



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2020 – 05:09 PM BST

PDB ID : 5MX2  
Title : Photosystem II depleted of the Mn<sub>4</sub>CaO<sub>5</sub> cluster at 2.55 Å resolution  
Authors : Zhang, M.; Bommer, M.; Chatterjee, R.; Hussain, R.; Kern, J.; Yano, J.; Dau, H.; Dobbek, H.; Zouni, A.  
Deposited on : 2017-01-20  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

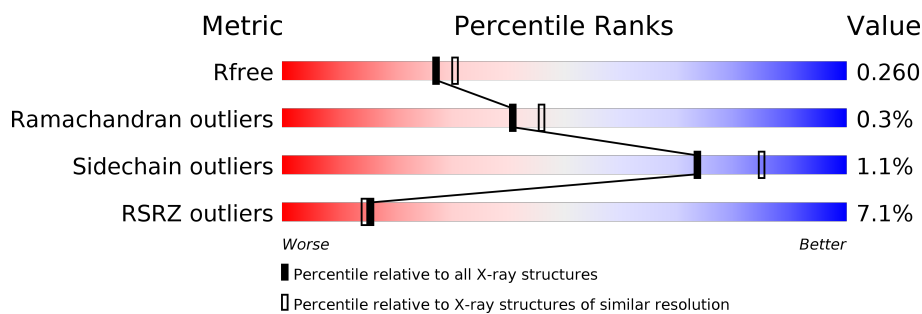
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



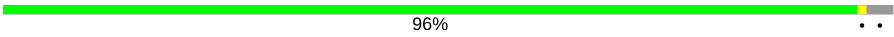
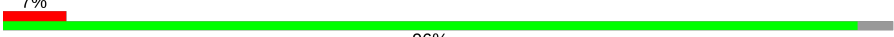

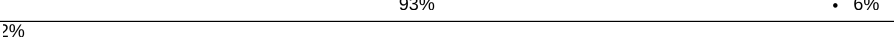


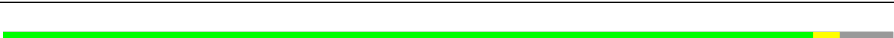
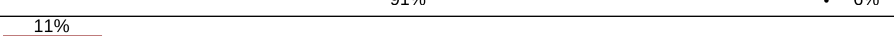



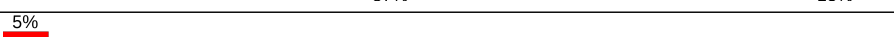





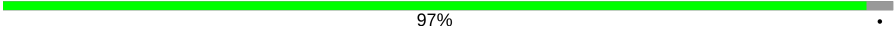






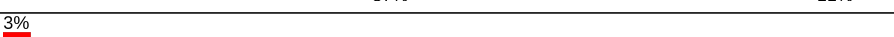
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
1	a	344	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
2	B	510	<div> <div>5%</div> <div>98%</div> <div>.</div> </div>
2	b	510	<div> <div>7%</div> <div>98%</div> <div>..</div> </div>
3	C	461	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>
3	c	461	<div> <div>3%</div> <div>95%</div> <div>..</div> </div>
4	D	352	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	

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Mol	Chain	Length	Quality of chain
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	412	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 50407 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 protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	0	0
			3980	2611	665	691	13			
2	b	503	Total	C	N	O	S	0	0	0
			3958	2599	657	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	13			
3	c	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			656	428	106	122			
5	e	79	Total	C	N	O	0	0	0
			645	422	104	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	62	Total	C	N	O	S	0	0	0
			493	330	79	82	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			
8	i	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			
9	j	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	35	Total	C	N	O	0	0	0
			272	192	37	43			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			284	198	41	45			

- 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 reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			
12	m	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1859	1162	314	379	4			
13	o	241	Total	C	N	O	S	0	0	0
			1852	1158	313	377	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	28	Total	C	N	O	S	0	0	0
			241	170	34	35	2			
14	t	29	Total	C	N	O	S	0	0	0
			249	176	35	36	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	96	Total	C	N	O	0	0	0
			765	486	128	151			

- 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 Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	21	Total	C	N	O	S	0	0	0
			155	102	28	23	2			
17	y	23	Total	C	N	O	S	0	0	0
			171	113	30	25	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			

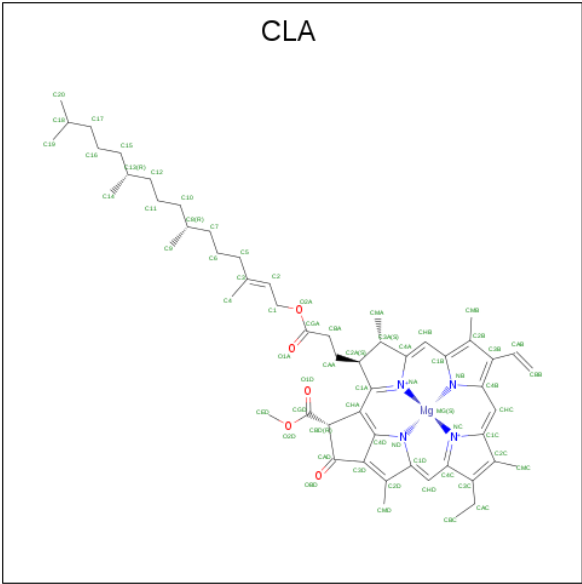
- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	35	Total	C	N	O		0	0	0
			282	191	49	42				
20	r	32	Total	C	N	O		0	0	0
			257	176	45	36				

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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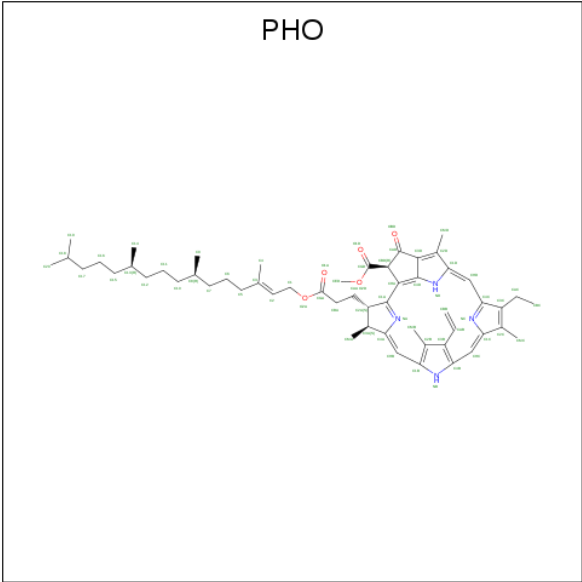
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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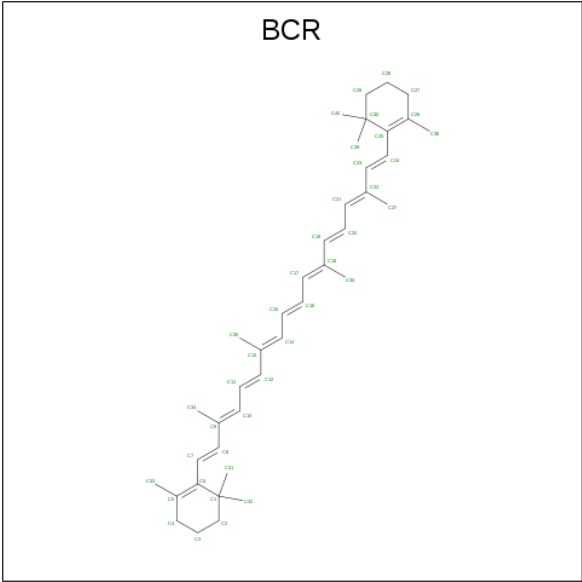
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



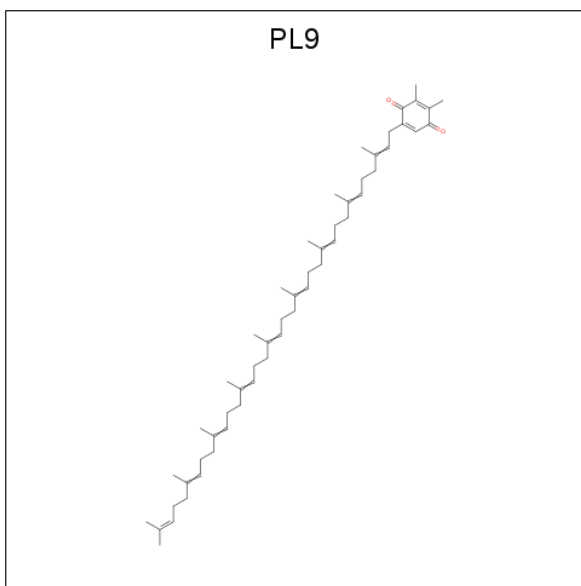
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



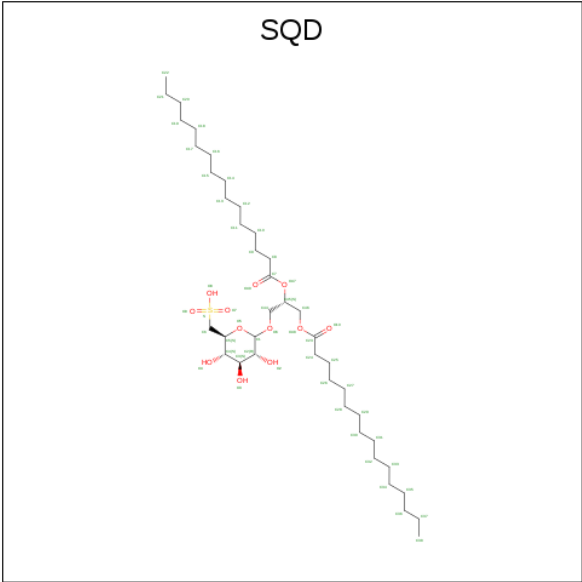
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total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

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



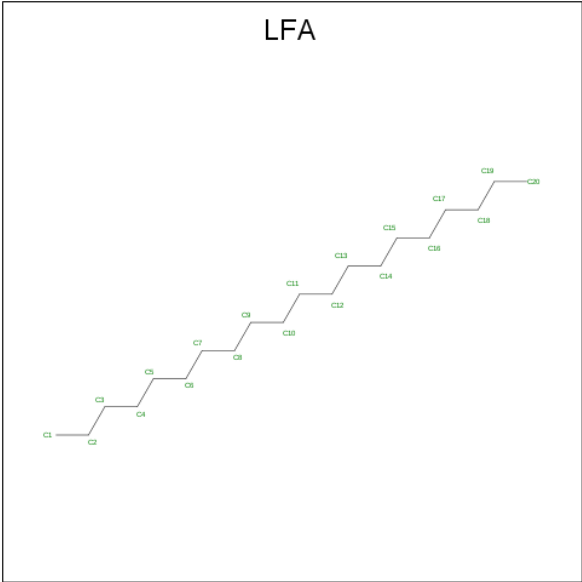
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			55	53	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	a	1	Total	C	O	0	0
			55	53	2		
25	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			48	35	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O		0	0
			50	41	9			
26	b	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 EICOSANE (three-letter code: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	1	Total	C	0	0
			14	14		
27	A	1	Total	C	0	0
			11	11		
27	B	1	Total	C	0	0
			10	10		
27	B	1	Total	C	0	0
			16	16		
27	B	1	Total	C	0	0
			13	13		
27	B	1	Total	C	0	0
			15	15		
27	B	1	Total	C	0	0
			9	9		
27	B	1	Total	C	0	0
			10	10		
27	B	1	Total	C	0	0
			14	14		
27	B	1	Total	C	0	0
			12	12		
27	C	1	Total	C	0	0
			15	15		
27	D	1	Total	C	0	0
			15	15		
27	D	1	Total	C	0	0
			8	8		
27	D	1	Total	C	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	1	Total C 14 14	0	0
27	J	1	Total C 11 11	0	0
27	M	1	Total C 10 10	0	0
27	M	1	Total C 16 16	0	0
27	T	1	Total C 12 12	0	0
27	a	1	Total C 7 7	0	0
27	b	1	Total C 15 15	0	0
27	b	1	Total C 10 10	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 16 16	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 11 11	0	0
27	b	1	Total C 9 9	0	0
27	b	1	Total C 15 15	0	0
27	c	1	Total C 9 9	0	0
27	c	1	Total C 15 15	0	0
27	d	1	Total C 15 15	0	0
27	d	1	Total C 9 9	0	0
27	d	1	Total C 16 16	0	0
27	i	1	Total C 16 16	0	0
27	i	1	Total C 7 7	0	0

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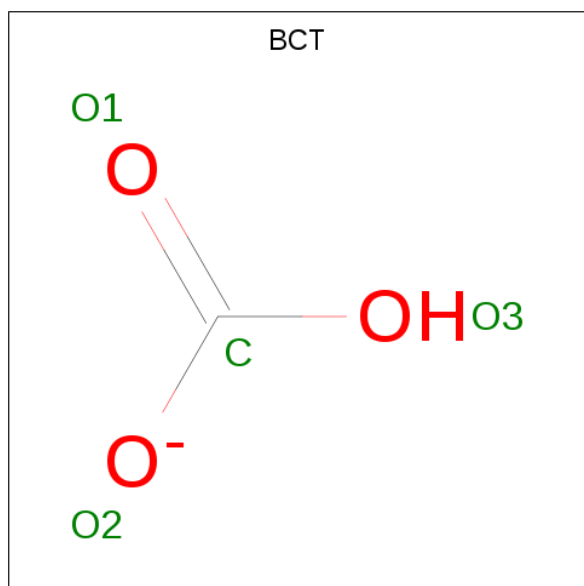
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	j	1	Total C 15 15	0	0
27	m	1	Total C 10 10	0	0
27	m	1	Total C 15 15	0	0
27	t	1	Total C 15 15	0	0

- Molecule 28 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

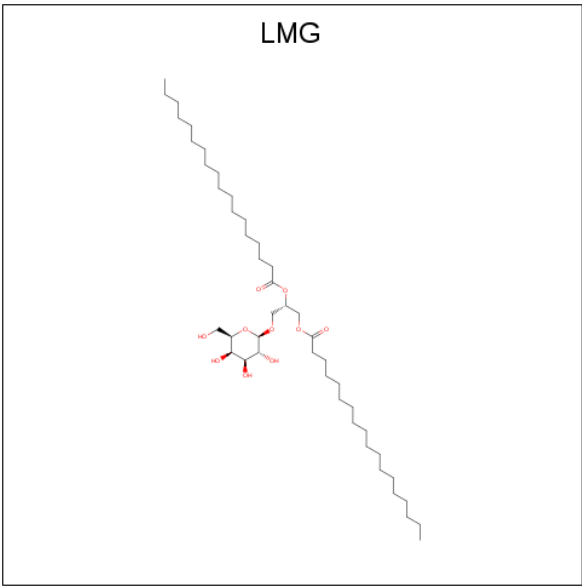
- Molecule 29 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3^-$ ).



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

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

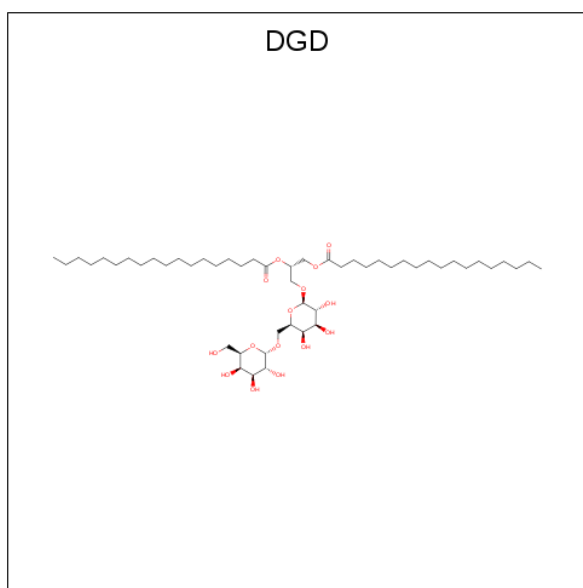
code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			51	41	10		
30	B	1	Total	C	O	0	0
			36	26	10		
30	C	1	Total	C	O	0	0
			51	41	10		
30	C	1	Total	C	O	0	0
			48	38	10		
30	C	1	Total	C	O	0	0
			44	34	10		
30	D	1	Total	C	O	0	0
			51	41	10		
30	b	1	Total	C	O	0	0
			39	29	10		
30	c	1	Total	C	O	0	0
			51	41	10		
30	c	1	Total	C	O	0	0
			51	41	10		
30	c	1	Total	C	O	0	0
			41	31	10		
30	f	1	Total	C	O	0	0
			51	41	10		
30	m	1	Total	C	O	0	0
			51	41	10		

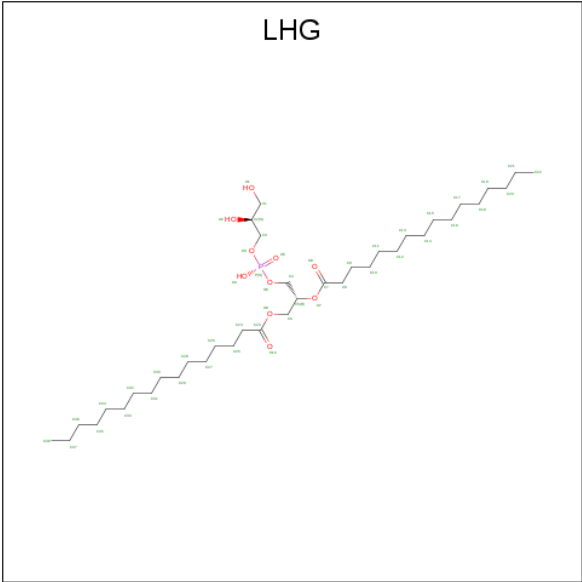
- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



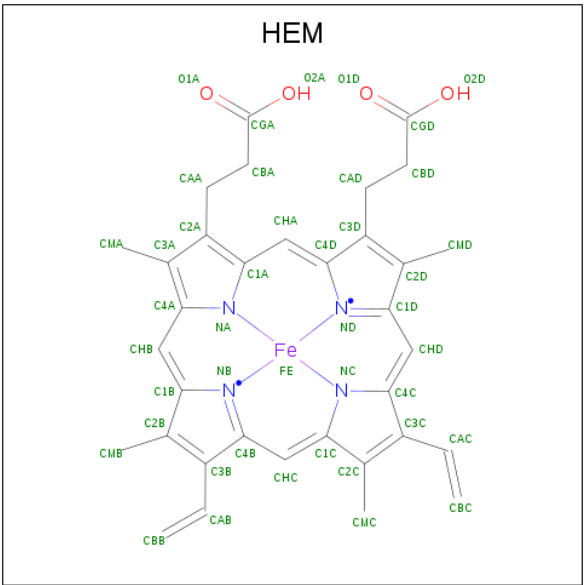
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			56	41	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	H	1	Total	C	O	0	0
			60	45	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			55	40	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 32 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
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			42	31	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	b	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		
32	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	70	Total	O	0	0
			70	70		
34	B	84	Total	O	0	0
			84	84		
34	C	62	Total	O	0	0
			62	62		
34	D	72	Total	O	0	0
			72	72		
34	E	5	Total	O	0	0
			5	5		
34	F	1	Total	O	0	0
			1	1		
34	H	17	Total	O	0	0
			17	17		
34	J	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	K	1	Total 1	O 1	0	0
34	L	5	Total 5	O 5	0	0
34	M	3	Total 3	O 3	0	0
34	O	30	Total 30	O 30	0	0
34	T	2	Total 2	O 2	0	0
34	U	2	Total 2	O 2	0	0
34	V	12	Total 12	O 12	0	0
34	X	3	Total 3	O 3	0	0
34	a	77	Total 77	O 77	0	0
34	b	72	Total 72	O 72	0	0
34	c	65	Total 65	O 65	0	0
34	d	51	Total 51	O 51	0	0
34	e	5	Total 5	O 5	0	0
34	f	2	Total 2	O 2	0	0
34	h	3	Total 3	O 3	0	0
34	l	5	Total 5	O 5	0	0
34	m	2	Total 2	O 2	0	0
34	o	25	Total 25	O 25	0	0
34	t	3	Total 3	O 3	0	0
34	u	12	Total 12	O 12	0	0
34	v	11	Total 11	O 11	0	0

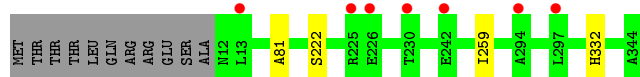
### 3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



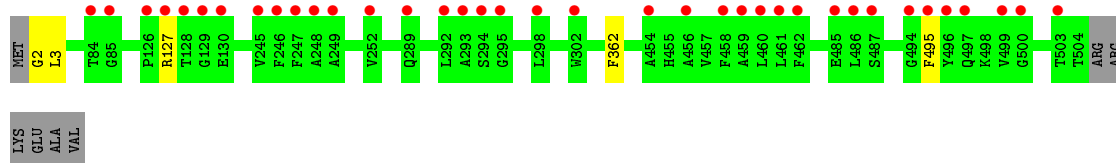
- Molecule 1: Photosystem II protein D1 1



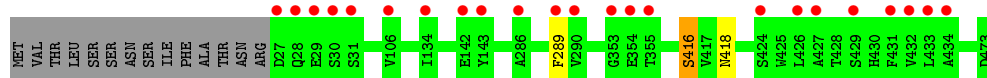
- Molecule 2: Photosystem II CP47 reaction center protein



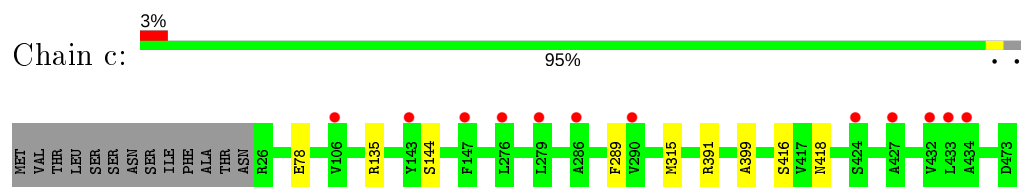
- Molecule 2: Photosystem II CP47 reaction center protein



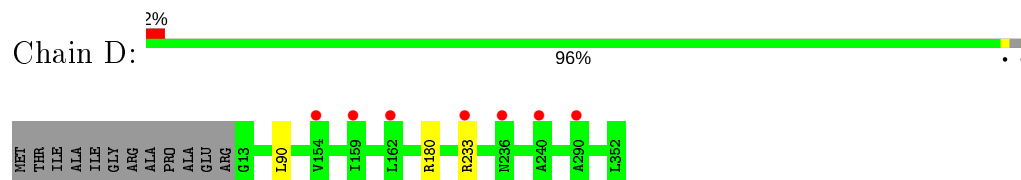
- Molecule 3: Photosystem II CP43 reaction center protein



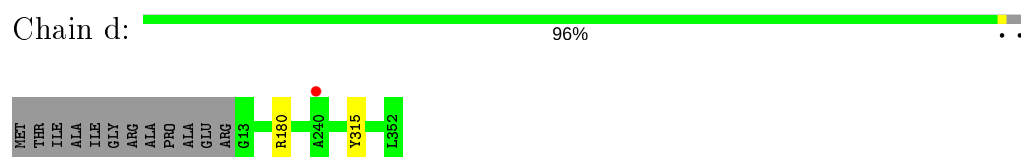
- Molecule 3: Photosystem II CP43 reaction center protein



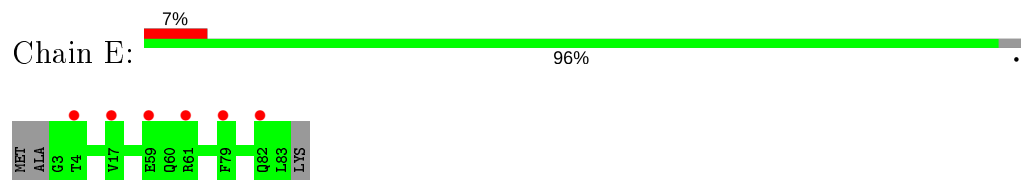
- Molecule 4: Photosystem II D2 protein



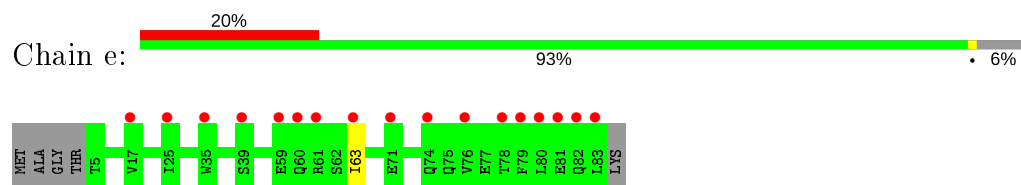
- Molecule 4: Photosystem II D2 protein



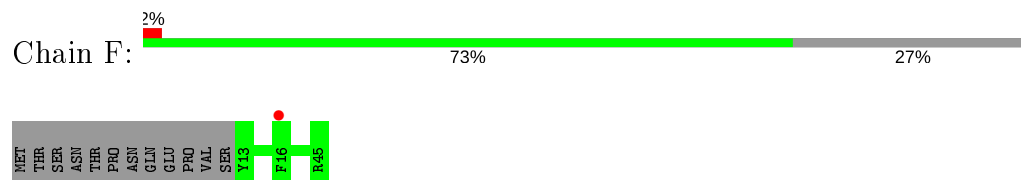
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

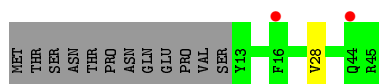


- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta





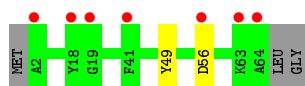
- Molecule 7: Photosystem II reaction center protein H

Chain H: 91% 6%



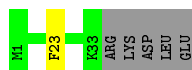
- Molecule 7: Photosystem II reaction center protein H

Chain h: 11% 92% 5%



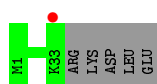
- Molecule 8: Photosystem II reaction center protein I

Chain I: 84% 13%



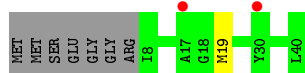
- Molecule 8: Photosystem II reaction center protein I

Chain i: 3% 87% 13%



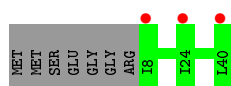
- Molecule 9: Photosystem II reaction center protein J

Chain J: 5% 80% 18%

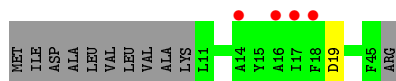
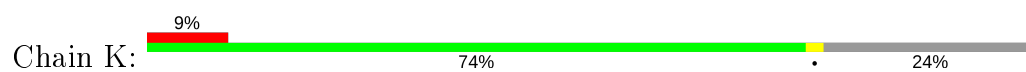


- Molecule 9: Photosystem II reaction center protein J

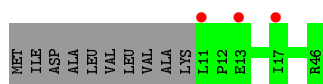
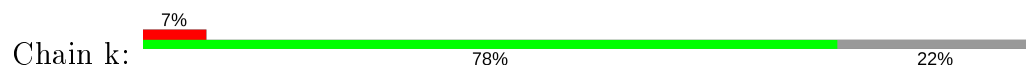
Chain j: 8% 83% 18%



- Molecule 10: Photosystem II reaction center protein K



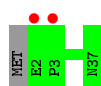
- Molecule 10: Photosystem II reaction center protein K



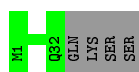
- Molecule 11: Photosystem II reaction center protein L



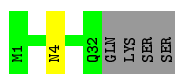
- Molecule 11: Photosystem II reaction center protein L



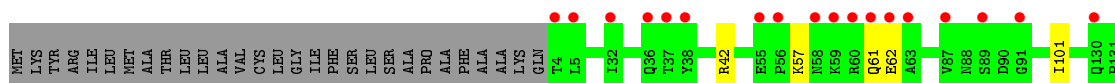
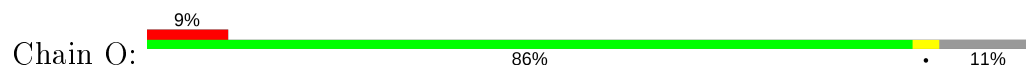
- Molecule 12: Photosystem II reaction center protein M

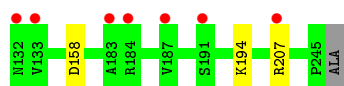


- Molecule 12: Photosystem II reaction center protein M

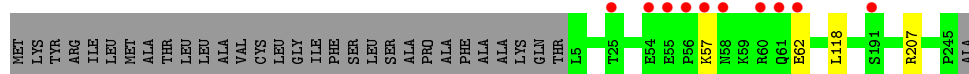
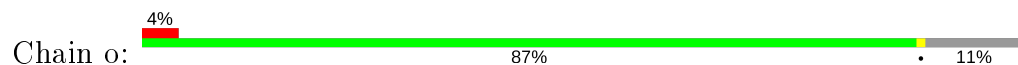


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

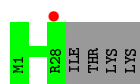
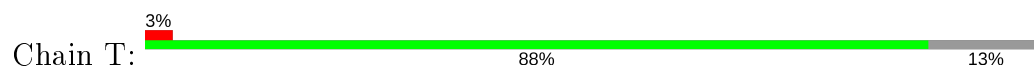




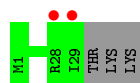
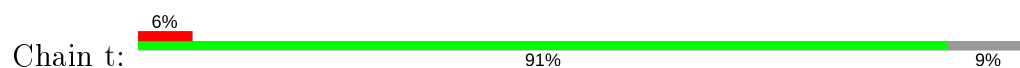
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



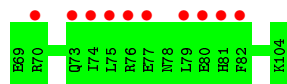
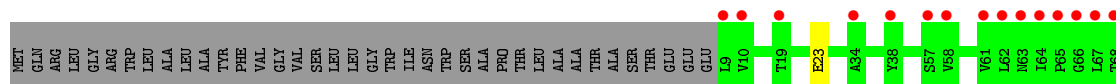
- Molecule 14: Photosystem II reaction center protein T



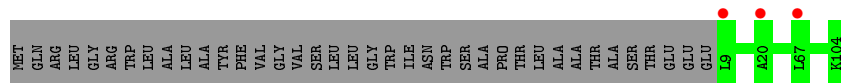
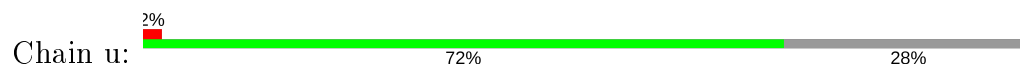
- Molecule 14: Photosystem II reaction center protein T



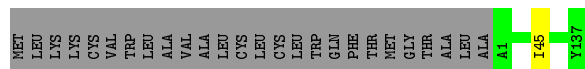
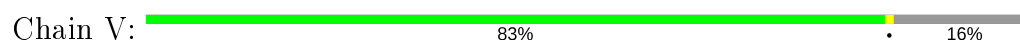
- Molecule 15: Photosystem II 12 kDa extrinsic protein



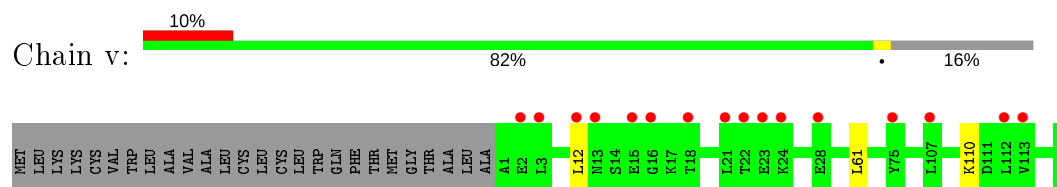
- Molecule 15: Photosystem II 12 kDa extrinsic protein



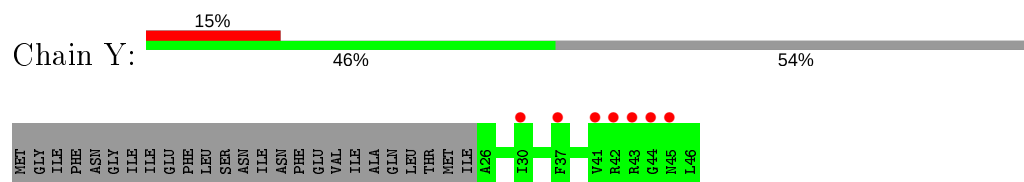
- Molecule 16: Cytochrome c-550



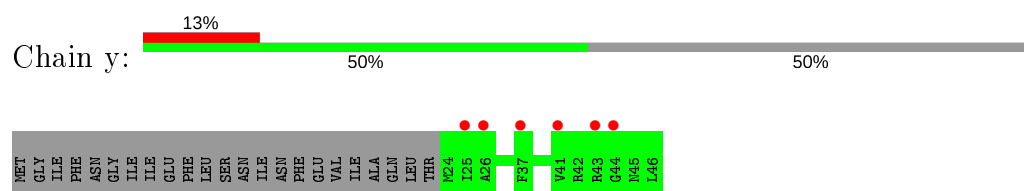
- Molecule 16: Cytochrome c-550



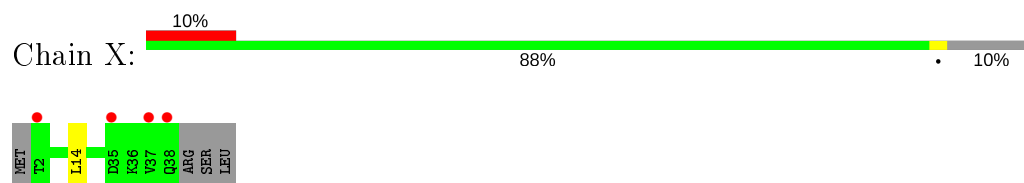
- Molecule 17: Photosystem II reaction center protein Ycf12



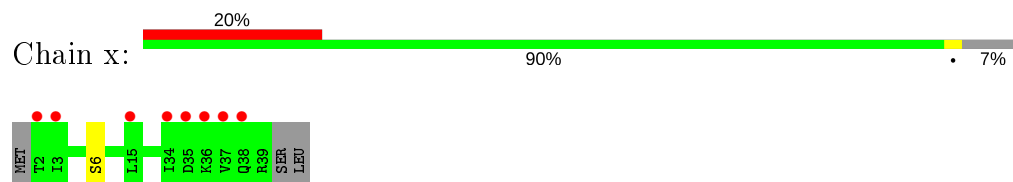
- Molecule 17: Photosystem II reaction center protein Ycf12



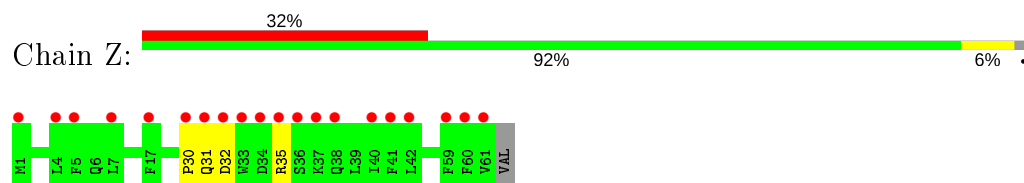
- Molecule 18: Photosystem II reaction center X protein



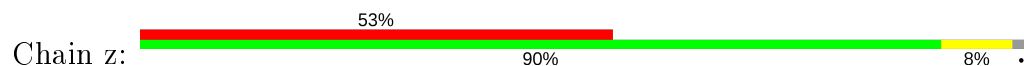
- Molecule 18: Photosystem II reaction center X protein

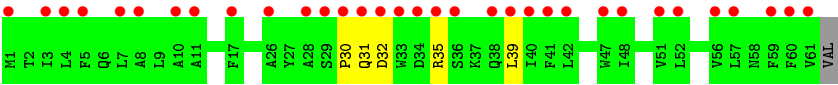


- Molecule 19: Photosystem II reaction center protein Z

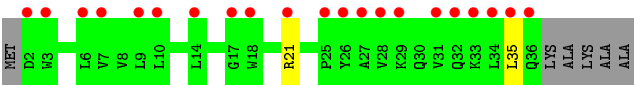
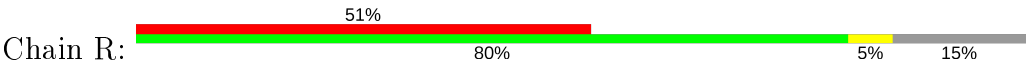


- Molecule 19: Photosystem II reaction center protein Z

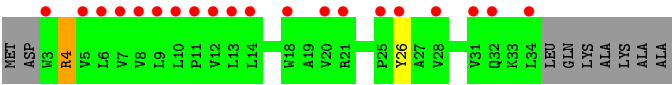




● Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.33Å 219.62Å 304.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.20 49.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.65-2.20) 92.6 (49.65-2.20)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.211 , 0.260 0.212 , 0.260	Depositor DCC
$R_{free}$ test set	18229 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LFA, DGD, CL, CLA, PL9, FE, HEM, BCT, PHO, SQD, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	0/2702	0.52	0/3685
1	a	0.53	0/2702	0.51	0/3685
2	B	0.54	0/4120	0.54	1/5614 (0.0%)
2	b	0.51	1/4098 (0.0%)	0.53	2/5586 (0.0%)
3	C	0.48	0/3568	0.51	0/4858
3	c	0.50	2/3579 (0.1%)	0.54	1/4872 (0.0%)
4	D	0.57	0/2801	0.54	1/3818 (0.0%)
4	d	0.52	0/2801	0.53	0/3818
5	E	0.41	0/675	0.48	0/922
5	e	0.58	1/664 (0.2%)	0.52	0/907
6	F	0.41	0/278	0.44	0/379
6	f	0.40	0/278	0.44	0/379
7	H	0.50	0/506	0.51	0/690
7	h	0.43	0/511	0.50	0/697
8	I	0.48	0/273	0.49	0/370
8	i	0.47	0/273	0.48	0/370
9	J	0.51	0/244	0.46	0/332
9	j	0.38	0/244	0.47	0/332
10	K	0.38	0/282	0.46	0/391
10	k	0.42	0/294	0.48	0/405
11	L	0.55	0/303	0.55	0/412
11	l	0.56	0/303	0.50	0/412
12	M	0.52	0/252	0.50	0/344
12	m	0.45	0/252	0.47	0/344
13	O	0.45	0/1890	0.56	1/2564 (0.0%)
13	o	0.46	0/1883	0.54	0/2554
14	T	0.60	0/250	0.41	0/338
14	t	0.51	0/258	0.45	0/349
15	U	0.33	0/776	0.49	0/1052
15	u	0.45	0/776	0.52	0/1052
16	V	0.43	0/1085	0.50	0/1473
16	v	0.40	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.28	0/156	0.43	0/207
17	y	0.31	0/172	0.47	0/228
18	X	0.38	0/273	0.45	0/370
18	x	0.31	0/284	0.43	0/384
19	Z	0.31	0/482	0.49	0/659
19	z	0.36	0/482	0.66	1/659 (0.2%)
20	R	0.31	0/288	0.44	0/395
20	r	0.37	0/263	0.69	1/361 (0.3%)
All	All	0.49	4/42406 (0.0%)	0.52	8/57740 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
19	z	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	-10.84	1.13	1.34
3	c	399	ALA	C-N	-7.65	1.19	1.34
2	b	2	GLY	C-N	-5.82	1.20	1.34
3	c	78	GLU	C-N	-5.37	1.21	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	135	ARG	NE-CZ-NH1	9.25	124.93	120.30
19	z	39	LEU	CA-CB-CG	9.14	136.31	115.30
2	B	476	ARG	NE-CZ-NH2	6.77	123.69	120.30
4	D	233	ARG	NE-CZ-NH1	6.47	123.54	120.30
20	r	4	ARG	NE-CZ-NH2	6.45	123.53	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	81	ALA	Peptide
19	z	35	ARG	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	41	46
1	a	331/344 (96%)	319 (96%)	11 (3%)	1 (0%)	41	46
2	B	503/510 (99%)	478 (95%)	25 (5%)	0	100	100
2	b	501/510 (98%)	479 (96%)	22 (4%)	0	100	100
3	C	445/461 (96%)	433 (97%)	11 (2%)	1 (0%)	47	55
3	c	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	47	55
4	D	338/352 (96%)	327 (97%)	11 (3%)	0	100	100
4	d	338/352 (96%)	321 (95%)	17 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
7	H	60/66 (91%)	56 (93%)	4 (7%)	0	100	100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100	100
8	I	31/38 (82%)	30 (97%)	1 (3%)	0	100	100
8	i	31/38 (82%)	31 (100%)	0	0	100	100
9	J	31/40 (78%)	30 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
10	K	33/46 (72%)	32 (97%)	1 (3%)	0	100	100
10	k	34/46 (74%)	33 (97%)	1 (3%)	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	30/36 (83%)	30 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	222 (92%)	15 (6%)	3 (1%)	12	9
13	o	239/272 (88%)	223 (93%)	14 (6%)	2 (1%)	19	19
14	T	26/32 (81%)	26 (100%)	0	0	100	100
14	t	27/32 (84%)	25 (93%)	2 (7%)	0	100	100
15	U	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
15	u	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	22
16	v	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
17	Y	19/46 (41%)	18 (95%)	1 (5%)	0	100	100
17	y	21/46 (46%)	21 (100%)	0	0	100	100
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	59/62 (95%)	54 (92%)	2 (3%)	3 (5%)	2	0
19	z	59/62 (95%)	53 (90%)	3 (5%)	3 (5%)	2	0
20	R	33/41 (80%)	32 (97%)	0	1 (3%)	4	2
20	r	30/41 (73%)	30 (100%)	0	0	100	100
All	All	5173/5700 (91%)	4951 (96%)	205 (4%)	17 (0%)	41	46

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	32	ASP
19	Z	35	ARG
3	c	416	SER
19	z	30	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	268 (99%)	2 (1%)	84	91
1	a	270/280 (96%)	268 (99%)	2 (1%)	84	91
2	B	403/407 (99%)	400 (99%)	3 (1%)	84	91
2	b	401/407 (98%)	399 (100%)	2 (0%)	88	94
3	C	349/362 (96%)	346 (99%)	3 (1%)	78	88
3	c	350/362 (97%)	345 (99%)	5 (1%)	67	80
4	D	275/283 (97%)	273 (99%)	2 (1%)	84	91
4	d	275/283 (97%)	273 (99%)	2 (1%)	84	91
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	26 (96%)	1 (4%)	34	43
7	H	53/55 (96%)	51 (96%)	2 (4%)	33	42
7	h	53/55 (96%)	51 (96%)	2 (4%)	33	42
8	I	30/35 (86%)	29 (97%)	1 (3%)	38	49
8	i	30/35 (86%)	30 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	29	36
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	28/37 (76%)	27 (96%)	1 (4%)	35	45
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	28 (97%)	1 (3%)	37	47
13	O	206/228 (90%)	202 (98%)	4 (2%)	57	71
13	o	205/228 (90%)	203 (99%)	2 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	25/29 (86%)	25 (100%)	0	100	100
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	82 (99%)	1 (1%)	71	83
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	114 (97%)	3 (3%)	46	58
17	Y	15/37 (40%)	15 (100%)	0	100	100
17	y	17/37 (46%)	17 (100%)	0	100	100
18	X	30/34 (88%)	29 (97%)	1 (3%)	38	49
18	x	31/34 (91%)	30 (97%)	1 (3%)	39	50
19	Z	51/52 (98%)	50 (98%)	1 (2%)	55	69
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	30/33 (91%)	29 (97%)	1 (3%)	38	49
20	r	27/33 (82%)	25 (93%)	2 (7%)	13	14
All	All	4297/4660 (92%)	4251 (99%)	46 (1%)	73	85

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	X	14	LEU
2	b	495	PHE
18	x	6	SER
19	Z	31	GLN
1	a	332	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	312	ASN
3	c	332	GLN
13	o	200	ASN
2	b	282	GLN
3	c	418	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
24	BCR	C	515	-	41,41,41	0.83	1 (2%)	56,56,56	1.80	17 (30%)
25	PL9	a	409	-	55,55,55	0.59	2 (3%)	68,69,69	1.78	18 (26%)
27	LFA	b	622	-	9,9,19	0.12	0	8,8,18	0.32	0
27	LFA	B	620	-	9,9,19	0.14	0	8,8,18	0.43	0
22	CLA	b	606	-	59,73,73	1.75	6 (10%)	67,113,113	1.53	9 (13%)
22	CLA	b	614	-	59,73,73	1.54	7 (11%)	67,113,113	1.39	8 (11%)
24	BCR	K	102	-	41,41,41	0.85	1 (2%)	56,56,56	1.90	12 (21%)
26	SQD	a	410	-	53,54,54	1.13	4 (7%)	62,65,65	1.37	11 (17%)
30	LMG	D	409	-	51,51,55	0.95	2 (3%)	59,59,63	0.94	2 (3%)
23	PHO	A	405	-	67,69,69	0.79	3 (4%)	85,99,99	1.02	5 (5%)
22	CLA	b	617	-	59,73,73	1.72	6 (10%)	67,113,113	1.31	7 (10%)
24	BCR	c	515	-	41,41,41	0.85	2 (4%)	56,56,56	1.39	6 (10%)
24	BCR	k	101	-	41,41,41	0.86	1 (2%)	56,56,56	1.83	13 (23%)
27	LFA	T	102	-	11,11,19	0.11	0	10,10,18	0.42	0
26	SQD	D	411	-	42,43,54	1.27	4 (9%)	51,54,65	1.80	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	606	34	59,73,73	1.68	8 (13%)	67,113,113	1.54	9 (13%)
31	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.23	8 (10%)
25	PL9	A	408	-	55,55,55	0.63	2 (3%)	68,69,69	1.98	19 (27%)
27	LFA	b	602	-	14,14,19	0.10	0	13,13,18	0.44	0
22	CLA	C	512	3	59,73,73	1.71	7 (11%)	67,113,113	1.35	8 (11%)
33	HEM	v	201	16	27,50,50	1.60	2 (7%)	17,82,82	2.21	4 (23%)
22	CLA	B	611	-	59,73,73	1.67	5 (8%)	67,113,113	1.31	7 (10%)
27	LFA	d	409	-	8,8,19	0.12	0	7,7,18	0.26	0
31	DGD	c	517	-	56,56,67	0.88	2 (3%)	70,70,81	1.10	5 (7%)
22	CLA	C	510	-	59,73,73	1.64	7 (11%)	67,113,113	1.33	8 (11%)
22	CLA	C	503	-	59,73,73	1.69	6 (10%)	67,113,113	1.28	11 (16%)
22	CLA	b	610	-	59,73,73	1.65	9 (15%)	67,113,113	1.45	7 (10%)
27	LFA	B	624	-	14,14,19	0.08	0	13,13,18	0.31	0
25	PL9	D	405	-	55,55,55	0.70	3 (5%)	68,69,69	1.64	17 (25%)
33	HEM	V	201	16	27,50,50	1.58	2 (7%)	17,82,82	2.02	5 (29%)
22	CLA	B	615	-	59,73,73	1.78	7 (11%)	67,113,113	1.53	6 (8%)
24	BCR	B	617	-	41,41,41	0.86	2 (4%)	56,56,56	1.61	12 (21%)
33	HEM	e	102	5,6	27,50,50	1.50	2 (7%)	17,82,82	1.47	3 (17%)
22	CLA	b	613	-	59,73,73	1.67	6 (10%)	67,113,113	1.39	6 (8%)
22	CLA	d	403	-	59,73,73	1.60	6 (10%)	67,113,113	1.35	8 (11%)
30	LMG	C	522	-	44,44,55	1.05	3 (6%)	52,52,63	1.59	8 (15%)
24	BCR	t	102	-	41,41,41	0.86	1 (2%)	56,56,56	1.93	14 (25%)
30	LMG	C	501	-	51,51,55	0.88	2 (3%)	59,59,63	1.09	3 (5%)
27	LFA	J	101	-	10,10,19	0.11	0	9,9,18	0.37	0
30	LMG	f	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	5 (8%)
22	CLA	b	605	-	59,73,73	1.75	8 (13%)	67,113,113	1.36	6 (8%)
32	LHG	D	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.19	4 (7%)
27	LFA	B	625	-	8,8,19	0.10	0	7,7,18	0.31	0
22	CLA	B	612	-	59,73,73	1.68	8 (13%)	67,113,113	1.35	7 (10%)
24	BCR	H	102	-	41,41,41	0.76	0	56,56,56	1.87	14 (25%)
22	CLA	B	613	-	59,73,73	1.95	8 (13%)	67,113,113	1.40	6 (8%)
27	LFA	b	623	-	11,11,19	0.10	0	10,10,18	0.39	0
22	CLA	b	603	34	59,73,73	1.82	7 (11%)	67,113,113	1.30	8 (11%)
22	CLA	H	101	34	59,73,73	1.81	7 (11%)	67,113,113	1.28	5 (7%)
27	LFA	A	410	-	13,13,19	0.10	0	12,12,18	0.33	0
27	LFA	C	521	-	14,14,19	0.08	0	13,13,18	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	505	34	59,73,73	1.49	5 (8%)	67,113,113	1.27	10 (14%)
22	CLA	B	605	-	59,73,73	1.81	6 (10%)	67,113,113	1.45	6 (8%)
29	BCT	A	415	28	0,3,3	0.00	-	0,3,3	0.00	-
31	DGD	c	516	-	63,63,67	0.83	3 (4%)	77,77,81	1.13	6 (7%)
26	SQD	A	409	-	53,54,54	1.12	4 (7%)	62,65,65	1.65	11 (17%)
22	CLA	C	513	-	59,73,73	1.80	8 (13%)	67,113,113	1.25	9 (13%)
27	LFA	d	408	-	14,14,19	0.10	0	13,13,18	0.42	0
22	CLA	c	514	-	59,73,73	1.69	8 (13%)	67,113,113	1.36	9 (13%)
24	BCR	A	407	-	41,41,41	0.83	0	56,56,56	1.57	13 (23%)
27	LFA	b	629	-	8,8,19	0.11	0	7,7,18	0.32	0
24	BCR	K	101	-	41,41,41	0.79	0	56,56,56	1.64	12 (21%)
24	BCR	D	404	-	41,41,41	0.90	2 (4%)	56,56,56	1.89	13 (23%)
22	CLA	a	407	-	59,73,73	1.63	7 (11%)	67,113,113	1.31	9 (13%)
22	CLA	b	615	-	59,73,73	1.90	10 (16%)	67,113,113	1.36	8 (11%)
27	LFA	i	101	-	15,15,19	0.10	0	14,14,18	0.38	0
24	BCR	h	101	-	41,41,41	0.78	0	56,56,56	1.83	14 (25%)
27	LFA	M	101	-	9,9,19	0.15	0	8,8,18	0.64	0
24	BCR	b	620	-	41,41,41	0.78	0	56,56,56	1.51	9 (16%)
30	LMG	B	619	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	2 (3%)
22	CLA	c	507	-	59,73,73	1.77	8 (13%)	67,113,113	1.48	7 (10%)
22	CLA	A	406	-	59,73,73	1.75	8 (13%)	67,113,113	1.29	8 (11%)
30	LMG	c	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	6 (10%)
22	CLA	c	504	-	59,73,73	1.91	7 (11%)	67,113,113	1.32	8 (11%)
24	BCR	C	516	-	41,41,41	0.98	3 (7%)	56,56,56	1.73	10 (17%)
22	CLA	b	607	-	59,73,73	2.00	8 (13%)	67,113,113	1.31	7 (10%)
22	CLA	b	608	-	59,73,73	1.78	8 (13%)	67,113,113	1.39	8 (11%)
23	PHO	a	414	-	67,69,69	0.76	2 (2%)	85,99,99	0.96	4 (4%)
23	PHO	D	401	-	67,69,69	0.79	2 (2%)	85,99,99	0.98	5 (5%)
24	BCR	B	616	-	41,41,41	0.85	1 (2%)	56,56,56	1.71	12 (21%)
22	CLA	c	502	-	59,73,73	1.73	7 (11%)	67,113,113	1.44	8 (11%)
27	LFA	c	521	-	14,14,19	0.08	0	13,13,18	0.35	0
30	LMG	c	501	-	51,51,55	0.86	2 (3%)	59,59,63	1.24	4 (6%)
22	CLA	a	404	-	59,73,73	1.60	7 (11%)	67,113,113	1.47	7 (10%)
33	HEM	E	102	5,6	27,50,50	1.57	2 (7%)	17,82,82	2.03	5 (29%)
22	CLA	a	405	34	59,73,73	1.70	8 (13%)	67,113,113	1.29	8 (11%)
22	CLA	B	607	-	59,73,73	1.89	7 (11%)	67,113,113	1.24	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	507	-	59,73,73	1.76	8 (13%)	67,113,113	1.46	7 (10%)
26	SQD	a	412	-	50,50,54	0.89	2 (4%)	58,58,65	1.17	6 (10%)
27	LFA	a	411	-	6,6,19	0.11	0	5,5,18	0.21	0
27	LFA	M	102	-	15,15,19	0.17	0	14,14,18	0.65	0
23	PHO	a	406	-	67,69,69	0.74	2 (2%)	85,99,99	1.02	6 (7%)
32	LHG	d	406	-	48,48,48	0.92	4 (8%)	51,54,54	1.16	4 (7%)
26	SQD	A	411	-	53,54,54	1.14	4 (7%)	62,65,65	1.34	8 (12%)
22	CLA	b	611	-	59,73,73	1.79	9 (15%)	67,113,113	1.38	7 (10%)
27	LFA	b	625	-	15,15,19	0.09	0	14,14,18	0.39	0
22	CLA	B	601	-	59,73,73	1.94	6 (10%)	67,113,113	1.41	6 (8%)
31	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	1.04	2 (2%)
22	CLA	C	514	-	59,73,73	1.62	7 (11%)	67,113,113	1.35	9 (13%)
27	LFA	c	520	-	8,8,19	0.11	0	7,7,18	0.37	0
22	CLA	B	603	-	59,73,73	1.71	4 (6%)	67,113,113	1.45	8 (11%)
27	LFA	b	627	-	10,10,19	0.10	0	9,9,18	0.35	0
22	CLA	B	614	-	59,73,73	1.77	7 (11%)	67,113,113	1.45	8 (11%)
27	LFA	D	410	-	14,14,19	0.09	0	13,13,18	0.25	0
26	SQD	b	601	-	53,54,54	1.14	4 (7%)	62,65,65	1.53	13 (20%)
22	CLA	B	604	-	59,73,73	1.99	5 (8%)	67,113,113	1.33	6 (8%)
22	CLA	A	403	-	59,73,73	1.73	7 (11%)	67,113,113	1.54	6 (8%)
22	CLA	d	402	-	59,73,73	1.63	6 (10%)	67,113,113	1.25	5 (7%)
22	CLA	c	513	-	59,73,73	1.72	7 (11%)	67,113,113	1.28	8 (11%)
22	CLA	c	510	-	59,73,73	1.67	7 (11%)	67,113,113	1.31	7 (10%)
31	DGD	H	103	-	61,61,67	0.84	2 (3%)	75,75,81	1.19	5 (6%)
22	CLA	C	502	-	59,73,73	1.67	8 (13%)	67,113,113	1.49	8 (11%)
22	CLA	c	512	3	59,73,73	1.64	7 (11%)	67,113,113	1.40	9 (13%)
32	LHG	D	407	-	48,48,48	0.86	3 (6%)	51,54,54	1.17	4 (7%)
24	BCR	d	404	-	41,41,41	0.90	1 (2%)	56,56,56	2.20	18 (32%)
30	LMG	C	520	-	48,48,55	0.94	2 (4%)	56,56,63	1.15	5 (8%)
22	CLA	C	511	-	59,73,73	1.72	6 (10%)	67,113,113	1.36	8 (11%)
22	CLA	b	612	34	59,73,73	1.89	8 (13%)	67,113,113	1.59	8 (11%)
22	CLA	C	504	-	59,73,73	1.84	6 (10%)	67,113,113	1.24	8 (11%)
22	CLA	b	609	34	59,73,73	1.65	10 (16%)	67,113,113	1.52	11 (16%)
27	LFA	m	101	-	9,9,19	0.12	0	8,8,18	0.44	0
22	CLA	A	412	34	59,73,73	1.49	8 (13%)	67,113,113	1.31	7 (10%)
27	LFA	B	623	-	12,12,19	0.09	0	11,11,18	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LFA	B	622	-	15,15,19	0.10	0	14,14,18	0.33	0
32	LHG	l	101	-	48,48,48	0.87	3 (6%)	51,54,54	1.22	5 (9%)
25	PL9	d	405	-	55,55,55	0.63	3 (5%)	68,69,69	1.73	14 (20%)
32	LHG	d	407	-	48,48,48	0.91	3 (6%)	51,54,54	1.10	3 (5%)
22	CLA	c	509	-	59,73,73	1.71	7 (11%)	67,113,113	1.41	7 (10%)
30	LMG	b	624	-	39,39,55	1.11	3 (7%)	47,47,63	1.12	6 (12%)
22	CLA	B	609	34	59,73,73	1.91	8 (13%)	67,113,113	1.49	8 (11%)
30	LMG	B	621	-	36,36,55	1.05	2 (5%)	44,44,63	1.22	4 (9%)
22	CLA	c	511	-	59,73,73	1.75	8 (13%)	67,113,113	1.36	6 (8%)
27	LFA	B	627	-	13,13,19	0.10	0	12,12,18	0.51	0
27	LFA	b	630	-	14,14,19	0.08	0	13,13,18	0.37	0
27	LFA	j	101	-	14,14,19	0.09	0	13,13,18	0.43	0
24	BCR	B	618	-	41,41,41	0.91	1 (2%)	56,56,56	1.97	16 (28%)
26	SQD	f	102	-	42,43,54	1.27	4 (9%)	51,54,65	1.68	10 (19%)
32	LHG	E	101	-	41,41,48	1.00	2 (4%)	44,47,54	1.08	3 (6%)
27	LFA	d	410	-	15,15,19	0.08	0	14,14,18	0.37	0
31	DGD	h	102	-	63,63,67	0.81	2 (3%)	77,77,81	1.01	4 (5%)
22	CLA	b	604	-	59,73,73	1.62	8 (13%)	67,113,113	1.45	7 (10%)
27	LFA	b	626	-	11,11,19	0.11	0	10,10,18	0.30	0
27	LFA	I	101	-	13,13,19	0.09	0	12,12,18	0.36	0
24	BCR	a	408	-	41,41,41	0.87	1 (2%)	56,56,56	1.45	12 (21%)
22	CLA	b	616	-	59,73,73	1.81	8 (13%)	67,113,113	1.17	6 (8%)
27	LFA	B	628	-	11,11,19	0.09	0	10,10,18	0.38	0
22	CLA	C	506	-	59,73,73	1.91	6 (10%)	67,113,113	1.26	7 (10%)
24	BCR	c	524	-	41,41,41	0.79	0	56,56,56	1.74	13 (23%)
24	BCR	c	523	-	41,41,41	0.84	1 (2%)	56,56,56	1.84	12 (21%)
24	BCR	T	101	-	41,41,41	0.90	1 (2%)	56,56,56	2.03	16 (28%)
24	BCR	b	621	-	41,41,41	0.84	1 (2%)	56,56,56	1.86	13 (23%)
30	LMG	m	103	-	51,51,55	0.83	2 (3%)	59,59,63	1.36	8 (13%)
31	DGD	C	518	-	57,57,67	0.85	2 (3%)	71,71,81	1.28	10 (14%)
31	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	1.09	7 (9%)
27	LFA	A	413	-	10,10,19	0.08	0	9,9,18	0.43	0
22	CLA	D	403	-	59,73,73	1.74	8 (13%)	67,113,113	1.34	8 (11%)
27	LFA	i	102	-	6,6,19	0.12	0	5,5,18	0.16	0
32	LHG	e	101	-	41,41,48	0.97	2 (4%)	44,47,54	1.06	3 (6%)
22	CLA	b	618	-	59,73,73	1.72	7 (11%)	67,113,113	1.44	8 (11%)
30	LMG	c	522	-	41,41,55	1.04	2 (4%)	49,49,63	1.60	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	508	34	59,73,73	1.71	7 (11%)	67,113,113	1.39	8 (11%)
26	SQD	L	101	-	47,48,54	1.22	4 (8%)	56,59,65	3.78	10 (17%)
22	CLA	c	506	-	59,73,73	1.78	7 (11%)	67,113,113	1.24	7 (10%)
29	BCT	a	413	28	0,3,3	0.00	-	0,3,3	0.00	-
32	LHG	D	408	-	48,48,48	0.86	3 (6%)	51,54,54	1.02	2 (3%)
22	CLA	A	404	34	59,73,73	1.68	7 (11%)	67,113,113	1.30	7 (10%)
27	LFA	m	102	-	14,14,19	0.11	0	13,13,18	0.40	0
22	CLA	C	509	-	59,73,73	1.65	8 (13%)	67,113,113	1.27	8 (11%)
32	LHG	b	628	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	5 (9%)
27	LFA	t	101	-	14,14,19	0.12	0	13,13,18	0.52	0
27	LFA	D	412	-	7,7,19	0.12	0	6,6,18	0.33	0
27	LFA	D	413	-	9,9,19	0.16	0	8,8,18	0.52	0
22	CLA	c	503	-	59,73,73	1.66	8 (13%)	67,113,113	1.33	8 (11%)
22	CLA	c	508	34	59,73,73	1.68	8 (13%)	67,113,113	1.57	7 (10%)
22	CLA	B	610	-	59,73,73	1.57	7 (11%)	67,113,113	1.56	8 (11%)
22	CLA	D	402	-	59,73,73	1.78	6 (10%)	67,113,113	1.56	8 (11%)
22	CLA	B	602	-	59,73,73	1.79	7 (11%)	67,113,113	1.41	7 (10%)
22	CLA	C	505	34	59,73,73	1.64	8 (13%)	67,113,113	1.36	9 (13%)
22	CLA	d	401	34	59,73,73	1.61	8 (13%)	67,113,113	1.28	8 (11%)
24	BCR	b	619	-	41,41,41	0.85	1 (2%)	56,56,56	1.79	12 (21%)
27	LFA	B	626	-	9,9,19	0.11	0	8,8,18	0.45	0
32	LHG	L	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.11	2 (3%)
22	CLA	B	608	-	59,73,73	1.72	7 (11%)	67,113,113	1.36	7 (10%)

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
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
25	PL9	a	409	-	-	17/53/73/73	0/1/1/1
27	LFA	b	622	-	-	3/7/7/17	-
27	LFA	B	620	-	-	5/7/7/17	-
22	CLA	b	606	-	3/3/20/25	8/37/135/135	-
22	CLA	b	614	-	3/3/20/25	4/37/135/135	-
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	410	-	-	14/49/69/69	0/1/1/1
30	LMG	D	409	-	-	4/46/66/70	0/1/1/1
23	PHO	A	405	-	-	1/53/103/103	0/5/6/6
22	CLA	b	617	-	3/3/20/25	3/37/135/135	-
22	CLA	c	507	-	3/3/20/25	6/37/135/135	-
24	BCR	k	101	-	-	5/29/63/63	0/2/2/2
22	CLA	b	613	-	3/3/20/25	6/37/135/135	-
26	SQD	D	411	-	-	6/38/58/69	0/1/1/1
22	CLA	B	606	34	3/3/20/25	7/37/135/135	-
31	DGD	C	517	-	-	14/51/91/95	0/2/2/2
25	PL9	A	408	-	-	9/53/73/73	0/1/1/1
27	LFA	b	602	-	-	5/12/12/17	-
22	CLA	C	512	3	3/3/20/25	1/37/135/135	-
33	HEM	v	201	16	-	0/6/54/54	-
22	CLA	B	611	-	3/3/20/25	4/37/135/135	-
27	LFA	d	409	-	-	2/6/6/17	-
31	DGD	c	517	-	-	14/44/84/95	0/2/2/2
22	CLA	C	510	-	3/3/20/25	6/37/135/135	-
22	CLA	C	503	-	3/3/20/25	4/37/135/135	-
22	CLA	b	610	-	3/3/20/25	3/37/135/135	-
27	LFA	B	624	-	-	8/12/12/17	-
25	PL9	D	405	-	-	13/53/73/73	0/1/1/1
33	HEM	V	201	16	-	0/6/54/54	-
22	CLA	B	615	-	3/3/20/25	6/37/135/135	-
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2
33	HEM	e	102	5,6	-	1/6/54/54	-
27	LFA	T	102	-	-	2/9/9/17	-
22	CLA	d	403	-	3/3/20/25	8/37/135/135	-
30	LMG	C	522	-	-	16/39/59/70	0/1/1/1
24	BCR	t	102	-	-	6/29/63/63	0/2/2/2
30	LMG	C	501	-	-	15/46/66/70	0/1/1/1
27	LFA	J	101	-	-	1/8/8/17	-
30	LMG	f	101	-	-	8/46/66/70	0/1/1/1
22	CLA	b	605	-	3/3/20/25	5/37/135/135	-
32	LHG	D	406	-	-	15/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LFA	B	625	-	-	0/6/6/17	-
22	CLA	B	612	-	3/3/20/25	2/37/135/135	-
22	CLA	c	504	-	3/3/20/25	2/37/135/135	-
22	CLA	B	613	-	3/3/20/25	11/37/135/135	-
27	LFA	b	623	-	-	0/9/9/17	-
22	CLA	b	603	34	3/3/20/25	8/37/135/135	-
22	CLA	H	101	34	3/3/20/25	7/37/135/135	-
22	CLA	C	514	-	3/3/20/25	2/37/135/135	-
27	LFA	C	521	-	-	5/12/12/17	-
22	CLA	c	505	34	3/3/20/25	5/37/135/135	-
22	CLA	B	605	-	3/3/20/25	6/37/135/135	-
30	LMG	c	522	-	-	10/36/56/70	0/1/1/1
31	DGD	c	516	-	-	13/51/91/95	0/2/2/2
26	SQD	A	409	-	-	10/49/69/69	0/1/1/1
22	CLA	C	513	-	3/3/20/25	5/37/135/135	-
27	LFA	d	408	-	-	5/12/12/17	-
22	CLA	c	514	-	3/3/20/25	2/37/135/135	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
27	LFA	b	629	-	-	0/6/6/17	-
24	BCR	K	101	-	-	4/29/63/63	0/2/2/2
24	BCR	D	404	-	-	6/29/63/63	0/2/2/2
22	CLA	a	407	-	3/3/20/25	4/37/135/135	-
22	CLA	b	615	-	3/3/20/25	5/37/135/135	-
27	LFA	i	101	-	-	6/13/13/17	-
24	BCR	h	101	-	-	4/29/63/63	0/2/2/2
27	LFA	M	101	-	-	2/7/7/17	-
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	LMG	B	619	-	-	15/46/66/70	0/1/1/1
24	BCR	c	515	-	-	1/29/63/63	0/2/2/2
22	CLA	A	406	-	3/3/20/25	2/37/135/135	-
30	LMG	c	519	-	-	12/46/66/70	0/1/1/1
27	LFA	c	520	-	-	0/6/6/17	-
24	BCR	H	102	-	-	3/29/63/63	0/2/2/2
24	BCR	C	516	-	-	1/29/63/63	0/2/2/2
22	CLA	b	607	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	608	-	3/3/20/25	4/37/135/135	-
22	CLA	c	510	-	3/3/20/25	4/37/135/135	-
23	PHO	D	401	-	-	6/53/103/103	0/5/6/6
22	CLA	C	511	-	3/3/20/25	2/37/135/135	-
22	CLA	c	502	-	3/3/20/25	2/37/135/135	-
27	LFA	c	521	-	-	4/12/12/17	-
30	LMG	c	501	-	-	17/46/66/70	0/1/1/1
22	CLA	a	404	-	3/3/20/25	2/37/135/135	-
33	HEM	E	102	5,6	-	2/6/54/54	-
22	CLA	a	405	34	3/3/20/25	5/37/135/135	-
22	CLA	B	607	-	3/3/20/25	2/37/135/135	-
22	CLA	C	507	-	3/3/20/25	6/37/135/135	-
26	SQD	a	412	-	-	15/44/64/69	0/1/1/1
27	LFA	a	411	-	-	1/4/4/17	-
27	LFA	M	102	-	-	5/13/13/17	-
23	PHO	a	406	-	-	4/53/103/103	0/5/6/6
32	LHG	d	406	-	-	16/53/53/53	-
26	SQD	A	411	-	-	23/49/69/69	0/1/1/1
22	CLA	b	611	-	3/3/20/25	7/37/135/135	-
27	LFA	b	625	-	-	6/13/13/17	-
22	CLA	B	601	-	3/3/20/25	6/37/135/135	-
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
27	LFA	A	410	-	-	6/11/11/17	-
22	CLA	b	618	-	3/3/20/25	5/37/135/135	-
22	CLA	B	603	-	3/3/20/25	2/37/135/135	-
27	LFA	b	627	-	-	3/8/8/17	-
22	CLA	B	614	-	3/3/20/25	7/37/135/135	-
27	LFA	D	410	-	-	5/12/12/17	-
26	SQD	b	601	-	-	11/49/69/69	0/1/1/1
22	CLA	B	604	-	3/3/20/25	9/37/135/135	-
22	CLA	A	403	-	3/3/20/25	1/37/135/135	-
24	BCR	B	618	-	-	4/29/63/63	0/2/2/2
22	CLA	c	513	-	3/3/20/25	2/37/135/135	-
23	PHO	a	414	-	-	0/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	H	103	-	-	12/49/89/95	0/2/2/2
22	CLA	C	502	-	3/3/20/25	0/37/135/135	-
22	CLA	c	512	3	3/3/20/25	0/37/135/135	-
32	LHG	D	407	-	-	11/53/53/53	-
24	BCR	d	404	-	-	6/29/63/63	0/2/2/2
30	LMG	C	520	-	-	10/43/63/70	0/1/1/1
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
22	CLA	b	612	34	3/3/20/25	6/37/135/135	-
22	CLA	C	504	-	3/3/20/25	6/37/135/135	-
22	CLA	b	609	34	3/3/20/25	7/37/135/135	-
27	LFA	m	101	-	-	1/7/7/17	-
22	CLA	A	412	34	3/3/20/25	2/37/135/135	-
27	LFA	B	623	-	-	6/10/10/17	-
27	LFA	B	622	-	-	2/13/13/17	-
32	LHG	l	101	-	-	20/53/53/53	-
25	PL9	d	405	-	-	11/53/73/73	0/1/1/1
32	LHG	d	407	-	-	25/53/53/53	-
22	CLA	c	509	-	3/3/20/25	5/37/135/135	-
30	LMG	b	624	-	-	13/34/54/70	0/1/1/1
22	CLA	B	609	34	3/3/20/25	4/37/135/135	-
30	LMG	B	621	-	-	7/31/51/70	0/1/1/1
22	CLA	c	511	-	3/3/20/25	4/37/135/135	-
27	LFA	B	627	-	-	8/11/11/17	-
27	LFA	b	630	-	-	6/12/12/17	-
27	LFA	j	101	-	-	3/12/12/17	-
22	CLA	d	402	-	3/3/20/25	1/37/135/135	-
26	SQD	f	102	-	-	18/38/58/69	0/1/1/1
32	LHG	E	101	-	-	20/46/46/53	-
27	LFA	d	410	-	-	5/13/13/17	-
31	DGD	h	102	-	-	18/51/91/95	0/2/2/2
22	CLA	b	604	-	3/3/20/25	8/37/135/135	-
27	LFA	b	626	-	-	6/9/9/17	-
27	LFA	I	101	-	-	6/11/11/17	-
24	BCR	a	408	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	616	-	3/3/20/25	11/37/135/135	-
27	LFA	B	628	-	-	2/9/9/17	-
22	CLA	C	506	-	3/3/20/25	6/37/135/135	-
24	BCR	c	524	-	-	2/29/63/63	0/2/2/2
24	BCR	c	523	-	-	2/29/63/63	0/2/2/2
24	BCR	T	101	-	-	8/29/63/63	0/2/2/2
24	BCR	b	621	-	-	8/29/63/63	0/2/2/2
30	LMG	m	103	-	-	17/46/66/70	0/1/1/1
31	DGD	C	518	-	-	16/45/85/95	0/2/2/2
31	DGD	C	519	-	-	6/51/91/95	0/2/2/2
27	LFA	A	413	-	-	5/8/8/17	-
22	CLA	D	403	-	3/3/20/25	6/37/135/135	-
27	LFA	i	102	-	-	1/4/4/17	-
32	LHG	e	101	-	-	13/46/46/53	-
22	CLA	c	506	-	3/3/20/25	6/37/135/135	-
22	CLA	C	508	34	3/3/20/25	1/37/135/135	-
26	SQD	L	101	-	-	18/43/63/69	0/1/1/1
32	LHG	D	408	-	-	17/53/53/53	-
22	CLA	A	404	34	3/3/20/25	2/37/135/135	-
27	LFA	m	102	-	-	4/12/12/17	-
22	CLA	C	509	-	3/3/20/25	4/37/135/135	-
32	LHG	b	628	-	-	12/53/53/53	-
27	LFA	t	101	-	-	3/12/12/17	-
27	LFA	D	412	-	-	2/5/5/17	-
27	LFA	D	413	-	-	0/7/7/17	-
22	CLA	c	503	-	3/3/20/25	3/37/135/135	-
22	CLA	c	508	34	3/3/20/25	4/37/135/135	-
22	CLA	B	610	-	3/3/20/25	4/37/135/135	-
22	CLA	D	402	-	3/3/20/25	3/37/135/135	-
22	CLA	B	602	-	3/3/20/25	4/37/135/135	-
22	CLA	C	505	34	3/3/20/25	7/37/135/135	-
22	CLA	d	401	34	3/3/20/25	4/37/135/135	-
24	BCR	b	619	-	-	2/29/63/63	0/2/2/2
27	LFA	B	626	-	-	4/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	L	102	-	-	16/53/53/53	-
22	CLA	B	608	-	3/3/20/25	7/37/135/135	-

The worst 5 of 655 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C4B-NB	11.88	1.45	1.35
22	B	613	CLA	C4B-NB	11.43	1.45	1.35
22	B	601	CLA	C4B-NB	11.36	1.45	1.35
22	c	504	CLA	C4B-NB	11.36	1.45	1.35
22	b	607	CLA	C4B-NB	11.25	1.45	1.35

The worst 5 of 1142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	SQD	O9-S-C6	-18.70	84.72	106.94
26	L	101	SQD	O8-S-O9	-10.90	84.64	111.27
26	L	101	SQD	O7-S-C6	10.80	119.78	106.94
26	L	101	SQD	O9-S-O7	-9.72	80.32	113.95
22	A	403	CLA	C4A-NA-C1A	-8.71	102.79	106.71

5 of 210 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND

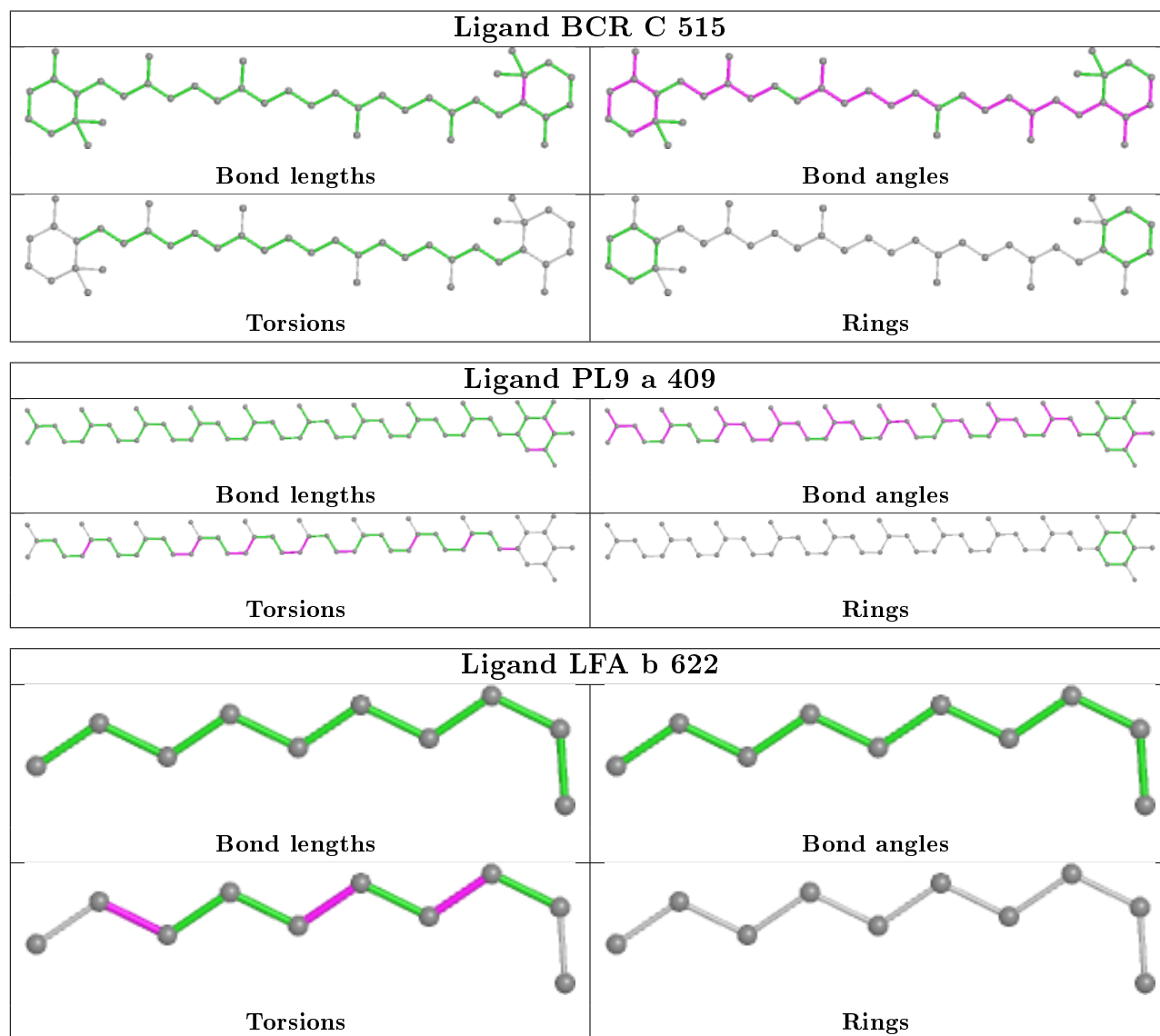
5 of 1127 torsion outliers are listed below:

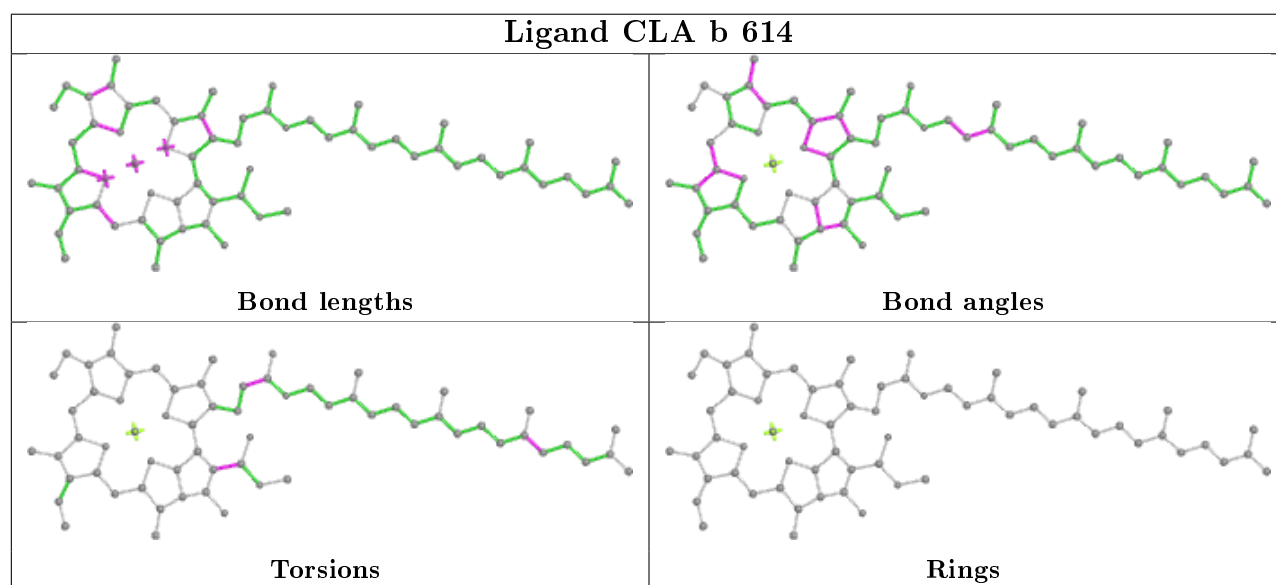
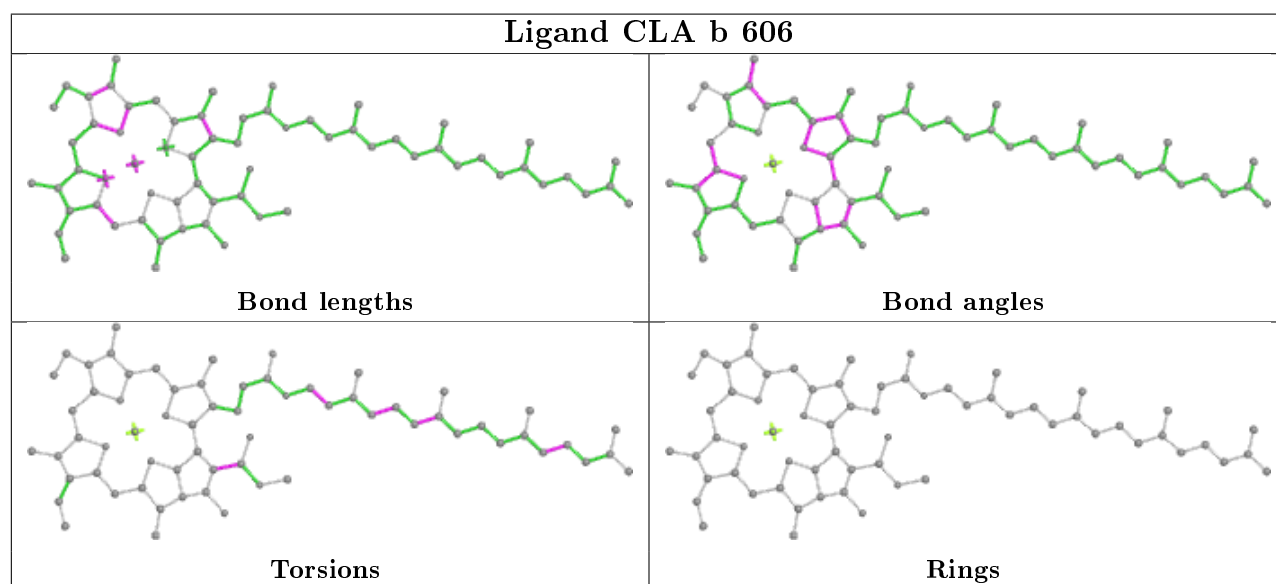
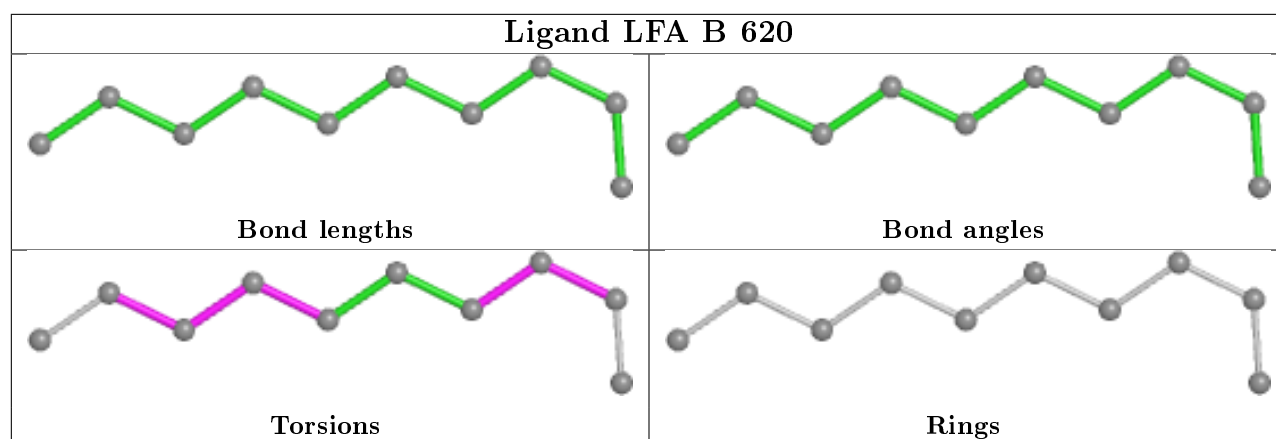
Mol	Chain	Res	Type	Atoms
25	a	409	PL9	C45-C44-C46-C47
24	K	102	BCR	C7-C8-C9-C10
24	K	102	BCR	C7-C8-C9-C34
25	A	408	PL9	C9-C11-C12-C13
25	A	408	PL9	C13-C14-C16-C17

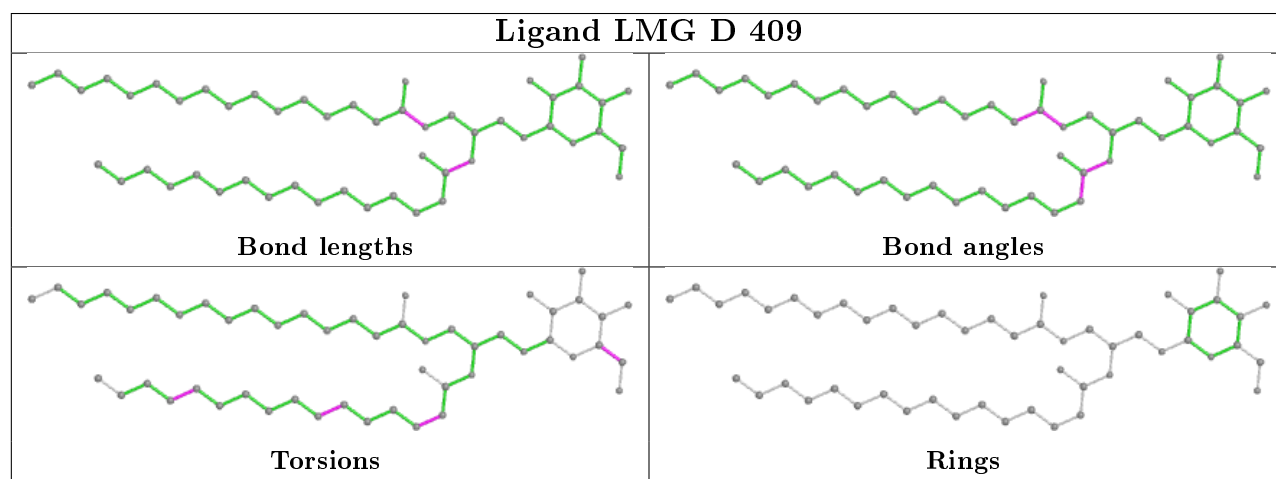
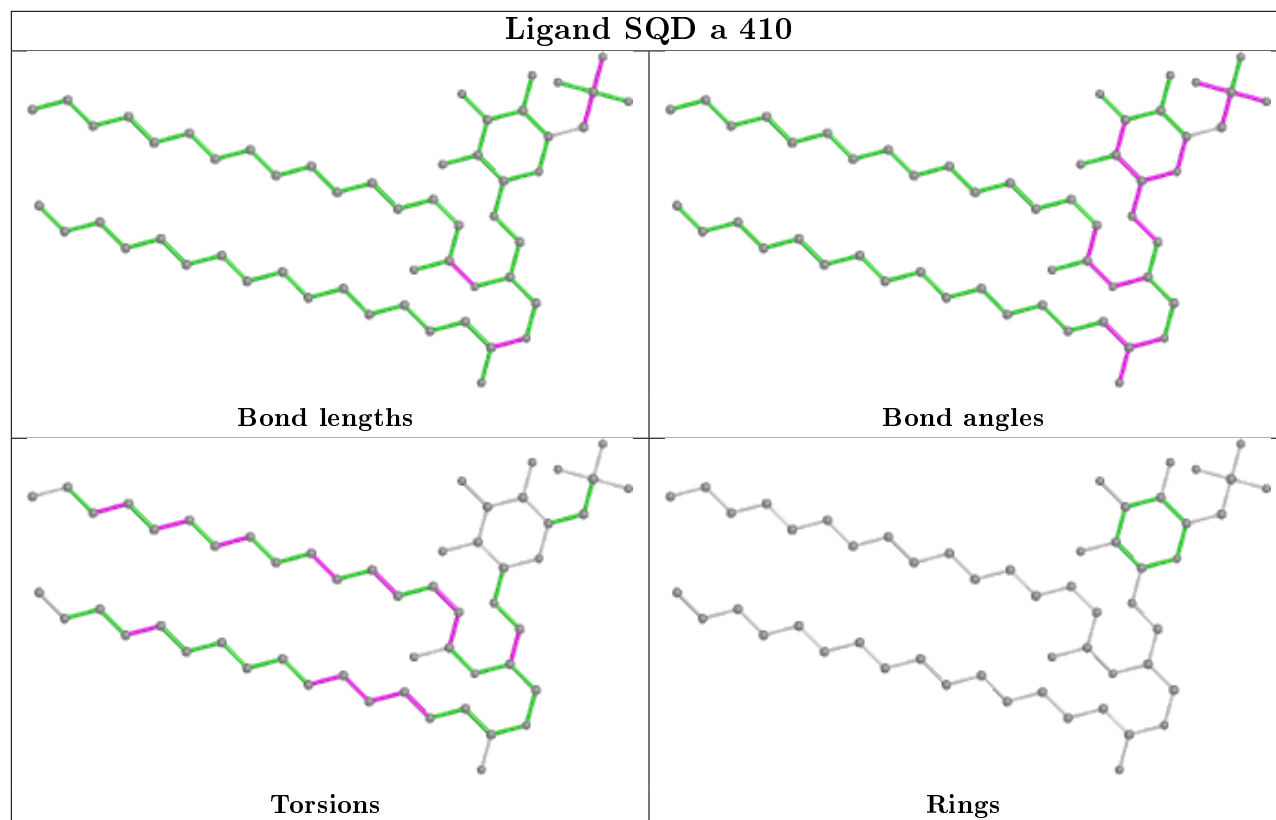
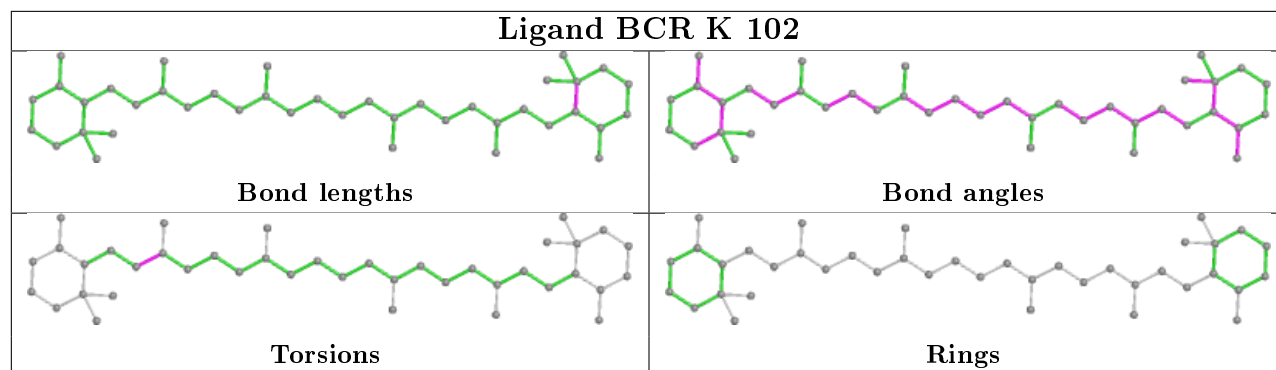
There are no ring outliers.

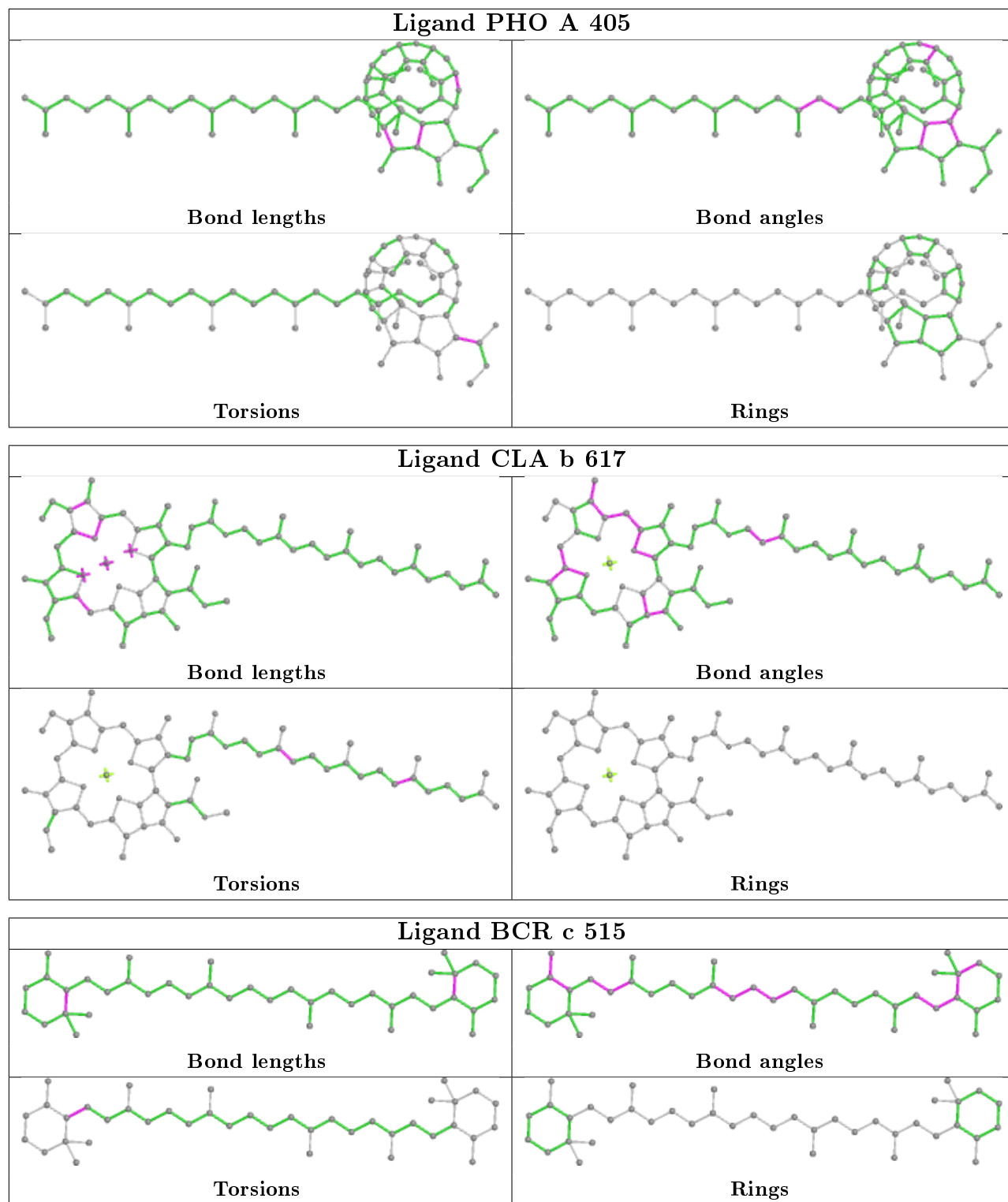
No monomer is involved in short contacts.

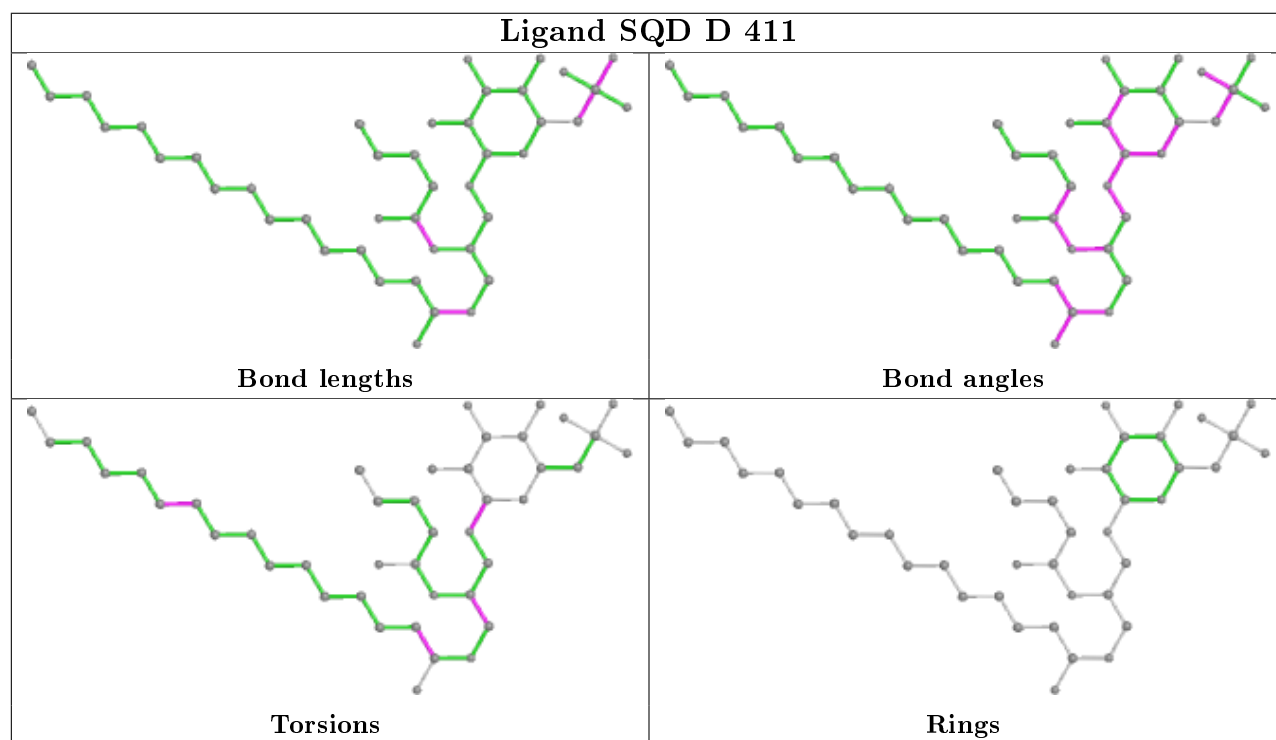
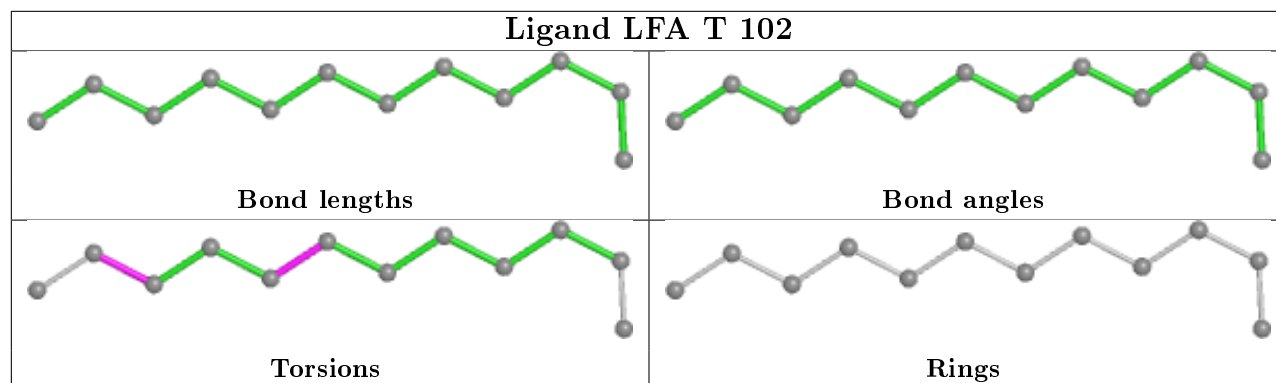
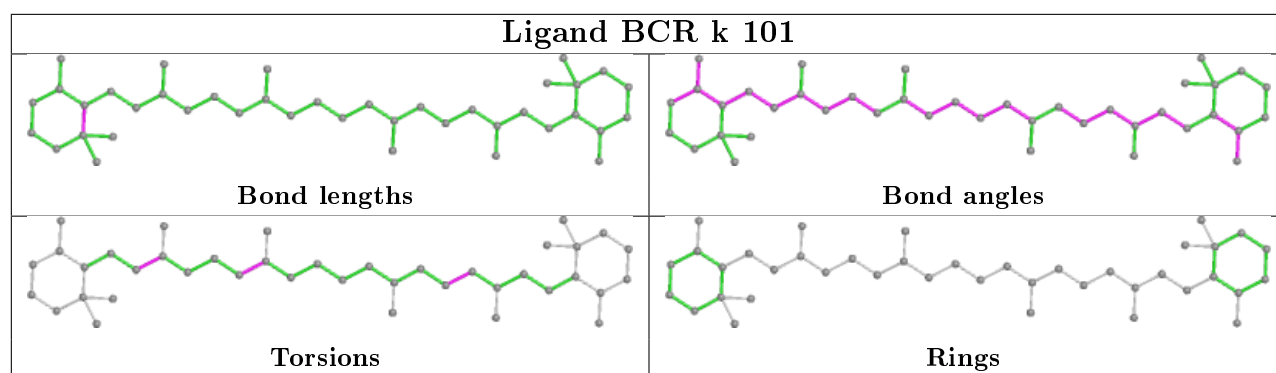
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

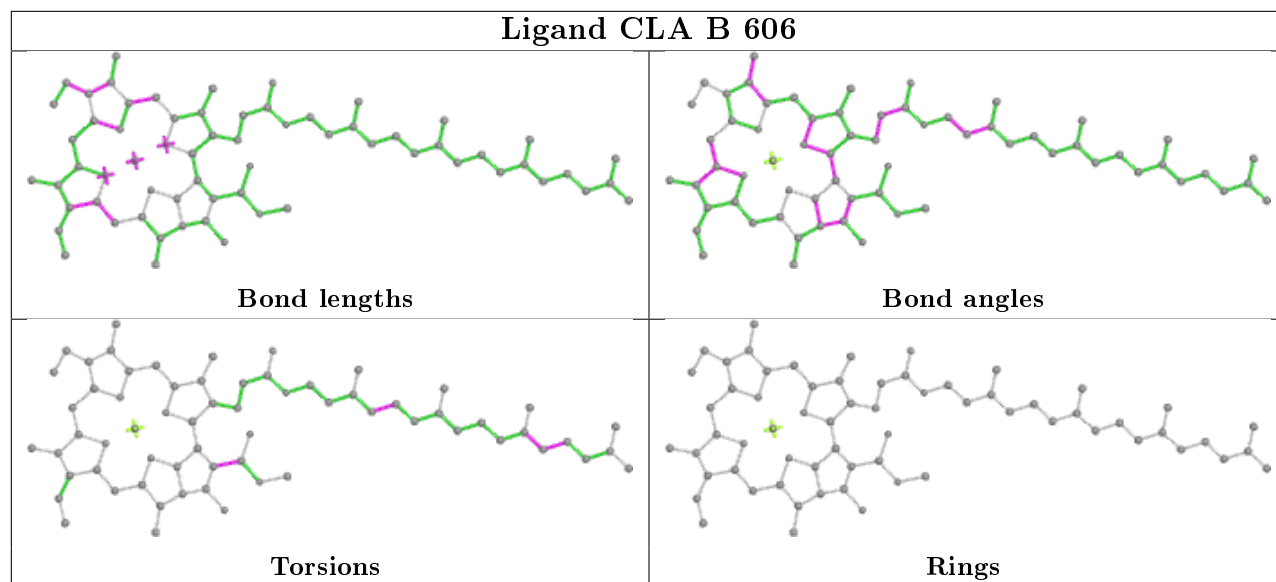
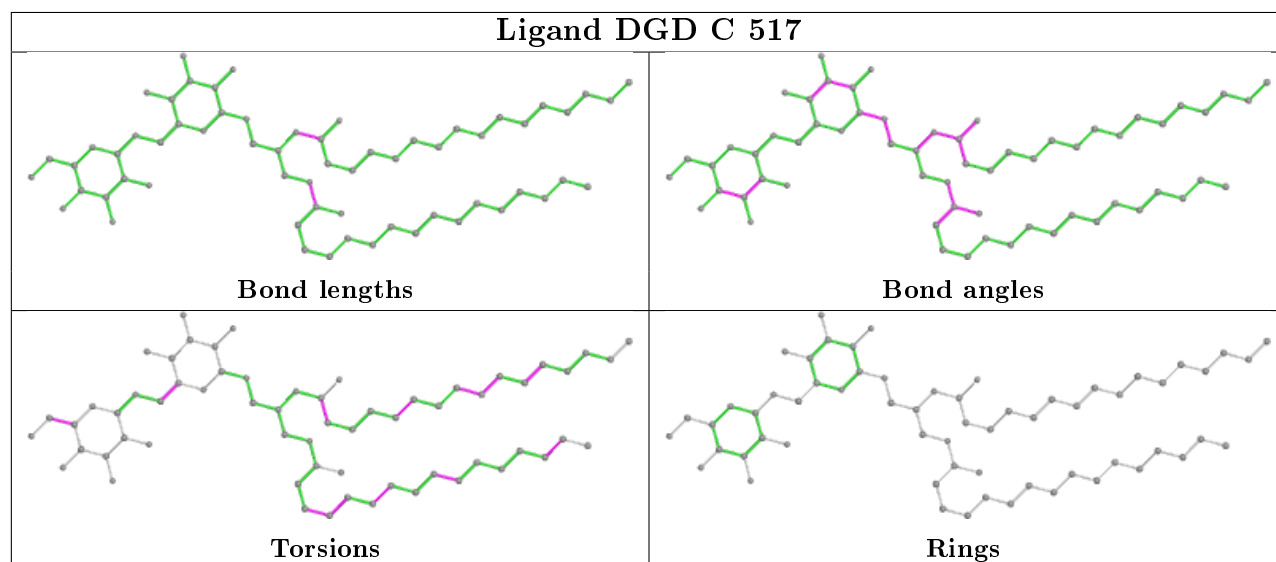
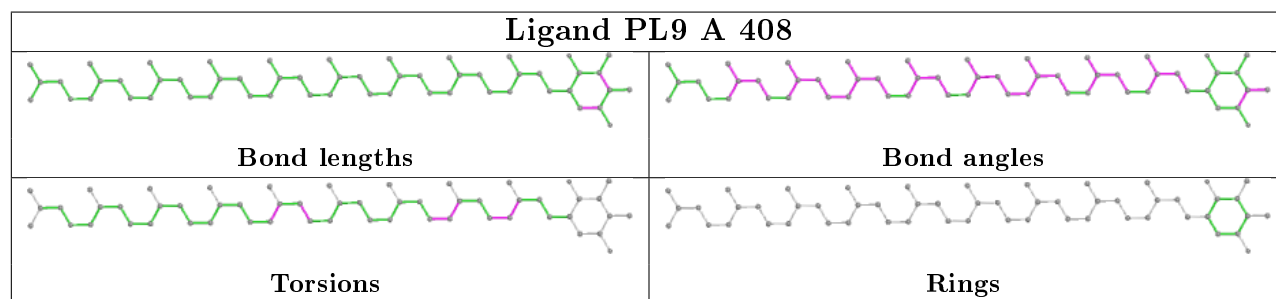


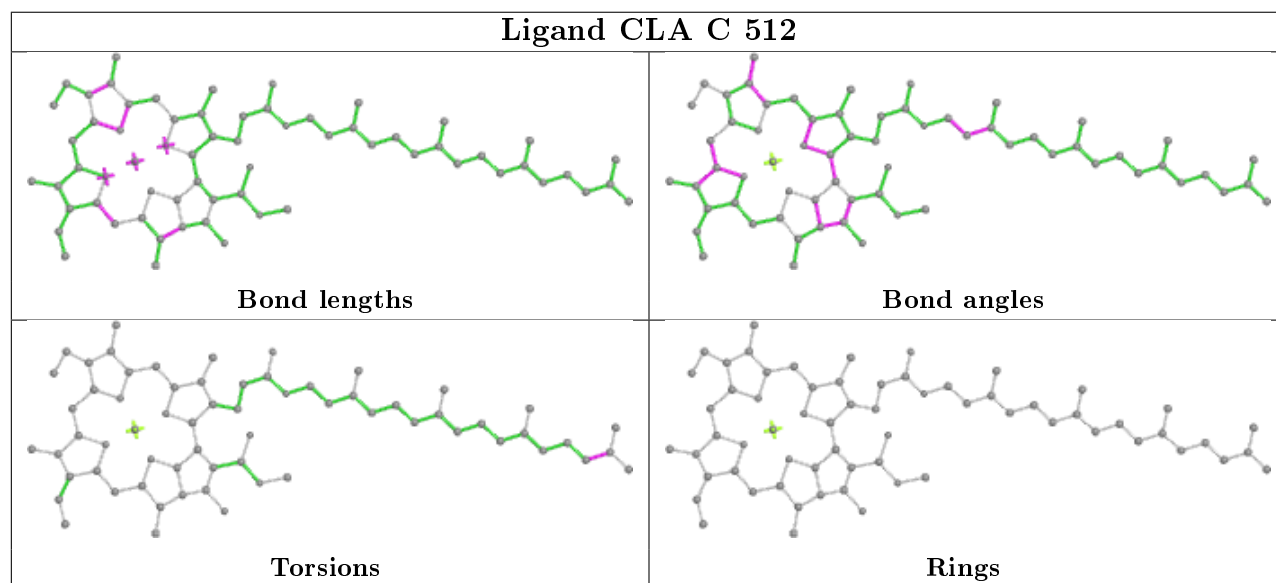
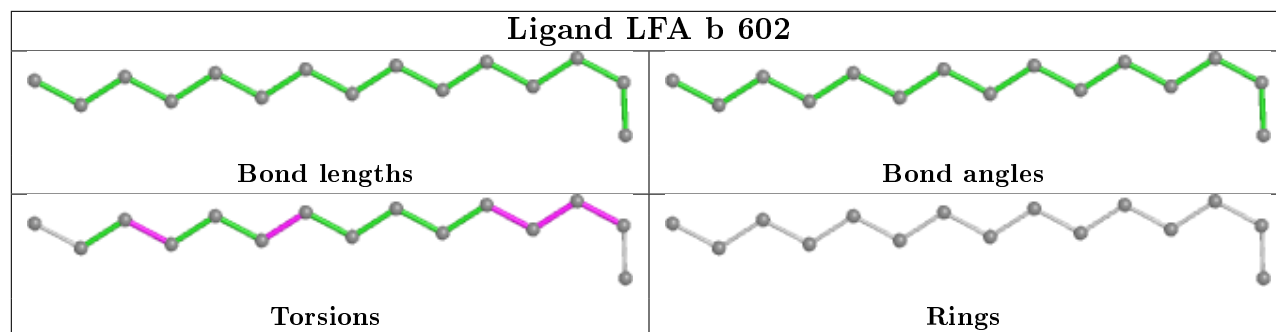


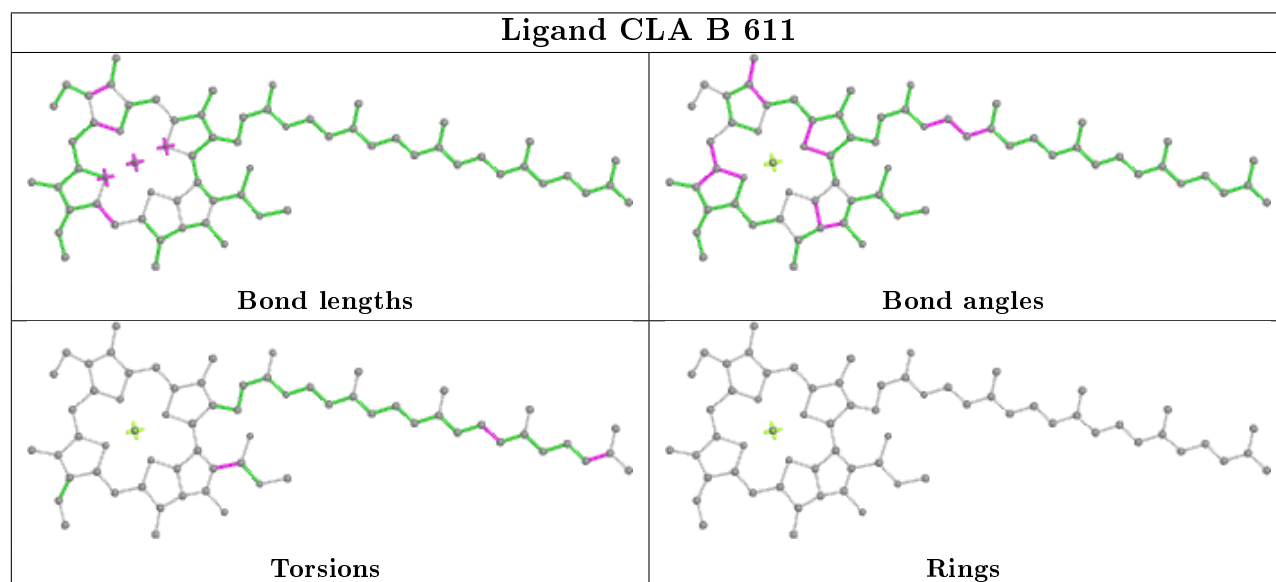
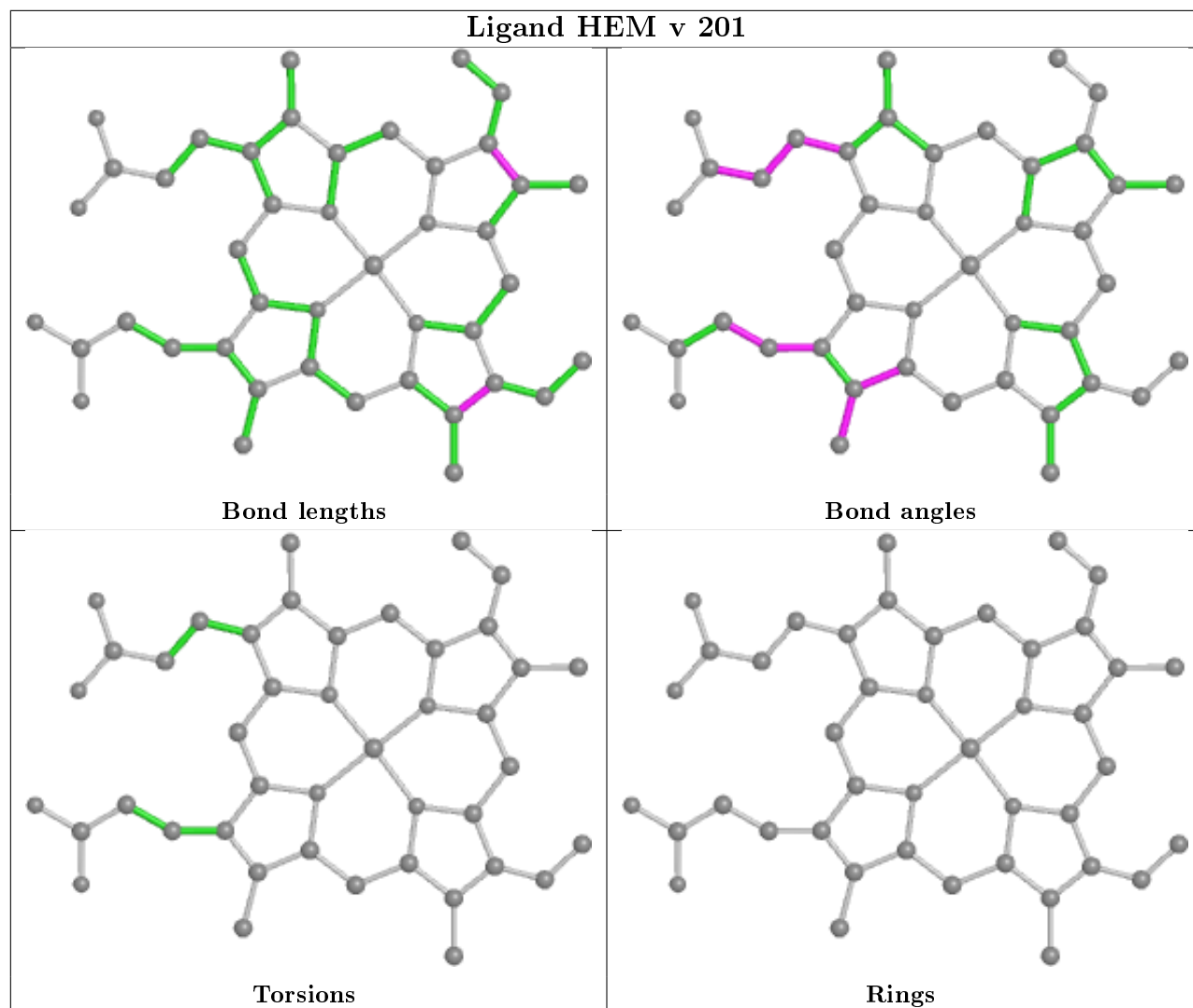


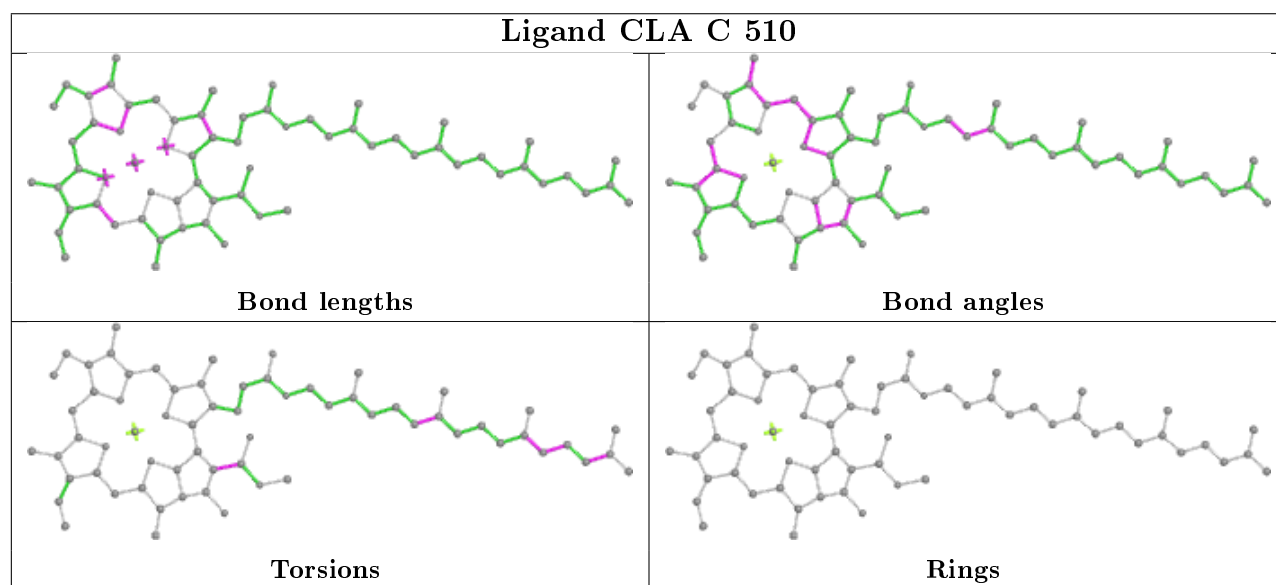
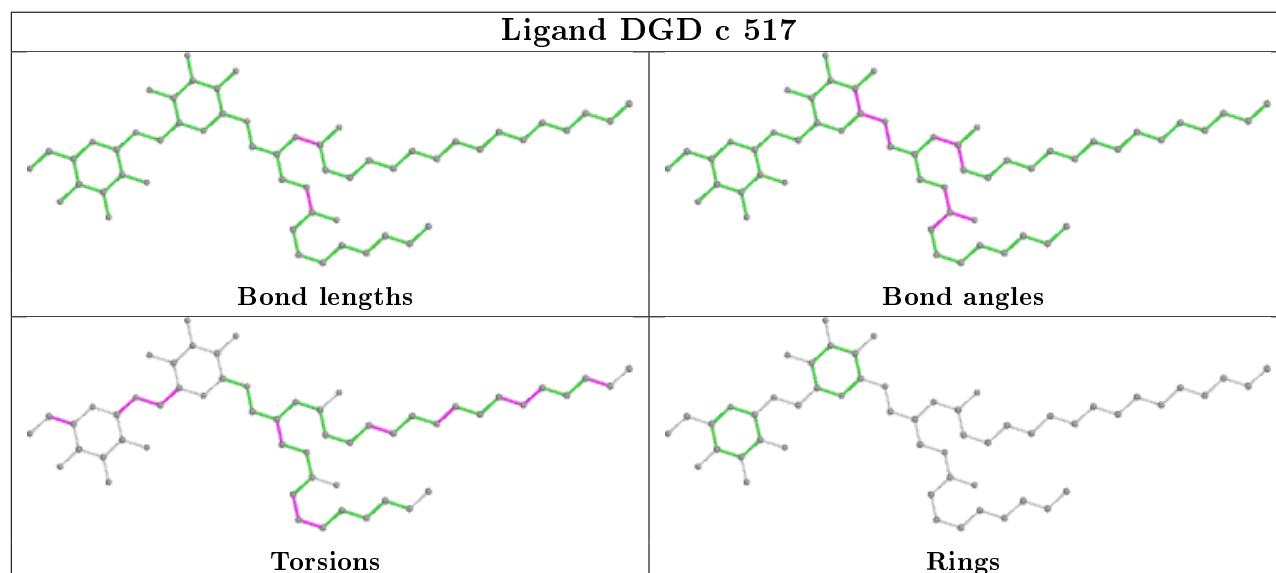
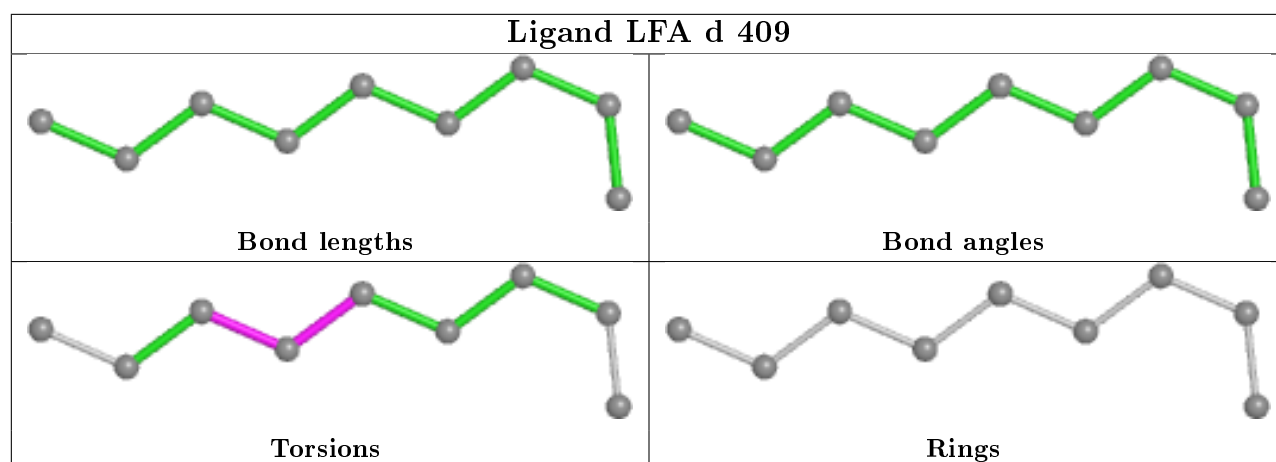


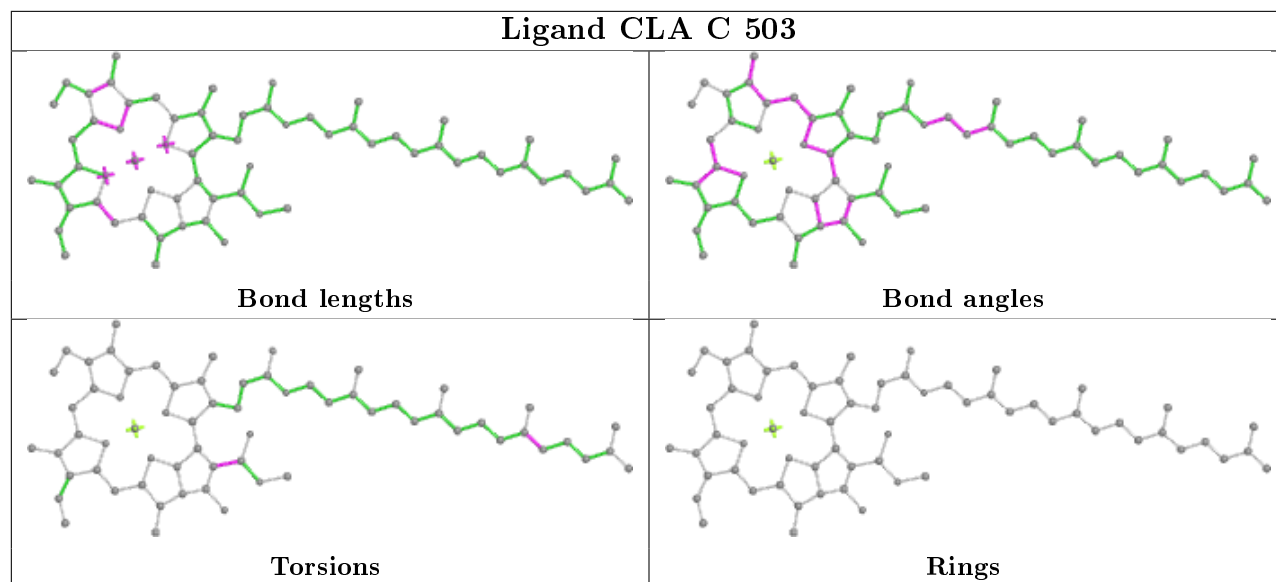
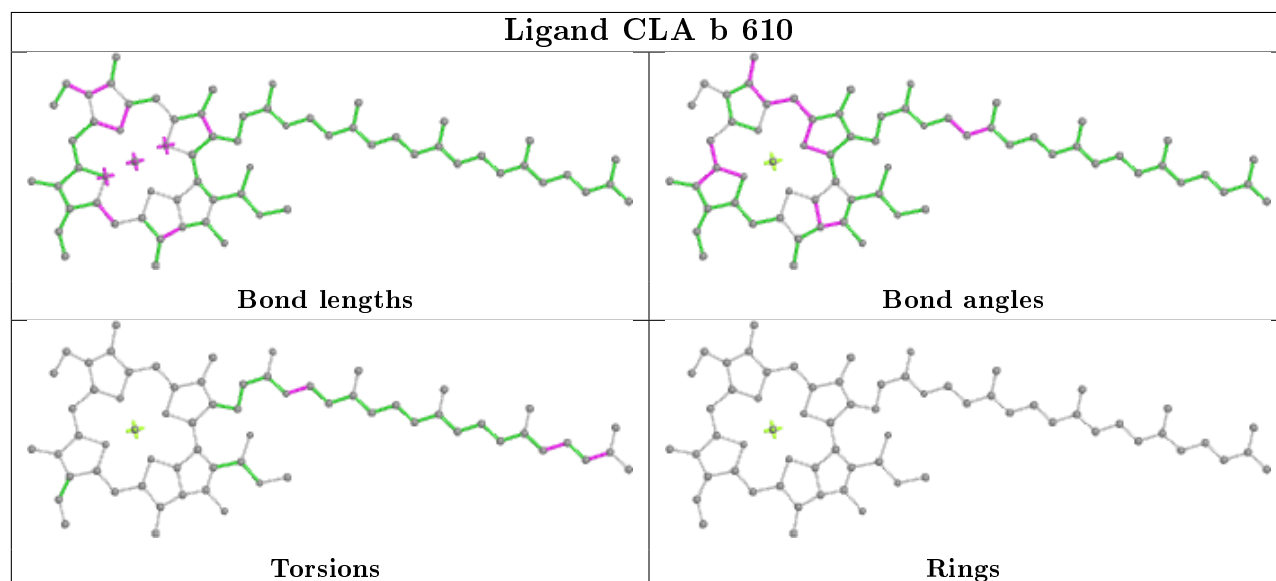
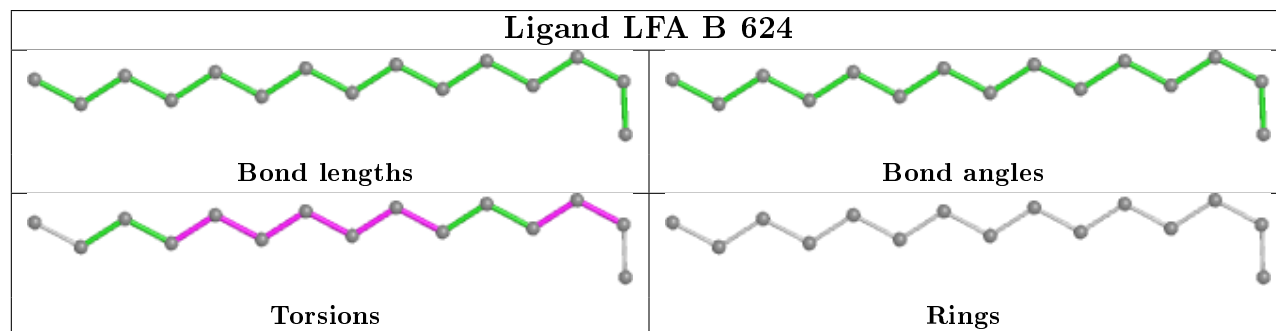


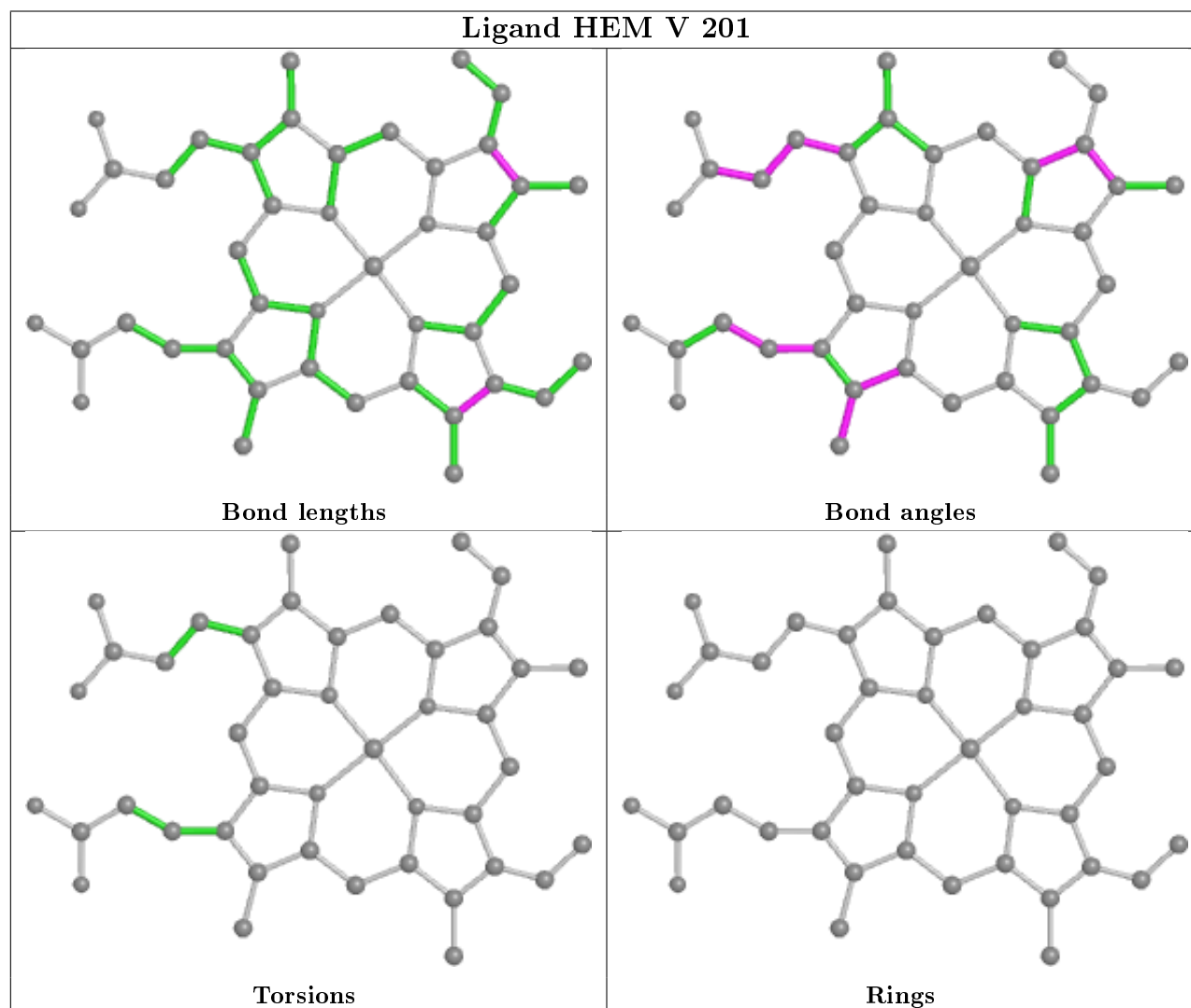
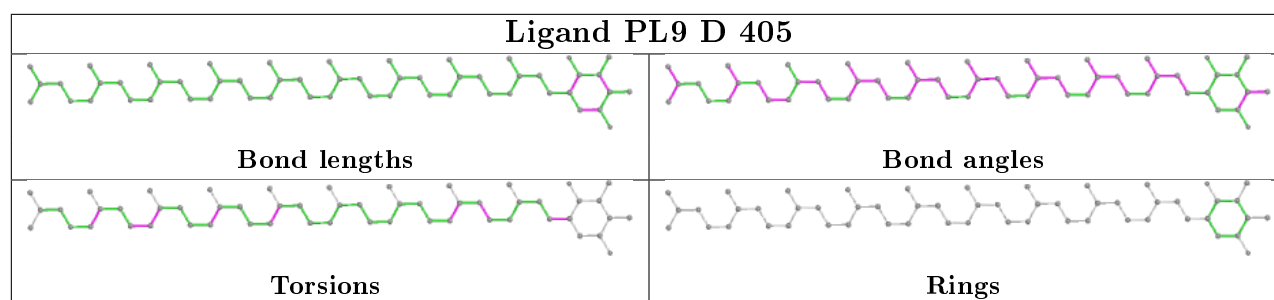
**Ligand CLA B 606****Ligand DGD C 517****Ligand PL9 A 408**

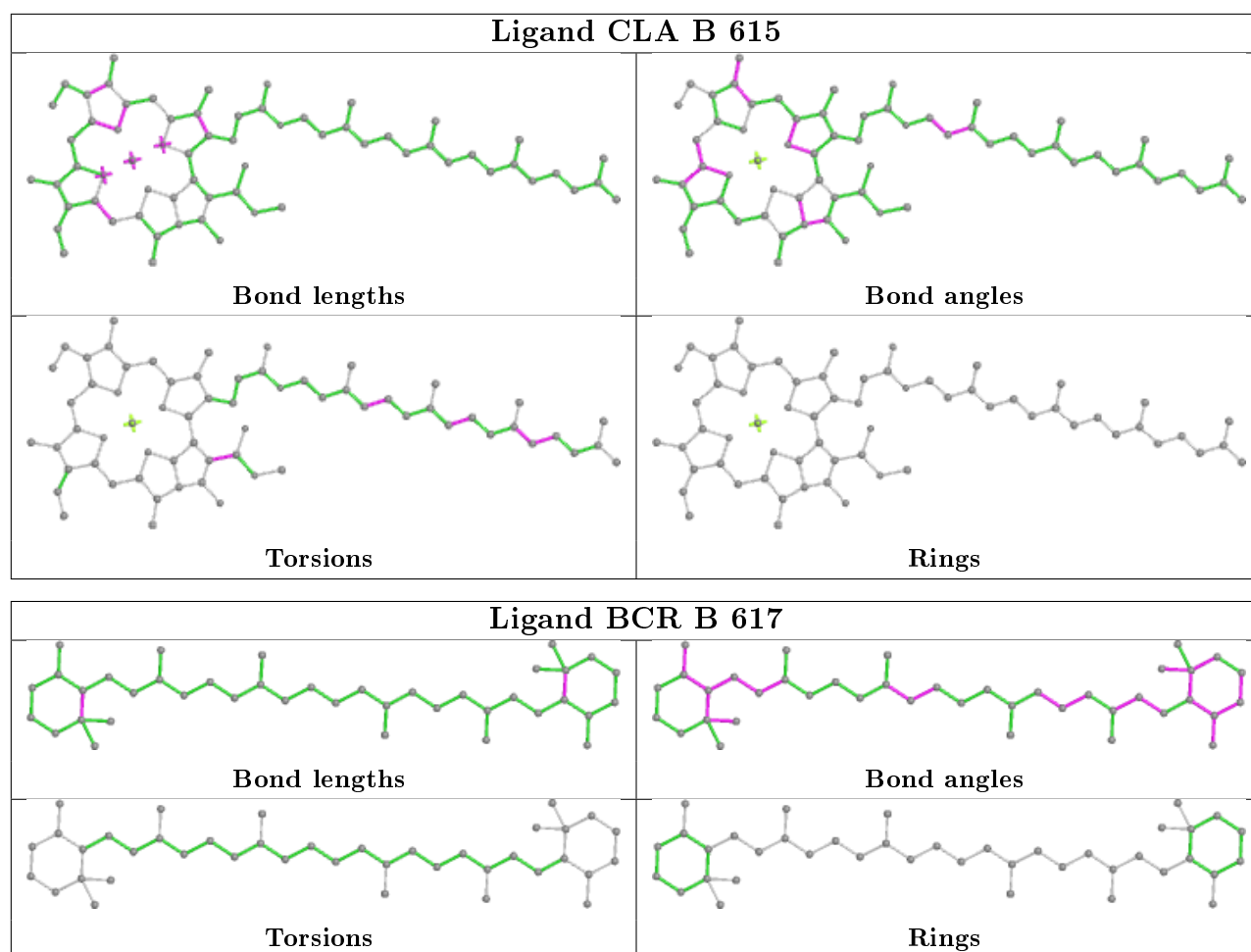


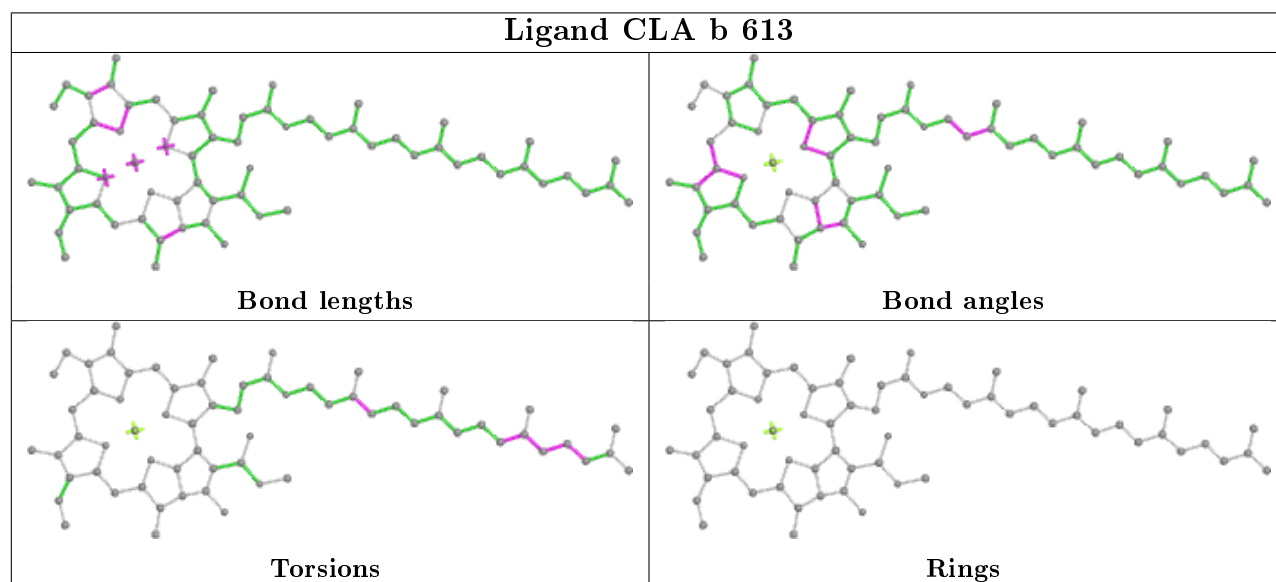
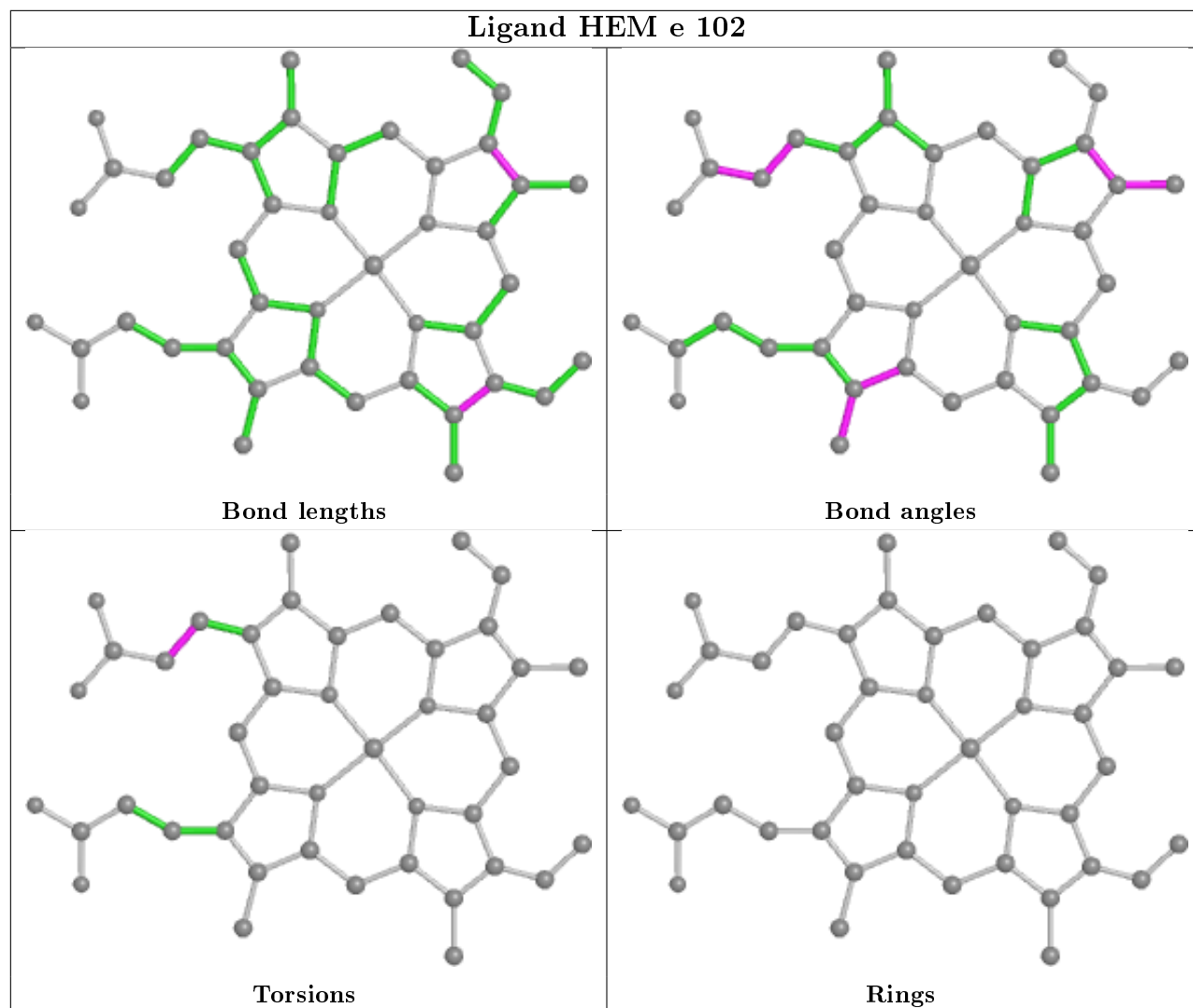


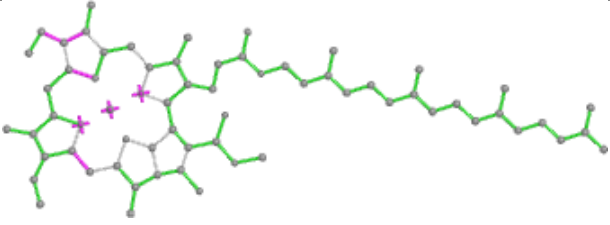
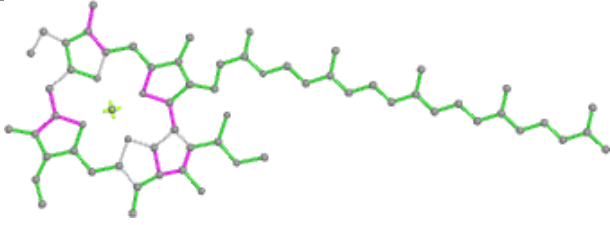
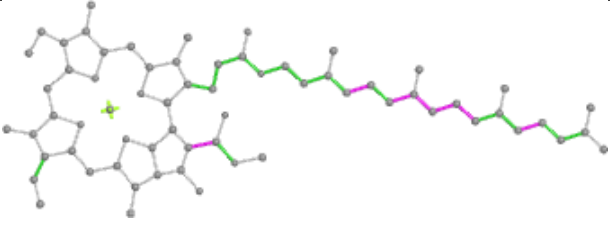
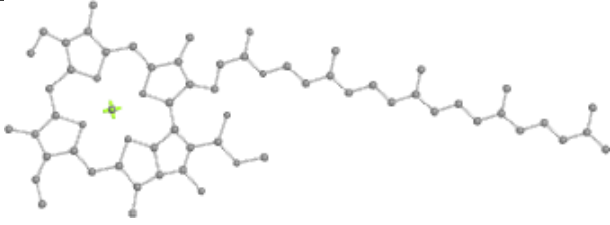
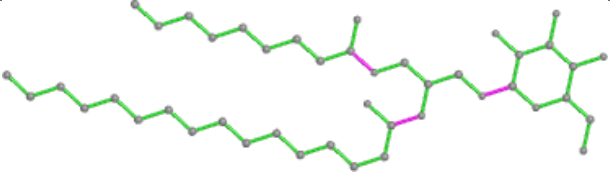
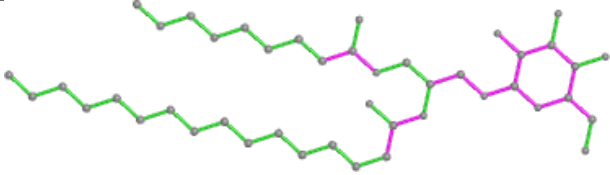
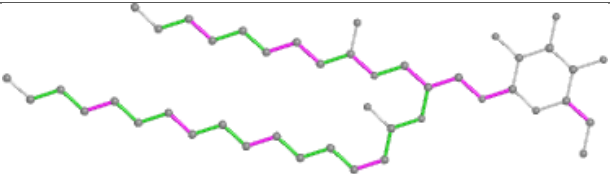
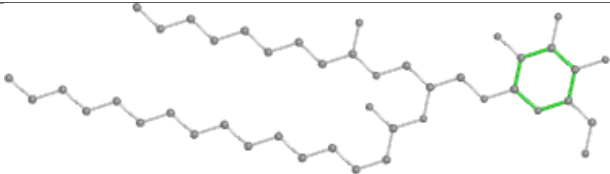
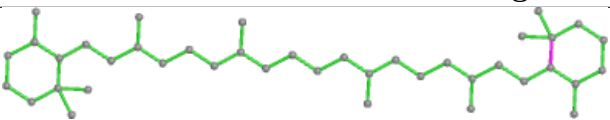
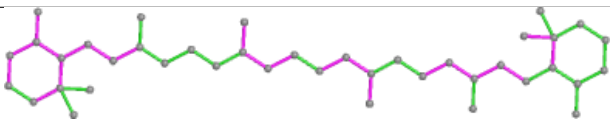
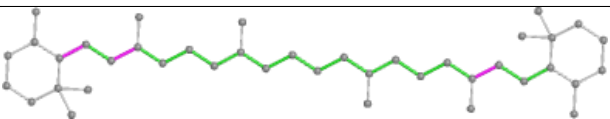
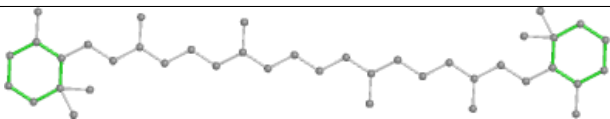


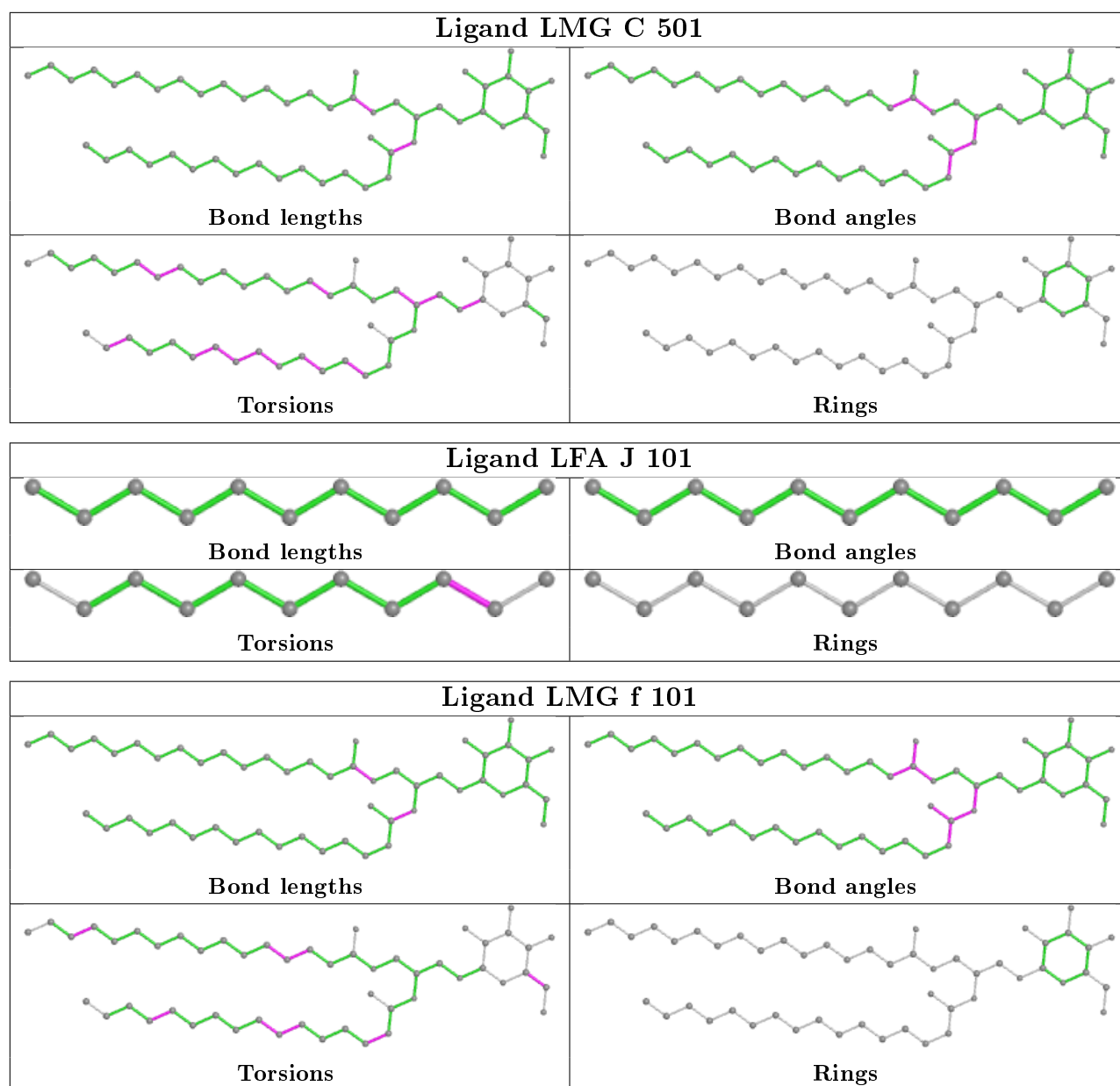
**Ligand CLA C 503****Ligand CLA b 610****Ligand LFA B 624**

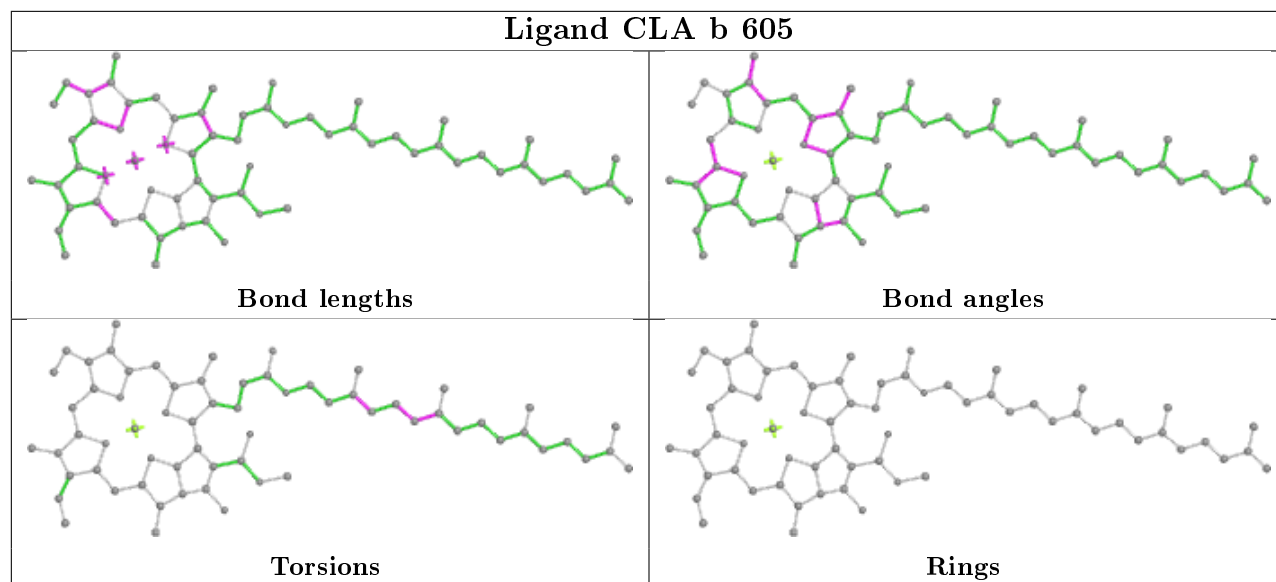
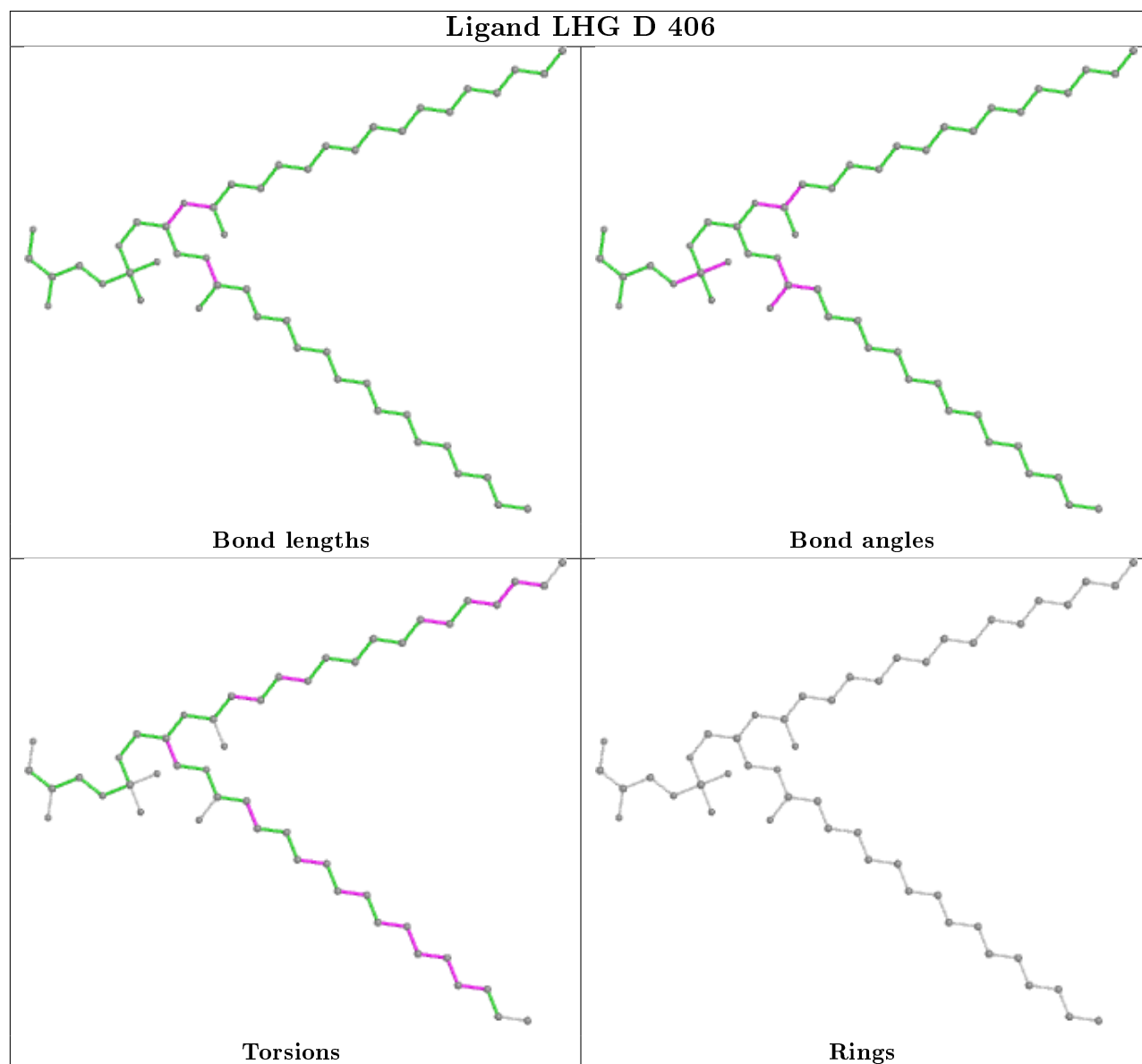


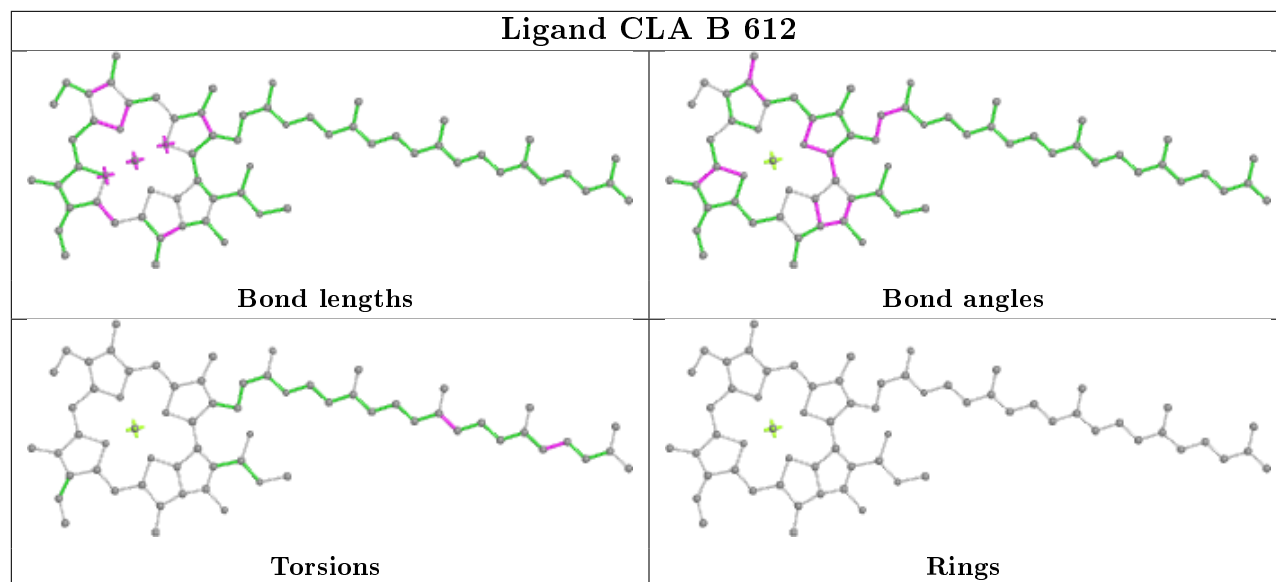
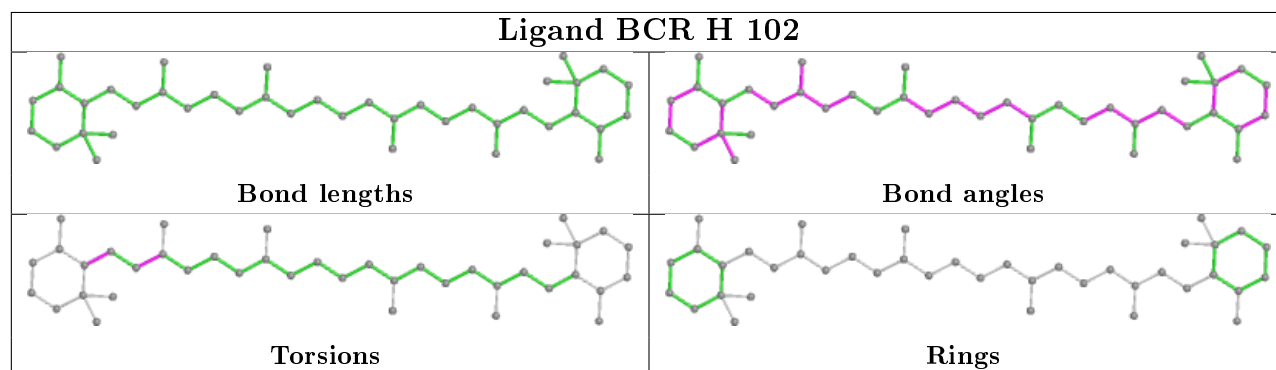
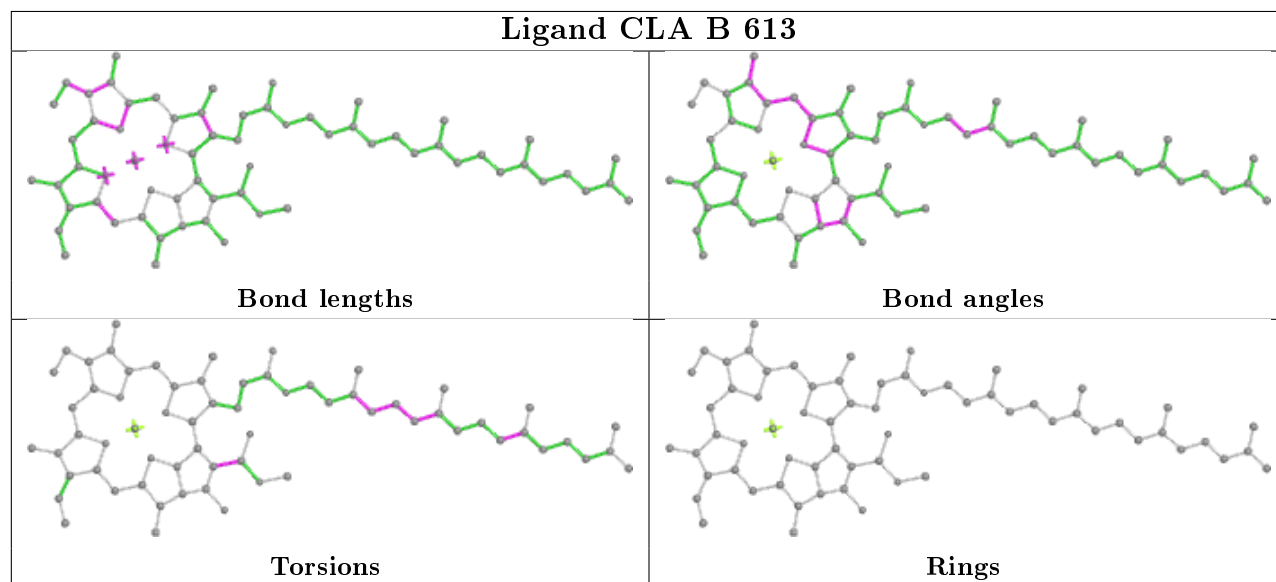




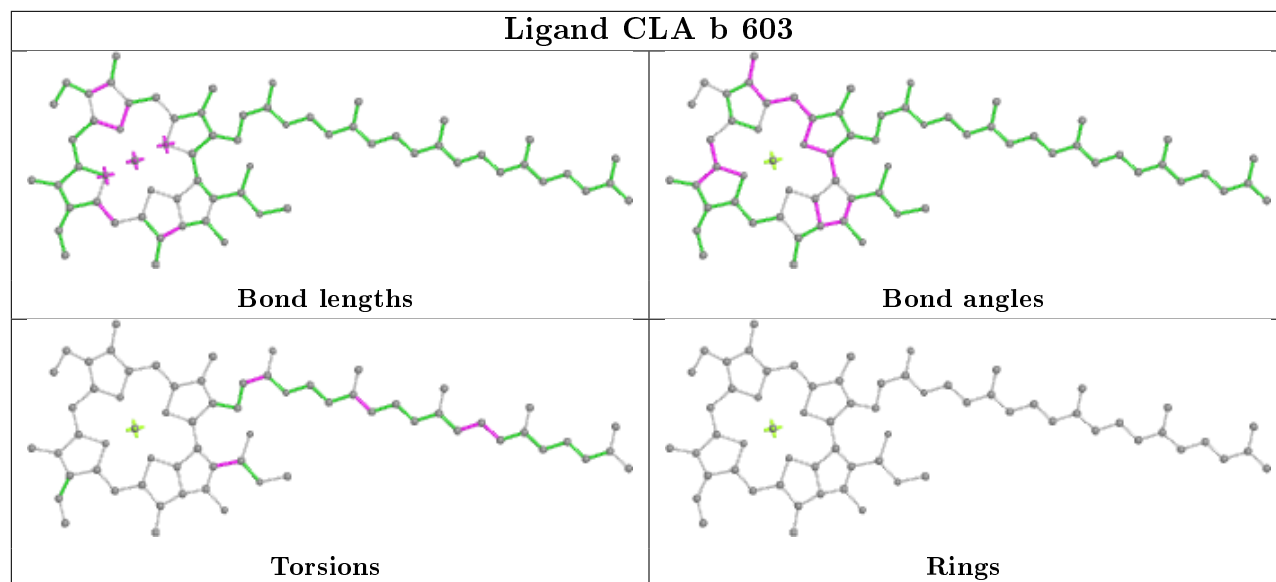
Ligand CLA d 403	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG C 522	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR t 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



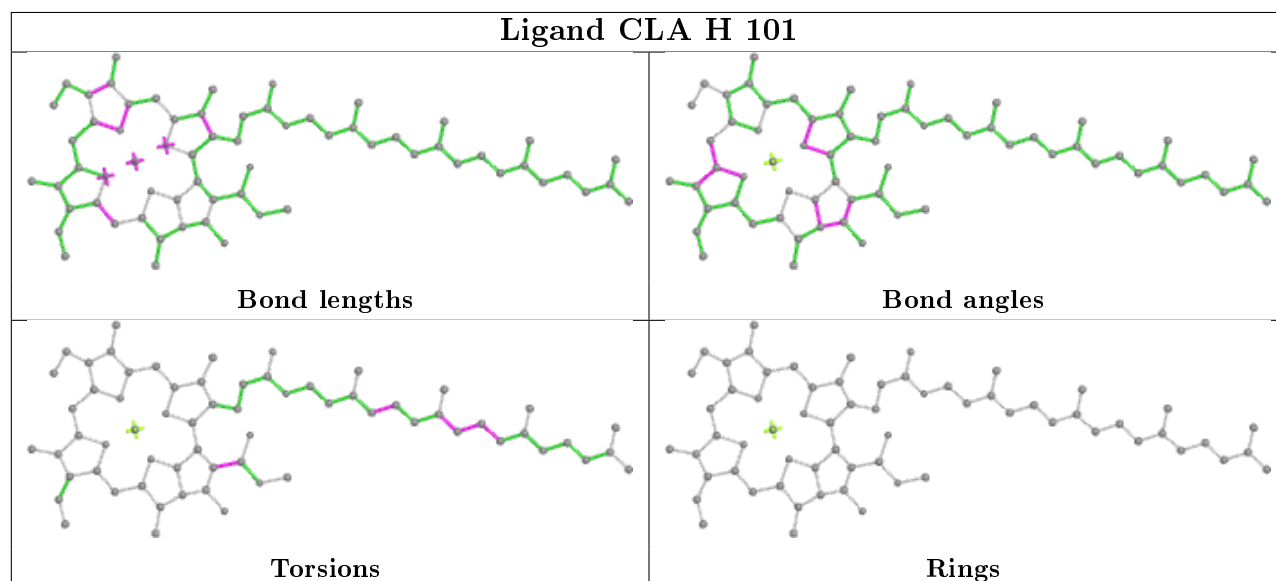
**Ligand CLA b 605****Ligand LHG D 406**

**Ligand CLA B 612****Ligand BCR H 102****Ligand CLA B 613**

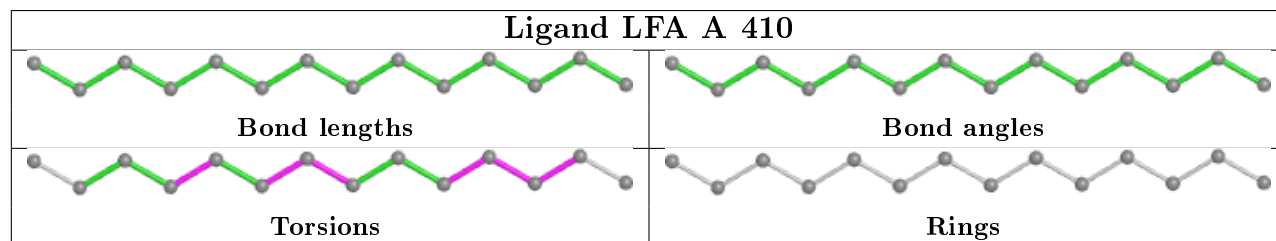
## Ligand CLA b 603



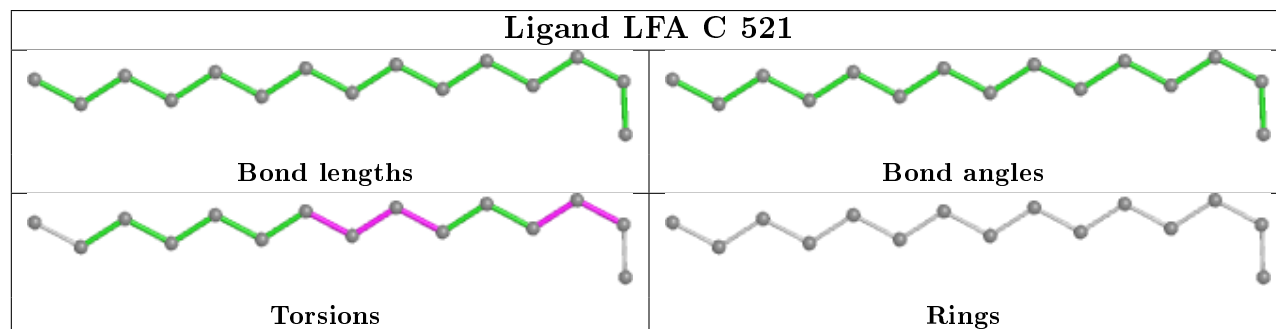
## Ligand CLA H 101



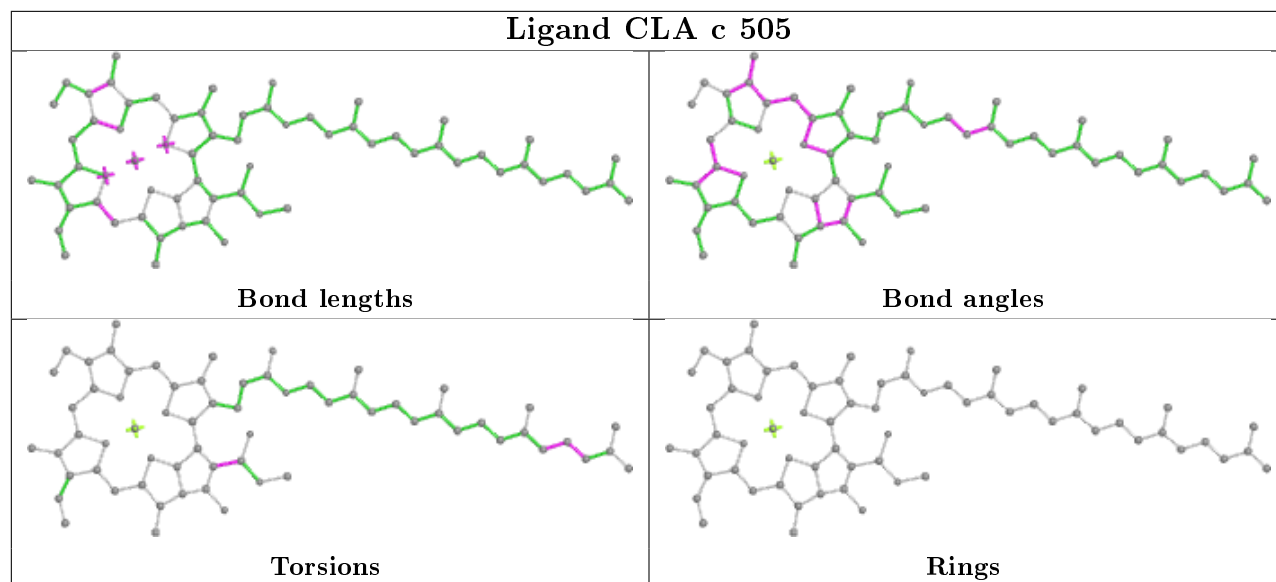
## Ligand LFA A 410



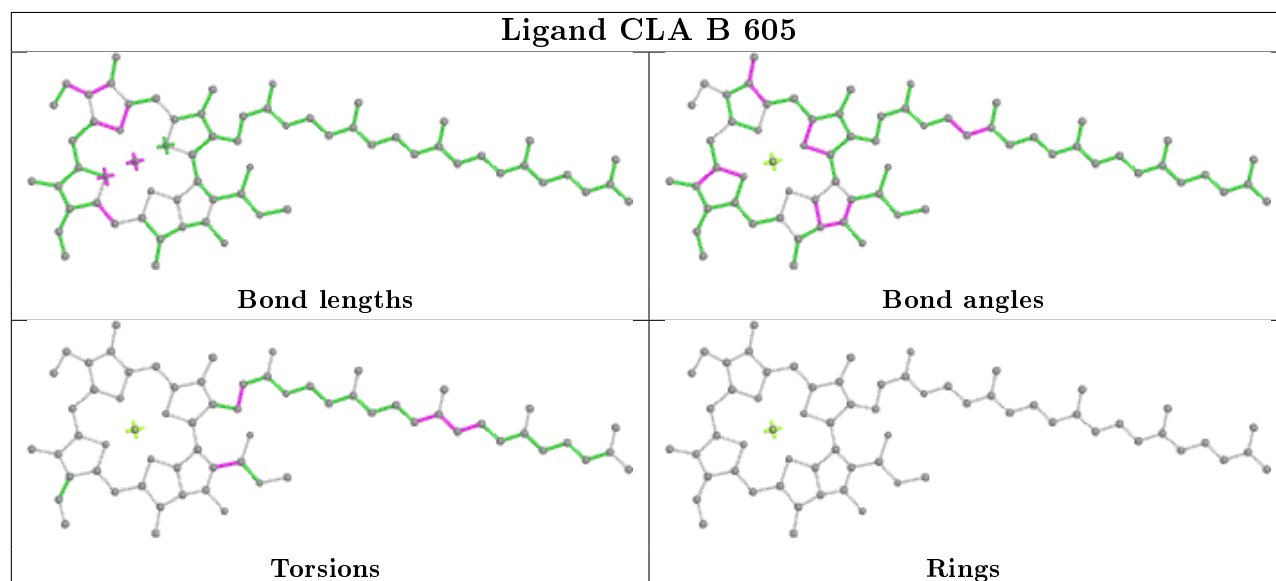
## Ligand LFA C 521



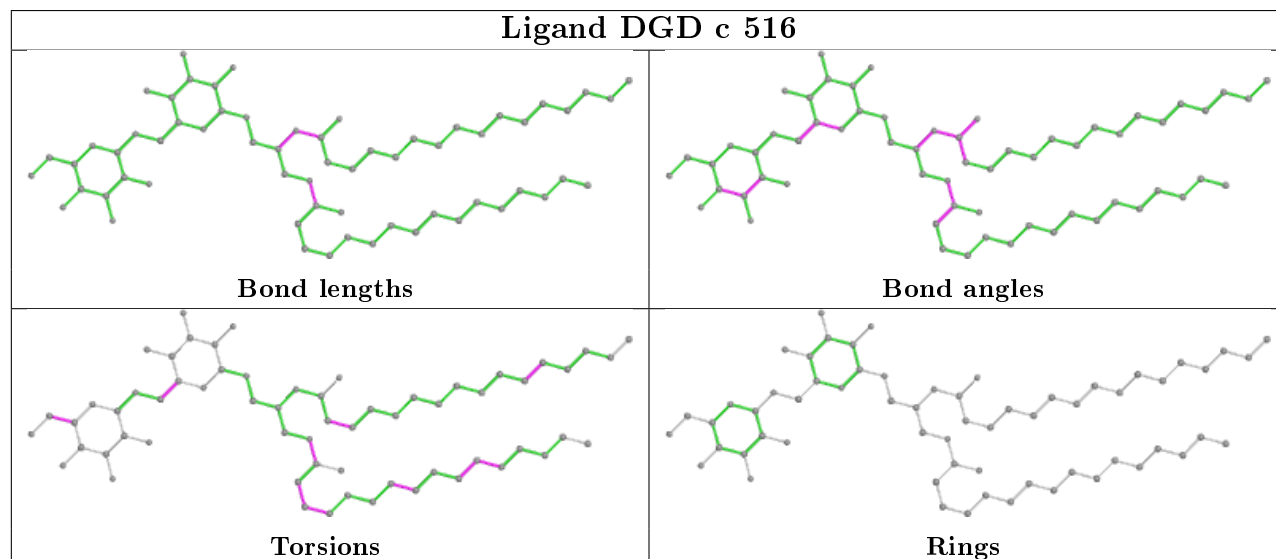
## Ligand CLA c 505

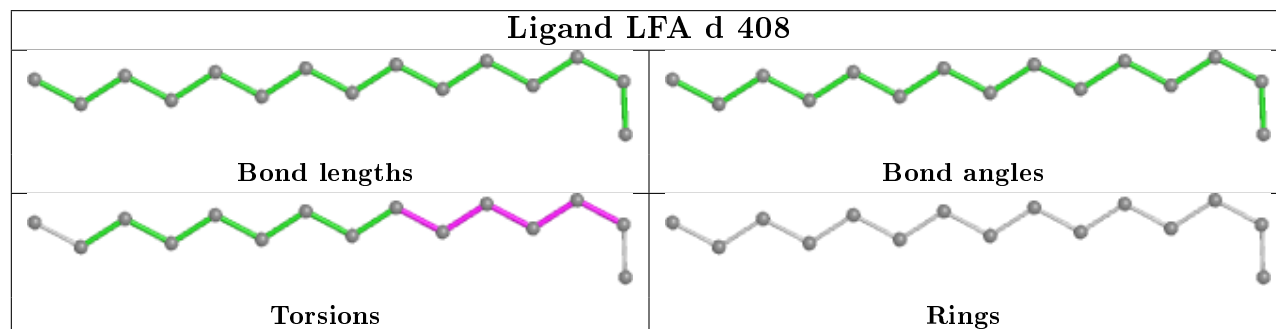
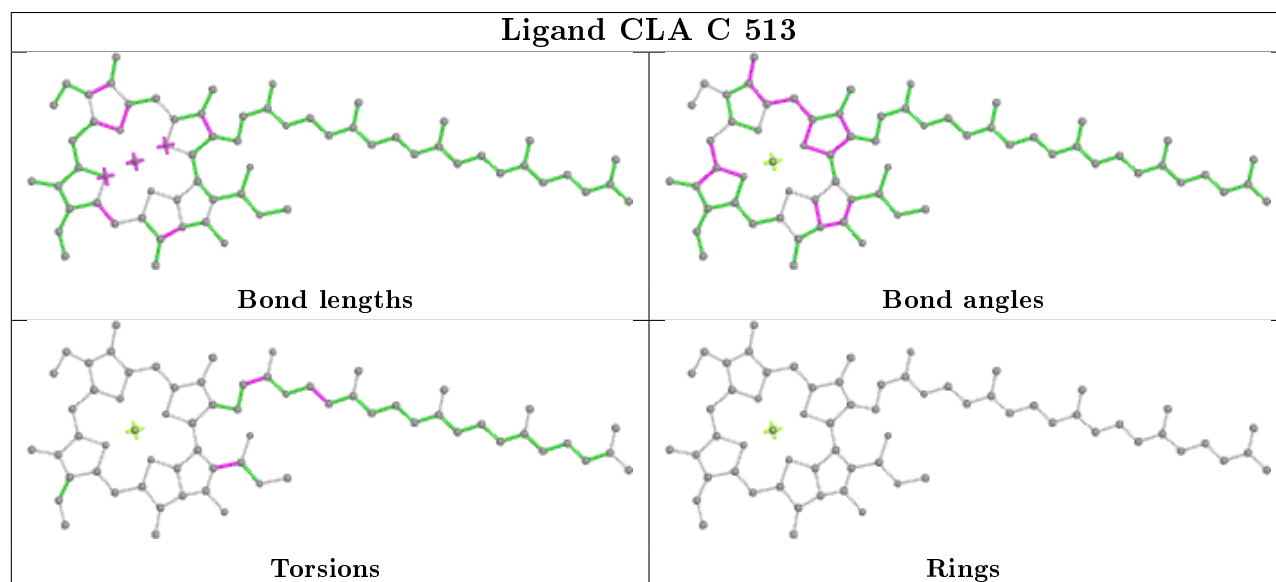
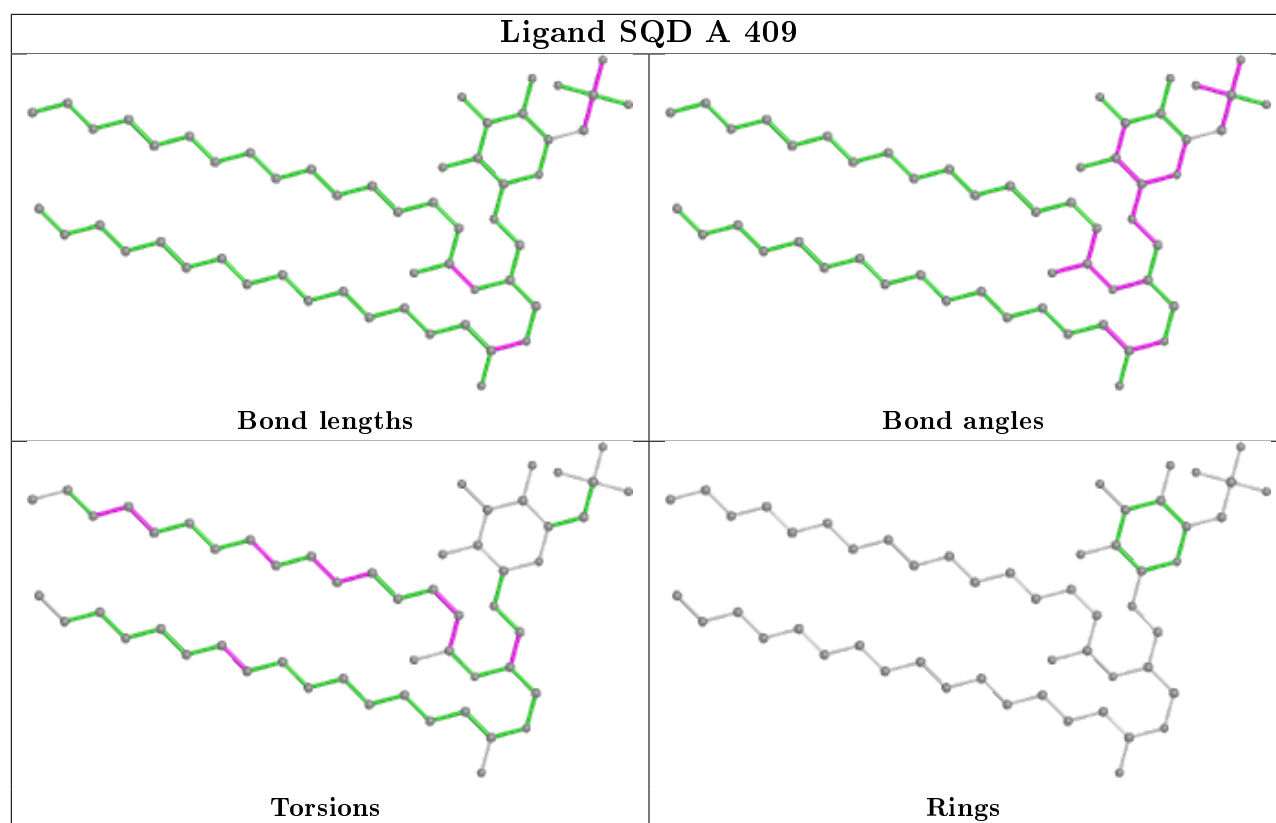


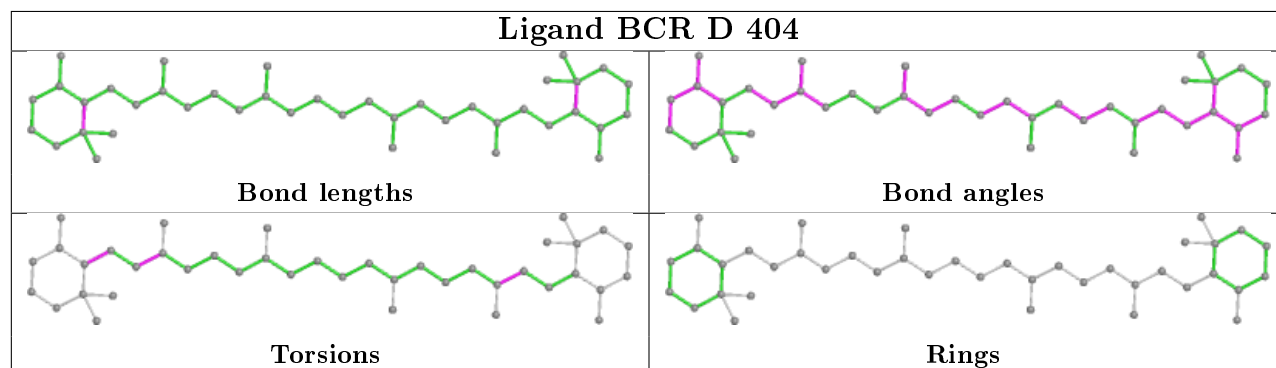
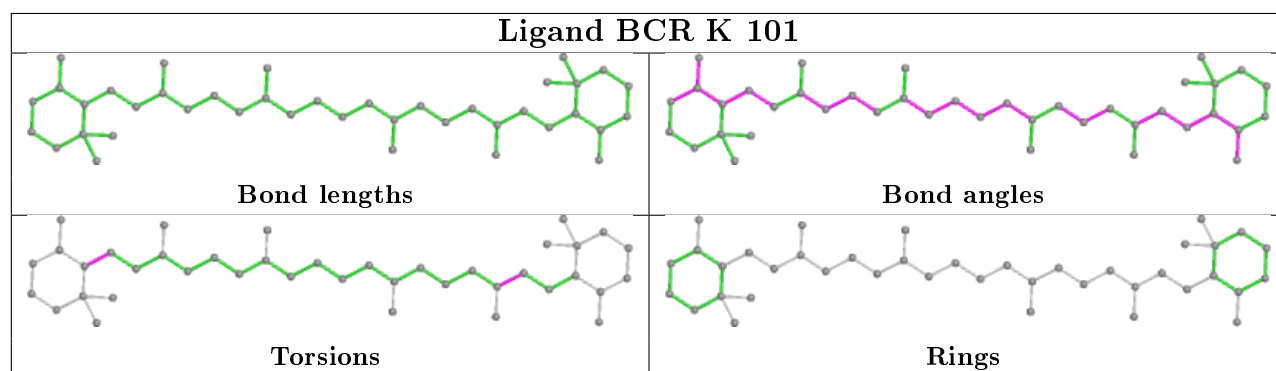
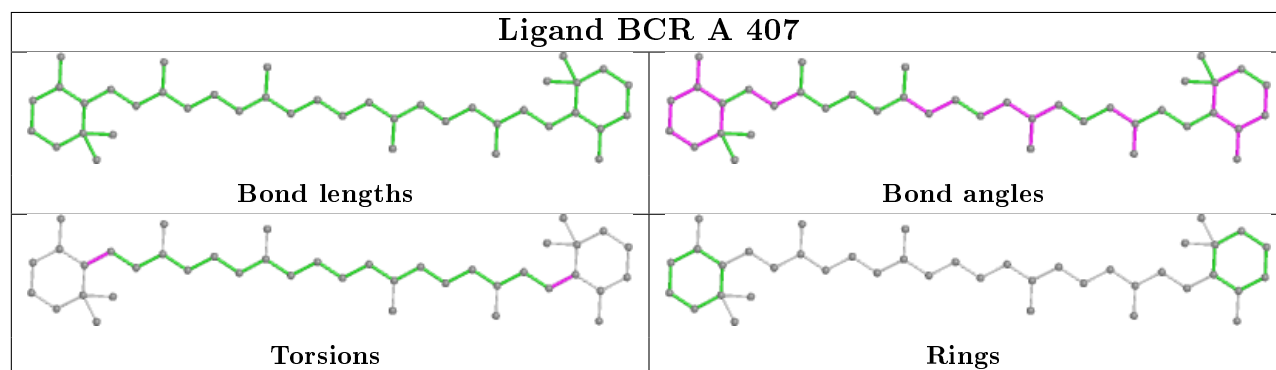
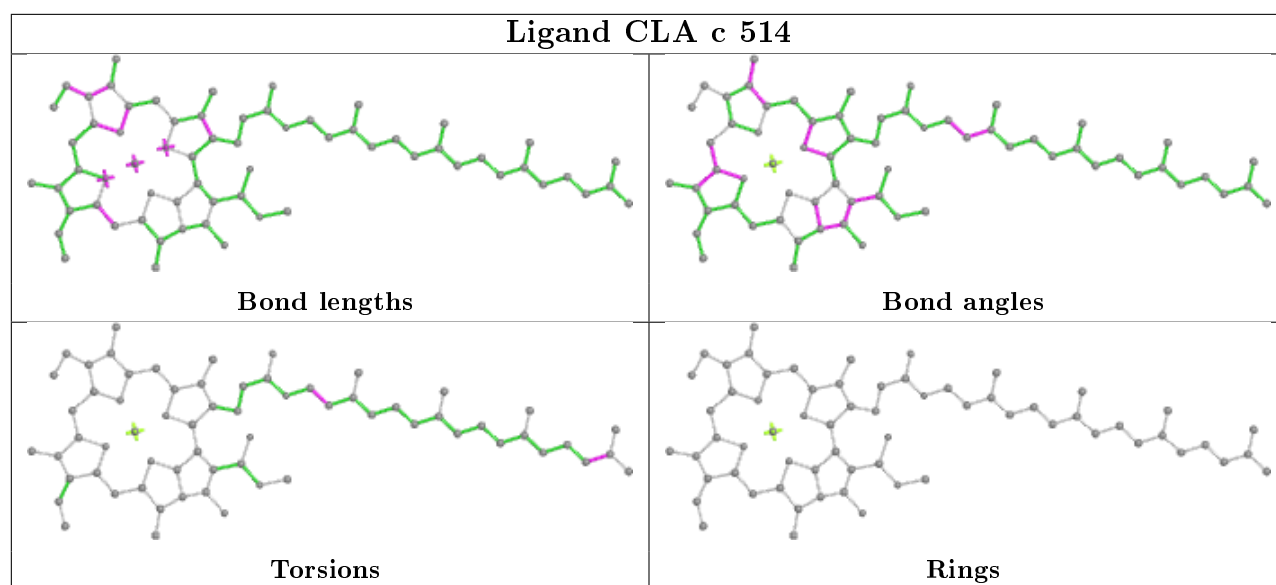
## Ligand CLA B 605



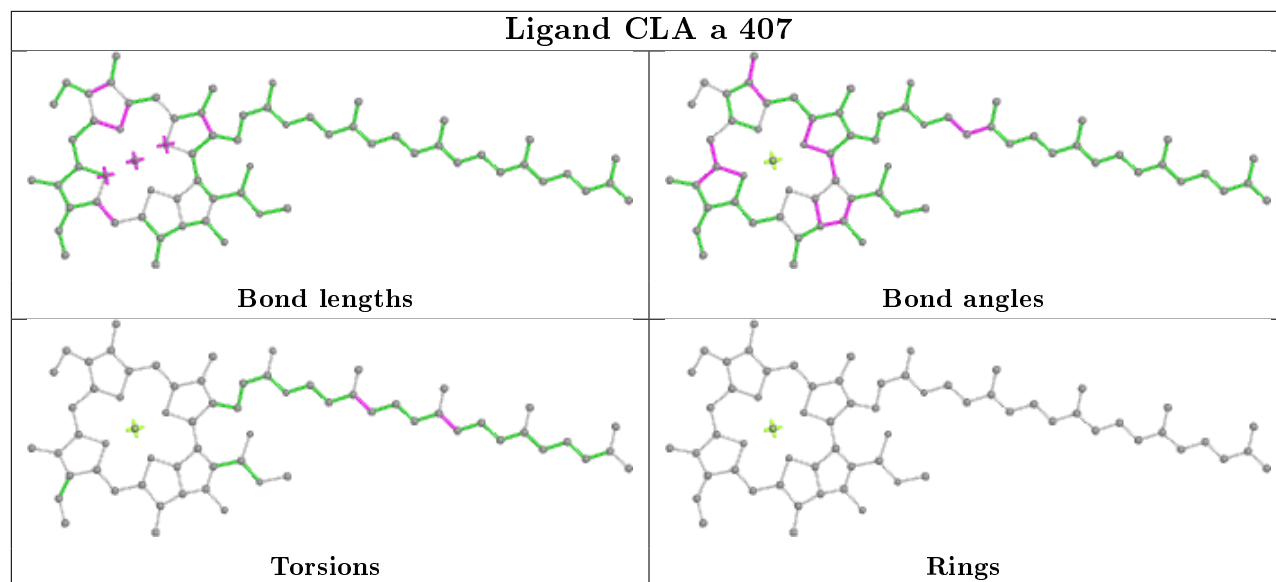
## Ligand DGD c 516



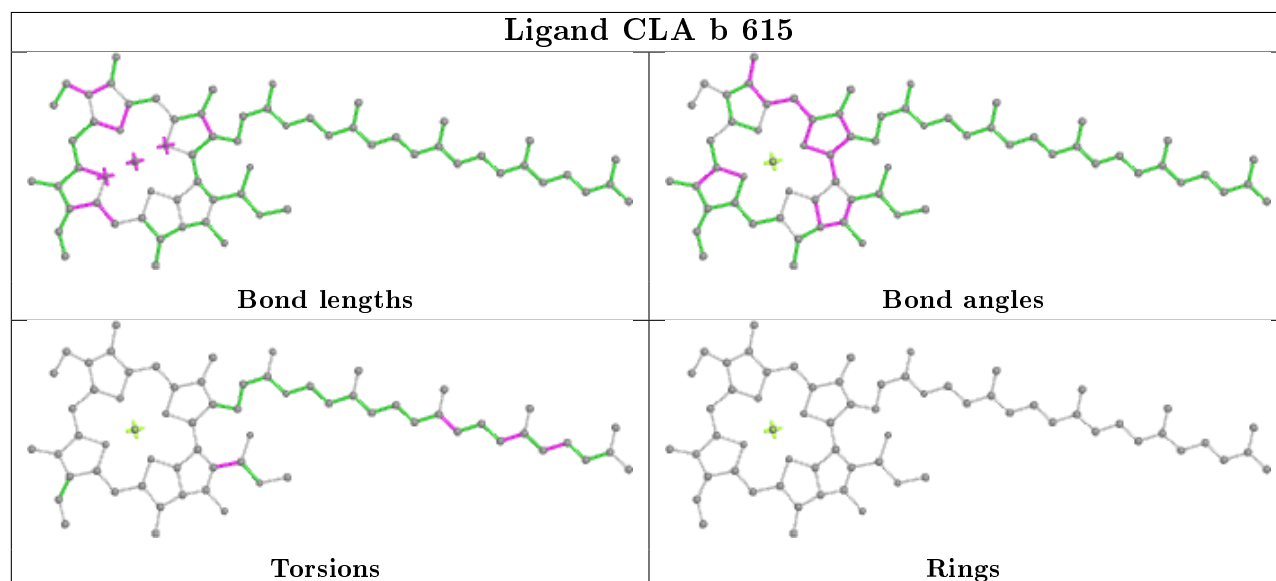




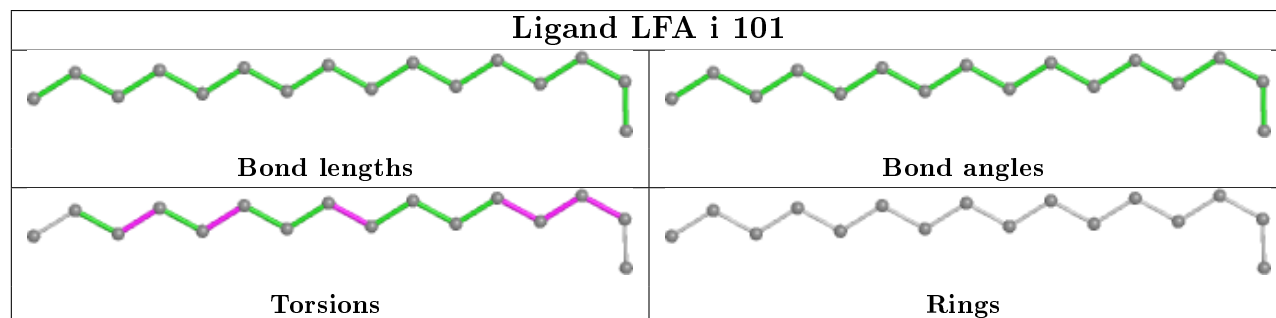
## Ligand CLA a 407

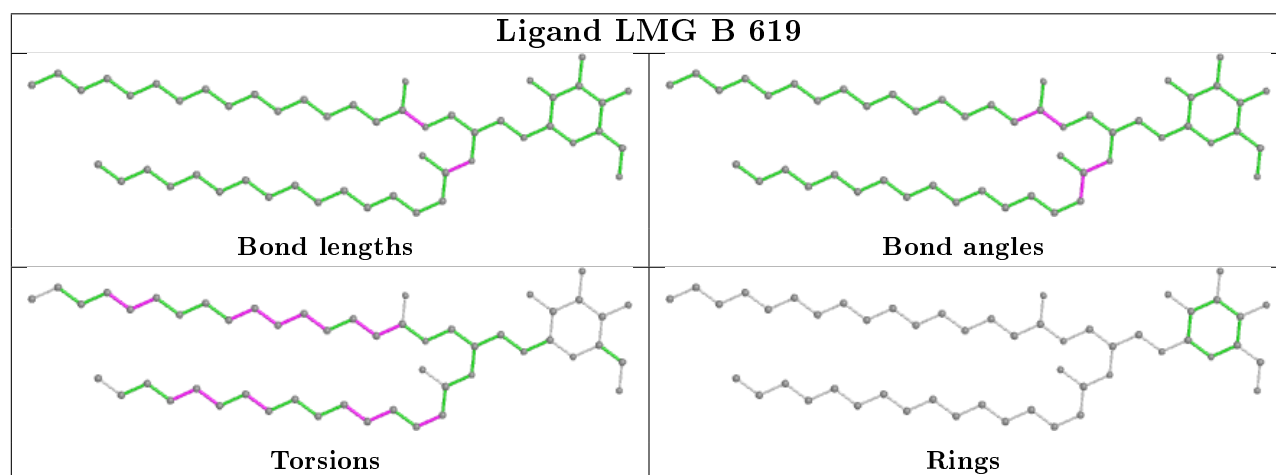
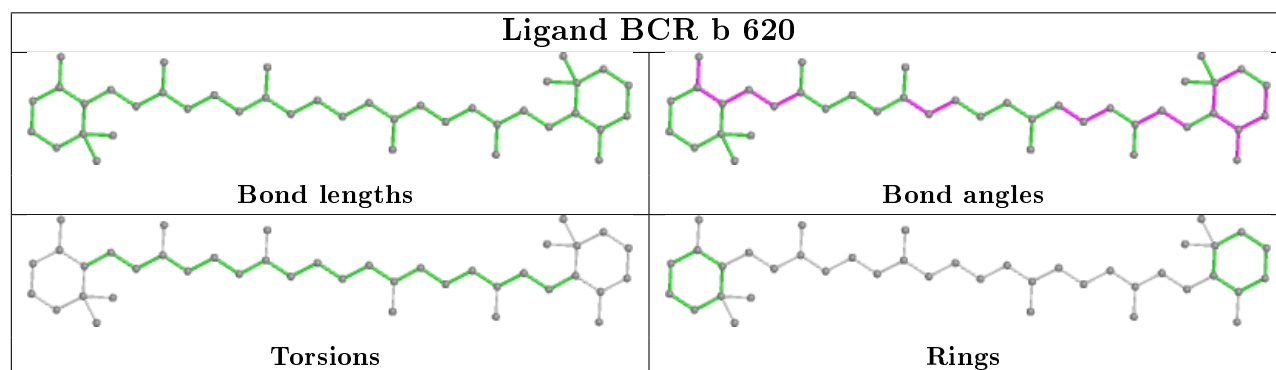
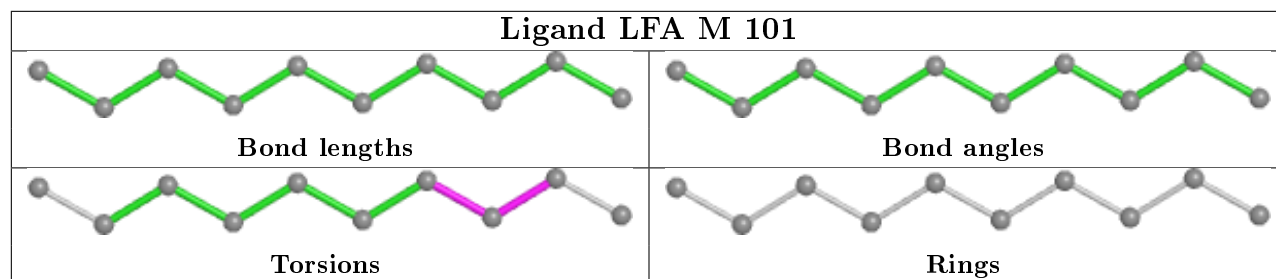
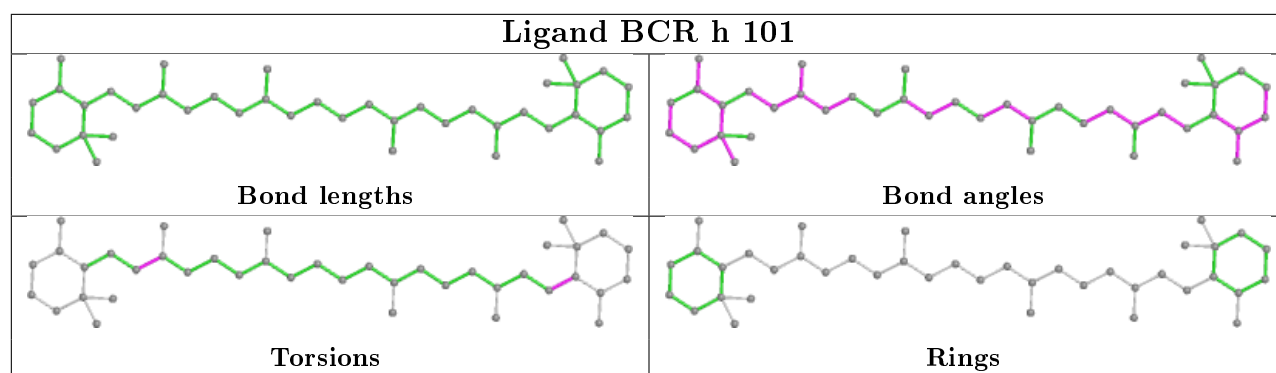


## Ligand CLA b 615

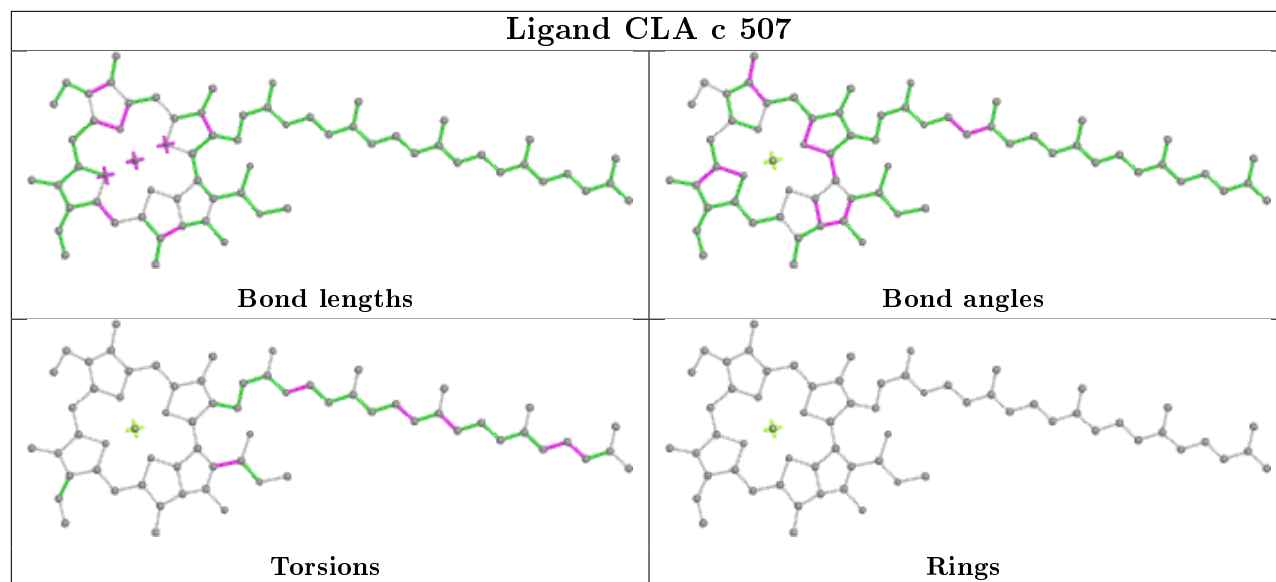


## Ligand LFA i 101

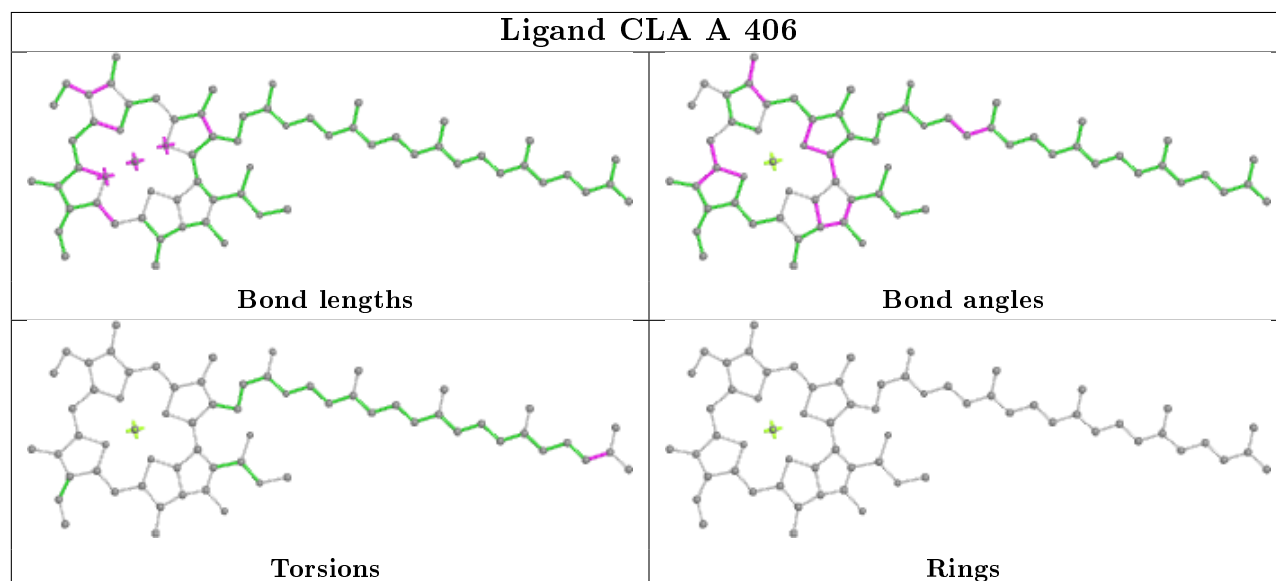




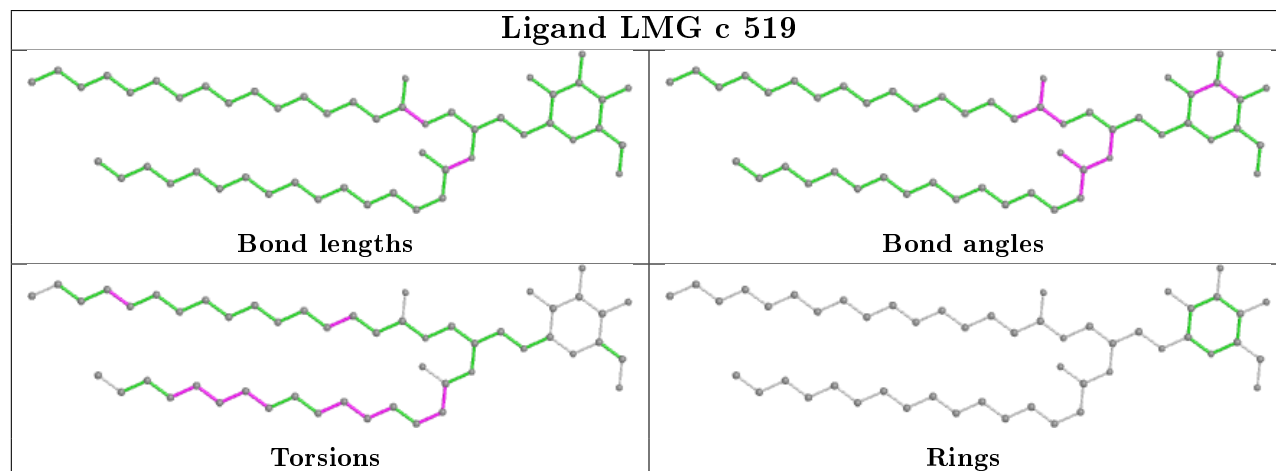
## Ligand CLA c 507

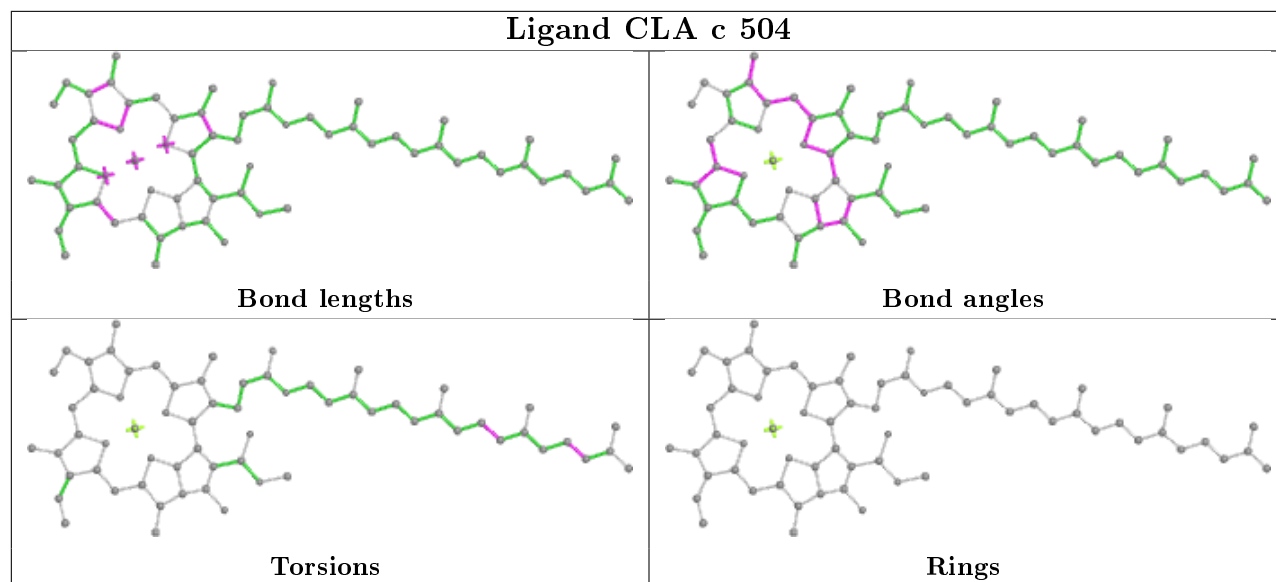
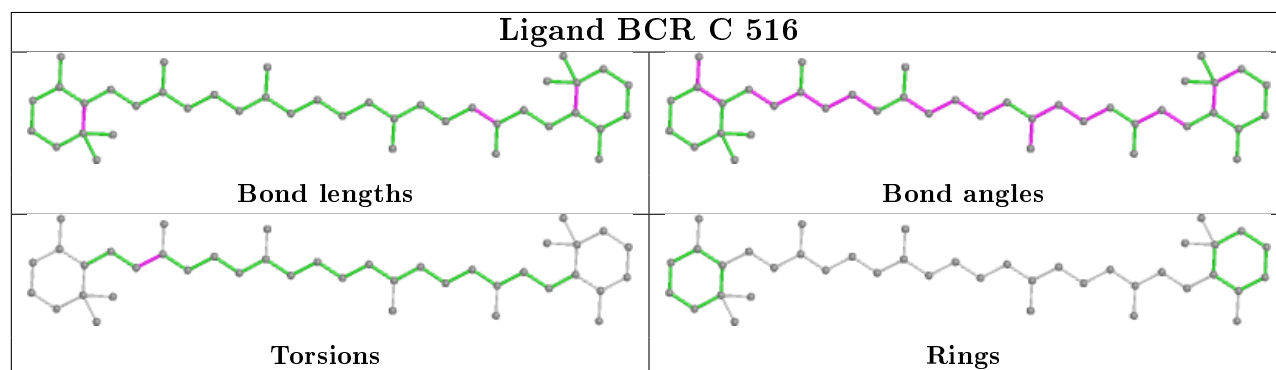
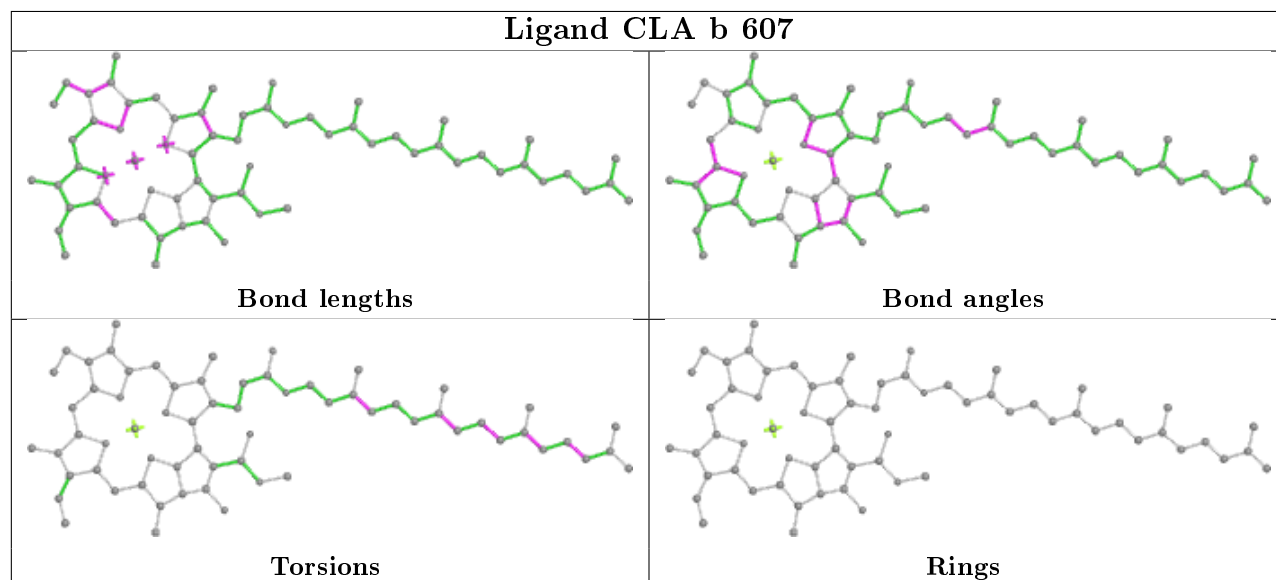


## Ligand CLA A 406

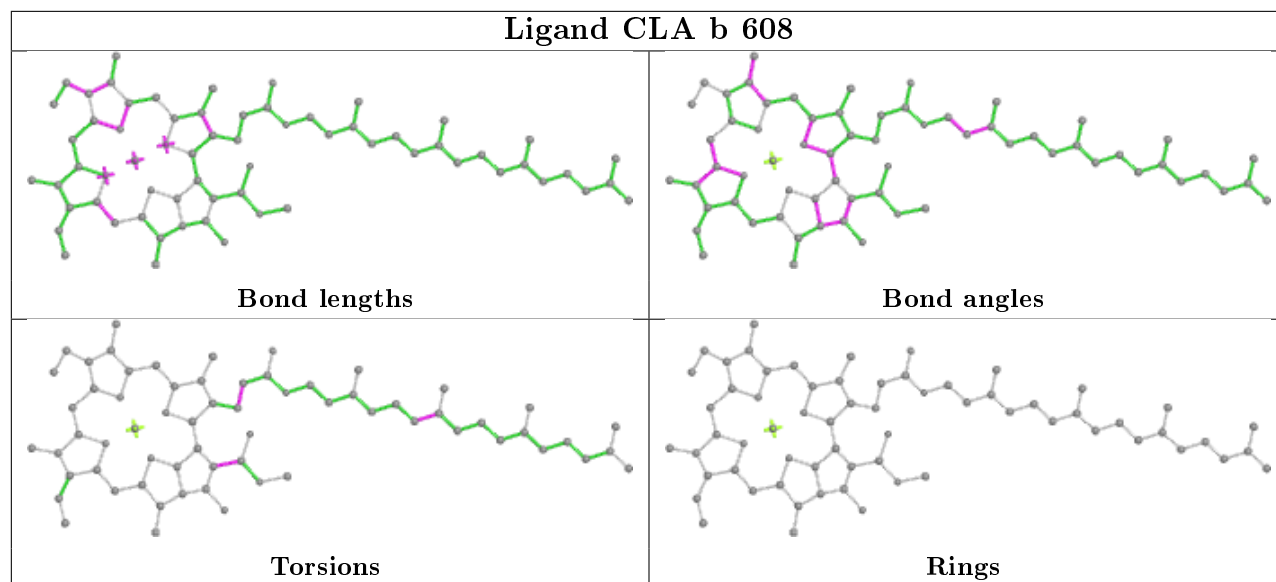


## Ligand LMG c 519

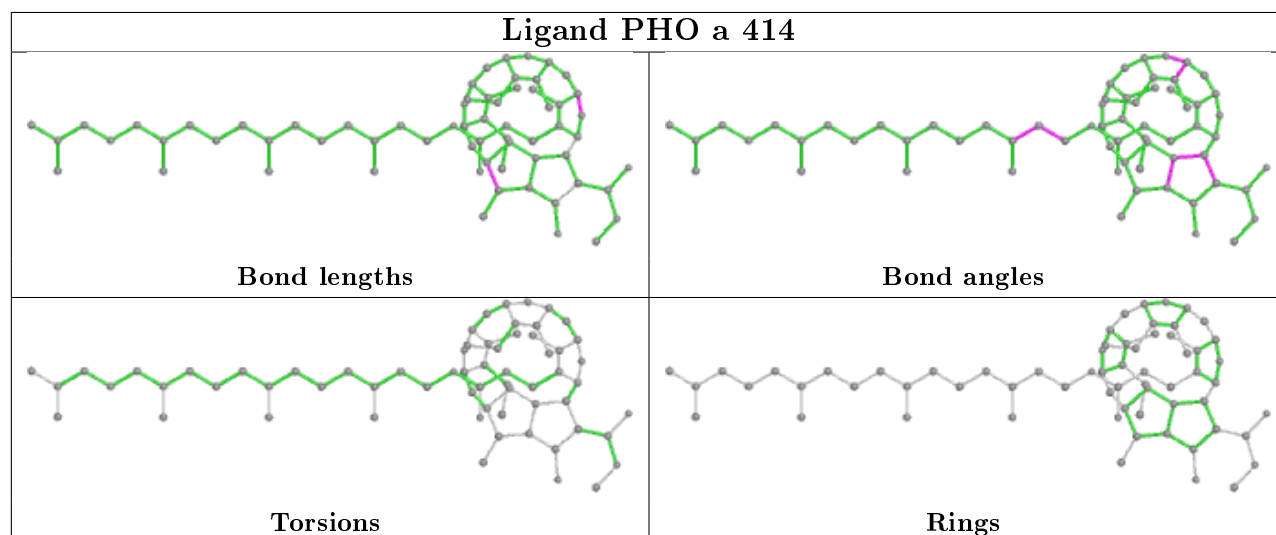


**Ligand CLA c 504****Ligand BCR C 516****Ligand CLA b 607**

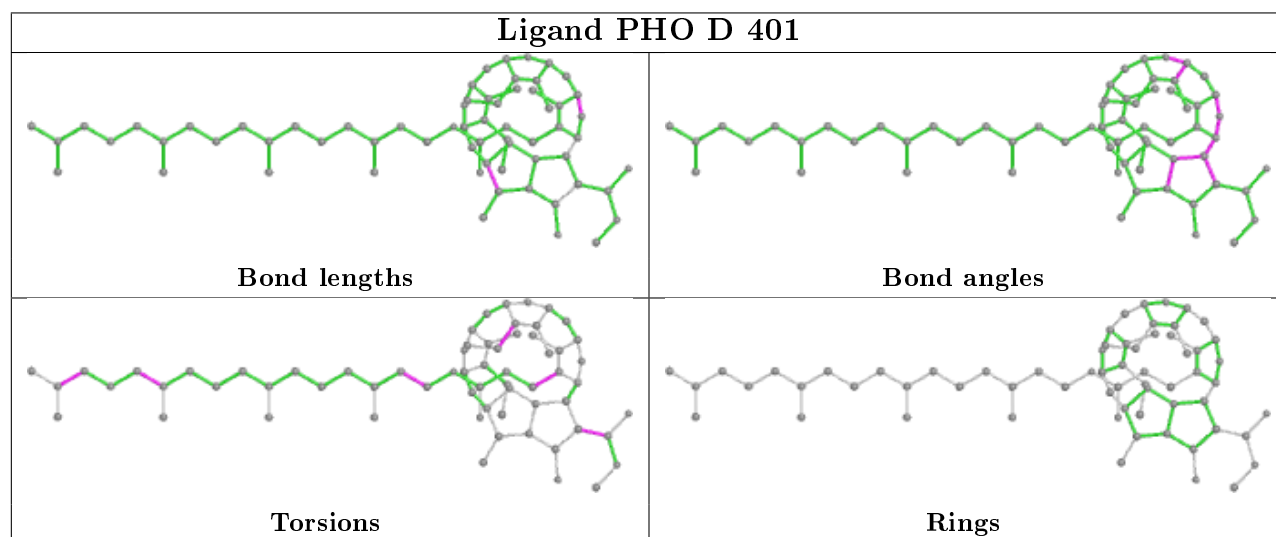
## Ligand CLA b 608

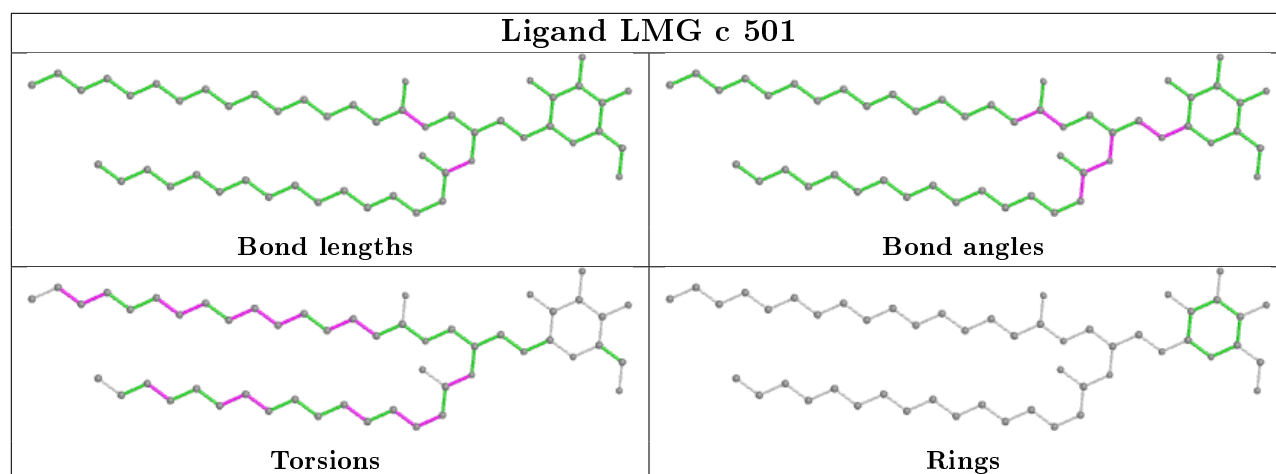
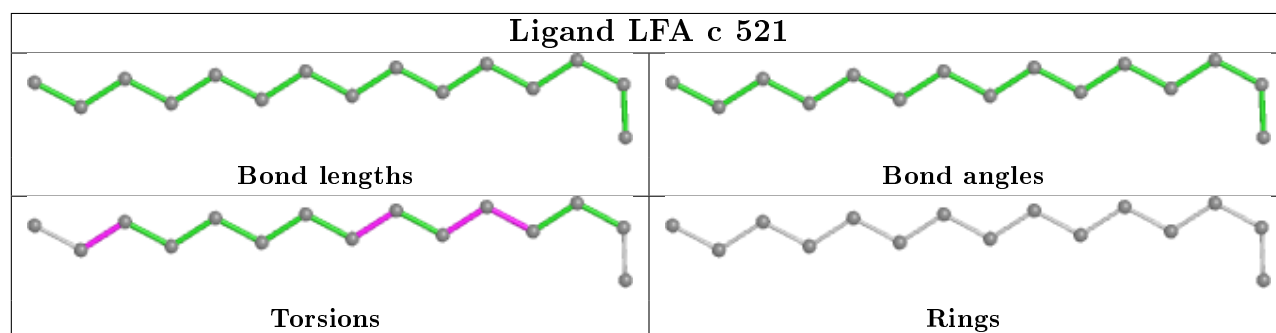
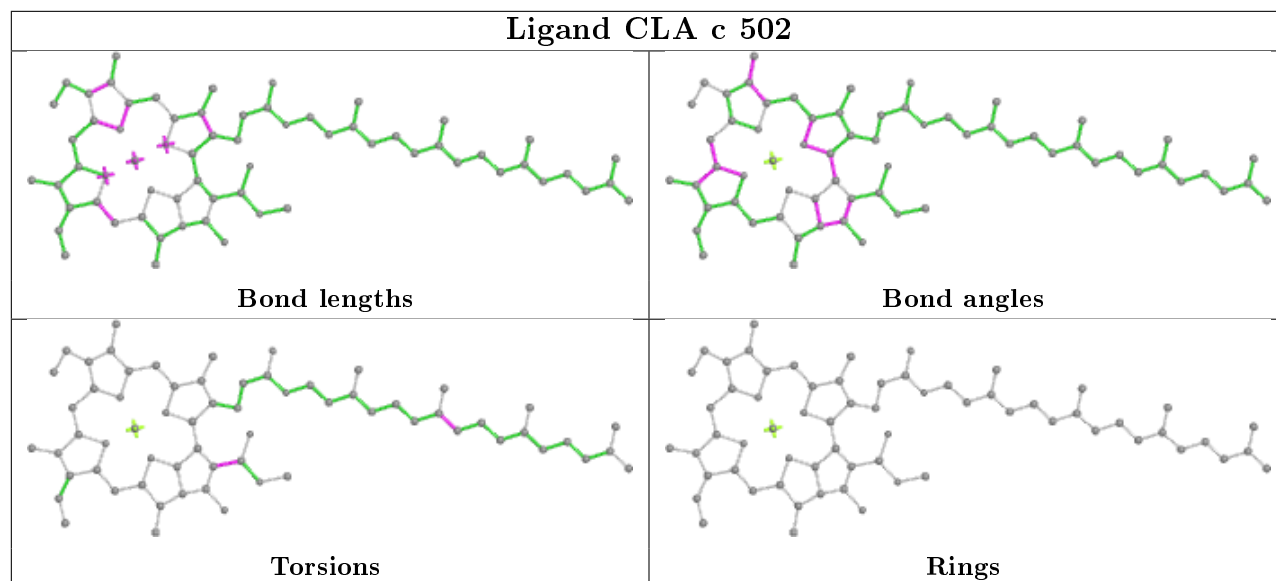
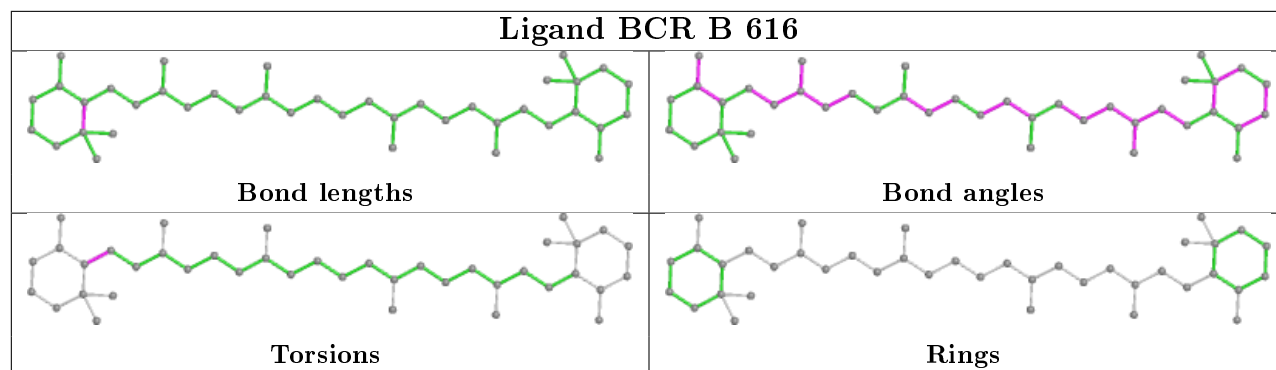


## Ligand PHO a 414

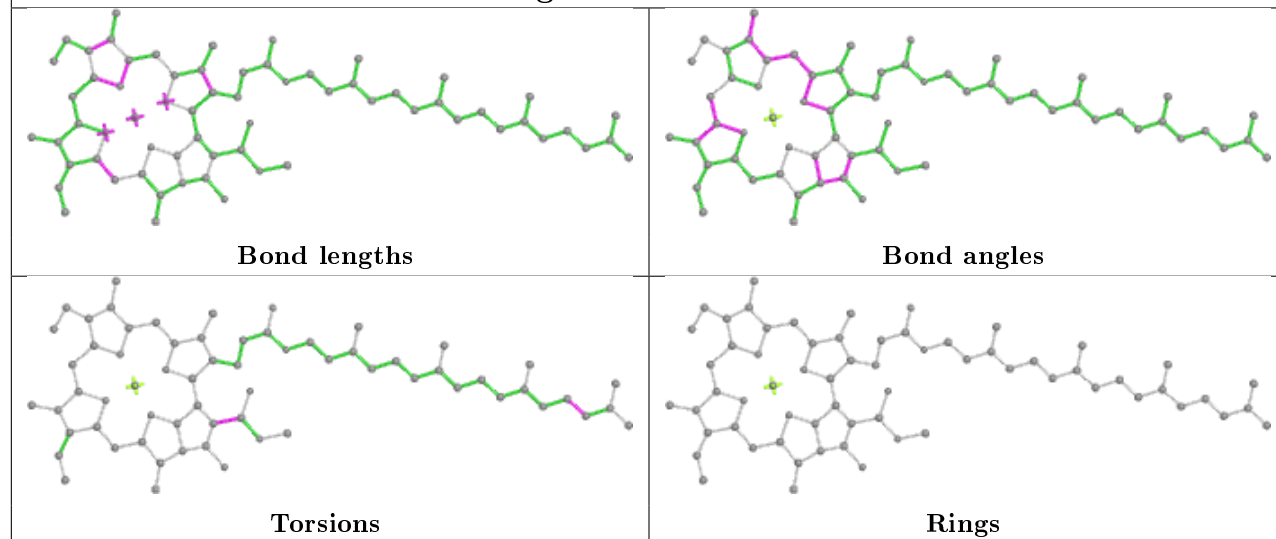


## Ligand PHO D 401

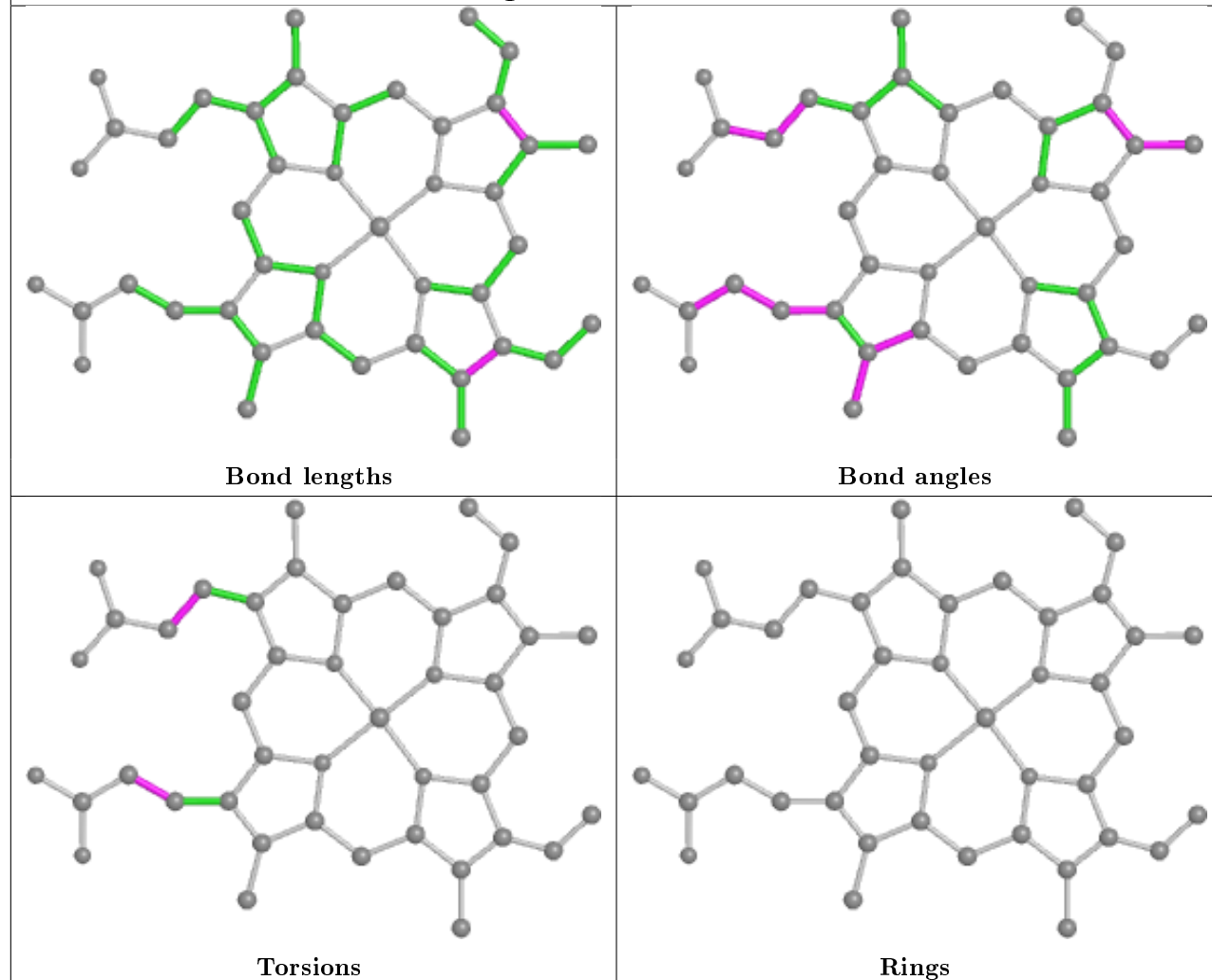


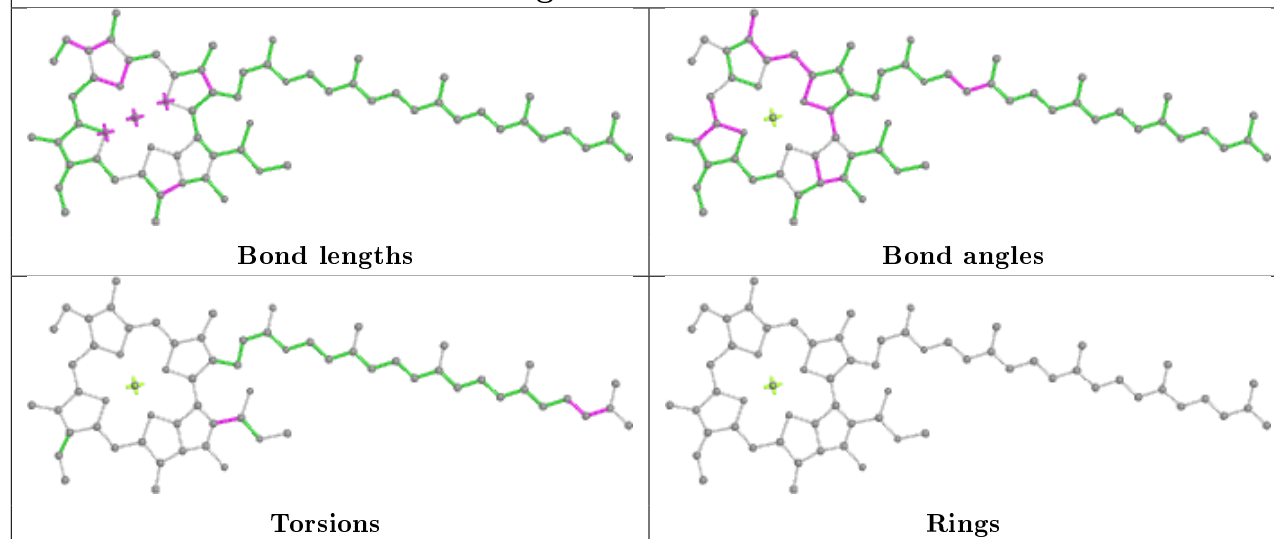
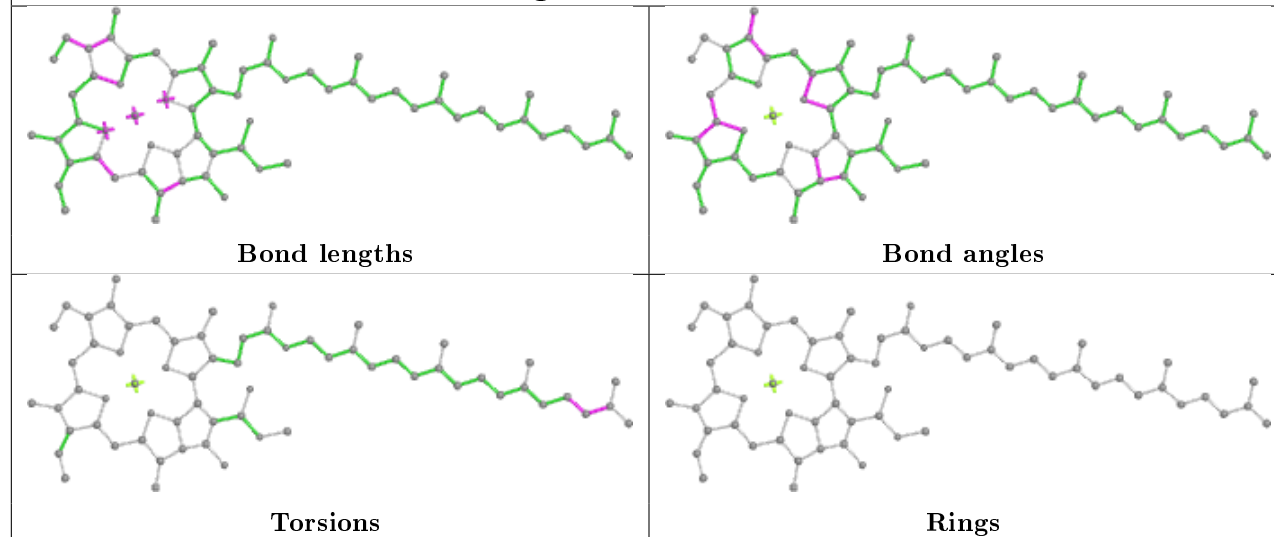
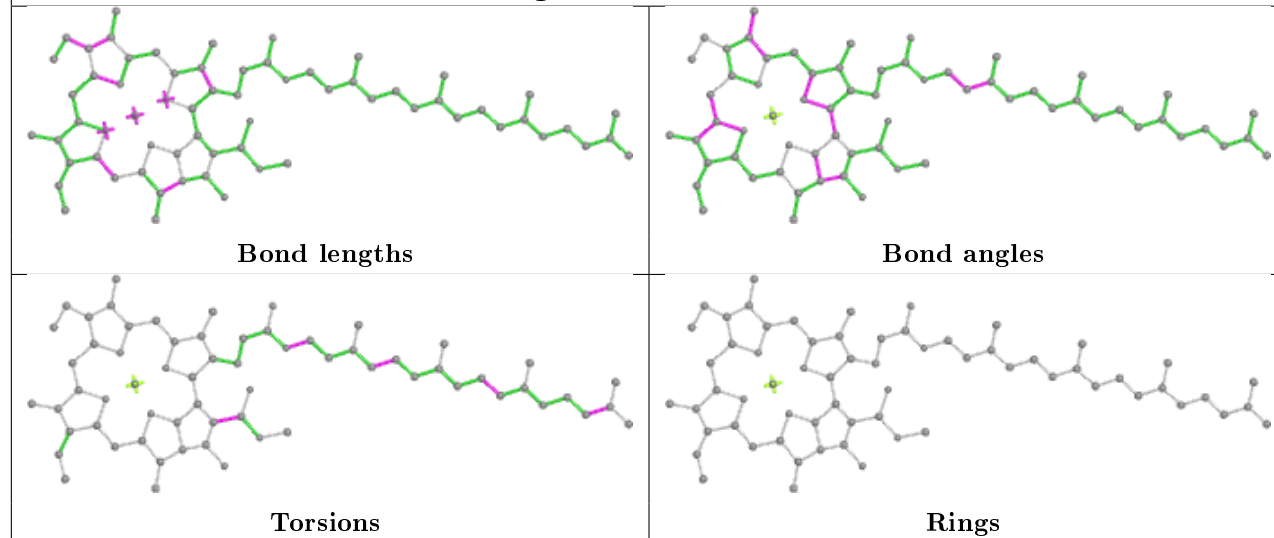


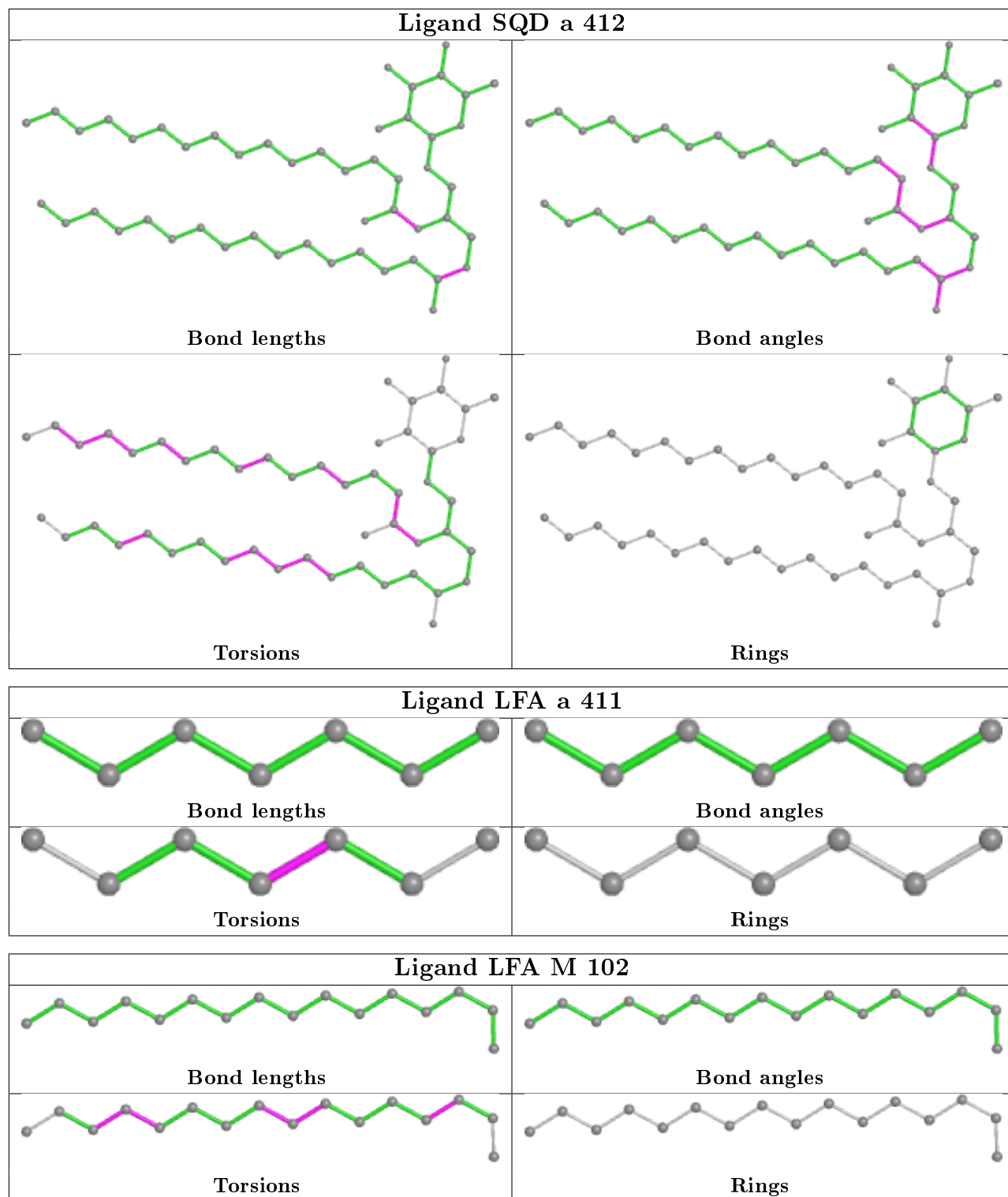
## Ligand CLA a 404

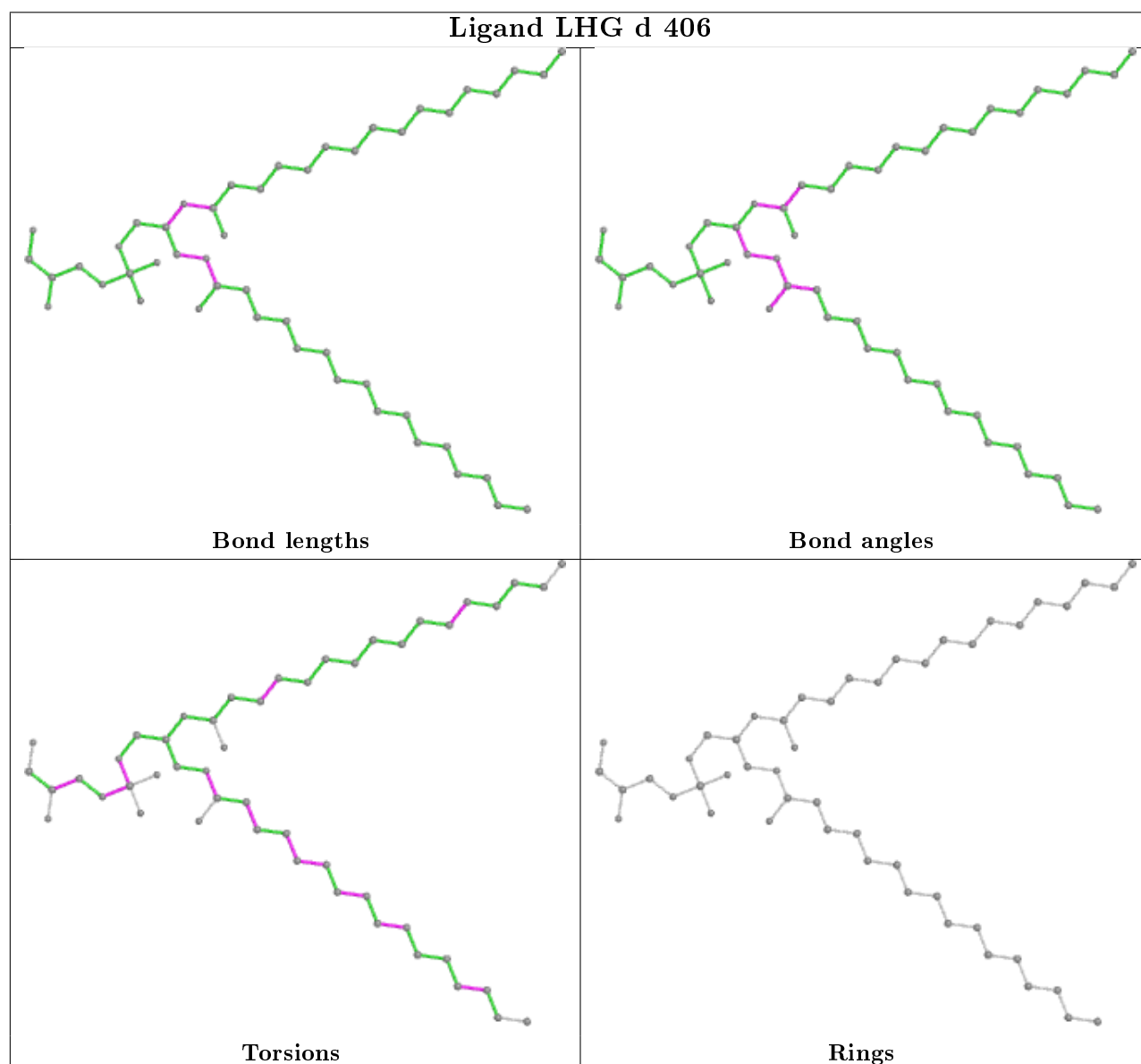
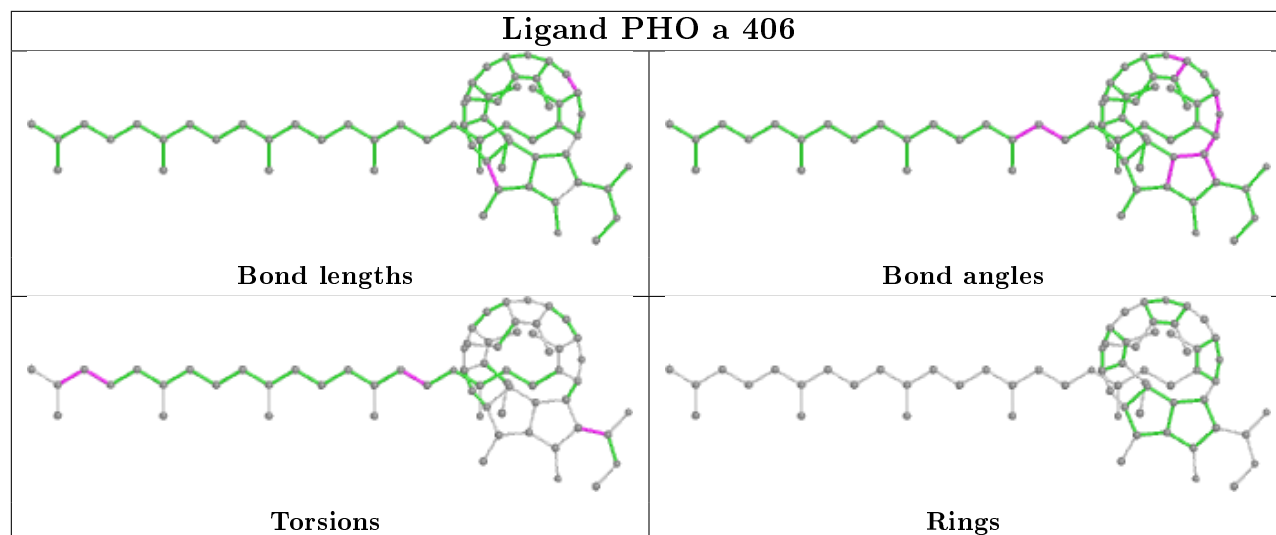


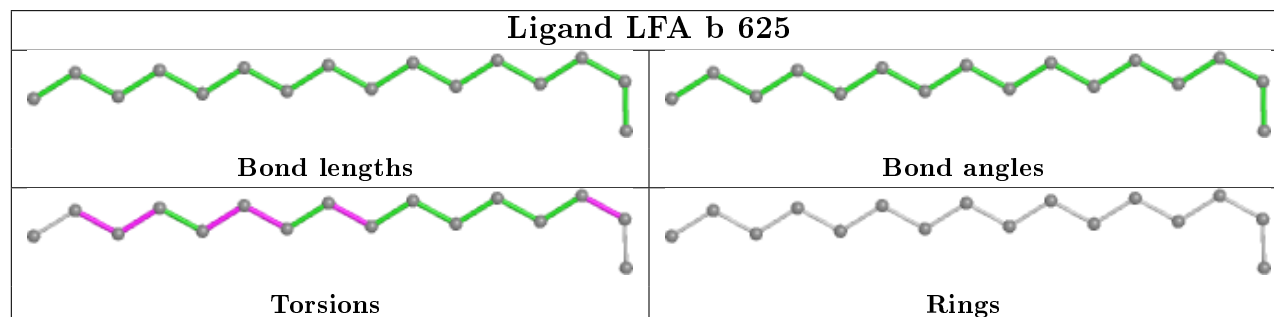
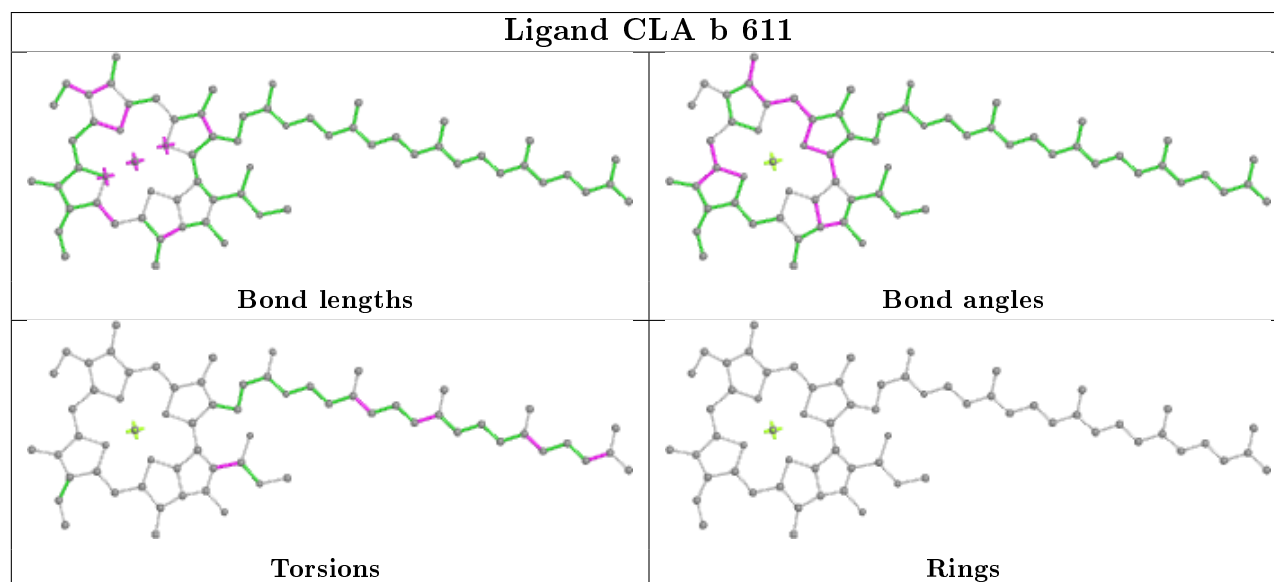
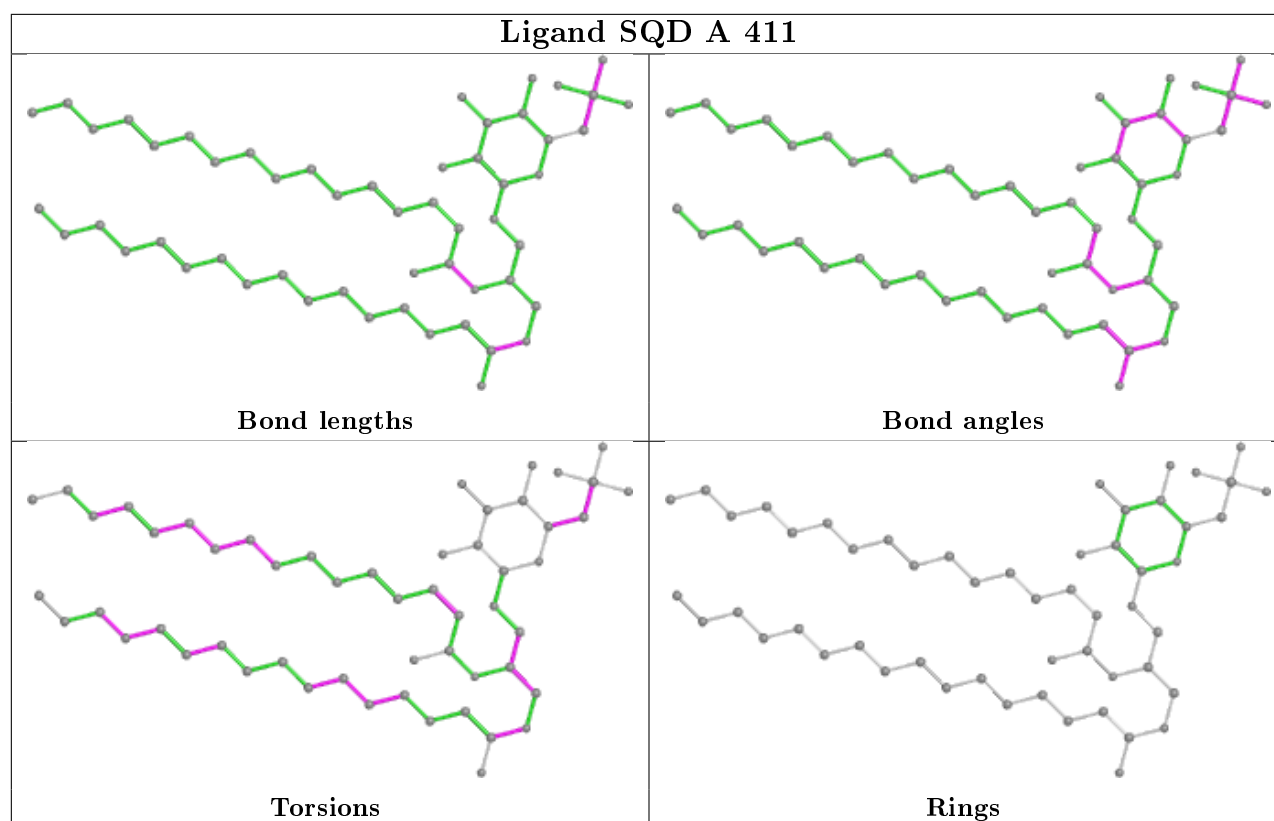
## Ligand HEM E 102

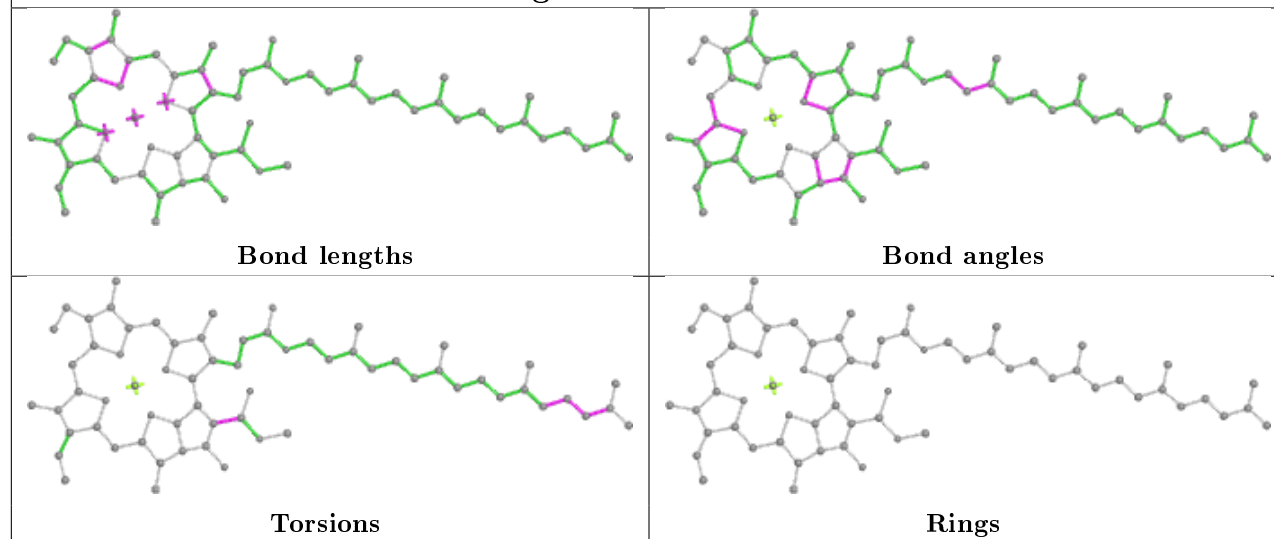
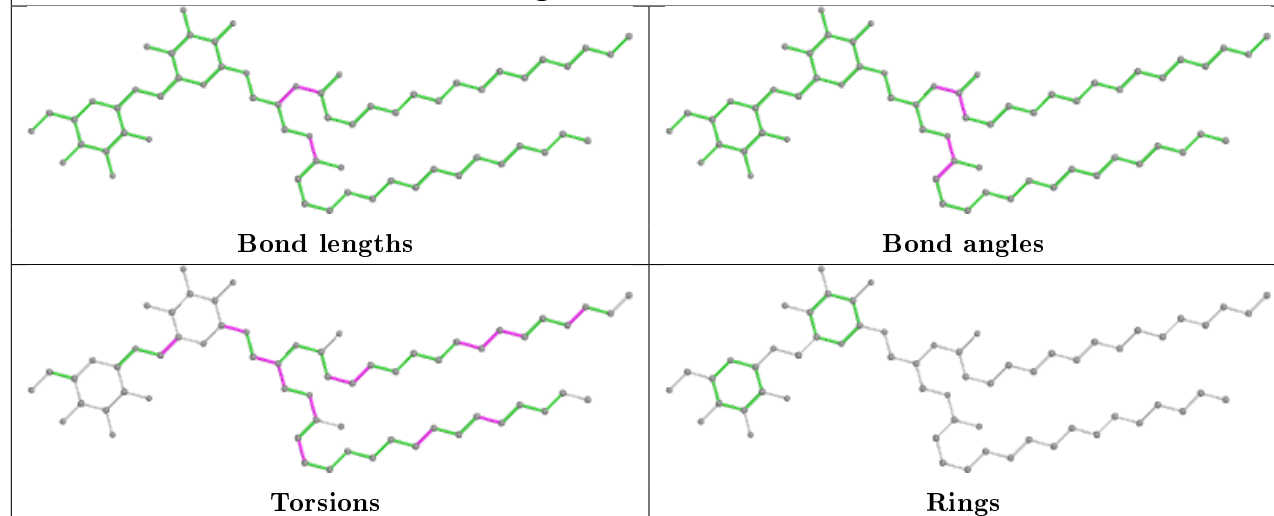
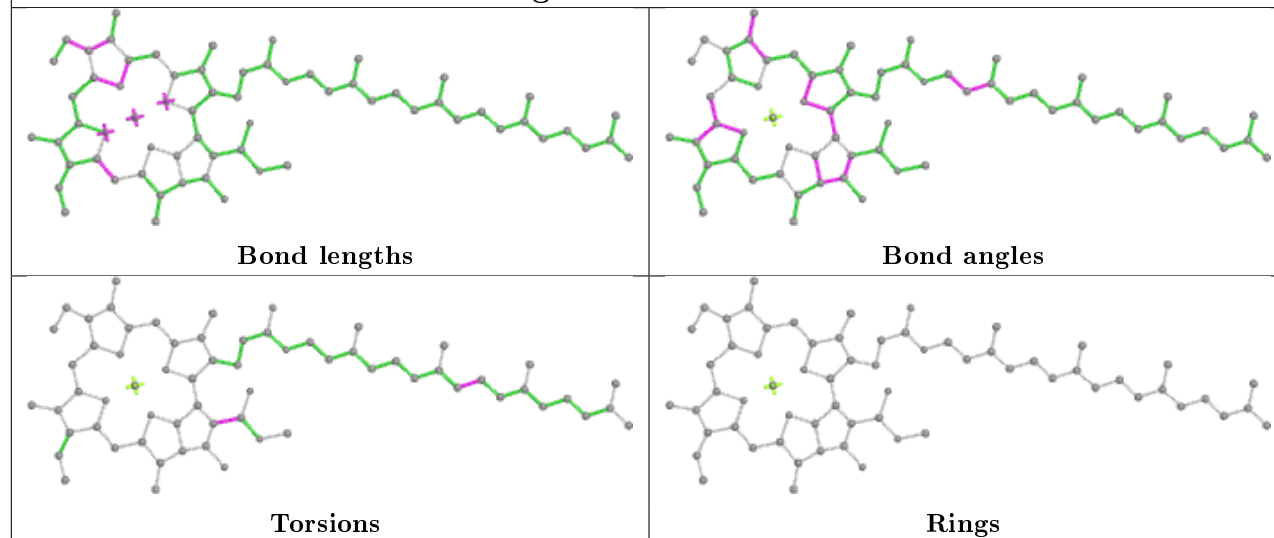


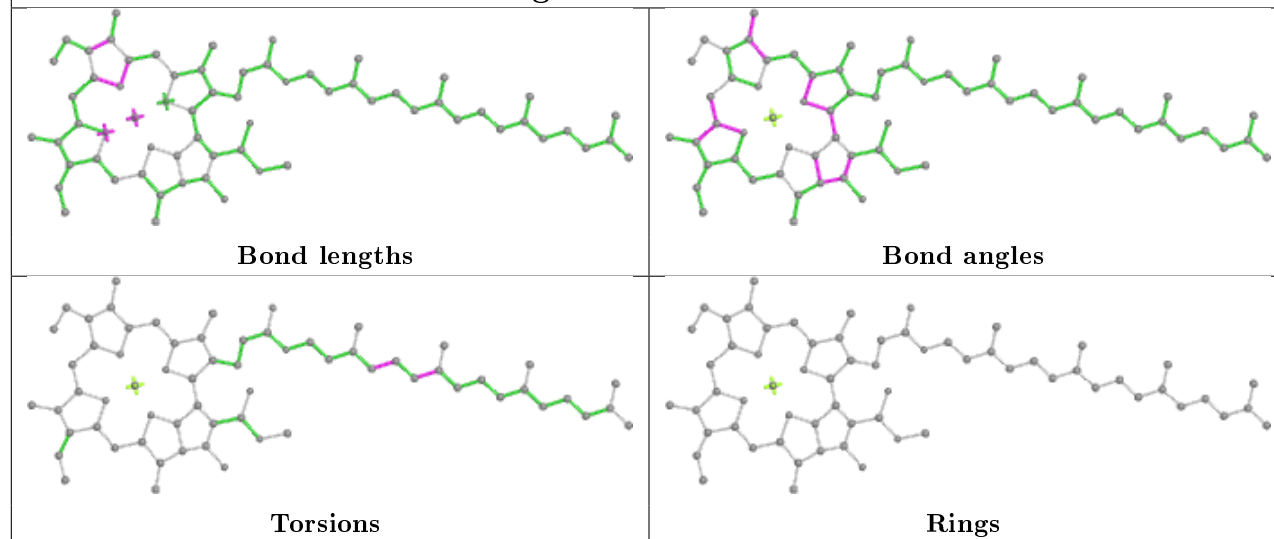
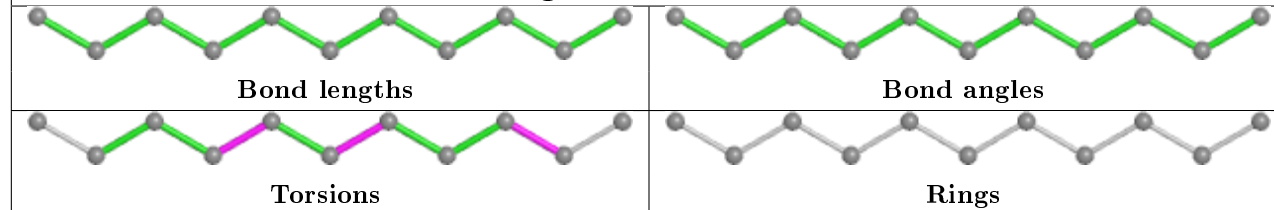
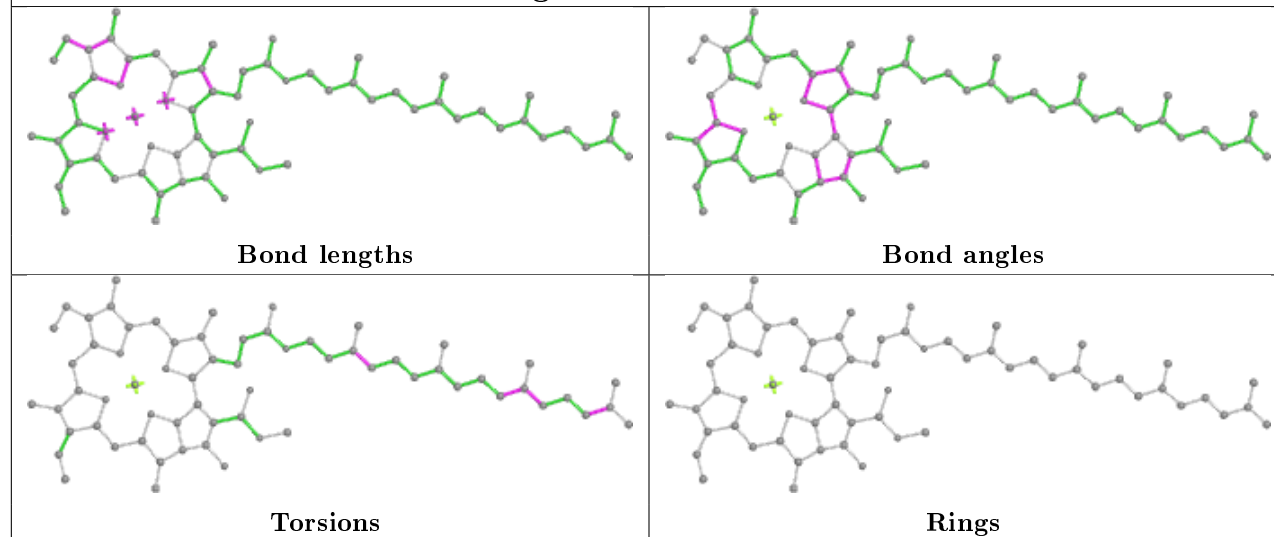
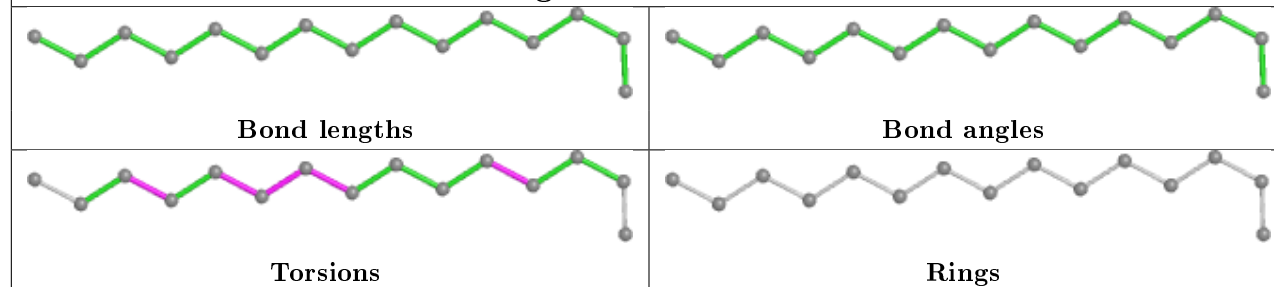
**Ligand CLA a 405****Ligand CLA B 607****Ligand CLA C 507**

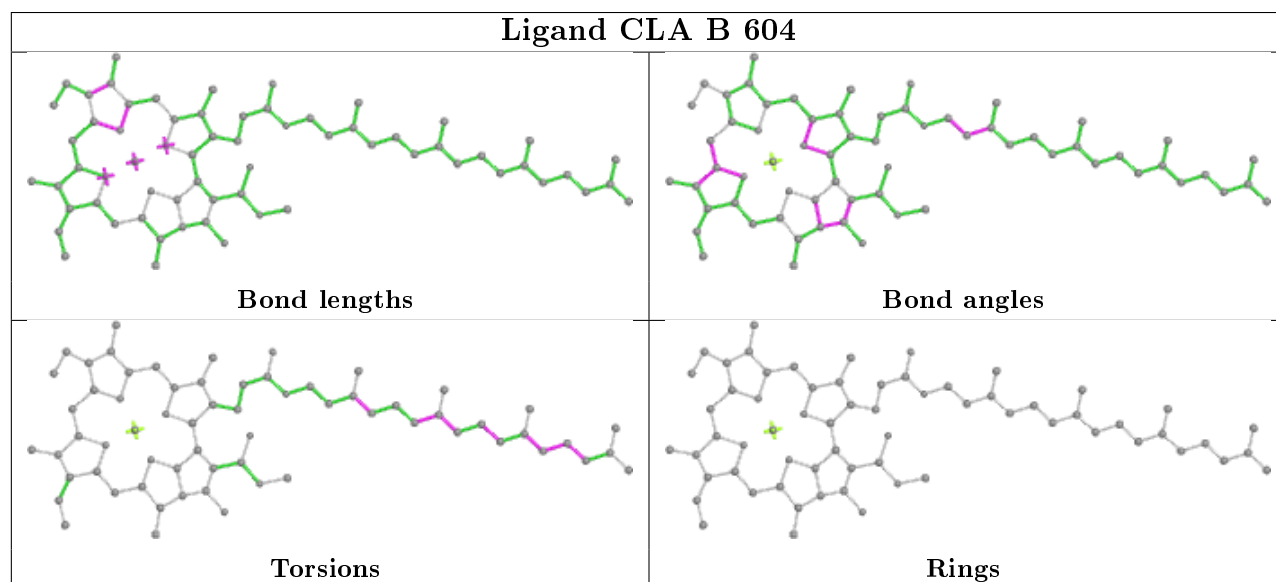
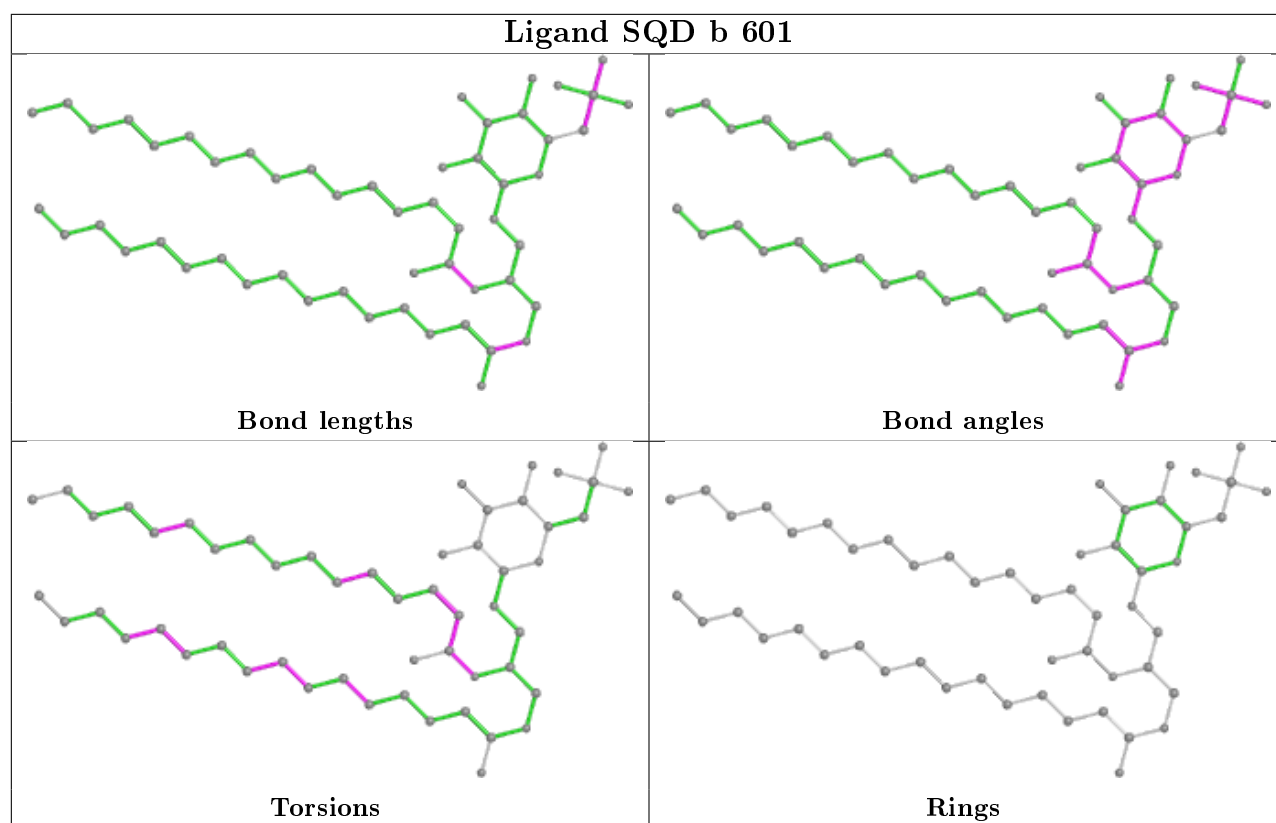


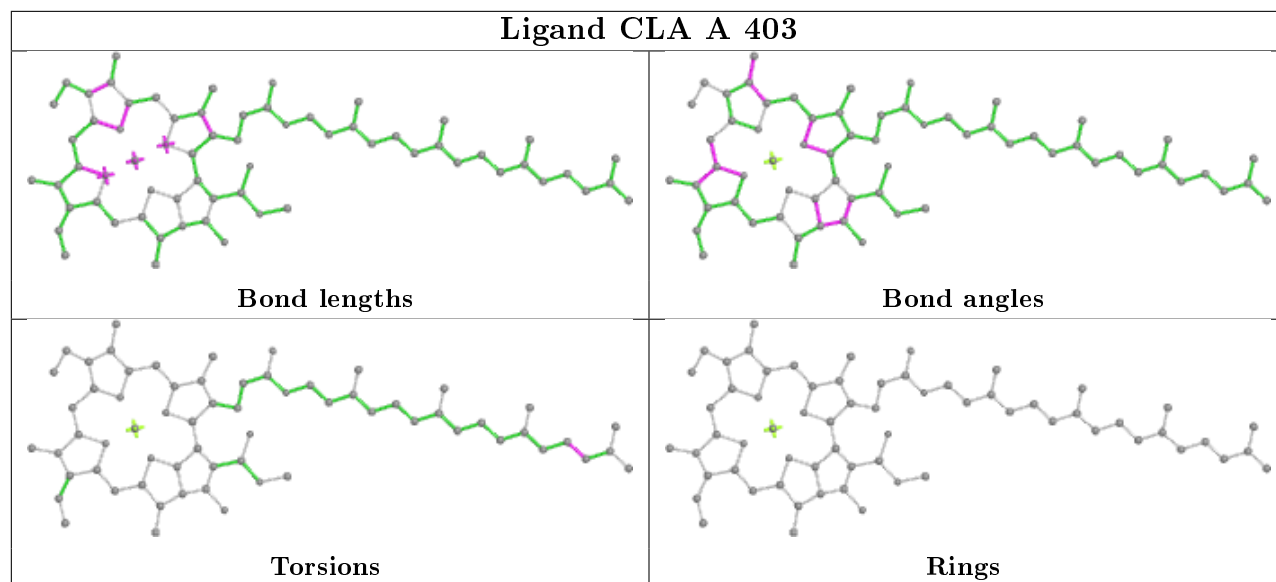
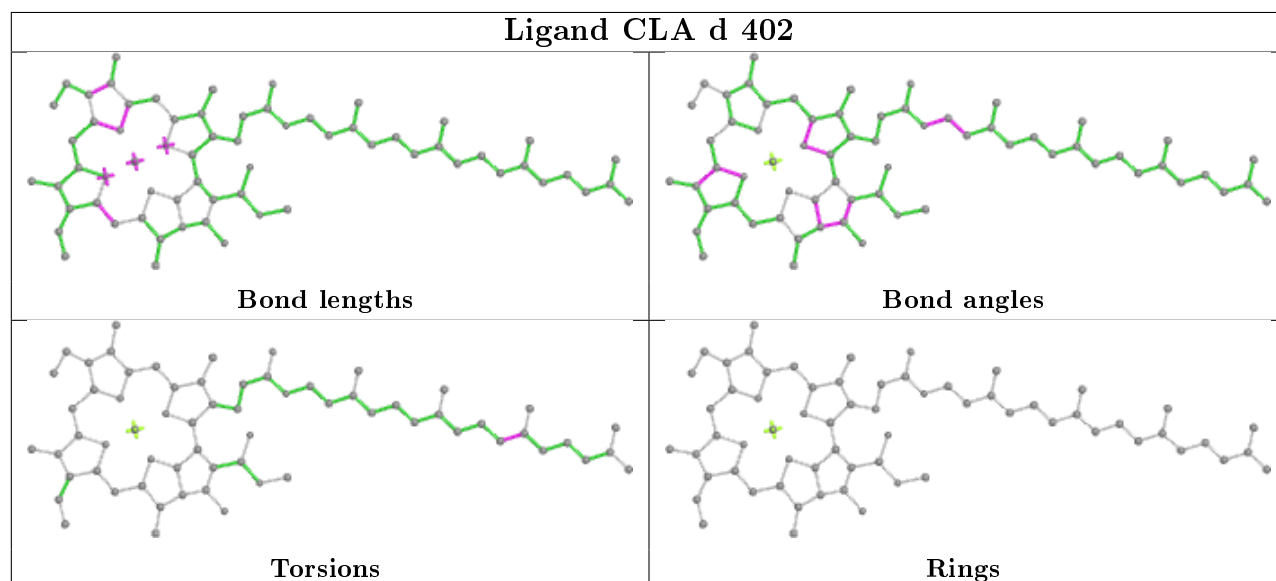
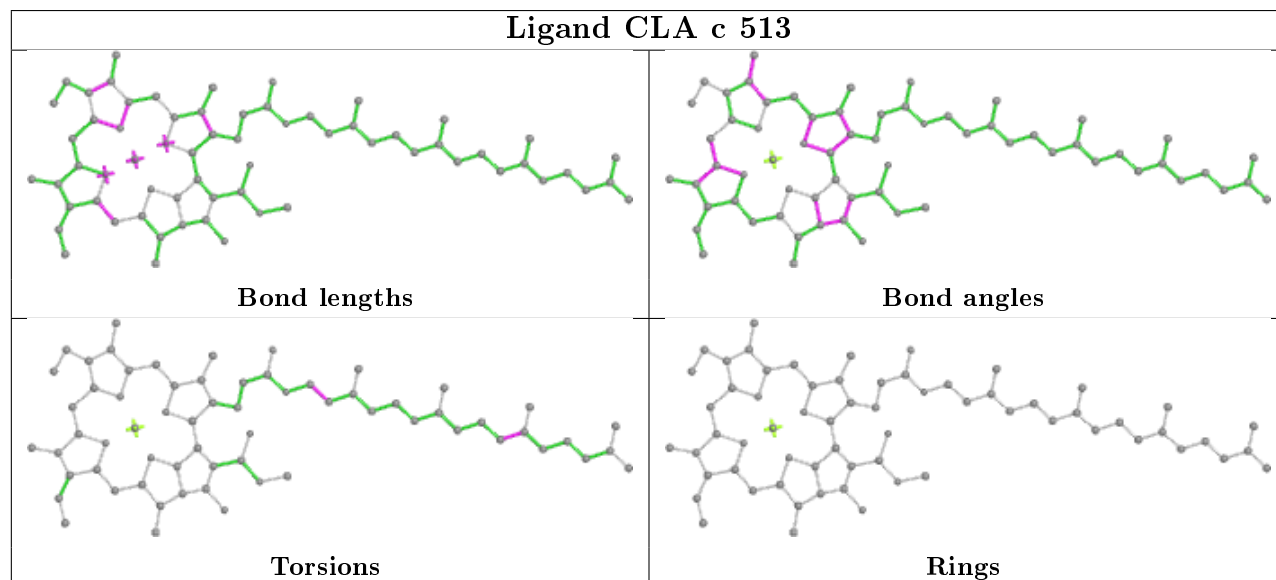




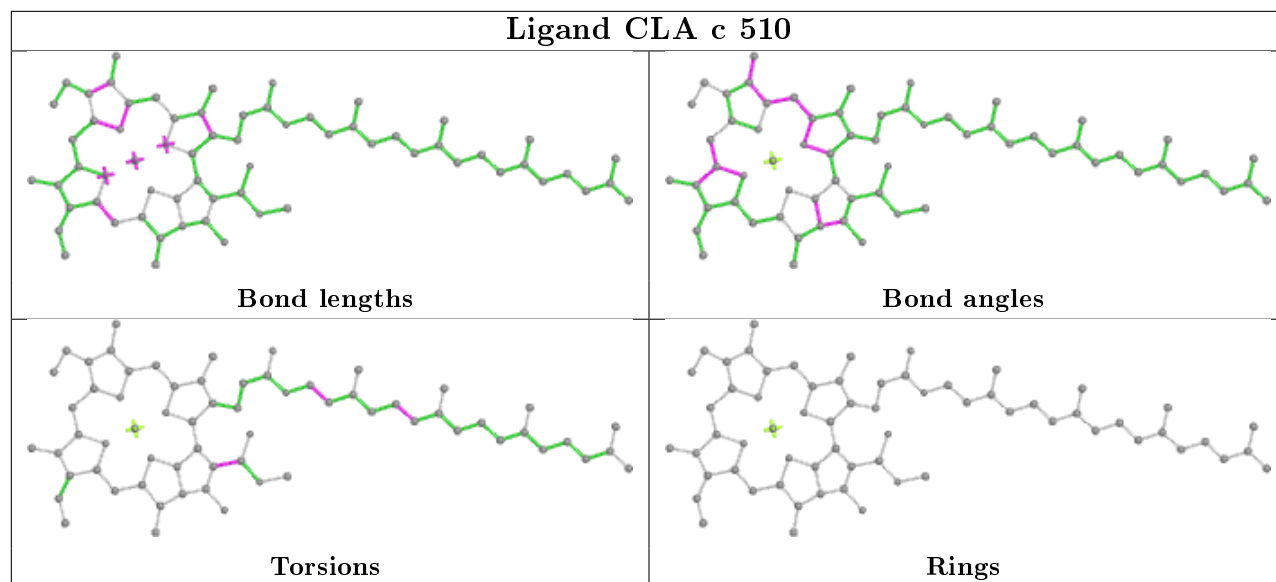
**Ligand CLA B 601****Ligand DGD c 518****Ligand CLA C 514**

**Ligand CLA B 603****Ligand LFA b 627****Ligand CLA B 614****Ligand LFA D 410**

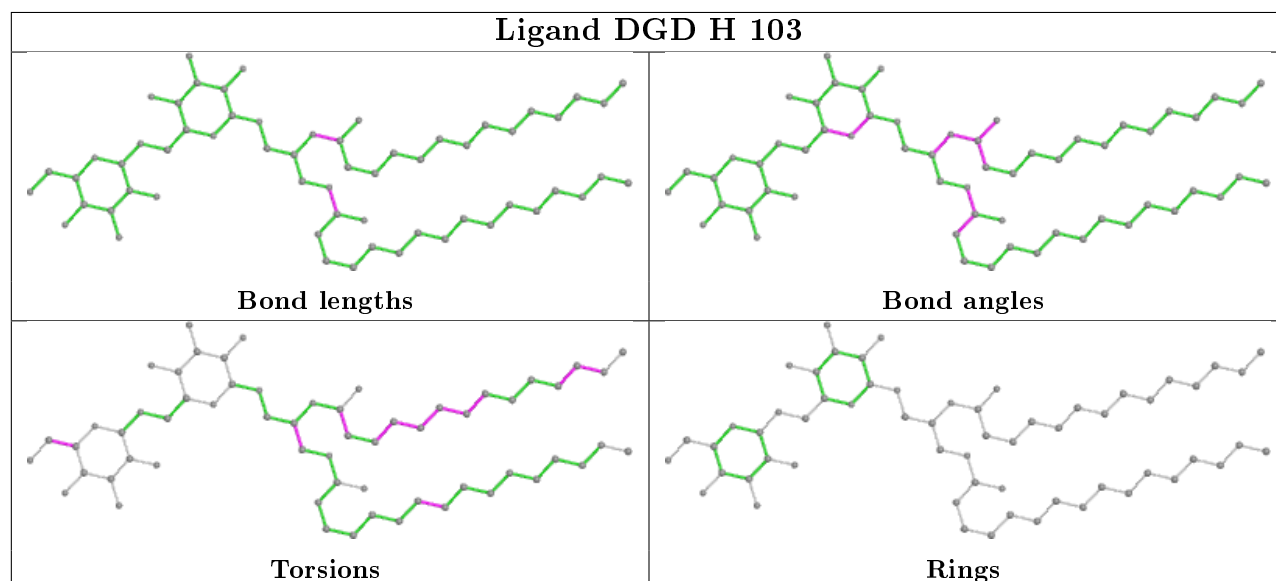


**Ligand CLA A 403****Ligand CLA d 402****Ligand CLA c 513**

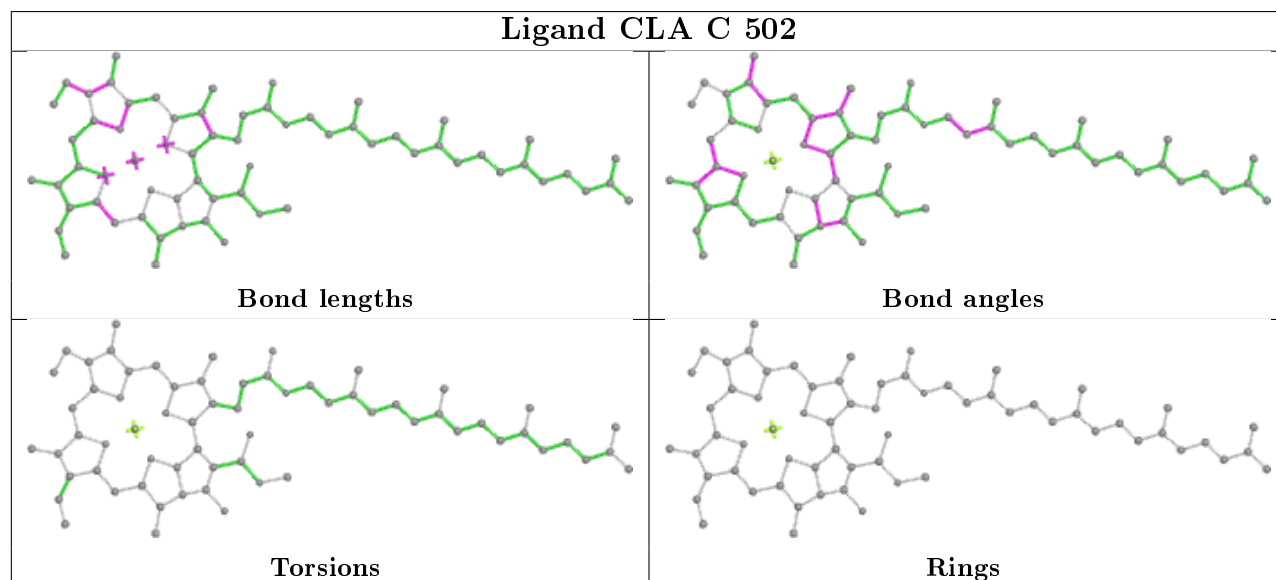
## Ligand CLA c 510

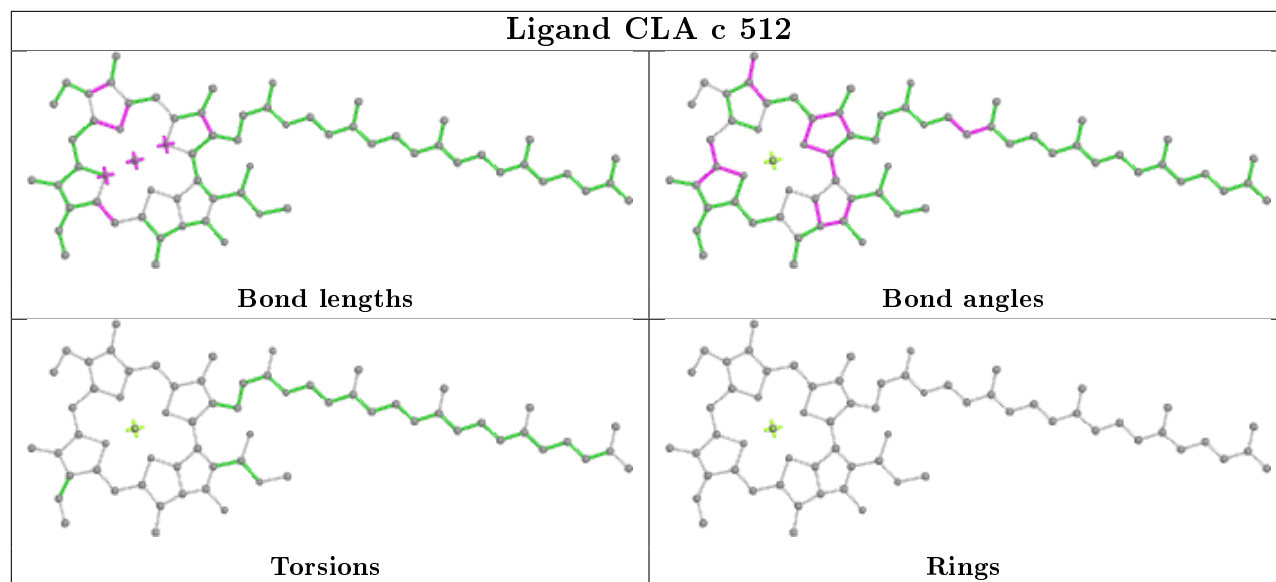
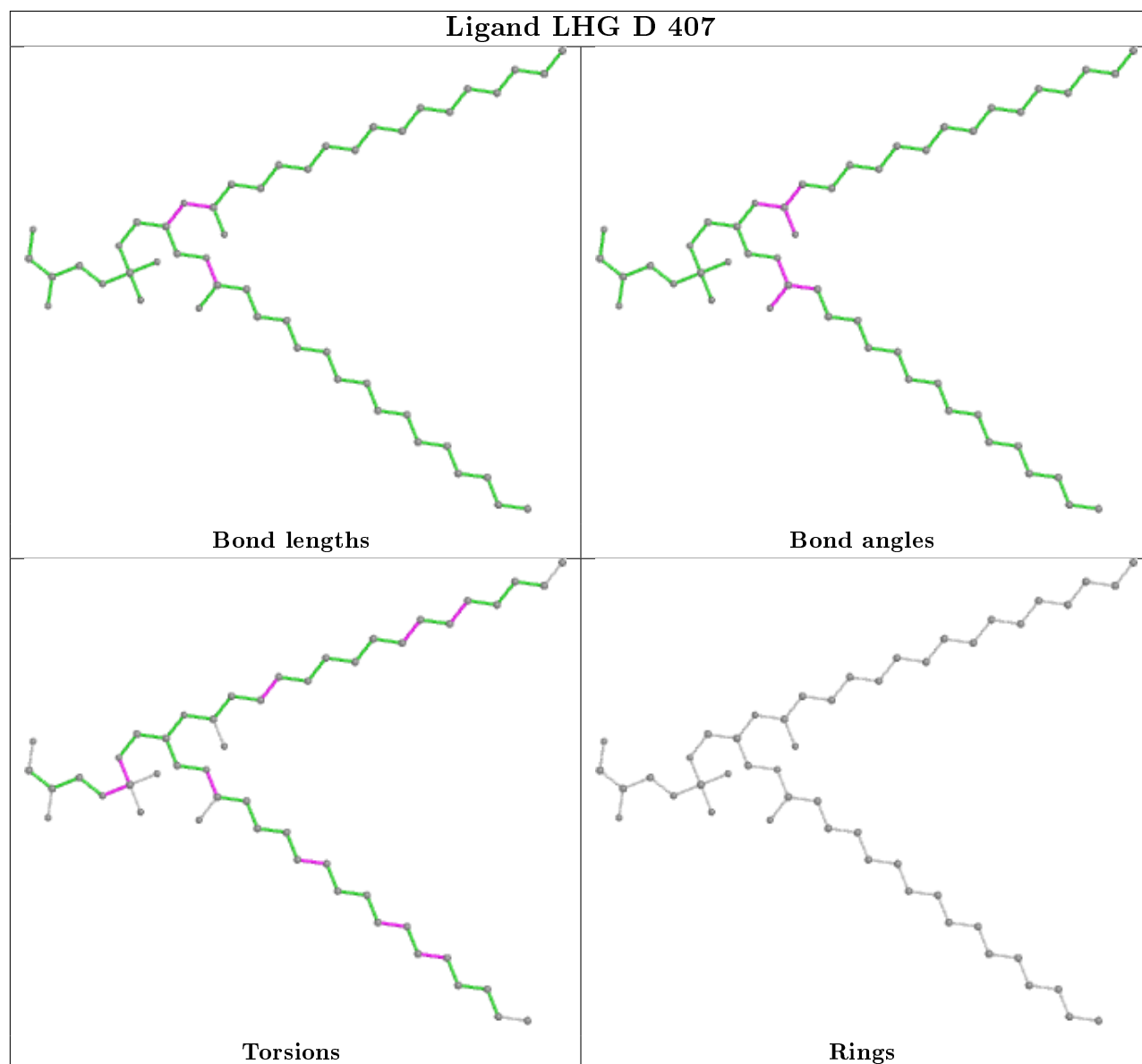


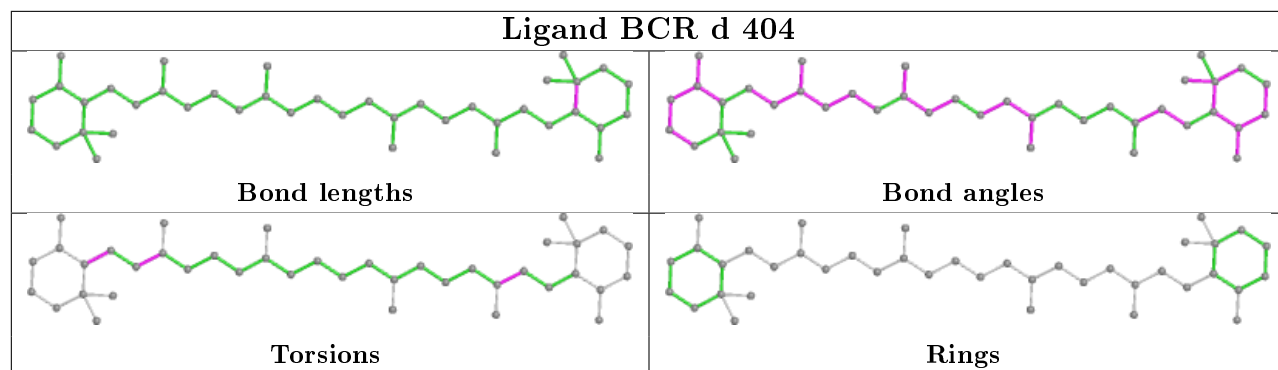
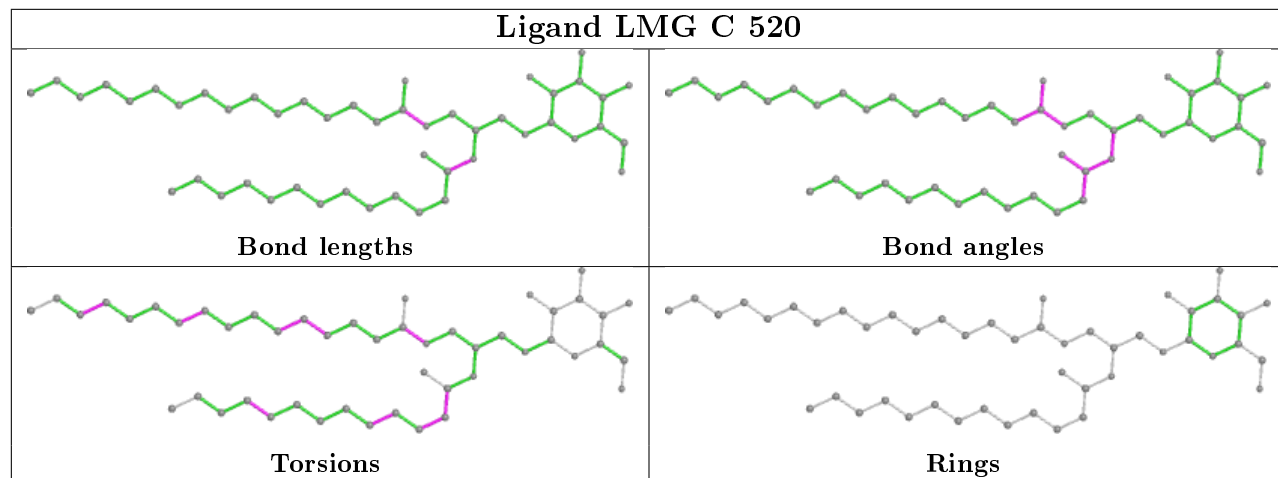
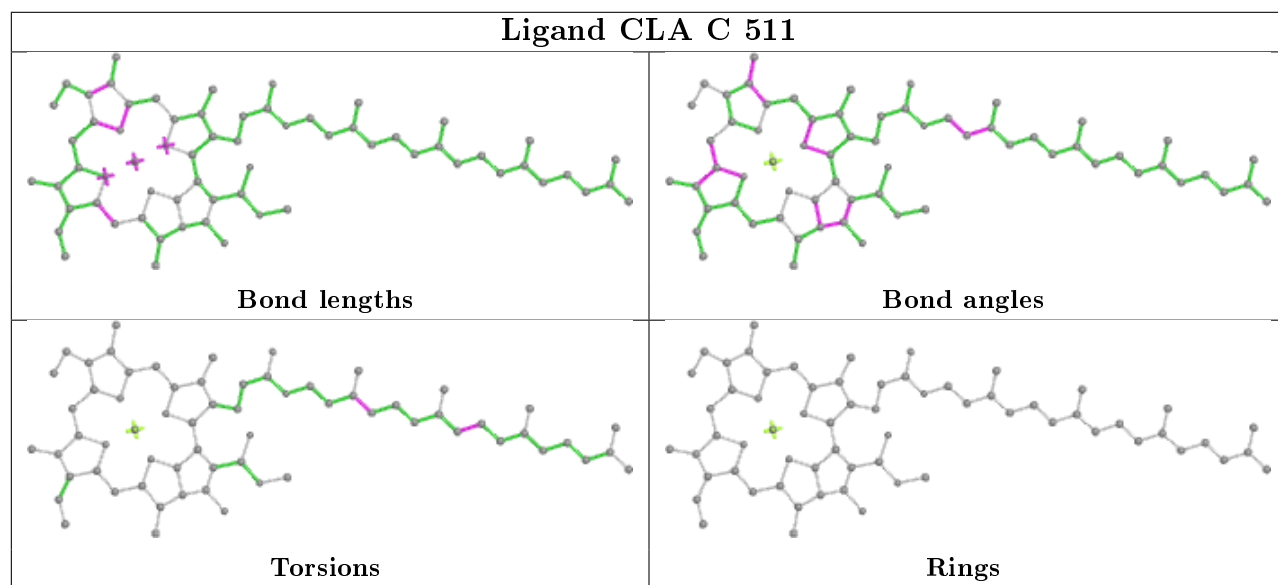
## Ligand DGD H 103

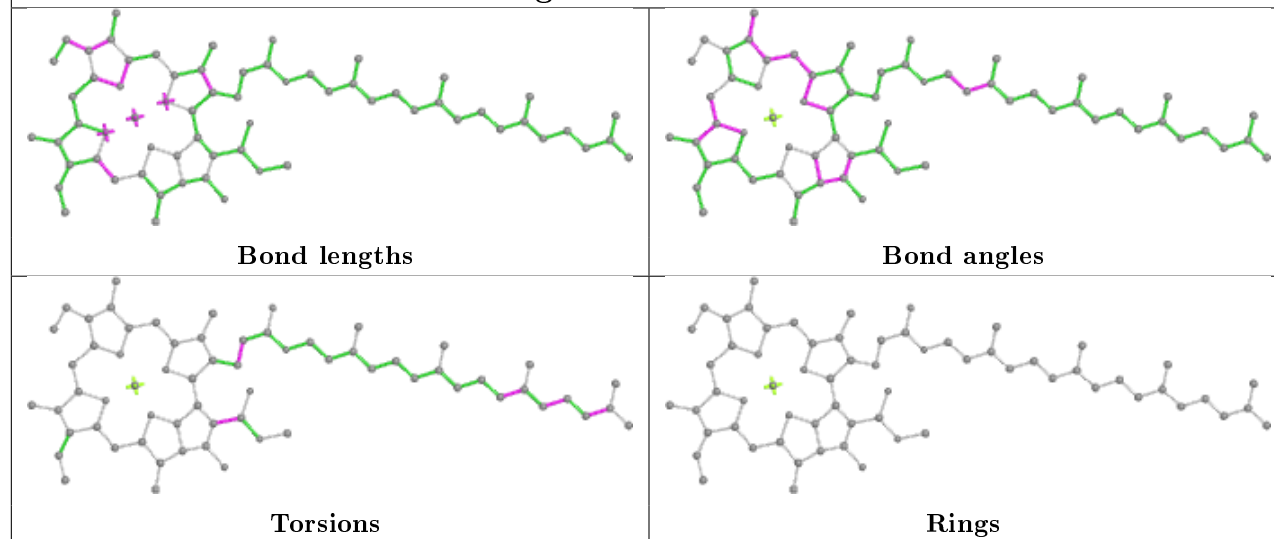
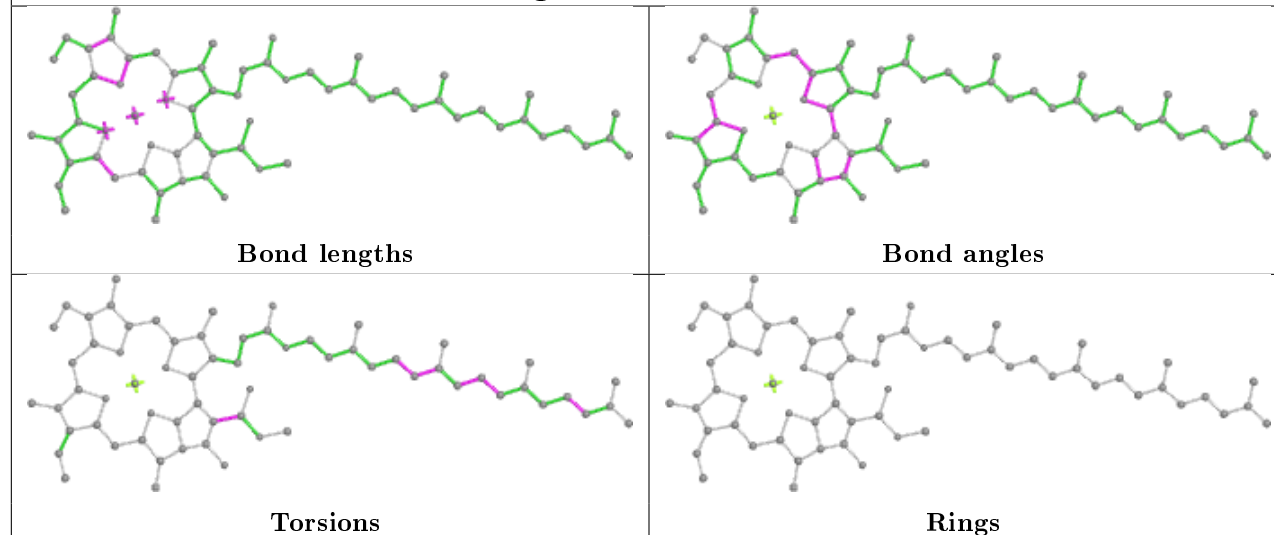
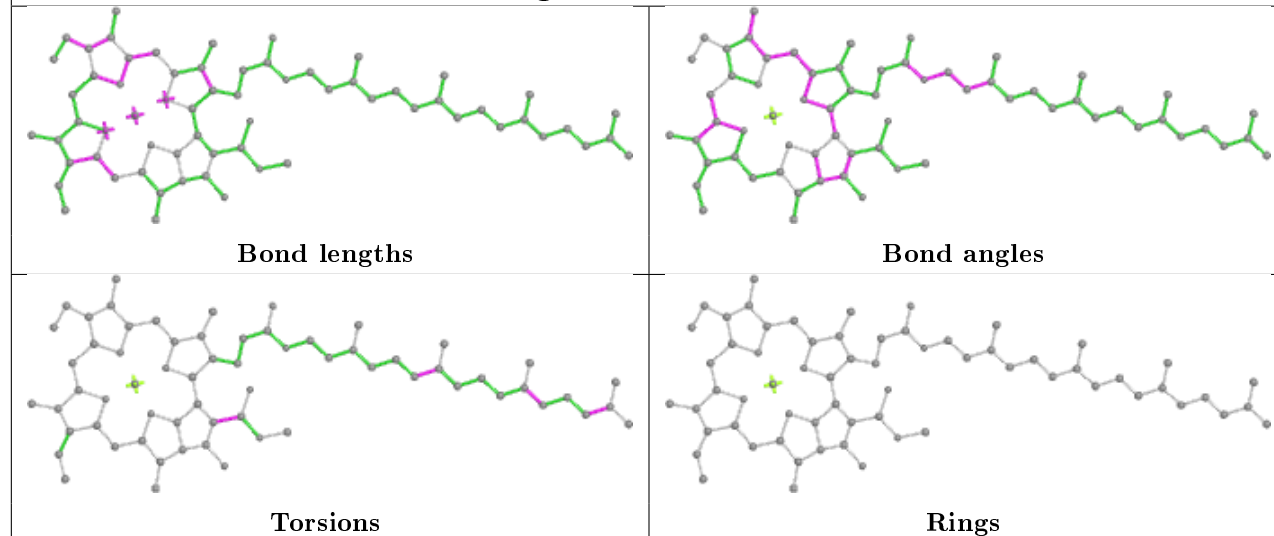


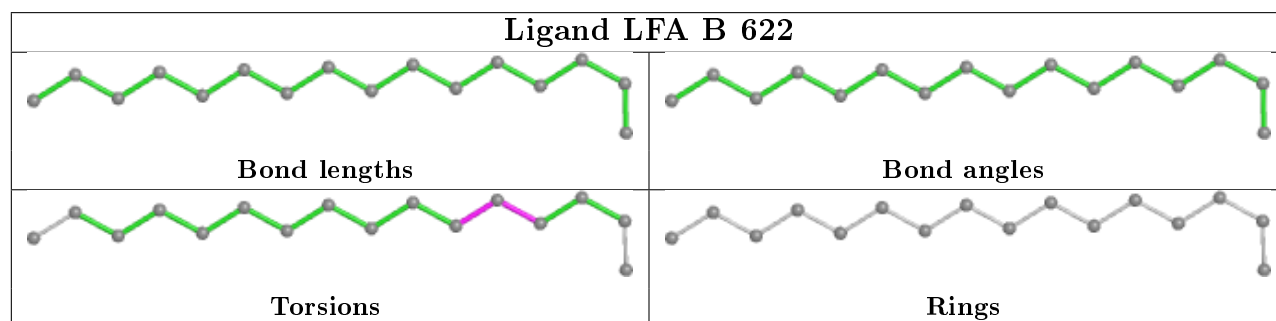
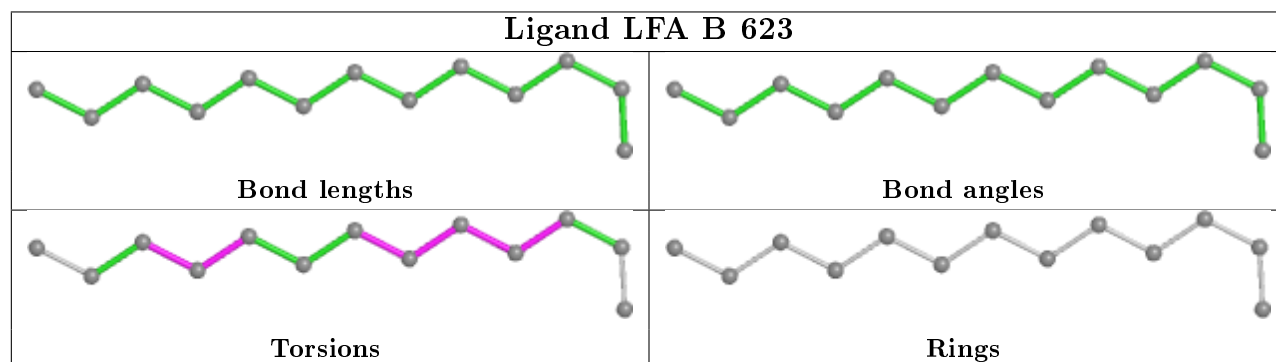
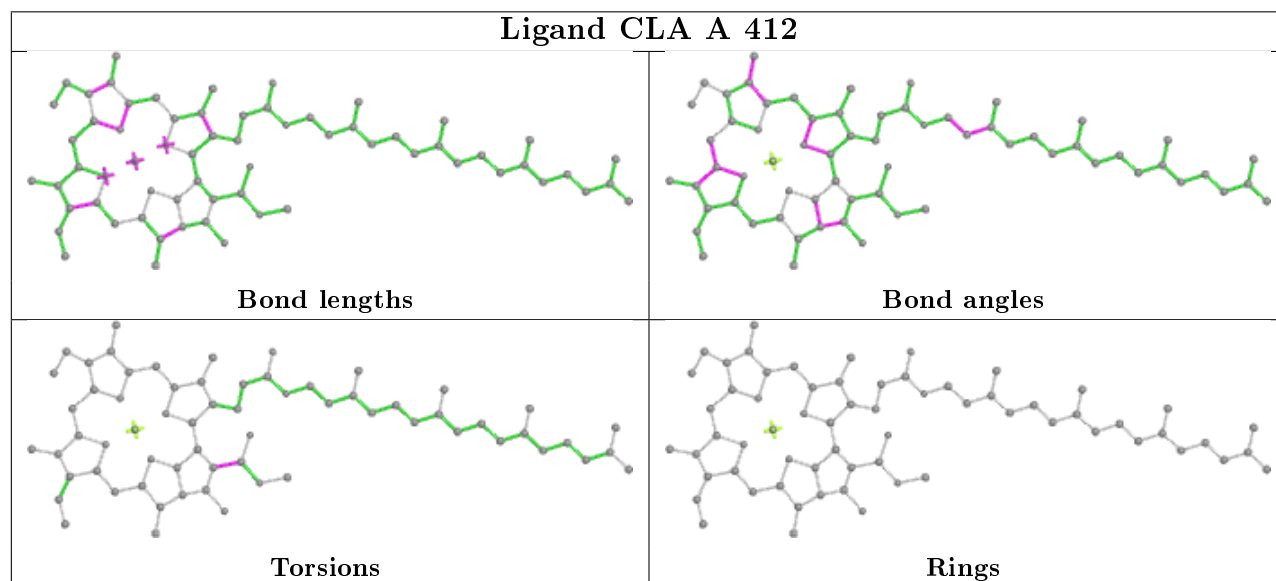
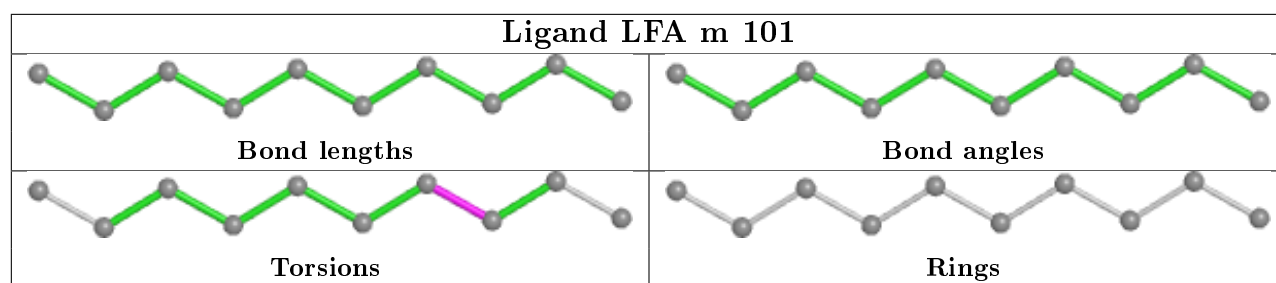
## Ligand CLA C 502

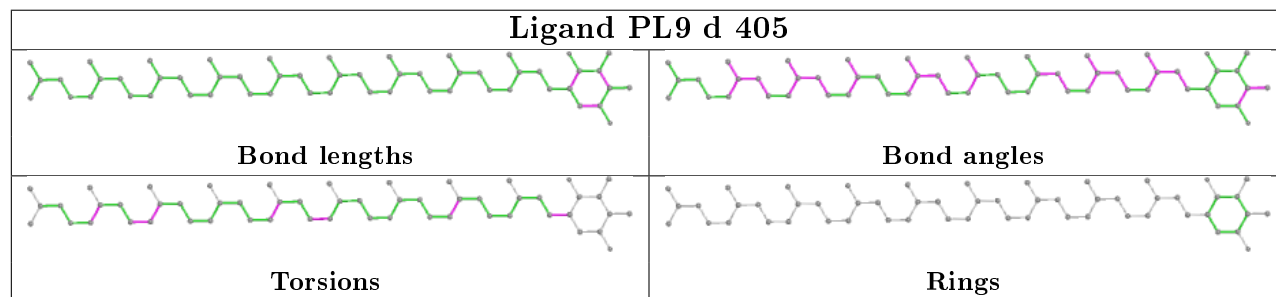
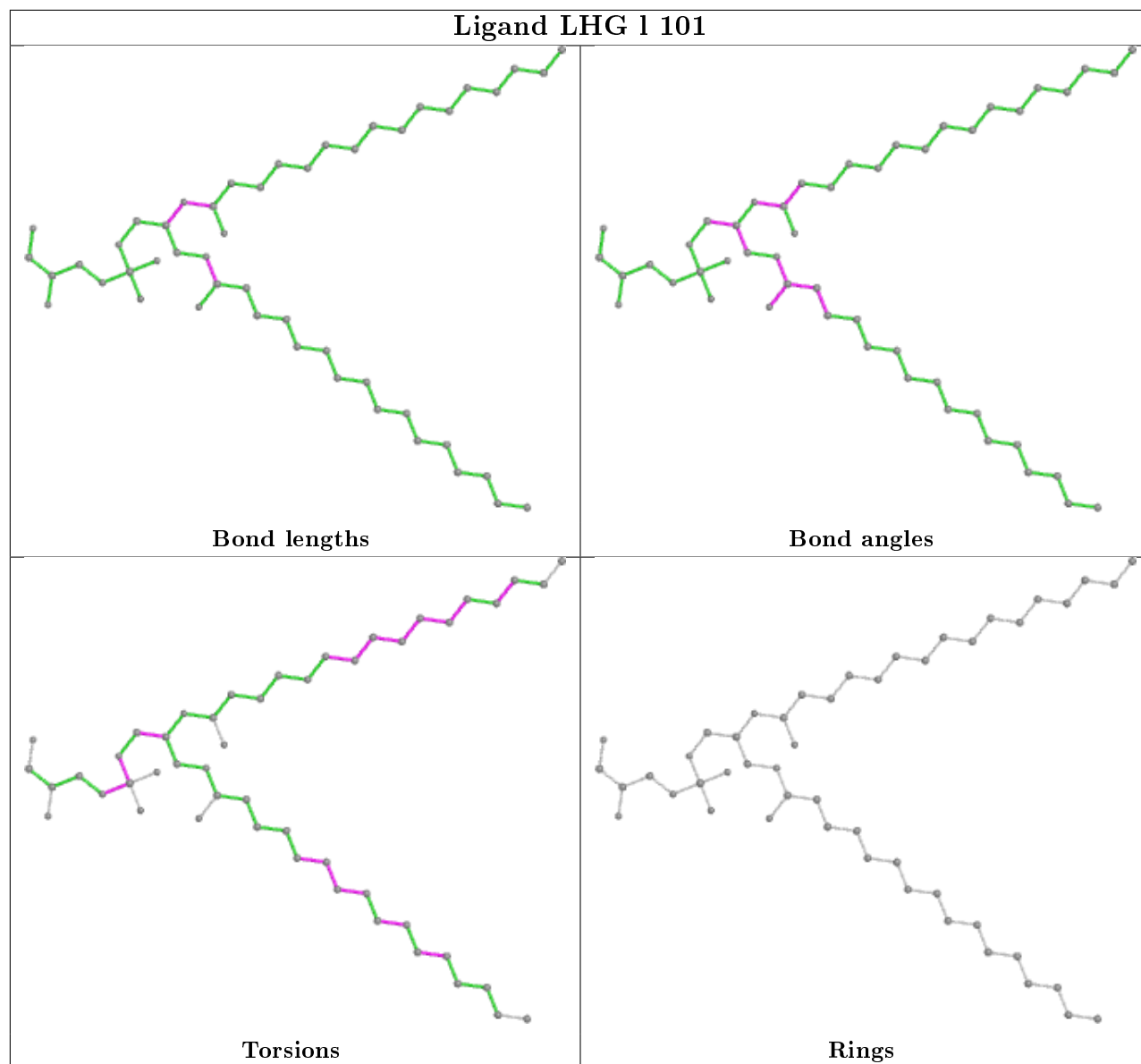


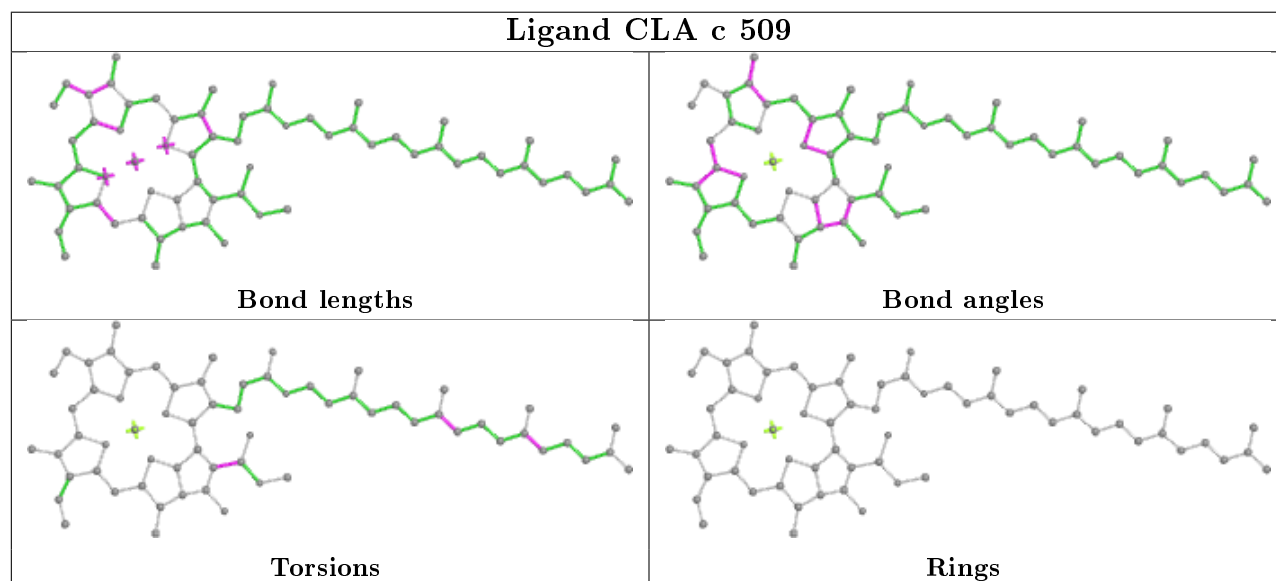
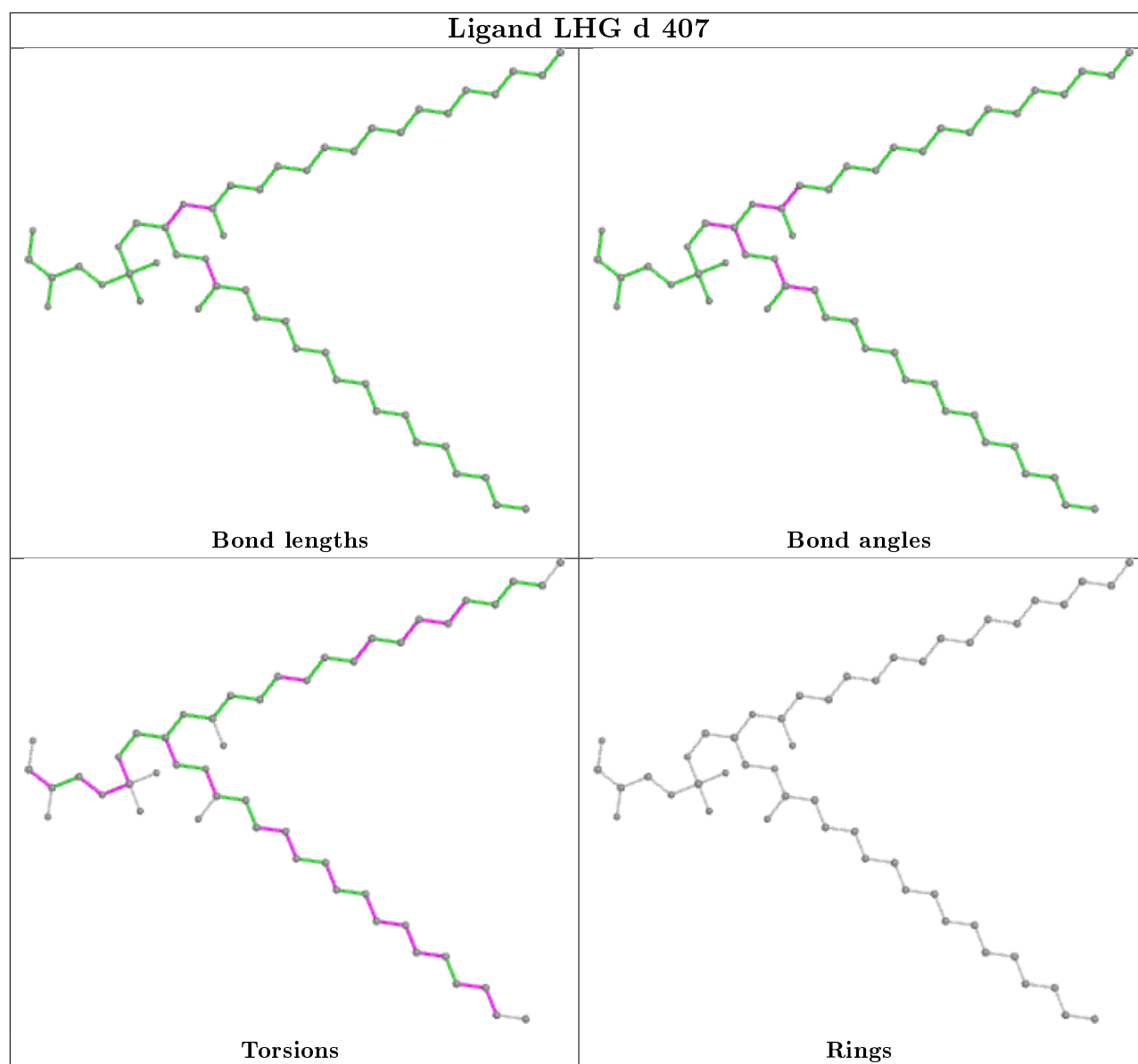
**Ligand CLA c 512****Ligand LHG D 407**

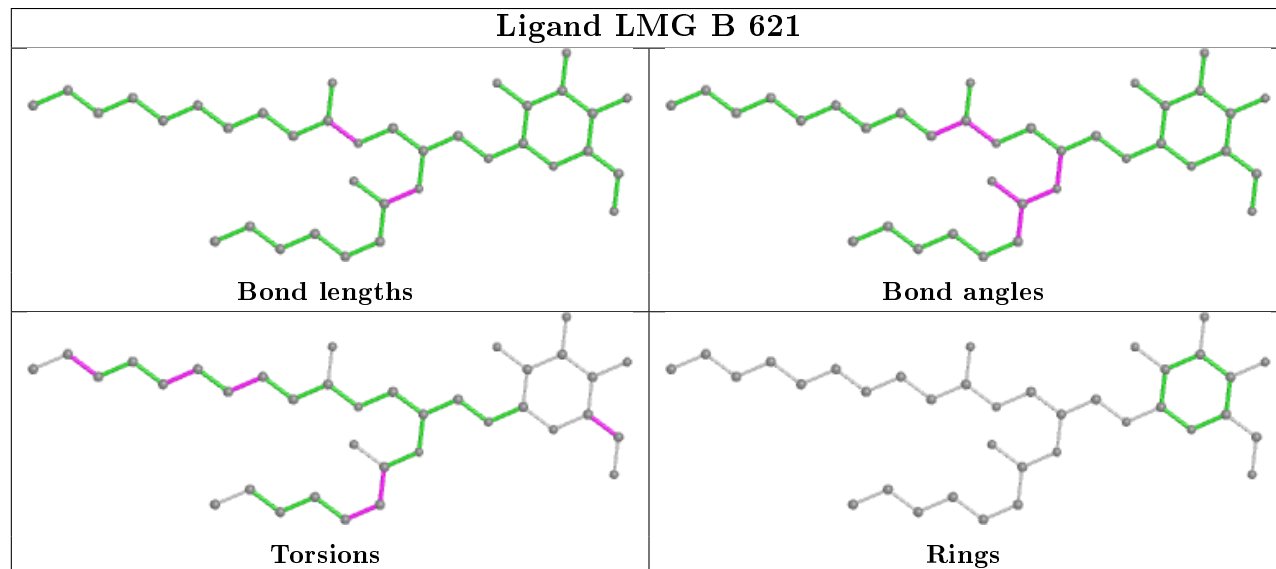
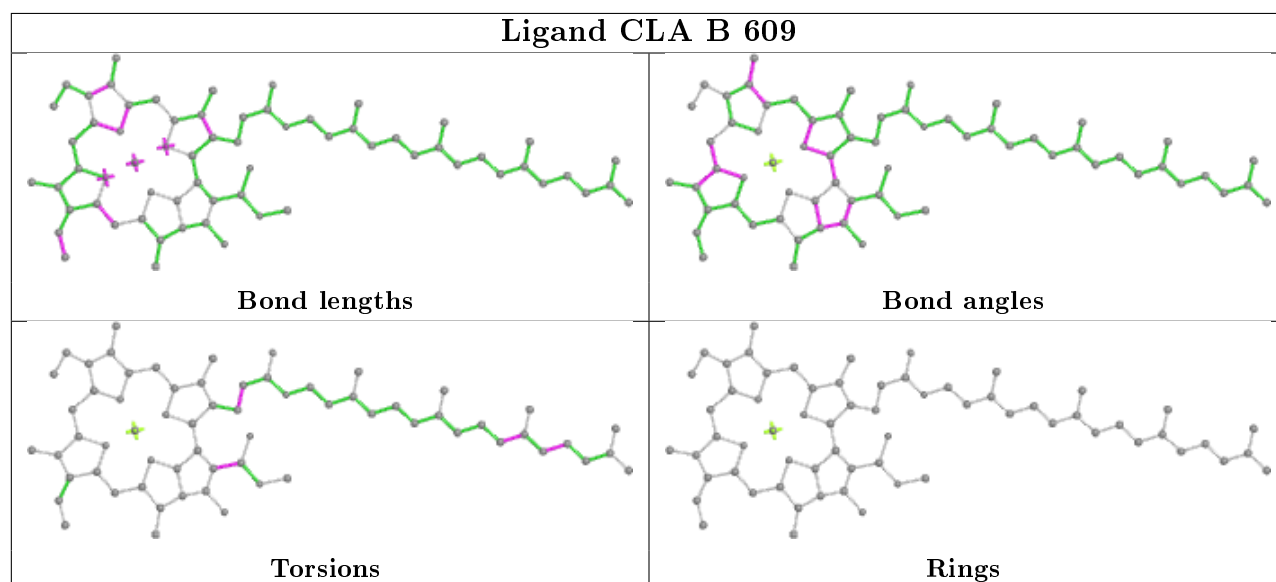
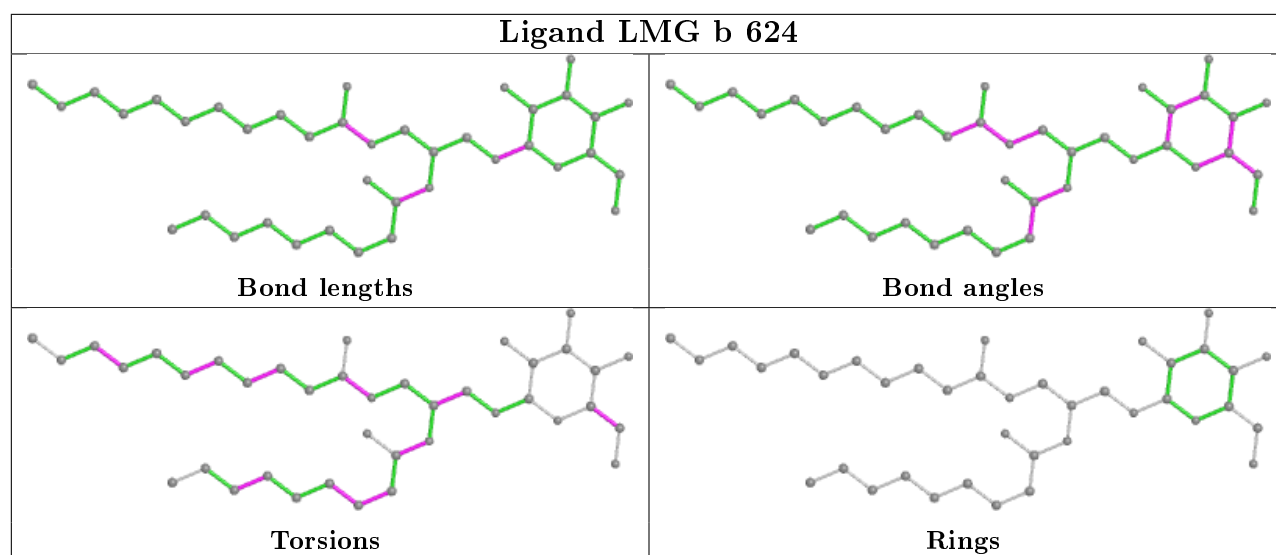
**Ligand BCR d 404****Ligand LMG C 520****Ligand CLA C 511**

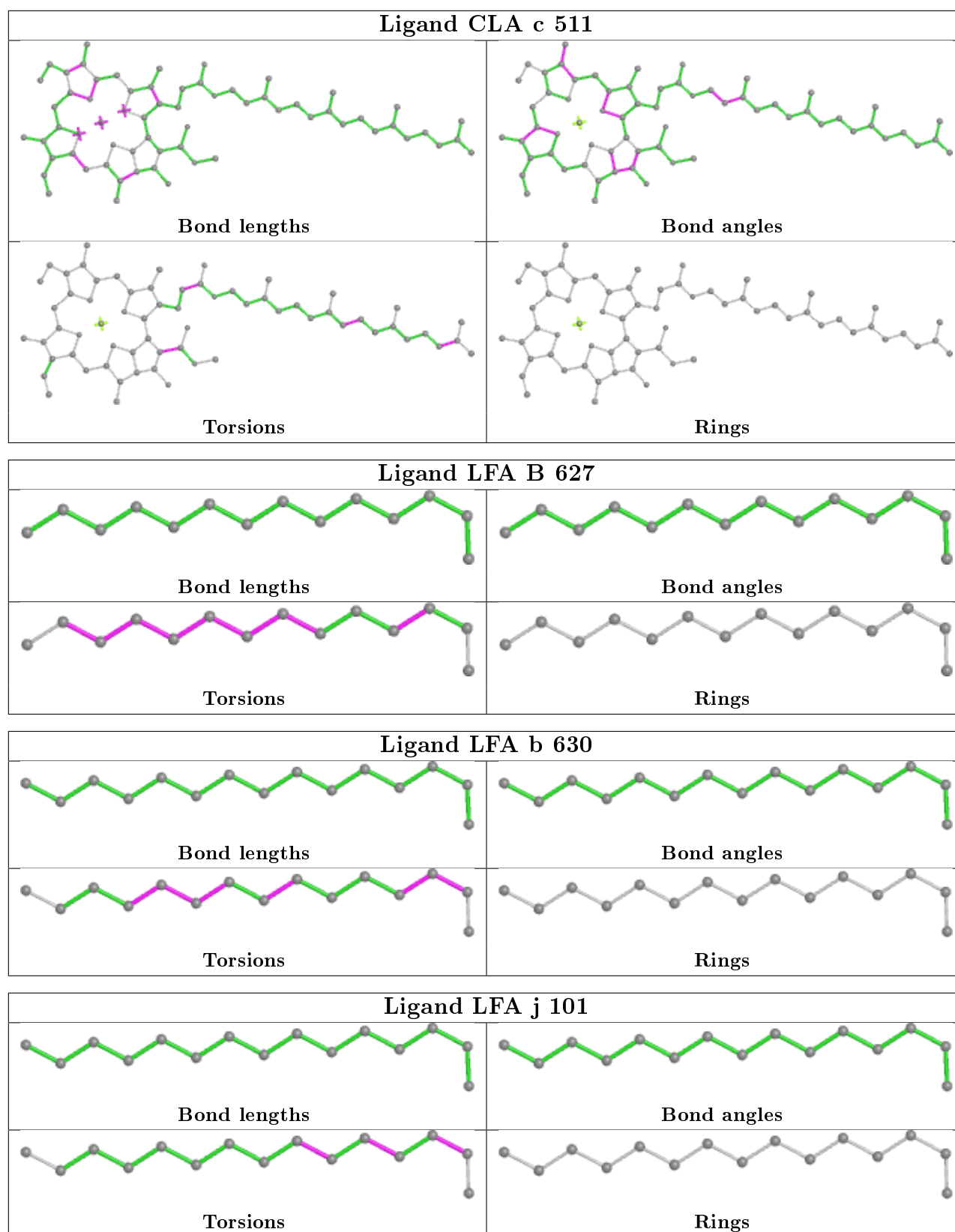
**Ligand CLA b 612****Ligand CLA C 504****Ligand CLA b 609**

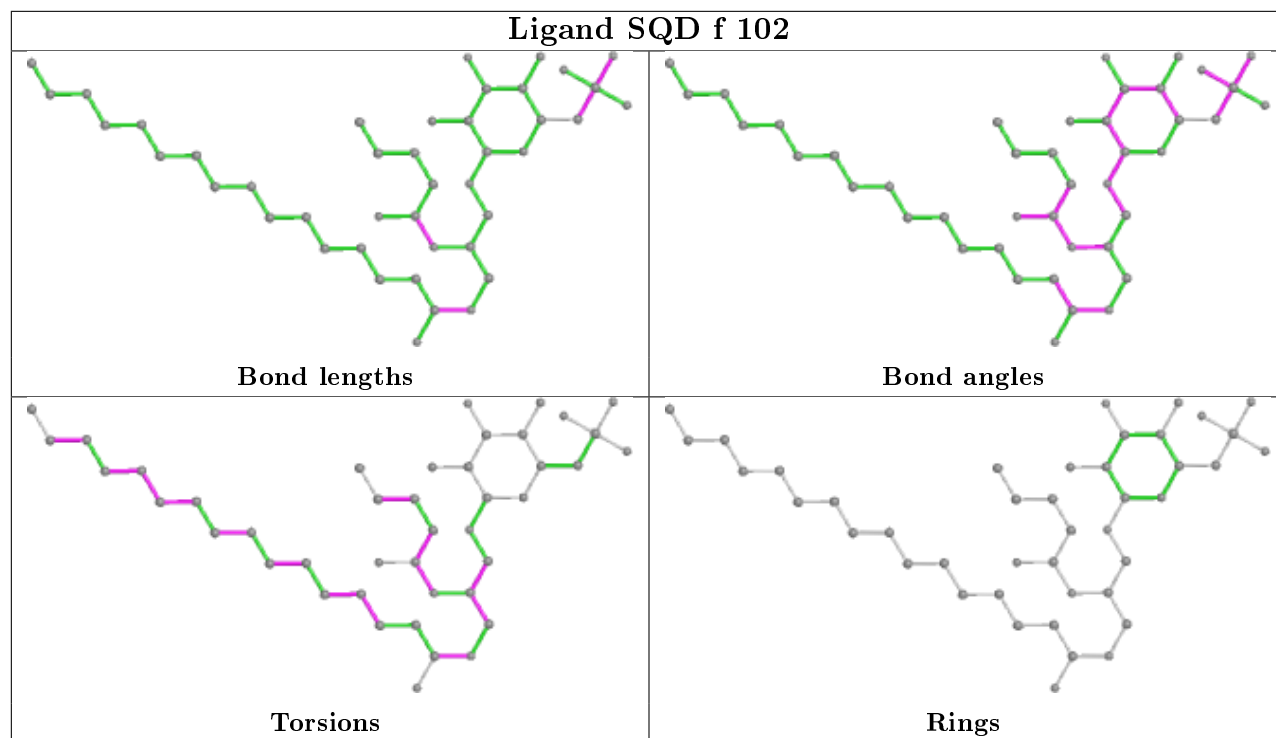
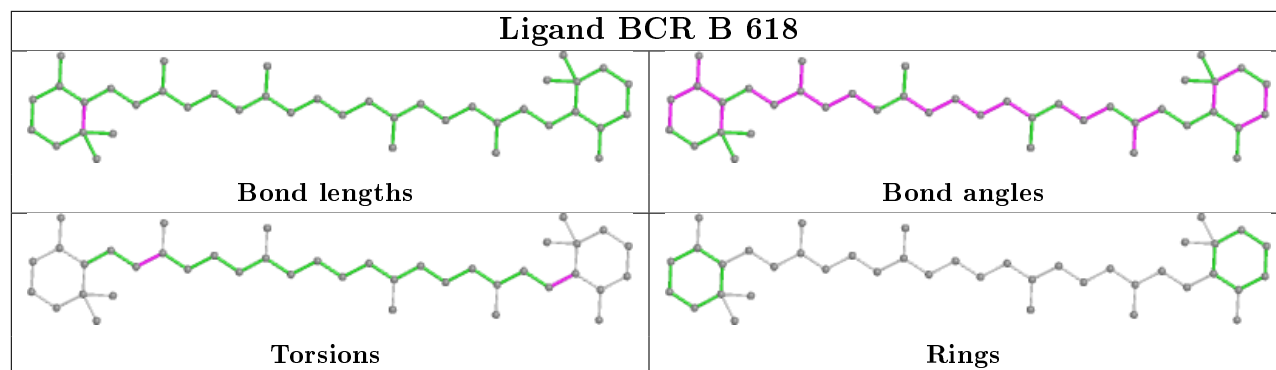


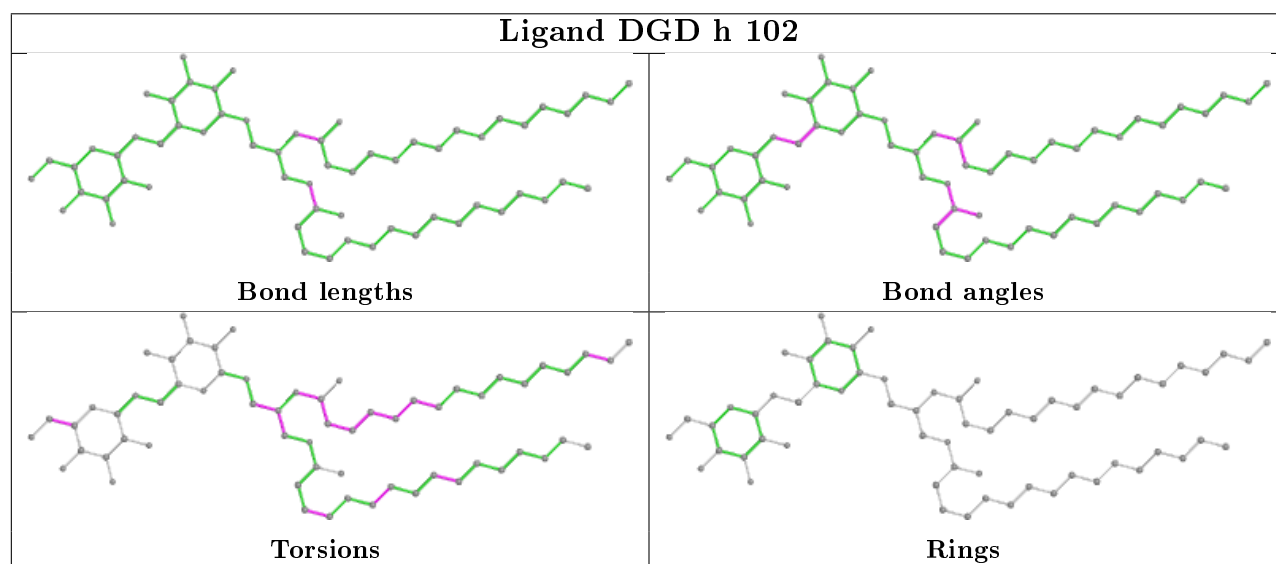
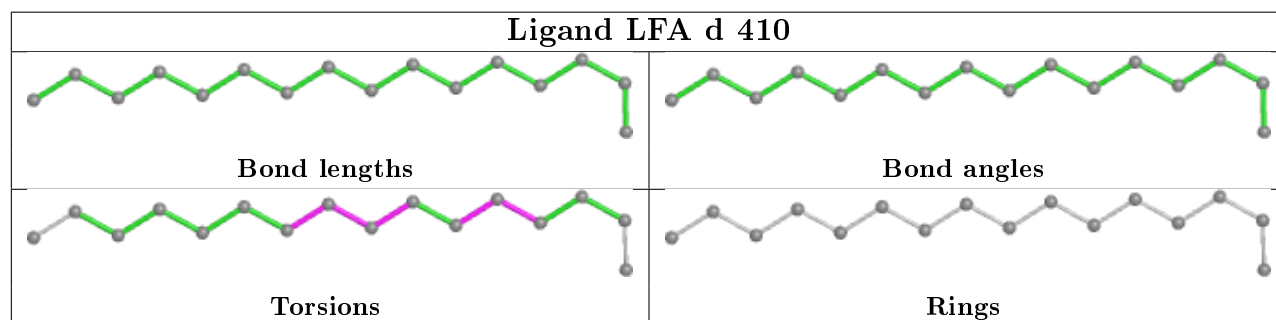
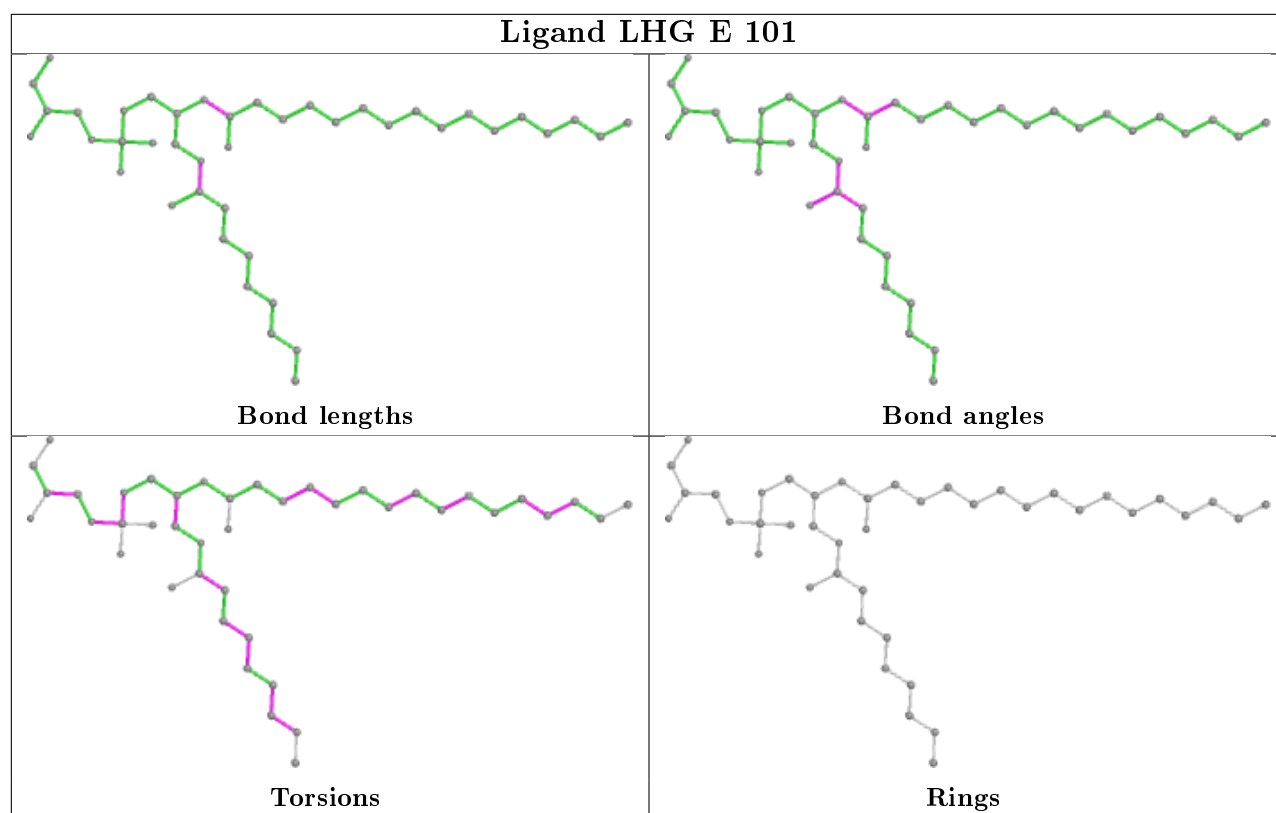


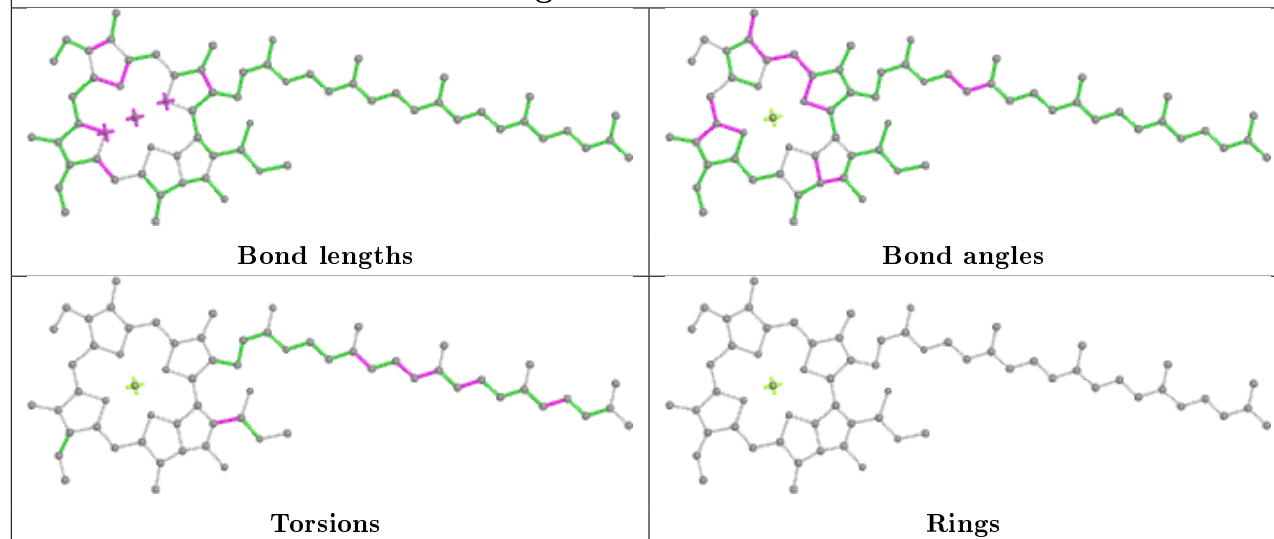
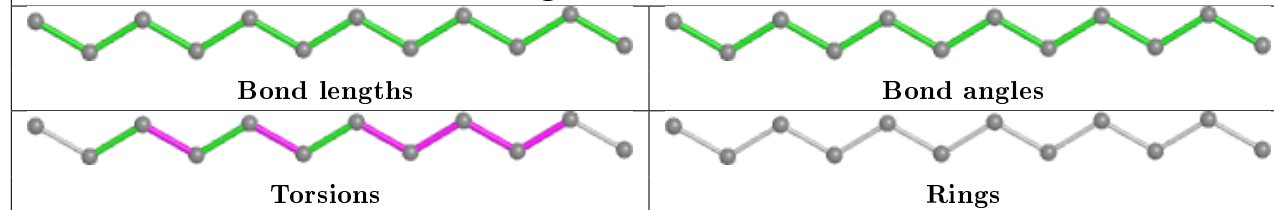
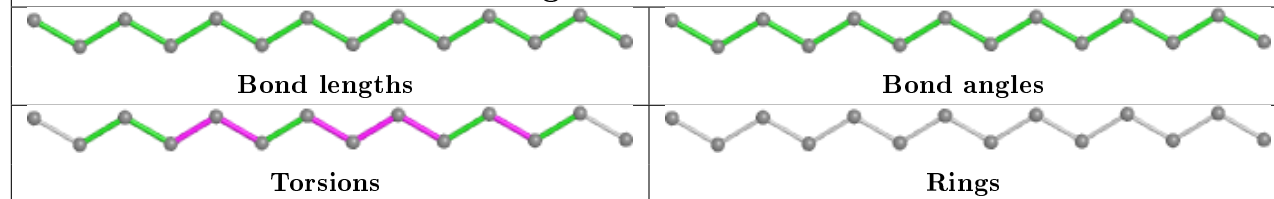
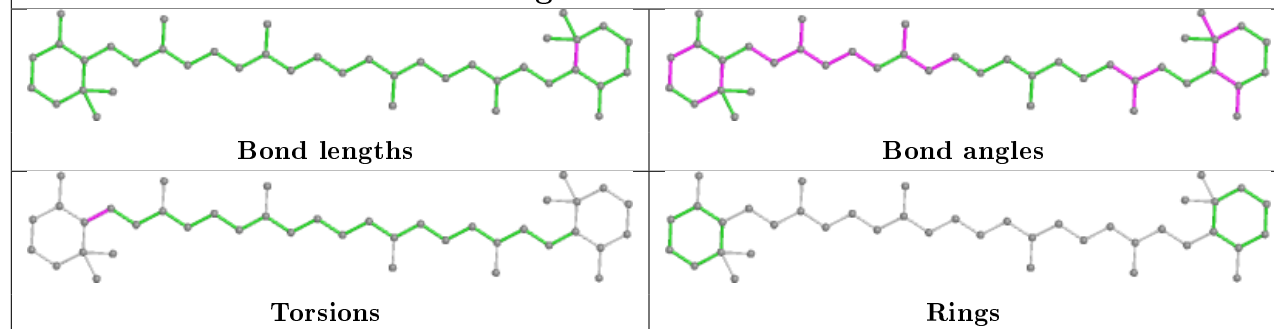


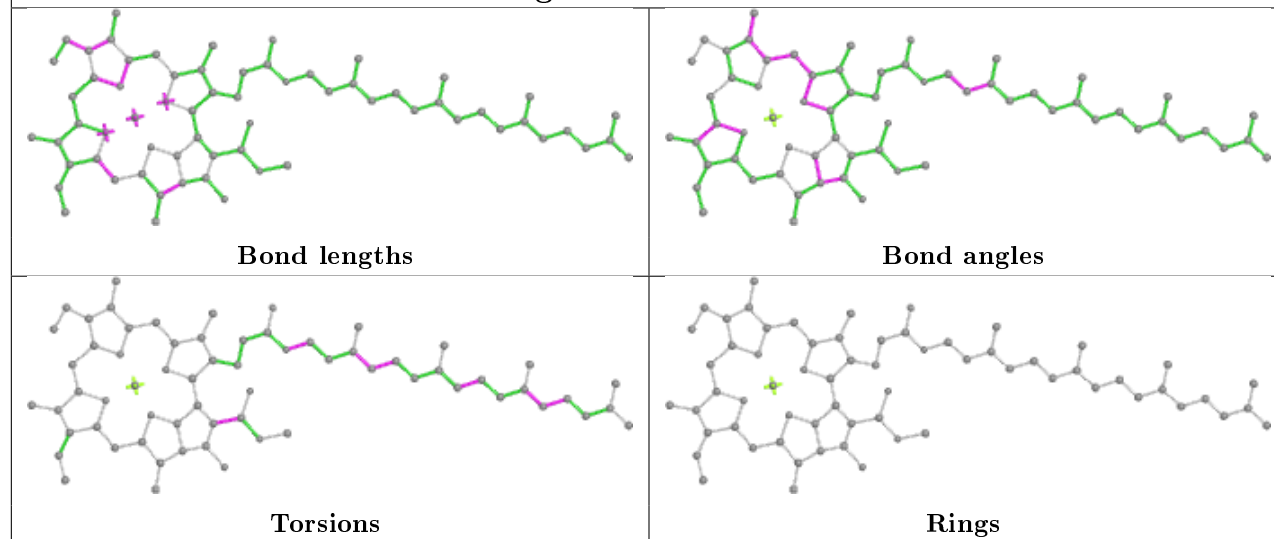
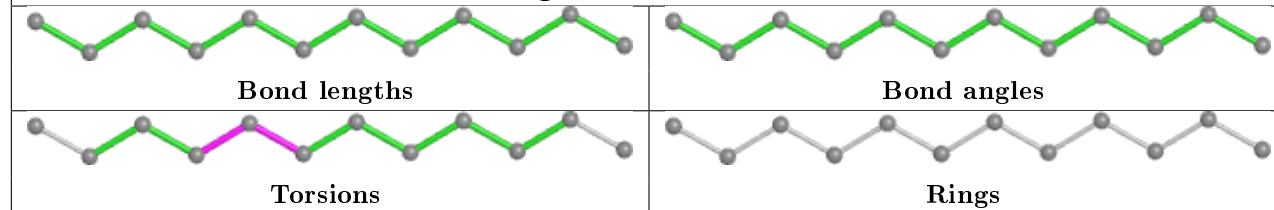
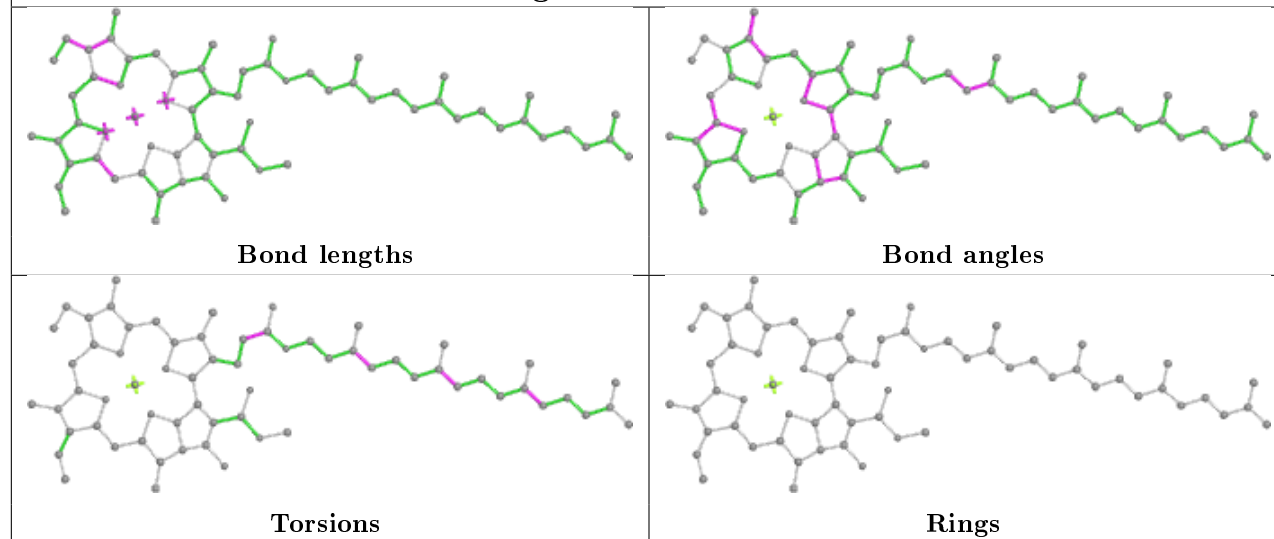


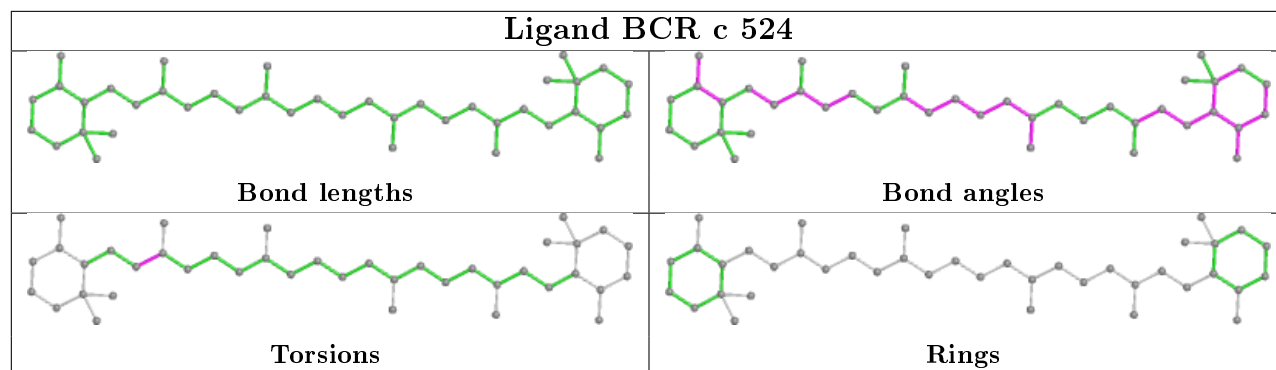
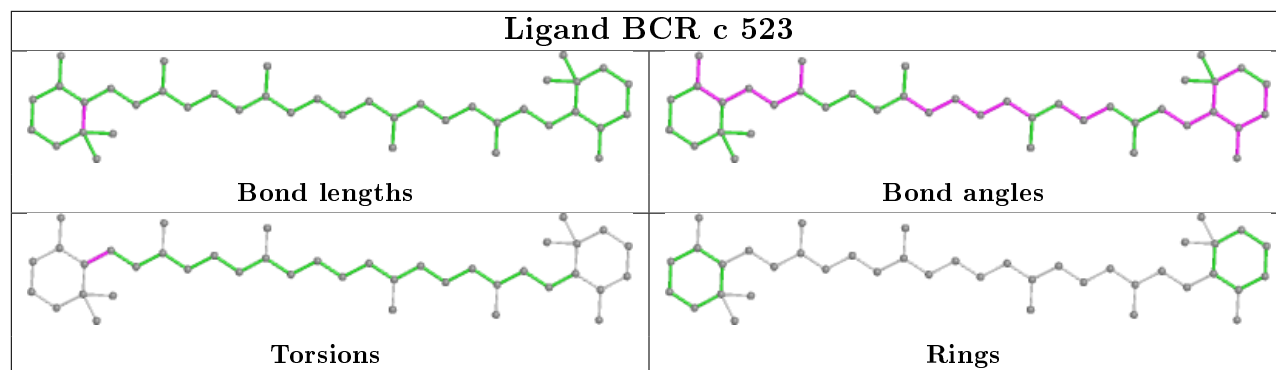
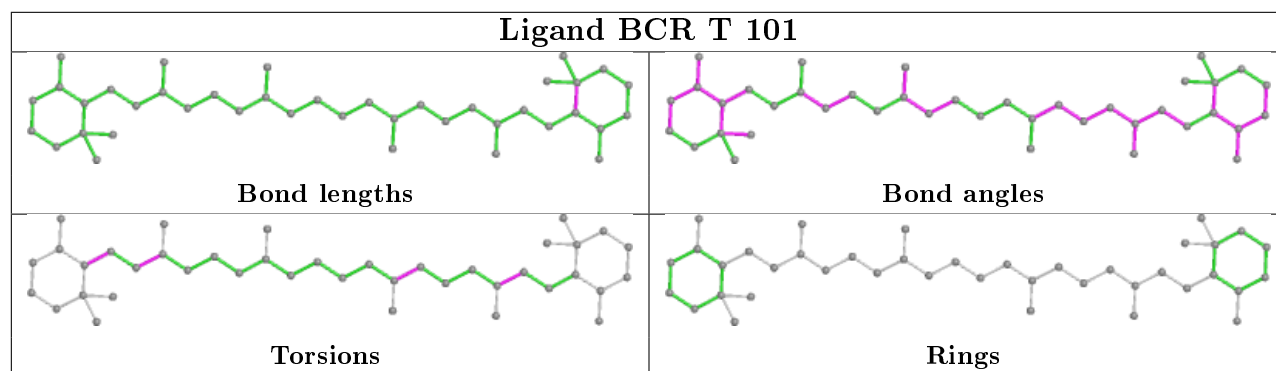
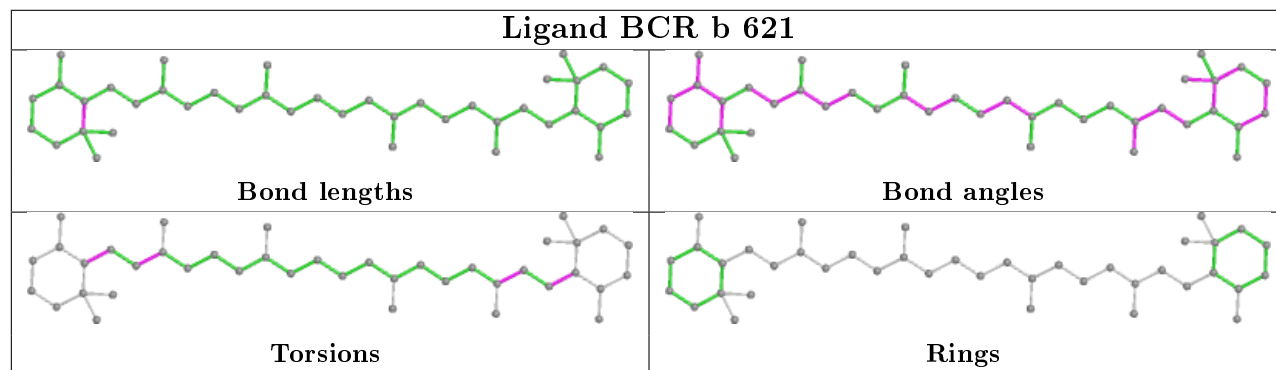


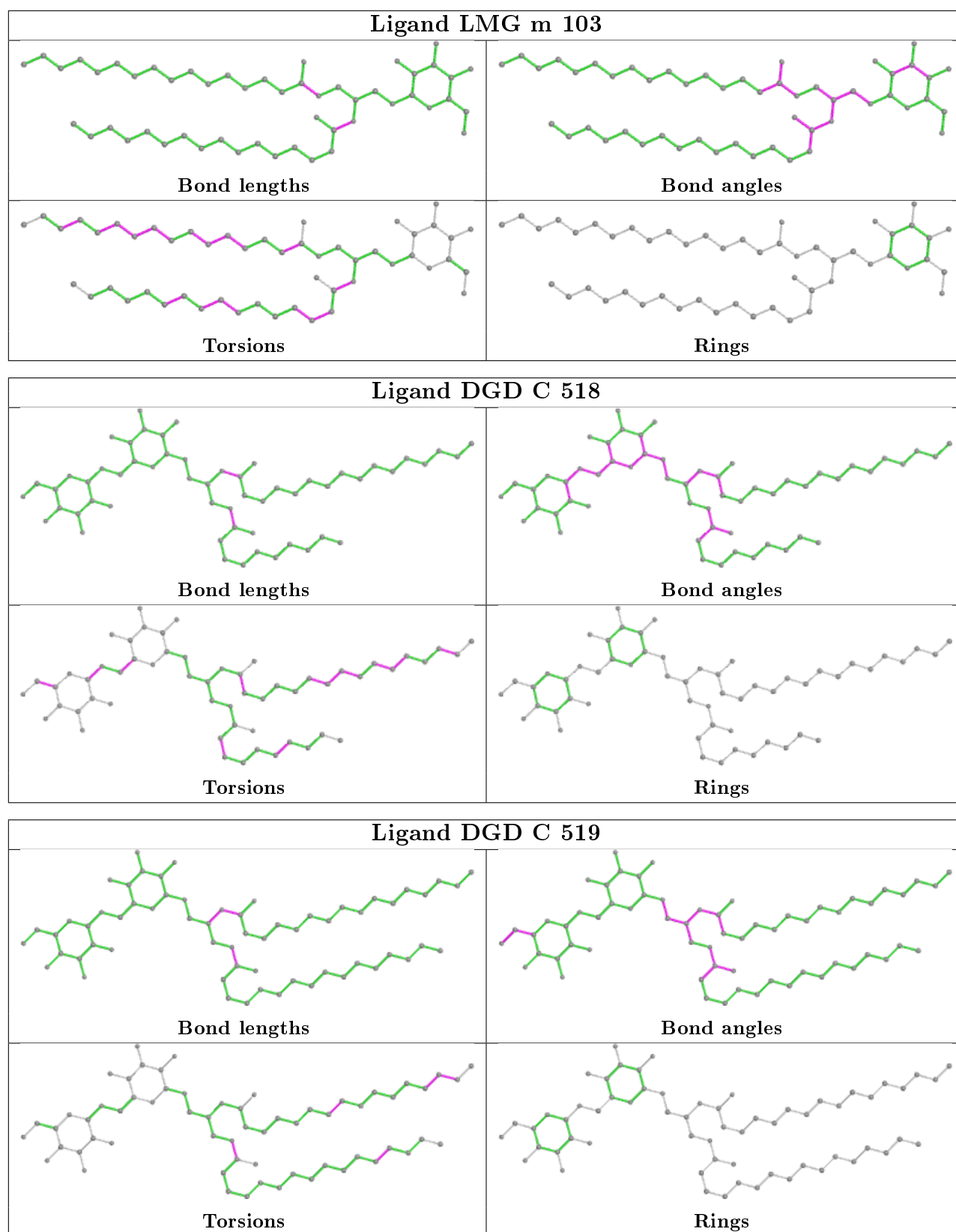


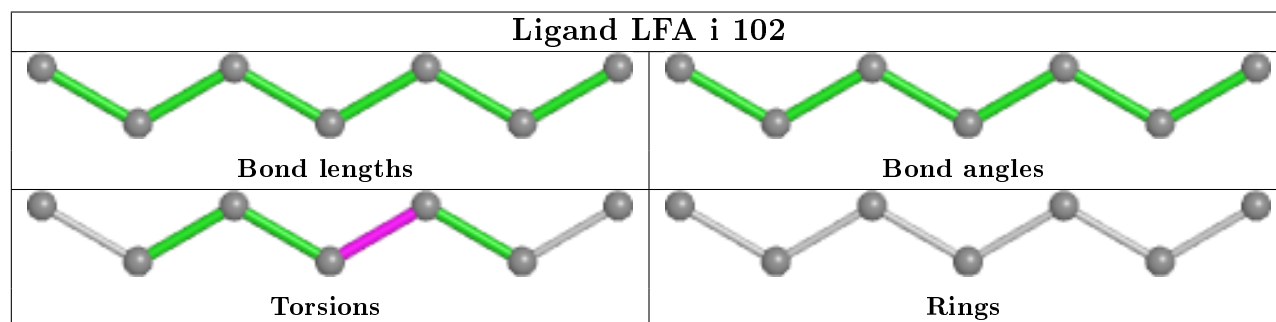
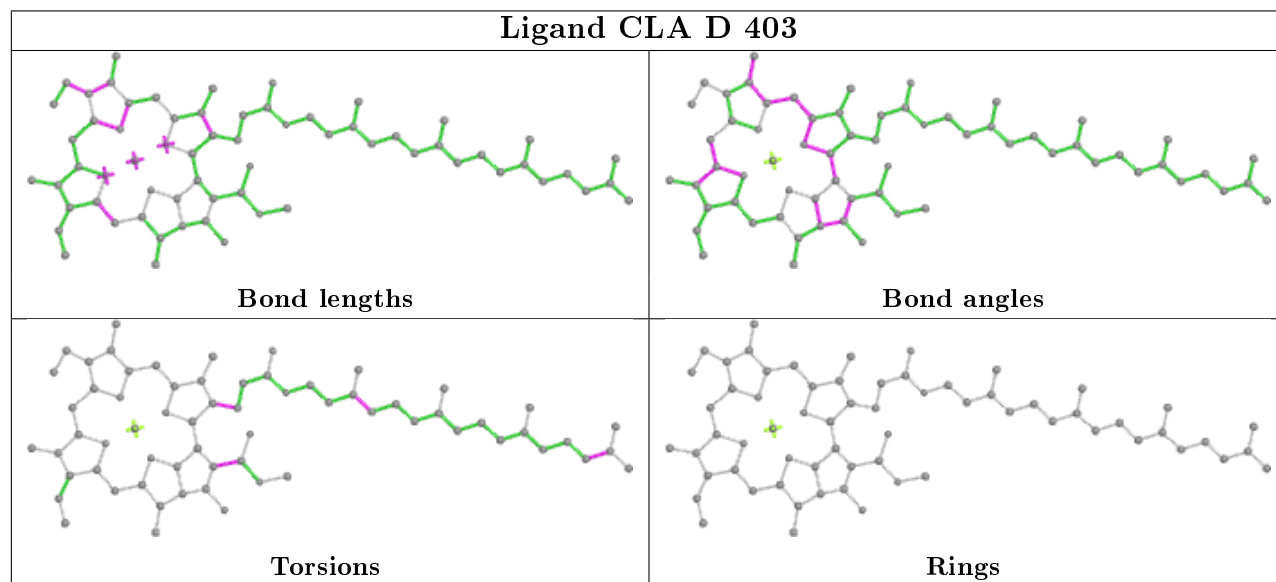
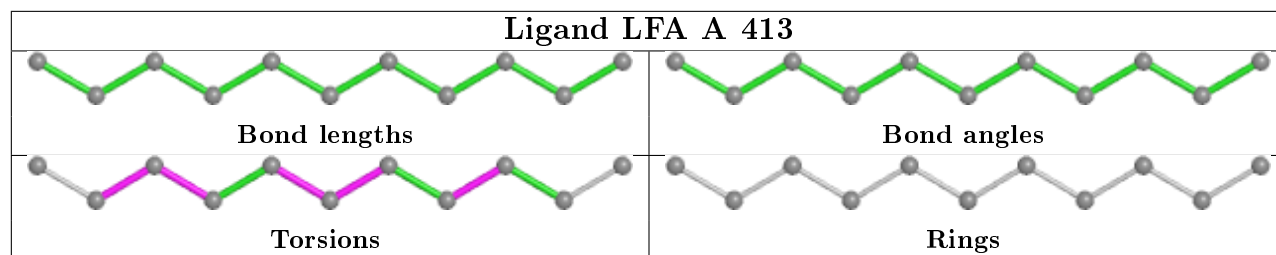


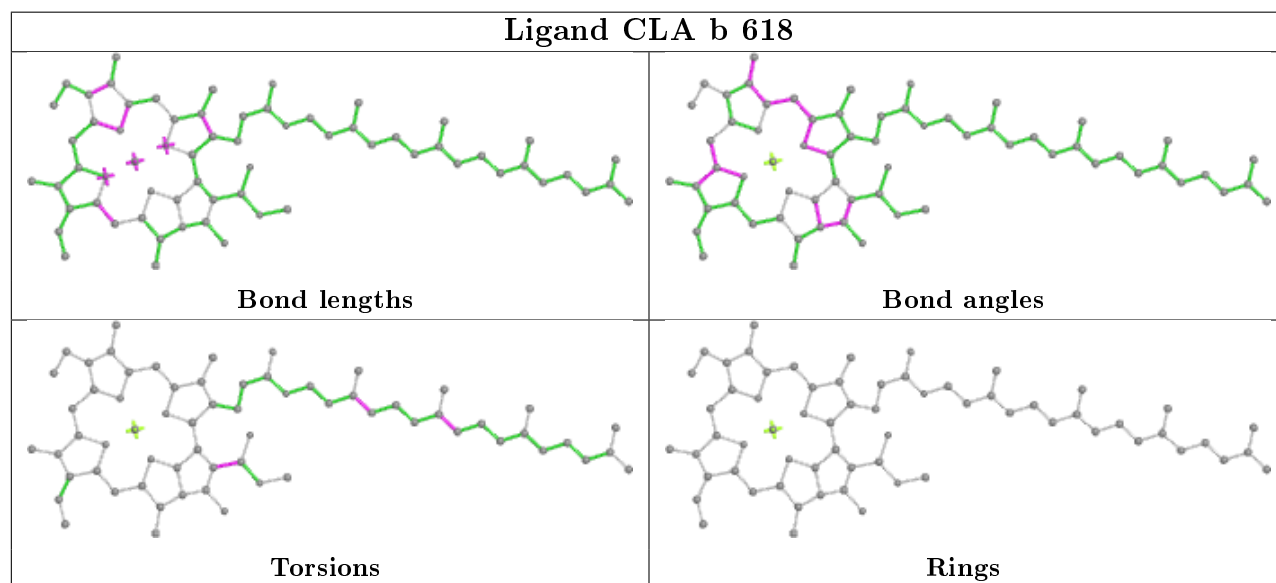
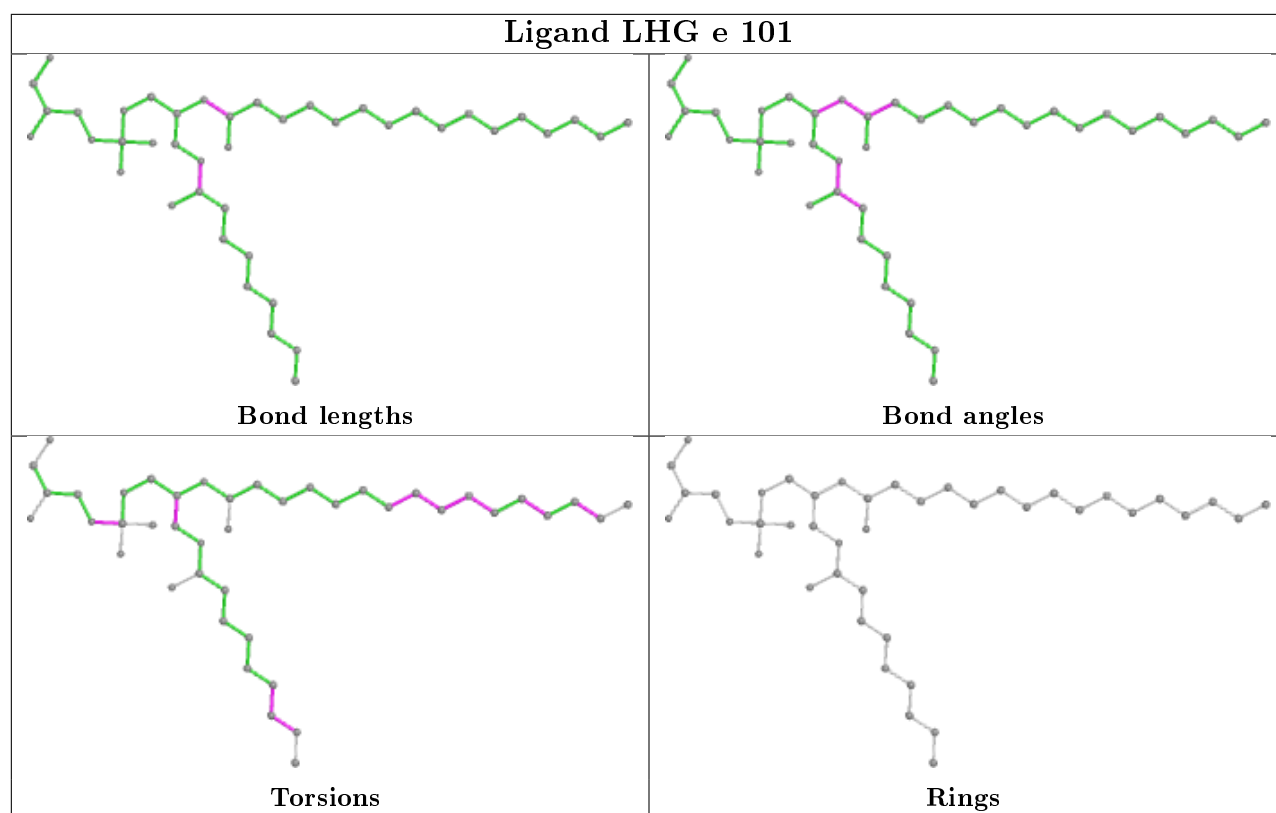
**Ligand CLA b 604****Ligand LFA b 626****Ligand LFA I 101****Ligand BCR a 408**

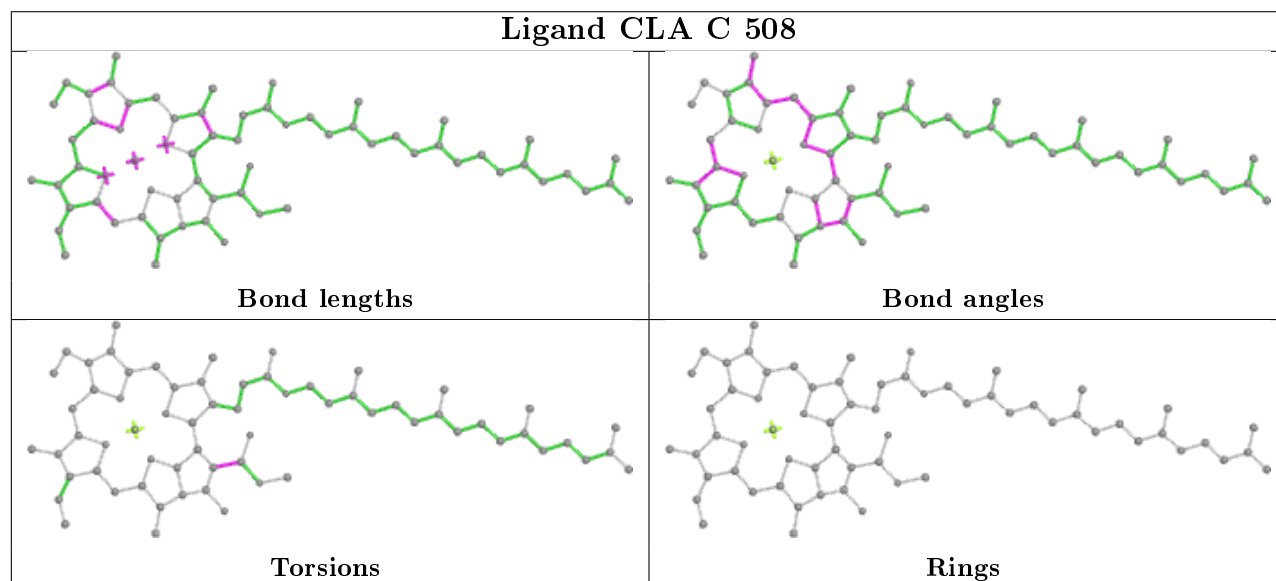
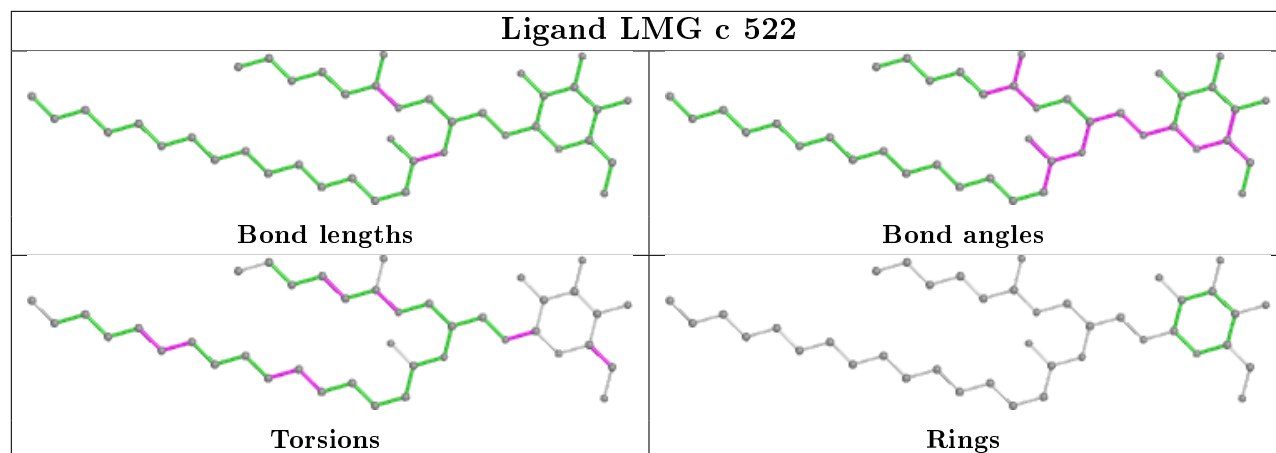
**Ligand CLA b 616****Ligand LFA B 628****Ligand CLA C 506**

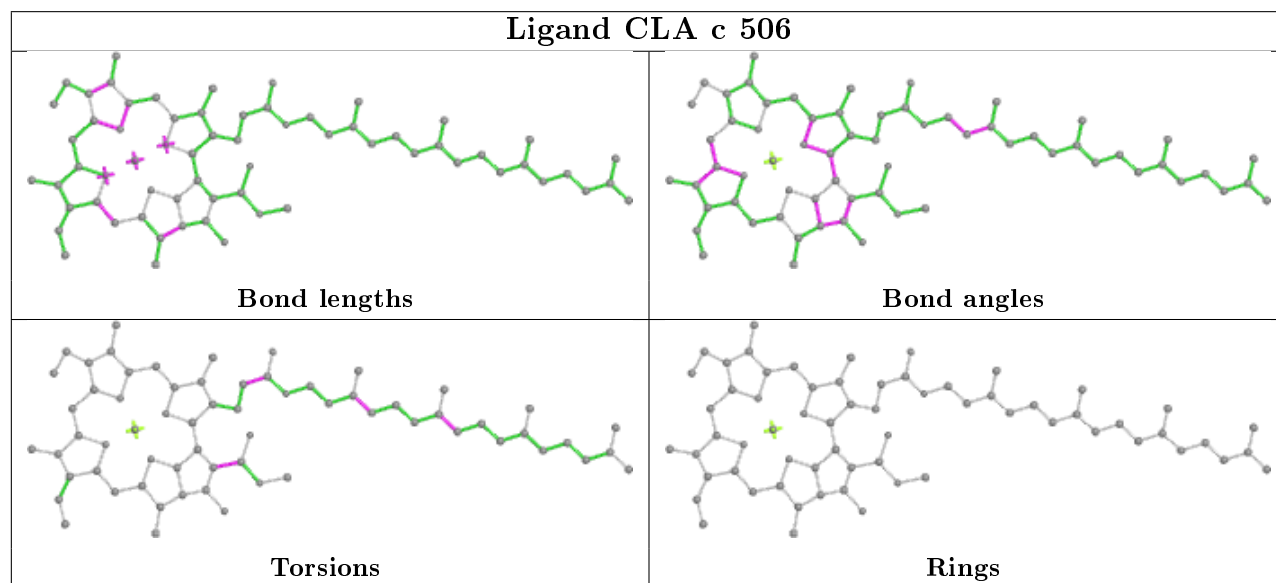
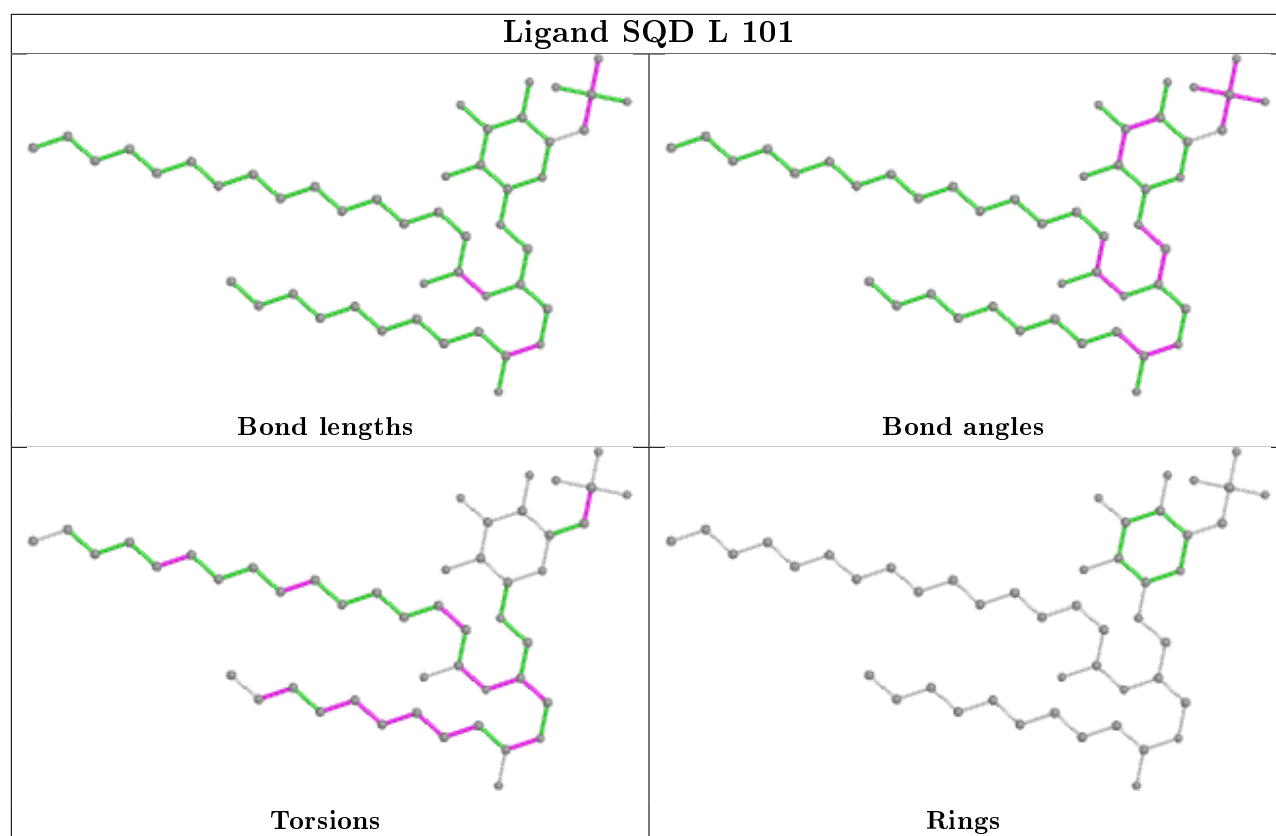
**Ligand BCR c 524****Ligand BCR c 523****Ligand BCR T 101****Ligand BCR b 621**

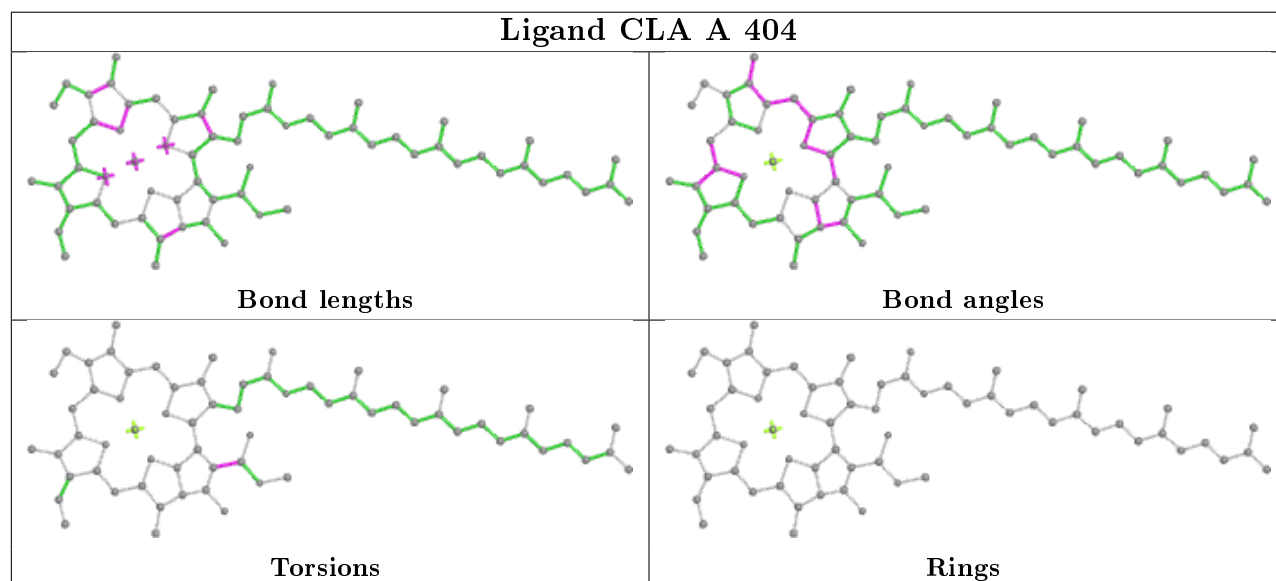
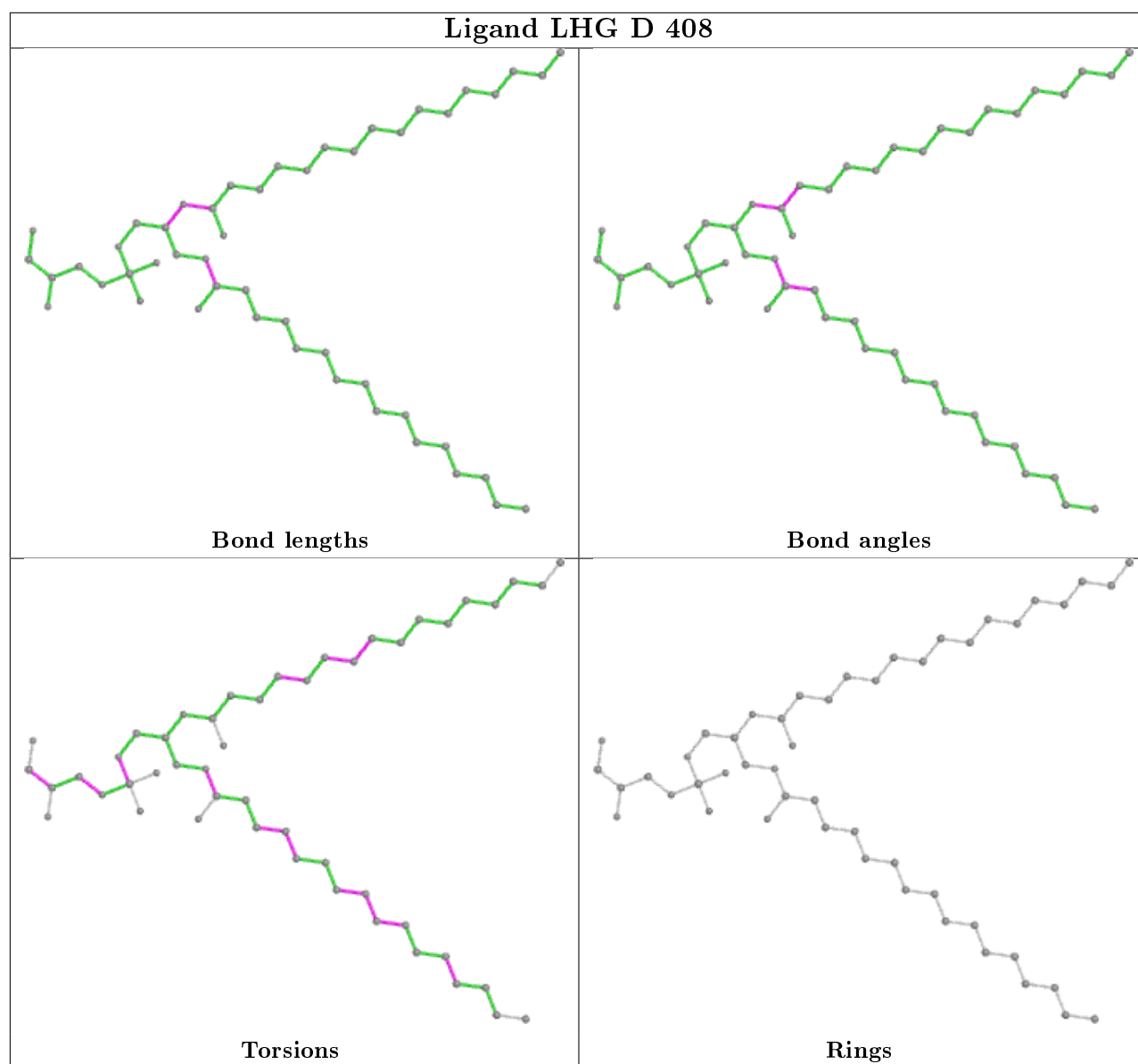


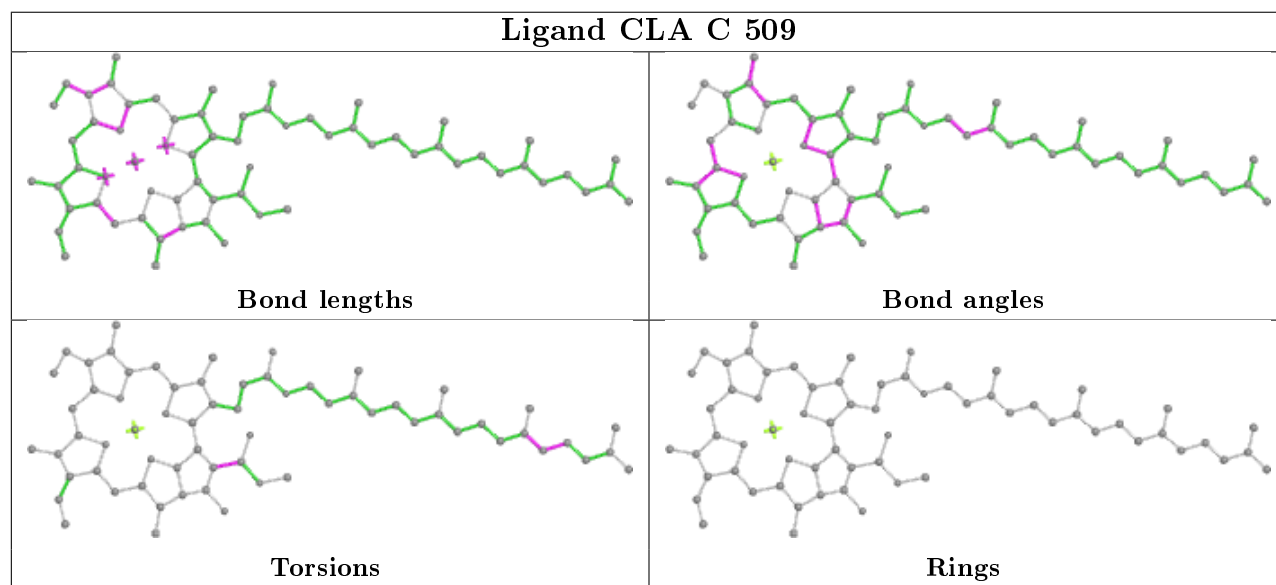
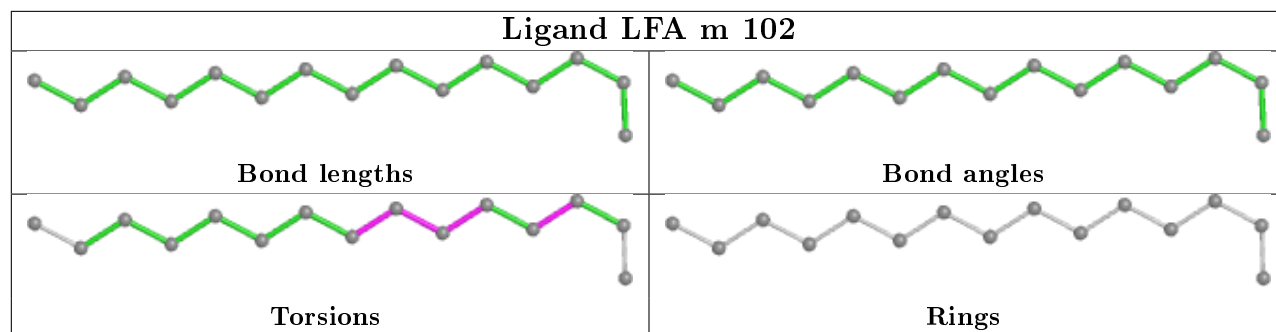


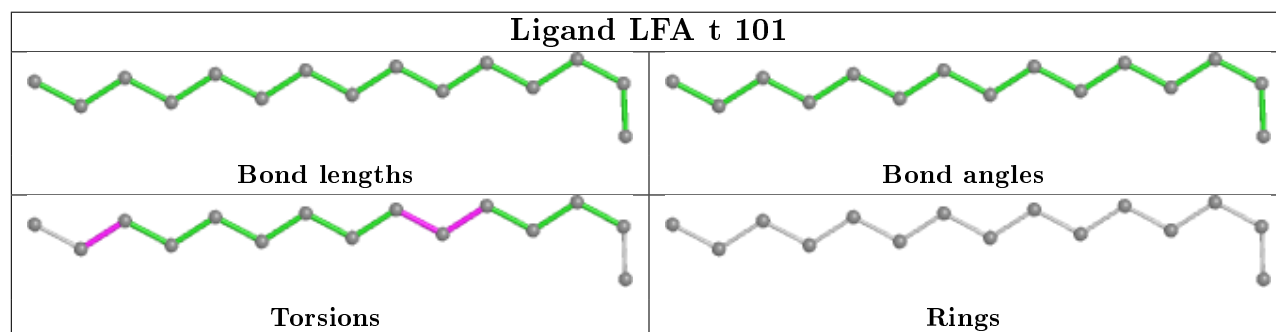
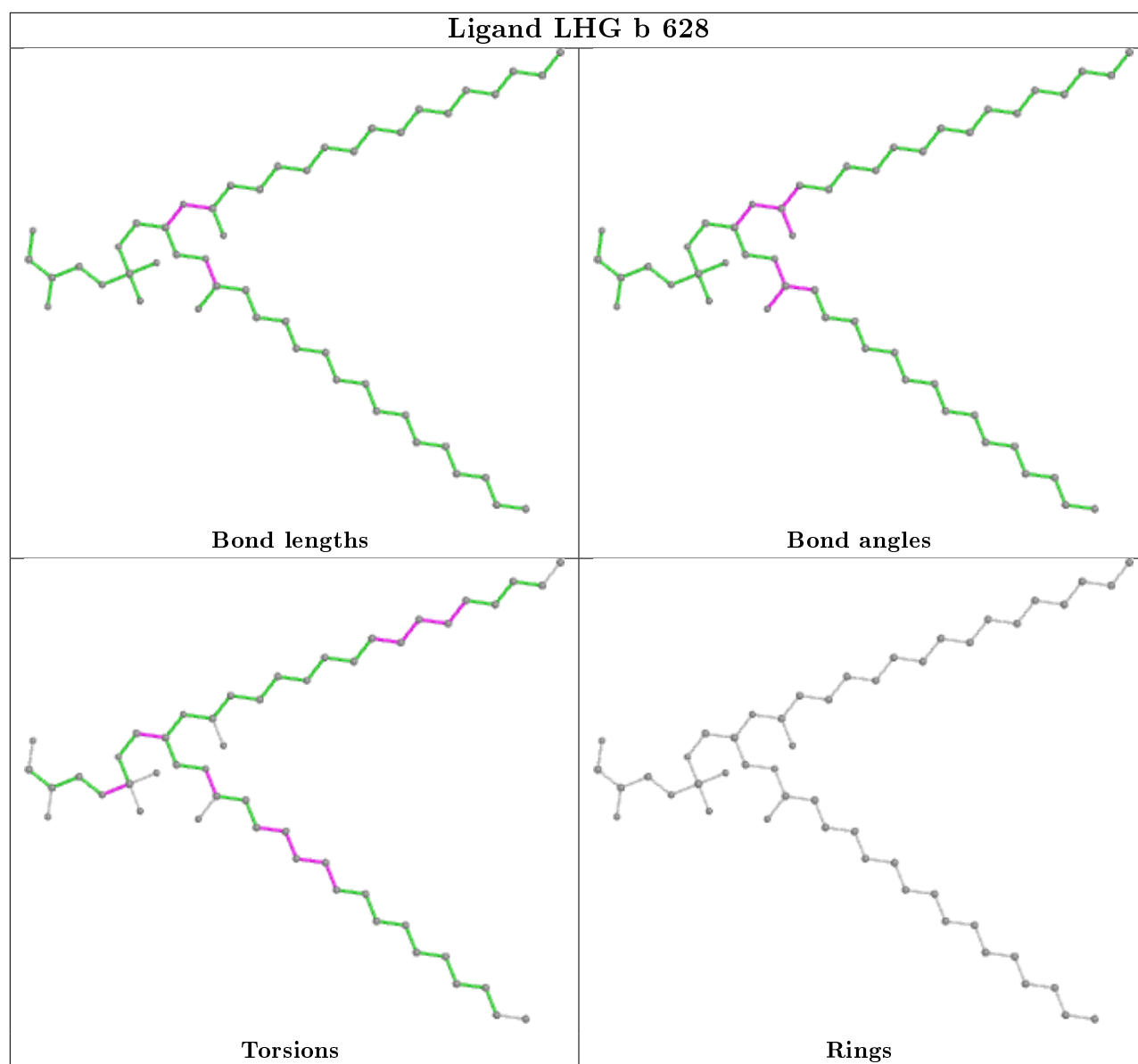




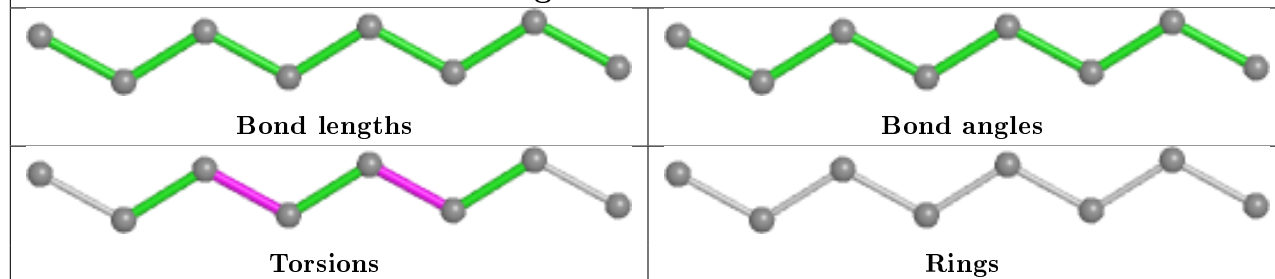




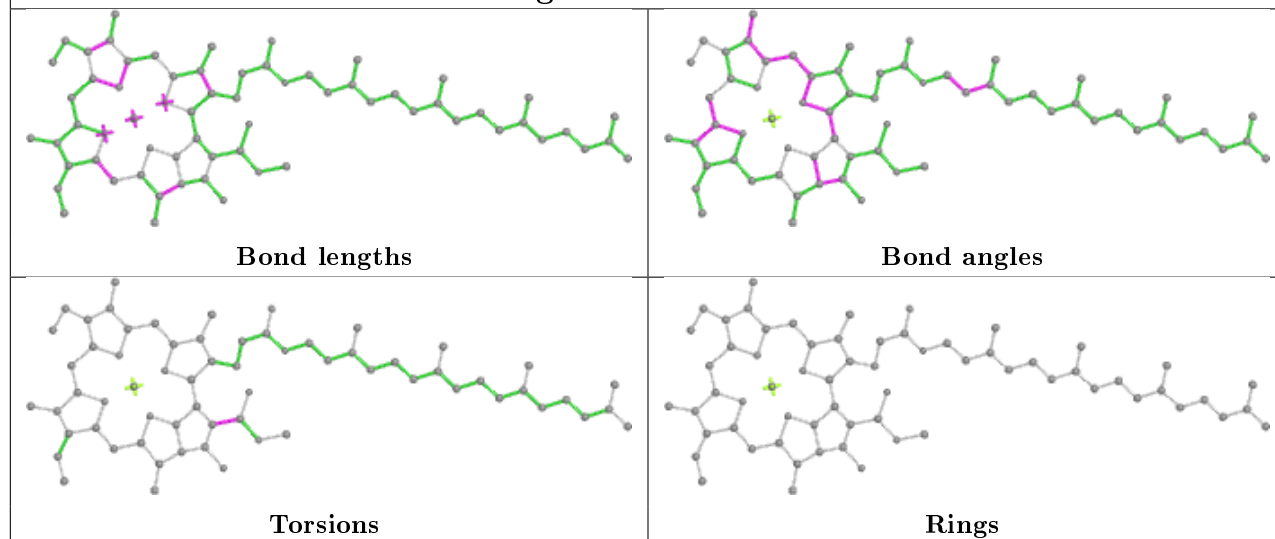




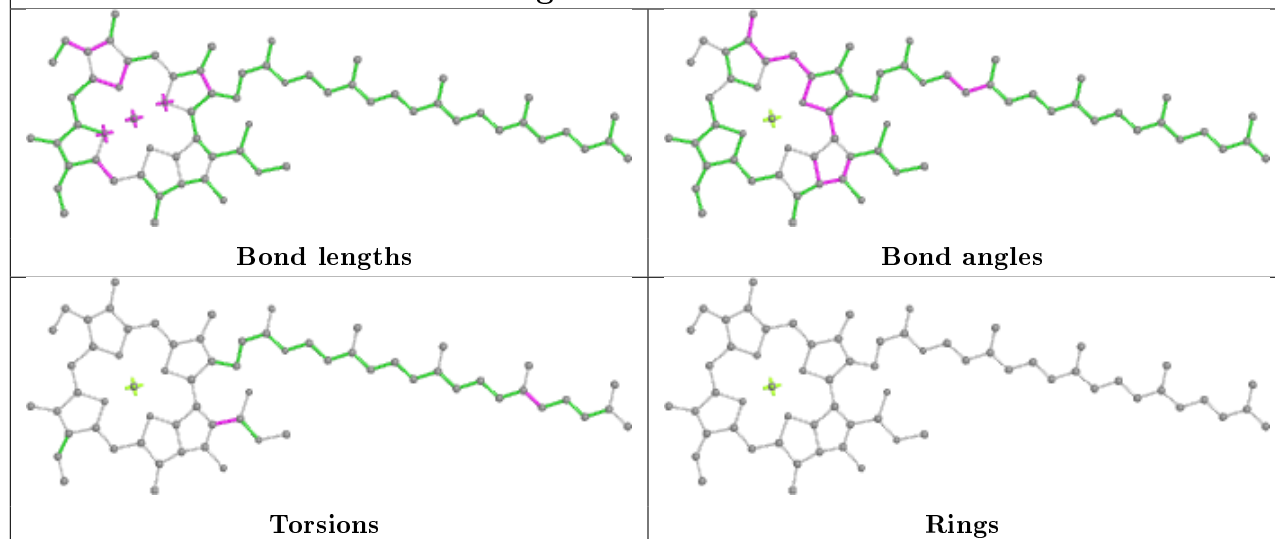
## Ligand LFA D 412

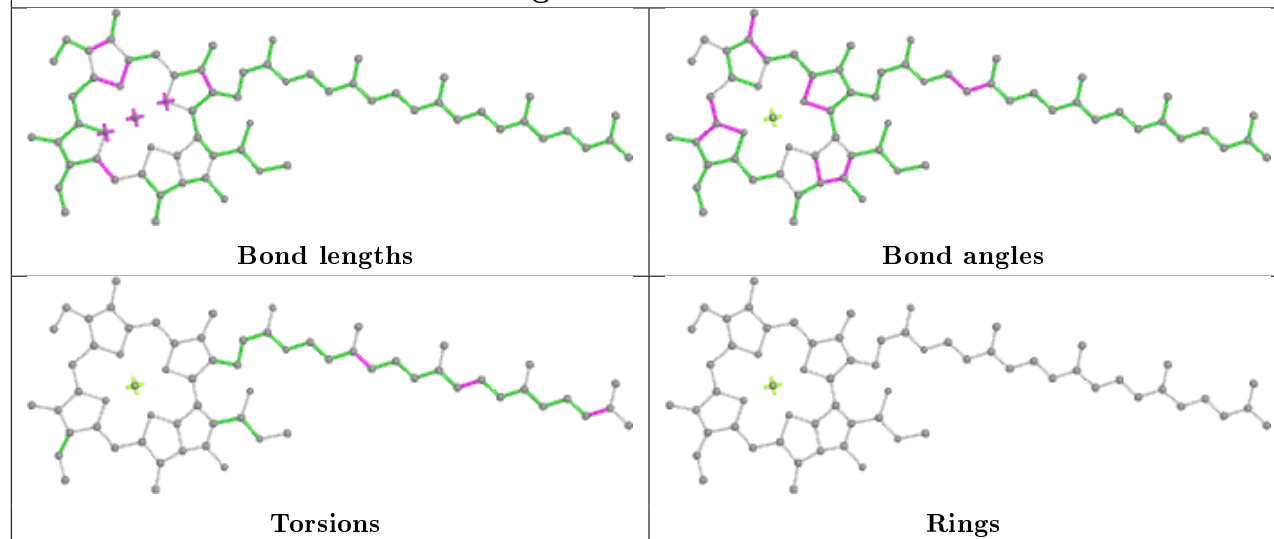
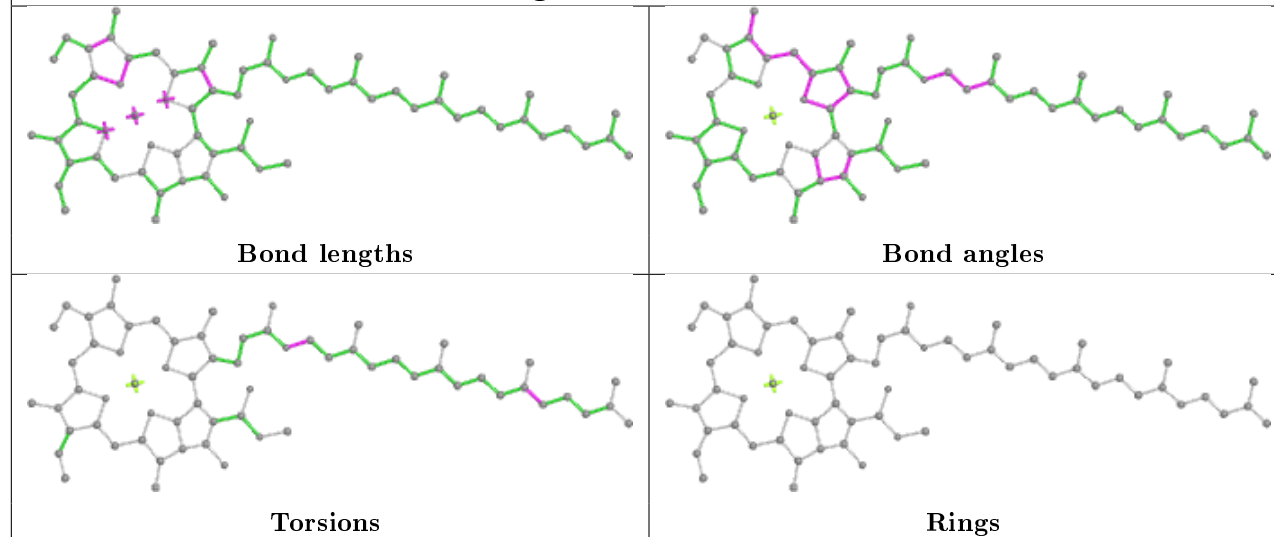
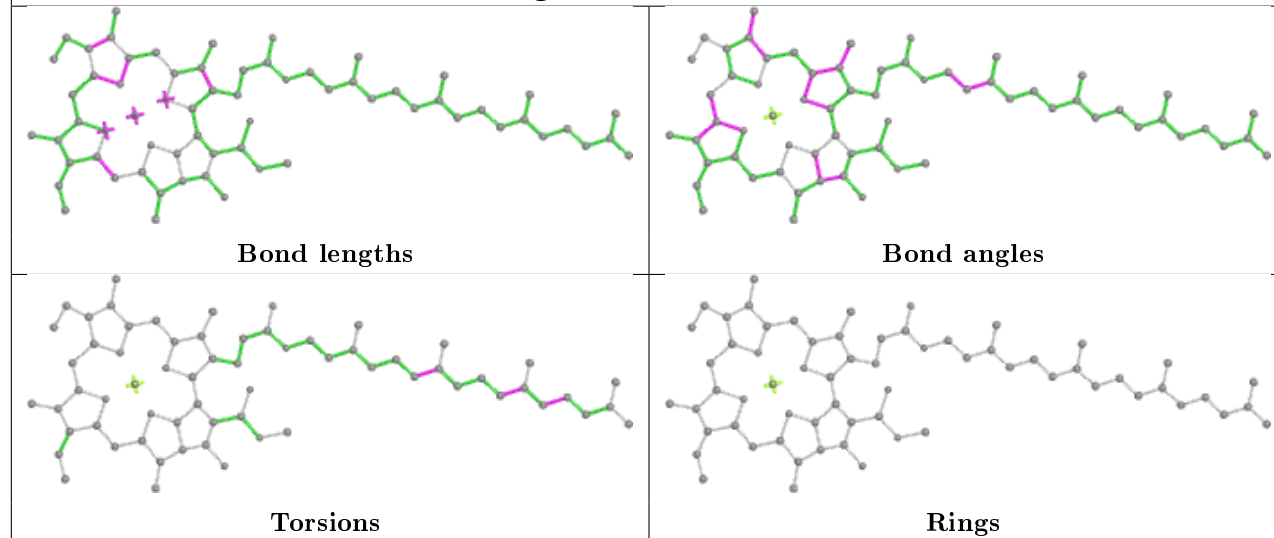


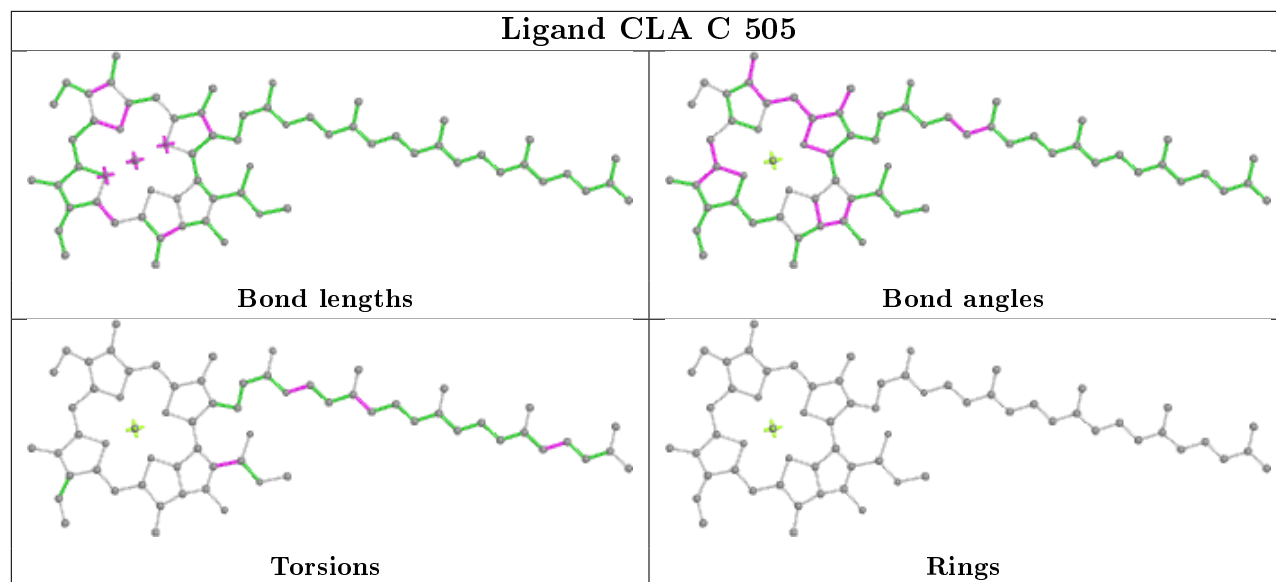
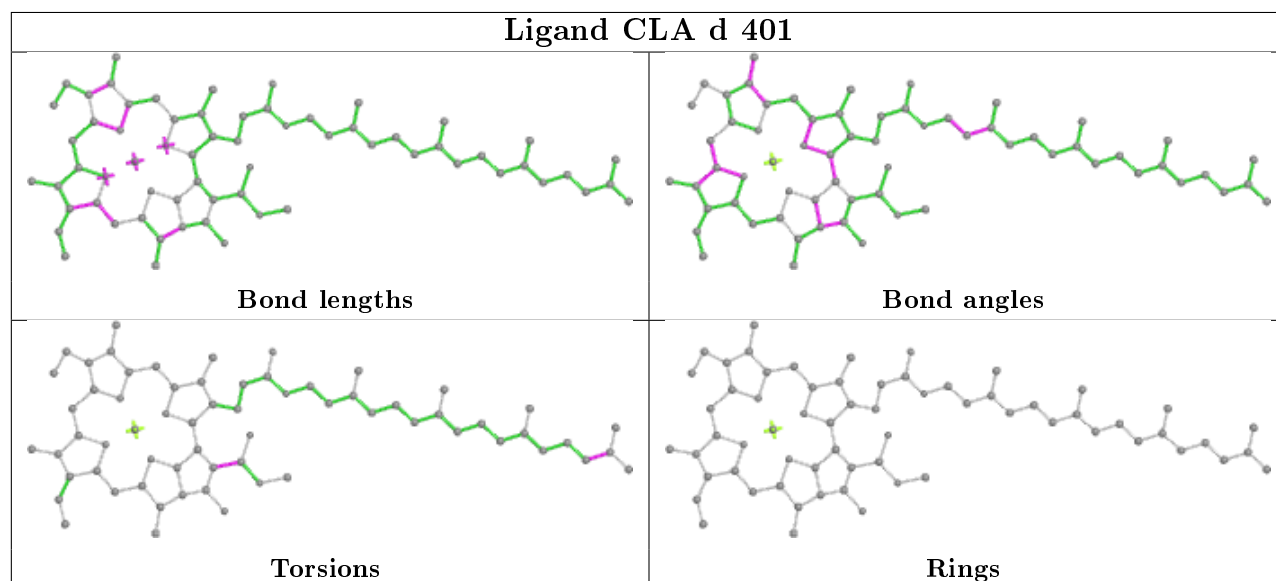
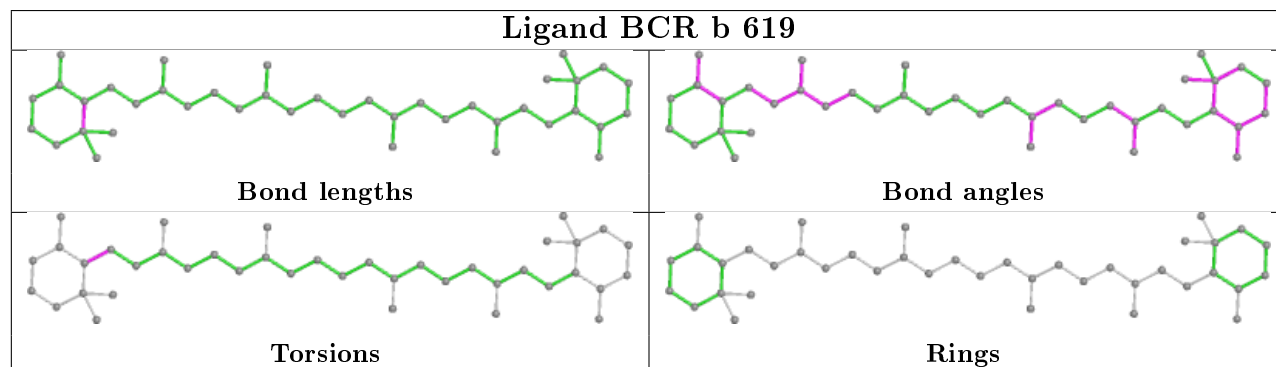
## Ligand CLA c 503

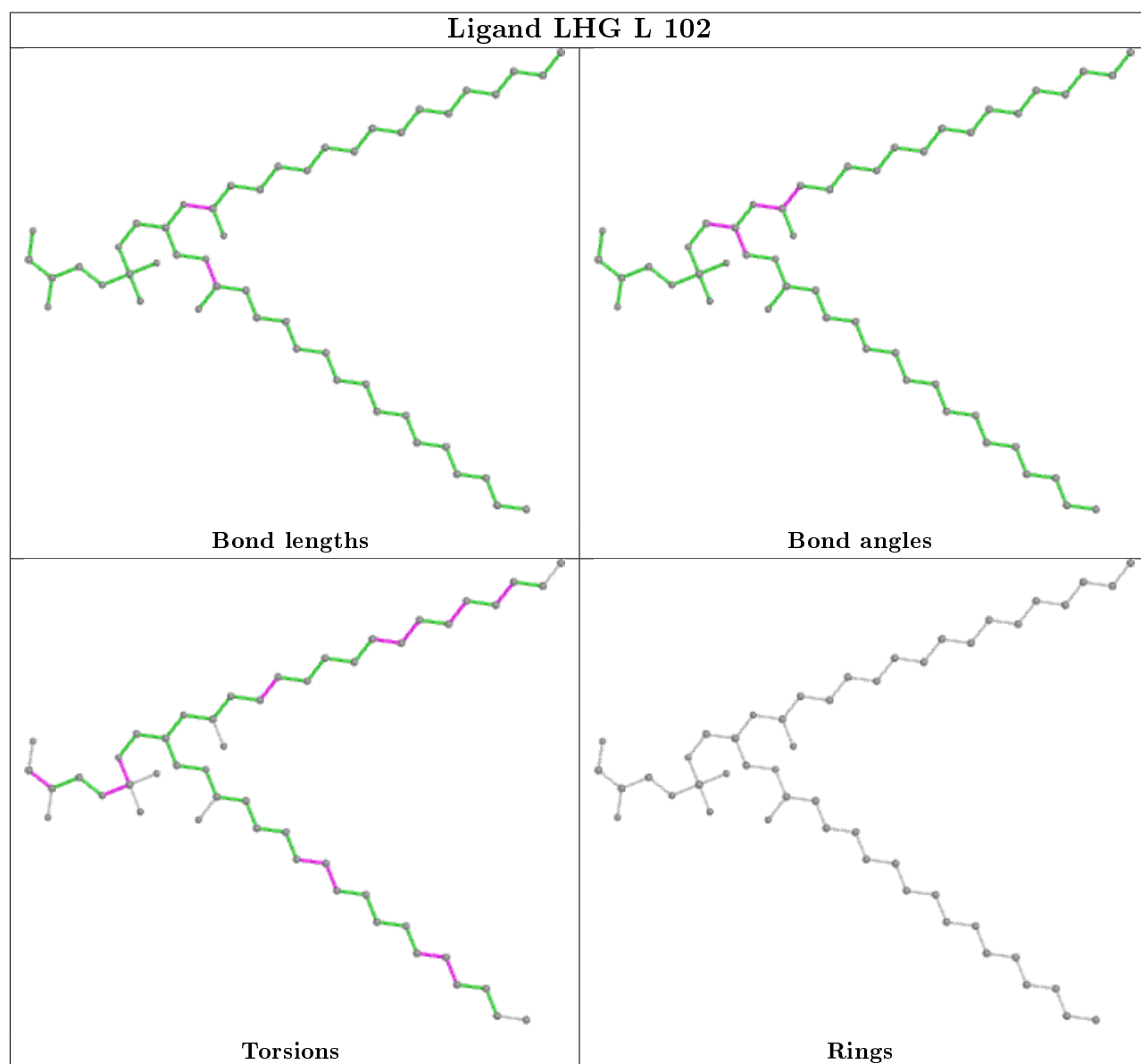
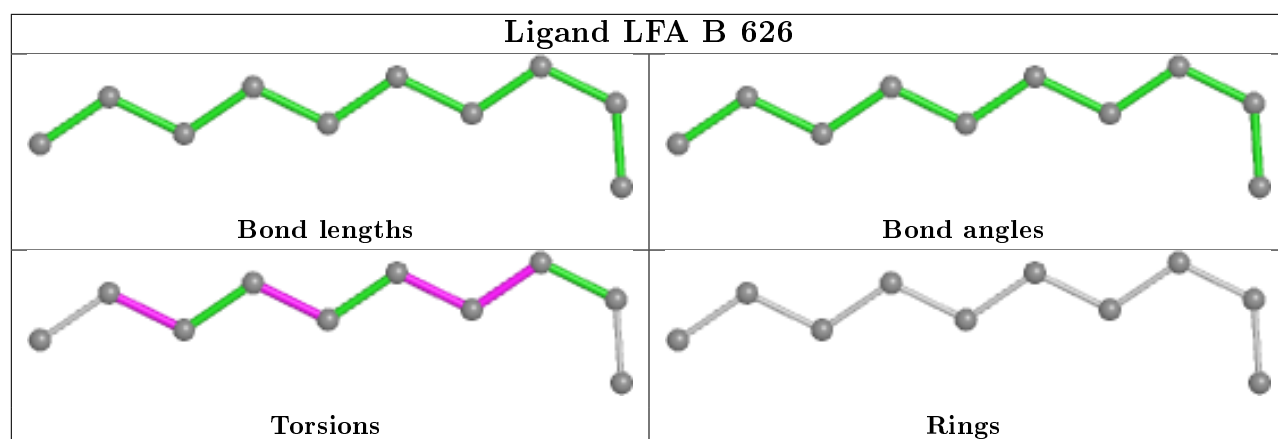


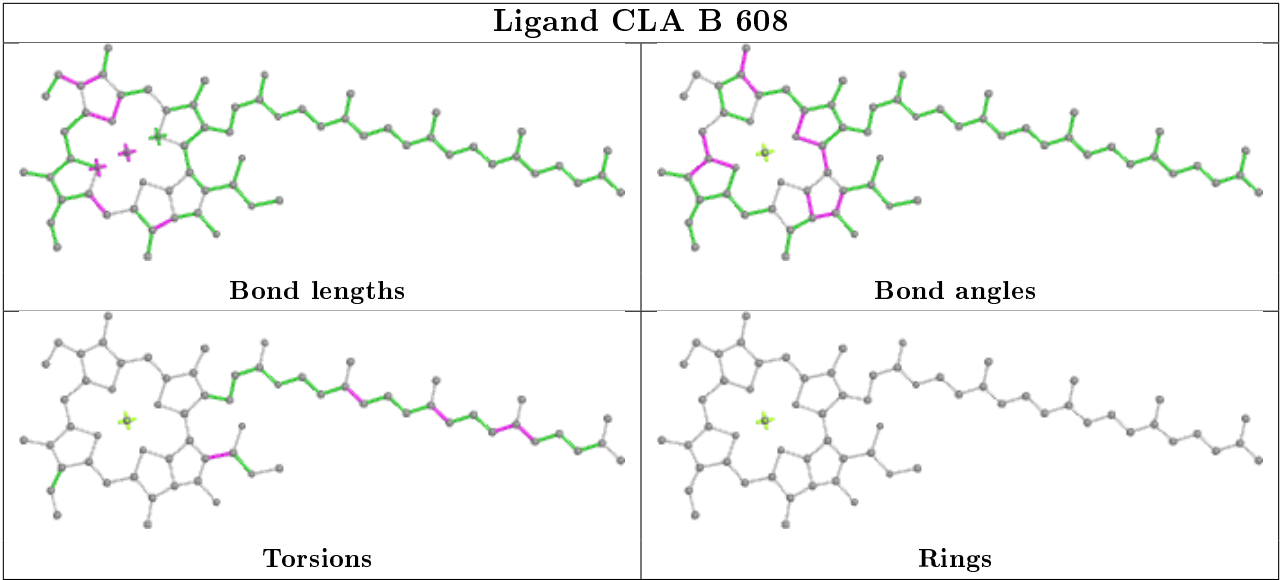
## Ligand CLA c 508



**Ligand CLA B 610****Ligand CLA D 402****Ligand CLA B 602**

**Ligand CLA C 505****Ligand CLA d 401****Ligand BCR b 619**





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	c	1
5	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	399:ALA	C	400:PRO	N	1.19
1	e	63:ILE	C	64:PRO	N	1.13

## 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	333/344 (96%)	0.33	15 (4%) 33 32	17, 24, 47, 70	0
1	a	333/344 (96%)	0.15	7 (2%) 63 61	16, 24, 48, 66	0
2	B	505/510 (99%)	0.16	23 (4%) 32 31	16, 25, 55, 73	0
2	b	503/510 (98%)	0.20	37 (7%) 14 13	19, 30, 59, 90	0
3	C	447/461 (96%)	0.23	23 (5%) 28 26	20, 32, 50, 83	0
3	c	448/461 (97%)	0.08	12 (2%) 54 52	21, 32, 46, 67	0
4	D	340/352 (96%)	0.08	7 (2%) 63 61	16, 25, 42, 62	0
4	d	340/352 (96%)	0.06	1 (0%) 94 93	17, 28, 48, 67	0
5	E	81/84 (96%)	0.60	6 (7%) 14 13	29, 46, 59, 76	0
5	e	79/84 (94%)	0.92	17 (21%) 0 0	34, 50, 68, 87	0
6	F	33/45 (73%)	0.02	1 (3%) 50 48	32, 39, 49, 58	0
6	f	33/45 (73%)	-0.03	2 (6%) 21 20	39, 44, 61, 63	0
7	H	62/66 (93%)	0.00	0 100 100	25, 30, 36, 45	0
7	h	63/66 (95%)	0.46	7 (11%) 5 4	34, 39, 50, 55	0
8	I	33/38 (86%)	-0.16	0 100 100	23, 28, 35, 43	0
8	i	33/38 (86%)	-0.22	1 (3%) 50 48	21, 28, 39, 45	0
9	J	33/40 (82%)	0.41	2 (6%) 21 20	33, 41, 49, 54	0
9	j	33/40 (82%)	0.34	3 (9%) 9 8	33, 41, 49, 56	0
10	K	35/46 (76%)	0.52	4 (11%) 5 4	41, 47, 69, 76	0
10	k	36/46 (78%)	0.17	3 (8%) 11 10	35, 45, 66, 77	0
11	L	36/37 (97%)	-0.30	0 100 100	18, 22, 46, 54	0
11	l	36/37 (97%)	-0.15	2 (5%) 24 23	17, 23, 43, 55	0
12	M	32/36 (88%)	-0.09	0 100 100	19, 24, 45, 51	0
12	m	32/36 (88%)	0.02	0 100 100	20, 25, 48, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	242/272 (88%)	0.48	25 (10%) 6 5	24, 43, 69, 124	0
13	o	241/272 (88%)	0.11	10 (4%) 37 35	25, 39, 68, 122	0
14	T	28/32 (87%)	0.06	1 (3%) 42 41	19, 23, 42, 72	0
14	t	29/32 (90%)	0.09	2 (6%) 16 15	20, 24, 46, 57	0
15	U	96/134 (71%)	1.33	25 (26%) 0 0	45, 61, 83, 90	0
15	u	96/134 (71%)	0.31	3 (3%) 49 47	32, 40, 51, 54	0
16	V	137/163 (84%)	0.00	0 100 100	32, 40, 50, 61	0
16	v	137/163 (84%)	0.56	16 (11%) 4 4	34, 43, 59, 75	0
17	Y	21/46 (45%)	1.76	7 (33%) 0 0	54, 65, 81, 85	0
17	y	23/46 (50%)	1.19	6 (26%) 0 0	50, 58, 79, 82	0
18	X	37/41 (90%)	0.33	4 (10%) 5 5	32, 38, 53, 65	0
18	x	38/41 (92%)	0.93	8 (21%) 1 1	38, 49, 68, 84	0
19	Z	61/62 (98%)	1.79	20 (32%) 0 0	50, 64, 121, 133	0
19	z	61/62 (98%)	2.46	33 (54%) 0 0	51, 72, 114, 128	0
20	R	35/41 (85%)	2.23	21 (60%) 0 0	49, 61, 81, 84	0
20	r	32/41 (78%)	2.40	20 (62%) 0 0	56, 65, 90, 97	0
All	All	5253/5700 (92%)	0.30	374 (7%) 16 14	16, 33, 65, 133	0

The worst 5 of 374 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	33	TRP	12.4
19	z	31	GLN	9.6
19	Z	30	PRO	8.4
13	O	58	ASN	7.9
3	C	29	GLU	7.6

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

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

## 6.3 Carbohydrates ⓘ

There are no 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
27	LFA	A	410	14/20	0.72	0.20	37,39,43,45	0
27	LFA	i	102	7/20	0.74	0.17	26,32,34,39	0
27	LFA	b	626	12/20	0.74	0.24	29,36,43,47	0
30	LMG	C	520	48/55	0.75	0.22	38,53,67,71	0
27	LFA	b	623	12/20	0.76	0.22	25,36,38,39	0
27	LFA	A	413	11/20	0.76	0.17	27,32,46,47	0
30	LMG	c	522	41/55	0.78	0.30	21,46,54,60	0
27	LFA	m	101	10/20	0.78	0.17	28,36,44,50	0
30	LMG	b	624	39/55	0.78	0.23	34,53,60,66	0
27	LFA	B	624	15/20	0.78	0.15	28,37,47,48	0
26	SQD	A	411	54/54	0.79	0.20	27,47,71,83	0
27	LFA	B	626	10/20	0.79	0.20	20,29,38,40	0
26	SQD	b	601	54/54	0.80	0.18	25,39,62,65	0
27	LFA	b	627	11/20	0.80	0.19	36,46,49,53	0
30	LMG	B	621	36/55	0.80	0.25	28,50,59,63	0
27	LFA	C	521	15/20	0.81	0.16	26,34,39,42	0
30	LMG	B	619	51/55	0.81	0.18	15,31,42,47	0
30	LMG	C	501	51/55	0.81	0.21	26,40,50,53	0
27	LFA	b	625	16/20	0.82	0.17	27,32,41,45	0
27	LFA	b	629	9/20	0.82	0.26	29,31,33,39	0
22	CLA	b	603	65/65	0.82	0.24	33,57,78,85	0
27	LFA	d	410	16/20	0.82	0.16	28,35,44,45	0
26	SQD	L	101	48/54	0.82	0.17	21,42,66,69	0
30	LMG	C	522	44/55	0.82	0.29	32,42,53,58	0
30	LMG	c	501	51/55	0.83	0.18	25,39,51,60	0
25	PL9	A	408	55/55	0.84	0.20	34,43,53,56	0
32	LHG	E	101	42/49	0.84	0.17	31,54,67,71	0
26	SQD	a	412	50/54	0.85	0.16	28,43,70,76	0
31	DGD	H	103	60/66	0.85	0.22	22,29,40,45	0
31	DGD	h	102	62/66	0.85	0.20	23,33,40,45	0
24	BCR	h	101	40/40	0.85	0.17	28,40,45,49	0
27	LFA	m	102	15/20	0.85	0.20	25,29,37,37	0
27	LFA	j	101	15/20	0.85	0.21	41,45,51,56	0
24	BCR	K	101	40/40	0.86	0.17	37,48,53,55	0
30	LMG	c	519	51/55	0.86	0.20	38,52,64,67	0
27	LFA	d	409	9/20	0.86	0.19	24,35,40,46	0
30	LMG	m	103	51/55	0.86	0.18	17,30,41,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LFA	b	630	15/20	0.86	0.13	31,39,42,42	0
27	LFA	B	623	13/20	0.87	0.16	21,31,34,36	0
27	LFA	B	627	14/20	0.87	0.17	20,31,36,39	0
27	LFA	B	622	16/20	0.87	0.14	27,32,36,37	0
25	PL9	a	409	55/55	0.87	0.20	38,48,59,65	0
26	SQD	D	411	43/54	0.88	0.21	38,50,58,69	0
27	LFA	i	101	16/20	0.88	0.16	23,32,40,41	0
27	LFA	D	410	15/20	0.88	0.17	23,28,40,47	0
27	LFA	T	102	12/20	0.88	0.13	22,28,32,32	0
27	LFA	d	408	15/20	0.88	0.18	25,32,37,37	0
31	DGD	C	518	56/66	0.88	0.17	29,38,48,53	0
22	CLA	C	513	65/65	0.89	0.16	34,41,54,63	0
32	LHG	e	101	42/49	0.89	0.16	40,62,80,94	0
27	LFA	M	102	16/20	0.89	0.13	25,27,46,47	0
27	LFA	b	622	10/20	0.89	0.13	27,31,37,38	0
22	CLA	H	101	65/65	0.89	0.15	30,45,64,72	0
27	LFA	t	101	15/20	0.89	0.18	25,31,42,43	0
24	BCR	t	102	40/40	0.89	0.17	21,26,38,40	0
24	BCR	c	523	40/40	0.90	0.15	39,46,52,55	0
24	BCR	T	101	40/40	0.90	0.14	22,29,34,37	0
22	CLA	c	513	65/65	0.90	0.15	36,42,55,62	0
26	SQD	A	409	54/54	0.90	0.15	24,42,54,56	0
22	CLA	b	618	65/65	0.90	0.15	23,32,58,64	0
22	CLA	C	511	65/65	0.90	0.18	25,34,41,49	0
22	CLA	C	504	65/65	0.90	0.14	20,35,38,42	0
22	CLA	B	603	65/65	0.90	0.17	14,21,35,44	0
22	CLA	c	504	65/65	0.90	0.16	26,34,39,40	0
24	BCR	H	102	40/40	0.90	0.13	22,28,42,43	0
22	CLA	b	606	65/65	0.90	0.20	16,23,38,45	0
24	BCR	c	524	40/40	0.90	0.18	36,43,53,53	0
24	BCR	d	404	40/40	0.91	0.14	25,36,53,56	0
27	LFA	I	101	14/20	0.91	0.10	21,29,32,32	0
24	BCR	B	616	40/40	0.91	0.15	19,25,31,32	0
27	LFA	B	620	10/20	0.91	0.14	22,24,28,33	0
22	CLA	B	605	65/65	0.91	0.12	17,25,38,44	0
21	CL	A	401	1/1	0.91	0.13	57,57,57,57	0
22	CLA	C	512	65/65	0.91	0.13	35,44,52,56	0
22	CLA	c	514	65/65	0.91	0.17	33,45,61,67	0
31	DGD	C	519	62/66	0.91	0.15	27,33,46,60	0
24	BCR	K	102	40/40	0.91	0.14	39,44,47,48	0
24	BCR	D	404	40/40	0.91	0.13	23,33,49,50	0
27	LFA	J	101	11/20	0.91	0.15	38,43,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	BCR	k	101	40/40	0.91	0.16	29,43,51,54	0
22	CLA	C	503	65/65	0.91	0.16	24,32,36,38	0
24	BCR	C	515	40/40	0.91	0.14	36,45,52,55	0
25	PL9	D	405	55/55	0.91	0.15	12,21,26,28	0
27	LFA	D	412	8/20	0.91	0.15	25,30,37,40	0
27	LFA	D	413	10/20	0.91	0.17	22,23,26,28	0
22	CLA	c	503	65/65	0.91	0.20	23,30,38,39	0
24	BCR	b	619	40/40	0.91	0.16	18,28,34,35	0
22	CLA	b	608	65/65	0.91	0.13	22,29,42,53	0
22	CLA	c	502	65/65	0.92	0.14	17,28,35,38	0
27	LFA	B	628	12/20	0.92	0.20	23,28,37,37	0
27	LFA	c	521	15/20	0.92	0.11	31,35,41,41	0
22	CLA	c	507	65/65	0.92	0.13	25,32,52,58	0
22	CLA	B	615	65/65	0.92	0.15	19,25,70,79	0
24	BCR	b	621	40/40	0.92	0.12	23,34,42,47	0
24	BCR	B	617	40/40	0.92	0.15	15,24,30,30	0
31	DGD	c	517	55/66	0.92	0.18	25,34,50,63	0
22	CLA	C	514	65/65	0.92	0.14	37,49,63,67	0
31	DGD	c	518	62/66	0.92	0.15	26,32,52,58	0
22	CLA	D	403	65/65	0.92	0.16	17,24,62,66	0
24	BCR	b	620	40/40	0.92	0.15	18,25,30,32	0
27	LFA	b	602	15/20	0.92	0.12	29,33,42,42	0
26	SQD	a	410	54/54	0.92	0.15	30,48,58,62	0
27	LFA	c	520	9/20	0.92	0.17	31,39,46,47	0
24	BCR	B	618	40/40	0.92	0.12	18,26,34,36	0
22	CLA	C	509	65/65	0.92	0.17	22,31,62,66	0
26	SQD	f	102	43/54	0.92	0.23	51,66,77,86	0
31	DGD	c	516	62/66	0.92	0.15	23,28,49,52	0
24	BCR	C	516	40/40	0.92	0.12	21,30,37,38	0
31	DGD	C	517	62/66	0.92	0.17	20,26,49,52	0
22	CLA	c	508	65/65	0.92	0.15	22,30,34,37	0
22	CLA	C	505	65/65	0.92	0.19	28,35,48,61	0
27	LFA	B	625	9/20	0.92	0.17	20,25,27,33	0
22	CLA	c	512	65/65	0.92	0.11	28,39,47,50	0
22	CLA	d	403	65/65	0.93	0.15	22,30,57,63	0
24	BCR	c	515	40/40	0.93	0.12	19,29,38,41	0
22	CLA	a	404	65/65	0.93	0.15	14,20,27,36	0
22	CLA	a	405	65/65	0.93	0.13	14,19,25,31	0
22	CLA	C	507	65/65	0.93	0.12	22,30,55,57	0
22	CLA	c	510	65/65	0.93	0.15	22,31,38,40	0
30	LMG	f	101	51/55	0.93	0.13	31,38,55,61	0
27	LFA	a	411	7/20	0.93	0.09	26,32,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	c	506	65/65	0.93	0.12	21,26,37,40	0
22	CLA	C	508	65/65	0.93	0.13	21,26,35,45	0
32	LHG	D	406	49/49	0.93	0.14	17,24,30,33	0
32	LHG	D	408	49/49	0.93	0.16	16,33,53,57	0
22	CLA	b	604	65/65	0.93	0.15	25,30,41,46	0
23	PHO	a	406	64/64	0.93	0.14	13,17,25,27	0
22	CLA	b	610	65/65	0.93	0.17	22,28,37,45	0
22	CLA	b	616	65/65	0.93	0.13	20,26,39,42	0
22	CLA	b	611	65/65	0.93	0.12	23,30,40,52	0
22	CLA	C	510	65/65	0.93	0.14	25,31,39,40	0
21	CL	a	403	1/1	0.93	0.10	40,40,40,40	0
22	CLA	B	613	65/65	0.93	0.14	18,25,46,57	0
32	LHG	l	101	49/49	0.93	0.13	17,25,34,39	0
22	CLA	B	611	65/65	0.93	0.16	14,19,25,28	0
32	LHG	L	102	49/49	0.93	0.13	18,24,31,34	0
22	CLA	C	506	65/65	0.94	0.12	17,27,32,40	0
22	CLA	b	615	65/65	0.94	0.20	16,21,36,39	0
23	PHO	a	414	64/64	0.94	0.14	21,28,33,39	0
22	CLA	c	505	65/65	0.94	0.23	21,33,49,53	0
22	CLA	A	412	65/65	0.94	0.12	16,20,25,27	0
22	CLA	B	601	65/65	0.94	0.15	17,26,32,36	0
22	CLA	b	617	65/65	0.94	0.11	21,27,39,50	0
27	LFA	M	101	10/20	0.94	0.17	26,31,41,42	0
25	PL9	d	405	55/55	0.94	0.12	16,23,27,30	0
22	CLA	c	509	65/65	0.94	0.18	24,30,59,66	0
33	HEM	e	102	43/43	0.94	0.13	37,48,57,60	0
21	CL	a	402	1/1	0.94	0.16	52,52,52,52	0
22	CLA	c	511	65/65	0.94	0.21	27,32,38,44	0
22	CLA	b	613	65/65	0.94	0.15	18,23,29,31	0
22	CLA	B	614	65/65	0.94	0.10	15,22,32,47	0
33	HEM	E	102	43/43	0.94	0.12	34,43,52,54	0
22	CLA	b	614	65/65	0.94	0.17	16,23,28,32	0
22	CLA	A	404	65/65	0.94	0.15	15,23,61,72	0
22	CLA	B	604	65/65	0.94	0.16	15,21,25,29	0
22	CLA	d	402	65/65	0.94	0.13	17,20,37,40	0
32	LHG	b	628	49/49	0.94	0.13	22,27,35,49	0
22	CLA	B	607	65/65	0.94	0.17	13,19,26,34	0
24	BCR	A	407	40/40	0.94	0.10	14,23,30,31	0
30	LMG	D	409	51/55	0.94	0.13	25,36,51,54	0
22	CLA	C	502	65/65	0.94	0.13	18,24,33,35	0
22	CLA	B	612	65/65	0.94	0.17	13,18,40,43	0
22	CLA	B	610	65/65	0.94	0.17	12,18,24,29	0

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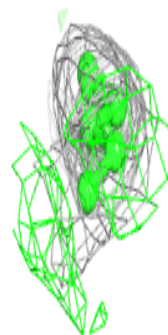
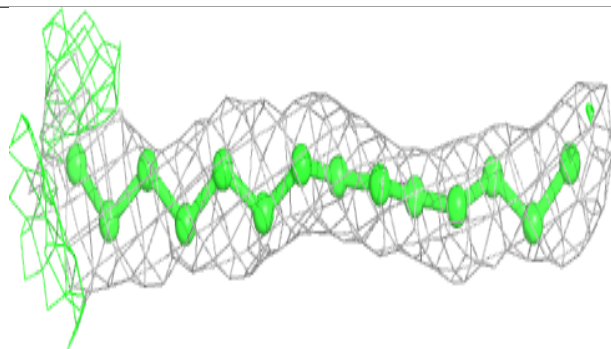
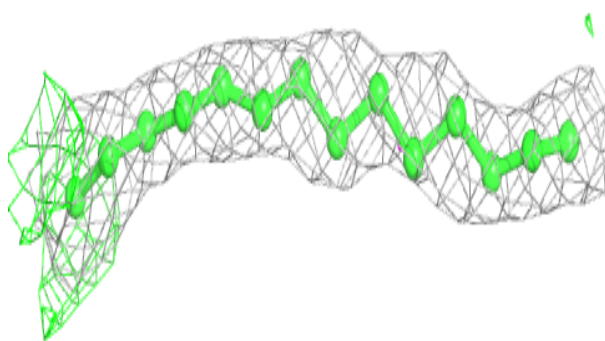
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	B	602	65/65	0.94	0.15	18,21,35,38	0
24	BCR	a	408	40/40	0.94	0.10	18,22,29,31	0
22	CLA	d	401	65/65	0.94	0.15	18,27,63,69	0
32	LHG	D	407	49/49	0.94	0.13	18,24,30,37	0
22	CLA	a	407	65/65	0.94	0.13	13,19,56,60	0
22	CLA	b	607	65/65	0.94	0.14	18,23,30,32	0
22	CLA	B	608	65/65	0.94	0.11	15,24,33,36	0
23	PHO	D	401	64/64	0.95	0.15	14,18,25,28	0
33	HEM	V	201	43/43	0.95	0.12	28,36,41,45	0
22	CLA	B	606	65/65	0.95	0.15	10,18,33,37	0
22	CLA	A	403	65/65	0.95	0.14	12,18,23,30	0
32	LHG	d	406	49/49	0.95	0.12	18,24,32,36	0
22	CLA	D	402	65/65	0.95	0.14	13,18,26,35	0
32	LHG	d	407	49/49	0.95	0.16	21,37,60,63	0
22	CLA	A	406	65/65	0.95	0.13	11,20,54,60	0
22	CLA	b	612	65/65	0.95	0.14	16,25,31,33	0
22	CLA	B	609	65/65	0.95	0.15	15,20,27,29	0
22	CLA	b	605	65/65	0.95	0.17	18,22,37,49	0
22	CLA	b	609	65/65	0.95	0.16	11,21,29,32	0
23	PHO	A	405	64/64	0.95	0.17	15,21,28,31	0
29	BCT	a	413	4/4	0.96	0.11	31,33,34,40	0
21	CL	A	402	1/1	0.96	0.12	57,57,57,57	0
33	HEM	v	201	43/43	0.97	0.09	28,34,38,41	0
29	BCT	A	415	4/4	0.97	0.09	25,29,31,32	0
28	FE	A	414	1/1	0.98	0.04	26,26,26,26	0
28	FE	a	401	1/1	0.99	0.10	39,39,39,39	0

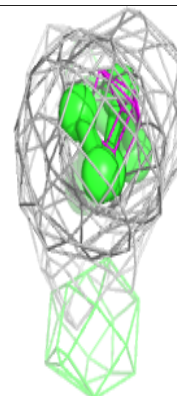
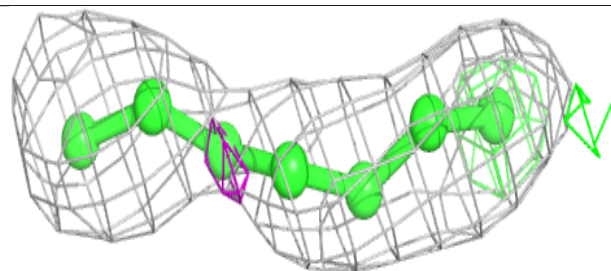
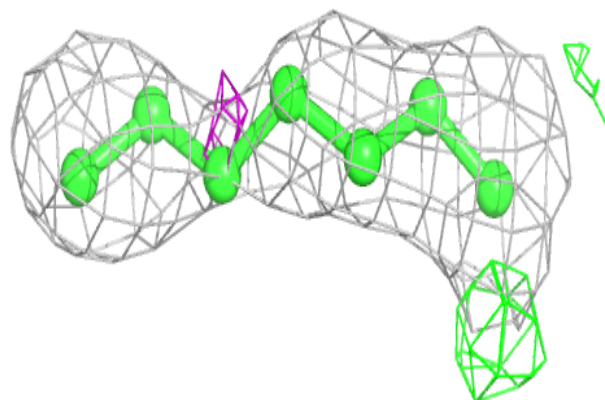
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LFA 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)

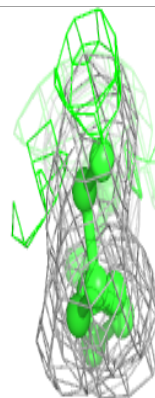
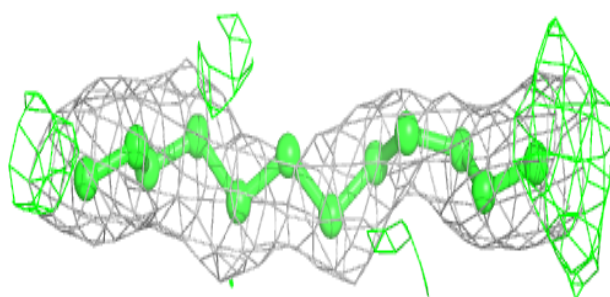
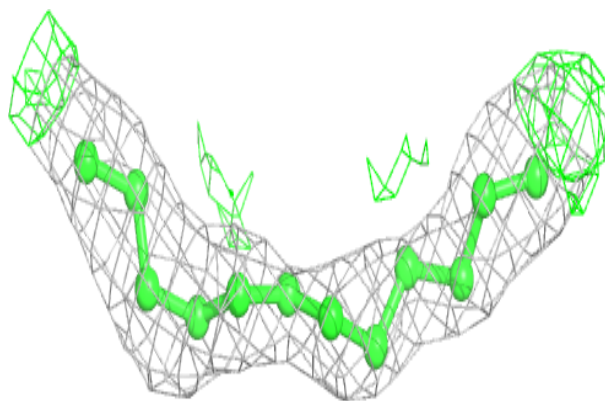
**Electron density around LFA i 102:**

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

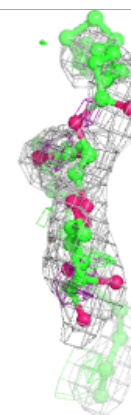
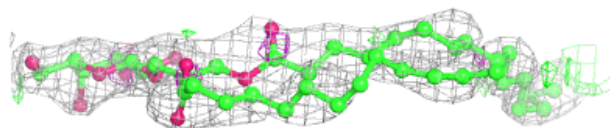
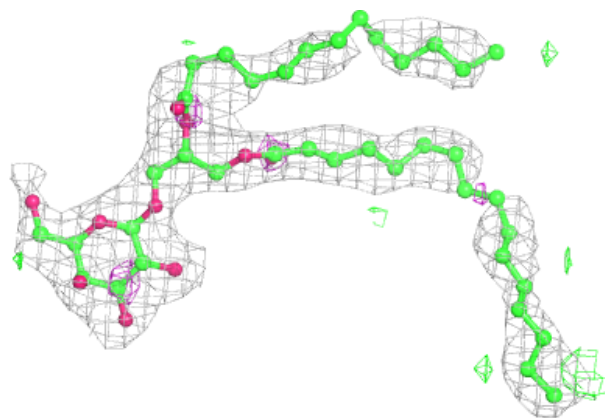


**Electron density around LFA b 626:**

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

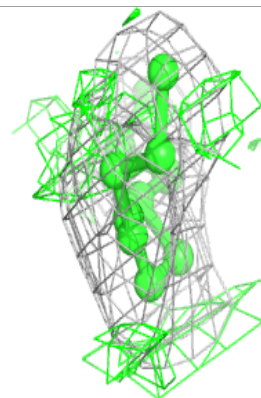
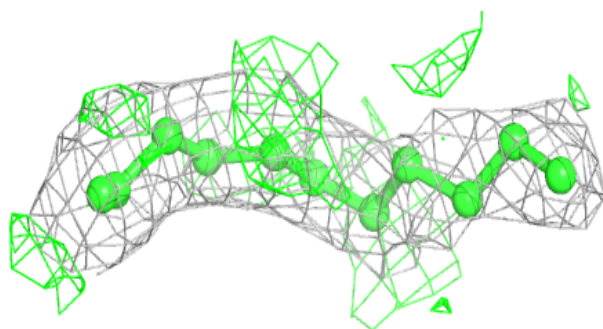
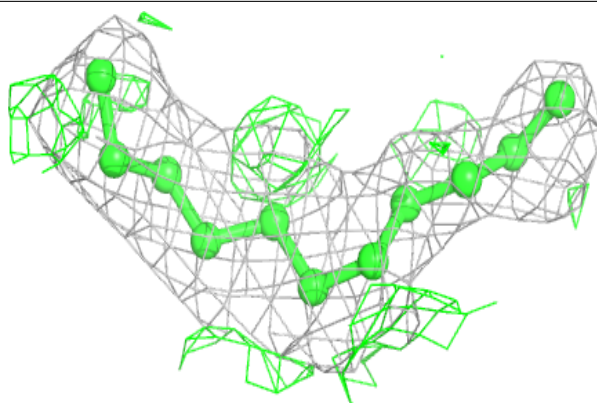
**Electron density around LMG C 520:**

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

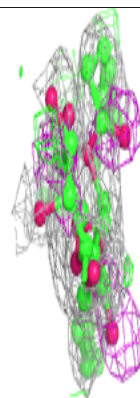
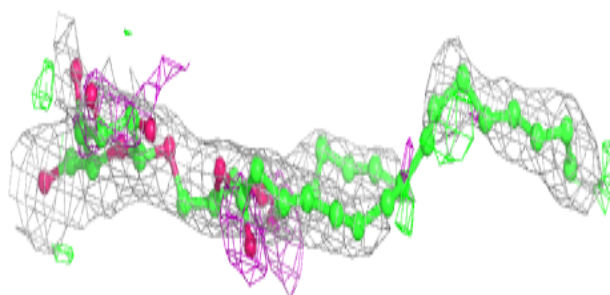
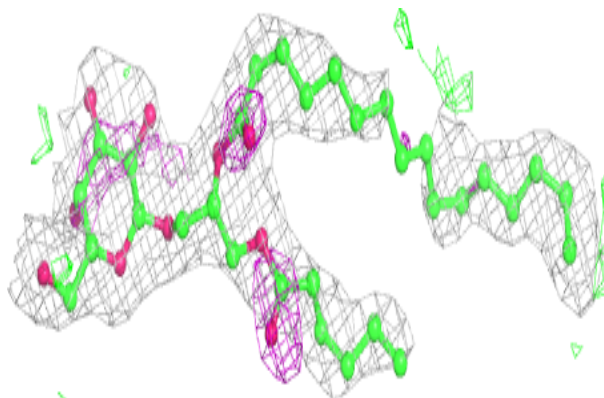


**Electron density around LFA A 413:**

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

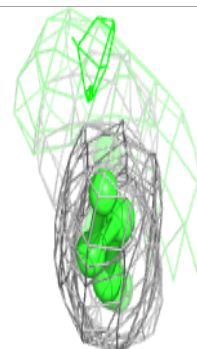
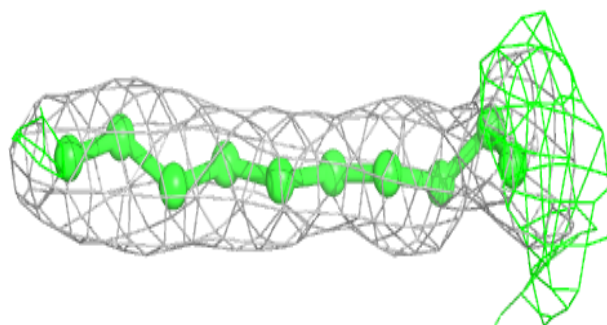
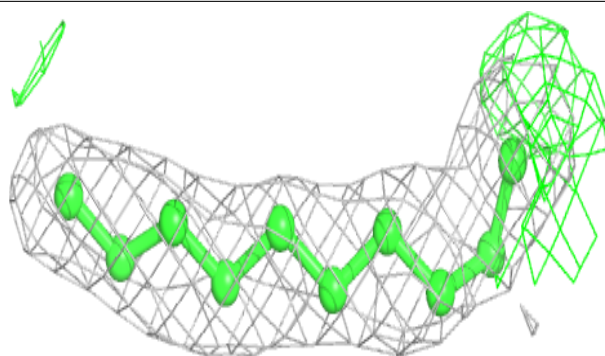
**Electron density around LMG c 522:**

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

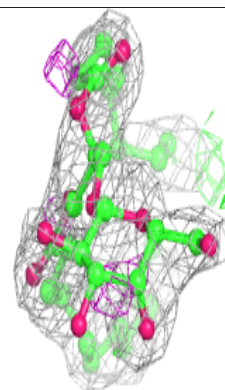
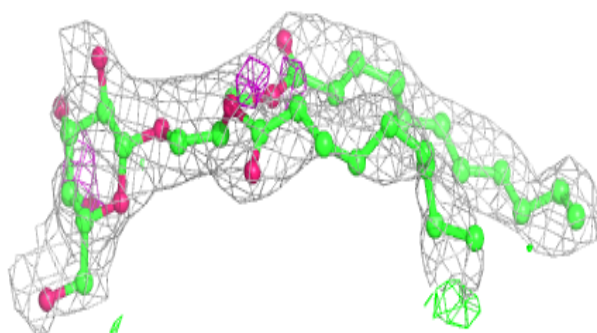
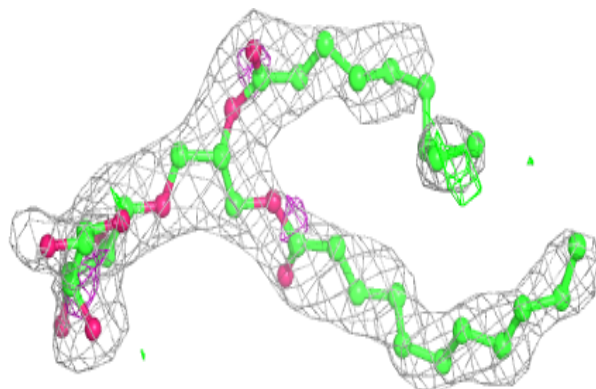


**Electron density around LFA m 101:**

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

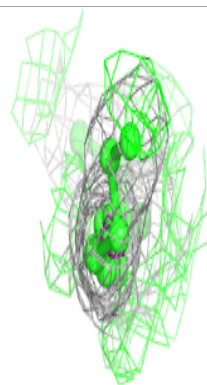
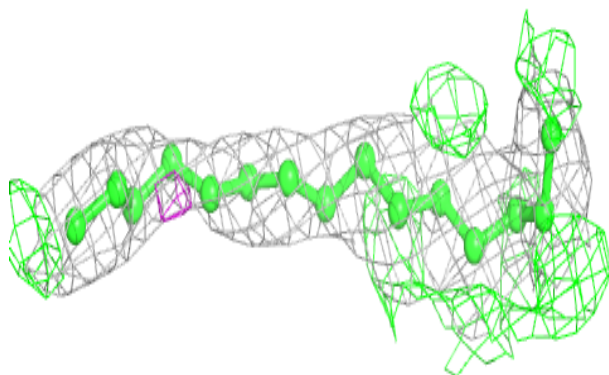
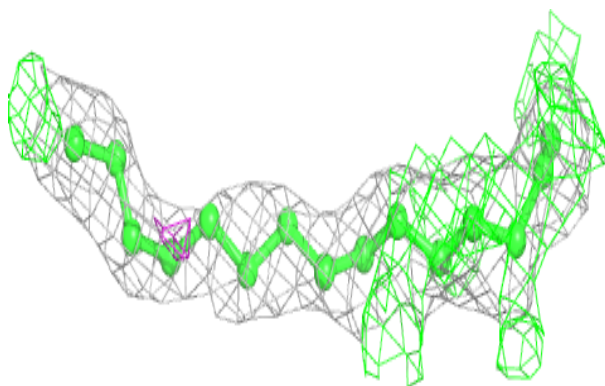
**Electron density around LMG b 624:**

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

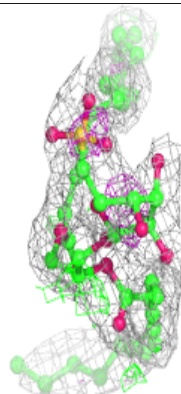
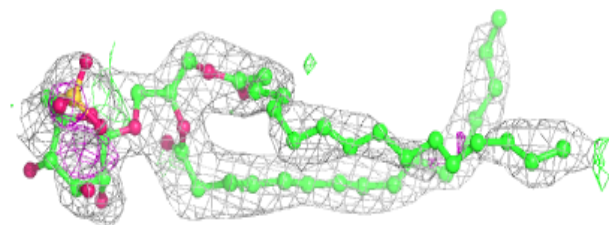
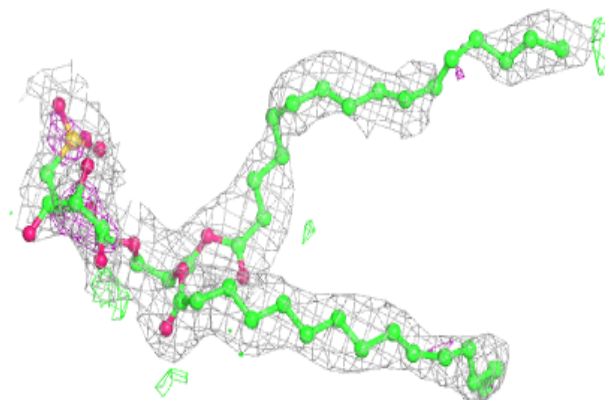


**Electron density around LFA B 624:**

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

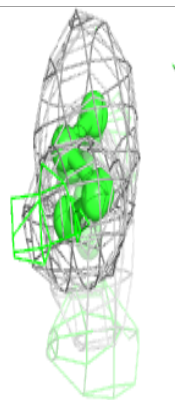
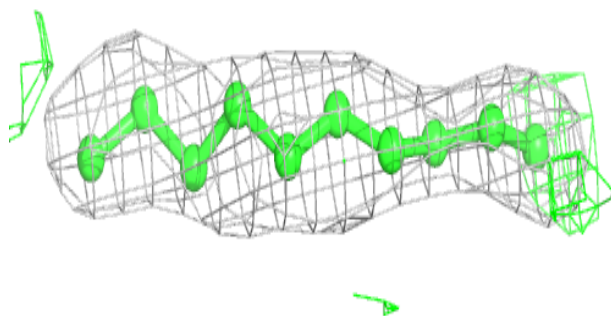
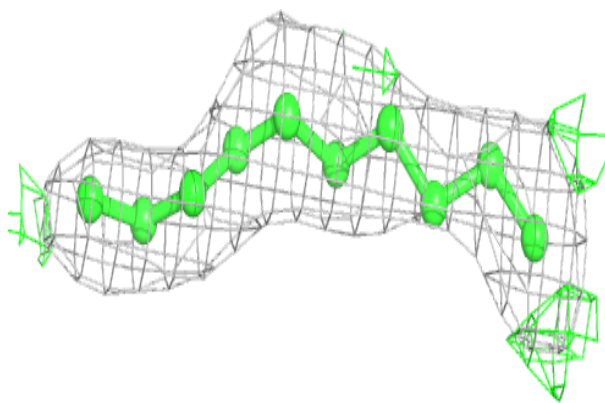
**Electron density around SQD A 411:**

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

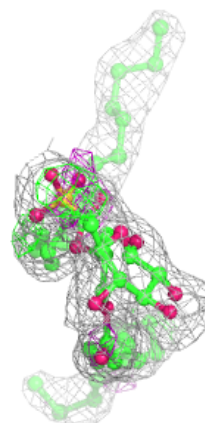
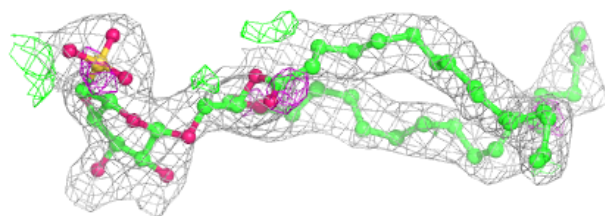
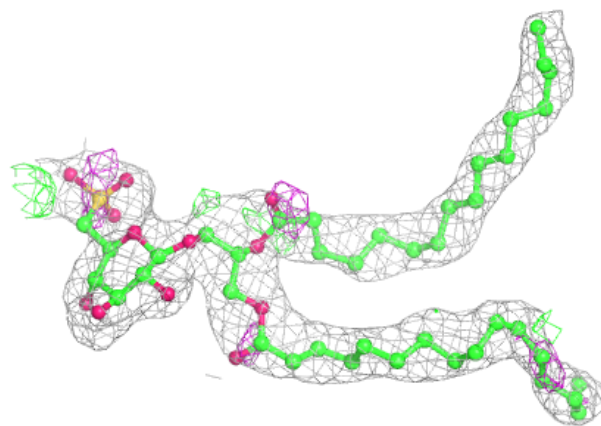


**Electron density around LFA B 626:**

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

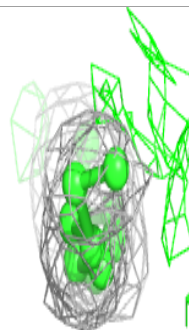
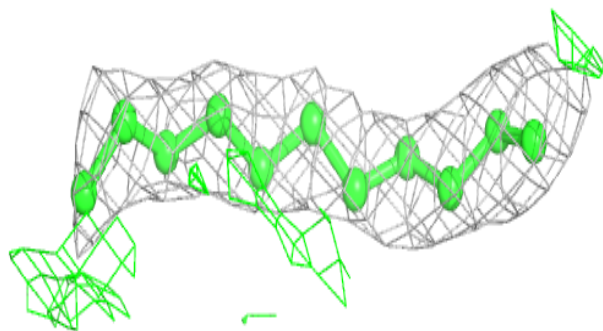
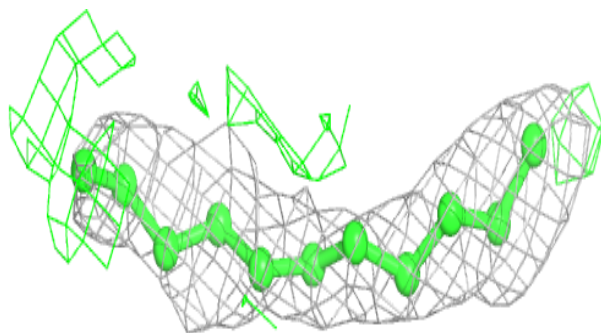
**Electron density around SQD b 601:**

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

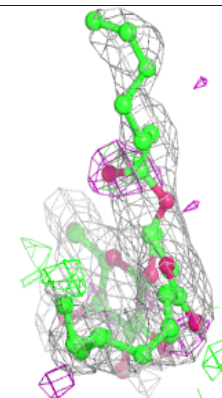
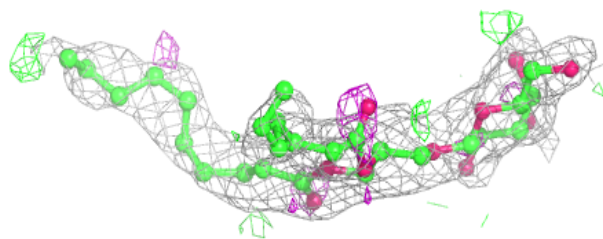
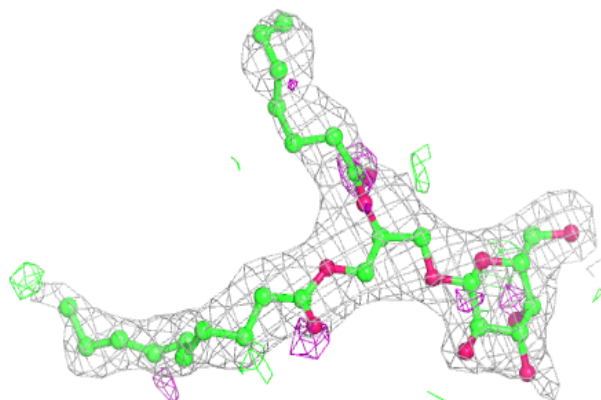


**Electron density around LFA b 627:**

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

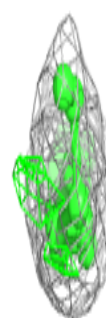
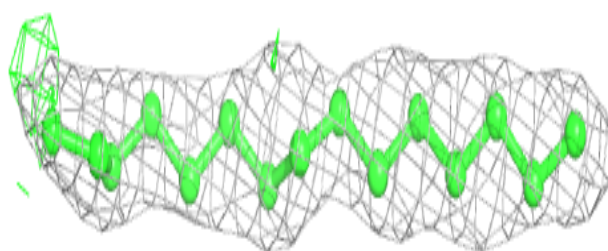
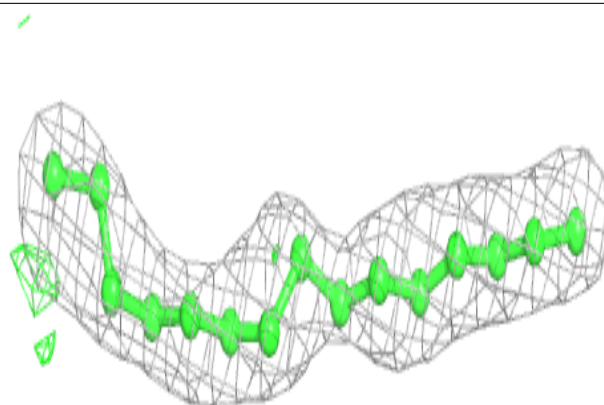
**Electron density around LMG B 621:**

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

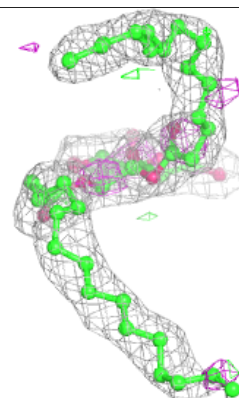
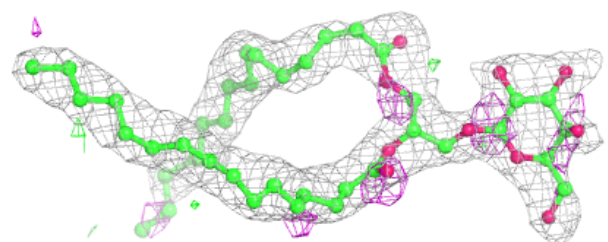
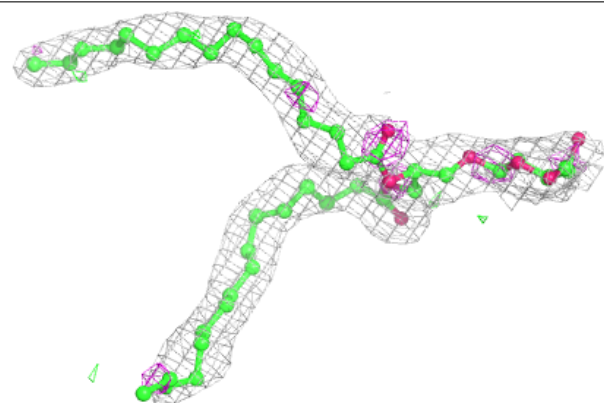


**Electron density around LFA C 521:**

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

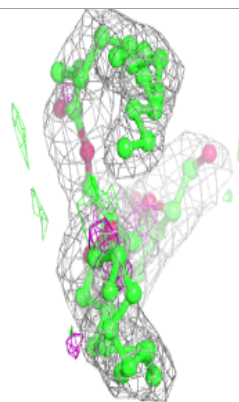
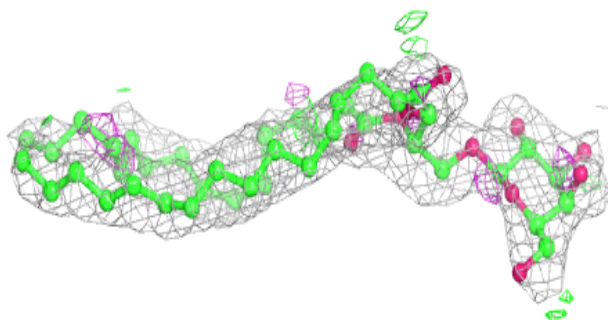
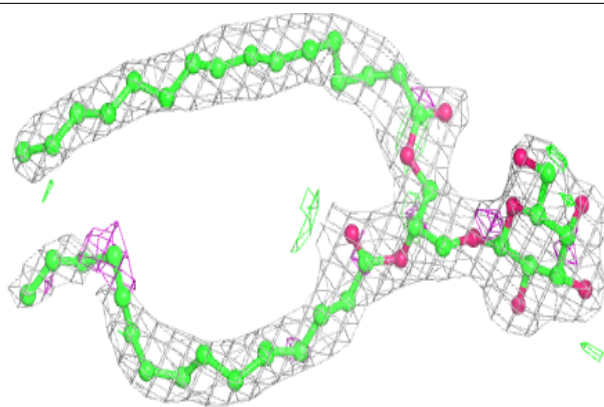
**Electron density around LMG B 619:**

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

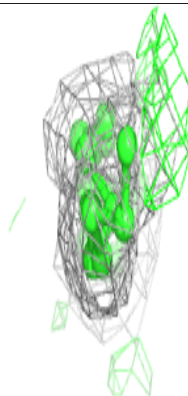
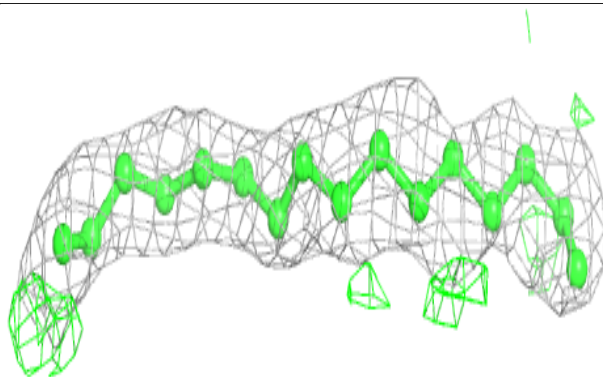
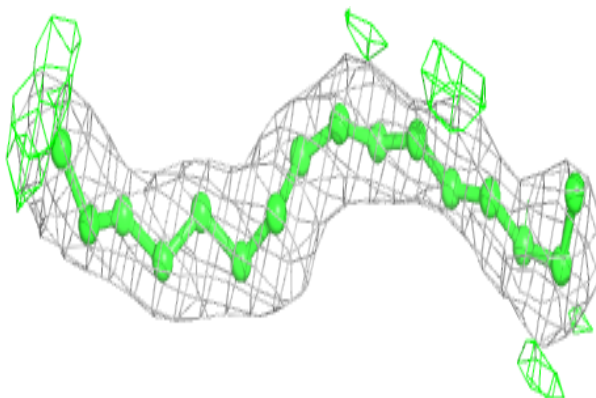


**Electron density around LMG C 501:**

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

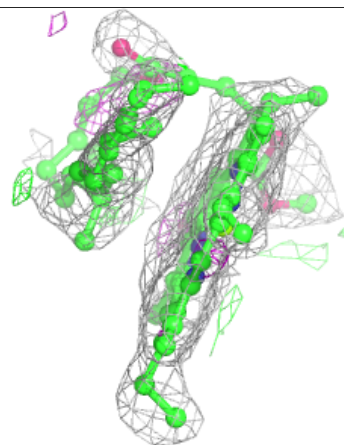
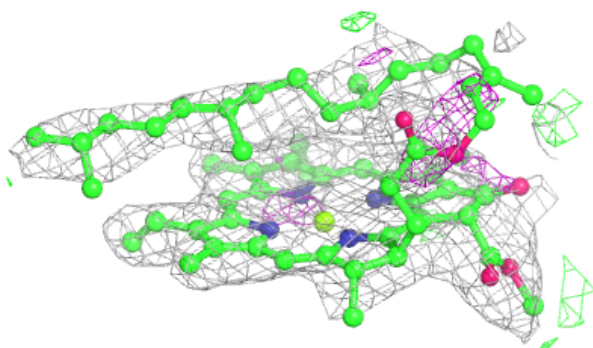
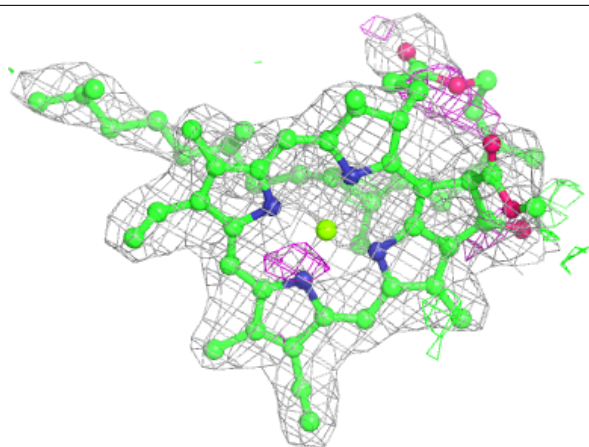
**Electron density around LFA b 625:**

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

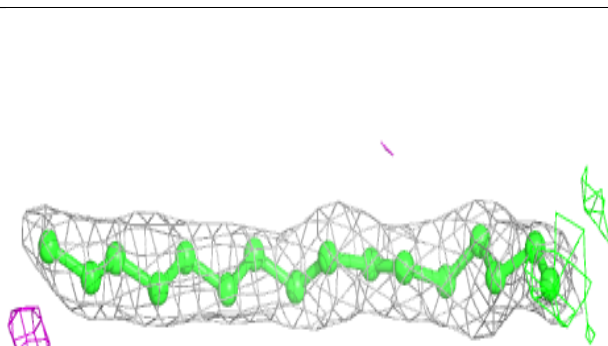
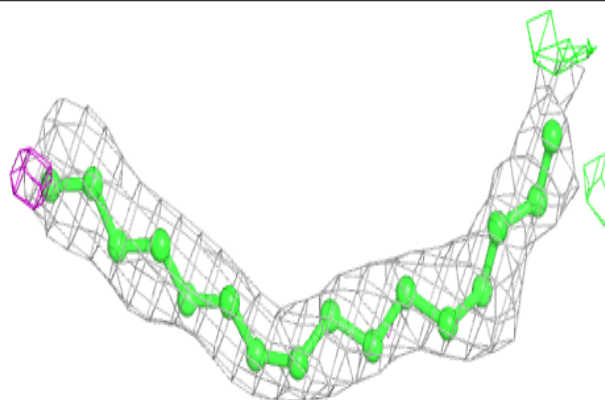


**Electron density around CLA b 603:**

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

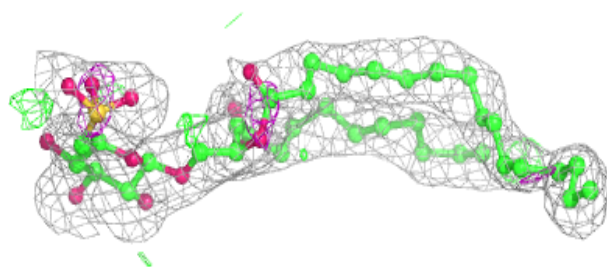
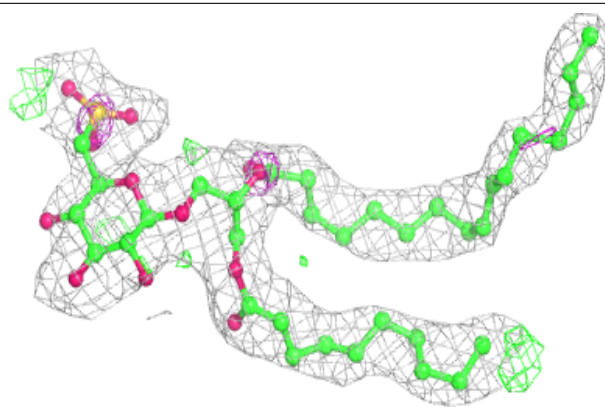
**Electron density around LFA d 410:**

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

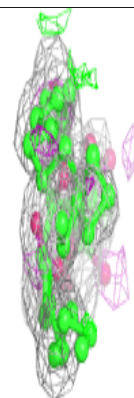
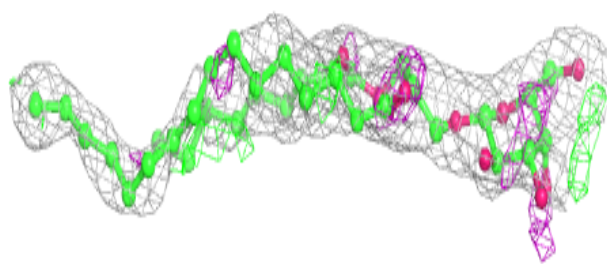
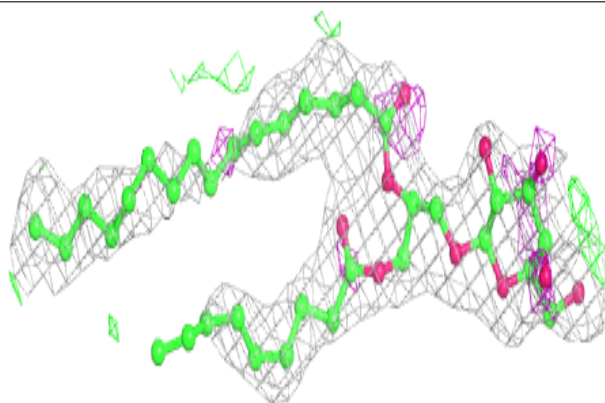


**Electron density around SQD L 101:**

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

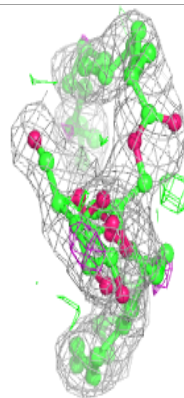
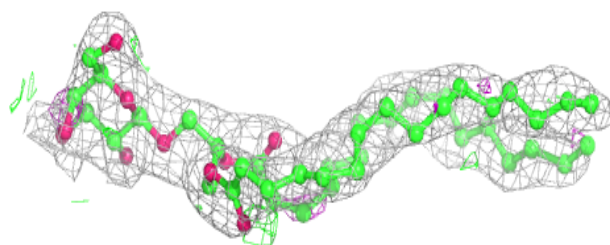
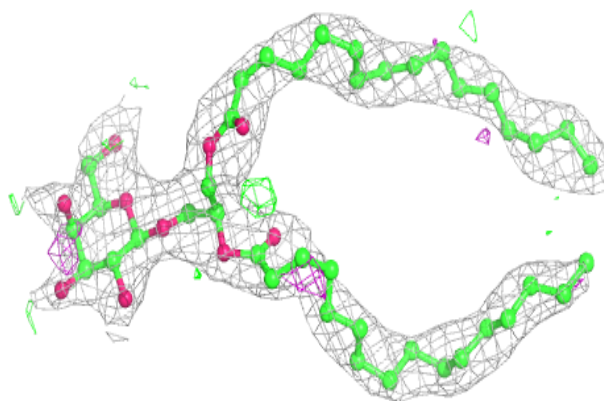
**Electron density around LMG C 522:**

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

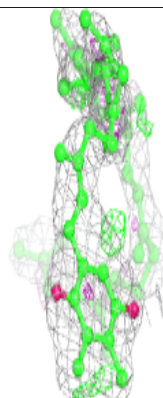
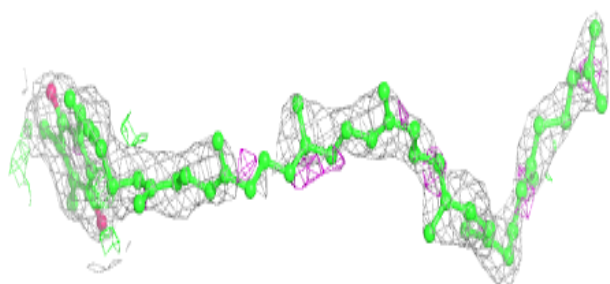
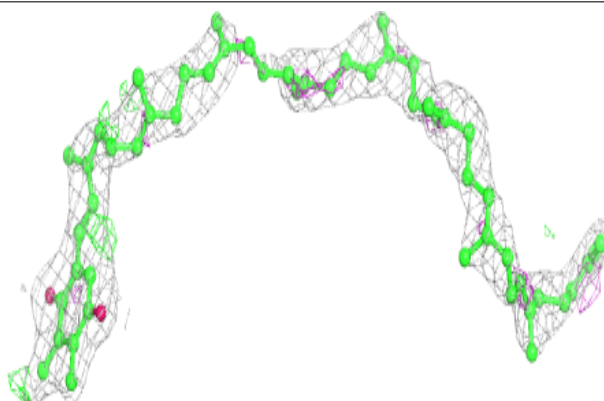


**Electron density around LMG c 501:**

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

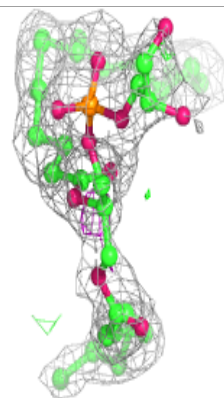
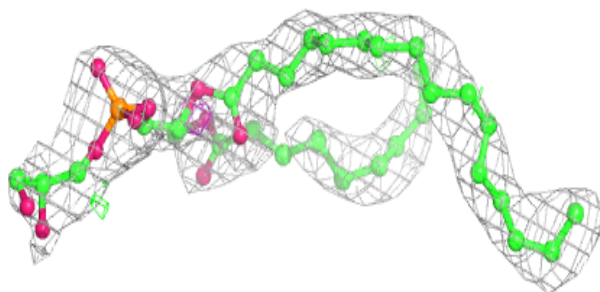
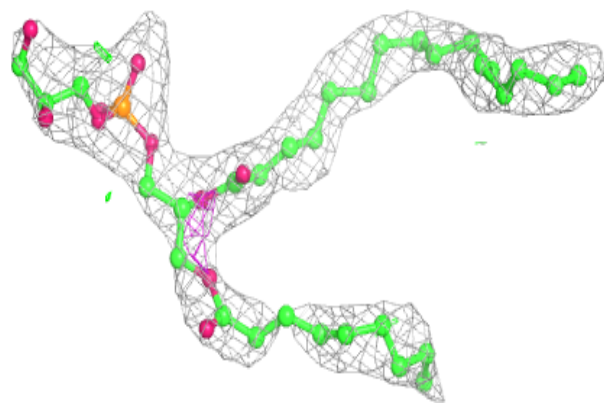
**Electron density around PL9 A 408:**

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

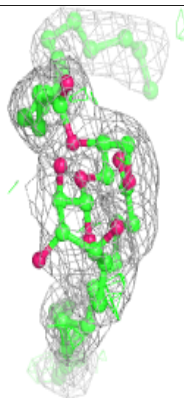
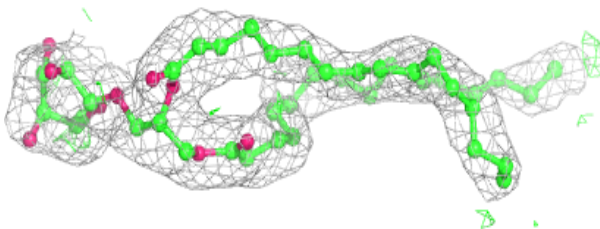
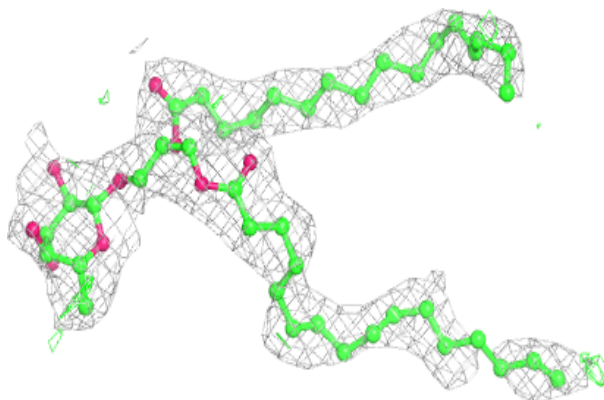


**Electron density around LHG E 101:**

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

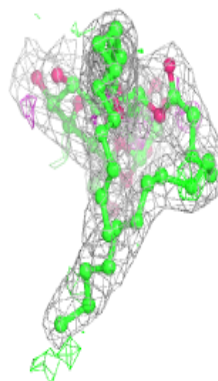
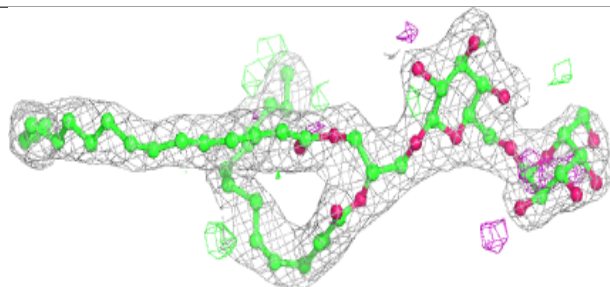
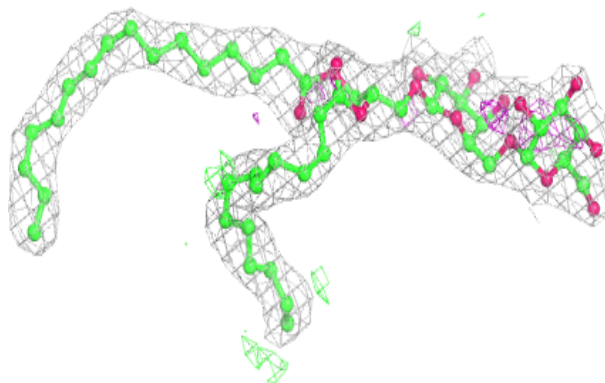
**Electron density around SQD a 412:**

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

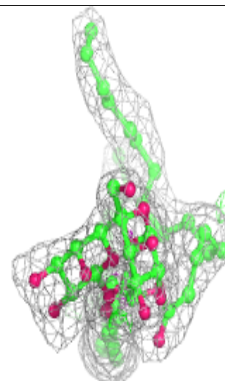
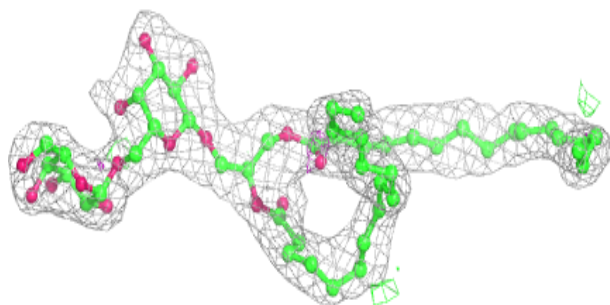
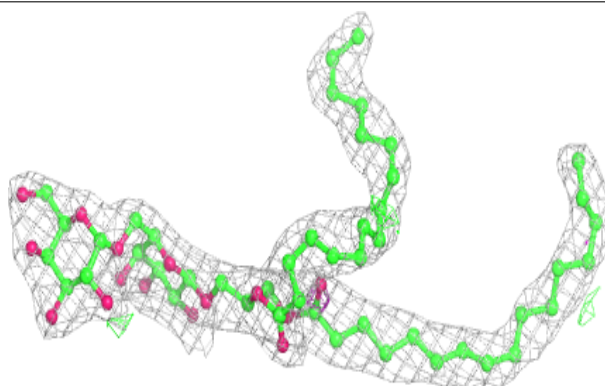


**Electron density around DGD H 103:**

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

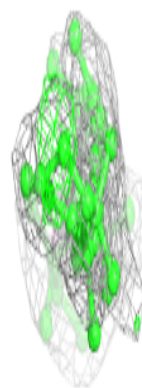
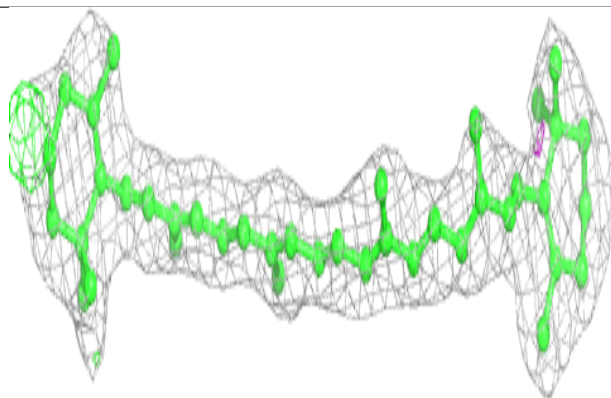
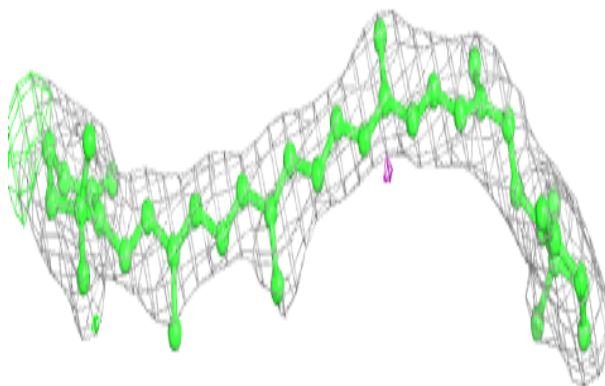
**Electron density around DGD h 102:**

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

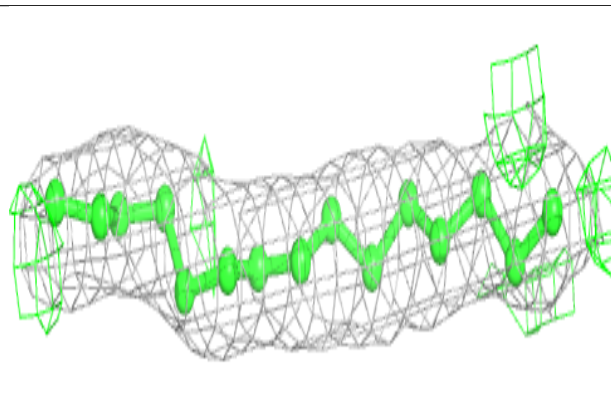
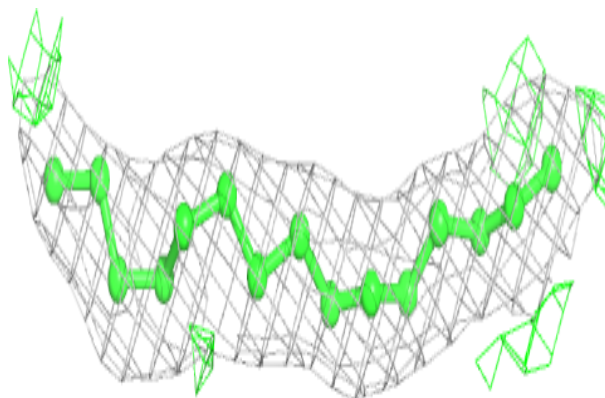


**Electron density around BCR h 101:**

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

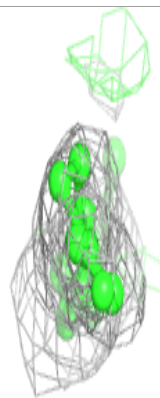
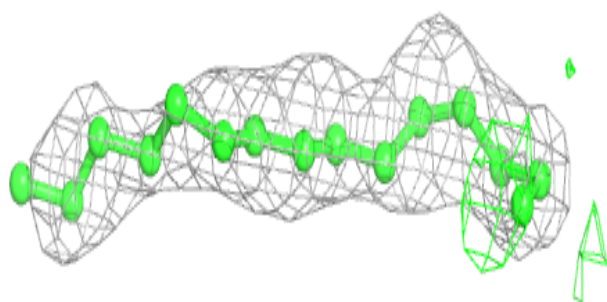
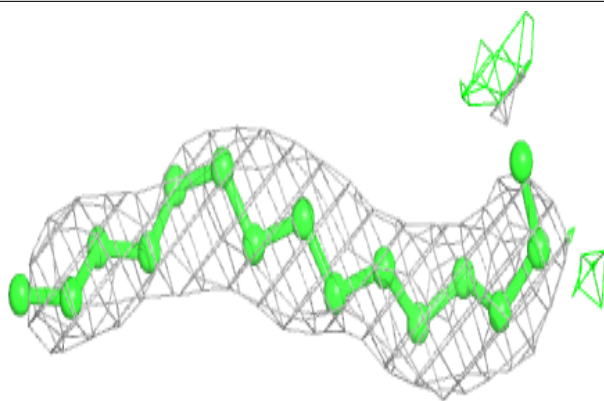
**Electron density around LFA m 102:**

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

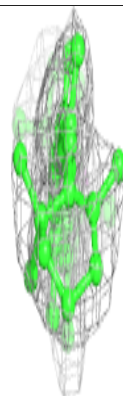
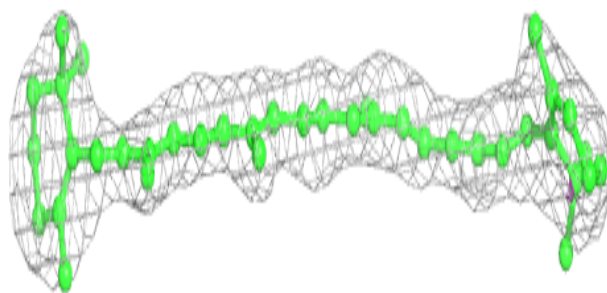
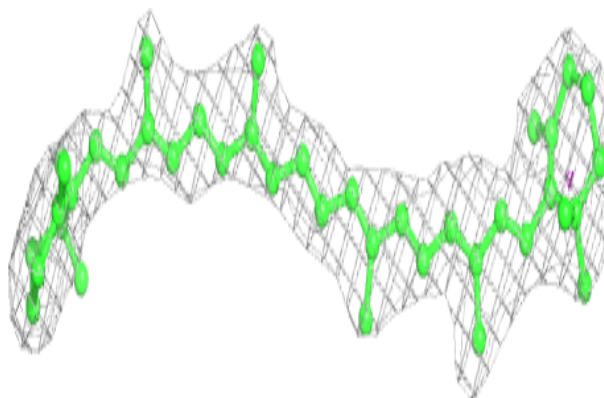


**Electron density around LFA j 101:**

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

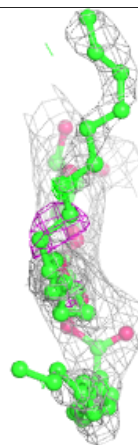
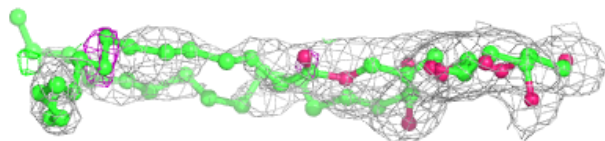
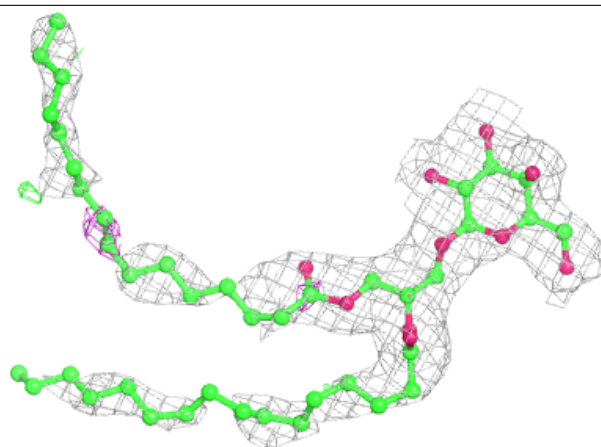
**Electron density around BCR K 101:**

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

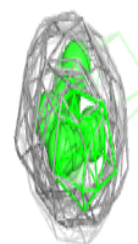
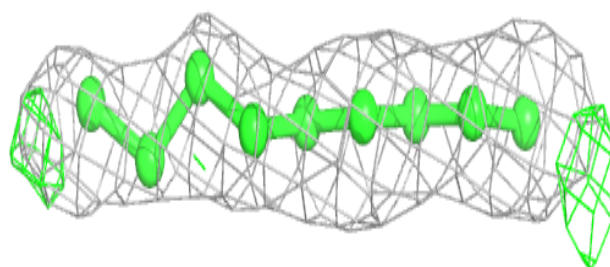
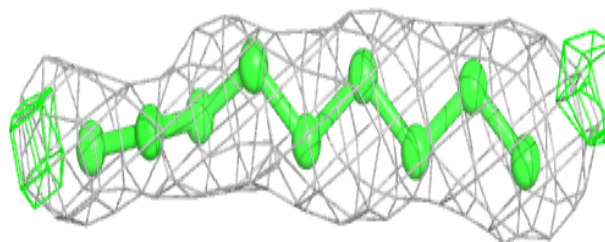


**Electron density around LMG c 519:**

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

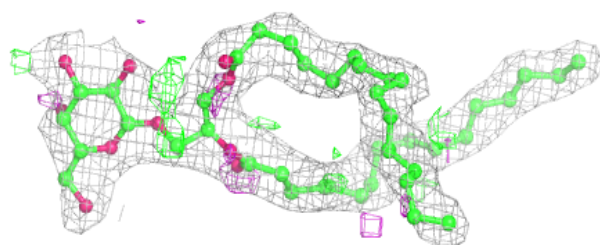
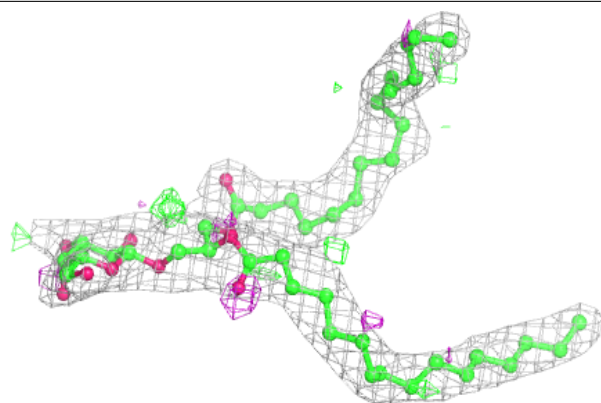
**Electron density around LFA d 409:**

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

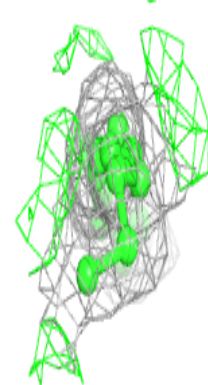
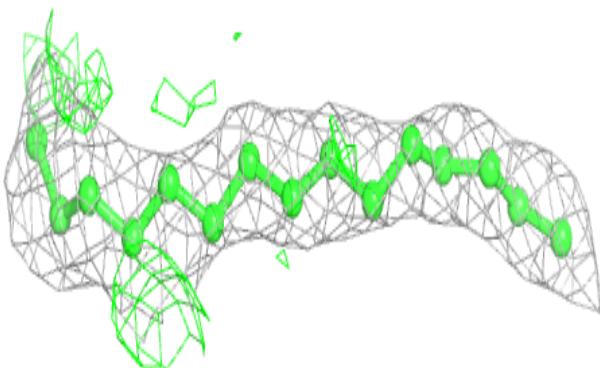
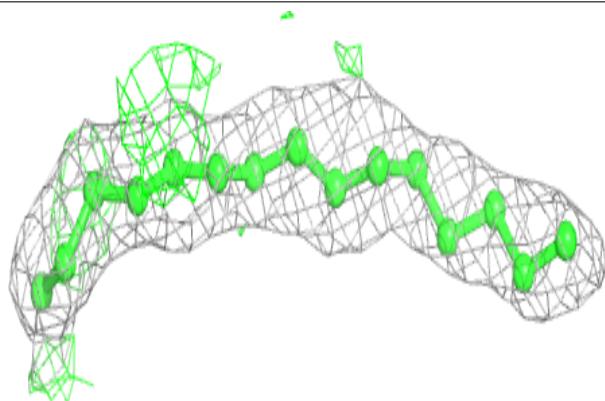


**Electron density around LMG m 103:**

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

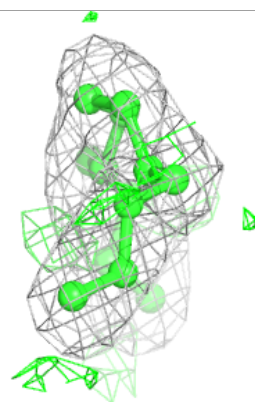
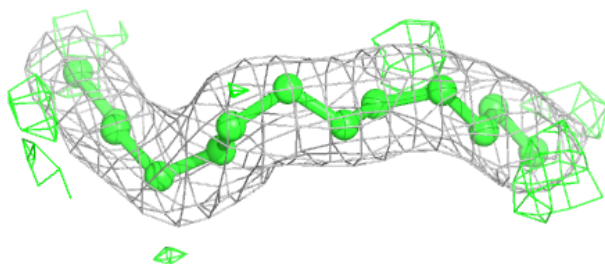
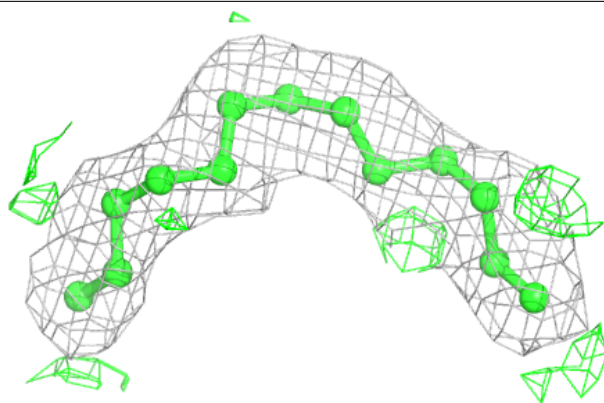
**Electron density around LFA b 630:**

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

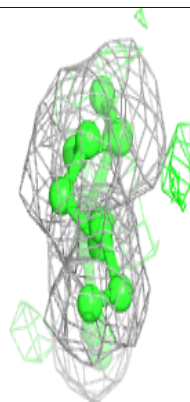
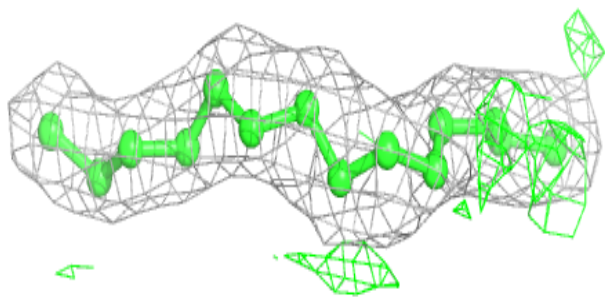
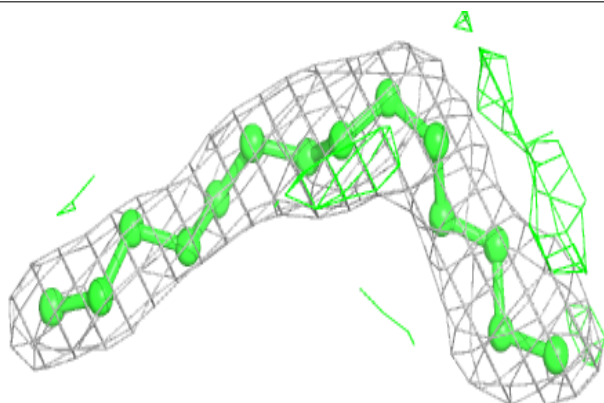


**Electron density around LFA B 623:**

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

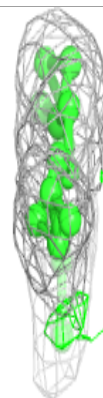
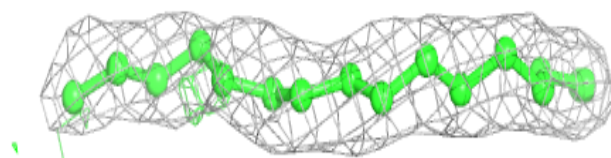
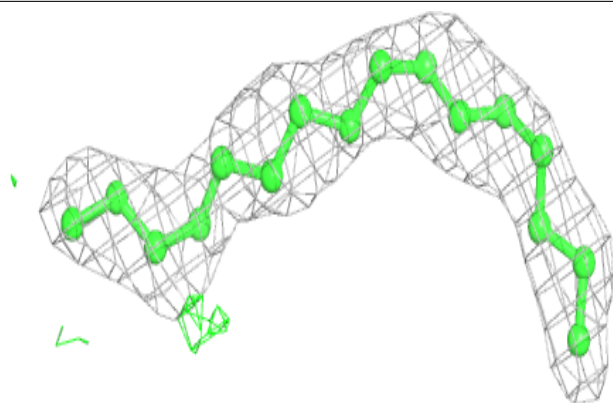
**Electron density around LFA B 627:**

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

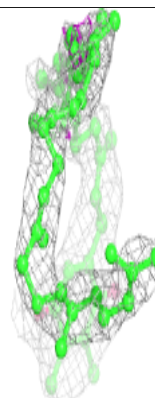
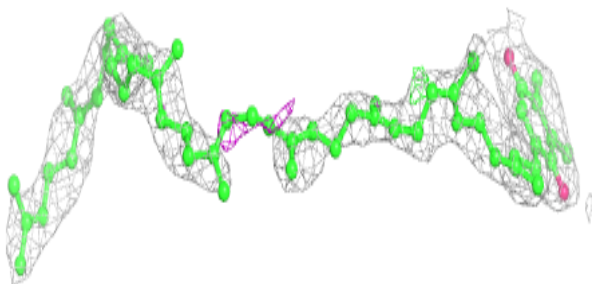
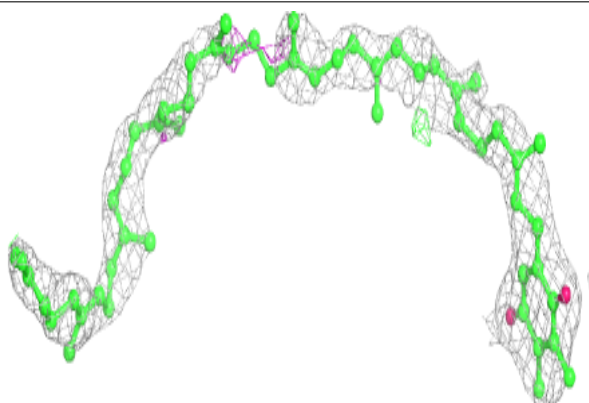


**Electron density around LFA B 622:**

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

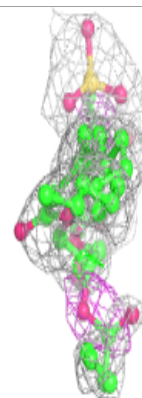
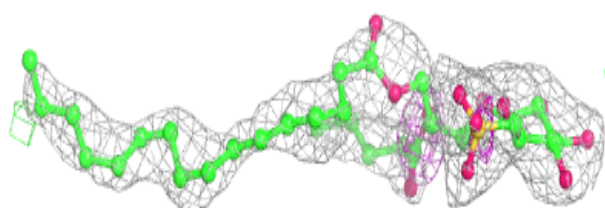
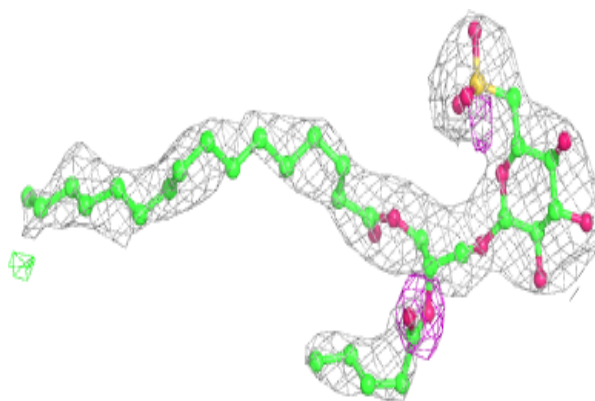
**Electron density around PL9 a 409:**

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

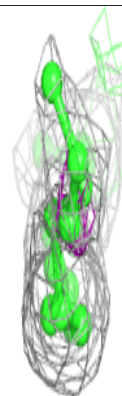
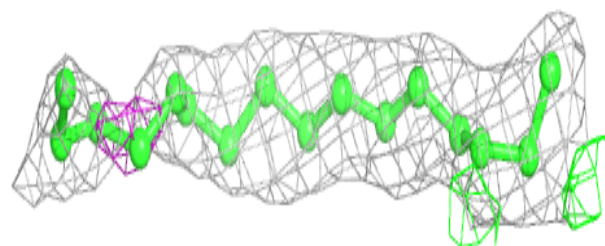
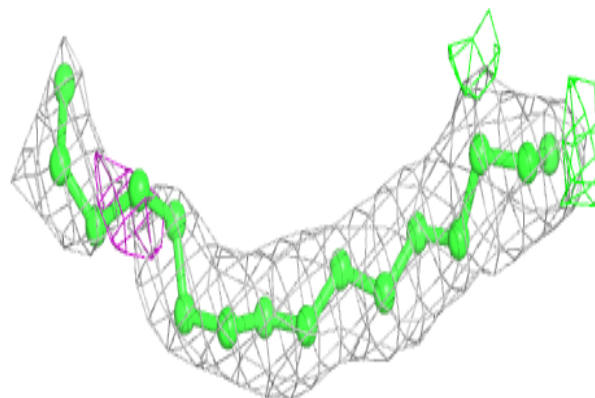


**Electron density around SQD D 411:**

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

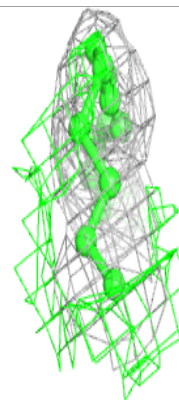
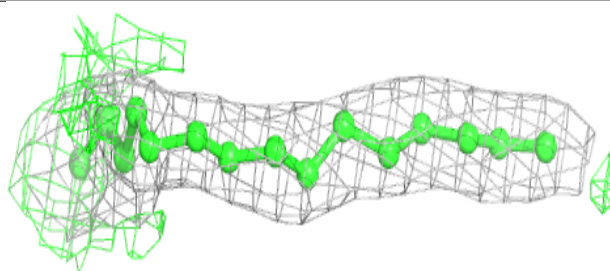
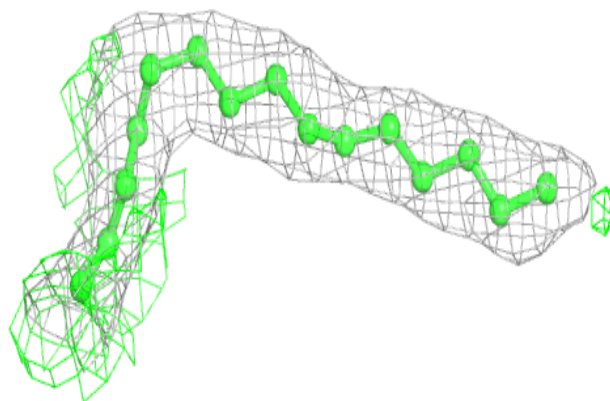
**Electron density around LFA i 101:**

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

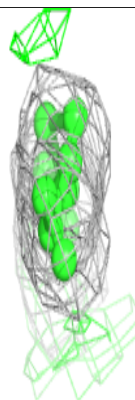
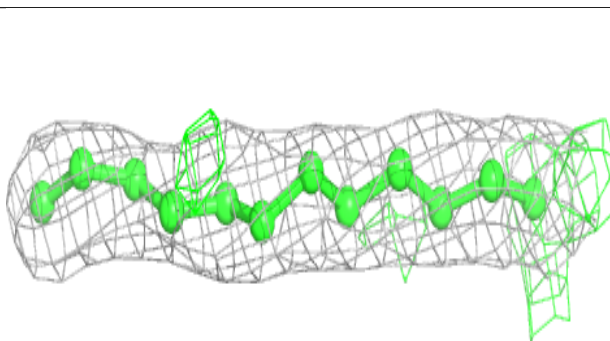
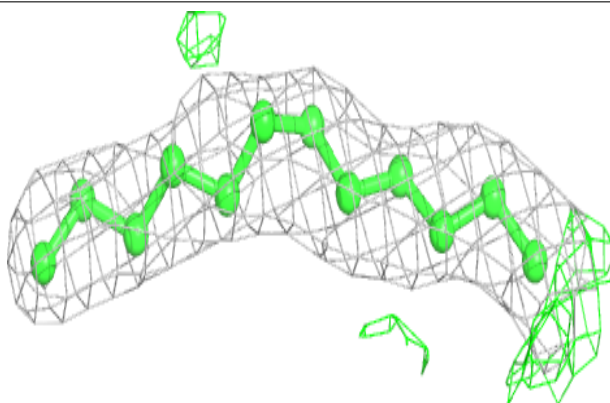


**Electron density around LFA D 410:**

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

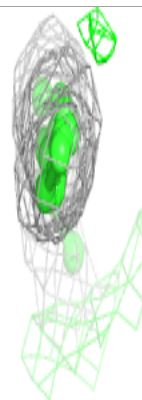
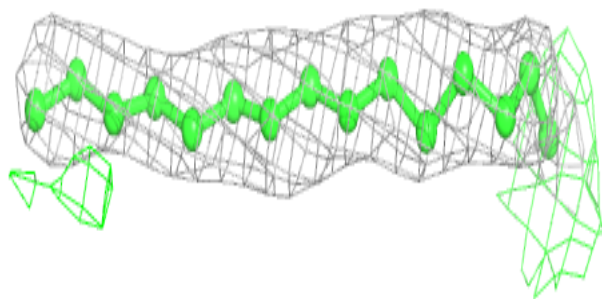
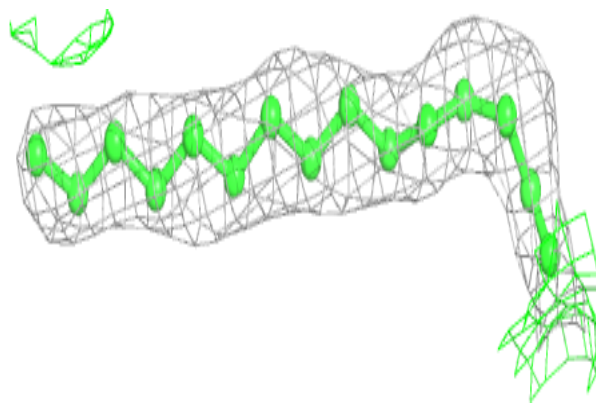
**Electron density around LFA T 102:**

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

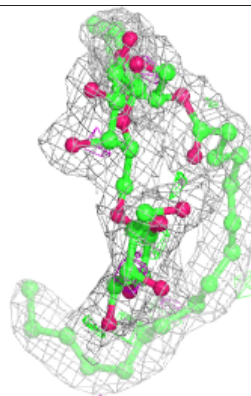
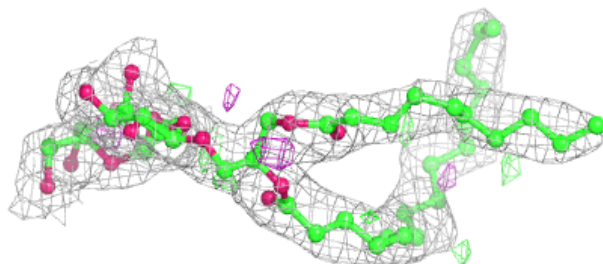
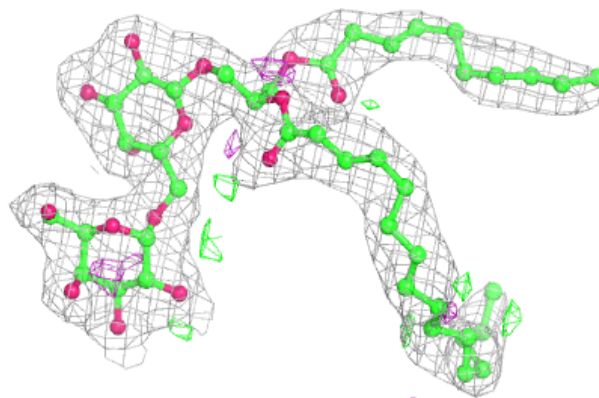


**Electron density around LFA d 408:**

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

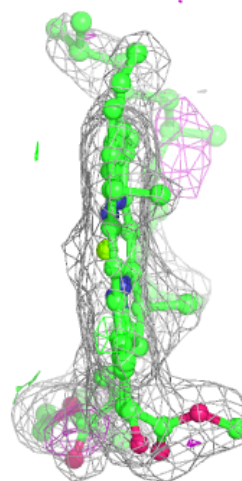
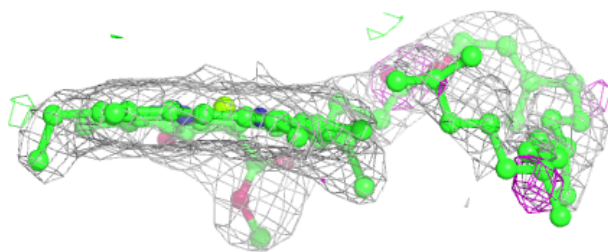
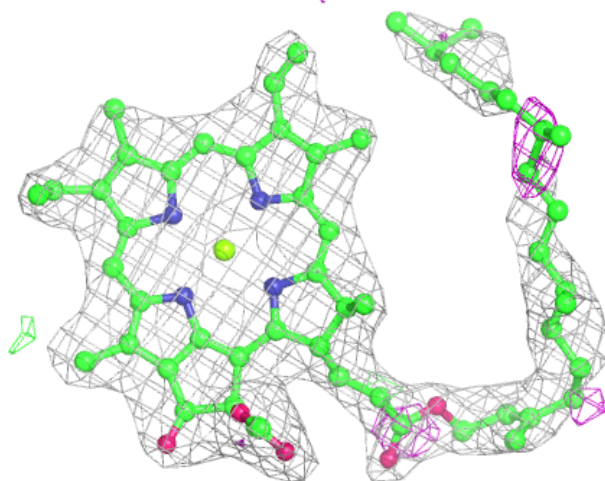
**Electron density around DGD C 518:**

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



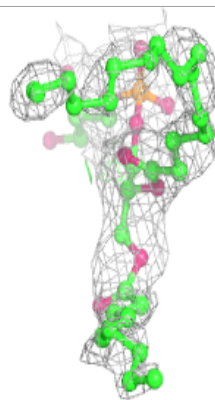
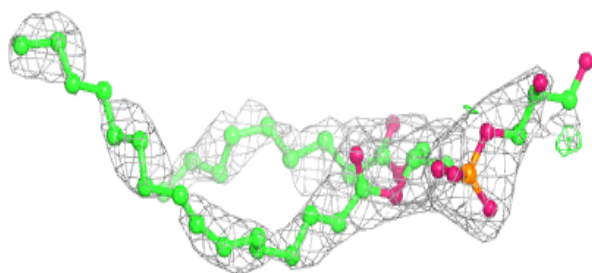
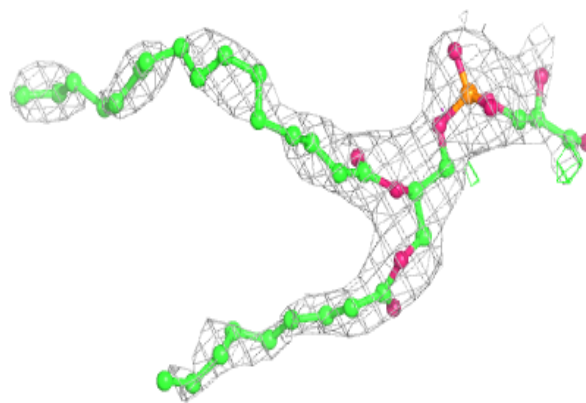
**Electron density around CLA C 513:**

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

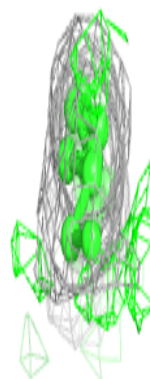
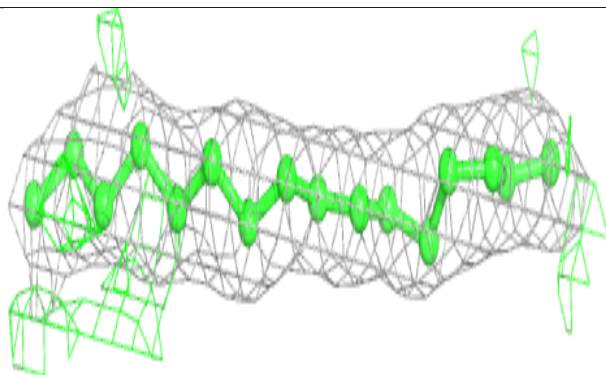
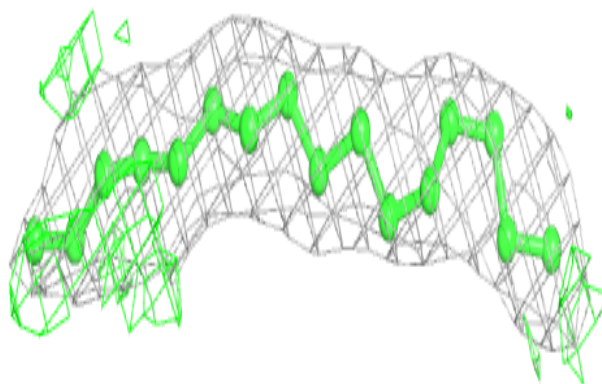


**Electron density around LHG e 101:**

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

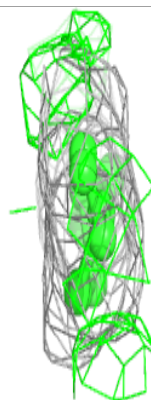
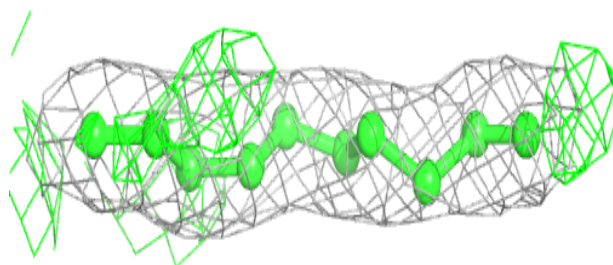
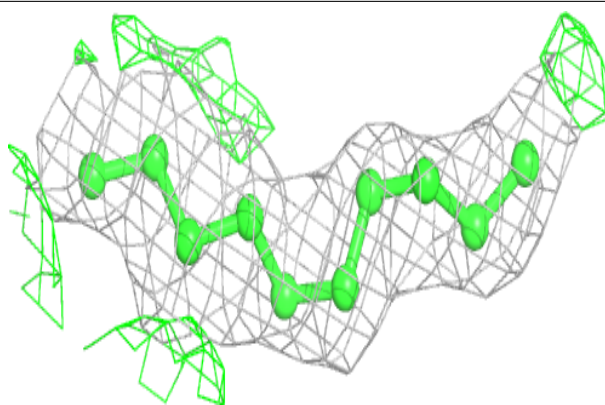
**Electron density around LFA M 102:**

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

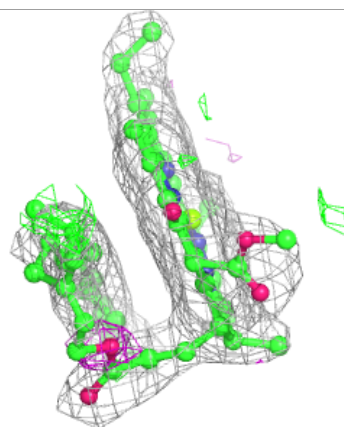
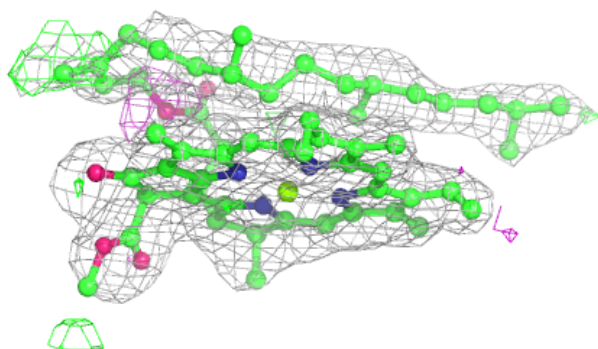
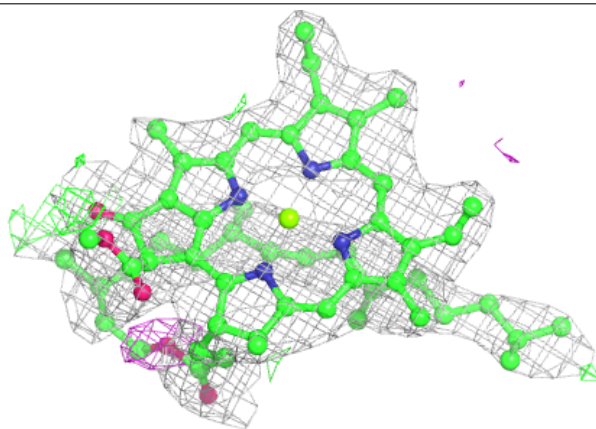


**Electron density around LFA b 622:**

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

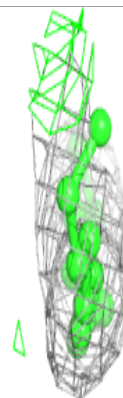
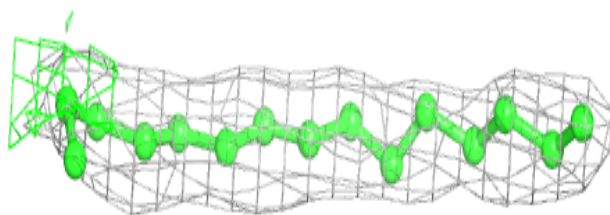
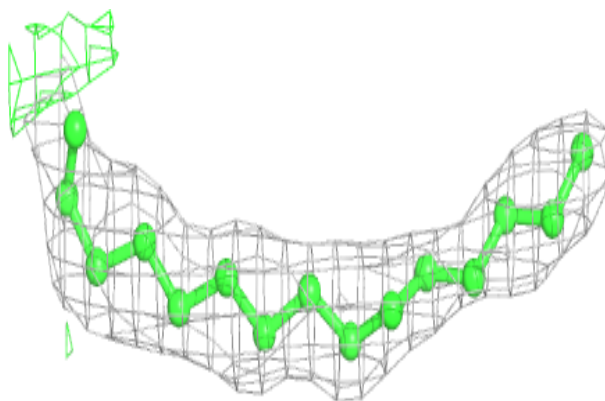
**Electron density around CLA H 101:**

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

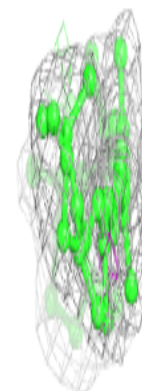
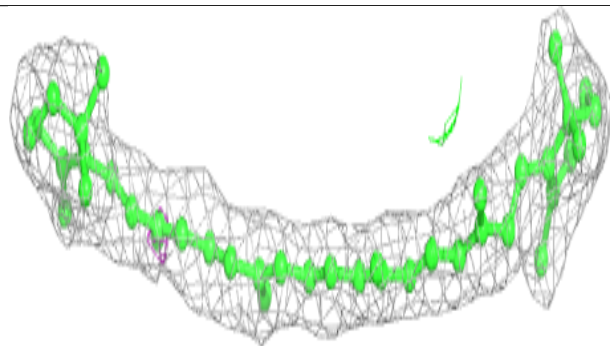
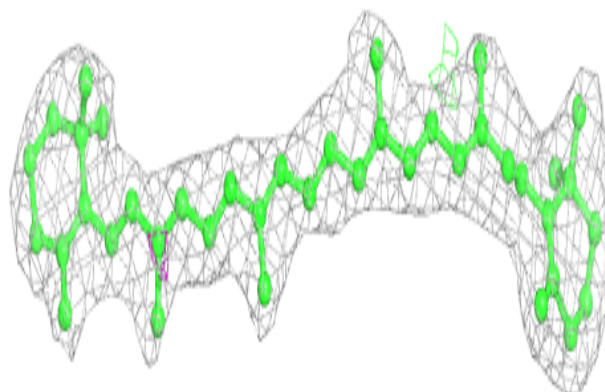


**Electron density around LFA t 101:**

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

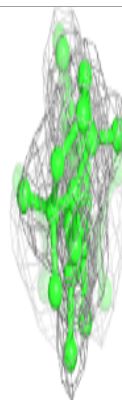
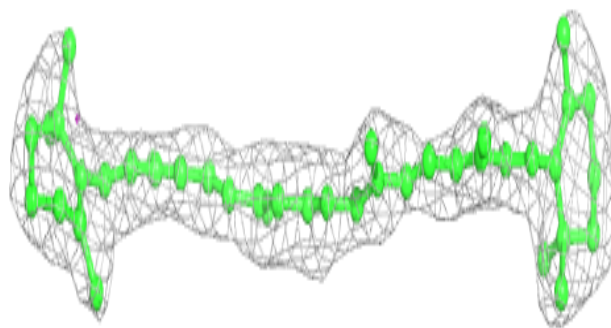
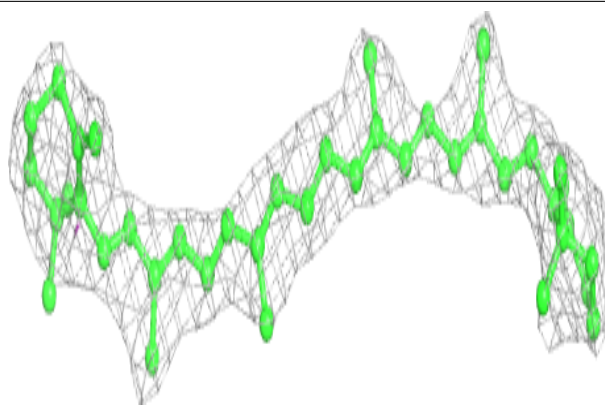
**Electron density around BCR t 102:**

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

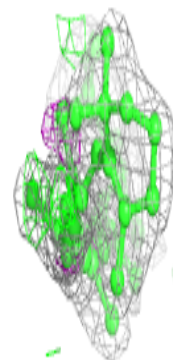
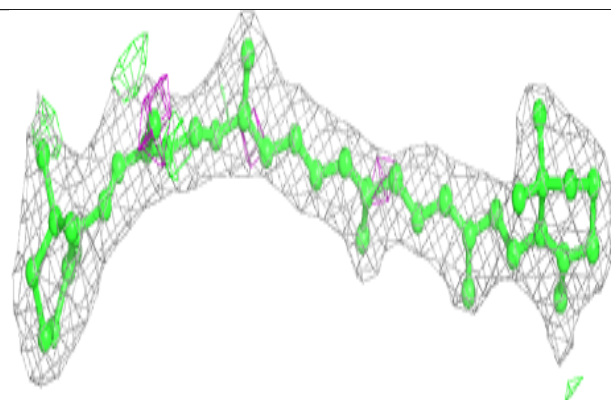
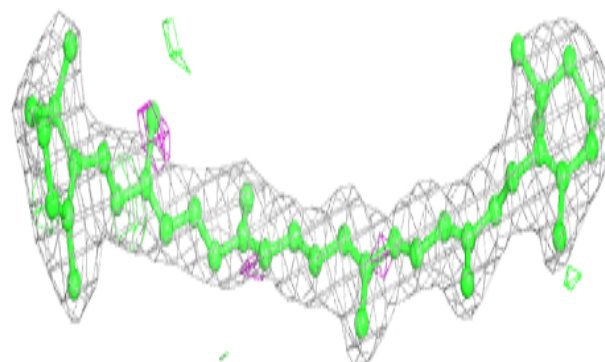


**Electron density around BCR c 523:**

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

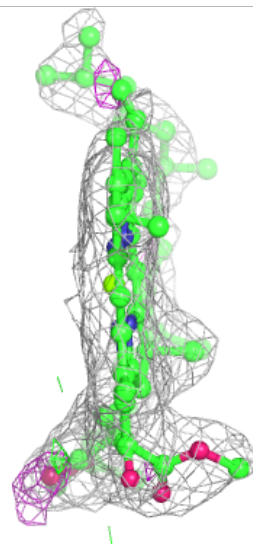
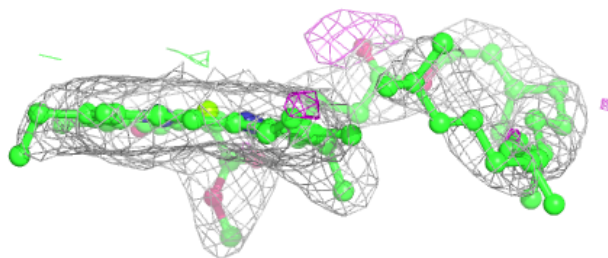
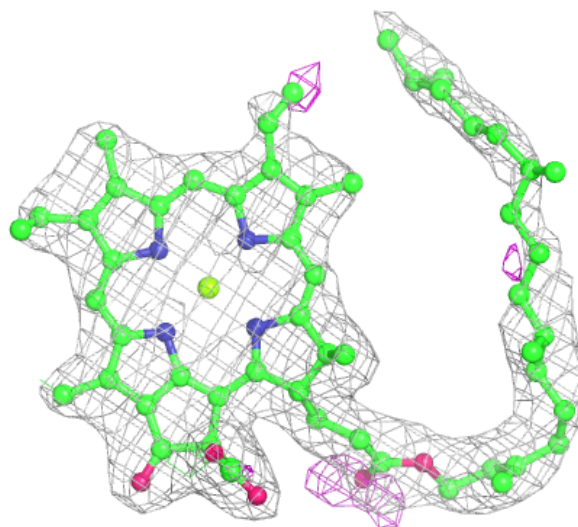
**Electron density around BCR T 101:**

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



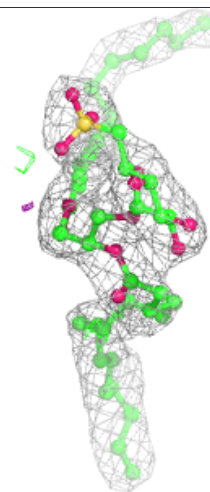
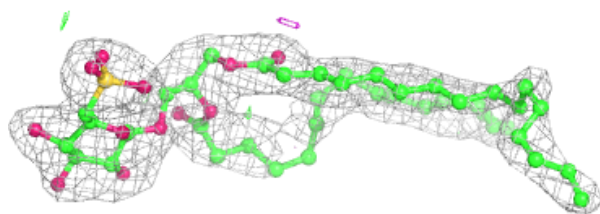
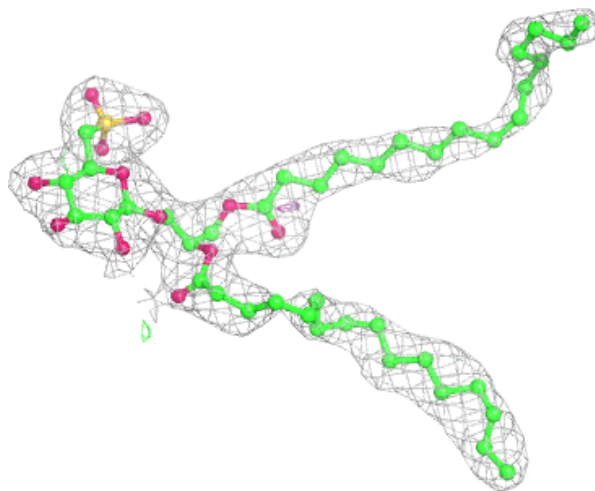
**Electron density around CLA c 513:**

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



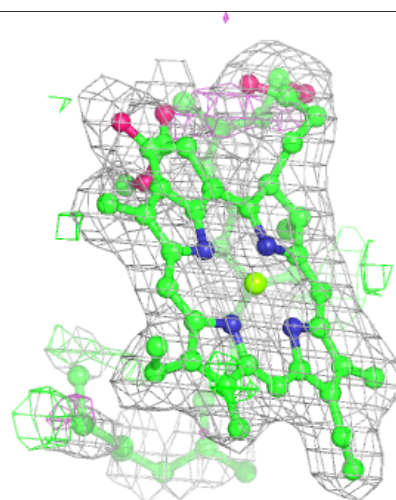
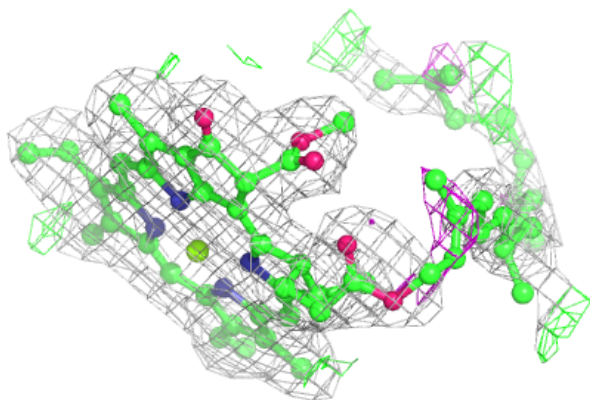
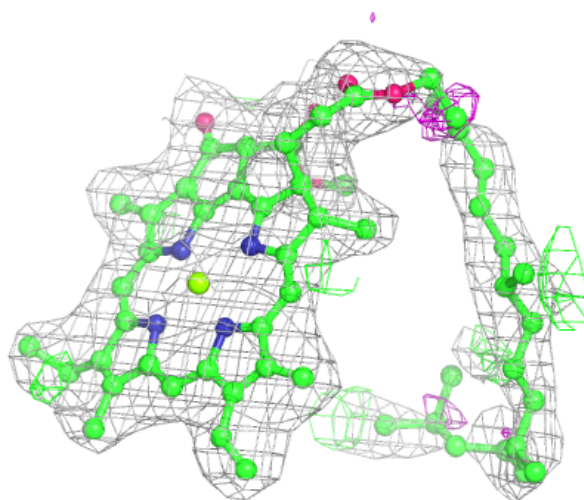
**Electron density around SQD A 409:**

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



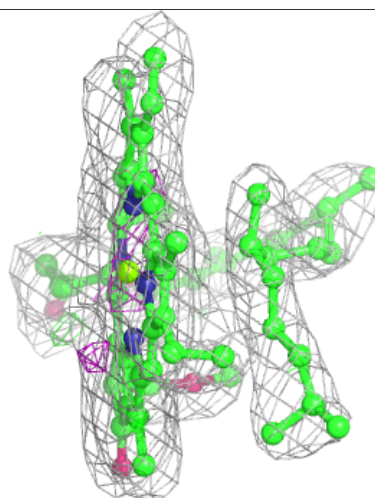
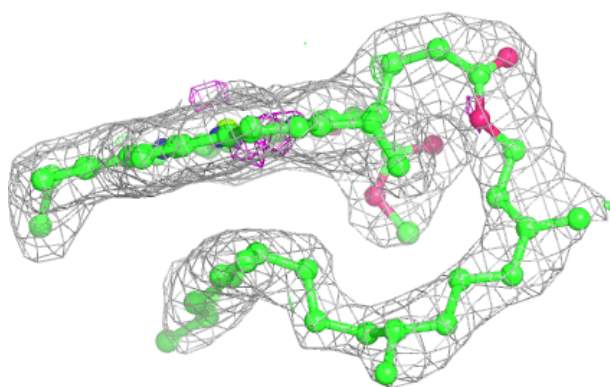
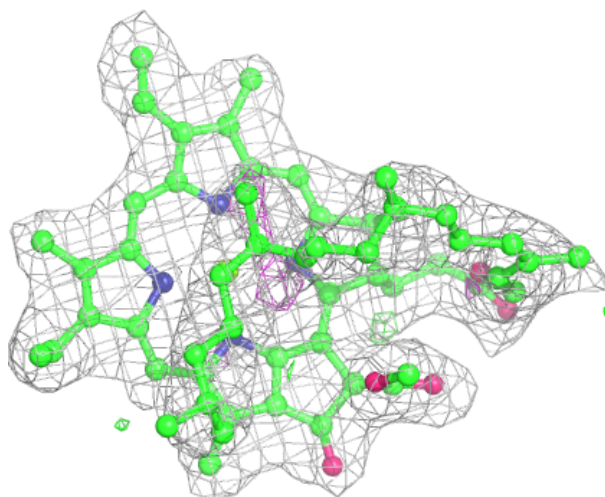
**Electron density around CLA b 618:**

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



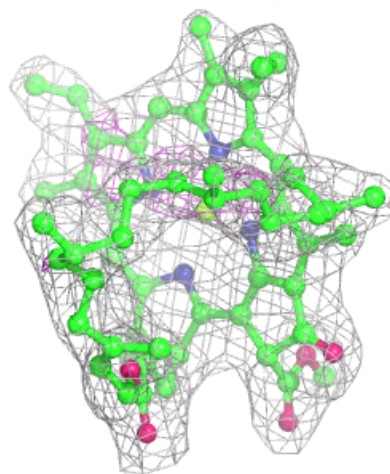
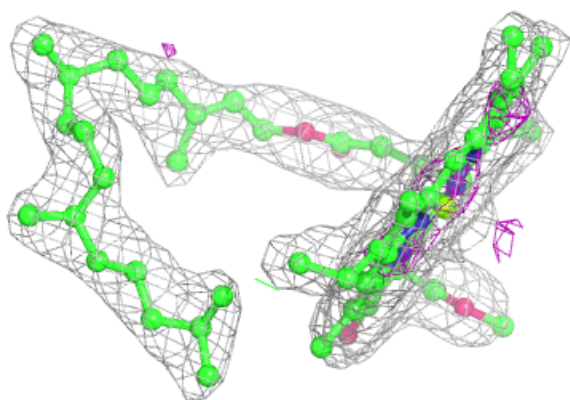
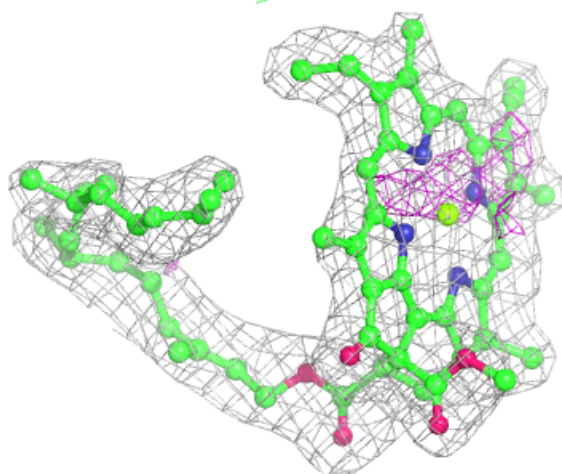
**Electron density around CLA C 511:**

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



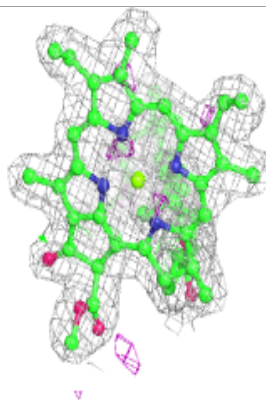
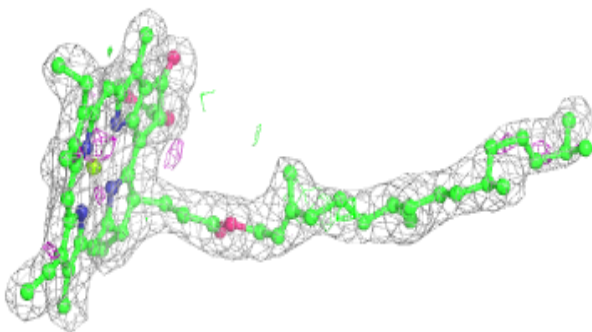
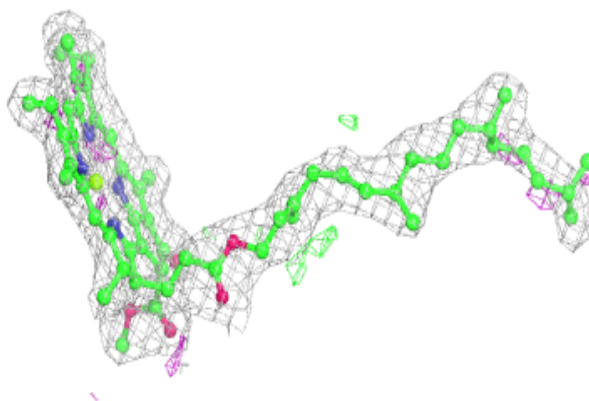
**Electron density around CLA C 504:**

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



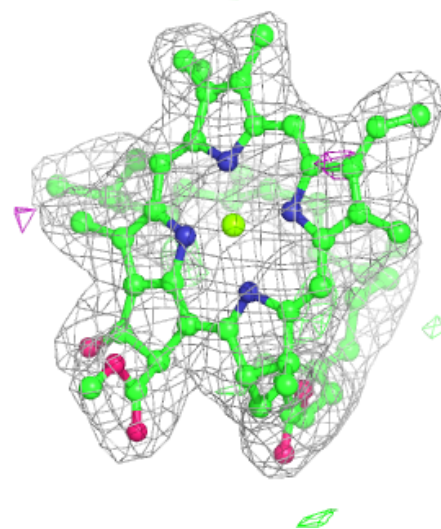
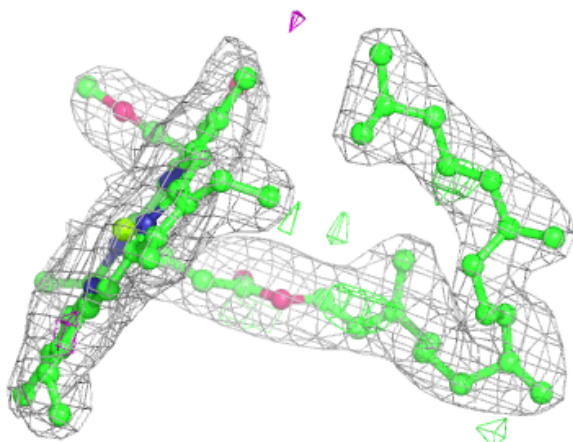
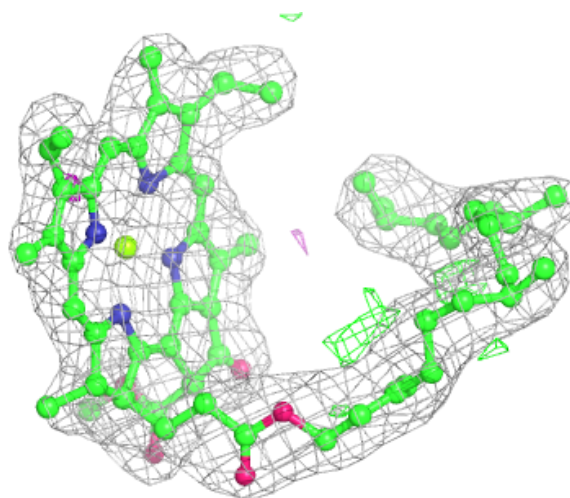
**Electron density around CLA B 603:**

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



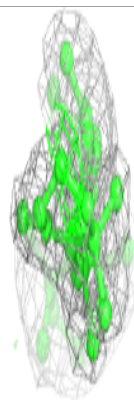
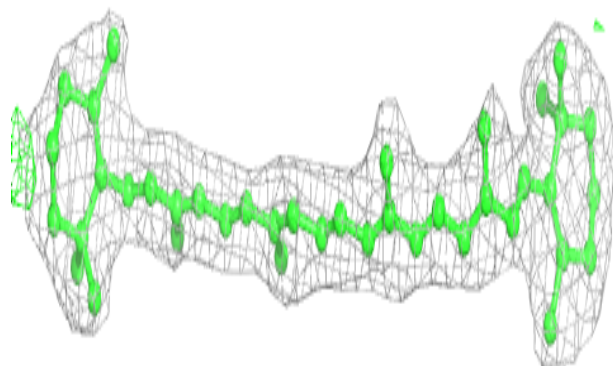
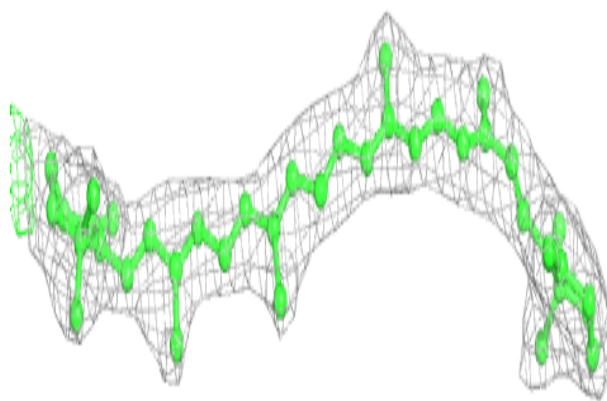
**Electron density around CLA c 504:**

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

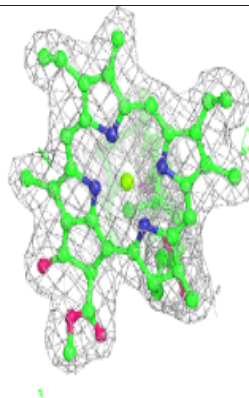
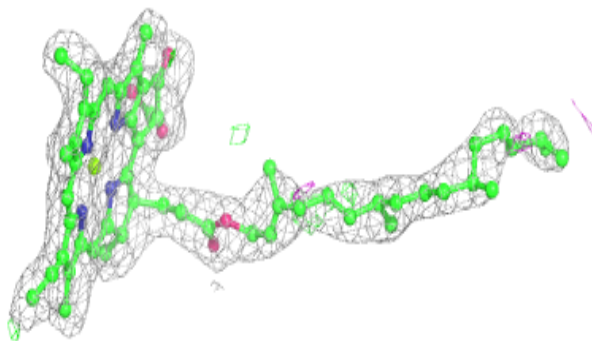
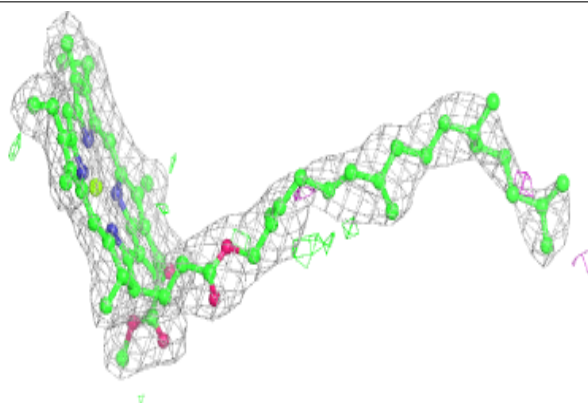


**Electron density around BCR H 102:**

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

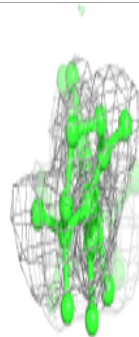
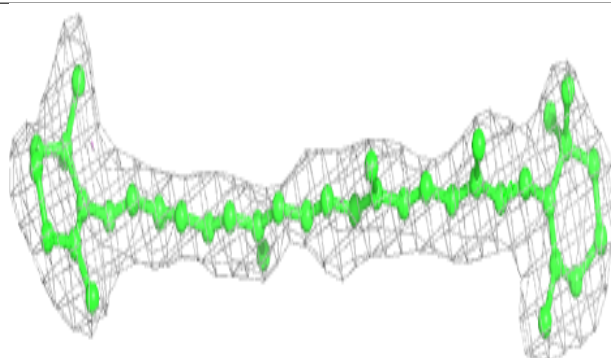
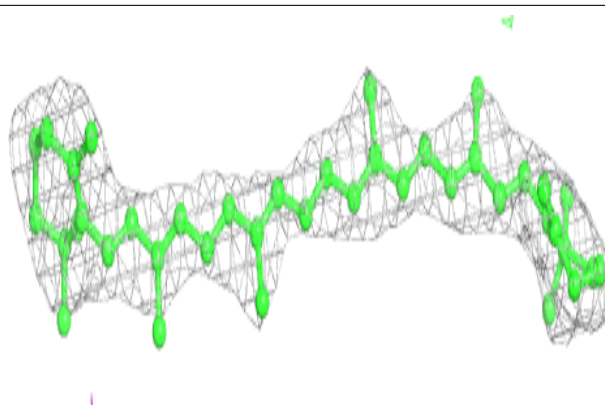
**Electron density around CLA b 606:**

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

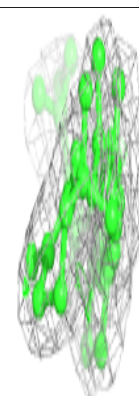
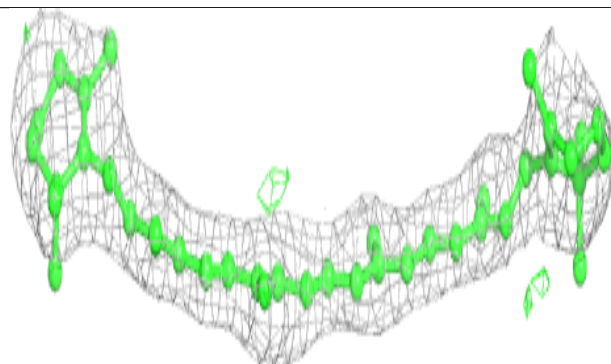
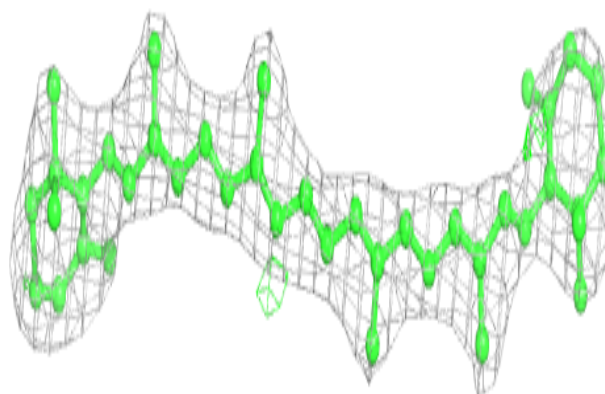


**Electron density around BCR c 524:**

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

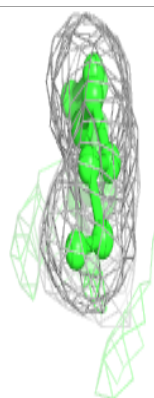
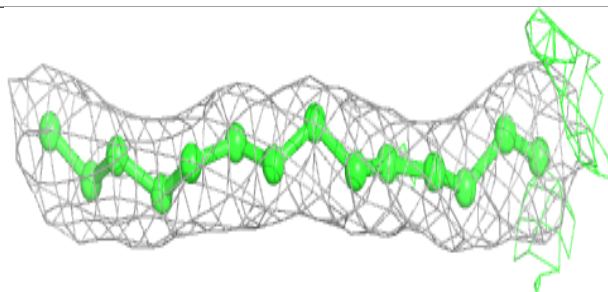
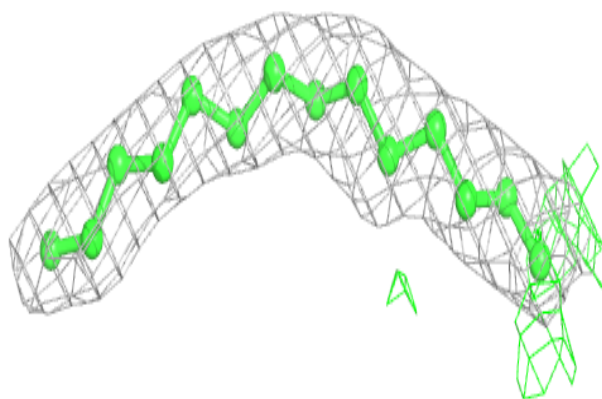
**Electron density around BCR d 404:**

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

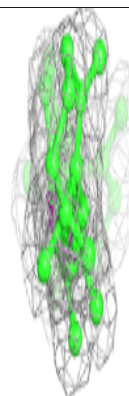
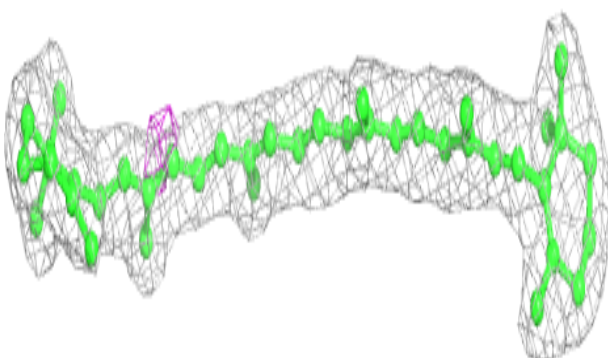
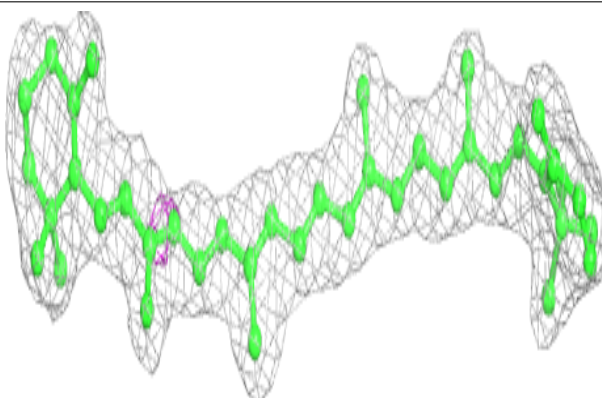


**Electron density around LFA I 101:**

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

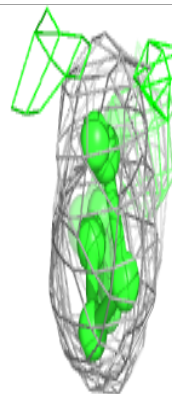
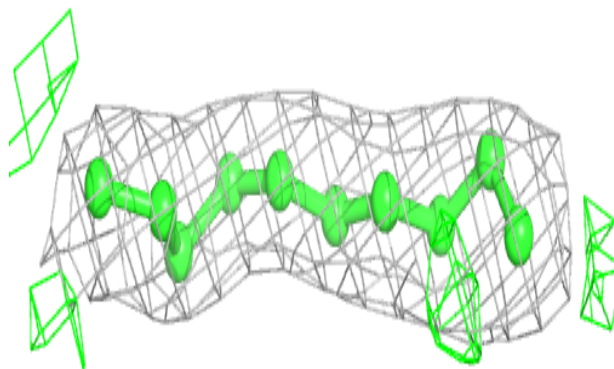
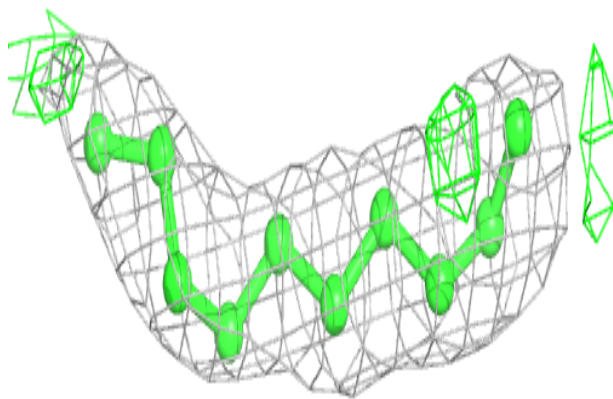
**Electron density around BCR B 616:**

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



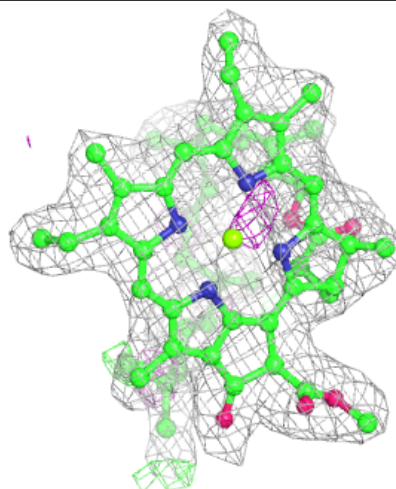
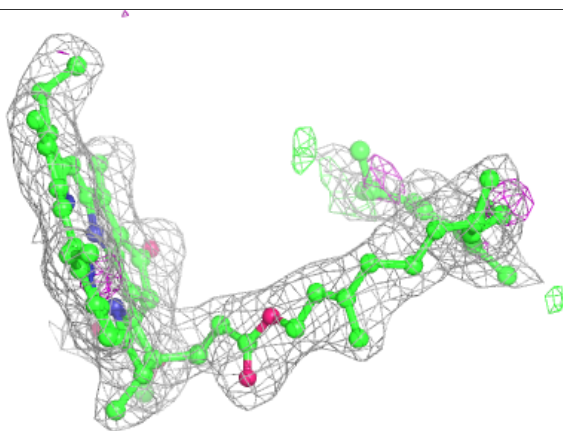
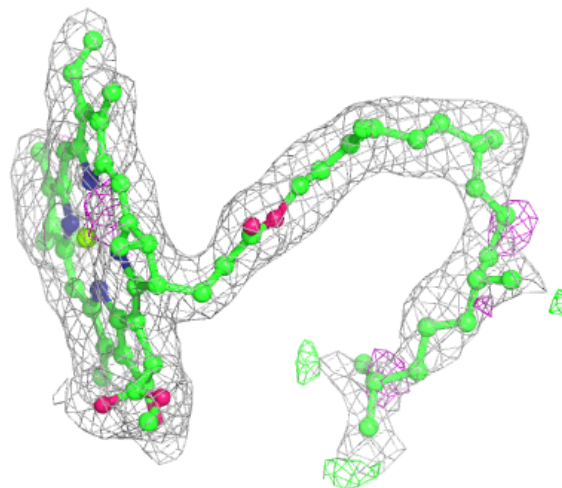
**Electron density around LFA B 620:**

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



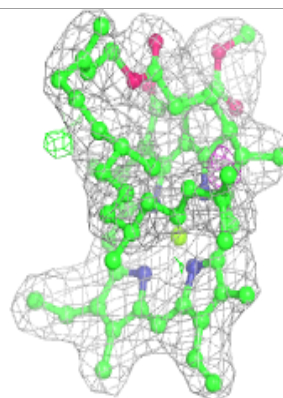
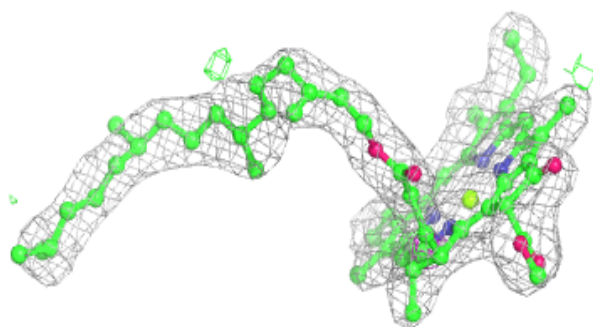
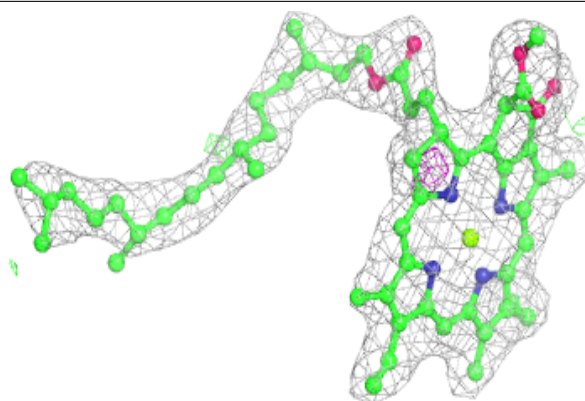
**Electron density around CLA B 605:**

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

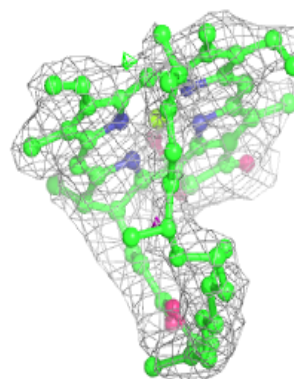
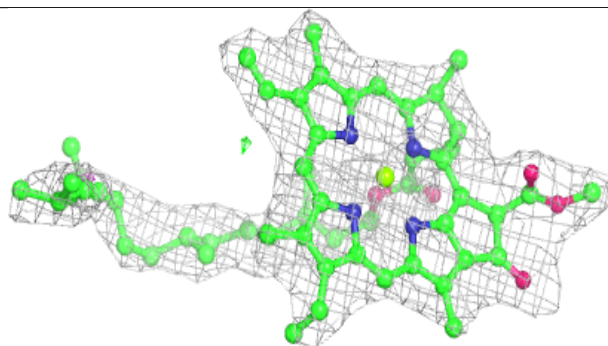
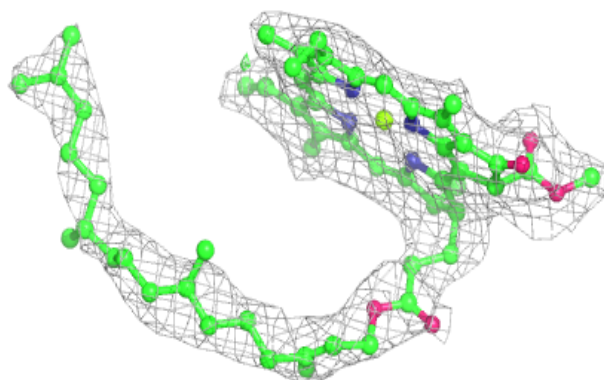


**Electron density around CLA C 512:**

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

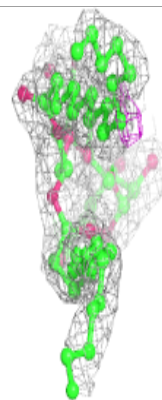
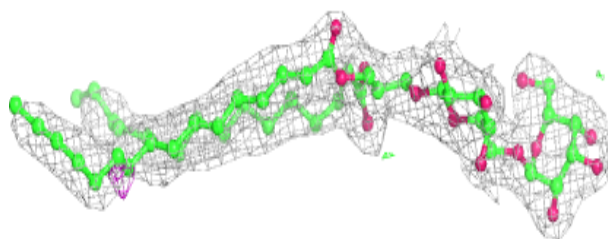
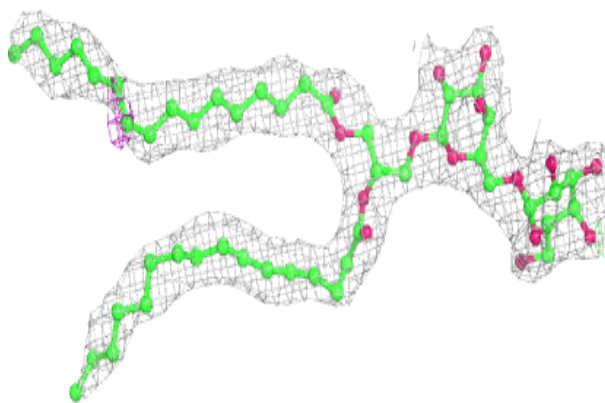
**Electron density around CLA c 514:**

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

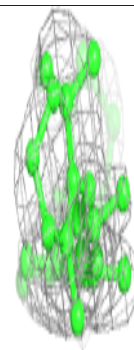
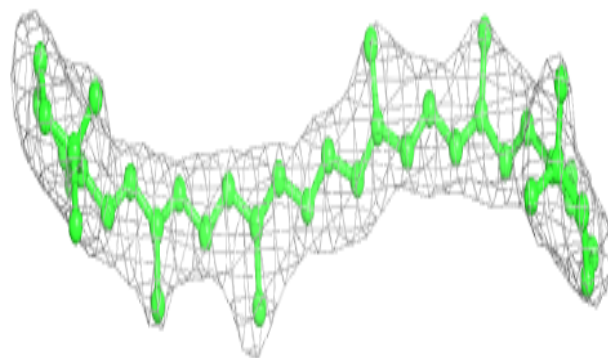
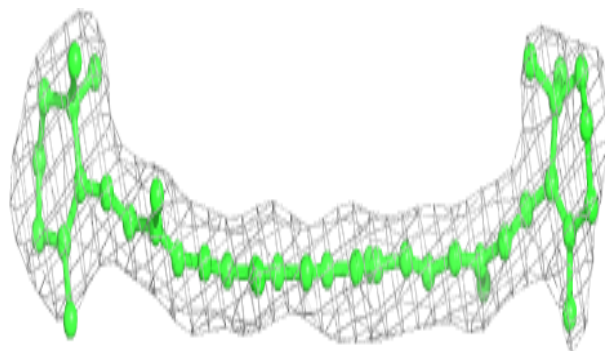


**Electron density around DGD C 519:**

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

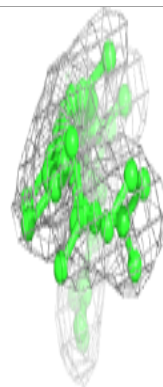
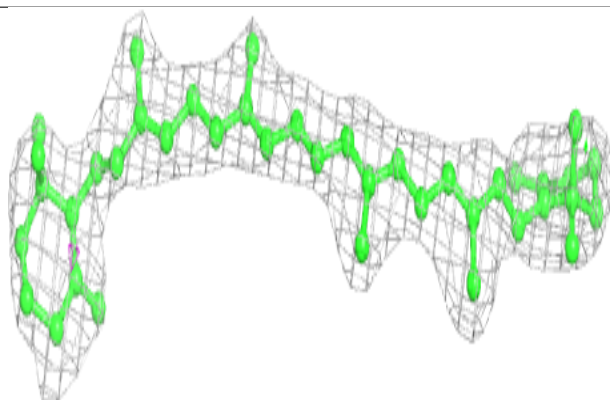
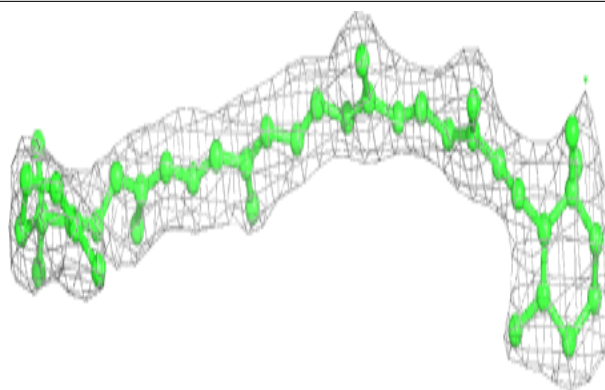
**Electron density around BCR K 102:**

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

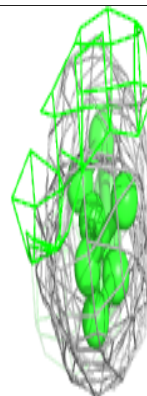
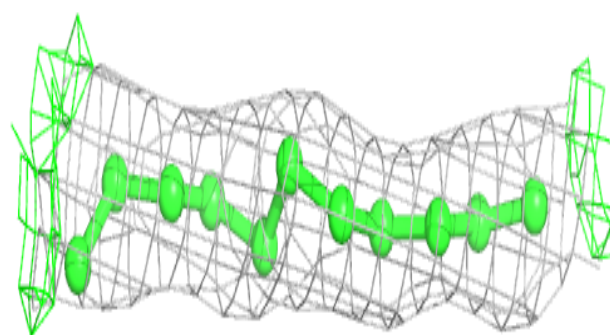
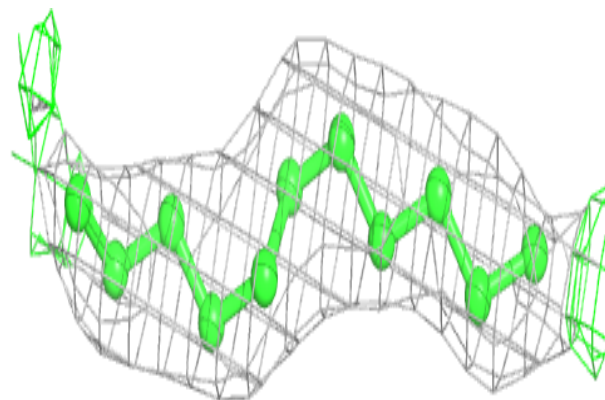


**Electron density around BCR D 404:**

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

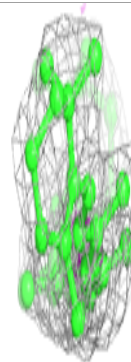
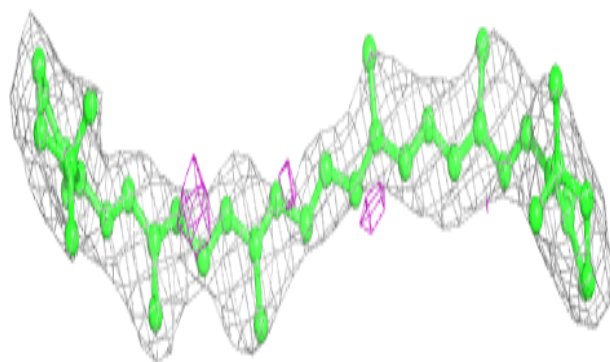
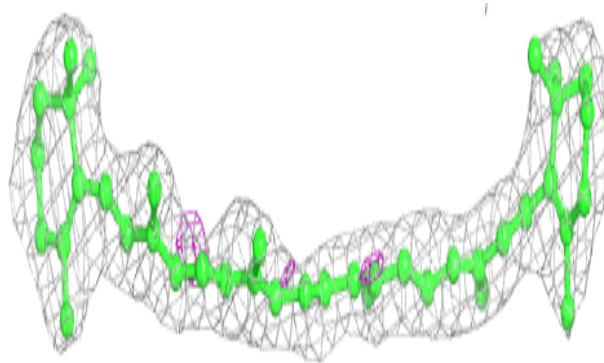
**Electron density around LFA J 101:**

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

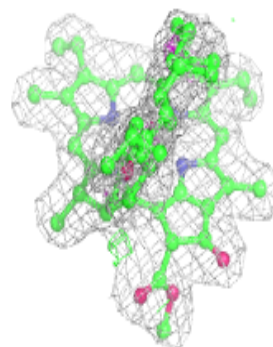
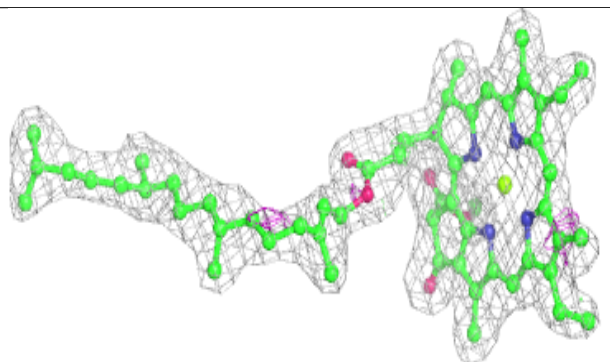
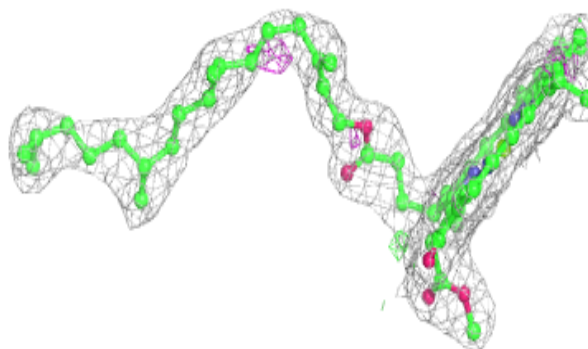


**Electron density around BCR k 101:**

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

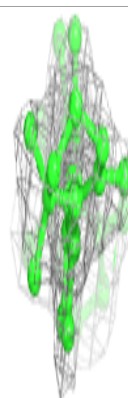
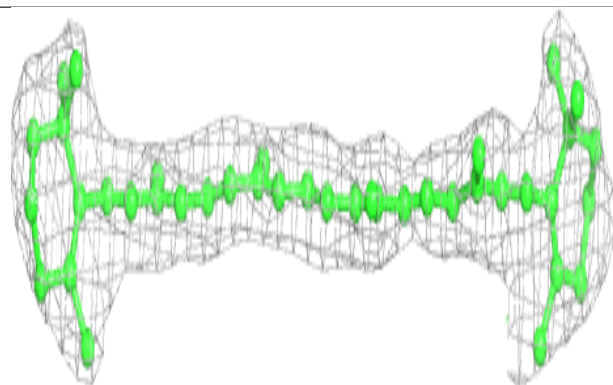
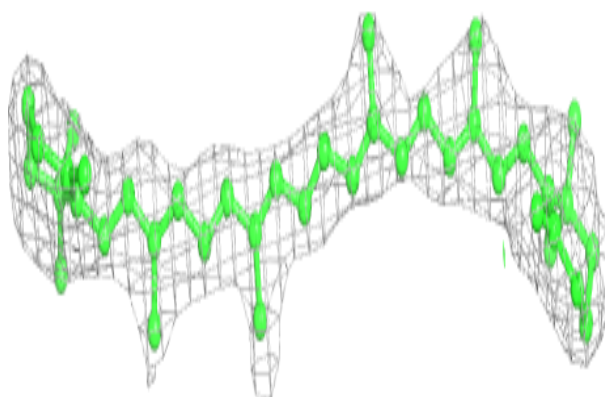
**Electron density around CLA C 503:**

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

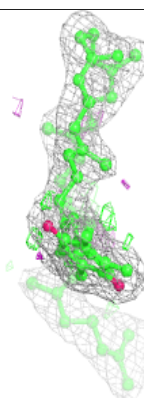
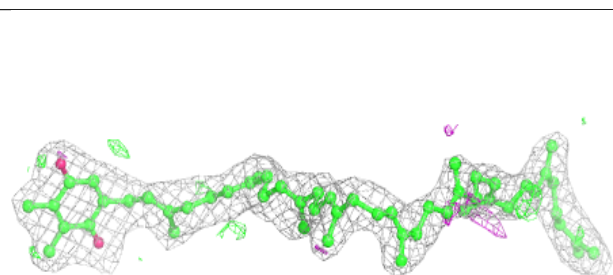
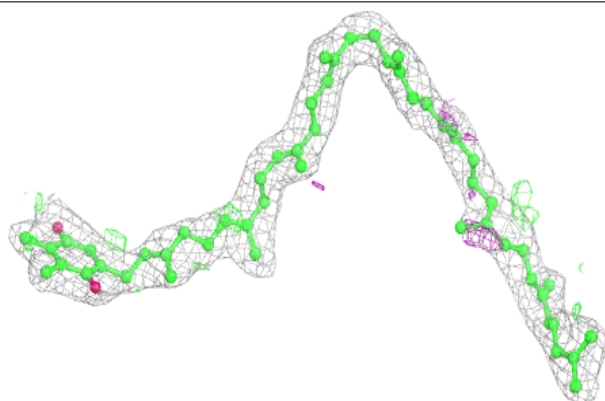


**Electron density around BCR C 515:**

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

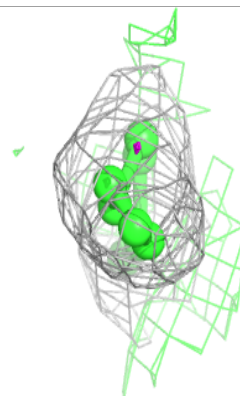
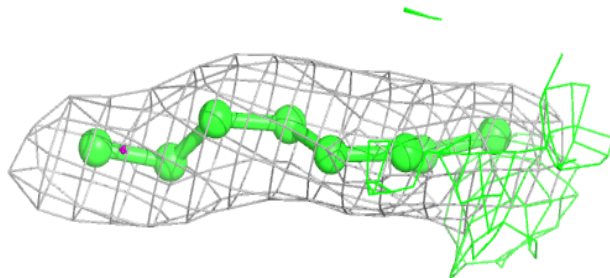
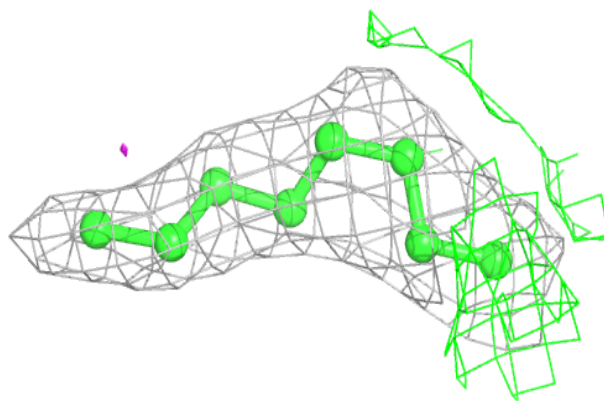
**Electron density around PL9 D 405:**

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

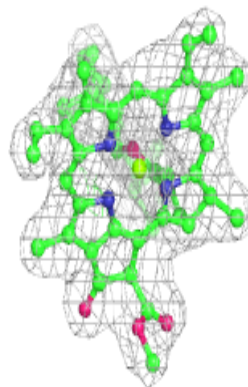
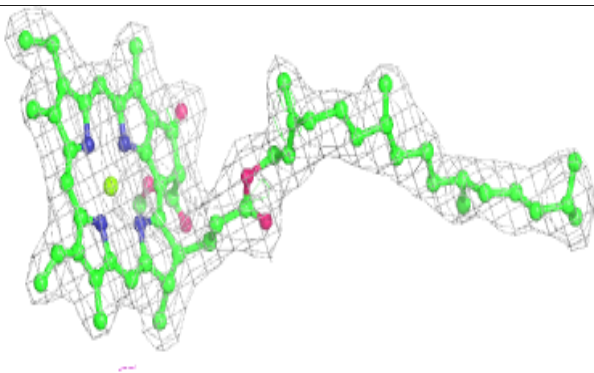
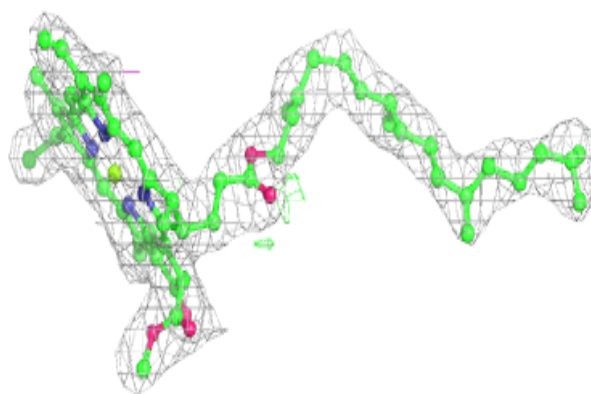


**Electron density around LFA D 412:**

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

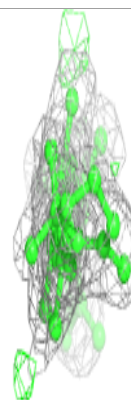
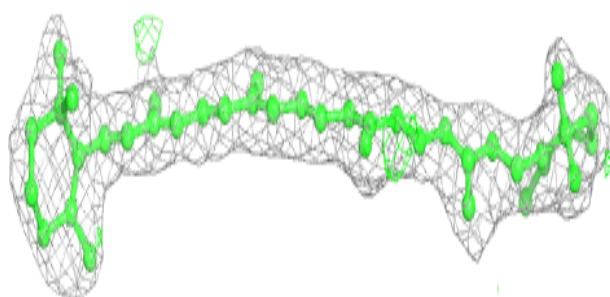
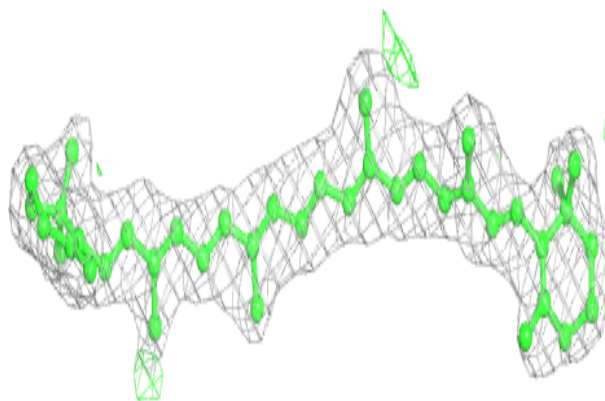
**Electron density around CLA c 503:**

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

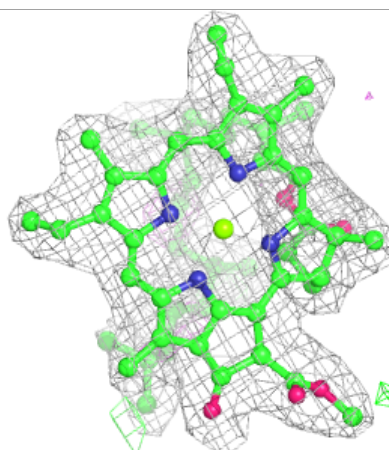
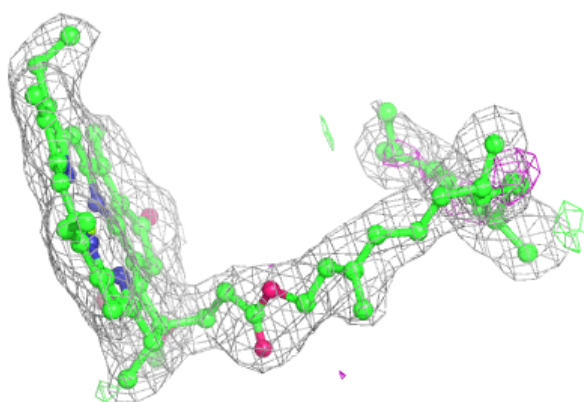
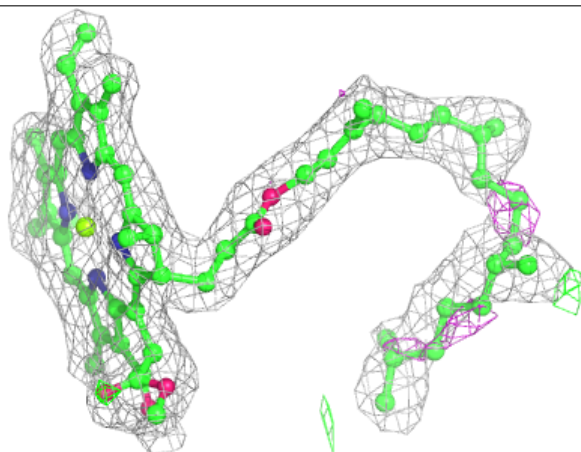


**Electron density around BCR b 619:**

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

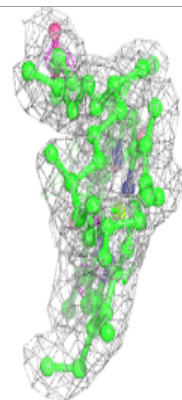
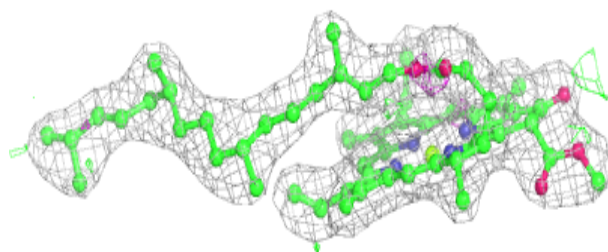
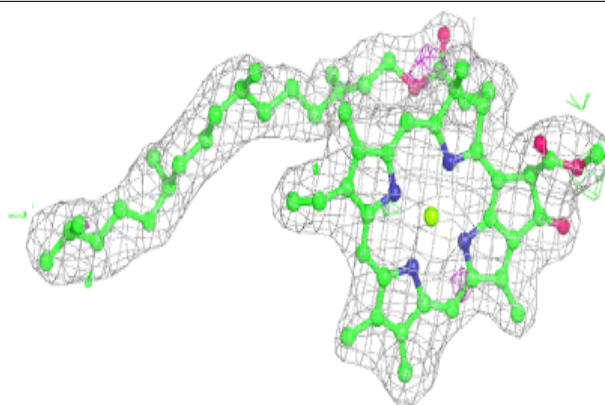
**Electron density around CLA b 608:**

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

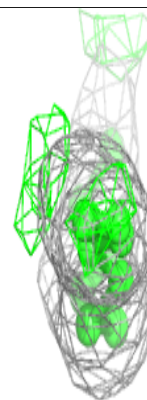
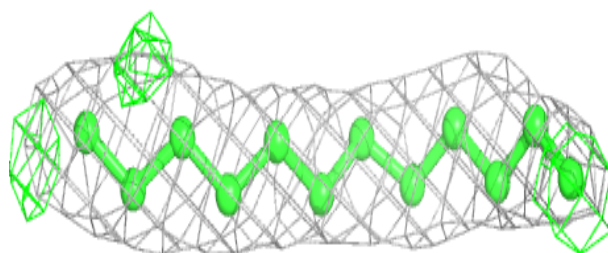
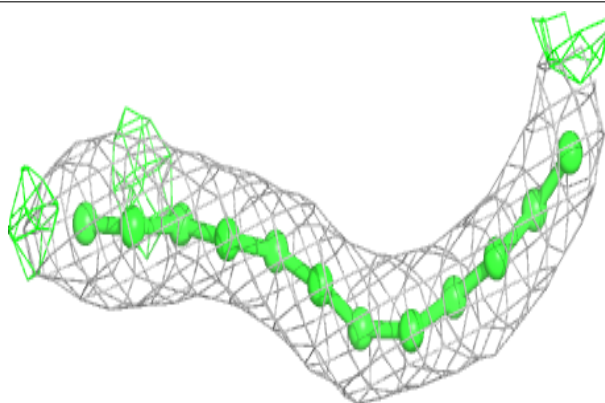


**Electron density around CLA c 502:**

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

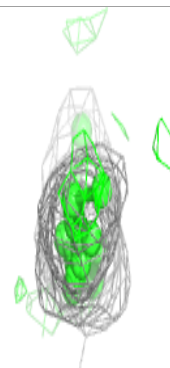
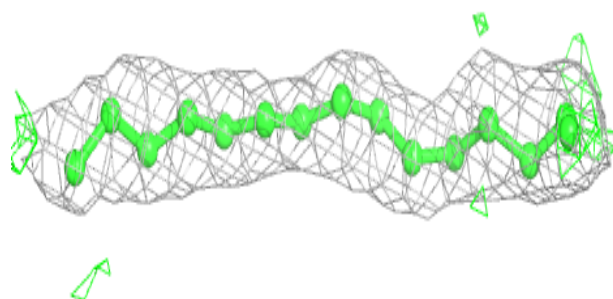
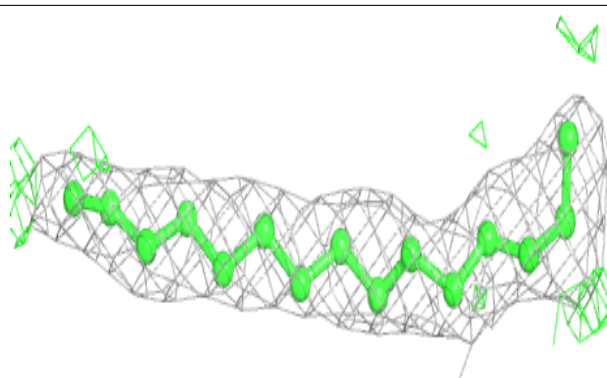
**Electron density around LFA B 628:**

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

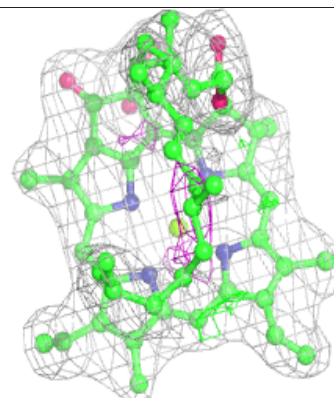
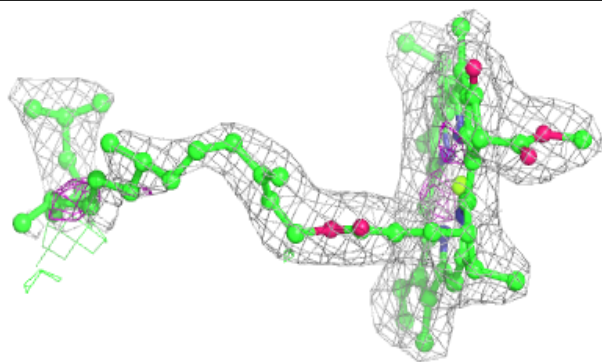
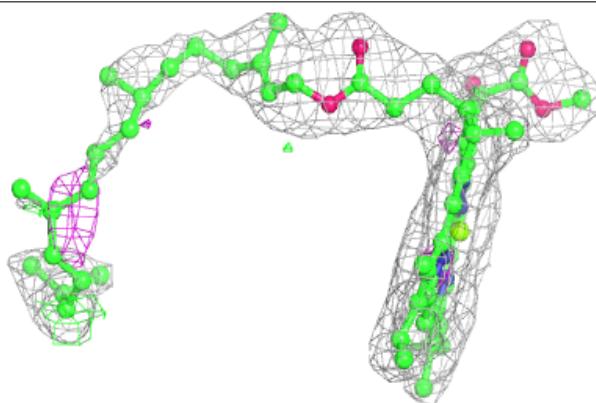


**Electron density around LFA c 521:**

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

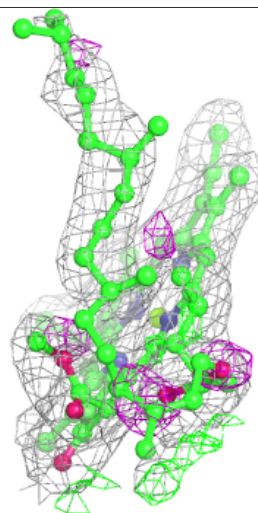
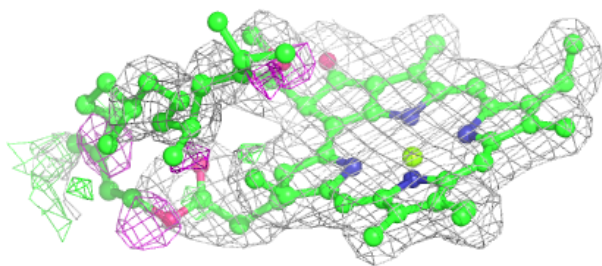
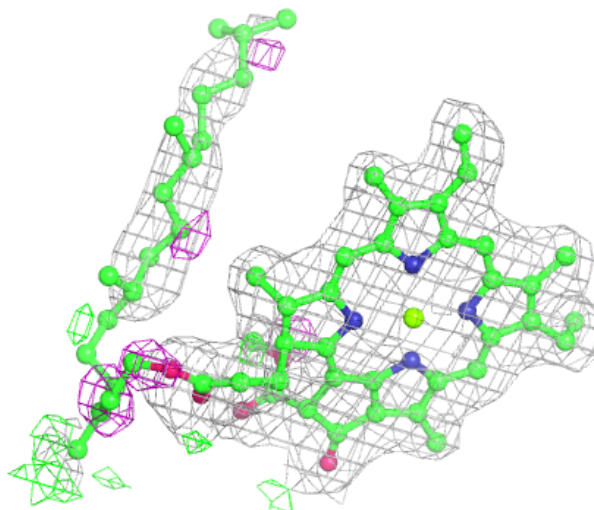
**Electron density around CLA c 507:**

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



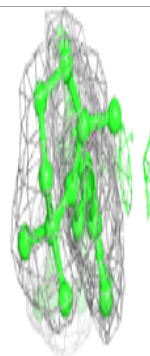
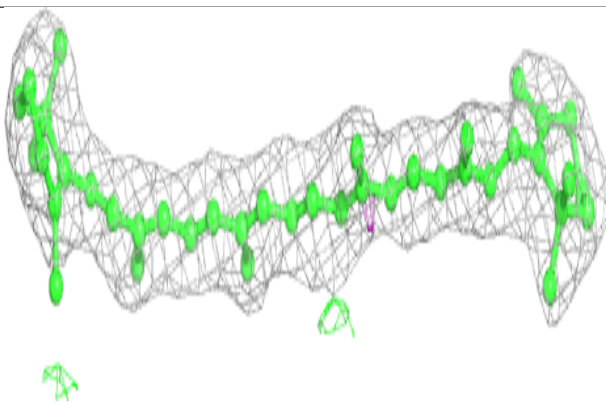
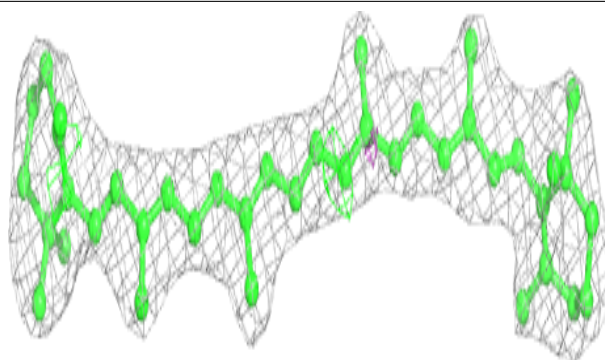
**Electron density around CLA B 615:**

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

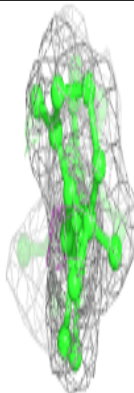
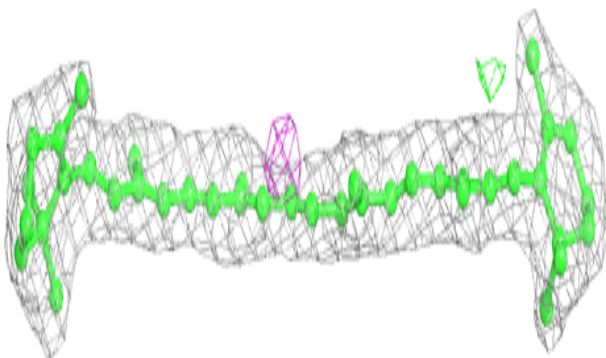
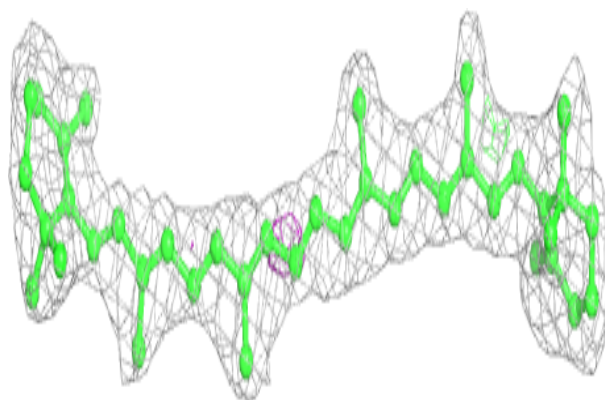


**Electron density around BCR b 621:**

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

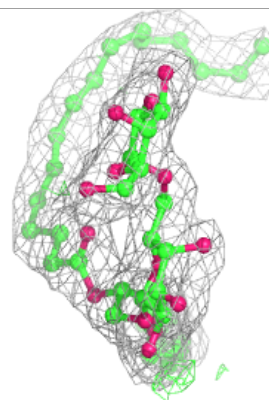
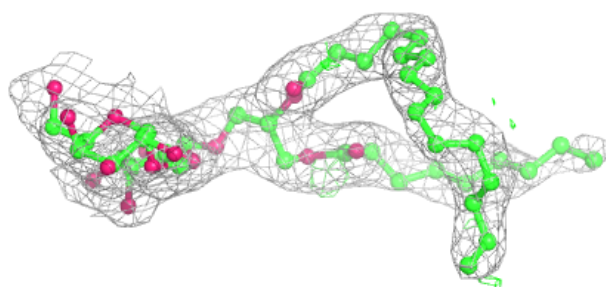
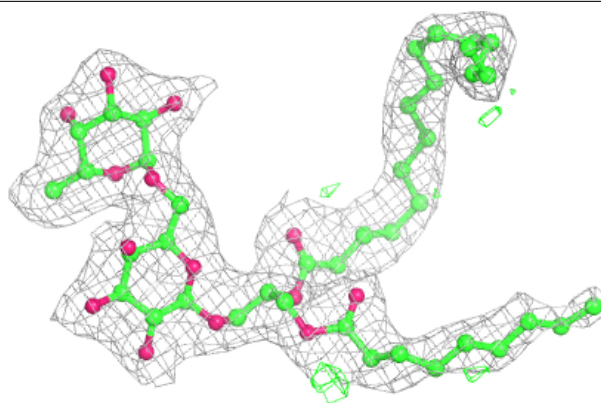
**Electron density around BCR B 617:**

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

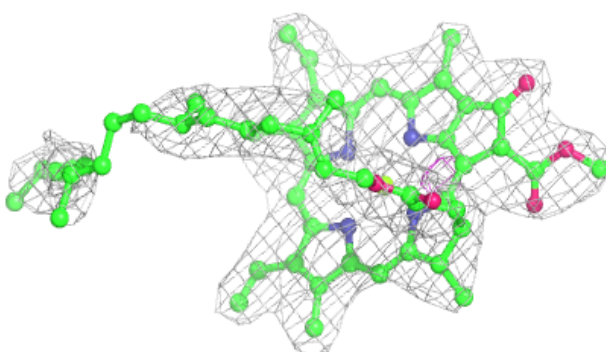
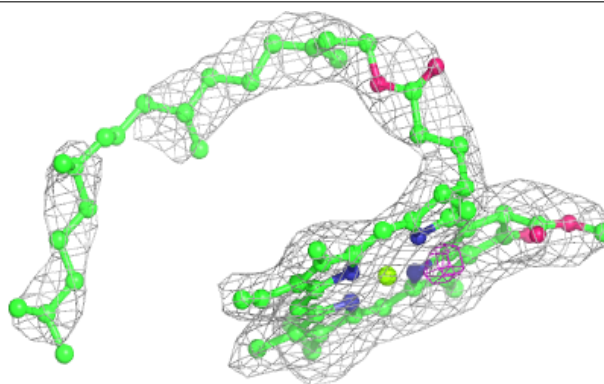


**Electron density around DGD c 517:**

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

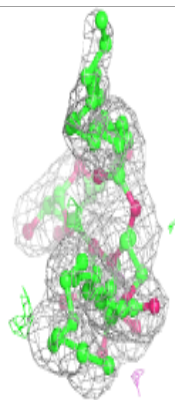
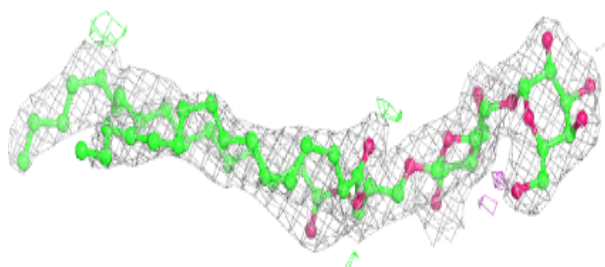
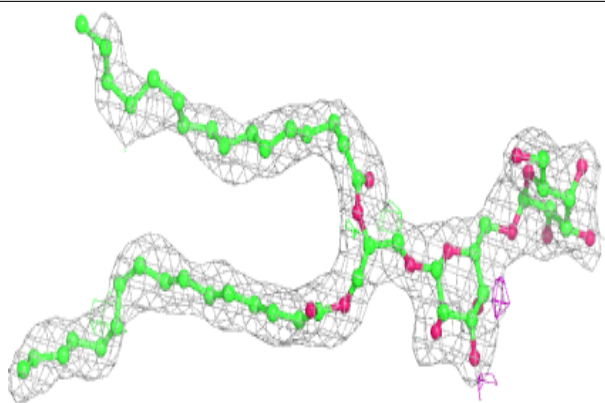
**Electron density around CLA C 514:**

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

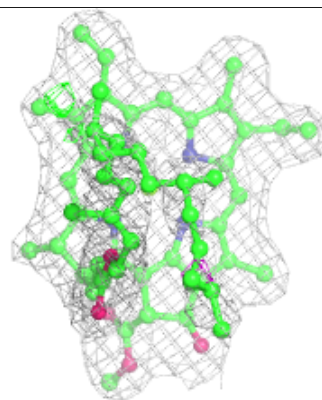
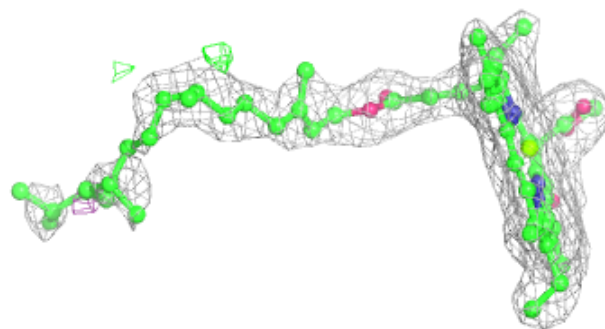
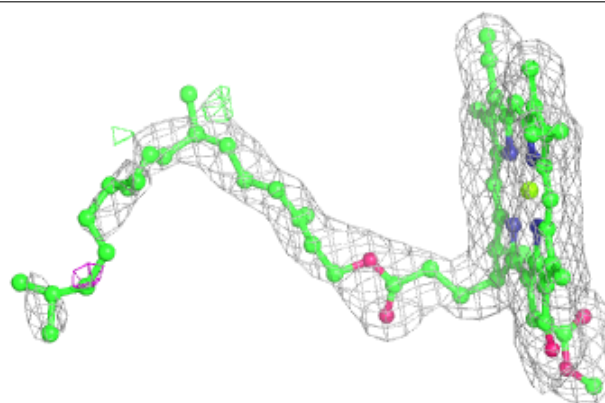


**Electron density around DGD c 518:**

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

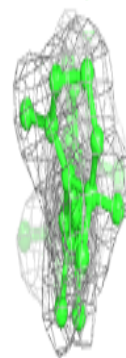
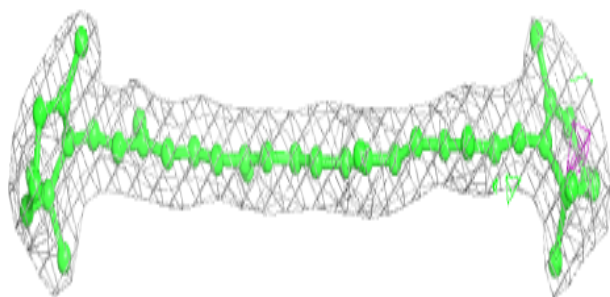
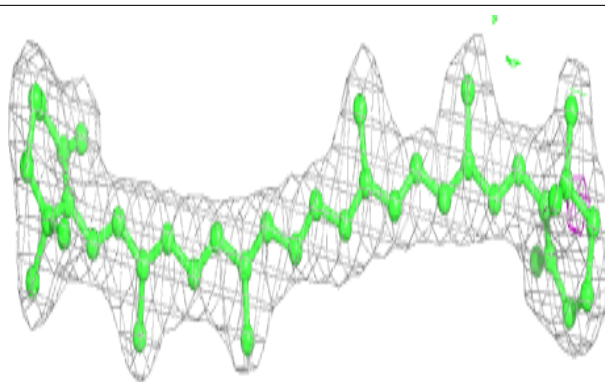
**Electron density around CLA D 403:**

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

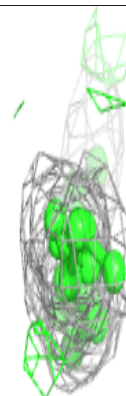
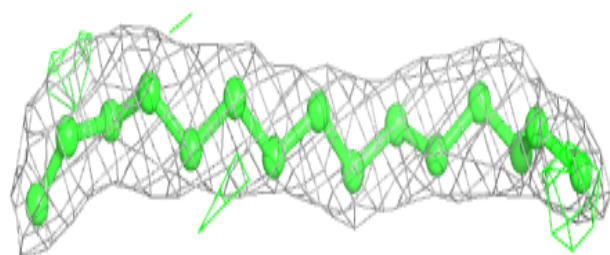
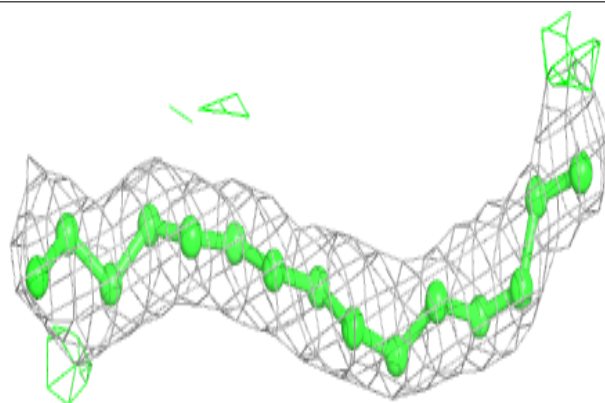


**Electron density around BCR b 620:**

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

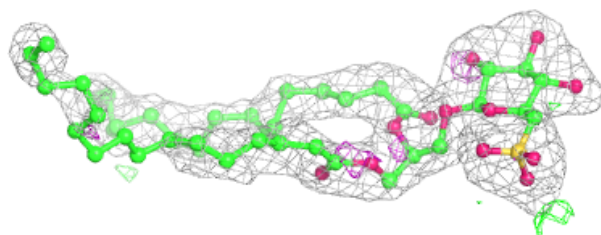
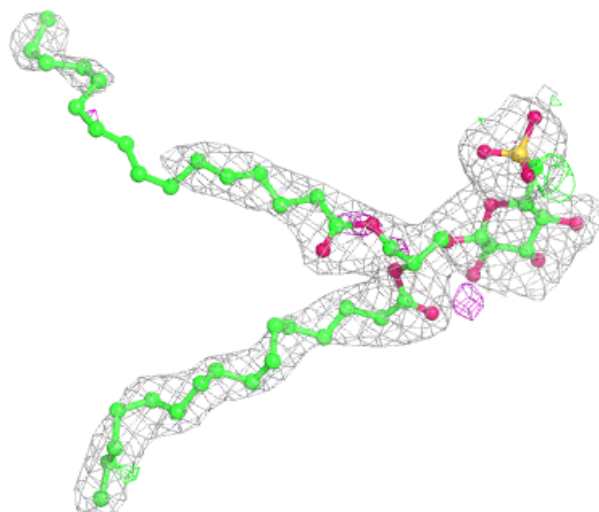
**Electron density around LFA b 602:**

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



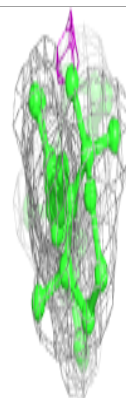
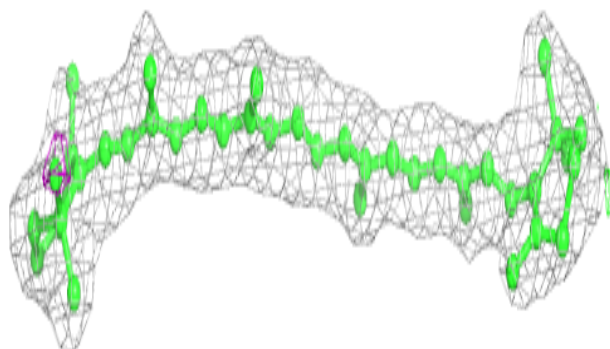
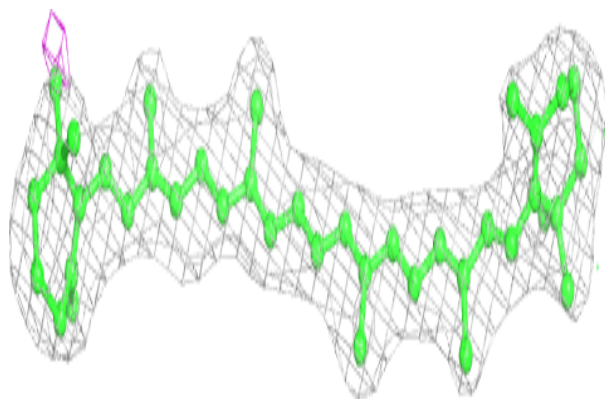
**Electron density around SQD a 410:**

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

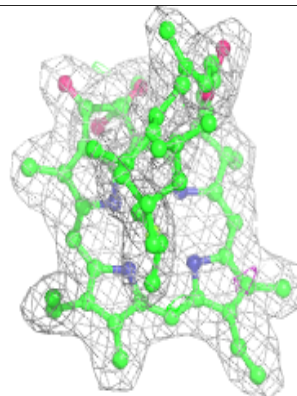
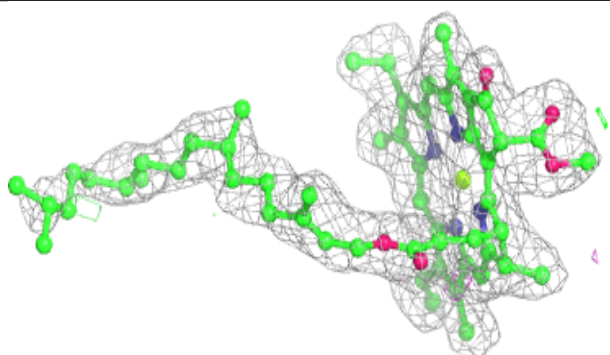
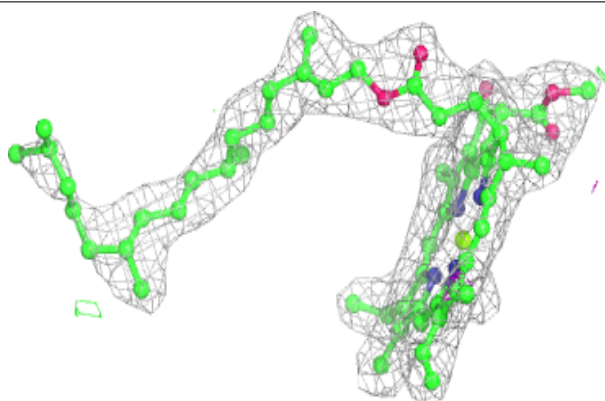


**Electron density around BCR B 618:**

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

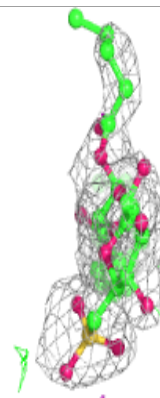
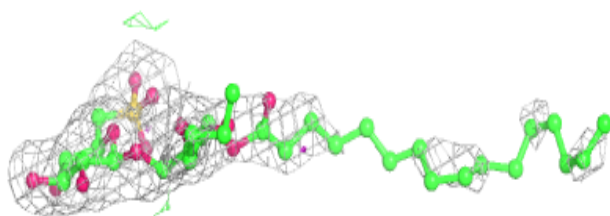
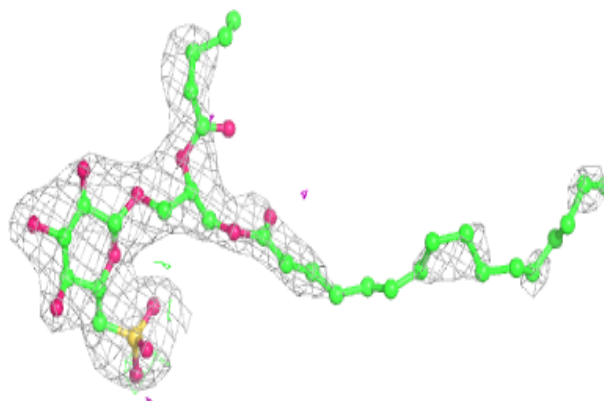
**Electron density around CLA C 509:**

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

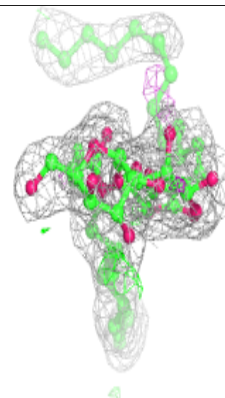
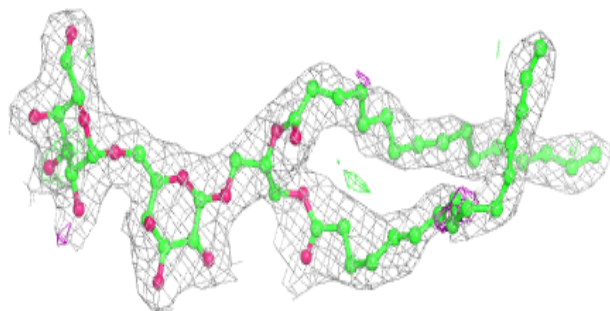
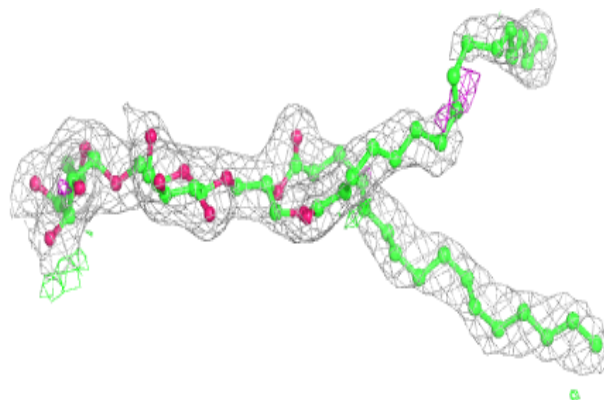


**Electron density around SQD f 102:**

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

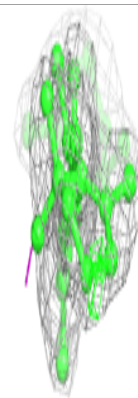
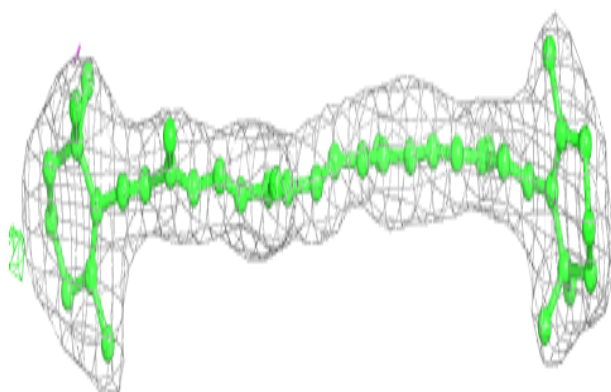
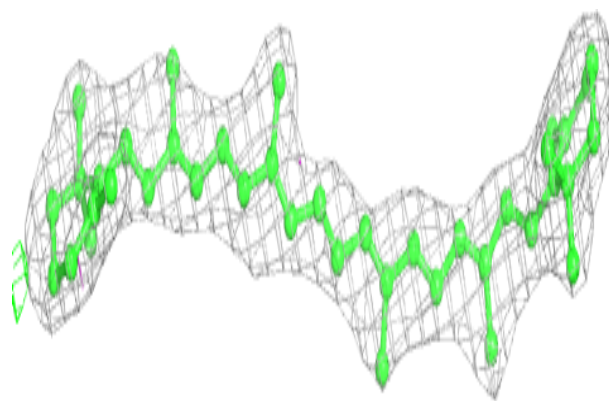
**Electron density around DGD c 516:**

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

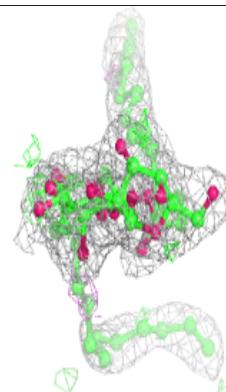
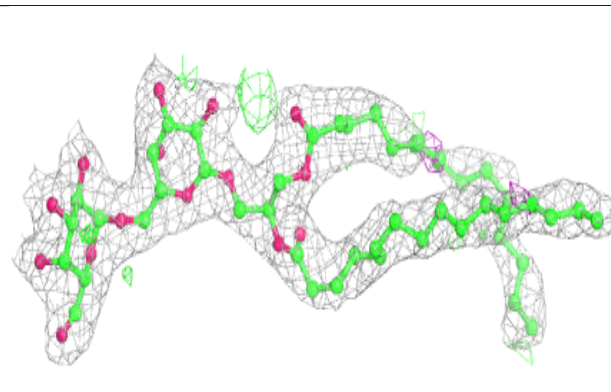
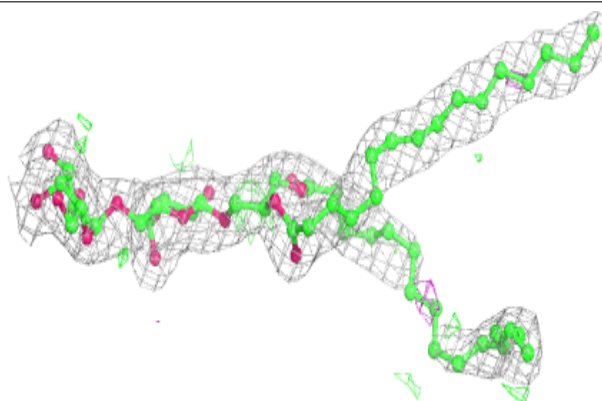


**Electron density around BCR C 516:**

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

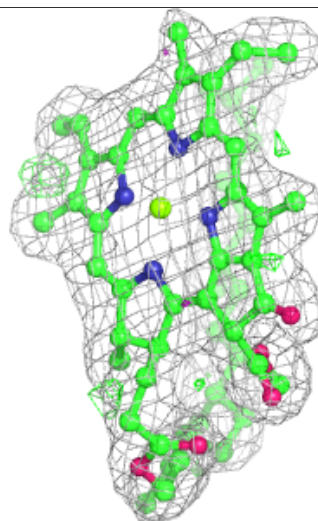
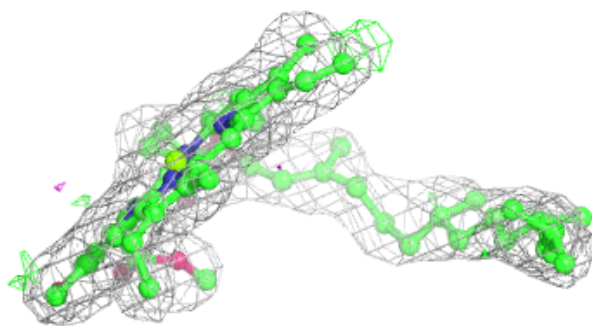
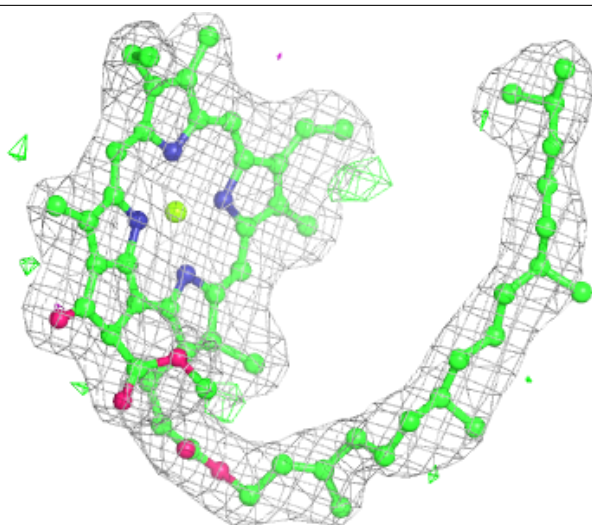
**Electron density around DGD C 517:**

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



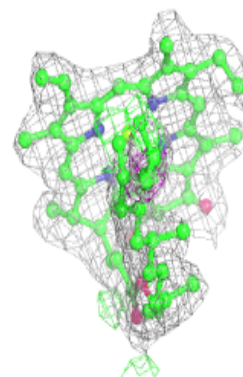
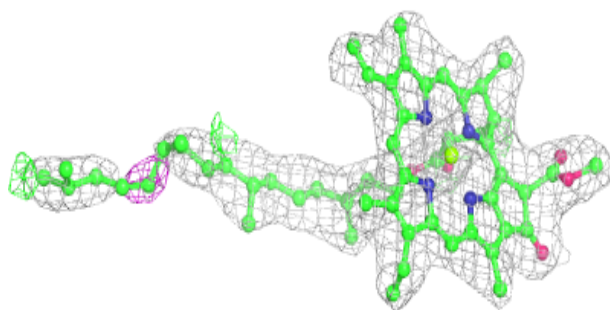
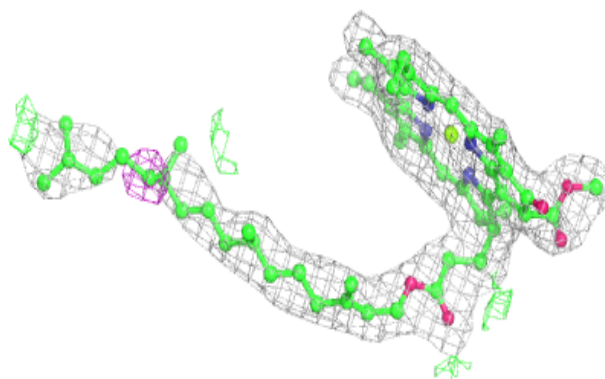
**Electron density around CLA c 508:**

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

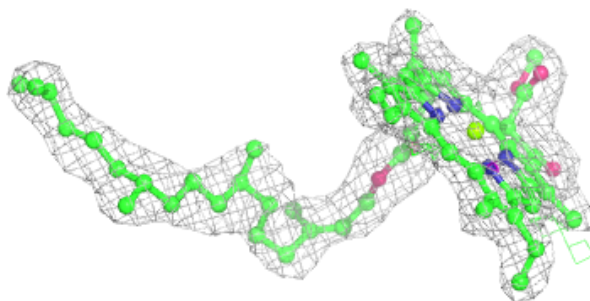
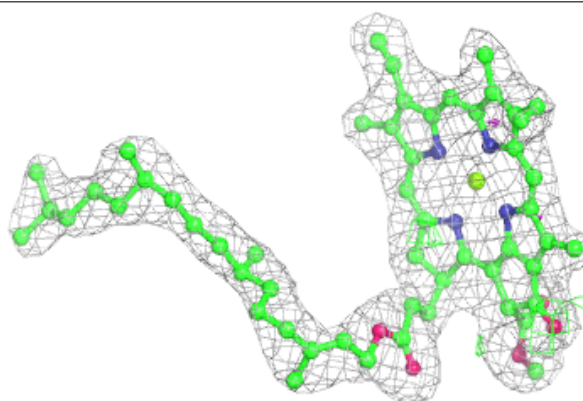


**Electron density around CLA C 505:**

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

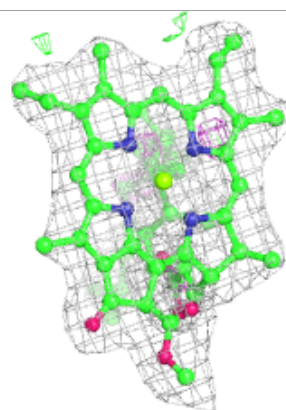
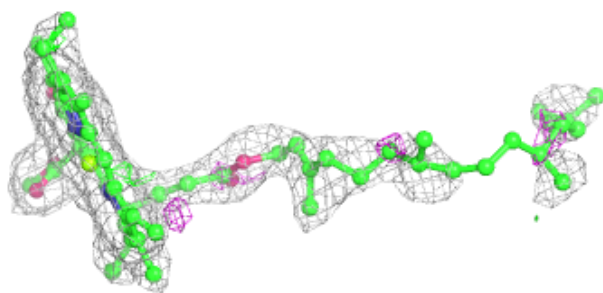
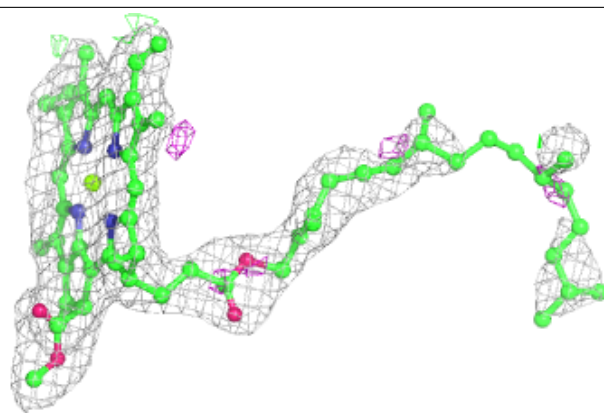
**Electron density around CLA c 512:**

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

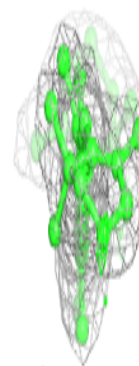
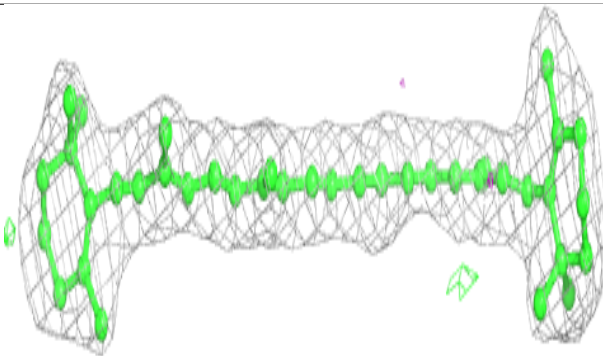
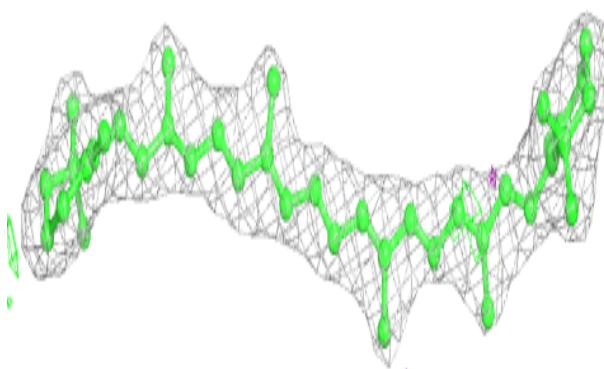


**Electron density around CLA d 403:**

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

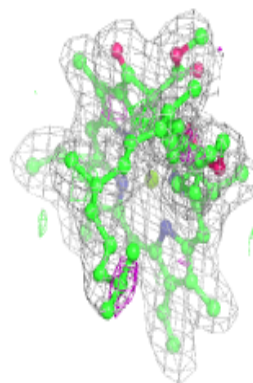
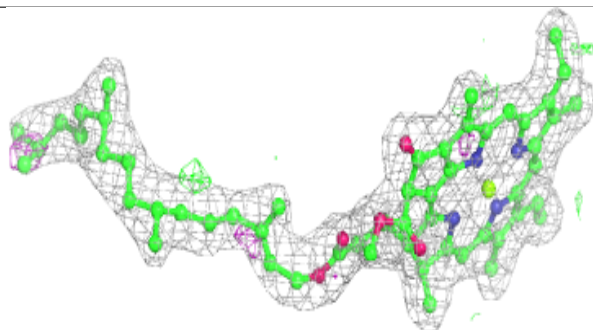
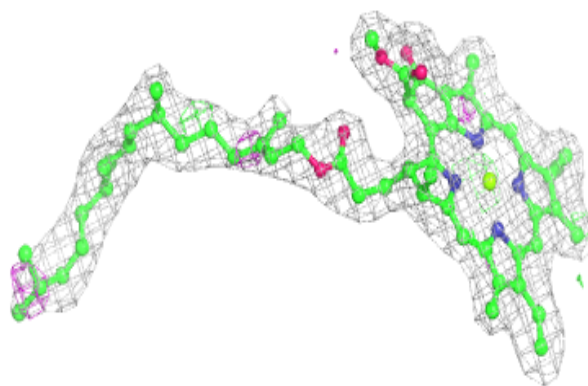
**Electron density around BCR c 515:**

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

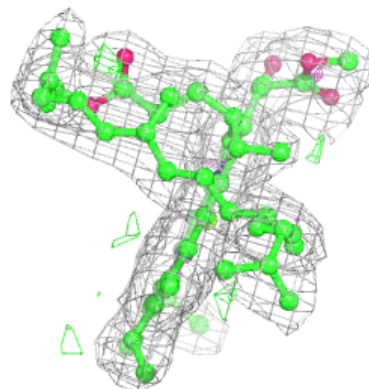
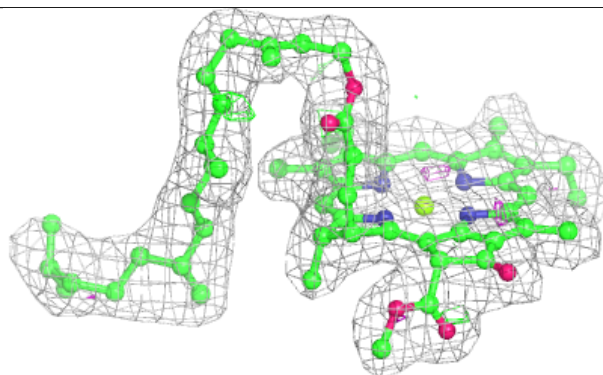
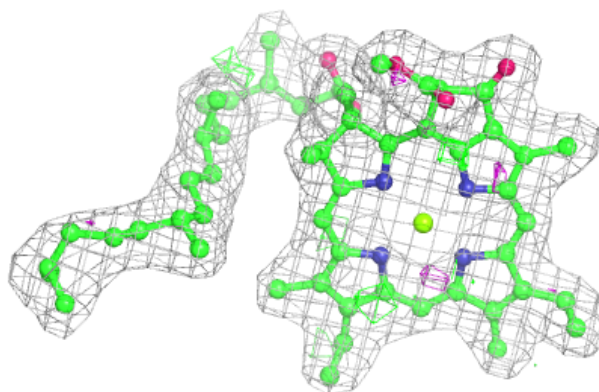


**Electron density around CLA a 404:**

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

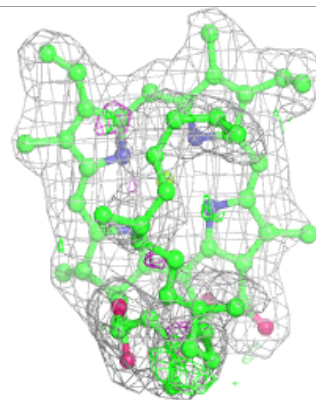
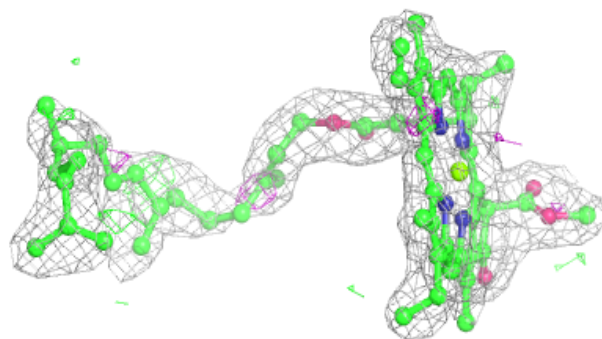
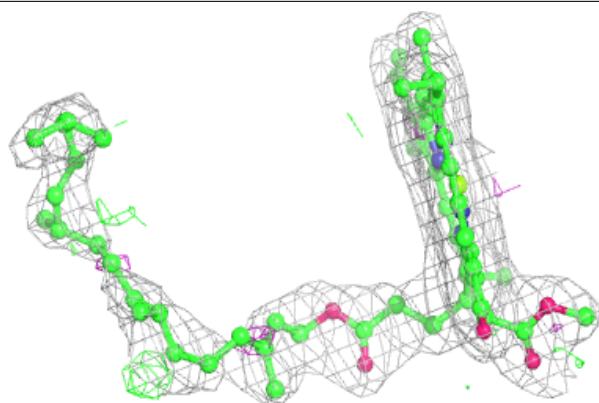
**Electron density around CLA a 405:**

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



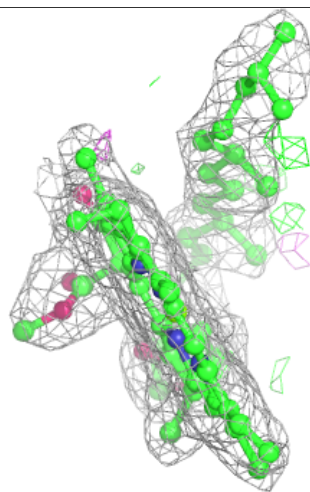
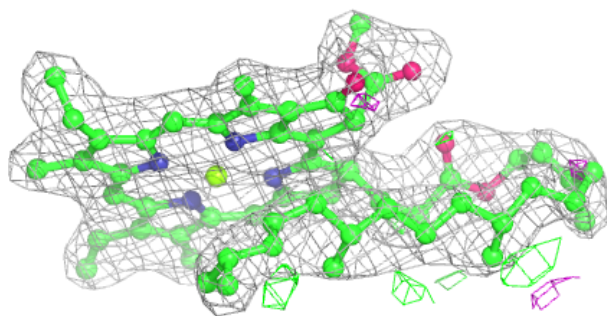
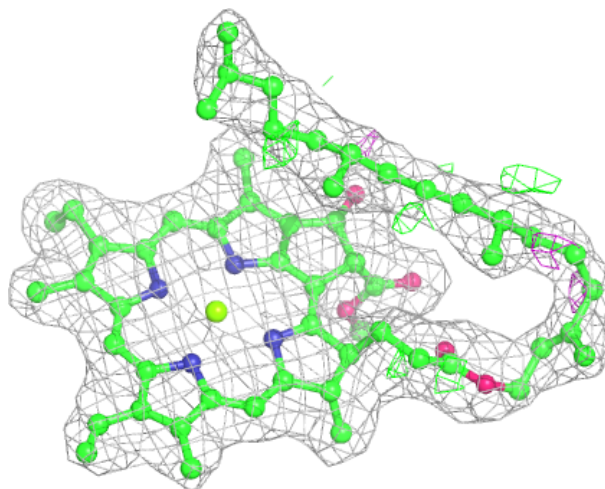
**Electron density around CLA C 507:**

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



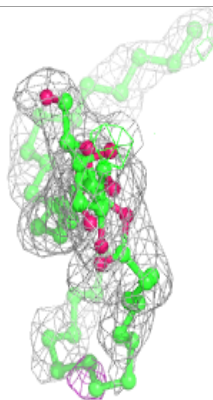
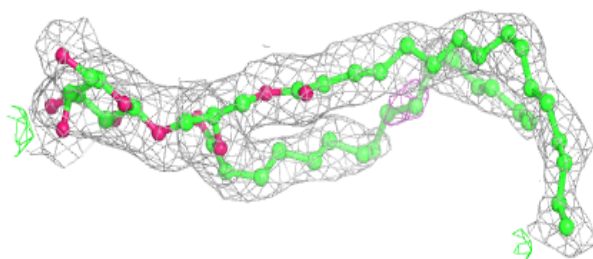
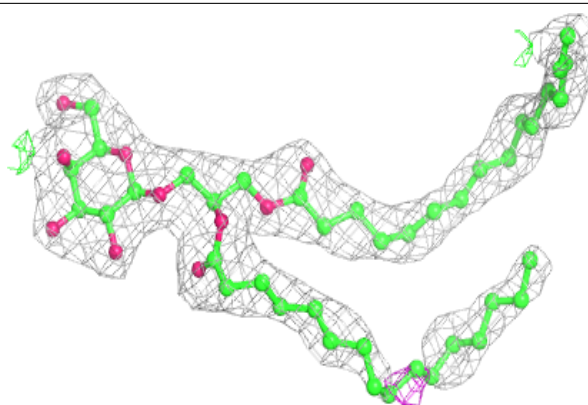
**Electron density around CLA c 510:**

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

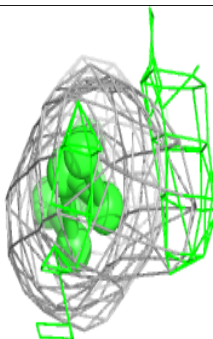
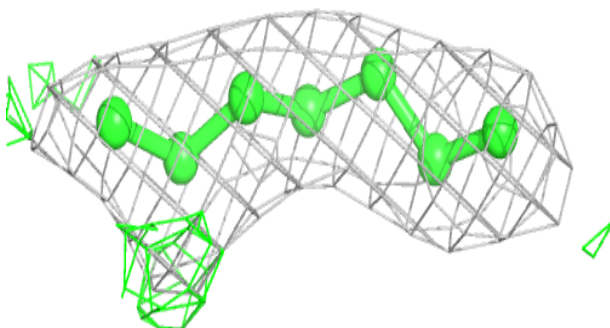
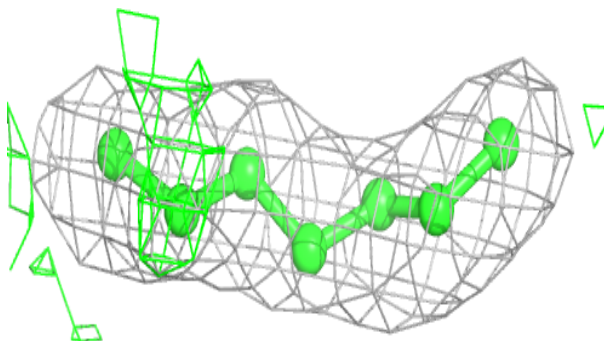


**Electron density around LMG f 101:**

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

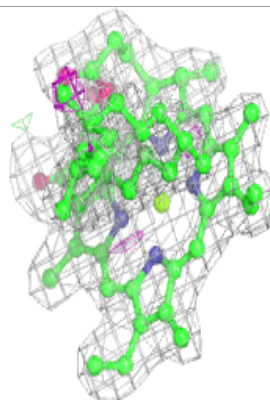
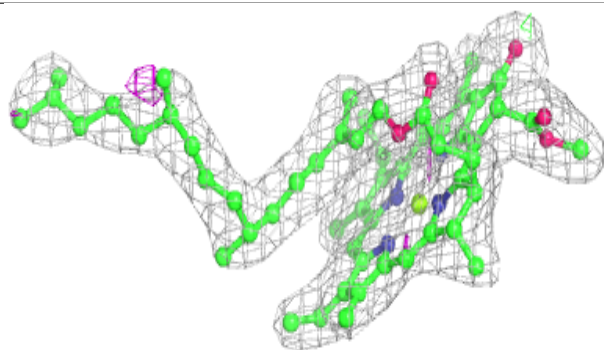
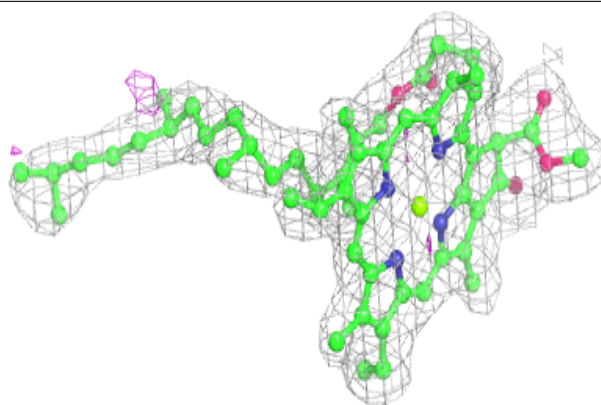
**Electron density around LFA a 411:**

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



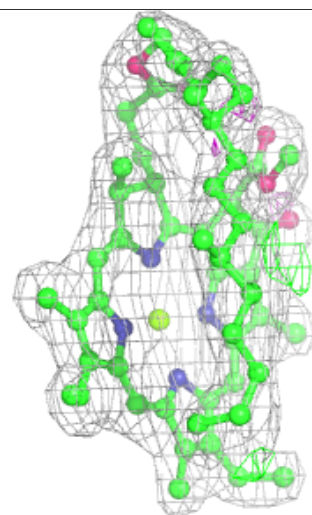
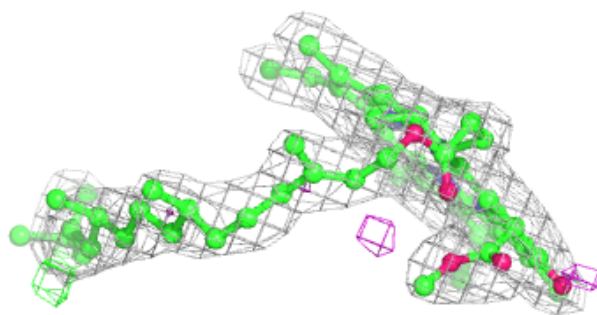
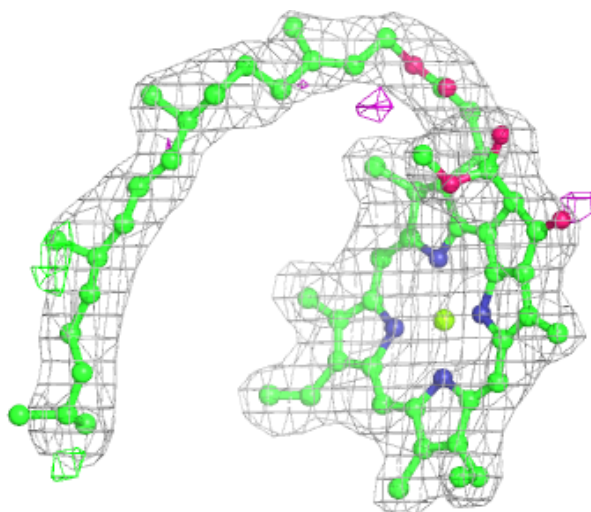
**Electron density around CLA c 506:**

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



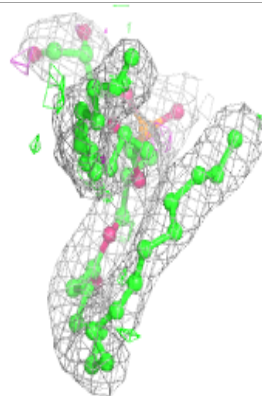
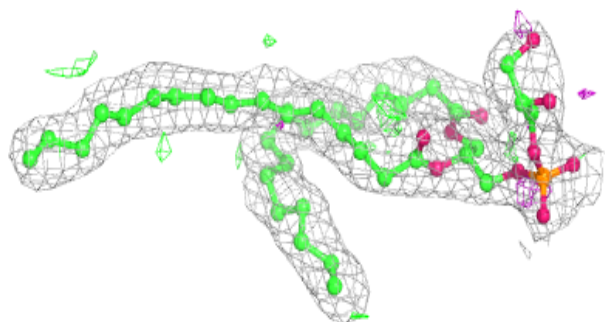
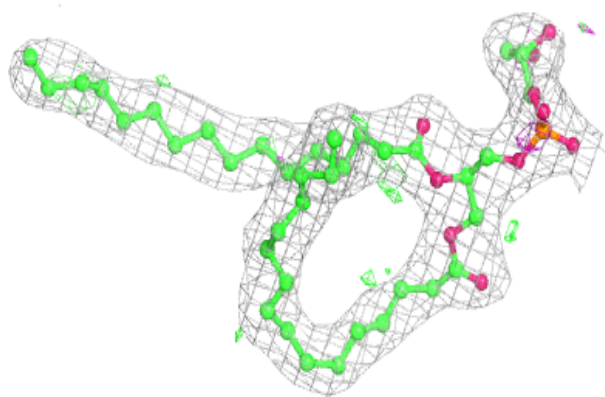
**Electron density around CLA C 508:**

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

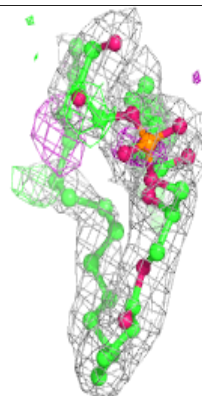
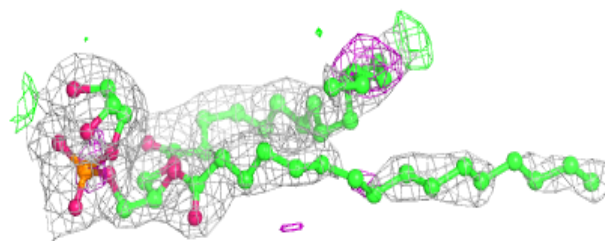
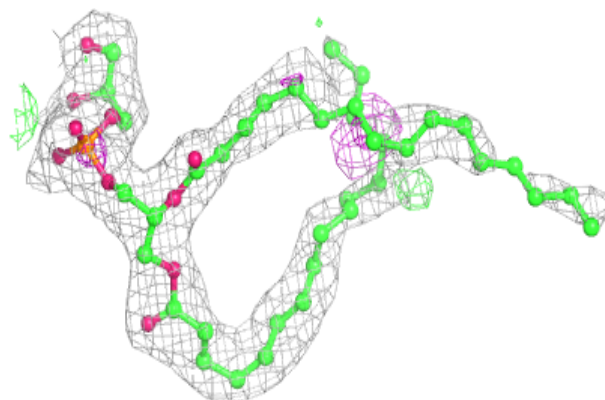


**Electron density around LHG D 406:**

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

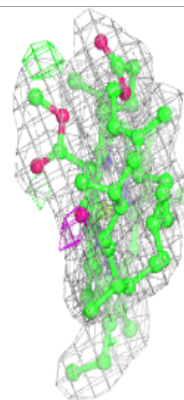
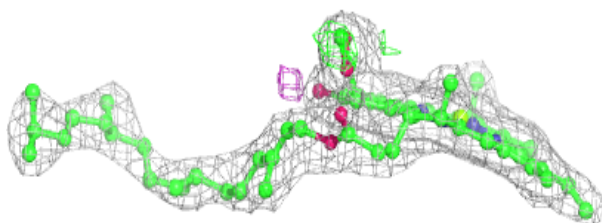
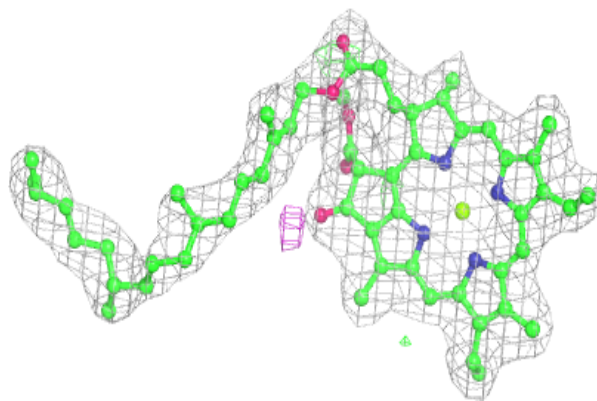
**Electron density around LHG D 408:**

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



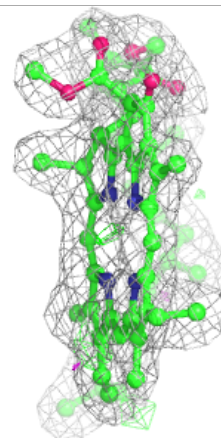
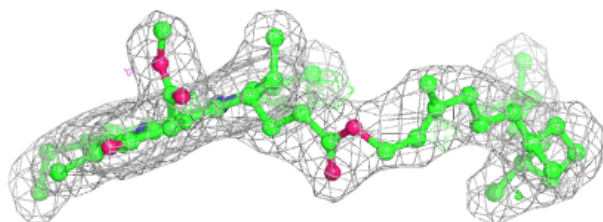
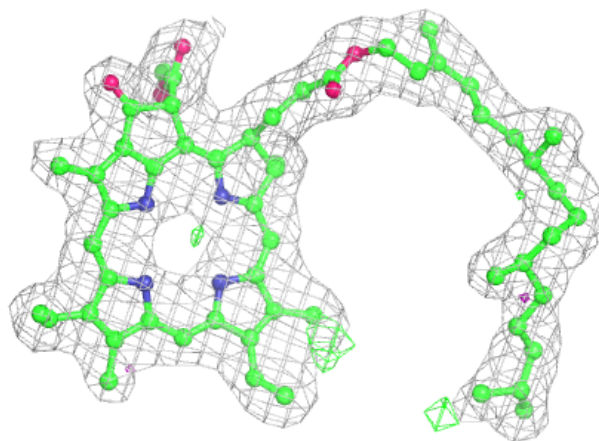
**Electron density around CLA b 604:**

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



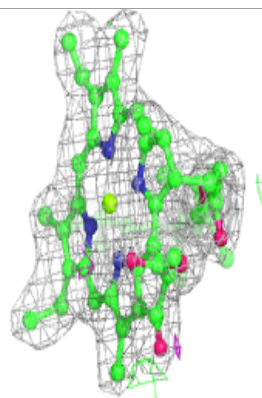
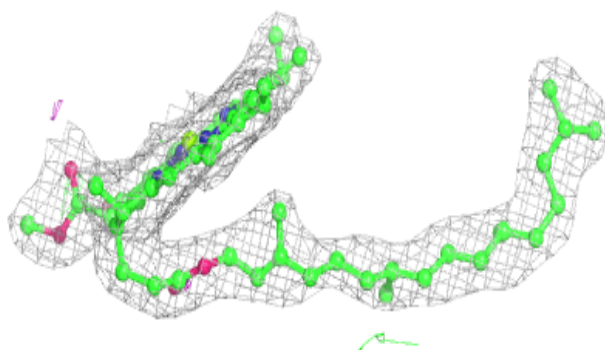
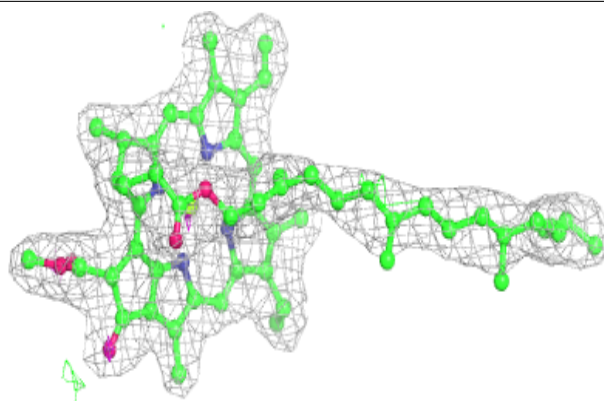
**Electron density around PHO a 406:**

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

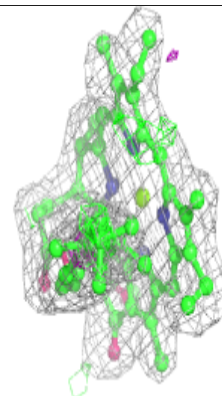
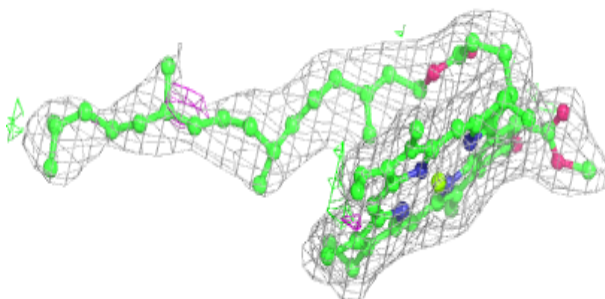
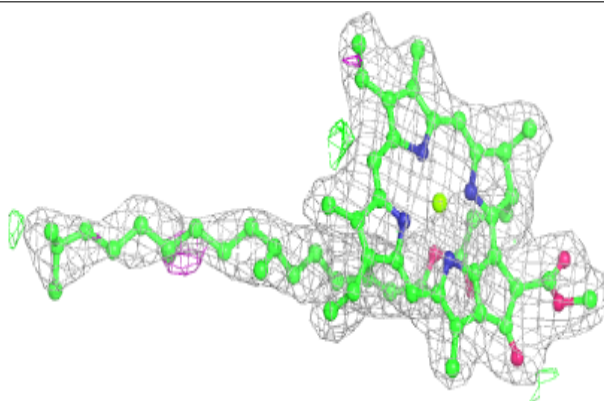


**Electron density around CLA b 610:**

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

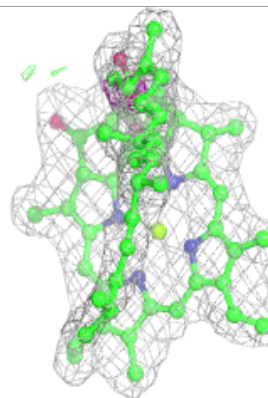
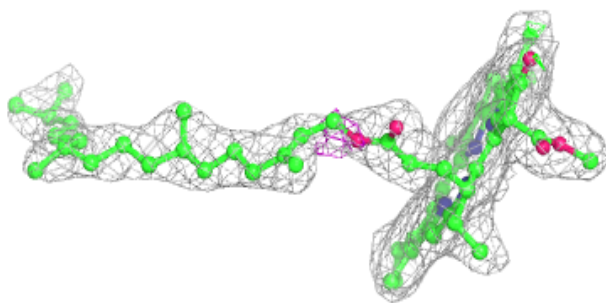
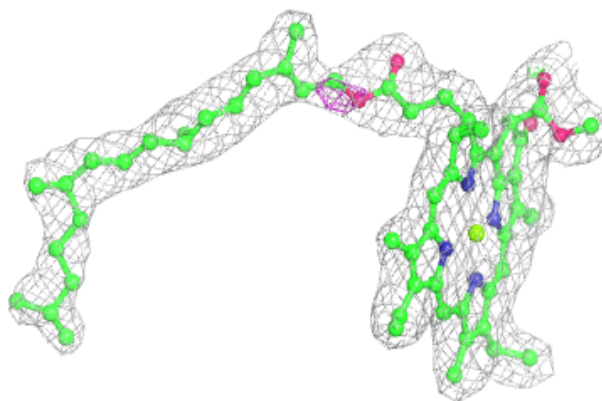
**Electron density around CLA b 616:**

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

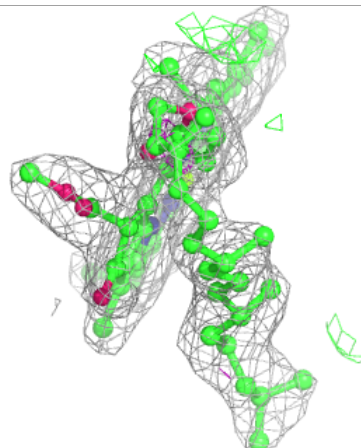
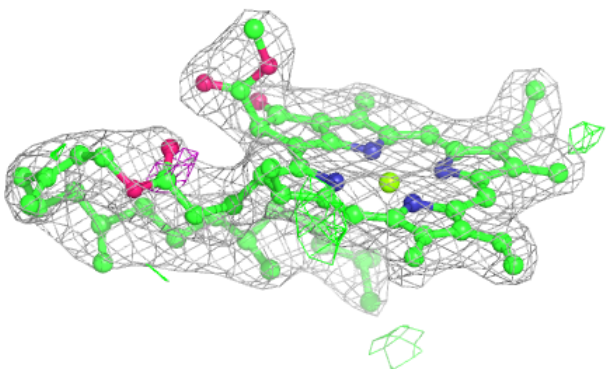
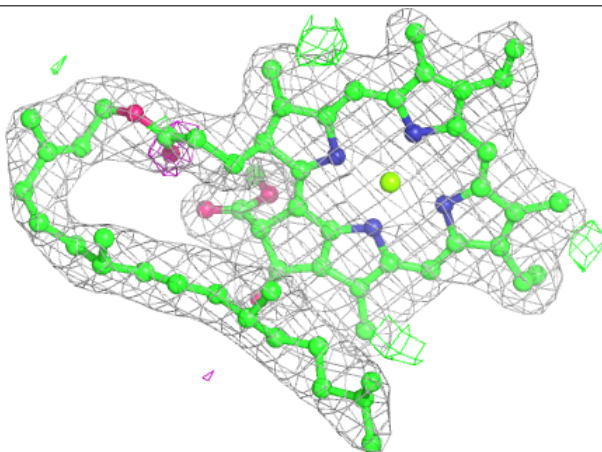


**Electron density around CLA b 611:**

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

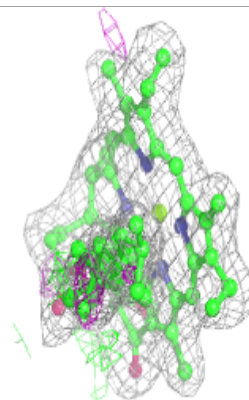
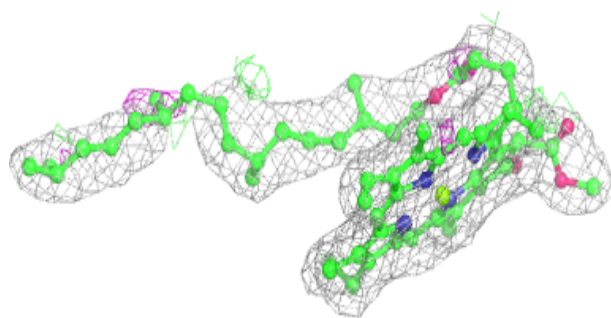
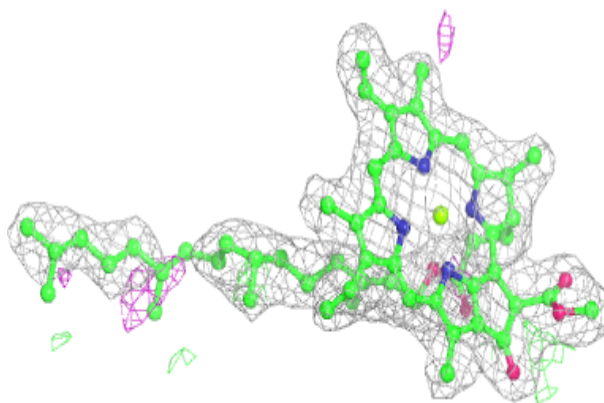
**Electron density around CLA C 510:**

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



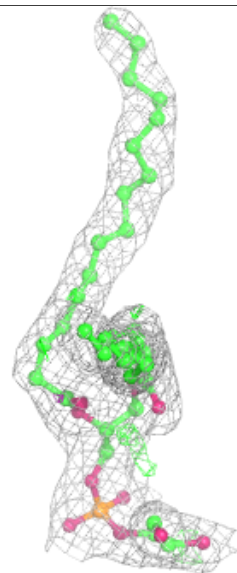
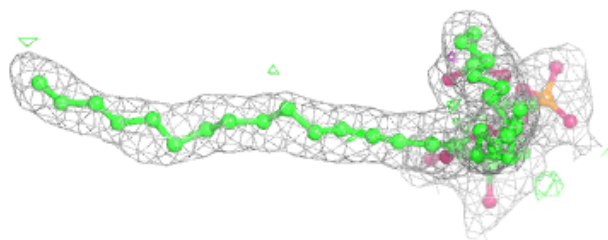
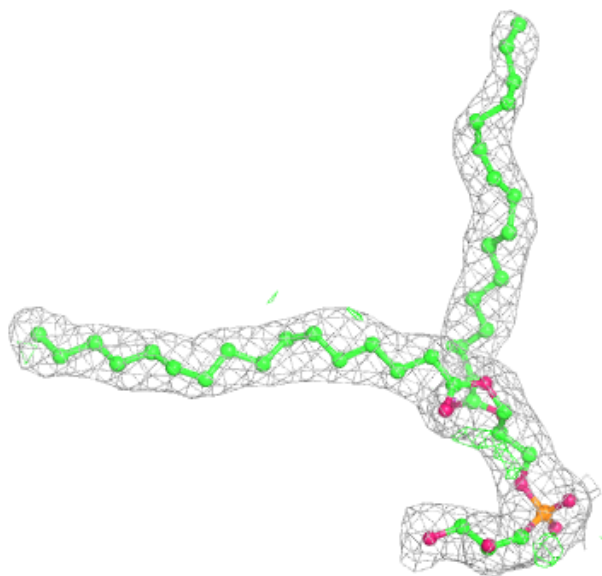
**Electron density around CLA B 613:**

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



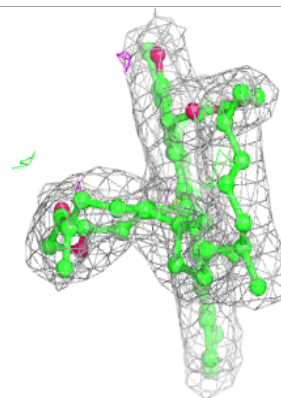
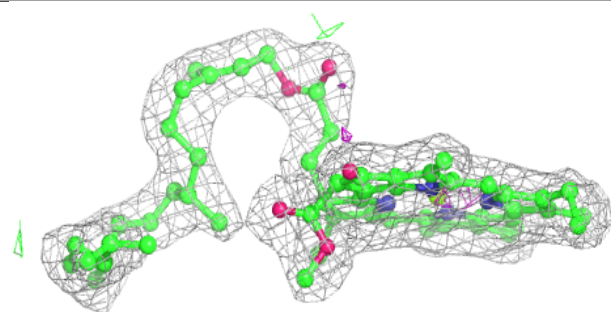
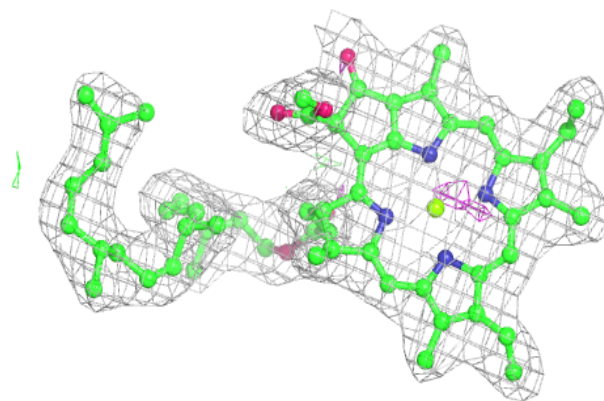
**Electron density around LHG 1 101:**

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



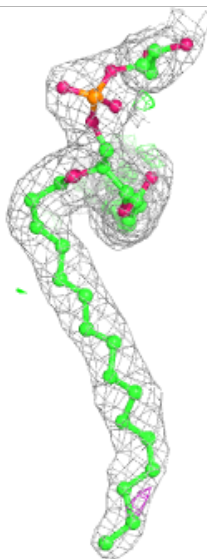
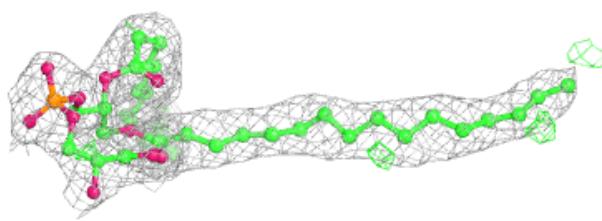
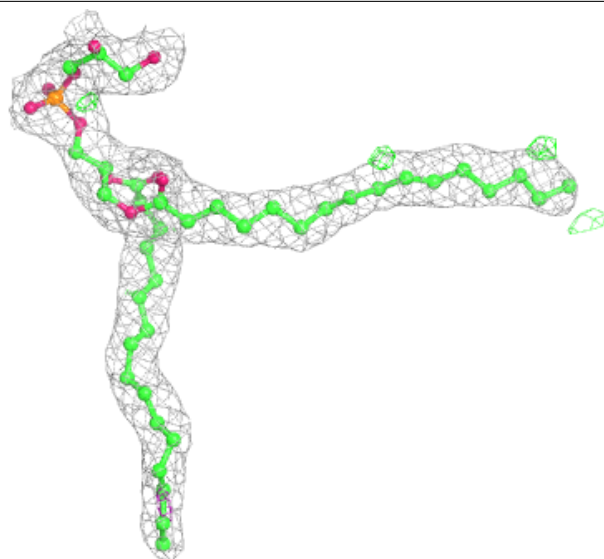
**Electron density around CLA B 611:**

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



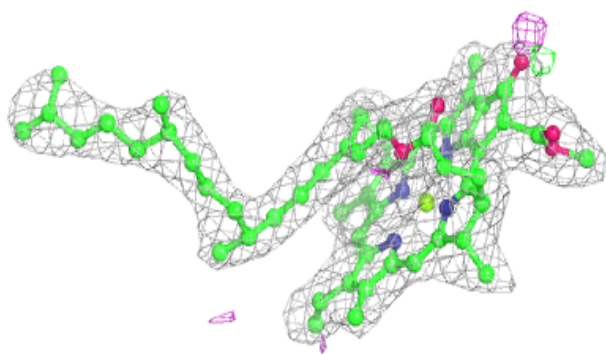
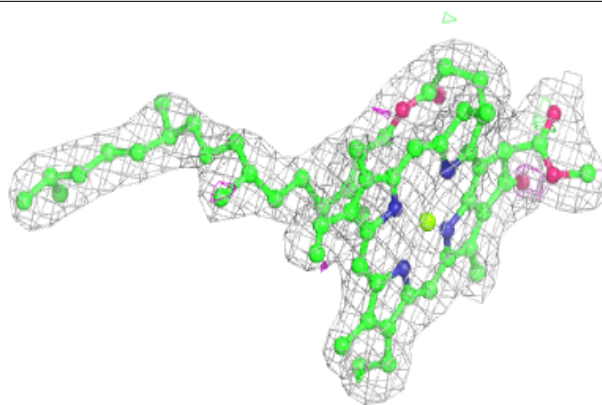
**Electron density around LHG L 102:**

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



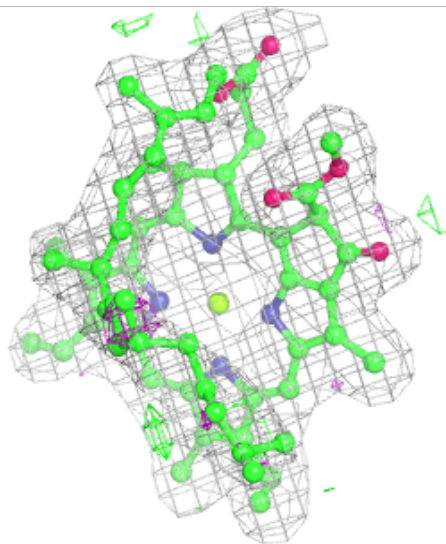
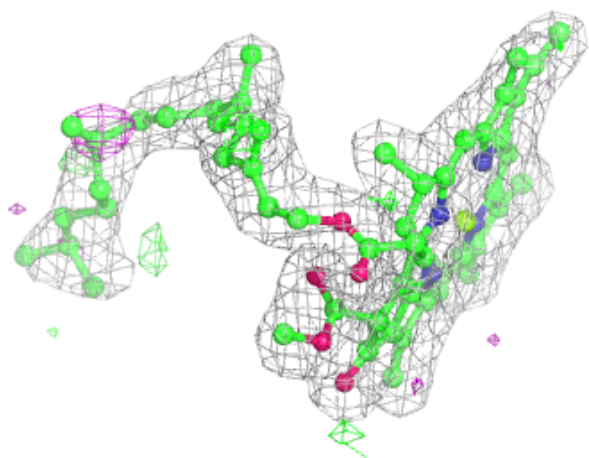
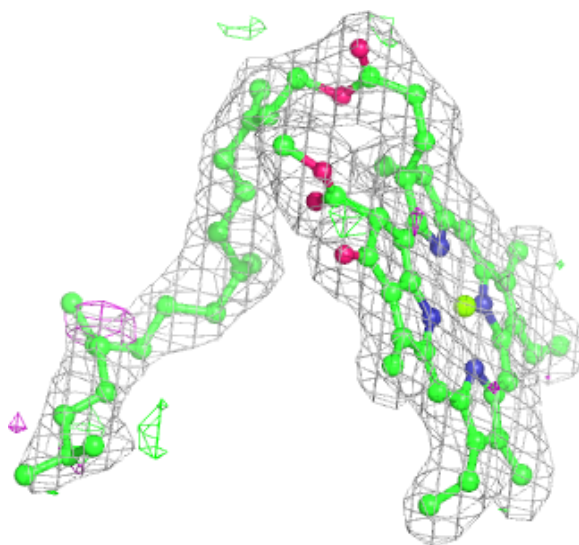
**Electron density around CLA C 506:**

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



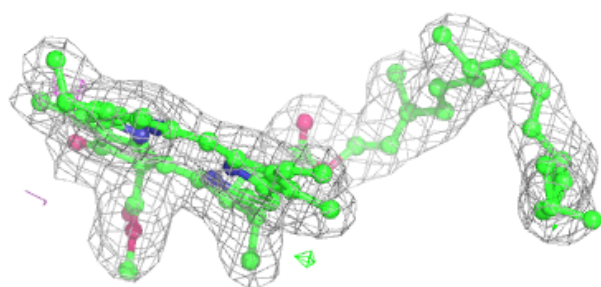
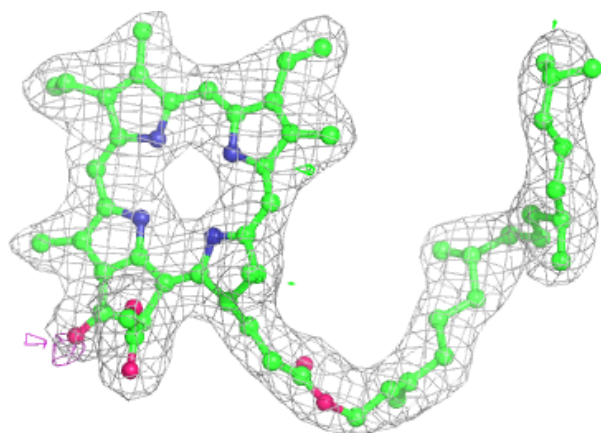
**Electron density around CLA b 615:**

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

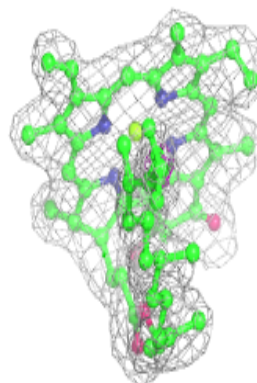
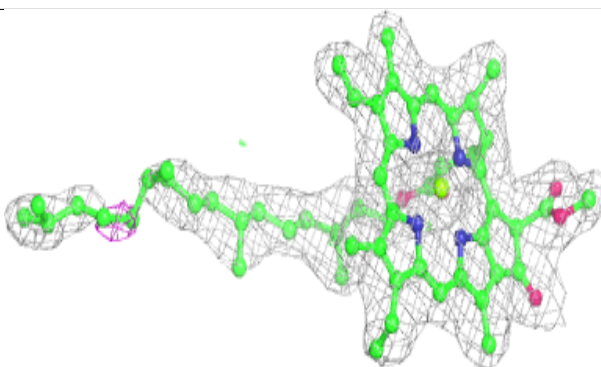
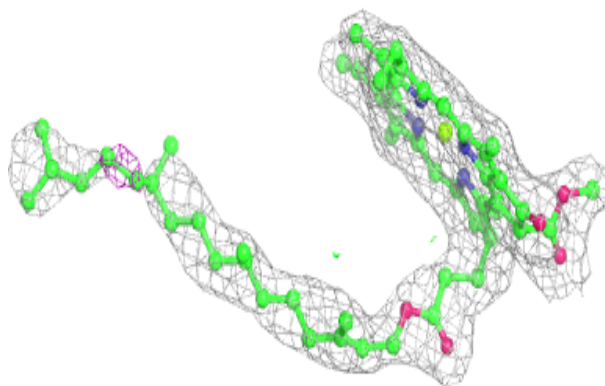


**Electron density around PHO a 414:**

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

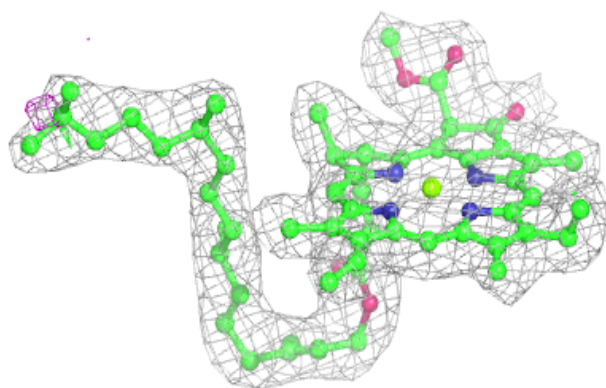
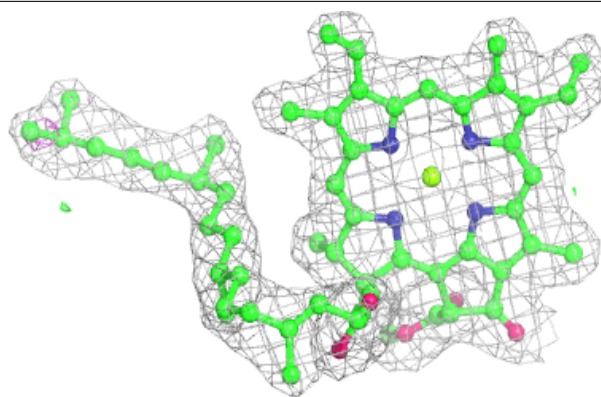
**Electron density around CLA c 505:**

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

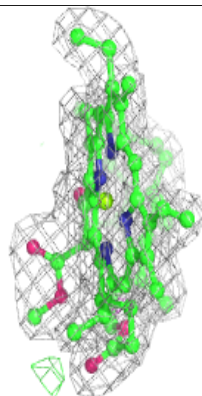
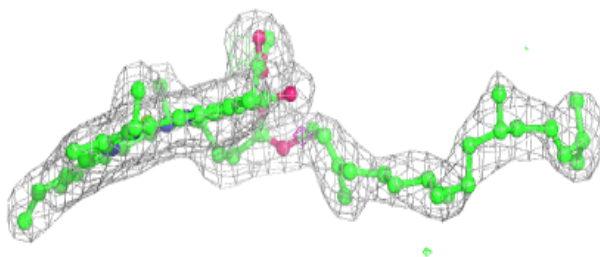
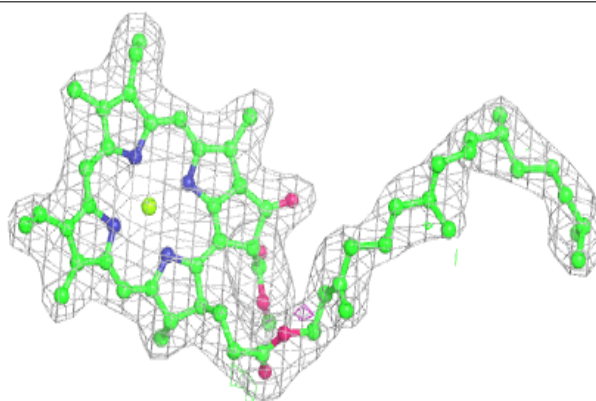


**Electron density around CLA A 412:**

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

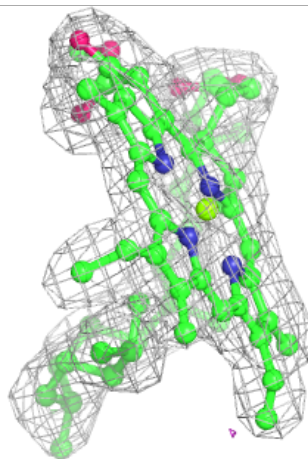
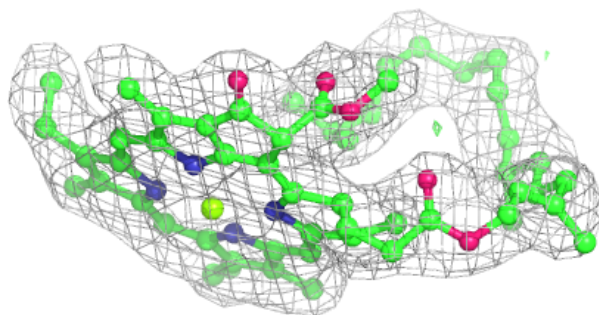
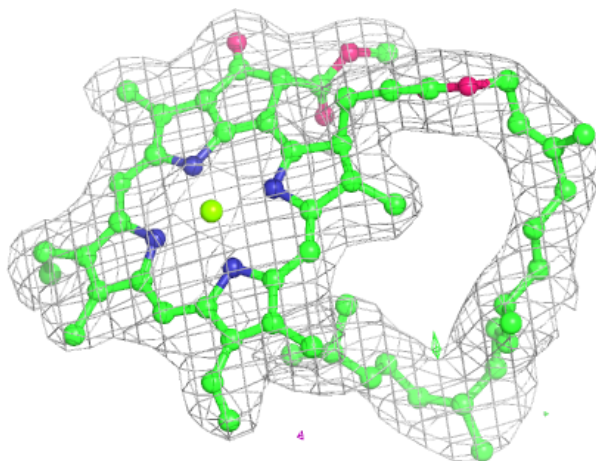
**Electron density around CLA B 601:**

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



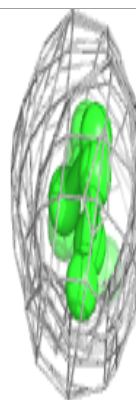
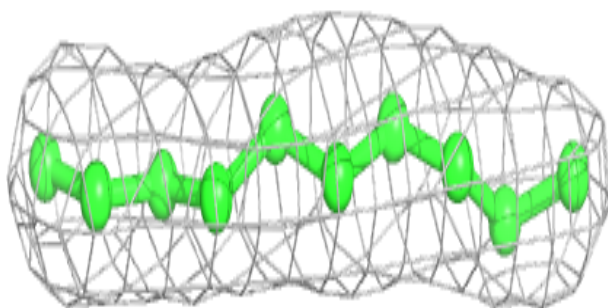
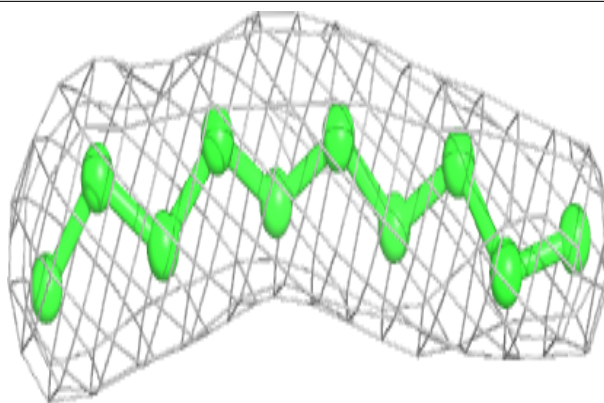
**Electron density around CLA b 617:**

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

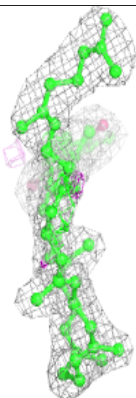
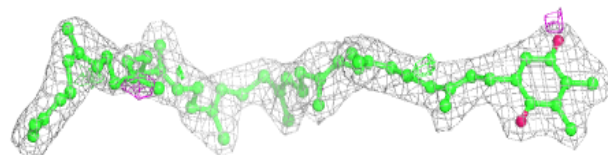
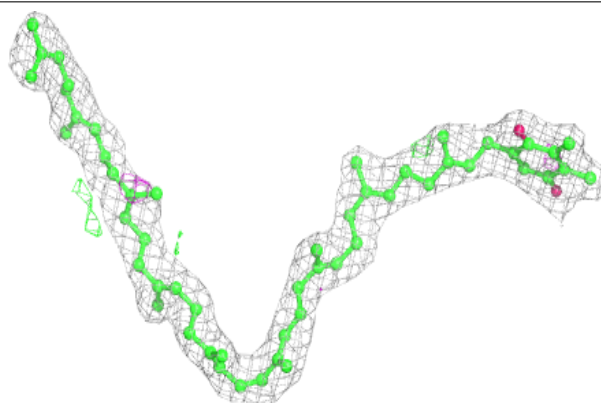


**Electron density around LFA M 101:**

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

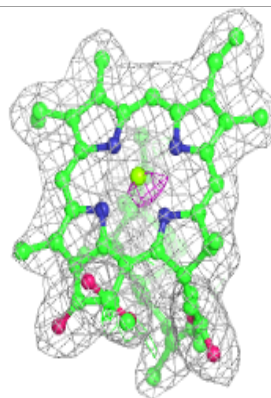
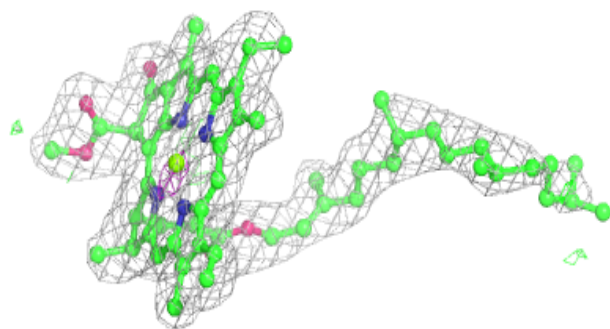
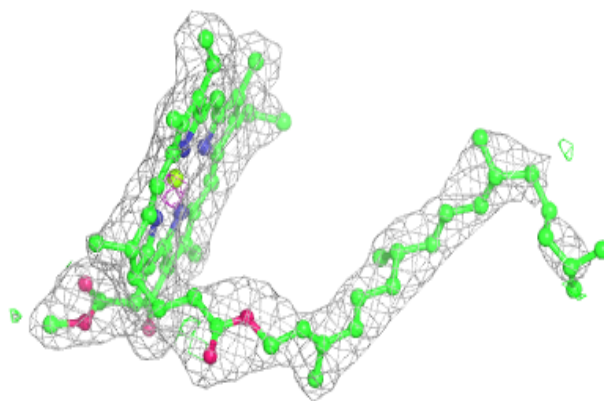
**Electron density around PL9 d 405:**

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



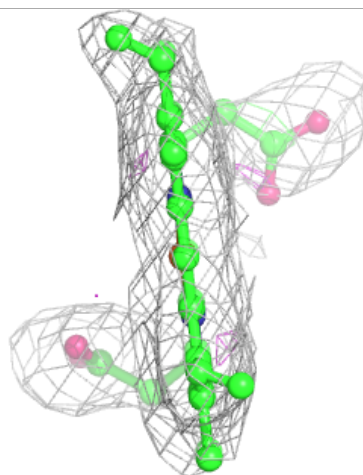
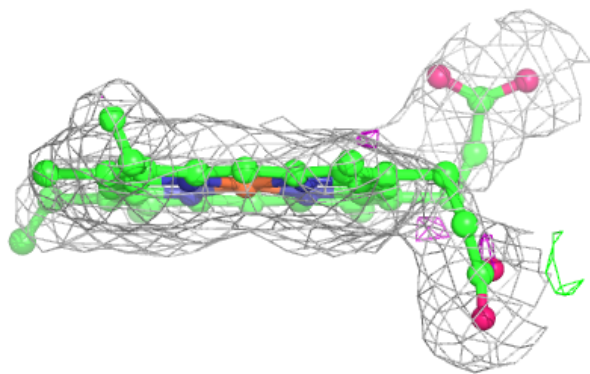
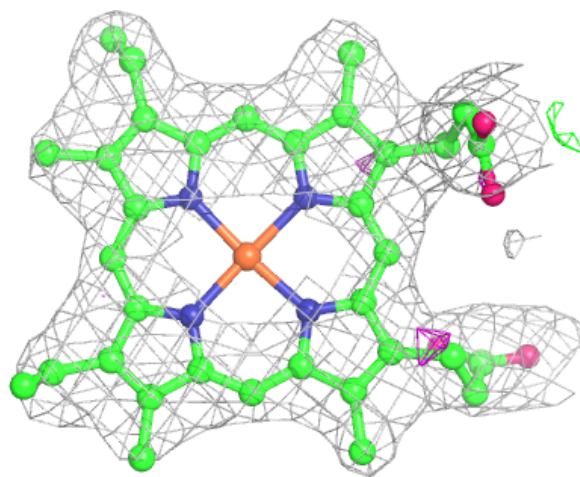
**Electron density around CLA c 509:**

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



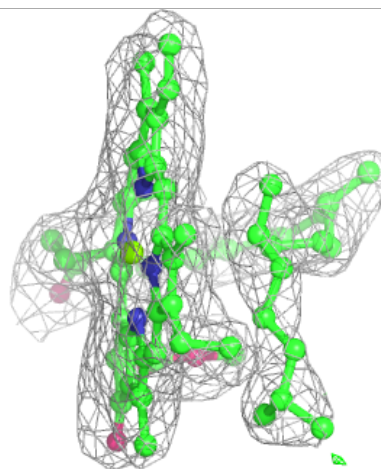
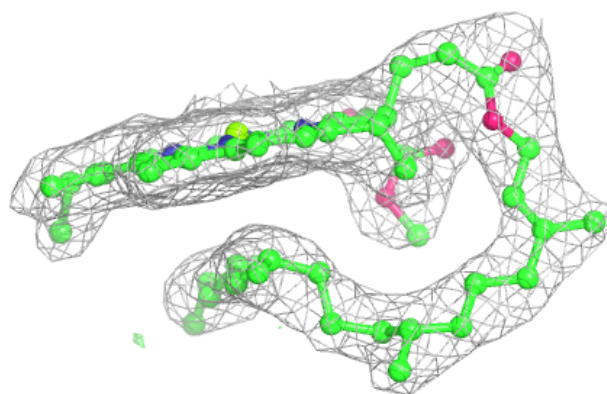
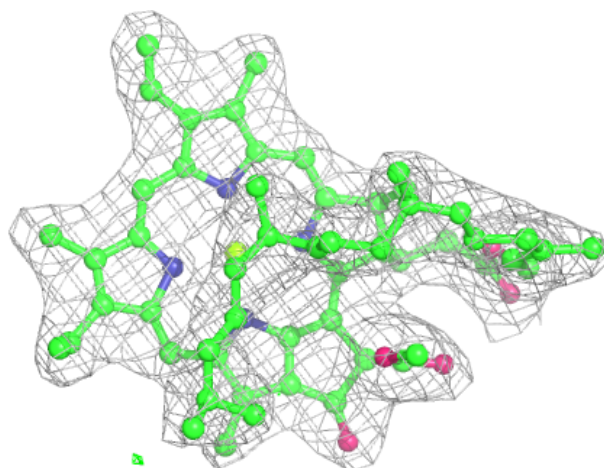
**Electron density around HEM e 102:**

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



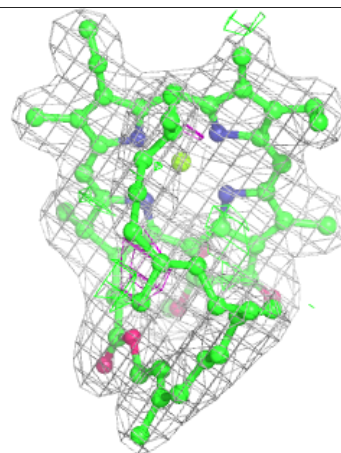
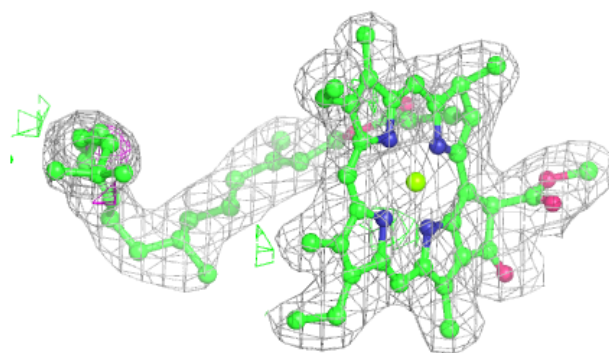
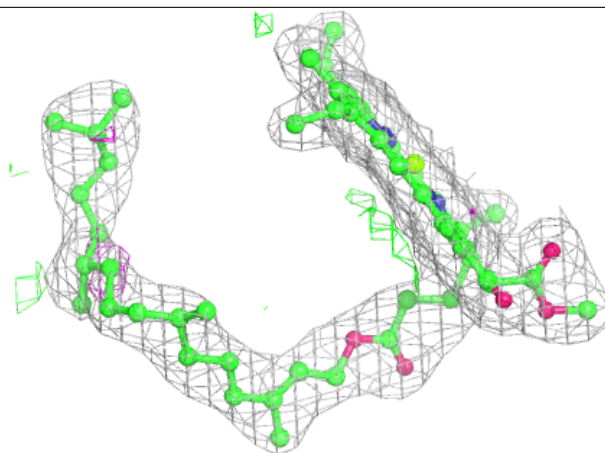
**Electron density around CLA c 511:**

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



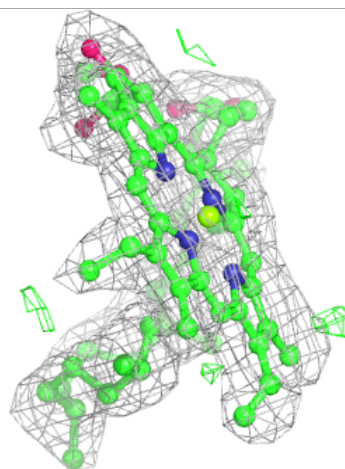
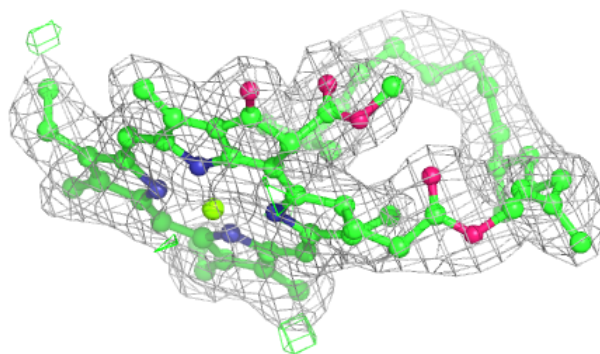
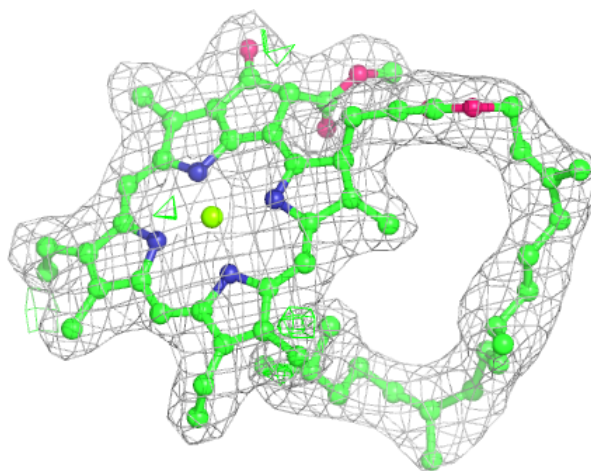
**Electron density around CLA b 613:**

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



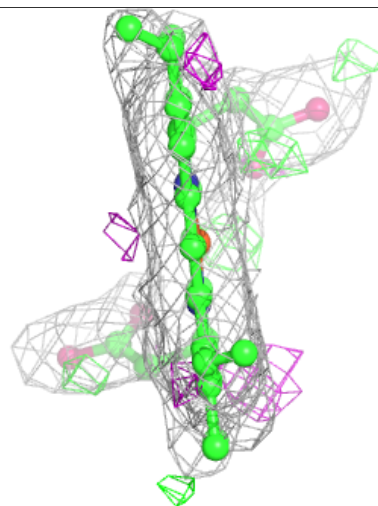
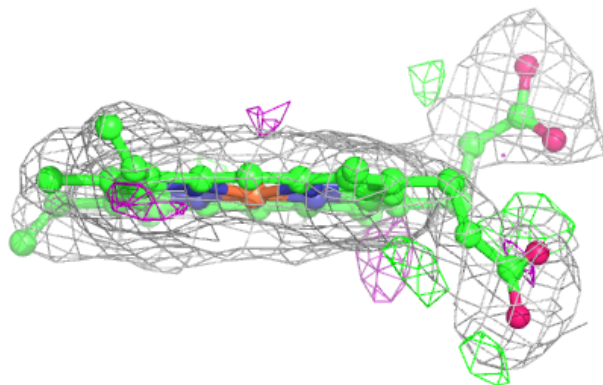
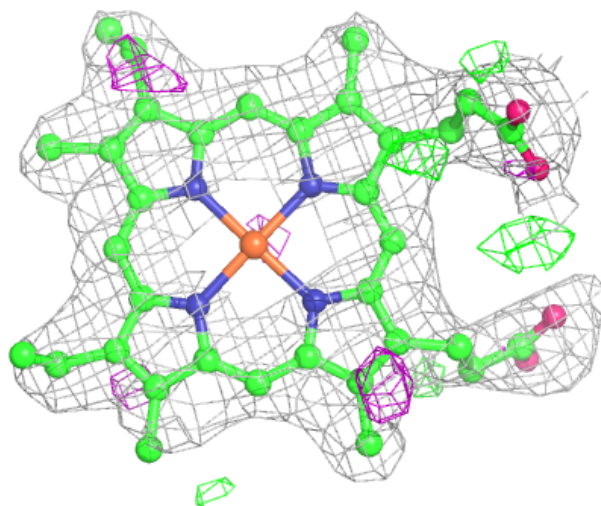
**Electron density around CLA B 614:**

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



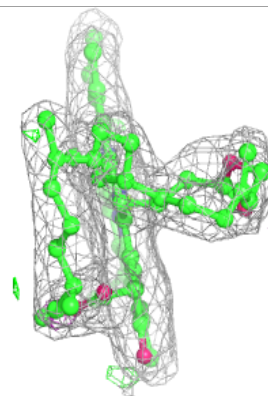
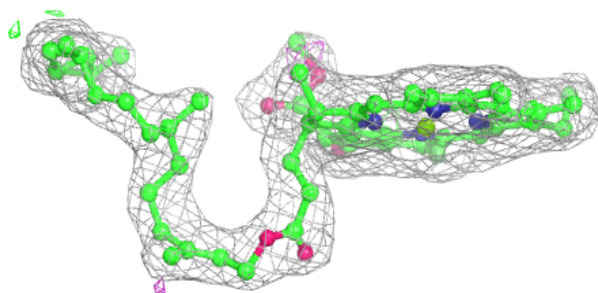
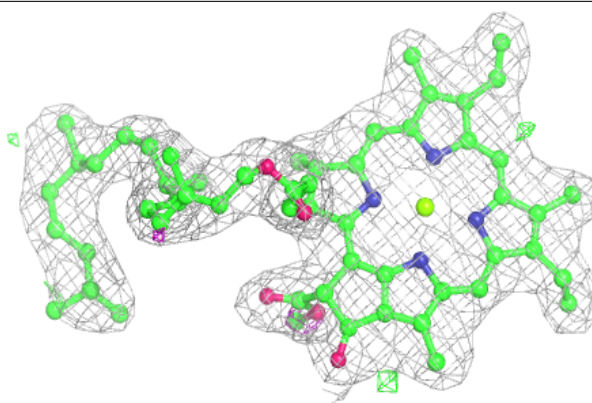
**Electron density around HEM E 102:**

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

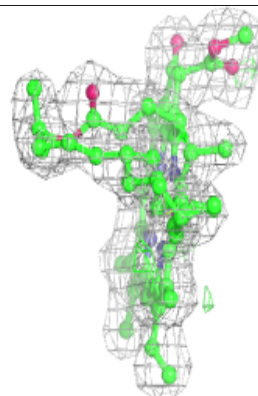
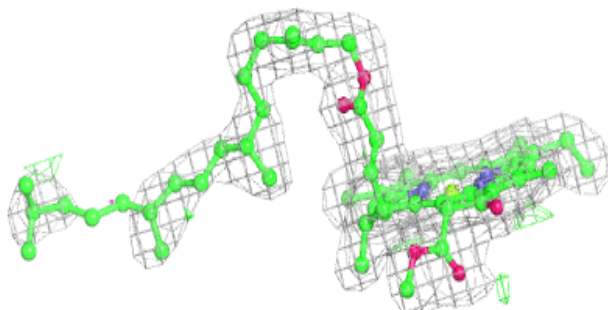
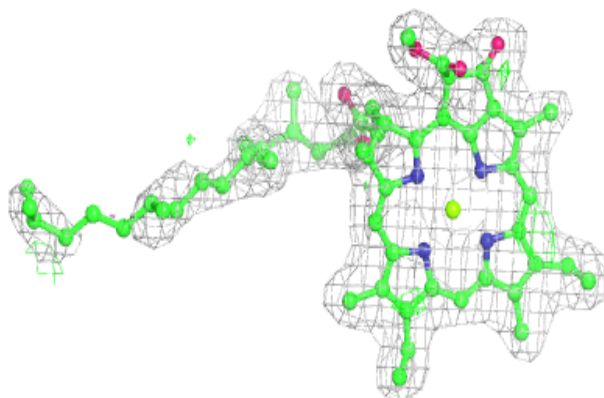


**Electron density around CLA b 614:**

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

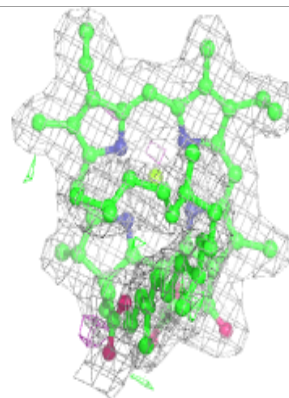
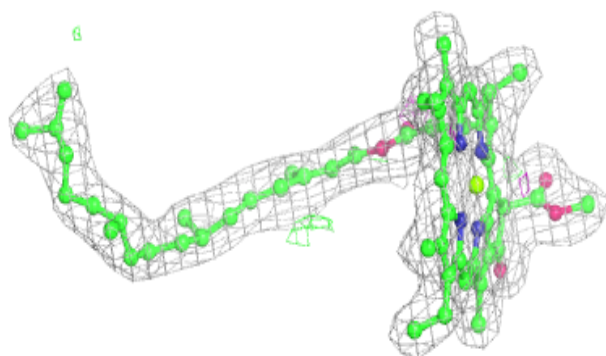
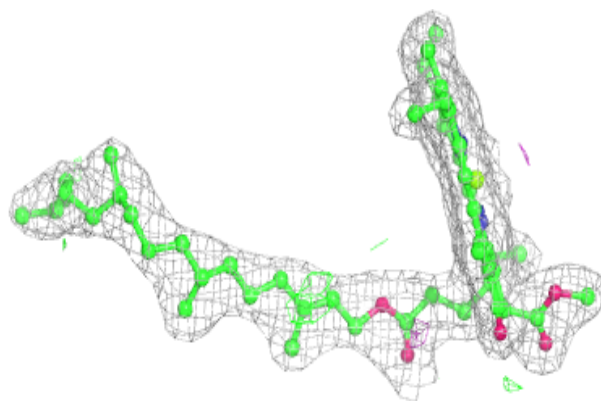
**Electron density around CLA A 404:**

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

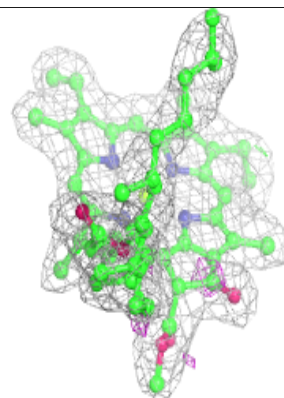
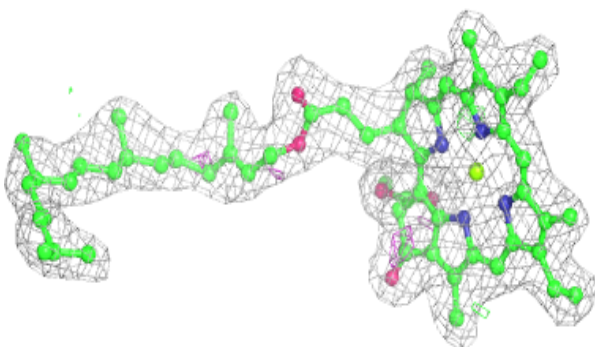
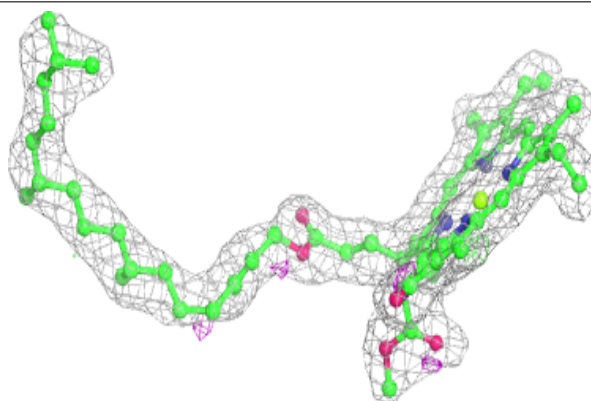


**Electron density around CLA B 604:**

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

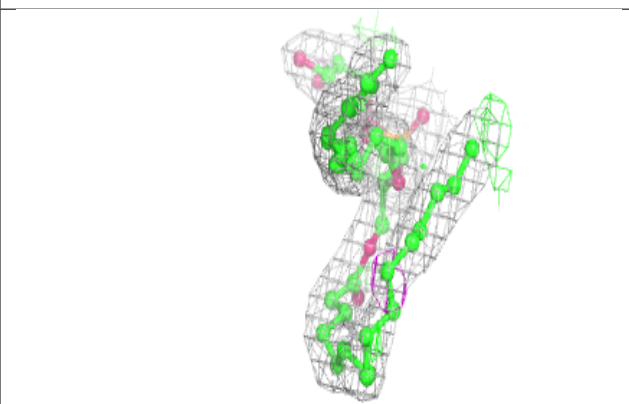
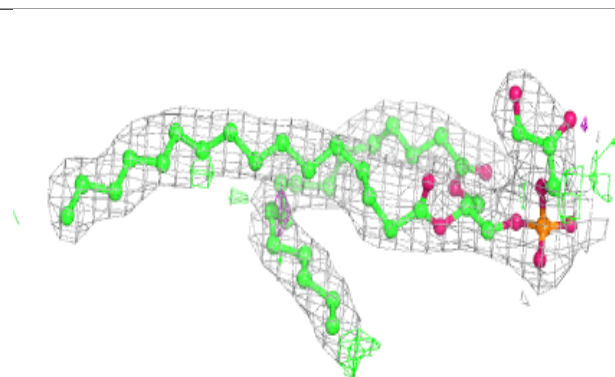
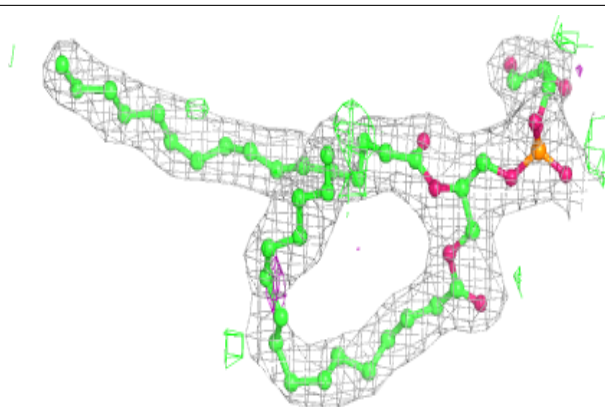
**Electron density around CLA d 402:**

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

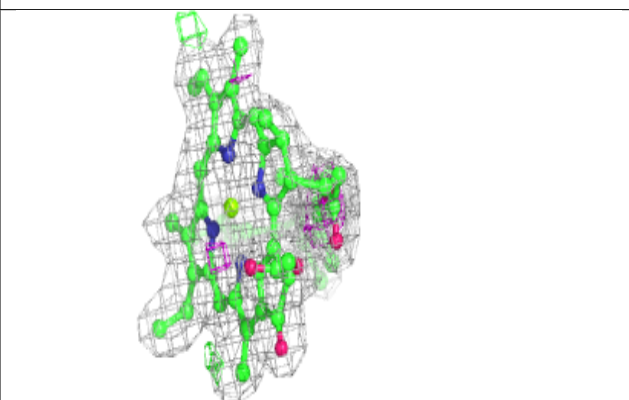
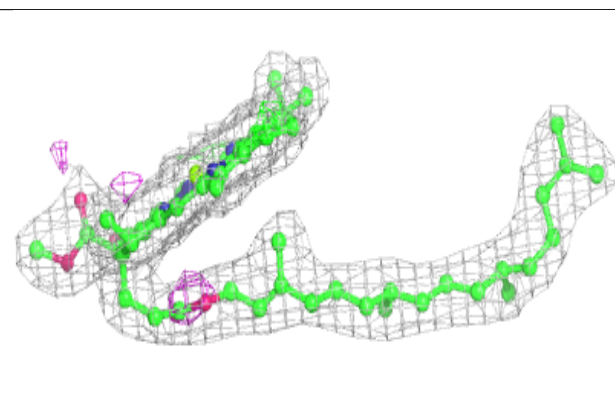
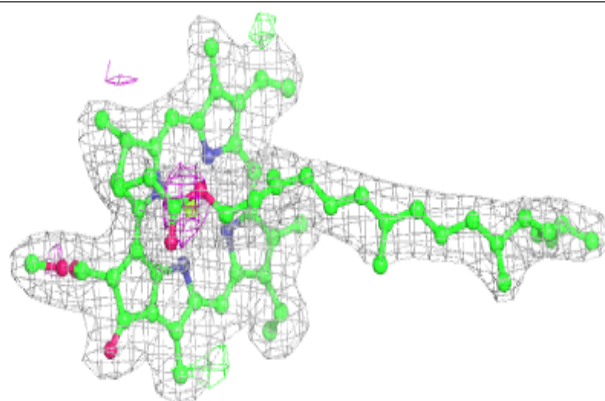


**Electron density around LHG b 628:**

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

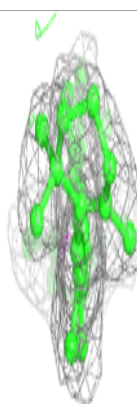
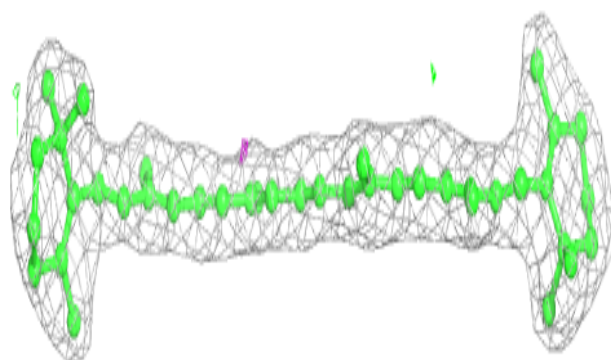
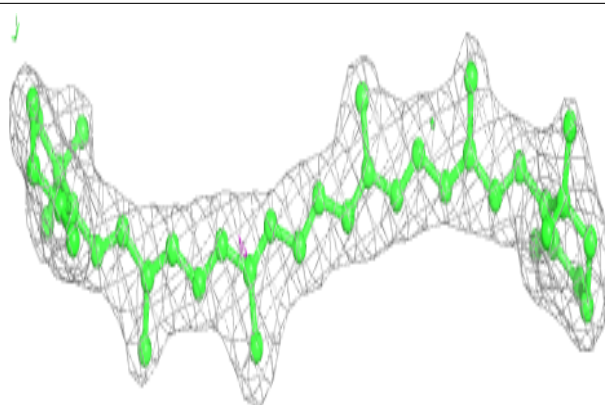
**Electron density around CLA B 607:**

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

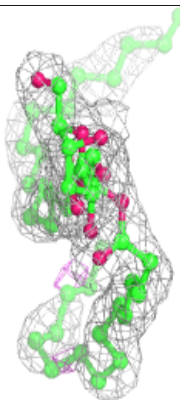
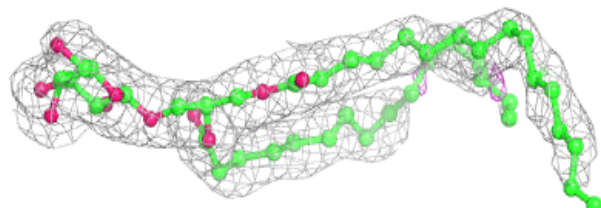
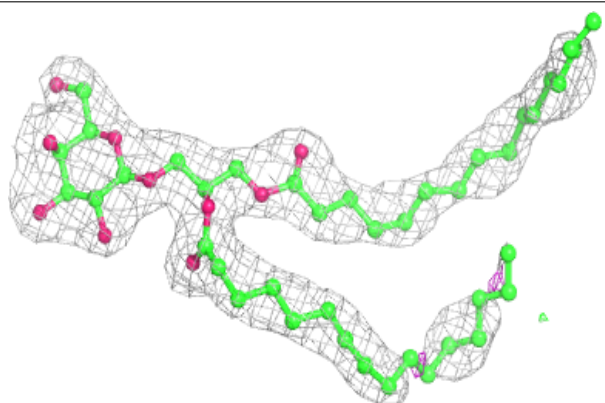


**Electron density around BCR A 407:**

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

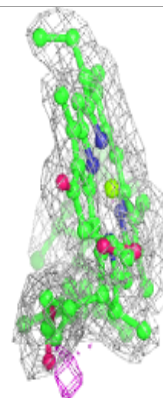
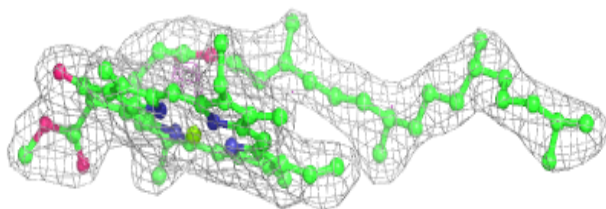
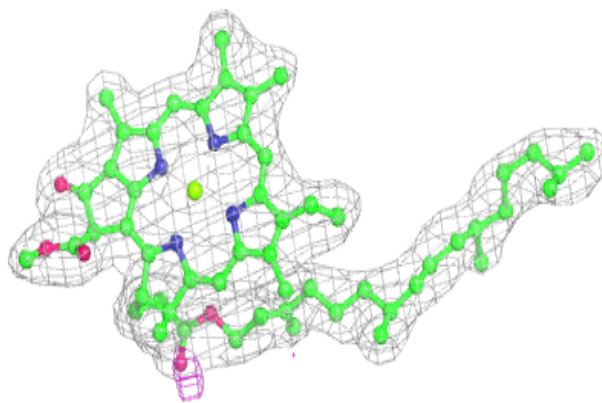
**Electron density around LMG D 409:**

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



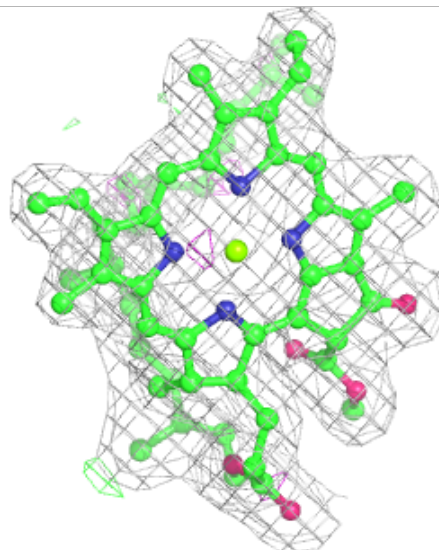
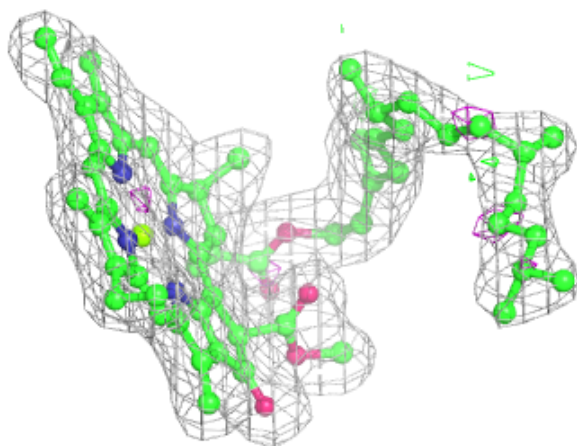
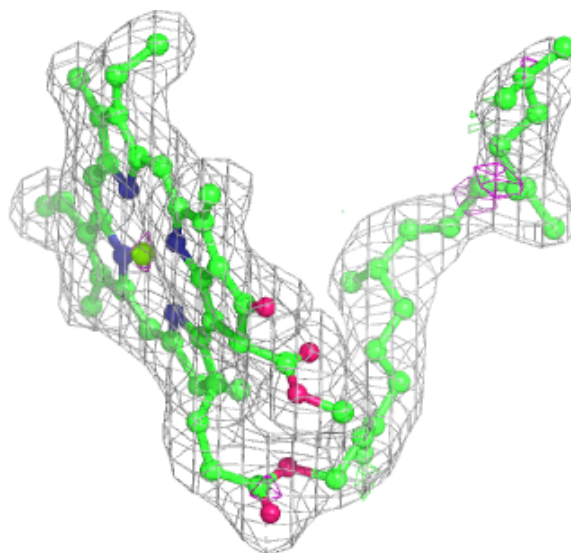
**Electron density around CLA C 502:**

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



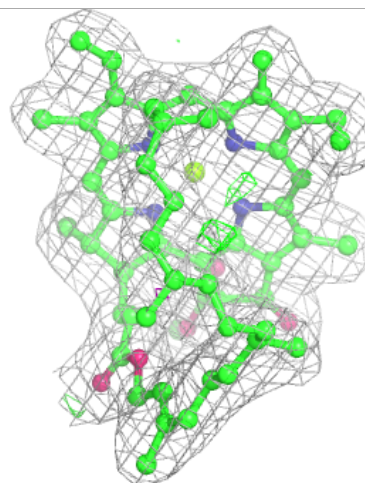
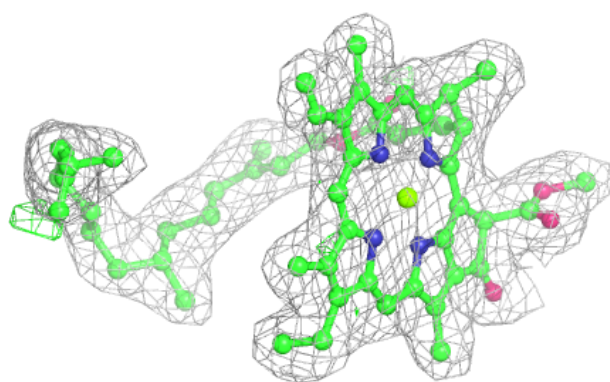
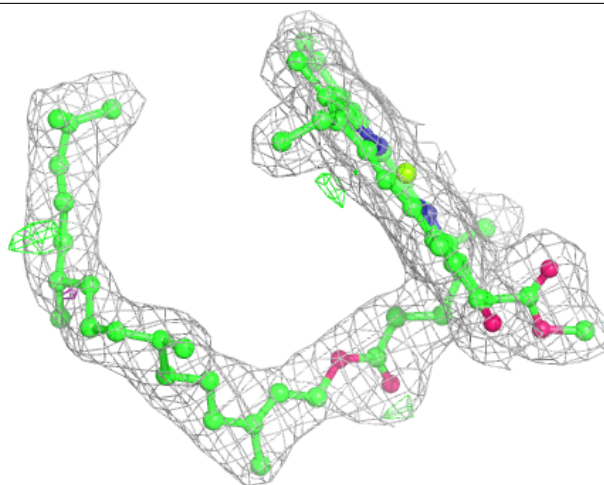
**Electron density around CLA B 612:**

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



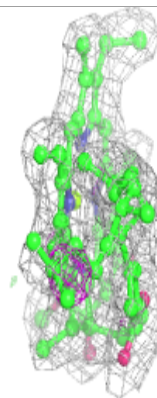
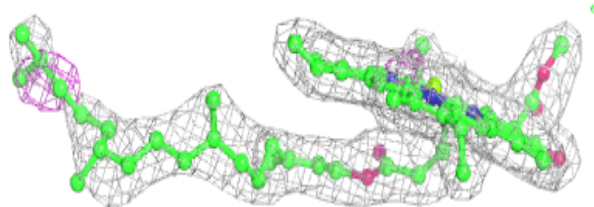
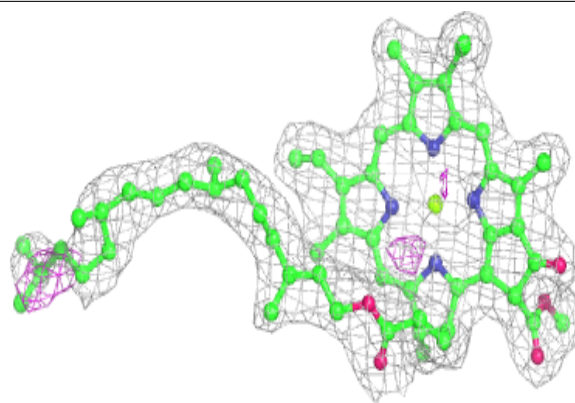
**Electron density around CLA B 610:**

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

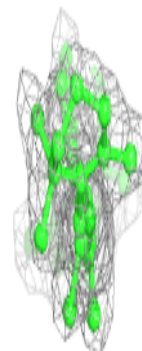
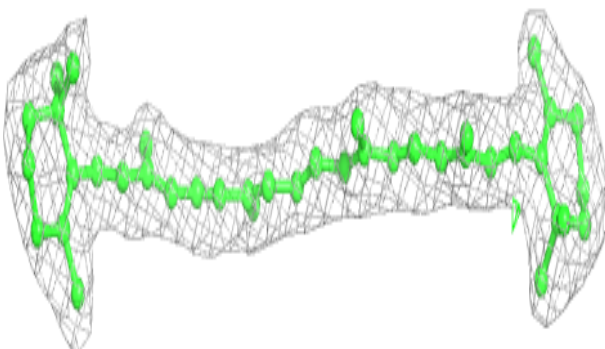
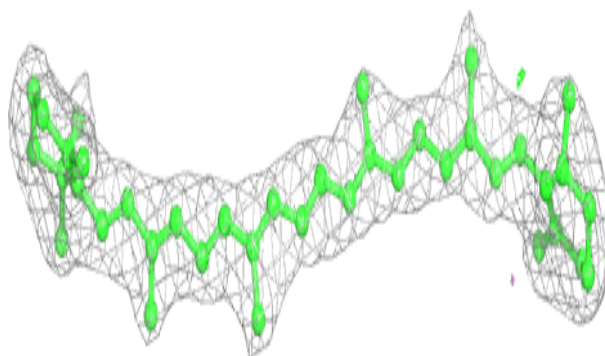


**Electron density around CLA B 602:**

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

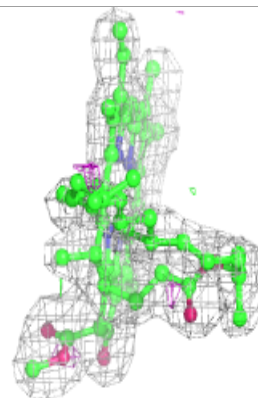
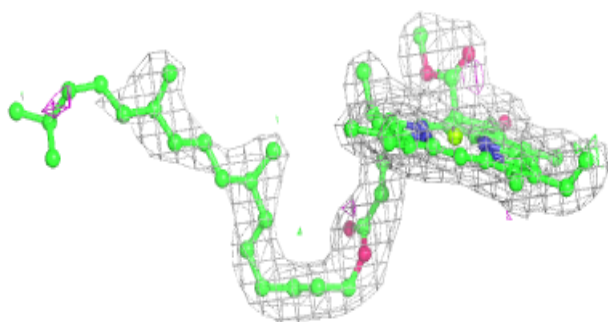
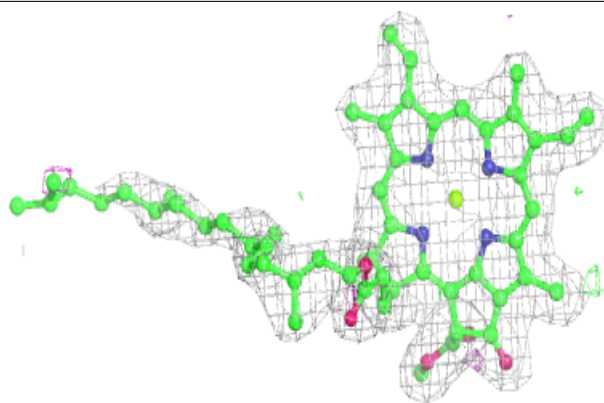
**Electron density around BCR a 408:**

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

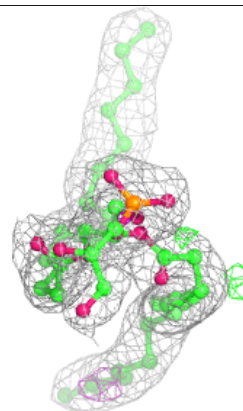
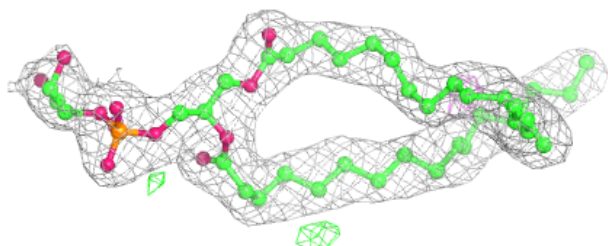
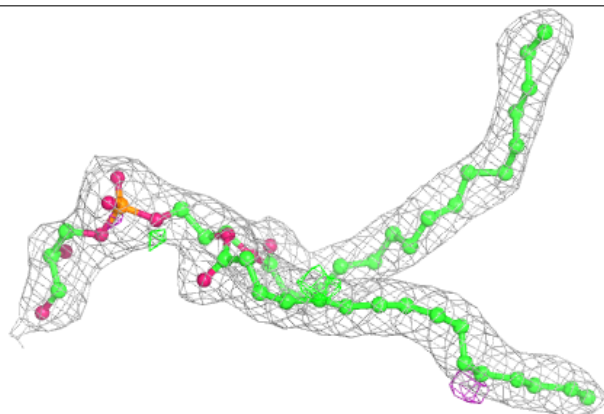


**Electron density around CLA d 401:**

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

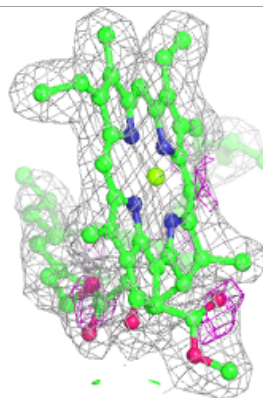
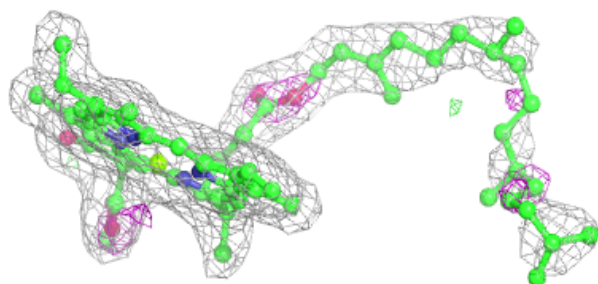
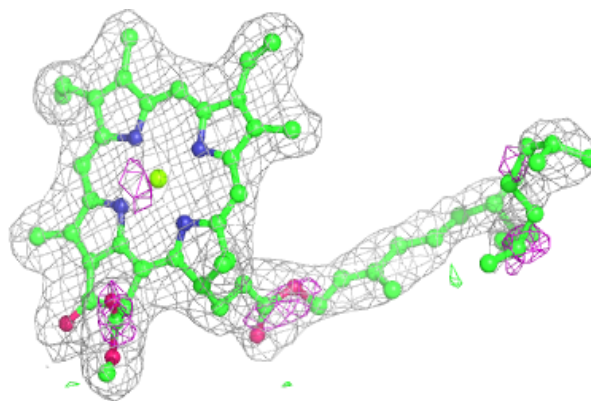
**Electron density around LHG D 407:**

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

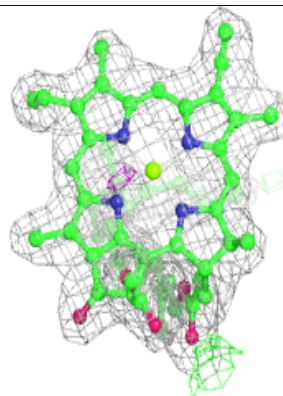
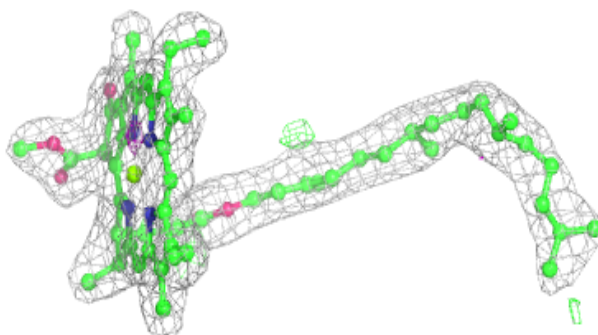
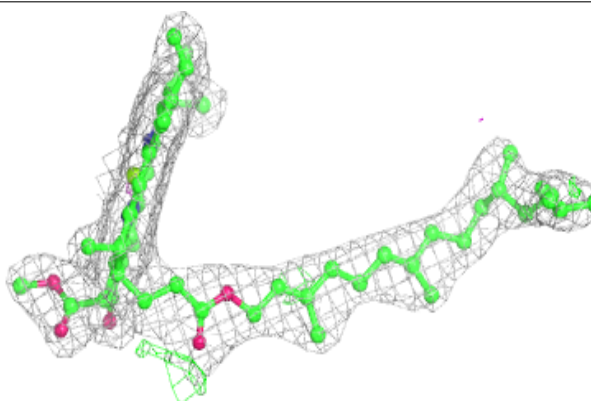


**Electron density around CLA a 407:**

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

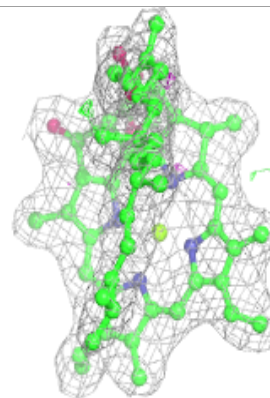
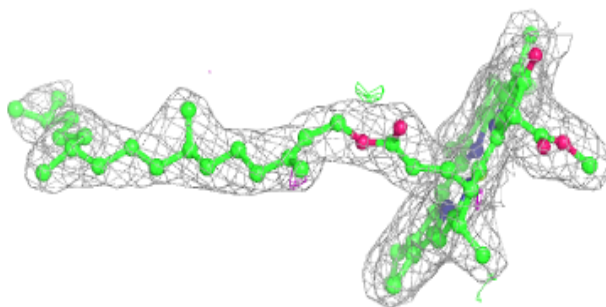
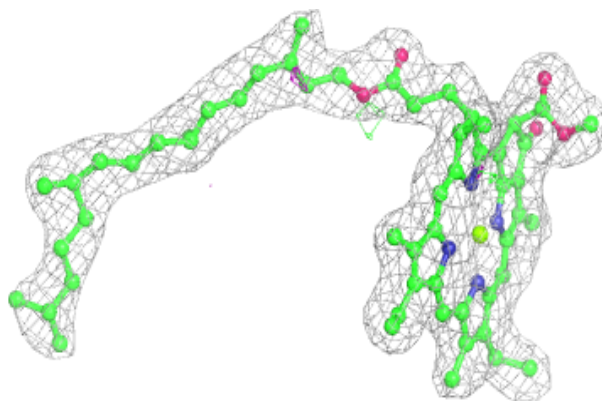
**Electron density around CLA b 607:**

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

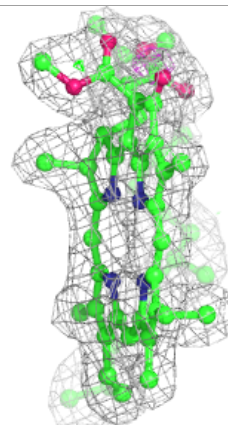
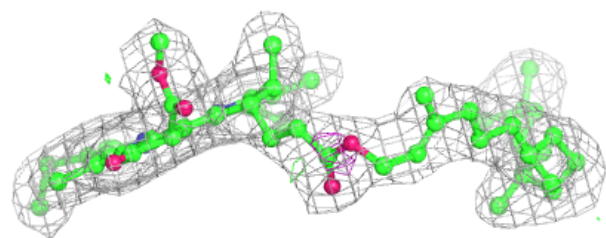
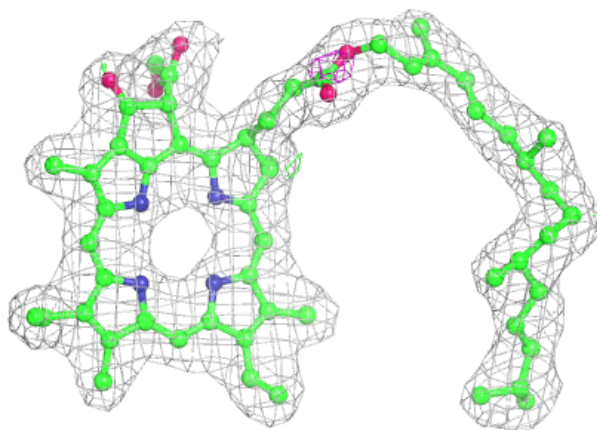


**Electron density around CLA B 608:**

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

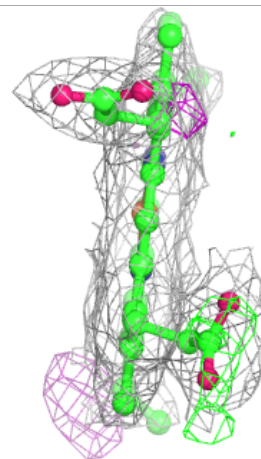
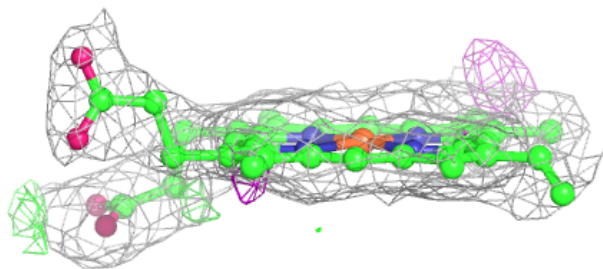
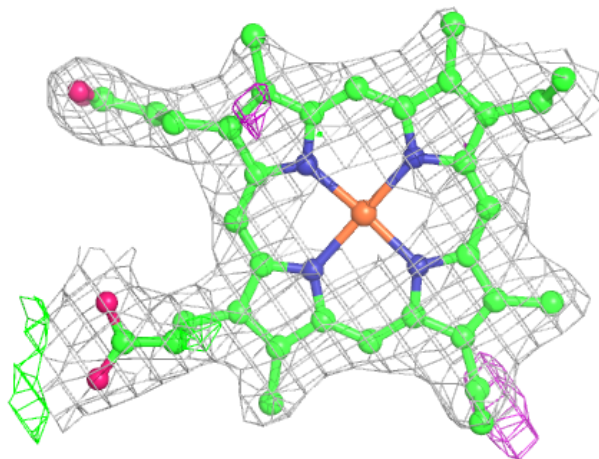
**Electron density around PHO D 401:**

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



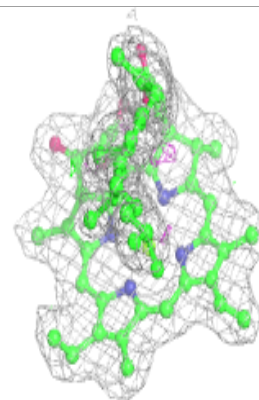
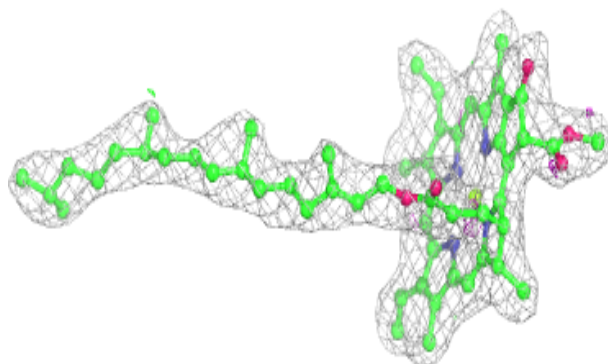
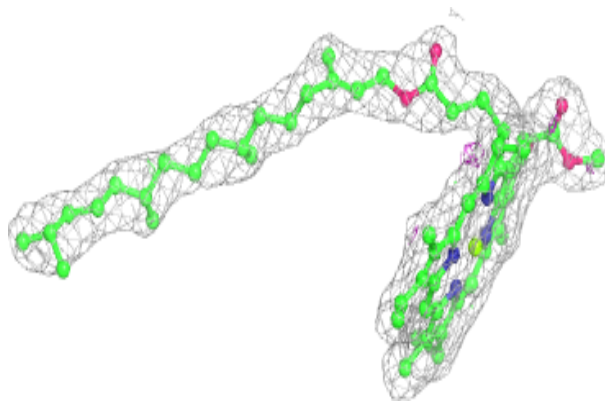
**Electron density around HEM V 201:**

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

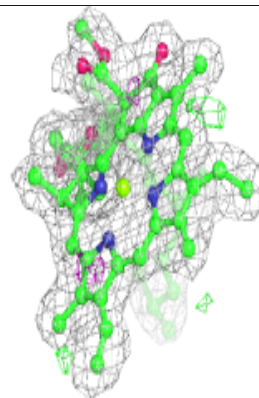
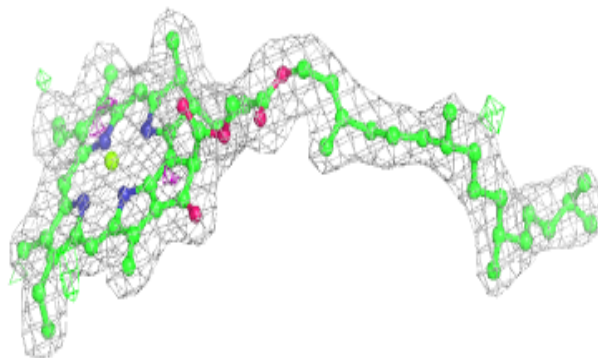
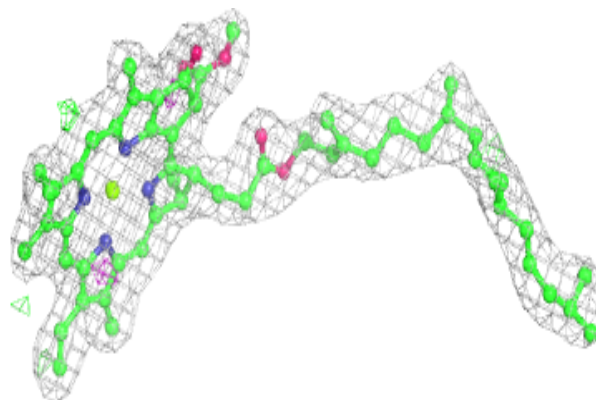


**Electron density around CLA B 606:**

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

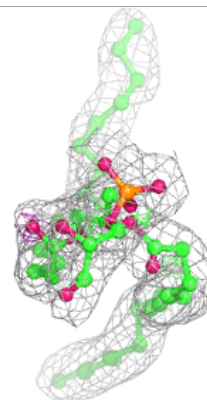
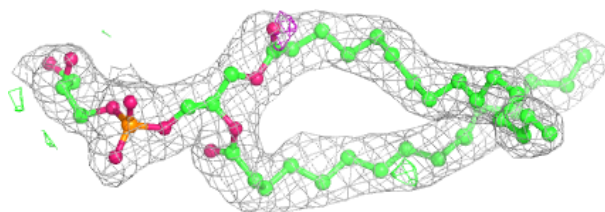
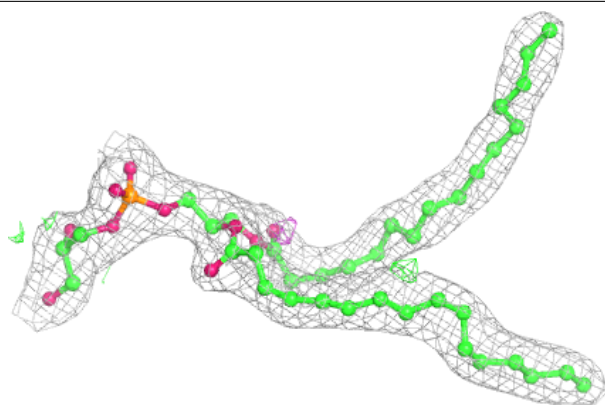
**Electron density around CLA A 403:**

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

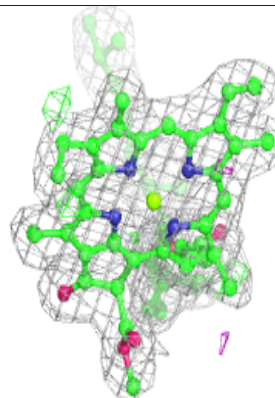
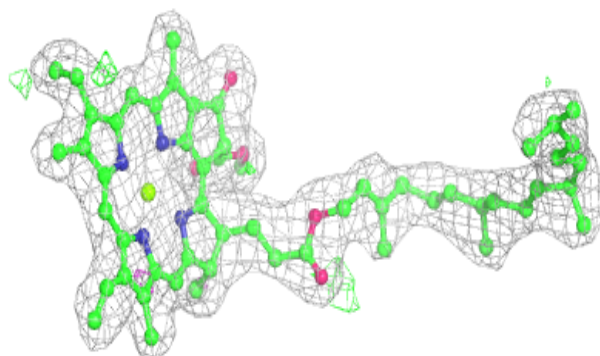
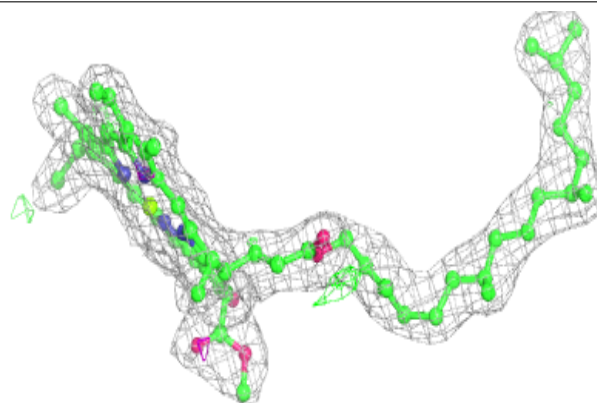


**Electron density around LHG d 406:**

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

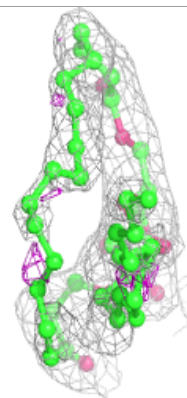
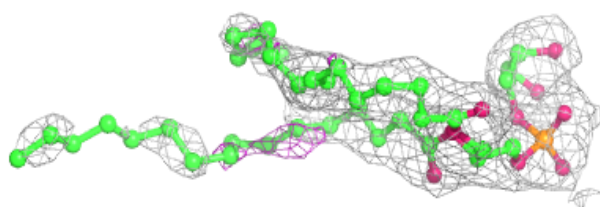
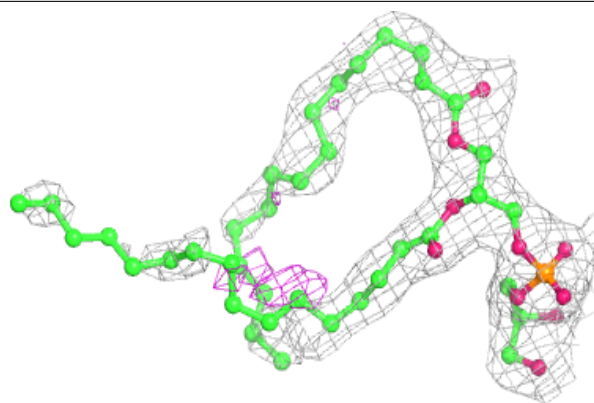
**Electron density around CLA D 402:**

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

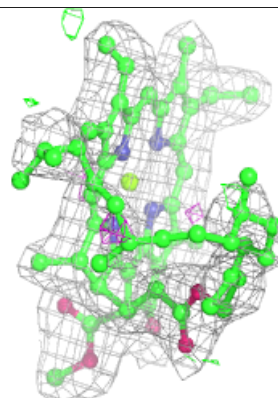
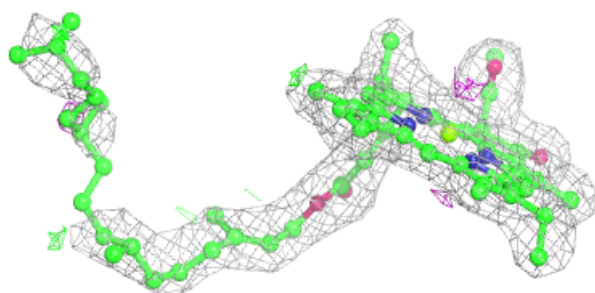
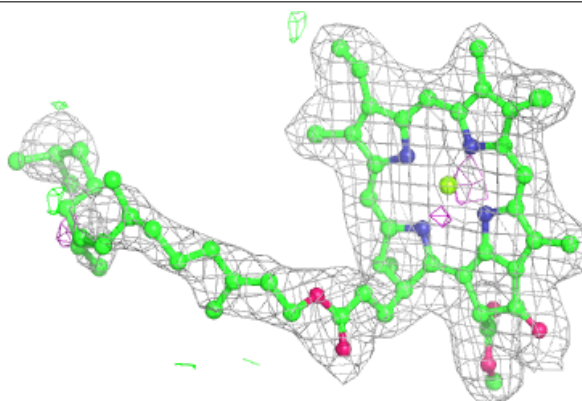


**Electron density around LHG d 407:**

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

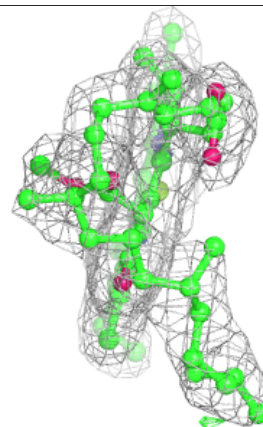
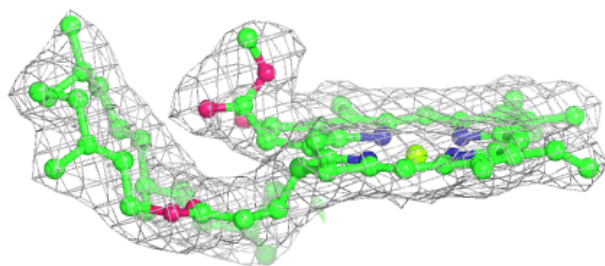
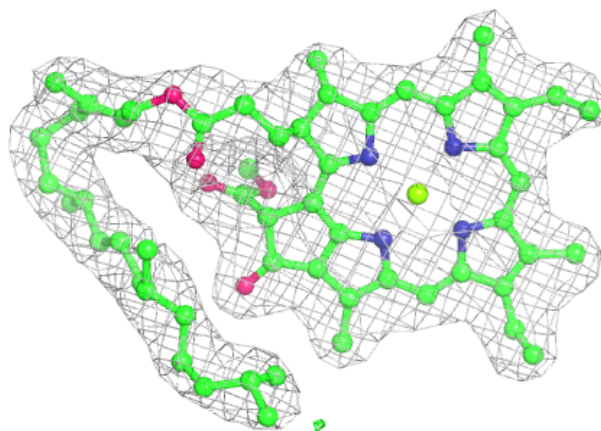
**Electron density around CLA A 406:**

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



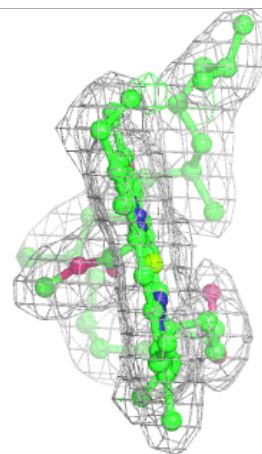
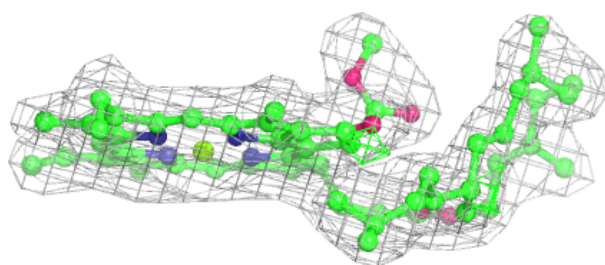
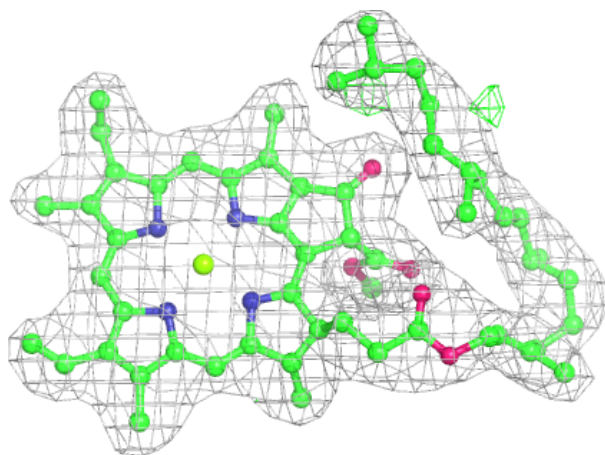
**Electron density around CLA b 612:**

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



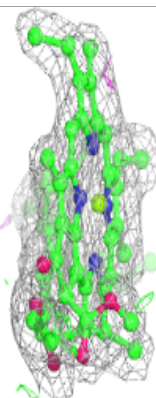
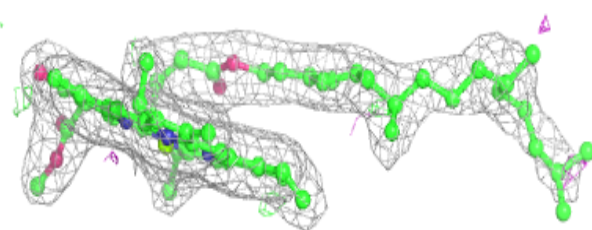
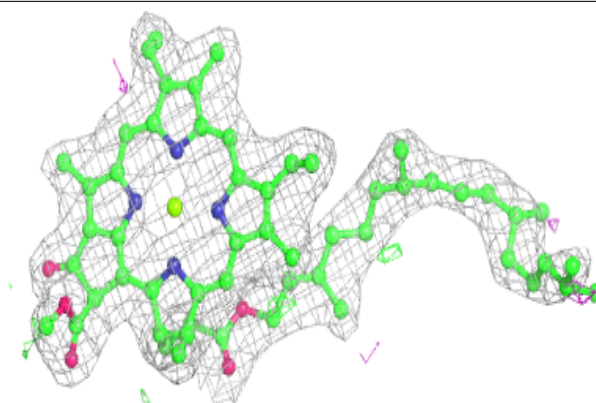
**Electron density around CLA B 609:**

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

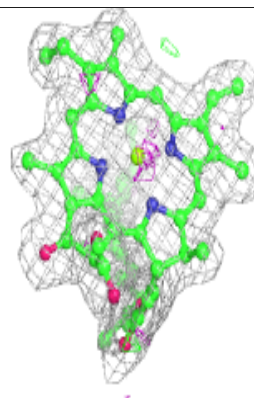
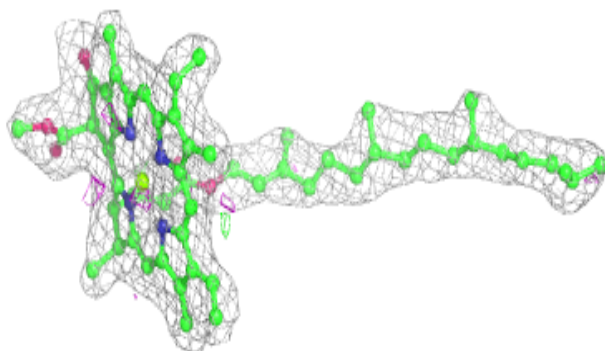
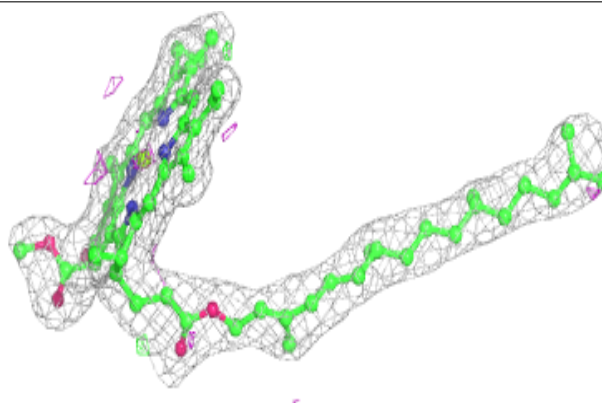


**Electron density around CLA b 605:**

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

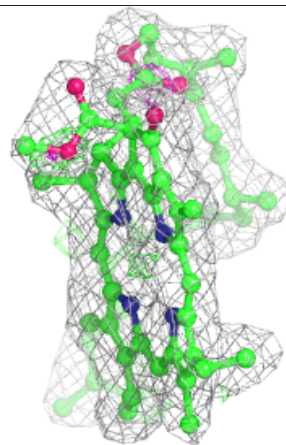
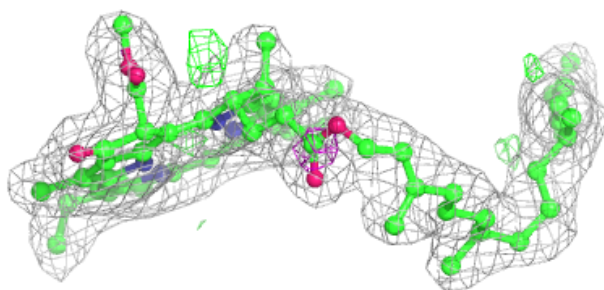
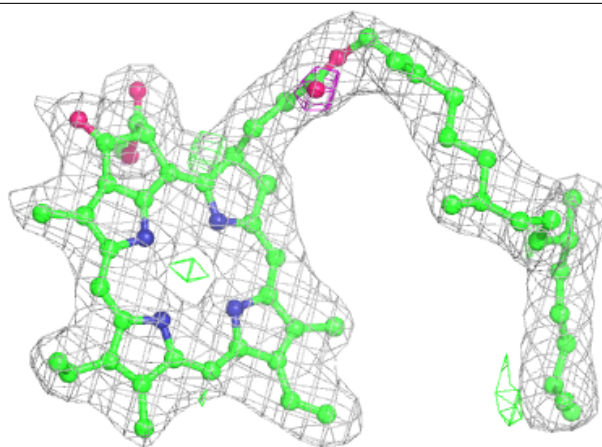
**Electron density around CLA b 609:**

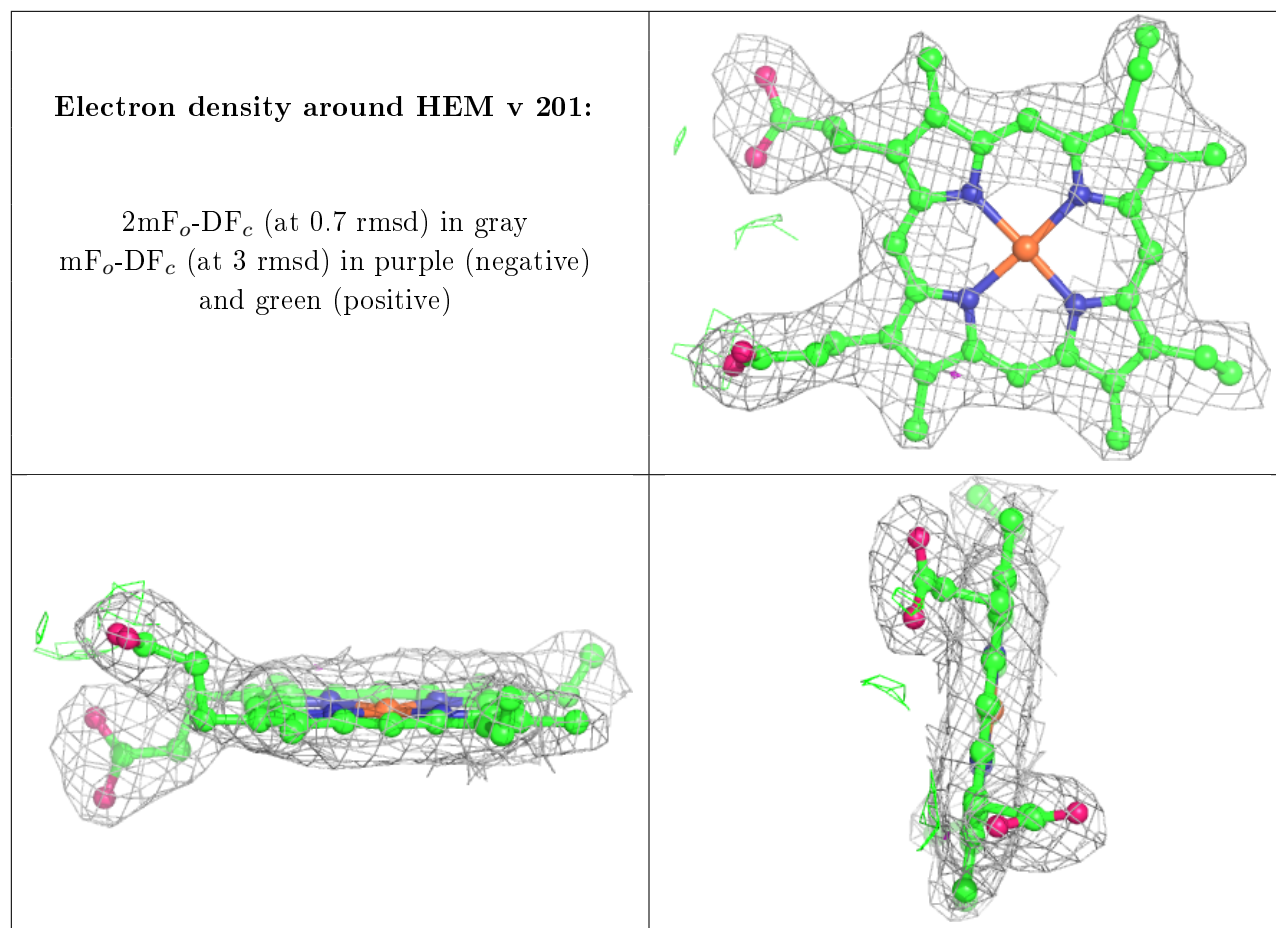
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO A 405:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.