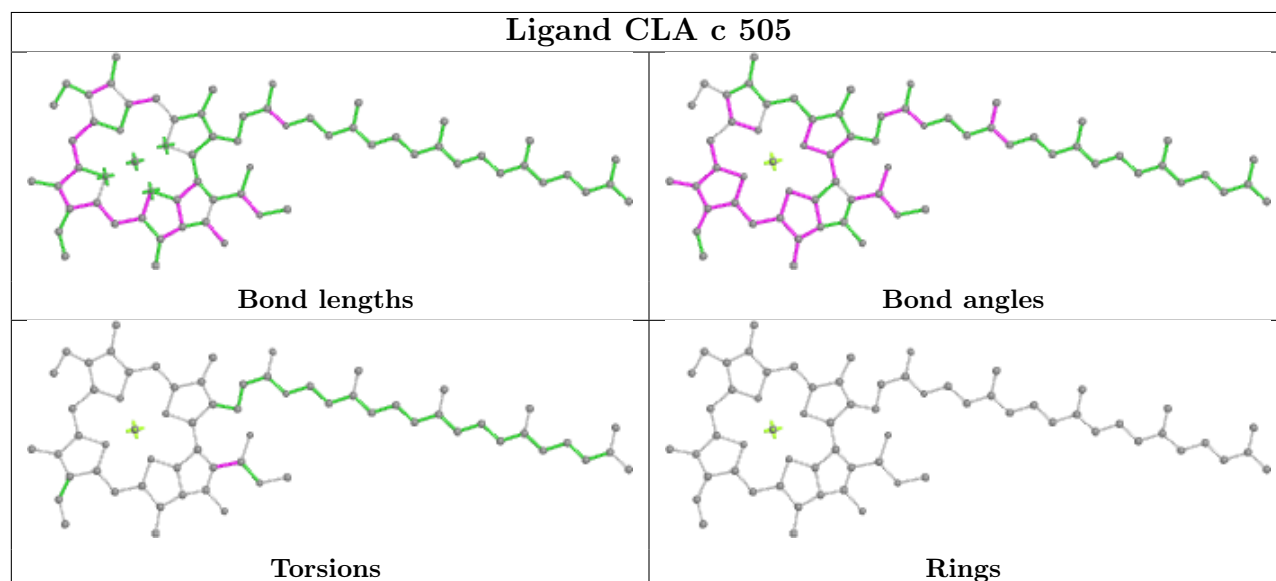
**Ligand CLA B 609****Ligand CLA B 616****Ligand CLA d 402**



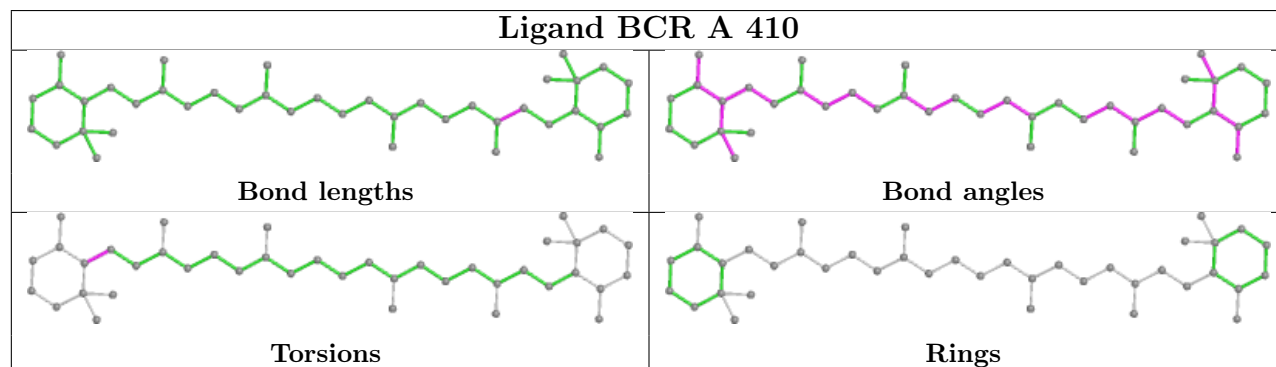
## Ligand CLA C 507

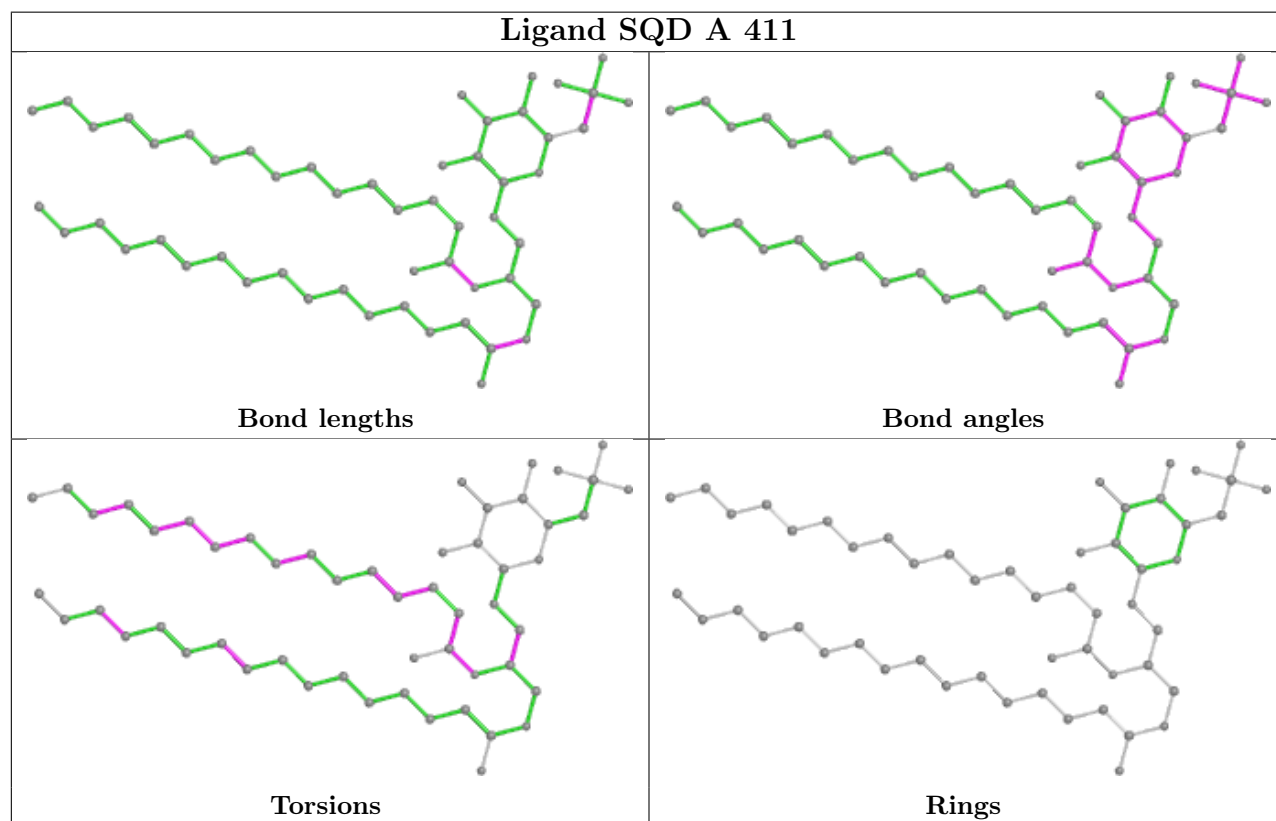
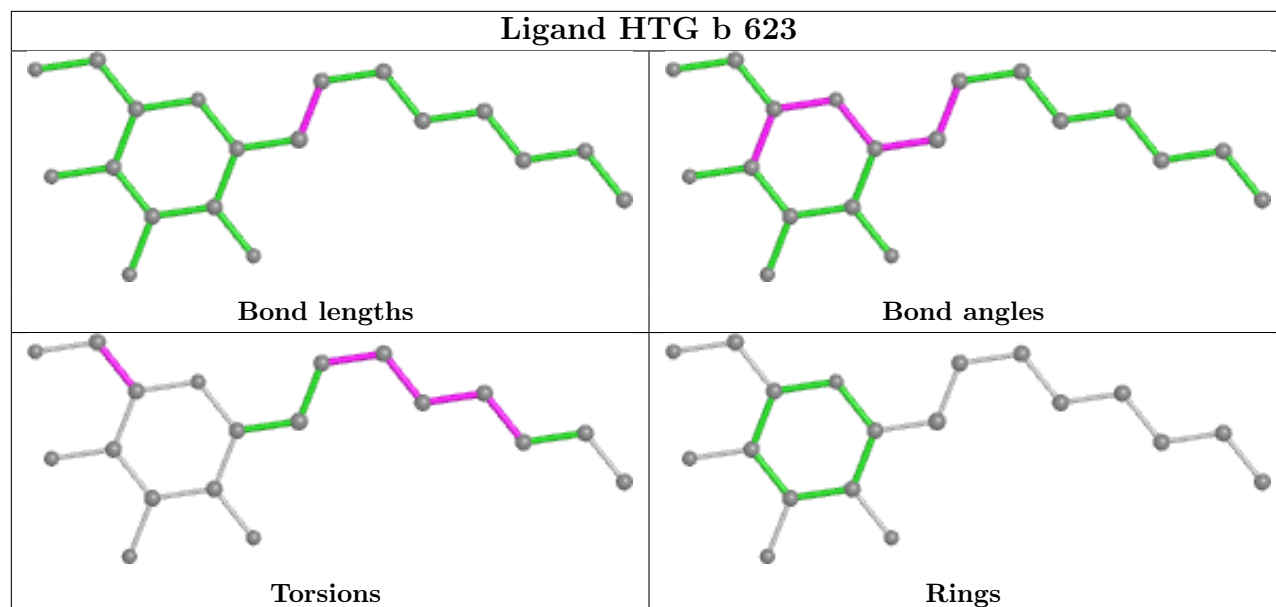


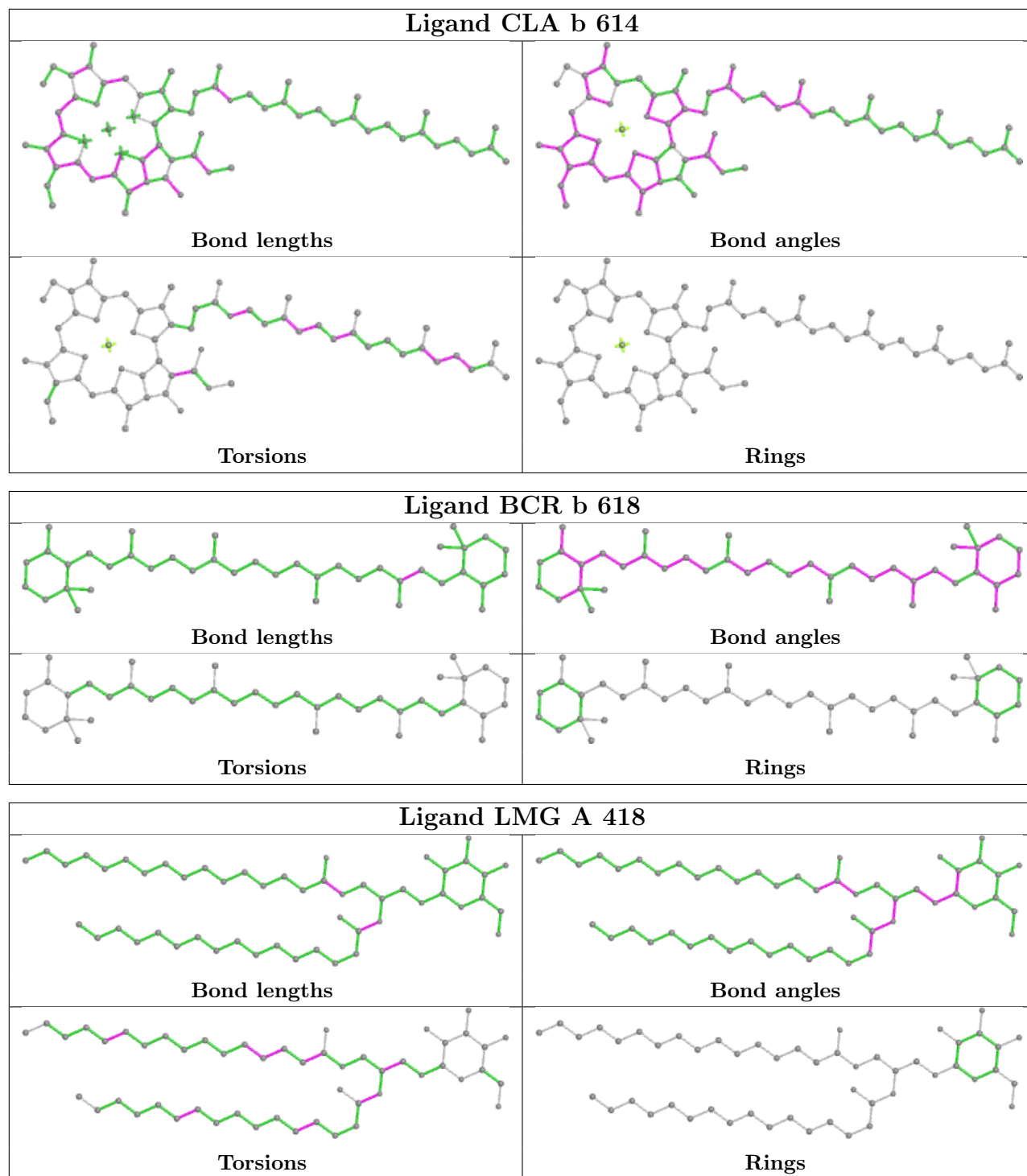
## Ligand CLA c 505

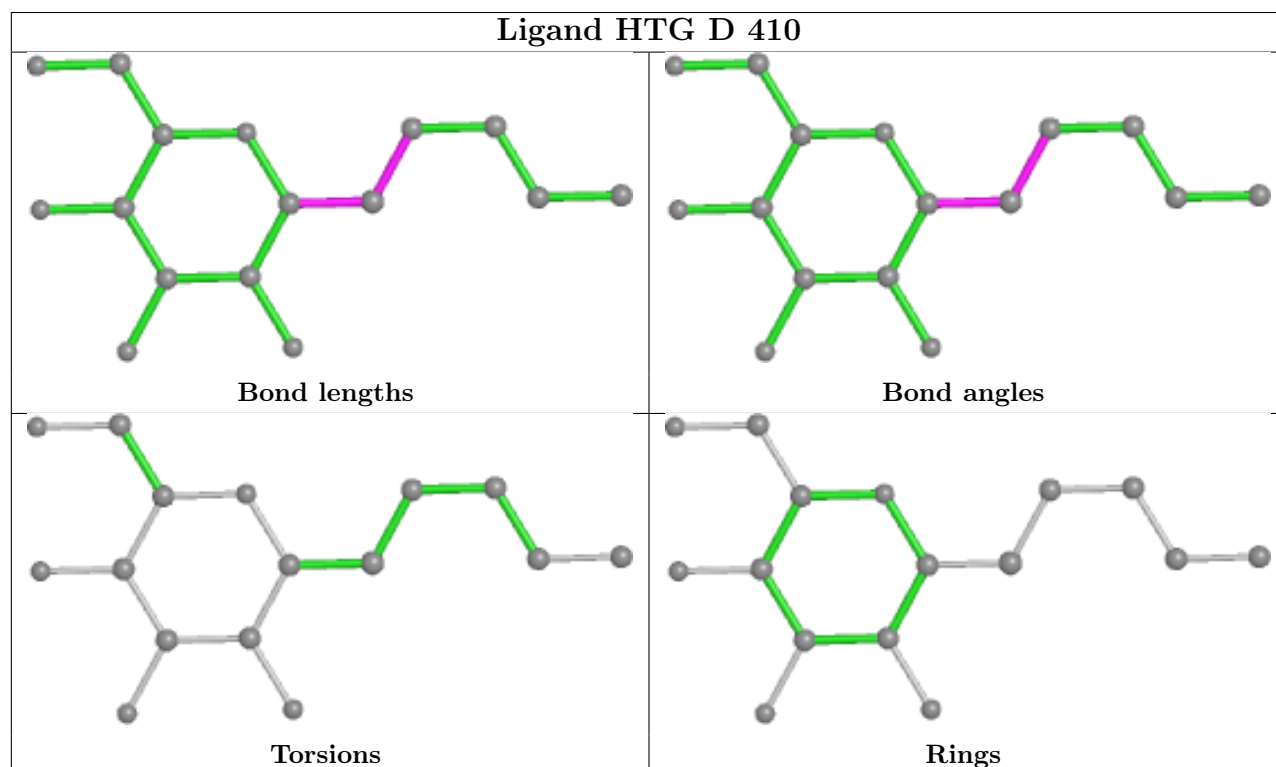
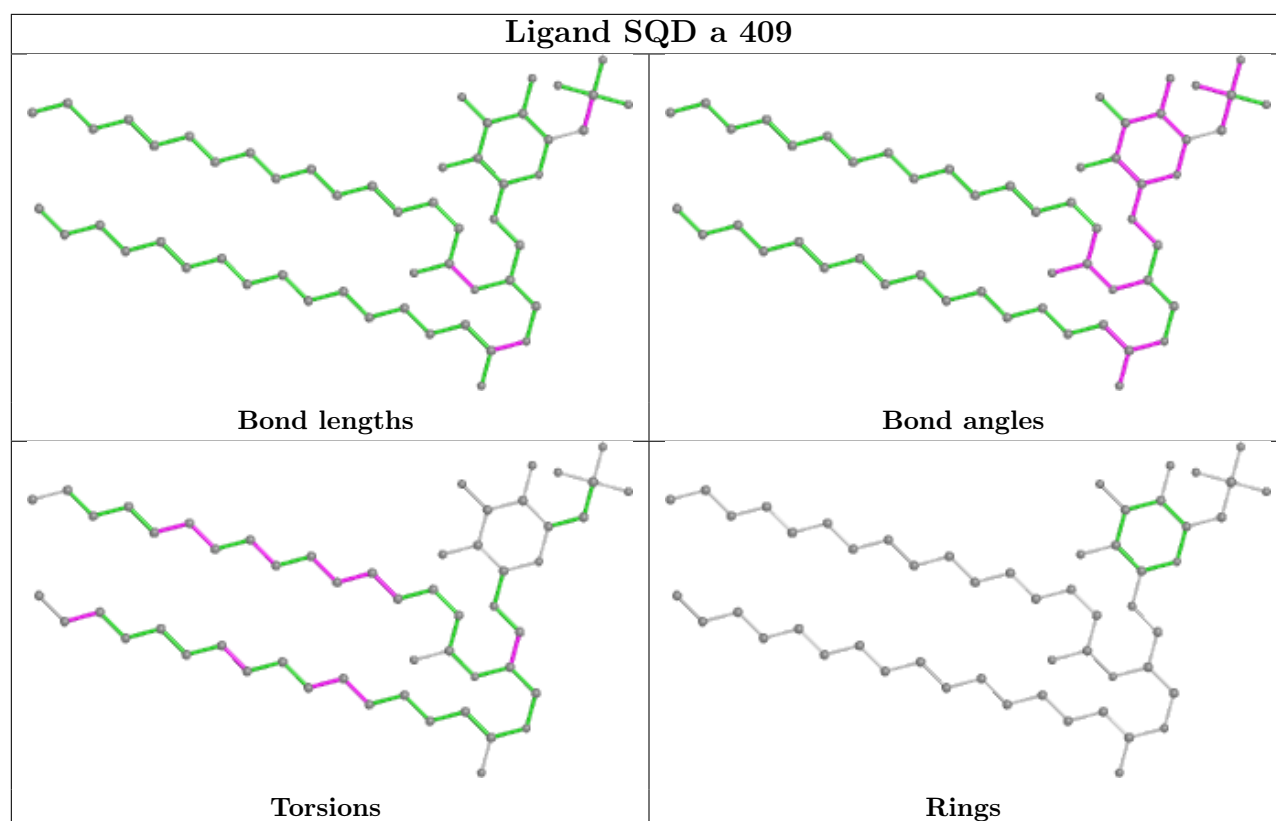


## Ligand BCR A 410

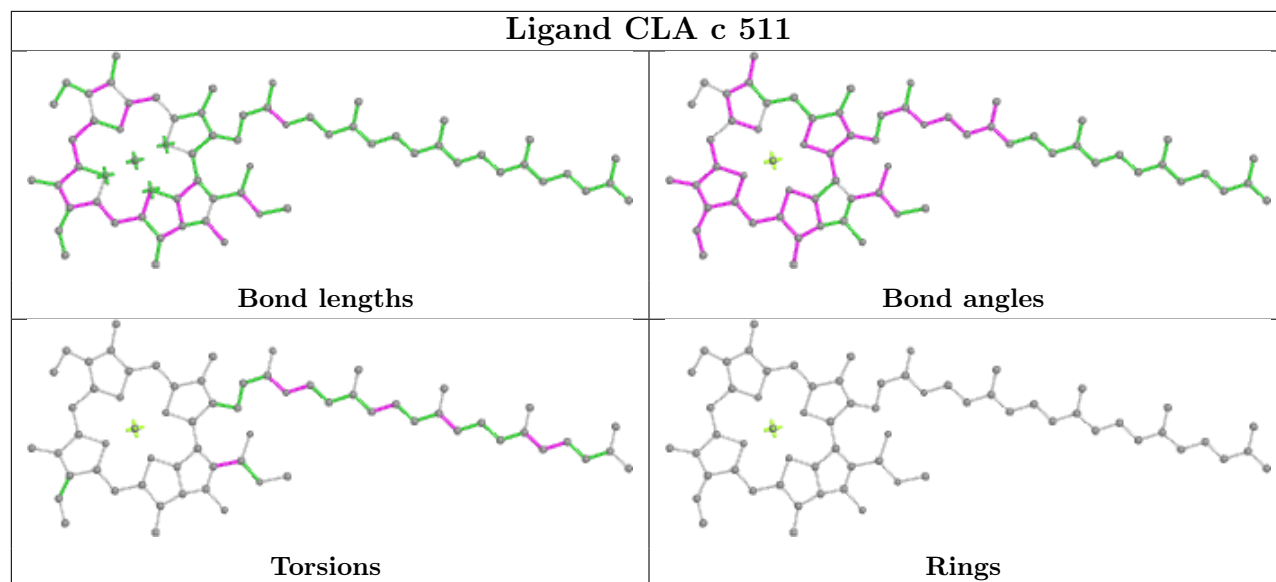




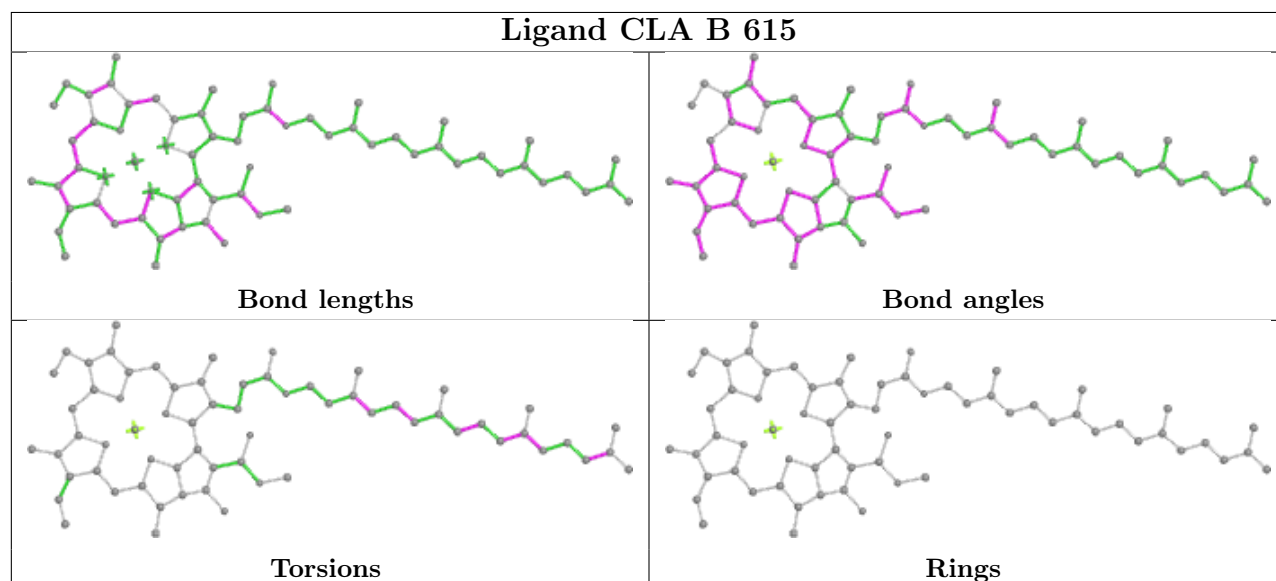




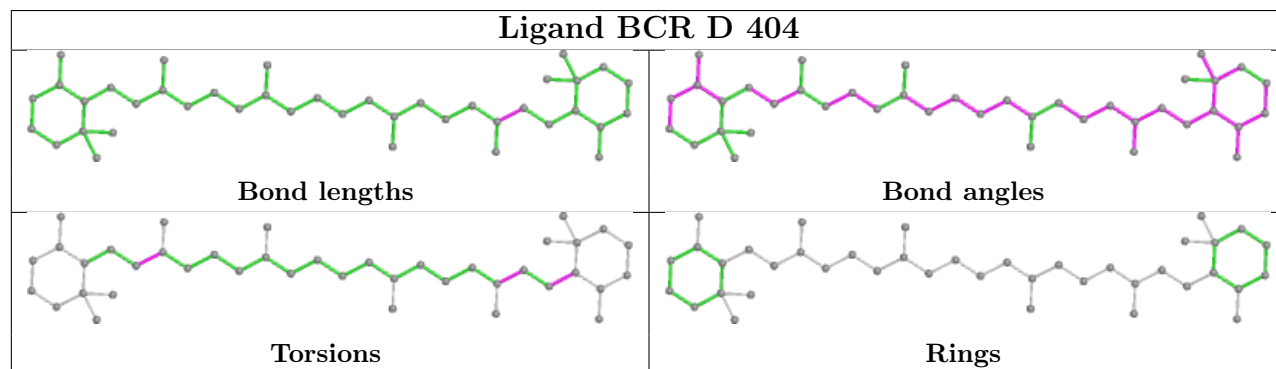
## Ligand CLA c 511

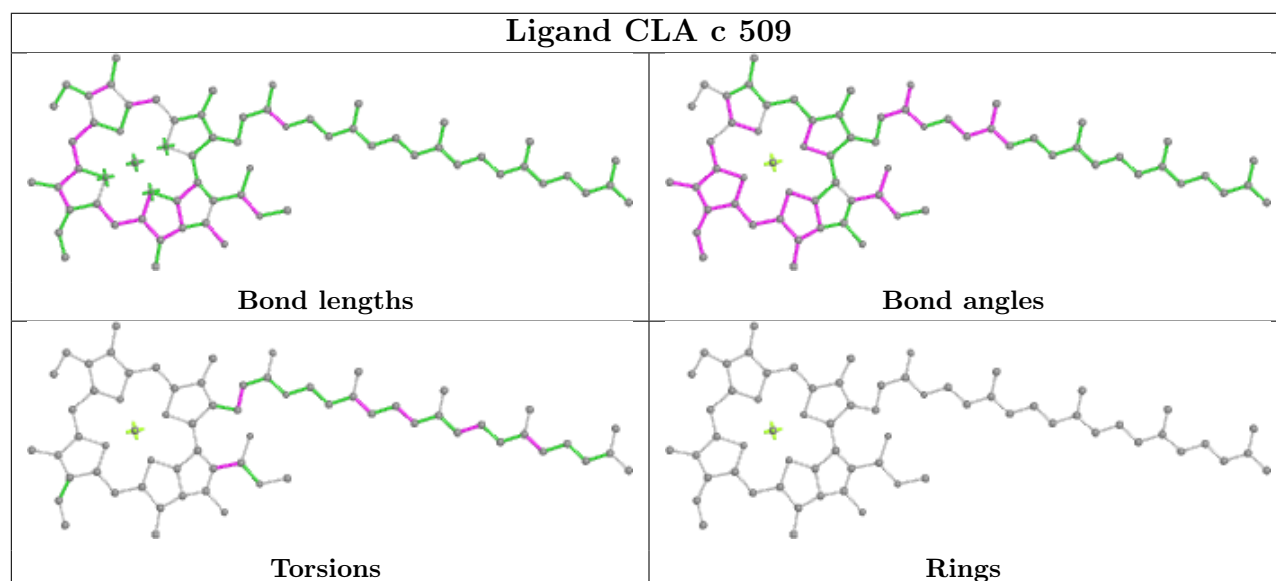
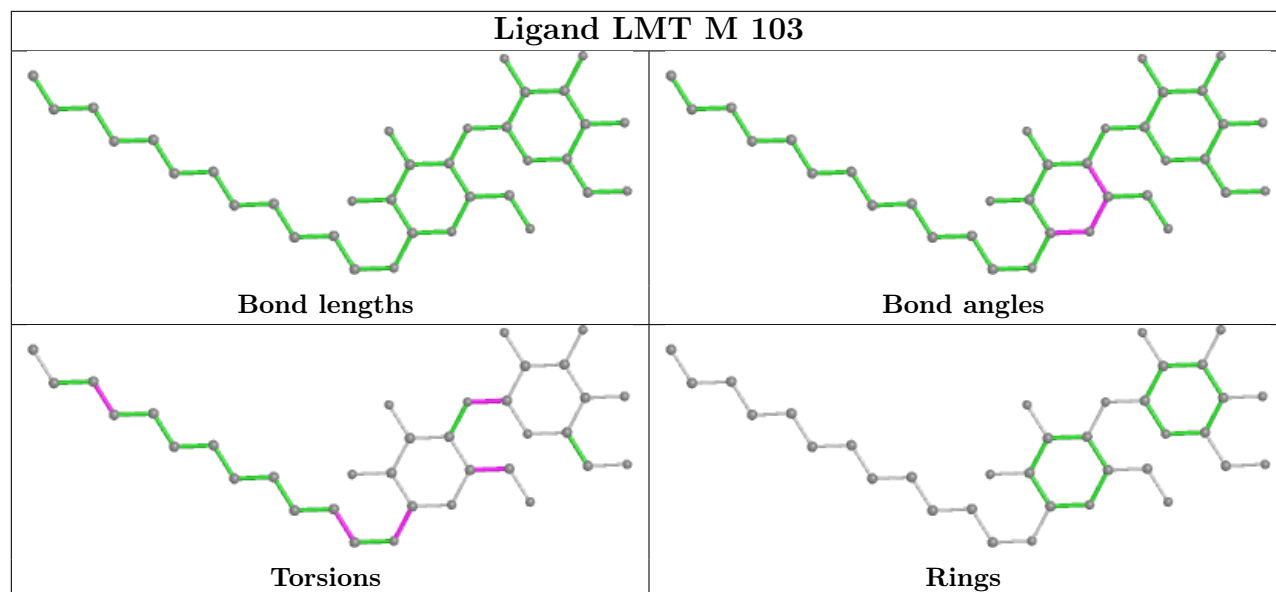
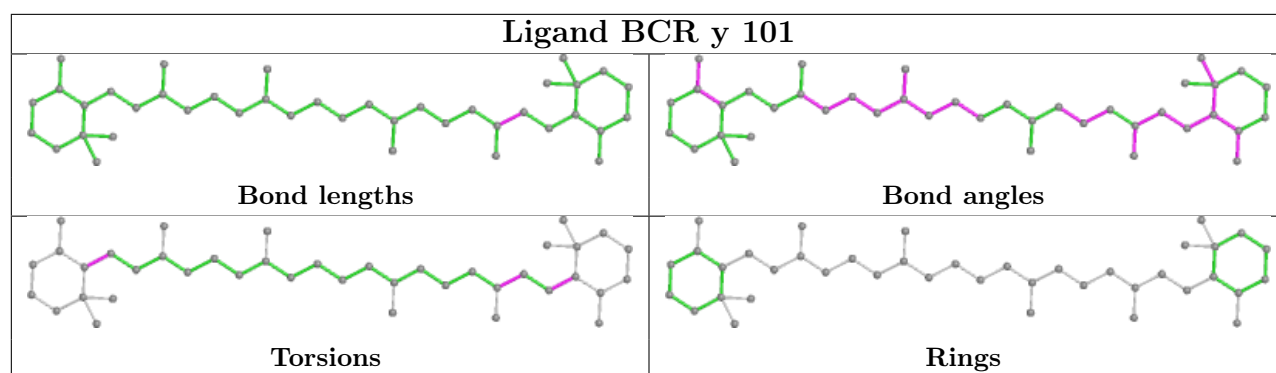


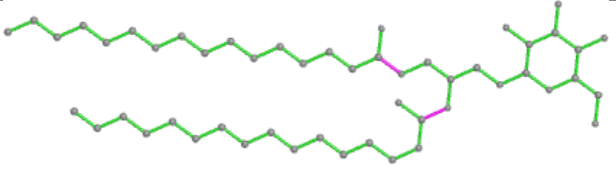
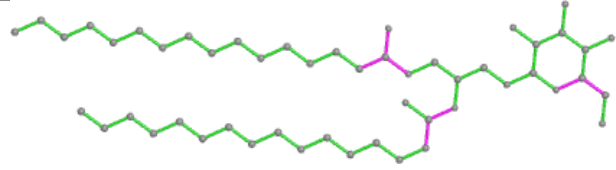
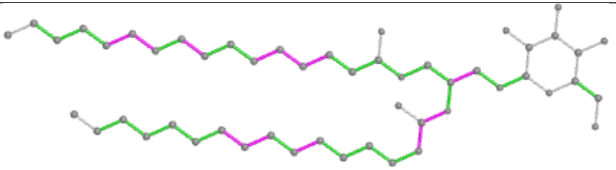
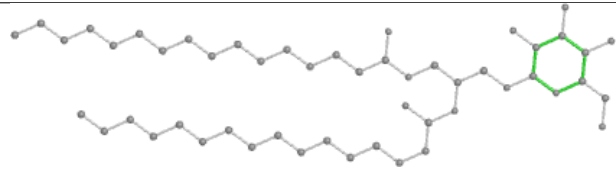
## Ligand CLA B 615

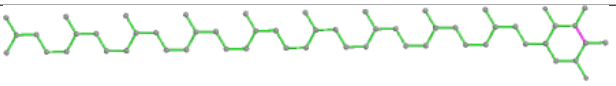
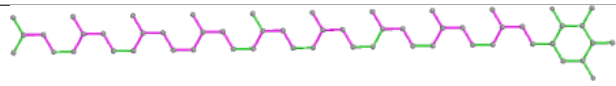
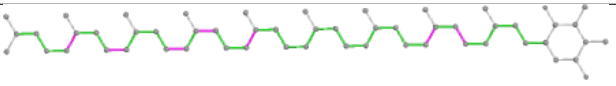
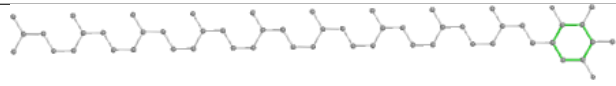


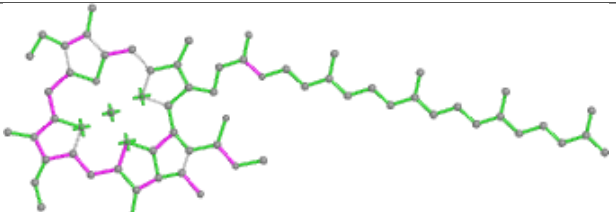
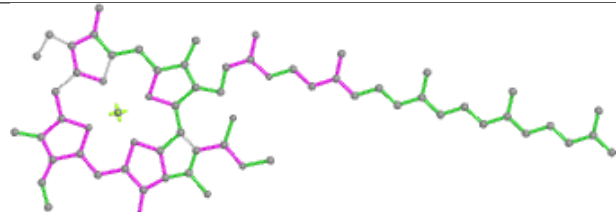
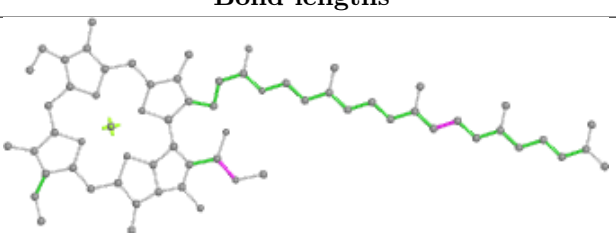
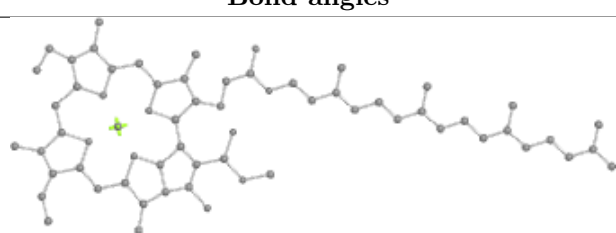
## Ligand BCR D 404

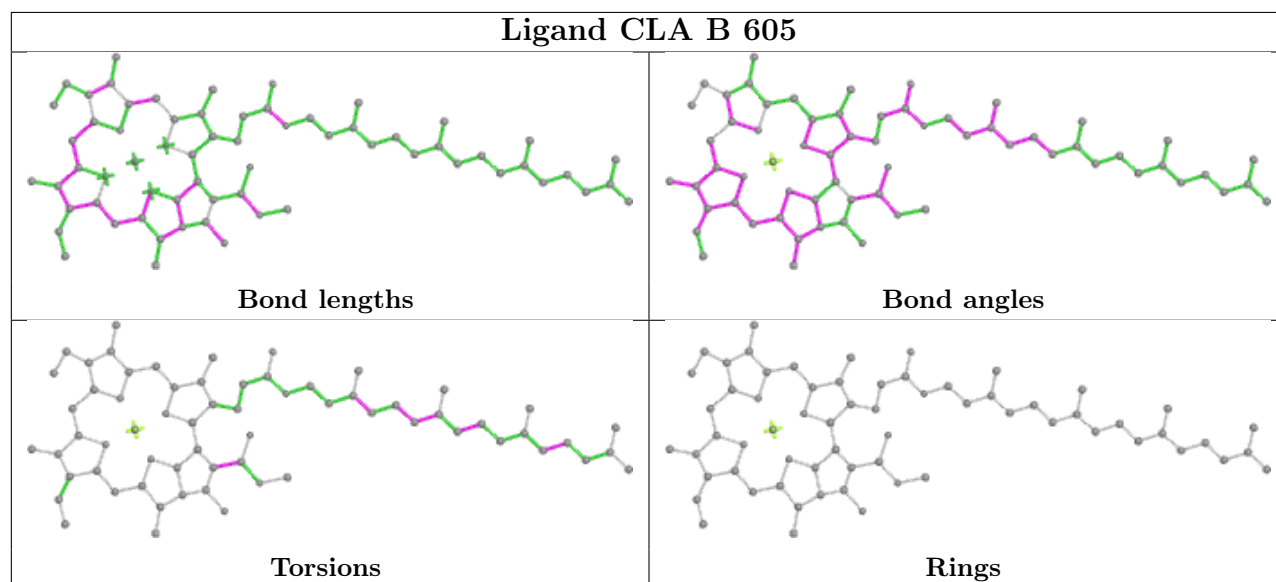
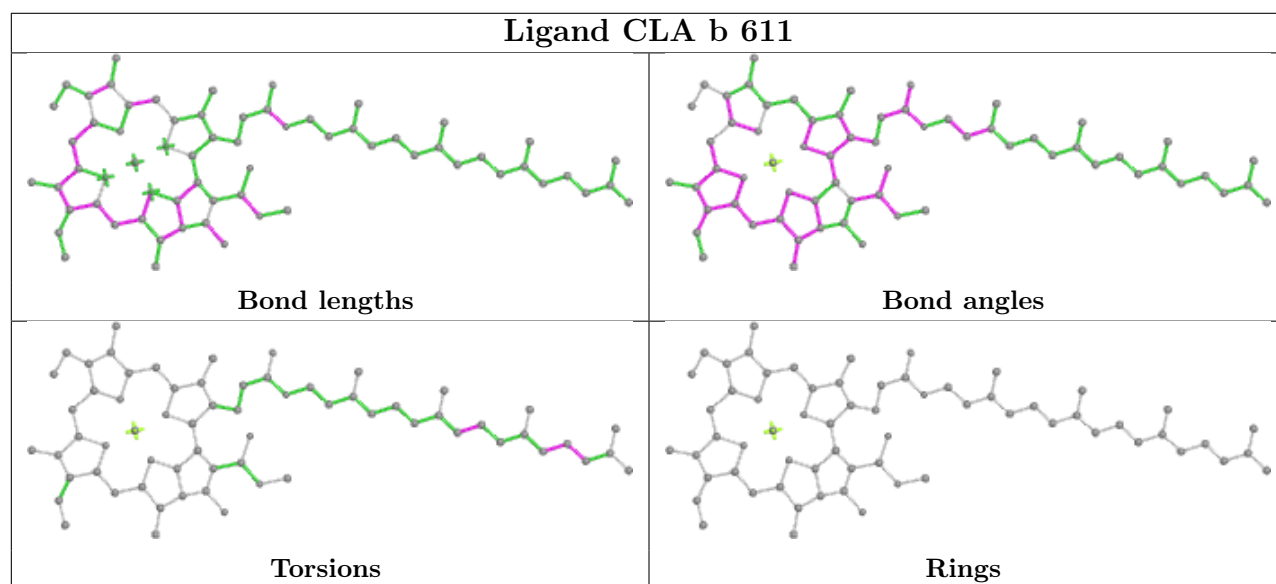
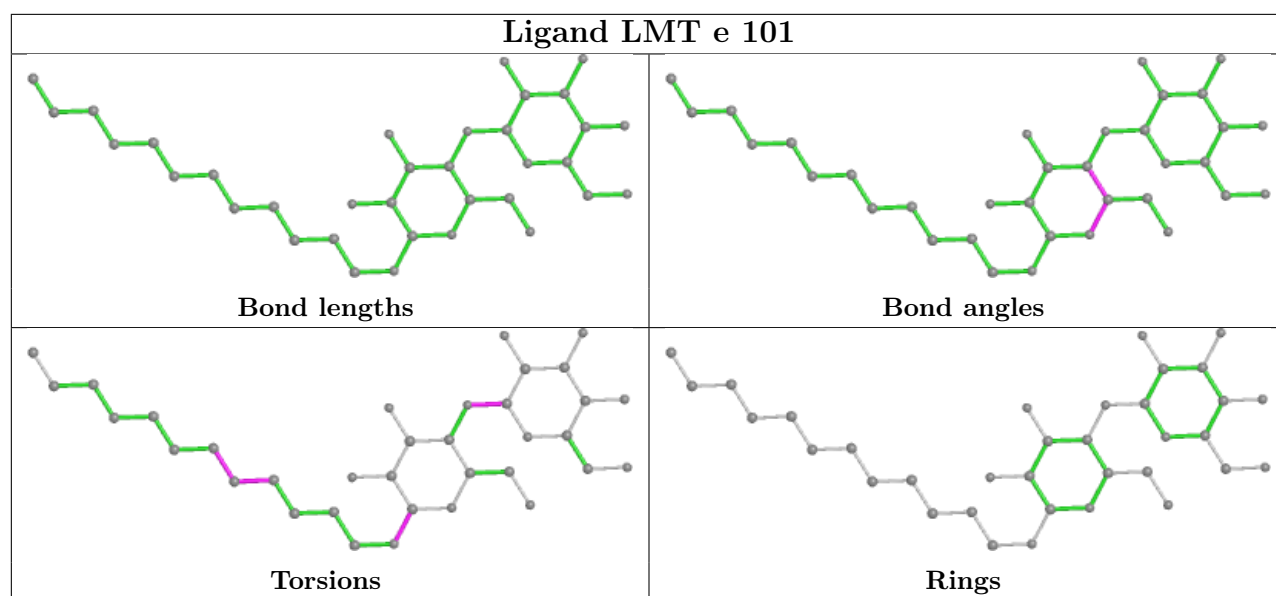




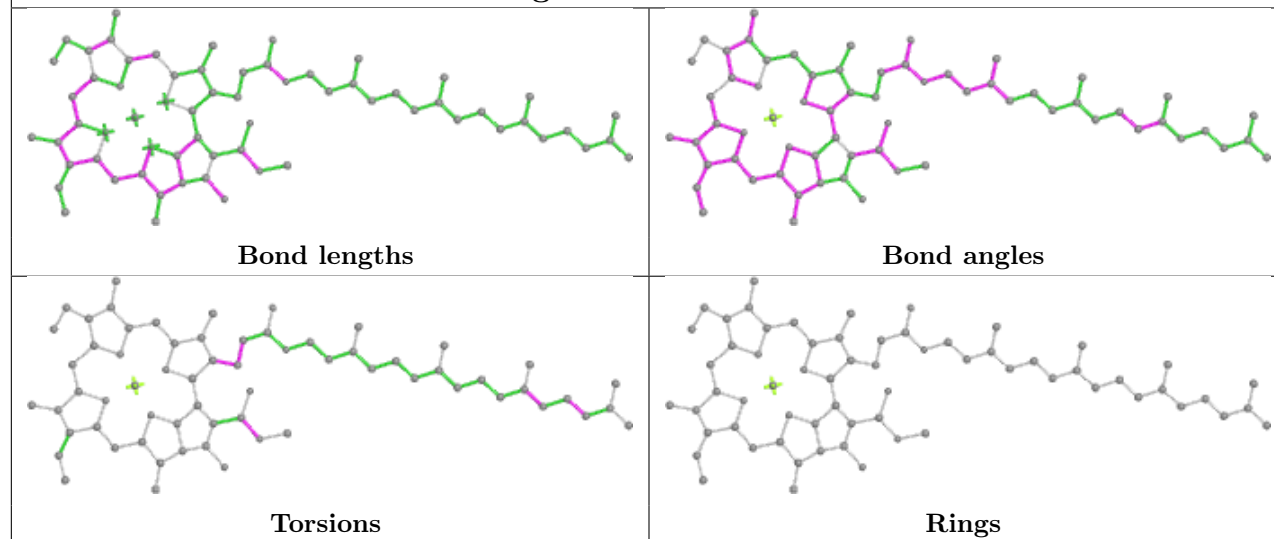
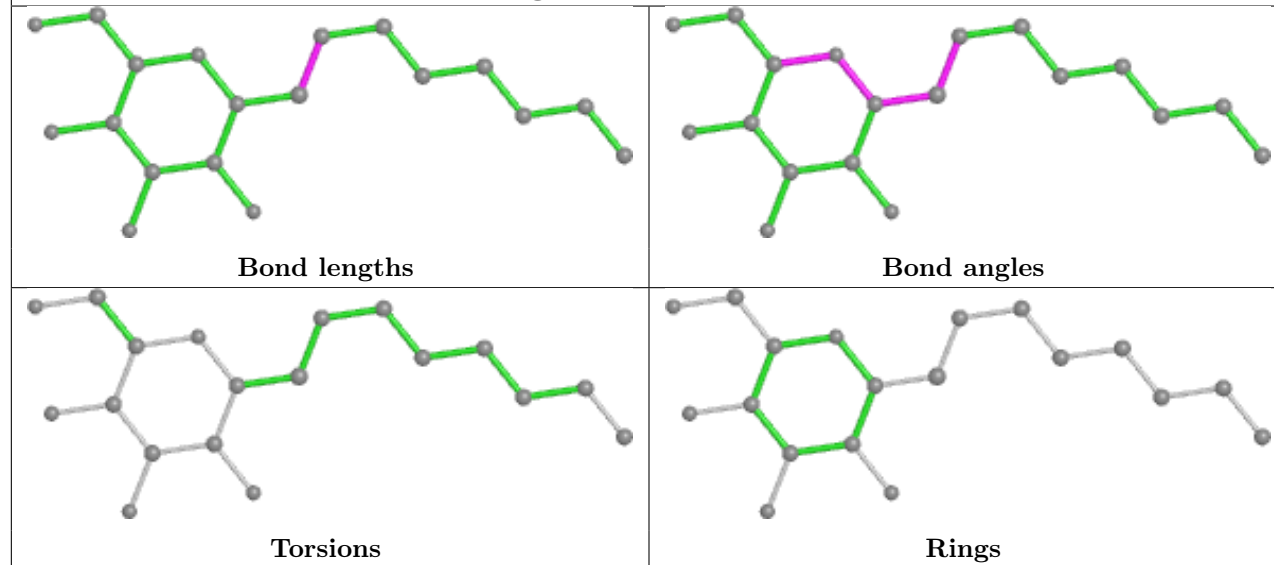
Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

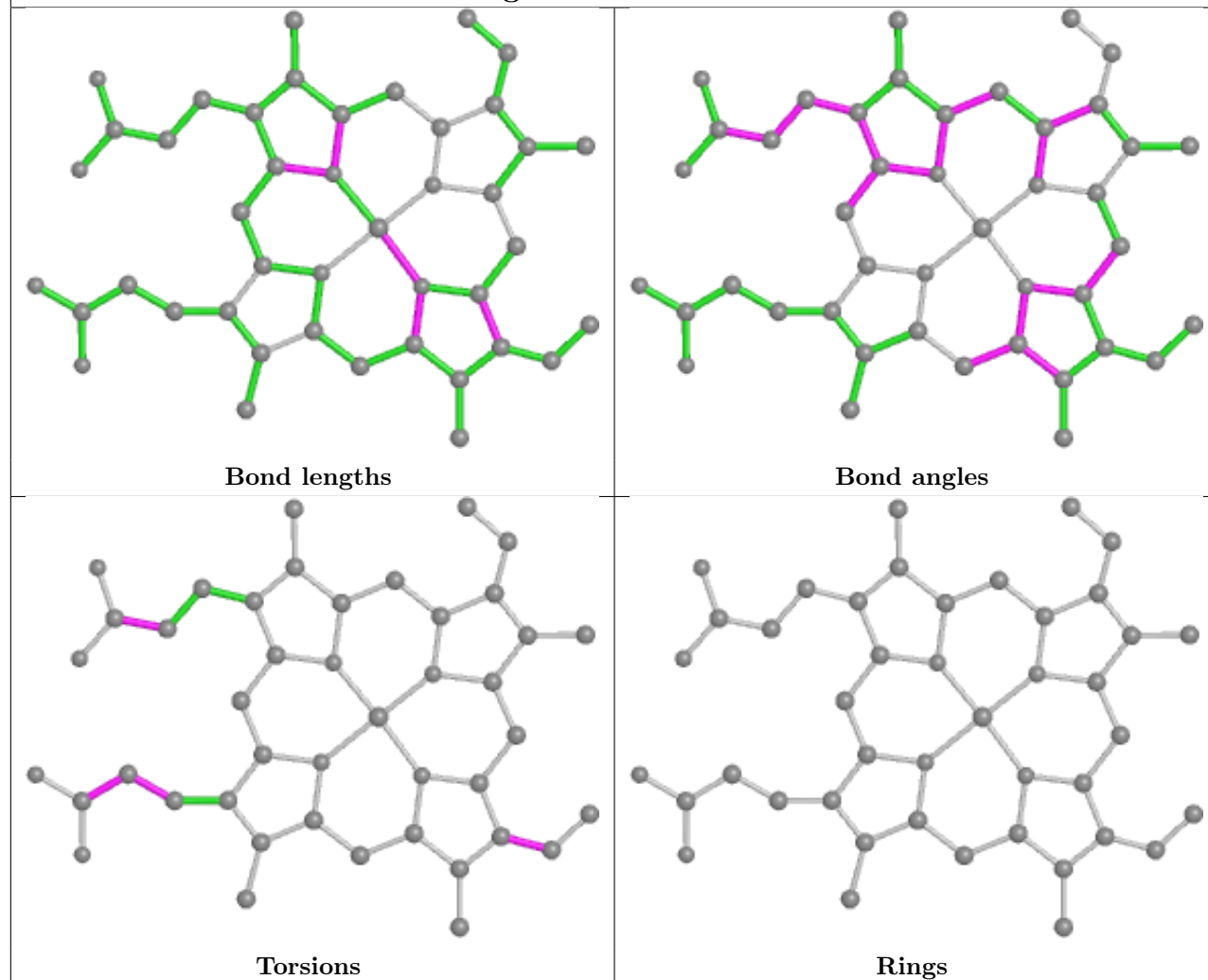
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings



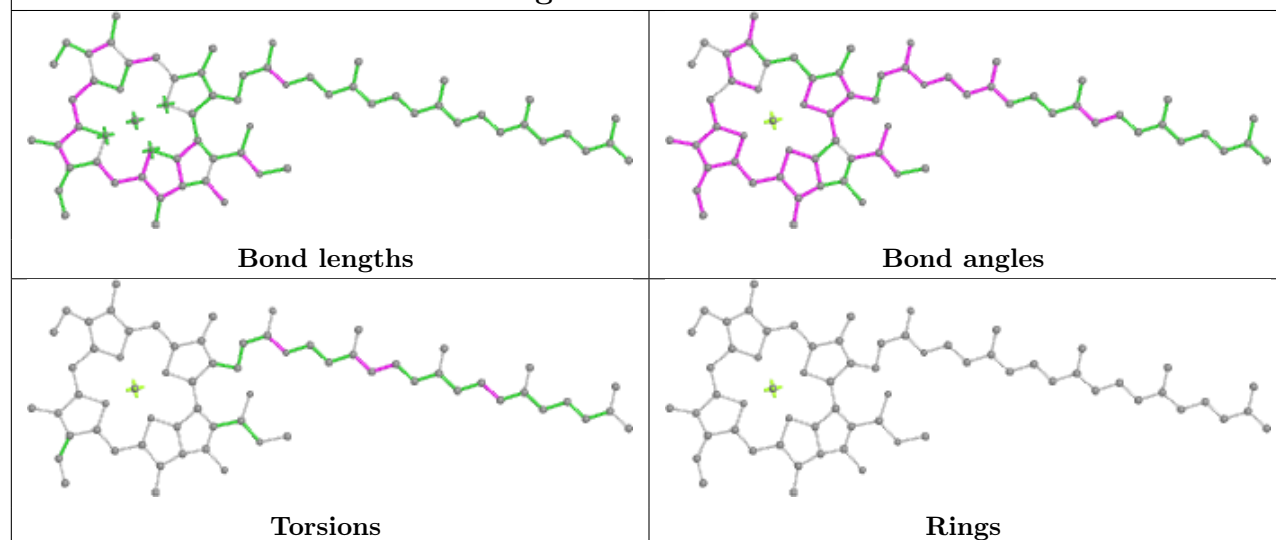


**Ligand CLA C 502****Ligand HTG C 522**

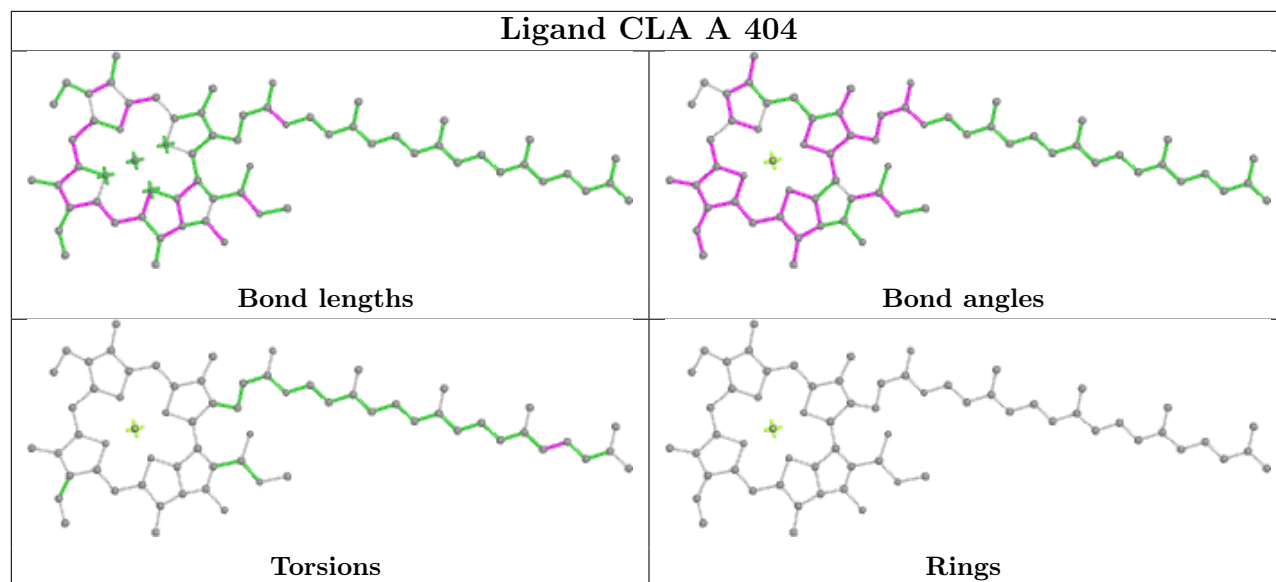
## Ligand HEM e 102



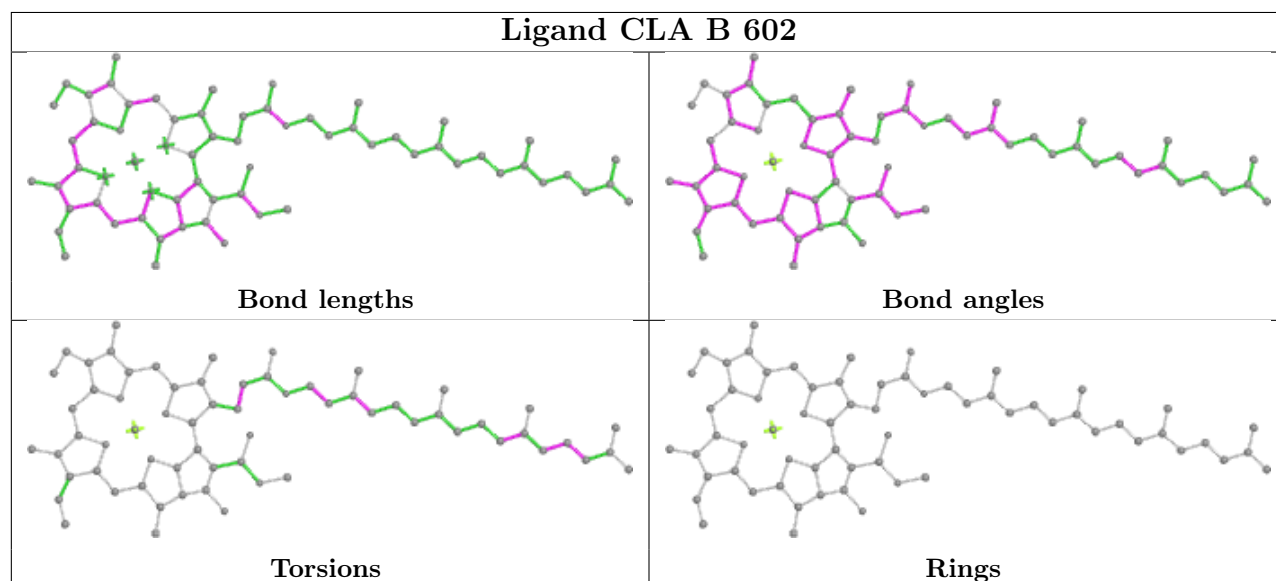
## Ligand CLA d 403



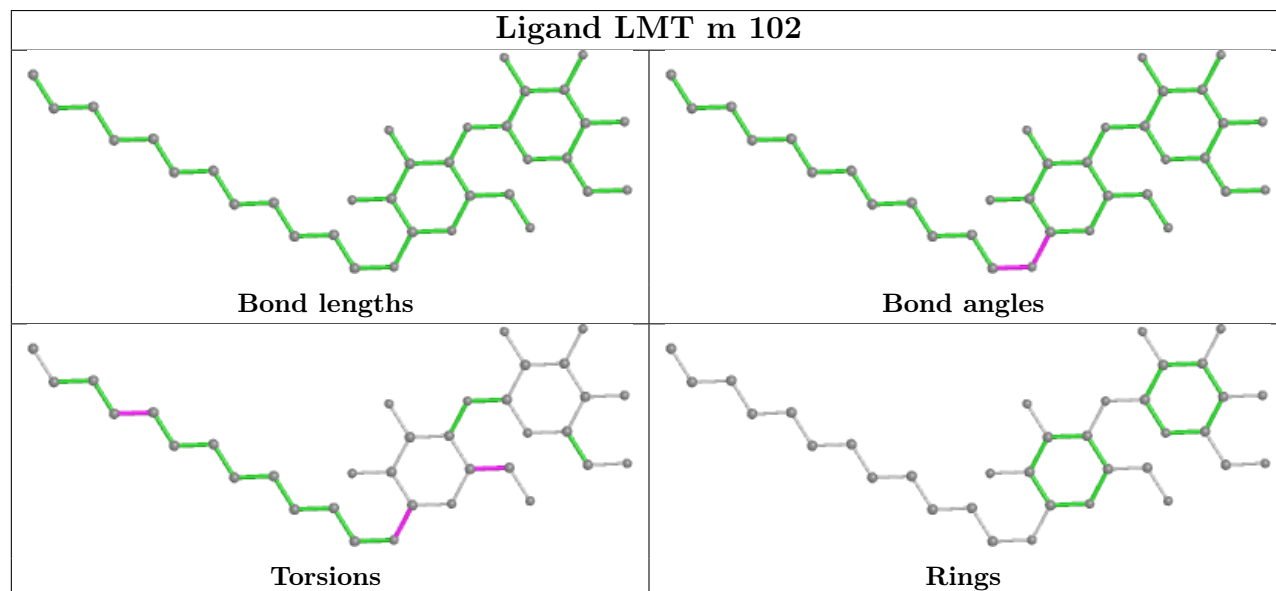
## Ligand CLA A 404

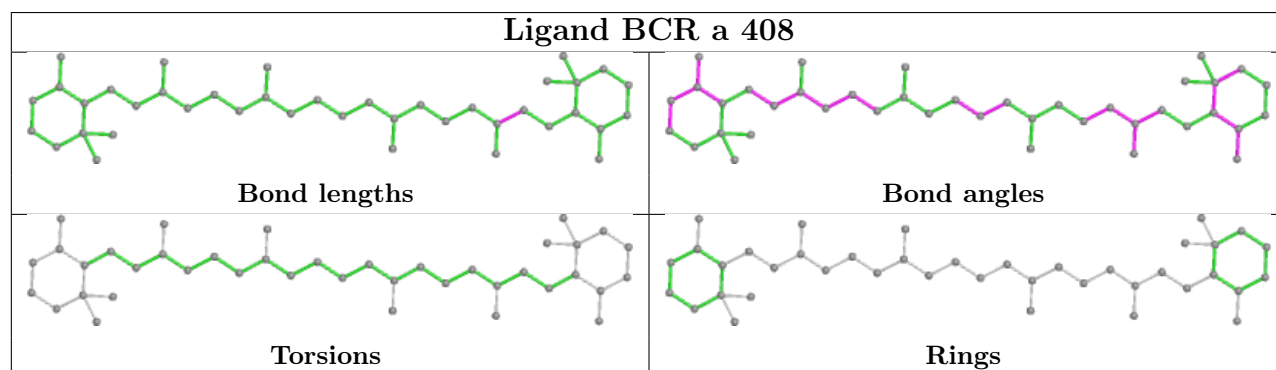
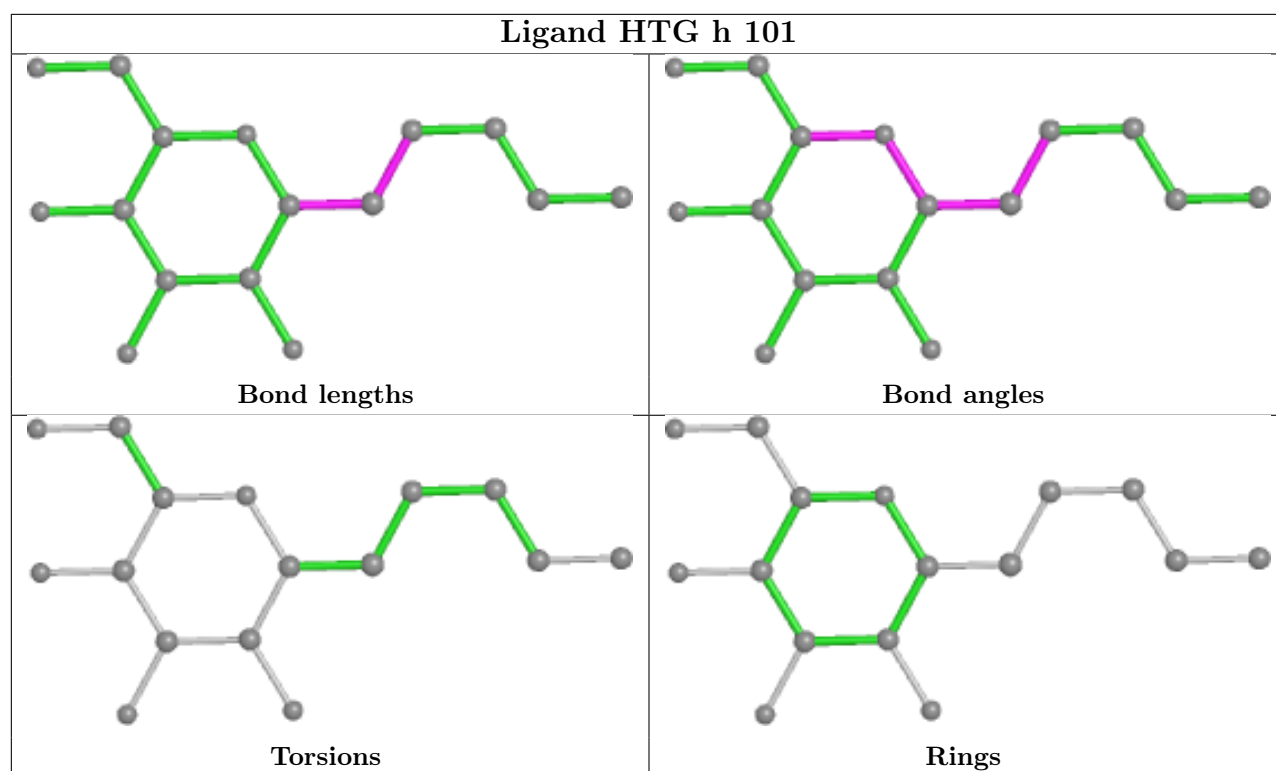


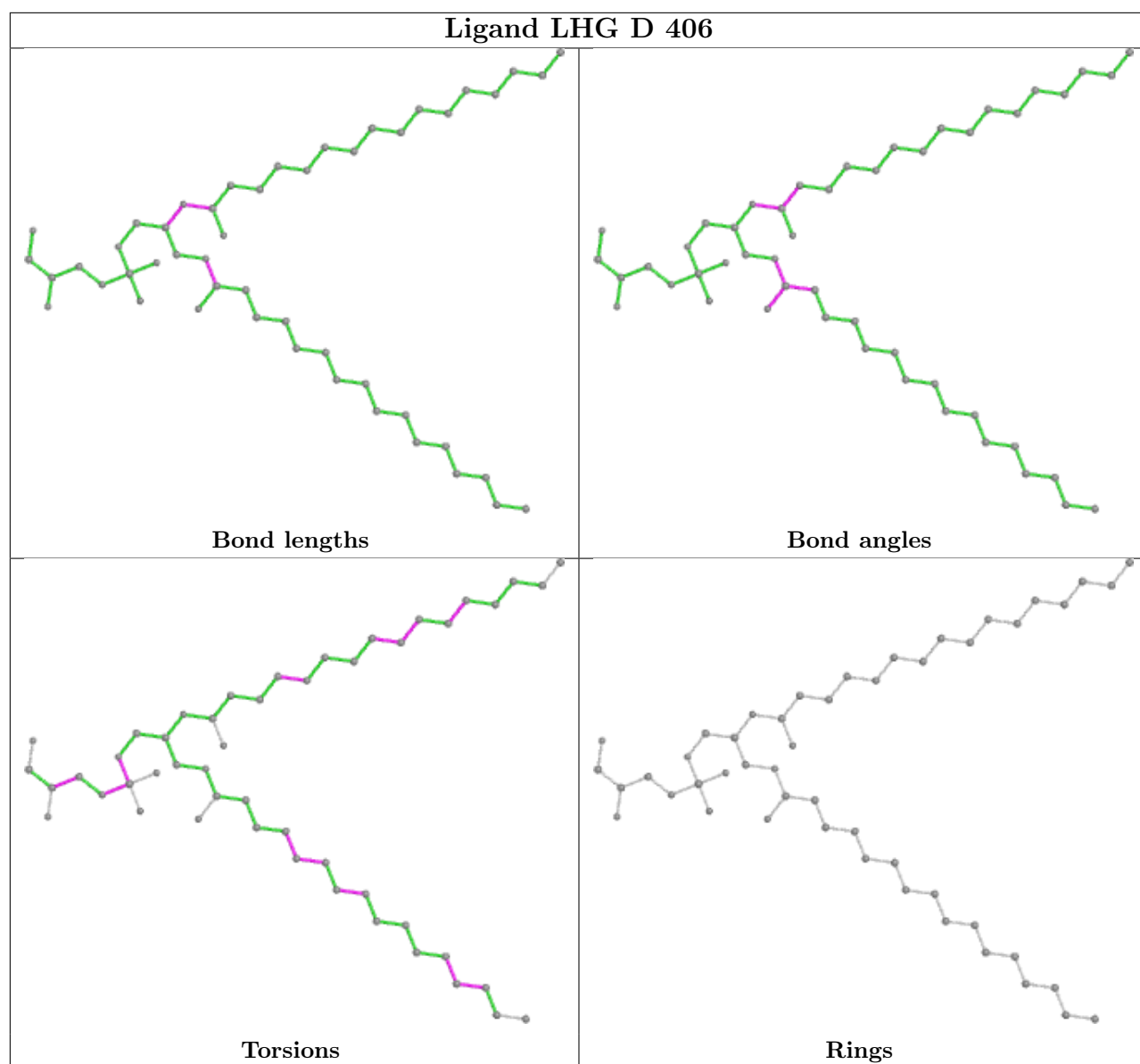
## Ligand CLA B 602

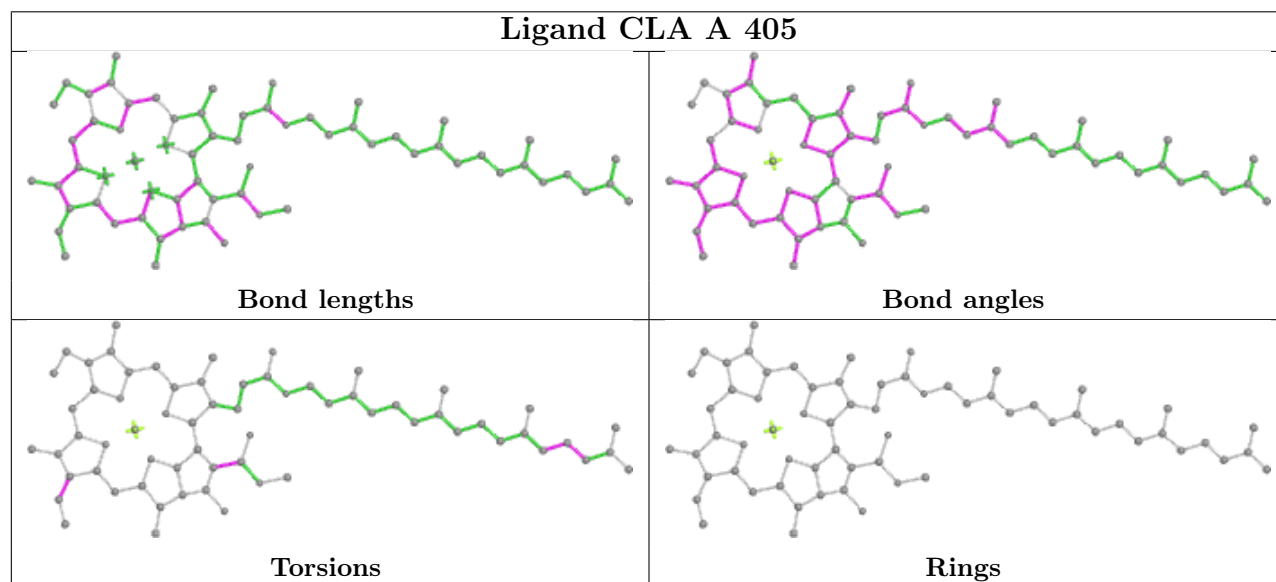
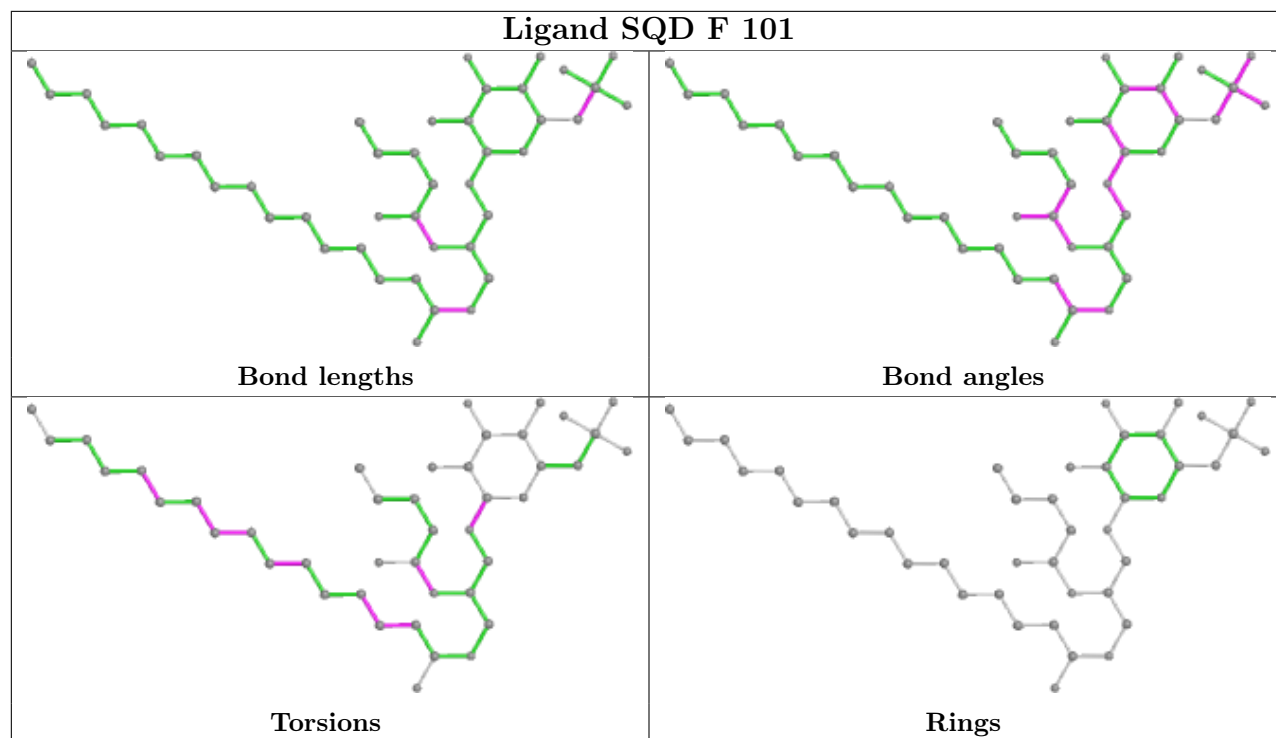


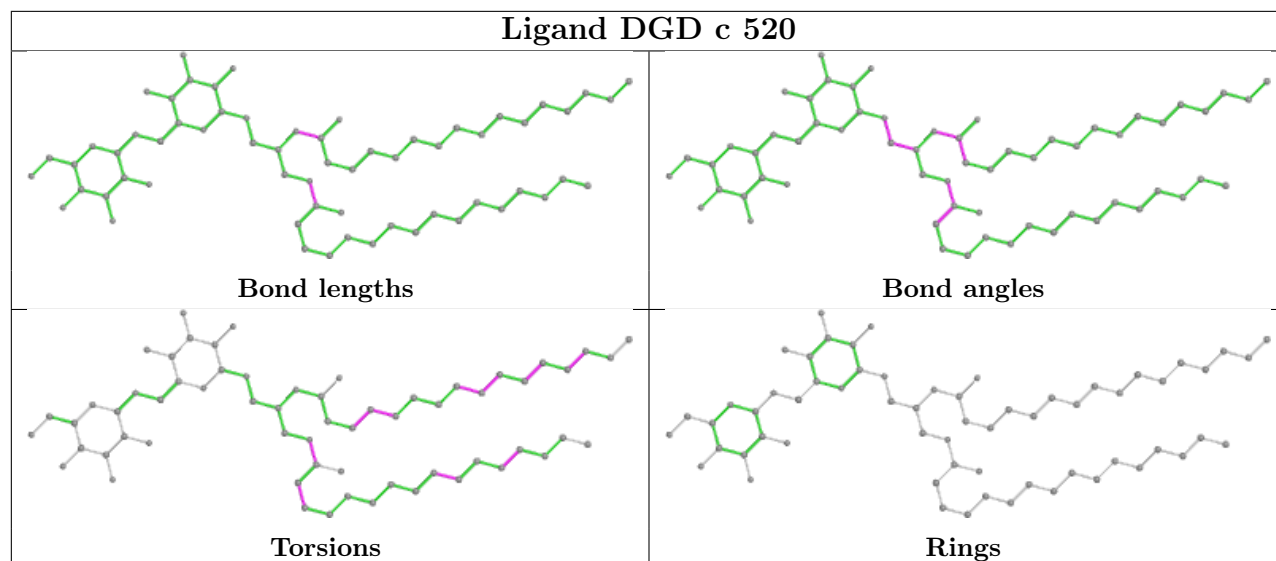
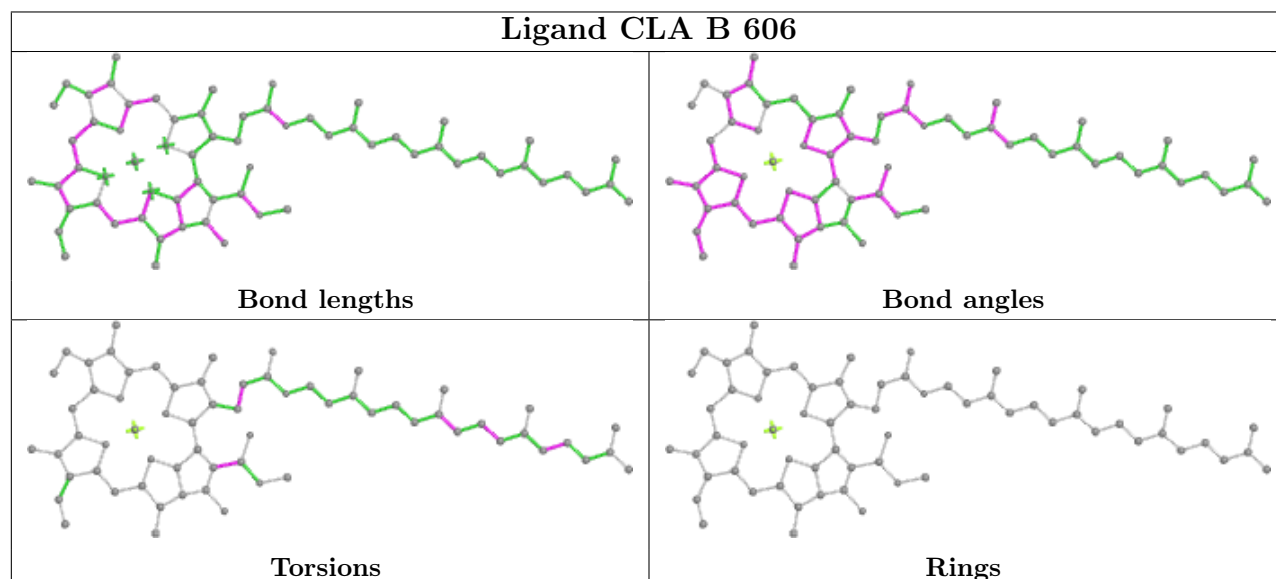
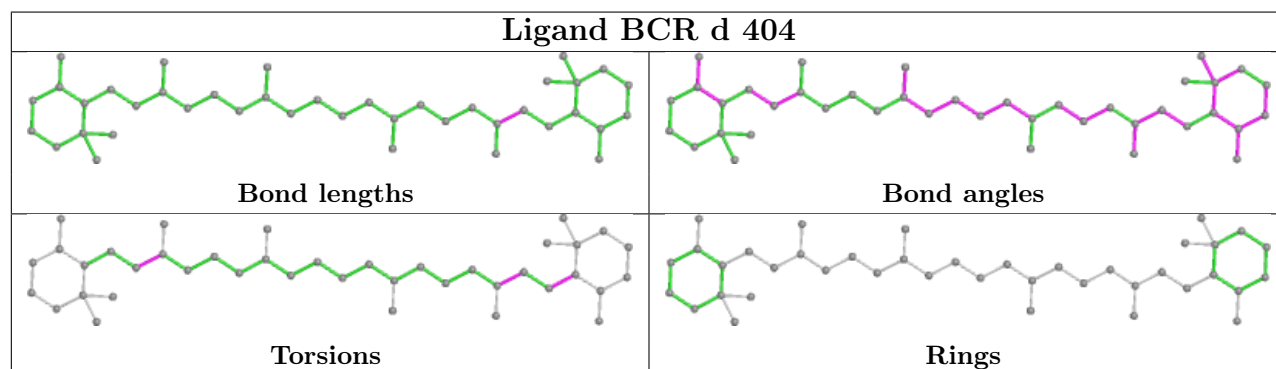
## Ligand LMT m 102



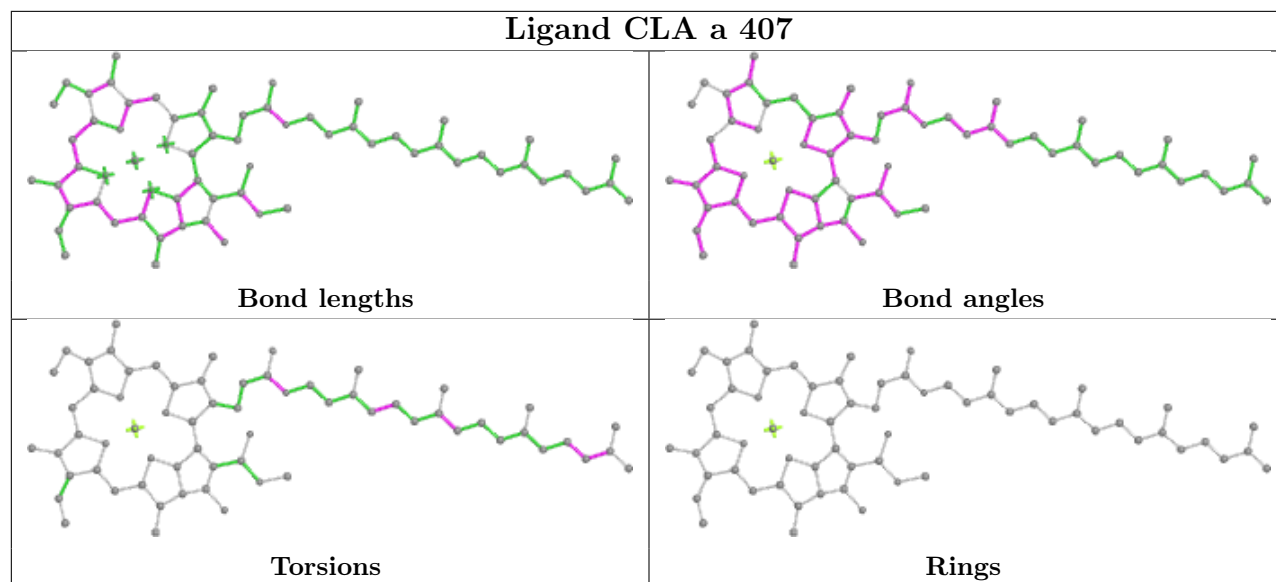




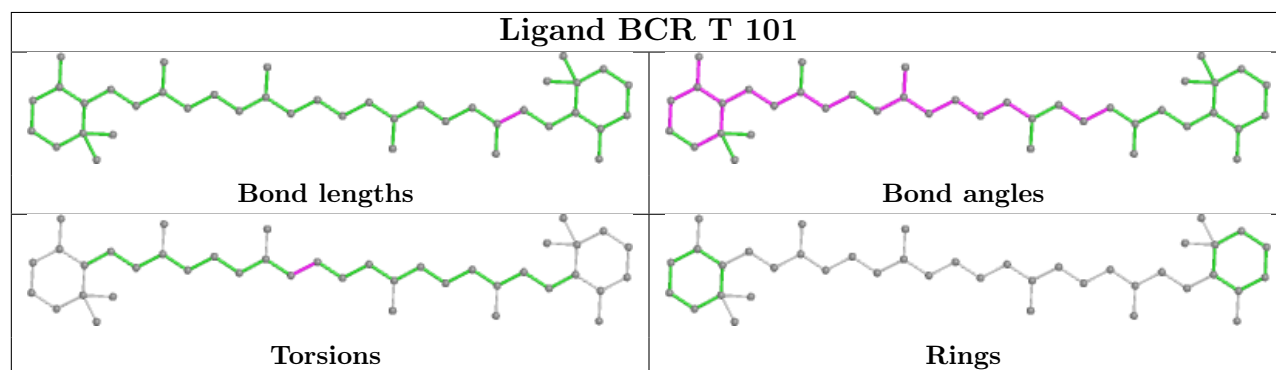


**Ligand DGD c 520****Ligand CLA B 606****Ligand BCR d 404**

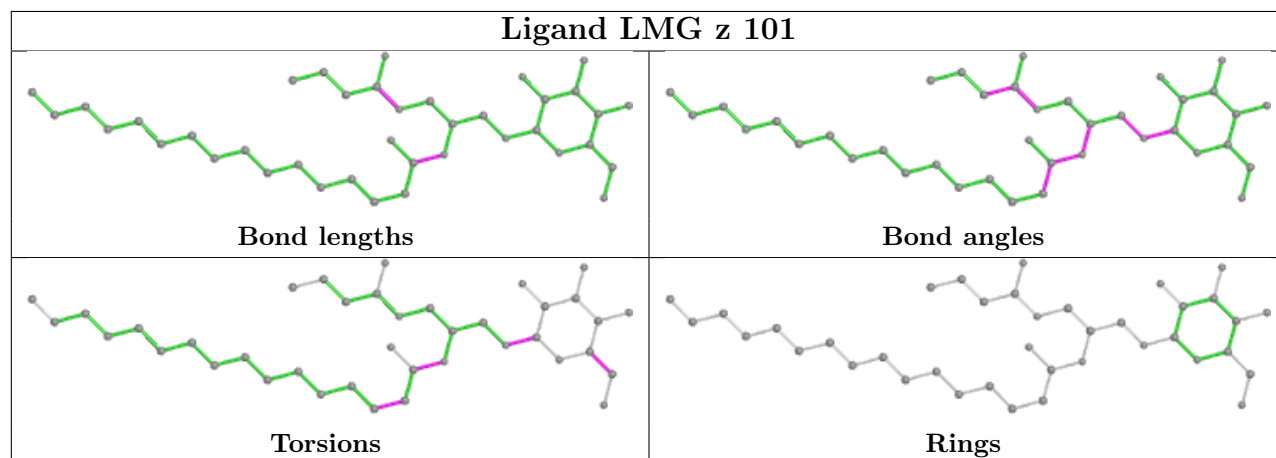
## Ligand CLA a 407



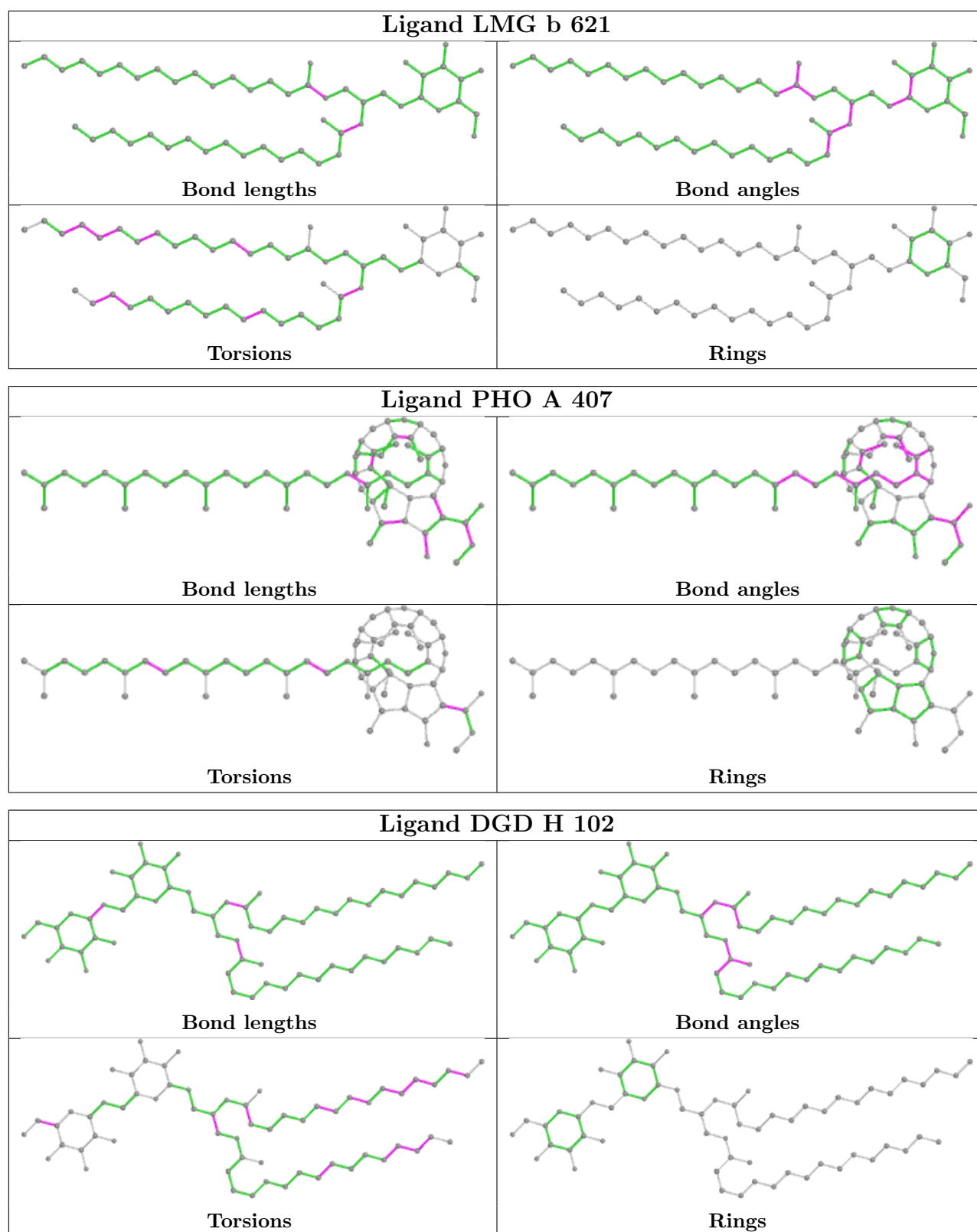
## Ligand BCR T 101

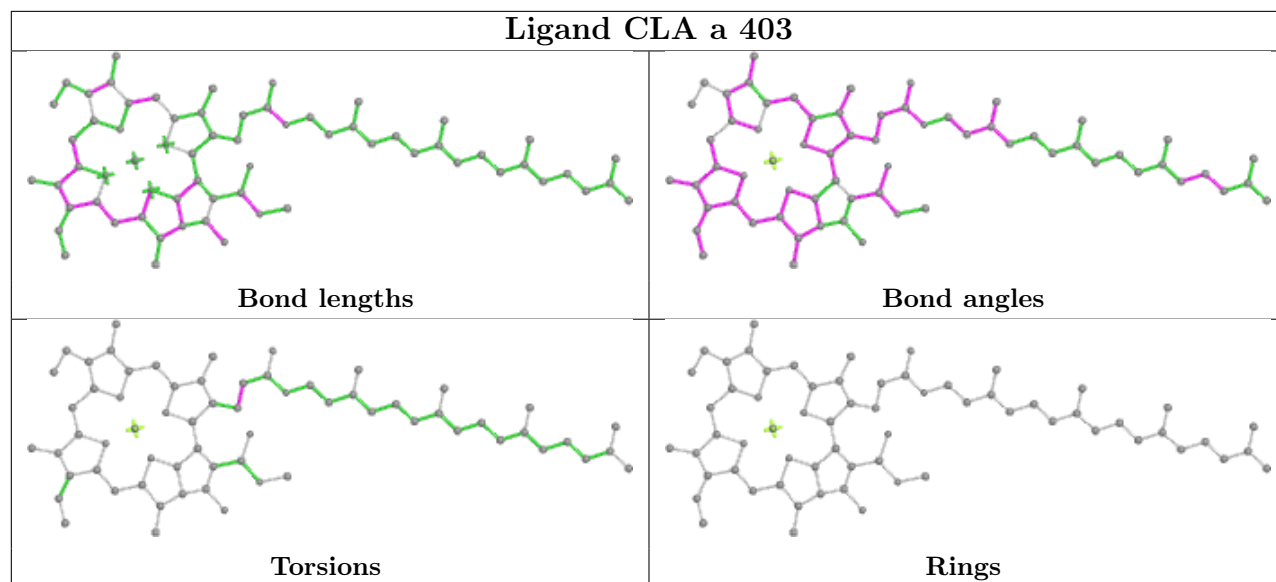
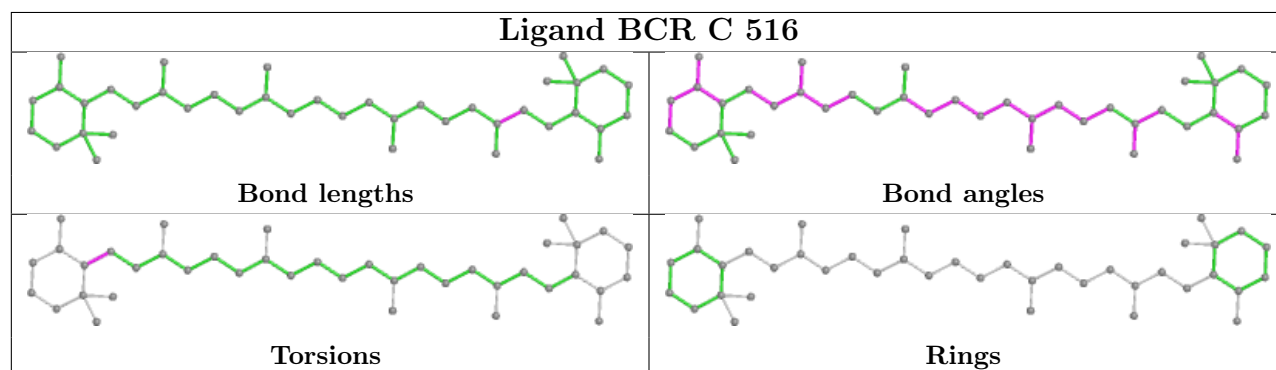
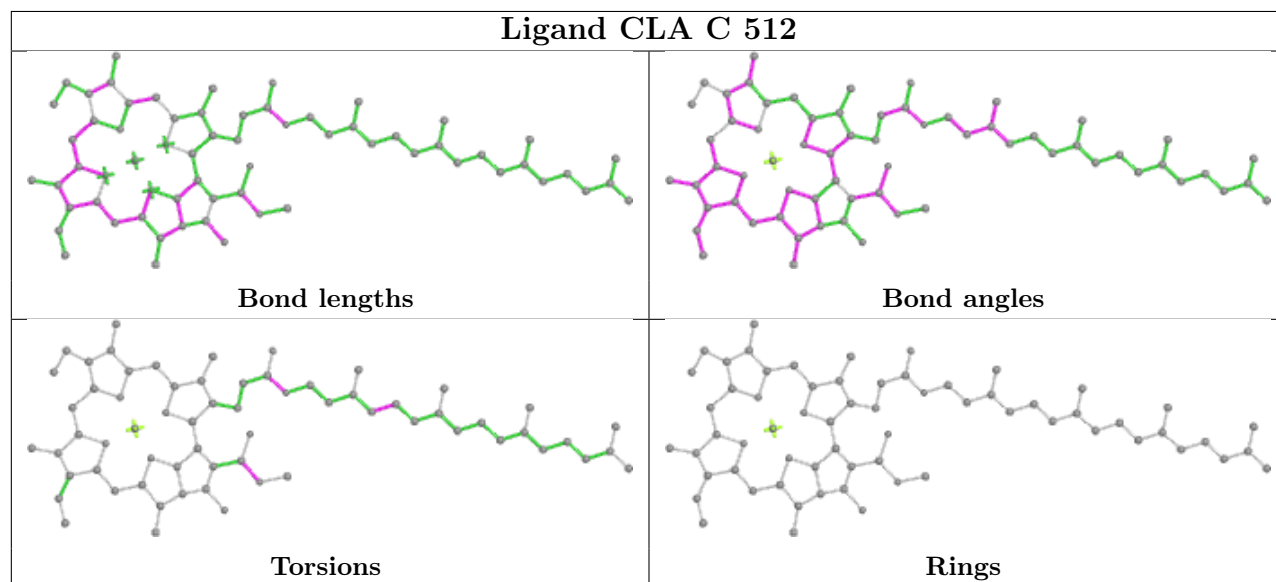


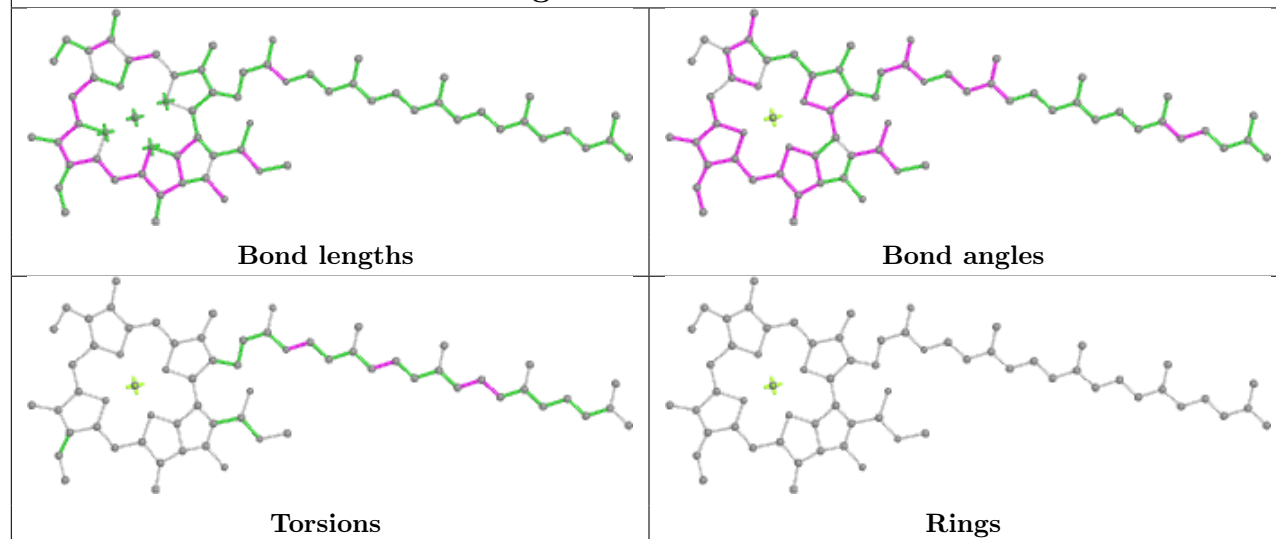
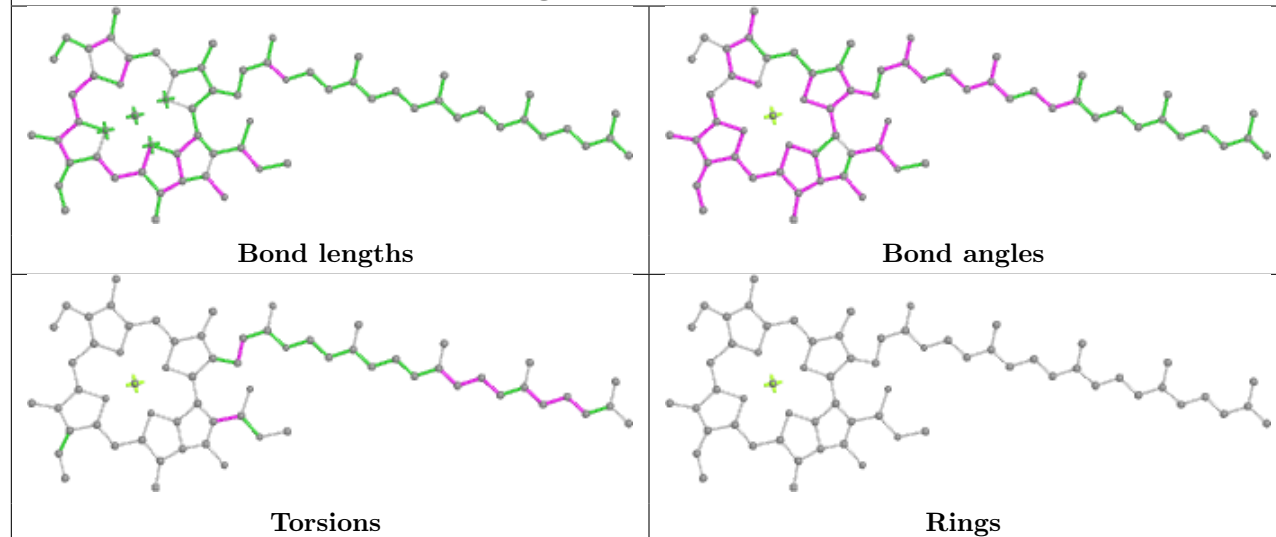
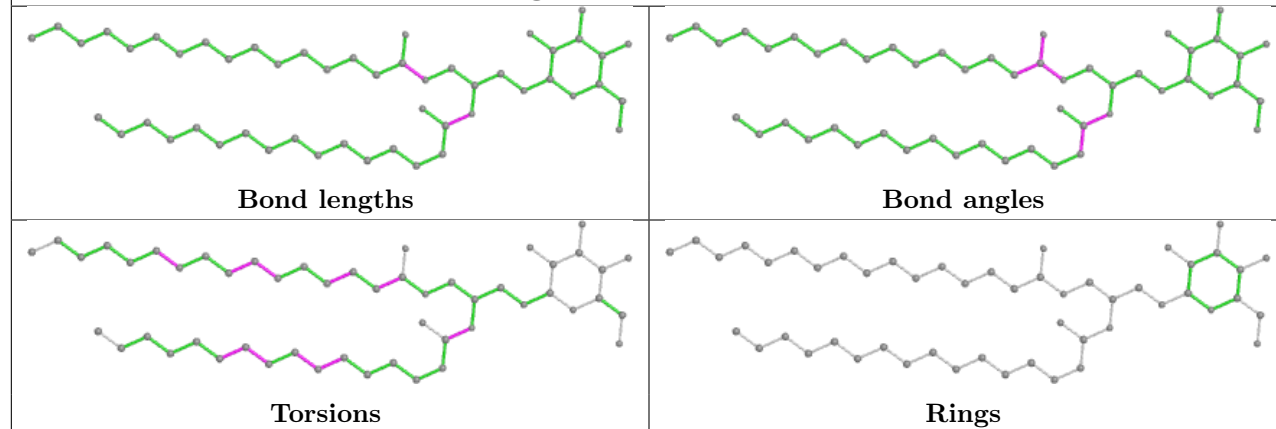
## Ligand LMG z 101

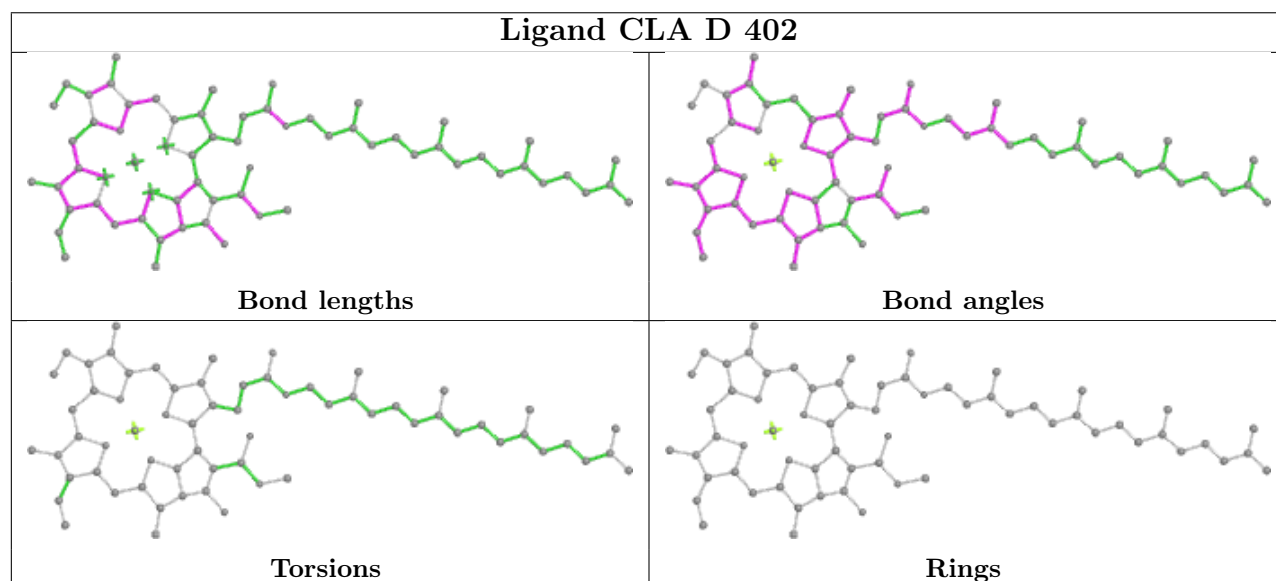
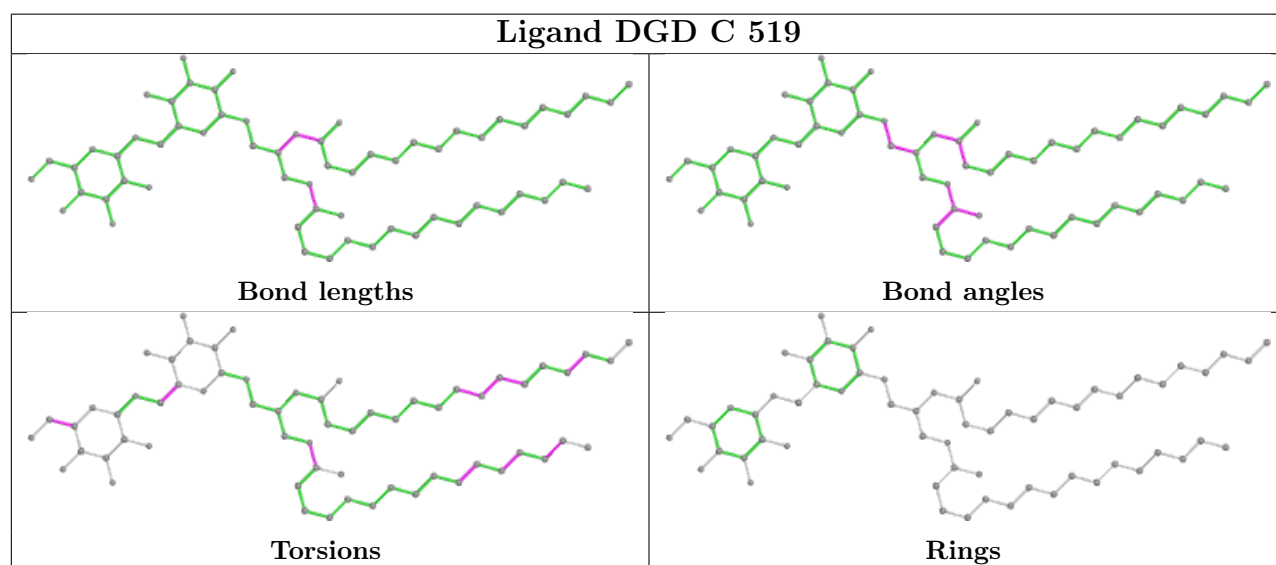
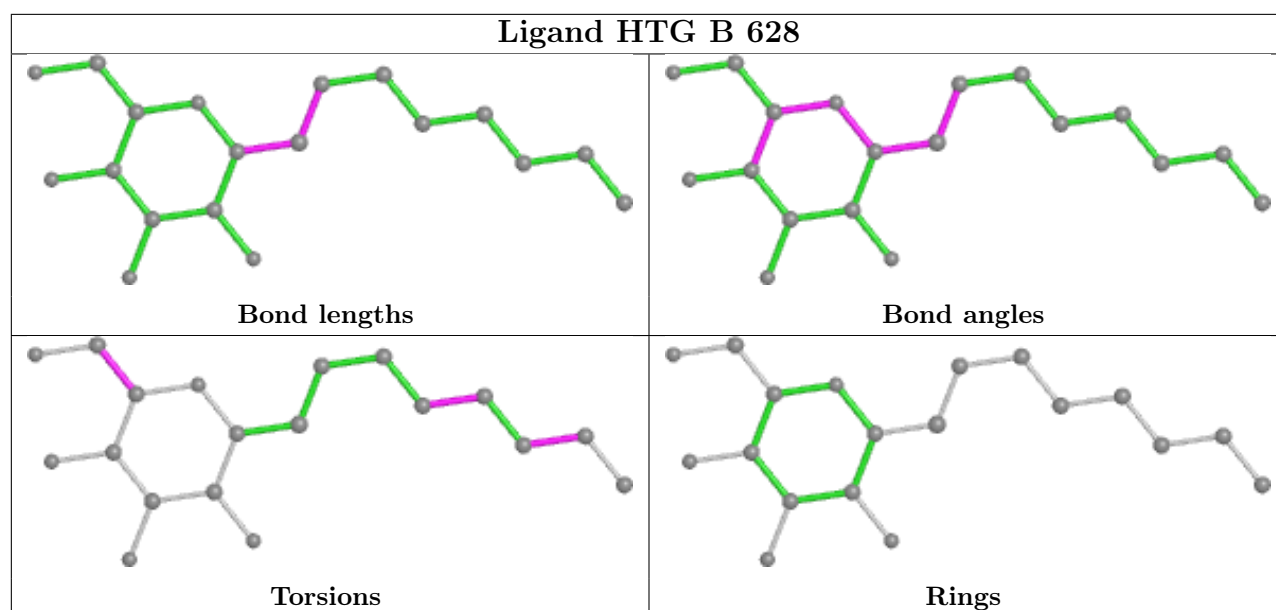




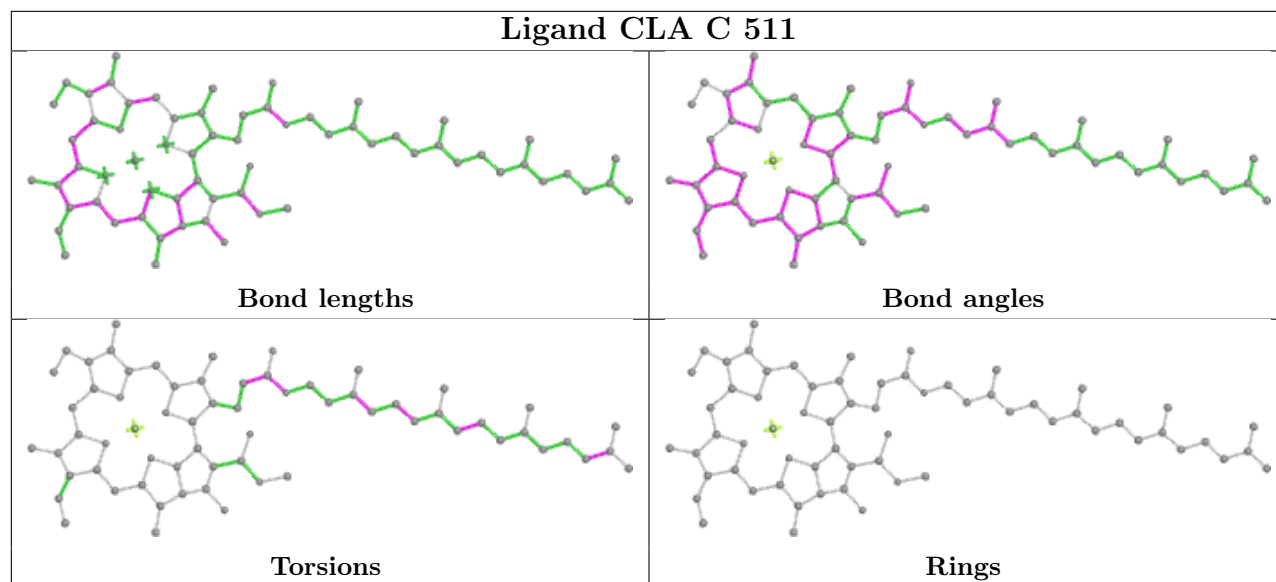


**Ligand CLA a 403****Ligand BCR C 516****Ligand CLA C 512**

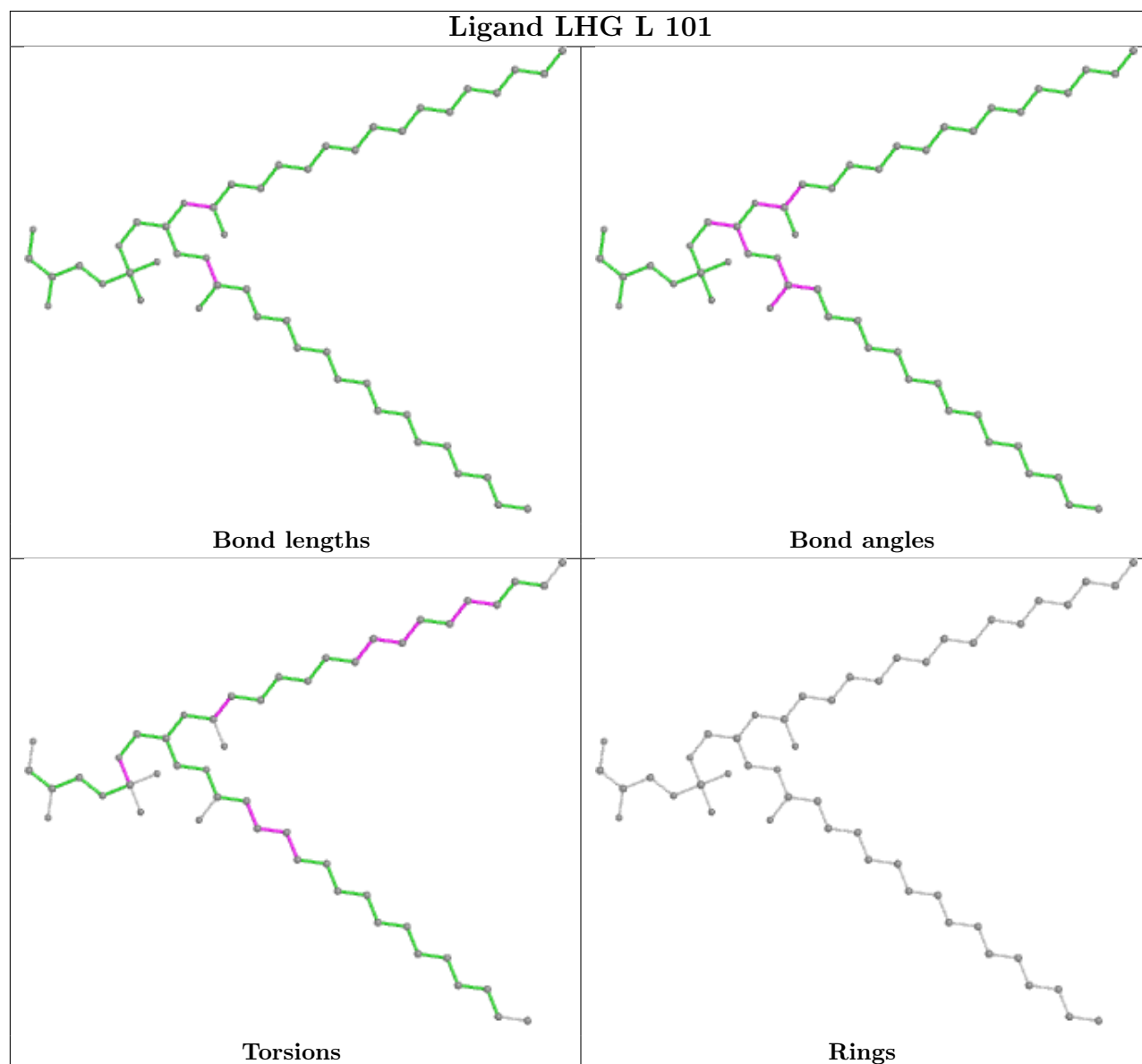
**Ligand CLA C 510****Ligand CLA b 606****Ligand LMG B 621**



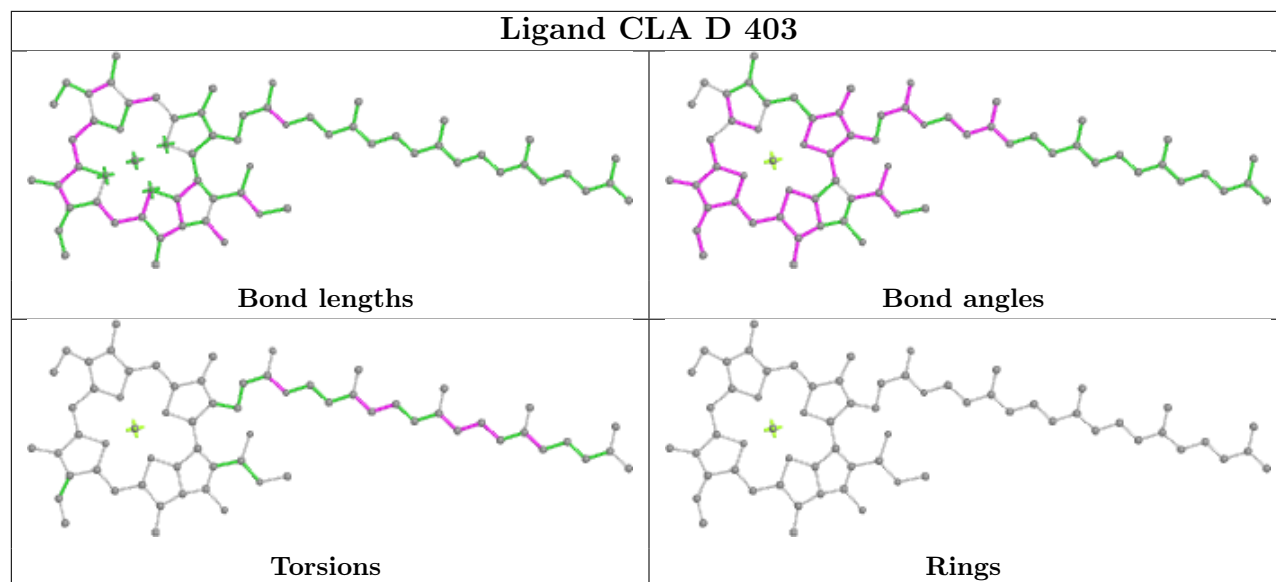
## Ligand CLA C 511



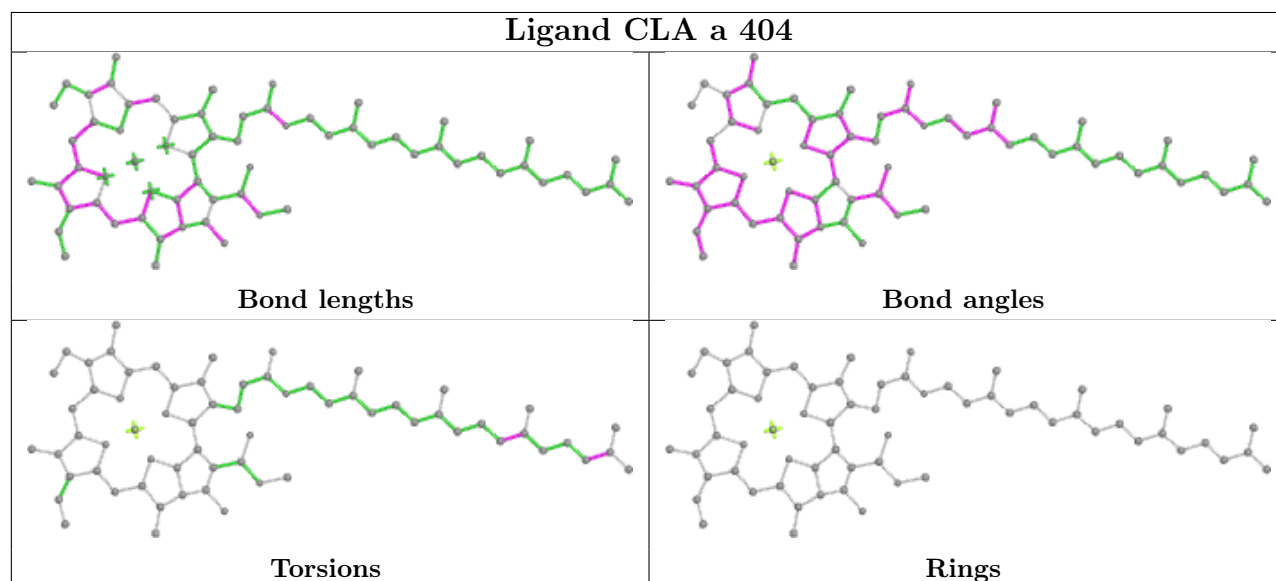
## Ligand LHG L 101



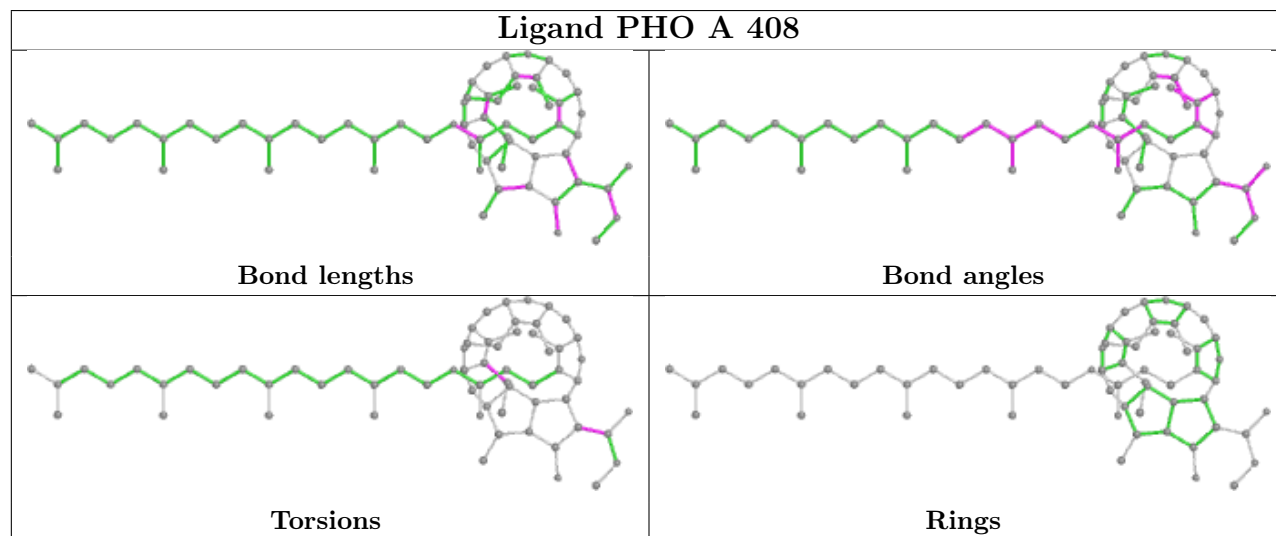
## Ligand CLA D 403

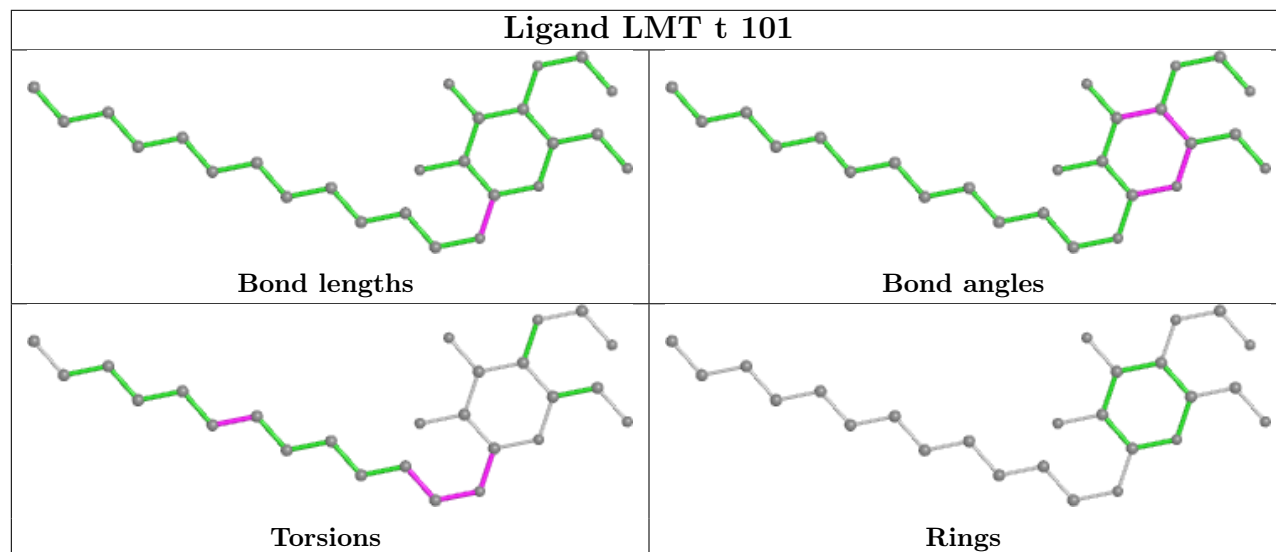
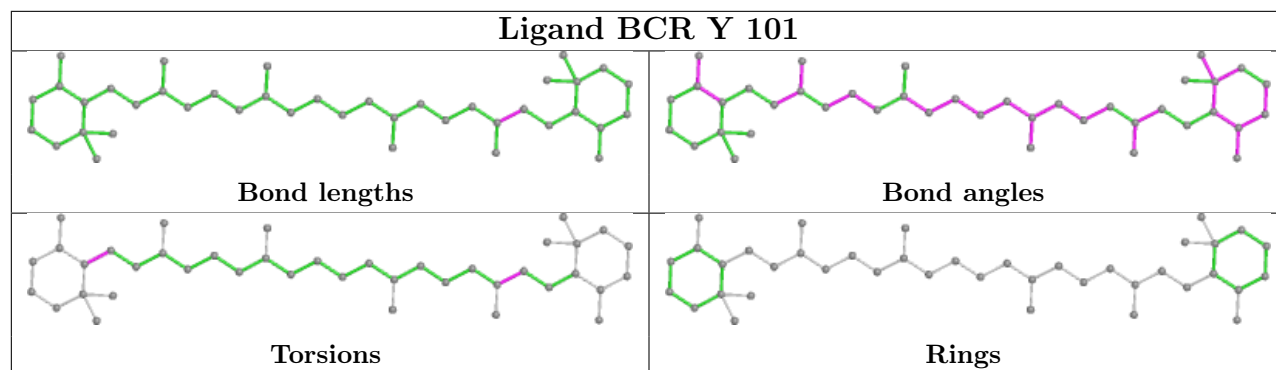
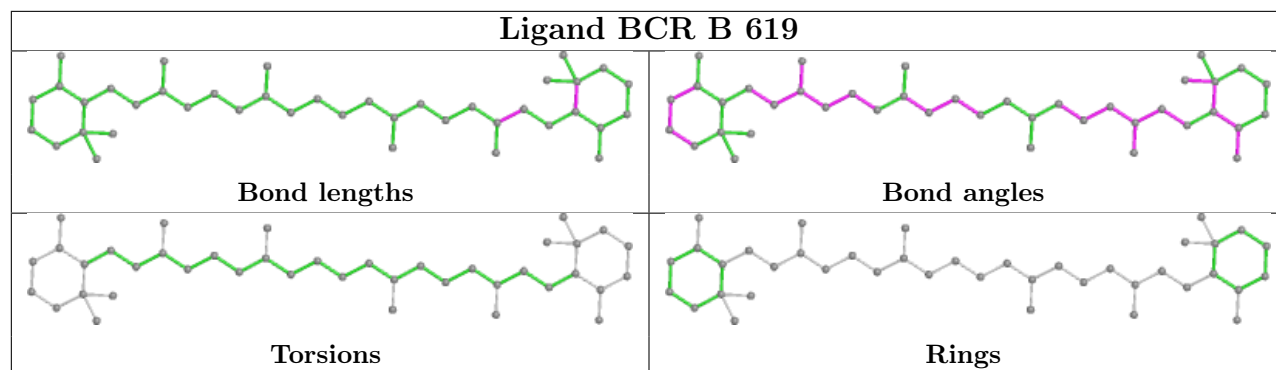


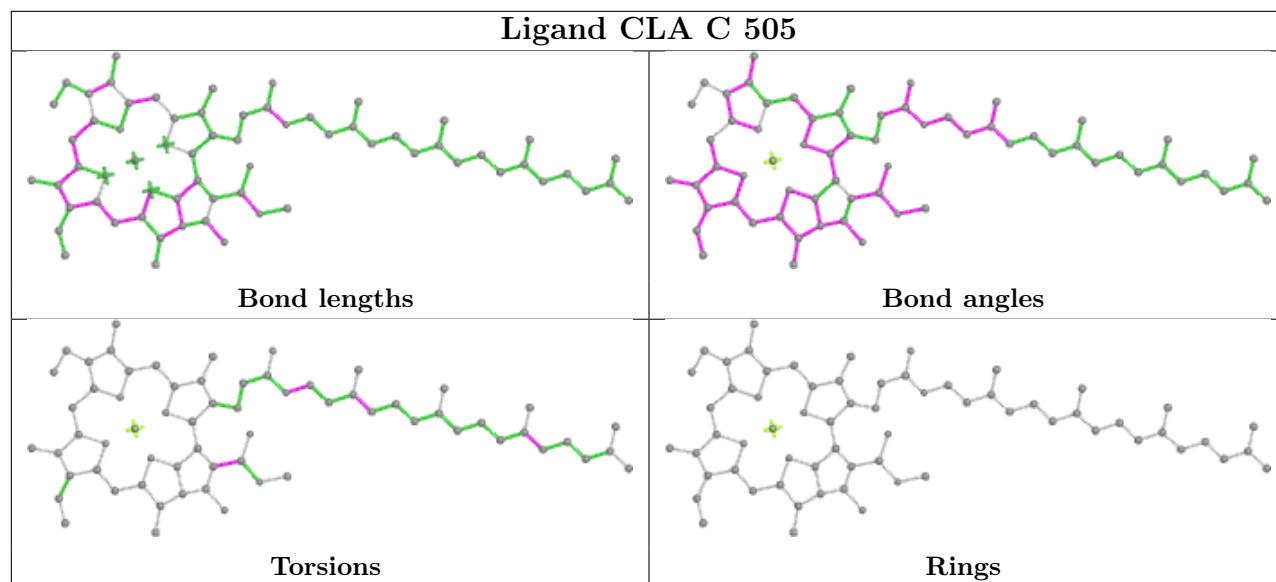
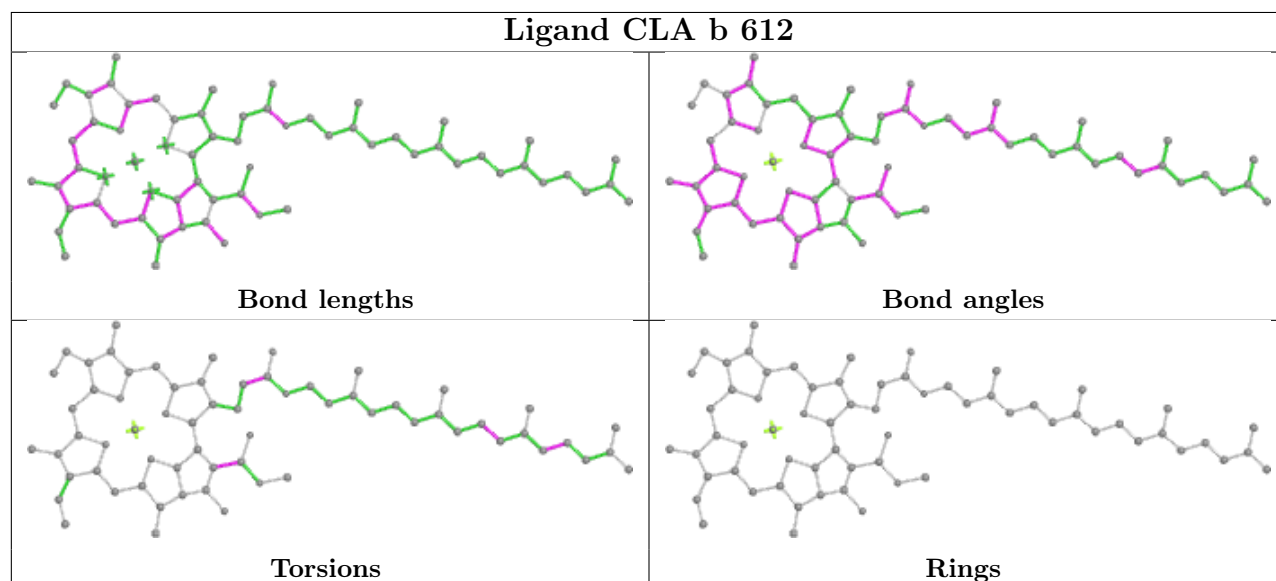
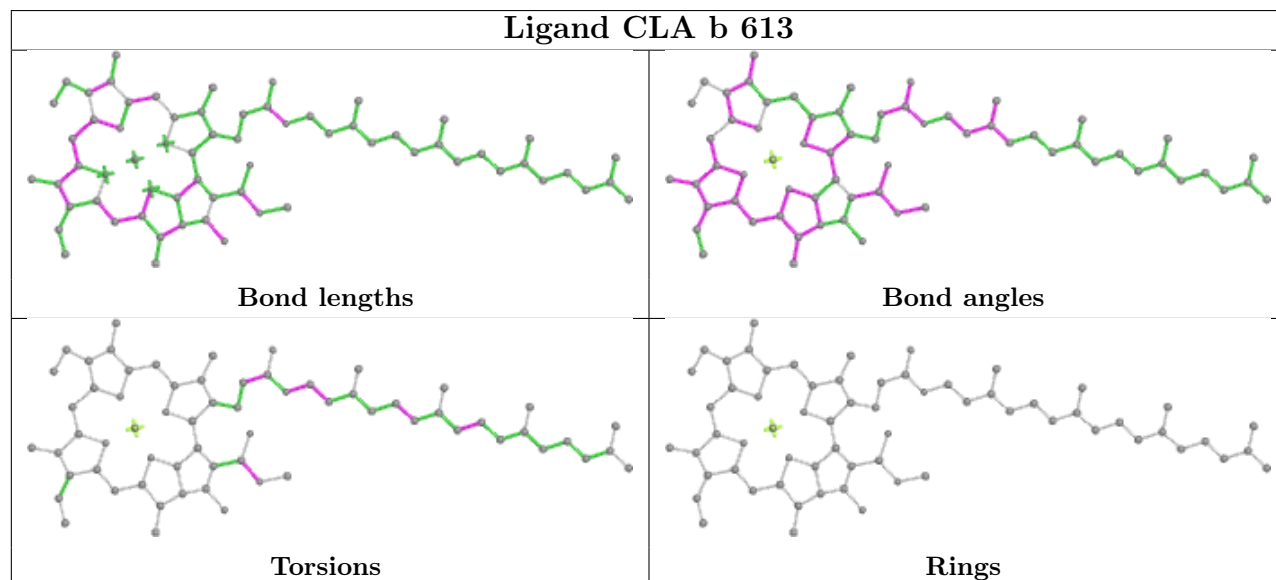
## Ligand CLA a 404



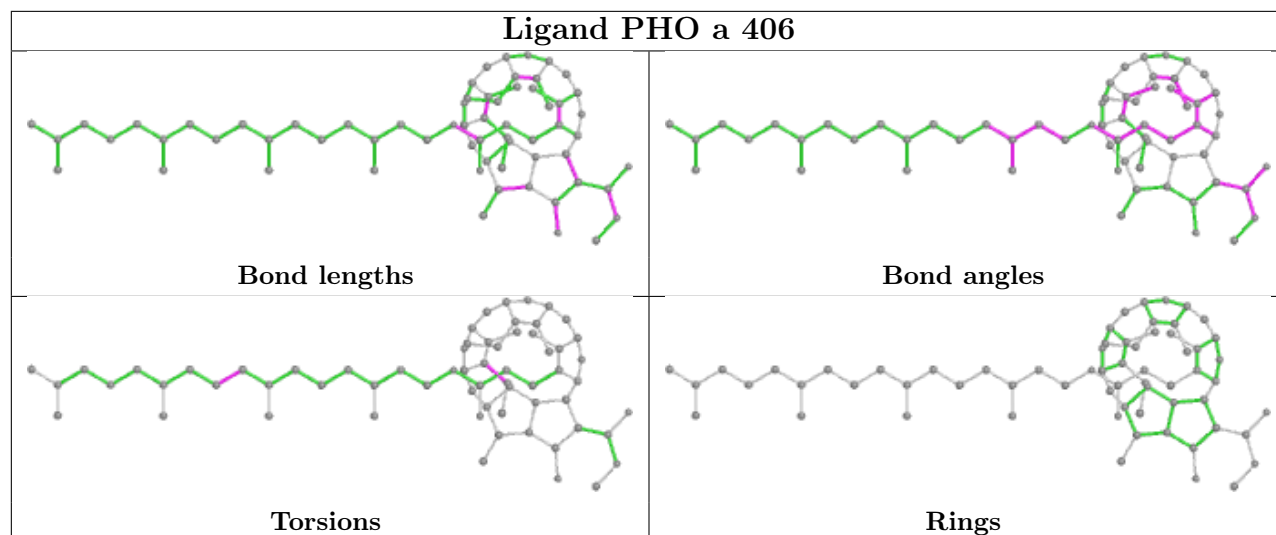
## Ligand PHO A 408





**Ligand CLA C 505****Ligand CLA b 612****Ligand CLA b 613**





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)	1.51	76 (22%) 0 1	40, 48, 69, 120	1 (0%)
1	a	334/344 (97%)	1.77	109 (32%) 0 0	41, 52, 84, 120	0
2	B	504/505 (99%)	1.66	154 (30%) 0 0	41, 53, 83, 128	0
2	b	504/505 (99%)	1.83	167 (33%) 0 0	44, 57, 97, 149	0
3	C	451/455 (99%)	1.83	162 (35%) 0 0	43, 59, 81, 142	0
3	c	455/455 (100%)	1.97	190 (41%) 0 0	48, 67, 90, 129	0
4	D	342/342 (100%)	1.45	88 (25%) 0 1	38, 49, 68, 139	0
4	d	341/342 (99%)	1.62	104 (30%) 0 0	43, 55, 78, 147	0
5	E	81/84 (96%)	2.35	40 (49%) 0 0	53, 70, 100, 151	0
5	e	79/84 (94%)	3.52	61 (77%) 0 0	62, 78, 122, 140	0
6	F	34/44 (77%)	1.45	10 (29%) 0 0	52, 63, 90, 117	0
6	f	31/44 (70%)	2.68	15 (48%) 0 0	62, 68, 100, 140	0
7	H	64/65 (98%)	1.93	24 (37%) 0 0	49, 62, 81, 129	0
7	h	64/65 (98%)	2.21	28 (43%) 0 0	58, 69, 95, 147	0
8	I	37/38 (97%)	2.05	12 (32%) 0 0	55, 62, 127, 147	0
8	i	37/38 (97%)	2.00	15 (40%) 0 0	57, 66, 123, 138	0
9	J	38/39 (97%)	2.17	16 (42%) 0 0	51, 71, 129, 175	0
9	j	39/39 (100%)	2.85	24 (61%) 0 0	56, 80, 149, 175	0
10	K	37/37 (100%)	1.70	13 (35%) 0 0	60, 67, 89, 101	0
10	k	37/37 (100%)	2.37	25 (67%) 0 0	70, 77, 101, 117	0
11	L	36/37 (97%)	1.88	10 (27%) 0 0	41, 47, 109, 162	0
11	l	36/37 (97%)	1.50	7 (19%) 1 2	43, 48, 103, 152	0
12	M	32/36 (88%)	1.37	6 (18%) 1 2	43, 49, 74, 134	0
12	m	33/36 (91%)	1.48	4 (12%) 4 7	43, 50, 86, 140	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	1.92	80 (32%) 0 0	40, 63, 115, 176	0
13	o	243/244 (99%)	2.05	96 (39%) 0 0	44, 65, 121, 161	0
14	T	29/32 (90%)	1.17	3 (10%) 6 10	42, 49, 81, 115	0
14	t	29/32 (90%)	1.13	2 (6%) 16 24	43, 50, 81, 130	0
15	U	96/104 (92%)	1.81	36 (37%) 0 0	47, 60, 90, 101	0
15	u	97/104 (93%)	1.36	20 (20%) 1 1	51, 62, 84, 121	0
16	V	137/137 (100%)	1.53	33 (24%) 0 1	46, 57, 82, 112	0
16	v	137/137 (100%)	2.40	74 (54%) 0 0	52, 71, 104, 137	0
17	X	38/40 (95%)	2.46	22 (57%) 0 0	59, 71, 96, 126	0
17	x	38/40 (95%)	3.14	25 (65%) 0 0	65, 78, 117, 154	0
18	Y	29/30 (96%)	4.41	24 (82%) 0 0	73, 87, 140, 155	0
18	y	29/30 (96%)	4.02	24 (82%) 0 0	79, 97, 126, 136	0
19	Z	62/62 (100%)	3.93	51 (82%) 0 0	67, 84, 131, 173	0
19	z	62/62 (100%)	4.79	55 (88%) 0 0	83, 99, 148, 185	0
20	R	34/34 (100%)	6.44	34 (100%) 0 0	97, 125, 149, 154	0
All	All	5283/5384 (98%)	1.95	1939 (36%) 0 0	38, 59, 104, 185	1 (0%)

The worst 5 of 1939 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	15.0
11	L	2	GLU	12.7
19	z	33	TRP	12.5
18	Y	19	ILE	12.3
6	f	15	ILE	12.3

## 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
8	FME	I	1	10/11	0.81	0.25	46,65,76,76	0
8	FME	i	1	10/11	0.81	0.28	59,64,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	FME	M	1	10/11	0.84	0.26	34,56,91,100	0
14	FME	T	1	10/11	0.88	0.19	44,50,74,88	0
14	FME	t	1	10/11	0.89	0.17	43,51,75,84	0
12	FME	m	1	10/11	0.89	0.20	47,60,91,103	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
35	HTG	c	523	19/19	-0.05	0.60	118,144,148,169	0
34	LMT	b	622	25/35	0.02	0.59	88,117,159,160	0
35	HTG	c	526	19/19	0.13	0.58	114,161,170,200	0
37	CA	V	201	1/1	0.13	0.20	141,141,141,141	0
35	HTG	b	625	19/19	0.16	0.45	91,138,154,196	0
32	UNL	i	101	40/-	0.20	0.44	77,109,164,165	0
34	LMT	B	622	35/35	0.21	0.46	78,125,142,144	0
32	UNL	b	629	33/-	0.22	0.40	72,108,162,162	0
34	LMT	m	102	35/35	0.22	0.45	63,95,117,121	0
33	LMG	c	522	51/55	0.23	0.53	80,127,154,158	0
34	LMT	I	101	35/35	0.23	0.47	110,145,160,162	0
27	SQD	f	101	43/54	0.24	0.51	118,136,170,175	0
35	HTG	D	410	16/19	0.24	0.50	82,121,136,138	0
32	UNL	A	417	28/-	0.24	0.44	98,110,128,144	0
38	LHG	a	419	42/49	0.24	0.51	78,141,167,179	0
34	LMT	A	359	35/35	0.26	0.55	73,134,144,148	0
34	LMT	e	101	35/35	0.27	0.67	121,166,181,186	0
33	LMG	C	521	51/55	0.27	0.46	68,121,155,157	0
34	LMT	a	359	35/35	0.28	0.50	65,144,151,154	0
35	HTG	h	101	16/19	0.28	0.50	98,133,140,163	0
32	UNL	B	629	33/-	0.29	0.46	57,103,166,173	0
32	UNL	K	101	34/-	0.30	0.61	83,119,134,150	0
35	HTG	B	625	19/19	0.31	0.34	82,167,178,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	LMT	M	101	35/35	0.31	0.41	61,99,123,126	0
33	LMG	Z	101	37/55	0.33	0.44	77,129,150,151	0
38	LHG	E	101	42/49	0.34	0.45	72,118,132,132	0
32	UNL	a	415	30/-	0.34	0.41	98,115,136,146	0
34	LMT	a	418	35/35	0.35	0.49	113,136,151,151	0
33	LMG	z	101	39/55	0.38	0.42	84,133,148,153	0
27	SQD	b	620	54/54	0.40	0.44	68,93,144,152	0
33	LMG	a	417	51/55	0.42	0.52	76,100,122,129	0
34	LMT	M	103	35/35	0.42	0.38	68,146,169,171	0
34	LMT	B	630	25/35	0.43	0.47	54,89,147,148	0
35	HTG	C	522	19/19	0.45	0.36	112,123,133,150	0
35	HTG	C	523	19/19	0.45	0.56	84,153,166,186	0
27	SQD	B	620	54/54	0.46	0.43	65,93,132,134	0
32	UNL	d	410	36/-	0.46	0.58	73,100,136,140	0
32	UNL	I	102	40/-	0.46	0.39	66,113,156,158	0
33	LMG	A	418	51/55	0.47	0.50	61,97,118,121	0
35	HTG	b	624	19/19	0.48	0.44	114,128,145,170	0
35	HTG	b	628	19/19	0.49	0.33	61,82,106,112	0
27	SQD	a	411	54/54	0.49	0.43	72,95,139,149	0
36	DGD	h	103	62/66	0.49	0.50	52,66,78,86	0
34	LMT	b	630	25/35	0.50	0.42	57,81,151,153	0
35	HTG	b	623	19/19	0.50	0.40	68,88,130,131	0
32	UNL	c	527	32/-	0.50	0.37	93,125,140,143	0
27	SQD	A	413	54/54	0.54	0.42	63,91,128,137	0
34	LMT	E	102	35/35	0.57	0.44	119,145,171,173	0
35	HTG	B	624	19/19	0.58	0.36	71,103,114,115	0
32	UNL	j	102	10/-	0.58	0.58	87,106,117,118	0
32	UNL	D	409	40/-	0.59	0.43	67,93,136,140	0
33	LMG	B	621	51/55	0.60	0.41	53,72,94,108	0
24	CLA	C	514	65/65	0.61	0.31	60,81,122,127	0
33	LMG	b	621	51/55	0.62	0.36	53,74,105,124	0
24	CLA	B	609	65/65	0.63	0.30	47,57,73,80	0
24	CLA	b	602	65/65	0.63	0.37	51,62,79,88	0
33	LMG	c	521	51/55	0.63	0.39	68,101,145,156	0
35	HTG	B	623	19/19	0.63	0.34	70,88,128,128	0
28	GOL	a	416	6/6	0.64	0.36	55,82,84,86	0
27	SQD	A	411	54/54	0.65	0.41	55,86,123,126	0
36	DGD	H	102	62/66	0.65	0.48	46,63,76,78	0
24	CLA	c	515	65/65	0.65	0.33	70,91,134,138	0
33	LMG	C	520	51/55	0.66	0.41	56,90,127,140	0
31	PL9	a	414[B]	55/55	0.66	0.43	97,107,120,124	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
31	PL9	a	414[A]	55/55	0.66	0.43	97,107,120,124	55
35	HTG	B	628	19/19	0.67	0.26	65,80,89,95	0
32	UNL	x	101	18/-	0.67	0.27	70,85,105,106	0
27	SQD	F	101	43/54	0.67	0.32	81,114,134,137	0
34	LMT	t	101	26/35	0.67	0.28	71,110,152,153	0
36	DGD	C	518	62/66	0.68	0.36	48,67,127,131	0
24	CLA	C	505	65/65	0.69	0.40	42,56,103,113	0
24	CLA	b	609	65/65	0.69	0.31	50,61,83,99	0
32	UNL	m	101	10/-	0.69	0.55	69,78,80,84	0
28	GOL	v	202	6/6	0.70	0.75	75,86,94,96	0
24	CLA	c	505	65/65	0.70	0.40	58,67,77,83	0
24	CLA	C	504	65/65	0.70	0.40	47,58,76,85	0
38	LHG	l	101	49/49	0.70	0.32	50,60,74,91	0
26	BCR	h	102	40/40	0.71	0.24	56,70,80,81	0
24	CLA	c	512	65/65	0.71	0.39	50,65,81,92	0
24	CLA	B	602	65/65	0.71	0.34	45,55,80,84	0
37	CA	O	301	1/1	0.71	0.32	119,119,119,119	0
24	CLA	C	512	65/65	0.72	0.23	52,63,79,86	0
36	DGD	c	518	62/66	0.72	0.37	49,67,95,103	0
31	PL9	A	416[A]	55/55	0.72	0.39	66,93,107,111	55
31	PL9	A	416[B]	55/55	0.72	0.39	66,93,108,113	55
36	DGD	C	517	62/66	0.73	0.40	43,63,104,106	0
24	CLA	c	507	65/65	0.73	0.29	49,61,91,95	0
28	GOL	a	410	6/6	0.73	0.31	79,81,90,95	0
24	CLA	b	601	65/65	0.73	0.30	58,85,115,130	0
28	GOL	b	627	6/6	0.73	0.29	97,106,113,116	0
24	CLA	c	513	65/65	0.74	0.24	57,71,91,97	0
36	DGD	c	519	62/66	0.74	0.34	56,73,136,145	0
32	UNL	X	101	18/-	0.74	0.26	57,76,100,100	0
24	CLA	b	603	65/65	0.74	0.38	46,56,85,92	0
27	SQD	a	409	54/54	0.75	0.30	63,85,127,131	0
24	CLA	C	513	65/65	0.75	0.25	60,73,118,123	0
24	CLA	c	508	65/65	0.75	0.26	60,72,120,133	0
24	CLA	B	605	65/65	0.76	0.32	39,48,65,68	0
24	CLA	c	510	65/65	0.76	0.29	53,63,141,145	0
24	CLA	B	611	65/65	0.76	0.33	37,47,63,73	0
24	CLA	C	506	65/65	0.76	0.36	49,57,92,100	0
24	CLA	b	614	65/65	0.76	0.25	41,49,116,120	0
24	CLA	b	615	65/65	0.76	0.22	46,59,81,86	0
38	LHG	D	357	49/49	0.76	0.49	49,64,86,102	0
24	CLA	a	350	65/65	0.76	0.27	36,46,63,77	0
24	CLA	C	507	65/65	0.76	0.27	53,69,137,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	LMG	J	101	51/55	0.76	0.30	48,73,119,126	0
33	LMG	j	101	51/55	0.77	0.27	60,70,121,138	0
24	CLA	C	509	65/65	0.77	0.34	44,57,115,131	0
24	CLA	B	606	65/65	0.77	0.25	41,52,104,114	0
24	CLA	b	606	65/65	0.77	0.24	45,58,114,129	0
24	CLA	b	608	65/65	0.77	0.40	46,58,81,84	0
24	CLA	B	608	65/65	0.77	0.35	41,54,68,71	0
39	HEM	E	103	43/43	0.77	0.26	60,70,80,93	0
24	CLA	A	404	65/65	0.78	0.27	36,43,66,80	0
24	CLA	A	405	65/65	0.78	0.26	34,45,54,63	0
28	GOL	V	202	6/6	0.78	0.74	64,74,85,92	0
24	CLA	B	612	65/65	0.78	0.32	35,47,57,74	0
36	DGD	C	519	62/66	0.78	0.28	43,60,94,116	0
24	CLA	c	514	65/65	0.78	0.26	59,80,123,128	0
24	CLA	b	610	65/65	0.78	0.33	47,58,73,75	0
24	CLA	b	612	65/65	0.78	0.34	43,54,64,75	0
38	LHG	D	407	49/49	0.79	0.42	53,61,120,125	0
32	UNL	d	409	17/-	0.79	0.65	68,83,111,114	0
26	BCR	H	101	40/40	0.79	0.20	50,65,77,82	0
38	LHG	L	101	49/49	0.79	0.36	45,55,67,96	0
24	CLA	B	601	65/65	0.79	0.30	53,77,112,132	0
38	LHG	d	406	49/49	0.79	0.37	50,66,90,106	0
38	LHG	d	407	49/49	0.79	0.36	48,59,73,85	0
24	CLA	B	614	65/65	0.79	0.26	38,49,103,113	0
24	CLA	C	502	65/65	0.79	0.32	48,59,73,83	0
24	CLA	C	511	65/65	0.80	0.42	49,61,74,88	0
38	LHG	d	408	49/49	0.80	0.34	53,68,121,125	0
24	CLA	c	504	65/65	0.80	0.36	45,65,86,89	0
24	CLA	b	605	65/65	0.80	0.33	43,52,70,74	0
24	CLA	D	402	65/65	0.81	0.24	31,45,68,82	0
32	UNL	J	102	10/-	0.81	0.50	77,81,99,104	0
37	CA	b	626	1/1	0.81	0.51	151,151,151,151	0
24	CLA	c	506	65/65	0.81	0.34	51,66,116,125	0
24	CLA	a	403	65/65	0.81	0.29	36,48,69,86	0
24	CLA	a	404	65/65	0.81	0.26	42,53,126,133	0
24	CLA	c	509	65/65	0.81	0.25	56,70,86,92	0
24	CLA	B	613	65/65	0.81	0.36	37,47,94,103	0
24	CLA	c	511	65/65	0.81	0.31	51,69,82,89	0
24	CLA	A	406	65/65	0.81	0.24	36,47,110,116	0
24	CLA	B	615	65/65	0.81	0.20	37,52,74,83	0
24	CLA	B	607	65/65	0.81	0.30	32,45,71,78	0
24	CLA	C	508	65/65	0.81	0.29	49,60,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	B	604	65/65	0.82	0.37	34,46,123,127	0
26	BCR	y	101	40/40	0.82	0.16	58,74,88,88	0
24	CLA	b	611	65/65	0.82	0.28	41,52,73,82	0
24	CLA	b	616	65/65	0.82	0.21	50,60,124,127	0
24	CLA	d	403	65/65	0.82	0.20	46,64,132,137	0
35	HTG	V	204	11/19	0.82	0.49	104,117,122,125	0
25	PHO	a	406	64/64	0.82	0.29	41,55,63,65	0
37	CA	c	525	1/1	0.82	0.16	92,92,92,92	0
24	CLA	b	607	65/65	0.82	0.30	35,49,77,87	0
39	HEM	e	102	43/43	0.82	0.42	67,93,128,137	0
38	LHG	D	406	49/49	0.83	0.40	47,57,76,93	0
26	BCR	c	516	40/40	0.83	0.21	77,86,93,96	0
32	UNL	D	408	17/-	0.83	0.56	66,85,107,110	0
32	UNL	M	102	10/-	0.83	0.47	62,72,86,92	0
24	CLA	d	402	65/65	0.83	0.28	39,48,74,86	0
24	CLA	B	603	65/65	0.83	0.34	42,52,69,76	0
26	BCR	B	618	40/40	0.84	0.34	44,57,70,77	0
28	GOL	C	525	6/6	0.84	0.39	66,73,76,78	0
26	BCR	k	101	40/40	0.84	0.26	58,73,84,90	0
37	CA	v	201	1/1	0.84	0.18	123,123,123,123	0
24	CLA	c	503	65/65	0.84	0.31	56,66,79,86	0
36	DGD	c	520	62/66	0.84	0.28	55,64,100,116	0
26	BCR	T	101	40/40	0.84	0.33	46,57,68,72	0
24	CLA	B	610	65/65	0.84	0.30	43,53,64,80	0
41	HEC	V	203	43/43	0.84	0.19	39,52,58,60	0
24	CLA	C	503	65/65	0.85	0.37	47,55,78,95	0
26	BCR	b	618	40/40	0.85	0.36	44,60,73,75	0
24	CLA	D	403	65/65	0.85	0.21	44,58,139,144	0
26	BCR	d	404	40/40	0.85	0.20	53,67,96,98	0
24	CLA	b	613	65/65	0.85	0.33	42,49,101,106	0
24	CLA	b	604	65/65	0.85	0.35	37,50,122,128	0
37	CA	o	301	1/1	0.85	0.23	108,108,108,108	0
26	BCR	K	102	40/40	0.86	0.22	56,67,74,81	0
25	PHO	A	407	64/64	0.86	0.30	35,45,54,58	0
26	BCR	C	515	40/40	0.86	0.16	63,75,82,85	0
40	MG	J	103	1/1	0.86	0.20	61,61,61,61	0
24	CLA	B	616	65/65	0.86	0.19	45,58,147,153	0
26	BCR	a	408	40/40	0.87	0.22	42,52,65,68	0
25	PHO	A	408	64/64	0.87	0.27	37,49,57,60	0
24	CLA	A	409	65/65	0.87	0.21	42,53,136,144	0
26	BCR	D	404	40/40	0.87	0.22	46,61,94,95	0
41	HEC	v	203	43/43	0.87	0.17	51,64,72,78	0

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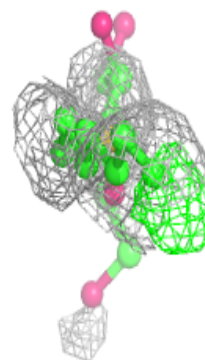
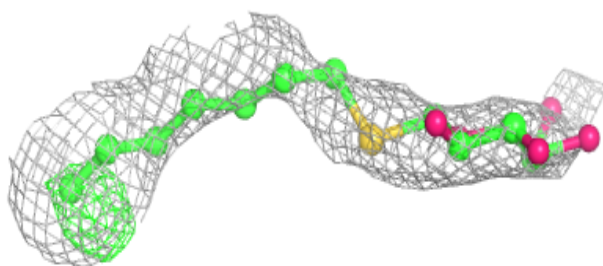
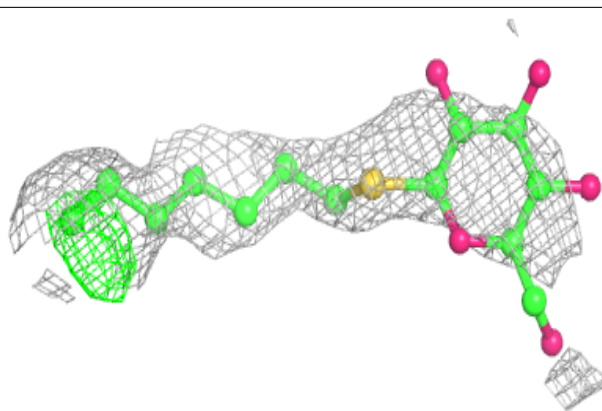
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	b	617	40/40	0.88	0.25	45,52,63,63	0
26	BCR	C	516	40/40	0.88	0.30	53,62,72,81	0
26	BCR	t	102	40/40	0.88	0.31	45,60,76,80	0
26	BCR	b	619	40/40	0.88	0.20	51,62,81,84	0
26	BCR	B	619	40/40	0.88	0.17	45,57,80,87	0
24	CLA	C	510	65/65	0.88	0.33	49,60,81,91	0
28	GOL	B	627	6/6	0.88	0.34	58,77,85,87	0
23	BCT	A	403[A]	4/4	0.89	0.23	58,60,60,69	4
31	PL9	d	405	55/55	0.89	0.29	41,50,66,85	0
23	BCT	A	403[B]	4/4	0.89	0.23	55,61,62,78	4
26	BCR	c	517	40/40	0.89	0.20	56,67,80,81	0
26	BCR	Y	101	40/40	0.89	0.18	57,68,74,81	0
28	GOL	A	412	6/6	0.89	0.17	80,82,86,98	0
25	PHO	a	405	64/64	0.90	0.30	41,49,56,64	0
24	CLA	a	407	65/65	0.90	0.19	44,57,134,140	0
26	BCR	B	617	40/40	0.90	0.29	44,52,59,65	0
26	BCR	A	410	40/40	0.91	0.22	42,51,61,62	0
28	GOL	c	502	6/6	0.91	0.55	68,70,71,75	0
30	OXY	A	415[B]	11/11	0.92	0.23	43,49,55,56	11
23	BCT	a	420[B]	4/4	0.92	0.21	54,63,64,72	4
23	BCT	a	420[A]	4/4	0.92	0.21	58,63,63,68	4
40	MG	j	103	1/1	0.92	0.18	64,64,64,64	0
31	PL9	D	405	55/55	0.92	0.34	37,49,62,78	0
29	OEX	a	412[A]	10/10	0.92	0.24	50,55,61,74	10
30	OXY	a	413[B]	11/11	0.93	0.24	50,54,58,74	11
29	OEX	A	414[A]	10/10	0.93	0.23	44,48,55,59	10
37	CA	c	524	1/1	0.94	0.20	78,78,78,78	0
28	GOL	B	626	6/6	0.95	0.34	85,88,90,95	0
22	CL	a	347	1/1	0.97	0.28	53,53,53,53	0
22	CL	A	402	1/1	0.98	0.32	44,44,44,44	0
22	CL	A	347	1/1	0.98	0.37	49,49,49,49	0
22	CL	a	402	1/1	0.98	0.40	51,51,51,51	0
21	FE2	a	401[A]	1/1	0.99	0.07	60,60,60,60	1
37	CA	C	524	1/1	0.99	0.19	72,72,72,72	0
21	FE2	a	401[B]	1/1	0.99	0.07	60,60,60,60	1
21	FE2	A	401[A]	1/1	0.99	0.05	62,62,62,62	1
21	FE2	A	401[B]	1/1	0.99	0.05	60,60,60,60	1

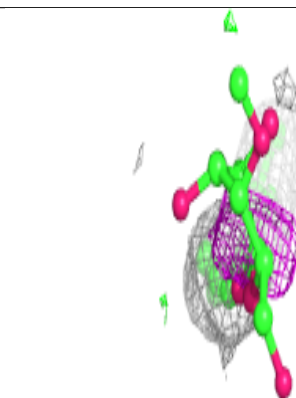
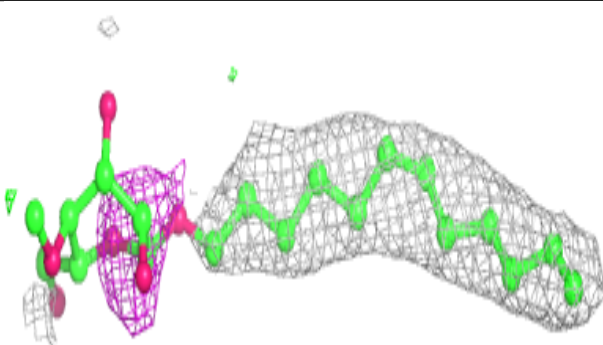
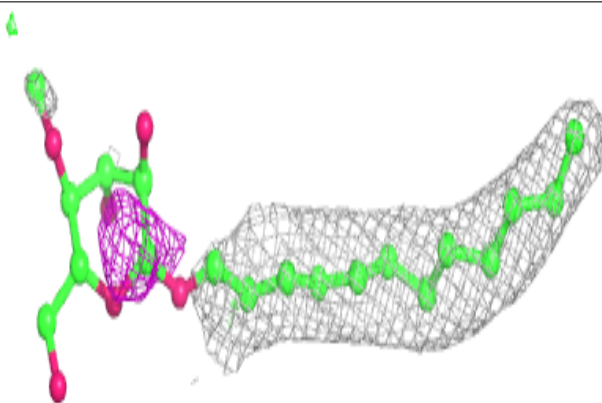
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HTG 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)

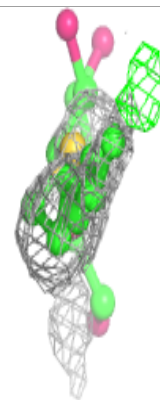
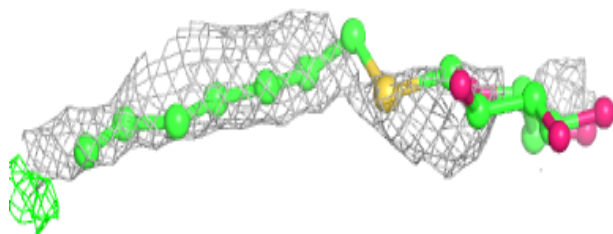
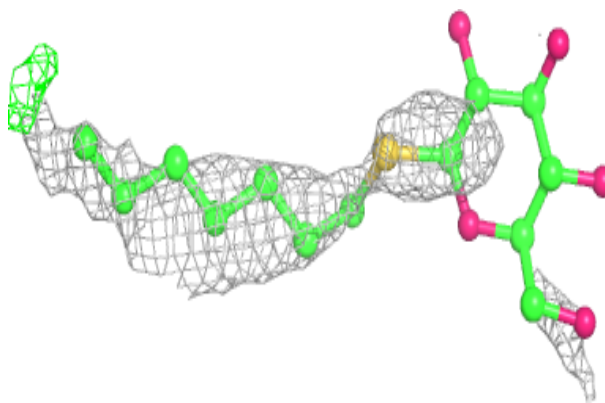
**Electron density around LMT b 622:**

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

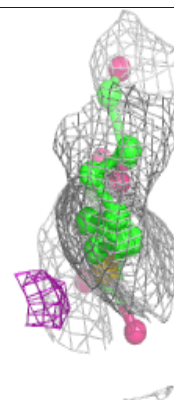
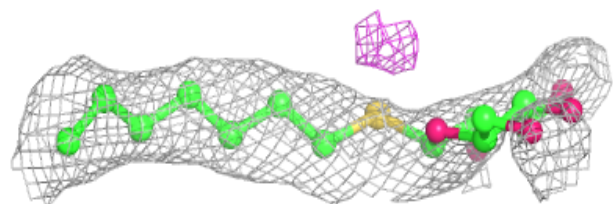
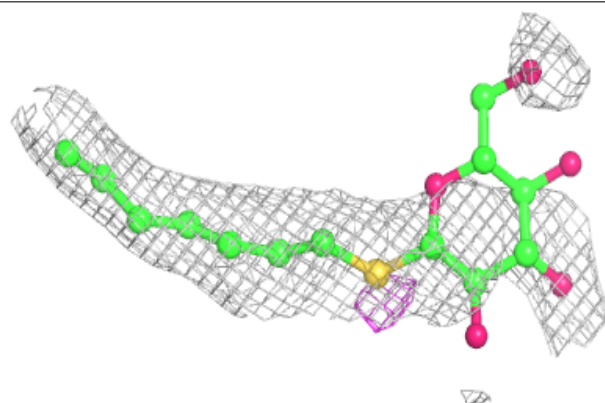


**Electron density around HTG c 526:**

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

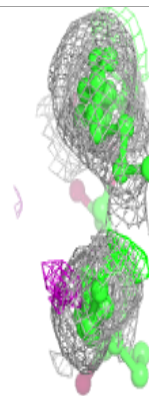
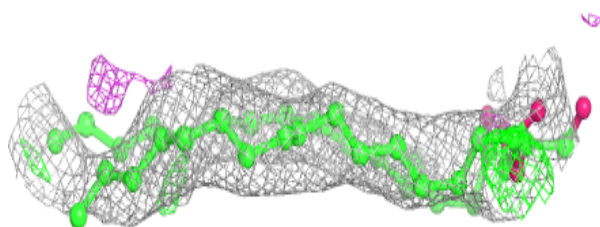
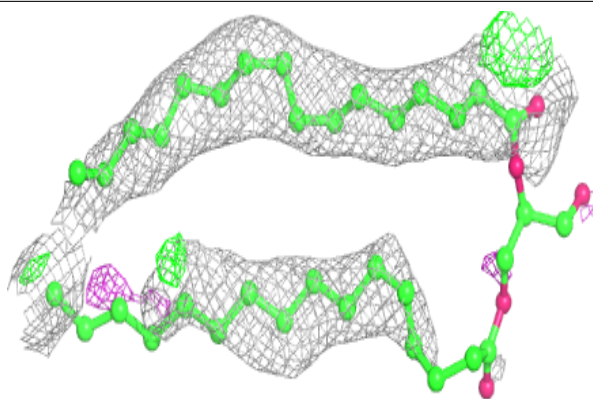
**Electron density around HTG b 625:**

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

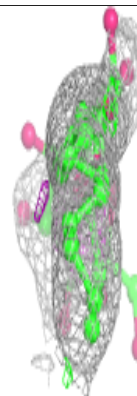
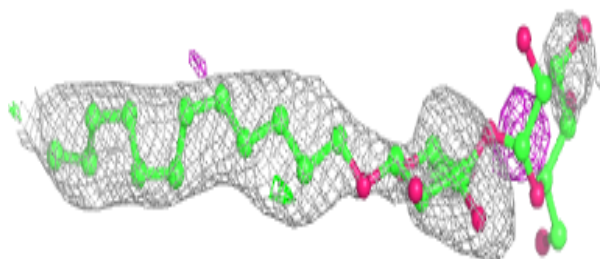
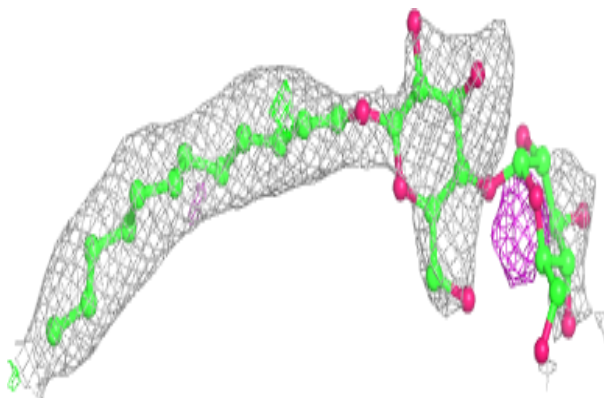


**Electron density around UNL i 101:**

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

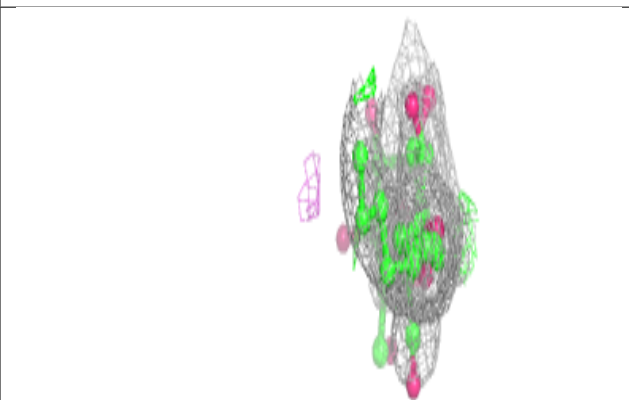
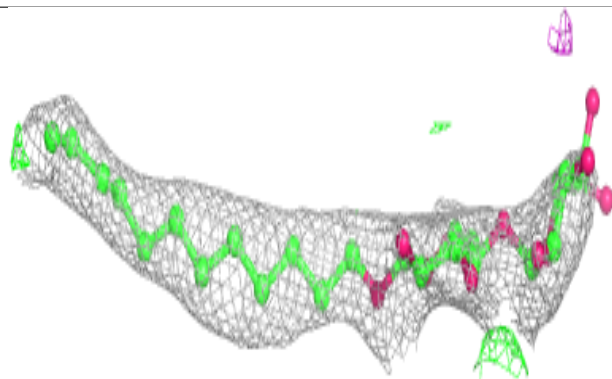
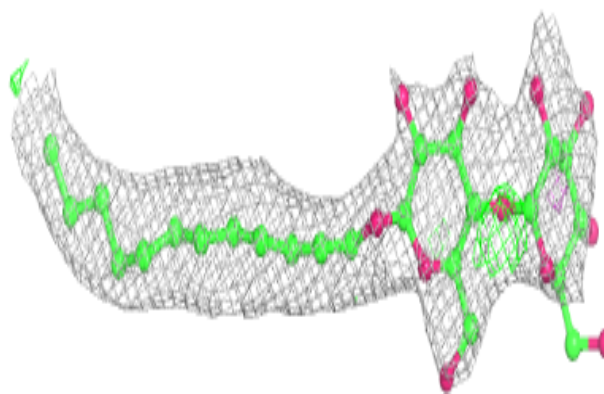
**Electron density around LMT B 622:**

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

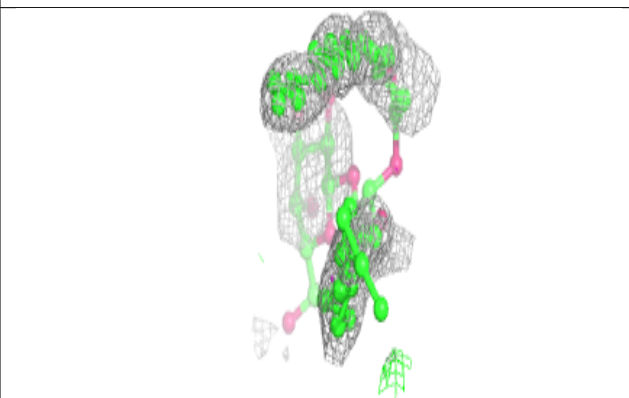
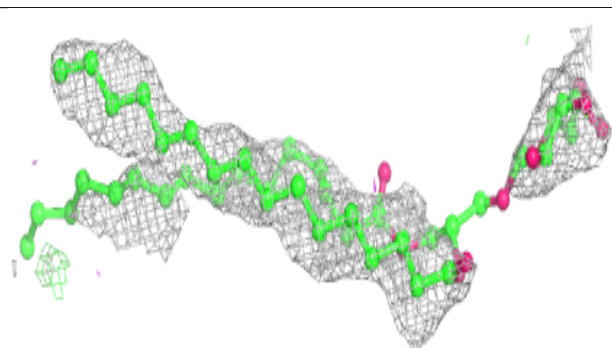
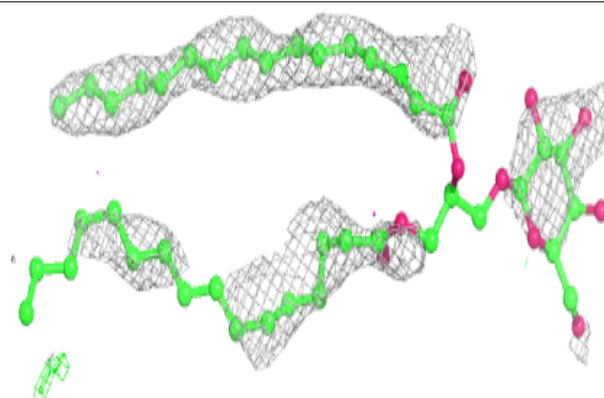


**Electron density around LMT m 102:**

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

**Electron density around LMG c 522:**

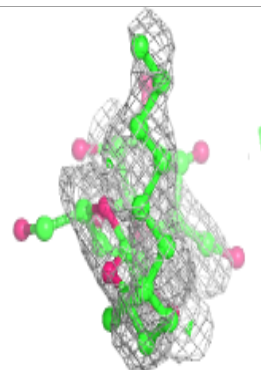
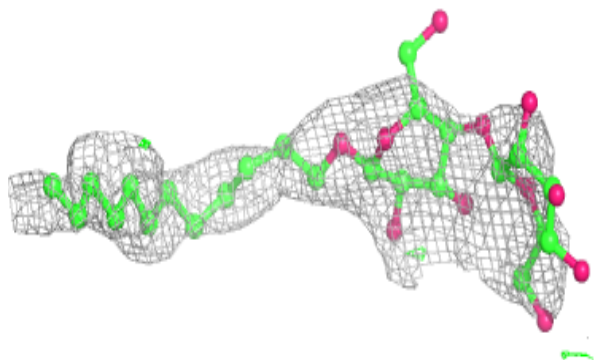
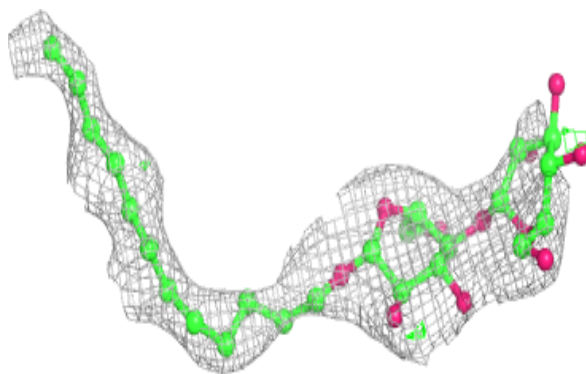
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



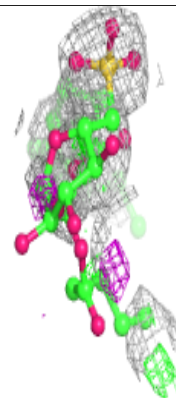
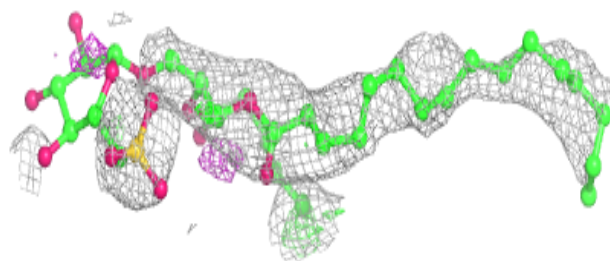
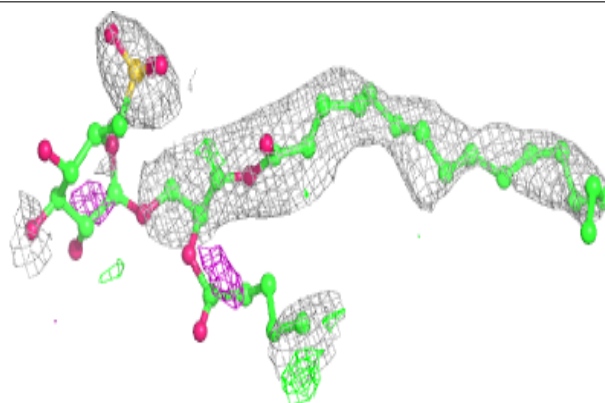


**Electron density around LMT I 101:**

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

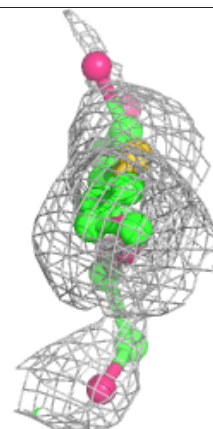
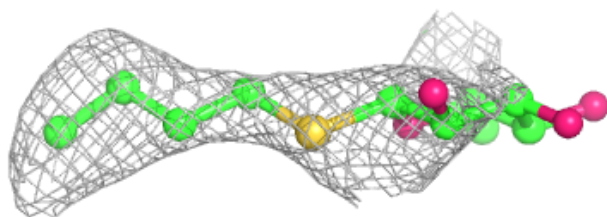
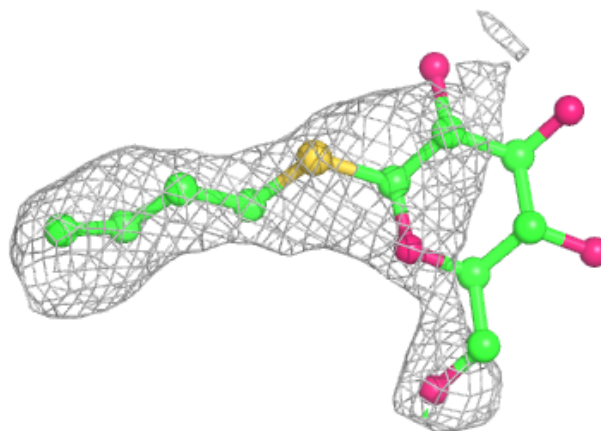
**Electron density around SQD f 101:**

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

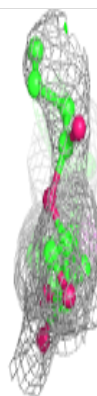
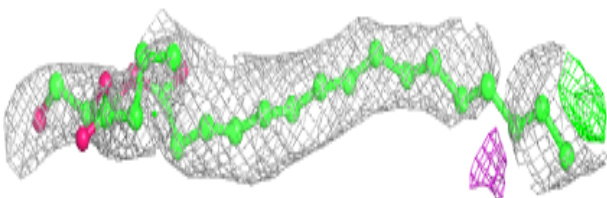
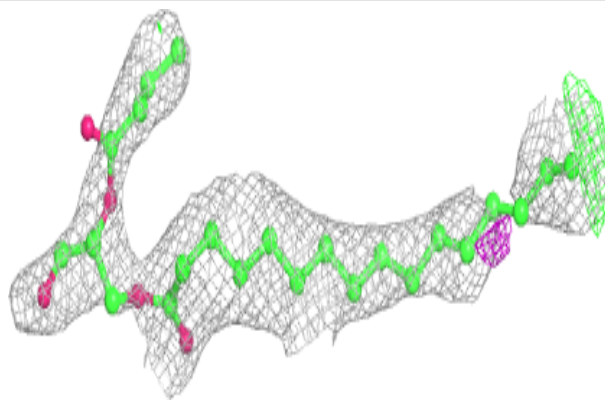


**Electron density around HTG D 410:**

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

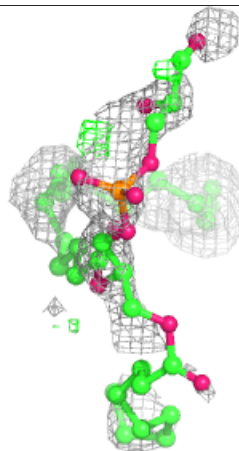
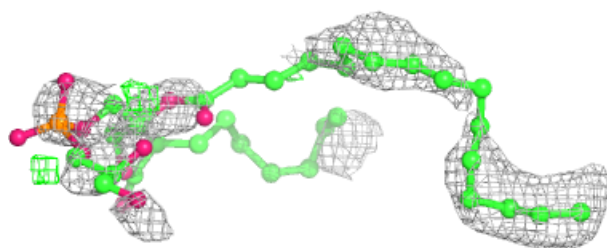
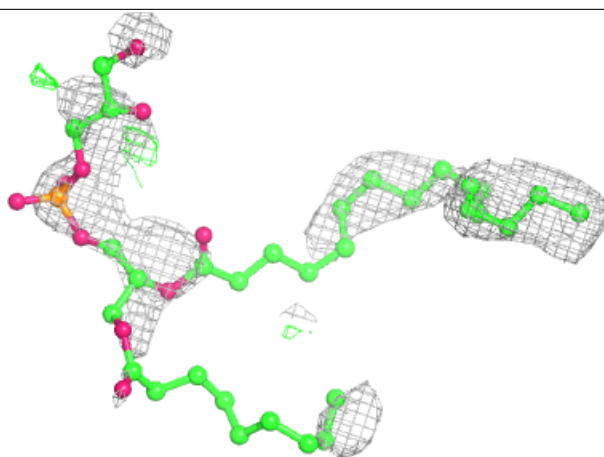
**Electron density around UNL A 417:**

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

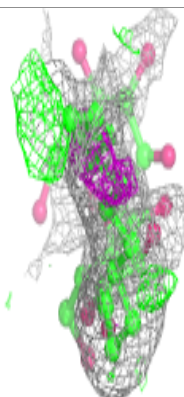
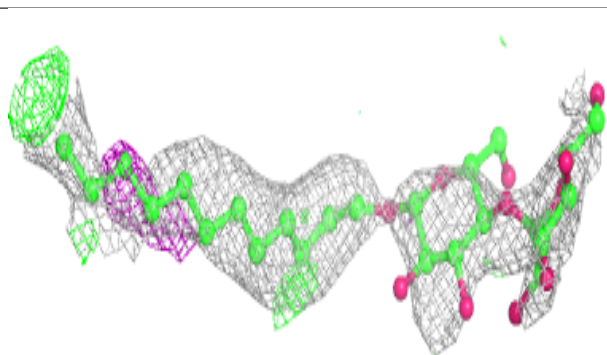
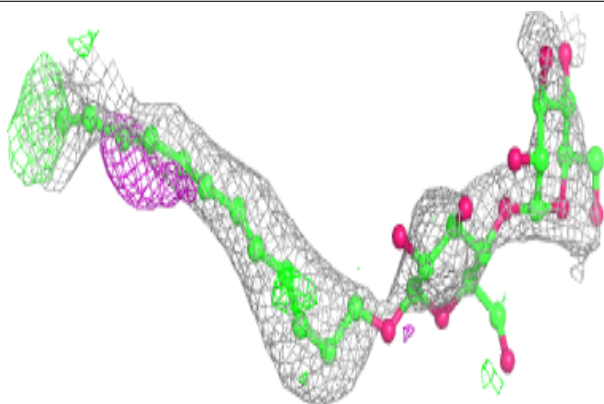


**Electron density around LHG a 419:**

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

**Electron density around LMT A 359:**

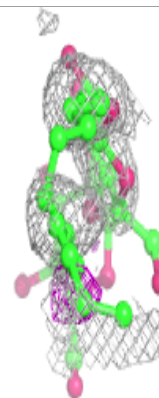
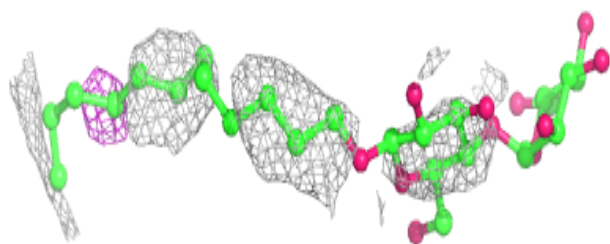
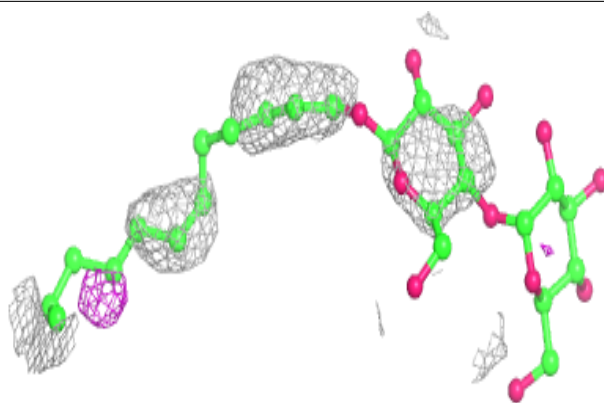
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



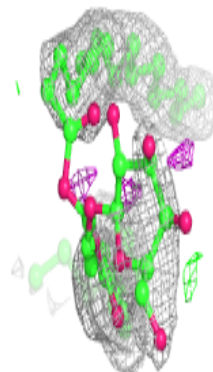
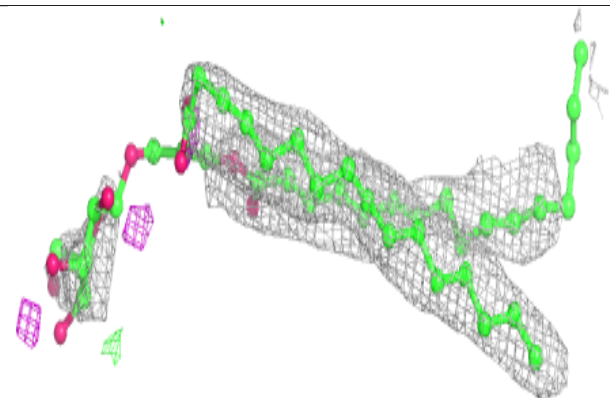
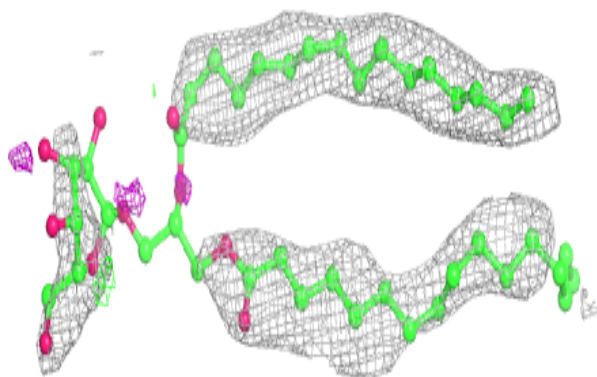


**Electron density around LMT e 101:**

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

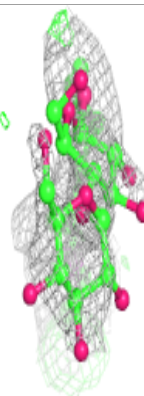
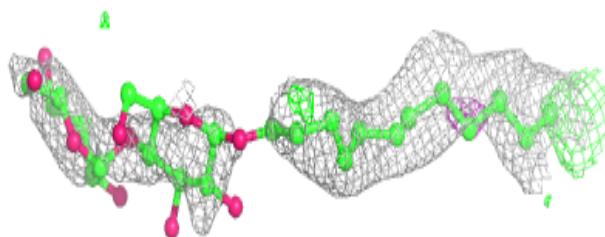
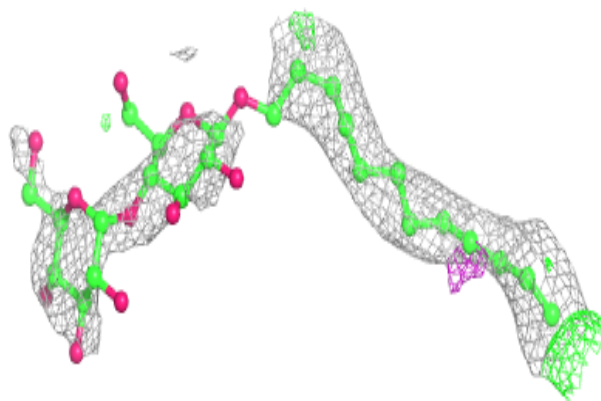
**Electron density around LMG C 521:**

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

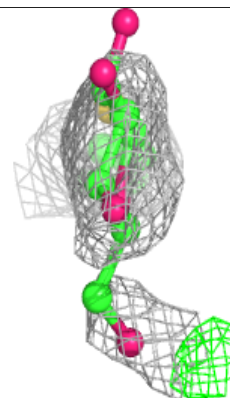
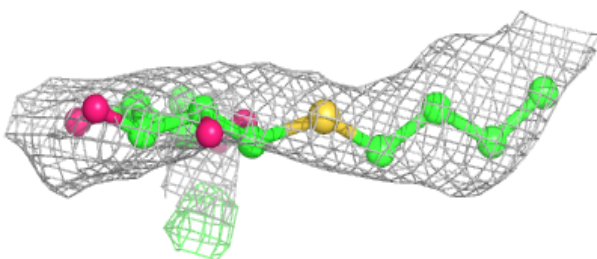
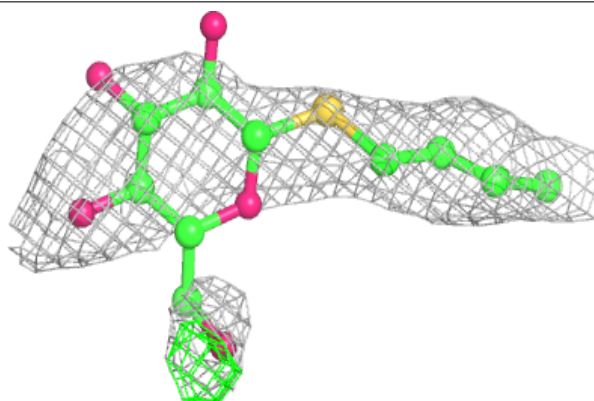


**Electron density around LMT a 359:**

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

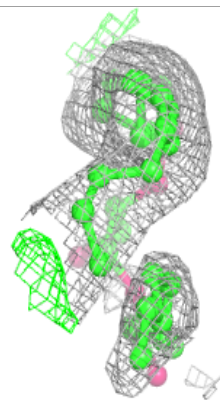
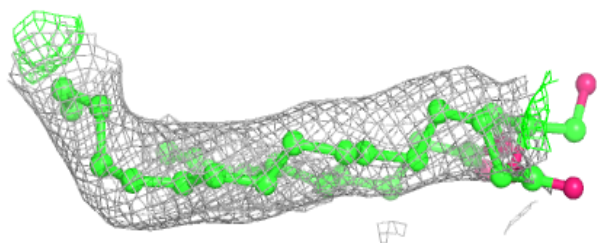
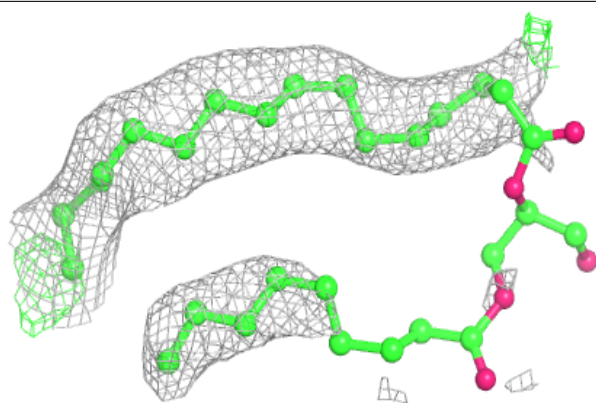
**Electron density around HTG h 101:**

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

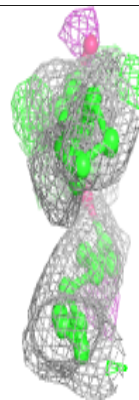
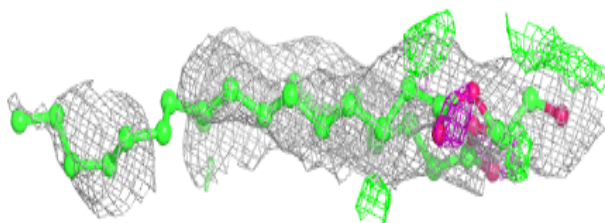
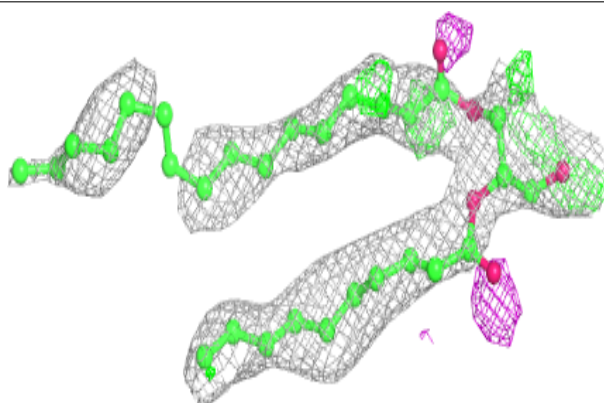


**Electron density around UNL B 629:**

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

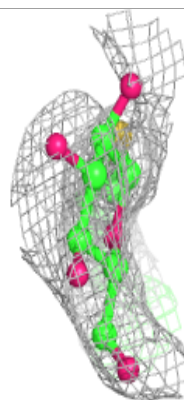
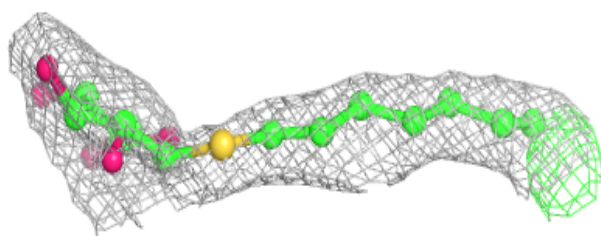
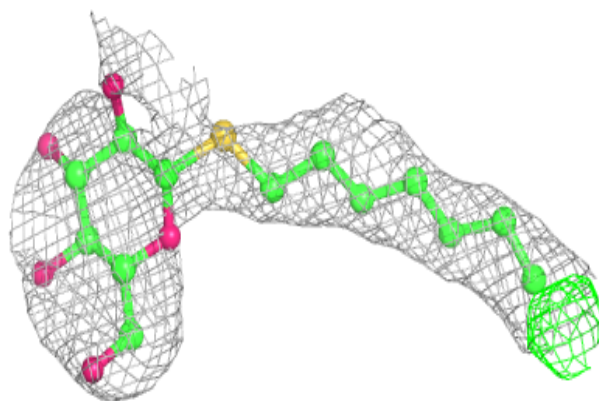
**Electron density around UNL K 101:**

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

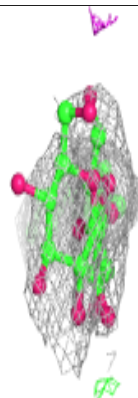
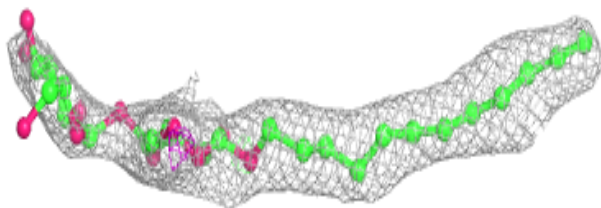
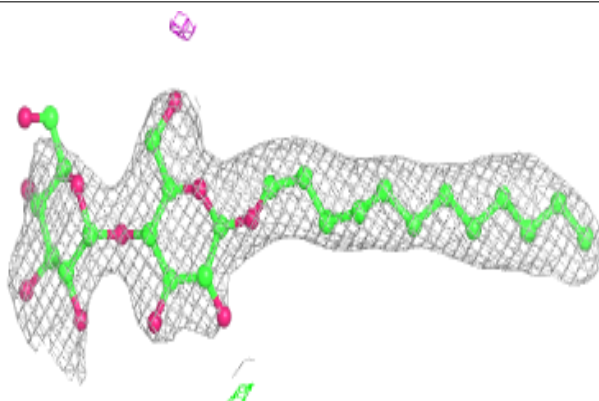


**Electron density around HTG B 625:**

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

**Electron density around LMT M 101:**

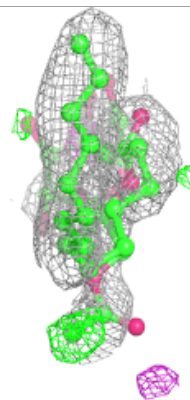
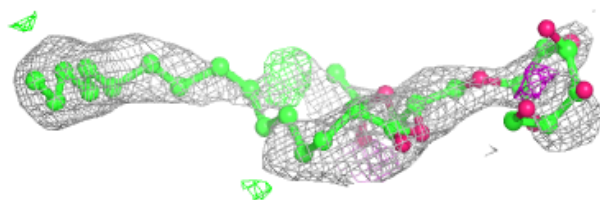
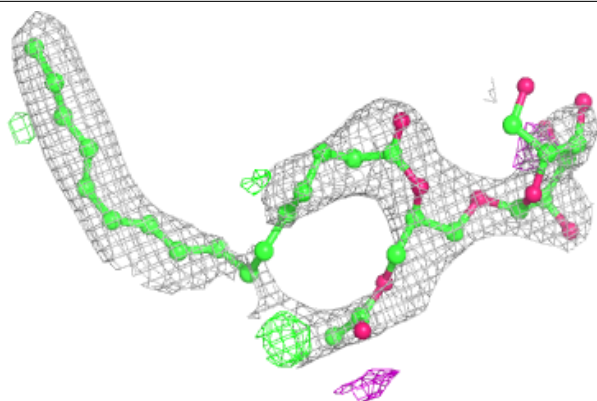
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



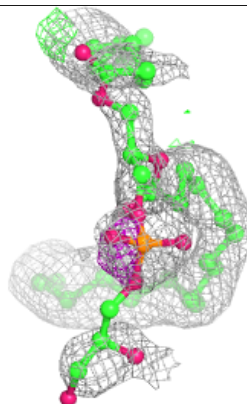
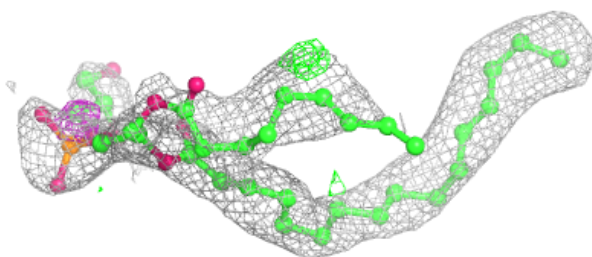
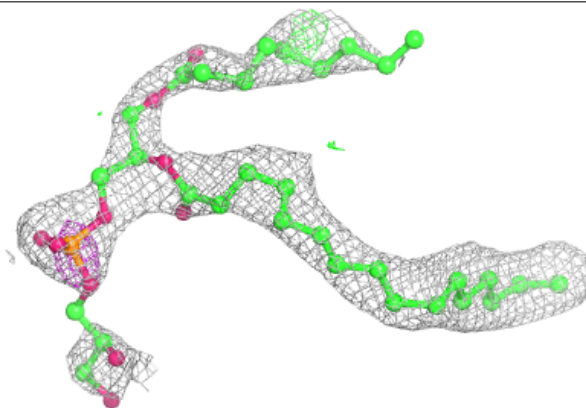


**Electron density around LMG Z 101:**

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

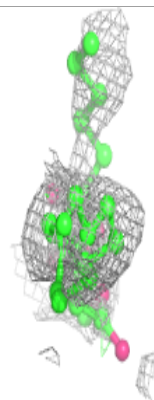
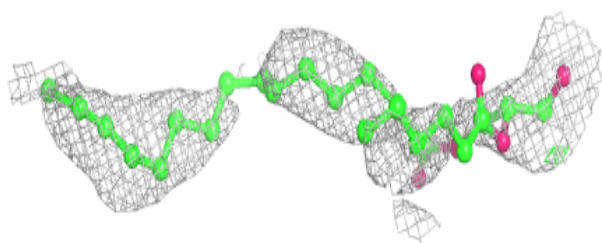
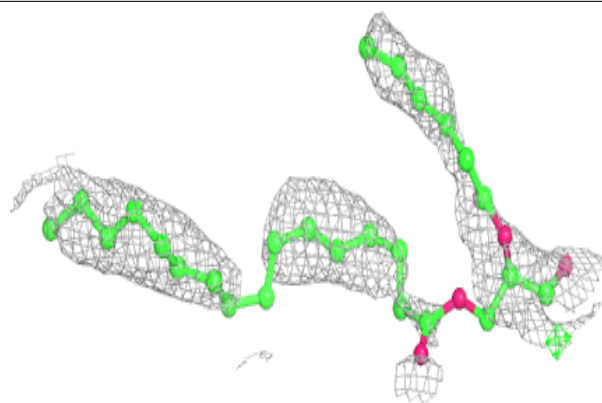
**Electron density around LHG E 101:**

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

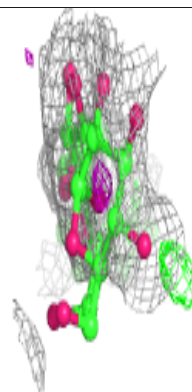
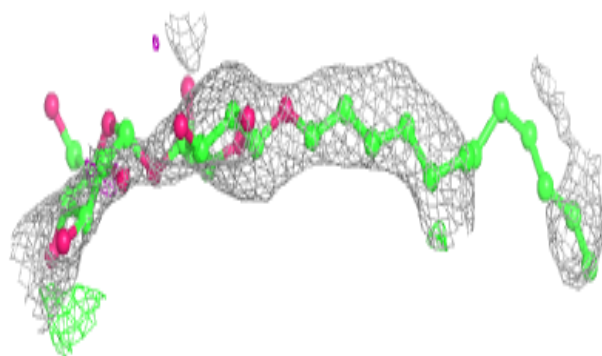
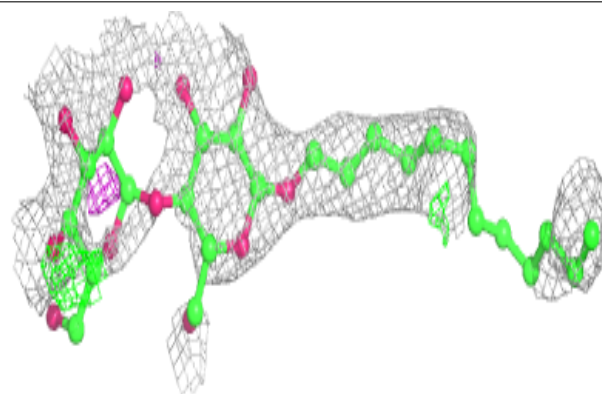


**Electron density around UNL a 415:**

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

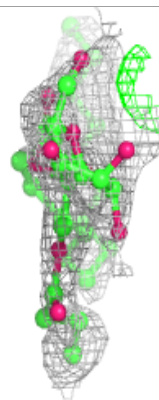
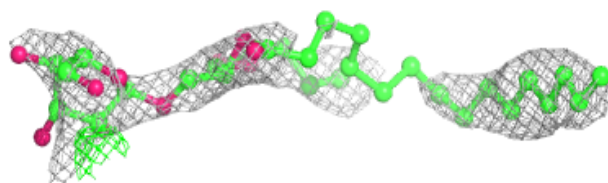
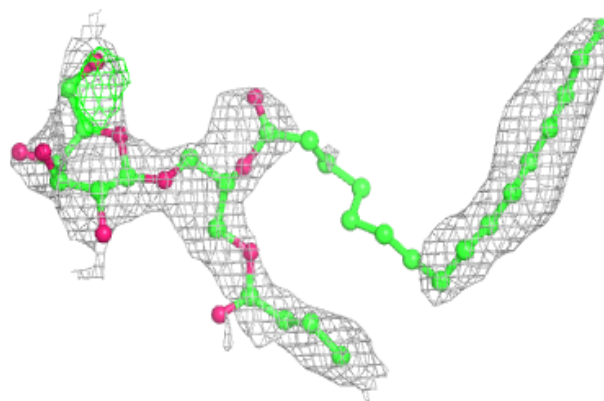
**Electron density around LMT a 418:**

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

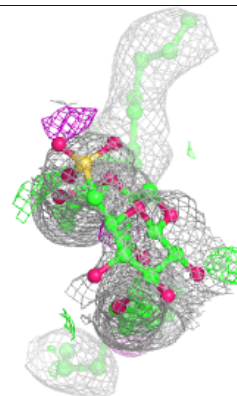
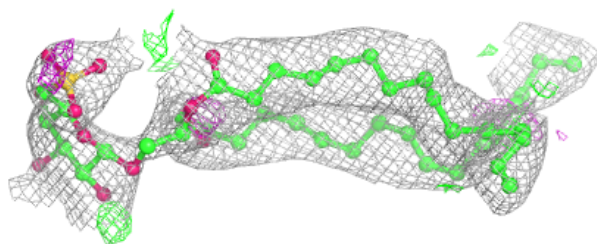
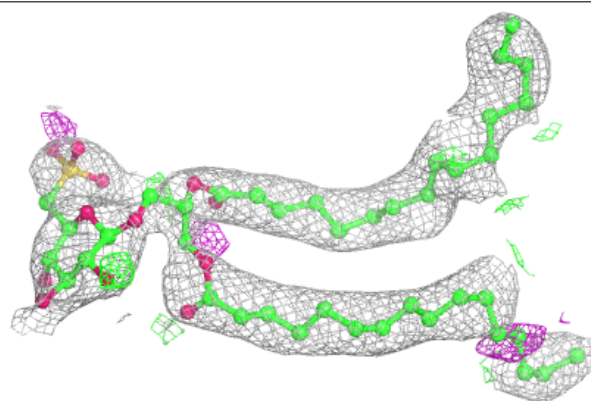


**Electron density around LMG z 101:**

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

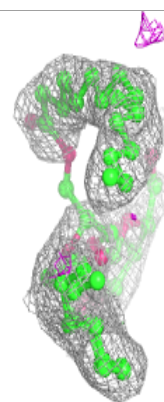
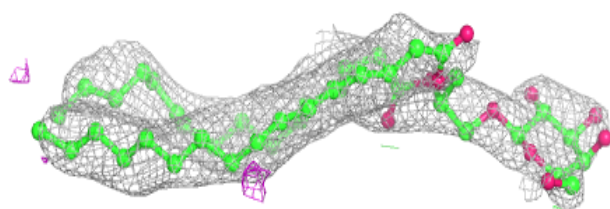
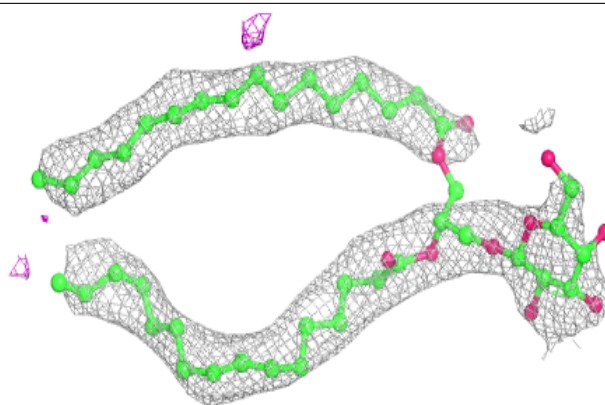
**Electron density around SQD b 620:**

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

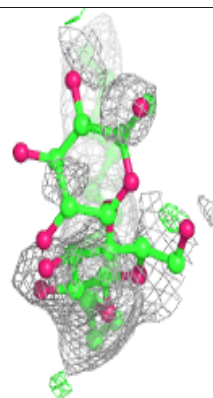
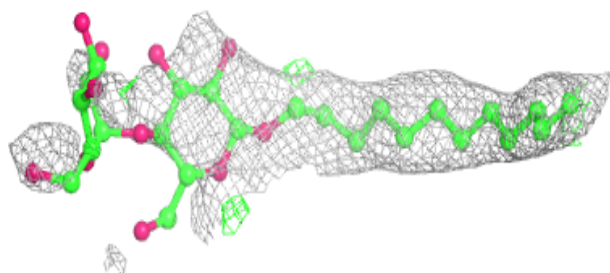
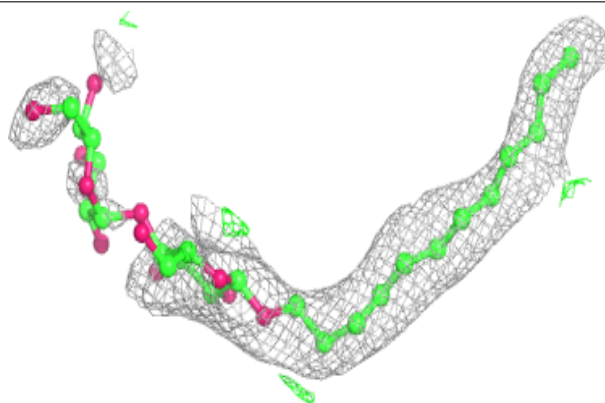


**Electron density around LMG a 417:**

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

**Electron density around LMT M 103:**

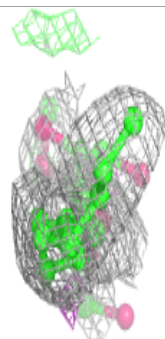
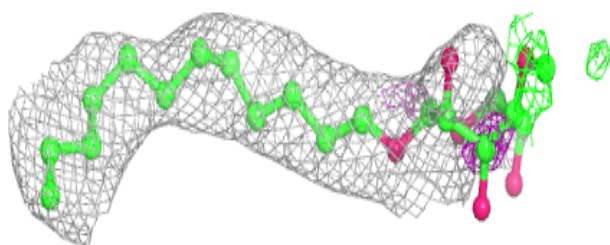
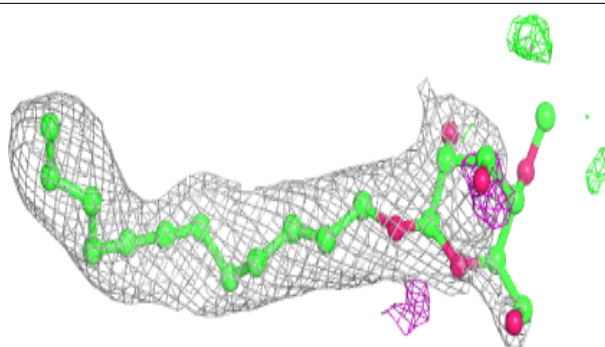
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



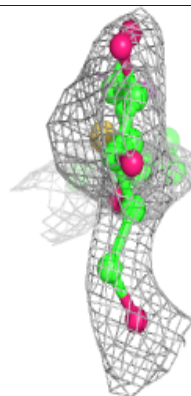
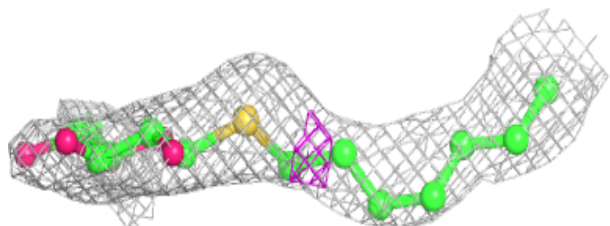
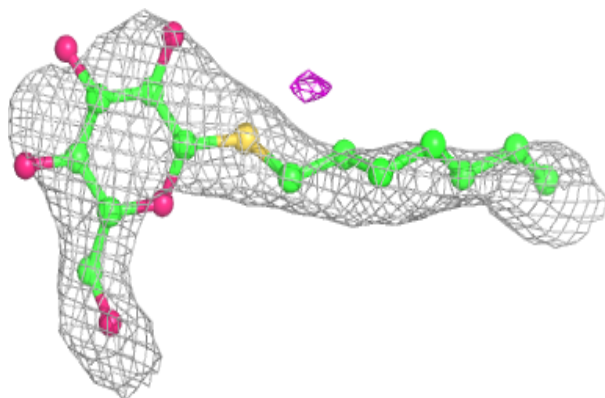


**Electron density around LMT B 630:**

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

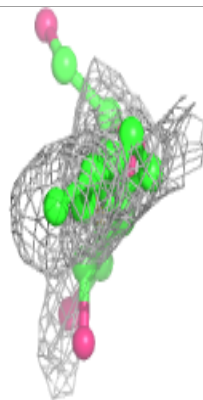
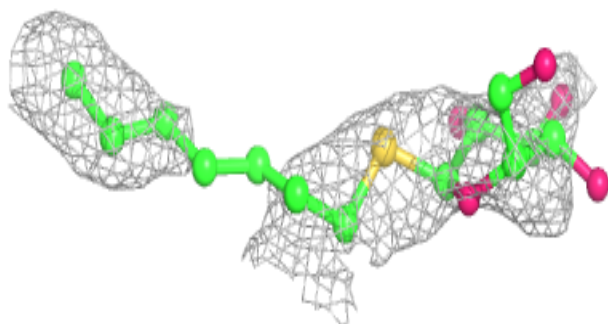
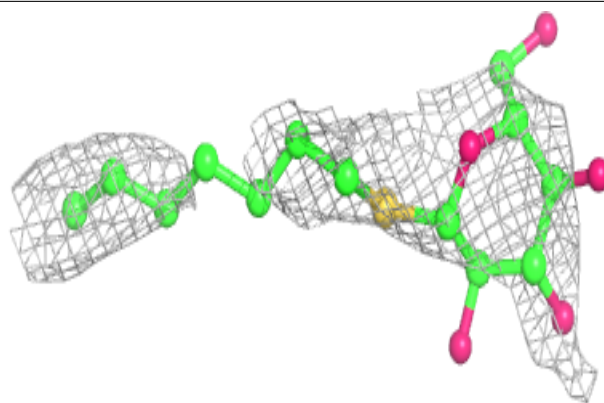
**Electron density around HTG C 522:**

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

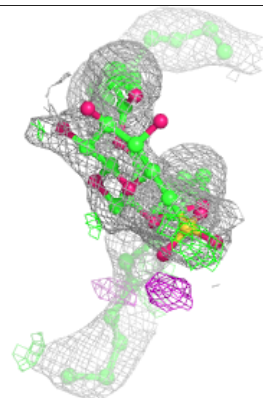
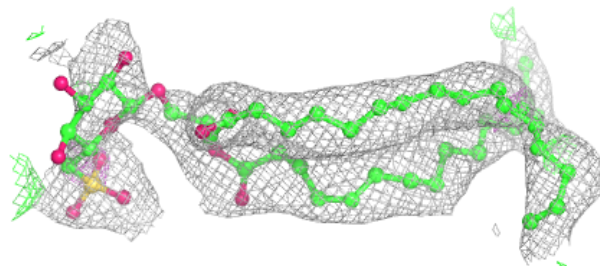
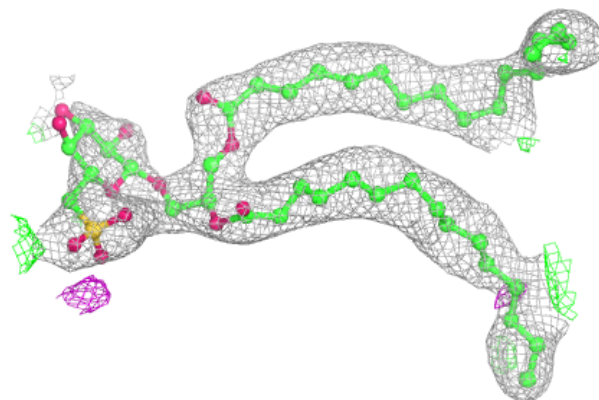


**Electron density around HTG C 523:**

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

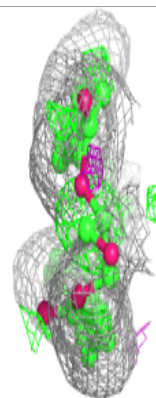
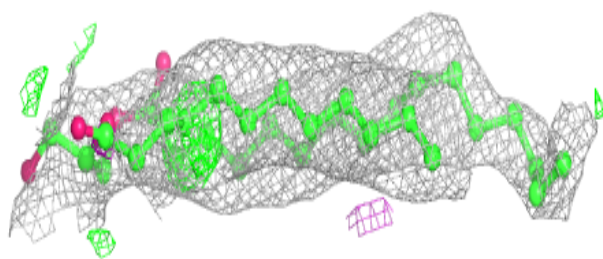
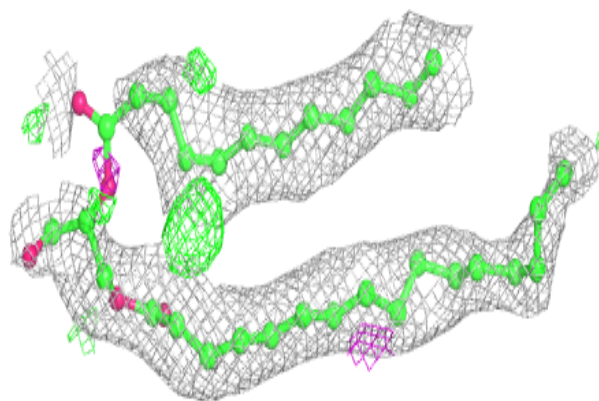
**Electron density around SQD B 620:**

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

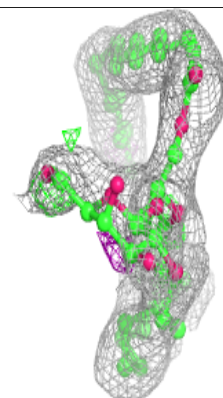
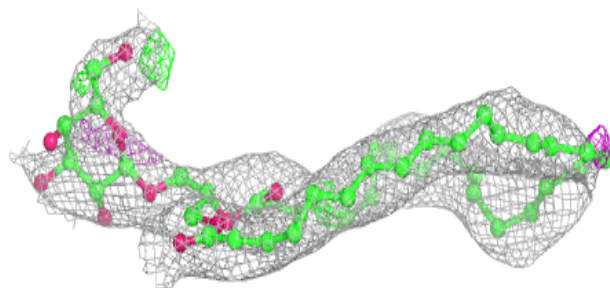
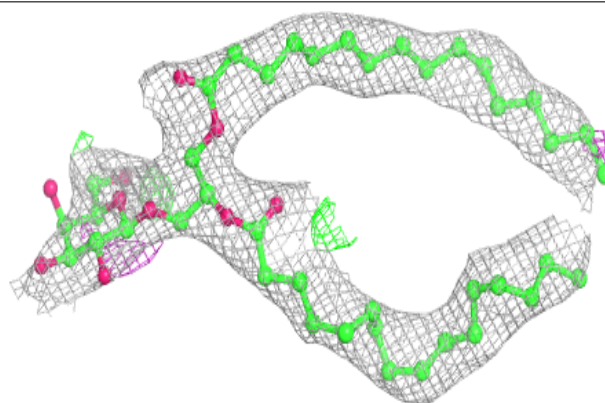


**Electron density around UNL d 410:**

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

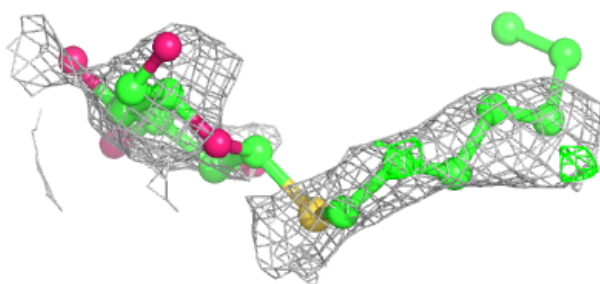
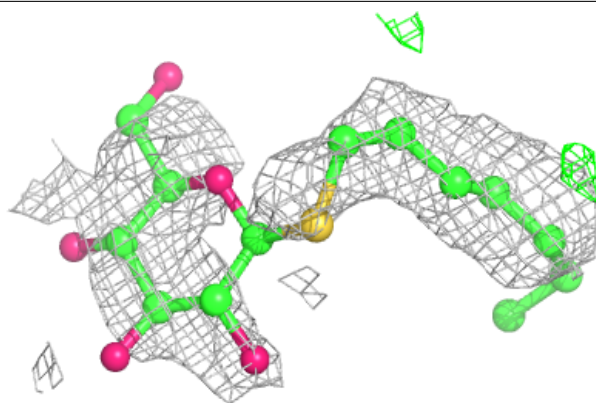
**Electron density around LMG A 418:**

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

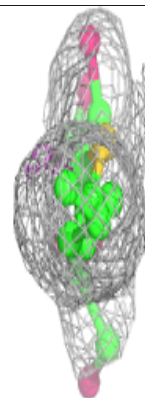
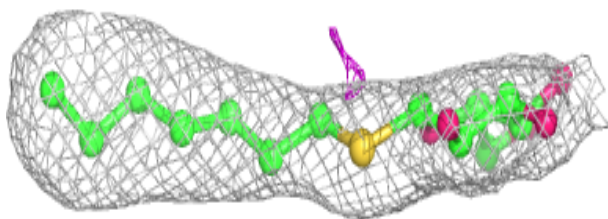
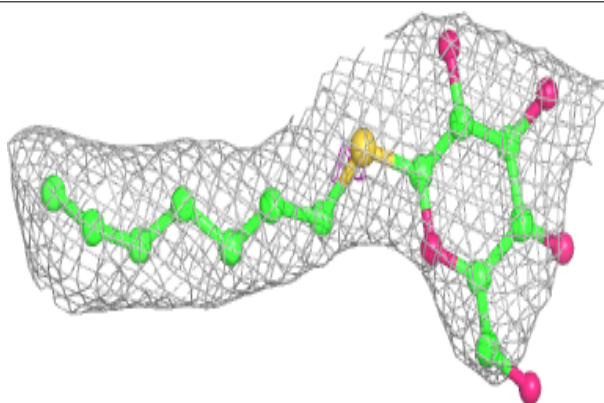


**Electron density around HTG b 624:**

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

**Electron density around HTG b 628:**

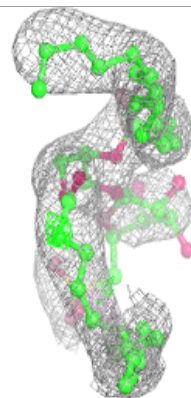
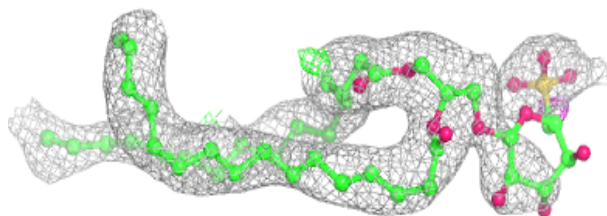
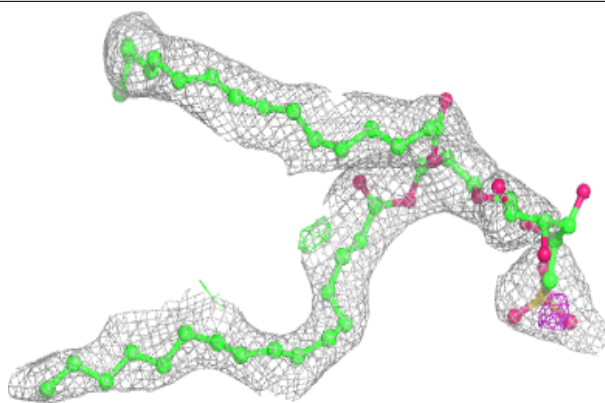
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



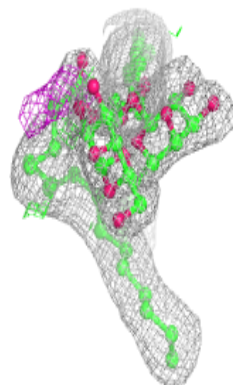
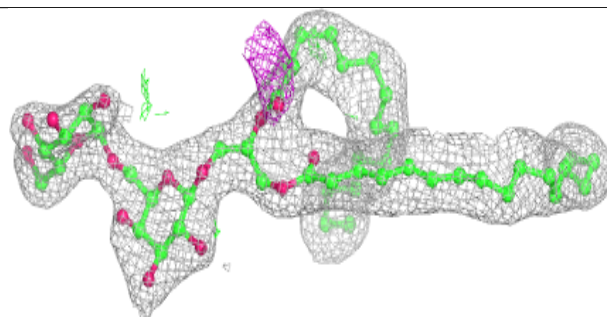
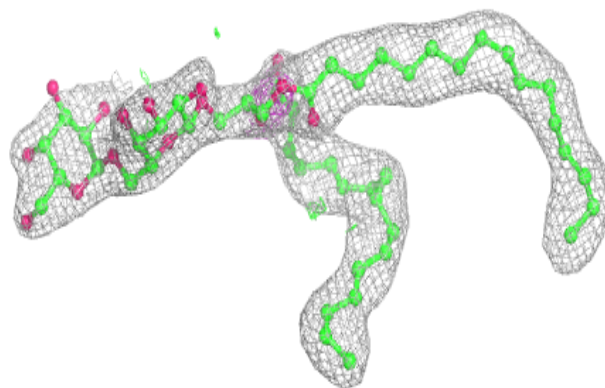


**Electron density around SQD a 411:**

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

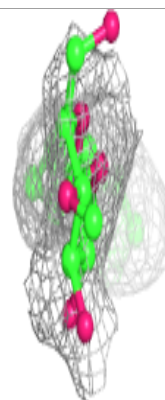
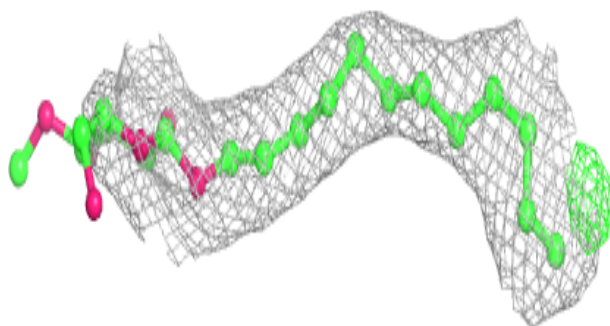
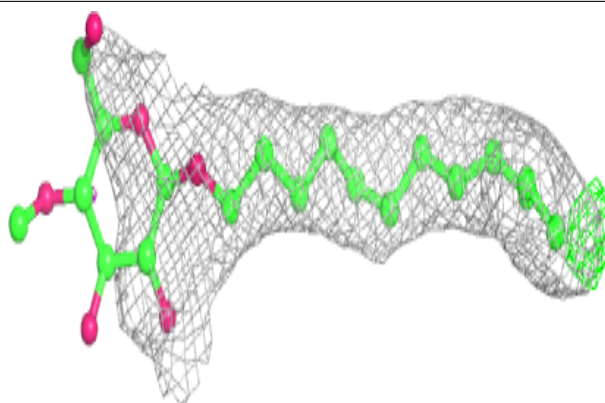
**Electron density around DGD h 103:**

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

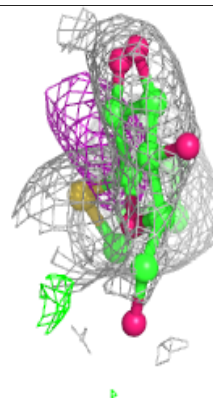
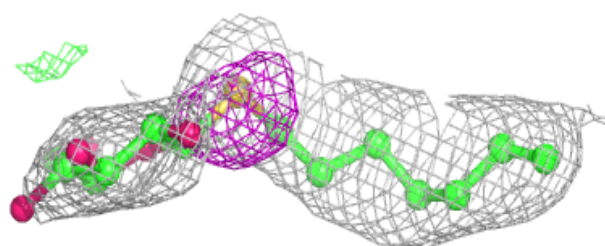
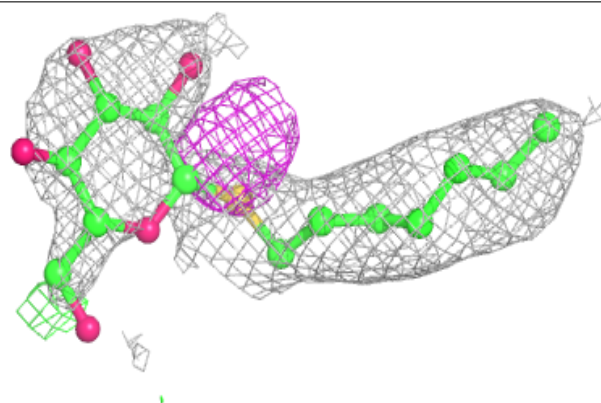


**Electron density around LMT b 630:**

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

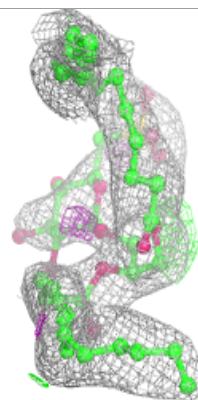
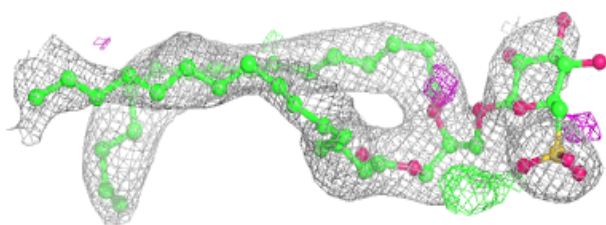
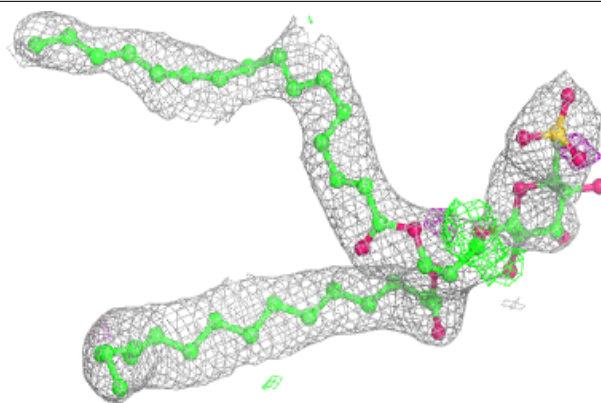
**Electron density around HTG b 623:**

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

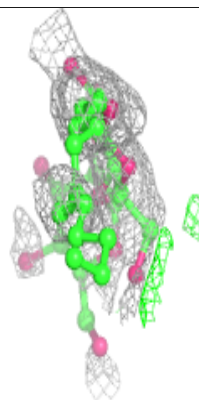
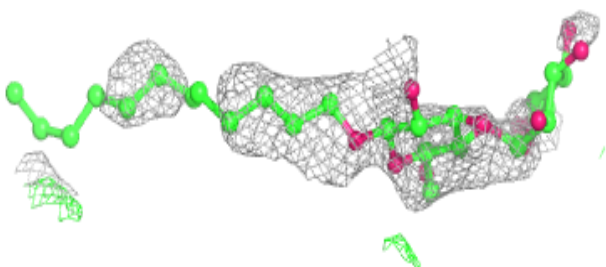
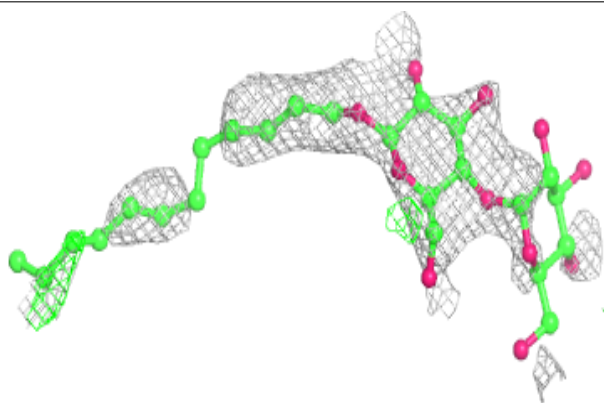


**Electron density around SQD A 413:**

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

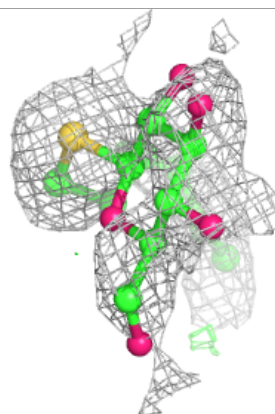
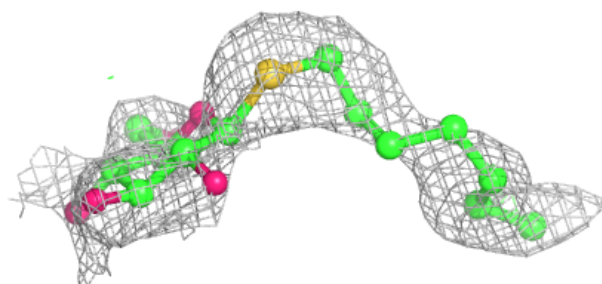
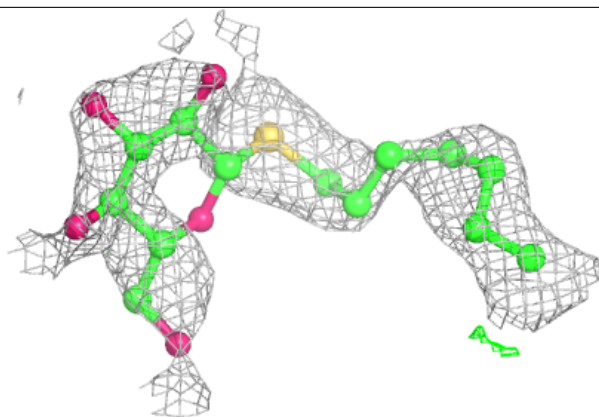
**Electron density around LMT E 102:**

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

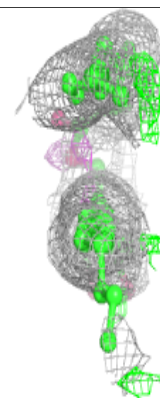
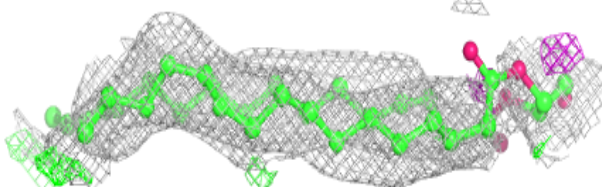
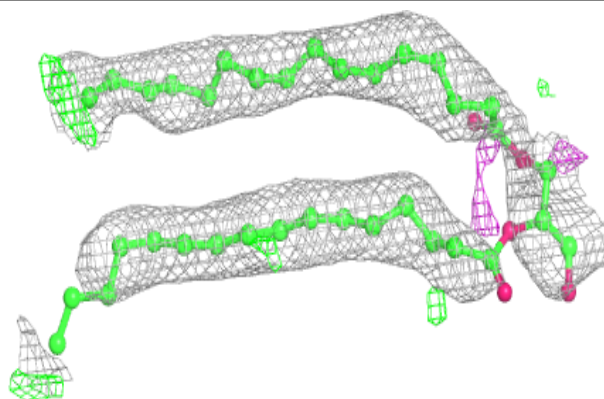


**Electron density around HTG B 624:**

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

**Electron density around UNL D 409:**

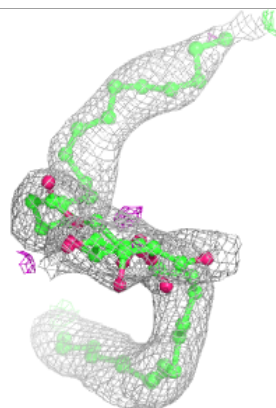
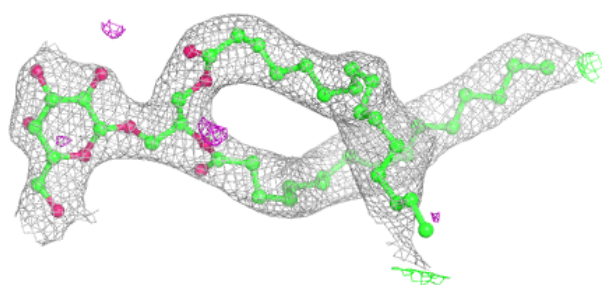
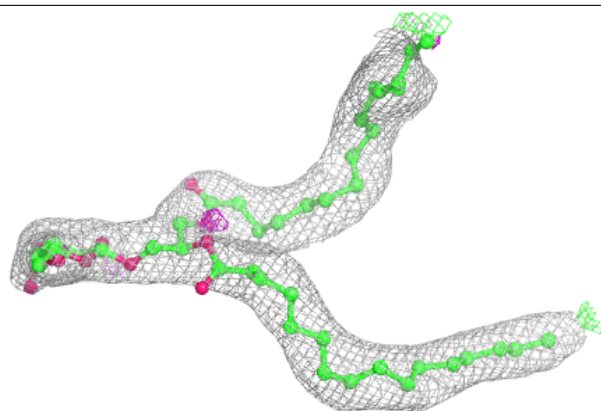
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



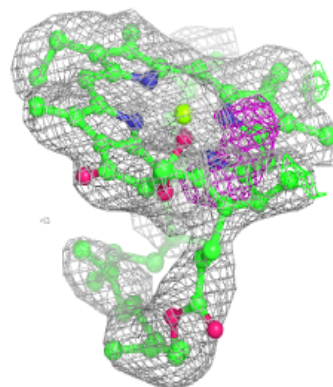
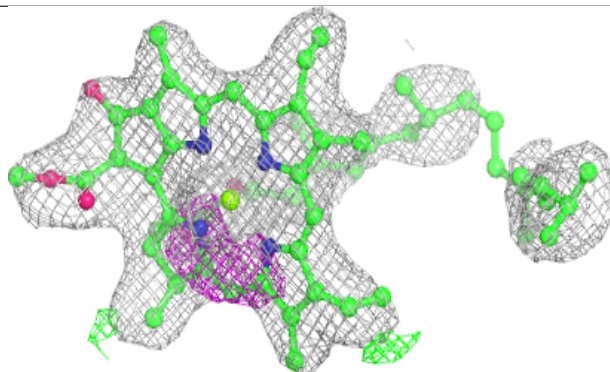
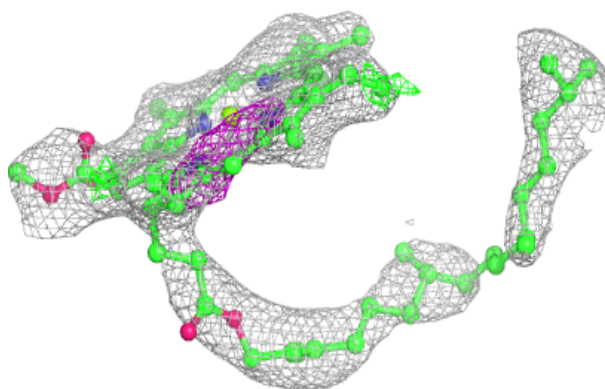


**Electron density around LMG B 621:**

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

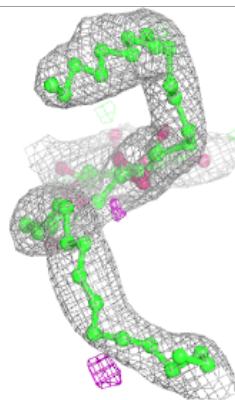
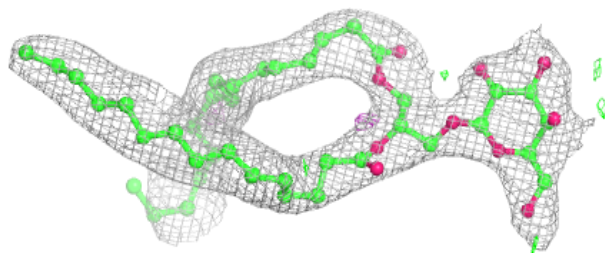
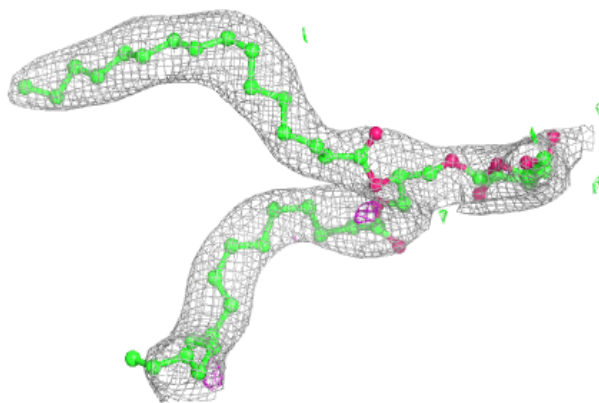
**Electron density around CLA C 514:**

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

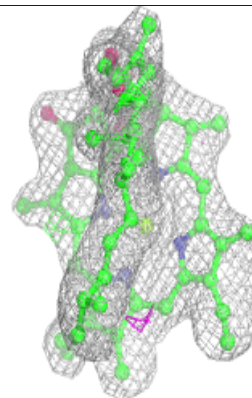
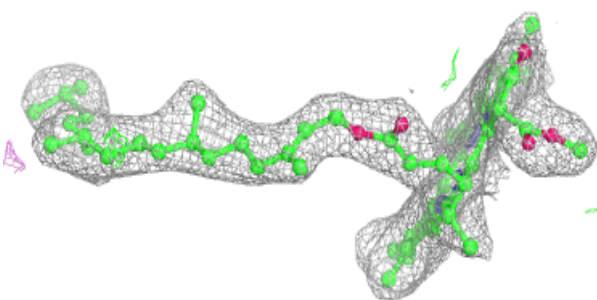
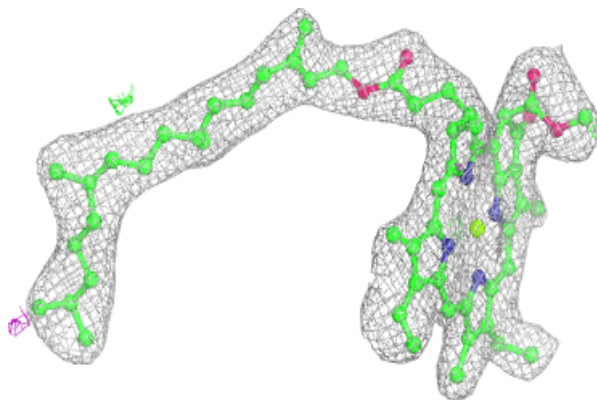


**Electron density around LMG b 621:**

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

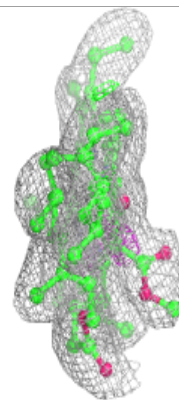
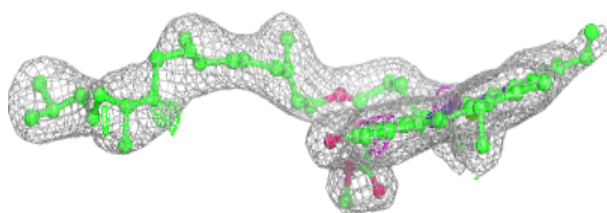
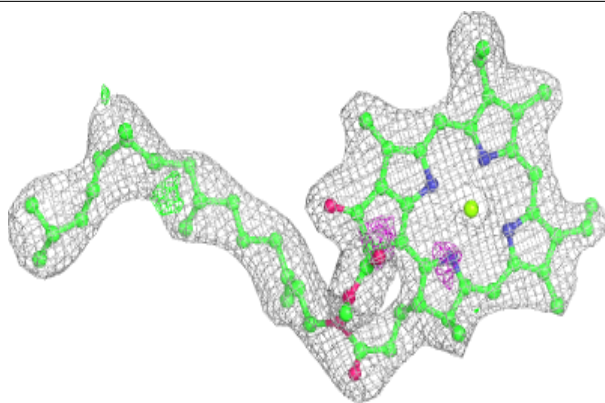
**Electron density around CLA B 609:**

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



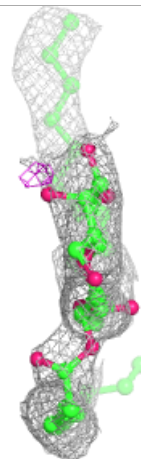
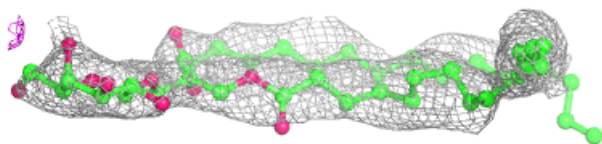
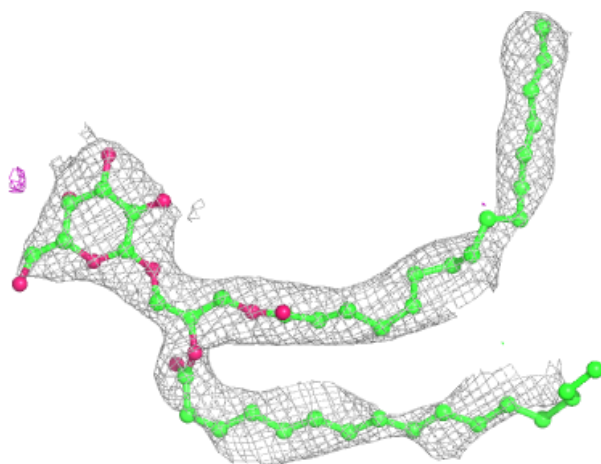
**Electron density around CLA b 602:**

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



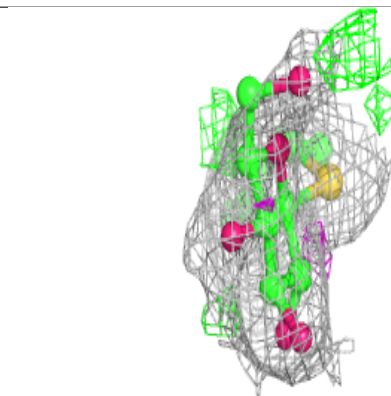
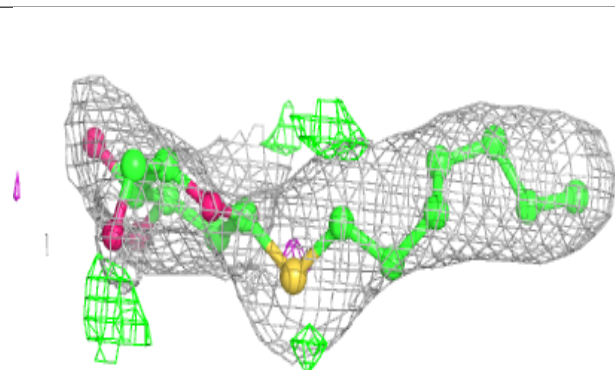
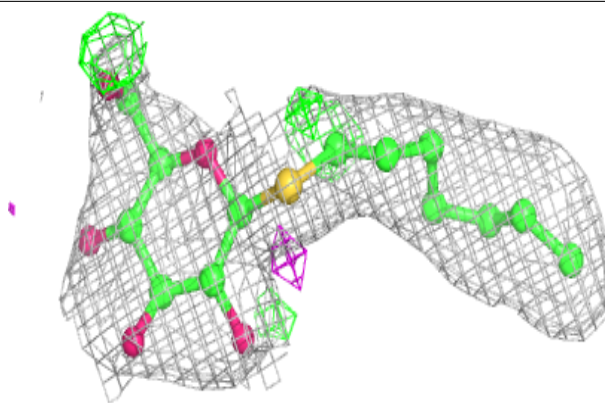
**Electron density around LMG c 521:**

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



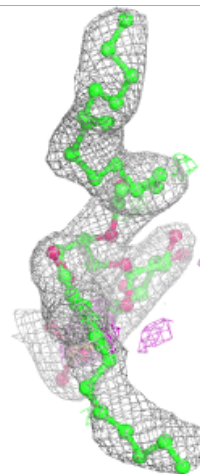
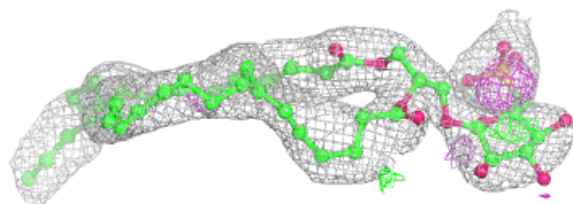
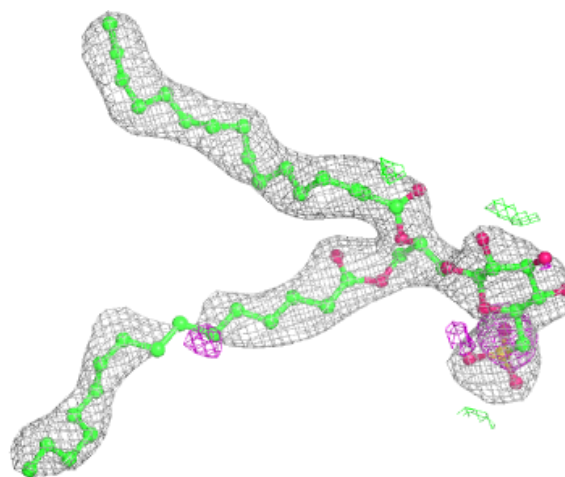
**Electron density around HTG B 623:**

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



**Electron density around SQD A 411:**

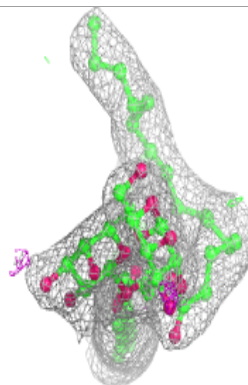
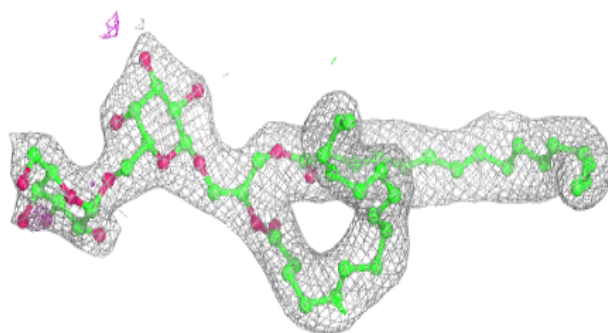
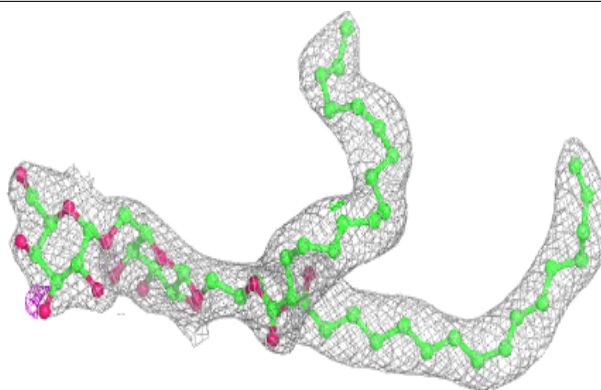
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



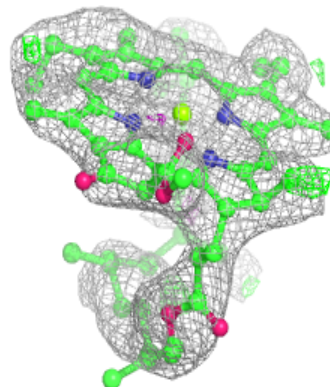
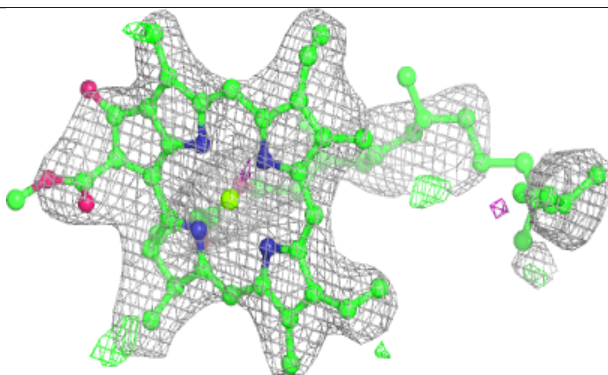
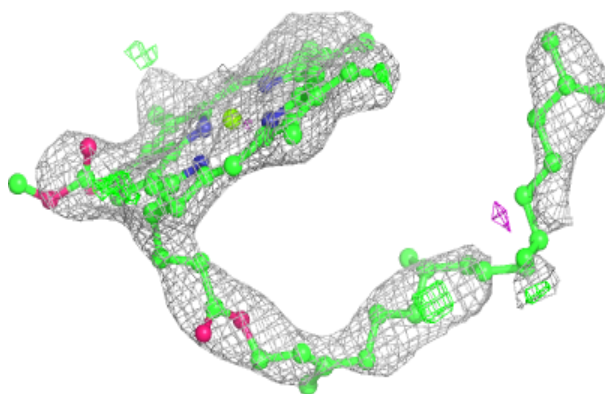


**Electron density around DGD H 102:**

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

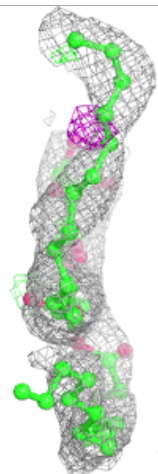
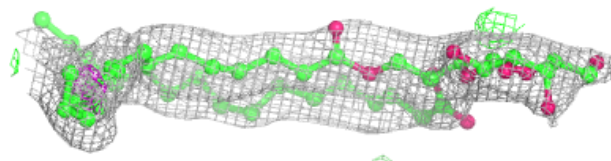
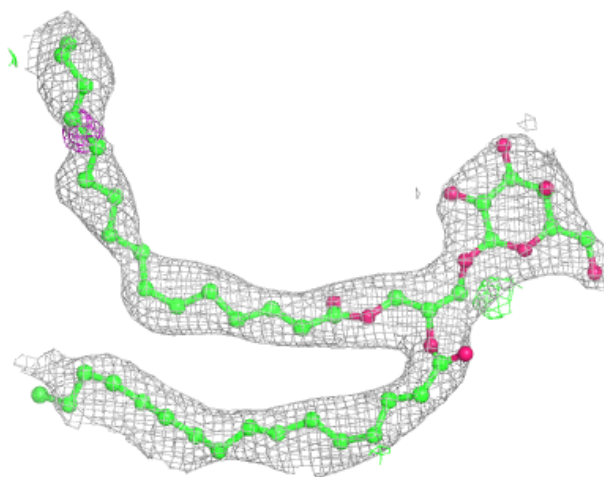
**Electron density around CLA c 515:**

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



**Electron density around LMG C 520:**

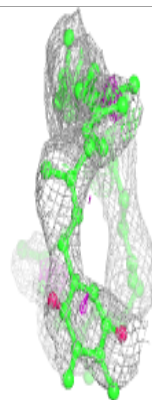
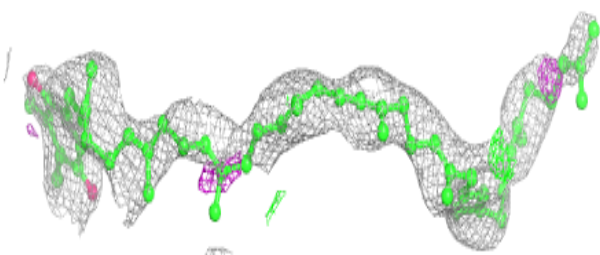
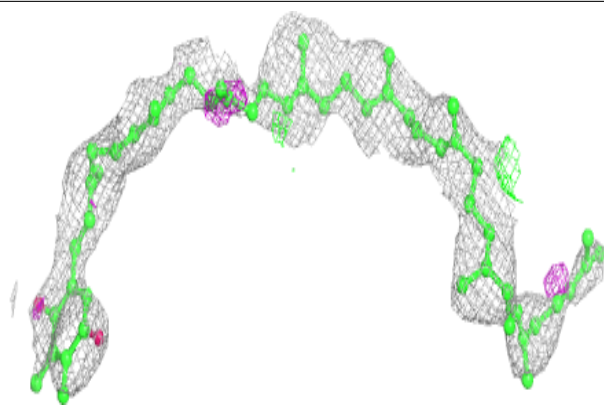
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



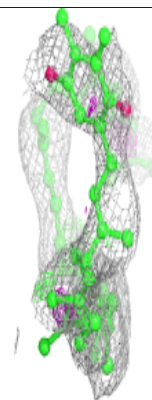
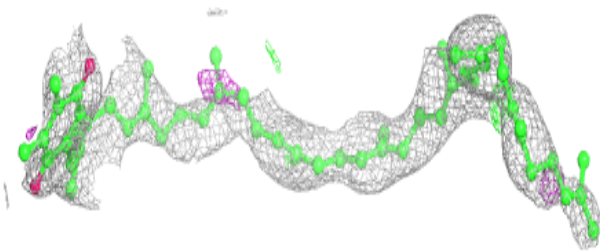
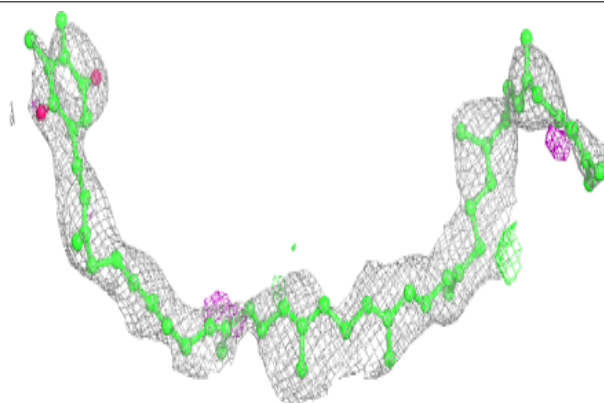


**Electron density around PL9 a 414 (B):**

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

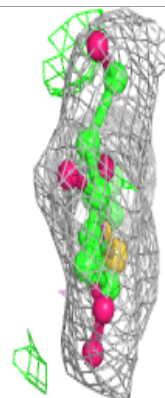
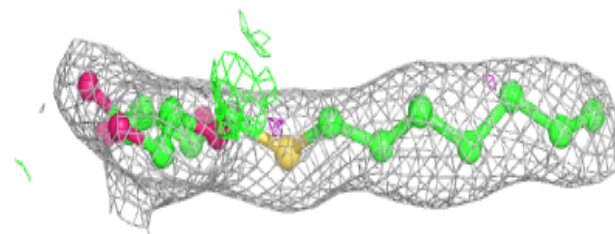
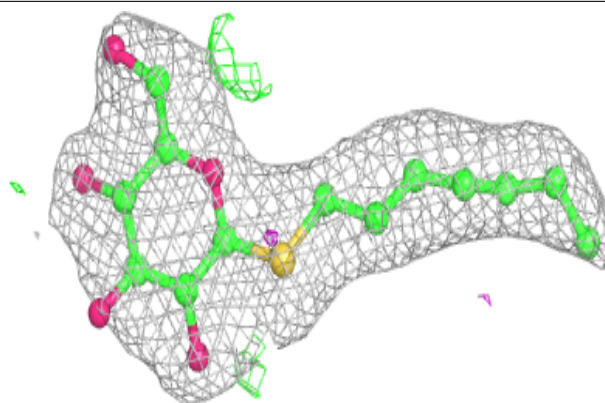
**Electron density around PL9 a 414 (A):**

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

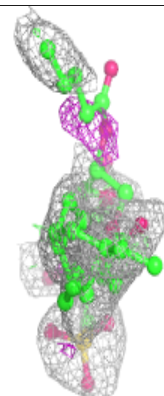
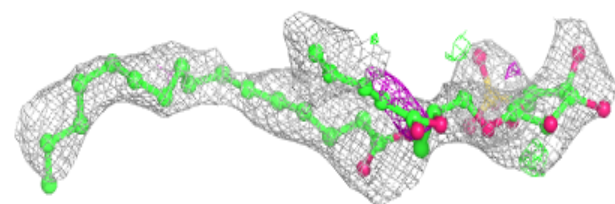
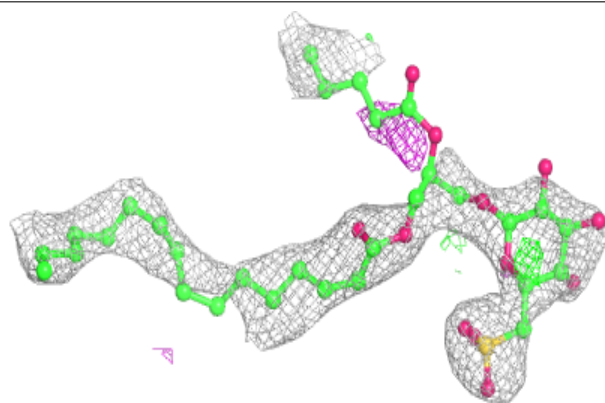


**Electron density around HTG B 628:**

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

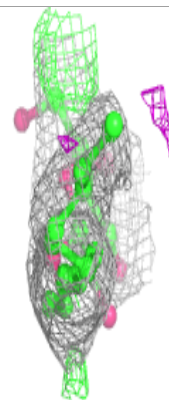
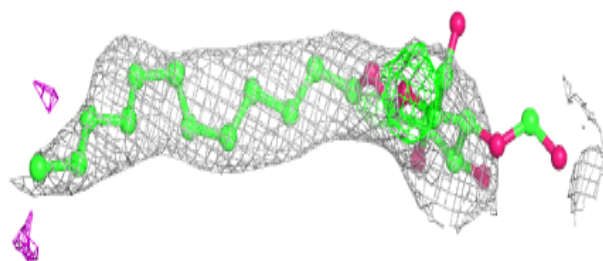
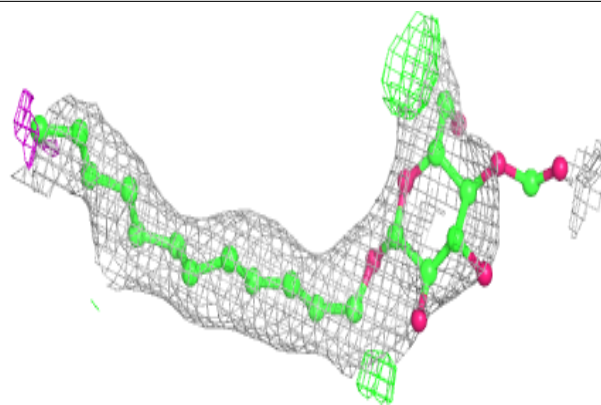
**Electron density around SQD F 101:**

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

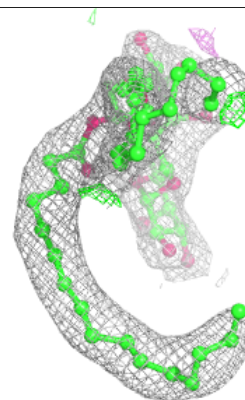
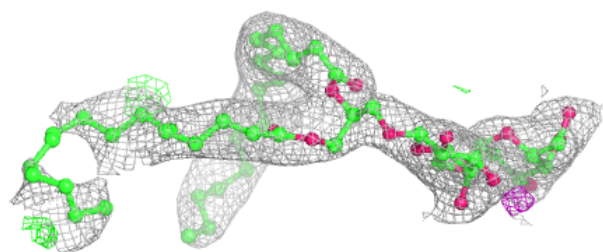
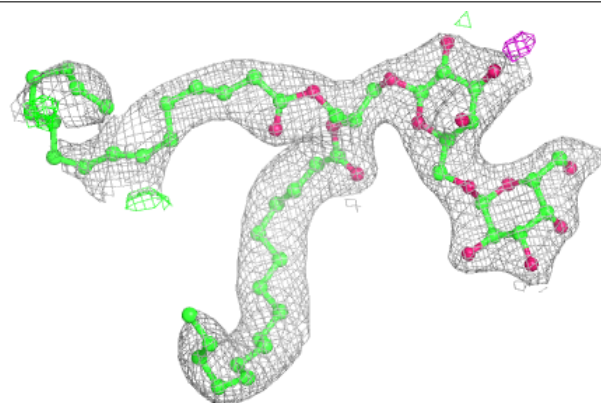


**Electron density around LMT t 101:**

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

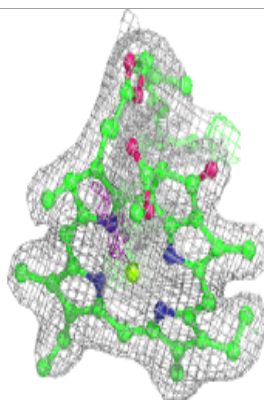
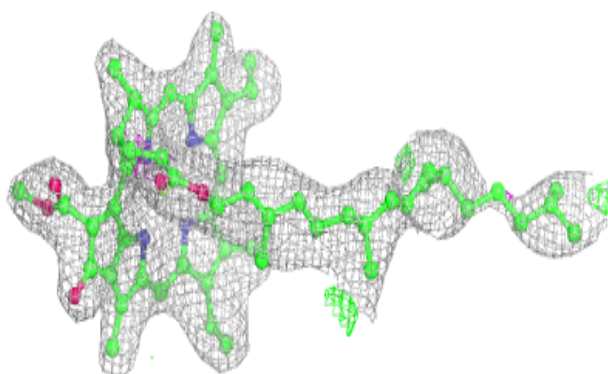
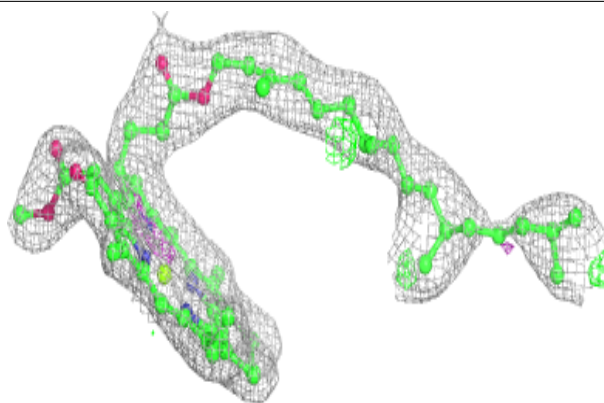
**Electron density around DGD C 518:**

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

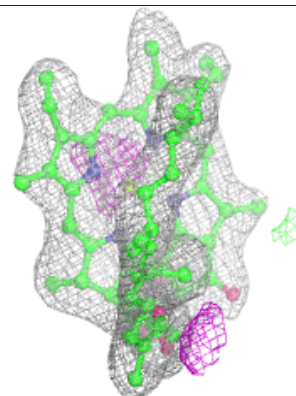
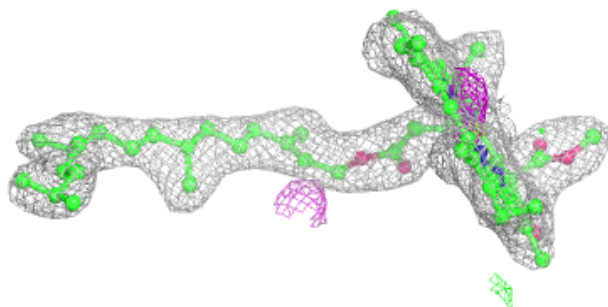
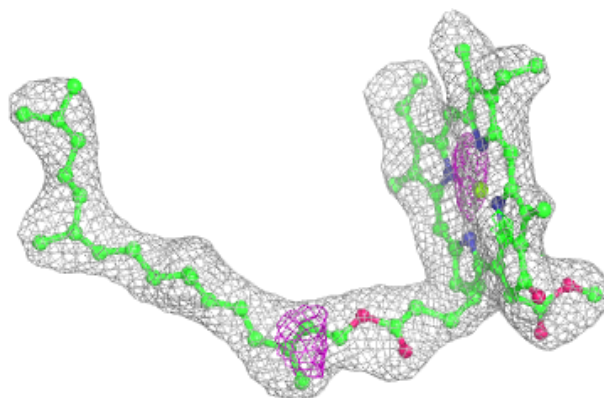


**Electron density around CLA C 505:**

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

**Electron density around CLA b 609:**

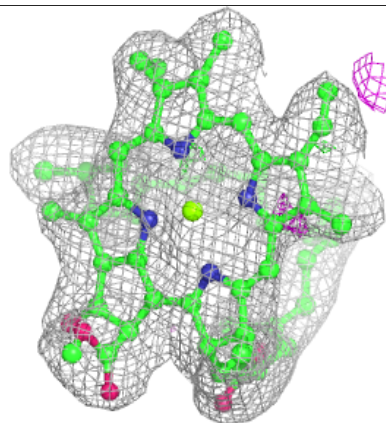
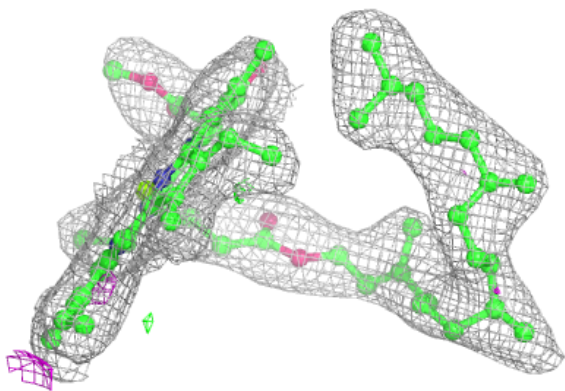
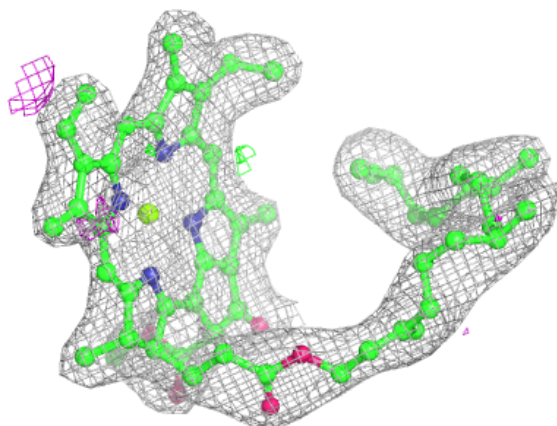
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





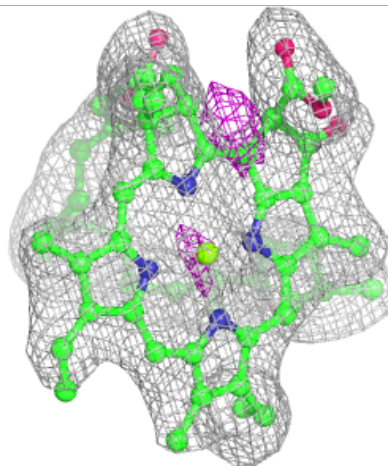
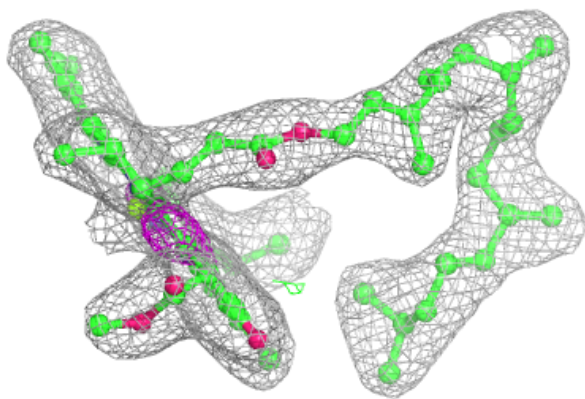
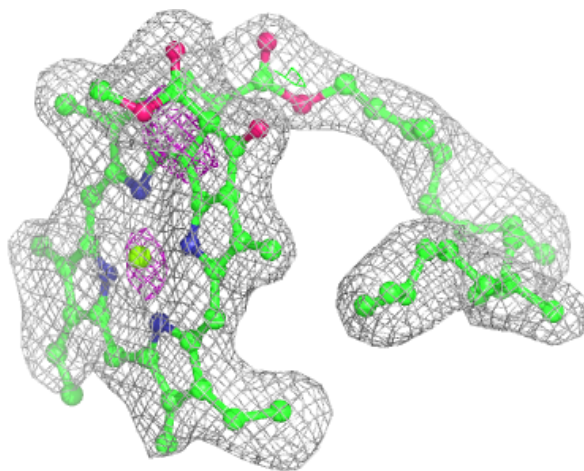
**Electron density around CLA c 505:**

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



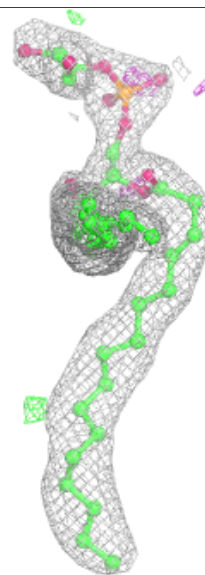
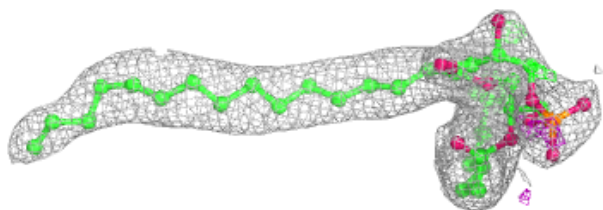
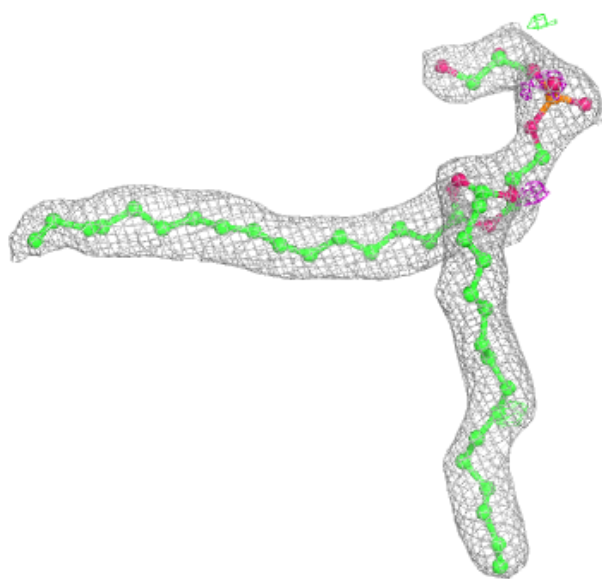
**Electron density around CLA C 504:**

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



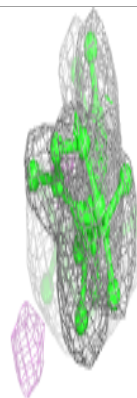
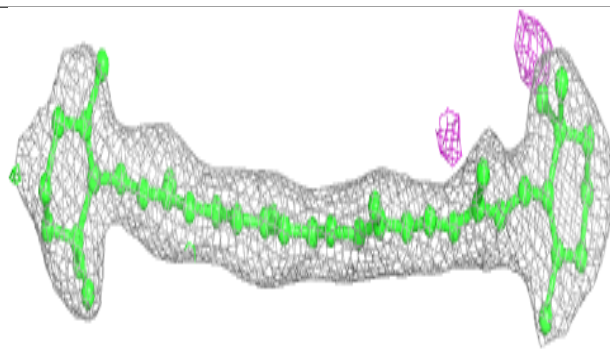
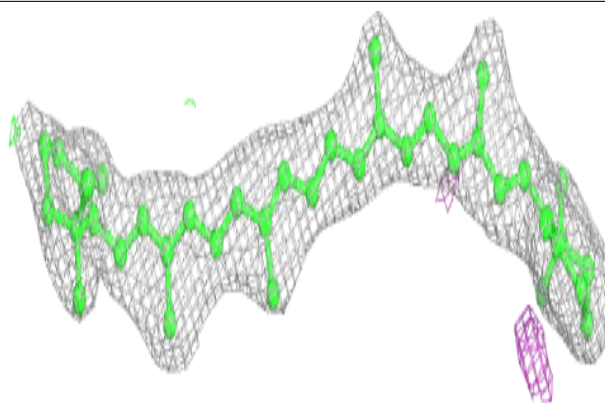
**Electron density around LHG 1 101:**

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



**Electron density around BCR h 102:**

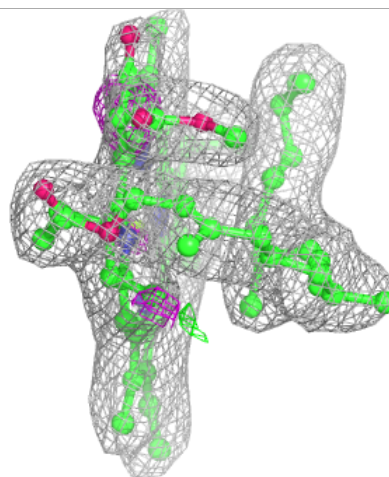
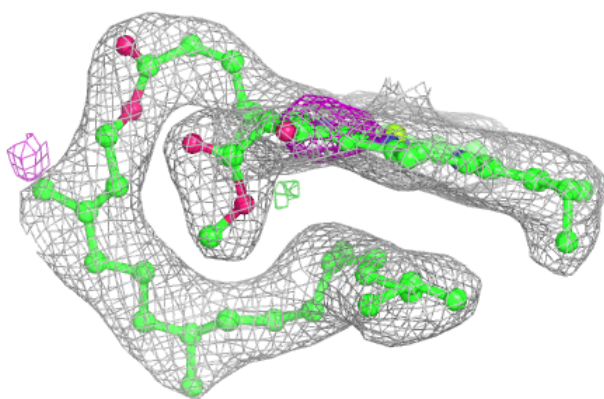
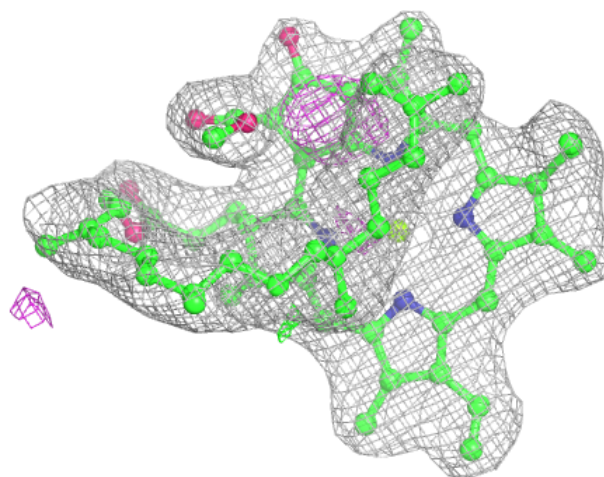
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





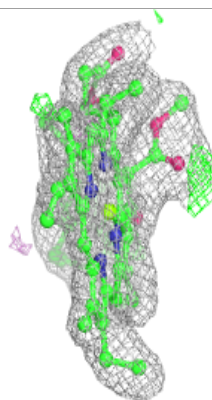
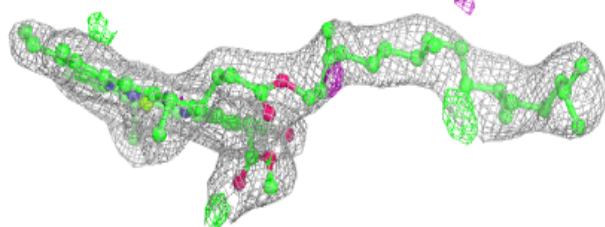
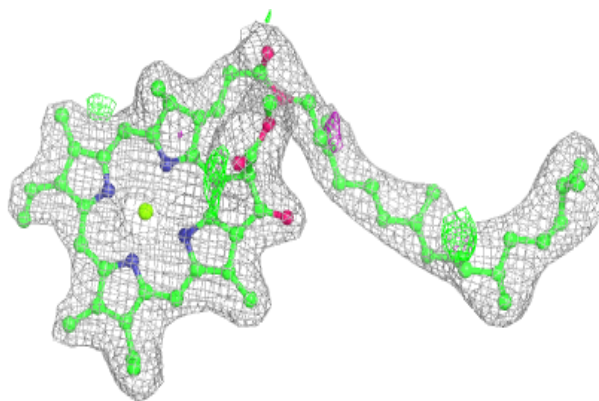
**Electron density around CLA c 512:**

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

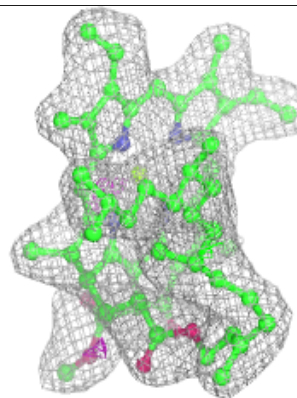
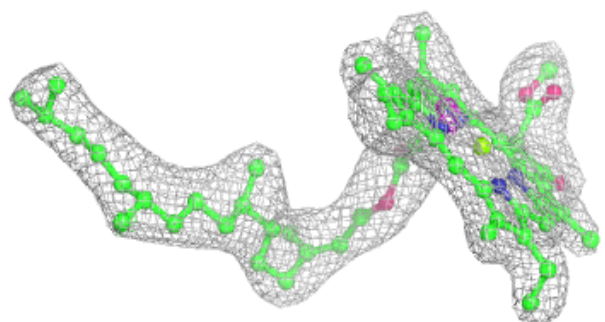
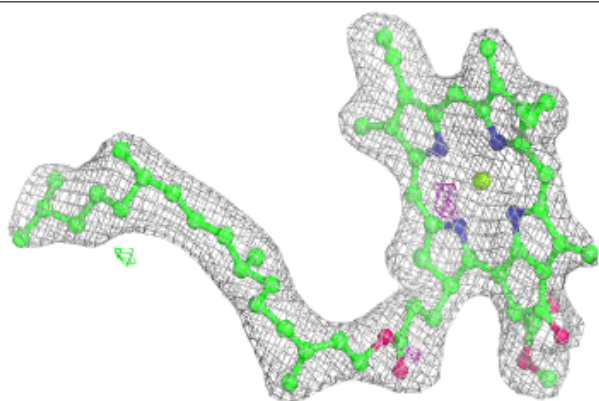


**Electron density around CLA B 602:**

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

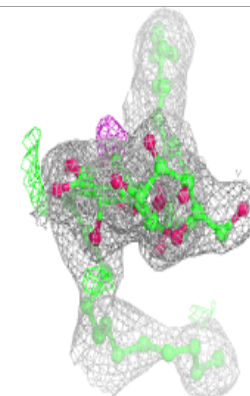
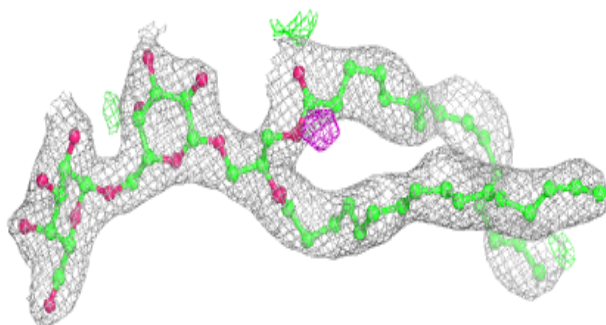
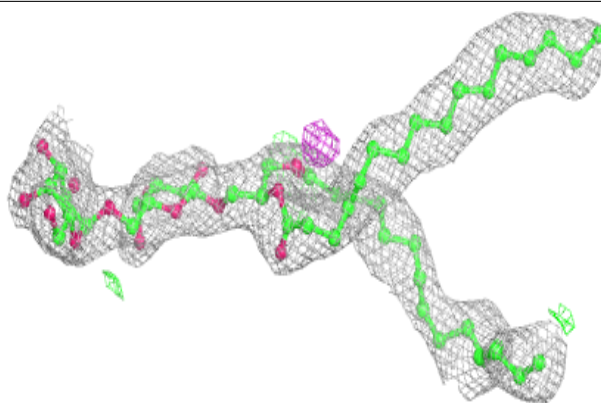
**Electron density around CLA C 512:**

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

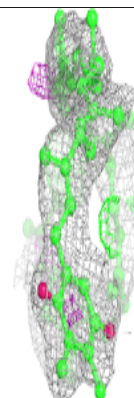
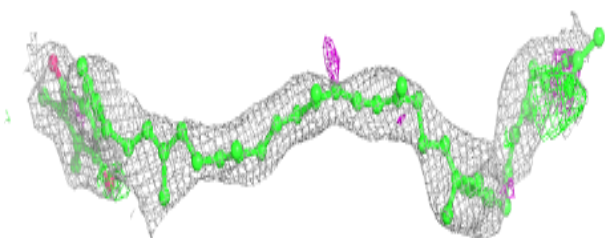
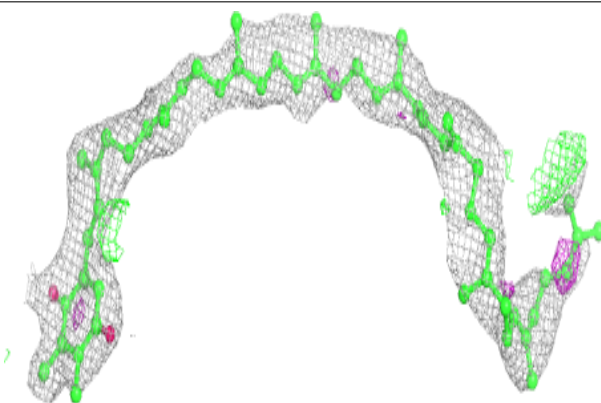


**Electron density around DGD c 518:**

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

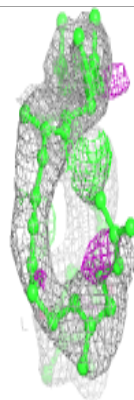
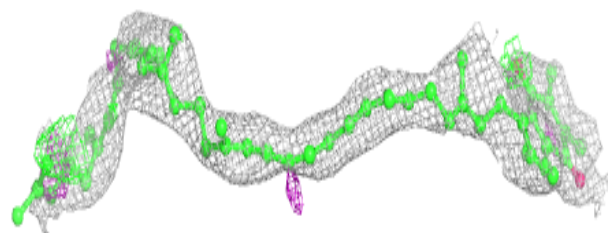
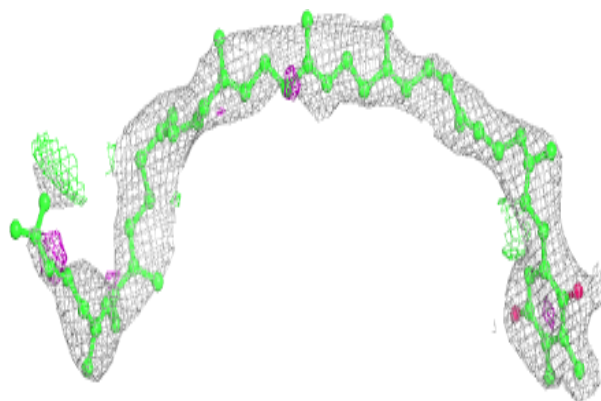
**Electron density around PL9 A 416 (A):**

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

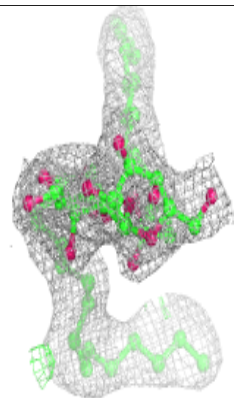
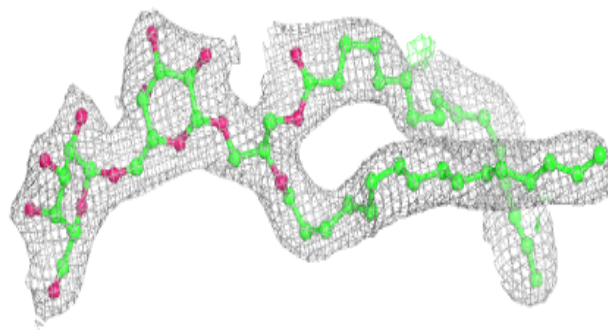
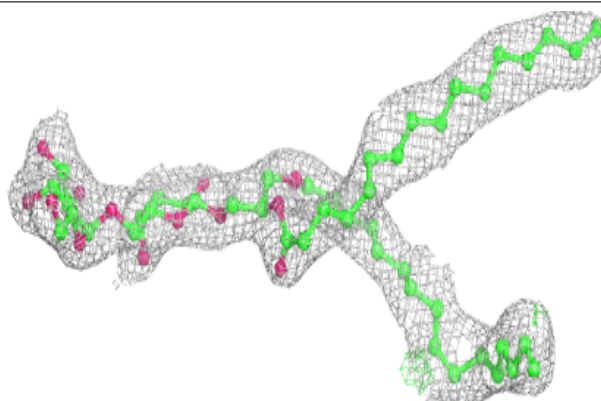


**Electron density around PL9 A 416 (B):**

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

**Electron density around DGD C 517:**

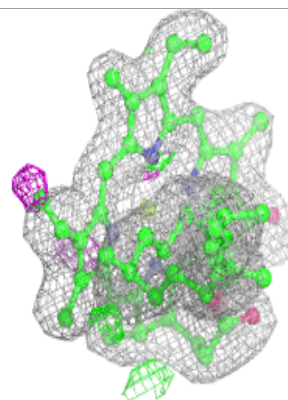
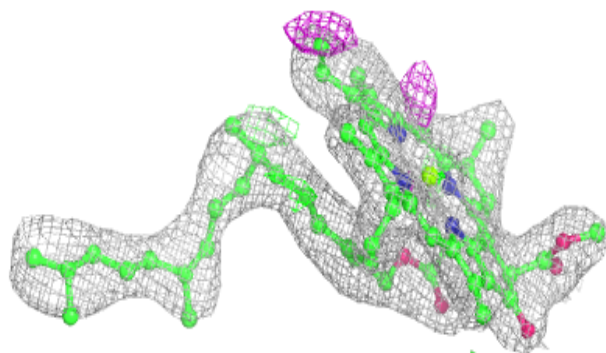
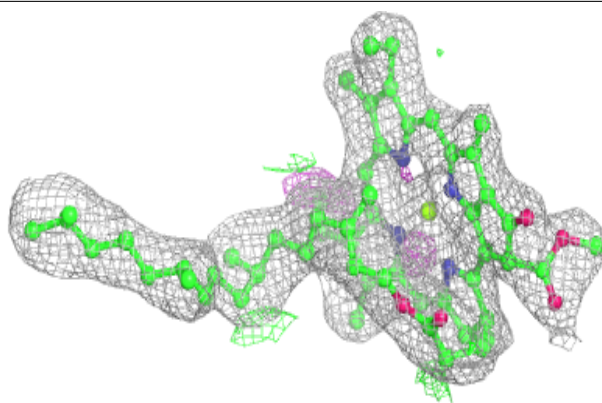
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





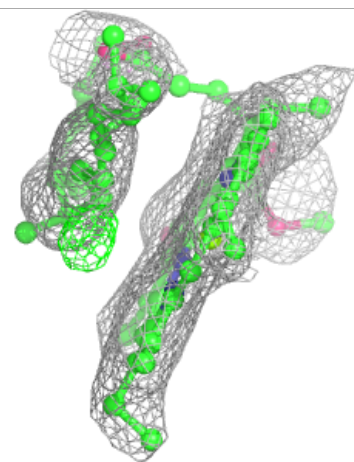
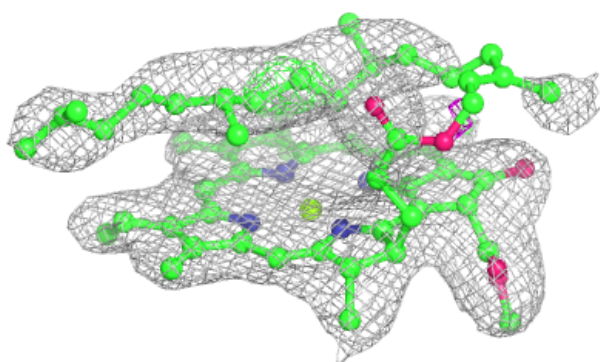
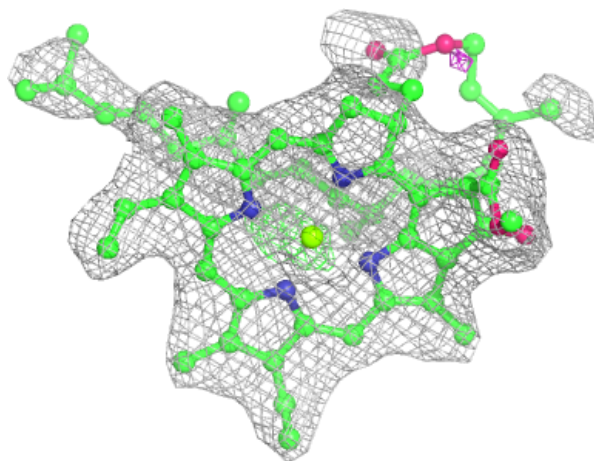
**Electron density around CLA c 507:**

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



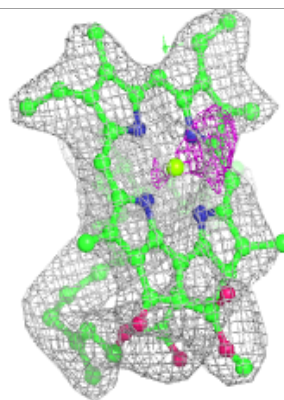
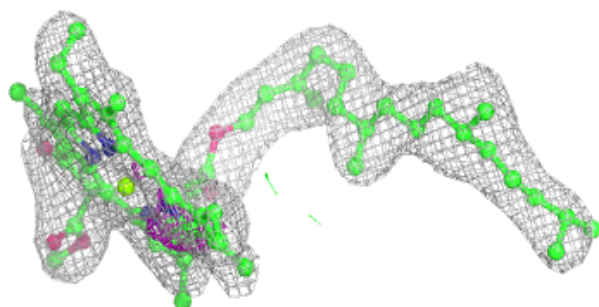
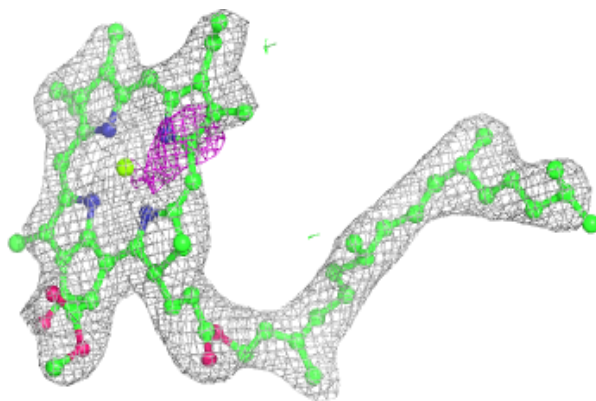
**Electron density around CLA b 601:**

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

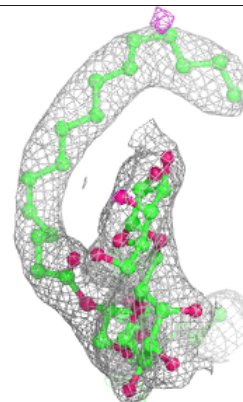
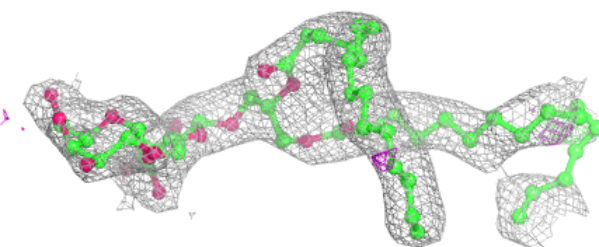
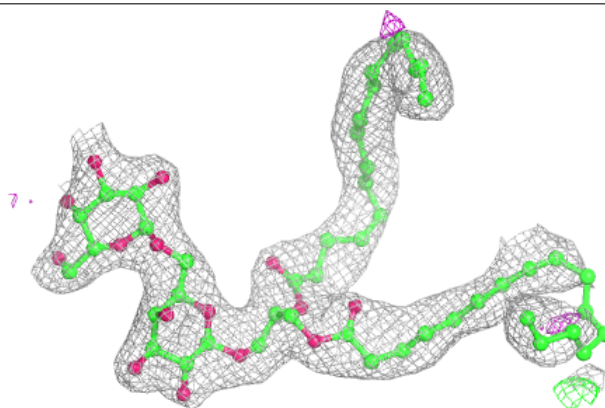


**Electron density around CLA c 513:**

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

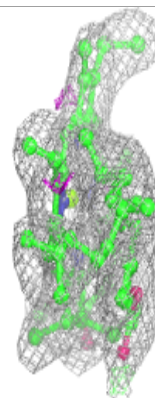
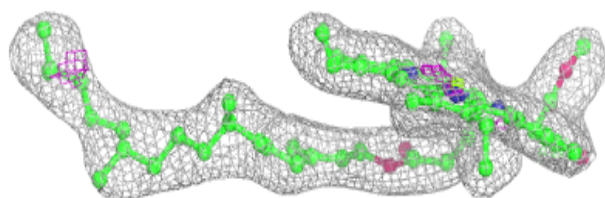
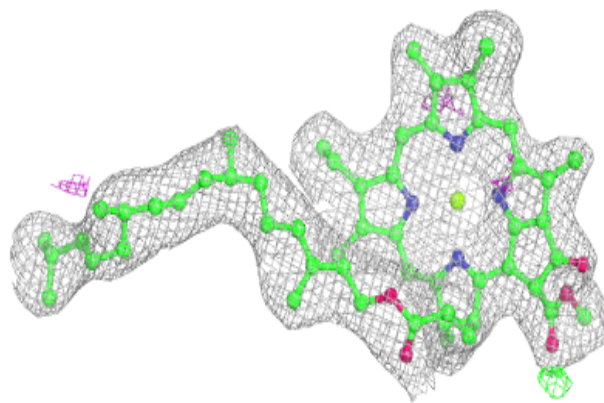
**Electron density around DGD c 519:**

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



**Electron density around CLA b 603:**

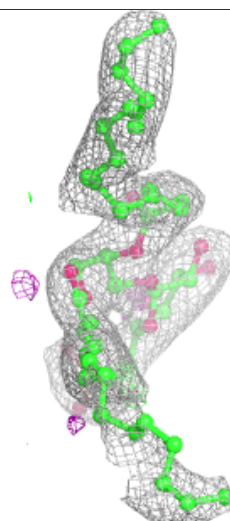
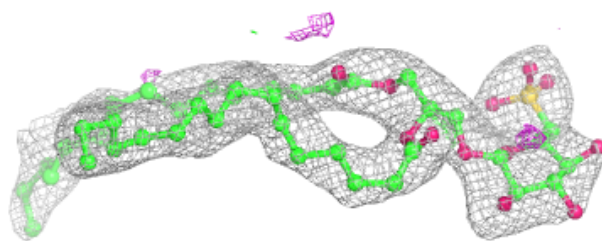
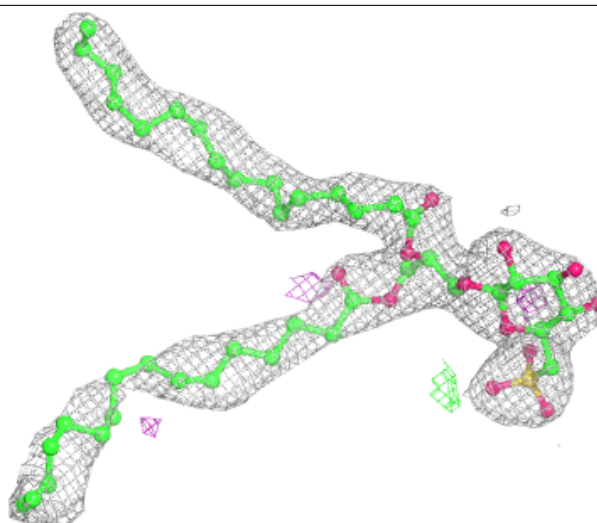
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





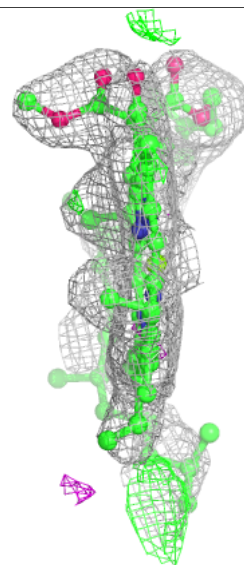
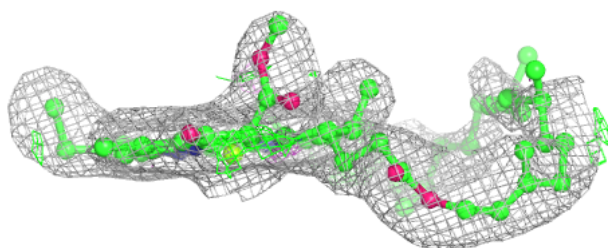
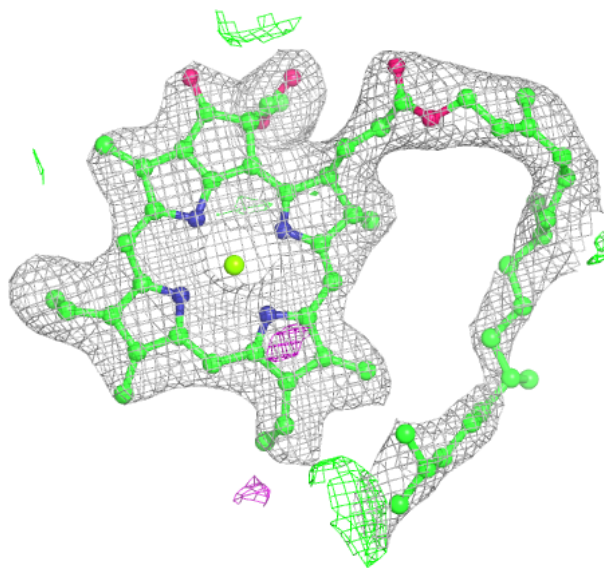
**Electron density around SQD a 409:**

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



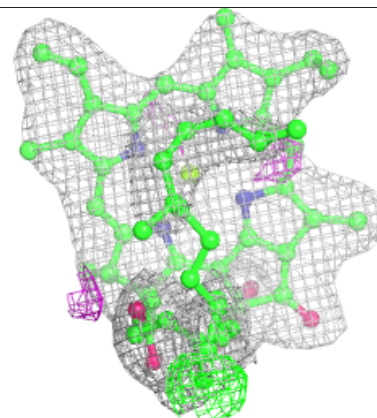
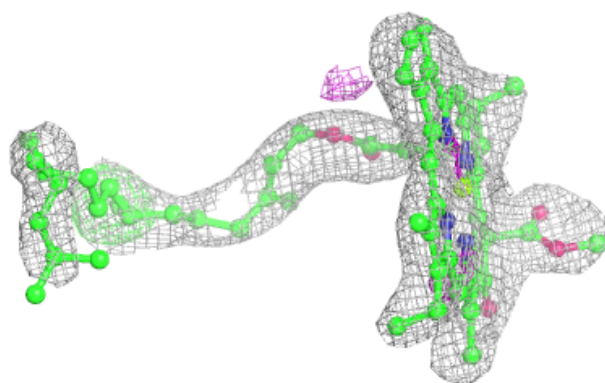
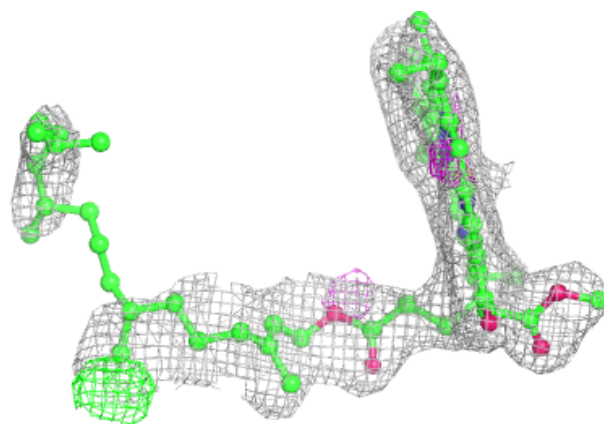
**Electron density around CLA C 513:**

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

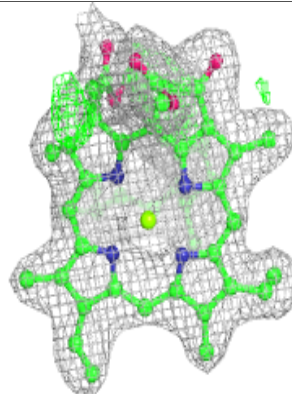
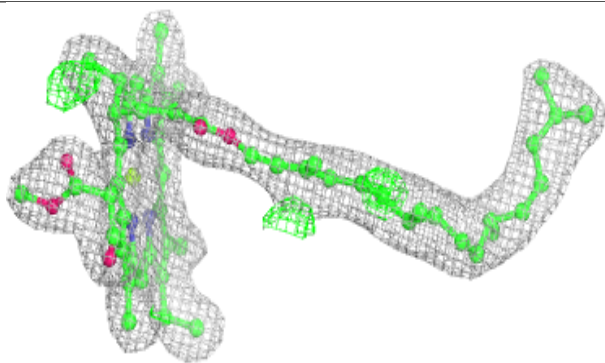
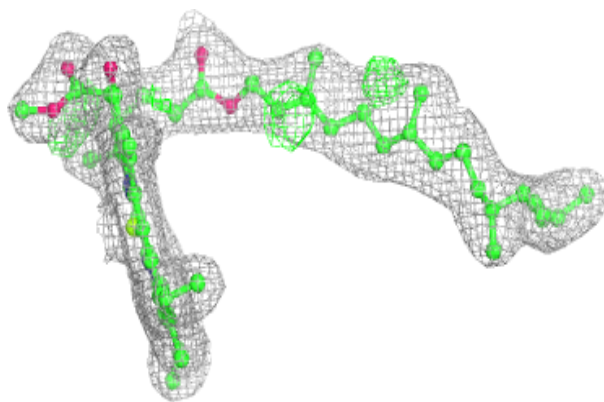


**Electron density around CLA c 508:**

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

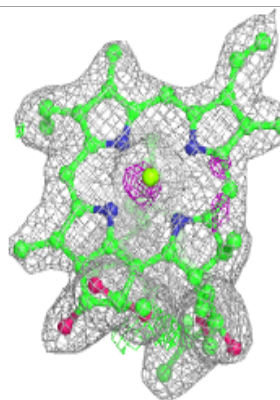
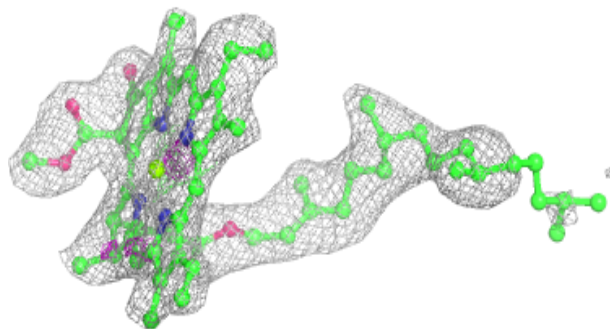
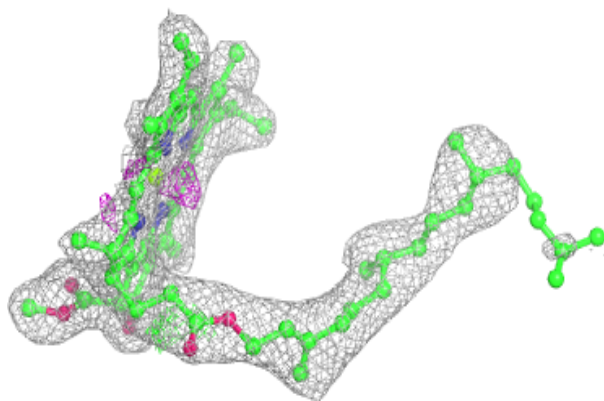
**Electron density around CLA B 605:**

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



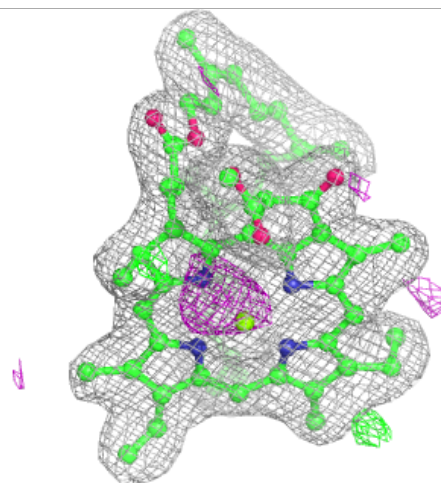
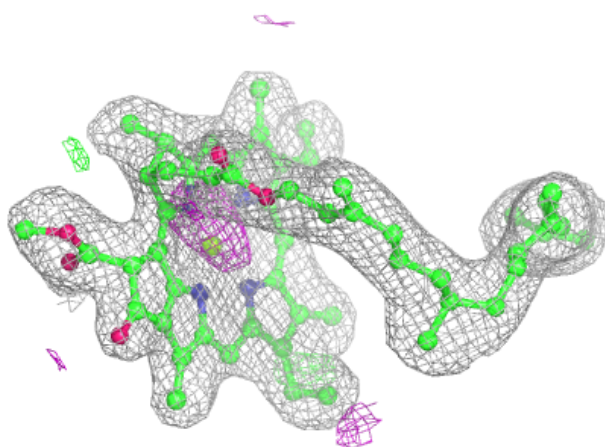
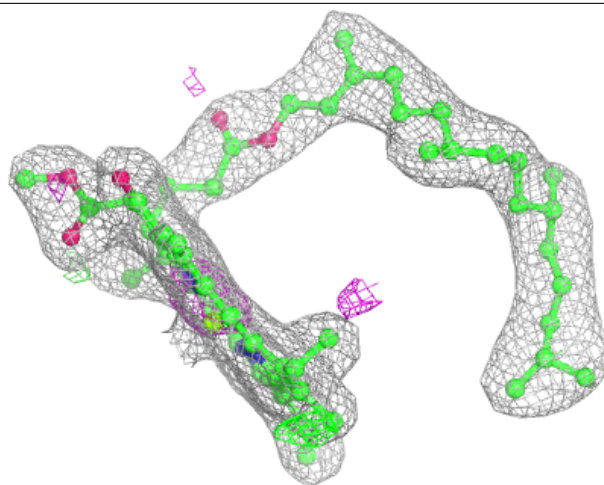
**Electron density around CLA c 510:**

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



**Electron density around CLA B 611:**

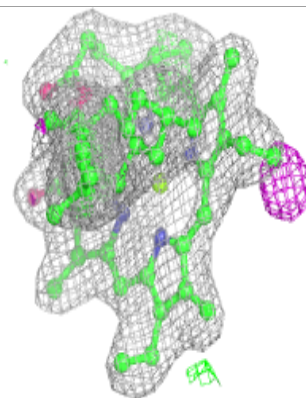
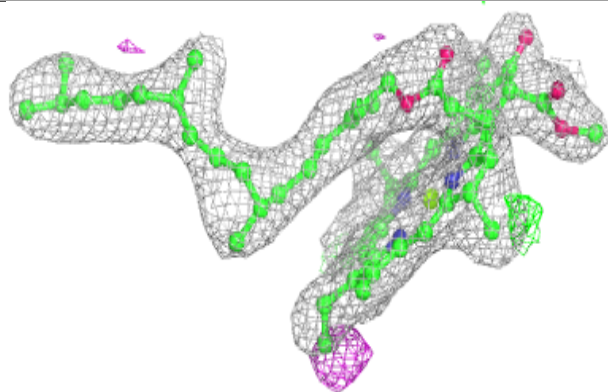
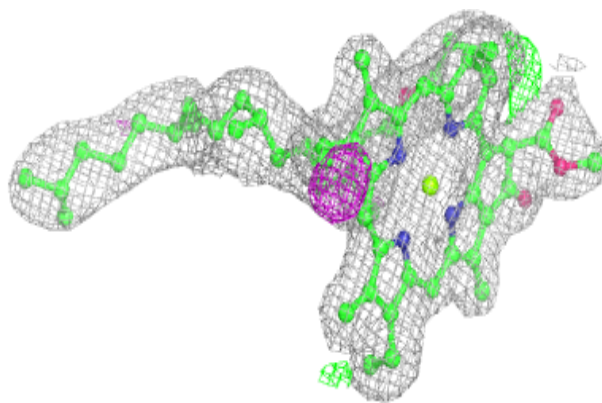
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



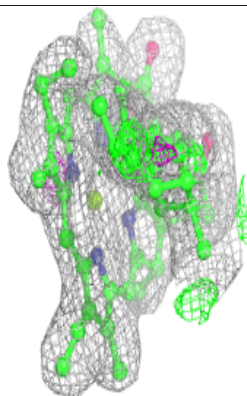
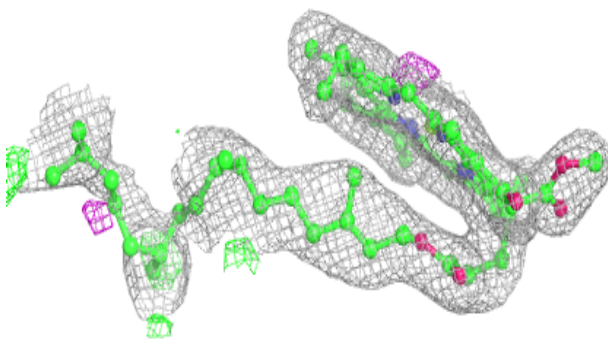
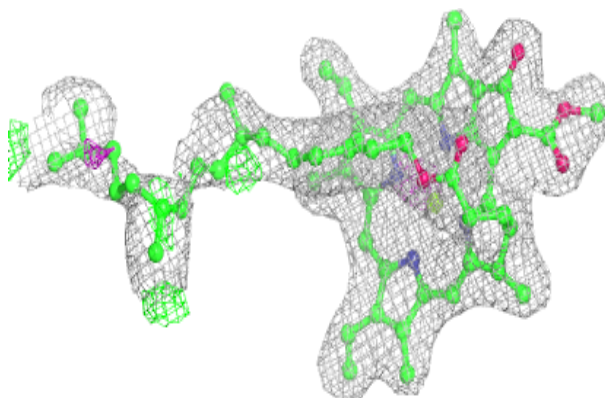


**Electron density around CLA C 506:**

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

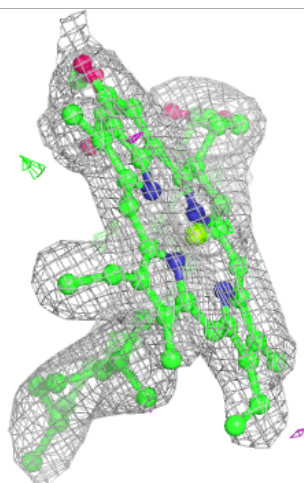
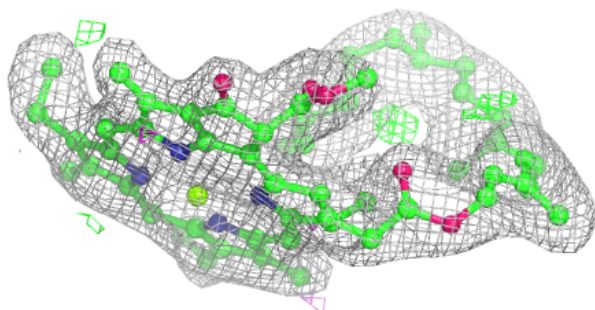
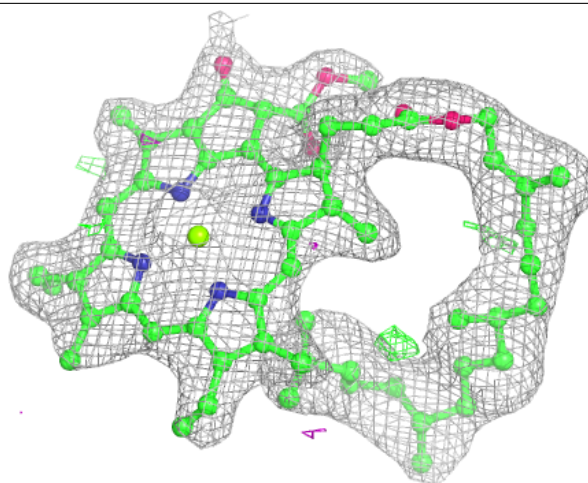
**Electron density around CLA b 614:**

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



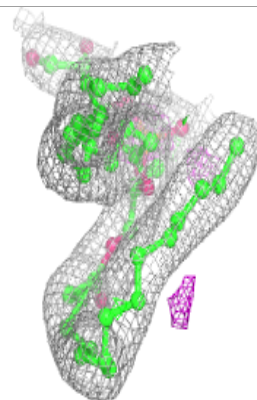
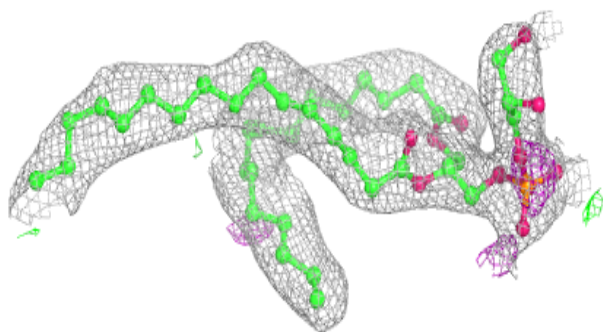
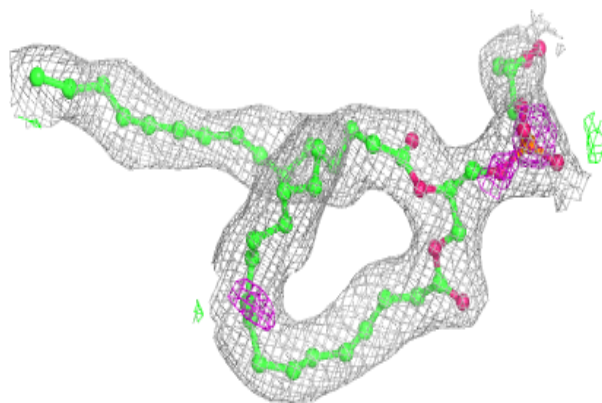
**Electron density around CLA b 615:**

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

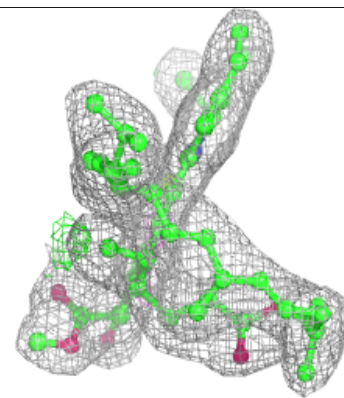
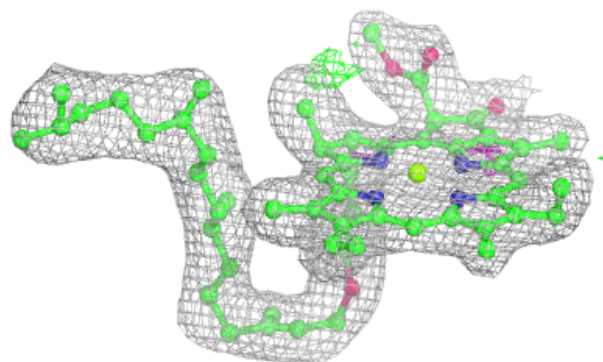
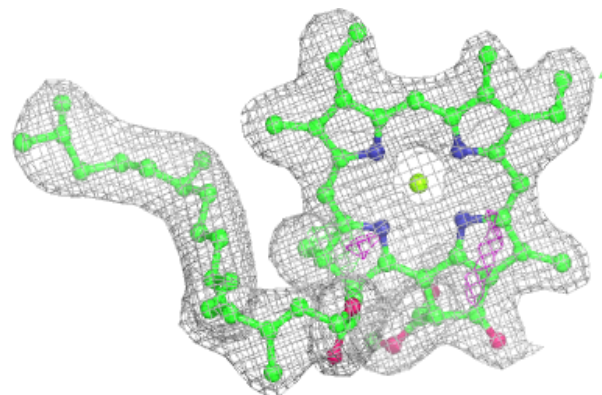


**Electron density around LHG D 357:**

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

**Electron density around CLA a 350:**

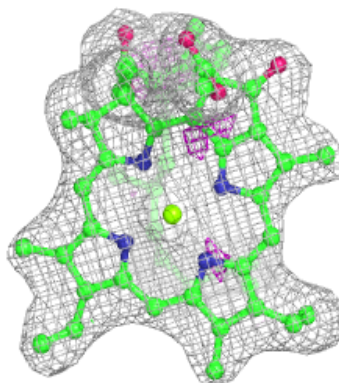
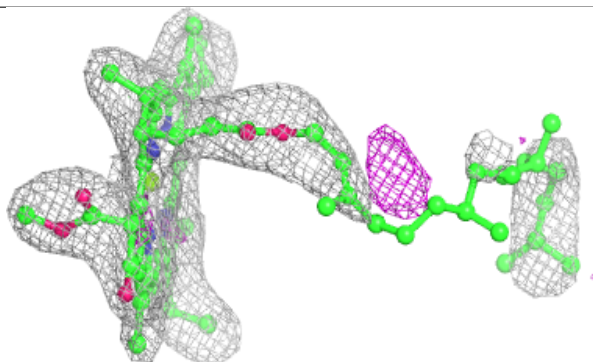
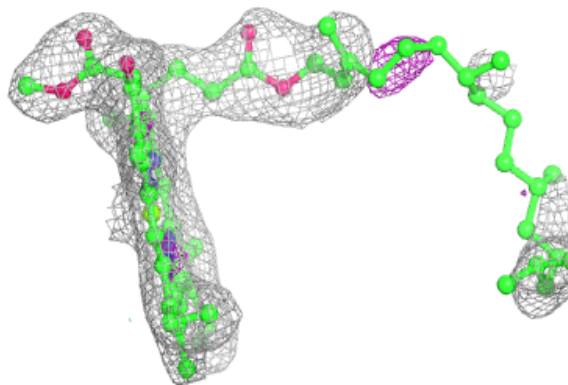
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



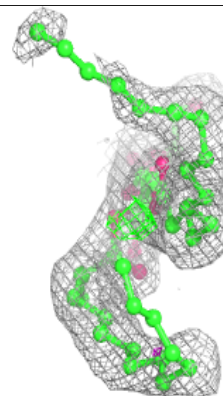
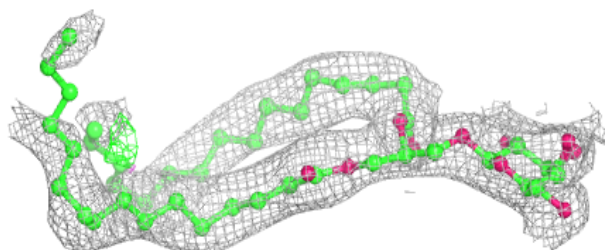
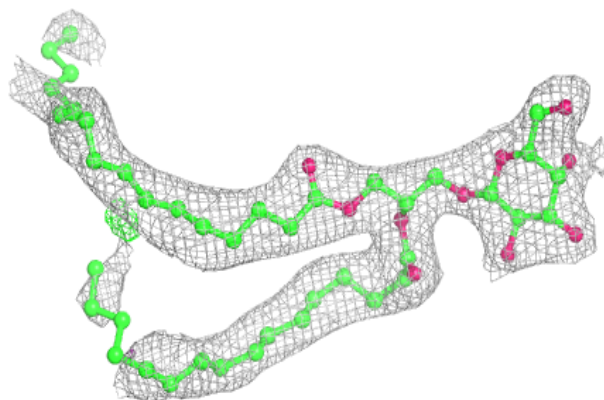


**Electron density around CLA C 507:**

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

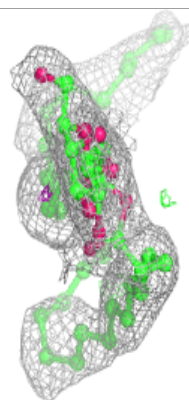
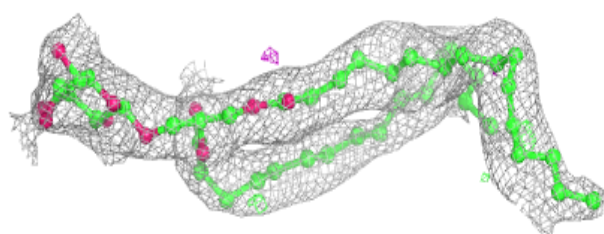
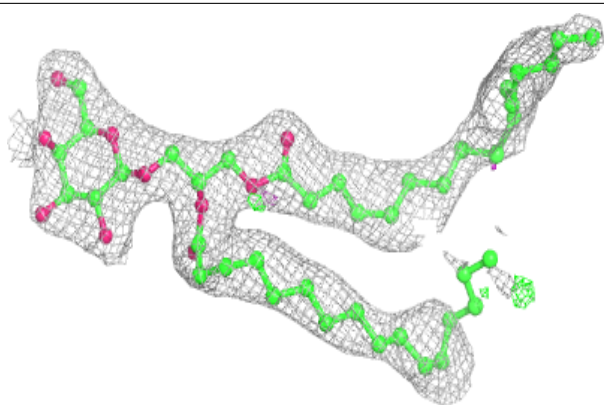
**Electron density around LMG J 101:**

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

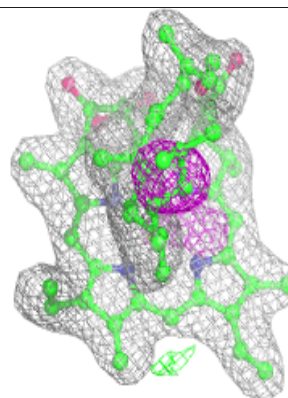
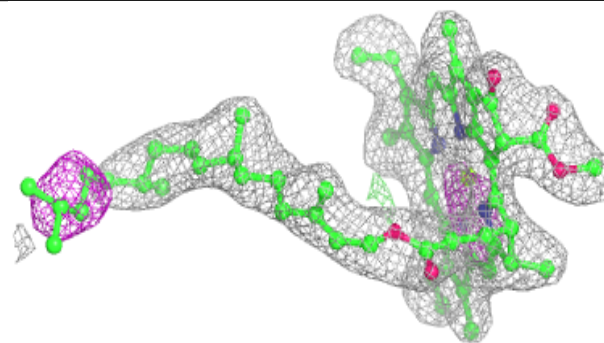
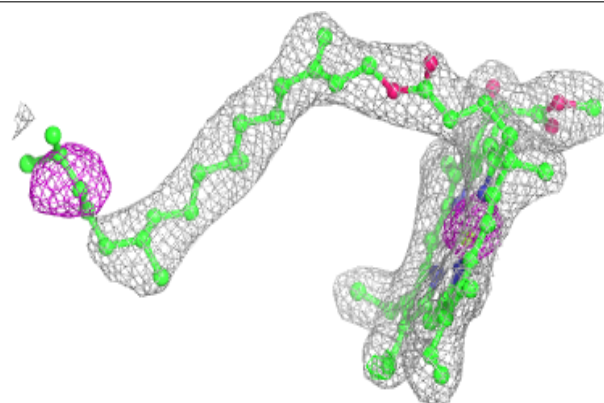


**Electron density around LMG j 101:**

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

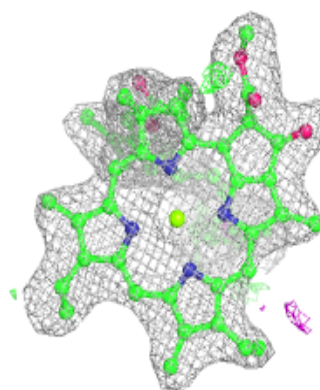
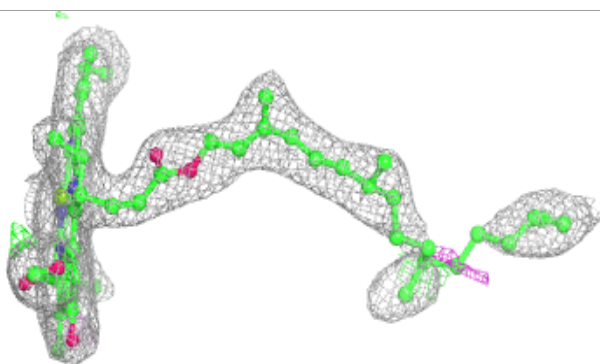
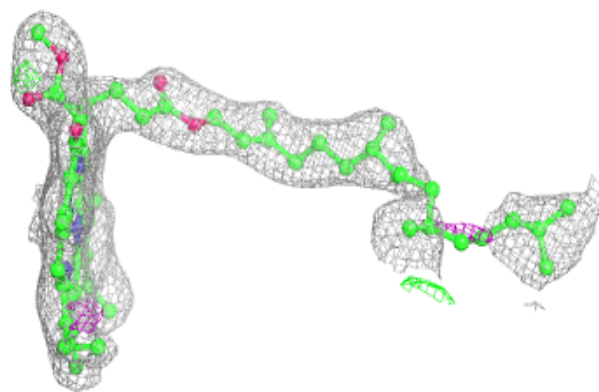
**Electron density around CLA C 509:**

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

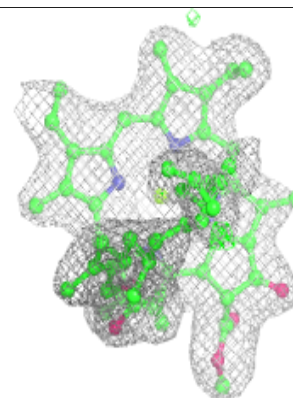
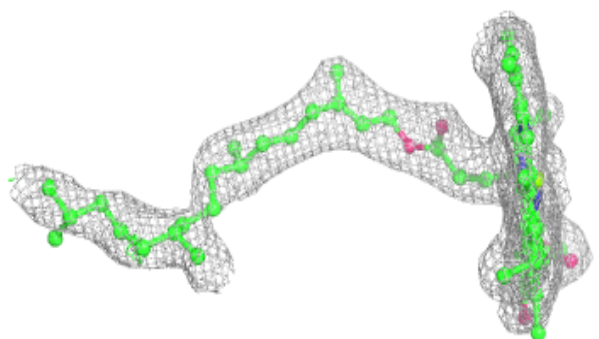
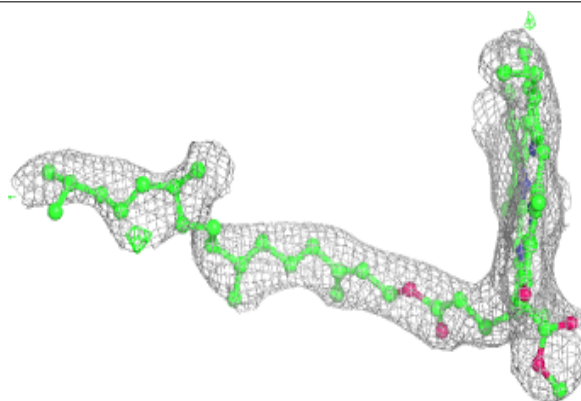


**Electron density around CLA B 606:**

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

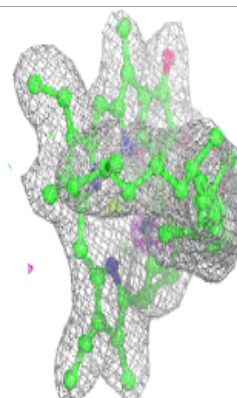
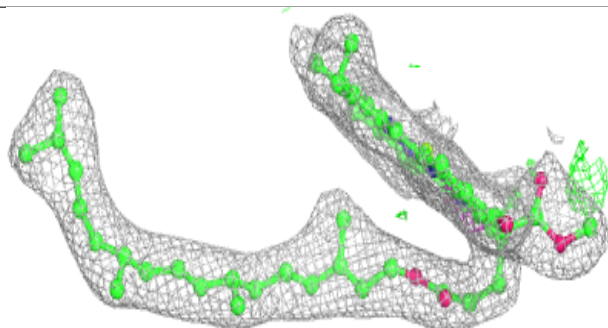
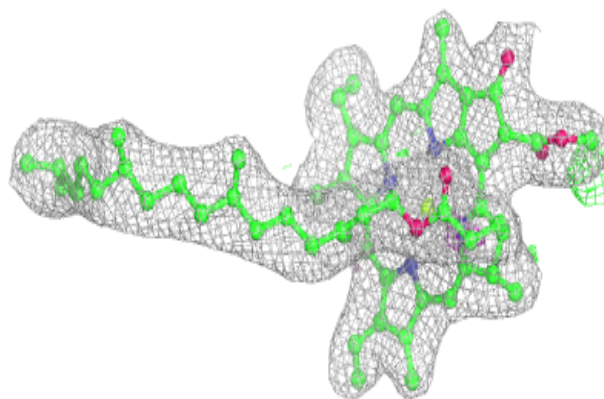
**Electron density around CLA b 606:**

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

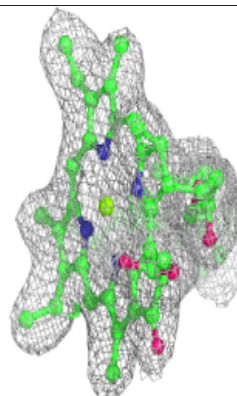
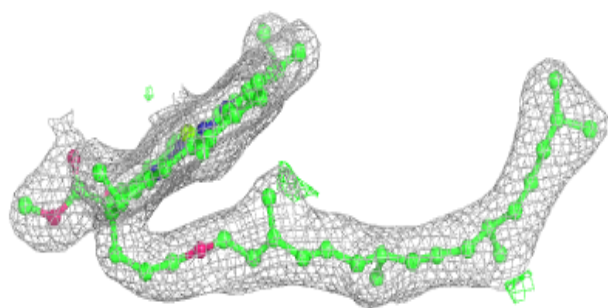
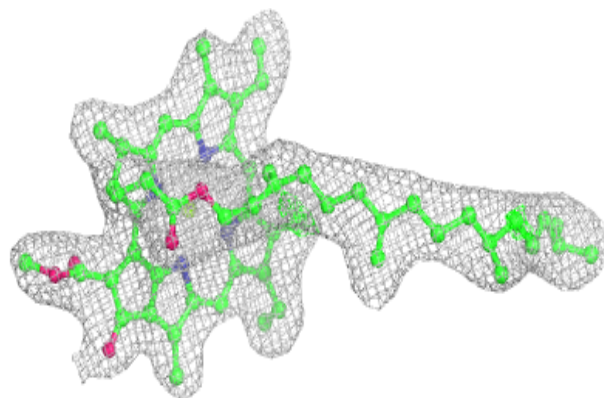


**Electron density around CLA b 608:**

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

**Electron density around CLA B 608:**

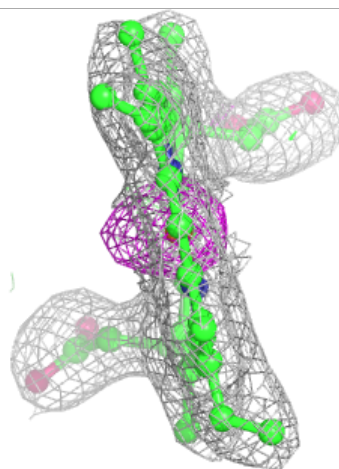
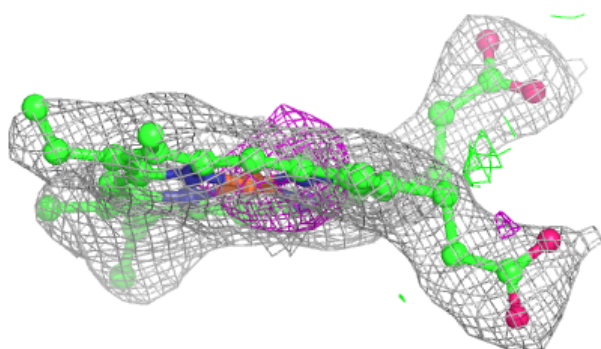
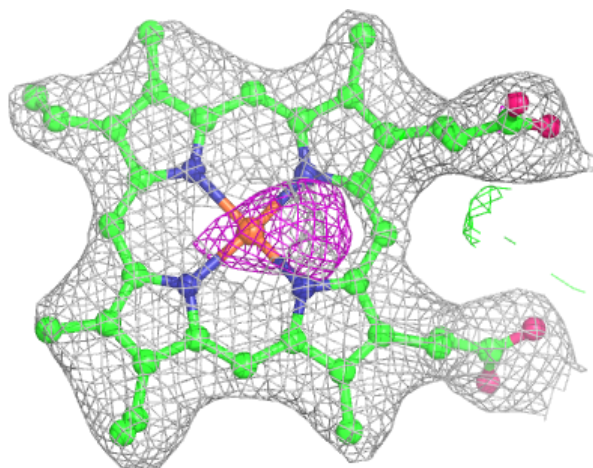
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





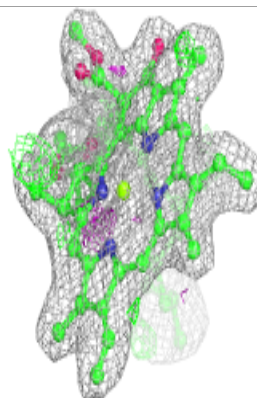
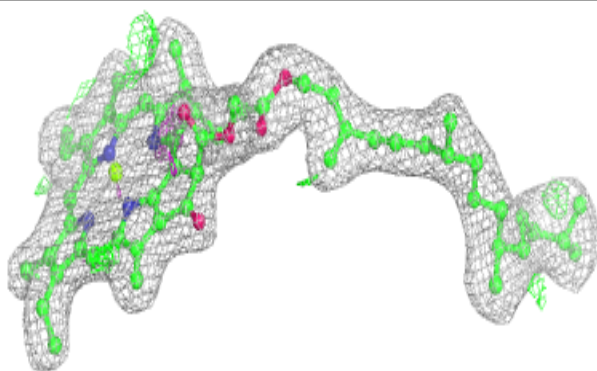
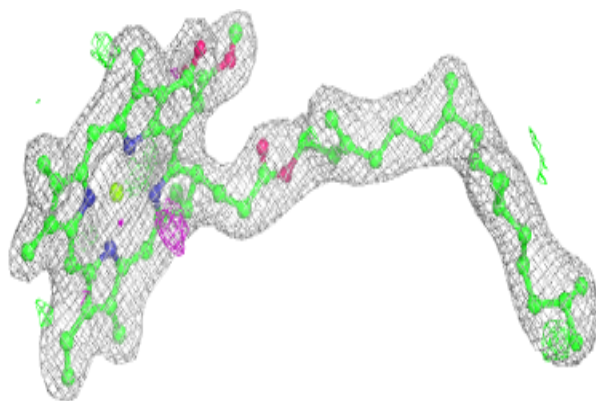
**Electron density around HEM E 103:**

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

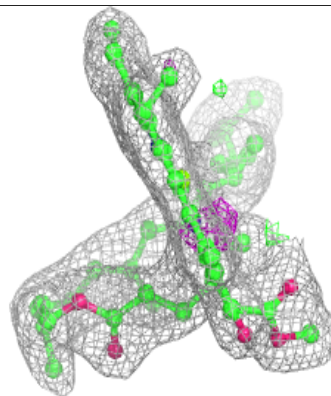
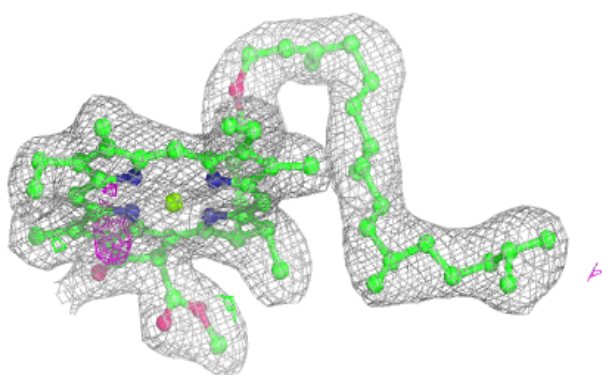
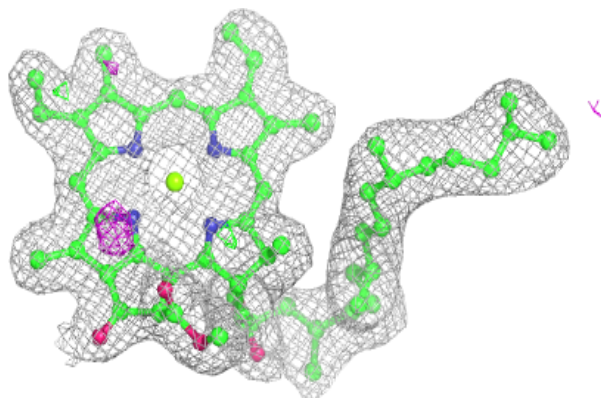


**Electron density around CLA A 404:**

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

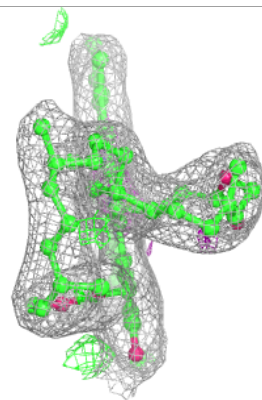
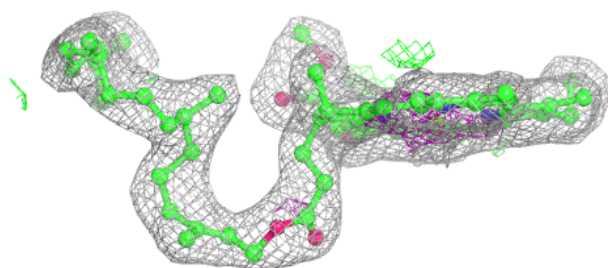
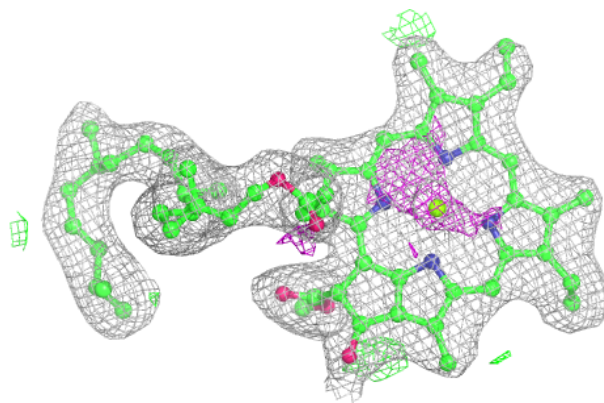
**Electron density around CLA A 405:**

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

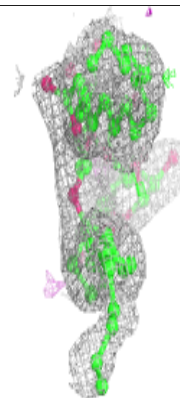
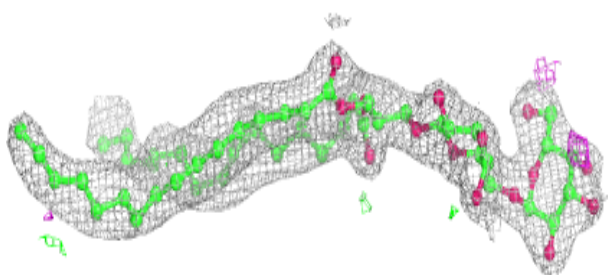
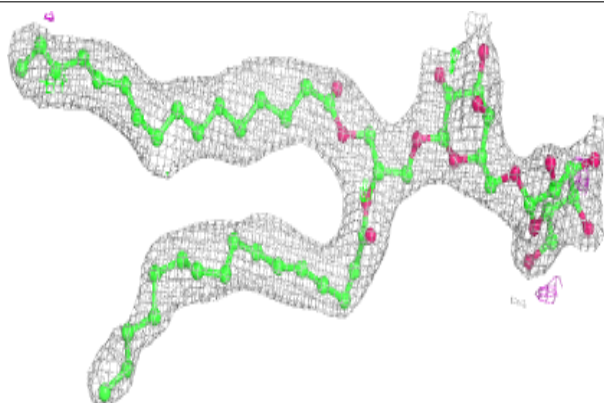


**Electron density around CLA B 612:**

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

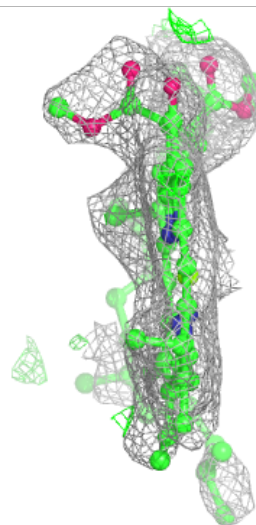
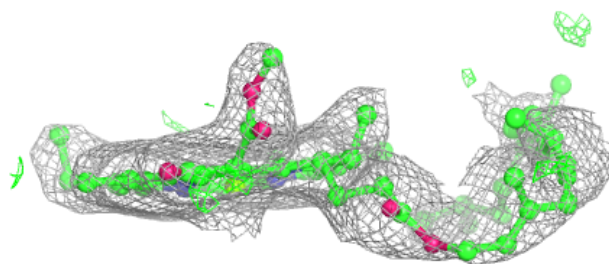
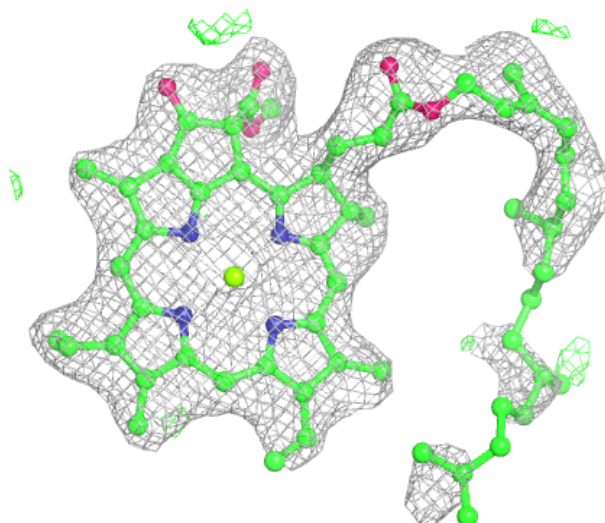
**Electron density around DGD C 519:**

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



**Electron density around CLA c 514:**

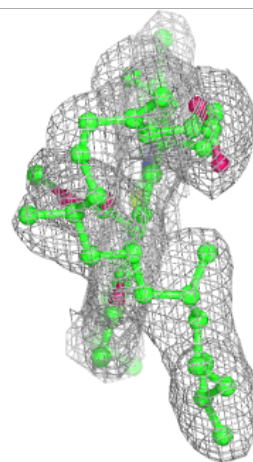
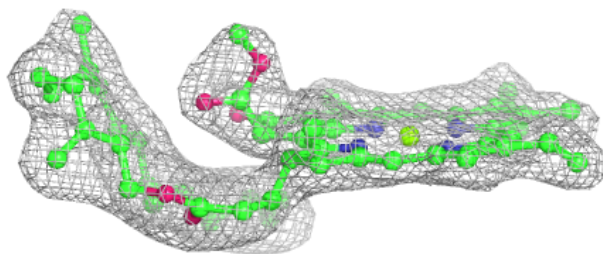
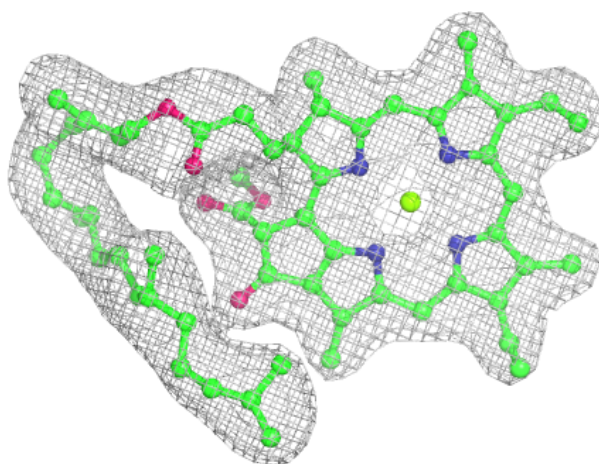
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





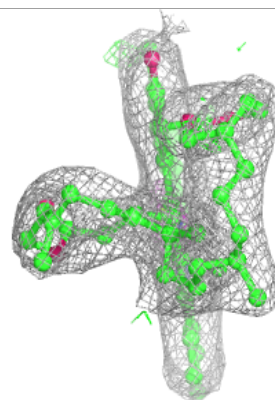
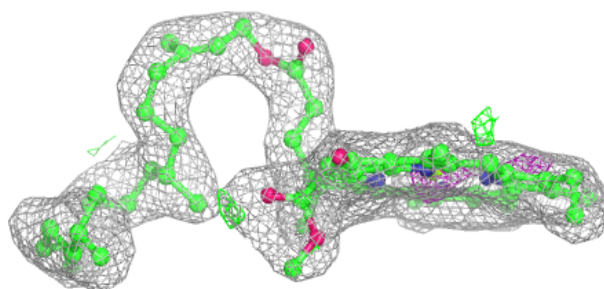
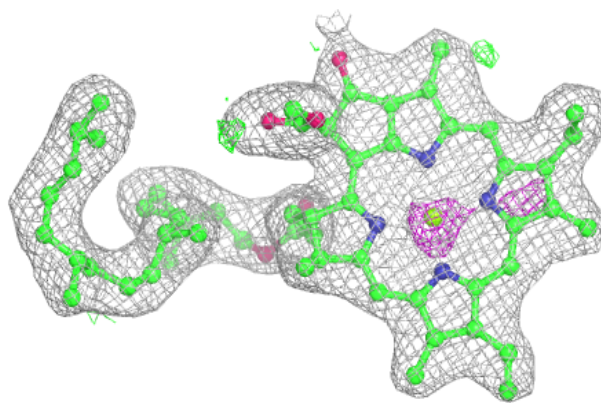
**Electron density around CLA b 610:**

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

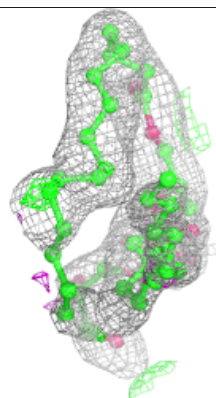
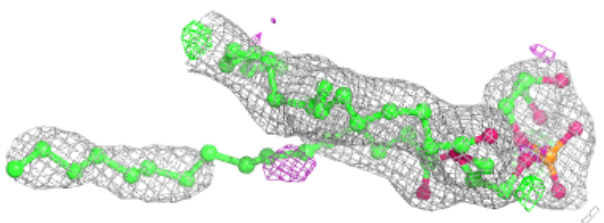
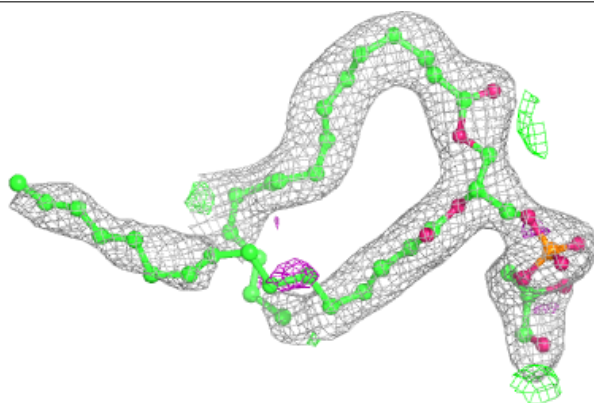


**Electron density around CLA b 612:**

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

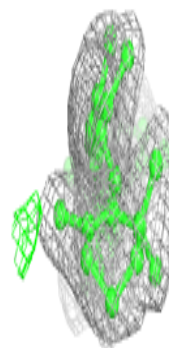
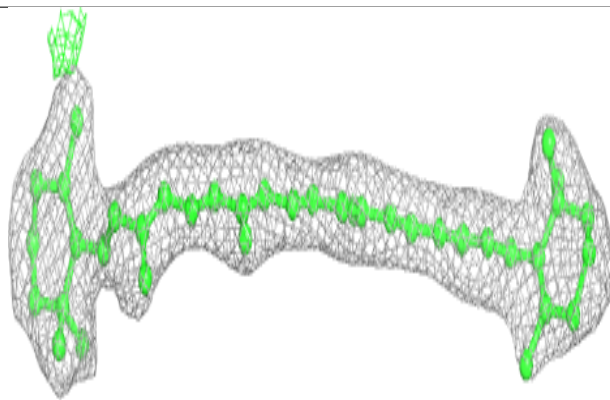
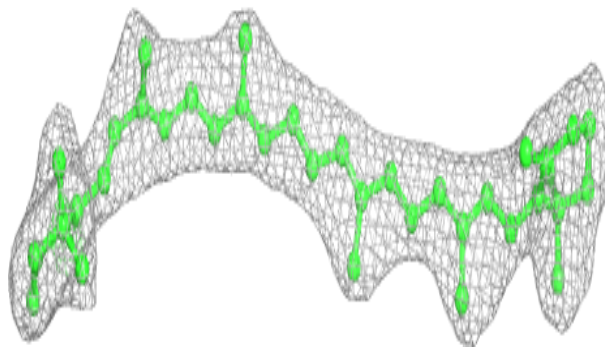
**Electron density around LHG D 407:**

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



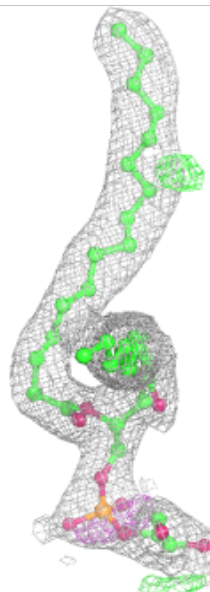
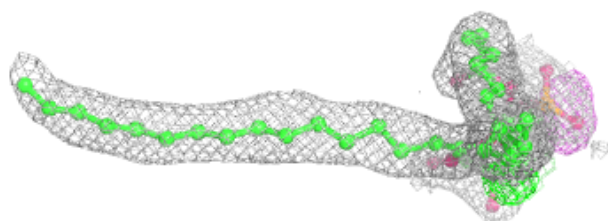
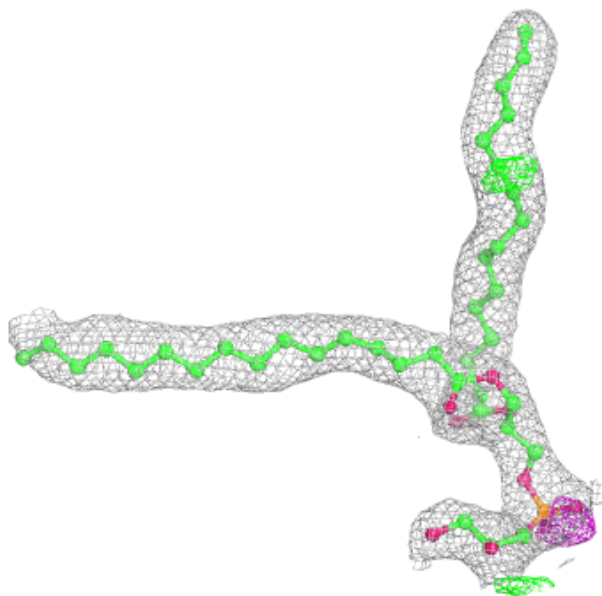
**Electron density around BCR H 101:**

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



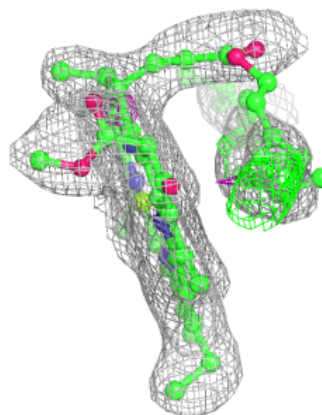
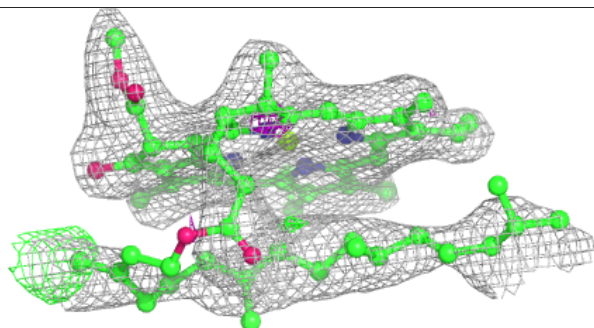
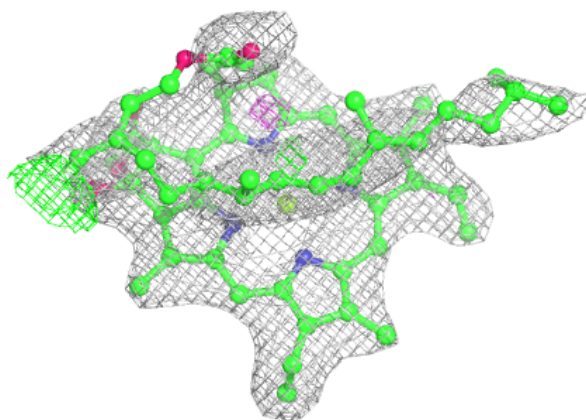
**Electron density around LHG L 101:**

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

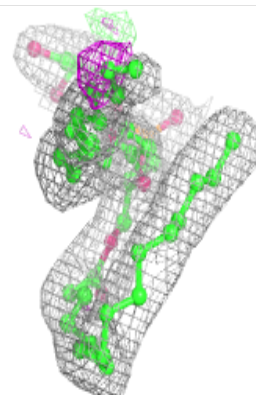
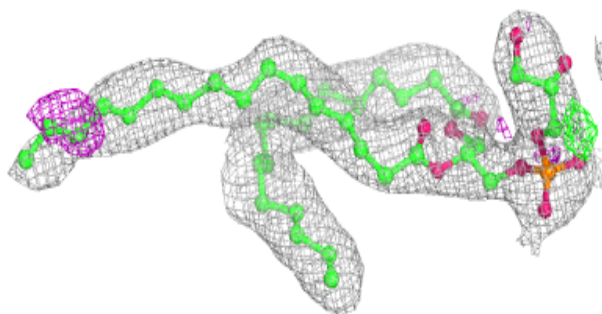
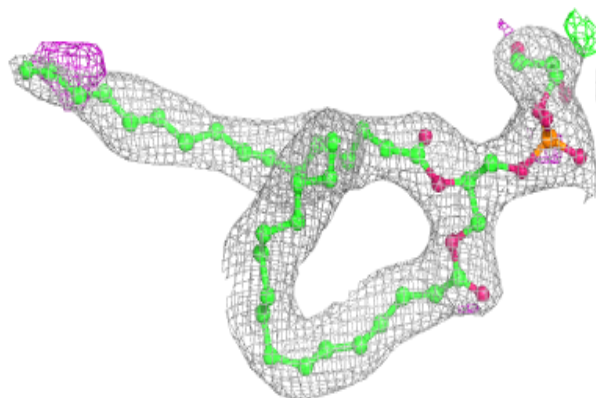


**Electron density around CLA B 601:**

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

**Electron density around LHG d 406:**

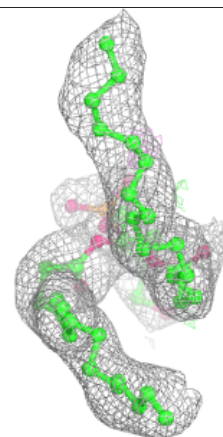
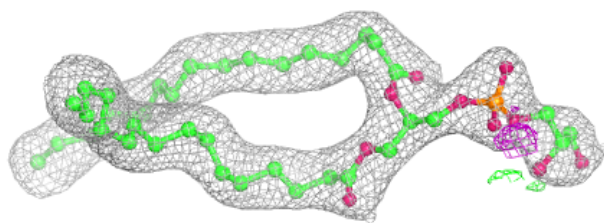
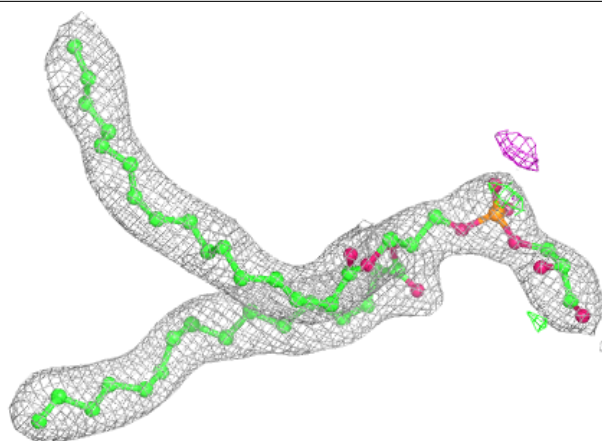
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



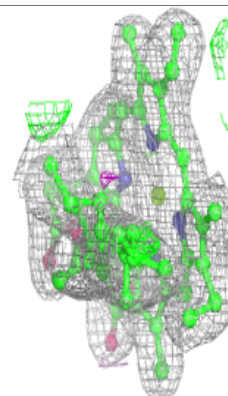
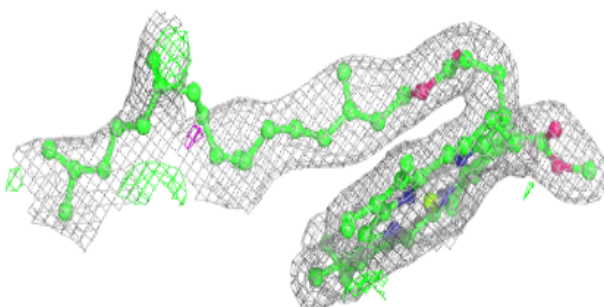
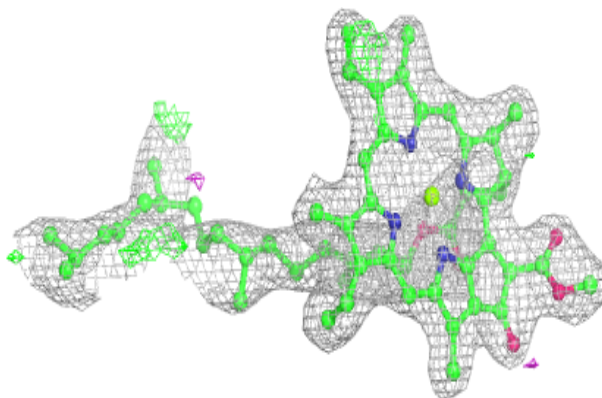


**Electron density around LHG d 407:**

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

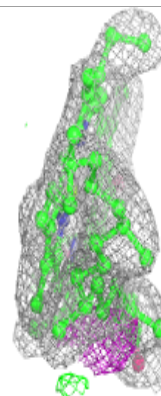
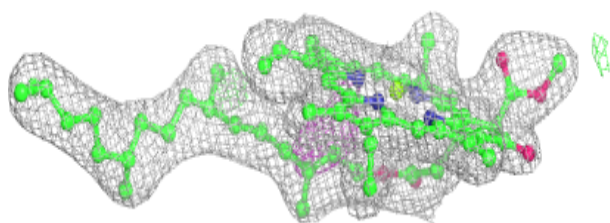
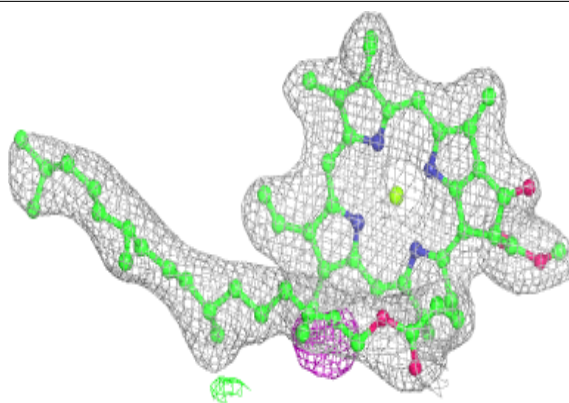
**Electron density around CLA B 614:**

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



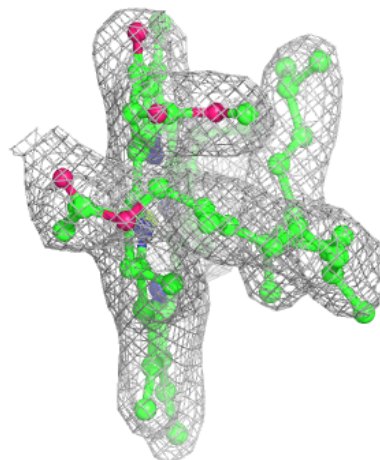
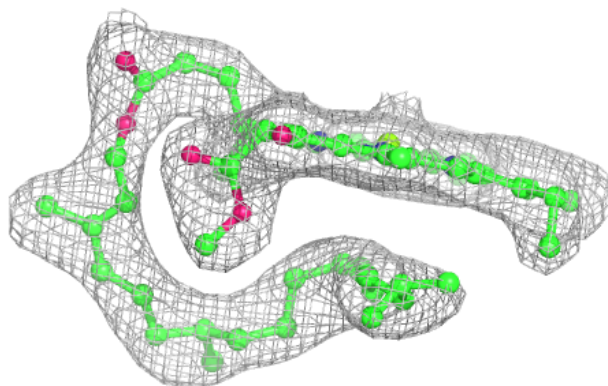
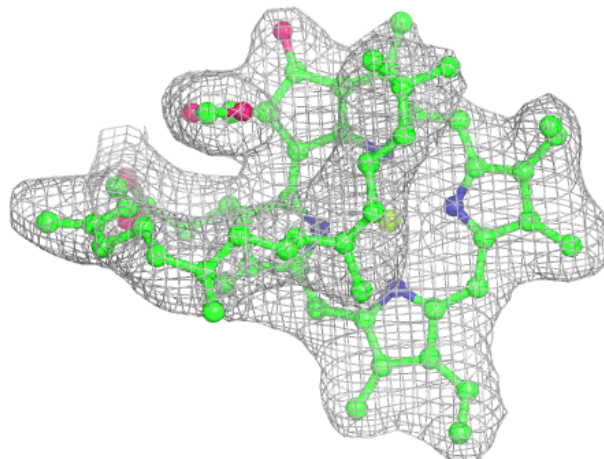
**Electron density around CLA C 502:**

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



**Electron density around CLA C 511:**

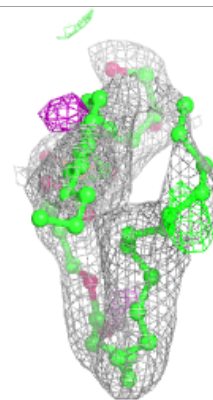
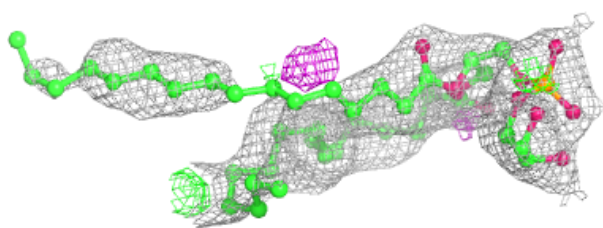
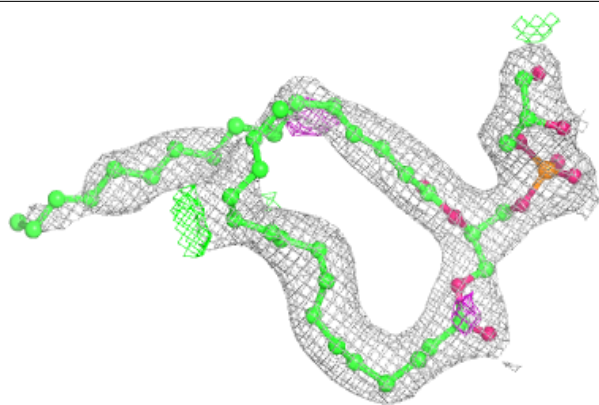
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



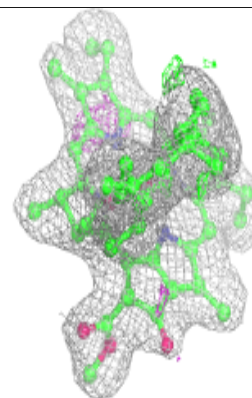
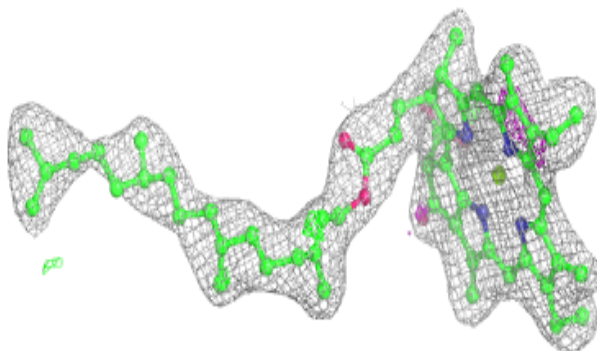
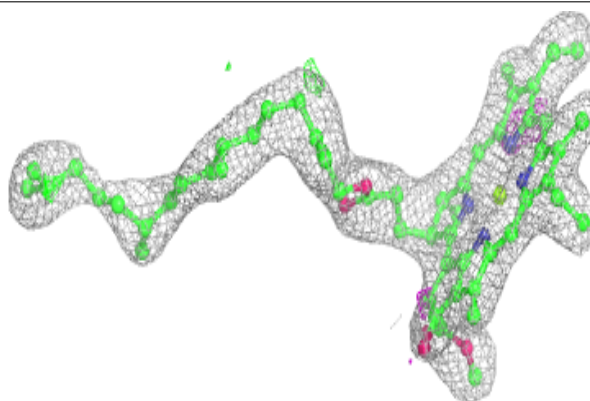


**Electron density around LHG d 408:**

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

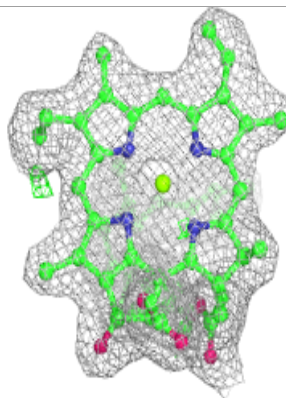
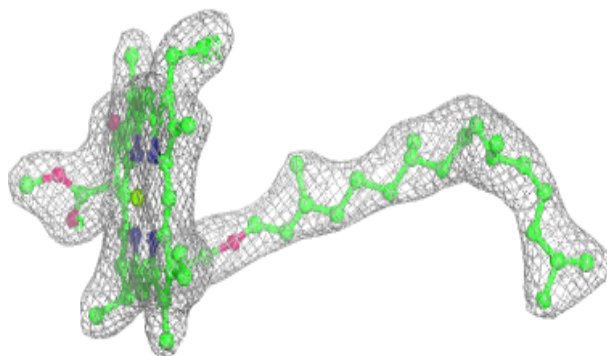
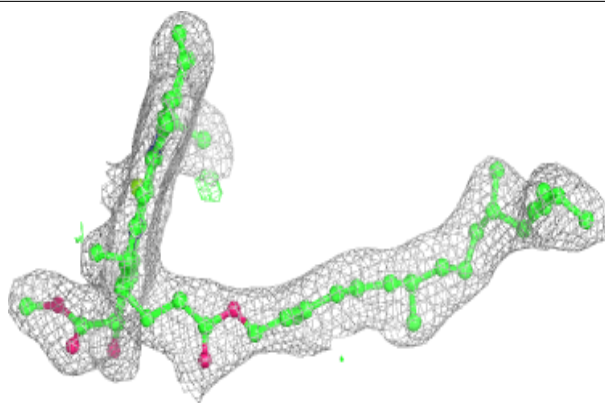
**Electron density around CLA c 504:**

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

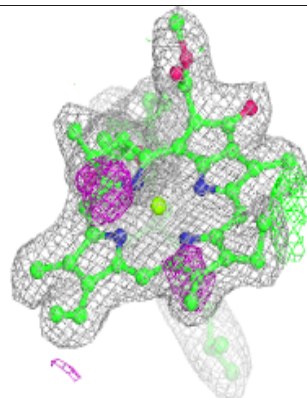
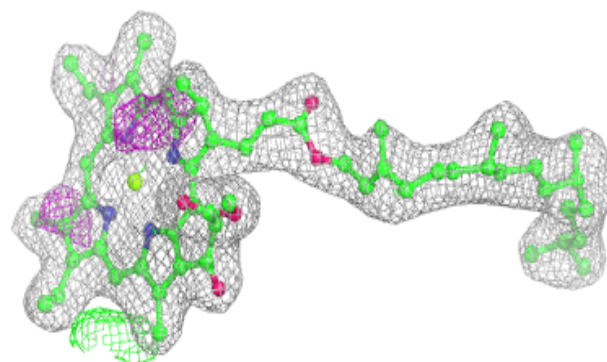
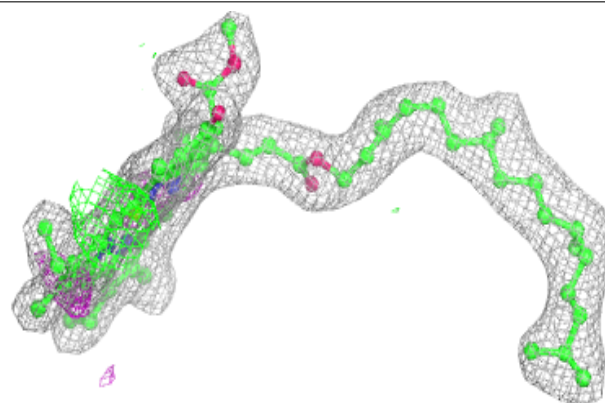


**Electron density around CLA b 605:**

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

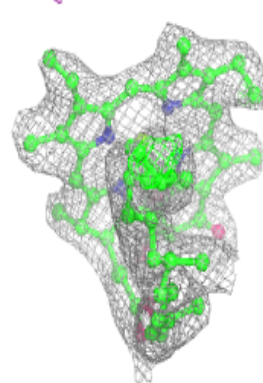
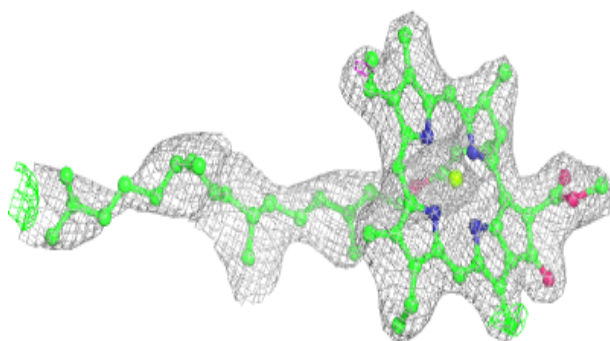
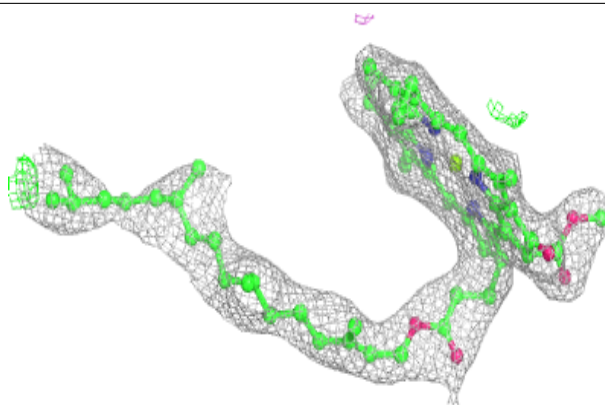
**Electron density around CLA D 402:**

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

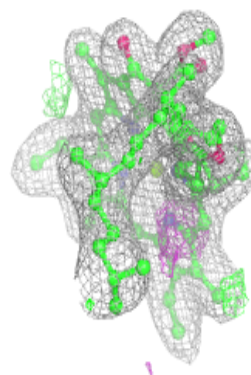
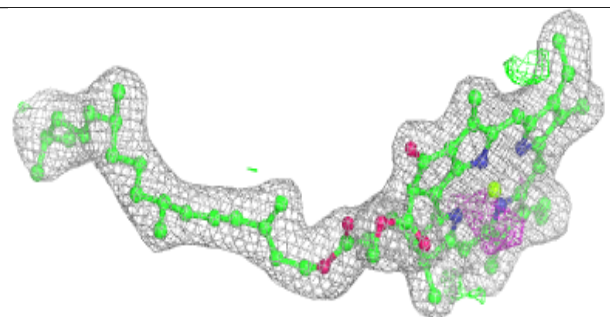
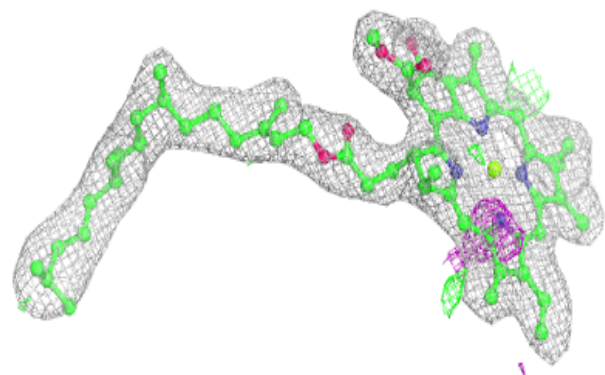


**Electron density around CLA c 506:**

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

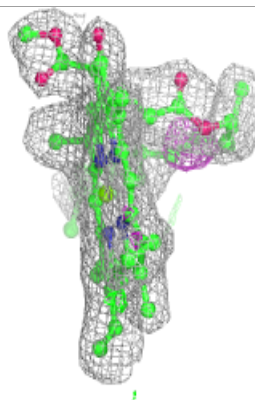
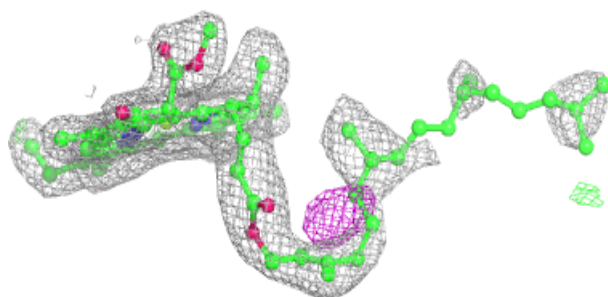
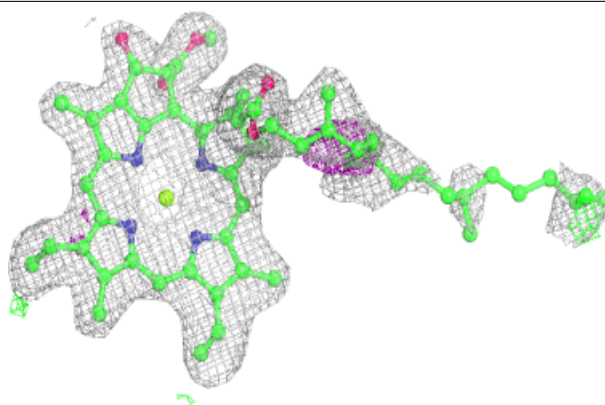
**Electron density around CLA a 403:**

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



**Electron density around CLA a 404:**

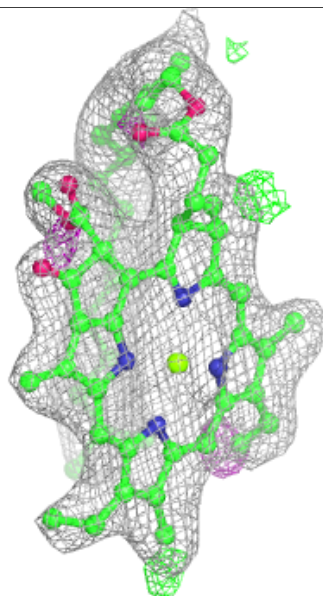
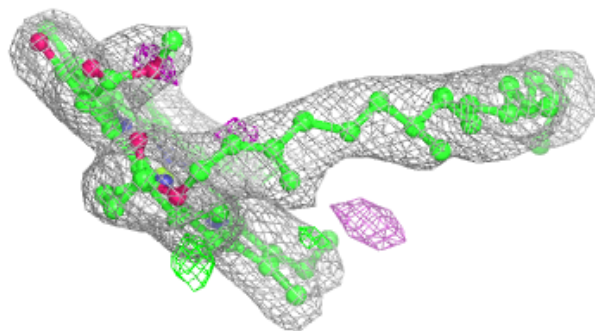
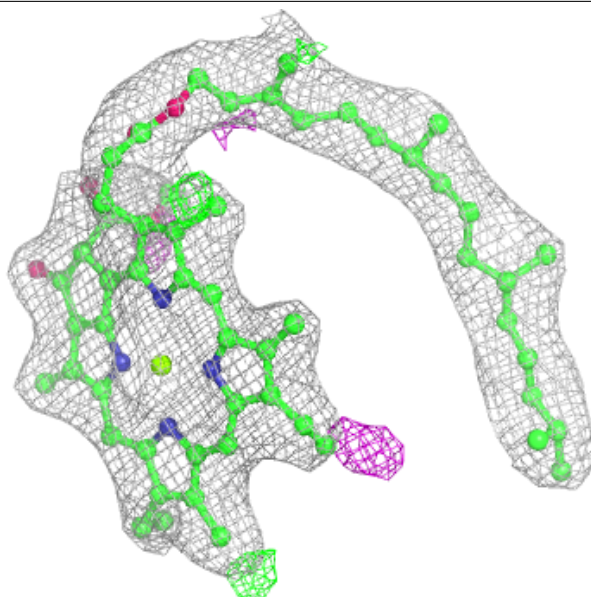
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





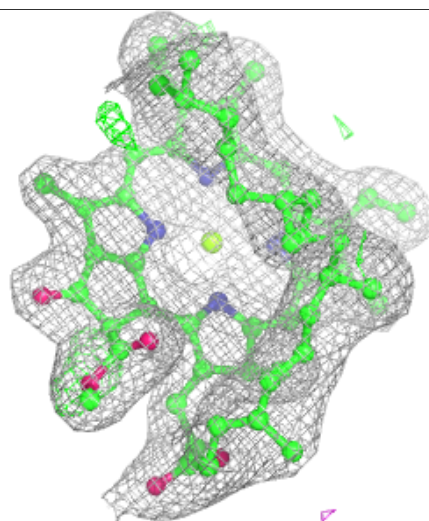
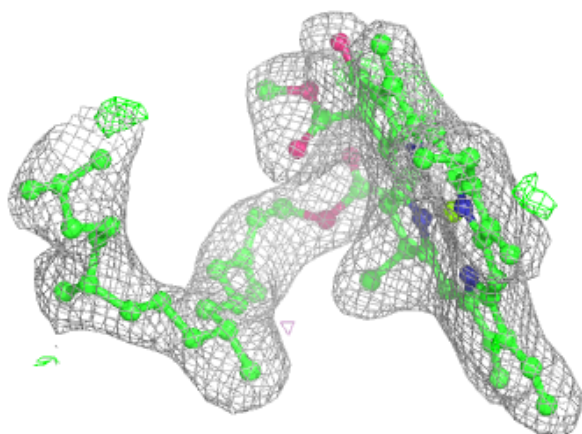
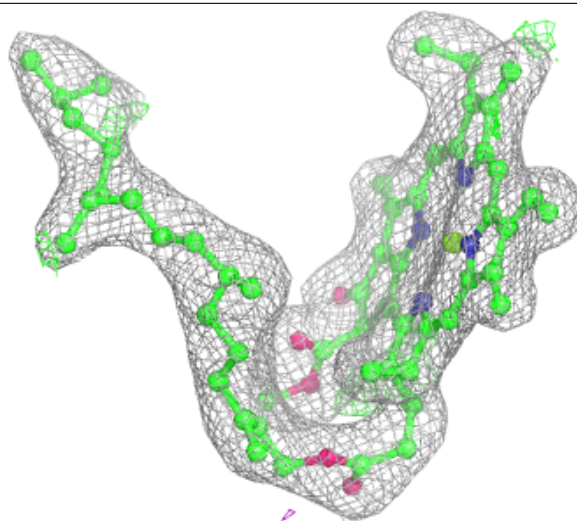
**Electron density around CLA c 509:**

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



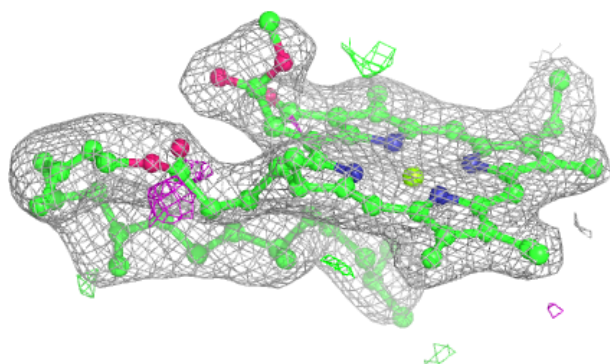
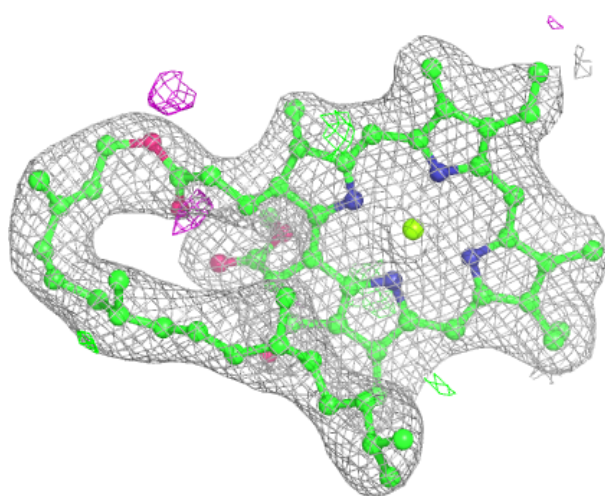
**Electron density around CLA B 613:**

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



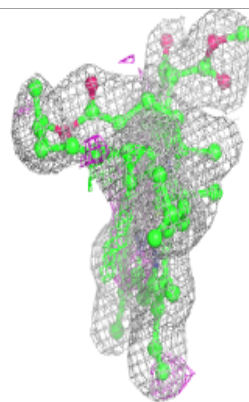
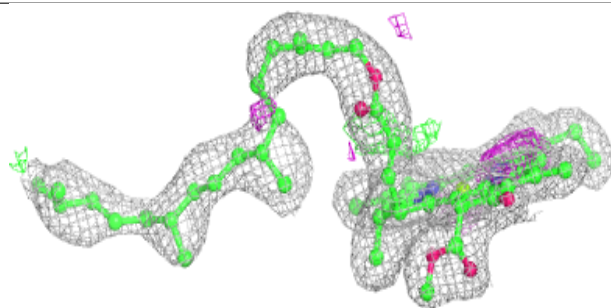
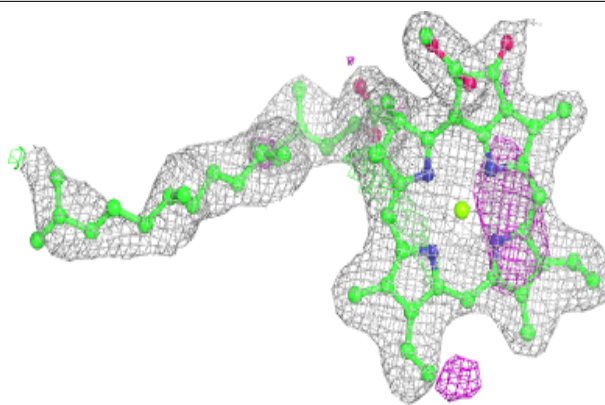
**Electron density around CLA c 511:**

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



**Electron density around CLA A 406:**

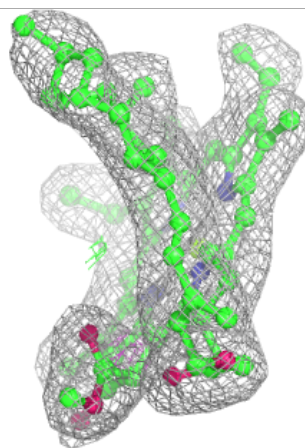
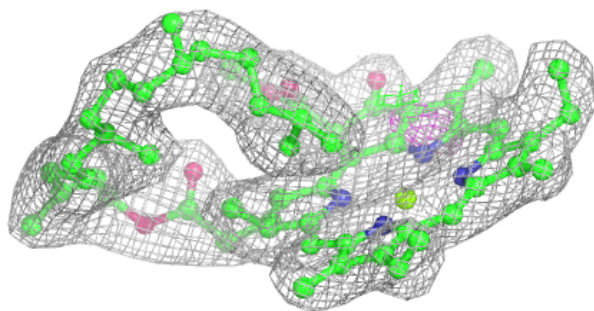
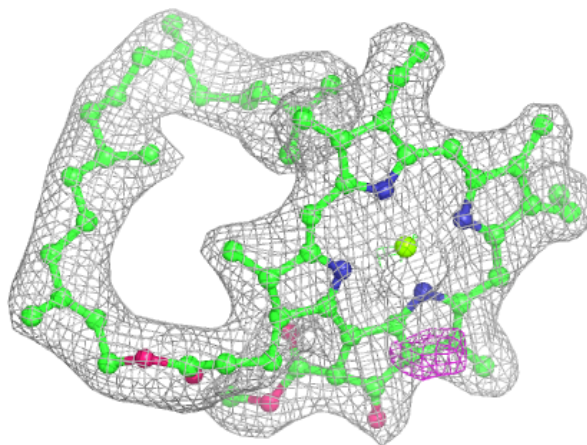
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





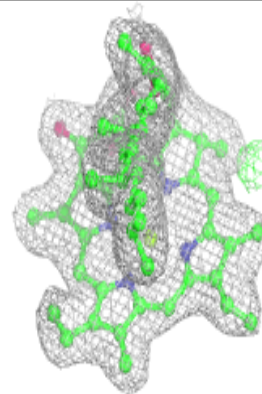
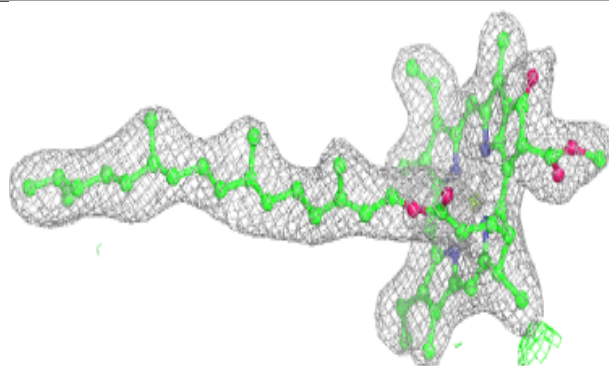
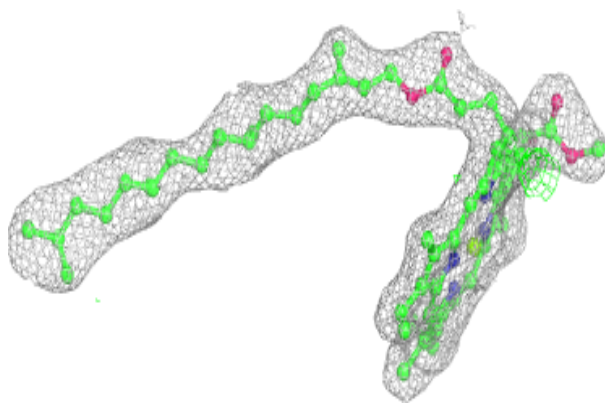
**Electron density around CLA B 615:**

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



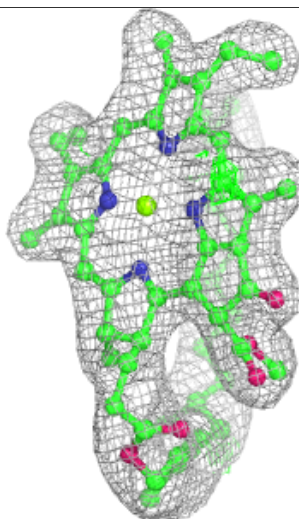
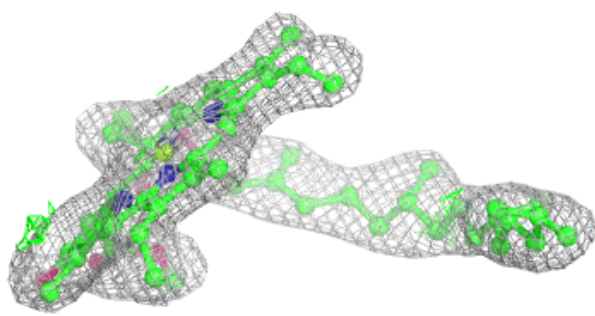
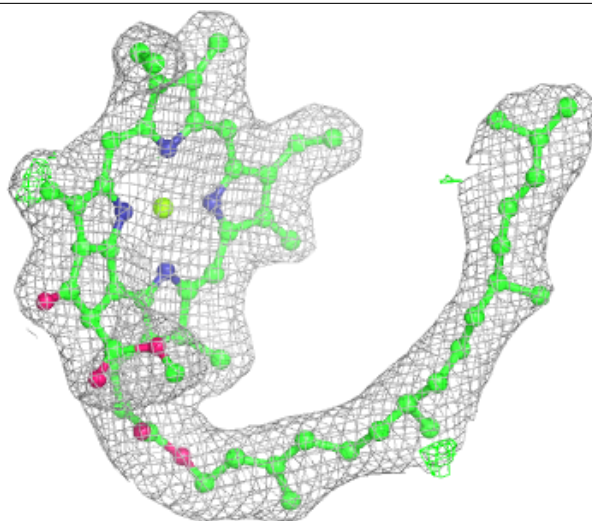
**Electron density around CLA B 607:**

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



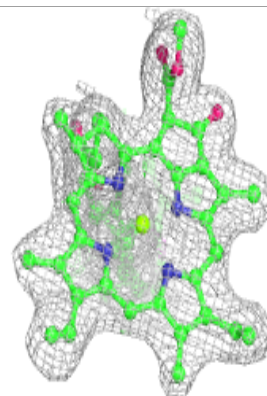
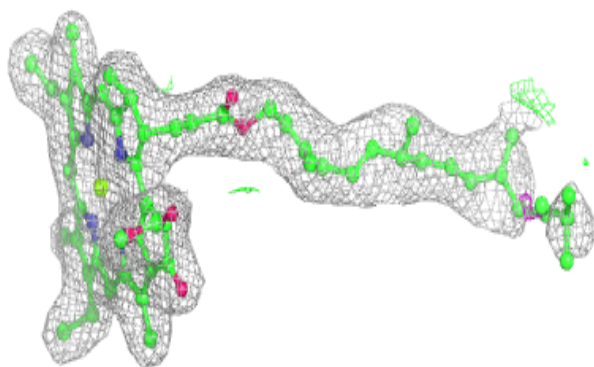
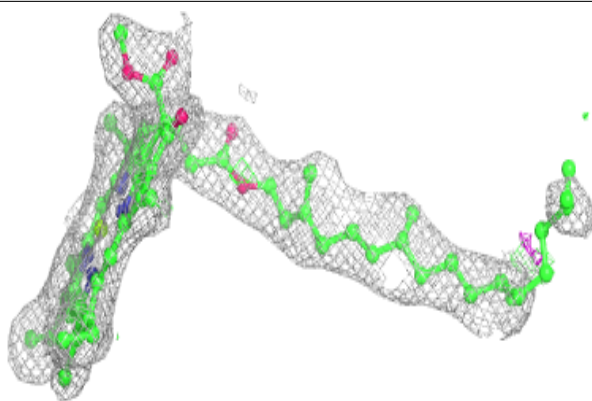
**Electron density around CLA C 508:**

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

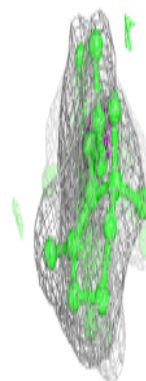
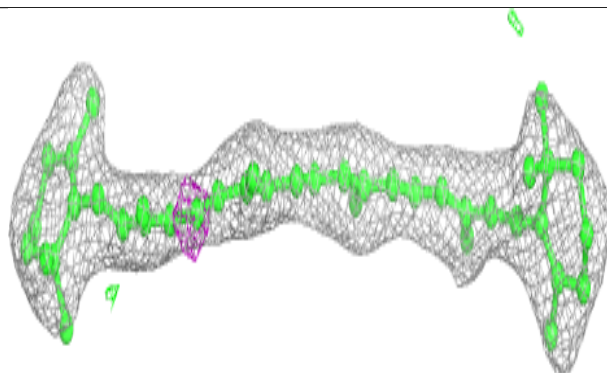
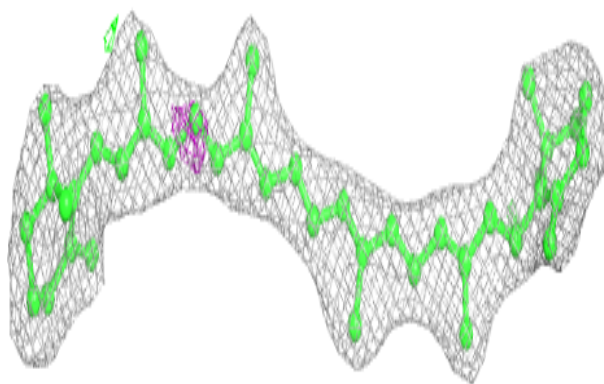


**Electron density around CLA B 604:**

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

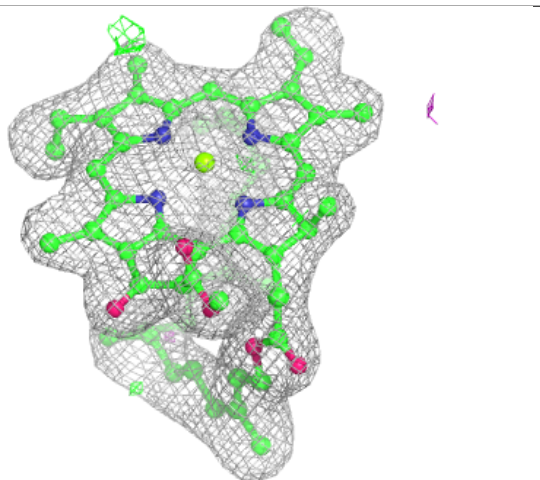
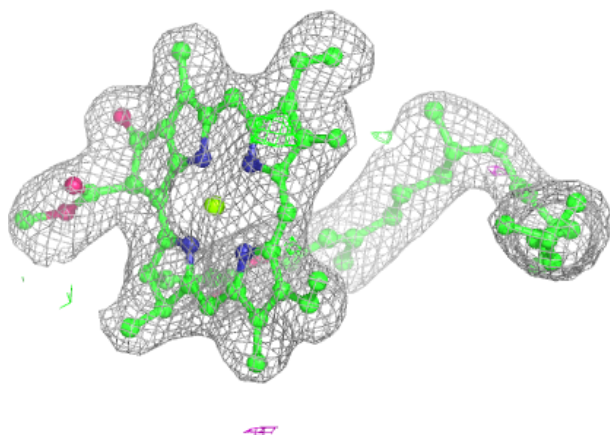
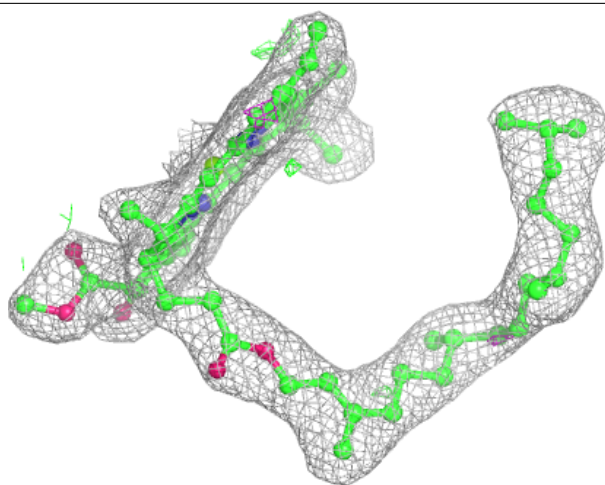
**Electron density around BCR y 101:**

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



**Electron density around CLA b 611:**

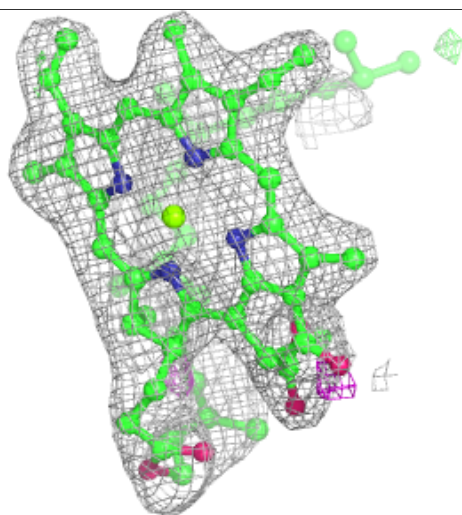
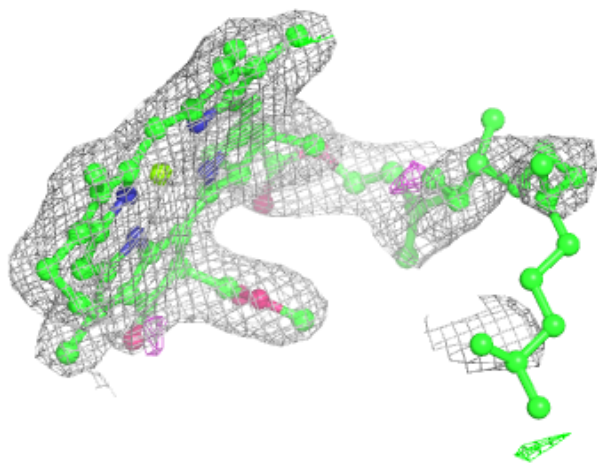
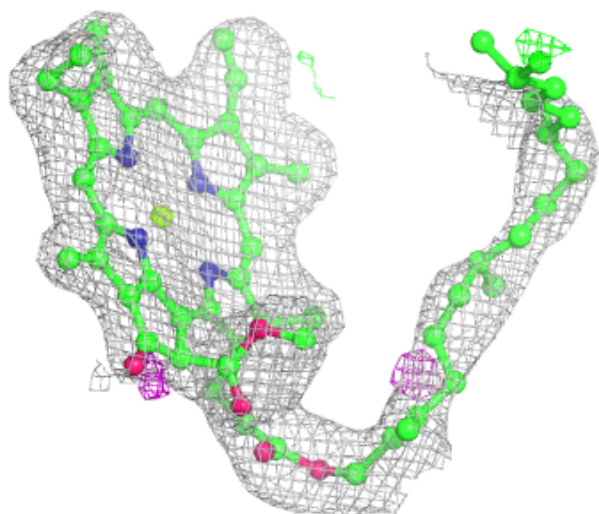
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





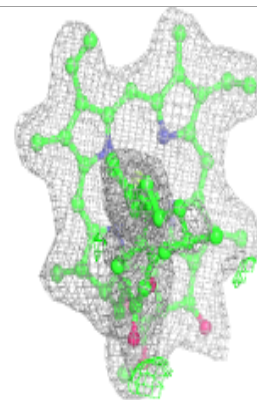
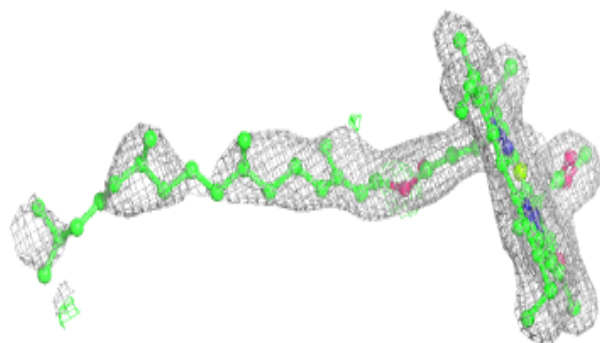
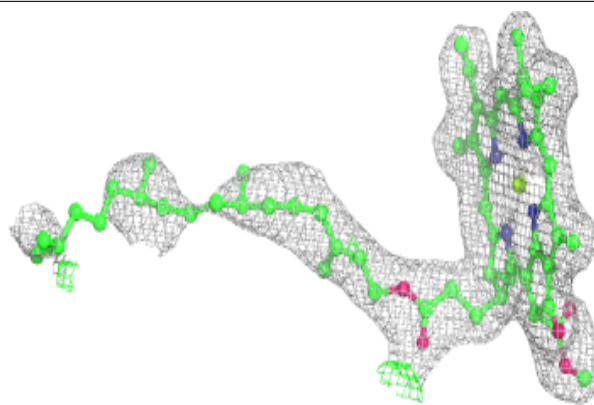
**Electron density around CLA b 616:**

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



**Electron density around CLA d 403:**

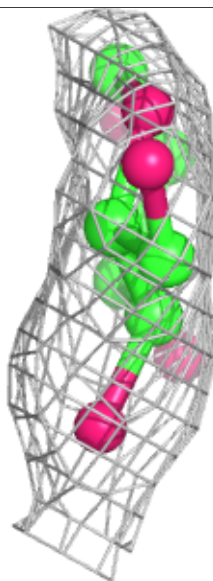
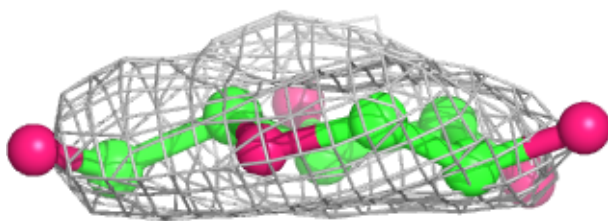
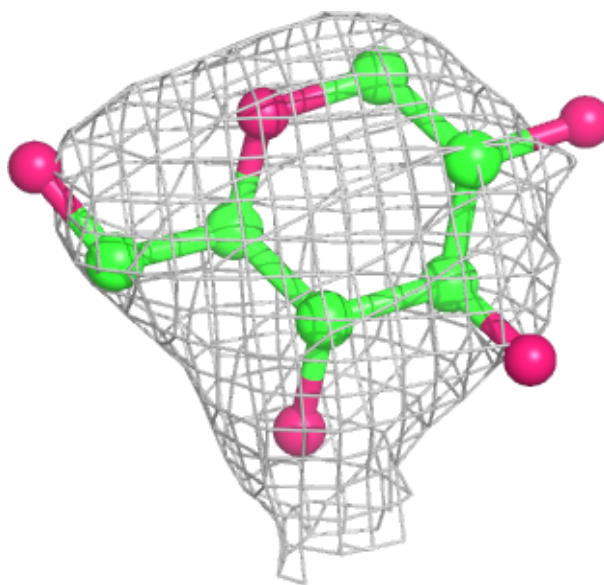
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





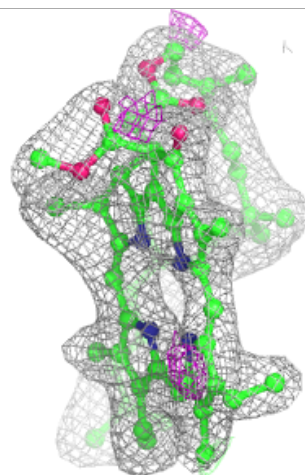
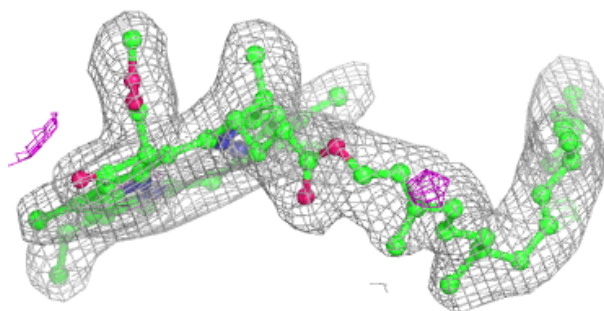
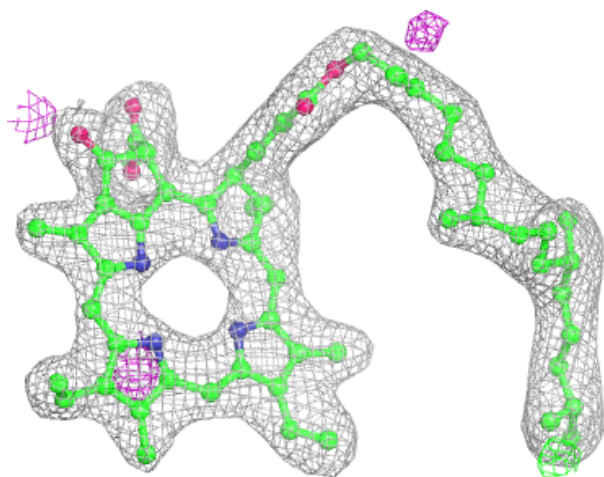
**Electron density around HTG V 204:**

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



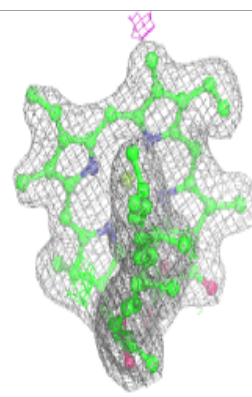
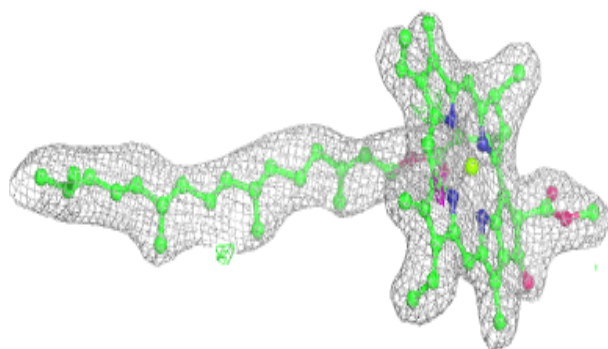
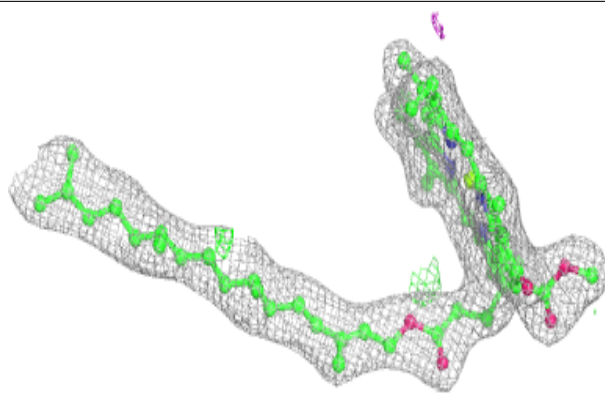
**Electron density around PHO a 406:**

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

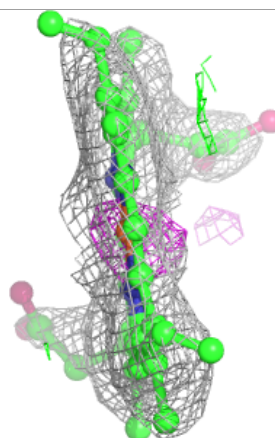
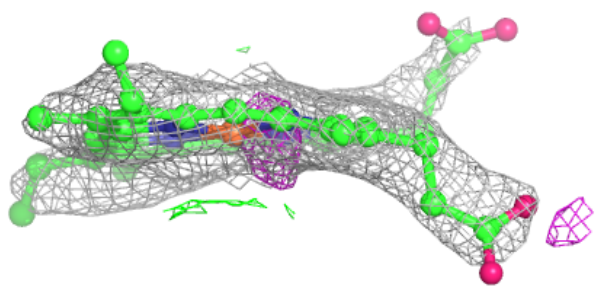
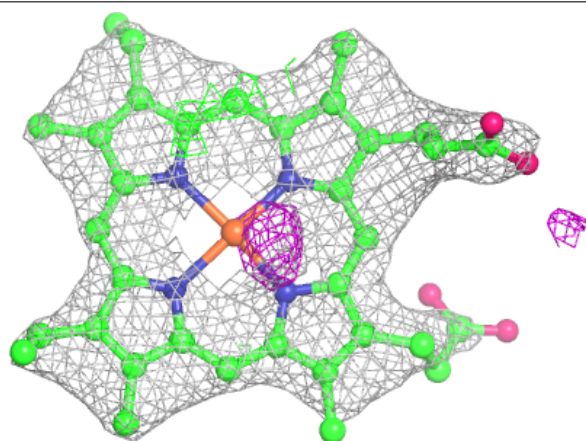


**Electron density around CLA b 607:**

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

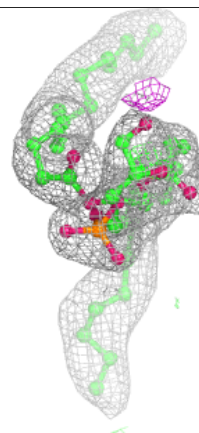
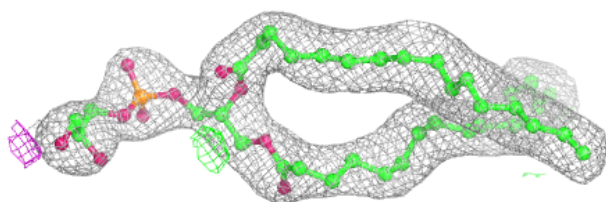
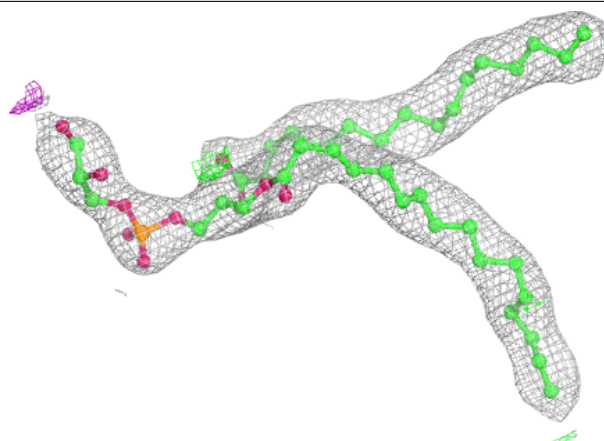
**Electron density around HEM e 102:**

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

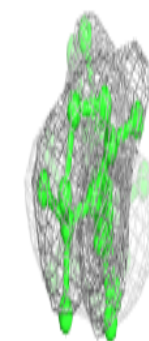
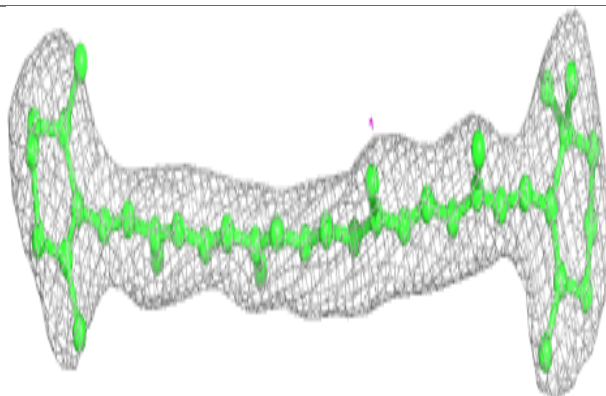
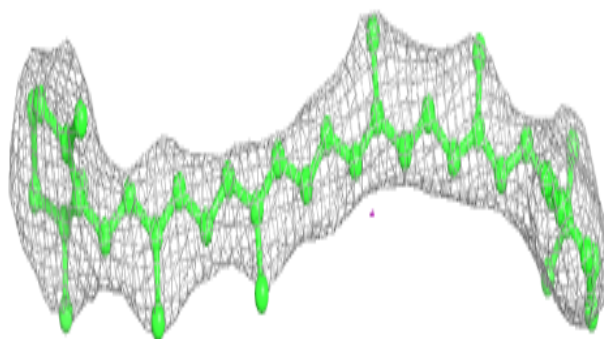


**Electron density around LHG D 406:**

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

**Electron density around BCR c 516:**

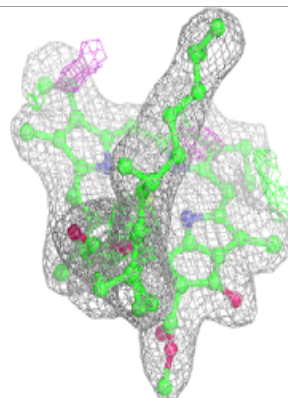
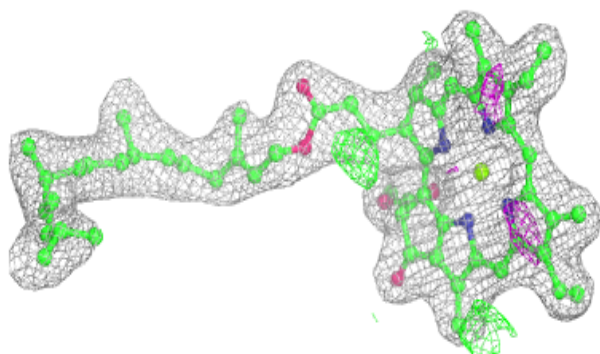
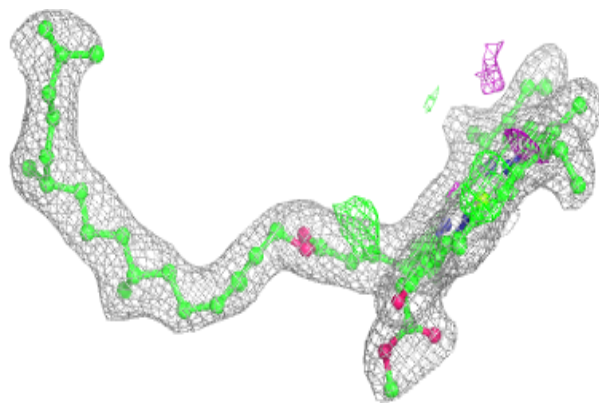
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



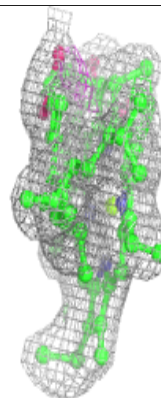
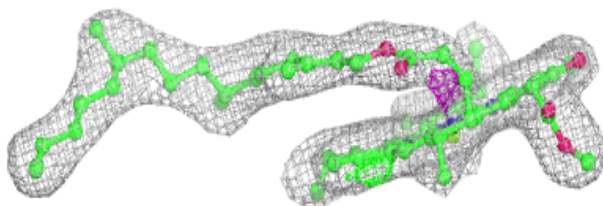
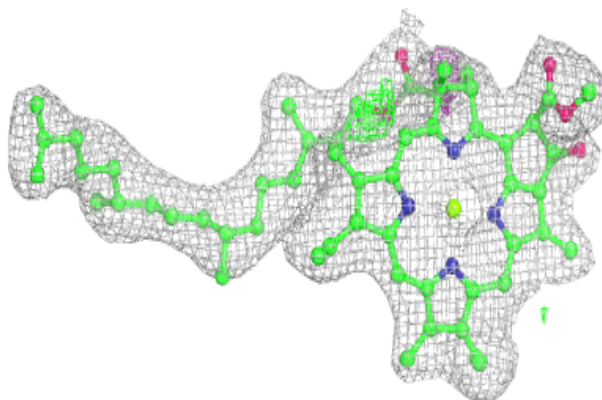


**Electron density around CLA d 402:**

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

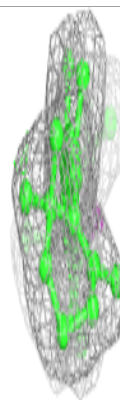
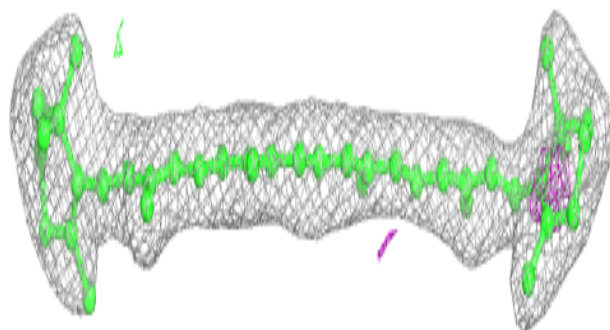
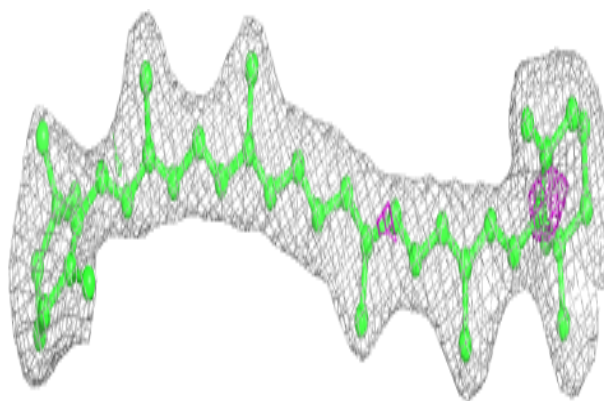
**Electron density around CLA B 603:**

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

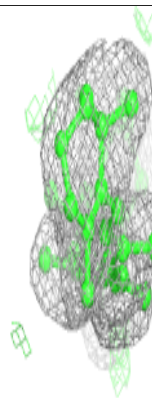
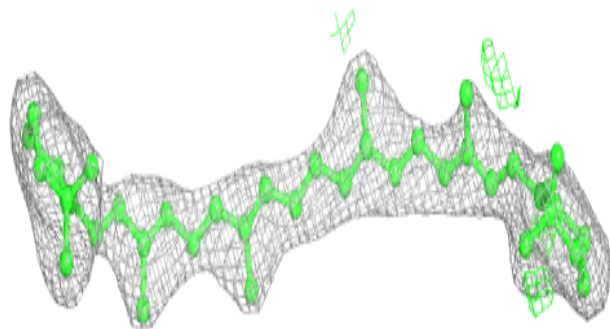
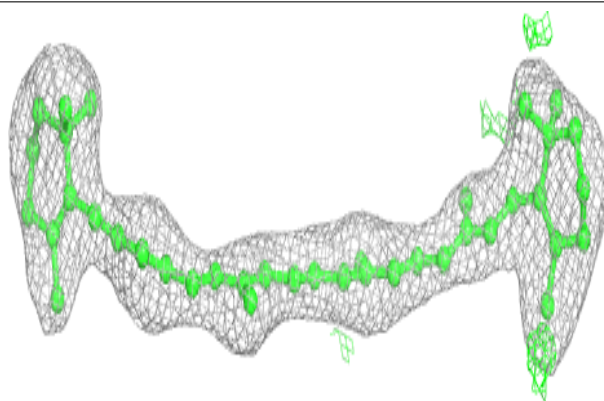


**Electron density around BCR B 618:**

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

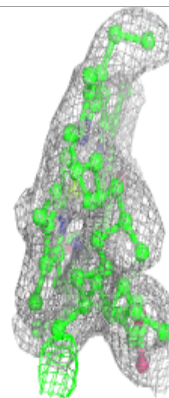
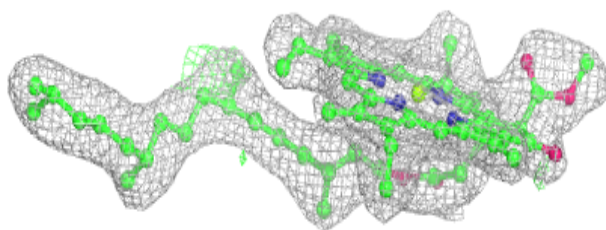
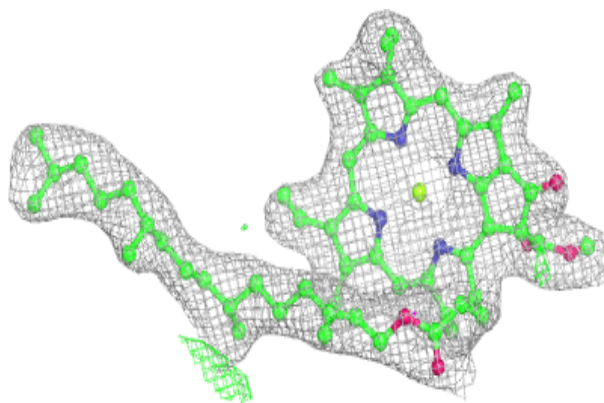
**Electron density around BCR k 101:**

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

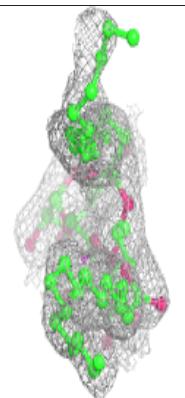
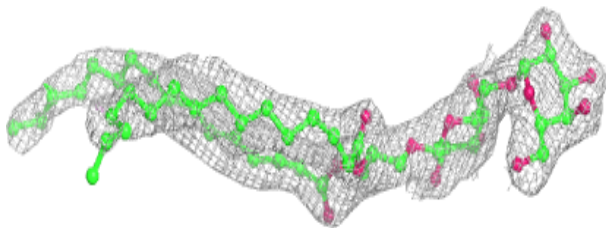
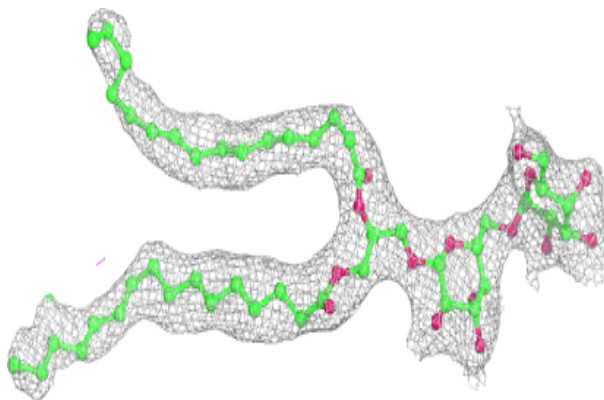


**Electron density around CLA c 503:**

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

**Electron density around DGD c 520:**

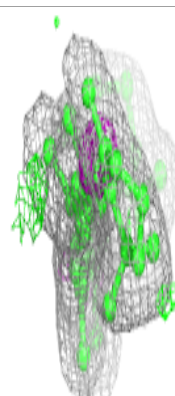
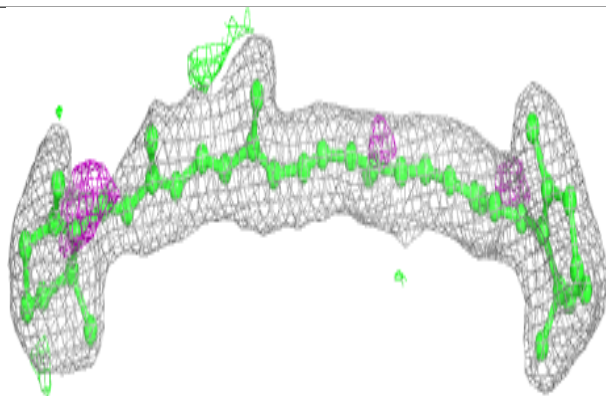
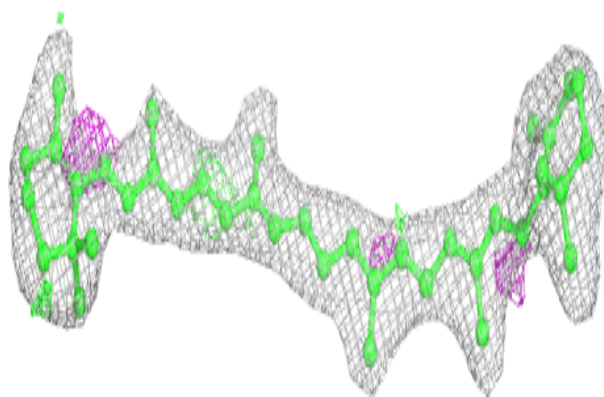
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



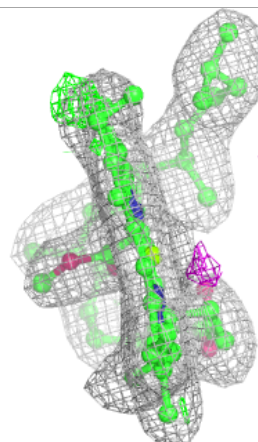
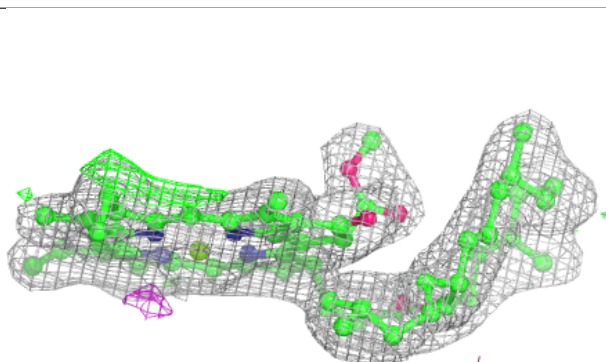
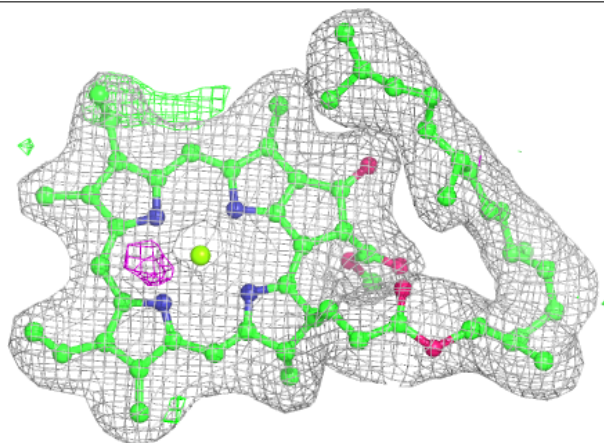


**Electron density around BCR T 101:**

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

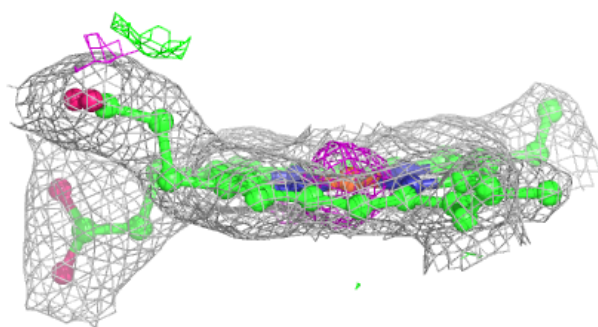
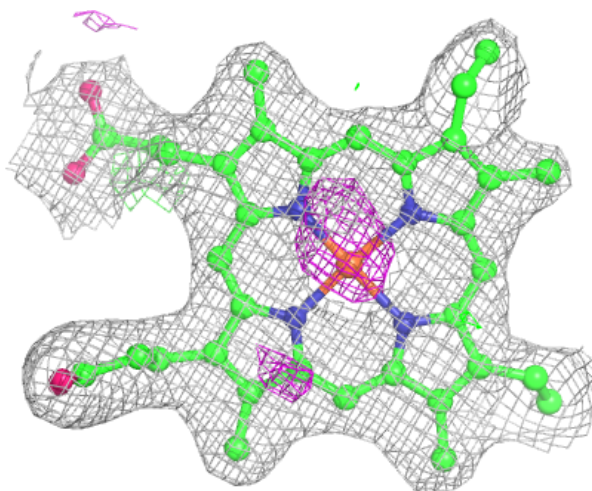
**Electron density around CLA B 610:**

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



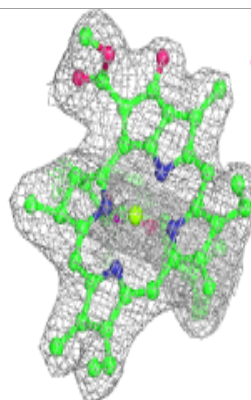
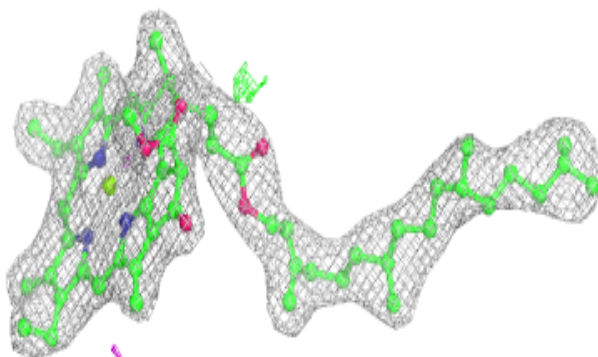
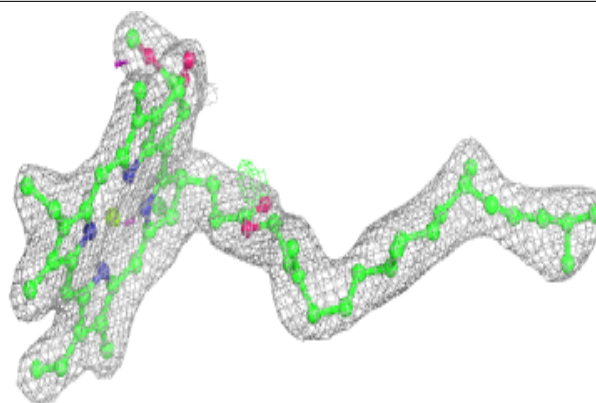
**Electron density around HEC V 203:**

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

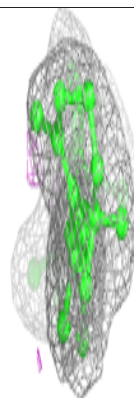
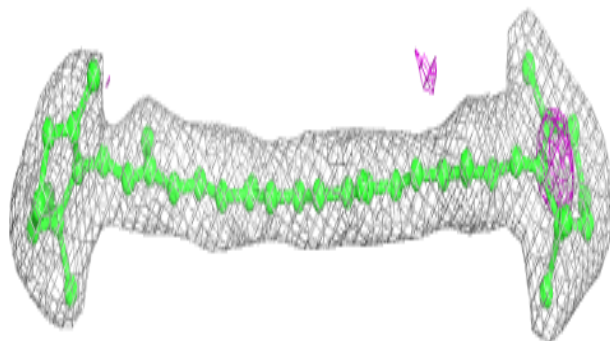
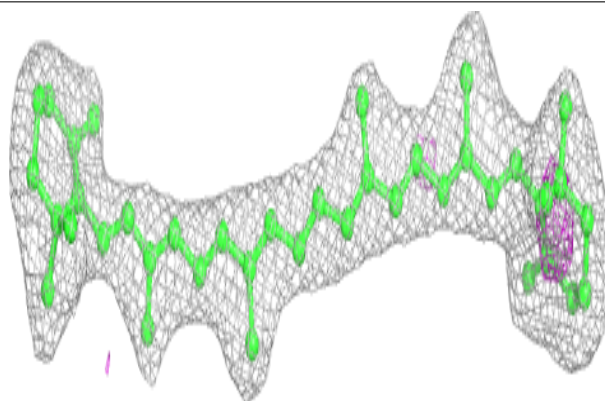


**Electron density around CLA C 503:**

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

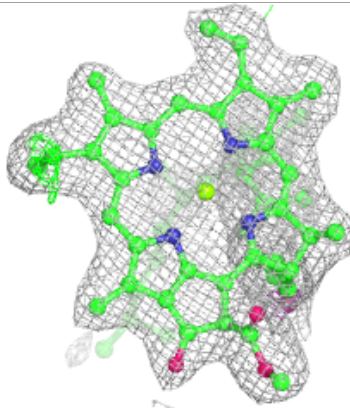
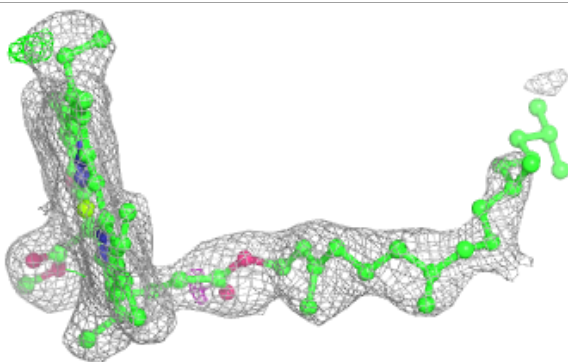
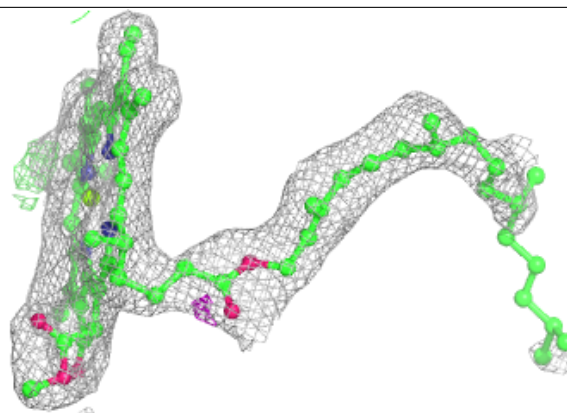
**Electron density around BCR b 618:**

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

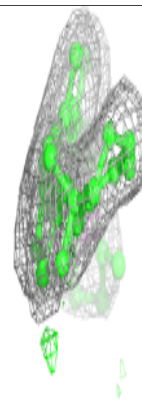
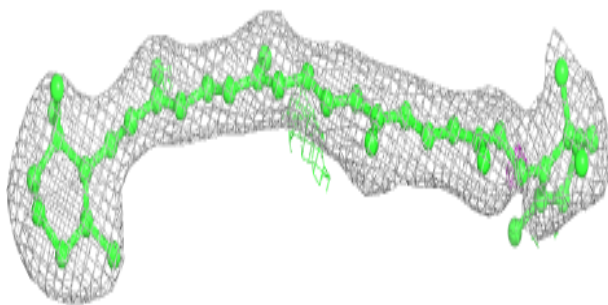
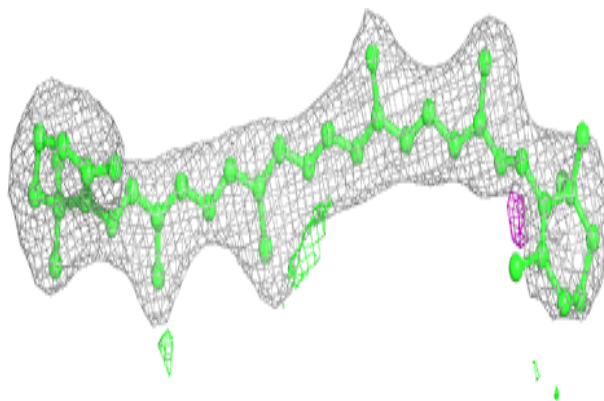


**Electron density around CLA D 403:**

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

**Electron density around BCR d 404:**

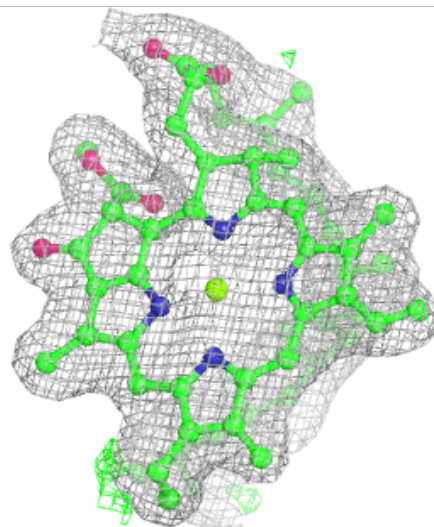
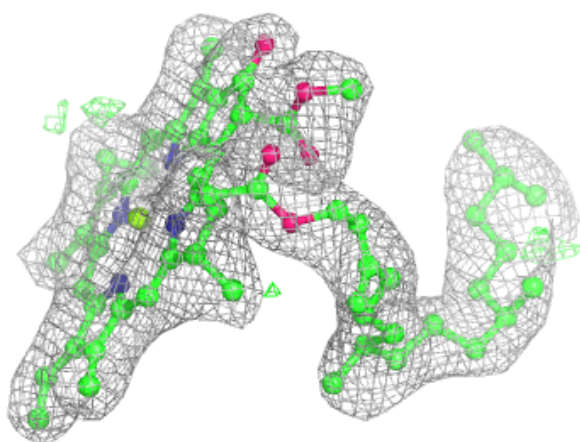
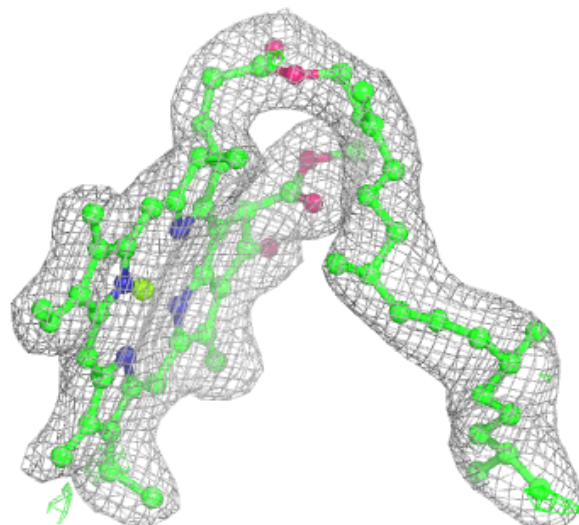
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





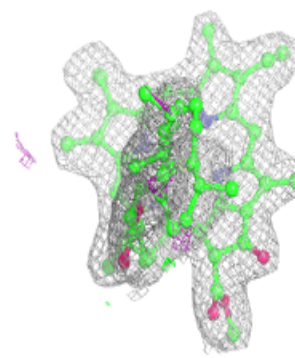
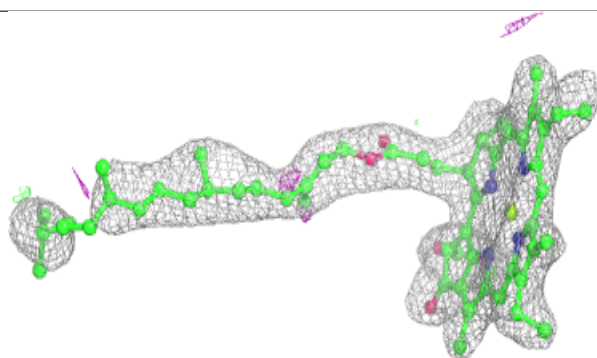
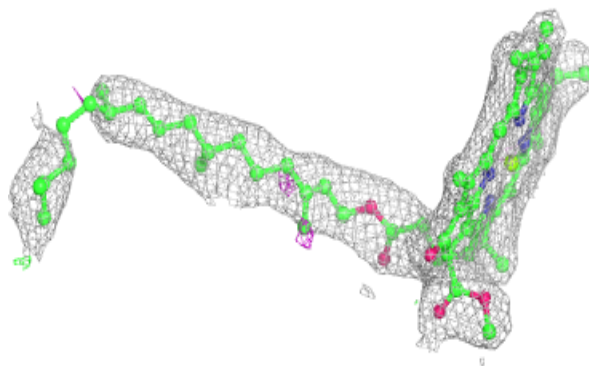
**Electron density around CLA b 613:**

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

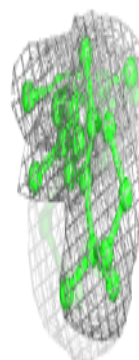
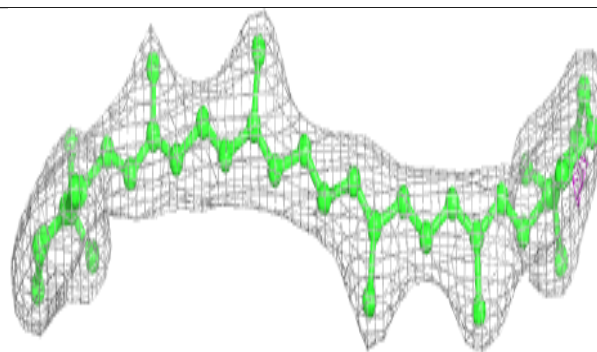
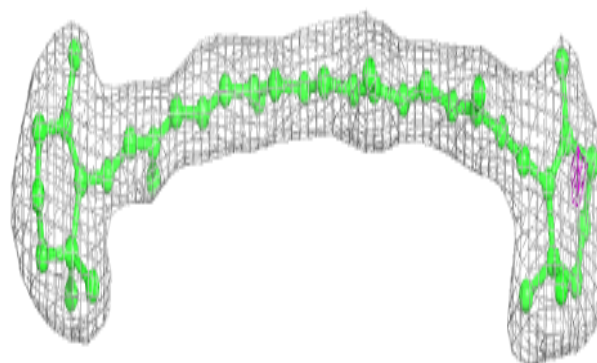


**Electron density around CLA b 604:**

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

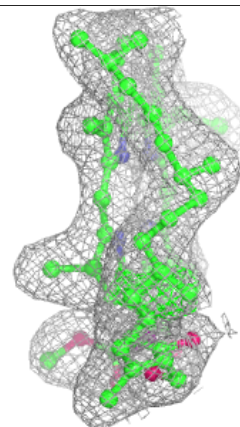
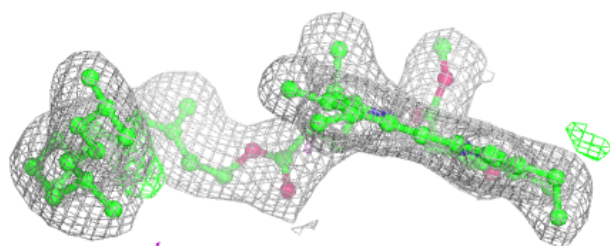
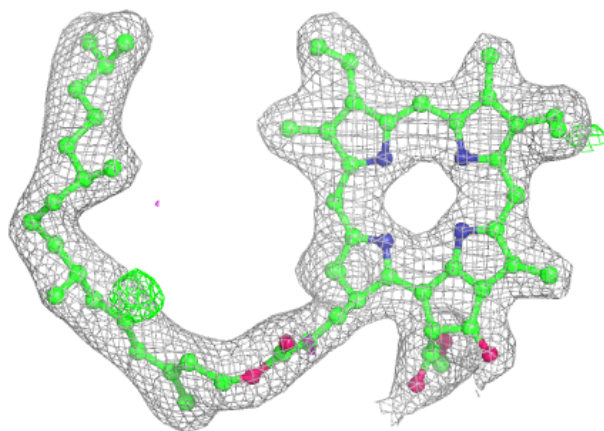
**Electron density around BCR K 102:**

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

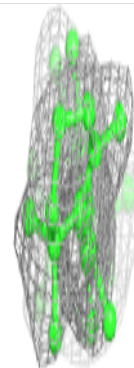
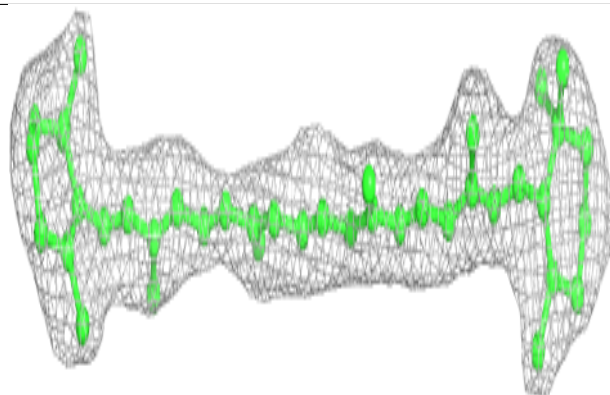
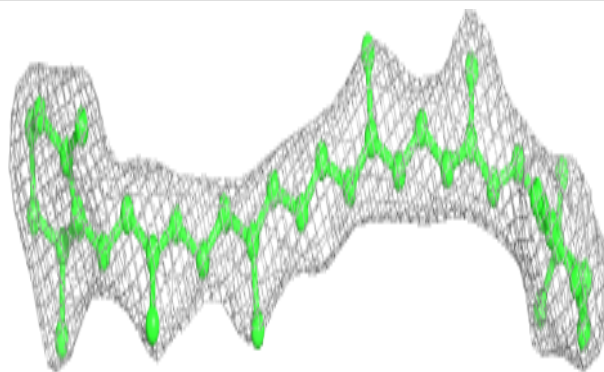


**Electron density around PHO A 407:**

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

**Electron density around BCR C 515:**

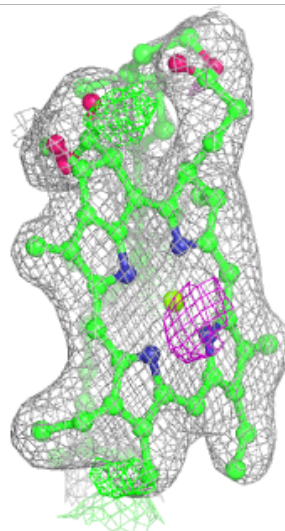
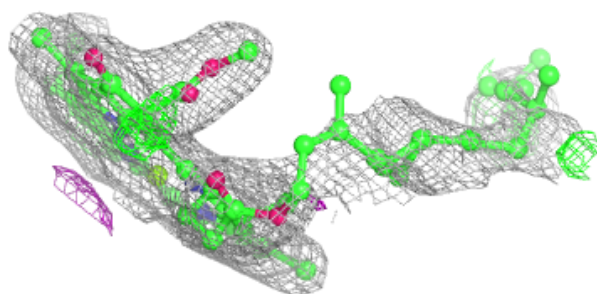
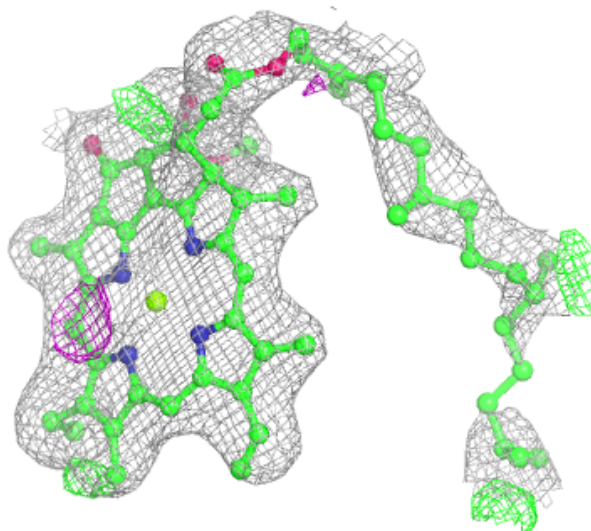
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





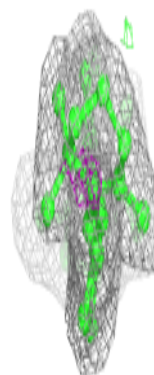
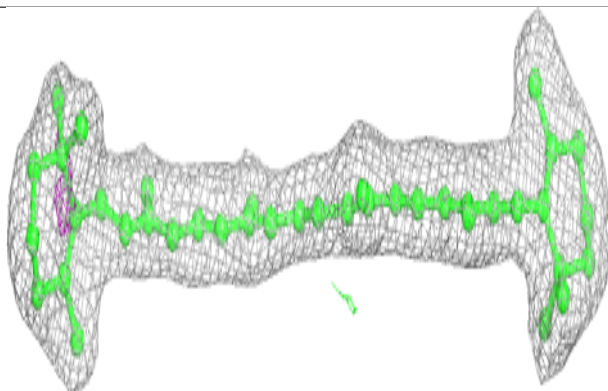
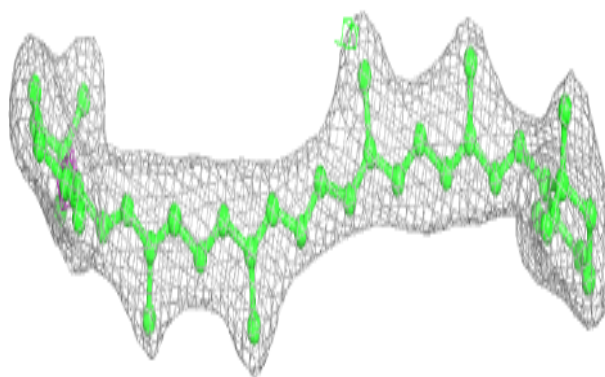
**Electron density around CLA B 616:**

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



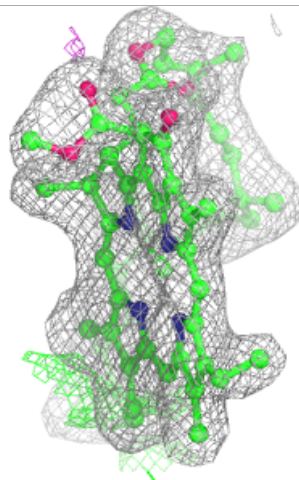
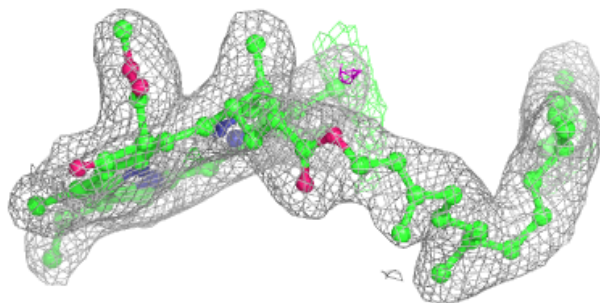
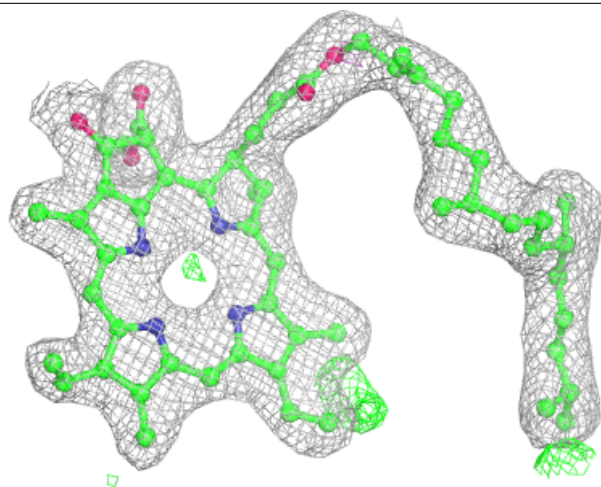
**Electron density around BCR a 408:**

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



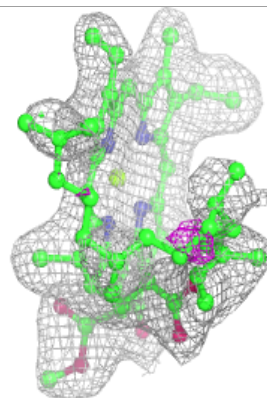
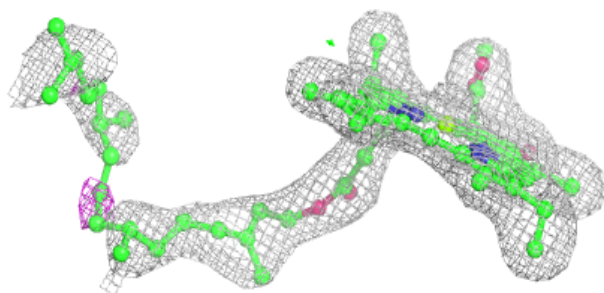
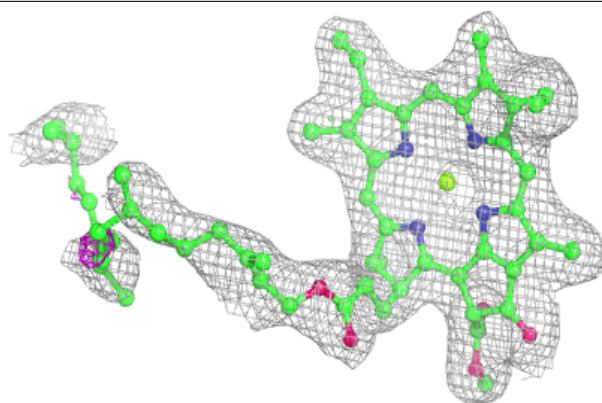
**Electron density around PHO A 408:**

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

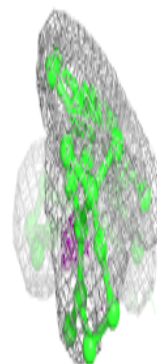
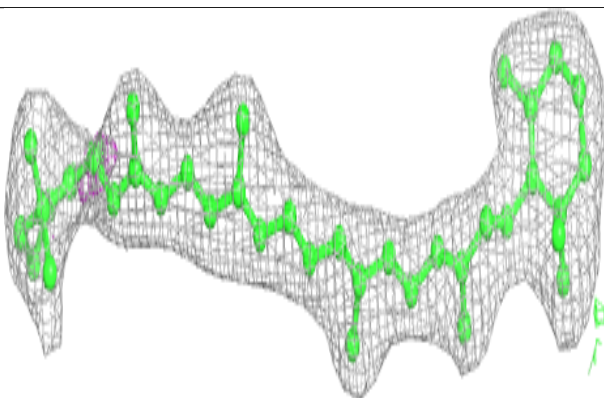
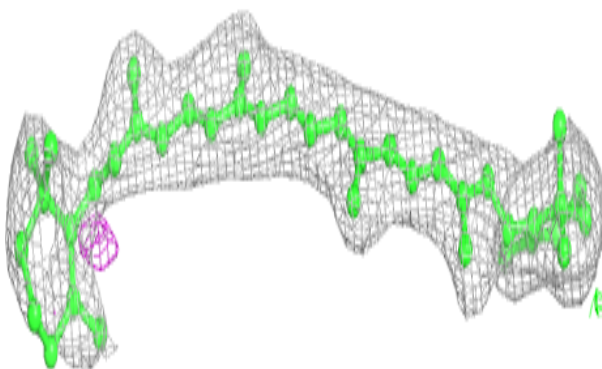


**Electron density around CLA A 409:**

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

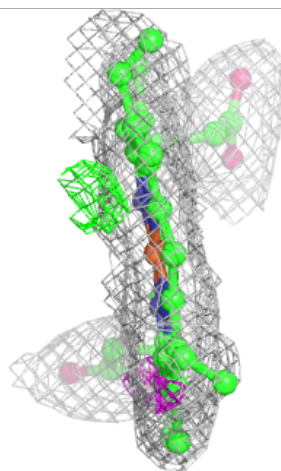
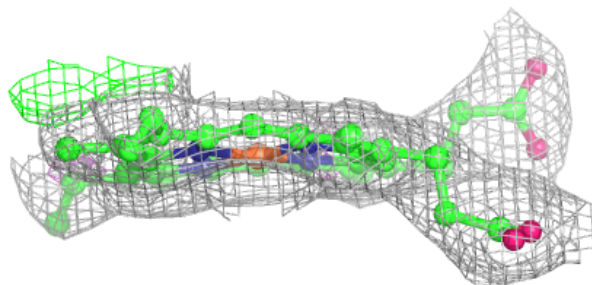
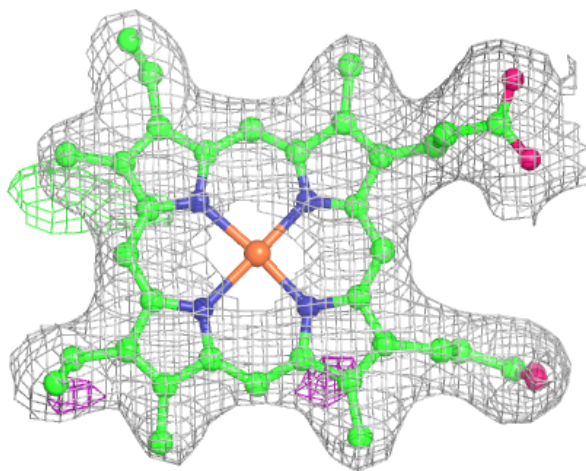
**Electron density around BCR D 404:**

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



**Electron density around HEC v 203:**

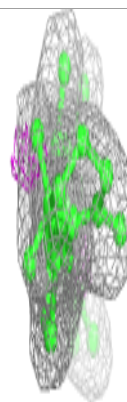
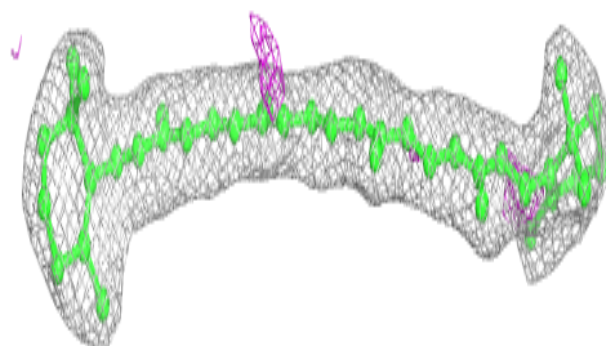
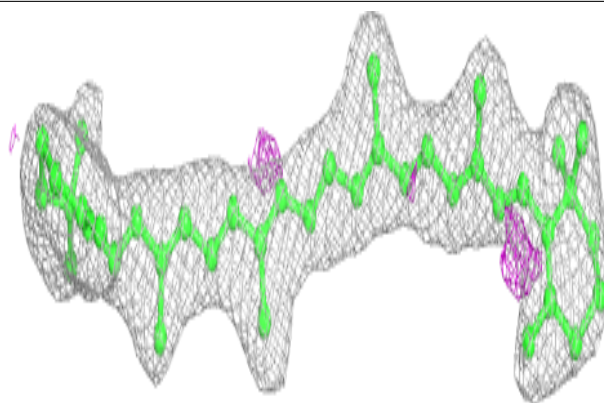
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



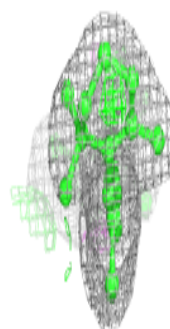
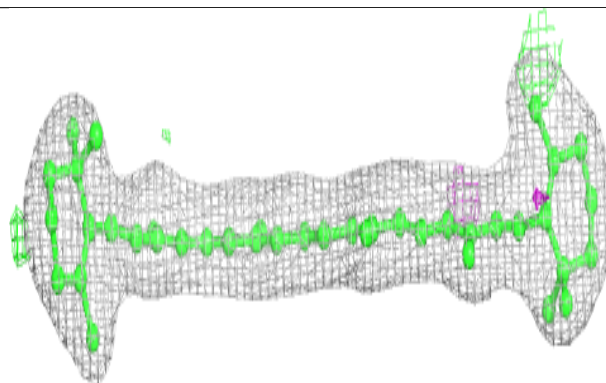
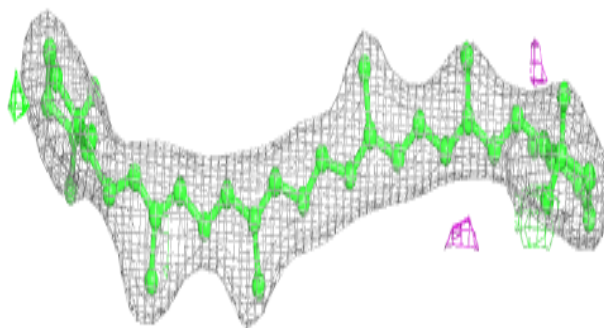


**Electron density around BCR b 617:**

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

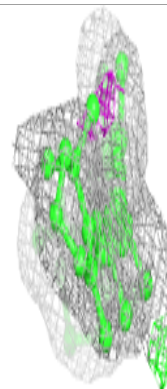
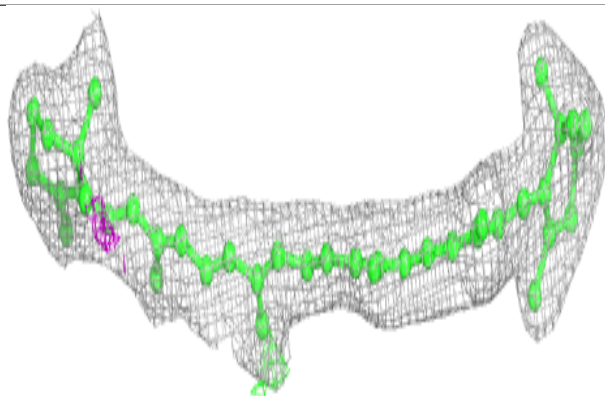
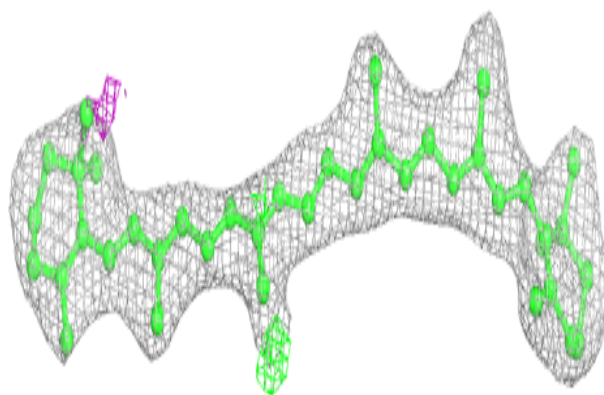
**Electron density around BCR C 516:**

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

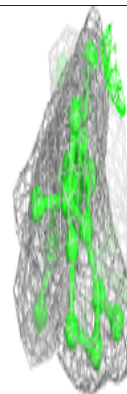
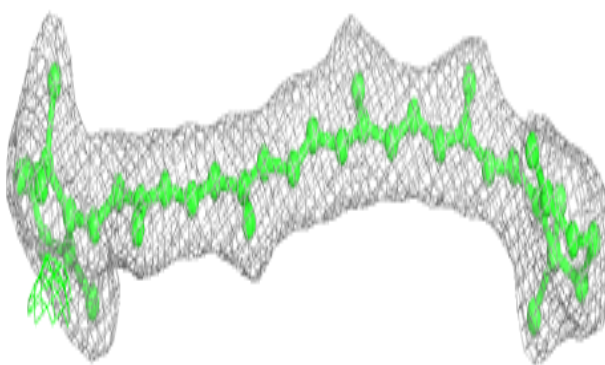
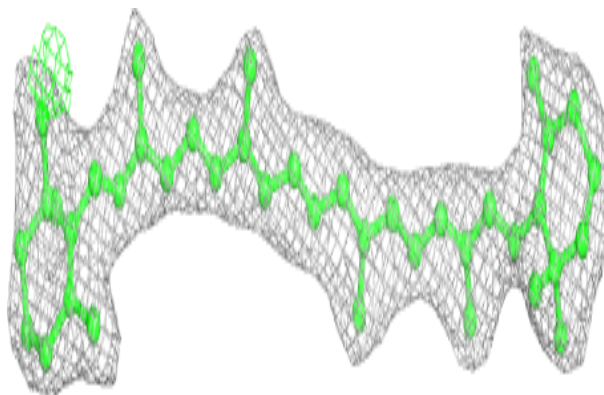


**Electron density around BCR t 102:**

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

**Electron density around BCR b 619:**

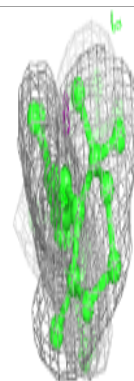
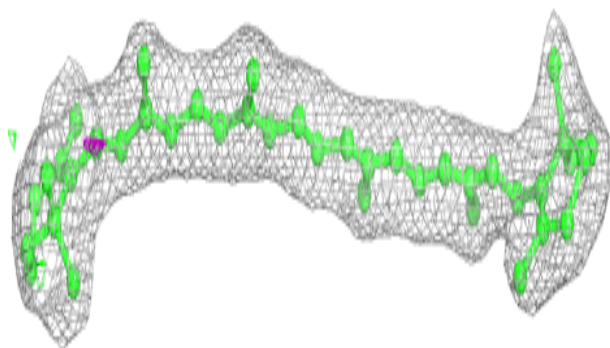
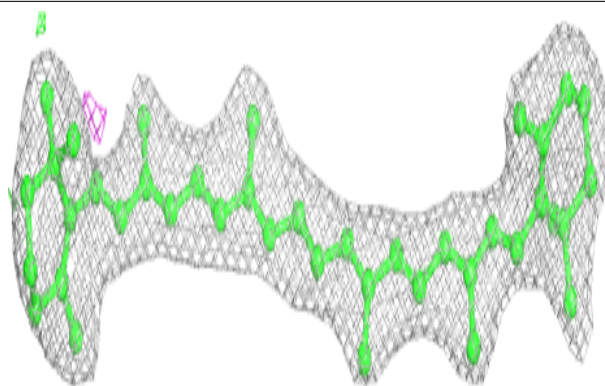
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





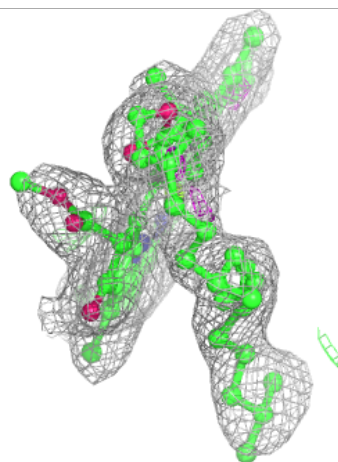
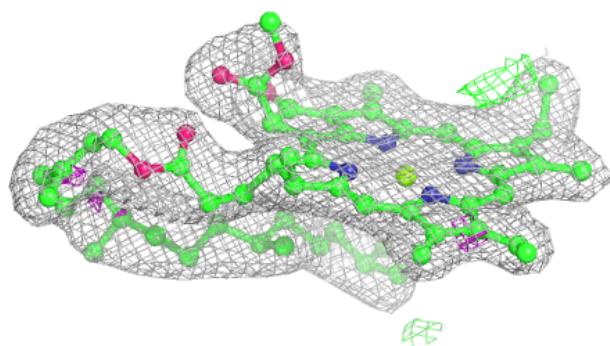
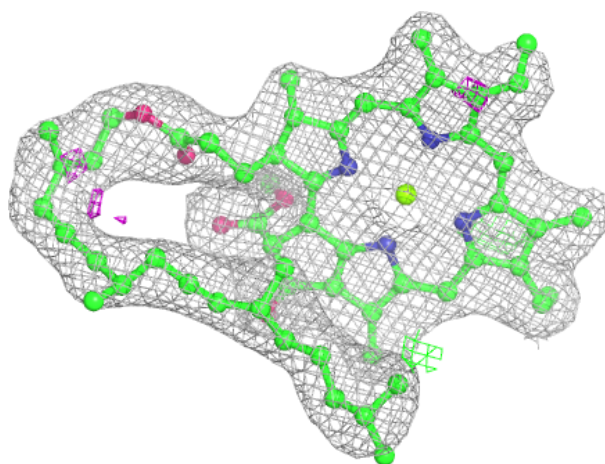
**Electron density around BCR B 619:**

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



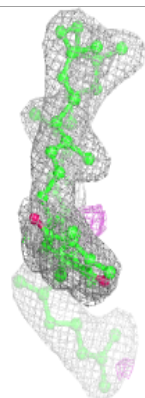
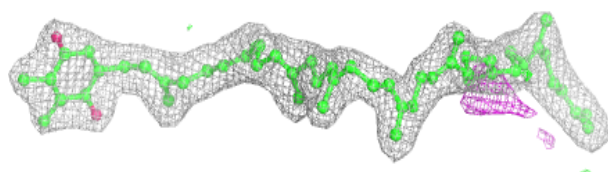
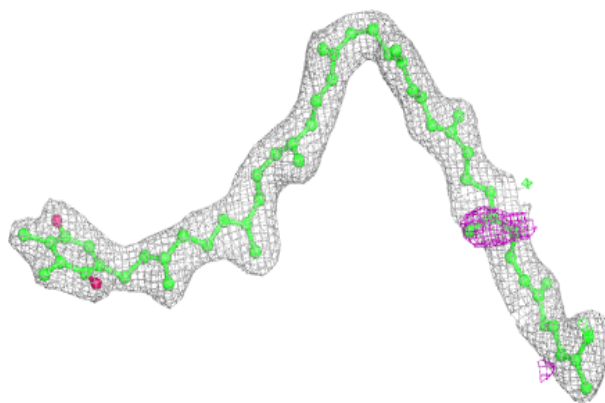
**Electron density around CLA C 510:**

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

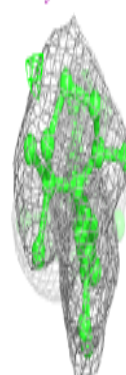
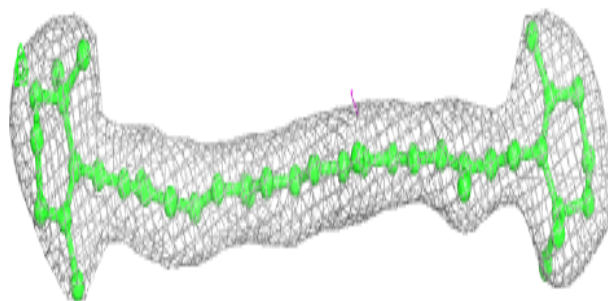
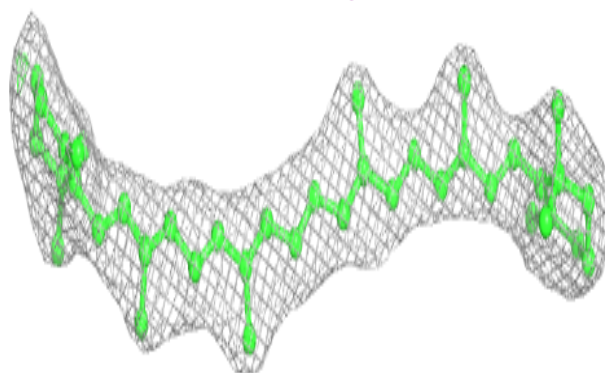


**Electron density around PL9 d 405:**

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

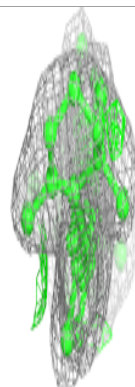
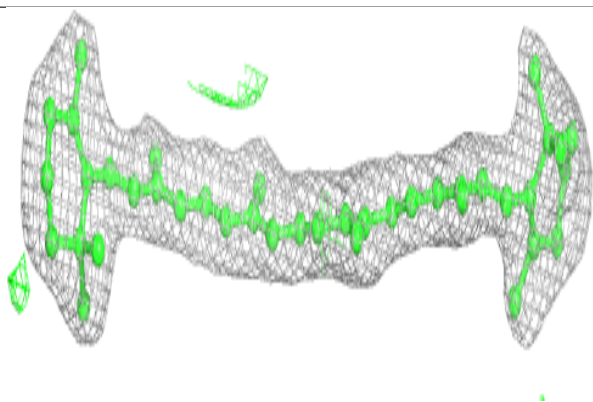
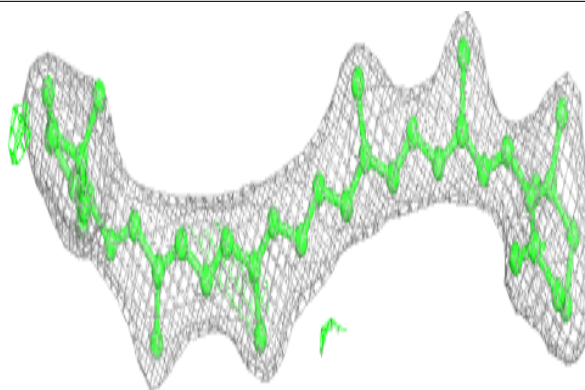
**Electron density around BCR c 517:**

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

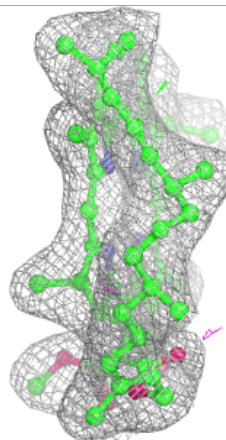
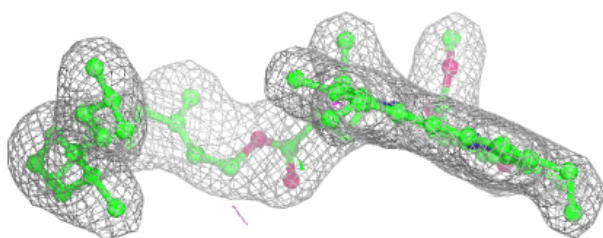
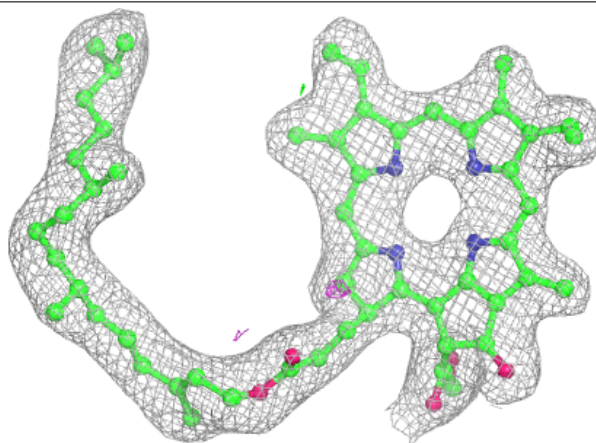


**Electron density around BCR Y 101:**

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

**Electron density around PHO a 405:**

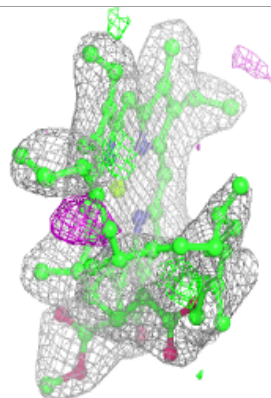
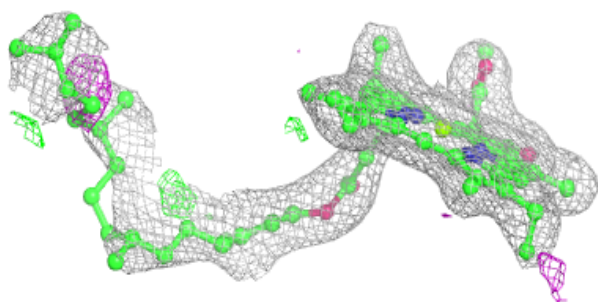
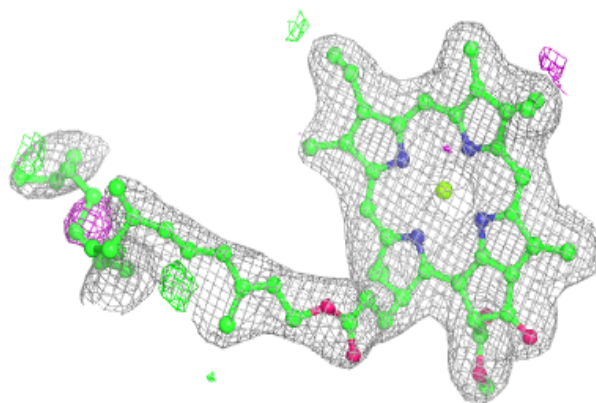
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



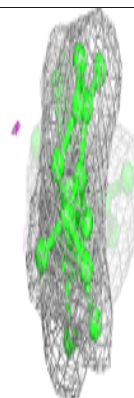
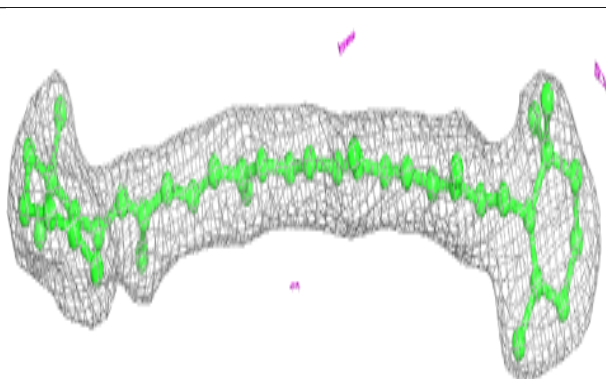
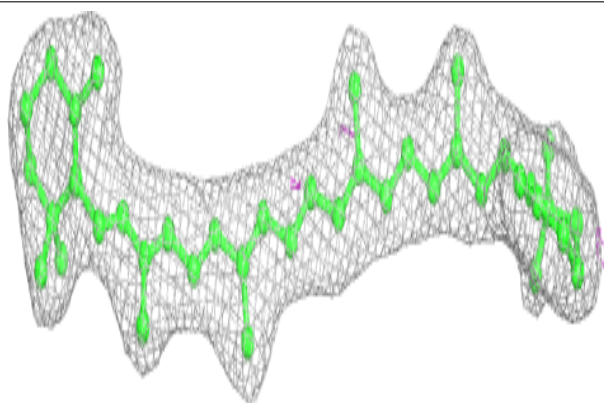


**Electron density around CLA a 407:**

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

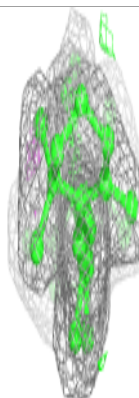
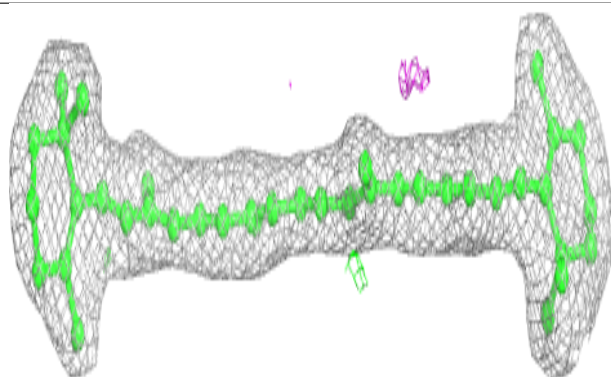
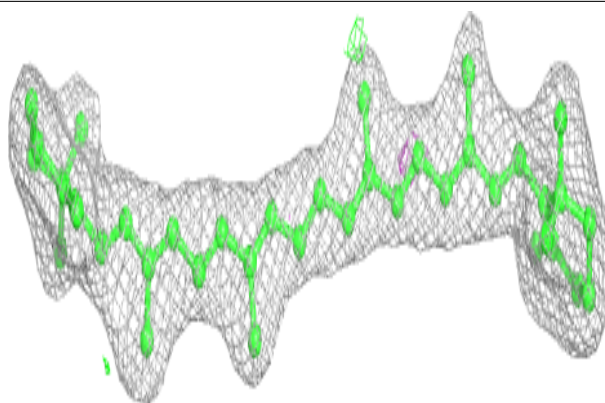
**Electron density around BCR B 617:**

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

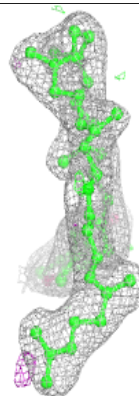
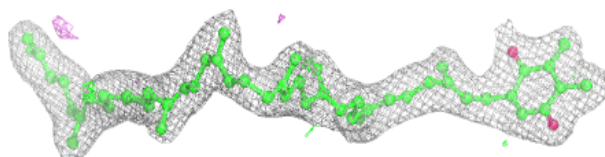
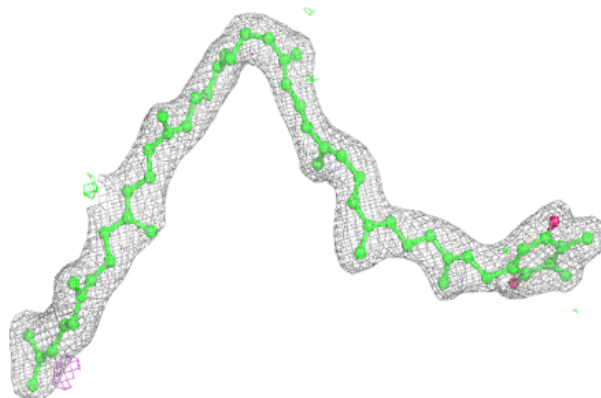


**Electron density around BCR A 410:**

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

**Electron density around PL9 D 405:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.