



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2024 – 06:18 PM JST

PDB ID : 5GTI  
Title : Native XFEL structure of photosystem II (two flash dataset)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2016-08-20  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

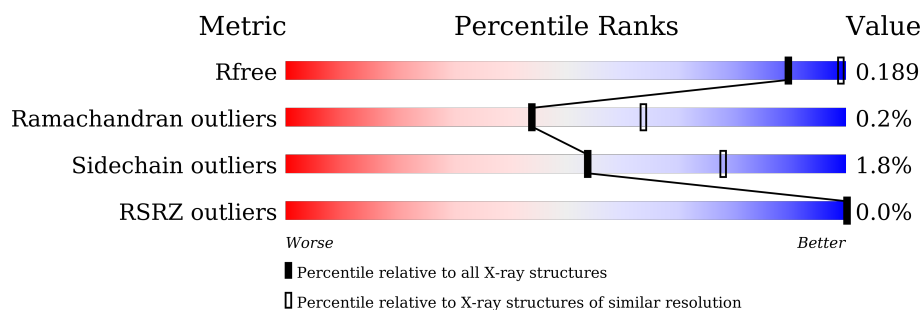
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5504 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	97% .
1	a	344	97% . .
2	B	505	98% .
2	b	505	97% .
3	C	455	98% .
3	c	455	98% .
4	D	342	100%

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Mol	Chain	Length	Quality of chain
4	d	342	99%
5	E	84	95% . .
5	e	84	90% . 6%
6	F	44	77% 23%
6	f	44	68% . 30%
7	H	65	2% 94% 5% .
7	h	65	97% .
8	I	38	95% 5%
8	i	38	92% 5% .
9	J	39	92% 5% .
9	j	39	100%
10	K	37	92% 8%
10	k	37	92% 8%
11	L	37	97% .
11	l	37	97% .
12	M	36	89% . 8%
12	m	36	89% 6% 6%
13	O	244	98% .
13	o	244	98% .
14	T	32	91% . 6%
14	t	32	88% 6% 6%
15	U	104	91% . 8%
15	u	104	91% . 7%
16	V	137	100%
16	v	137	100%

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Mol	Chain	Length	Quality of chain
17	X	40	 92% 5%
17	x	40	 95% 5%
18	Y	30	 97% .
18	y	30	 93% . .
19	Z	62	 94% 6%
19	z	62	 92% 8%
20	R	34	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52752 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	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			

- 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	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	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	0	0
			2726	1805	445	464	12			
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	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	0	0
			662	432	107	123			
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	0	0
			506	339	81	84	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	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 PsbK protein.

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	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

- Molecule 12 is a protein called Photosystem II PsbM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			260	173	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	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

- 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	0
			1	1		

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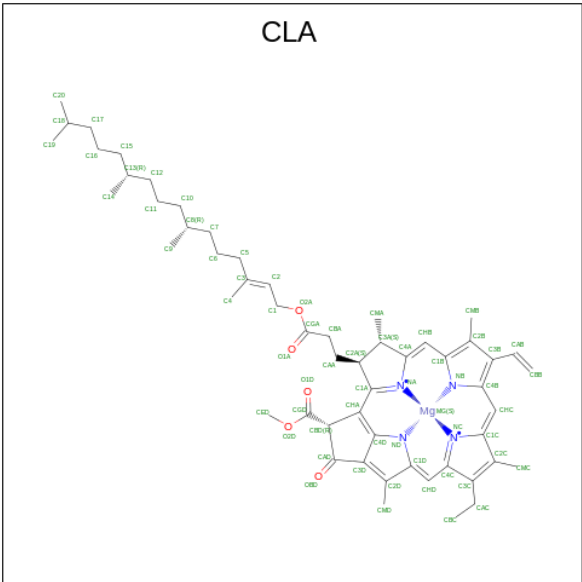
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

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

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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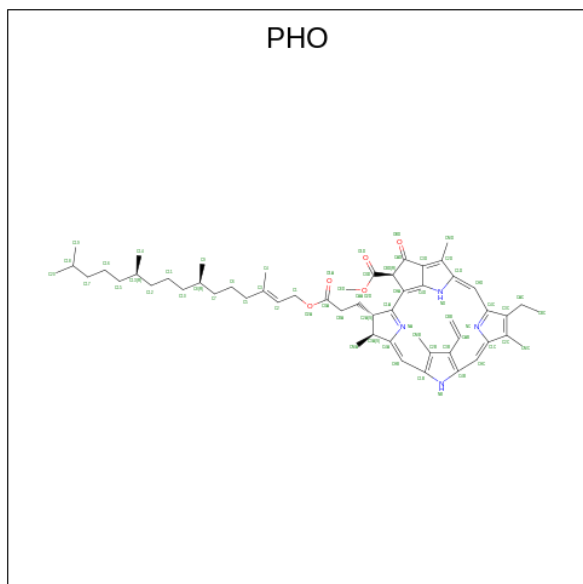
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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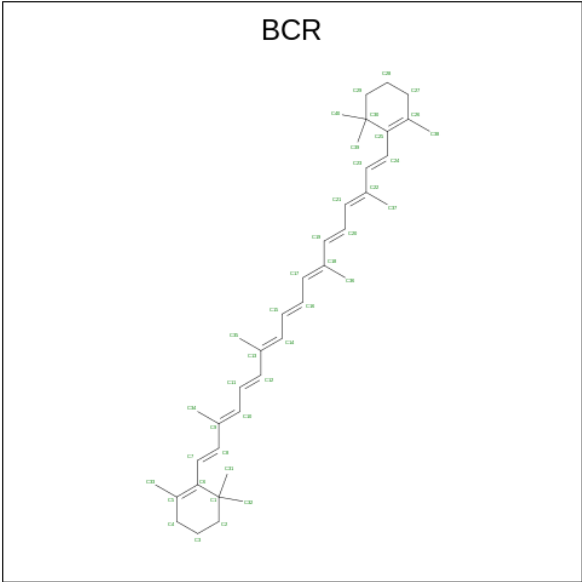
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



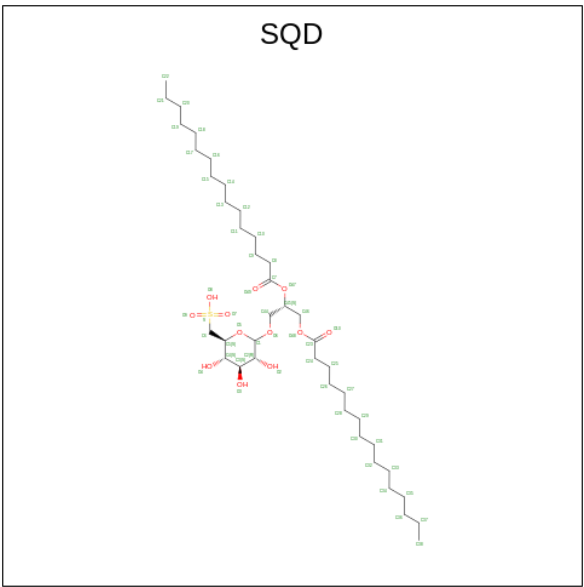
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



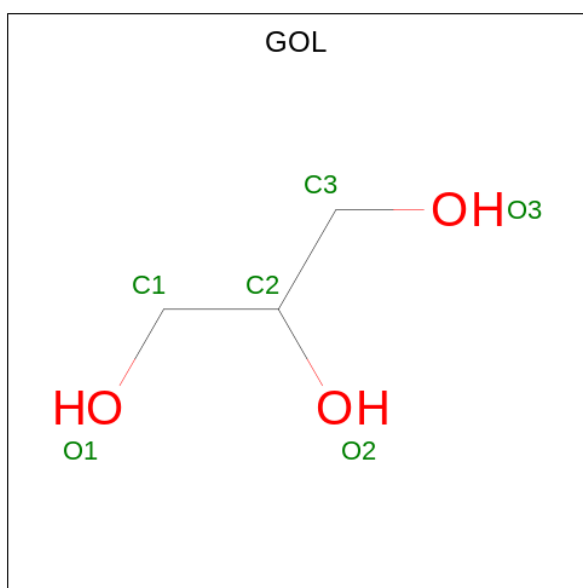
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



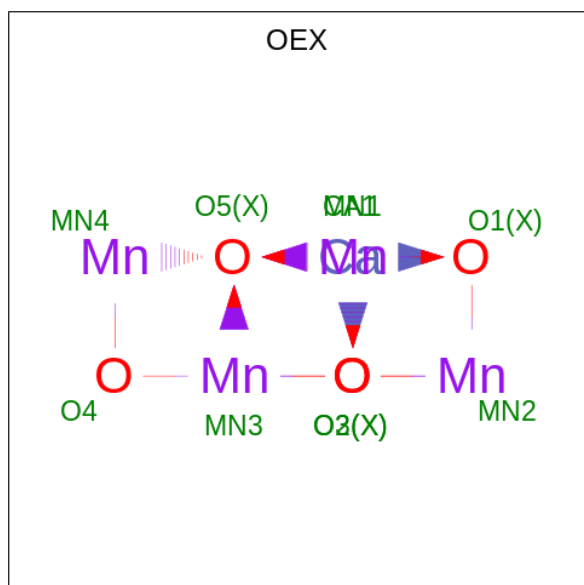
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	b	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		

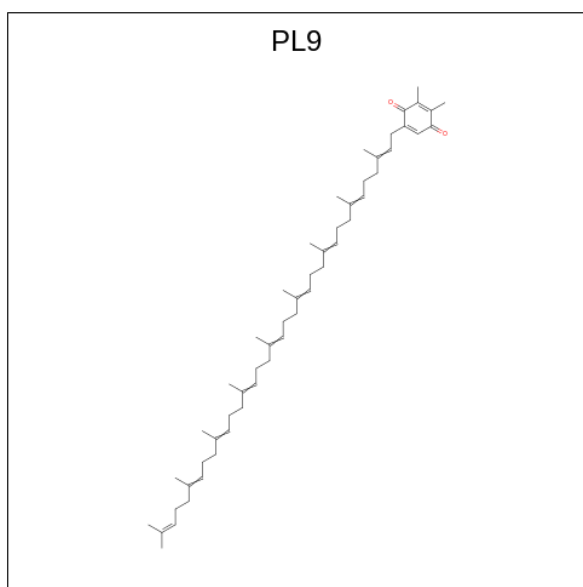
- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 29 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:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

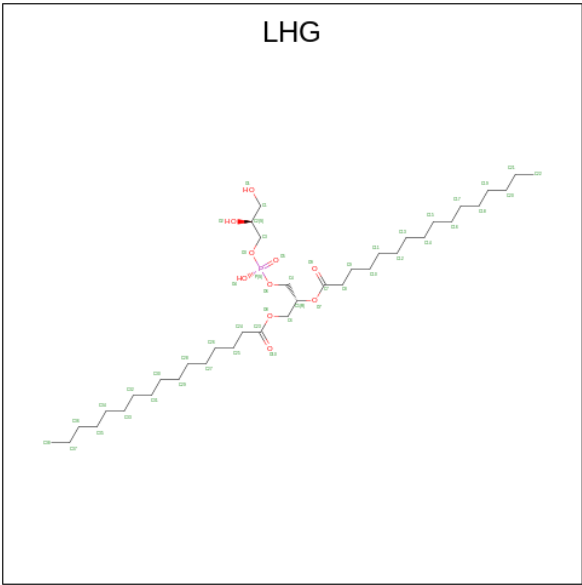
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	2	Total	C	O	0	0
			69	59	10		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	1	Total	C	O	0	0
			17	16	1		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



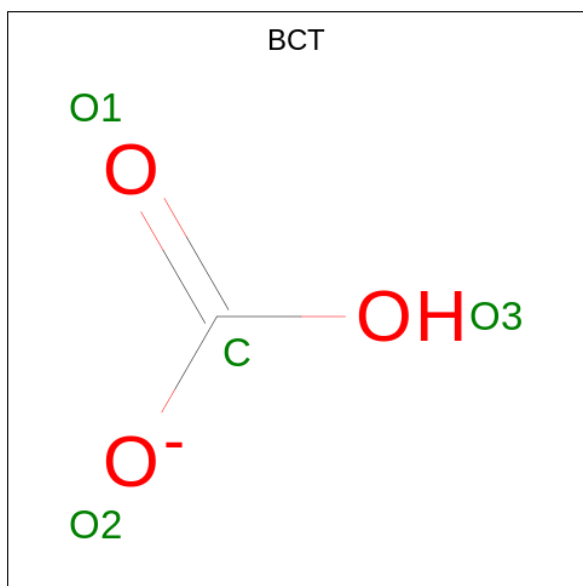
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	b	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).

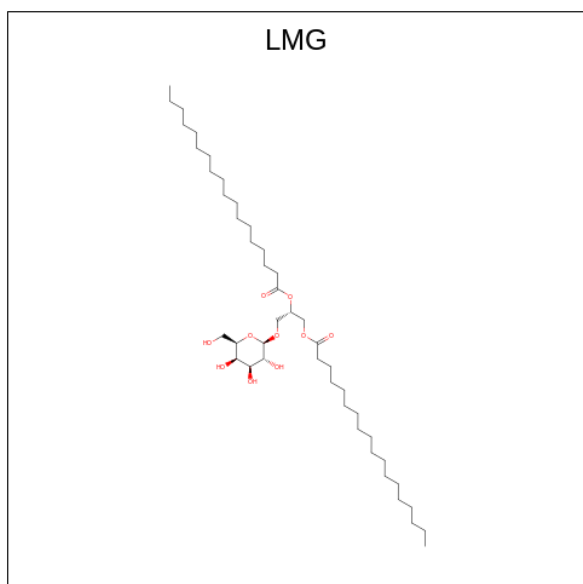


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		
33	C	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	V	1	Total	Ca	0	0
			1	1		
33	c	2	Total	Ca	0	0
			2	2		
33	o	1	Total	Ca	0	0
			1	1		

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



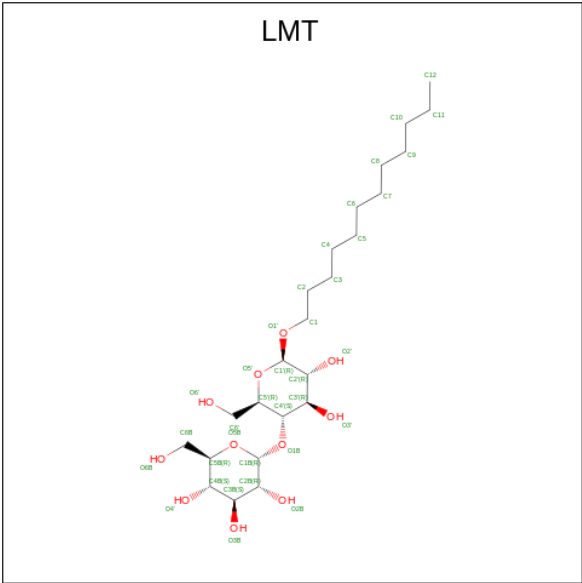
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



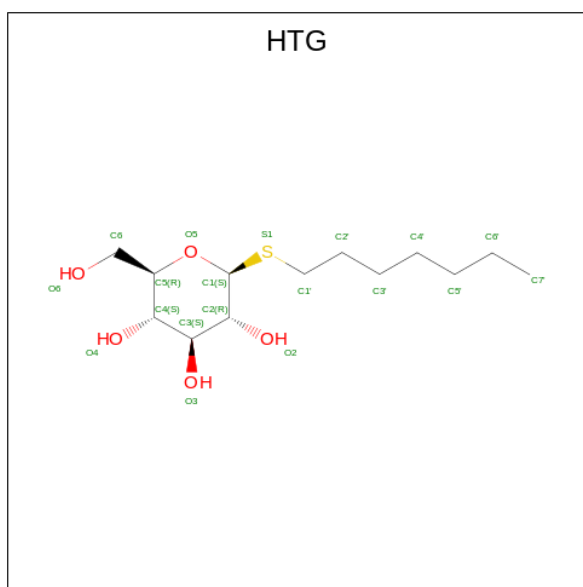
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			25	19	6		
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			26	19	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			35	24	11		
35	D	1	Total	C	O	0	0
			35	24	11		
35	E	1	Total	C	O	0	0
			35	24	11		
35	M	1	Total	C	O	0	0
			35	24	11		
35	M	1	Total	C	O	0	0
			35	24	11		
35	a	1	Total	C	O	0	0
			35	24	11		
35	b	1	Total	C	O	0	0
			25	19	6		
35	b	1	Total	C	O	0	0
			25	19	6		
35	e	1	Total	C	O	0	0
			35	24	11		
35	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



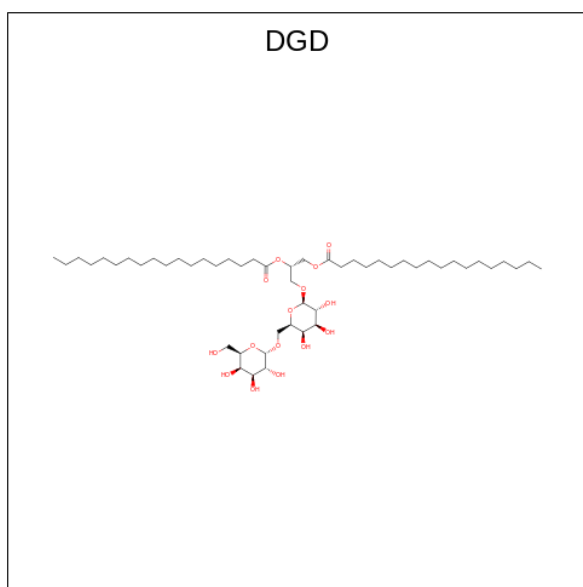
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	S		0	0
			9	8	1			
36	D	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O		0	0
			11	6	5			
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).

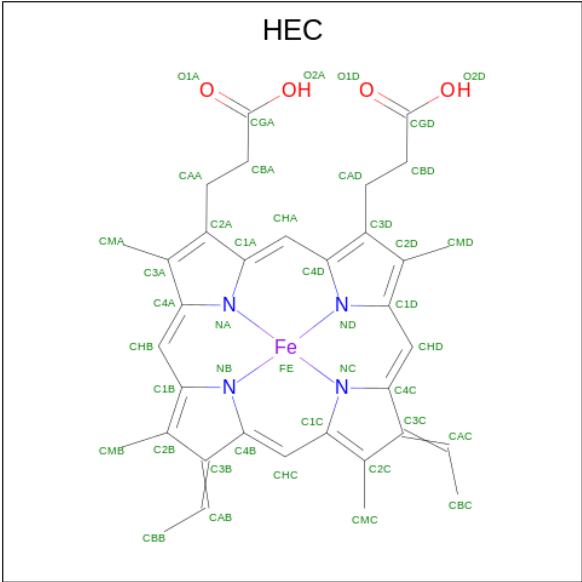


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	h	1	Total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

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).







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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	135	Total	O	0	0
			135	135		
41	B	195	Total	O	0	0
			195	195		
41	C	151	Total	O	0	0
			151	151		
41	D	118	Total	O	0	0
			118	118		
41	E	25	Total	O	0	0
			25	25		
41	F	5	Total	O	0	0
			5	5		
41	H	22	Total	O	0	0
			22	22		
41	I	6	Total	O	0	0
			6	6		
41	J	4	Total	O	0	0
			4	4		
41	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	6	Total 6	O 6	0	0
41	M	15	Total 15	O 15	0	0
41	O	105	Total 105	O 105	0	0
41	T	13	Total 13	O 13	0	0
41	U	51	Total 51	O 51	0	0
41	V	81	Total 81	O 81	0	0
41	X	4	Total 4	O 4	0	0
41	Y	1	Total 1	O 1	0	0
41	Z	1	Total 1	O 1	0	0
41	R	1	Total 1	O 1	0	0
41	a	132	Total 132	O 132	0	0
41	b	206	Total 206	O 206	0	0
41	c	153	Total 153	O 153	0	0
41	d	115	Total 115	O 115	0	0
41	e	16	Total 16	O 16	0	0
41	f	5	Total 5	O 5	0	0
41	h	27	Total 27	O 27	0	0
41	i	3	Total 3	O 3	0	0
41	j	3	Total 3	O 3	0	0
41	k	6	Total 6	O 6	0	0
41	l	9	Total 9	O 9	0	0

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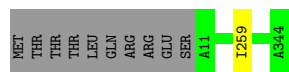
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	m	18	Total 18	O 18	0	0
41	o	115	Total 115	O 115	0	0
41	t	9	Total 9	O 9	0	0
41	u	62	Total 62	O 62	0	0
41	v	78	Total 78	O 78	0	0
41	x	8	Total 8	O 8	0	0
41	z	1	Total 1	O 1	0	0

### 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.

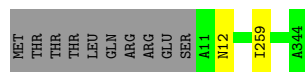
- Molecule 1: Photosystem II D1 protein

Chain A:  97%



- Molecule 1: Photosystem II D1 protein

Chain a:  97%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  98%



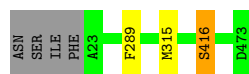
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  97%



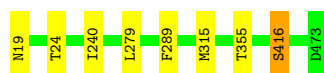
- Molecule 3: Photosystem II CP43 protein

Chain C:  98%



- Molecule 3: Photosystem II CP43 protein

Chain c:  98%



- Molecule 4: Photosystem II D2 protein

Chain D: 100%



- Molecule 4: Photosystem II D2 protein

Chain d: 99%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 95%



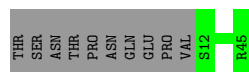
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 90%



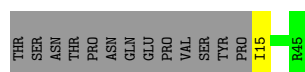
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 77%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 68%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 94%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 97% .



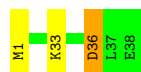
- Molecule 8: Photosystem II reaction center protein I

Chain I: 95% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain i: 92% 5% .



- Molecule 9: Photosystem II reaction center protein J

Chain J: 92% 5% .



- Molecule 9: Photosystem II reaction center protein J

Chain j: 100%

There are no outlier residues recorded for this chain.

- Molecule 10: Photosystem II PsbK protein

Chain K: 92% 8%



- Molecule 10: Photosystem II PsbK protein

Chain k: 92% 8%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 97% .



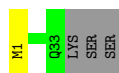
- Molecule 11: Photosystem II reaction center protein L

Chain l: 97% .



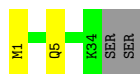
- Molecule 12: Photosystem II PsbM protein

Chain M: 89% . 8%



- Molecule 12: Photosystem II PsbM protein

Chain m: 89% 6% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 98% .



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

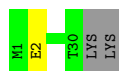
Chain o: 98% .



- Molecule 14: Photosystem II reaction center protein T

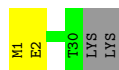
Chain T: 91% . 6%





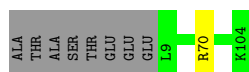
- Molecule 14: Photosystem II reaction center protein T

Chain t: 88% 6% 6%



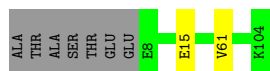
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 91% • 8%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 91% • 7%



- Molecule 16: Cytochrome c-550

Chain V: 100%

There are no outlier residues recorded for this chain.

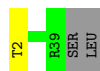
- Molecule 16: Cytochrome c-550

Chain v: 100%

There are no outlier residues recorded for this chain.

- Molecule 17: Photosystem II reaction center protein X

Chain X: 92% • 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x: 95% 5%



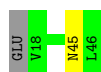
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  97% .



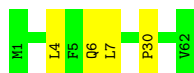
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  93% . .



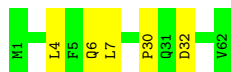
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  94% 6%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  92% 8%



- Molecule 20: Photosystem II protein Y

Chain R:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 99.7 (19.98-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.139 , 0.187 0.142 , 0.189	Depositor DCC
$R_{free}$ test set	14585 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	52752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.44	0/2705	0.56	0/3689
1	a	0.43	0/2705	0.54	0/3689
2	B	0.42	0/4109	0.54	0/5600
2	b	0.41	0/4109	0.54	0/5600
3	C	0.39	0/3599	0.51	0/4900
3	c	0.39	0/3633	0.53	0/4946
4	D	0.43	0/2821	0.54	0/3844
4	d	0.43	0/2812	0.54	0/3832
5	E	0.35	0/681	0.53	0/928
5	e	0.37	0/667	0.49	0/908
6	F	0.34	0/284	0.48	0/387
6	f	0.40	0/257	0.49	0/349
7	H	0.36	0/519	0.53	0/708
7	h	0.35	0/524	0.49	0/713
8	I	0.37	0/311	0.51	0/419
8	i	0.36	0/311	0.54	0/419
9	J	0.36	0/278	0.46	0/376
9	j	0.35	0/283	0.47	0/383
10	K	0.35	0/303	0.53	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.42	0/303	0.51	0/412
11	l	0.38	0/303	0.53	0/412
12	M	0.44	0/253	0.58	0/346
12	m	0.42	0/262	0.58	0/357
13	O	0.38	0/1896	0.58	0/2571
13	o	0.39	0/1896	0.58	0/2571
14	T	0.54	0/257	0.56	0/349
14	t	0.52	0/257	0.52	0/349
15	U	0.40	0/776	0.57	0/1052
15	u	0.41	0/785	0.57	0/1064
16	V	0.37	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.37	0/1085	0.53	0/1473
17	X	0.33	0/284	0.49	0/384
17	x	0.31	0/284	0.46	0/384
18	Y	0.30	0/216	0.44	0/289
18	y	0.31	0/216	0.50	0/289
19	Z	0.32	0/490	0.46	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.27	0/279	0.43	0/383
All	All	0.40	0/42631	0.53	0/58018

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	37	56
1	a	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	37	56
2	B	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
2	b	502/505 (99%)	494 (98%)	8 (2%)	0	100	100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	44	64
3	c	453/455 (100%)	442 (98%)	10 (2%)	1 (0%)	44	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (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	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	6
9	J	36/39 (92%)	36 (100%)	0	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	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
13	o	241/244 (99%)	232 (96%)	9 (4%)	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%)	89 (95%)	5 (5%)	0	100	100
15	u	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	2	3
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	7	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	14
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5212/5384 (97%)	5097 (98%)	107 (2%)	8 (0%)	44	64

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416	SER
3	c	416	SER
19	Z	30	PRO
1	a	259	ILE

### 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	269/279 (96%)	269 (100%)	0	100	100
1	a	269/279 (96%)	268 (100%)	1 (0%)	89	96
2	B	402/403 (100%)	395 (98%)	7 (2%)	56	79
2	b	402/403 (100%)	390 (97%)	12 (3%)	36	63
3	C	352/356 (99%)	349 (99%)	3 (1%)	75	90
3	c	356/356 (100%)	348 (98%)	8 (2%)	47	73
4	D	277/277 (100%)	276 (100%)	1 (0%)	89	96
4	d	276/277 (100%)	275 (100%)	1 (0%)	89	96
5	E	72/73 (99%)	71 (99%)	1 (1%)	62	83
5	e	70/73 (96%)	67 (96%)	3 (4%)	25	48
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	27	51
7	H	54/54 (100%)	51 (94%)	3 (6%)	17	36
7	h	54/54 (100%)	52 (96%)	2 (4%)	29	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	64
8	i	34/34 (100%)	32 (94%)	2 (6%)	16	33
9	J	26/27 (96%)	24 (92%)	2 (8%)	10	22
9	j	26/27 (96%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	6	13
10	k	30/30 (100%)	27 (90%)	3 (10%)	6	13
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	59
13	O	206/207 (100%)	201 (98%)	5 (2%)	44	70
13	o	206/207 (100%)	203 (98%)	3 (2%)	60	82
14	T	26/28 (93%)	25 (96%)	1 (4%)	28	53
14	t	26/28 (93%)	25 (96%)	1 (4%)	28	53
15	U	83/89 (93%)	82 (99%)	1 (1%)	67	86
15	u	84/89 (94%)	82 (98%)	2 (2%)	44	70
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	117 (100%)	0	100	100
17	X	31/33 (94%)	30 (97%)	1 (3%)	34	60
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	22 (100%)	0	100	100
19	Z	52/52 (100%)	49 (94%)	3 (6%)	17	34
19	z	52/52 (100%)	48 (92%)	4 (8%)	10	22
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4317/4403 (98%)	4241 (98%)	76 (2%)	54	78

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	f	15	ILE
15	u	61	VAL
7	h	56	ASP

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Mol	Chain	Res	Type
12	m	5	GLN
19	z	32	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	331	ASN
4	d	142	ASN
19	z	58	ASN
4	d	83	ASN
5	e	60	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	FME	M	1	12	8,9,10	0.55	0	7,9,11	1.35	1 (14%)
14	FME	t	1	14	8,9,10	0.68	0	7,9,11	1.72	2 (28%)
12	FME	m	1	12	8,9,10	0.61	0	7,9,11	1.64	3 (42%)
8	FME	i	1	8	8,9,10	0.61	0	7,9,11	1.26	1 (14%)
14	FME	T	1	14	8,9,10	0.64	0	7,9,11	1.22	0
8	FME	I	1	8	8,9,10	0.64	0	7,9,11	1.00	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	-
14	FME	t	1	14	-	0/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-2.74	118.61	122.82
14	t	1	FME	O-C-CA	-2.68	117.76	124.78
12	M	1	FME	O-C-CA	-2.52	118.17	124.78
12	m	1	FME	CA-N-CN	-2.39	119.15	122.82
8	i	1	FME	O-C-CA	-2.30	118.75	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	O1-CN-N-CA
14	T	1	FME	C-CA-CB-CG
12	m	1	FME	O1-CN-N-CA
12	m	1	FME	CB-CA-N-CN
14	T	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 218 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
31	LHG	D	409	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
23	CLA	c	506	3	65,73,73	2.03	17 (26%)	76,113,113	2.68	28 (36%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.39	6 (10%)
25	BCR	C	527	-	41,41,41	1.01	1 (2%)	56,56,56	1.57	12 (21%)
36	HTG	b	625	-	19,19,19	0.99	2 (10%)	23,24,24	1.48	3 (13%)
23	CLA	B	611	41	65,73,73	2.06	16 (24%)	76,113,113	2.84	29 (38%)
35	LMT	M	101	-	36,36,36	0.56	0	47,47,47	1.10	3 (6%)
36	HTG	B	625	-	19,19,19	0.83	1 (5%)	23,24,24	1.60	1 (4%)
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.50	11 (19%)
23	CLA	C	504	3	65,73,73	2.03	16 (24%)	76,113,113	2.74	24 (31%)
25	BCR	b	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.53	12 (21%)
27	GOL	d	401	-	5,5,5	0.35	0	5,5,5	0.52	0
31	LHG	e	101	-	41,41,48	1.03	2 (4%)	44,47,54	0.94	2 (4%)
37	DGD	C	519	-	63,63,67	0.83	2 (3%)	77,77,81	0.99	4 (5%)
25	BCR	B	619	-	41,41,41	0.97	1 (2%)	56,56,56	1.56	13 (23%)
27	GOL	O	302	-	5,5,5	0.34	0	5,5,5	0.34	0
40	HEC	v	201	16	32,50,50	1.47	4 (12%)	24,82,82	1.53	6 (25%)
23	CLA	b	602	2	65,73,73	2.07	16 (24%)	76,113,113	2.85	32 (42%)
26	SQD	A	409	-	53,54,54	0.98	3 (5%)	62,65,65	1.84	13 (20%)
23	CLA	c	509	3	65,73,73	2.11	17 (26%)	76,113,113	2.76	27 (35%)
37	DGD	c	517	-	63,63,67	0.91	3 (4%)	77,77,81	0.98	4 (5%)
23	CLA	d	403	4	65,73,73	2.06	16 (24%)	76,113,113	2.83	27 (35%)
31	LHG	A	415	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	6 (11%)
23	CLA	b	611	2	65,73,73	2.05	15 (23%)	76,113,113	2.80	27 (35%)
26	SQD	A	411	-	53,54,54	1.03	3 (5%)	62,65,65	1.11	4 (6%)
23	CLA	a	406	41	65,73,73	2.03	13 (20%)	76,113,113	2.83	27 (35%)
23	CLA	b	613	2	65,73,73	2.10	16 (24%)	76,113,113	2.73	28 (36%)
23	CLA	D	401	41	65,73,73	2.05	16 (24%)	76,113,113	2.86	29 (38%)
26	SQD	f	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.53	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	502	3	65,73,73	2.08	15 (23%)	76,113,113	2.77	25 (32%)
31	LHG	b	630	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	2 (3%)
23	CLA	D	404	4	65,73,73	2.06	16 (24%)	76,113,113	2.87	28 (36%)
35	LMT	b	628	-	25,25,36	0.54	1 (4%)	30,30,47	1.21	4 (13%)
23	CLA	A	407	1	65,73,73	2.06	17 (26%)	76,113,113	2.82	26 (34%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.12	4 (8%)
23	CLA	B	612	2	65,73,73	2.05	15 (23%)	76,113,113	2.84	29 (38%)
36	HTG	D	412	-	16,16,19	1.03	2 (12%)	20,21,24	1.40	1 (5%)
23	CLA	a	405	41	65,73,73	2.11	15 (23%)	76,113,113	2.77	30 (39%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.82	17 (30%)
34	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.17	6 (10%)
23	CLA	c	505	3	65,73,73	2.03	16 (24%)	76,113,113	2.69	25 (32%)
25	BCR	H	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.59	11 (19%)
26	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.53	10 (16%)
23	CLA	B	603	2	65,73,73	2.12	17 (26%)	76,113,113	2.74	27 (35%)
34	LMG	c	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.21	7 (11%)
23	CLA	b	616	2	65,73,73	2.08	16 (24%)	76,113,113	2.66	29 (38%)
34	LMG	c	519	-	51,51,55	0.96	3 (5%)	59,59,63	1.05	5 (8%)
23	CLA	b	612	2	65,73,73	2.06	16 (24%)	76,113,113	2.73	27 (35%)
29	PL9	D	407	-	55,55,55	0.67	2 (3%)	68,69,69	1.66	19 (27%)
35	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.84	3 (6%)
23	CLA	B	614	2	65,73,73	2.07	16 (24%)	76,113,113	2.66	27 (35%)
31	LHG	d	408	-	48,48,48	0.96	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	c	504	41	65,73,73	2.10	18 (27%)	76,113,113	2.77	28 (36%)
23	CLA	c	513	3	65,73,73	2.08	17 (26%)	76,113,113	2.86	28 (36%)
27	GOL	B	627	-	5,5,5	0.35	0	5,5,5	0.37	0
23	CLA	c	510	3	65,73,73	2.03	16 (24%)	76,113,113	2.76	32 (42%)
23	CLA	b	615	2	65,73,73	2.00	16 (24%)	76,113,113	2.76	28 (36%)
23	CLA	B	609	2	65,73,73	1.95	16 (24%)	76,113,113	2.77	27 (35%)
23	CLA	C	506	3	65,73,73	2.04	16 (24%)	76,113,113	2.72	27 (35%)
23	CLA	C	513	3	65,73,73	2.06	15 (23%)	76,113,113	2.71	29 (38%)
35	LMT	D	403	-	36,36,36	0.57	1 (2%)	47,47,47	1.20	4 (8%)
23	CLA	b	601	41	65,73,73	2.12	16 (24%)	76,113,113	2.68	26 (34%)
23	CLA	B	610	2	65,73,73	2.01	17 (26%)	76,113,113	2.74	23 (30%)
28	OEX	a	414	41,3,1	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	B	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.63	10 (17%)
24	PHO	D	402	-	51,69,69	1.87	8 (15%)	47,99,99	1.85	11 (23%)
27	GOL	A	410	-	5,5,5	0.37	0	5,5,5	0.25	0
37	DGD	H	102	-	63,63,67	0.89	2 (3%)	77,77,81	0.98	3 (3%)
23	CLA	A	404	1	65,73,73	2.11	15 (23%)	76,113,113	2.79	30 (39%)
23	CLA	D	405	4	65,73,73	2.06	15 (23%)	76,113,113	2.82	27 (35%)
26	SQD	D	413	-	42,43,54	1.14	3 (7%)	51,54,65	1.63	12 (23%)
36	HTG	b	621	-	19,19,19	1.24	2 (10%)	23,24,24	1.76	5 (21%)
25	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	7 (12%)
23	CLA	d	402	4	65,73,73	2.01	17 (26%)	76,113,113	2.70	28 (36%)
23	CLA	C	514	3	65,73,73	2.06	17 (26%)	76,113,113	2.83	28 (36%)
26	SQD	a	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.60	11 (17%)
35	LMT	B	632	-	25,25,36	0.45	0	30,30,47	0.71	0
35	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.74	1 (2%)
23	CLA	C	509	3	65,73,73	2.07	17 (26%)	76,113,113	2.76	28 (36%)
23	CLA	C	505	41	65,73,73	2.09	16 (24%)	76,113,113	2.69	29 (38%)
29	PL9	d	405	-	55,55,55	0.64	2 (3%)	68,69,69	1.86	22 (32%)
23	CLA	B	613	2	65,73,73	2.03	17 (26%)	76,113,113	2.71	28 (36%)
23	CLA	c	503	3	65,73,73	2.06	16 (24%)	76,113,113	2.73	27 (35%)
36	HTG	V	203	-	11,11,19	0.28	0	15,15,24	1.35	1 (6%)
23	CLA	C	503	3	65,73,73	2.04	16 (24%)	76,113,113	2.65	25 (32%)
23	CLA	B	605	2	65,73,73	2.01	15 (23%)	76,113,113	2.76	28 (36%)
34	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.26	6 (10%)
38	HEM	e	103	6,5	41,50,50	1.32	6 (14%)	45,82,82	1.83	10 (22%)
25	BCR	k	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.61	13 (23%)
23	CLA	B	616	2	65,73,73	2.03	14 (21%)	76,113,113	2.67	29 (38%)
23	CLA	c	508	3	65,73,73	2.10	16 (24%)	76,113,113	2.74	25 (32%)
37	DGD	c	518	-	63,63,67	0.86	3 (4%)	77,77,81	1.09	4 (5%)
37	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.19	7 (9%)
23	CLA	b	614	2	65,73,73	2.05	16 (24%)	76,113,113	2.77	27 (35%)
31	LHG	d	407	-	48,48,48	0.91	2 (4%)	51,54,54	0.93	3 (5%)
34	LMG	B	622	-	51,51,55	0.90	2 (3%)	59,59,63	1.15	5 (8%)
23	CLA	C	502	3	65,73,73	2.05	16 (24%)	76,113,113	2.75	27 (35%)
25	BCR	d	404	-	41,41,41	1.12	1 (2%)	56,56,56	1.68	13 (23%)
35	LMT	B	623	-	36,36,36	0.42	0	47,47,47	1.14	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	512	3	65,73,73	2.03	16 (24%)	76,113,113	2.77	27 (35%)
23	CLA	b	604	2	65,73,73	2.00	15 (23%)	76,113,113	2.74	27 (35%)
28	OEX	A	412	41,3,1	0,15,15	-	-	-	-	-
23	CLA	A	405	41	65,73,73	2.05	17 (26%)	76,113,113	2.75	29 (38%)
23	CLA	B	604	2	65,73,73	2.04	16 (24%)	76,113,113	2.82	28 (36%)
26	SQD	a	413	-	53,54,54	1.09	4 (7%)	62,65,65	1.23	8 (12%)
38	HEM	E	103	6,5	41,50,50	1.34	6 (14%)	45,82,82	1.88	13 (28%)
36	HTG	B	630	-	19,19,19	1.01	2 (10%)	23,24,24	1.33	1 (4%)
23	CLA	B	607	2	65,73,73	1.98	15 (23%)	76,113,113	2.81	28 (36%)
31	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	a	409	1	65,73,73	2.08	17 (26%)	76,113,113	2.70	32 (42%)
35	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.86	0
35	LMT	C	522	-	36,36,36	0.53	1 (2%)	47,47,47	1.02	4 (8%)
23	CLA	b	603	2	65,73,73	2.03	15 (23%)	76,113,113	2.83	27 (35%)
27	GOL	C	525	-	5,5,5	0.39	0	5,5,5	0.20	0
23	CLA	B	606	2	65,73,73	2.05	17 (26%)	76,113,113	2.78	29 (38%)
23	CLA	c	511	3	65,73,73	2.09	15 (23%)	76,113,113	2.76	26 (34%)
35	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.78	1 (2%)
25	BCR	c	514	-	41,41,41	1.01	1 (2%)	56,56,56	1.87	15 (26%)
25	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.81	12 (21%)
27	GOL	b	624	-	5,5,5	0.36	0	5,5,5	0.41	0
23	CLA	b	608	2	65,73,73	2.06	16 (24%)	76,113,113	2.74	28 (36%)
25	BCR	c	515	-	41,41,41	0.98	1 (2%)	56,56,56	1.67	14 (25%)
31	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.09	3 (6%)
36	HTG	b	623	-	19,19,19	1.08	2 (10%)	23,24,24	1.63	3 (13%)
34	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.08	3 (5%)
25	BCR	A	408	-	41,41,41	0.99	1 (2%)	56,56,56	1.65	16 (28%)
23	CLA	b	607	41	65,73,73	1.96	17 (26%)	76,113,113	2.75	27 (35%)
34	LMG	J	101	39	51,51,55	0.91	3 (5%)	59,59,63	1.07	5 (8%)
34	LMG	Z	101	-	37,37,55	0.99	3 (8%)	45,45,63	1.54	8 (17%)
32	BCT	a	419	21	2,3,3	0.65	0	2,3,3	0.46	0
37	DGD	c	516	-	63,63,67	0.85	2 (3%)	77,77,81	1.08	6 (7%)
23	CLA	c	501	3	65,73,73	2.07	17 (26%)	76,113,113	2.72	27 (35%)
36	HTG	B	624	-	19,19,19	0.98	1 (5%)	23,24,24	1.38	4 (17%)
23	CLA	b	606	2	65,73,73	1.99	16 (24%)	76,113,113	2.81	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	610	41	65,73,73	2.11	16 (24%)	76,113,113	2.78	28 (36%)
36	HTG	B	629	-	19,19,19	0.97	2 (10%)	23,24,24	1.35	3 (13%)
36	HTG	h	101	-	16,16,19	1.09	2 (12%)	20,21,24	1.30	1 (5%)
25	BCR	h	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	10 (17%)
23	CLA	C	510	3	65,73,73	2.09	17 (26%)	76,113,113	2.83	27 (35%)
36	HTG	C	523	-	19,19,19	0.96	1 (5%)	23,24,24	1.50	3 (13%)
35	LMT	B	634	-	26,26,36	0.49	0	31,31,47	0.90	1 (3%)
35	LMT	m	103	-	36,36,36	0.50	0	47,47,47	0.93	1 (2%)
40	HEC	V	202	16	32,50,50	1.46	4 (12%)	24,82,82	1.49	5 (20%)
23	CLA	b	605	2	65,73,73	2.04	17 (26%)	76,113,113	2.79	28 (36%)
23	CLA	C	508	41	65,73,73	2.04	15 (23%)	76,113,113	2.68	27 (35%)
25	BCR	B	620	-	41,41,41	1.06	1 (2%)	56,56,56	1.50	12 (21%)
31	LHG	d	406	-	48,48,48	0.87	3 (6%)	51,54,54	1.09	5 (9%)
34	LMG	a	417	-	51,51,55	0.96	3 (5%)	59,59,63	1.11	4 (6%)
23	CLA	C	507	3	65,73,73	2.06	17 (26%)	76,113,113	2.76	29 (38%)
34	LMG	j	101	39	51,51,55	0.91	2 (3%)	59,59,63	1.08	6 (10%)
24	PHO	A	406	-	51,69,69	1.88	7 (13%)	47,99,99	1.90	12 (25%)
35	LMT	b	620	-	25,25,36	0.46	0	30,30,47	0.66	0
25	BCR	t	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.84	13 (23%)
25	BCR	a	410	-	41,41,41	0.99	1 (2%)	56,56,56	1.57	13 (23%)
36	HTG	C	524	-	8,8,19	0.39	0	7,7,24	1.15	1 (14%)
26	SQD	B	621	-	53,54,54	1.04	3 (5%)	62,65,65	1.45	8 (12%)
36	HTG	B	626	-	19,19,19	0.96	1 (5%)	23,24,24	1.59	2 (8%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.98	5 (6%)
27	GOL	B	628	-	5,5,5	0.54	0	5,5,5	0.49	0
24	PHO	a	408	-	51,69,69	1.96	8 (15%)	47,99,99	1.88	12 (25%)
23	CLA	B	617	2	65,73,73	2.05	16 (24%)	76,113,113	2.79	27 (35%)
23	CLA	c	507	41	65,73,73	2.08	17 (26%)	76,113,113	2.79	29 (38%)
27	GOL	a	412	-	5,5,5	0.43	0	5,5,5	0.27	0
29	PL9	a	415	-	55,55,55	0.65	1 (1%)	68,69,69	2.00	20 (29%)
31	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.17	4 (7%)
36	HTG	b	622	-	19,19,19	1.01	2 (10%)	23,24,24	1.39	2 (8%)
23	CLA	B	602	41	65,73,73	2.06	16 (24%)	76,113,113	2.76	29 (38%)
23	CLA	B	615	2	65,73,73	2.00	16 (24%)	76,113,113	2.86	26 (34%)
24	PHO	a	407	-	51,69,69	1.85	7 (13%)	47,99,99	1.92	12 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	T	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.85	10 (17%)
25	BCR	y	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.66	12 (21%)
23	CLA	C	512	3	65,73,73	2.08	17 (26%)	76,113,113	2.69	27 (35%)
34	LMG	C	521	-	51,51,55	0.98	3 (5%)	59,59,63	1.21	4 (6%)
37	DGD	h	103	-	63,63,67	0.89	3 (4%)	77,77,81	0.96	3 (3%)
23	CLA	b	609	2	65,73,73	2.08	17 (26%)	76,113,113	2.80	26 (34%)
36	HTG	c	521	-	19,19,19	0.93	1 (5%)	23,24,24	1.46	1 (4%)
25	BCR	D	406	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	13 (23%)
36	HTG	b	626	-	19,19,19	1.08	2 (10%)	23,24,24	1.28	2 (8%)
23	CLA	a	404	1	65,73,73	2.05	15 (23%)	76,113,113	2.73	32 (42%)
23	CLA	C	511	3	65,73,73	2.05	14 (21%)	76,113,113	2.73	26 (34%)
29	PL9	A	413	-	55,55,55	0.63	2 (3%)	68,69,69	1.96	22 (32%)
32	BCT	A	416	21	2,3,3	0.66	0	2,3,3	0.33	0
23	CLA	B	608	41	65,73,73	2.07	17 (26%)	76,113,113	2.76	29 (38%)
36	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.47	3 (13%)
35	LMT	B	633	-	36,36,36	0.56	1 (2%)	47,47,47	0.97	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	D	409	-	-	14/53/53/53	-
23	CLA	c	506	3	1/1/15/20	12/37/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	C	527	-	-	1/29/63/63	0/2/2/2
36	HTG	b	625	-	-	5/10/30/30	0/1/1/1
23	CLA	B	611	41	1/1/15/20	7/37/115/115	-
35	LMT	M	101	-	-	2/21/61/61	0/2/2/2
36	HTG	B	625	-	-	5/10/30/30	0/1/1/1
25	BCR	C	516	-	-	1/29/63/63	0/2/2/2
23	CLA	C	504	3	1/1/15/20	3/37/115/115	-
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
27	GOL	d	401	-	-	2/4/4/4	-
31	LHG	e	101	-	-	14/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	C	519	-	-	7/51/91/95	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	GOL	O	302	-	-	2/4/4/4	-
40	HEC	v	201	16	-	2/10/54/54	-
23	CLA	b	602	2	1/1/15/20	4/37/115/115	-
26	SQD	A	409	-	-	14/49/69/69	0/1/1/1
23	CLA	c	509	3	1/1/15/20	15/37/115/115	-
37	DGD	c	517	-	-	14/51/91/95	0/2/2/2
23	CLA	d	403	4	1/1/15/20	6/37/115/115	-
31	LHG	A	415	-	-	11/53/53/53	-
23	CLA	b	611	2	1/1/15/20	10/37/115/115	-
26	SQD	A	411	-	-	14/49/69/69	0/1/1/1
23	CLA	a	406	41	-	8/37/115/115	-
23	CLA	b	613	2	1/1/15/20	7/37/115/115	-
23	CLA	D	401	41	1/1/15/20	8/37/115/115	-
26	SQD	f	101	-	-	16/38/58/69	0/1/1/1
23	CLA	c	502	3	1/1/15/20	8/37/115/115	-
31	LHG	b	630	-	-	19/53/53/53	-
23	CLA	D	404	4	1/1/15/20	2/37/115/115	-
35	LMT	b	628	-	-	9/17/37/61	0/1/1/2
23	CLA	A	407	1	1/1/15/20	8/37/115/115	-
34	LMG	z	101	-	-	15/34/54/70	0/1/1/1
23	CLA	B	612	2	1/1/15/20	4/37/115/115	-
36	HTG	D	412	-	-	1/7/27/30	0/1/1/1
23	CLA	a	405	41	1/1/15/20	5/37/115/115	-
25	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
34	LMG	m	101	-	-	16/46/66/70	0/1/1/1
23	CLA	c	505	3	1/1/15/20	7/37/115/115	-
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
26	SQD	L	102	-	-	22/49/69/69	0/1/1/1
23	CLA	B	603	2	1/1/15/20	8/37/115/115	-
34	LMG	c	520	-	-	8/46/66/70	0/1/1/1
23	CLA	b	616	2	1/1/15/20	12/37/115/115	-
34	LMG	c	519	-	-	13/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	612	2	1/1/15/20	5/37/115/115	-
29	PL9	D	407	-	-	7/53/73/73	0/1/1/1
35	LMT	e	102	-	-	8/21/61/61	0/2/2/2
23	CLA	B	614	2	1/1/15/20	5/37/115/115	-
31	LHG	d	408	-	-	17/53/53/53	-
23	CLA	c	504	41	1/1/15/20	12/37/115/115	-
23	CLA	c	513	3	-	6/37/115/115	-
27	GOL	B	627	-	-	4/4/4/4	-
23	CLA	c	510	3	1/1/15/20	8/37/115/115	-
23	CLA	b	615	2	1/1/15/20	7/37/115/115	-
23	CLA	B	609	2	1/1/15/20	4/37/115/115	-
23	CLA	C	506	3	1/1/15/20	7/37/115/115	-
23	CLA	C	513	3	1/1/15/20	7/37/115/115	-
35	LMT	D	403	-	-	8/21/61/61	0/2/2/2
23	CLA	b	601	41	1/1/15/20	19/37/115/115	-
23	CLA	B	610	2	1/1/15/20	9/37/115/115	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	PHO	D	402	-	-	5/37/103/103	0/5/6/6
27	GOL	A	410	-	-	4/4/4/4	-
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2
23	CLA	A	404	1	1/1/15/20	3/37/115/115	-
23	CLA	D	405	4	1/1/15/20	7/37/115/115	-
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
36	HTG	b	621	-	-	2/10/30/30	0/1/1/1
25	BCR	C	515	-	-	1/29/63/63	0/2/2/2
23	CLA	d	402	4	1/1/15/20	3/37/115/115	-
23	CLA	C	514	3	-	8/37/115/115	-
26	SQD	a	411	-	-	14/49/69/69	0/1/1/1
35	LMT	B	632	-	-	7/17/37/61	0/1/1/2
35	LMT	a	418	-	-	3/21/61/61	0/2/2/2
23	CLA	C	509	3	1/1/15/20	6/37/115/115	-
23	CLA	C	505	41	1/1/15/20	6/37/115/115	-
29	PL9	d	405	-	-	6/53/73/73	0/1/1/1
23	CLA	B	613	2	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	503	3	1/1/15/20	3/37/115/115	-
36	HTG	V	203	-	-	0/2/19/30	0/1/1/1
23	CLA	C	503	3	1/1/15/20	9/37/115/115	-
23	CLA	B	605	2	1/1/15/20	13/37/115/115	-
34	LMG	C	501	-	-	11/46/66/70	0/1/1/1
38	HEM	e	103	6,5	-	6/12/54/54	-
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	616	2	1/1/15/20	10/37/115/115	-
23	CLA	c	508	3	1/1/15/20	6/37/115/115	-
37	DGD	c	518	-	-	6/51/91/95	0/2/2/2
37	DGD	C	517	-	-	15/51/91/95	0/2/2/2
23	CLA	b	614	2	1/1/15/20	15/37/115/115	-
31	LHG	d	407	-	-	23/53/53/53	-
34	LMG	B	622	-	-	12/46/66/70	0/1/1/1
23	CLA	C	502	3	1/1/15/20	5/37/115/115	-
25	BCR	d	404	-	-	8/29/63/63	0/2/2/2
35	LMT	B	623	-	-	8/21/61/61	0/2/2/2
23	CLA	c	512	3	1/1/15/20	9/37/115/115	-
23	CLA	b	604	2	1/1/15/20	9/37/115/115	-
23	CLA	B	604	2	1/1/15/20	6/37/115/115	-
23	CLA	A	405	41	-	8/37/115/115	-
26	SQD	a	413	-	-	16/49/69/69	0/1/1/1
38	HEM	E	103	6,5	-	4/12/54/54	-
36	HTG	B	630	-	-	1/10/30/30	0/1/1/1
23	CLA	B	607	2	1/1/15/20	5/37/115/115	-
31	LHG	D	408	-	-	18/53/53/53	-
23	CLA	a	409	1	1/1/15/20	7/37/115/115	-
35	LMT	E	102	-	-	10/21/61/61	0/2/2/2
35	LMT	C	522	-	-	9/21/61/61	0/2/2/2
23	CLA	b	603	2	1/1/15/20	4/37/115/115	-
27	GOL	C	525	-	-	2/4/4/4	-
23	CLA	B	606	2	1/1/15/20	11/37/115/115	-
23	CLA	c	511	3	1/1/15/20	5/37/115/115	-
35	LMT	M	103	-	-	14/21/61/61	0/2/2/2
25	BCR	c	514	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	b	608	2	-	5/37/115/115	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
31	LHG	E	101	-	-	17/46/46/53	-
36	HTG	b	623	-	-	2/10/30/30	0/1/1/1
34	LMG	C	520	-	-	16/46/66/70	0/1/1/1
25	BCR	A	408	-	-	1/29/63/63	0/2/2/2
23	CLA	b	607	41	1/1/15/20	9/37/115/115	-
34	LMG	J	101	39	-	10/46/66/70	0/1/1/1
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
37	DGD	c	516	-	-	15/51/91/95	0/2/2/2
23	CLA	c	501	3	1/1/15/20	8/37/115/115	-
36	HTG	B	624	-	-	4/10/30/30	0/1/1/1
23	CLA	b	606	2	1/1/15/20	10/37/115/115	-
23	CLA	b	610	41	1/1/15/20	7/37/115/115	-
36	HTG	B	629	-	-	1/10/30/30	0/1/1/1
36	HTG	h	101	-	-	3/7/27/30	0/1/1/1
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
23	CLA	C	510	3	1/1/15/20	14/37/115/115	-
36	HTG	C	523	-	-	0/10/30/30	0/1/1/1
35	LMT	B	634	-	-	6/17/38/61	0/1/1/2
35	LMT	m	103	-	-	8/21/61/61	0/2/2/2
40	HEC	V	202	16	-	2/10/54/54	-
23	CLA	b	605	2	1/1/15/20	13/37/115/115	-
23	CLA	C	508	41	1/1/15/20	7/37/115/115	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
31	LHG	d	406	-	-	12/53/53/53	-
34	LMG	a	417	-	-	14/46/66/70	0/1/1/1
23	CLA	C	507	3	1/1/15/20	14/37/115/115	-
34	LMG	j	101	39	-	8/46/66/70	0/1/1/1
24	PHO	A	406	-	-	5/37/103/103	0/5/6/6
35	LMT	b	620	-	-	5/17/37/61	0/1/1/2
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
36	HTG	C	524	-	-	1/6/6/30	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	B	621	-	-	21/49/69/69	0/1/1/1
36	HTG	B	626	-	-	4/10/30/30	0/1/1/1
37	DGD	C	518	-	-	15/51/91/95	0/2/2/2
27	GOL	B	628	-	-	4/4/4/4	-
24	PHO	a	408	-	-	2/37/103/103	0/5/6/6
23	CLA	B	617	2	1/1/15/20	7/37/115/115	-
23	CLA	c	507	41	1/1/15/20	8/37/115/115	-
27	GOL	a	412	-	-	2/4/4/4	-
29	PL9	a	415	-	-	16/53/73/73	0/1/1/1
31	LHG	L	101	-	-	16/53/53/53	-
36	HTG	b	622	-	-	1/10/30/30	0/1/1/1
23	CLA	B	602	41	1/1/15/20	13/37/115/115	-
23	CLA	B	615	2	1/1/15/20	12/37/115/115	-
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
25	BCR	T	101	-	-	5/29/63/63	0/2/2/2
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	C	512	3	1/1/15/20	6/37/115/115	-
34	LMG	C	521	-	-	9/46/66/70	0/1/1/1
37	DGD	h	103	-	-	11/51/91/95	0/2/2/2
23	CLA	b	609	2	1/1/15/20	8/37/115/115	-
36	HTG	c	521	-	-	3/10/30/30	0/1/1/1
25	BCR	D	406	-	-	7/29/63/63	0/2/2/2
36	HTG	b	626	-	-	0/10/30/30	0/1/1/1
23	CLA	a	404	1	1/1/15/20	5/37/115/115	-
23	CLA	C	511	3	1/1/15/20	13/37/115/115	-
29	PL9	A	413	-	-	11/53/73/73	0/1/1/1
23	CLA	B	608	41	1/1/15/20	3/37/115/115	-
36	HTG	c	522	-	-	2/10/30/30	0/1/1/1
35	LMT	B	633	-	-	5/21/61/61	0/2/2/2

The worst 5 of 1328 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C3B-C2B	6.96	1.50	1.40
23	B	614	CLA	C3B-C2B	6.74	1.49	1.40
24	a	407	PHO	C3B-C2B	6.71	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	PHO	C3B-C2B	6.68	1.49	1.40
23	A	404	CLA	C3B-C2B	6.65	1.49	1.40

The worst 5 of 2636 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	C1D-ND-C4D	-10.30	99.02	106.33
23	D	401	CLA	C1D-ND-C4D	-10.24	99.06	106.33
23	C	514	CLA	C1D-ND-C4D	-10.04	99.20	106.33
23	d	403	CLA	C1D-ND-C4D	-9.92	99.29	106.33
23	A	407	CLA	C1D-ND-C4D	-9.85	99.33	106.33

5 of 65 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND

5 of 1353 torsion outliers are listed below:

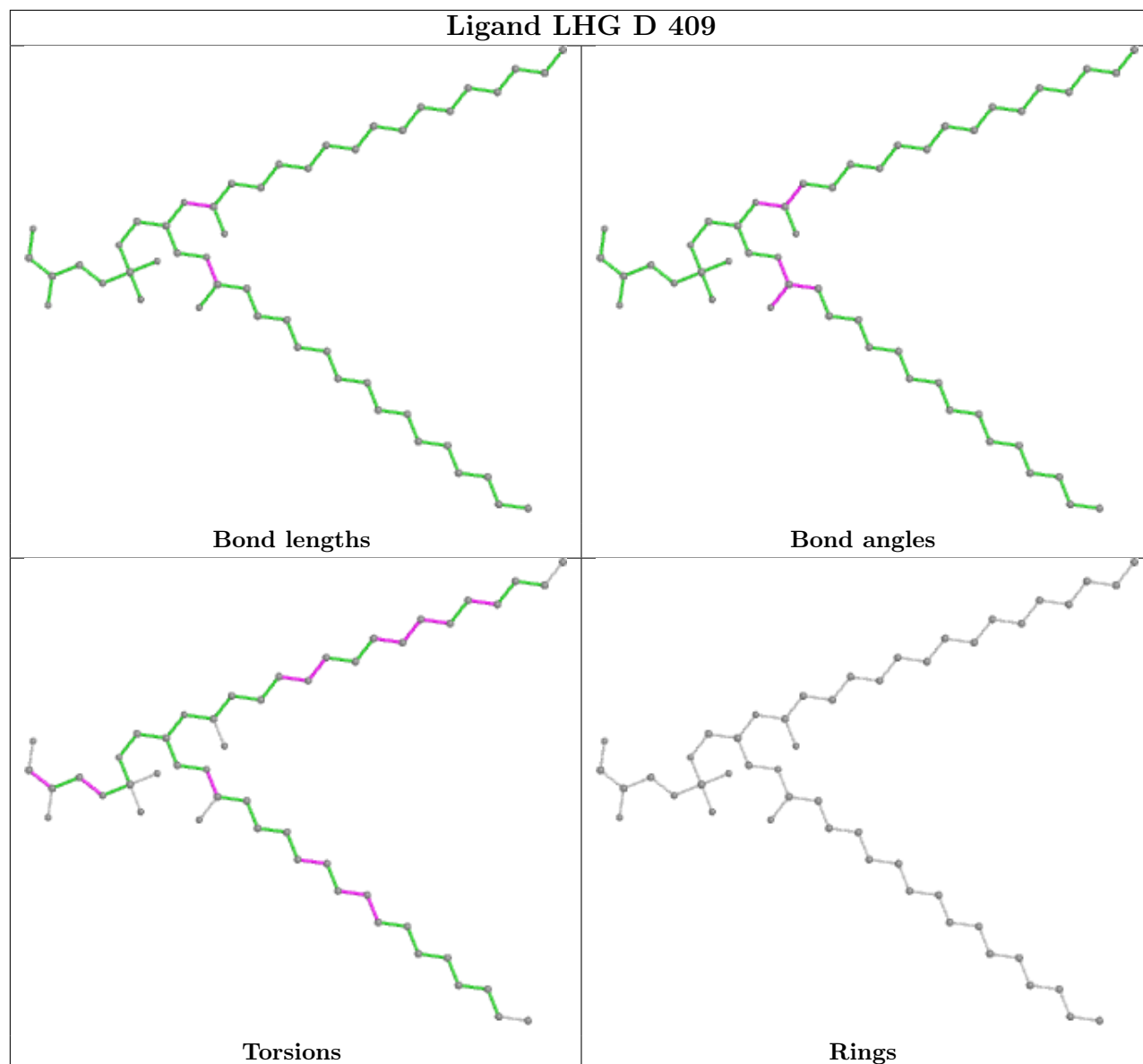
Mol	Chain	Res	Type	Atoms
23	B	604	CLA	C2-C3-C5-C6
23	B	604	CLA	C4-C3-C5-C6
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O1D

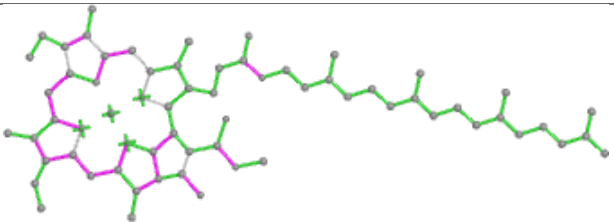
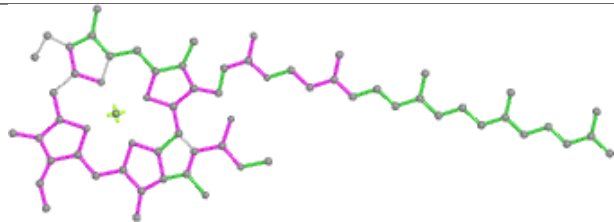
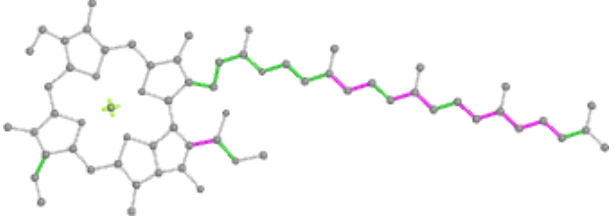
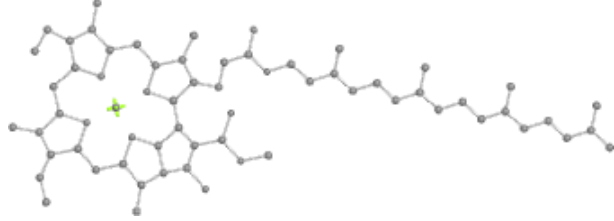
There are no ring outliers.

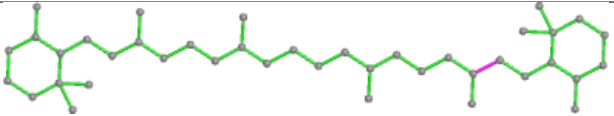
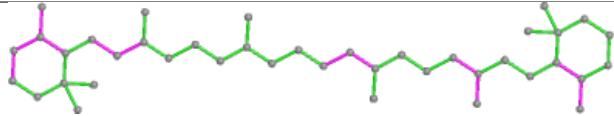
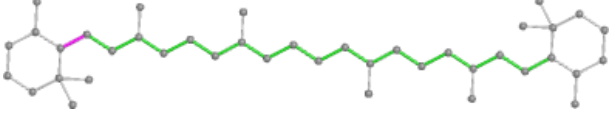
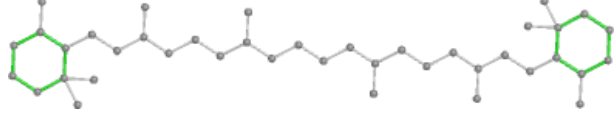
No monomer is involved in short contacts.

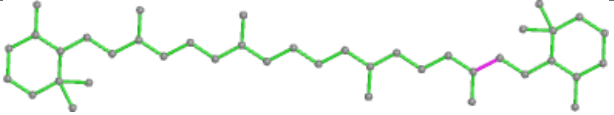
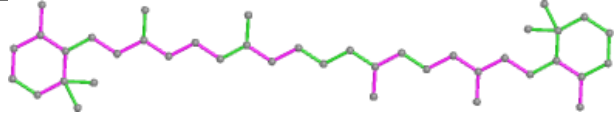
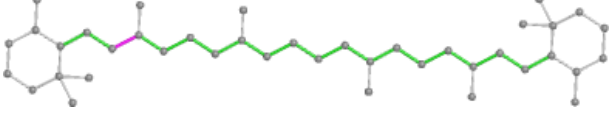
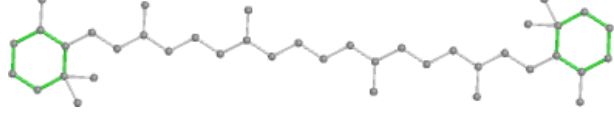
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

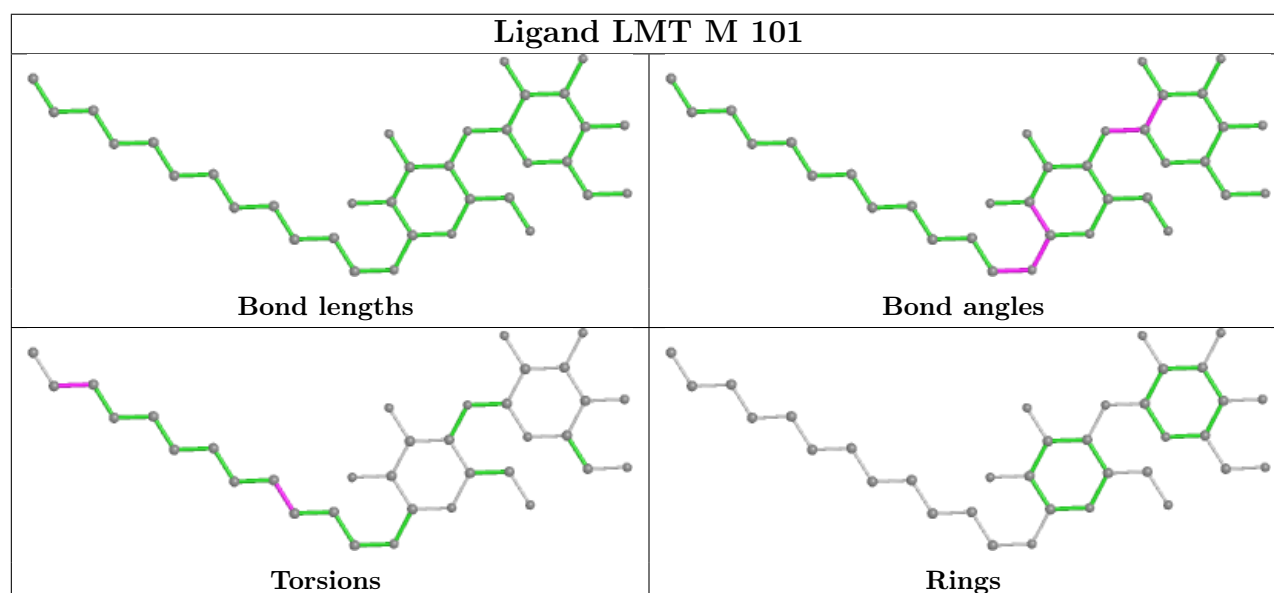
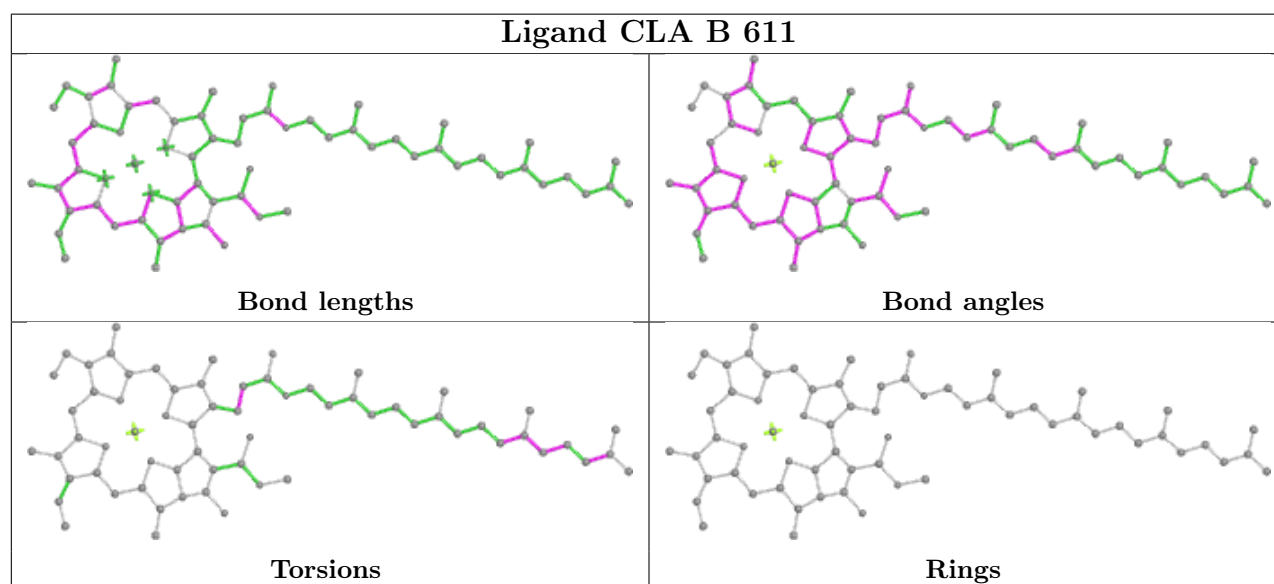
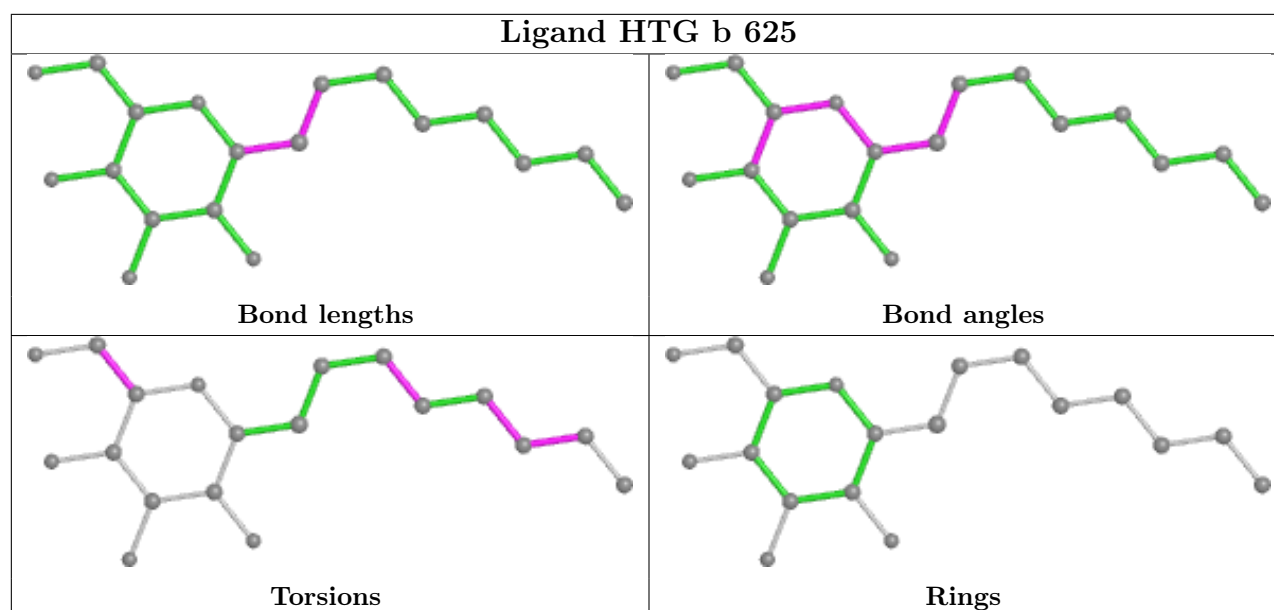


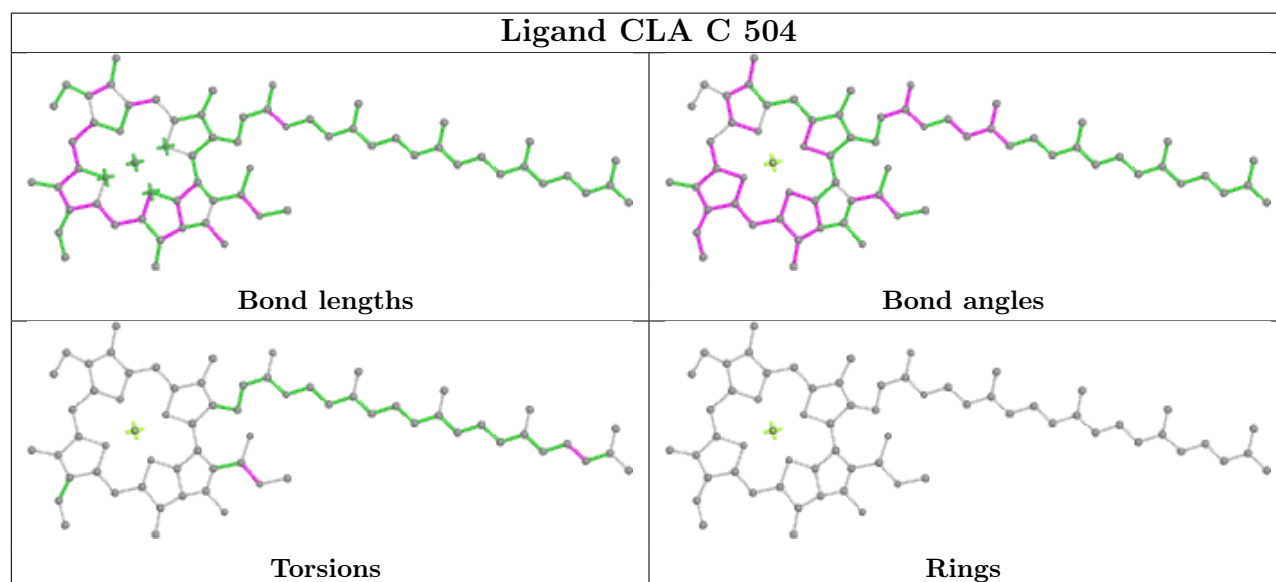
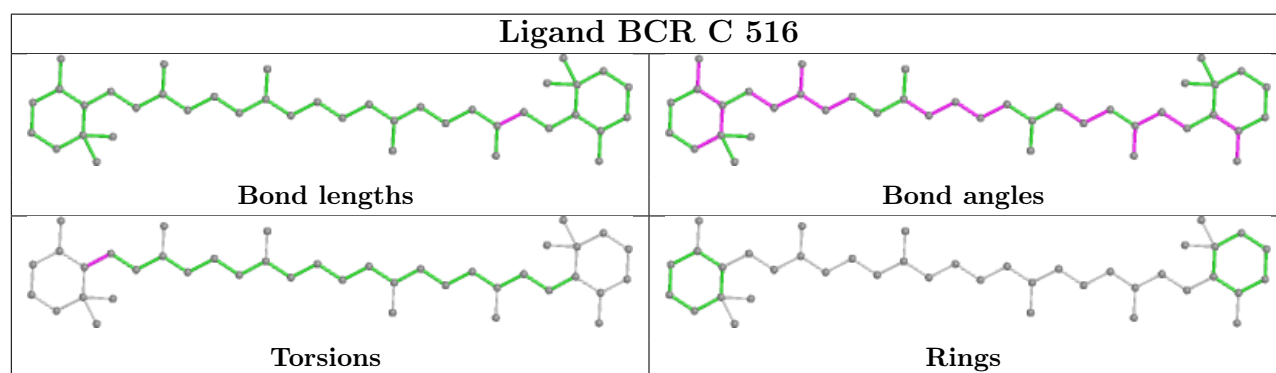
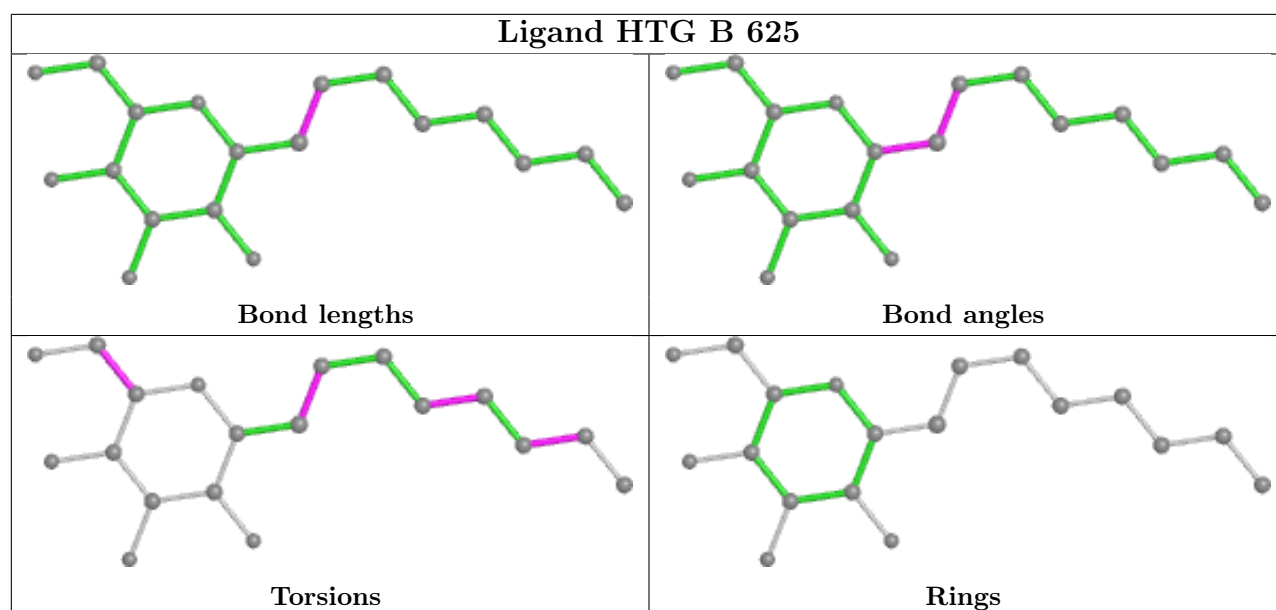
Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

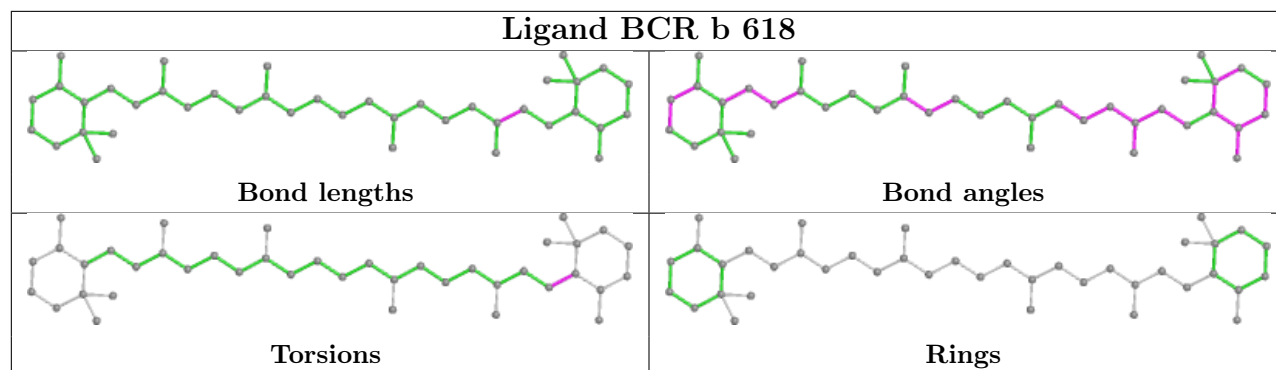
Ligand BCR C 527	
	
Bond lengths	Bond angles
	
Torsions	Rings



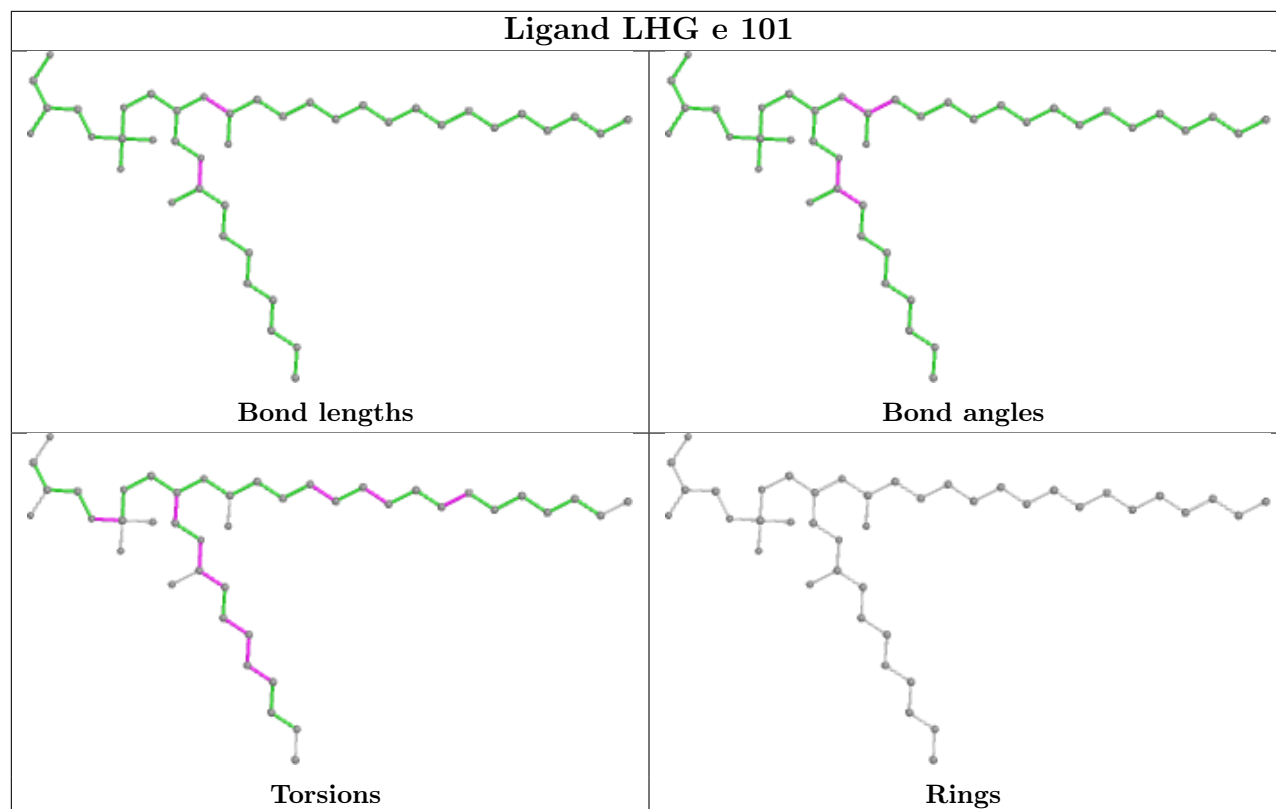




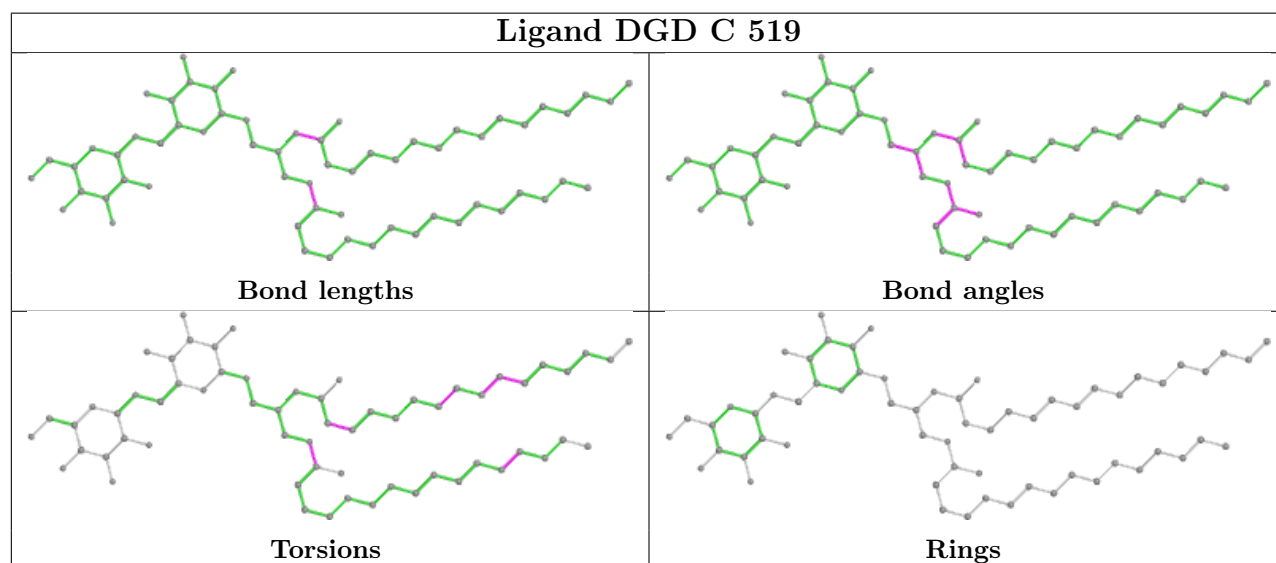
## Ligand BCR b 618

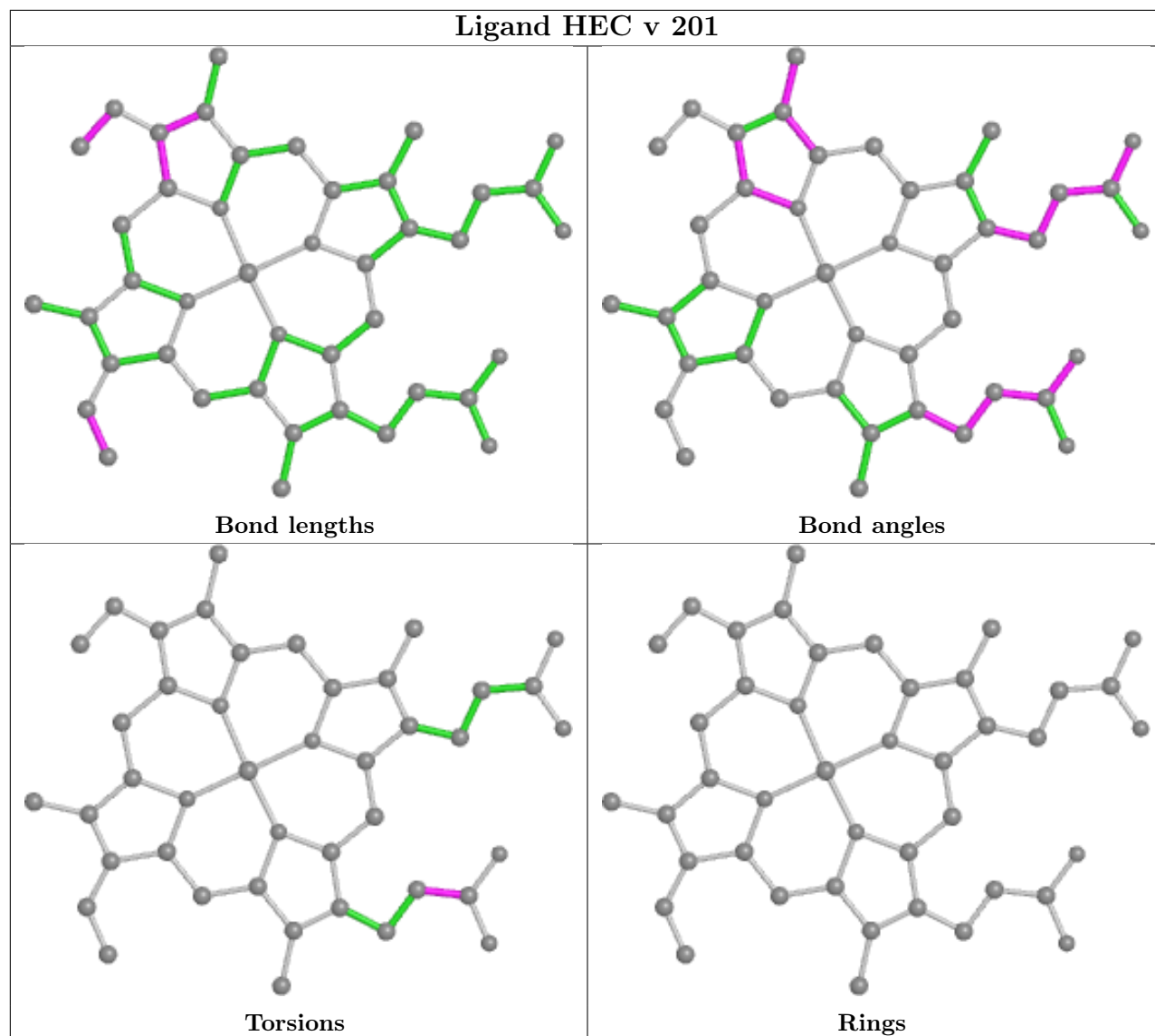
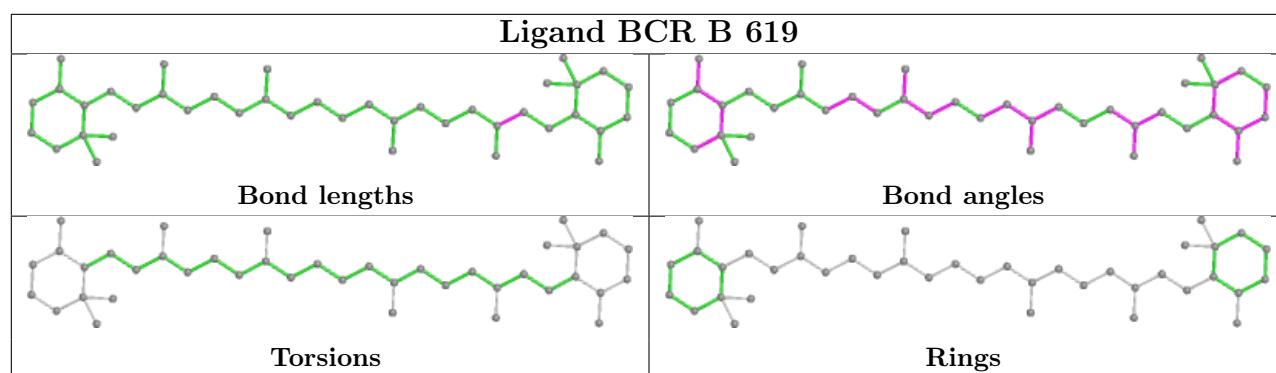


## Ligand LHG e 101

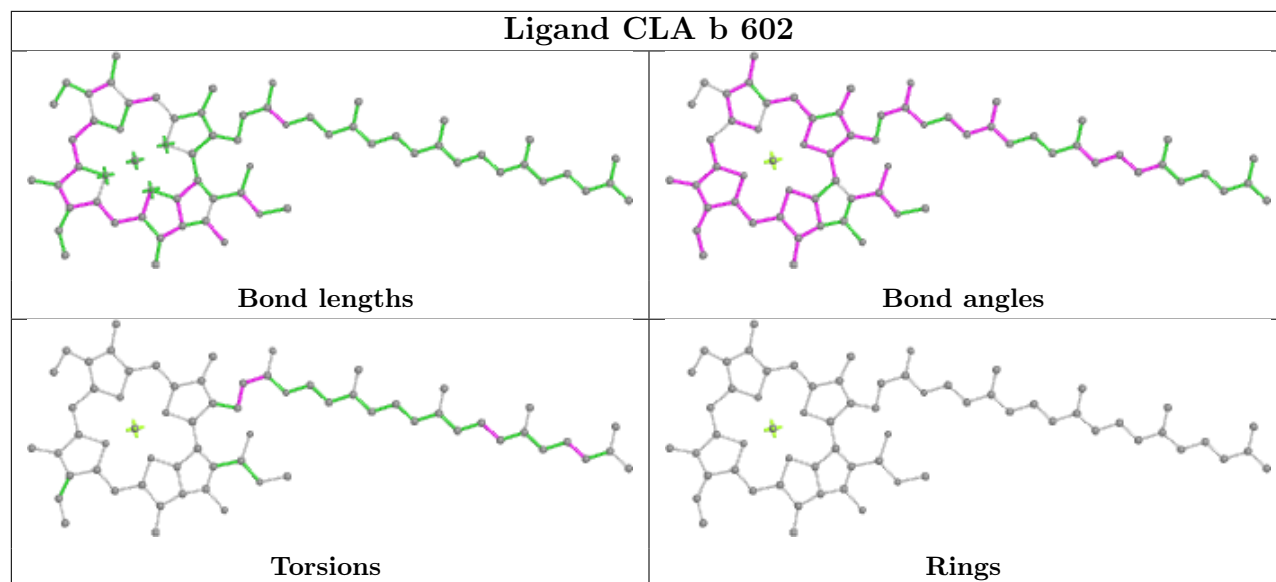


## Ligand DGD C 519

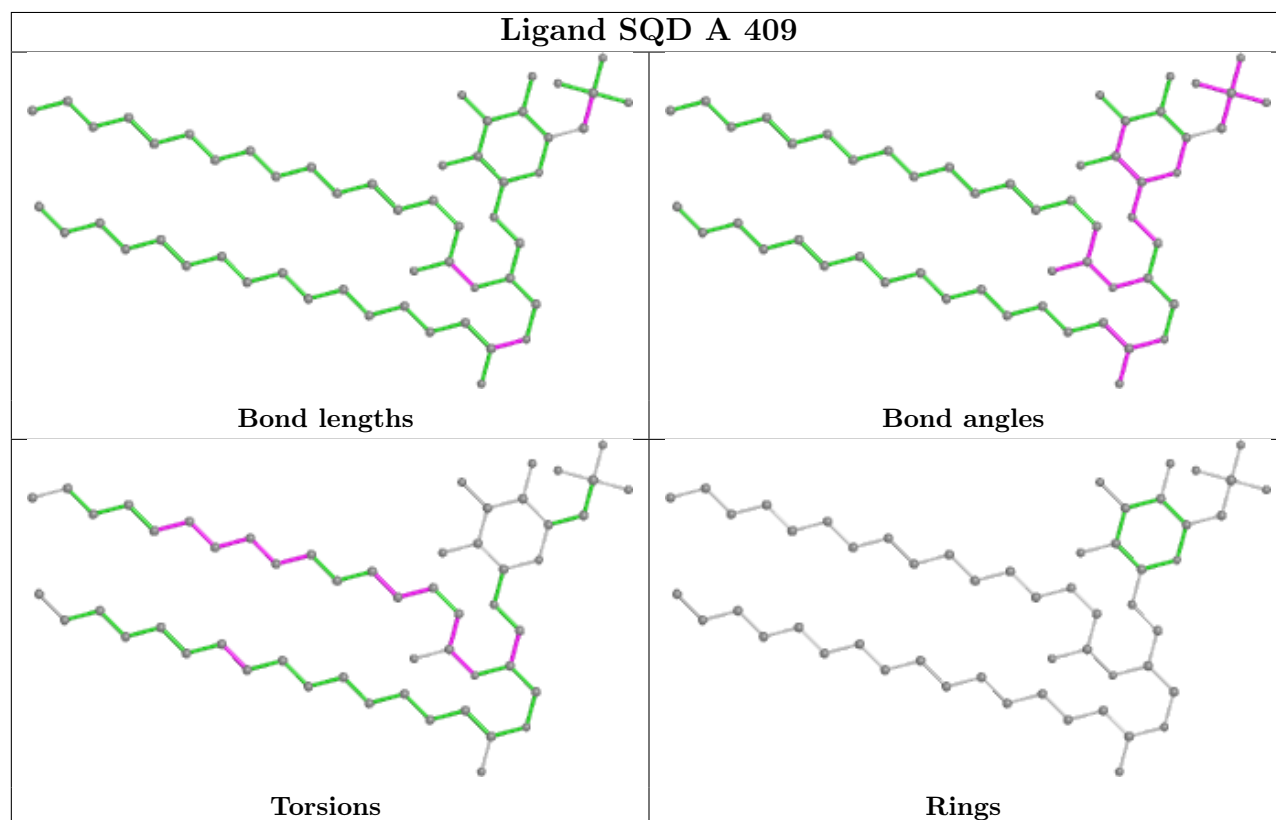




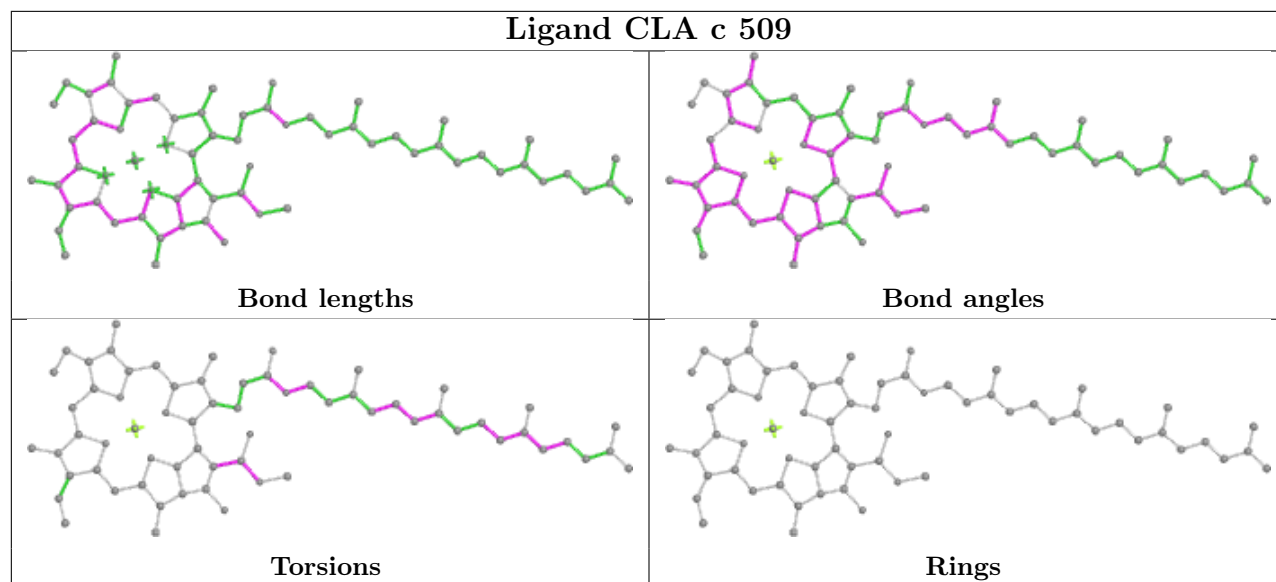
## Ligand CLA b 602



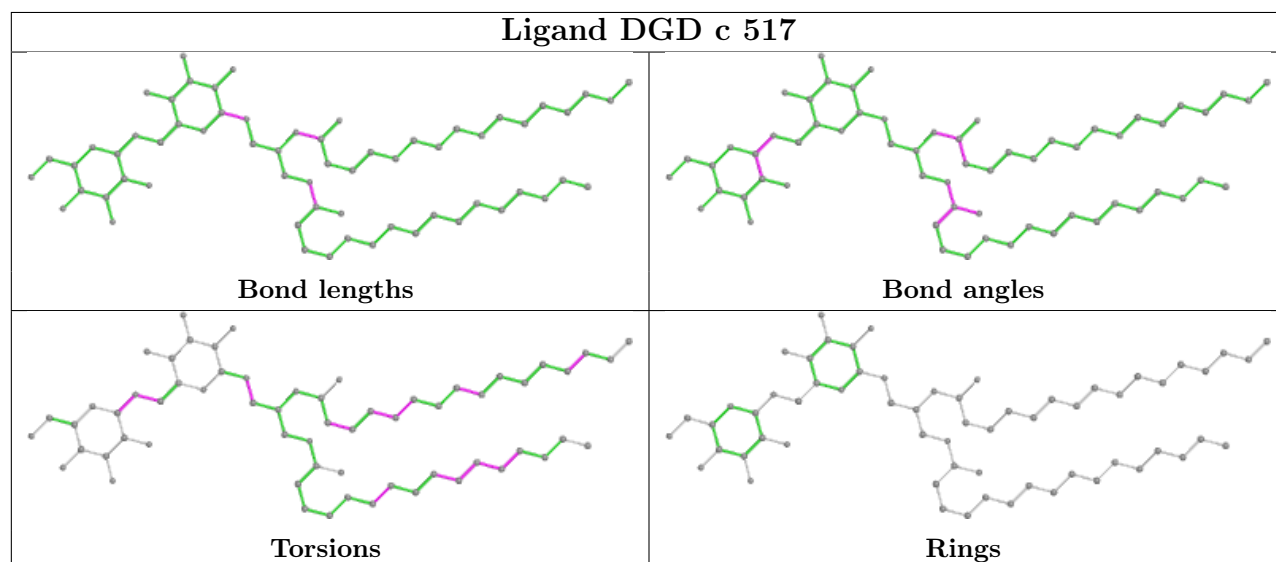
## Ligand SQD A 409



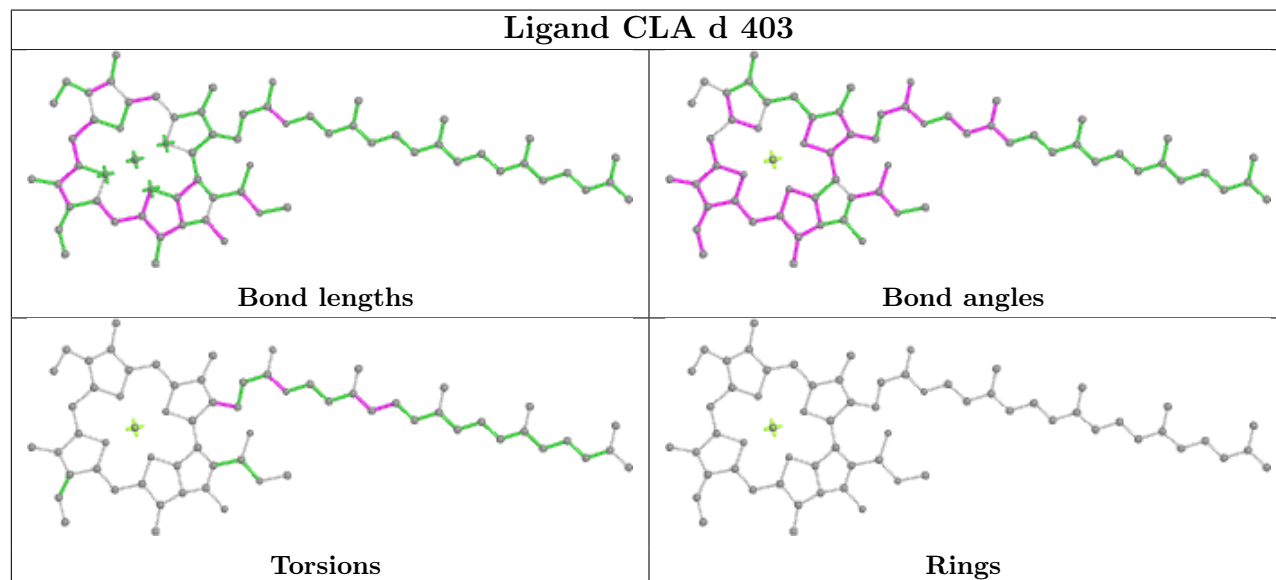
## Ligand CLA c 509

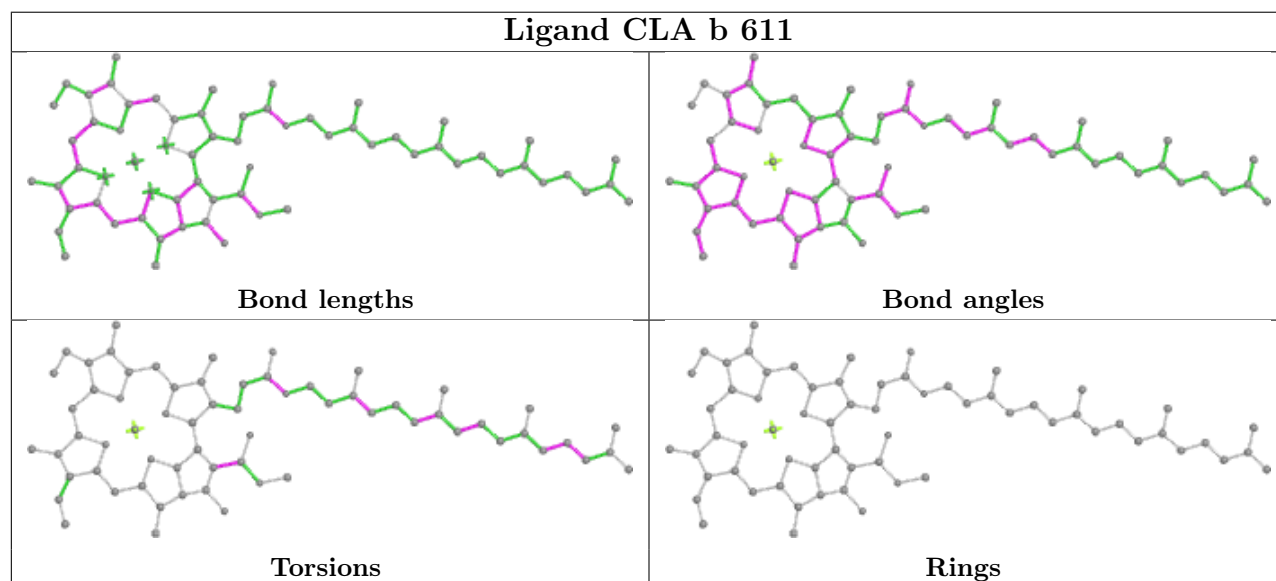
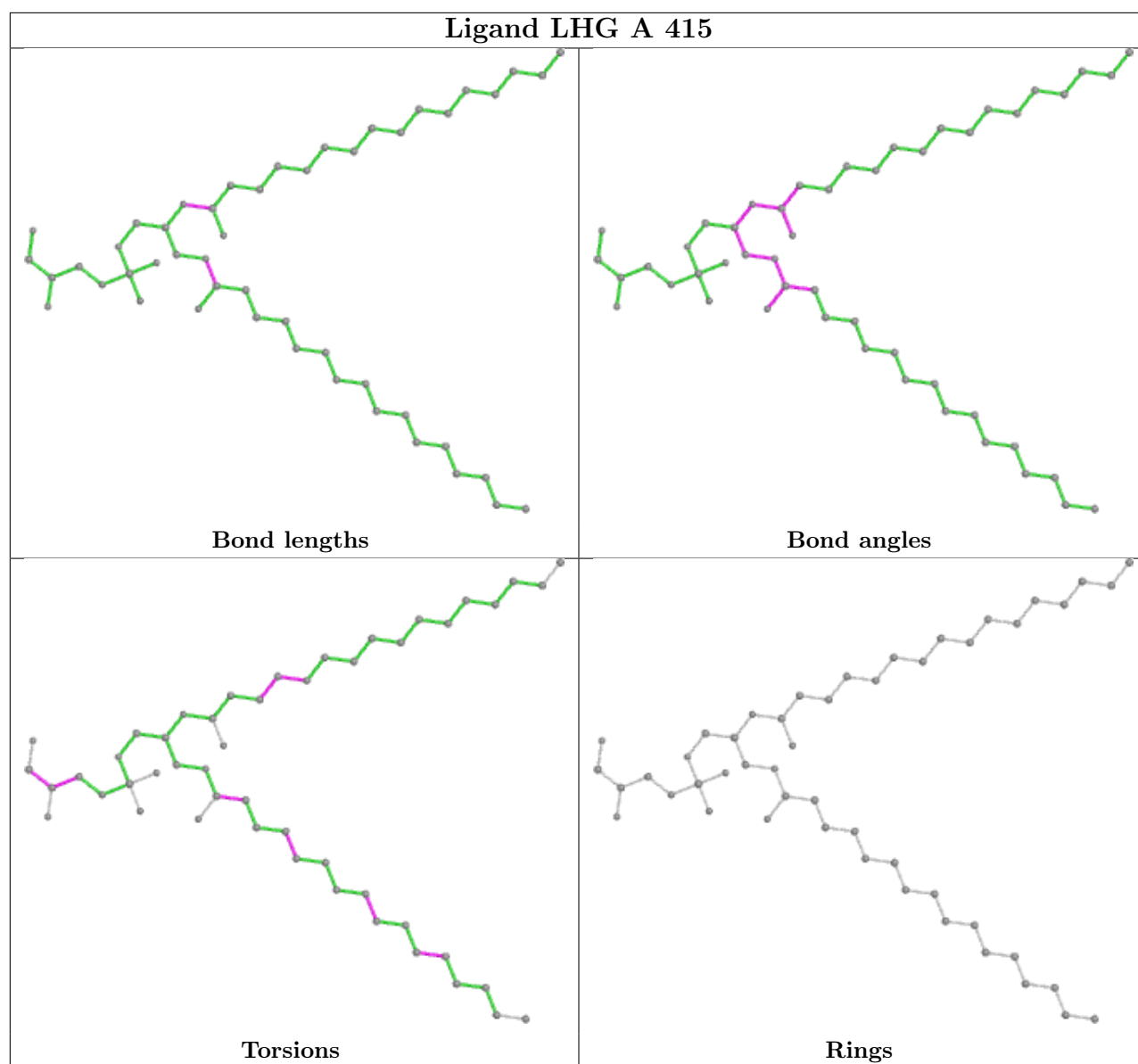


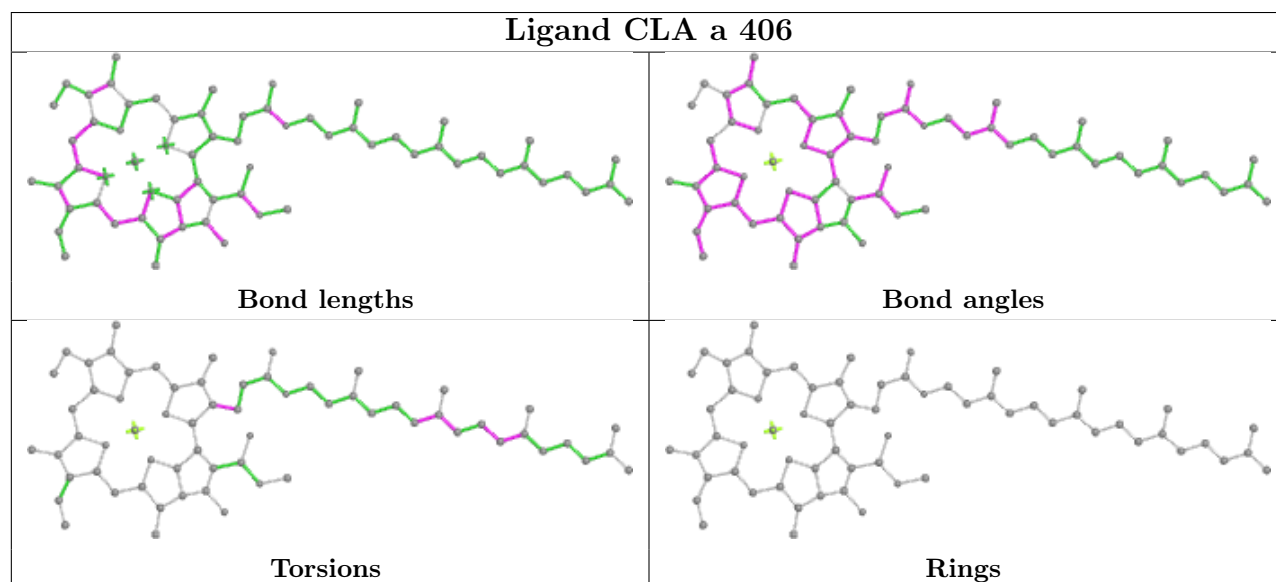
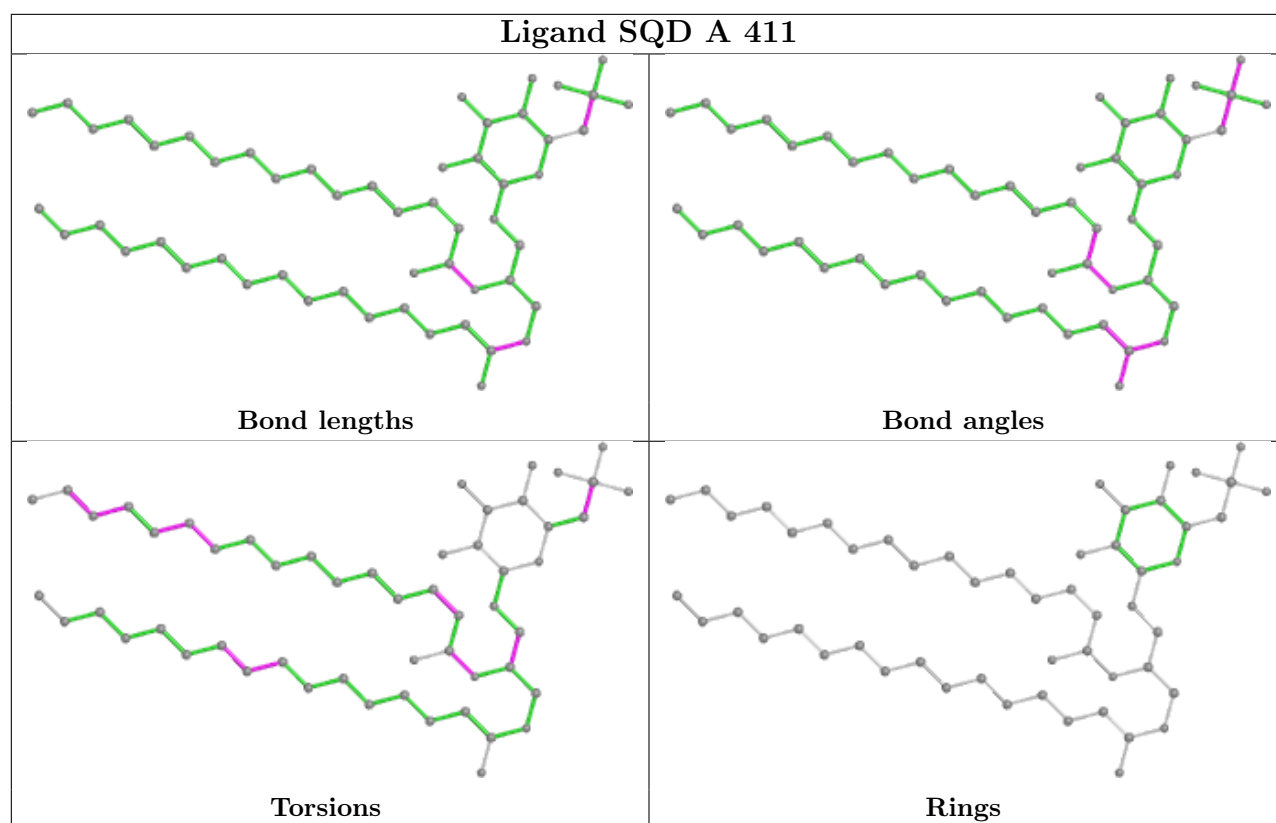
## Ligand DGD c 517



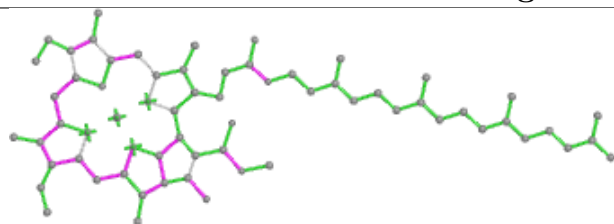
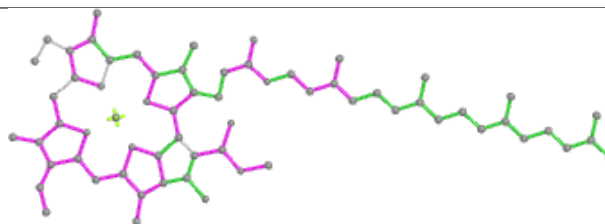
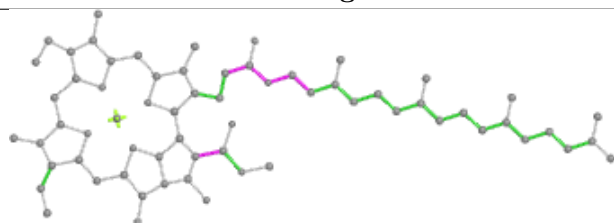
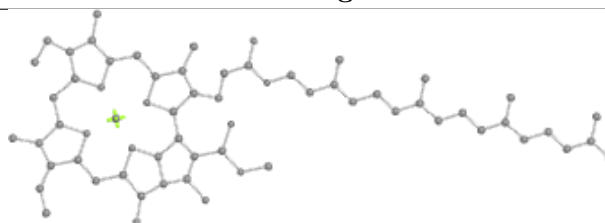
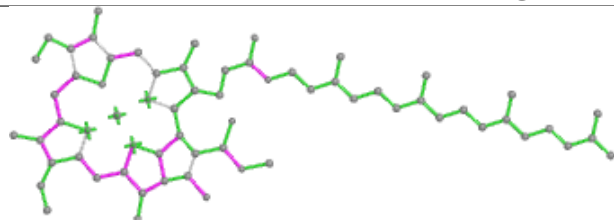
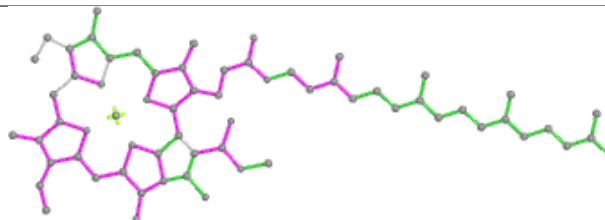
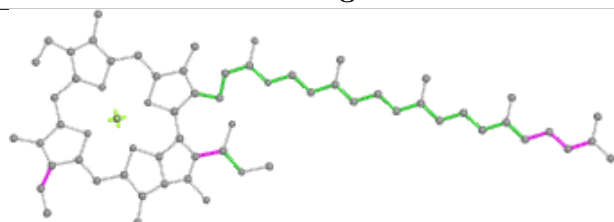
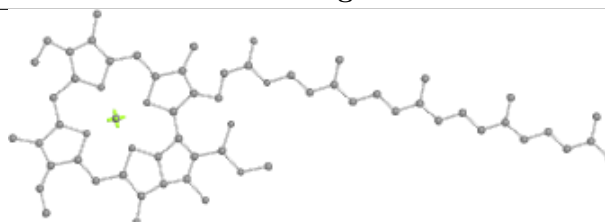
## Ligand CLA d 403

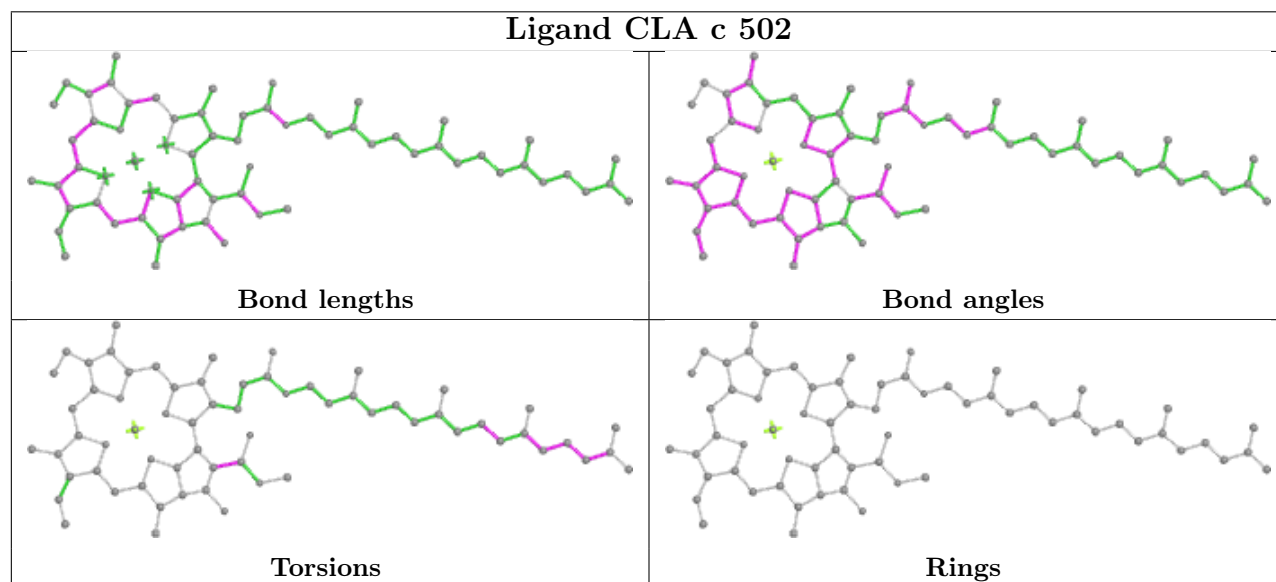
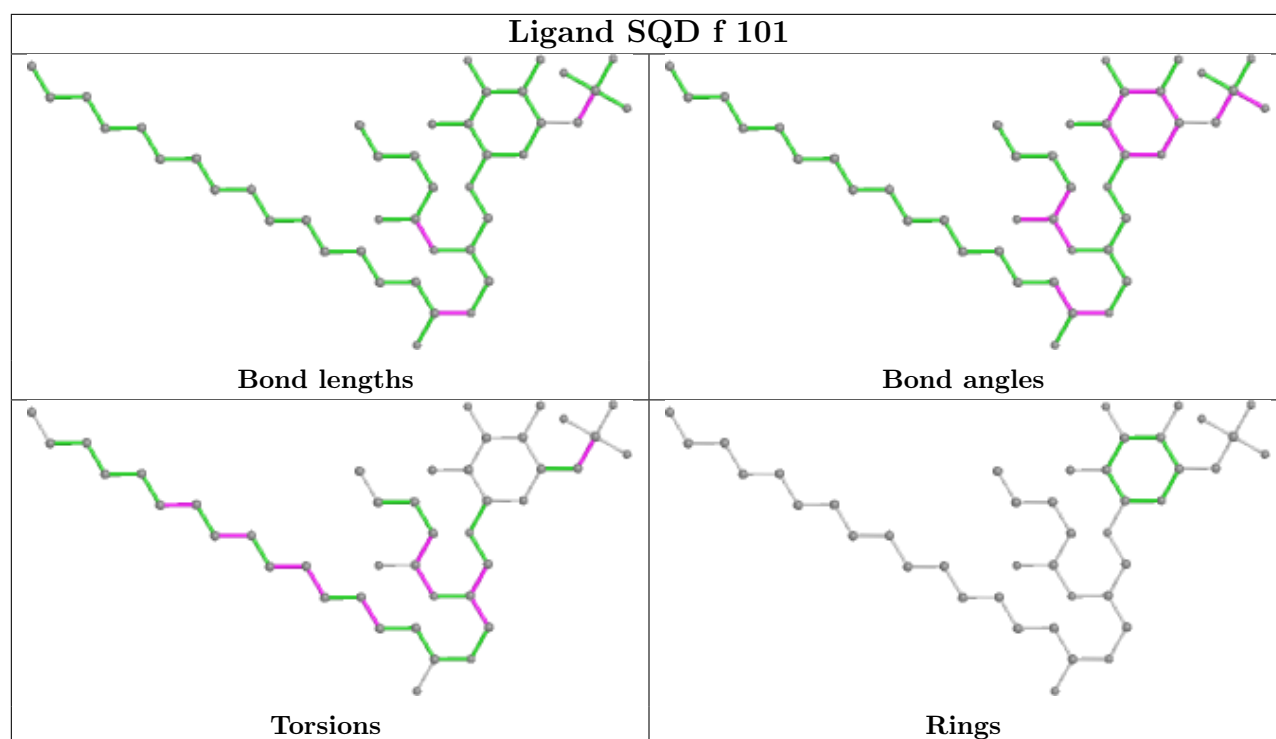




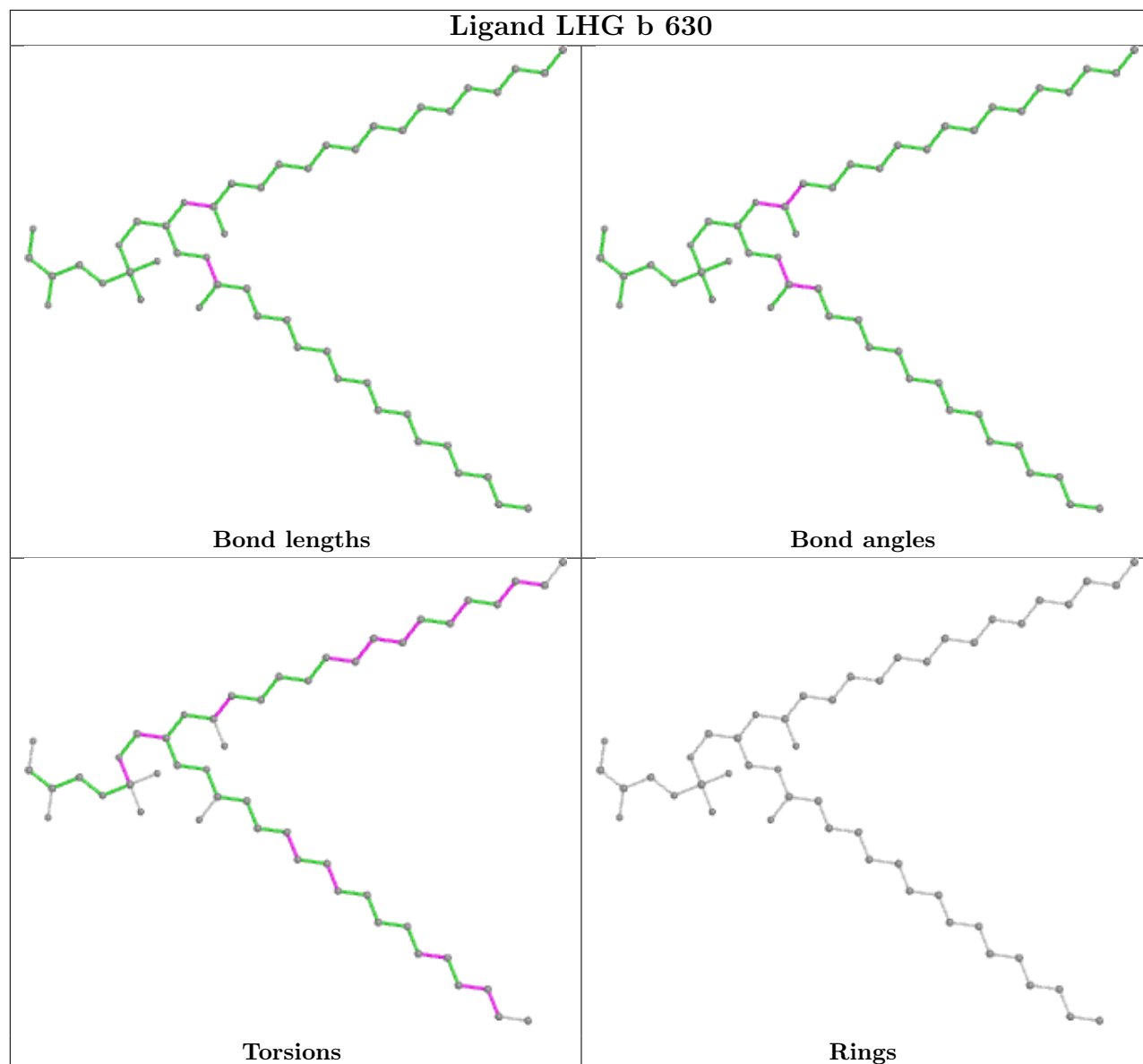




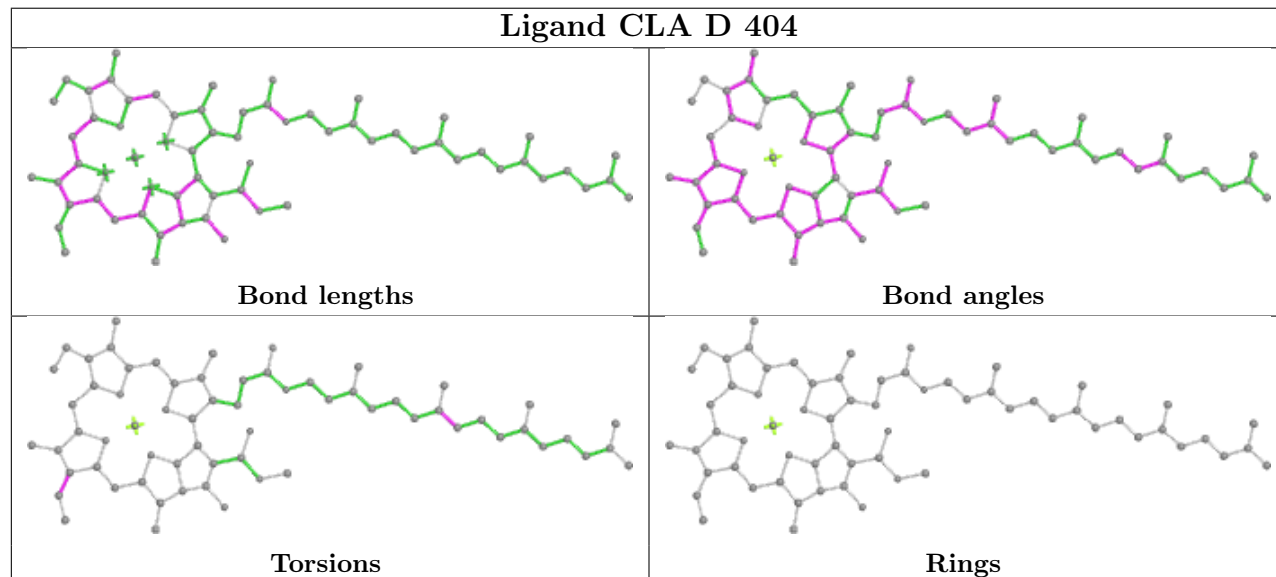
**Ligand CLA b 613****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA D 401****Bond lengths****Bond angles****Torsions****Rings**



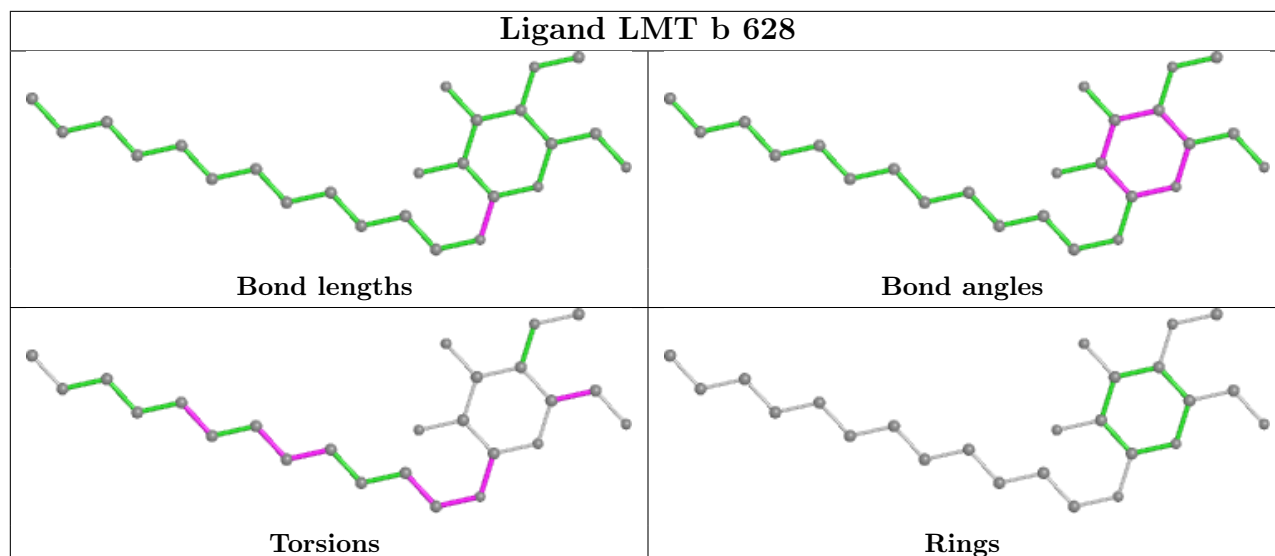
## Ligand LHG b 630



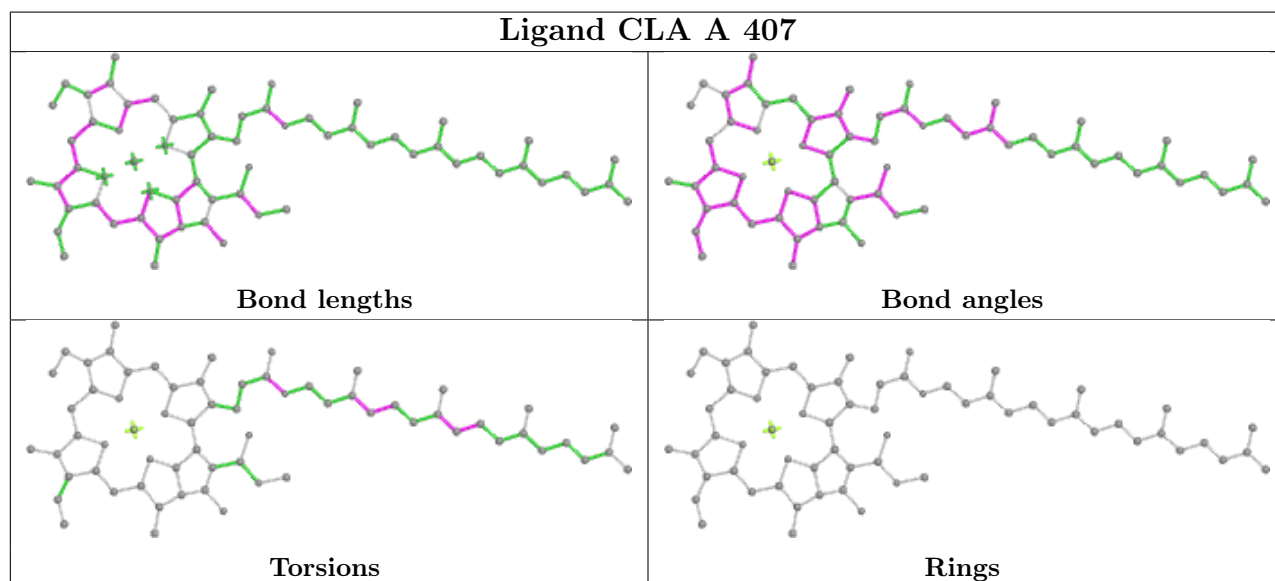
## Ligand CLA D 404



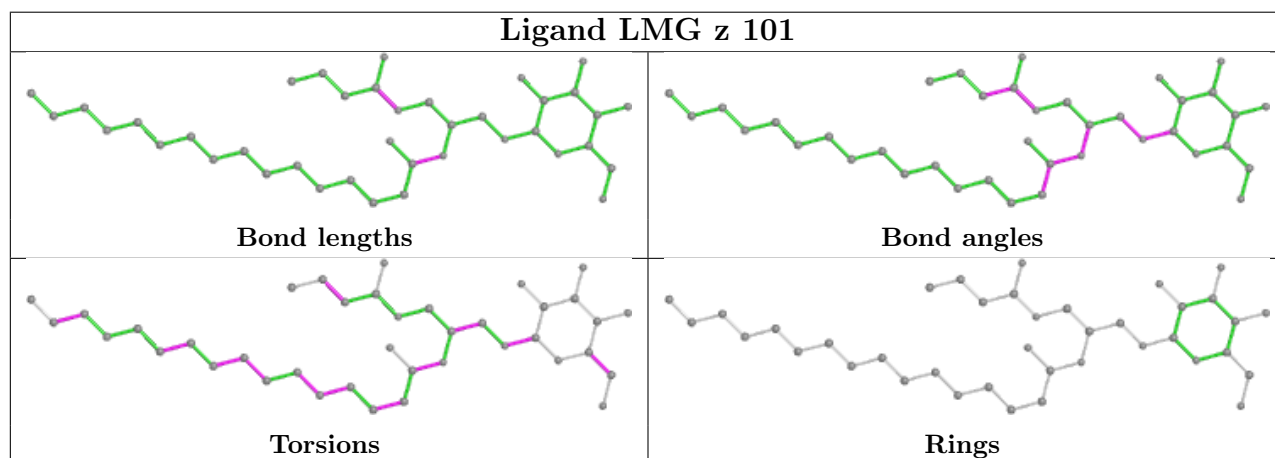
## Ligand LMT b 628

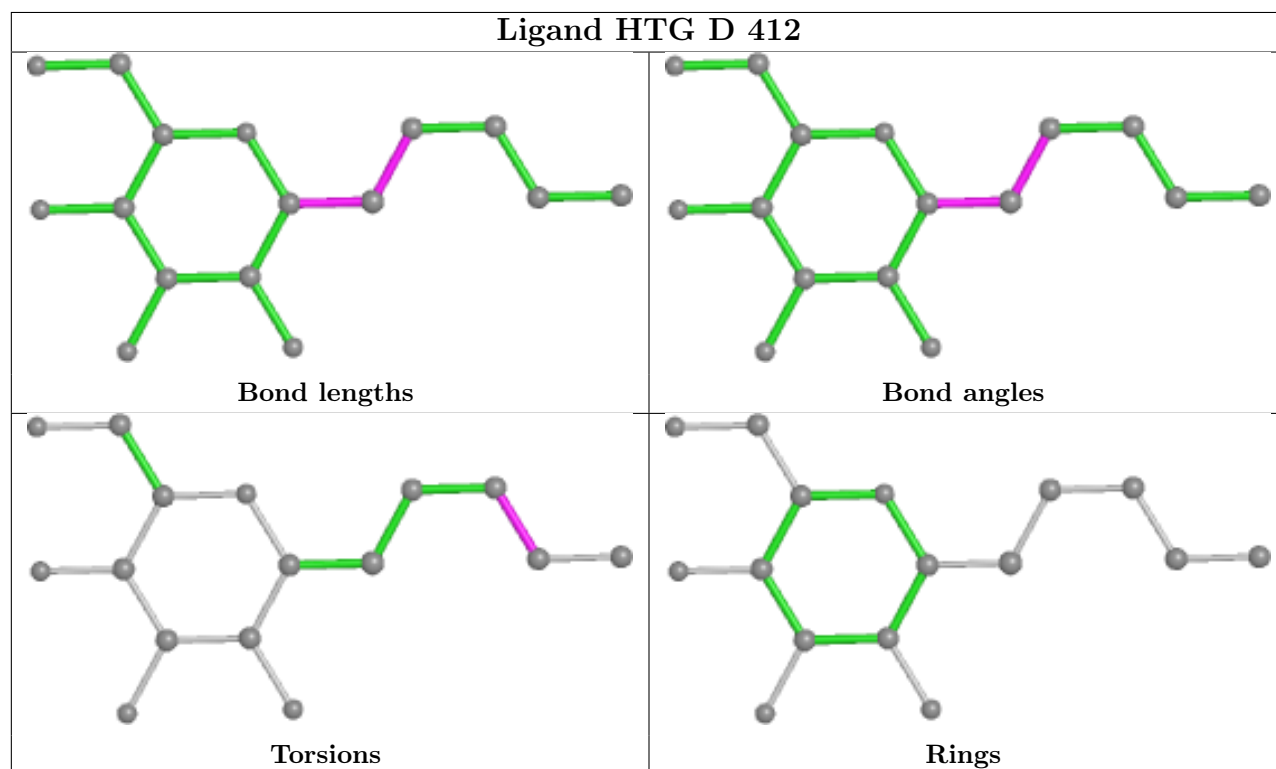
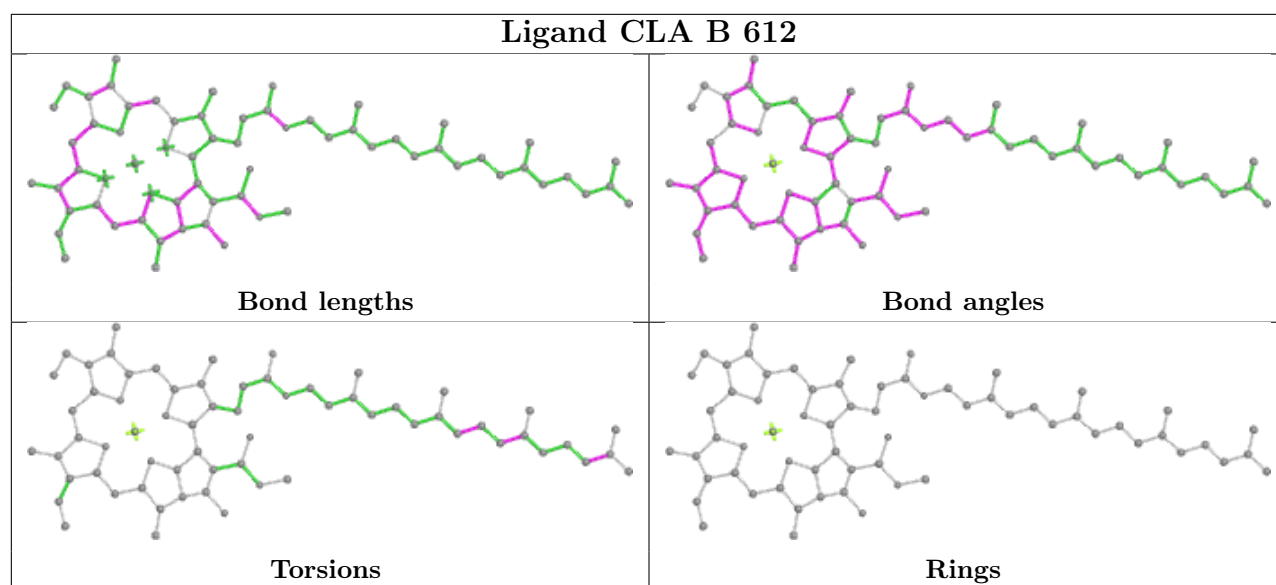


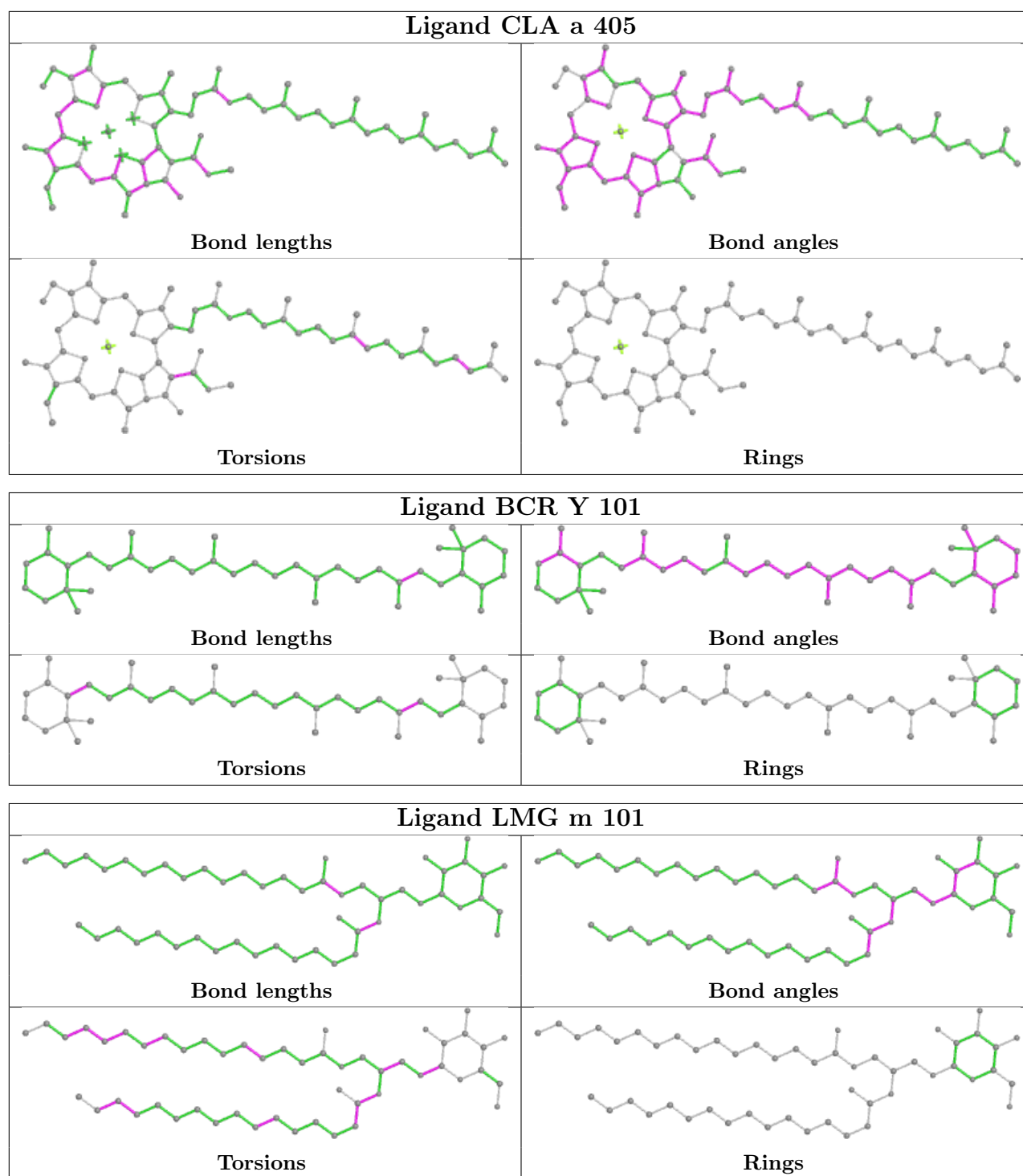
## Ligand CLA A 407



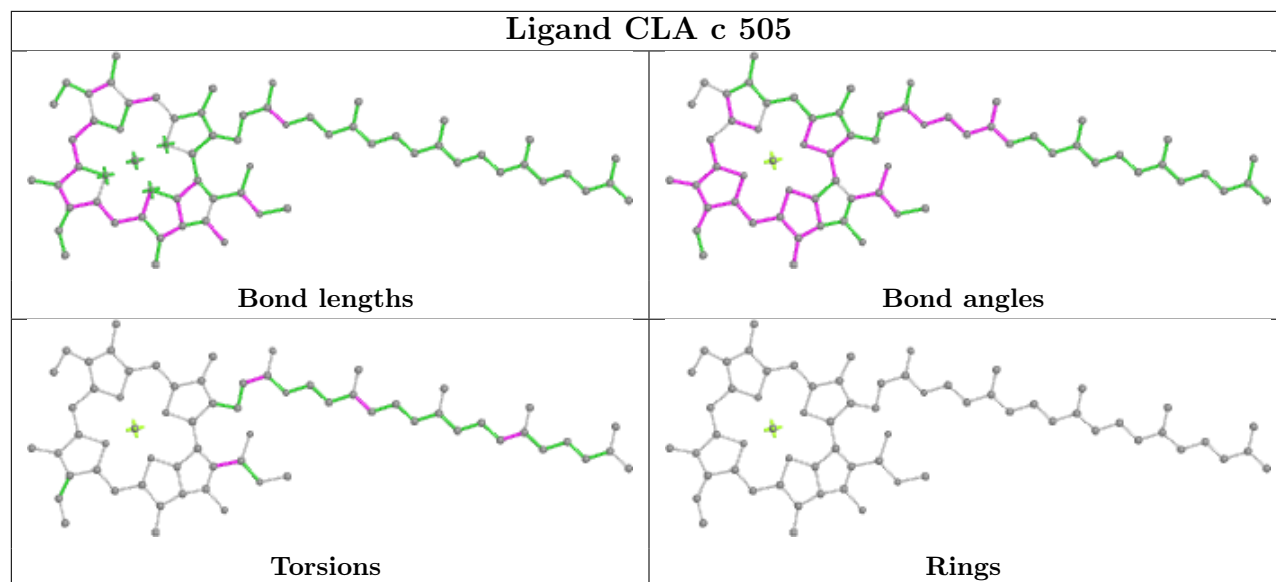
## Ligand LMG z 101



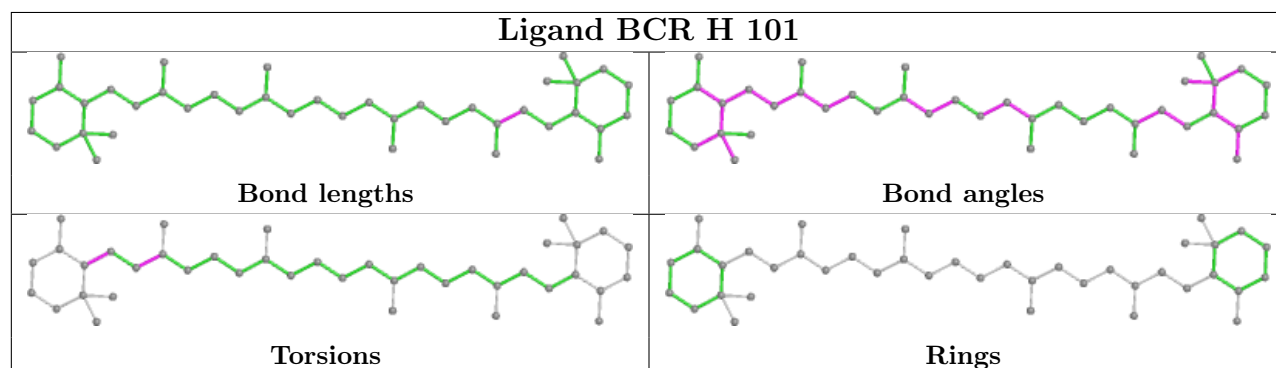




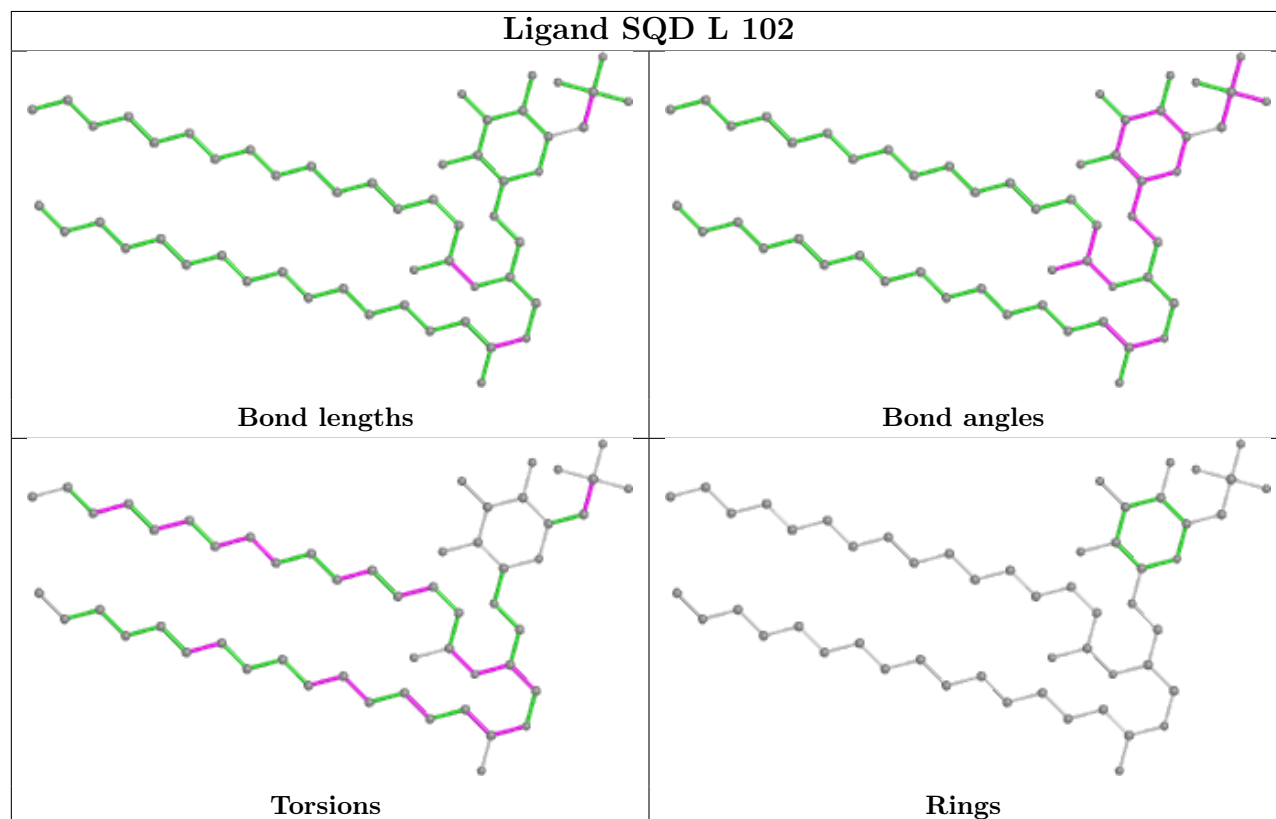
## Ligand CLA c 505

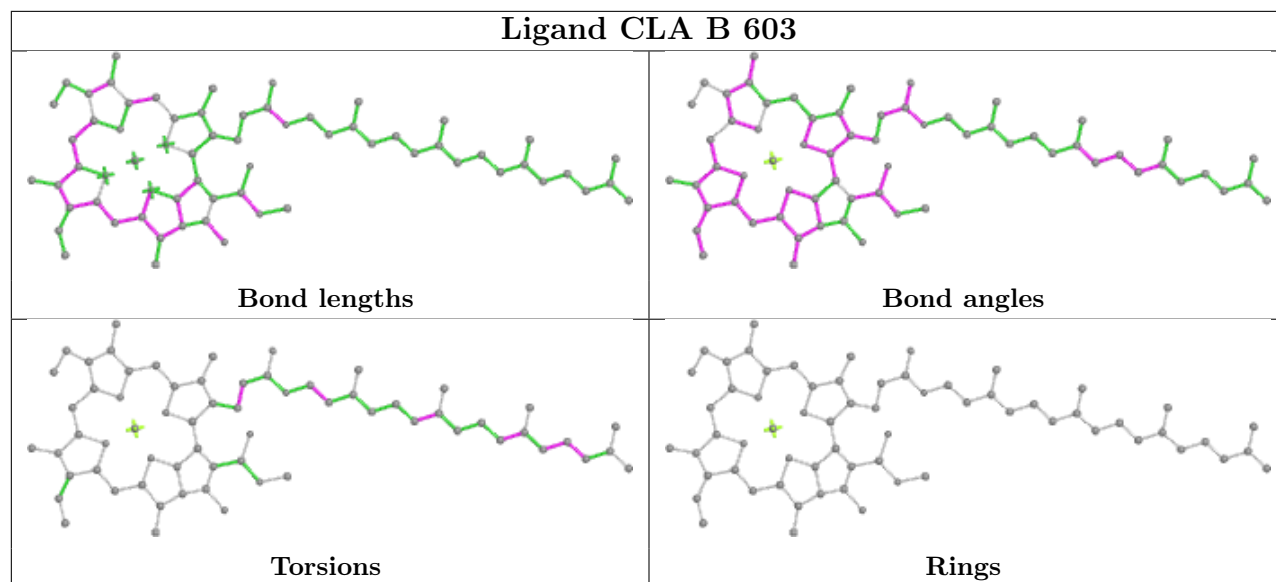
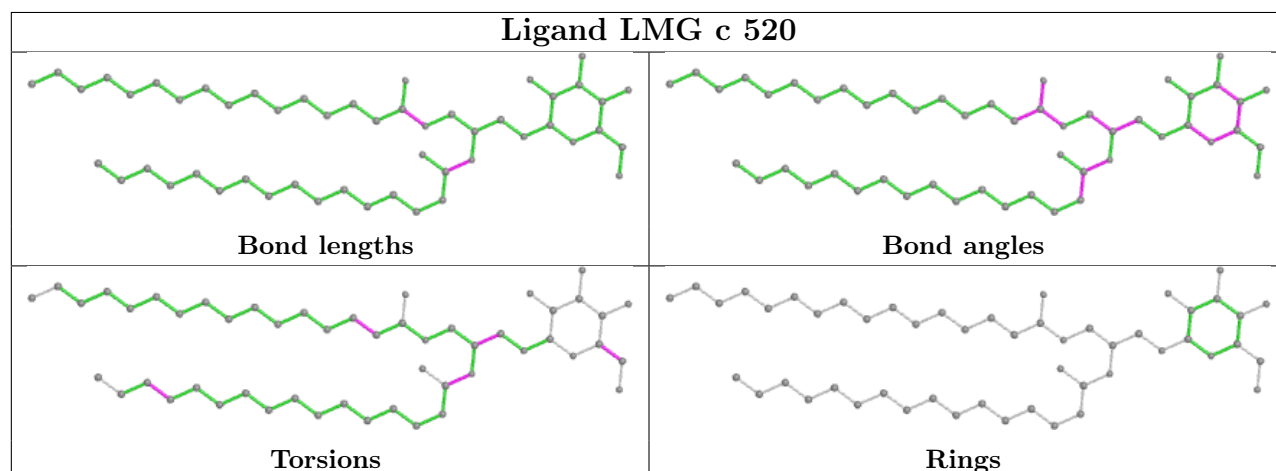
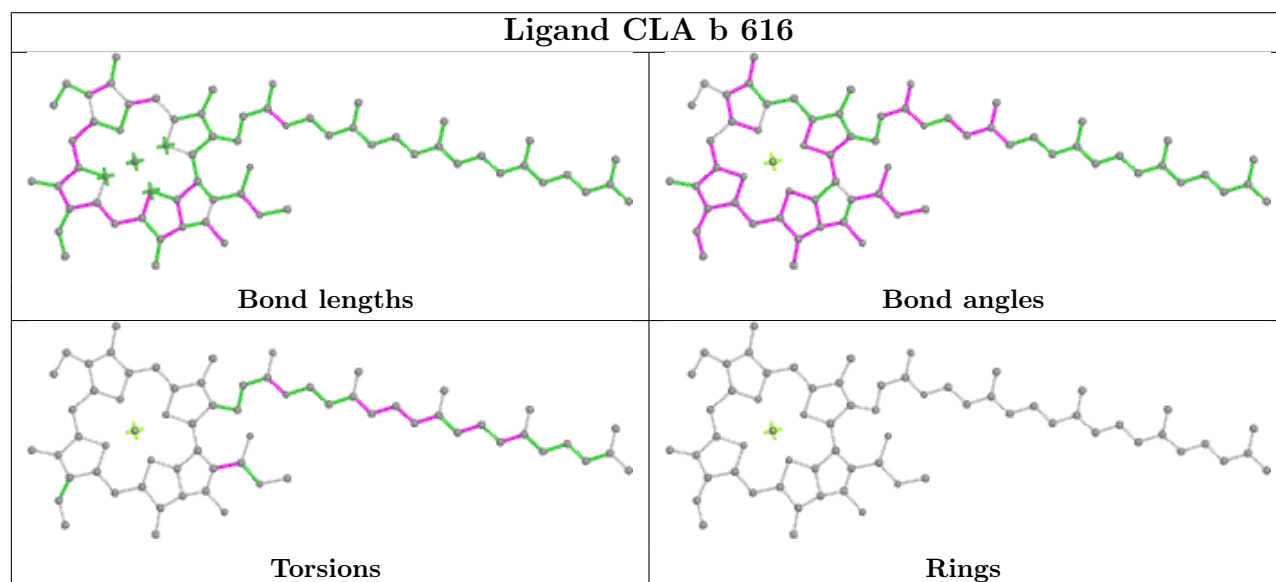


## Ligand BCR H 101

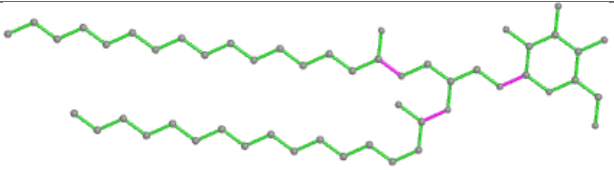
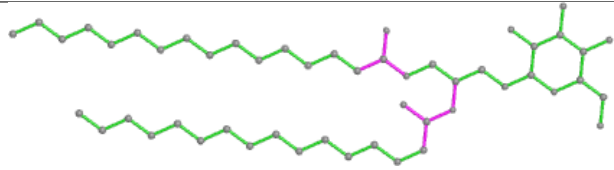
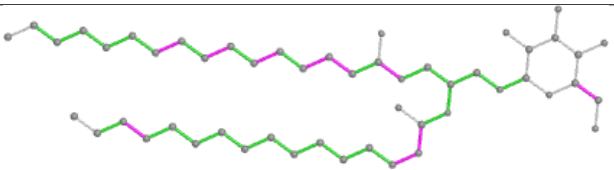
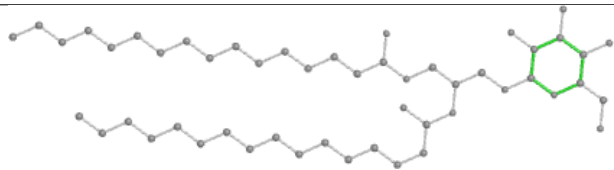


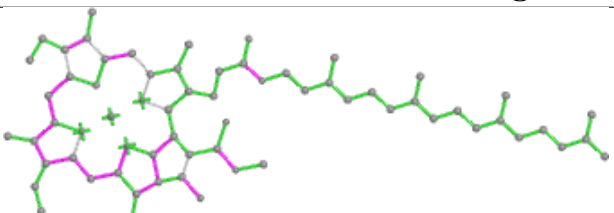
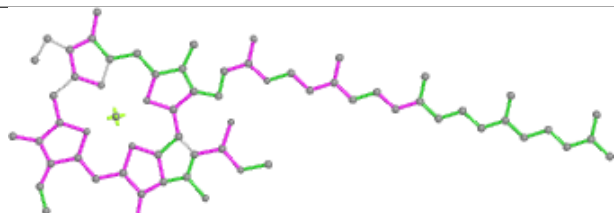
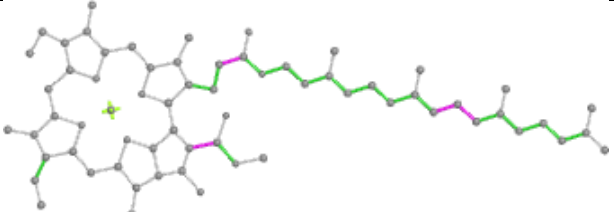
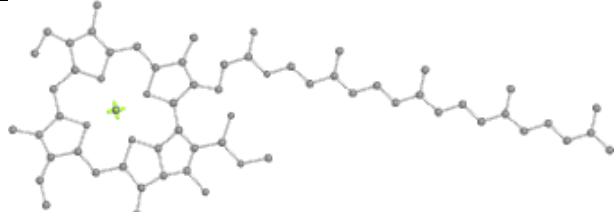
## Ligand SQD L 102

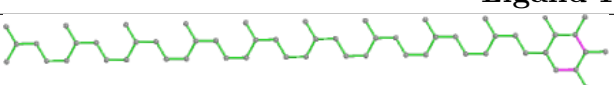
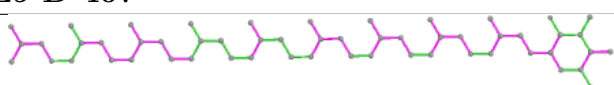
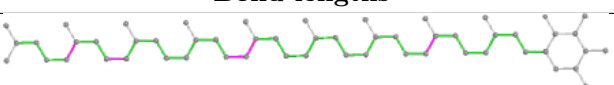
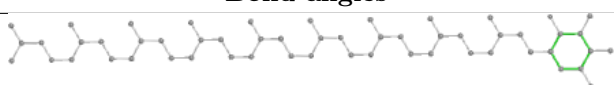


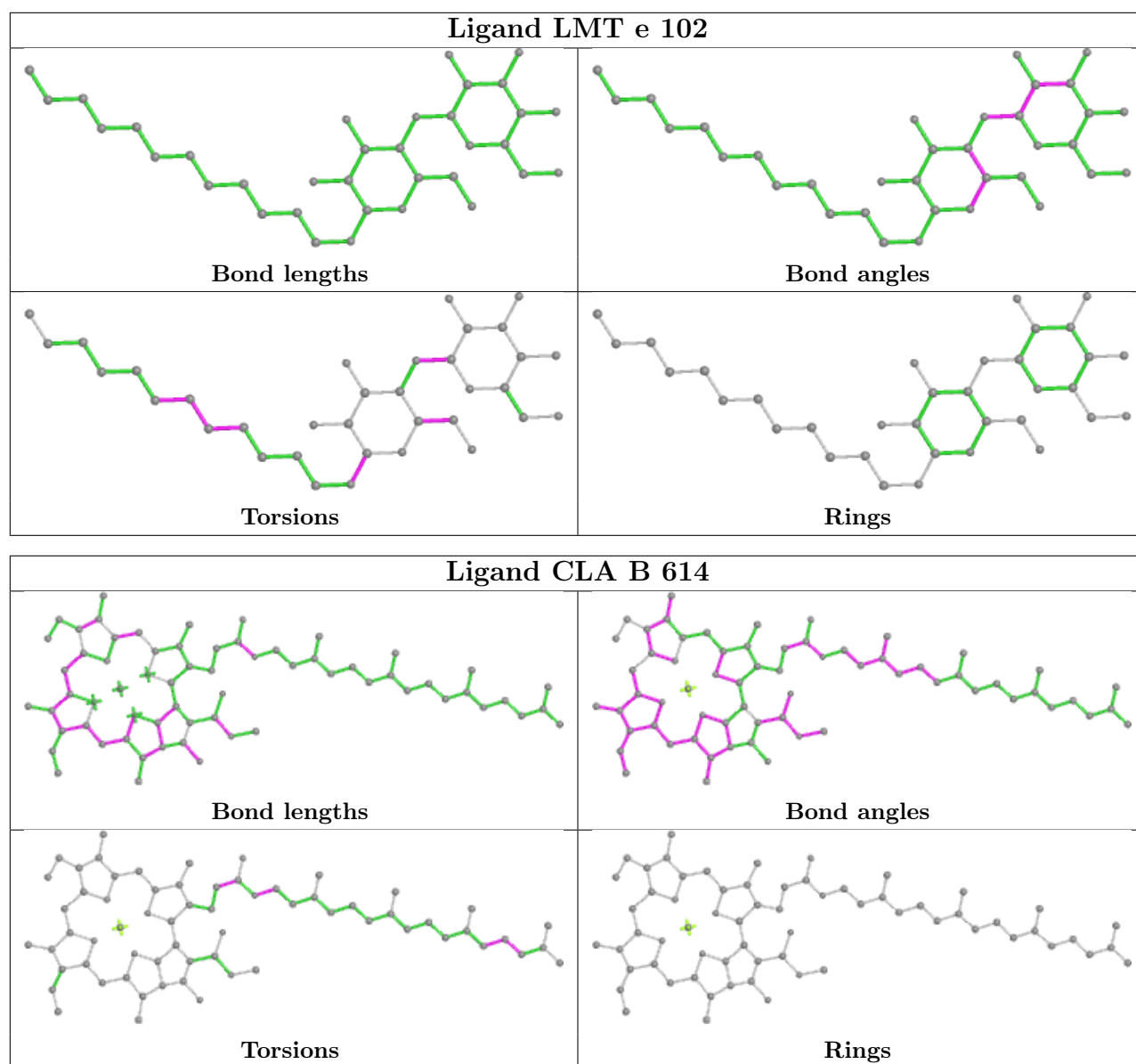
**Ligand CLA B 603****Ligand LMG c 520****Ligand CLA b 616**

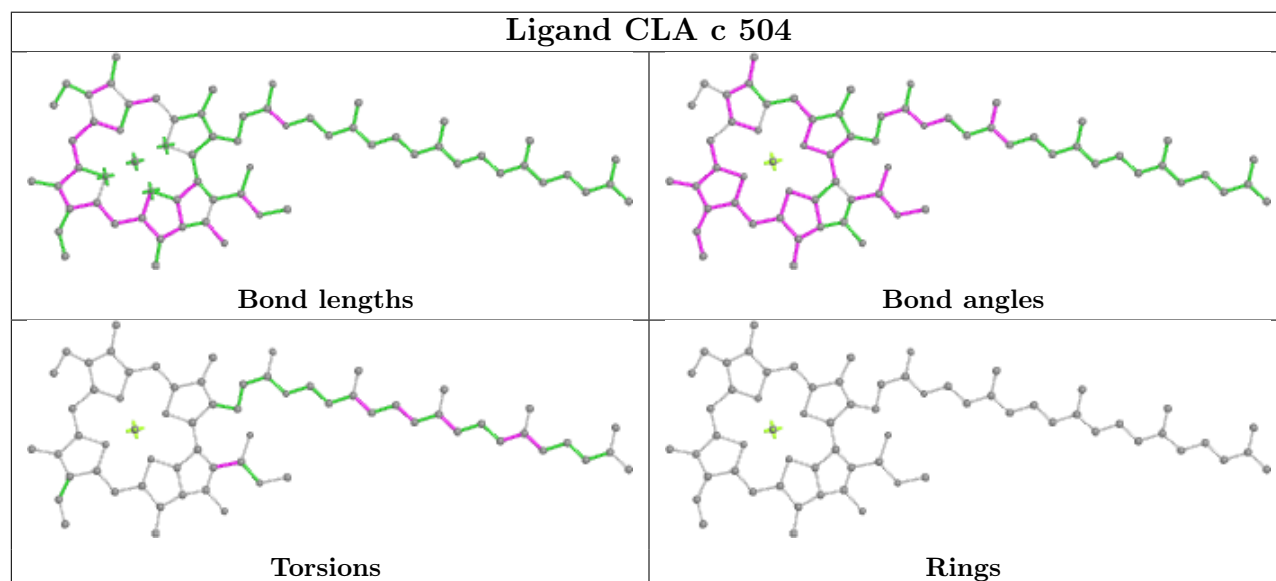
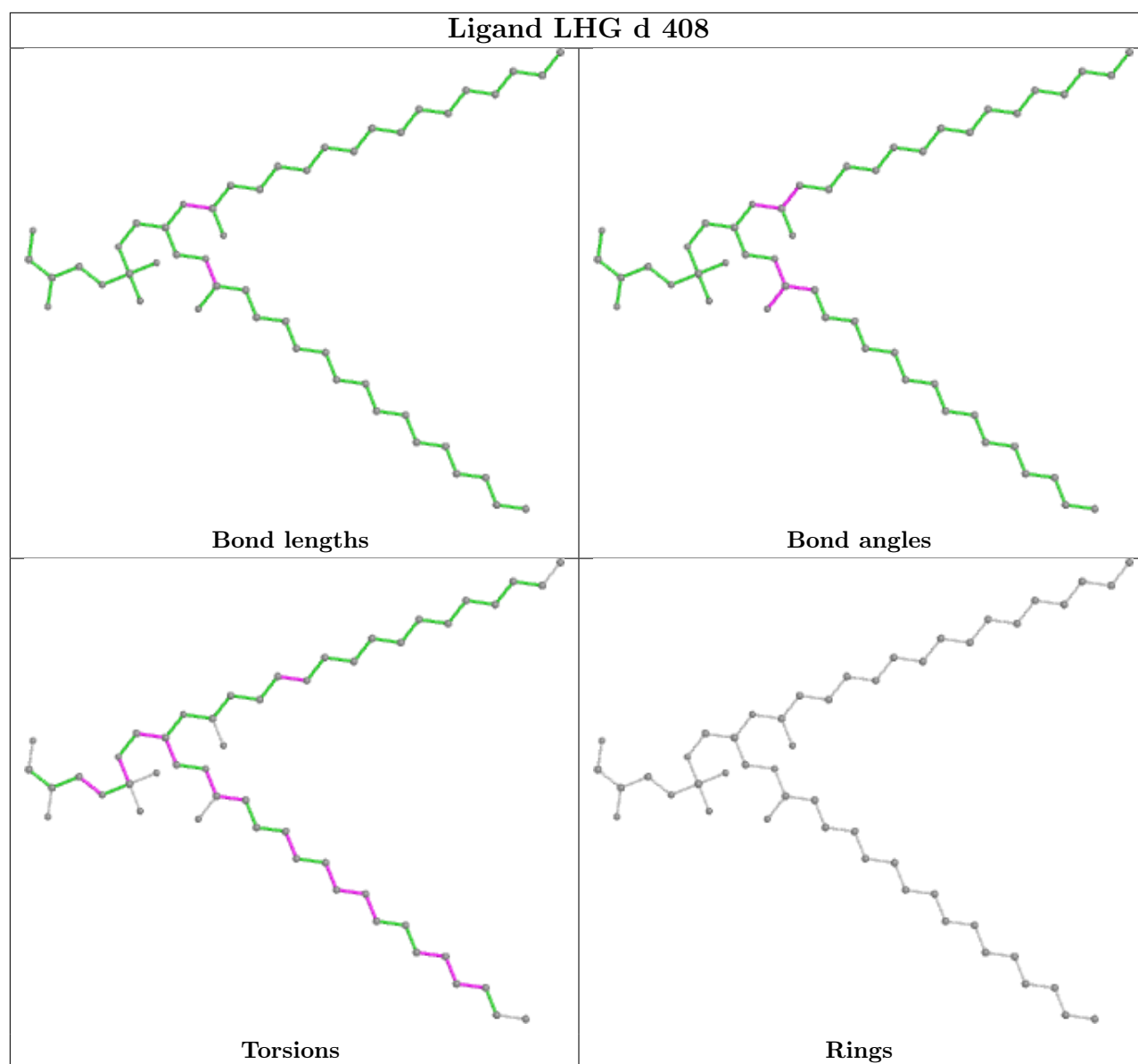


Ligand LMG c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

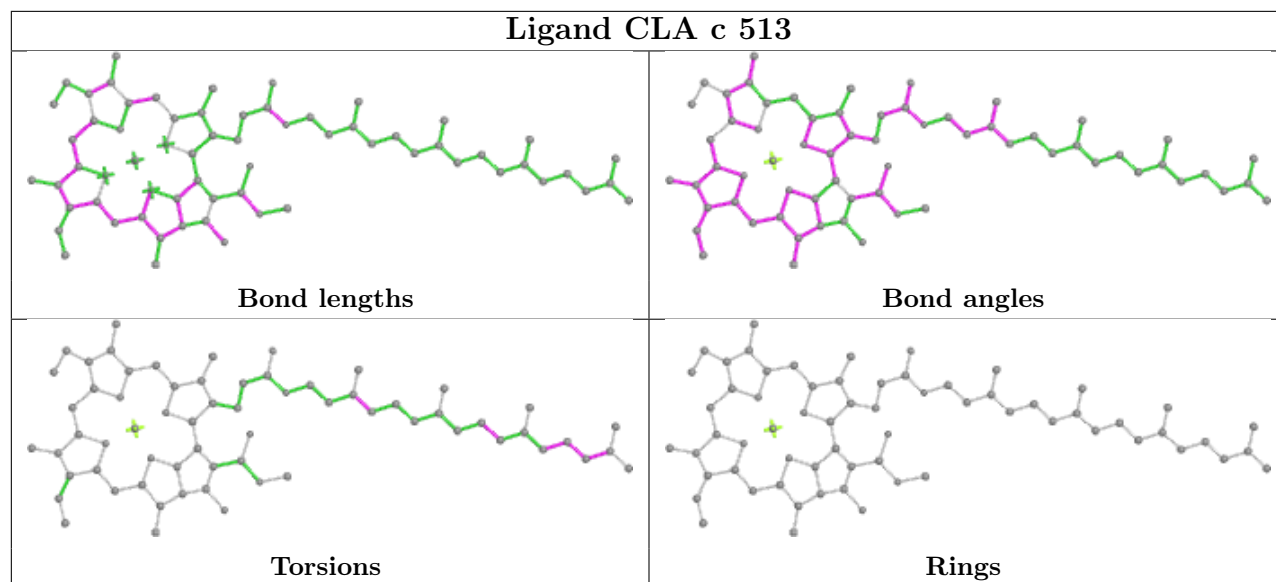
Ligand CLA b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

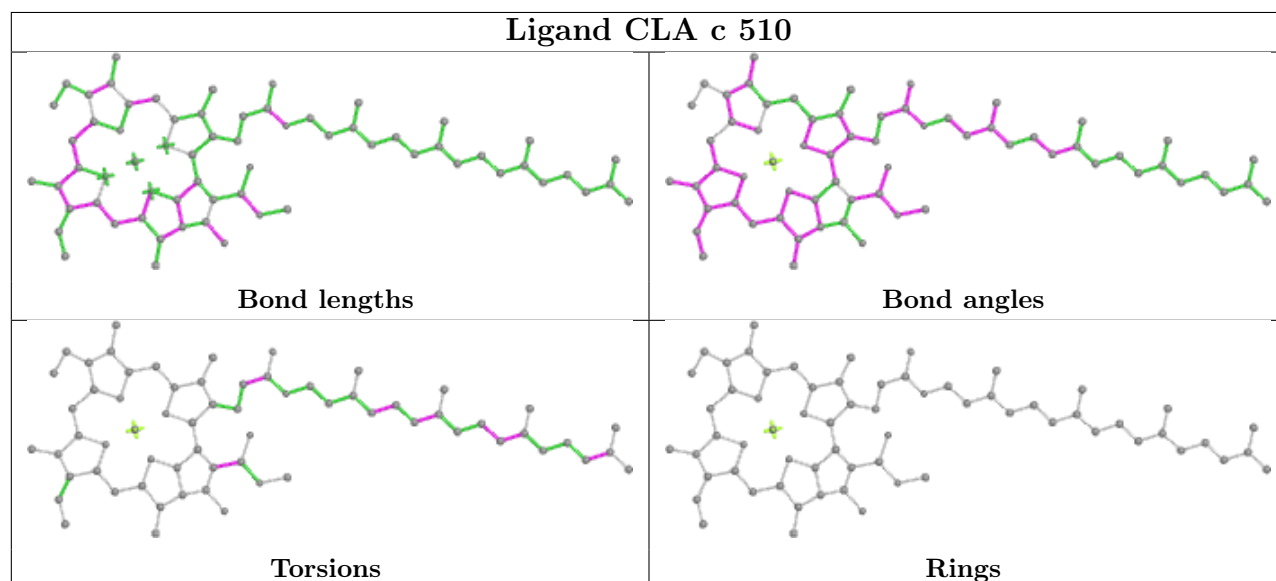




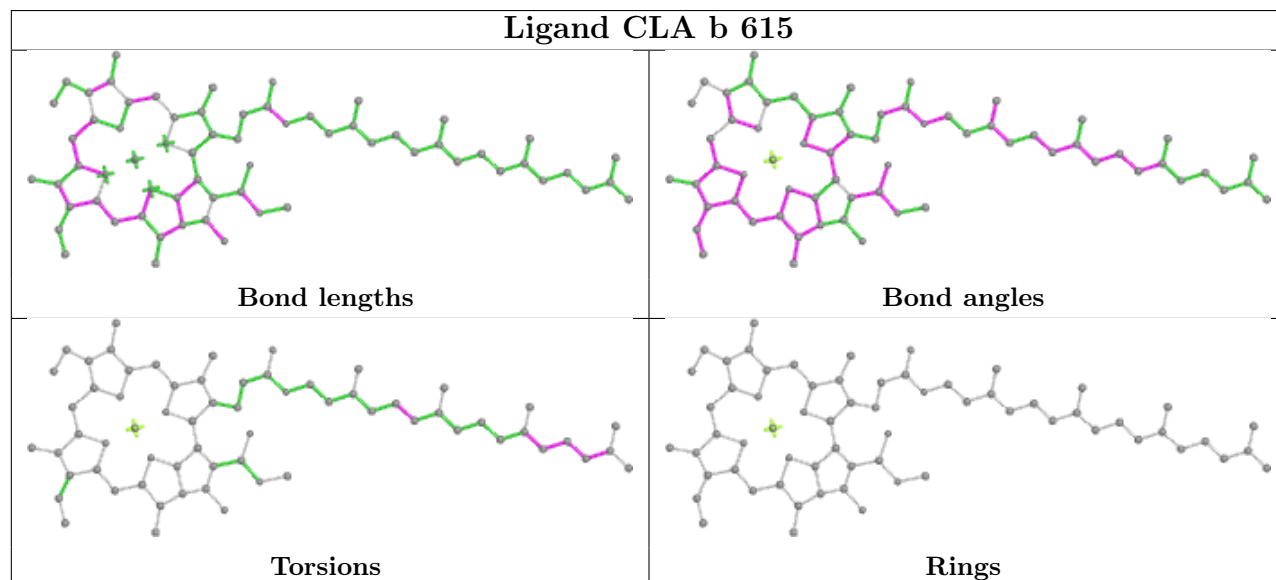
## Ligand CLA c 513

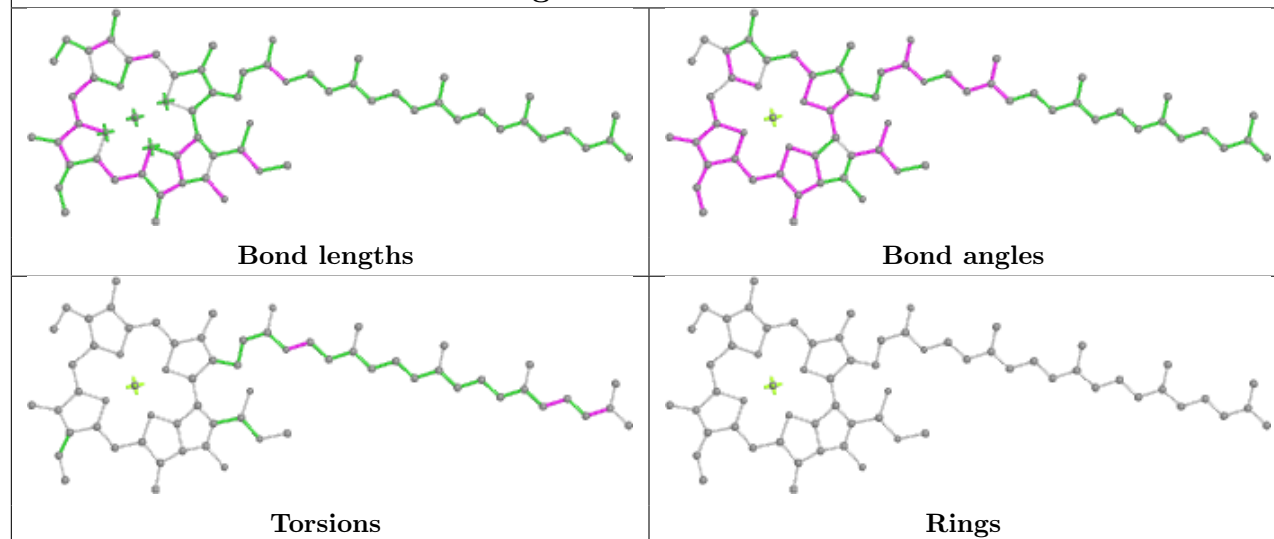
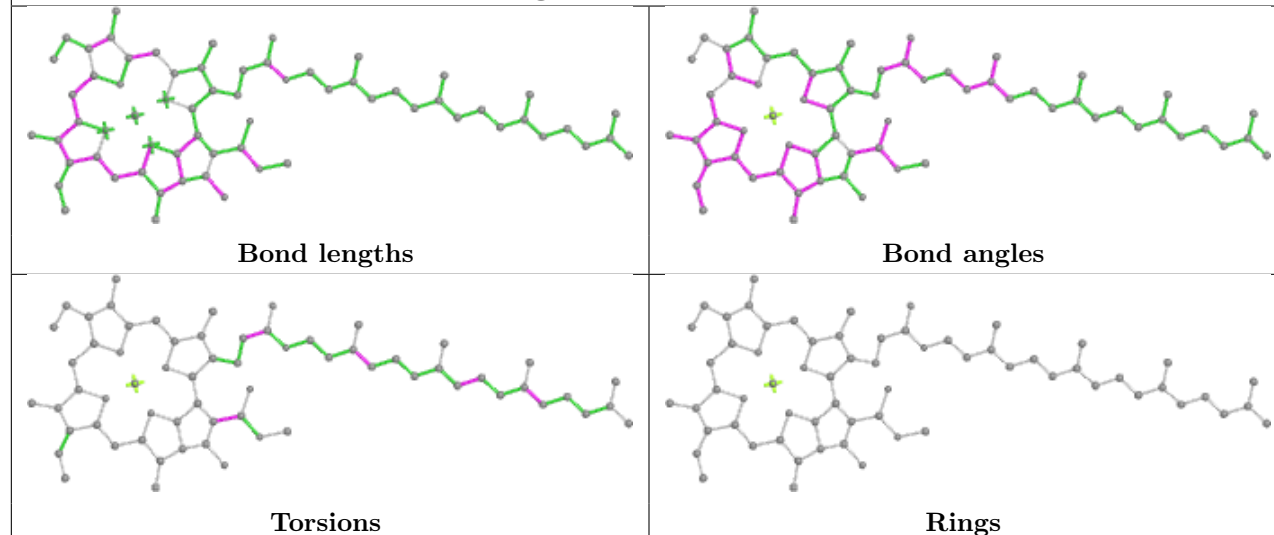
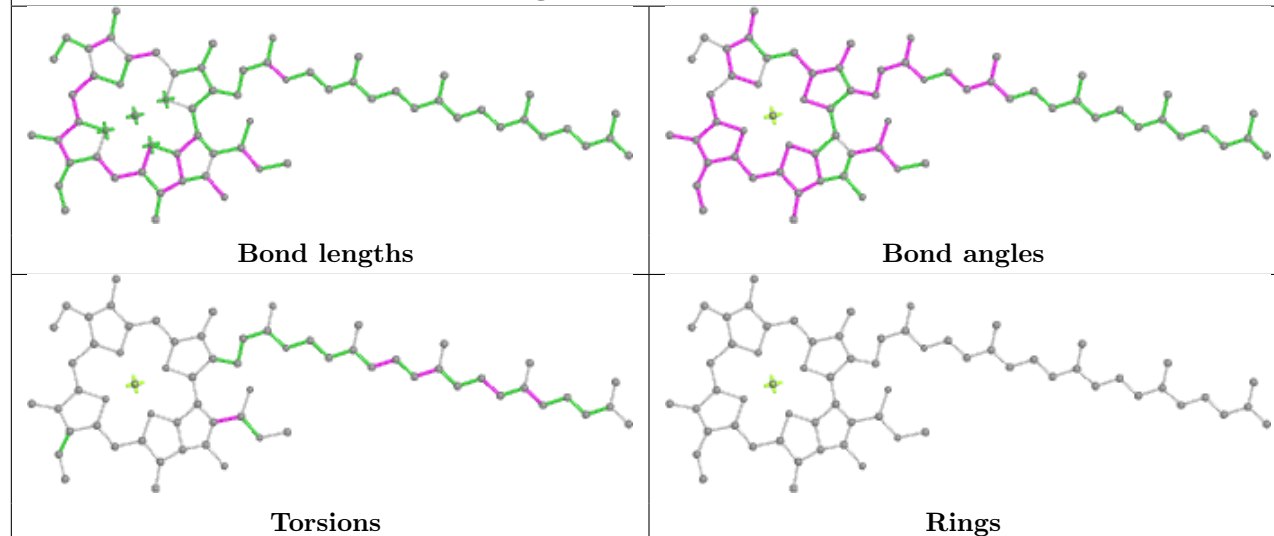


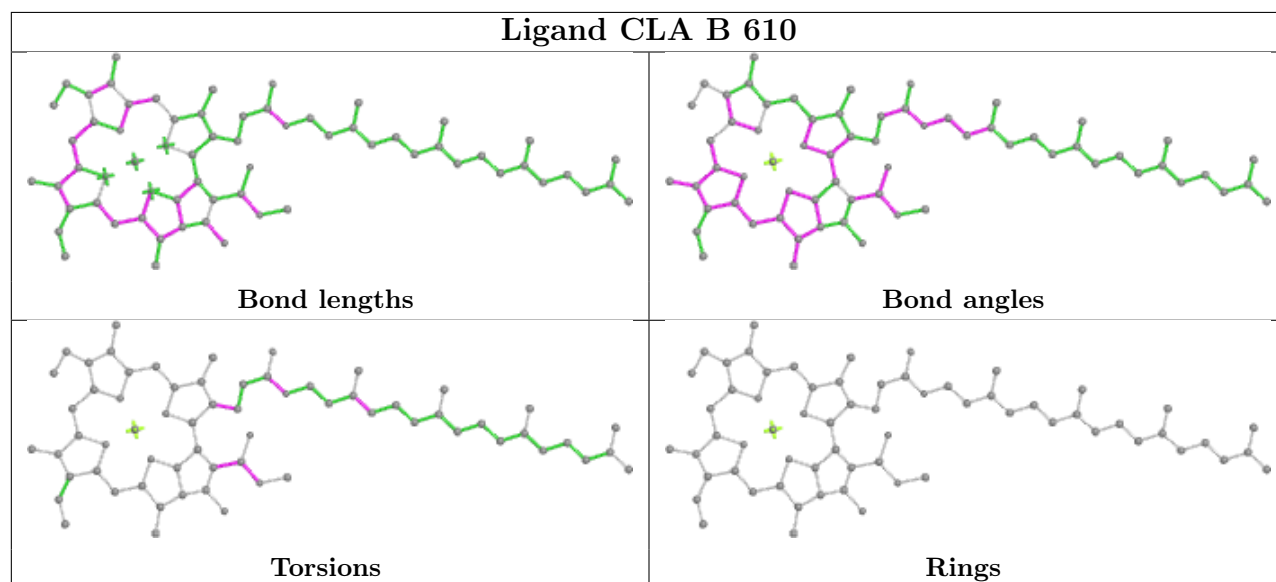
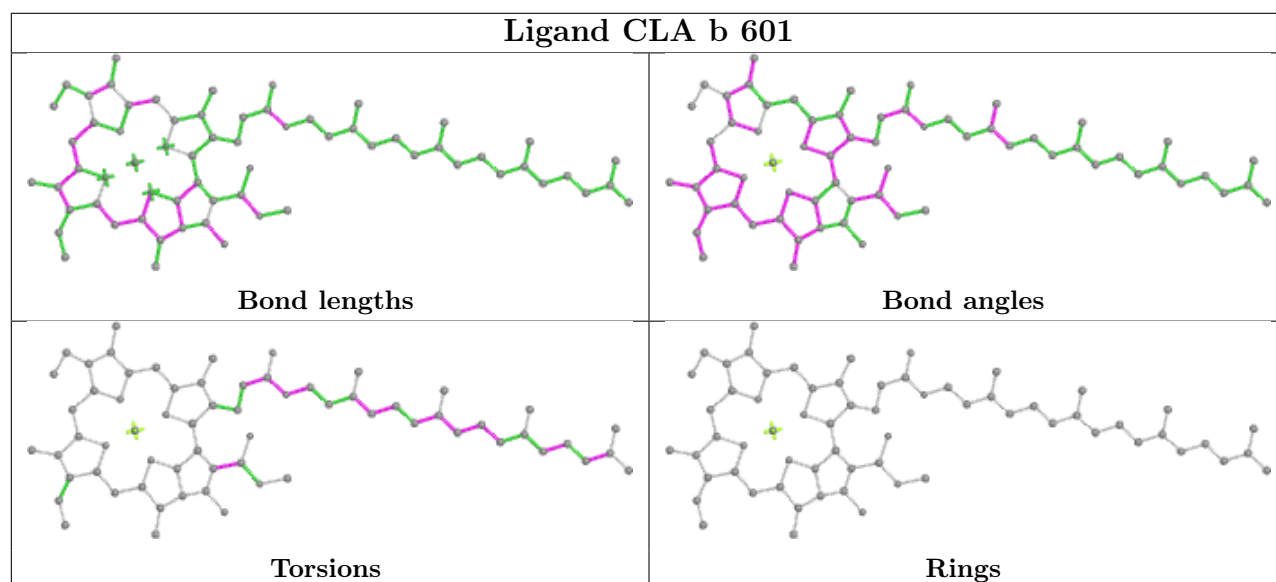
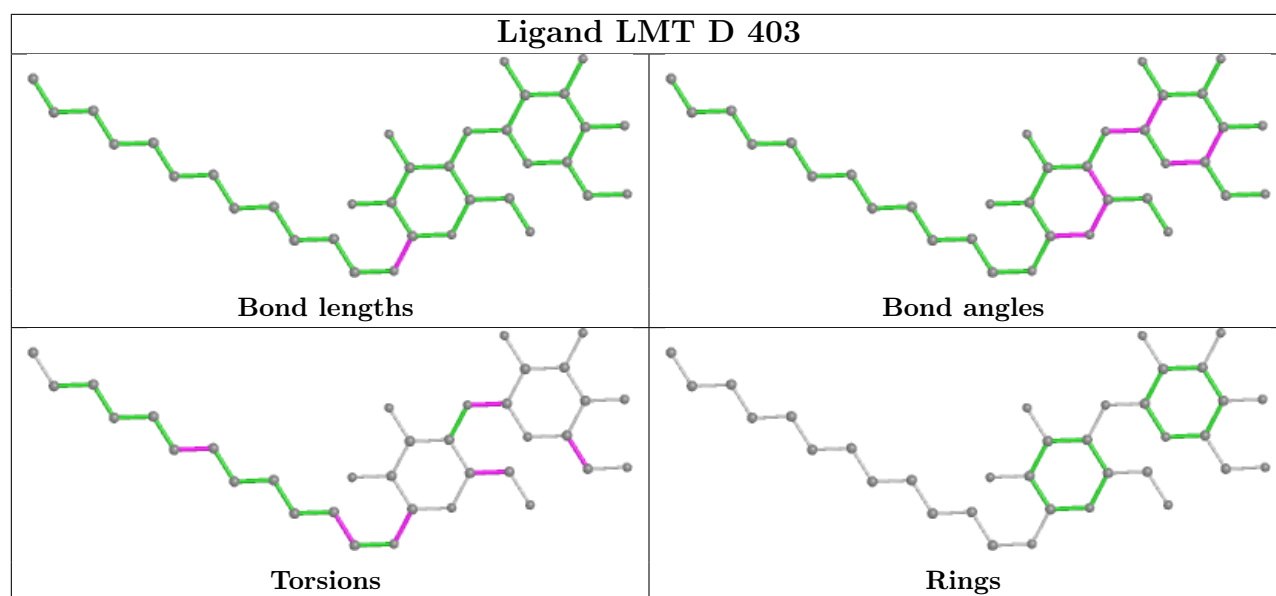
## Ligand CLA c 510

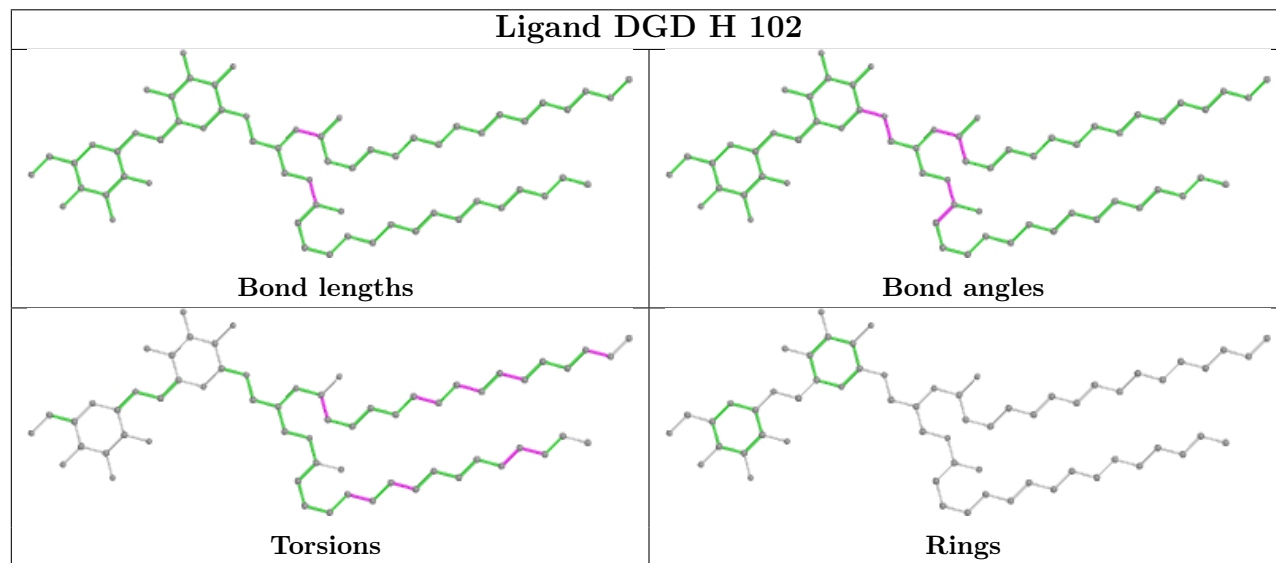
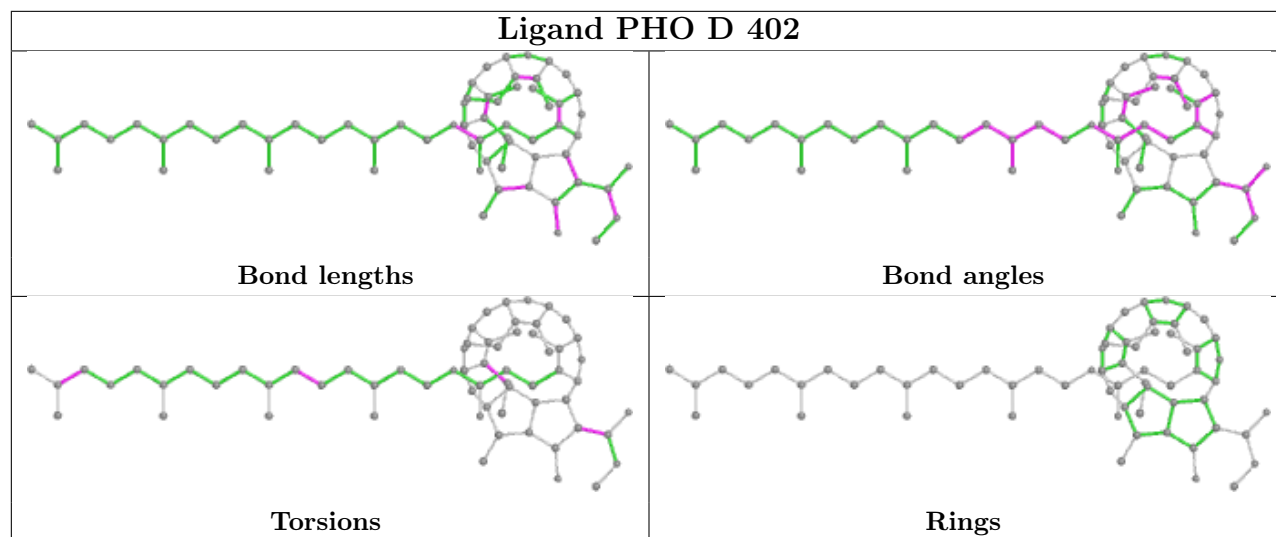
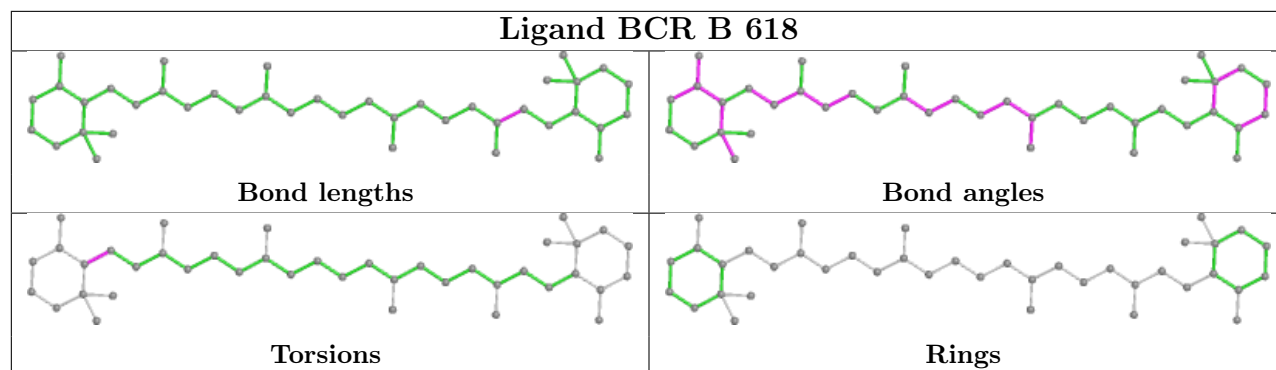


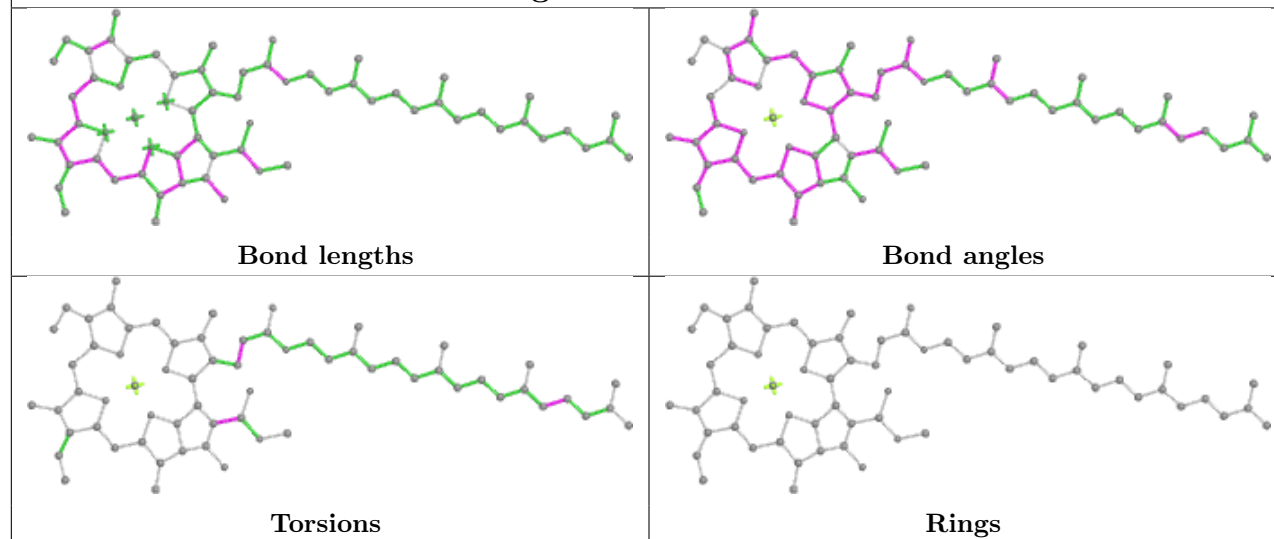
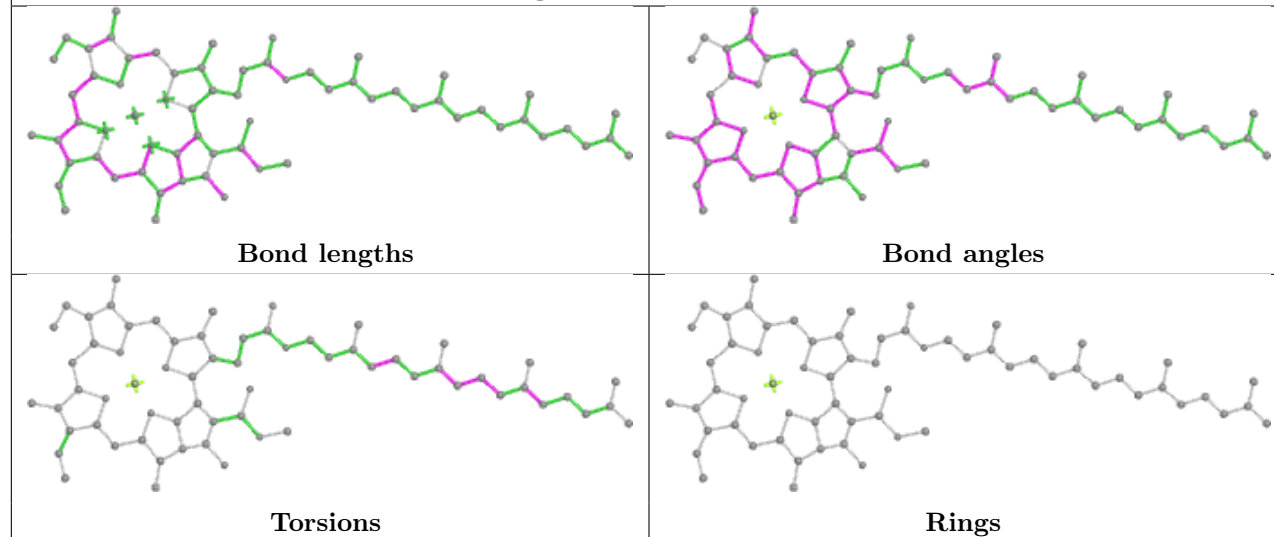
## Ligand CLA b 615



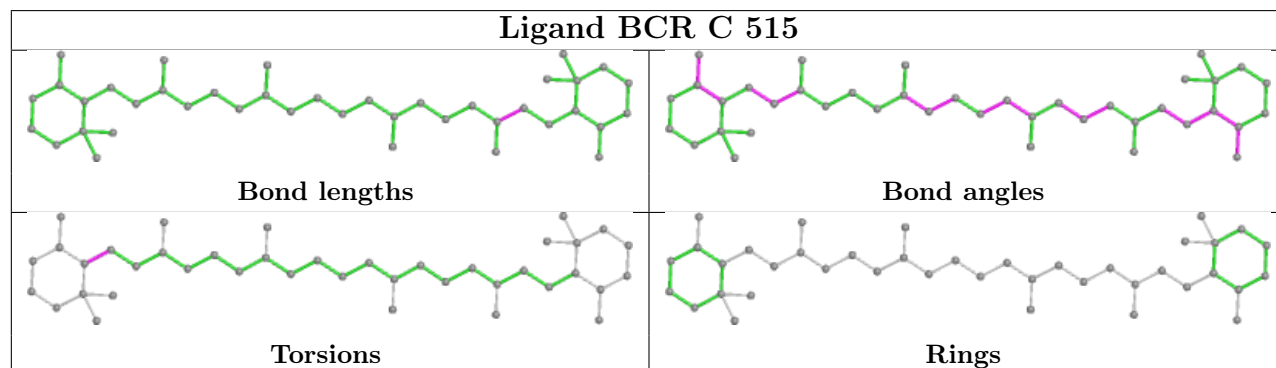
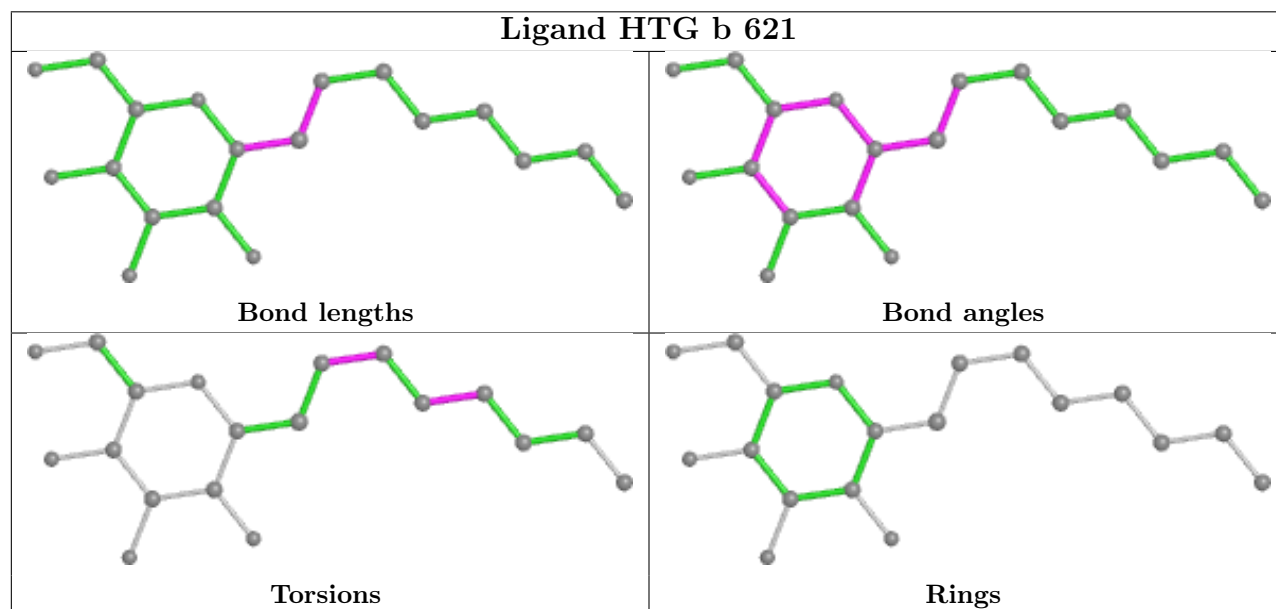
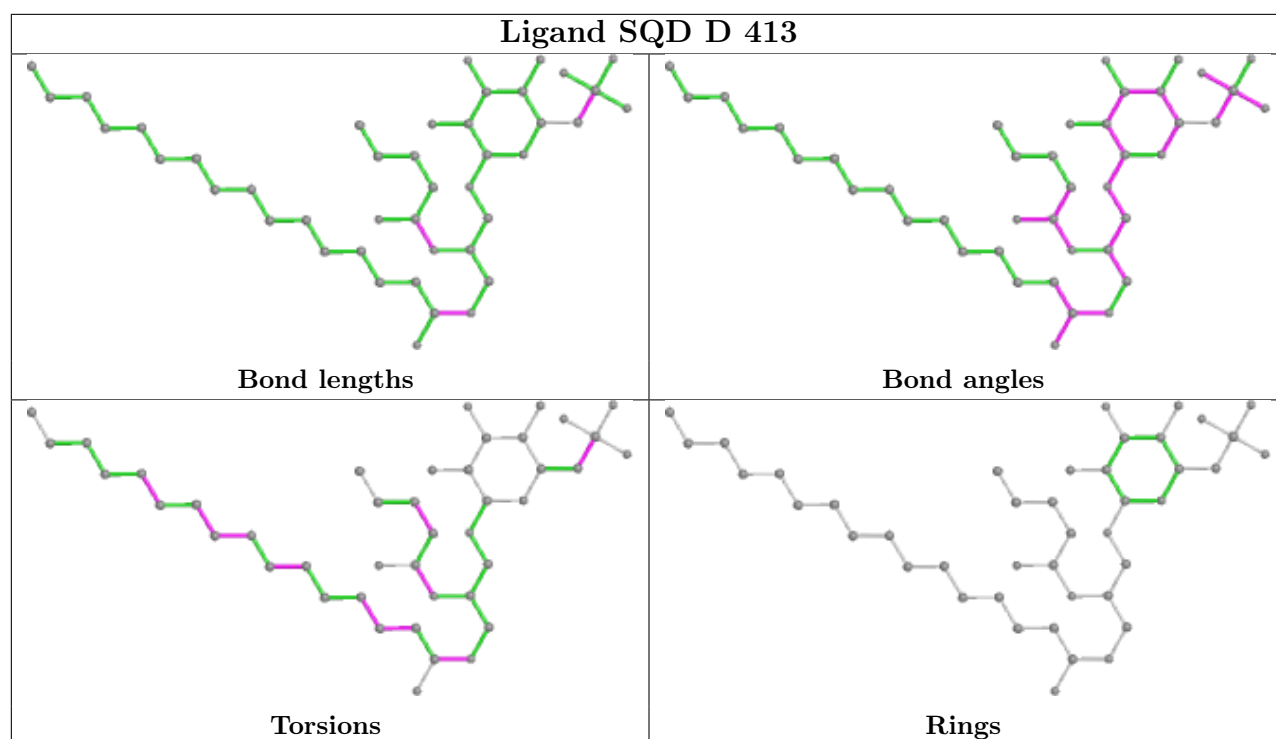
**Ligand CLA B 609****Ligand CLA C 506****Ligand CLA C 513**

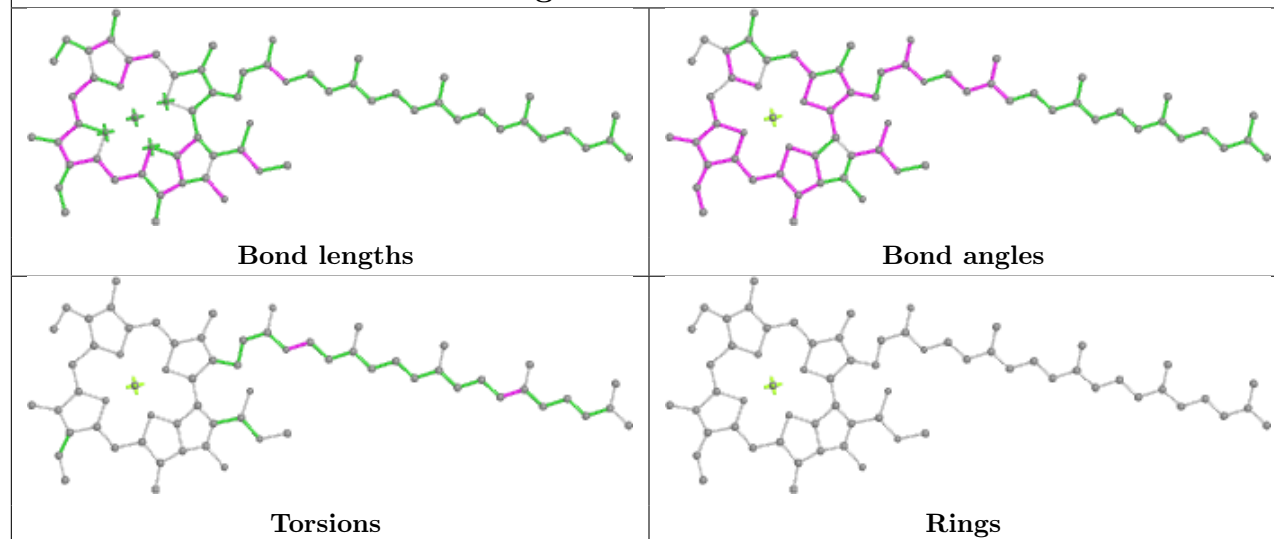
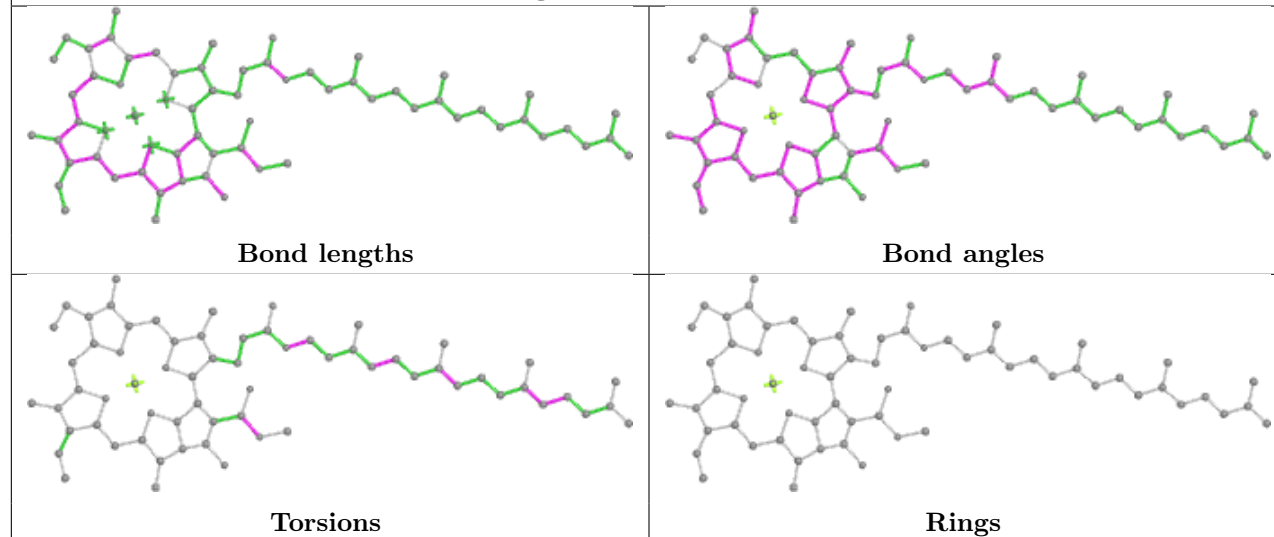


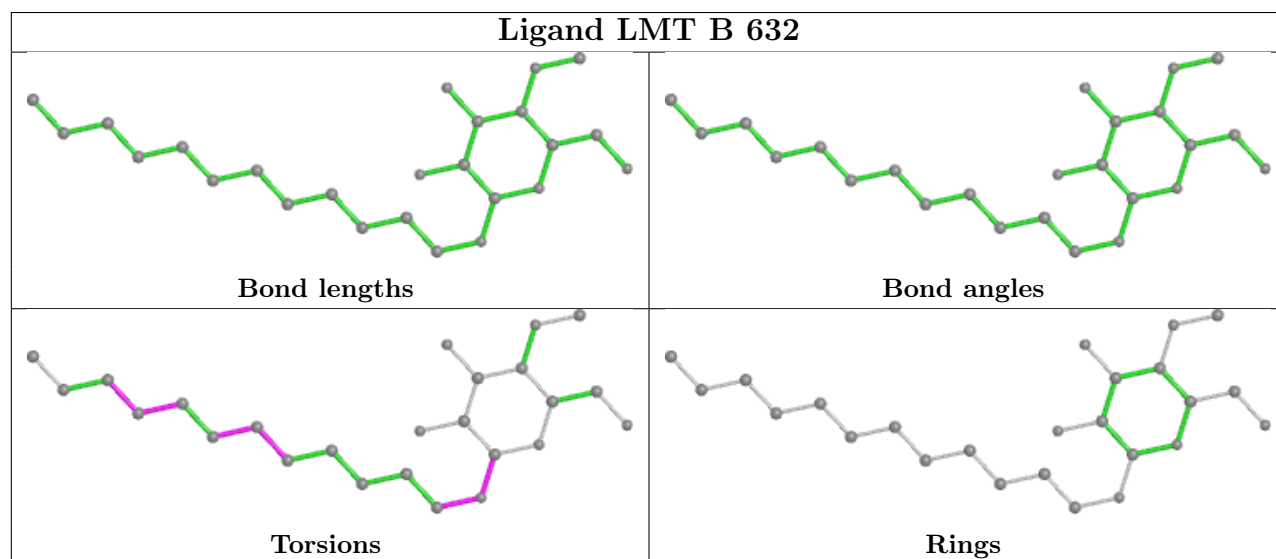
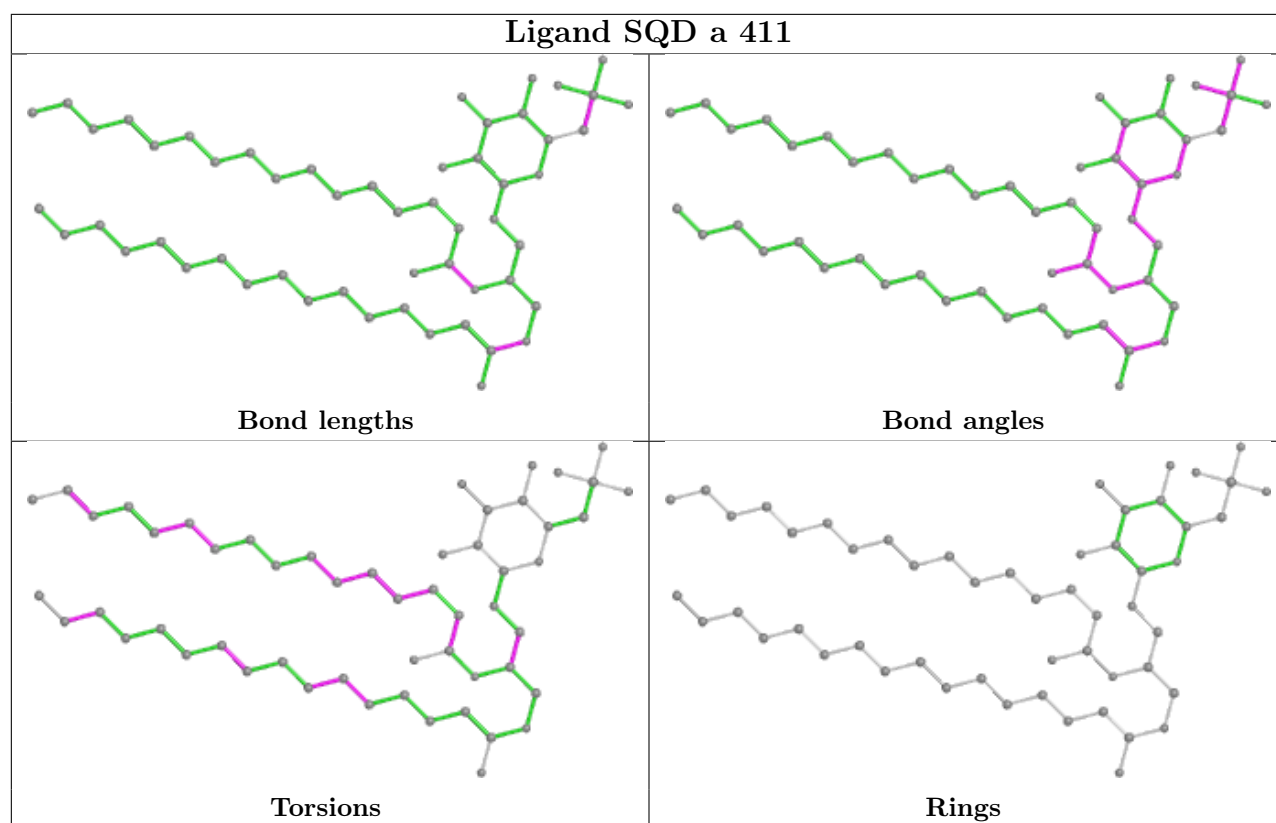


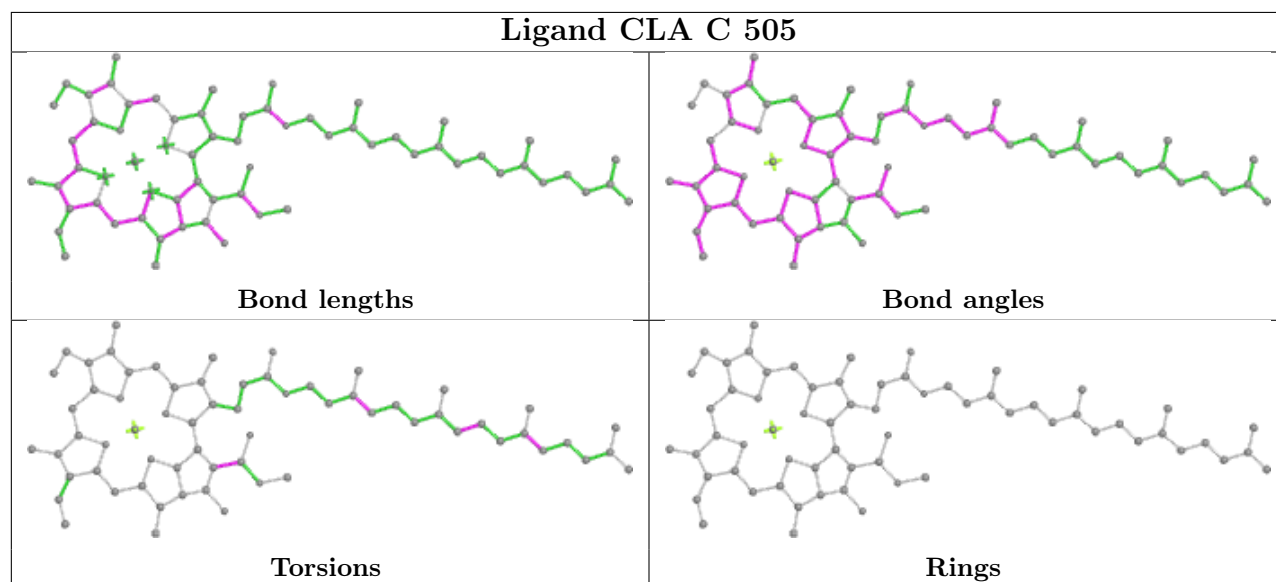
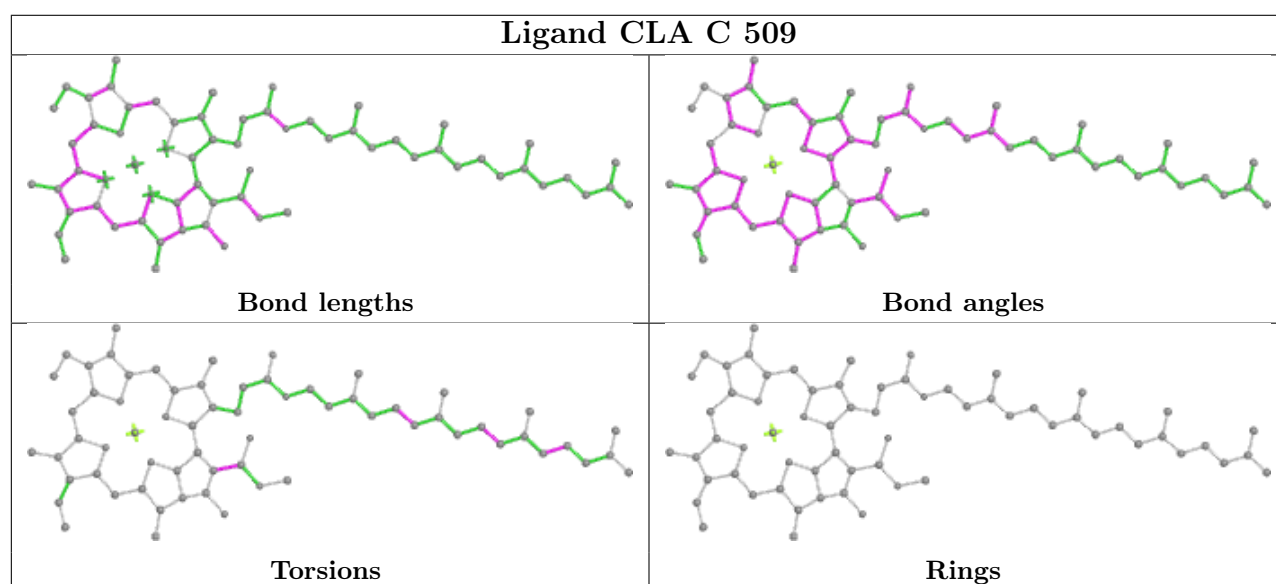
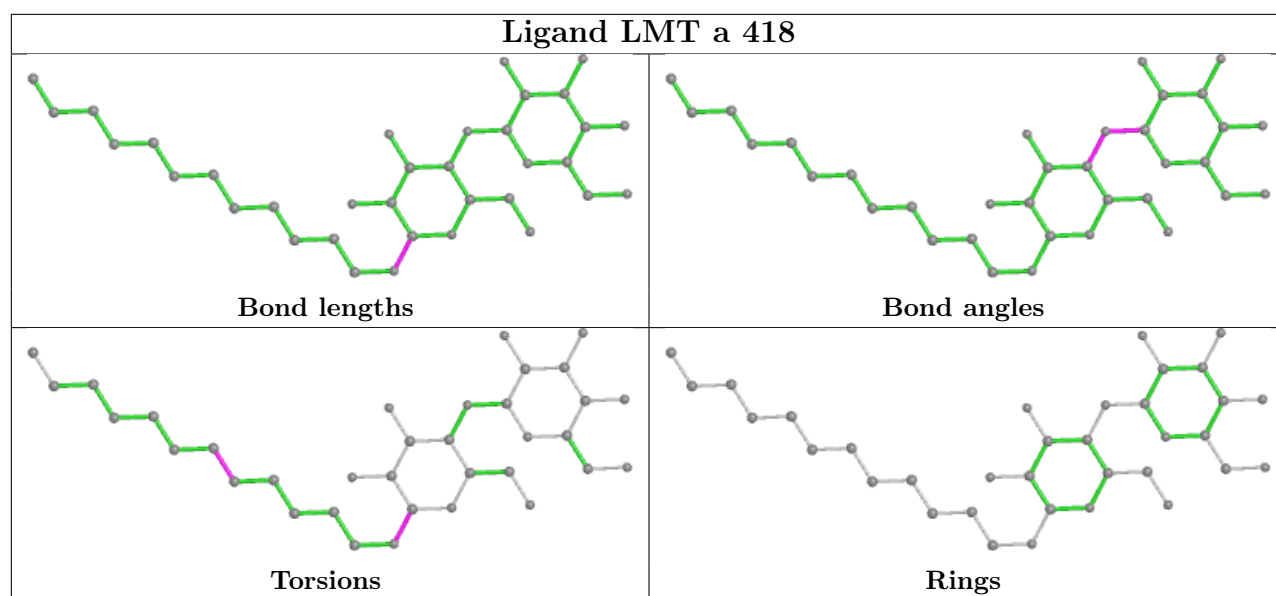
**Ligand CLA A 404****Ligand CLA D 405**

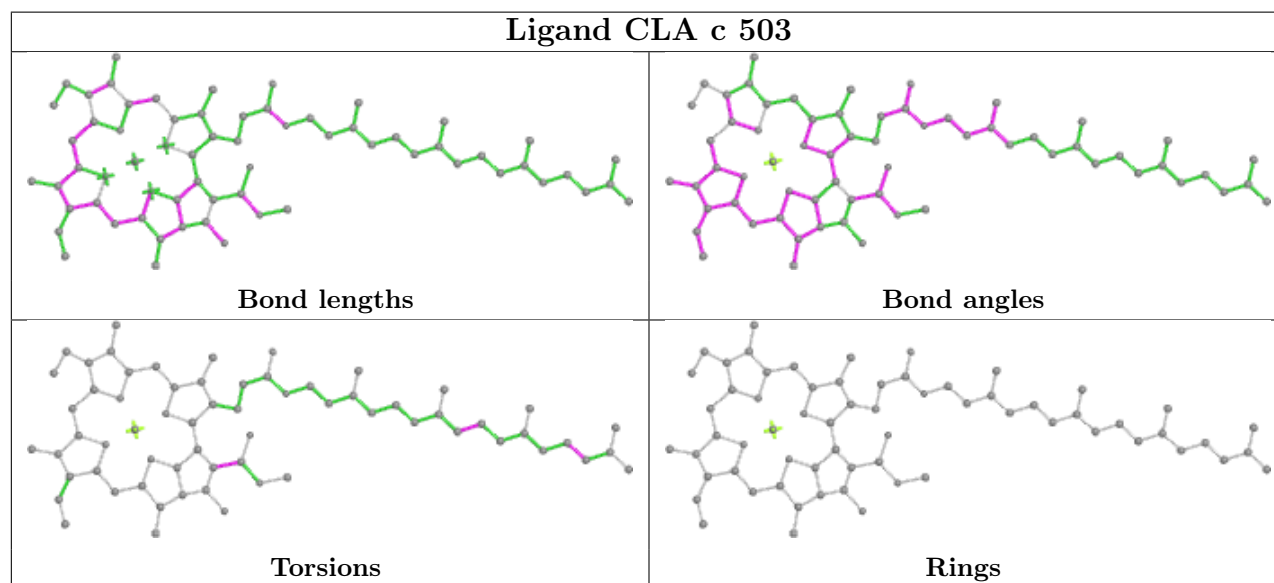
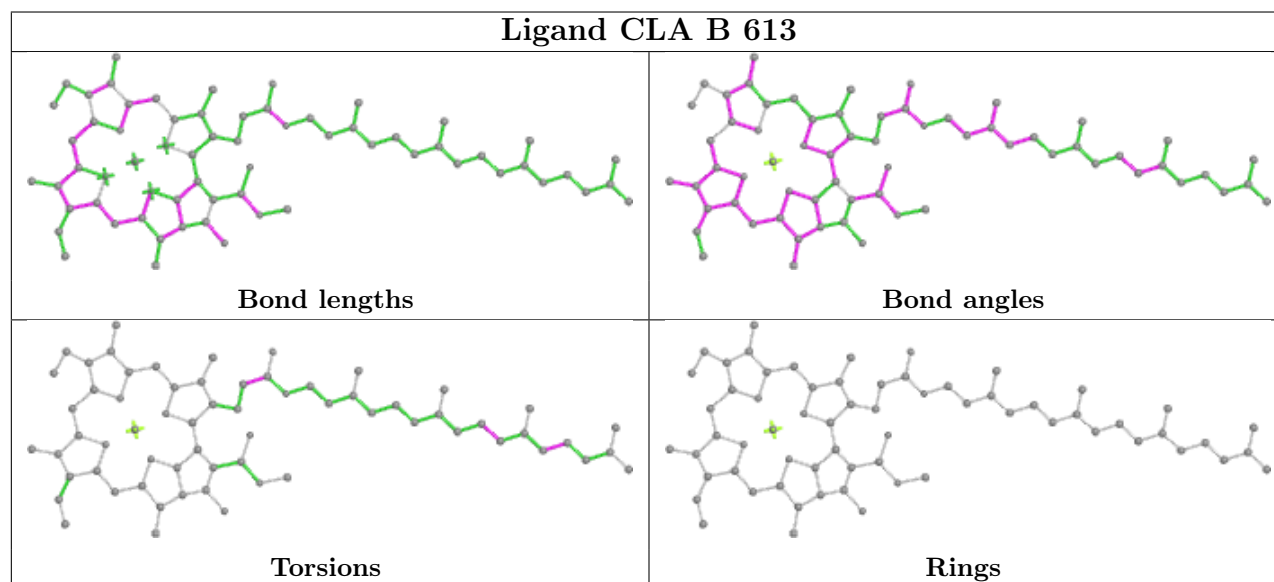
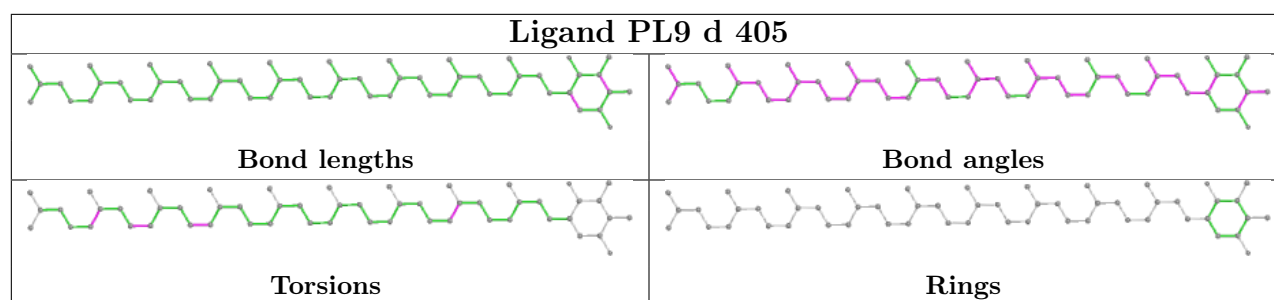


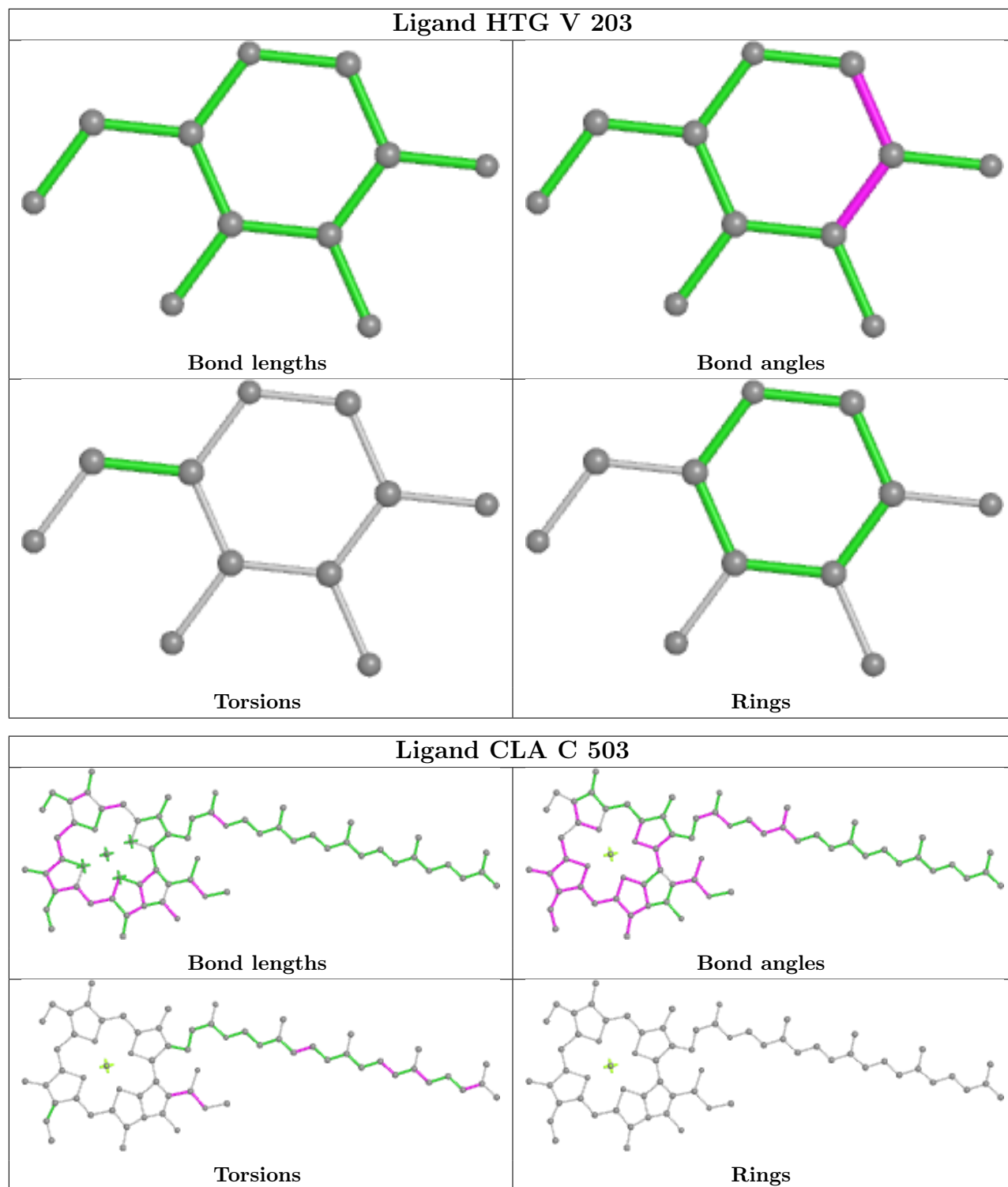


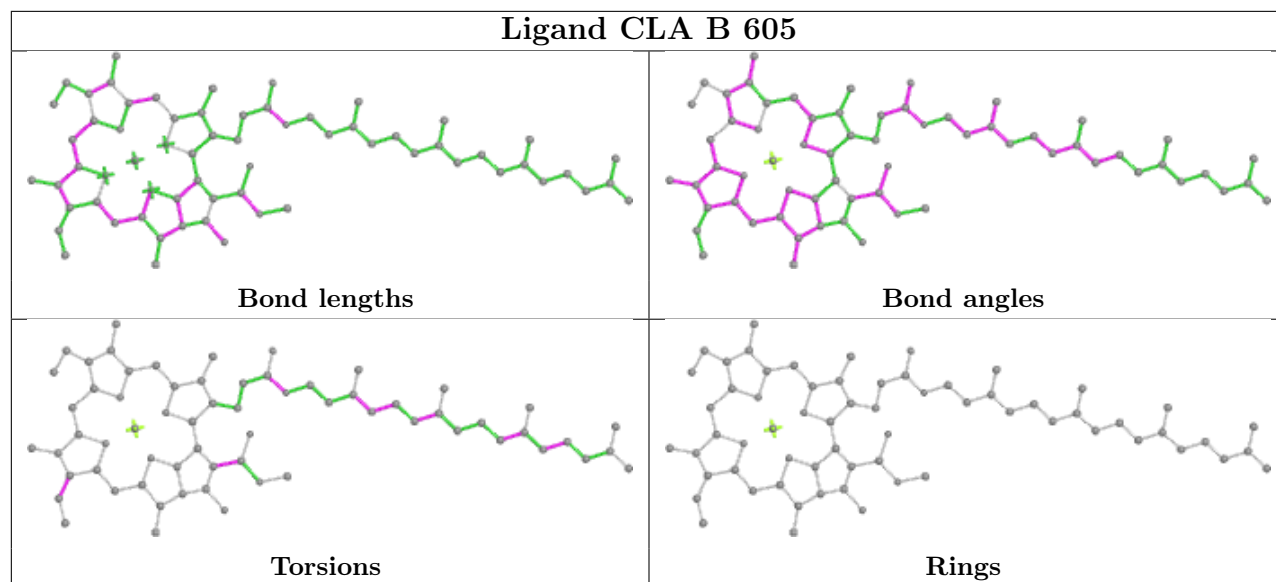
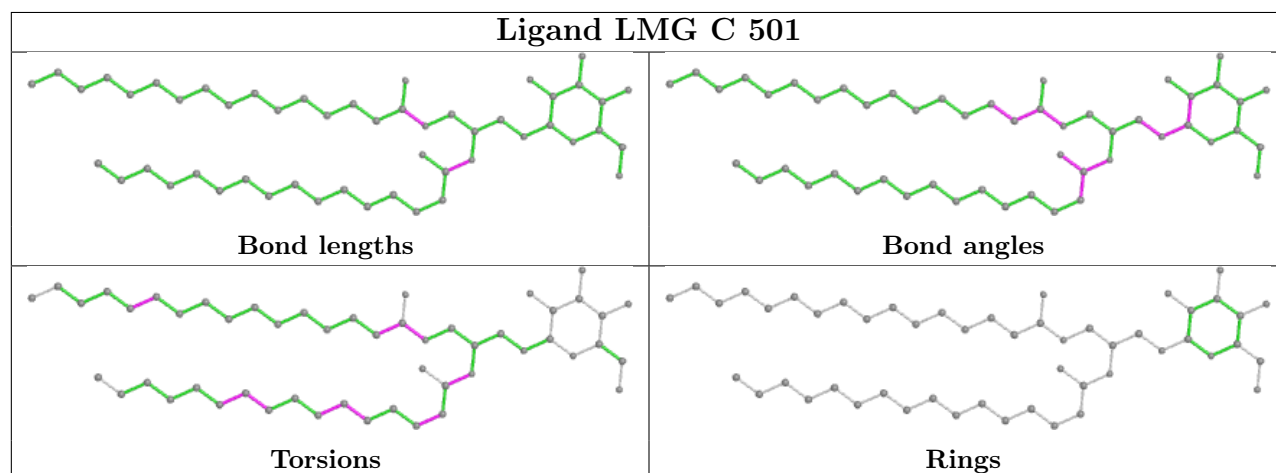
**Ligand CLA d 402****Ligand CLA C 514**



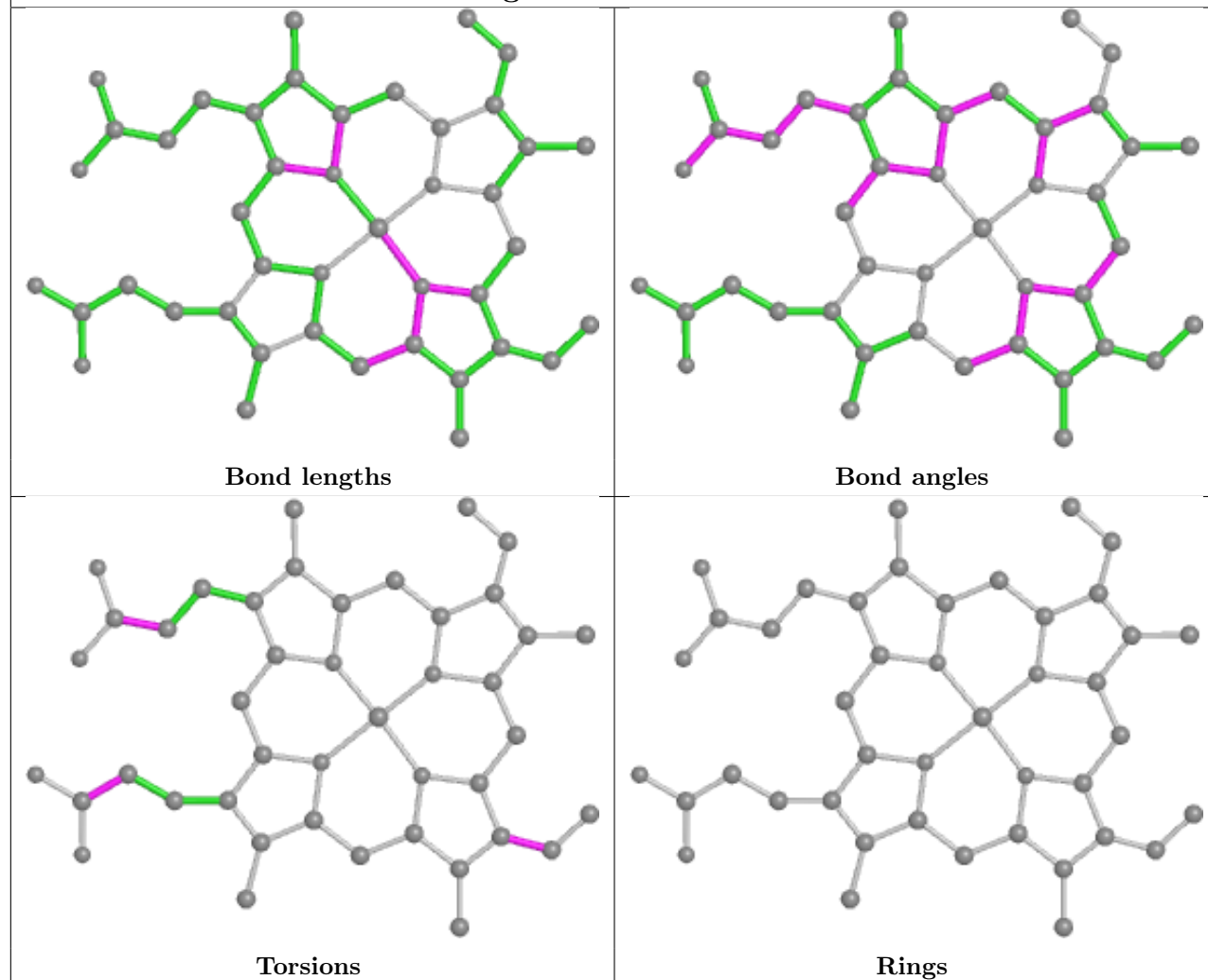




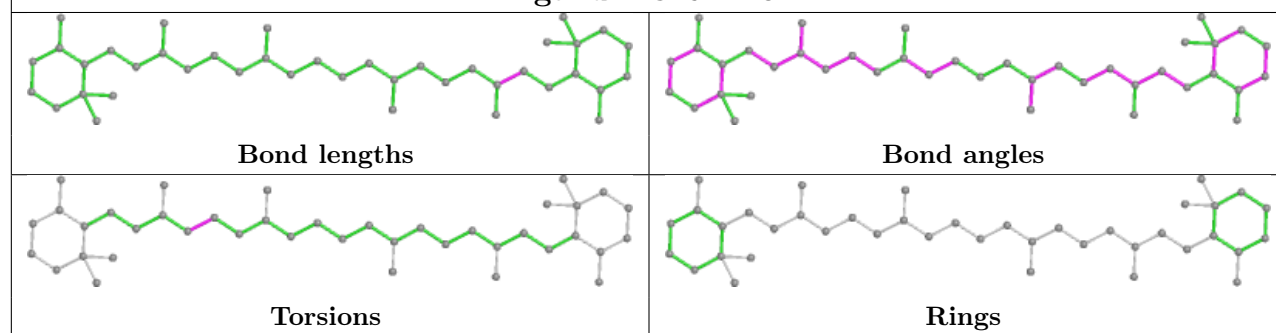


**Ligand CLA B 605****Ligand LMG C 501**

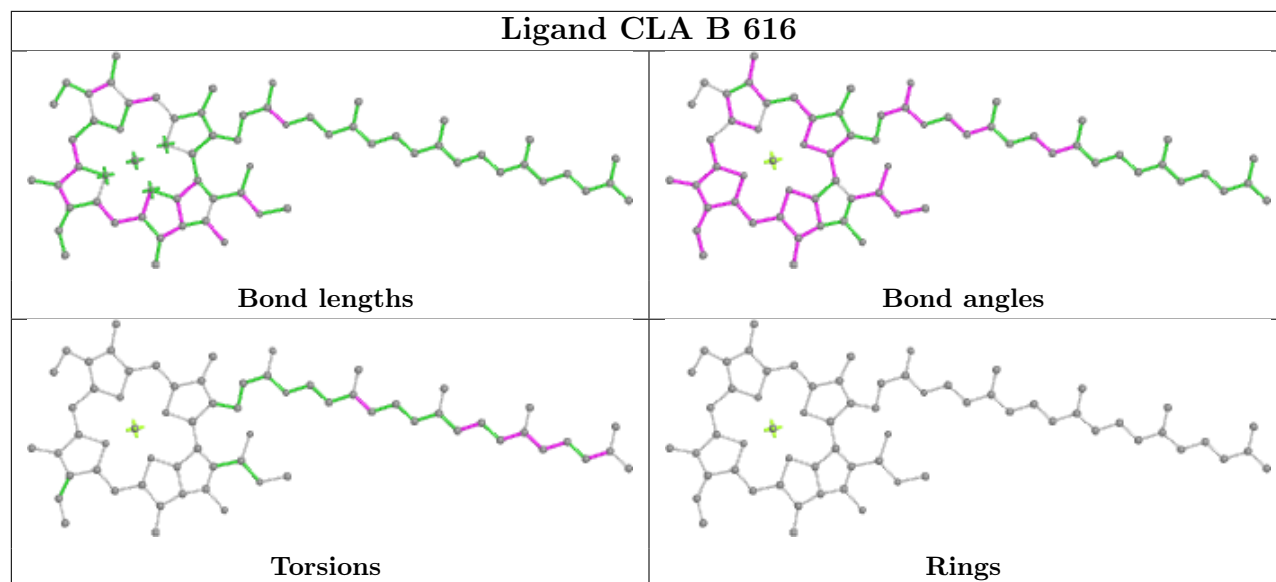
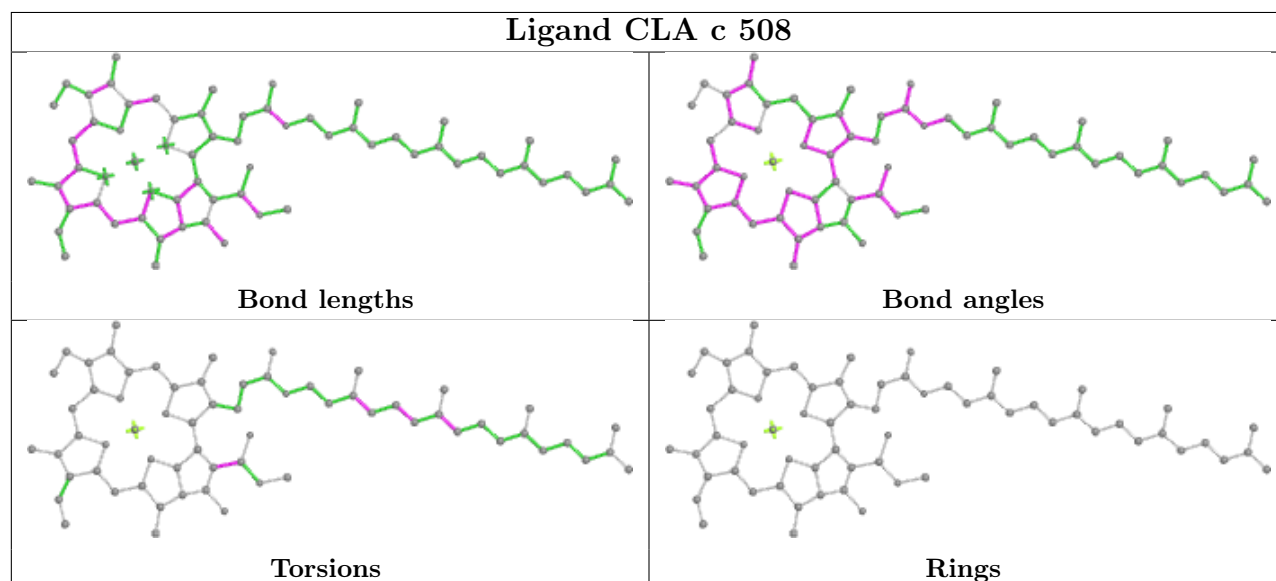
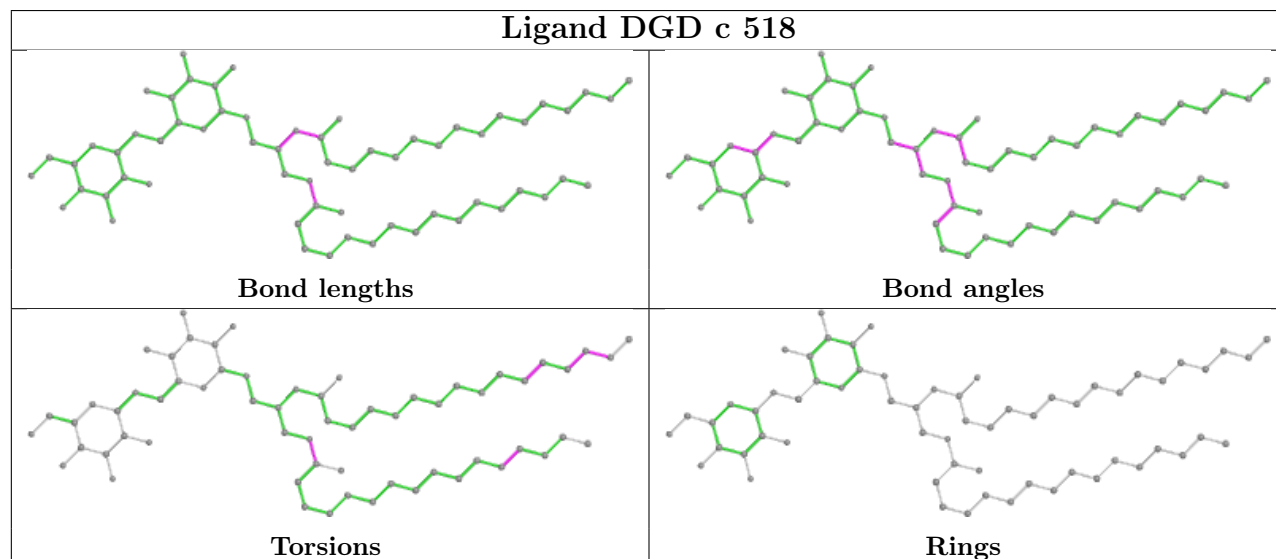
## Ligand HEM e 103

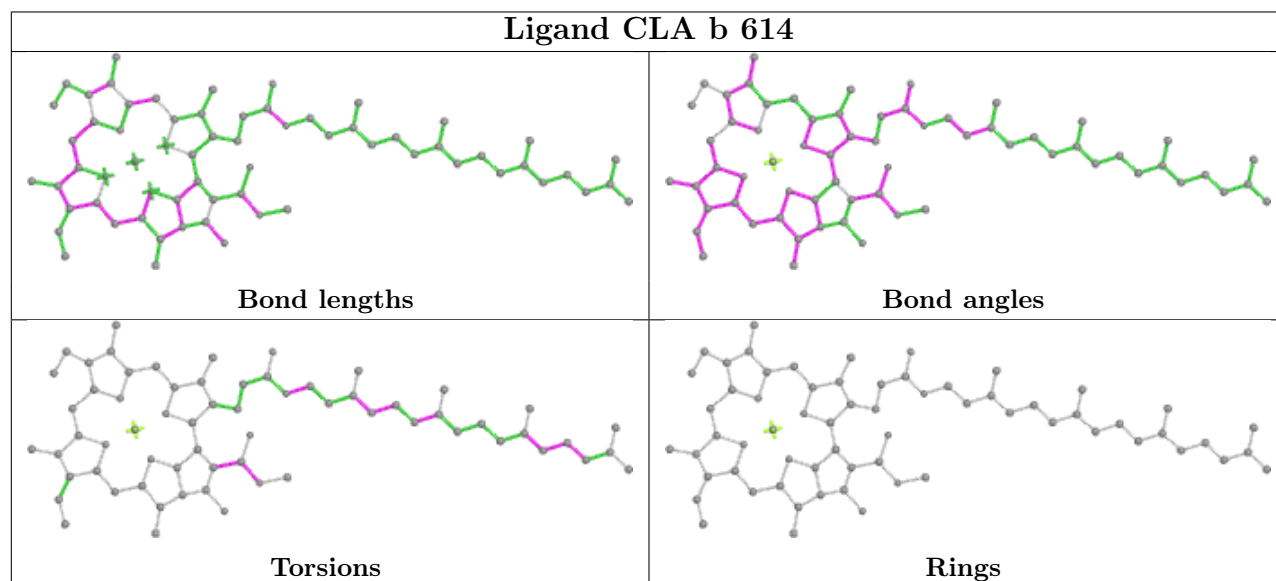
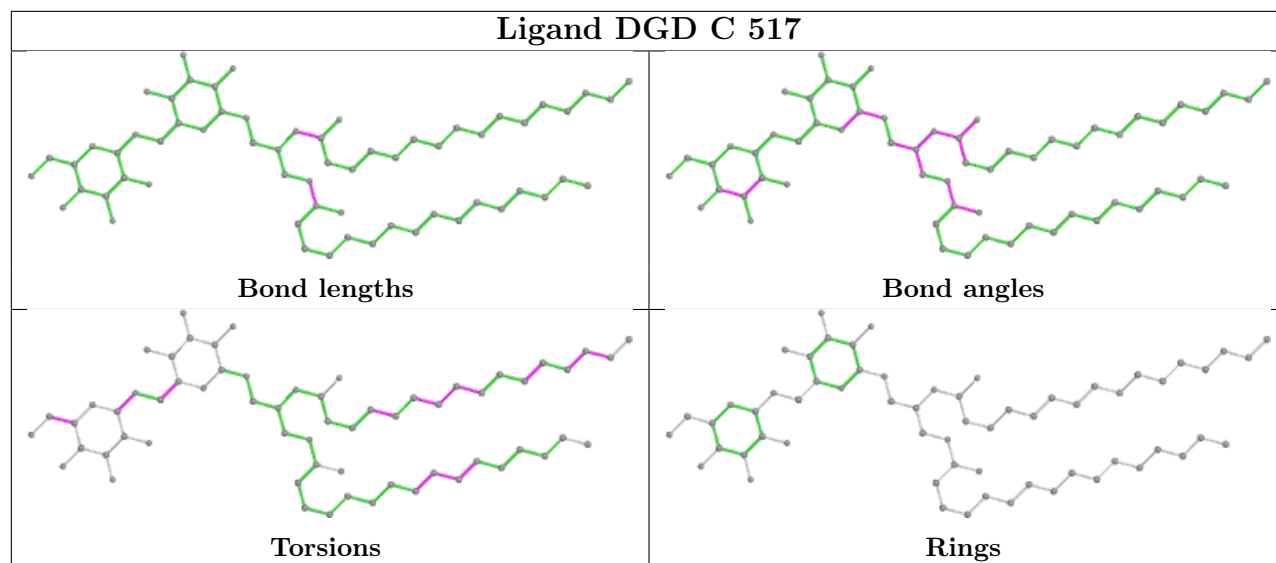


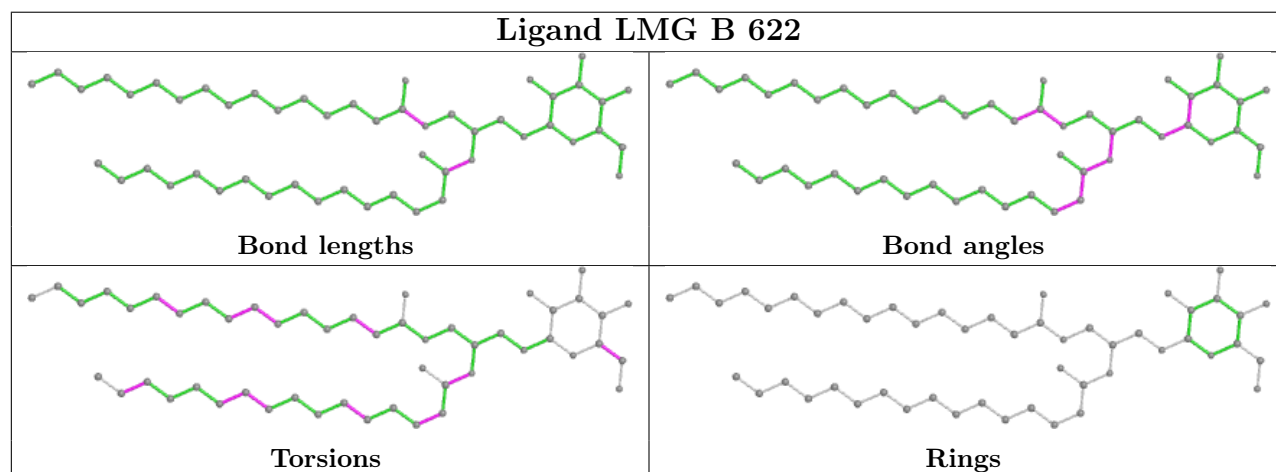
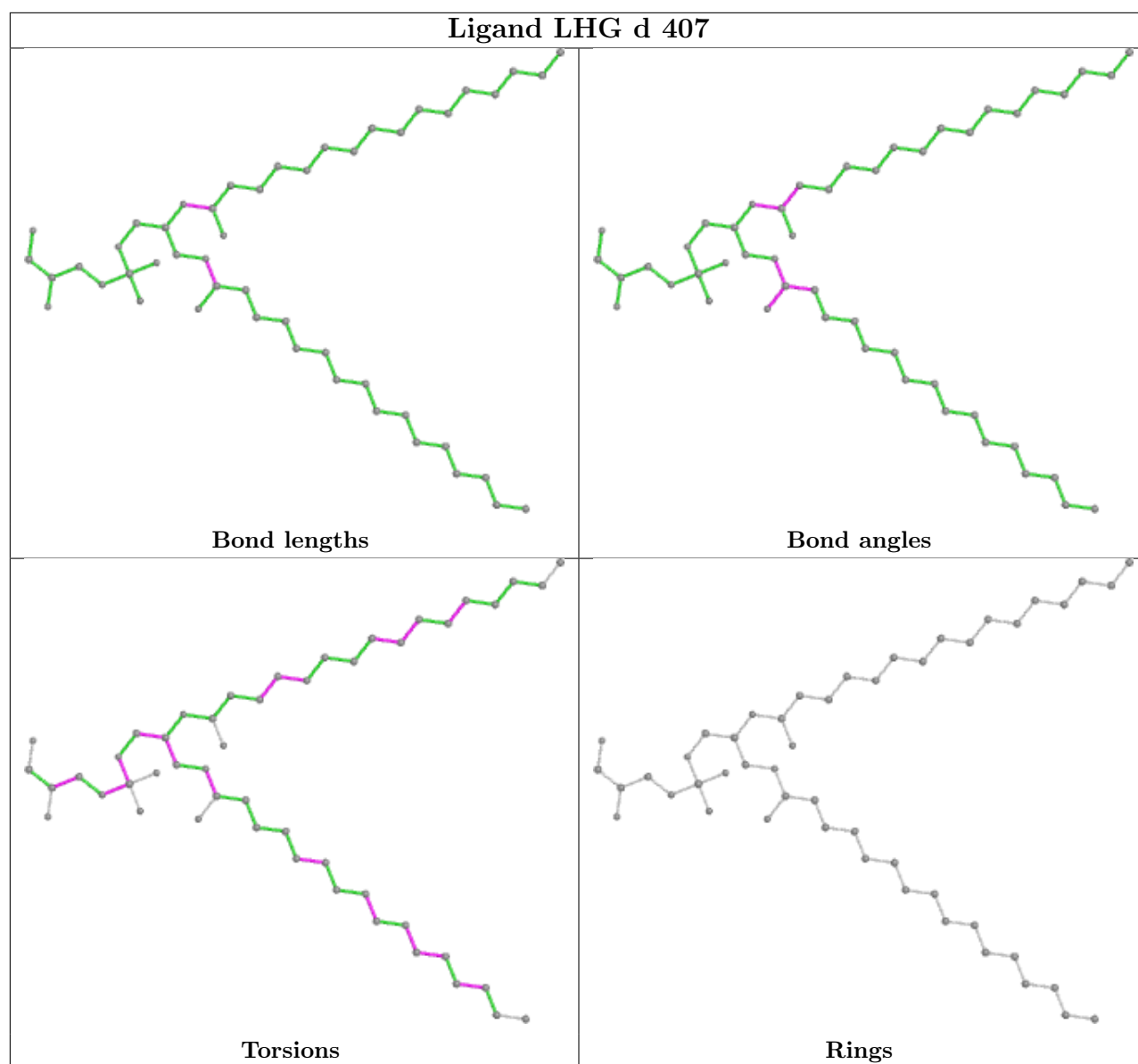
## Ligand BCR k 101

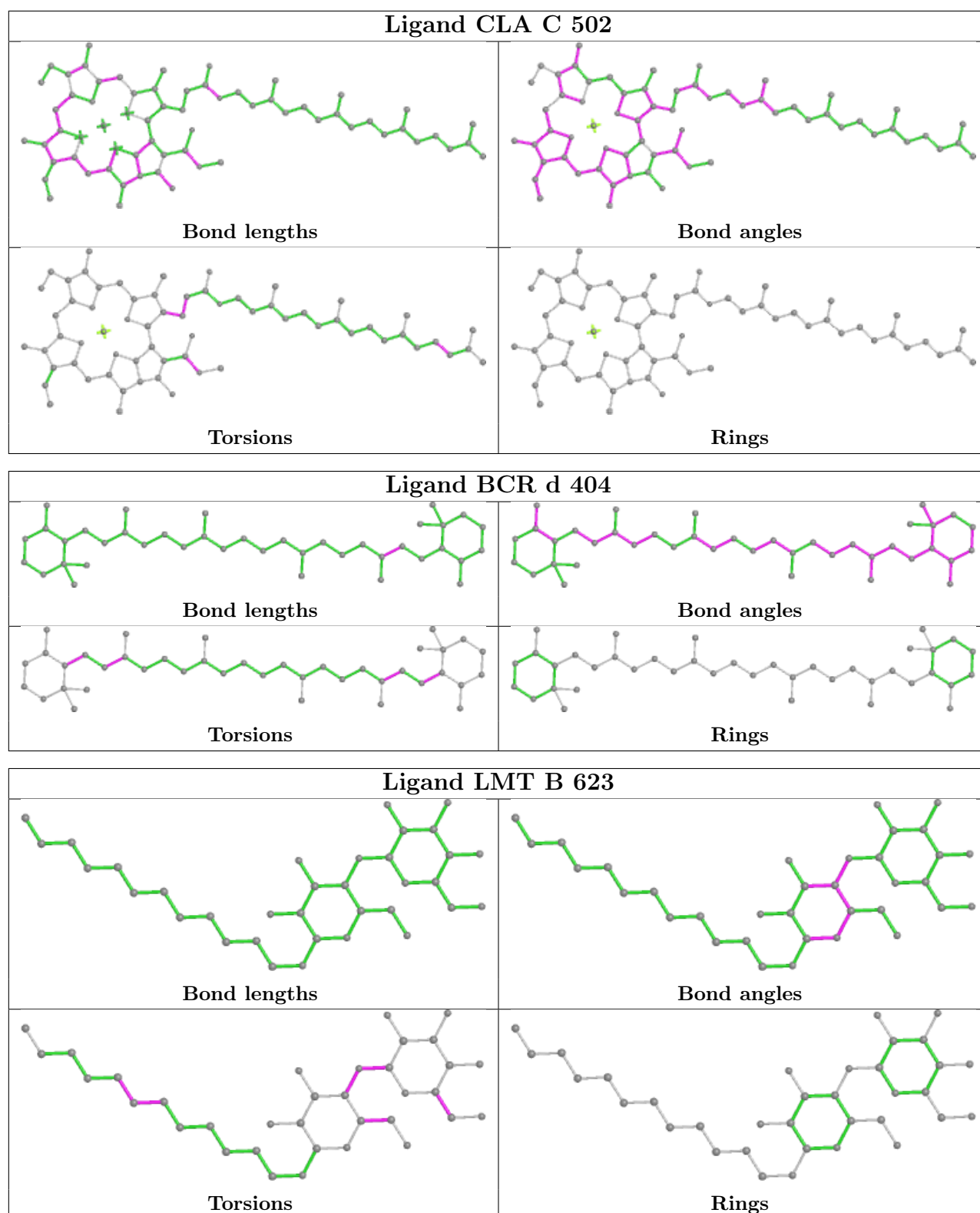


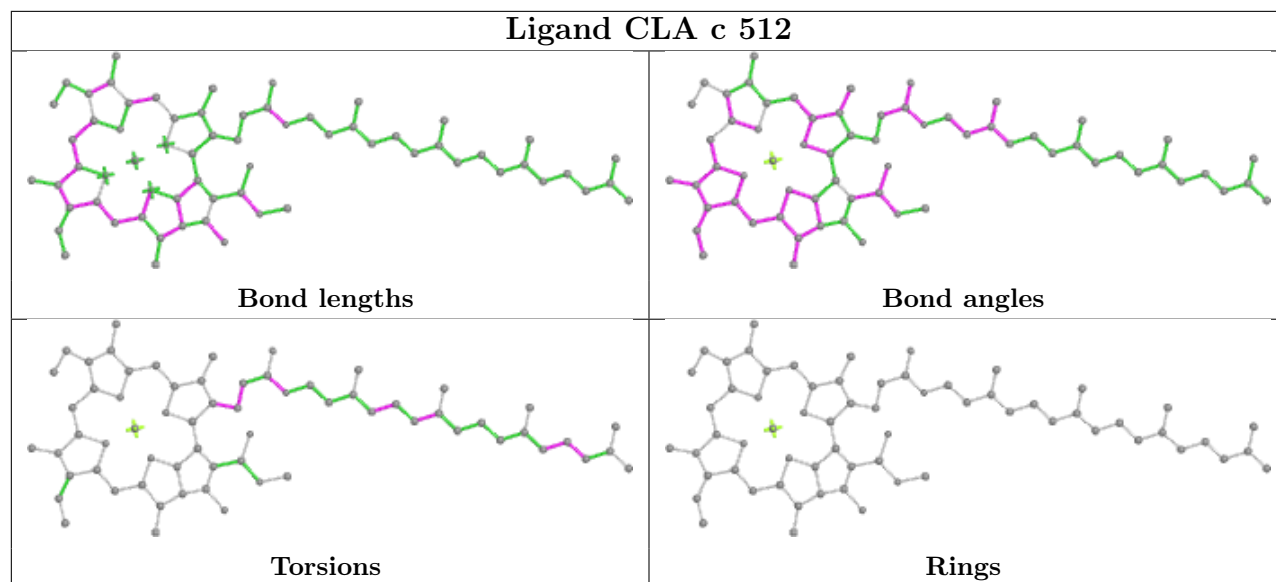
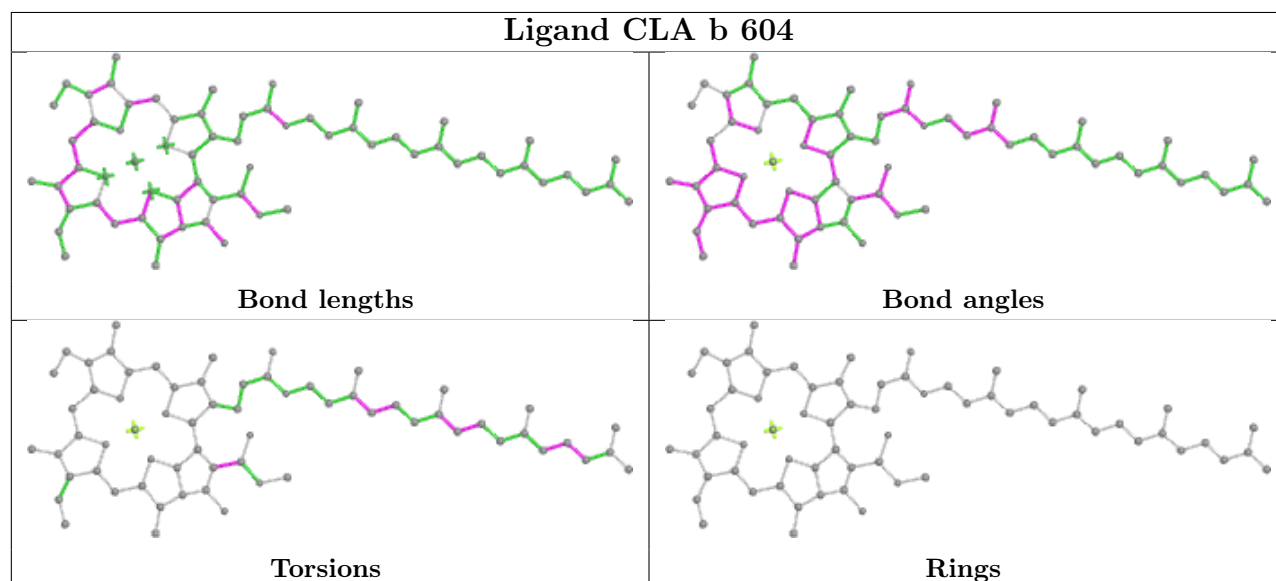
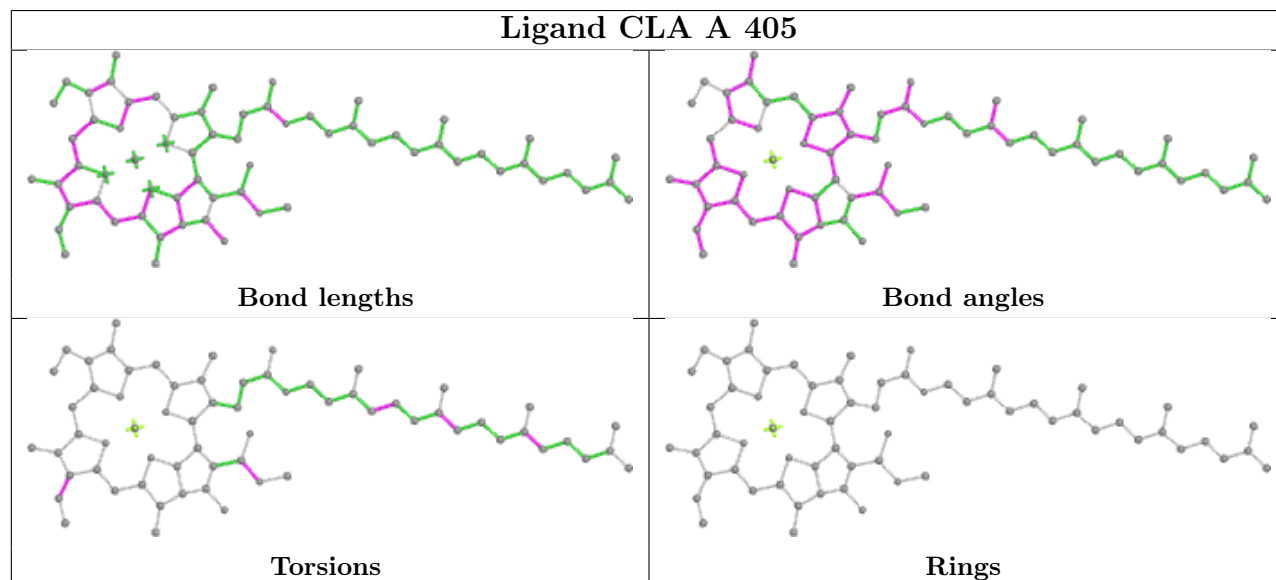


**Ligand CLA B 616****Ligand CLA c 508****Ligand DGD c 518**

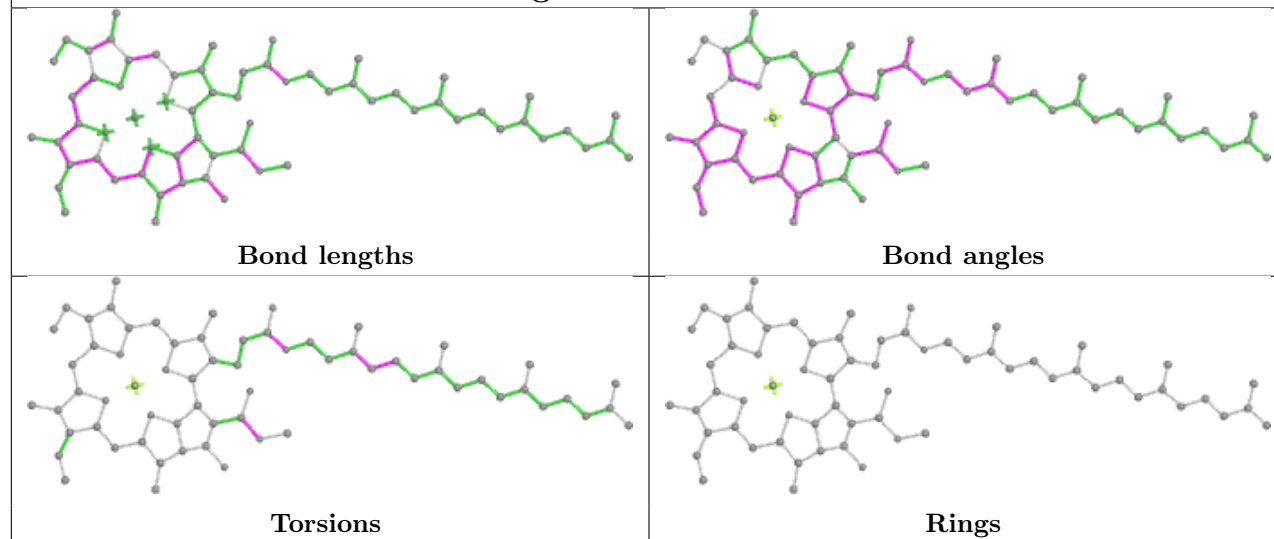




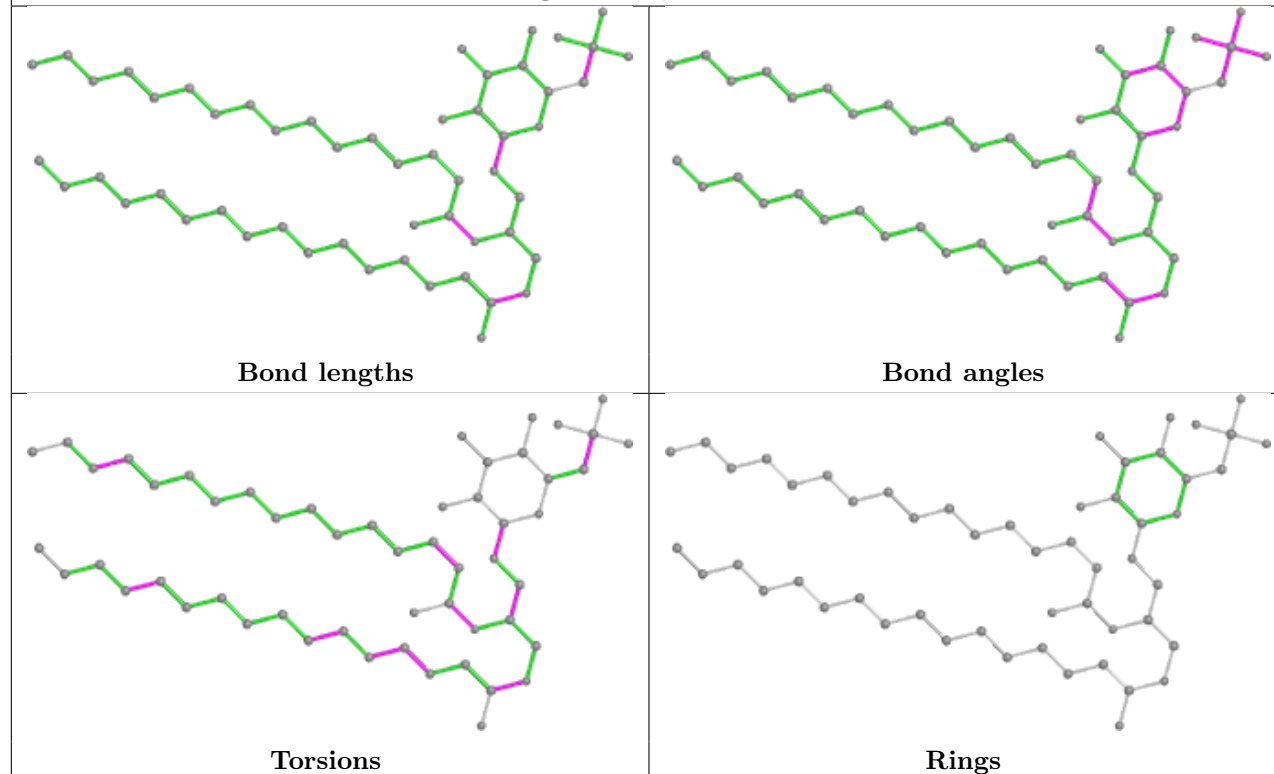


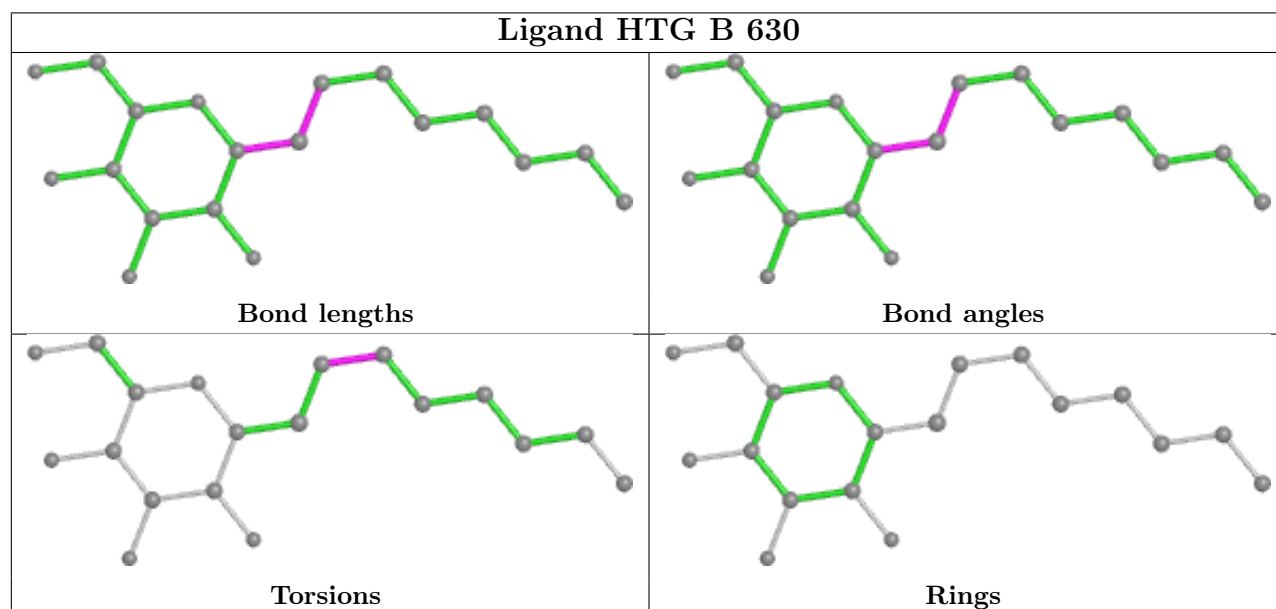
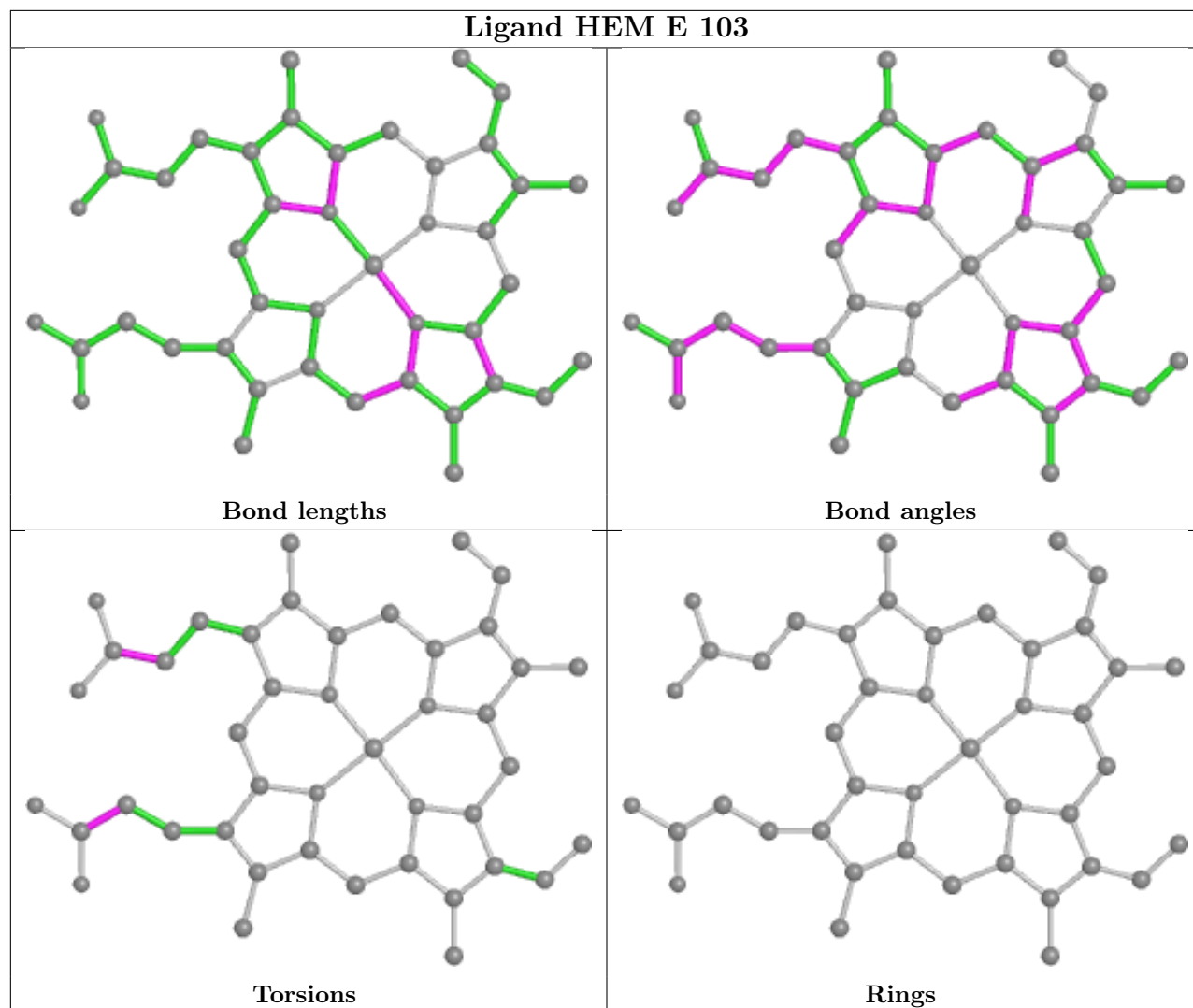
**Ligand CLA c 512****Ligand CLA b 604****Ligand CLA A 405**

## Ligand CLA B 604

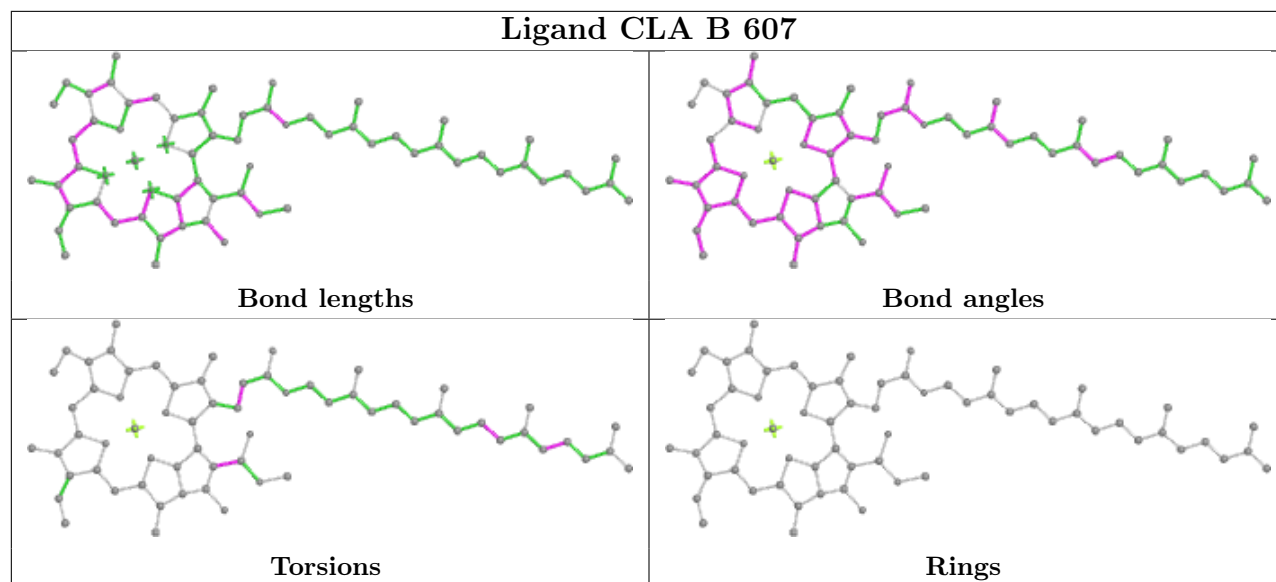


## Ligand SQD a 413

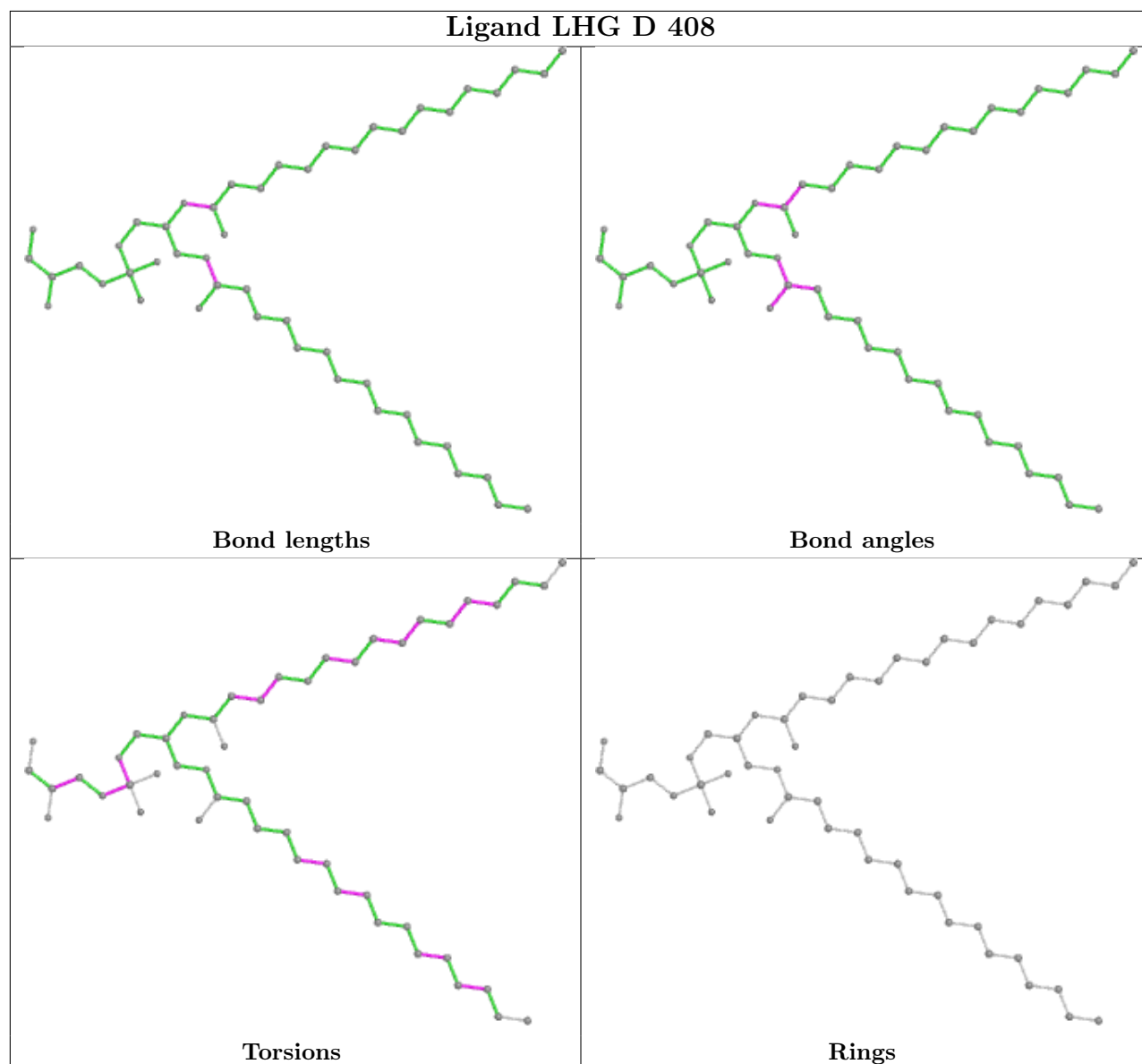




## Ligand CLA B 607

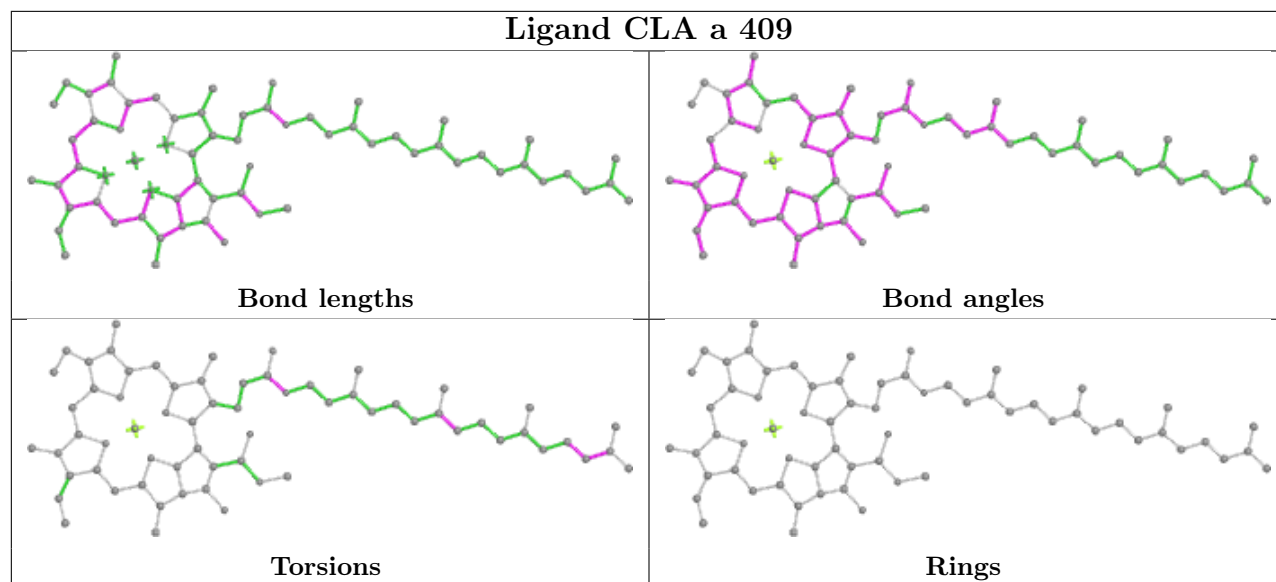


## Ligand LHG D 408

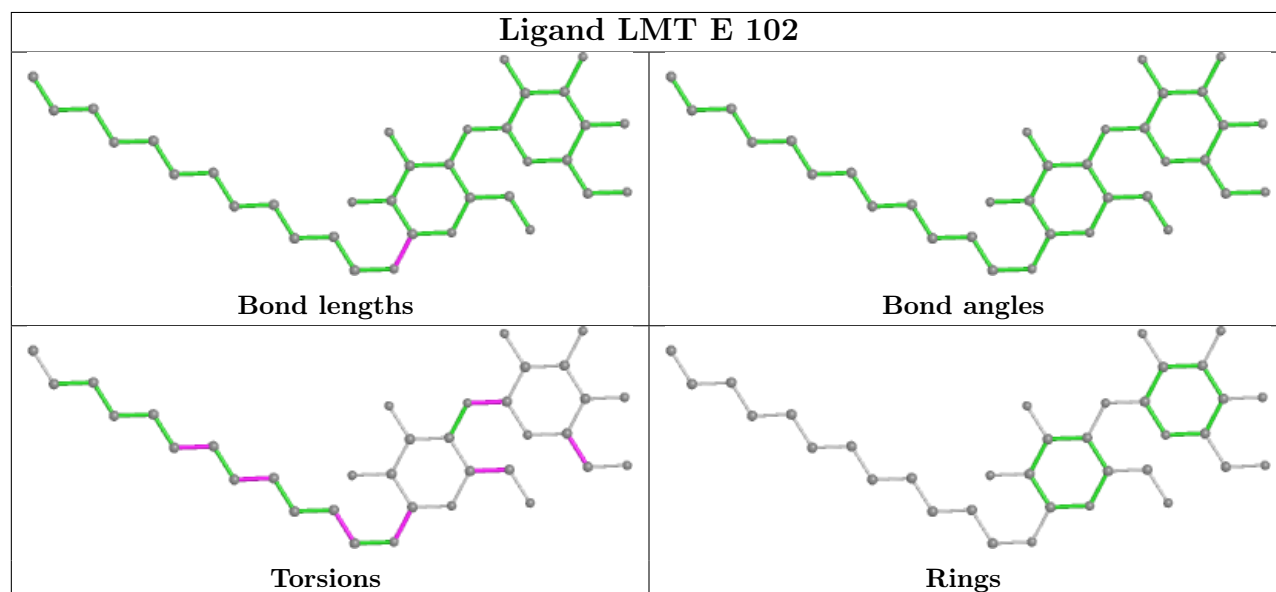




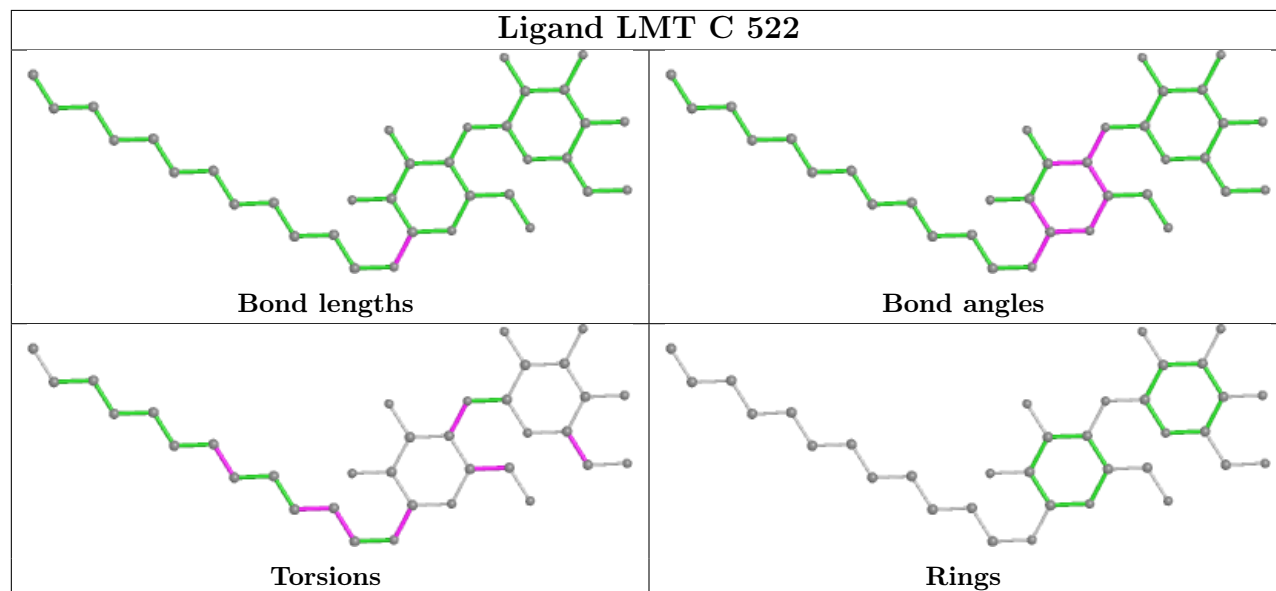
## Ligand CLA a 409

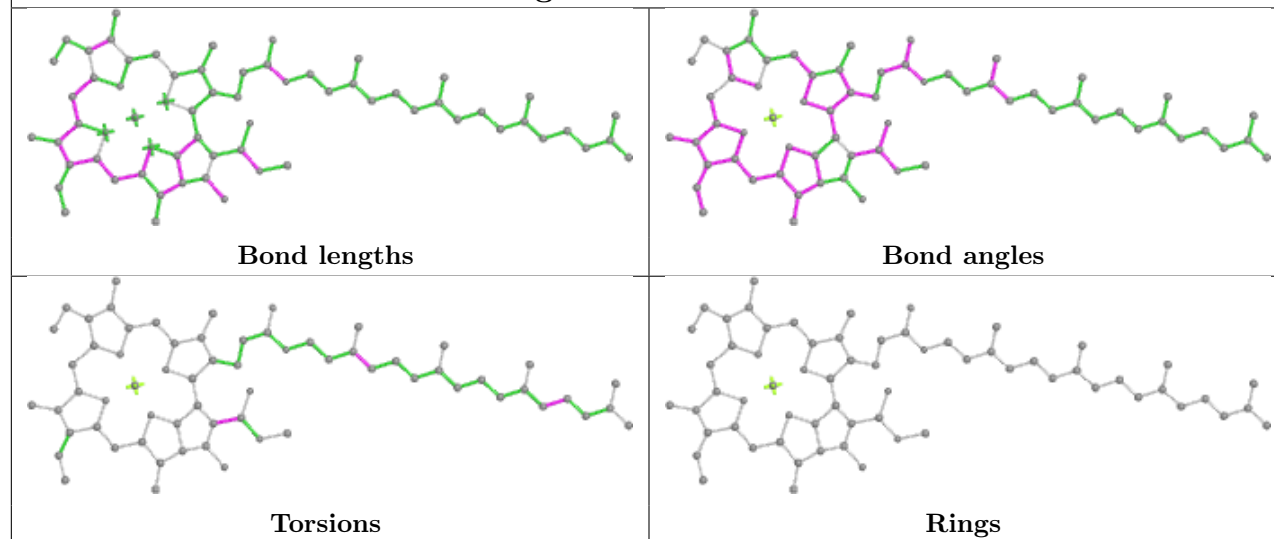
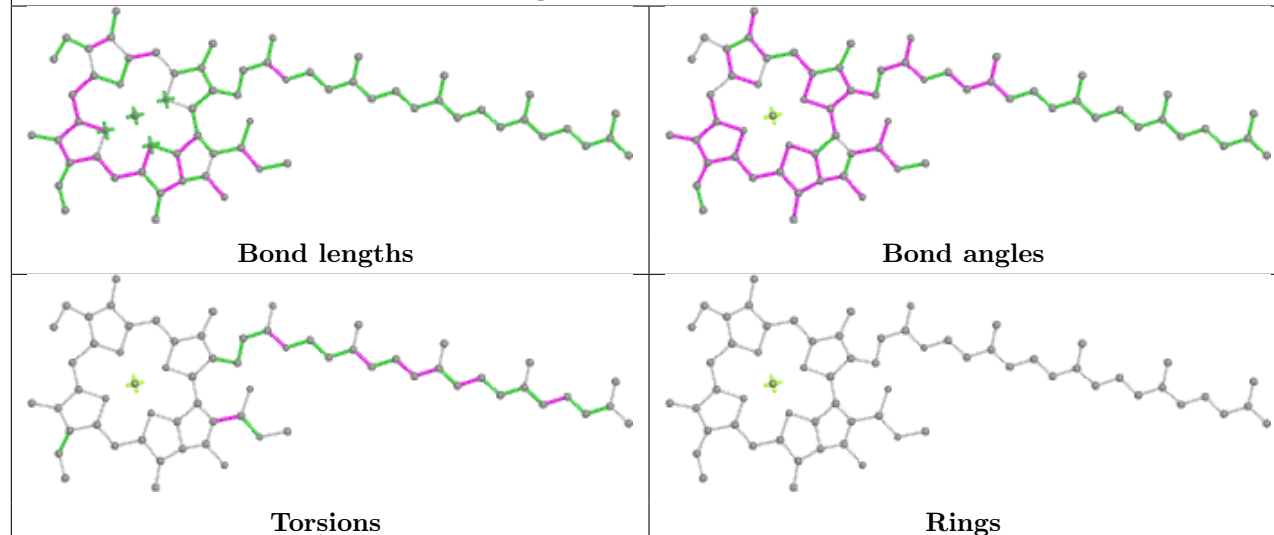
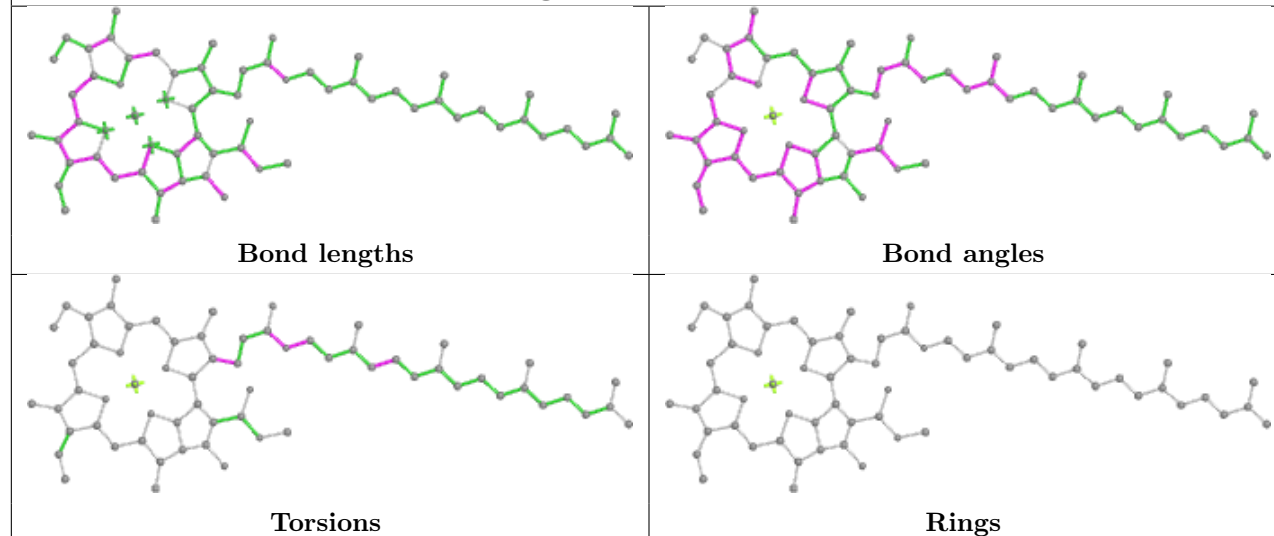


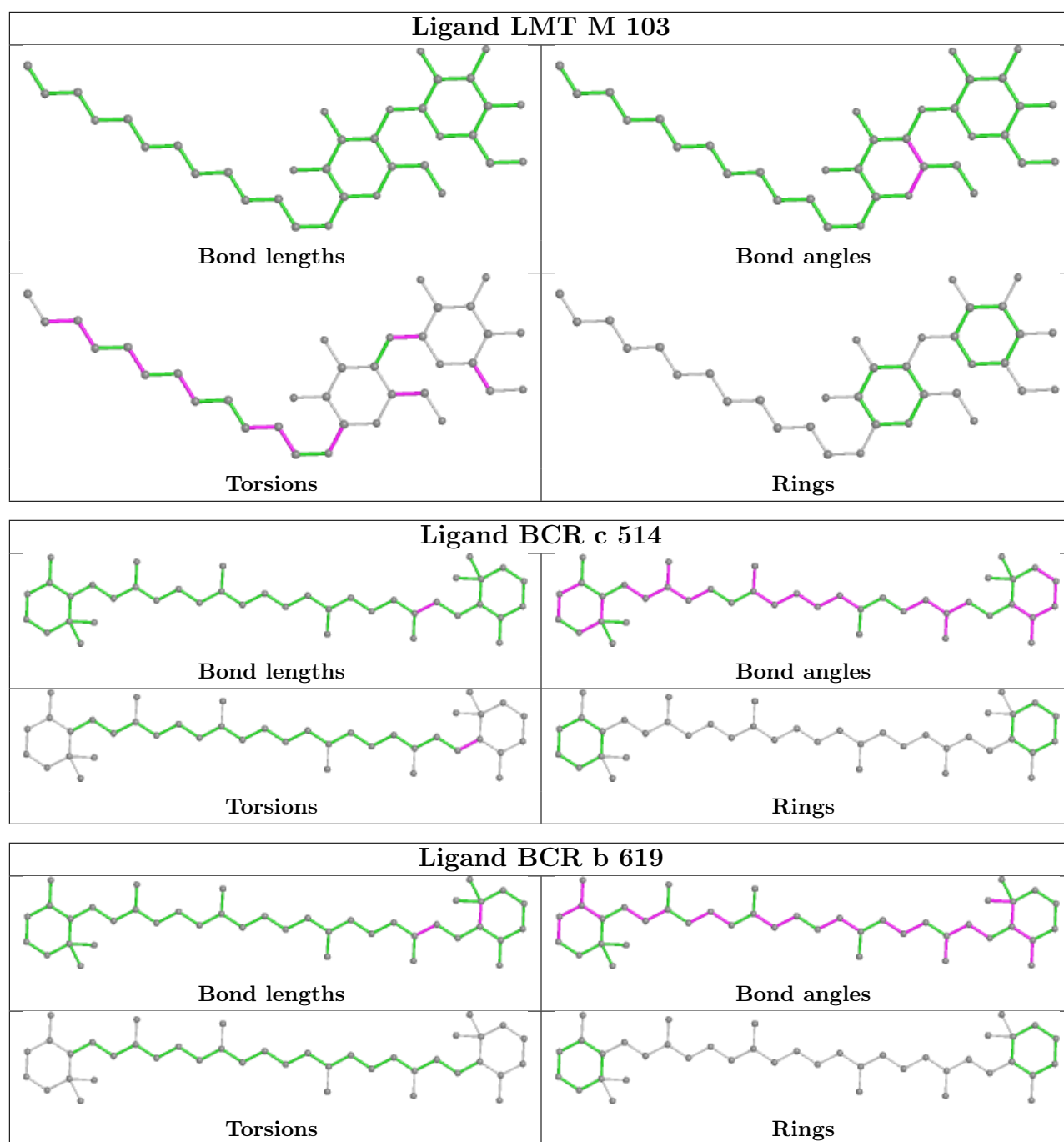
## Ligand LMT E 102



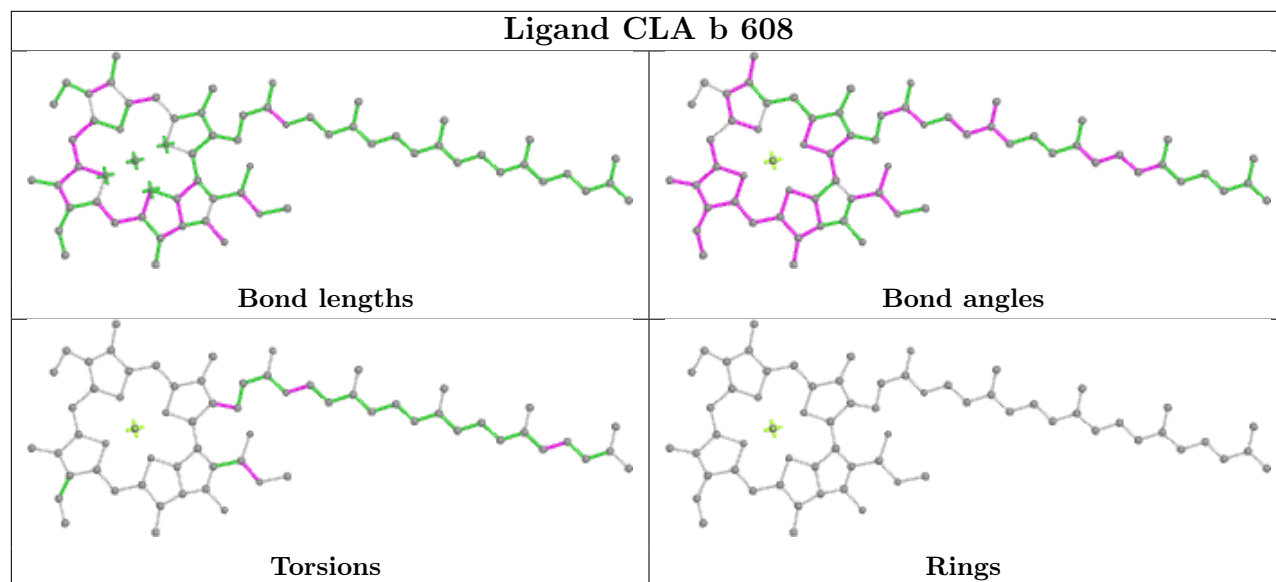
## Ligand LMT C 522



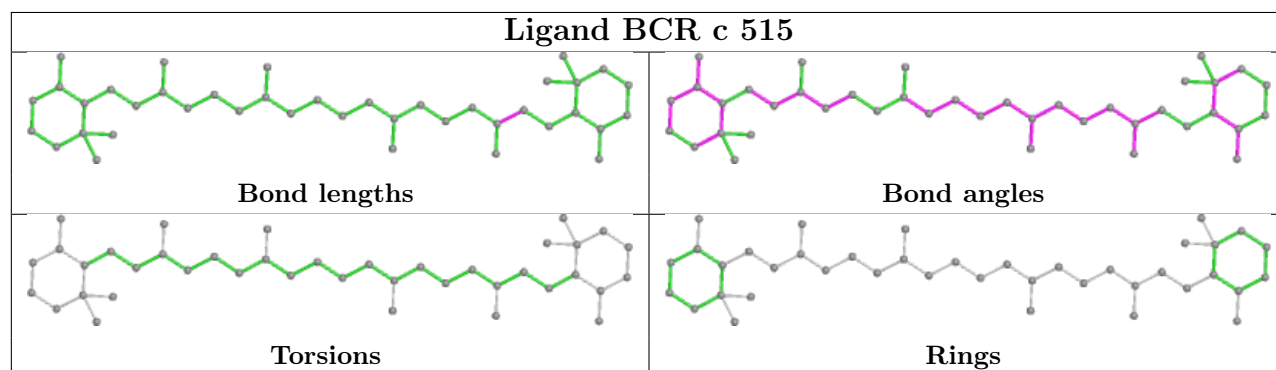
**Ligand CLA b 603****Ligand CLA B 606****Ligand CLA c 511**



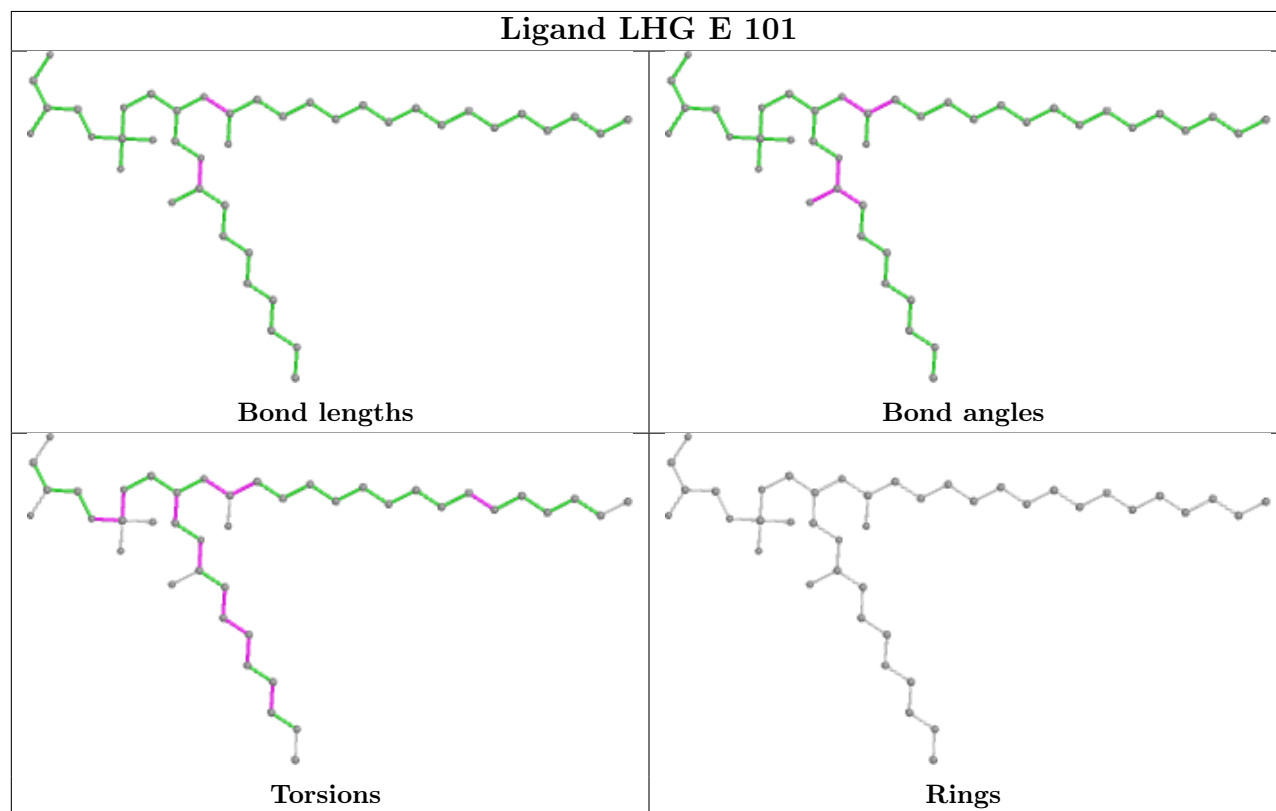
## Ligand CLA b 608

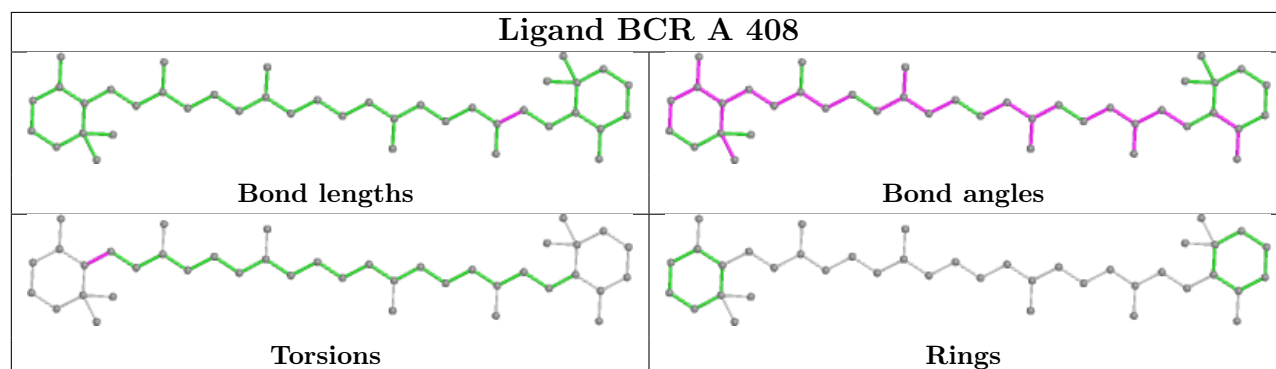
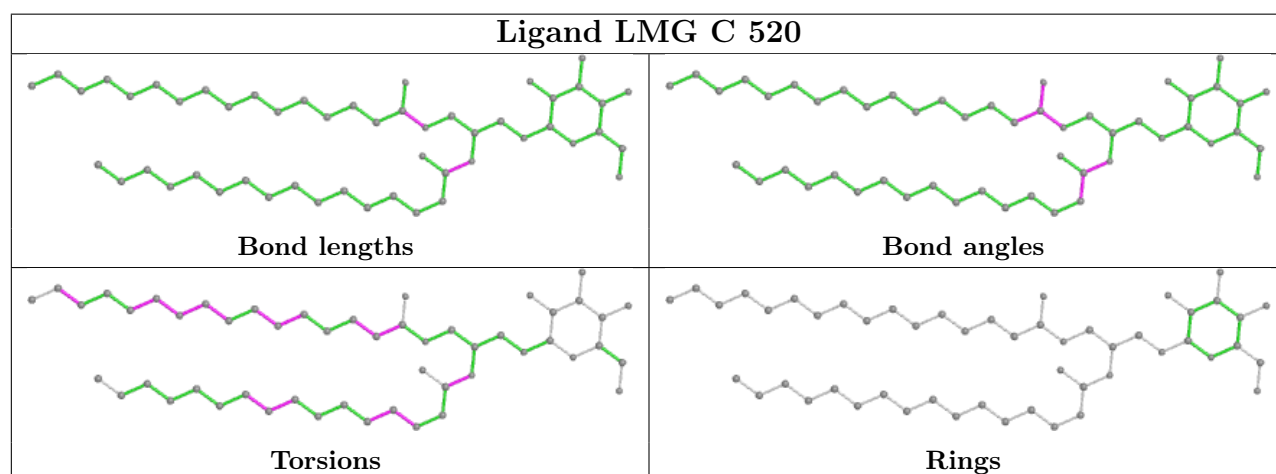
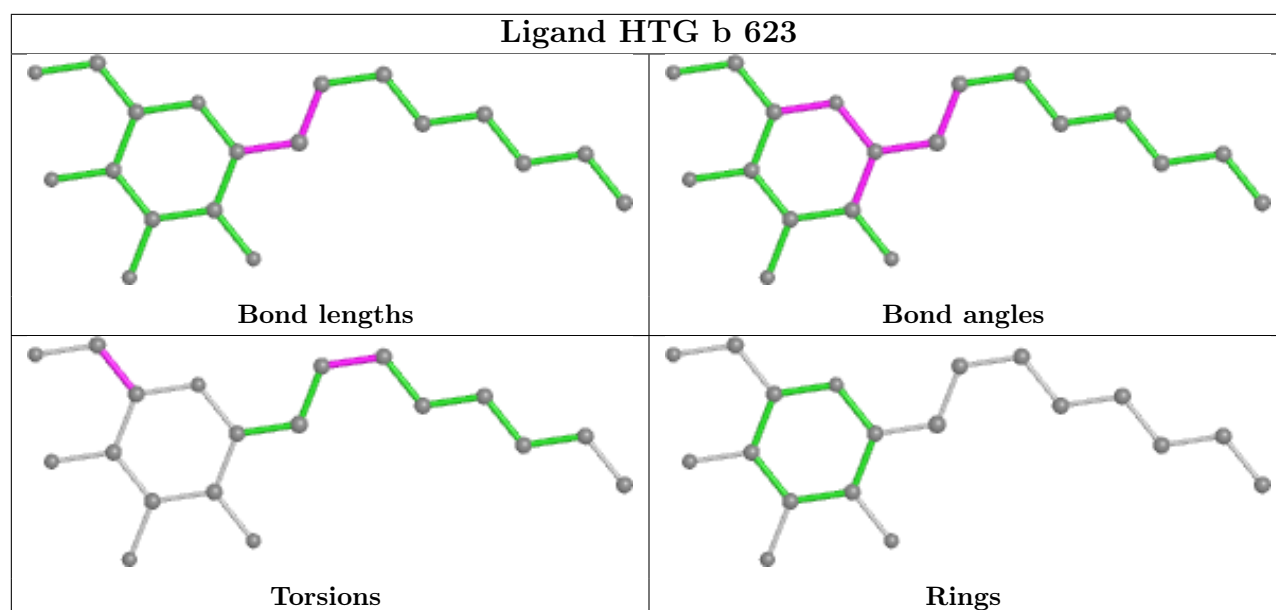


## Ligand BCR c 515

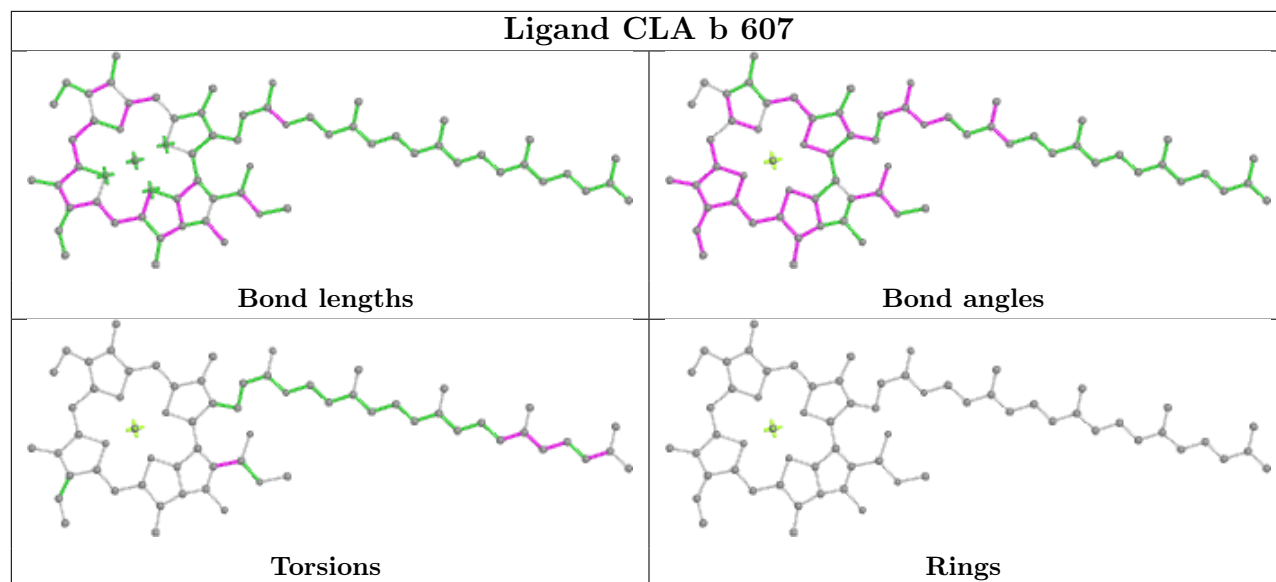


## Ligand LHG E 101

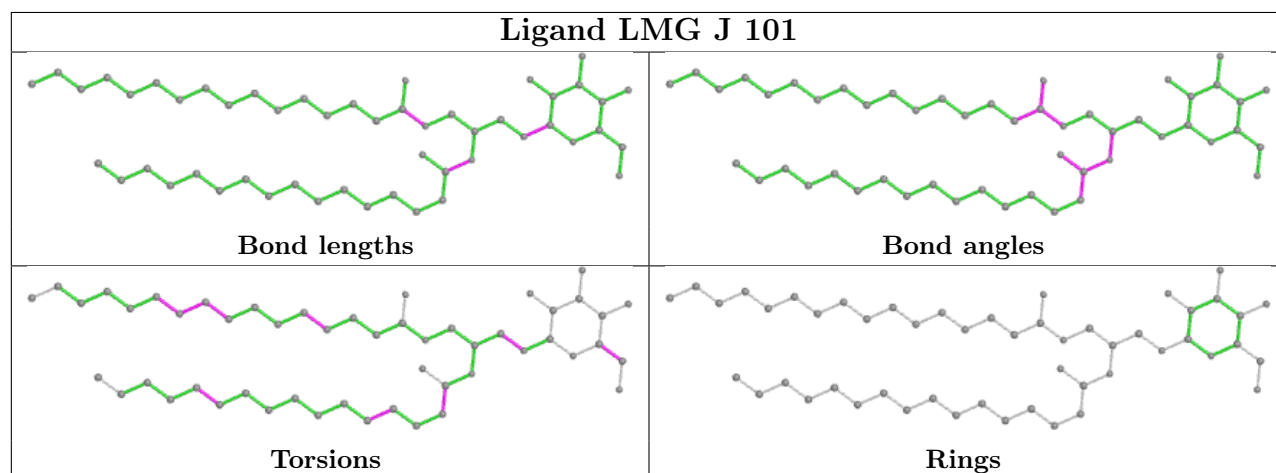




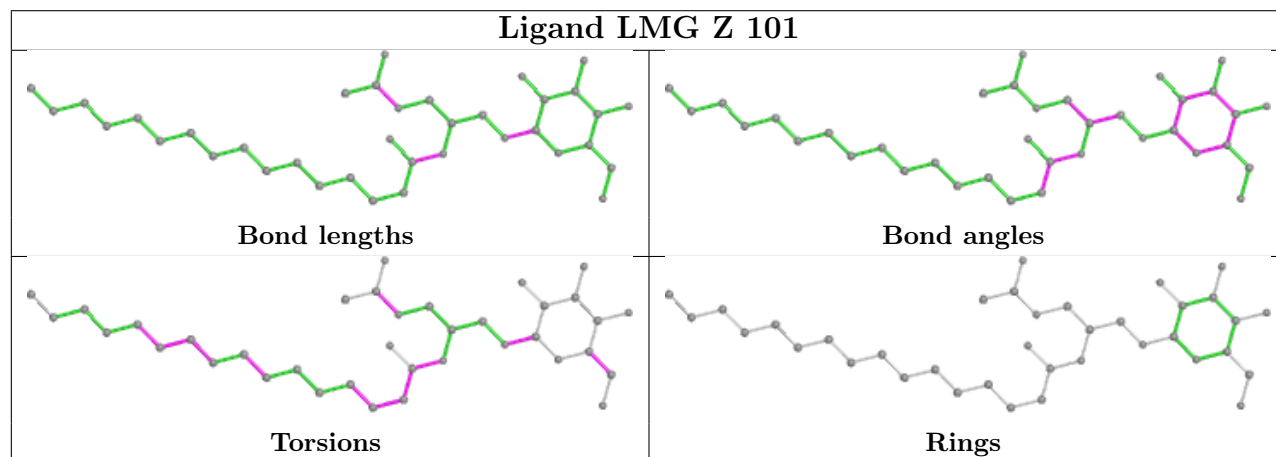
## Ligand CLA b 607

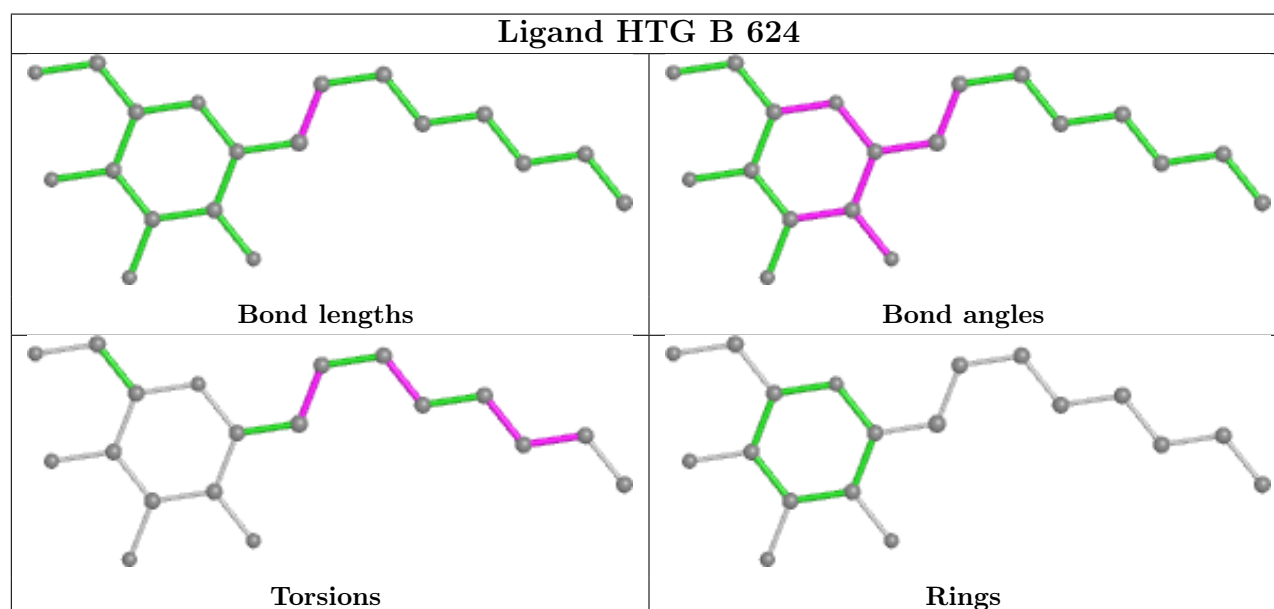
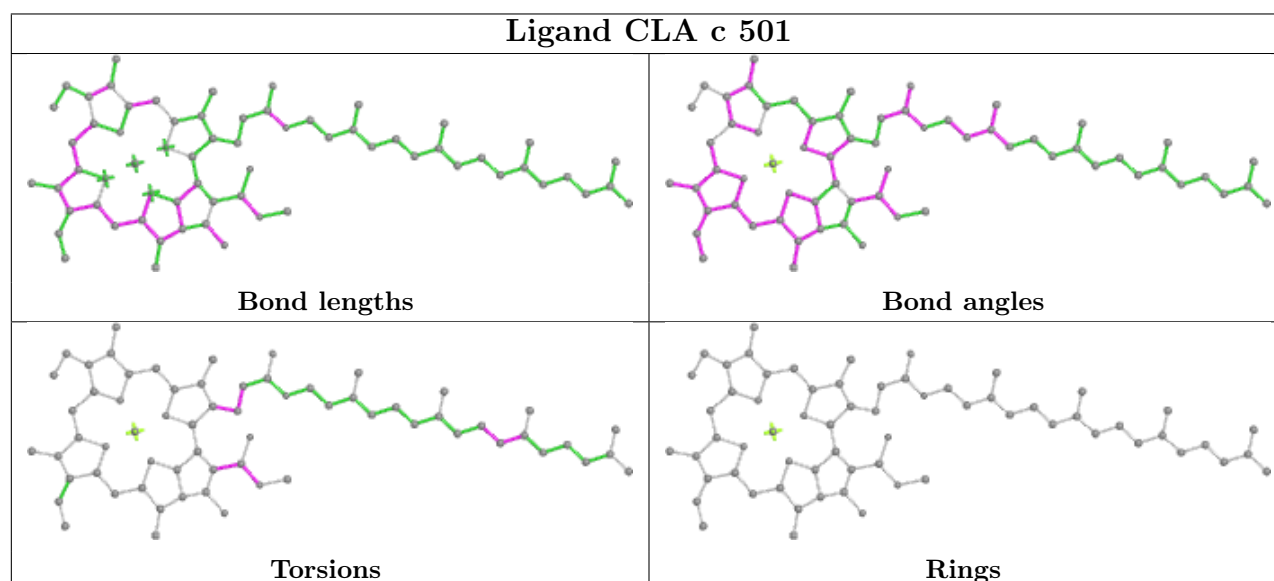
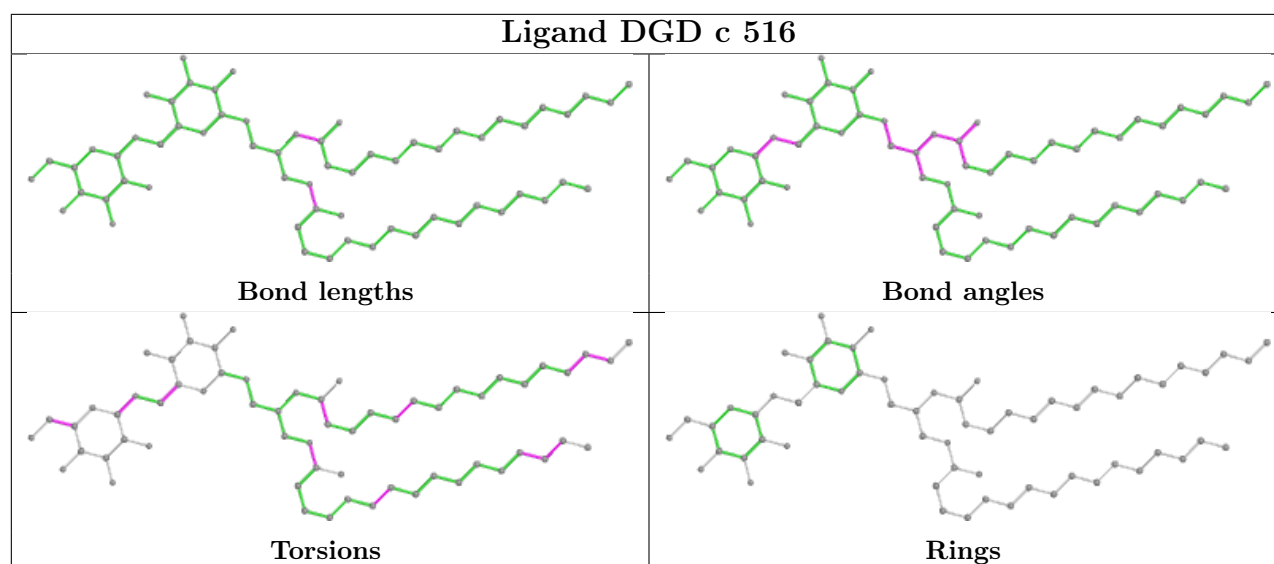


## Ligand LMG J 101

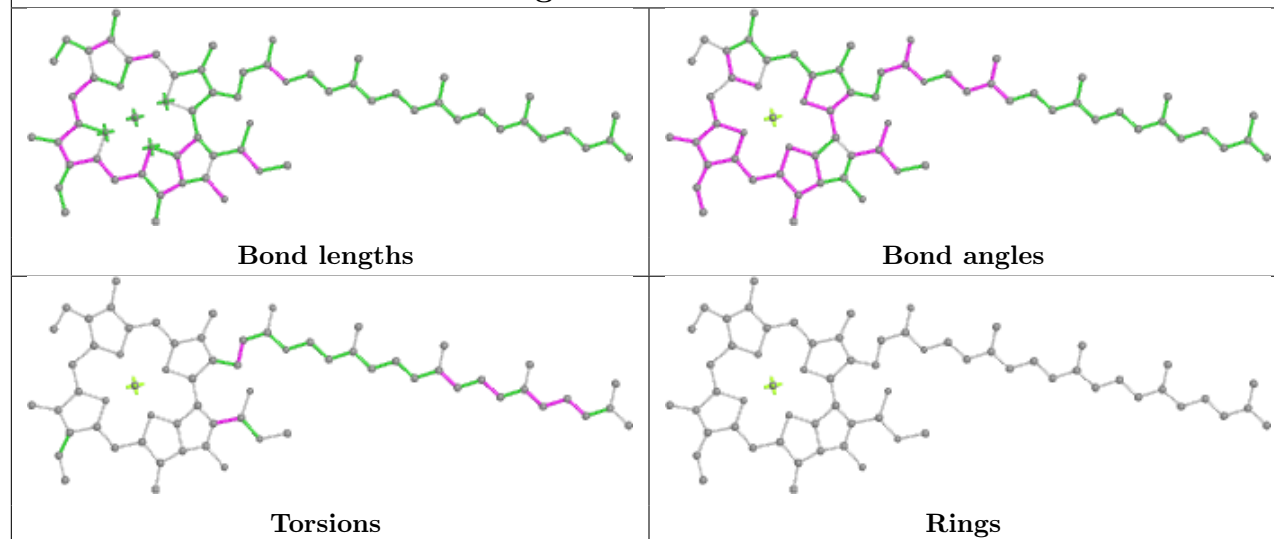


## Ligand LMG Z 101

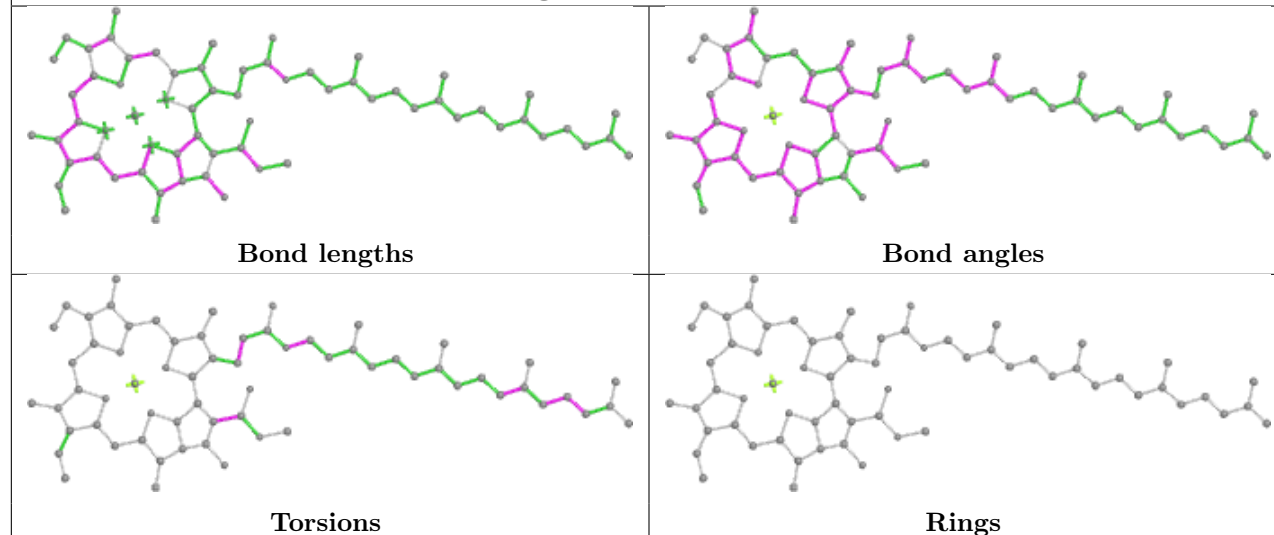




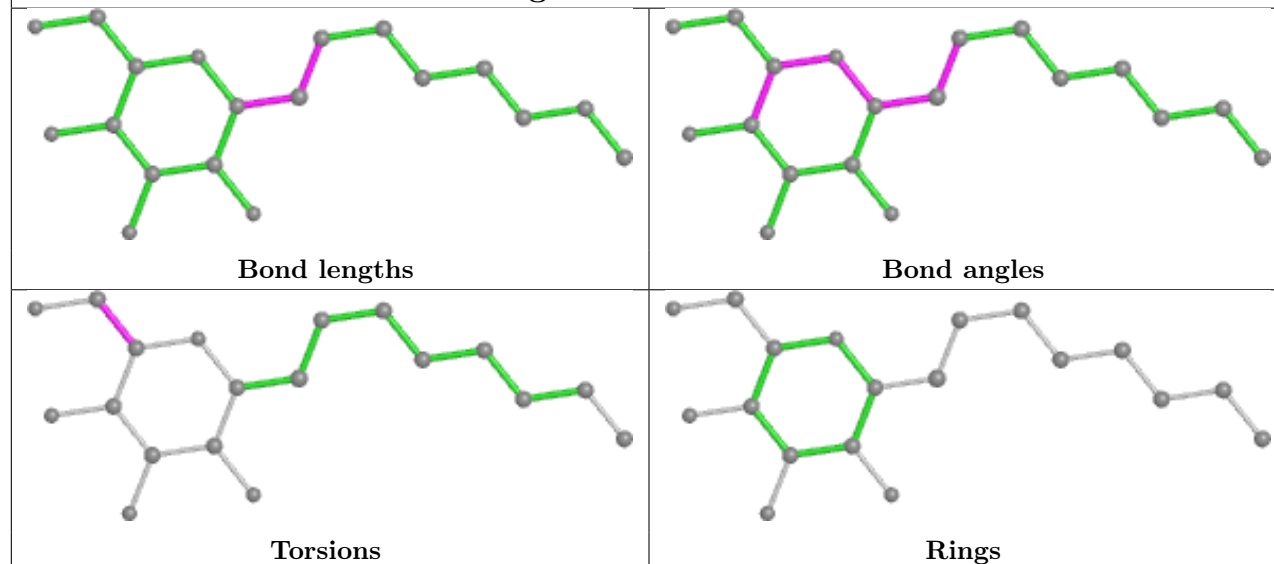
## Ligand CLA b 606



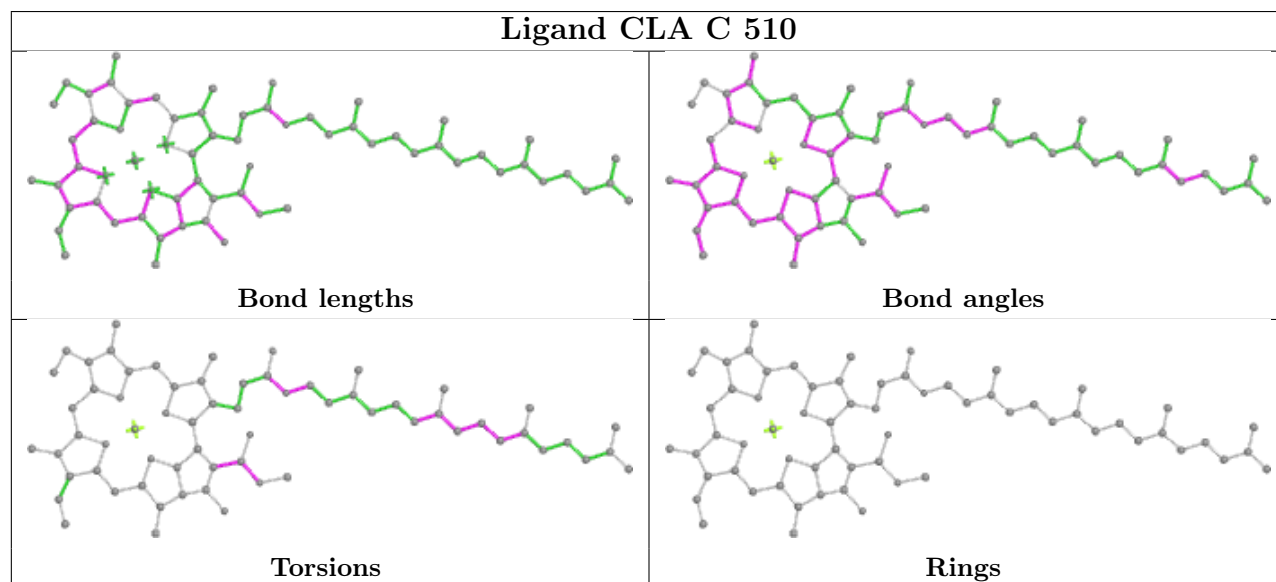
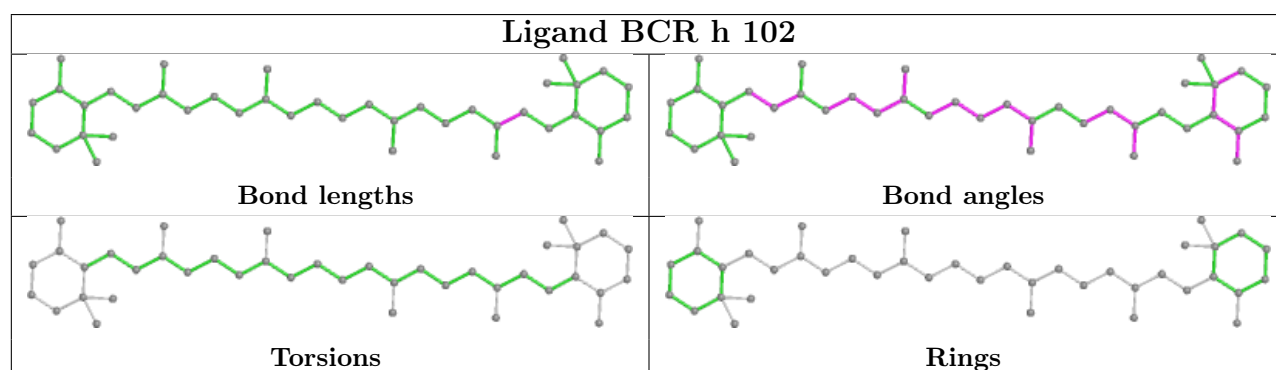
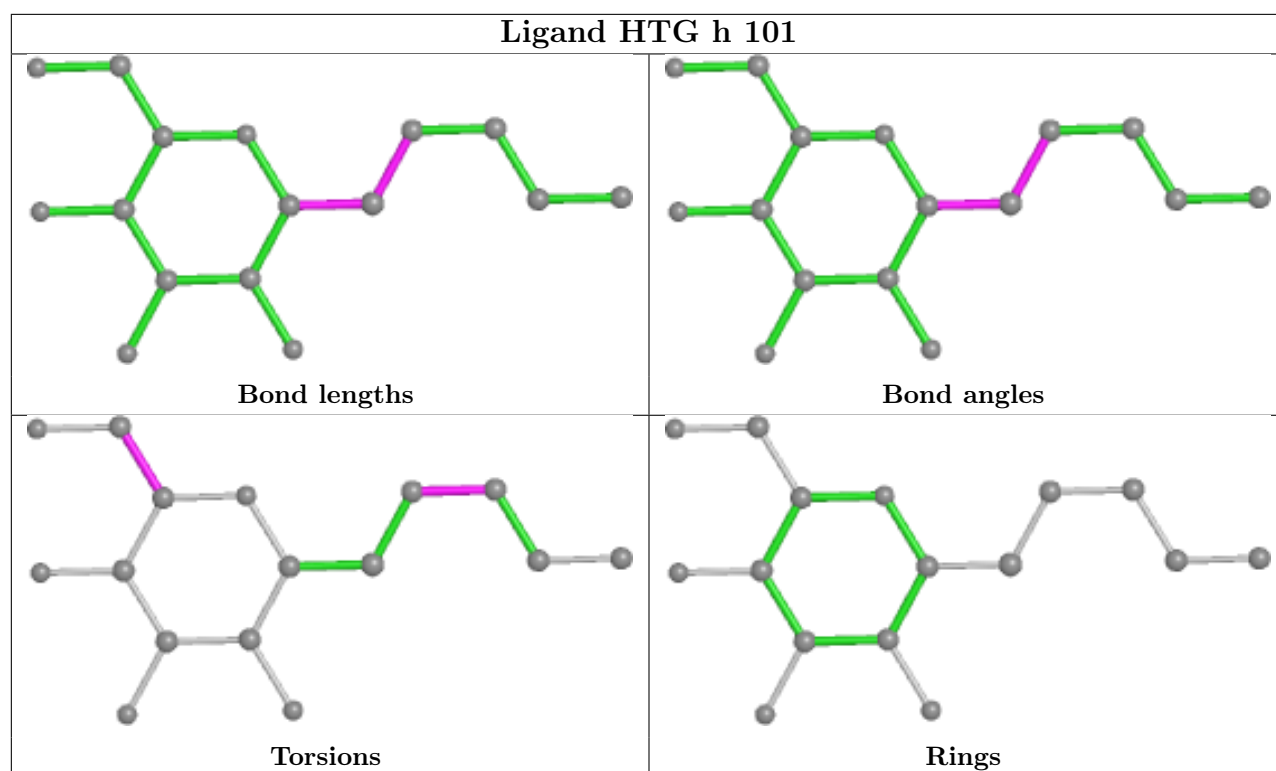
## Ligand CLA b 610

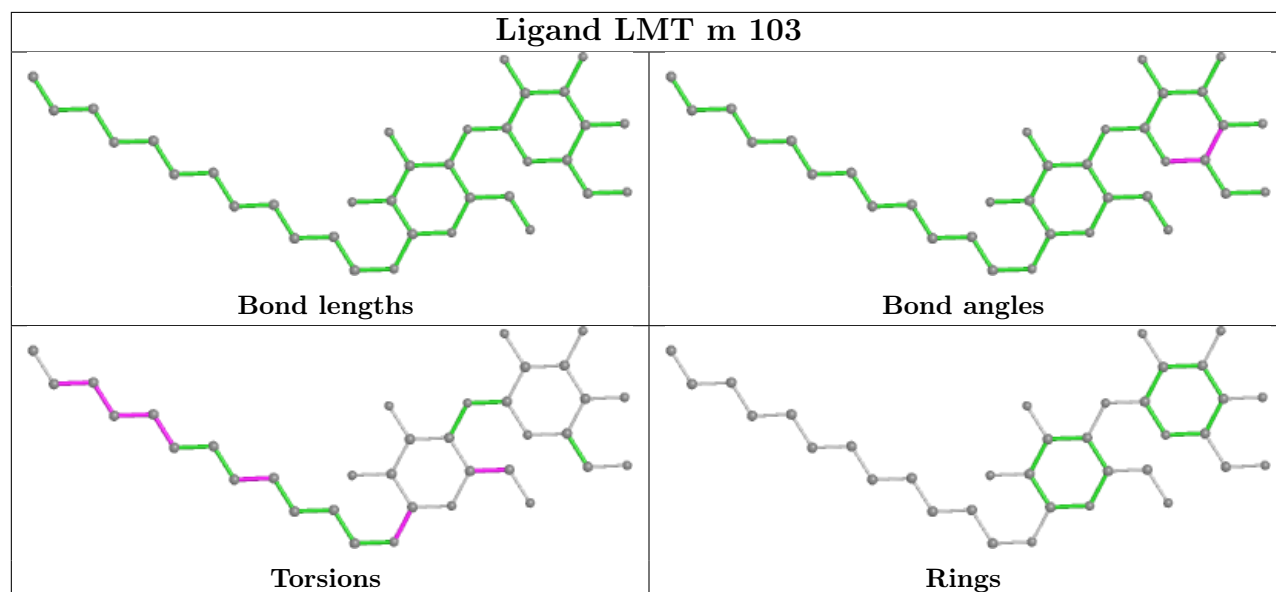
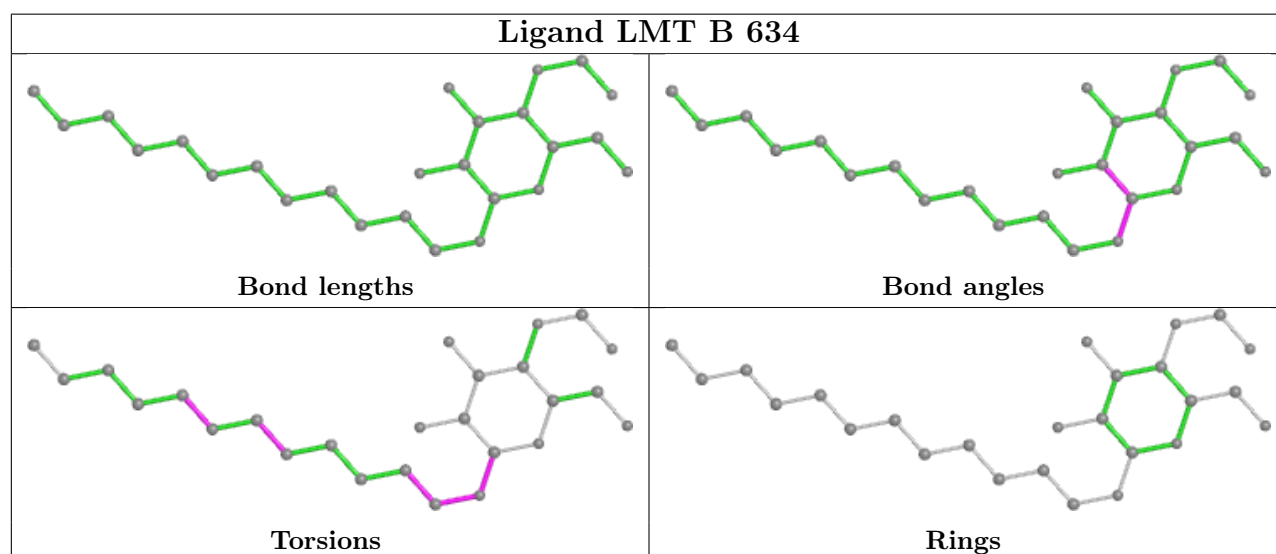
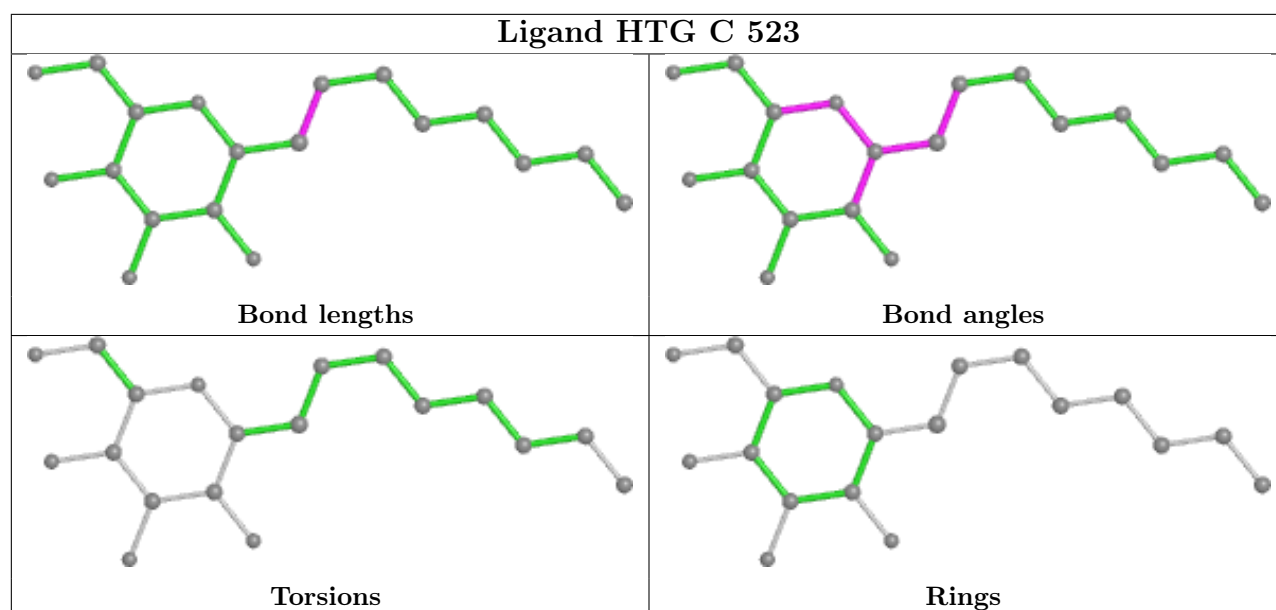


## Ligand HTG B 629

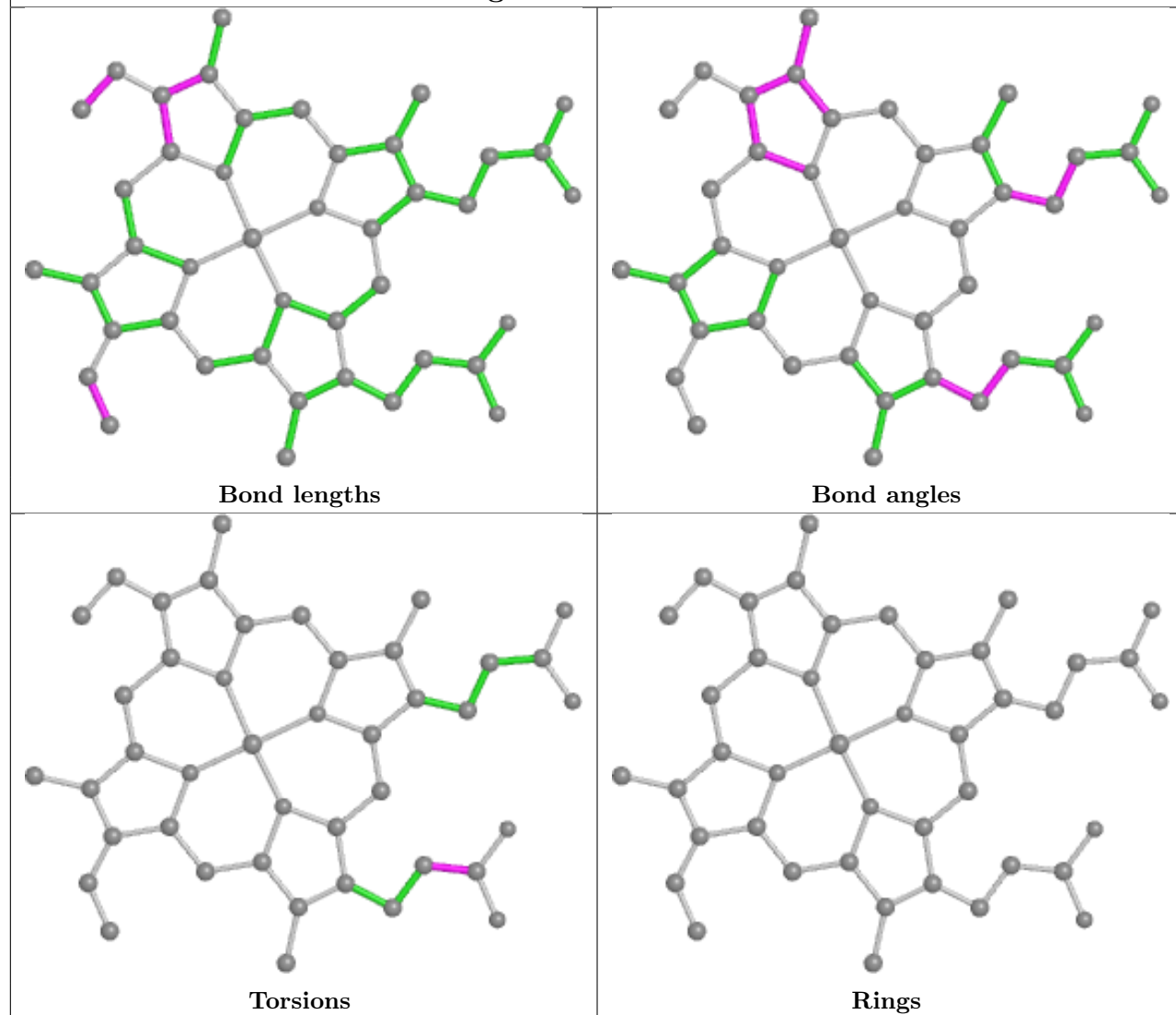




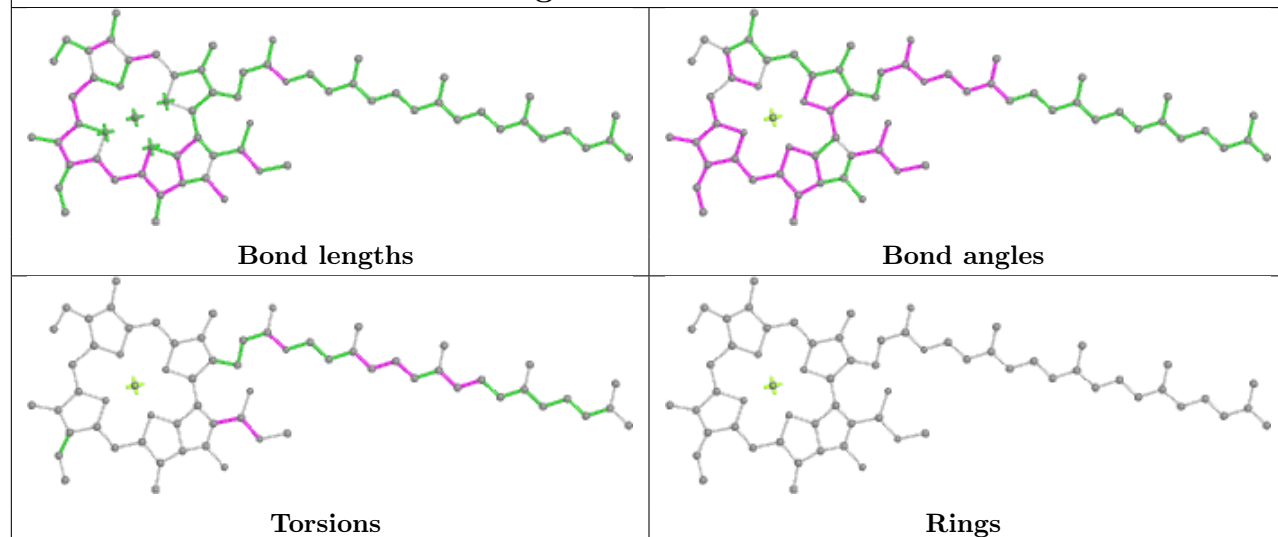


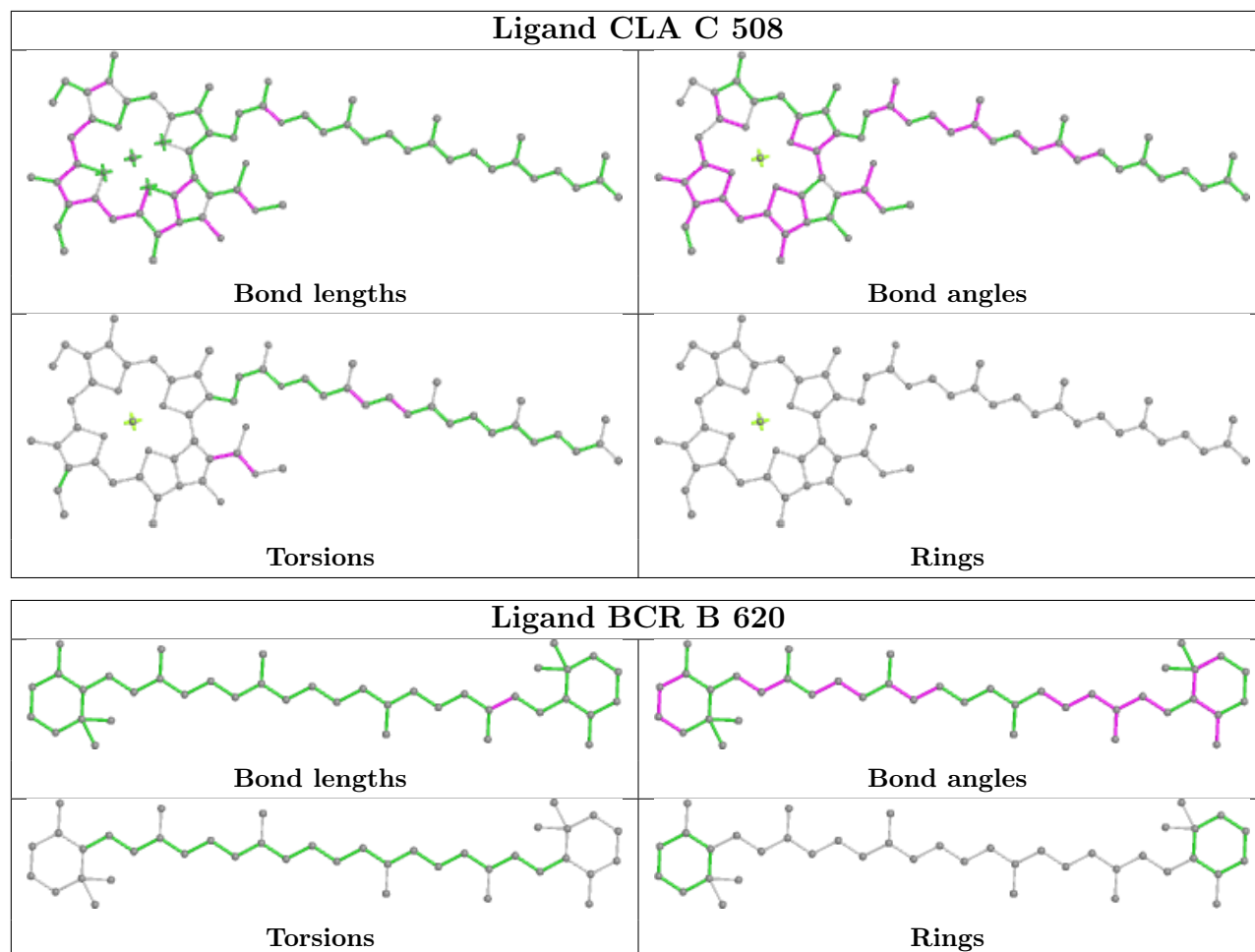


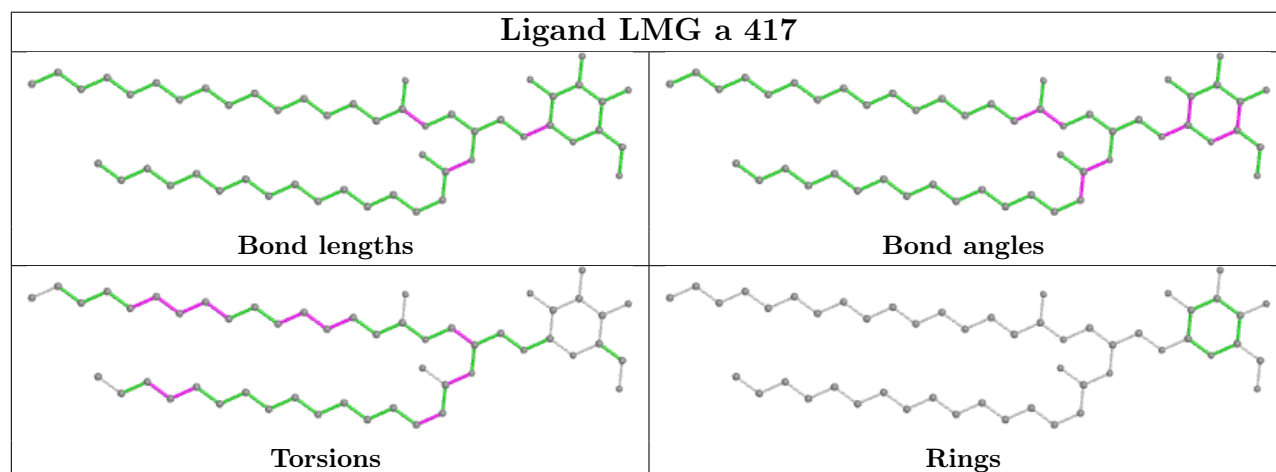
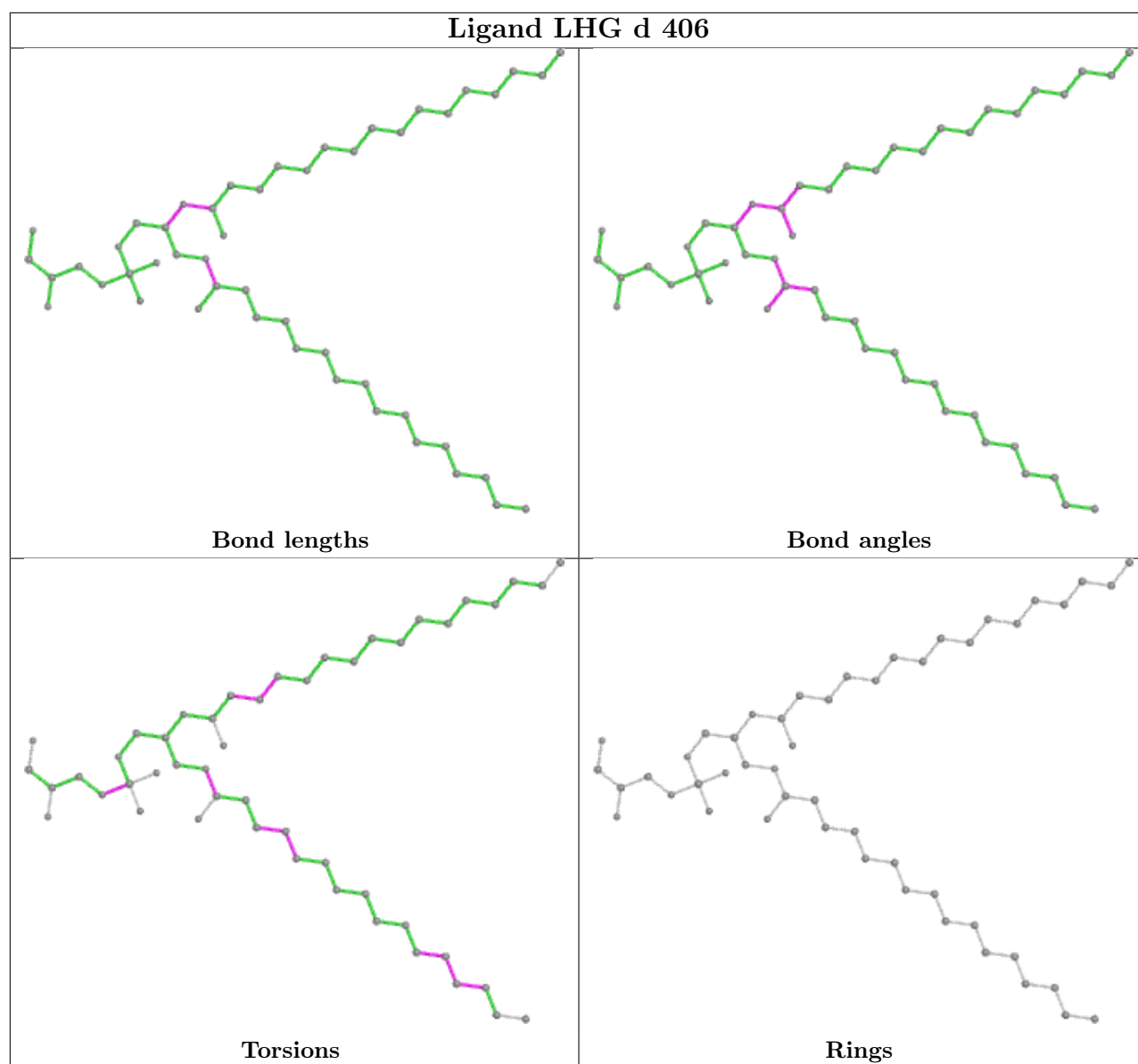
## Ligand HEC V 202



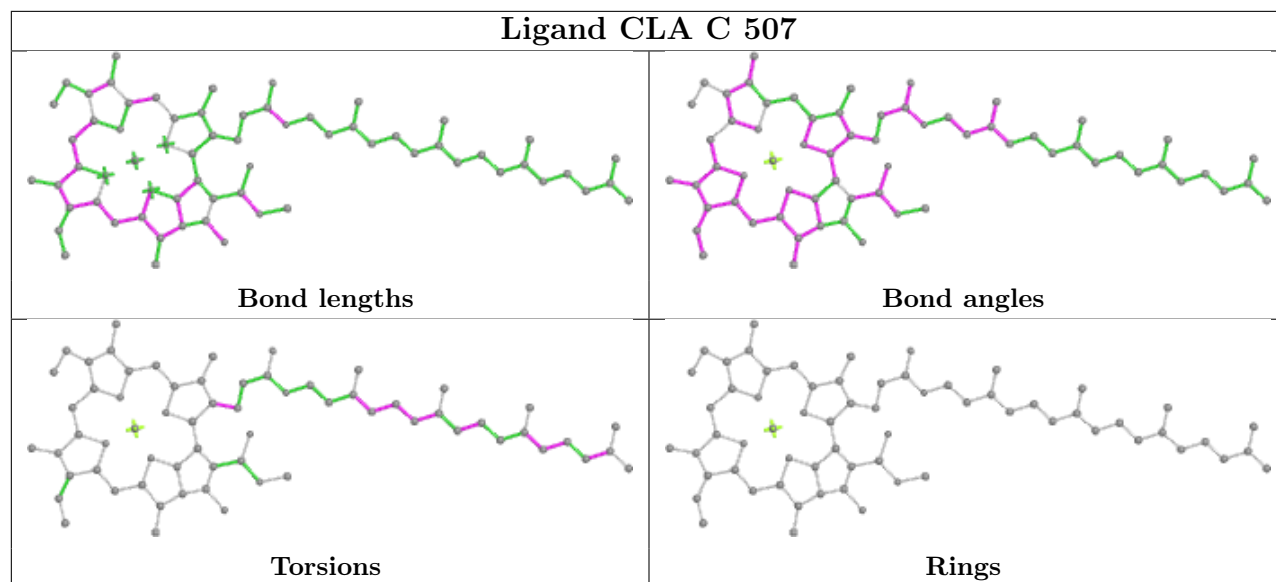
## Ligand CLA b 605



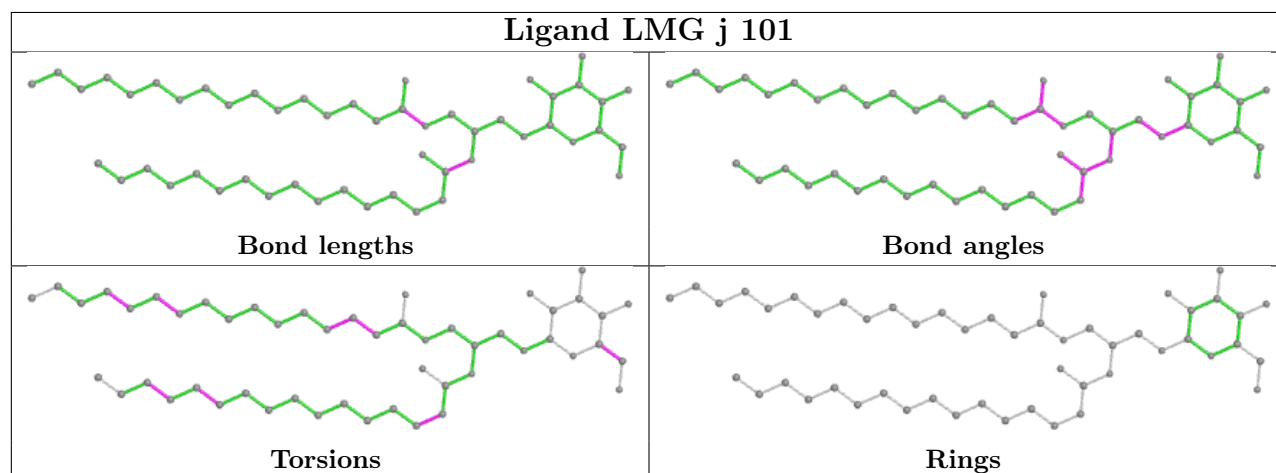




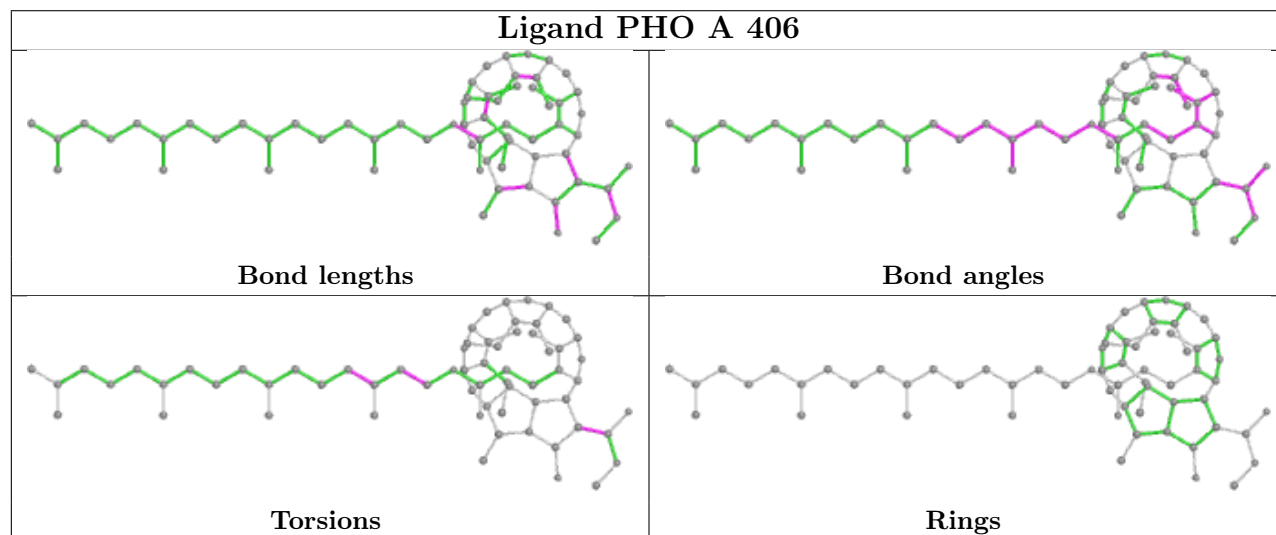
## Ligand CLA C 507

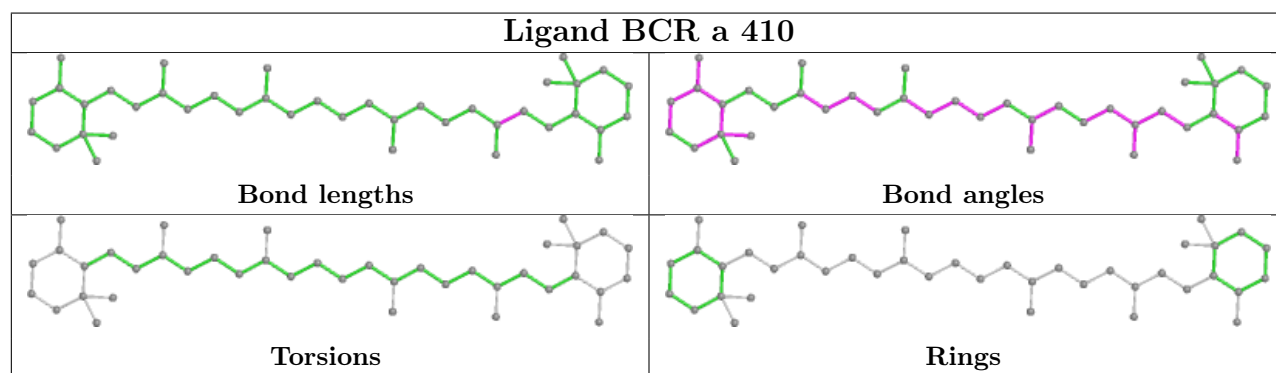
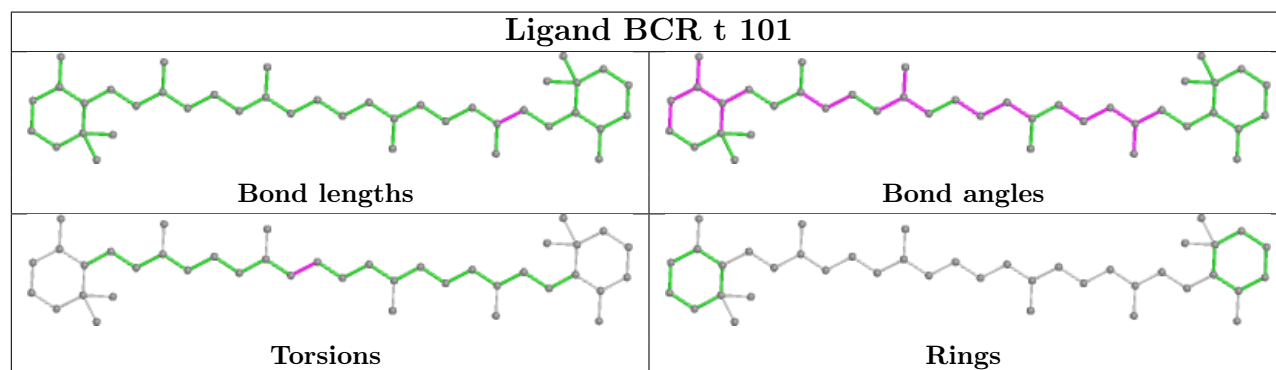
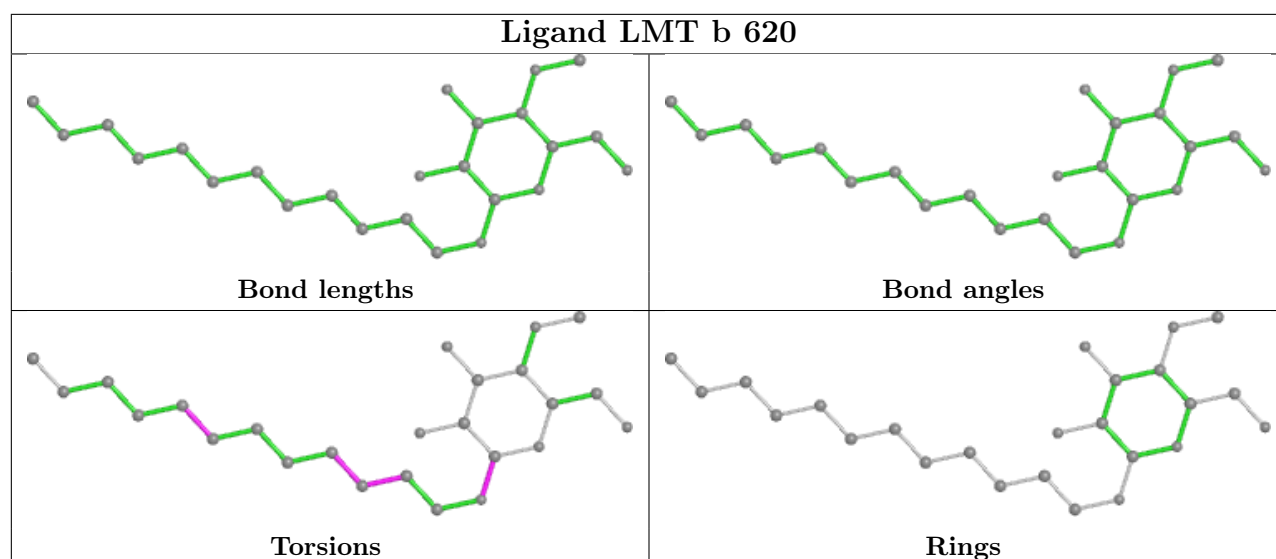


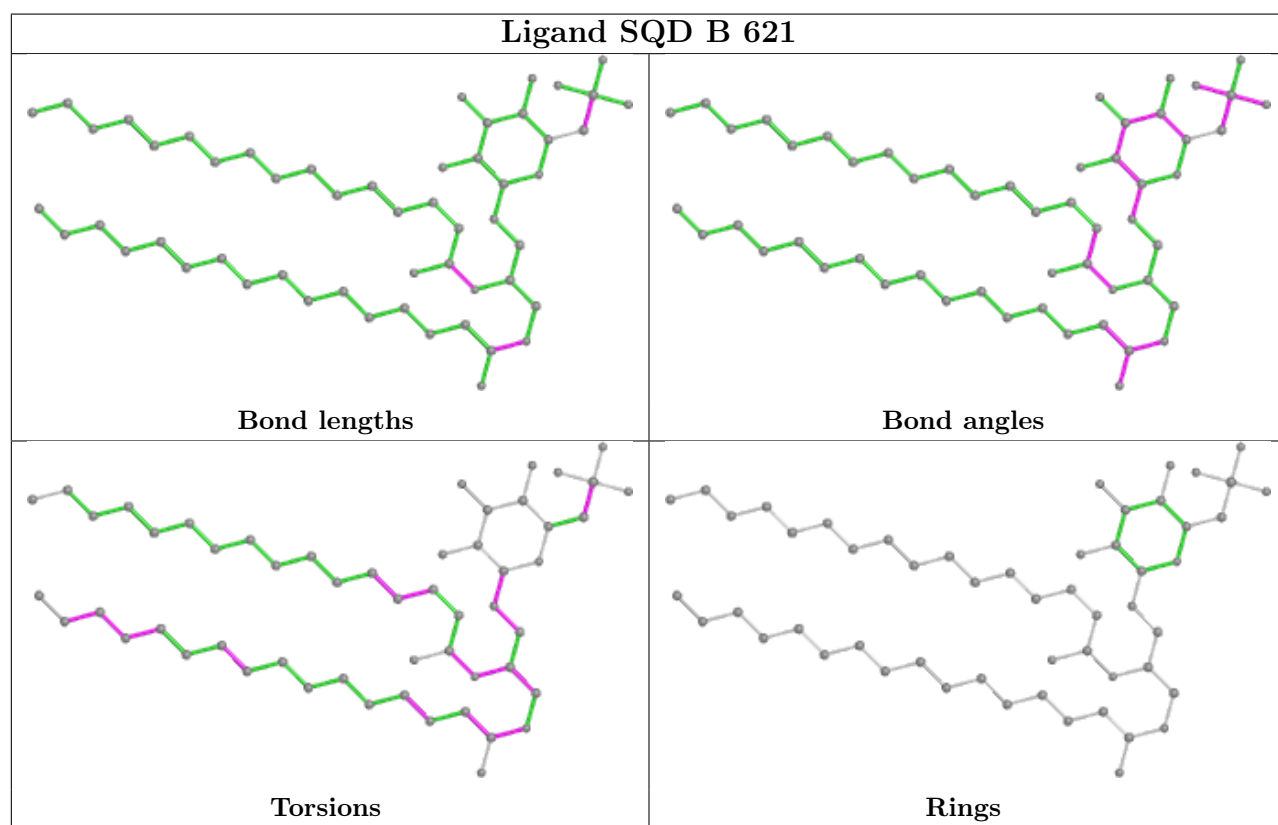
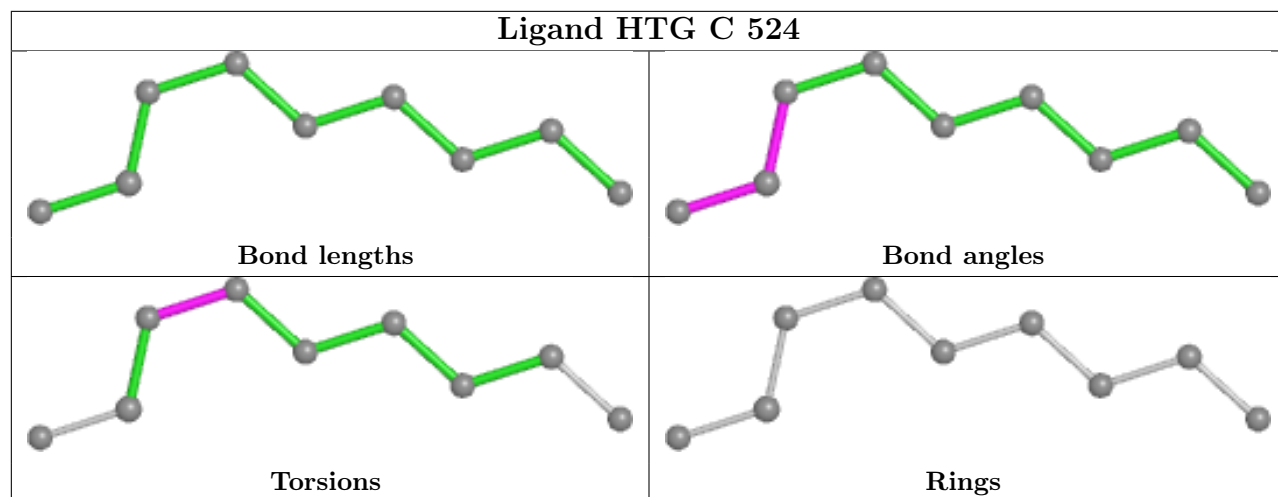
## Ligand LMG j 101



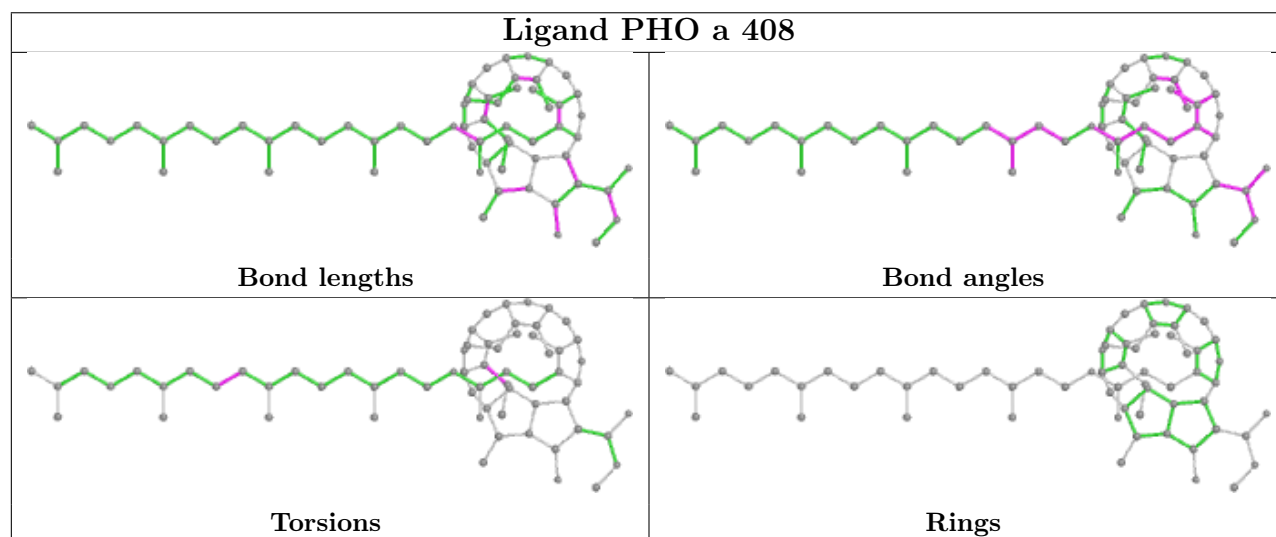
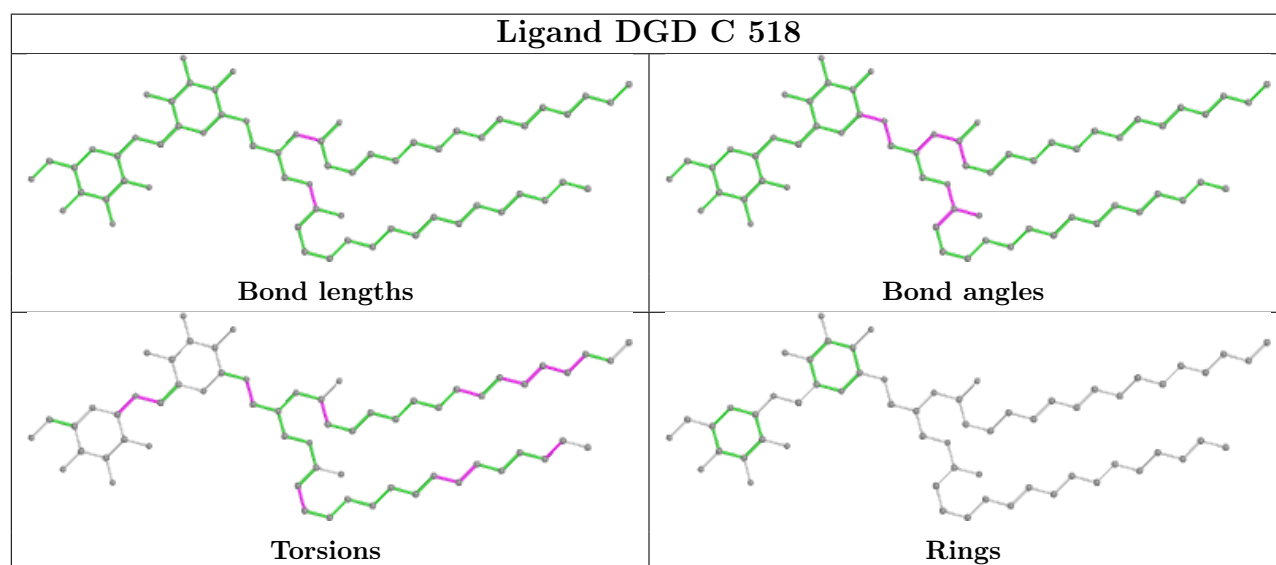
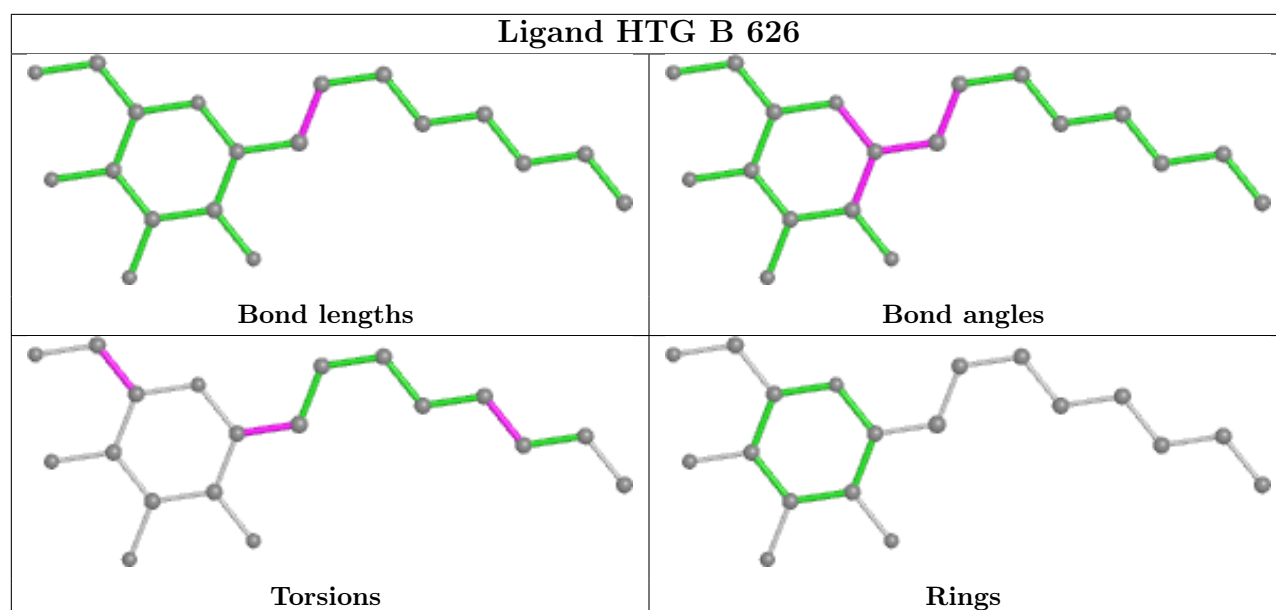
## Ligand PHO A 406

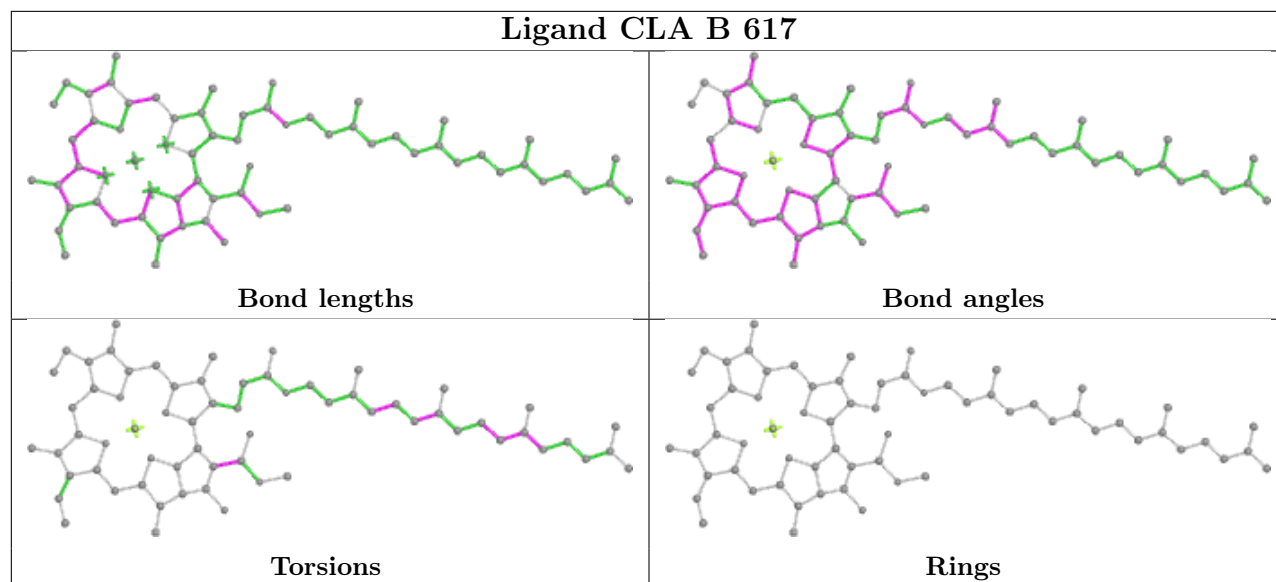
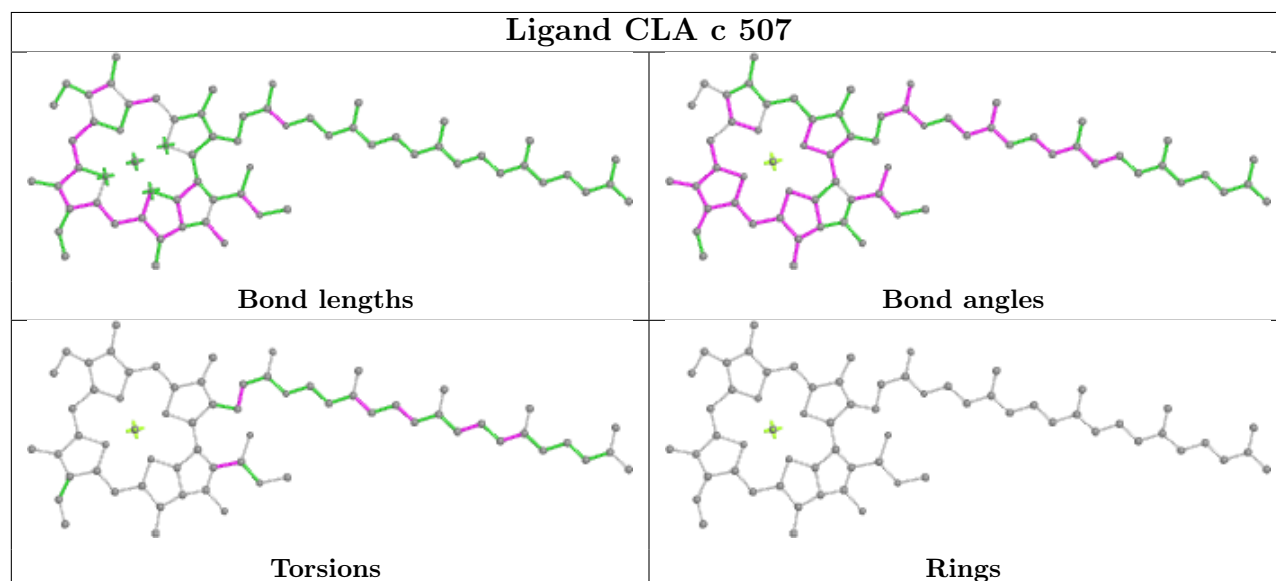
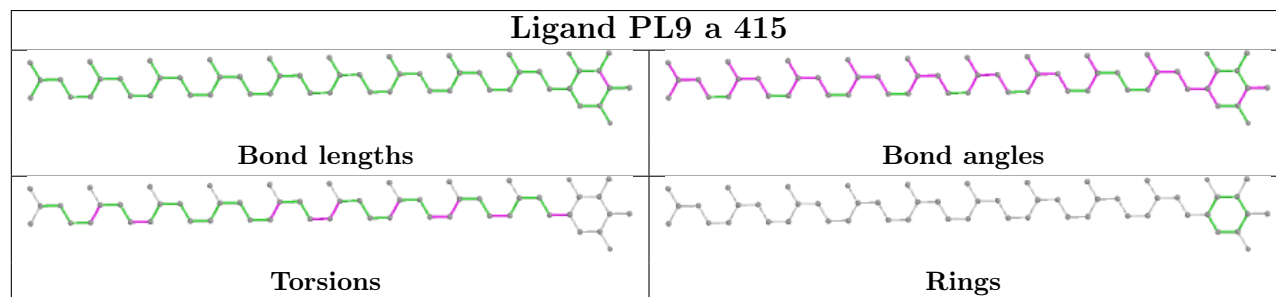




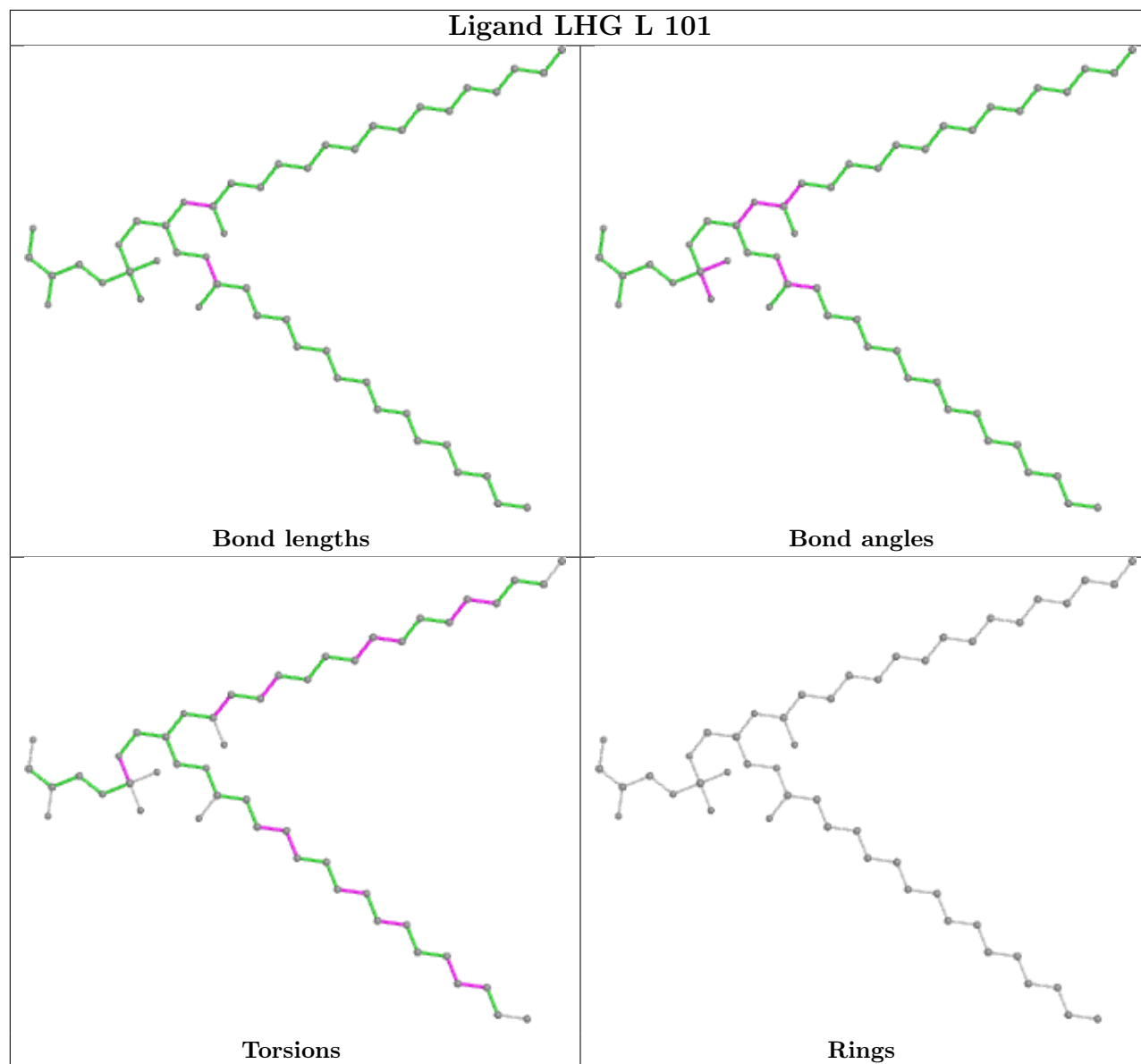




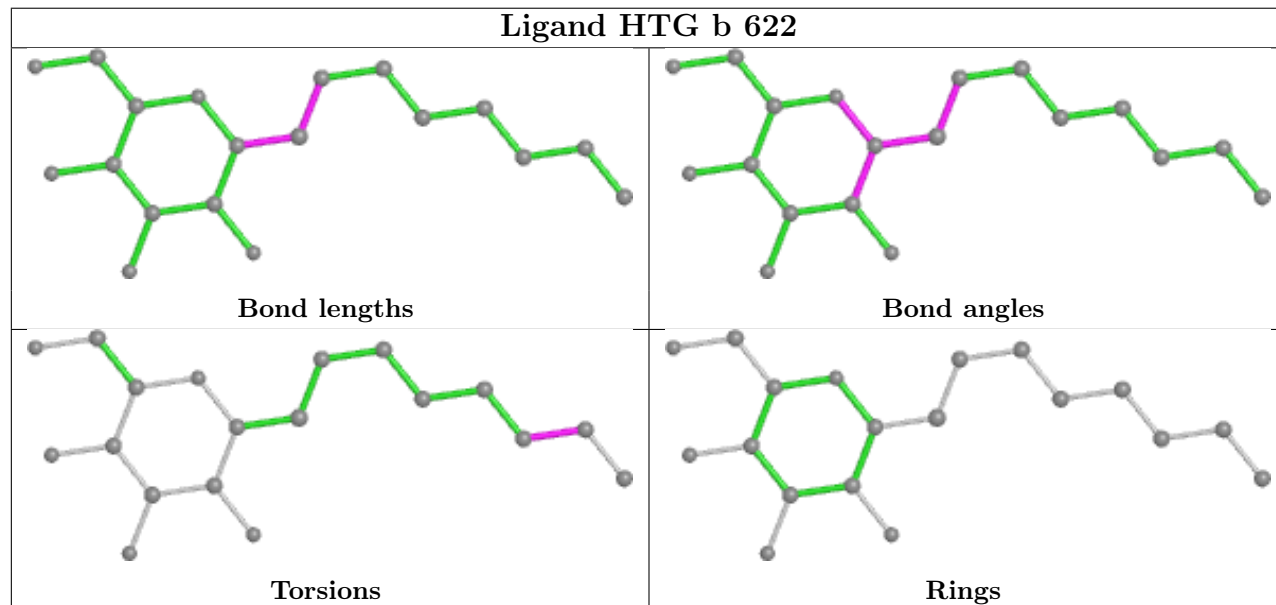


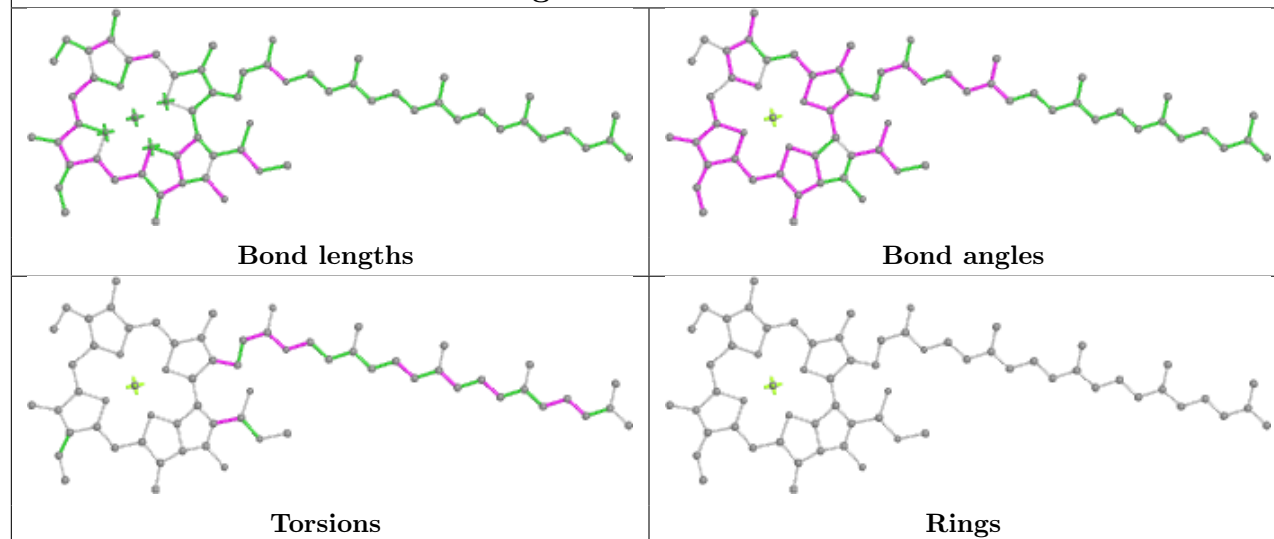
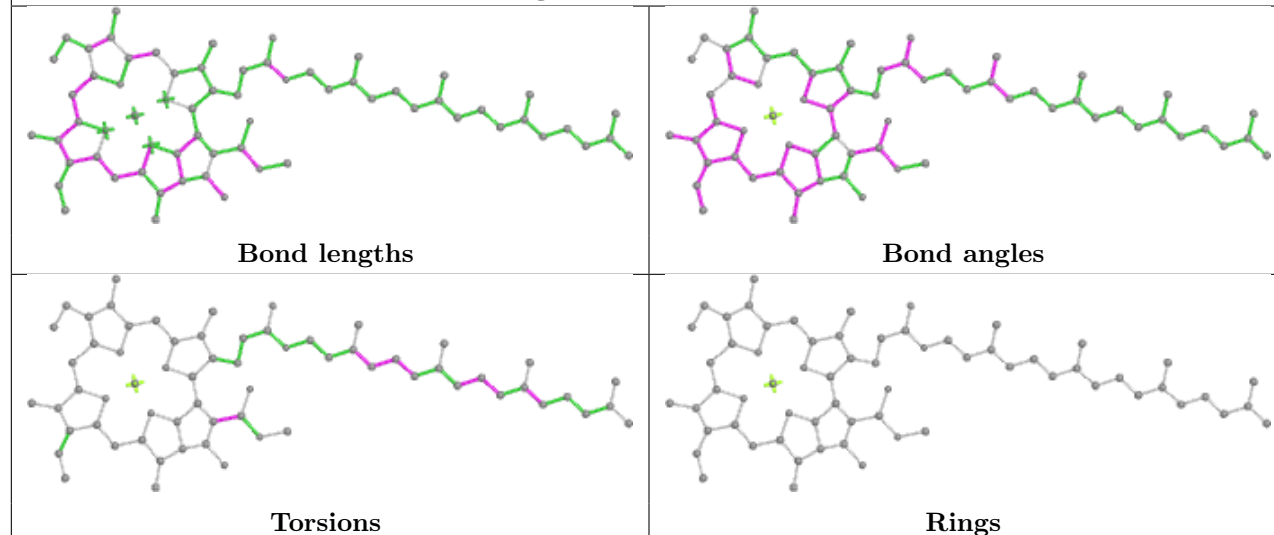
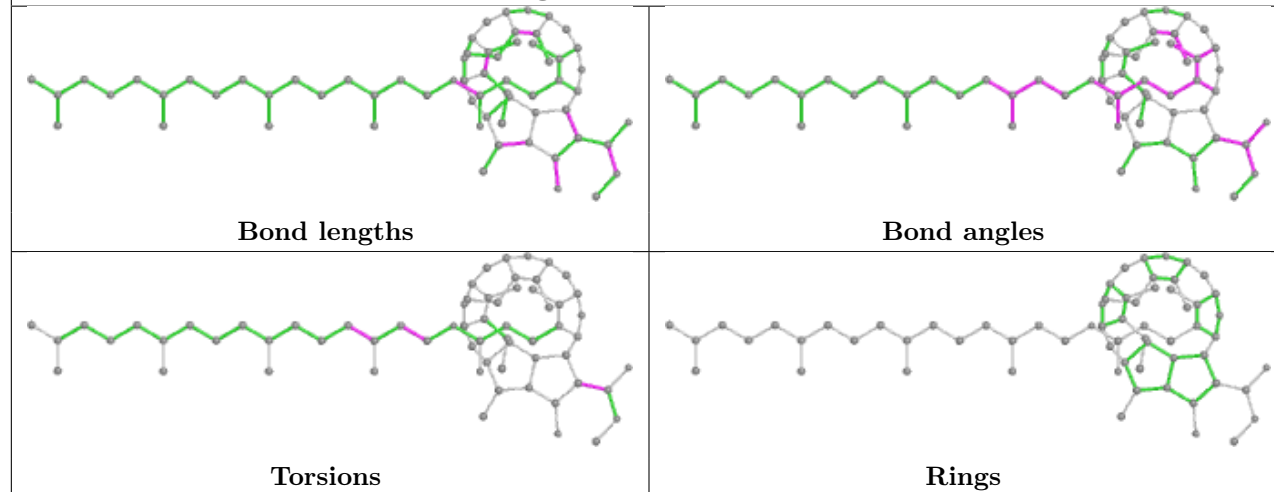
**Ligand CLA B 617****Ligand CLA c 507****Ligand PL9 a 415**

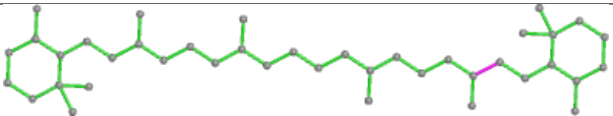
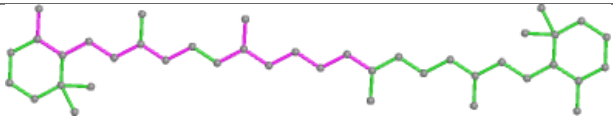
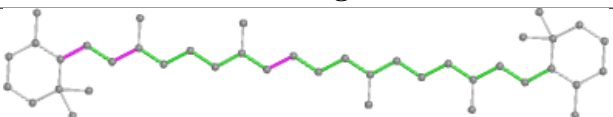
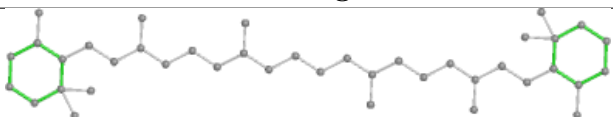
## Ligand LHG L 101

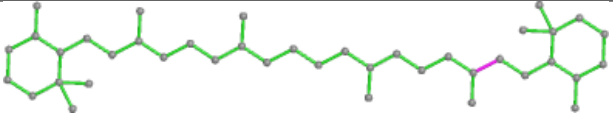
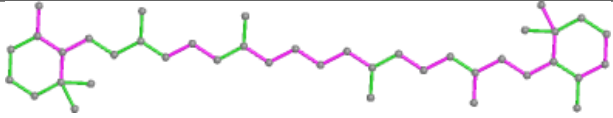
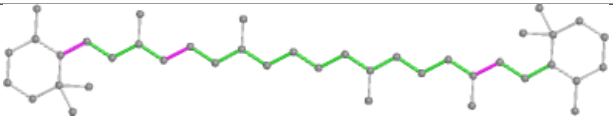
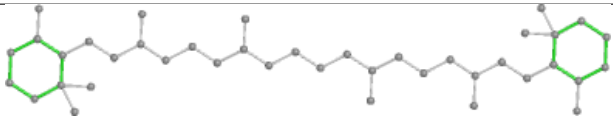


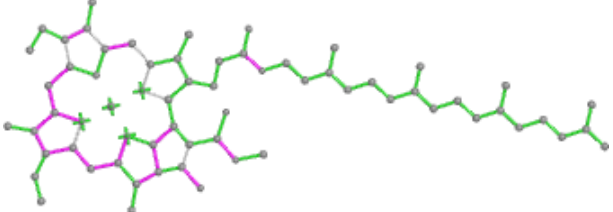
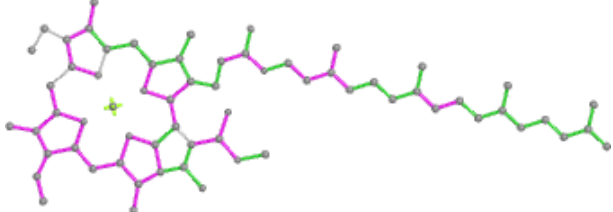
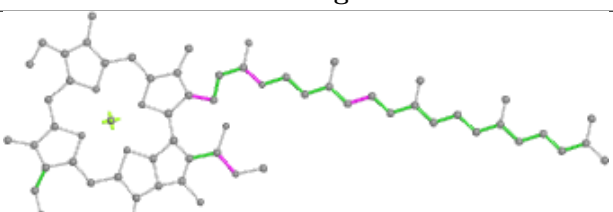
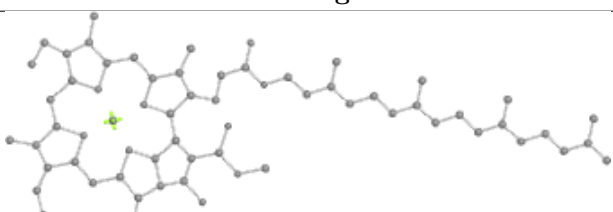
## Ligand HTG b 622

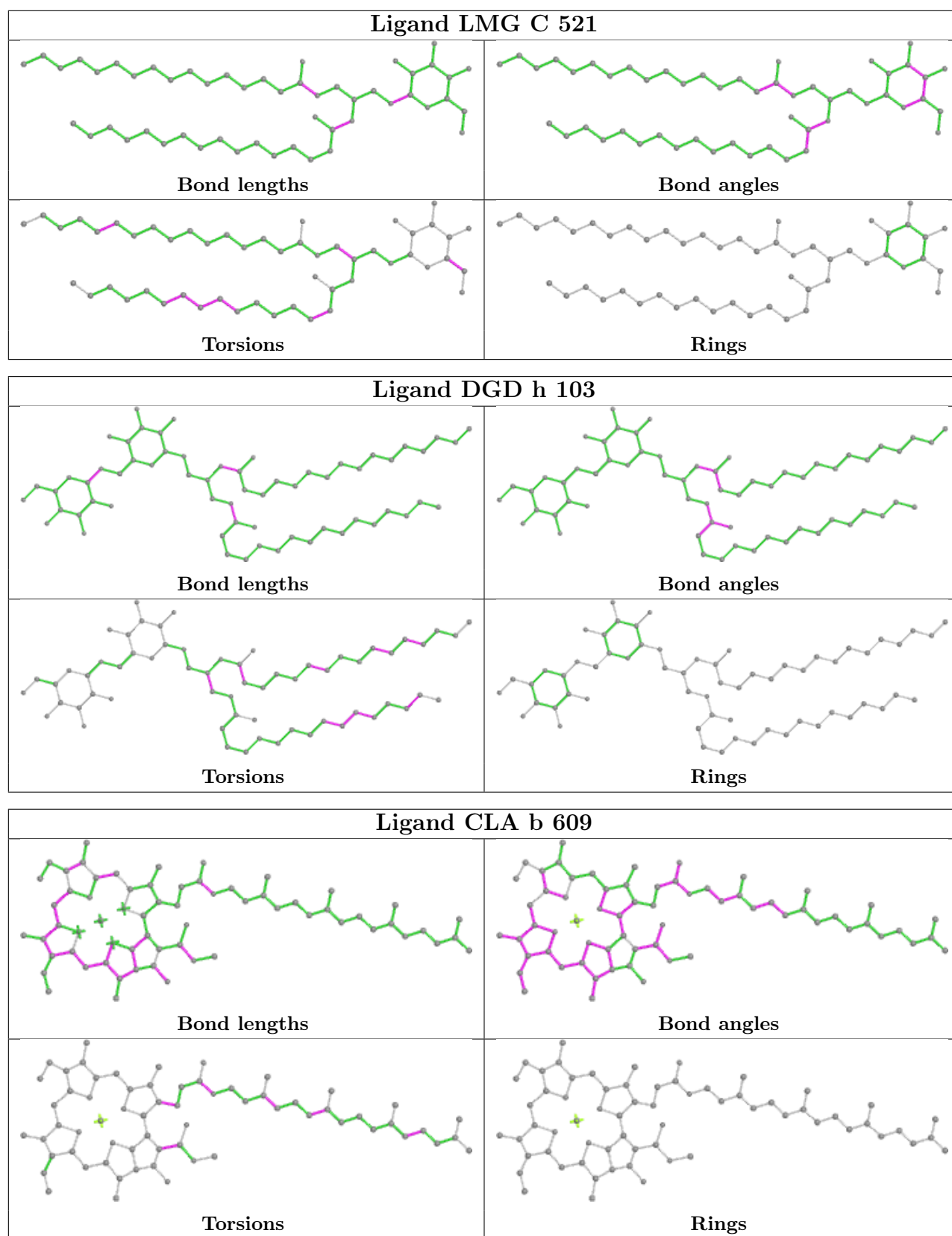


**Ligand CLA B 602****Ligand CLA B 615****Ligand PHO a 407**

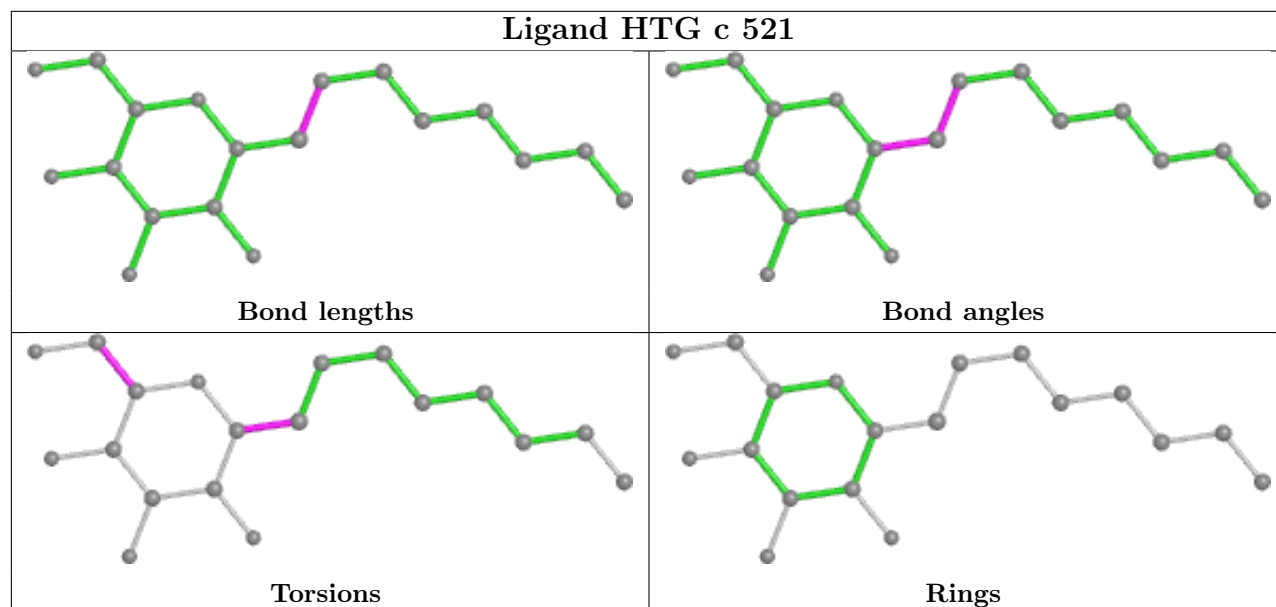
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

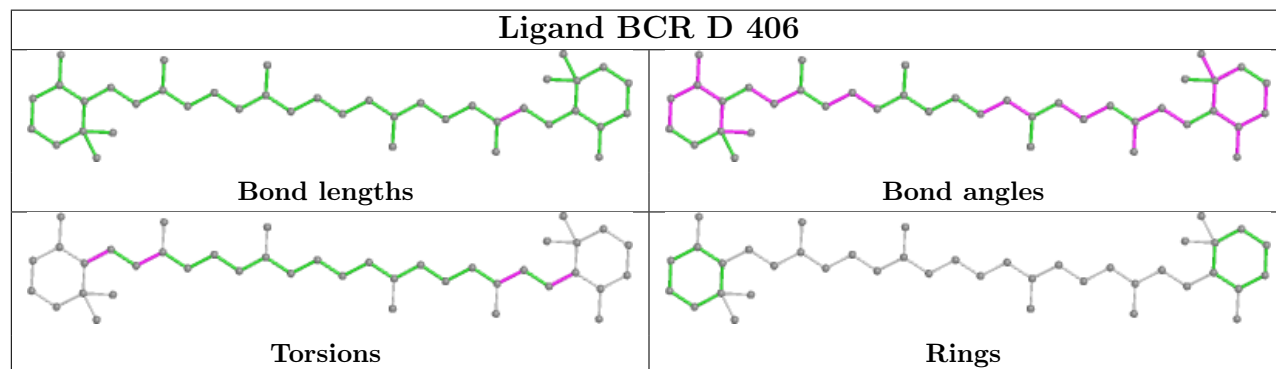
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings



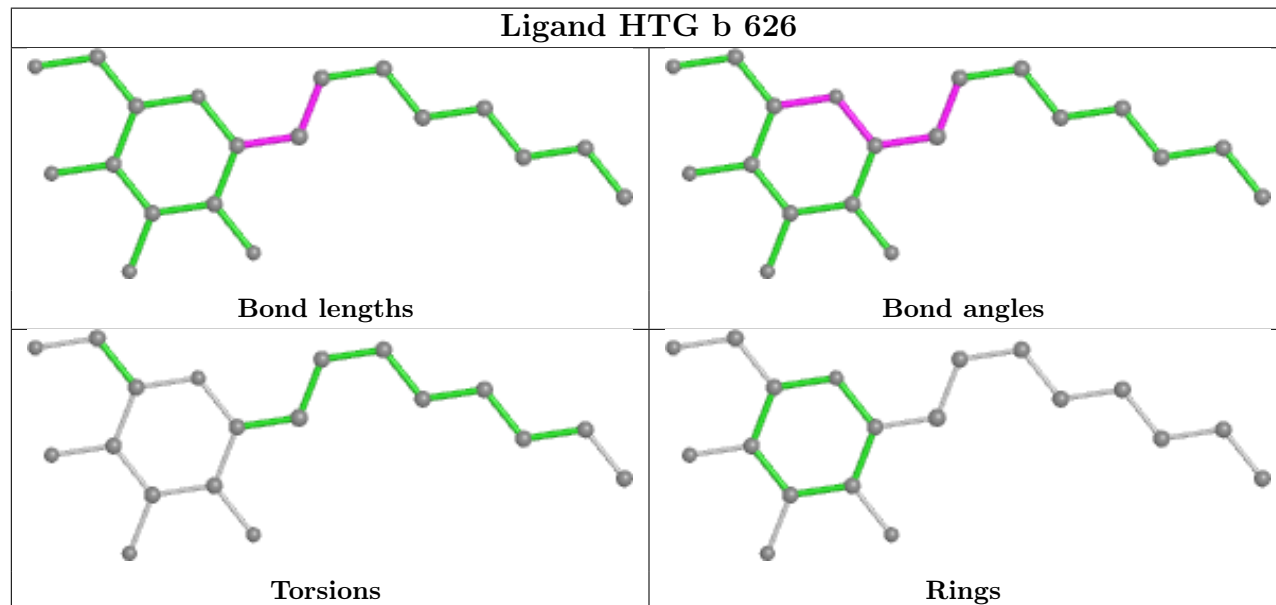
## Ligand HTG c 521

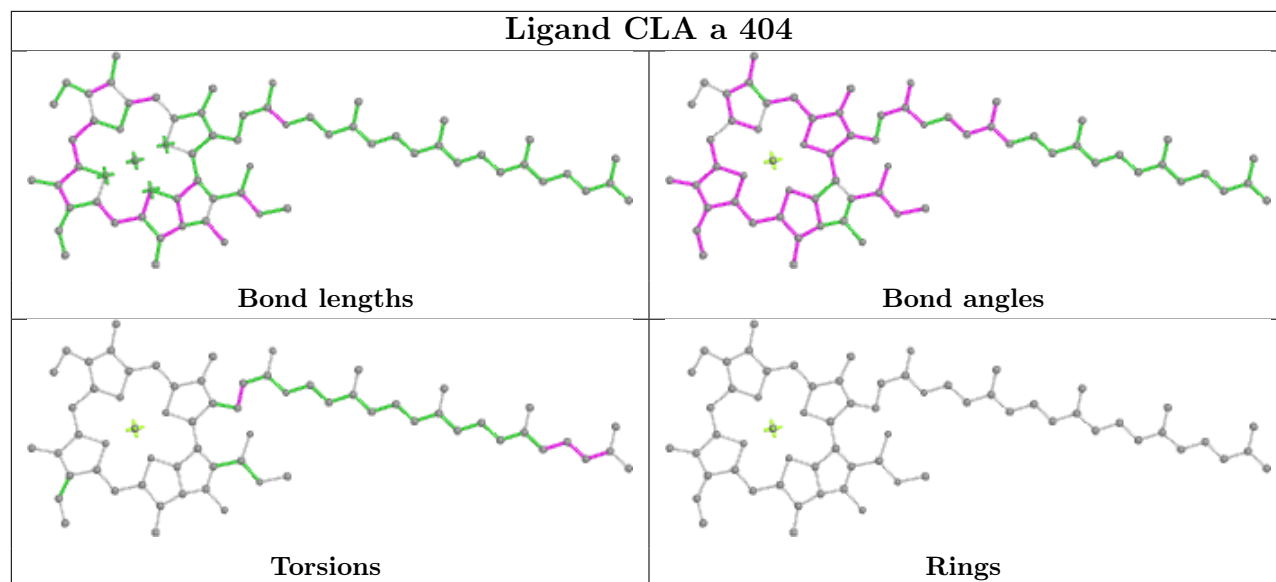
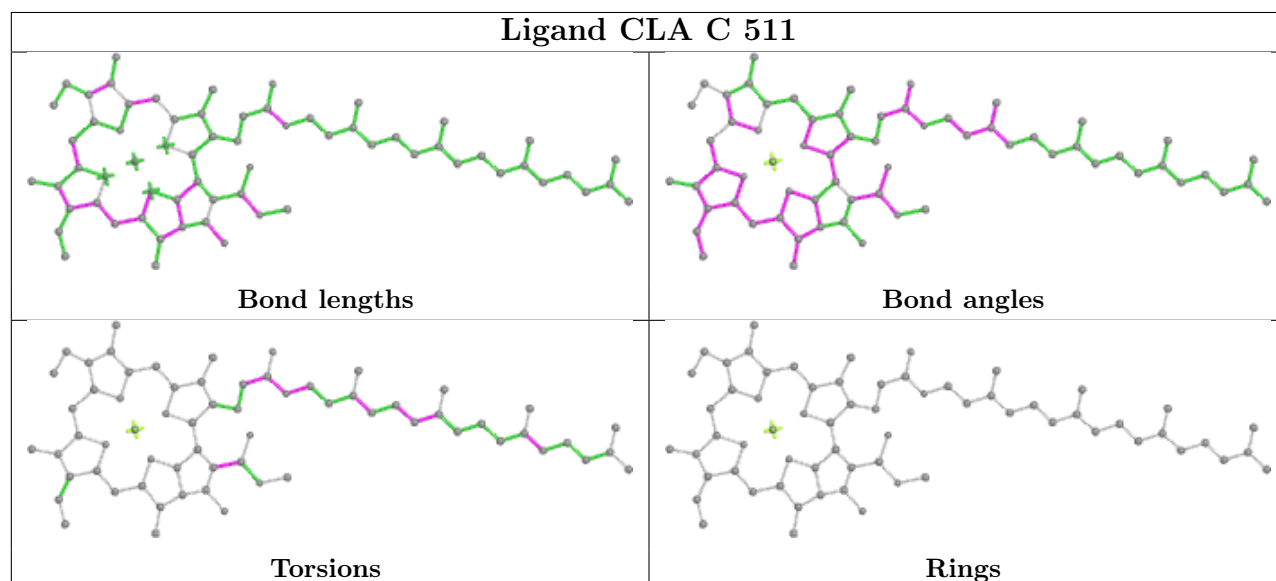
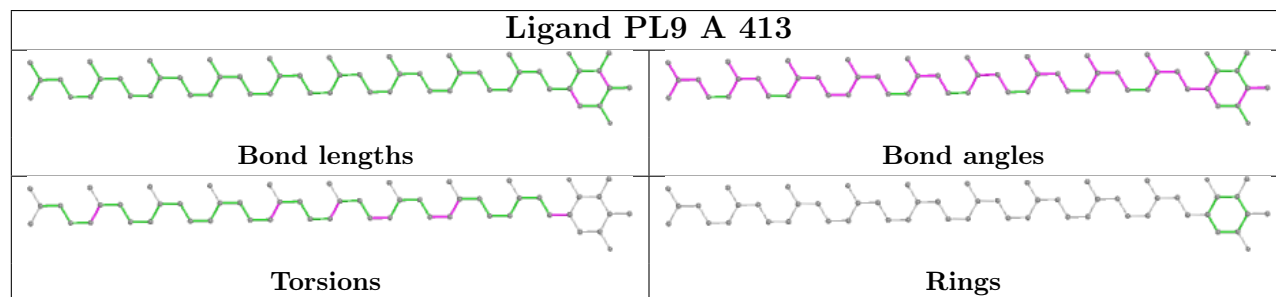


## Ligand BCR D 406



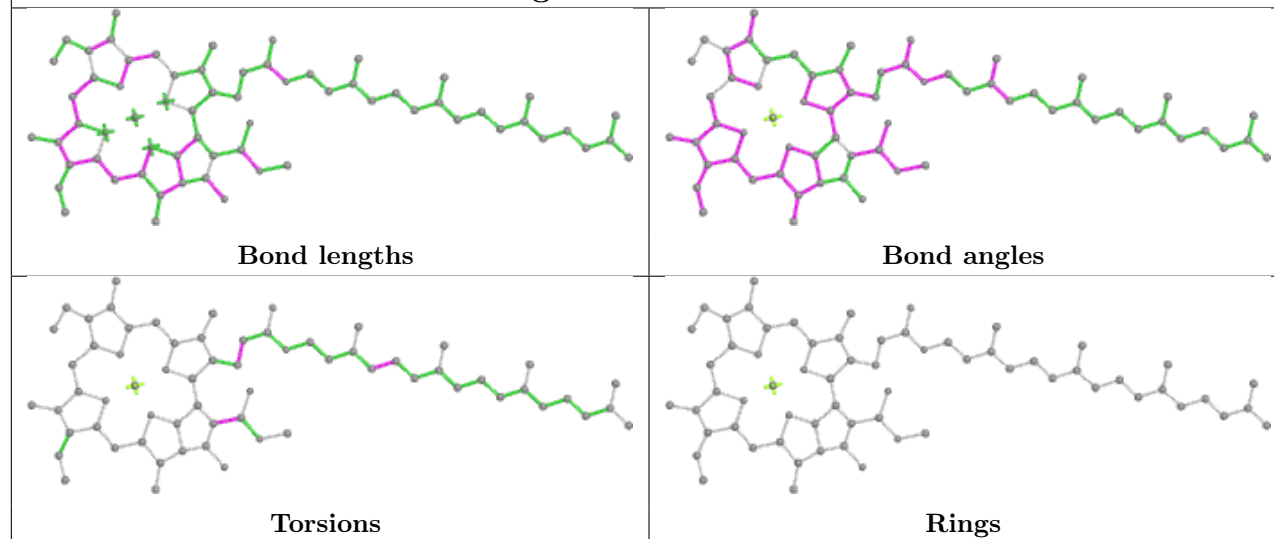
## Ligand HTG b 626



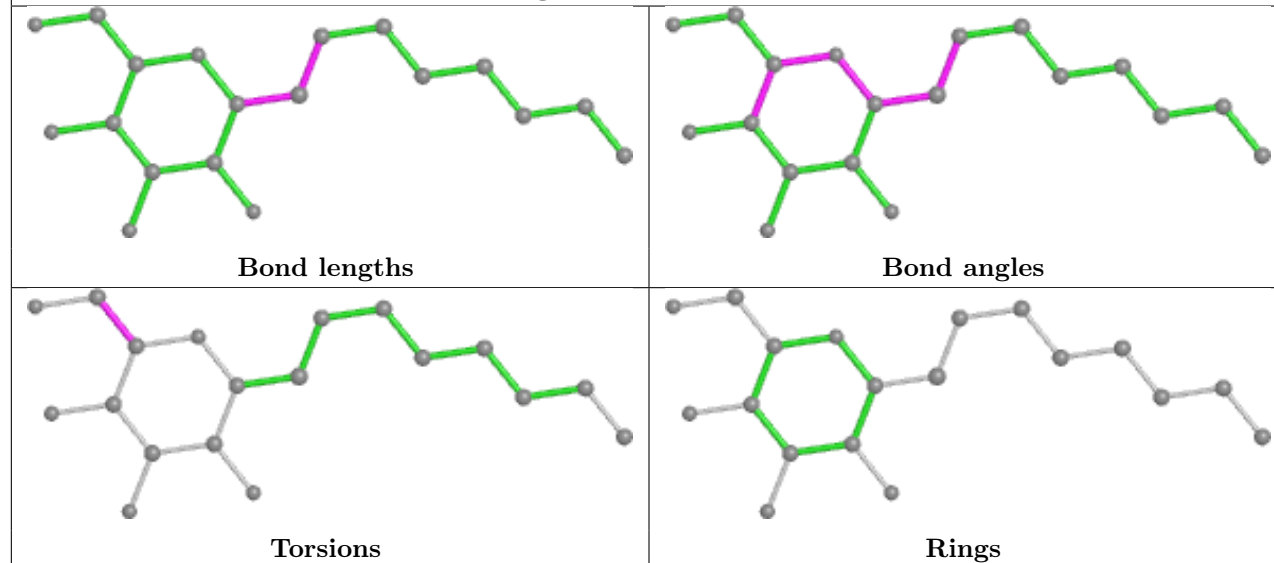
**Ligand CLA a 404****Ligand CLA C 511****Ligand PL9 A 413**



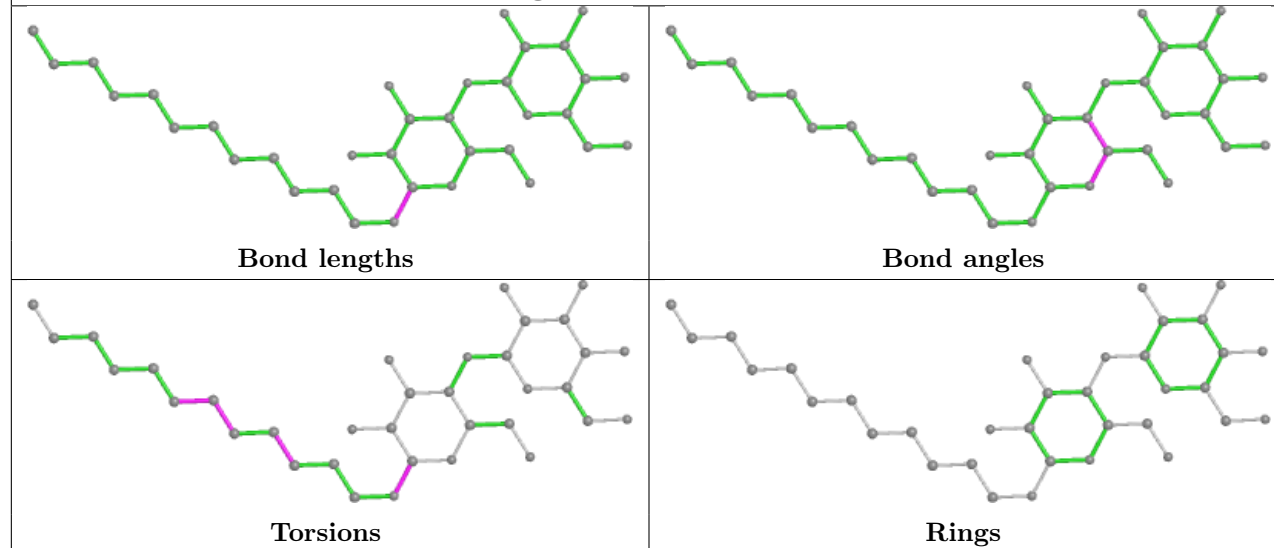
## Ligand CLA B 608



## Ligand HTG c 522



## Ligand LMT B 633



## 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%)	-1.23	0 100 100	22, 33, 58, 97	0
1	a	334/344 (97%)	-1.22	0 100 100	24, 36, 65, 113	0
2	B	504/505 (99%)	-1.16	0 100 100	24, 38, 68, 118	0
2	b	504/505 (99%)	-1.14	0 100 100	25, 40, 77, 122	0
3	C	451/455 (99%)	-1.12	0 100 100	27, 48, 70, 108	0
3	c	455/455 (100%)	-1.11	0 100 100	32, 52, 72, 118	0
4	D	342/342 (100%)	-1.23	0 100 100	22, 35, 58, 113	0
4	d	341/342 (99%)	-1.23	0 100 100	24, 39, 59, 124	0
5	E	81/84 (96%)	-1.01	0 100 100	40, 59, 90, 125	0
5	e	79/84 (94%)	-0.99	0 100 100	45, 62, 100, 125	0
6	F	34/44 (77%)	-1.04	0 100 100	41, 51, 81, 96	0
6	f	31/44 (70%)	-0.93	0 100 100	48, 53, 84, 128	0
7	H	64/65 (98%)	-1.00	1 (1%) 70 67	37, 51, 72, 104	0
7	h	65/65 (100%)	-1.10	0 100 100	40, 54, 79, 152	0
8	I	37/38 (97%)	-1.04	0 100 100	36, 48, 98, 129	0
8	i	37/38 (97%)	-0.90	0 100 100	38, 49, 107, 137	0
9	J	38/39 (97%)	-1.07	0 100 100	37, 55, 113, 156	0
9	j	39/39 (100%)	-0.96	0 100 100	46, 56, 109, 137	0
10	K	37/37 (100%)	-1.17	0 100 100	49, 58, 81, 98	0
10	k	37/37 (100%)	-1.15	0 100 100	52, 60, 82, 99	0
11	L	36/37 (97%)	-1.28	0 100 100	23, 30, 98, 143	0
11	l	36/37 (97%)	-1.26	0 100 100	24, 31, 97, 143	0
12	M	32/36 (88%)	-1.23	0 100 100	24, 31, 53, 125	0
12	m	33/36 (91%)	-1.21	0 100 100	24, 32, 66, 126	0

*Continued on next page...*

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	-1.13	0 100 100	22, 50, 103, 163	0
13	o	243/244 (99%)	-1.14	0 100 100	26, 50, 108, 151	0
14	T	29/32 (90%)	-1.22	0 100 100	26, 31, 68, 97	0
14	t	29/32 (90%)	-1.22	0 100 100	26, 31, 69, 98	0
15	U	96/104 (92%)	-1.19	0 100 100	32, 44, 72, 86	0
15	u	97/104 (93%)	-1.27	0 100 100	37, 47, 72, 105	0
16	V	137/137 (100%)	-1.16	0 100 100	30, 46, 74, 111	0
16	v	137/137 (100%)	-1.14	0 100 100	37, 54, 79, 112	0
17	X	38/40 (95%)	-0.88	0 100 100	49, 58, 80, 121	0
17	x	38/40 (95%)	-0.70	0 100 100	50, 60, 84, 123	0
18	Y	29/30 (96%)	-0.61	0 100 100	60, 76, 112, 120	0
18	y	29/30 (96%)	-0.85	0 100 100	63, 76, 107, 118	0
19	Z	62/62 (100%)	-0.94	0 100 100	57, 77, 127, 161	0
19	z	62/62 (100%)	-0.70	0 100 100	61, 79, 127, 161	0
20	R	34/34 (100%)	0.36	0 100 100	92, 116, 145, 149	0
All	All	5284/5384 (98%)	-1.13	1 (0%) 100 100	22, 45, 88, 163	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	m	1	10/11	0.96	0.06	26,43,69,74	0
14	FME	t	1	10/11	0.97	0.04	22,34,47,66	0
14	FME	T	1	10/11	0.97	0.05	19,37,45,52	0
8	FME	I	1	10/11	0.98	0.04	29,49,53,54	0
12	FME	M	1	10/11	0.98	0.06	33,41,72,72	0
8	FME	i	1	10/11	0.98	0.04	38,50,63,74	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	UNL	m	102	10/-	0.70	0.13	36,47,64,66	0
36	HTG	D	412	16/19	0.72	0.11	43,118,136,138	0
35	LMT	E	102	35/35	0.73	0.13	91,129,157,163	0
36	HTG	B	626	19/19	0.73	0.11	51,135,163,189	0
30	UNL	J	102	10/-	0.73	0.17	59,66,85,90	0
36	HTG	b	622	19/19	0.73	0.15	77,105,127,134	0
34	LMG	C	521	51/55	0.74	0.11	50,107,149,153	0
36	HTG	B	630	19/19	0.74	0.09	67,116,145,154	0
36	HTG	C	524	9/19	0.74	0.18	70,90,106,139	0
35	LMT	D	403	35/35	0.74	0.11	40,112,125,126	0
30	UNL	A	414	28/-	0.74	0.13	66,93,121,126	0
27	GOL	O	302	6/6	0.75	0.09	63,68,72,78	0
30	UNL	i	101	40/-	0.76	0.12	56,91,147,151	0
35	LMT	B	633	35/35	0.76	0.12	39,117,133,139	0
30	UNL	a	416	30/-	0.76	0.11	86,102,121,129	0
35	LMT	a	418	35/35	0.77	0.11	97,118,139,139	0
35	LMT	e	102	35/35	0.77	0.11	75,139,161,171	0
36	HTG	C	523	19/19	0.77	0.10	95,107,121,133	0
30	UNL	j	102	10/-	0.78	0.11	57,81,94,94	0
30	UNL	K	101	34/-	0.78	0.10	62,102,116,137	0
36	HTG	b	626	19/19	0.78	0.09	66,114,151,181	0
36	HTG	B	625	19/19	0.79	0.15	43,101,109,111	0
35	LMT	C	522	35/35	0.79	0.10	83,119,141,151	0
30	UNL	M	102	10/-	0.81	0.09	38,51,60,60	0
36	HTG	c	521	19/19	0.81	0.08	71,125,137,163	0
26	SQD	f	101	43/54	0.82	0.10	86,117,154,157	0
30	UNL	B	631	33/-	0.83	0.12	36,92,134,151	0
30	UNL	b	629	36/-	0.83	0.09	46,85,130,141	0
35	LMT	M	103	35/35	0.83	0.09	37,128,152,157	0
34	LMG	c	520	51/55	0.83	0.09	62,104,135,147	0
35	LMT	B	623	35/35	0.83	0.09	50,95,120,122	0
36	HTG	b	623	19/19	0.83	0.10	73,116,140,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	UNL	D	411	40/-	0.83	0.10	49,76,125,128	0
30	UNL	I	101	40/-	0.83	0.10	39,89,141,148	0
36	HTG	c	522	19/19	0.83	0.10	83,139,149,158	0
31	LHG	e	101	42/49	0.84	0.09	63,119,140,150	0
30	UNL	b	627	33/-	0.85	0.09	53,80,145,147	0
35	LMT	b	620	25/35	0.85	0.09	55,88,143,147	0
35	LMT	M	101	35/35	0.85	0.08	40,85,105,107	0
35	LMT	m	103	35/35	0.85	0.10	40,85,113,117	0
30	UNL	c	525	32/-	0.85	0.10	74,104,124,132	0
36	HTG	h	101	16/19	0.85	0.09	71,110,125,143	0
27	GOL	a	412	6/6	0.86	0.12	56,70,85,86	0
31	LHG	E	101	42/49	0.86	0.09	47,95,114,121	0
36	HTG	b	621	19/19	0.86	0.10	33,91,127,144	0
34	LMG	Z	101	37/55	0.87	0.10	57,103,134,149	0
26	SQD	B	621	54/54	0.87	0.09	44,82,109,118	0
26	SQD	a	413	54/54	0.87	0.07	37,73,134,146	0
27	GOL	d	401	6/6	0.87	0.24	36,51,76,77	0
36	HTG	V	203	11/19	0.87	0.08	88,101,107,108	0
26	SQD	A	411	54/54	0.87	0.07	41,71,114,129	0
33	CA	B	601	1/1	0.88	0.07	144,144,144,144	0
35	LMT	B	632	25/35	0.88	0.10	41,68,135,136	0
30	UNL	D	410	17/-	0.89	0.09	46,64,94,102	0
27	GOL	B	628	6/6	0.89	0.12	47,58,65,72	0
29	PL9	a	415	55/55	0.89	0.10	56,82,108,115	0
26	SQD	D	413	43/54	0.90	0.10	58,106,117,124	0
35	LMT	b	628	25/35	0.90	0.08	37,63,135,142	0
36	HTG	B	629	19/19	0.90	0.07	47,59,78,83	0
26	SQD	L	102	54/54	0.90	0.07	39,73,114,123	0
34	LMG	z	101	39/55	0.90	0.10	69,117,144,151	0
29	PL9	A	413	55/55	0.91	0.10	44,83,100,110	0
27	GOL	b	624	6/6	0.91	0.10	75,92,97,104	0
34	LMG	C	501	51/55	0.91	0.09	40,81,110,113	0
30	UNL	x	101	18/-	0.91	0.09	47,66,104,105	0
25	BCR	D	406	40/40	0.91	0.07	35,46,78,84	0
35	LMT	B	634	26/35	0.92	0.08	48,90,109,115	0
34	LMG	C	520	51/55	0.92	0.08	43,75,125,134	0
23	CLA	b	601	65/65	0.92	0.07	46,70,107,135	0
30	UNL	X	101	18/-	0.92	0.10	39,66,83,87	0
34	LMG	a	417	51/55	0.92	0.07	42,79,99,115	0
36	HTG	B	624	19/19	0.92	0.07	33,71,128,130	0
34	LMG	c	519	51/55	0.92	0.08	47,78,122,143	0
27	GOL	C	525	6/6	0.93	0.12	45,56,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	C	507	65/65	0.93	0.07	42,57,106,115	0
23	CLA	B	602	65/65	0.93	0.08	39,61,93,123	0
36	HTG	b	625	19/19	0.93	0.06	40,60,90,94	0
23	CLA	c	513	65/65	0.93	0.07	58,74,112,119	0
27	GOL	A	410	6/6	0.93	0.08	45,57,60,90	0
25	BCR	C	515	40/40	0.93	0.07	49,60,74,82	0
34	LMG	J	101	51/55	0.93	0.07	33,54,96,105	0
23	CLA	C	505	65/65	0.94	0.07	32,46,91,111	0
25	BCR	C	527	40/40	0.94	0.07	43,55,71,72	0
23	CLA	C	514	65/65	0.94	0.07	50,65,100,107	0
25	BCR	Y	101	40/40	0.94	0.06	40,51,62,71	0
25	BCR	y	101	40/40	0.94	0.06	48,60,74,77	0
25	BCR	B	620	40/40	0.94	0.06	30,43,67,78	0
27	GOL	B	627	6/6	0.94	0.09	60,77,93,95	0
34	LMG	j	101	51/55	0.94	0.06	41,56,92,119	0
34	LMG	B	622	51/55	0.94	0.06	35,53,83,101	0
30	UNL	d	409	17/-	0.94	0.06	48,58,94,99	0
37	DGD	c	517	62/66	0.94	0.06	42,55,110,126	0
23	CLA	C	513	65/65	0.95	0.06	46,60,106,112	0
31	LHG	d	406	49/49	0.95	0.07	27,48,81,84	0
26	SQD	A	409	54/54	0.95	0.07	41,66,99,109	0
23	CLA	b	616	65/65	0.95	0.06	34,51,101,111	0
23	CLA	c	504	65/65	0.95	0.06	41,52,94,117	0
23	CLA	c	506	65/65	0.95	0.06	47,65,98,117	0
23	CLA	c	507	65/65	0.95	0.07	43,57,70,72	0
29	PL9	D	407	55/55	0.95	0.05	20,30,44,53	0
26	SQD	a	411	54/54	0.95	0.07	44,69,108,113	0
23	CLA	c	512	65/65	0.95	0.07	53,66,96,104	0
25	BCR	b	619	40/40	0.95	0.05	33,46,69,80	0
25	BCR	d	404	40/40	0.95	0.06	43,55,79,81	0
25	BCR	k	101	40/40	0.95	0.07	50,60,84,87	0
25	BCR	t	101	40/40	0.95	0.05	23,43,64,68	0
34	LMG	m	101	51/55	0.95	0.05	33,52,85,99	0
37	DGD	C	518	62/66	0.95	0.06	35,51,111,119	0
37	DGD	c	516	62/66	0.95	0.06	35,47,74,93	0
31	LHG	A	415	49/49	0.95	0.06	29,46,67,82	0
37	DGD	c	518	62/66	0.95	0.05	39,50,74,97	0
23	CLA	C	508	65/65	0.96	0.06	40,51,66,78	0
23	CLA	C	509	65/65	0.96	0.05	33,46,93,103	0
23	CLA	d	403	65/65	0.96	0.06	41,52,102,116	0
24	PHO	a	408	64/64	0.96	0.05	30,40,53,60	0
25	BCR	A	408	40/40	0.96	0.05	23,34,48,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	B	619	40/40	0.96	0.04	21,36,52,60	0
23	CLA	C	511	65/65	0.96	0.05	36,48,61,67	0
23	CLA	B	607	65/65	0.96	0.06	28,37,76,93	0
31	LHG	D	409	49/49	0.96	0.07	32,50,107,117	0
25	BCR	C	516	40/40	0.96	0.06	38,50,63,68	0
31	LHG	b	630	49/49	0.96	0.05	26,43,59,64	0
23	CLA	B	617	65/65	0.96	0.07	33,45,121,132	0
31	LHG	d	408	49/49	0.96	0.07	40,55,105,111	0
23	CLA	D	405	65/65	0.96	0.07	33,48,111,119	0
25	BCR	H	101	40/40	0.96	0.05	35,46,66,73	0
25	BCR	T	101	40/40	0.96	0.04	21,37,55,60	0
23	CLA	a	409	65/65	0.96	0.07	30,44,124,130	0
25	BCR	b	617	40/40	0.96	0.04	21,35,45,51	0
25	BCR	b	618	40/40	0.96	0.04	22,36,51,56	0
29	PL9	d	405	55/55	0.96	0.05	24,33,49,66	0
23	CLA	C	502	65/65	0.96	0.06	36,45,67,70	0
25	BCR	c	514	40/40	0.96	0.05	58,68,80,83	0
25	BCR	c	515	40/40	0.96	0.05	41,54,66,70	0
23	CLA	b	602	65/65	0.96	0.06	36,48,68,77	0
25	BCR	h	102	40/40	0.96	0.06	42,57,71,74	0
23	CLA	C	503	65/65	0.96	0.06	33,43,60,67	0
23	CLA	c	501	65/65	0.96	0.05	43,53,67,72	0
23	CLA	C	504	65/65	0.96	0.06	37,47,66,75	0
37	DGD	C	519	62/66	0.96	0.05	30,44,80,109	0
37	DGD	H	102	62/66	0.96	0.06	29,42,64,68	0
23	CLA	A	407	65/65	0.96	0.06	28,38,98,117	0
23	CLA	B	603	65/65	0.96	0.05	31,41,57,69	0
23	CLA	c	511	65/65	0.96	0.06	47,56,78,89	0
23	CLA	b	605	65/65	0.97	0.05	26,34,51,76	0
23	CLA	b	606	65/65	0.97	0.05	29,42,91,110	0
23	CLA	b	607	65/65	0.97	0.05	21,30,58,67	0
23	CLA	b	608	65/65	0.97	0.05	34,44,67,72	0
23	CLA	b	609	65/65	0.97	0.05	39,48,63,74	0
25	BCR	a	410	40/40	0.97	0.05	28,38,55,58	0
23	CLA	b	610	65/65	0.97	0.05	35,44,56,61	0
23	CLA	b	611	65/65	0.97	0.05	27,35,57,62	0
23	CLA	b	612	65/65	0.97	0.06	28,35,48,69	0
23	CLA	b	613	65/65	0.97	0.05	24,36,79,89	0
23	CLA	b	614	65/65	0.97	0.05	25,35,93,107	0
23	CLA	b	615	65/65	0.97	0.05	33,43,65,87	0
23	CLA	C	506	65/65	0.97	0.05	33,44,75,82	0
23	CLA	B	611	65/65	0.97	0.06	29,41,55,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	c	502	65/65	0.97	0.05	40,55,70,74	0
23	CLA	c	503	65/65	0.97	0.05	44,55,67,84	0
23	CLA	B	612	65/65	0.97	0.05	24,32,49,54	0
23	CLA	c	505	65/65	0.97	0.06	36,46,76,82	0
23	CLA	B	613	65/65	0.97	0.05	26,33,45,65	0
23	CLA	B	614	65/65	0.97	0.04	23,31,72,87	0
31	LHG	D	408	49/49	0.97	0.06	25,37,56,78	0
23	CLA	c	508	65/65	0.97	0.05	39,53,121,131	0
23	CLA	c	509	65/65	0.97	0.06	46,56,73,79	0
31	LHG	L	101	49/49	0.97	0.04	26,39,54,75	0
23	CLA	c	510	65/65	0.97	0.05	39,51,67,71	0
23	CLA	C	512	65/65	0.97	0.06	39,54,77,85	0
31	LHG	d	407	49/49	0.97	0.06	24,38,58,65	0
23	CLA	B	615	65/65	0.97	0.05	23,32,86,95	0
23	CLA	B	604	65/65	0.97	0.05	30,43,56,67	0
32	BCT	a	419	4/4	0.97	0.05	41,45,48,58	0
23	CLA	B	605	65/65	0.97	0.05	22,31,101,111	0
33	CA	O	301	1/1	0.97	0.06	101,101,101,101	0
33	CA	V	201	1/1	0.97	0.04	94,94,94,94	0
24	PHO	D	402	64/64	0.97	0.04	25,31,44,55	0
23	CLA	a	406	65/65	0.97	0.05	30,38,98,103	0
37	DGD	C	517	62/66	0.97	0.05	30,41,77,88	0
23	CLA	A	405	65/65	0.97	0.05	24,33,85,94	0
25	BCR	B	618	40/40	0.97	0.04	24,37,48,49	0
23	CLA	B	608	65/65	0.97	0.05	20,28,59,67	0
23	CLA	B	610	65/65	0.97	0.05	31,42,53,89	0
23	CLA	b	603	65/65	0.97	0.05	32,44,61,70	0
23	CLA	b	604	65/65	0.97	0.05	24,33,95,101	0
37	DGD	h	103	62/66	0.97	0.05	34,46,67,76	0
23	CLA	D	404	65/65	0.98	0.05	21,29,50,56	0
22	CL	a	403	1/1	0.98	0.04	41,41,41,41	0
23	CLA	a	404	65/65	0.98	0.05	27,33,52,66	0
32	BCT	A	416	4/4	0.98	0.05	32,45,46,51	0
23	CLA	a	405	65/65	0.98	0.04	23,29,52,60	0
23	CLA	C	510	65/65	0.98	0.06	39,53,71,79	0
23	CLA	d	402	65/65	0.98	0.05	27,32,58,72	0
23	CLA	B	616	65/65	0.98	0.04	29,38,60,67	0
33	CA	c	523	1/1	0.98	0.10	68,68,68,68	0
24	PHO	A	406	64/64	0.98	0.04	22,29,39,46	0
23	CLA	A	404	65/65	0.98	0.04	22,25,39,58	0
24	PHO	a	407	64/64	0.98	0.04	24,31,45,50	0
23	CLA	B	609	65/65	0.98	0.04	30,42,56,66	0

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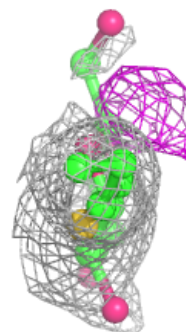
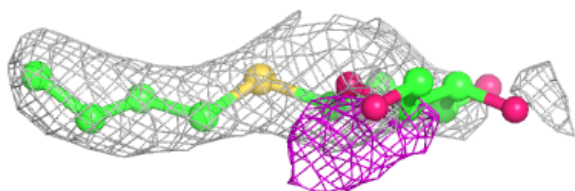
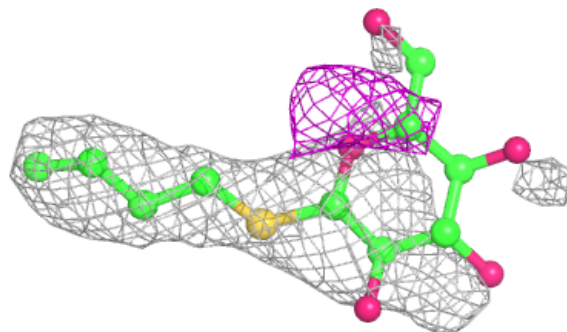
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	B	606	65/65	0.98	0.05	24,33,46,51	0
23	CLA	D	401	65/65	0.98	0.04	21,28,43,47	0
38	HEM	E	103	43/43	0.98	0.06	43,56,69,83	0
38	HEM	e	103	43/43	0.98	0.06	52,78,106,116	0
39	MG	J	103	1/1	0.98	0.10	43,43,43,43	0
40	HEC	v	201	43/43	0.98	0.05	44,53,63,82	0
33	CA	o	301	1/1	0.99	0.02	89,89,89,89	0
21	FE2	a	401	1/1	0.99	0.03	47,47,47,47	0
22	CL	A	402	1/1	0.99	0.07	24,24,24,24	0
33	CA	C	526	1/1	0.99	0.10	59,59,59,59	0
22	CL	A	403	1/1	0.99	0.03	27,27,27,27	0
22	CL	a	402	1/1	0.99	0.06	28,28,28,28	0
39	MG	j	103	1/1	0.99	0.06	48,48,48,48	0
40	HEC	V	202	43/43	0.99	0.05	33,36,48,70	0
21	FE2	A	401	1/1	0.99	0.03	46,46,46,46	0
28	OEX	A	412	10/10	1.00	0.03	23,32,46,47	0
33	CA	c	524	1/1	1.00	0.03	66,66,66,66	0
28	OEX	a	414	10/10	1.00	0.02	29,36,46,48	0

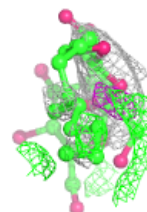
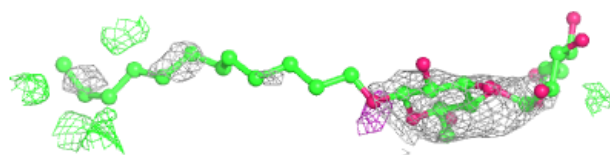
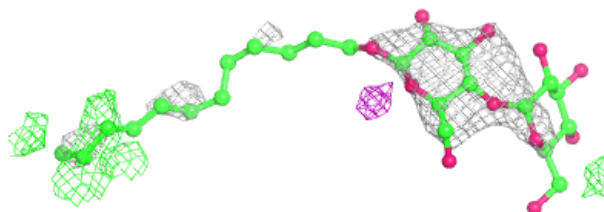
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HTG D 412:**

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

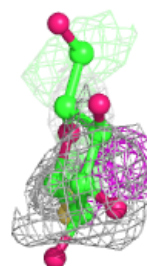
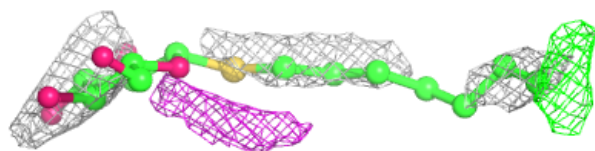
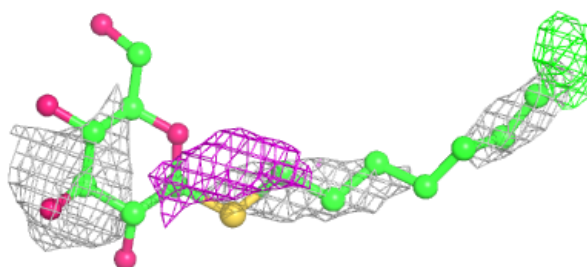
**Electron density around LMT E 102:**

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

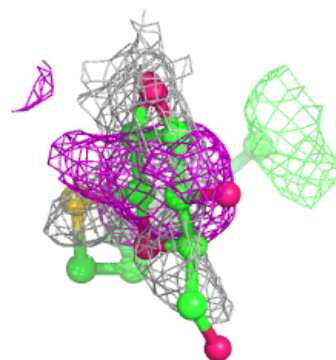
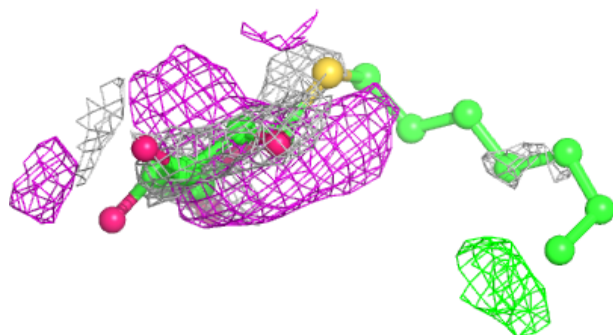
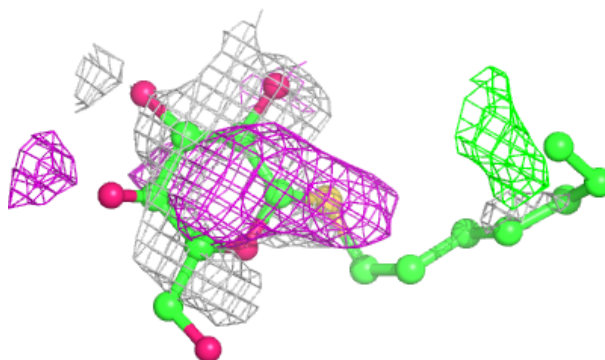


**Electron density around HTG B 626:**

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

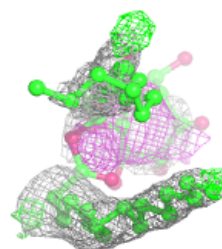
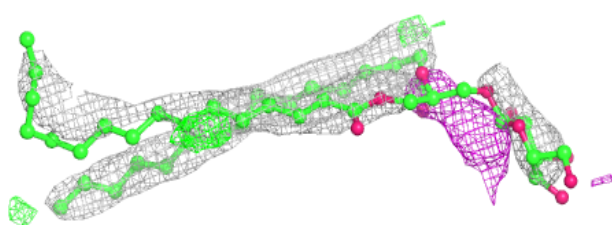
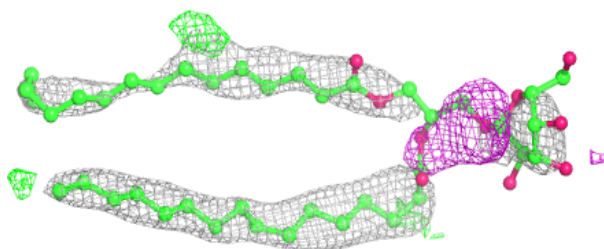
**Electron density around HTG b 622:**

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

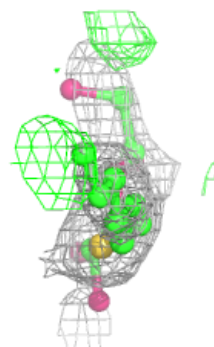
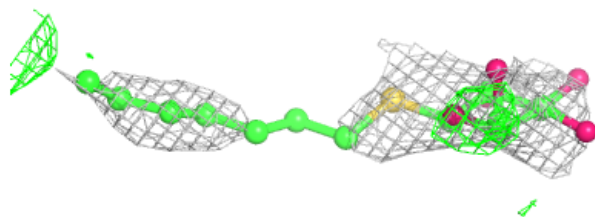
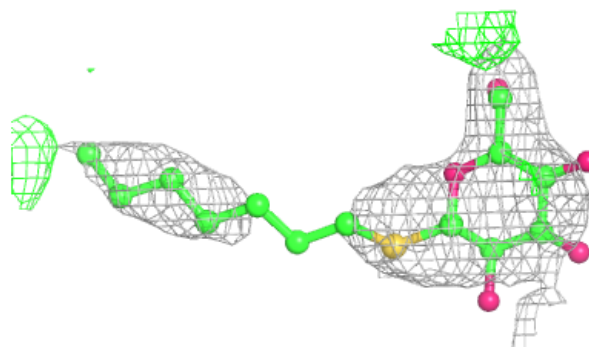


**Electron density around LMG C 521:**

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

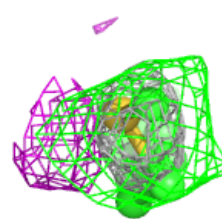
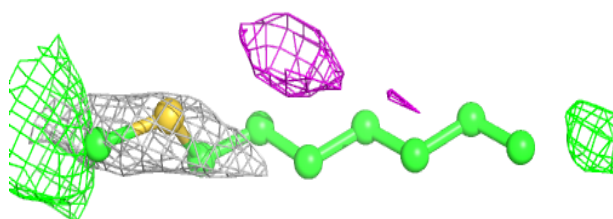
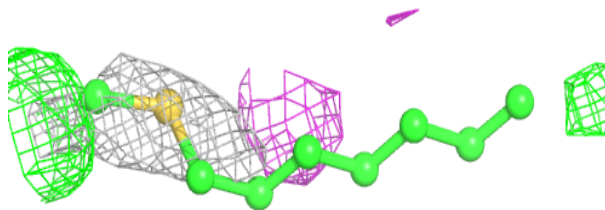
**Electron density around HTG B 630:**

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

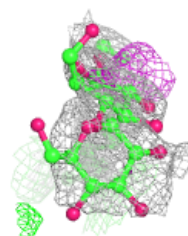
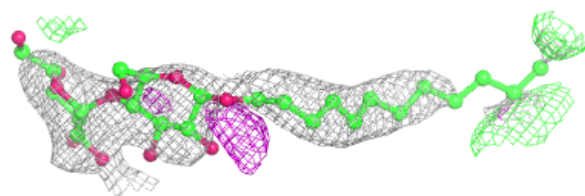
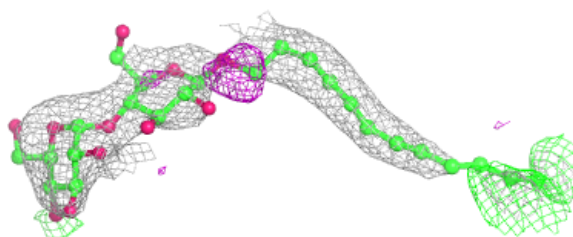


**Electron density around HTG C 524:**

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

**Electron density around LMT D 403:**

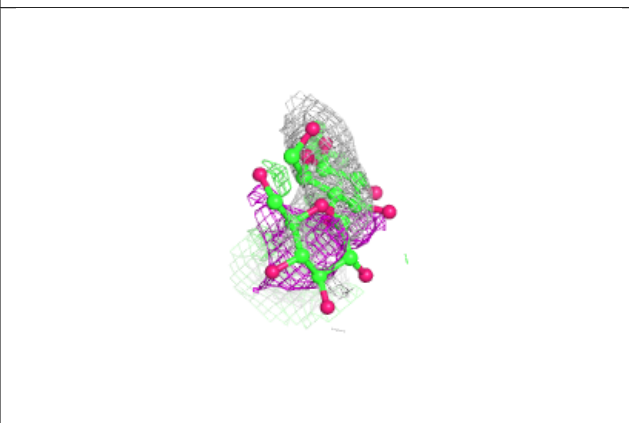
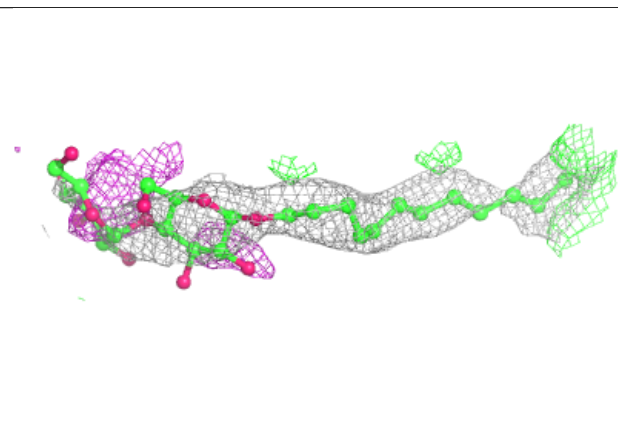
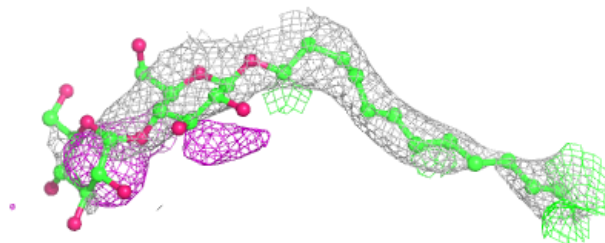
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



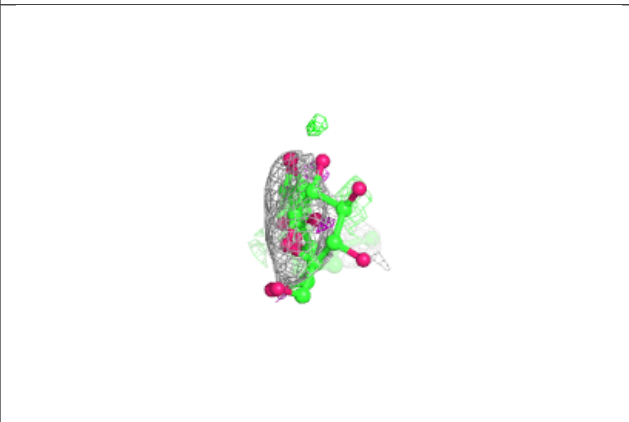
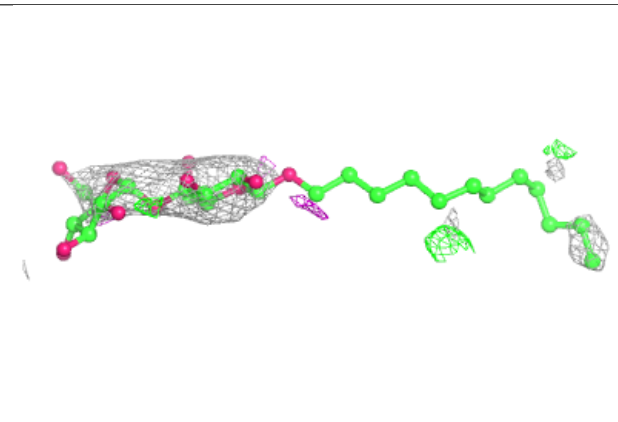
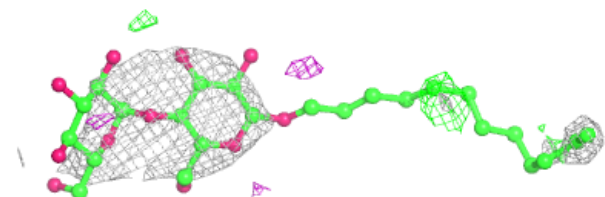


**Electron density around LMT B 633:**

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

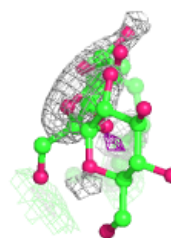
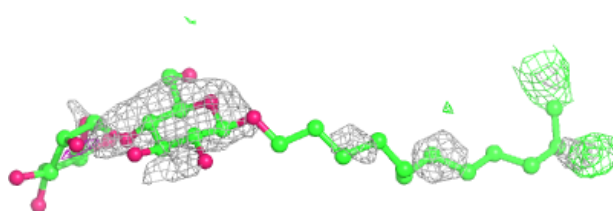
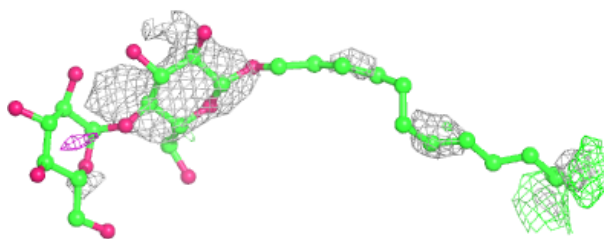
**Electron density around LMT a 418:**

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

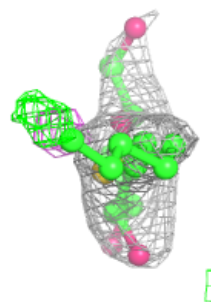
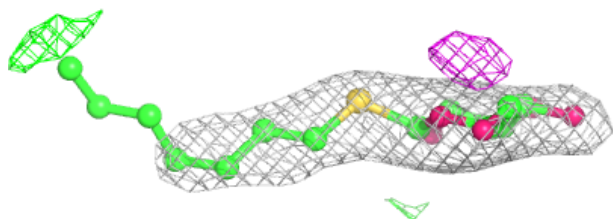
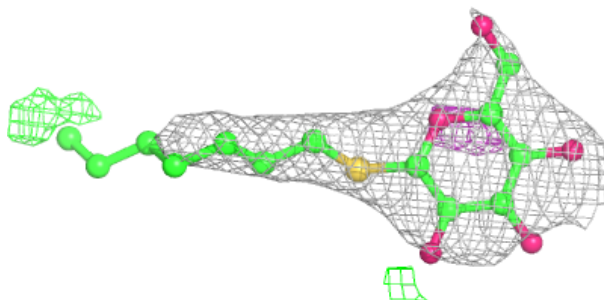


**Electron density around LMT e 102:**

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

**Electron density around HTG C 523:**

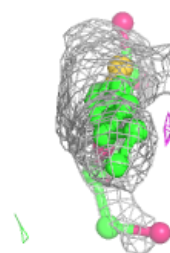
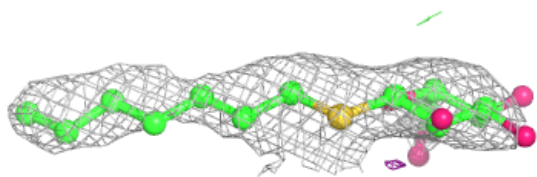
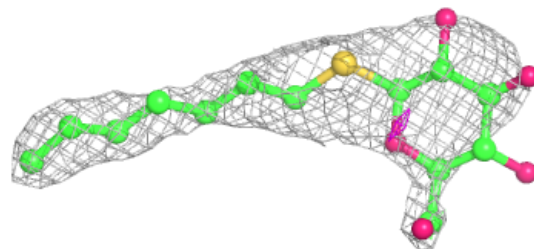
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



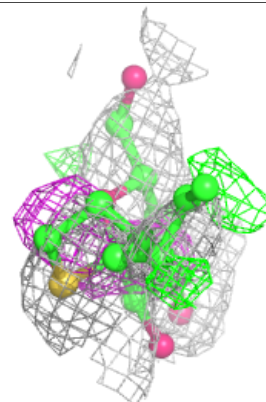
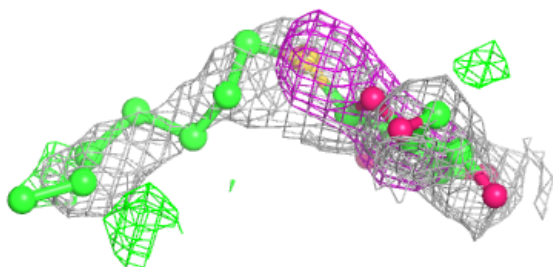
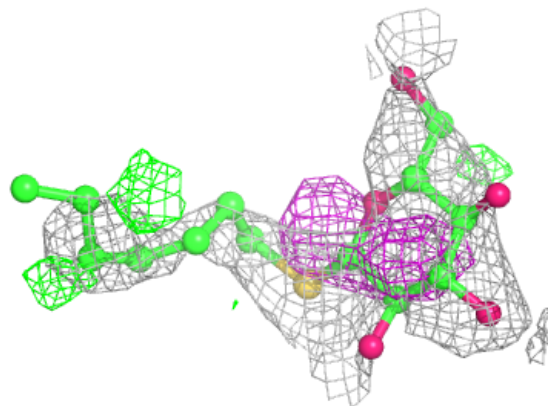


**Electron density around HTG b 626:**

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

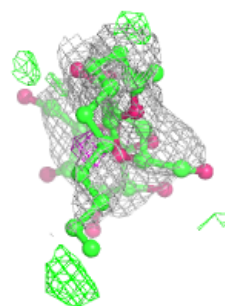
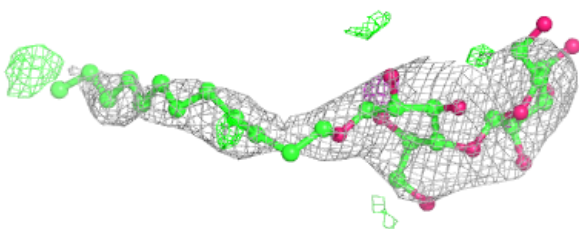
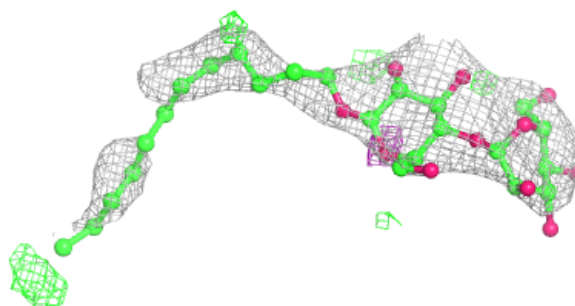
**Electron density around HTG B 625:**

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

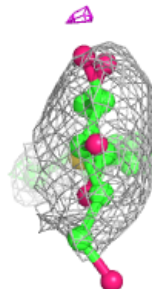
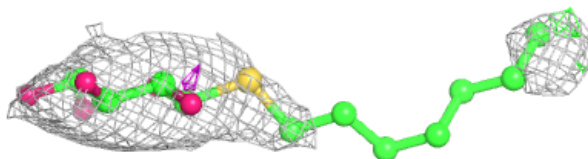
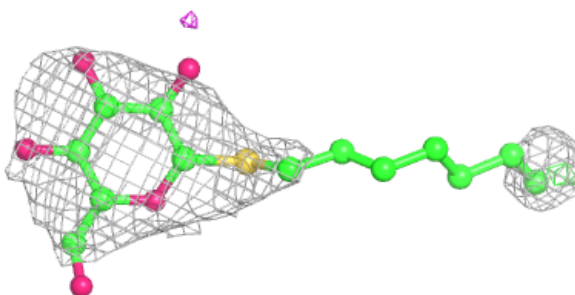


**Electron density around LMT C 522:**

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

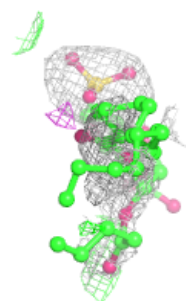
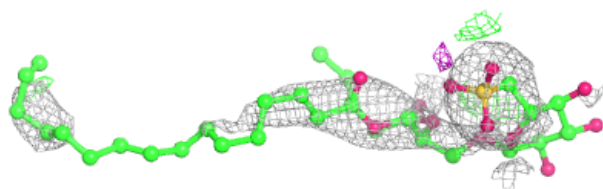
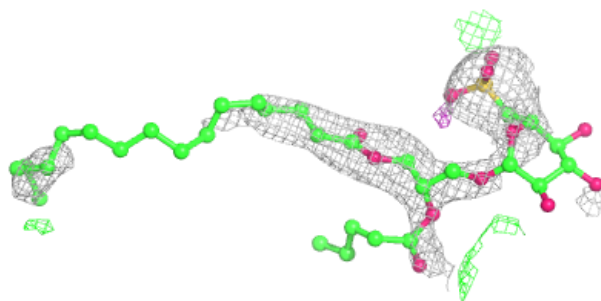
**Electron density around HTG c 521:**

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

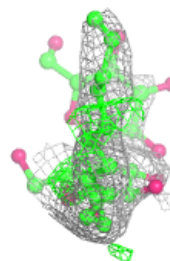
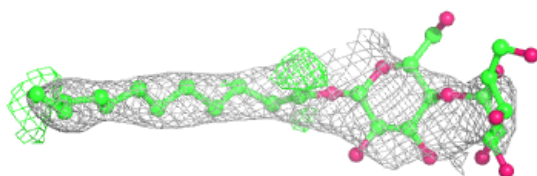
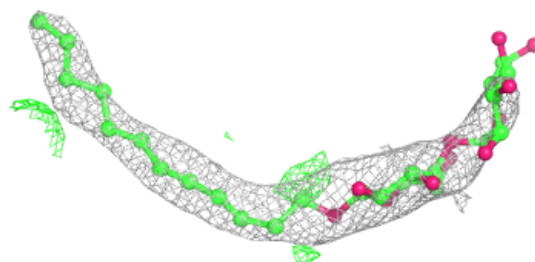


**Electron density around SQD f 101:**

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

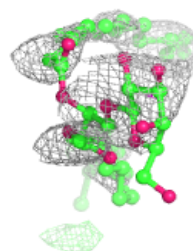
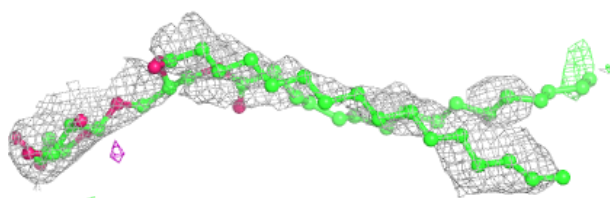
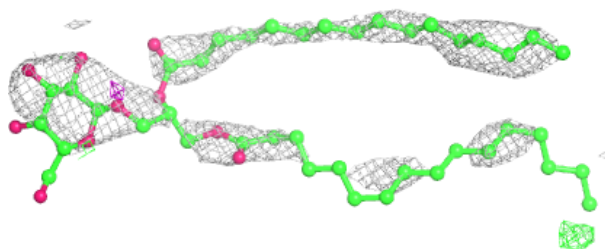
**Electron density around LMT M 103:**

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

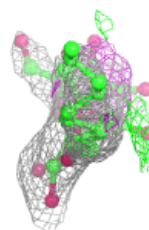
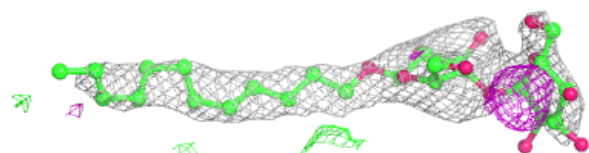
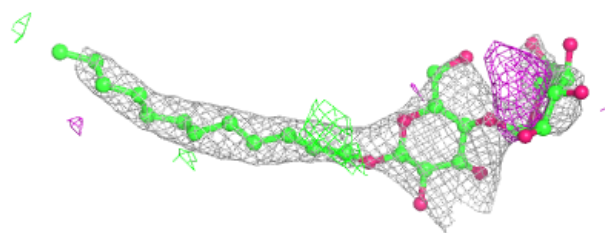


**Electron density around LMG c 520:**

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

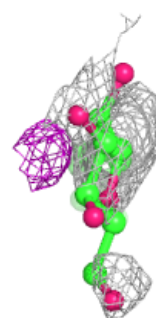
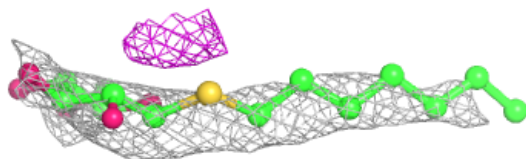
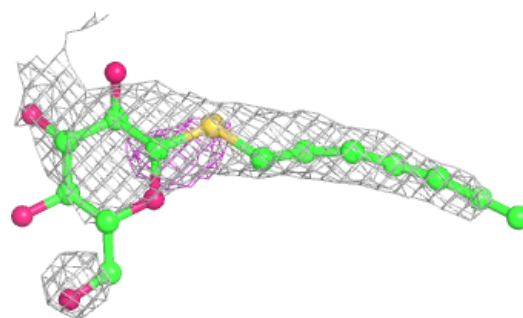
**Electron density around LMT B 623:**

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

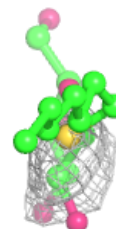
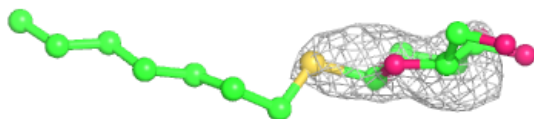
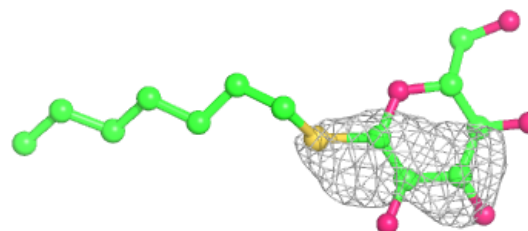


**Electron density around HTG b 623:**

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

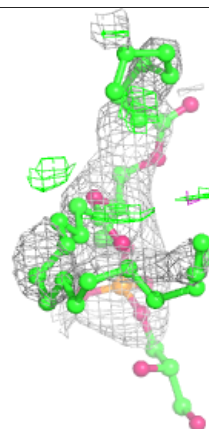
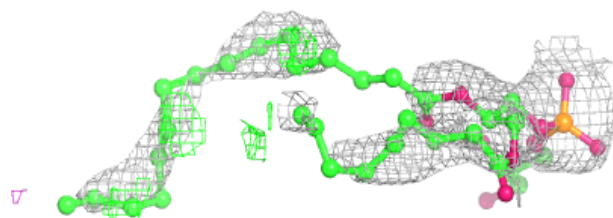
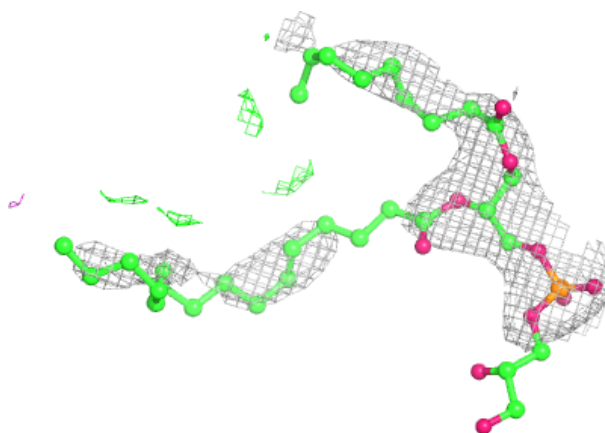
**Electron density around HTG c 522:**

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

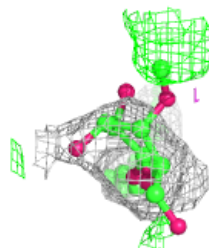
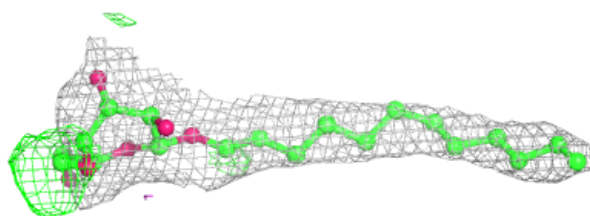
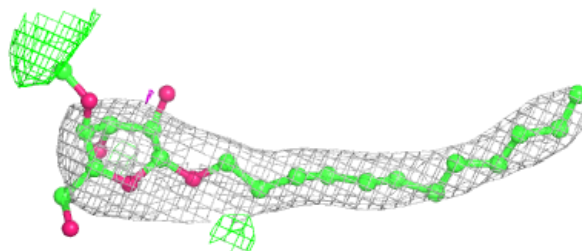


**Electron density around LHG e 101:**

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

**Electron density around LMT b 620:**

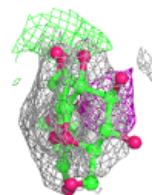
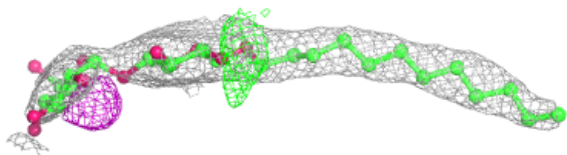
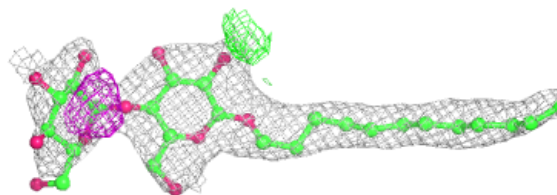
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



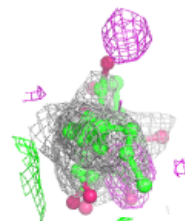
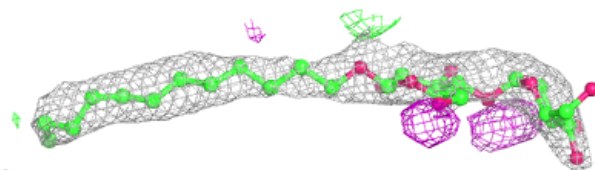
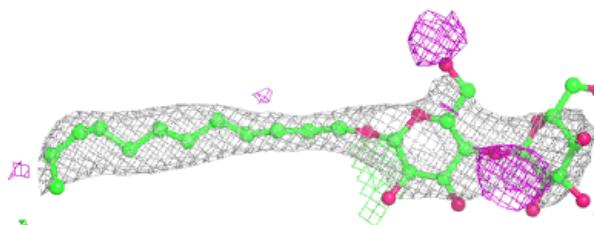


**Electron density around LMT M 101:**

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

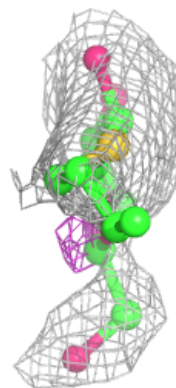
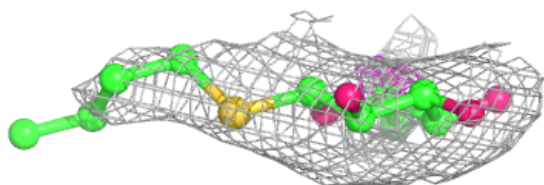
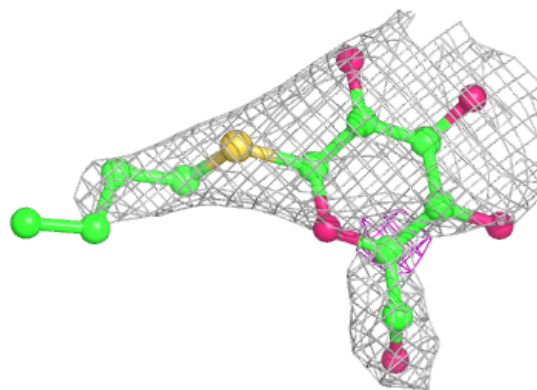
**Electron density around LMT m 103:**

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

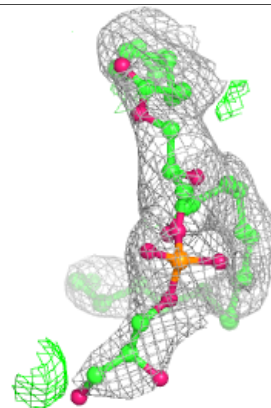
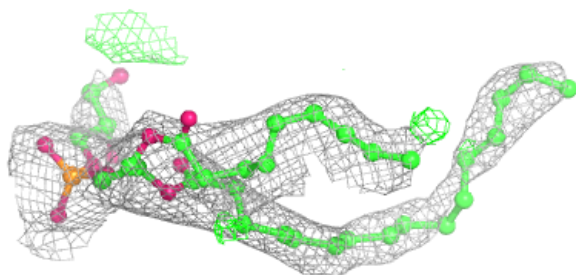
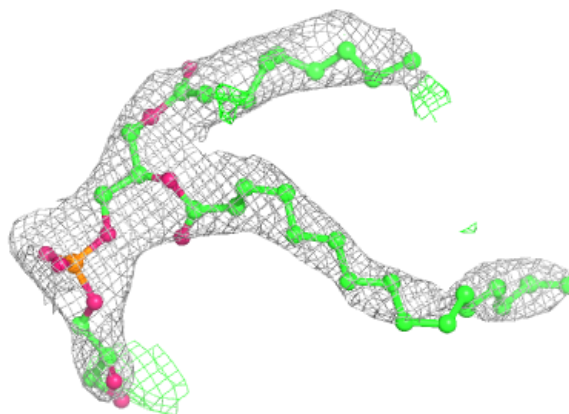


**Electron density around HTG h 101:**

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

**Electron density around LHG E 101:**

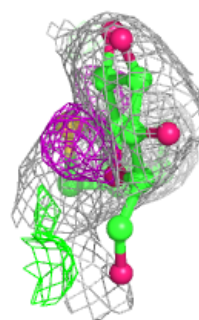
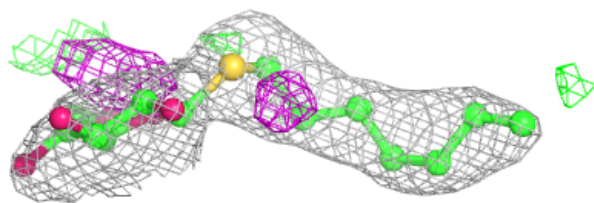
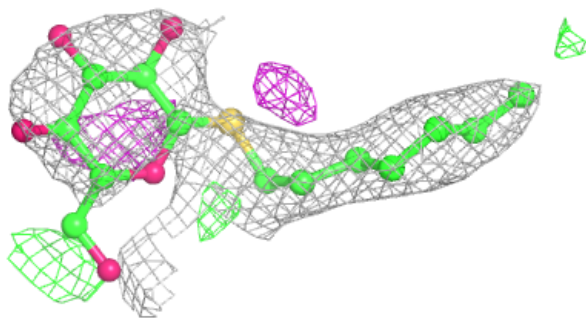
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



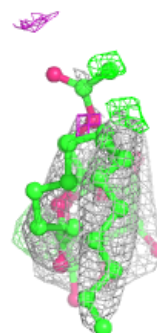
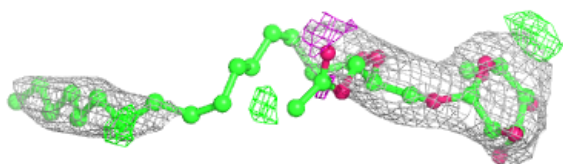
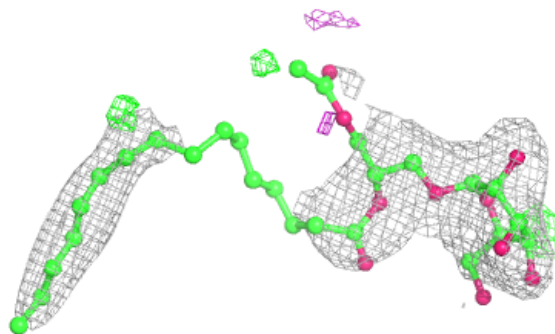


**Electron density around HTG b 621:**

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

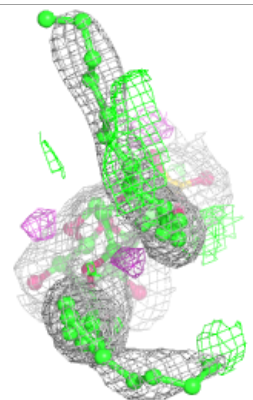
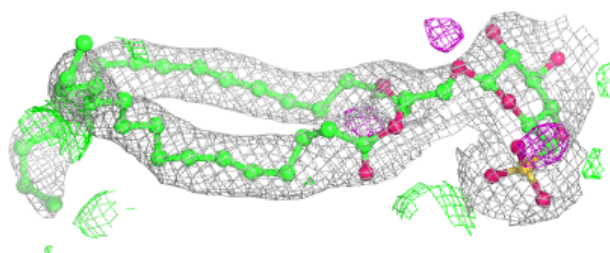
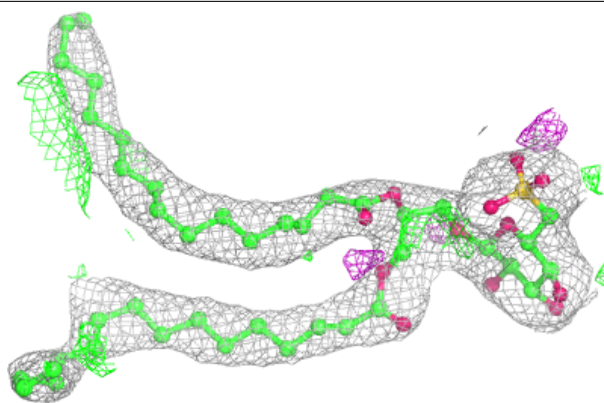
**Electron density around LMG Z 101:**

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

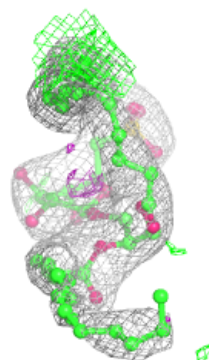
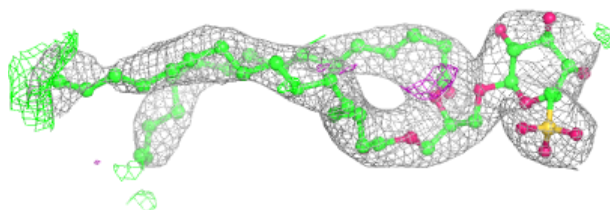
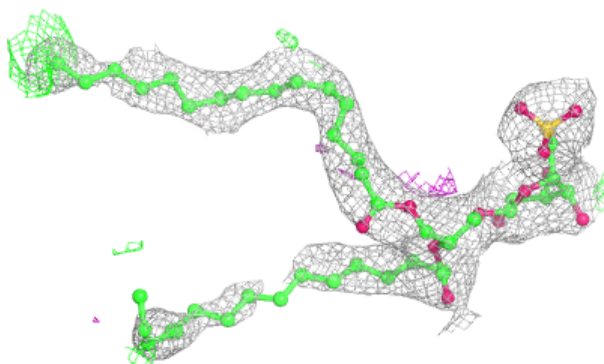


**Electron density around SQD B 621:**

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

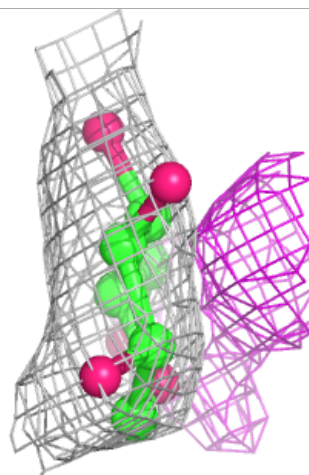
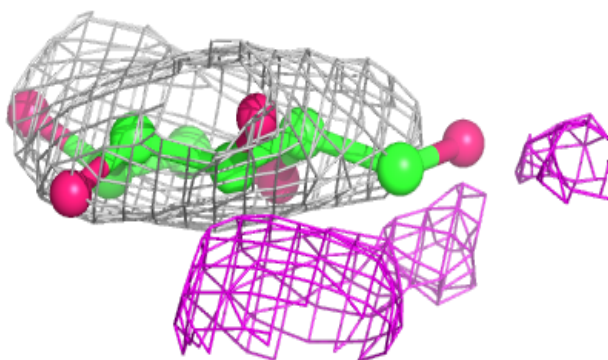
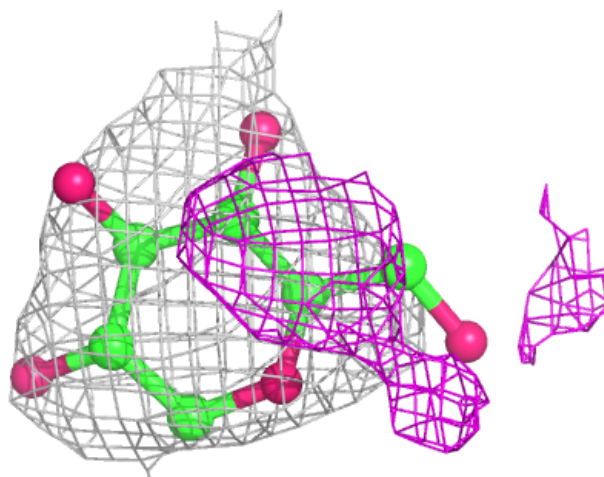
**Electron density around SQD a 413:**

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



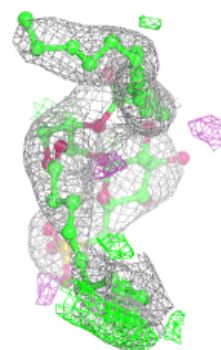
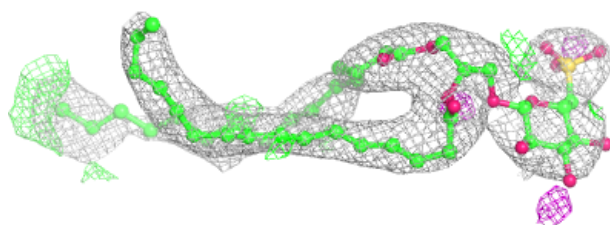
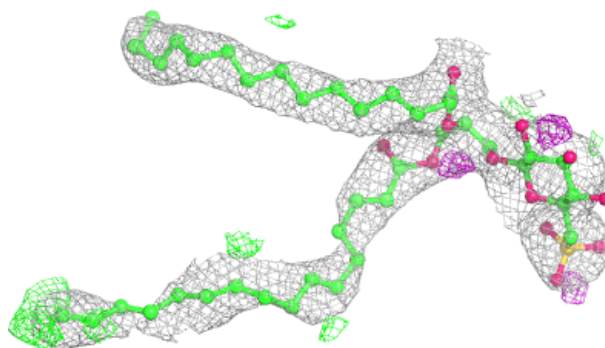
**Electron density around HTG V 203:**

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

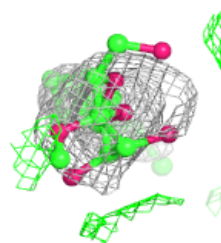
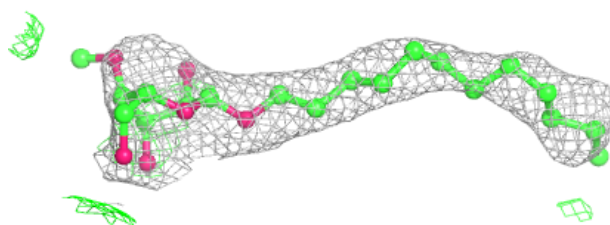
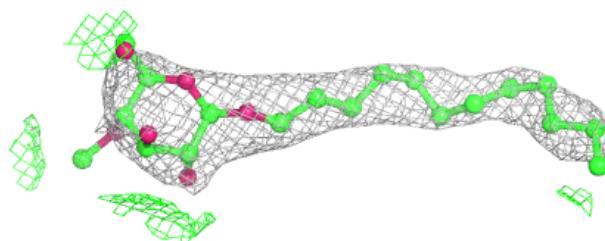


**Electron density around SQD A 411:**

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

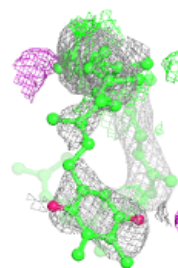
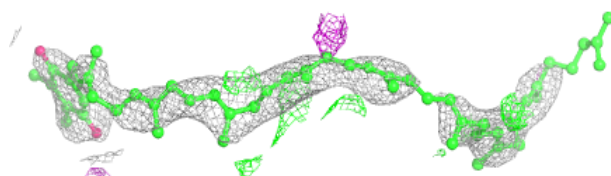
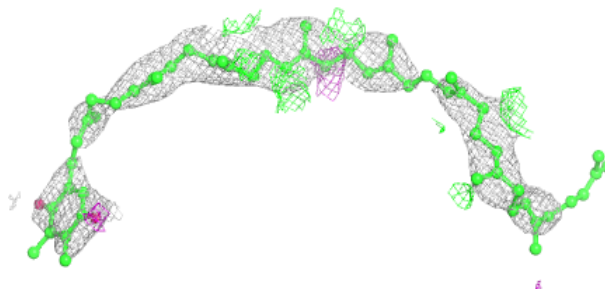
**Electron density around LMT B 632:**

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

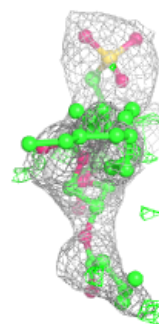
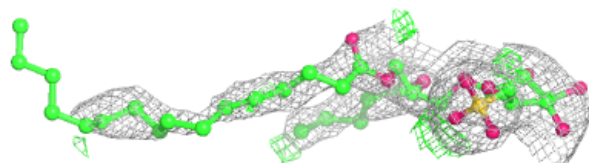
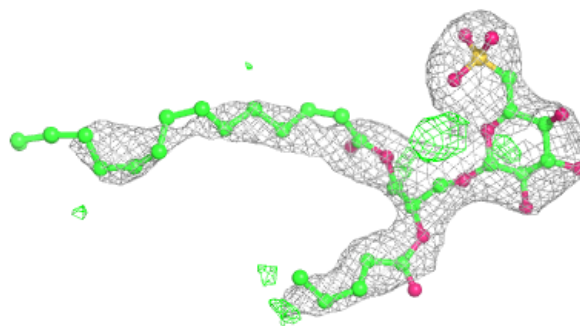


**Electron density around PL9 a 415:**

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

**Electron density around SQD D 413:**

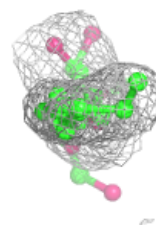
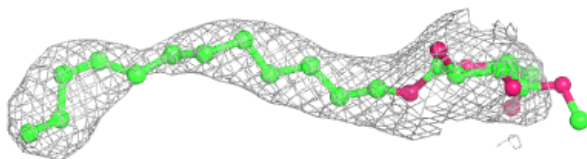
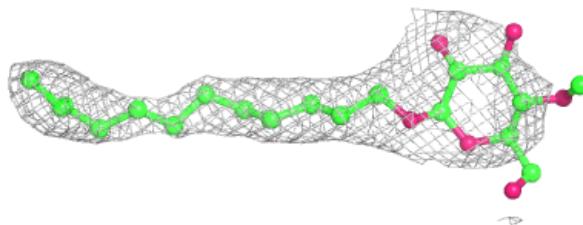
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



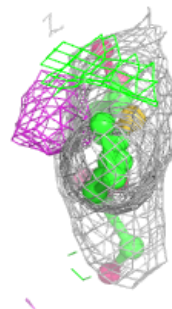
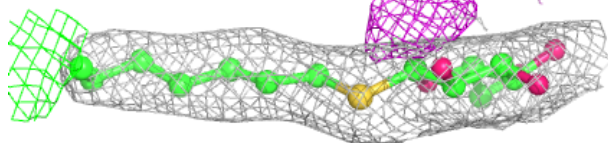
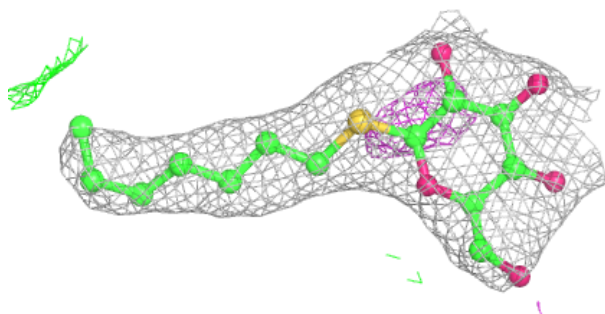


**Electron density around LMT b 628:**

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

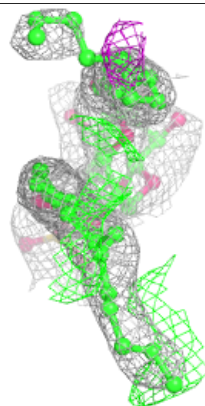
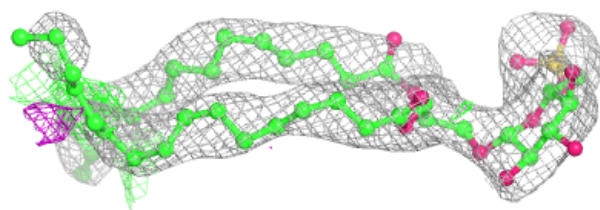
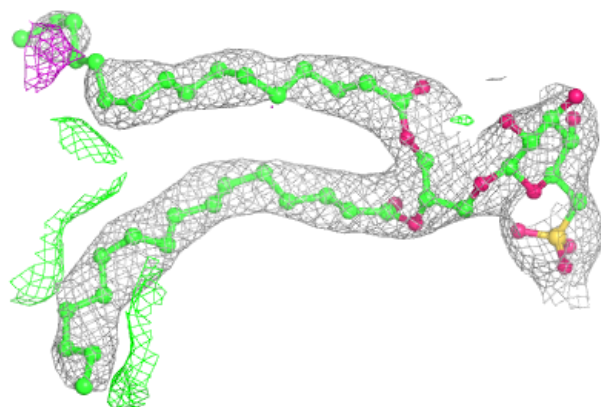
**Electron density around HTG B 629:**

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

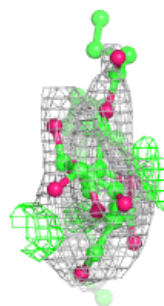
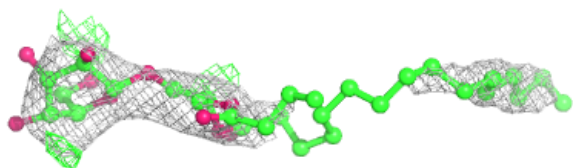
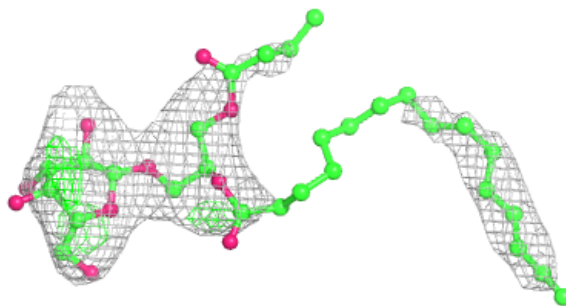


**Electron density around SQD L 102:**

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

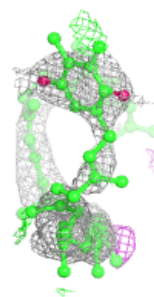
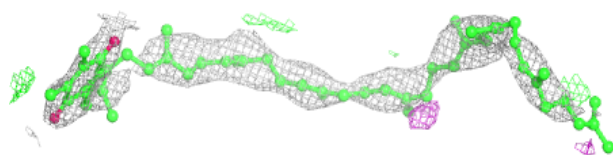
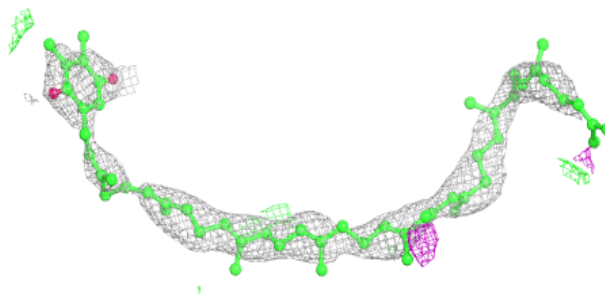
**Electron density around LMG z 101:**

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

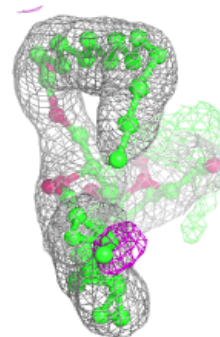
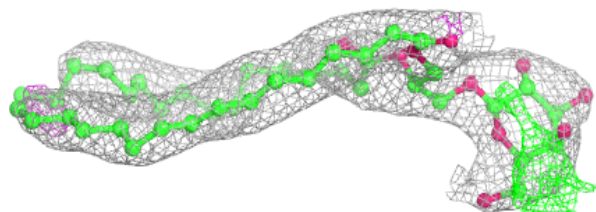
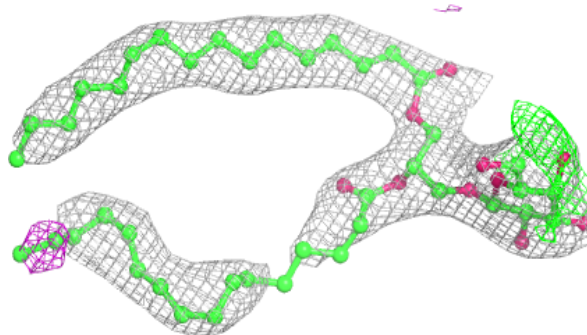


**Electron density around PL9 A 413:**

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

**Electron density around LMG C 501:**

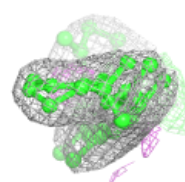
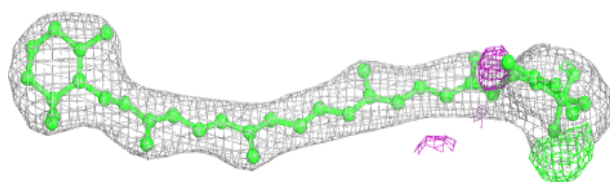
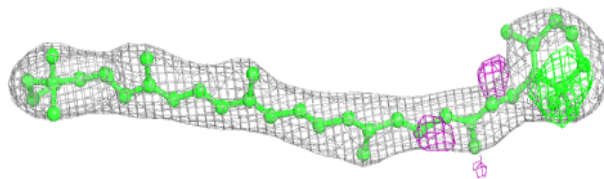
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



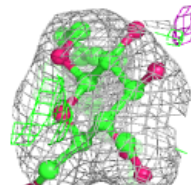
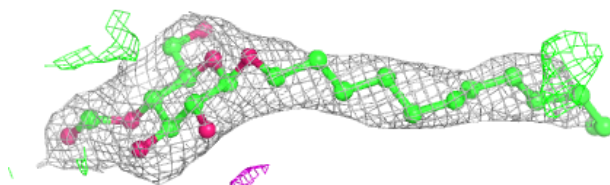
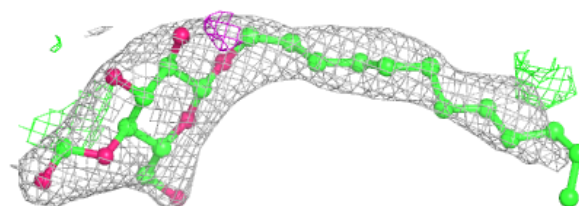


**Electron density around BCR D 406:**

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

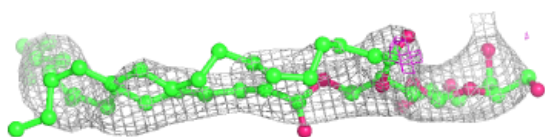
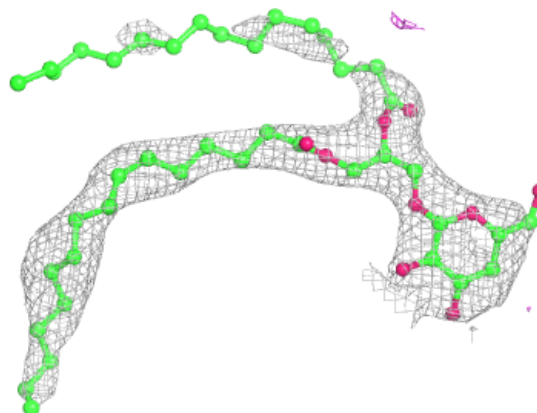
**Electron density around LMT B 634:**

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

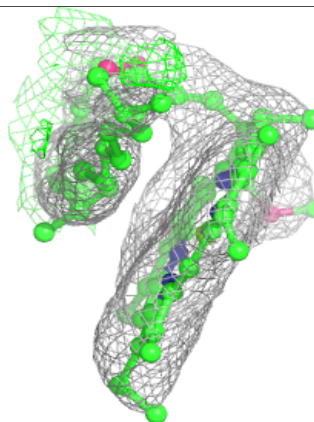
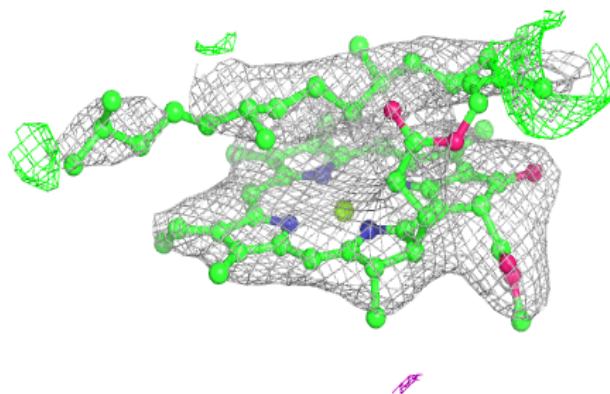
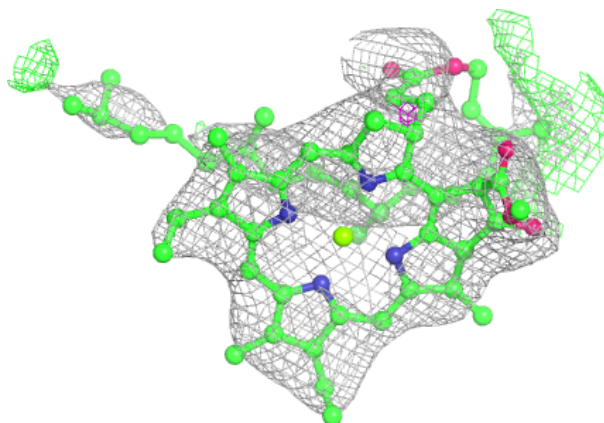


**Electron density around LMG C 520:**

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

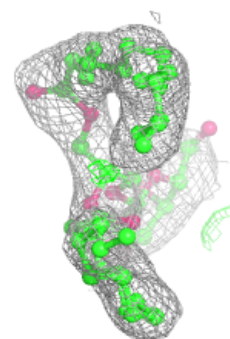
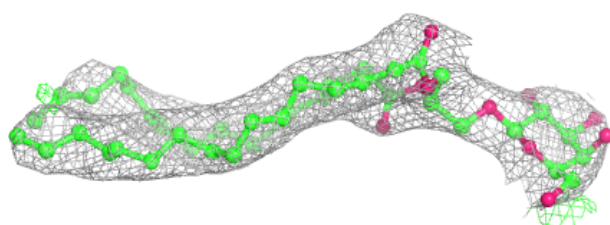
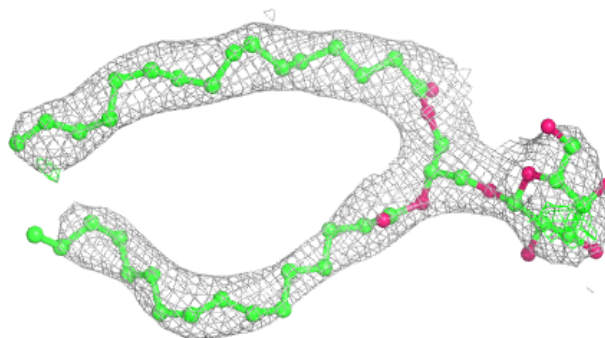
**Electron density around CLA b 601:**

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

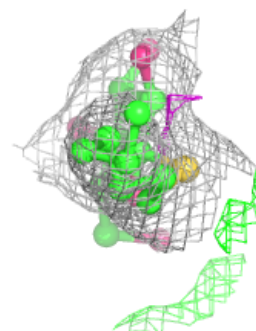
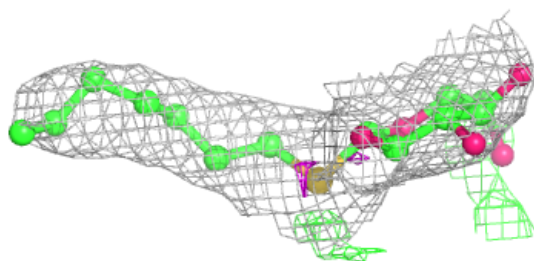
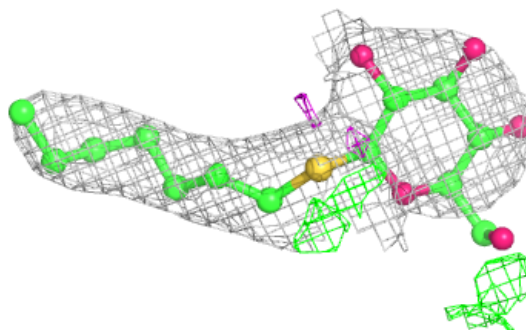


**Electron density around LMG a 417:**

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

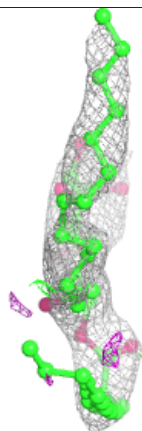
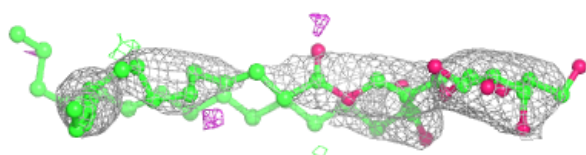
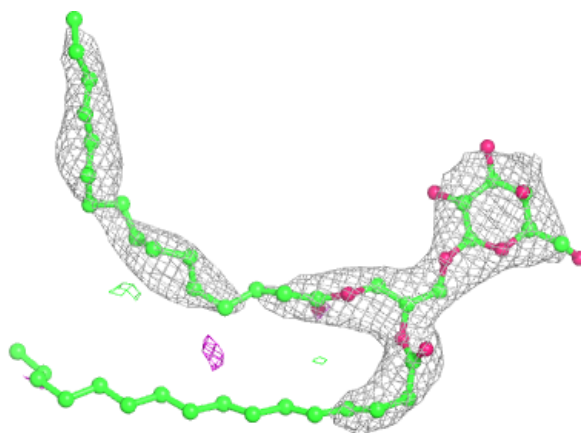
**Electron density around HTG B 624:**

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

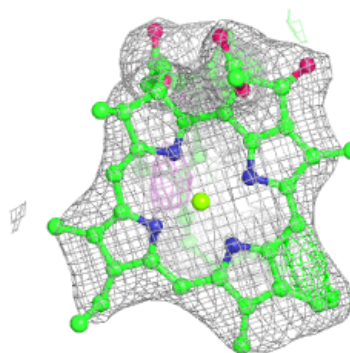
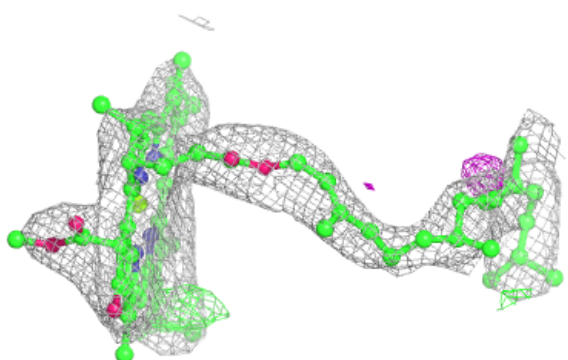
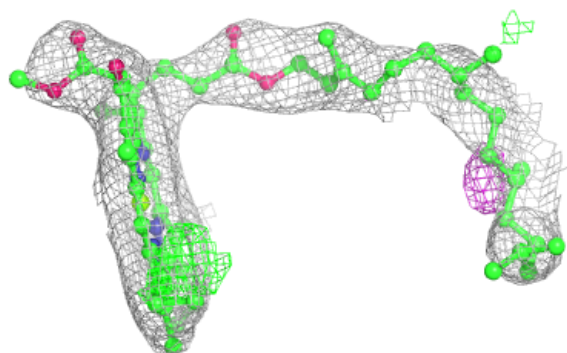


**Electron density around LMG c 519:**

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

**Electron density around CLA C 507:**

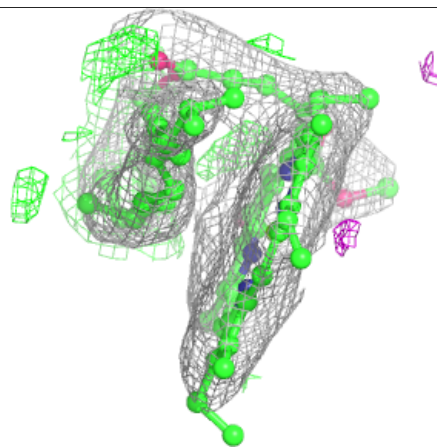
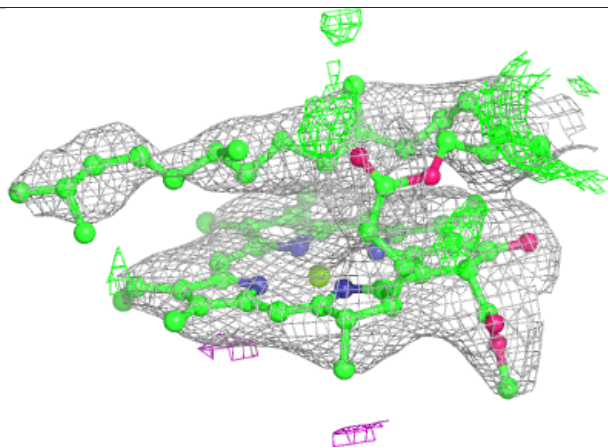
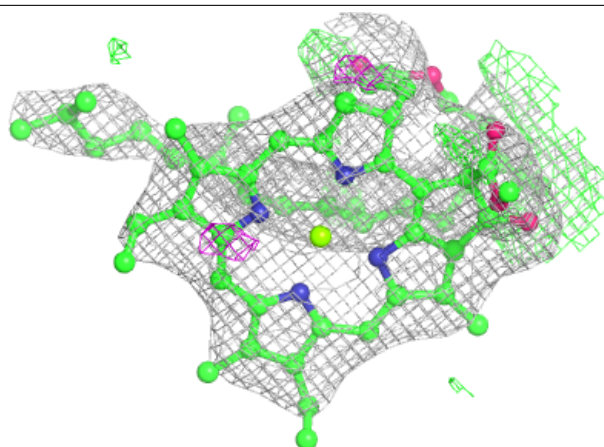
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



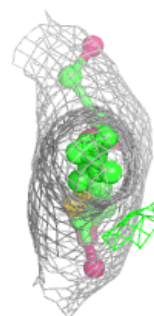
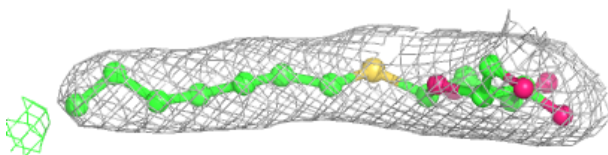
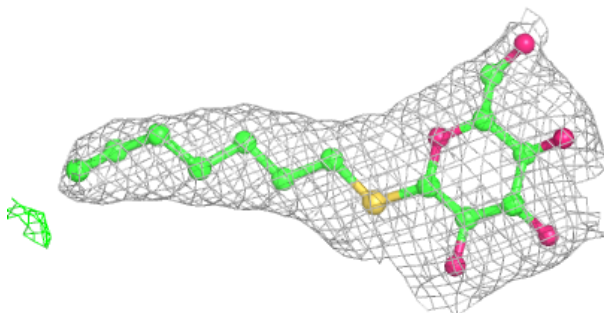


**Electron density around CLA B 602:**

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

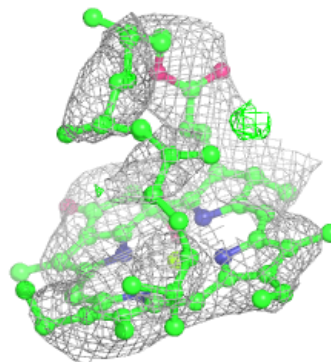
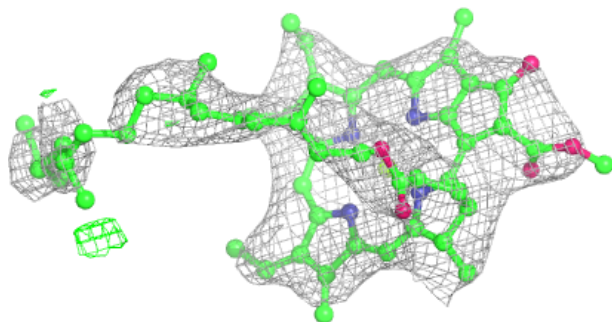
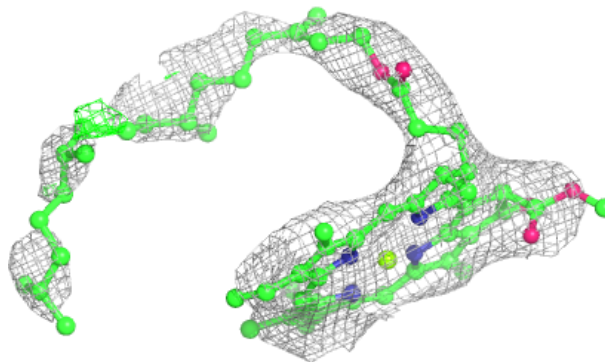
**Electron density around HTG b 625:**

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

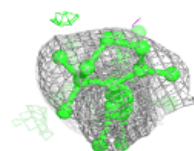
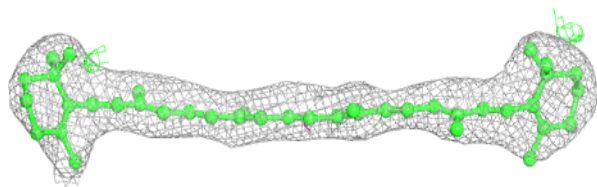
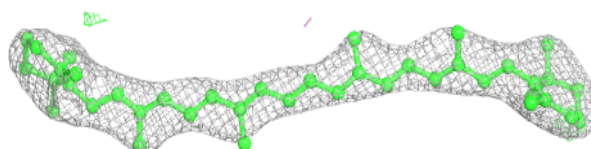


**Electron density around CLA c 513:**

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

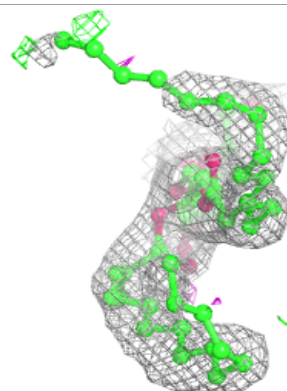
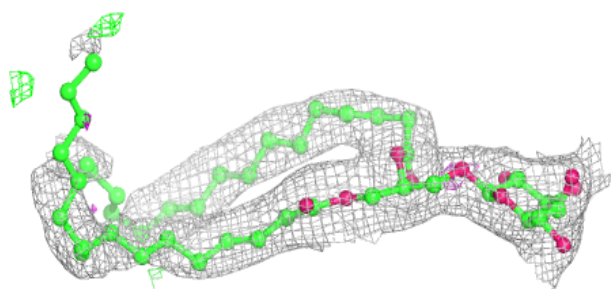
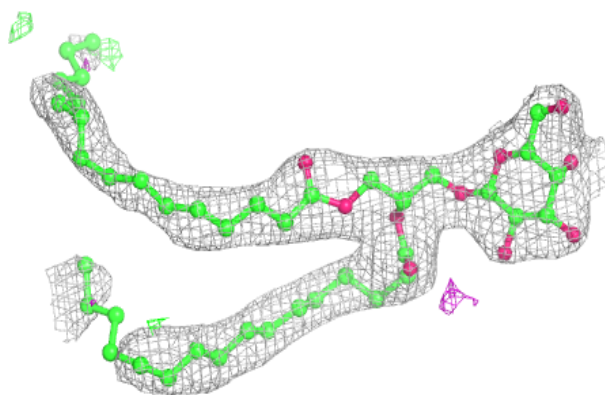
**Electron density around BCR C 515:**

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

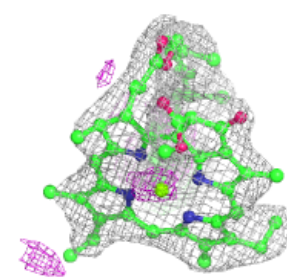
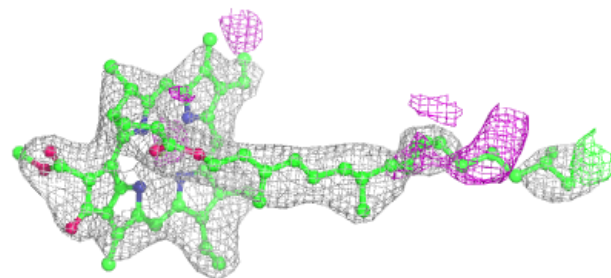
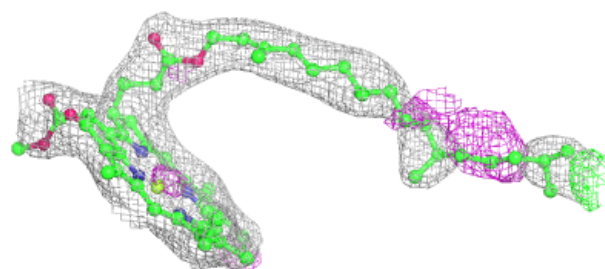


**Electron density around LMG J 101:**

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

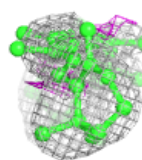
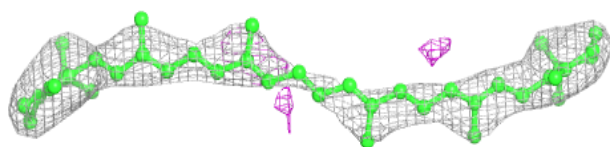
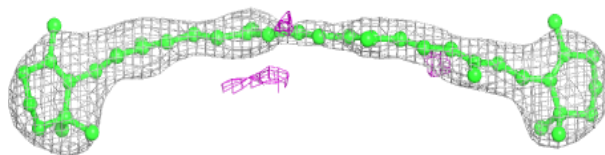
**Electron density around CLA C 505:**

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

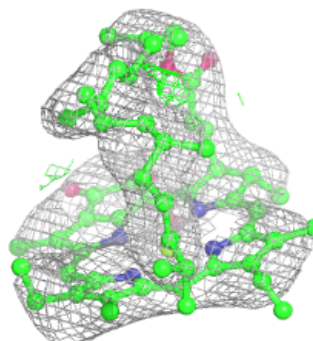
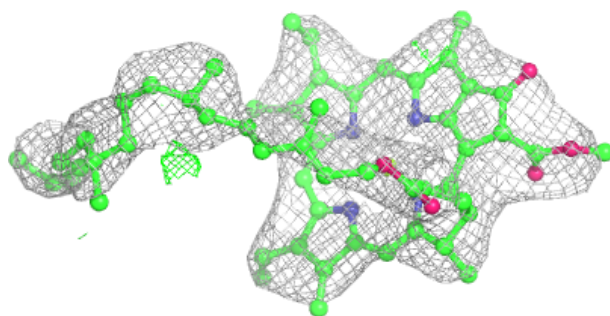
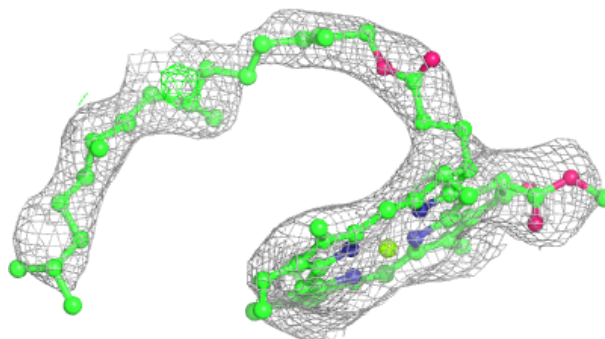


**Electron density around BCR C 527:**

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

**Electron density around CLA C 514:**

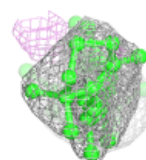
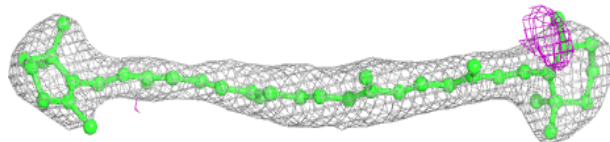
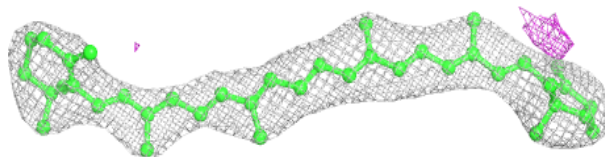
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



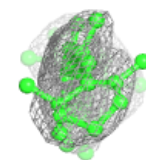
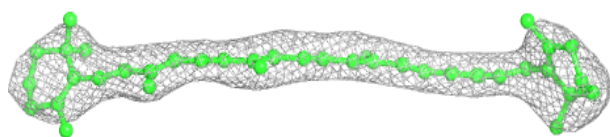
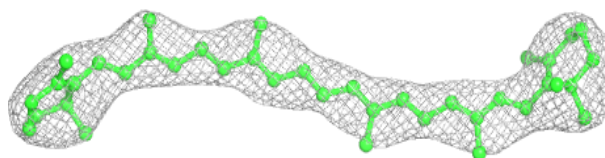


**Electron density around BCR Y 101:**

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

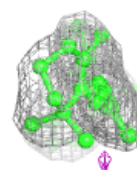
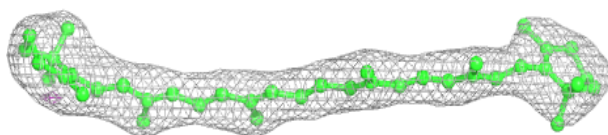
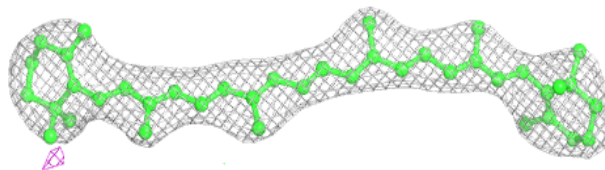
**Electron density around BCR y 101:**

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

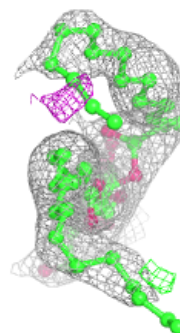
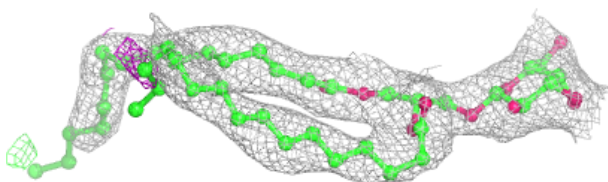
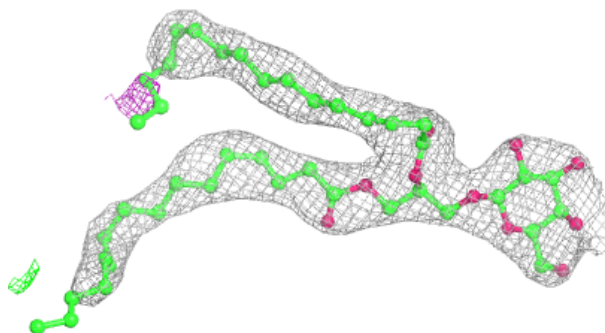


**Electron density around BCR B 620:**

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

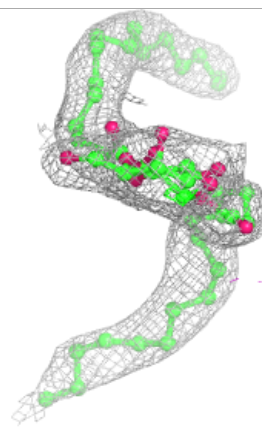
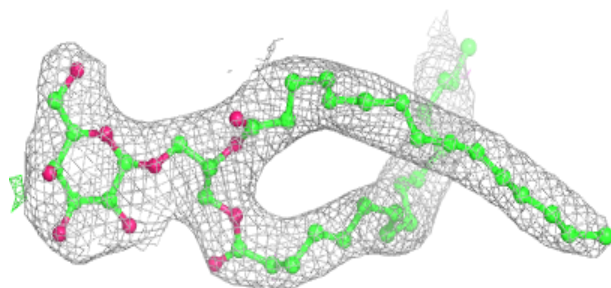
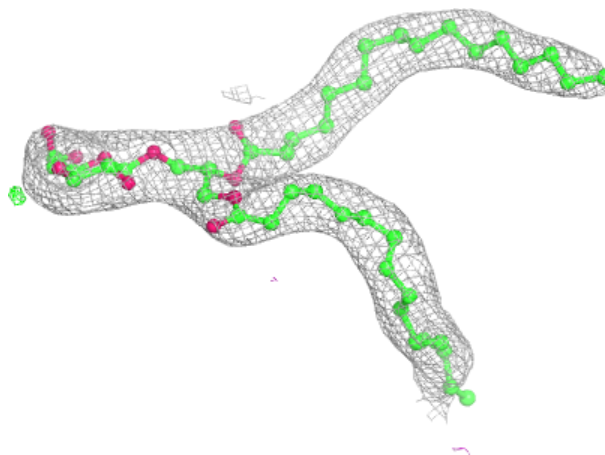
**Electron density around LMG j 101:**

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



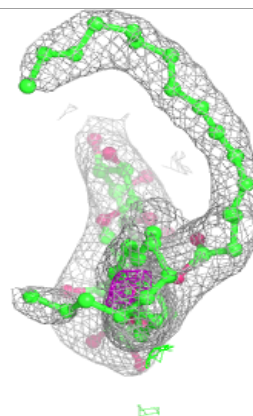
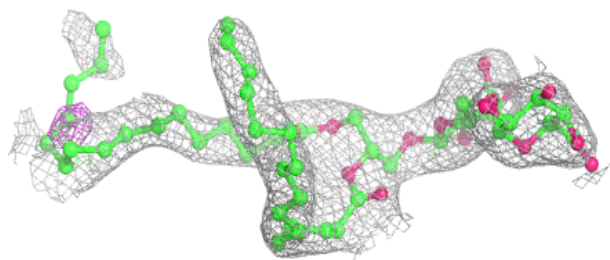
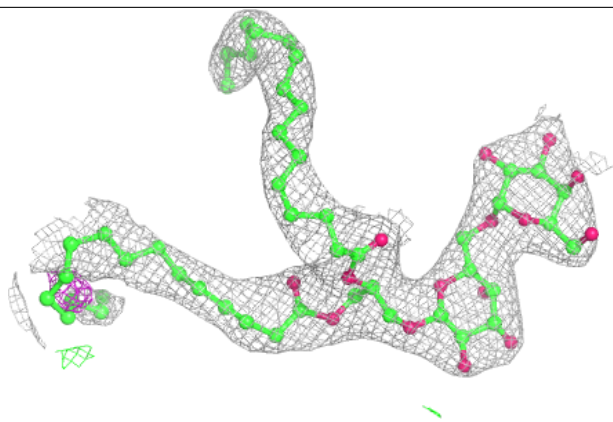
**Electron density around LMG B 622:**

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



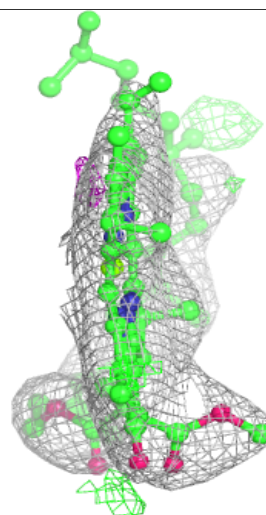
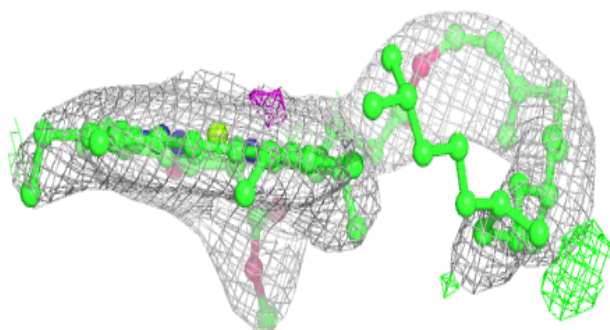
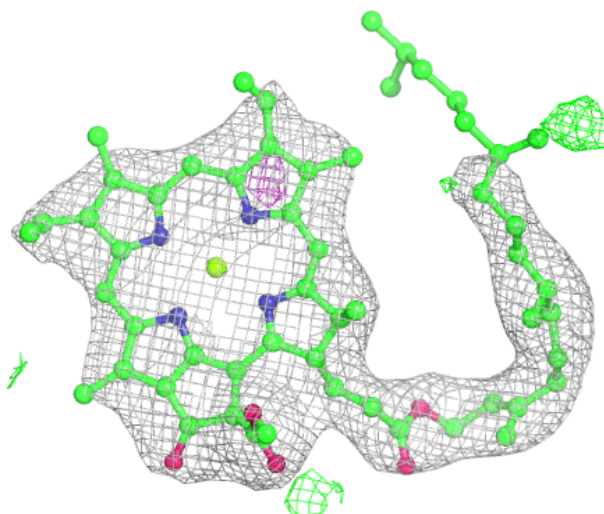
**Electron density around DGD c 517:**

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



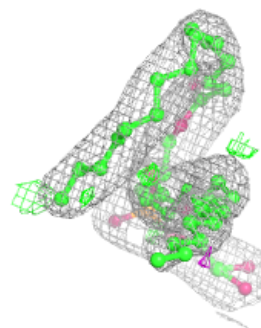
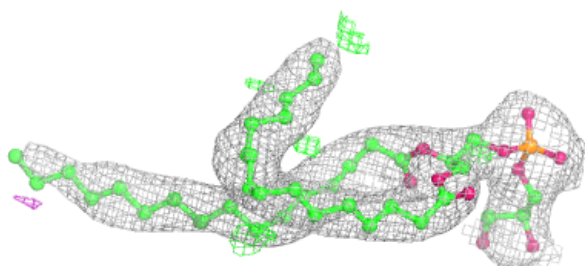
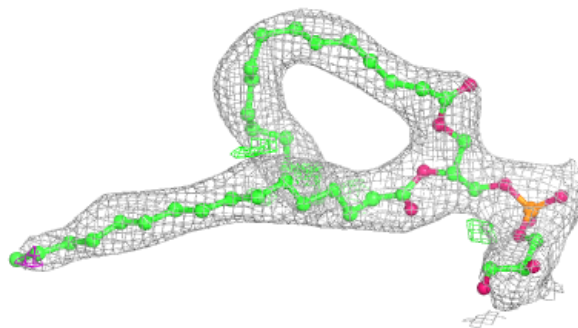
**Electron density around CLA C 513:**

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



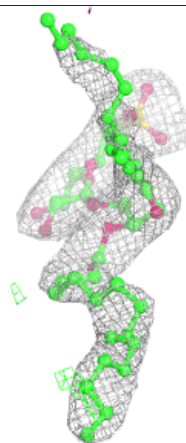
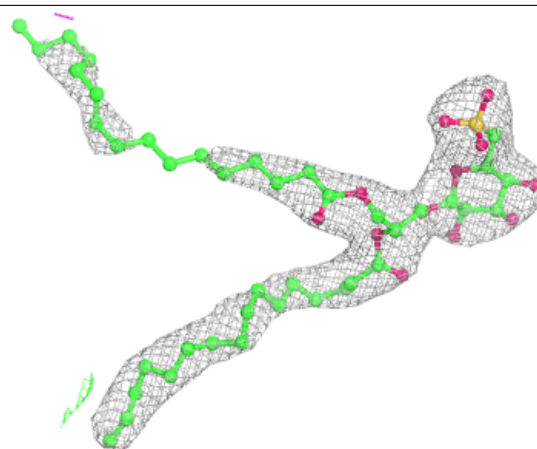
**Electron density around LHG d 406:**

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



**Electron density around SQD A 409:**

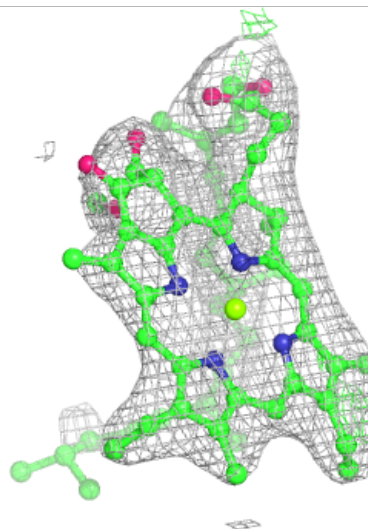
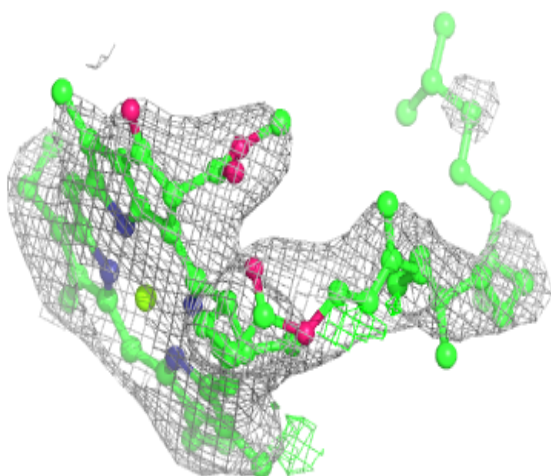
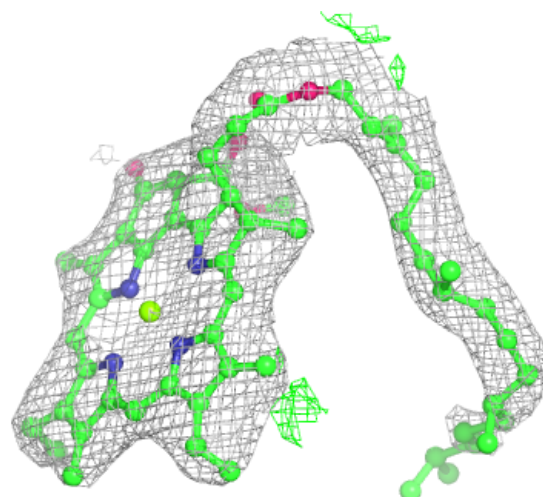
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA b 616:**

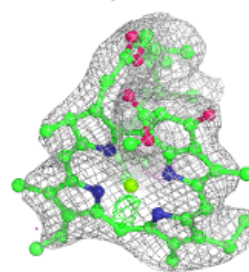
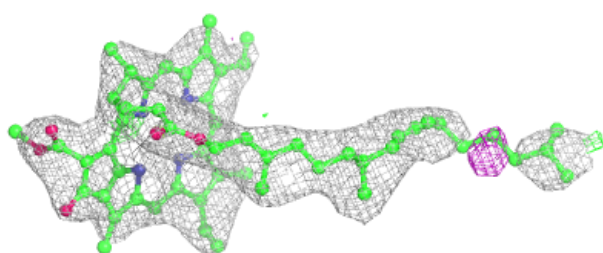
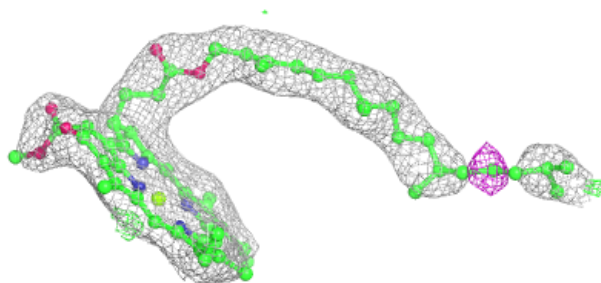
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



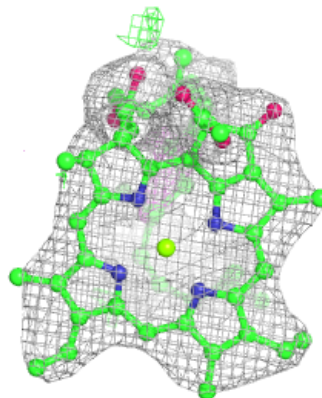
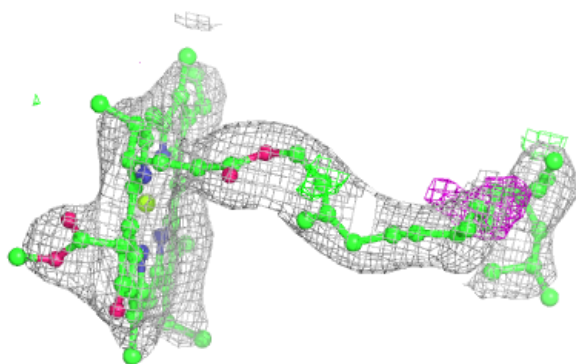
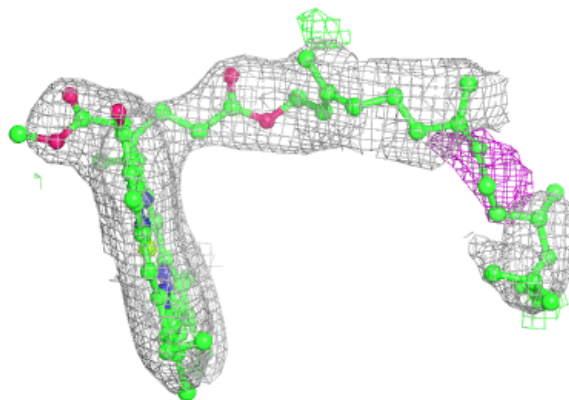


**Electron density around CLA c 504:**

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

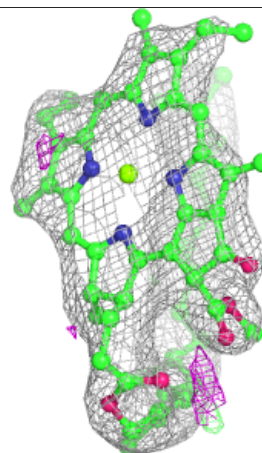
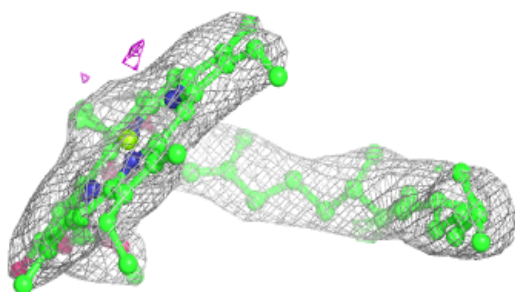
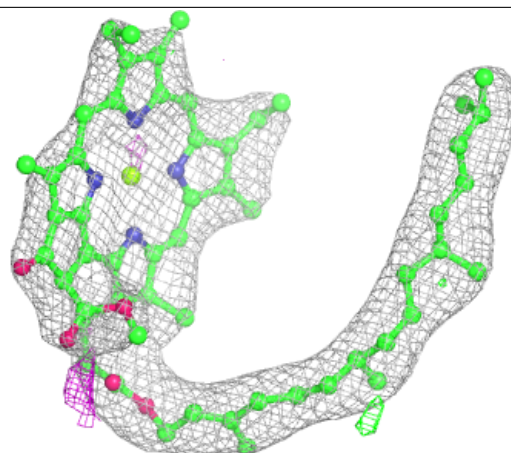
**Electron density around CLA c 506:**

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

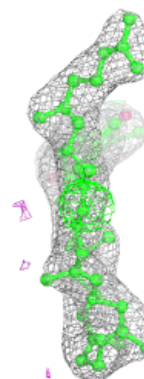
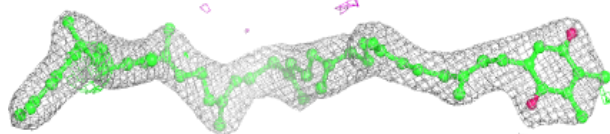
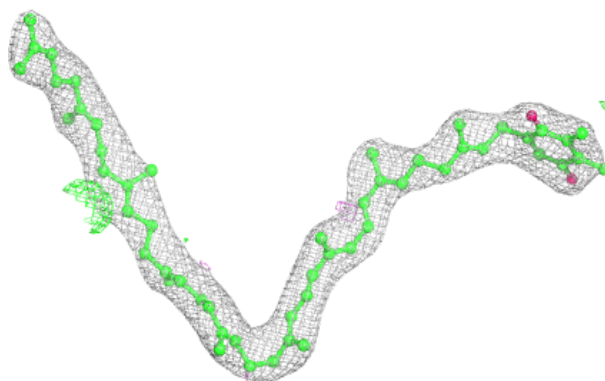


**Electron density around CLA c 507:**

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

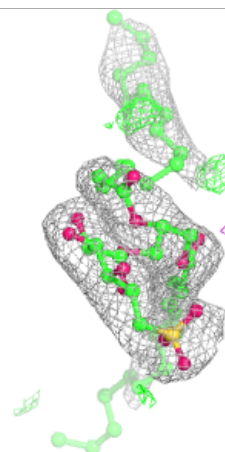
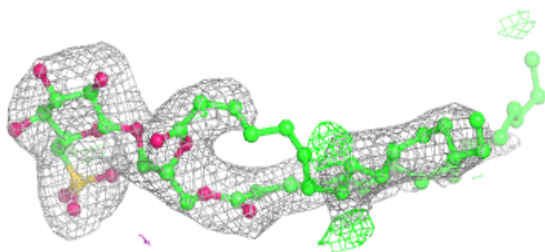
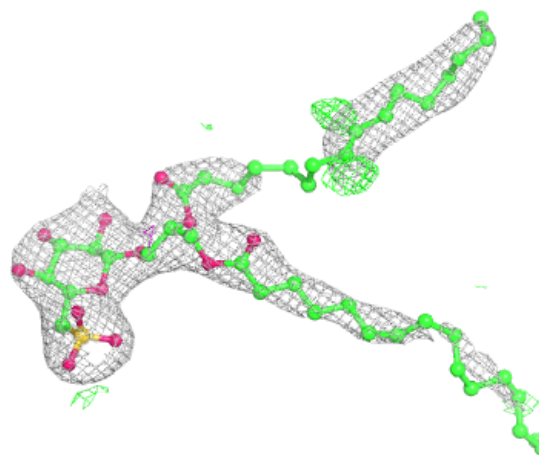
**Electron density around PL9 D 407:**

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



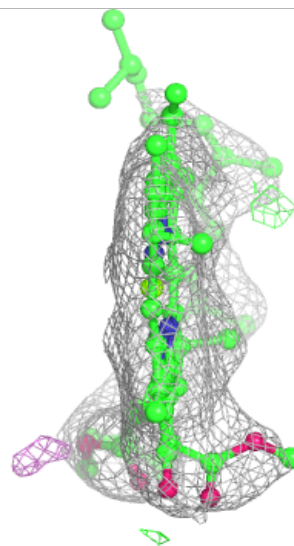
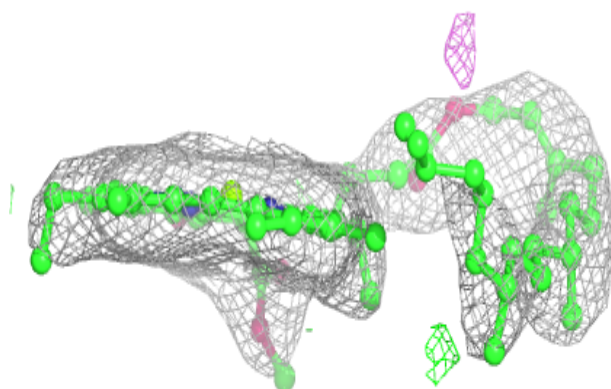
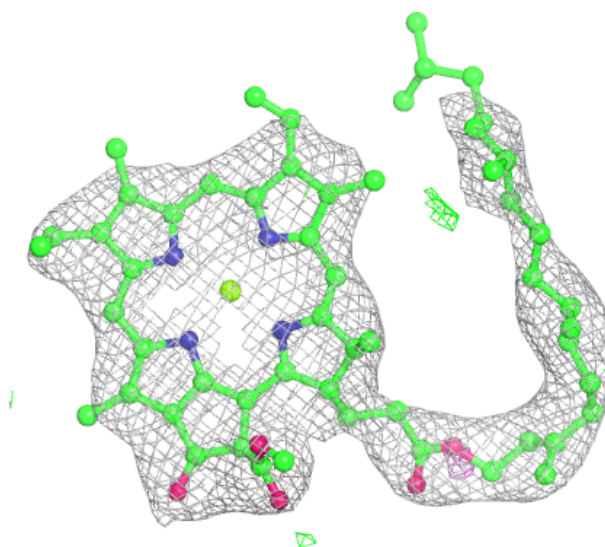
**Electron density around SQD a 411:**

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



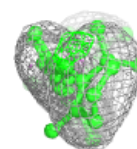
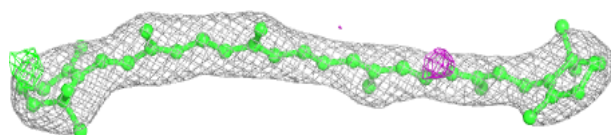
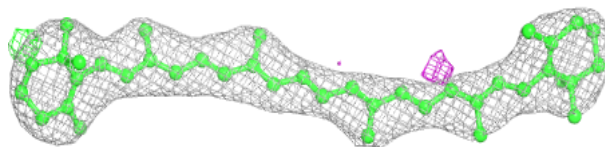
**Electron density around CLA c 512:**

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

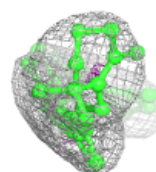
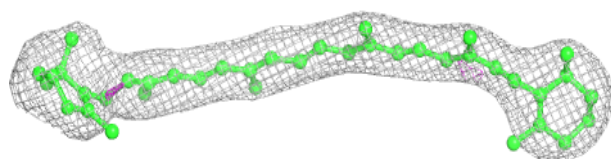
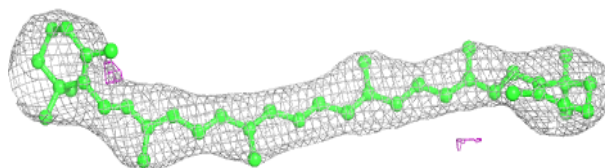


**Electron density around BCR b 619:**

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

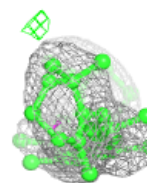
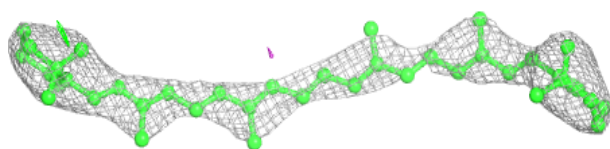
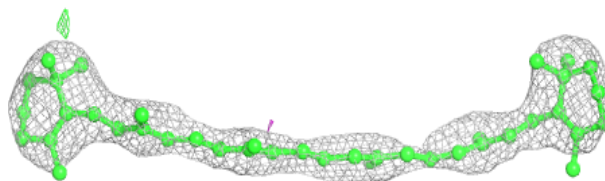
**Electron density around BCR d 404:**

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

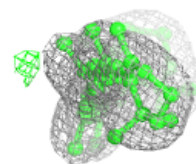
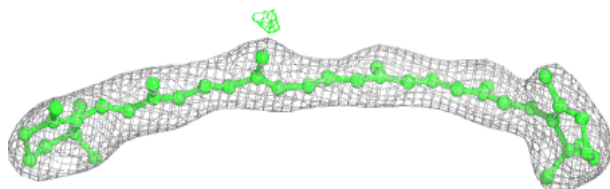
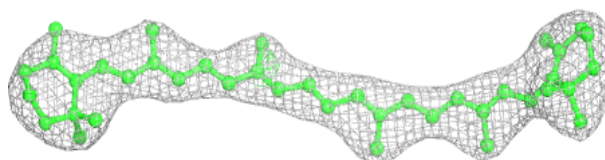


**Electron density around BCR k 101:**

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

**Electron density around BCR t 101:**

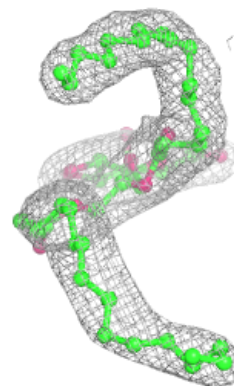
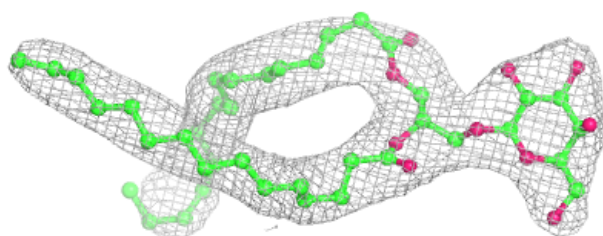
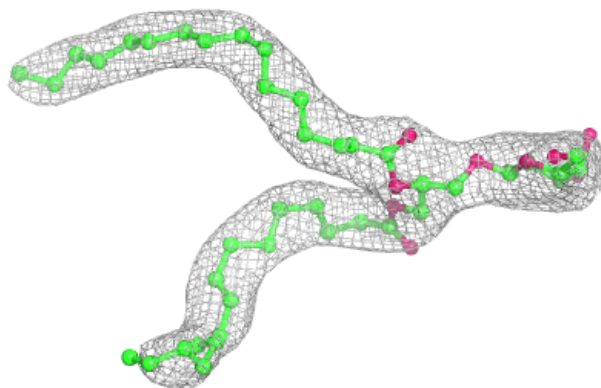
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



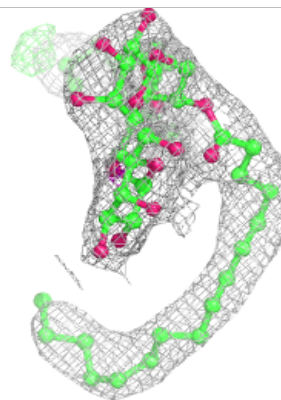
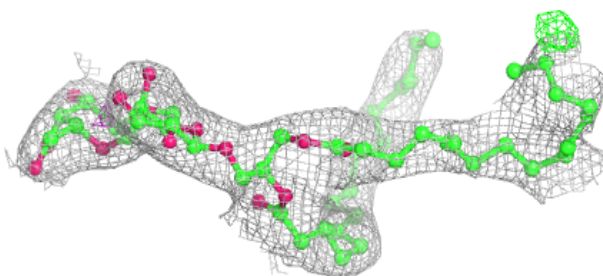
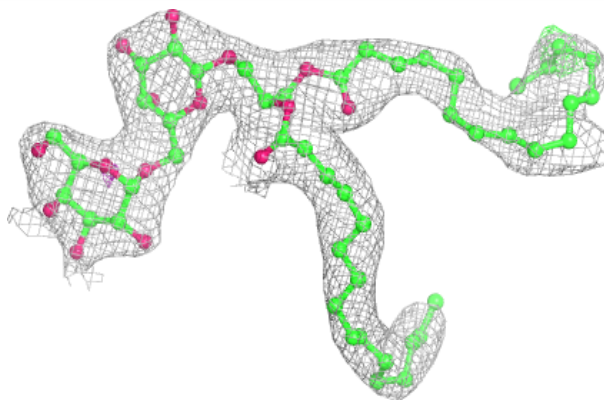


**Electron density around LMG m 101:**

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

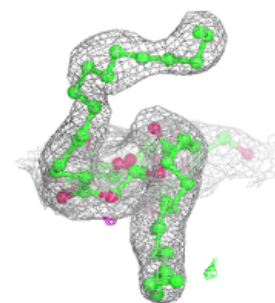
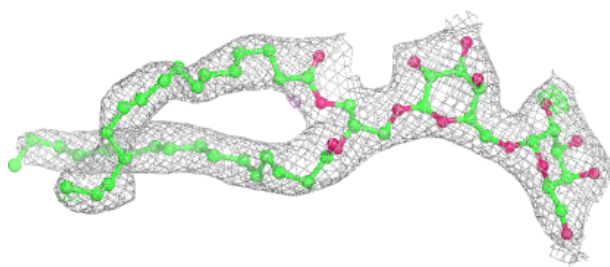
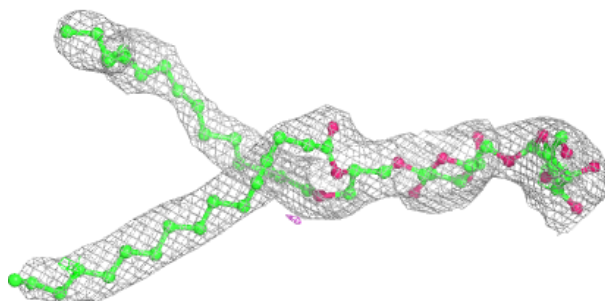
**Electron density around DGD C 518:**

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

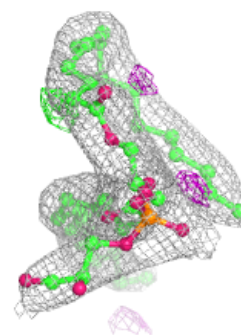
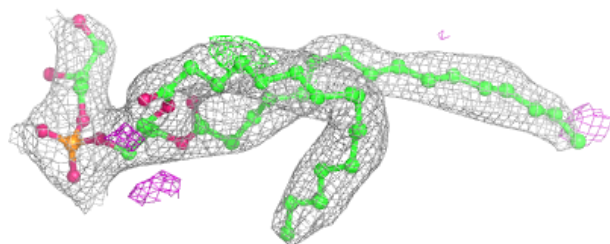
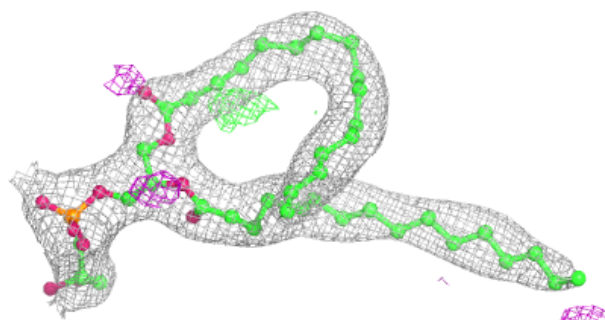


**Electron density around DGD c 516:**

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

**Electron density around LHG A 415:**

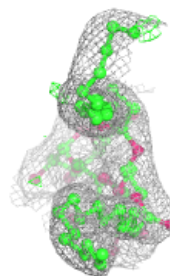
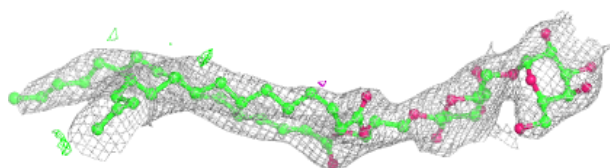
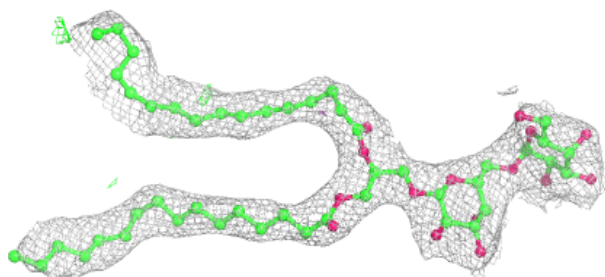
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



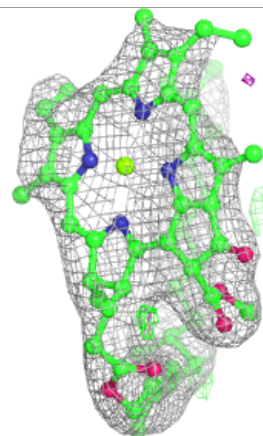
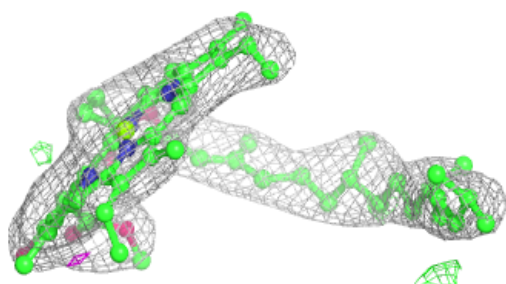
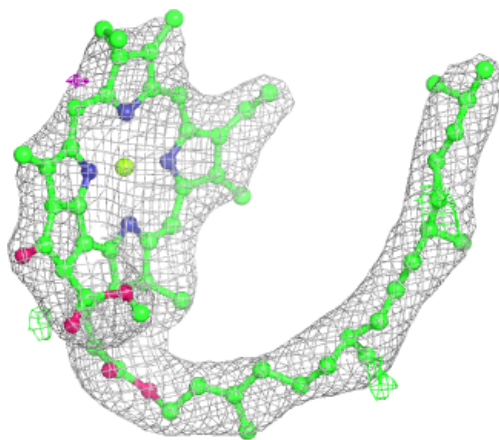


**Electron density around DGD c 518:**

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

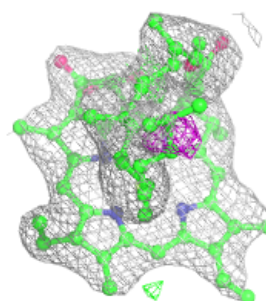
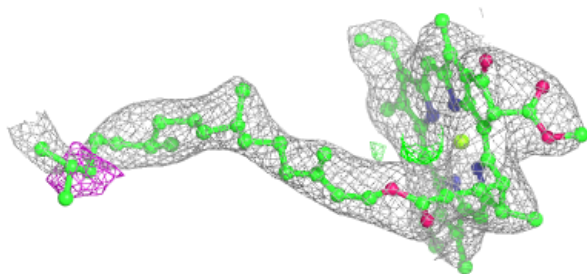
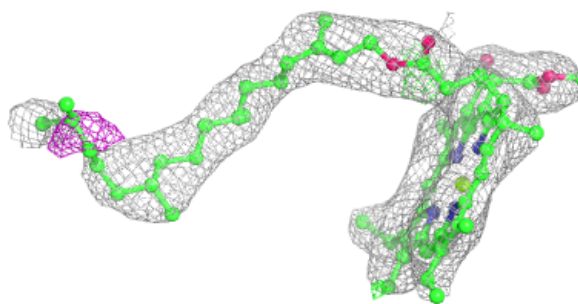
**Electron density around CLA C 508:**

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

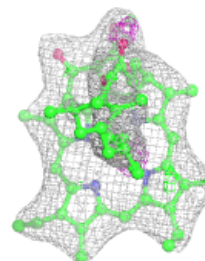
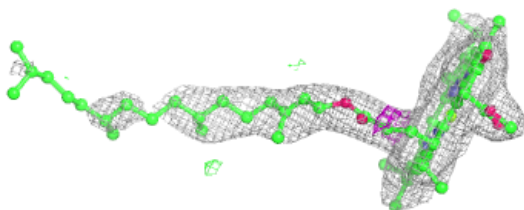
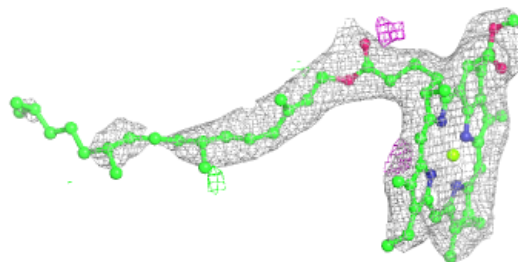


**Electron density around CLA C 509:**

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

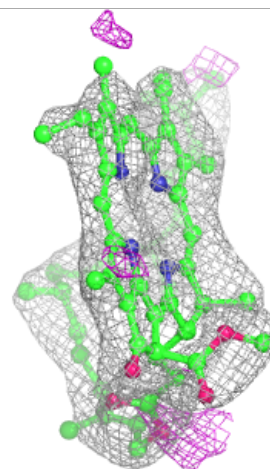
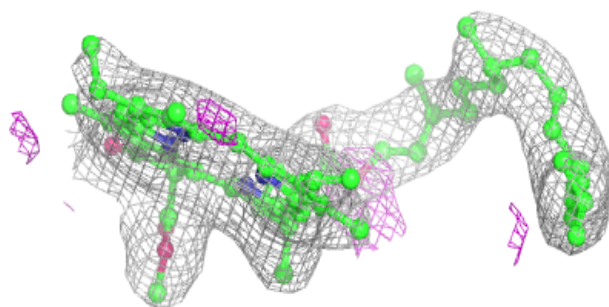
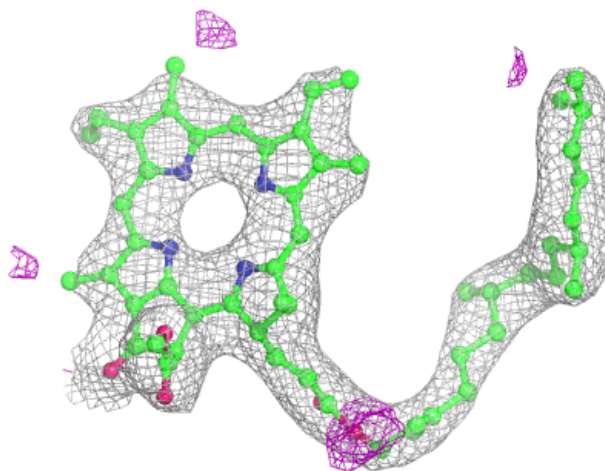
**Electron density around CLA d 403:**

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



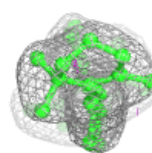
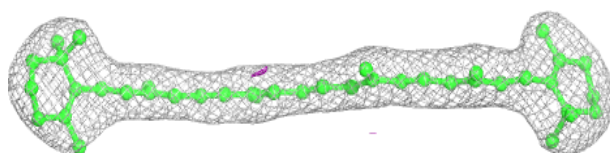
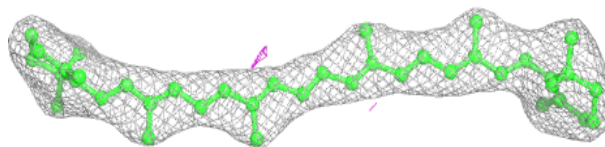
**Electron density around PHO a 408:**

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

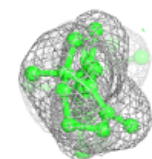
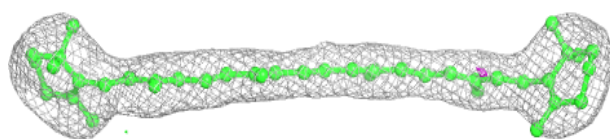
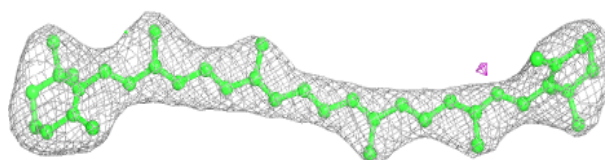


**Electron density around BCR A 408:**

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

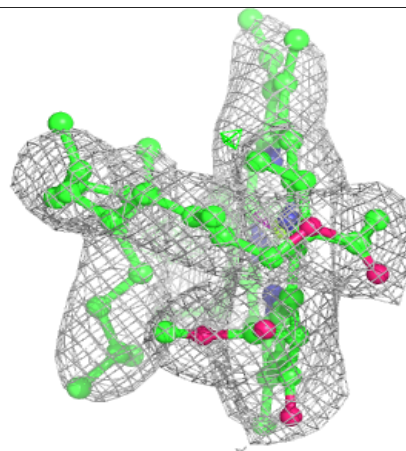
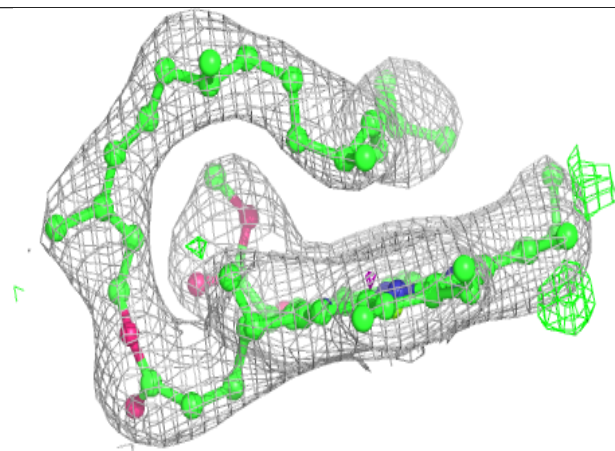
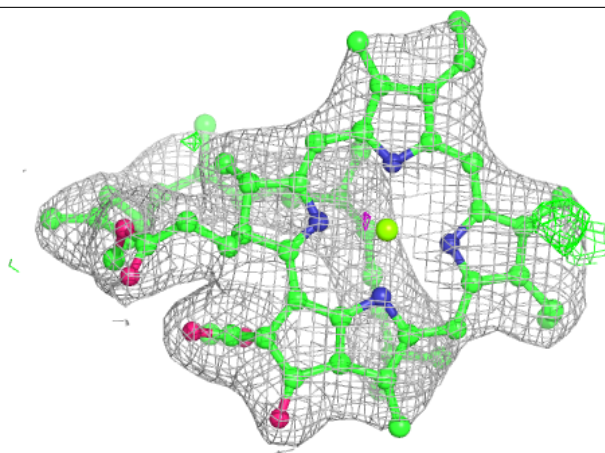
**Electron density around BCR B 619:**

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



**Electron density around CLA C 511:**

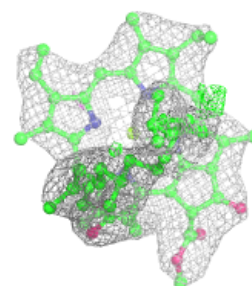
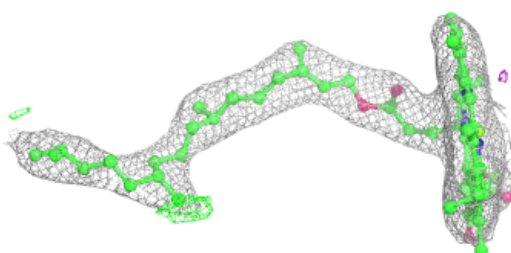
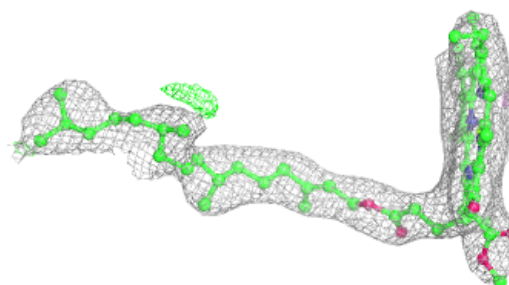
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



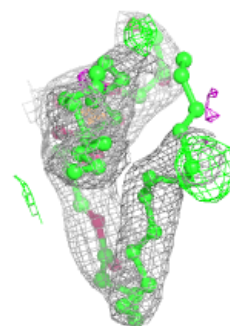
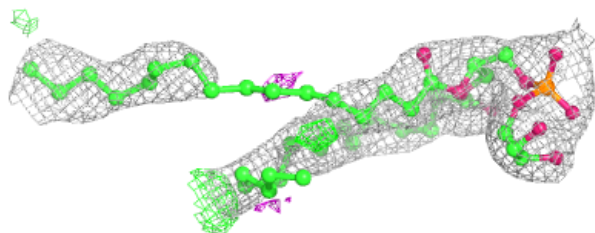
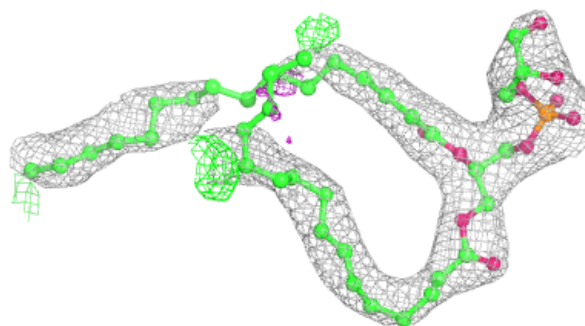


**Electron density around CLA B 607:**

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

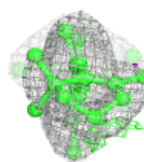
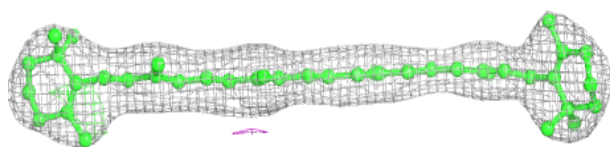
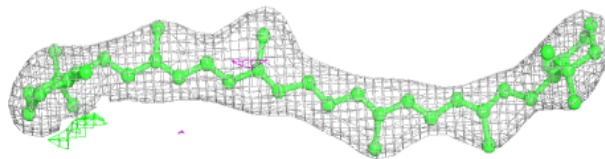
**Electron density around LHG D 409:**

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



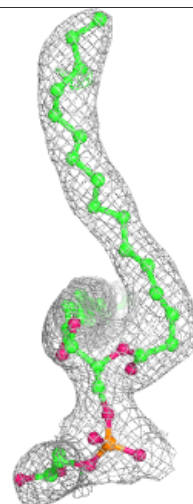
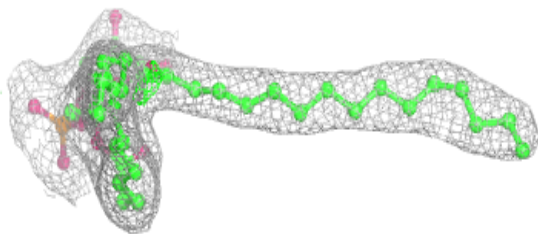
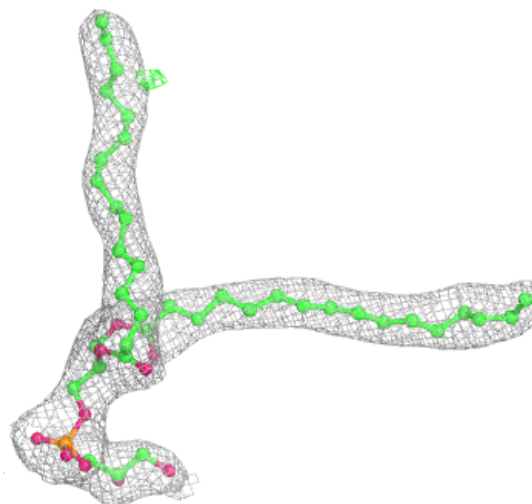
**Electron density around BCR C 516:**

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



**Electron density around LHG b 630:**

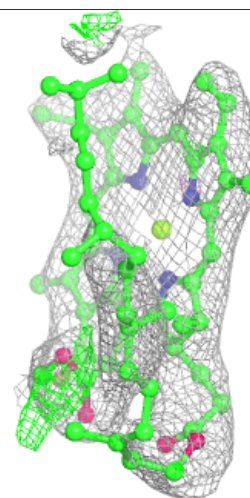
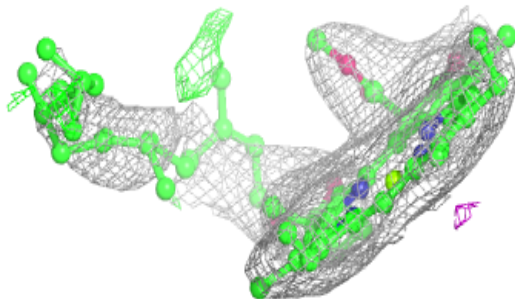
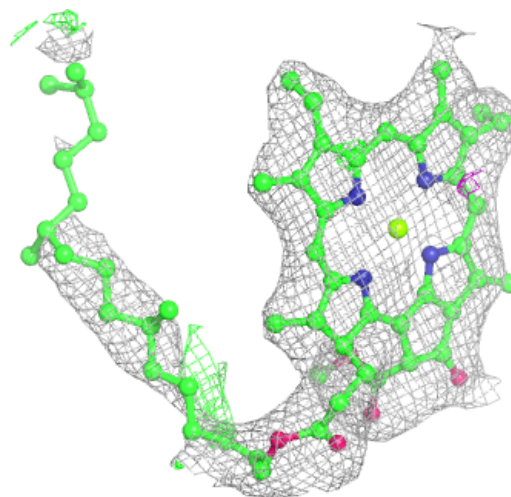
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





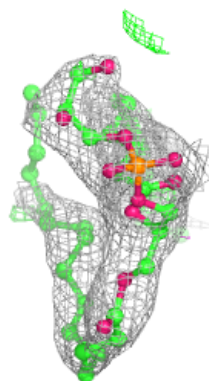
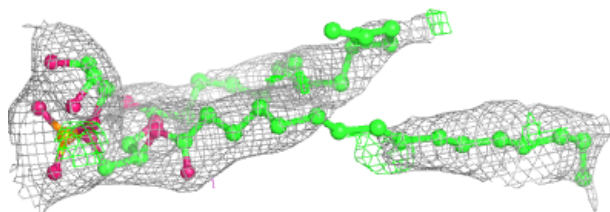
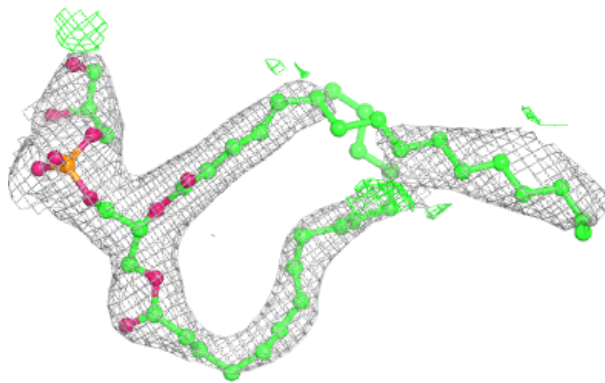
**Electron density around CLA B 617:**

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

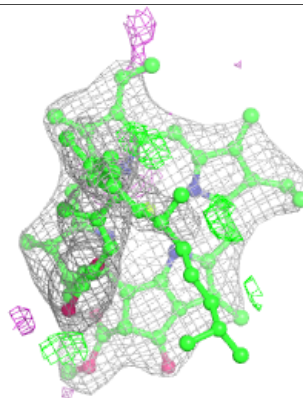
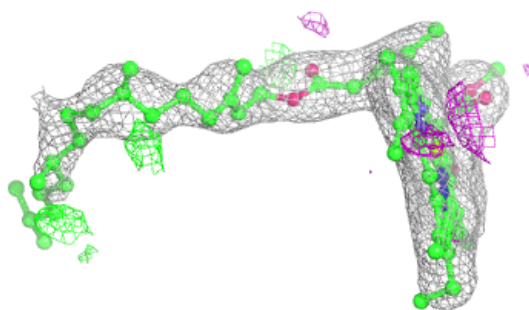
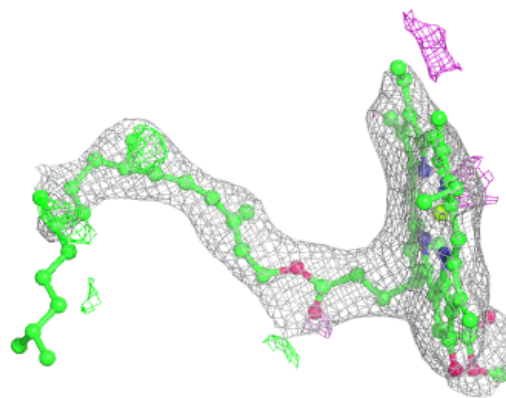


**Electron density around LHG d 408:**

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

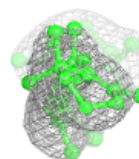
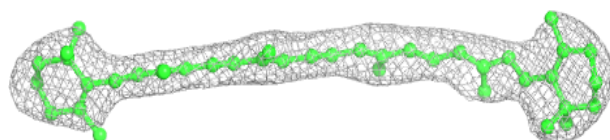
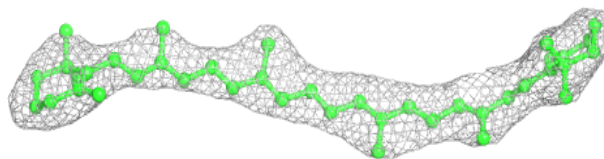
**Electron density around CLA D 405:**

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

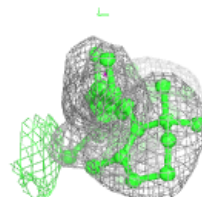
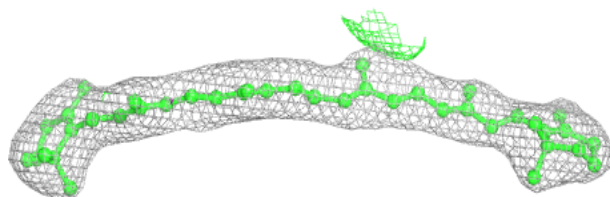
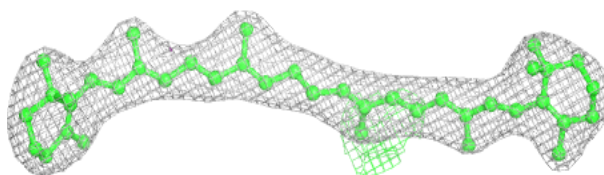


**Electron density around BCR H 101:**

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

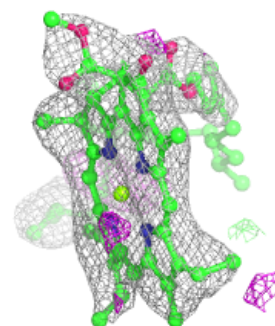
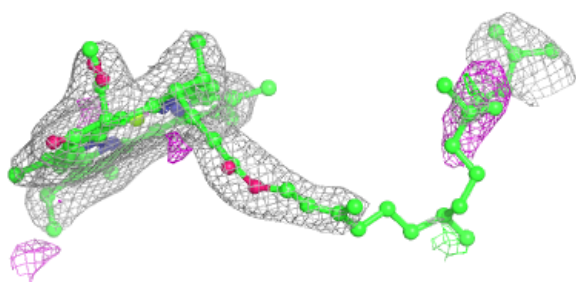
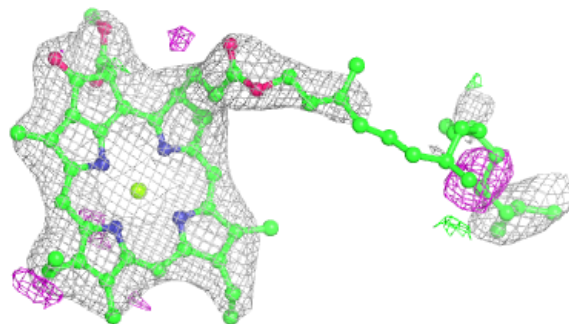
**Electron density around BCR T 101:**

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

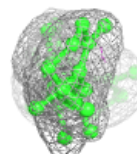
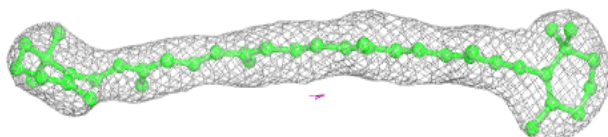
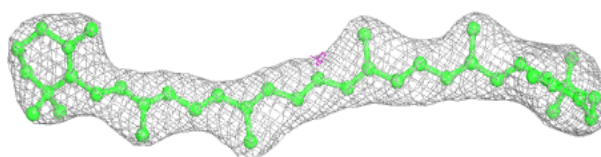


**Electron density around CLA a 409:**

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

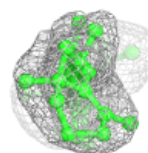
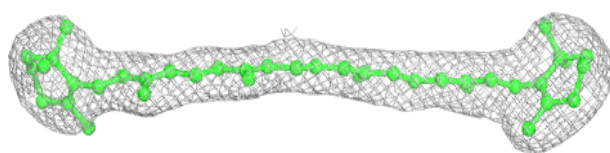
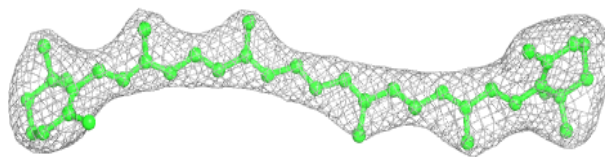
**Electron density around BCR b 617:**

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

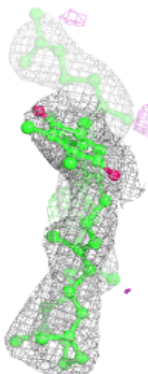
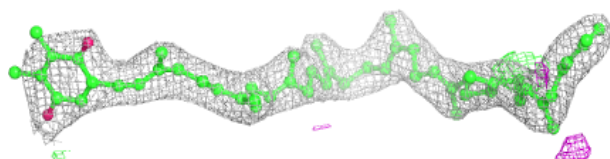
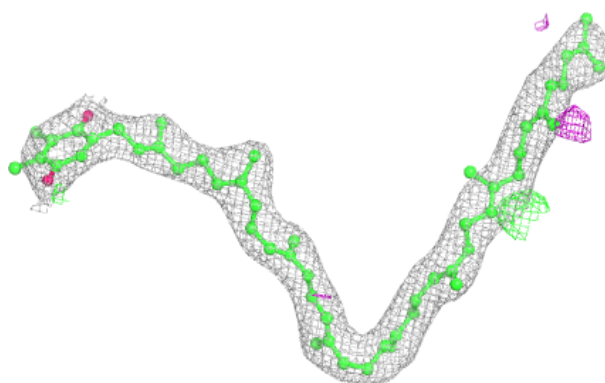


**Electron density around BCR b 618:**

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

**Electron density around PL9 d 405:**

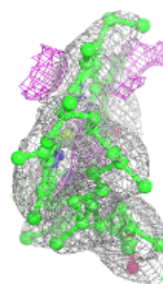
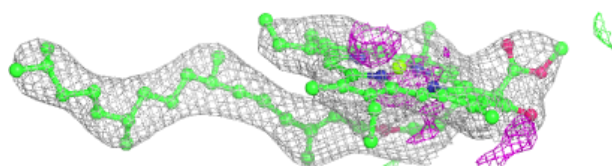
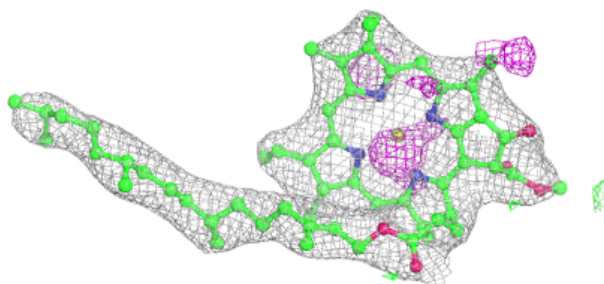
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



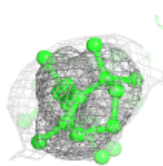
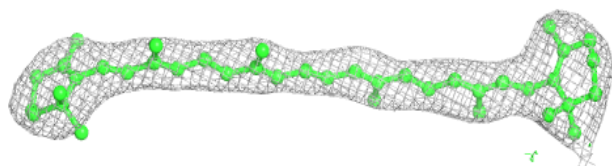
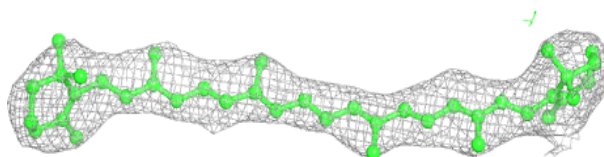


**Electron density around CLA C 502:**

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

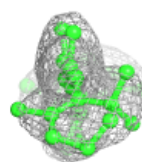
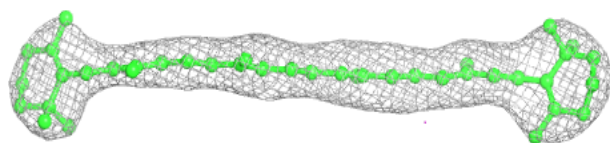
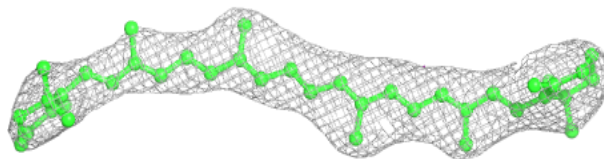
**Electron density around BCR c 514:**

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

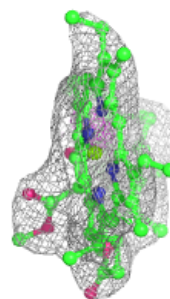
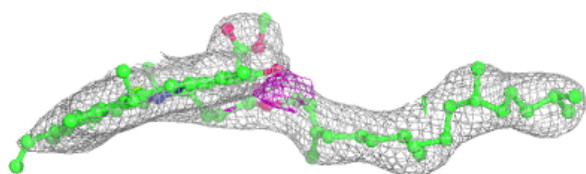
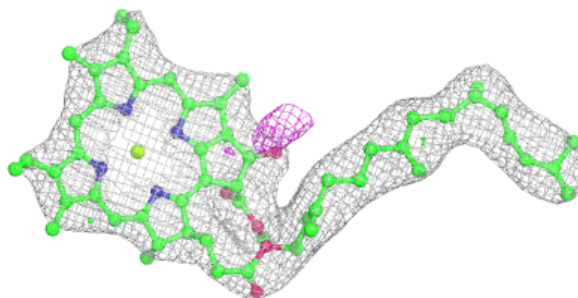


**Electron density around BCR c 515:**

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

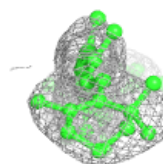
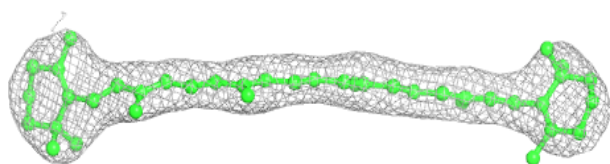
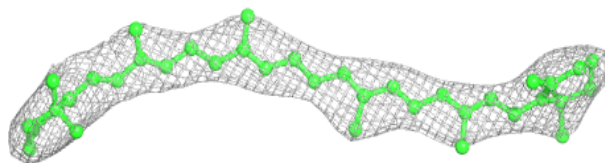
**Electron density around CLA b 602:**

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

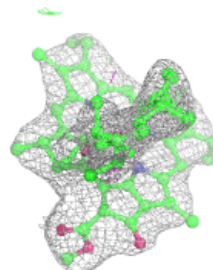
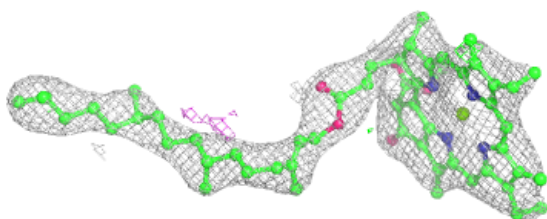
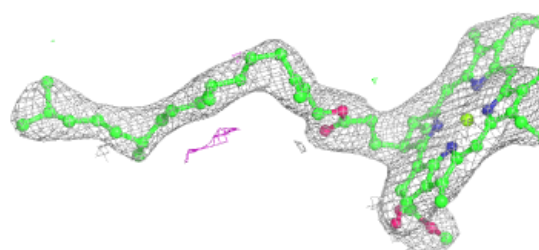


**Electron density around BCR h 102:**

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

**Electron density around CLA C 503:**

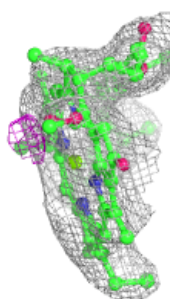
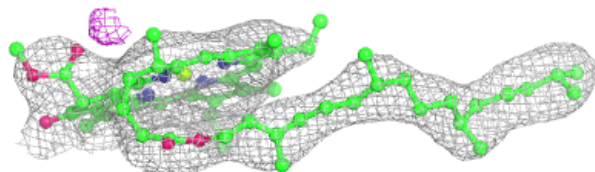
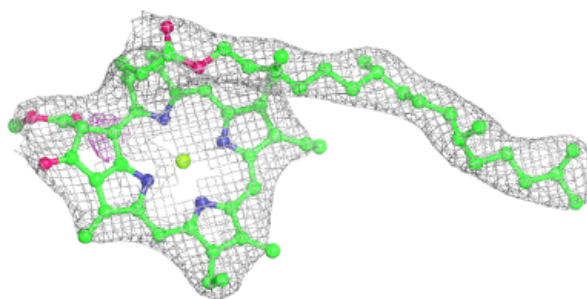
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



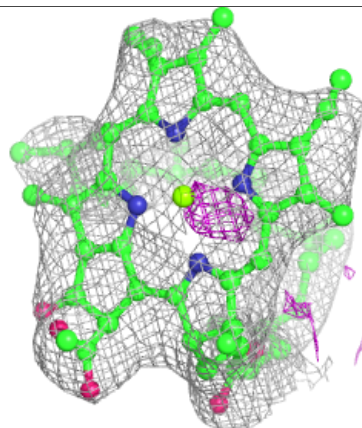
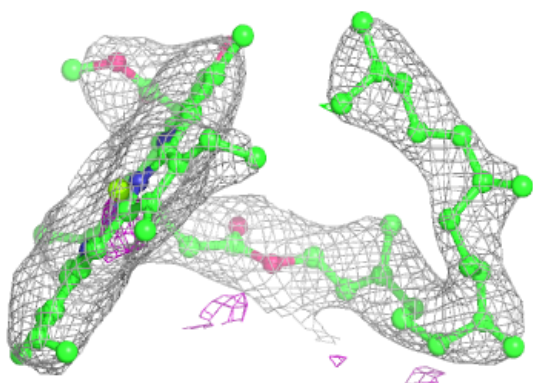
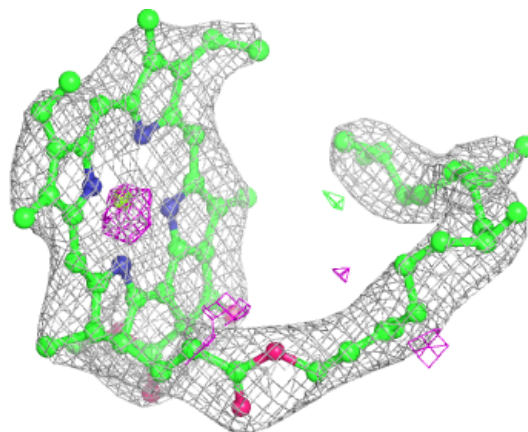


**Electron density around CLA c 501:**

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

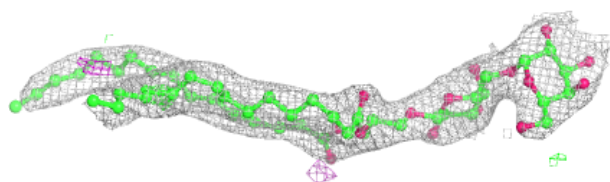
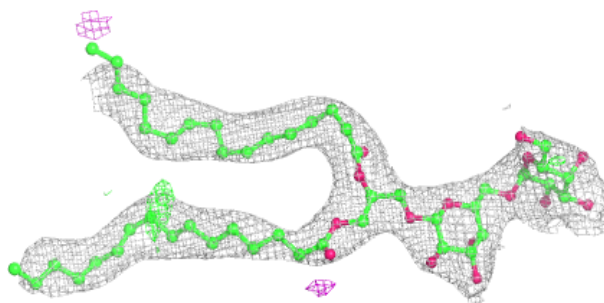
**Electron density around CLA C 504:**

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

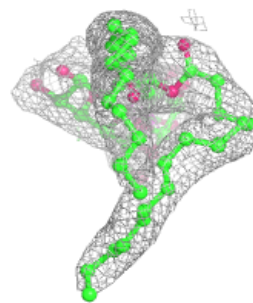
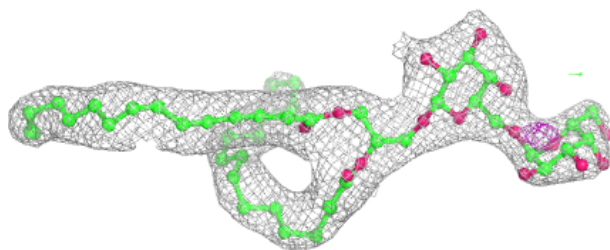
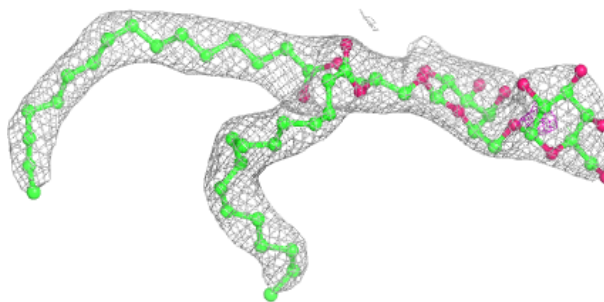


**Electron density around DGD C 519:**

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

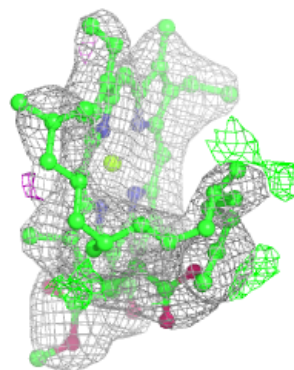
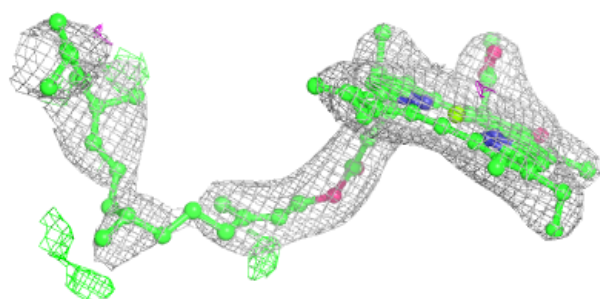
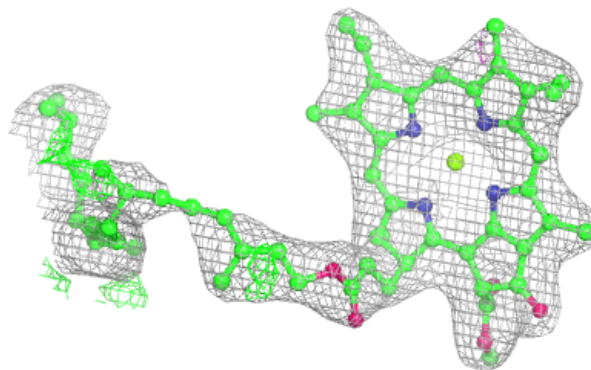
**Electron density around DGD H 102:**

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

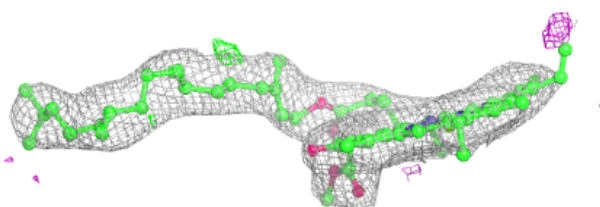
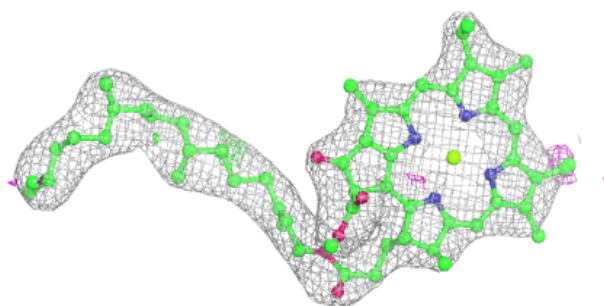


**Electron density around CLA A 407:**

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

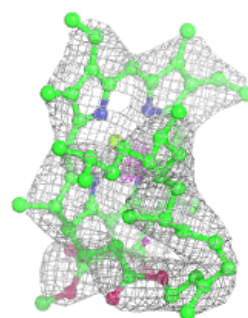
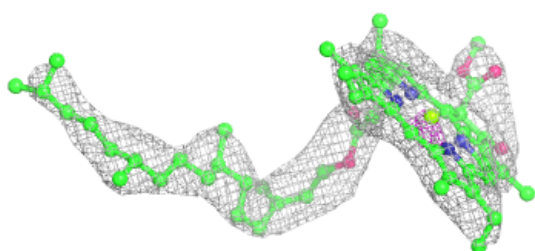
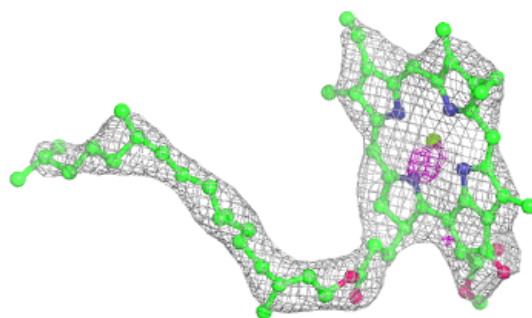
**Electron density around CLA B 603:**

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

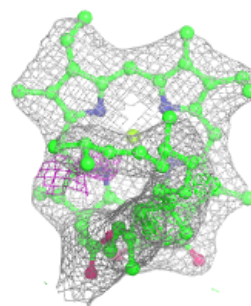
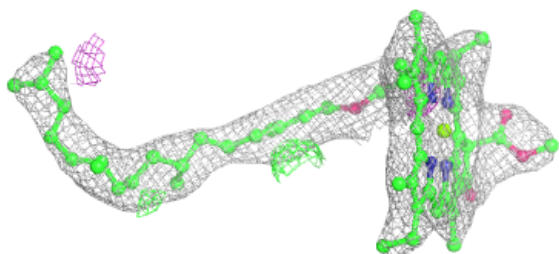
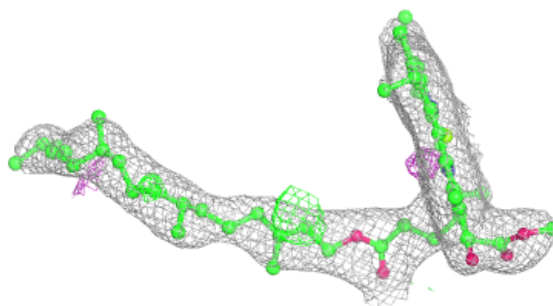


**Electron density around CLA c 511:**

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

**Electron density around CLA b 605:**

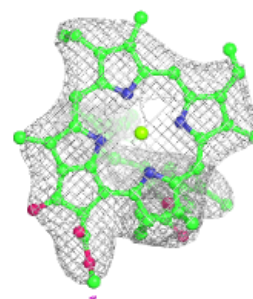
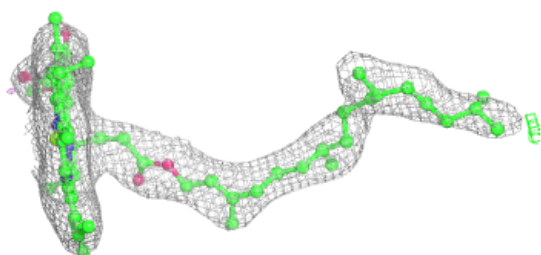
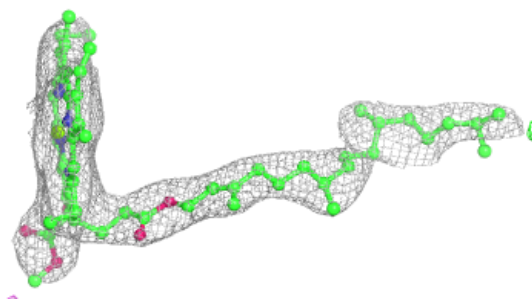
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



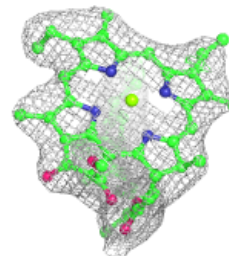
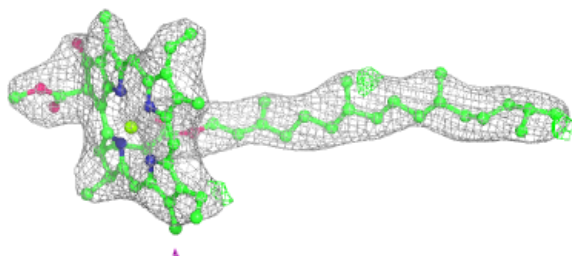
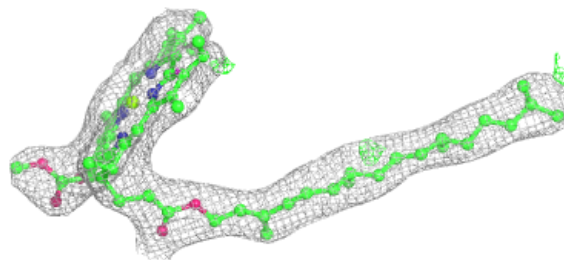


**Electron density around CLA b 606:**

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

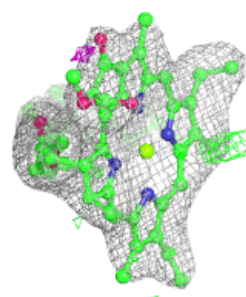
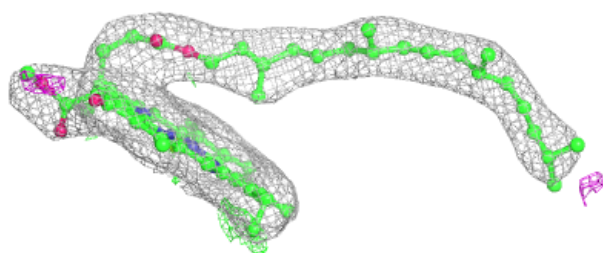
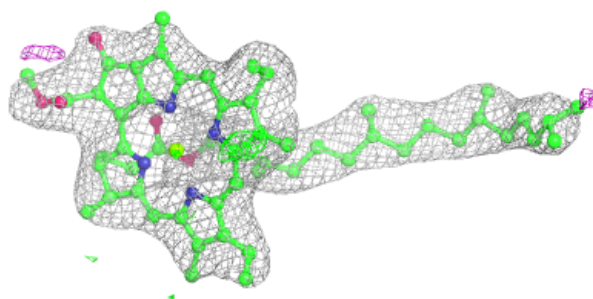
**Electron density around CLA b 607:**

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

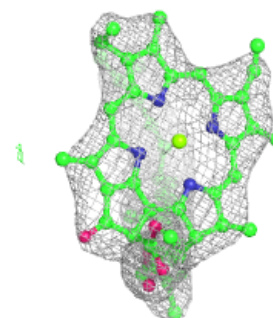
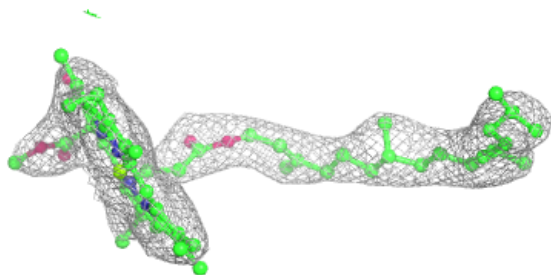
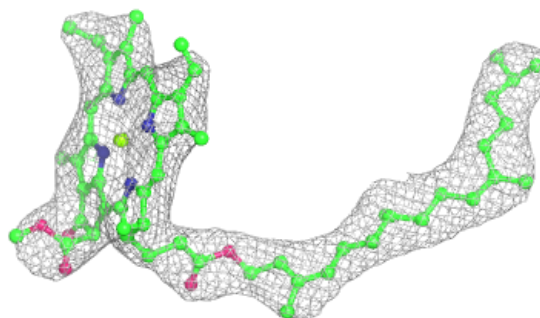


**Electron density around CLA b 608:**

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

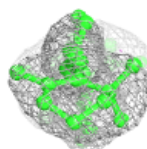
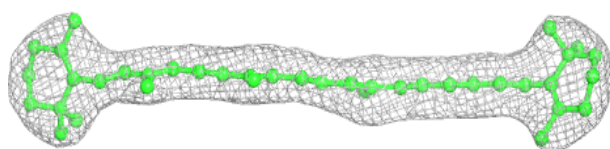
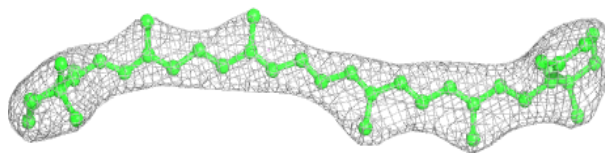
**Electron density around CLA b 609:**

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

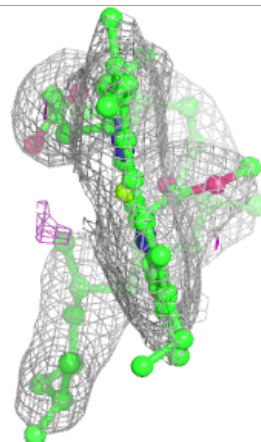
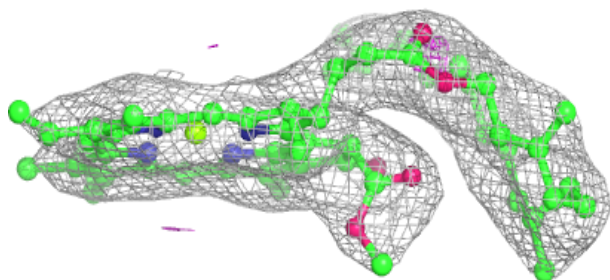
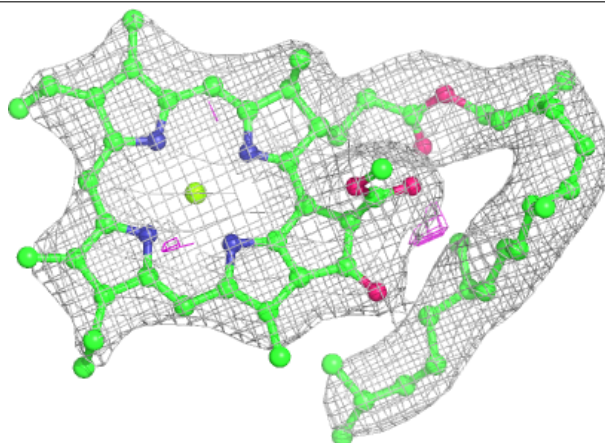


**Electron density around BCR a 410:**

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

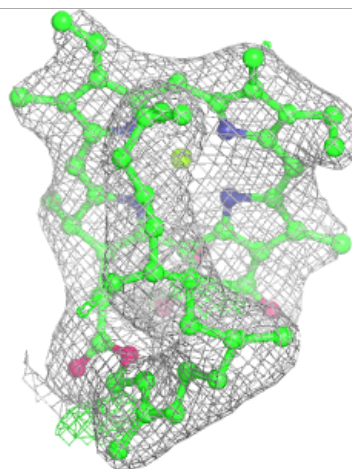
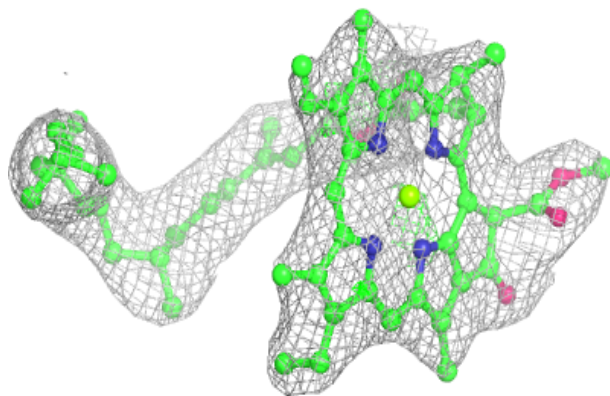
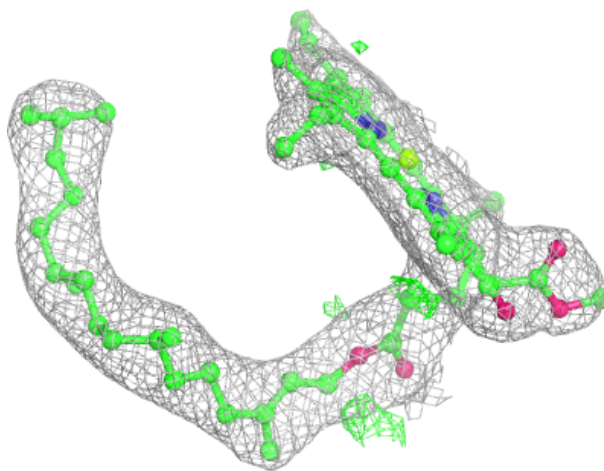
**Electron density around CLA b 610:**

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



**Electron density around CLA b 611:**

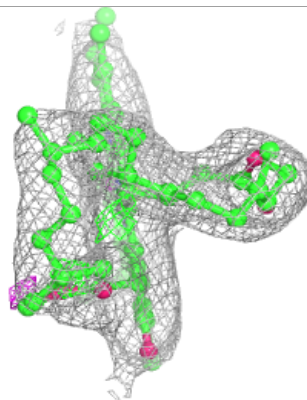
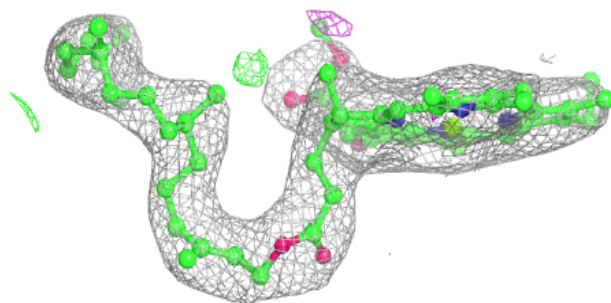
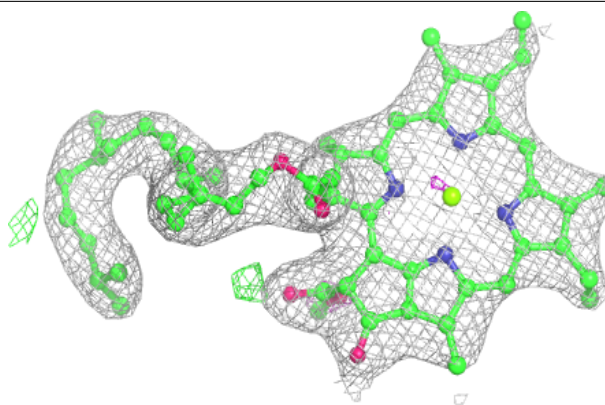
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





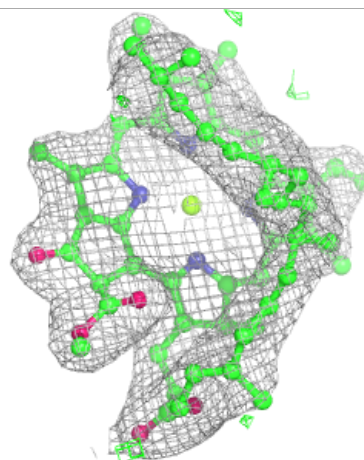
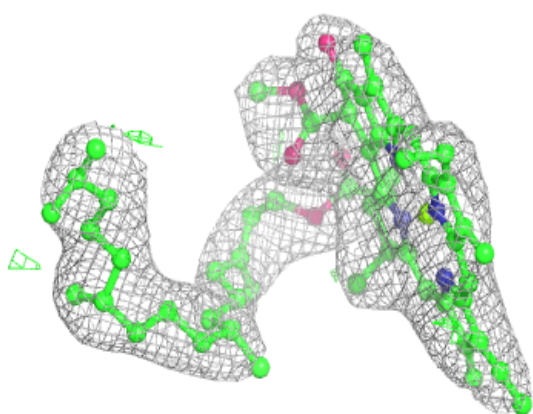
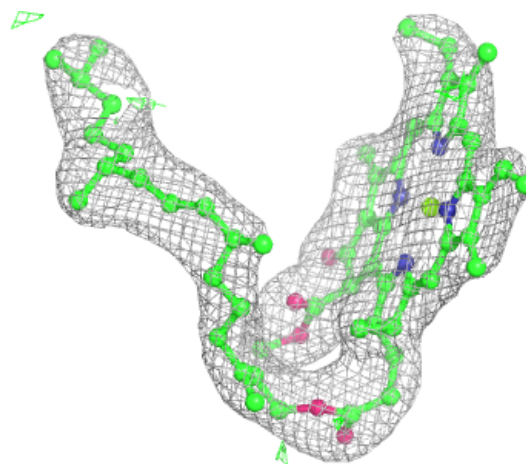
**Electron density around CLA b 612:**

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



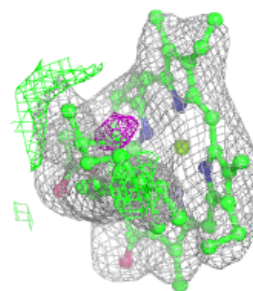
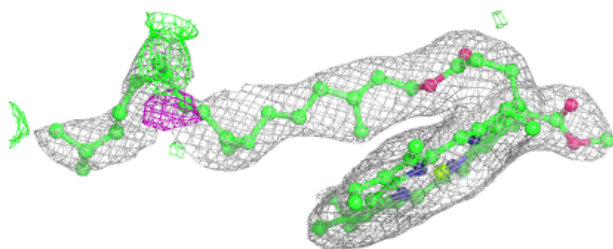
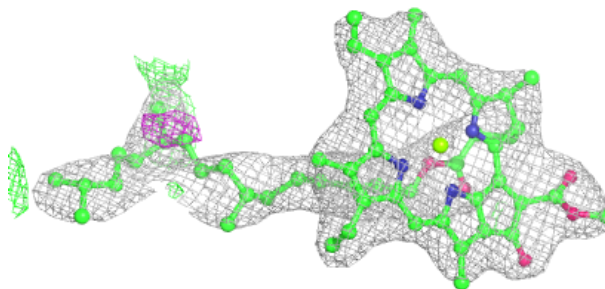
**Electron density around CLA b 613:**

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



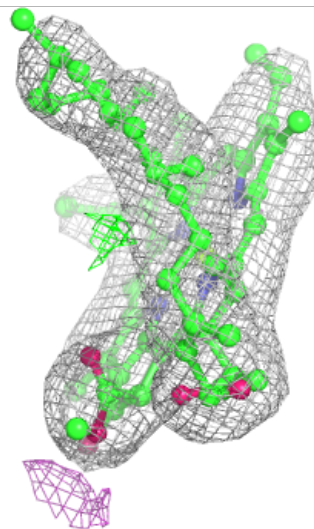
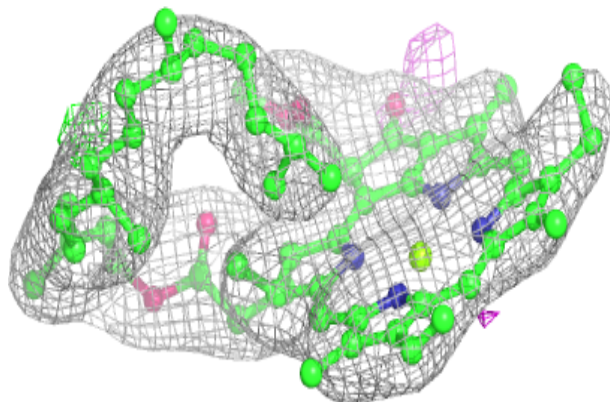
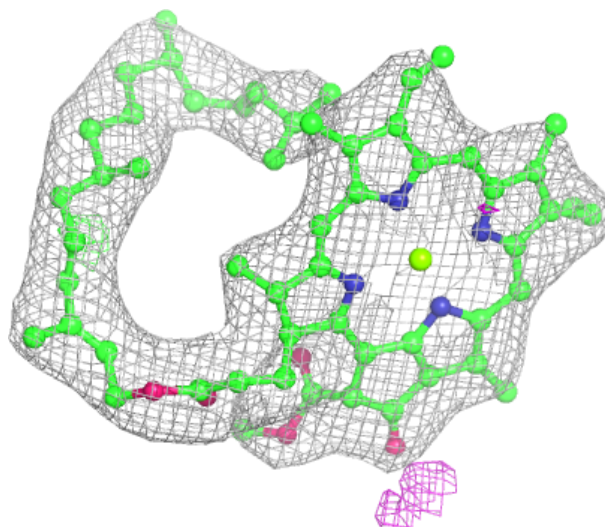
**Electron density around CLA b 614:**

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



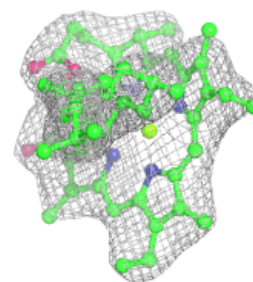
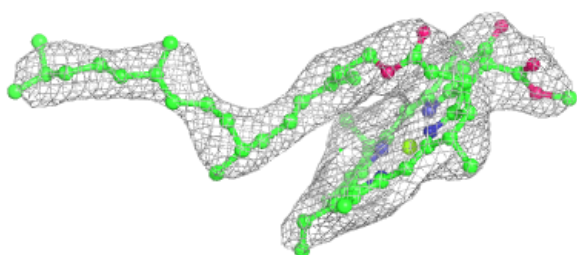
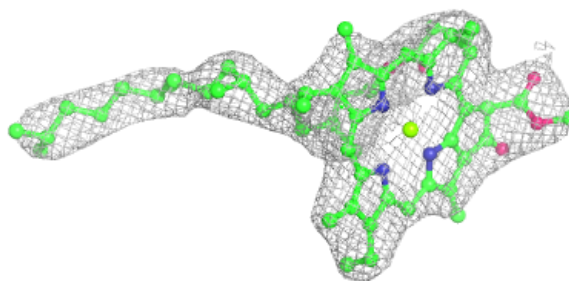
**Electron density around CLA b 615:**

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

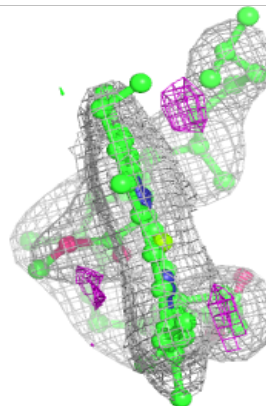
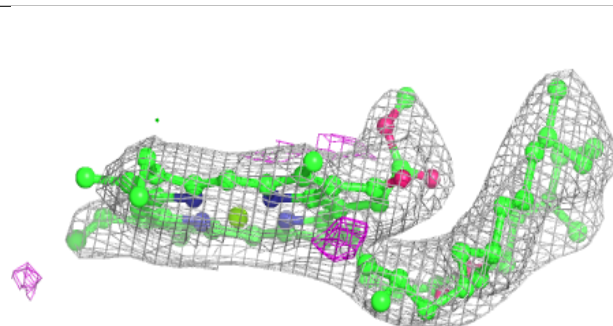
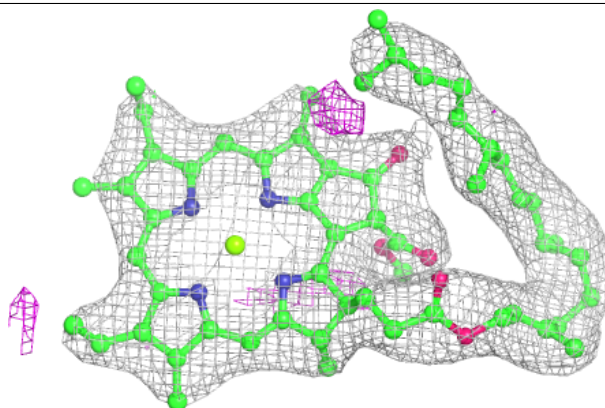


**Electron density around CLA C 506:**

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

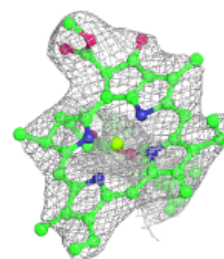
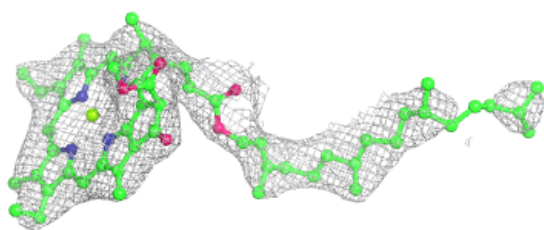
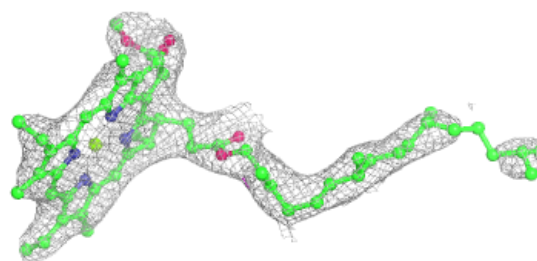
**Electron density around CLA B 611:**

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



**Electron density around CLA c 502:**

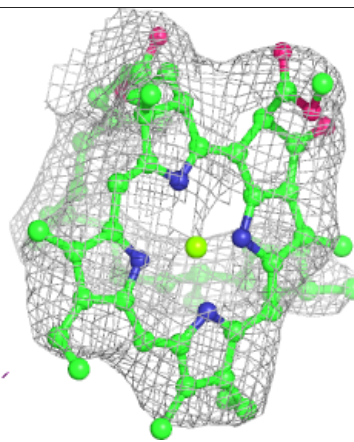
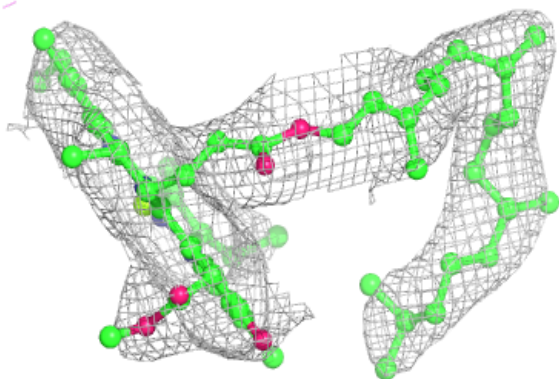
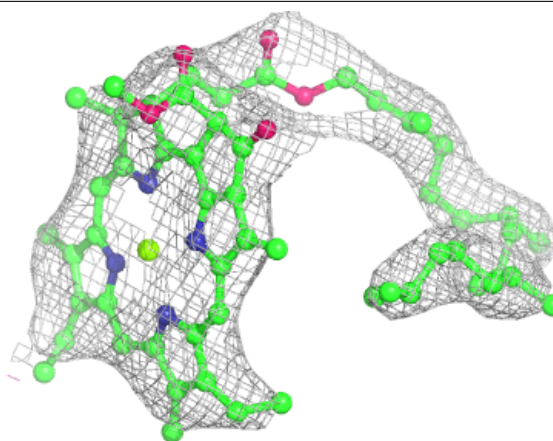
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





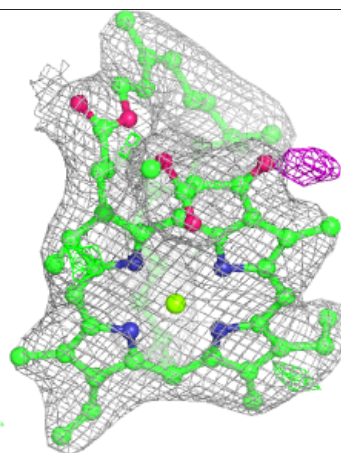
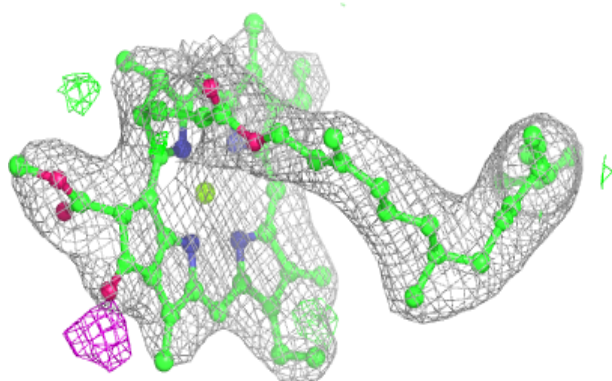
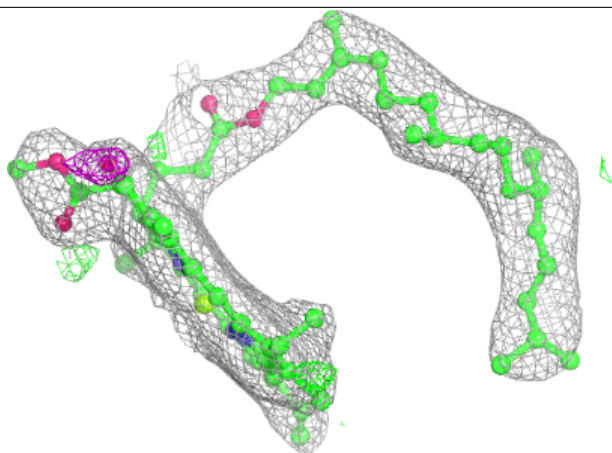
**Electron density around CLA c 503:**

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



**Electron density around CLA B 612:**

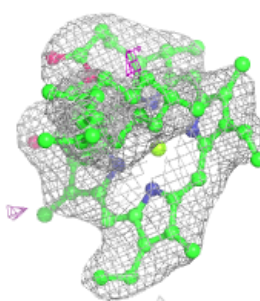
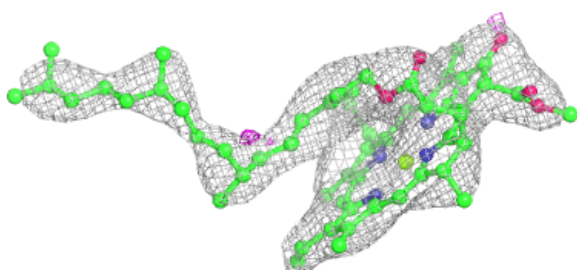
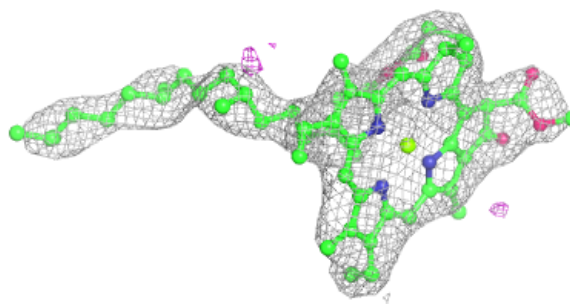
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



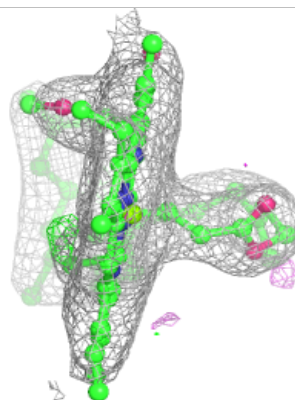
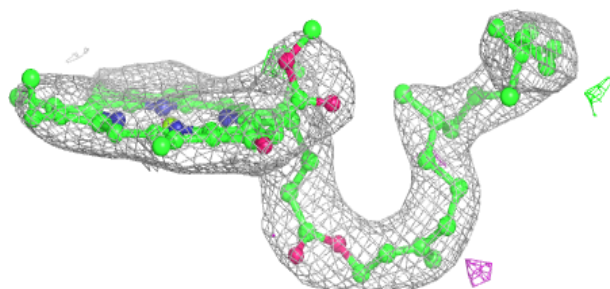
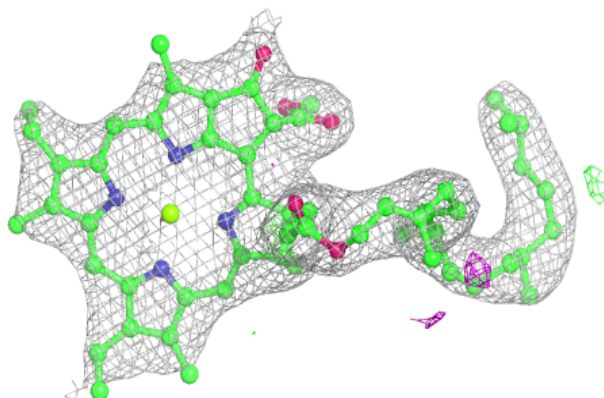


**Electron density around CLA c 505:**

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

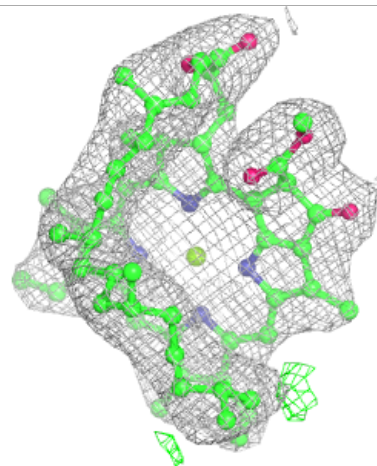
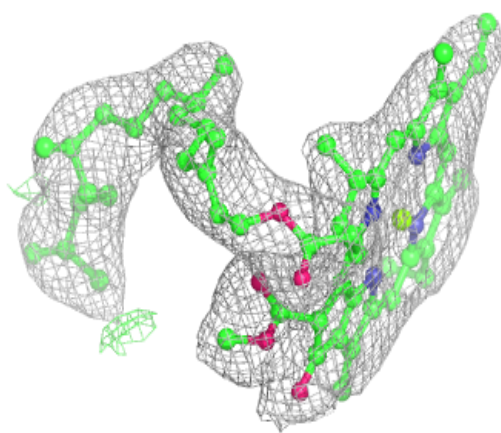
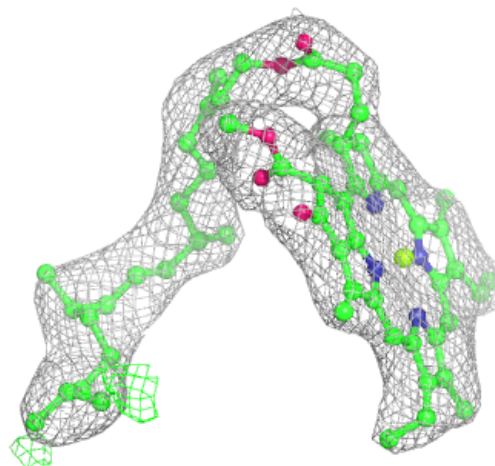
**Electron density around CLA B 613:**

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



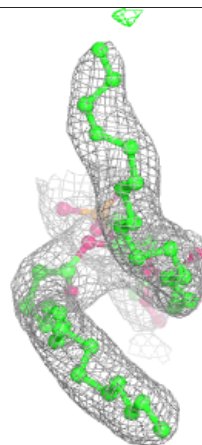
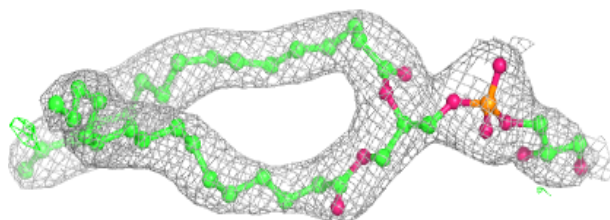
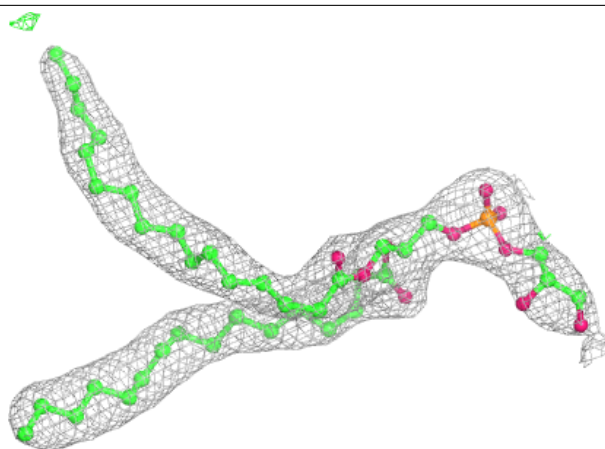
**Electron density around CLA B 614:**

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



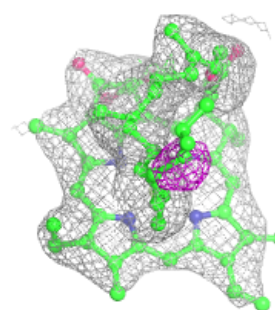
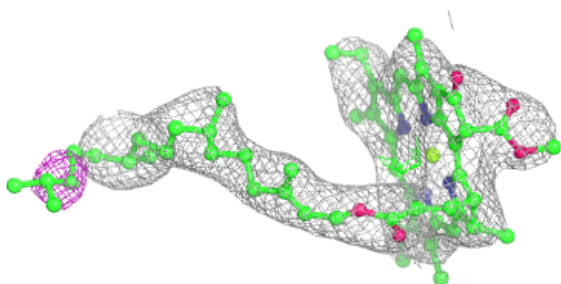
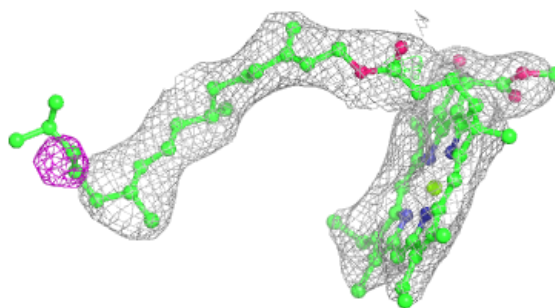
**Electron density around LHG D 408:**

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

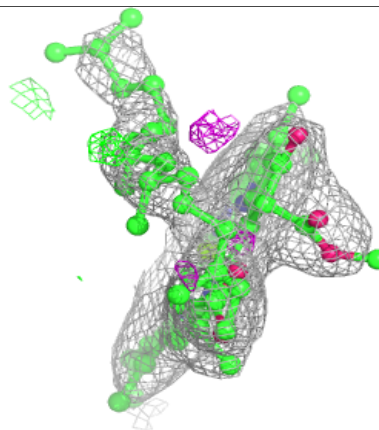
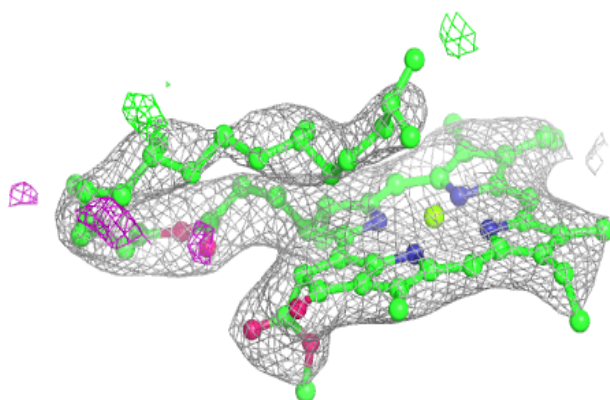
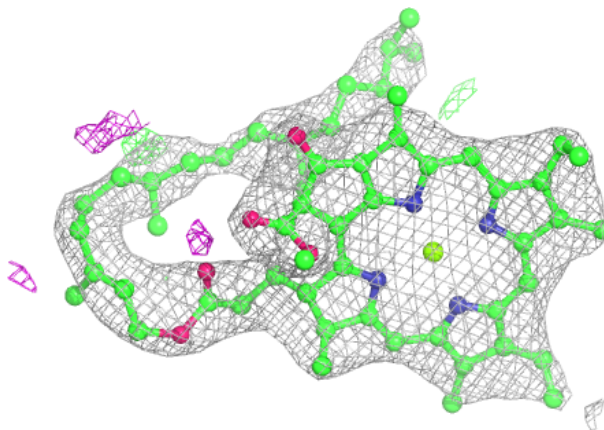


**Electron density around CLA c 508:**

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

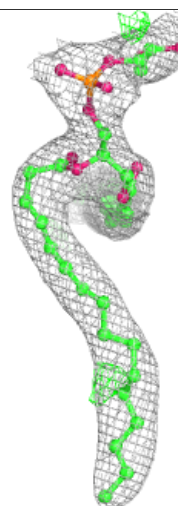
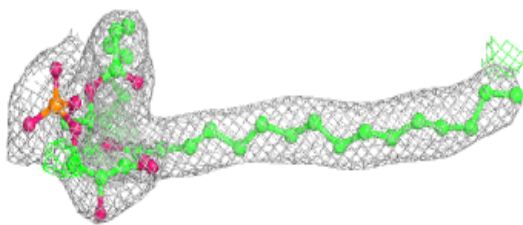
**Electron density around CLA c 509:**

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



**Electron density around LHG L 101:**

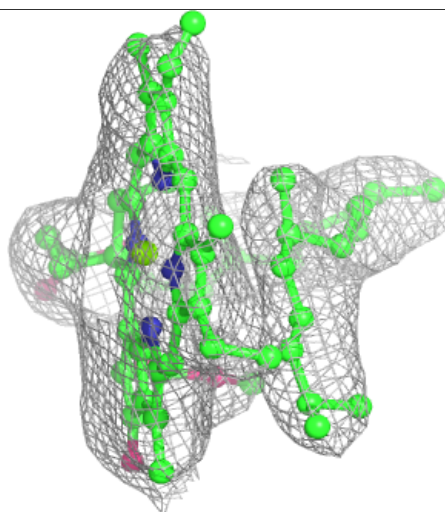
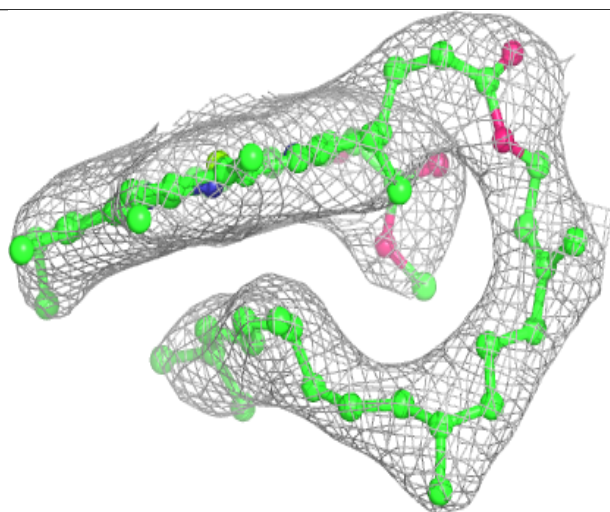
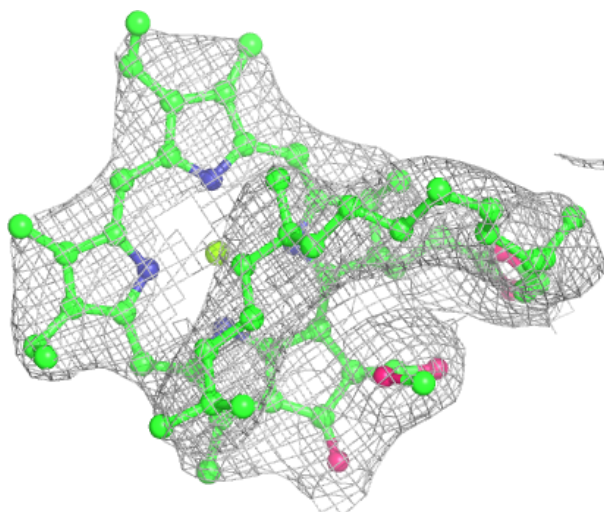
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





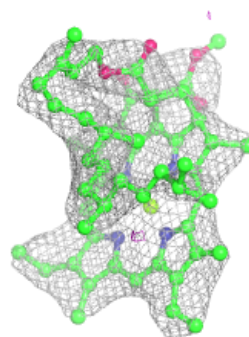
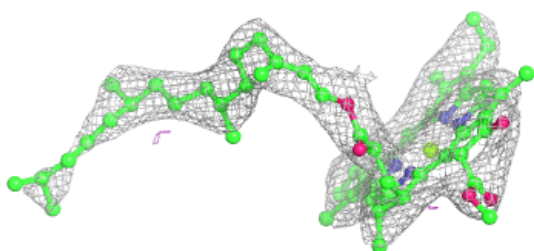
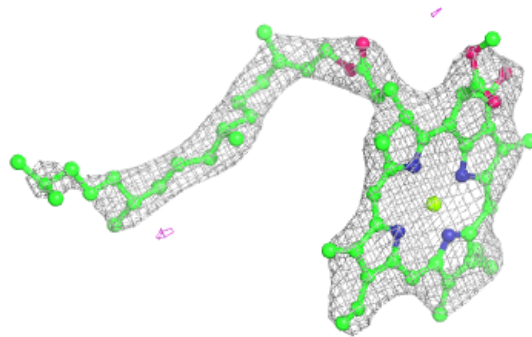
**Electron density around CLA c 510:**

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

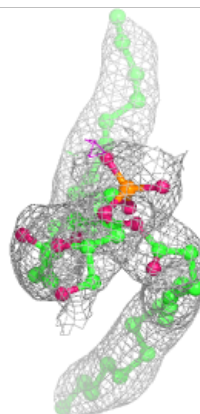
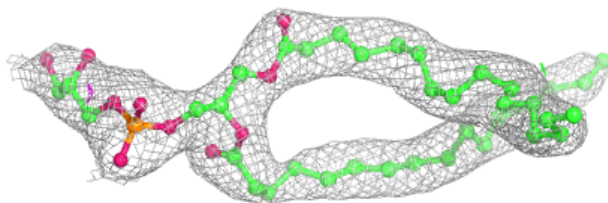
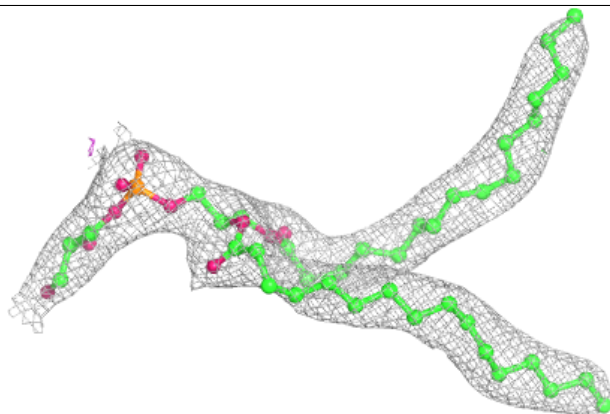


**Electron density around CLA C 512:**

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

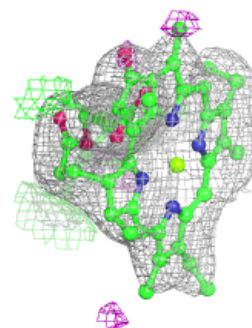
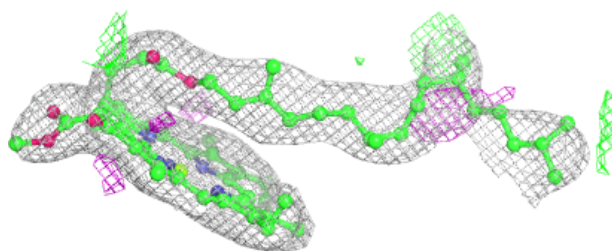
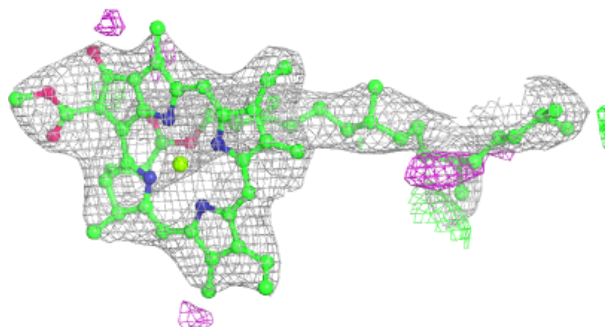
**Electron density around LHG d 407:**

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

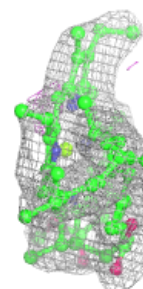
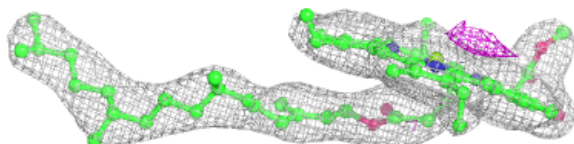
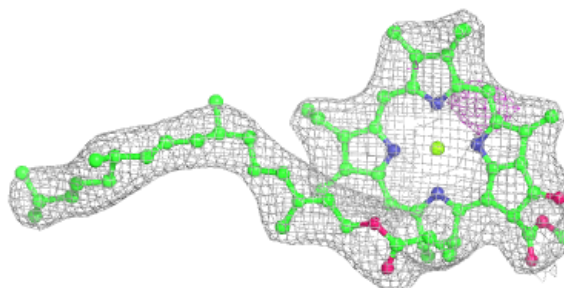


**Electron density around CLA B 615:**

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

**Electron density around CLA B 604:**

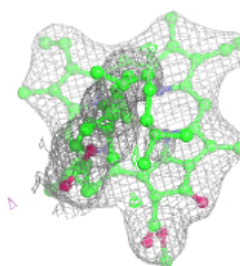
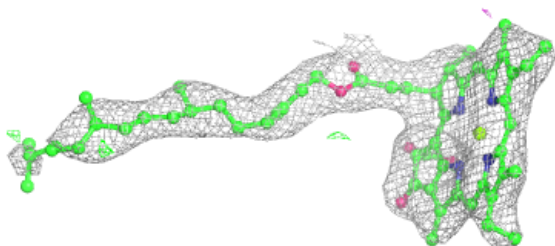
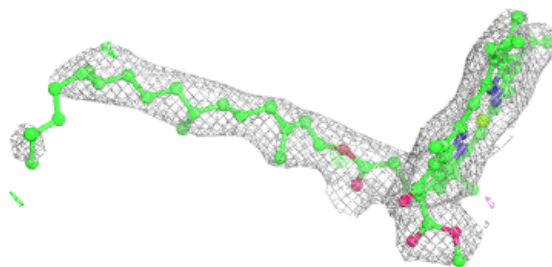
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





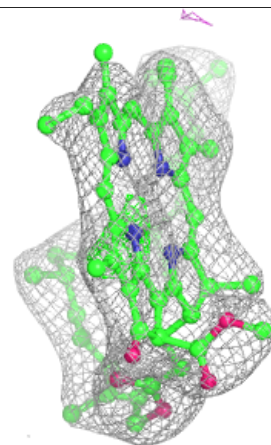
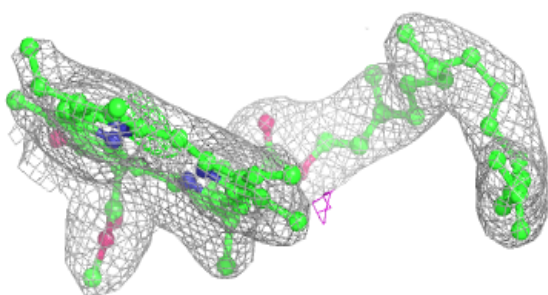
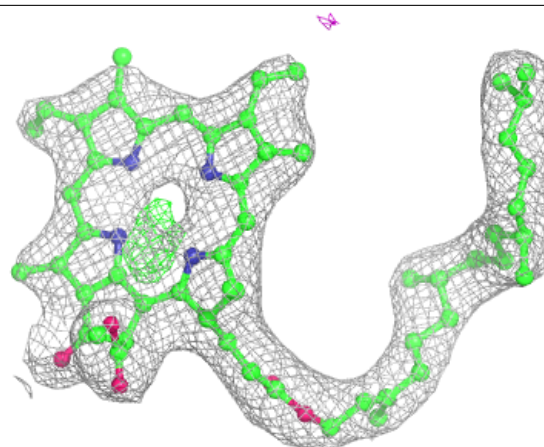
**Electron density around CLA B 605:**

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



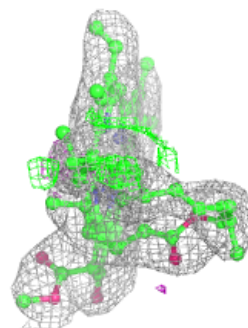
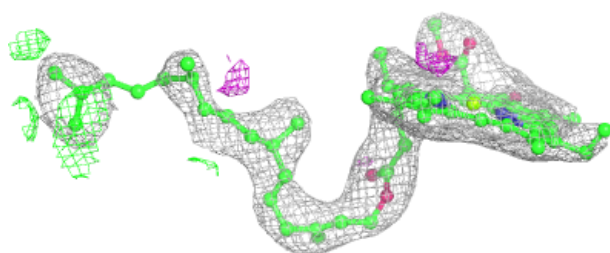
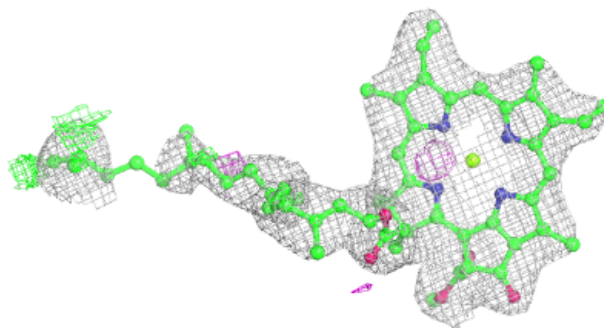
**Electron density around PHO D 402:**

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

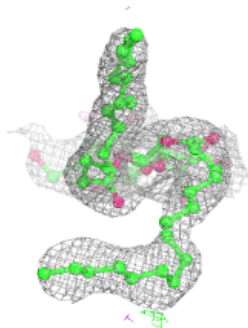
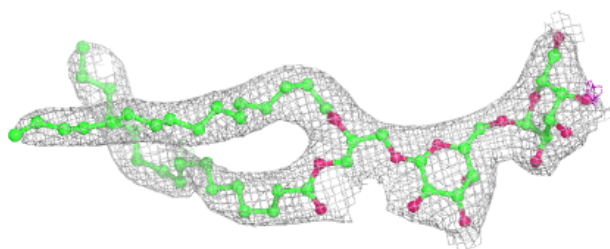
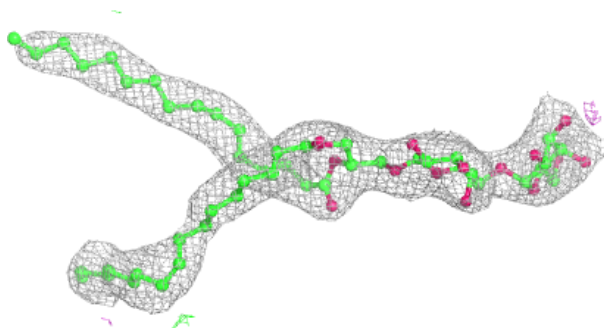


**Electron density around CLA a 406:**

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

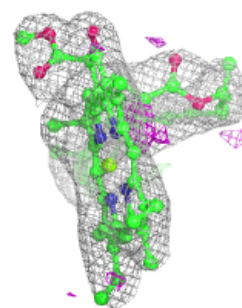
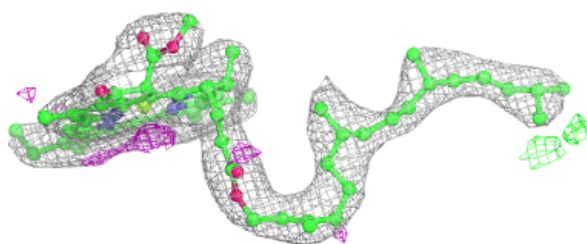
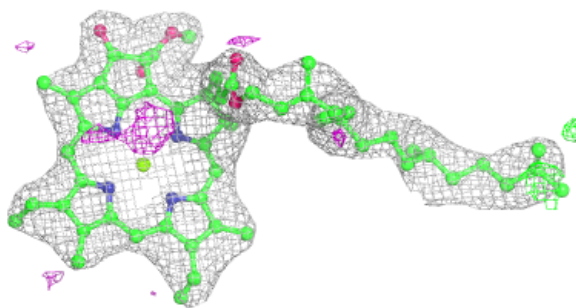
**Electron density around DGD C 517:**

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

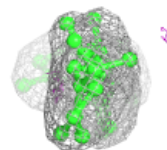
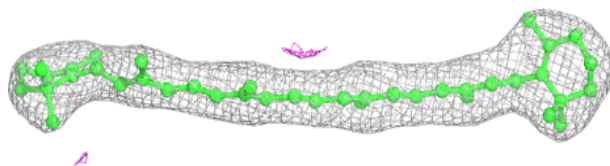
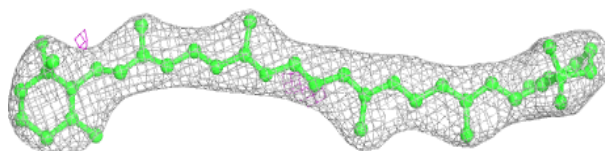


**Electron density around CLA A 405:**

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

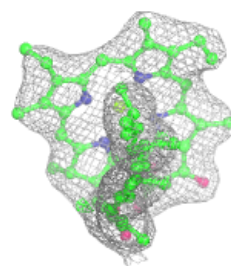
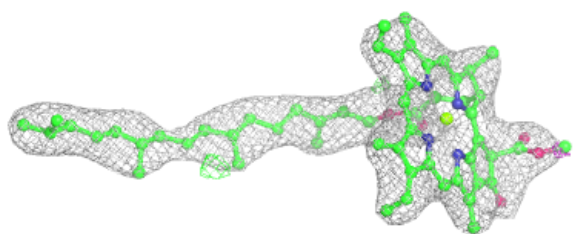
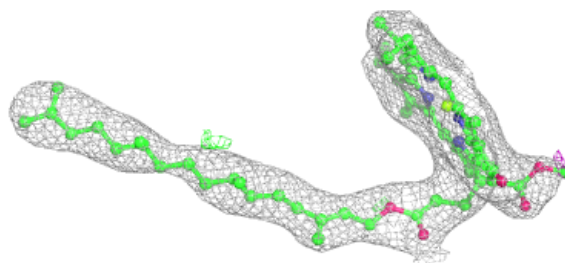
**Electron density around BCR B 618:**

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

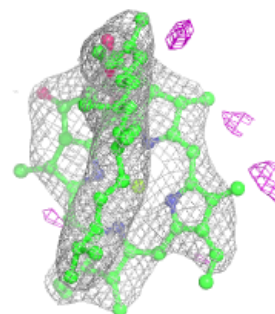
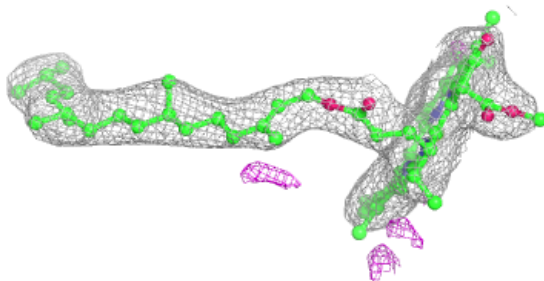
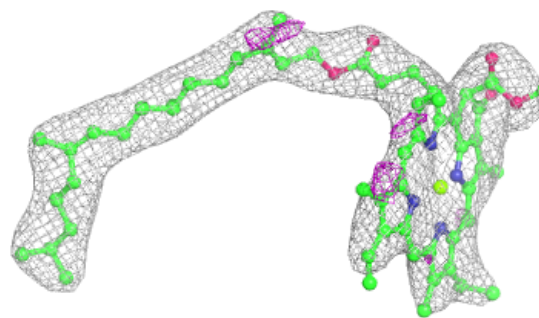


**Electron density around CLA B 608:**

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

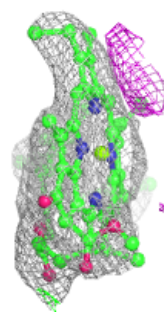
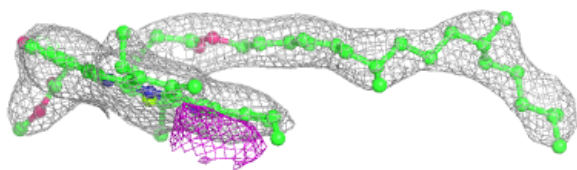
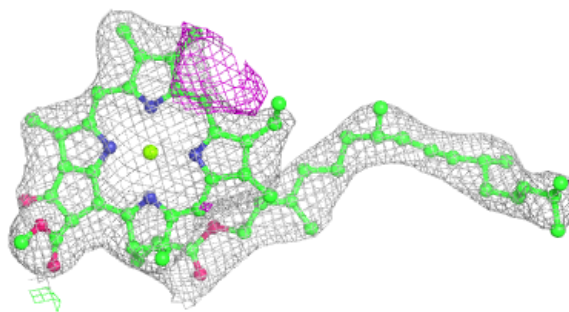
**Electron density around CLA B 610:**

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

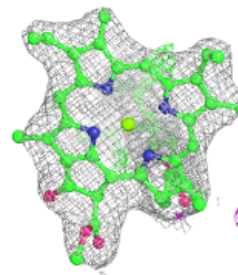
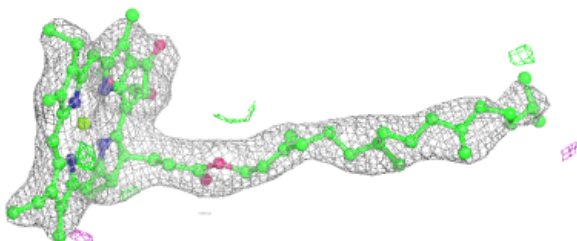
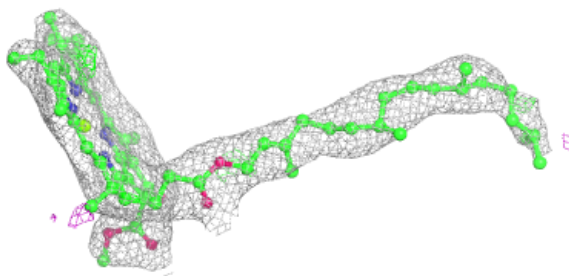


**Electron density around CLA b 603:**

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

**Electron density around CLA b 604:**

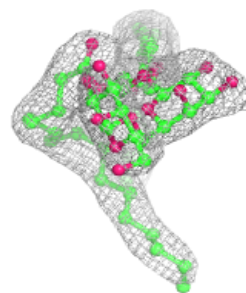
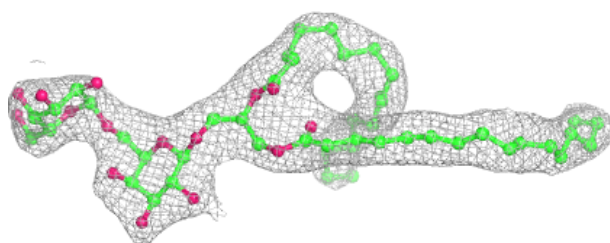
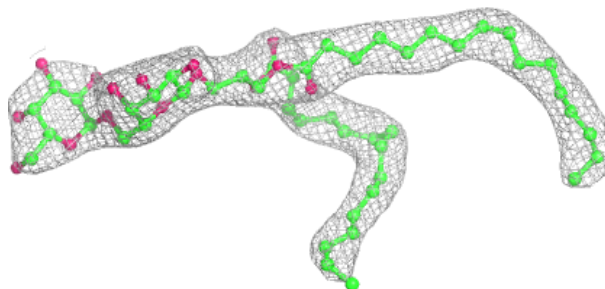
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



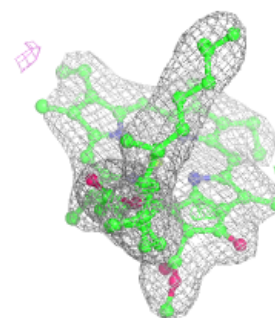
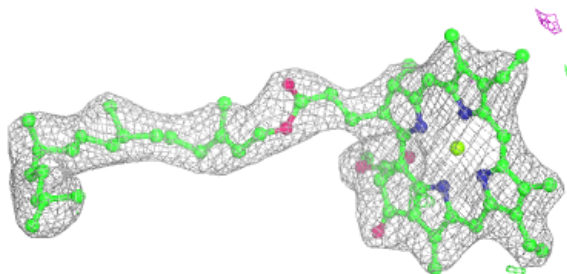
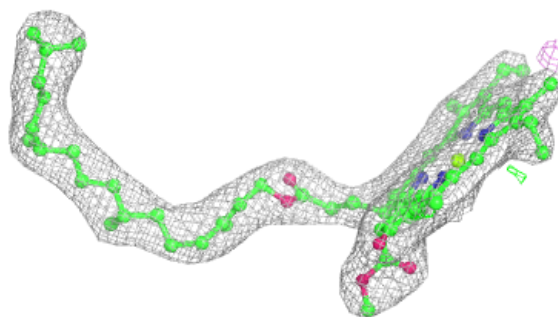


**Electron density around DGD h 103:**

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

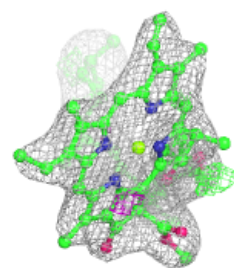
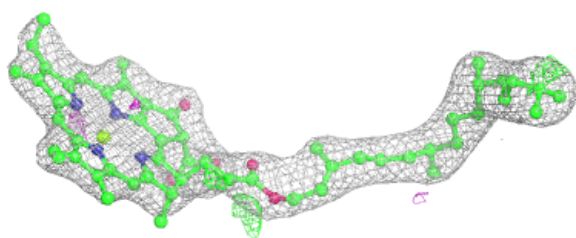
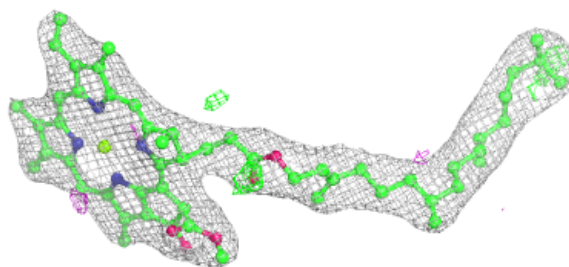
**Electron density around CLA D 404:**

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

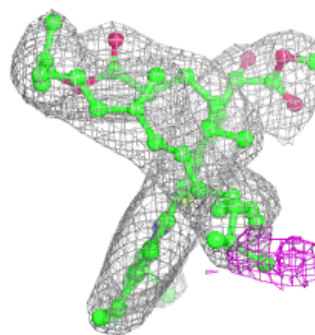
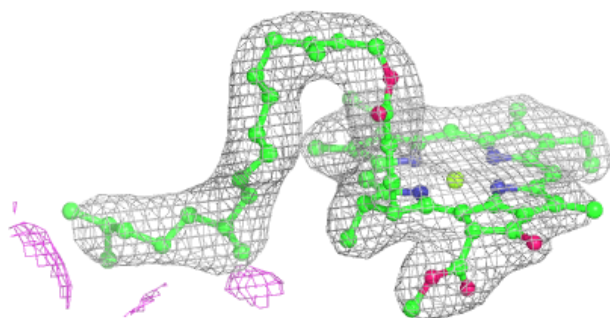
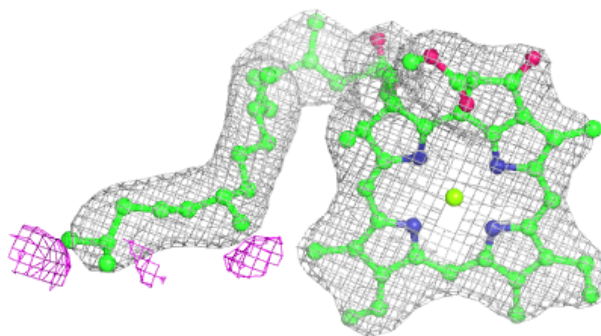


**Electron density around CLA a 404:**

$2mF_o-DF_c$  (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:**

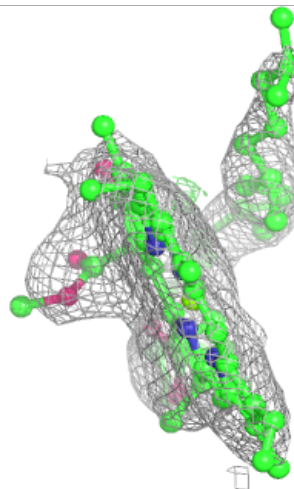
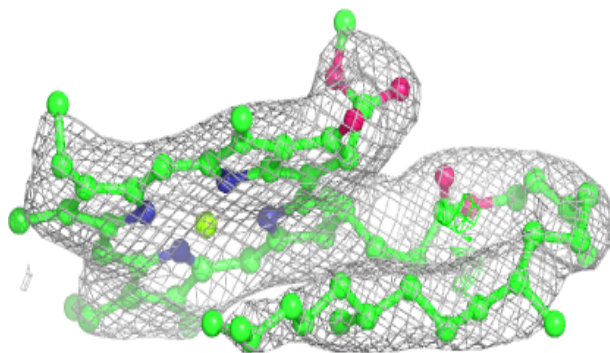
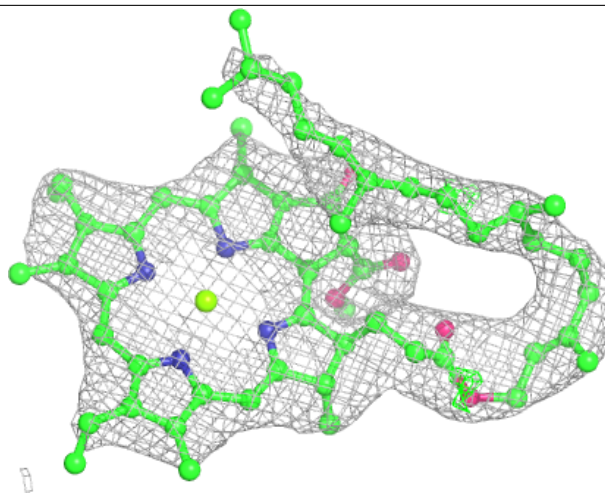
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





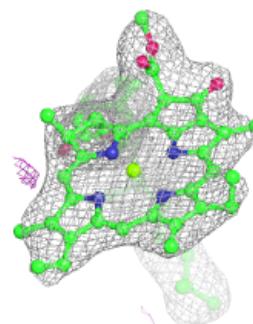
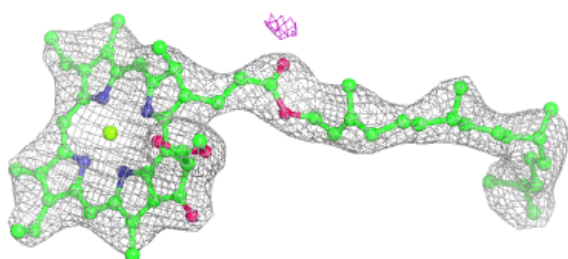
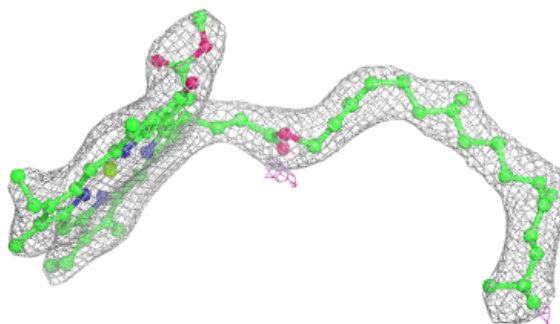
**Electron density around CLA C 510:**

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



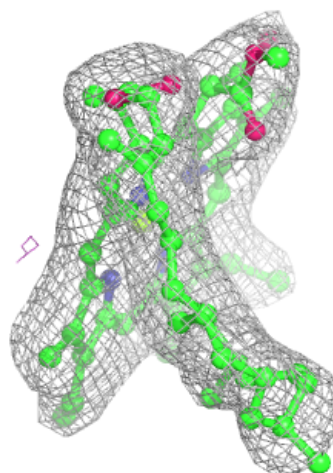
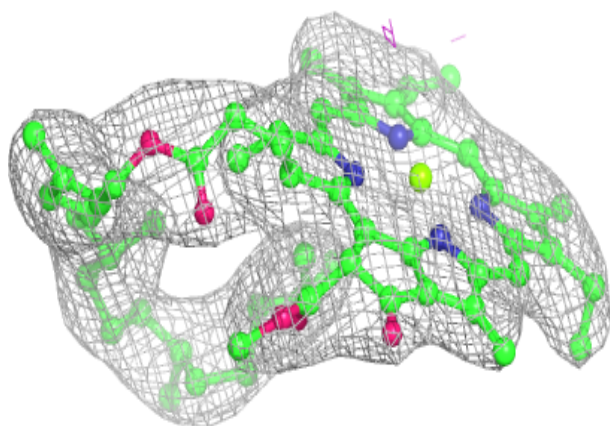
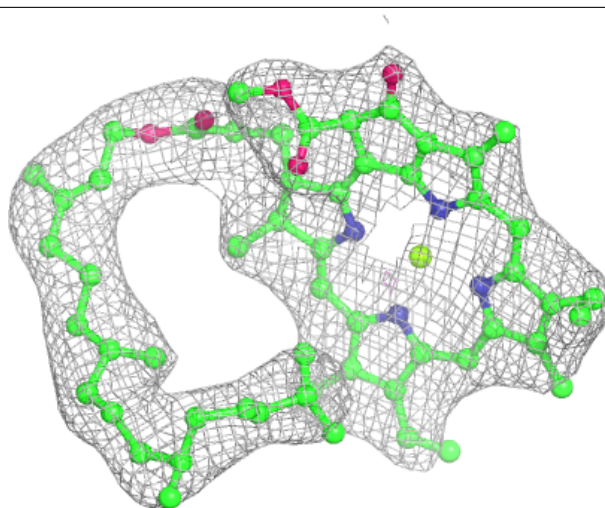
**Electron density around CLA d 402:**

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



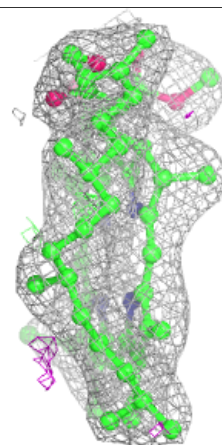
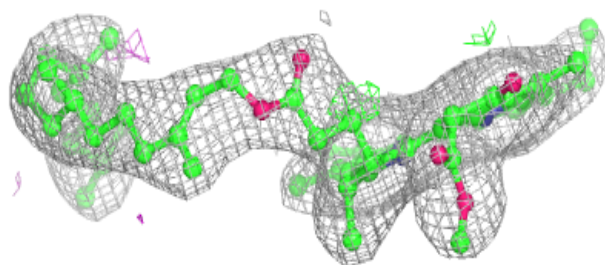
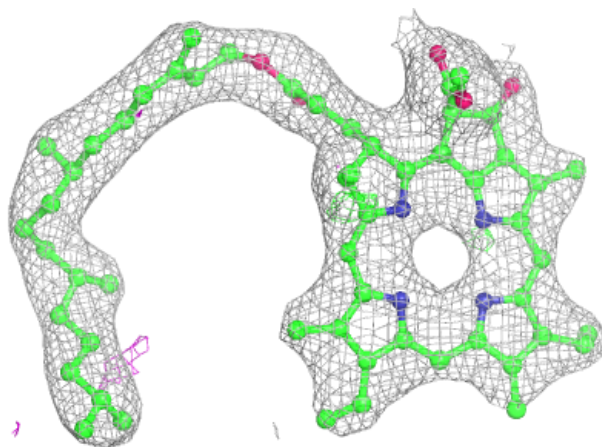
**Electron density around CLA B 616:**

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



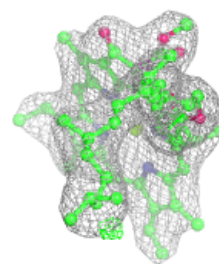
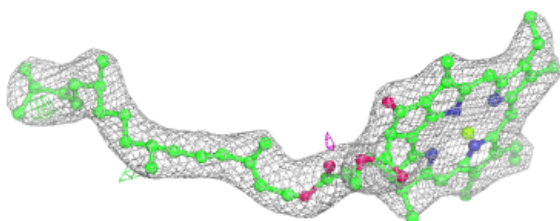
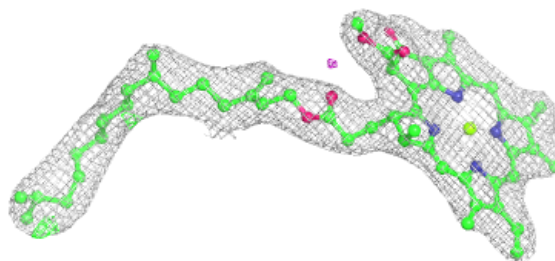
**Electron density around PHO A 406:**

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



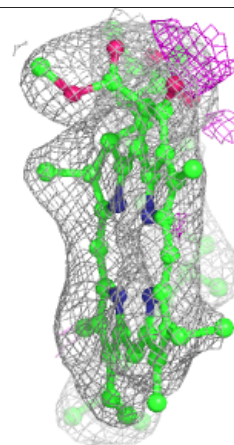
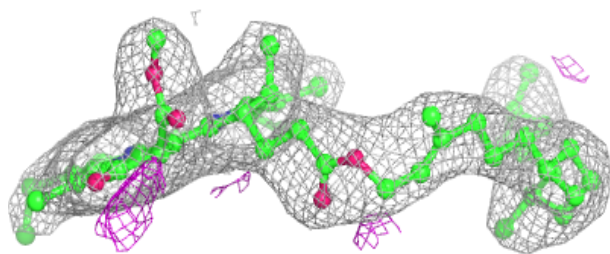
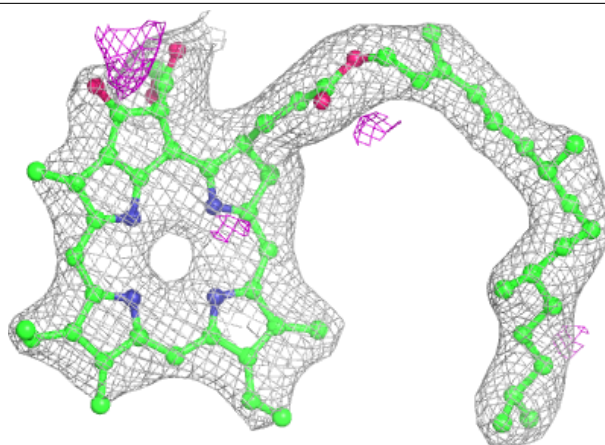
**Electron density around CLA A 404:**

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



**Electron density around PHO a 407:**

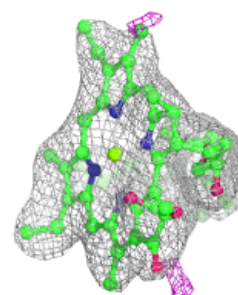
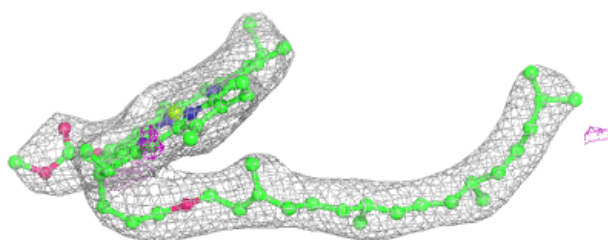
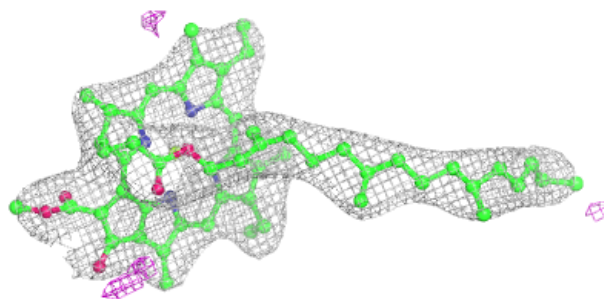
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



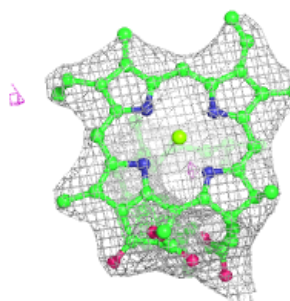
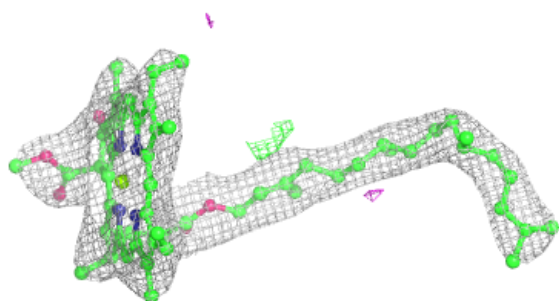
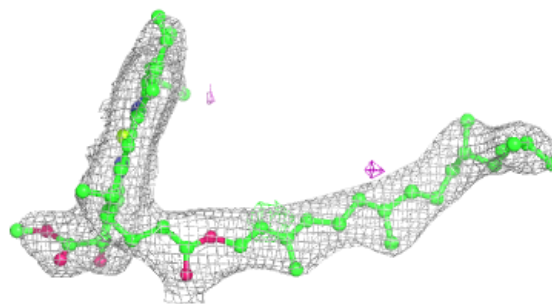


**Electron density around CLA B 609:**

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

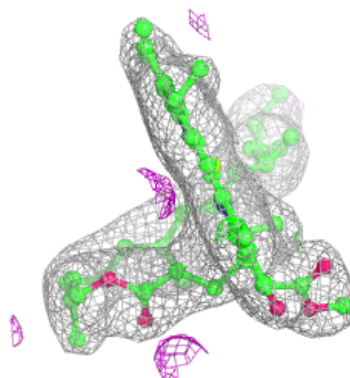
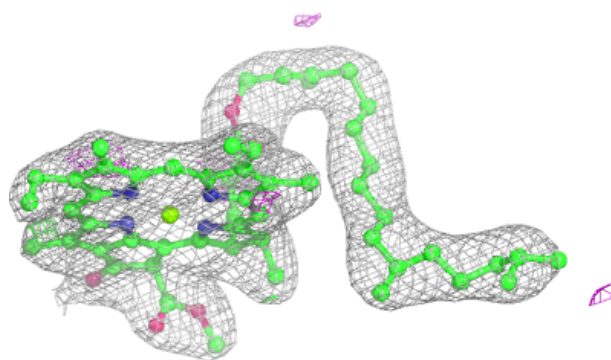
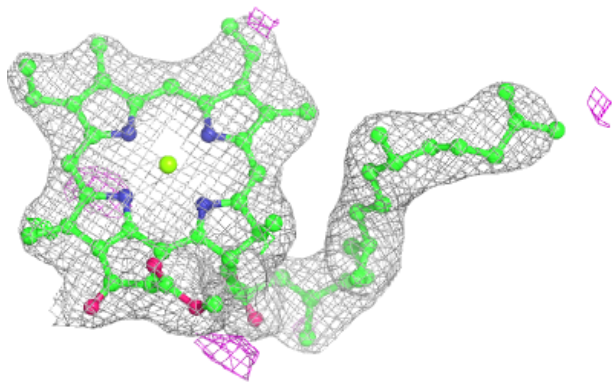
**Electron density around CLA B 606:**

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



**Electron density around CLA D 401:**

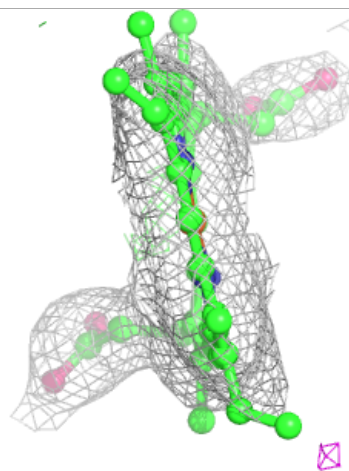
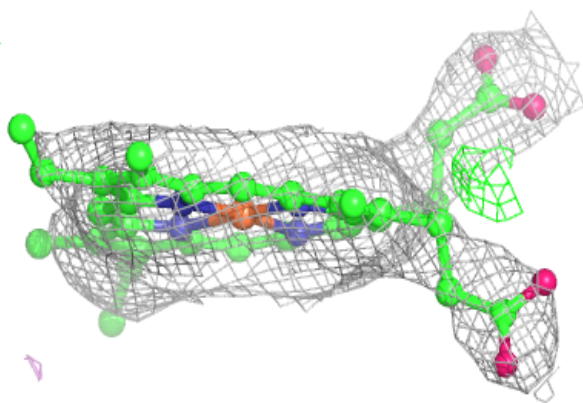
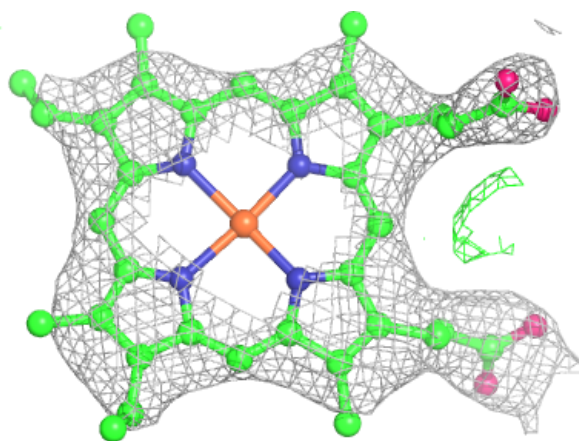
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





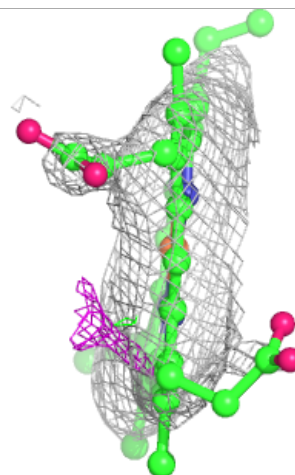
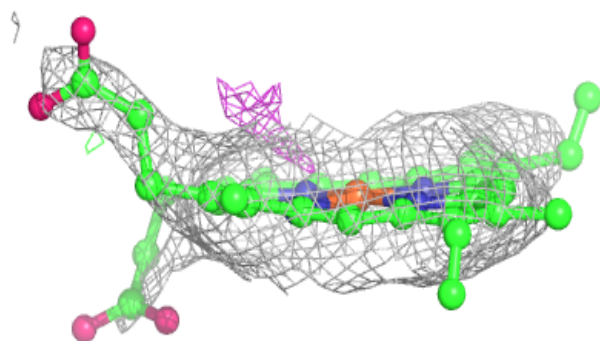
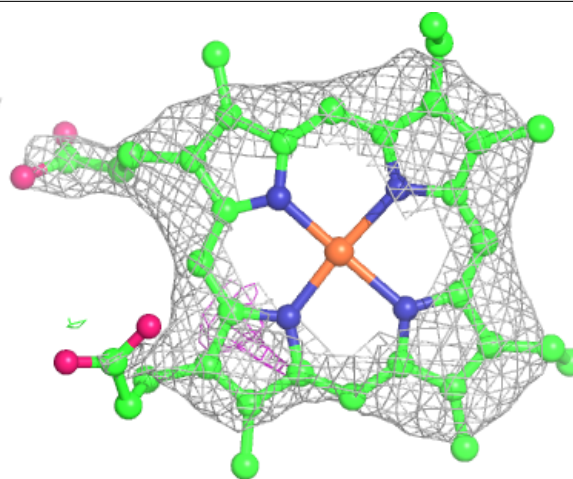
**Electron density around HEM E 103:**

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



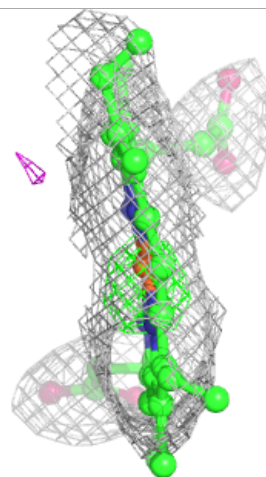
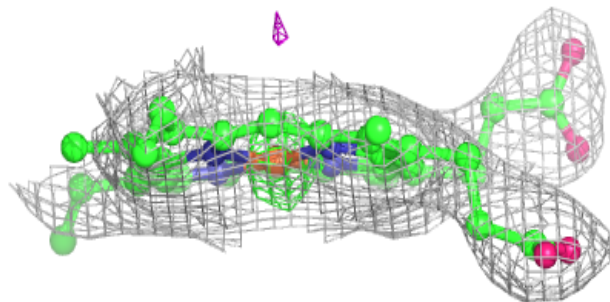
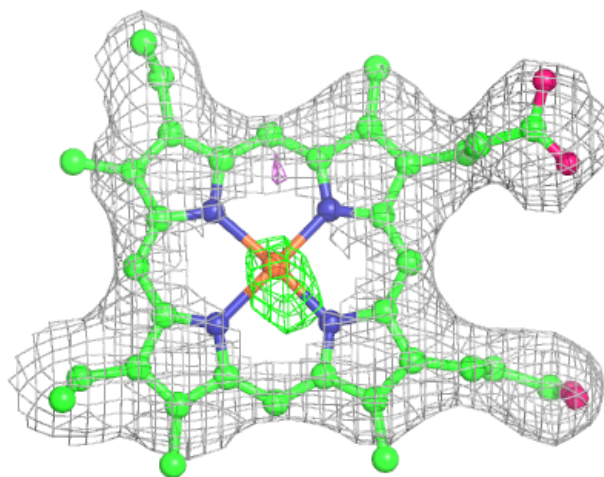
**Electron density around HEM e 103:**

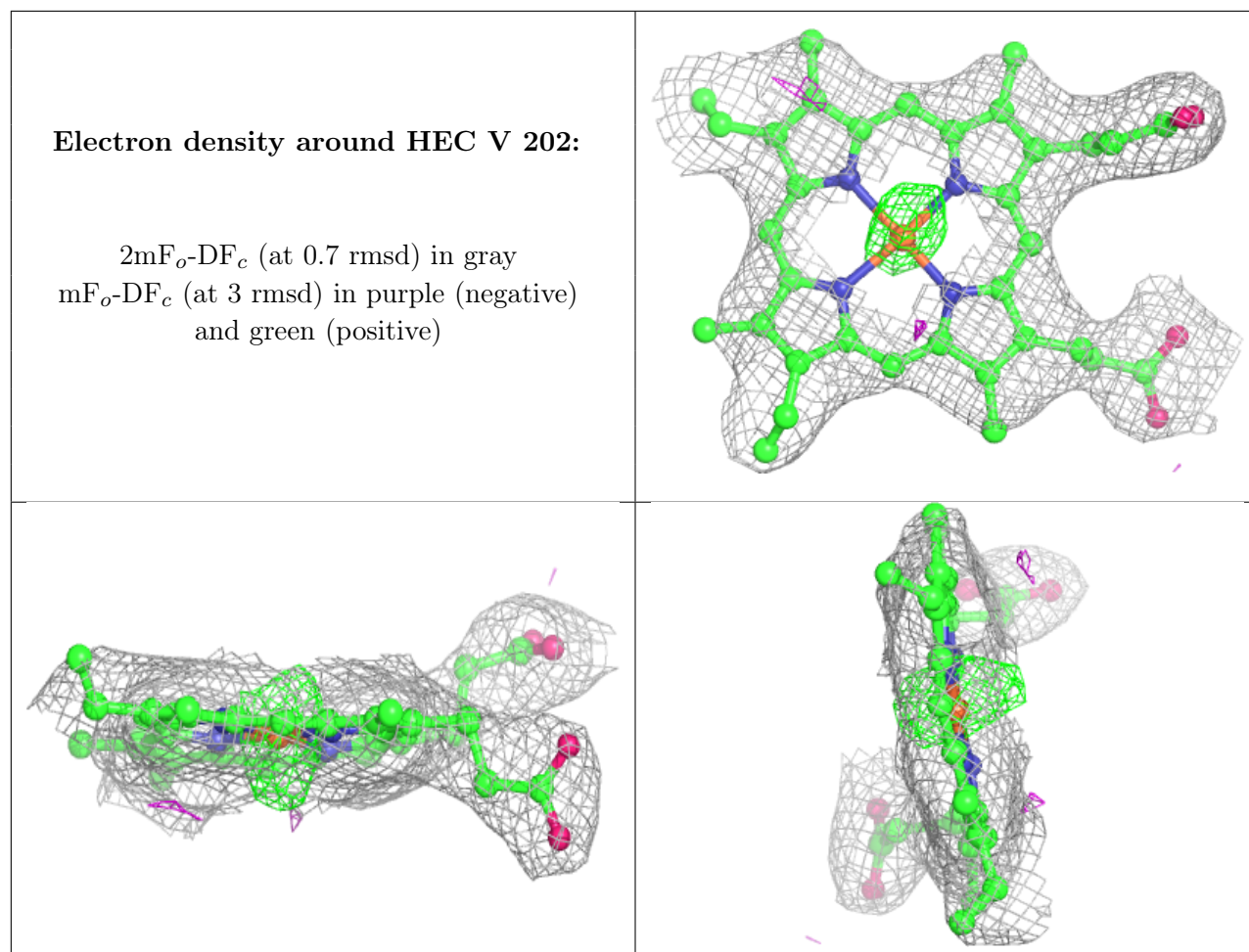
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC v 201:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.