



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 01:06 AM EDT

PDB ID : 4PBU  
Title : Serial Time-resolved crystallography of Photosystem II using a femtosecond X-ray laser The S1 state  
Authors : Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.A.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.  
Deposited on : 2014-04-13  
Resolution : 5.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467

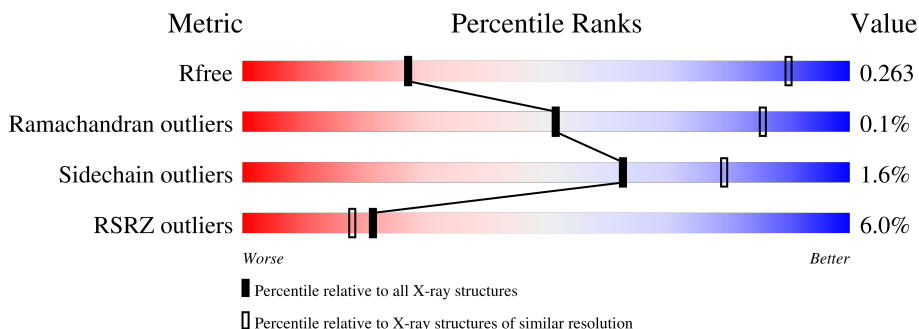
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 5.00 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	1140 (6.20-3.80)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RSRZ outliers	127900	1010 (6.22-3.72)

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

Mol	Chain	Length	Quality of chain
1	A	334	

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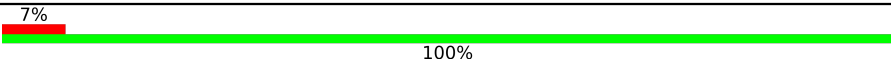
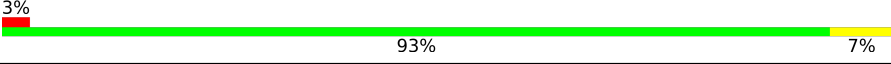
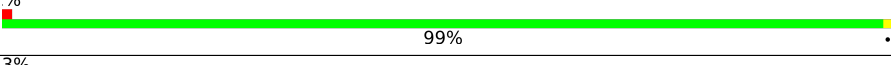
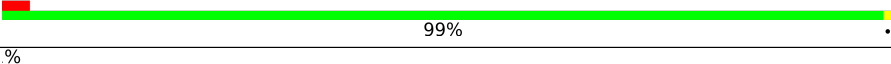
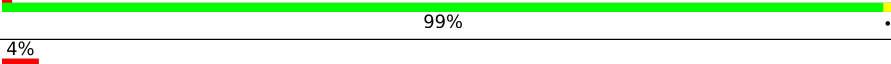
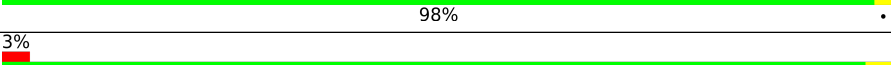
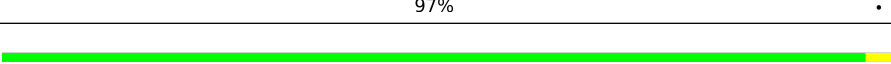
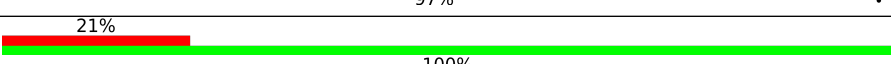
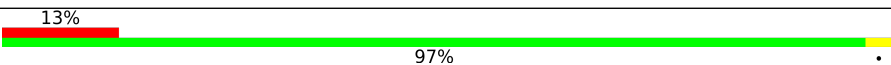
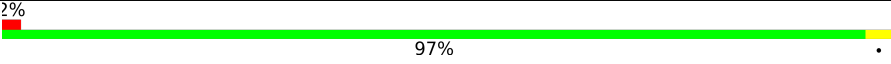
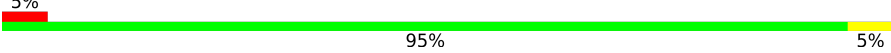

Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

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Mol	Chain	Length	Quality of chain
1	a	334	
2	B	504	
2	b	504	
3	C	455	
3	c	455	
4	D	342	
4	d	342	
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	243	
13	o	243	

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Mol	Chain	Length	Quality of chain
14	T	30	
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	29	
17	y	29	
18	X	39	
18	x	39	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	A	603	-	-	-	X
24	CLA	A	606	X	-	-	-
24	CLA	A	607	-	-	-	X
24	CLA	B	602	X	-	-	X
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	-	-	-	X
24	CLA	B	608	X	-	-	X
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	X
24	CLA	B	617	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	X
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	X
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	512	X	-	-	X
24	CLA	C	513	-	-	-	X
24	CLA	D	402	X	-	-	-
24	CLA	D	403	-	-	-	X
24	CLA	a	406	X	-	-	-
24	CLA	a	407	-	-	-	X
24	CLA	a	408	-	-	-	X
24	CLA	b	602	X	-	-	X
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	X
24	CLA	b	608	X	-	-	X
24	CLA	b	611	X	-	-	-
24	CLA	b	612	-	-	-	X
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	X
24	CLA	c	902	X	-	-	X
24	CLA	c	903	-	-	-	X
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	913	X	-	-	X
24	CLA	c	914	-	-	-	X
24	CLA	d	403	X	-	-	-
25	PHO	A	608	-	-	-	X
26	BCR	A	610	-	-	-	X
26	BCR	B	620	-	-	-	X
26	BCR	C	514	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	BCR	D	404	-	-	-	X
26	BCR	H	101	-	-	-	X
26	BCR	K	101	-	X	-	-
26	BCR	T	101	-	-	-	X
26	BCR	T	102	-	-	-	X
26	BCR	Y	101	-	-	-	X
26	BCR	a	409	-	-	-	X
26	BCR	b	618	-	-	-	X
26	BCR	b	619	-	-	-	X
26	BCR	c	915	-	-	-	X
26	BCR	c	918	-	-	-	X
26	BCR	f	101	-	X	-	X
26	BCR	h	101	-	-	-	X
26	BCR	k	101	-	-	-	X
26	BCR	k	102	-	X	-	X
27	PL9	A	611	-	-	-	X
27	PL9	D	405	-	-	-	X
27	PL9	a	410	-	-	-	X
27	PL9	d	405	-	-	-	X
28	SQD	A	612	-	-	-	X
28	SQD	A	613	-	-	-	X
28	SQD	a	411	-	-	-	X
28	SQD	d	407	-	-	-	X
28	SQD	l	101	-	-	-	X
29	LHG	A	615	-	-	-	X
29	LHG	D	408	-	-	-	X
29	LHG	a	413	-	-	-	X
30	CA	B	601	-	-	-	X
30	CA	F	102	-	-	-	X
30	CA	b	601	-	-	-	X
30	CA	c	901	-	-	-	X
31	DGD	C	517	-	-	-	X
31	DGD	D	406	-	-	-	X
31	DGD	d	406	-	-	-	X

## 2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 48924 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			662	432	107	123				
5	e	81	Total	C	N	O		0	0	0
			662	432	107	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	40	Total	C	N	O	S	0	0	0
			288	192	44	49	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

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

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

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

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

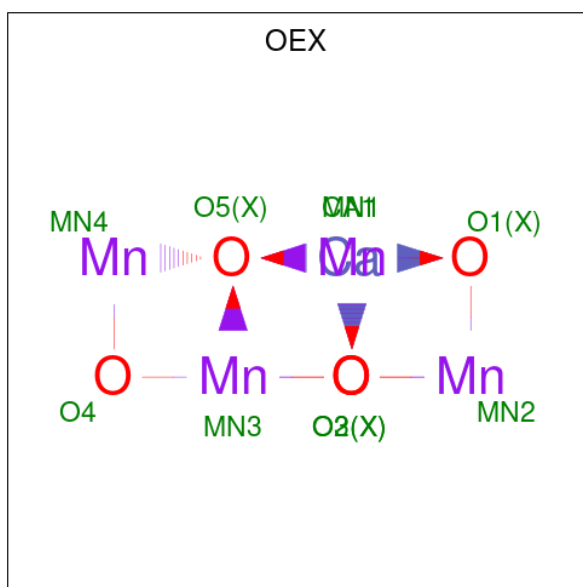
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	0	0
			287	191	46	50			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

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

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

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

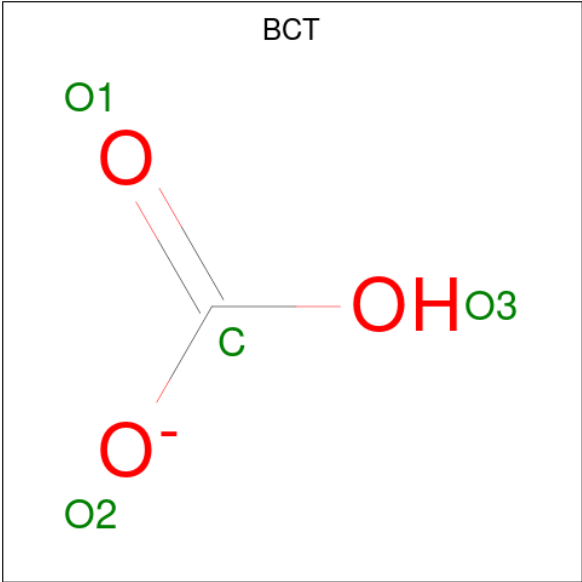
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

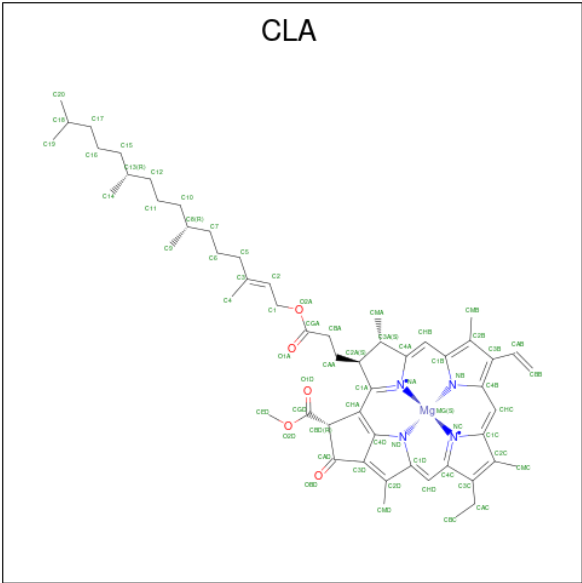
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	V	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

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

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

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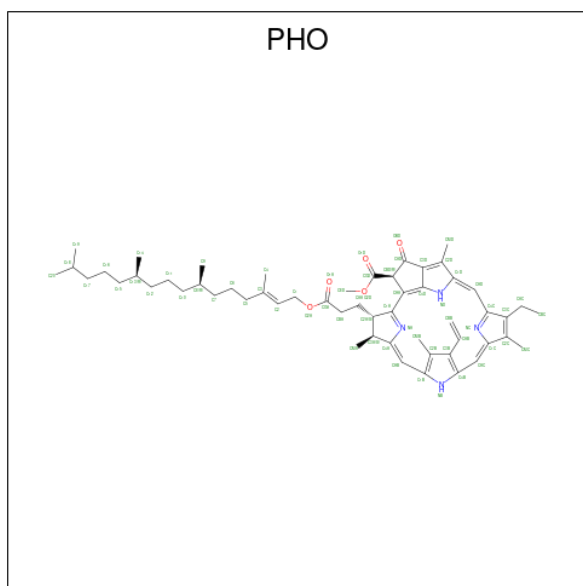
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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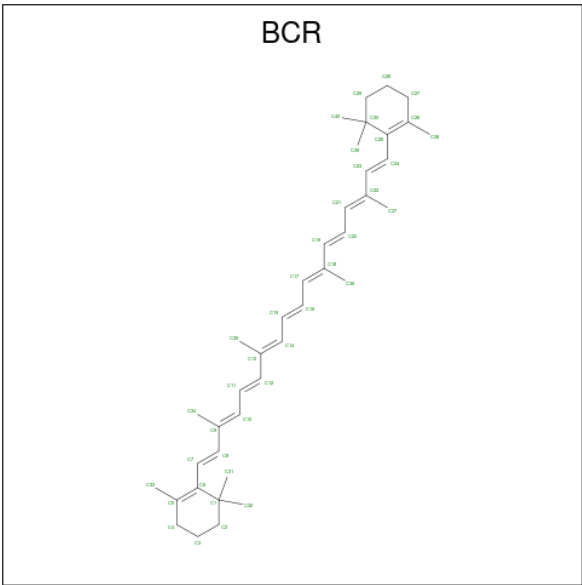
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



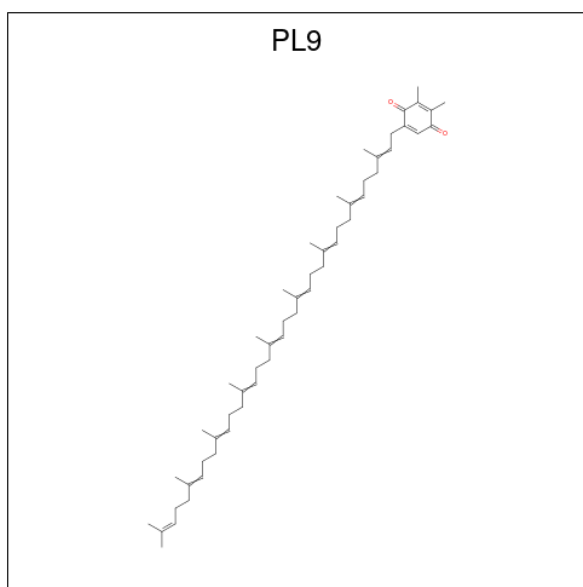
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	f	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0

- Molecule 27 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:  $C_{53}H_{80}O_2$ ).



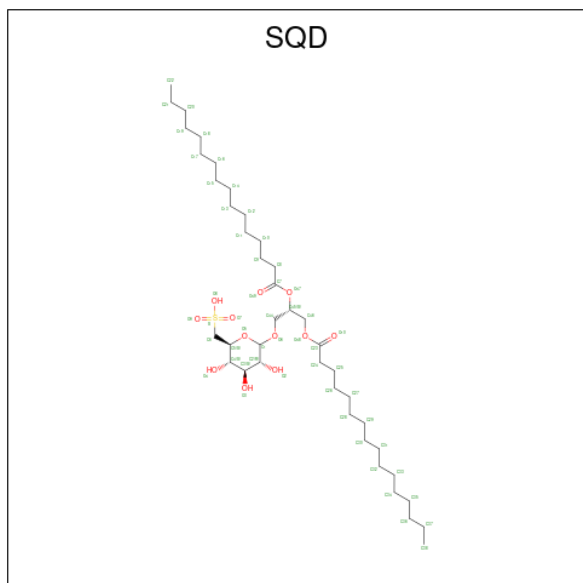
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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

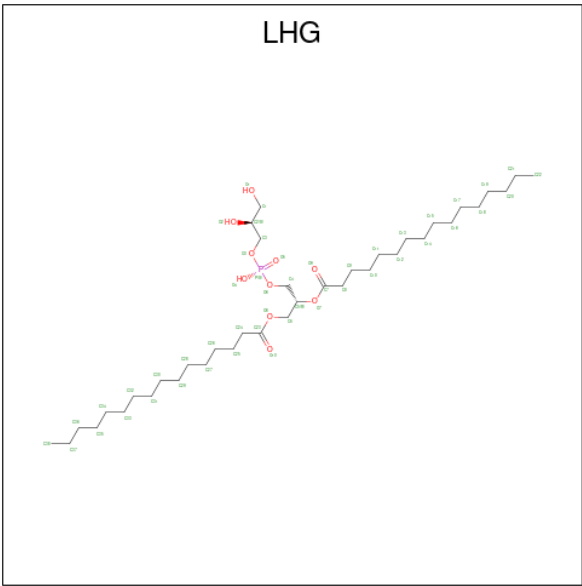
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			43	30	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	d	1	Total	C	O	S	0	0
			43	30	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 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
29	A	1	Total	C	O	P	0	0
			42	31	10	1		
29	B	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			42	31	10	1		
29	b	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	Ca	0	0
			1	1		

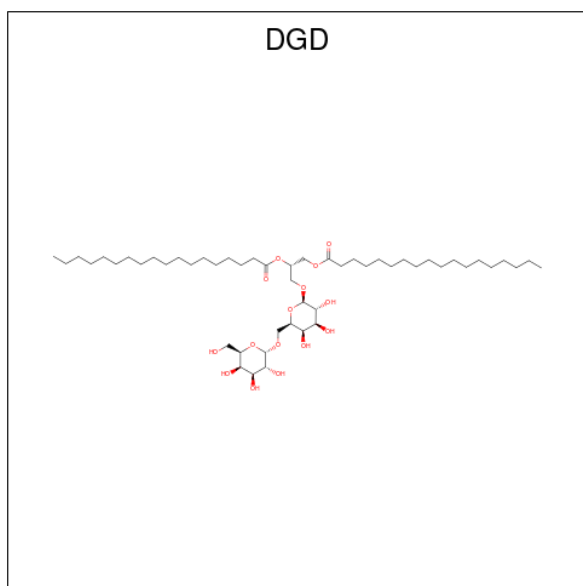
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	F	1	Total 1	Ca 1	0	0
30	O	1	Total 1	Ca 1	0	0
30	b	1	Total 1	Ca 1	0	0
30	c	1	Total 1	Ca 1	0	0
30	f	1	Total 1	Ca 1	0	0
30	o	1	Total 1	Ca 1	0	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total 62	C 47	O 15	0	0
31	C	1	Total 62	C 47	O 15	0	0
31	C	1	Total 62	C 47	O 15	0	0
31	D	1	Total 62	C 47	O 15	0	0
31	H	1	Total 62	C 47	O 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	d	1	Total C O 62 47 15	0	0
31	h	1	Total C O 62 47 15	0	0
31	j	1	Total C O 62 47 15	0	0

- # HEM

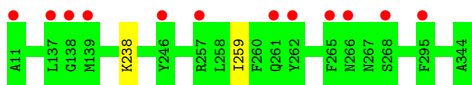
- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

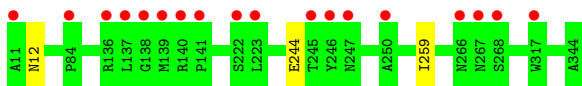
### 3 Residue-property plots

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.

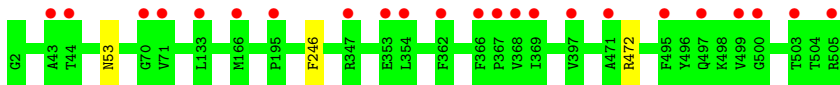
- Molecule 1: Photosystem Q(B) protein 1



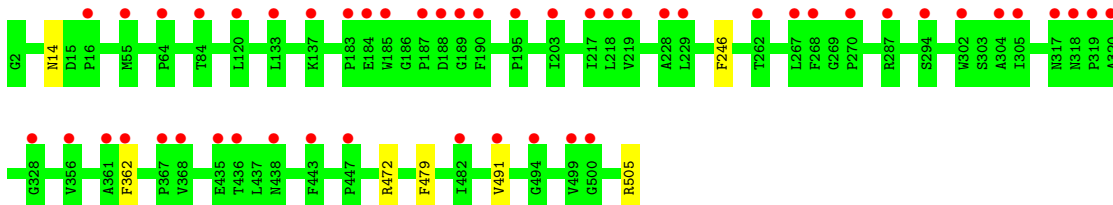
- Molecule 1: Photosystem Q(B) protein 1



- Molecule 2: Photosystem II core light harvesting protein

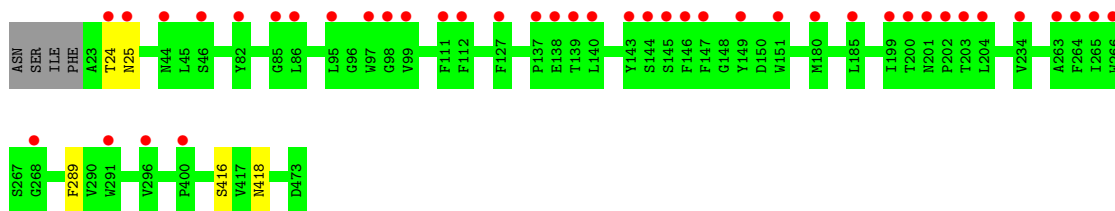


- Molecule 2: Photosystem II core light harvesting protein

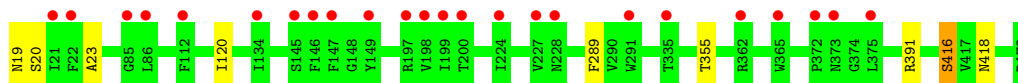


- Molecule 3: Photosystem II CP43 protein

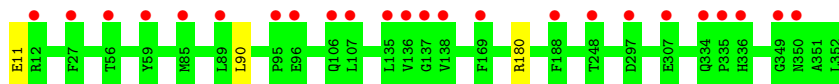




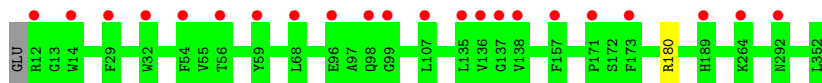
● Molecule 3: Photosystem II CP43 protein



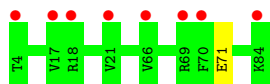
● Molecule 4: Photosystem II D2 protein



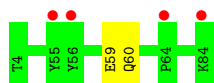
● Molecule 4: Photosystem II D2 protein



● Molecule 5: Cytochrome b559 subunit alpha



● Molecule 5: Cytochrome b559 subunit alpha

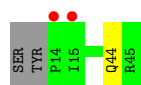


● Molecule 6: Cytochrome b559 subunit beta

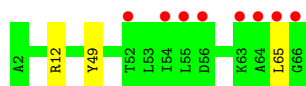




- Molecule 6: Cytochrome b559 subunit beta



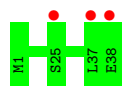
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



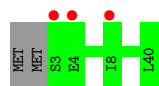
- Molecule 8: Photosystem II reaction center protein I



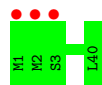
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



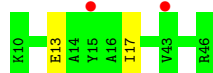
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



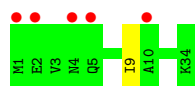
- Molecule 11: Photosystem II reaction center protein L



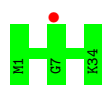
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



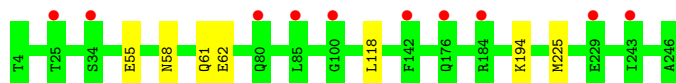
- Molecule 12: Photosystem II reaction center protein M



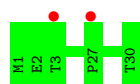
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



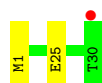
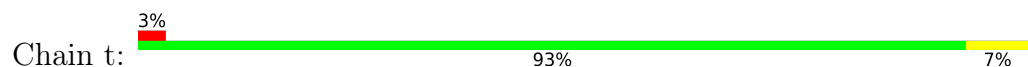
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



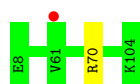
- Molecule 14: Photosystem II reaction center protein T



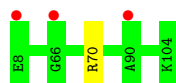
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



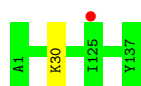
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550



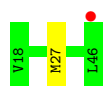




- Molecule 16: Cytochrome c-550



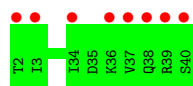
- Molecule 17: Photosystem II reaction center protein Ycf12



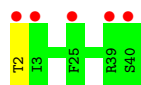
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



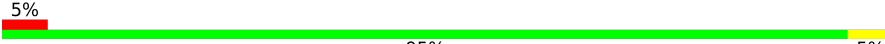
- Molecule 18: Photosystem II reaction center X protein

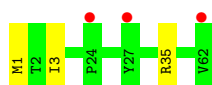


- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  5% 95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.64 – 5.00 100.64 – 5.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.64-5.00) 100.0 (100.64-5.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.261 , 0.262 0.259 , 0.263	Depositor DCC
$R_{free}$ test set	2056 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	285.1	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.0	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	0.88	EDS
Total number of atoms	48924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.52	0/2705	0.55	0/3689
1	a	0.51	0/2705	0.54	0/3689
2	B	0.50	0/4109	0.54	0/5600
2	b	0.49	0/4109	0.53	0/5600
3	C	0.47	0/3599	0.51	0/4900
3	c	0.44	0/3633	0.50	0/4946
4	D	0.53	0/2821	0.55	0/3844
4	d	0.49	0/2812	0.53	0/3832
5	E	0.43	0/681	0.51	0/928
5	e	0.42	0/681	0.50	0/928
6	F	0.49	0/284	0.45	0/387
6	f	0.47	0/265	0.44	0/360
7	H	0.47	0/524	0.50	0/713
7	h	0.44	0/524	0.49	0/713
8	I	0.47	0/319	0.51	0/429
8	i	0.46	0/319	0.47	0/429
9	J	0.46	0/278	0.43	0/376
9	j	0.39	0/294	0.45	0/396
10	K	0.43	0/303	0.50	0/416
10	k	0.43	0/303	0.51	0/416
11	L	0.55	0/311	0.51	0/422
11	l	0.54	0/311	0.52	0/422
12	M	0.47	0/270	0.58	0/367
12	m	0.49	0/270	0.52	0/367
13	O	0.45	0/1896	0.58	0/2571
13	o	0.43	0/1896	0.56	0/2571
14	T	0.54	0/265	0.52	0/359
14	t	0.55	0/265	0.52	0/359
15	U	0.46	0/785	0.55	0/1064
15	u	0.45	0/785	0.55	0/1064
16	V	0.47	0/1085	0.53	0/1473
16	v	0.42	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.41	0/216	0.45	0/289
17	y	0.35	0/216	0.52	0/289
18	X	0.43	0/290	0.46	0/392
18	x	0.42	0/290	0.48	0/392
19	Z	0.41	0/490	0.45	0/669
19	z	0.40	0/490	0.47	0/669
All	All	0.48	0/42484	0.53	0/57803

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	41	76
1	a	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	41	76
2	B	502/504 (100%)	496 (99%)	6 (1%)	0	100	100
2	b	502/504 (100%)	492 (98%)	10 (2%)	0	100	100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	47	81
3	c	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	47	81
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
5	e	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/40 (90%)	36 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/34 (94%)	32 (100%)	0	0	100	100
12	m	32/34 (94%)	32 (100%)	0	0	100	100
13	O	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	34	72
13	o	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	34	72
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
18	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
18	x	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5191/5276 (98%)	5072 (98%)	113 (2%)	6 (0%)	51	86

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416	SER
3	c	416	SER
1	A	259	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/269 (100%)	268 (100%)	1 (0%)	91	94
1	a	269/269 (100%)	267 (99%)	2 (1%)	84	90
2	B	402/402 (100%)	399 (99%)	3 (1%)	84	90
2	b	402/402 (100%)	395 (98%)	7 (2%)	60	78
3	C	352/356 (99%)	348 (99%)	4 (1%)	73	85
3	c	356/356 (100%)	350 (98%)	6 (2%)	60	78
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	85
4	d	276/277 (100%)	275 (100%)	1 (0%)	91	94
5	E	72/72 (100%)	71 (99%)	1 (1%)	67	81
5	e	72/72 (100%)	70 (97%)	2 (3%)	43	65
6	F	28/28 (100%)	27 (96%)	1 (4%)	35	59
6	f	26/28 (93%)	25 (96%)	1 (4%)	33	57
7	H	54/54 (100%)	51 (94%)	3 (6%)	21	48
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	75
8	I	35/35 (100%)	35 (100%)	0	100	100
8	i	35/35 (100%)	35 (100%)	0	100	100
9	J	26/28 (93%)	26 (100%)	0	100	100
9	j	28/28 (100%)	28 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	42
11	L	35/35 (100%)	33 (94%)	2 (6%)	20	47
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	M	31/31 (100%)	30 (97%)	1 (3%)	39	61
12	m	31/31 (100%)	31 (100%)	0	100	100
13	O	206/206 (100%)	202 (98%)	4 (2%)	57	75
13	o	206/206 (100%)	200 (97%)	6 (3%)	42	64
14	T	27/27 (100%)	27 (100%)	0	100	100
14	t	27/27 (100%)	25 (93%)	2 (7%)	13	40
15	U	84/84 (100%)	83 (99%)	1 (1%)	71	84
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	84
16	V	117/117 (100%)	116 (99%)	1 (1%)	78	88
16	v	117/117 (100%)	114 (97%)	3 (3%)	46	67
17	Y	22/22 (100%)	21 (96%)	1 (4%)	27	53
17	y	22/22 (100%)	21 (96%)	1 (4%)	27	53
18	X	32/32 (100%)	32 (100%)	0	100	100
18	x	32/32 (100%)	31 (97%)	1 (3%)	40	62
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	57
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	46
All	All	4305/4314 (100%)	4235 (98%)	70 (2%)	62	79

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	194	LYS
14	t	1	MET
17	y	42	ARG
13	O	234	LYS
13	O	181	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	82	GLN

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Mol	Chain	Res	Type
13	o	124	ASN
13	O	82	GLN
11	L	13	ASN
13	o	147	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 152 ligands modelled in this entry, 16 are monoatomic - leaving 136 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	$\# Z  > 2$
26	BCR	T	102	-	41,41,41	3.67	15 (36%)	56,56,56	7.23	37 (66%)
24	CLA	b	607	-	65,73,73	2.60	18 (27%)	76,113,113	2.70	22 (28%)
24	CLA	C	512	-	65,73,73	2.70	18 (27%)	76,113,113	2.45	23 (30%)
29	LHG	A	615	-	41,41,48	1.05	2 (4%)	44,47,54	1.06	3 (6%)
27	PL9	A	611	-	55,55,55	0.71	2 (3%)	68,69,69	1.56	13 (19%)
29	LHG	d	410	-	48,48,48	0.92	2 (4%)	51,54,54	0.95	4 (7%)
24	CLA	b	603	-	65,73,73	2.34	18 (27%)	76,113,113	2.42	20 (26%)
31	DGD	C	516	-	63,63,67	0.87	3 (4%)	77,77,81	0.98	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	k	102	-	41,41,41	3.80	14 (34%)	56,56,56	8.42	42 (75%)
31	DGD	D	406	-	63,63,67	0.99	4 (6%)	77,77,81	1.02	6 (7%)
24	CLA	C	503	-	65,73,73	2.52	17 (26%)	76,113,113	2.50	19 (25%)
24	CLA	b	604	-	65,73,73	2.21	14 (21%)	76,113,113	2.50	22 (28%)
24	CLA	B	615	-	65,73,73	2.24	18 (27%)	76,113,113	2.56	22 (28%)
29	LHG	d	409	-	48,48,48	0.84	2 (4%)	51,54,54	0.91	3 (5%)
25	PHO	A	608	-	51,69,69	1.59	7 (13%)	47,99,99	1.52	6 (12%)
24	CLA	b	602	-	65,73,73	2.57	19 (29%)	76,113,113	2.52	24 (31%)
26	BCR	b	618	-	41,41,41	3.70	14 (34%)	56,56,56	7.96	41 (73%)
28	SQD	d	407	-	42,43,54	1.20	3 (7%)	51,54,65	1.43	7 (13%)
24	CLA	B	612	-	65,73,73	2.13	16 (24%)	76,113,113	2.60	21 (27%)
24	CLA	d	401	-	65,73,73	2.34	16 (24%)	76,113,113	2.58	21 (27%)
24	CLA	D	402	-	65,73,73	2.14	19 (29%)	76,113,113	2.52	24 (31%)
29	LHG	a	413	-	41,41,48	1.05	2 (4%)	44,47,54	0.90	2 (4%)
24	CLA	b	610	-	65,73,73	2.47	18 (27%)	76,113,113	2.39	18 (23%)
24	CLA	c	909	-	65,73,73	2.40	19 (29%)	76,113,113	2.56	19 (25%)
24	CLA	d	403	-	65,73,73	2.15	17 (26%)	76,113,113	2.48	19 (25%)
24	CLA	c	910	-	65,73,73	2.46	19 (29%)	76,113,113	2.70	23 (30%)
24	CLA	A	609	-	65,73,73	2.20	15 (23%)	76,113,113	2.61	22 (28%)
28	SQD	L	101	-	53,54,54	1.08	4 (7%)	62,65,65	1.43	9 (14%)
24	CLA	B	602	-	65,73,73	2.56	19 (29%)	76,113,113	2.66	21 (27%)
31	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	2 (2%)
24	CLA	B	614	-	65,73,73	2.28	18 (27%)	76,113,113	2.59	22 (28%)
29	LHG	D	409	-	48,48,48	0.94	2 (4%)	51,54,54	0.90	3 (5%)
24	CLA	b	605	-	65,73,73	2.41	19 (29%)	76,113,113	2.66	21 (27%)
24	CLA	B	607	-	65,73,73	2.47	18 (27%)	76,113,113	2.65	24 (31%)
26	BCR	C	515	-	41,41,41	3.82	14 (34%)	56,56,56	8.21	38 (67%)
25	PHO	D	401	-	51,69,69	1.73	7 (13%)	47,99,99	1.60	7 (14%)
24	CLA	C	513	-	65,73,73	2.68	19 (29%)	76,113,113	2.47	22 (28%)
24	CLA	b	609	-	65,73,73	2.36	17 (26%)	76,113,113	2.49	20 (26%)
24	CLA	c	903	-	65,73,73	2.34	17 (26%)	76,113,113	2.65	21 (27%)
26	BCR	f	101	-	41,41,41	3.82	14 (34%)	56,56,56	7.95	45 (80%)
24	CLA	B	610	-	65,73,73	2.22	18 (27%)	76,113,113	2.51	20 (26%)
24	CLA	C	510	-	65,73,73	2.30	18 (27%)	76,113,113	2.62	23 (30%)
31	DGD	d	406	-	63,63,67	0.97	3 (4%)	77,77,81	0.95	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	HEM	e	101	6,5	41,50,50	2.01	8 (19%)	45,82,82	1.72	7 (15%)
24	CLA	b	615	-	65,73,73	2.21	16 (24%)	76,113,113	2.75	25 (32%)
28	SQD	l	101	-	53,54,54	1.04	4 (7%)	62,65,65	1.36	8 (12%)
29	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.95	3 (5%)
29	LHG	b	620	-	48,48,48	0.89	2 (4%)	51,54,54	0.98	3 (5%)
23	BCT	A	605	21	2,3,3	0.90	0	2,3,3	0.21	0
28	SQD	F	101	-	42,43,54	1.21	3 (7%)	51,54,65	1.46	7 (13%)
24	CLA	B	605	-	65,73,73	2.39	16 (24%)	76,113,113	2.64	21 (27%)
24	CLA	b	613	-	65,73,73	2.47	15 (23%)	76,113,113	2.59	22 (28%)
24	CLA	B	609	-	65,73,73	2.11	15 (23%)	76,113,113	2.49	24 (31%)
24	CLA	B	606	-	65,73,73	2.32	16 (24%)	76,113,113	2.48	21 (27%)
24	CLA	C	502	-	65,73,73	2.22	17 (26%)	76,113,113	2.47	19 (25%)
24	CLA	b	614	-	65,73,73	2.17	16 (24%)	76,113,113	2.64	22 (28%)
24	CLA	B	616	-	65,73,73	2.45	18 (27%)	76,113,113	2.55	20 (26%)
26	BCR	B	620	-	41,41,41	3.72	14 (34%)	56,56,56	8.42	41 (73%)
24	CLA	B	603	-	65,73,73	2.34	17 (26%)	76,113,113	2.43	19 (25%)
24	CLA	c	908	-	65,73,73	2.49	17 (26%)	76,113,113	2.73	20 (26%)
24	CLA	d	404	-	65,73,73	2.41	19 (29%)	76,113,113	2.51	23 (30%)
24	CLA	C	505	-	65,73,73	2.34	19 (29%)	76,113,113	2.41	19 (25%)
26	BCR	a	409	-	41,41,41	3.65	14 (34%)	56,56,56	7.80	33 (58%)
29	LHG	D	407	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	4 (7%)
31	DGD	H	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.94	4 (5%)
32	HEM	E	101	6,5	41,50,50	1.92	7 (17%)	45,82,82	1.79	9 (20%)
26	BCR	B	622	-	41,41,41	3.78	15 (36%)	56,56,56	7.59	36 (64%)
20	OEX	a	401	1,3	0,15,15	-	-	-	-	-
24	CLA	C	508	-	65,73,73	2.48	20 (30%)	76,113,113	2.50	17 (22%)
24	CLA	B	604	-	65,73,73	2.23	18 (27%)	76,113,113	2.63	22 (28%)
29	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.84	2 (3%)
24	CLA	a	407	-	65,73,73	2.21	18 (27%)	76,113,113	2.48	22 (28%)
24	CLA	b	616	-	65,73,73	2.38	16 (24%)	76,113,113	2.52	20 (26%)
28	SQD	a	402	-	53,54,54	1.06	3 (5%)	62,65,65	1.22	5 (8%)
26	BCR	C	514	-	41,41,41	3.86	15 (36%)	56,56,56	8.41	36 (64%)
24	CLA	c	906	-	65,73,73	2.29	17 (26%)	76,113,113	2.53	21 (27%)
26	BCR	K	101	-	41,41,41	3.76	14 (34%)	56,56,56	7.77	41 (73%)
31	DGD	c	916	-	63,63,67	0.85	3 (4%)	77,77,81	0.90	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	B	619	-	41,41,41	3.65	14 (34%)	56,56,56	7.72	41 (73%)
24	CLA	b	608	-	65,73,73	2.33	15 (23%)	76,113,113	2.47	22 (28%)
26	BCR	A	610	-	41,41,41	3.71	14 (34%)	56,56,56	7.75	37 (66%)
24	CLA	b	611	-	65,73,73	2.36	18 (27%)	76,113,113	2.54	20 (26%)
29	LHG	B	621	-	48,48,48	0.89	2 (4%)	51,54,54	0.97	2 (3%)
28	SQD	A	612	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
26	BCR	Y	101	-	41,41,41	3.83	14 (34%)	56,56,56	8.02	36 (64%)
24	CLA	c	914	-	65,73,73	2.74	19 (29%)	76,113,113	2.41	23 (30%)
24	CLA	B	613	-	65,73,73	2.36	17 (26%)	76,113,113	2.55	20 (26%)
31	DGD	j	101	-	63,63,67	0.87	3 (4%)	77,77,81	0.87	3 (3%)
24	CLA	D	403	-	65,73,73	2.39	18 (27%)	76,113,113	2.57	20 (26%)
25	PHO	a	412	-	51,69,69	1.67	7 (13%)	47,99,99	1.74	7 (14%)
24	CLA	A	606	-	65,73,73	2.16	16 (24%)	76,113,113	2.44	21 (27%)
24	CLA	c	911	-	65,73,73	2.29	18 (27%)	76,113,113	2.55	21 (27%)
26	BCR	k	101	-	41,41,41	3.88	14 (34%)	56,56,56	8.48	41 (73%)
26	BCR	h	101	-	41,41,41	3.79	14 (34%)	56,56,56	8.35	41 (73%)
28	SQD	A	613	-	53,54,54	1.05	3 (5%)	62,65,65	1.22	6 (9%)
23	BCT	a	414	21	2,3,3	0.90	0	2,3,3	0.70	0
24	CLA	C	506	-	65,73,73	2.37	18 (27%)	76,113,113	2.59	20 (26%)
24	CLA	b	617	-	65,73,73	2.33	17 (26%)	76,113,113	2.57	24 (31%)
24	CLA	b	606	-	65,73,73	2.26	18 (27%)	76,113,113	2.56	20 (26%)
27	PL9	a	410	-	55,55,55	0.70	2 (3%)	68,69,69	1.57	17 (25%)
24	CLA	c	912	3	65,73,73	2.61	18 (27%)	76,113,113	2.58	21 (27%)
24	CLA	c	905	-	65,73,73	2.51	20 (30%)	76,113,113	2.65	21 (27%)
20	OEX	A	601	1,3	0,15,15	-	-	-	-	-
24	CLA	B	617	-	65,73,73	2.19	15 (23%)	76,113,113	2.56	24 (31%)
24	CLA	C	509	-	65,73,73	2.40	17 (26%)	76,113,113	2.62	24 (31%)
26	BCR	c	918	-	41,41,41	3.61	15 (36%)	56,56,56	7.55	36 (64%)
24	CLA	b	612	-	65,73,73	2.26	15 (23%)	76,113,113	2.54	20 (26%)
24	CLA	c	913	-	65,73,73	2.71	19 (29%)	76,113,113	2.52	24 (31%)
32	HEM	v	202	16	41,50,50	1.96	5 (12%)	45,82,82	1.82	7 (15%)
26	BCR	T	101	-	41,41,41	3.80	14 (34%)	56,56,56	7.07	39 (69%)
27	PL9	d	405	-	55,55,55	0.81	2 (3%)	68,69,69	1.32	10 (14%)
32	HEM	V	202	16	41,50,50	1.95	8 (19%)	45,82,82	1.74	8 (17%)
26	BCR	B	618	-	41,41,41	3.65	14 (34%)	56,56,56	7.51	38 (67%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	c	907	-	65,73,73	2.41	18 (27%)	76,113,113	2.59	20 (26%)
24	CLA	C	507	-	65,73,73	2.50	17 (26%)	76,113,113	2.66	22 (28%)
24	CLA	A	614	-	65,73,73	1.97	17 (26%)	76,113,113	2.47	21 (27%)
24	CLA	C	504	-	65,73,73	2.37	17 (26%)	76,113,113	2.59	20 (26%)
24	CLA	B	608	-	65,73,73	2.29	18 (27%)	76,113,113	2.47	20 (26%)
24	CLA	c	902	-	65,73,73	2.35	18 (27%)	76,113,113	2.75	22 (28%)
26	BCR	c	915	-	41,41,41	3.79	15 (36%)	56,56,56	8.54	39 (69%)
24	CLA	A	607	-	65,73,73	2.28	15 (23%)	76,113,113	2.61	22 (28%)
28	SQD	a	411	-	53,54,54	1.00	3 (5%)	62,65,65	1.57	10 (16%)
26	BCR	H	101	-	41,41,41	3.80	14 (34%)	56,56,56	8.25	40 (71%)
27	PL9	D	405	-	55,55,55	0.80	1 (1%)	68,69,69	1.33	9 (13%)
24	CLA	a	406	-	65,73,73	2.12	18 (27%)	76,113,113	2.59	22 (28%)
24	CLA	C	501	-	65,73,73	2.33	17 (26%)	76,113,113	2.58	21 (27%)
24	CLA	B	611	-	65,73,73	2.31	18 (27%)	76,113,113	2.56	21 (27%)
26	BCR	b	619	-	41,41,41	3.80	15 (36%)	56,56,56	8.49	42 (75%)
25	PHO	d	402	-	51,69,69	1.63	8 (15%)	47,99,99	1.65	6 (12%)
24	CLA	c	904	-	65,73,73	2.62	18 (27%)	76,113,113	2.54	22 (28%)
31	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.85	3 (3%)
31	DGD	c	917	-	63,63,67	0.88	2 (3%)	77,77,81	0.81	2 (2%)
26	BCR	D	404	-	41,41,41	3.80	14 (34%)	56,56,56	7.77	40 (71%)
24	CLA	C	511	3	65,73,73	2.49	16 (24%)	76,113,113	2.65	19 (25%)
24	CLA	a	408	-	65,73,73	2.19	17 (26%)	76,113,113	2.52	23 (30%)
31	DGD	C	518	-	63,63,67	0.79	3 (4%)	77,77,81	0.90	3 (3%)

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
26	BCR	T	102	-	-	3/29/63/63	0/2/2/2
24	CLA	b	607	-	1/1/15/20	12/37/115/115	-
24	CLA	C	512	-	1/1/15/20	10/37/115/115	-
29	LHG	A	615	-	-	25/46/46/53	-
27	PL9	A	611	-	-	9/53/73/73	0/1/1/1
29	LHG	d	410	-	-	17/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	603	-	1/1/15/20	4/37/115/115	-
31	DGD	C	516	-	-	24/51/91/95	0/2/2/2
26	BCR	k	102	-	-	12/29/63/63	0/2/2/2
31	DGD	D	406	-	-	32/51/91/95	0/2/2/2
24	CLA	C	503	-	1/1/15/20	1/37/115/115	-
24	CLA	b	604	-	1/1/15/20	8/37/115/115	-
24	CLA	B	615	-	1/1/15/20	12/37/115/115	-
29	LHG	d	409	-	-	11/53/53/53	-
25	PHO	A	608	-	-	4/37/103/103	0/5/6/6
24	CLA	b	602	-	1/1/15/20	20/37/115/115	-
26	BCR	b	618	-	-	3/29/63/63	0/2/2/2
28	SQD	d	407	-	-	22/38/58/69	0/1/1/1
24	CLA	B	612	-	-	3/37/115/115	-
24	CLA	d	401	-	-	6/37/115/115	-
24	CLA	D	402	-	1/1/15/20	4/37/115/115	-
29	LHG	a	413	-	-	25/46/46/53	-
24	CLA	b	610	-	-	0/37/115/115	-
24	CLA	c	909	-	-	8/37/115/115	-
24	CLA	d	403	-	1/1/15/20	3/37/115/115	-
24	CLA	A	609	-	-	16/37/115/115	-
24	CLA	c	910	-	1/1/15/20	10/37/115/115	-
28	SQD	L	101	-	-	29/49/69/69	0/1/1/1
24	CLA	B	602	-	1/1/15/20	17/37/115/115	-
31	DGD	C	517	-	-	25/51/91/95	0/2/2/2
24	CLA	B	614	-	1/1/15/20	2/37/115/115	-
29	LHG	D	409	-	-	13/53/53/53	-
24	CLA	b	605	-	1/1/15/20	6/37/115/115	-
24	CLA	B	607	-	-	9/37/115/115	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	PHO	D	401	-	-	5/37/103/103	0/5/6/6
24	CLA	C	513	-	-	10/37/115/115	-
24	CLA	b	609	-	-	1/37/115/115	-
24	CLA	c	903	-	-	7/37/115/115	-
26	BCR	f	101	-	-	7/29/63/63	0/2/2/2
24	CLA	B	610	-	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	510	-	1/1/15/20	9/37/115/115	-
31	DGD	d	406	-	-	33/51/91/95	0/2/2/2
32	HEM	e	101	6,5	-	4/12/54/54	-
24	CLA	b	615	-	1/1/15/20	19/37/115/115	-
28	SQD	l	101	-	-	28/49/69/69	0/1/1/1
29	LHG	d	408	-	-	11/53/53/53	-
29	LHG	b	620	-	-	17/53/53/53	-
28	SQD	F	101	-	-	16/38/58/69	0/1/1/1
24	CLA	B	605	-	1/1/15/20	7/37/115/115	-
24	CLA	b	613	-	1/1/15/20	5/37/115/115	-
24	CLA	B	609	-	-	2/37/115/115	-
24	CLA	B	606	-	1/1/15/20	6/37/115/115	-
24	CLA	C	502	-	-	8/37/115/115	-
24	CLA	b	614	-	1/1/15/20	6/37/115/115	-
24	CLA	B	616	-	1/1/15/20	10/37/115/115	-
26	BCR	B	620	-	-	2/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/15/20	4/37/115/115	-
24	CLA	c	908	-	1/1/15/20	9/37/115/115	-
24	CLA	d	404	-	-	9/37/115/115	-
24	CLA	C	505	-	1/1/15/20	4/37/115/115	-
26	BCR	a	409	-	-	2/29/63/63	0/2/2/2
29	LHG	D	407	-	-	13/53/53/53	-
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
32	HEM	E	101	6,5	-	3/12/54/54	-
26	BCR	B	622	-	-	4/29/63/63	0/2/2/2
24	CLA	C	508	-	-	7/37/115/115	-
24	CLA	B	604	-	1/1/15/20	5/37/115/115	-
29	LHG	D	408	-	-	14/53/53/53	-
24	CLA	b	616	-	1/1/15/20	11/37/115/115	-
24	CLA	a	407	-	-	10/37/115/115	-
28	SQD	a	402	-	-	23/49/69/69	0/1/1/1
26	BCR	C	514	-	-	5/29/63/63	0/2/2/2
24	CLA	c	906	-	1/1/15/20	6/37/115/115	-
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	c	916	-	-	23/51/91/95	0/2/2/2
26	BCR	B	619	-	-	4/29/63/63	0/2/2/2
24	CLA	b	608	-	1/1/15/20	2/37/115/115	-
26	BCR	A	610	-	-	4/29/63/63	0/2/2/2
24	CLA	b	611	-	1/1/15/20	4/37/115/115	-
29	LHG	B	621	-	-	17/53/53/53	-
28	SQD	A	612	-	-	16/49/69/69	0/1/1/1
26	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
24	CLA	c	914	-	-	16/37/115/115	-
24	CLA	B	613	-	1/1/15/20	4/37/115/115	-
31	DGD	j	101	-	-	18/51/91/95	0/2/2/2
24	CLA	D	403	-	-	15/37/115/115	-
25	PHO	a	412	-	-	3/37/103/103	0/5/6/6
24	CLA	A	606	-	1/1/15/20	3/37/115/115	-
24	CLA	c	911	-	1/1/15/20	9/37/115/115	-
26	BCR	k	101	-	-	8/29/63/63	0/2/2/2
26	BCR	h	101	-	-	9/29/63/63	0/2/2/2
28	SQD	A	613	-	-	23/49/69/69	0/1/1/1
24	CLA	C	506	-	1/1/15/20	14/37/115/115	-
24	CLA	b	617	-	1/1/15/20	12/37/115/115	-
24	CLA	b	606	-	1/1/15/20	5/37/115/115	-
27	PL9	a	410	-	-	9/53/73/73	0/1/1/1
24	CLA	c	912	3	-	7/37/115/115	-
24	CLA	c	905	-	-	10/37/115/115	-
26	BCR	c	918	-	-	13/29/63/63	0/2/2/2
24	CLA	B	617	-	1/1/15/20	16/37/115/115	-
24	CLA	C	509	-	1/1/15/20	9/37/115/115	-
24	CLA	b	612	-	-	4/37/115/115	-
24	CLA	c	913	-	1/1/15/20	14/37/115/115	-
32	HEM	v	202	16	-	4/12/54/54	-
26	BCR	T	101	-	-	2/29/63/63	0/2/2/2
27	PL9	d	405	-	-	3/53/73/73	0/1/1/1
32	HEM	V	202	16	-	4/12/54/54	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	907	-	1/1/15/20	11/37/115/115	-
24	CLA	C	507	-	1/1/15/20	10/37/115/115	-
24	CLA	A	614	-	-	5/37/115/115	-
24	CLA	C	504	-	1/1/15/20	9/37/115/115	-
24	CLA	B	608	-	1/1/15/20	2/37/115/115	-
24	CLA	c	902	-	1/1/15/20	5/37/115/115	-
26	BCR	c	915	-	-	9/29/63/63	0/2/2/2
24	CLA	A	607	-	-	8/37/115/115	-
28	SQD	a	411	-	-	23/49/69/69	0/1/1/1
26	BCR	H	101	-	-	8/29/63/63	0/2/2/2
27	PL9	D	405	-	-	1/53/73/73	0/1/1/1
24	CLA	a	406	-	1/1/15/20	3/37/115/115	-
24	CLA	C	501	-	-	11/37/115/115	-
24	CLA	B	611	-	1/1/15/20	8/37/115/115	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	PHO	d	402	-	-	2/37/103/103	0/5/6/6
24	CLA	c	904	-	-	4/37/115/115	-
31	DGD	h	102	-	-	12/51/91/95	0/2/2/2
31	DGD	c	917	-	-	18/51/91/95	0/2/2/2
26	BCR	D	404	-	-	6/29/63/63	0/2/2/2
24	CLA	C	511	3	-	2/37/115/115	-
24	CLA	a	408	-	-	12/37/115/115	-
31	DGD	C	518	-	-	16/51/91/95	0/2/2/2

The worst 5 of 1669 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	14.06	2.39	2.06
24	c	914	CLA	MG-NC	12.56	2.36	2.06
24	b	613	CLA	MG-NA	12.54	2.36	2.06
24	c	913	CLA	MG-NA	12.23	2.35	2.06
24	B	605	CLA	MG-NA	12.05	2.34	2.06

The worst 5 of 2580 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C20-C21-C22	30.20	170.41	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C20-C21-C22	26.89	165.69	127.31
26	c	915	BCR	C20-C21-C22	26.83	165.60	127.31
26	C	514	BCR	C15-C16-C17	26.78	178.33	123.47
26	k	101	BCR	C16-C17-C18	26.63	165.32	127.31

5 of 45 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	606	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND

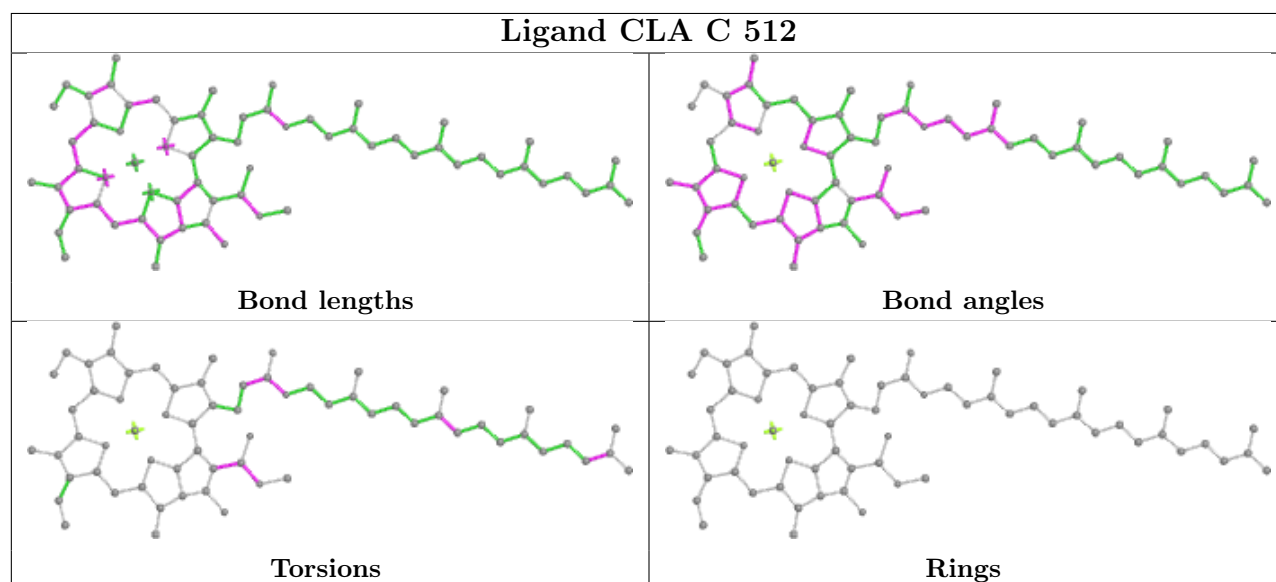
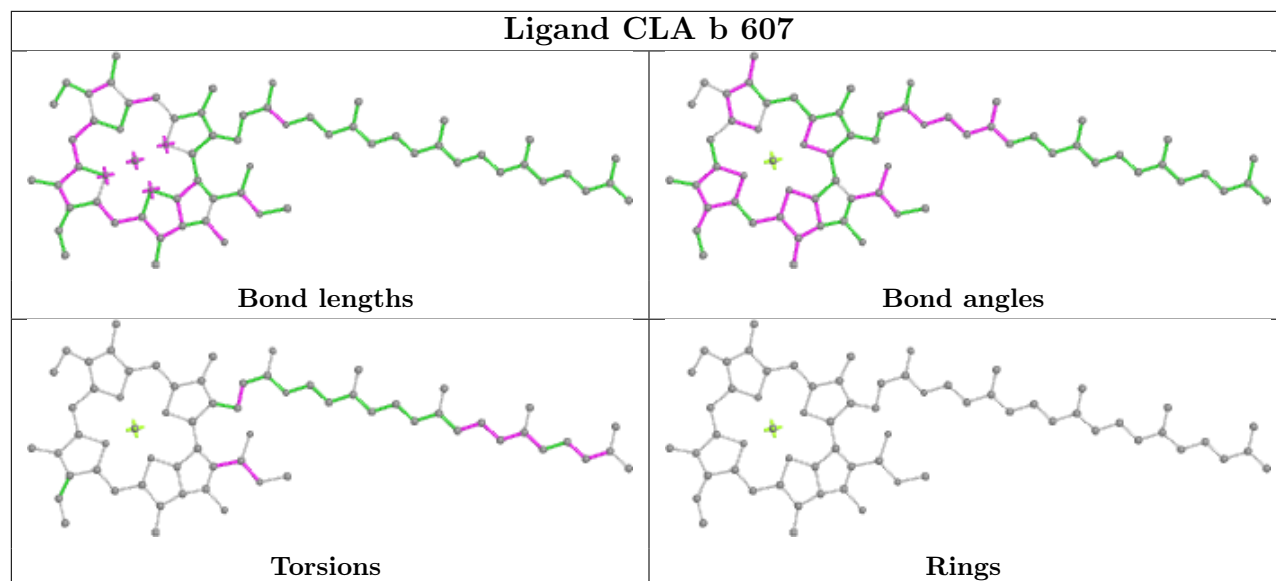
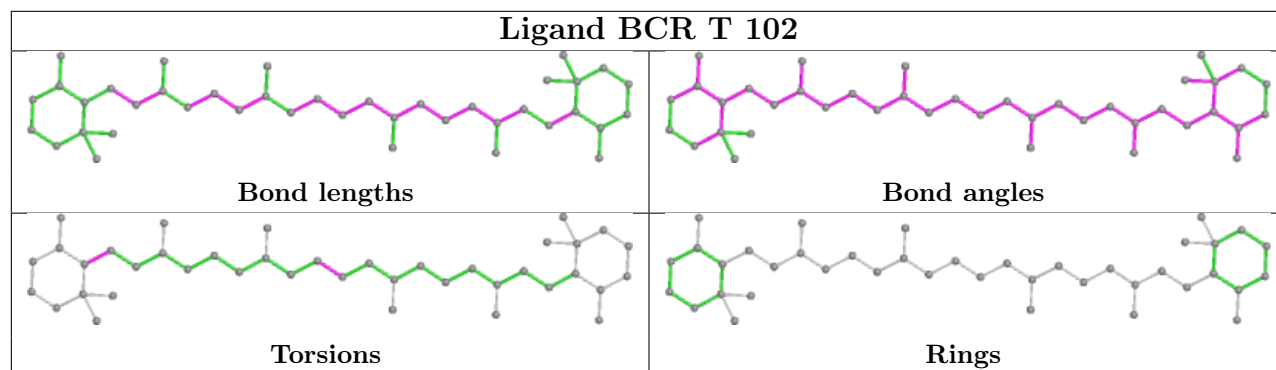
5 of 1279 torsion outliers are listed below:

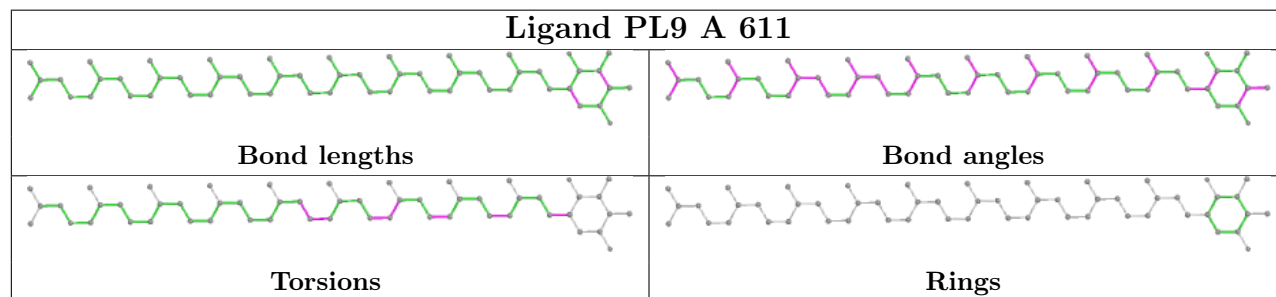
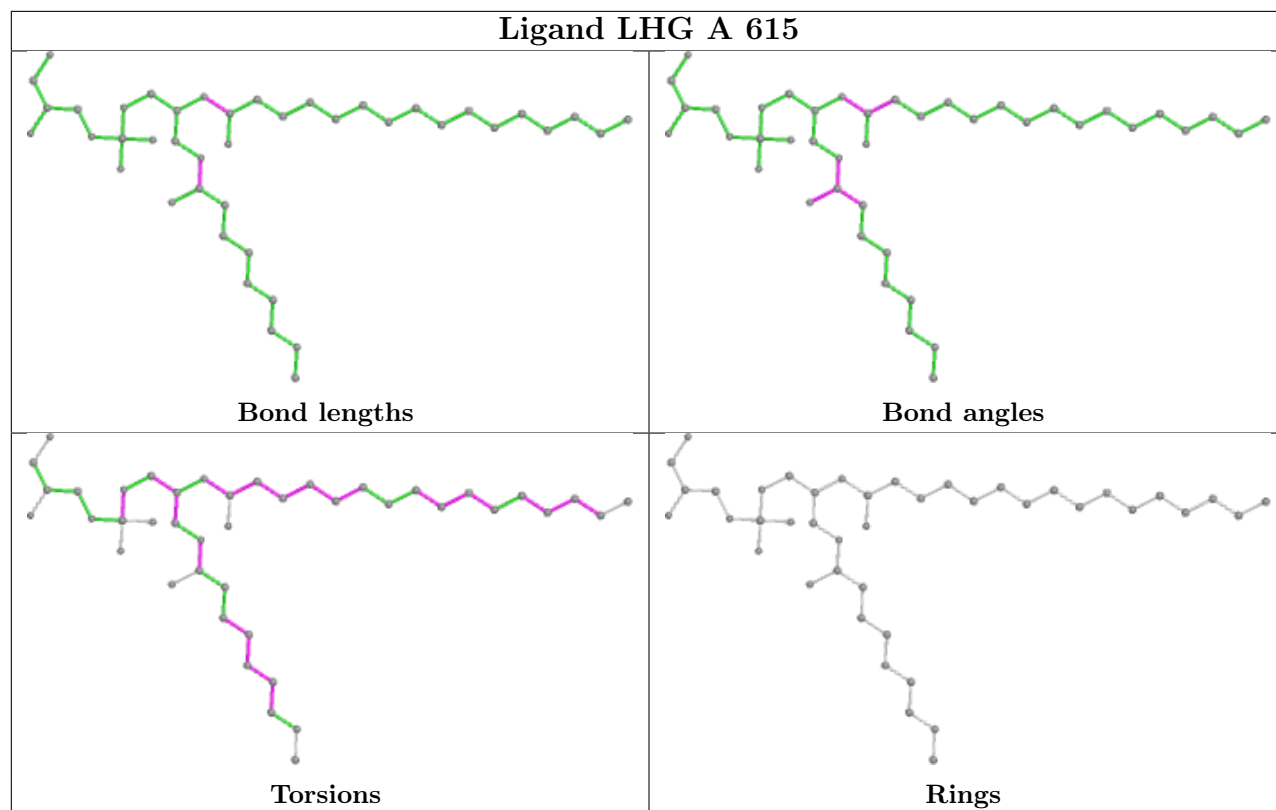
Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O1D

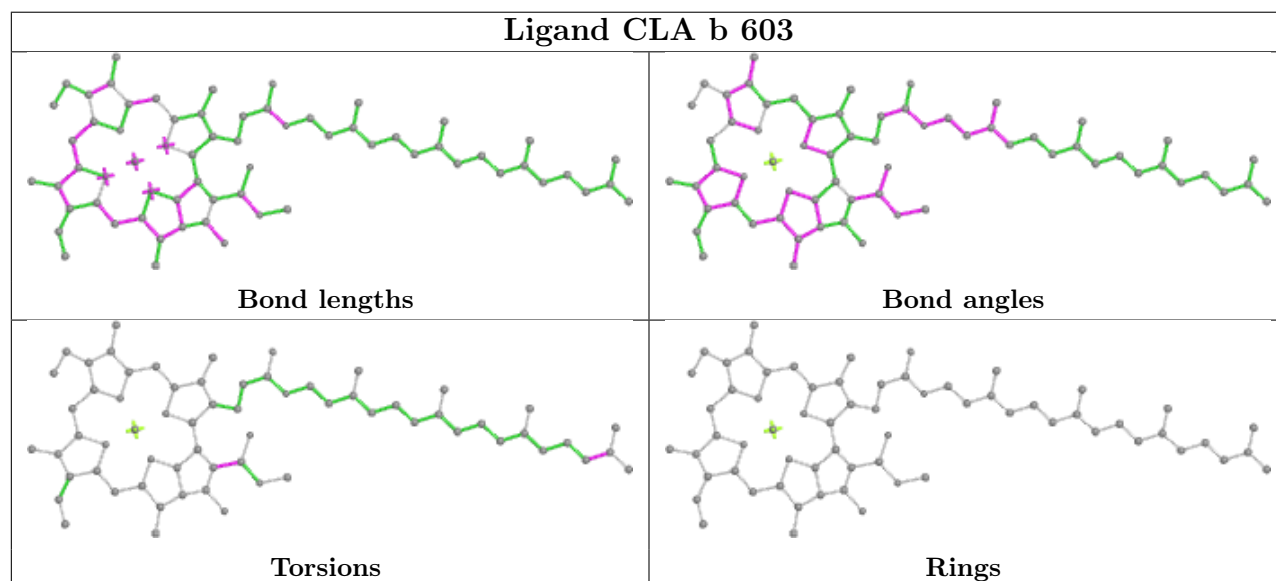
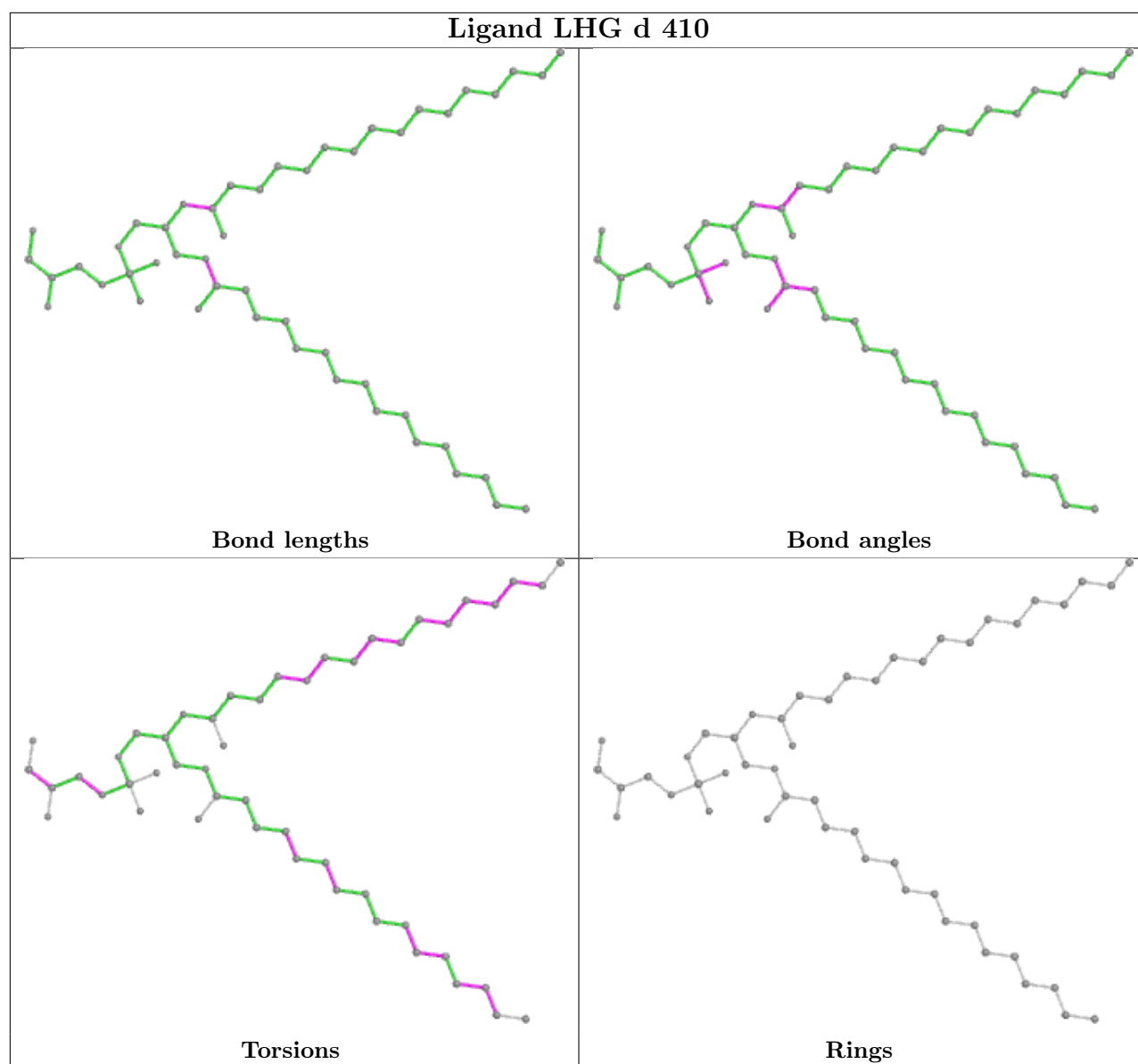
There are no ring outliers.

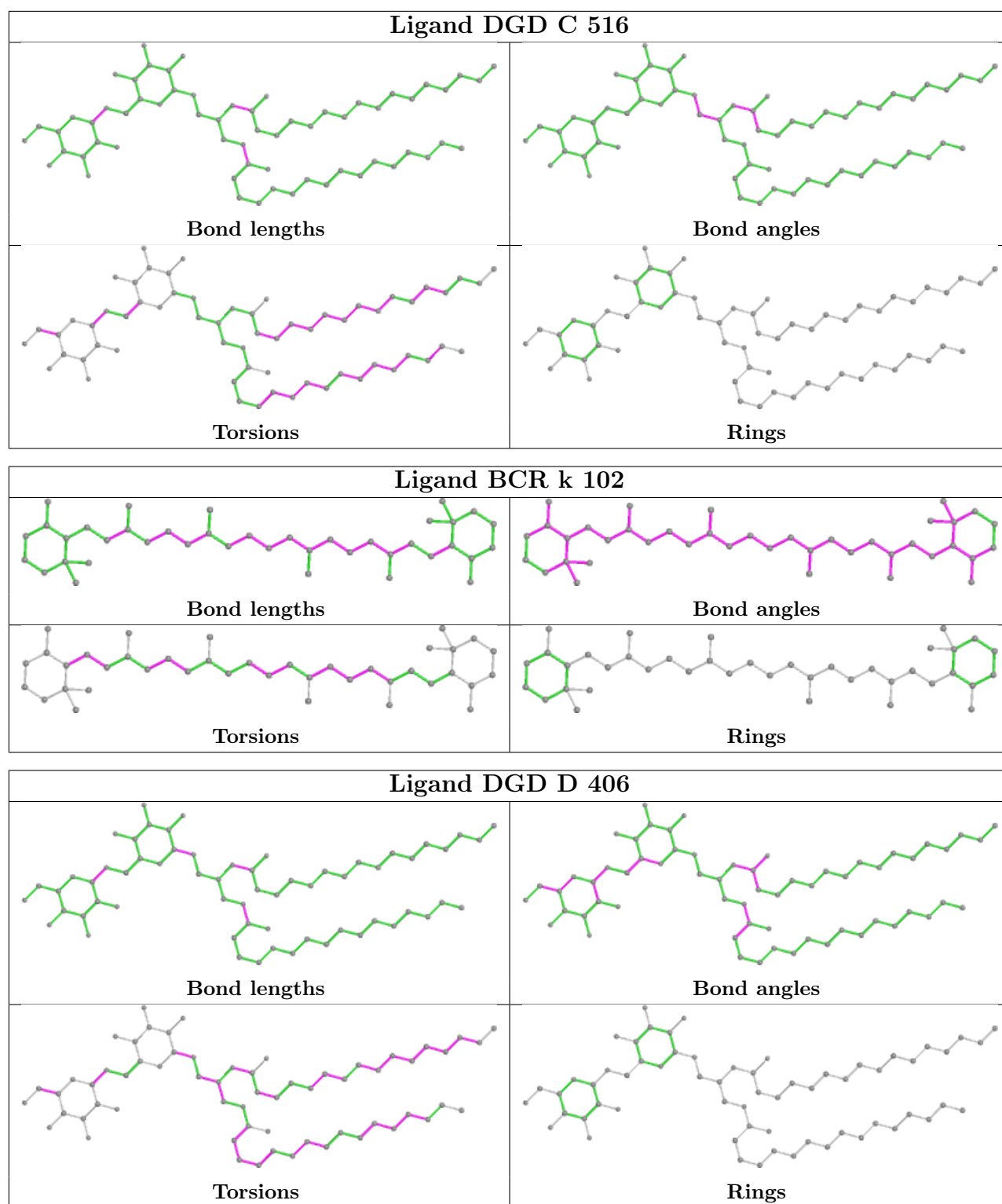
No monomer is involved in short contacts.

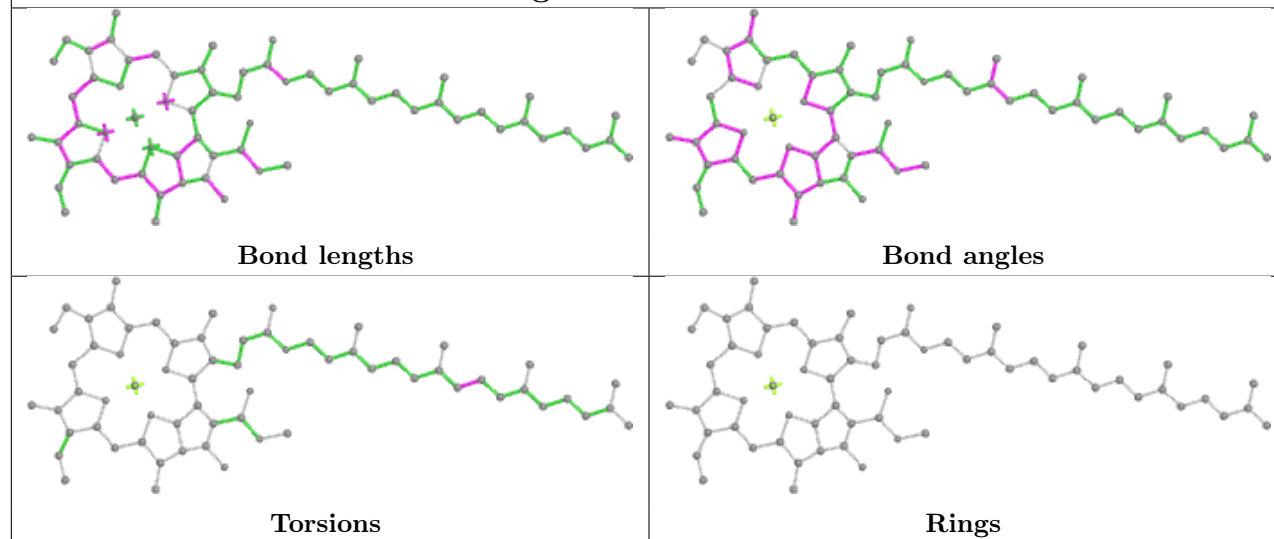
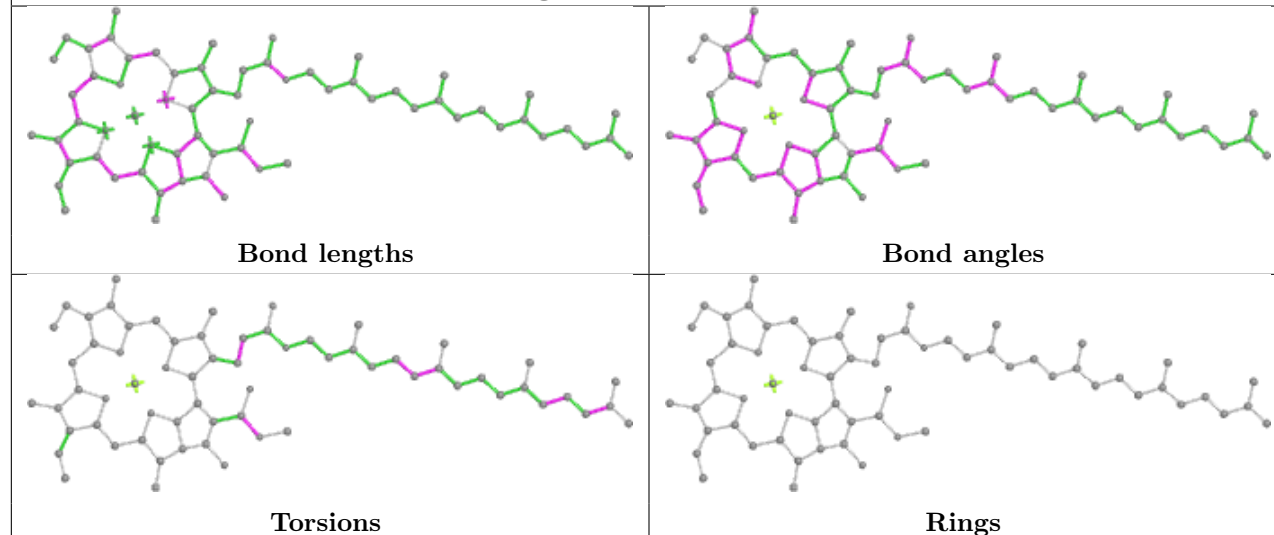
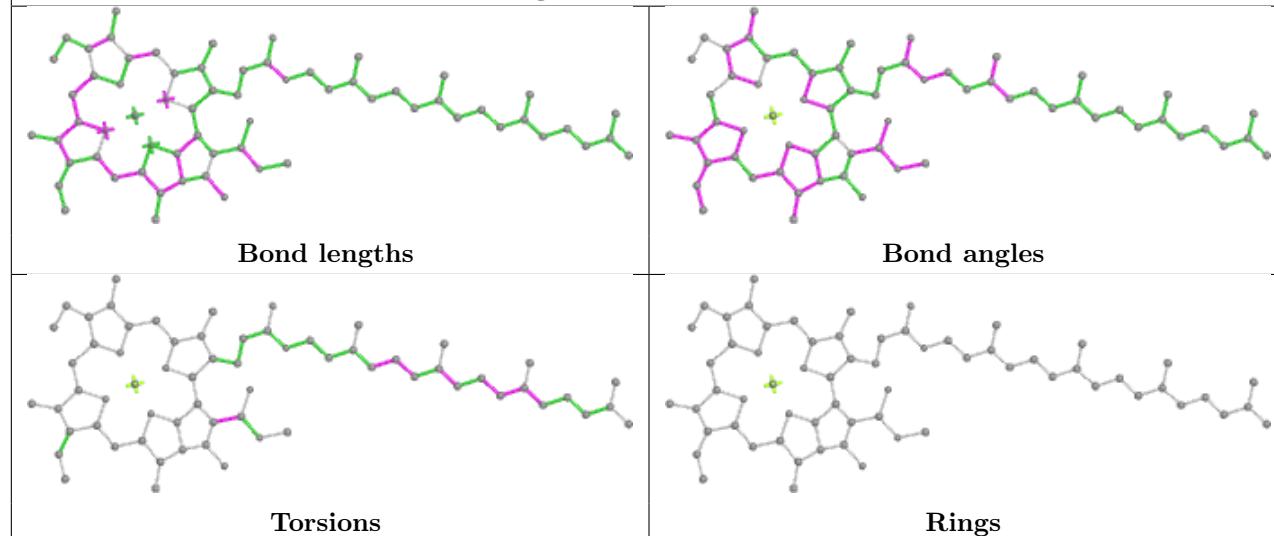
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



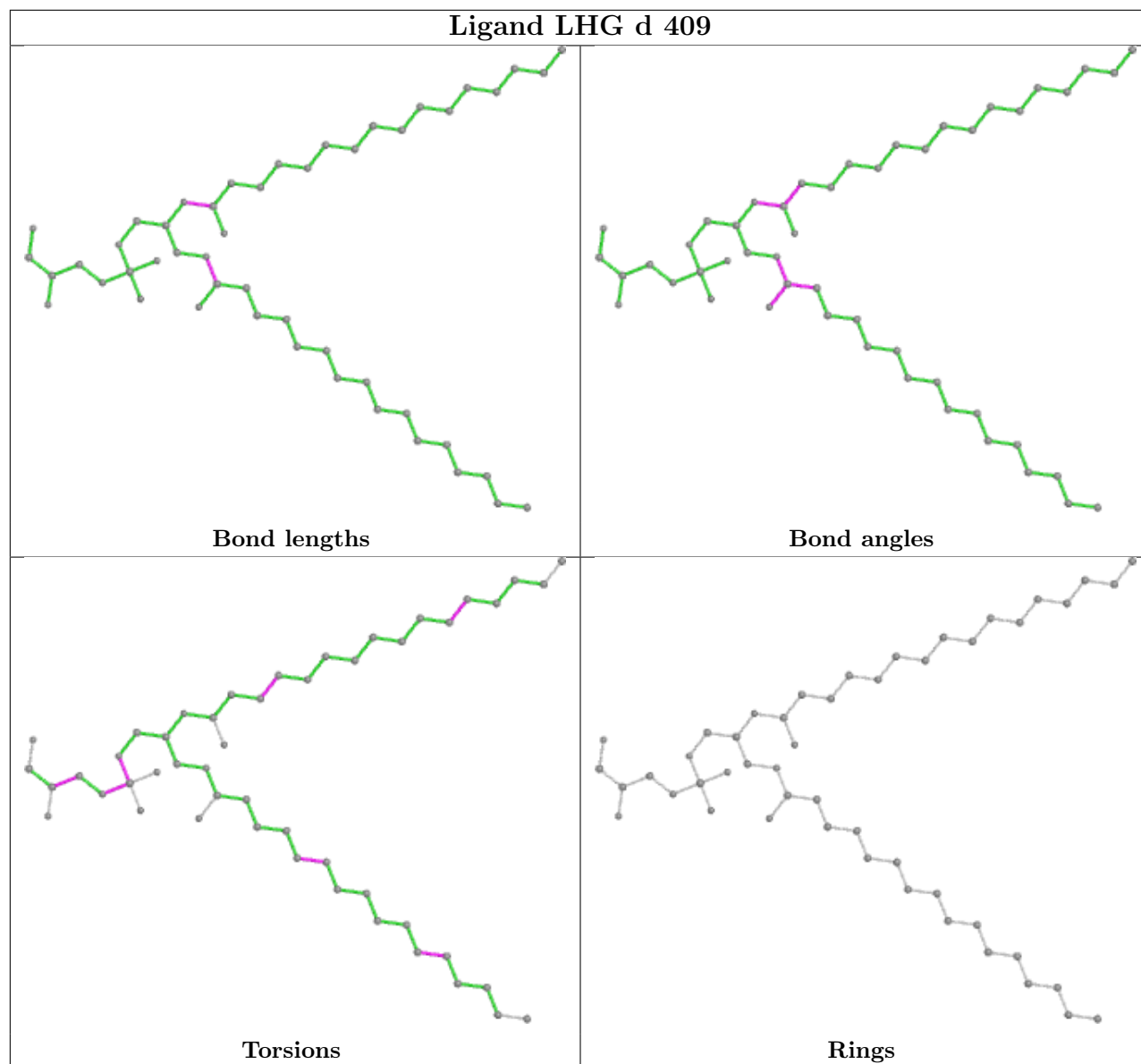




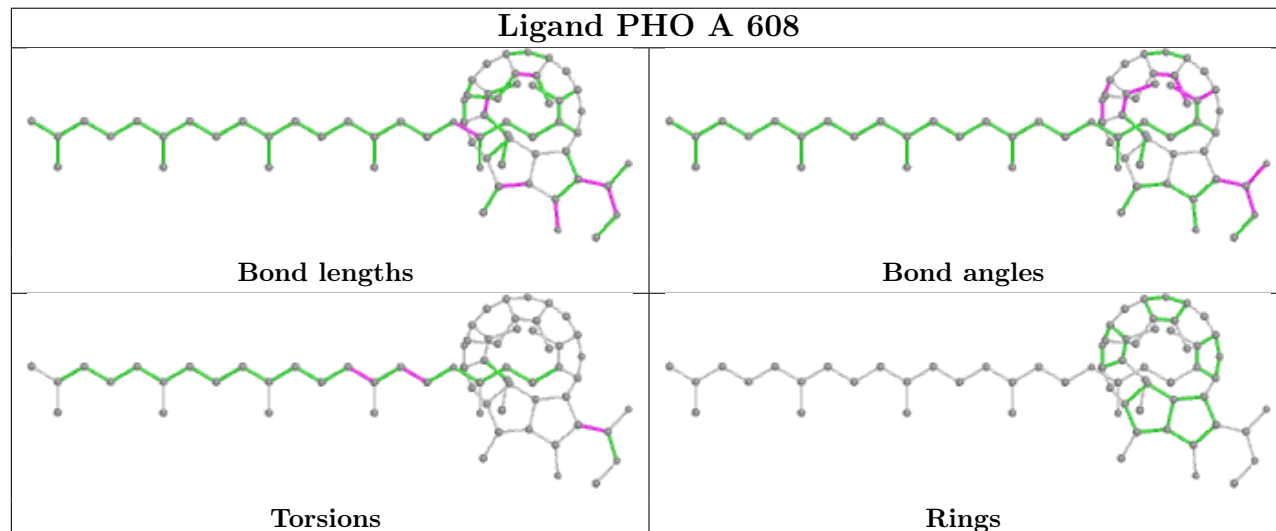


**Ligand CLA C 503****Ligand CLA b 604****Ligand CLA B 615**

## Ligand LHG d 409

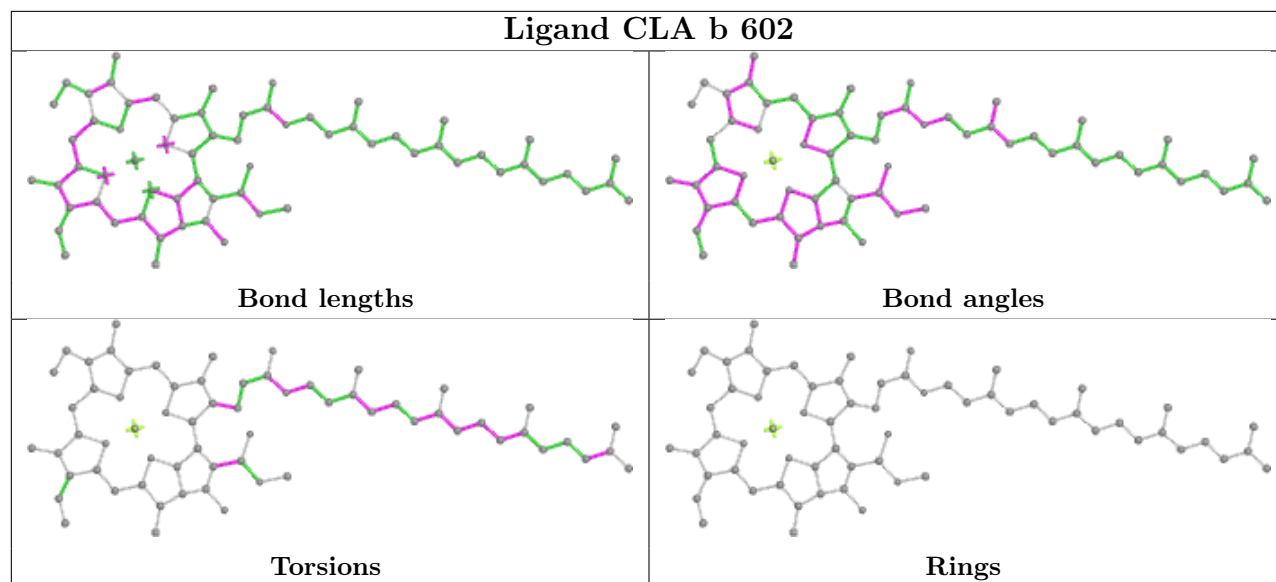


## Ligand PHO A 608

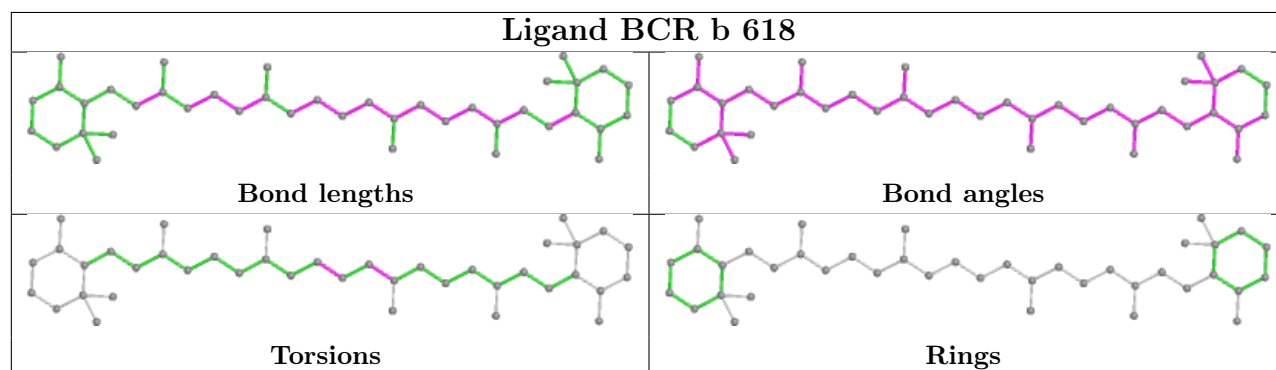




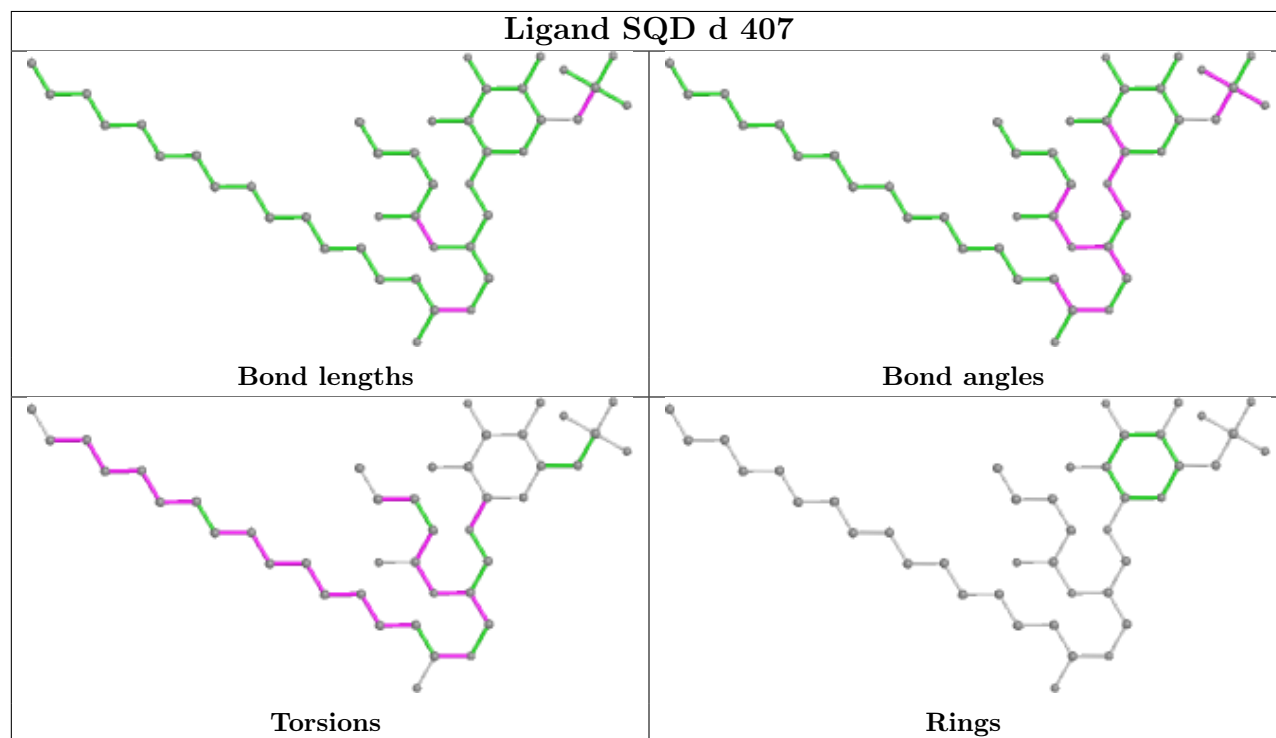
## Ligand CLA b 602



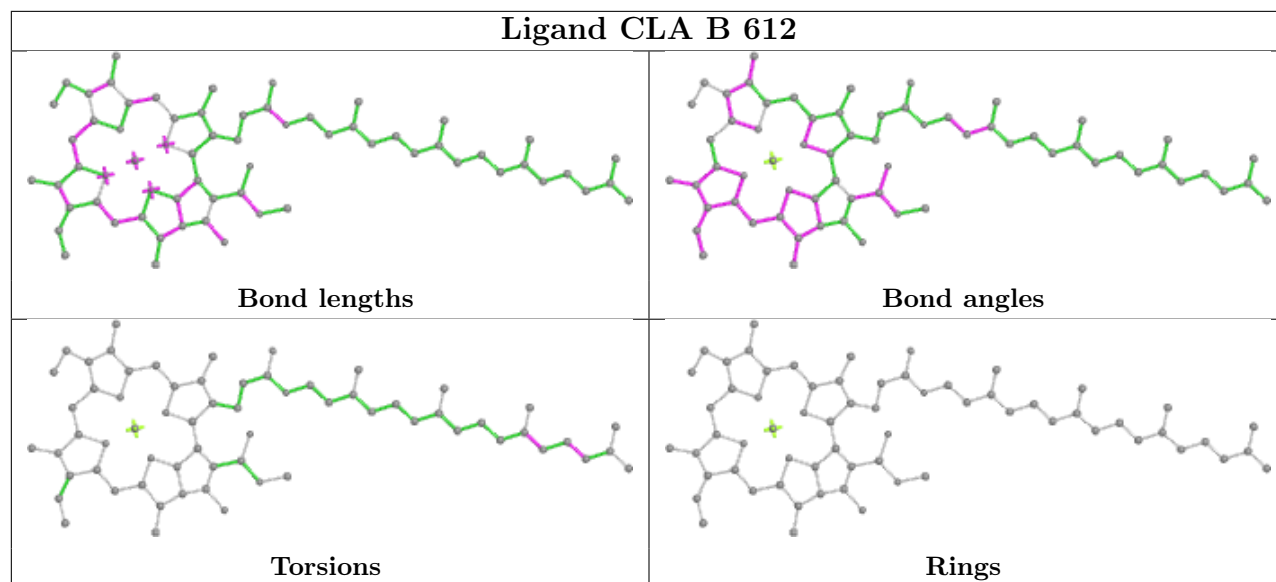
## Ligand BCR b 618



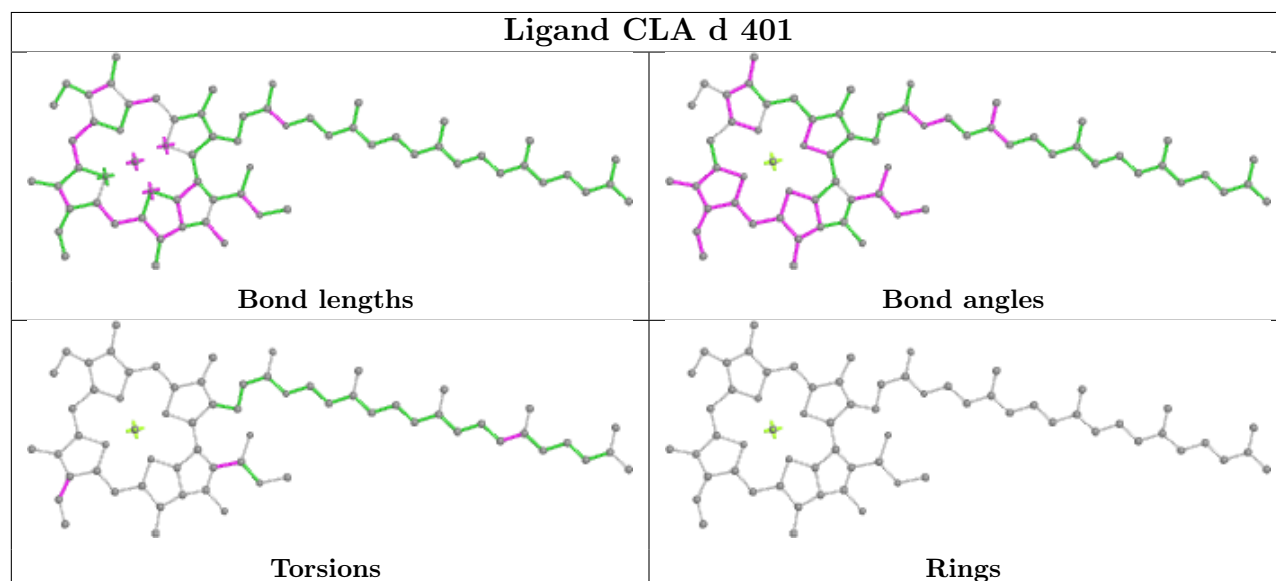
## Ligand SQD d 407



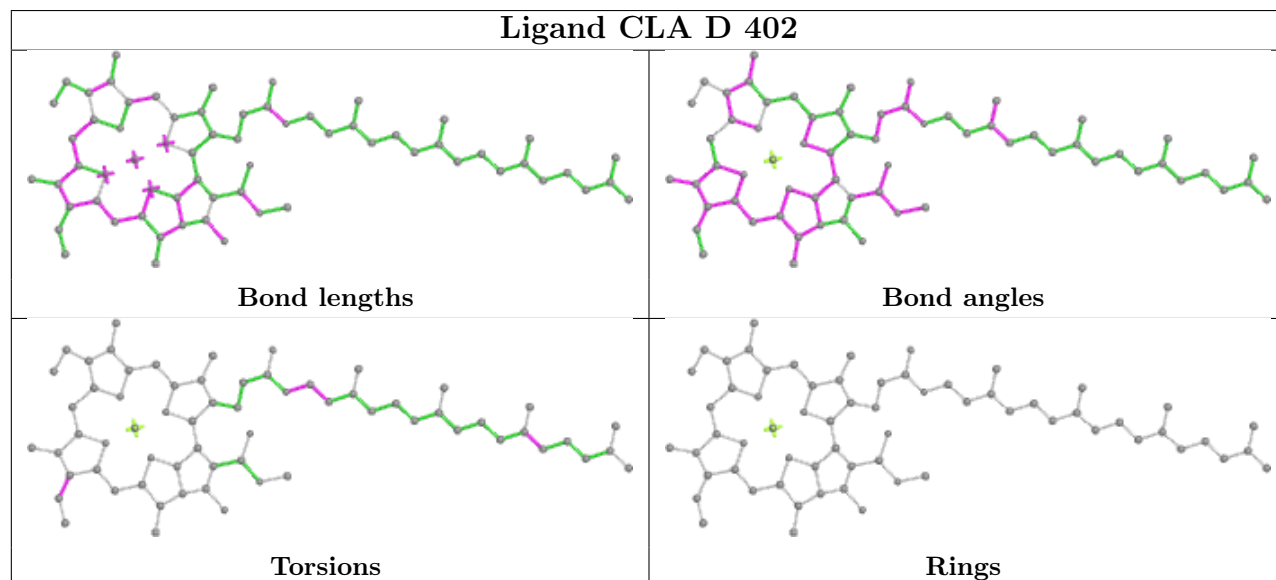
## Ligand CLA B 612

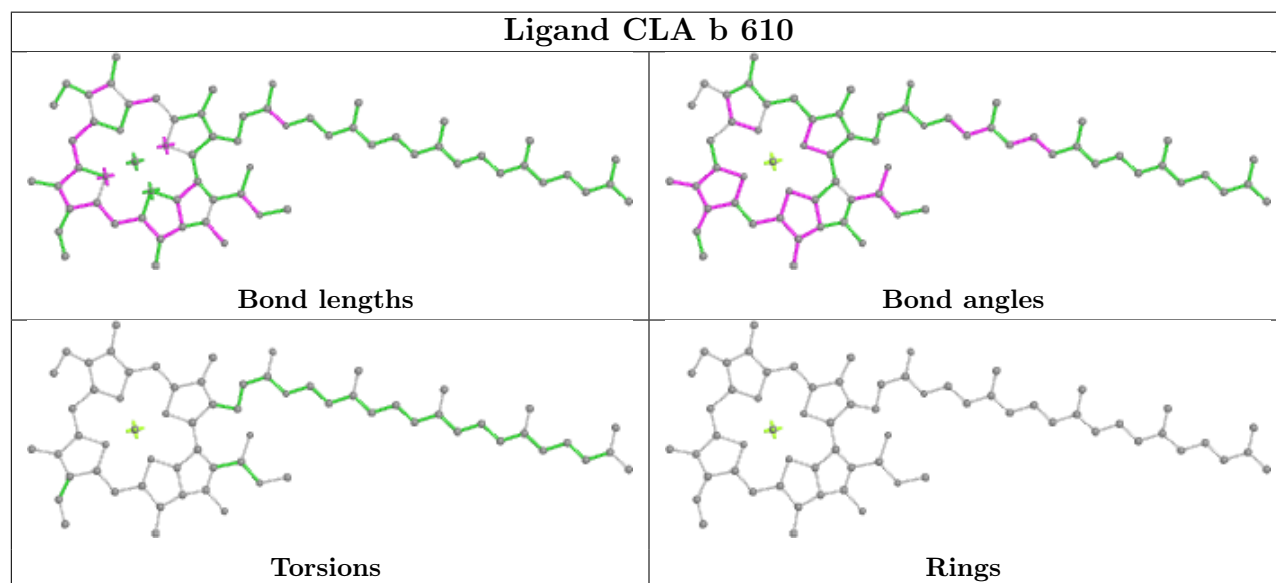
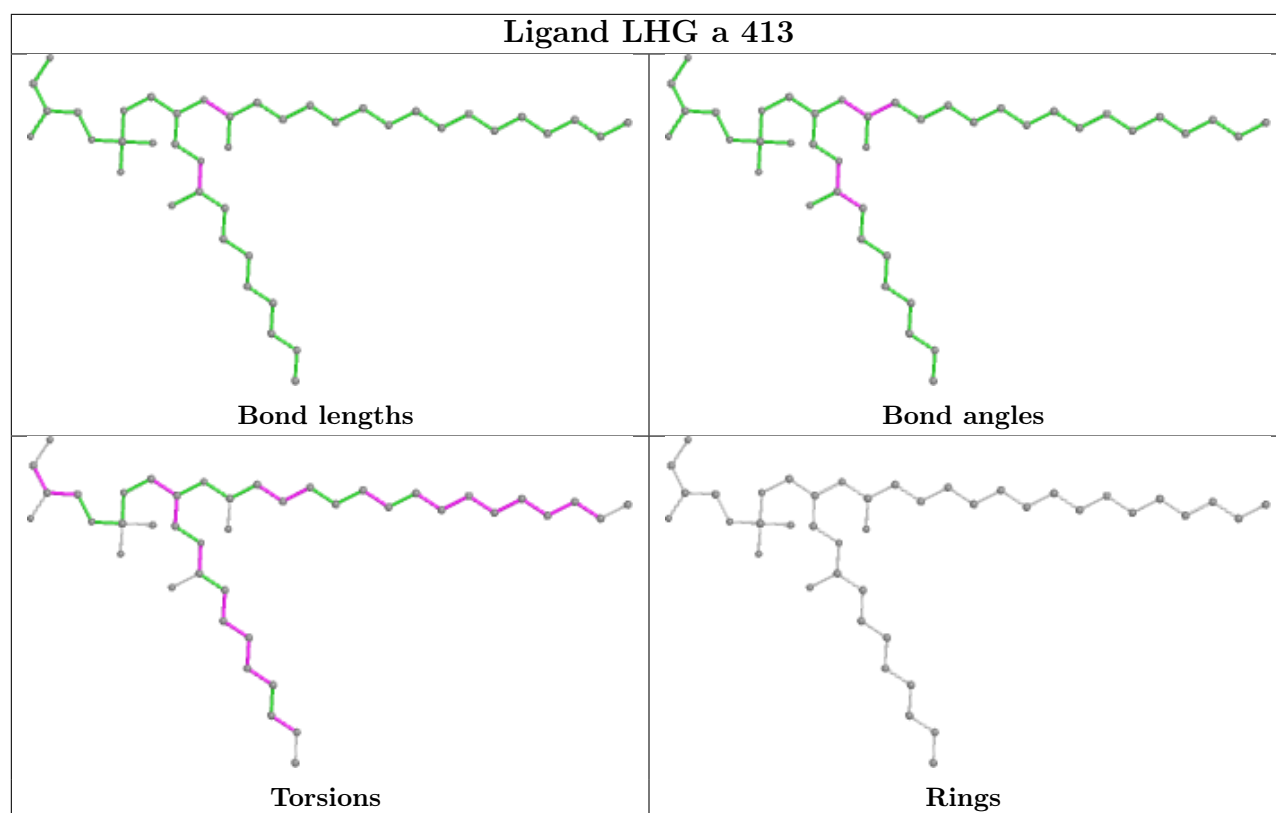


## Ligand CLA d 401

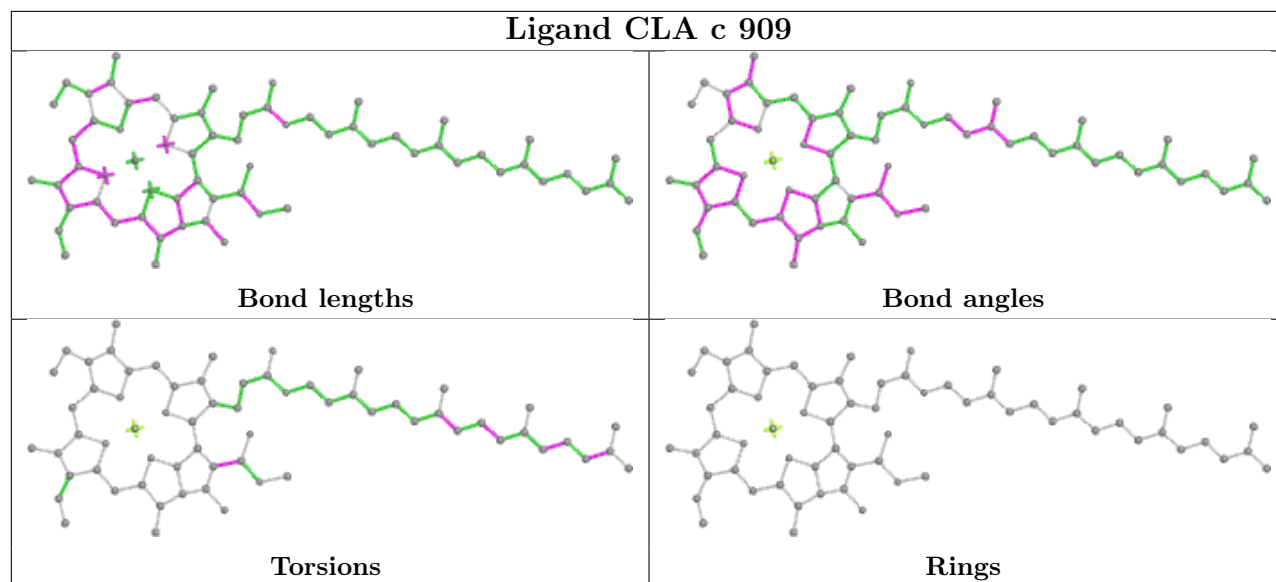


## Ligand CLA D 402

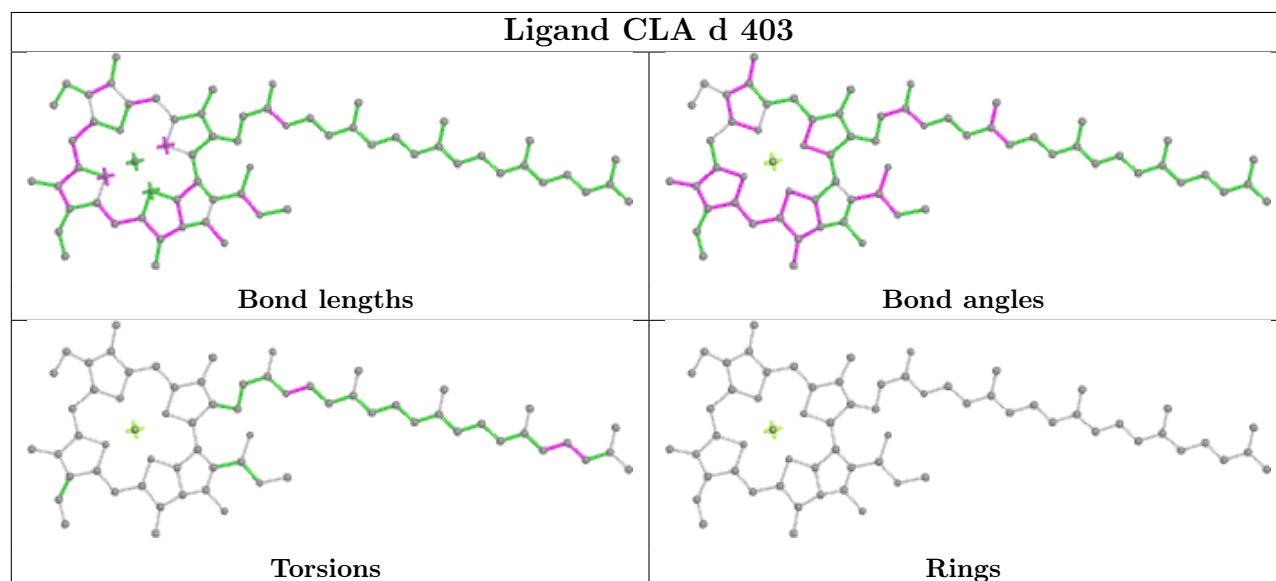




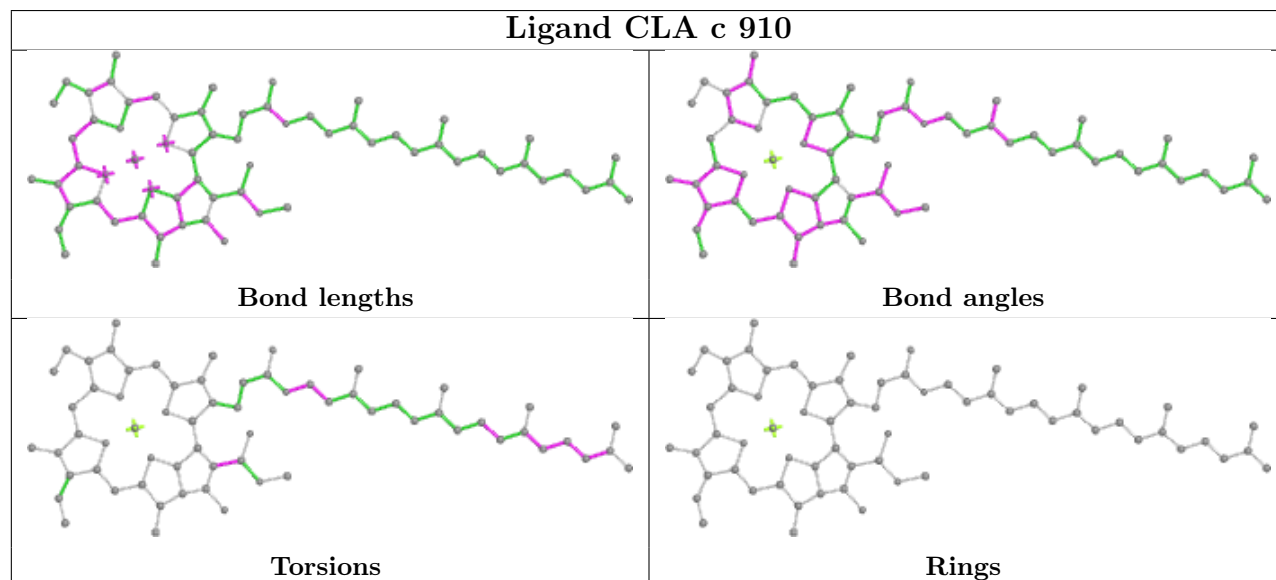
## Ligand CLA c 909



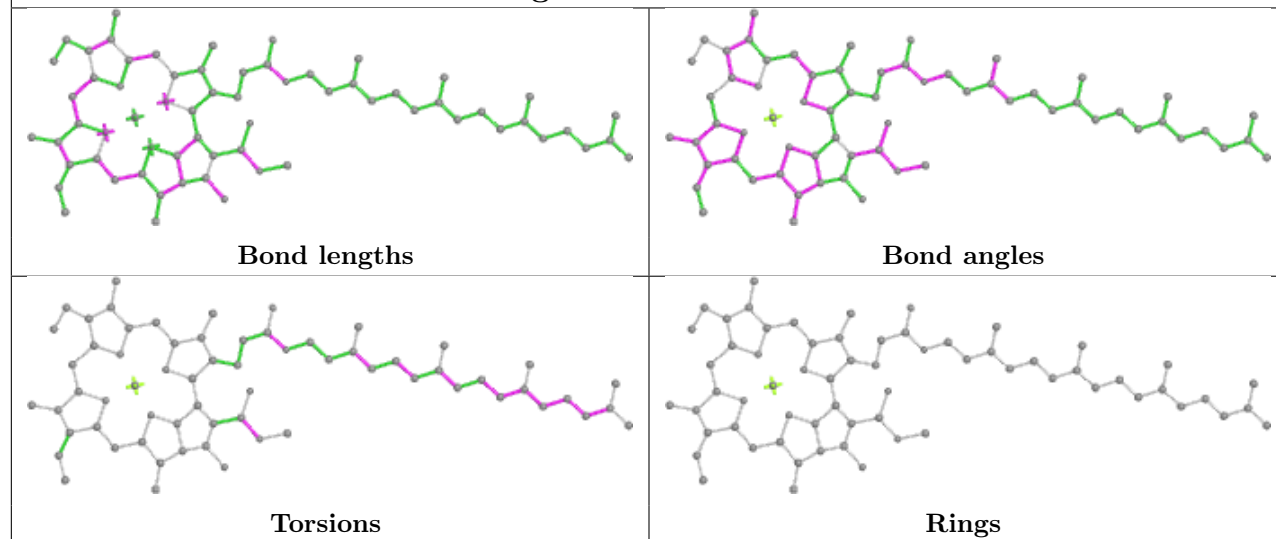
## Ligand CLA d 403



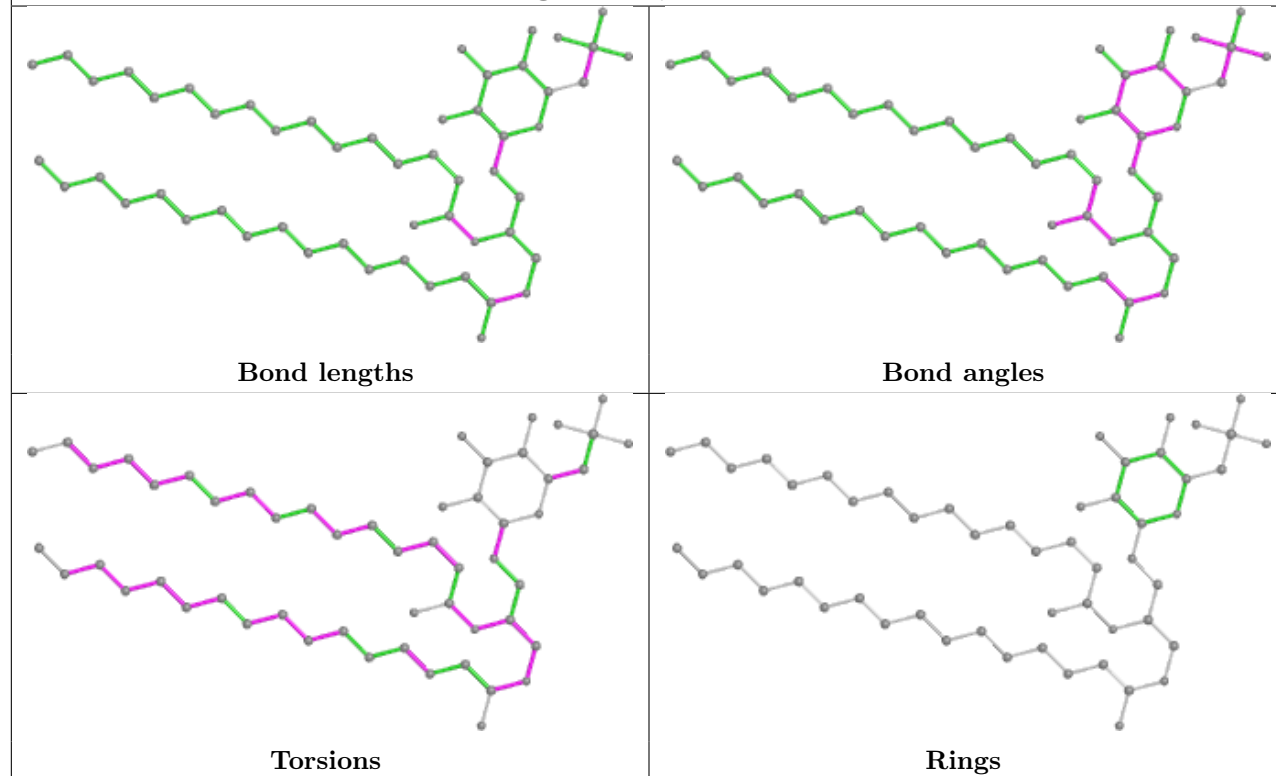
## Ligand CLA c 910

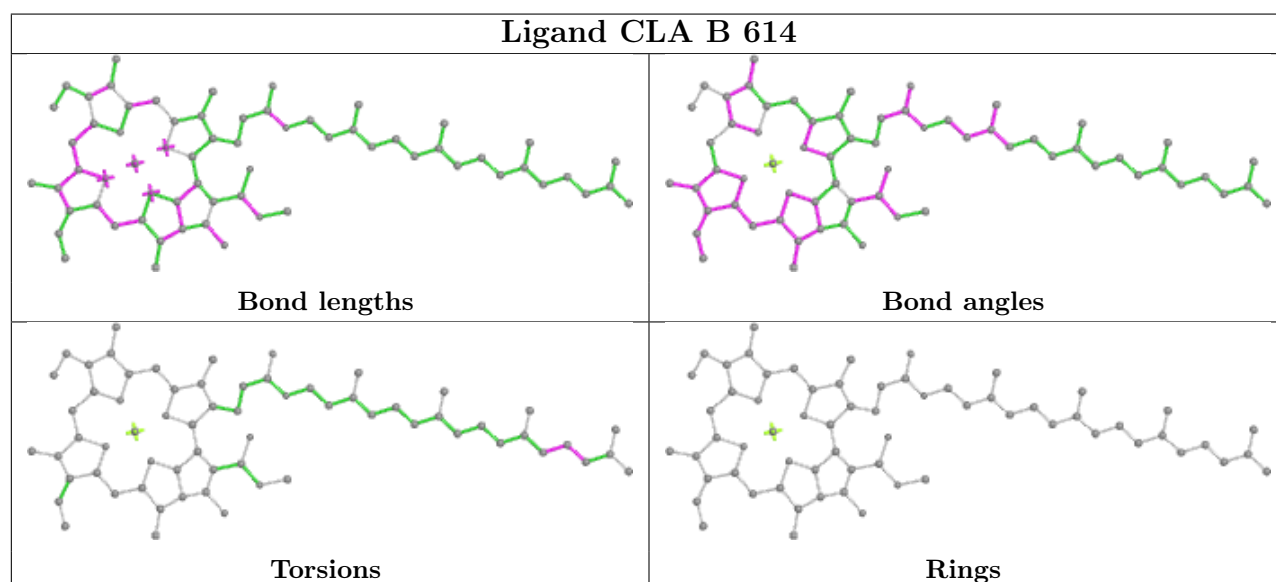
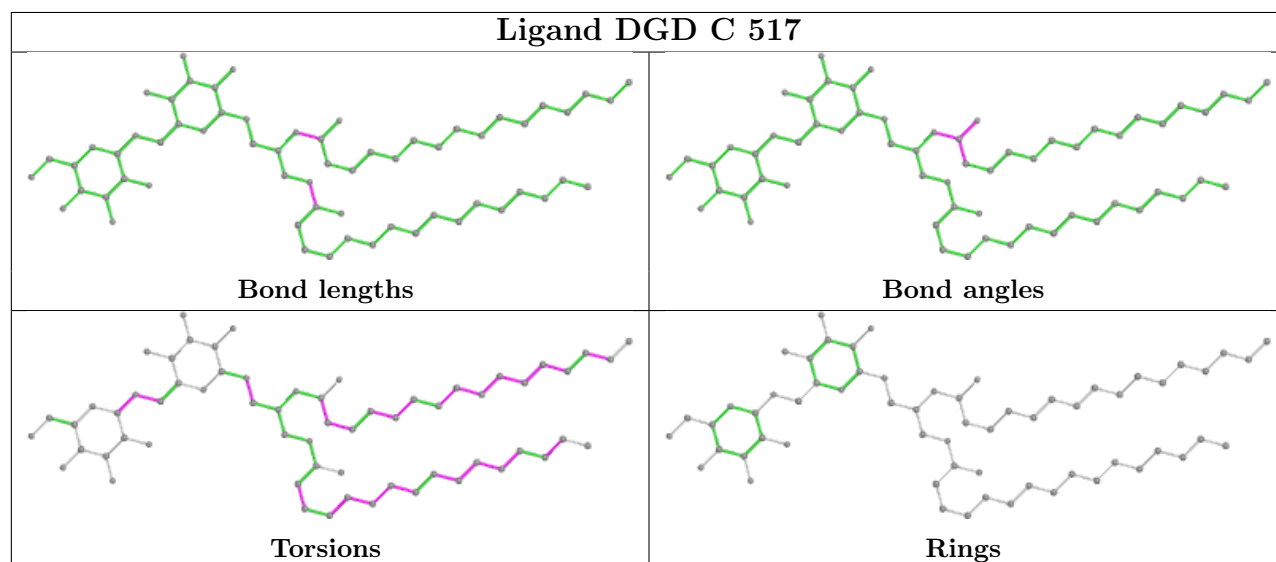
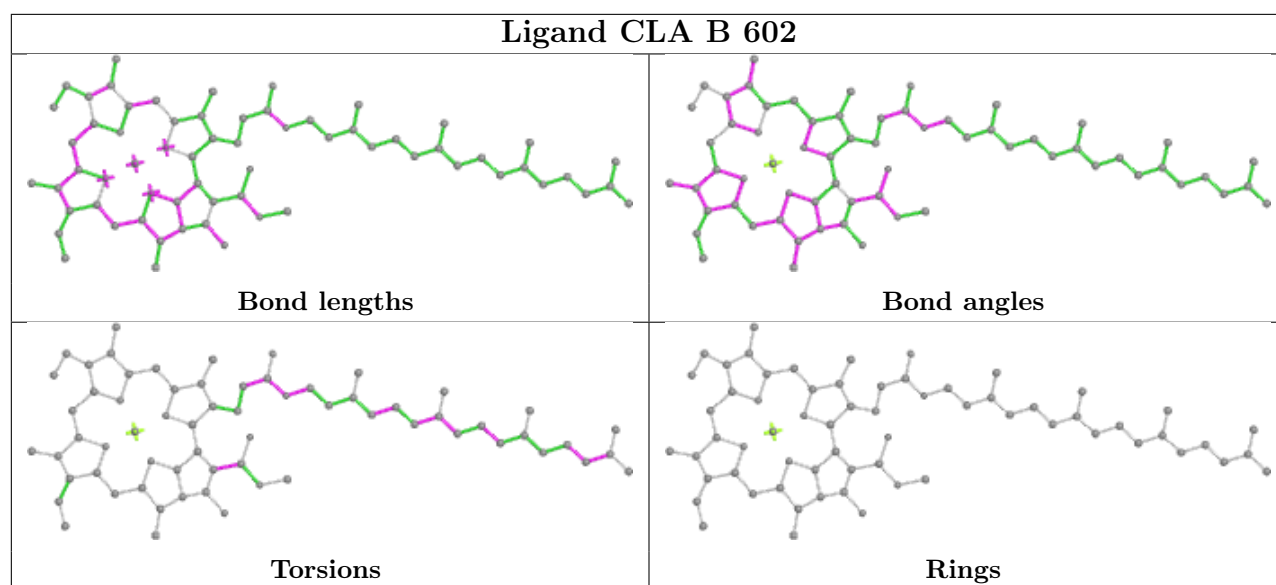


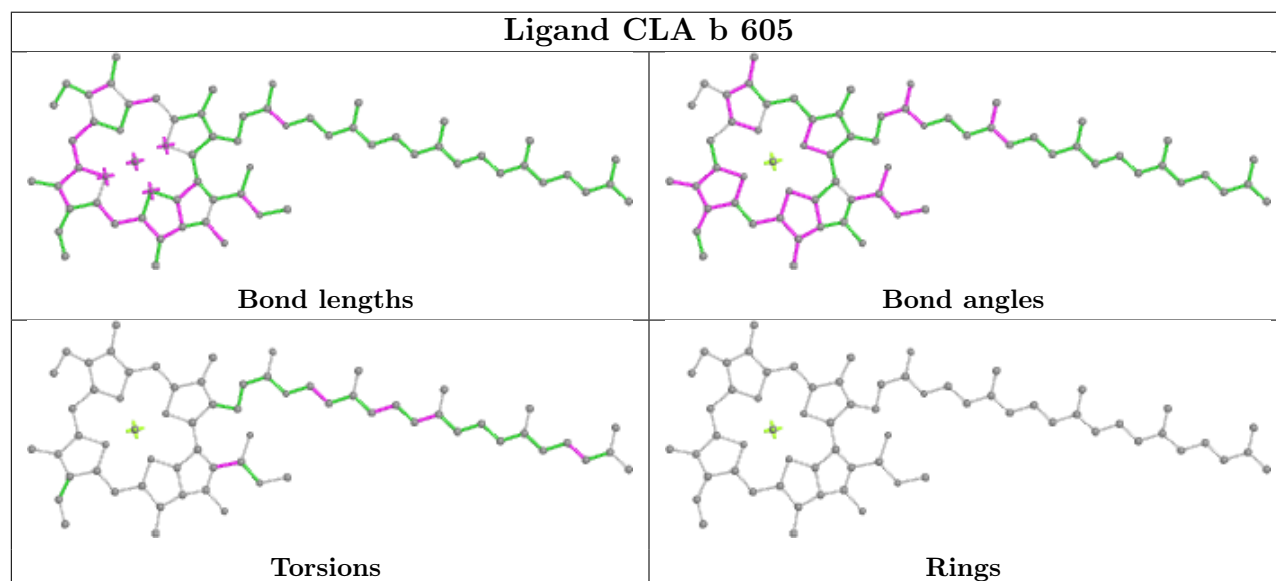
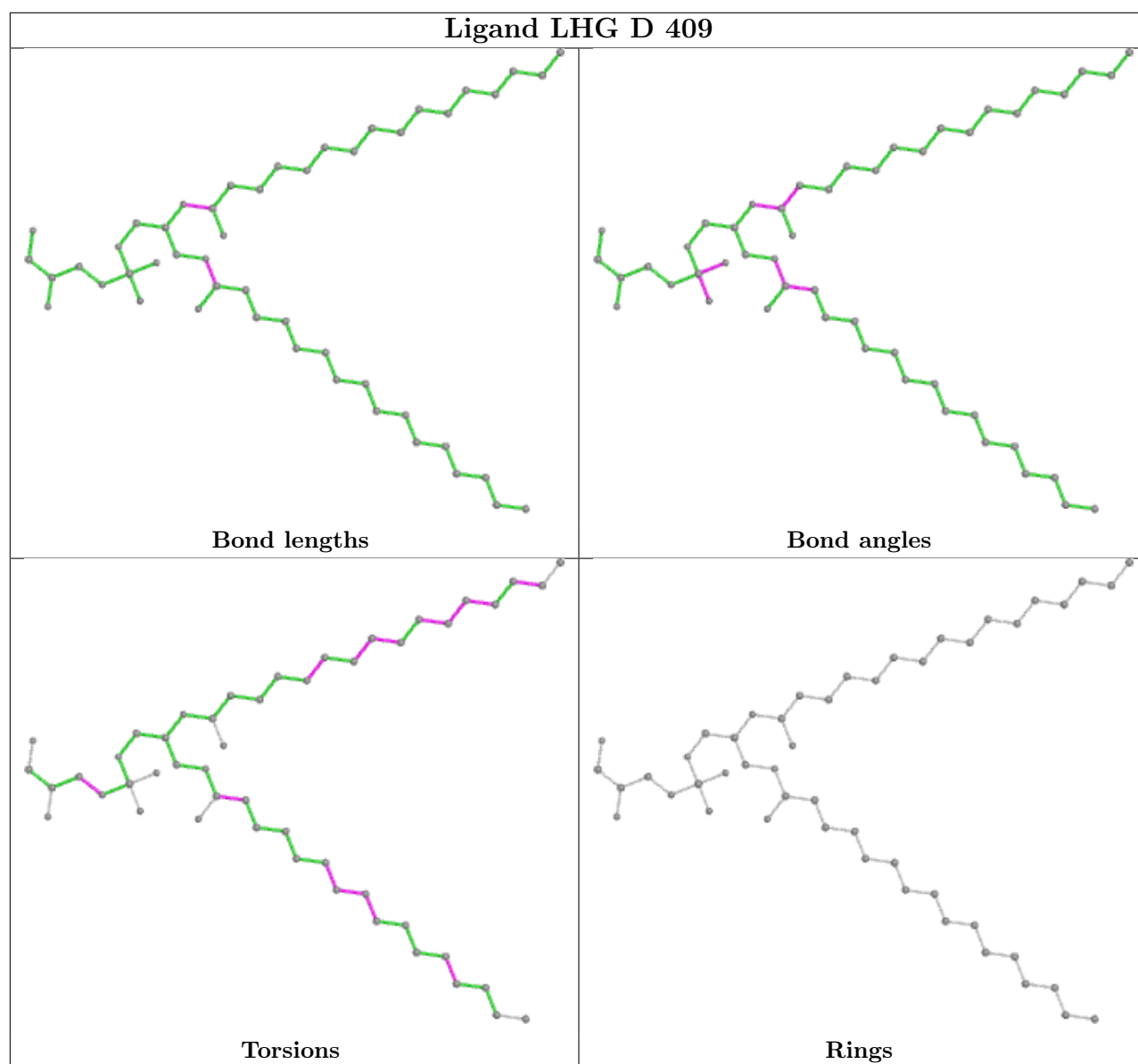
## Ligand CLA A 609

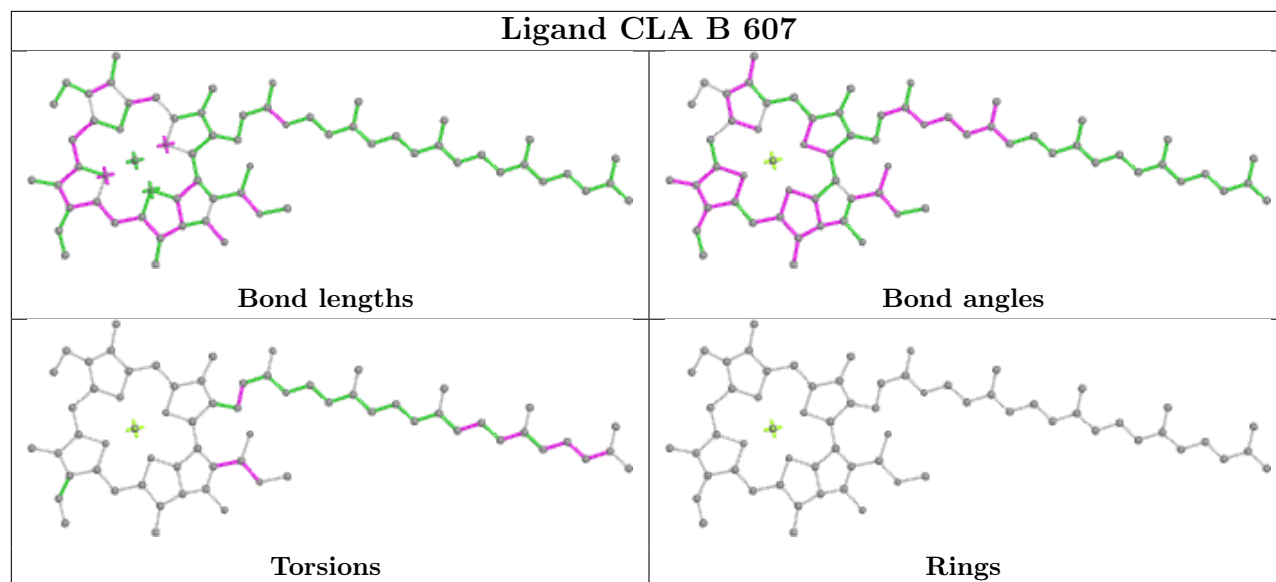
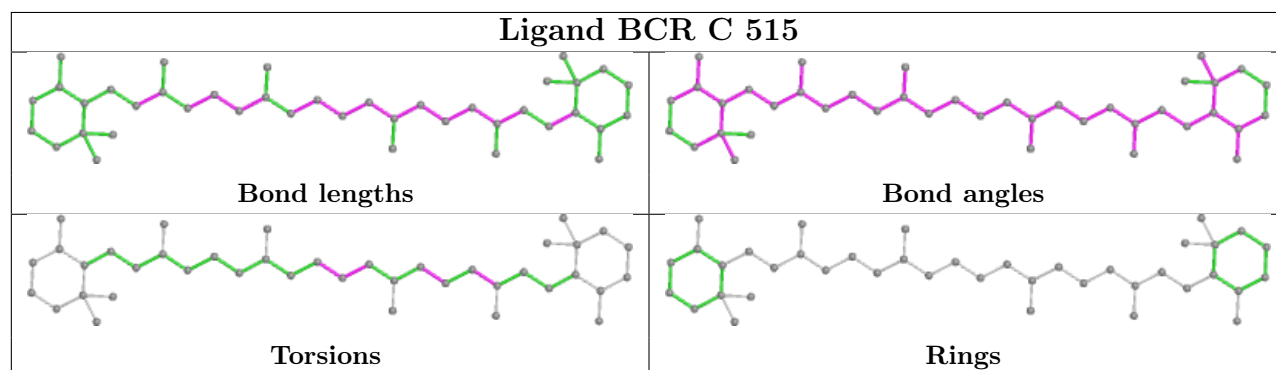
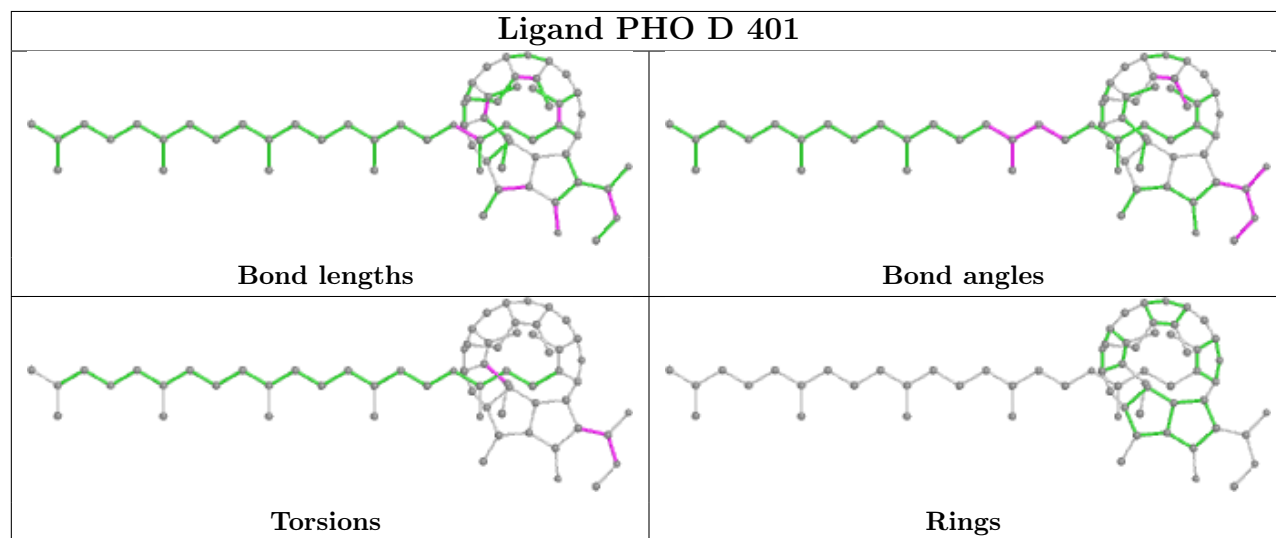


## Ligand SQD L 101

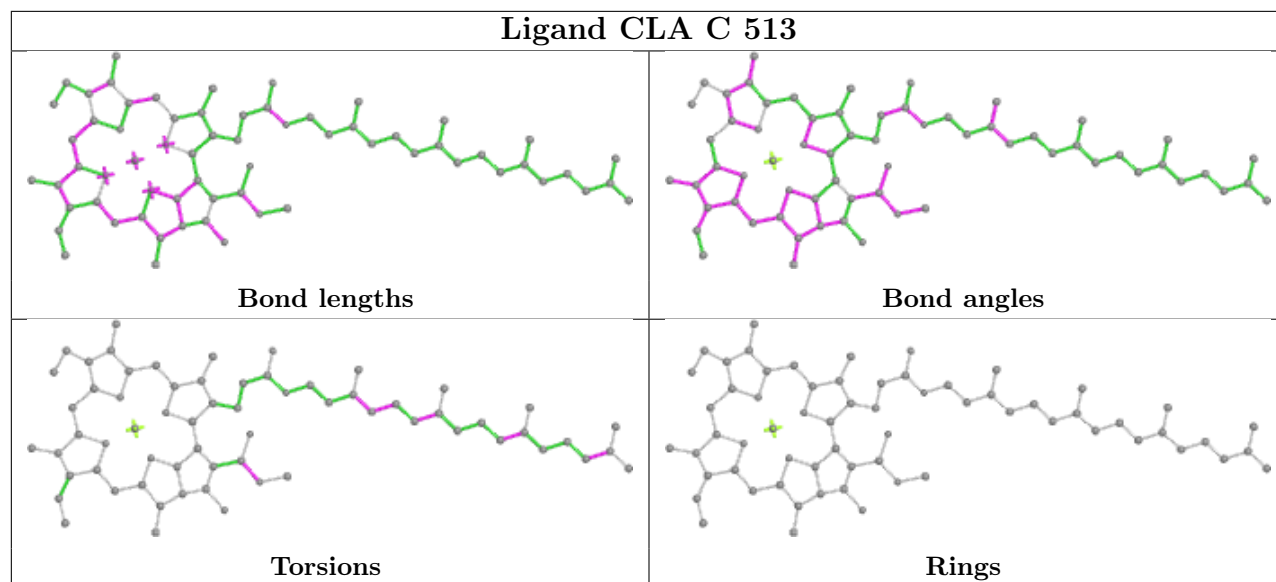
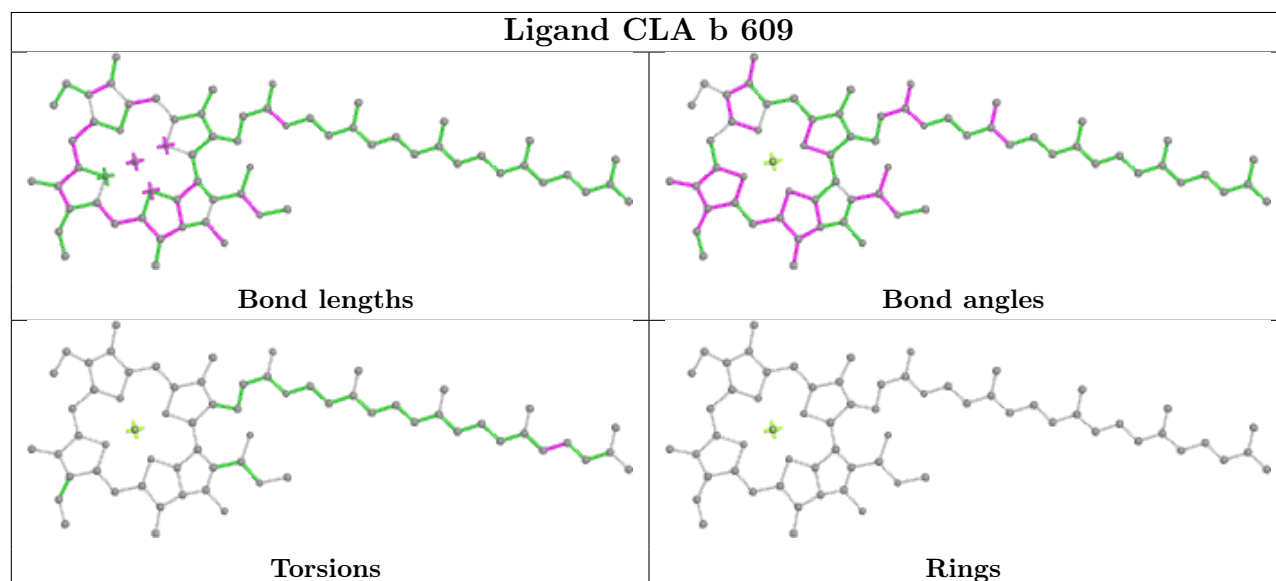
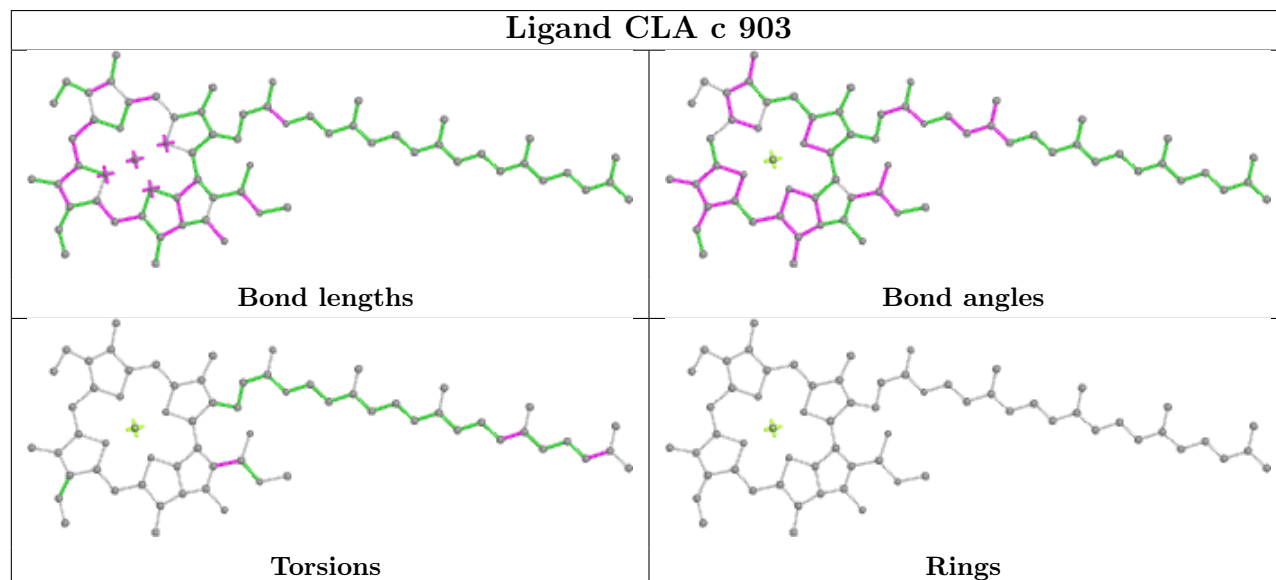


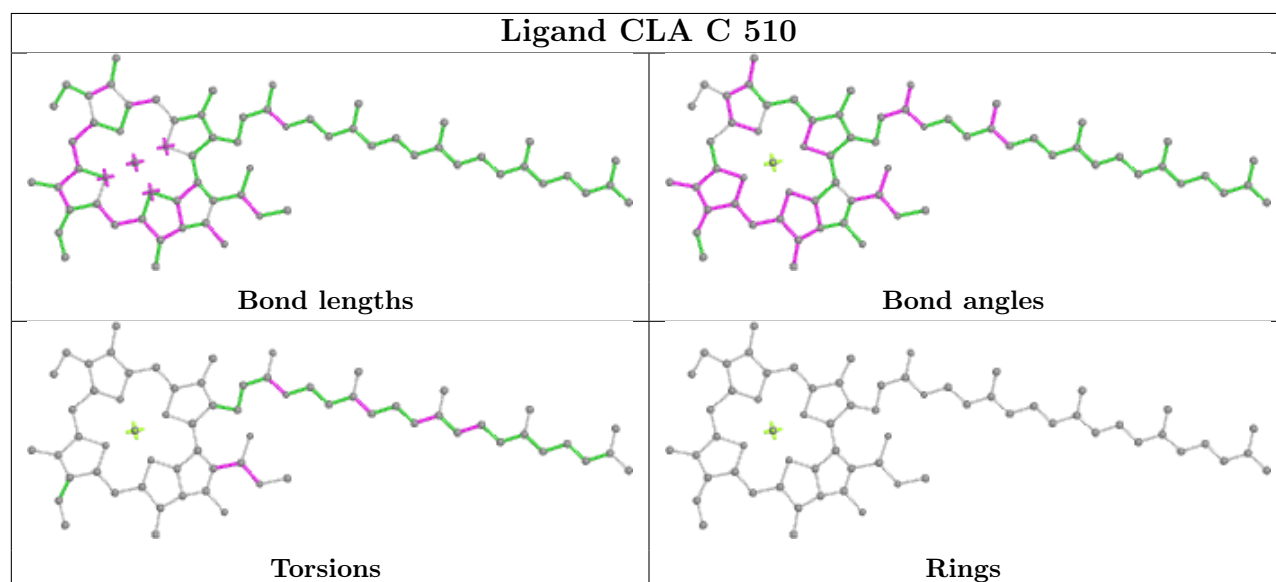
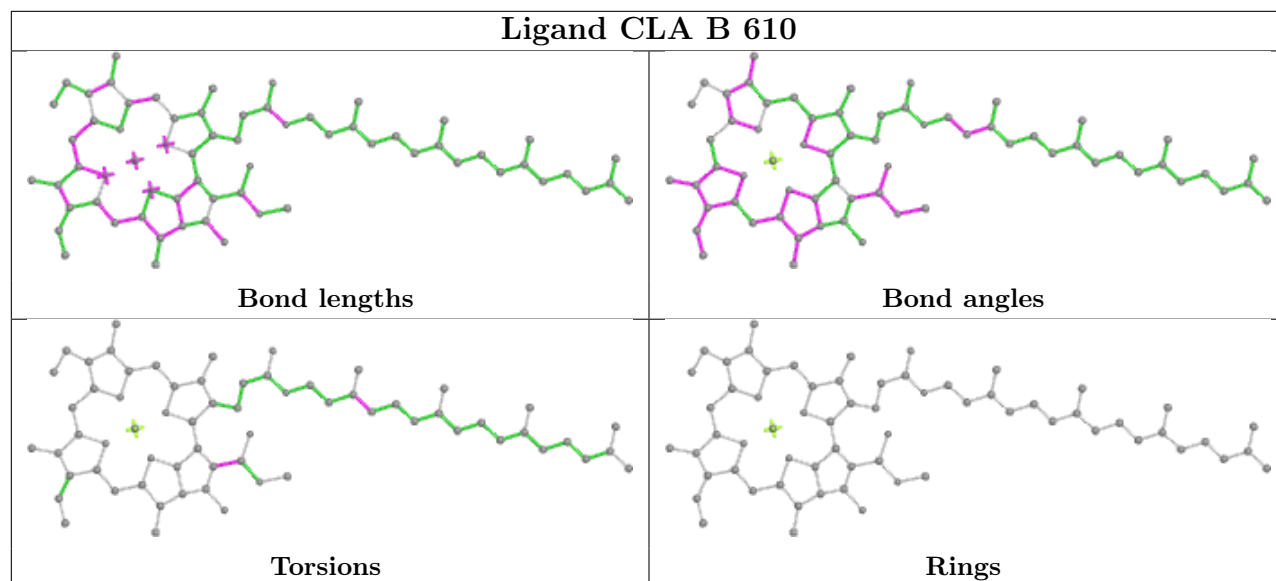
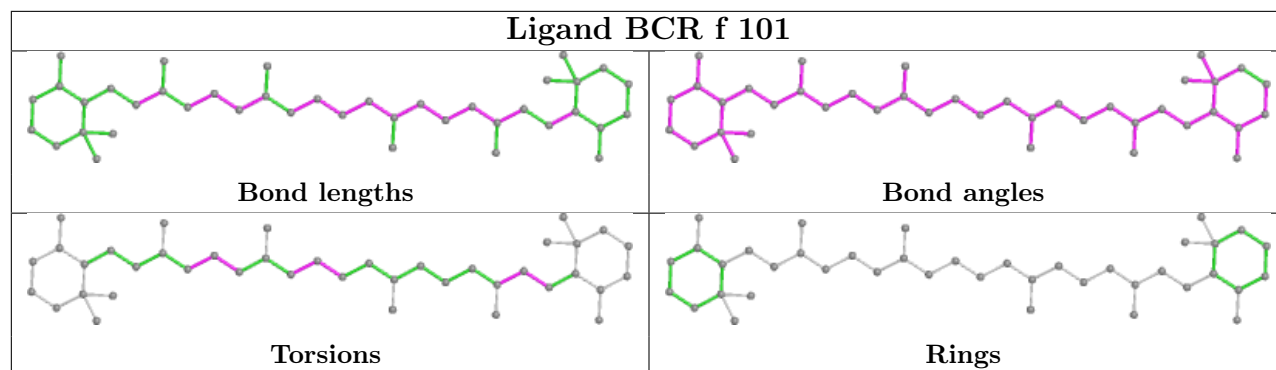


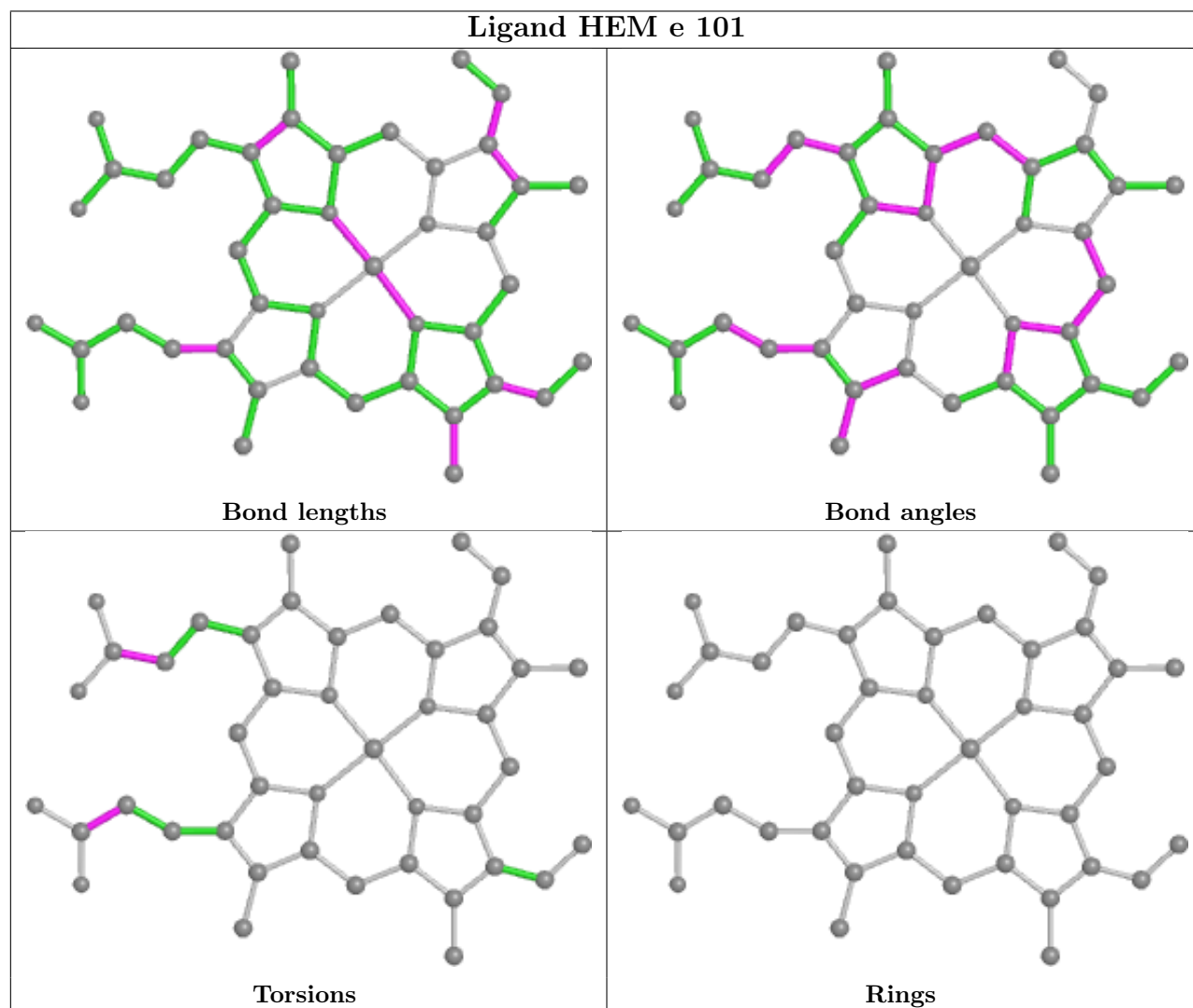
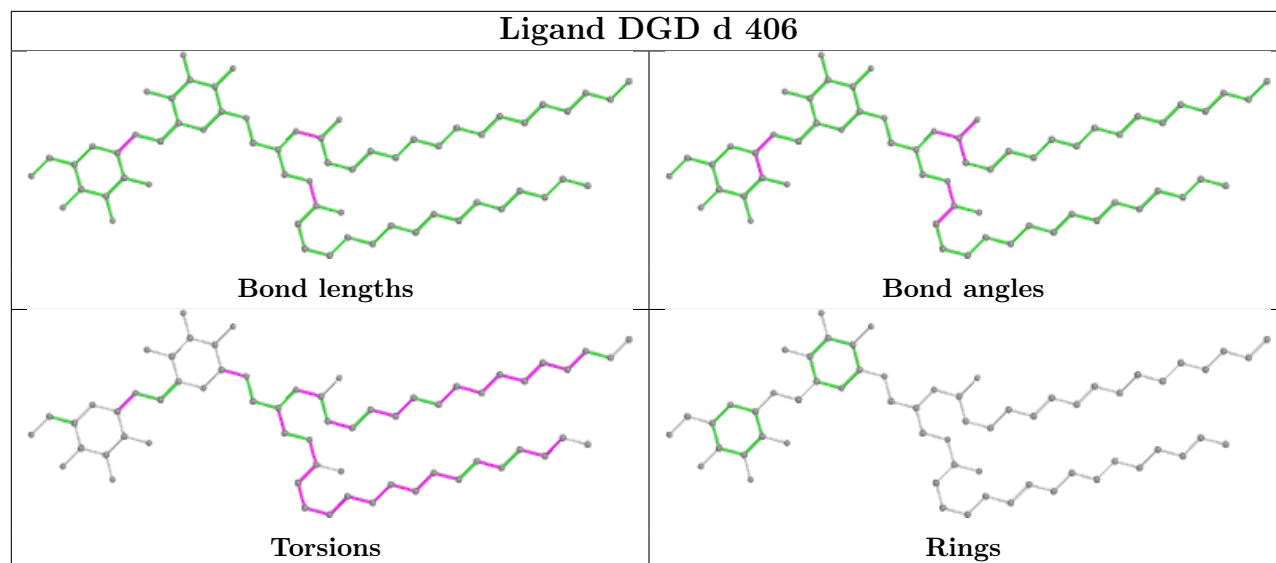


**Ligand CLA B 607****Ligand BCR C 515****Ligand PHO D 401**

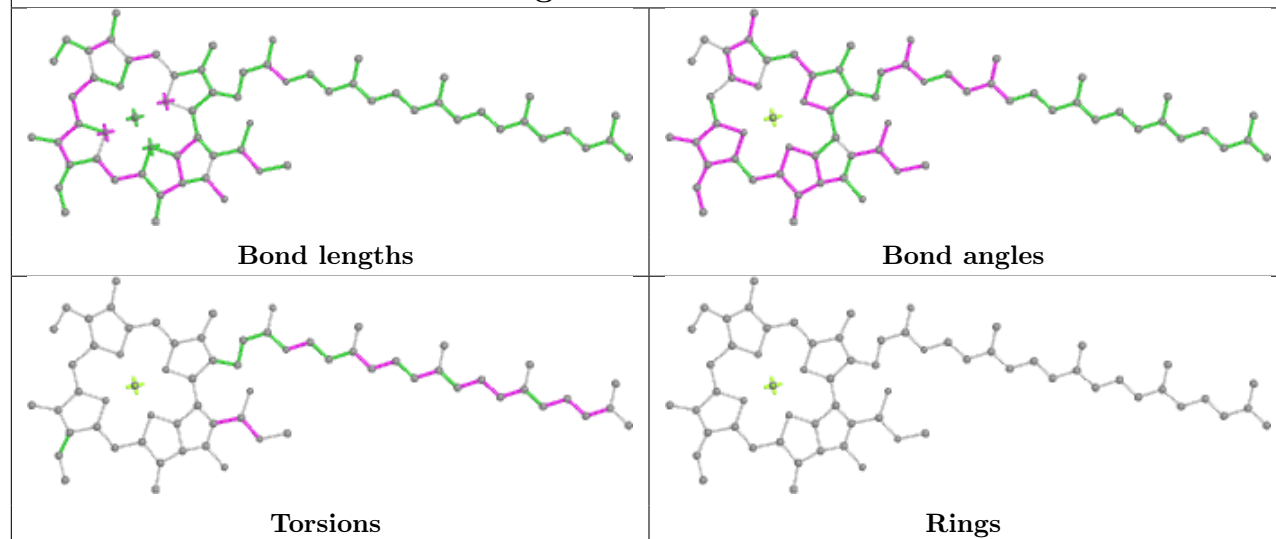


**Ligand CLA C 513****Ligand CLA b 609****Ligand CLA c 903**

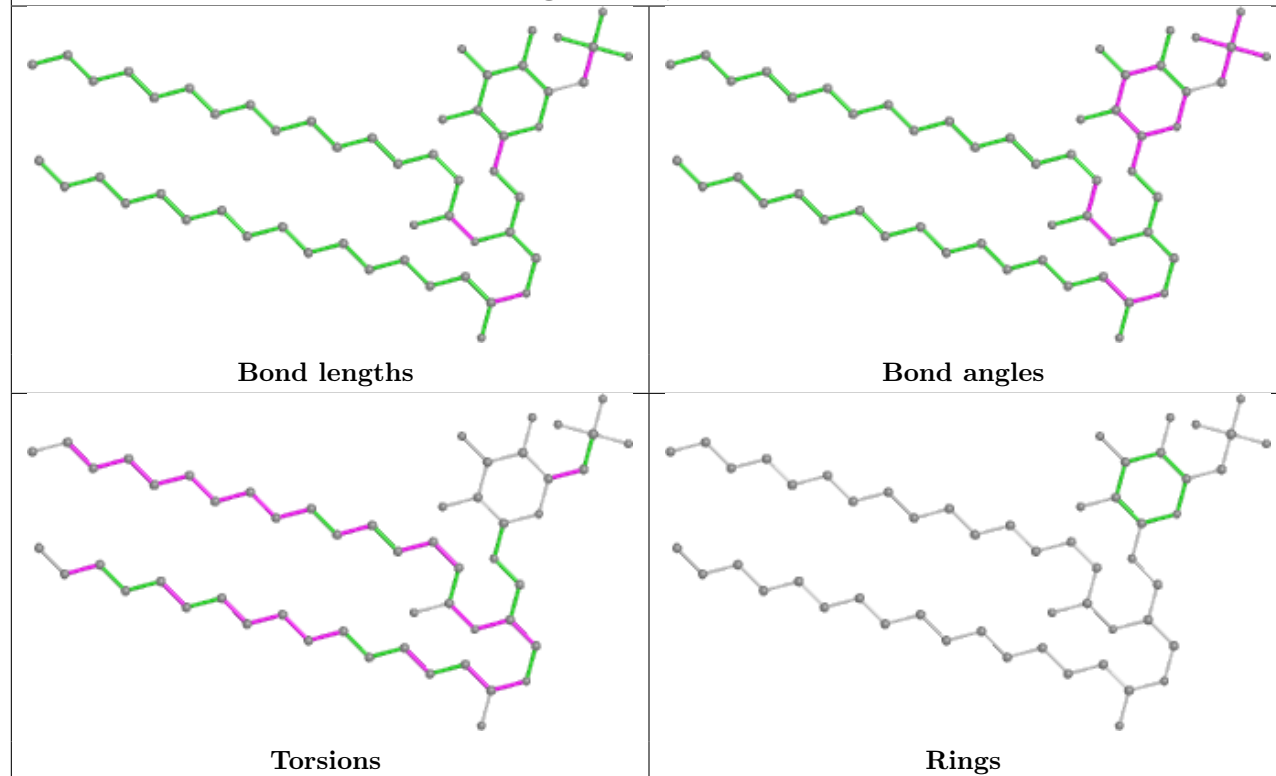


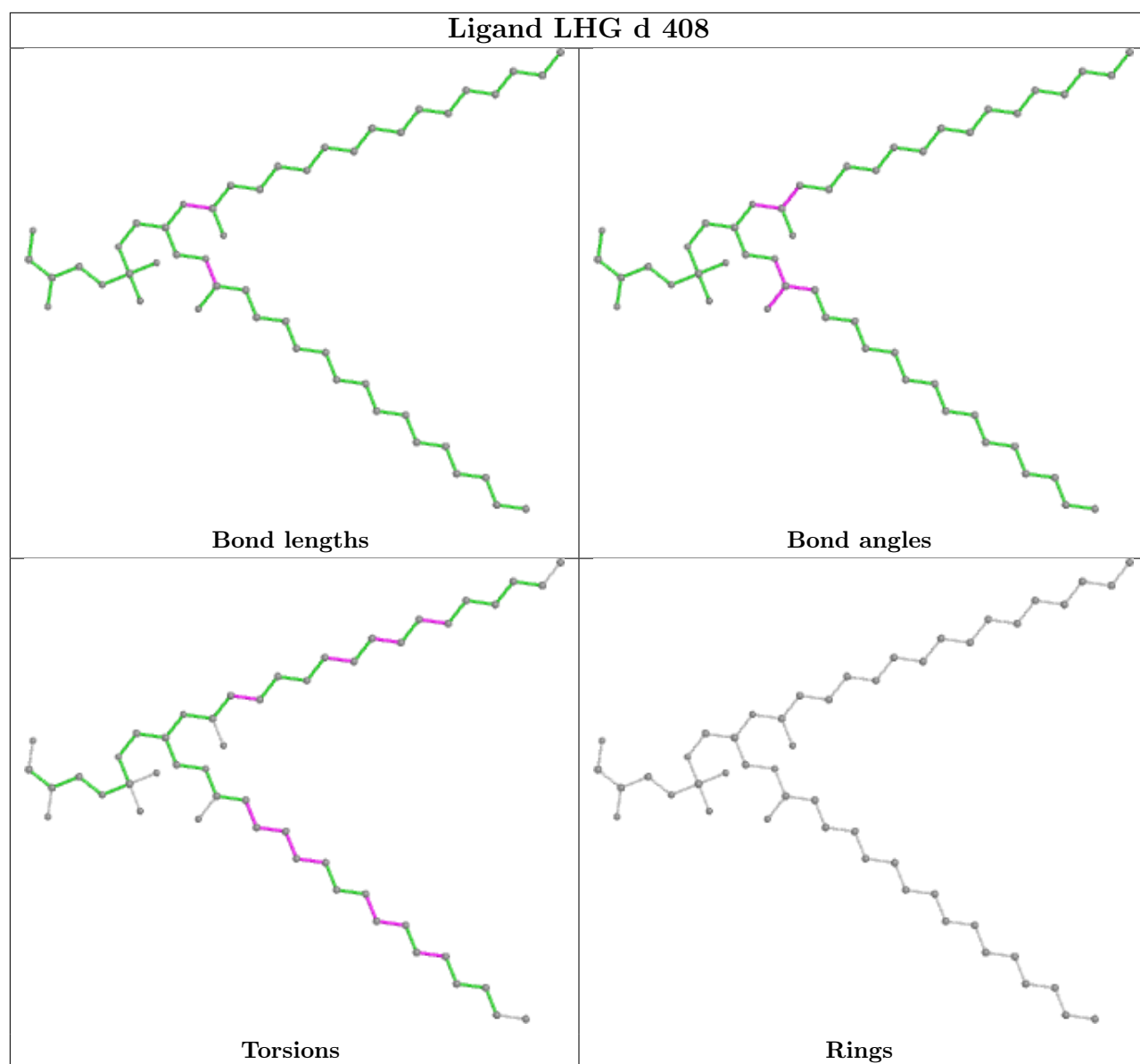


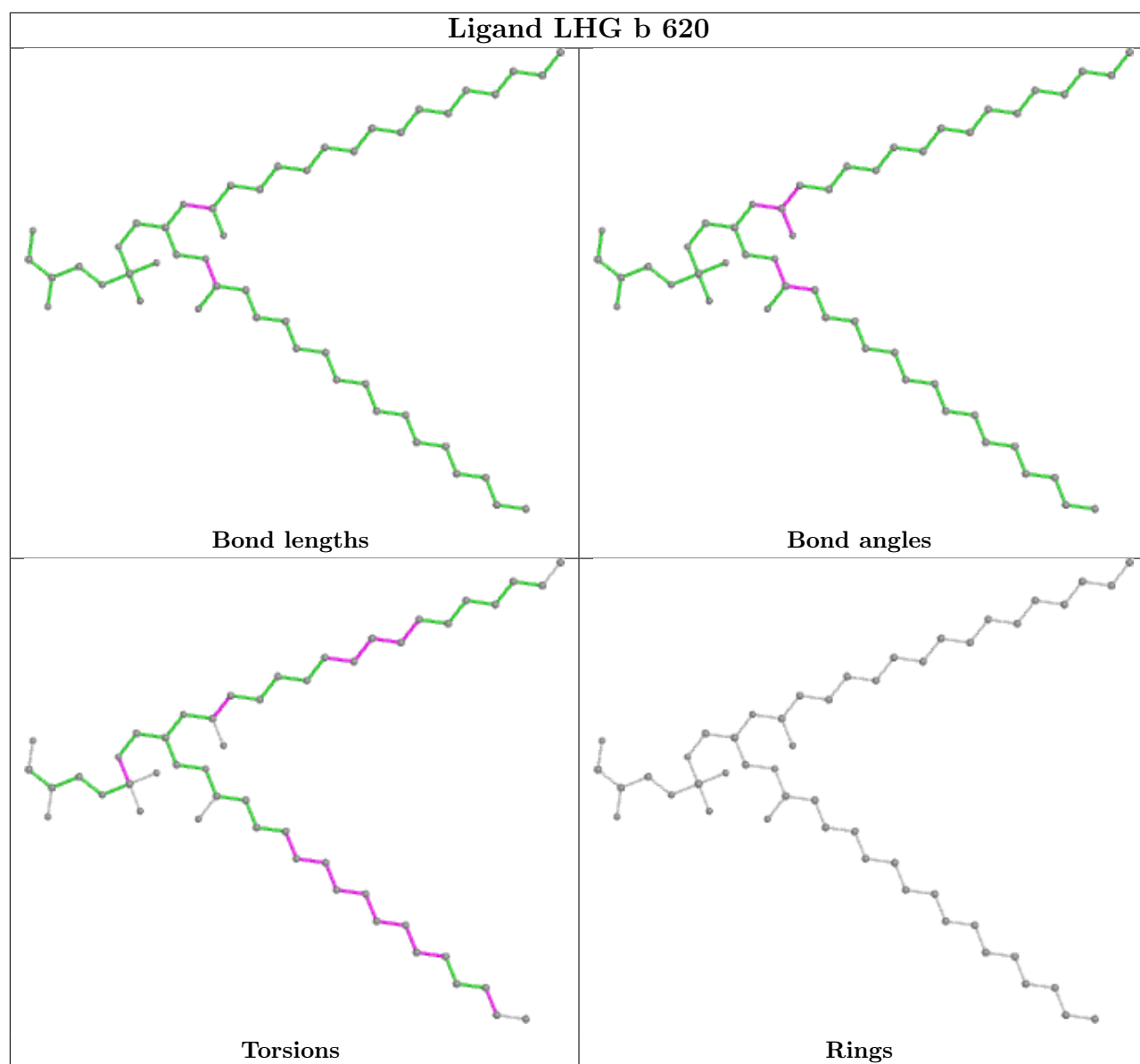
## Ligand CLA b 615

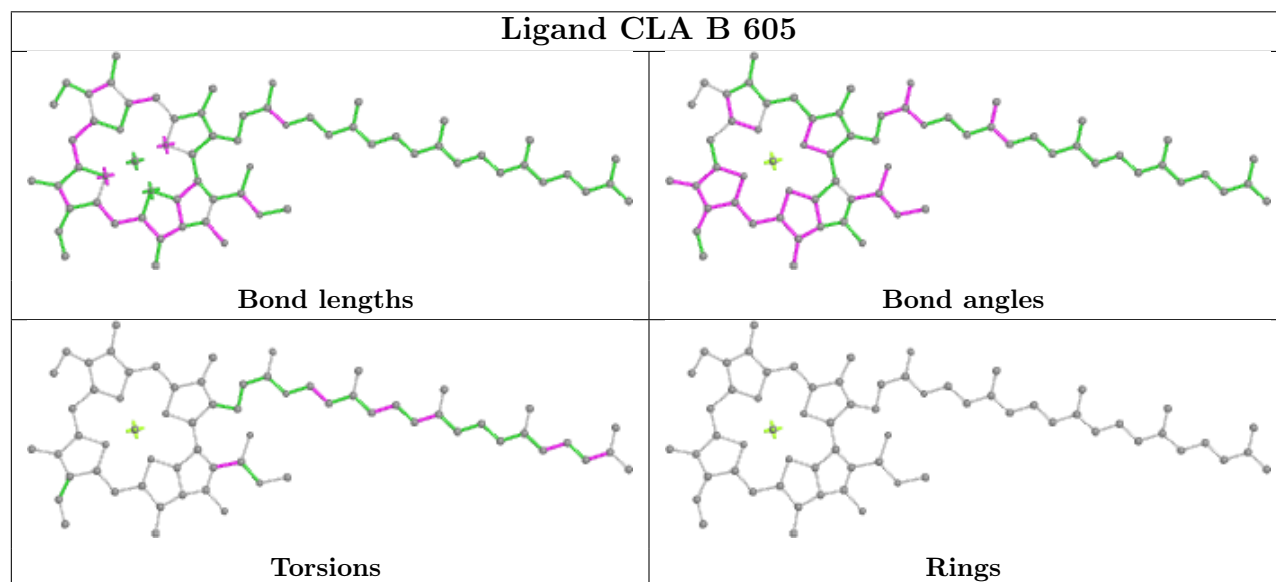
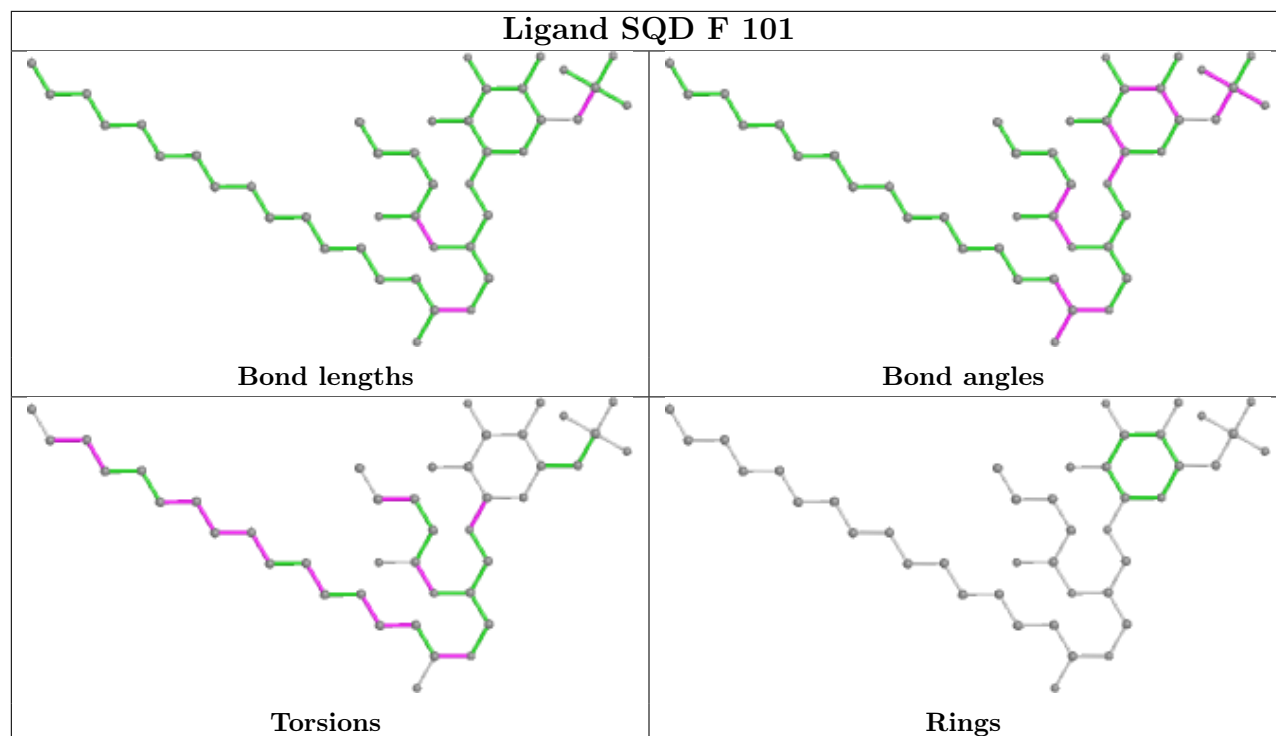


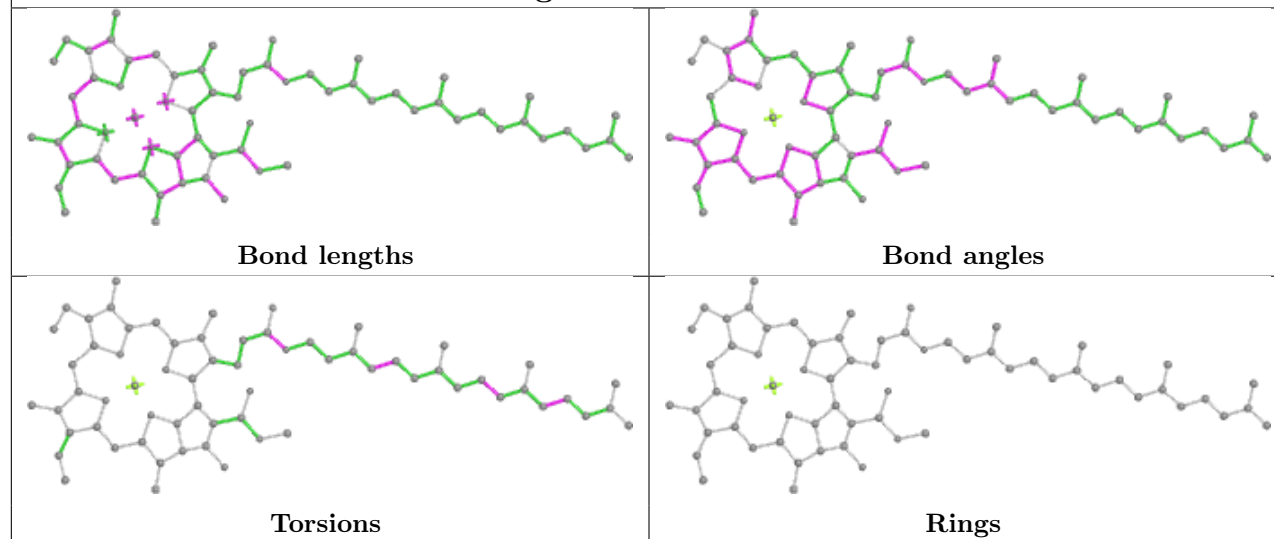
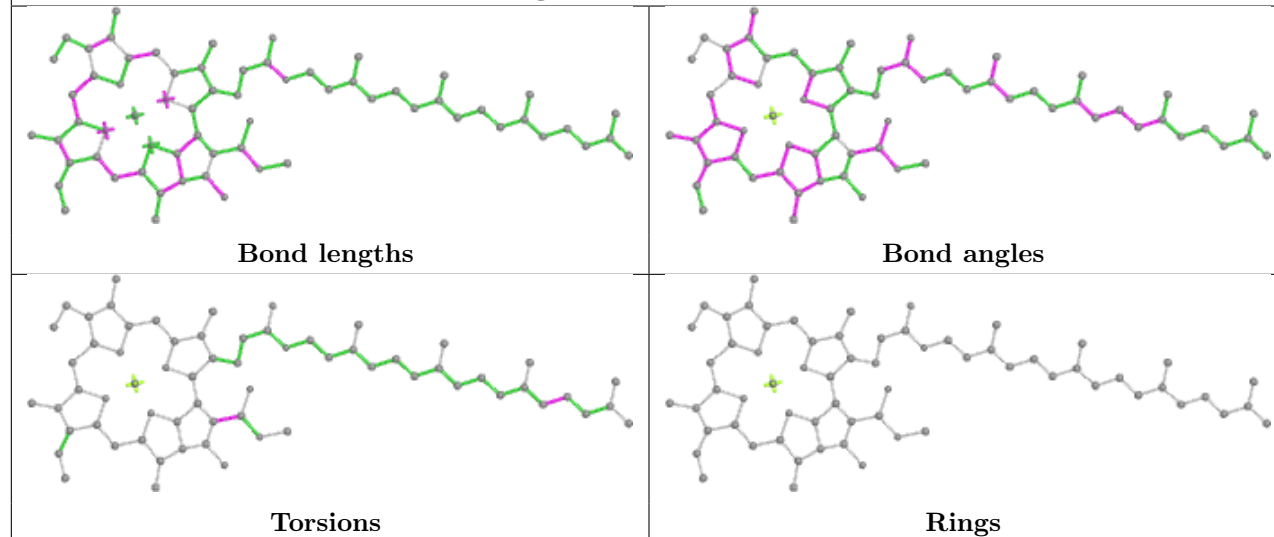
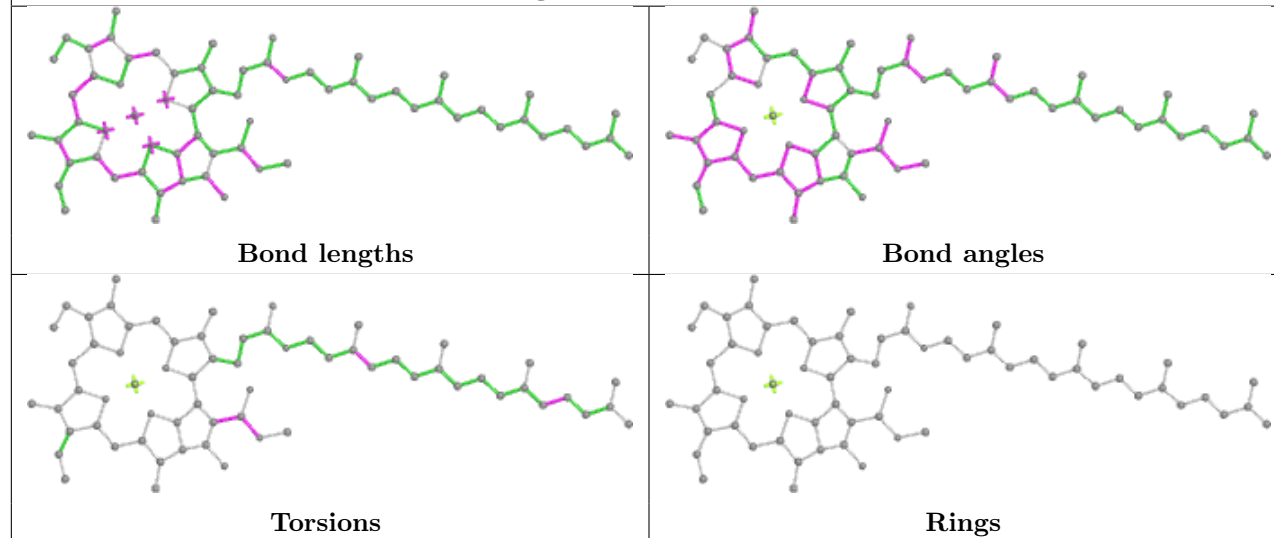
## Ligand SQD 1 101



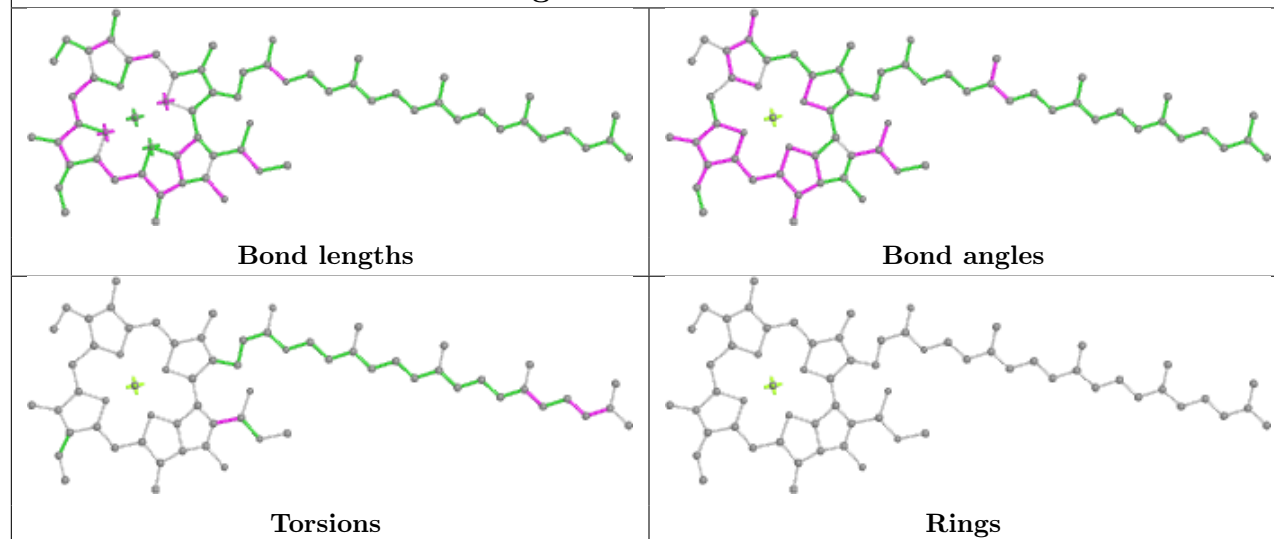
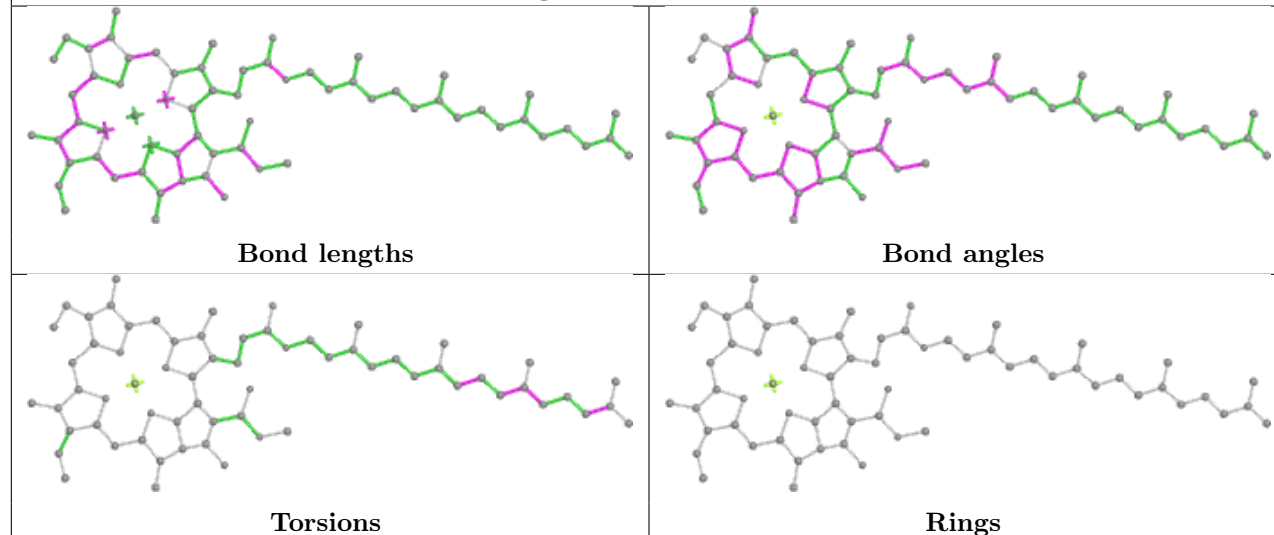
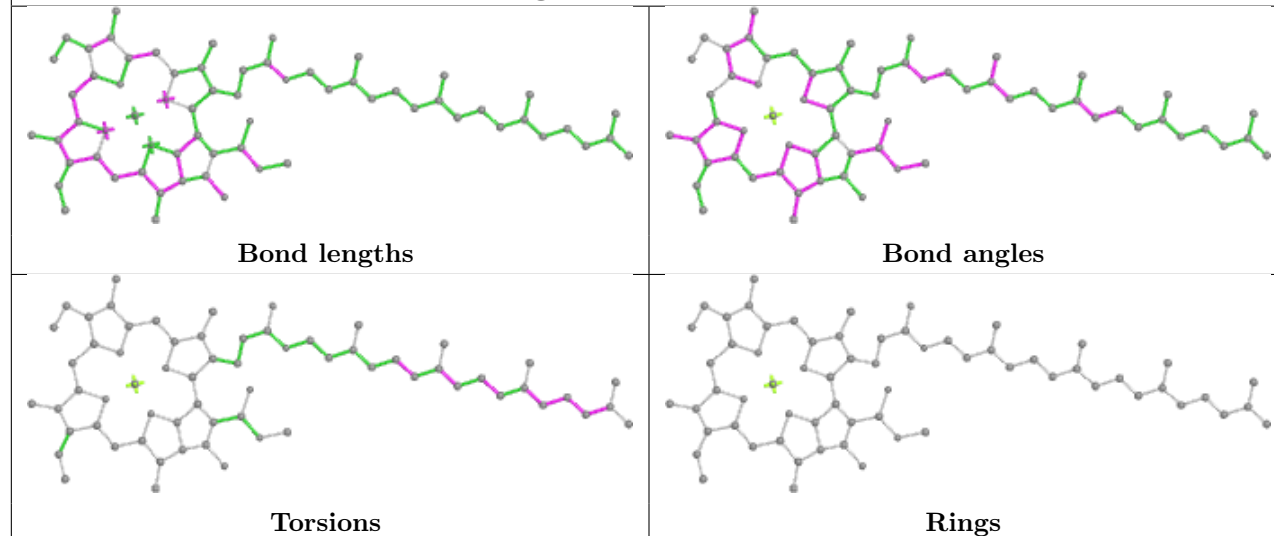


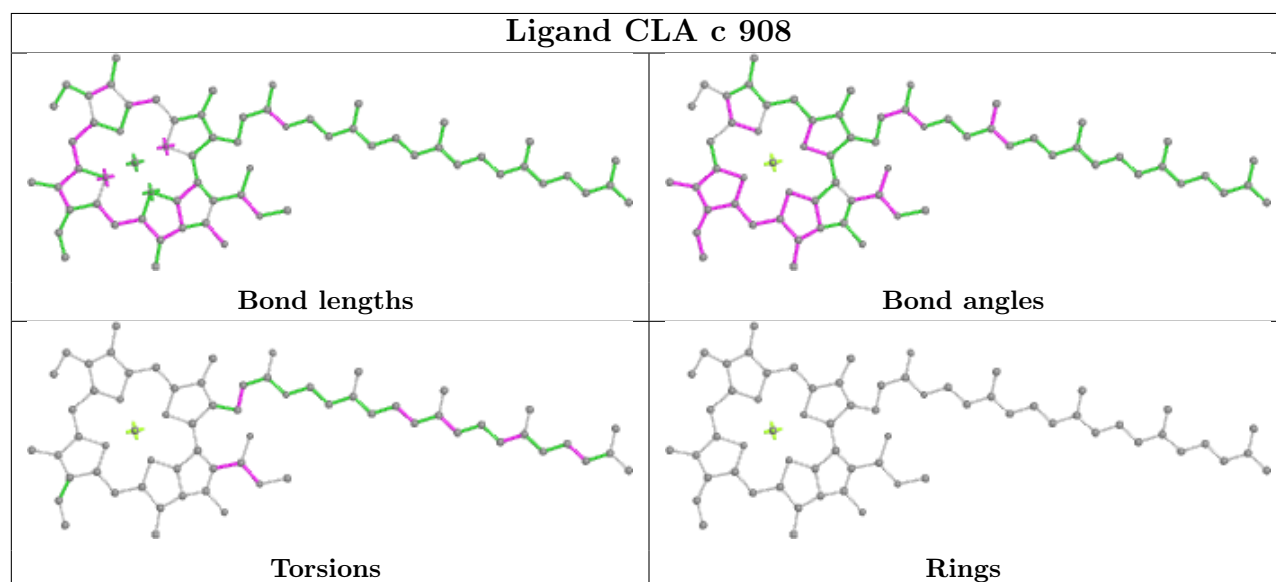
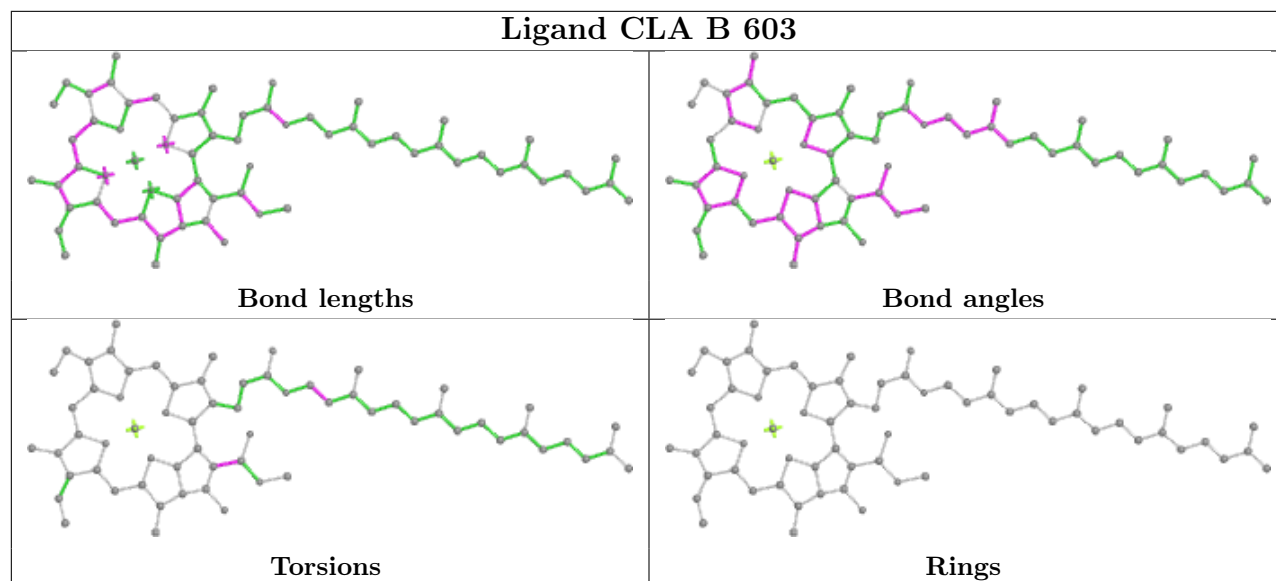
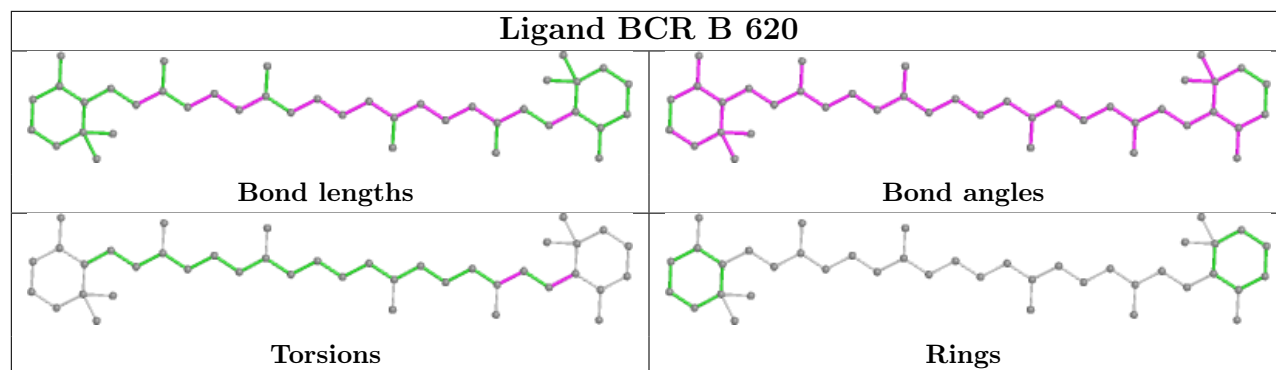




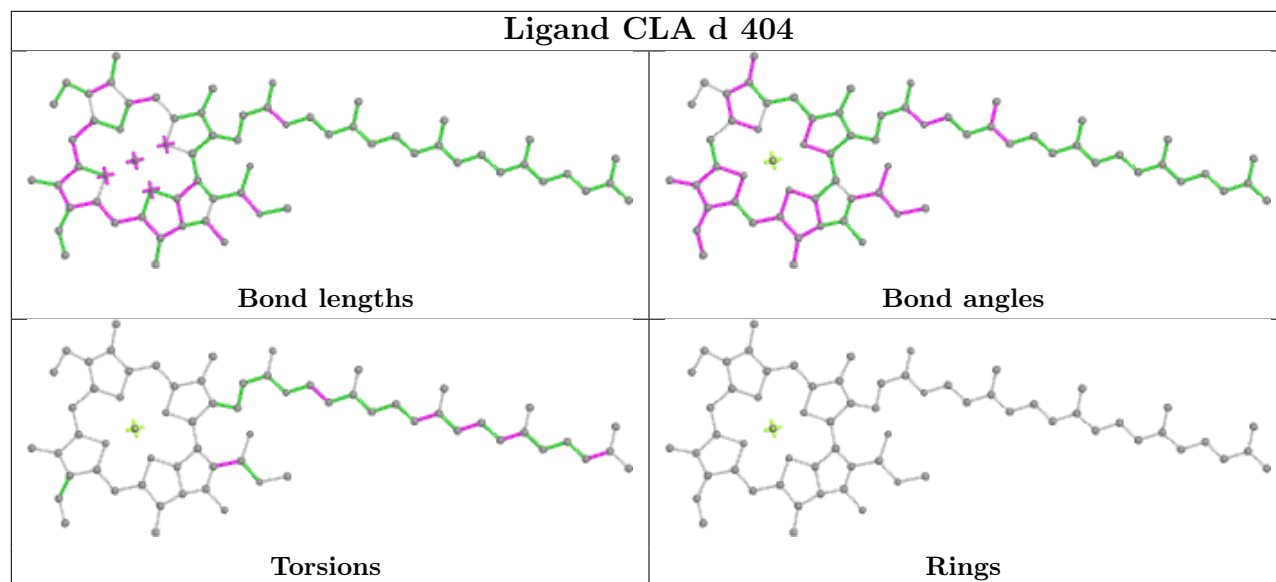
**Ligand CLA b 613****Ligand CLA B 609****Ligand CLA B 606**



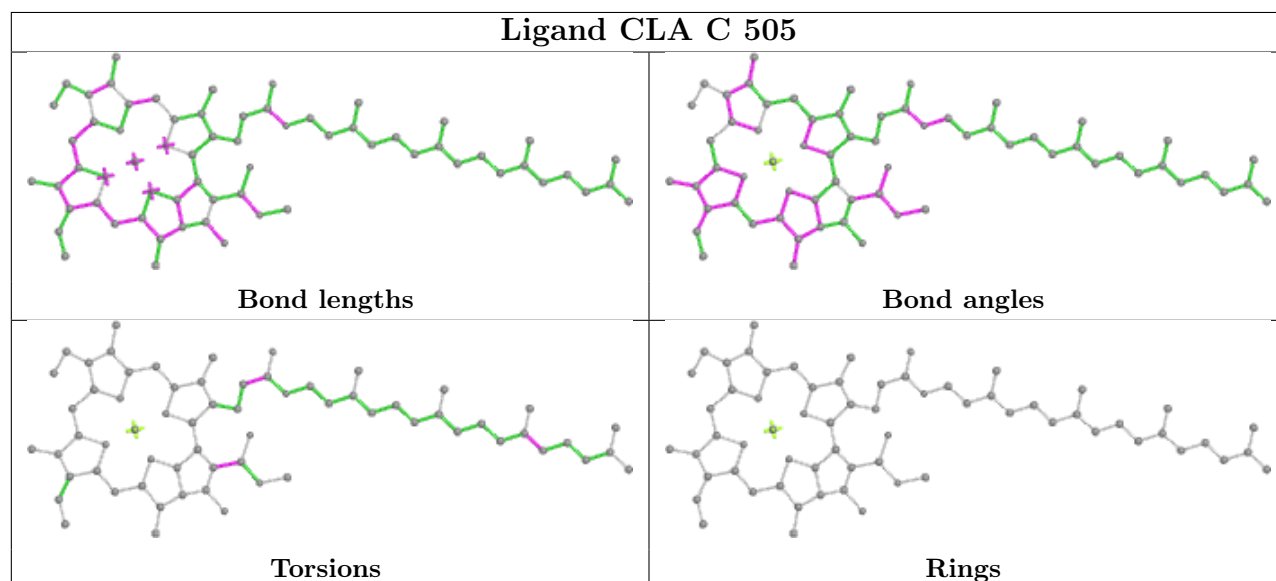
**Ligand CLA C 502****Ligand CLA b 614****Ligand CLA B 616**



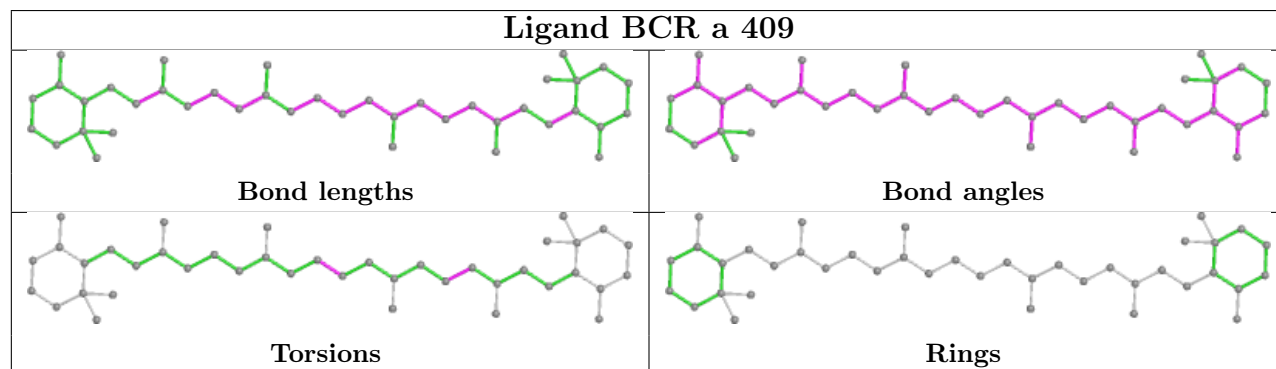
## Ligand CLA d 404

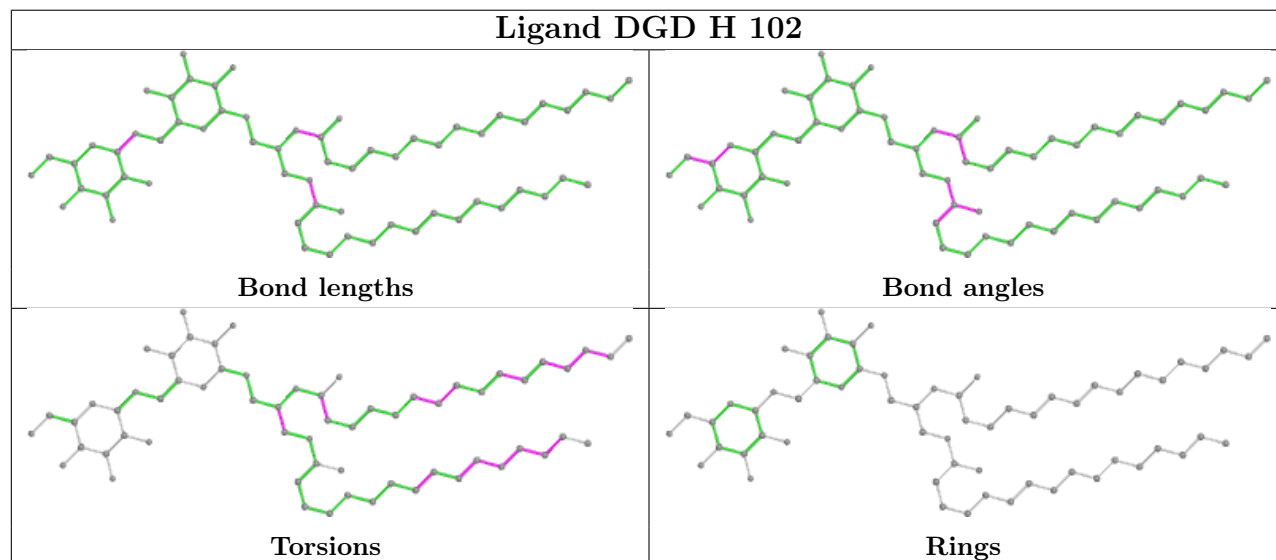
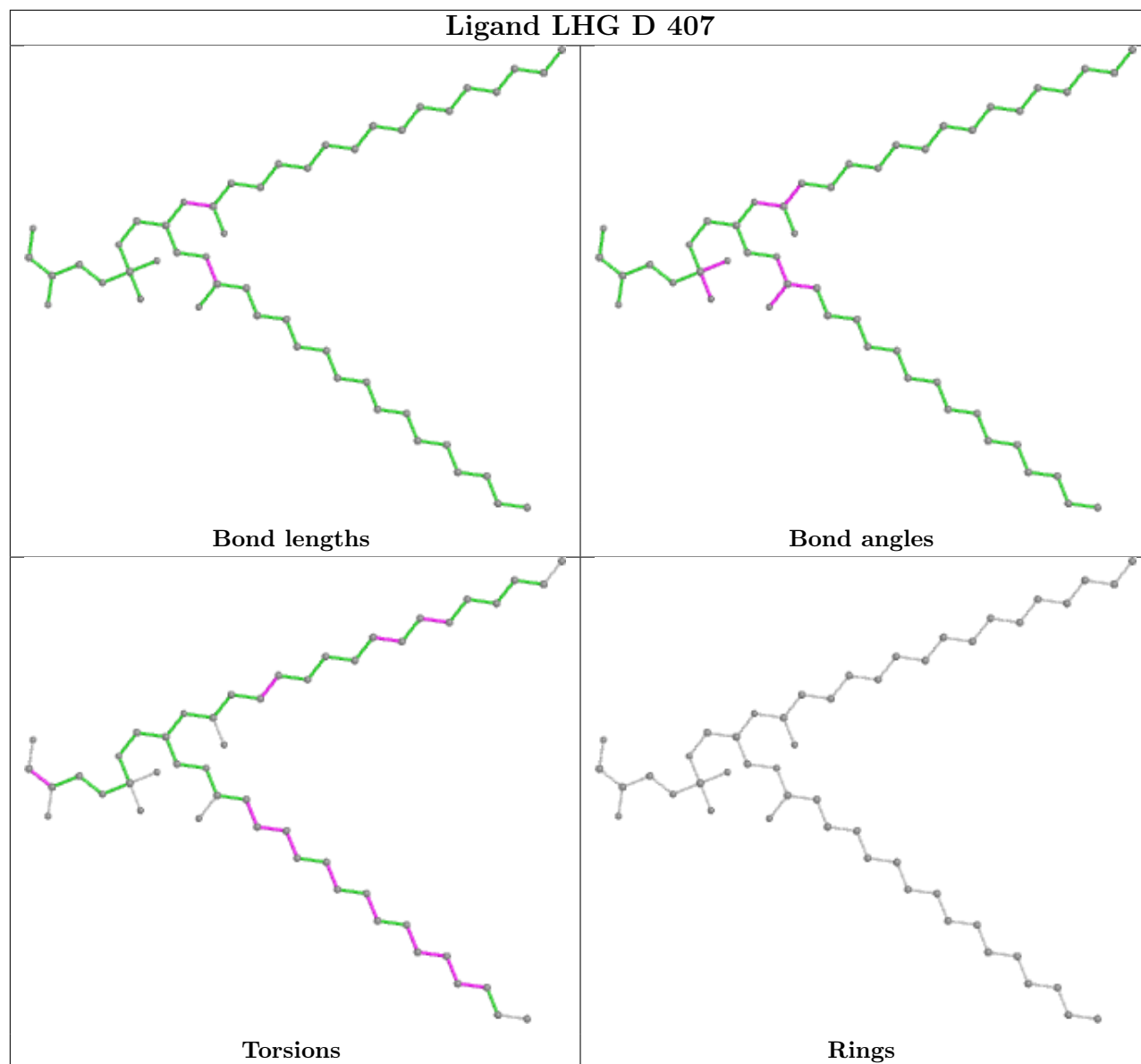


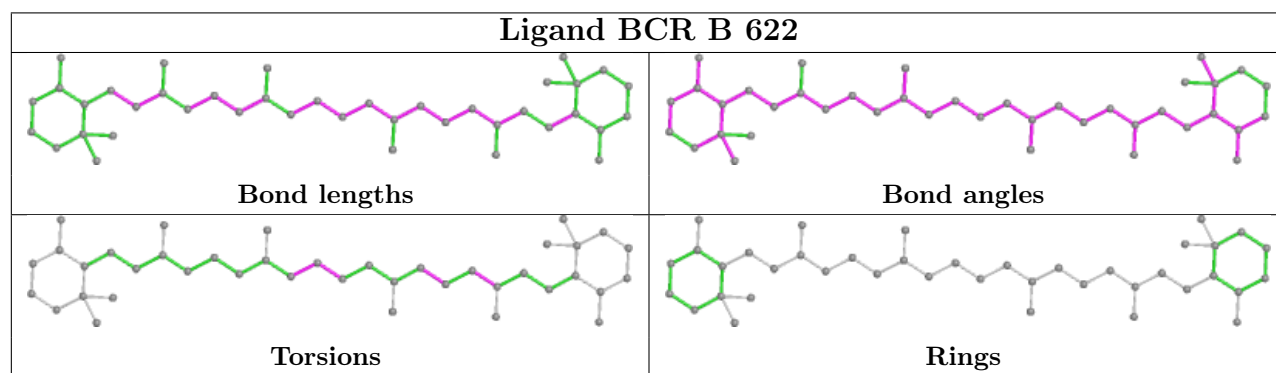
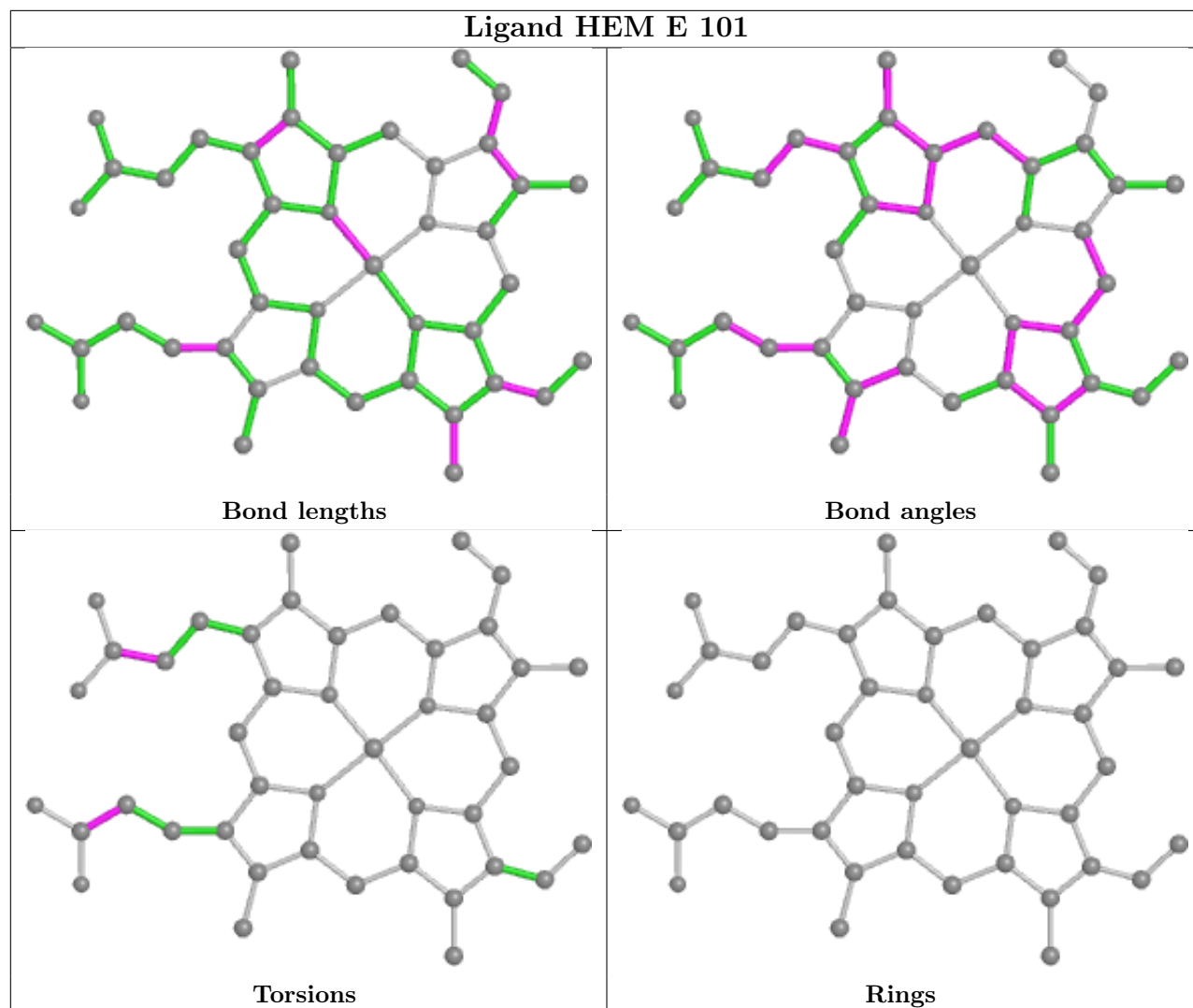
## Ligand CLA C 505

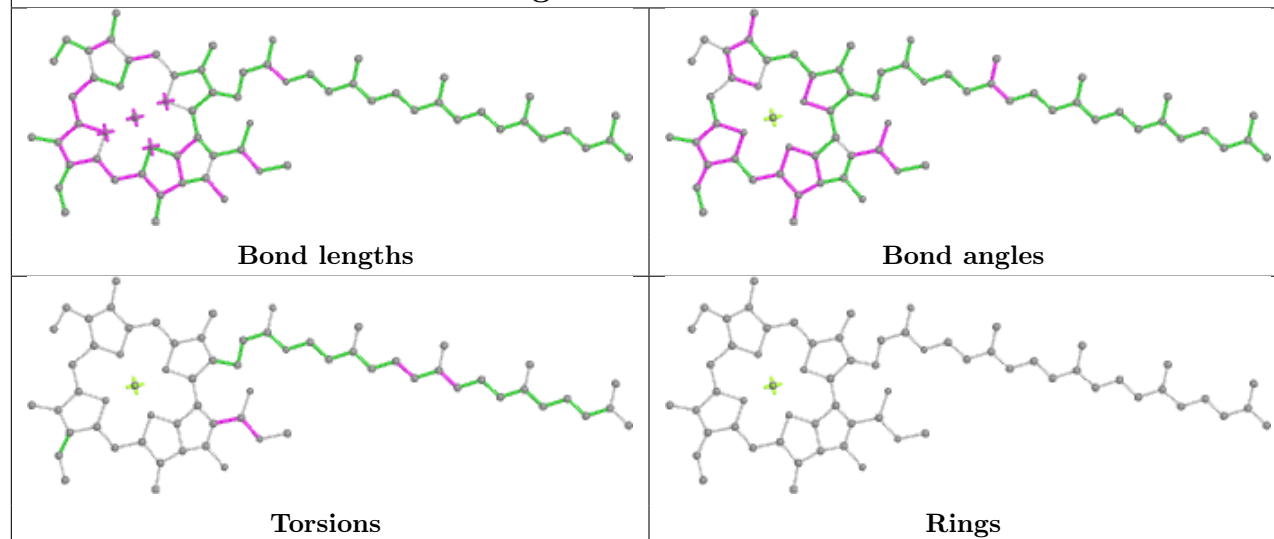
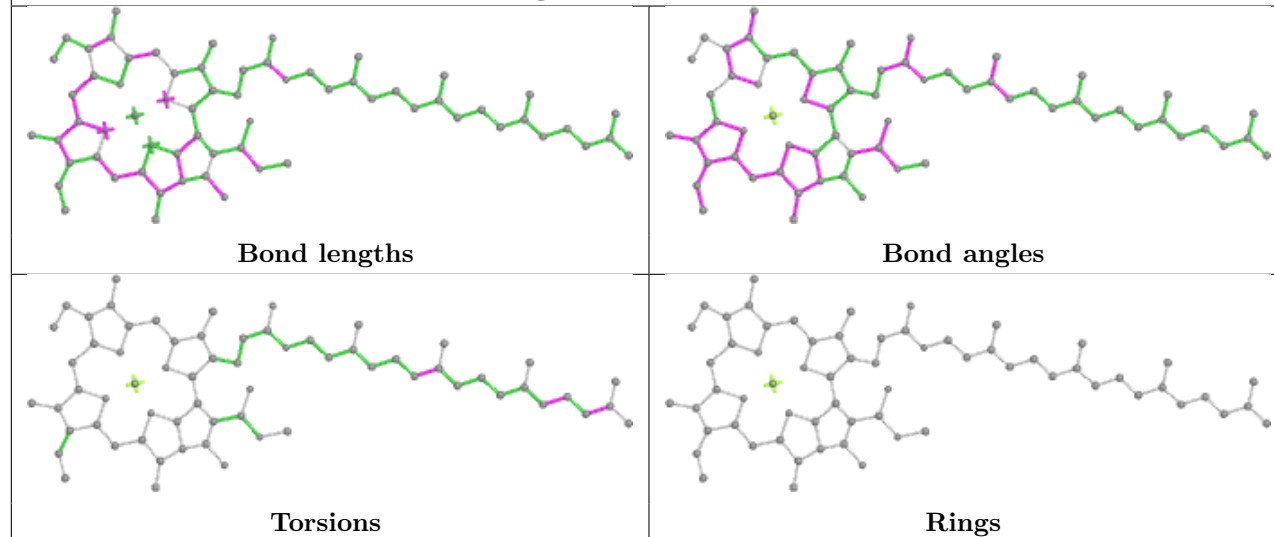


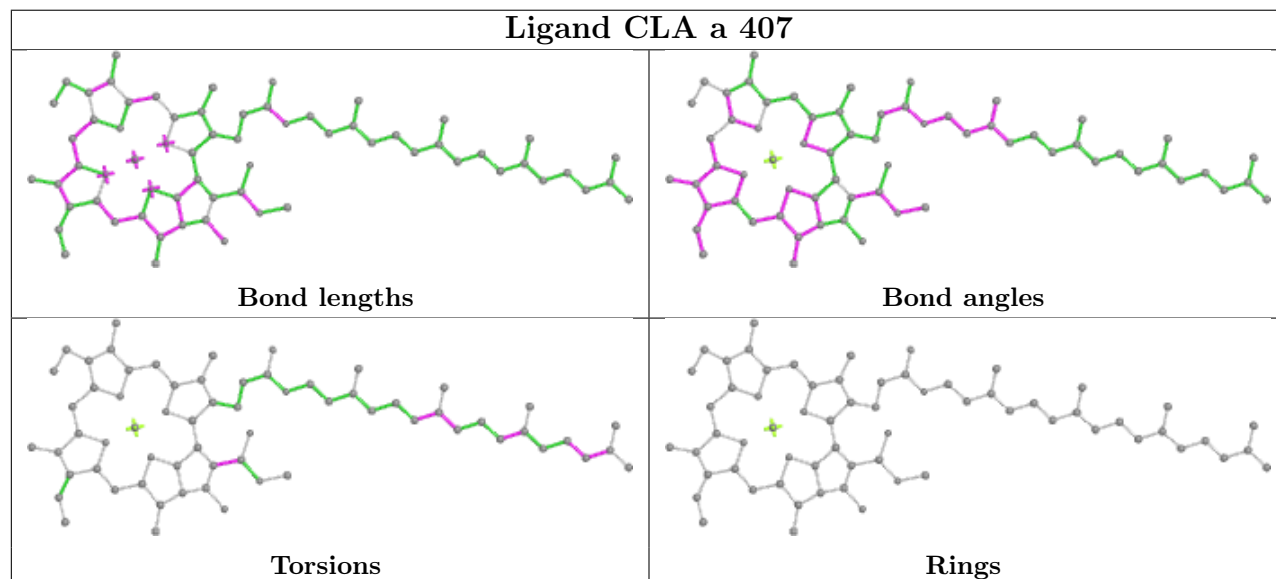
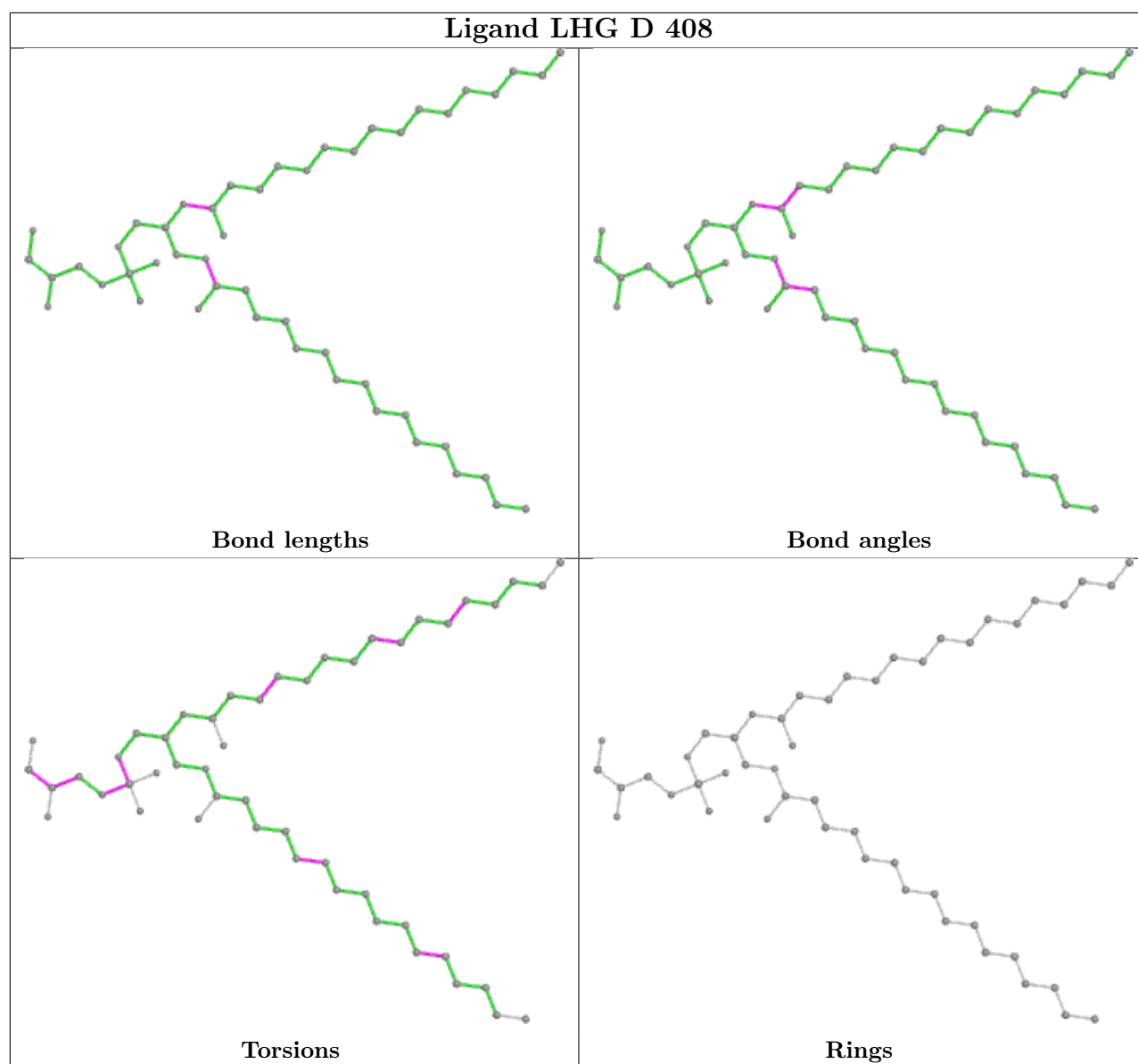
## Ligand BCR a 409



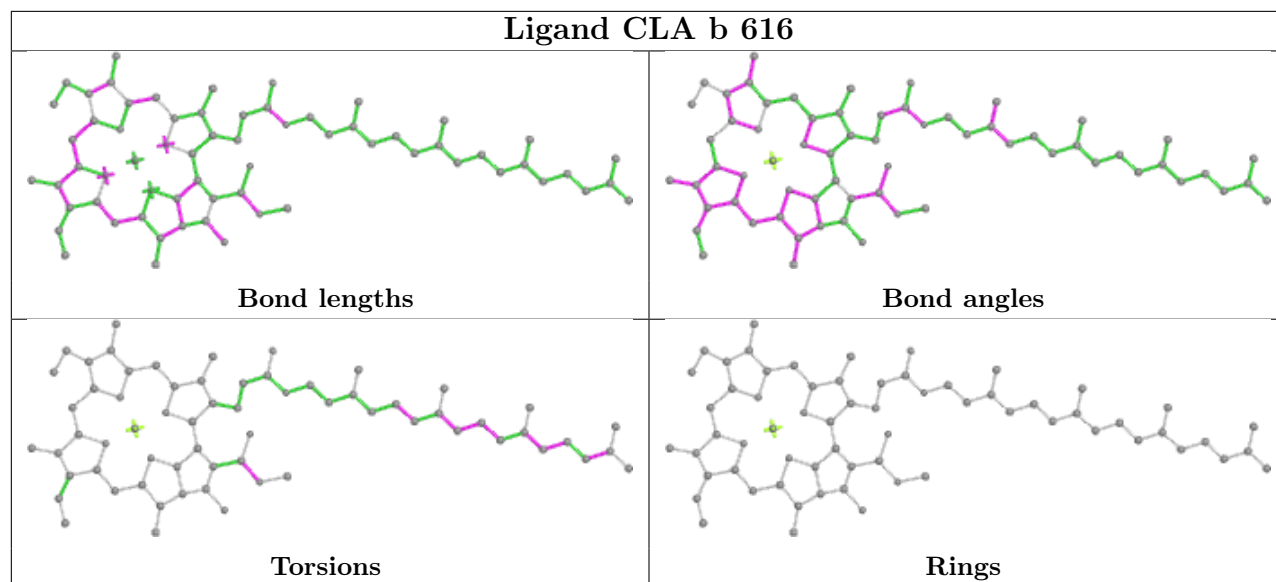




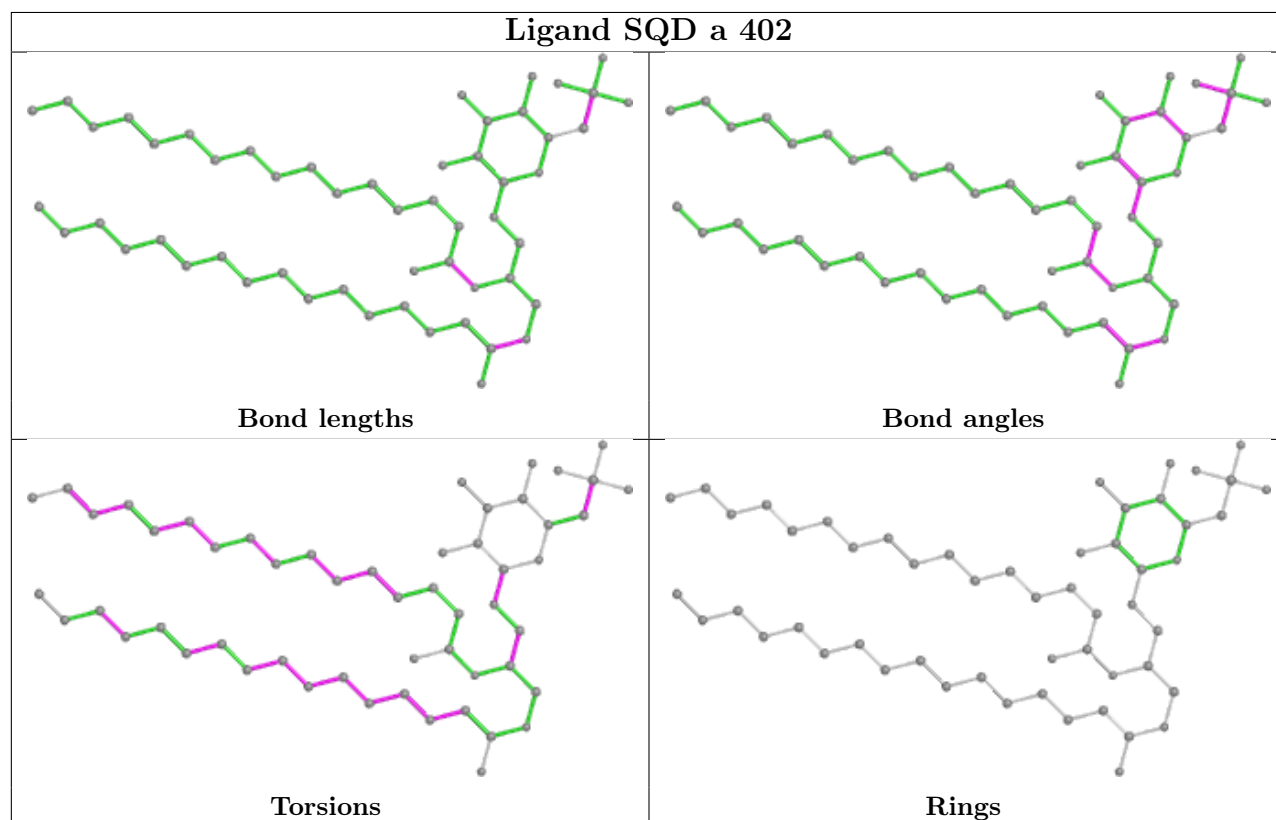
**Ligand CLA C 508****Ligand CLA B 604**



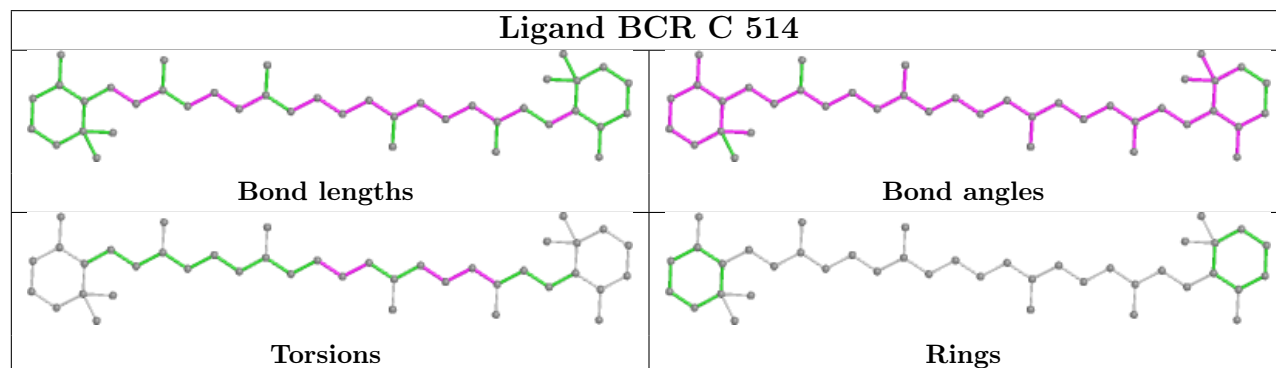
## Ligand CLA b 616



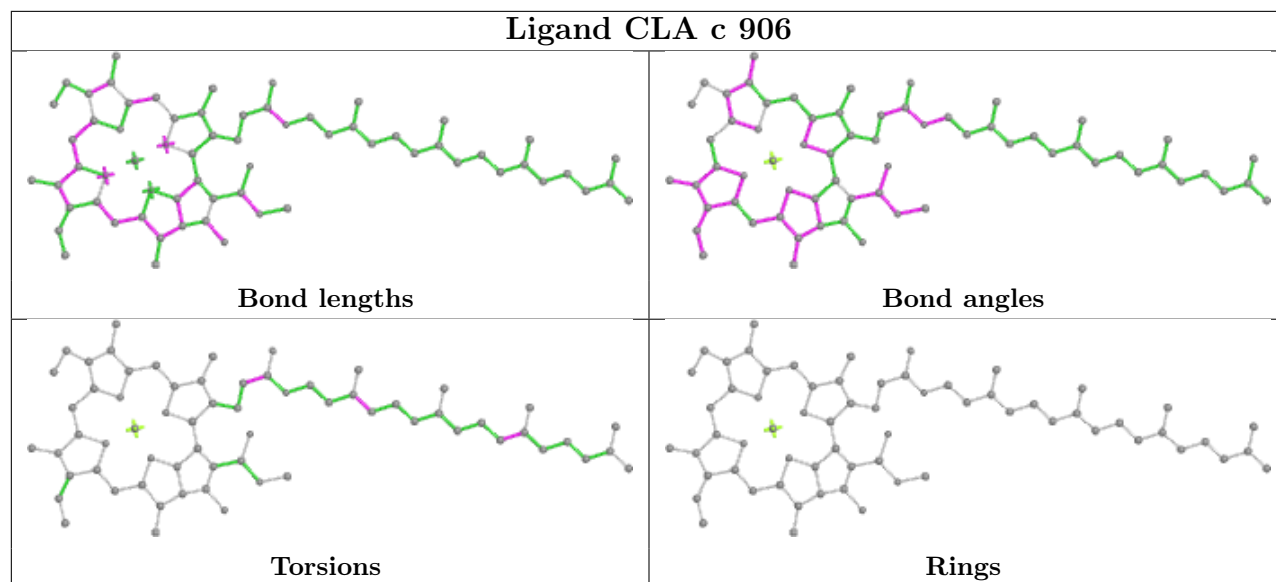
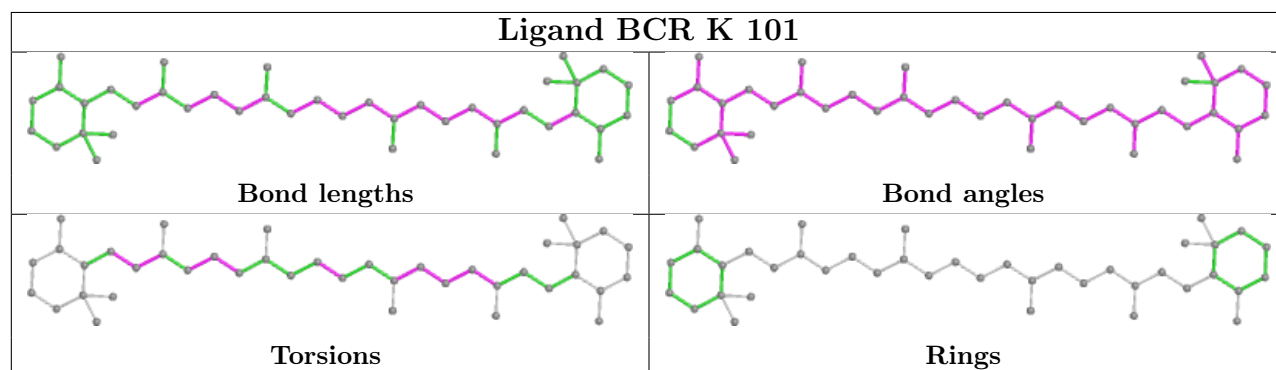
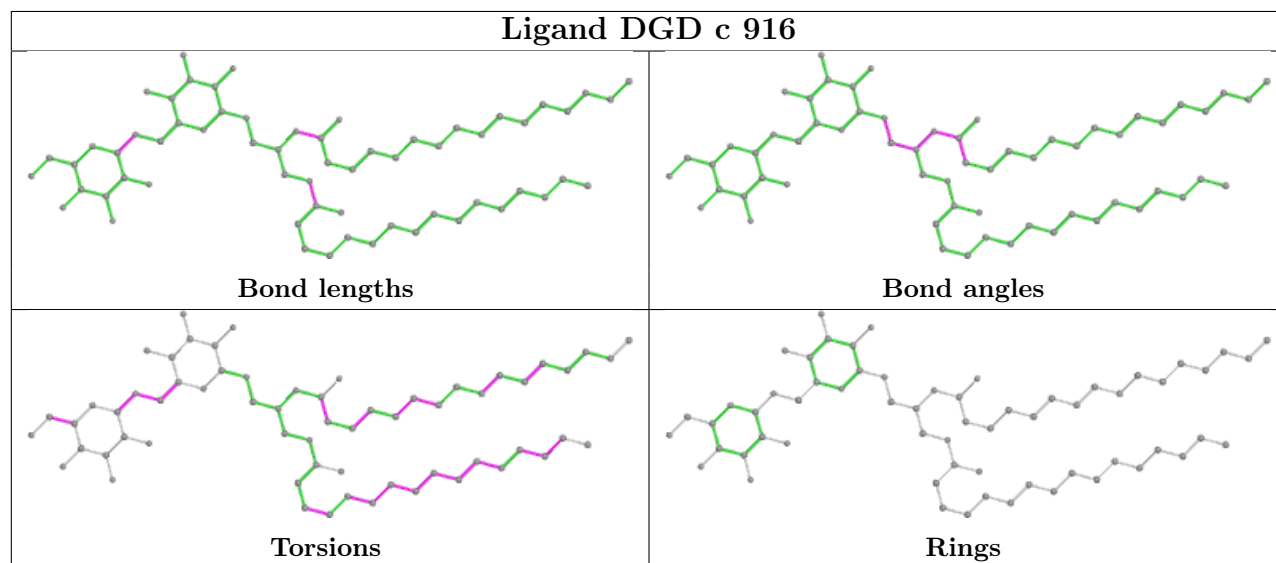
## Ligand SQD a 402

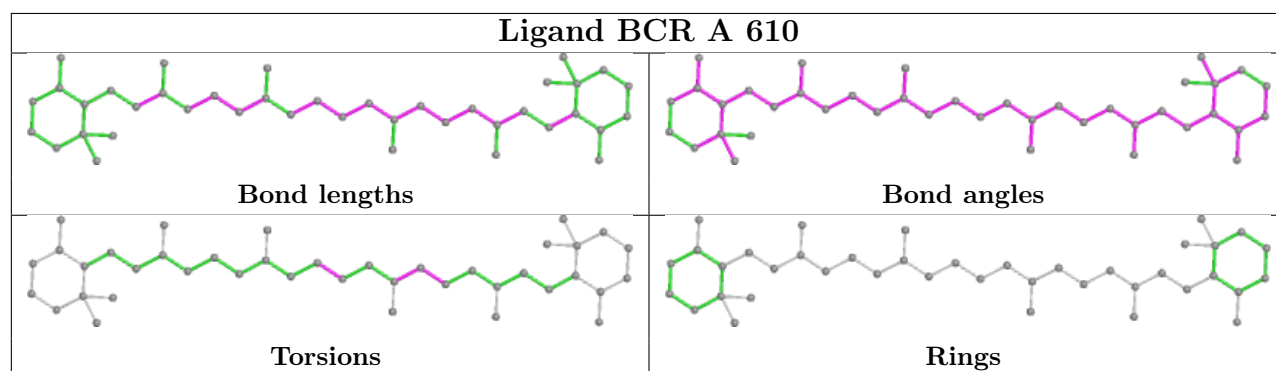
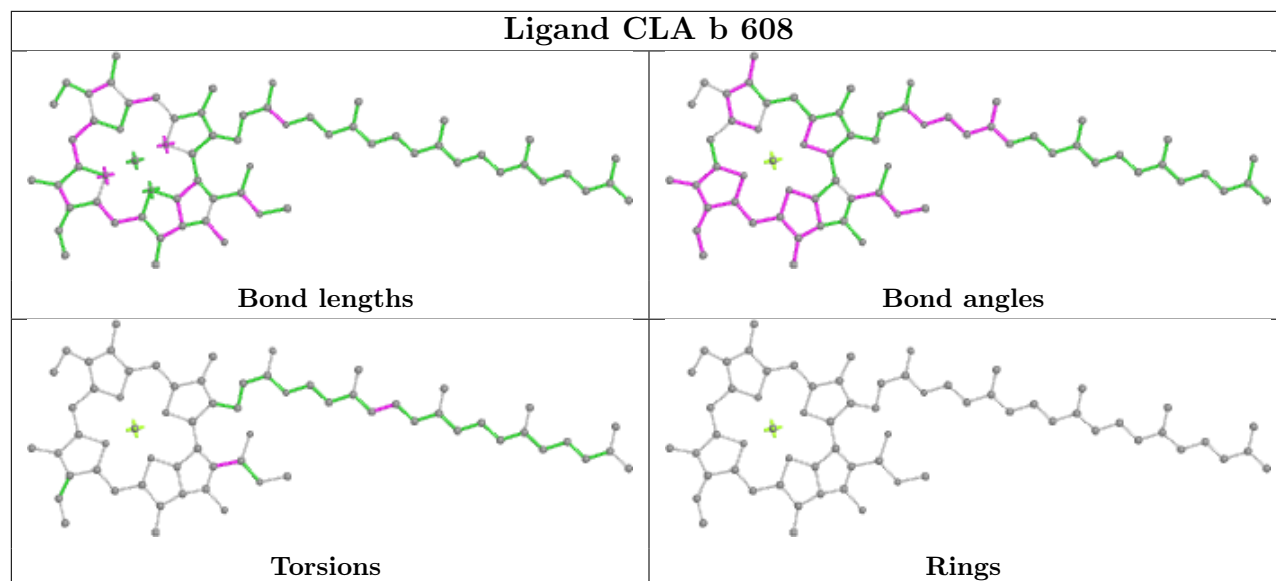
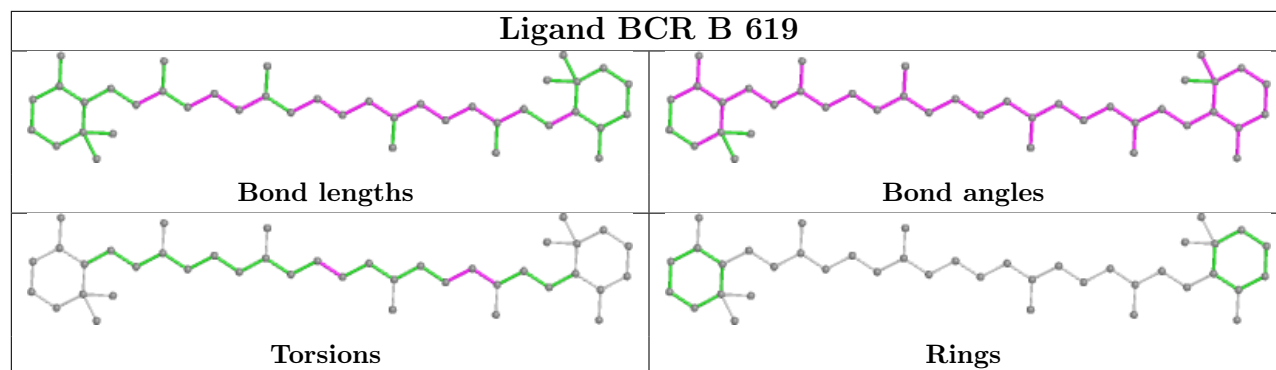


## Ligand BCR C 514

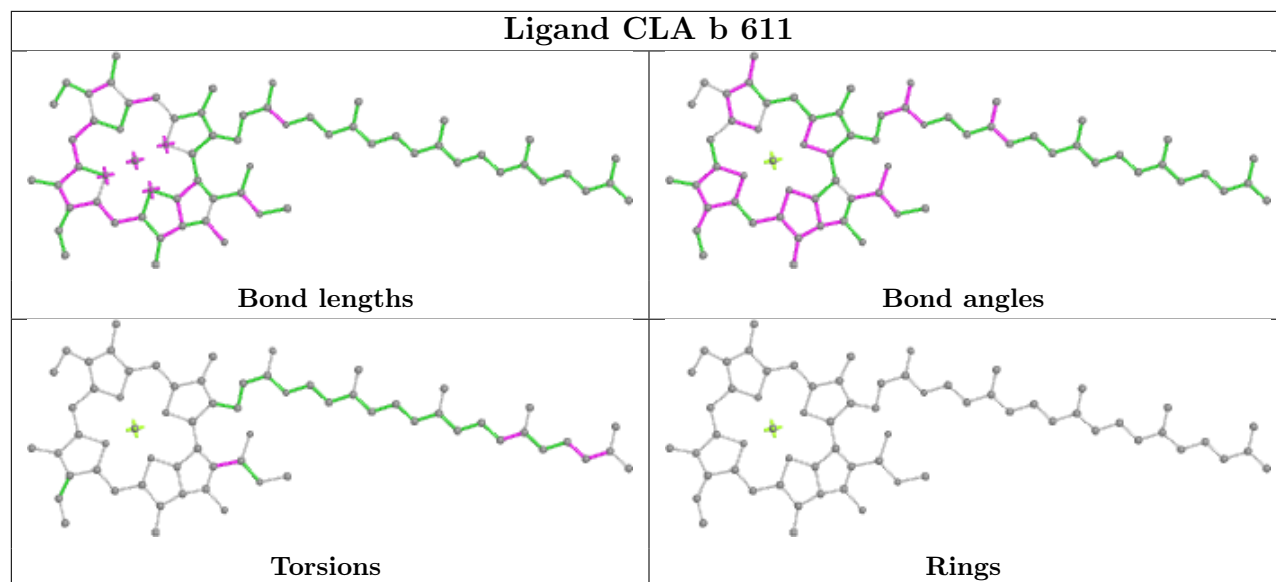




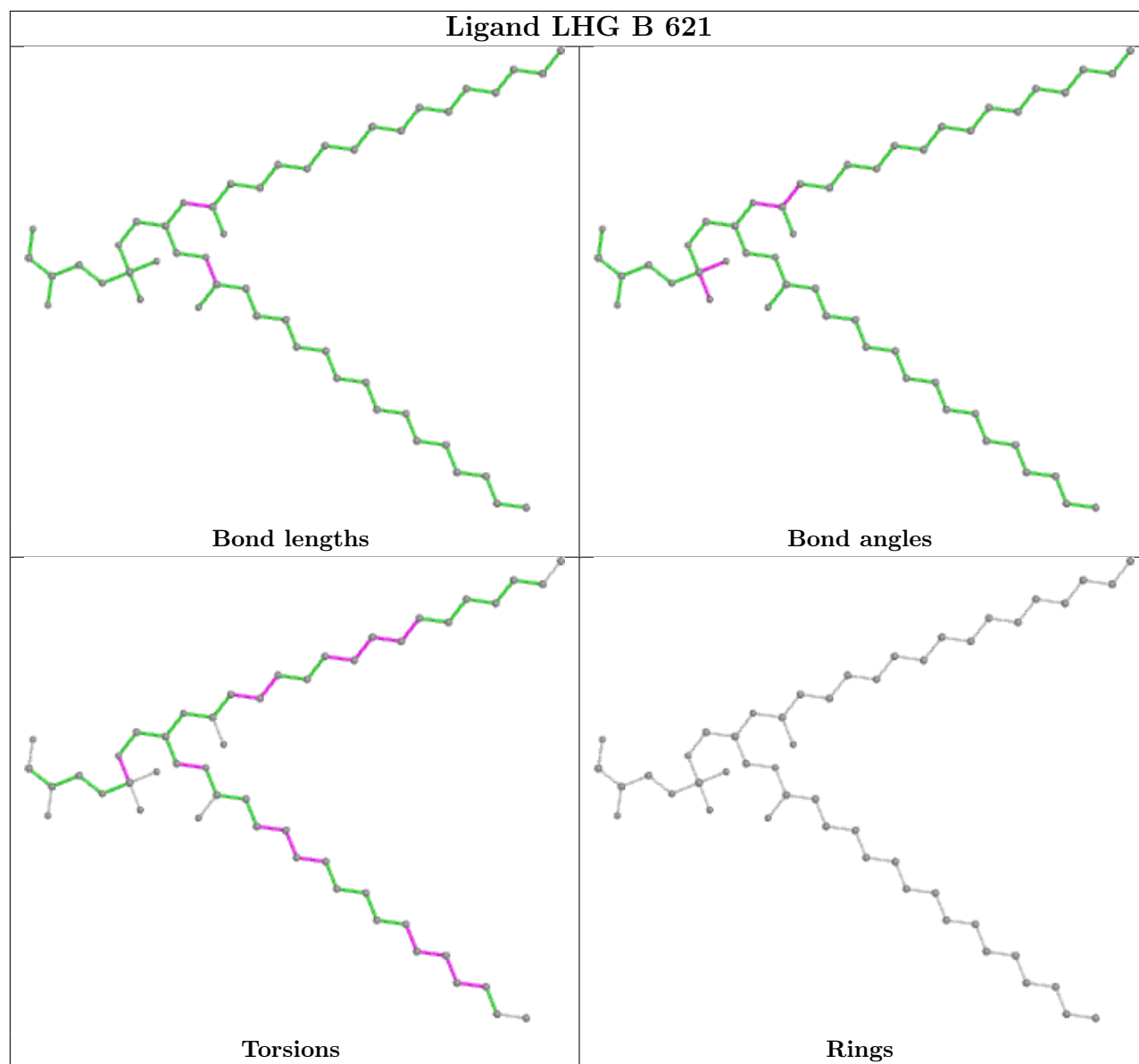
**Ligand CLA c 906****Ligand BCR K 101****Ligand DGD c 916**

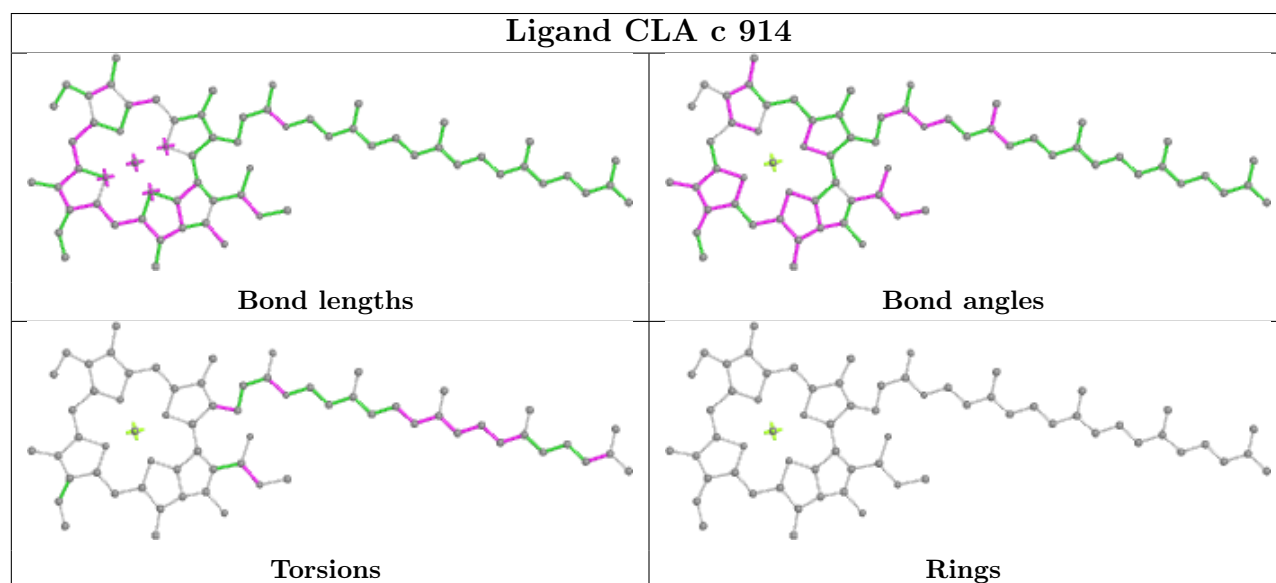
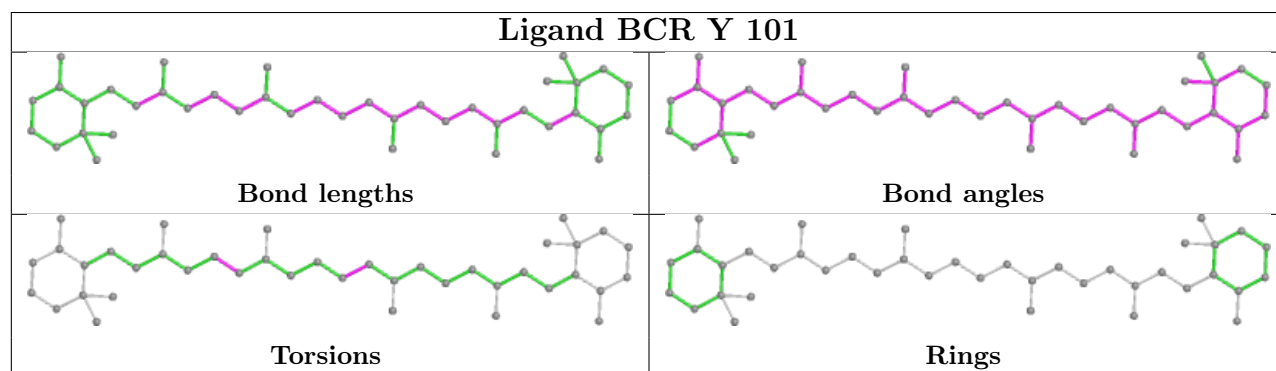
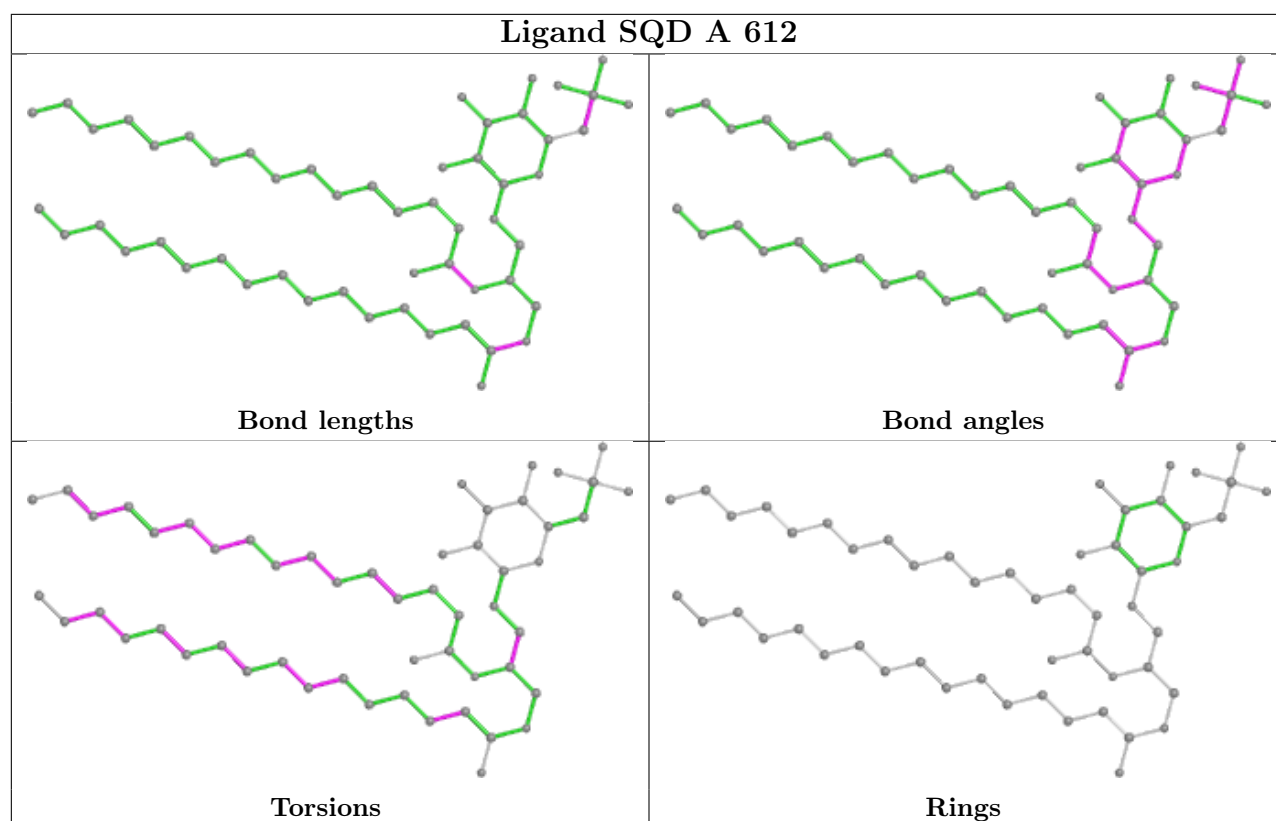


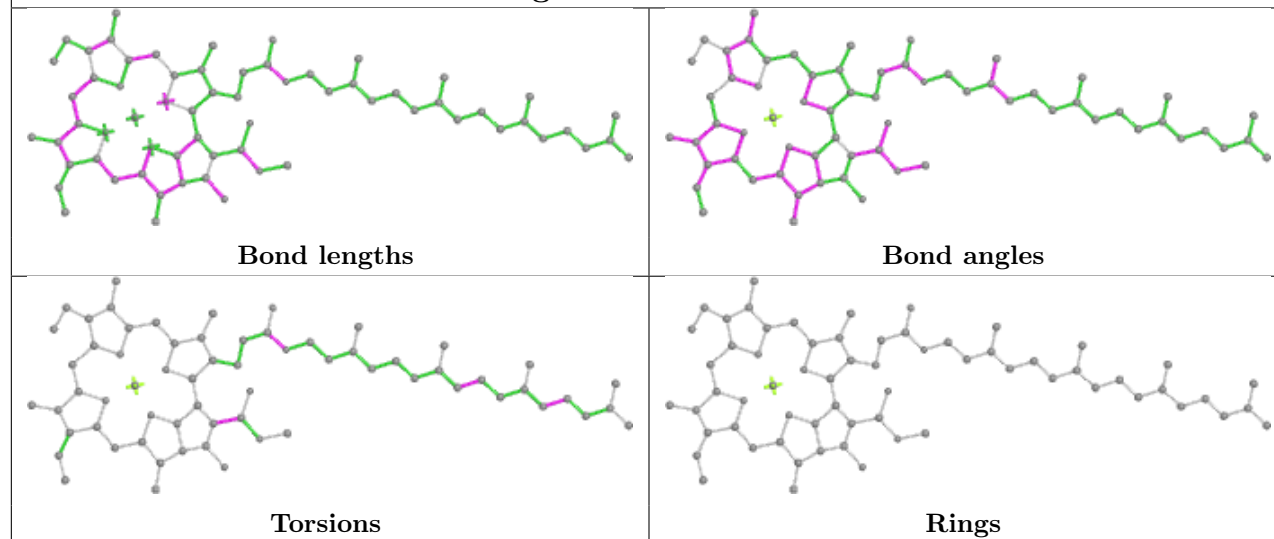
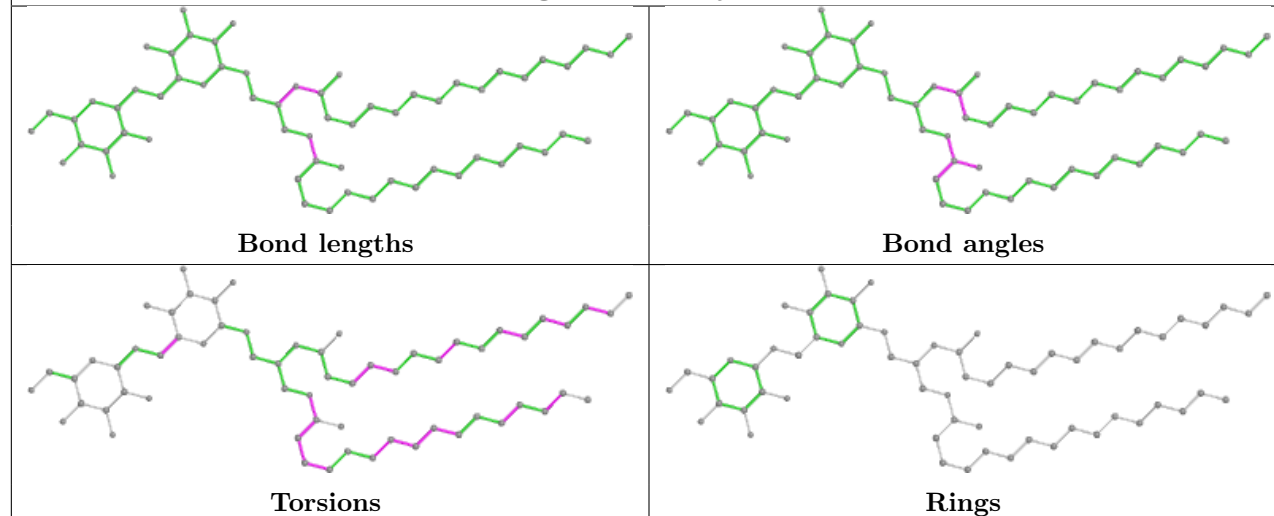
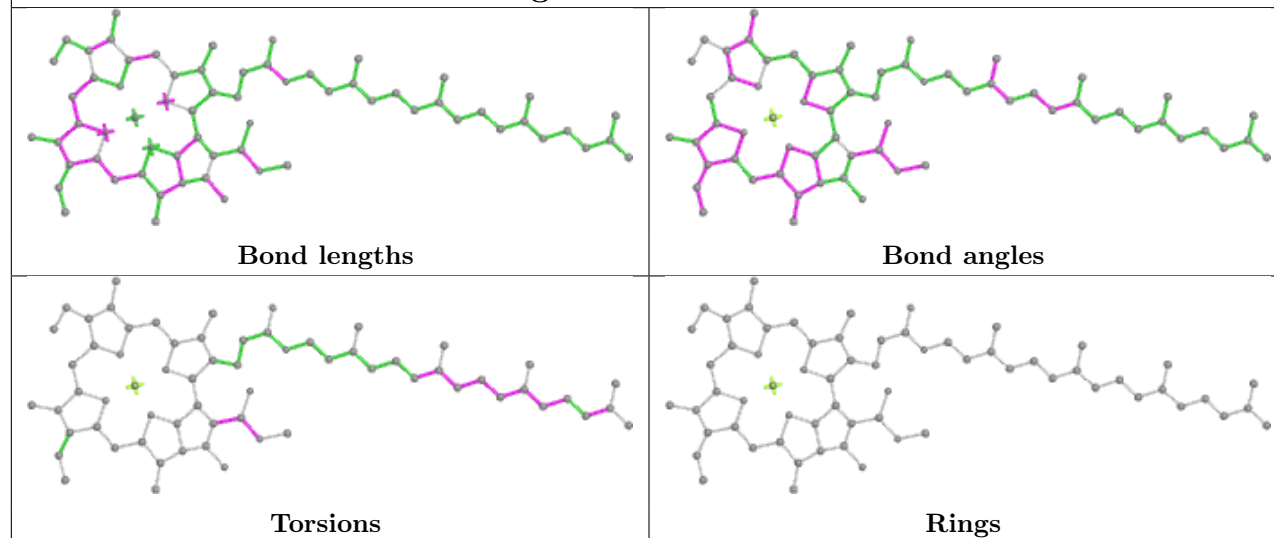
## Ligand CLA b 611

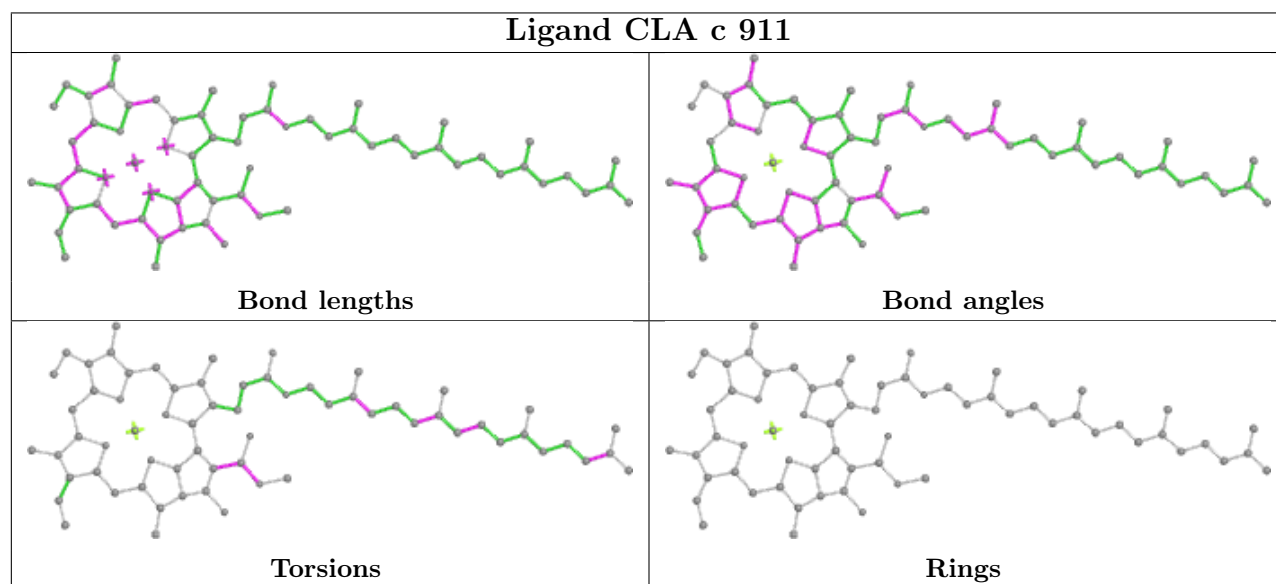
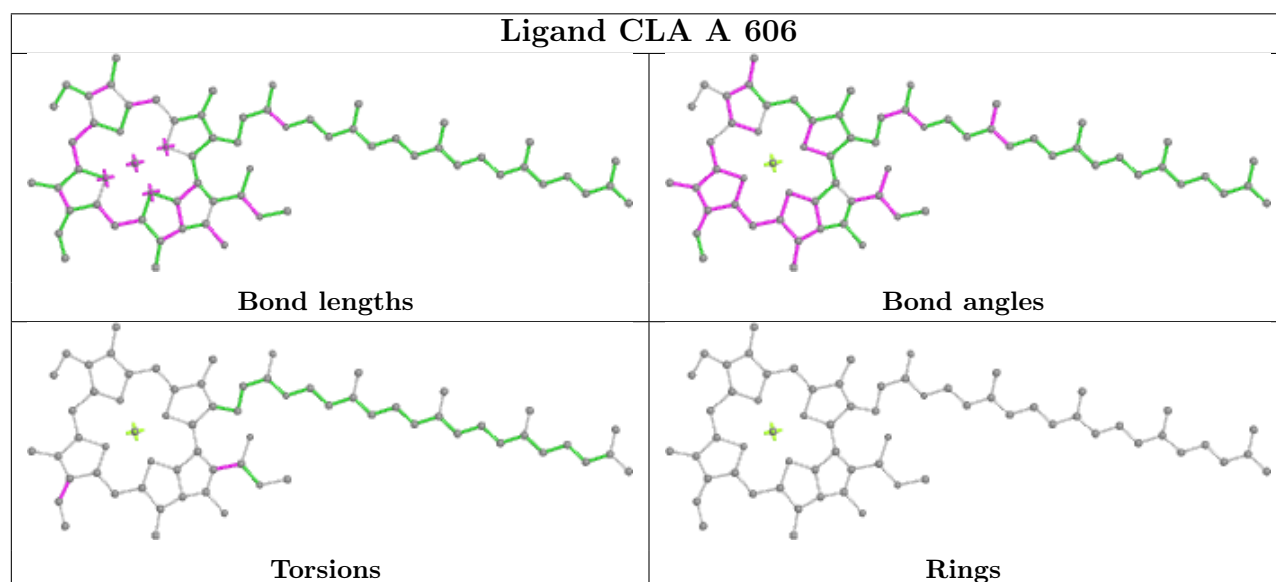
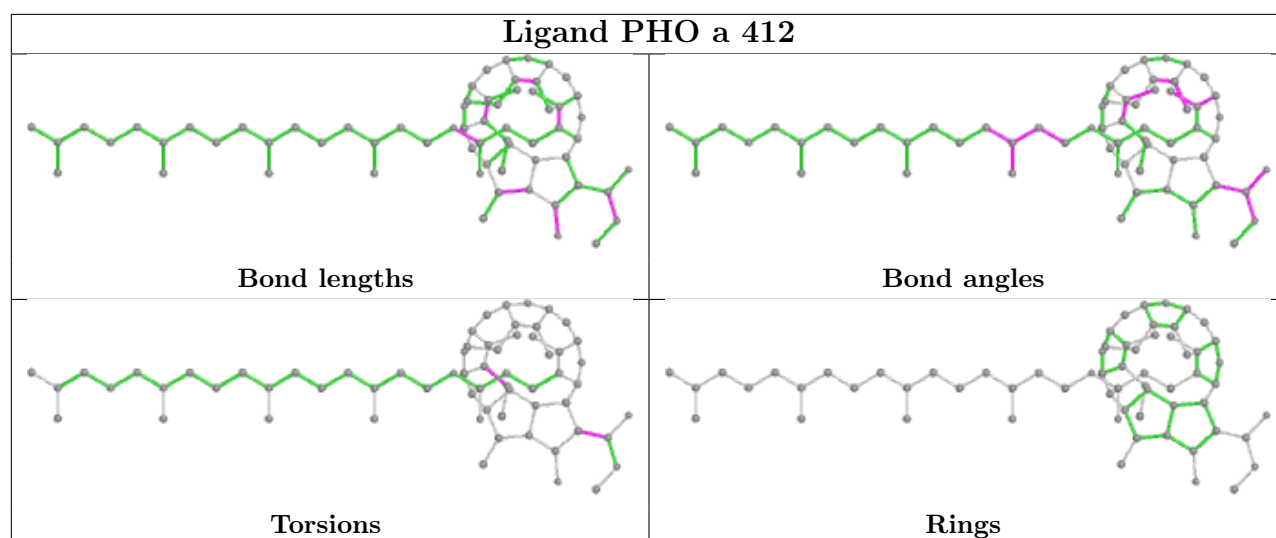


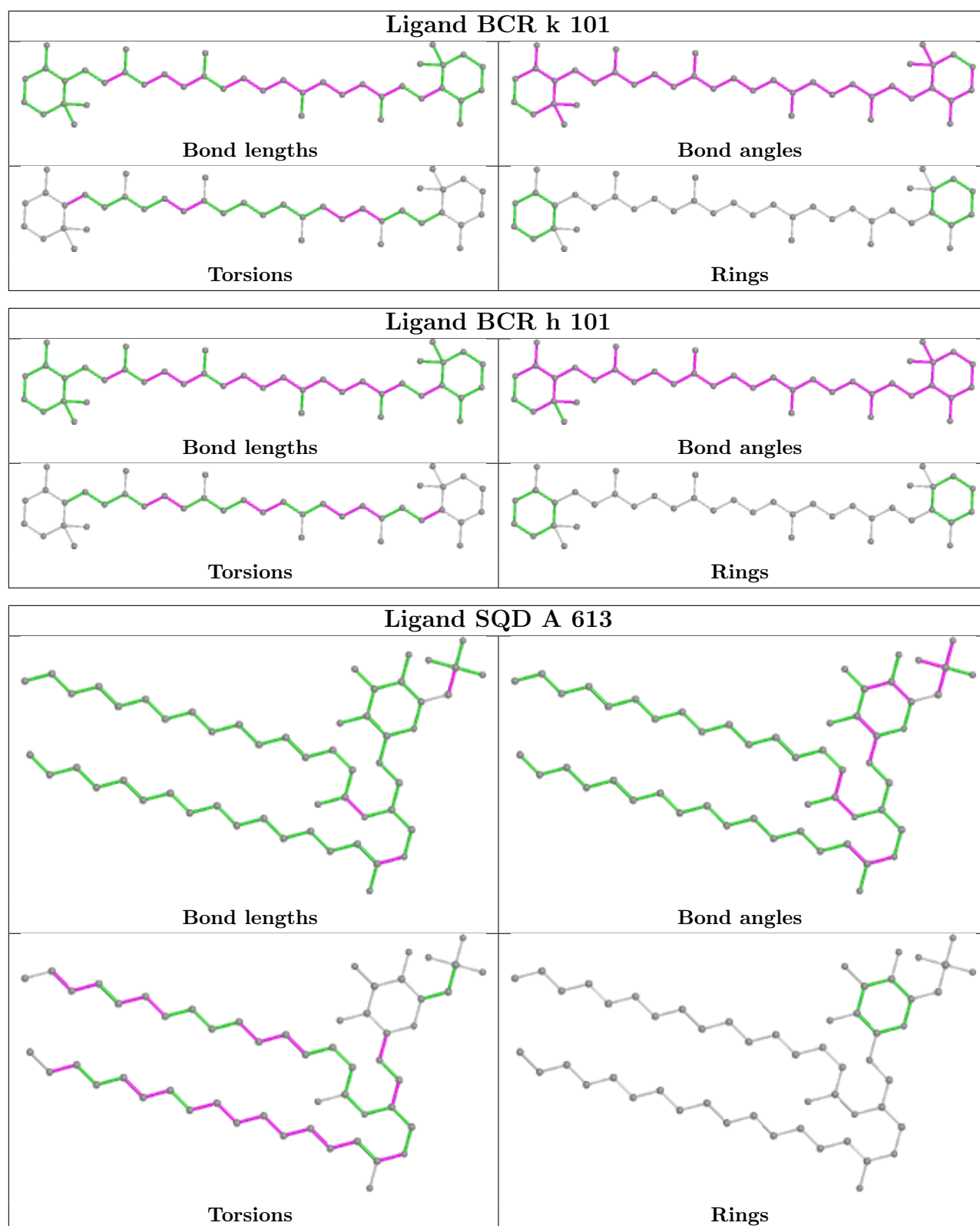
## Ligand LHG B 621

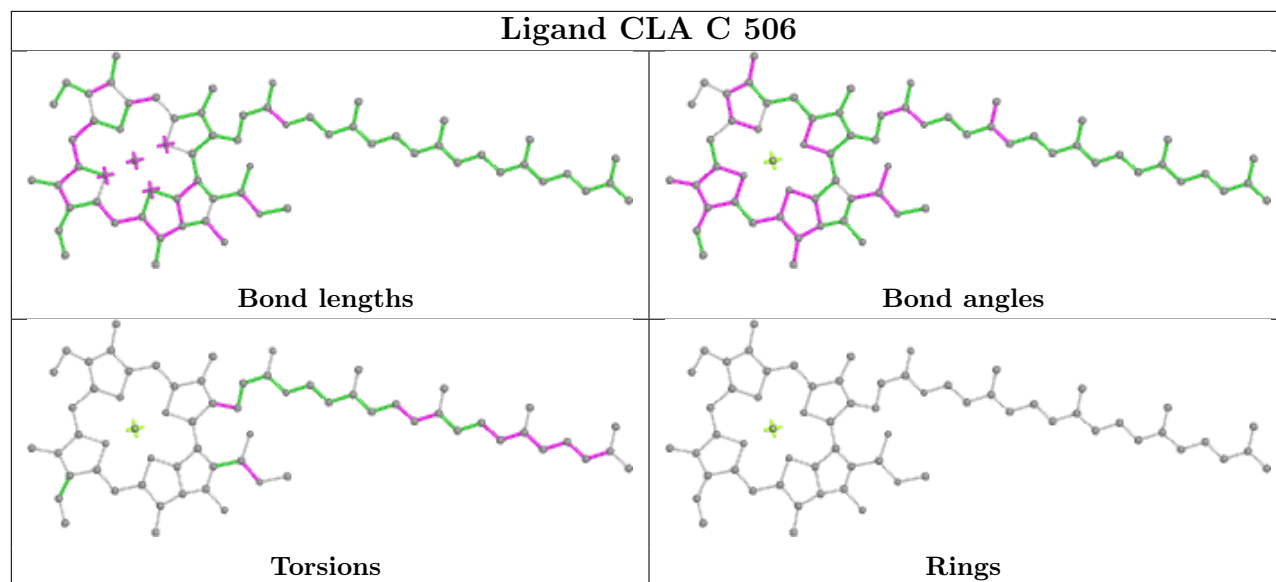
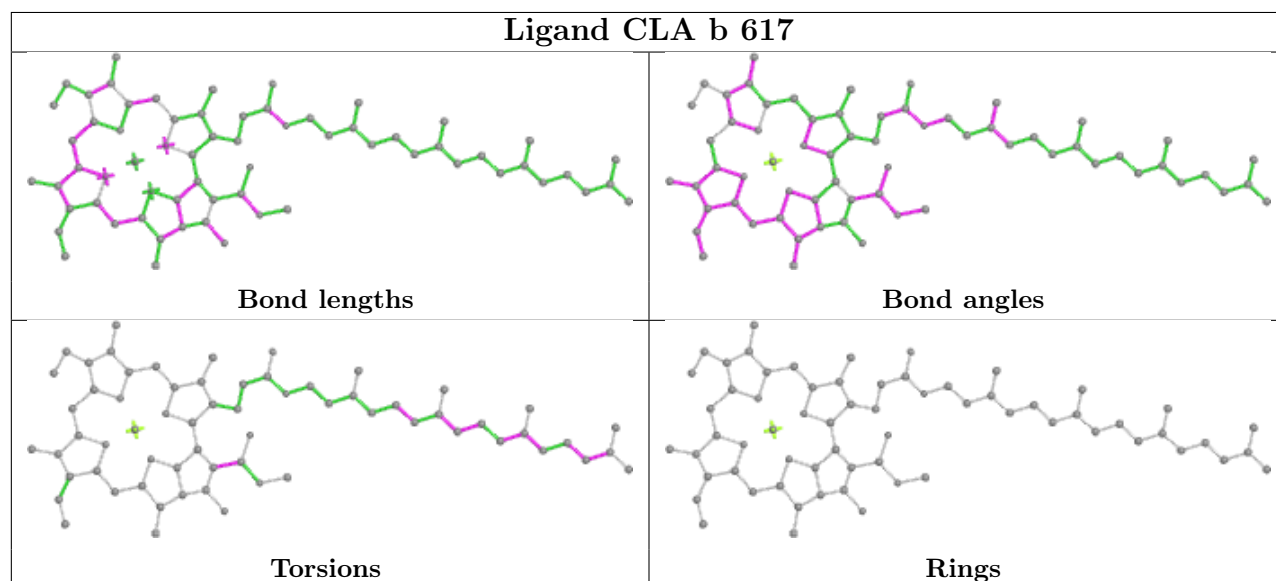
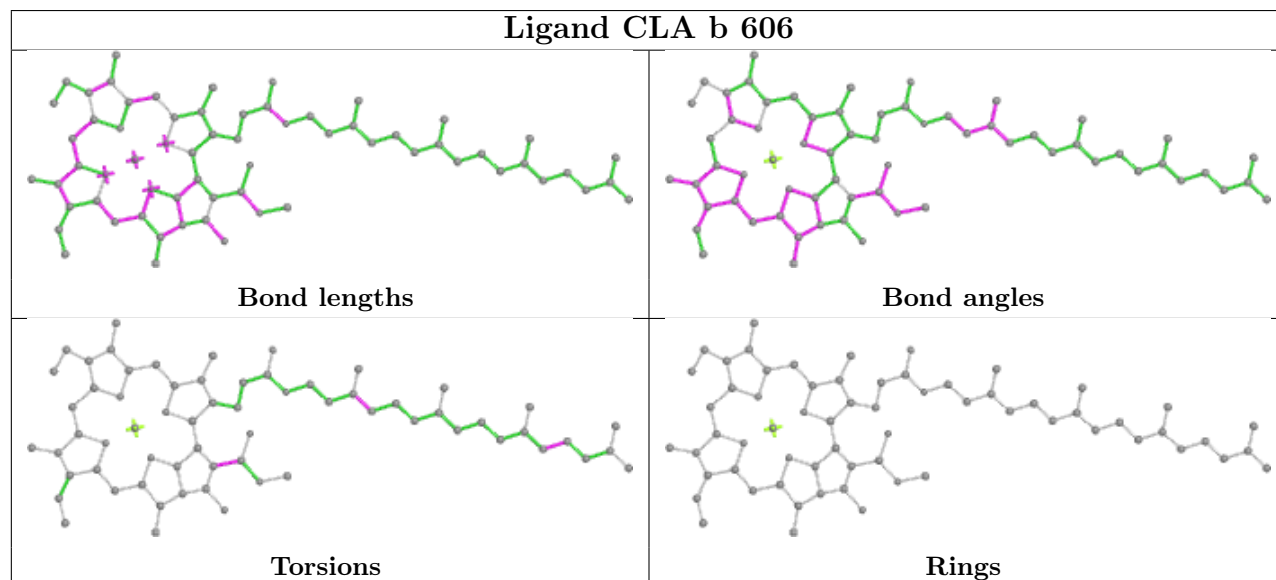




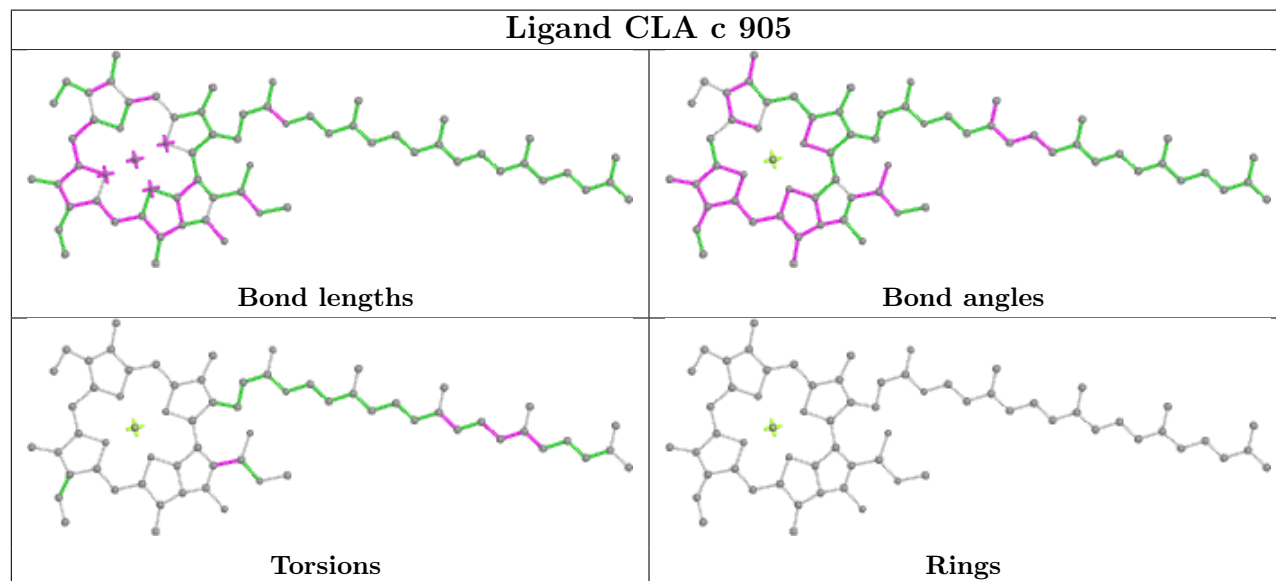
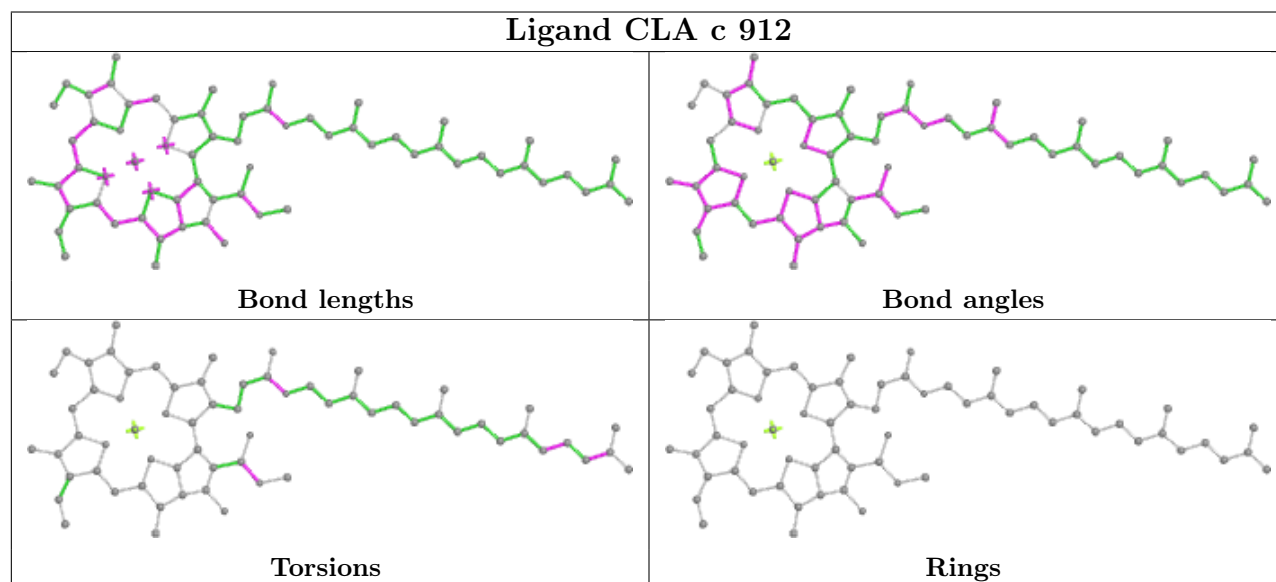
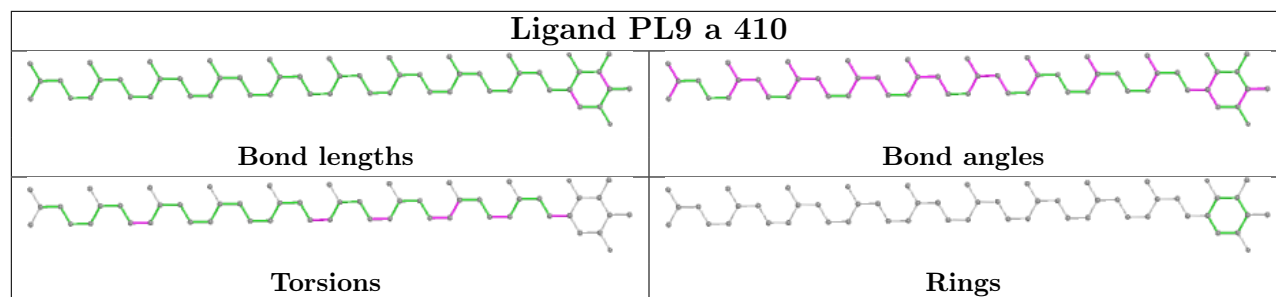
**Ligand CLA B 613****Ligand DGD j 101****Ligand CLA D 403**



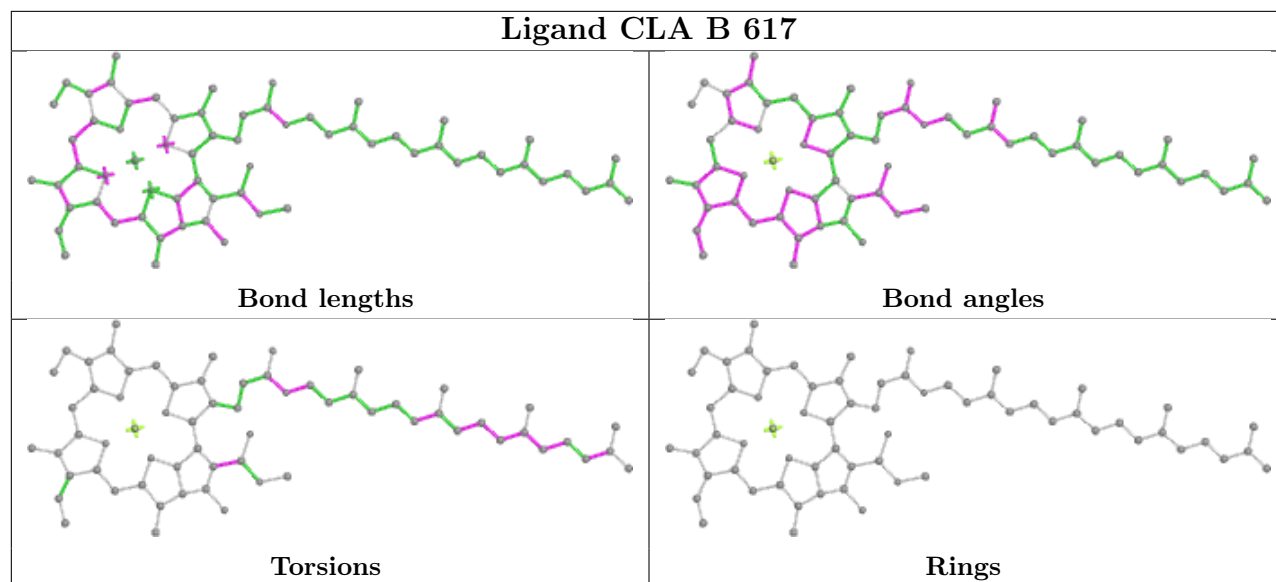


**Ligand CLA C 506****Ligand CLA b 617****Ligand CLA b 606**

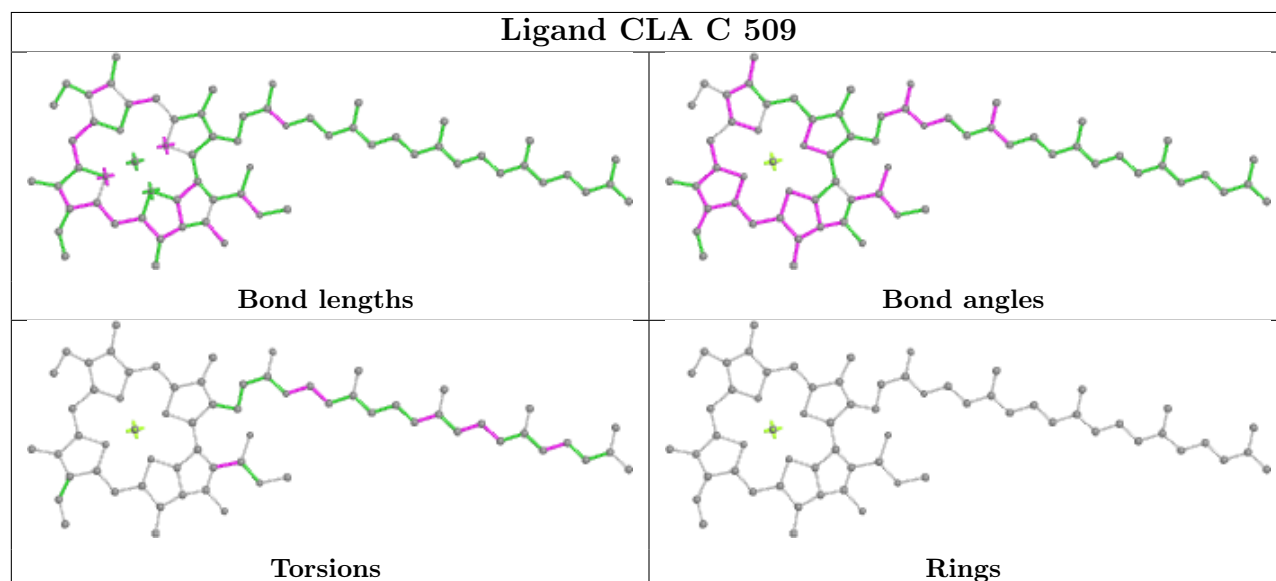




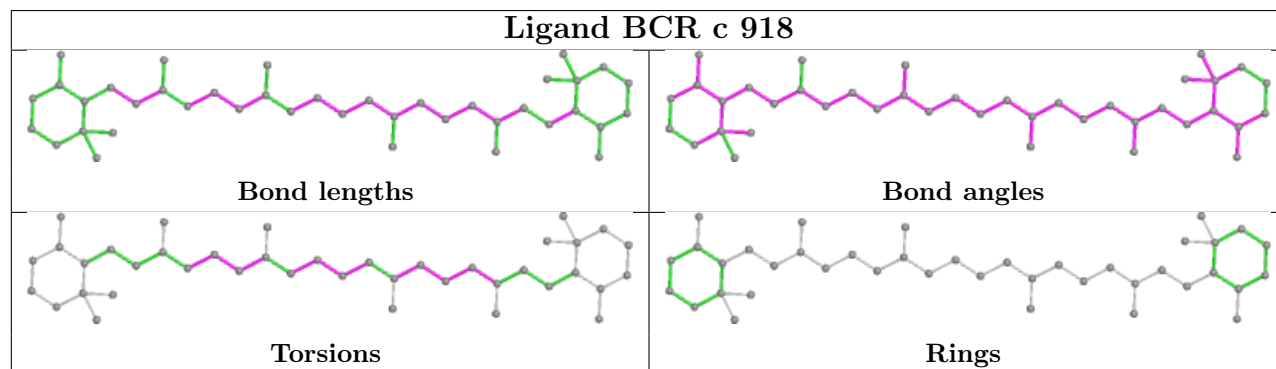
## Ligand CLA B 617

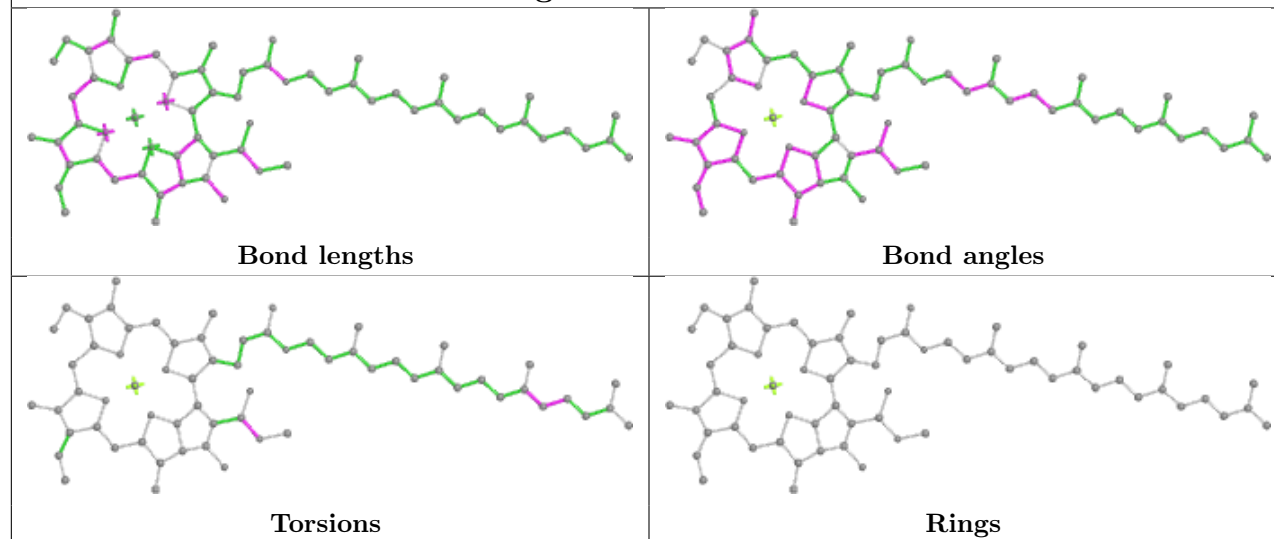
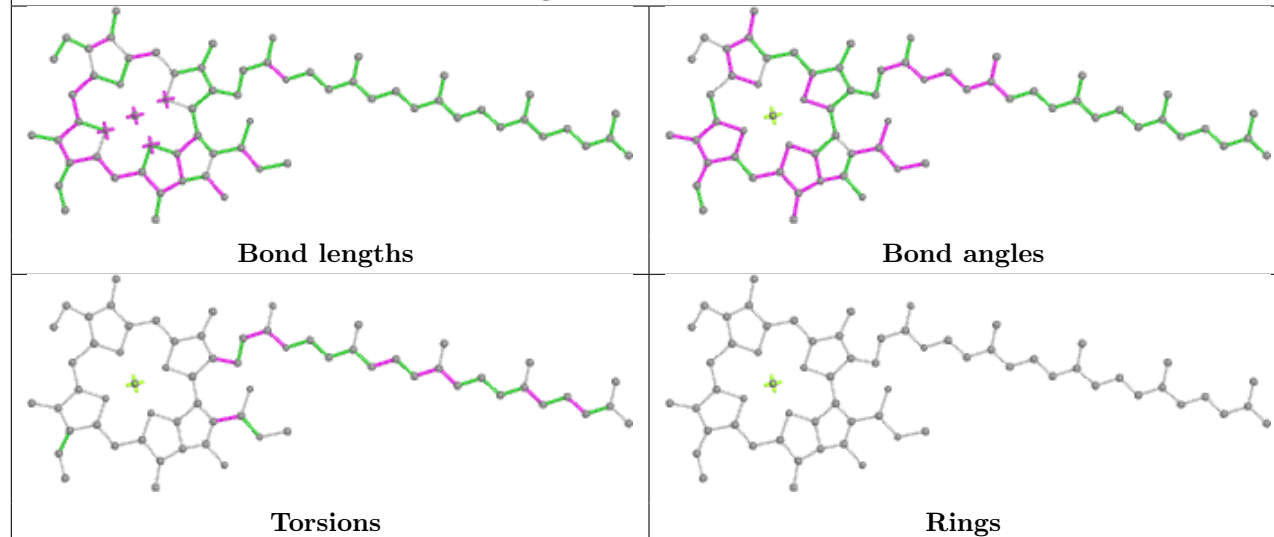


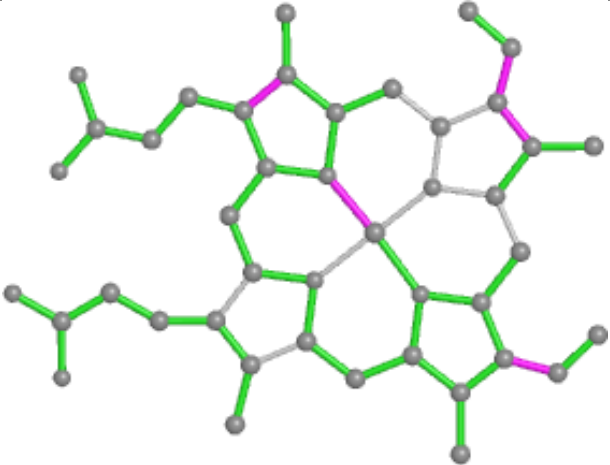
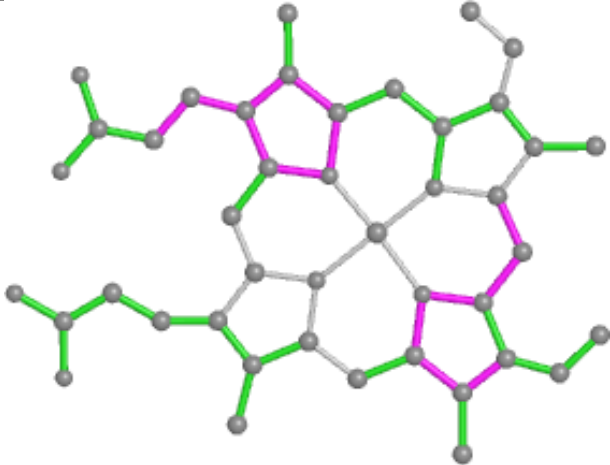
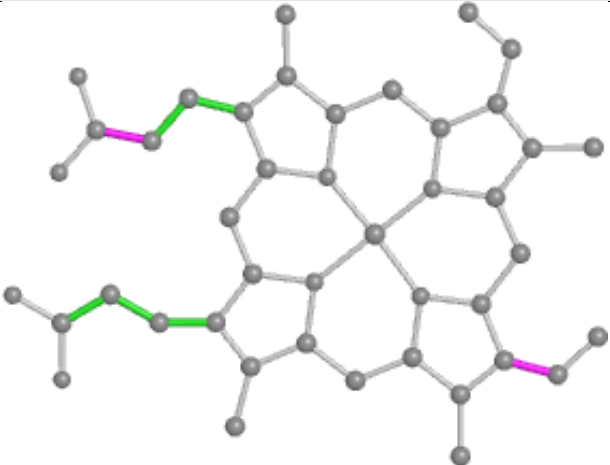
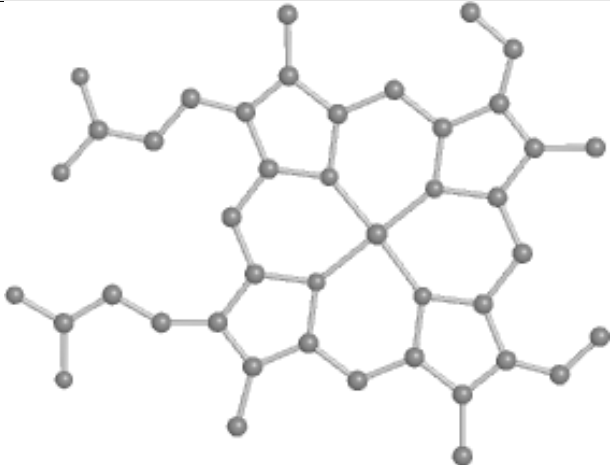
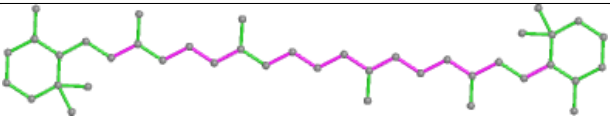
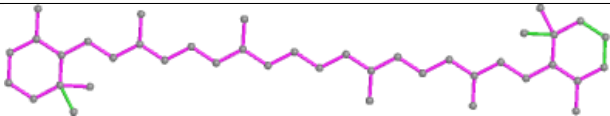
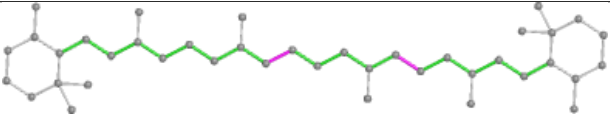
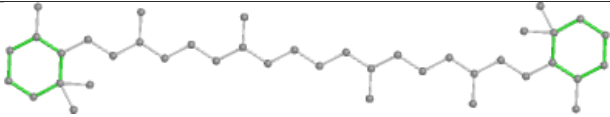
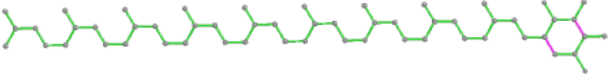
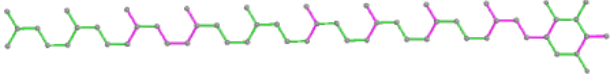
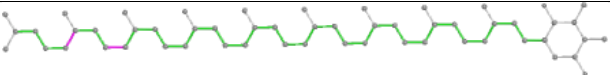
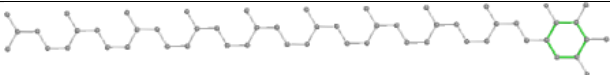
## Ligand CLA C 509

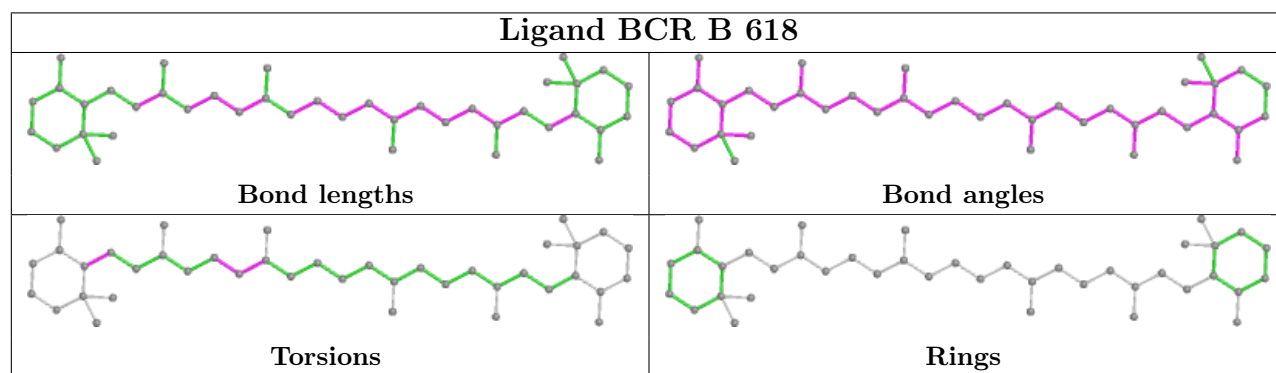
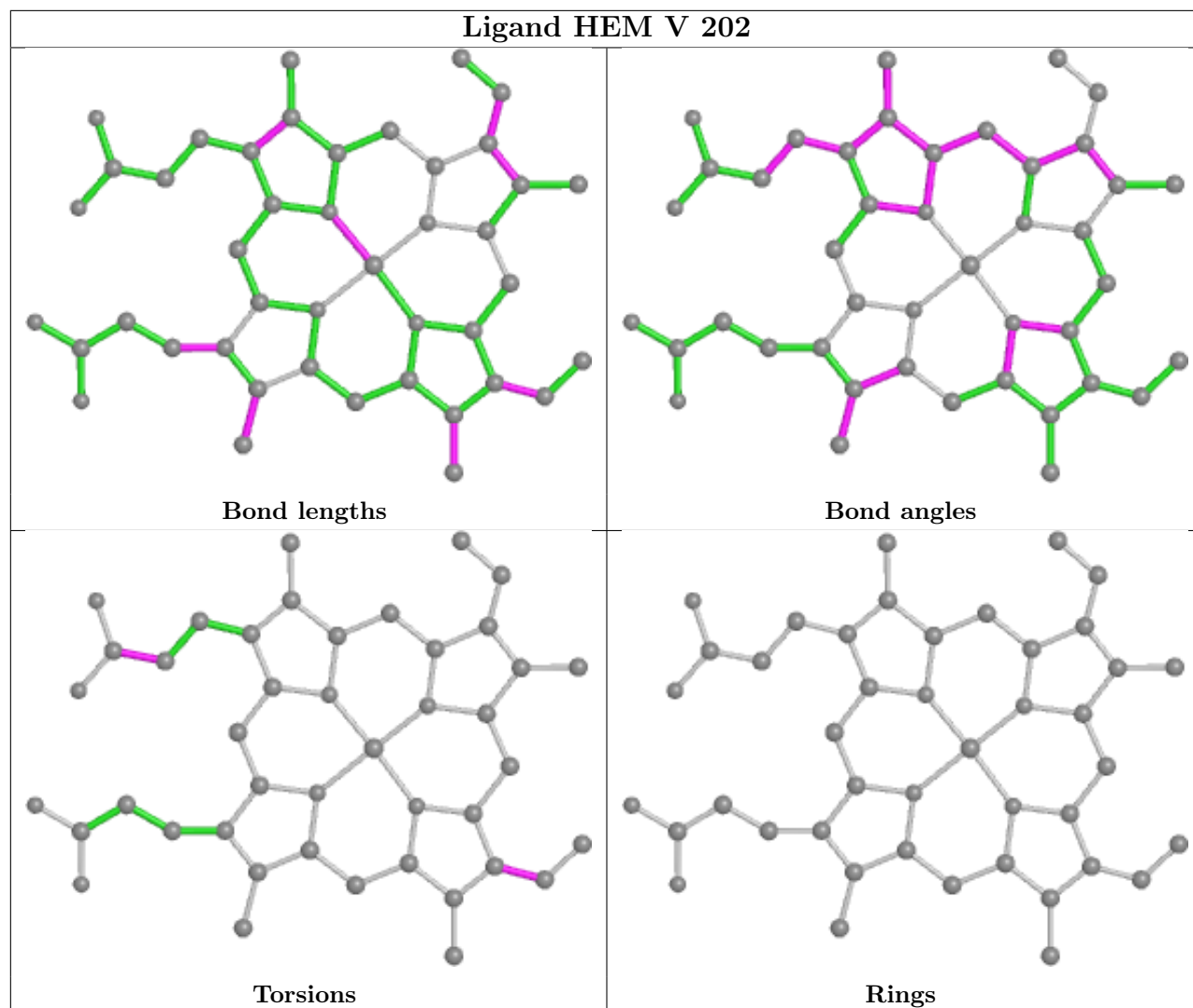


## Ligand BCR c 918

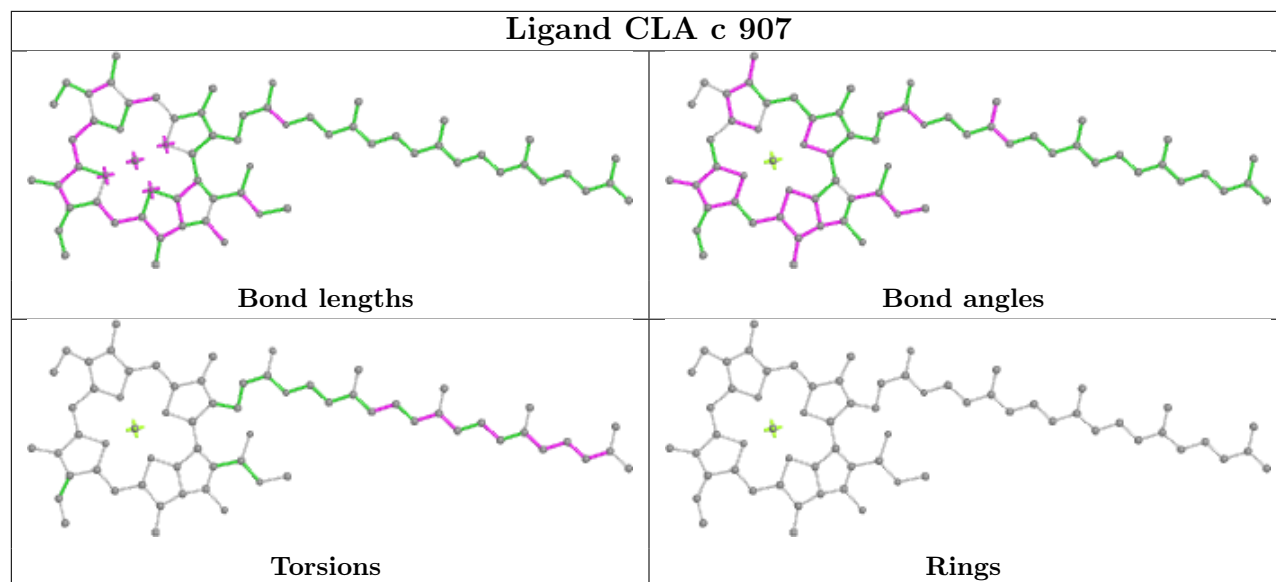


**Ligand CLA b 612****Ligand CLA c 913**

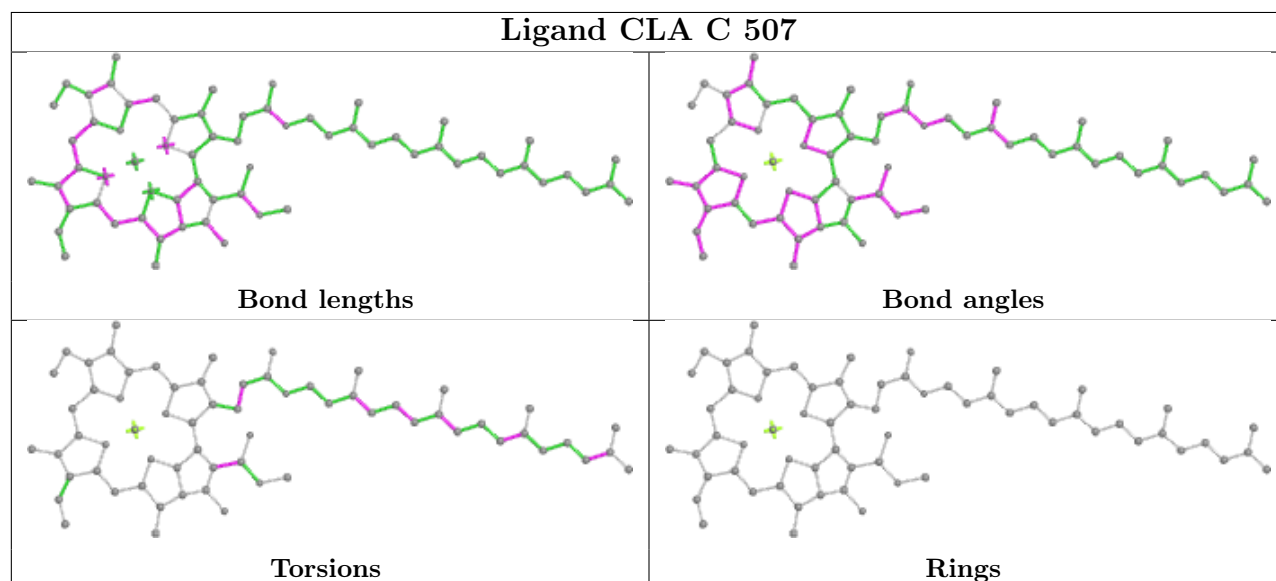
Ligand HEM v 202	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings



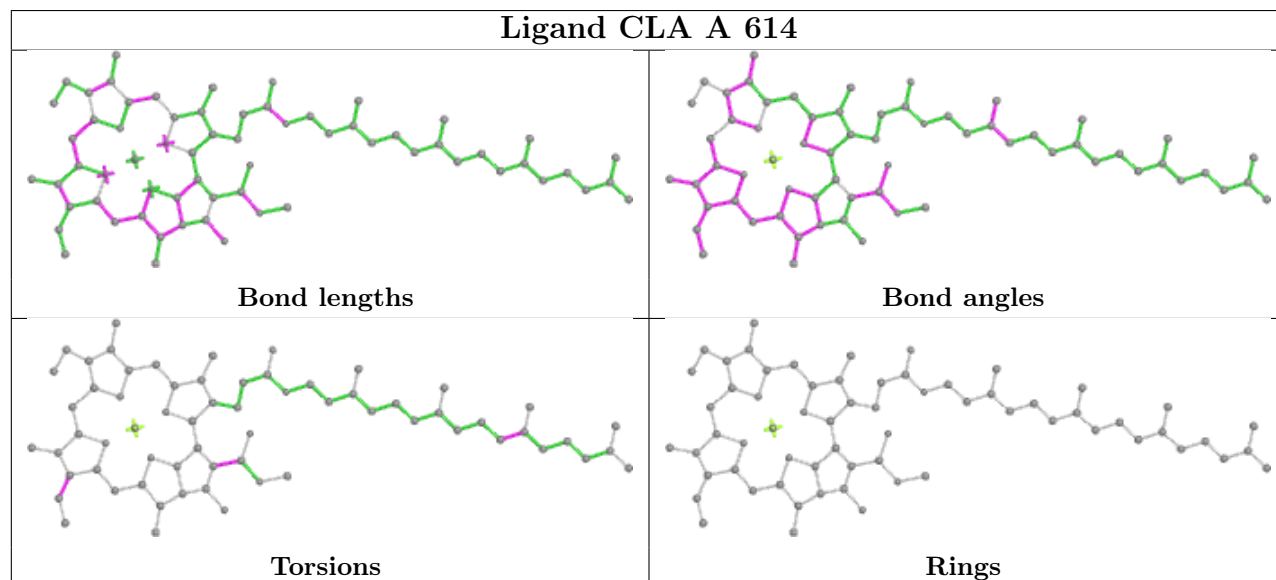
## Ligand CLA c 907

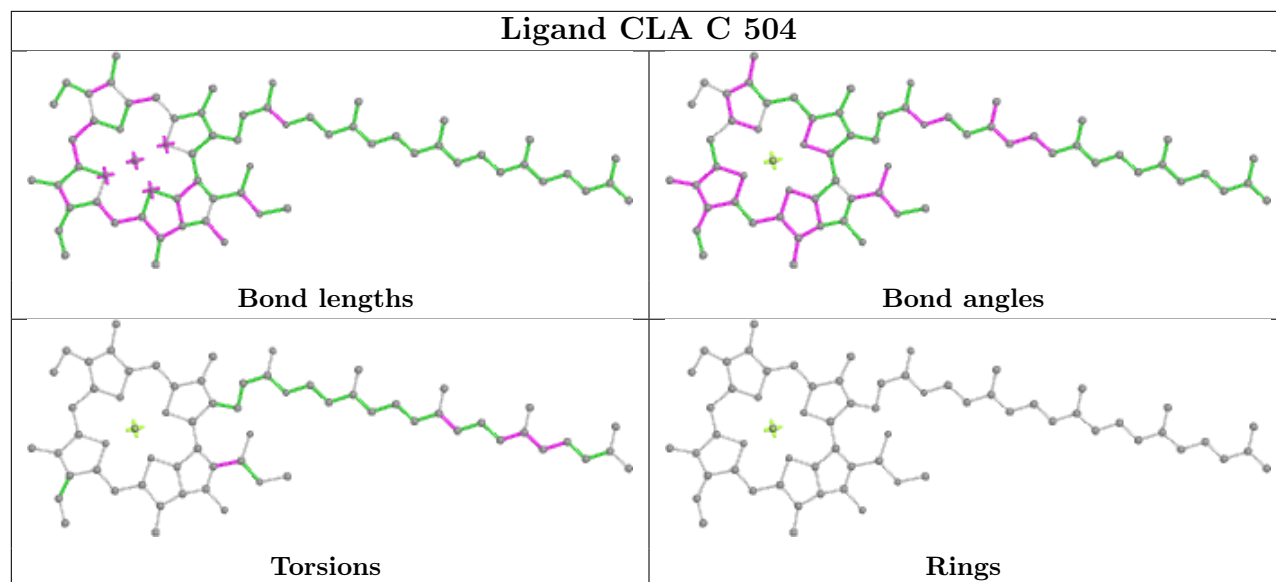
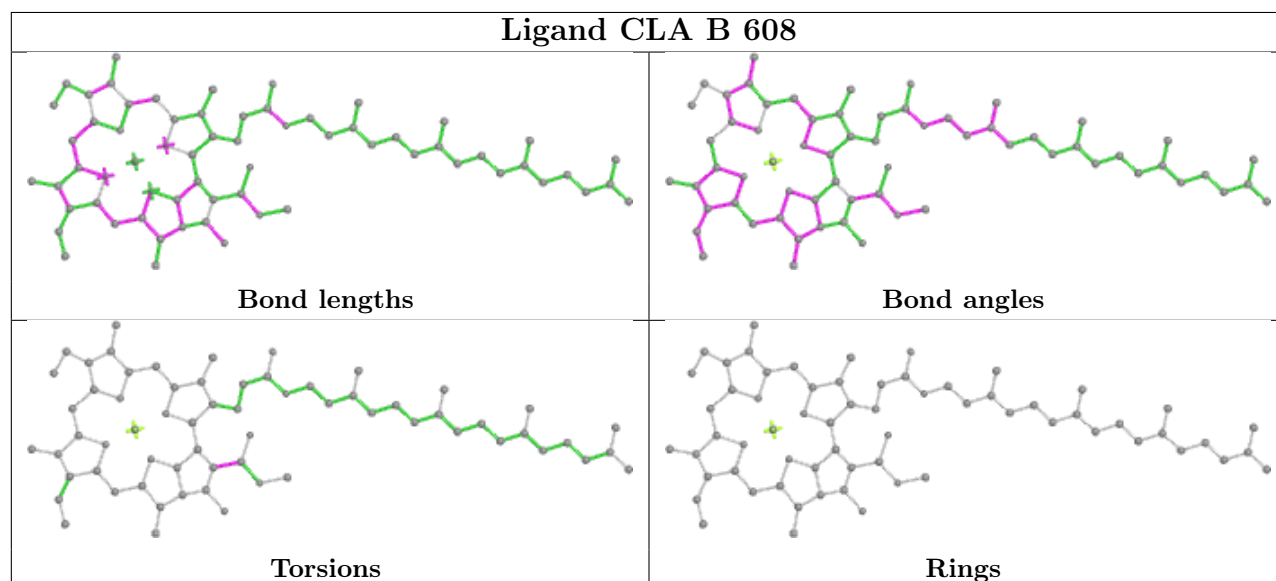
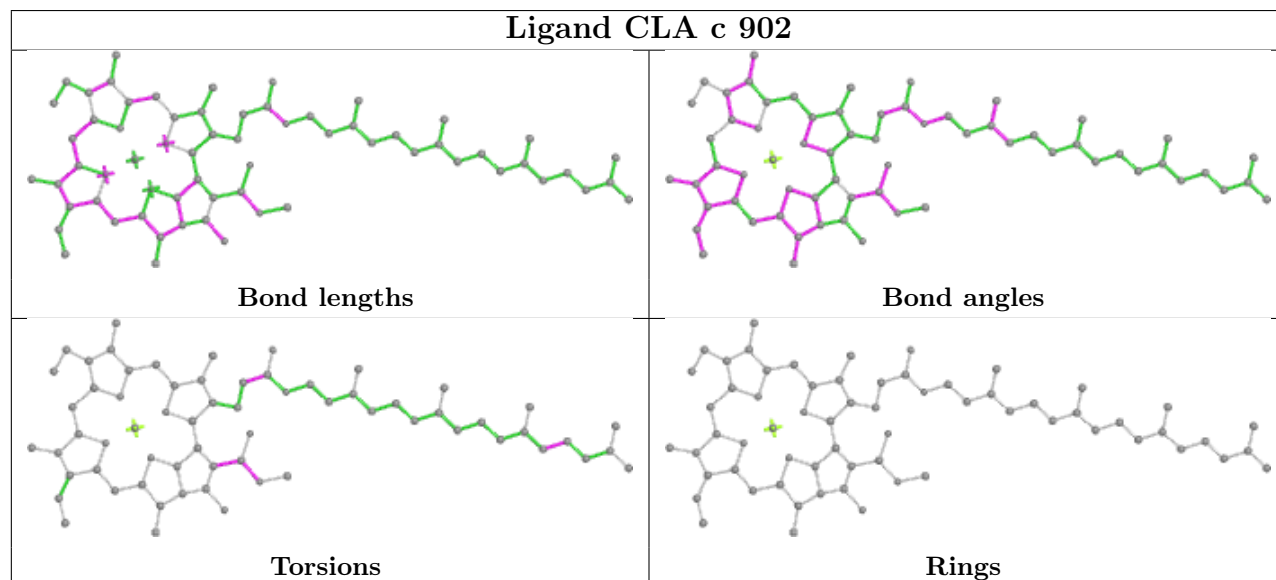


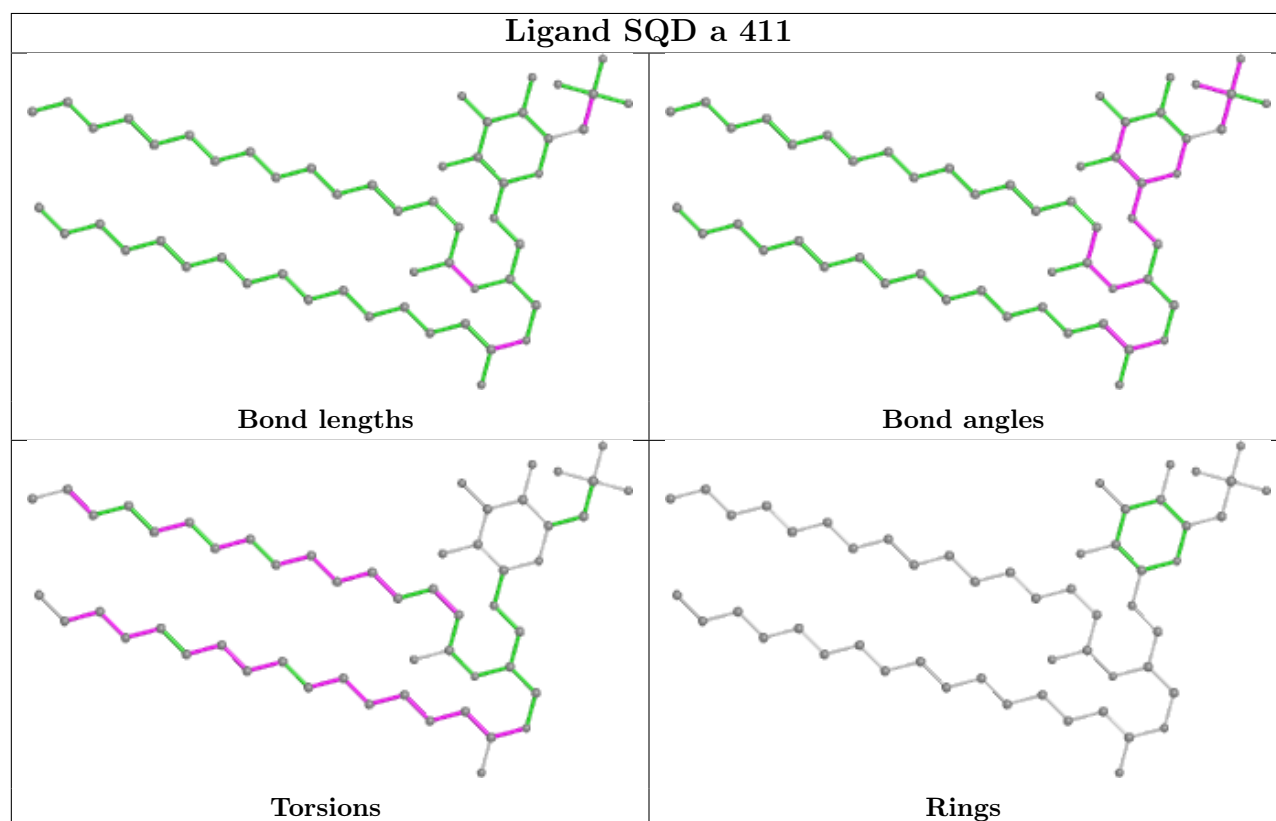
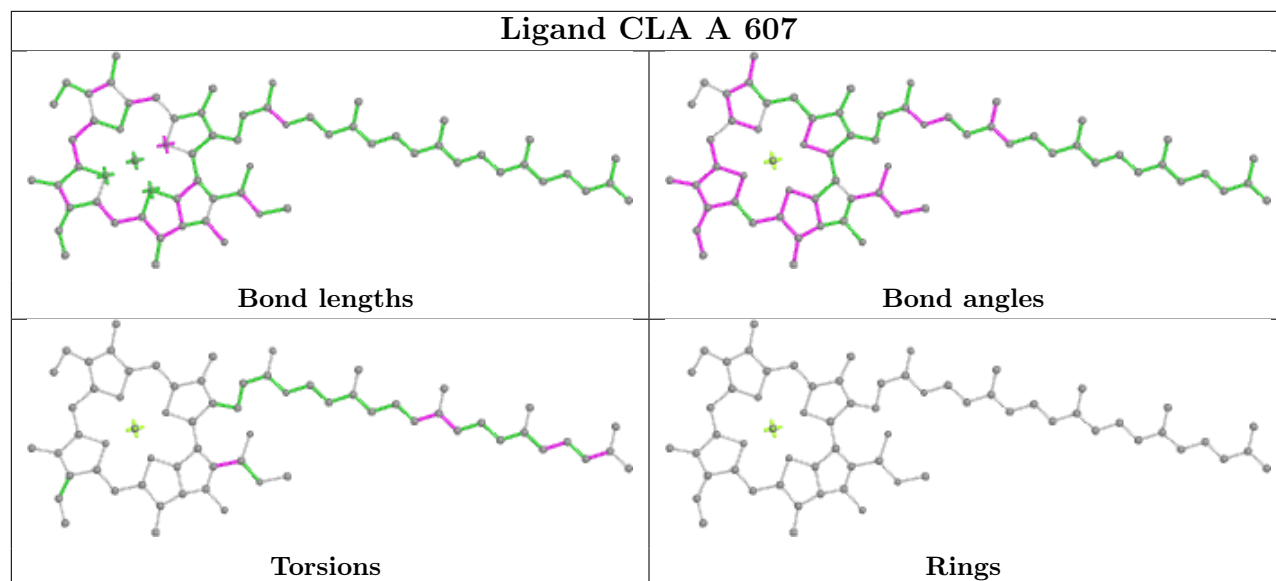
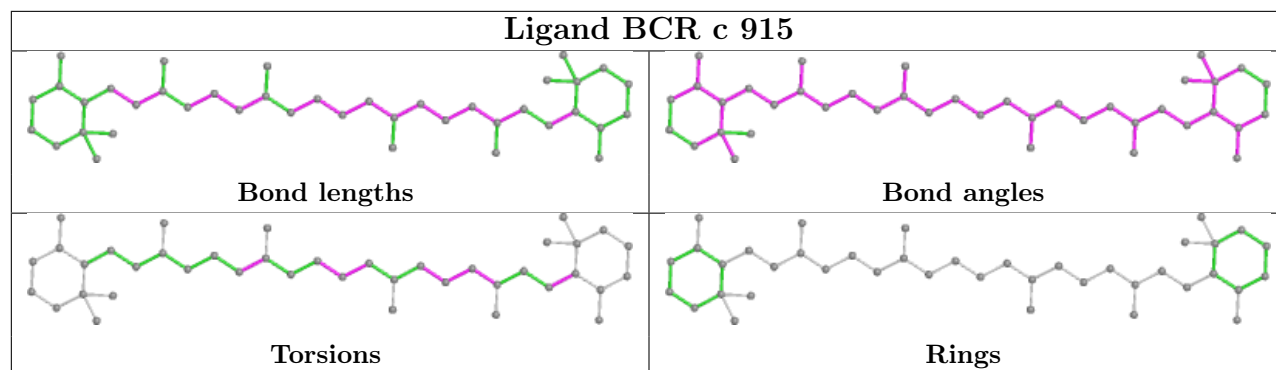
## Ligand CLA C 507



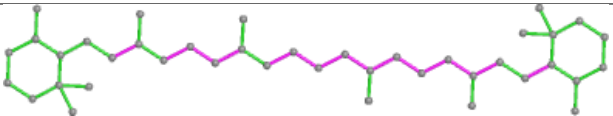
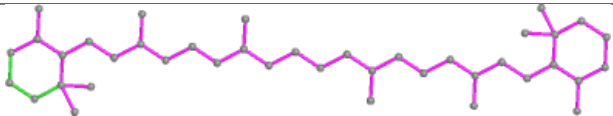
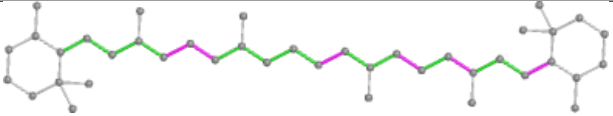
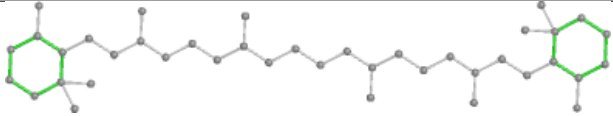
## Ligand CLA A 614

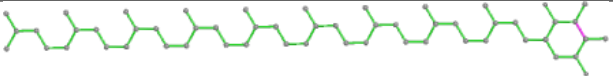
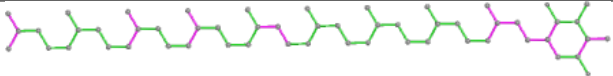
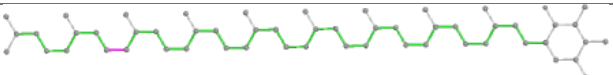
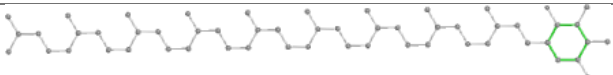


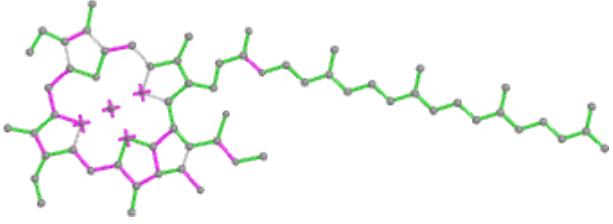
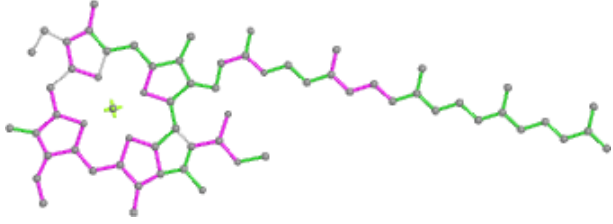
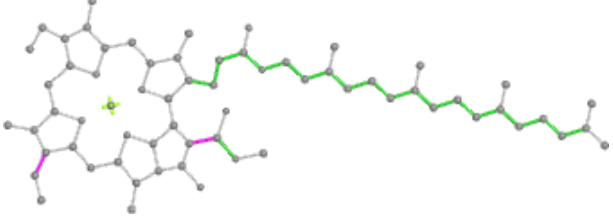
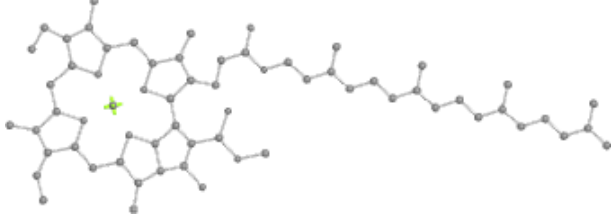
**Ligand CLA C 504****Ligand CLA B 608****Ligand CLA c 902**



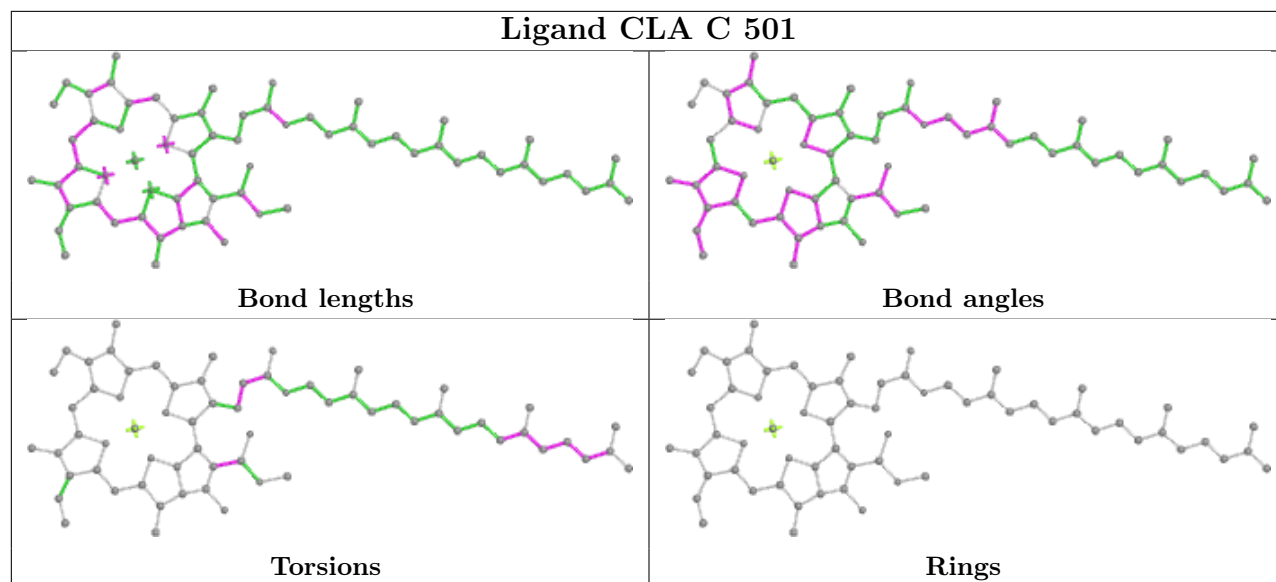


Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

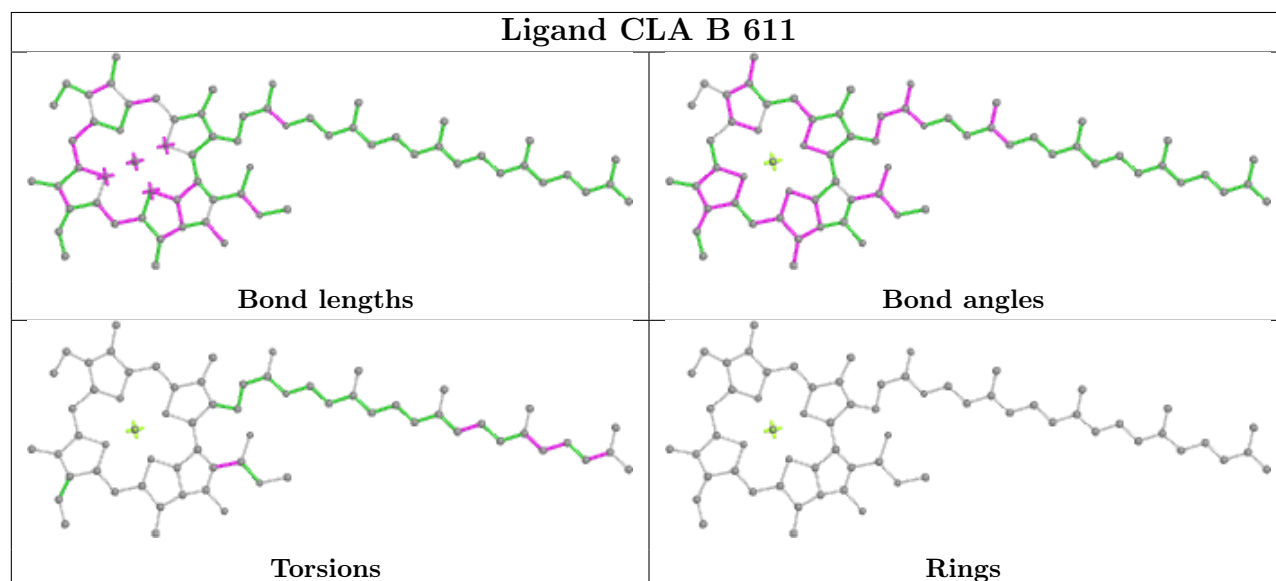
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

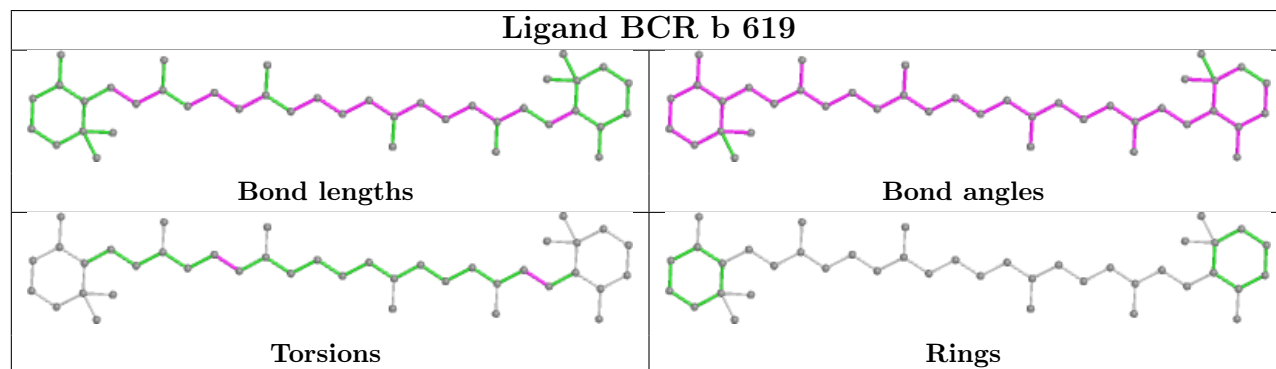
## Ligand CLA C 501

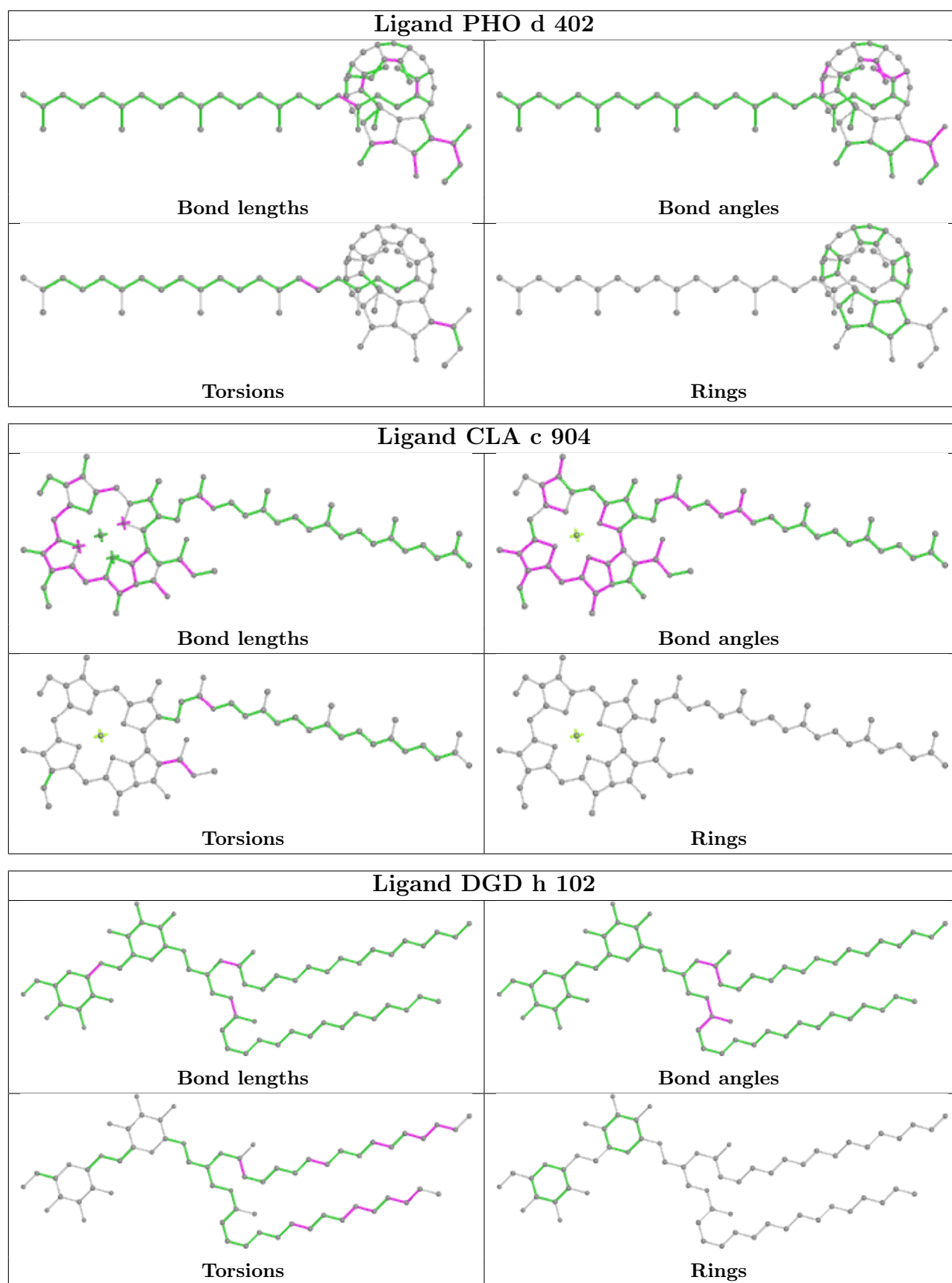


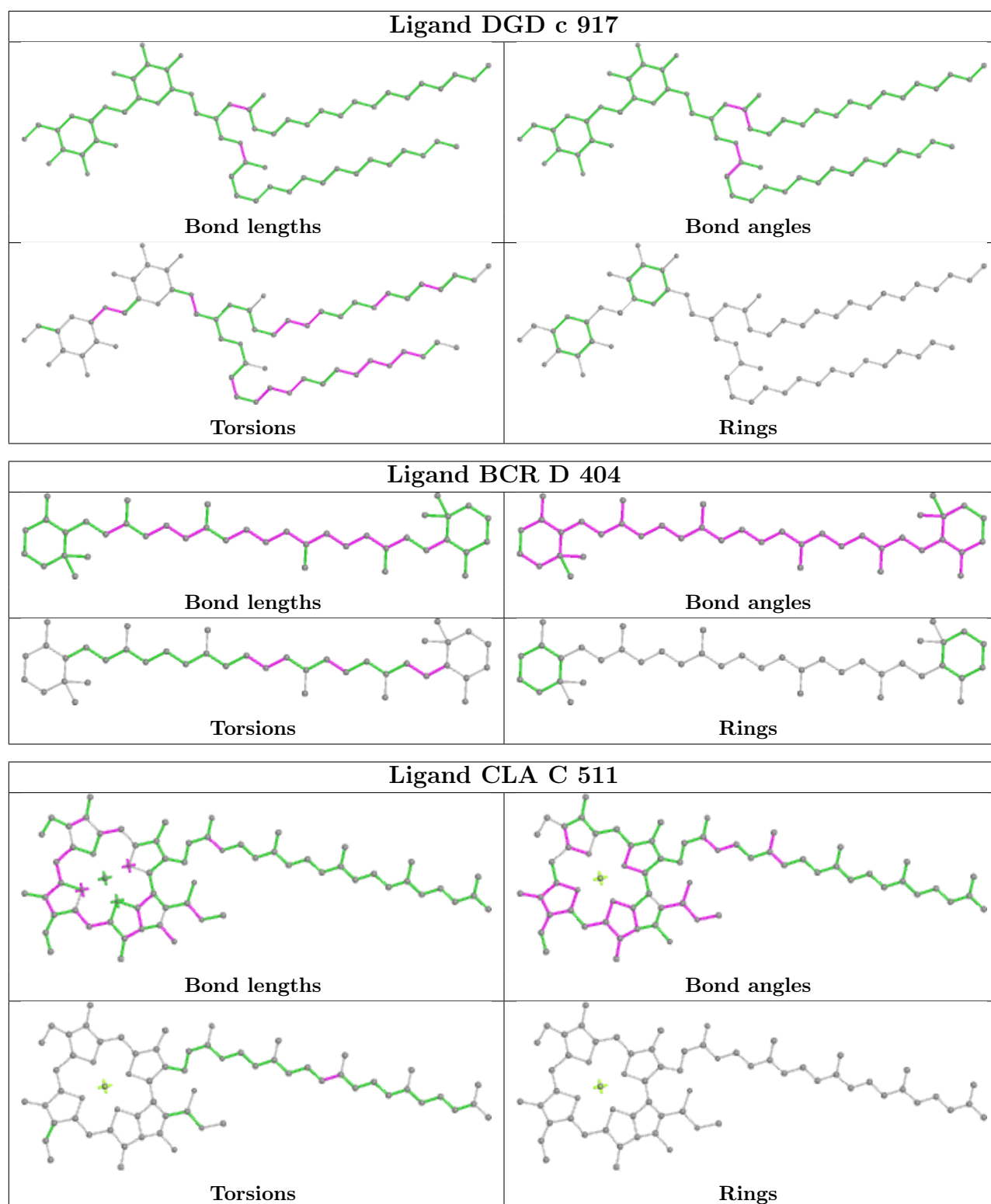
## Ligand CLA B 611

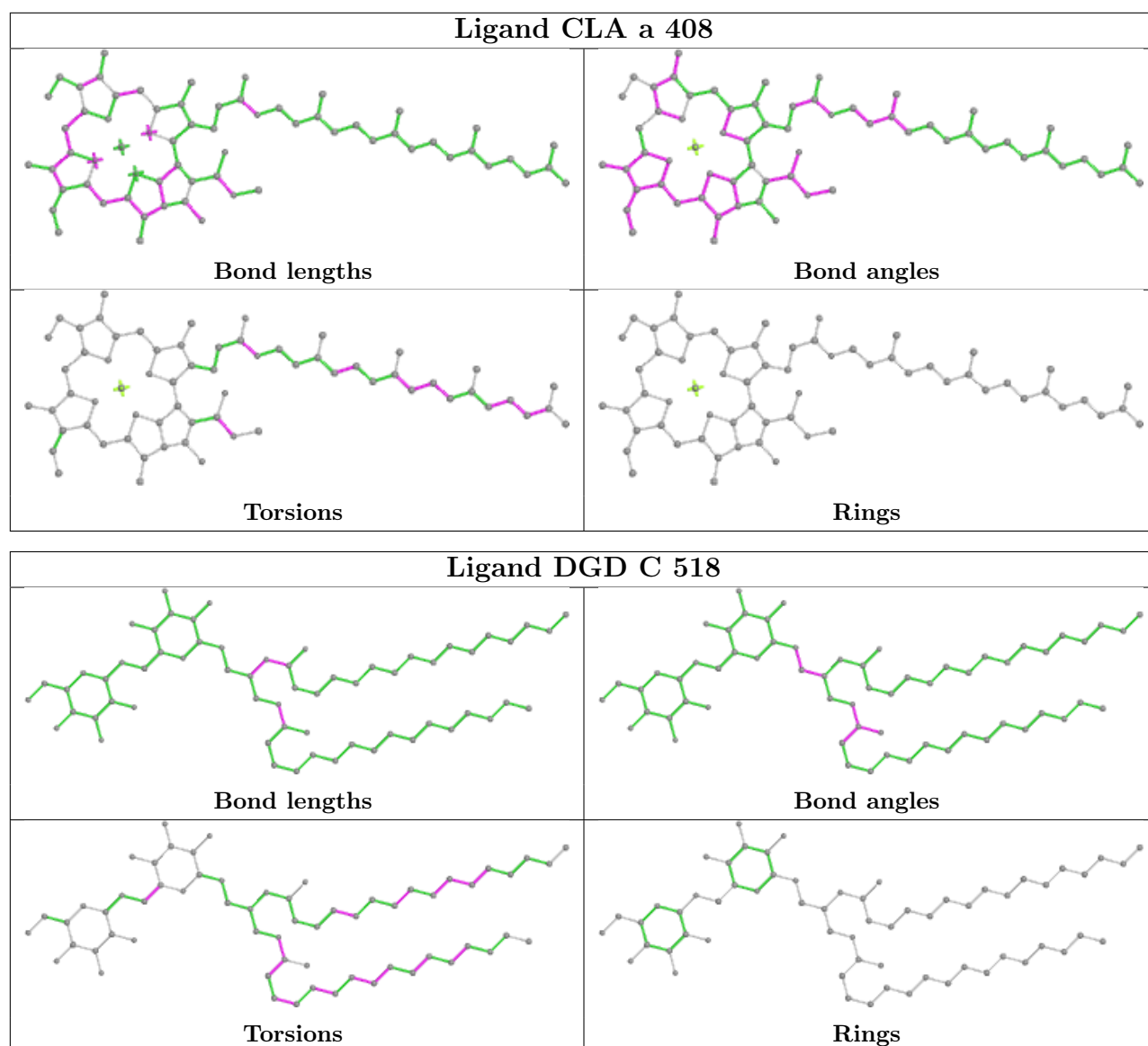


## Ligand BCR b 619









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	0.38	12 (3%) 42 35	16, 22, 43, 53	0
1	a	334/334 (100%)	0.39	18 (5%) 25 22	19, 24, 45, 62	0
2	B	504/504 (100%)	0.26	23 (4%) 32 27	18, 27, 49, 70	0
2	b	504/504 (100%)	0.53	50 (9%) 7 7	20, 29, 52, 93	0
3	C	451/455 (99%)	0.44	42 (9%) 8 8	21, 31, 44, 56	0
3	c	455/455 (100%)	0.27	24 (5%) 26 23	24, 34, 45, 59	0
4	D	342/342 (100%)	0.60	24 (7%) 16 13	17, 23, 39, 61	0
4	d	341/342 (99%)	0.52	22 (6%) 18 15	19, 26, 42, 59	0
5	E	81/81 (100%)	0.58	8 (9%) 7 7	27, 40, 57, 63	0
5	e	81/81 (100%)	0.23	4 (4%) 29 26	34, 45, 67, 76	0
6	F	34/34 (100%)	-0.10	1 (2%) 51 41	28, 33, 58, 61	0
6	f	32/34 (94%)	-0.05	2 (6%) 20 16	30, 36, 60, 62	0
7	H	65/65 (100%)	0.57	8 (12%) 4 5	23, 34, 40, 58	0
7	h	65/65 (100%)	1.06	11 (16%) 1 2	28, 37, 48, 58	0
8	I	38/38 (100%)	0.30	3 (7%) 12 11	26, 33, 65, 68	0
8	i	38/38 (100%)	-0.01	2 (5%) 26 23	29, 34, 62, 65	0
9	J	38/40 (95%)	0.50	3 (7%) 12 11	26, 37, 68, 72	0
9	j	40/40 (100%)	-0.10	3 (7%) 14 12	31, 42, 76, 80	0
10	K	37/37 (100%)	0.05	0 100 100	33, 38, 45, 47	0
10	k	37/37 (100%)	0.23	2 (5%) 25 22	38, 43, 55, 58	0
11	L	37/37 (100%)	0.53	3 (8%) 12 11	17, 22, 50, 59	0
11	l	37/37 (100%)	0.39	0 100 100	19, 22, 55, 62	0
12	M	34/34 (100%)	0.96	5 (14%) 2 3	21, 23, 36, 52	0
12	m	34/34 (100%)	0.67	1 (2%) 51 41	21, 25, 37, 53	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/243 (100%)	0.18	3 (1%) 79 70	18, 32, 55, 71	0
13	o	243/243 (100%)	0.31	10 (4%) 37 31	21, 35, 61, 72	0
14	T	30/30 (100%)	0.65	2 (6%) 17 15	19, 23, 44, 52	0
14	t	30/30 (100%)	0.66	1 (3%) 46 37	20, 24, 44, 50	0
15	U	97/97 (100%)	0.04	1 (1%) 82 74	23, 30, 48, 50	0
15	u	97/97 (100%)	0.25	3 (3%) 49 39	25, 31, 37, 47	0
16	V	137/137 (100%)	0.05	1 (0%) 87 82	23, 28, 39, 48	0
16	v	137/137 (100%)	0.07	6 (4%) 34 29	27, 37, 51, 57	0
17	Y	29/29 (100%)	0.44	1 (3%) 45 37	42, 48, 75, 77	0
17	y	29/29 (100%)	0.04	0 100 100	50, 56, 75, 76	0
18	X	39/39 (100%)	0.63	8 (20%) 1 1	33, 40, 66, 68	0
18	x	39/39 (100%)	0.87	5 (12%) 3 5	37, 43, 75, 77	0
19	Z	62/62 (100%)	0.28	1 (1%) 72 62	39, 48, 68, 72	0
19	z	62/62 (100%)	0.32	3 (4%) 30 26	53, 61, 82, 87	0
All	All	5267/5276 (99%)	0.37	316 (5%) 21 18	16, 30, 56, 93	0

The worst 5 of 316 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	40	SER	8.2
7	H	65	LEU	6.5
4	D	137	GLY	6.0
4	D	136	VAL	5.9
6	f	14	PRO	5.7

## 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
30	CA	f	102	1/1	0.22	0.38	58,58,58,58	0
27	PL9	a	410	55/55	0.27	1.66	63,80,85,85	0
26	BCR	k	101	40/40	0.34	1.07	37,41,45,45	0
30	CA	b	601	1/1	0.44	1.04	77,77,77,77	0
26	BCR	f	101	40/40	0.46	0.98	30,34,48,49	0
22	CL	v	201	1/1	0.49	0.40	60,60,60,60	0
29	LHG	a	413	42/49	0.50	0.71	95,107,110,111	0
30	CA	B	601	1/1	0.52	0.59	76,76,76,76	0
26	BCR	a	409	40/40	0.53	0.47	21,26,29,29	0
31	DGD	D	406	62/66	0.54	1.28	77,89,103,103	0
26	BCR	D	404	40/40	0.55	0.92	25,30,48,49	0
26	BCR	k	102	40/40	0.55	2.00	33,44,47,48	0
26	BCR	b	619	40/40	0.57	1.00	30,34,41,42	0
30	CA	F	102	1/1	0.58	0.44	56,56,56,56	0
33	MG	j	102	1/1	0.58	0.19	34,34,34,34	0
30	CA	c	901	1/1	0.59	0.43	46,46,46,46	0
31	DGD	d	406	62/66	0.59	0.91	80,91,105,105	0
27	PL9	A	611	55/55	0.59	2.02	52,69,78,78	0
24	CLA	b	607	65/65	0.62	0.56	26,30,41,42	0
26	BCR	B	620	40/40	0.63	0.52	27,33,39,39	0
24	CLA	b	617	65/65	0.63	0.85	27,33,74,75	0
26	BCR	A	610	40/40	0.63	0.63	22,27,32,32	0
29	LHG	A	615	42/49	0.64	1.14	69,83,86,86	0
26	BCR	B	622	40/40	0.64	0.37	23,34,41,41	0
26	BCR	Y	101	40/40	0.65	1.59	34,38,39,39	0
24	CLA	B	602	65/65	0.65	0.84	32,41,66,66	0
24	CLA	a	407	65/65	0.65	0.73	19,23,63,65	0
28	SQD	A	612	54/54	0.66	0.81	49,57,66,67	0
26	BCR	T	101	40/40	0.67	0.44	25,37,44,45	0
26	BCR	H	101	40/40	0.67	1.31	26,33,42,42	0
22	CL	V	201	1/1	0.69	0.15	50,50,50,50	0
26	BCR	B	618	40/40	0.70	0.35	23,27,28,29	0
27	PL9	D	405	55/55	0.70	0.55	19,23,29,32	0
24	CLA	b	602	65/65	0.71	1.20	38,46,68,68	0
28	SQD	d	407	43/54	0.71	0.94	84,90,93,94	0
24	CLA	C	513	65/65	0.71	1.17	39,45,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	T	102	40/40	0.71	0.42	25,29,31,31	0
28	SQD	a	411	54/54	0.72	0.51	50,60,75,76	0
24	CLA	D	403	65/65	0.72	0.95	24,27,65,67	0
26	BCR	c	915	40/40	0.72	1.72	30,37,41,42	0
26	BCR	b	618	40/40	0.72	0.43	24,28,39,39	0
26	BCR	C	514	40/40	0.73	1.35	37,43,47,47	0
28	SQD	l	101	54/54	0.73	0.41	57,69,84,85	0
24	CLA	b	608	65/65	0.73	0.46	19,23,30,32	0
24	CLA	B	607	65/65	0.73	0.55	24,28,40,41	0
27	PL9	d	405	55/55	0.74	0.41	19,25,29,31	0
24	CLA	a	408	65/65	0.74	0.72	20,24,75,75	0
29	LHG	D	407	49/49	0.74	0.39	29,34,41,41	0
24	CLA	B	608	65/65	0.75	0.41	17,20,32,34	0
28	SQD	A	613	54/54	0.76	0.49	50,63,68,68	0
24	CLA	c	914	65/65	0.76	1.06	46,51,73,74	0
24	CLA	B	617	65/65	0.76	0.44	22,29,77,78	0
24	CLA	C	512	65/65	0.76	1.32	37,41,62,63	0
26	BCR	c	918	40/40	0.76	1.72	50,52,58,58	0
25	PHO	A	608	64/64	0.77	0.55	16,21,25,26	0
24	CLA	c	902	65/65	0.77	1.47	30,33,41,45	0
24	CLA	b	612	65/65	0.77	0.48	20,23,37,41	0
24	CLA	c	903	65/65	0.78	0.85	25,28,42,45	0
24	CLA	c	913	65/65	0.78	1.24	38,42,62,63	0
28	SQD	L	101	54/54	0.78	0.39	58,66,80,80	0
31	DGD	C	517	62/66	0.78	0.47	23,35,62,63	0
28	SQD	a	402	54/54	0.78	0.38	51,67,75,76	0
24	CLA	b	615	65/65	0.78	0.35	22,26,65,66	0
26	BCR	B	619	40/40	0.78	0.31	21,28,40,40	0
26	BCR	h	101	40/40	0.79	1.14	29,37,45,45	0
29	LHG	D	408	49/49	0.79	0.52	24,28,37,40	0
24	CLA	A	607	65/65	0.79	0.85	19,21,63,65	0
22	CL	A	603	1/1	0.79	0.47	24,24,24,24	0
24	CLA	a	406	65/65	0.80	0.50	18,20,28,33	0
24	CLA	C	507	65/65	0.80	1.13	29,33,52,53	0
24	CLA	b	614	65/65	0.80	0.38	21,24,44,45	0
24	CLA	B	616	65/65	0.80	0.59	25,27,45,46	0
25	PHO	D	401	64/64	0.80	1.05	19,22,28,32	0
24	CLA	b	616	65/65	0.80	1.05	27,30,45,46	0
24	CLA	B	615	65/65	0.80	0.39	20,24,60,61	0
24	CLA	C	504	65/65	0.80	0.68	25,28,54,54	0
29	LHG	d	408	49/49	0.80	0.40	29,37,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	C	515	40/40	0.81	1.82	30,37,40,41	0
24	CLA	d	404	65/65	0.81	0.78	26,31,67,68	0
24	CLA	b	605	65/65	0.81	0.81	20,25,53,55	0
22	CL	a	404	1/1	0.81	0.64	28,28,28,28	0
24	CLA	C	508	65/65	0.82	0.75	25,29,54,58	0
31	DGD	c	917	62/66	0.82	0.41	28,36,64,65	0
25	PHO	d	402	64/64	0.83	0.50	18,22,24,25	0
28	SQD	F	101	43/54	0.83	0.81	67,74,78,79	0
29	LHG	D	409	49/49	0.83	0.81	26,33,62,64	0
24	CLA	B	606	65/65	0.83	0.70	19,23,34,35	0
24	CLA	b	606	65/65	0.83	0.81	21,24,32,33	0
24	CLA	A	614	65/65	0.84	0.49	14,18,29,35	0
25	PHO	a	412	64/64	0.84	0.80	20,25,30,33	0
29	LHG	d	409	49/49	0.84	0.35	23,27,38,40	0
31	DGD	C	518	62/66	0.84	0.54	22,31,52,56	0
24	CLA	c	908	65/65	0.85	0.98	28,32,50,51	0
24	CLA	D	402	65/65	0.85	0.82	13,18,34,35	0
31	DGD	c	916	62/66	0.85	0.48	24,35,60,61	0
24	CLA	b	613	65/65	0.85	0.66	21,26,33,35	0
24	CLA	d	401	65/65	0.85	0.44	17,20,27,31	0
24	CLA	c	904	65/65	0.85	0.89	26,37,39,40	0
26	BCR	K	101	40/40	0.86	1.83	29,33,37,37	0
24	CLA	A	606	65/65	0.86	0.65	15,19,25,34	0
29	LHG	b	620	49/49	0.86	0.32	24,31,46,50	0
24	CLA	B	609	65/65	0.86	0.97	20,24,31,31	0
24	CLA	B	612	65/65	0.86	0.45	19,21,32,34	0
29	LHG	d	410	49/49	0.86	0.72	28,34,66,67	0
24	CLA	c	907	65/65	0.87	0.78	30,35,64,64	0
24	CLA	c	910	65/65	0.87	0.88	27,30,46,46	0
24	CLA	c	912	65/65	0.87	0.77	32,37,43,44	0
31	DGD	h	102	62/66	0.87	0.89	29,36,43,44	0
24	CLA	d	403	65/65	0.87	0.72	18,21,38,39	0
24	CLA	A	609	65/65	0.88	0.63	21,24,71,72	0
24	CLA	C	501	65/65	0.88	0.92	29,32,44,46	0
24	CLA	b	603	65/65	0.88	0.97	26,29,36,37	0
24	CLA	B	613	65/65	0.88	0.54	20,24,30,31	0
24	CLA	C	506	65/65	0.88	0.68	31,38,74,75	0
24	CLA	C	503	65/65	0.89	0.64	27,31,35,36	0
31	DGD	C	516	62/66	0.89	0.43	23,33,61,62	0
30	CA	O	301	1/1	0.89	0.17	49,49,49,49	0
24	CLA	C	509	65/65	0.89	1.01	29,32,46,47	0
24	CLA	c	905	65/65	0.89	0.56	28,30,55,56	0

*Continued on next page...*

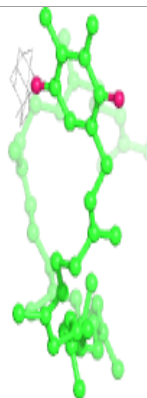
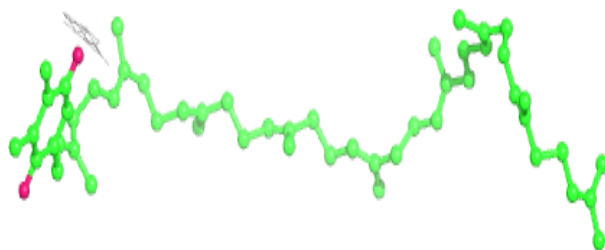
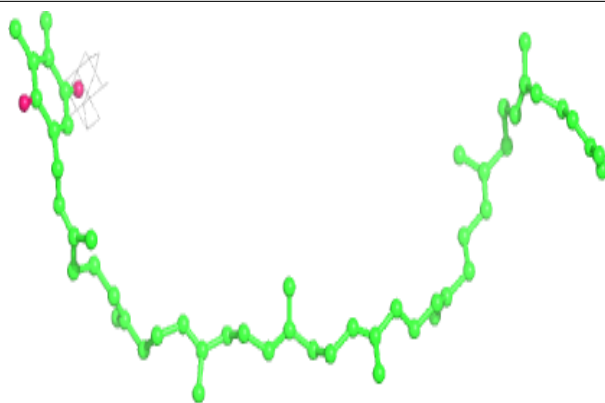
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	B	604	65/65	0.90	0.88	18,22,31,35	0
31	DGD	H	102	62/66	0.90	1.04	26,32,38,40	0
24	CLA	b	611	65/65	0.90	0.74	25,28,34,37	0
24	CLA	c	909	65/65	0.90	0.59	27,29,57,60	0
24	CLA	B	611	65/65	0.90	0.80	21,25,32,37	0
24	CLA	C	510	65/65	0.90	0.72	24,28,35,37	0
31	DGD	j	101	62/66	0.90	0.43	25,34,52,55	0
32	HEM	V	202	43/43	0.90	0.52	23,24,27,29	0
24	CLA	c	906	65/65	0.90	0.77	28,31,44,44	0
24	CLA	B	603	65/65	0.91	1.10	23,26,32,32	0
29	LHG	B	621	49/49	0.91	0.31	23,31,43,44	0
24	CLA	C	502	65/65	0.91	0.65	24,26,39,42	0
24	CLA	B	610	65/65	0.91	0.80	23,28,31,32	0
24	CLA	c	911	65/65	0.91	0.68	26,30,39,40	0
22	CL	A	604	1/1	0.91	0.33	21,21,21,21	0
24	CLA	B	605	65/65	0.91	0.49	19,22,50,51	0
24	CLA	b	610	65/65	0.92	0.93	28,31,33,36	0
24	CLA	B	614	65/65	0.92	0.33	19,22,45,47	0
32	HEM	e	101	43/43	0.92	0.41	43,46,52,55	0
24	CLA	b	609	65/65	0.92	1.10	22,27,38,39	0
32	HEM	E	101	43/43	0.93	0.67	39,42,45,47	0
24	CLA	C	505	65/65	0.93	0.78	28,30,44,45	0
20	OEX	A	601	10/10	0.93	0.34	22,23,26,26	0
32	HEM	v	202	43/43	0.93	0.57	28,31,34,36	0
24	CLA	C	511	65/65	0.93	0.96	29,34,37,38	0
22	CL	a	405	1/1	0.94	0.26	26,26,26,26	0
24	CLA	b	604	65/65	0.95	1.07	23,26,35,38	0
21	FE2	a	403	1/1	0.95	0.22	27,27,27,27	0
23	BCT	A	605	4/4	0.95	0.44	39,39,40,42	0
20	OEX	a	401	10/10	0.95	0.35	25,27,28,28	0
30	CA	o	301	1/1	0.95	0.09	51,51,51,51	0
23	BCT	a	414	4/4	0.97	0.96	34,34,35,37	0
21	FE2	A	602	1/1	0.99	0.10	26,26,26,26	0

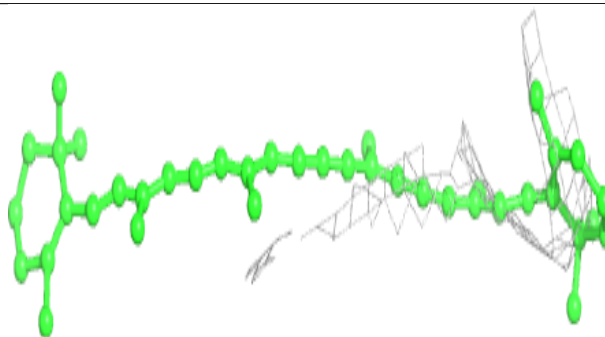
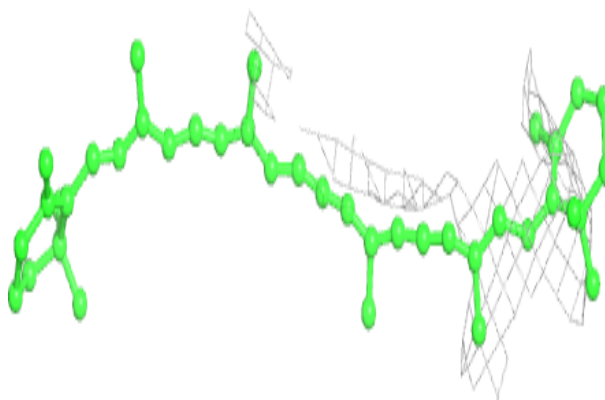
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PL9 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)

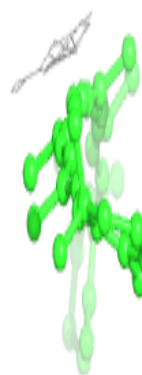
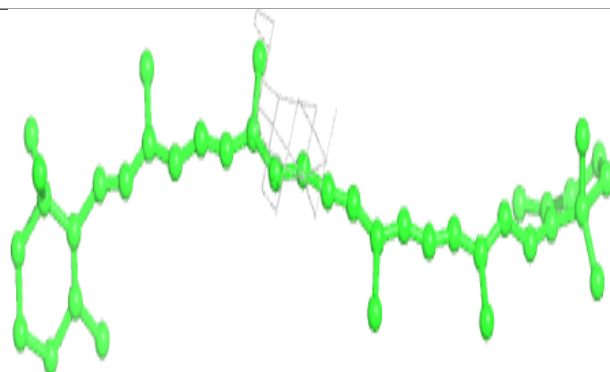
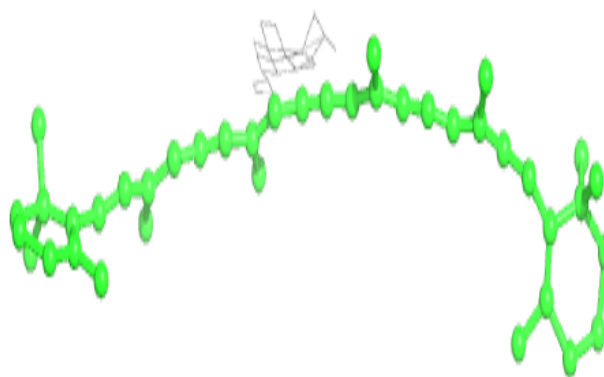
**Electron density around BCR k 101:**

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

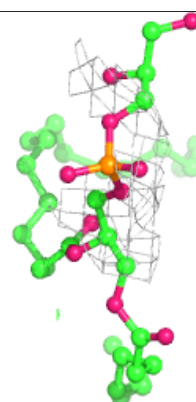
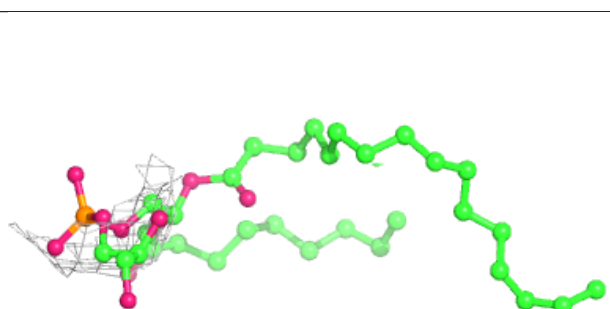
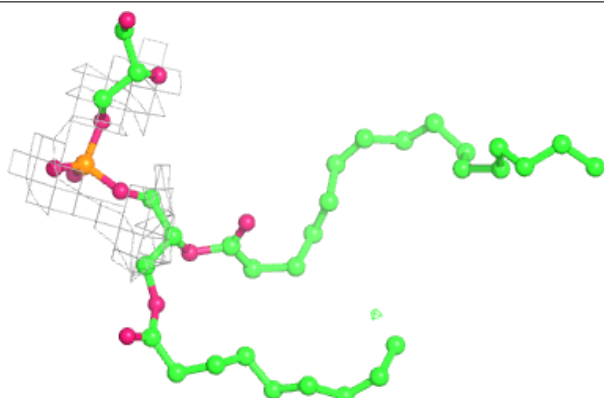


**Electron density around BCR f 101:**

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

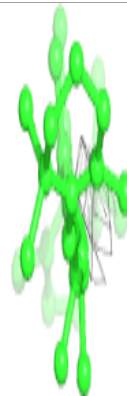
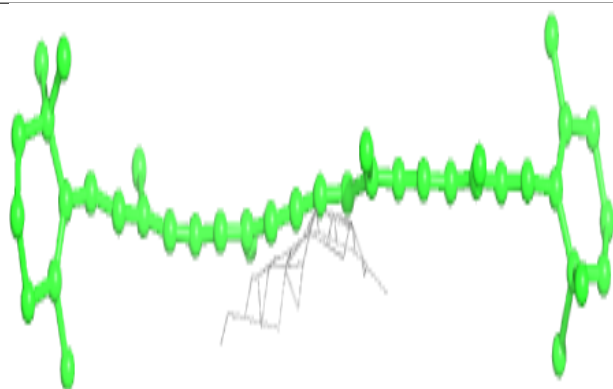
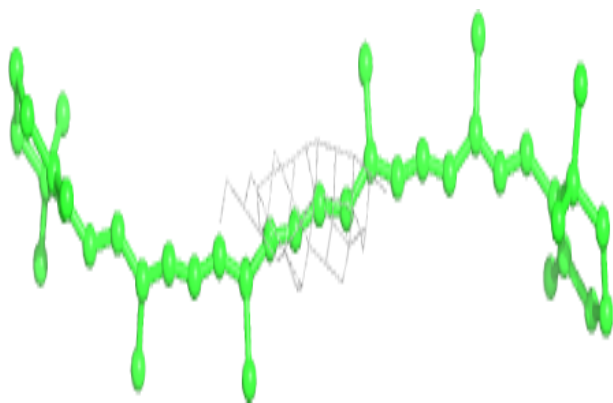
**Electron density around LHG a 413:**

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

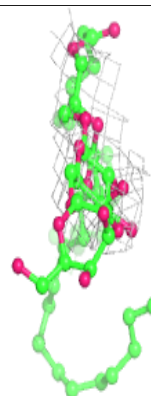
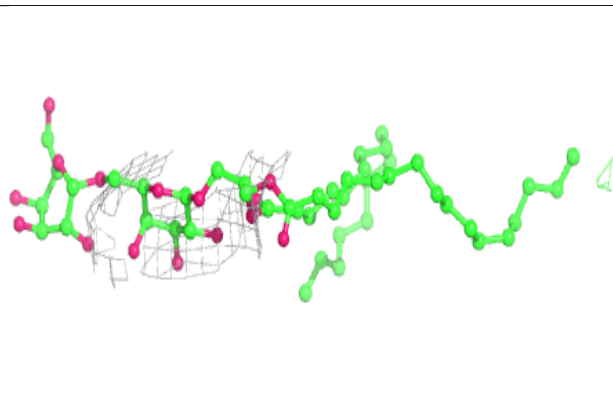
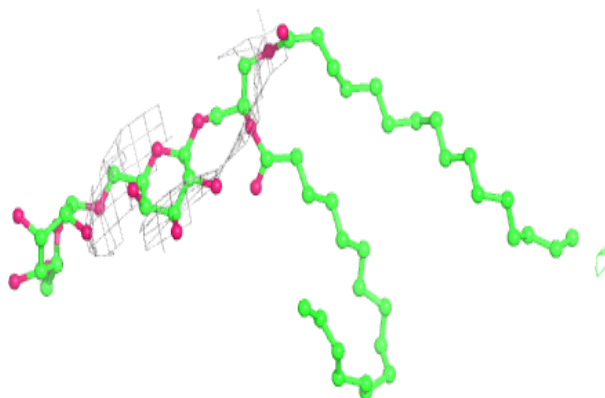


**Electron density around BCR a 409:**

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

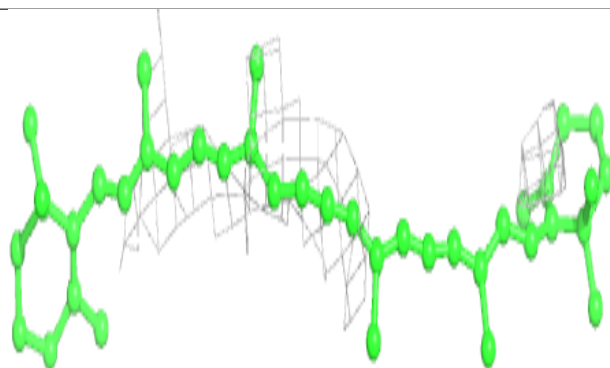
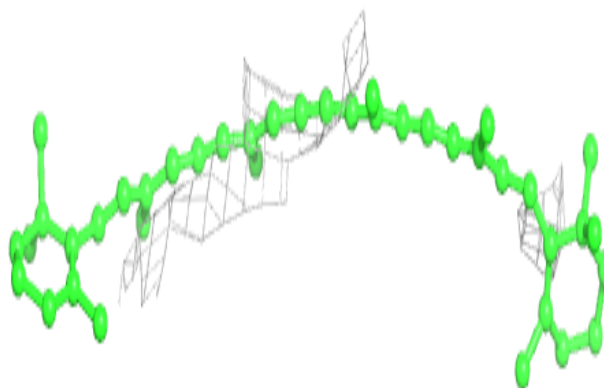
**Electron density around DGD D 406:**

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

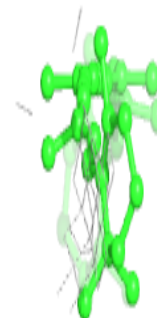
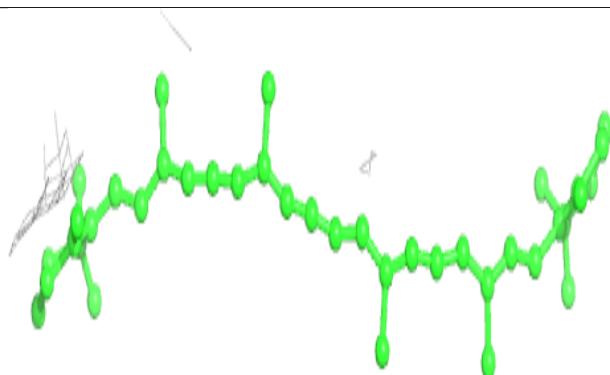
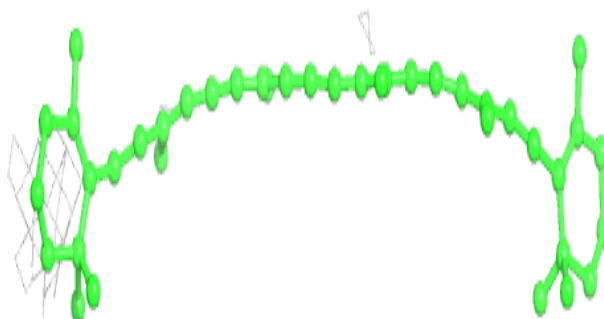


**Electron density around BCR D 404:**

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

**Electron density around BCR k 102:**

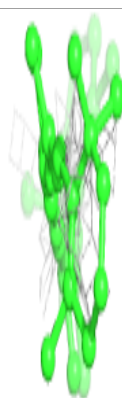
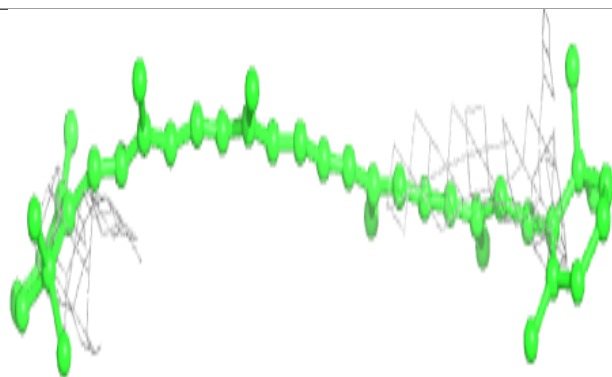
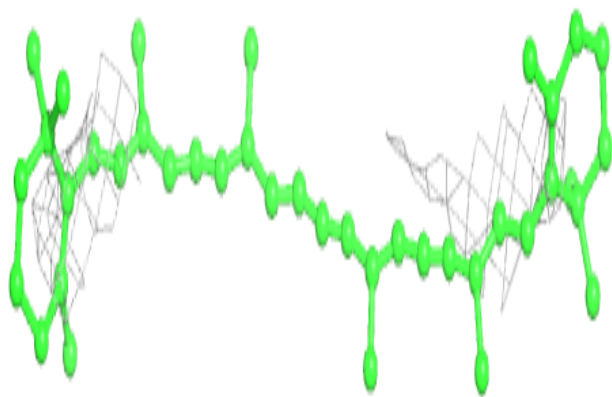
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



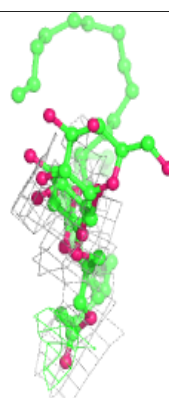
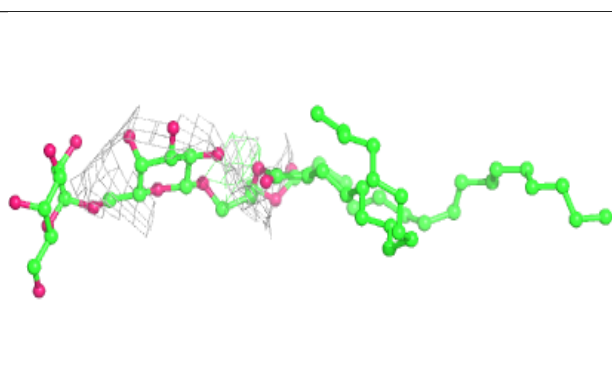
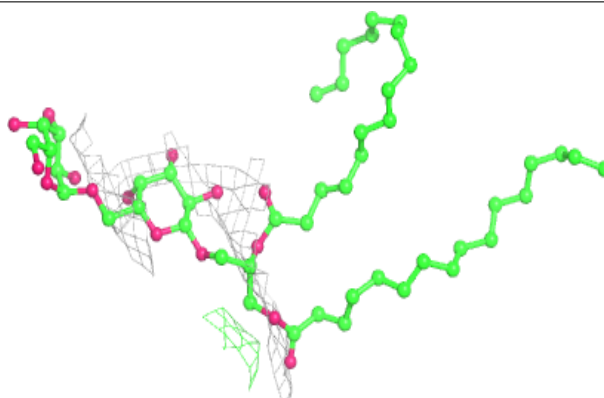


**Electron density around BCR b 619:**

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

**Electron density around DGD d 406:**

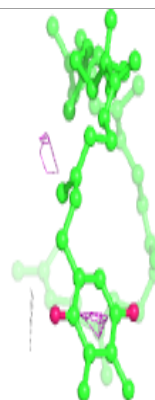
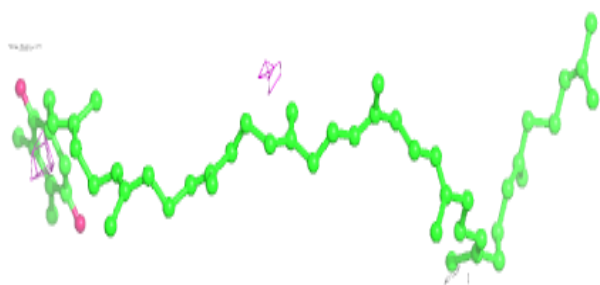
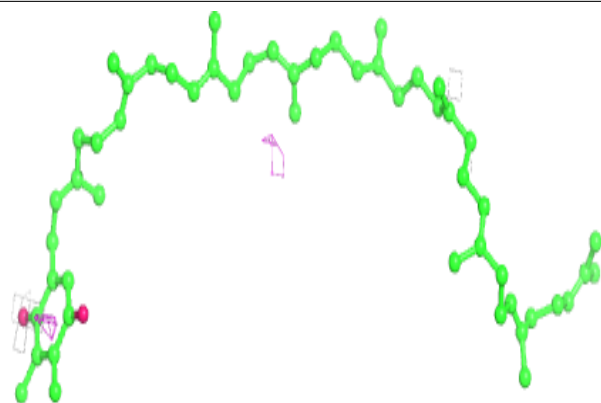
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



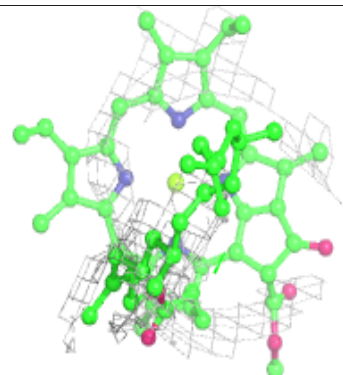
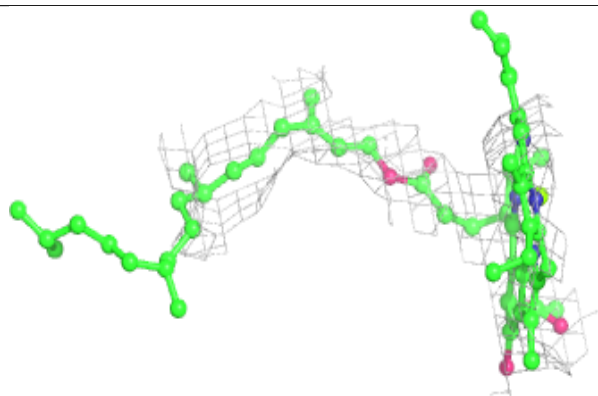
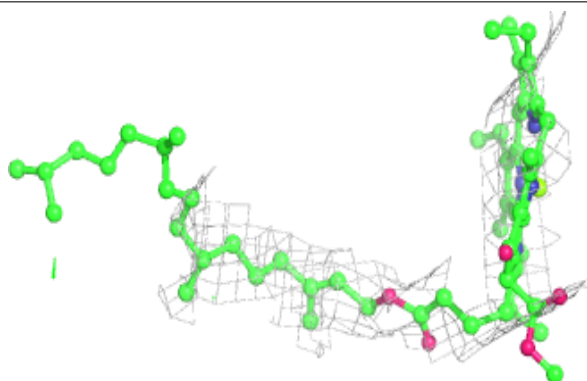


**Electron density around PL9 A 611:**

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

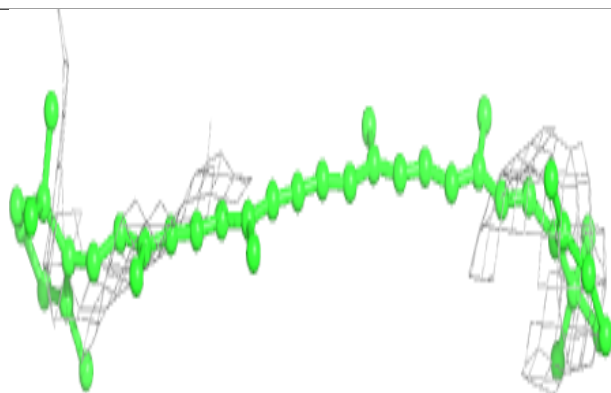
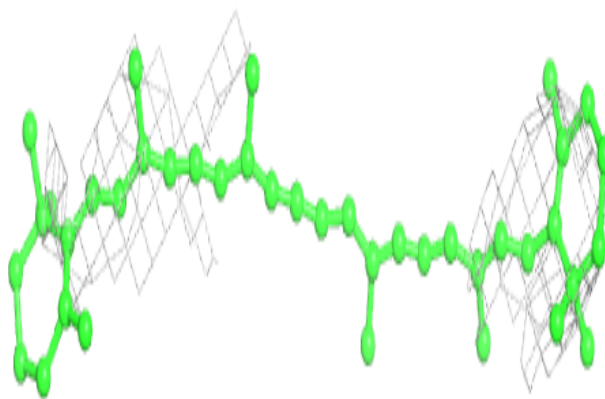
**Electron density around CLA b 607:**

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



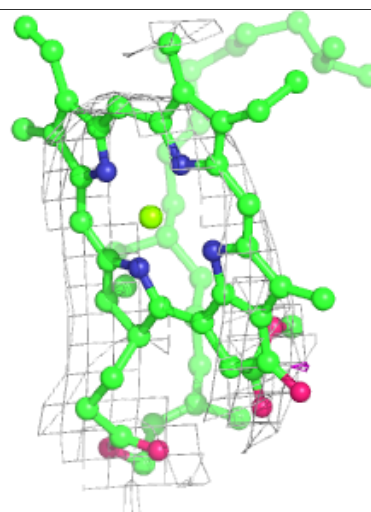
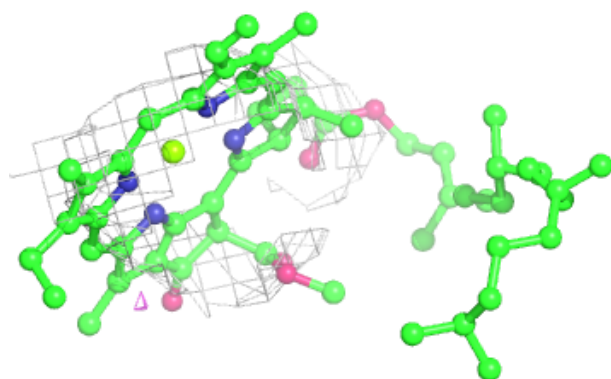
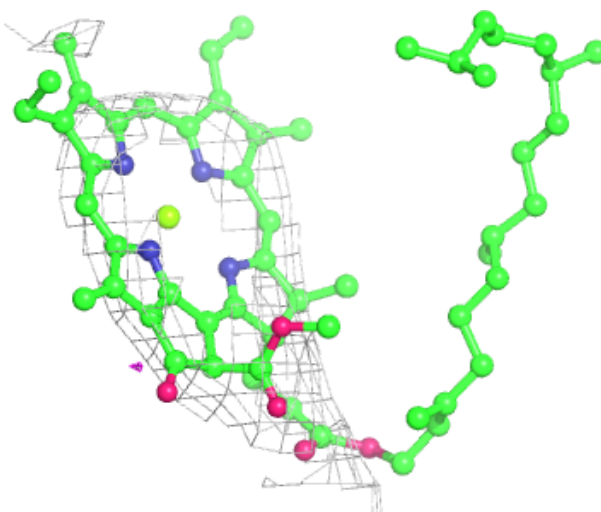
**Electron density around BCR B 620:**

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



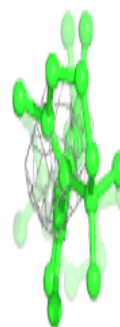
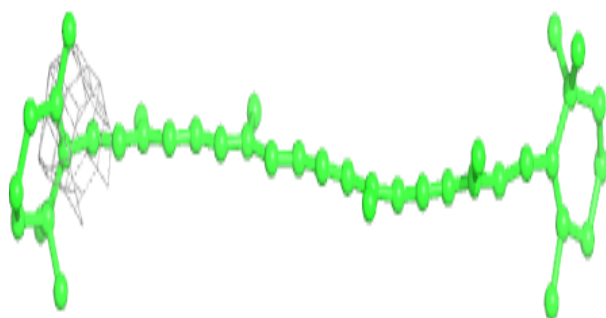
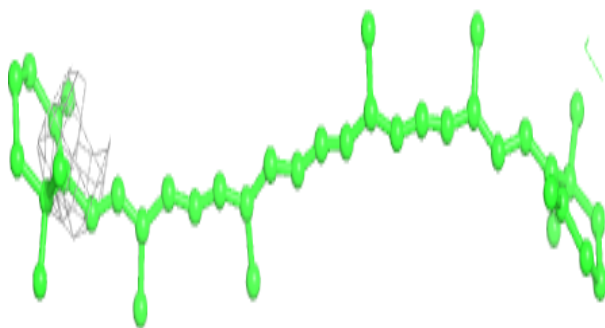
**Electron density around CLA b 617:**

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

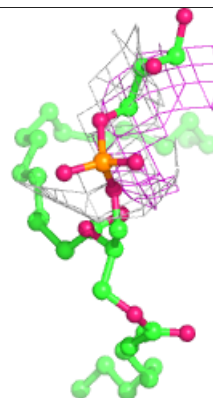
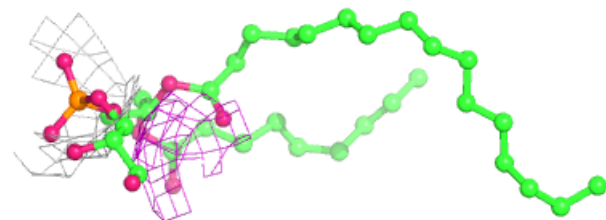
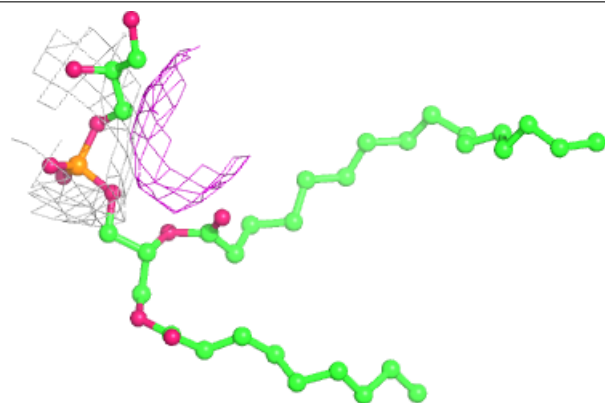


**Electron density around BCR A 610:**

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

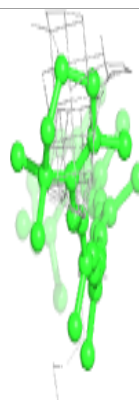
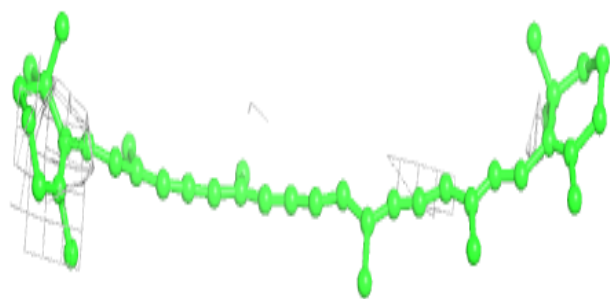
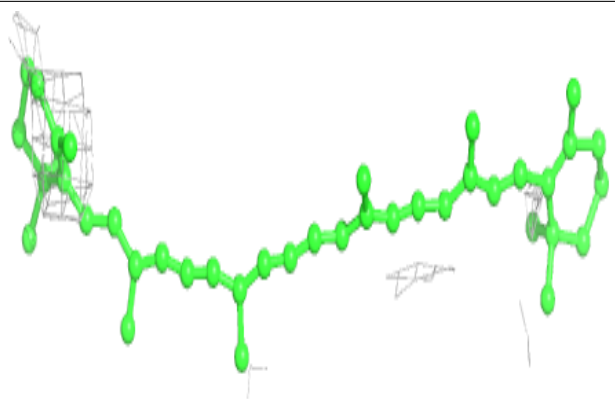
**Electron density around LHG A 615:**

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

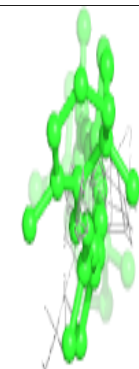
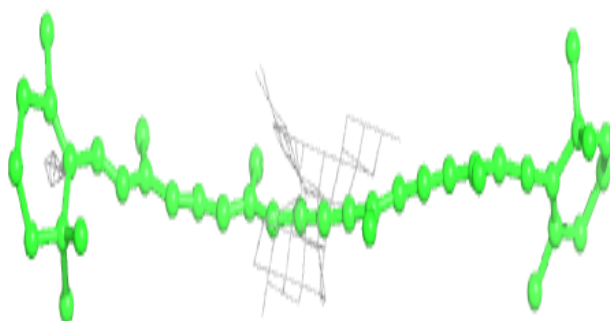
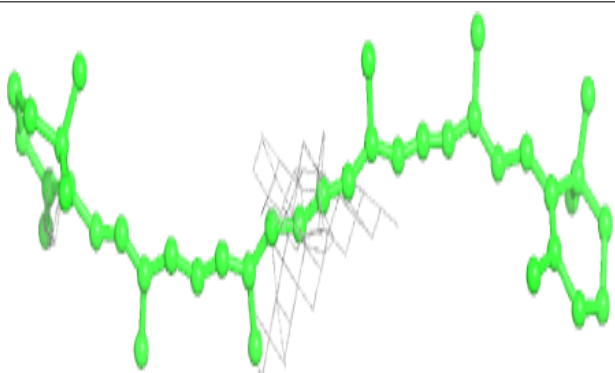


**Electron density around BCR B 622:**

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

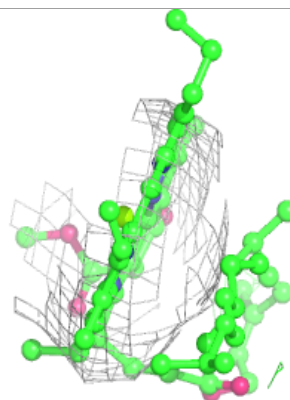
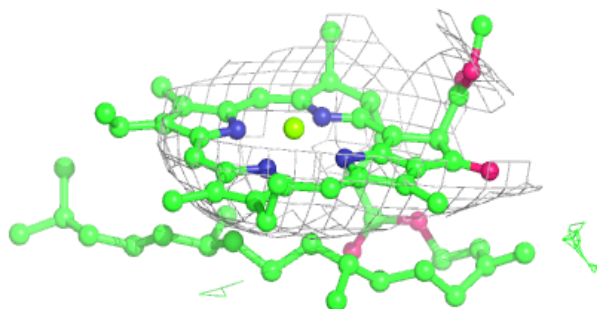
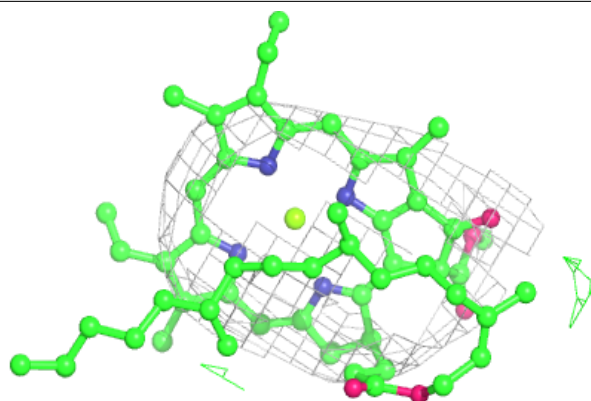
**Electron density around BCR Y 101:**

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

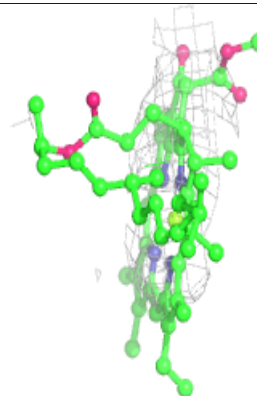
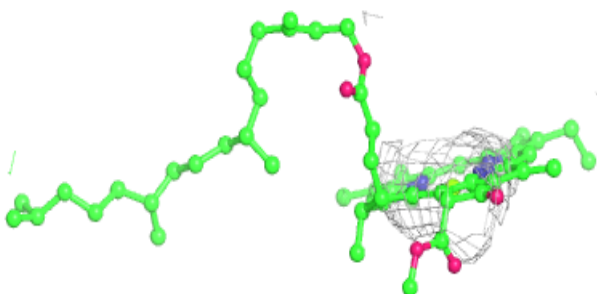
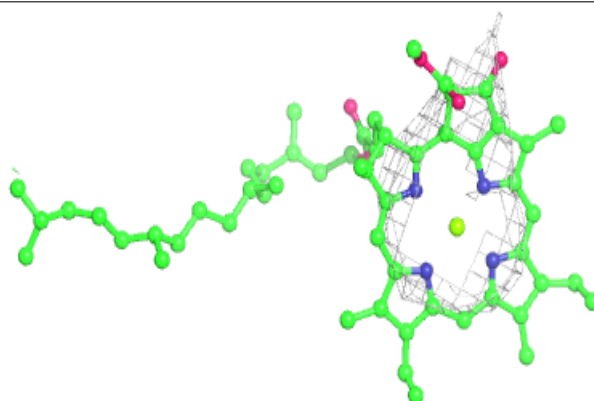


**Electron density around CLA B 602:**

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

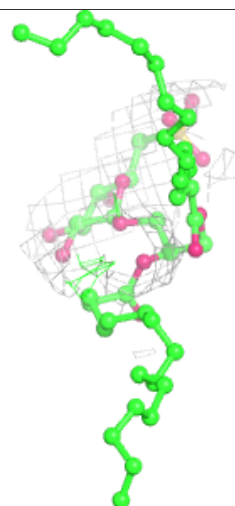
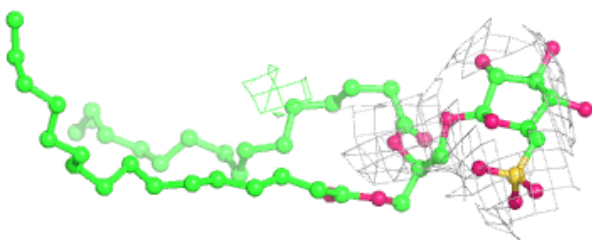
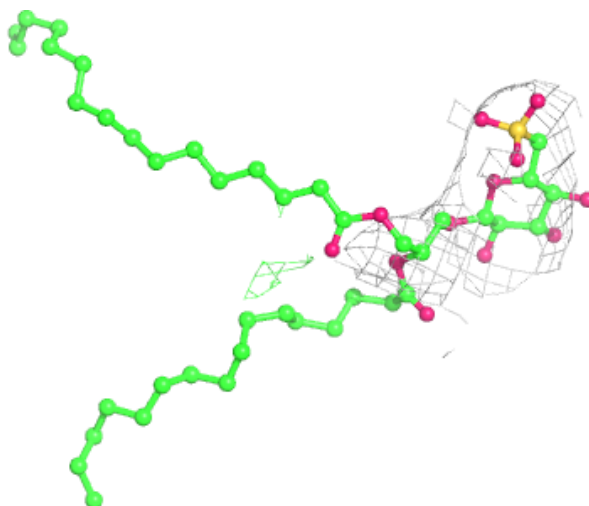
**Electron density around CLA a 407:**

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



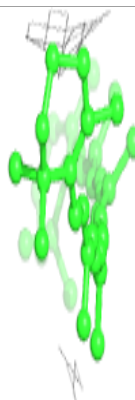
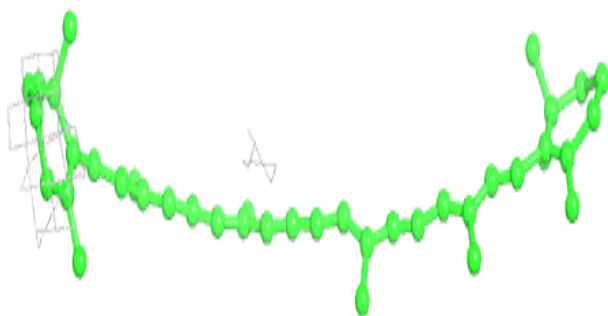
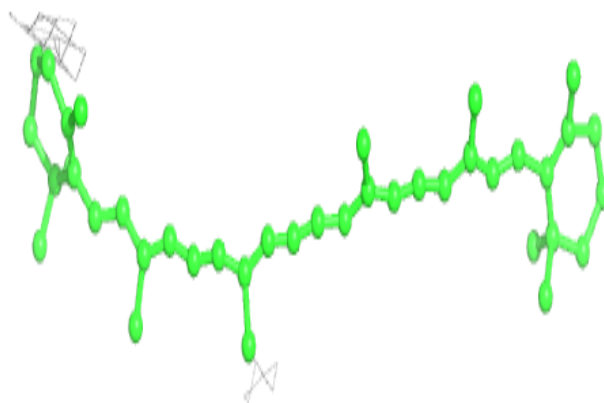
**Electron density around SQD A 612:**

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

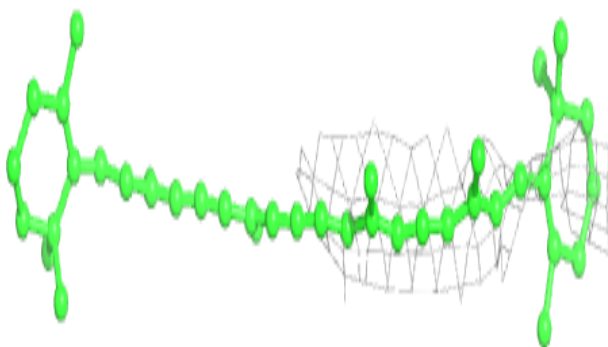
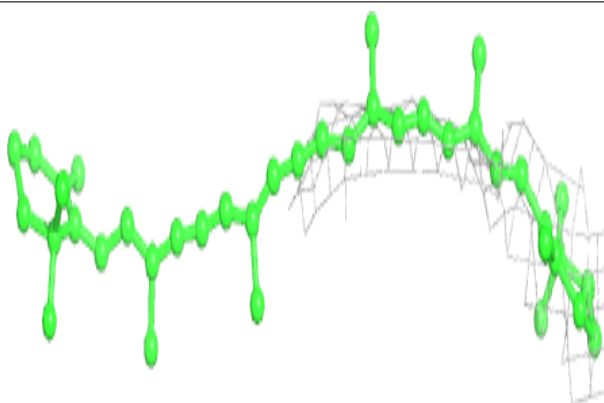


**Electron density around BCR T 101:**

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

**Electron density around BCR H 101:**

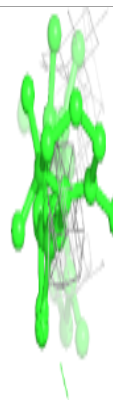
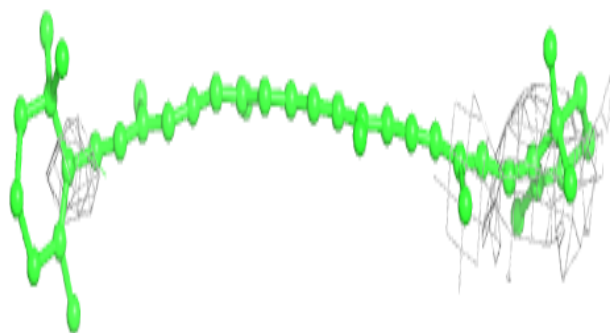
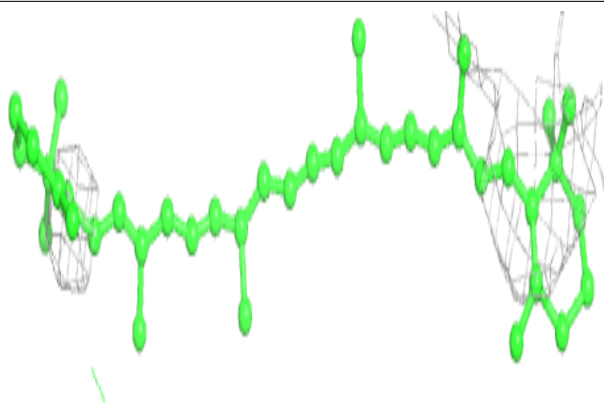
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



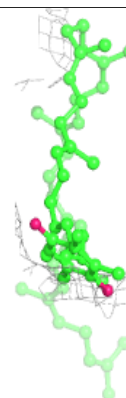
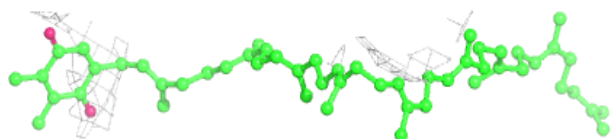
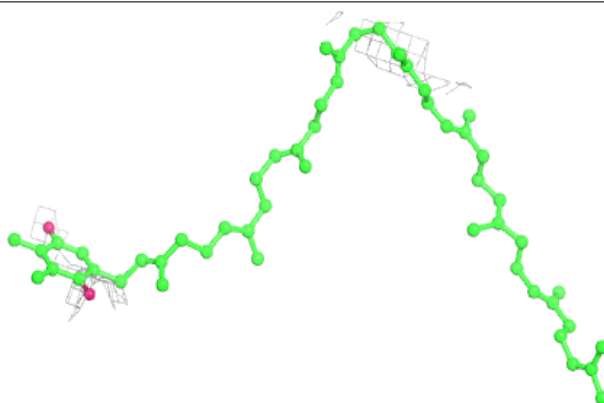


**Electron density around BCR B 618:**

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

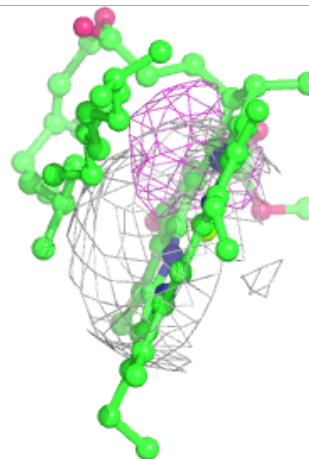
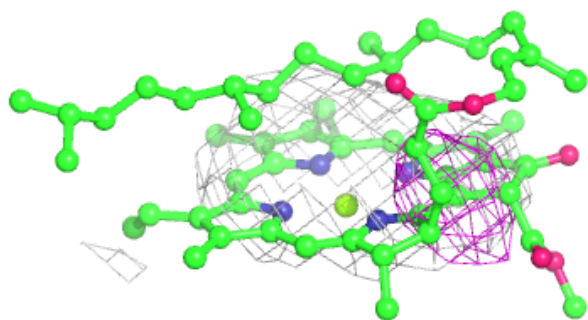
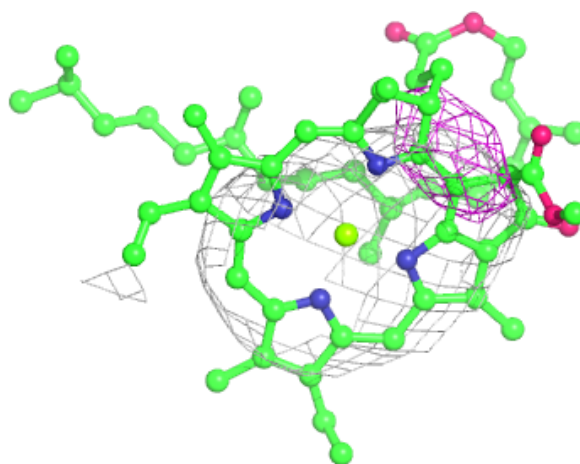
**Electron density around PL9 D 405:**

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



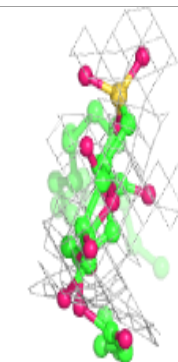
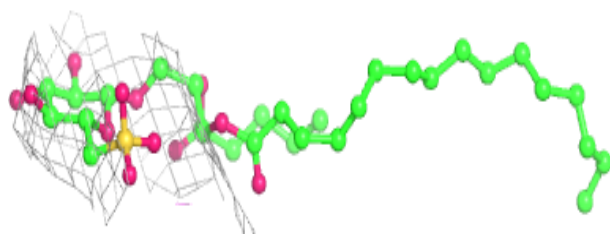
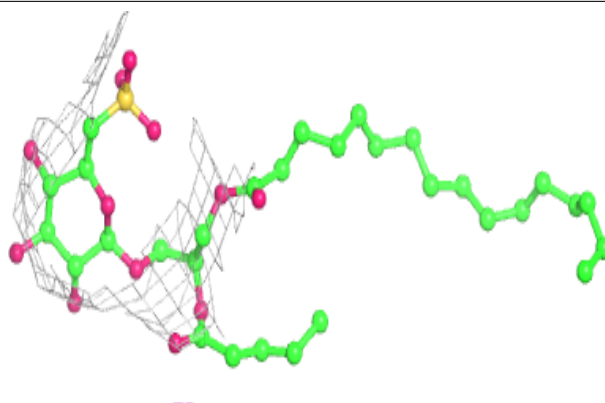
**Electron density around CLA b 602:**

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

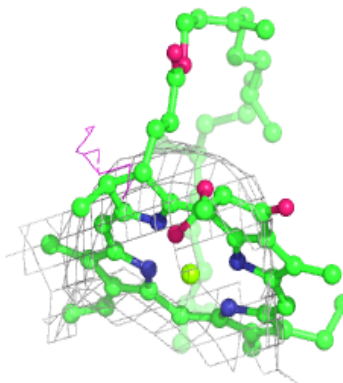
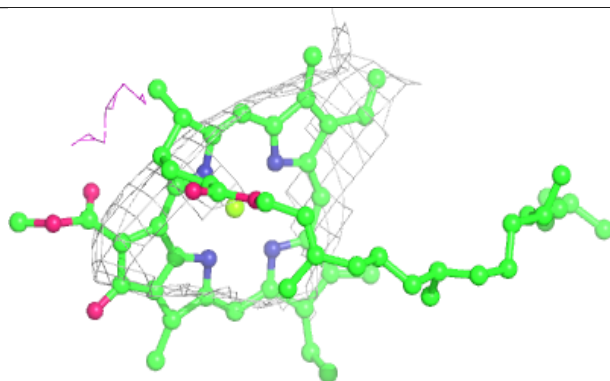
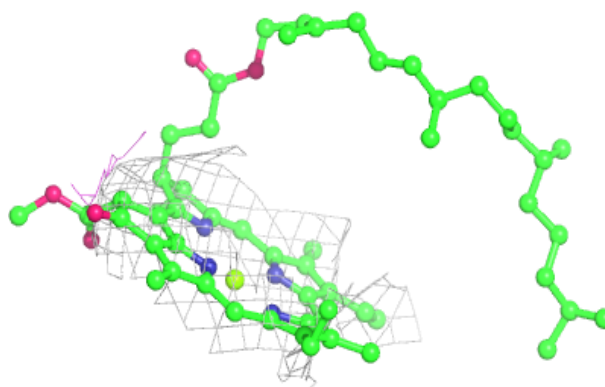


**Electron density around SQD d 407:**

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

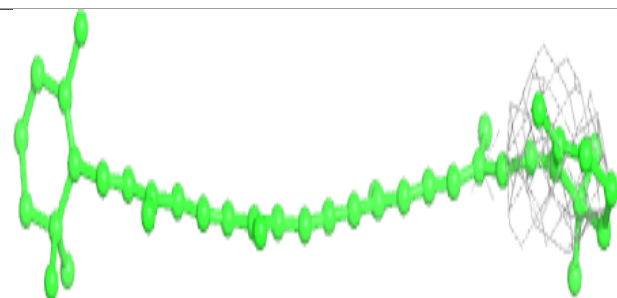
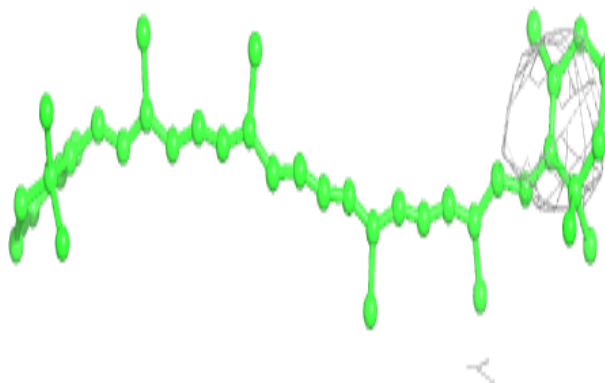
**Electron density around CLA C 513:**

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



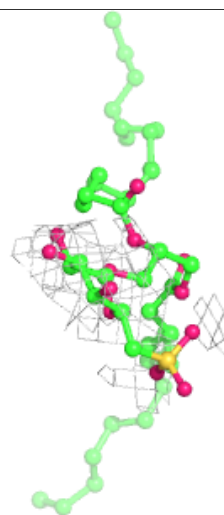
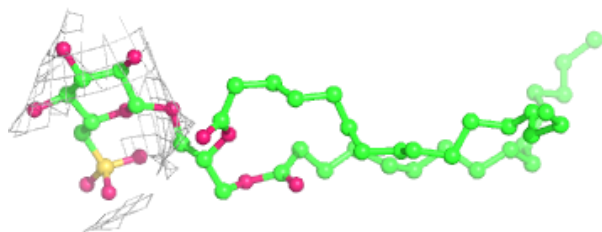
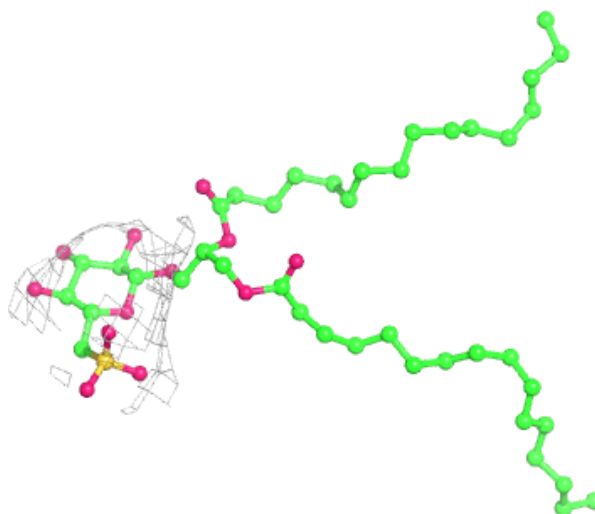
**Electron density around BCR T 102:**

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



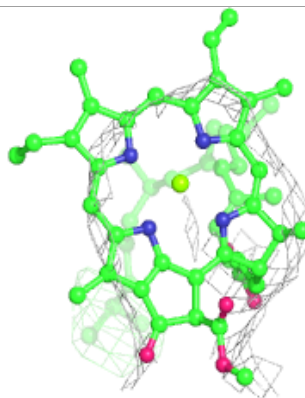
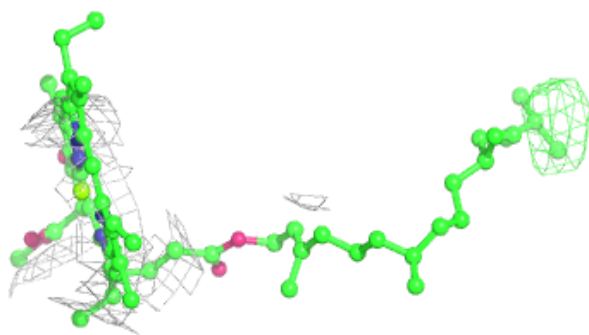
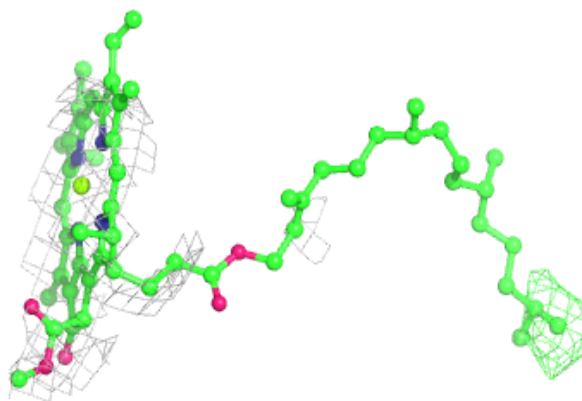
**Electron density around SQD a 411:**

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

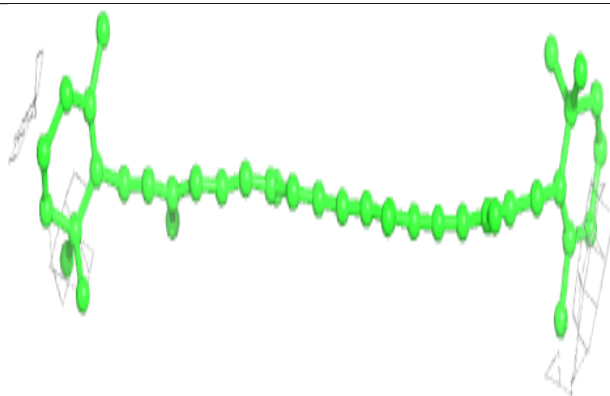
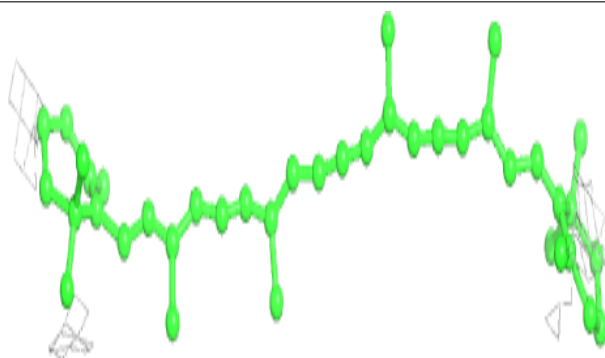


**Electron density around CLA D 403:**

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

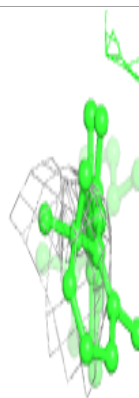
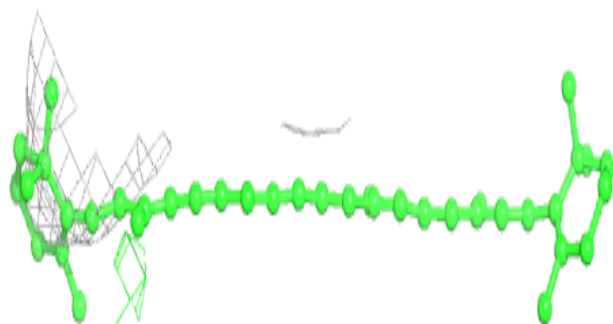
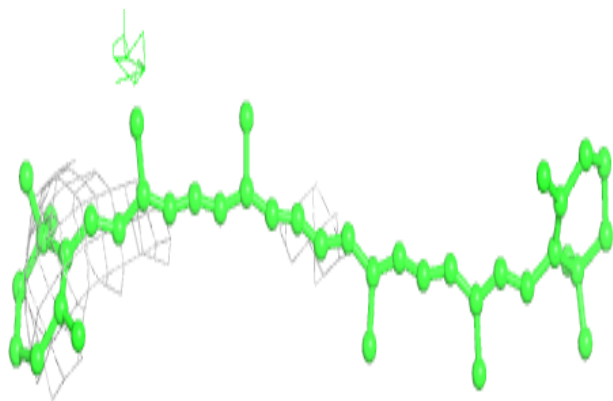
**Electron density around BCR c 915:**

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

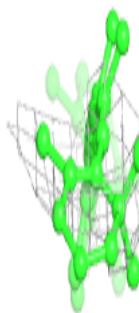
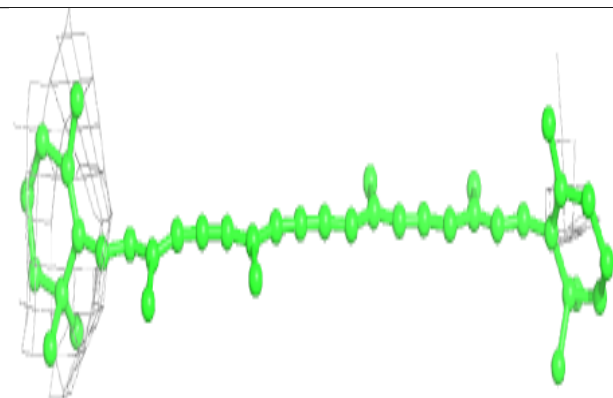
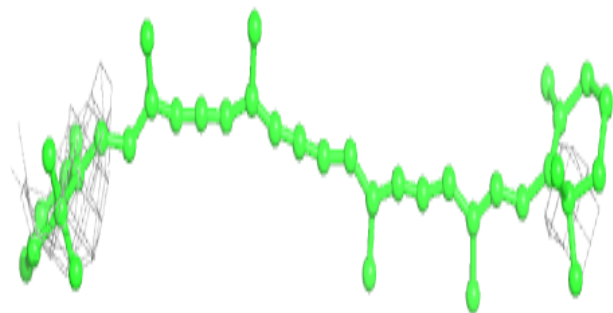


**Electron density around BCR b 618:**

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

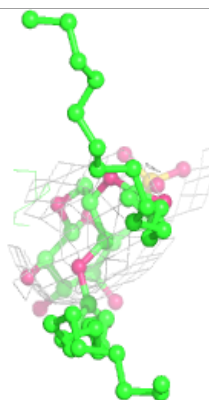
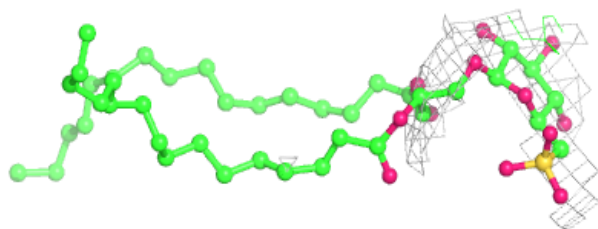
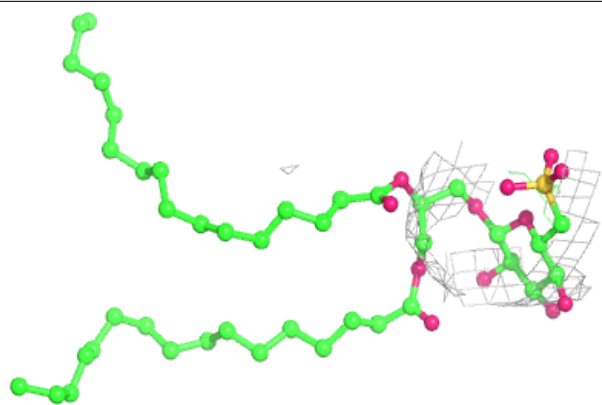
**Electron density around BCR C 514:**

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

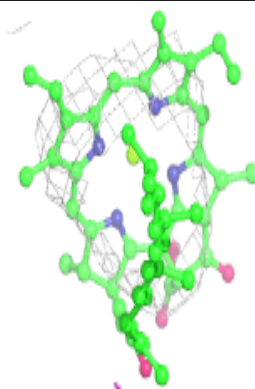
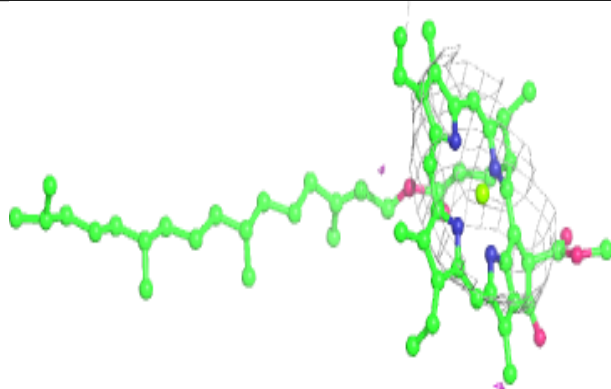
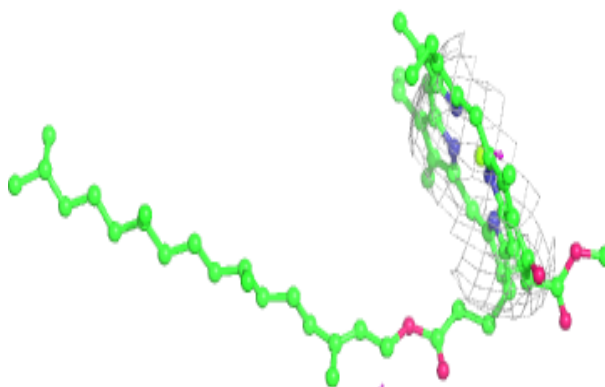


**Electron density around SQD 1 101:**

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

**Electron density around CLA b 608:**

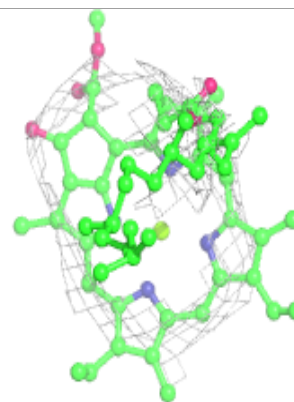
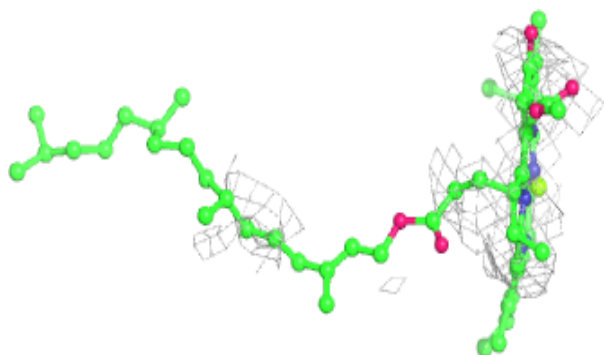
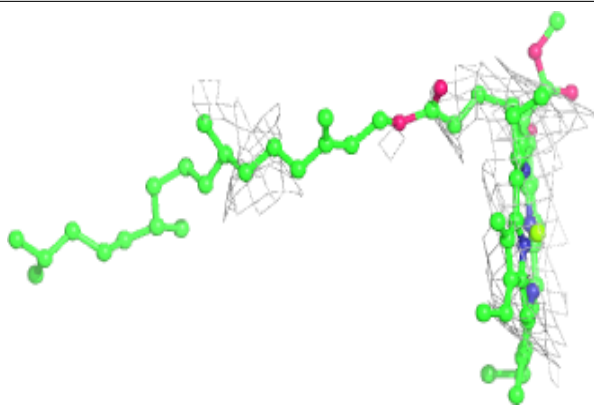
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



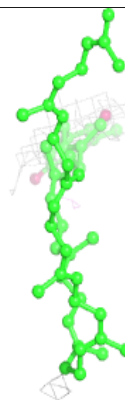
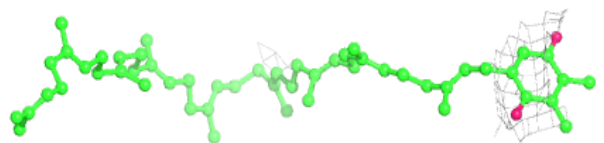
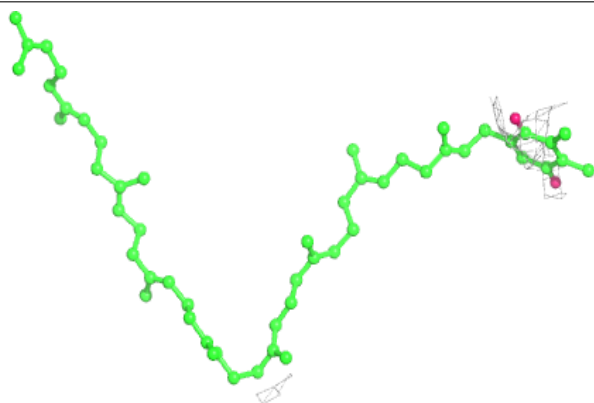


**Electron density around CLA B 607:**

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

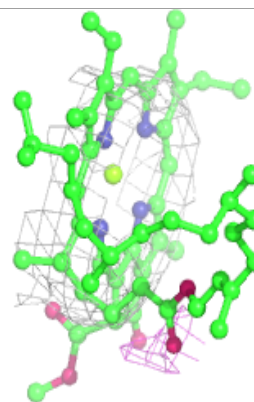
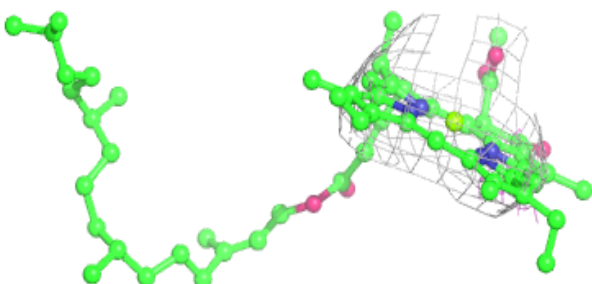
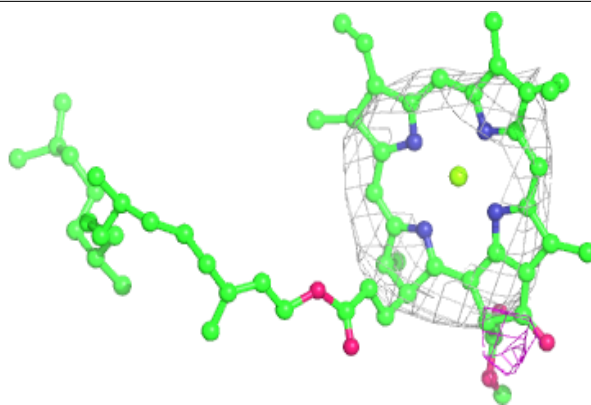
**Electron density around PL9 d 405:**

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

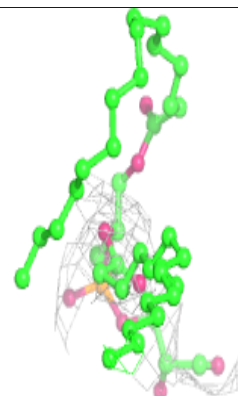
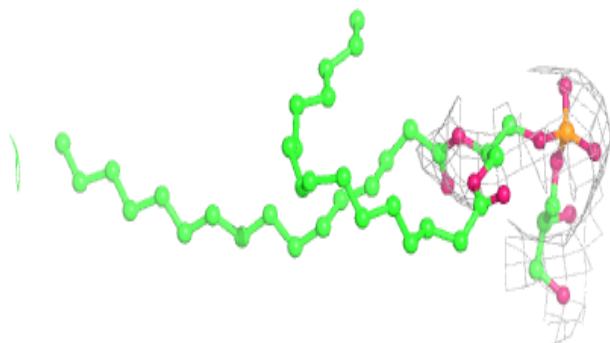
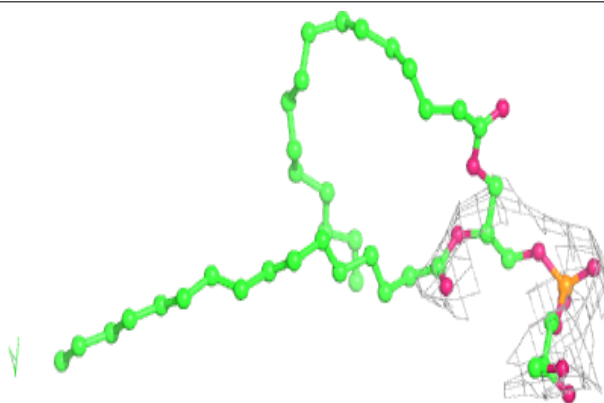


**Electron density around CLA a 408:**

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

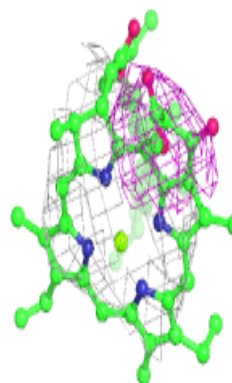
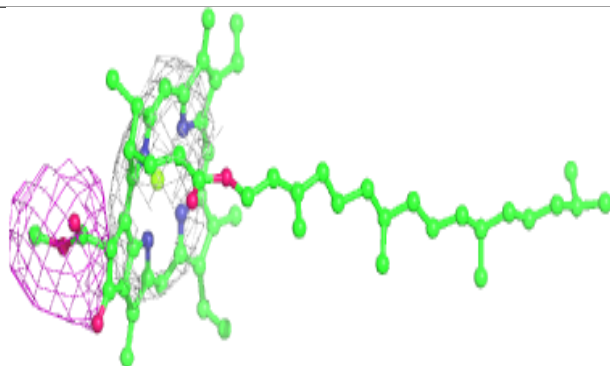
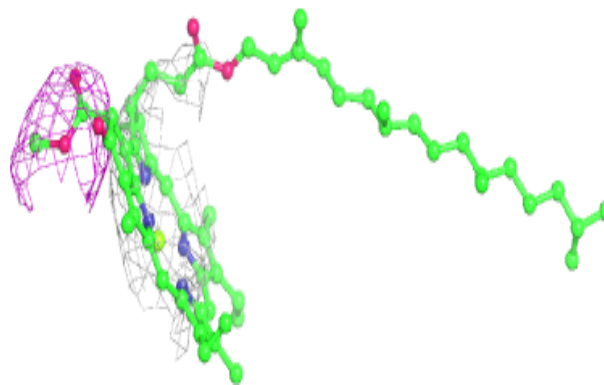
**Electron density around LHG D 407:**

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

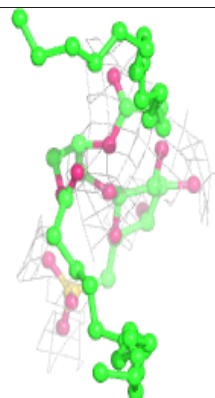
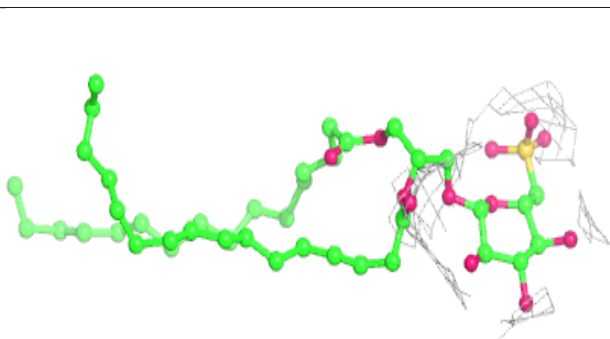
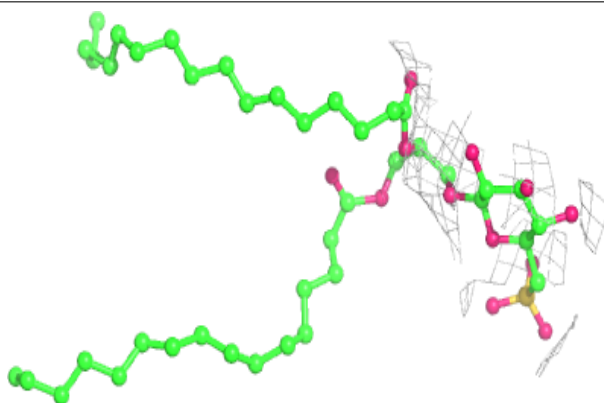


**Electron density around CLA B 608:**

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

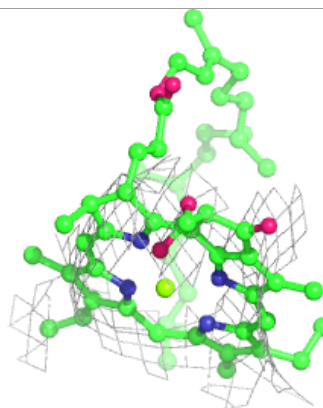
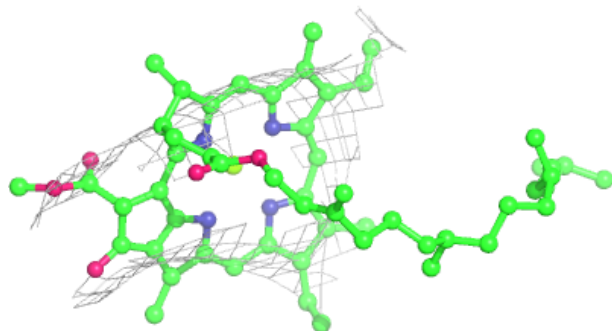
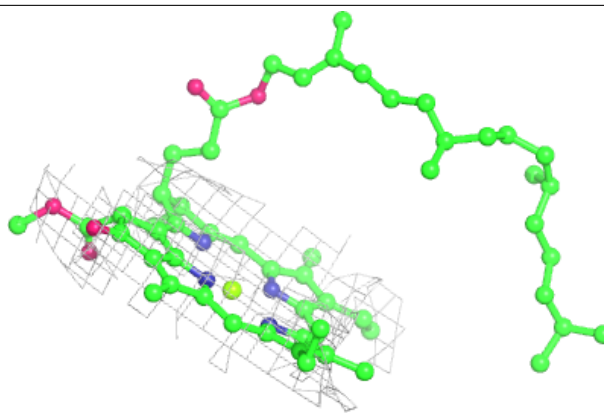
**Electron density around SQD A 613:**

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



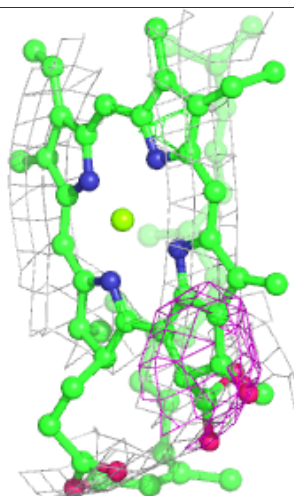
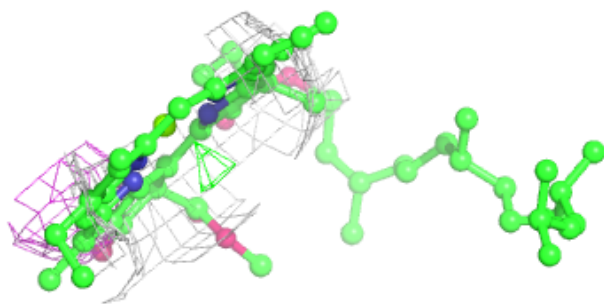
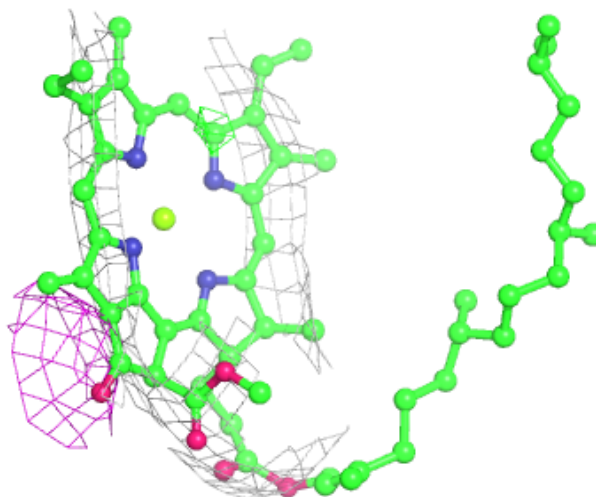
**Electron density around CLA c 914:**

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



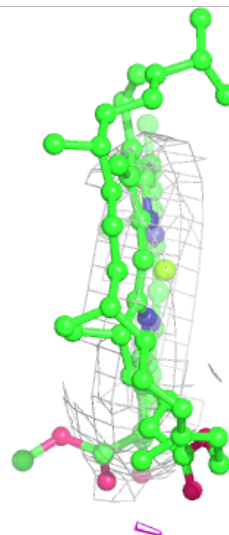
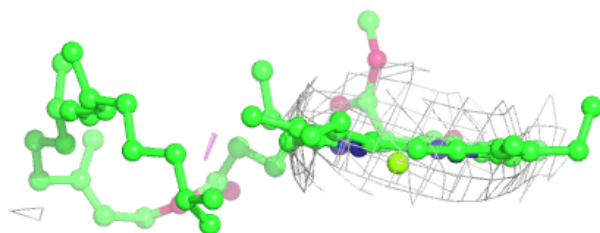
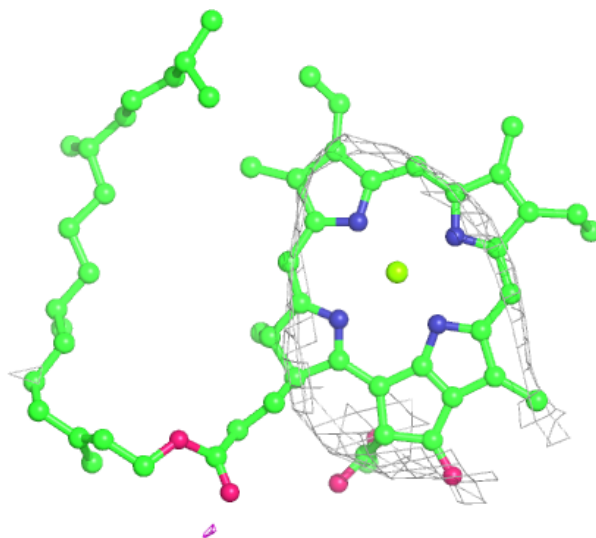
**Electron density around CLA B 617:**

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



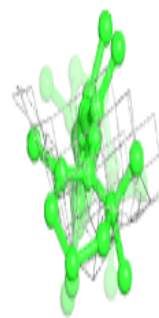
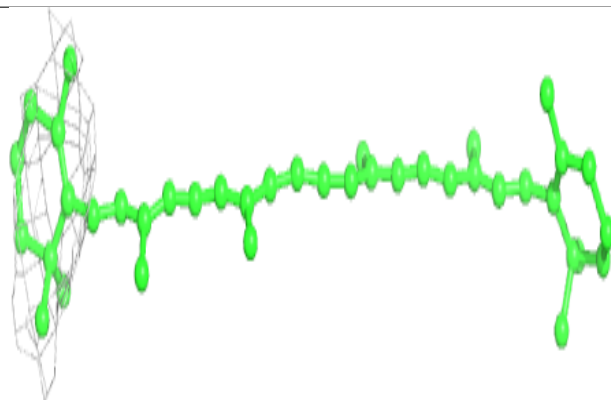
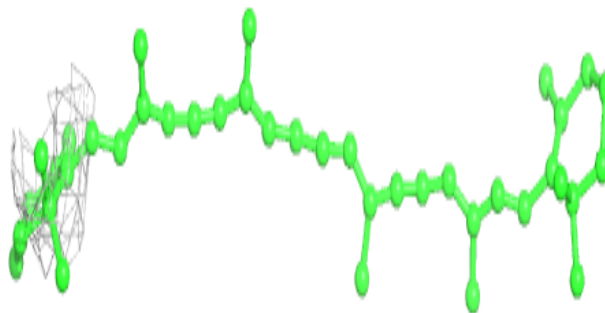
**Electron density around CLA C 512:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

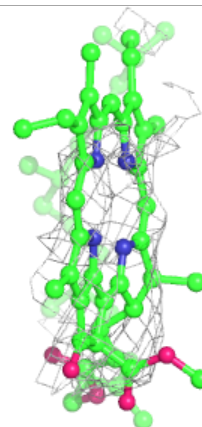
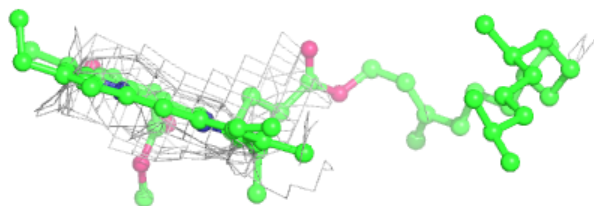
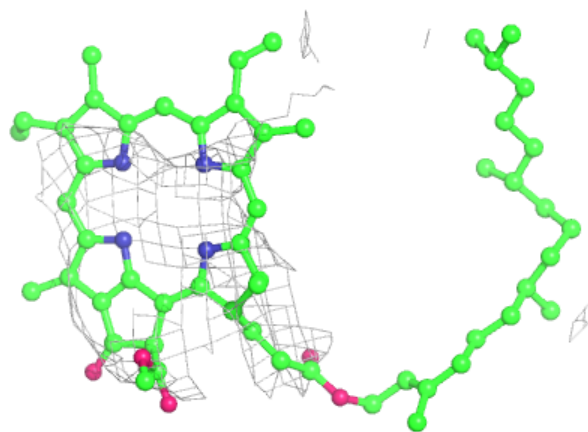


**Electron density around BCR c 918:**

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

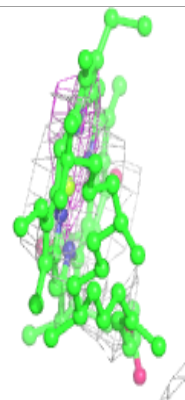
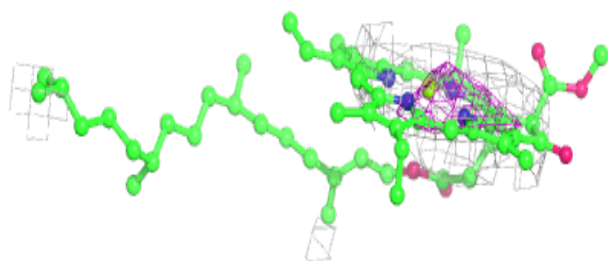
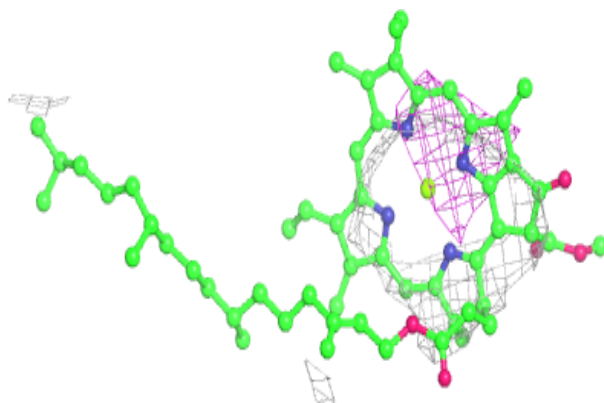
**Electron density around PHO A 608:**

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



**Electron density around CLA c 902:**

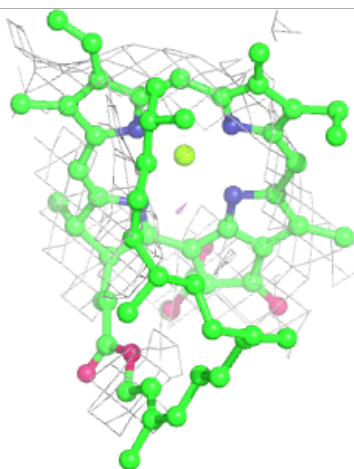
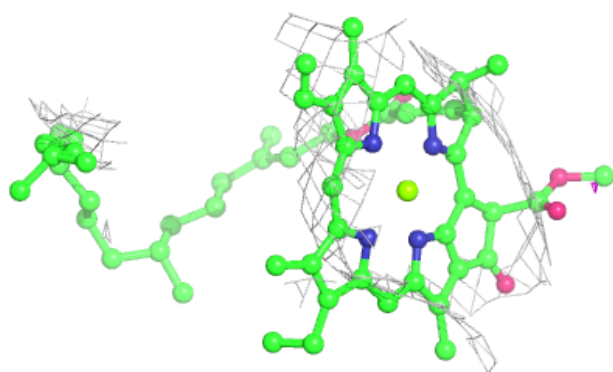
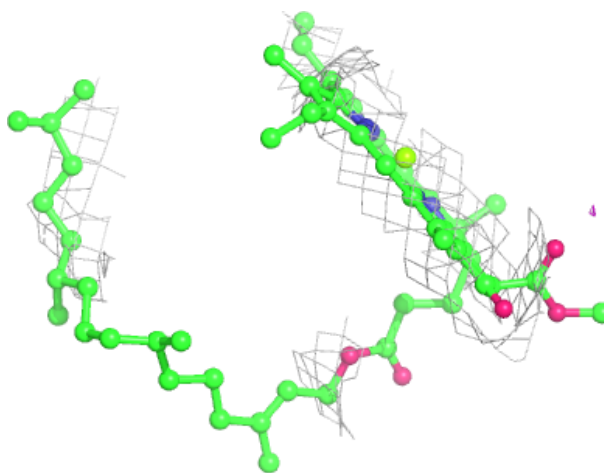
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





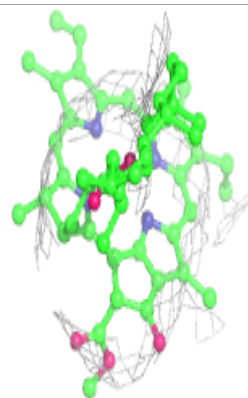
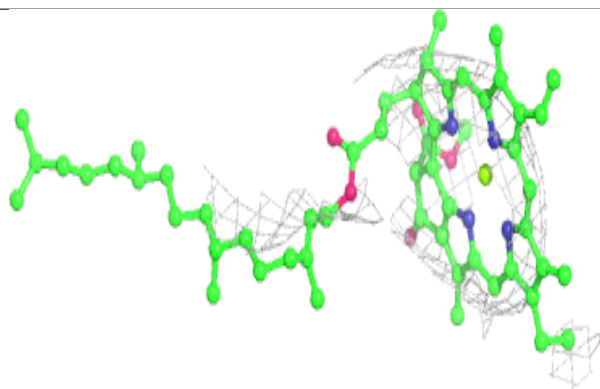
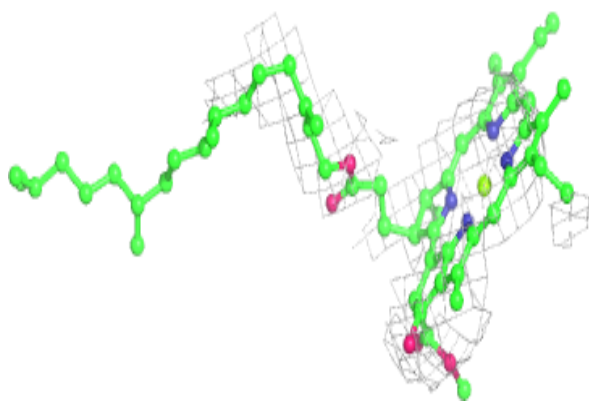
**Electron density around CLA b 612:**

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



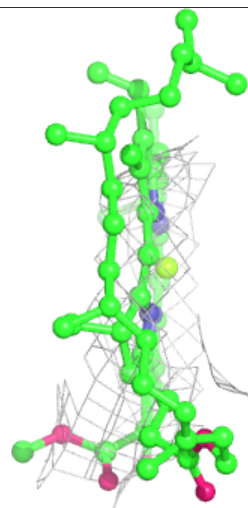
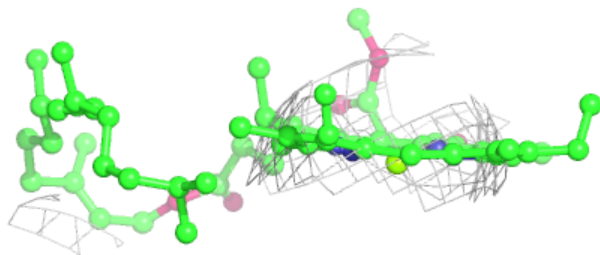
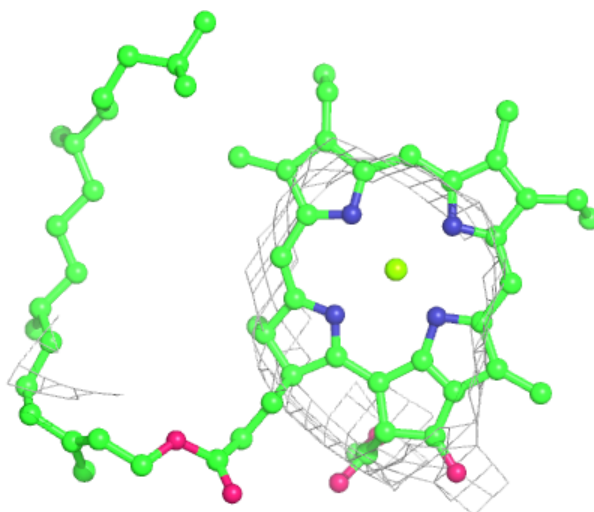
**Electron density around CLA c 903:**

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



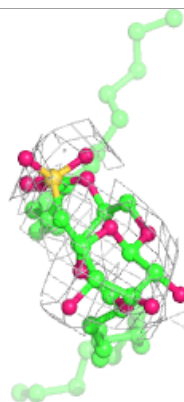
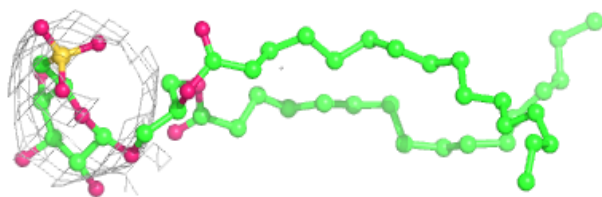
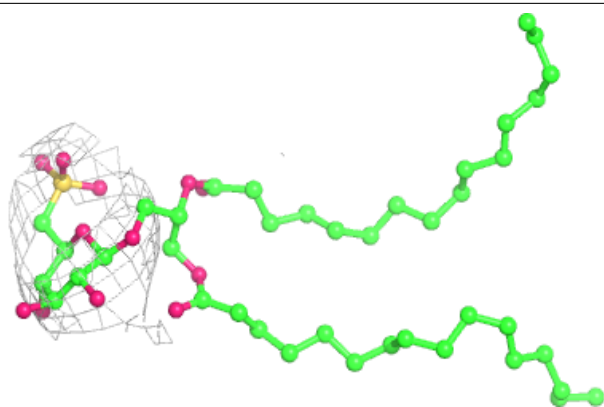
**Electron density around CLA c 913:**

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

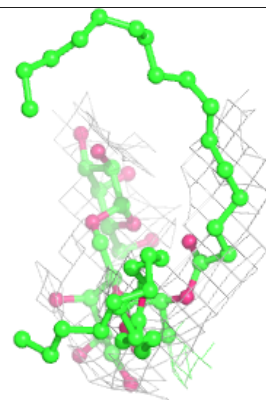
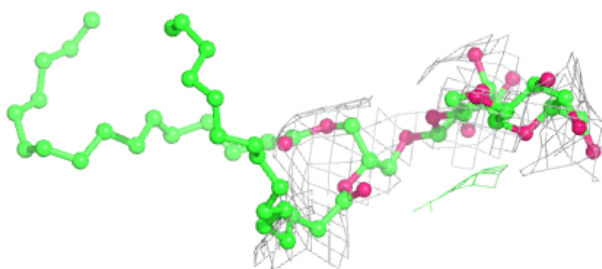
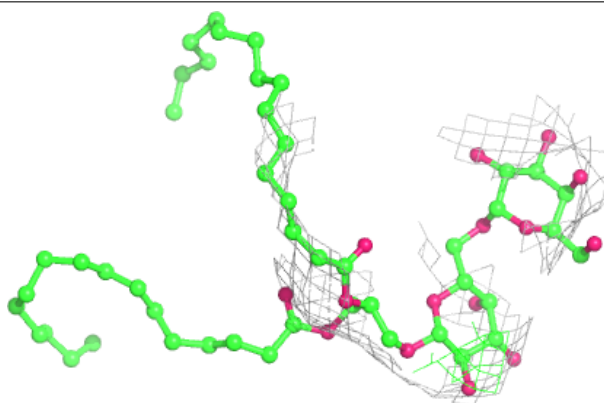


**Electron density around SQD L 101:**

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

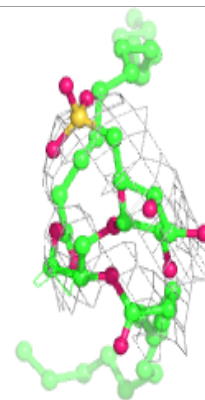
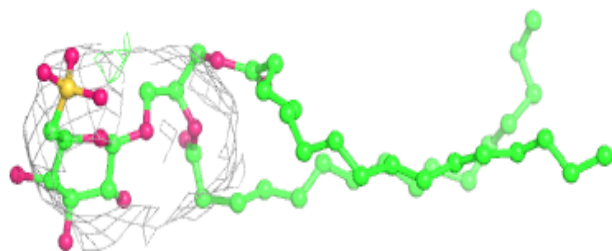
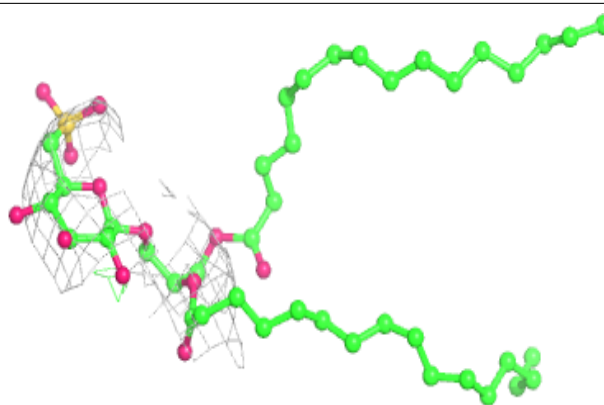
**Electron density around DGD C 517:**

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

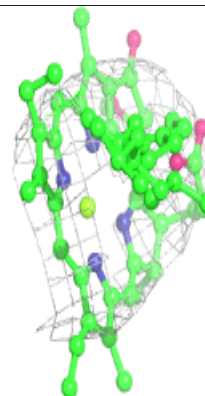
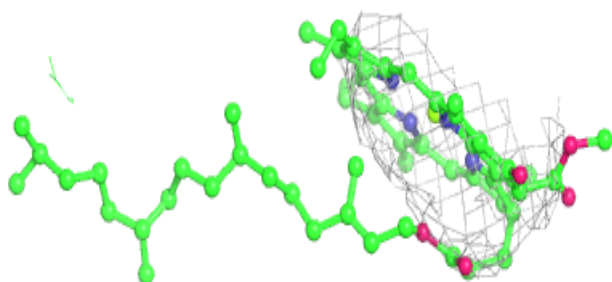
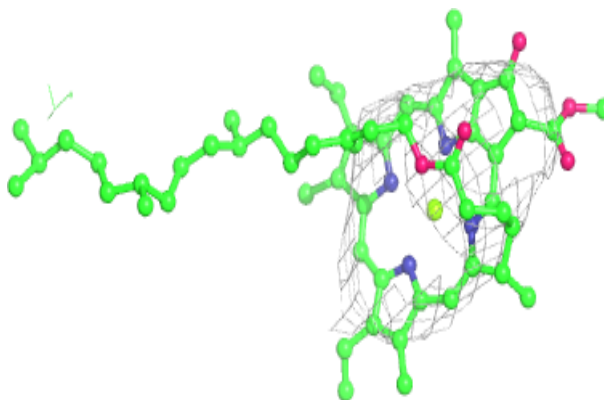


**Electron density around SQD a 402:**

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

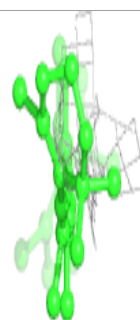
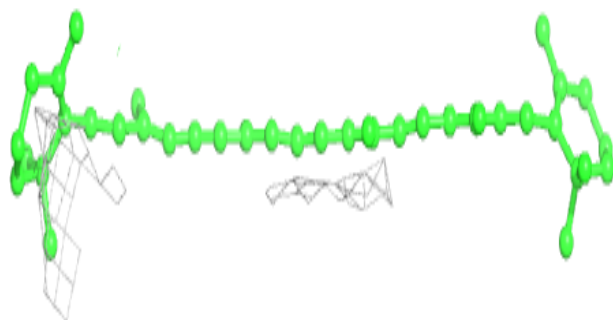
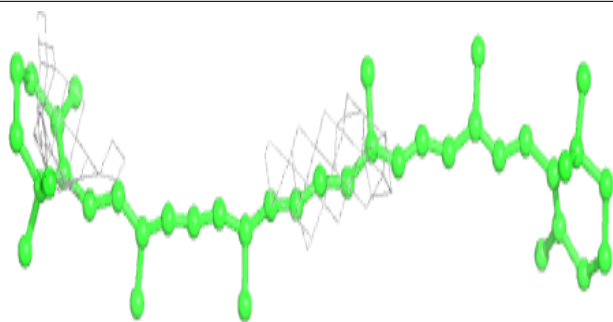
**Electron density around CLA b 615:**

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

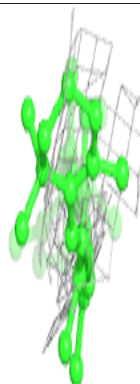
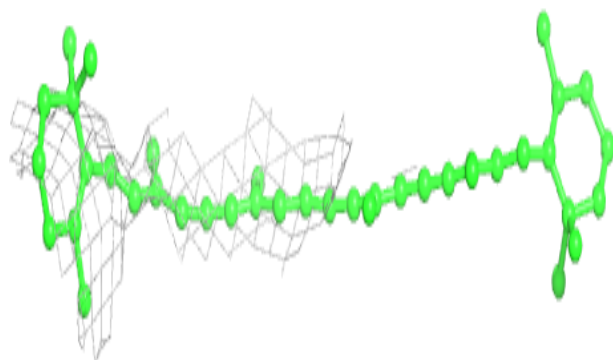
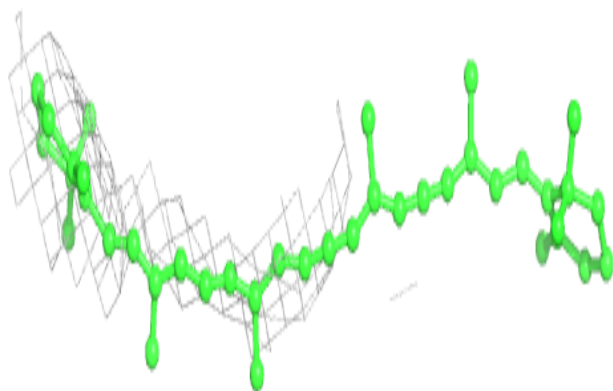


**Electron density around BCR B 619:**

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

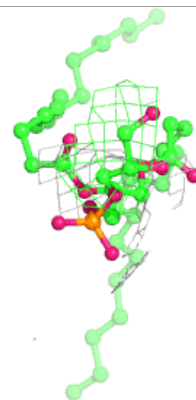
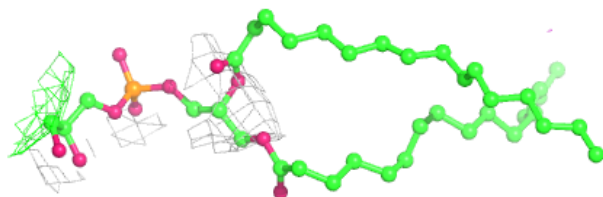
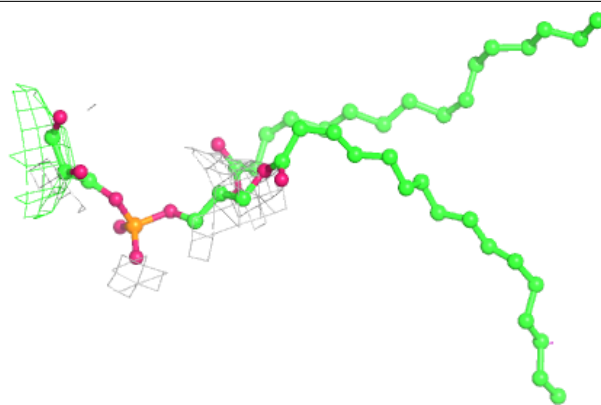
**Electron density around BCR h 101:**

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

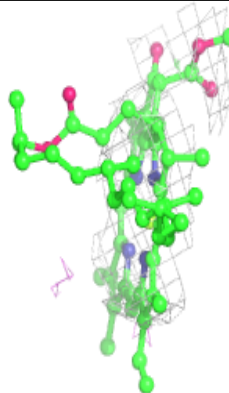
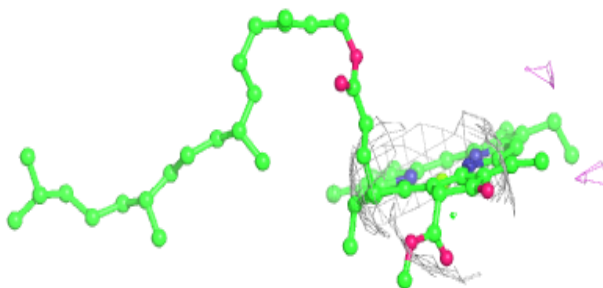
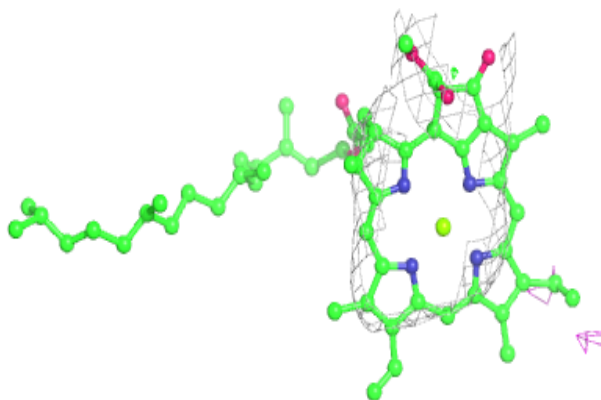


**Electron density around LHG D 408:**

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

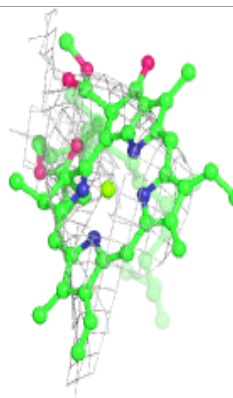
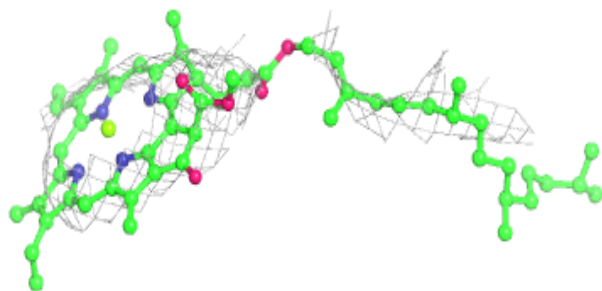
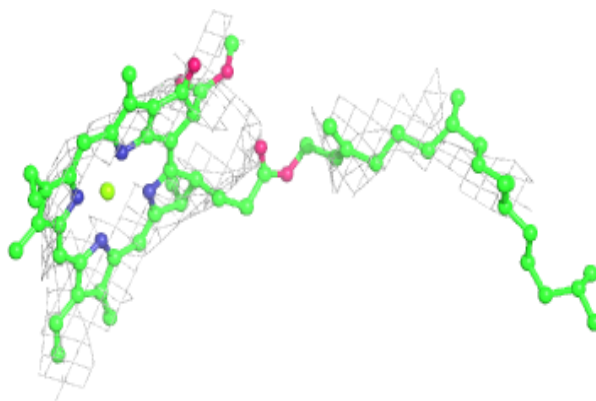
**Electron density around CLA A 607:**

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



**Electron density around CLA a 406:**

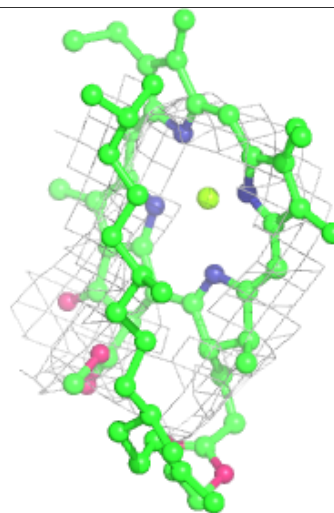
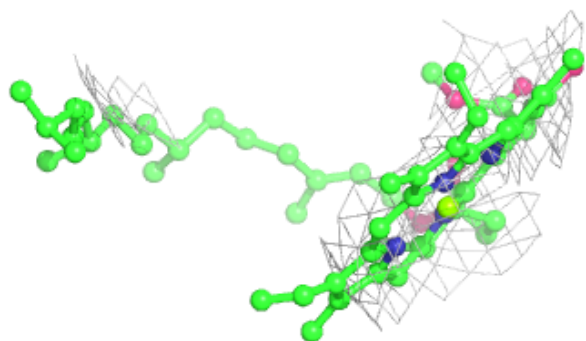
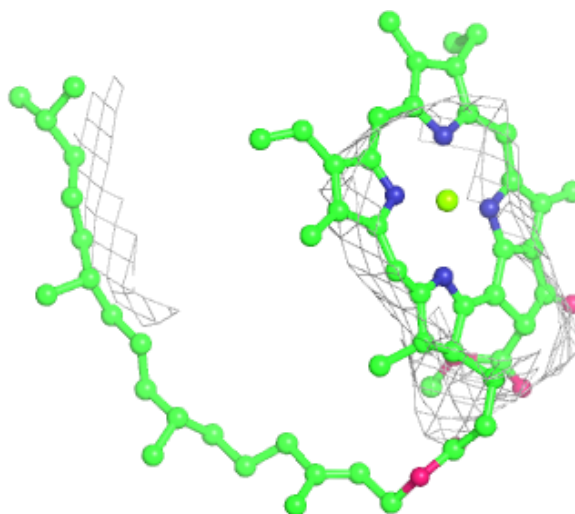
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





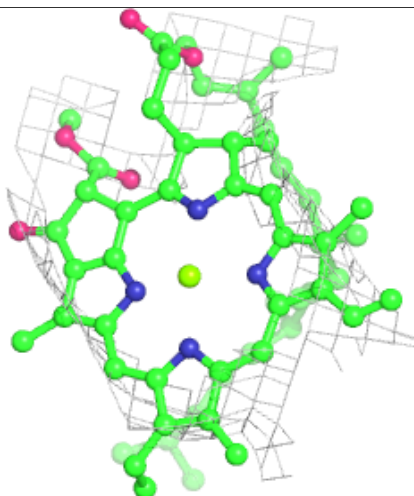
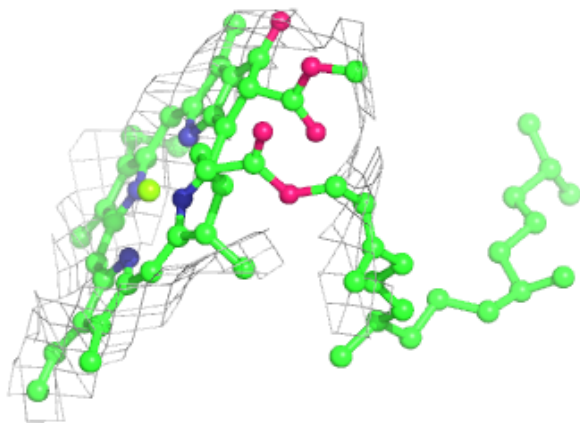
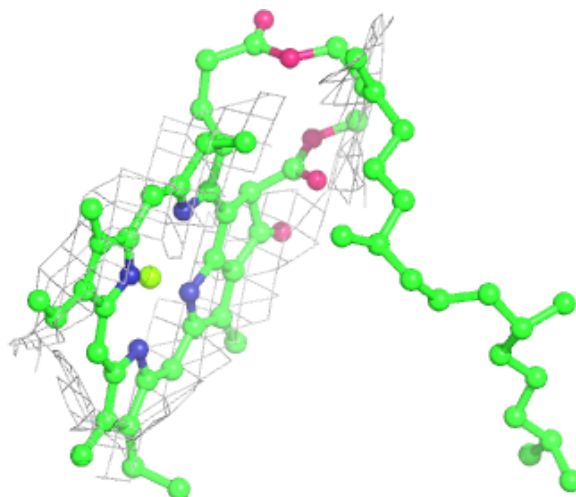
**Electron density around CLA C 507:**

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



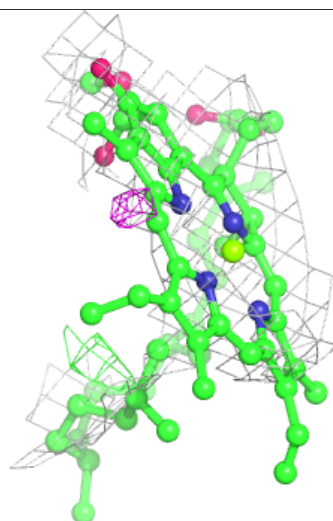
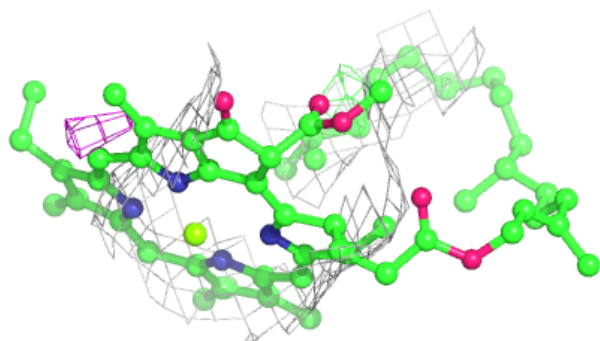
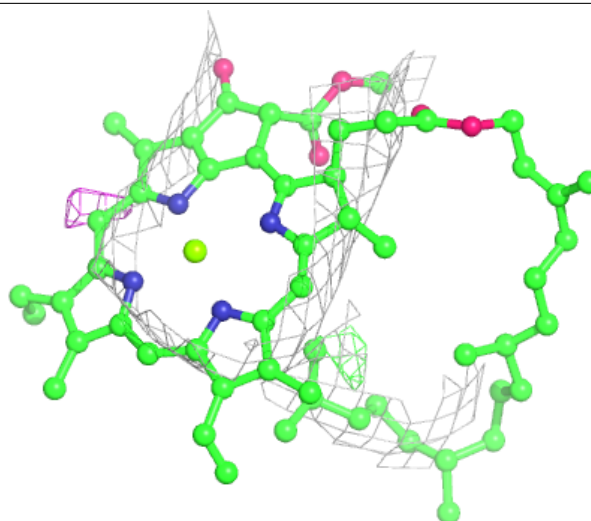
**Electron density around CLA b 614:**

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



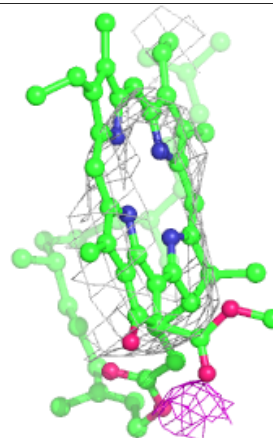
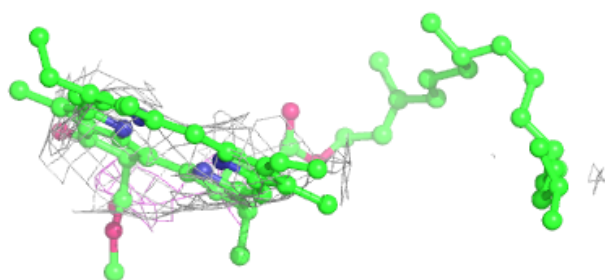
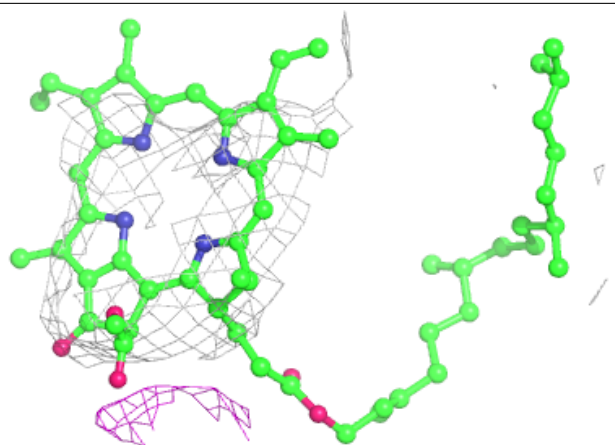
**Electron density around CLA B 616:**

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



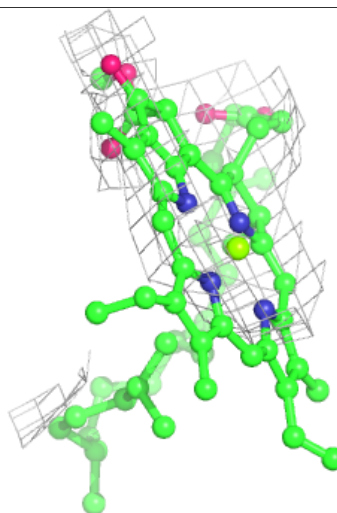
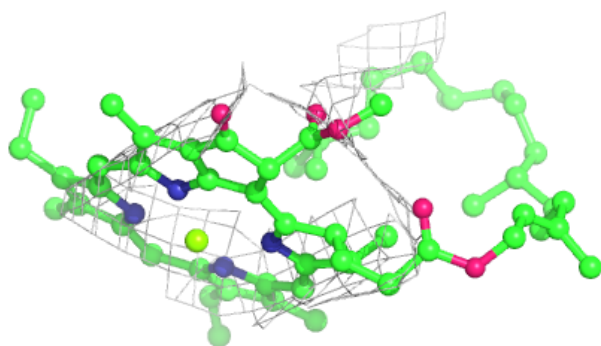
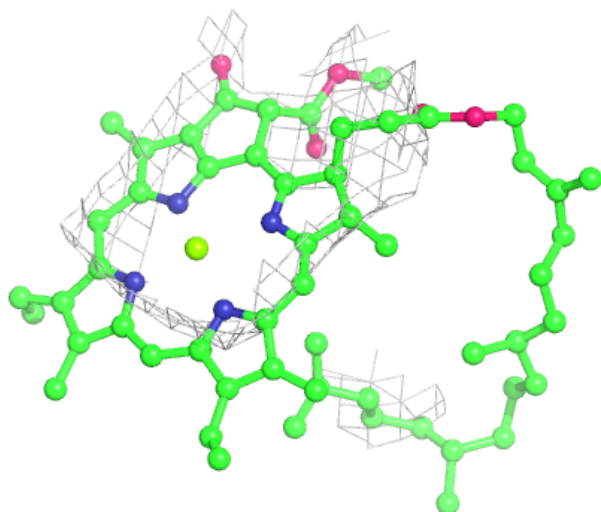
**Electron density around PHO D 401:**

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



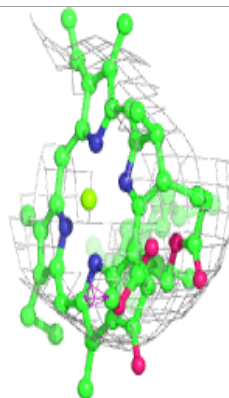
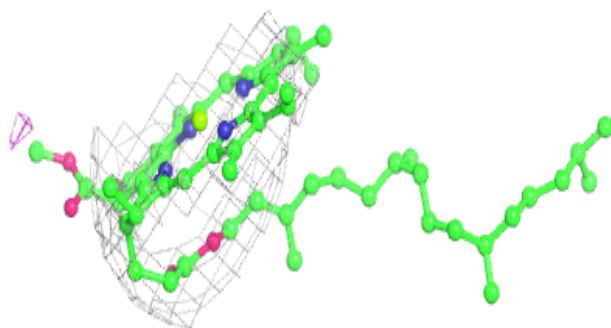
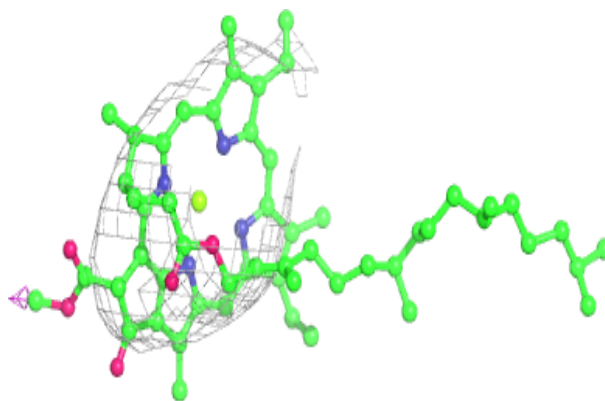
**Electron density around CLA b 616:**

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

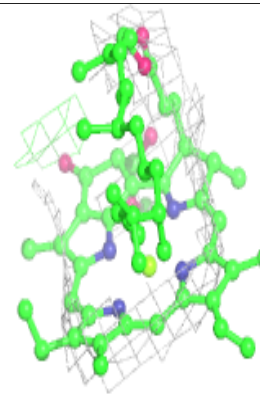
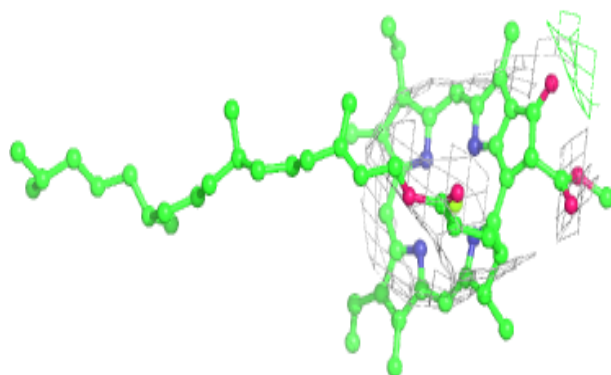
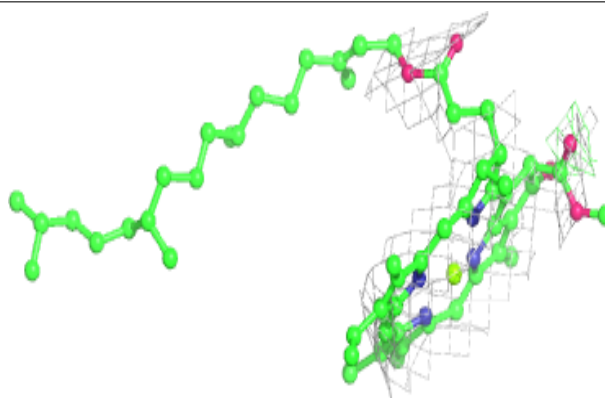


**Electron density around CLA B 615:**

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

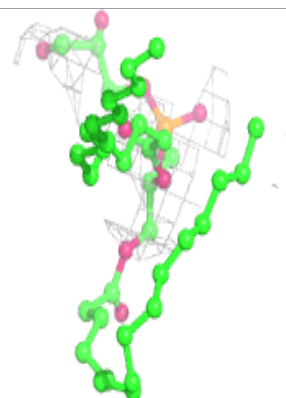
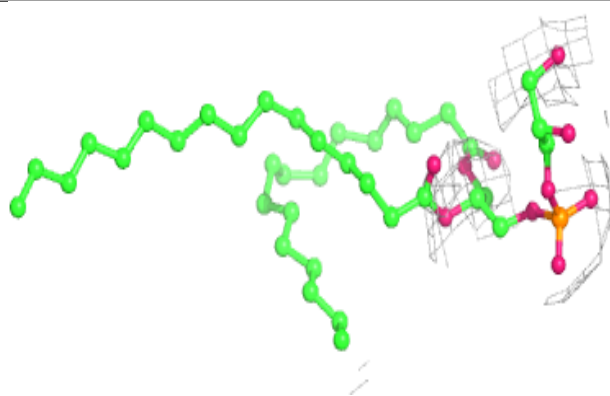
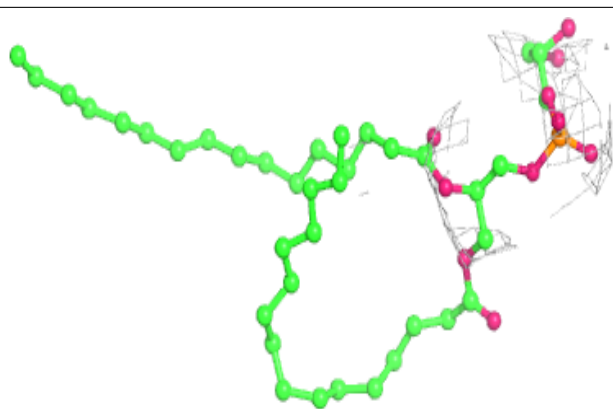
**Electron density around CLA C 504:**

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

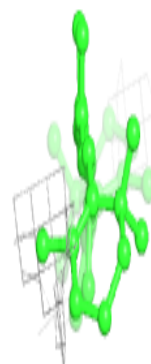
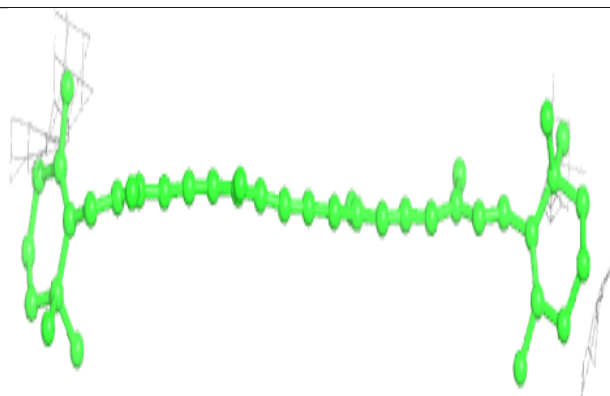
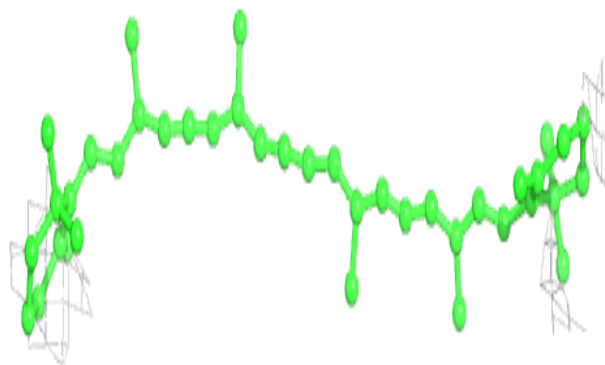


**Electron density around LHG d 408:**

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

**Electron density around BCR C 515:**

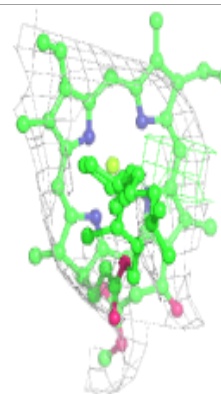
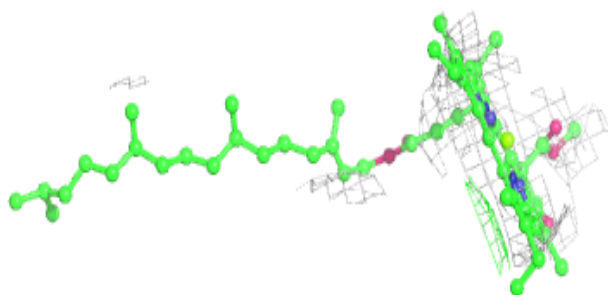
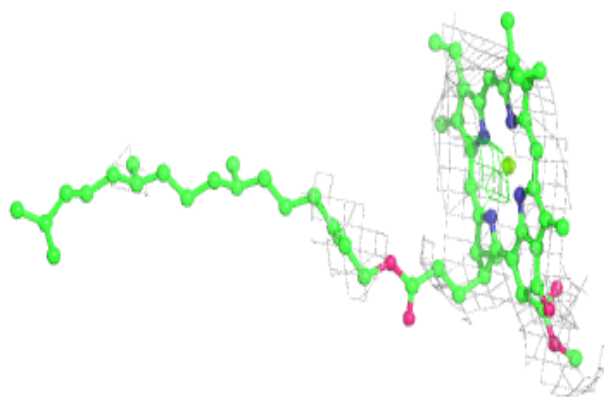
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



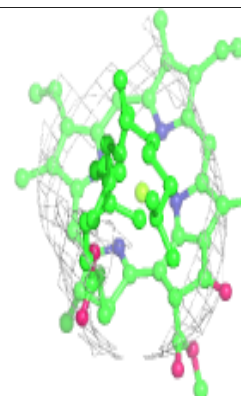
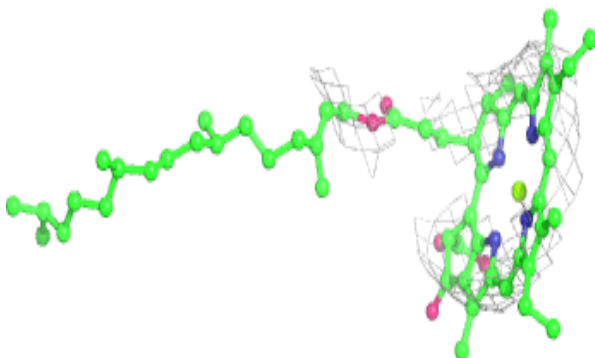
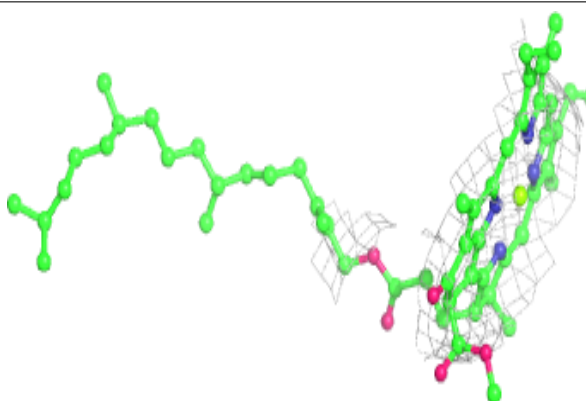


**Electron density around CLA d 404:**

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

**Electron density around CLA b 605:**

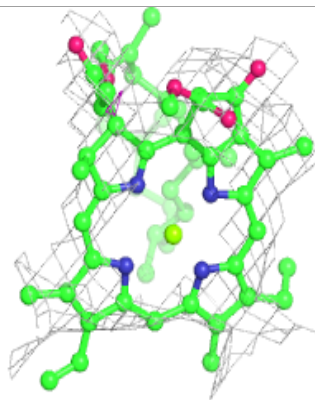
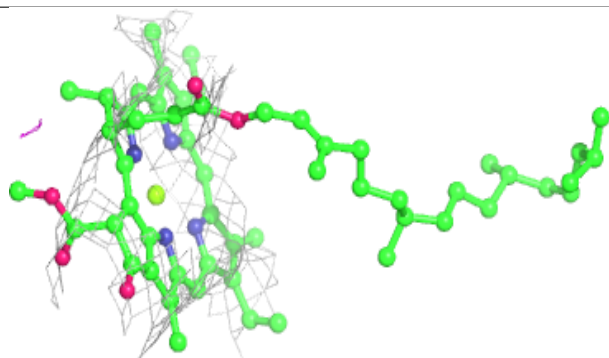
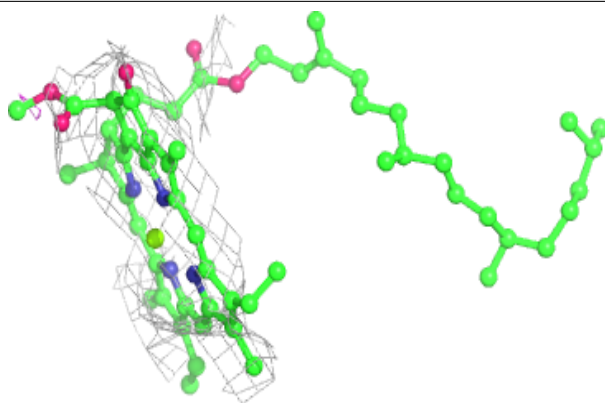
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



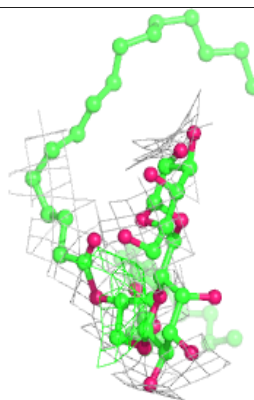
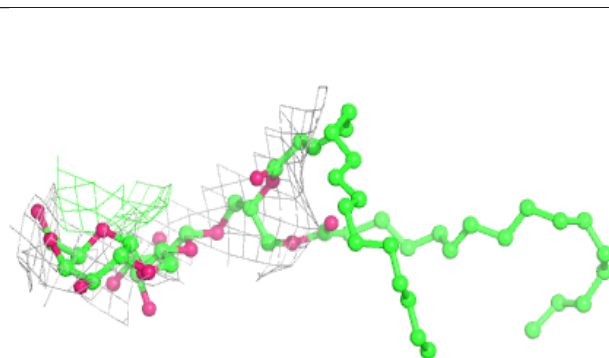
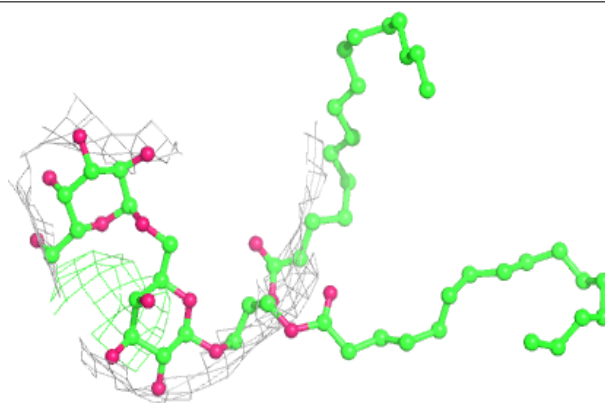


**Electron density around CLA C 508:**

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

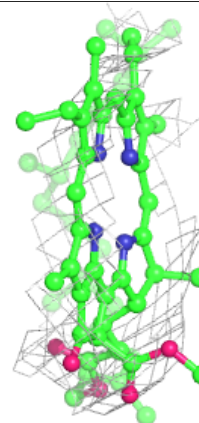
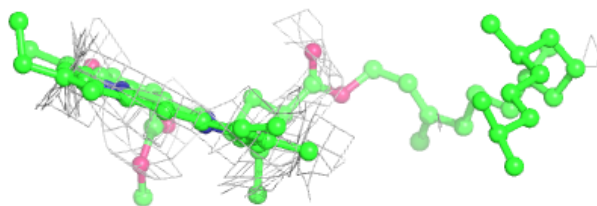
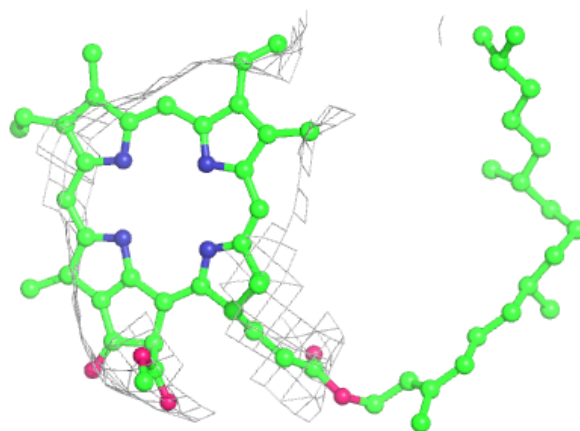
**Electron density around DGD c 917:**

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

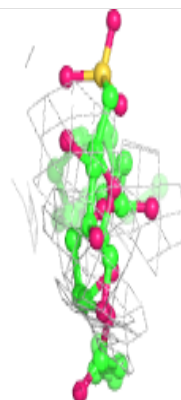
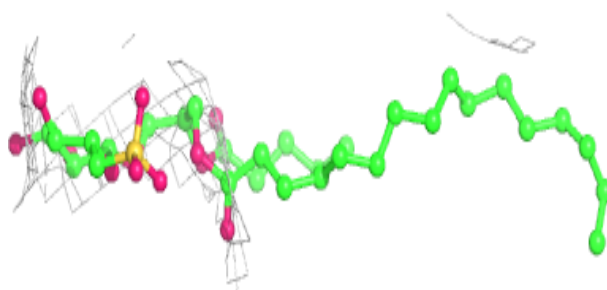
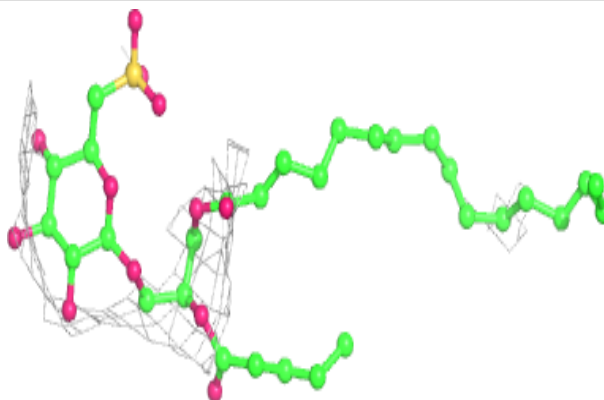


**Electron density around PHO d 402:**

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

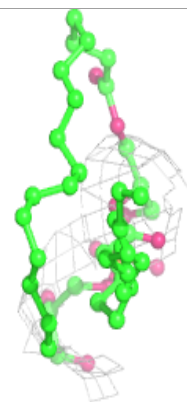
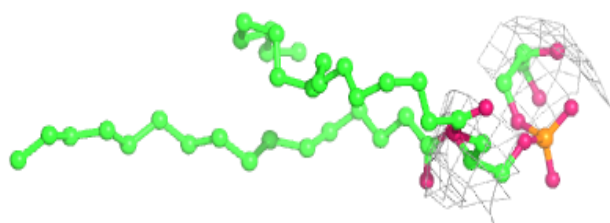
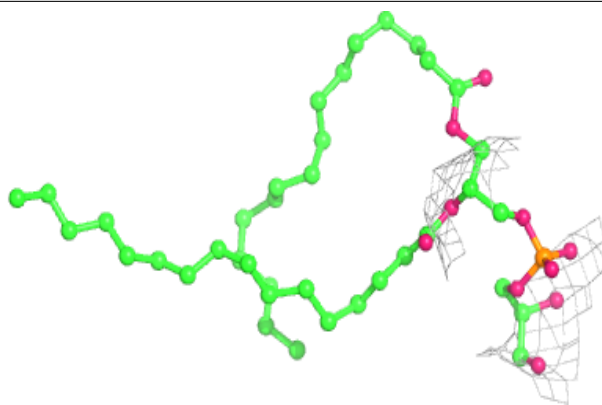
**Electron density around SQD F 101:**

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

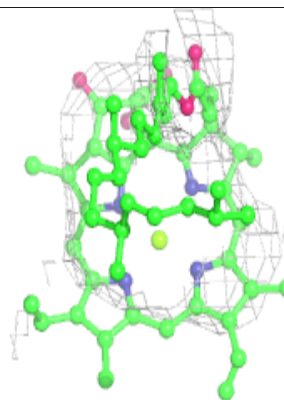
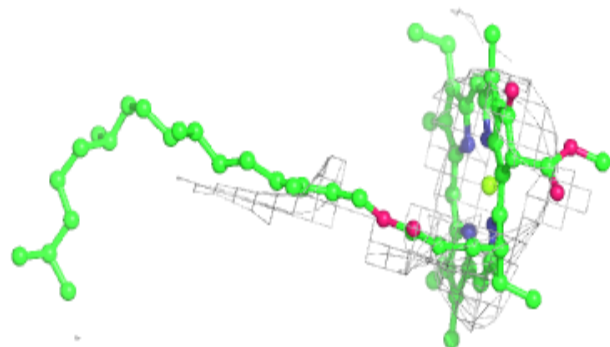
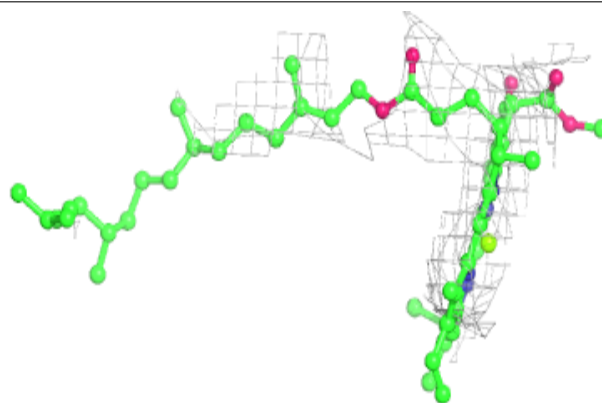


**Electron density around LHG D 409:**

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

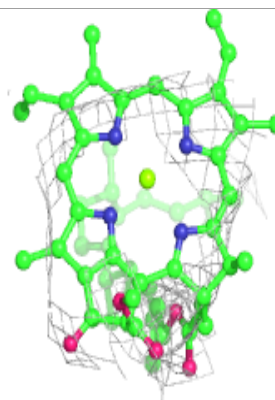
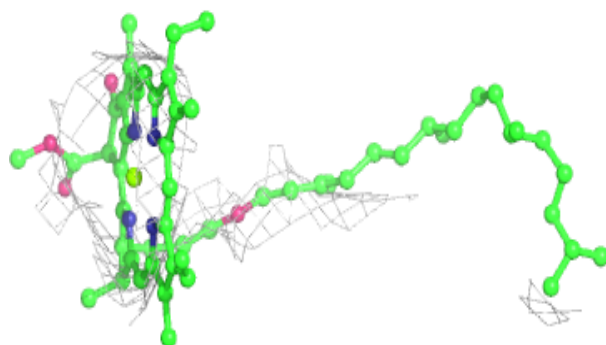
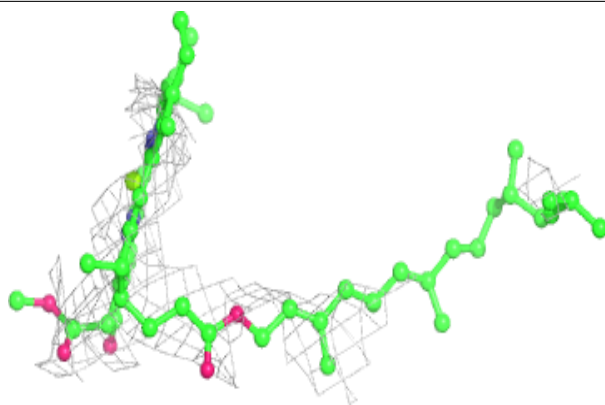
**Electron density around CLA B 606:**

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

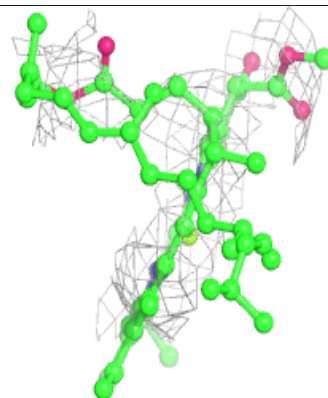
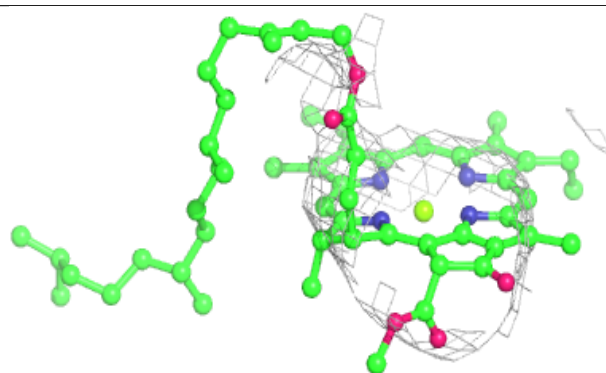
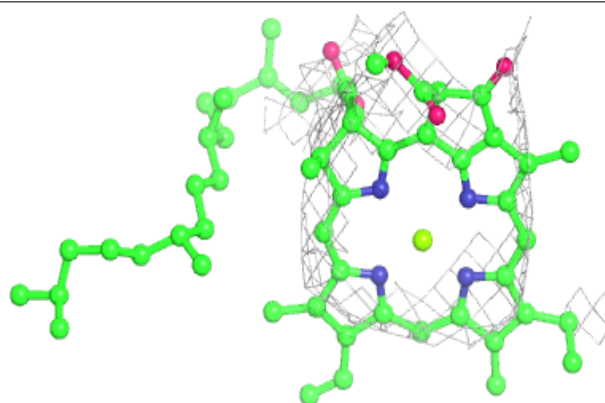


**Electron density around CLA b 606:**

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

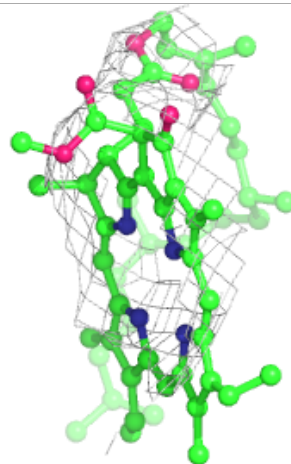
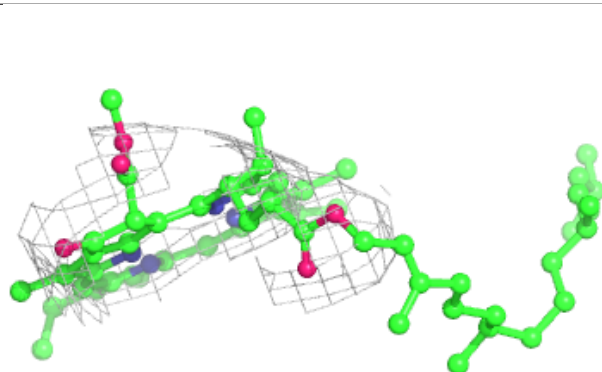
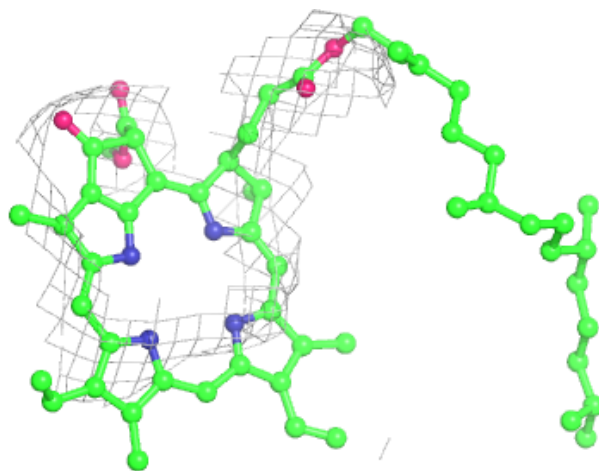
**Electron density around CLA A 614:**

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



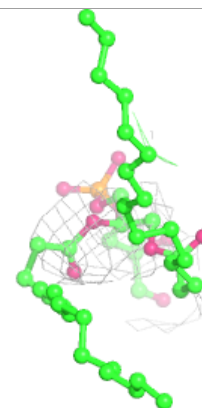
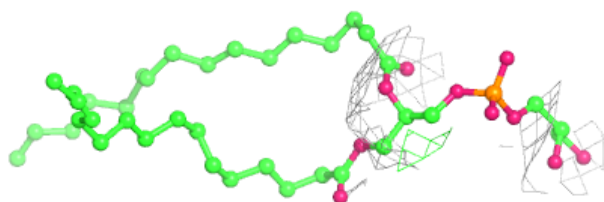
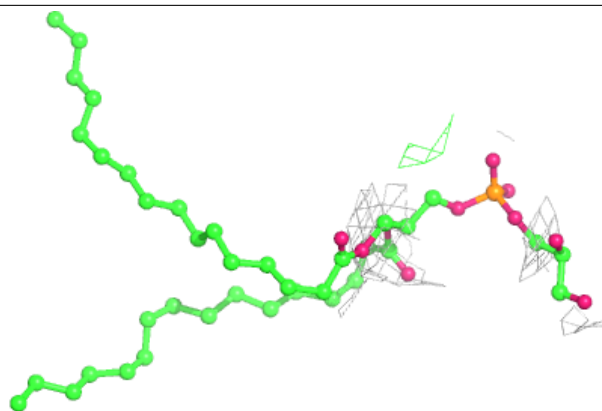
**Electron density around PHO a 412:**

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

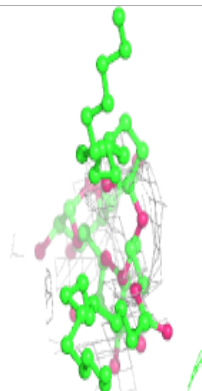
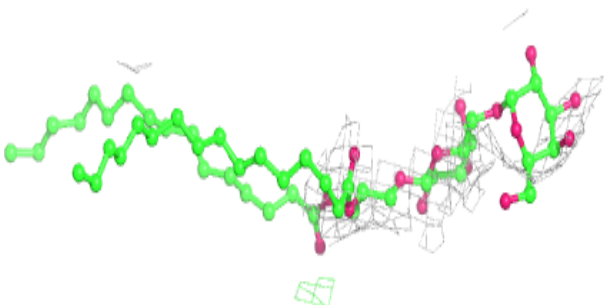
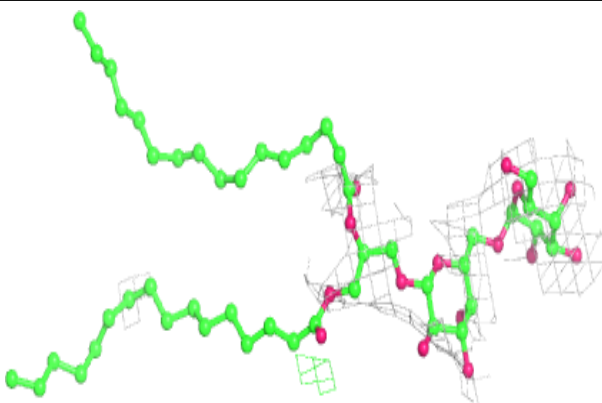


**Electron density around LHG d 409:**

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

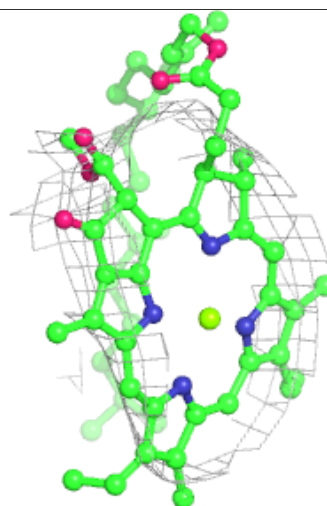
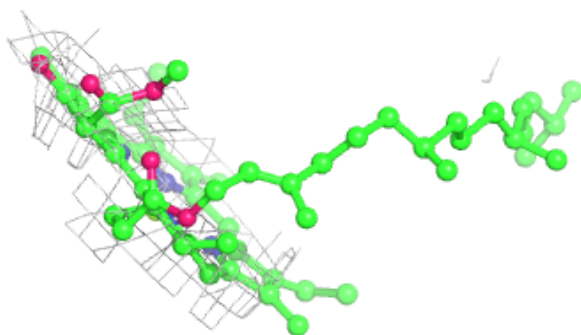
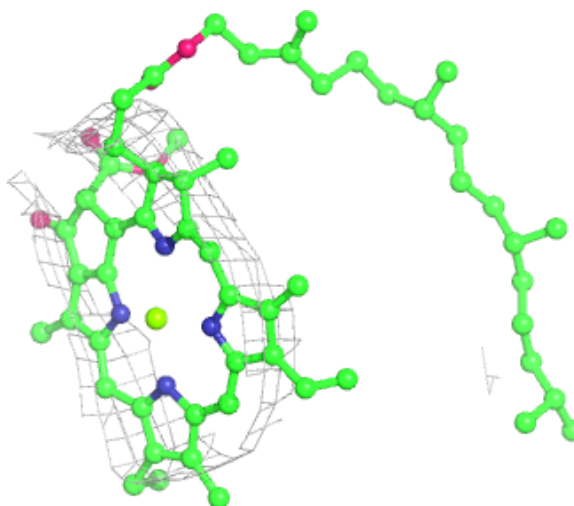
**Electron density around DGD C 518:**

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



**Electron density around CLA c 908:**

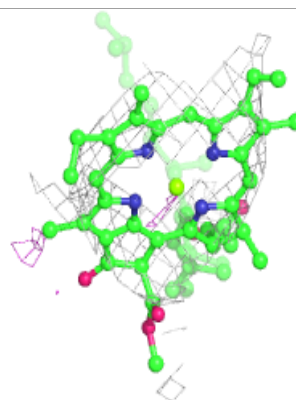
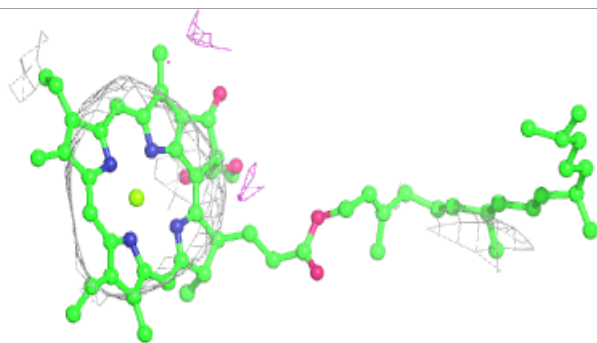
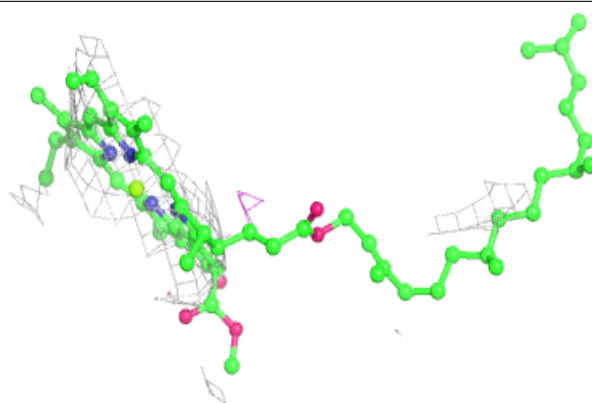
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



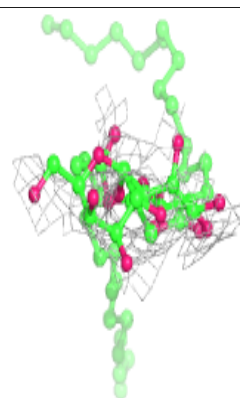
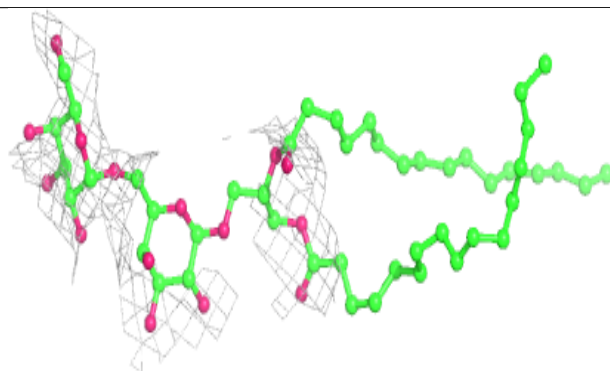
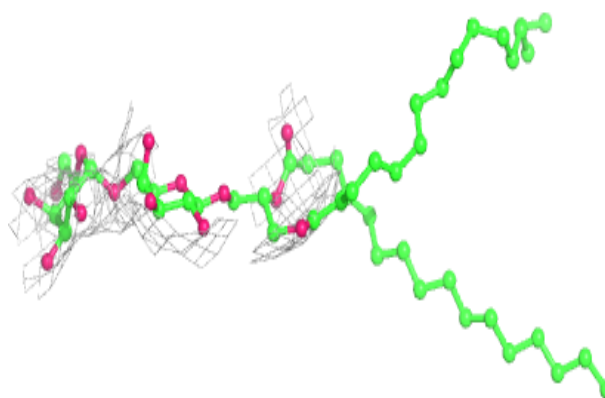


**Electron density around CLA D 402:**

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

**Electron density around DGD c 916:**

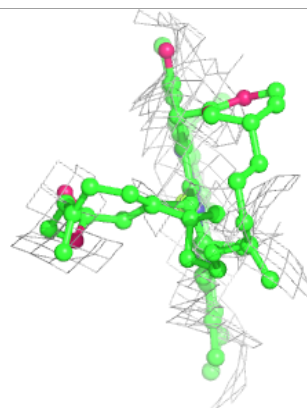
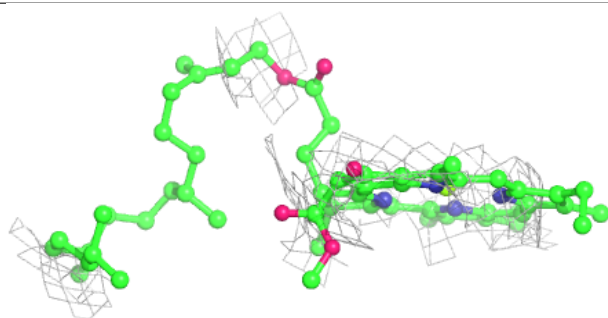
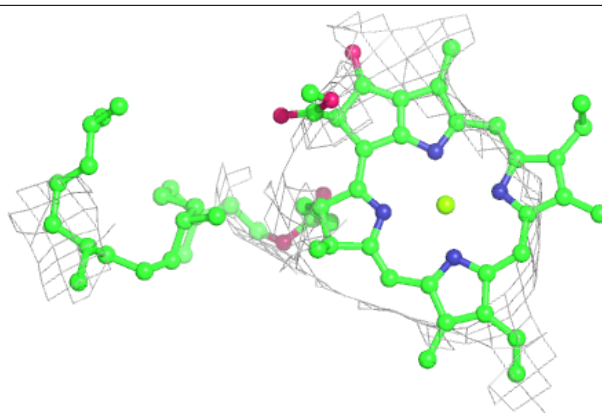
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



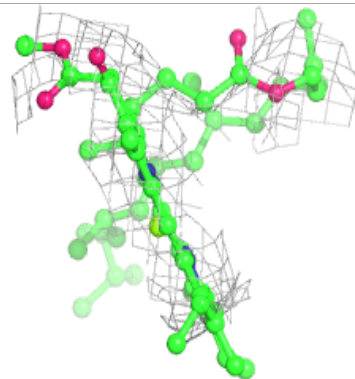
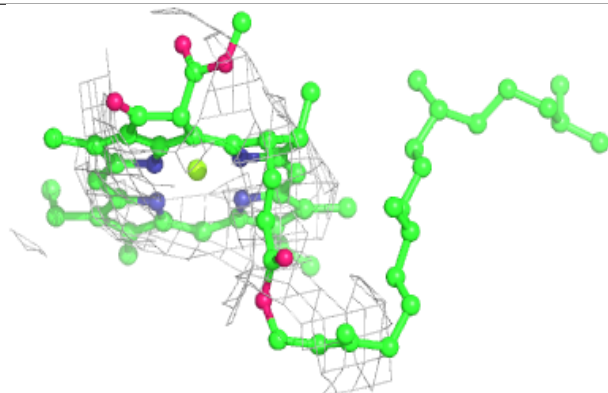
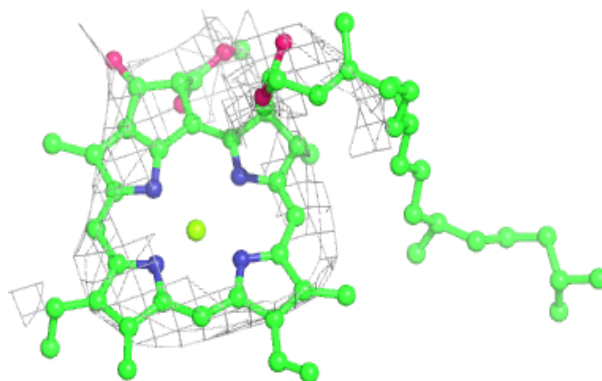


**Electron density around CLA b 613:**

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

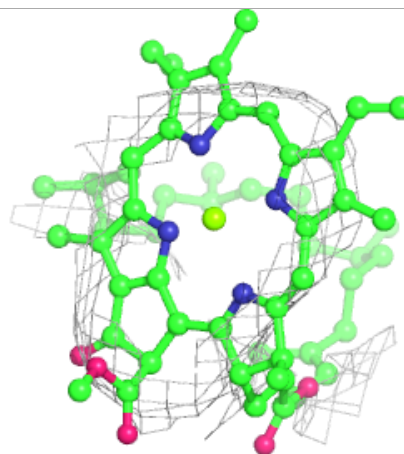
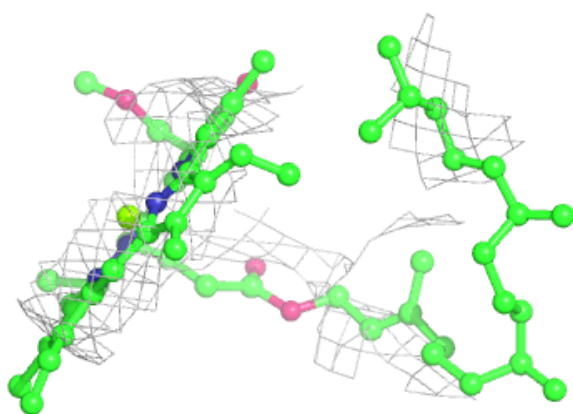
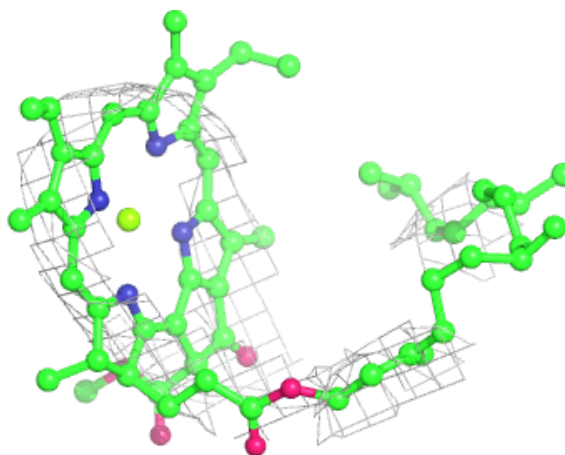
**Electron density around CLA d 401:**

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



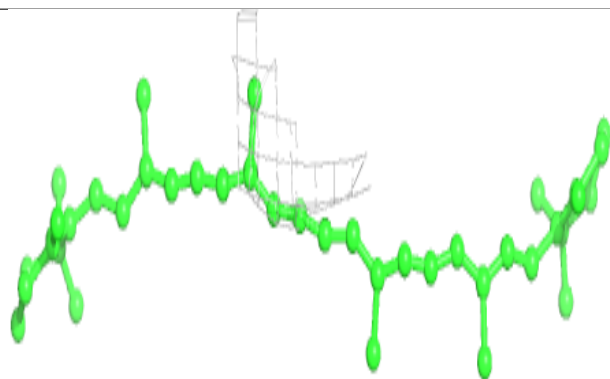
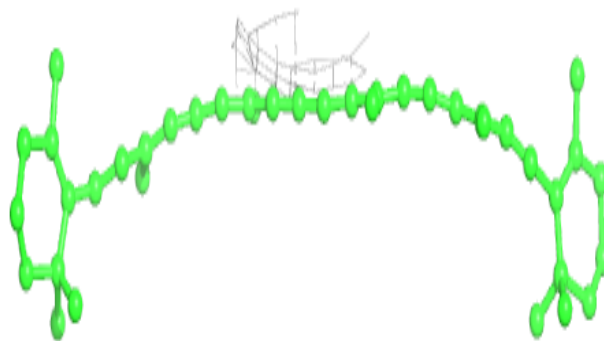
**Electron density around CLA c 904:**

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

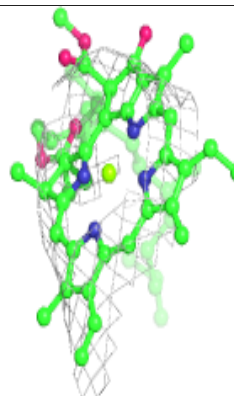
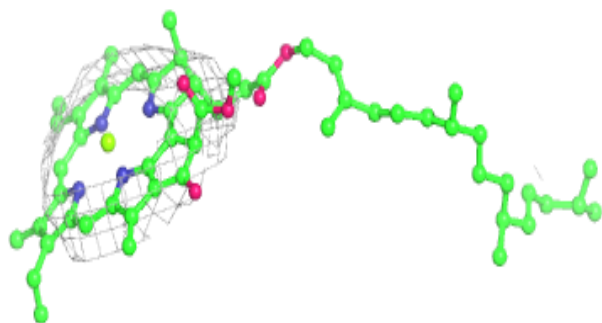
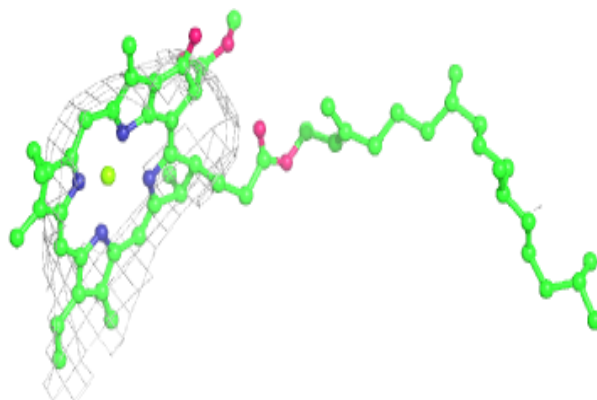


**Electron density around BCR K 101:**

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

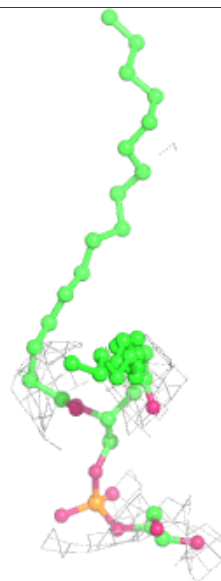
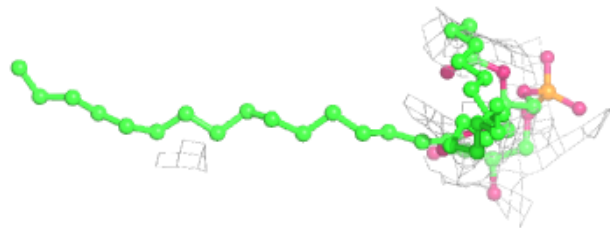
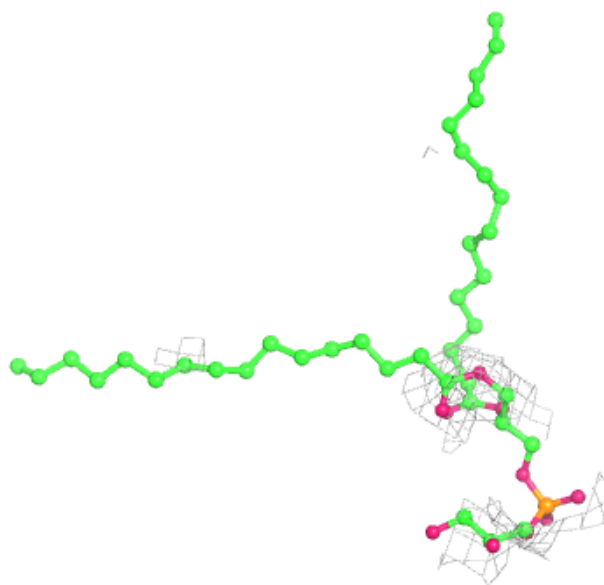
**Electron density around CLA A 606:**

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



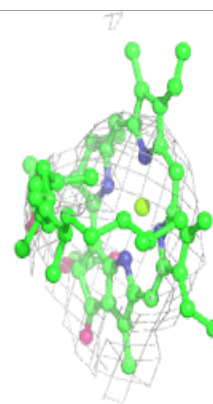
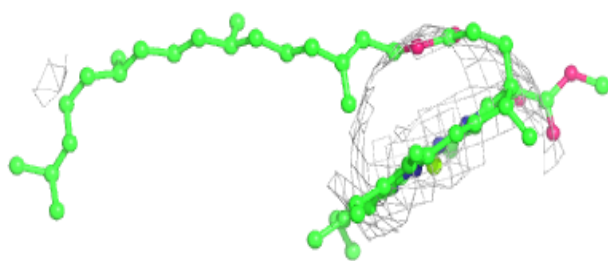
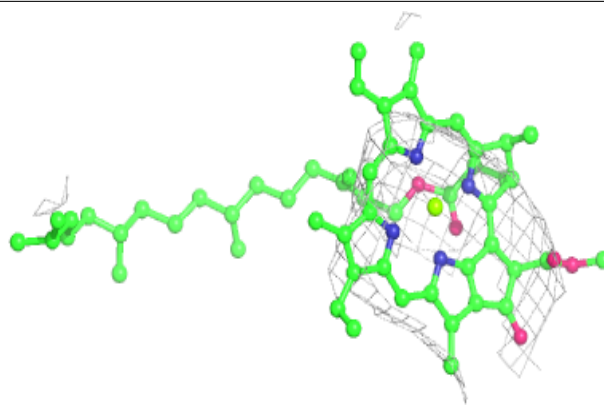
**Electron density around LHG b 620:**

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



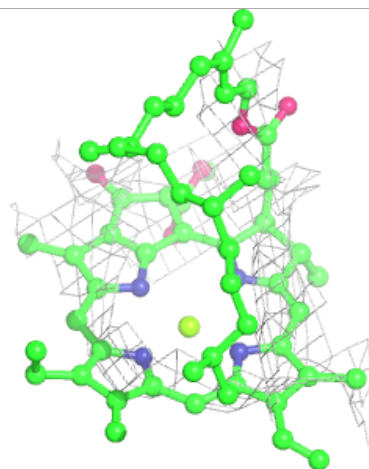
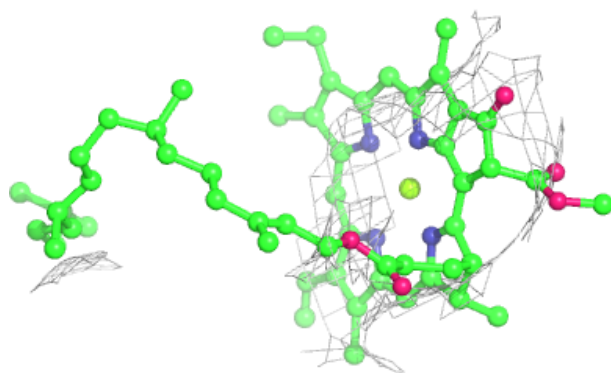
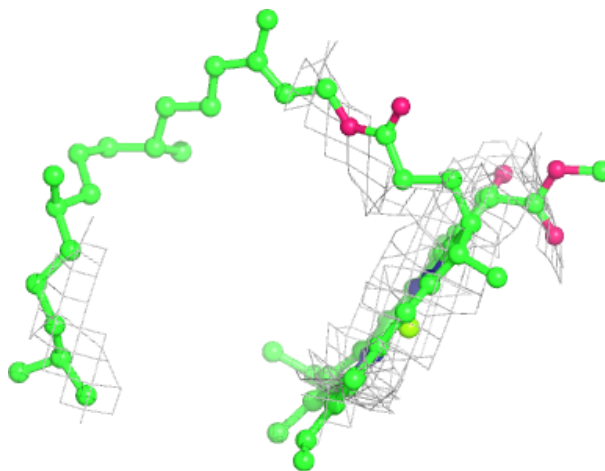
**Electron density around CLA B 609:**

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



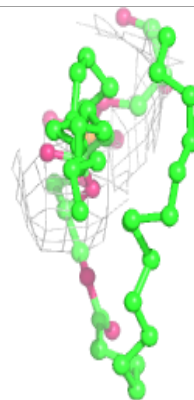
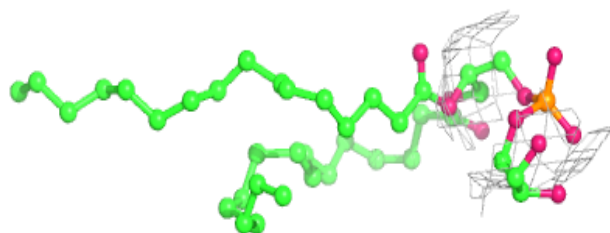
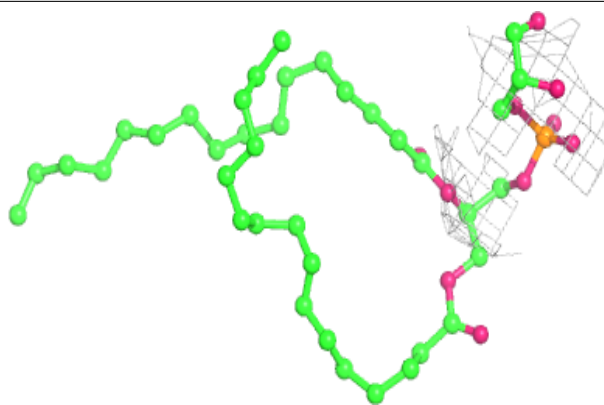
**Electron density around CLA B 612:**

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

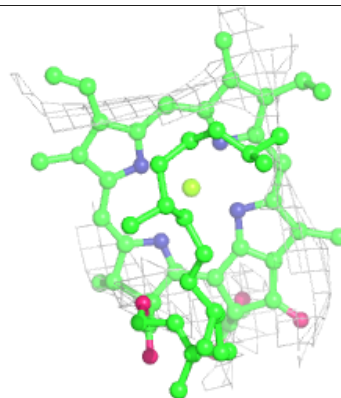
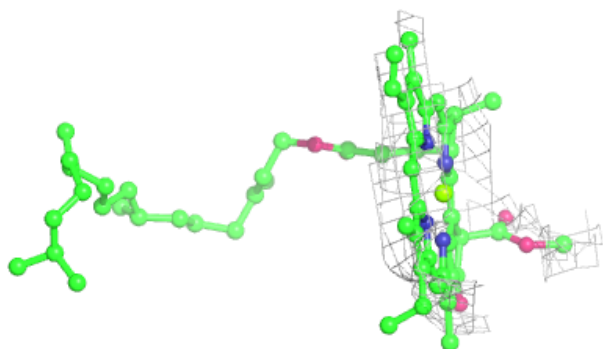
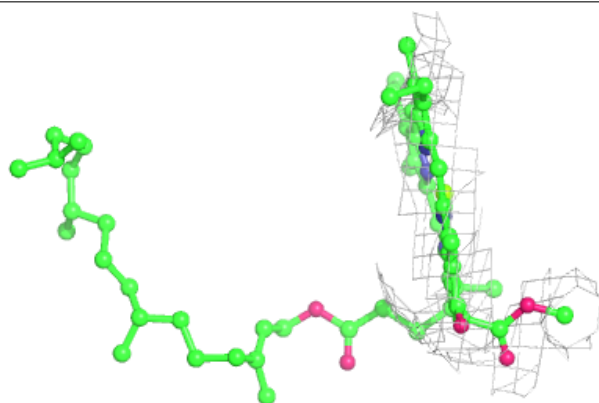


**Electron density around LHG d 410:**

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

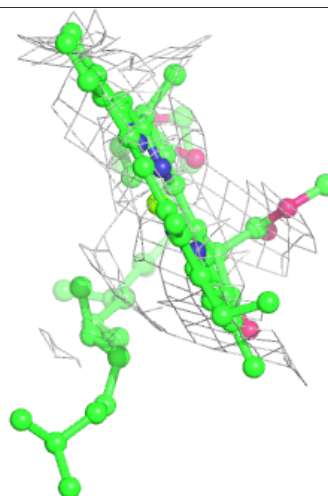
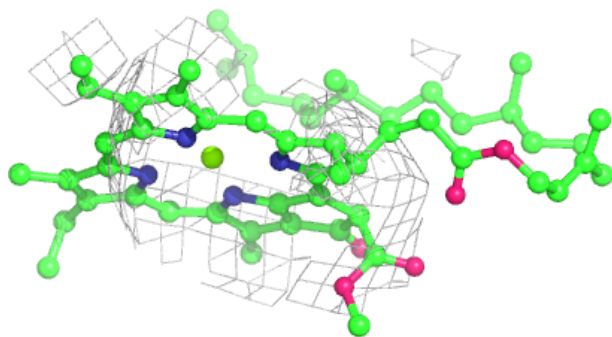
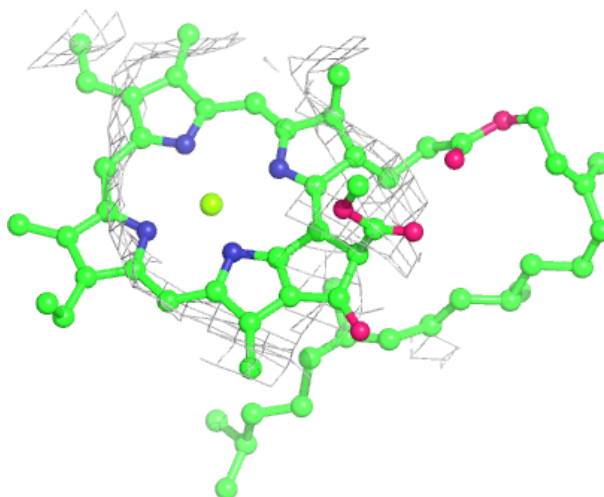
**Electron density around CLA c 907:**

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



**Electron density around CLA c 910:**

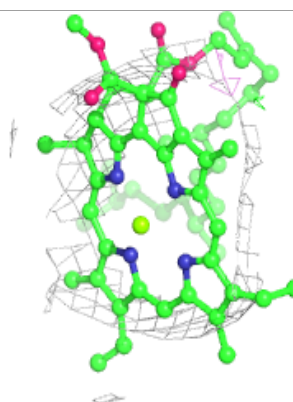
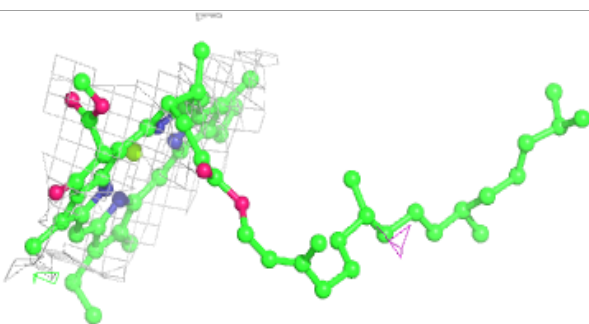
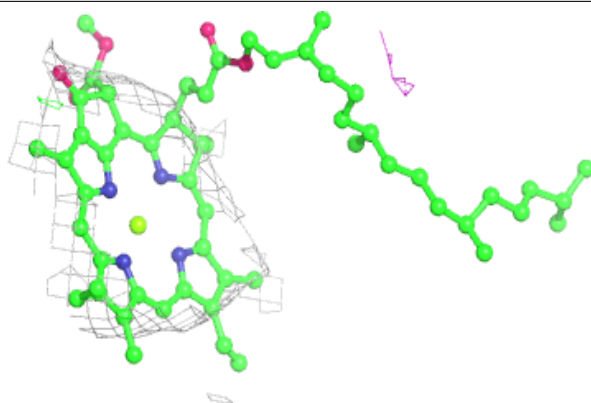
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



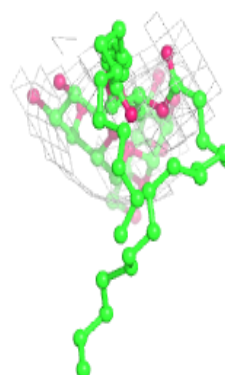
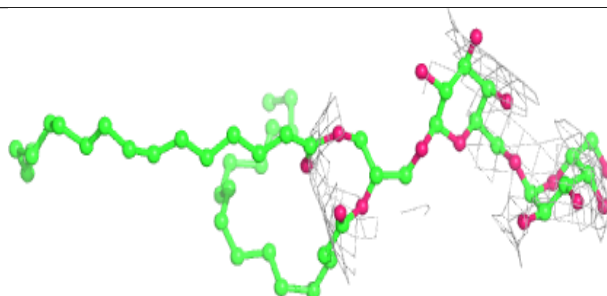
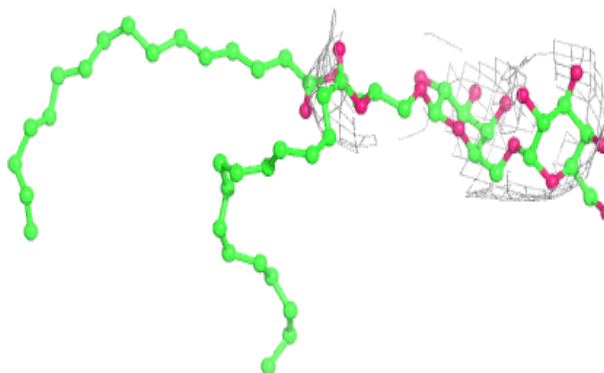


**Electron density around CLA c 912:**

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

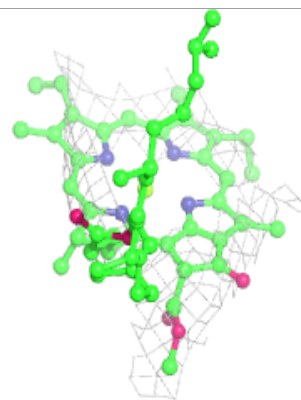
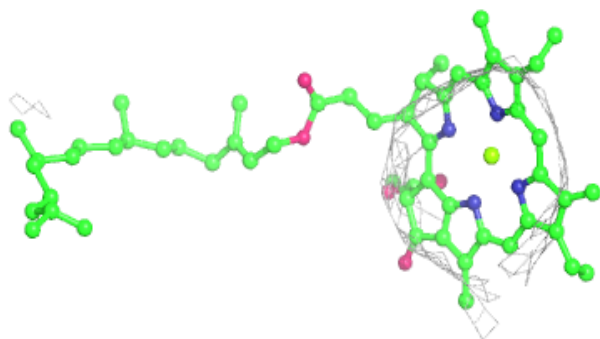
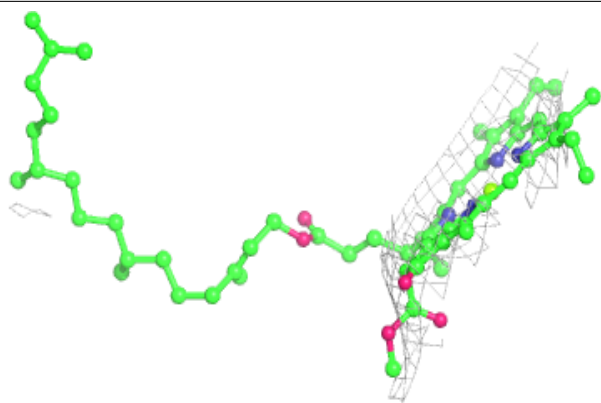
**Electron density around DGD h 102:**

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

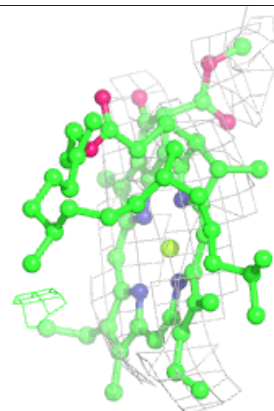
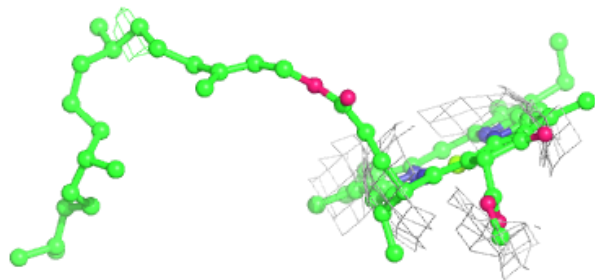
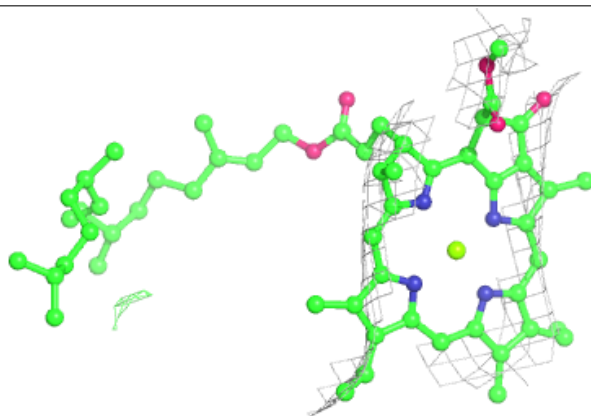


**Electron density around CLA d 403:**

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

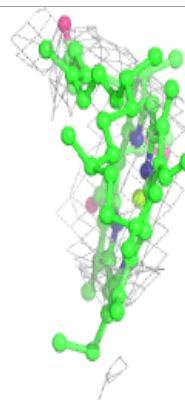
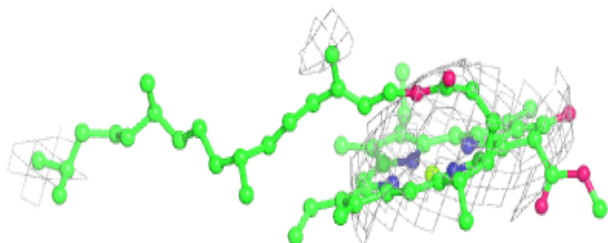
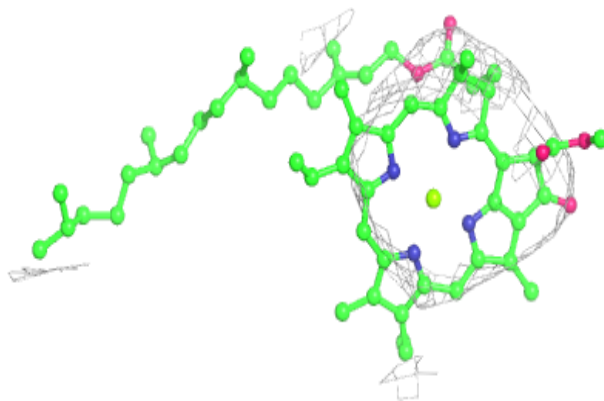
**Electron density around CLA A 609:**

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

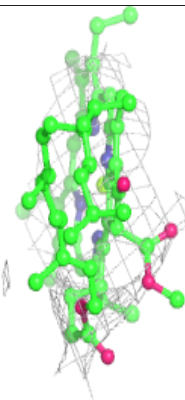
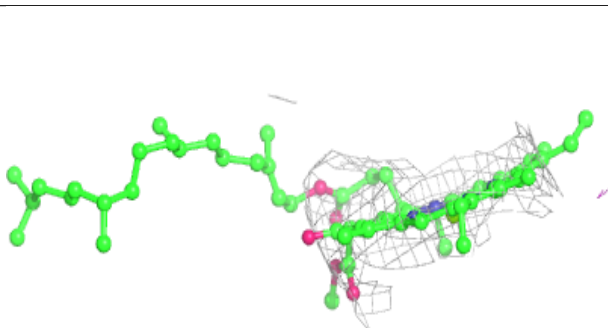
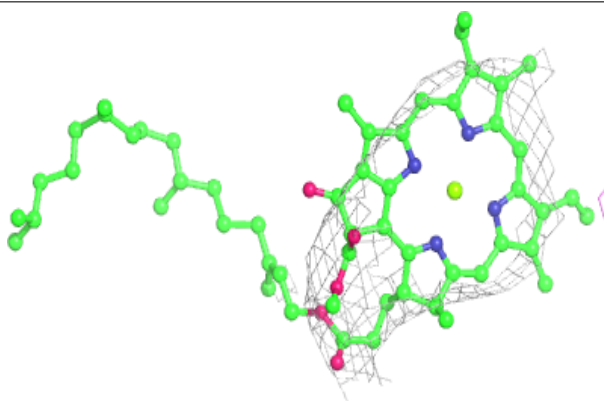


**Electron density around CLA C 501:**

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

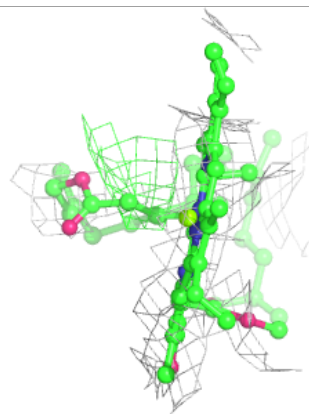
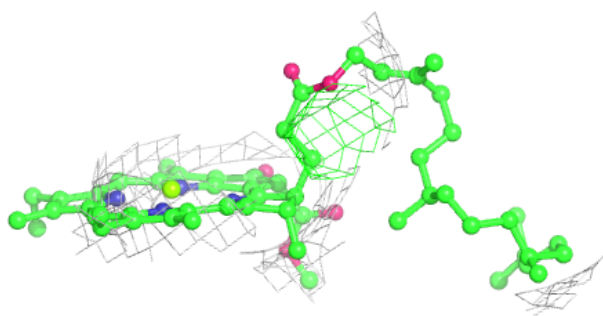
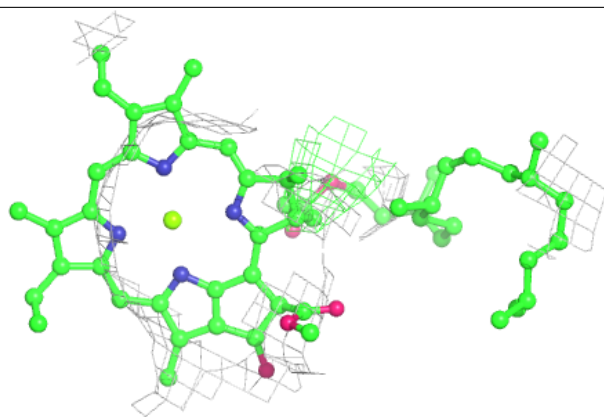
**Electron density around CLA b 603:**

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

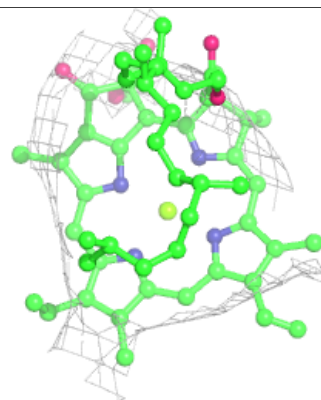
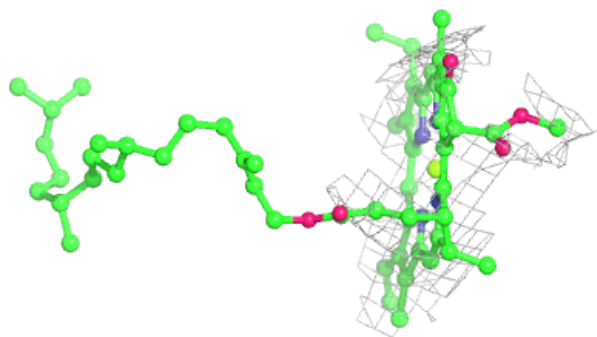
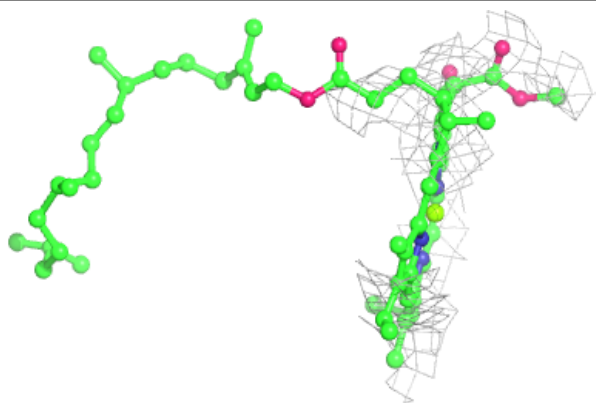


**Electron density around CLA B 613:**

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

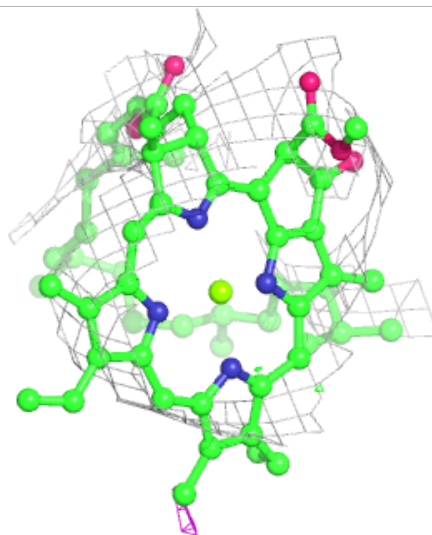
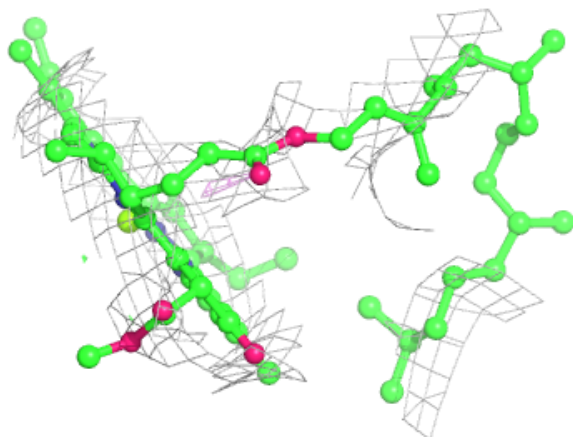
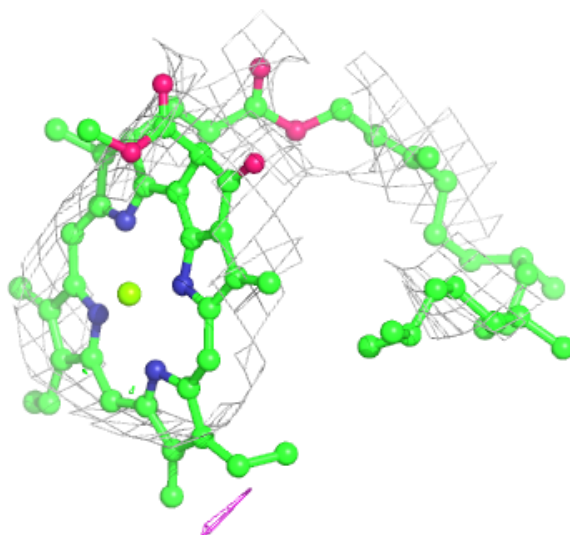
**Electron density around CLA C 506:**

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



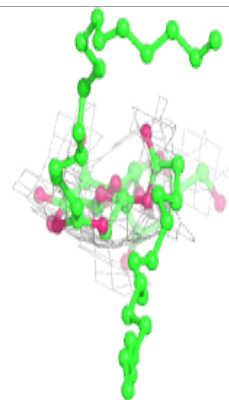
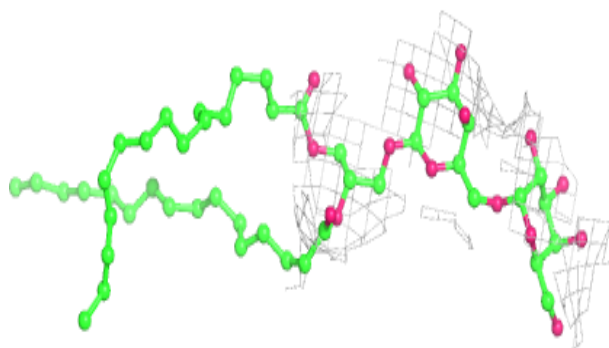
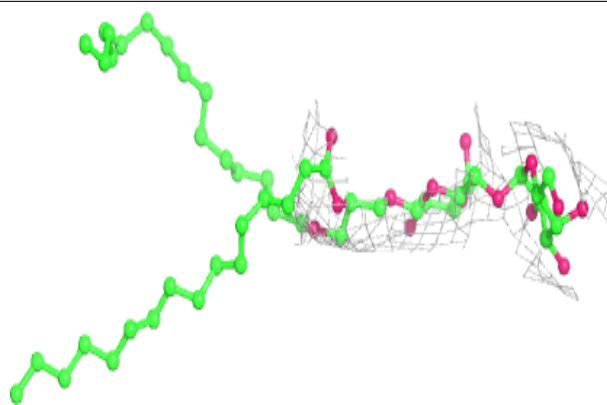
**Electron density around CLA C 503:**

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



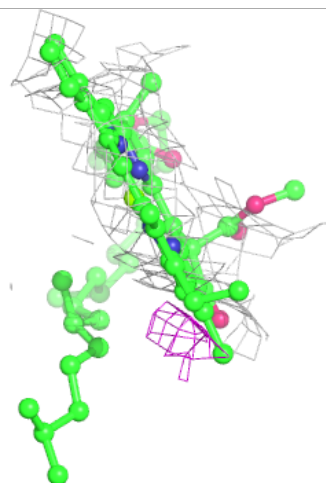
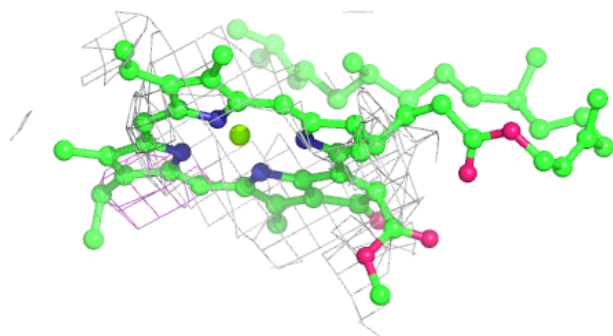
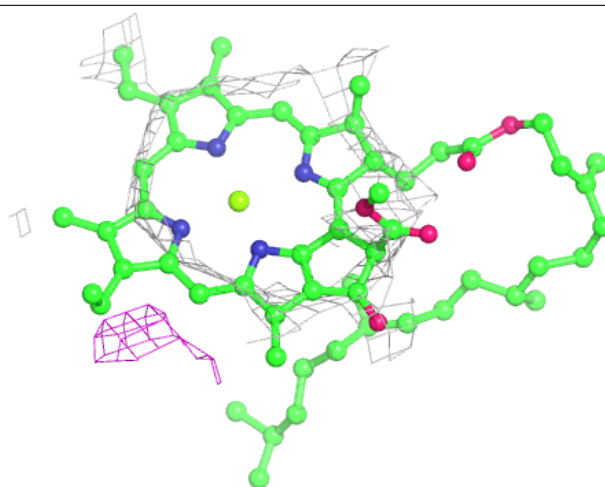
**Electron density around DGD C 516:**

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



**Electron density around CLA C 509:**

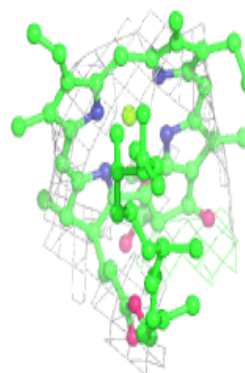
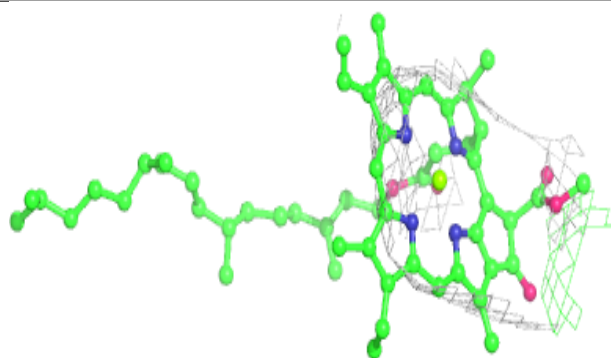
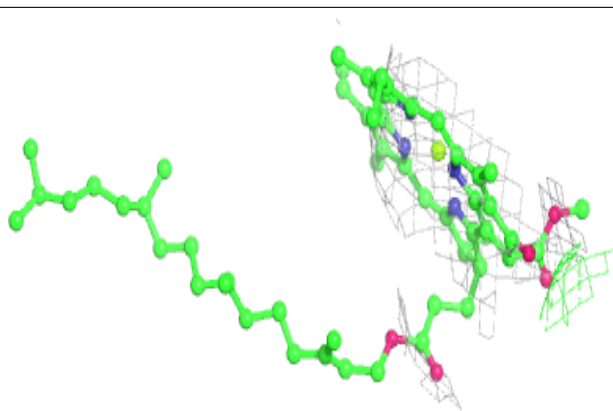
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



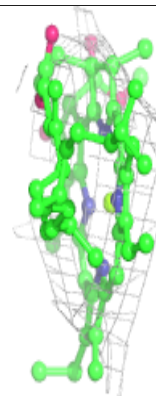
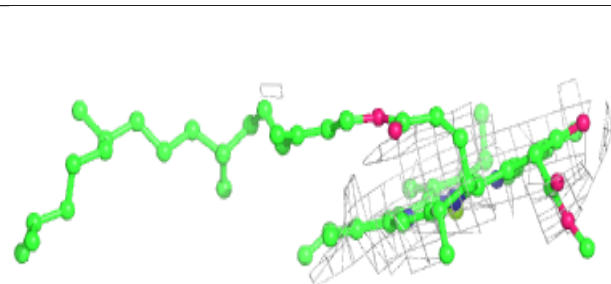
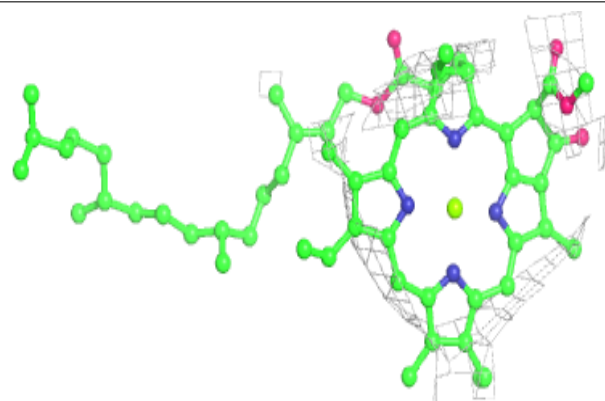


**Electron density around CLA c 905:**

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

**Electron density around CLA B 604:**

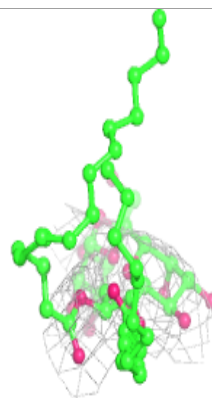
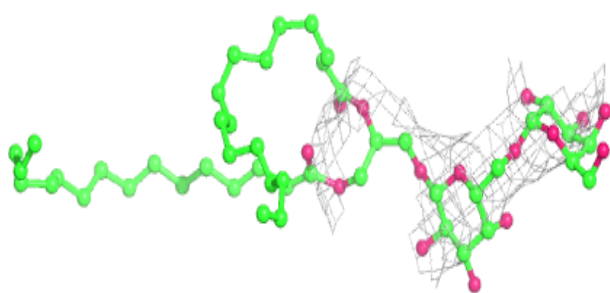
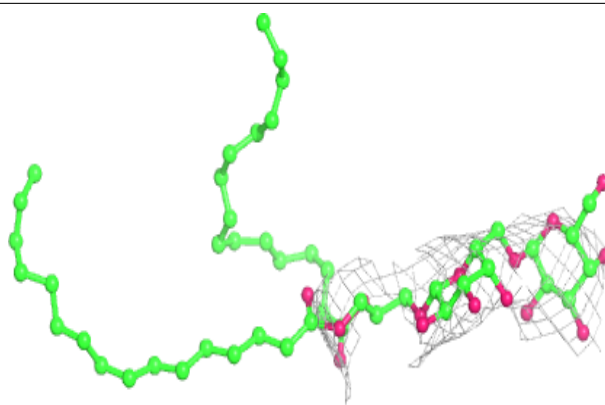
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



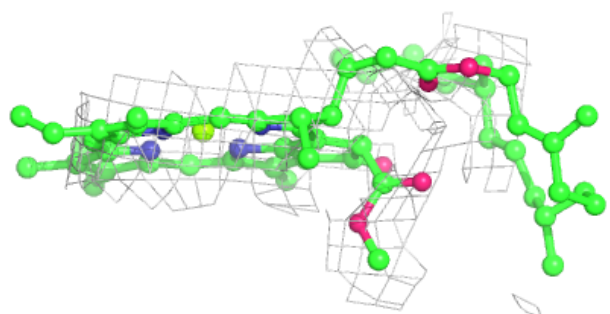
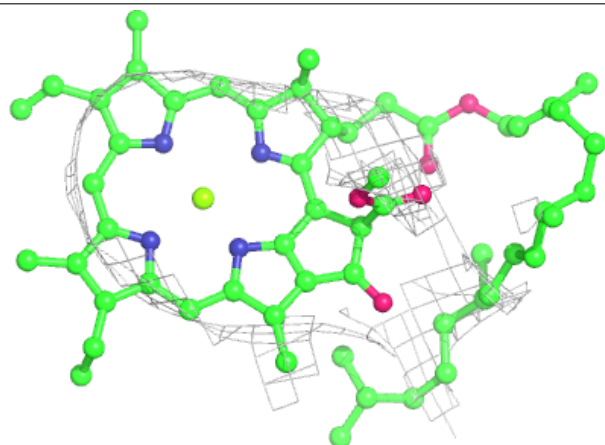


**Electron density around DGD H 102:**

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

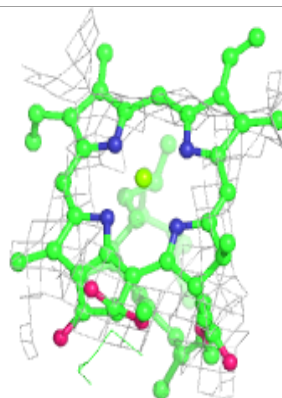
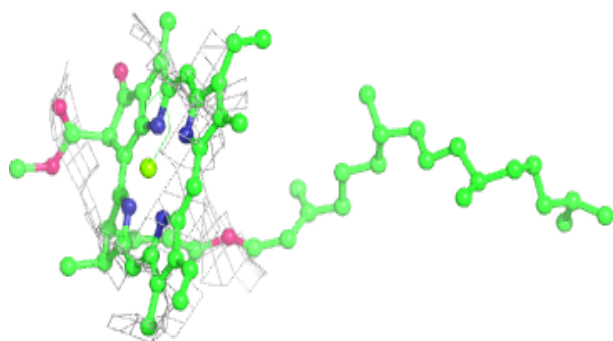
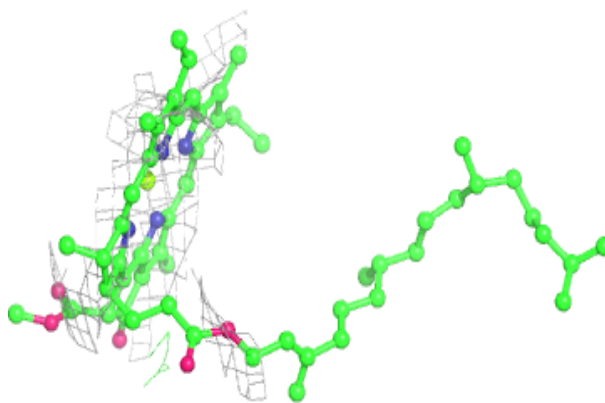
**Electron density around CLA b 611:**

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

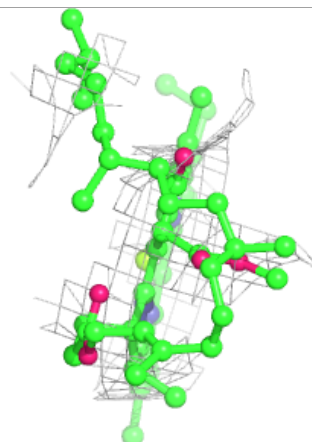
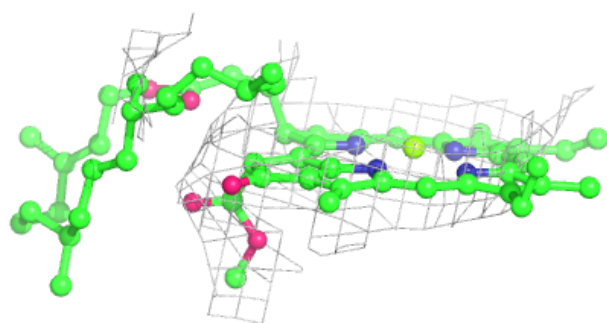
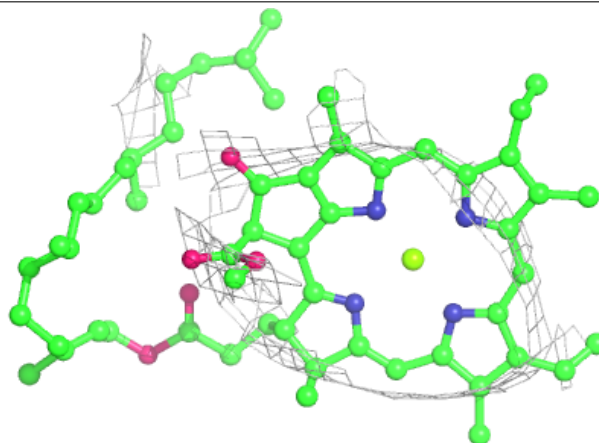


**Electron density around CLA c 909:**

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

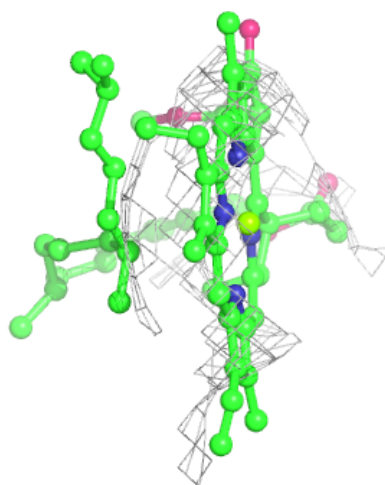
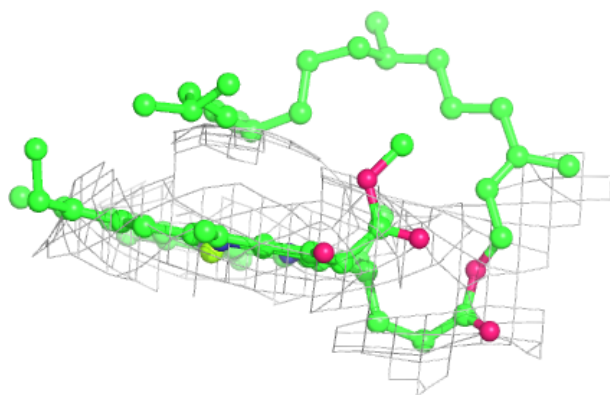
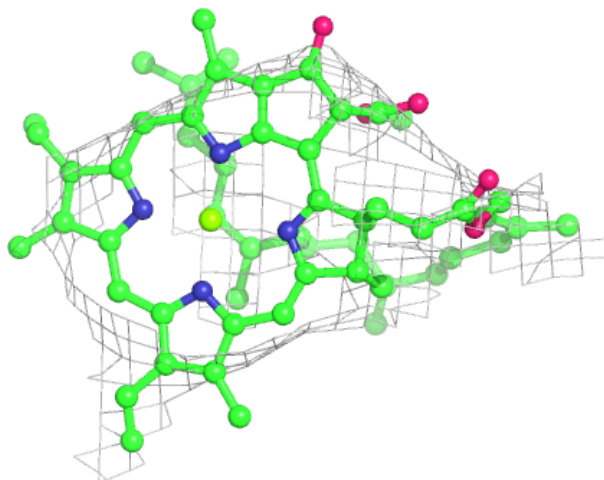
**Electron density around CLA B 611:**

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



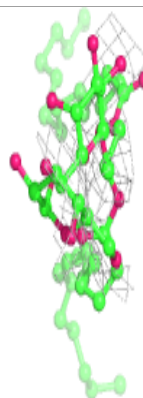
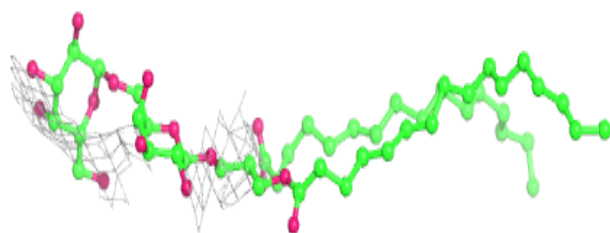
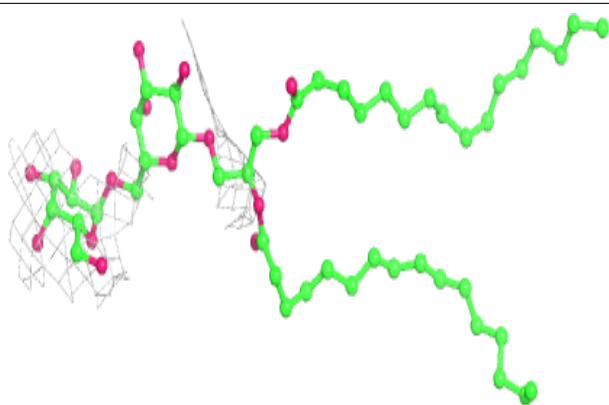
**Electron density around CLA C 510:**

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



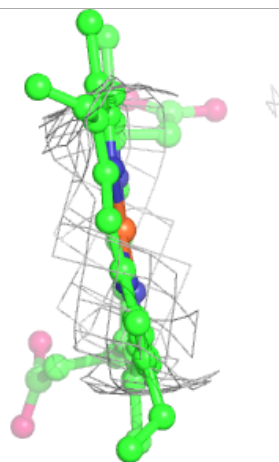
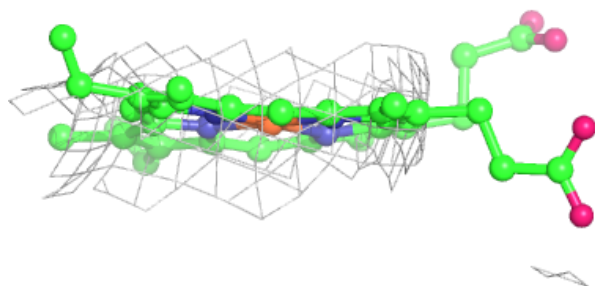
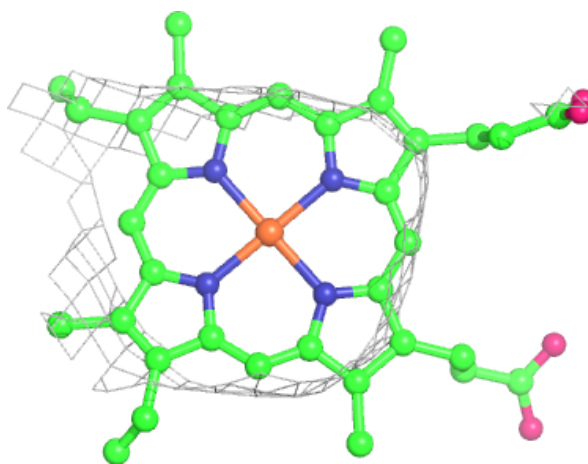
**Electron density around DGD j 101:**

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



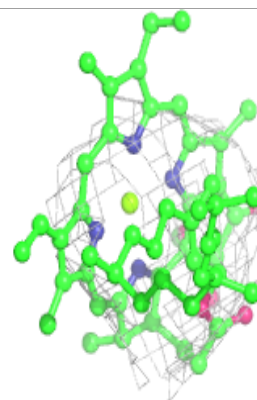
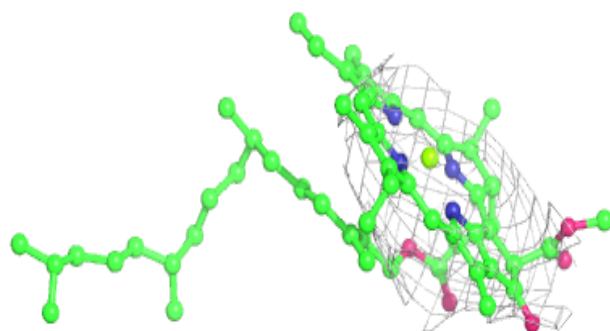
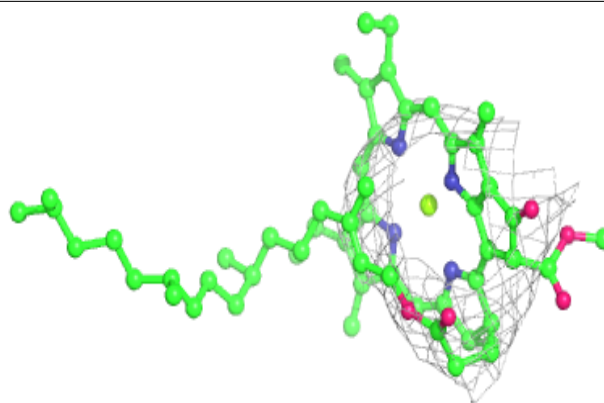
**Electron density around HEM V 202:**

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

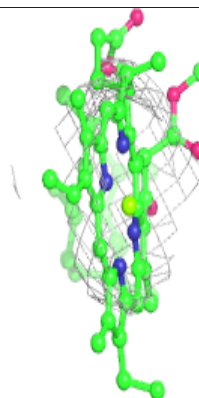
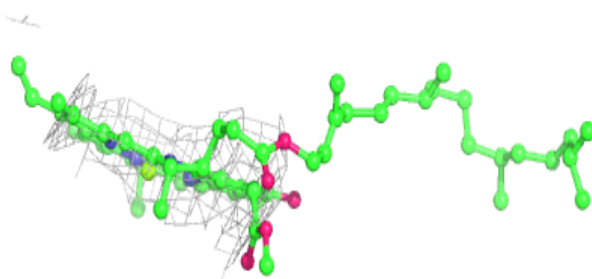
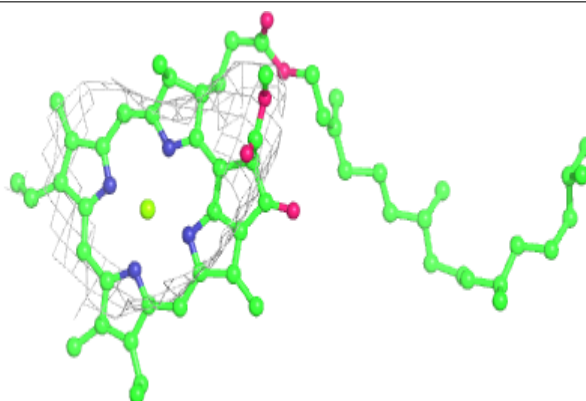


**Electron density around CLA c 906:**

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

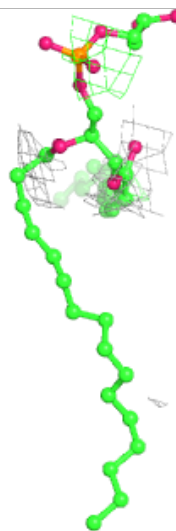
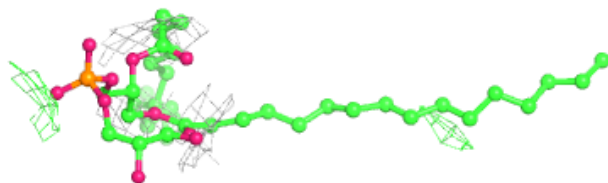
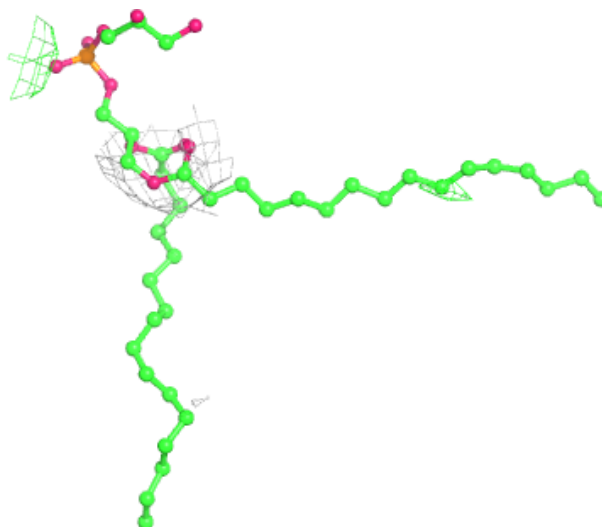
**Electron density around CLA B 603:**

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



**Electron density around LHG B 621:**

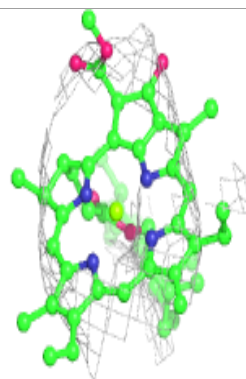
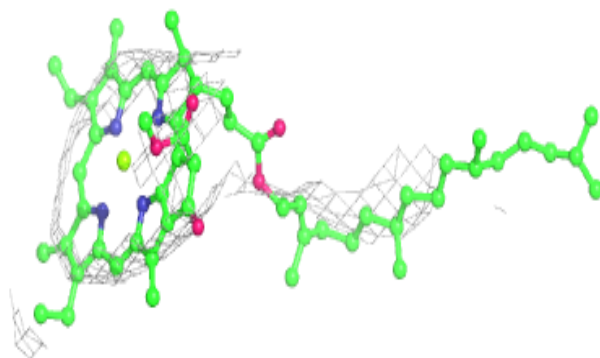
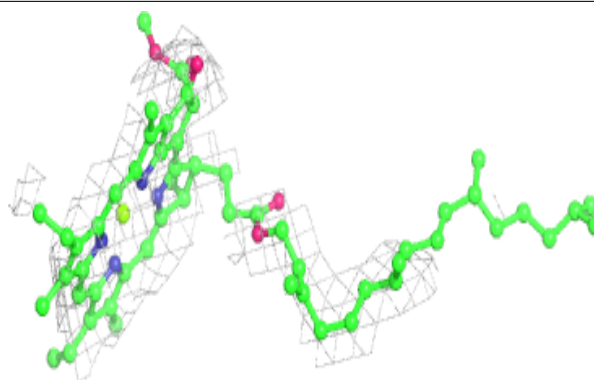
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



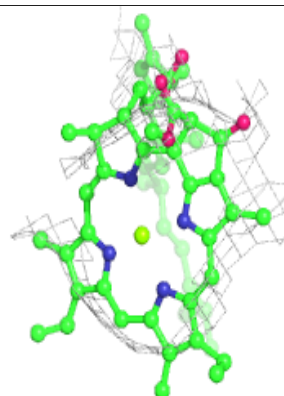
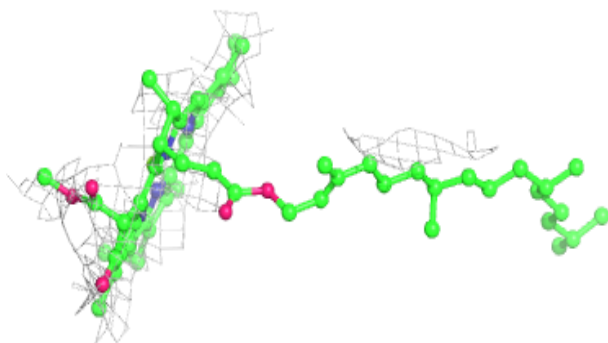
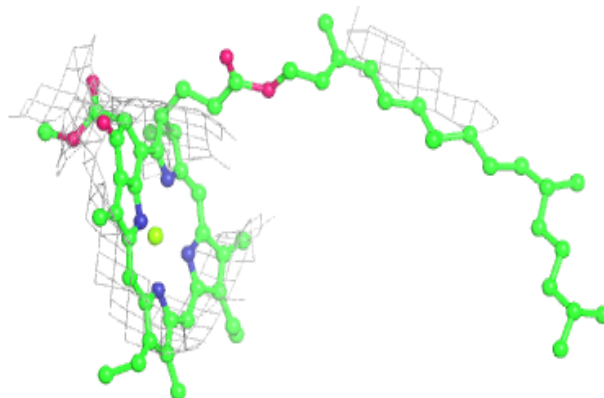


**Electron density around CLA C 502:**

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

**Electron density around CLA B 610:**

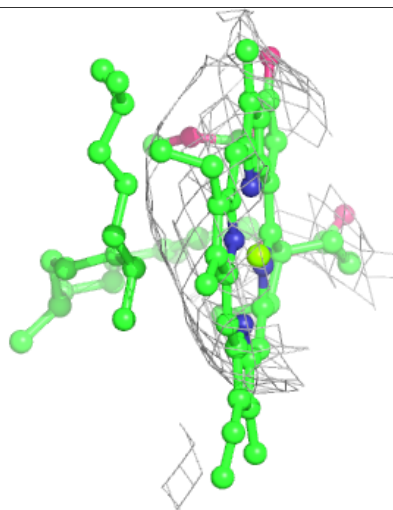
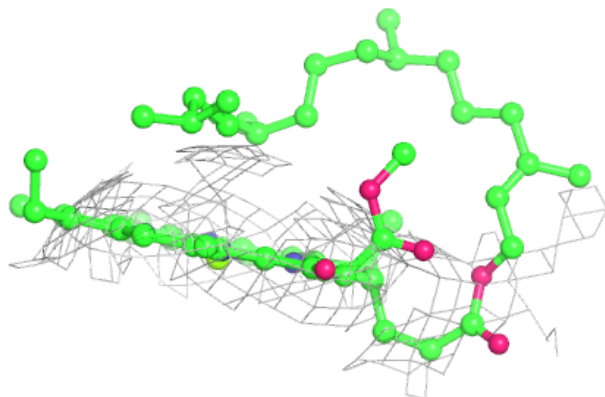
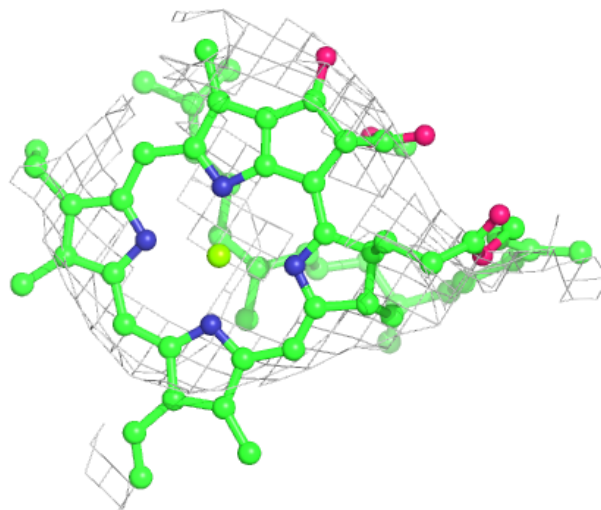
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





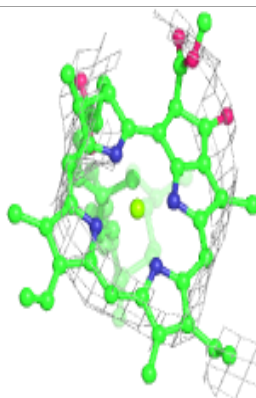
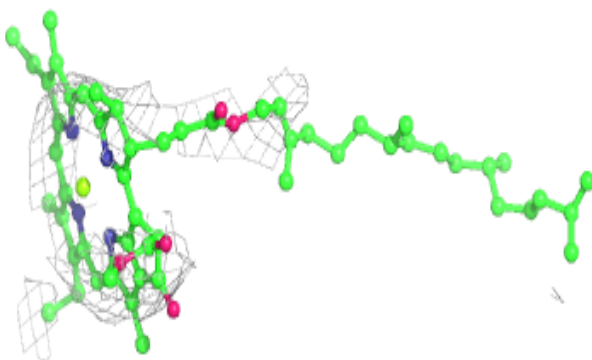
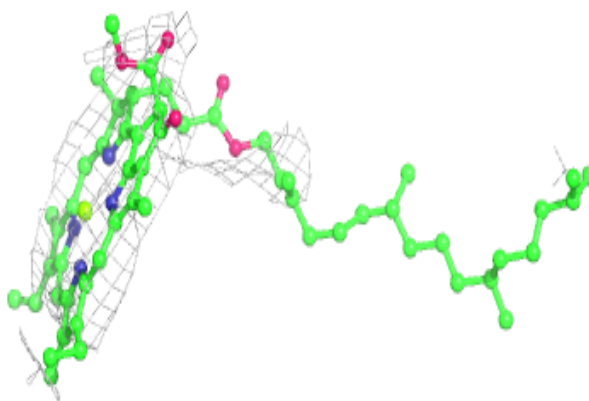
**Electron density around CLA c 911:**

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

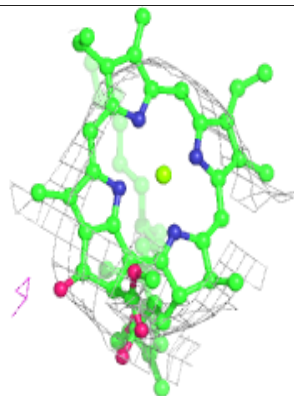
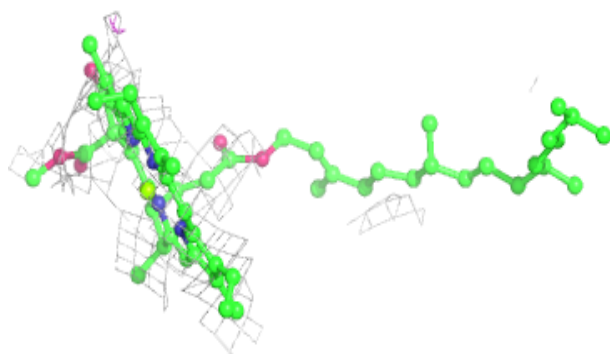
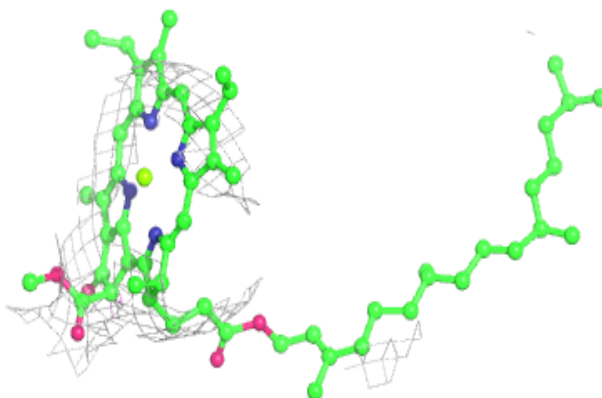


**Electron density around CLA B 605:**

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

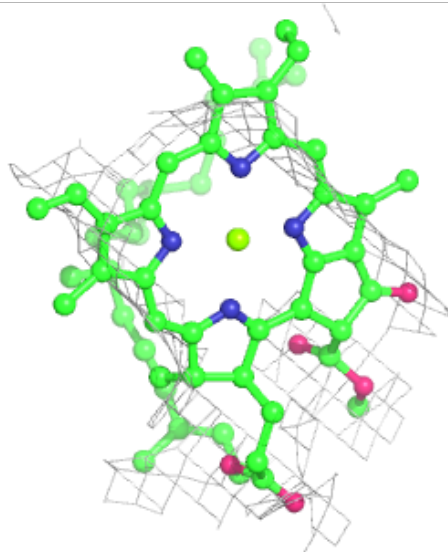
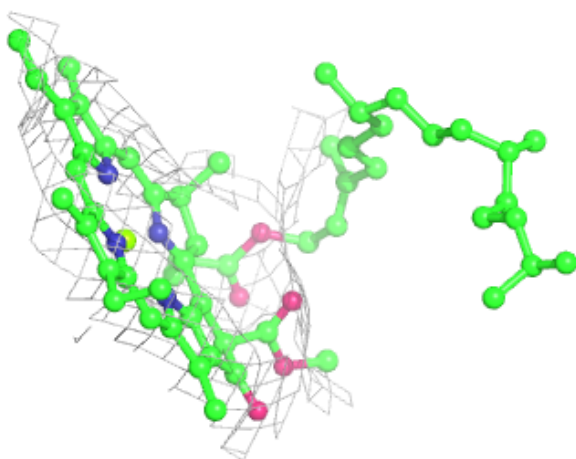
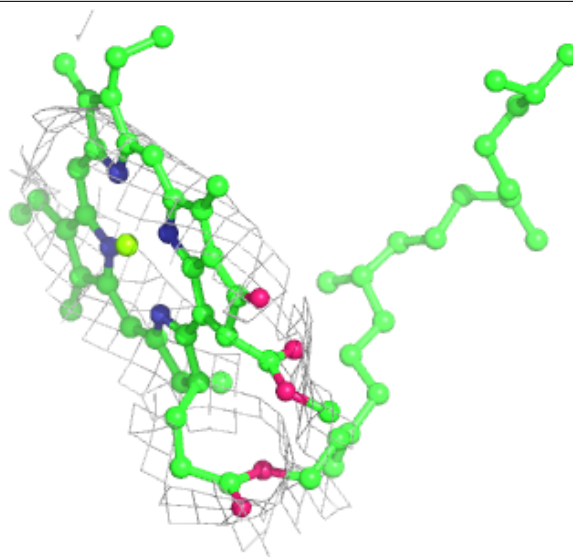
**Electron density around CLA b 610:**

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



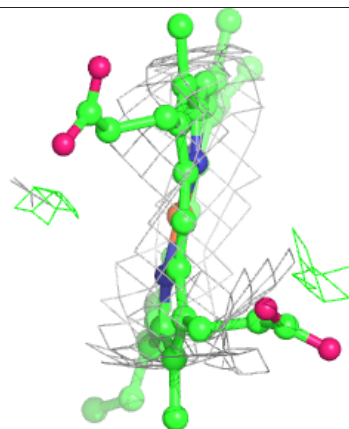
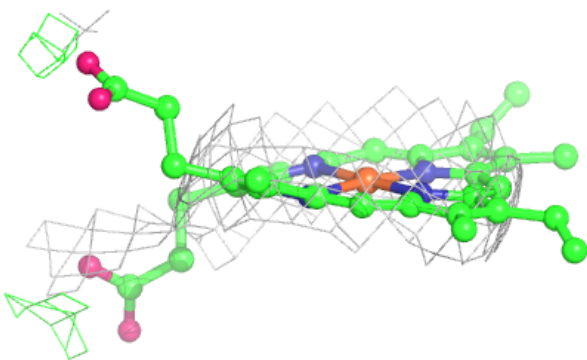
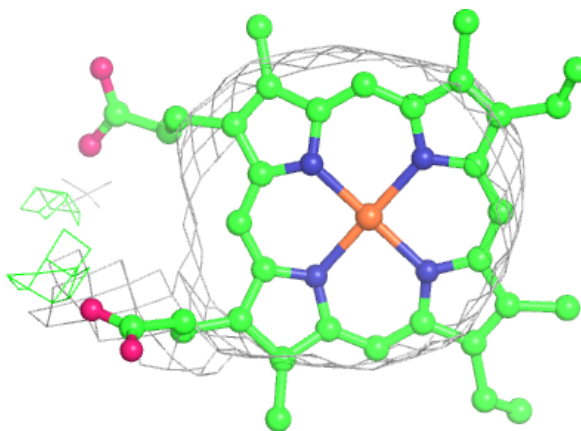
**Electron density around CLA B 614:**

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

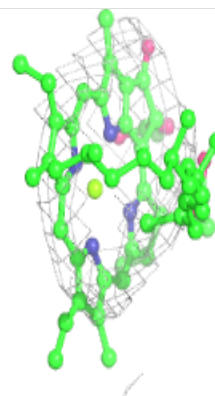
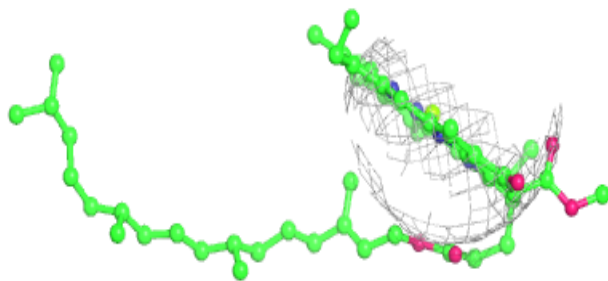
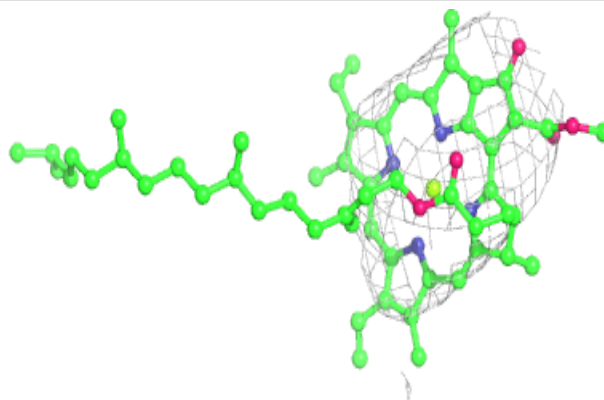


**Electron density around HEM e 101:**

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

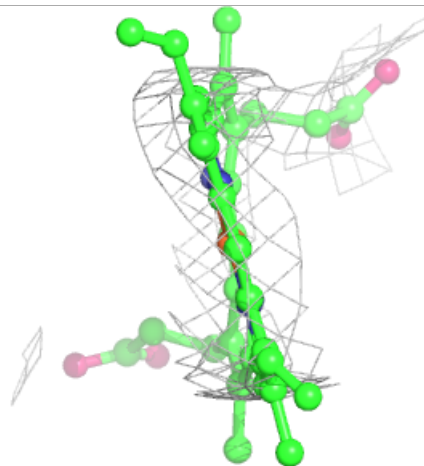
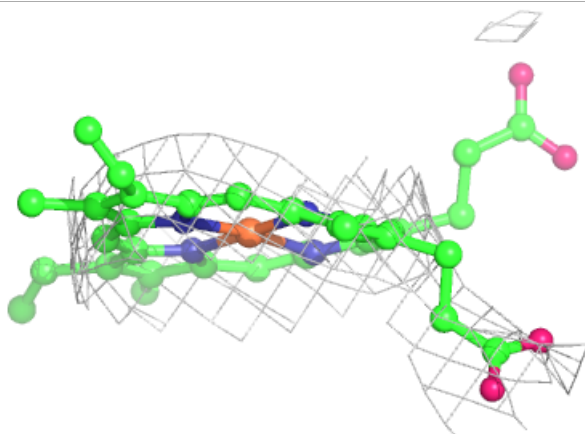
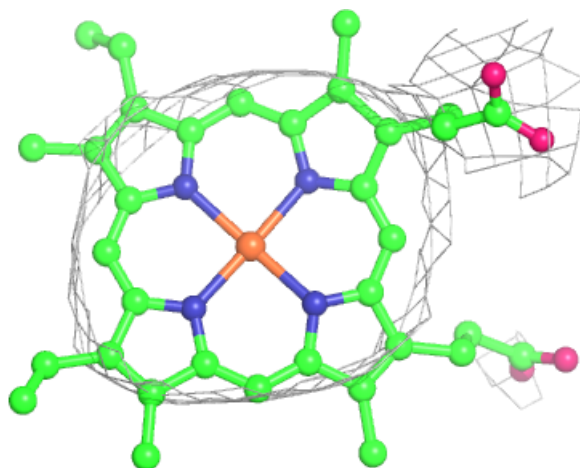
**Electron density around CLA b 609:**

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



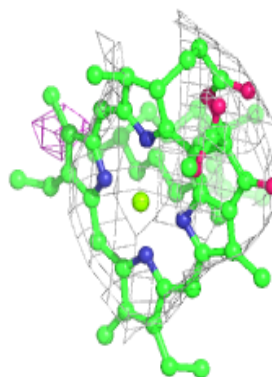
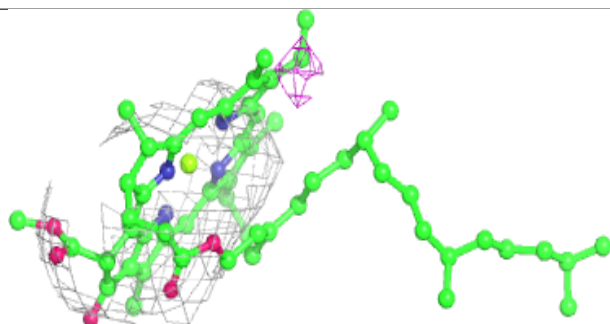
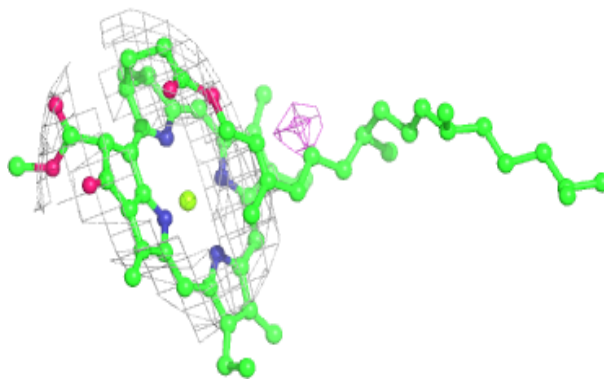
**Electron density around HEM E 101:**

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

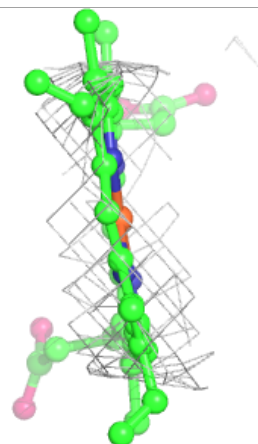
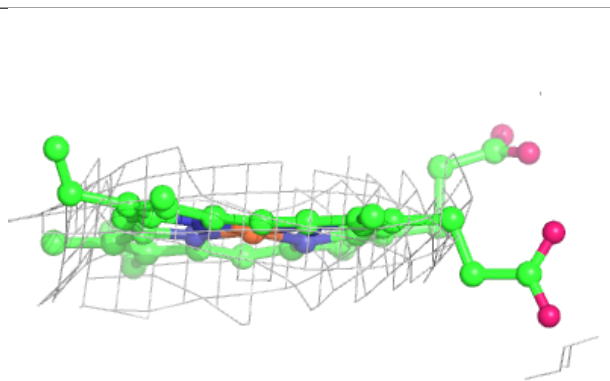
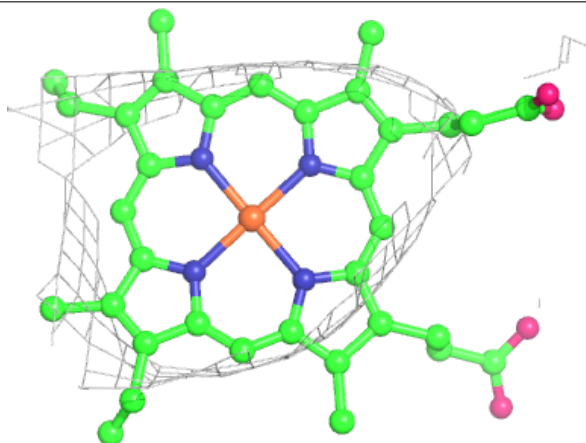


**Electron density around CLA C 505:**

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

**Electron density around HEM v 202:**

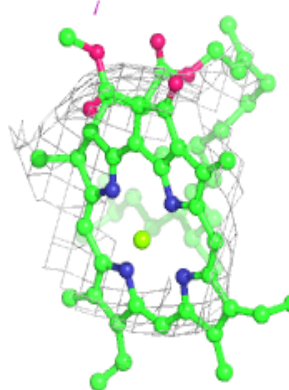
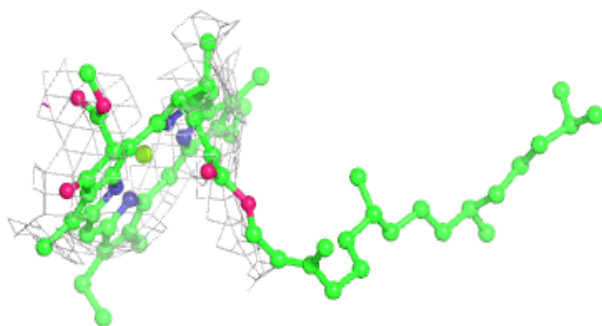
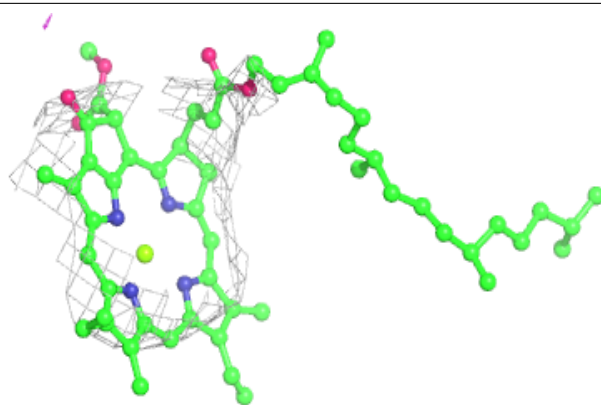
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



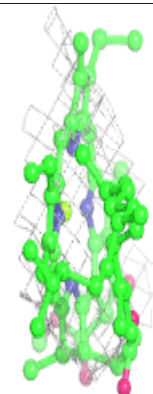
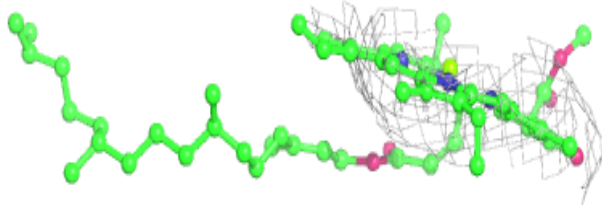
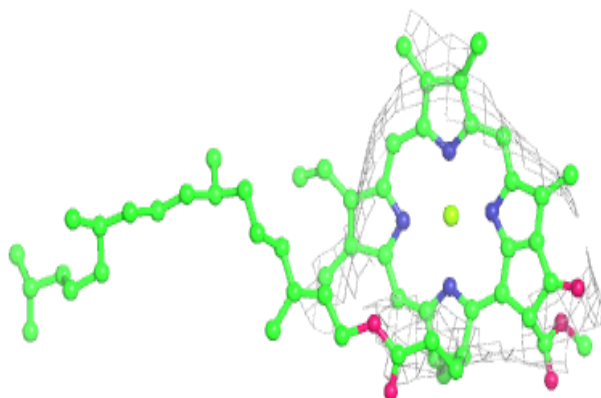


**Electron density around CLA C 511:**

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

**Electron density around CLA b 604:**

$2mF_o-DF_c$  (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.