



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 19, 2020 – 05:28 AM BST

PDB ID : 4YUU  
Title : Crystal structure of oxygen-evolving photosystem II from a red alga  
Authors : Ago, H.; Shen, J.-R.  
Deposited on : 2015-03-19  
Resolution : 2.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

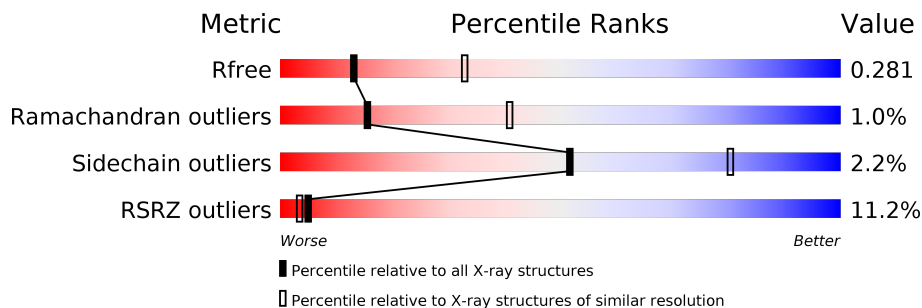
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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

Mol	Chain	Length	Quality of chain
1	A1	344	 3% 99%
1	A2	344	 7% 95%
1	a1	344	 3% 96%
1	a2	344	 5% 95%
2	B1	509	 6% 93% 5%
2	B2	509	 11% 96%
2	b1	509	 6% 96%

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Mol	Chain	Length	Quality of chain
2	b2	509	8% 92% 6%
3	C1	460	6% 96% ..
3	C2	460	17% 96% ..
3	c1	460	5% 96% ..
3	c2	460	6% 96% ..
4	D1	351	6% 95% ..
4	D2	351	9% 96% ..
4	d1	351	2% 96% ..
4	d2	351	5% 96% ..
5	E1	84	29% 73% 27%
5	E2	84	37% 75% 25%
5	e1	84	15% 67% 32%
5	e2	84	26% 71% 29%
6	F1	43	5% 63% 35%
6	F2	43	19% 70% 28%
6	f1	43	7% 65% 33%
6	f2	43	16% 65% 33%
7	H1	67	13% 87% 10%
7	H2	67	15% 91% 7%
7	h1	67	4% 90% 7%
7	h2	67	19% 90% 7%
8	I1	38	5% 87% 11%
8	I2	38	5% 89% 8%
8	i1	38	3% 87% 11%
8	i2	38	5% 84% 13%

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Mol	Chain	Length	Quality of chain
9	J1	39	8% 82% 18%
9	J2	39	23% 90% 10%
9	j1	39	13% 82% 18%
9	j2	39	3% 85% 15%
10	K1	41	7% 85% 5% 10%
10	K2	41	22% 85% 5% 10%
10	k1	41	15% 85% 5% 10%
10	k2	41	22% 85% 5% 10%
11	L1	38	8% 95% • •
11	L2	38	3% 95% • •
11	l1	38	3% 95% • •
11	l2	38	95% • •
12	M1	108	% 36% • 63%
12	M2	108	36% • 63%
12	m1	108	36% • 63%
12	m2	108	4% 36% • 63%
13	O1	329	11% 65% 6% • 27%
13	O2	329	16% 57% • • 38%
13	o1	329	11% 65% 5% • 28%
13	o2	329	12% 66% 6% • 26%
14	T1	32	3% 94% 6%
14	T2	32	3% 94% 6%
14	t1	32	9% 94% 6%
14	t2	32	6% 88% • 9%
15	U1	155	% 57% • 40%

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Mol	Chain	Length	Quality of chain
15	U2	155	13% 55% 42%
15	u1	155	8% 57% 40%
15	u2	155	3% 56% 40%
16	V1	155	3% 79% 17%
16	V2	155	25% 79% 17%
16	v1	155	8% 78% 17%
16	v2	155	8% 79% 17%
17	Y1	35	9% 77% 23%
17	Y2	35	23% 71% 29%
17	y1	35	17% 77% 23%
17	y2	35	14% 77% 23%
18	X1	40	25% 70% 28%
18	X2	40	28% 75% 23%
18	x1	40	15% 85% 5% 10%
18	x2	40	33% 78% 20%
19	S1	46	11% 54% 46%
19	S2	46	35% 65% 35%
19	s1	46	24% 87% 13%
19	s2	46	28% 100%
20	W1	25	4% 84% 16%
20	W2	25	84% 16%
20	w1	25	16% 100%
20	w2	25	4% 80% 20%
21	Q2	218	25% 49% 49%
21	q1	218	21% 47% 52%

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Mol	Chain	Length	Quality of chain
22	Z2	62	
22	z2	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
23	BCR	K1	101	-	-	-	X
23	BCR	K2	102	-	-	-	X
23	BCR	k1	101	-	-	-	X
23	BCR	z2	101	-	-	-	X
25	CLA	A1	403	X	-	-	-
25	CLA	A1	404	X	-	-	-
25	CLA	A1	405	X	-	-	-
25	CLA	A1	406	X	-	-	-
25	CLA	A2	402	X	-	-	-
25	CLA	A2	403	X	-	-	-
25	CLA	A2	404	X	-	-	-
25	CLA	B1	604	X	-	-	-
25	CLA	B1	605	X	-	-	-
25	CLA	B1	606	X	-	-	-
25	CLA	B1	607	X	-	-	-
25	CLA	B1	608	X	-	-	-
25	CLA	B1	609	X	-	-	-
25	CLA	B1	610	X	-	-	-
25	CLA	B1	611	X	-	-	-
25	CLA	B1	612	X	-	-	-
25	CLA	B1	613	X	-	-	-
25	CLA	B1	614	X	-	-	-
25	CLA	B1	615	X	-	-	-
25	CLA	B1	616	X	-	-	-
25	CLA	B1	617	X	-	-	-
25	CLA	B1	618	X	-	-	-
25	CLA	B1	619	X	-	-	-
25	CLA	B2	604	X	-	-	-
25	CLA	B2	605	X	-	-	-
25	CLA	B2	606	X	-	-	-
25	CLA	B2	607	X	-	-	-
25	CLA	B2	608	X	-	-	-
25	CLA	B2	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B2	610	X	-	-	-
25	CLA	B2	611	X	-	-	-
25	CLA	B2	612	X	-	-	-
25	CLA	B2	613	X	-	-	-
25	CLA	B2	614	X	-	-	-
25	CLA	B2	615	X	-	-	-
25	CLA	B2	616	X	-	-	-
25	CLA	B2	617	X	-	-	-
25	CLA	B2	618	X	-	-	-
25	CLA	B2	619	X	-	-	-
25	CLA	C1	502	X	-	-	-
25	CLA	C1	503	X	-	-	-
25	CLA	C1	504	X	-	-	-
25	CLA	C1	505	X	-	-	-
25	CLA	C1	506	X	-	-	-
25	CLA	C1	507	X	-	-	-
25	CLA	C1	508	X	-	-	-
25	CLA	C1	509	X	-	-	-
25	CLA	C1	510	X	-	-	-
25	CLA	C1	511	X	-	-	-
25	CLA	C1	512	X	-	-	-
25	CLA	C1	513	X	-	-	-
25	CLA	C1	514	X	-	-	-
25	CLA	C2	503	X	-	-	-
25	CLA	C2	504	X	-	-	-
25	CLA	C2	505	X	-	-	-
25	CLA	C2	506	X	-	-	-
25	CLA	C2	507	X	-	-	-
25	CLA	C2	508	X	-	-	-
25	CLA	C2	509	X	-	-	-
25	CLA	C2	510	X	-	-	-
25	CLA	C2	511	X	-	-	-
25	CLA	C2	513	X	-	-	-
25	CLA	C2	516	X	-	-	-
25	CLA	C2	518	X	-	-	-
25	CLA	D1	402	X	-	-	-
25	CLA	D1	403	X	-	-	-
25	CLA	D2	401	X	-	-	-
25	CLA	D2	404	X	-	-	-
25	CLA	D2	406	X	-	-	-
25	CLA	K2	101	X	-	-	-
25	CLA	a1	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	a1	404	X	-	-	-
25	CLA	a1	405	X	-	-	-
25	CLA	a2	404	X	-	-	-
25	CLA	a2	405	X	-	-	-
25	CLA	a2	413	X	-	-	-
25	CLA	b1	604	X	-	-	-
25	CLA	b1	605	X	-	-	-
25	CLA	b1	606	X	-	-	-
25	CLA	b1	607	X	-	-	-
25	CLA	b1	608	X	-	-	-
25	CLA	b1	609	X	-	-	-
25	CLA	b1	610	X	-	-	-
25	CLA	b1	611	X	-	-	-
25	CLA	b1	612	X	-	-	-
25	CLA	b1	613	X	-	-	-
25	CLA	b1	614	X	-	-	-
25	CLA	b1	615	X	-	-	-
25	CLA	b1	616	X	-	-	-
25	CLA	b1	617	X	-	-	-
25	CLA	b1	619	X	-	-	-
25	CLA	b1	620	X	-	-	-
25	CLA	b2	604	X	-	-	-
25	CLA	b2	606	X	-	-	-
25	CLA	b2	608	X	-	-	-
25	CLA	b2	609	X	-	-	-
25	CLA	b2	610	X	-	-	-
25	CLA	b2	611	X	-	-	-
25	CLA	b2	612	X	-	-	-
25	CLA	b2	613	X	-	-	-
25	CLA	b2	614	X	-	-	-
25	CLA	b2	615	X	-	-	-
25	CLA	b2	616	X	-	-	-
25	CLA	b2	617	X	-	-	-
25	CLA	b2	618	X	-	-	-
25	CLA	b2	619	X	-	-	-
25	CLA	b2	620	X	-	-	-
25	CLA	b2	624	X	-	-	-
25	CLA	c1	503	X	-	-	-
25	CLA	c1	504	X	-	-	-
25	CLA	c1	505	X	-	-	-
25	CLA	c1	506	X	-	-	-
25	CLA	c1	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c1	508	X	-	-	-
25	CLA	c1	509	X	-	-	-
25	CLA	c1	510	X	-	-	-
25	CLA	c1	511	X	-	-	-
25	CLA	c1	512	X	-	-	-
25	CLA	c1	513	X	-	-	-
25	CLA	c1	515	X	-	-	-
25	CLA	c1	516	X	-	-	-
25	CLA	c2	502	X	-	-	-
25	CLA	c2	503	X	-	-	-
25	CLA	c2	504	X	-	-	-
25	CLA	c2	505	X	-	-	-
25	CLA	c2	506	X	-	-	-
25	CLA	c2	507	X	-	-	-
25	CLA	c2	508	X	-	-	-
25	CLA	c2	509	X	-	-	-
25	CLA	c2	510	X	-	-	-
25	CLA	c2	511	X	-	-	-
25	CLA	c2	512	X	-	-	-
25	CLA	c2	513	X	-	-	-
25	CLA	c2	515	X	-	-	-
25	CLA	d1	401	X	-	-	-
25	CLA	d1	404	X	-	-	-
25	CLA	d1	406	X	-	-	-
25	CLA	d2	402	X	-	-	-
25	CLA	d2	404	X	-	-	-
25	CLA	d2	405	X	-	-	-
28	UNL	C2	501	-	-	-	X
28	UNL	C2	517	-	-	-	X
28	UNL	D1	410	-	-	-	X
28	UNL	H2	102	-	-	-	X
28	UNL	J2	101	-	-	-	X
28	UNL	X2	101	-	-	-	X
28	UNL	b1	623	-	-	-	X
28	UNL	b1	630	-	-	-	X
28	UNL	d2	410	-	-	-	X
28	UNL	j1	101	-	-	-	X
29	LMG	C2	515	-	-	-	X
29	LMG	j2	101	-	-	-	X
32	GOL	C1	518	-	-	-	X
33	LHG	b2	625	-	-	-	X
35	LMT	c1	517	-	-	-	X

## 2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 92765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A1	344	Total 2609	C 1708	N 425	O 462	S 14	0	0	0
1	a1	334	Total 2564	C 1676	N 421	O 454	S 13	0	0	0
1	A2	332	Total 2475	C 1607	N 411	O 444	S 13	0	1	0
1	a2	334	Total 2513	C 1638	N 410	O 452	S 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B1	483	Total 3703	C 2426	N 624	O 641	S 12	0	0	0
2	b1	503	Total 3881	C 2549	N 646	O 674	S 12	0	1	0
2	B2	503	Total 3770	C 2460	N 645	O 654	S 11	0	0	0
2	b2	481	Total 3681	C 2418	N 620	O 631	S 12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C1	449	Total 3392	C 2215	N 573	O 594	S 10	0	0	0
3	c1	449	Total 3439	C 2241	N 577	O 611	S 10	0	2	0
3	C2	444	Total 3145	C 2028	N 545	O 564	S 8	0	0	0
3	c2	448	Total 3386	C 2201	N 578	O 597	S 10	0	0	0



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D1	337	Total	C	N	O	S	0	0	0
			2615	1736	422	447	10			
4	d1	339	Total	C	N	O	S	0	0	0
			2678	1775	433	460	10			
4	D2	340	Total	C	N	O	S	0	0	0
			2585	1713	422	440	10			
4	d2	340	Total	C	N	O	S	0	0	0
			2643	1756	425	452	10			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E1	61	Total	C	N	O	0	0	0
			405	264	68	73			
5	e1	57	Total	C	N	O	0	0	0
			427	280	71	76			
5	E2	63	Total	C	N	O	0	0	0
			430	279	72	79			
5	e2	60	Total	C	N	O	0	0	0
			421	279	71	71			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F1	28	Total	C	N	O	S	0	0	0
			213	144	36	32	1			
6	f1	29	Total	C	N	O	S	0	0	0
			227	158	36	32	1			
6	F2	31	Total	C	N	O	S	0	0	0
			229	153	41	34	1			
6	f2	29	Total	C	N	O	S	0	0	0
			225	157	34	33	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H1	60	Total	C	N	O	S	0	0	0
			433	289	69	73	2			
7	h1	62	Total	C	N	O	S	0	0	0
			470	317	71	80	2			
7	H2	62	Total	C	N	O	S	0	0	0
			443	294	72	75	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	h2	62	Total	C	N	O	S	0	0	0
			450	302	69	77	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I1	34	Total	C	N	O	S	0	0	0
			274	184	42	45	3			
8	i1	34	Total	C	N	O	S	0	0	0
			280	188	44	45	3			
8	I2	35	Total	C	N	O	S	0	0	0
			265	177	41	45	2			
8	i2	33	Total	C	N	O	S	0	0	0
			261	174	40	44	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J1	32	Total	C	N	O	0	0	0
			220	148	33	39			
9	j1	32	Total	C	N	O	0	0	0
			224	152	33	39			
9	J2	35	Total	C	N	O	0	0	0
			231	154	36	41			
9	j2	33	Total	C	N	O	0	0	0
			228	153	34	41			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K1	37	Total	C	N	O	S	0	0	0
			279	195	39	44	1			
10	k1	37	Total	C	N	O	S	0	0	0
			280	198	39	42	1			
10	K2	37	Total	C	N	O	0	0	0	
			250	171	39	40				
10	k2	37	Total	C	N	O	S	0	0	0
			269	185	40	43	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L1	37	Total	C	N	O	0	0	0
			292	197	46	49			
11	l1	37	Total	C	N	O	0	0	0
			299	203	47	49			
11	L2	37	Total	C	N	O	0	0	0
			299	202	46	51			
11	l2	37	Total	C	N	O	0	0	0
			299	202	46	51			

- Molecule 12 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M1	40	Total	C	N	O	S	0	0	0
			285	189	44	50	2			
12	m1	40	Total	C	N	O	S	0	0	0
			285	189	44	50	2			
12	M2	40	Total	C	N	O	S	0	0	0
			284	188	46	48	2			
12	m2	40	Total	C	N	O	S	0	0	0
			287	189	46	50	2			

- Molecule 13 is a protein called PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O1	240	Total	C	N	O	S	0	0	0
			1674	1074	276	316	8			
13	o1	238	Total	C	N	O	S	0	0	0
			1692	1070	282	332	8			
13	O2	205	Total	C	N	O	S	0	0	0
			1376	870	237	262	7			
13	o2	245	Total	C	N	O	S	0	0	0
			1768	1123	296	341	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T1	30	Total	C	N	O	S	0	0	0
			241	168	36	36	1			
14	t1	30	Total	C	N	O	S	0	0	0
			246	173	36	36	1			
14	T2	30	Total	C	N	O	S	0	0	0
			240	170	33	36	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	t2	29	235	167	32	35	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	U1	93	691	445	116	129	1	0	0	0
15	u1	93	703	449	119	134	1	0	0	0
15	U2	90	577	355	103	118	1	0	0	0
15	u2	93	708	455	120	132	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U1	-51	MET	-	initiating methionine	UNP Q9ZQS5
u1	-51	MET	-	initiating methionine	UNP Q9ZQS5
U2	-51	MET	-	initiating methionine	UNP Q9ZQS5
u2	-51	MET	-	initiating methionine	UNP Q9ZQS5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V1	129	917	579	159	175	4	0	0	0
16	v1	129	921	577	163	177	4	0	0	0
16	V2	129	845	521	152	168	4	0	0	0
16	v2	129	963	608	168	183	4	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	Y1	27	170	111	29	30	0	0	0
17	y1	27	195	133	30	32	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Y2	25	Total	C	N	O	0	0	0
			159	104	27	28			
17	y2	27	Total	C	N	O	0	0	0
			188	126	30	32			

- Molecule 18 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X1	29	Total	C	N	O	0	0	0	
			197	135	30	32				
18	x1	36	Total	C	N	O	S	0	0	0
			255	174	38	42	1			
18	X2	31	Total	C	N	O	S	0	0	0
			215	149	33	32	1			
18	x2	32	Total	C	N	O	0	0	0	
			218	147	35	36				

- Molecule 19 is a protein called PEPTIDE CHAIN UNASSIGNED.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S1	25	Total	C	N	O	0	0	0
			164	113	26	25			
19	s1	40	Total	C	N	O	0	0	0
			263	182	41	40			
19	S2	30	Total	C	N	O	0	0	0
			191	130	31	30			
19	s2	46	Total	C	N	O	0	0	0
			281	188	47	46			

- Molecule 20 is a protein called PEPTIDE CHAIN UNASSIGNED.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	W1	21	Total	C	N	O	0	0	0
			134	91	21	22			
20	w1	25	Total	C	N	O	0	0	0
			152	101	25	26			
20	W2	21	Total	C	N	O	0	0	0
			129	86	21	22			
20	w2	20	Total	C	N	O	0	0	0
			127	86	20	21			

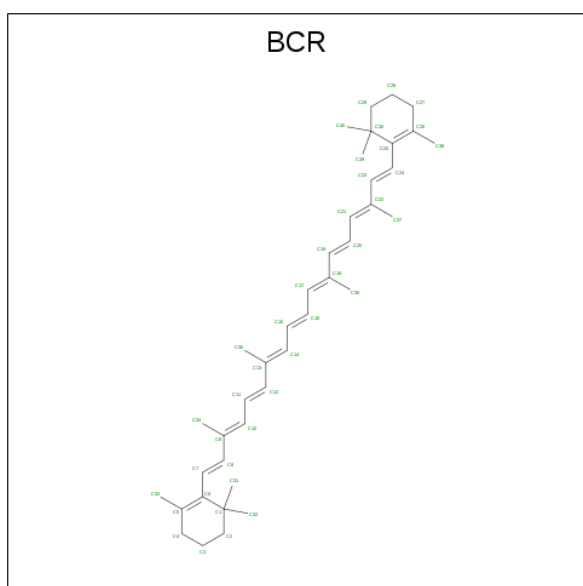
- Molecule 21 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	q1	105	Total	C	N	O	S	0	0	0
			645	399	115	127	4			
21	Q2	111	Total	C	N	O	S	0	0	0
			676	417	123	133	3			

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z2	59	Total	C	N	O	S	0	0	0
			351	224	61	65	1			
22	z2	59	Total	C	N	O	S	0	0	0
			381	250	63	67	1			

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	C1	1	Total	C	0	0
			40	40		
23	C1	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D1	1	Total C 40 40	0	0
23	H1	1	Total C 22 22	0	0
23	J1	1	Total C 40 40	0	0
23	K1	1	Total C 31 31	0	0
23	a1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	c1	1	Total C 40 40	0	0
23	c1	1	Total C 40 40	0	0
23	d1	1	Total C 40 40	0	0
23	h1	1	Total C 40 40	0	0
23	k1	1	Total C 40 40	0	0
23	A2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	C2	1	Total C 40 40	0	0
23	F2	1	Total C 40 40	0	0
23	H2	1	Total C 24 24	0	0
23	K2	1	Total C 40 40	0	0

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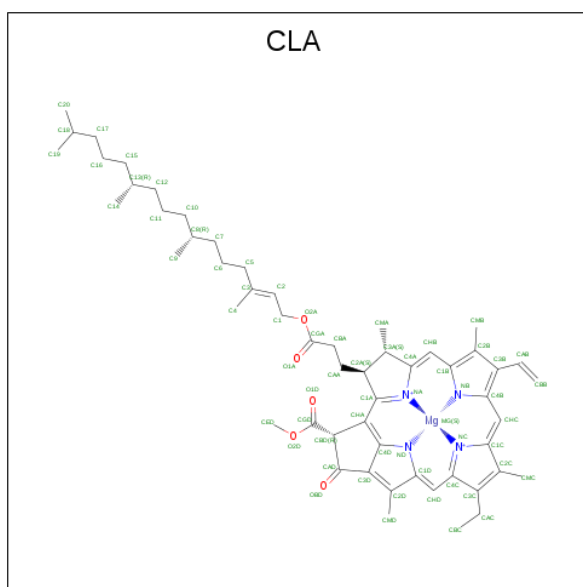
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	K2	1	Total C 29 29	0	0
23	a2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	c2	1	Total C 40 40	0	0
23	d2	1	Total C 40 40	0	0
23	h2	1	Total C 40 40	0	0
23	j2	1	Total C 40 40	0	0
23	k2	1	Total C 40 40	0	0
23	z2	1	Total C 40 40	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	a1	1	Total Cl 1 1	0	0
24	A2	1	Total Cl 1 1	0	0
24	A1	1	Total Cl 1 1	0	0
24	a2	1	Total Cl 1 1	0	0

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
25	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	C1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
25	D1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	a1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	a1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	A2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
25	B2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
25	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N	O		
25	B2	1	65	55	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	B2	1	54	44	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	B2	1	60	50	1	4	5	0	0
25	B2	1	65	55	1	4	5	0	0
25	C2	1	65	55	1	4	5	0	0
25	C2	1	46	36	1	4	5	0	0
25	C2	1	65	55	1	4	5	0	0
25	C2	1	65	55	1	4	5	0	0
25	C2	1	45	35	1	4	5	0	0
25	C2	1	50	40	1	4	5	0	0
25	C2	1	65	55	1	4	5	0	0
25	C2	1	45	35	1	4	5	0	0
25	C2	1	50	40	1	4	5	0	0

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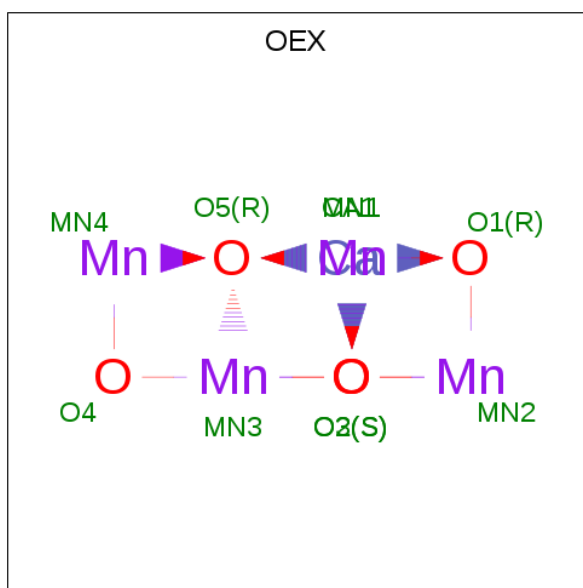
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
25	C2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
25	C2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
25	D2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	D2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	K2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
25	a2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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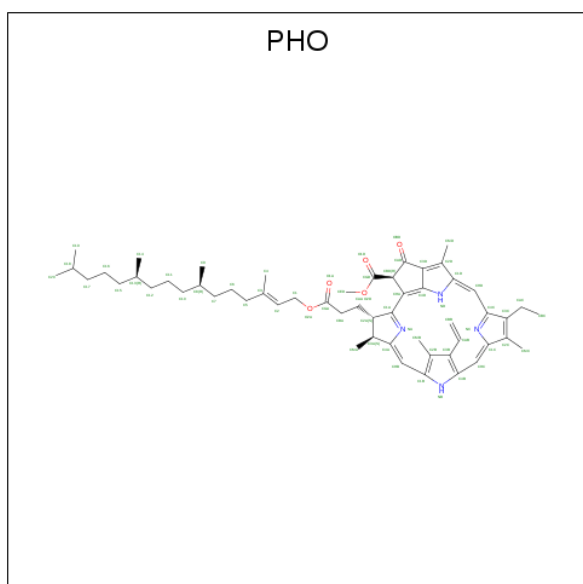
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	b2	1	65	55	1	4	5	0	0
25	b2	1	65	55	1	4	5	0	0
25	b2	1	59	49	1	4	5	0	0
25	b2	1	65	55	1	4	5	0	0
25	b2	1	65	55	1	4	5	0	0
25	c2	1	65	55	1	4	5	0	0
25	c2	1	65	55	1	4	5	0	0
25	c2	1	65	55	1	4	5	0	0
25	c2	1	65	55	1	4	5	0	0
25	c2	1	61	51	1	4	5	0	0
25	c2	1	54	44	1	4	5	0	0
25	c2	1	65	55	1	4	5	0	0
25	c2	1	65	55	1	4	5	0	0
25	c2	1	54	44	1	4	5	0	0
25	c2	1	65	55	1	4	5	0	0
25	c2	1	65	55	1	4	5	0	0
25	c2	1	54	44	1	4	5	0	0
25	c2	1	46	36	1	4	5	0	0
25	d2	1	65	55	1	4	5	0	0
25	d2	1	50	40	1	4	5	0	0
25	d2	1	65	55	1	4	5	0	0

- Molecule 26 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
26	A1	1	10	1	4	5	0	0
26	a1	1	10	1	4	5	0	0
26	A2	1	10	1	4	5	0	0
26	a2	1	10	1	4	5	0	0

- Molecule 27 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A1	1	Total	C	N	O	0	0
			64	55	4	5		
27	D1	1	Total	C	N	O	0	0
			63	54	4	5		
27	a1	1	Total	C	N	O	0	0
			64	55	4	5		
27	d1	1	Total	C	N	O	0	0
			64	55	4	5		
27	A2	1	Total	C	N	O	0	0
			64	55	4	5		
27	D2	1	Total	C	N	O	0	0
			64	55	4	5		
27	a2	1	Total	C	N	O	0	0
			64	55	4	5		
27	d2	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 28 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

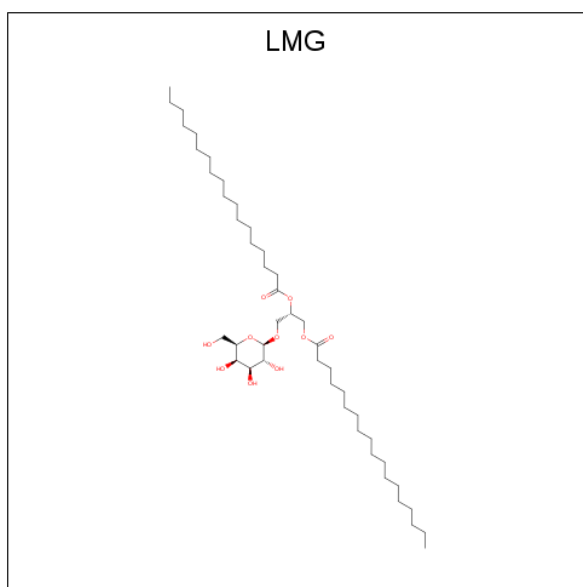
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	I2	2	Total	C	0	0
			31	31		
28	d1	1	Total	C	0	0
			12	12		
28	F2	1	Total	C	0	0
			16	16		
28	m2	2	Total	C	0	0
			36	36		
28	W2	1	Total	C	0	0
			9	9		
28	c2	1	Total	C	0	0
			15	15		
28	J2	1	Total	C	0	0
			10	10		
28	A2	2	Total	C	0	0
			28	28		
28	j1	1	Total	C	0	0
			17	17		
28	i2	1	Total	C	0	0
			14	14		
28	d2	2	Total	C	0	0
			25	25		
28	B2	4	Total	C	0	0
			58	58		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	b1	7	Total C 92 92	0	0
28	t1	2	Total C 27 27	0	0
28	m1	1	Total C 6 6	0	0
28	a2	4	Total C 55 55	0	0
28	K2	1	Total C 5 5	0	0
28	A1	1	Total C 14 14	0	0
28	l1	1	Total C 12 12	0	0
28	b2	1	Total C 12 12	0	0
28	x1	1	Total C 15 15	0	0
28	X2	1	Total C 7 7	0	0
28	k2	4	Total C 30 30	0	0
28	a1	1	Total C 11 11	0	0
28	D1	1	Total C 6 6	0	0
28	H2	1	Total C 5 5	0	0
28	M2	1	Total C 11 11	0	0
28	C2	2	Total C 24 24	0	0
28	B1	3	Total C 41 41	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	A1	1	43	33	10	0	0
29	A1	1	41	31	10	0	0
29	B1	1	31	21	10	0	0
29	B1	1	48	38	10	0	0
29	C1	1	48	38	10	0	0
29	D1	1	35	25	10	0	0
29	M1	1	31	27	4	0	0
29	a1	1	51	41	10	0	0
29	b1	1	38	28	10	0	0
29	b1	1	39	29	10	0	0
29	b1	1	40	30	10	0	0
29	c1	1	55	45	10	0	0
29	d1	1	33	23	10	0	0
29	d1	1	35	30	5	0	0

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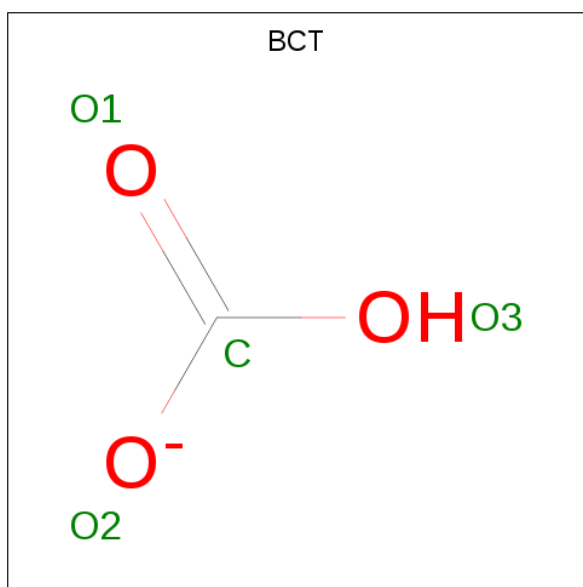
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A2	1	Total	C	O	0	0
			29	19	10		
29	B2	1	Total	C	O	0	0
			40	30	10		
29	B2	1	Total	C	O	0	0
			37	27	10		
29	C2	1	Total	C	O	0	0
			24	14	10		
29	F2	1	Total	C	O	0	0
			35	25	10		
29	I2	1	Total	C	O	0	0
			34	24	10		
29	a2	1	Total	C	O	0	0
			44	34	10		
29	b2	1	Total	C	O	0	0
			39	29	10		
29	c2	1	Total	C	O	0	0
			26	16	10		
29	d2	1	Total	C	O	0	0
			27	17	10		
29	j2	1	Total	C	O	0	0
			50	40	10		

- Molecule 30 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	a1	1	Total	Fe	0	0
			1	1		
30	A2	1	Total	Fe	0	0
			1	1		
30	A1	1	Total	Fe	0	0
			1	1		
30	a2	1	Total	Fe	0	0
			1	1		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



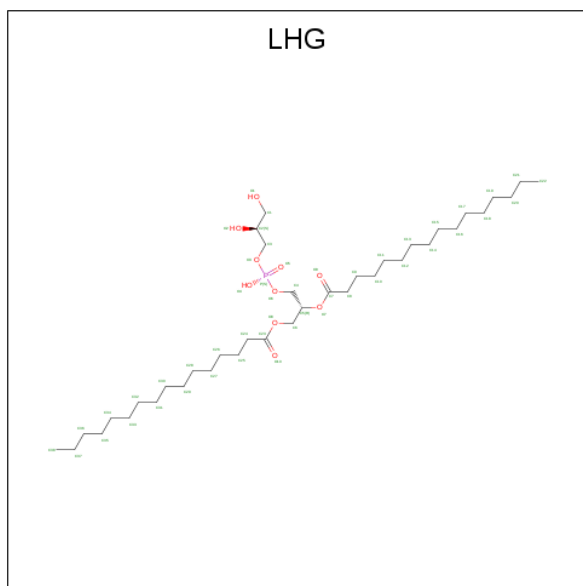
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A1	1	Total	C	O	0	0
			4	1	3		
31	a1	1	Total	C	O	0	0
			4	1	3		
31	A2	1	Total	C	O	0	0
			4	1	3		
31	a2	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B1	1	Total	C	O	0	0
			6	3	3		
32	C1	1	Total	C	O	0	0
			6	3	3		
32	a1	1	Total	C	O	0	0
			6	3	3		
32	b1	1	Total	C	O	0	0
			6	3	3		
32	c1	1	Total	C	O	0	0
			6	3	3		
32	i1	1	Total	C	O	0	0
			6	3	3		
32	C2	1	Total	C	O	0	0
			6	3	3		
32	a2	1	Total	C	O	0	0
			6	3	3		
32	c2	1	Total	C	O	0	0
			6	3	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



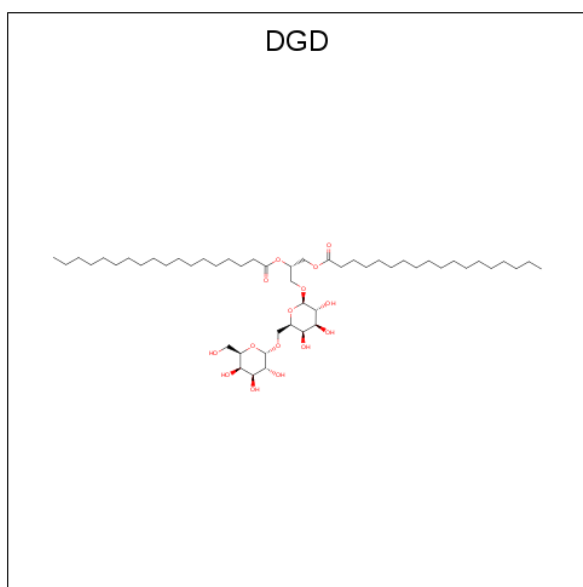
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B1	1	Total	C	O	P	0	0
			49	38	10	1		
33	D1	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
33	D1	1	49	38	10	1	0	0
33	L1	1	41	30	10	1	0	0
33	a1	1	43	32	10	1	0	0
33	b1	1	49	38	10	1	0	0
33	d1	1	32	21	10	1	0	0
33	d1	1	49	38	10	1	0	0
33	l1	1	49	38	10	1	0	0
33	A2	1	33	22	10	1	0	0
33	B2	1	42	31	10	1	0	0
33	D2	1	49	38	10	1	0	0
33	D2	1	49	38	10	1	0	0
33	L2	1	49	38	10	1	0	0
33	a2	1	30	19	10	1	0	0
33	b2	1	43	32	10	1	0	0
33	d2	1	49	38	10	1	0	0
33	d2	1	49	38	10	1	0	0
33	l2	1	44	33	10	1	0	0

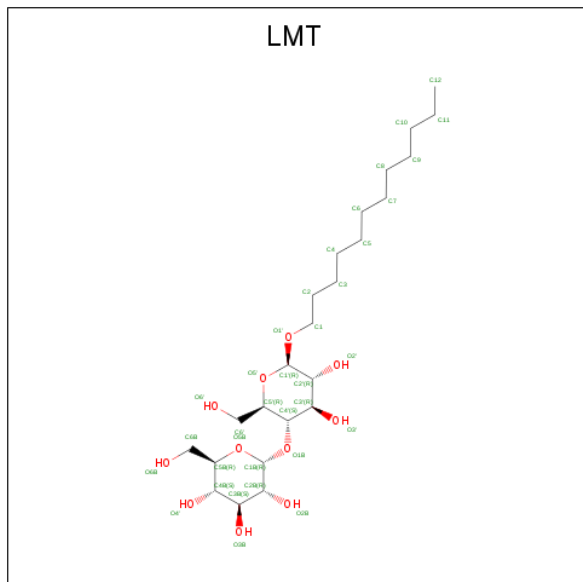
- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	C1	1	Total	C	O	0	0
			52	37	15		
34	C1	1	Total	C	O	0	0
			62	47	15		
34	C1	1	Total	C	O	0	0
			64	49	15		
34	H1	1	Total	C	O	0	0
			62	47	15		
34	c1	1	Total	C	O	0	0
			51	36	15		
34	c1	1	Total	C	O	0	0
			62	47	15		
34	c1	1	Total	C	O	0	0
			62	47	15		
34	h1	1	Total	C	O	0	0
			62	47	15		
34	C2	1	Total	C	O	0	0
			33	18	15		
34	H2	1	Total	C	O	0	0
			62	47	15		
34	c2	1	Total	C	O	0	0
			62	47	15		
34	c2	1	Total	C	O	0	0
			52	37	15		
34	c2	1	Total	C	O	0	0
			62	47	15		
34	h2	1	Total	C	O	0	0
			62	47	15		



- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



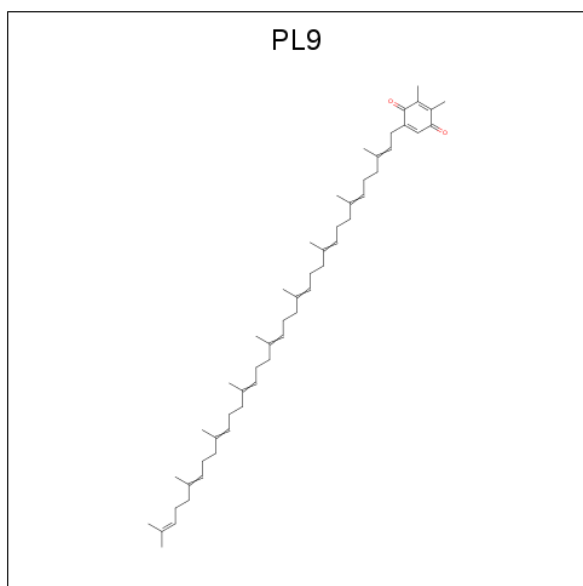
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C1	1	Total C O 35 24 11	0	0
35	L1	1	Total C 12 12	0	0
35	M1	1	Total C 11 11	0	0
35	M1	1	Total C O 24 18 6	0	0
35	T1	1	Total C 12 12	0	0
35	c1	1	Total C O 33 22 11	0	0
35	l1	1	Total C O 24 18 6	0	0
35	m1	1	Total C O 35 24 11	0	0
35	a2	1	Total C O 35 24 11	0	0
35	b2	1	Total C O 35 24 11	0	0
35	b2	1	Total C O 35 24 11	0	0
35	i2	1	Total C 7 7	0	0

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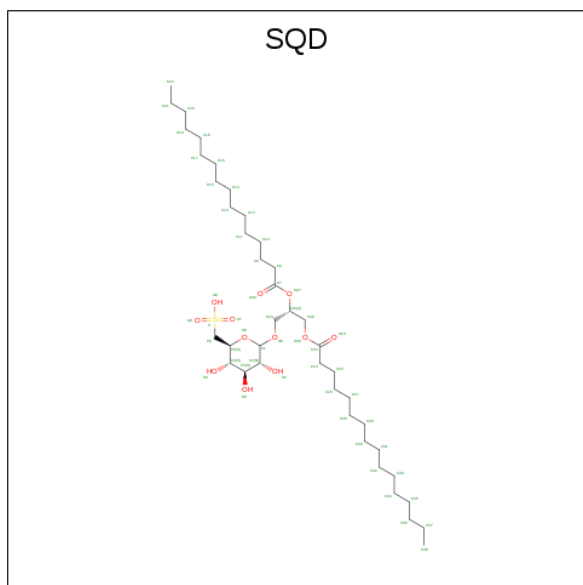
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	m2	1	Total	C	O	0	0
			30	19	11		
35	m2	1	Total	C	O	0	0
			29	18	11		

- Molecule 36 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:  $C_{53}H_{80}O_2$ ).



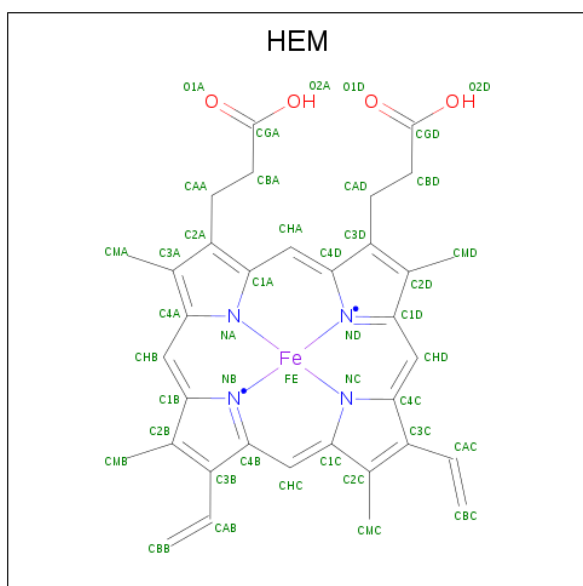
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	D1	1	Total	C	O	0	0
			55	53	2		
36	d1	1	Total	C	O	0	0
			55	53	2		
36	D2	1	Total	C	O	0	0
			55	53	2		
36	d2	1	Total	C	O	0	0
			55	53	2		

- Molecule 37 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	
			Total	C	O			S
37	D1	1	35	22	12	1	0	0
37	B2	1	45	32	12	1	0	0
37	D2	1	25	12	12	1	0	0
37	b2	1	45	32	12	1	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	E1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	V1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	f1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	v1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	E2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	V2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	v2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O1	1	Total	Ca	0	0
			1	1		
39	o2	1	Total	Ca	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A1	2	Total	O	0	0
			2	2		
40	B1	1	Total	O	0	0
			1	1		
40	a1	4	Total	O	0	0
			4	4		
40	c1	2	Total	O	0	0
			2	2		
40	A2	2	Total	O	0	0
			2	2		
40	a2	4	Total	O	0	0
			4	4		
40	b2	1	Total	O	0	0
			1	1		
40	c2	1	Total	O	0	0
			1	1		

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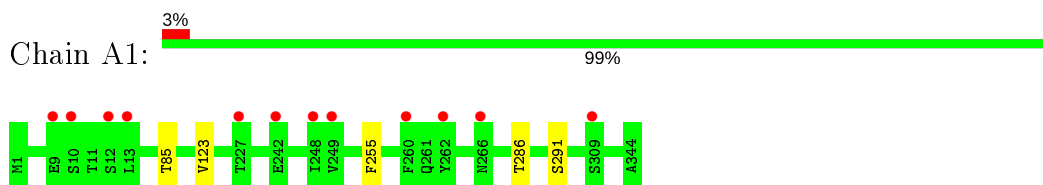
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
40	d2	1	Total	O	0	0
			1	1		

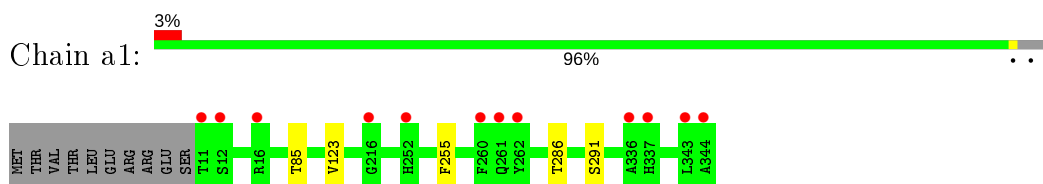
### 3 Residue-property plots [i](#)

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

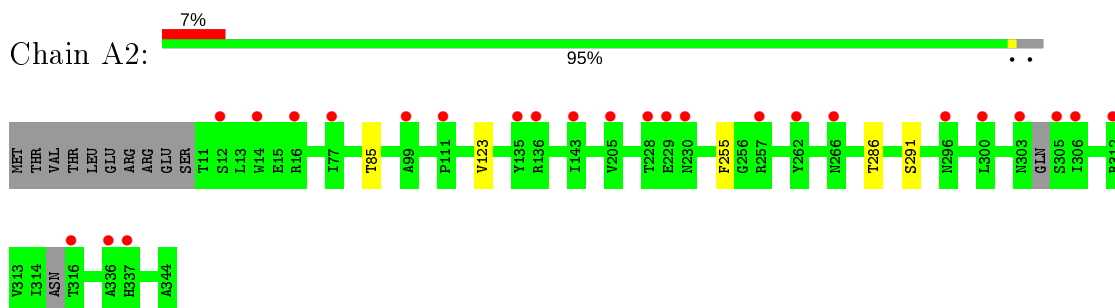
- Molecule 1: Photosystem II protein D1



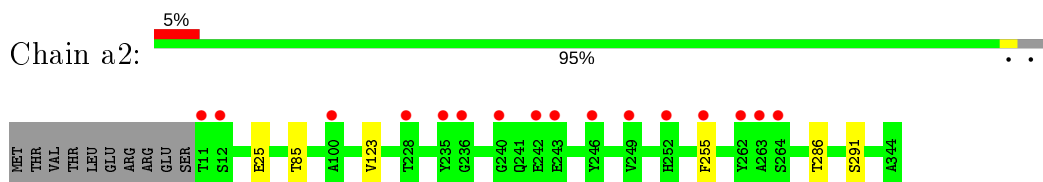
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

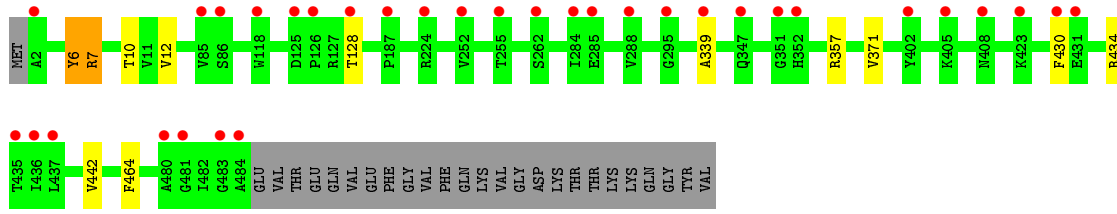


- Molecule 1: Photosystem II protein D1

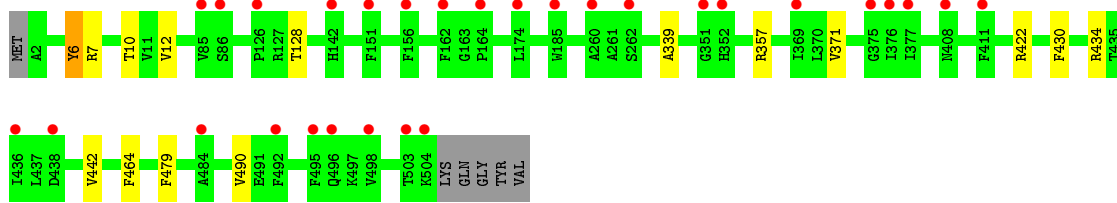


- Molecule 2: Photosystem II CP47 reaction center protein

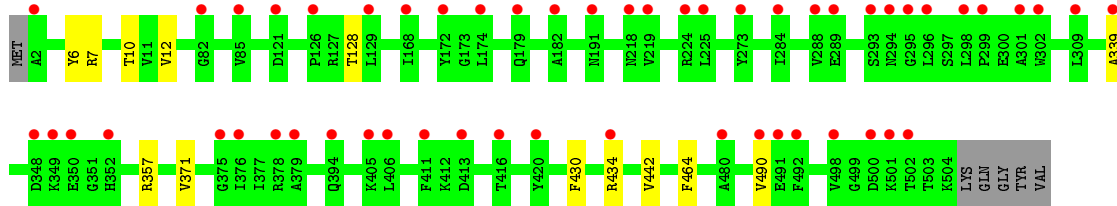




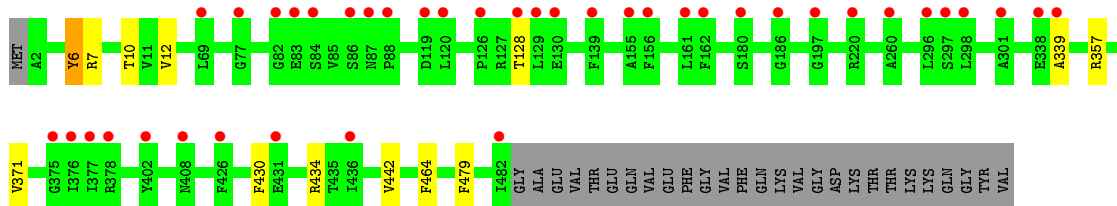
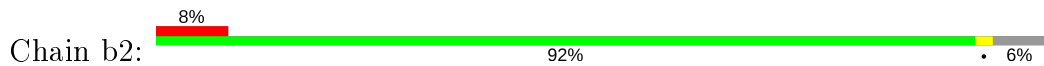
• Molecule 2: Photosystem II CP47 reaction center protein



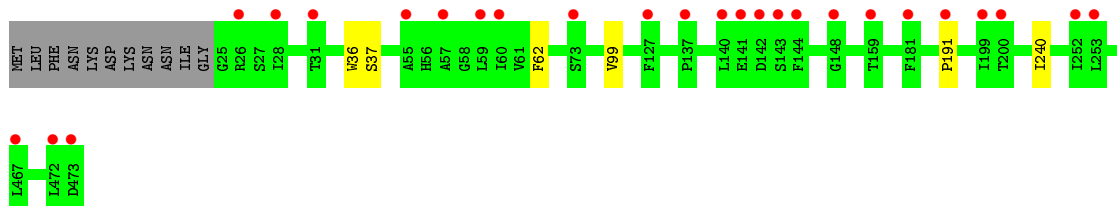
• Molecule 2: Photosystem II CP47 reaction center protein



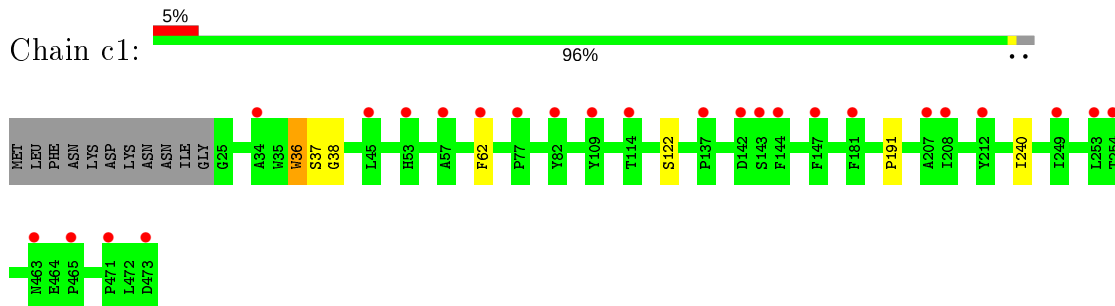
• Molecule 2: Photosystem II CP47 reaction center protein



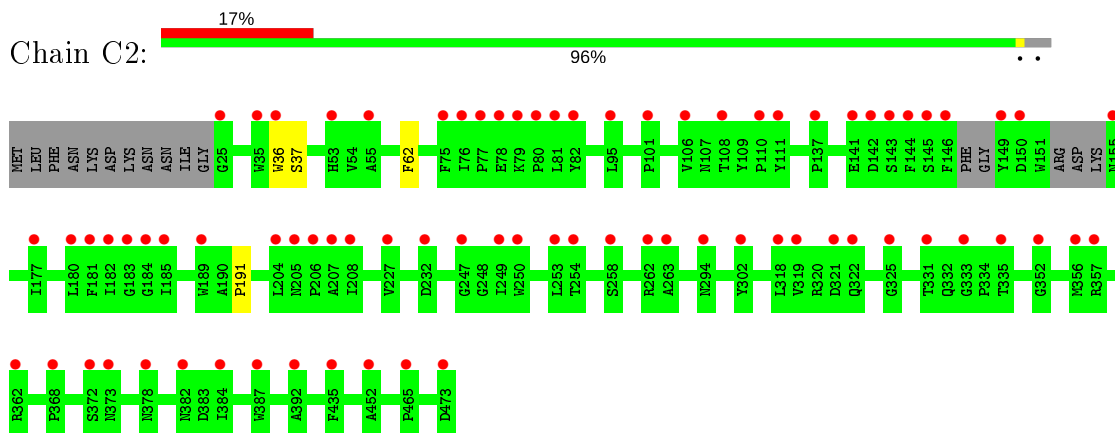
• Molecule 3: Photosystem II CP43 reaction center protein



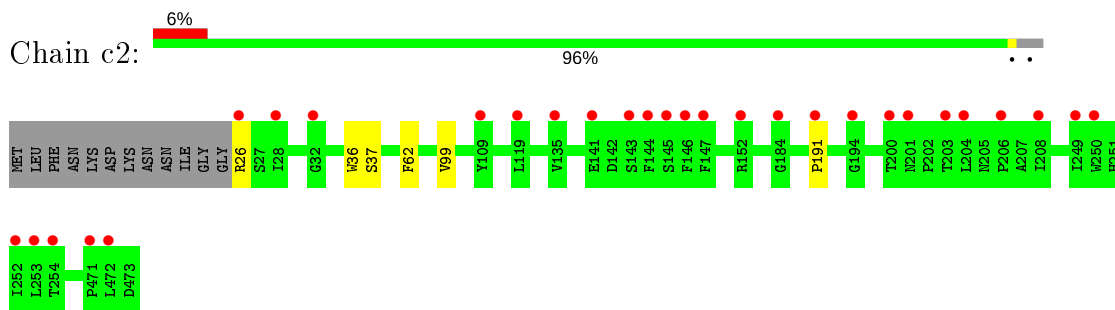
- Molecule 3: Photosystem II CP43 reaction center protein



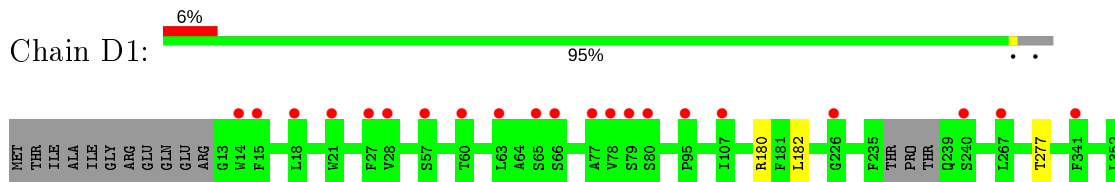
- Molecule 3: Photosystem II CP43 reaction center protein



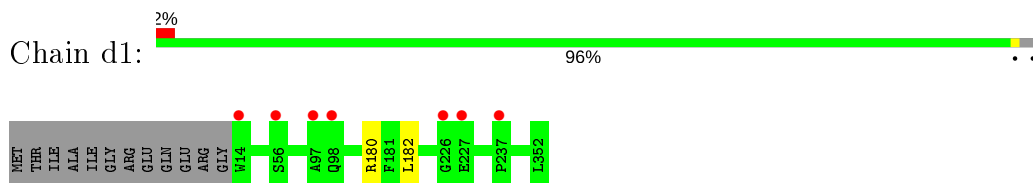
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein

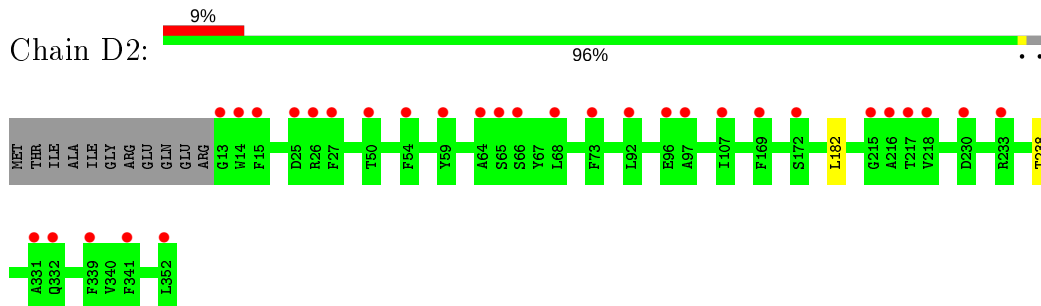


- Molecule 4: Photosystem II D2 protein

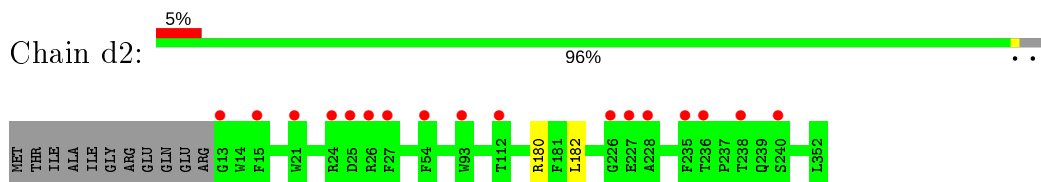




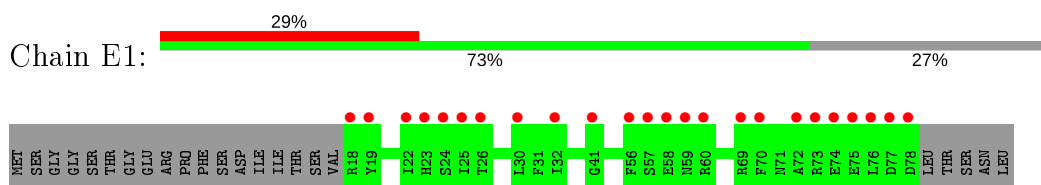
- Molecule 4: Photosystem II D2 protein



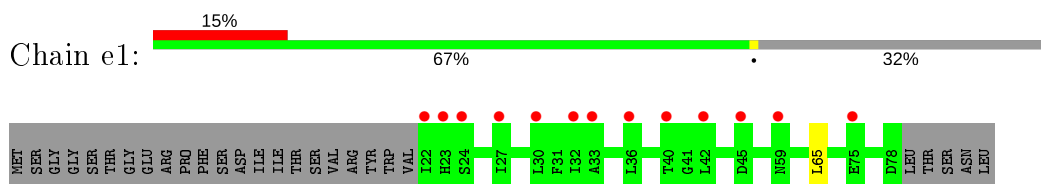
- Molecule 4: Photosystem II D2 protein



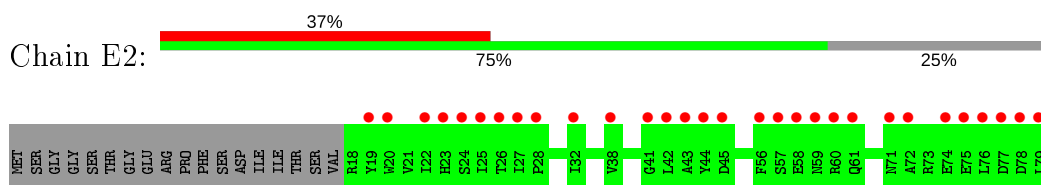
- Molecule 5: Cytochrome b559 subunit alpha



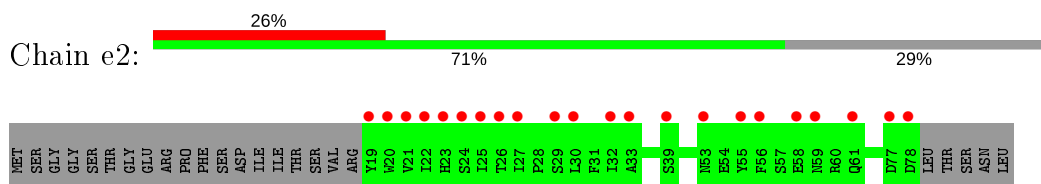
- Molecule 5: Cytochrome b559 subunit alpha



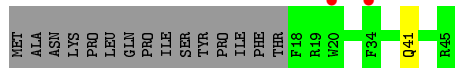
- Molecule 5: Cytochrome b559 subunit alpha



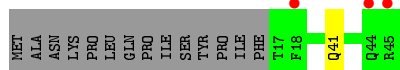
- Molecule 5: Cytochrome b559 subunit alpha



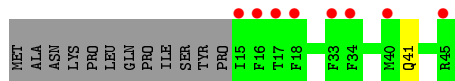
- Molecule 6: Cytochrome b559 subunit beta



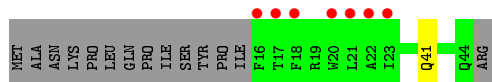
• Molecule 6: Cytochrome b559 subunit beta



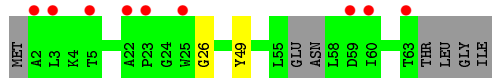
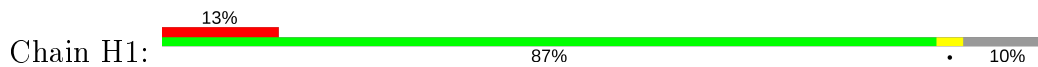
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta



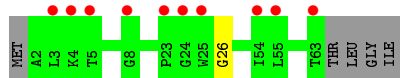
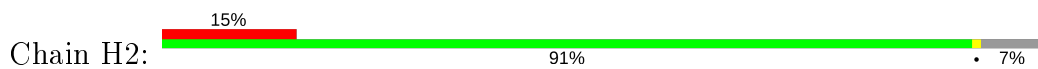
• Molecule 7: Photosystem II reaction center protein H



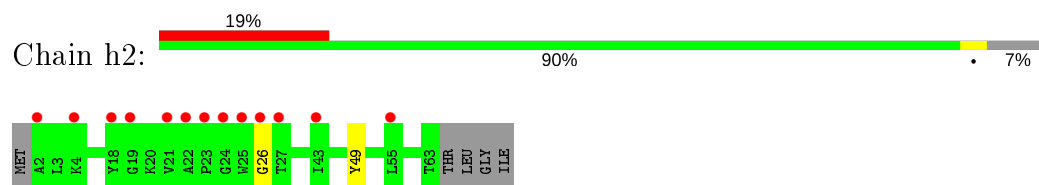
• Molecule 7: Photosystem II reaction center protein H



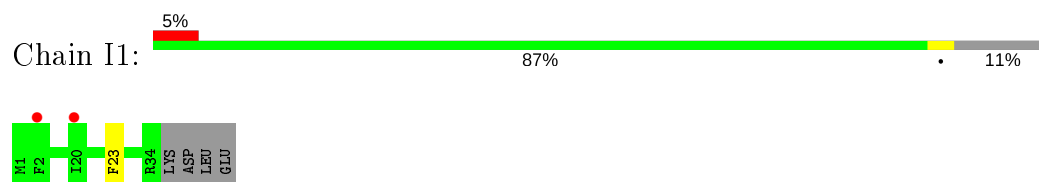
• Molecule 7: Photosystem II reaction center protein H



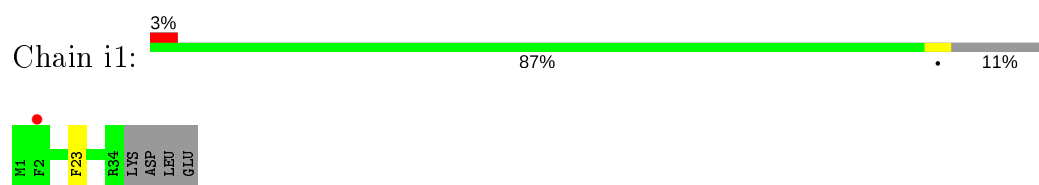
- Molecule 7: Photosystem II reaction center protein H



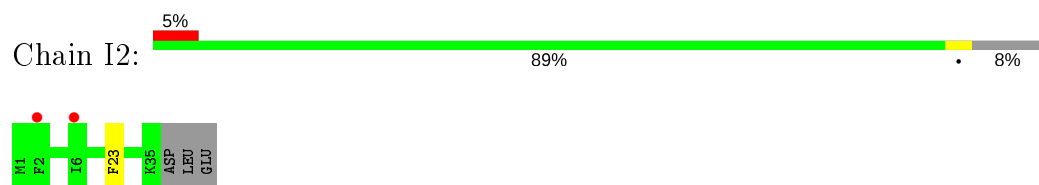
- Molecule 8: Photosystem II reaction center protein I



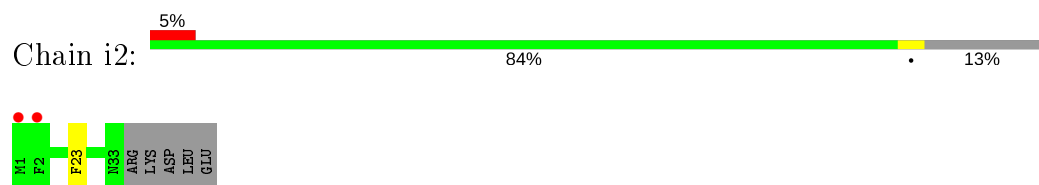
- Molecule 8: Photosystem II reaction center protein I



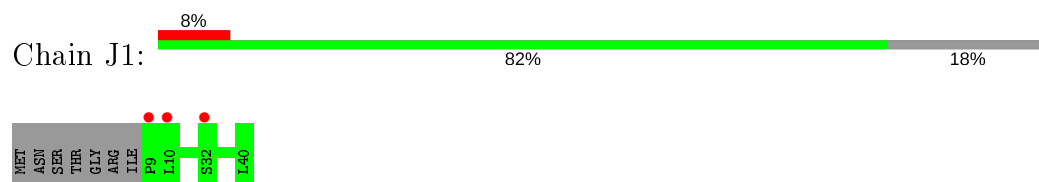
- Molecule 8: Photosystem II reaction center protein I



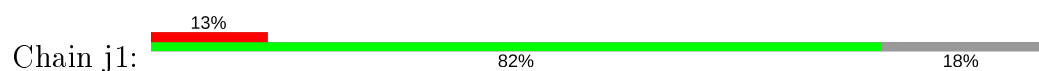
- Molecule 8: Photosystem II reaction center protein I

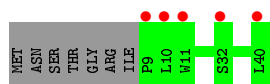


- Molecule 9: Photosystem II reaction center protein J

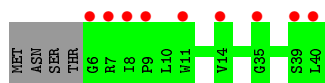
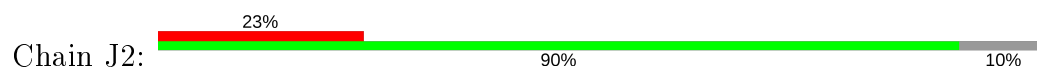


- Molecule 9: Photosystem II reaction center protein J

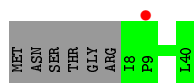
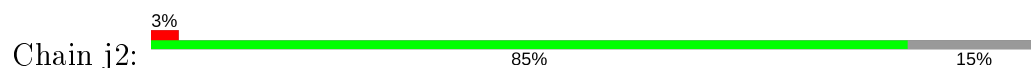




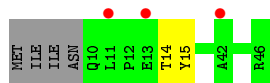
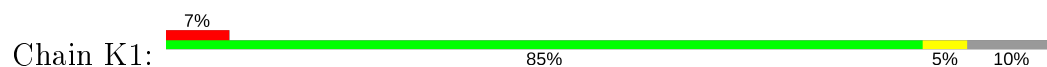
- Molecule 9: Photosystem II reaction center protein J



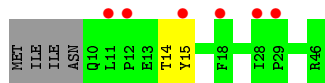
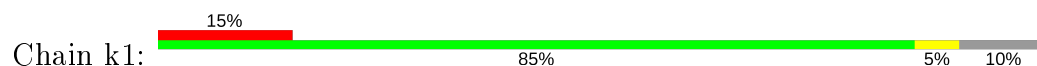
- Molecule 9: Photosystem II reaction center protein J



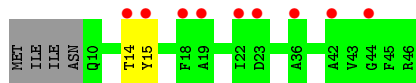
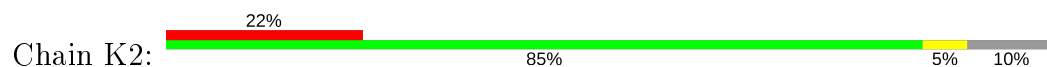
- Molecule 10: Photosystem II reaction center protein K



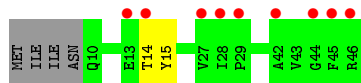
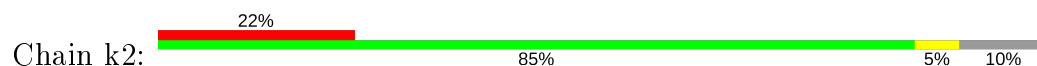
- Molecule 10: Photosystem II reaction center protein K



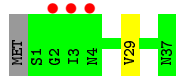
- Molecule 10: Photosystem II reaction center protein K



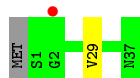
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



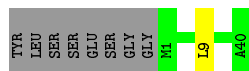
• Molecule 11: Photosystem II reaction center protein L



• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

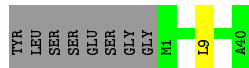
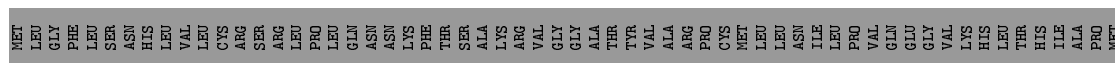


• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M



• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

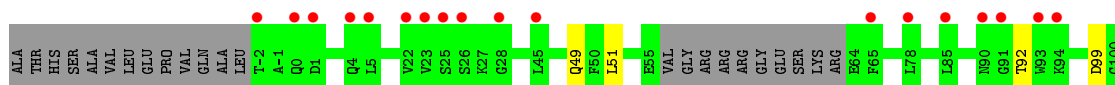




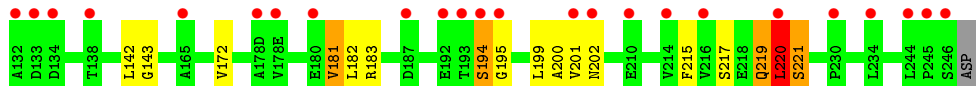
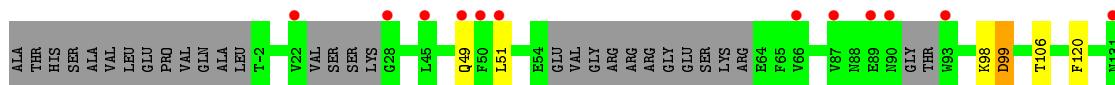
● Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M



● Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO

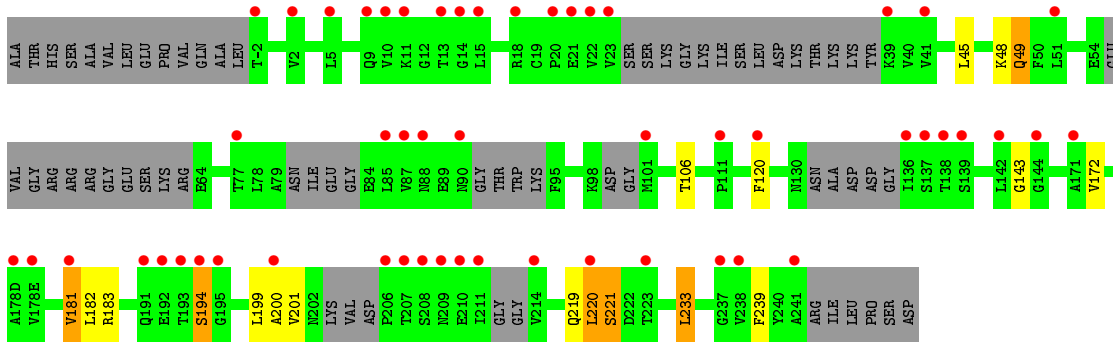


● Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO

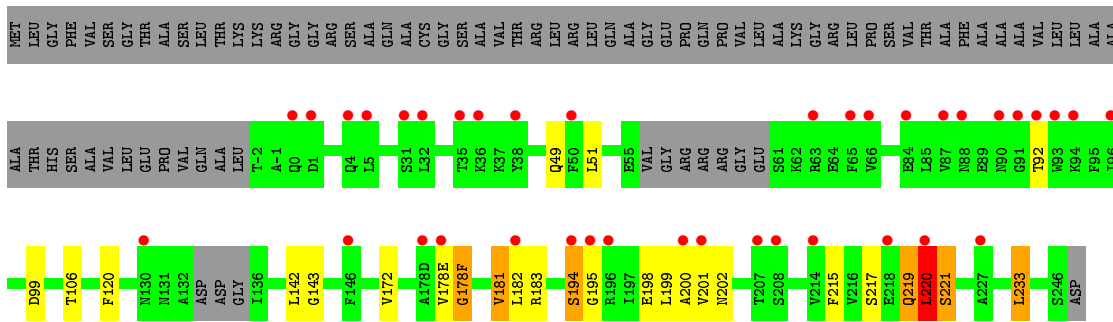


● Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO





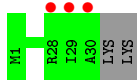
• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO



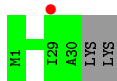
• Molecule 14: Photosystem II reaction center protein T



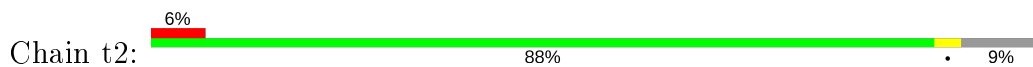
• Molecule 14: Photosystem II reaction center protein T

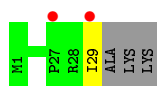


• Molecule 14: Photosystem II reaction center protein T

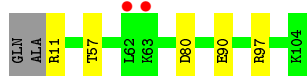


• Molecule 14: Photosystem II reaction center protein T

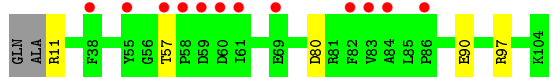




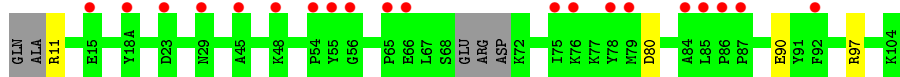
• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



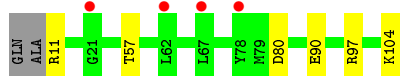
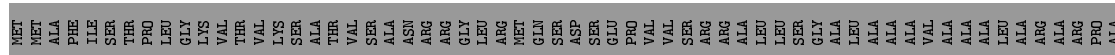
• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



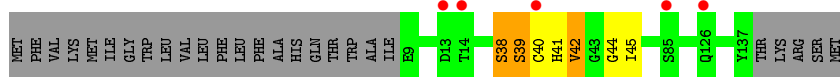
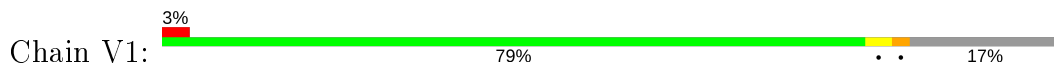
• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

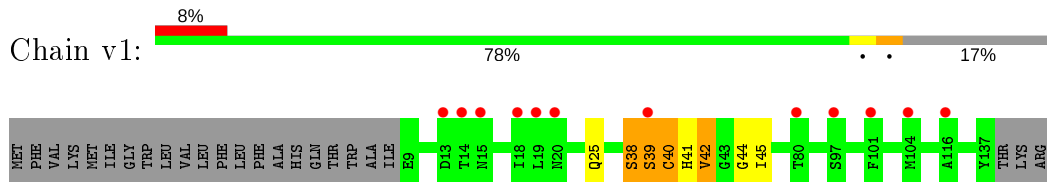


• Molecule 16: Cytochrome c-550

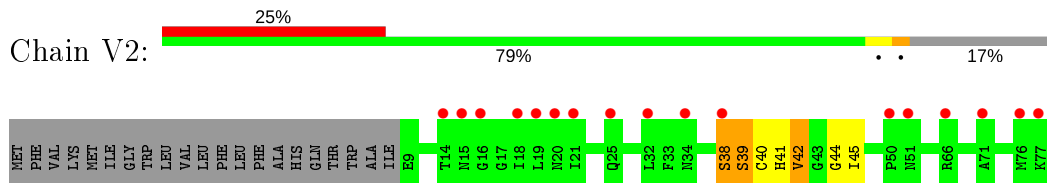




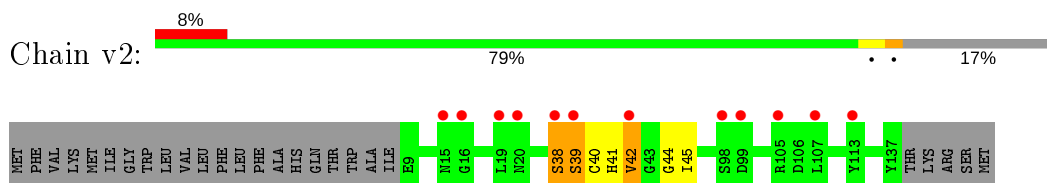
- Molecule 16: Cytochrome c-550



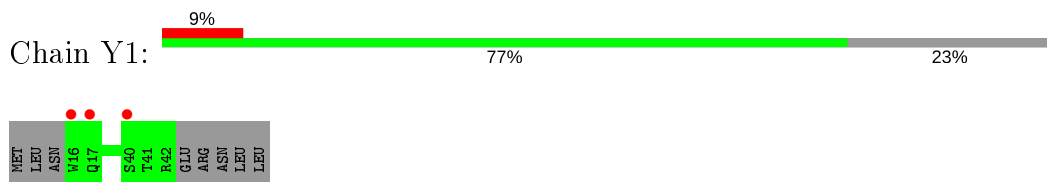
- Molecule 16: Cytochrome c-550



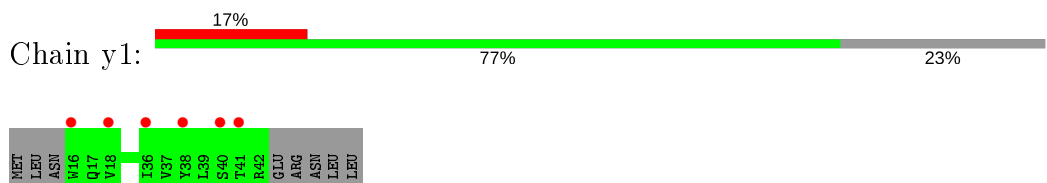
- Molecule 16: Cytochrome c-550



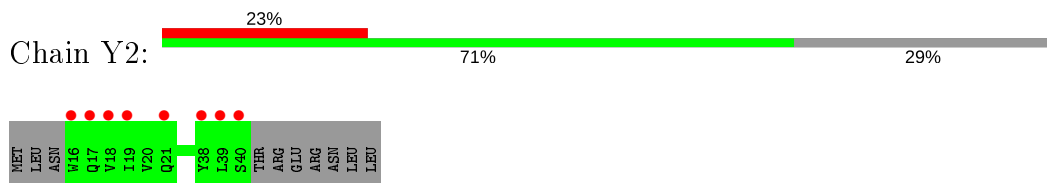
- Molecule 17: Photosystem II reaction center protein Ycf12



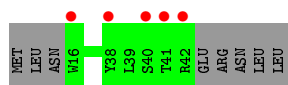
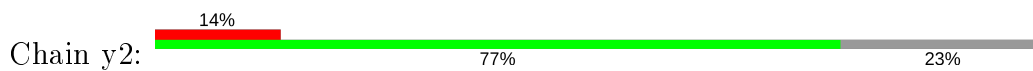
- Molecule 17: Photosystem II reaction center protein Ycf12



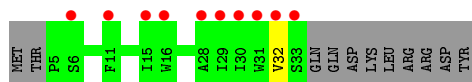
- Molecule 17: Photosystem II reaction center protein Ycf12



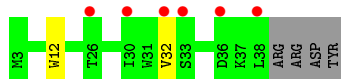
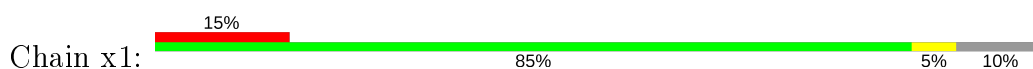
- Molecule 17: Photosystem II reaction center protein Ycf12



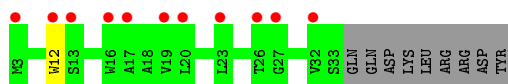
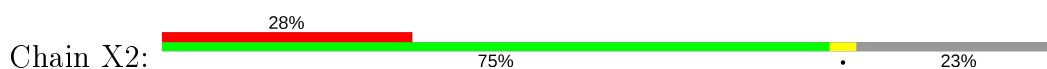
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



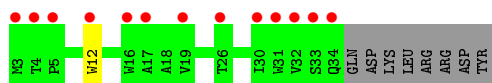
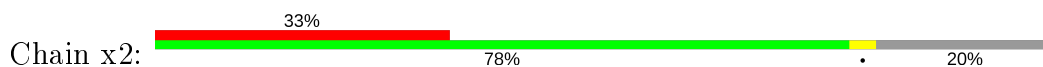
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



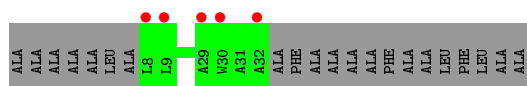
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



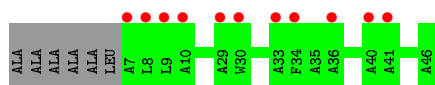
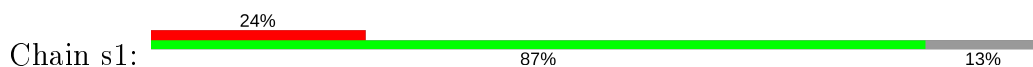
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



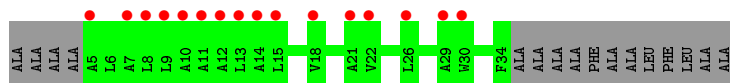
• Molecule 19: PEPTIDE CHAIN UNASSIGNED



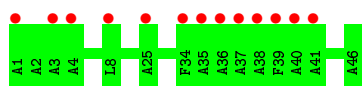
• Molecule 19: PEPTIDE CHAIN UNASSIGNED



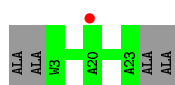
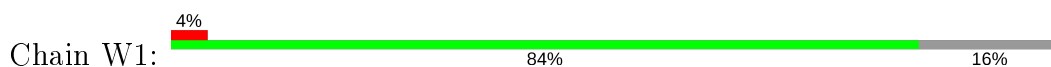
• Molecule 19: PEPTIDE CHAIN UNASSIGNED



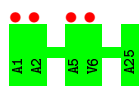
• Molecule 19: PEPTIDE CHAIN UNASSIGNED



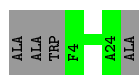
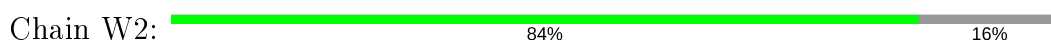
• Molecule 20: PEPTIDE CHAIN UNASSIGNED



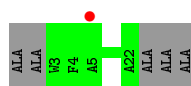
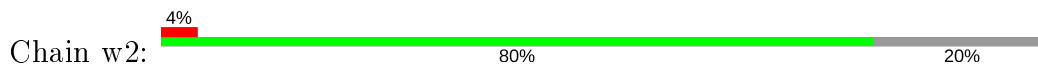
• Molecule 20: PEPTIDE CHAIN UNASSIGNED



• Molecule 20: PEPTIDE CHAIN UNASSIGNED

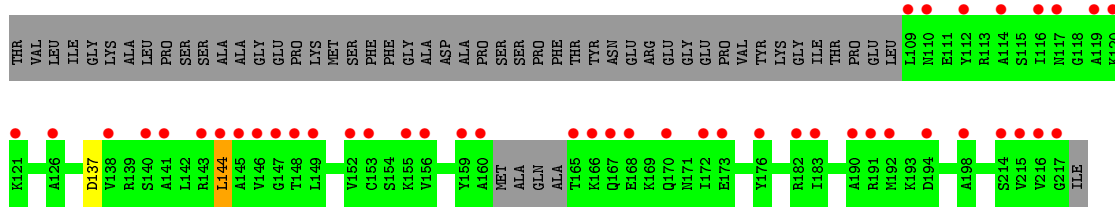


• Molecule 20: PEPTIDE CHAIN UNASSIGNED

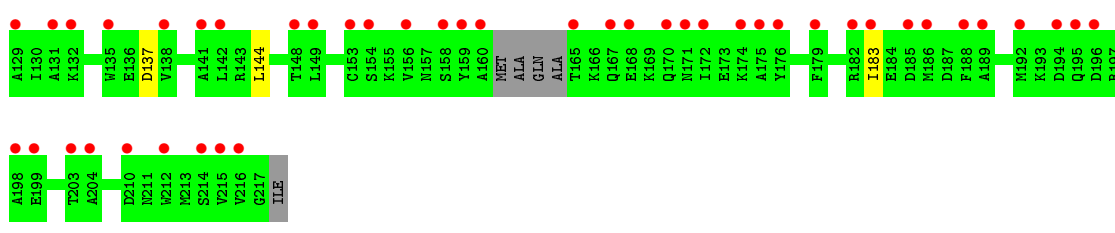
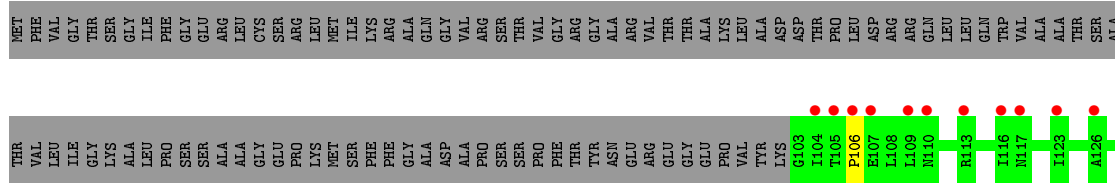


• Molecule 21: Extrinsic protein in photosystem II

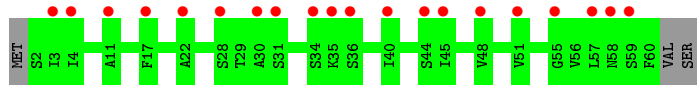




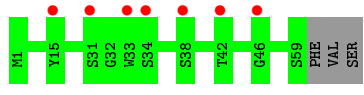
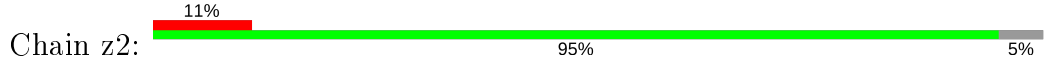
• Molecule 21: Extrinsic protein in photosystem II



• Molecule 22: Photosystem II reaction center protein Z



• Molecule 22: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.44Å 240.31Å 300.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.77 29.78 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.7 (10.00-2.77) 99.5 (29.78-2.77)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.76Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.249 , 0.278 0.254 , 0.281	Depositor DCC
$R_{free}$ test set	19164 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.0	Xtrriage
Anisotropy	0.616	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 69.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	92765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	A1	0.28	0/2685	0.43	0/3673
1	A2	0.29	0/2548	0.43	0/3481
1	a1	0.28	0/2642	0.42	0/3612
1	a2	0.28	0/2586	0.43	0/3538
2	B1	0.33	0/3830	0.48	3/5227 (0.1%)
2	B2	0.33	0/3897	0.48	2/5323 (0.0%)
2	b1	0.36	1/4015 (0.0%)	0.49	2/5473 (0.0%)
2	b2	0.33	0/3808	0.48	2/5197 (0.0%)
3	C1	0.28	0/3501	0.43	0/4782
3	C2	0.27	0/3242	0.42	0/4441
3	c1	0.30	0/3555	0.43	0/4850
3	c2	0.27	0/3495	0.42	0/4773
4	D1	0.35	0/2704	0.46	0/3688
4	D2	0.34	0/2675	0.46	0/3655
4	d1	0.35	0/2772	0.46	0/3783
4	d2	0.35	0/2736	0.46	0/3734
5	E1	0.24	0/418	0.38	0/577
5	E2	0.25	0/443	0.39	0/614
5	e1	0.24	0/440	0.39	0/603
5	e2	0.24	0/434	0.37	0/598
6	F1	0.45	0/220	0.51	0/299
6	F2	0.43	0/236	0.51	0/320
6	f1	0.44	0/235	0.50	0/319
6	f2	0.45	0/234	0.49	0/318
7	H1	0.23	0/443	0.40	0/606
7	H2	0.23	0/453	0.38	0/619
7	h1	0.23	0/481	0.41	0/657
7	h2	0.23	0/461	0.38	0/631
8	I1	0.26	0/283	0.35	0/381
8	I2	0.26	0/273	0.35	0/371
8	i1	0.26	0/289	0.36	0/389

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	i2	0.27	0/270	0.34	0/364
9	J1	0.23	0/225	0.35	0/307
9	J2	0.22	0/236	0.35	0/324
9	j1	0.23	0/229	0.34	0/313
9	j2	0.22	0/233	0.36	0/319
10	K1	0.38	0/289	0.53	0/399
10	K2	0.38	0/258	0.52	0/359
10	k1	0.37	0/290	0.53	0/401
10	k2	0.38	0/278	0.52	0/385
11	L1	0.49	0/301	0.58	0/410
11	L2	0.47	0/308	0.57	0/419
11	l1	0.49	0/308	0.58	0/418
11	l2	0.48	0/308	0.58	0/418
12	M1	0.39	0/288	0.59	0/391
12	M2	0.38	0/287	0.58	0/390
12	m1	0.38	0/288	0.59	0/391
12	m2	0.38	0/290	0.59	0/394
13	O1	0.66	2/1700 (0.1%)	0.91	15/2315 (0.6%)
13	O2	0.63	1/1387 (0.1%)	0.85	7/1881 (0.4%)
13	o1	0.63	2/1716 (0.1%)	0.90	13/2330 (0.6%)
13	o2	0.65	2/1794 (0.1%)	0.91	14/2434 (0.6%)
14	T1	0.26	0/248	0.39	0/337
14	T2	0.25	0/247	0.38	0/337
14	t1	0.25	0/253	0.39	0/344
14	t2	0.26	0/242	0.39	0/330
15	U1	0.46	0/709	0.68	2/970 (0.2%)
15	U2	0.45	0/588	1.15	3/809 (0.4%)
15	u1	0.46	0/721	0.67	2/981 (0.2%)
15	u2	0.44	0/726	0.66	2/988 (0.2%)
16	V1	0.48	0/937	0.67	4/1281 (0.3%)
16	V2	0.46	1/858 (0.1%)	0.62	1/1177 (0.1%)
16	v1	0.47	0/941	0.67	4/1284 (0.3%)
16	v2	0.46	0/983	0.66	4/1337 (0.3%)
17	Y1	0.43	0/171	0.52	0/236
17	Y2	0.44	0/159	0.53	0/219
17	y1	0.41	0/198	0.50	0/274
17	y2	0.42	0/191	0.50	0/264
18	X1	0.26	0/202	0.43	0/278
18	X2	0.25	0/222	0.43	0/307
18	x1	0.29	0/262	0.44	0/363
18	x2	0.34	0/225	0.46	0/312
19	S1	0.25	0/167	0.36	0/231
19	S2	0.25	0/194	0.36	0/268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	s1	0.26	0/269	0.33	0/371
19	s2	0.24	0/285	0.34	0/395
20	W1	0.20	0/134	0.37	0/186
20	W2	0.20	0/129	0.38	0/179
20	w1	0.20	0/152	0.36	0/211
20	w2	0.21	0/127	0.37	0/176
21	Q2	0.41	0/682	0.47	0/937
21	q1	0.40	0/650	0.50	1/893 (0.1%)
22	Z2	0.20	0/353	0.37	0/487
22	z2	0.22	0/387	0.38	0/532
All	All	0.37	9/79929 (0.0%)	0.53	81/109188 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	O1	0	2
13	O2	0	4
13	o1	0	3
13	o2	0	3
16	V1	0	3
16	V2	0	3
16	v1	0	3
16	v2	0	3
All	All	0	24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O1	221	SER	N-CA	6.20	1.58	1.46
13	o2	221	SER	N-CA	6.10	1.58	1.46
13	o1	221	SER	N-CA	6.00	1.58	1.46
13	O1	220	LEU	N-CA	5.81	1.57	1.46
13	o2	220	LEU	N-CA	5.81	1.57	1.46

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	U2	11	ARG	NE-CZ-NH1	-19.49	110.56	120.30
15	U2	11	ARG	NE-CZ-NH2	17.62	129.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o1	99	ASP	CB-CG-OD1	-10.04	109.26	118.30
15	U2	11	ARG	CD-NE-CZ	9.31	136.64	123.60
13	o1	195	GLY	CA-C-O	-8.28	105.69	120.60

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	O1	194	SER	Peptide
13	O1	220	LEU	Peptide
16	V1	38	SER	Peptide
16	V1	41	HIS	Peptide
16	V1	44	GLY	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	342/344 (99%)	328 (96%)	14 (4%)	0	100	100
1	A2	327/344 (95%)	318 (97%)	9 (3%)	0	100	100
1	a1	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
1	a2	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
2	B1	481/509 (94%)	456 (95%)	23 (5%)	2 (0%)	34	64
2	B2	501/509 (98%)	474 (95%)	26 (5%)	1 (0%)	47	76
2	b1	502/509 (99%)	474 (94%)	26 (5%)	2 (0%)	34	64
2	b2	479/509 (94%)	454 (95%)	23 (5%)	2 (0%)	34	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C1	447/460 (97%)	424 (95%)	20 (4%)	3 (1%)	22	50
3	C2	438/460 (95%)	416 (95%)	19 (4%)	3 (1%)	22	50
3	c1	449/460 (98%)	426 (95%)	19 (4%)	4 (1%)	17	44
3	c2	446/460 (97%)	424 (95%)	19 (4%)	3 (1%)	22	50
4	D1	333/351 (95%)	318 (96%)	15 (4%)	0	100	100
4	D2	338/351 (96%)	322 (95%)	16 (5%)	0	100	100
4	d1	337/351 (96%)	321 (95%)	16 (5%)	0	100	100
4	d2	338/351 (96%)	323 (96%)	15 (4%)	0	100	100
5	E1	59/84 (70%)	57 (97%)	2 (3%)	0	100	100
5	E2	61/84 (73%)	59 (97%)	2 (3%)	0	100	100
5	e1	55/84 (66%)	54 (98%)	1 (2%)	0	100	100
5	e2	58/84 (69%)	57 (98%)	1 (2%)	0	100	100
6	F1	26/43 (60%)	26 (100%)	0	0	100	100
6	F2	29/43 (67%)	29 (100%)	0	0	100	100
6	f1	27/43 (63%)	27 (100%)	0	0	100	100
6	f2	27/43 (63%)	26 (96%)	1 (4%)	0	100	100
7	H1	56/67 (84%)	53 (95%)	2 (4%)	1 (2%)	8	25
7	H2	60/67 (90%)	54 (90%)	5 (8%)	1 (2%)	9	27
7	h1	60/67 (90%)	57 (95%)	2 (3%)	1 (2%)	9	27
7	h2	60/67 (90%)	56 (93%)	3 (5%)	1 (2%)	9	27
8	I1	32/38 (84%)	32 (100%)	0	0	100	100
8	I2	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i1	32/38 (84%)	32 (100%)	0	0	100	100
8	i2	31/38 (82%)	31 (100%)	0	0	100	100
9	J1	30/39 (77%)	30 (100%)	0	0	100	100
9	J2	33/39 (85%)	33 (100%)	0	0	100	100
9	j1	30/39 (77%)	30 (100%)	0	0	100	100
9	j2	31/39 (80%)	31 (100%)	0	0	100	100
10	K1	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	4
10	K2	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	4
10	k1	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k2	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	4
11	L1	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	4	14
11	L2	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	4	14
11	l1	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	4	14
11	l2	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	4	14
12	M1	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
12	M2	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
12	m1	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
12	m2	38/108 (35%)	30 (79%)	8 (21%)	0	100	100
13	O1	234/329 (71%)	210 (90%)	14 (6%)	10 (4%)	2	7
13	O2	187/329 (57%)	165 (88%)	14 (8%)	8 (4%)	2	7
13	o1	230/329 (70%)	204 (89%)	16 (7%)	10 (4%)	2	7
13	o2	239/329 (73%)	212 (89%)	15 (6%)	12 (5%)	2	5
14	T1	28/32 (88%)	28 (100%)	0	0	100	100
14	T2	28/32 (88%)	28 (100%)	0	0	100	100
14	t1	28/32 (88%)	28 (100%)	0	0	100	100
14	t2	27/32 (84%)	27 (100%)	0	0	100	100
15	U1	91/155 (59%)	85 (93%)	6 (7%)	0	100	100
15	U2	86/155 (56%)	81 (94%)	5 (6%)	0	100	100
15	u1	91/155 (59%)	87 (96%)	4 (4%)	0	100	100
15	u2	91/155 (59%)	85 (93%)	6 (7%)	0	100	100
16	V1	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	3	9
16	V2	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	3	9
16	v1	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	3	9
16	v2	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	3	9
17	Y1	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
17	Y2	23/35 (66%)	22 (96%)	1 (4%)	0	100	100
17	y1	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
17	y2	25/35 (71%)	24 (96%)	1 (4%)	0	100	100
18	X1	27/40 (68%)	27 (100%)	0	0	100	100
18	X2	29/40 (72%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x1	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
18	x2	30/40 (75%)	30 (100%)	0	0	100	100
19	S1	23/46 (50%)	23 (100%)	0	0	100	100
19	S2	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
19	s1	38/46 (83%)	34 (90%)	4 (10%)	0	100	100
19	s2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
20	W1	19/25 (76%)	19 (100%)	0	0	100	100
20	W2	19/25 (76%)	19 (100%)	0	0	100	100
20	w1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
20	w2	18/25 (72%)	18 (100%)	0	0	100	100
21	Q2	107/218 (49%)	102 (95%)	3 (3%)	2 (2%)	8	23
21	q1	101/218 (46%)	97 (96%)	3 (3%)	1 (1%)	15	41
22	Z2	57/62 (92%)	55 (96%)	2 (4%)	0	100	100
22	z2	57/62 (92%)	55 (96%)	2 (4%)	0	100	100
All	All	10304/12316 (84%)	9726 (94%)	479 (5%)	99 (1%)	15	41

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C1	36	TRP
3	C1	37	SER
10	K1	14	THR
13	O1	49	GLN
13	O1	99	ASP

### 5.3.2 Protein sidechains [i](#)

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	A1	261/282 (93%)	256 (98%)	5 (2%)	57	83
1	A2	239/282 (85%)	234 (98%)	5 (2%)	53	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a1	261/282 (93%)	256 (98%)	5 (2%)	57	83
1	a2	249/282 (88%)	243 (98%)	6 (2%)	49	78
2	B1	360/415 (87%)	351 (98%)	9 (2%)	47	77
2	B2	351/415 (85%)	341 (97%)	10 (3%)	43	74
2	b1	380/415 (92%)	369 (97%)	11 (3%)	42	73
2	b2	352/415 (85%)	342 (97%)	10 (3%)	43	74
3	C1	320/364 (88%)	317 (99%)	3 (1%)	78	92
3	C2	261/364 (72%)	260 (100%)	1 (0%)	91	96
3	c1	338/364 (93%)	334 (99%)	4 (1%)	71	90
3	c2	323/364 (89%)	320 (99%)	3 (1%)	78	92
4	D1	255/283 (90%)	252 (99%)	3 (1%)	71	90
4	D2	238/283 (84%)	236 (99%)	2 (1%)	81	93
4	d1	267/283 (94%)	265 (99%)	2 (1%)	84	94
4	d2	258/283 (91%)	256 (99%)	2 (1%)	81	93
5	E1	28/75 (37%)	28 (100%)	0	100	100
5	E2	34/75 (45%)	34 (100%)	0	100	100
5	e1	38/75 (51%)	37 (97%)	1 (3%)	46	76
5	e2	33/75 (44%)	33 (100%)	0	100	100
6	F1	18/36 (50%)	17 (94%)	1 (6%)	21	48
6	F2	17/36 (47%)	16 (94%)	1 (6%)	19	46
6	f1	20/36 (56%)	19 (95%)	1 (5%)	24	53
6	f2	19/36 (53%)	18 (95%)	1 (5%)	22	51
7	H1	39/58 (67%)	38 (97%)	1 (3%)	46	76
7	H2	38/58 (66%)	38 (100%)	0	100	100
7	h1	47/58 (81%)	46 (98%)	1 (2%)	53	81
7	h2	42/58 (72%)	41 (98%)	1 (2%)	49	78
8	I1	30/36 (83%)	29 (97%)	1 (3%)	38	69
8	I2	26/36 (72%)	25 (96%)	1 (4%)	33	64
8	i1	32/36 (89%)	31 (97%)	1 (3%)	40	71
8	i2	28/36 (78%)	27 (96%)	1 (4%)	35	66
9	J1	20/32 (62%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J2	19/32 (59%)	19 (100%)	0	100	100
9	j1	22/32 (69%)	22 (100%)	0	100	100
9	j2	22/32 (69%)	22 (100%)	0	100	100
10	K1	26/36 (72%)	26 (100%)	0	100	100
10	K2	18/36 (50%)	18 (100%)	0	100	100
10	k1	27/36 (75%)	27 (100%)	0	100	100
10	k2	24/36 (67%)	24 (100%)	0	100	100
11	L1	31/35 (89%)	31 (100%)	0	100	100
11	L2	33/35 (94%)	33 (100%)	0	100	100
11	l1	33/35 (94%)	33 (100%)	0	100	100
11	l2	32/35 (91%)	32 (100%)	0	100	100
12	M1	26/88 (30%)	25 (96%)	1 (4%)	33	64
12	M2	26/88 (30%)	25 (96%)	1 (4%)	33	64
12	m1	26/88 (30%)	25 (96%)	1 (4%)	33	64
12	m2	27/88 (31%)	26 (96%)	1 (4%)	34	65
13	O1	148/266 (56%)	138 (93%)	10 (7%)	16	39
13	O2	110/266 (41%)	103 (94%)	7 (6%)	17	42
13	o1	156/266 (59%)	148 (95%)	8 (5%)	24	53
13	o2	168/266 (63%)	159 (95%)	9 (5%)	22	50
14	T1	24/28 (86%)	24 (100%)	0	100	100
14	T2	25/28 (89%)	25 (100%)	0	100	100
14	t1	26/28 (93%)	26 (100%)	0	100	100
14	t2	25/28 (89%)	24 (96%)	1 (4%)	31	62
15	U1	63/122 (52%)	59 (94%)	4 (6%)	18	43
15	U2	40/122 (33%)	37 (92%)	3 (8%)	13	34
15	u1	66/122 (54%)	62 (94%)	4 (6%)	18	45
15	u2	69/122 (57%)	64 (93%)	5 (7%)	14	36
16	V1	88/132 (67%)	87 (99%)	1 (1%)	73	90
16	V2	70/132 (53%)	69 (99%)	1 (1%)	67	87
16	v1	88/132 (67%)	85 (97%)	3 (3%)	37	68
16	v2	100/132 (76%)	99 (99%)	1 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y1	11/33 (33%)	11 (100%)	0	100	100
17	Y2	13/33 (39%)	13 (100%)	0	100	100
17	y1	18/33 (54%)	18 (100%)	0	100	100
17	y2	16/33 (48%)	16 (100%)	0	100	100
18	X1	17/34 (50%)	16 (94%)	1 (6%)	19	46
18	X2	16/34 (47%)	15 (94%)	1 (6%)	18	43
18	x1	23/34 (68%)	21 (91%)	2 (9%)	10	27
18	x2	17/34 (50%)	16 (94%)	1 (6%)	19	46
19	S1	10/20 (50%)	10 (100%)	0	100	100
19	S2	10/20 (50%)	10 (100%)	0	100	100
19	s1	15/20 (75%)	15 (100%)	0	100	100
19	s2	13/20 (65%)	13 (100%)	0	100	100
20	W1	12/13 (92%)	12 (100%)	0	100	100
20	W2	10/13 (77%)	10 (100%)	0	100	100
20	w1	11/13 (85%)	11 (100%)	0	100	100
20	w2	11/13 (85%)	11 (100%)	0	100	100
21	Q2	35/175 (20%)	33 (94%)	2 (6%)	20	48
21	q1	33/175 (19%)	32 (97%)	1 (3%)	41	72
22	Z2	22/54 (41%)	22 (100%)	0	100	100
22	z2	28/54 (52%)	28 (100%)	0	100	100
All	All	7221/10010 (72%)	7059 (98%)	162 (2%)	52	80

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o1	220	LEU
2	B2	6	TYR
13	o2	183	ARG
15	u1	57	THR
18	x1	12	TRP

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

Mol	Chain	Res	Type
2	b1	489	GLN
3	c1	418	ASN
13	o2	109	GLN
3	c1	56	HIS
13	o1	109	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 353 ligands modelled in this entry, 52 are unknown and 10 are monoatomic - leaving 291 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	$\# Z  > 2$
25	CLA	B1	613	-	59,73,73	1.47	6 (10%)	67,113,113	1.51	9 (13%)
25	CLA	D2	404	-	55,69,73	1.49	4 (7%)	62,108,113	1.52	10 (16%)
25	CLA	C1	506	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	9 (13%)
25	CLA	B1	608	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
29	LMG	b1	631	-	40,40,55	1.08	2 (5%)	48,48,63	1.23	5 (10%)
23	BCR	J1	101	-	41,41,41	0.75	0	56,56,56	2.10	16 (28%)
38	HEM	v2	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.35	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LMG	D1	406	-	35,35,55	1.11	2 (5%)	43,43,63	1.07	3 (6%)
25	CLA	b2	613	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	8 (11%)
25	CLA	b2	620	40	59,73,73	1.44	5 (8%)	67,113,113	1.51	9 (13%)
25	CLA	B1	606	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	9 (13%)
23	BCR	j2	102	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
33	LHG	b1	622	-	48,48,48	0.92	2 (4%)	51,54,54	1.04	5 (9%)
23	BCR	B2	603	-	41,41,41	0.69	0	56,56,56	1.84	12 (21%)
27	PHO	d1	403	-	67,69,69	2.13	16 (23%)	85,99,99	1.91	19 (22%)
25	CLA	C2	511	-	44,58,73	1.64	6 (13%)	49,95,113	1.78	9 (18%)
25	CLA	A1	403	-	59,73,73	1.50	8 (13%)	67,113,113	1.39	8 (11%)
25	CLA	a1	405	-	44,58,73	1.62	5 (11%)	49,95,113	1.73	10 (20%)
25	CLA	b2	611	-	59,73,73	1.42	5 (8%)	67,113,113	1.49	9 (13%)
31	BCT	A2	413	30	0,3,3	0.00	-	0,3,3	0.00	-
26	OEX	A1	407	1,3,40	0,15,15	0.00	-	-	-	-
29	LMG	F2	402	-	35,35,55	1.13	2 (5%)	43,43,63	1.03	3 (6%)
23	BCR	k1	101	-	41,41,41	0.71	0	56,56,56	2.03	15 (26%)
35	LMT	l1	101	-	24,24,36	0.47	0	29,29,47	0.83	2 (6%)
25	CLA	B2	609	-	59,73,73	1.42	6 (10%)	67,113,113	1.54	9 (13%)
25	CLA	c1	507	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	8 (11%)
32	GOL	a2	415	-	5,5,5	0.36	0	5,5,5	0.39	0
25	CLA	d2	402	-	59,73,73	1.43	5 (8%)	67,113,113	1.53	9 (13%)
35	LMT	M1	103	-	24,24,36	0.46	0	29,29,47	0.56	0
25	CLA	B2	619	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	9 (13%)
33	LHG	B1	621	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
29	LMG	B2	620	-	40,40,55	1.07	3 (7%)	48,48,63	1.05	4 (8%)
25	CLA	b2	604	-	36,50,73	1.80	5 (13%)	39,85,113	1.76	7 (17%)
27	PHO	D1	407	-	66,68,69	2.15	16 (24%)	83,97,99	1.96	21 (25%)
23	BCR	C1	501	-	41,41,41	0.70	0	56,56,56	1.80	14 (25%)
23	BCR	b2	603	-	41,41,41	0.70	0	56,56,56	1.91	13 (23%)
33	LHG	d1	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
34	DGD	C2	512	-	34,34,67	1.16	2 (5%)	46,47,81	1.06	2 (4%)
25	CLA	c2	506	-	55,69,73	1.50	5 (9%)	62,108,113	1.62	11 (17%)
26	OEX	A2	406	1,3,40	0,15,15	0.00	-	-	-	-
25	CLA	A2	403	-	55,69,73	1.51	5 (9%)	62,108,113	1.45	8 (12%)
25	CLA	K2	101	-	49,63,73	1.57	5 (10%)	55,101,113	1.56	9 (16%)
36	PL9	D1	408	-	55,55,55	0.64	2 (3%)	68,69,69	1.76	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	C2	516	-	40,54,73	1.70	5 (12%)	44,90,113	1.70	8 (18%)
35	LMT	M1	102	-	10,10,36	0.24	0	9,9,47	0.57	0
33	LHG	D2	403	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	3 (5%)
25	CLA	C2	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.46	8 (11%)
25	CLA	b1	605	-	59,73,73	1.44	5 (8%)	67,113,113	1.51	7 (10%)
27	PHO	a1	411	-	67,69,69	2.11	17 (25%)	85,99,99	1.88	20 (23%)
25	CLA	d1	406	-	59,73,73	1.44	5 (8%)	67,113,113	1.51	9 (13%)
37	SQD	D1	409	-	34,35,54	1.53	4 (11%)	43,46,65	1.41	6 (13%)
25	CLA	c1	504	-	59,73,73	1.40	5 (8%)	67,113,113	1.48	8 (11%)
25	CLA	B1	619	40	59,73,73	1.44	4 (6%)	67,113,113	1.51	9 (13%)
25	CLA	b2	610	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	9 (13%)
25	CLA	B1	610	-	59,73,73	1.44	5 (8%)	67,113,113	1.42	9 (13%)
23	BCR	d1	405	-	41,41,41	0.71	0	56,56,56	1.86	12 (21%)
25	CLA	C1	502	-	59,73,73	1.38	4 (6%)	67,113,113	1.51	8 (11%)
23	BCR	a2	402	-	41,41,41	0.67	0	56,56,56	1.64	12 (21%)
25	CLA	c1	506	40	59,73,73	1.43	5 (8%)	67,113,113	1.52	9 (13%)
25	CLA	c2	515	-	40,54,73	1.69	5 (12%)	44,90,113	1.72	7 (15%)
25	CLA	b1	617	-	59,73,73	1.45	5 (8%)	67,113,113	1.45	8 (11%)
23	BCR	b1	602	-	41,41,41	0.69	0	56,56,56	2.05	18 (32%)
23	BCR	C1	521	-	41,41,41	0.69	0	56,56,56	1.94	13 (23%)
35	LMT	b2	623	-	36,36,36	0.38	0	47,47,47	0.84	0
25	CLA	c1	503	-	59,73,73	1.37	5 (8%)	67,113,113	1.51	9 (13%)
25	CLA	c2	512	3	59,73,73	1.43	5 (8%)	67,113,113	1.41	9 (13%)
23	BCR	z2	101	-	41,41,41	0.70	0	56,56,56	1.76	10 (17%)
23	BCR	b2	601	-	41,41,41	0.70	0	56,56,56	1.97	16 (28%)
33	LHG	a2	407	-	29,29,48	1.09	2 (6%)	30,34,54	1.02	1 (3%)
37	SQD	D2	402	-	24,25,54	1.94	4 (16%)	31,35,65	1.66	6 (19%)
35	LMT	C1	519	-	36,36,36	0.35	0	47,47,47	0.70	1 (2%)
29	LMG	d1	411	-	34,34,55	1.10	2 (5%)	36,36,63	1.14	3 (8%)
25	CLA	c2	510	-	48,62,73	1.63	5 (10%)	53,99,113	1.53	8 (15%)
25	CLA	B2	616	-	48,62,73	1.61	5 (10%)	53,99,113	1.60	9 (16%)
29	LMG	b1	621	-	38,38,55	1.11	2 (5%)	46,46,63	1.07	2 (4%)
23	BCR	D1	401	-	41,41,41	0.72	0	56,56,56	1.98	13 (23%)
32	GOL	a1	406	-	5,5,5	0.35	0	5,5,5	0.28	0
33	LHG	L2	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.10	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	BCR	b1	601	-	41,41,41	0.69	0	56,56,56	1.83	14 (25%)
25	CLA	a2	404	-	59,73,73	1.46	7 (11%)	67,113,113	1.41	9 (13%)
23	BCR	h1	102	-	41,41,41	0.68	0	56,56,56	1.89	17 (30%)
29	LMG	a2	412	-	44,44,55	1.01	2 (4%)	52,52,63	1.11	5 (9%)
29	LMG	A1	410	-	43,43,55	1.03	2 (4%)	51,51,63	1.11	4 (7%)
25	CLA	c1	509	40	59,73,73	1.43	5 (8%)	67,113,113	1.46	8 (11%)
32	GOL	i1	101	-	5,5,5	0.42	0	5,5,5	0.20	0
25	CLA	b2	606	-	59,73,73	1.42	5 (8%)	67,113,113	1.49	8 (11%)
33	LHG	L1	101	-	40,40,48	1.01	2 (5%)	43,46,54	1.10	4 (9%)
25	CLA	C2	503	-	59,73,73	1.42	5 (8%)	67,113,113	1.51	7 (10%)
25	CLA	C1	509	-	59,73,73	1.43	5 (8%)	67,113,113	1.60	10 (14%)
25	CLA	b2	614	-	59,73,73	1.40	5 (8%)	67,113,113	1.47	9 (13%)
33	LHG	d1	402	-	31,31,48	1.16	2 (6%)	34,37,54	1.35	3 (8%)
25	CLA	b1	613	-	59,73,73	1.43	7 (11%)	67,113,113	1.51	10 (14%)
33	LHG	b2	625	-	42,42,48	1.00	2 (4%)	45,48,54	1.08	3 (6%)
33	LHG	A2	405	-	32,32,48	1.13	2 (6%)	35,38,54	1.07	2 (5%)
26	OEX	a1	408	1,3,40	0,15,15	0.00	-	-	-	-
25	CLA	b1	608	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	8 (11%)
25	CLA	d1	401	-	59,73,73	1.45	5 (8%)	67,113,113	1.48	10 (14%)
29	LMG	B1	626	-	48,48,55	0.98	2 (4%)	56,56,63	1.18	3 (5%)
23	BCR	B2	602	-	41,41,41	0.68	0	56,56,56	2.02	14 (25%)
25	CLA	c2	509	-	59,73,73	1.41	5 (8%)	67,113,113	1.59	10 (14%)
25	CLA	C2	513	-	47,61,73	1.64	5 (10%)	52,98,113	1.56	7 (13%)
25	CLA	b1	606	-	59,73,73	1.41	5 (8%)	67,113,113	1.47	9 (13%)
23	BCR	F2	401	-	41,41,41	0.72	0	56,56,56	2.18	18 (32%)
25	CLA	B2	610	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	8 (11%)
25	CLA	C1	504	-	59,73,73	1.45	4 (6%)	67,113,113	1.41	9 (13%)
25	CLA	D2	401	-	59,73,73	1.42	5 (8%)	67,113,113	1.50	9 (13%)
25	CLA	B2	611	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	9 (13%)
25	CLA	c2	507	-	48,62,73	1.59	5 (10%)	53,99,113	1.62	8 (15%)
27	PHO	A1	408	-	67,69,69	2.09	17 (25%)	85,99,99	1.92	20 (23%)
33	LHG	a1	407	-	42,42,48	1.01	2 (4%)	45,48,54	1.09	3 (6%)
25	CLA	C1	511	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	8 (11%)
38	HEM	v1	201	16	27,50,50	2.18	6 (22%)	17,82,82	1.44	3 (17%)
25	CLA	B1	607	-	54,68,73	1.52	5 (9%)	61,107,113	1.45	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	BCR	B1	602	-	41,41,41	0.69	0	56,56,56	1.95	12 (21%)
29	LMG	b2	622	-	39,39,55	1.07	2 (5%)	47,47,63	1.01	3 (6%)
25	CLA	b2	609	-	55,69,73	1.46	6 (10%)	62,108,113	1.54	8 (12%)
25	CLA	D2	406	-	59,73,73	1.45	5 (8%)	67,113,113	1.48	9 (13%)
25	CLA	C1	507	-	59,73,73	1.47	6 (10%)	67,113,113	1.43	10 (14%)
33	LHG	D1	405	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
34	DGD	C1	517	-	65,65,67	0.86	2 (3%)	79,79,81	0.85	3 (3%)
23	BCR	b2	602	-	41,41,41	0.70	0	56,56,56	2.13	17 (30%)
23	BCR	c2	501	-	41,41,41	0.80	1 (2%)	56,56,56	3.50	20 (35%)
25	CLA	b2	619	-	53,67,73	1.53	6 (11%)	59,105,113	1.52	7 (11%)
33	LHG	D1	404	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	4 (7%)
23	BCR	B1	603	-	41,41,41	0.69	0	56,56,56	1.72	11 (19%)
25	CLA	d2	404	-	44,58,73	1.66	5 (11%)	49,95,113	1.68	8 (16%)
36	PL9	D2	408	-	55,55,55	0.62	1 (1%)	68,69,69	1.73	19 (27%)
25	CLA	B2	612	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	10 (14%)
29	LMG	B1	622	-	31,31,55	1.20	2 (6%)	39,39,63	1.19	4 (10%)
23	BCR	B1	601	-	41,41,41	0.69	0	56,56,56	1.90	15 (26%)
25	CLA	B2	614	-	59,73,73	1.40	5 (8%)	67,113,113	1.48	10 (14%)
23	BCR	H1	102	-	22,22,41	0.69	0	29,29,56	1.71	6 (20%)
23	BCR	c1	501	-	41,41,41	0.70	0	56,56,56	2.10	13 (23%)
25	CLA	a1	404	-	54,68,73	1.55	6 (11%)	61,107,113	1.42	10 (16%)
25	CLA	B1	611	-	56,70,73	1.50	4 (7%)	63,109,113	1.49	11 (17%)
34	DGD	c1	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.00	5 (6%)
34	DGD	h2	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.91	2 (2%)
31	BCT	a1	413	30	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	C2	504	-	40,54,73	1.70	5 (12%)	44,90,113	1.68	7 (15%)
25	CLA	b2	624	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	8 (11%)
25	CLA	c2	503	-	59,73,73	1.44	5 (8%)	67,113,113	1.49	8 (11%)
25	CLA	b1	610	-	59,73,73	1.43	5 (8%)	67,113,113	1.49	11 (16%)
34	DGD	H2	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.91	3 (3%)
25	CLA	c2	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	8 (11%)
38	HEM	E2	101	5	27,50,50	2.17	6 (22%)	17,82,82	1.40	2 (11%)
25	CLA	c1	515	-	49,63,73	1.56	5 (10%)	55,101,113	1.62	8 (14%)
25	CLA	c2	504	-	59,73,73	1.43	5 (8%)	67,113,113	1.45	8 (11%)
34	DGD	C1	515	-	53,53,67	0.96	2 (3%)	67,67,81	1.01	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DGD	h1	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	4 (5%)
25	CLA	A1	406	-	59,73,73	1.48	5 (8%)	67,113,113	1.55	11 (16%)
25	CLA	B1	609	-	59,73,73	1.43	5 (8%)	67,113,113	1.74	12 (17%)
23	BCR	c1	502	-	41,41,41	0.75	0	56,56,56	2.09	14 (25%)
25	CLA	b2	616	-	54,68,73	1.53	5 (9%)	61,107,113	1.52	10 (16%)
35	LMT	m2	103	-	31,31,36	0.44	0	42,42,47	0.91	1 (2%)
25	CLA	b1	611	-	59,73,73	1.42	5 (8%)	67,113,113	1.41	9 (13%)
23	BCR	K2	102	-	41,41,41	0.72	0	56,56,56	2.07	16 (28%)
25	CLA	B1	615	-	59,73,73	1.40	5 (8%)	67,113,113	1.47	9 (13%)
25	CLA	c1	513	3	54,68,73	1.50	5 (9%)	61,107,113	1.51	7 (11%)
23	BCR	h2	101	-	41,41,41	0.68	0	56,56,56	1.79	14 (25%)
25	CLA	d2	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.42	9 (13%)
35	LMT	c1	517	-	34,34,36	0.43	0	45,45,47	0.68	1 (2%)
38	HEM	e2	101	5,6	27,50,50	2.18	5 (18%)	17,82,82	1.39	3 (17%)
25	CLA	b2	615	-	54,68,73	1.49	5 (9%)	61,107,113	1.54	10 (16%)
25	CLA	B1	618	-	52,66,73	1.53	6 (11%)	58,104,113	1.55	7 (12%)
25	CLA	c1	511	-	59,73,73	1.39	5 (8%)	67,113,113	1.50	9 (13%)
33	LHG	l2	101	-	43,43,48	1.00	2 (4%)	46,49,54	1.07	4 (8%)
27	PHO	D2	407	-	67,69,69	2.12	17 (25%)	85,99,99	2.01	21 (24%)
25	CLA	B1	605	-	59,73,73	1.44	5 (8%)	67,113,113	1.44	8 (11%)
32	GOL	c1	521	-	5,5,5	0.36	0	5,5,5	0.31	0
29	LMG	B2	621	-	37,37,55	0.95	3 (8%)	45,45,63	1.11	3 (6%)
23	BCR	H2	103	-	24,24,41	0.71	0	31,31,56	1.67	8 (25%)
23	BCR	K1	101	-	31,31,41	0.70	0	40,40,56	2.32	14 (35%)
25	CLA	c1	516	-	59,73,73	1.40	4 (6%)	67,113,113	1.45	9 (13%)
25	CLA	C2	518	-	35,49,73	1.81	5 (14%)	38,84,113	1.91	9 (23%)
34	DGD	c1	514	-	52,52,67	0.96	2 (3%)	66,66,81	1.04	4 (6%)
25	CLA	C2	508	-	44,58,73	1.64	5 (11%)	49,95,113	1.72	9 (18%)
32	GOL	c2	518	-	5,5,5	0.37	0	5,5,5	0.26	0
32	GOL	C2	514	-	5,5,5	0.36	0	5,5,5	0.31	0
33	LHG	l1	102	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
27	PHO	a2	416	-	67,69,69	2.11	16 (23%)	85,99,99	1.88	22 (25%)
37	SQD	B2	623	-	44,45,54	1.31	4 (9%)	53,56,65	1.22	6 (11%)
25	CLA	C1	514	-	36,53,73	1.79	4 (11%)	39,89,113	1.76	7 (17%)
25	CLA	B1	617	-	59,73,73	1.41	5 (8%)	67,113,113	1.47	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	b1	620	-	59,73,73	1.46	5 (8%)	67,113,113	1.48	9 (13%)
33	LHG	d2	406	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	4 (7%)
31	BCT	a2	417	30	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	b1	604	-	59,73,73	1.47	5 (8%)	67,113,113	1.39	8 (11%)
23	BCR	a1	401	-	41,41,41	0.69	0	56,56,56	1.73	14 (25%)
35	LMT	i2	102	-	6,6,36	0.28	0	5,5,47	0.44	0
25	CLA	C1	510	-	59,73,73	1.45	5 (8%)	67,113,113	1.40	7 (10%)
35	LMT	L1	102	-	11,11,36	0.25	0	10,10,47	0.57	0
23	BCR	C2	502	-	41,41,41	0.70	0	56,56,56	1.88	12 (21%)
25	CLA	B2	608	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	9 (13%)
29	LMG	c2	519	-	26,26,55	1.60	3 (11%)	32,33,63	1.30	2 (6%)
33	LHG	D2	405	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	4 (7%)
25	CLA	B1	614	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	9 (13%)
25	CLA	C2	509	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	9 (13%)
25	CLA	C2	506	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	10 (14%)
25	CLA	a1	403	-	59,73,73	1.51	7 (11%)	67,113,113	1.37	8 (11%)
29	LMG	d2	407	-	27,27,55	1.36	2 (7%)	35,35,63	1.29	3 (8%)
25	CLA	b1	616	-	59,73,73	1.43	6 (10%)	67,113,113	1.46	8 (11%)
35	LMT	m1	101	-	36,36,36	0.42	0	47,47,47	0.68	0
25	CLA	c2	508	40	59,73,73	1.44	5 (8%)	67,113,113	1.43	9 (13%)
29	LMG	c1	519	-	55,55,55	0.91	2 (3%)	63,63,63	0.95	2 (3%)
33	LHG	d2	403	-	48,48,48	0.94	2 (4%)	51,54,54	1.02	3 (5%)
25	CLA	a2	405	-	59,73,73	1.38	5 (8%)	67,113,113	1.46	10 (14%)
25	CLA	B2	613	-	59,73,73	1.44	5 (8%)	67,113,113	1.59	10 (14%)
27	PHO	A2	407	-	67,69,69	2.10	17 (25%)	85,99,99	1.93	21 (24%)
25	CLA	b2	608	-	59,73,73	1.47	5 (8%)	67,113,113	1.40	8 (11%)
25	CLA	b1	619	-	59,73,73	1.45	6 (10%)	67,113,113	1.46	8 (11%)
23	BCR	A1	401	-	41,41,41	0.68	0	56,56,56	1.74	11 (19%)
29	LMG	I2	101	-	34,34,55	1.15	2 (5%)	42,42,63	1.13	3 (7%)
23	BCR	k2	501	-	41,41,41	0.68	0	56,56,56	2.04	16 (28%)
29	LMG	d1	408	-	33,33,55	1.15	2 (6%)	41,41,63	1.10	3 (7%)
32	GOL	b1	618	-	5,5,5	0.35	0	5,5,5	0.39	0
23	BCR	K2	104	-	29,29,41	0.55	0	40,41,56	1.67	10 (25%)
25	CLA	B2	617	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	8 (11%)
35	LMT	T1	101	-	11,11,36	0.25	0	10,10,47	0.58	0
29	LMG	C1	520	-	48,48,55	0.97	2 (4%)	56,56,63	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	C1	503	-	54,68,73	1.47	5 (9%)	61,107,113	1.52	8 (13%)
25	CLA	A2	404	-	45,59,73	1.71	5 (11%)	50,96,113	1.58	9 (18%)
25	CLA	A1	404	-	45,59,73	1.64	5 (11%)	50,96,113	1.65	8 (16%)
25	CLA	c1	510	-	59,73,73	1.42	6 (10%)	67,113,113	1.56	11 (16%)
25	CLA	B2	618	-	54,68,73	1.53	6 (11%)	61,107,113	1.55	9 (14%)
25	CLA	D1	402	-	59,73,73	1.40	5 (8%)	67,113,113	1.48	8 (11%)
25	CLA	b1	612	-	59,73,73	1.43	5 (8%)	67,113,113	1.50	9 (13%)
31	BCT	A1	413	30	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	c2	513	-	48,62,73	1.57	5 (10%)	53,99,113	1.64	9 (16%)
25	CLA	c1	512	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	7 (10%)
25	CLA	C1	508	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	7 (10%)
34	DGD	c1	520	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	2 (2%)
38	HEM	E1	101	5,6	27,50,50	2.18	6 (22%)	17,82,82	1.40	2 (11%)
25	CLA	C2	510	-	36,53,73	1.76	5 (13%)	39,89,113	1.80	7 (17%)
29	LMG	C2	515	-	24,24,55	1.18	2 (8%)	32,32,63	1.05	2 (6%)
25	CLA	b1	607	-	59,73,73	1.50	5 (8%)	67,113,113	1.46	10 (14%)
38	HEM	V1	201	16	27,50,50	2.18	6 (22%)	17,82,82	1.42	3 (17%)
23	BCR	A2	401	-	41,41,41	0.69	0	56,56,56	2.02	16 (28%)
25	CLA	b2	612	-	59,73,73	1.48	7 (11%)	67,113,113	1.51	8 (11%)
25	CLA	b1	609	-	59,73,73	1.45	5 (8%)	67,113,113	1.45	9 (13%)
25	CLA	B1	604	-	36,50,73	1.82	5 (13%)	39,85,113	1.74	7 (17%)
29	LMG	b1	624	-	39,39,55	1.08	2 (5%)	47,47,63	1.31	5 (10%)
25	CLA	c2	505	-	59,73,73	1.40	5 (8%)	67,113,113	1.49	9 (13%)
25	CLA	B1	616	-	59,73,73	1.49	5 (8%)	67,113,113	1.40	9 (13%)
25	CLA	C1	512	-	59,73,73	1.40	5 (8%)	67,113,113	1.50	10 (14%)
25	CLA	b2	618	-	59,73,73	1.44	5 (8%)	67,113,113	1.46	9 (13%)
25	CLA	b1	615	-	53,67,73	1.46	5 (9%)	59,105,113	1.56	10 (16%)
25	CLA	b2	617	-	59,73,73	1.44	5 (8%)	67,113,113	1.42	9 (13%)
29	LMG	M1	101	-	30,30,55	1.20	3 (10%)	32,32,63	1.33	3 (9%)
32	GOL	C1	518	-	5,5,5	0.37	0	5,5,5	0.23	0
26	OEX	a2	408	1,3,40	0,15,15	0.00	-	-	-	-
27	PHO	d2	408	-	67,69,69	2.12	17 (25%)	85,99,99	1.93	19 (22%)
25	CLA	B2	605	-	59,73,73	1.43	5 (8%)	67,113,113	1.49	9 (13%)
29	LMG	a1	412	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	4 (6%)
37	SQD	b2	605	-	44,45,54	1.30	4 (9%)	53,56,65	1.16	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DGD	H1	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.92	3 (3%)
29	LMG	j2	101	-	50,50,55	0.94	2 (4%)	58,58,63	1.03	2 (3%)
34	DGD	c2	514	-	63,63,67	0.87	2 (3%)	77,77,81	0.97	4 (5%)
25	CLA	c2	511	-	59,73,73	1.43	5 (8%)	67,113,113	1.44	7 (10%)
29	LMG	A2	412	-	29,29,55	1.07	2 (6%)	37,37,63	1.10	2 (5%)
34	DGD	c2	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.84	2 (2%)
33	LHG	B2	627	-	41,41,48	1.03	2 (4%)	44,47,54	1.08	3 (6%)
36	PL9	d1	409	-	55,55,55	0.64	2 (3%)	68,69,69	1.78	20 (29%)
32	GOL	B1	620	-	5,5,5	0.35	0	5,5,5	0.32	0
25	CLA	B1	612	-	59,73,73	1.47	5 (8%)	67,113,113	1.47	8 (11%)
34	DGD	c2	516	-	53,53,67	0.96	2 (3%)	67,67,81	1.03	3 (4%)
25	CLA	c1	505	-	59,73,73	1.43	4 (6%)	67,113,113	1.44	8 (11%)
34	DGD	C1	516	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	4 (5%)
25	CLA	C2	507	-	36,53,73	1.81	5 (13%)	39,89,113	1.82	7 (17%)
25	CLA	D1	403	-	45,59,73	1.62	4 (8%)	50,96,113	1.63	7 (14%)
35	LMT	m2	104	-	30,30,36	0.47	0	41,41,47	0.81	1 (2%)
25	CLA	d1	404	40	59,73,73	1.50	4 (6%)	67,113,113	1.50	10 (14%)
25	CLA	B2	607	-	59,73,73	1.45	5 (8%)	67,113,113	1.47	10 (14%)
35	LMT	a2	406	-	36,36,36	0.45	0	47,47,47	0.66	1 (2%)
25	CLA	A2	402	-	59,73,73	1.53	7 (11%)	67,113,113	1.41	8 (11%)
25	CLA	A1	405	-	49,63,73	1.64	6 (12%)	55,101,113	1.56	11 (20%)
25	CLA	B2	604	-	35,49,73	1.83	4 (11%)	38,84,113	1.80	8 (21%)
23	BCR	d2	401	-	41,41,41	0.70	0	56,56,56	2.11	16 (28%)
29	LMG	A1	412	-	41,41,55	1.06	2 (4%)	49,49,63	1.02	3 (6%)
36	PL9	d2	409	-	55,55,55	0.64	1 (1%)	68,69,69	1.72	16 (23%)
38	HEM	V2	201	16	27,50,50	2.21	5 (18%)	17,82,82	1.37	2 (11%)
25	CLA	a2	413	-	44,58,73	1.66	5 (11%)	49,95,113	1.59	8 (16%)
25	CLA	B2	606	-	59,73,73	1.43	5 (8%)	67,113,113	1.44	7 (10%)
38	HEM	f1	101	6	27,50,50	2.18	6 (22%)	17,82,82	1.34	2 (11%)
25	CLA	C1	505	-	59,73,73	1.39	5 (8%)	67,113,113	1.53	8 (11%)
25	CLA	c1	508	-	44,58,73	1.69	5 (11%)	49,95,113	1.69	11 (22%)
35	LMT	b2	621	-	36,36,36	0.41	0	47,47,47	0.69	0
23	BCR	b1	603	-	41,41,41	0.72	0	56,56,56	1.75	11 (19%)
25	CLA	B2	615	-	59,73,73	1.42	5 (8%)	67,113,113	1.49	10 (14%)
25	CLA	b1	614	-	59,73,73	1.40	5 (8%)	67,113,113	1.52	9 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	BCR	B2	601	-	41,41,41	0.70	0	56,56,56	1.92	15 (26%)
25	CLA	C1	513	3	55,69,73	1.49	5 (9%)	62,108,113	1.48	8 (12%)

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
25	CLA	B1	613	-	3/3/20/25	13/37/135/135	-
25	CLA	D2	404	-	3/3/19/25	11/33/131/135	-
25	CLA	C1	506	-	3/3/20/25	15/37/135/135	-
25	CLA	B1	608	-	3/3/20/25	14/37/135/135	-
29	LMG	b1	631	-	-	7/35/55/70	0/1/1/1
23	BCR	J1	101	-	-	9/29/63/63	0/2/2/2
38	HEM	v2	201	16	-	1/6/54/54	-
29	LMG	D1	406	-	-	4/30/50/70	0/1/1/1
25	CLA	b2	613	-	3/3/20/25	6/37/135/135	-
25	CLA	b2	620	40	3/3/20/25	20/37/135/135	-
25	CLA	B1	606	-	3/3/20/25	18/37/135/135	-
23	BCR	j2	102	-	-	9/29/63/63	0/2/2/2
33	LHG	b1	622	-	-	14/53/53/53	-
23	BCR	B2	603	-	-	2/29/63/63	0/2/2/2
27	PHO	d1	403	-	-	5/53/103/103	0/5/6/6
25	CLA	C2	511	-	3/3/17/25	4/19/117/135	-
25	CLA	A1	403	-	3/3/20/25	10/37/135/135	-
25	CLA	a1	405	-	3/3/17/25	6/19/117/135	-
33	LHG	D2	405	-	-	16/53/53/53	-
25	CLA	B2	612	-	3/3/20/25	9/37/135/135	-
29	LMG	F2	402	-	-	2/30/50/70	0/1/1/1
23	BCR	k1	101	-	-	5/29/63/63	0/2/2/2
35	LMT	l1	101	-	-	3/15/35/61	0/1/1/2
25	CLA	B2	609	-	3/3/20/25	9/37/135/135	-
25	CLA	c1	507	-	3/3/20/25	16/37/135/135	-
32	GOL	a2	415	-	-	2/4/4/4	-
25	CLA	d2	402	-	3/3/20/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	a2	412	-	-	6/39/59/70	0/1/1/1
35	LMT	M1	103	-	-	3/15/35/61	0/1/1/2
25	CLA	B2	619	-	3/3/20/25	17/37/135/135	-
25	CLA	C1	513	3	3/3/19/25	13/33/131/135	-
29	LMG	B2	620	-	-	8/35/55/70	0/1/1/1
23	BCR	c1	502	-	-	5/29/63/63	0/2/2/2
27	PHO	D1	407	-	-	6/51/101/103	0/5/6/6
32	GOL	C2	514	-	-	2/4/4/4	-
23	BCR	C1	501	-	-	4/29/63/63	0/2/2/2
23	BCR	b2	603	-	-	0/29/63/63	0/2/2/2
33	LHG	d1	407	-	-	14/53/53/53	-
34	DGD	C2	512	-	-	1/20/60/95	0/2/2/2
25	CLA	c2	506	-	3/3/19/25	11/33/131/135	-
35	LMT	L1	102	-	-	1/9/9/61	-
25	CLA	A2	403	-	3/3/19/25	7/33/131/135	-
25	CLA	K2	101	-	3/3/18/25	11/25/123/135	-
25	CLA	b1	612	-	3/3/20/25	11/37/135/135	-
25	CLA	C2	516	-	3/3/16/25	6/15/113/135	-
25	CLA	B1	616	-	3/3/20/25	9/37/135/135	-
33	LHG	D2	403	-	-	10/53/53/53	-
25	CLA	C2	505	-	3/3/20/25	15/37/135/135	-
25	CLA	b1	605	-	3/3/20/25	7/37/135/135	-
27	PHO	a1	411	-	-	7/53/103/103	0/5/6/6
25	CLA	d1	406	-	3/3/20/25	14/37/135/135	-
37	SQD	D1	409	-	-	2/29/49/69	0/1/1/1
25	CLA	c1	504	-	3/3/20/25	7/37/135/135	-
25	CLA	B1	619	40	3/3/20/25	16/37/135/135	-
25	CLA	b2	610	-	3/3/20/25	7/37/135/135	-
25	CLA	B1	610	-	3/3/20/25	13/37/135/135	-
23	BCR	d1	405	-	-	8/29/63/63	0/2/2/2
25	CLA	C1	502	-	3/3/20/25	15/37/135/135	-
23	BCR	a2	402	-	-	3/29/63/63	0/2/2/2
25	CLA	c1	506	40	3/3/20/25	15/37/135/135	-
25	CLA	c2	515	-	3/3/16/25	5/15/113/135	-
25	CLA	b1	617	-	3/3/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	b1	602	-	-	3/29/63/63	0/2/2/2
23	BCR	C1	521	-	-	0/29/63/63	0/2/2/2
35	LMT	b2	623	-	-	1/21/61/61	0/2/2/2
25	CLA	c1	503	-	3/3/20/25	15/37/135/135	-
25	CLA	c2	512	3	3/3/20/25	13/37/135/135	-
25	CLA	a2	404	-	3/3/20/25	7/37/135/135	-
23	BCR	b2	601	-	-	0/29/63/63	0/2/2/2
33	LHG	a2	407	-	-	11/33/33/53	-
37	SQD	D2	402	-	-	4/18/38/69	0/1/1/1
35	LMT	C1	519	-	-	2/21/61/61	0/2/2/2
29	LMG	d1	411	-	-	2/36/36/70	-
25	CLA	c2	510	-	3/3/17/25	8/24/122/135	-
25	CLA	B2	616	-	3/3/17/25	7/24/122/135	-
29	LMG	b1	621	-	-	6/33/53/70	0/1/1/1
35	LMT	T1	101	-	-	0/9/9/61	-
23	BCR	D1	401	-	-	8/29/63/63	0/2/2/2
32	GOL	a1	406	-	-	2/4/4/4	-
33	LHG	L2	101	-	-	16/53/53/53	-
35	LMT	M1	102	-	-	1/8/8/61	-
25	CLA	C2	508	-	3/3/17/25	7/19/117/135	-
23	BCR	h1	102	-	-	5/29/63/63	0/2/2/2
25	CLA	A1	405	-	3/3/18/25	3/25/123/135	-
29	LMG	A1	410	-	-	4/38/58/70	0/1/1/1
32	GOL	i1	101	-	-	2/4/4/4	-
25	CLA	b2	606	-	3/3/20/25	14/37/135/135	-
33	LHG	L1	101	-	-	14/45/45/53	-
25	CLA	C2	503	-	3/3/20/25	16/37/135/135	-
25	CLA	C1	509	-	3/3/20/25	18/37/135/135	-
25	CLA	b2	614	-	3/3/20/25	17/37/135/135	-
33	LHG	d1	402	-	-	12/36/36/53	-
25	CLA	b1	613	-	3/3/20/25	6/37/135/135	-
33	LHG	b2	625	-	-	5/47/47/53	-
33	LHG	A2	405	-	-	10/37/37/53	-
25	CLA	B1	612	-	3/3/20/25	9/37/135/135	-
25	CLA	b1	608	-	3/3/20/25	15/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d1	401	-	3/3/20/25	10/37/135/135	-
29	LMG	B1	626	-	-	12/43/63/70	0/1/1/1
23	BCR	a1	401	-	-	2/29/63/63	0/2/2/2
23	BCR	B2	602	-	-	2/29/63/63	0/2/2/2
25	CLA	C2	513	-	3/3/17/25	0/23/121/135	-
25	CLA	b1	606	-	3/3/20/25	17/37/135/135	-
23	BCR	F2	401	-	-	9/29/63/63	0/2/2/2
25	CLA	B2	610	-	3/3/20/25	6/37/135/135	-
27	PHO	A2	407	-	-	10/53/103/103	0/5/6/6
25	CLA	D2	401	-	3/3/20/25	6/37/135/135	-
25	CLA	B2	611	-	3/3/20/25	8/37/135/135	-
25	CLA	c2	507	-	3/3/17/25	5/24/122/135	-
27	PHO	A1	408	-	-	7/53/103/103	0/5/6/6
33	LHG	a1	407	-	-	14/47/47/53	-
25	CLA	C1	511	-	3/3/20/25	12/37/135/135	-
38	HEM	v1	201	16	-	1/6/54/54	-
33	LHG	D1	404	-	-	11/53/53/53	-
25	CLA	b1	619	-	3/3/20/25	17/37/135/135	-
29	LMG	b2	622	-	-	0/34/54/70	0/1/1/1
25	CLA	b2	609	-	3/3/19/25	10/33/131/135	-
25	CLA	D2	406	-	3/3/20/25	14/37/135/135	-
25	CLA	C1	507	-	3/3/20/25	20/37/135/135	-
33	LHG	D1	405	-	-	14/53/53/53	-
34	DGD	C1	517	-	-	6/53/93/95	0/2/2/2
23	BCR	b2	602	-	-	6/29/63/63	0/2/2/2
23	BCR	c2	501	-	-	14/29/63/63	0/2/2/2
25	CLA	b2	619	-	3/3/18/25	10/30/128/135	-
25	CLA	c2	504	-	3/3/20/25	10/37/135/135	-
23	BCR	B1	603	-	-	1/29/63/63	0/2/2/2
25	CLA	d2	404	-	3/3/17/25	2/19/117/135	-
36	PL9	D2	408	-	-	7/53/73/73	0/1/1/1
29	LMG	B1	622	-	-	2/26/46/70	0/1/1/1
23	BCR	B1	601	-	-	0/29/63/63	0/2/2/2
25	CLA	B2	614	-	3/3/20/25	12/37/135/135	-
23	BCR	H1	102	-	-	3/15/32/63	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	B1	602	-	-	5/29/63/63	0/2/2/2
23	BCR	c1	501	-	-	0/29/63/63	0/2/2/2
25	CLA	a1	404	-	3/3/19/25	7/31/129/135	-
25	CLA	B1	611	-	2/2/19/25	10/34/132/135	-
34	DGD	c1	518	-	-	10/51/91/95	0/2/2/2
34	DGD	h2	102	-	-	9/51/91/95	0/2/2/2
25	CLA	C2	504	-	3/3/16/25	8/15/113/135	-
25	CLA	b2	624	-	3/3/20/25	9/37/135/135	-
25	CLA	c2	503	-	3/3/20/25	13/37/135/135	-
25	CLA	b1	610	-	3/3/20/25	2/37/135/135	-
34	DGD	H2	101	-	-	7/51/91/95	0/2/2/2
25	CLA	c2	502	-	3/3/20/25	13/37/135/135	-
38	HEM	E2	101	5	-	0/6/54/54	-
25	CLA	c1	515	-	3/3/18/25	9/25/123/135	-
25	CLA	B2	615	-	3/3/20/25	11/37/135/135	-
36	PL9	d2	409	-	-	8/53/73/73	0/1/1/1
34	DGD	C1	515	-	-	10/41/81/95	0/2/2/2
34	DGD	h1	101	-	-	9/51/91/95	0/2/2/2
25	CLA	A1	406	-	3/3/20/25	11/37/135/135	-
25	CLA	B1	609	-	3/3/20/25	10/37/135/135	-
25	CLA	b2	604	-	3/3/15/25	4/10/108/135	-
25	CLA	b2	616	-	3/3/19/25	9/31/129/135	-
35	LMT	m2	103	-	-	5/16/56/61	0/2/2/2
25	CLA	b1	611	-	3/3/20/25	6/37/135/135	-
23	BCR	K2	102	-	-	7/29/63/63	0/2/2/2
25	CLA	B1	615	-	3/3/20/25	15/37/135/135	-
25	CLA	c1	513	3	3/3/19/25	5/31/129/135	-
23	BCR	h2	101	-	-	4/29/63/63	0/2/2/2
25	CLA	d2	405	-	3/3/20/25	9/37/135/135	-
35	LMT	c1	517	-	-	1/19/59/61	0/2/2/2
38	HEM	e2	101	5,6	-	0/6/54/54	-
25	CLA	b2	615	-	3/3/19/25	8/31/129/135	-
25	CLA	B1	618	-	3/3/18/25	3/29/127/135	-
25	CLA	c1	511	-	3/3/20/25	10/37/135/135	-
33	LHG	l2	101	-	-	20/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PHO	D2	407	-	-	10/53/103/103	0/5/6/6
25	CLA	B1	605	-	3/3/20/25	9/37/135/135	-
32	GOL	c1	521	-	-	2/4/4/4	-
29	LMG	B2	621	-	-	8/31/51/70	0/1/1/1
23	BCR	H2	103	-	-	3/17/34/63	0/1/1/2
23	BCR	b1	601	-	-	0/29/63/63	0/2/2/2
25	CLA	c1	516	-	3/3/20/25	11/37/135/135	-
25	CLA	C2	518	-	3/3/15/25	4/8/106/135	-
25	CLA	b1	620	-	3/3/20/25	16/37/135/135	-
32	GOL	c2	518	-	-	2/4/4/4	-
33	LHG	B1	621	-	-	11/53/53/53	-
33	LHG	l1	102	-	-	18/53/53/53	-
25	CLA	c2	509	-	3/3/20/25	11/37/135/135	-
37	SQD	B2	623	-	-	2/40/60/69	0/1/1/1
25	CLA	B1	617	-	3/3/20/25	12/37/135/135	-
34	DGD	c1	514	-	-	9/40/80/95	0/2/2/2
25	CLA	b2	612	-	3/3/20/25	10/37/135/135	-
25	CLA	b1	604	-	3/3/20/25	14/37/135/135	-
25	CLA	C1	514	-	3/3/16/25	2/11/111/135	-
35	LMT	i2	102	-	-	0/4/4/61	-
25	CLA	C1	510	-	3/3/20/25	8/37/135/135	-
25	CLA	B2	607	-	3/3/20/25	7/37/135/135	-
23	BCR	z2	101	-	-	0/29/63/63	0/2/2/2
35	LMT	a2	406	-	-	5/21/61/61	0/2/2/2
23	BCR	C2	502	-	-	0/29/63/63	0/2/2/2
25	CLA	B2	608	-	3/3/20/25	18/37/135/135	-
29	LMG	c2	519	-	-	3/20/40/70	0/1/1/1
25	CLA	b2	611	-	3/3/20/25	5/37/135/135	-
25	CLA	B1	614	-	3/3/20/25	12/37/135/135	-
25	CLA	C2	509	-	3/3/20/25	14/37/135/135	-
25	CLA	C2	506	-	3/3/20/25	14/37/135/135	-
25	CLA	a1	403	-	3/3/20/25	6/37/135/135	-
27	PHO	a2	416	-	-	8/53/103/103	0/5/6/6
29	LMG	d2	407	-	-	3/21/41/70	0/1/1/1
25	CLA	b1	616	-	3/3/20/25	15/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	m1	101	-	-	8/21/61/61	0/2/2/2
25	CLA	c2	508	40	3/3/20/25	14/37/135/135	-
29	LMG	c1	519	-	-	9/50/70/70	0/1/1/1
33	LHG	d2	403	-	-	13/53/53/53	-
25	CLA	a2	405	-	3/3/20/25	13/37/135/135	-
25	CLA	B2	613	-	3/3/20/25	12/37/135/135	-
25	CLA	C1	504	-	3/3/20/25	6/37/135/135	-
25	CLA	b2	608	-	3/3/20/25	12/37/135/135	-
25	CLA	A2	402	-	3/3/20/25	10/37/135/135	-
23	BCR	A1	401	-	-	2/29/63/63	0/2/2/2
29	LMG	I2	101	-	-	3/29/49/70	0/1/1/1
23	BCR	k2	501	-	-	0/29/63/63	0/2/2/2
29	LMG	d1	408	-	-	2/28/48/70	0/1/1/1
32	GOL	b1	618	-	-	4/4/4/4	-
23	BCR	K2	104	-	-	2/12/46/63	0/2/2/2
25	CLA	B2	617	-	3/3/20/25	7/37/135/135	-
25	CLA	b1	607	-	3/3/20/25	10/37/135/135	-
29	LMG	C1	520	-	-	8/43/63/70	0/1/1/1
25	CLA	C1	503	-	3/3/19/25	11/31/129/135	-
25	CLA	A2	404	-	3/3/17/25	8/21/119/135	-
25	CLA	A1	404	-	3/3/17/25	7/21/119/135	-
29	LMG	M1	101	-	-	4/31/31/70	-
25	CLA	B2	618	-	3/3/19/25	4/31/129/135	-
25	CLA	D1	402	-	3/3/20/25	7/37/135/135	-
36	PL9	D1	408	-	-	7/53/73/73	0/1/1/1
25	CLA	c2	513	-	3/3/17/25	7/24/122/135	-
25	CLA	c1	512	-	3/3/20/25	15/37/135/135	-
25	CLA	C1	508	-	3/3/20/25	11/37/135/135	-
34	DGD	c1	520	-	-	8/51/91/95	0/2/2/2
38	HEM	E1	101	5,6	-	0/6/54/54	-
25	CLA	C2	510	-	3/3/16/25	4/11/111/135	-
29	LMG	C2	515	-	-	0/18/38/70	0/1/1/1
29	LMG	A1	412	-	-	7/36/56/70	0/1/1/1
38	HEM	V1	201	16	-	1/6/54/54	-
23	BCR	A2	401	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	d2	406	-	-	10/53/53/53	-
25	CLA	b1	609	-	3/3/20/25	11/37/135/135	-
25	CLA	B1	604	-	3/3/15/25	4/10/108/135	-
29	LMG	b1	624	-	-	3/34/54/70	0/1/1/1
25	CLA	c2	505	-	3/3/20/25	14/37/135/135	-
25	CLA	b2	618	-	3/3/20/25	4/37/135/135	-
25	CLA	b1	615	-	3/3/18/25	7/30/128/135	-
25	CLA	b2	617	-	3/3/20/25	16/37/135/135	-
25	CLA	C1	512	-	3/3/20/25	14/37/135/135	-
27	PHO	d2	408	-	-	6/53/103/103	0/5/6/6
25	CLA	B2	605	-	3/3/20/25	9/37/135/135	-
29	LMG	a1	412	-	-	12/46/66/70	0/1/1/1
37	SQD	b2	605	-	-	10/40/60/69	0/1/1/1
34	DGD	H1	101	-	-	12/51/91/95	0/2/2/2
29	LMG	j2	101	-	-	7/45/65/70	0/1/1/1
34	DGD	c2	514	-	-	16/51/91/95	0/2/2/2
29	LMG	A2	412	-	-	5/23/43/70	0/1/1/1
34	DGD	c2	517	-	-	7/51/91/95	0/2/2/2
33	LHG	B2	627	-	-	8/46/46/53	-
32	GOL	B1	620	-	-	2/4/4/4	-
36	PL9	d1	409	-	-	9/53/73/73	0/1/1/1
23	BCR	K1	101	-	-	5/26/43/63	0/1/1/2
34	DGD	c2	516	-	-	6/41/81/95	0/2/2/2
25	CLA	c1	505	-	3/3/20/25	5/37/135/135	-
34	DGD	C1	516	-	-	9/51/91/95	0/2/2/2
25	CLA	C2	507	-	3/3/16/25	4/11/111/135	-
25	CLA	D1	403	-	3/3/17/25	4/21/119/135	-
35	LMT	m2	104	-	-	4/15/55/61	0/2/2/2
25	CLA	d1	404	40	3/3/20/25	8/37/135/135	-
25	CLA	B1	607	-	3/3/19/25	7/31/129/135	-
25	CLA	c1	509	40	3/3/20/25	15/37/135/135	-
32	GOL	C1	518	-	-	2/4/4/4	-
25	CLA	B2	604	-	3/3/15/25	4/8/106/135	-
23	BCR	d2	401	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c1	510	-	3/3/20/25	10/37/135/135	-
38	HEM	V2	201	16	-	1/6/54/54	-
25	CLA	a2	413	-	3/3/17/25	5/19/117/135	-
25	CLA	B2	606	-	3/3/20/25	11/37/135/135	-
38	HEM	f1	101	6	-	2/6/54/54	-
25	CLA	C1	505	-	3/3/20/25	11/37/135/135	-
25	CLA	c1	508	-	3/3/17/25	5/19/117/135	-
35	LMT	b2	621	-	-	1/21/61/61	0/2/2/2
23	BCR	b1	603	-	-	4/29/63/63	0/2/2/2
25	CLA	c2	511	-	3/3/20/25	15/37/135/135	-
25	CLA	b1	614	-	3/3/20/25	14/37/135/135	-
23	BCR	B2	601	-	-	0/29/63/63	0/2/2/2

The worst 5 of 1037 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d1	404	CLA	C4B-NB	8.30	1.42	1.35
25	A2	402	CLA	C4B-NB	8.28	1.42	1.35
25	A2	404	CLA	C4B-NB	8.24	1.42	1.35
25	b1	607	CLA	C4B-NB	8.19	1.42	1.35
25	A1	406	CLA	C4B-NB	8.16	1.42	1.35

The worst 5 of 2211 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c2	501	BCR	C36-C18-C17	-10.87	107.70	122.92
23	c2	501	BCR	C24-C23-C22	-9.36	112.09	126.23
27	A2	407	PHO	CMD-C2D-C1D	9.25	139.31	125.06
27	D2	407	PHO	CMD-C2D-C1D	9.14	139.13	125.06
23	c2	501	BCR	C16-C17-C18	9.01	140.16	127.31

5 of 419 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	D2	404	CLA	NC
25	D2	404	CLA	ND
25	D2	404	CLA	NA
25	B1	608	CLA	NC
25	B1	608	CLA	ND

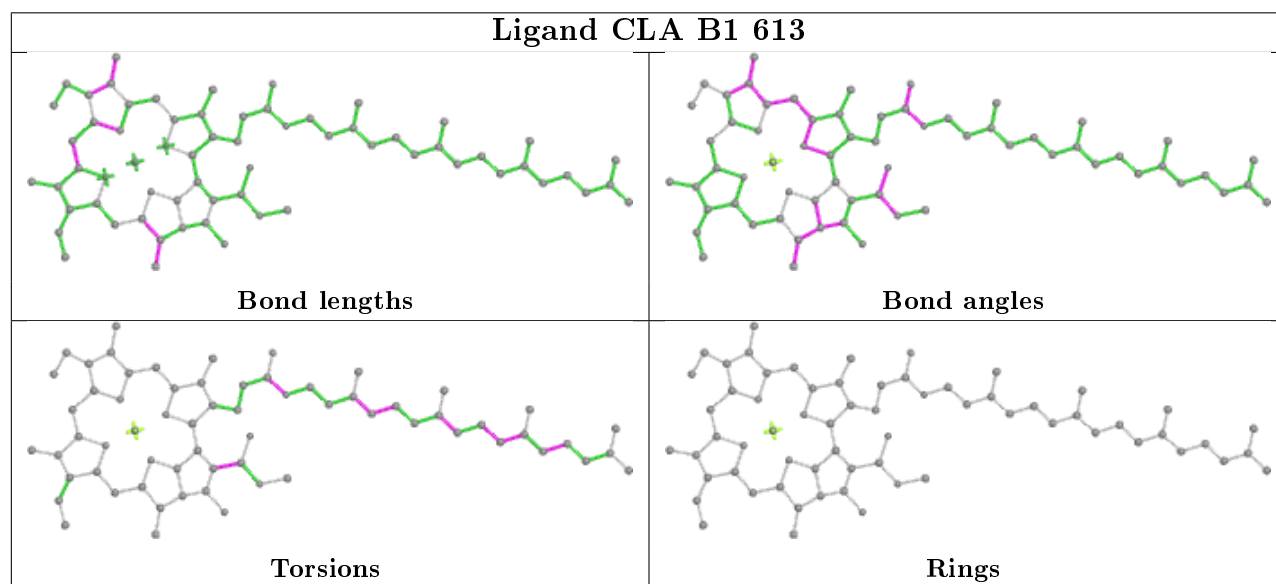
5 of 2187 torsion outliers are listed below:

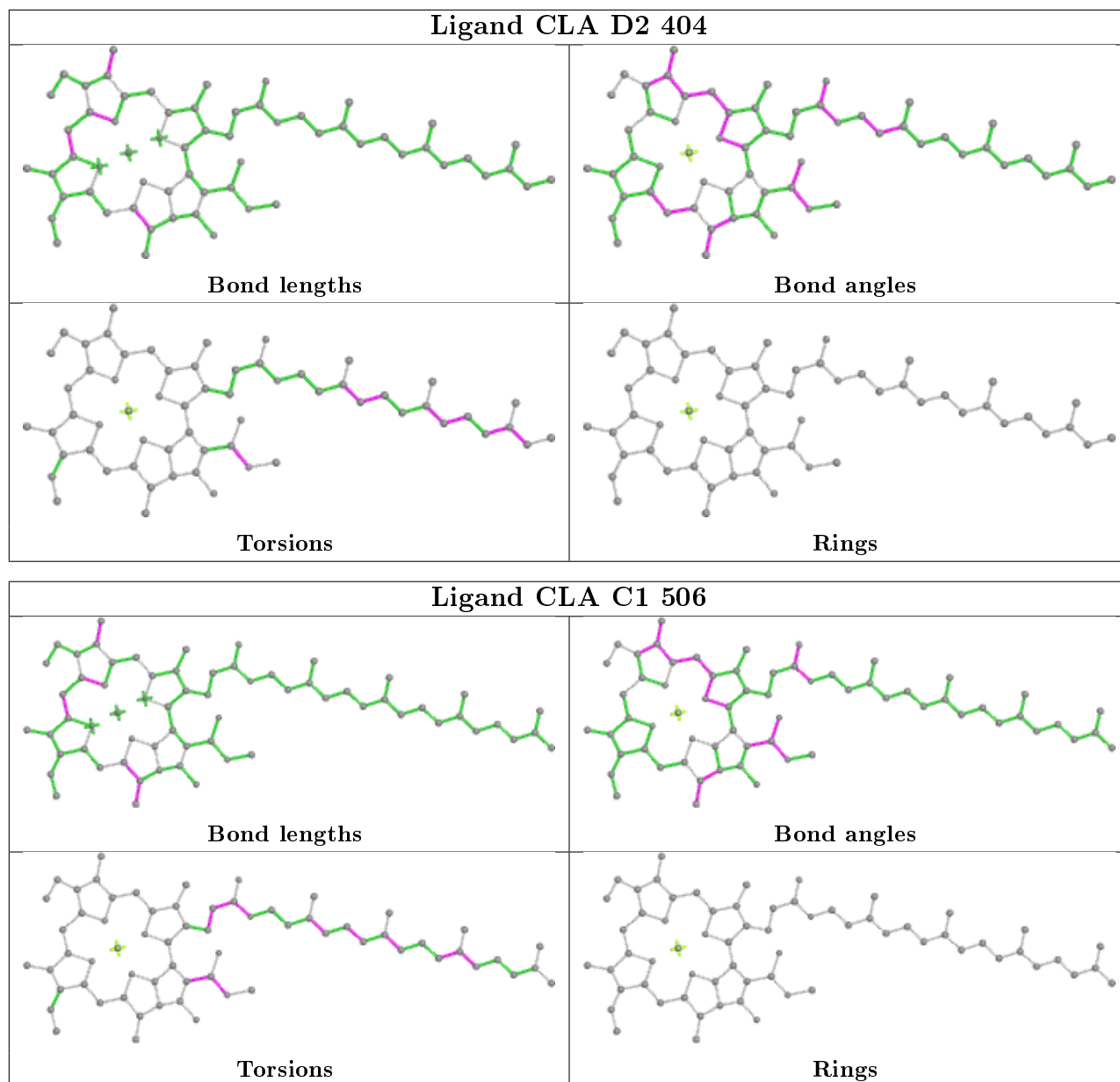
Mol	Chain	Res	Type	Atoms
25	b2	620	CLA	CBD-CGD-O2D-CED
25	a1	405	CLA	C1A-C2A-CAA-CBA
25	a1	405	CLA	C3A-C2A-CAA-CBA
33	B1	621	LHG	C3-O3-P-O4
33	B1	621	LHG	C3-O3-P-O5

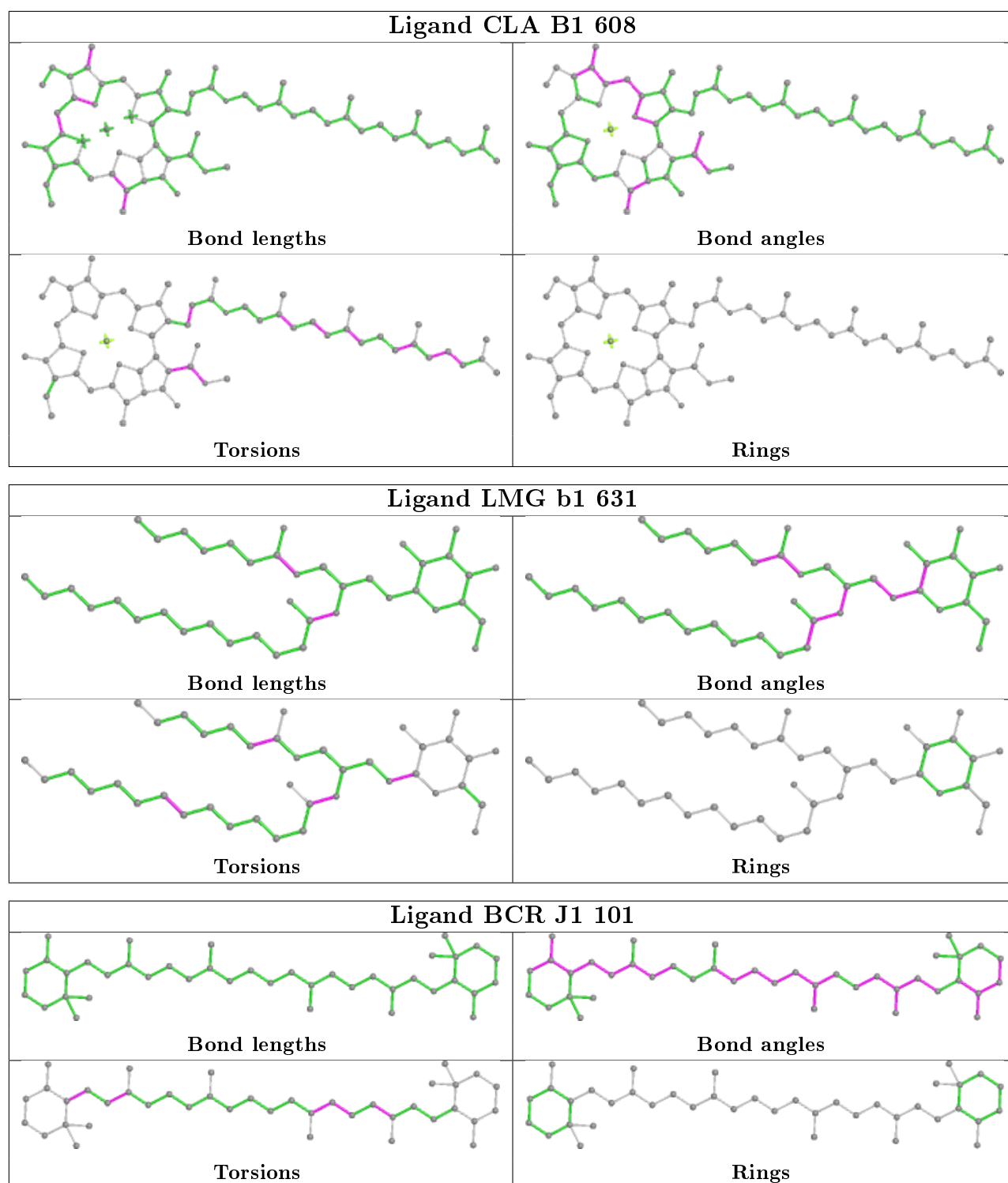
There are no ring outliers.

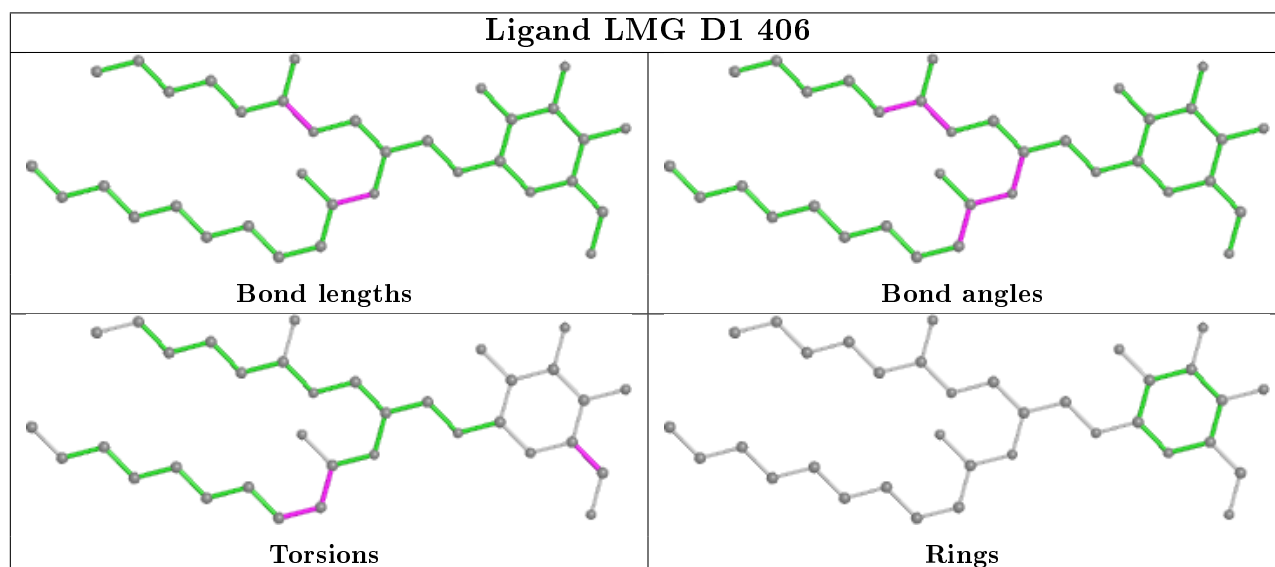
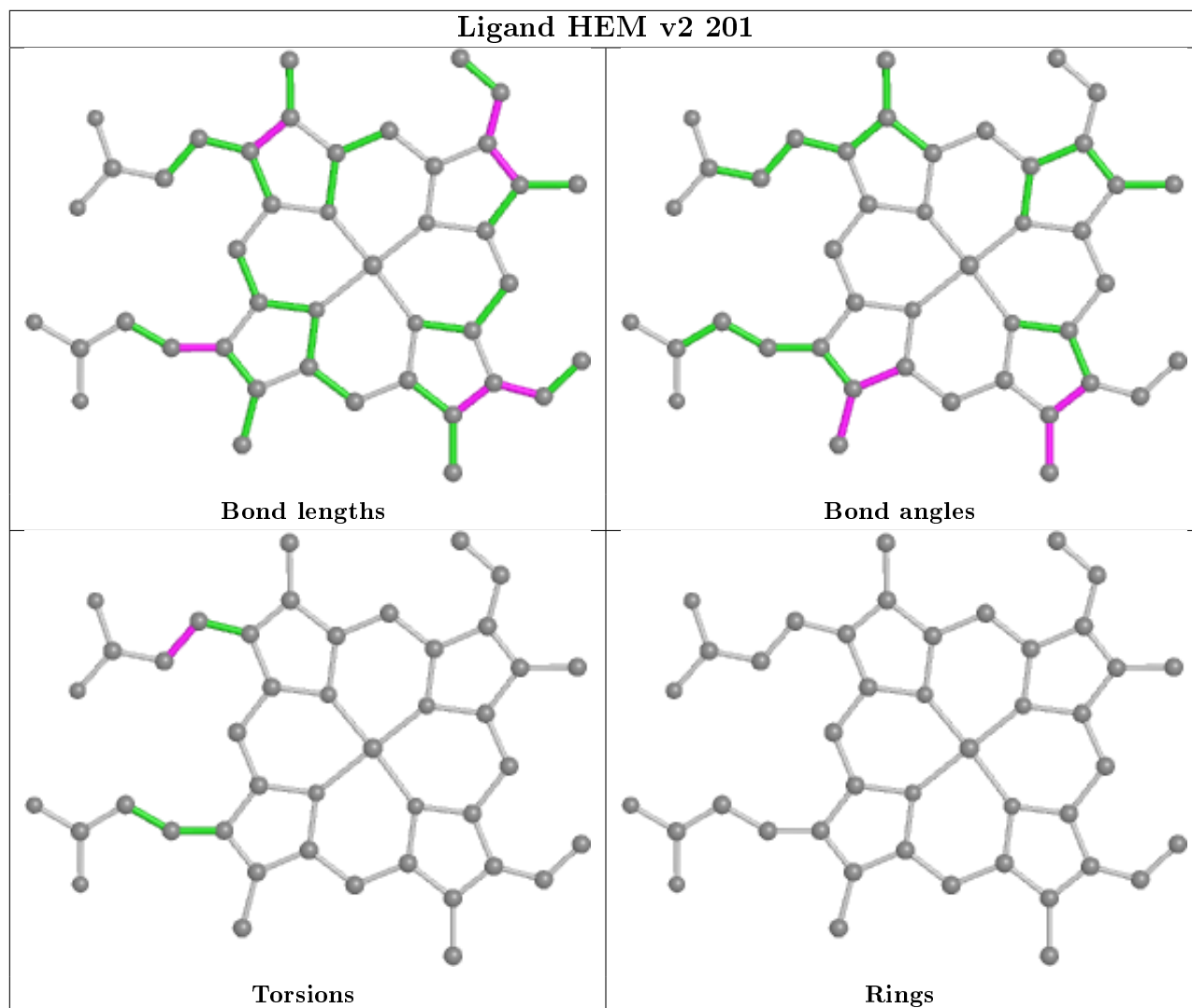
No monomer is involved in short contacts.

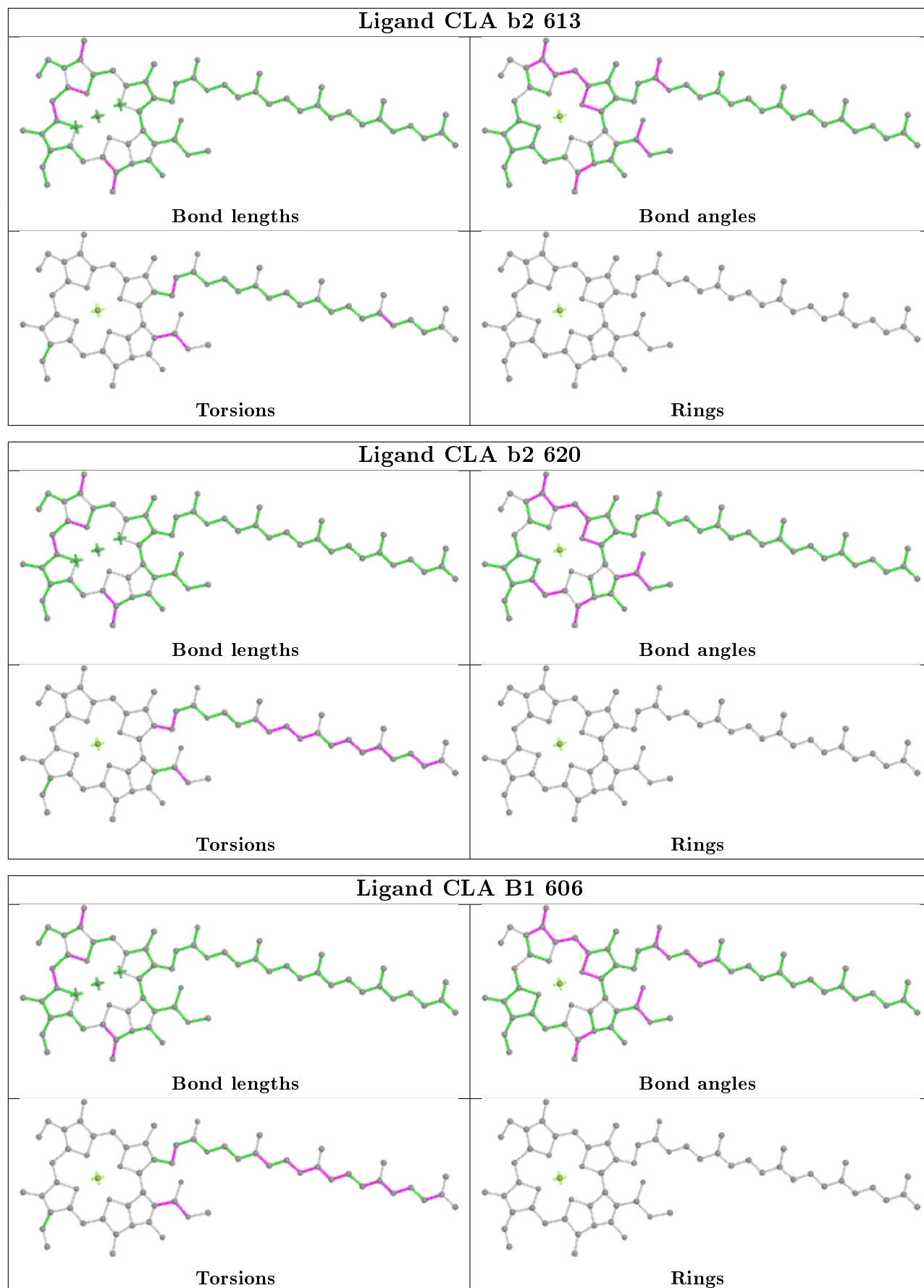
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

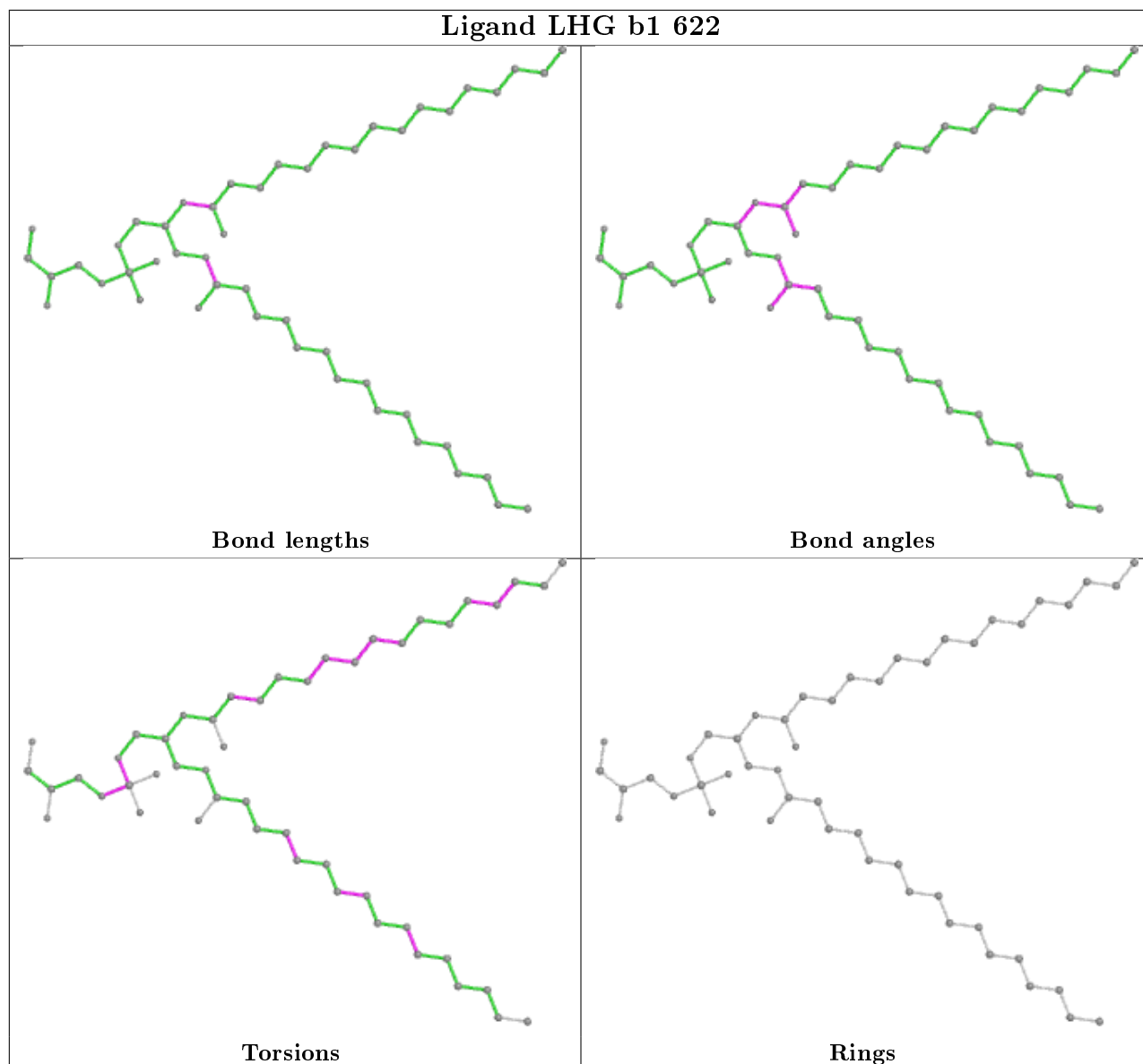
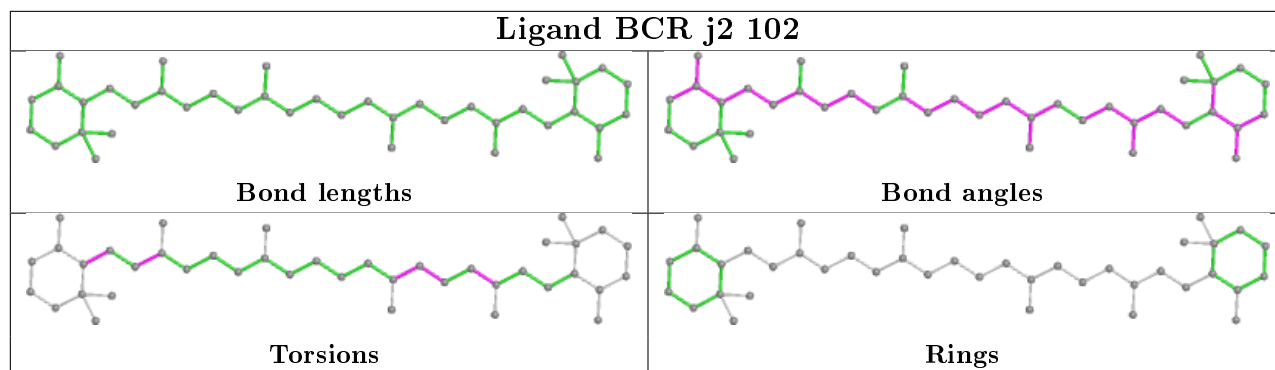


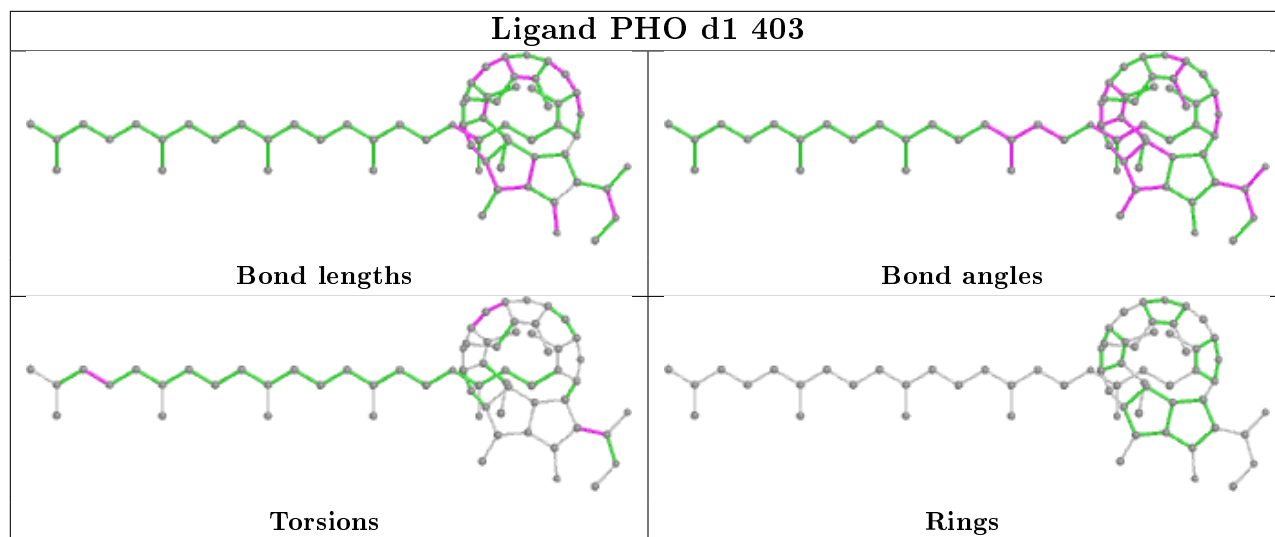
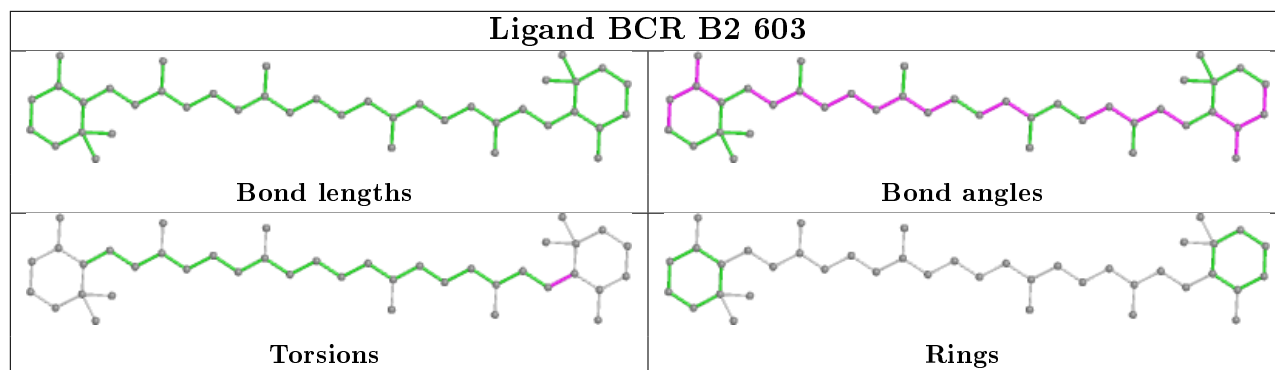




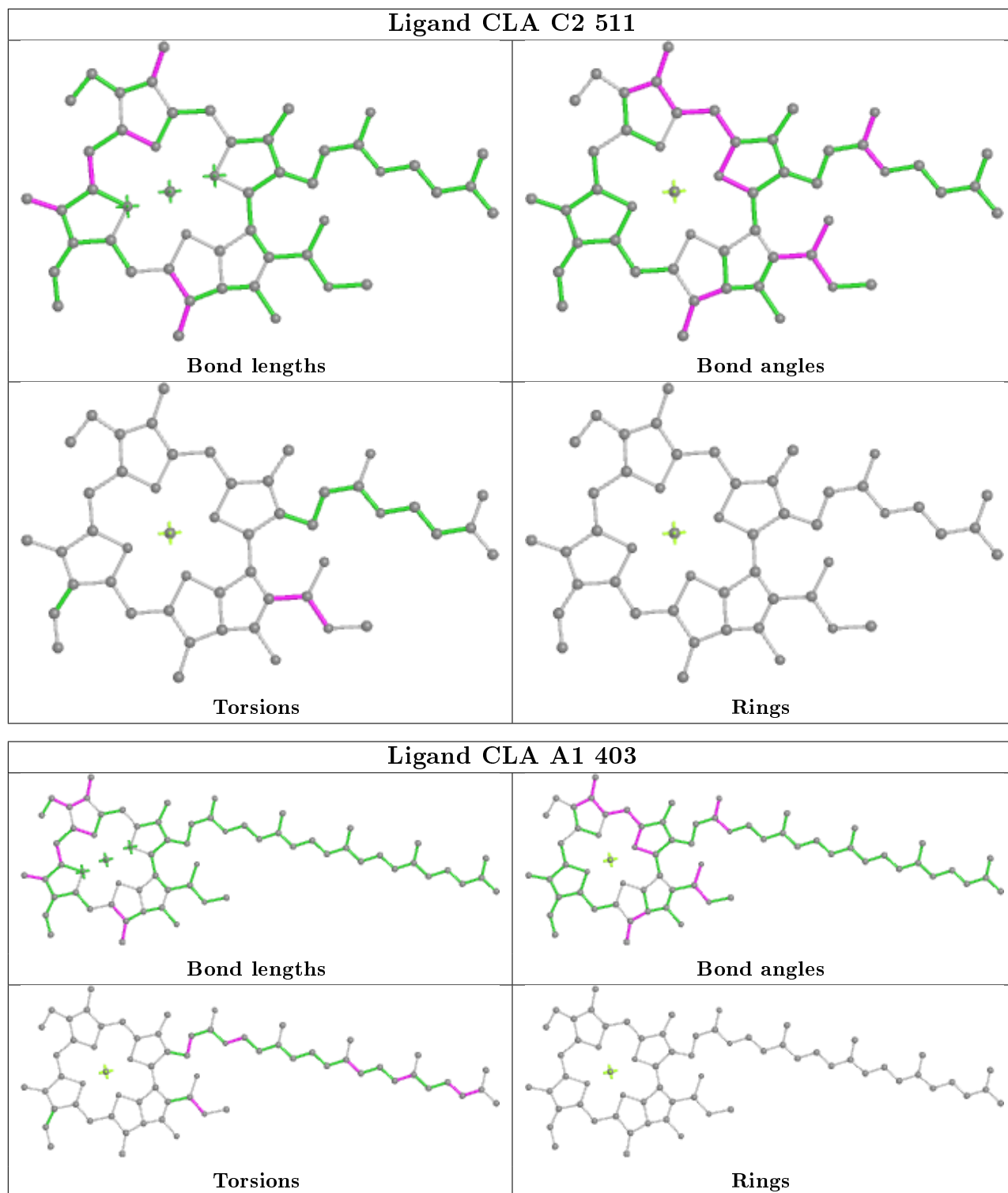


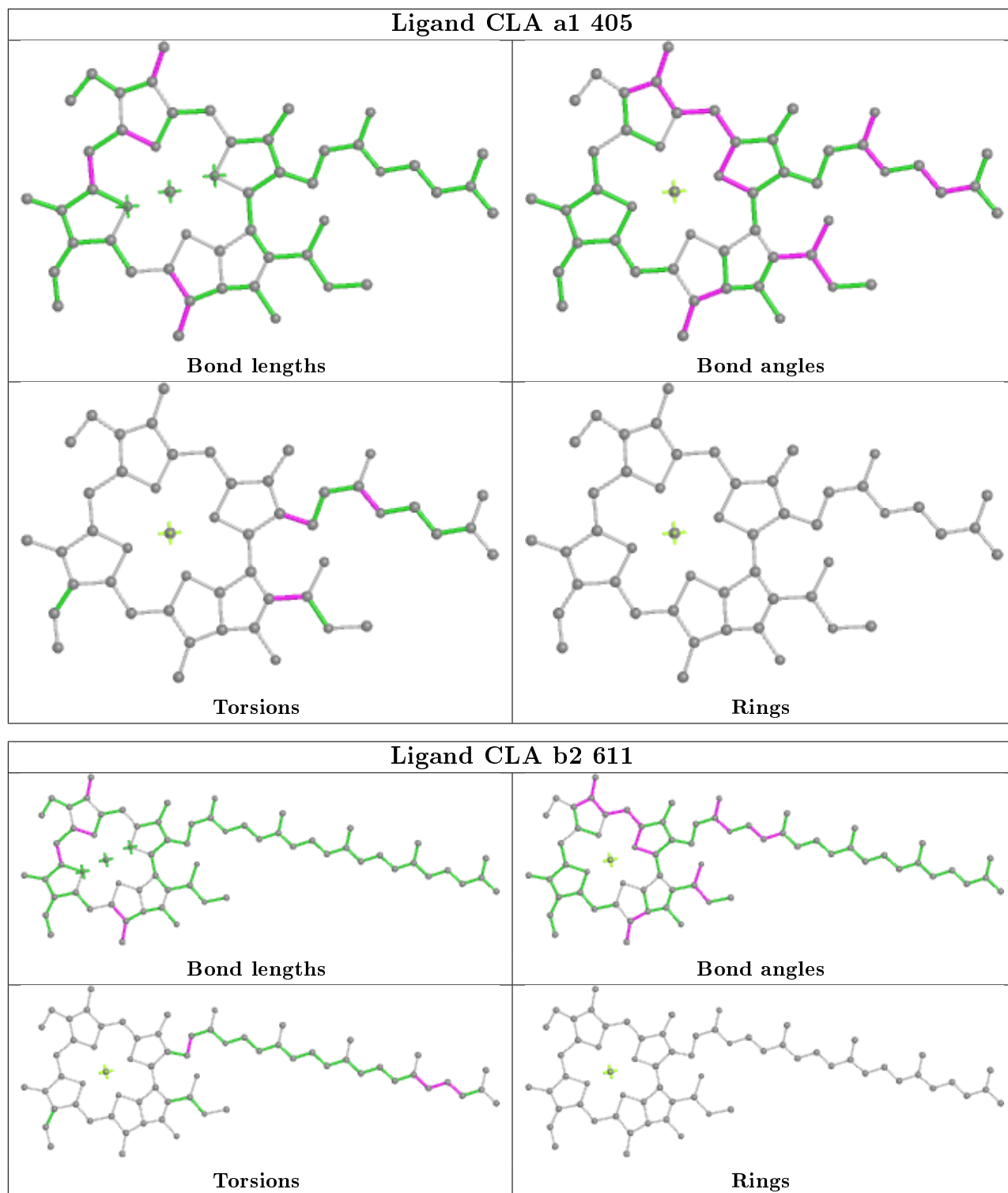


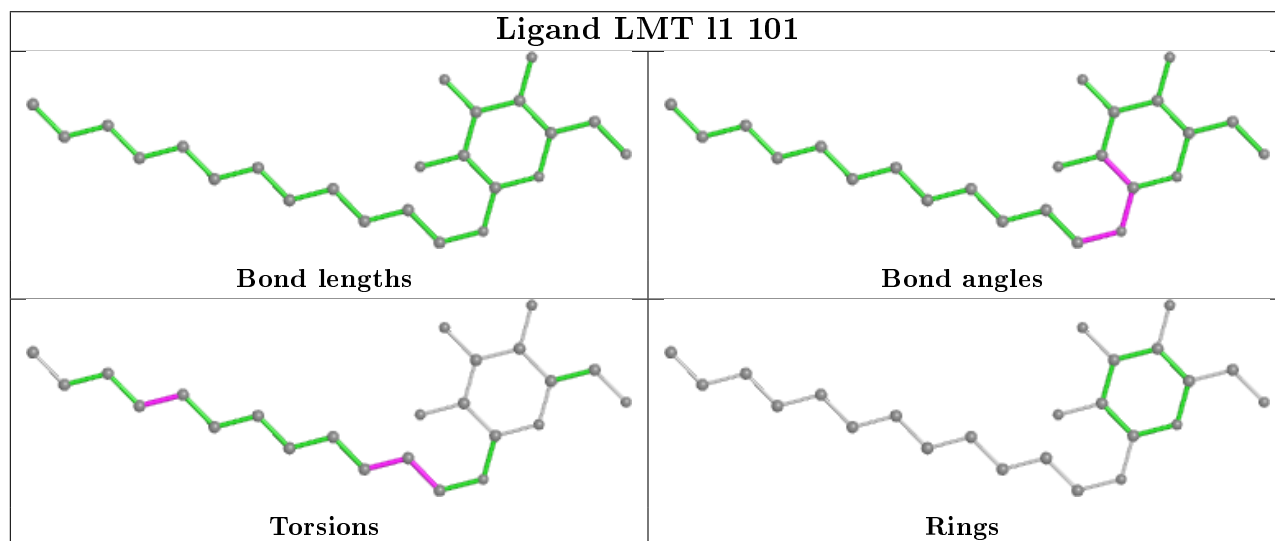
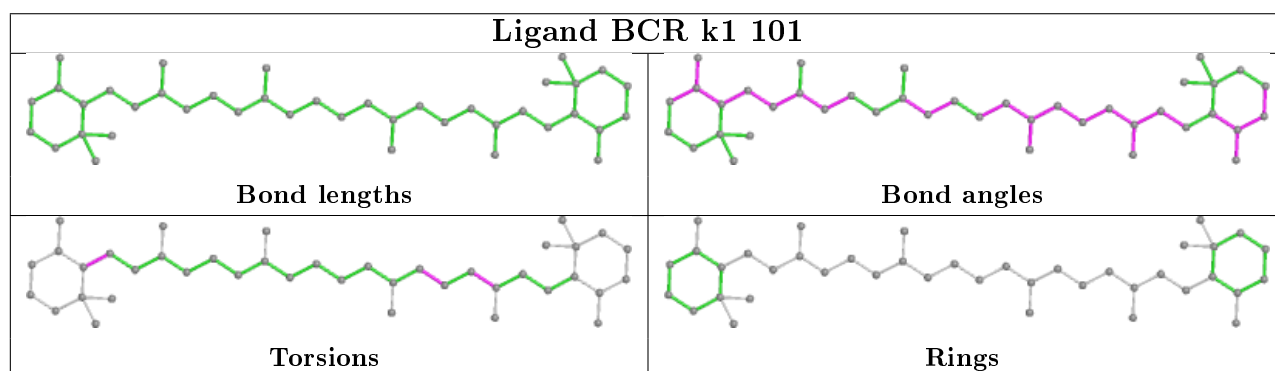
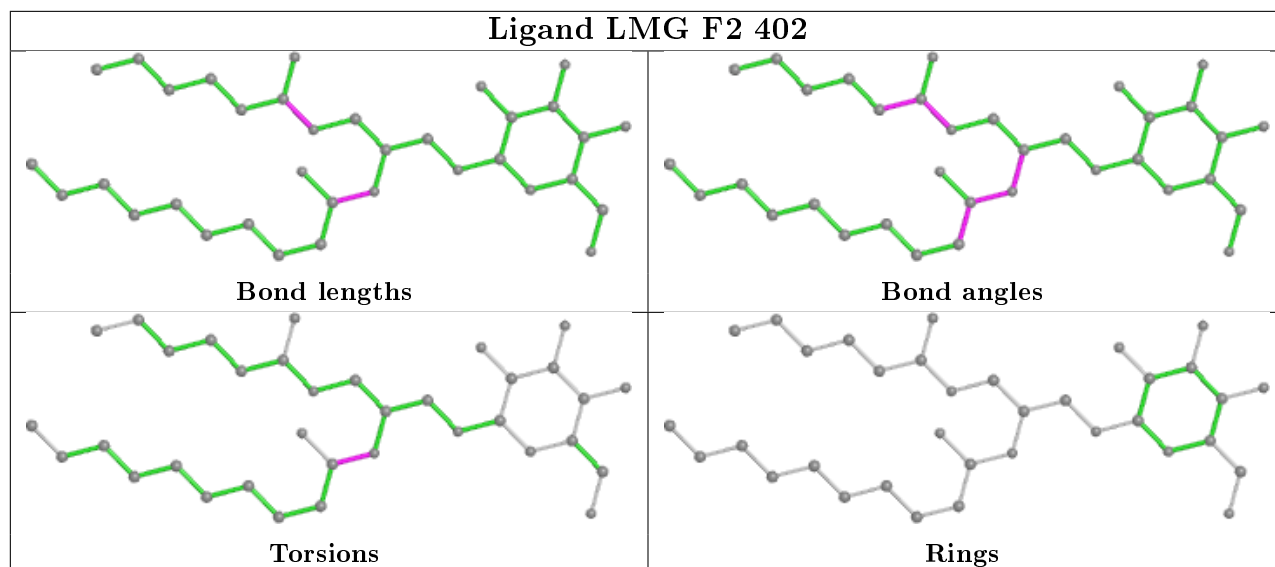


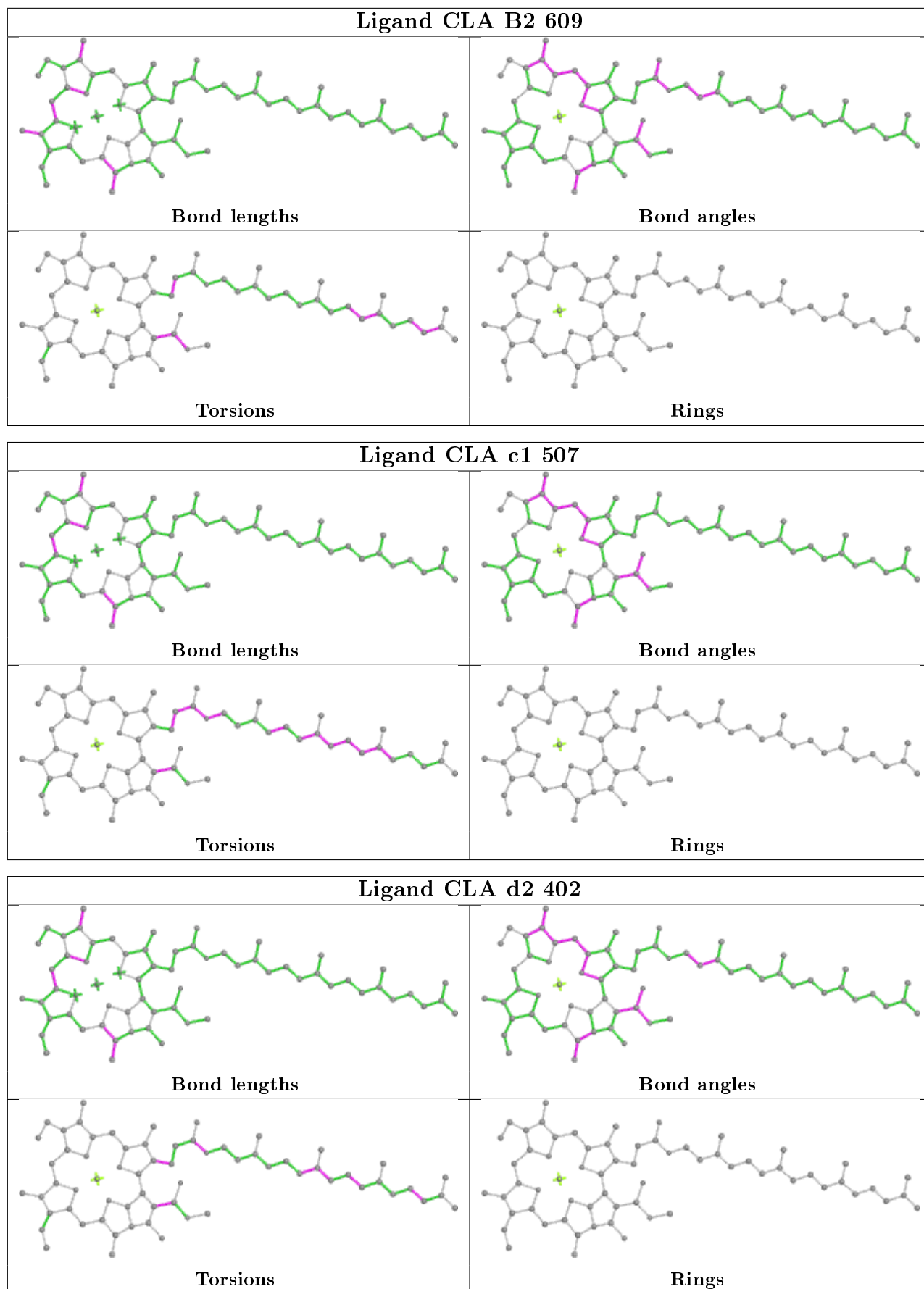


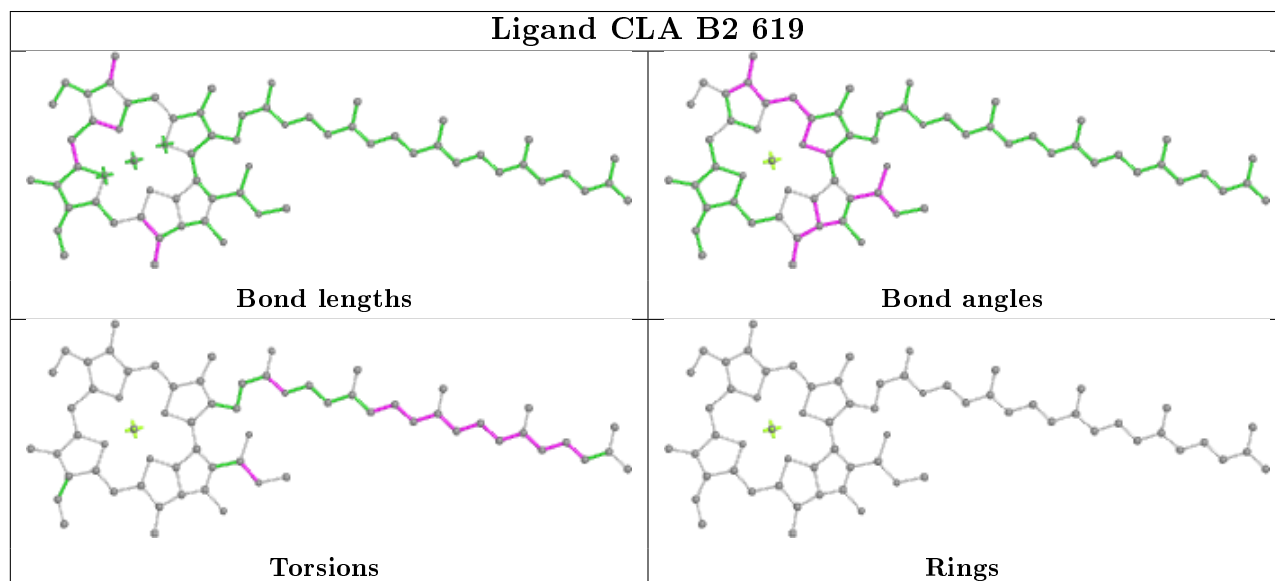
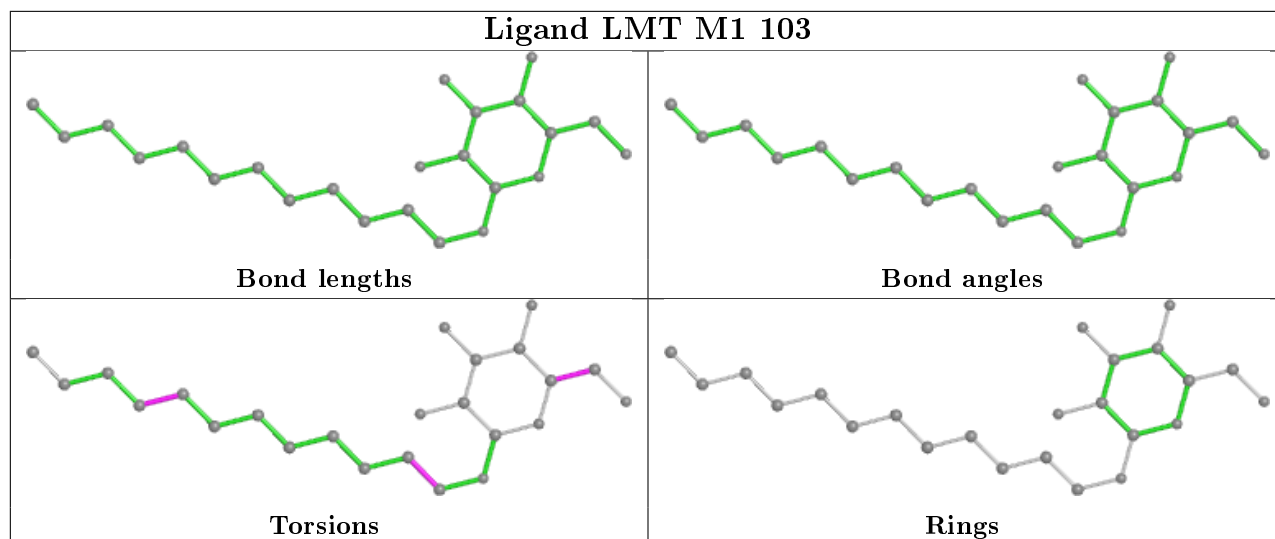


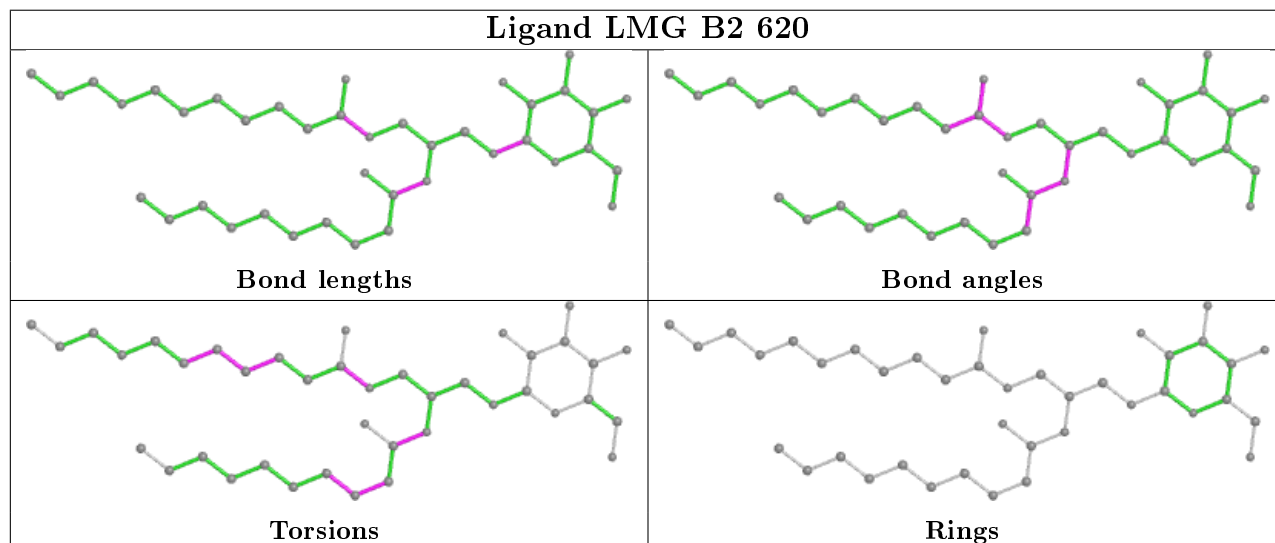
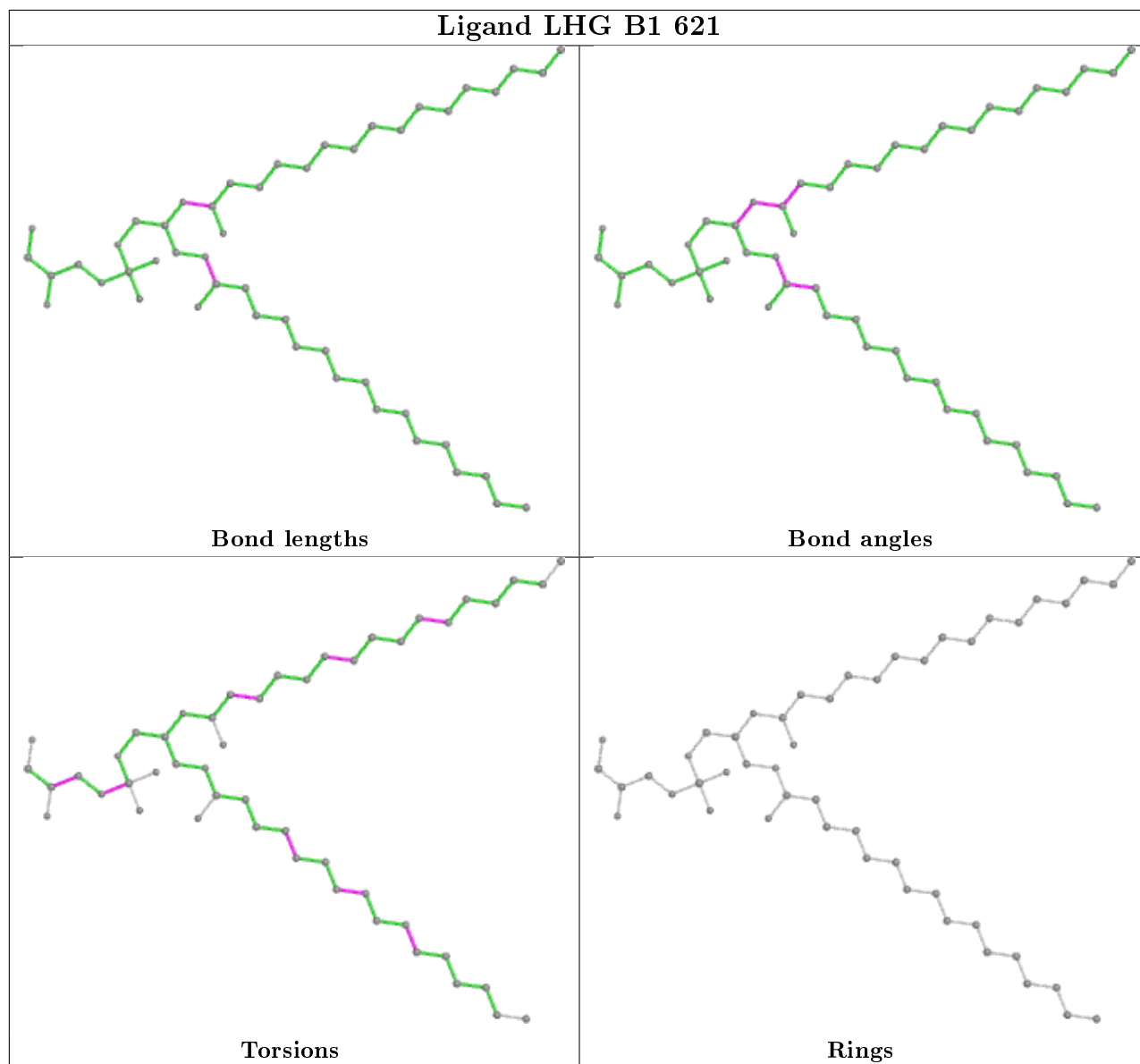


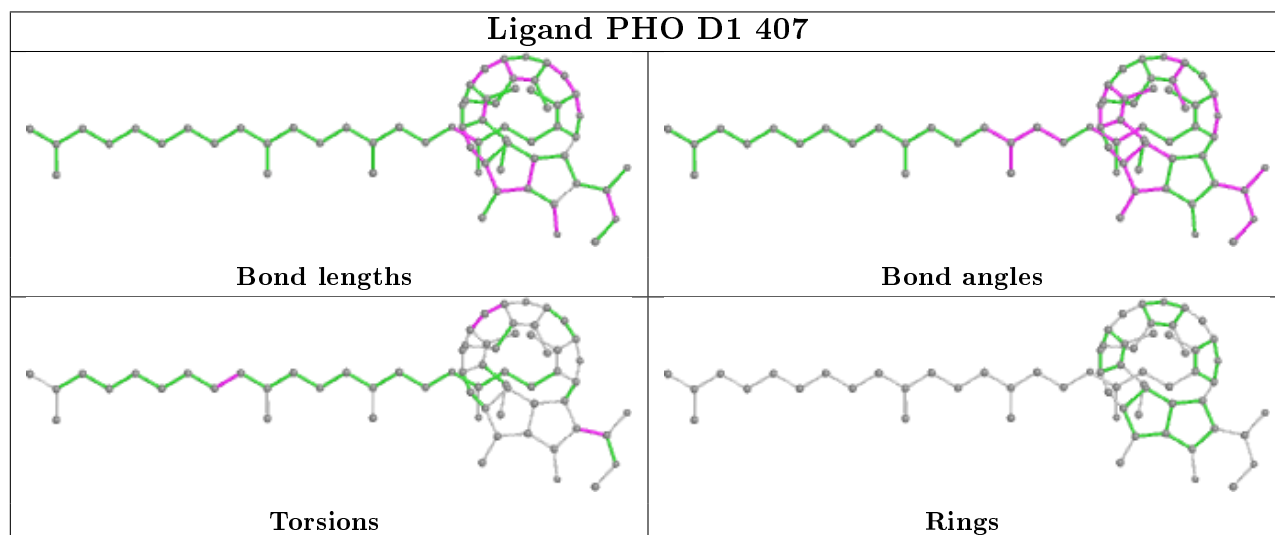
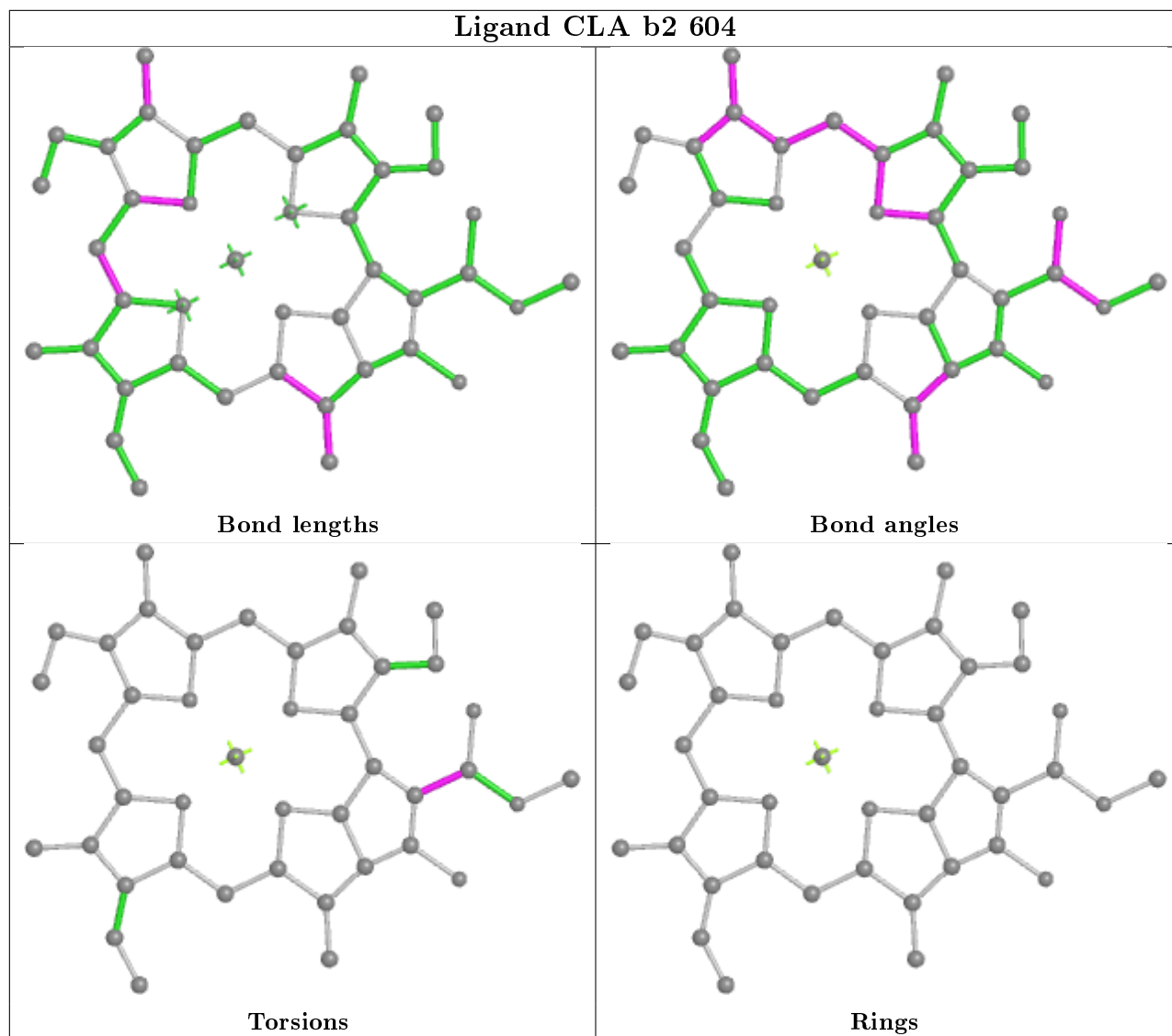


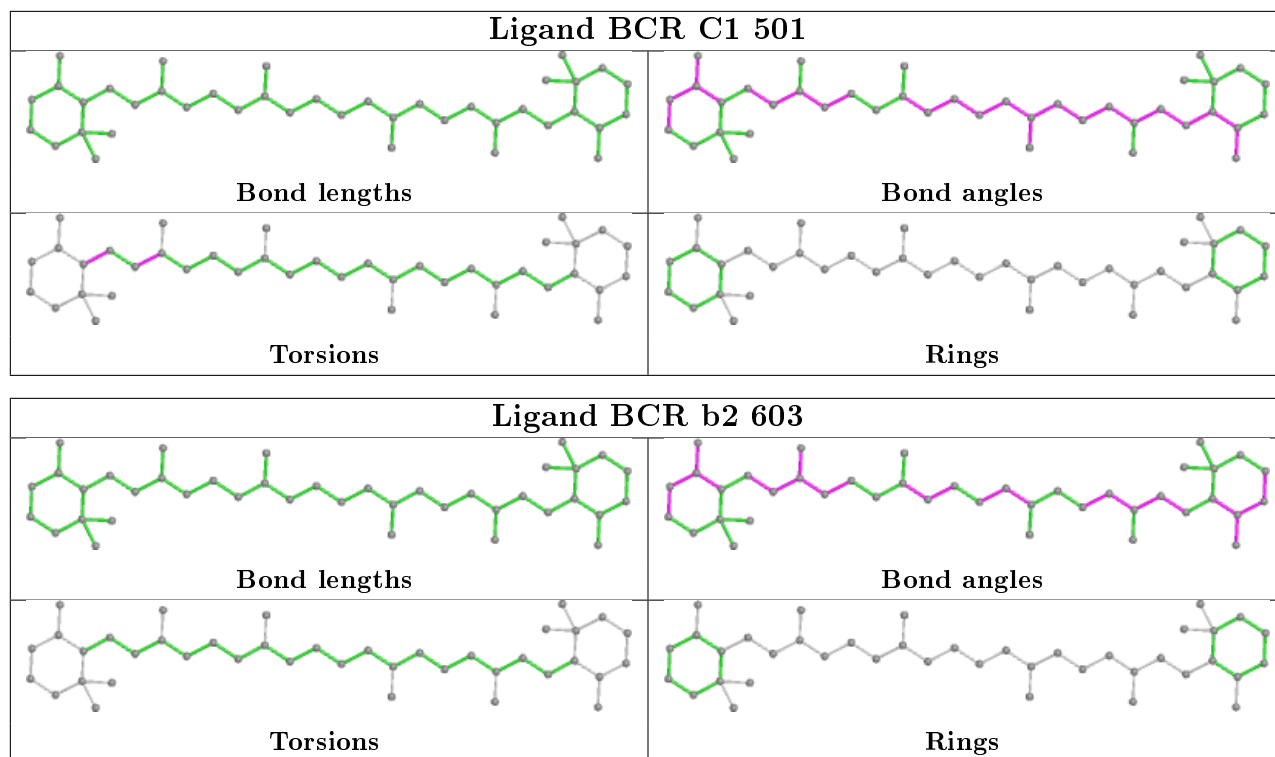




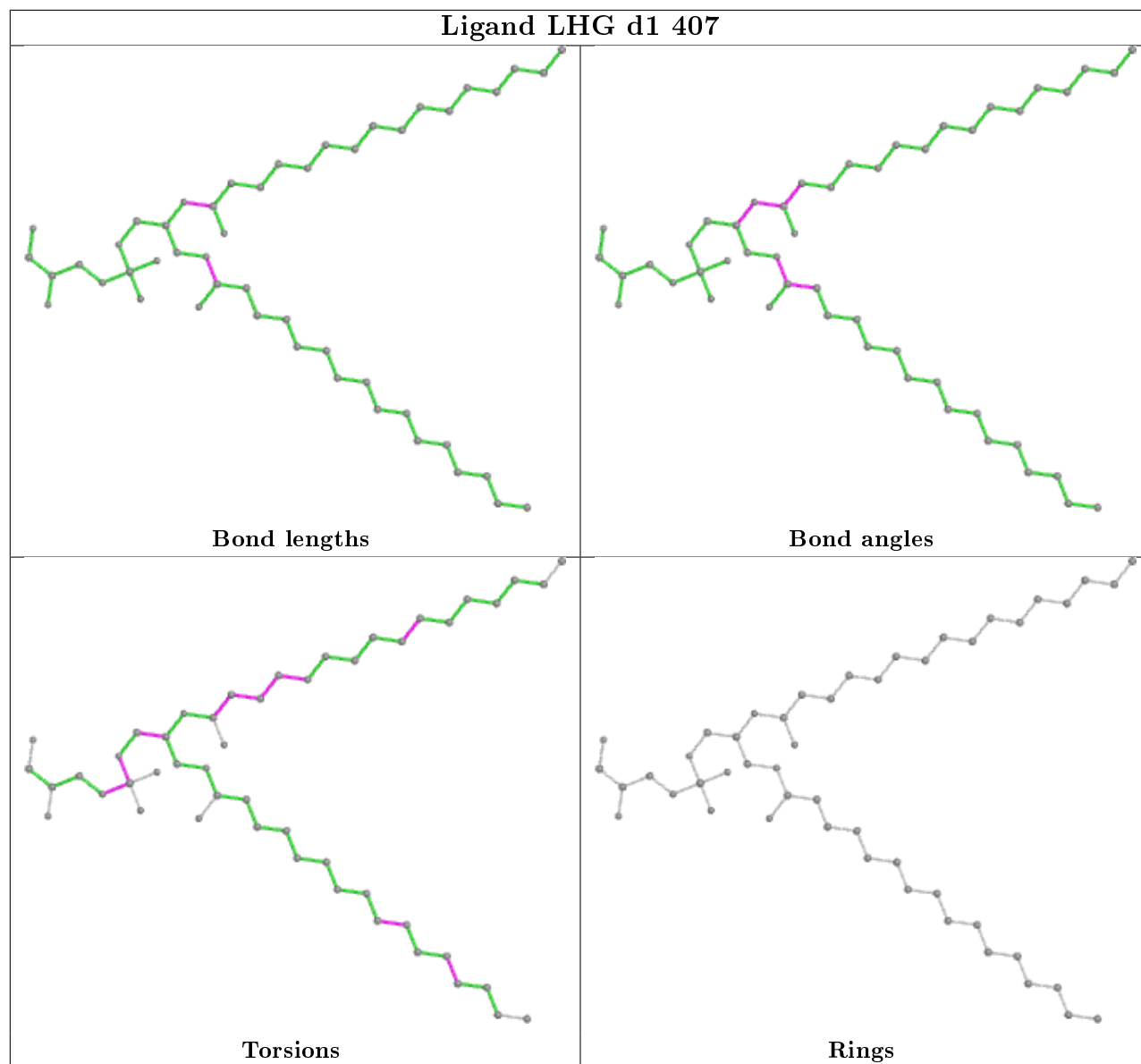


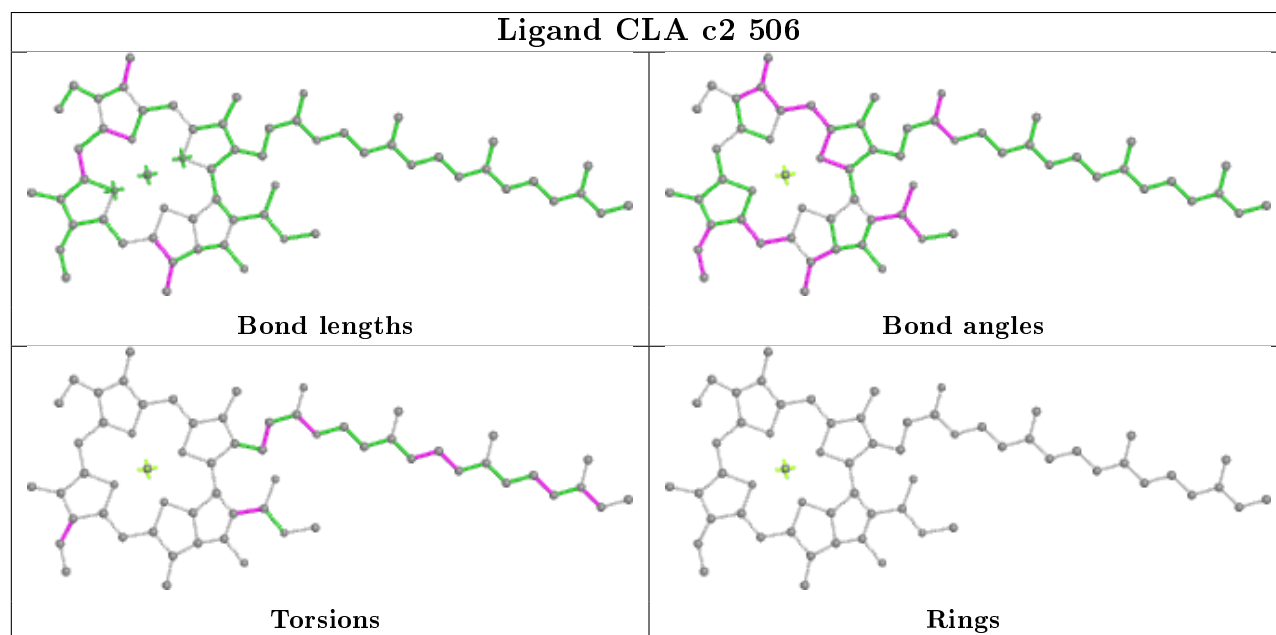
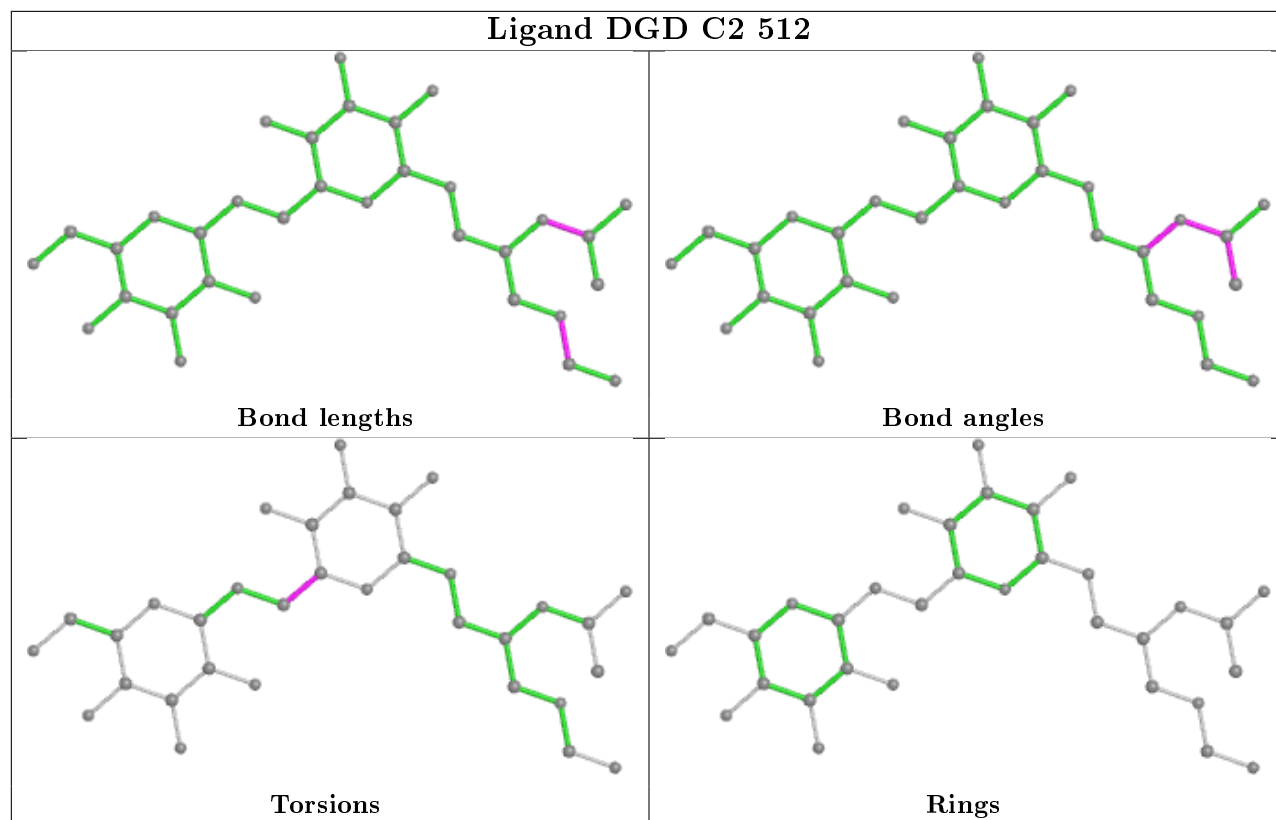


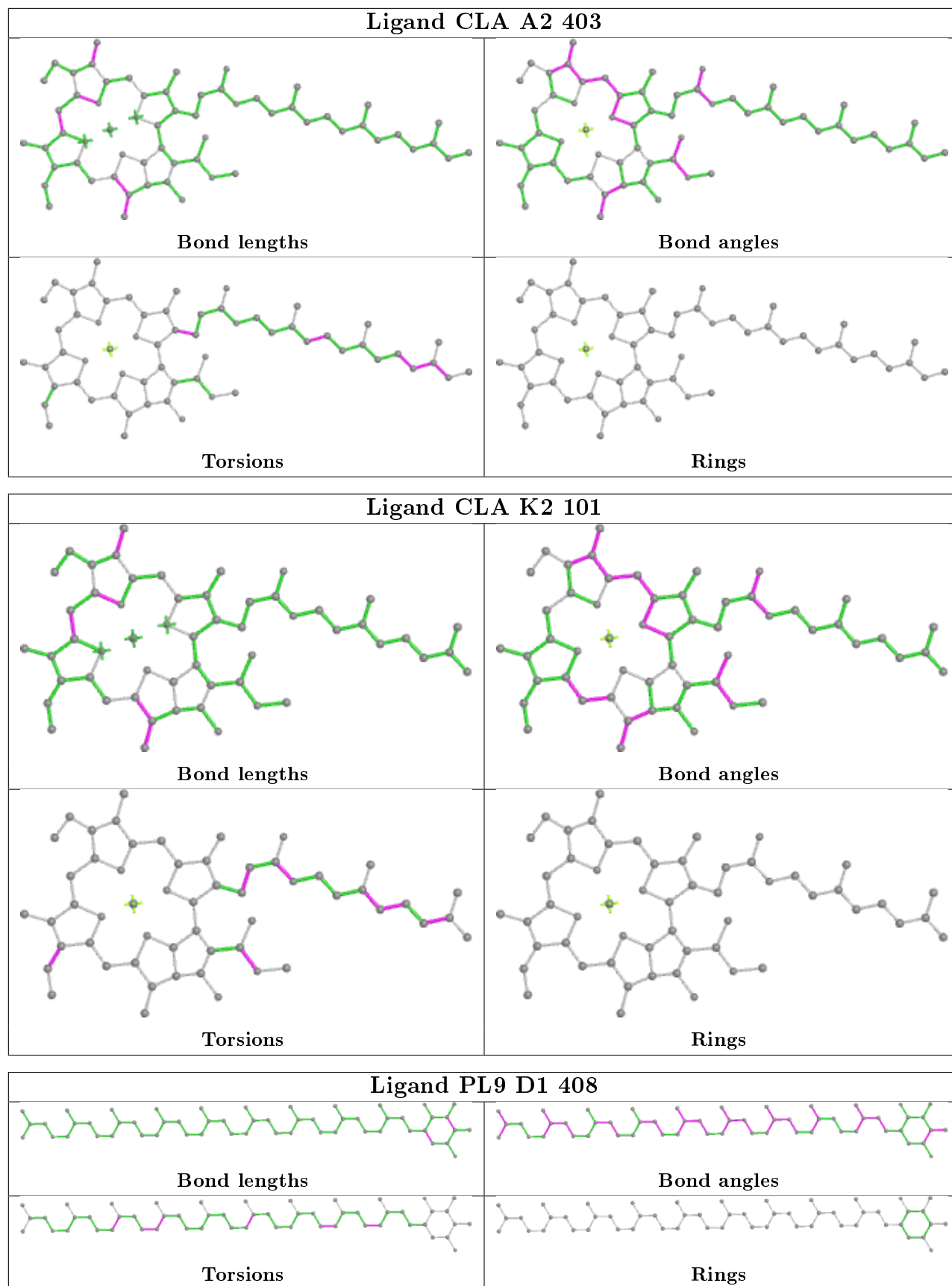


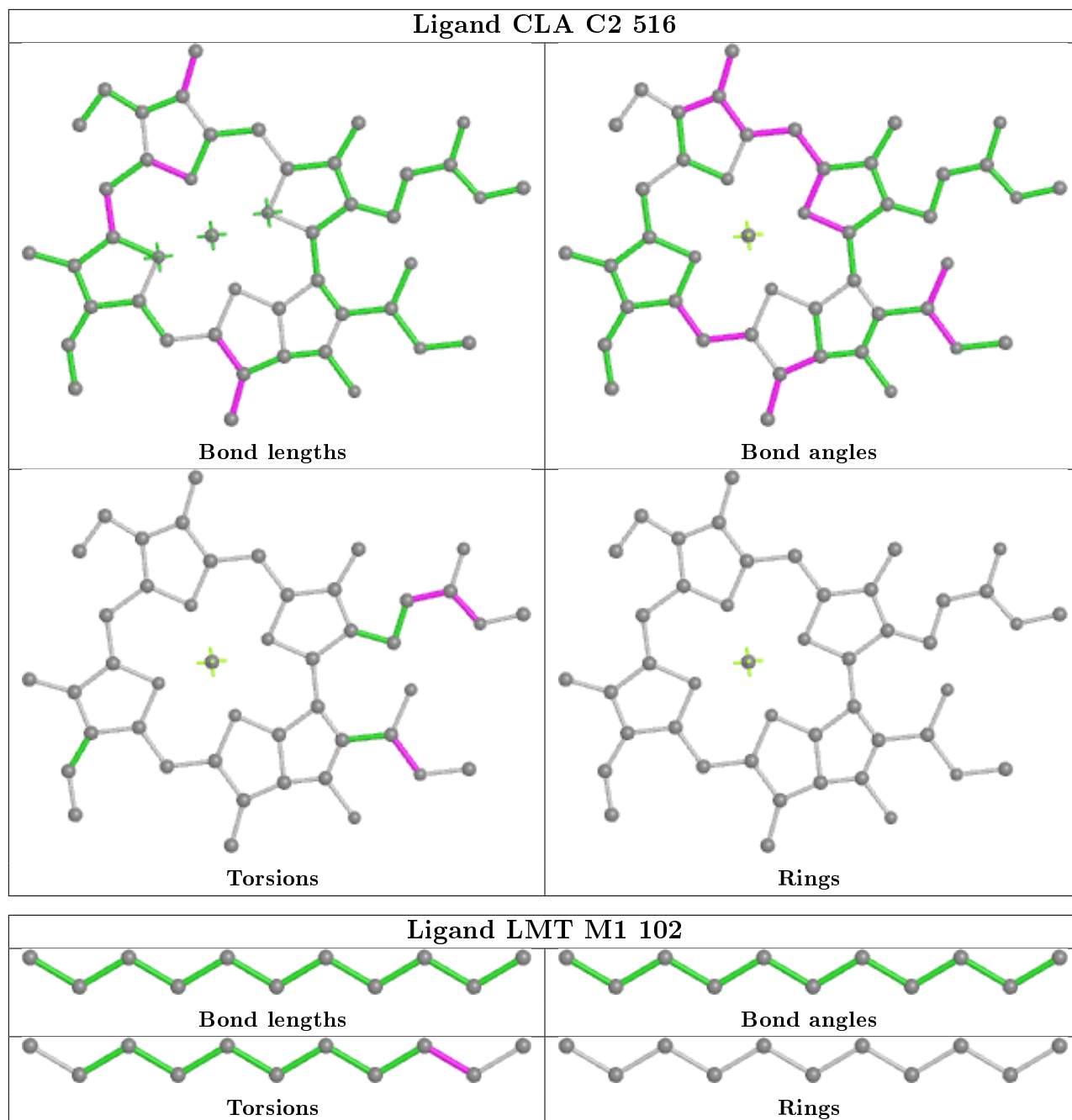


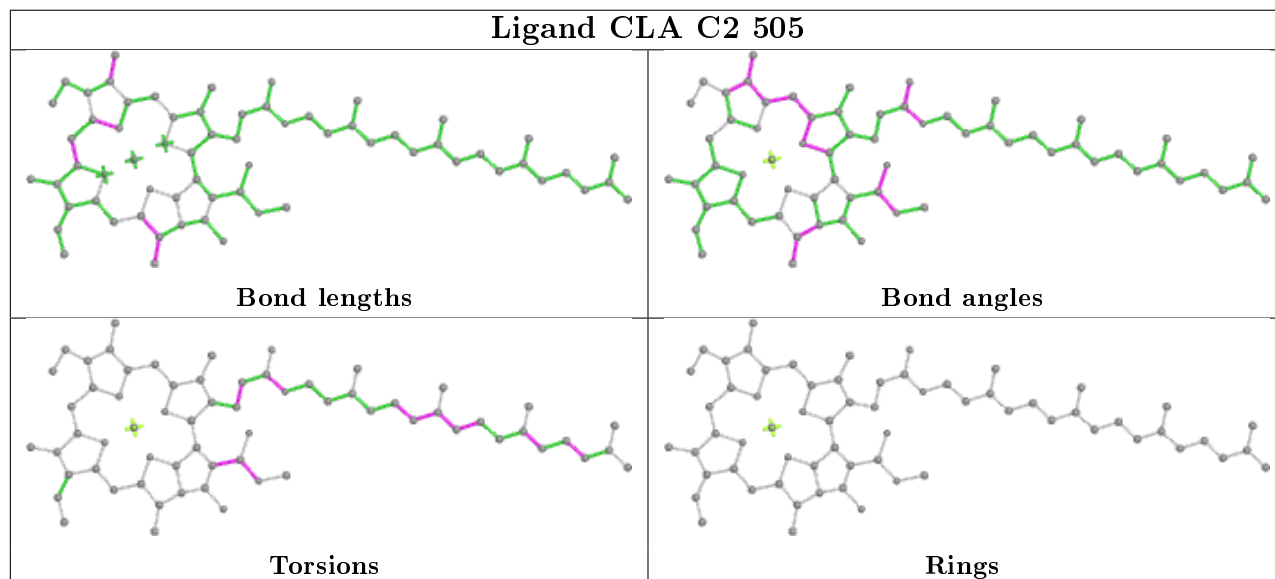
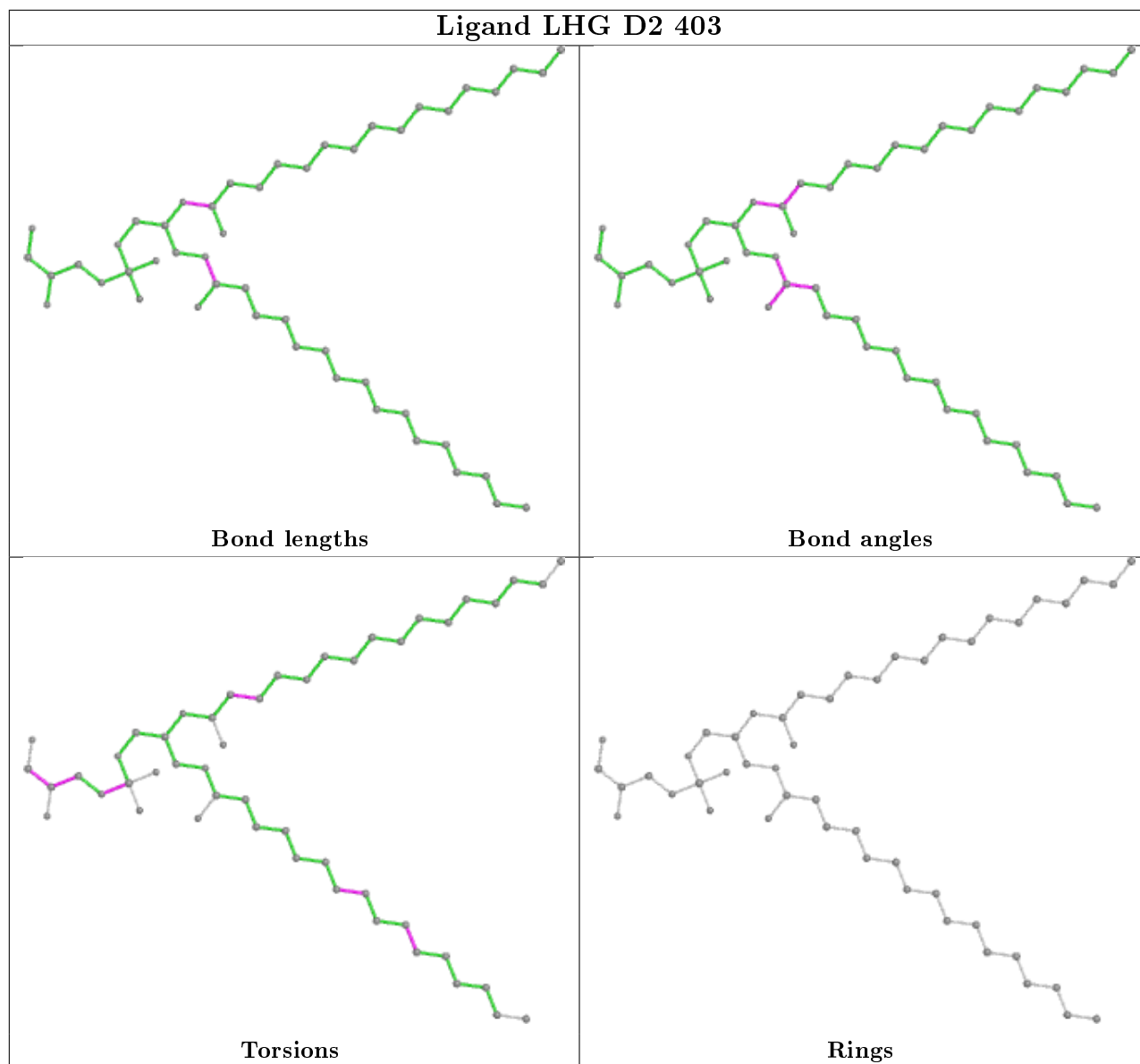


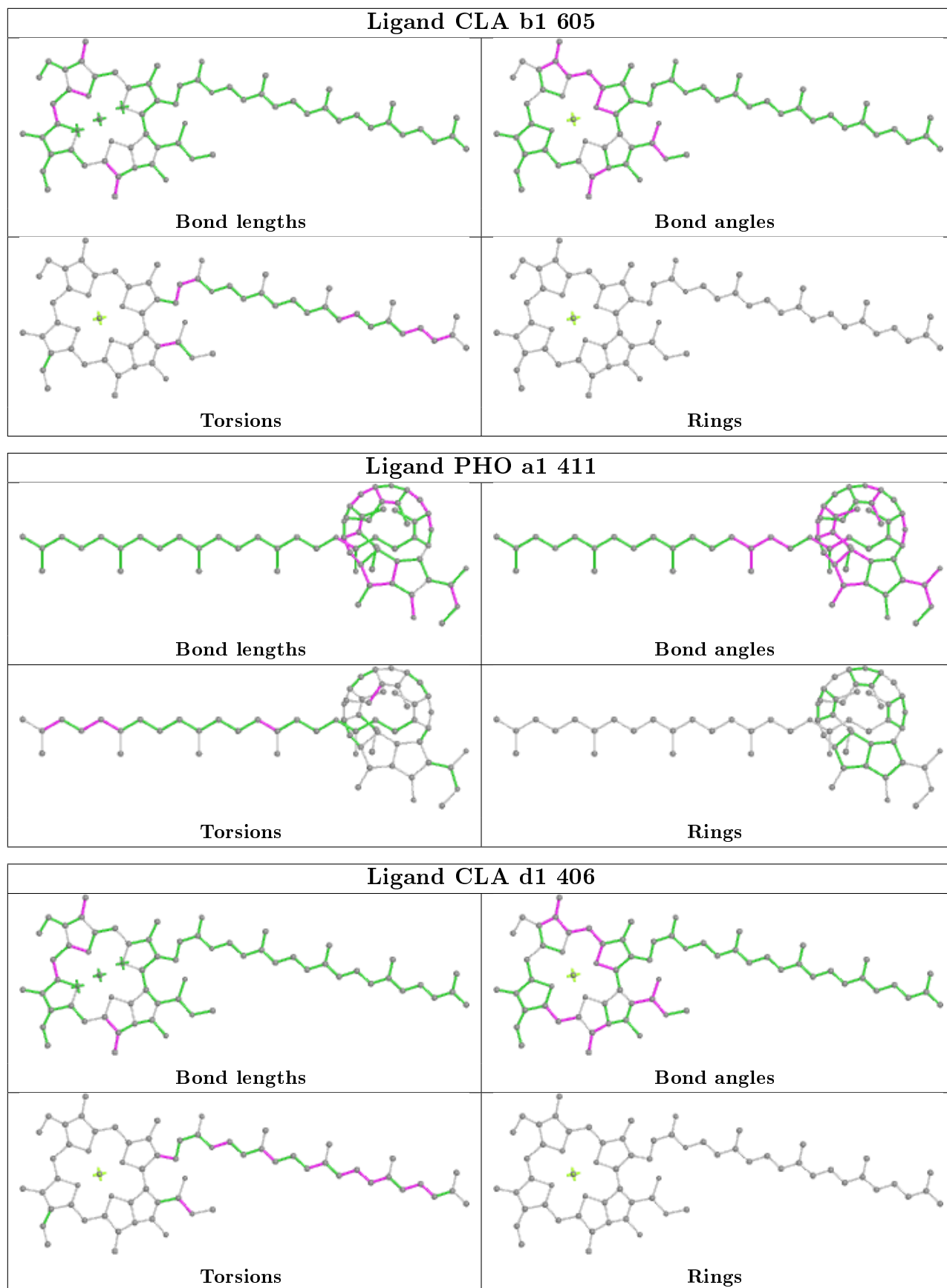


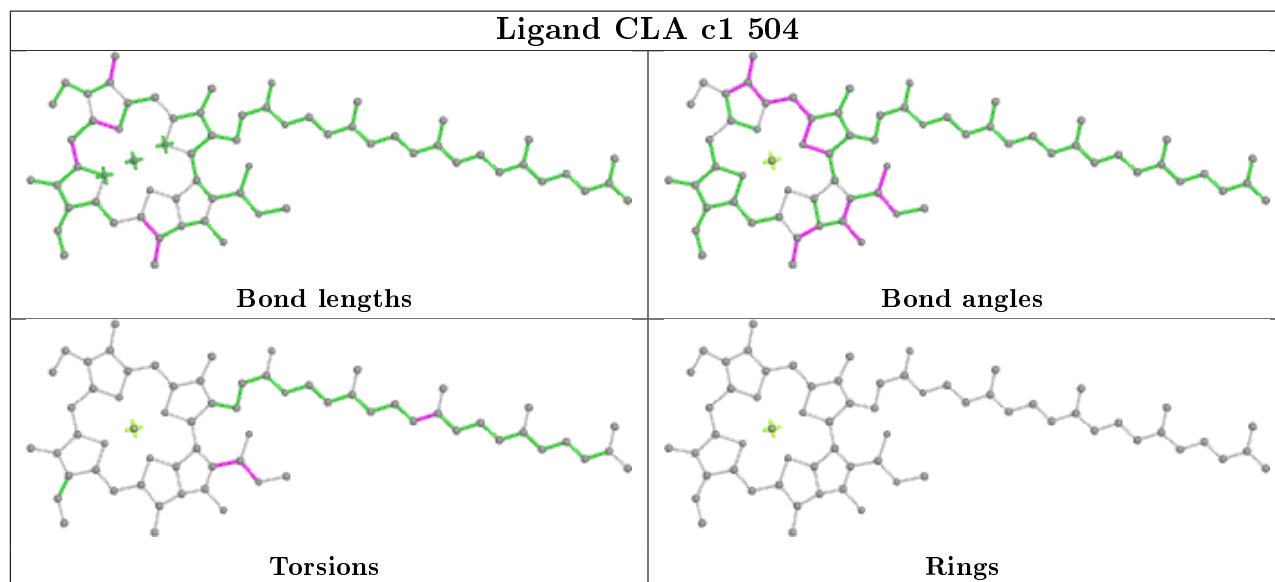
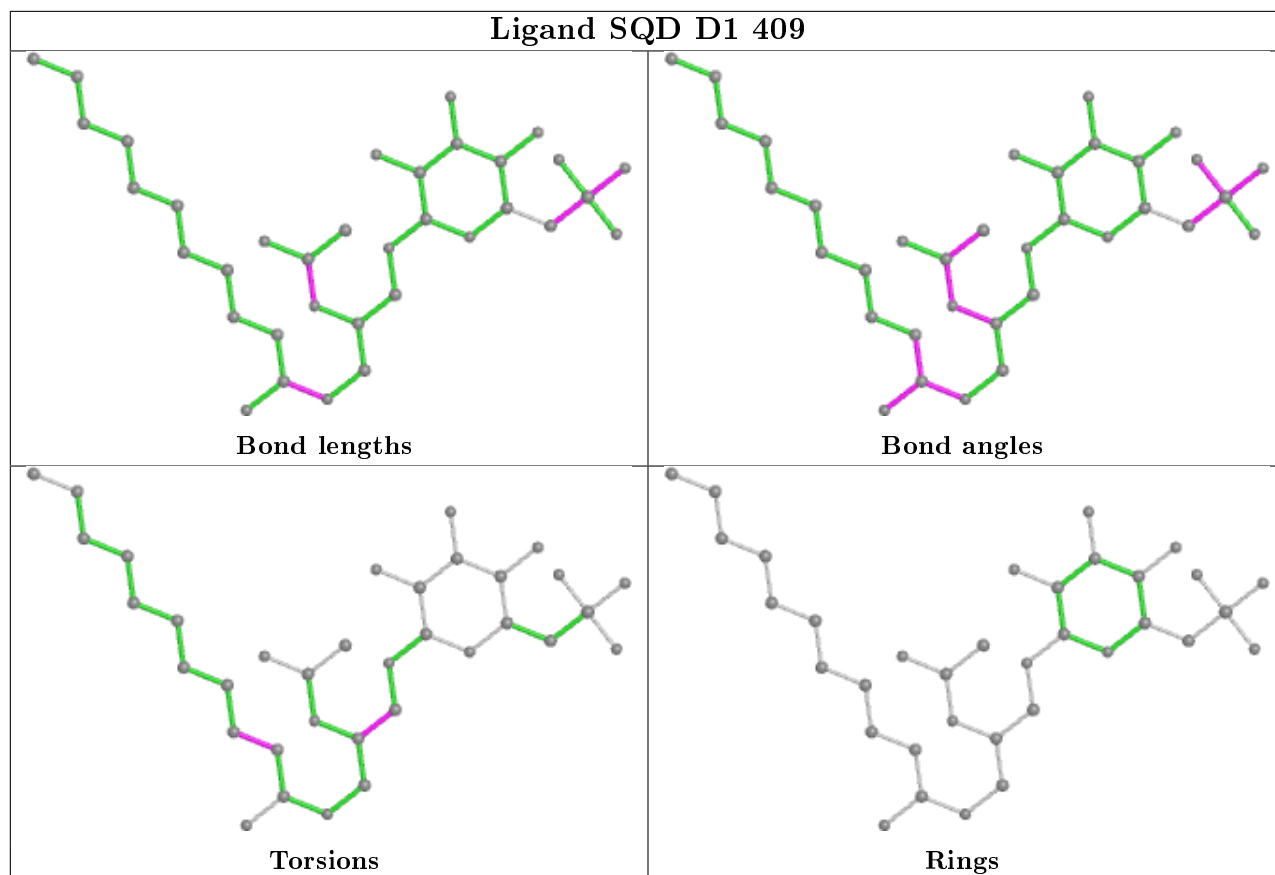


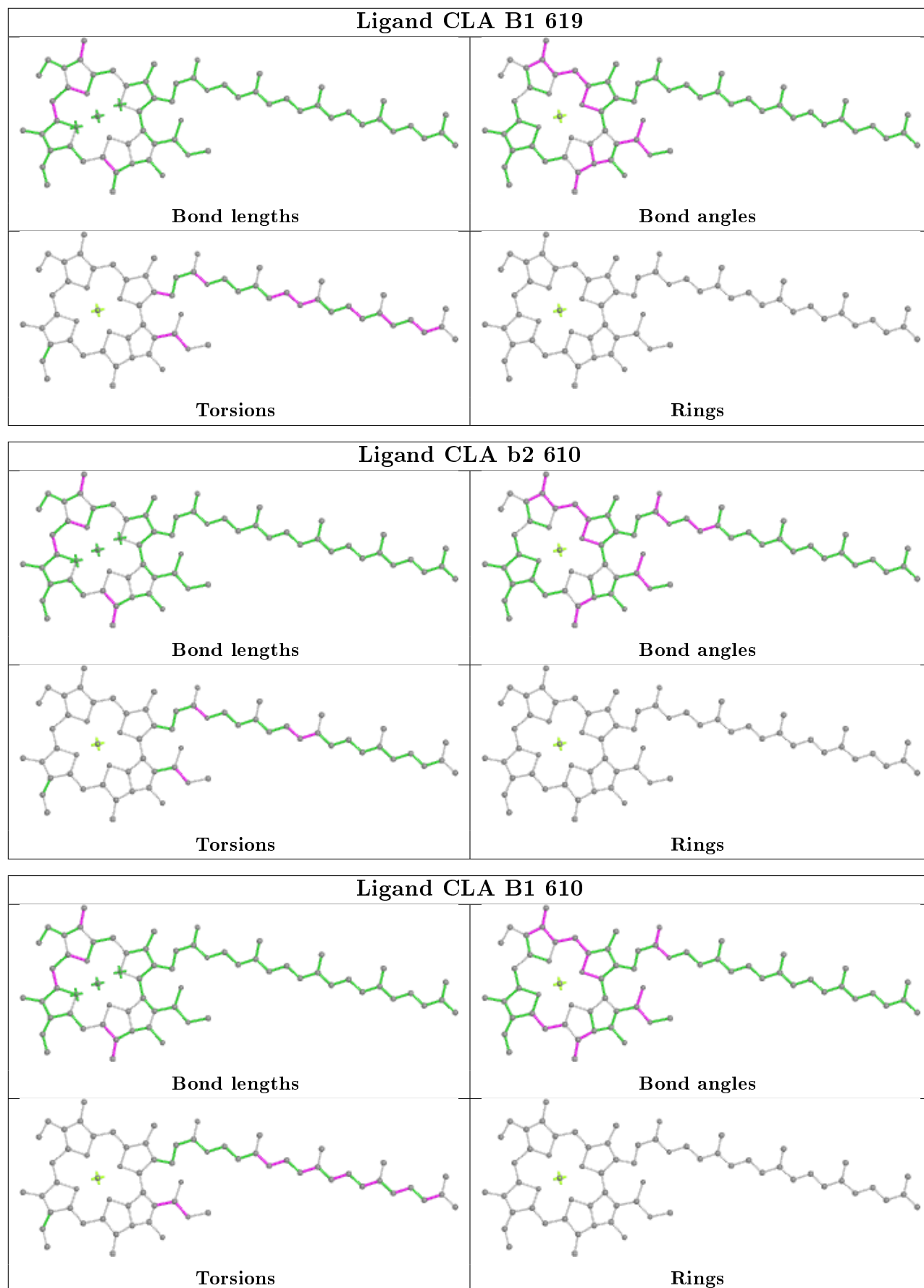




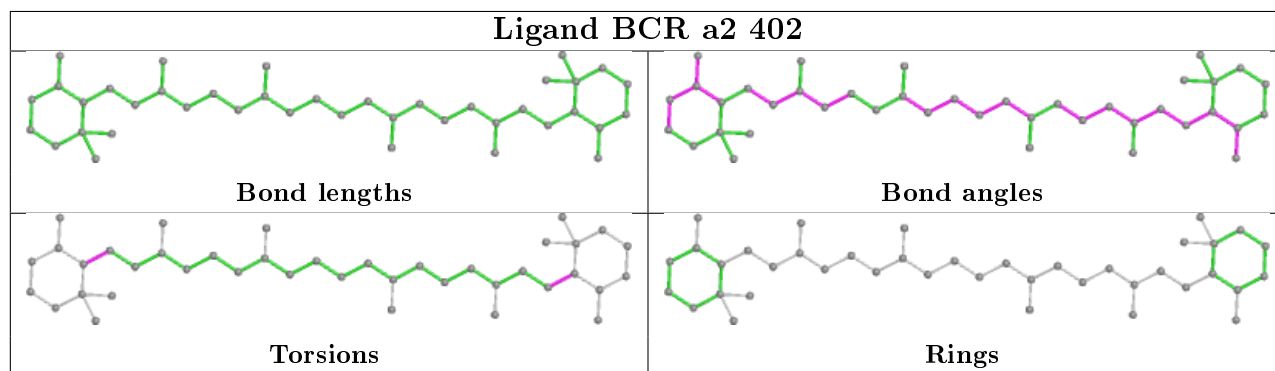
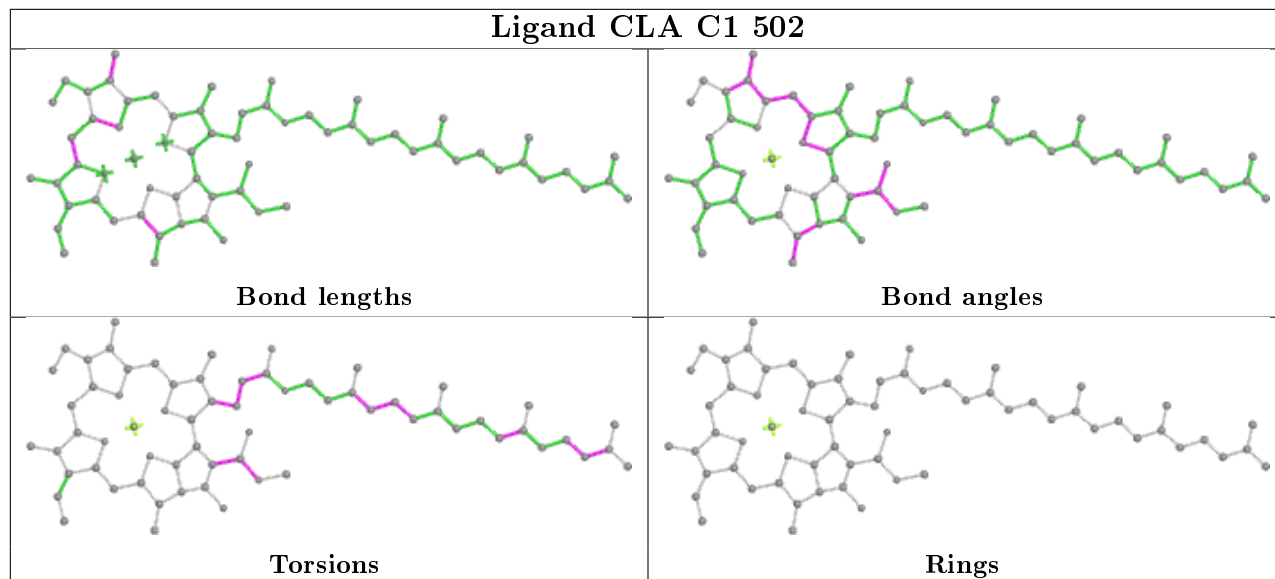
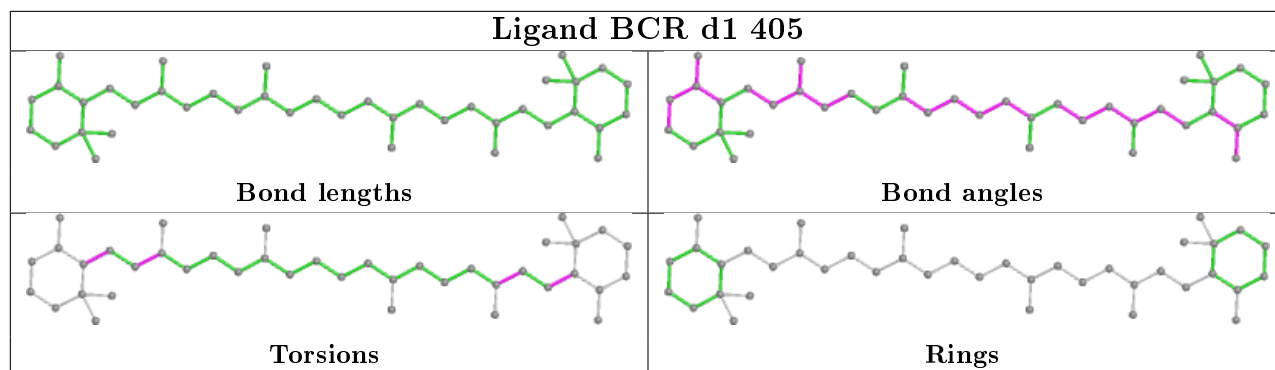


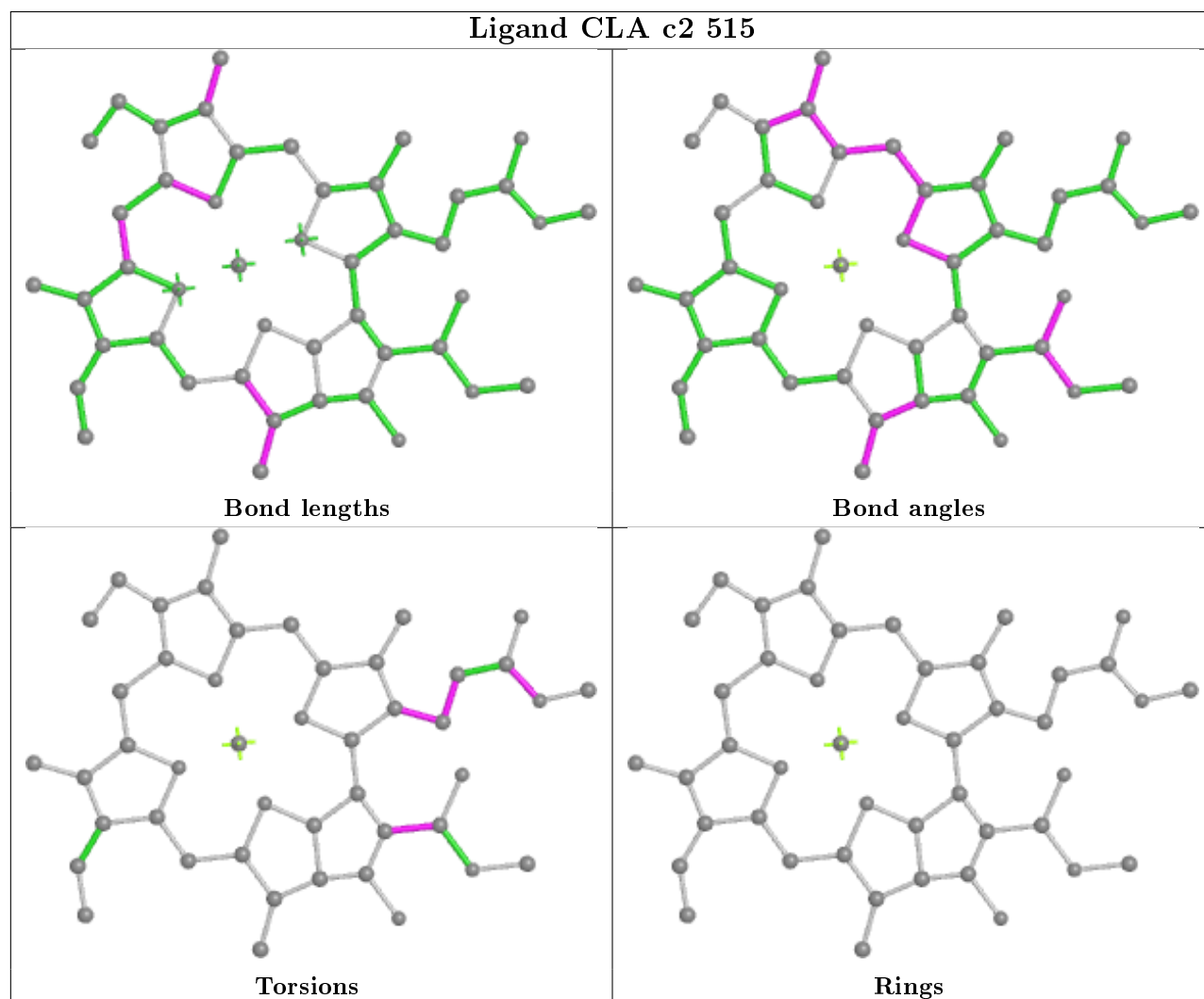
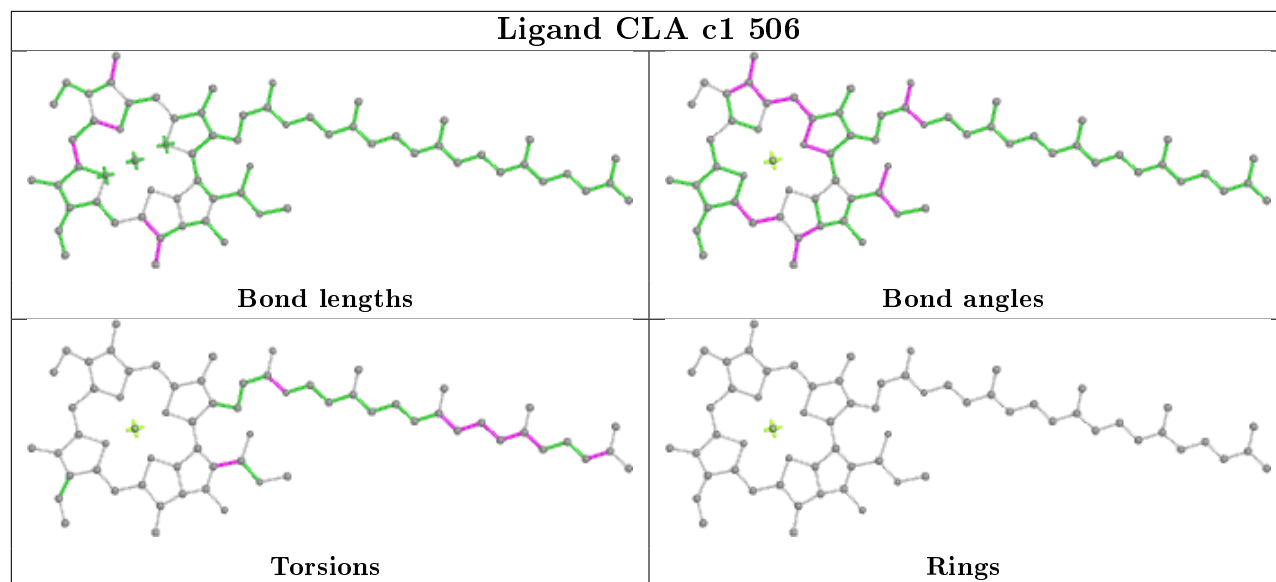


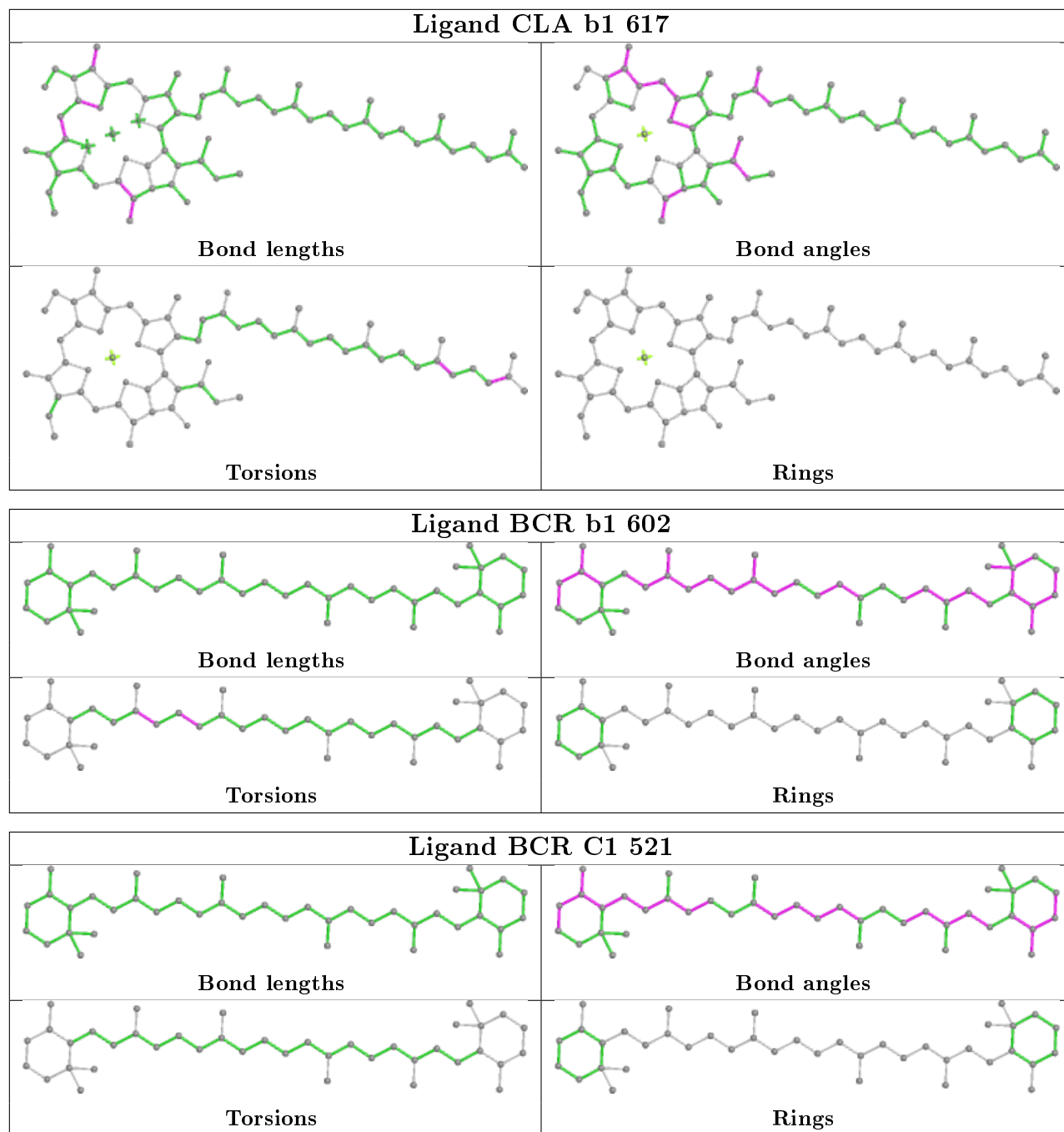


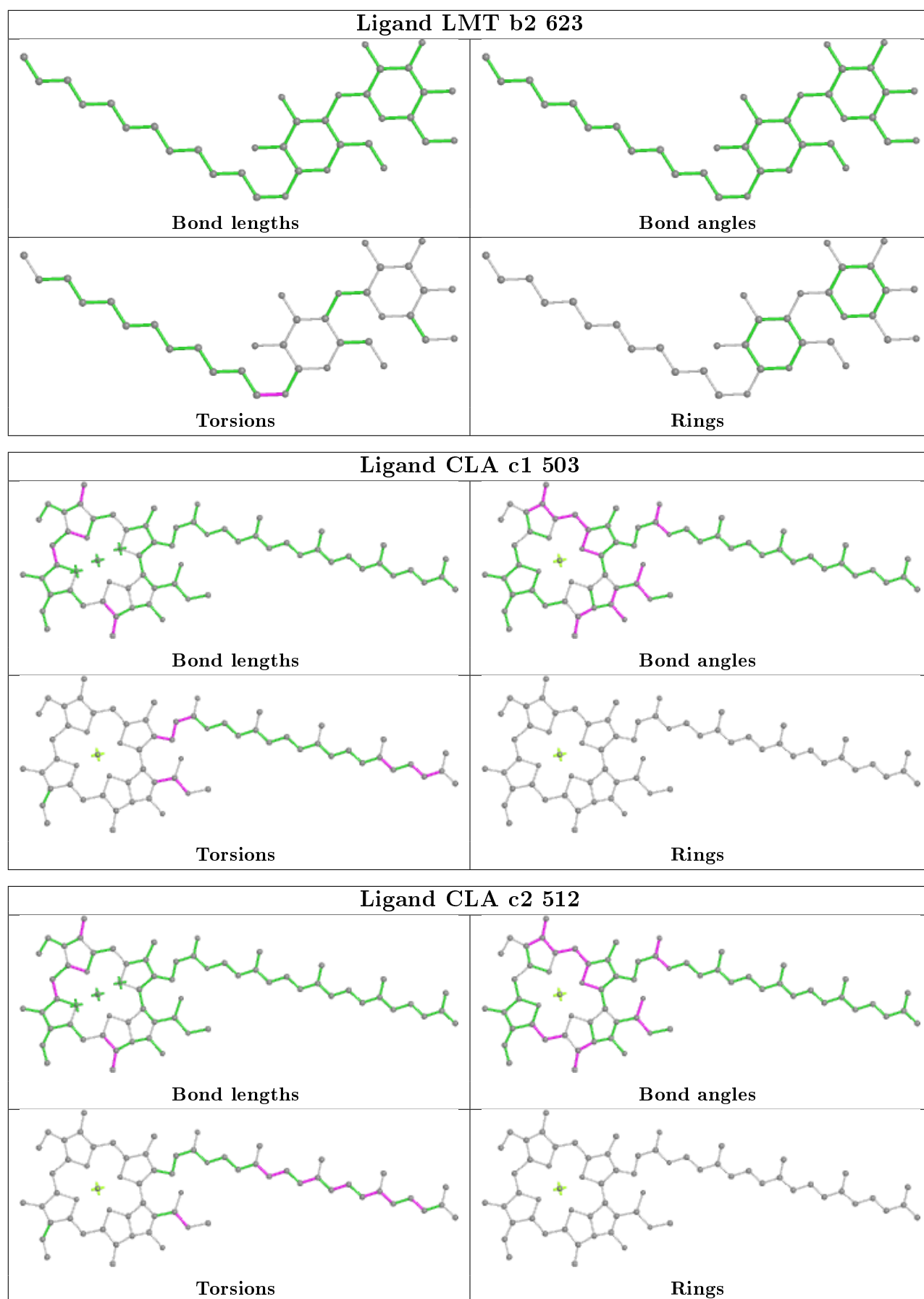


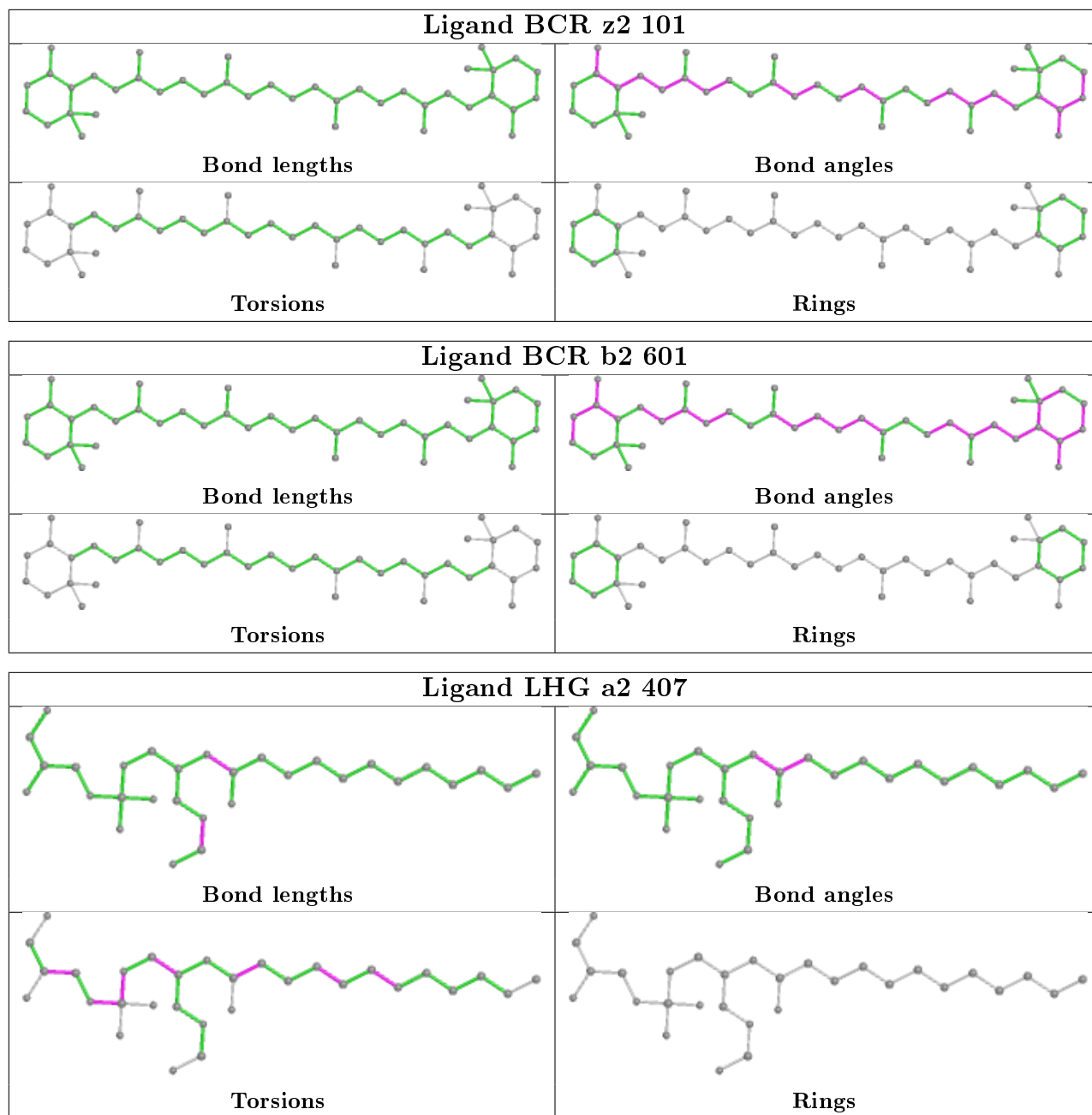


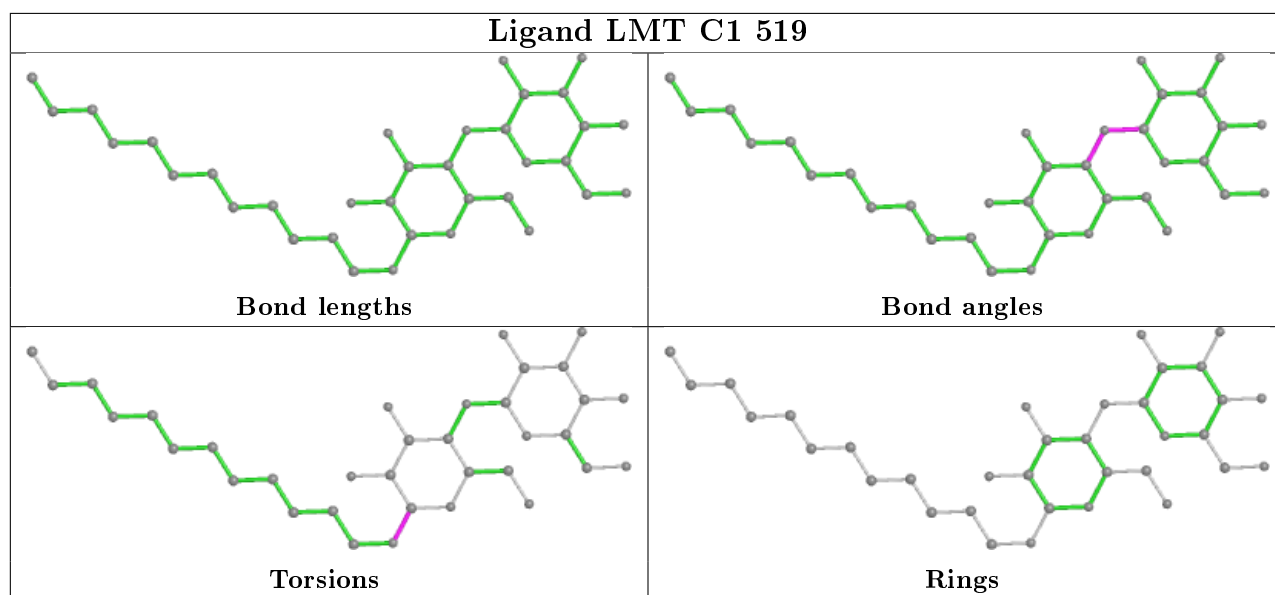
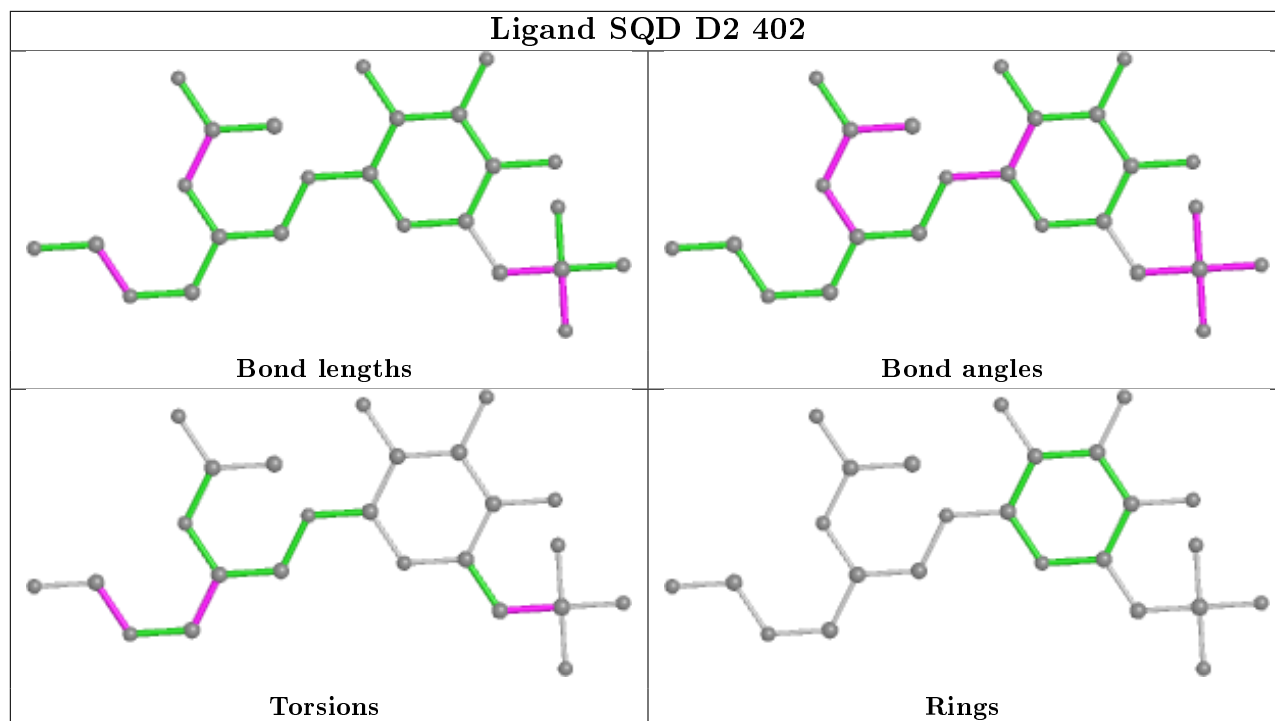


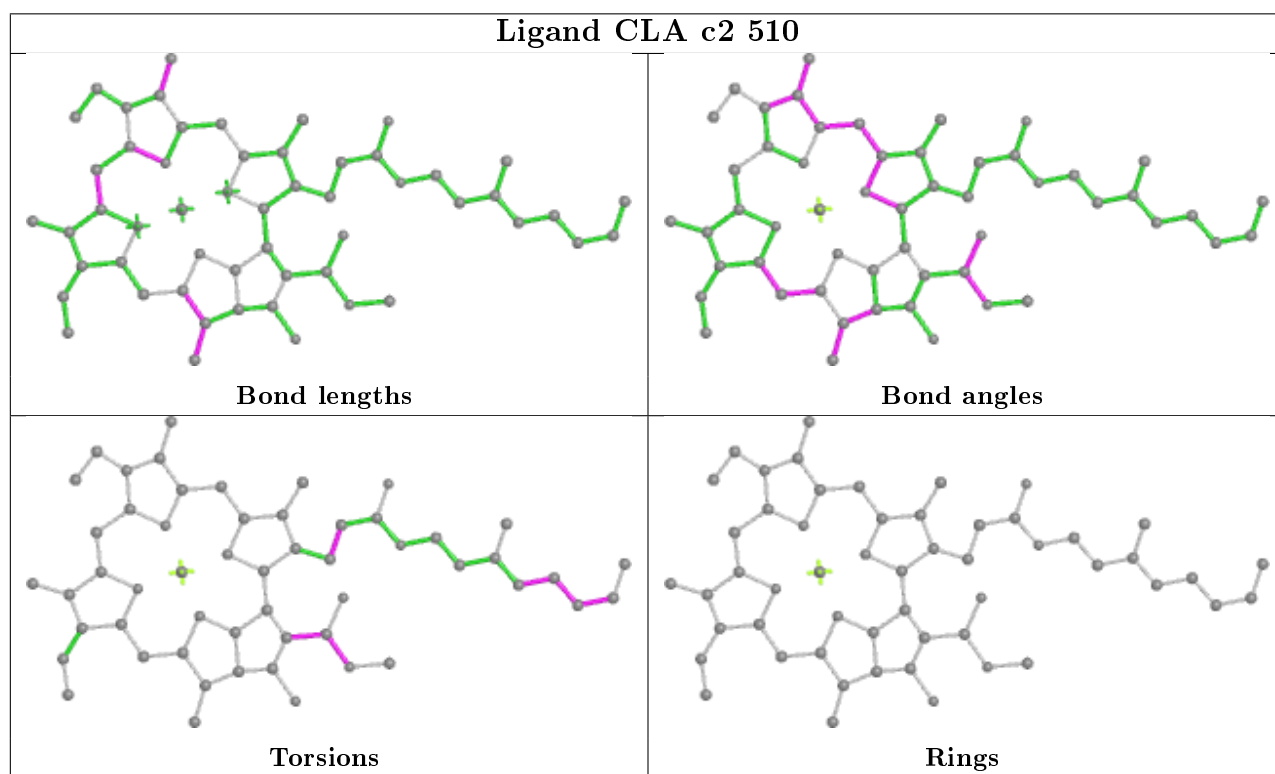
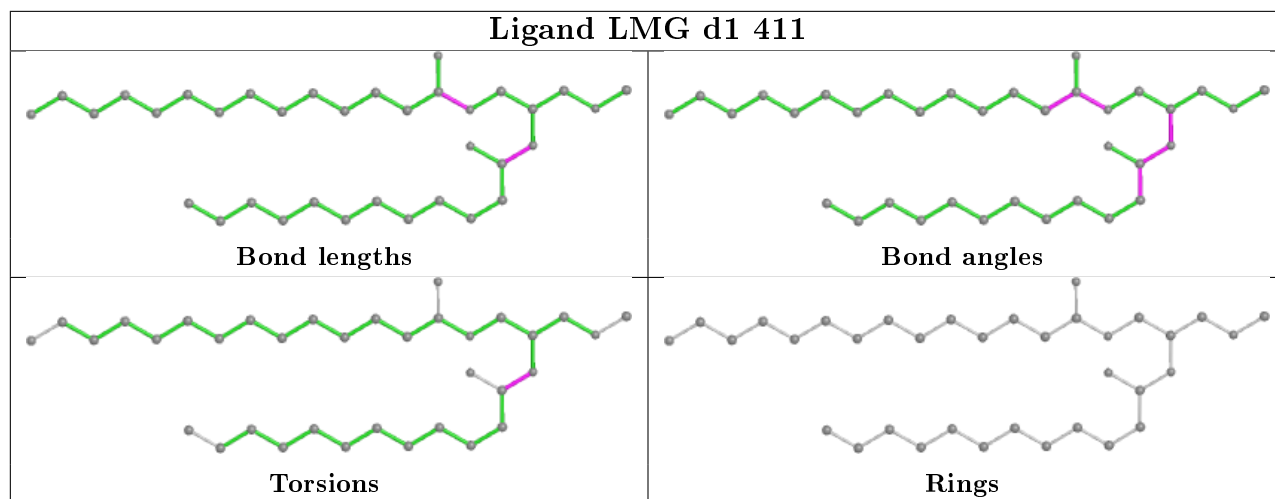


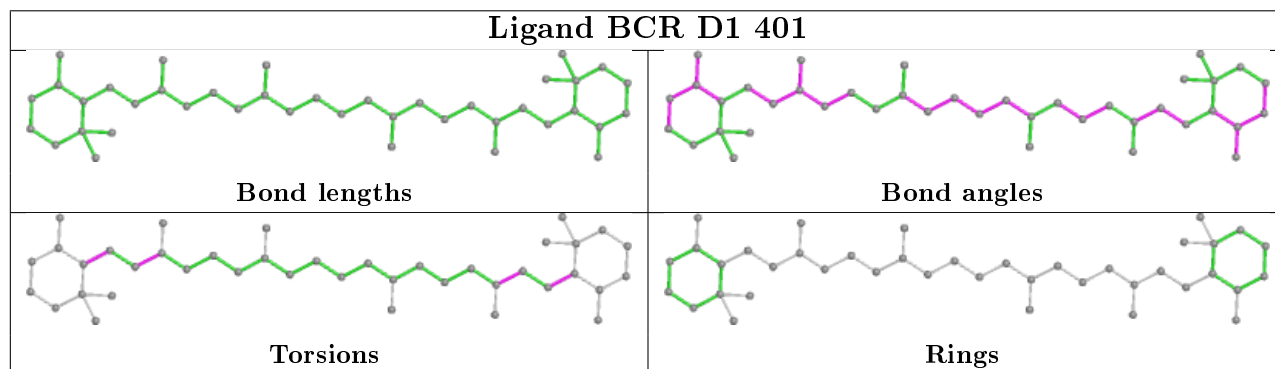
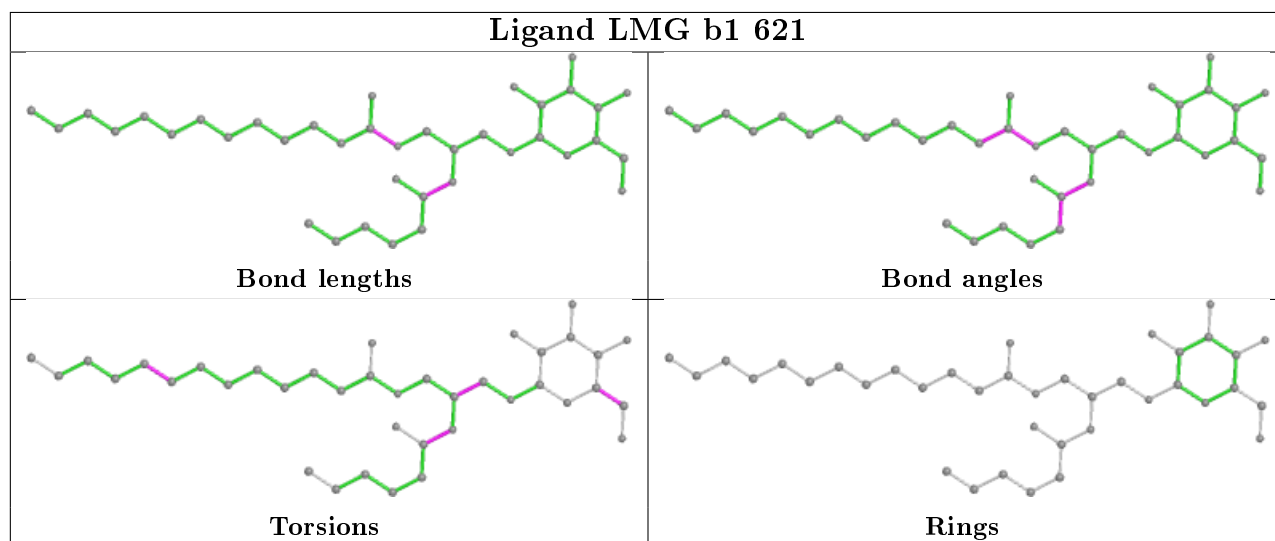
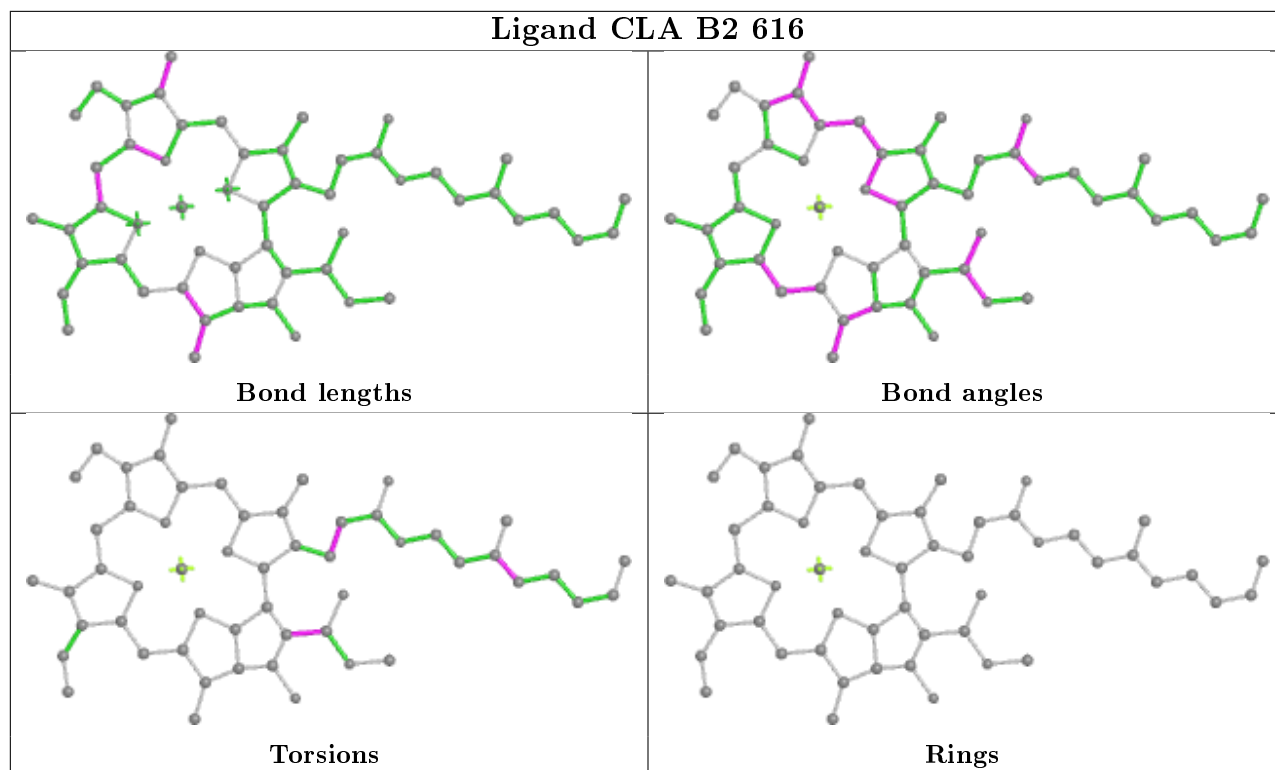




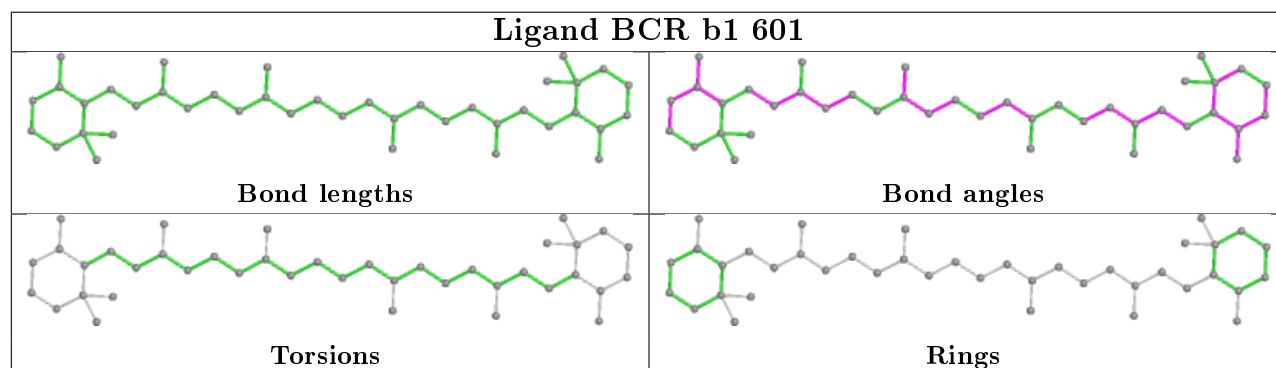
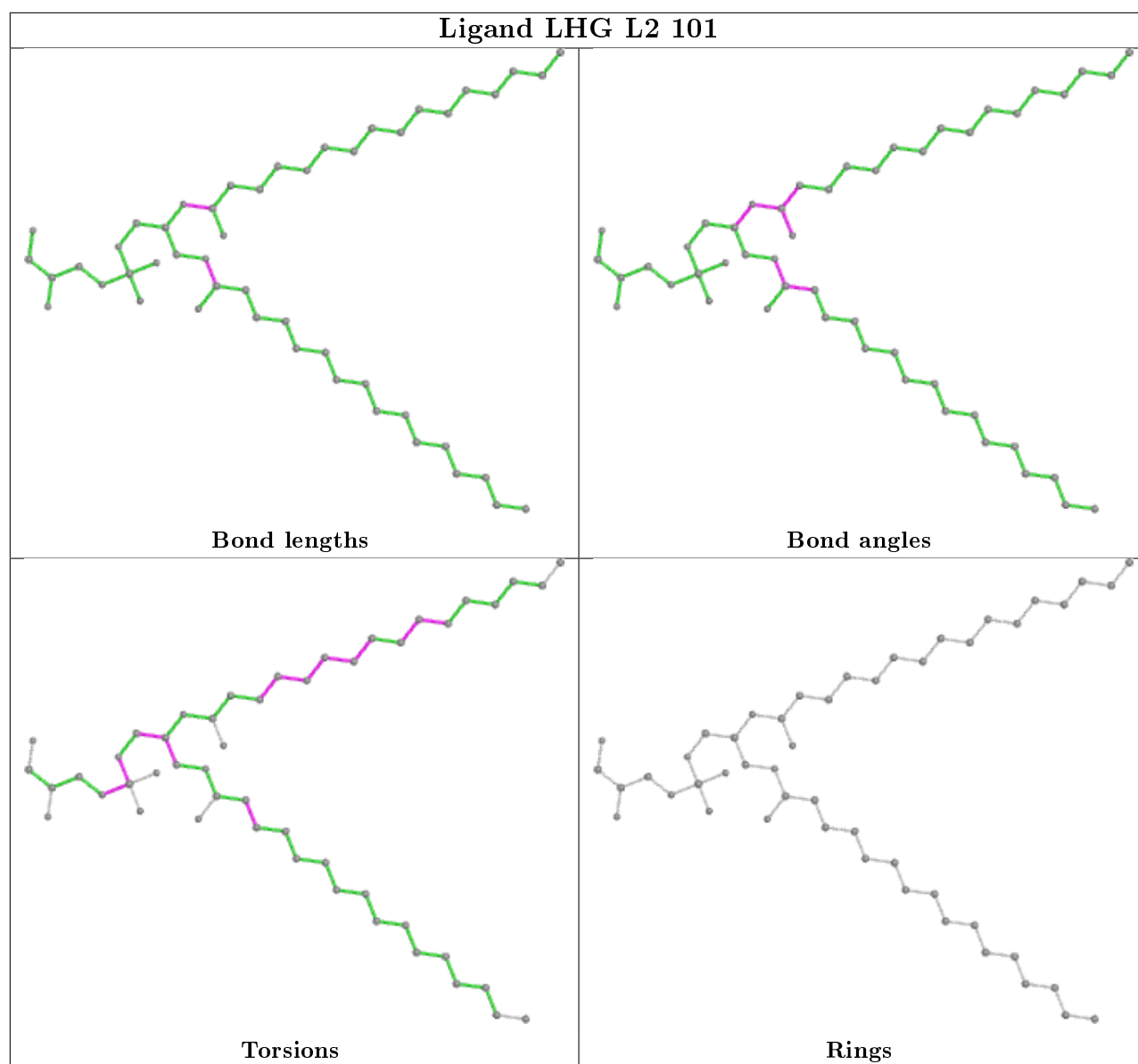


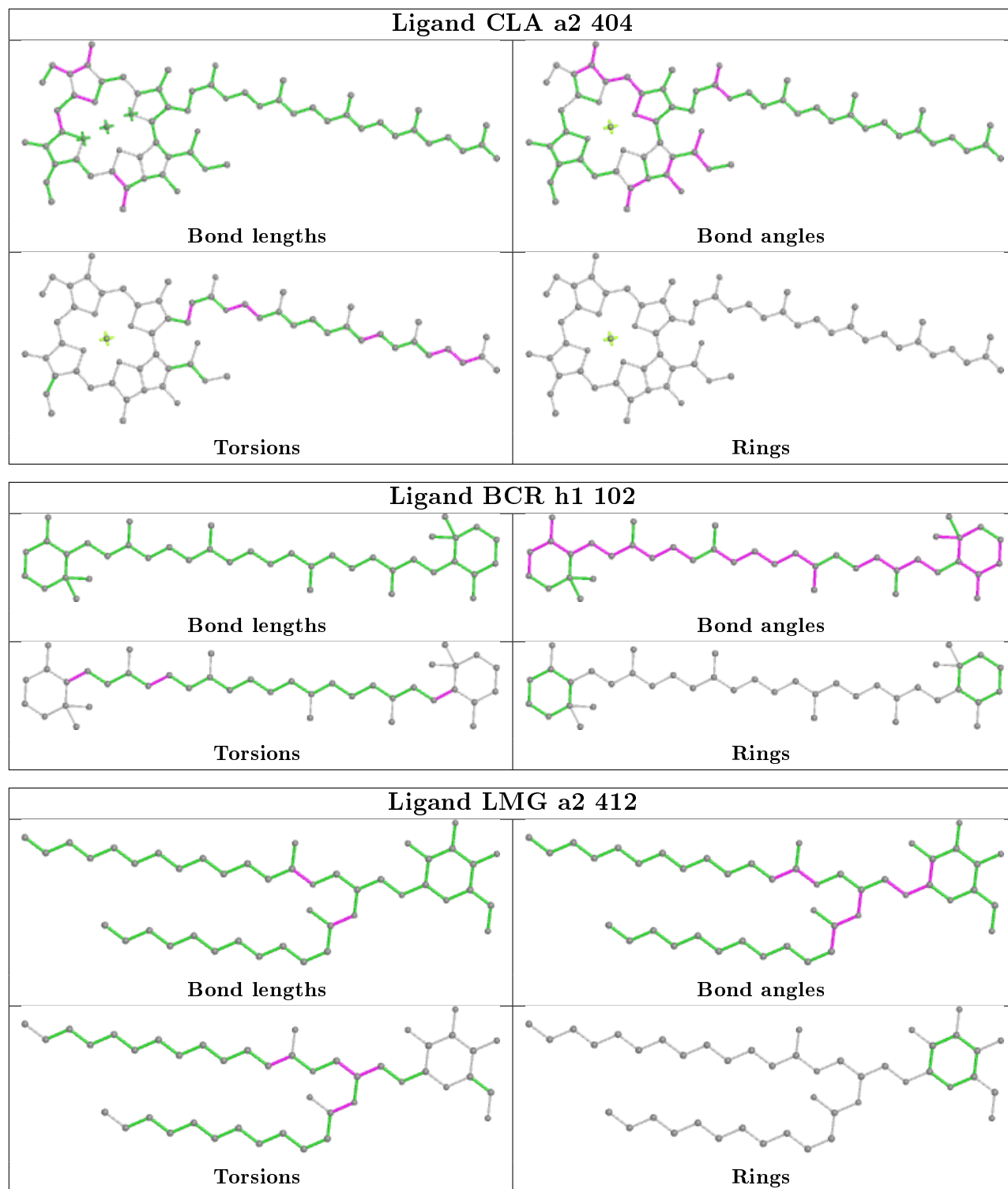


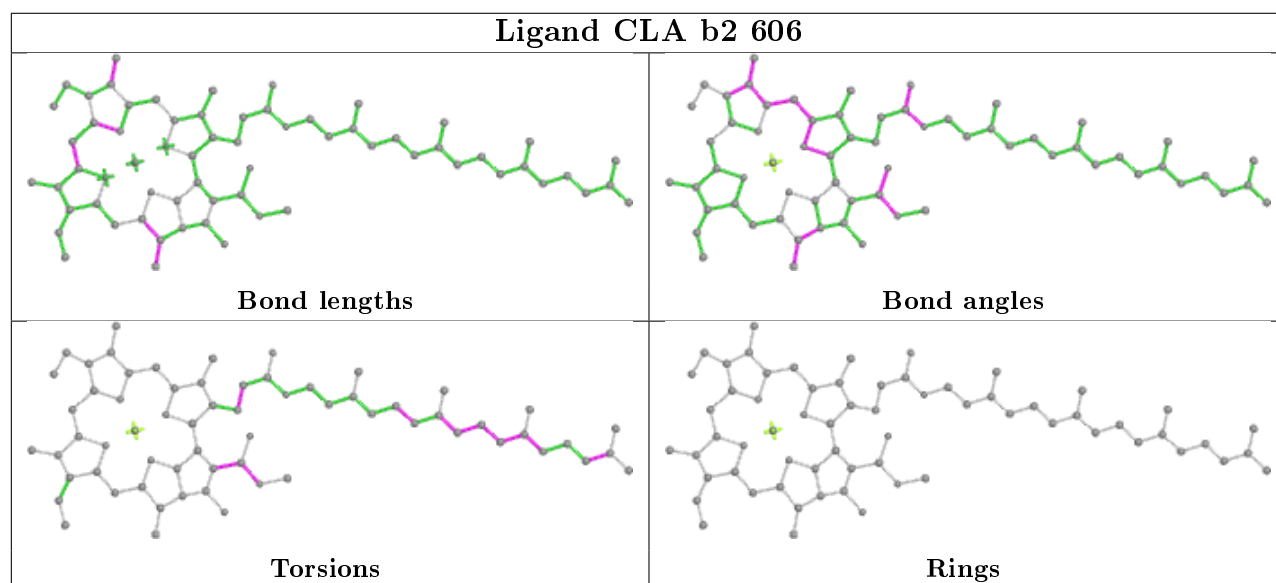
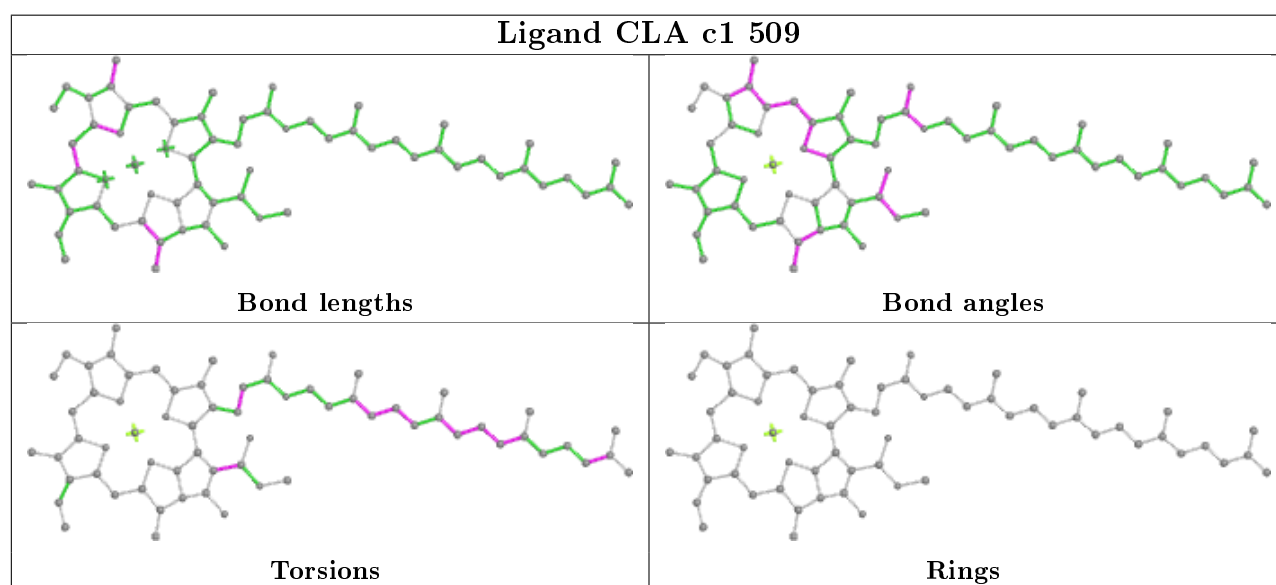
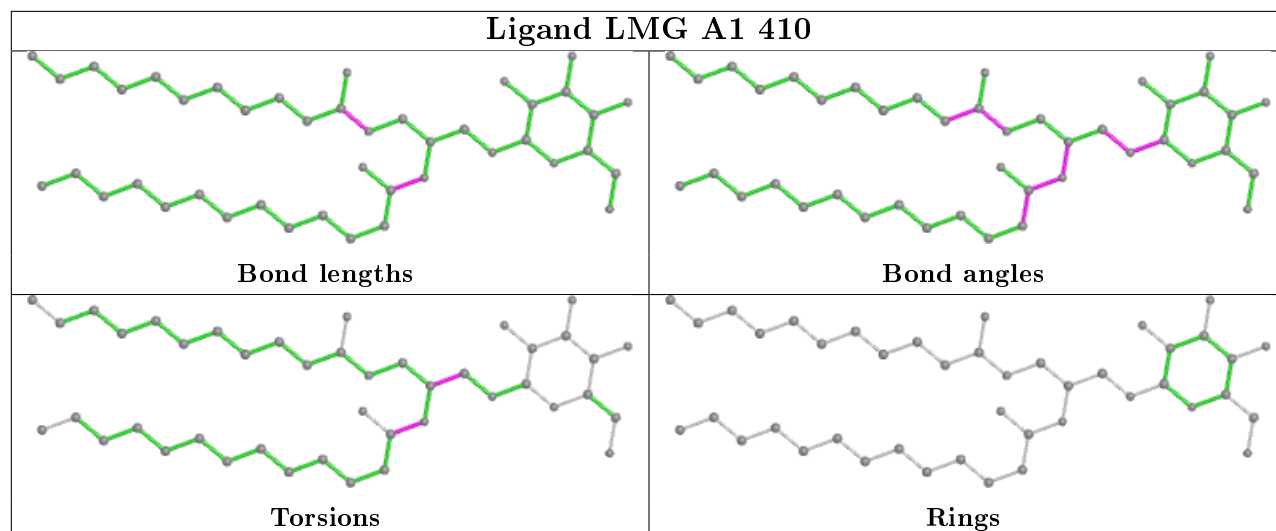


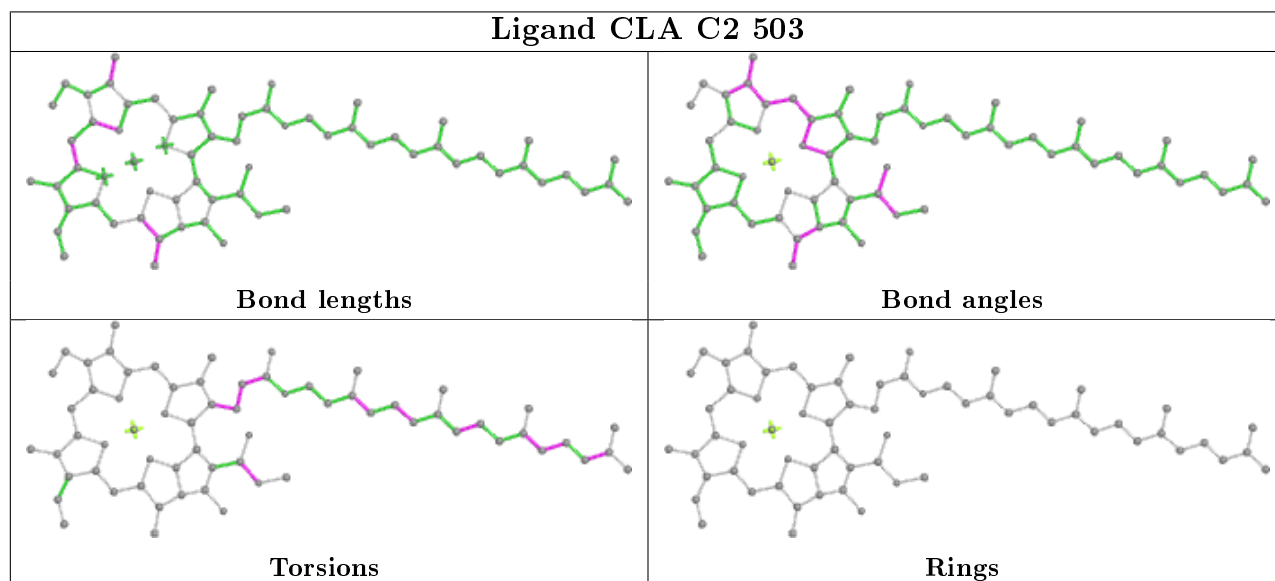
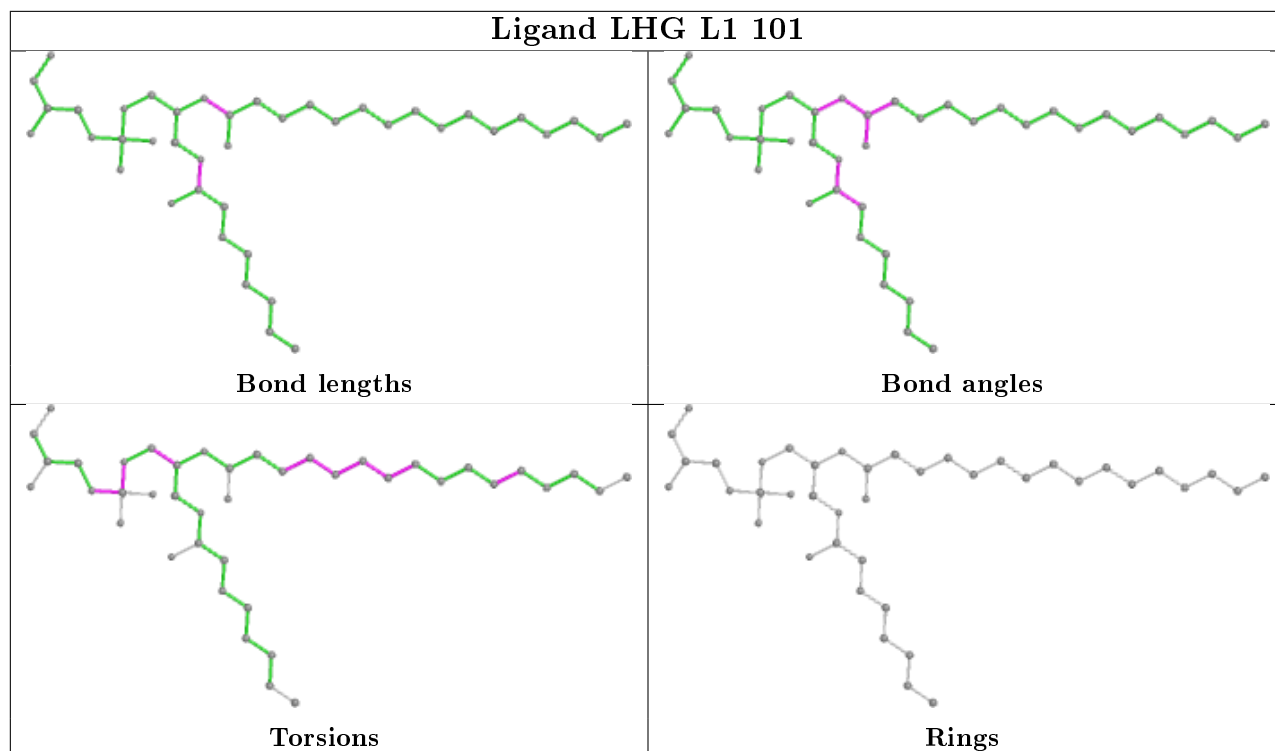


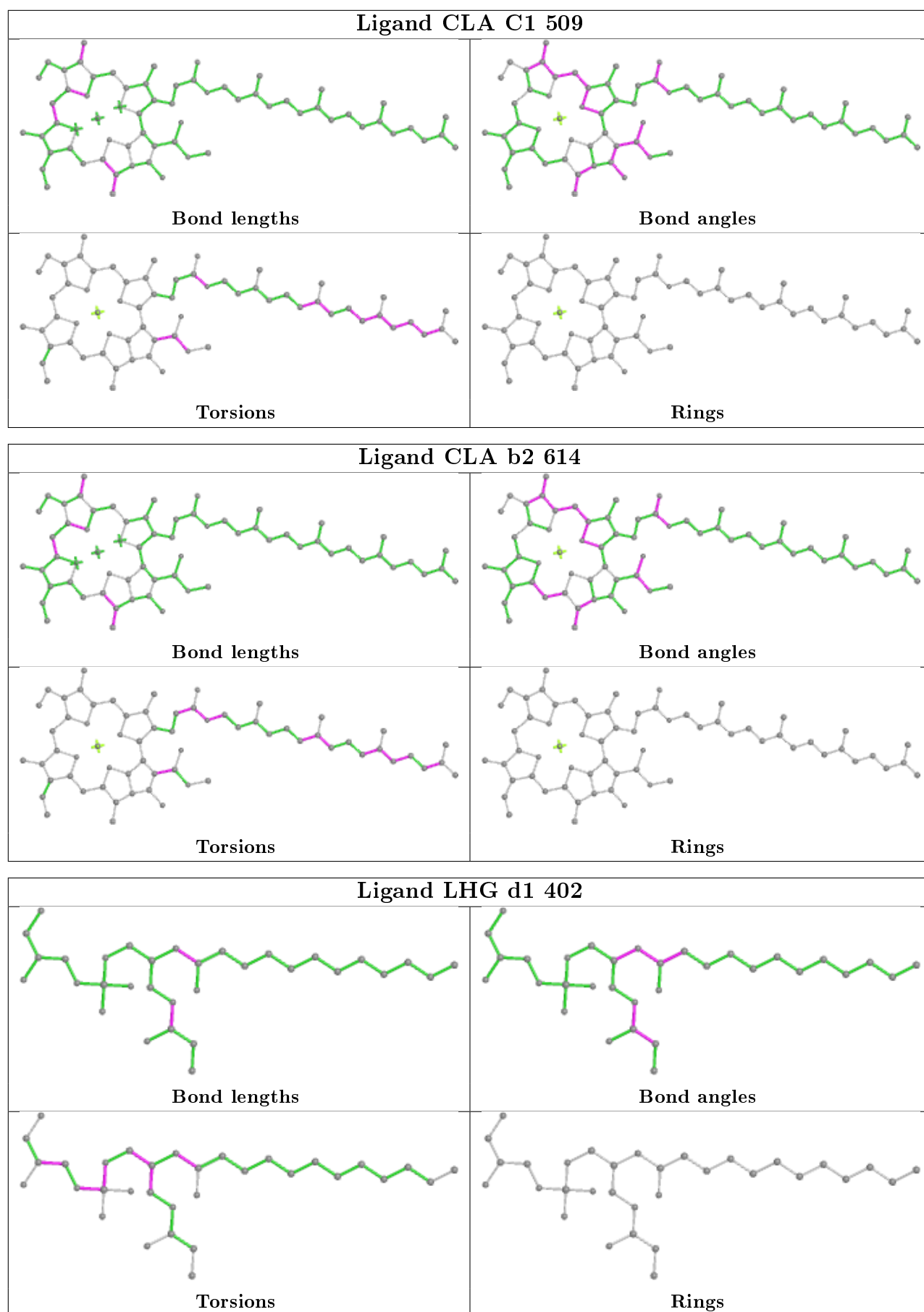


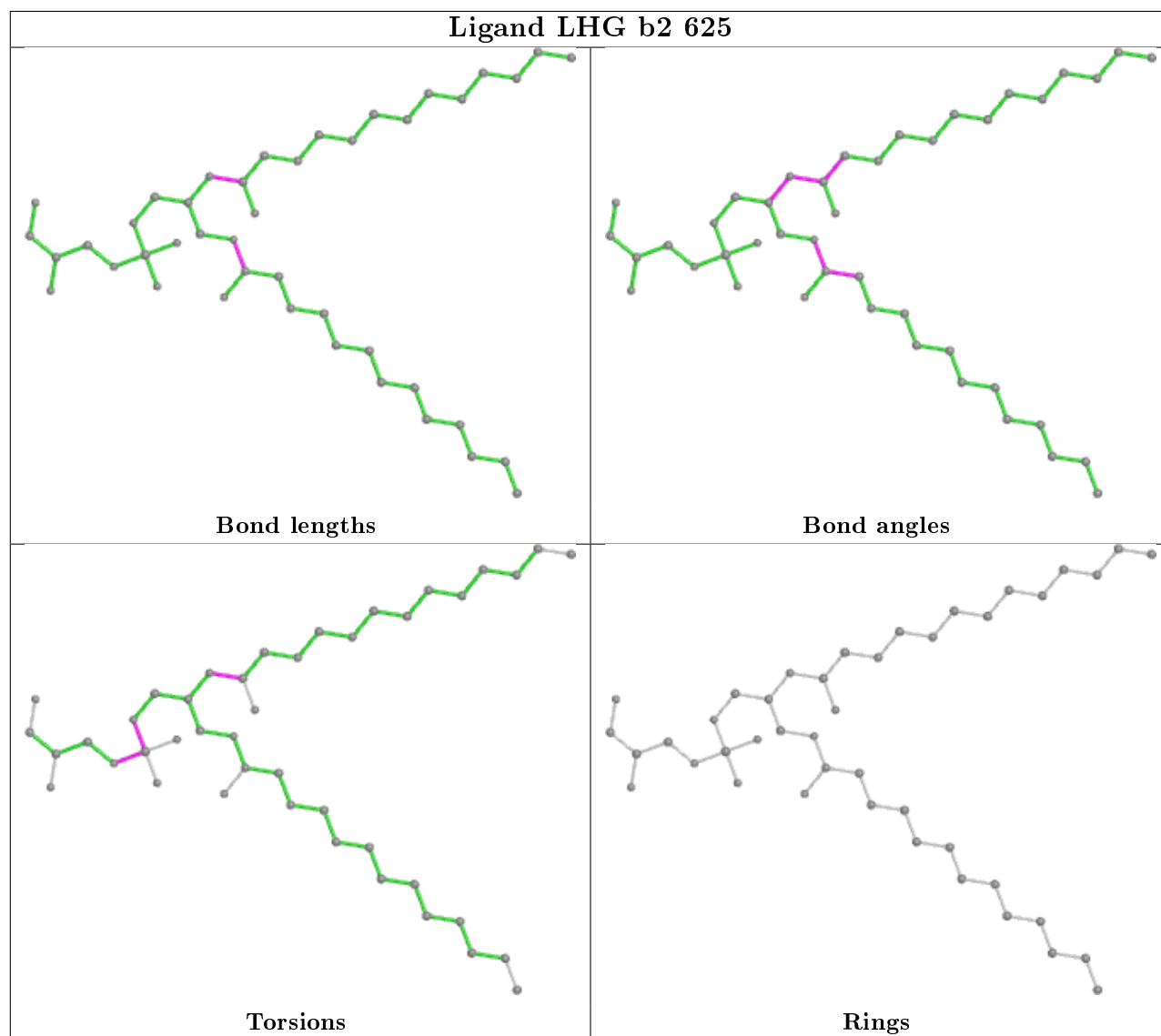
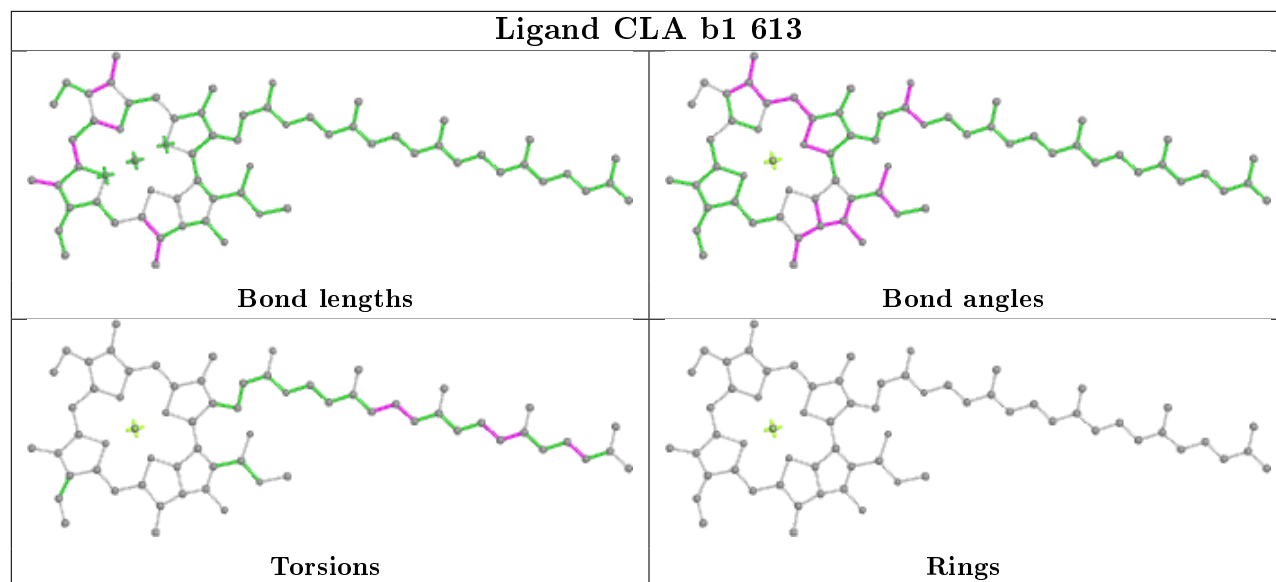


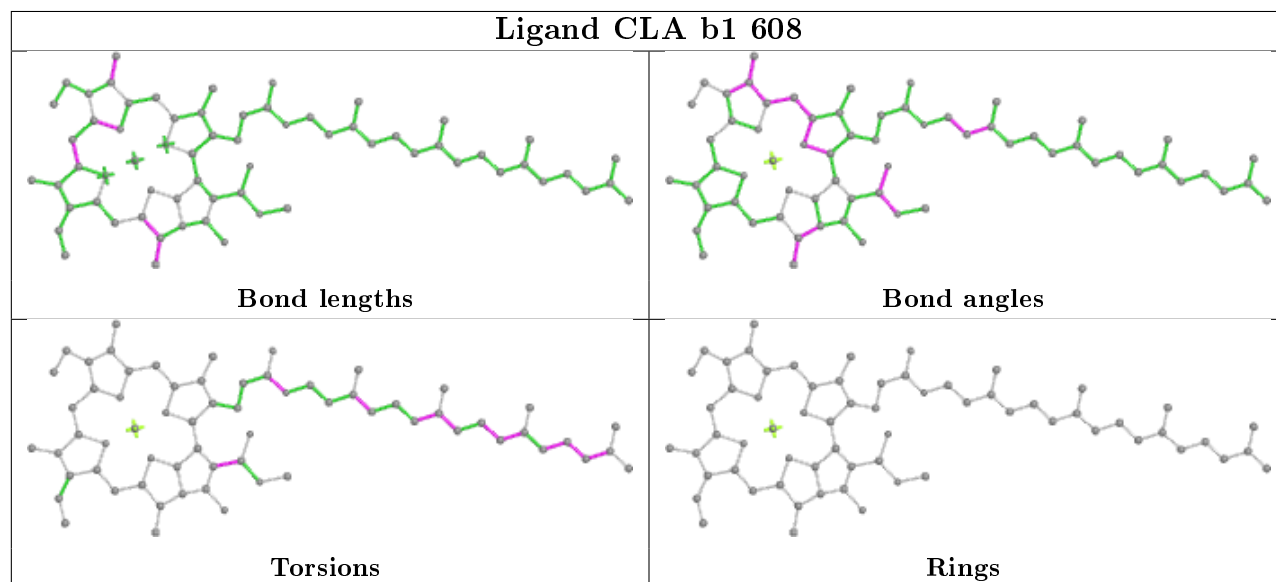
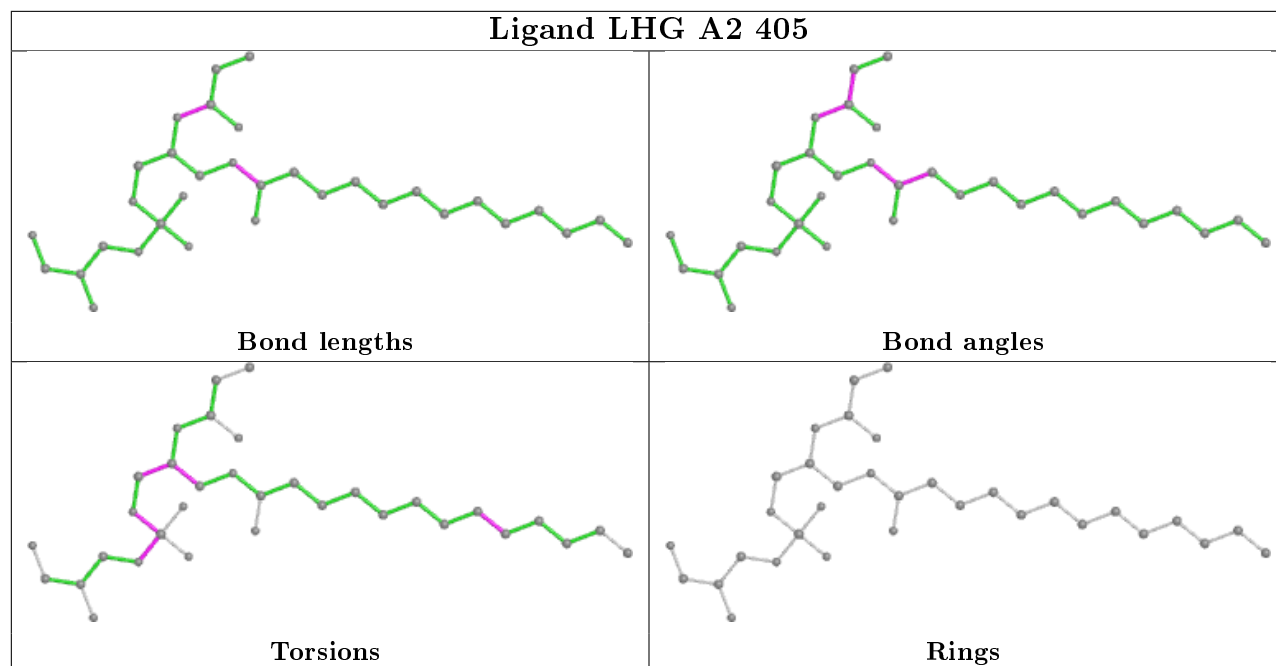


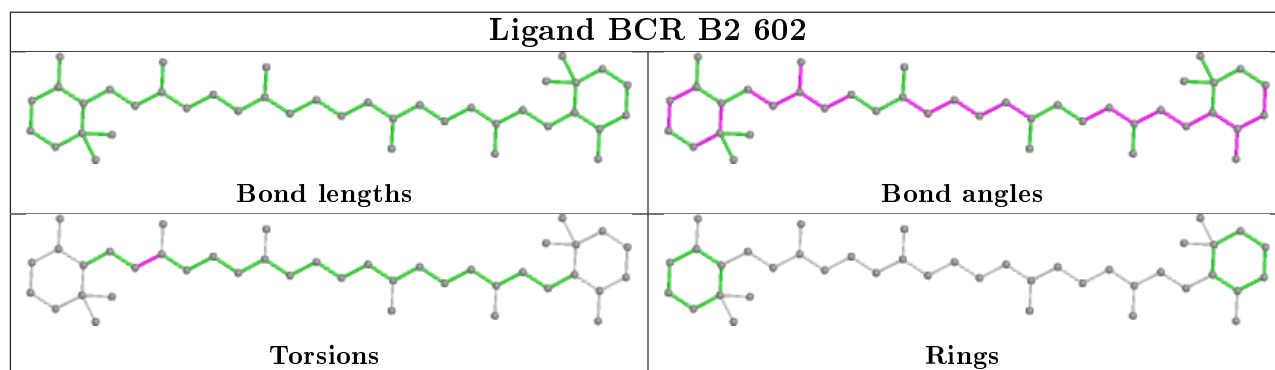
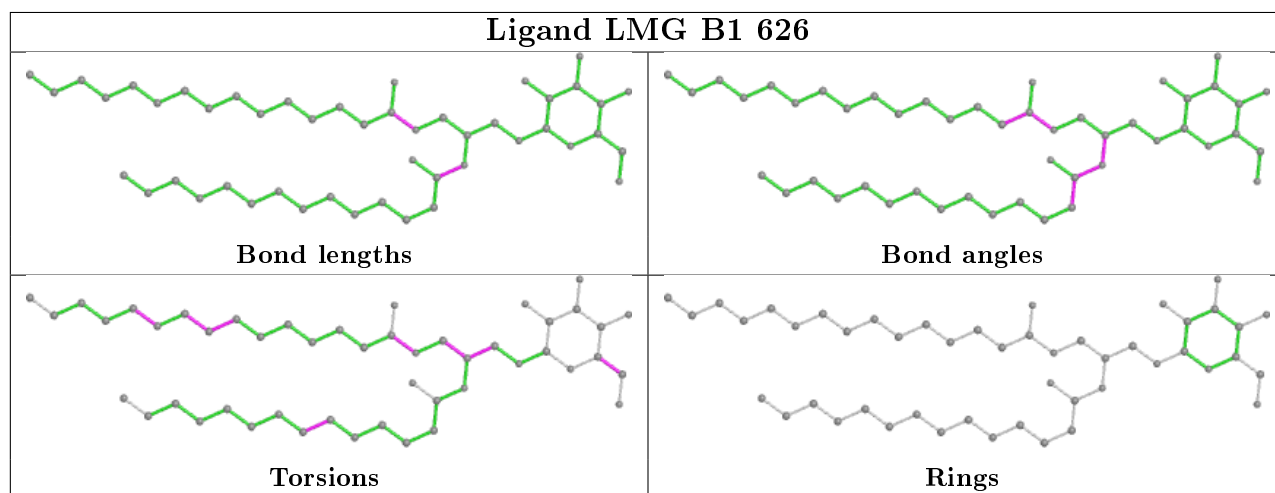
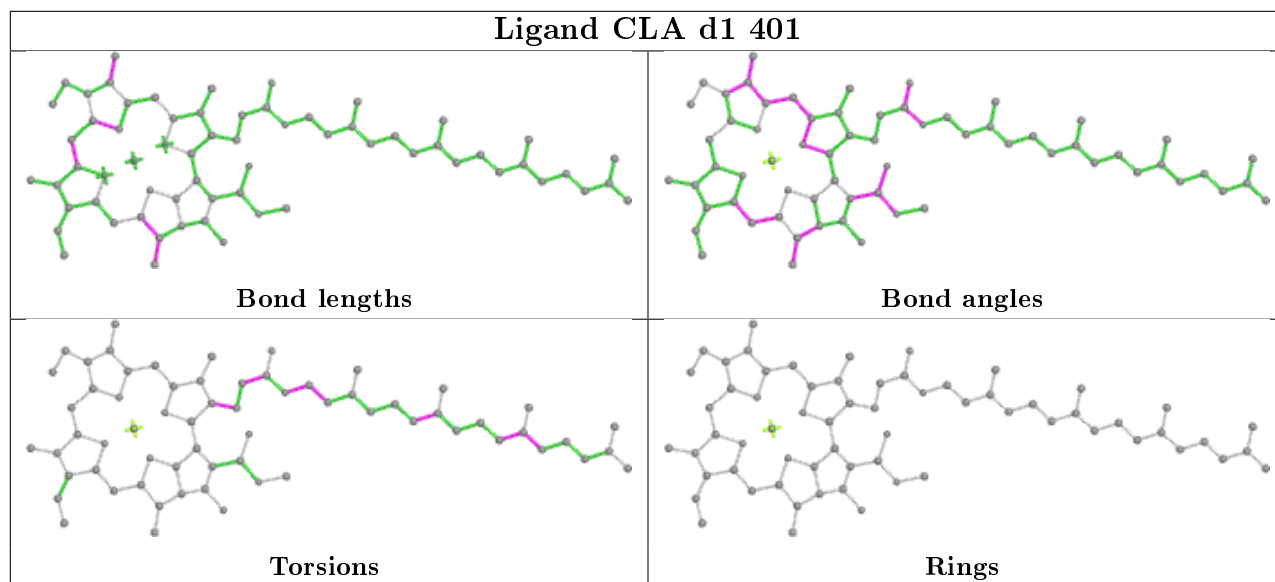




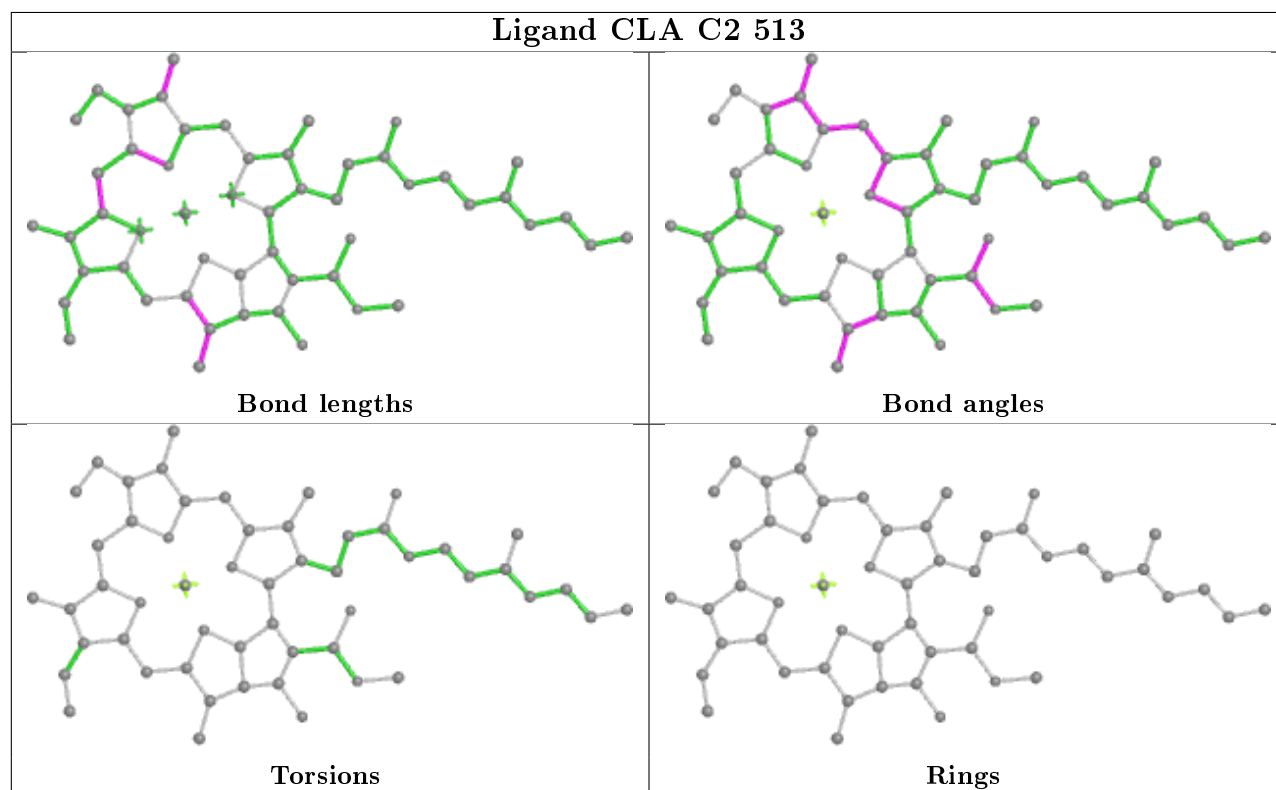
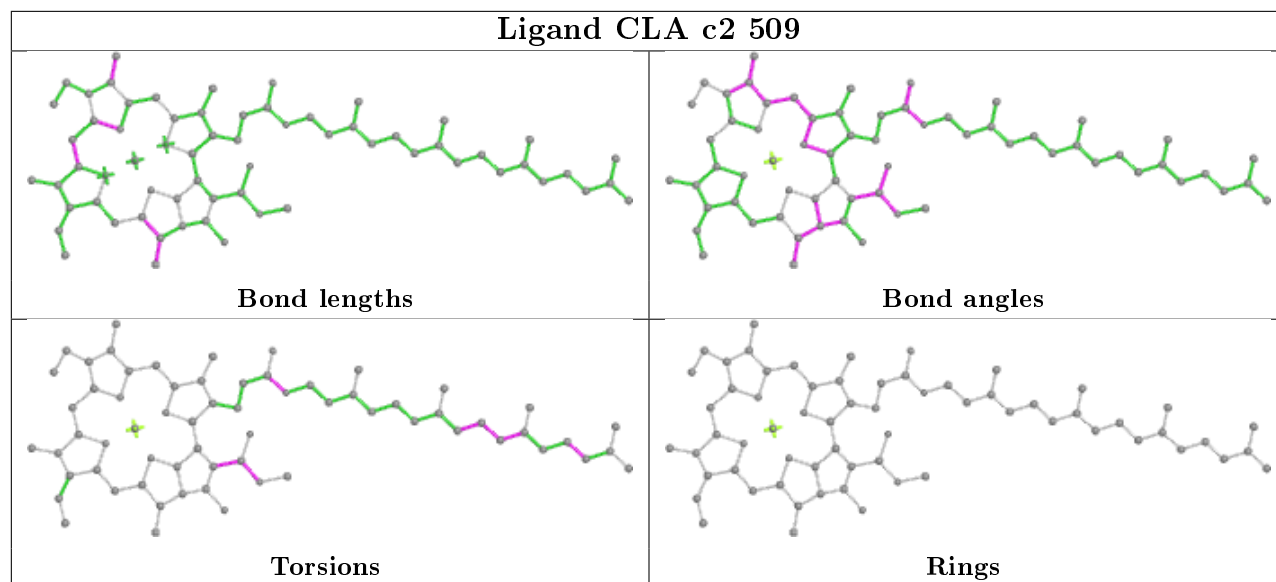


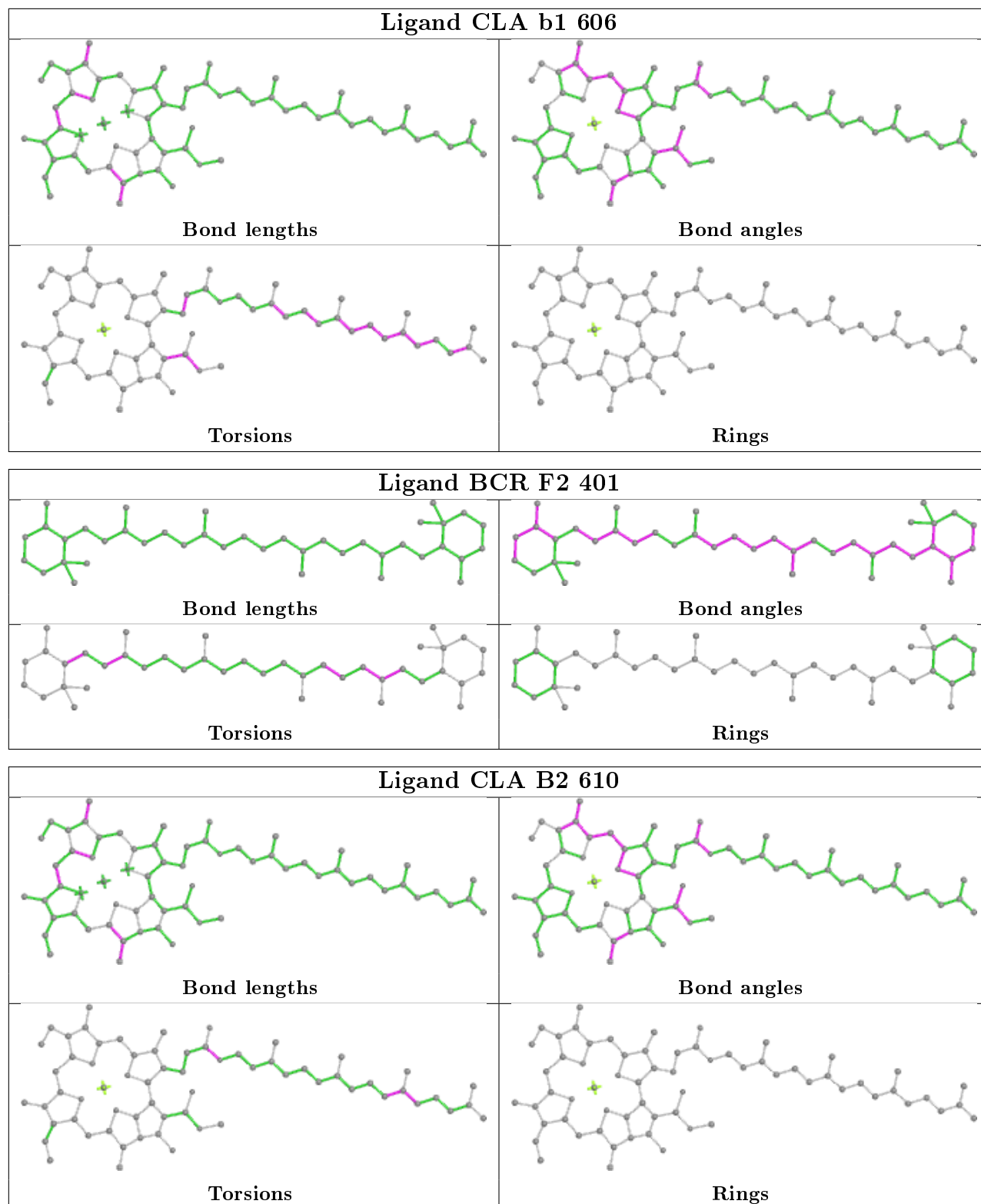


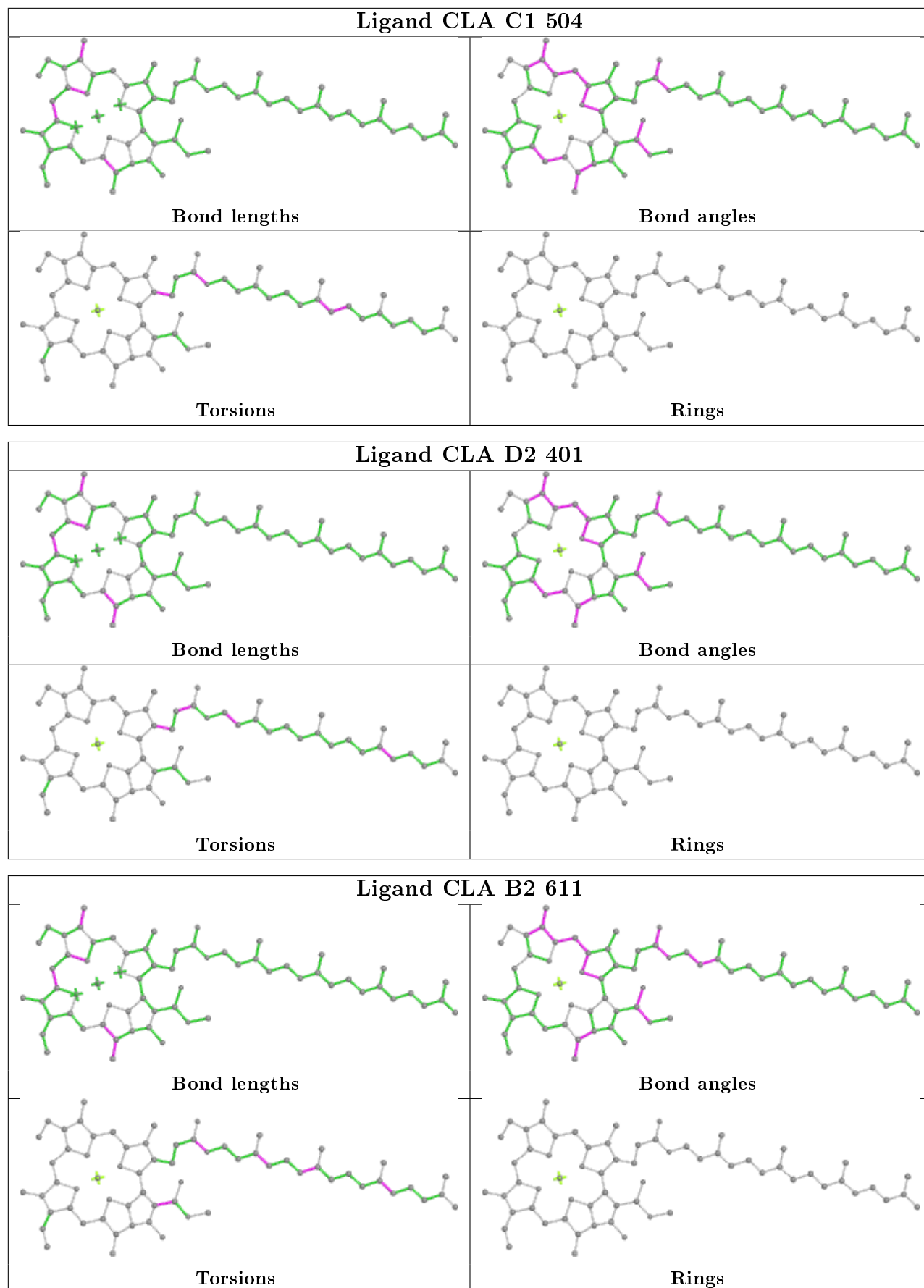


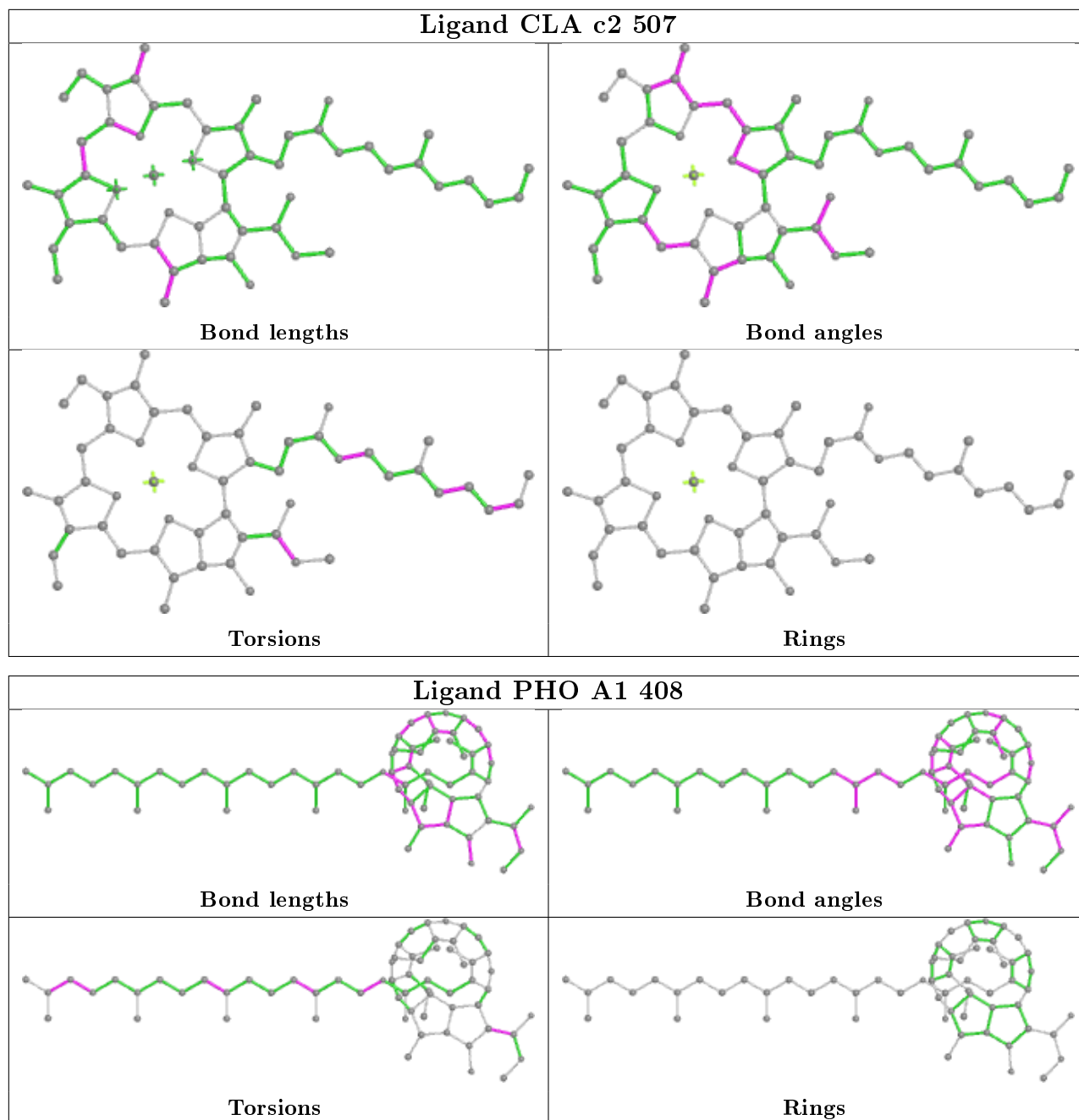


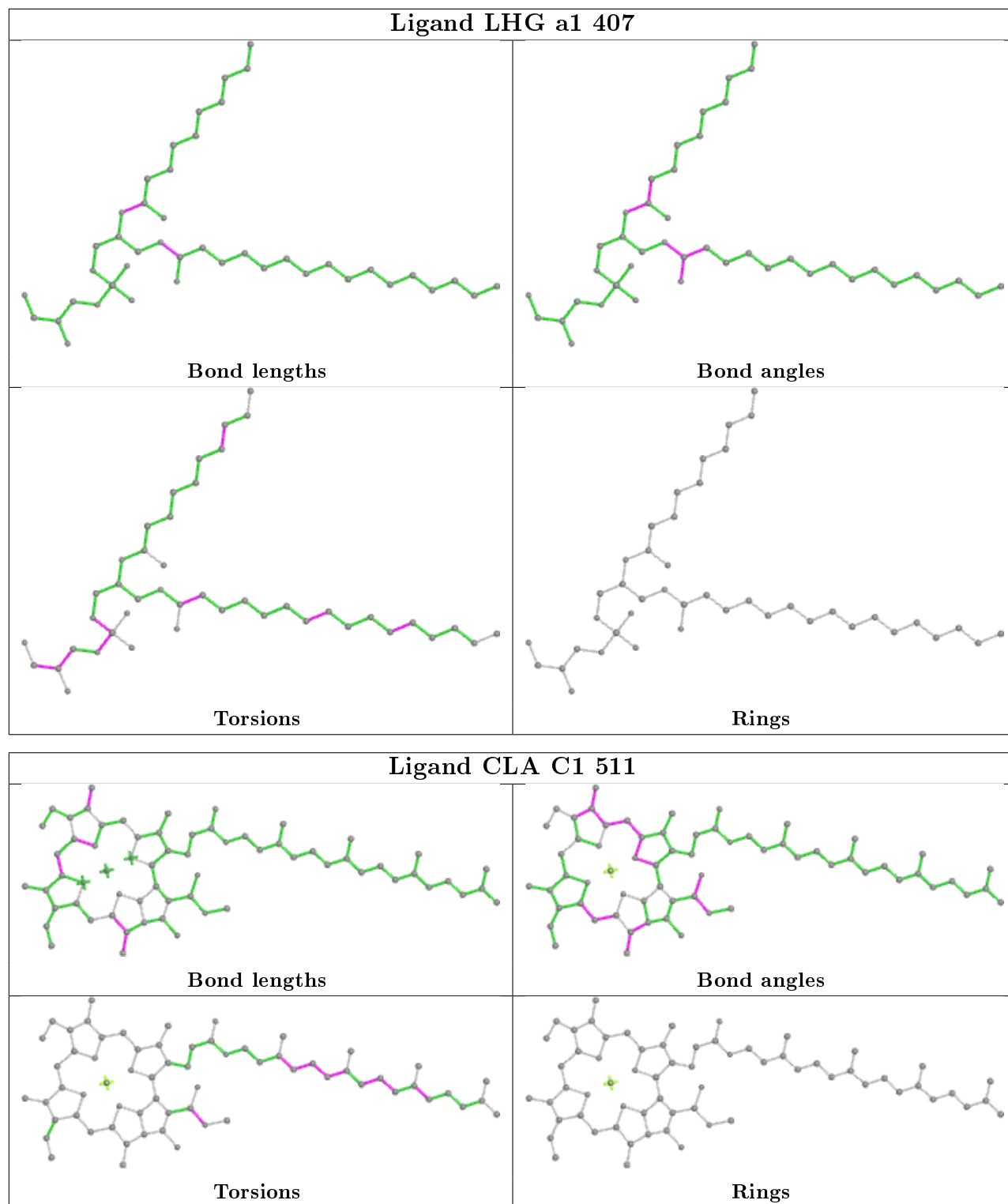


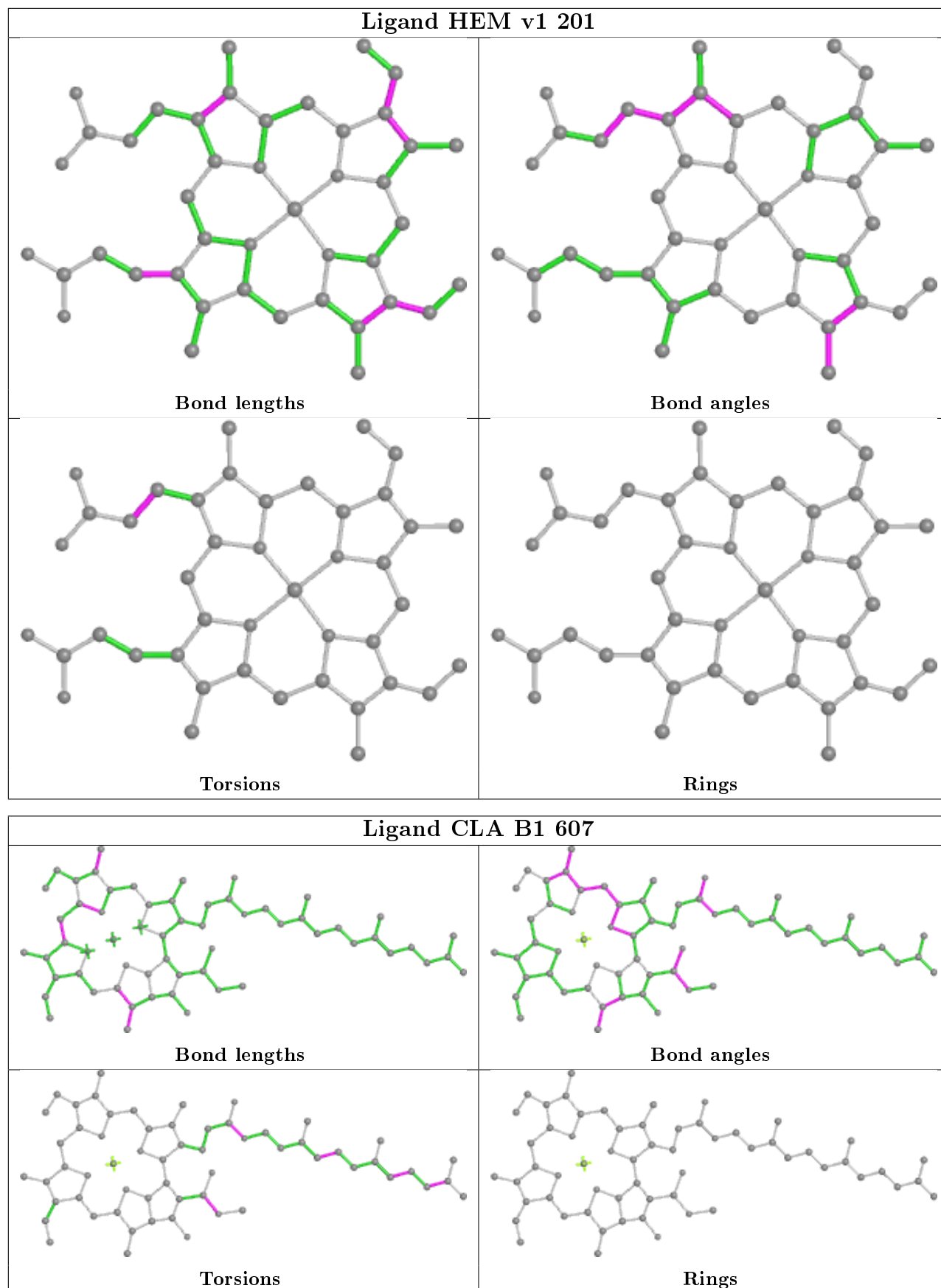


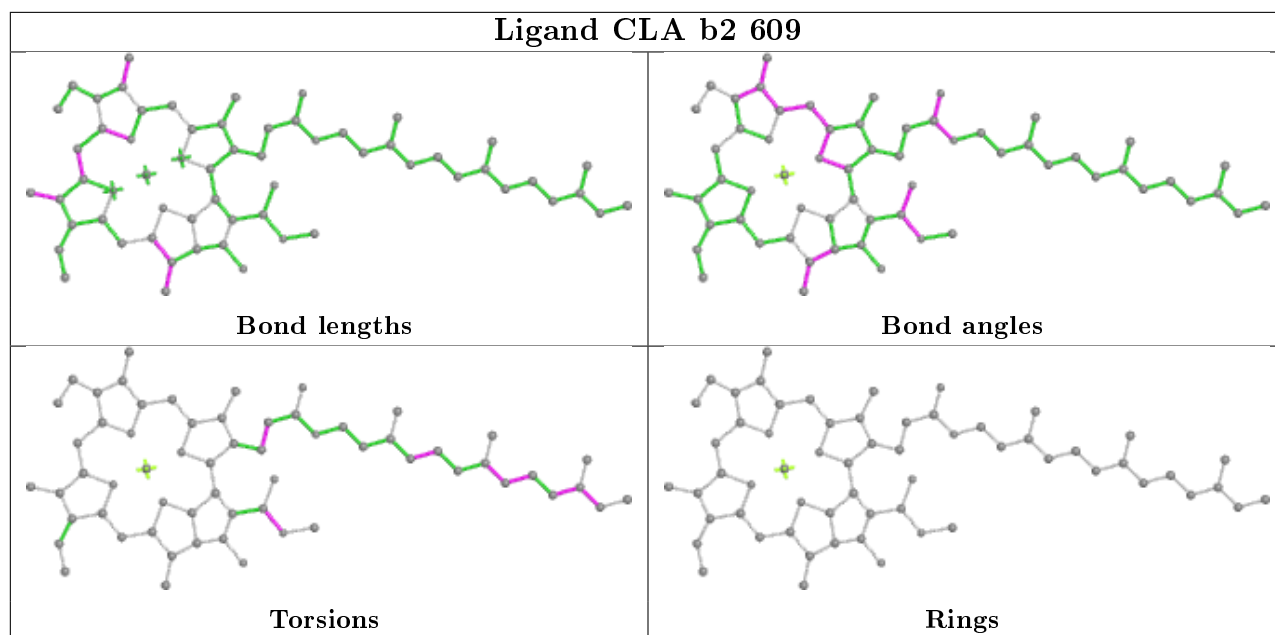
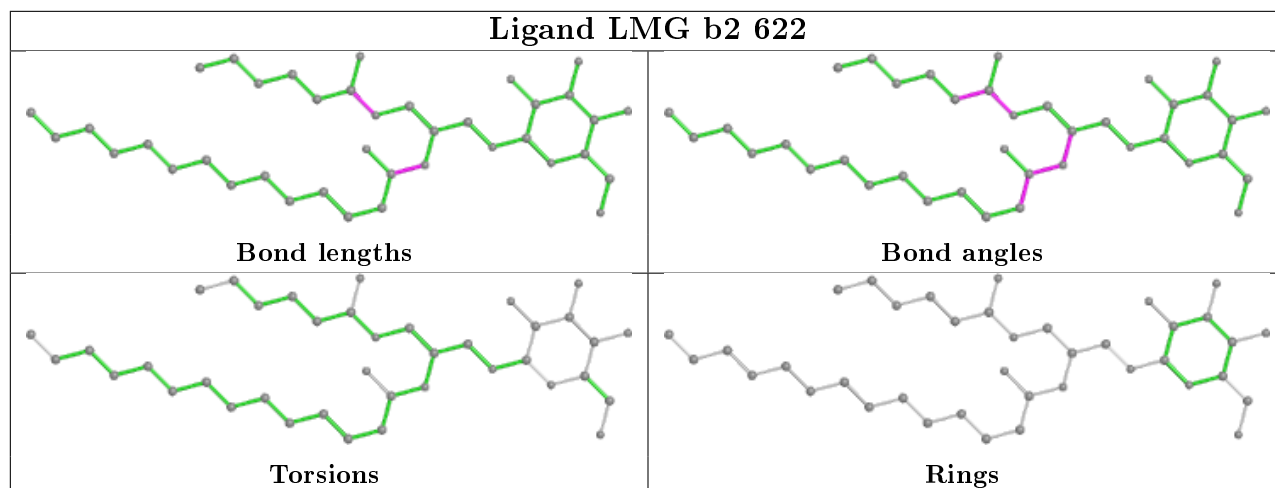
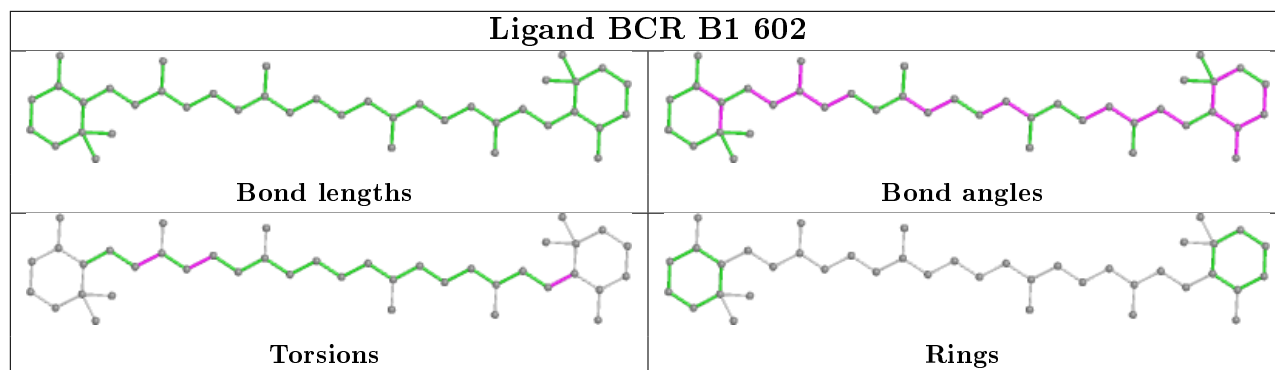


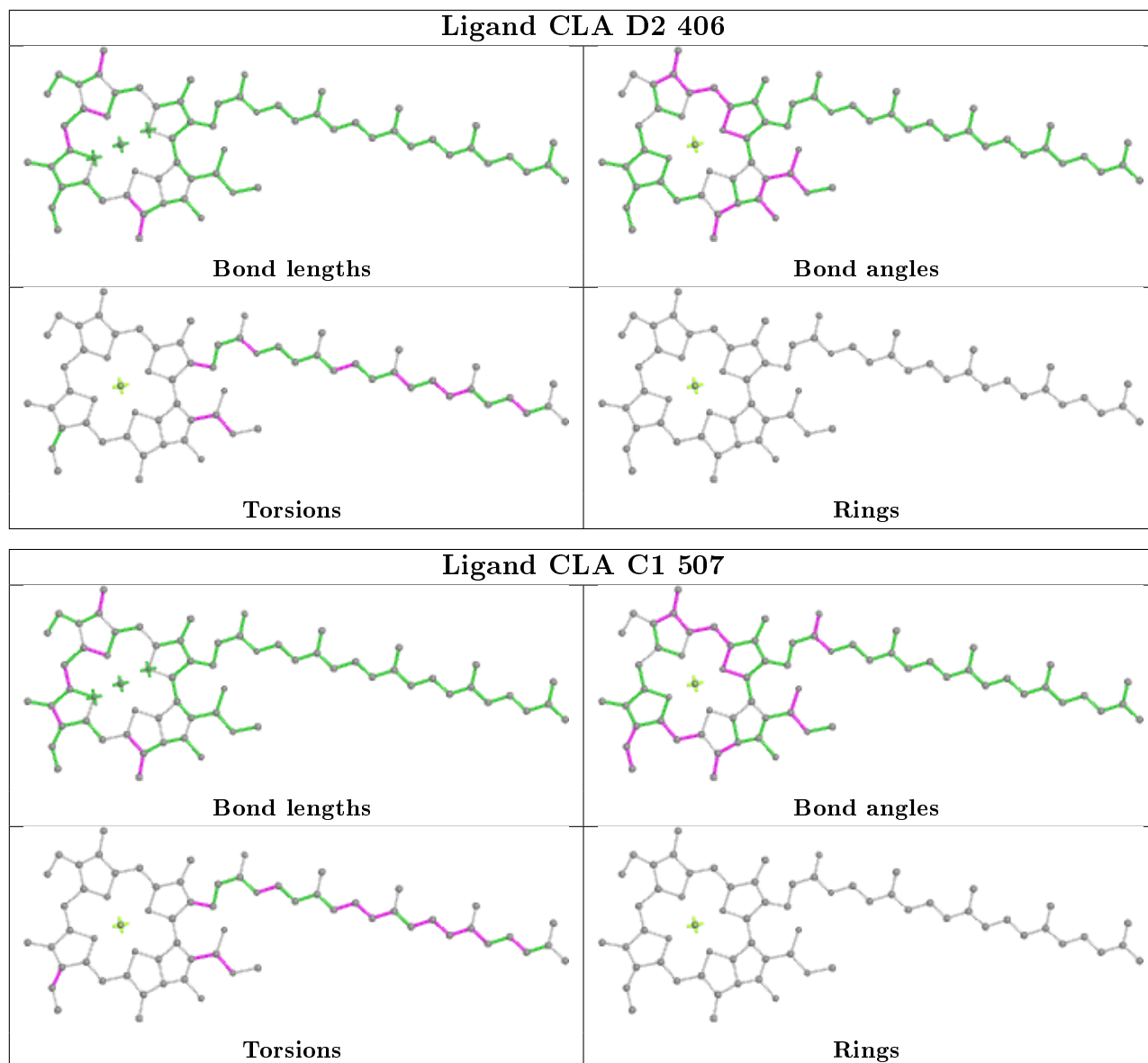




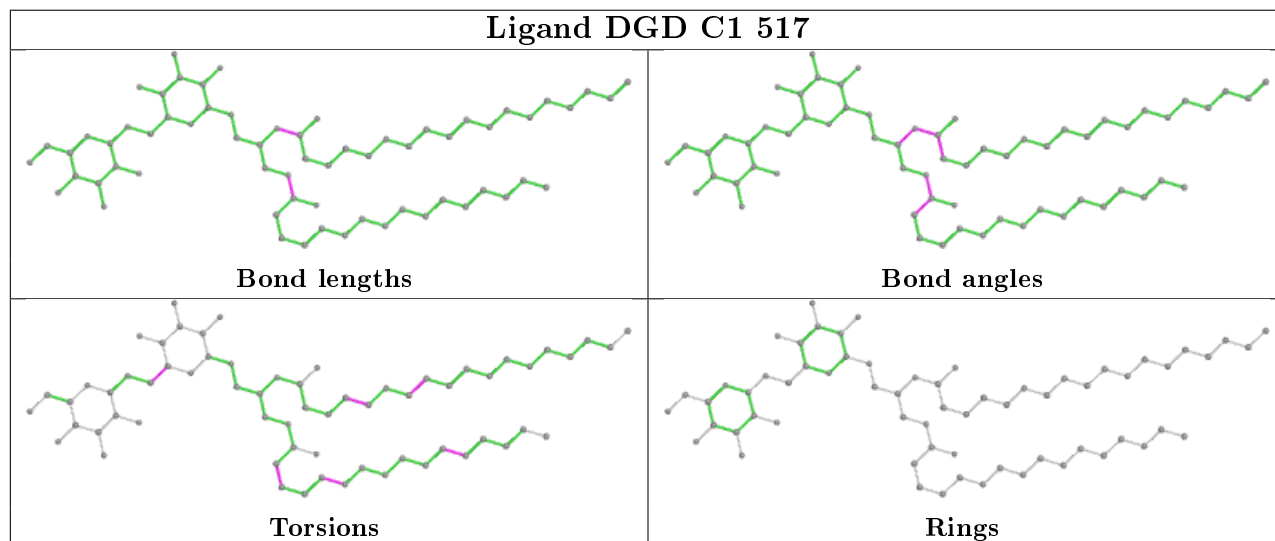
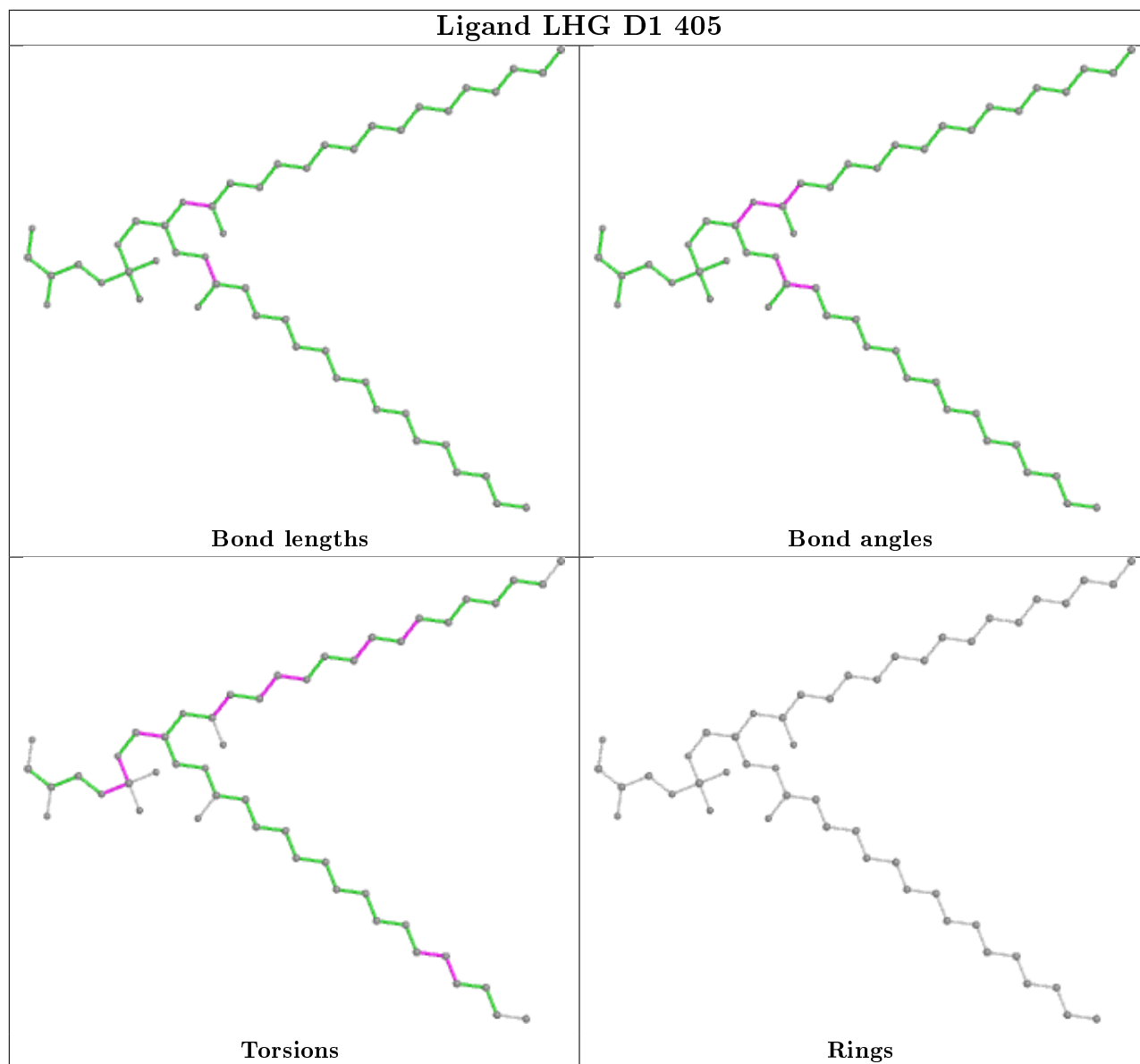


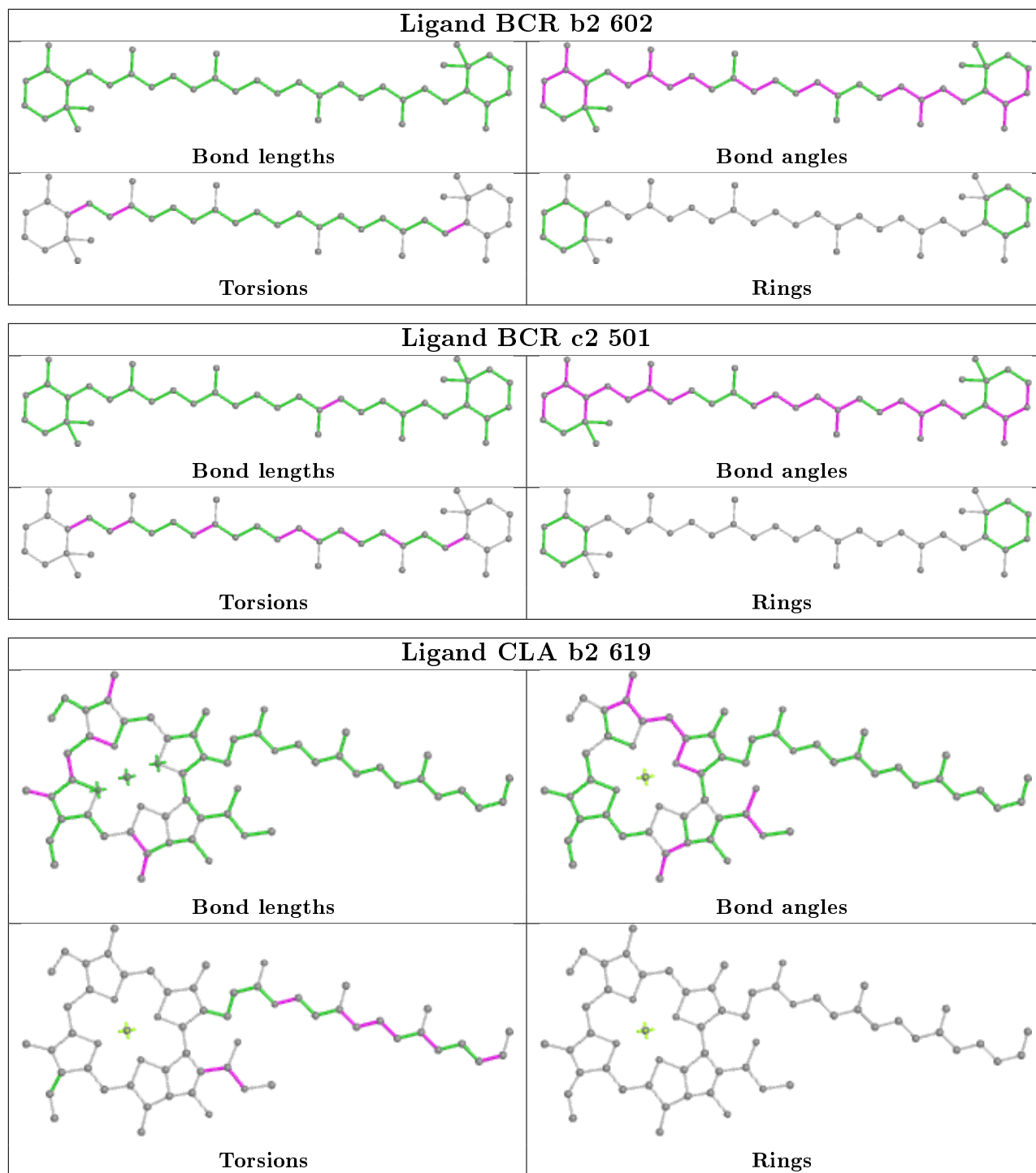


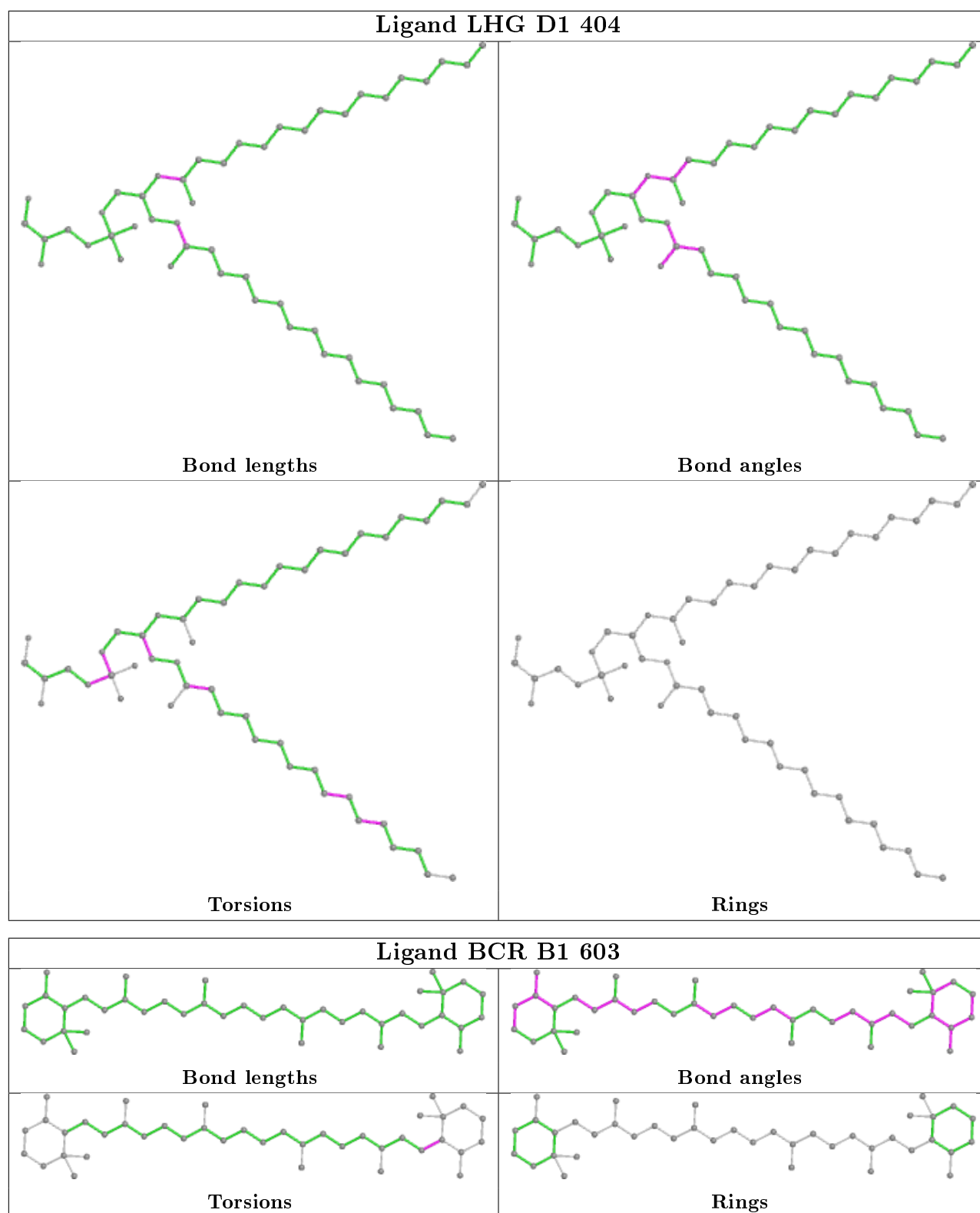


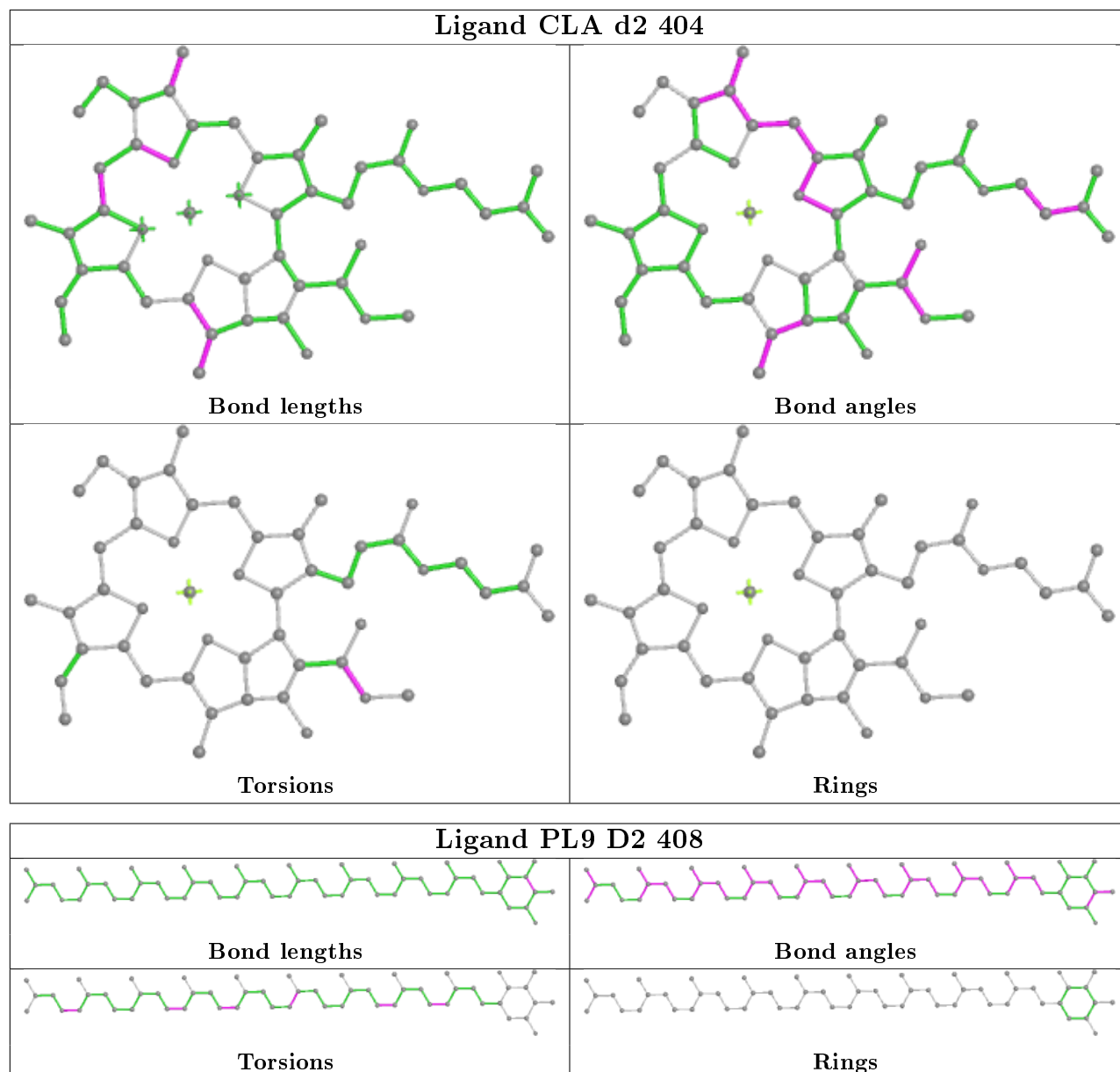


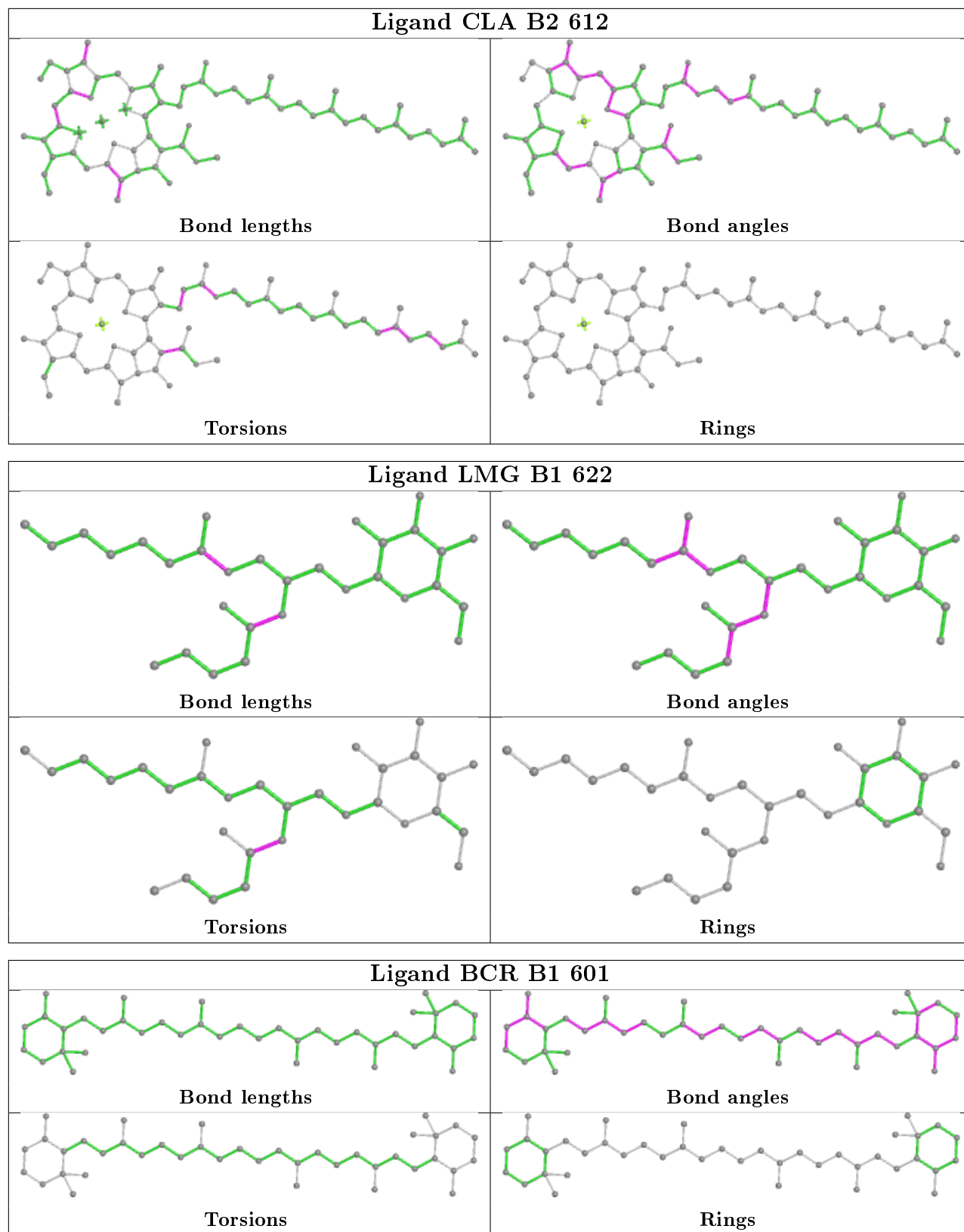


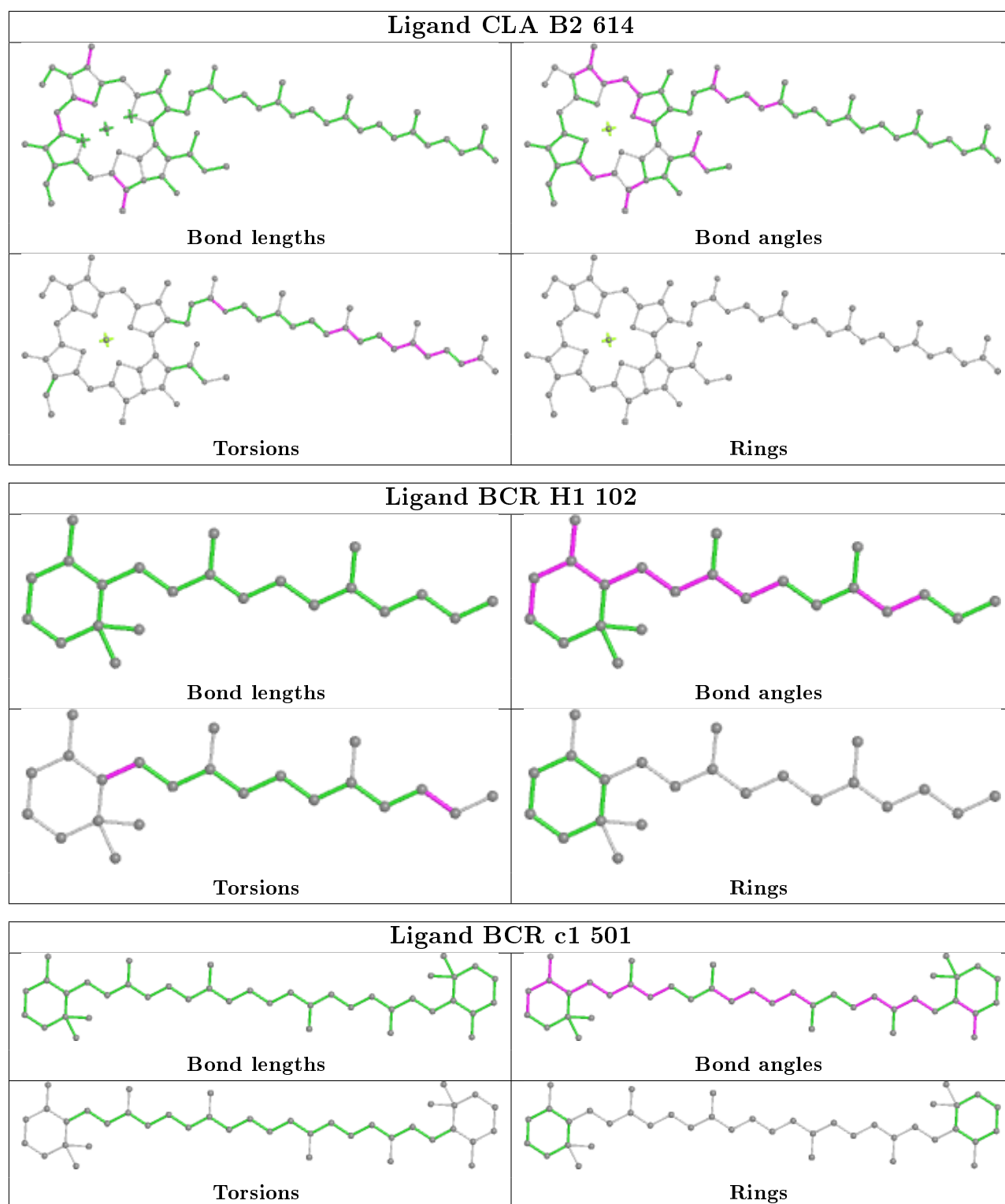


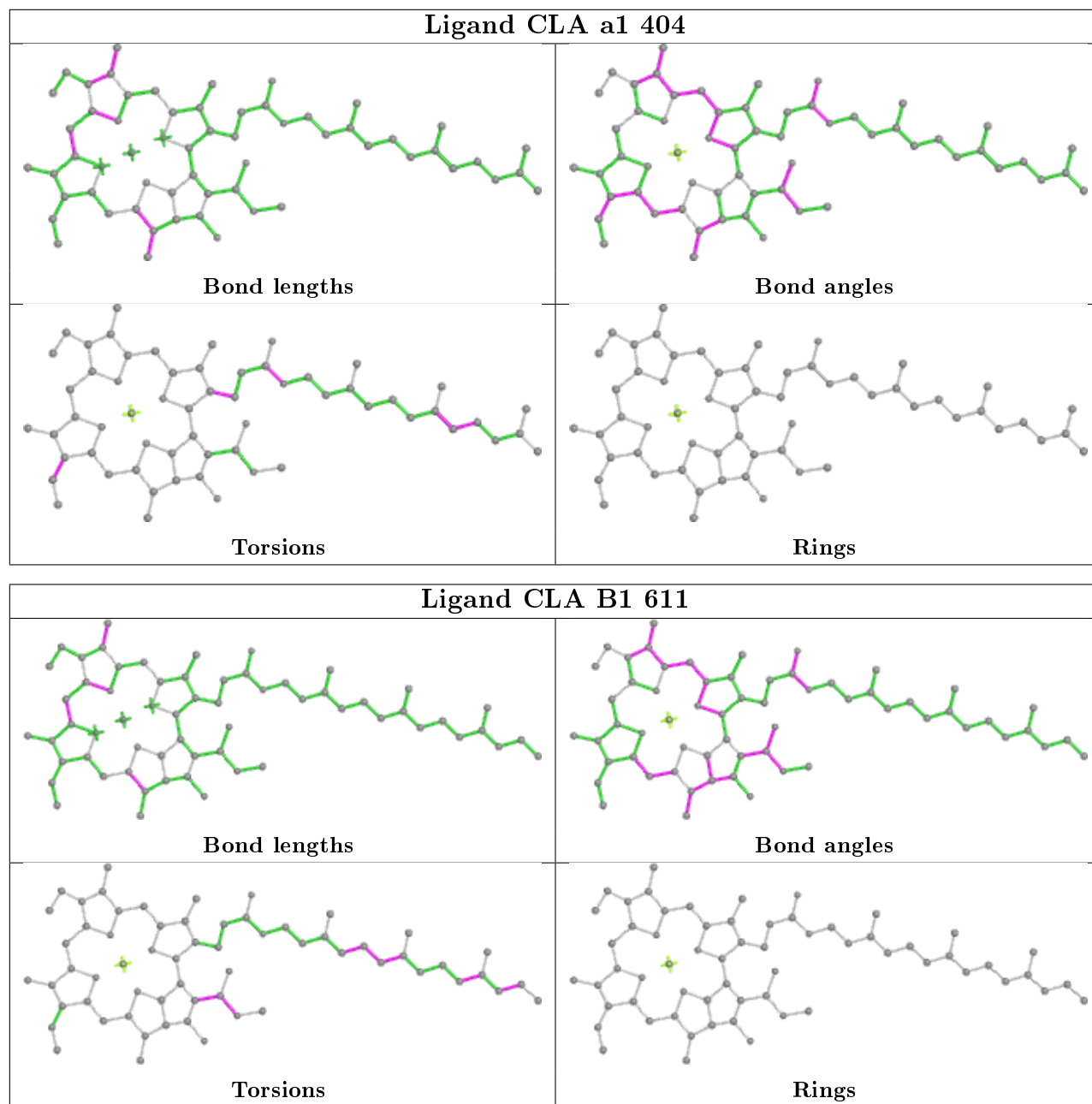


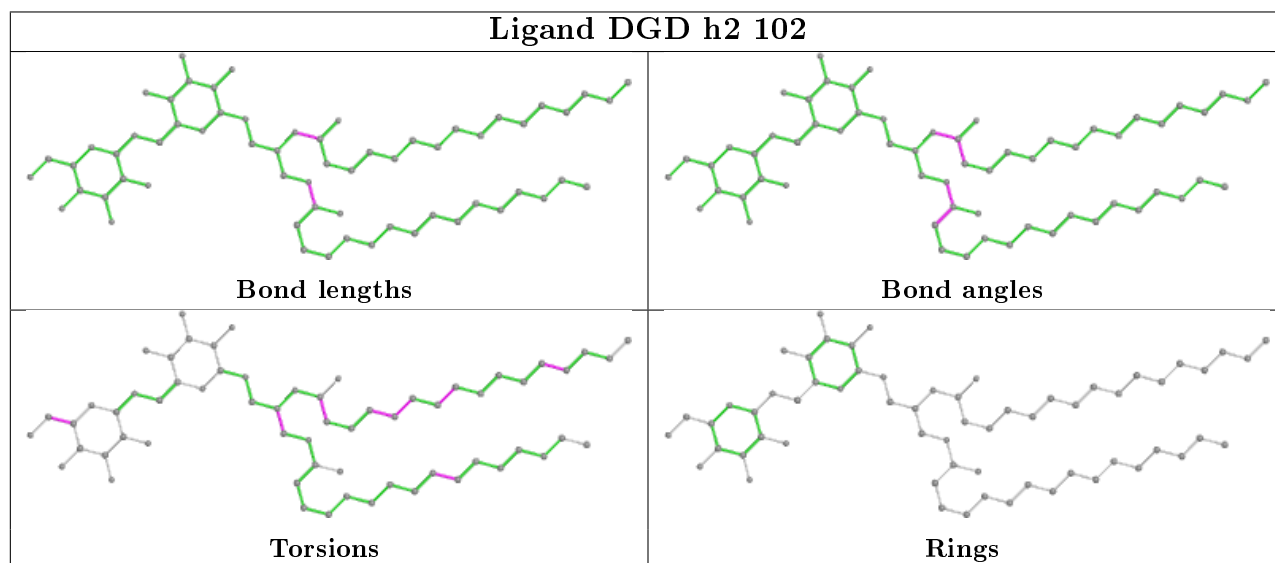
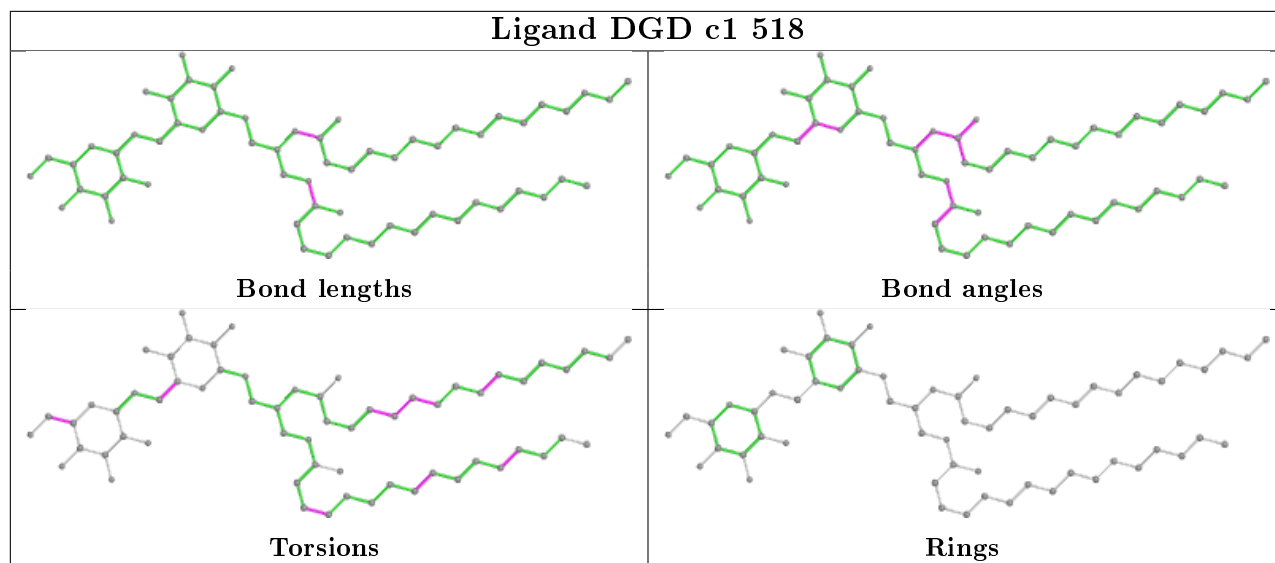




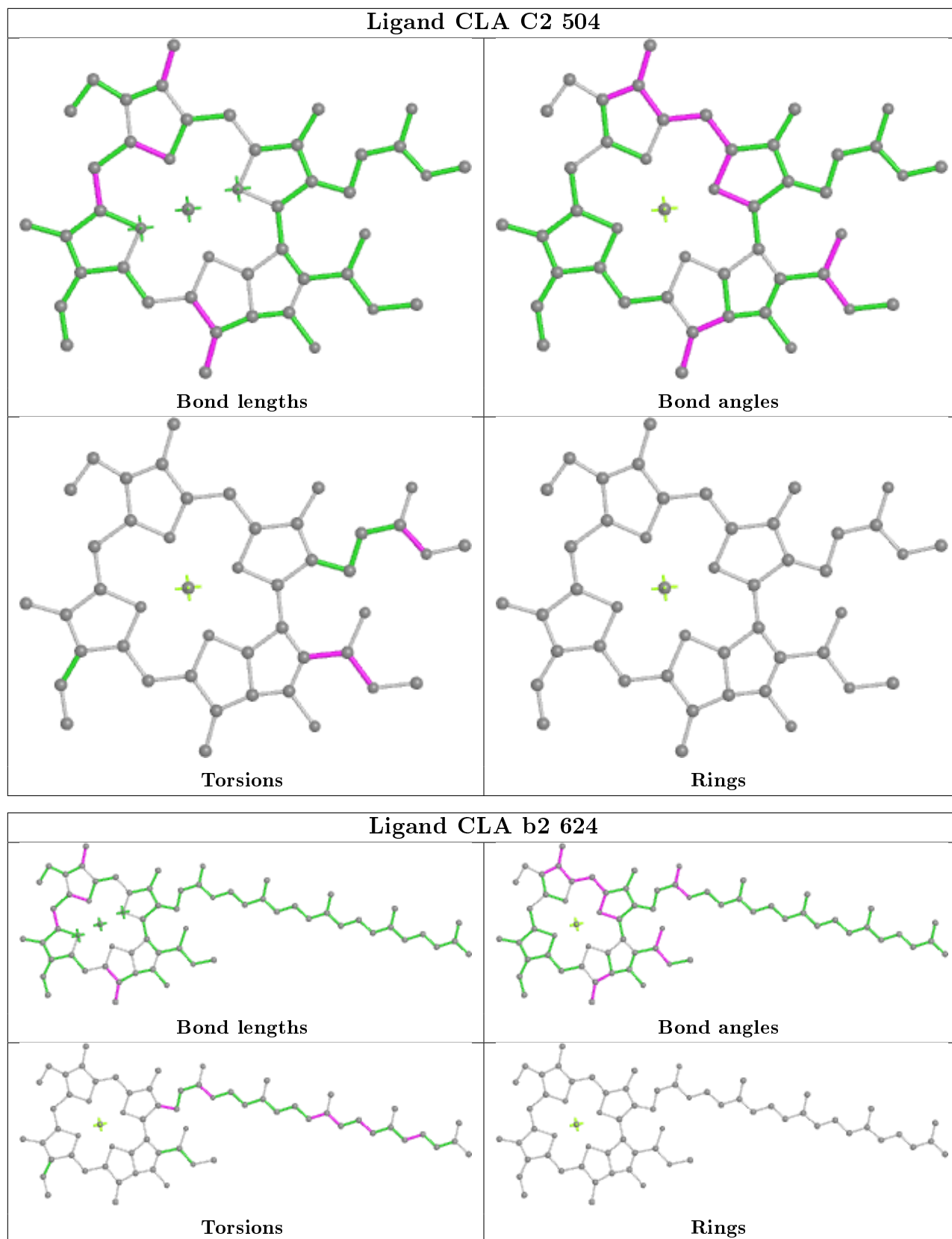


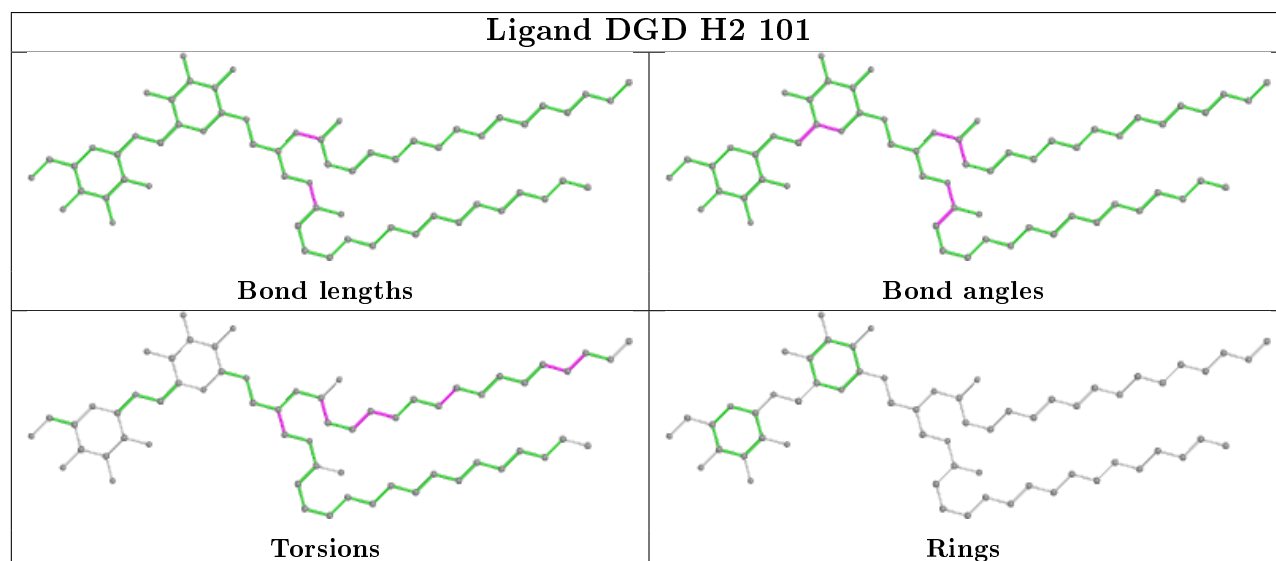
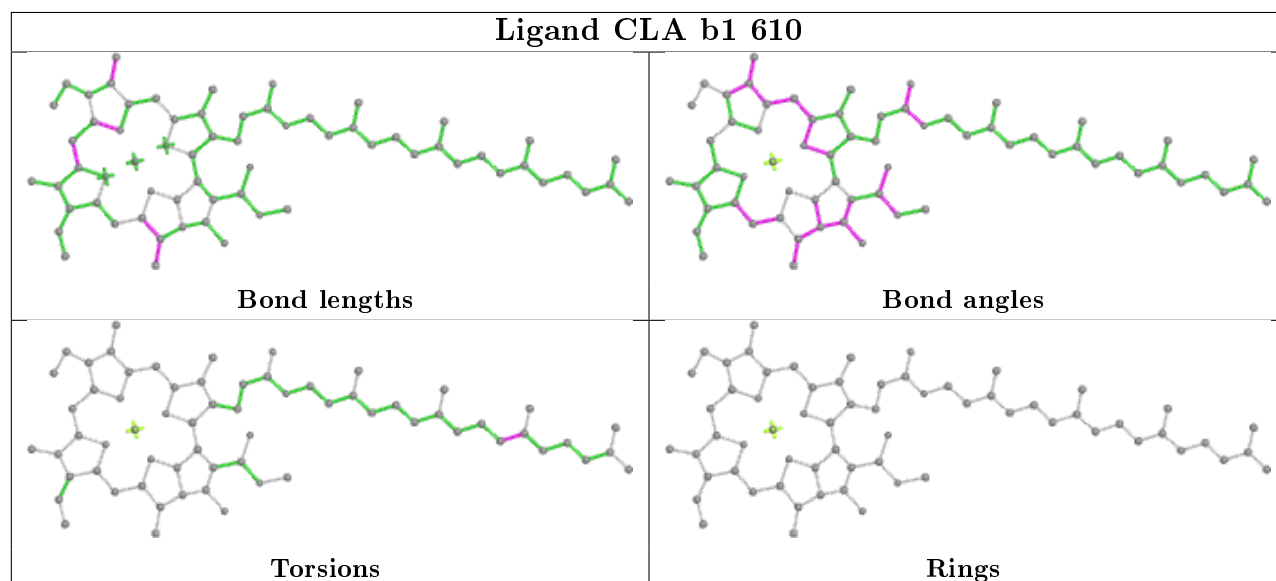
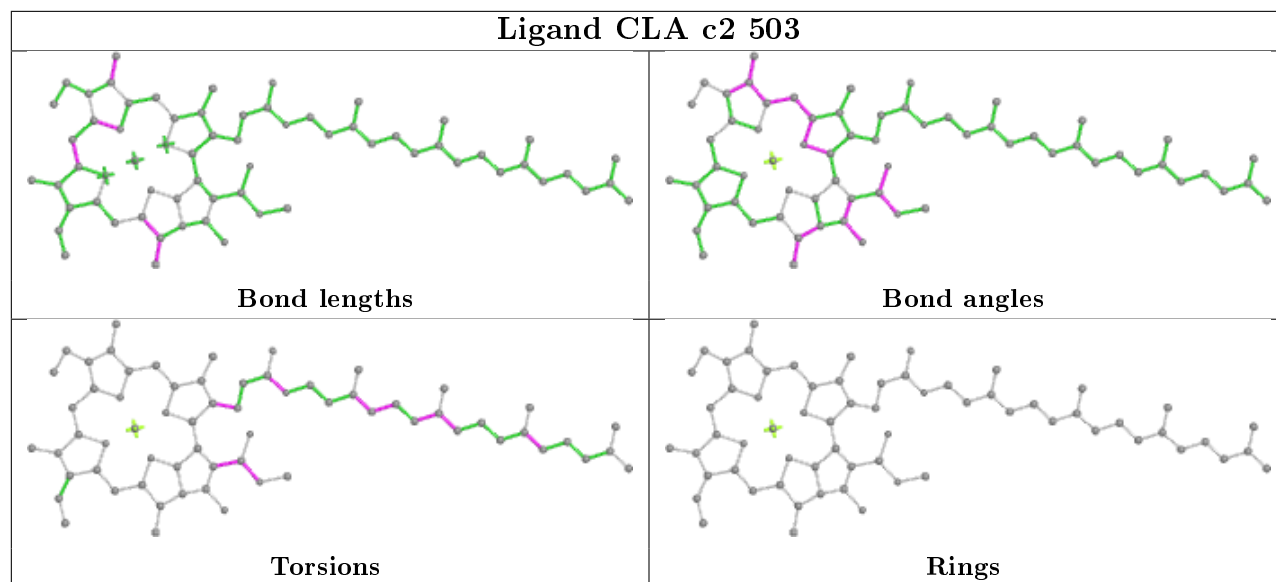


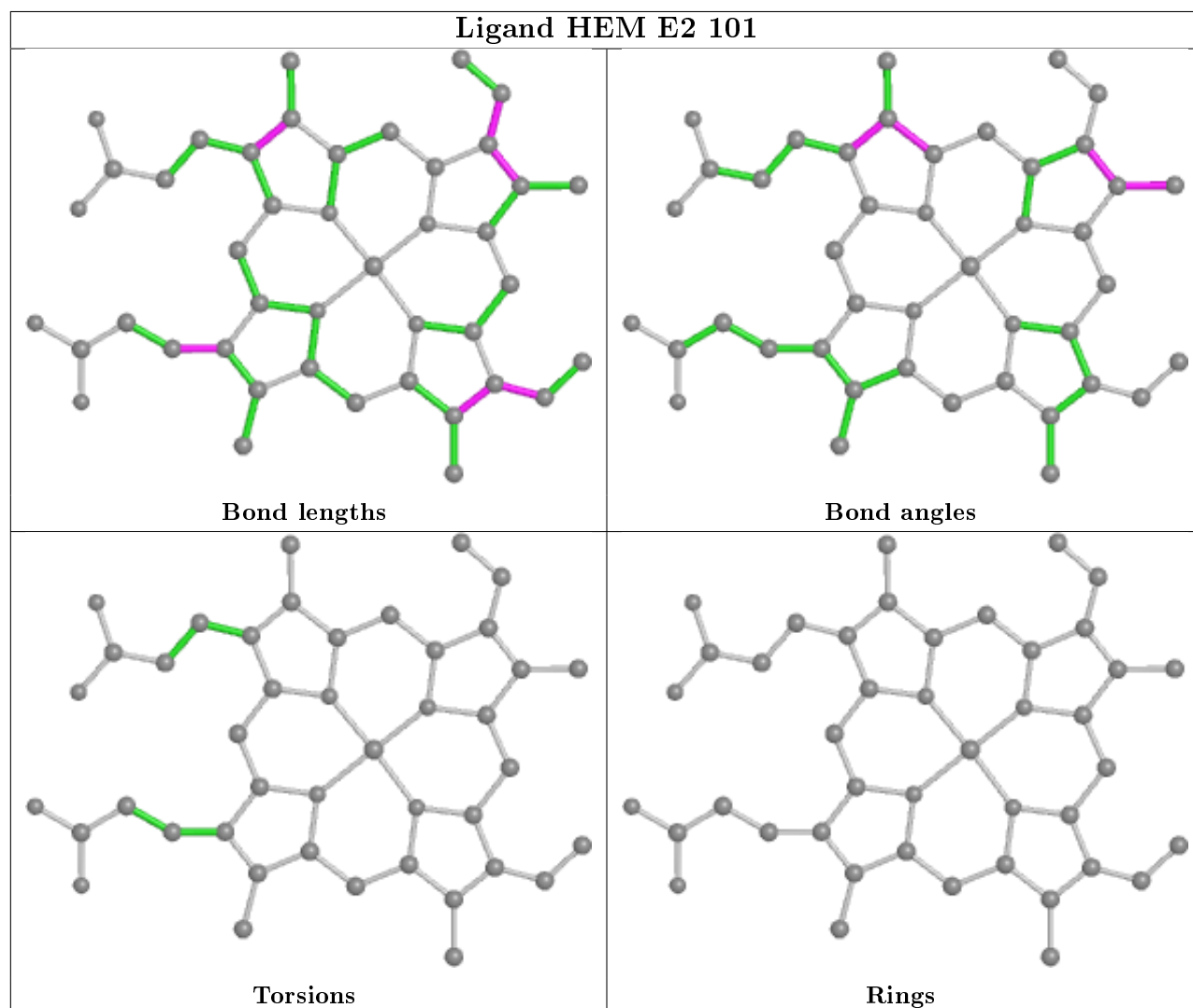
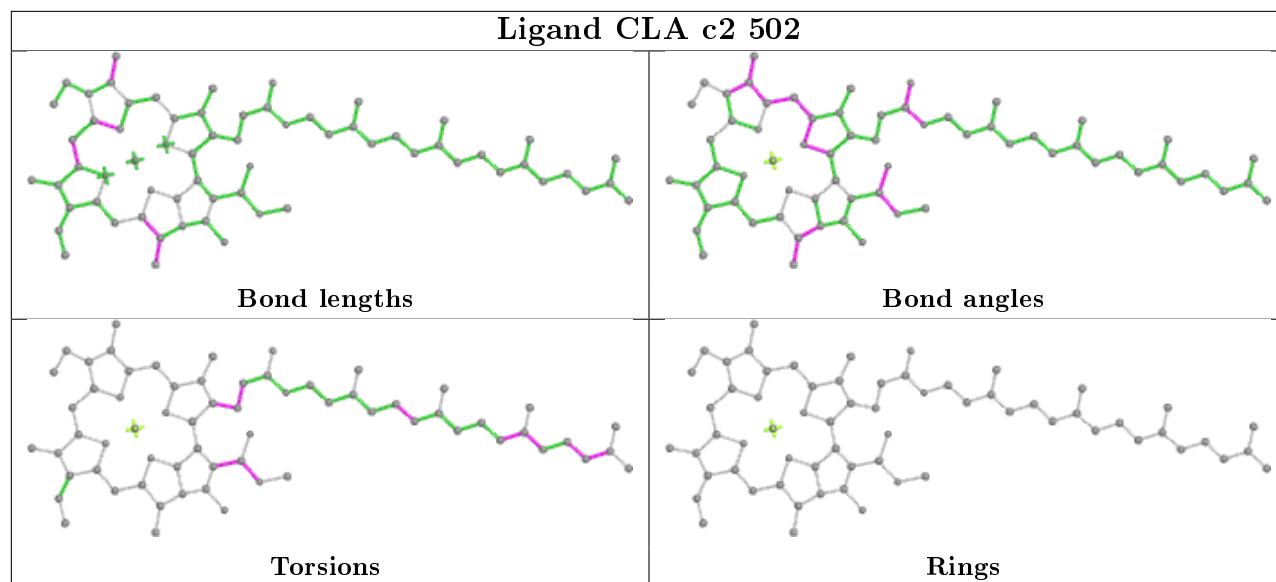


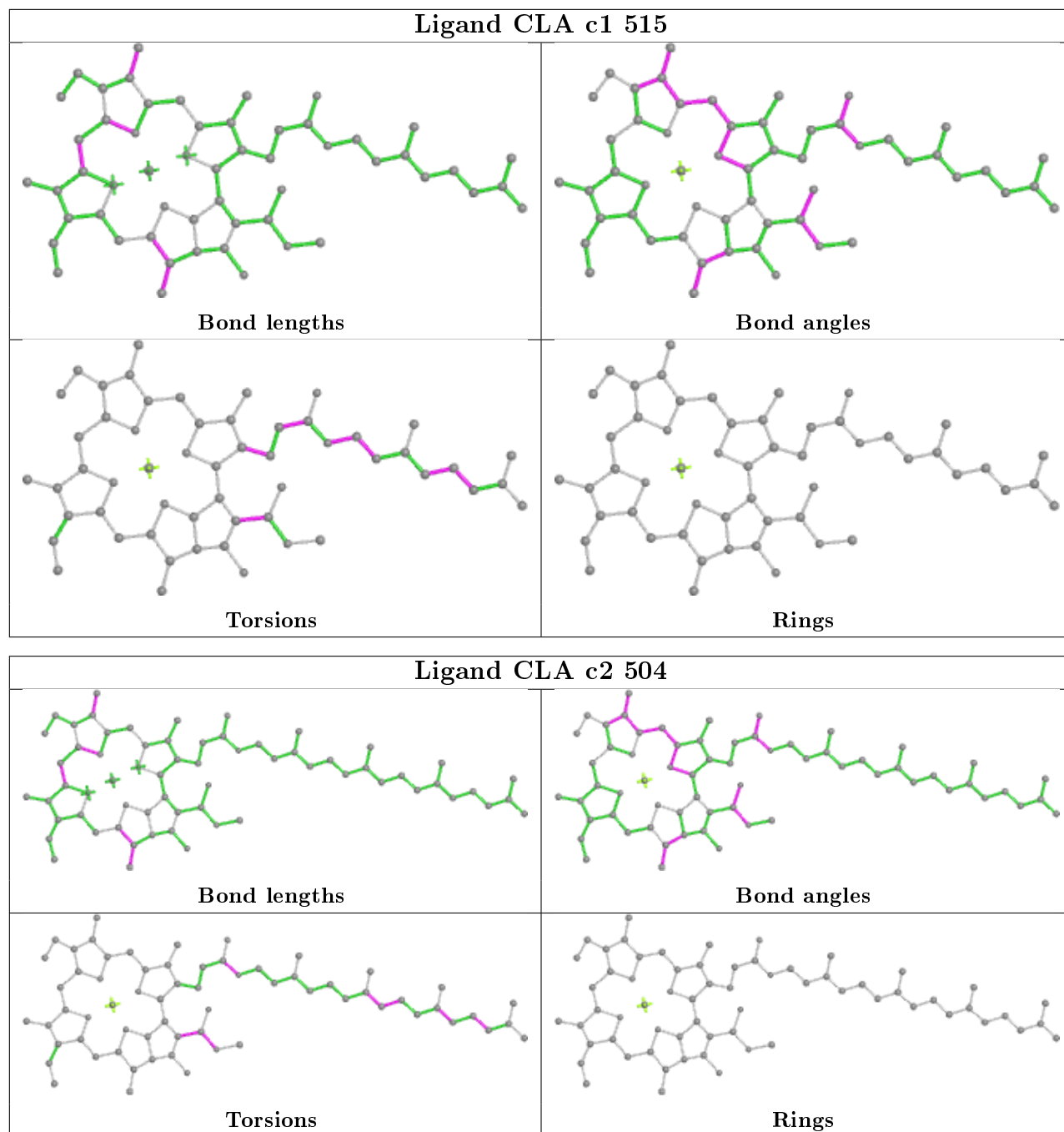


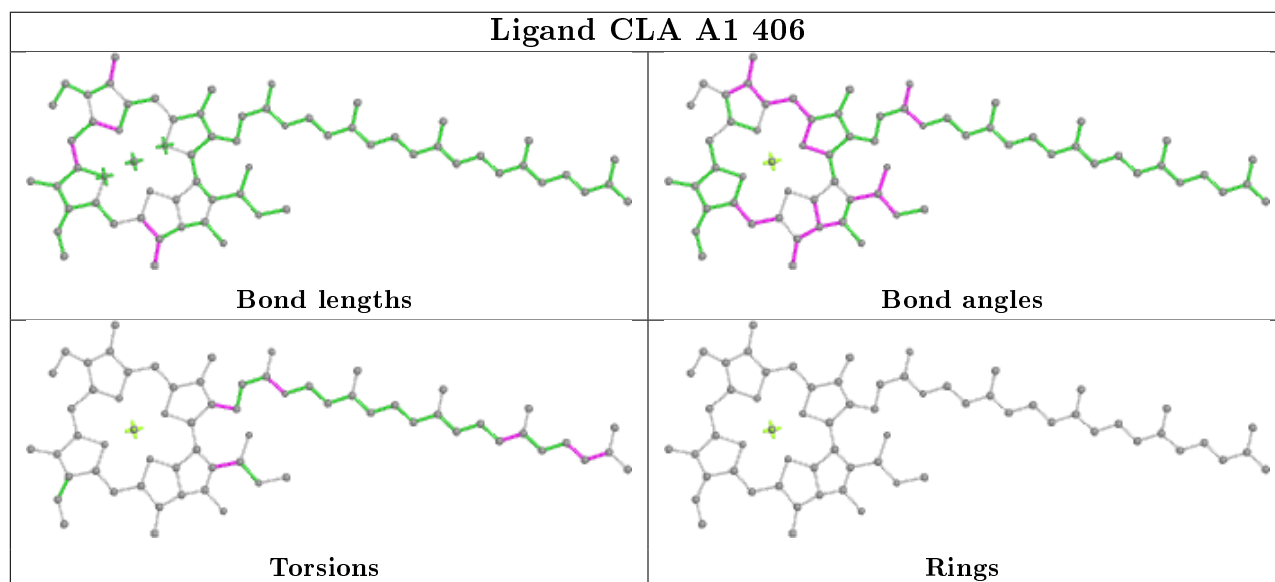
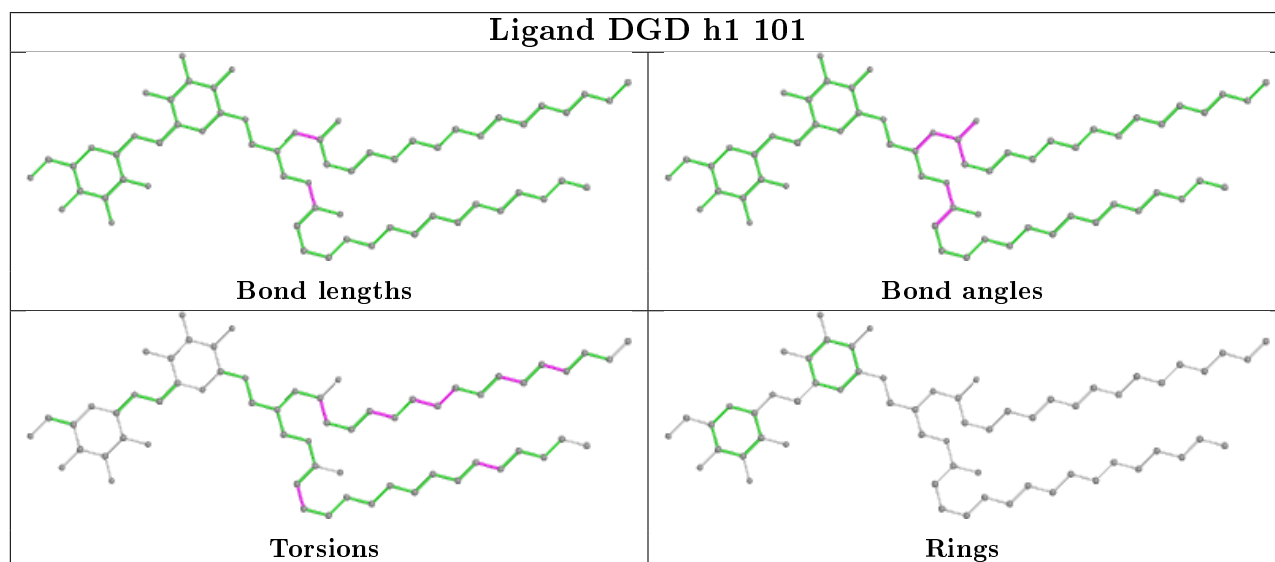
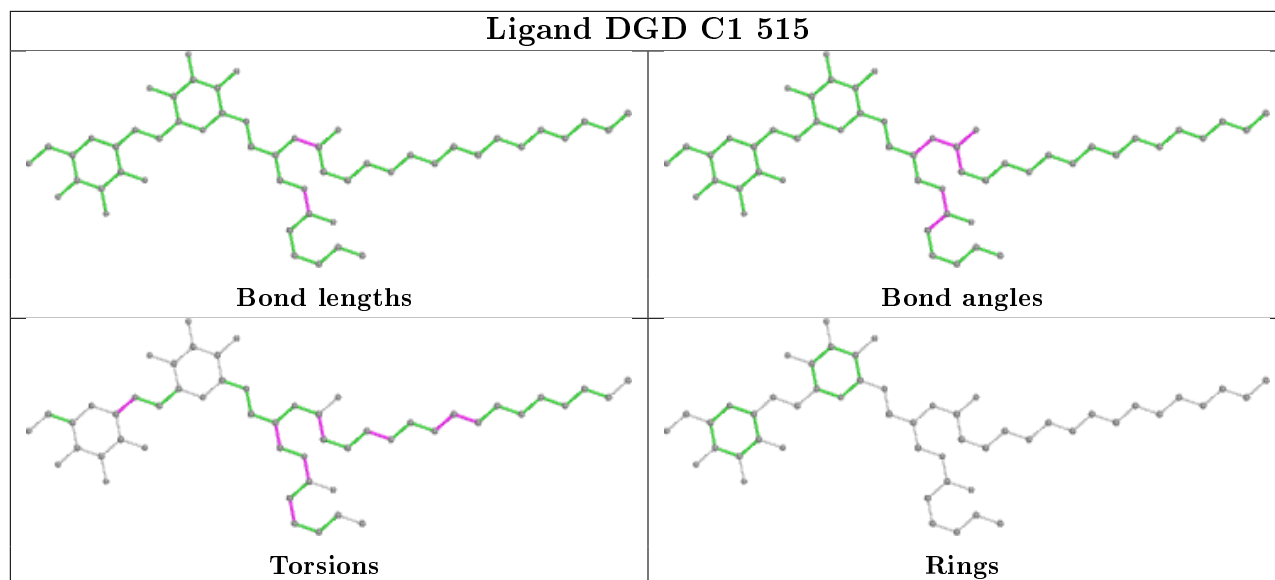


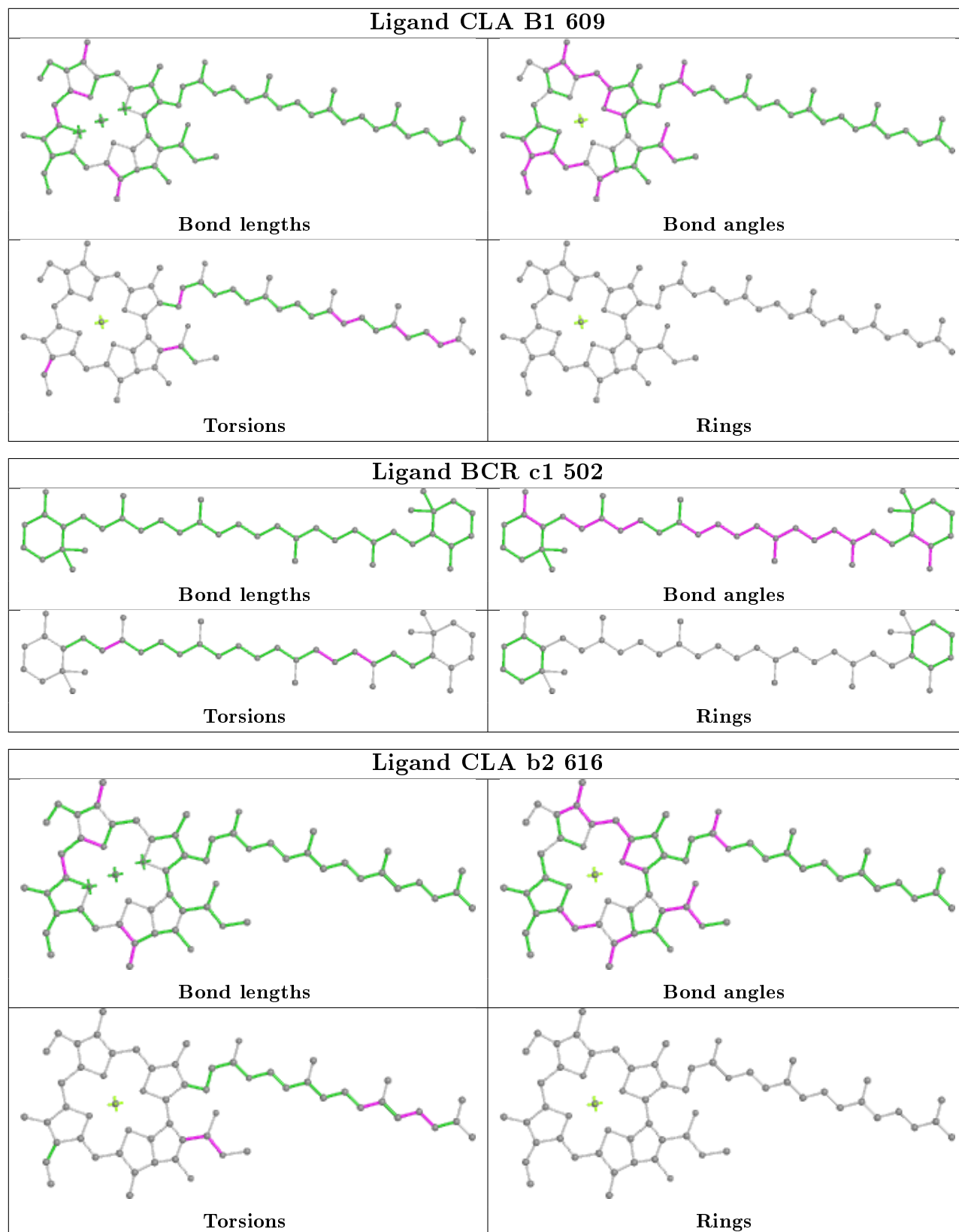


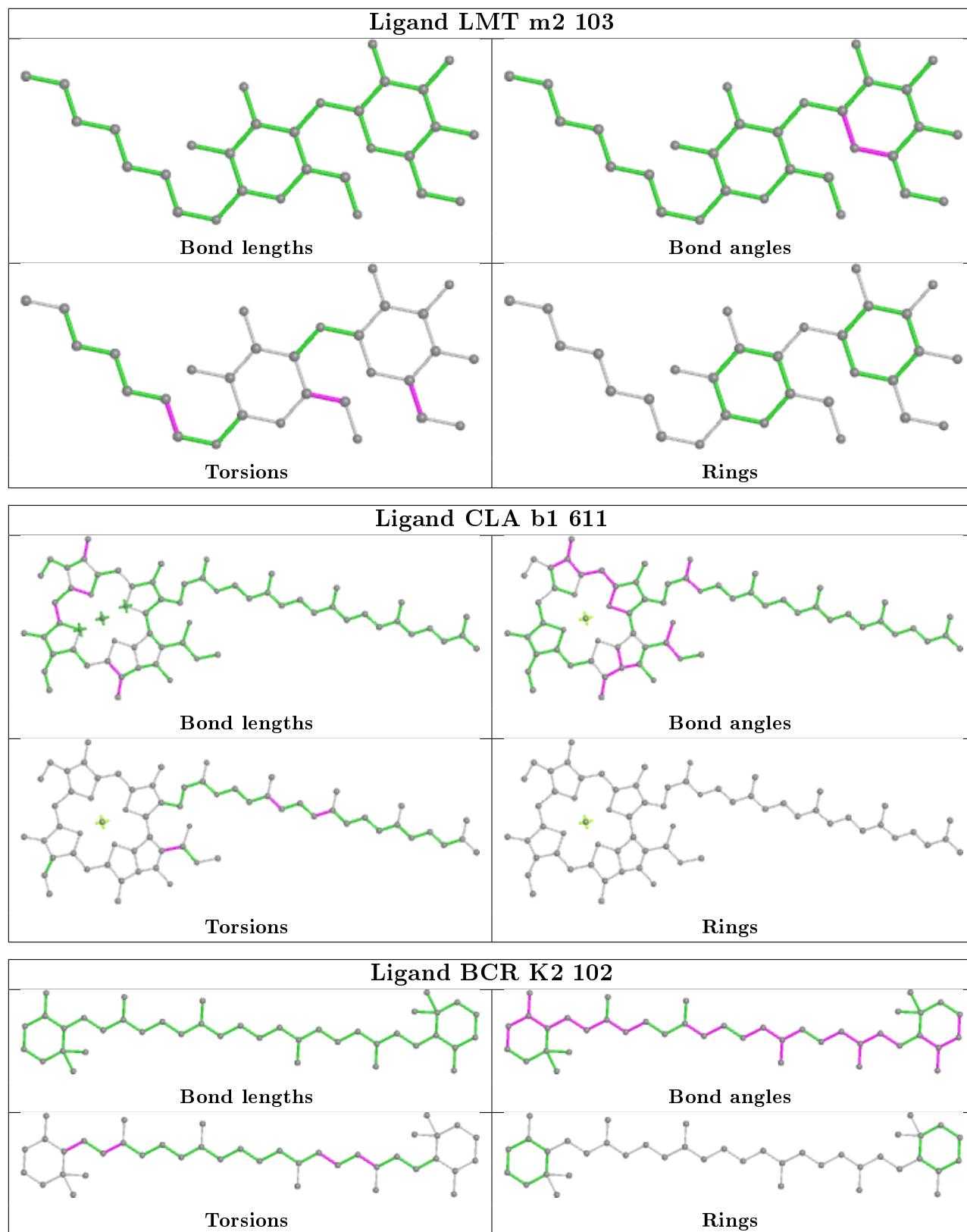


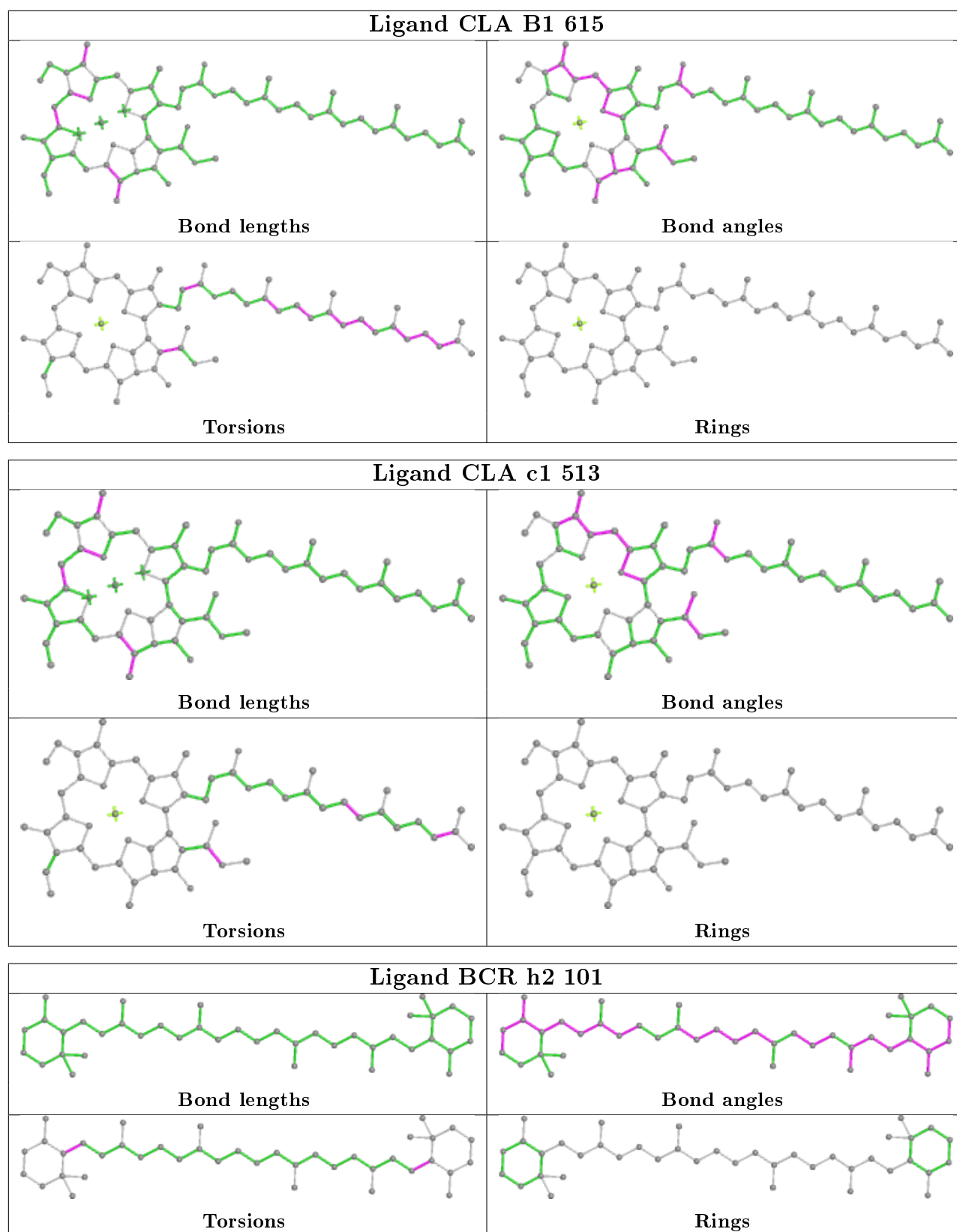




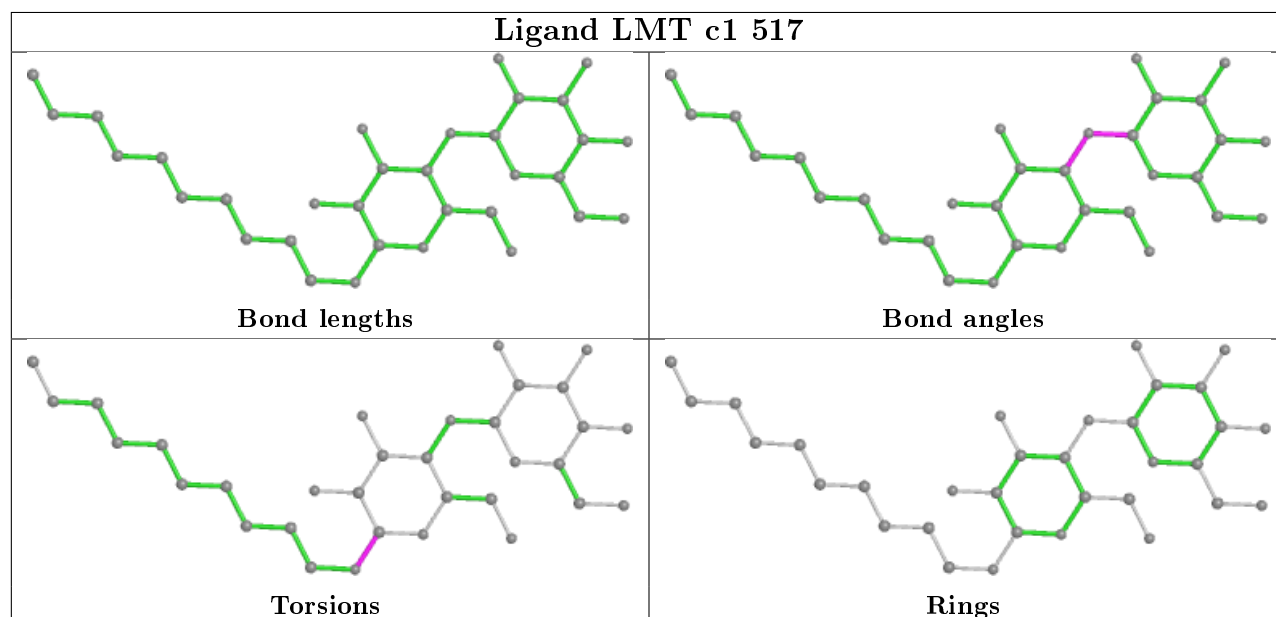
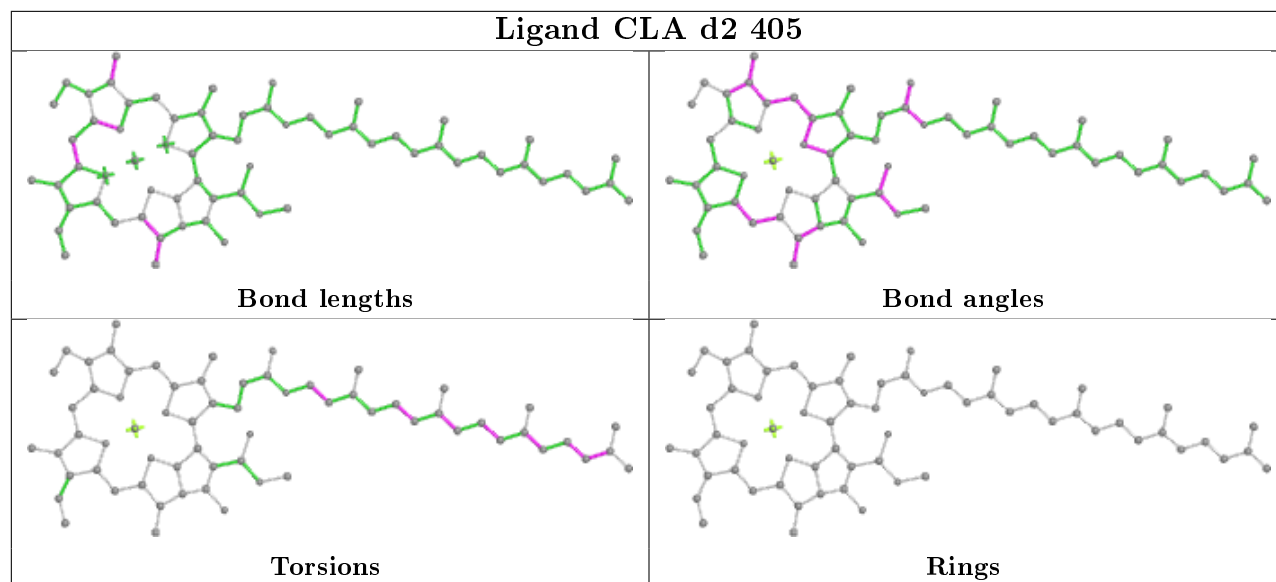


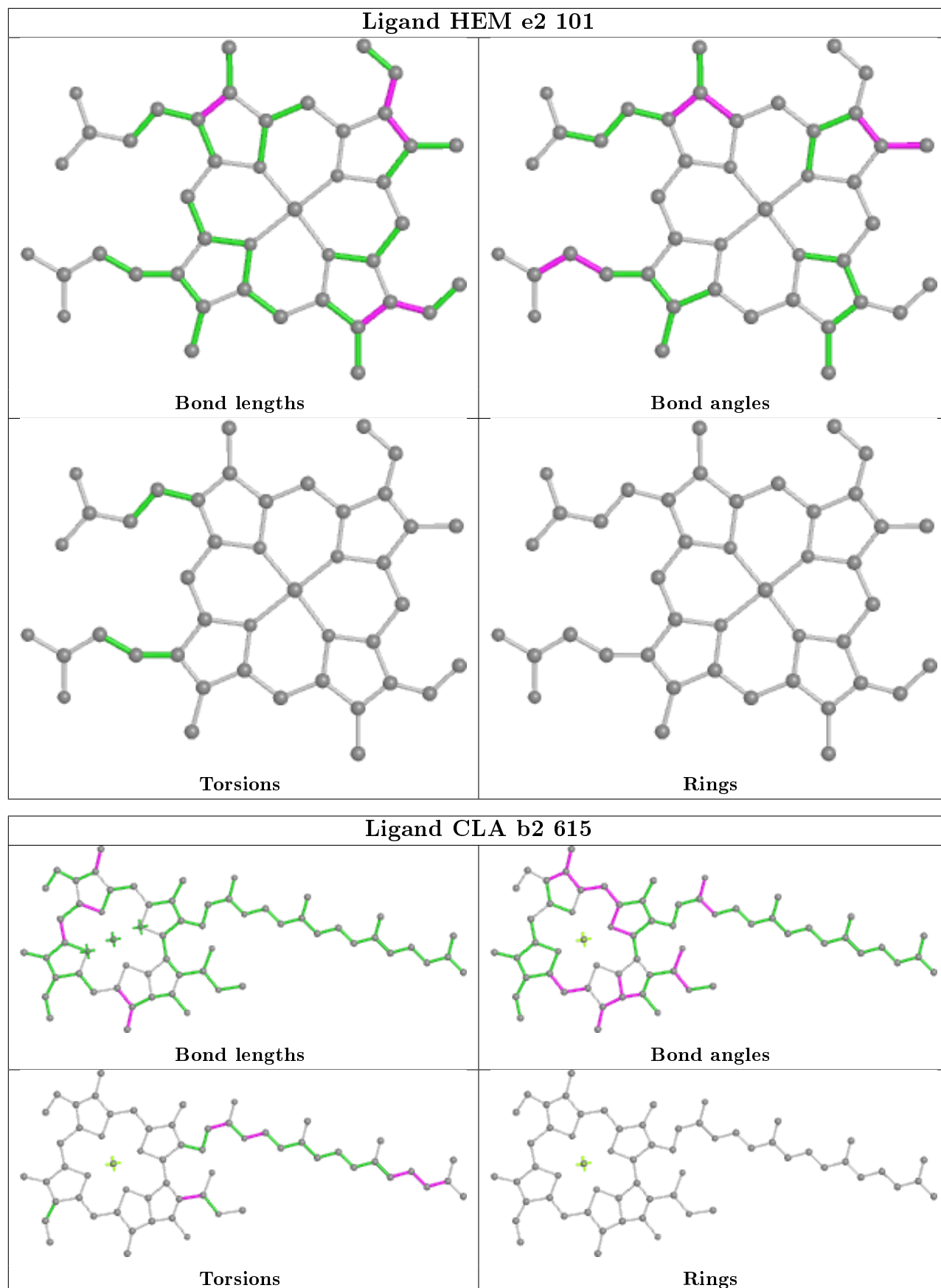


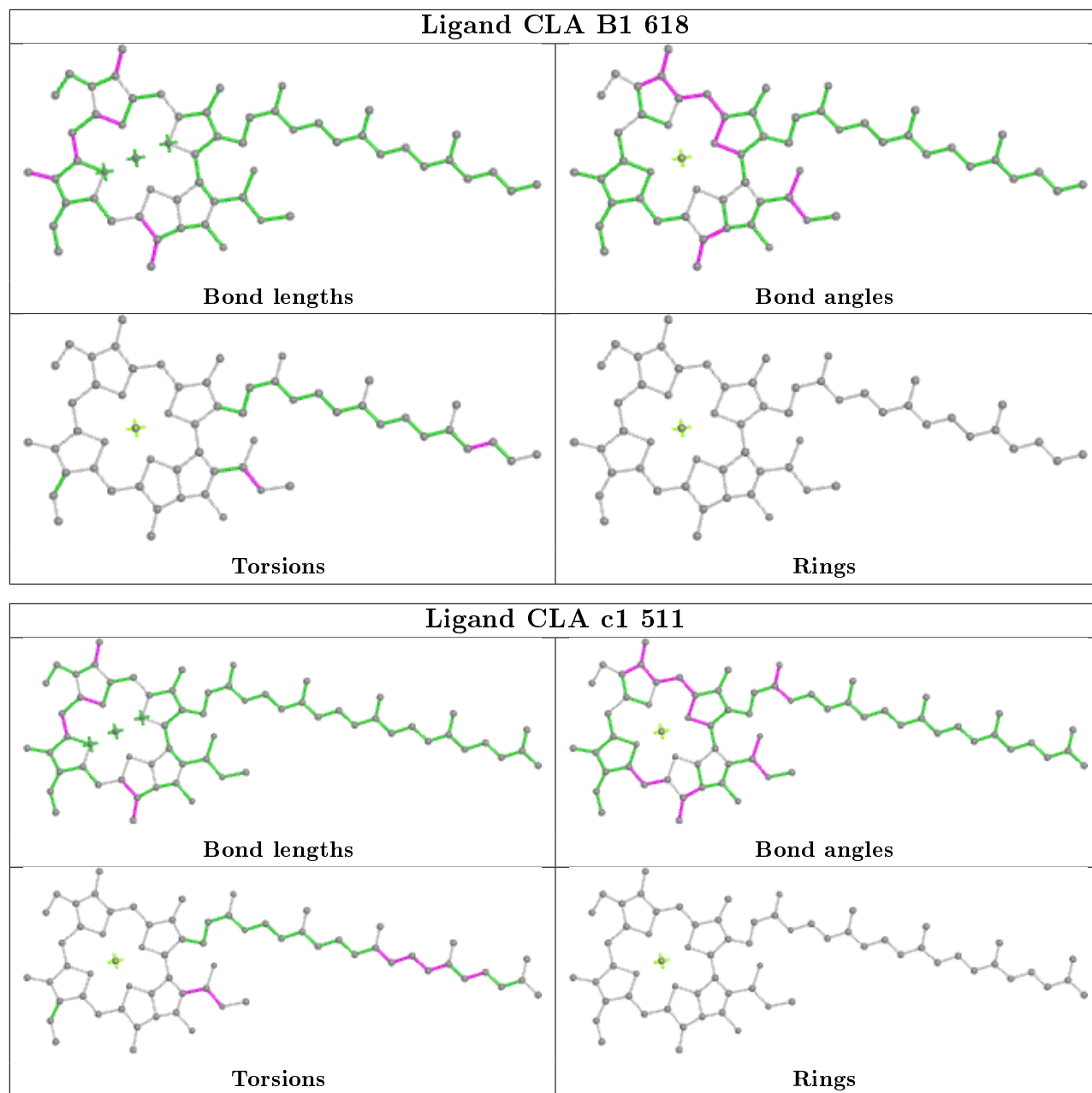


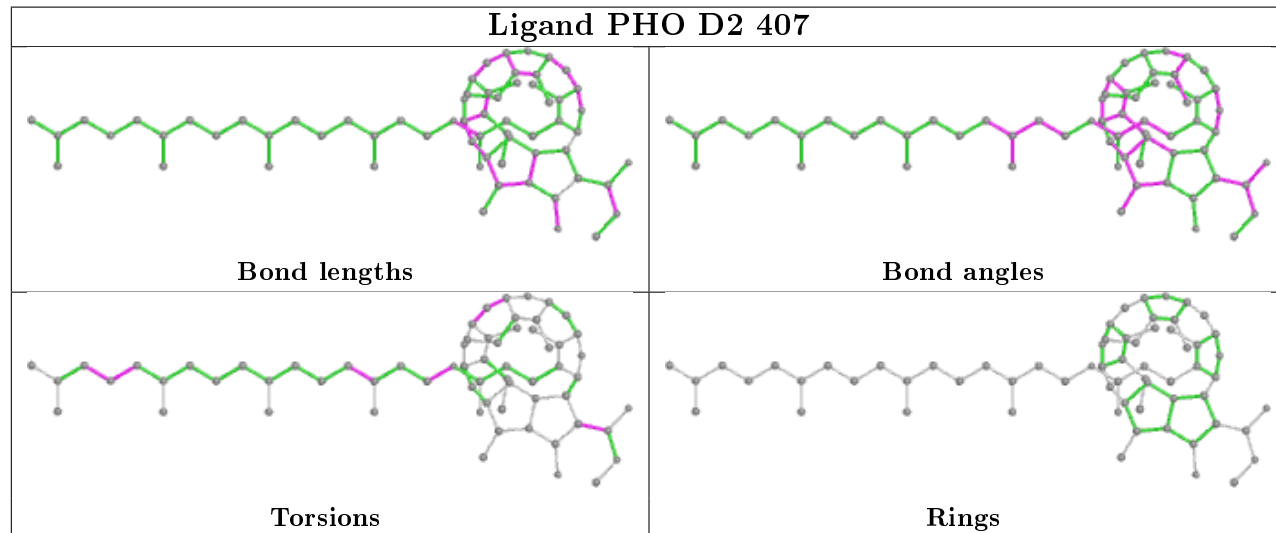
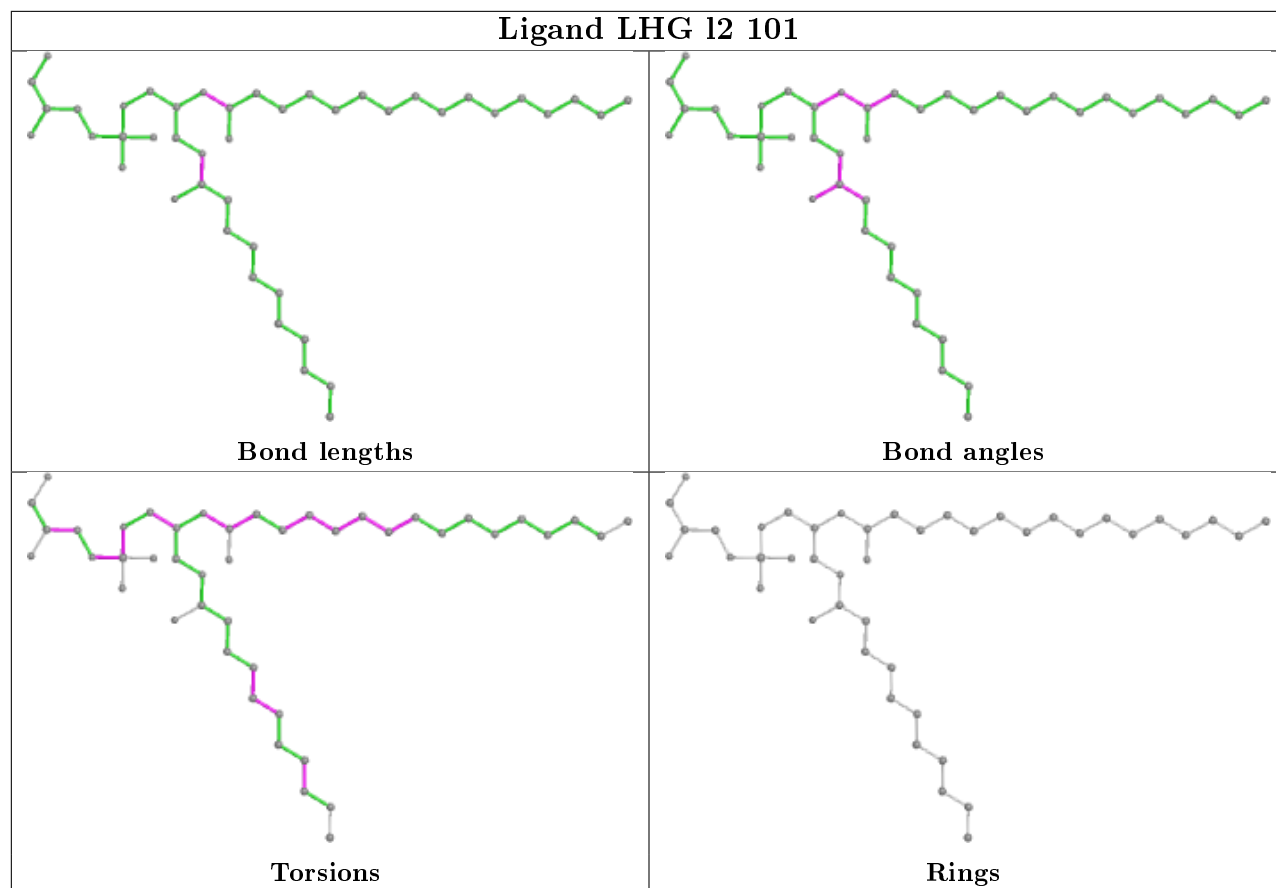


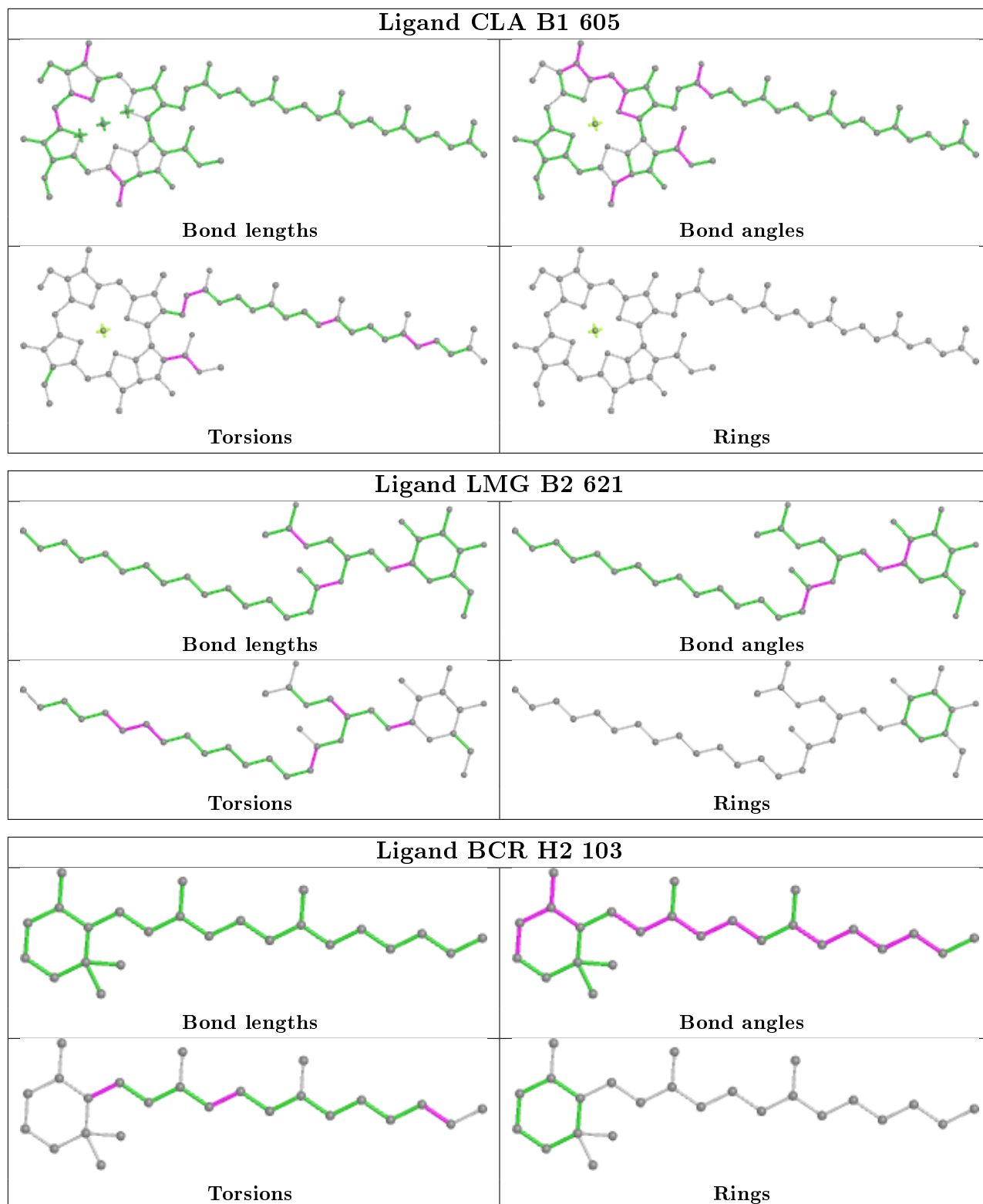


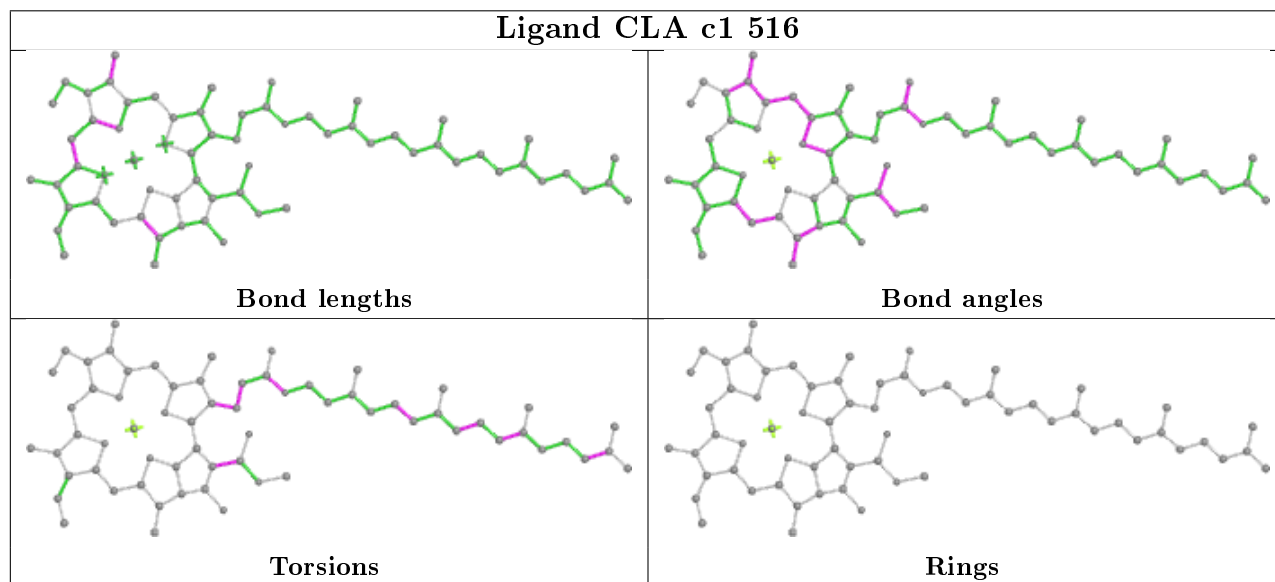
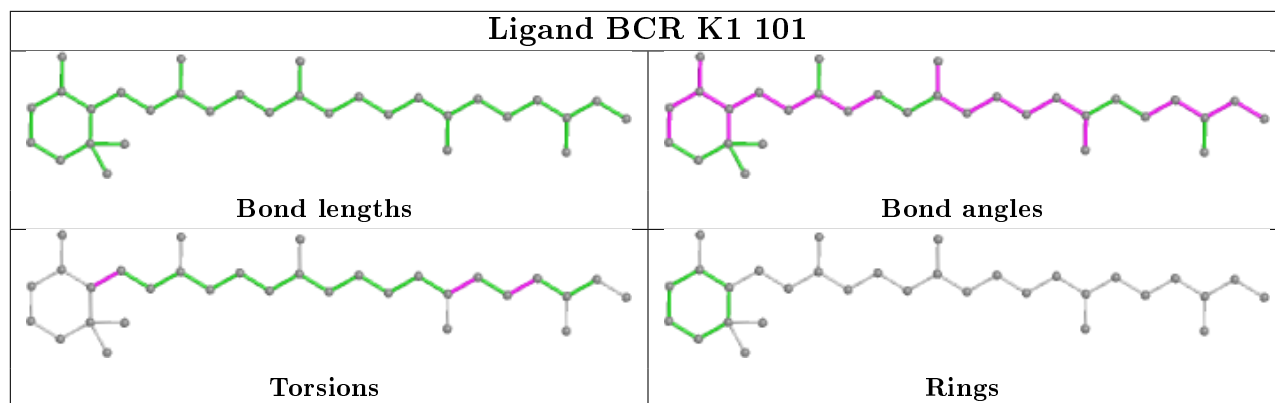


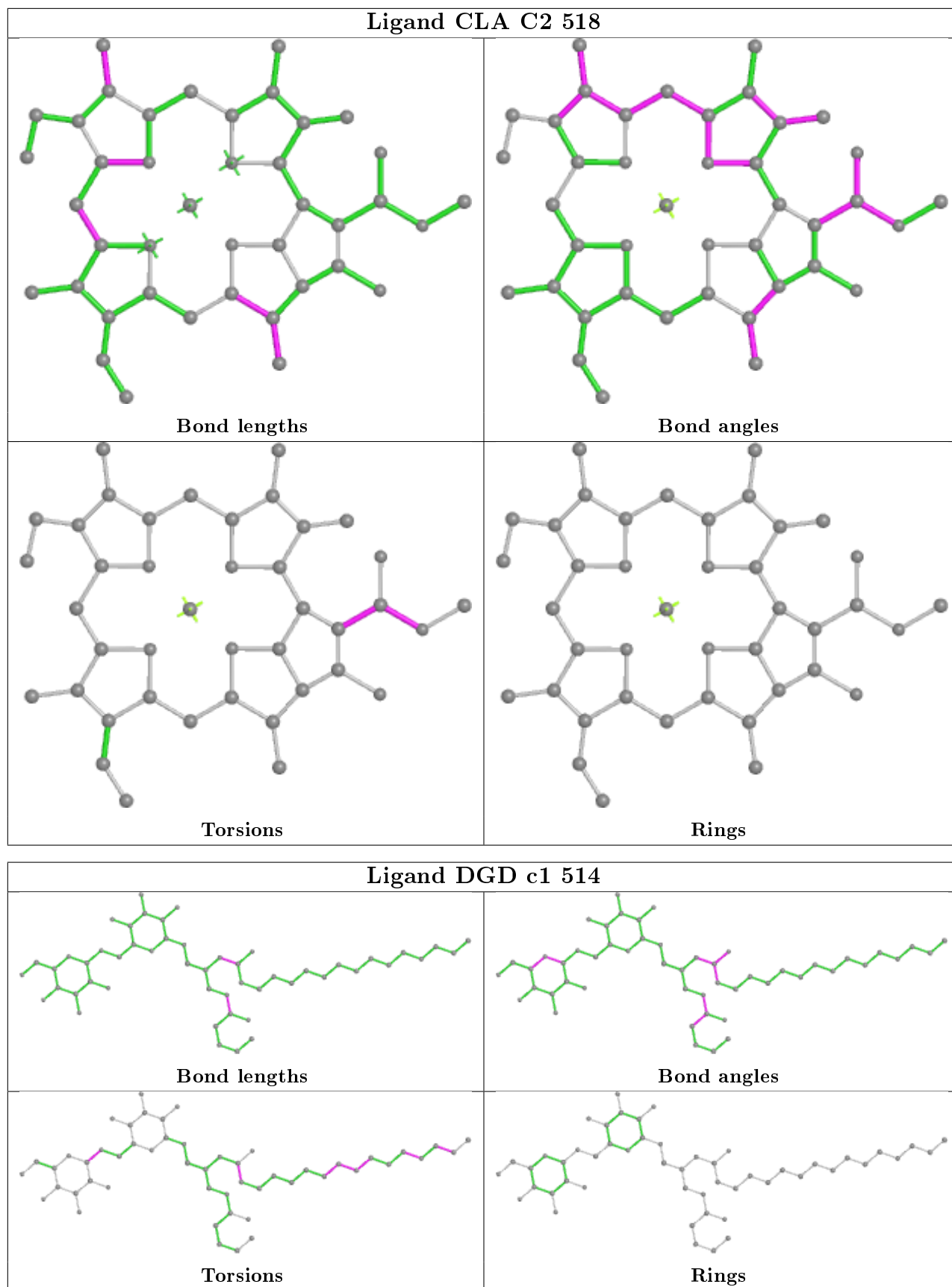


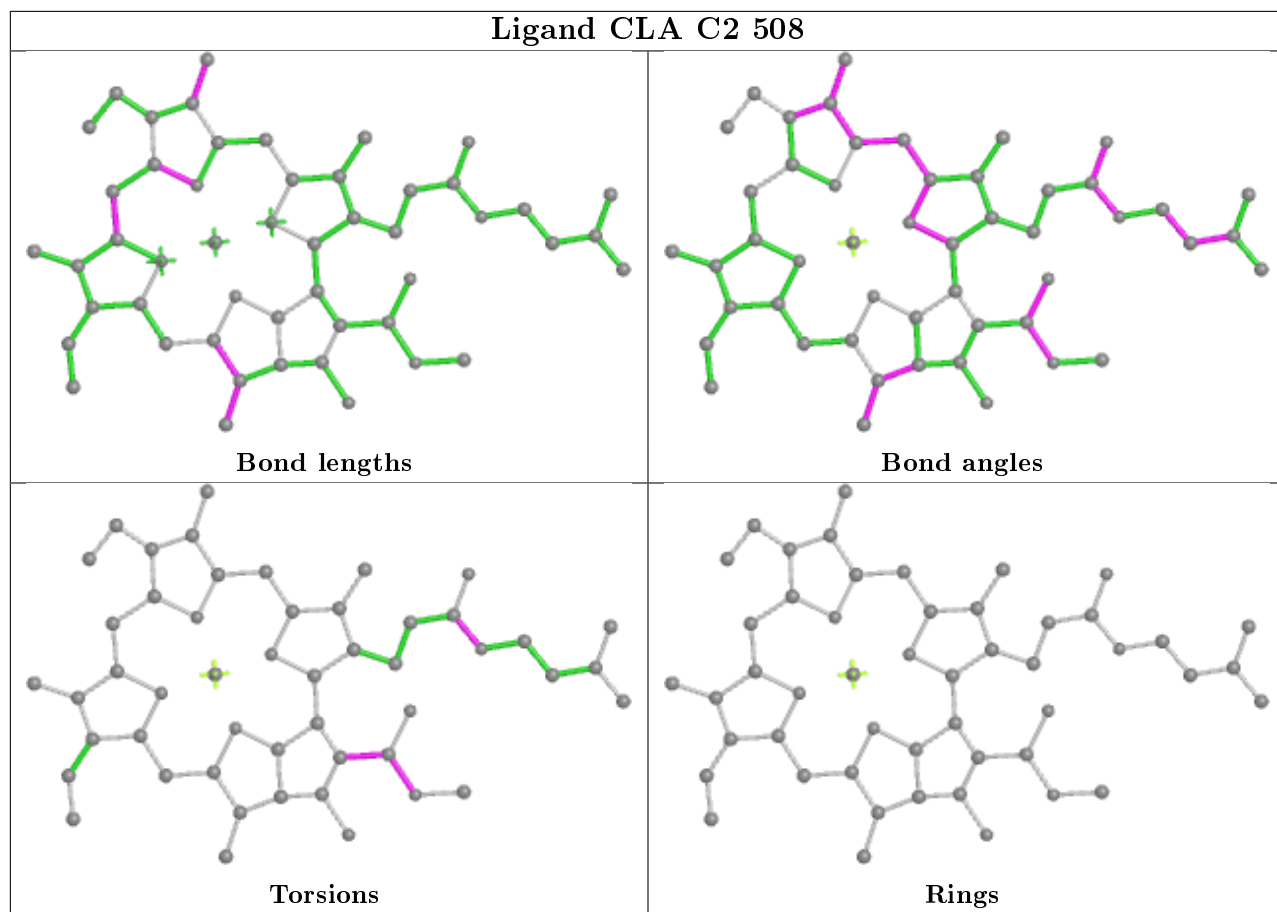




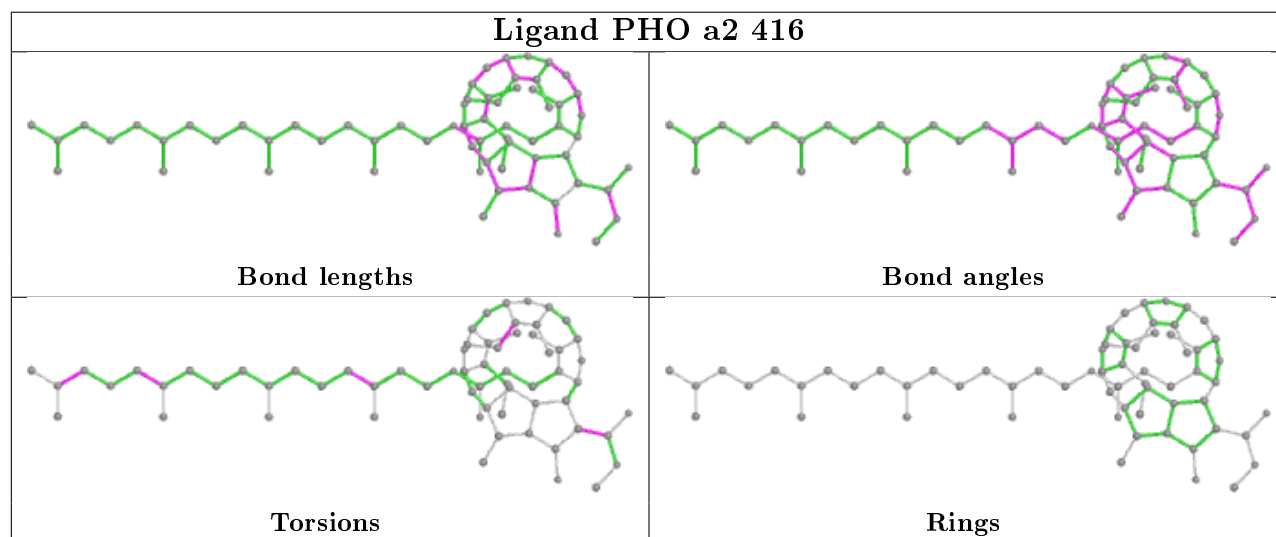
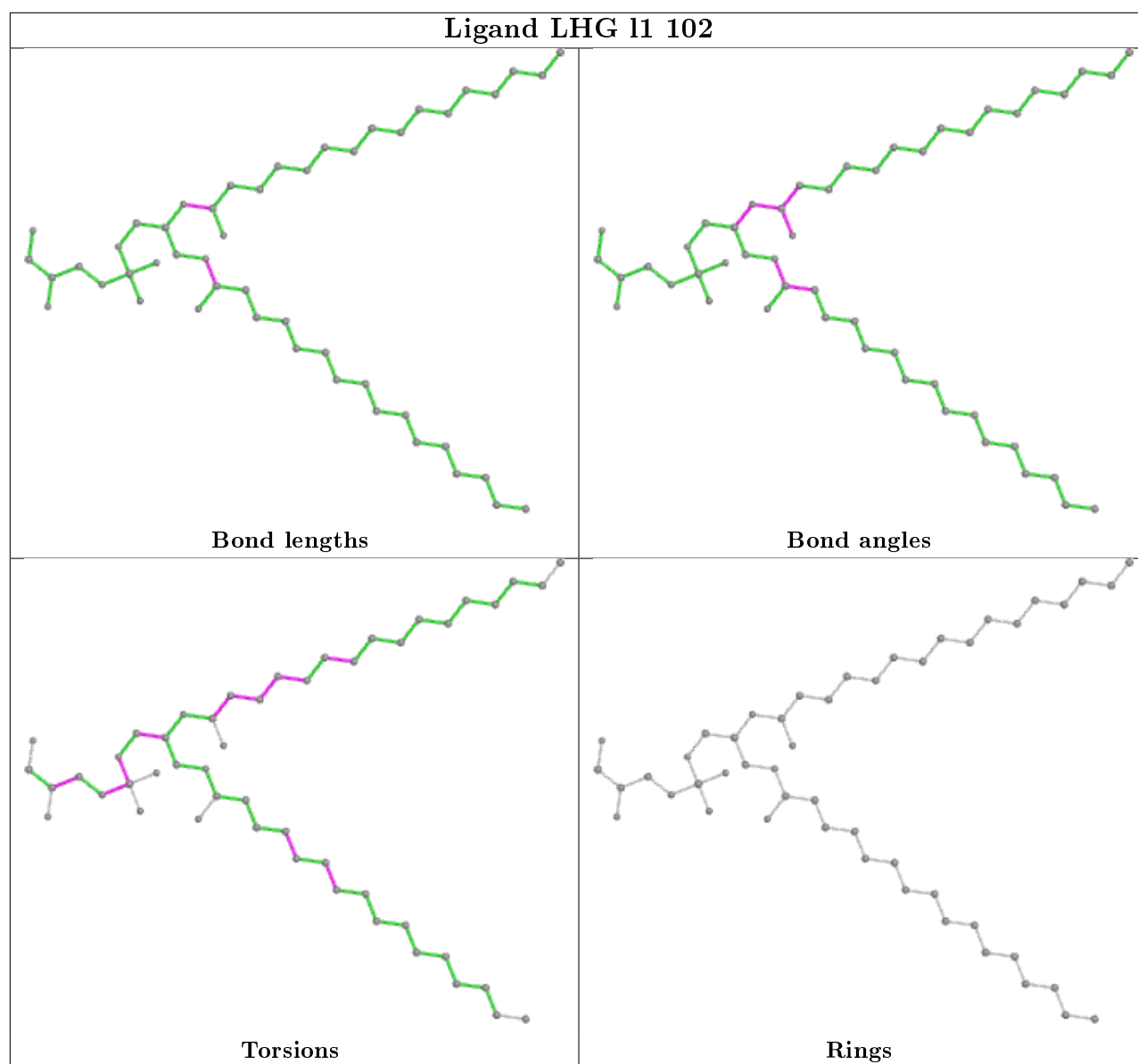


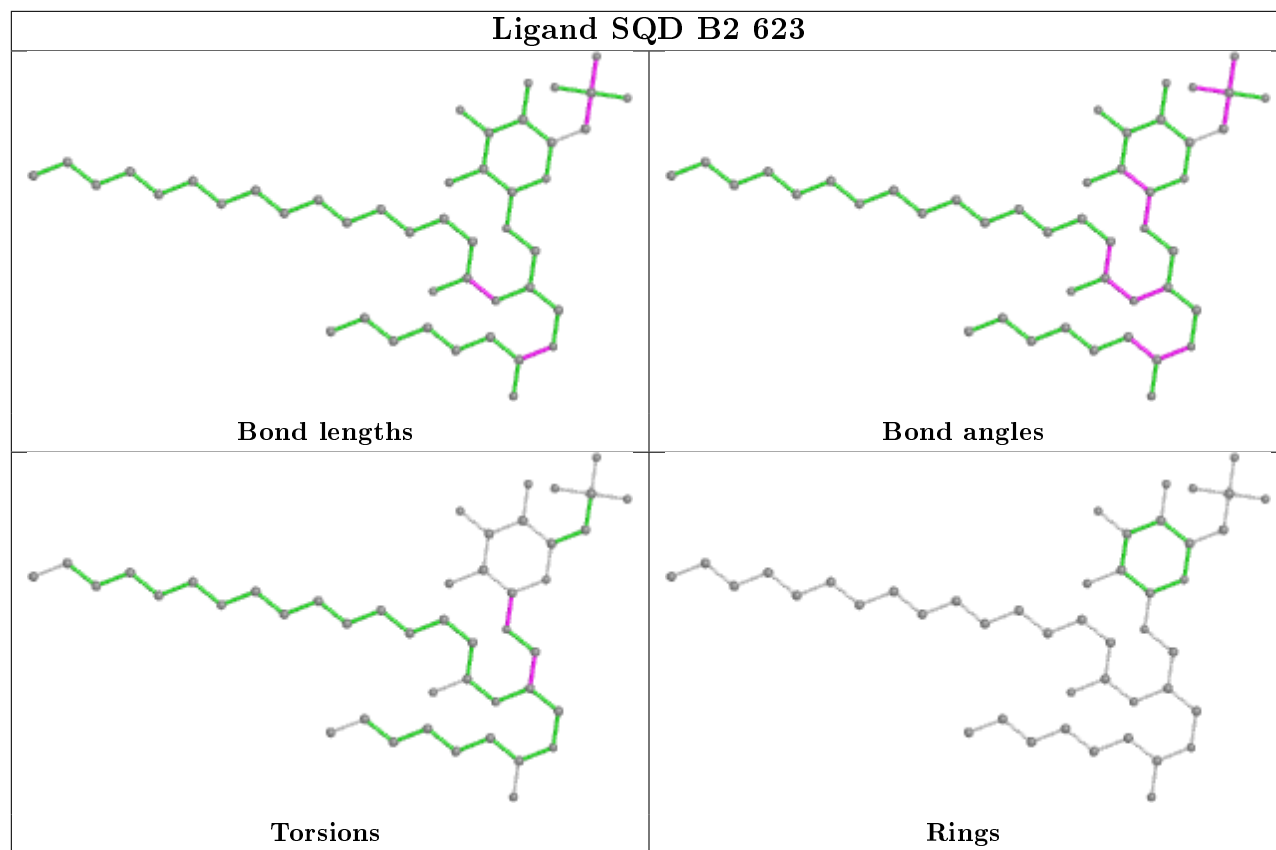


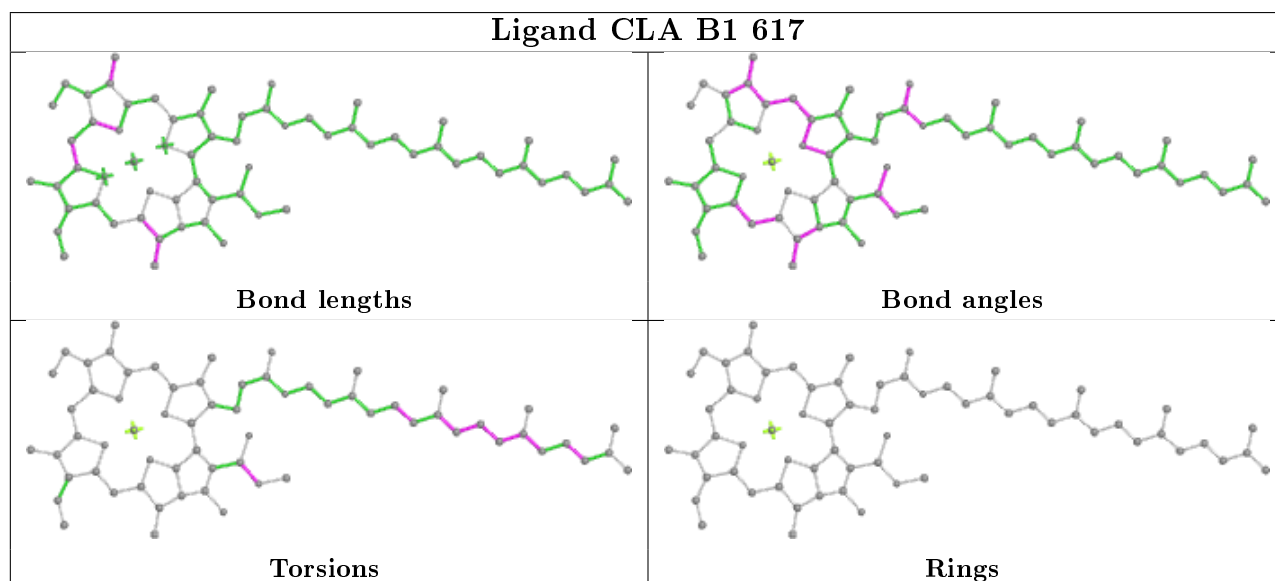
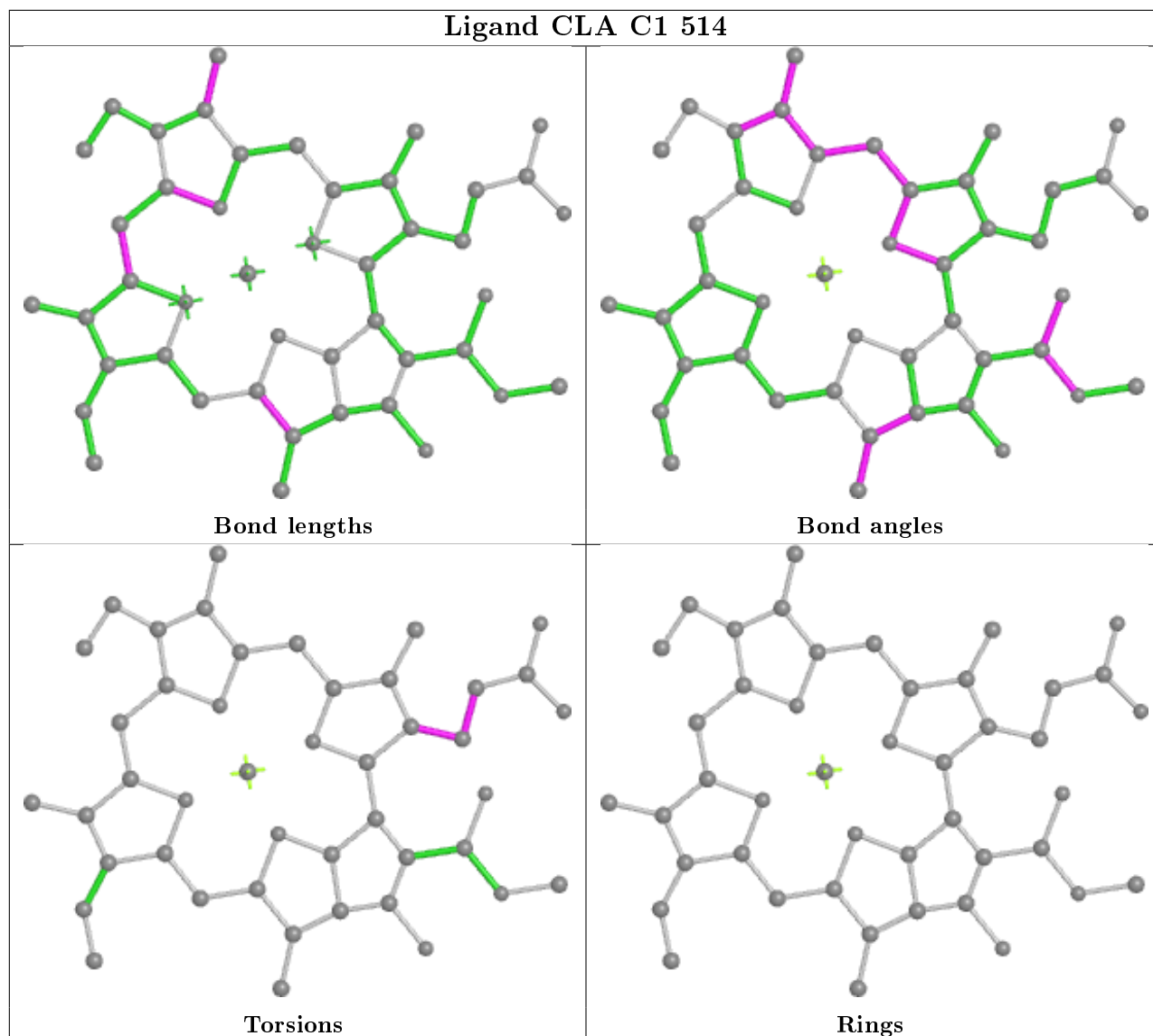


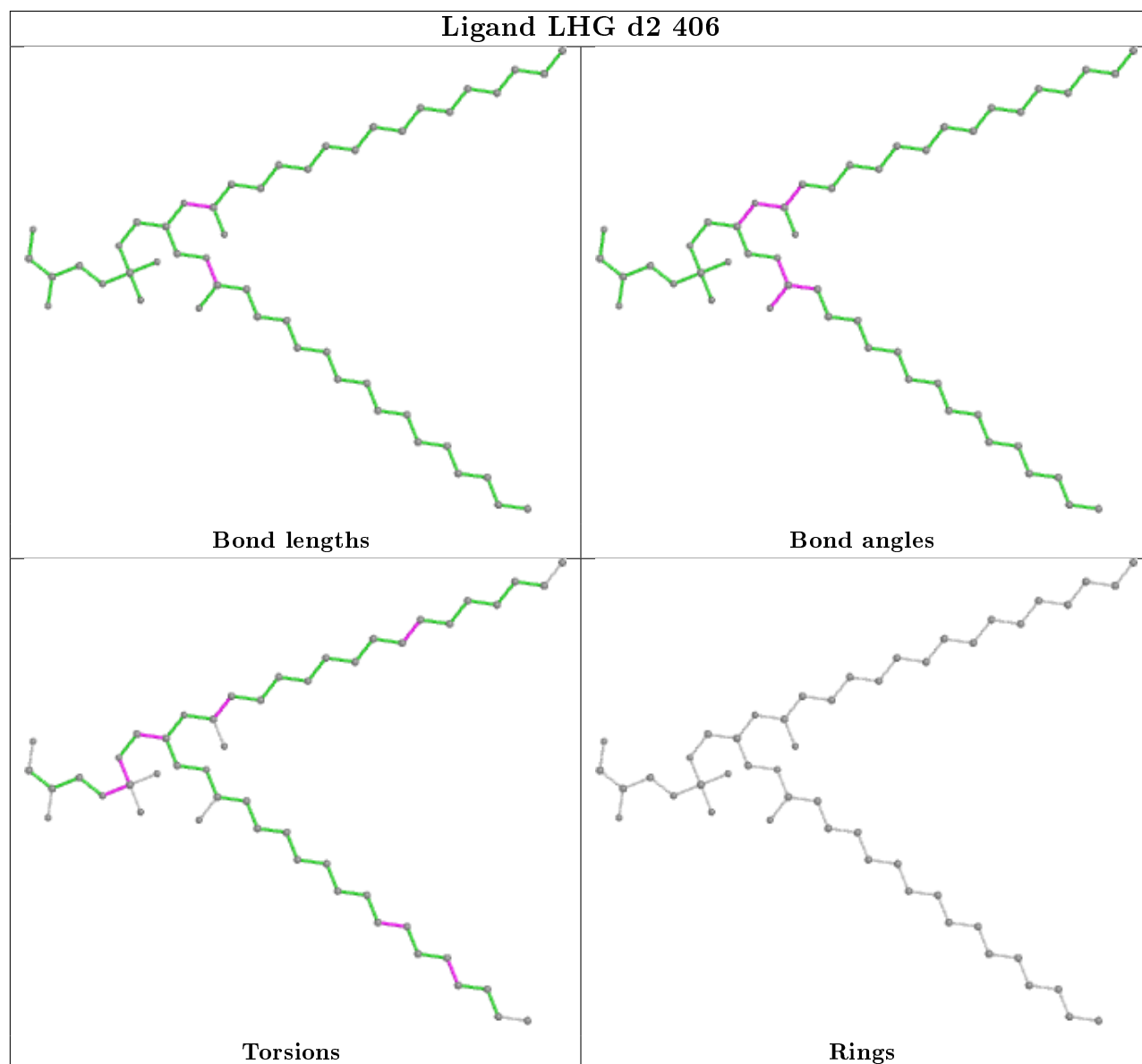
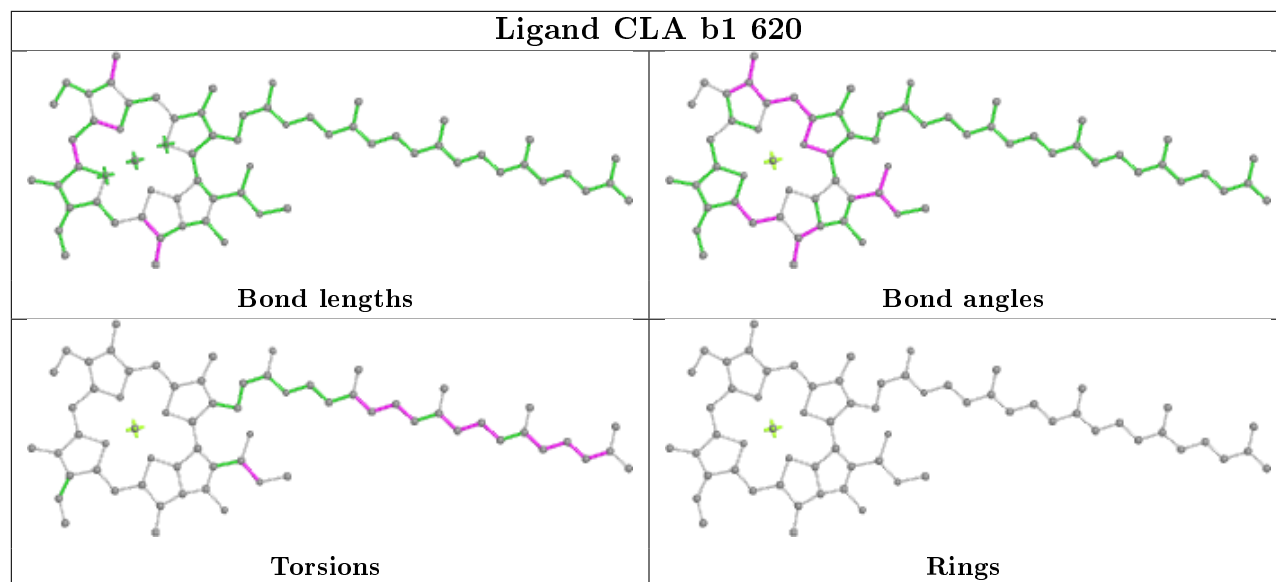


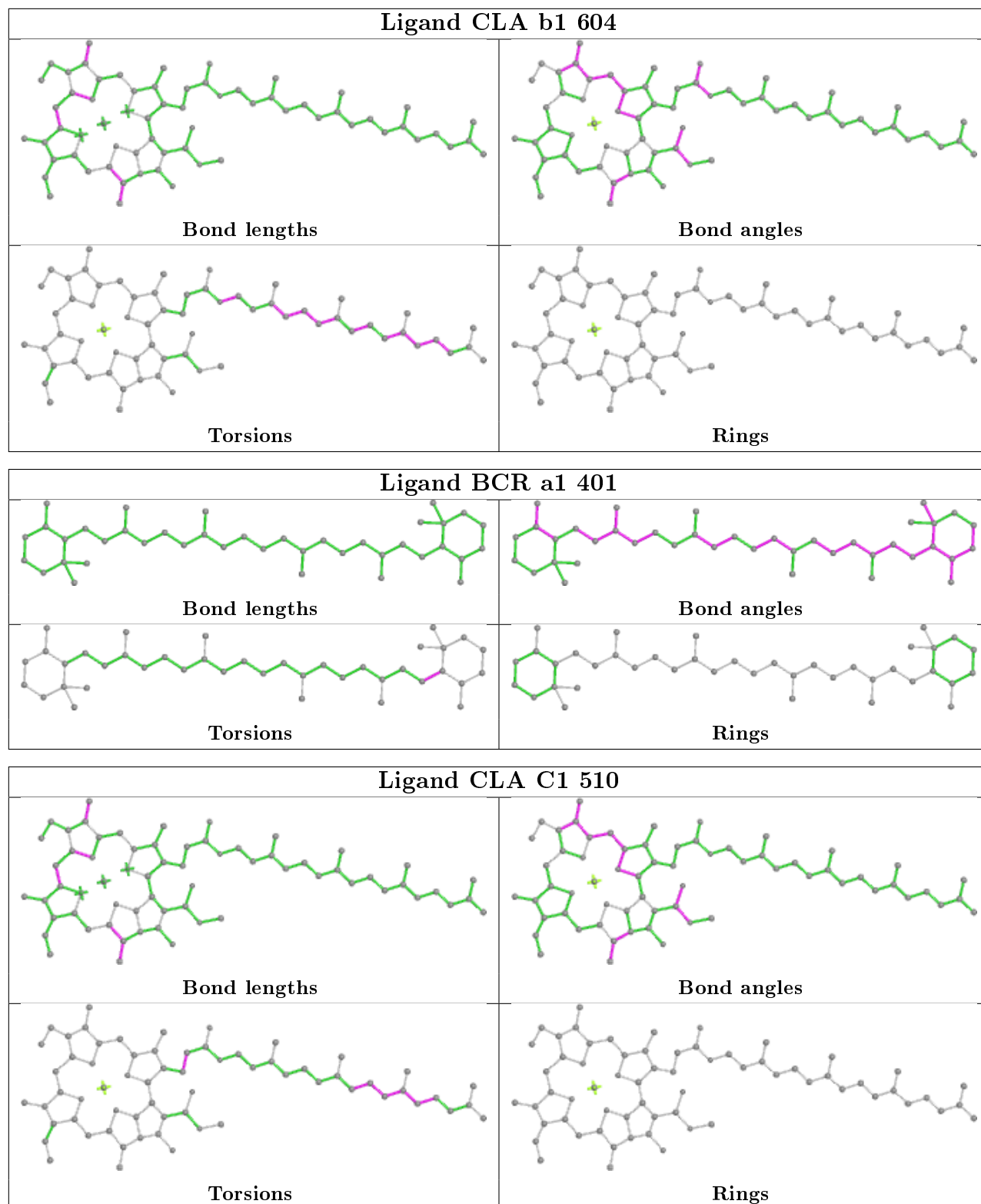


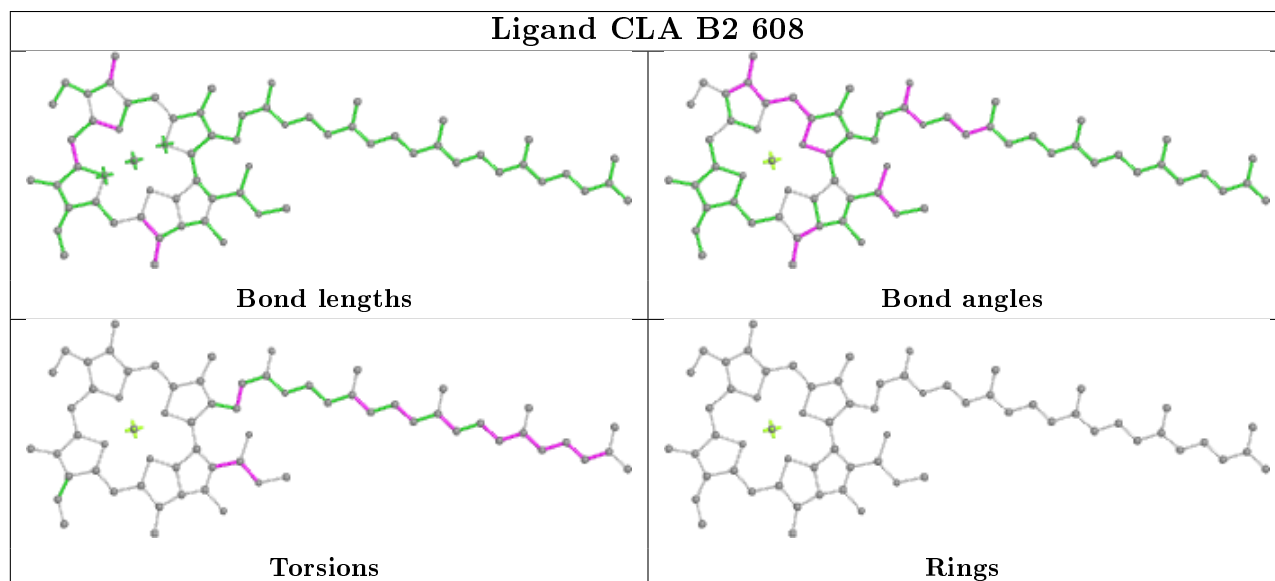
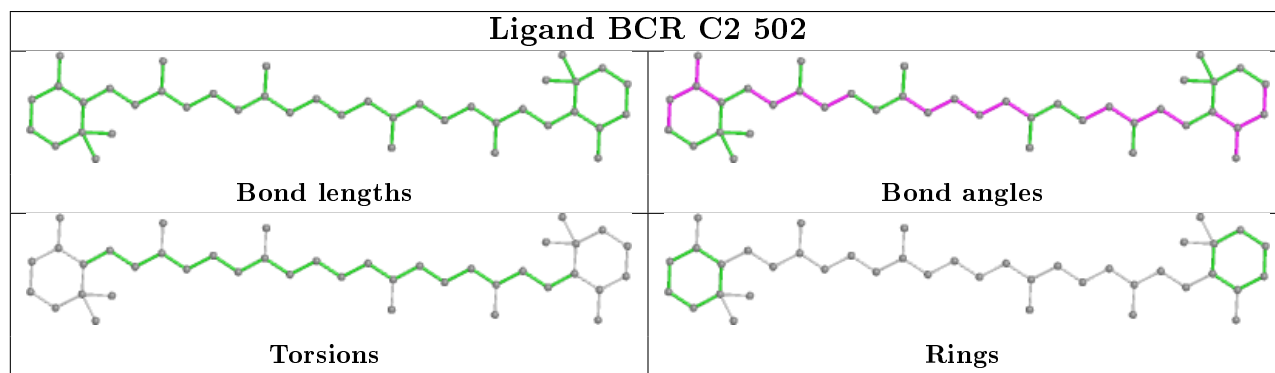
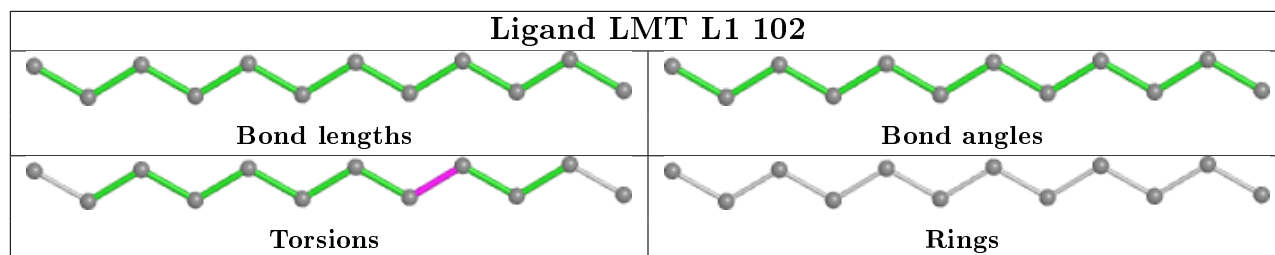


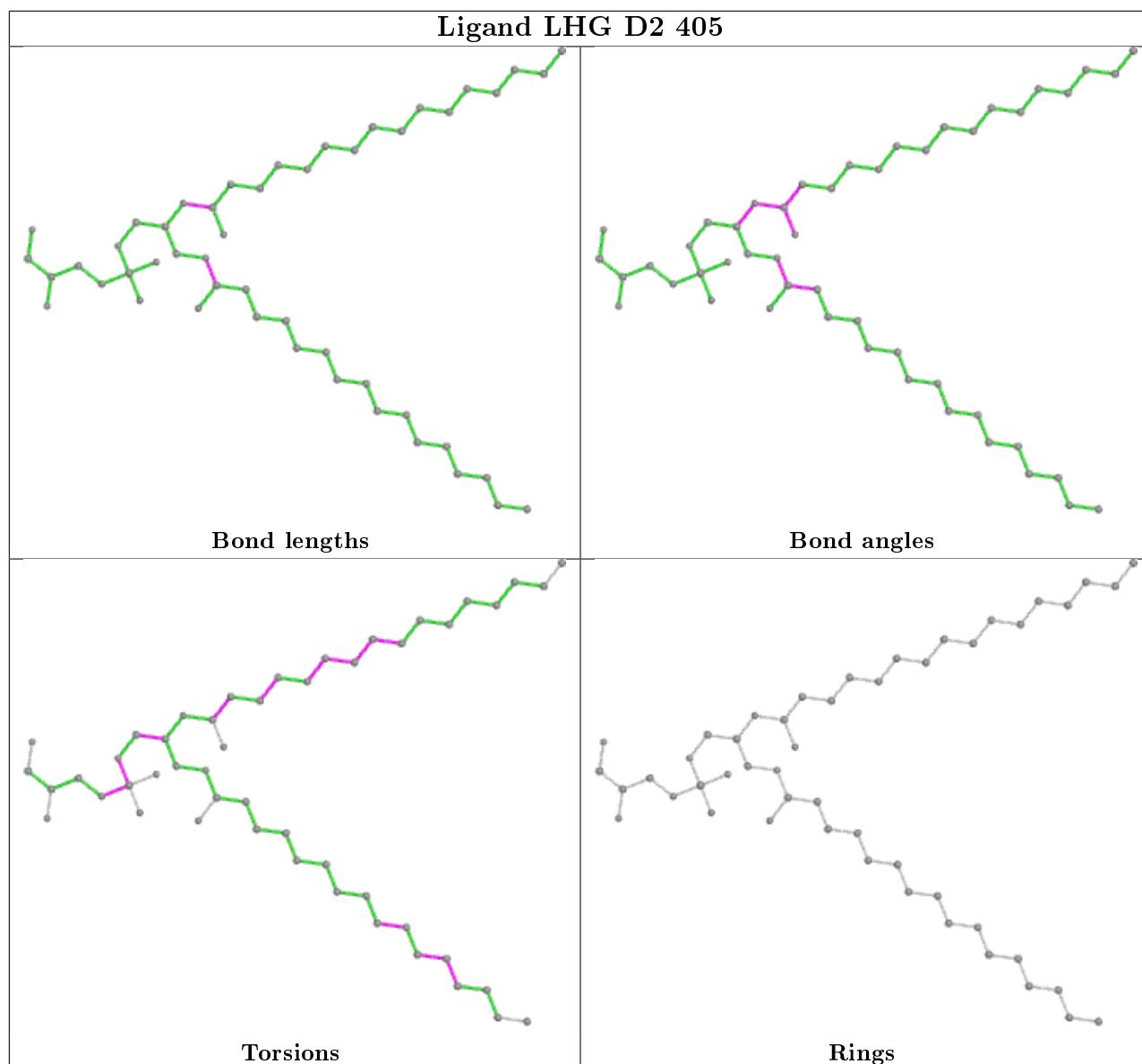
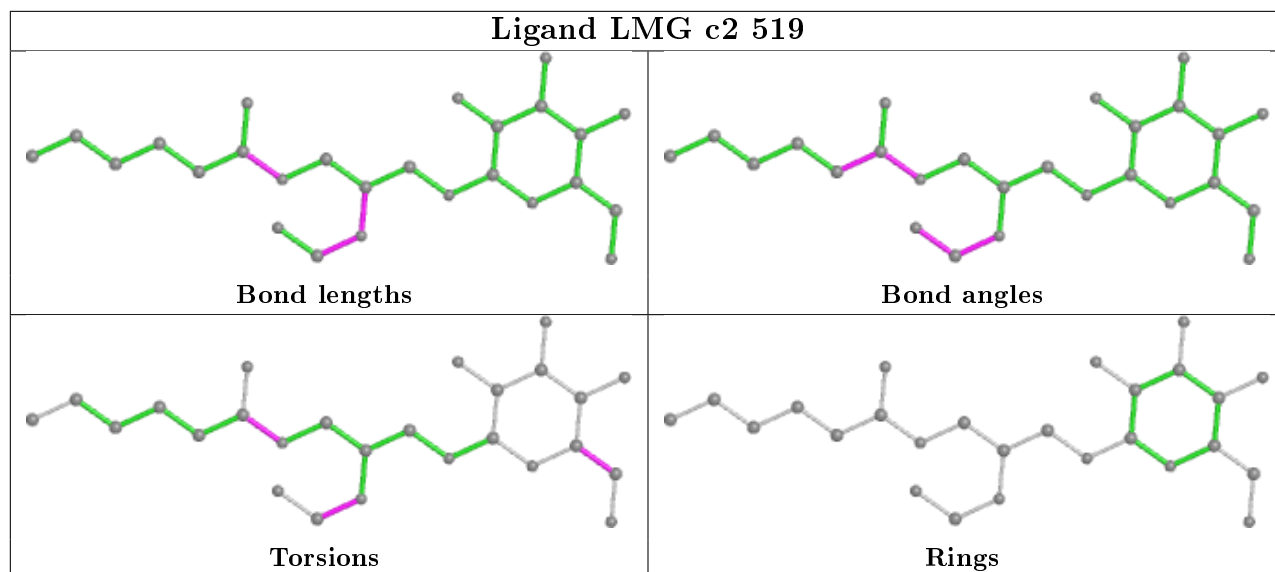


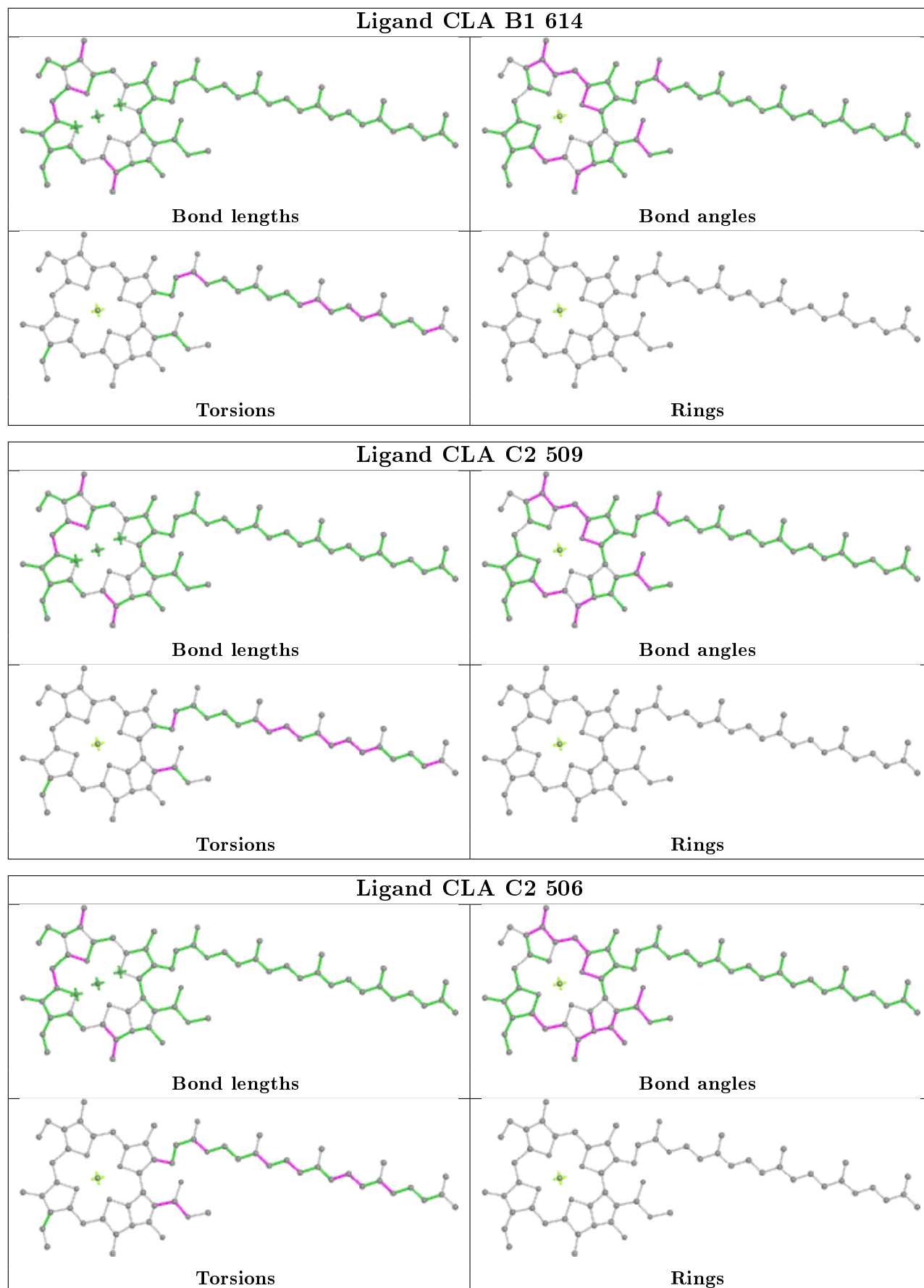




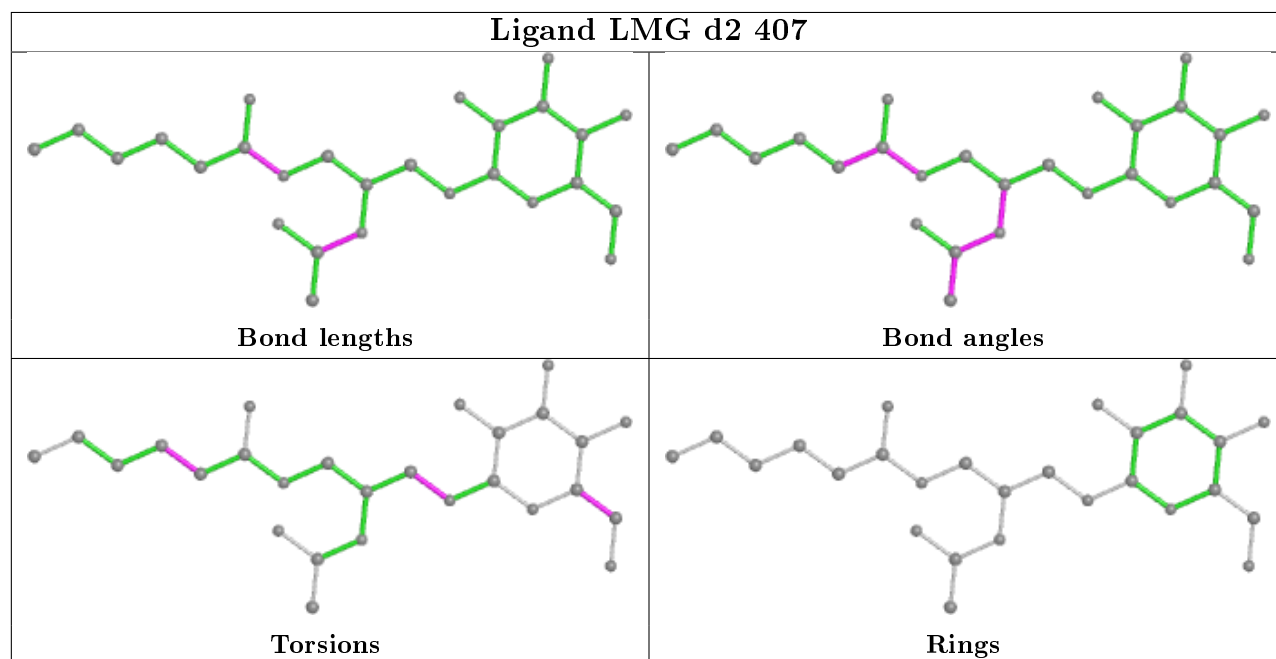
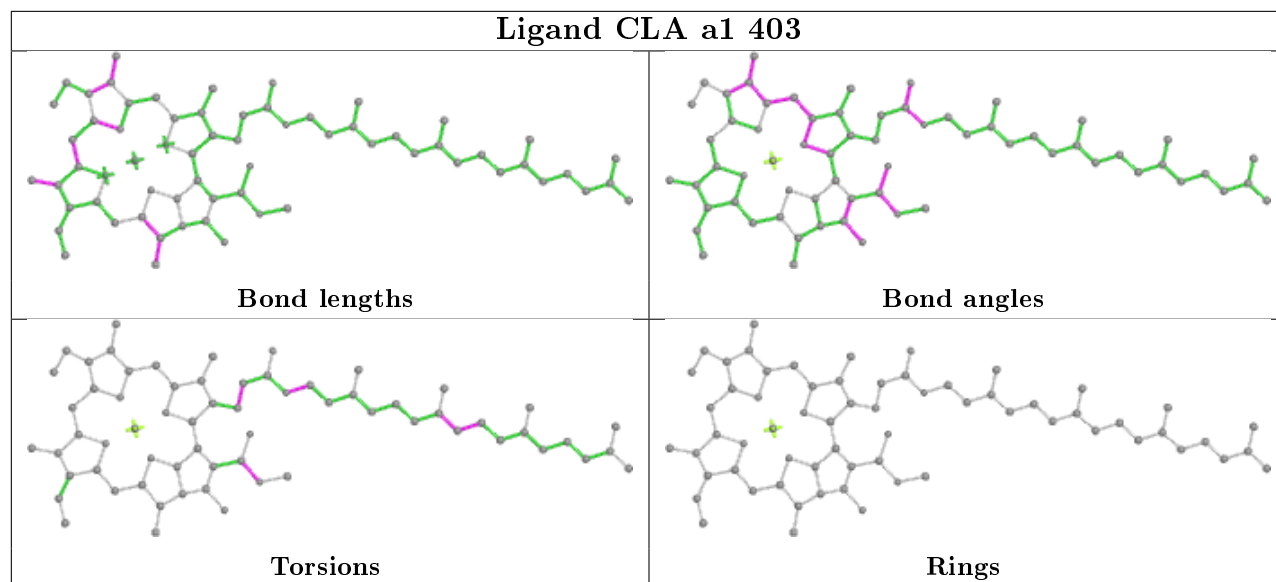


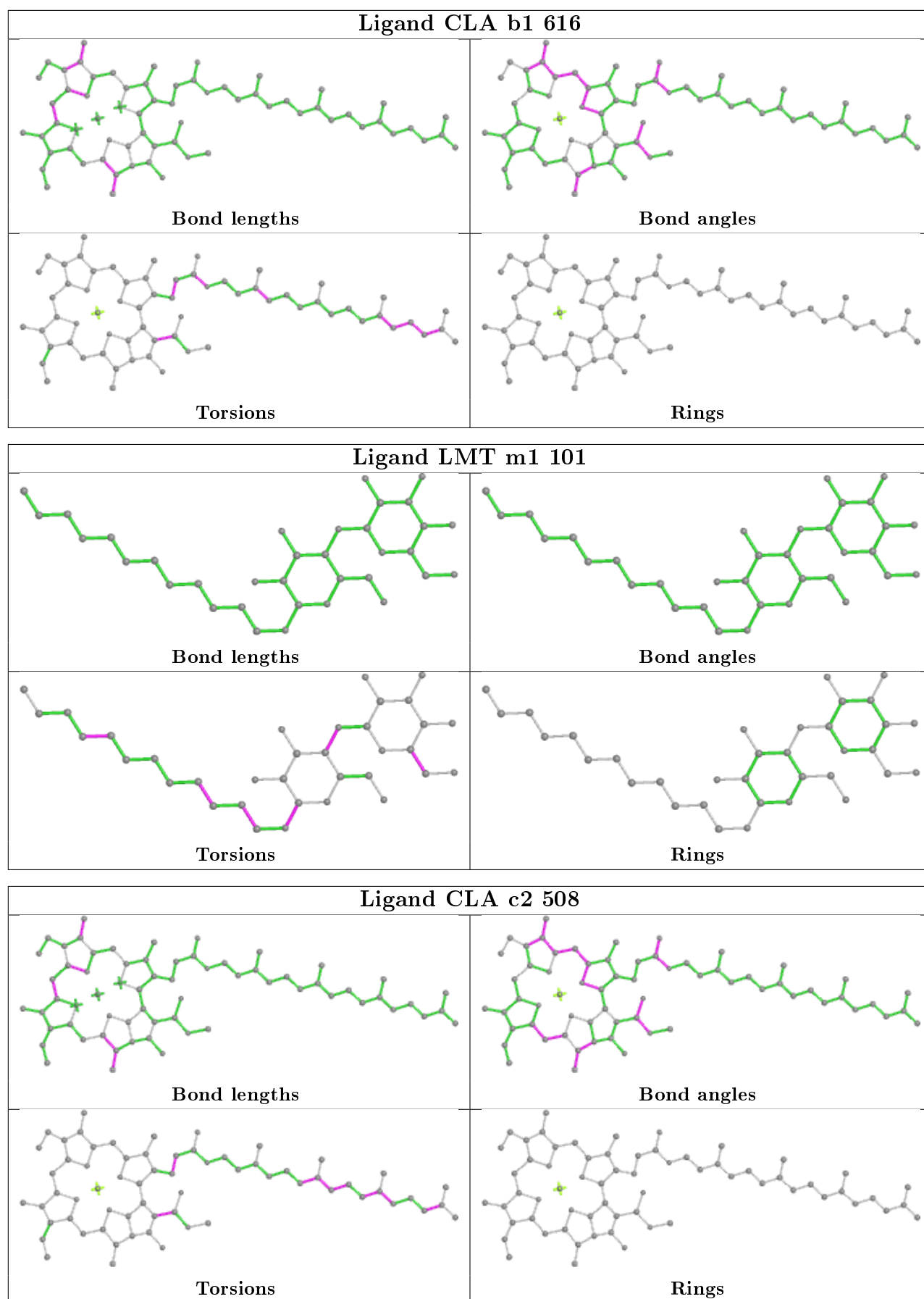


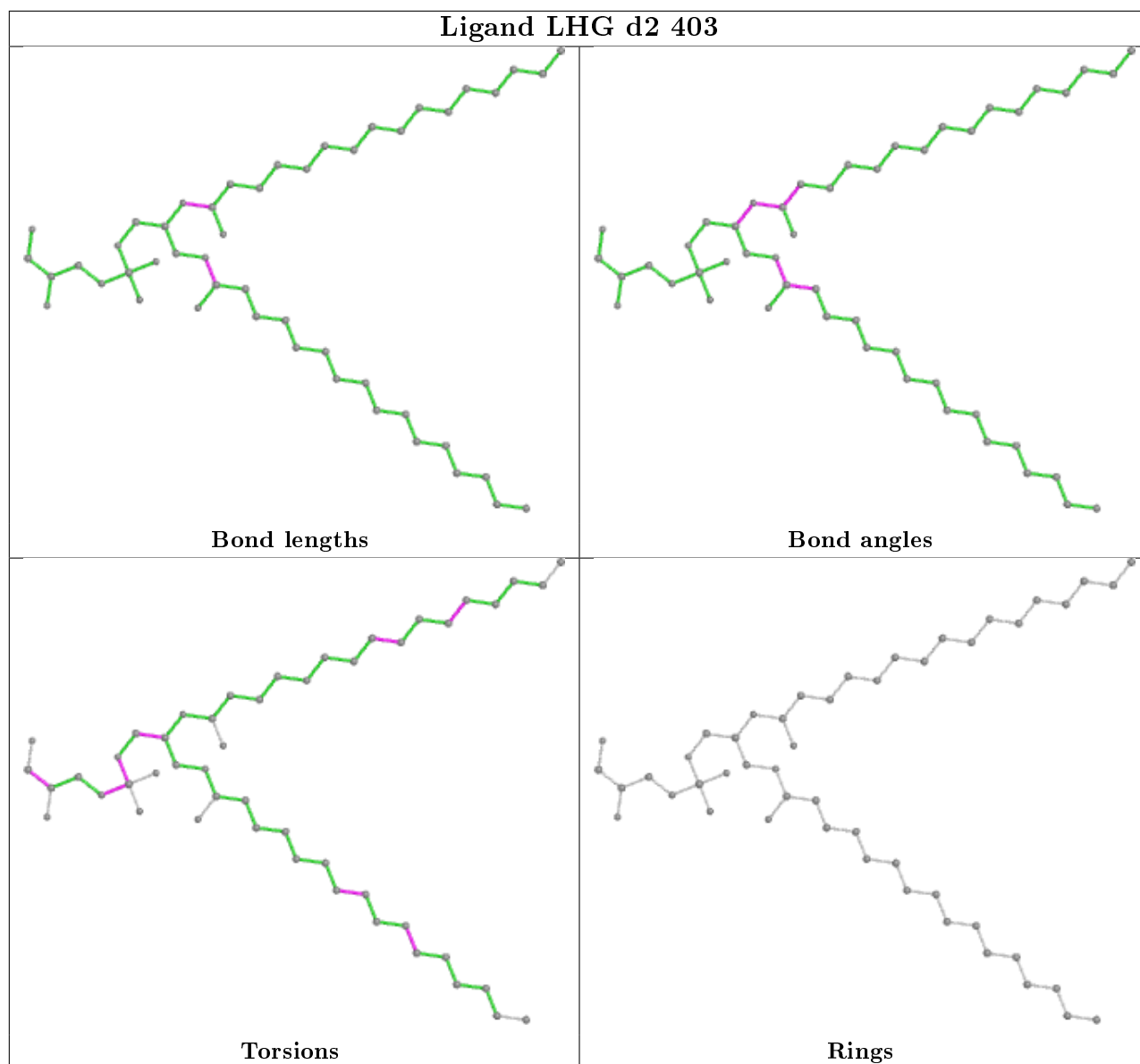
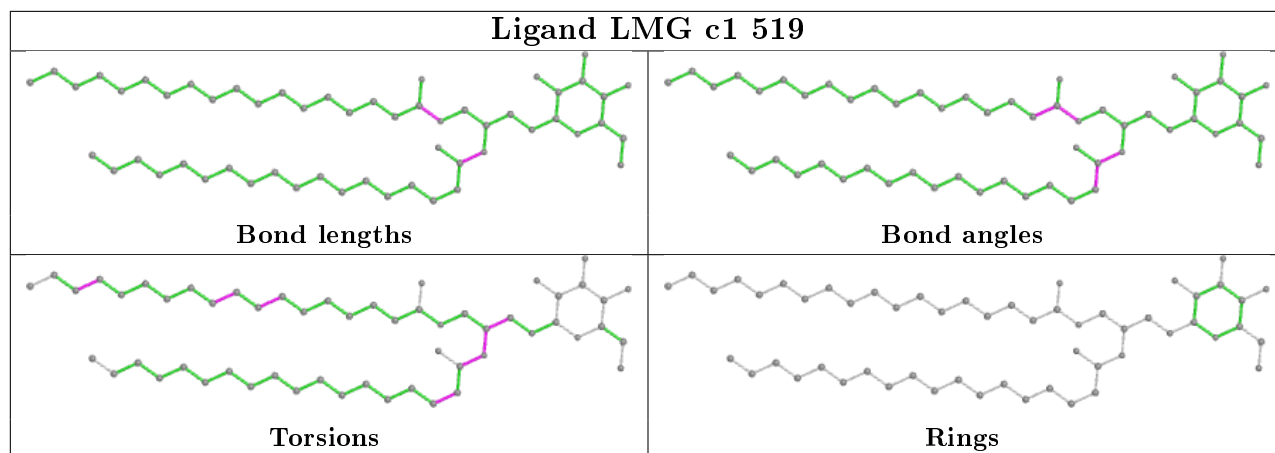


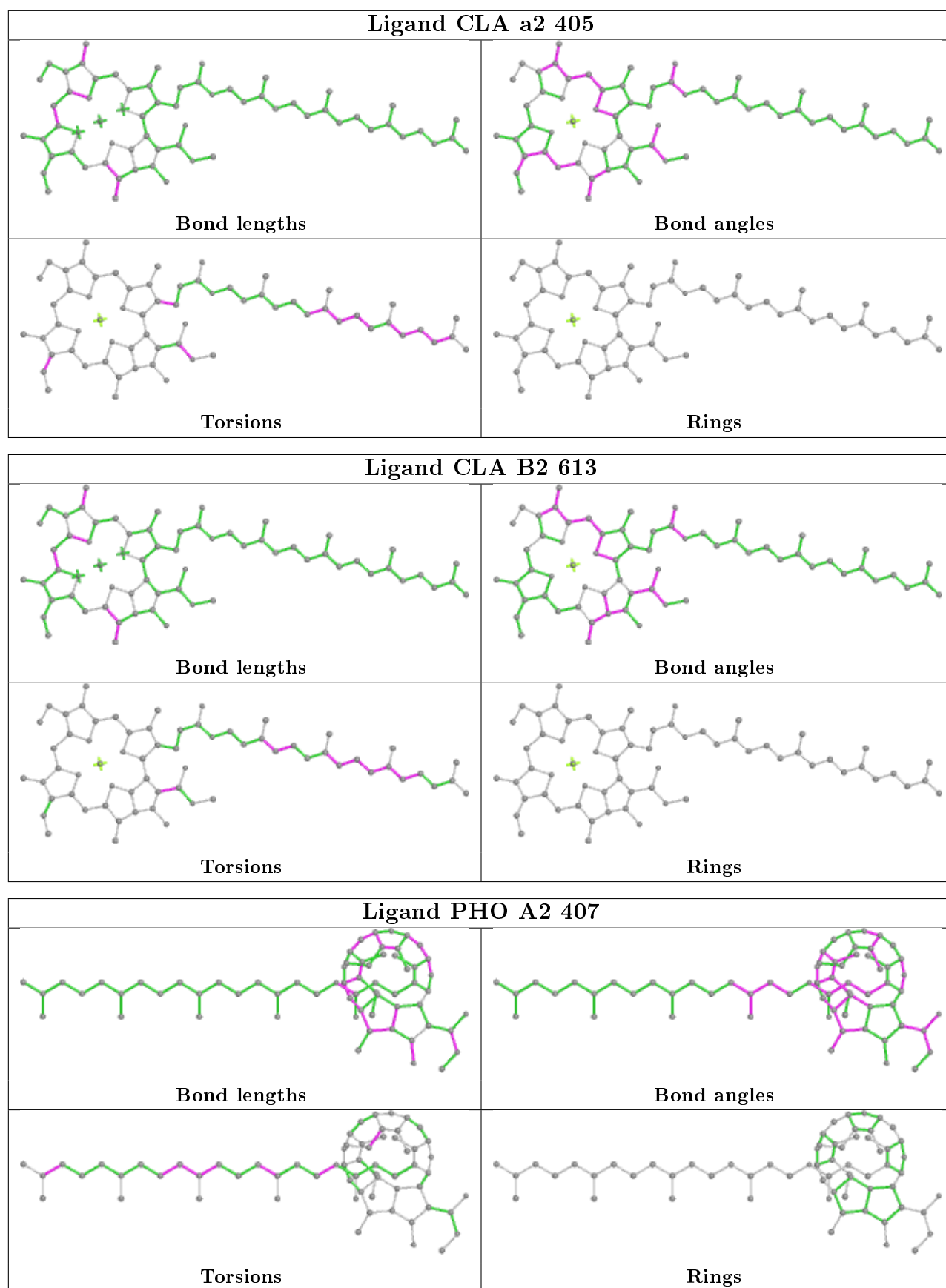


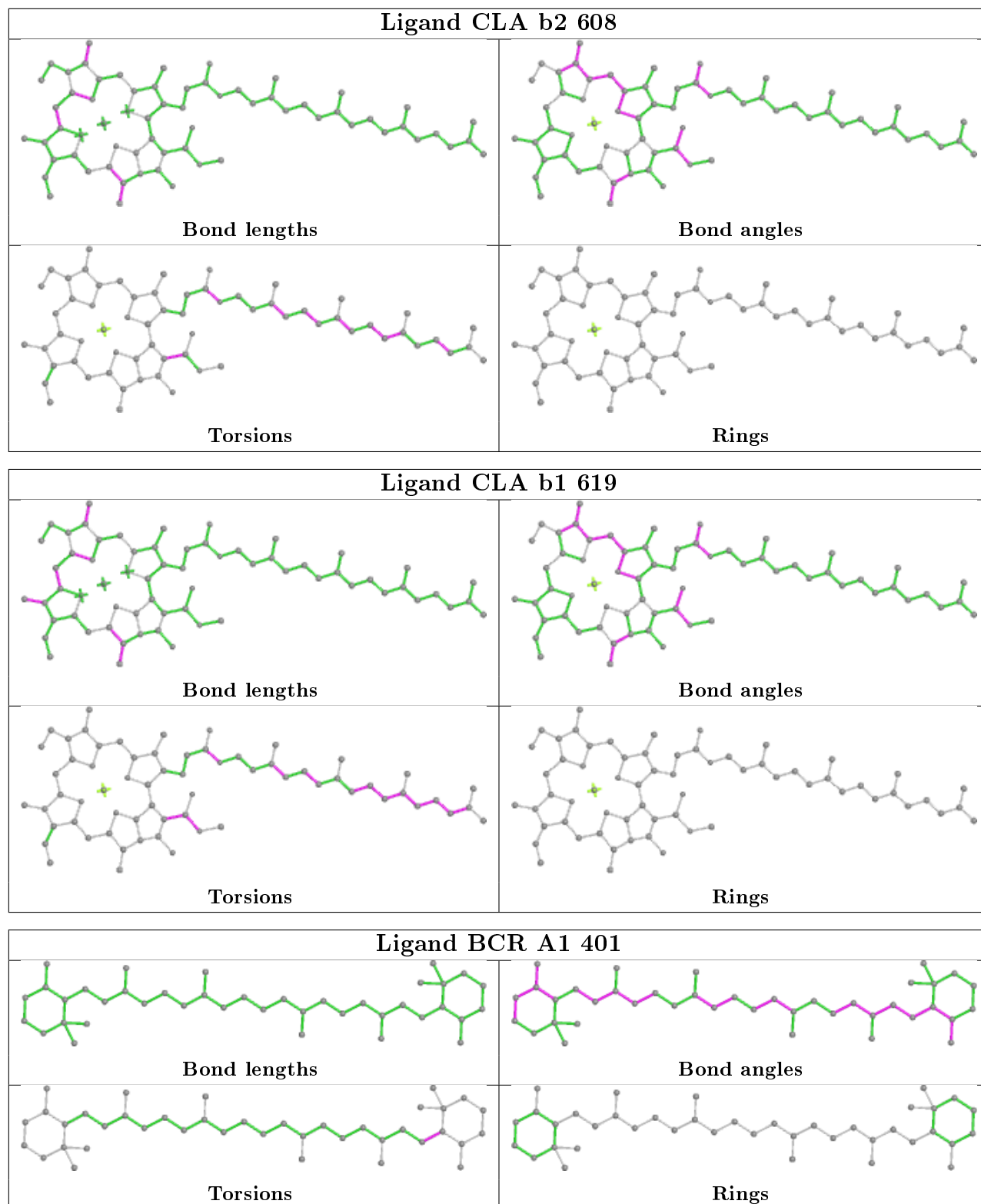


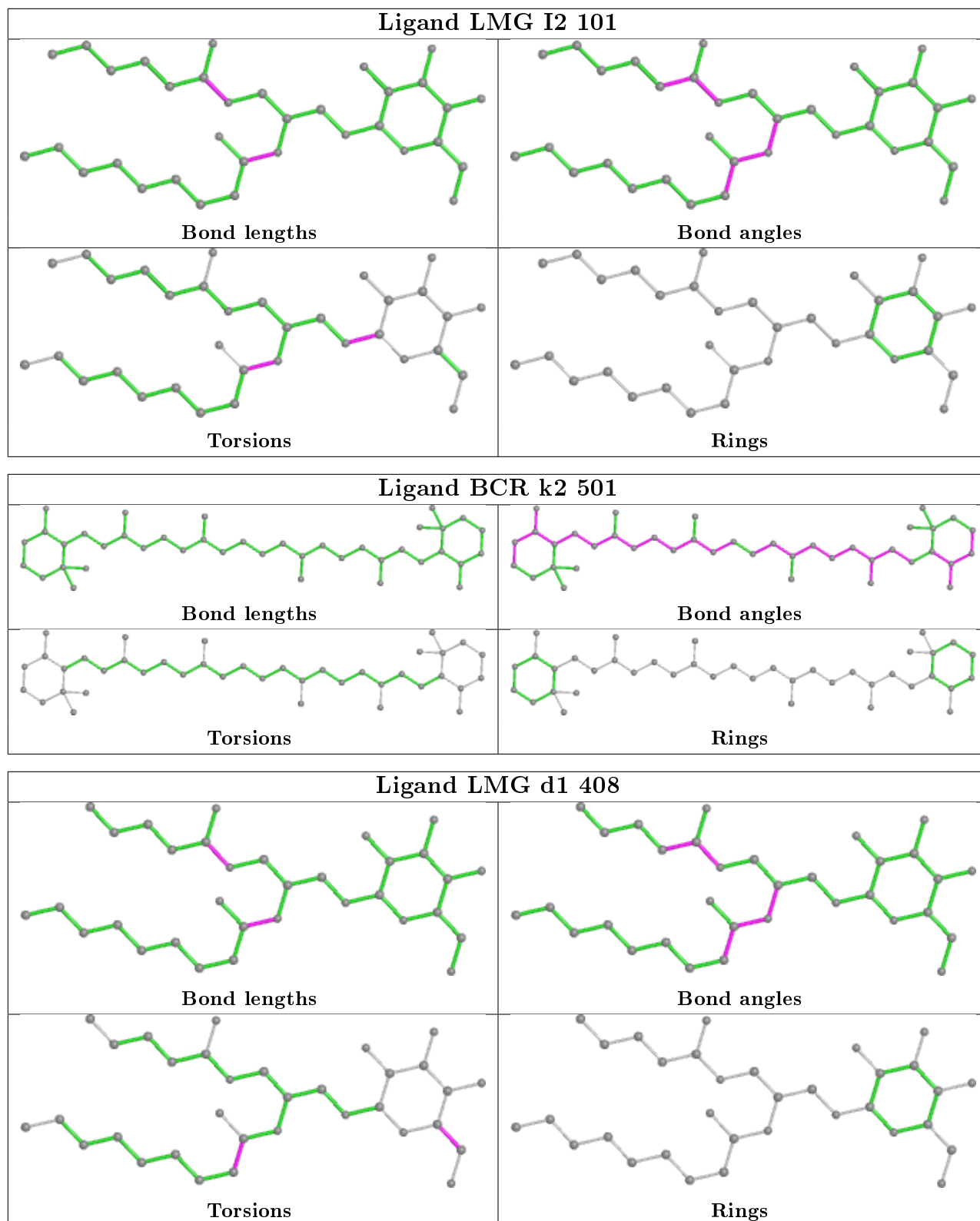


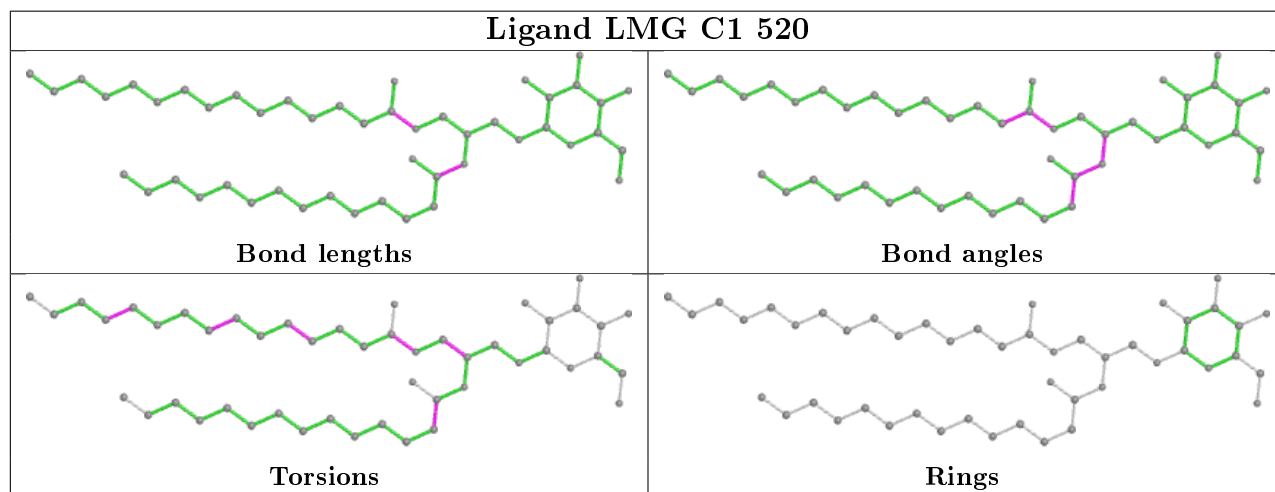
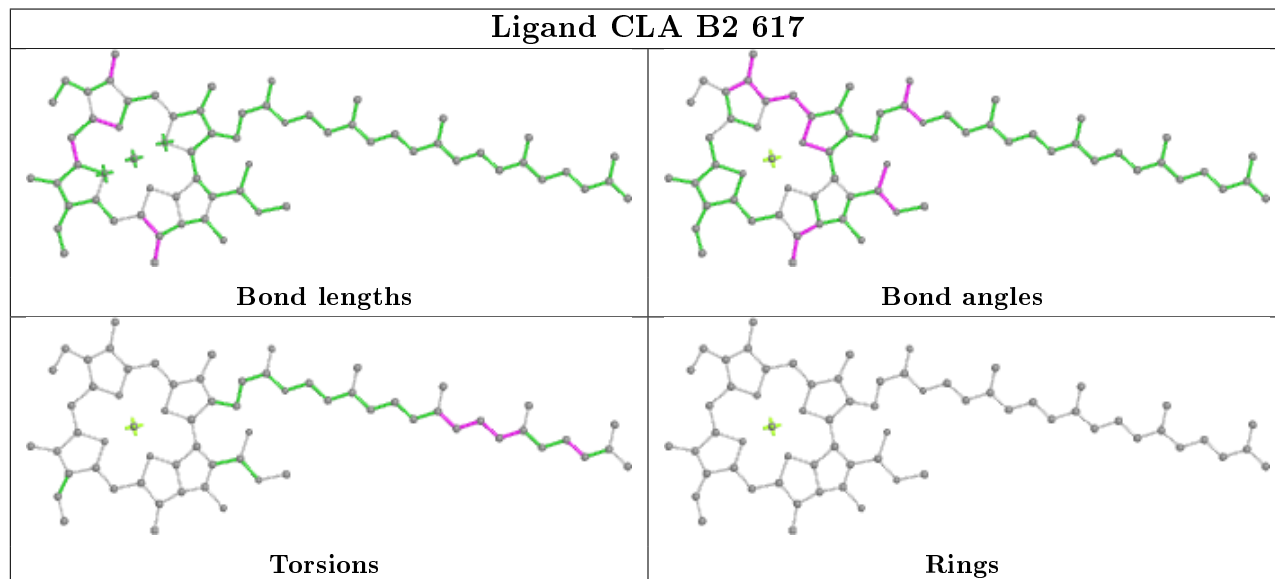
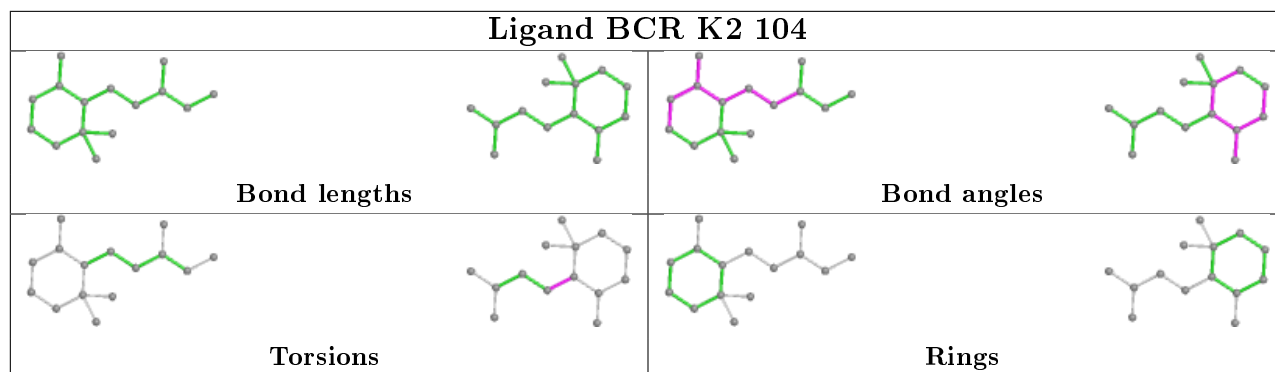


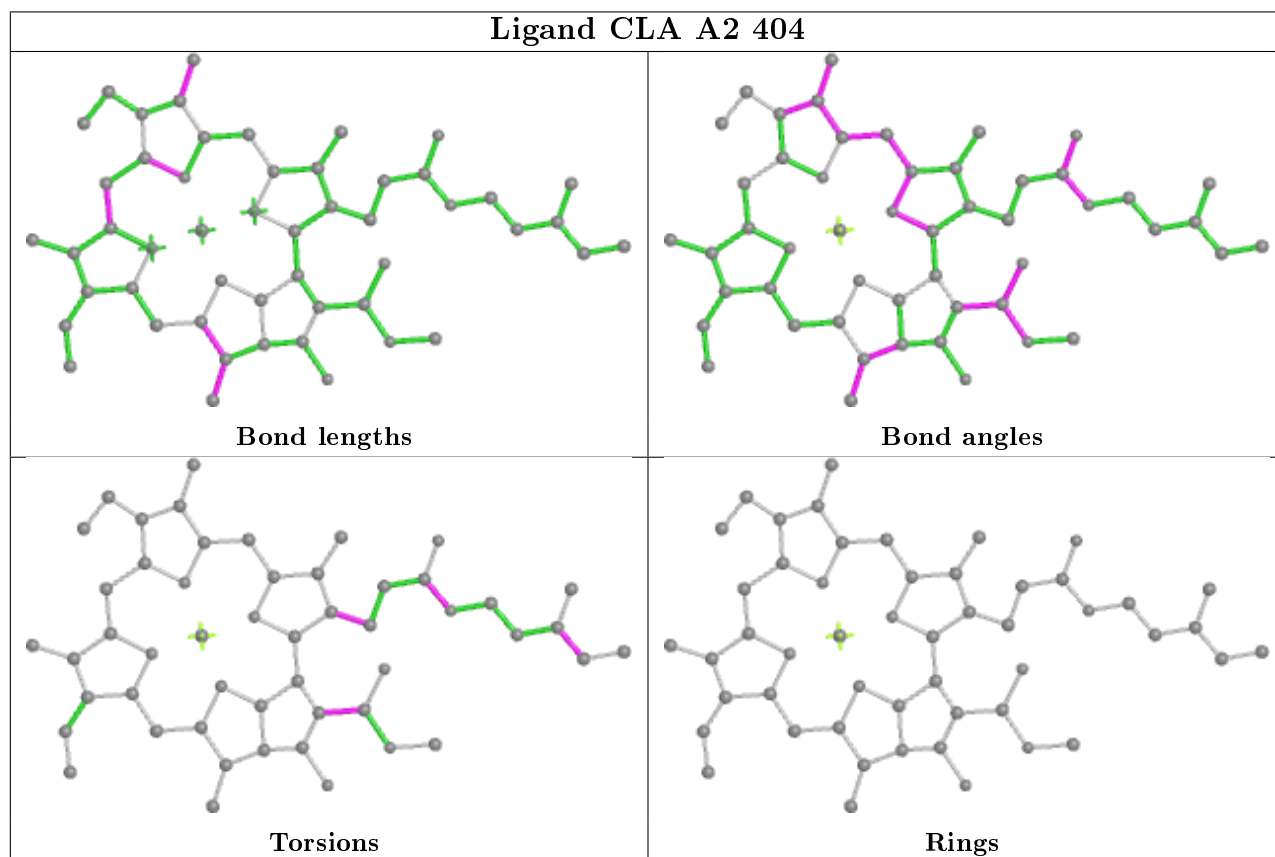
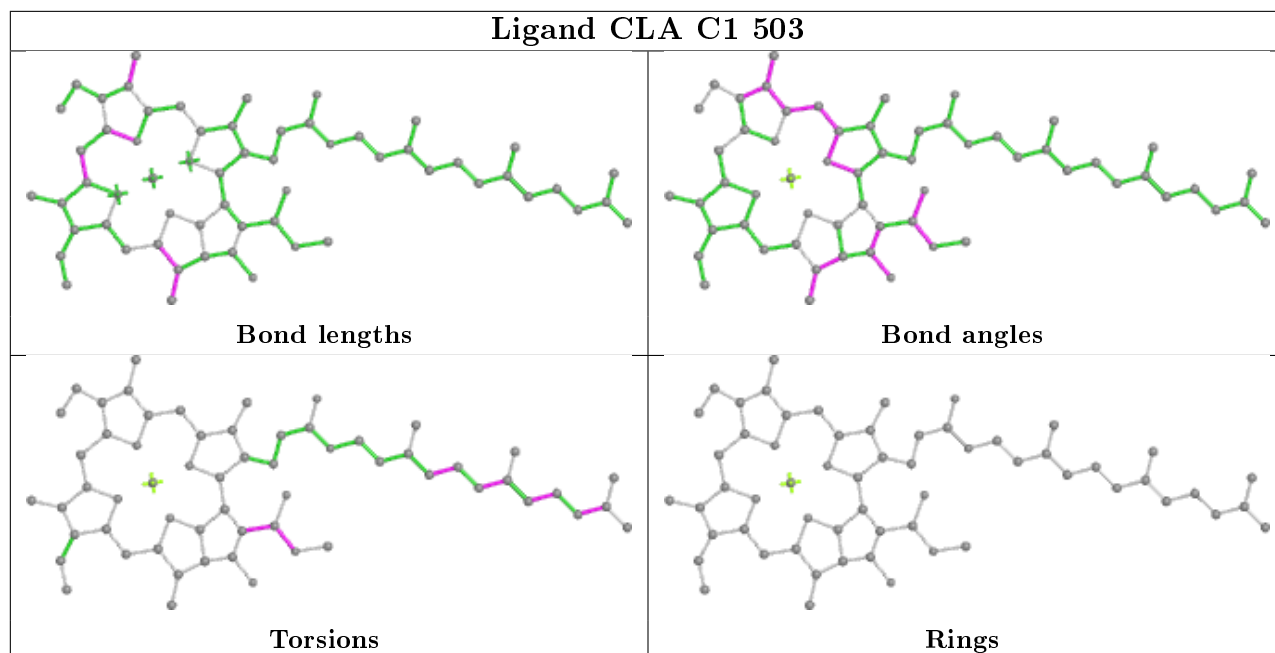




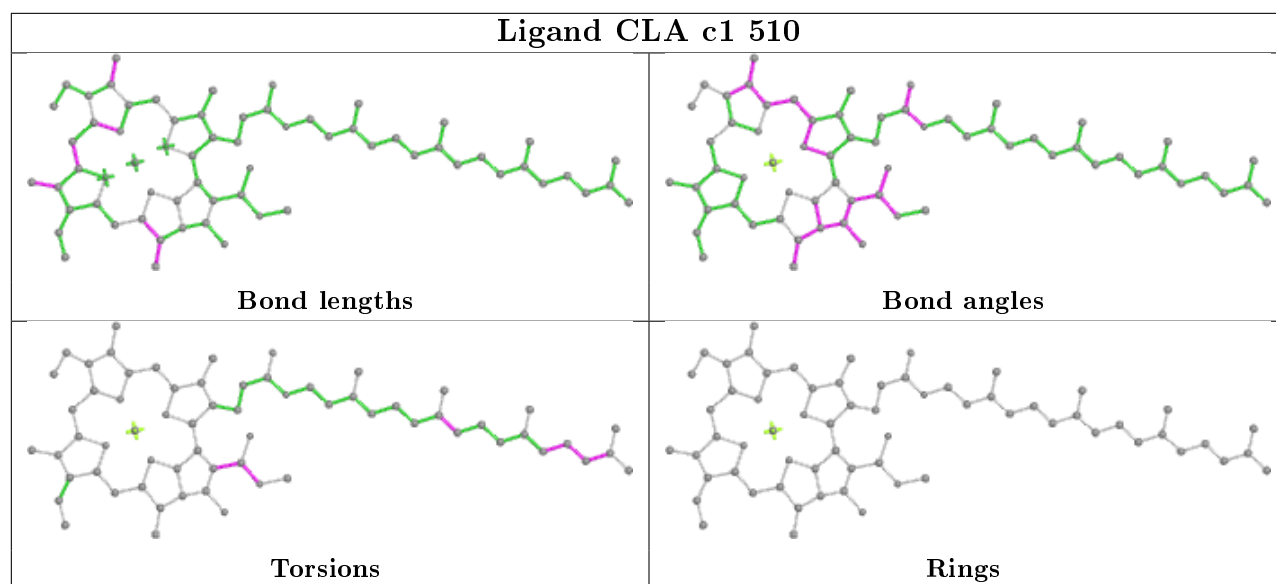
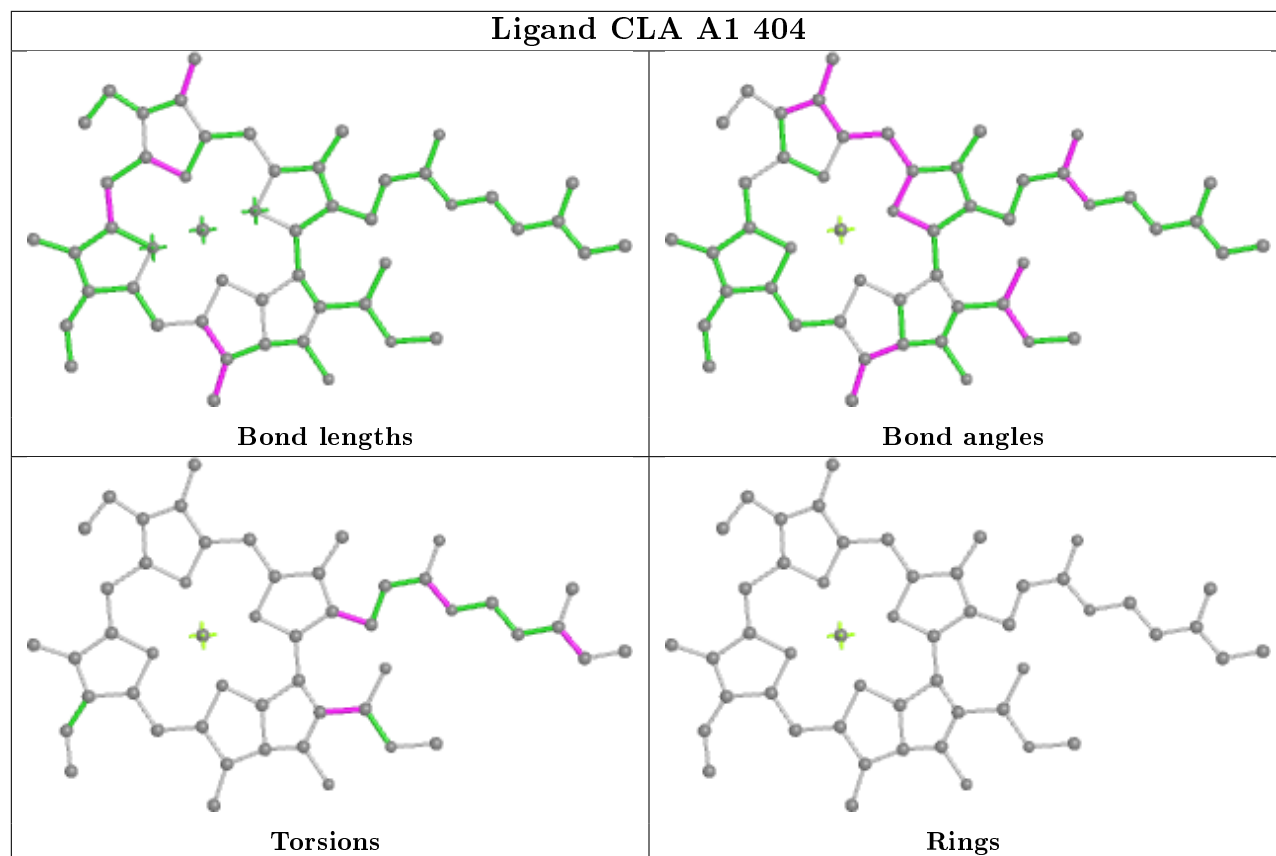


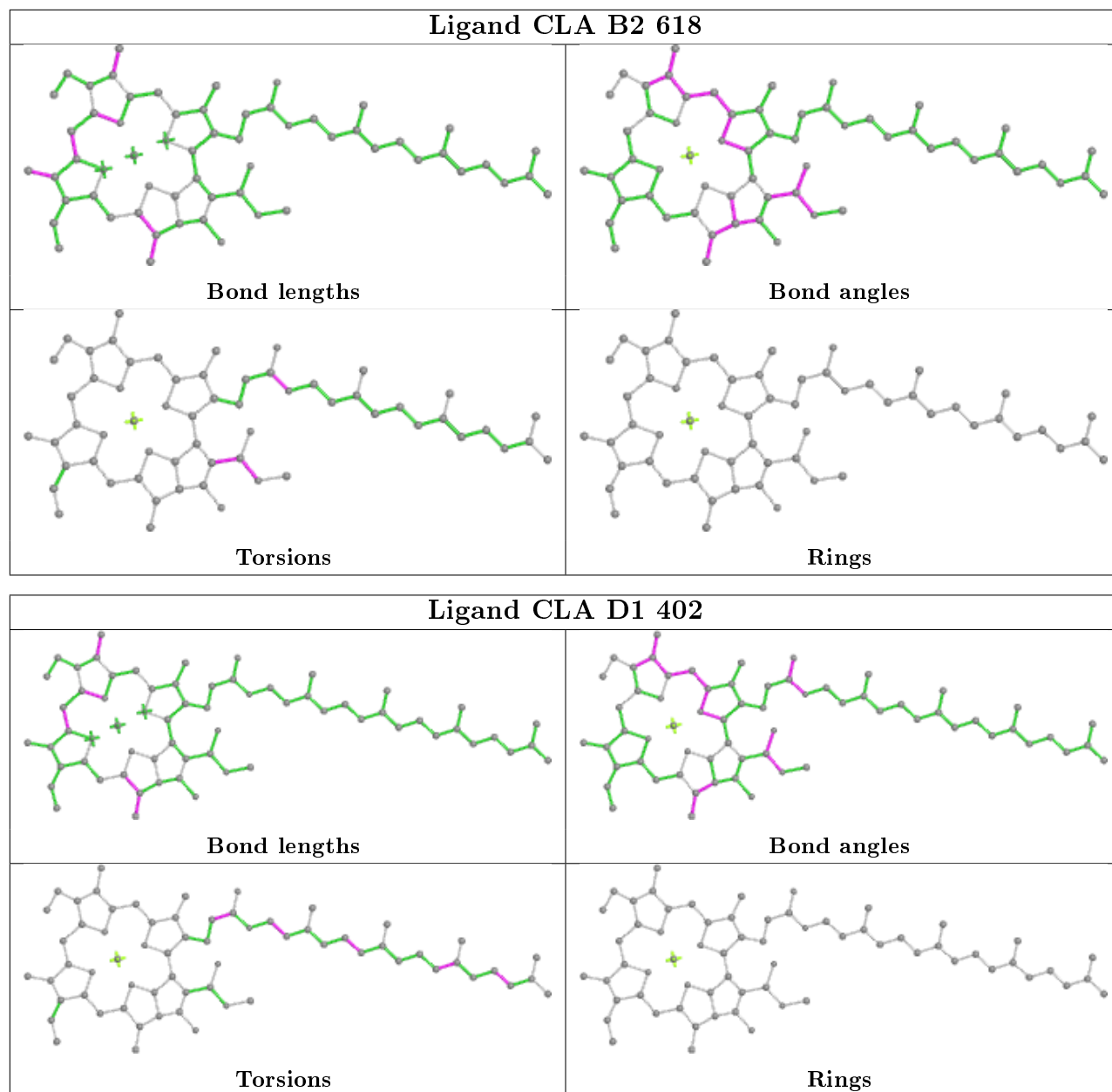


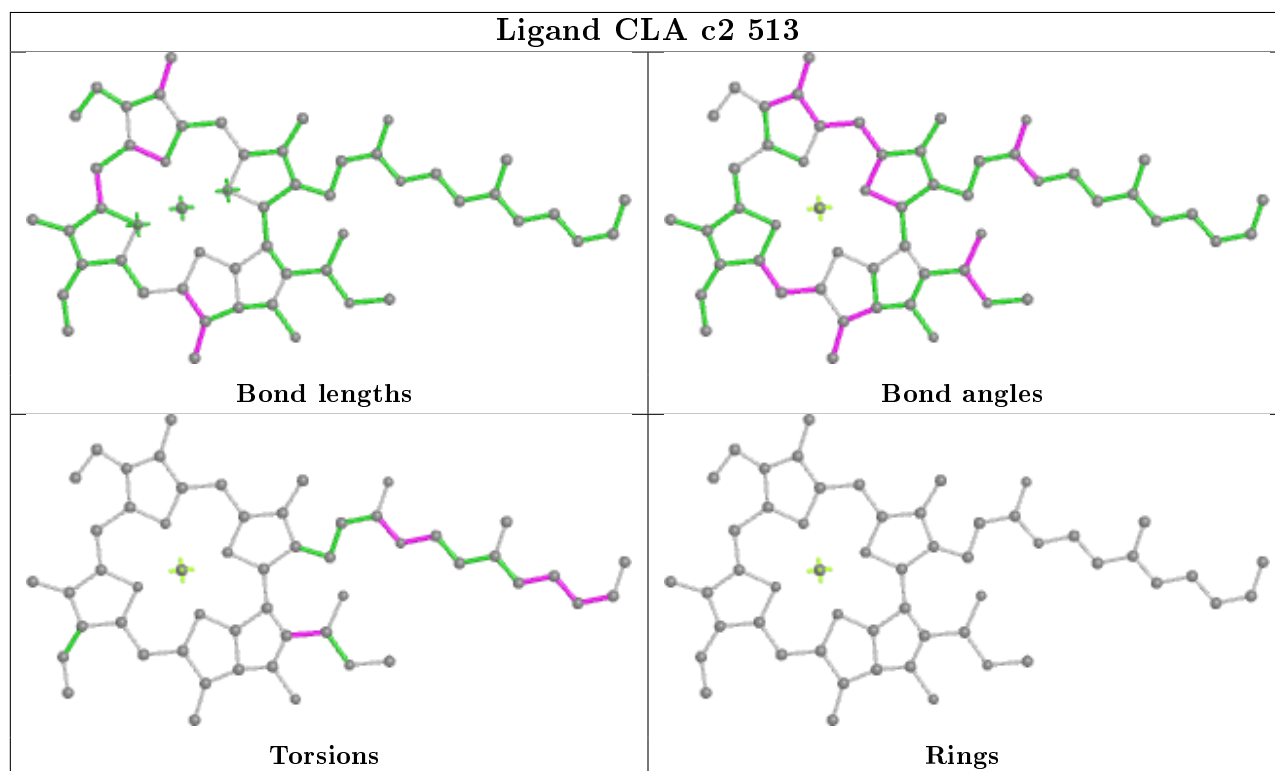
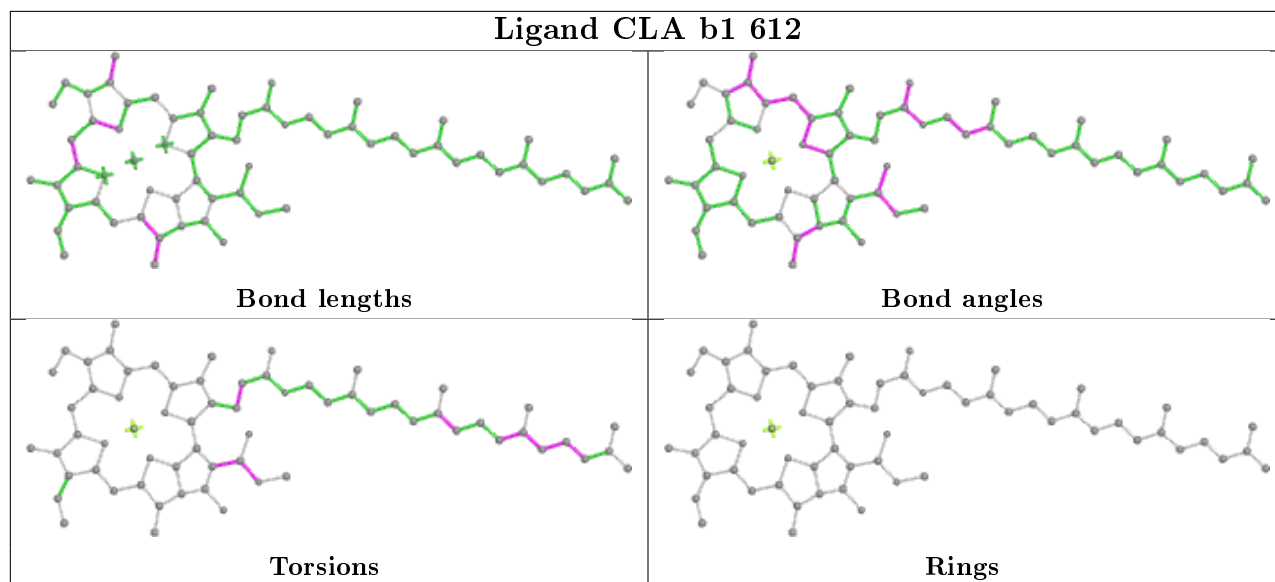


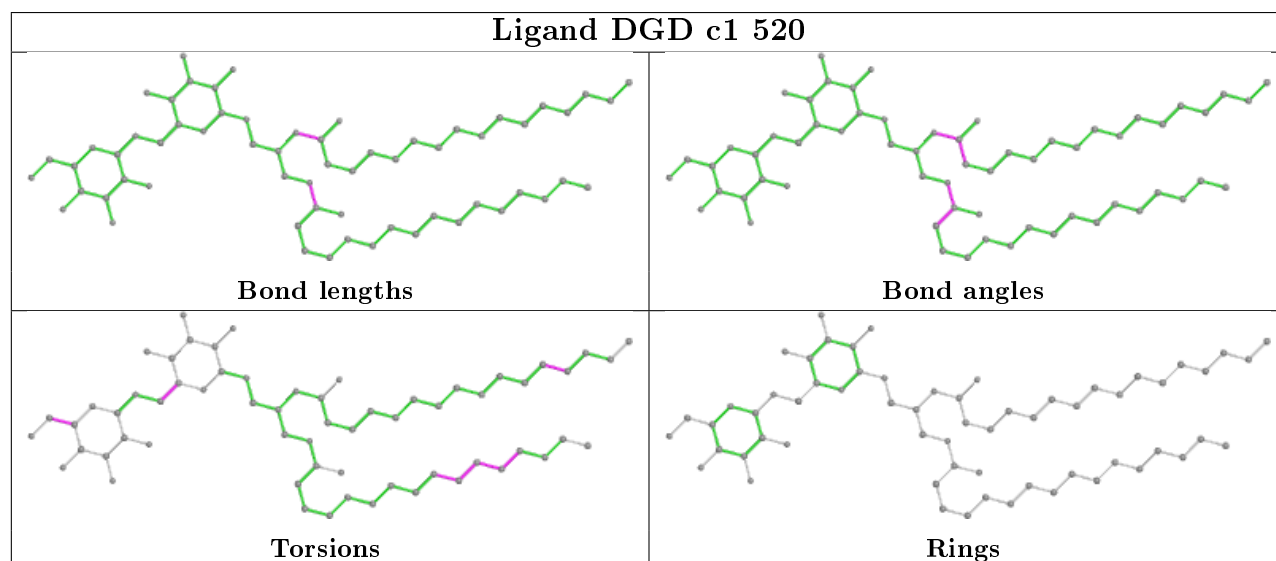
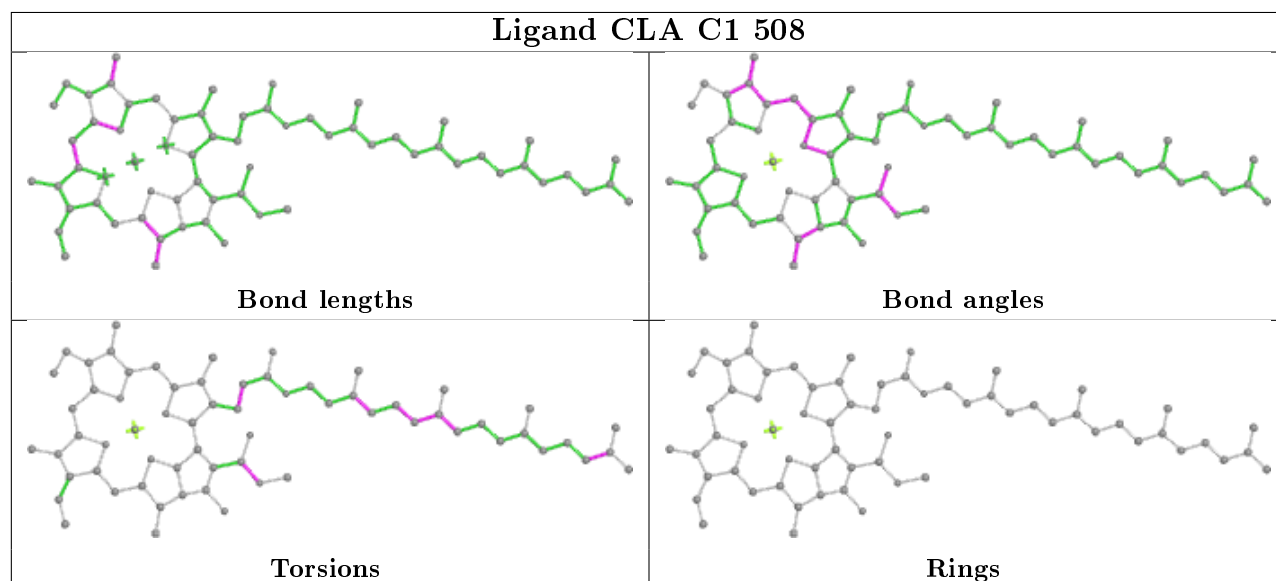
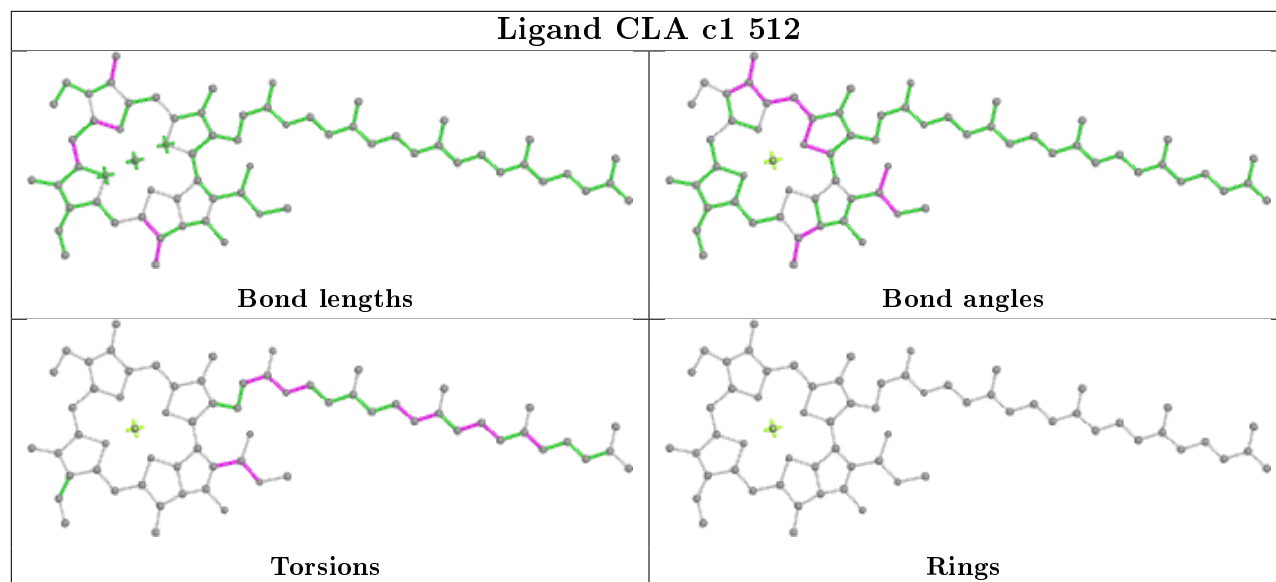


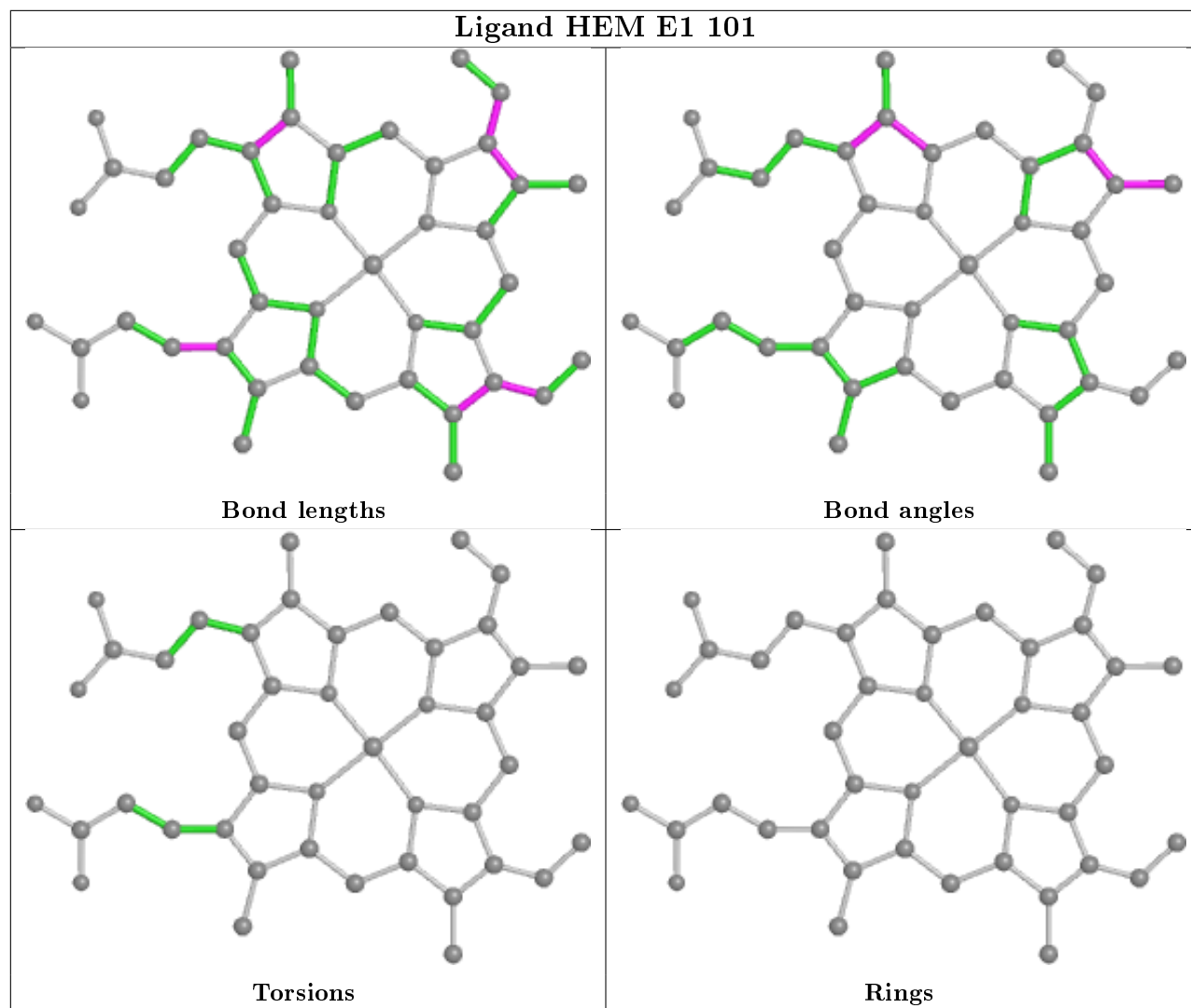


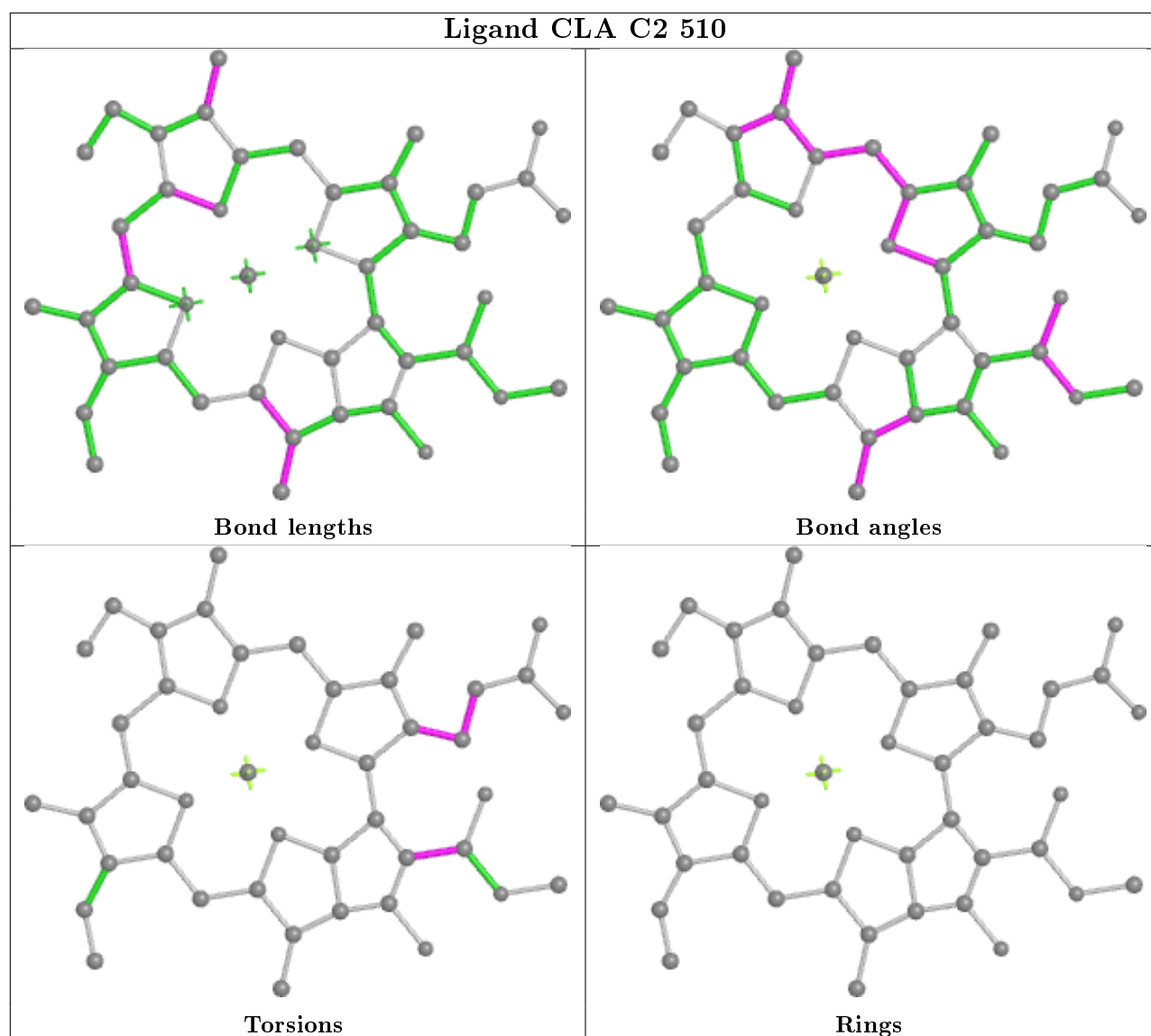


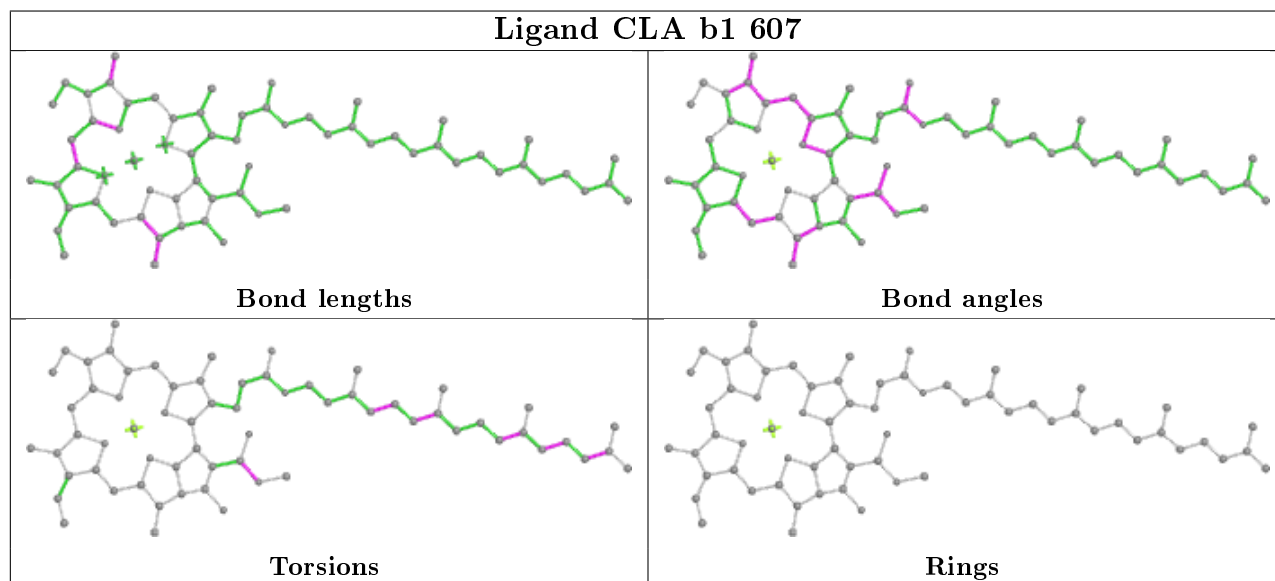
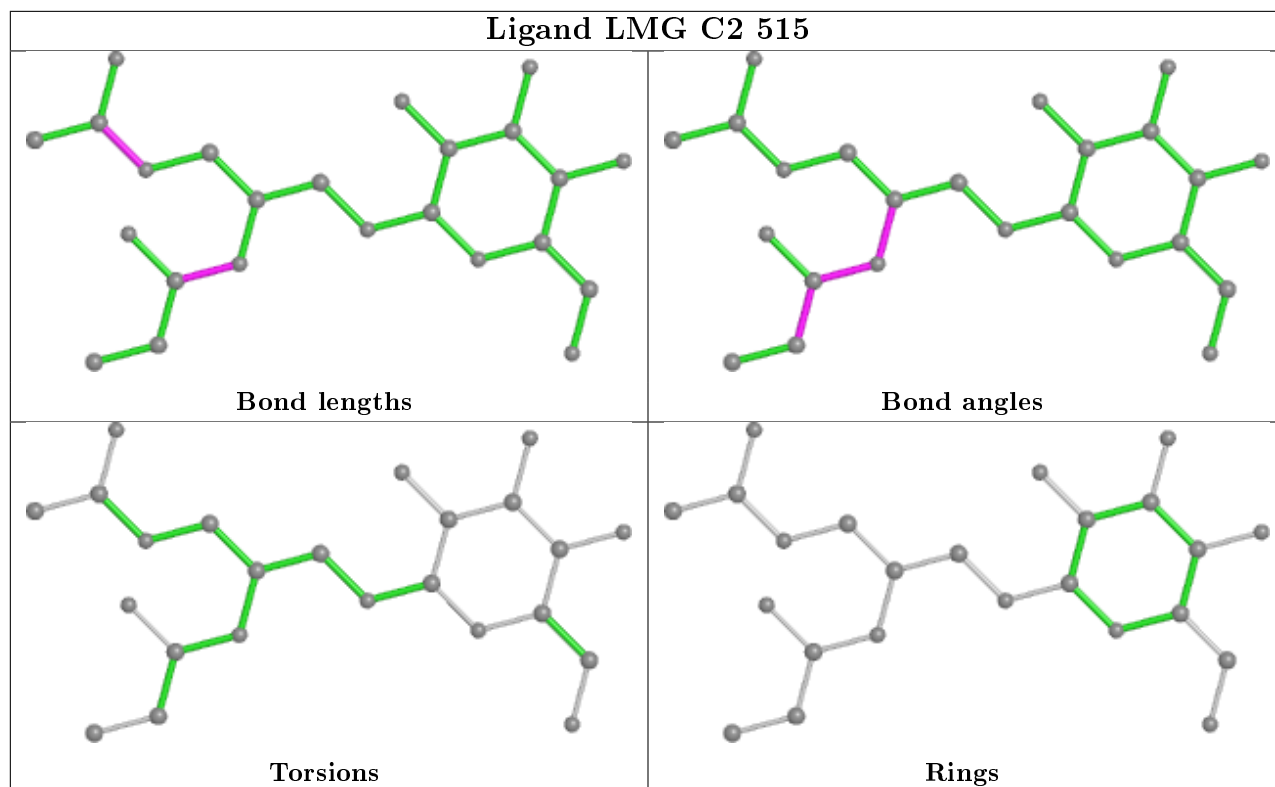


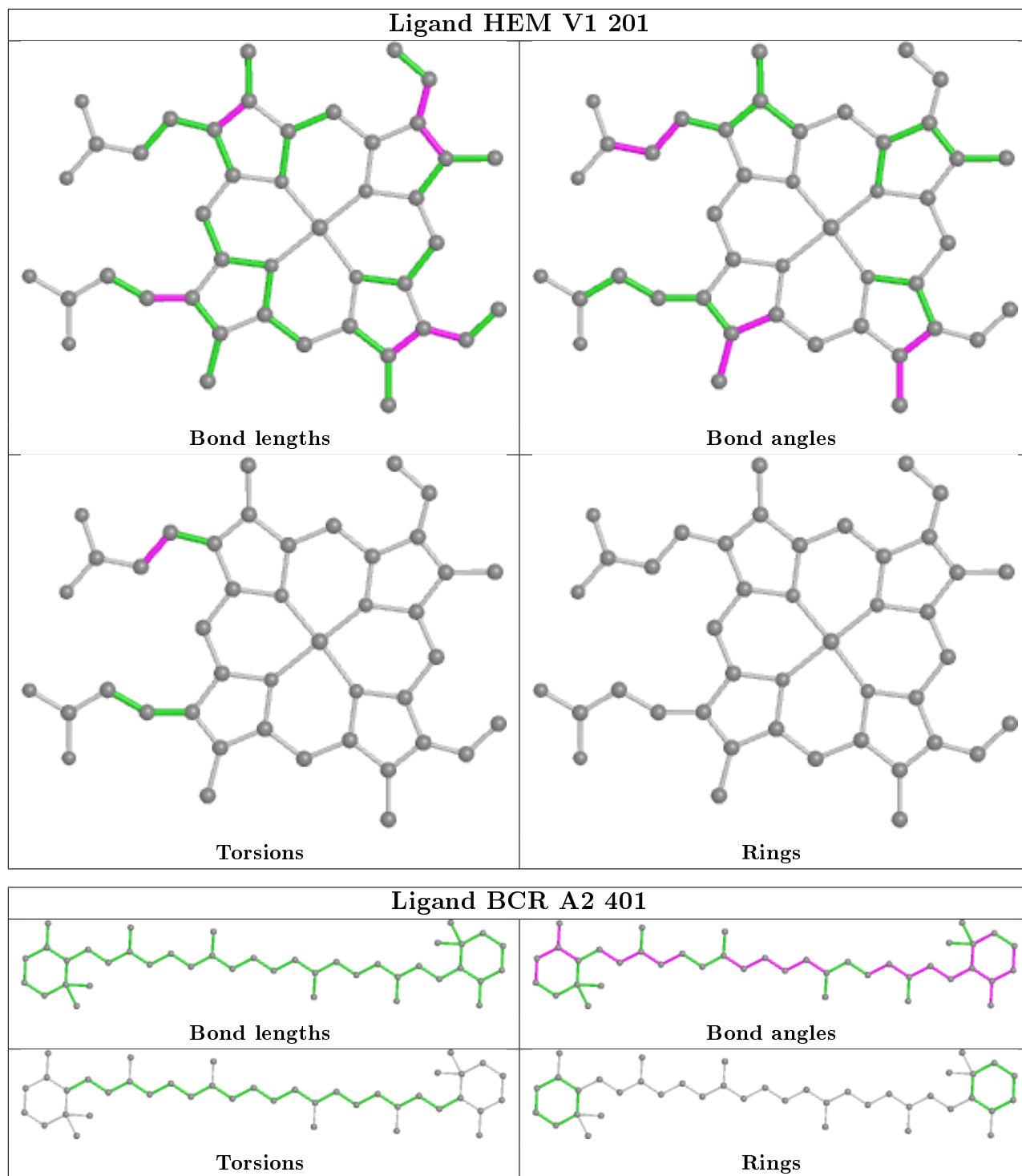




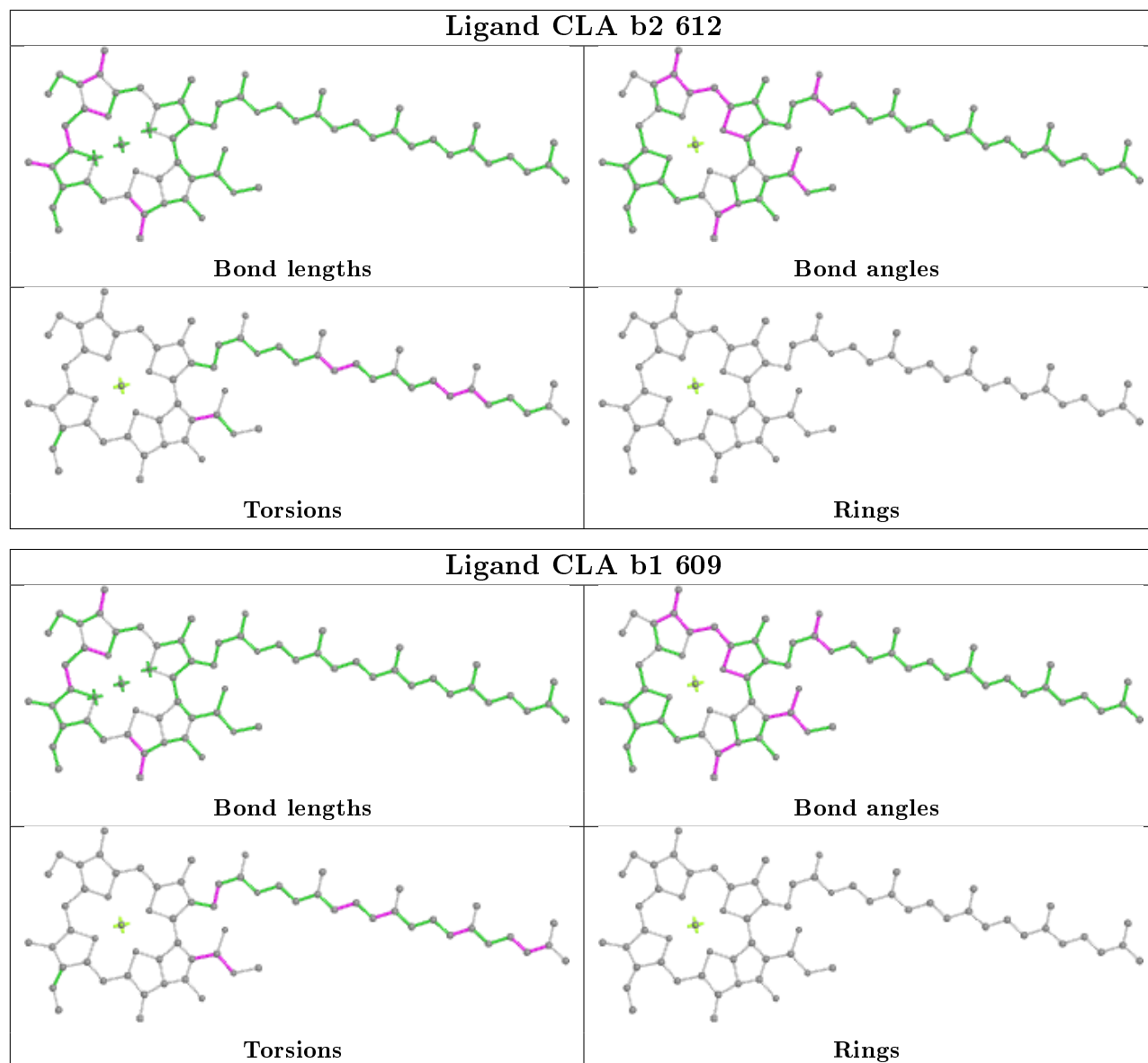


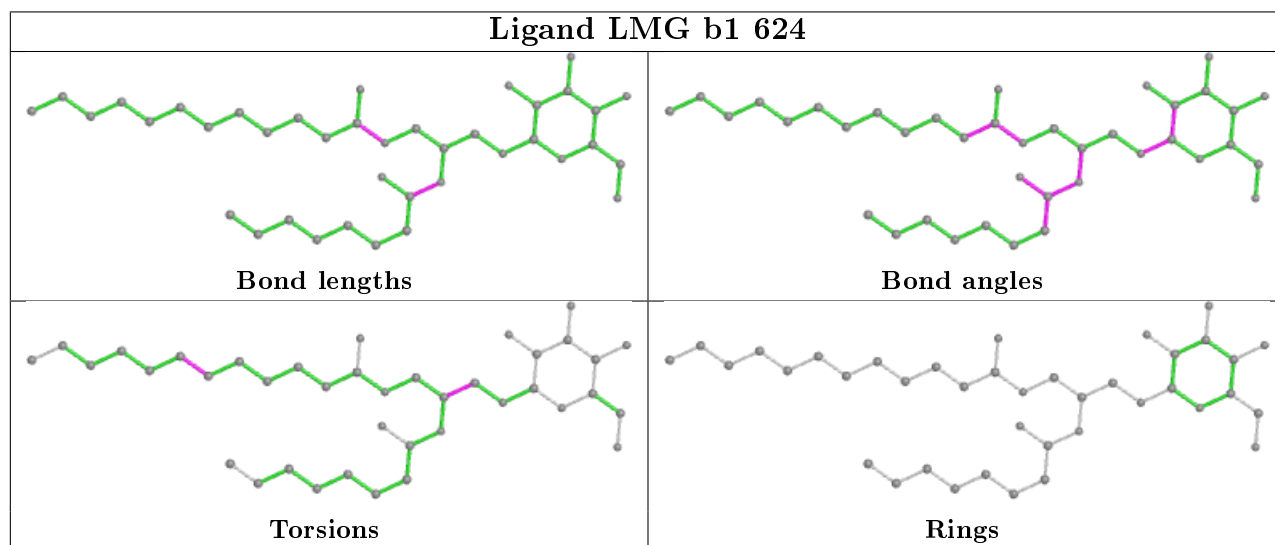
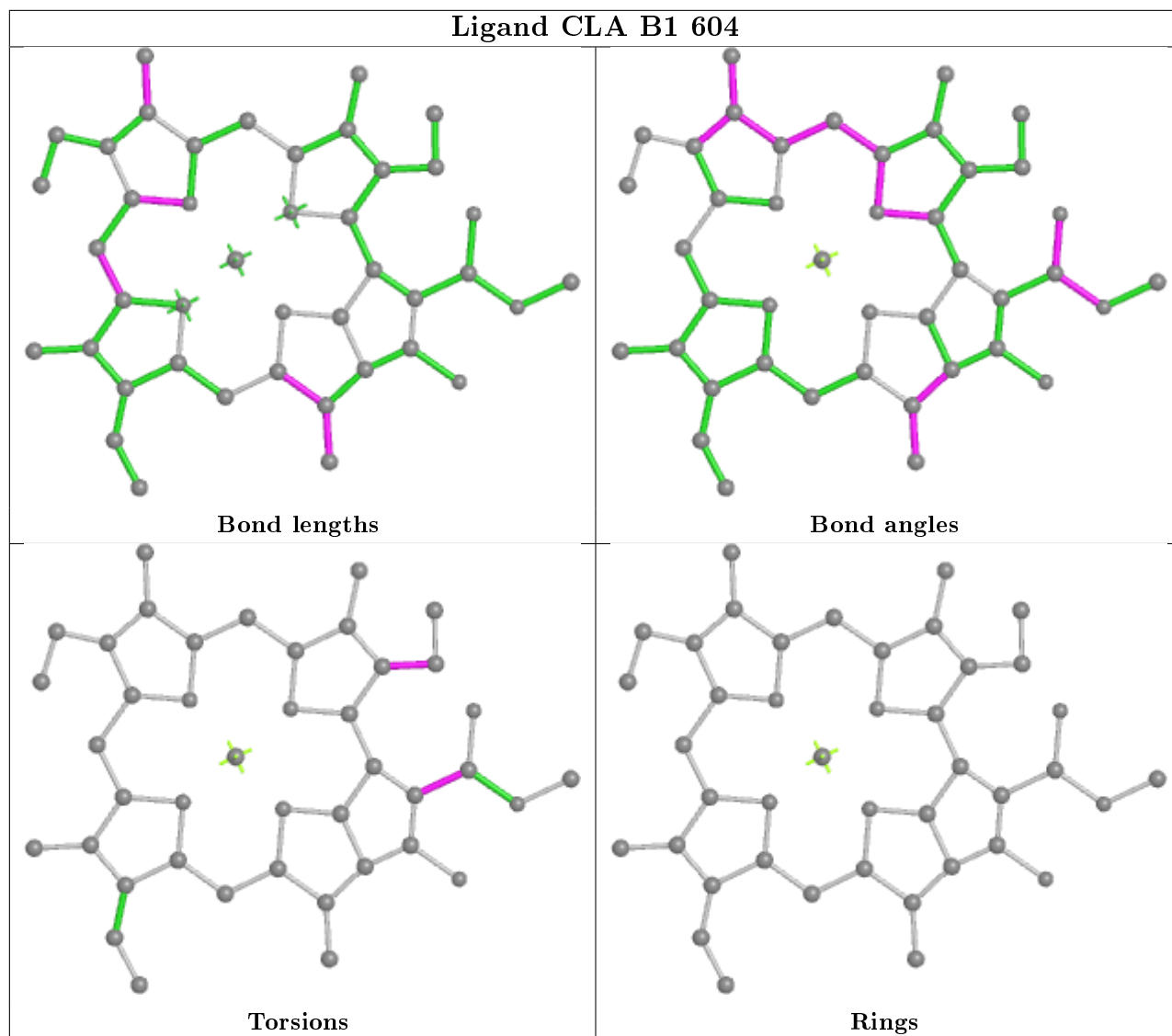


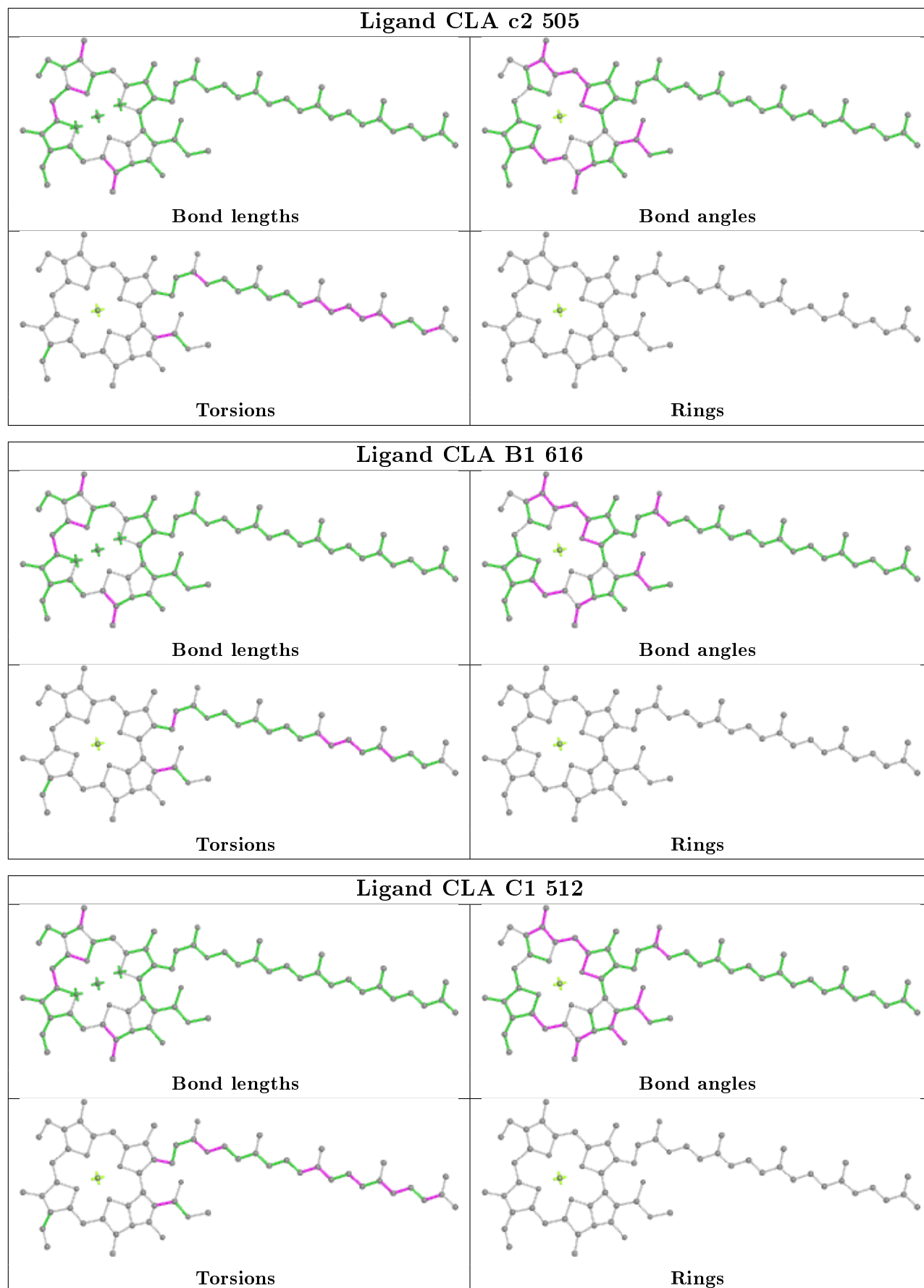


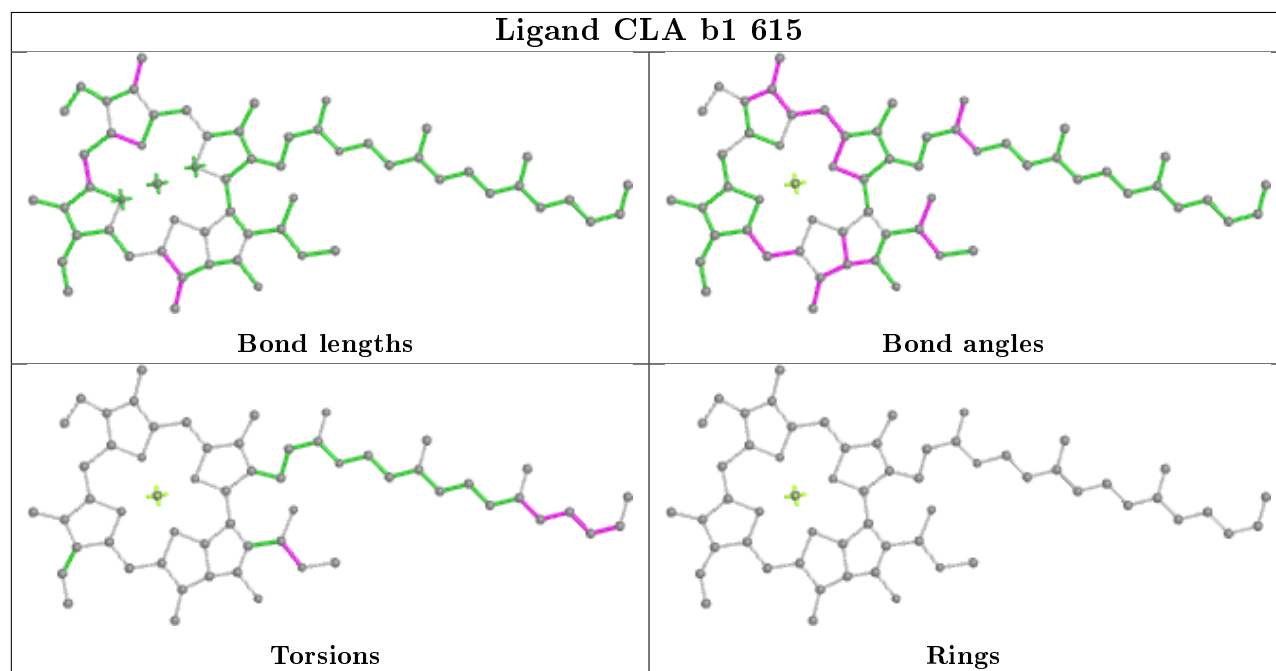
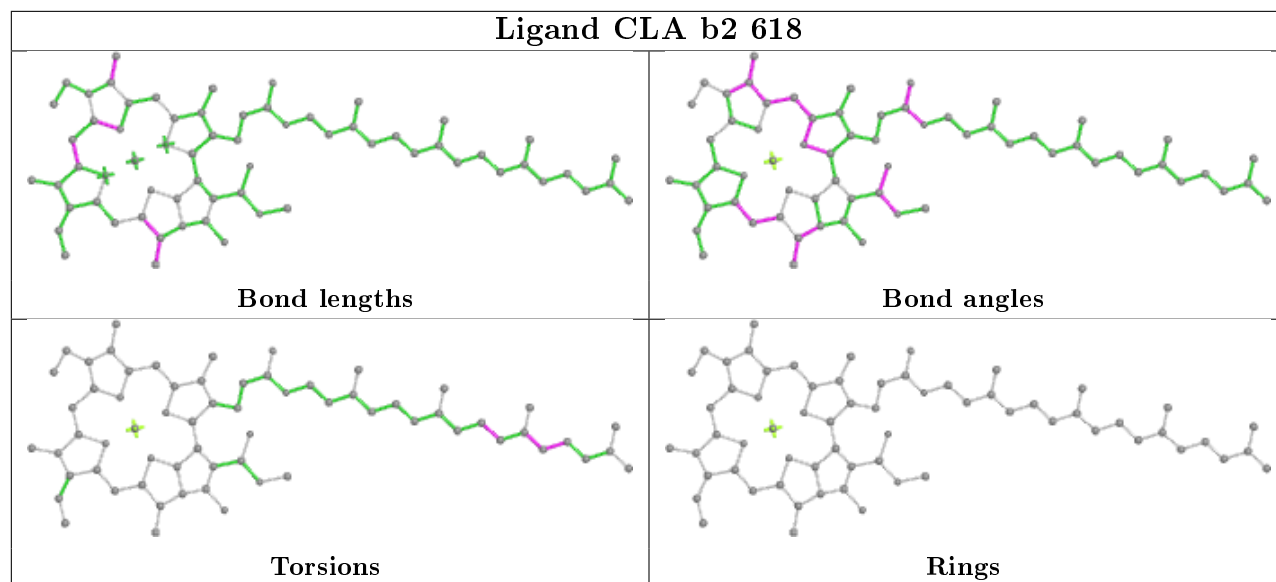


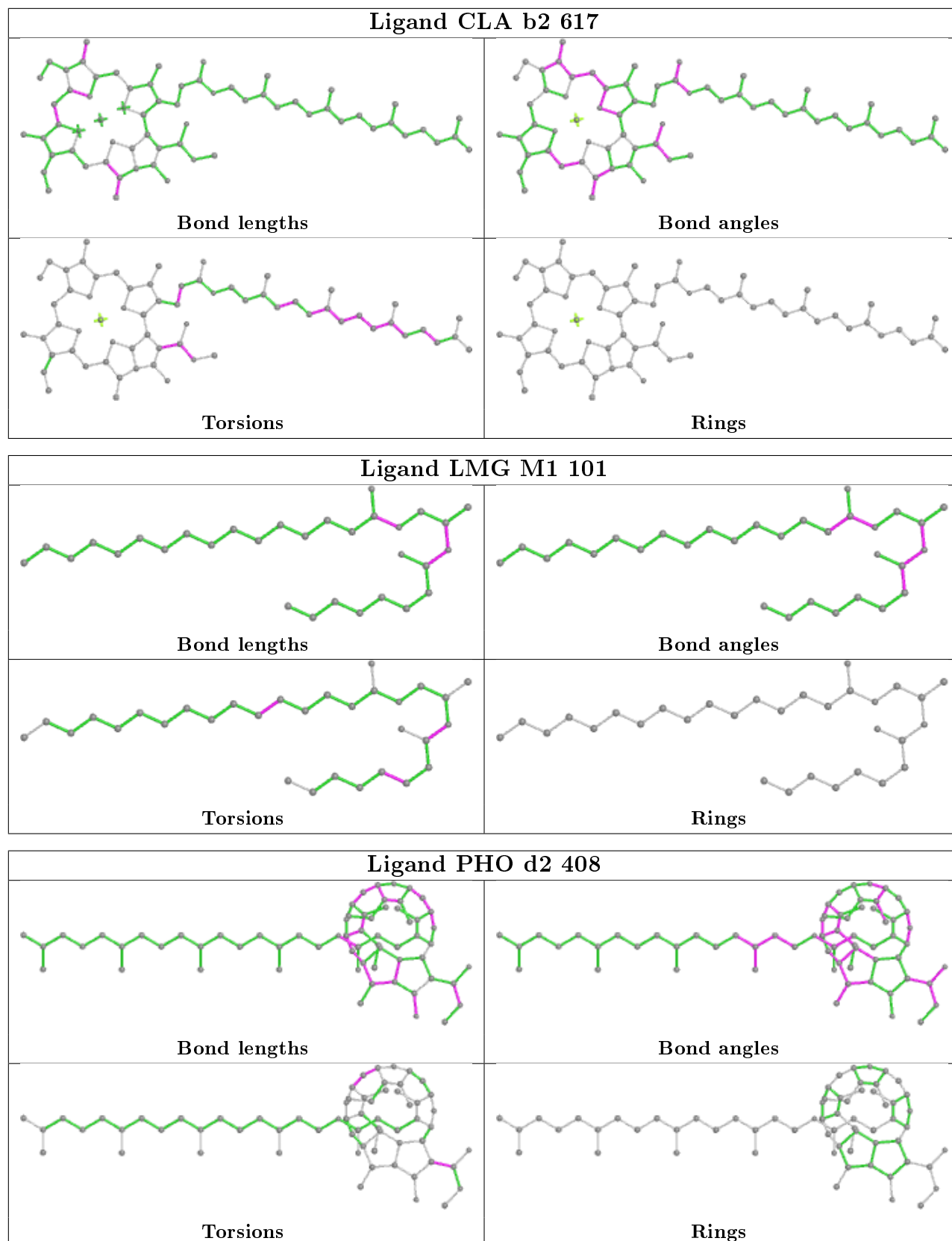


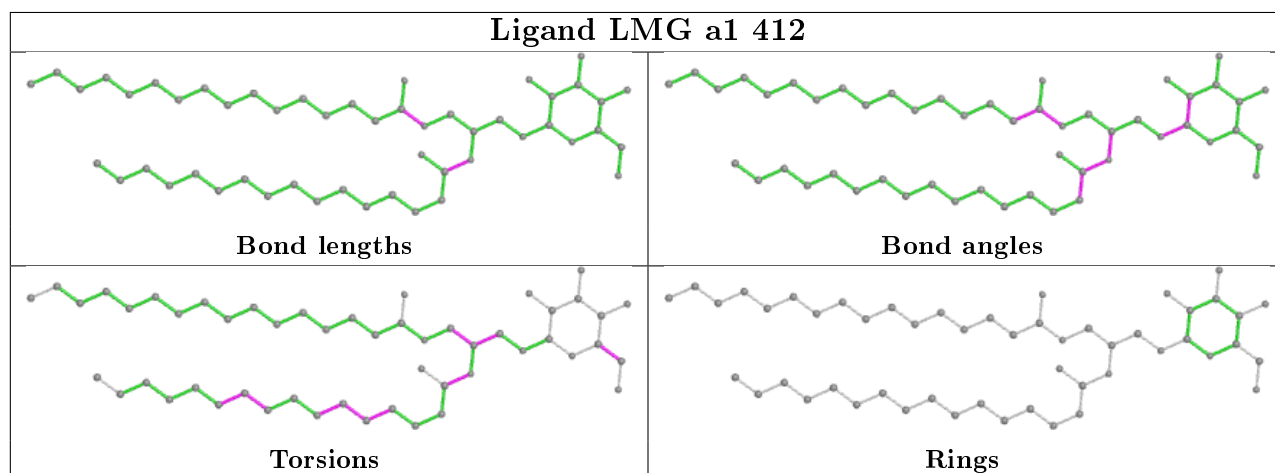
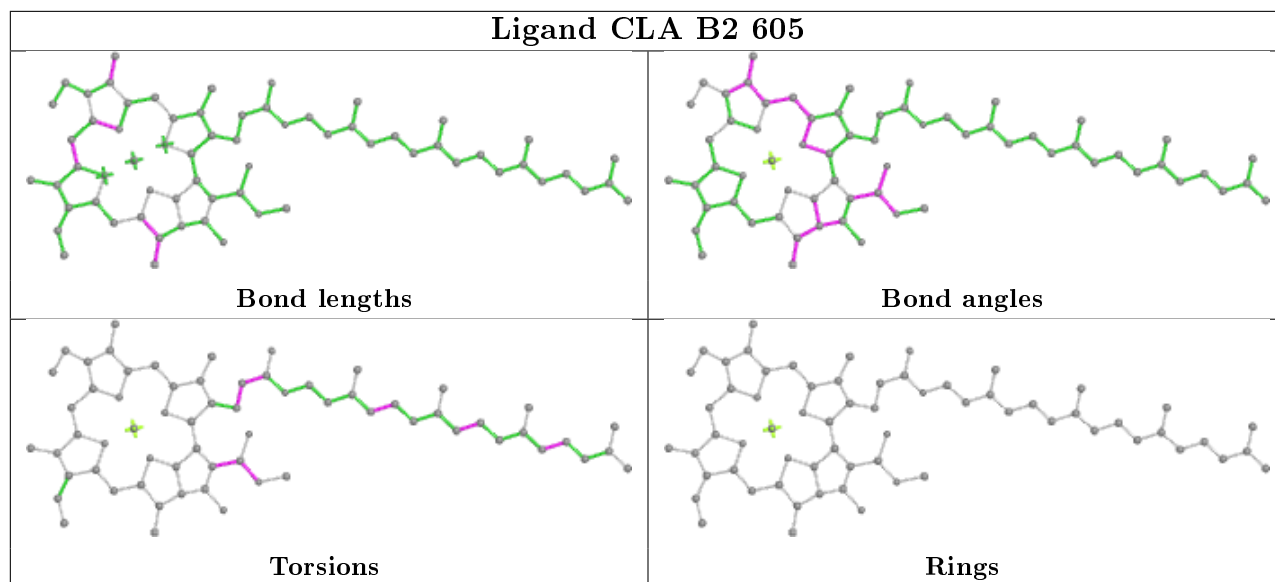


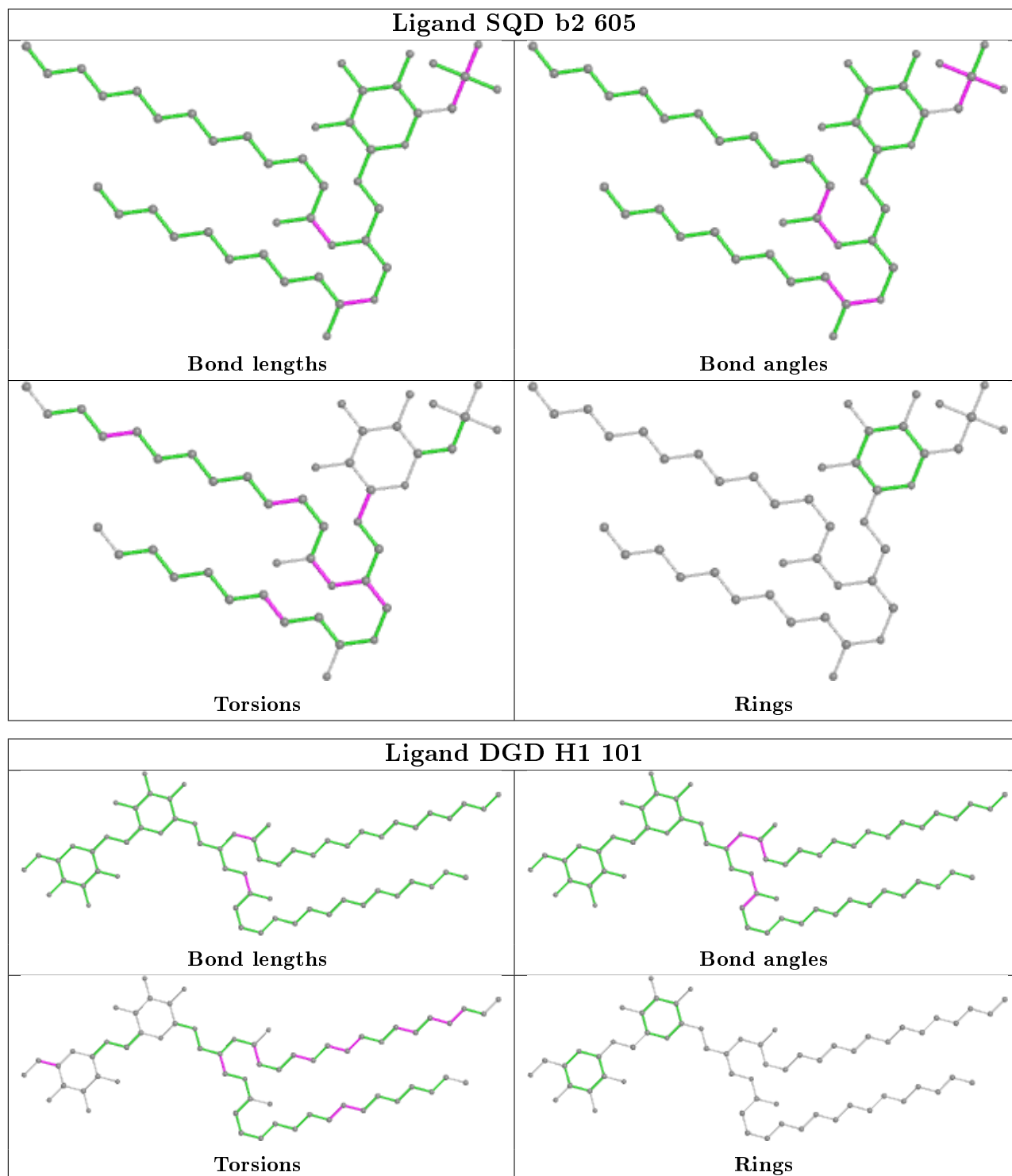


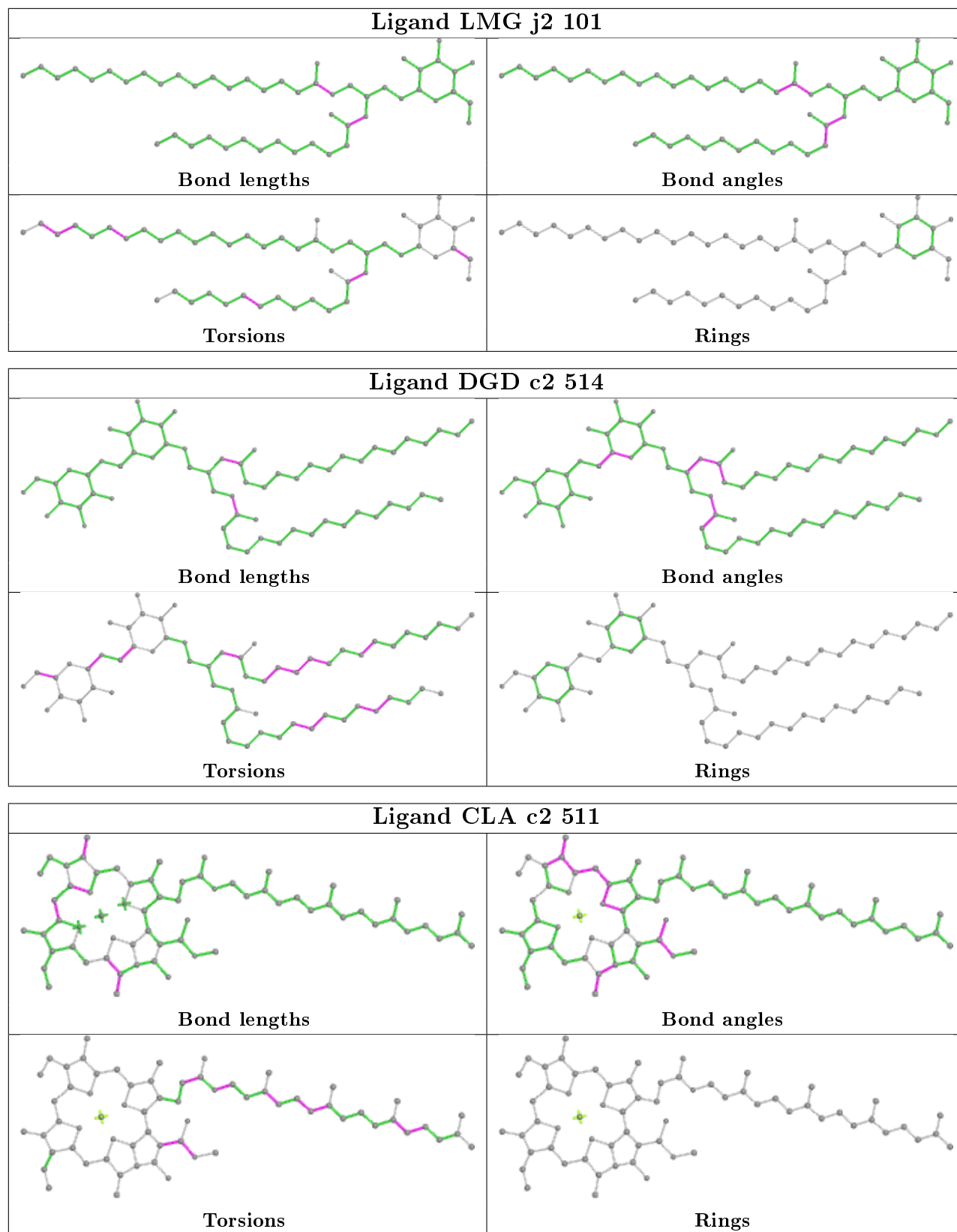




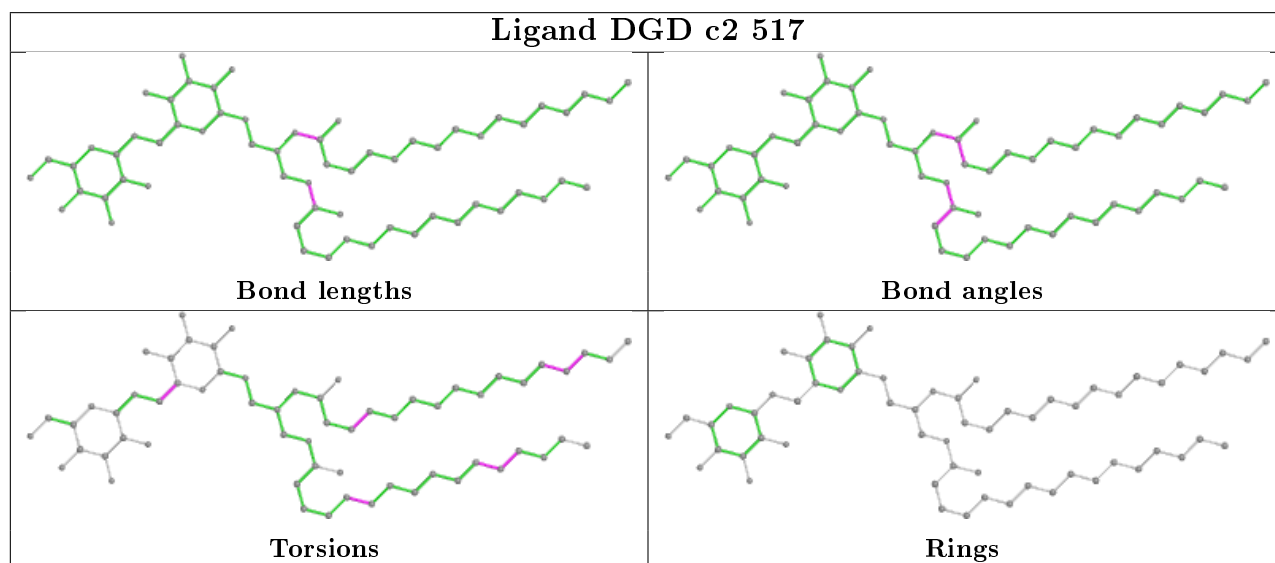
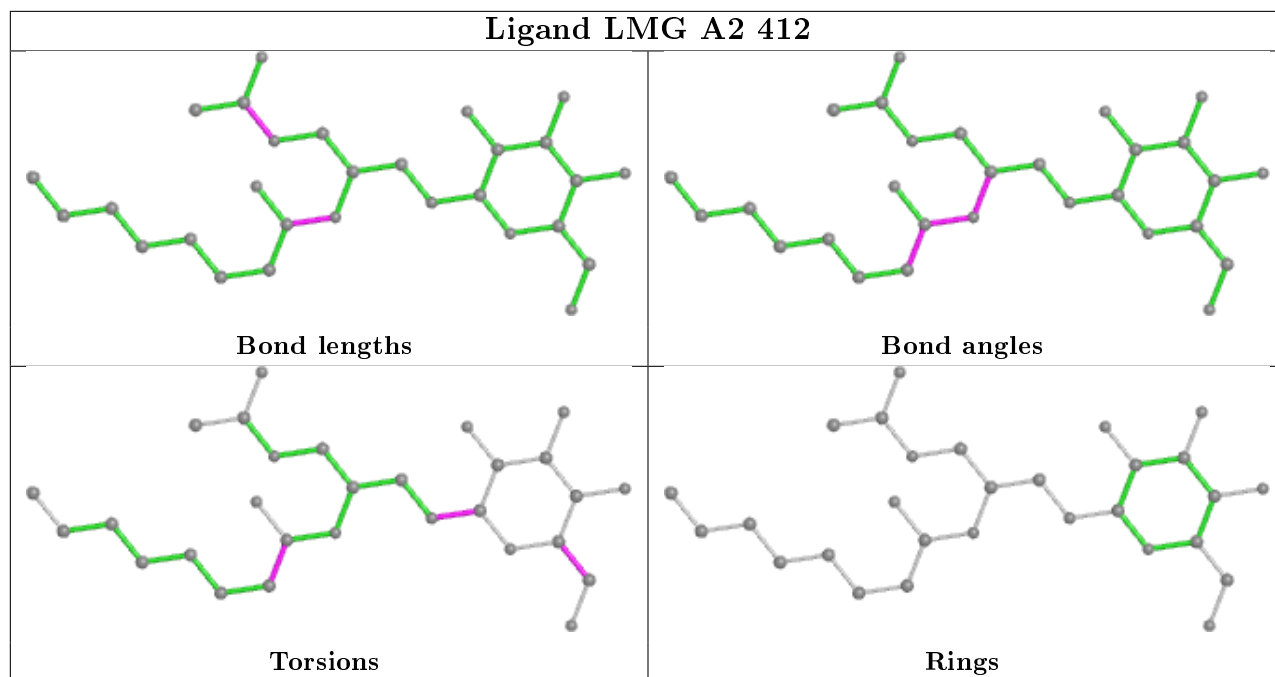


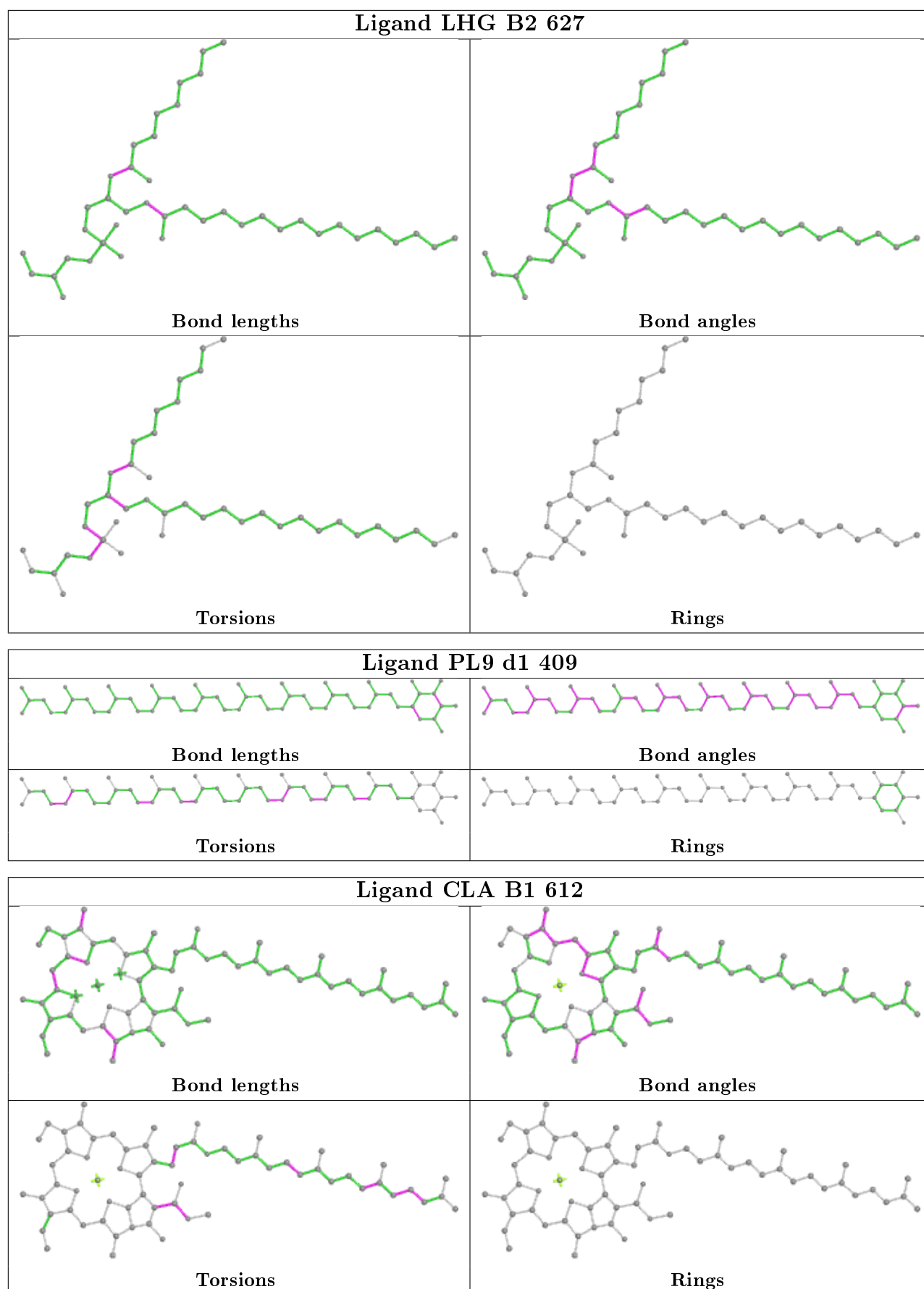


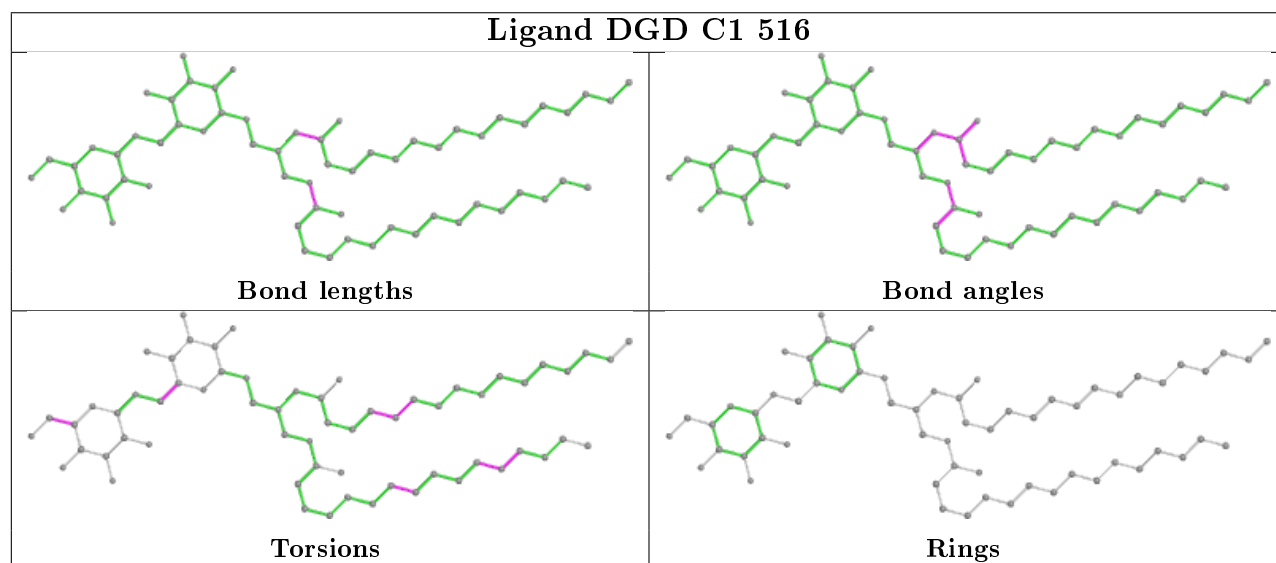
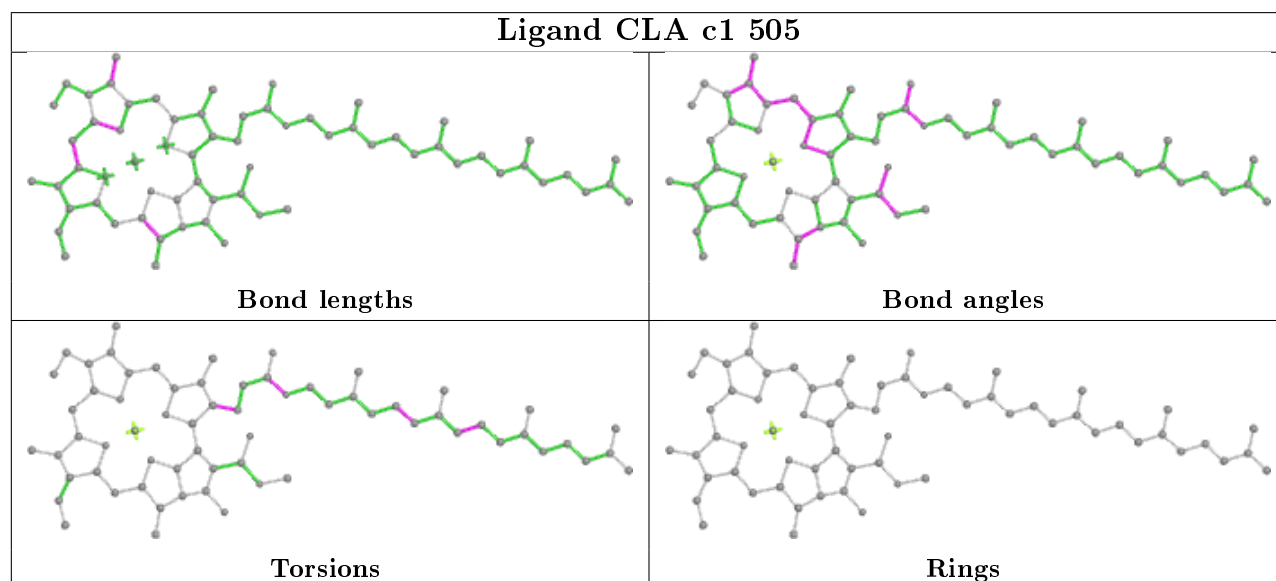
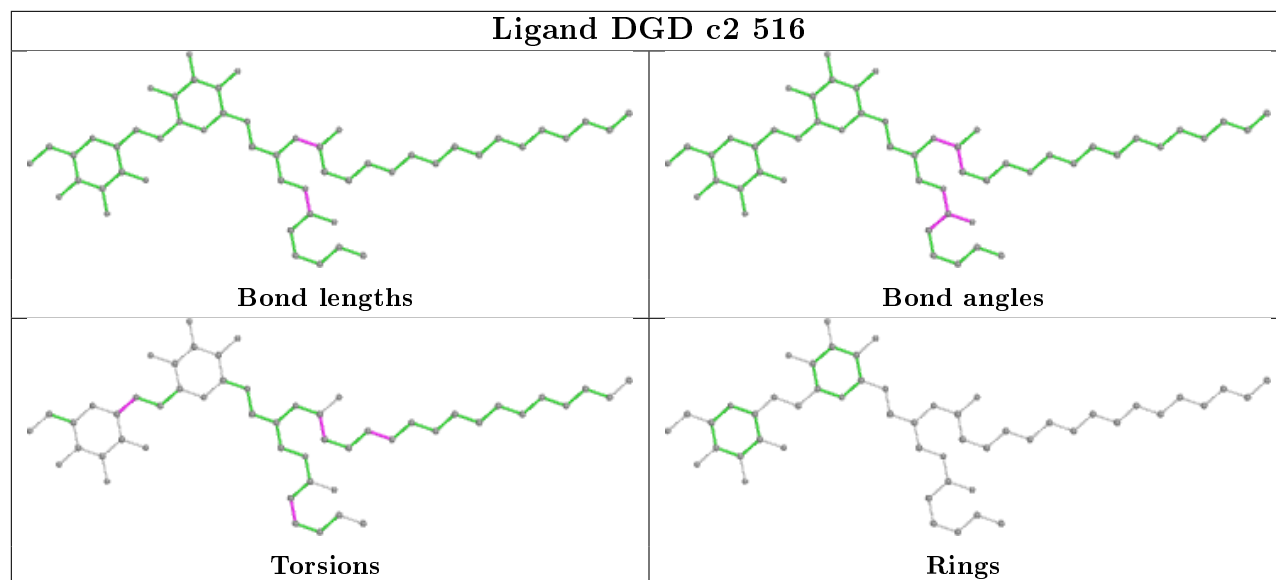


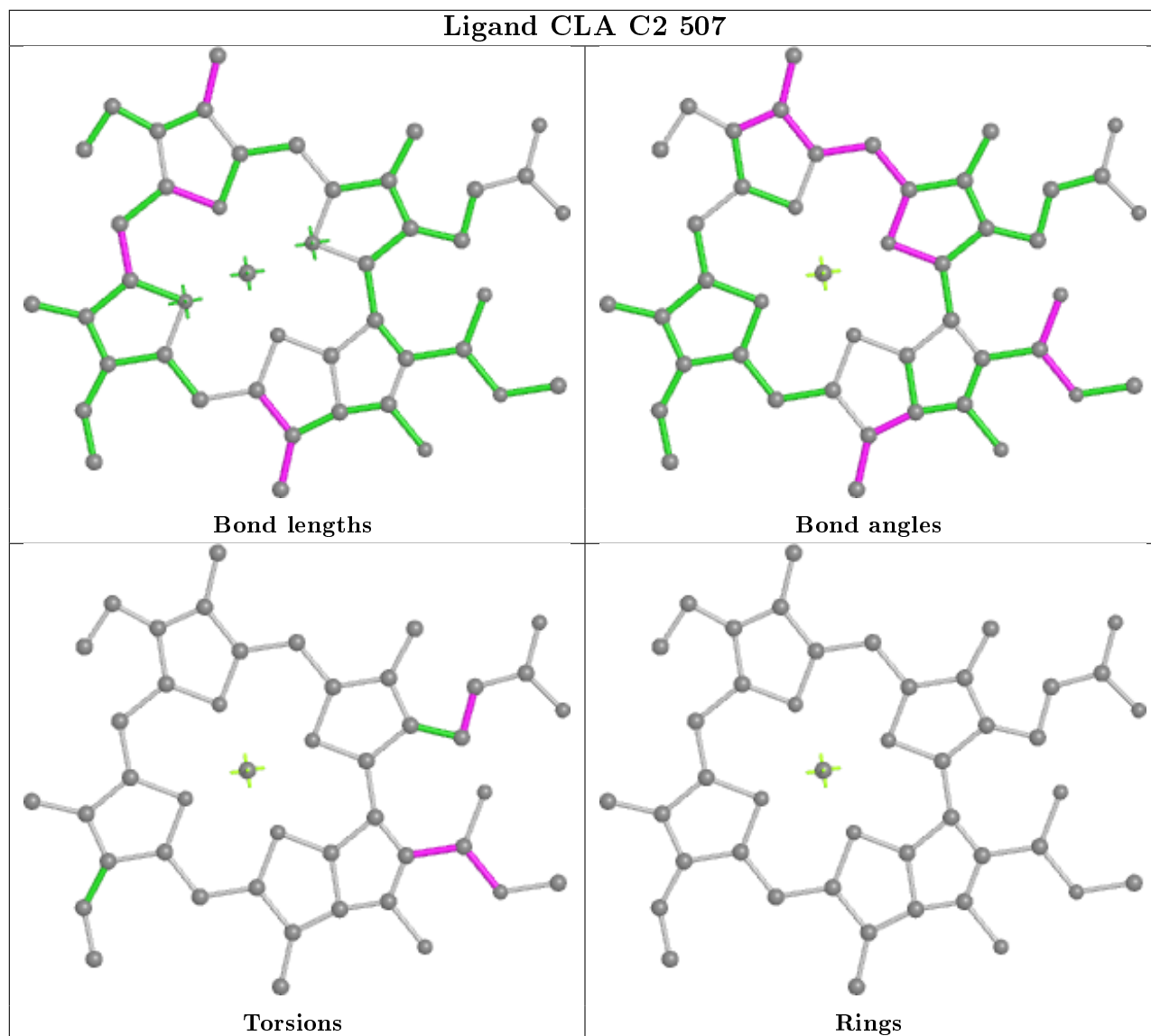


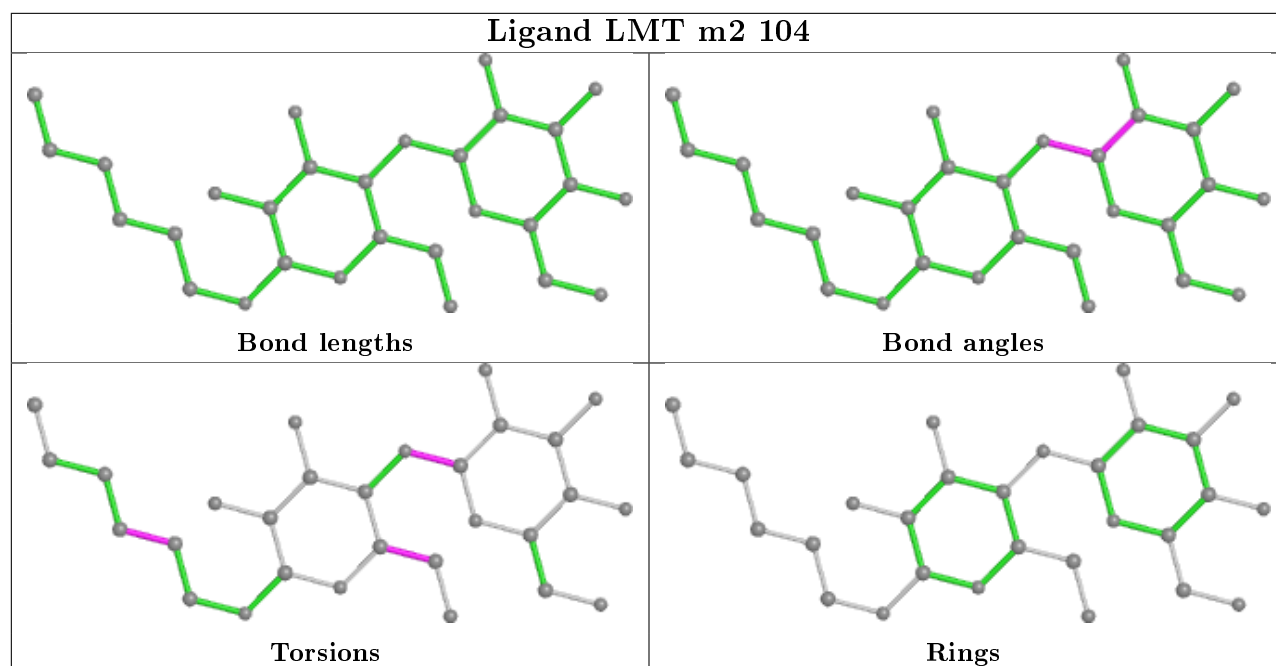
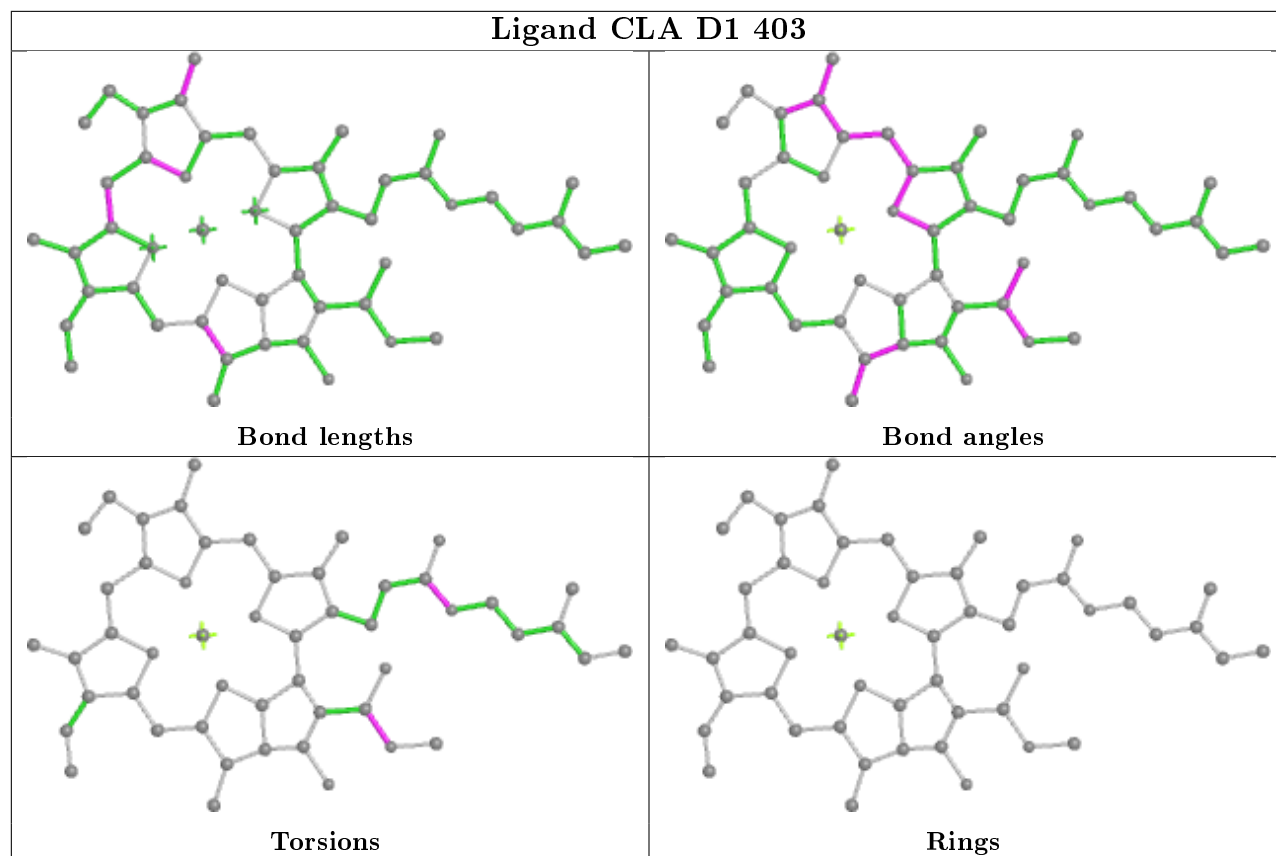


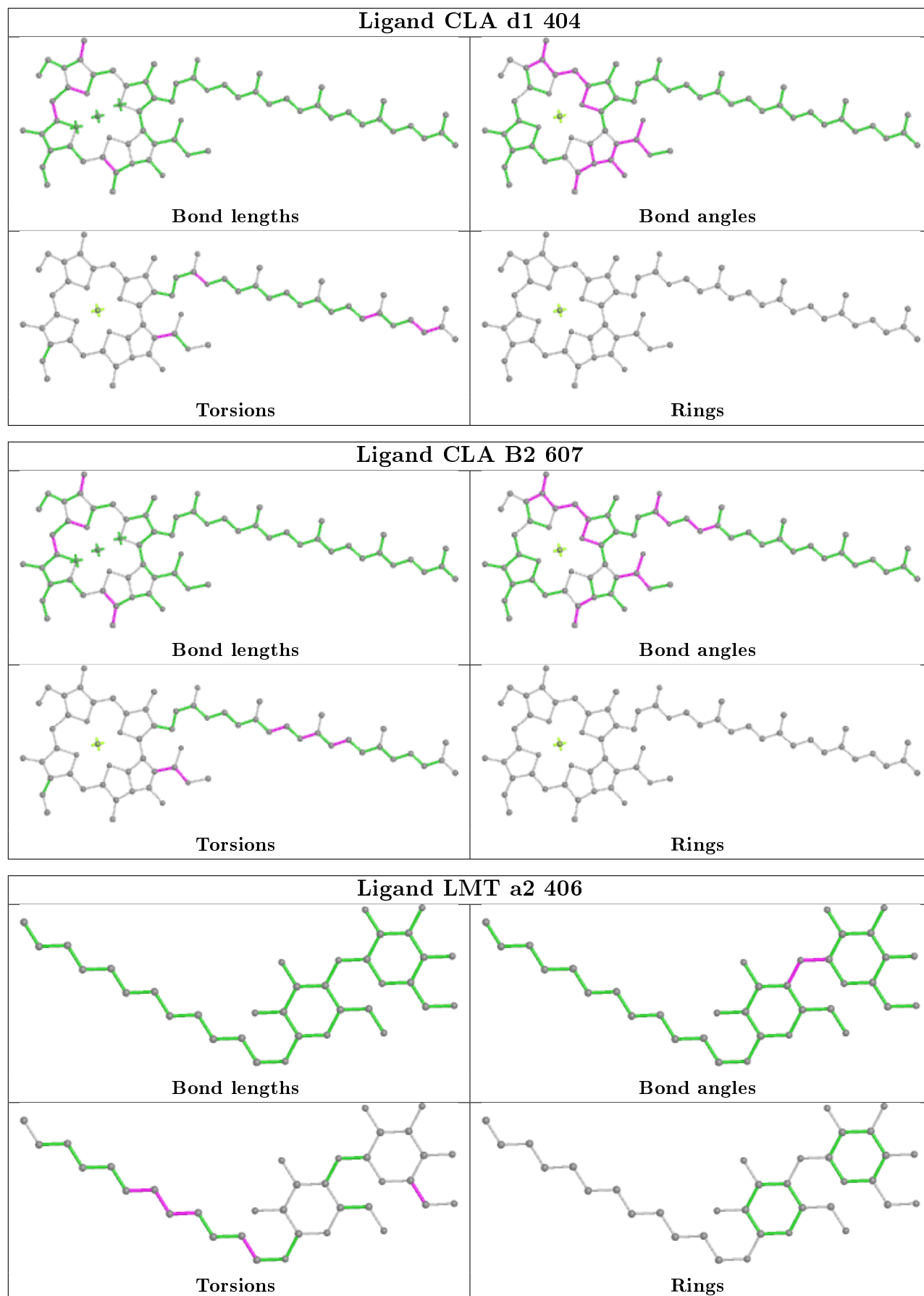


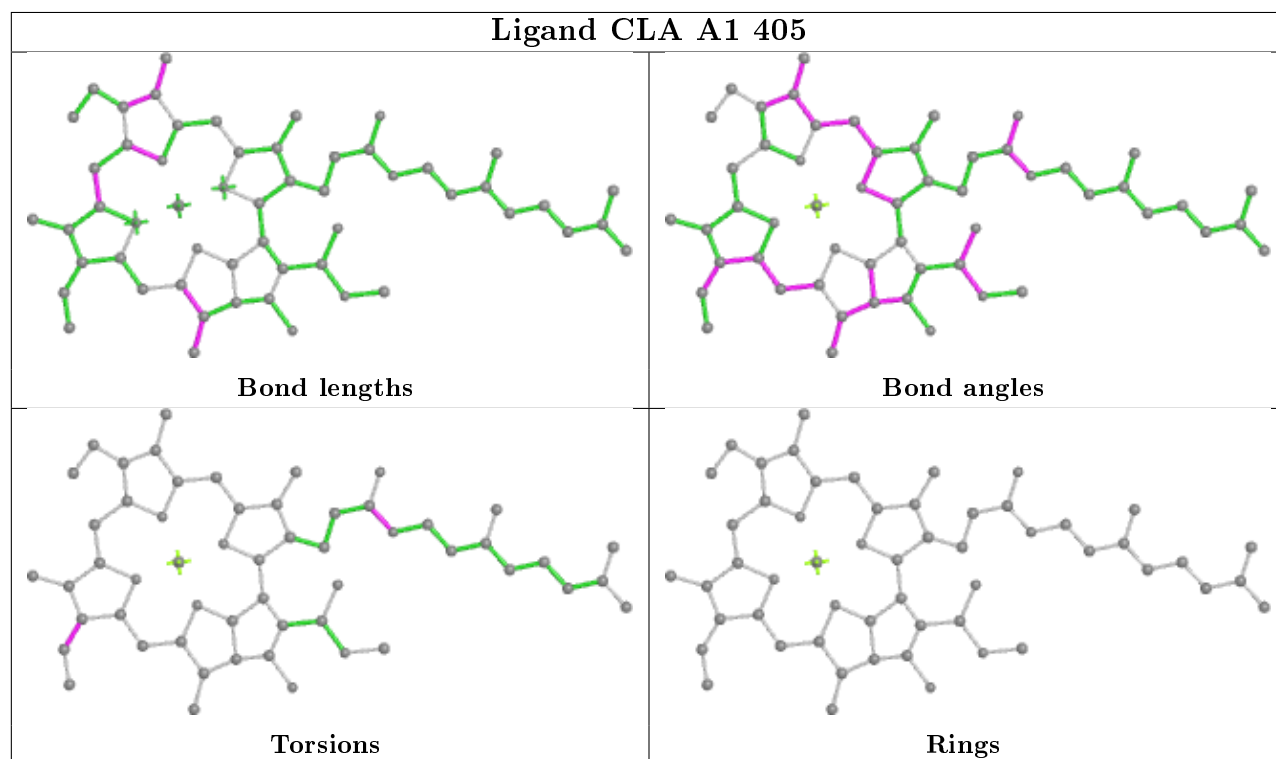
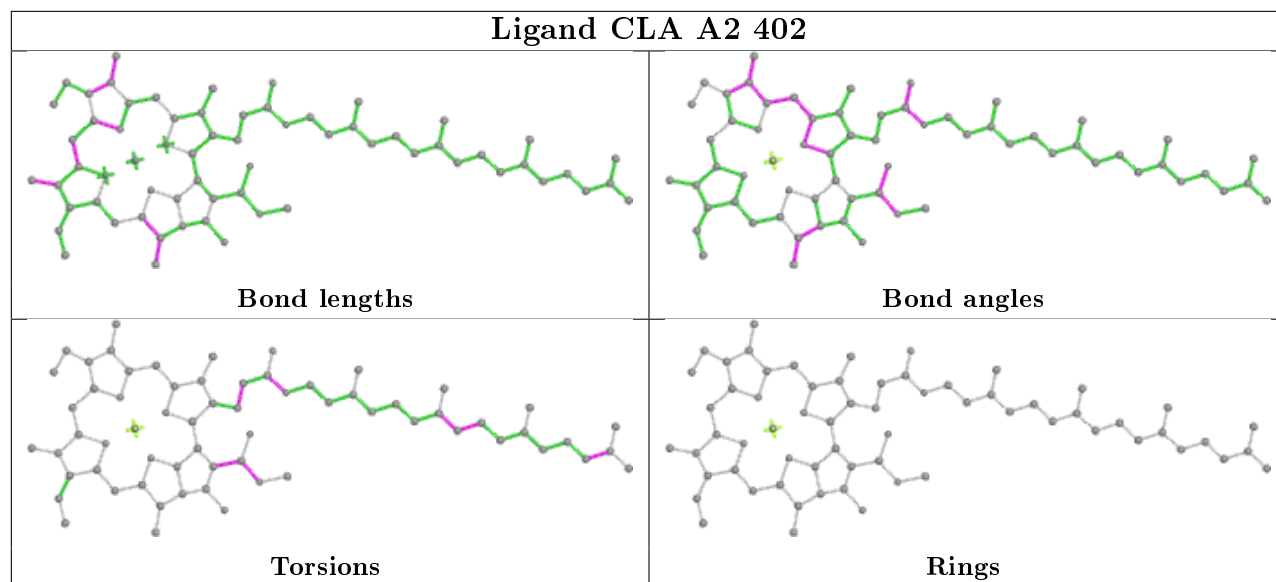


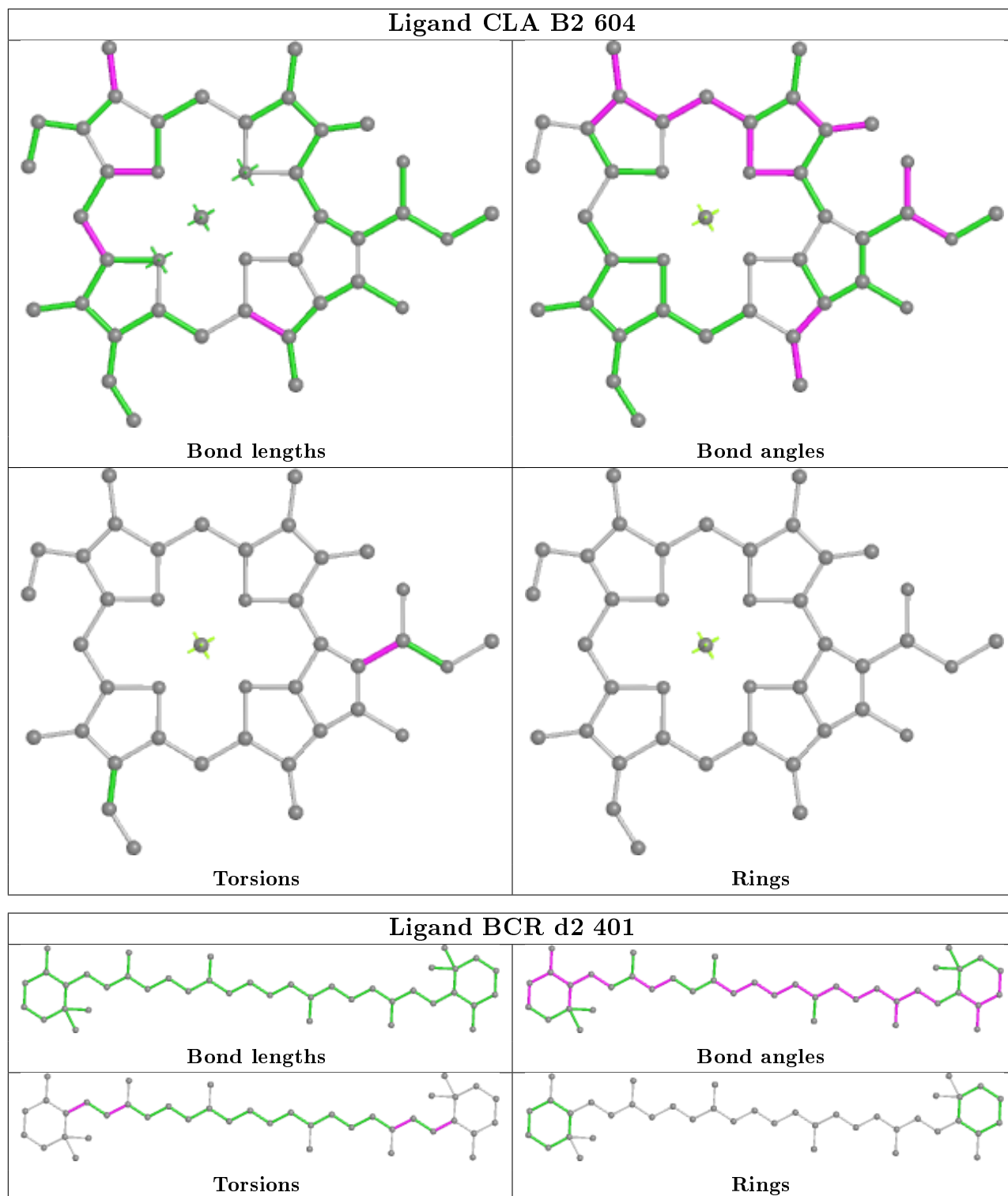




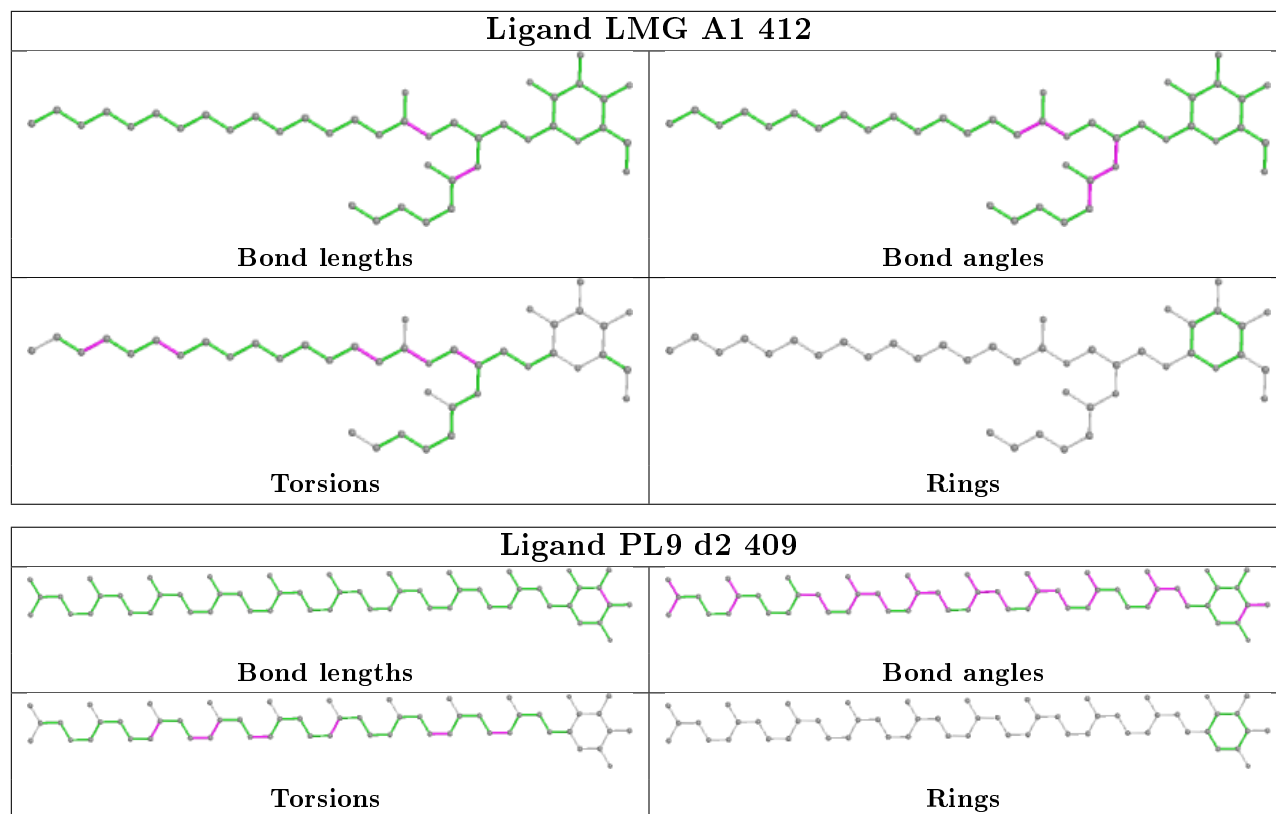


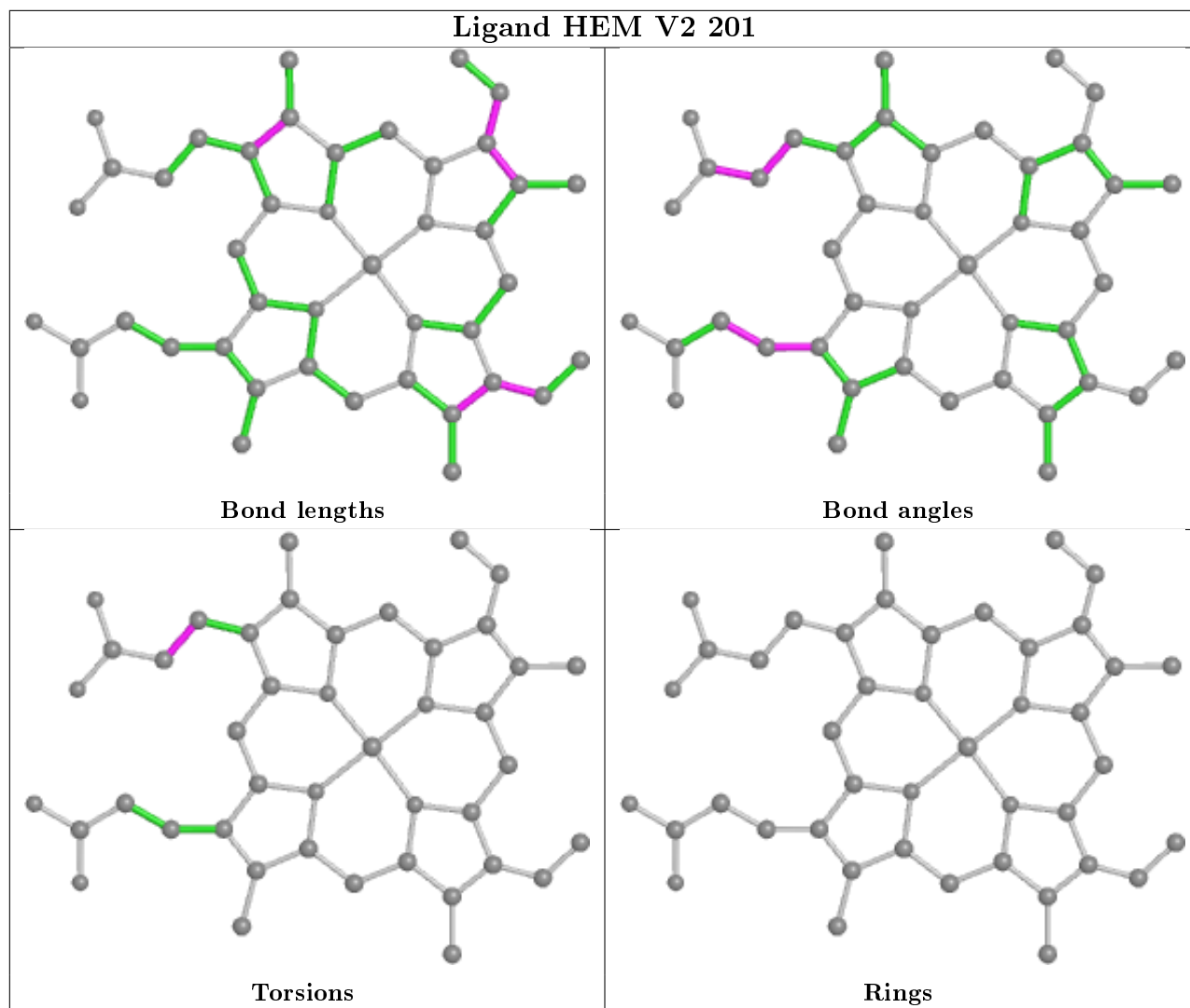


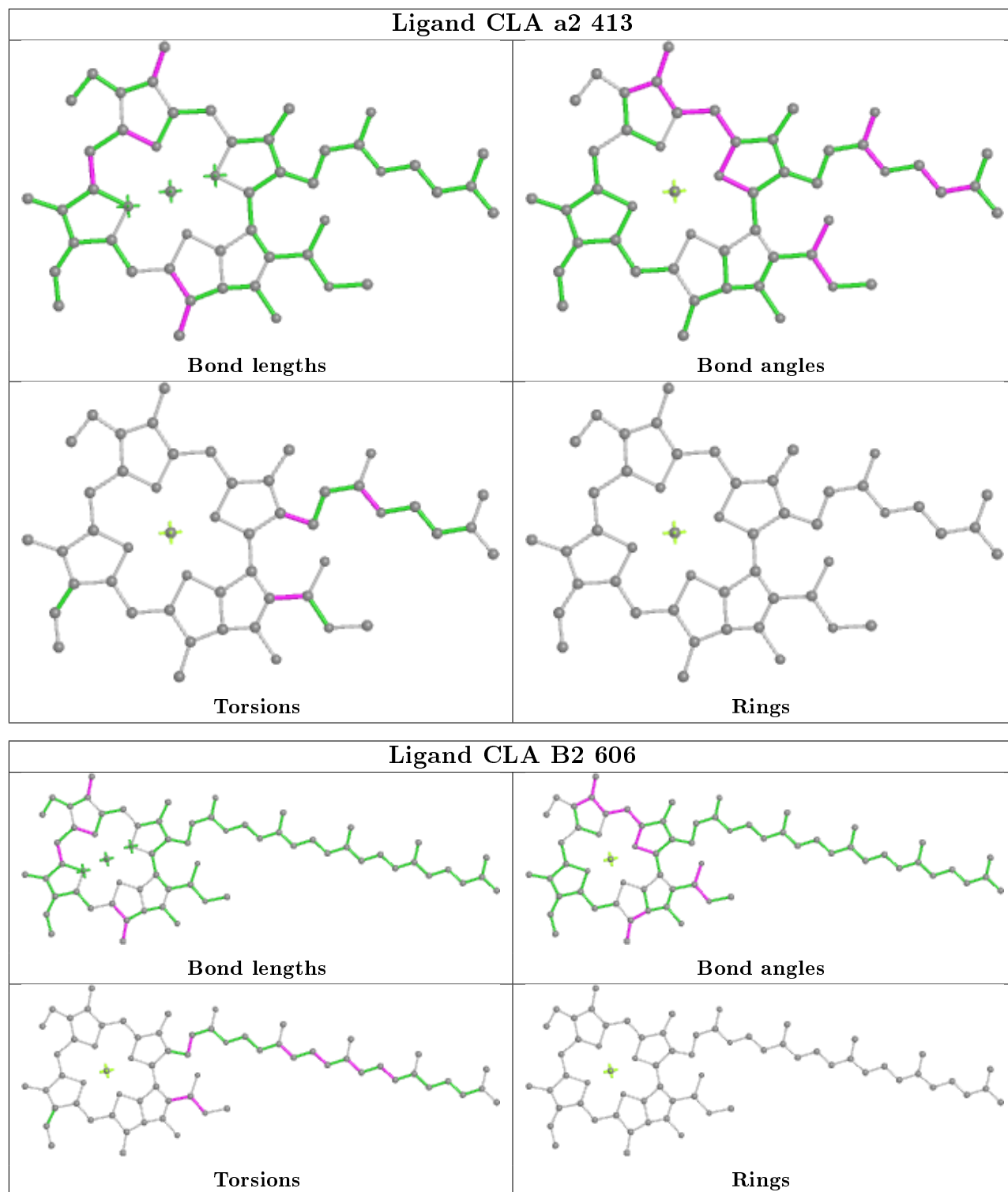


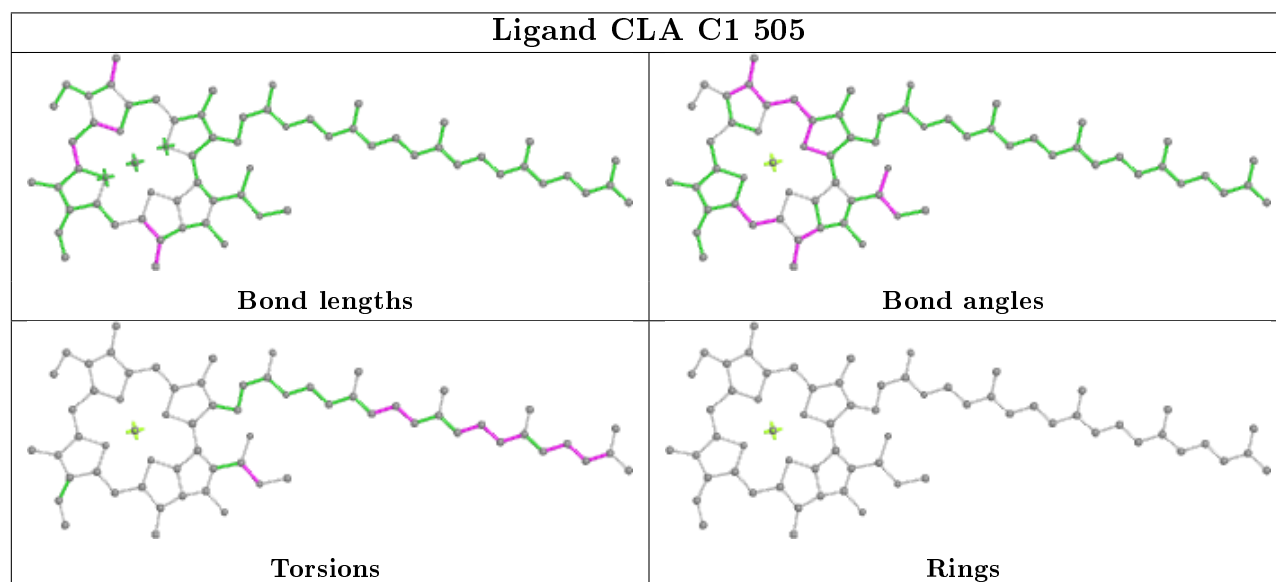
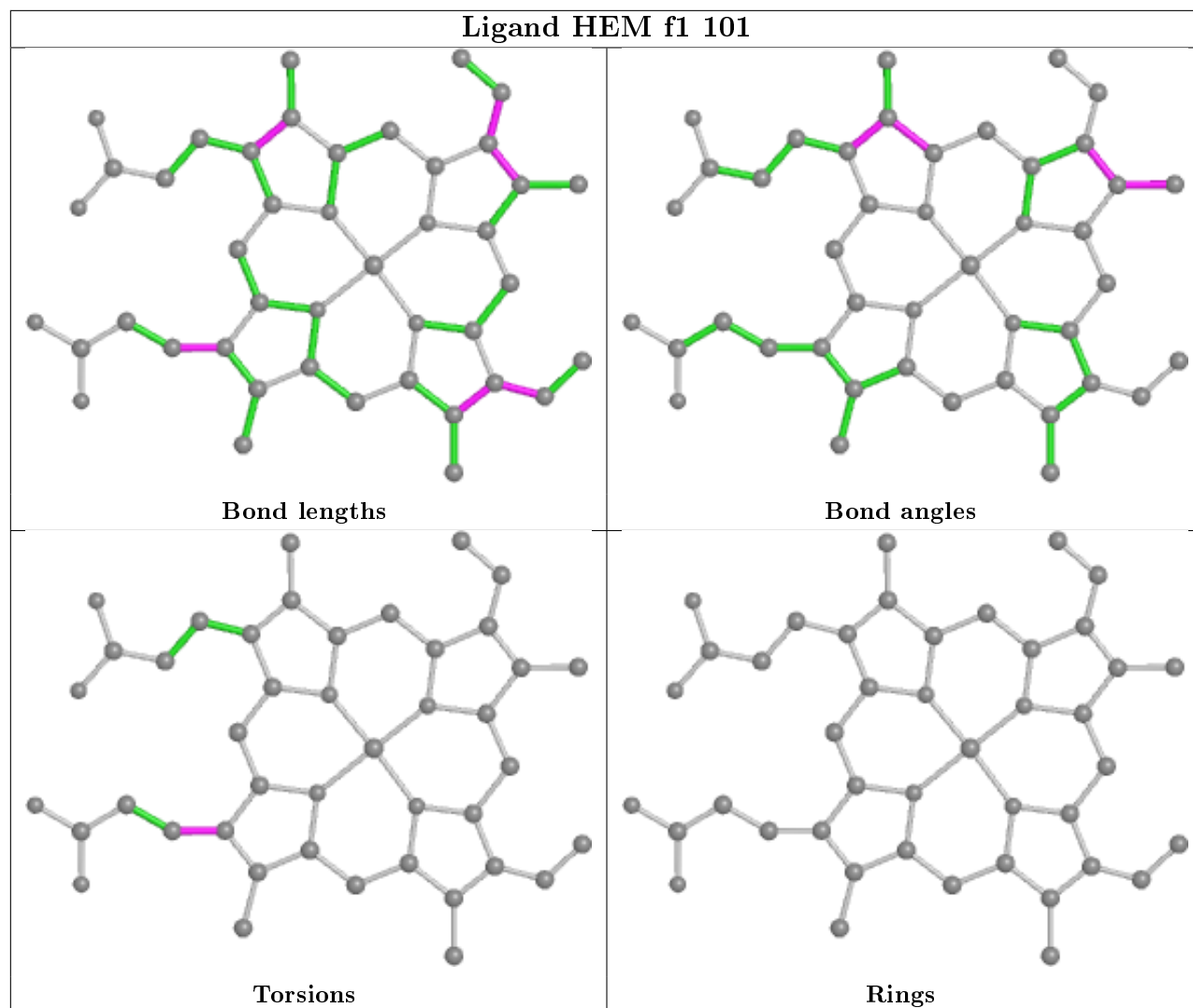


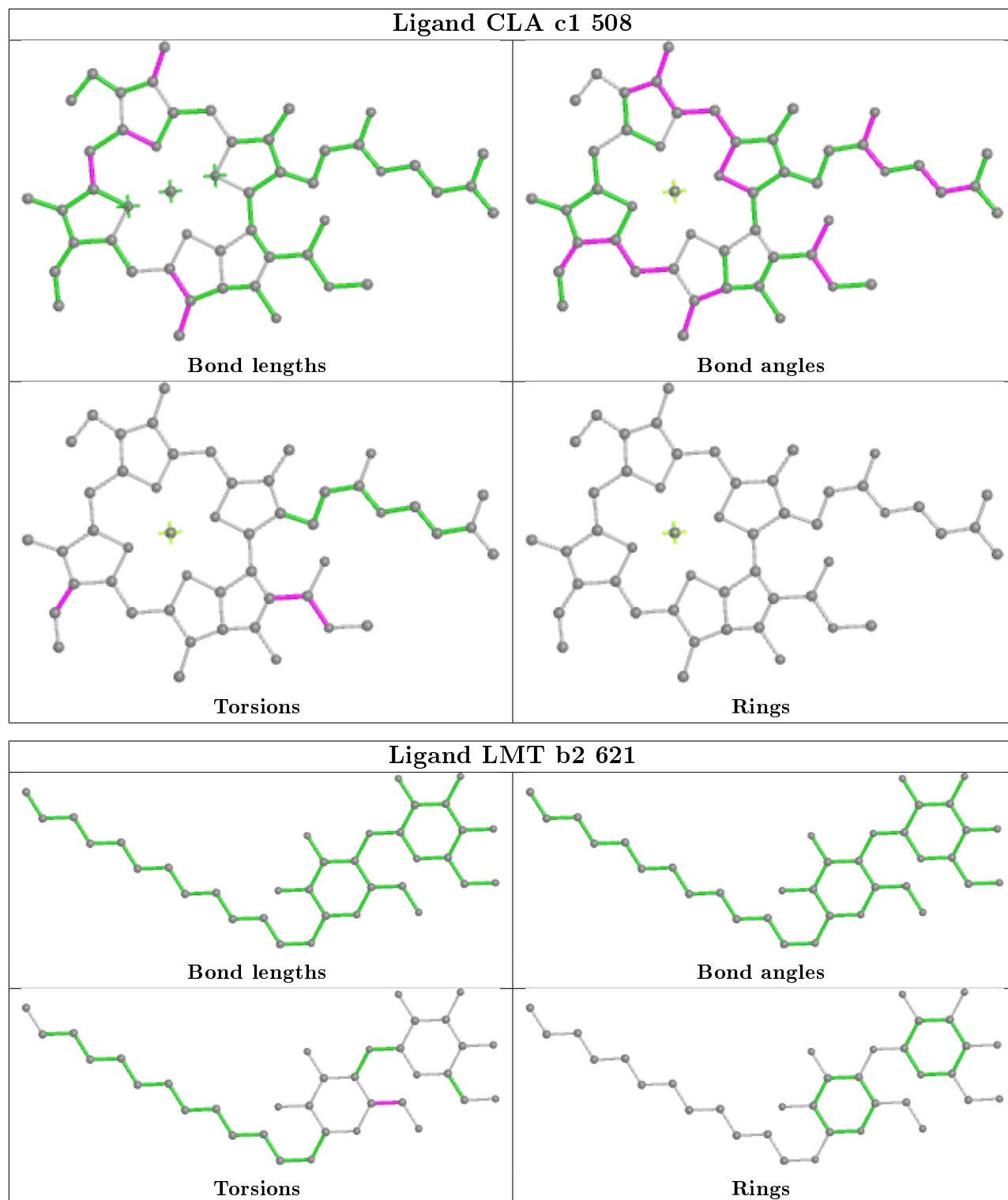


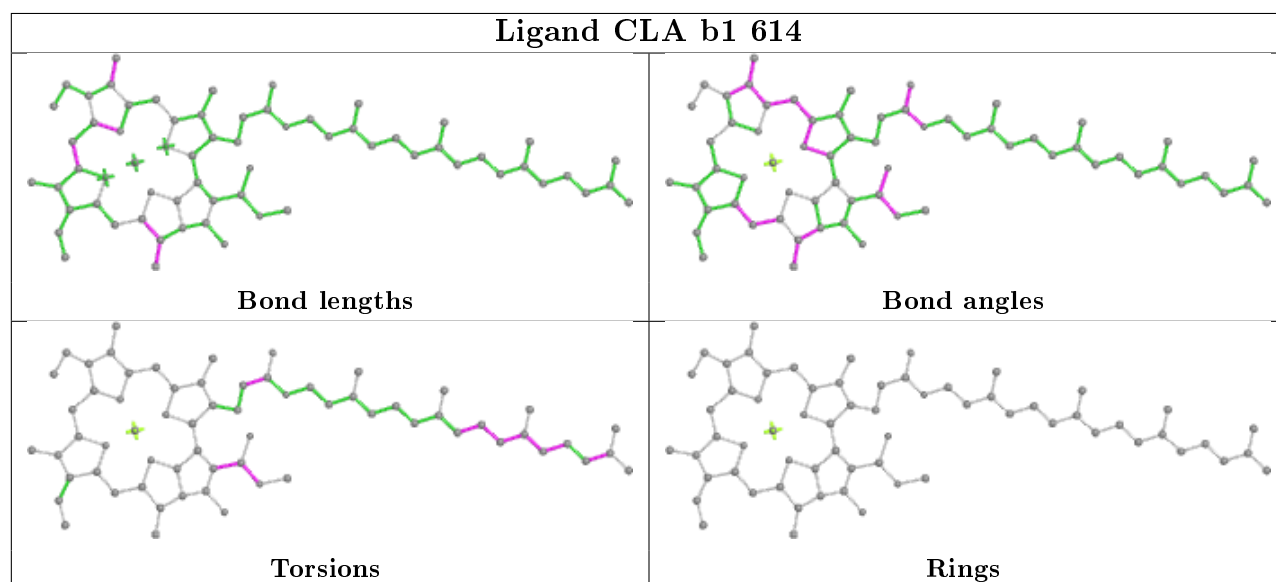
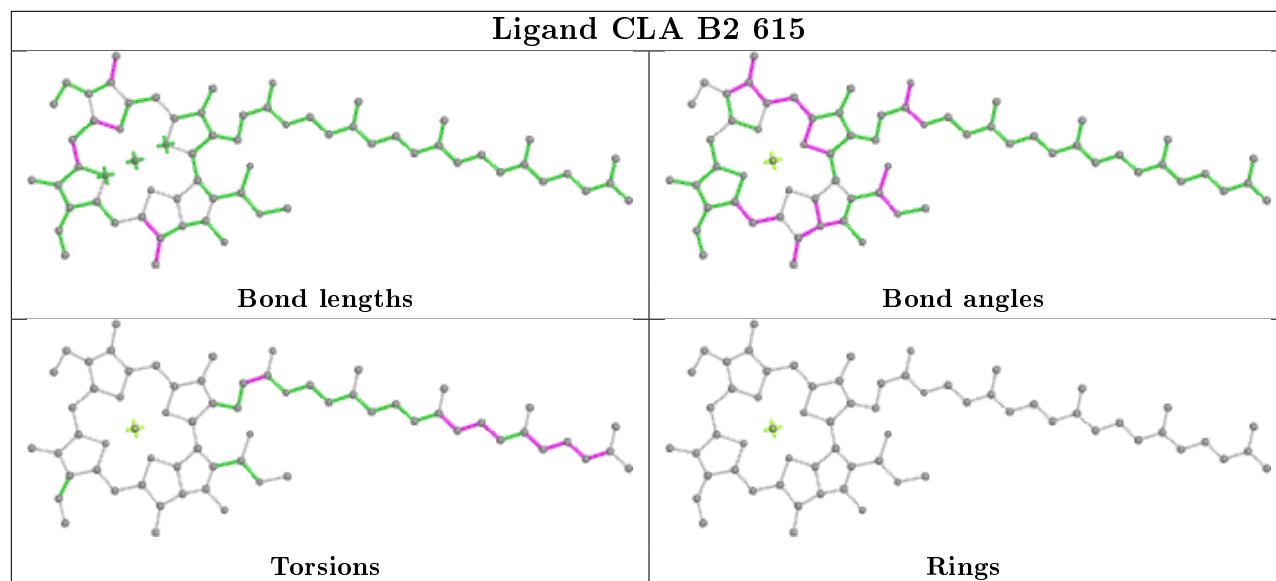
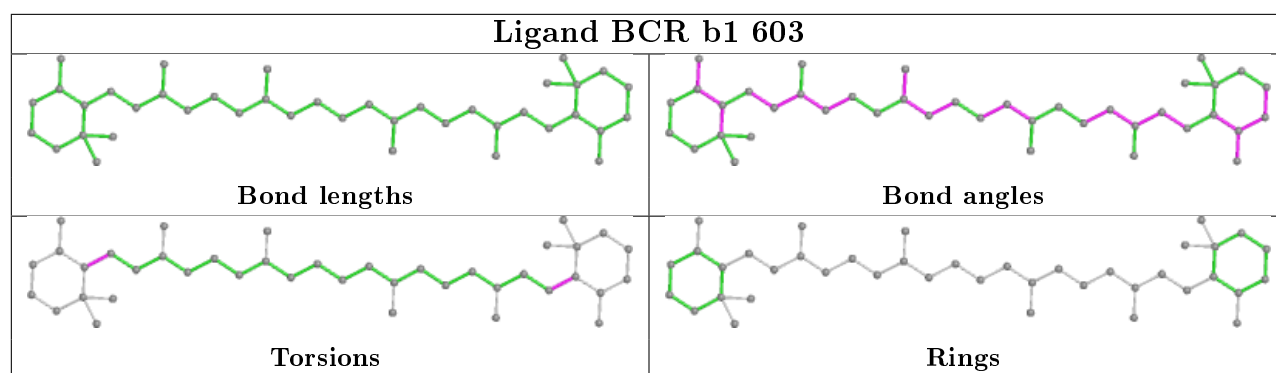


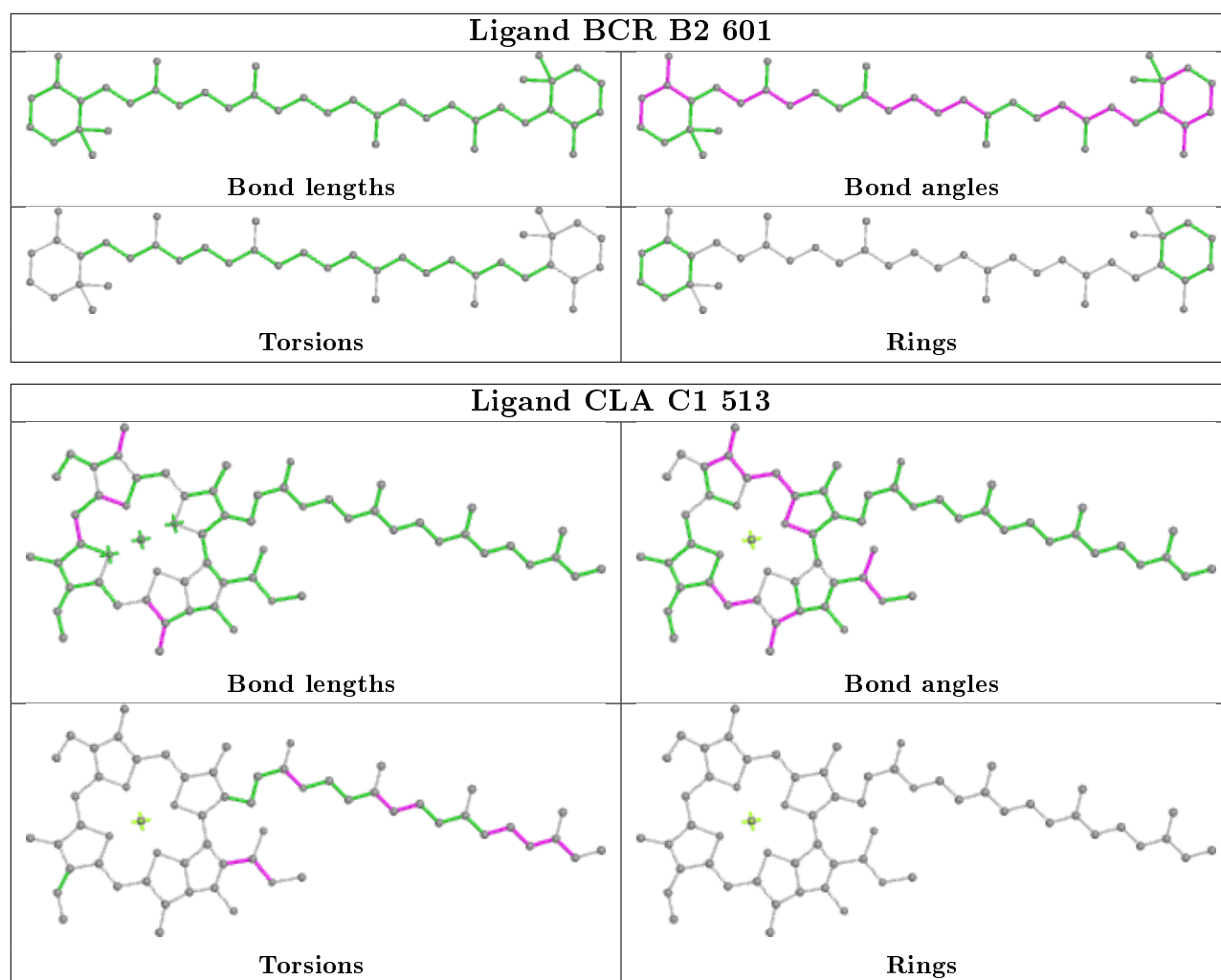












## 5.7 Other polymers [\(i\)](#)

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 i

### 6.1 Protein, DNA and RNA chains i

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	A1	344/344 (100%)	0.11	12 (3%) 44 38	31, 48, 79, 104	0
1	A2	332/344 (96%)	0.50	25 (7%) 14 10	51, 75, 91, 112	0
1	a1	334/344 (97%)	0.01	12 (3%) 42 37	36, 48, 68, 105	0
1	a2	334/344 (97%)	0.05	16 (4%) 30 24	34, 50, 83, 107	0
2	B1	483/509 (94%)	0.30	33 (6%) 17 12	40, 63, 93, 108	0
2	B2	503/509 (98%)	0.51	54 (10%) 6 4	46, 65, 93, 112	0
2	b1	503/509 (98%)	0.23	29 (5%) 23 18	36, 53, 80, 99	0
2	b2	481/509 (94%)	0.46	40 (8%) 11 7	43, 70, 99, 115	0
3	C1	449/460 (97%)	0.15	26 (5%) 23 18	33, 59, 78, 93	0
3	C2	444/460 (96%)	0.99	78 (17%) 1 1	73, 97, 117, 128	0
3	c1	449/460 (97%)	0.29	25 (5%) 24 19	41, 62, 85, 101	0
3	c2	448/460 (97%)	0.42	29 (6%) 18 14	39, 70, 93, 110	0
4	D1	337/351 (96%)	0.39	21 (6%) 20 15	36, 56, 88, 94	0
4	D2	340/351 (96%)	0.62	33 (9%) 7 5	51, 69, 85, 96	0
4	d1	339/351 (96%)	0.11	7 (2%) 63 59	34, 45, 65, 94	0
4	d2	340/351 (96%)	0.27	17 (5%) 28 23	36, 56, 88, 118	0
5	E1	61/84 (72%)	1.62	24 (39%) 0 0	64, 87, 141, 158	0
5	E2	63/84 (75%)	2.54	31 (49%) 0 0	77, 98, 131, 144	0
5	e1	57/84 (67%)	1.05	13 (22%) 0 0	49, 65, 87, 91	0
5	e2	60/84 (71%)	1.89	22 (36%) 0 0	59, 80, 144, 159	0
6	F1	28/43 (65%)	0.33	2 (7%) 16 11	62, 75, 123, 131	0
6	F2	31/43 (72%)	1.54	8 (25%) 0 0	81, 92, 144, 146	0
6	f1	29/43 (67%)	0.30	3 (10%) 6 4	50, 60, 95, 108	0
6	f2	29/43 (67%)	0.94	7 (24%) 0 0	64, 73, 128, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	H1	60/67 (89%)	0.52	9 (15%) 2 1	70, 84, 93, 101	0
7	H2	62/67 (92%)	0.75	10 (16%) 1 1	63, 75, 92, 124	0
7	h1	62/67 (92%)	0.31	3 (4%) 30 24	47, 67, 78, 84	0
7	h2	62/67 (92%)	1.14	13 (20%) 1 0	72, 87, 98, 122	0
8	I1	34/38 (89%)	0.07	2 (5%) 22 17	53, 61, 70, 71	0
8	I2	35/38 (92%)	0.51	2 (5%) 23 18	82, 93, 105, 109	0
8	i1	34/38 (89%)	0.05	1 (2%) 51 46	54, 61, 71, 76	0
8	i2	33/38 (86%)	0.19	2 (6%) 21 16	60, 67, 75, 77	0
9	J1	32/39 (82%)	0.22	3 (9%) 8 6	51, 65, 89, 105	0
9	J2	35/39 (89%)	1.29	9 (25%) 0 0	75, 87, 125, 136	0
9	j1	32/39 (82%)	0.27	5 (15%) 2 1	49, 63, 74, 81	0
9	j2	33/39 (84%)	0.11	1 (3%) 50 45	54, 70, 88, 110	0
10	K1	37/41 (90%)	0.70	3 (8%) 12 8	56, 66, 78, 79	0
10	K2	37/41 (90%)	1.04	9 (24%) 0 0	86, 96, 111, 117	0
10	k1	37/41 (90%)	0.78	6 (16%) 1 1	56, 67, 81, 81	0
10	k2	37/41 (90%)	1.28	9 (24%) 0 0	67, 76, 89, 92	0
11	L1	37/38 (97%)	0.00	3 (8%) 12 8	39, 43, 67, 77	0
11	L2	37/38 (97%)	-0.03	1 (2%) 54 49	49, 56, 61, 73	0
11	l1	37/38 (97%)	-0.07	1 (2%) 54 49	36, 43, 63, 73	0
11	l2	37/38 (97%)	0.16	0 100 100	43, 47, 73, 79	0
12	M1	40/108 (37%)	0.02	1 (2%) 57 52	32, 46, 62, 67	0
12	M2	40/108 (37%)	0.03	0 100 100	45, 54, 67, 69	0
12	m1	40/108 (37%)	-0.03	0 100 100	34, 44, 65, 67	0
12	m2	40/108 (37%)	0.25	4 (10%) 7 5	44, 51, 65, 71	0
13	O1	240/329 (72%)	0.57	35 (14%) 2 1	38, 61, 96, 107	0
13	O2	205/329 (62%)	1.54	53 (25%) 0 0	54, 91, 119, 151	0
13	o1	238/329 (72%)	0.72	36 (15%) 2 1	38, 76, 121, 145	0
13	o2	245/329 (74%)	0.68	38 (15%) 2 1	41, 64, 103, 127	0
14	T1	30/32 (93%)	-0.19	1 (3%) 46 41	37, 44, 60, 68	0
14	T2	30/32 (93%)	0.09	1 (3%) 46 41	54, 63, 76, 82	0
14	t1	30/32 (93%)	-0.02	3 (10%) 7 5	40, 46, 60, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	t2	29/32 (90%)	-0.22	2 (6%) 16 12	38, 48, 68, 84	0
15	U1	93/155 (60%)	0.25	2 (2%) 62 57	44, 59, 75, 104	0
15	U2	90/155 (58%)	1.15	20 (22%) 0 0	74, 91, 104, 115	0
15	u1	93/155 (60%)	0.60	12 (12%) 3 2	53, 68, 88, 95	0
15	u2	93/155 (60%)	0.32	4 (4%) 35 30	44, 58, 71, 86	0
16	V1	129/155 (83%)	0.22	5 (3%) 39 34	47, 62, 87, 93	0
16	V2	129/155 (83%)	1.54	39 (30%) 0 0	75, 96, 114, 127	0
16	v1	129/155 (83%)	0.60	12 (9%) 8 6	47, 69, 108, 124	0
16	v2	129/155 (83%)	0.41	12 (9%) 8 6	47, 63, 90, 105	0
17	Y1	27/35 (77%)	0.09	3 (11%) 5 3	64, 74, 103, 118	0
17	Y2	25/35 (71%)	1.41	8 (32%) 0 0	96, 100, 107, 109	0
17	y1	27/35 (77%)	0.94	6 (22%) 0 0	64, 71, 105, 107	0
17	y2	27/35 (77%)	0.61	5 (18%) 1 1	72, 79, 92, 106	0
18	X1	29/40 (72%)	1.88	10 (34%) 0 0	98, 113, 130, 135	0
18	X2	31/40 (77%)	1.70	11 (35%) 0 0	83, 101, 115, 121	0
18	x1	36/40 (90%)	0.75	6 (16%) 1 1	61, 83, 96, 102	0
18	x2	32/40 (80%)	1.64	13 (40%) 0 0	83, 104, 122, 126	0
19	S1	25/46 (54%)	0.96	5 (20%) 1 0	73, 79, 85, 98	0
19	S2	30/46 (65%)	2.28	16 (53%) 0 0	98, 114, 120, 122	0
19	s1	40/46 (86%)	1.30	11 (27%) 0 0	54, 78, 94, 95	0
19	s2	46/46 (100%)	1.56	13 (28%) 0 0	75, 90, 106, 112	0
20	W1	21/25 (84%)	-0.34	1 (4%) 30 24	71, 79, 86, 90	0
20	W2	21/25 (84%)	-0.72	0 100 100	66, 76, 84, 89	0
20	w1	25/25 (100%)	0.27	4 (16%) 1 1	73, 79, 96, 101	0
20	w2	20/25 (80%)	-0.13	1 (5%) 28 23	91, 96, 103, 111	0
21	Q2	111/218 (50%)	1.91	55 (49%) 0 0	122, 132, 145, 151	0
21	q1	105/218 (48%)	1.94	45 (42%) 0 0	103, 125, 138, 144	0
22	Z2	59/62 (95%)	1.61	20 (33%) 0 0	108, 121, 134, 140	0
22	z2	59/62 (95%)	0.51	7 (11%) 4 3	83, 101, 116, 127	0
All	All	10516/12316 (85%)	0.53	1179 (11%) 5 3	31, 66, 113, 159	0

The worst 5 of 1179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e2	21	VAL	13.3
13	O2	194	SER	10.3
6	F2	15	ILE	9.3
9	J2	7	ARG	9.1
13	O2	195	GLY	8.6

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
28	UNL	J2	101	10/-	0.43	0.86	71,82,86,88	0
28	UNL	c2	520	15/-	0.44	0.32	86,97,106,108	0
28	UNL	I2	103	14/-	0.54	0.38	62,93,102,104	0
33	LHG	a2	407	30/49	0.55	0.37	55,75,94,102	0
28	UNL	d2	410	13/-	0.55	0.59	74,92,108,111	0
23	BCR	K1	101	31/40	0.57	0.54	64,82,93,96	0
28	UNL	j1	101	17/-	0.59	0.46	60,69,71,77	0
33	LHG	b2	625	43/49	0.60	0.41	62,87,109,126	0
39	CA	o2	401	1/1	0.61	0.34	101,101,101,101	0
35	LMT	a2	406	35/35	0.61	0.36	43,80,92,94	0
28	UNL	I2	102	17/-	0.62	0.37	80,92,102,103	0
32	GOL	a1	406	6/6	0.63	0.29	68,75,86,90	0
28	UNL	a2	409	18/-	0.63	0.34	61,74,86,90	0
28	UNL	C2	517	18/-	0.64	0.45	74,83,87,89	0
35	LMT	c1	517	33/35	0.64	0.43	63,100,117,119	0
35	LMT	b2	621	35/35	0.65	0.35	69,110,123,123	0
23	BCR	K2	102	40/40	0.65	0.44	84,99,113,115	0
28	UNL	B2	626	15/-	0.65	0.36	79,83,92,95	0
28	UNL	X2	101	7/-	0.66	0.43	83,85,91,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
28	UNL	A2	409	10/-	0.67	0.39	72,82,85,87	0
28	UNL	A2	408	18/-	0.68	0.38	62,83,92,93	0
28	UNL	D1	410	6/-	0.68	0.49	59,62,66,66	0
32	GOL	C1	518	6/6	0.68	0.45	65,73,77,81	0
28	UNL	F2	403	16/-	0.68	0.19	51,76,86,89	0
28	UNL	d1	410	12/-	0.68	0.31	49,72,77,79	0
29	LMG	C2	515	24/55	0.70	0.60	82,97,104,105	0
28	UNL	t1	101	18/-	0.70	0.40	43,60,66,67	0
28	UNL	b1	626	13/-	0.70	0.29	53,64,83,86	0
28	UNL	k2	505	6/-	0.70	0.22	70,80,84,87	0
28	UNL	b1	623	11/-	0.70	0.41	59,74,83,84	0
29	LMG	d1	411	35/55	0.70	0.34	58,76,94,99	0
28	UNL	m2	102	18/-	0.70	0.38	46,65,79,79	0
28	UNL	C2	501	6/-	0.71	0.44	72,74,78,87	0
29	LMG	j2	101	50/55	0.72	0.41	60,78,97,107	0
28	UNL	B2	622	17/-	0.73	0.30	57,71,76,78	0
28	UNL	b2	607	12/-	0.73	0.36	64,75,80,87	0
23	BCR	K2	104	29/40	0.74	0.38	92,100,109,112	0
28	UNL	k2	504	9/-	0.74	0.35	66,74,80,88	0
29	LMG	I2	101	34/55	0.74	0.26	82,103,109,114	0
33	LHG	B2	627	42/49	0.74	0.32	67,88,120,132	0
35	LMT	m2	103	30/35	0.74	0.29	52,89,111,113	0
28	UNL	b1	629	15/-	0.74	0.29	46,59,71,83	0
28	UNL	B1	623	16/-	0.74	0.28	53,68,72,74	0
32	GOL	c2	518	6/6	0.75	0.35	50,55,59,64	0
35	LMT	m2	104	29/35	0.75	0.27	49,104,119,122	0
28	UNL	b1	627	16/-	0.76	0.27	42,56,75,77	0
23	BCR	h2	101	40/40	0.76	0.36	71,85,107,109	0
25	CLA	B1	604	42/65	0.77	0.31	83,98,107,113	0
23	BCR	c2	501	40/40	0.77	0.36	66,82,89,92	0
28	UNL	H2	102	5/-	0.77	0.56	72,81,84,85	0
28	UNL	x1	101	15/-	0.77	0.38	55,73,79,82	0
28	UNL	B2	625	18/-	0.77	0.35	37,56,68,68	0
28	UNL	k2	502	9/-	0.77	0.39	72,78,84,86	0
29	LMG	b2	622	39/55	0.78	0.30	47,60,85,90	0
23	BCR	C2	502	40/40	0.78	0.35	95,106,118,120	0
23	BCR	C1	521	40/40	0.78	0.29	59,68,80,84	0
23	BCR	c1	502	40/40	0.78	0.33	57,66,72,72	0
28	UNL	b1	630	17/-	0.78	0.42	48,57,74,75	0
25	CLA	D2	404	61/65	0.79	0.26	67,87,113,120	0
37	SQD	B2	623	45/54	0.79	0.34	58,79,89,96	0
29	LMG	F2	402	35/55	0.79	0.29	68,81,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	UNL	a2	401	18/-	0.79	0.30	46,56,70,86	0
24	CL	A2	410	1/1	0.80	0.18	87,87,87,87	0
23	BCR	j2	102	40/40	0.80	0.28	59,75,86,87	0
23	BCR	k1	101	40/40	0.80	0.43	56,70,82,85	0
35	LMT	b2	623	35/35	0.80	0.30	63,90,98,101	0
28	UNL	M2	101	11/-	0.80	0.30	59,68,73,74	0
35	LMT	l1	101	24/35	0.80	0.28	42,55,89,90	0
29	LMG	A1	412	41/55	0.80	0.24	50,75,96,100	0
23	BCR	z2	101	40/40	0.80	0.41	80,95,100,101	0
25	CLA	C2	510	45/65	0.80	0.34	107,116,121,126	0
28	UNL	k2	503	6/-	0.81	0.46	67,76,79,80	0
29	LMG	b1	621	38/55	0.81	0.24	52,63,76,82	0
25	CLA	C1	514	45/65	0.81	0.31	73,84,92,96	0
23	BCR	b2	603	40/40	0.81	0.26	60,74,102,104	0
35	LMT	m1	101	35/35	0.81	0.24	44,80,103,112	0
28	UNL	m1	102	6/-	0.81	0.33	54,55,63,66	0
33	LHG	A2	405	33/49	0.81	0.34	70,80,90,97	0
32	GOL	B1	620	6/6	0.81	0.32	63,75,81,82	0
29	LMG	a1	412	51/55	0.81	0.26	54,67,77,91	0
25	CLA	c1	516	65/65	0.81	0.32	66,82,104,109	0
28	UNL	a2	410	8/-	0.81	0.26	61,68,70,76	0
29	LMG	C1	520	48/55	0.82	0.26	59,69,78,86	0
35	LMT	i2	102	7/35	0.82	0.29	68,71,76,79	0
23	BCR	H2	103	24/40	0.82	0.30	65,76,82,85	0
37	SQD	b2	605	45/54	0.82	0.31	54,83,114,124	0
25	CLA	c2	513	54/65	0.82	0.29	75,94,102,105	0
33	LHG	d1	402	32/49	0.82	0.27	45,63,76,86	0
28	UNL	m2	101	18/-	0.82	0.34	44,57,79,85	0
29	LMG	B1	626	48/55	0.82	0.25	55,70,89,94	0
28	UNL	a2	411	11/-	0.82	0.31	51,55,65,67	0
23	BCR	F2	401	40/40	0.82	0.23	67,81,107,113	0
29	LMG	b1	624	39/55	0.83	0.36	58,73,84,87	0
29	LMG	a2	412	44/55	0.83	0.26	55,70,78,93	0
35	LMT	M1	103	24/35	0.83	0.21	42,68,97,101	0
25	CLA	d2	404	50/65	0.83	0.23	57,74,83,88	0
25	CLA	K2	101	55/65	0.83	0.28	86,98,104,109	0
28	UNL	B1	624	18/-	0.83	0.28	43,71,79,81	0
34	DGD	H2	101	62/66	0.83	0.26	51,74,83,85	0
28	UNL	b1	625	10/-	0.83	0.42	50,62,68,69	0
25	CLA	C2	508	50/65	0.83	0.32	87,103,112,115	0
25	CLA	C2	518	41/65	0.83	0.29	105,121,127,134	0
25	CLA	C1	513	61/65	0.84	0.28	49,68,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
25	CLA	C2	509	65/65	0.84	0.25	90,101,106,108	0
29	LMG	b1	631	40/55	0.84	0.23	29,52,85,92	0
25	CLA	C2	505	65/65	0.84	0.23	78,100,112,118	0
23	BCR	c1	501	40/40	0.84	0.24	56,66,79,82	0
29	LMG	A2	412	29/55	0.84	0.22	86,94,100,102	0
23	BCR	b1	602	40/40	0.84	0.25	35,57,65,73	0
32	GOL	b1	618	6/6	0.84	0.25	60,69,80,80	0
25	CLA	C1	512	65/65	0.85	0.25	63,82,102,121	0
23	BCR	D1	401	40/40	0.85	0.23	54,67,89,95	0
34	DGD	H1	101	62/66	0.85	0.24	50,71,84,89	0
39	CA	O1	401	1/1	0.85	0.07	82,82,82,82	0
25	CLA	C2	506	65/65	0.85	0.34	78,90,97,100	0
25	CLA	C2	503	65/65	0.85	0.28	94,104,112,116	0
23	BCR	k2	501	40/40	0.85	0.29	61,84,95,98	0
25	CLA	B1	611	62/65	0.85	0.25	58,78,87,89	0
29	LMG	B2	621	37/55	0.85	0.25	53,68,80,96	0
25	CLA	B1	618	58/65	0.85	0.25	53,64,80,86	0
23	BCR	C1	501	40/40	0.85	0.24	47,61,72,75	0
32	GOL	C2	514	6/6	0.85	0.22	87,93,100,101	0
28	UNL	W2	101	9/-	0.85	0.21	64,77,83,87	0
25	CLA	c2	515	46/65	0.85	0.27	81,100,104,109	0
25	CLA	C2	513	53/65	0.85	0.26	78,91,106,110	0
37	SQD	D1	409	35/54	0.85	0.36	61,75,92,97	0
23	BCR	J1	101	40/40	0.86	0.33	50,70,86,88	0
23	BCR	B1	602	40/40	0.86	0.21	49,62,74,78	0
23	BCR	B2	602	40/40	0.86	0.20	47,59,80,86	0
25	CLA	b1	604	65/65	0.86	0.26	52,78,110,115	0
23	BCR	H1	102	22/40	0.86	0.23	75,88,95,100	0
25	CLA	c1	515	55/65	0.86	0.24	69,82,90,94	0
28	UNL	d2	411	12/-	0.86	0.42	55,67,73,79	0
28	UNL	B2	624	8/-	0.86	0.24	46,51,54,55	0
29	LMG	c2	519	26/55	0.86	0.21	58,67,73,74	0
35	LMT	T1	101	12/35	0.86	0.28	46,51,54,56	0
25	CLA	c1	508	50/65	0.86	0.22	57,66,77,81	0
29	LMG	B2	620	40/55	0.87	0.26	62,74,97,98	0
25	CLA	D1	403	51/65	0.87	0.21	64,74,88,90	0
25	CLA	d1	406	65/65	0.87	0.23	44,58,94,99	0
25	CLA	b2	619	59/65	0.87	0.23	71,80,106,109	0
25	CLA	b2	610	65/65	0.87	0.21	60,82,90,92	0
25	CLA	c2	512	65/65	0.87	0.26	61,76,86,93	0
23	BCR	b2	602	40/40	0.87	0.21	51,70,78,82	0
23	BCR	d2	401	40/40	0.87	0.22	48,67,81,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	UNL	a1	409	11/-	0.87	0.23	43,51,60,63	0
35	LMT	C1	519	35/35	0.87	0.24	57,76,85,93	0
34	DGD	C2	512	33/66	0.87	0.20	63,77,83,93	0
25	CLA	b2	613	65/65	0.87	0.23	59,84,96,99	0
28	UNL	l1	103	12/-	0.87	0.35	35,47,53,55	0
32	GOL	i1	101	6/6	0.87	0.49	55,57,60,64	0
29	LMG	c1	519	55/55	0.87	0.26	47,70,84,91	0
29	LMG	B1	622	31/55	0.87	0.18	66,74,81,83	0
28	UNL	i2	101	14/-	0.87	0.21	62,66,73,75	0
25	CLA	b2	604	42/65	0.88	0.29	82,109,116,127	0
36	PL9	d2	409	55/55	0.88	0.28	33,44,56,57	0
28	UNL	B1	625	7/-	0.88	0.27	45,52,55,63	0
25	CLA	b2	618	65/65	0.88	0.25	68,82,90,92	0
28	UNL	b1	628	10/-	0.88	0.35	51,57,61,67	0
25	CLA	A2	403	61/65	0.88	0.26	80,89,98,102	0
33	LHG	D1	404	49/49	0.88	0.26	48,60,84,90	0
25	CLA	B2	611	65/65	0.88	0.21	51,73,81,86	0
34	DGD	h2	102	62/66	0.88	0.22	47,67,82,96	0
34	DGD	c2	516	52/66	0.88	0.20	37,63,71,75	0
25	CLA	C1	505	65/65	0.89	0.20	43,55,64,68	0
25	CLA	b1	609	65/65	0.89	0.21	42,58,84,104	0
28	UNL	A1	409	14/-	0.89	0.21	44,48,57,68	0
28	UNL	K2	103	5/-	0.89	0.40	79,83,88,90	0
29	LMG	M1	101	31/55	0.89	0.25	41,52,63,70	0
23	BCR	d1	405	40/40	0.89	0.18	38,51,94,99	0
25	CLA	D2	401	65/65	0.89	0.24	43,53,71,76	0
25	CLA	b1	619	65/65	0.89	0.21	48,62,81,85	0
34	DGD	C1	515	52/66	0.89	0.19	36,58,67,71	0
25	CLA	B2	618	60/65	0.89	0.23	59,65,80,85	0
29	LMG	A1	410	43/55	0.89	0.19	52,59,65,76	0
25	CLA	C2	516	46/65	0.89	0.17	70,92,97,100	0
25	CLA	C1	502	65/65	0.89	0.23	51,63,68,70	0
36	PL9	D2	408	55/55	0.89	0.26	43,59,64,74	0
25	CLA	c2	502	65/65	0.89	0.22	60,78,85,90	0
25	CLA	C2	507	45/65	0.89	0.23	73,93,102,113	0
24	CL	A1	402	1/1	0.89	0.15	39,39,39,39	0
25	CLA	C2	504	46/65	0.89	0.18	72,88,95,96	0
38	HEM	V2	201	43/43	0.89	0.25	83,98,102,107	0
25	CLA	c2	507	54/65	0.90	0.22	76,81,86,92	0
25	CLA	B2	604	41/65	0.90	0.33	68,79,92,97	0
25	CLA	C2	511	50/65	0.90	0.18	85,93,100,104	0
27	PHO	D2	407	64/64	0.90	0.21	58,68,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	c1	509	65/65	0.90	0.21	51,62,68,72	0
25	CLA	B1	617	65/65	0.90	0.24	59,67,74,75	0
37	SQD	D2	402	25/54	0.90	0.25	85,90,96,98	0
28	UNL	t1	102	9/-	0.90	0.26	45,57,68,69	0
38	HEM	e2	101	43/43	0.90	0.47	126,145,163,171	0
38	HEM	E1	101	43/43	0.90	0.43	108,134,152,155	0
25	CLA	B1	609	65/65	0.90	0.23	54,71,81,90	0
23	BCR	B2	603	40/40	0.90	0.25	46,59,76,81	0
25	CLA	B2	606	65/65	0.90	0.26	53,67,75,78	0
34	DGD	h1	101	62/66	0.90	0.19	37,48,59,65	0
23	BCR	b2	601	40/40	0.91	0.22	51,61,69,72	0
38	HEM	E2	101	43/43	0.91	0.35	116,132,146,152	0
25	CLA	B2	609	65/65	0.91	0.19	51,67,76,82	0
25	CLA	c2	508	65/65	0.91	0.22	68,78,84,88	0
25	CLA	b2	606	65/65	0.91	0.26	68,77,84,90	0
25	CLA	C1	511	65/65	0.91	0.23	45,56,62,68	0
25	CLA	C1	508	65/65	0.91	0.18	47,66,76,80	0
25	CLA	a1	404	60/65	0.91	0.19	49,57,82,89	0
25	CLA	b2	609	61/65	0.91	0.20	77,89,95,100	0
36	PL9	d1	409	55/55	0.91	0.24	28,41,50,61	0
25	CLA	C1	507	65/65	0.91	0.19	46,67,86,105	0
27	PHO	D1	407	63/64	0.91	0.20	40,56,63,67	0
29	LMG	d1	408	33/55	0.91	0.19	41,50,61,63	0
32	GOL	c1	521	6/6	0.91	0.20	54,56,60,65	0
34	DGD	c1	514	51/66	0.91	0.20	46,54,62,64	0
25	CLA	a2	405	65/65	0.91	0.20	51,60,81,87	0
25	CLA	c2	510	54/65	0.91	0.23	64,69,77,79	0
25	CLA	C1	506	65/65	0.91	0.21	49,62,70,73	0
23	BCR	A2	401	40/40	0.91	0.22	58,84,90,91	0
25	CLA	B2	614	65/65	0.91	0.23	46,58,66,68	0
25	CLA	B2	607	65/65	0.91	0.21	49,59,73,78	0
34	DGD	c1	520	62/66	0.91	0.22	36,59,73,87	0
25	CLA	c1	510	65/65	0.91	0.16	41,54,62,72	0
35	LMT	L1	102	12/35	0.91	0.21	35,45,59,62	0
25	CLA	c2	509	65/65	0.91	0.18	54,70,82,85	0
25	CLA	B2	605	65/65	0.91	0.18	63,71,77,82	0
35	LMT	M1	102	11/35	0.91	0.27	47,52,56,58	0
29	LMG	D1	406	35/55	0.91	0.22	50,57,71,74	0
25	CLA	c1	506	65/65	0.91	0.18	40,54,68,73	0
25	CLA	B1	606	65/65	0.91	0.25	60,71,77,82	0
25	CLA	B2	612	65/65	0.91	0.23	58,64,71,83	0
25	CLA	c1	503	65/65	0.91	0.22	55,66,71,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	c2	511	65/65	0.92	0.22	54,65,72,75	0
25	CLA	b2	617	65/65	0.92	0.19	47,58,65,72	0
25	CLA	c1	505	65/65	0.92	0.21	47,70,79,88	0
32	GOL	a2	415	6/6	0.92	0.46	47,55,59,63	0
34	DGD	c2	517	62/66	0.92	0.16	45,57,70,75	0
25	CLA	b2	612	65/65	0.92	0.17	39,54,64,70	0
23	BCR	B1	601	40/40	0.92	0.20	41,55,65,65	0
25	CLA	C1	509	65/65	0.92	0.20	48,59,71,80	0
25	CLA	A2	404	51/65	0.92	0.16	47,58,70,73	0
25	CLA	c1	513	60/65	0.92	0.19	49,59,71,72	0
25	CLA	b1	611	65/65	0.92	0.17	37,59,68,73	0
29	LMG	d2	407	27/55	0.92	0.17	49,60,64,70	0
33	LHG	B1	621	49/49	0.92	0.22	41,57,67,73	0
23	BCR	h1	102	40/40	0.92	0.21	53,60,67,69	0
33	LHG	L2	101	49/49	0.92	0.21	42,57,70,78	0
25	CLA	b2	611	65/65	0.92	0.29	66,72,80,83	0
25	CLA	B1	612	65/65	0.92	0.21	52,66,71,77	0
25	CLA	B1	607	60/65	0.92	0.20	45,56,68,72	0
25	CLA	c2	506	61/65	0.92	0.21	55,70,77,83	0
27	PHO	d2	408	64/64	0.92	0.19	45,56,62,64	0
34	DGD	C1	517	64/66	0.92	0.17	38,55,75,92	0
25	CLA	d2	405	65/65	0.92	0.20	34,44,61,77	0
27	PHO	A2	407	64/64	0.92	0.23	53,64,72,80	0
27	PHO	a2	416	64/64	0.92	0.20	35,46,53,62	0
25	CLA	c2	505	65/65	0.92	0.18	48,61,71,80	0
33	LHG	d2	403	49/49	0.92	0.22	42,59,69,73	0
25	CLA	B2	619	65/65	0.92	0.17	46,55,63,71	0
34	DGD	c1	518	62/66	0.93	0.19	41,61,69,79	0
25	CLA	b2	624	65/65	0.93	0.21	47,60,75,82	0
36	PL9	D1	408	55/55	0.93	0.25	28,42,52,63	0
25	CLA	C1	510	65/65	0.93	0.24	47,59,77,82	0
25	CLA	b1	616	65/65	0.93	0.19	39,46,57,69	0
23	BCR	a1	401	40/40	0.93	0.20	47,56,64,65	0
23	BCR	B1	603	40/40	0.93	0.17	45,56,78,85	0
25	CLA	c1	507	65/65	0.93	0.21	49,62,72,80	0
26	OEX	A2	406	10/10	0.93	0.10	68,84,93,94	0
25	CLA	c2	503	65/65	0.93	0.22	53,62,83,89	0
25	CLA	B2	615	65/65	0.93	0.16	44,56,73,86	0
33	LHG	D2	405	49/49	0.93	0.20	52,60,66,68	0
33	LHG	d2	406	49/49	0.93	0.20	36,50,59,66	0
25	CLA	c1	504	65/65	0.93	0.21	36,53,83,98	0
25	CLA	B1	619	65/65	0.93	0.20	32,50,57,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	C1	504	65/65	0.93	0.19	49,64,74,77	0
25	CLA	b2	608	65/65	0.93	0.20	65,77,85,86	0
25	CLA	A2	402	65/65	0.93	0.20	47,57,69,77	0
34	DGD	c2	514	62/66	0.93	0.20	47,59,67,69	0
25	CLA	C1	503	60/65	0.93	0.21	38,53,67,73	0
33	LHG	D2	403	49/49	0.93	0.19	45,60,68,73	0
33	LHG	b1	622	49/49	0.93	0.22	36,49,57,69	0
25	CLA	B2	610	65/65	0.93	0.20	44,59,82,86	0
38	HEM	v1	201	43/43	0.93	0.24	60,66,72,75	0
34	DGD	C1	516	62/66	0.93	0.17	44,53,60,61	0
25	CLA	d1	401	65/65	0.93	0.19	30,36,44,47	0
25	CLA	d1	404	65/65	0.93	0.19	31,43,49,51	0
25	CLA	B1	605	65/65	0.93	0.21	60,75,87,88	0
25	CLA	D2	406	65/65	0.93	0.20	45,57,65,67	0
23	BCR	b1	603	40/40	0.93	0.18	40,58,69,77	0
33	LHG	a1	407	43/49	0.93	0.20	36,52,66,70	0
25	CLA	c2	504	65/65	0.93	0.21	46,78,92,100	0
25	CLA	A1	405	55/65	0.93	0.17	38,46,59,65	0
38	HEM	f1	101	43/43	0.93	0.38	62,82,124,136	0
25	CLA	B2	616	54/65	0.93	0.18	43,51,57,59	0
25	CLA	B2	617	65/65	0.94	0.20	52,63,70,74	0
23	BCR	a2	402	40/40	0.94	0.19	33,51,62,67	0
25	CLA	B1	610	65/65	0.94	0.19	46,58,73,76	0
38	HEM	v2	201	43/43	0.94	0.21	47,60,66,78	0
25	CLA	c1	512	65/65	0.94	0.24	36,50,57,60	0
25	CLA	c1	511	65/65	0.94	0.23	38,53,71,78	0
25	CLA	B1	616	65/65	0.94	0.17	39,49,58,66	0
23	BCR	B2	601	40/40	0.94	0.18	41,56,66,68	0
23	BCR	A1	401	40/40	0.94	0.17	36,48,54,58	0
25	CLA	A1	404	51/65	0.94	0.17	37,48,58,70	0
25	CLA	b1	606	65/65	0.94	0.23	44,53,61,63	0
25	CLA	D1	402	65/65	0.94	0.17	31,40,58,63	0
25	CLA	b1	620	65/65	0.94	0.18	31,43,56,60	0
25	CLA	b1	617	65/65	0.94	0.23	47,56,65,68	0
25	CLA	b2	620	65/65	0.94	0.21	42,56,63,72	0
27	PHO	d1	403	64/64	0.94	0.16	32,41,50,54	0
25	CLA	b2	616	60/65	0.94	0.20	51,64,82,82	0
25	CLA	a1	403	65/65	0.94	0.18	29,37,48,51	0
23	BCR	b1	601	40/40	0.94	0.18	36,47,56,57	0
25	CLA	b1	605	65/65	0.94	0.24	38,52,60,66	0
33	LHG	L1	101	41/49	0.94	0.16	30,46,61,85	0
25	CLA	b2	614	65/65	0.94	0.18	51,66,73,75	0

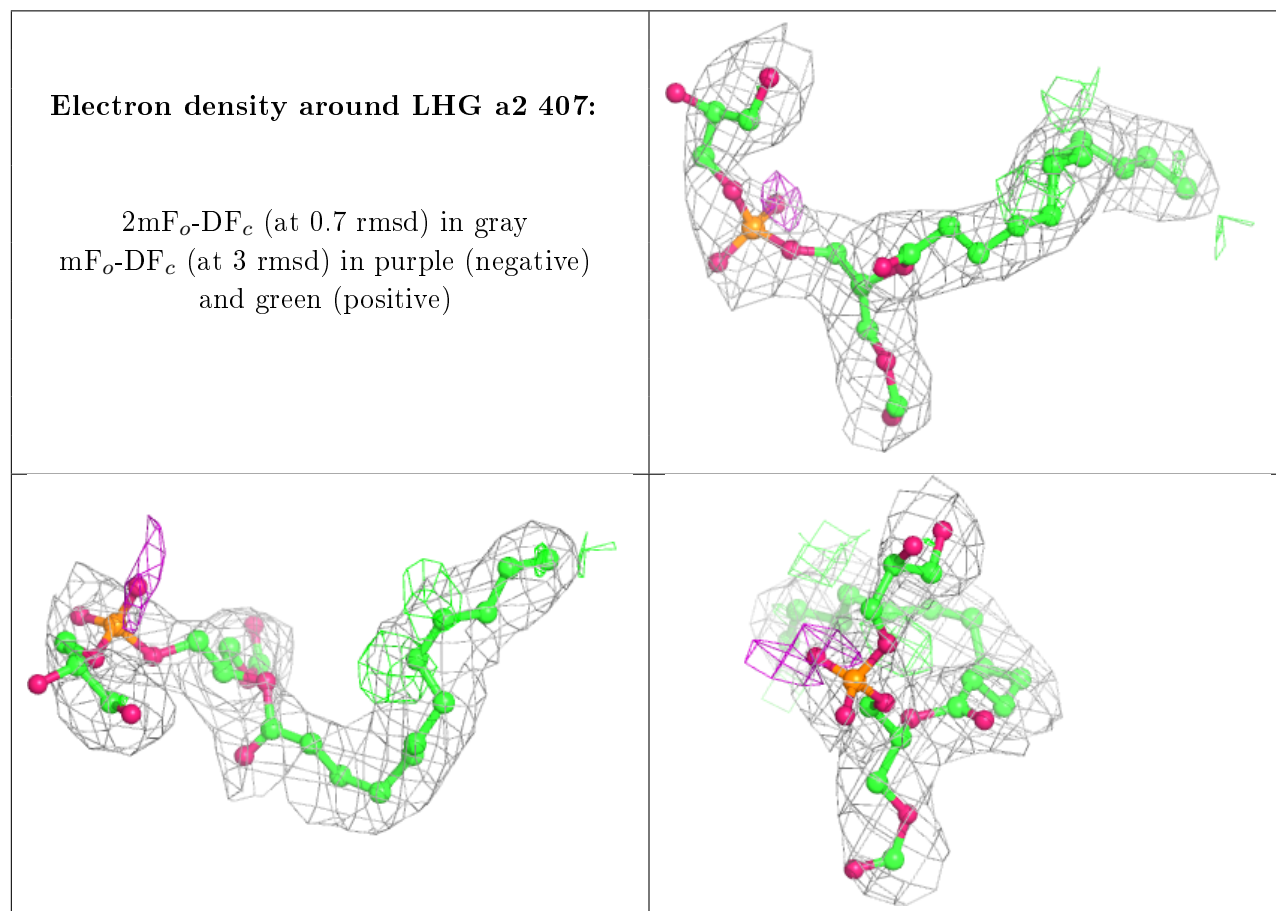
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	d2	402	65/65	0.94	0.18	24,37,48,52	0
25	CLA	B2	608	65/65	0.94	0.22	43,53,70,76	0
25	CLA	b1	613	65/65	0.94	0.17	36,44,54,68	0
25	CLA	b1	607	65/65	0.95	0.20	33,46,69,76	0
25	CLA	b1	610	65/65	0.95	0.16	37,47,56,63	0
25	CLA	a2	404	65/65	0.95	0.17	30,42,52,53	0
33	LHG	l2	101	44/49	0.95	0.16	36,53,66,72	0
27	PHO	a1	411	64/64	0.95	0.17	33,41,47,50	0
25	CLA	B1	615	65/65	0.95	0.18	35,47,73,80	0
25	CLA	b1	615	59/65	0.95	0.16	31,43,58,64	0
25	CLA	B2	613	65/65	0.95	0.16	41,52,68,70	0
25	CLA	a1	405	50/65	0.95	0.14	25,33,49,55	0
25	CLA	A1	406	65/65	0.95	0.19	28,37,46,55	0
38	HEM	V1	201	43/43	0.95	0.21	35,61,66,71	0
25	CLA	a2	413	50/65	0.95	0.14	33,46,57,66	0
25	CLA	b1	608	65/65	0.95	0.20	37,48,58,63	0
25	CLA	b1	614	65/65	0.95	0.20	35,45,54,56	0
25	CLA	b1	612	65/65	0.95	0.21	45,54,60,68	0
27	PHO	A1	408	64/64	0.95	0.18	30,42,50,56	0
33	LHG	D1	405	49/49	0.95	0.18	35,45,54,56	0
25	CLA	B1	614	65/65	0.95	0.19	43,55,62,67	0
25	CLA	B1	613	65/65	0.95	0.18	38,49,57,64	0
25	CLA	B1	608	65/65	0.95	0.18	46,58,71,81	0
24	CL	a1	402	1/1	0.95	0.09	49,49,49,49	0
33	LHG	d1	407	49/49	0.95	0.19	34,44,53,67	0
30	FE	A1	411	1/1	0.96	0.12	52,52,52,52	0
31	BCT	a1	413	4/4	0.96	0.38	43,48,48,50	0
26	OEX	A1	407	10/10	0.96	0.19	45,49,63,68	0
31	BCT	A1	413	4/4	0.96	0.27	54,60,62,63	0
25	CLA	b2	615	60/65	0.96	0.15	45,54,67,74	0
33	LHG	l1	102	49/49	0.96	0.18	25,43,67,75	0
25	CLA	A1	403	65/65	0.96	0.18	27,37,49,54	0
31	BCT	A2	413	4/4	0.97	0.27	65,69,71,72	0
26	OEX	a1	408	10/10	0.97	0.15	39,49,62,70	0
30	FE	a1	410	1/1	0.98	0.19	49,49,49,49	0
31	BCT	a2	417	4/4	0.98	0.27	59,65,67,73	0
24	CL	a2	403	1/1	0.98	0.06	37,37,37,37	0
26	OEX	a2	408	10/10	0.98	0.15	42,49,58,61	0
30	FE	a2	414	1/1	0.99	0.15	57,57,57,57	0
30	FE	A2	411	1/1	0.99	0.18	63,63,63,63	0

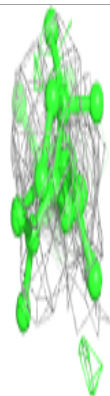
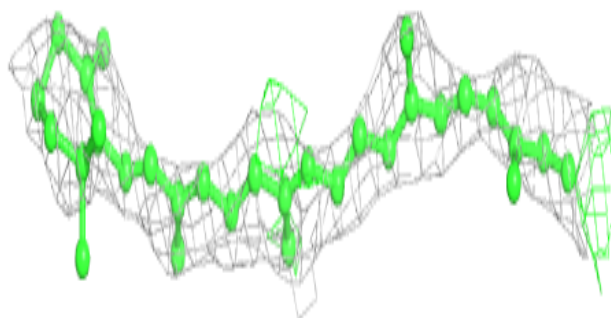
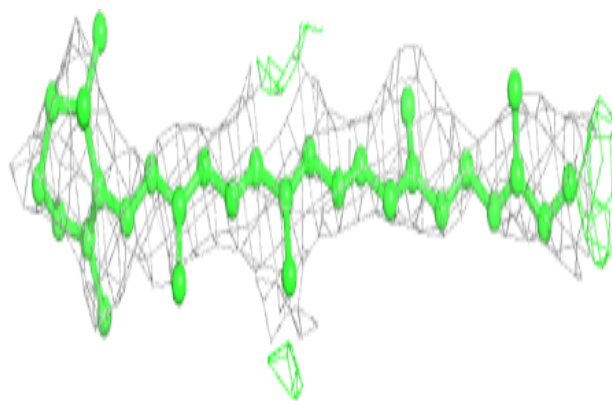
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

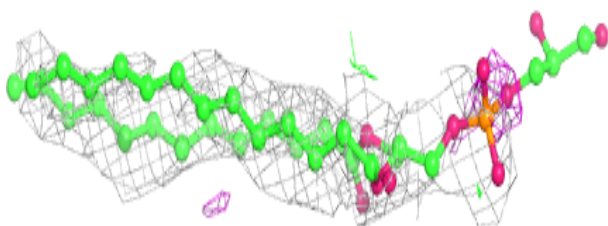
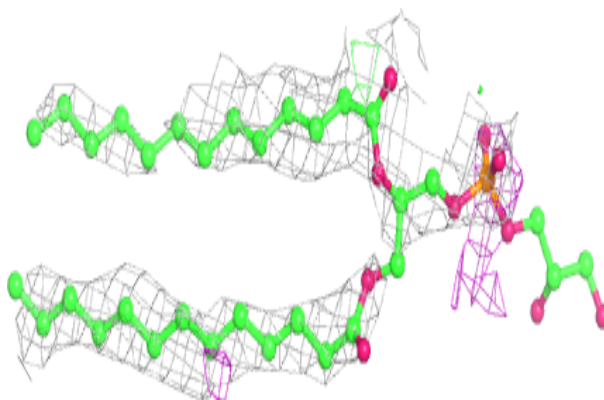


**Electron density around BCR K1 101:**

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

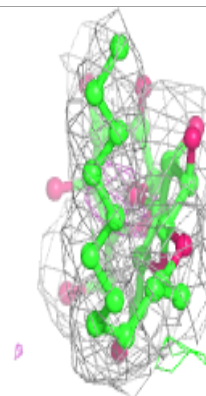
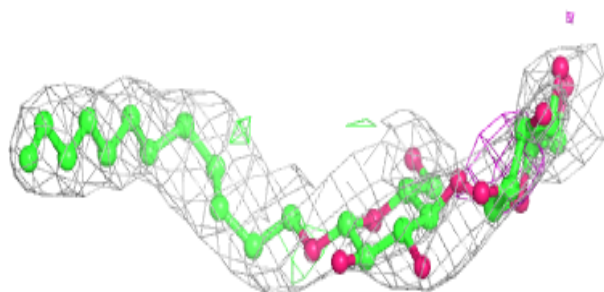
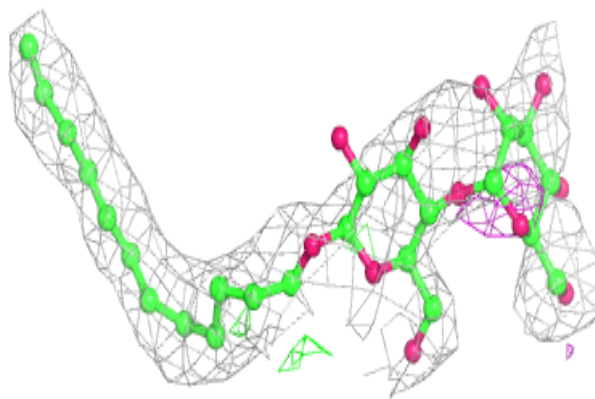
**Electron density around LHG b2 625:**

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

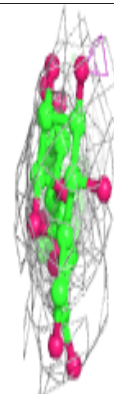
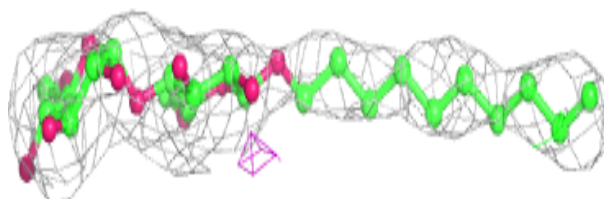
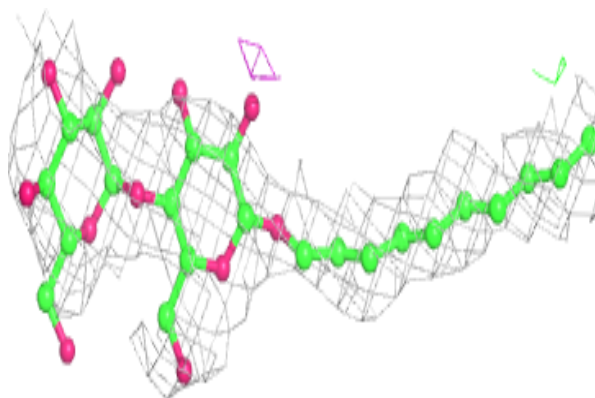


**Electron density around LMT a2 406:**

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

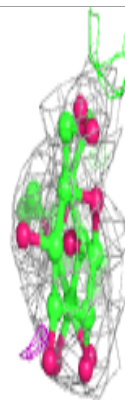
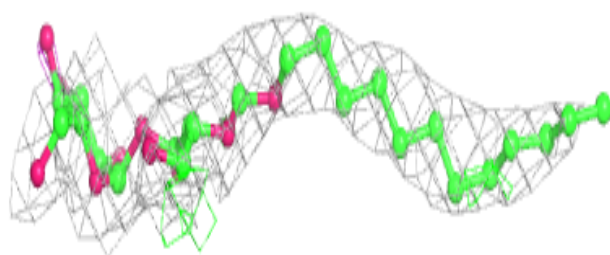
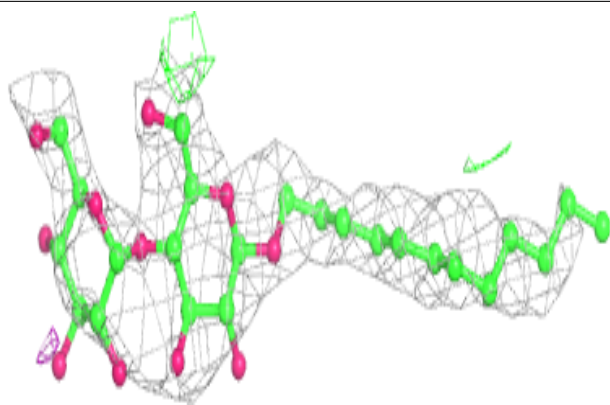
**Electron density around LMT c1 517:**

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

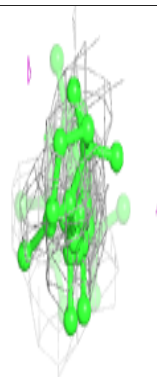
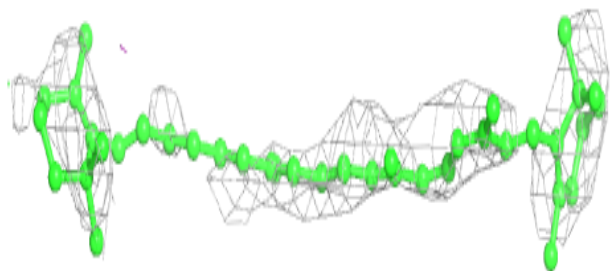
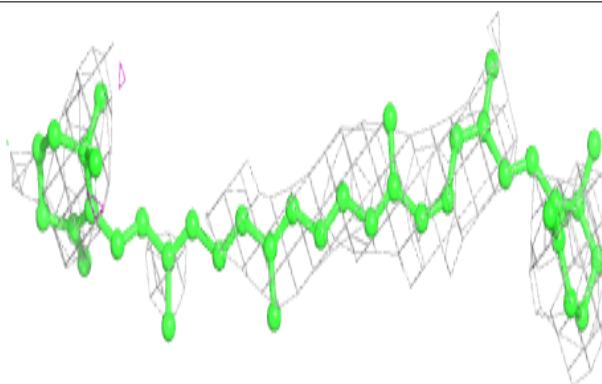


**Electron density around LMT b2 621:**

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

**Electron density around BCR K2 102:**

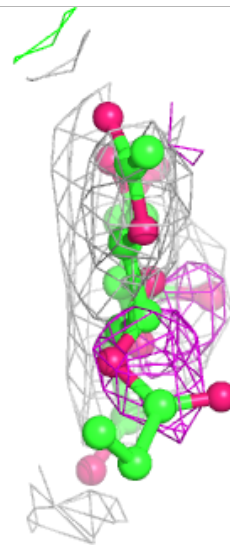
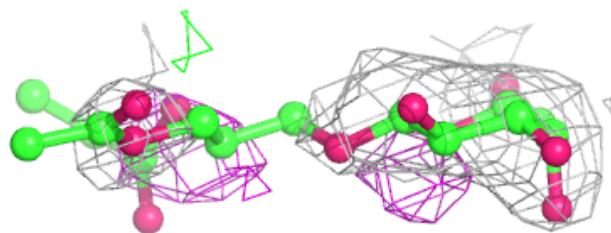
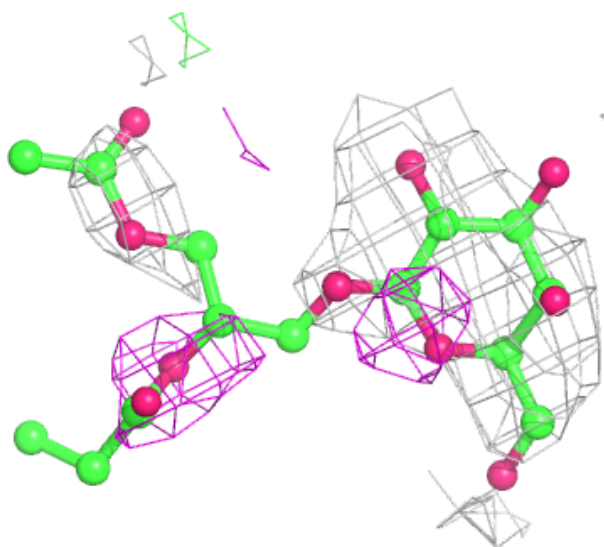
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around LMG C2 515:**

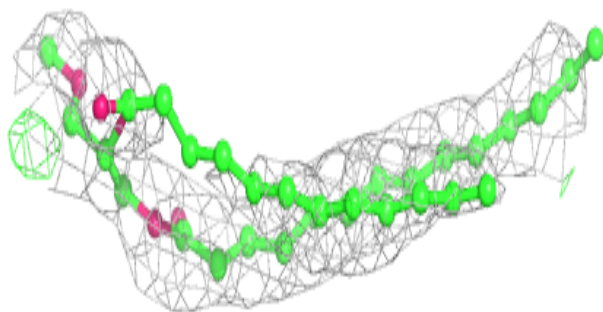
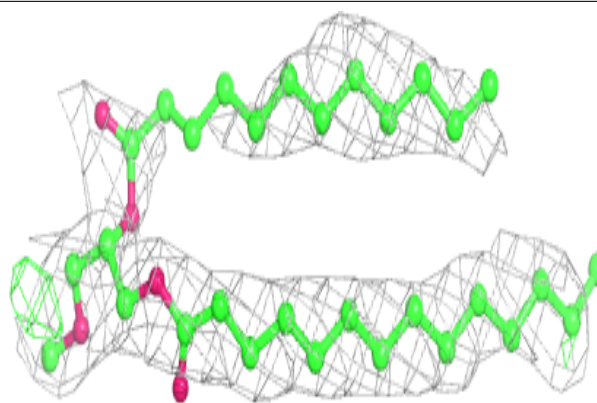
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



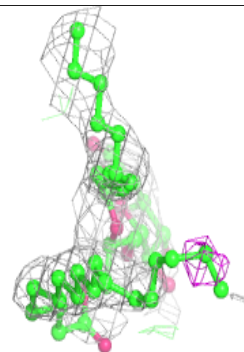
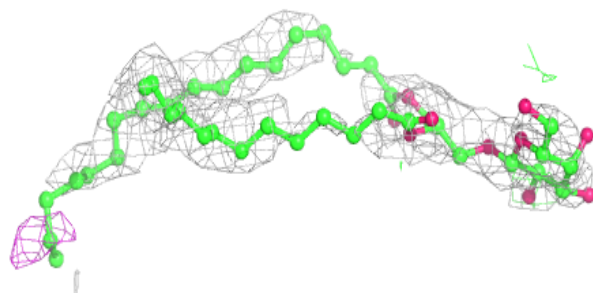
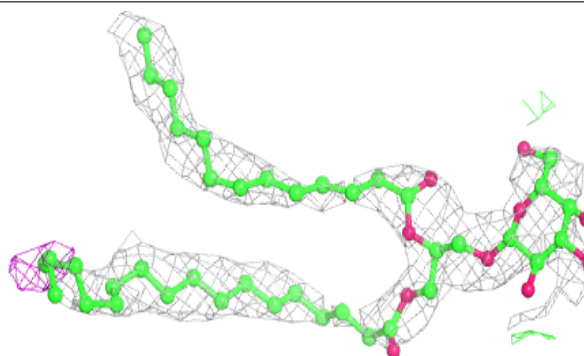


**Electron density around LMG d1 411:**

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

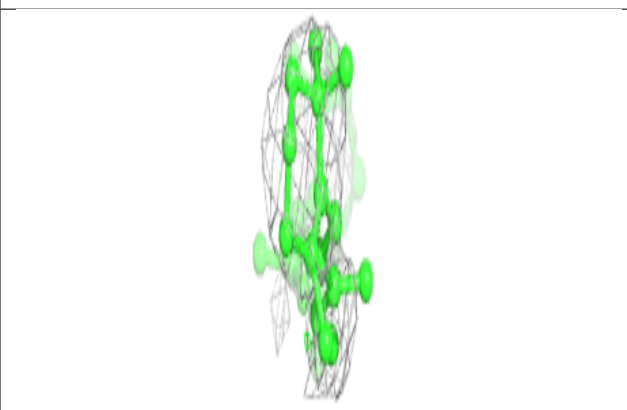
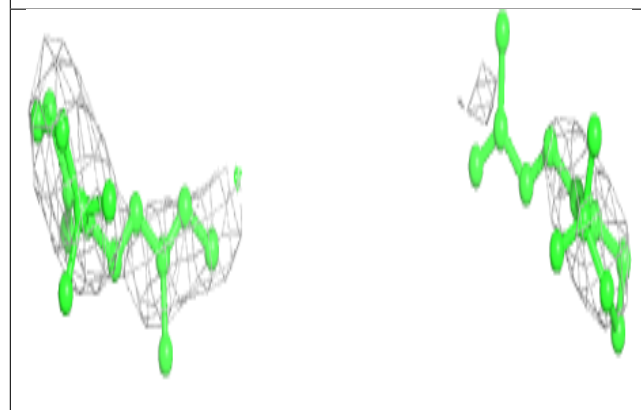
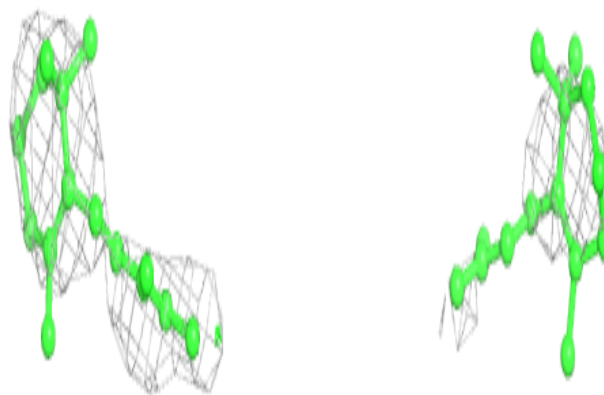
**Electron density around LMG j2 101:**

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

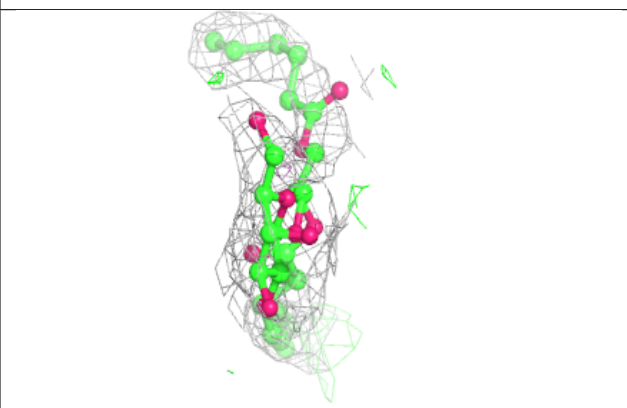
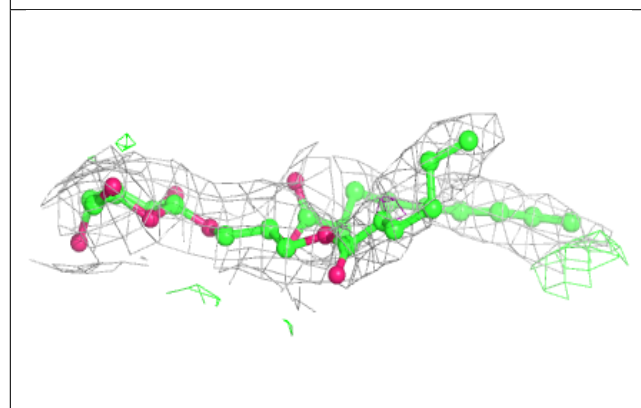
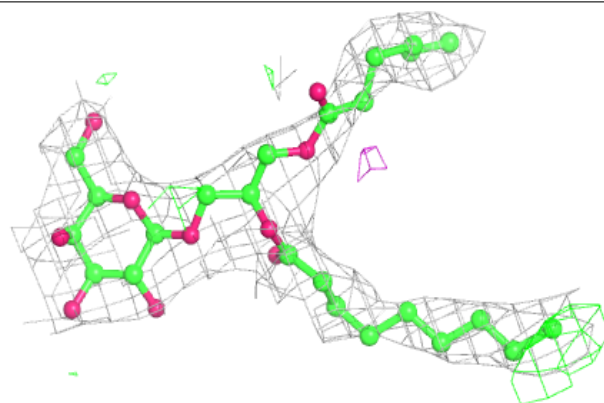


**Electron density around BCR K2 104:**

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

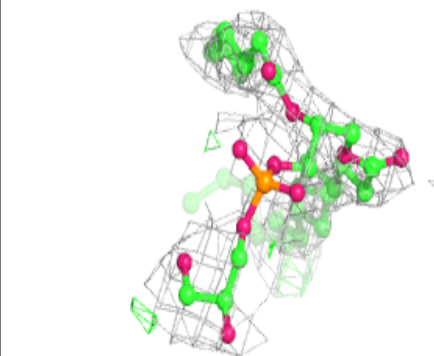
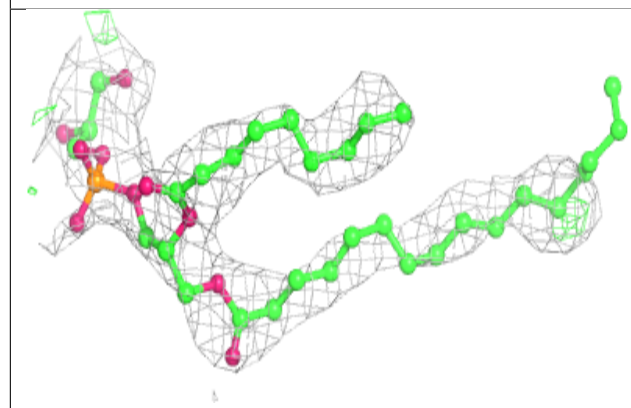
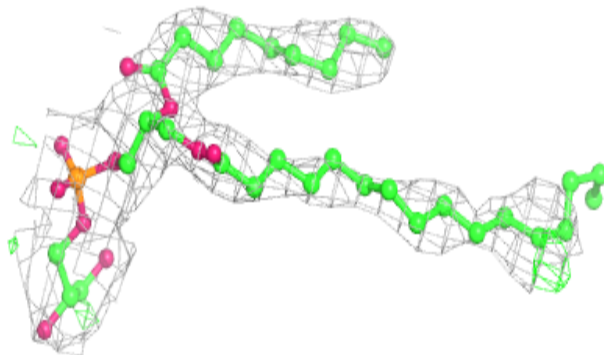
**Electron density around LMG I2 101:**

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

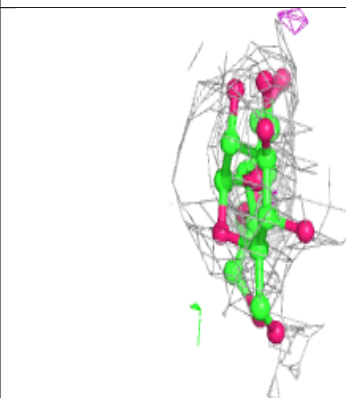
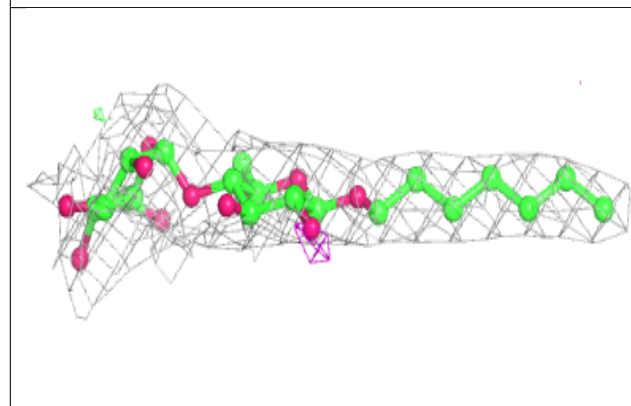
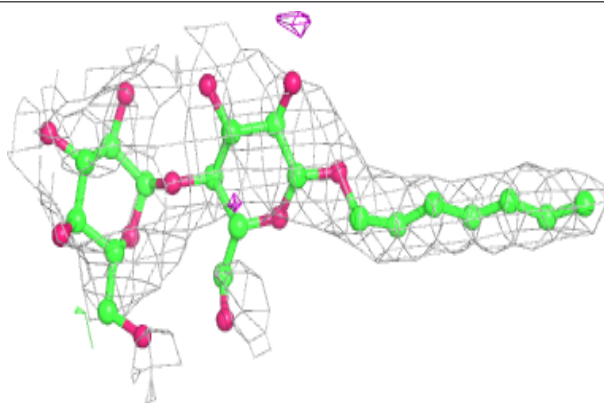


**Electron density around LHG B2 627:**

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

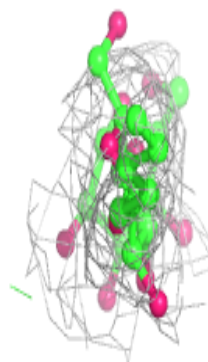
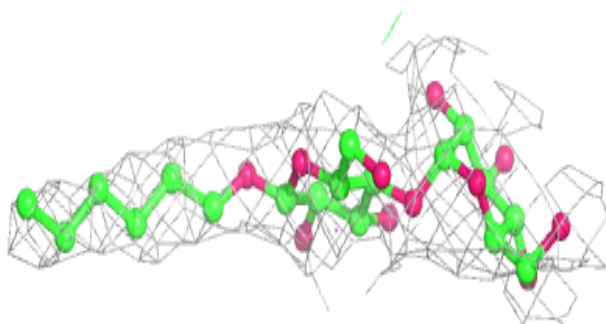
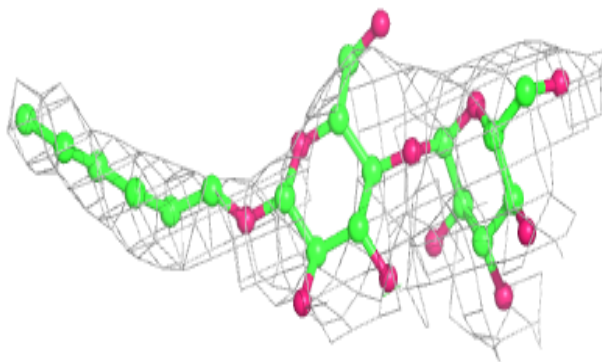
**Electron density around LMT m2 103:**

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

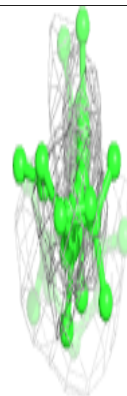
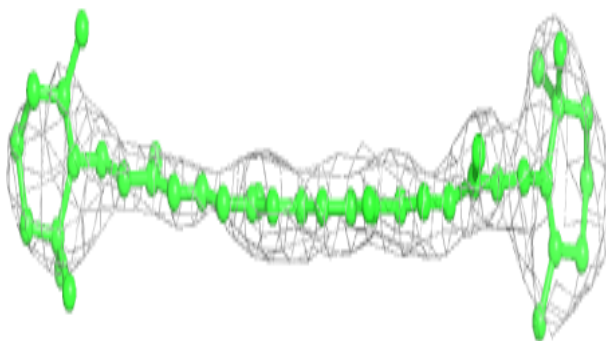
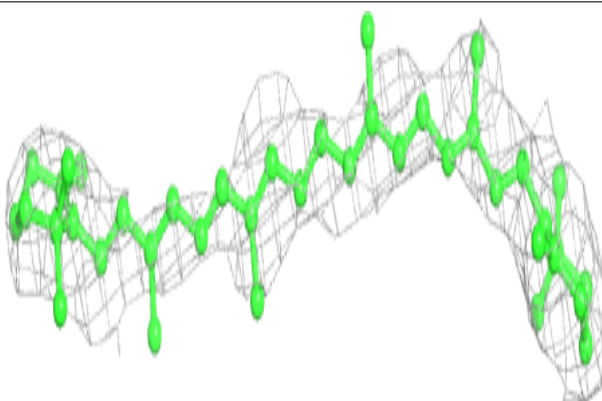


**Electron density around LMT m2 104:**

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

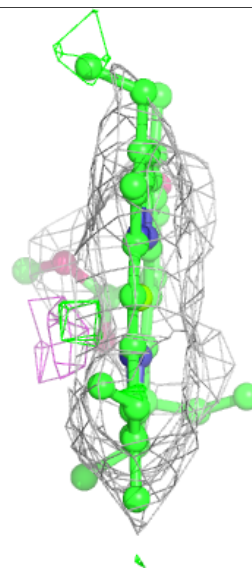
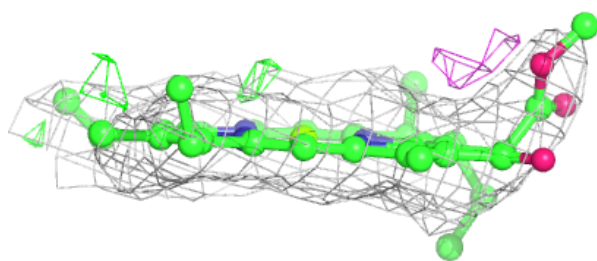
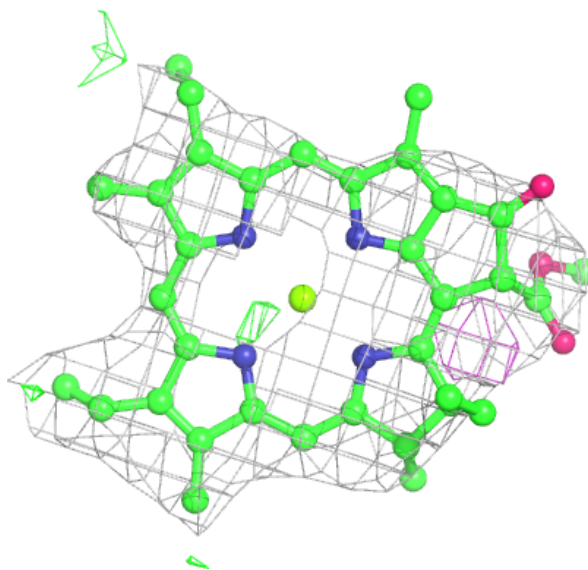
**Electron density around BCR h2 101:**

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



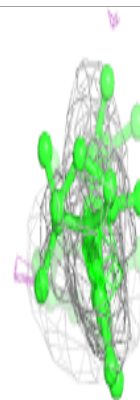
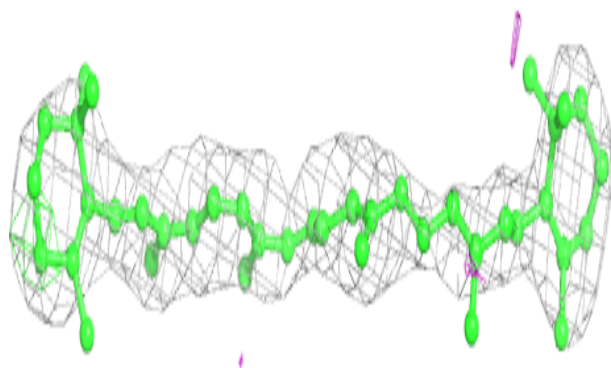
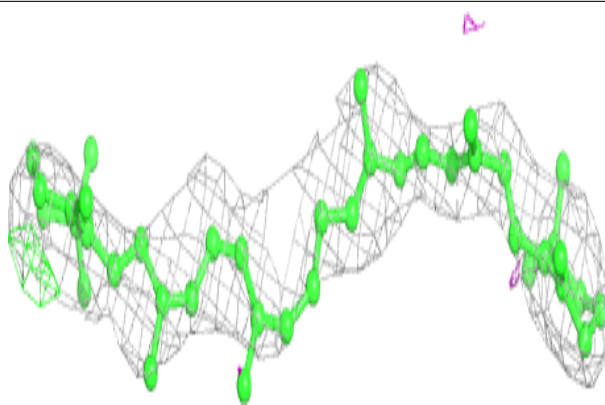
**Electron density around CLA B1 604:**

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

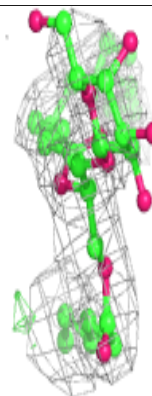
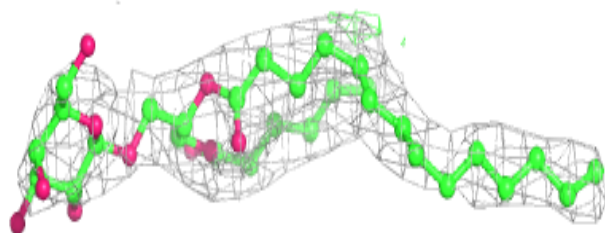
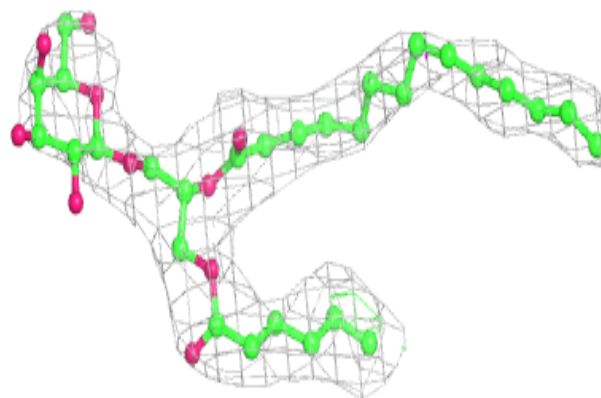


**Electron density around BCR c2 501:**

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

**Electron density around LMG b2 622:**

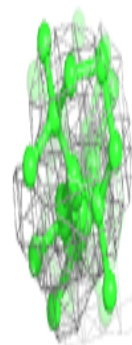
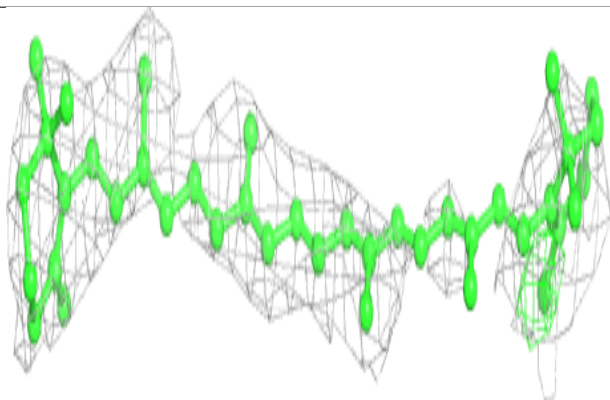
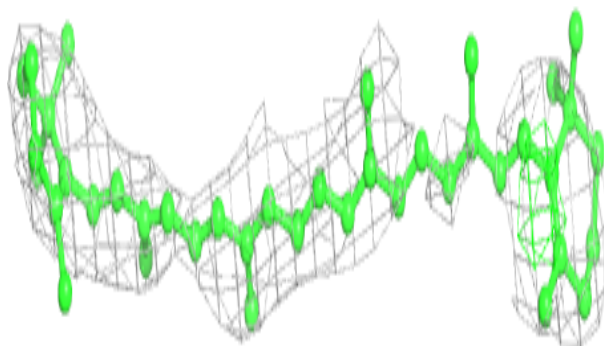
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



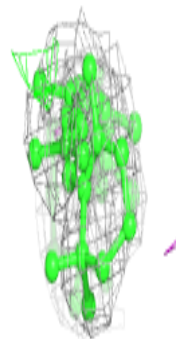
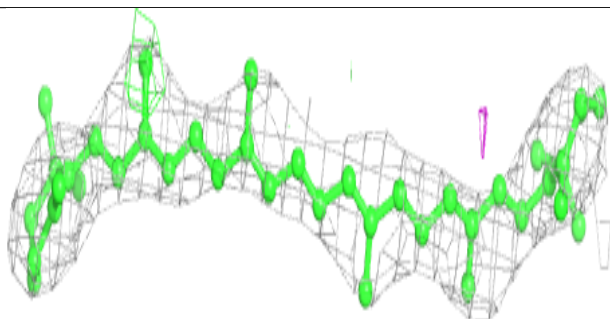
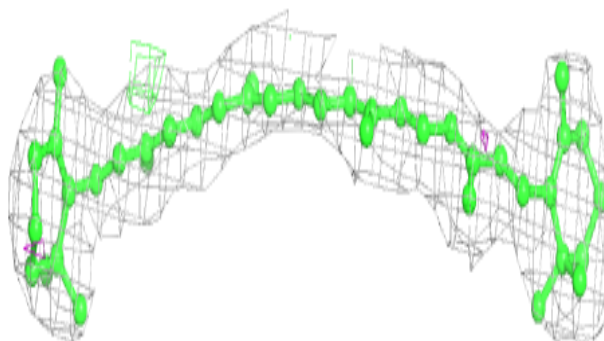


**Electron density around BCR C2 502:**

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

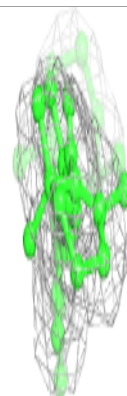
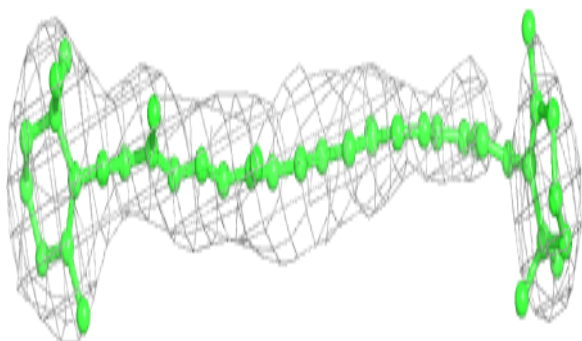
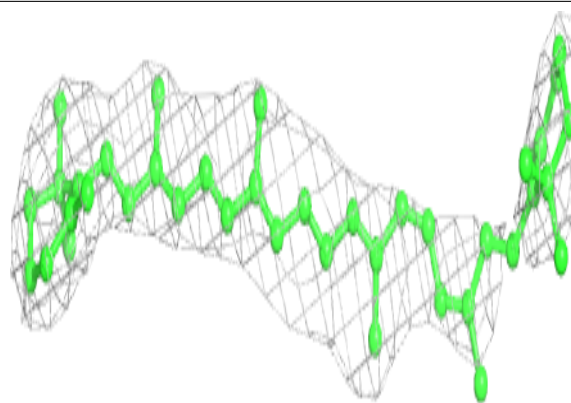
**Electron density around BCR C1 521:**

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

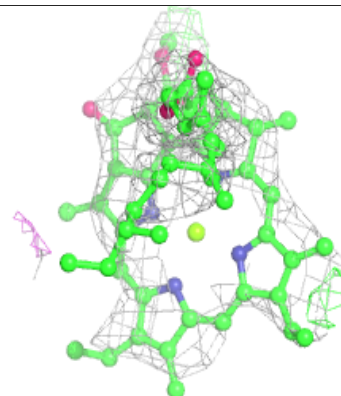
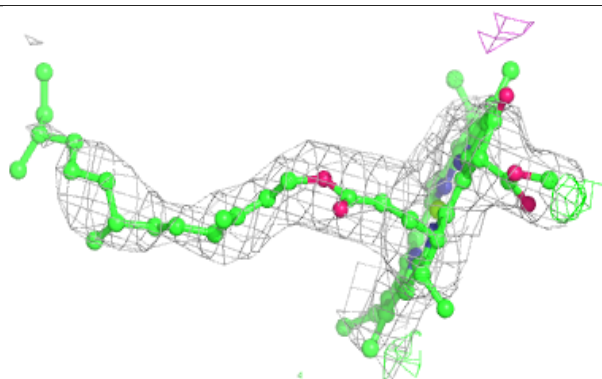
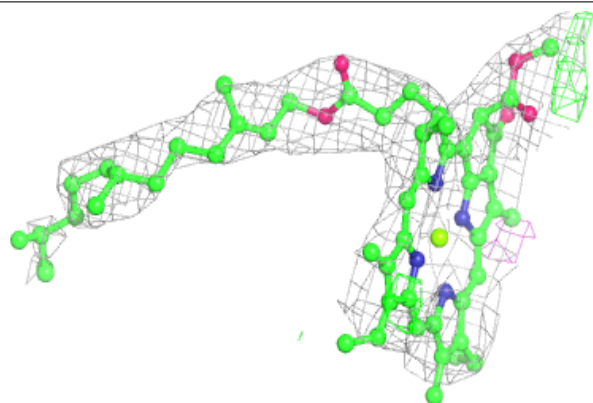


**Electron density around BCR c1 502:**

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

**Electron density around CLA D2 404:**

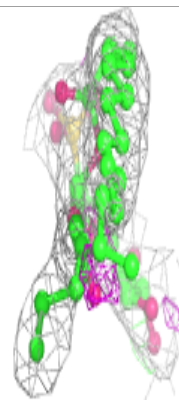
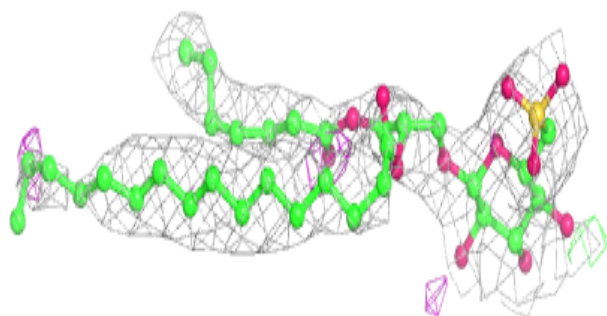
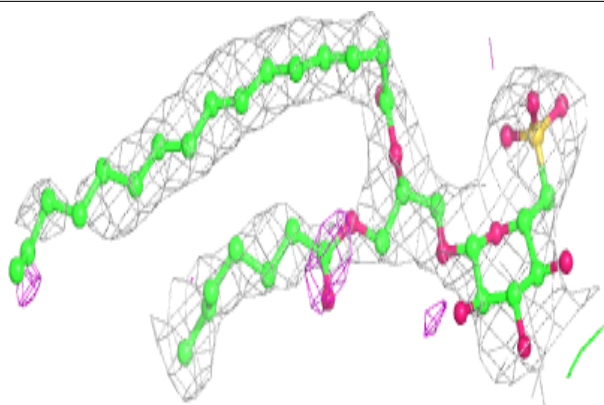
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



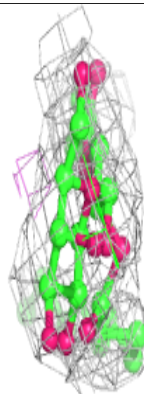
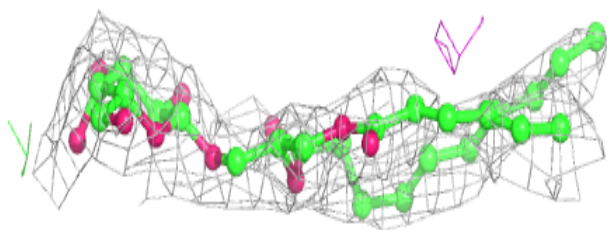
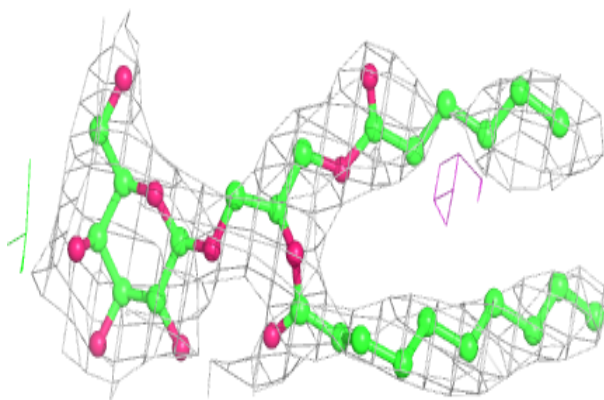


**Electron density around SQD B2 623:**

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

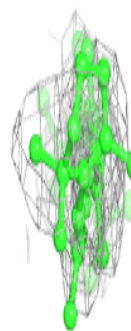
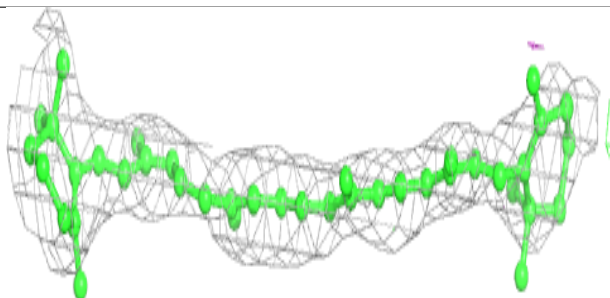
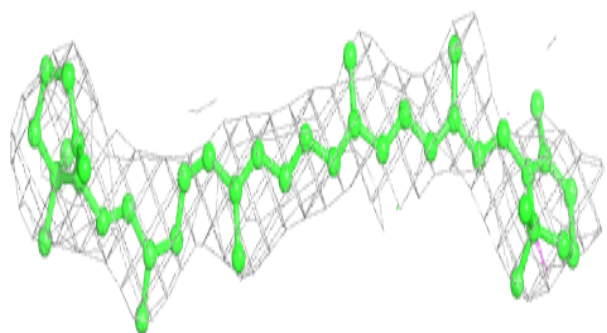
**Electron density around LMG F2 402:**

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

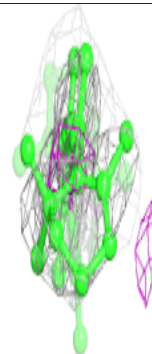
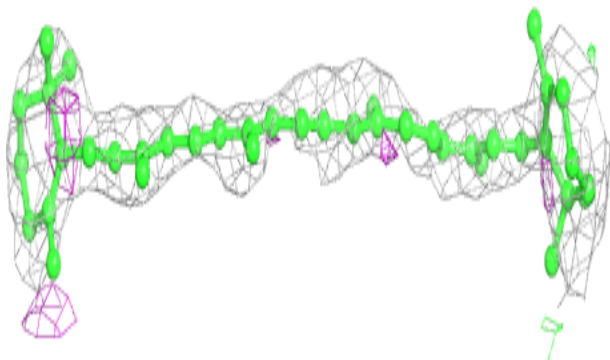
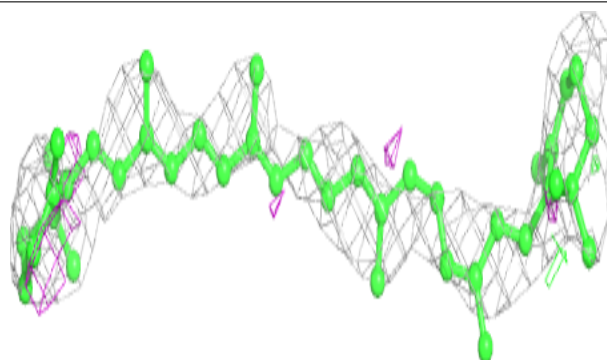


**Electron density around BCR j2 102:**

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

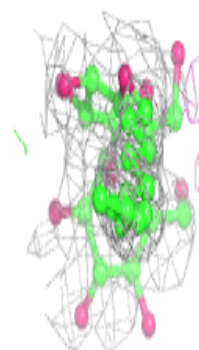
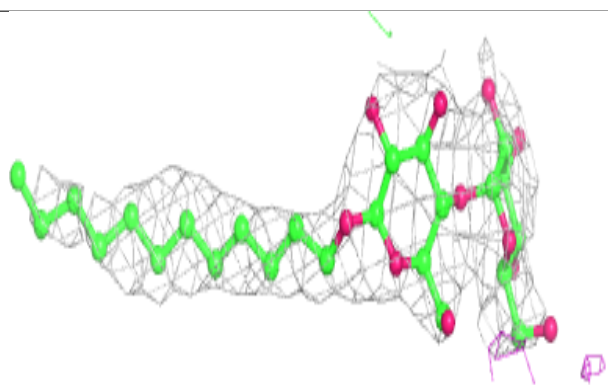
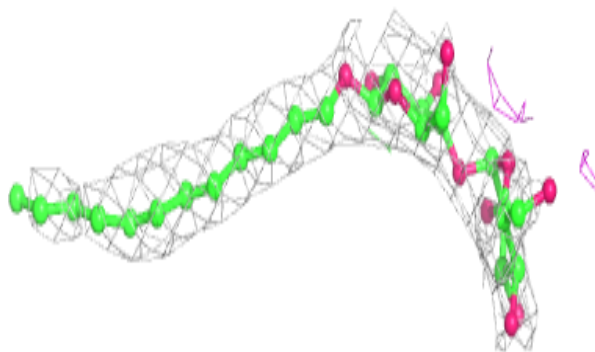
**Electron density around BCR k1 101:**

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

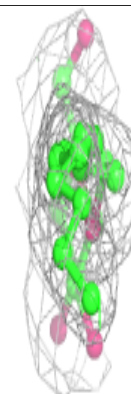
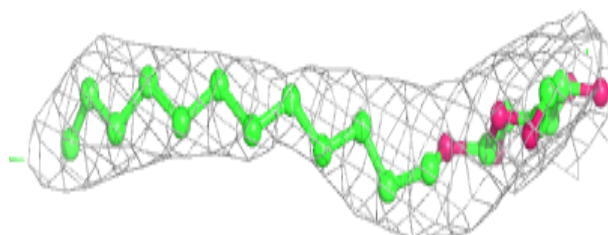
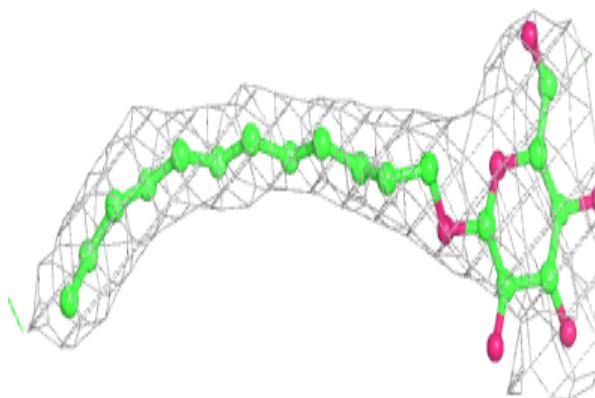


**Electron density around LMT b2 623:**

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

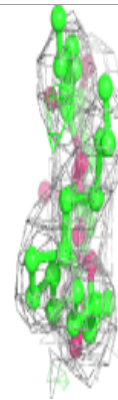
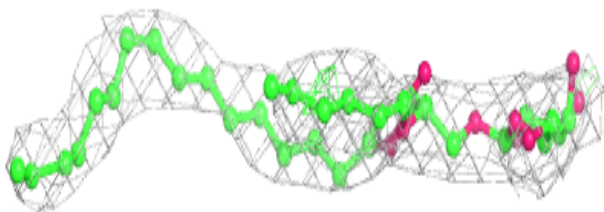
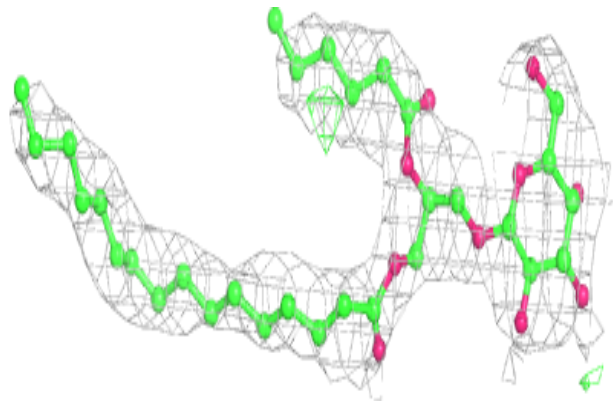
**Electron density around LMT 11 101:**

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

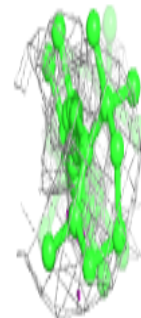
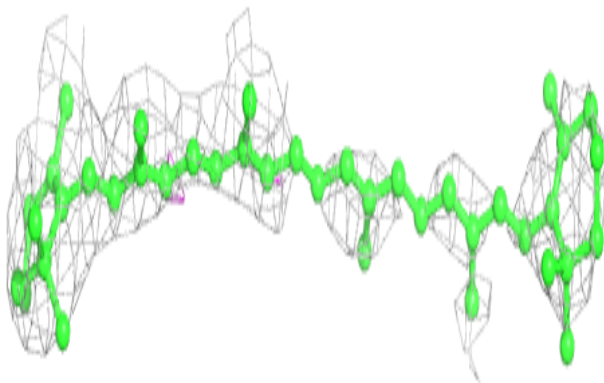
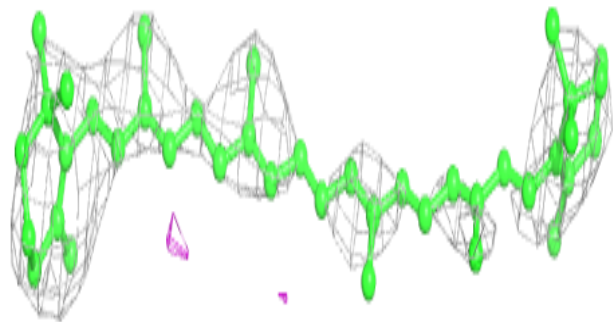


**Electron density around LMG A1 412:**

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

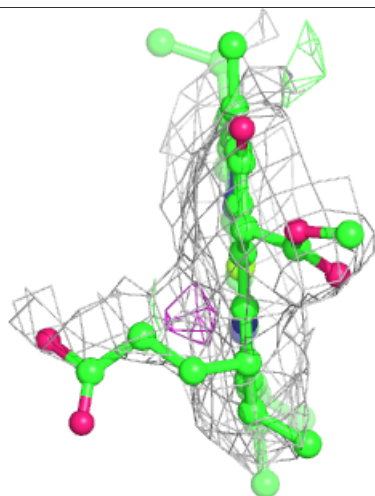
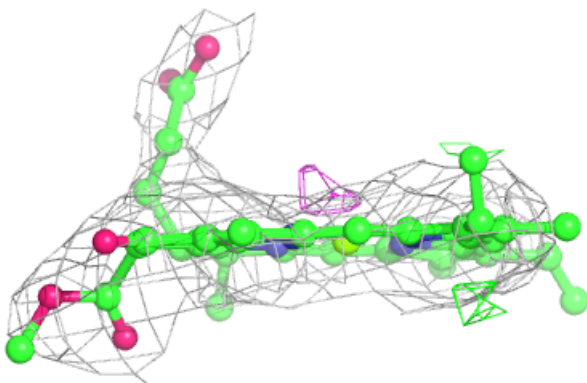
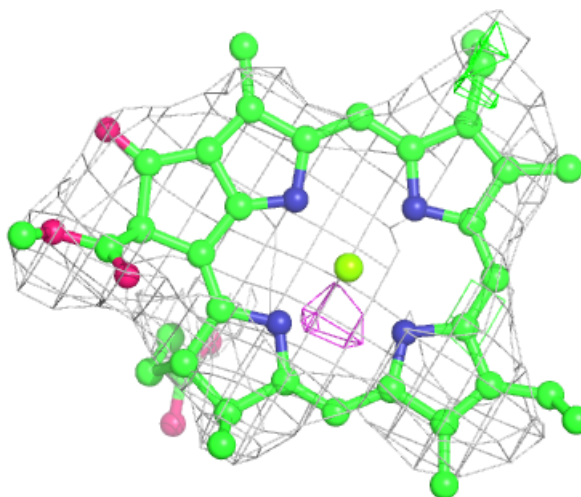
**Electron density around BCR z2 101:**

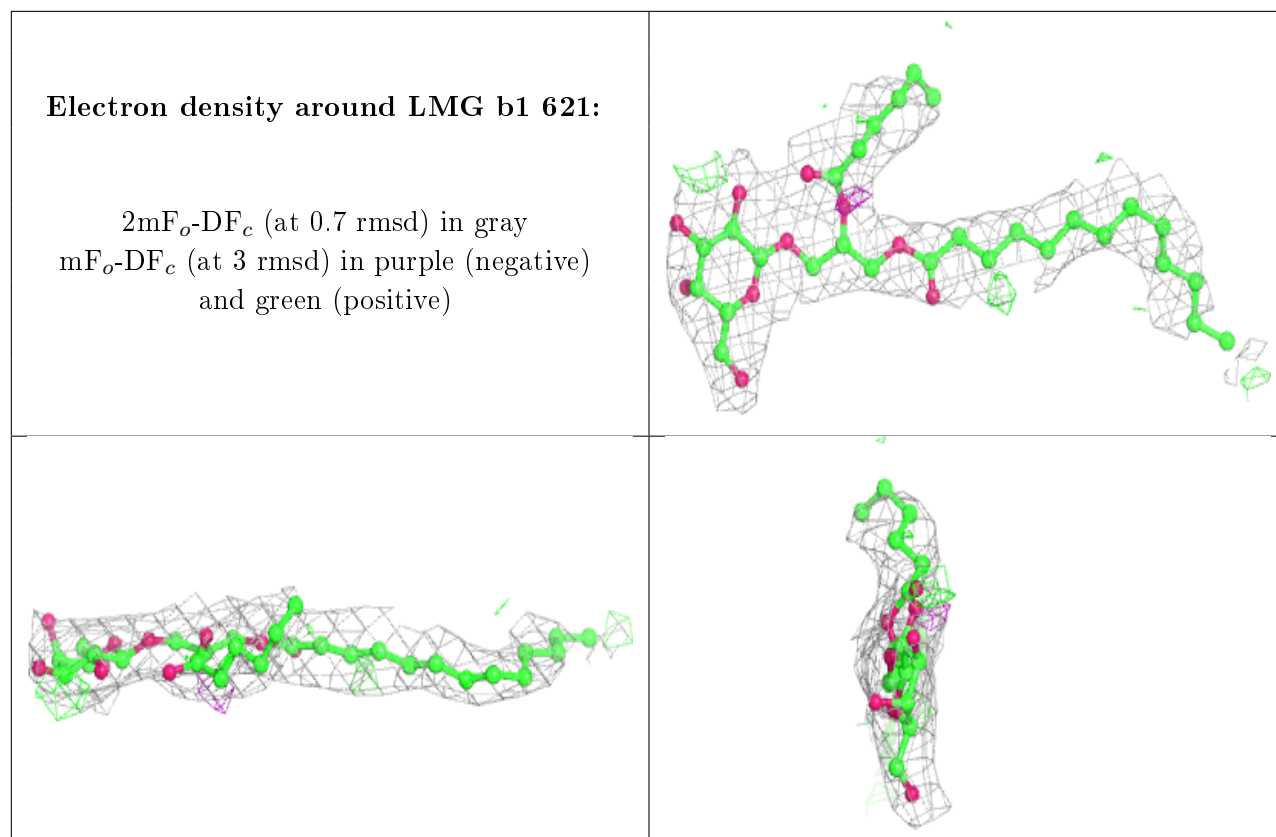
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C2 510:**

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

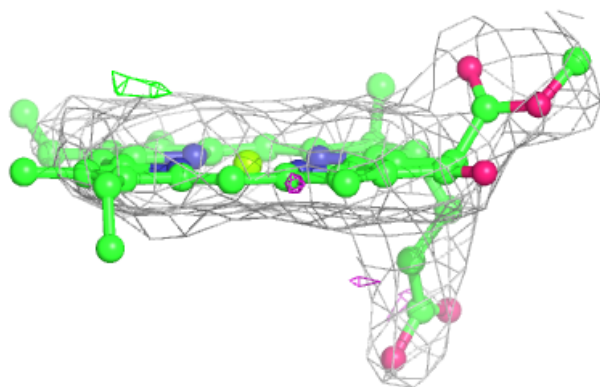
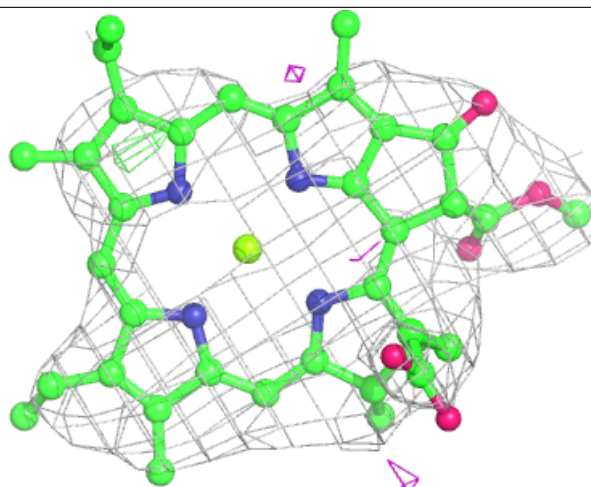


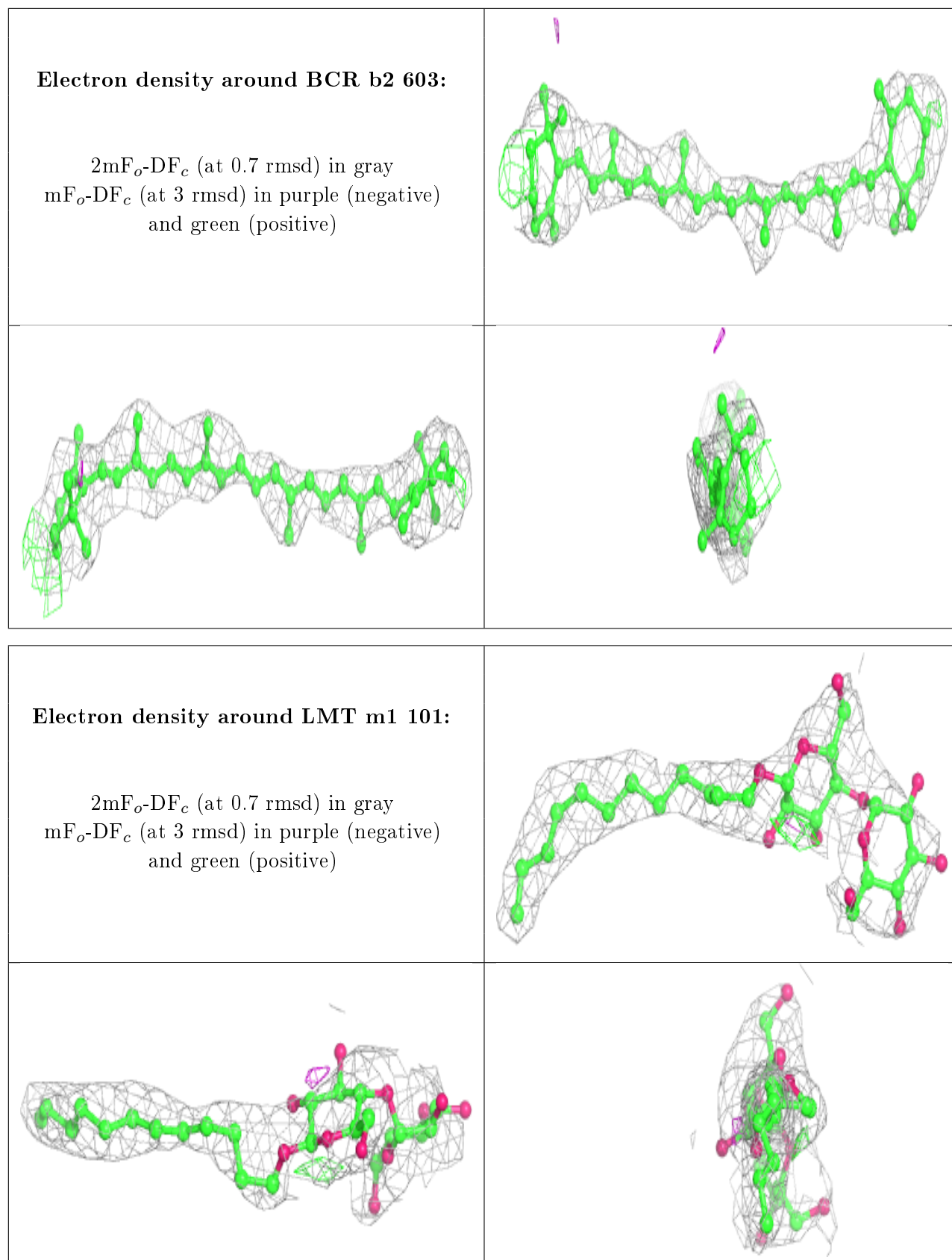




**Electron density around CLA C1 514:**

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

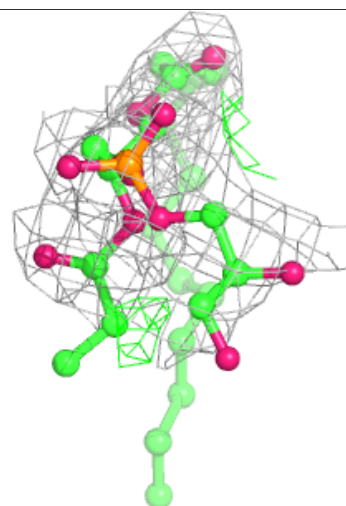
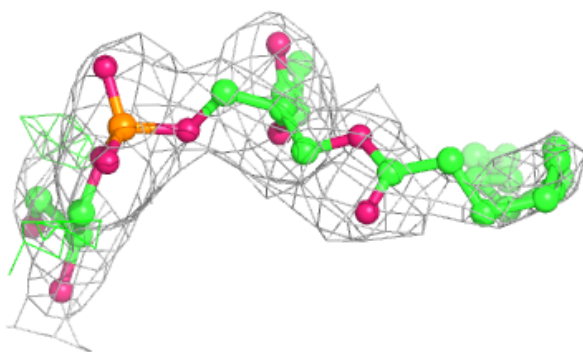
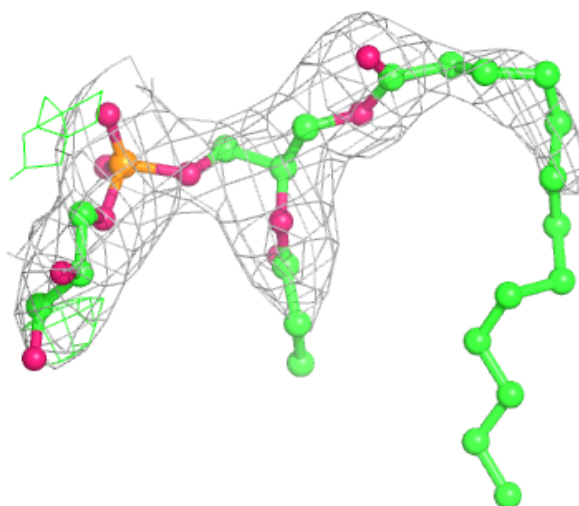






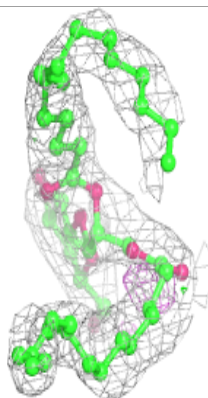
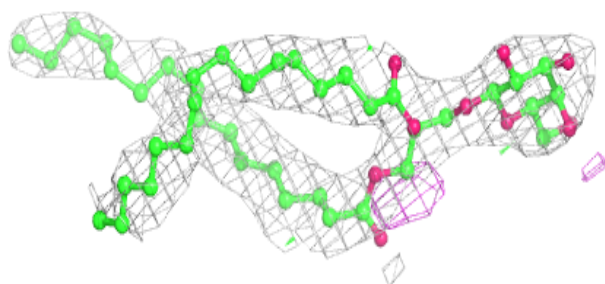
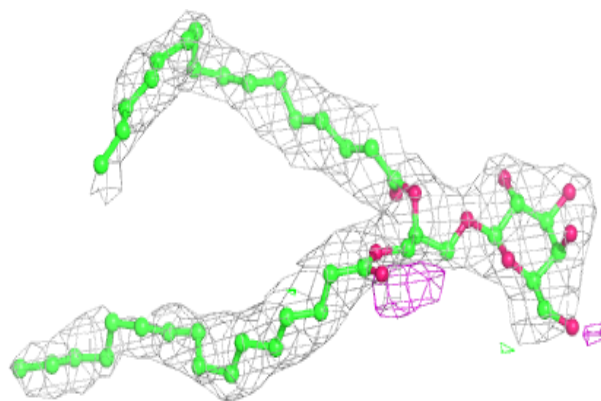
**Electron density around LHG A2 405:**

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

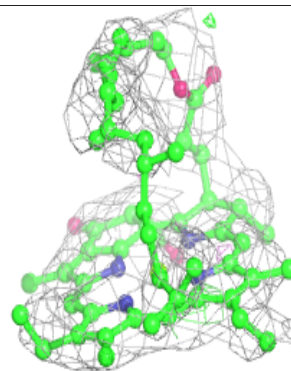
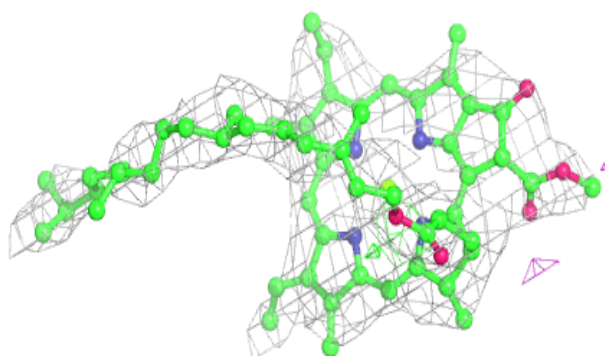
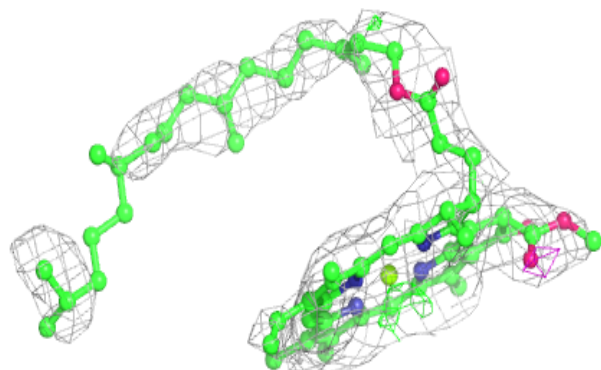


**Electron density around LMG a1 412:**

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

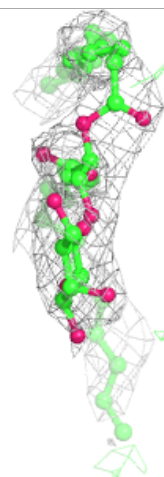
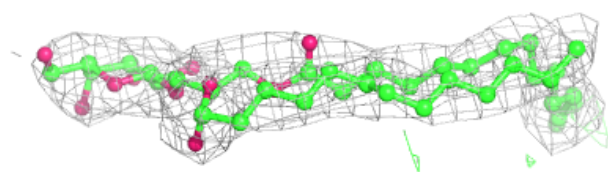
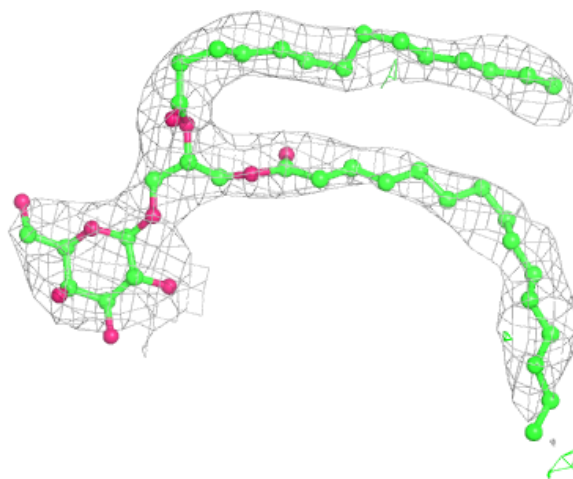
**Electron density around CLA c1 516:**

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



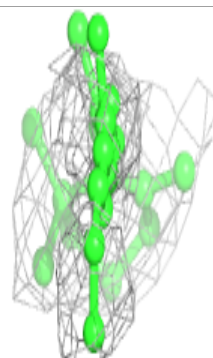
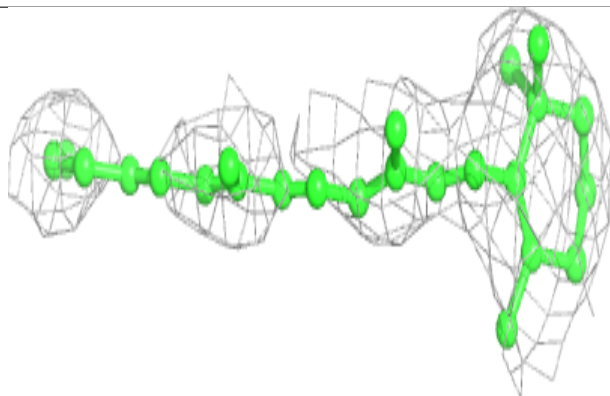
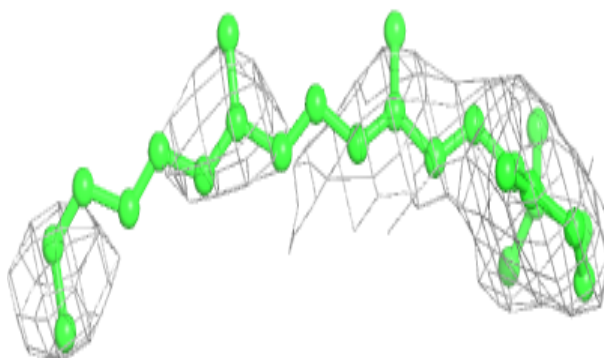
**Electron density around LMG C1 520:**

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

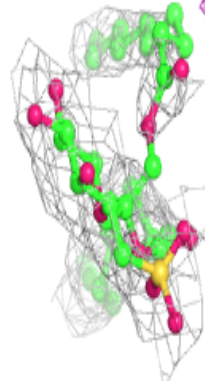
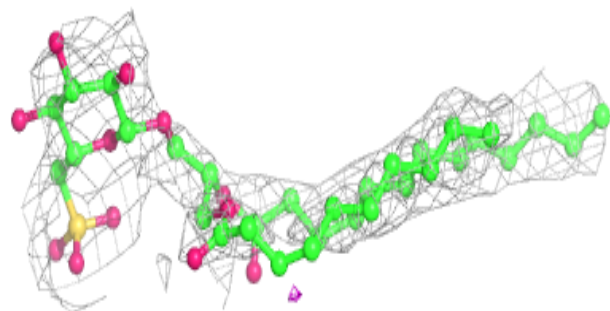
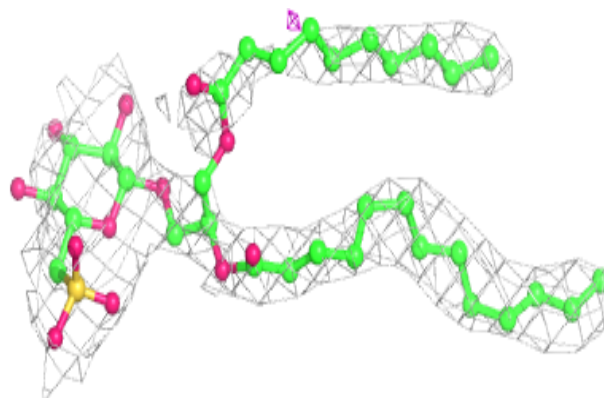


**Electron density around BCR H2 103:**

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

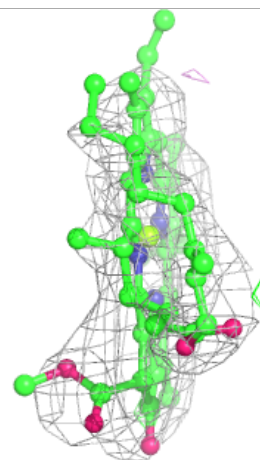
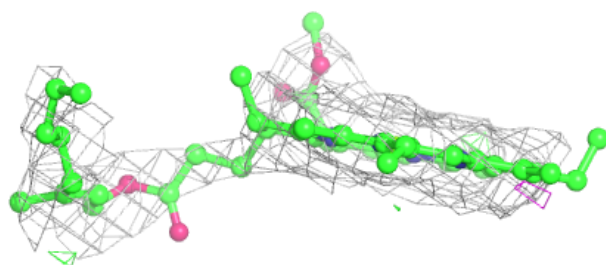
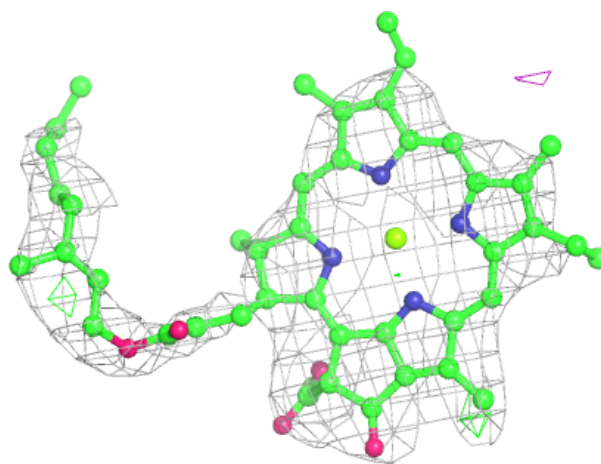
**Electron density around SQD b2 605:**

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



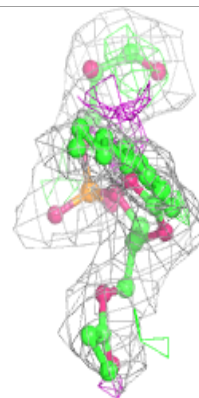
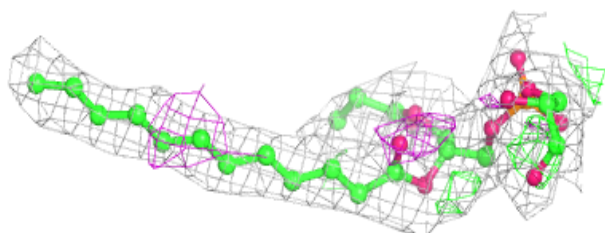
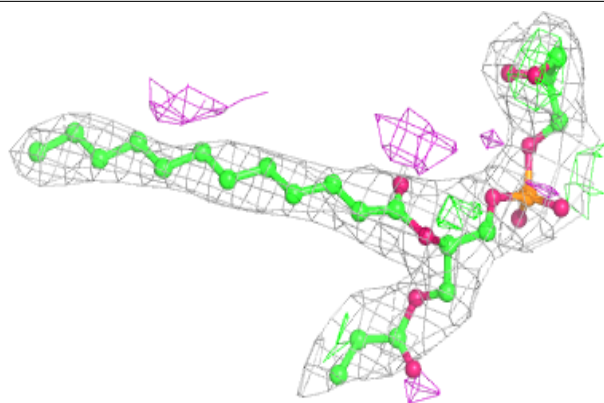
**Electron density around CLA c2 513:**

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

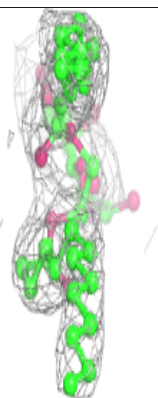
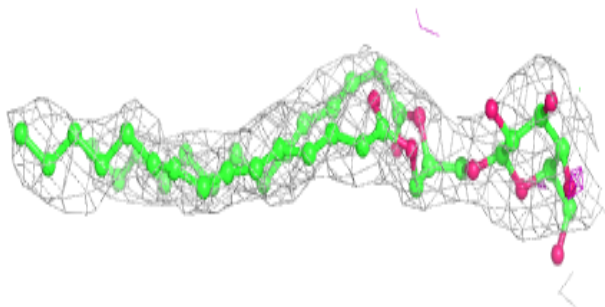
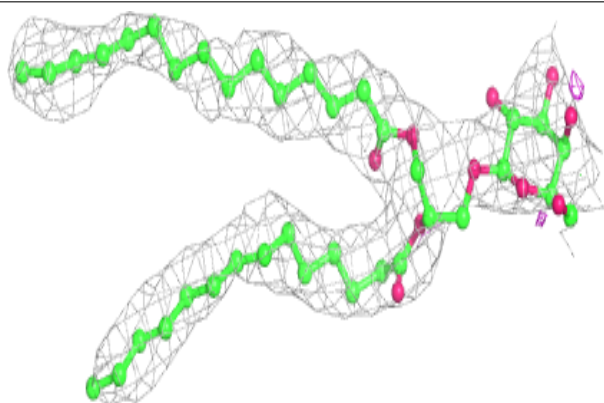


**Electron density around LHG d1 402:**

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

**Electron density around LMG B1 626:**

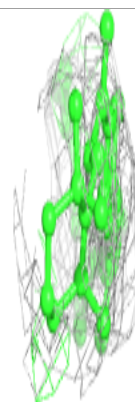
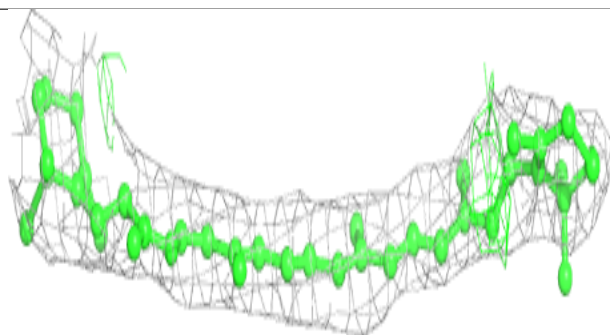
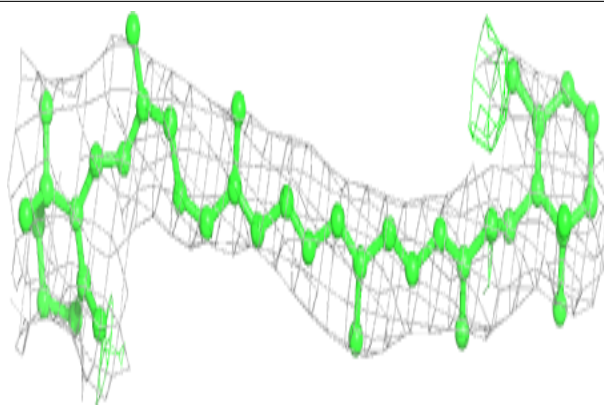
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



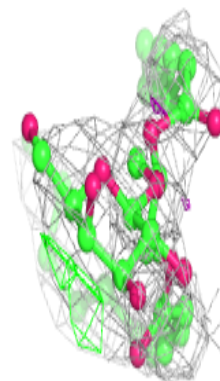
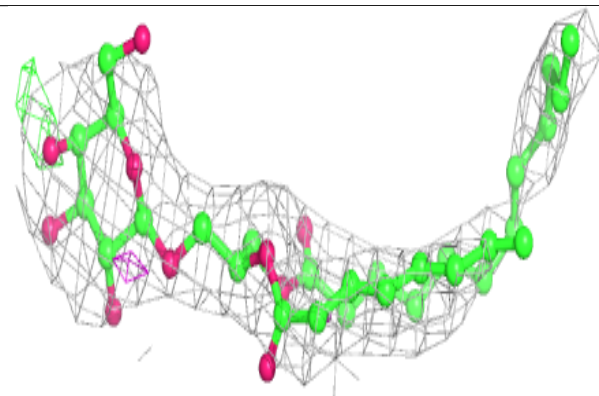
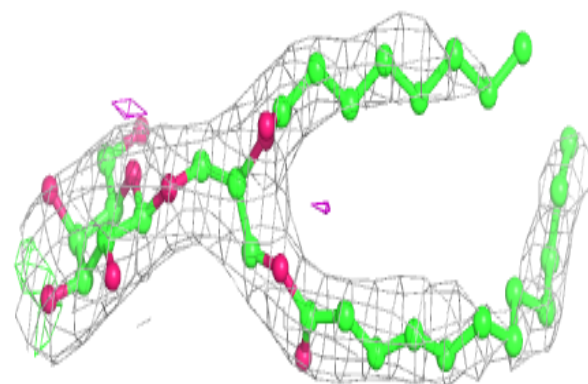


**Electron density around BCR F2 401:**

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

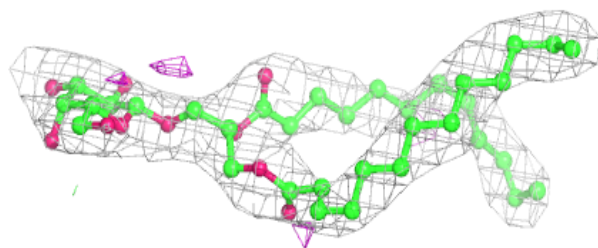
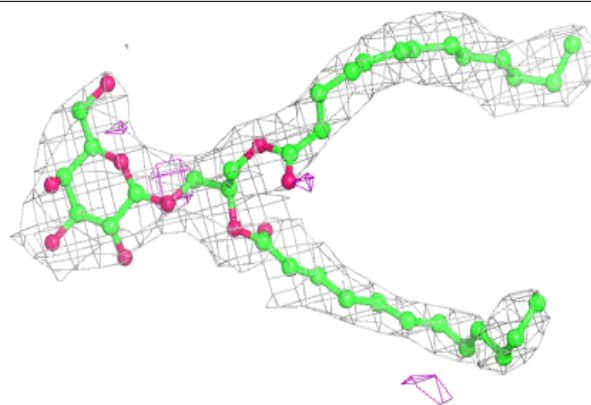
**Electron density around LMG b1 624:**

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

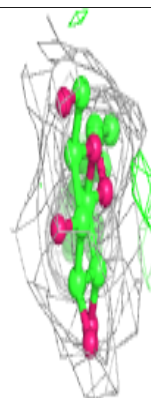
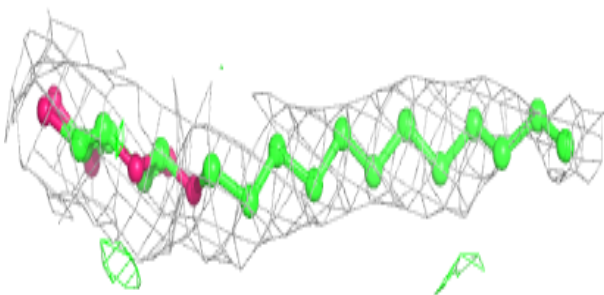
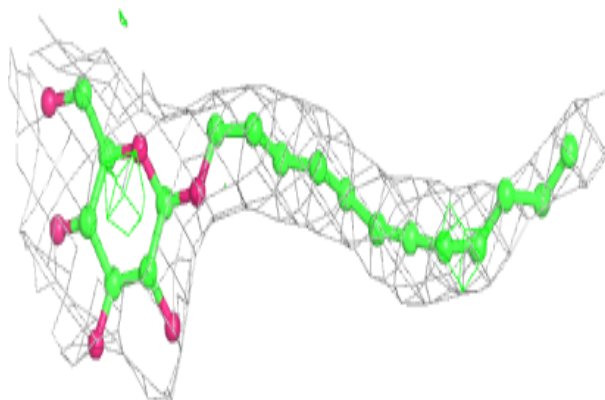


**Electron density around LMG a2 412:**

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

**Electron density around LMT M1 103:**

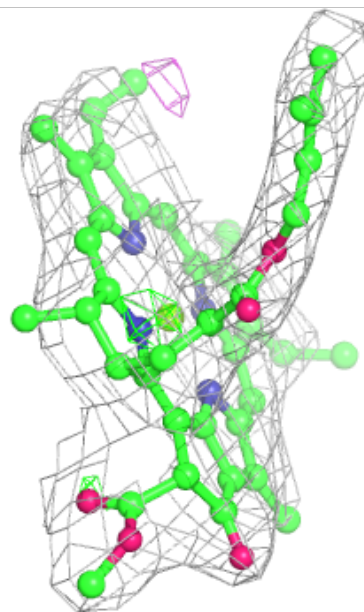
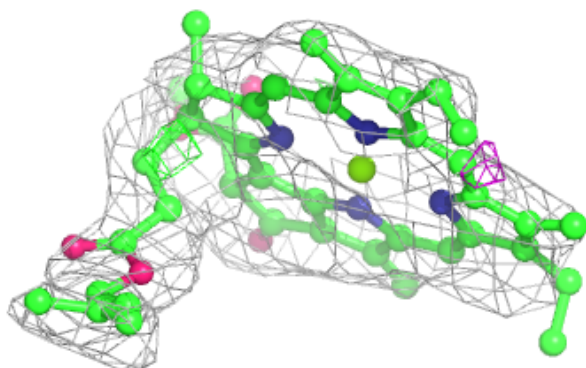
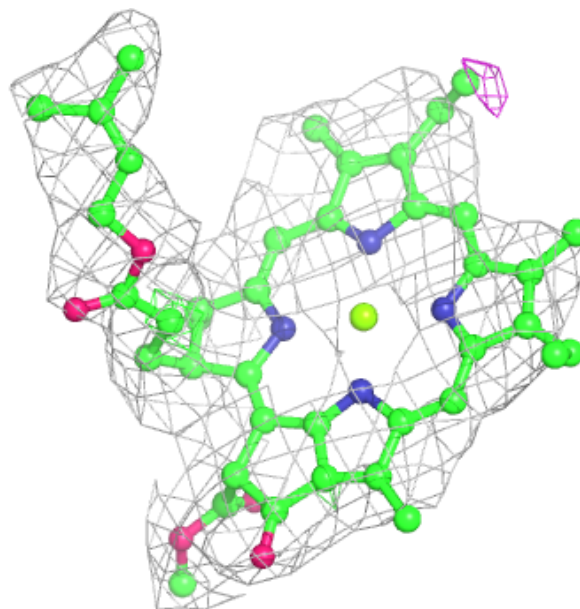
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





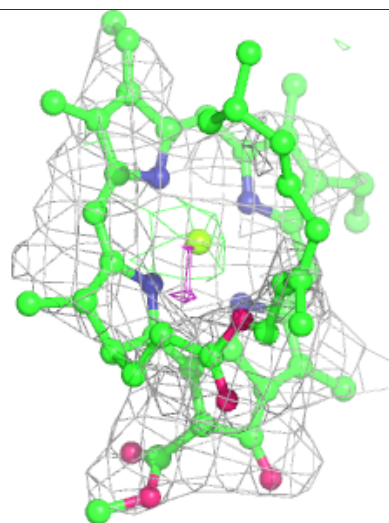
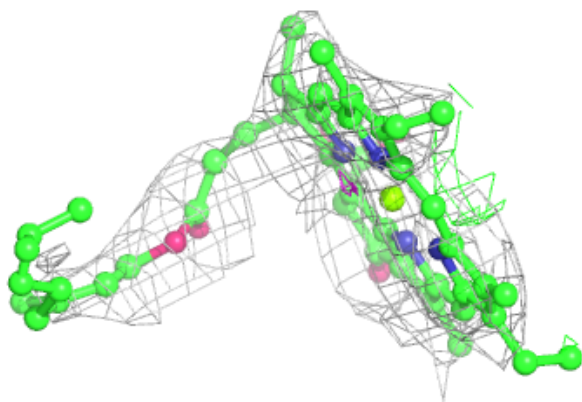
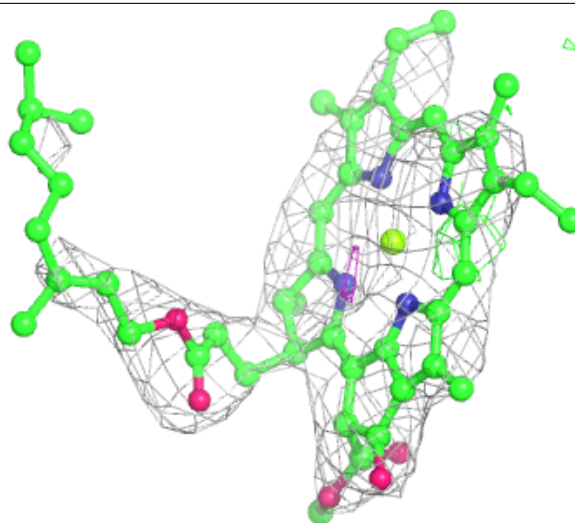
**Electron density around CLA d2 404:**

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



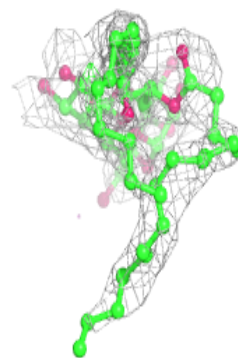
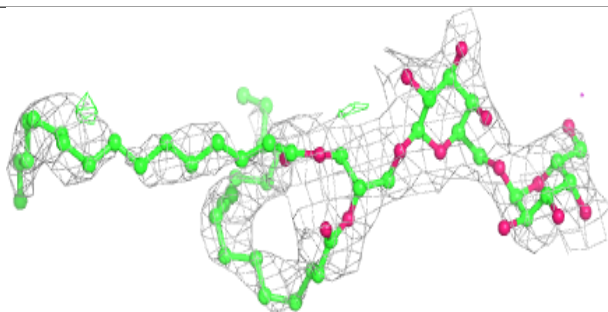
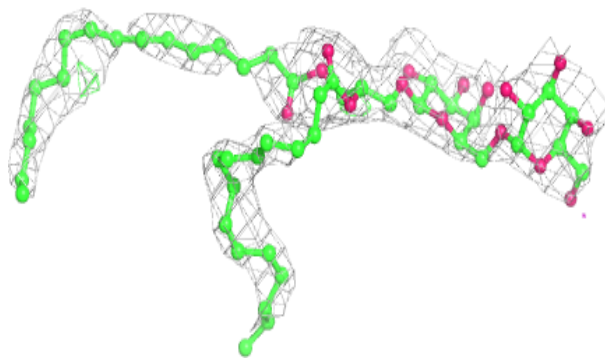
**Electron density around CLA K2 101:**

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



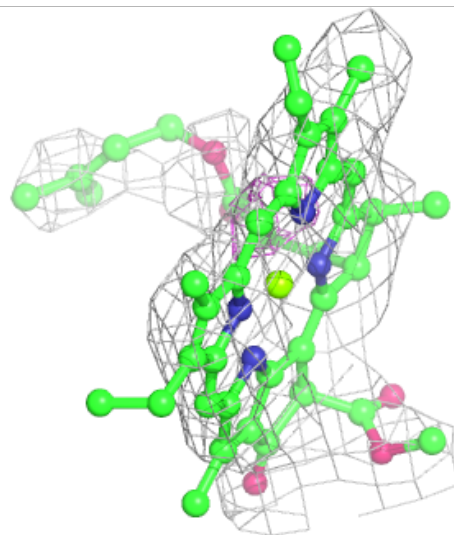
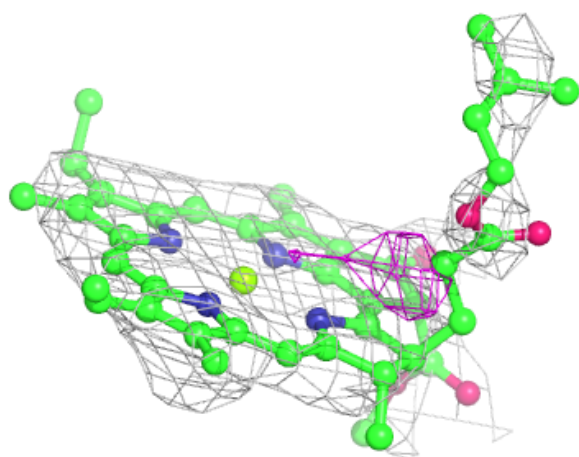
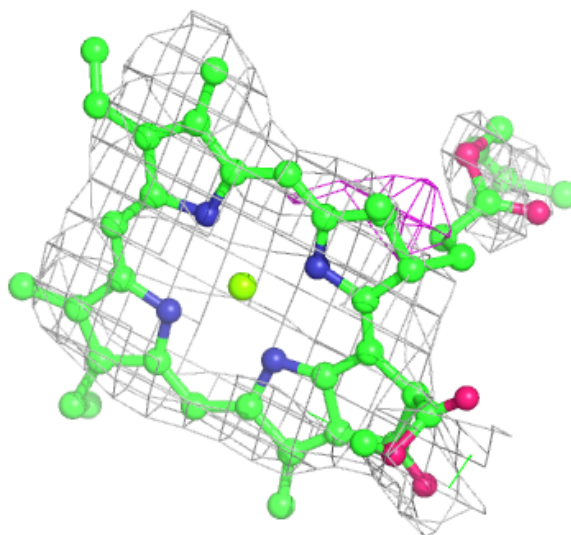
**Electron density around DGD H2 101:**

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



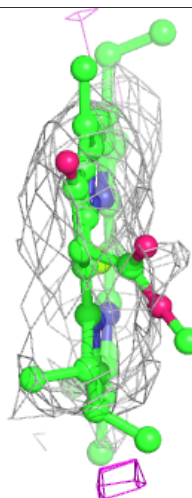
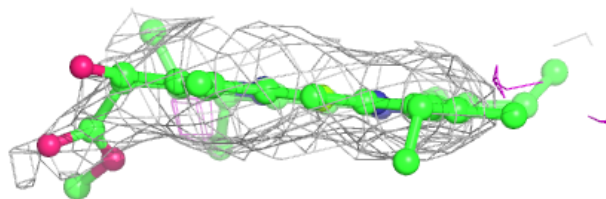
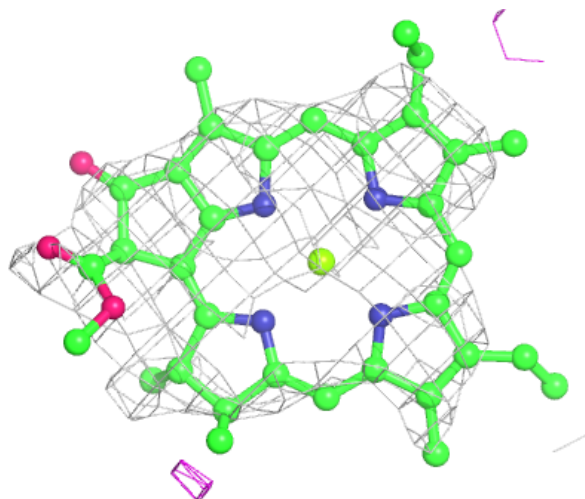
**Electron density around CLA C2 508:**

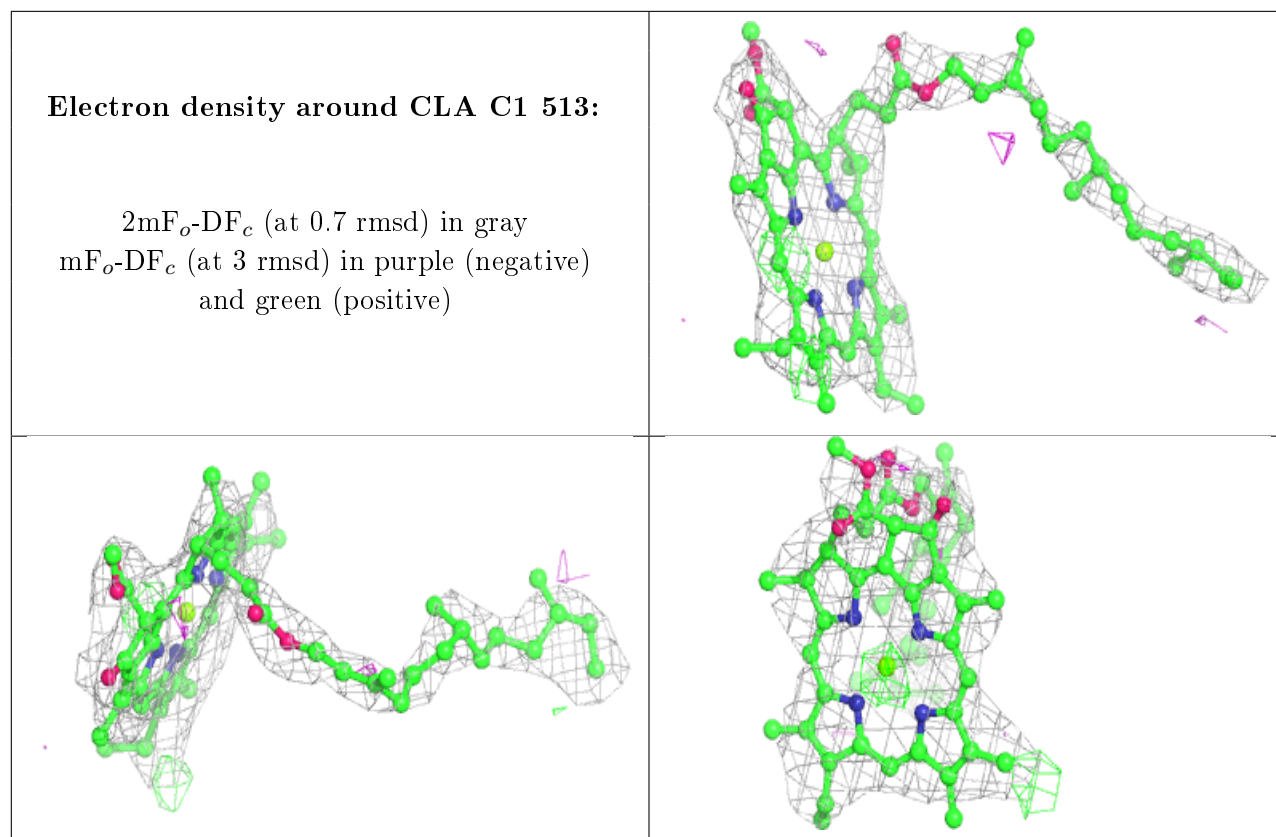
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C2 518:**

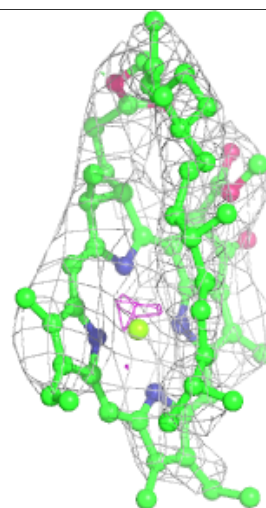
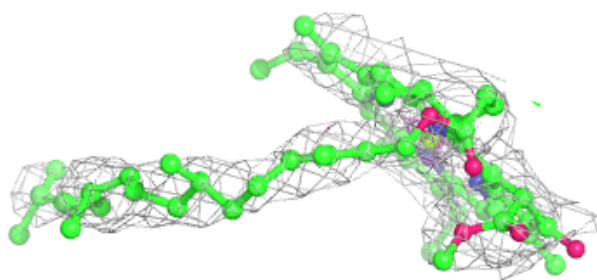
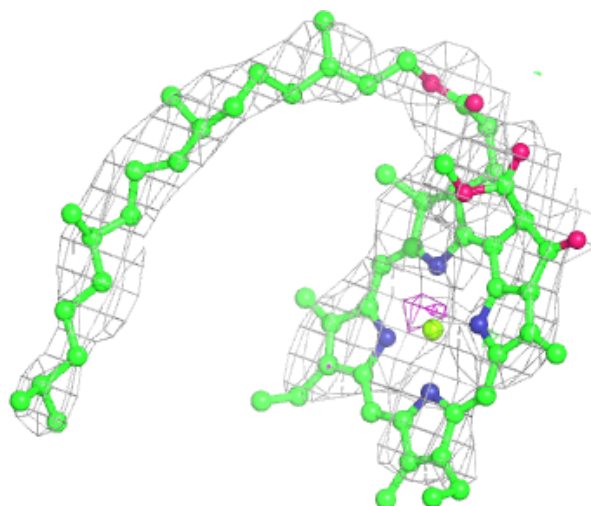
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



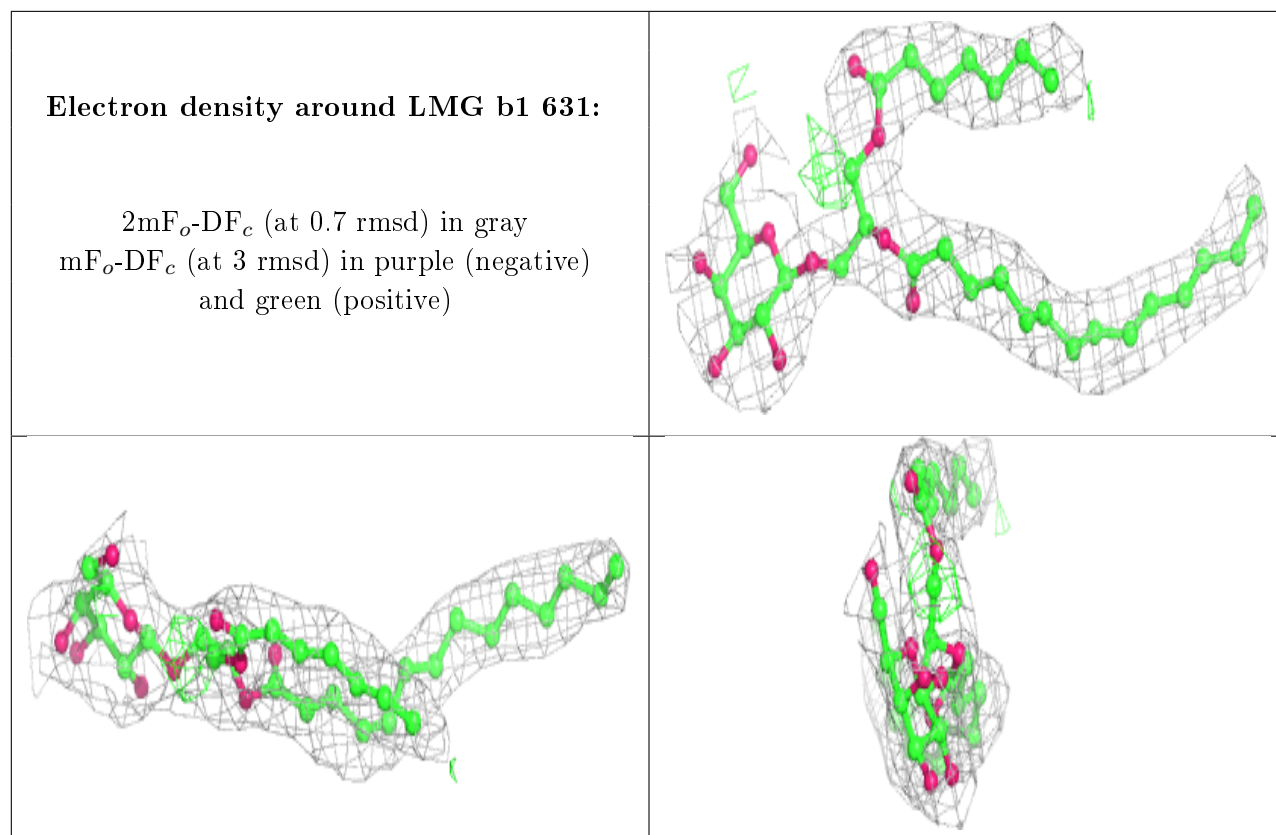


**Electron density around CLA C2 509:**

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



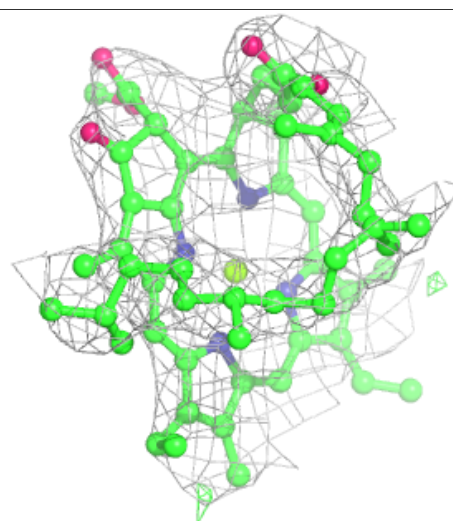
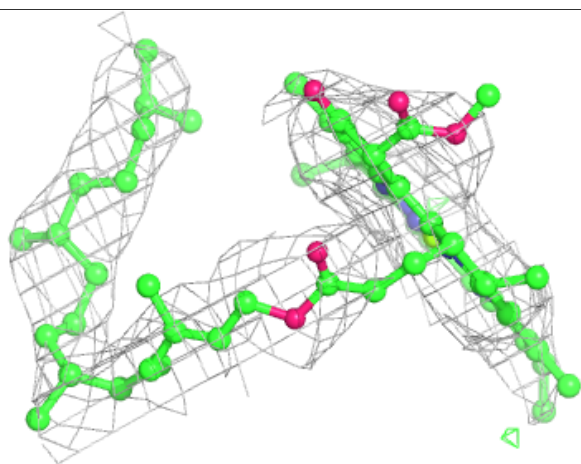
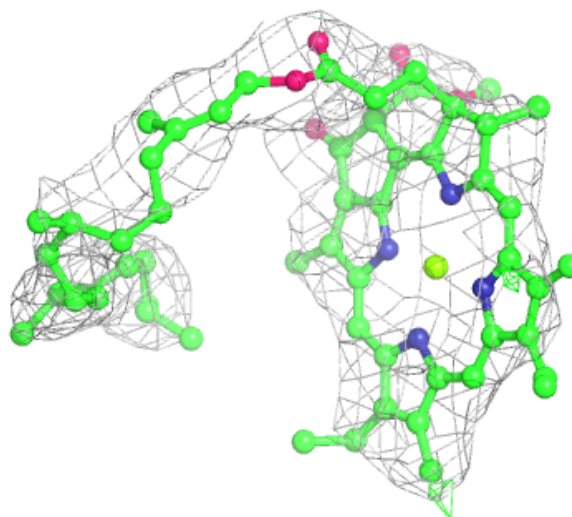






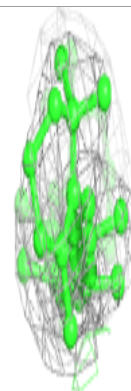
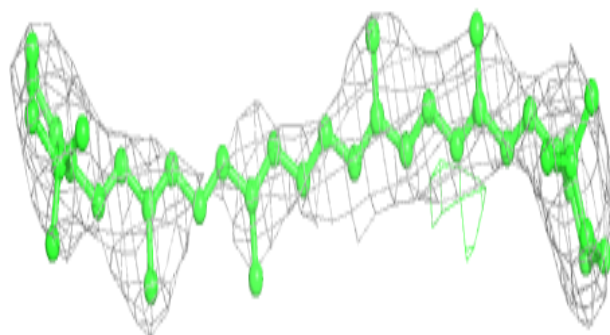
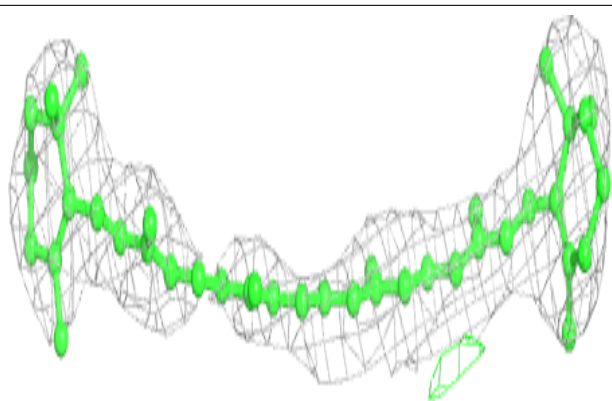
**Electron density around CLA C2 505:**

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

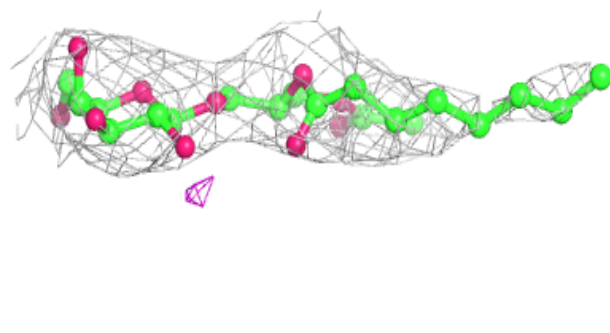
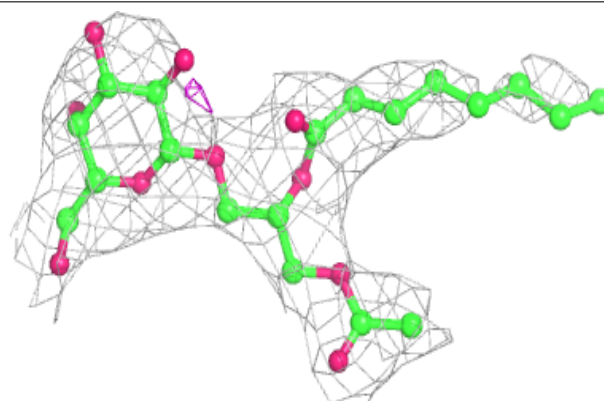


**Electron density around BCR c1 501:**

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

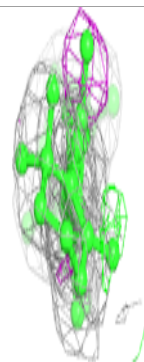
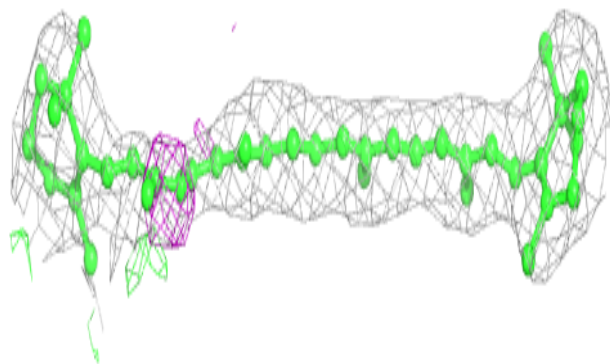
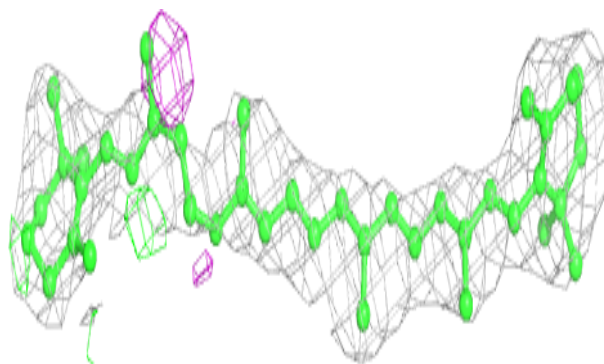
**Electron density around LMG A2 412:**

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



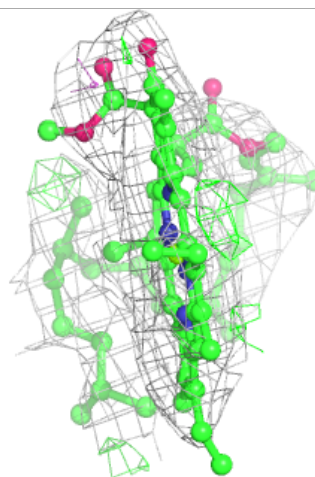
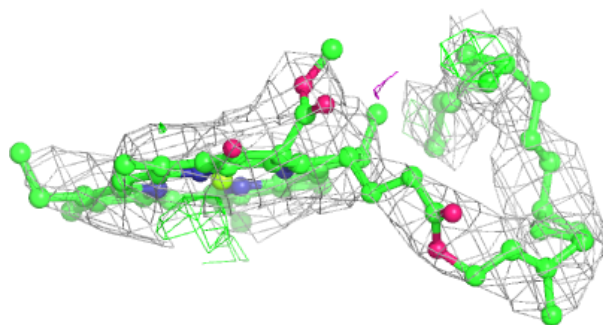
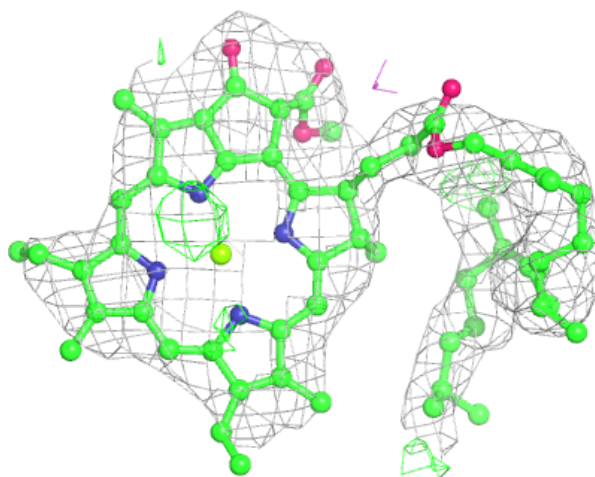
**Electron density around BCR b1 602:**

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



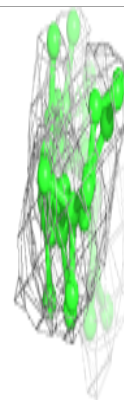
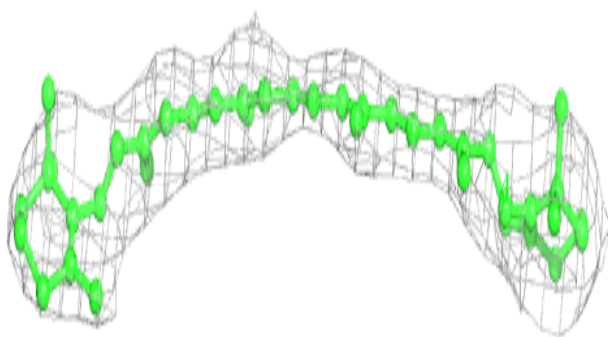
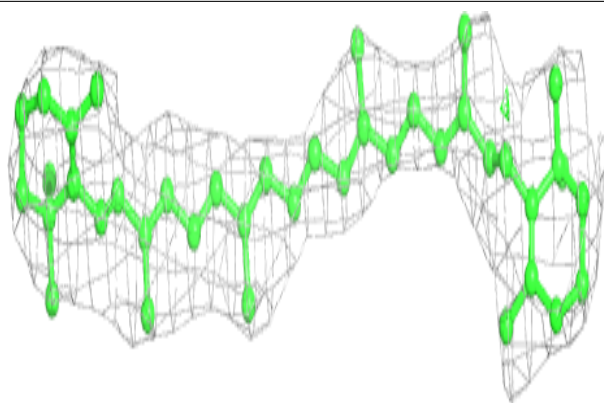
**Electron density around CLA C1 512:**

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

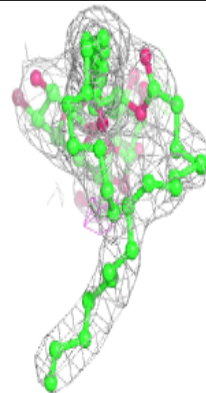
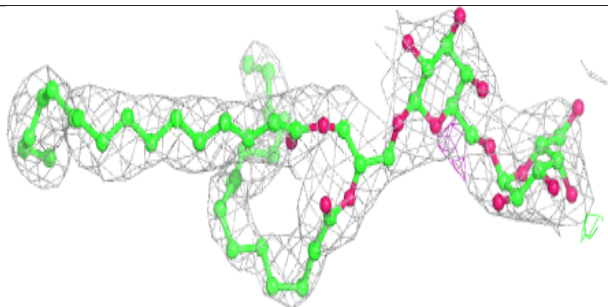
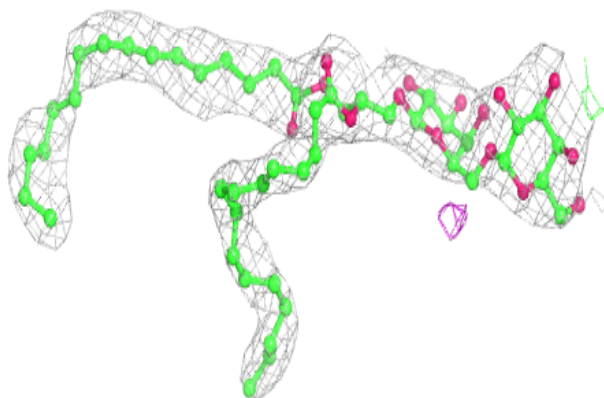


**Electron density around BCR D1 401:**

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

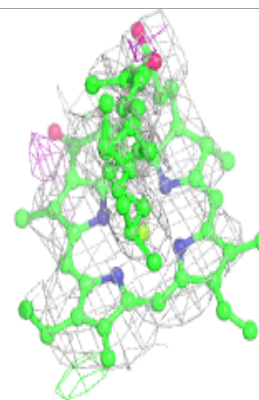
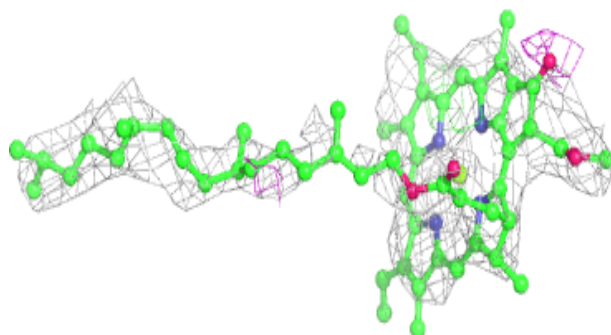
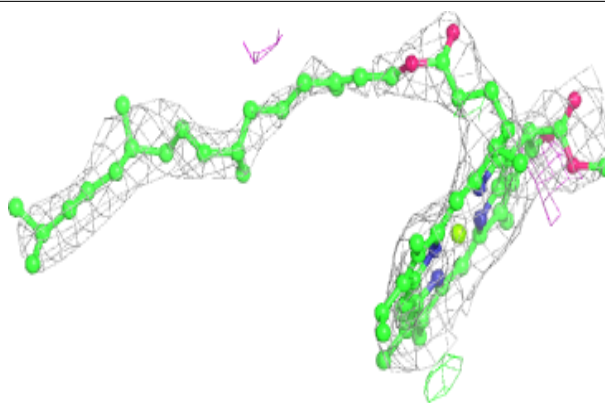
**Electron density around DGD H1 101:**

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

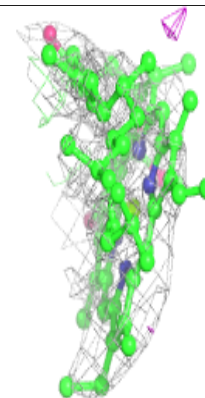
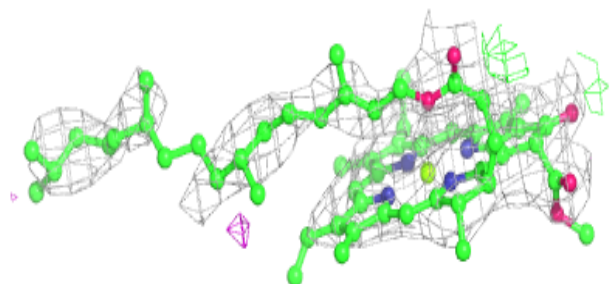
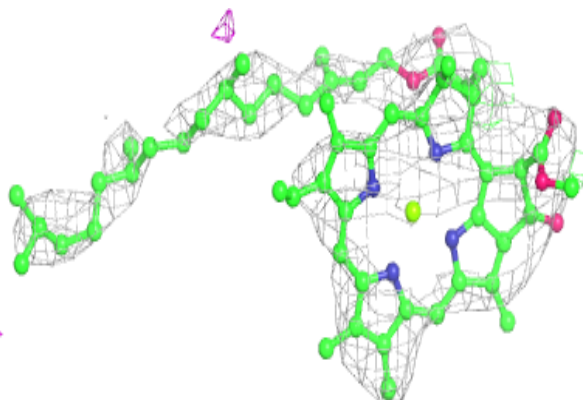


**Electron density around CLA C2 506:**

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

**Electron density around CLA C2 503:**

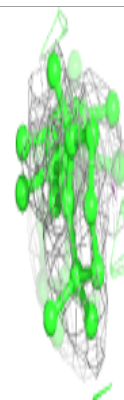
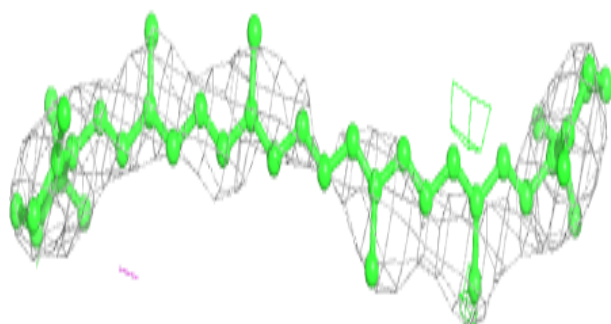
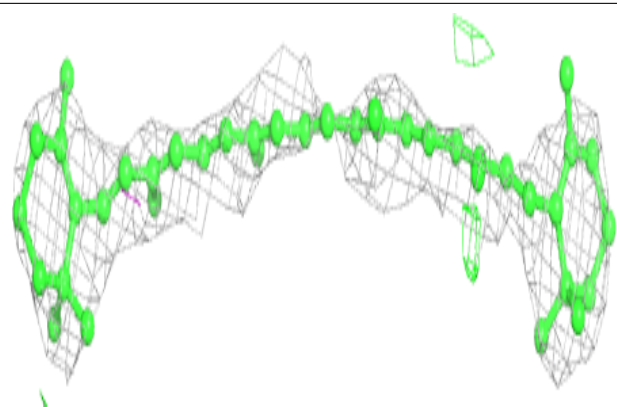
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



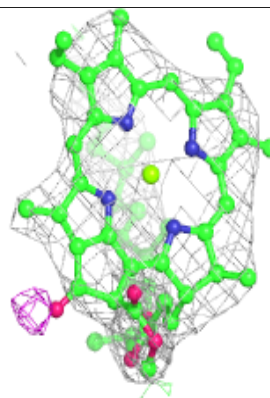
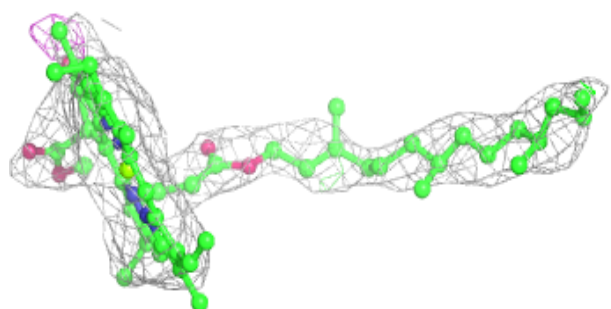
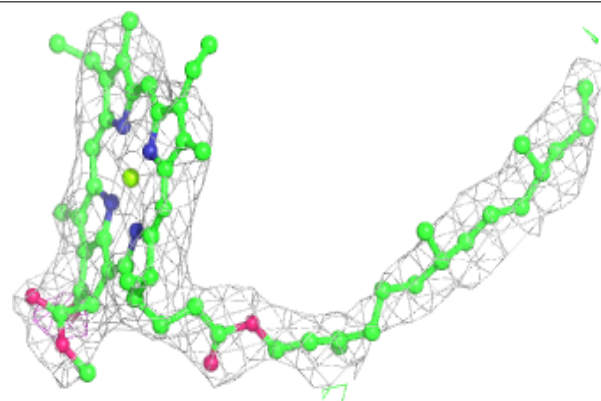


**Electron density around BCR k2 501:**

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

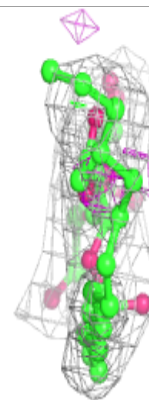
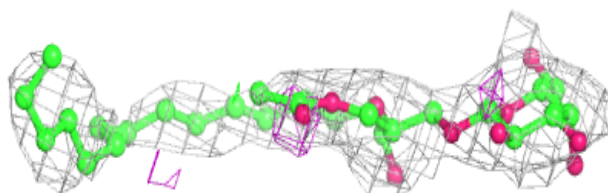
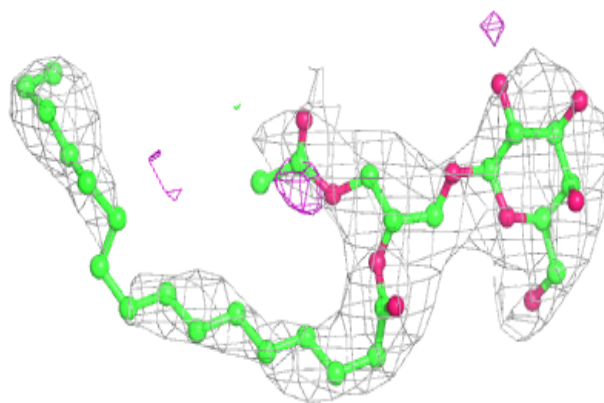
**Electron density around CLA B1 611:**

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

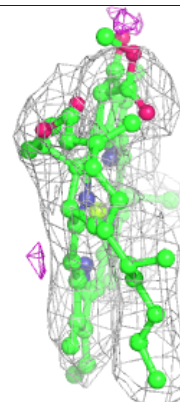
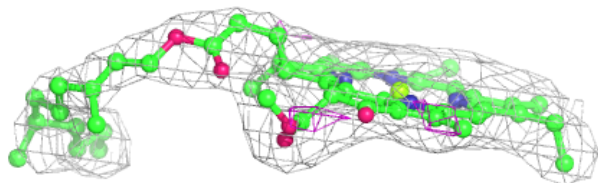
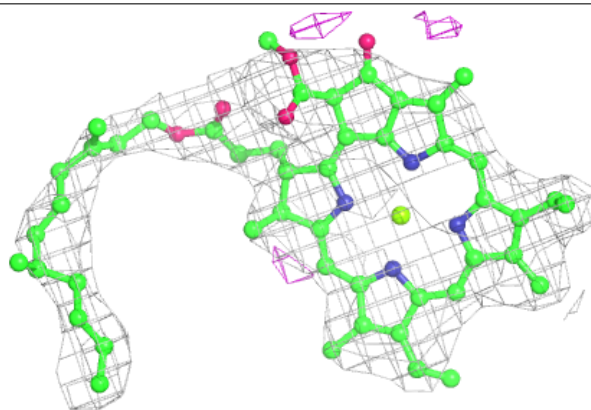


**Electron density around LMG B2 621:**

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

**Electron density around CLA B1 618:**

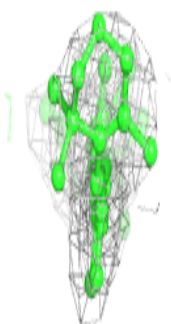
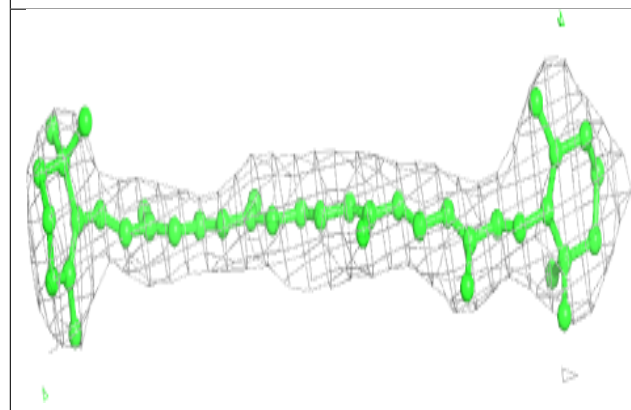
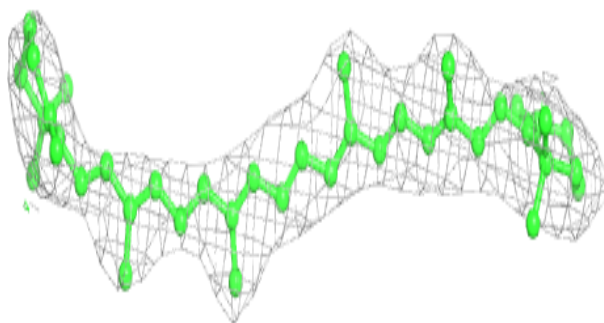
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





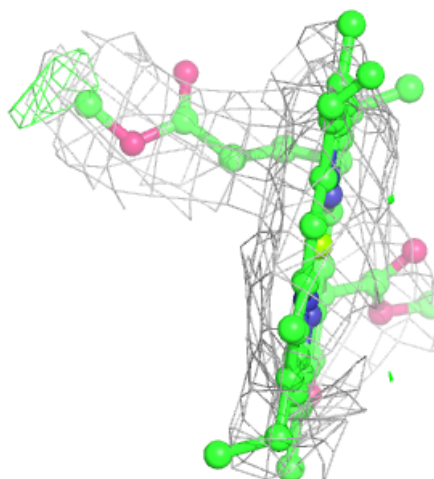
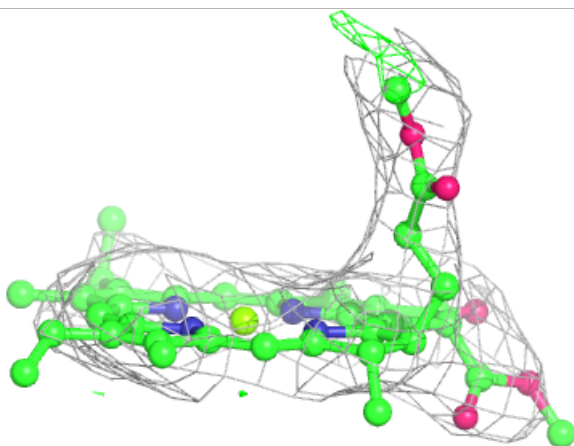
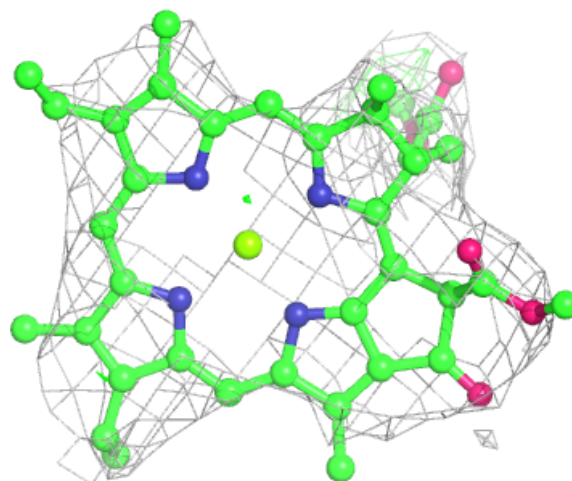
**Electron density around BCR C1 501:**

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



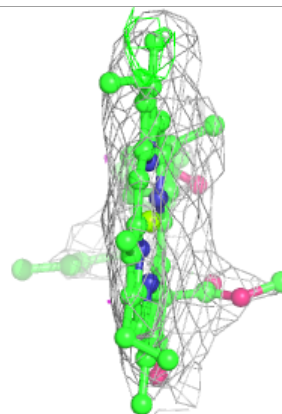
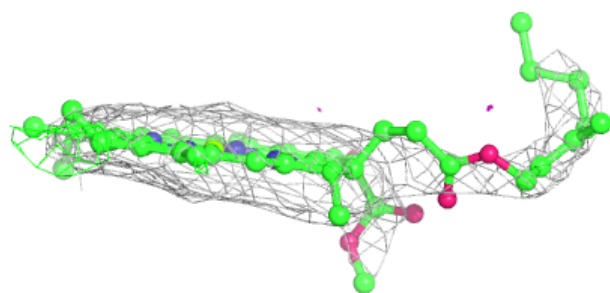
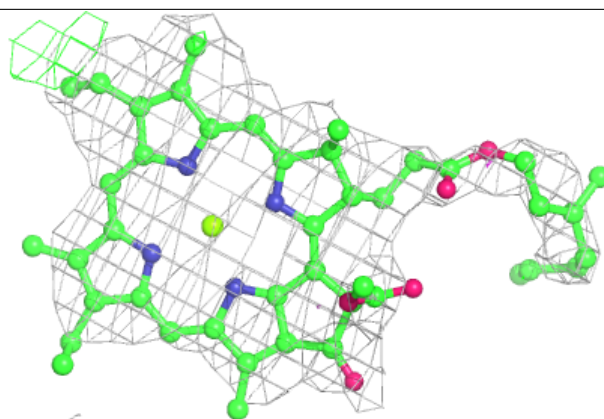
**Electron density around CLA c2 515:**

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

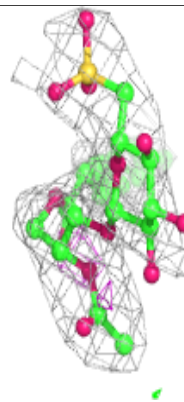
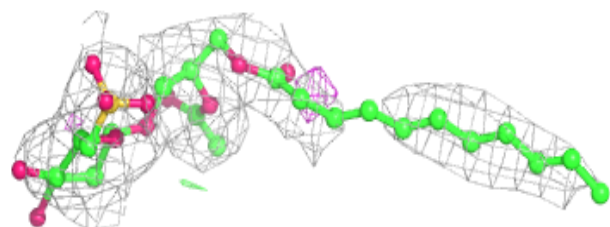
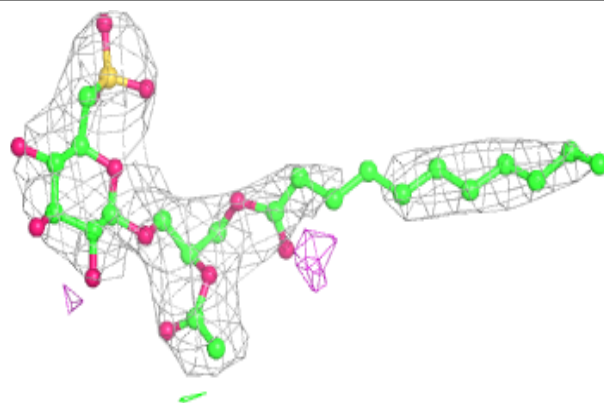


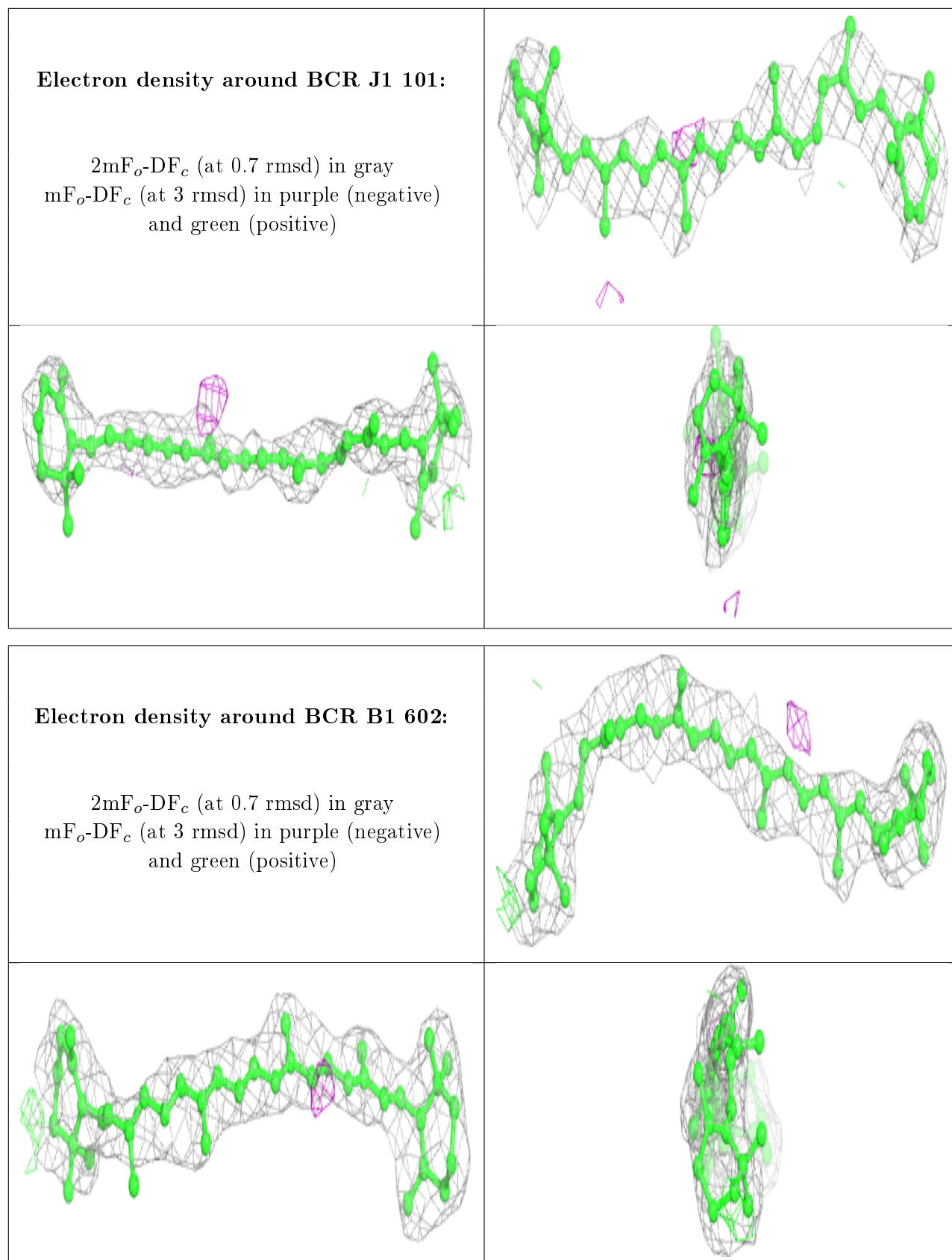
**Electron density around CLA C2 513:**

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

**Electron density around SQD D1 409:**

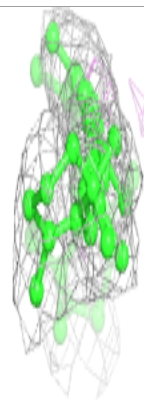
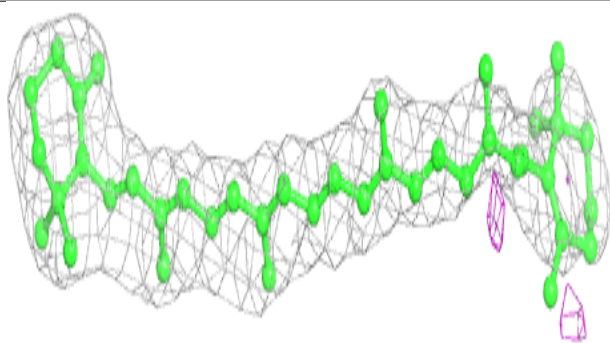
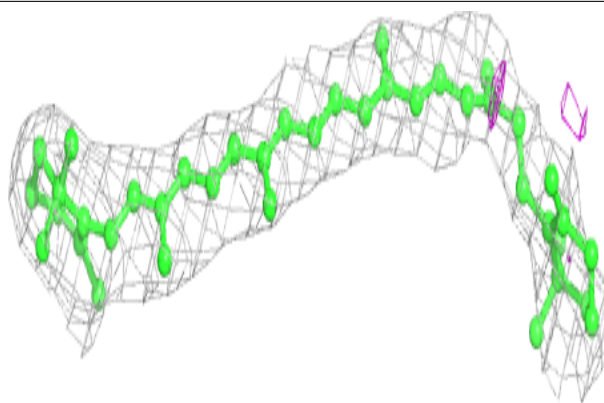
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



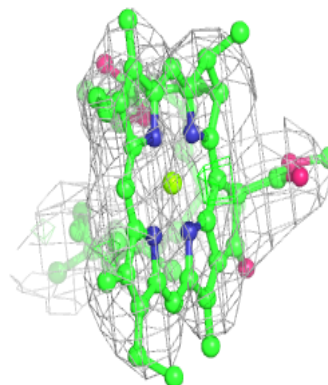
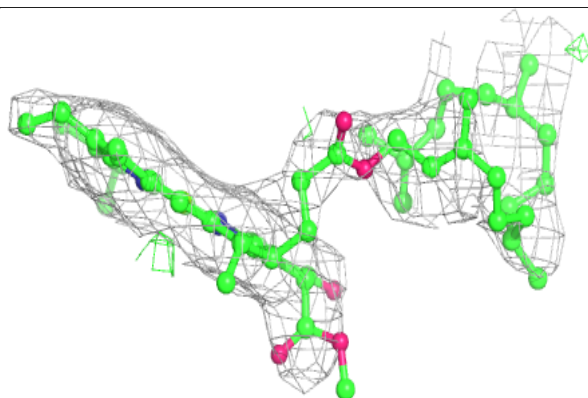
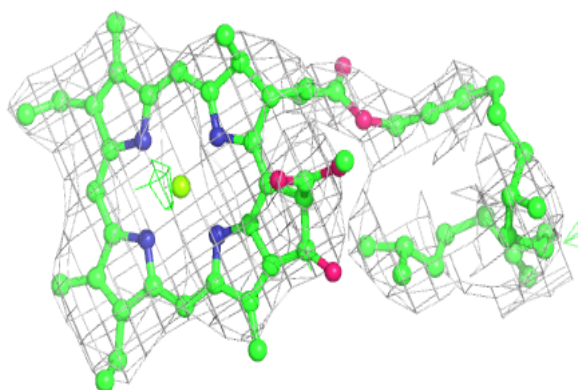


**Electron density around BCR B2 602:**

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

**Electron density around CLA b1 604:**

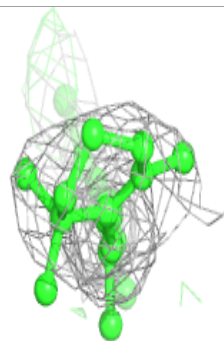
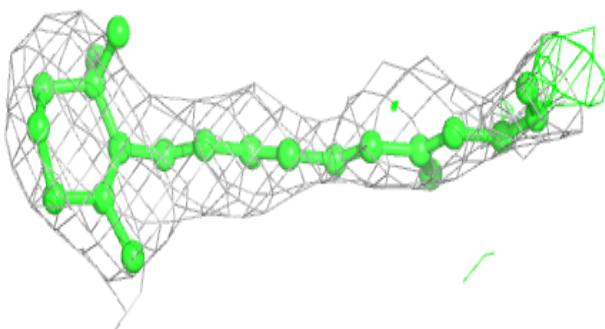
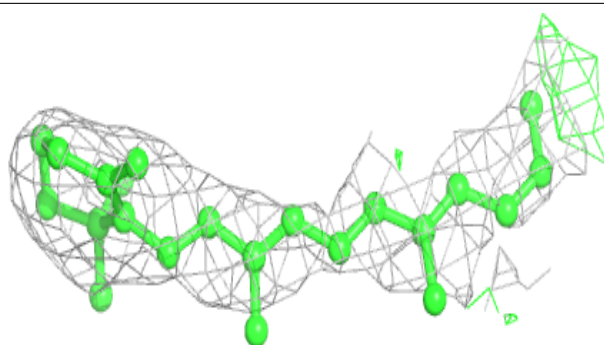
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



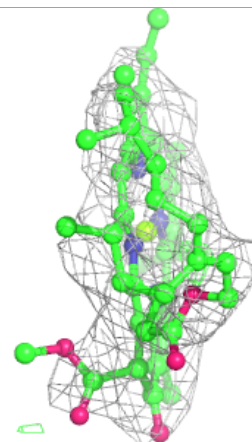
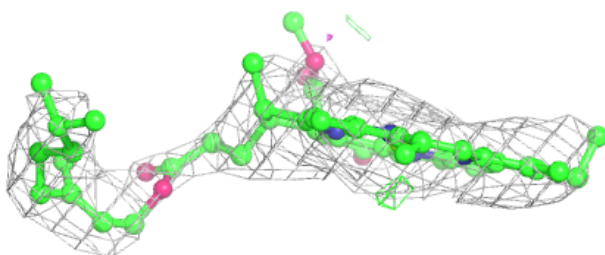
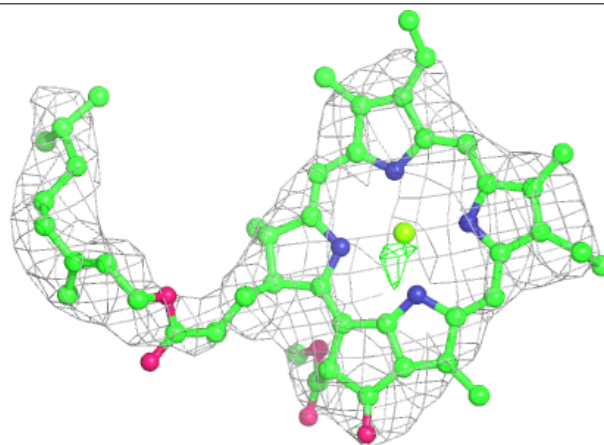


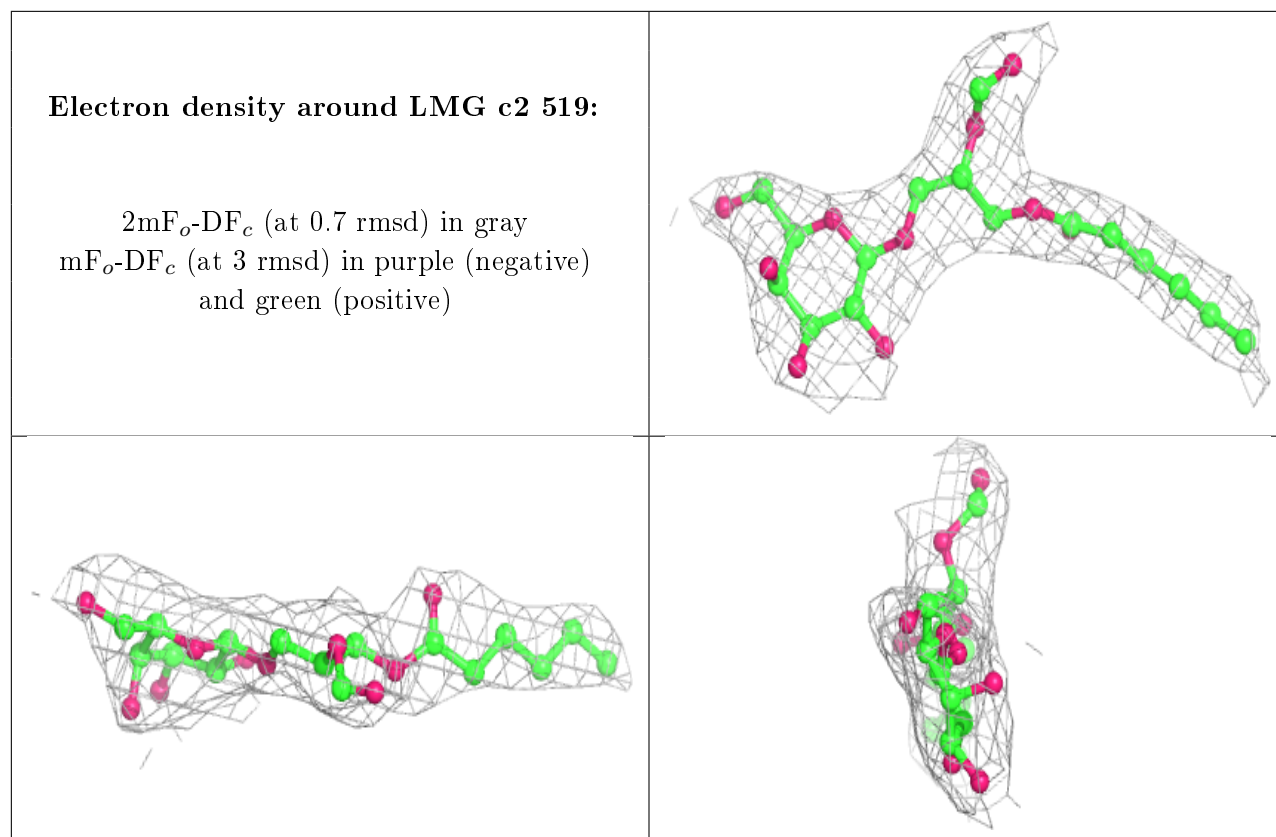
**Electron density around BCR H1 102:**

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

**Electron density around CLA c1 515:**

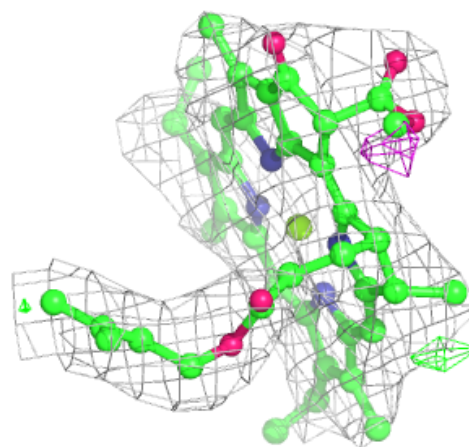
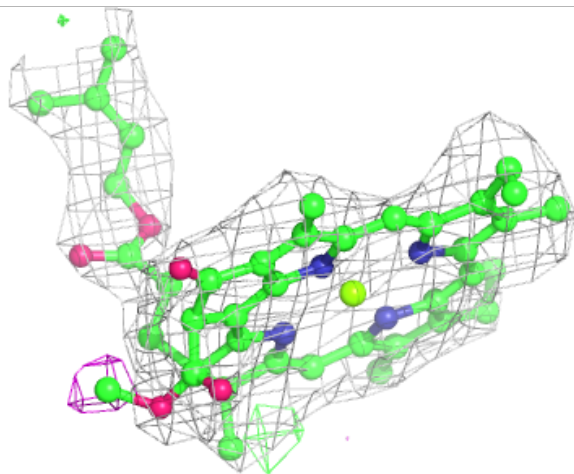
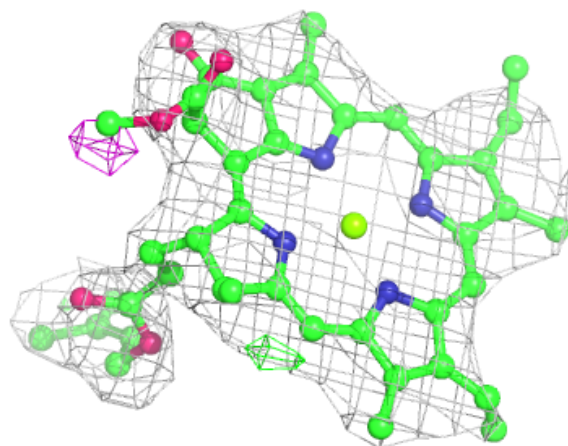
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA c1 508:**

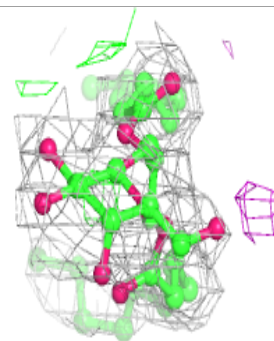
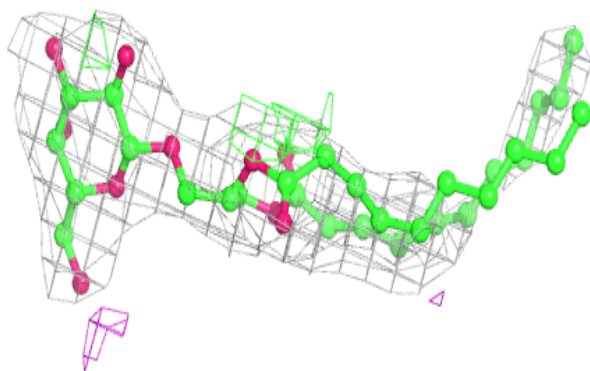
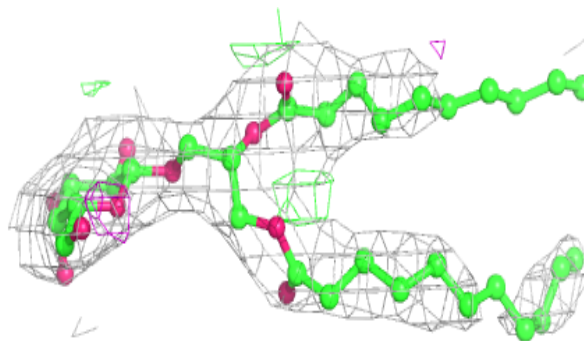
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





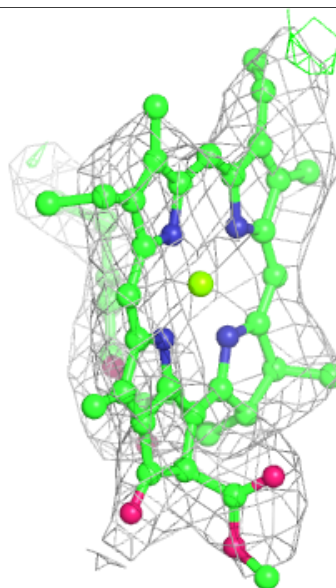
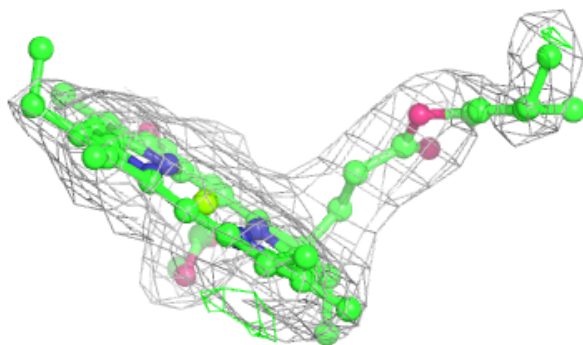
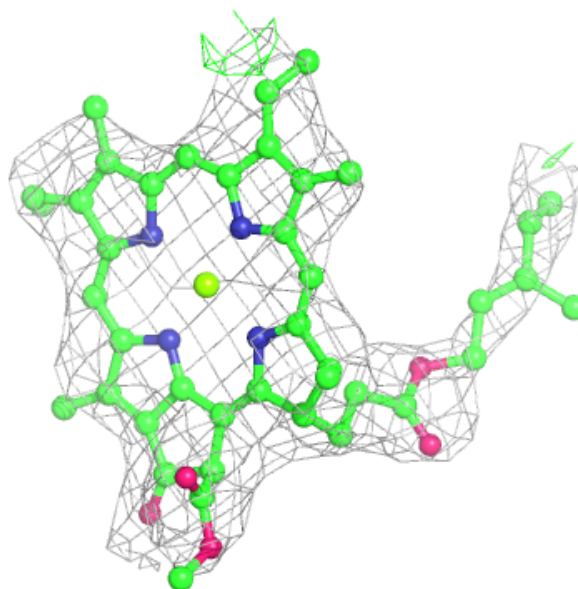
**Electron density around LMG B2 620:**

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



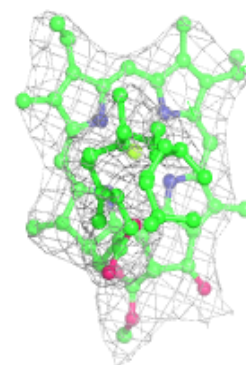
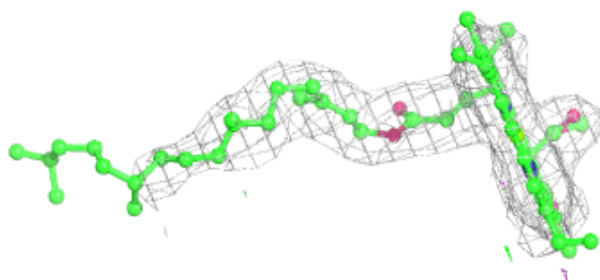
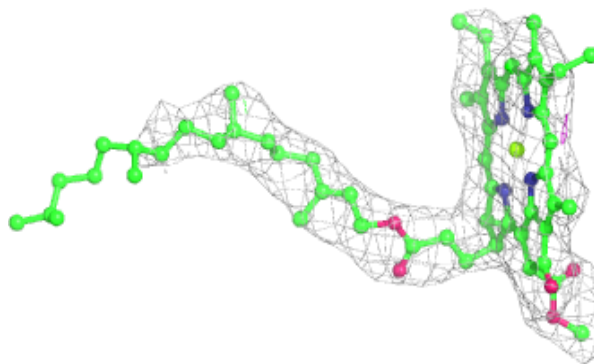
**Electron density around CLA D1 403:**

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

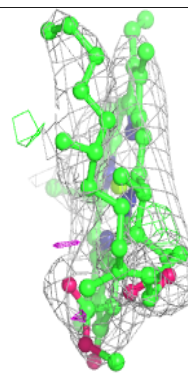
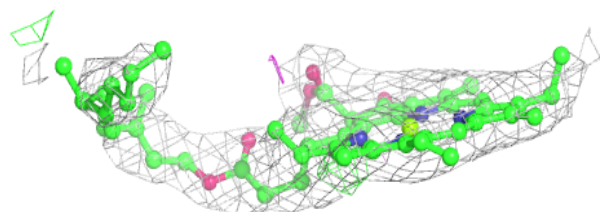
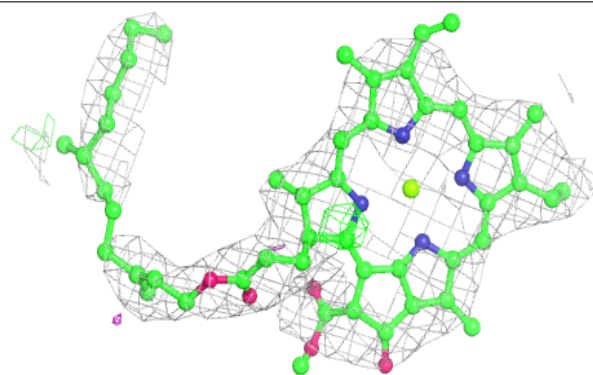


**Electron density around CLA d1 406:**

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

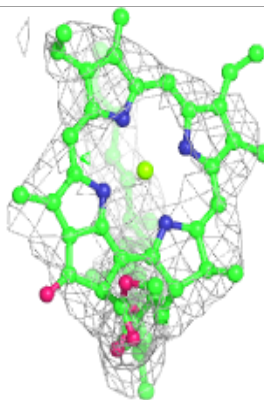
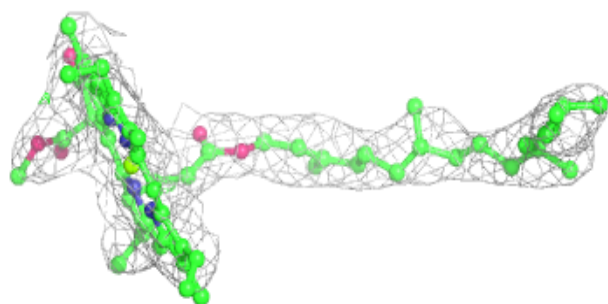
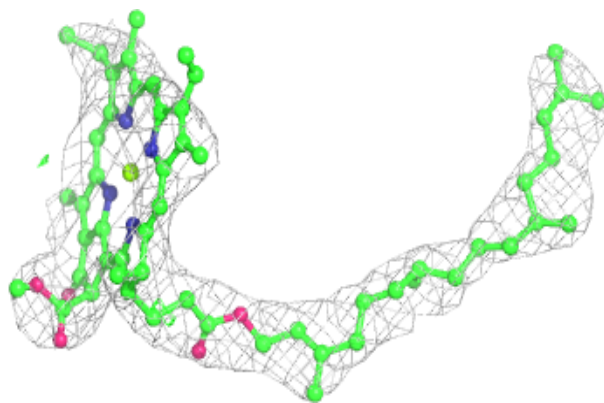
**Electron density around CLA b2 619:**

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

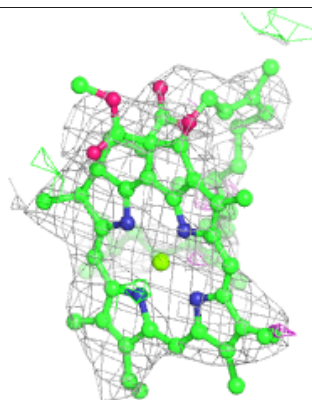
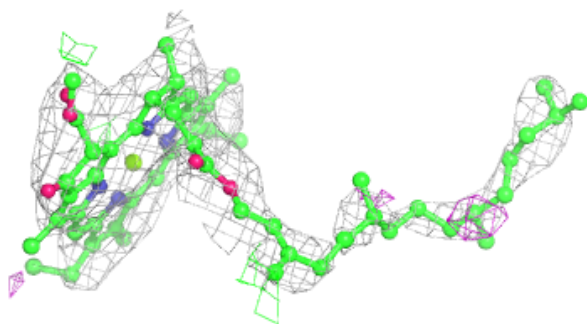
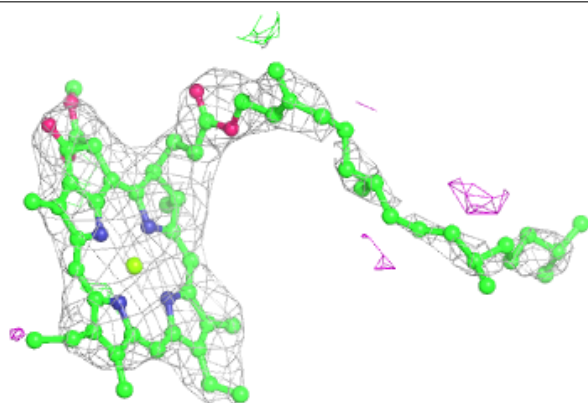


**Electron density around CLA b2 610:**

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

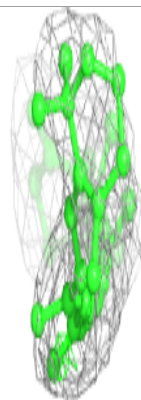
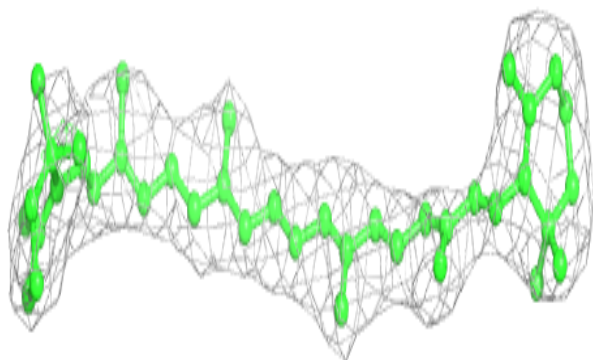
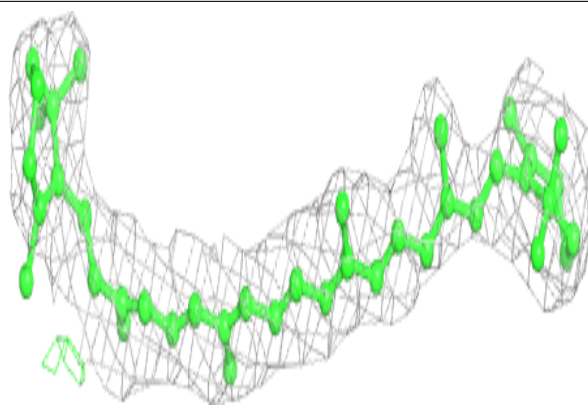
**Electron density around CLA c2 512:**

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

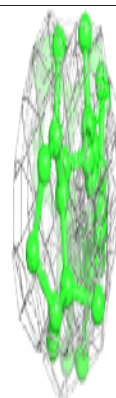
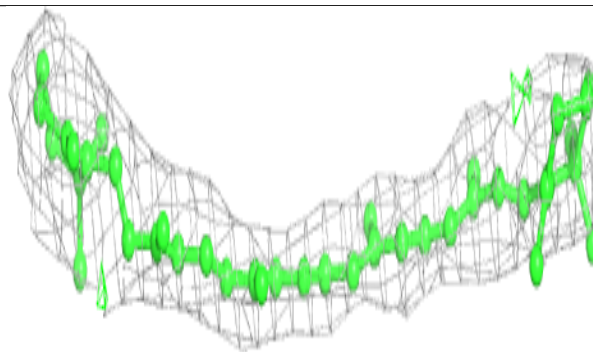
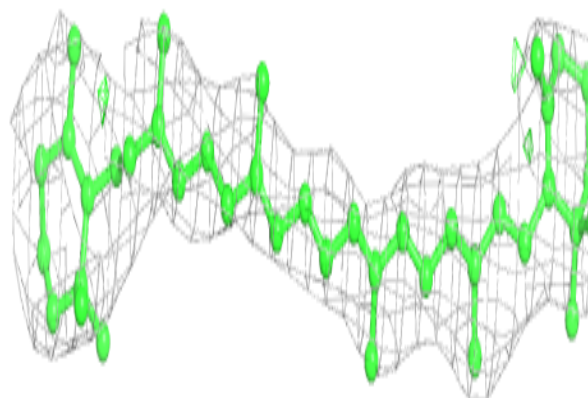


**Electron density around BCR b2 602:**

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

**Electron density around BCR d2 401:**

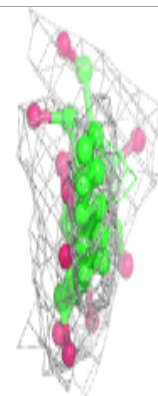
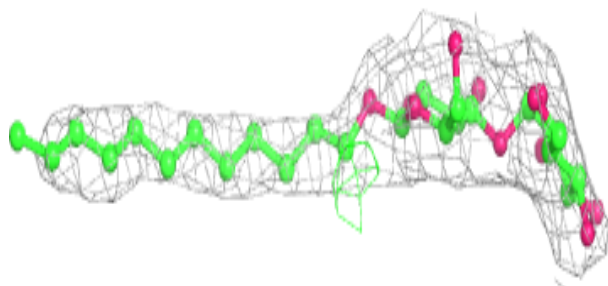
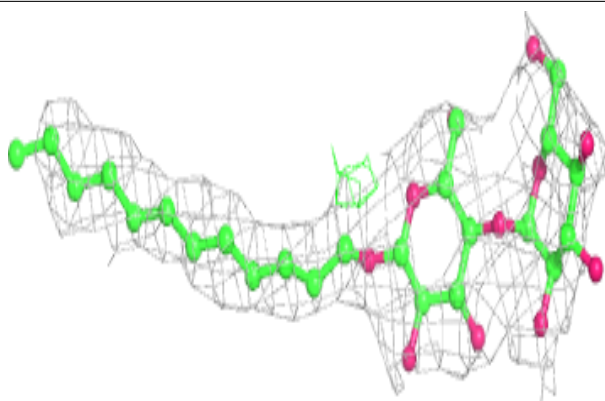
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



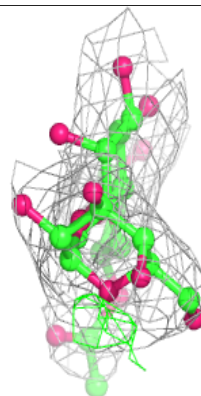
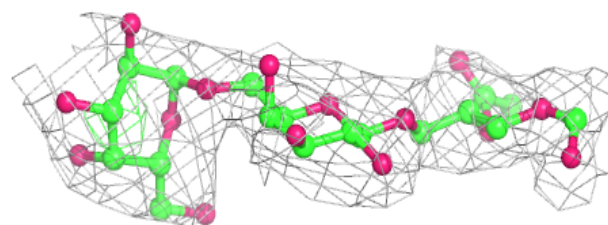
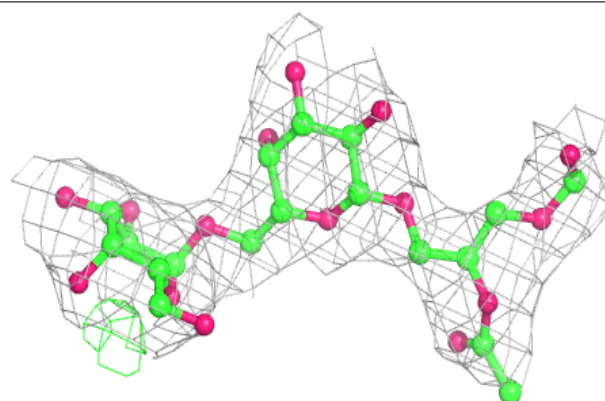


**Electron density around LMT C1 519:**

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

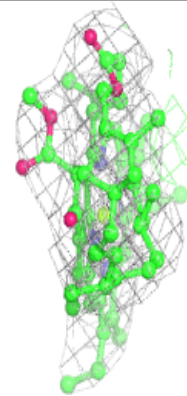
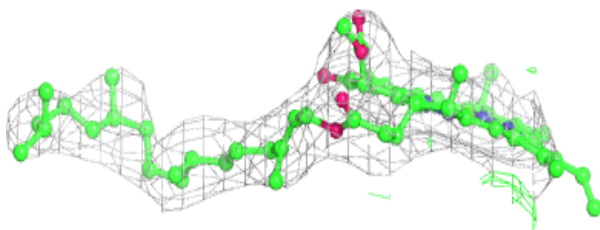
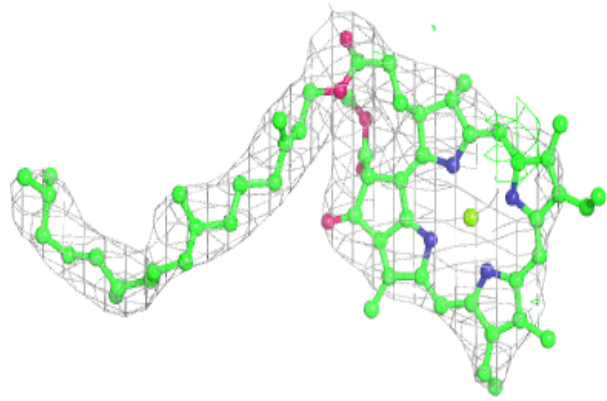
**Electron density around DGD C2 512:**

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

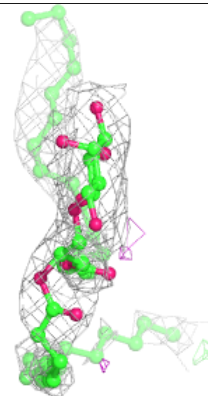
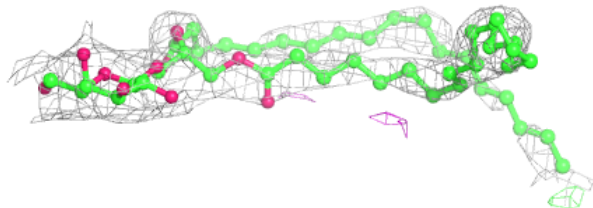
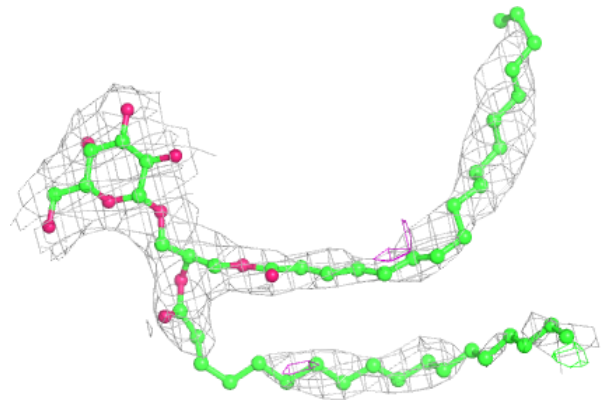


**Electron density around CLA b2 613:**

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

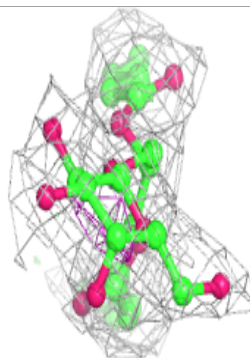
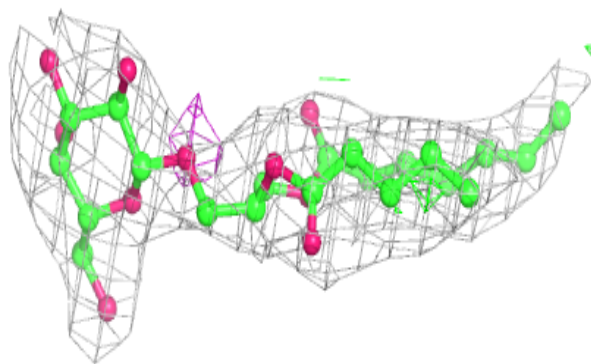
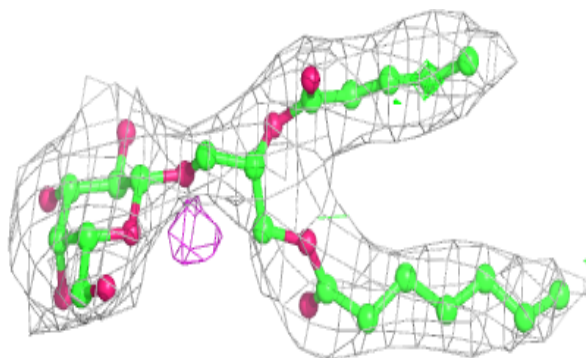
**Electron density around LMG c1 519:**

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



**Electron density around LMG B1 622:**

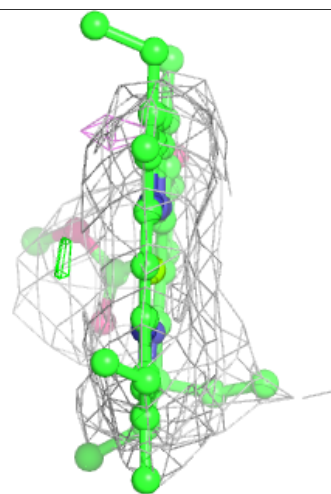
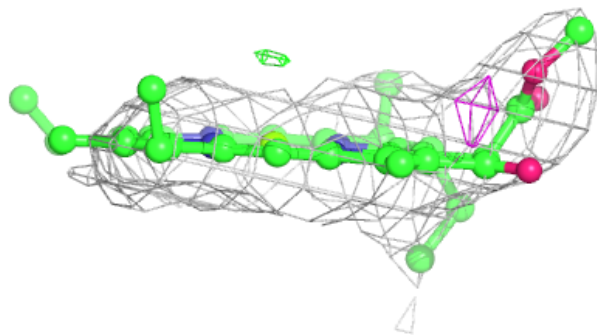
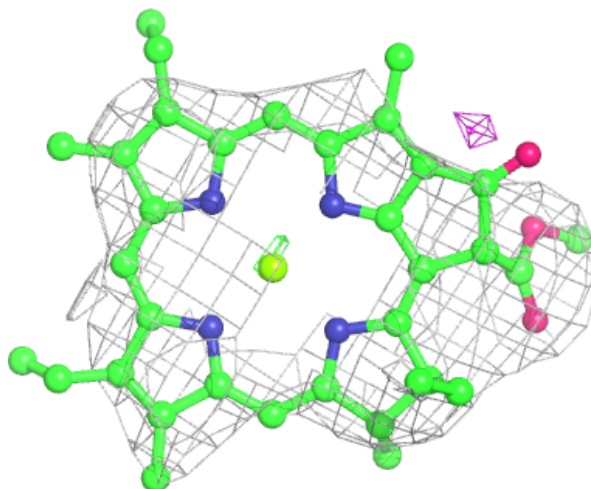
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

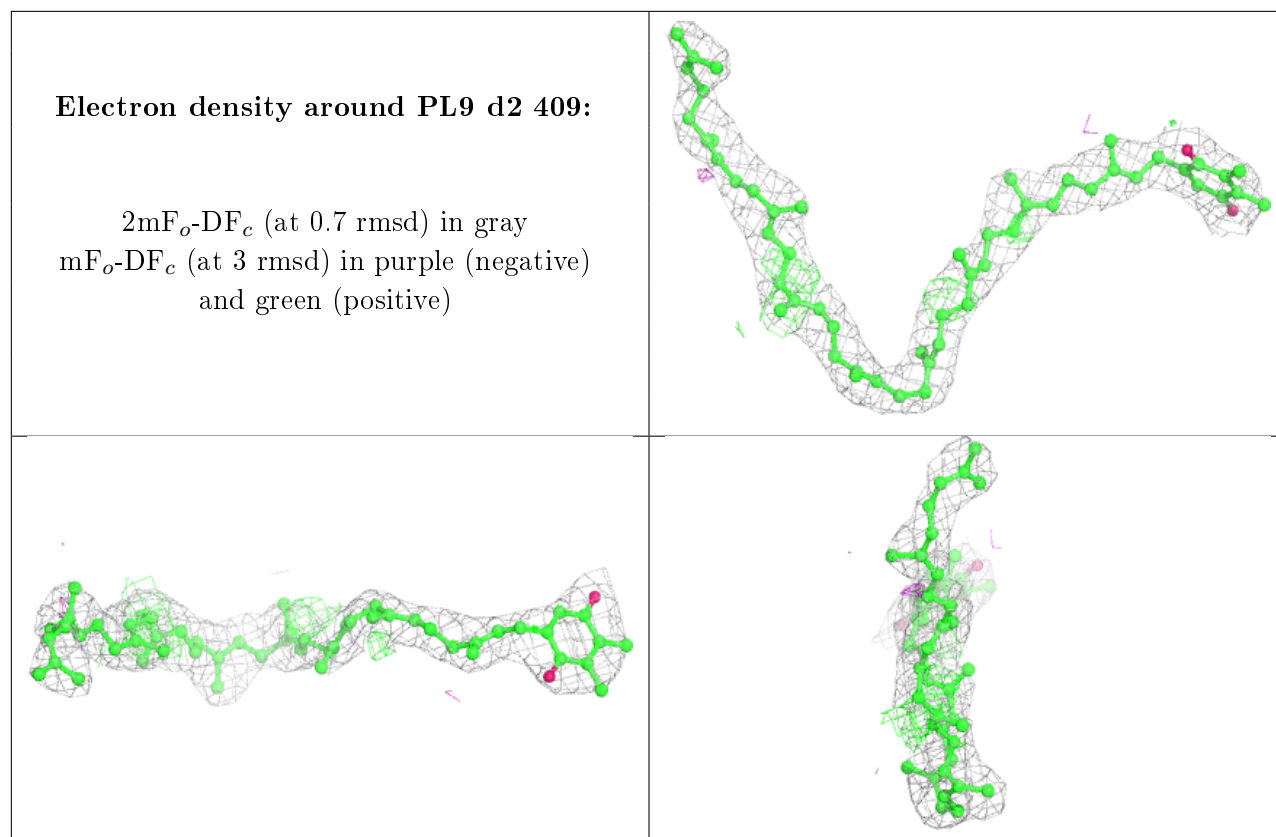




**Electron density around CLA b2 604:**

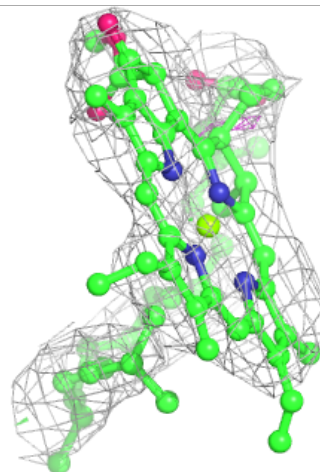
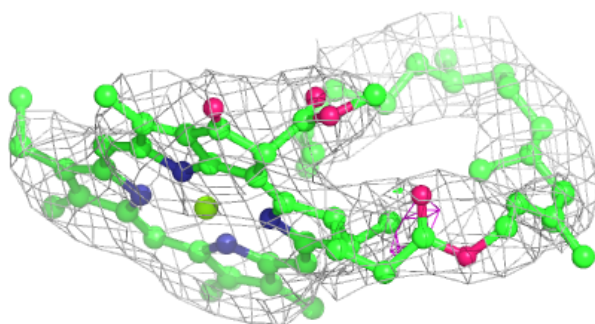
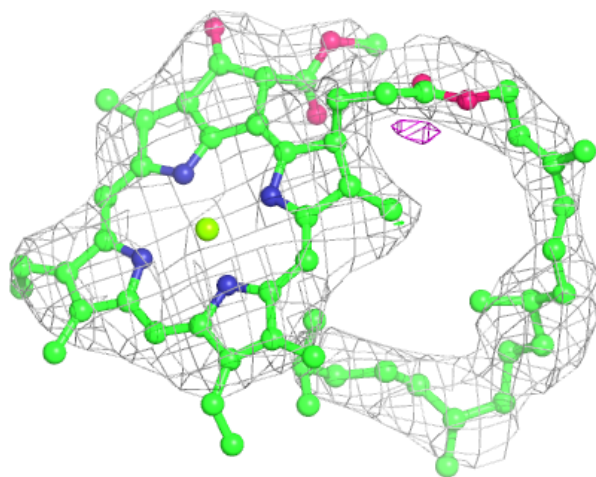
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





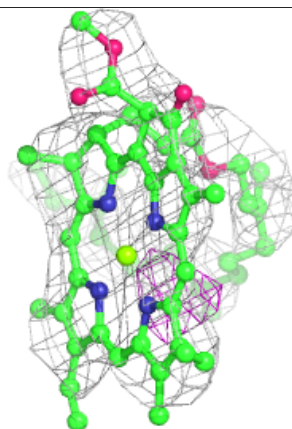
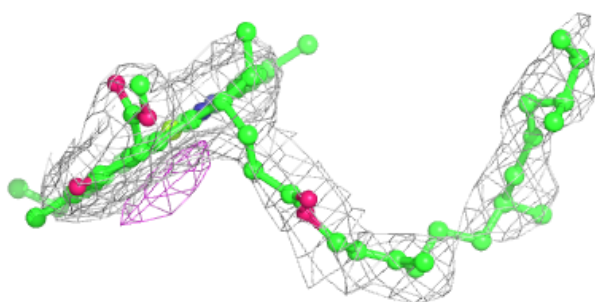
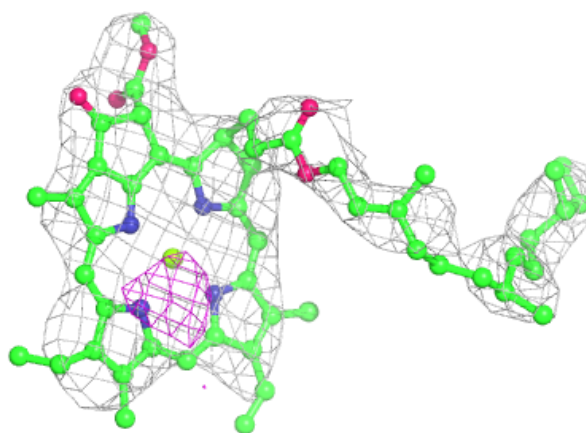
**Electron density around CLA b2 618:**

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

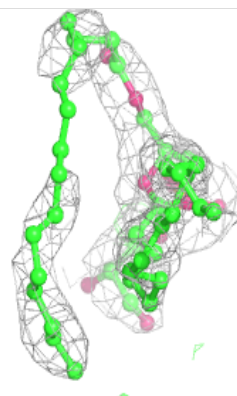
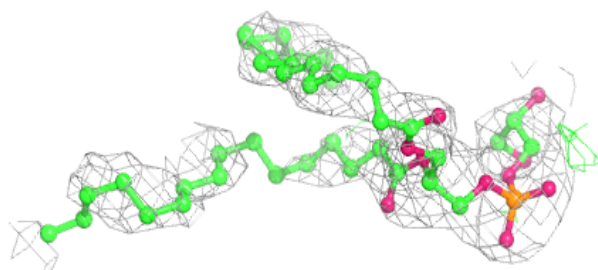
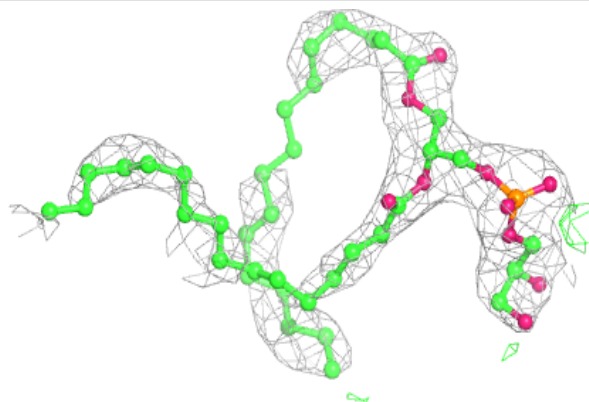


**Electron density around CLA A2 403:**

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

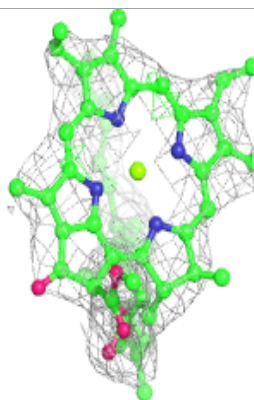
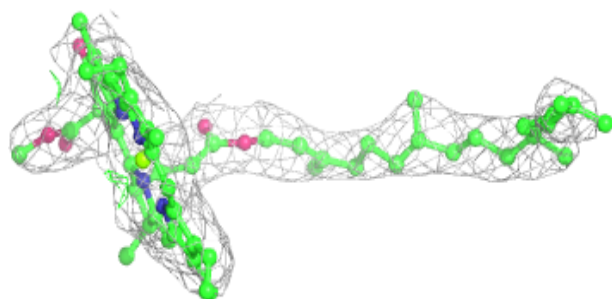
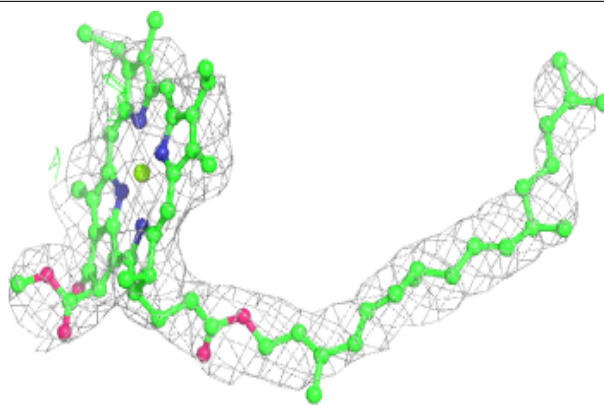
**Electron density around LHG D1 404:**

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

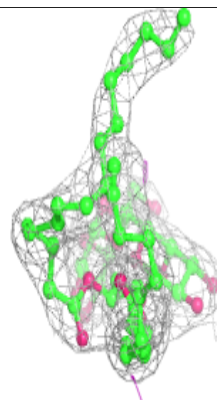
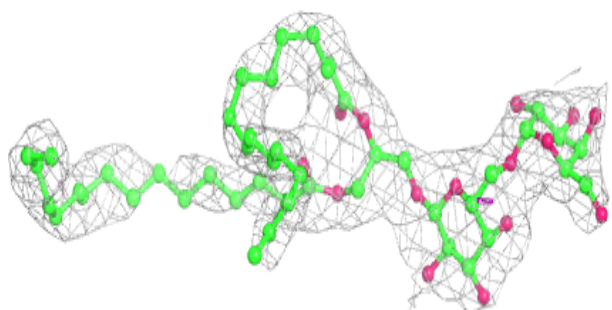
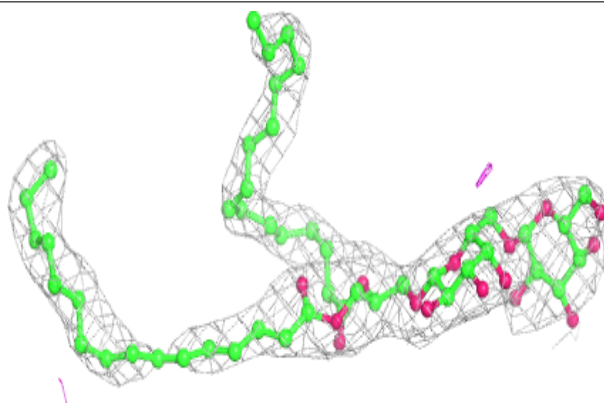


**Electron density around CLA B2 611:**

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

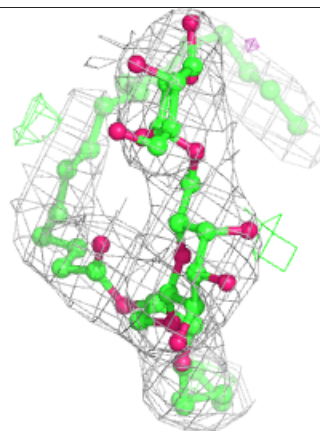
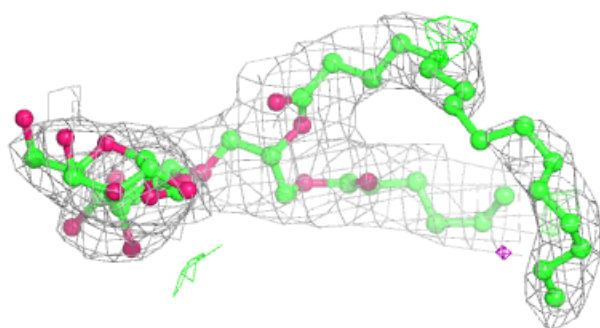
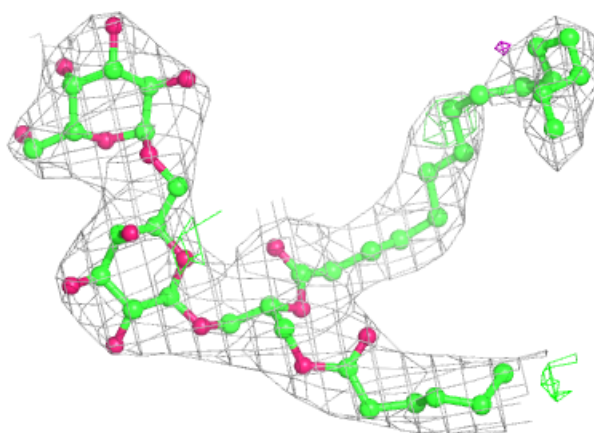
**Electron density around DGD h2 102:**

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

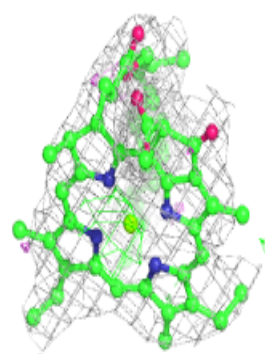
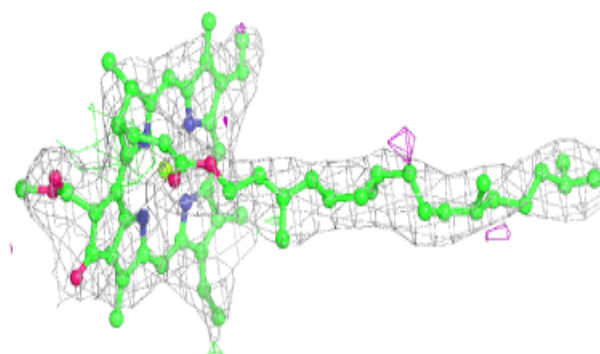
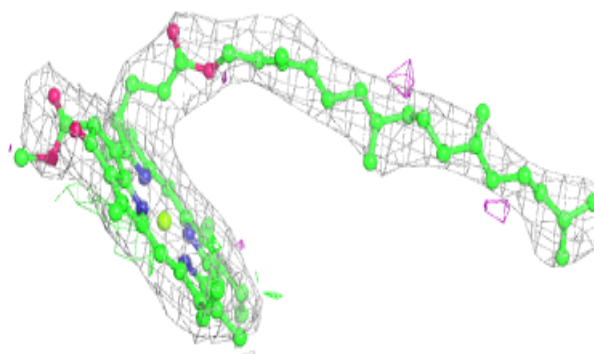


**Electron density around DGD c2 516:**

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

**Electron density around CLA C1 505:**

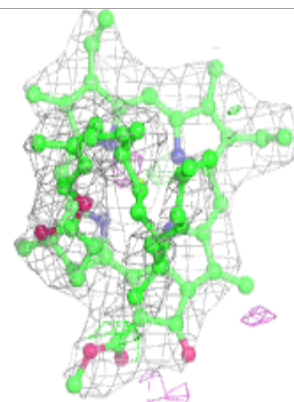
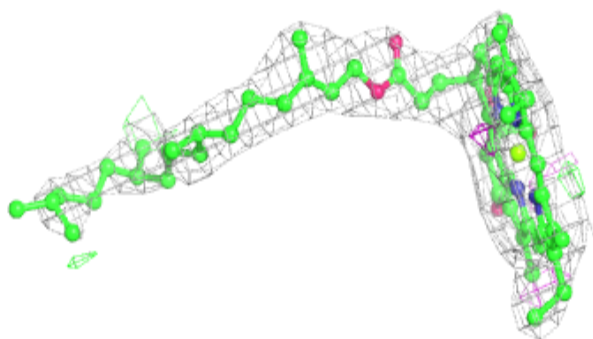
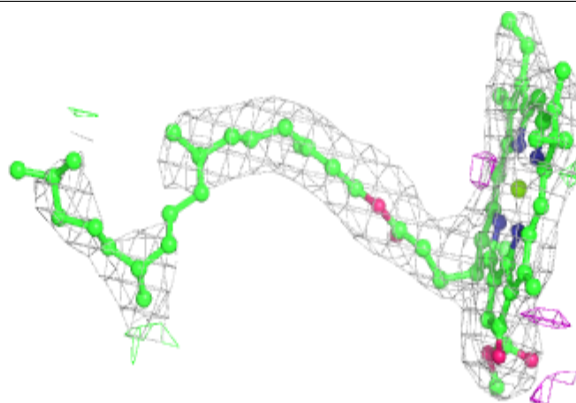
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



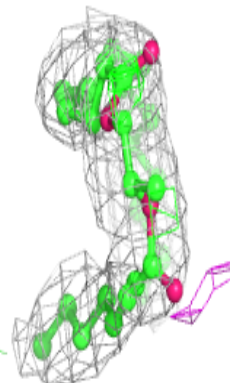
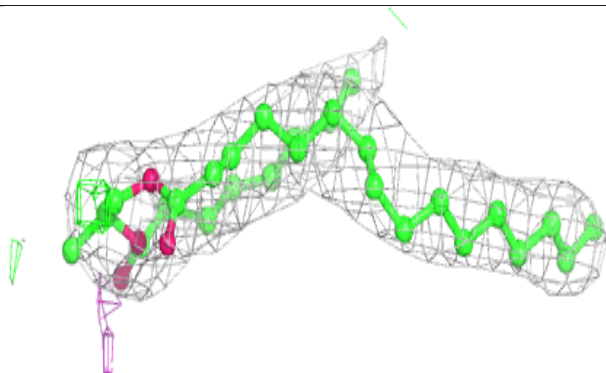
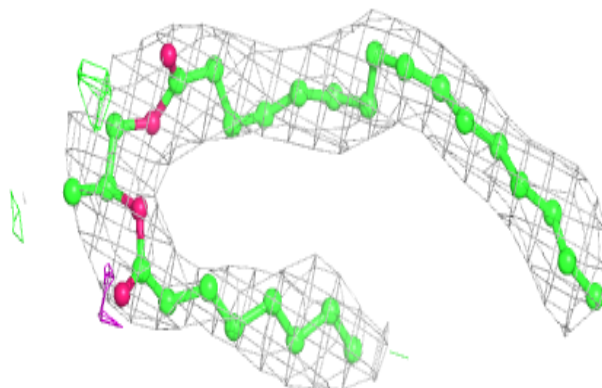


**Electron density around CLA b1 609:**

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

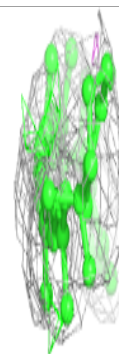
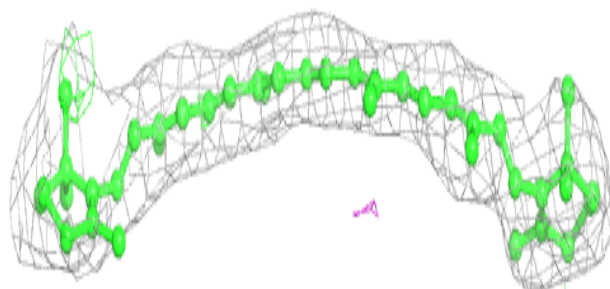
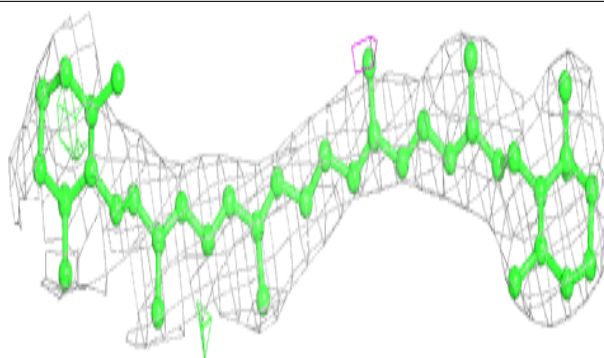
**Electron density around LMG M1 101:**

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

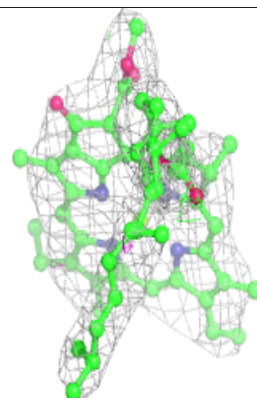
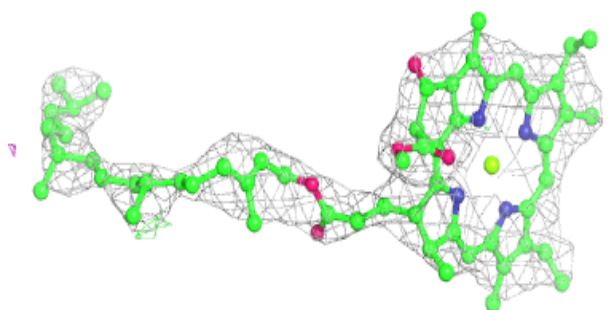
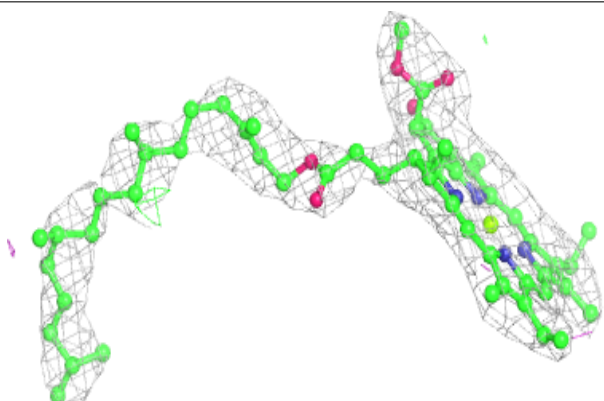


**Electron density around BCR d1 405:**

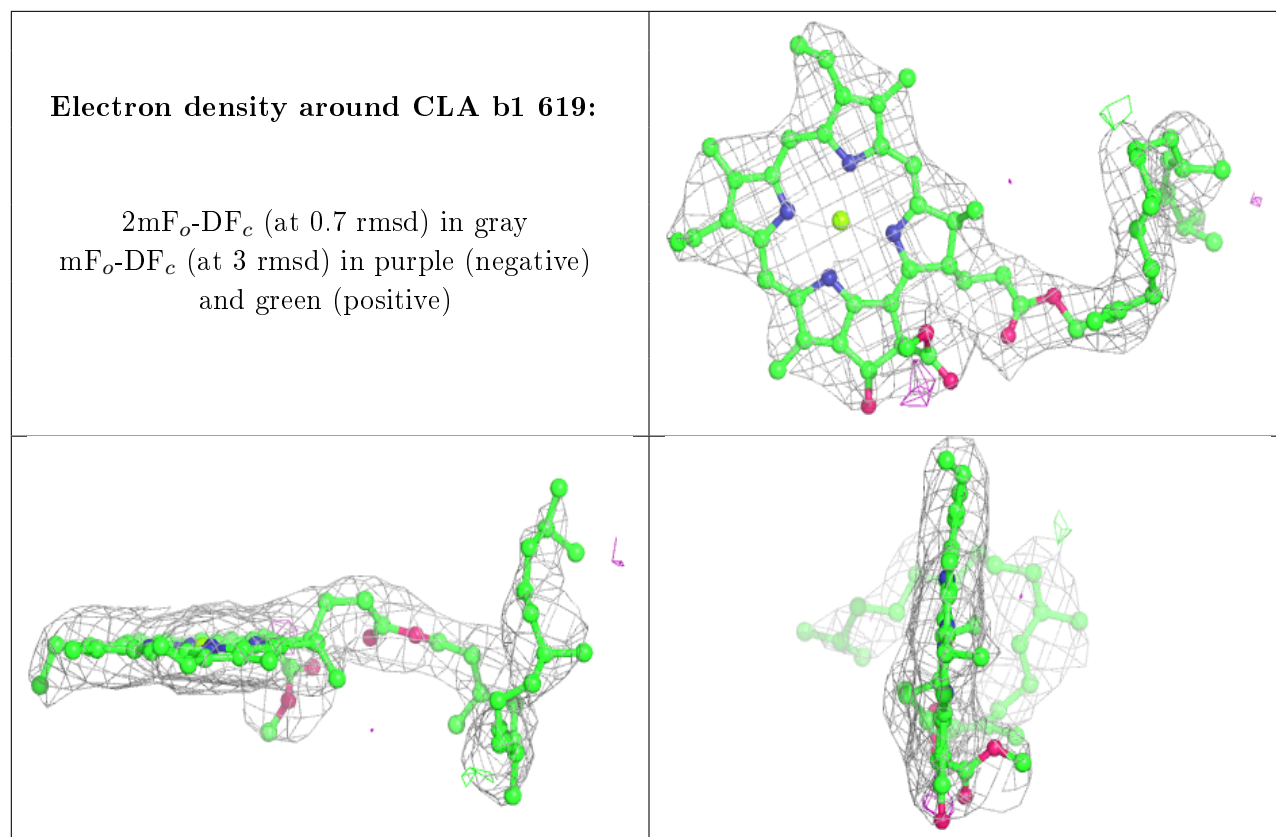
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA D2 401:**

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

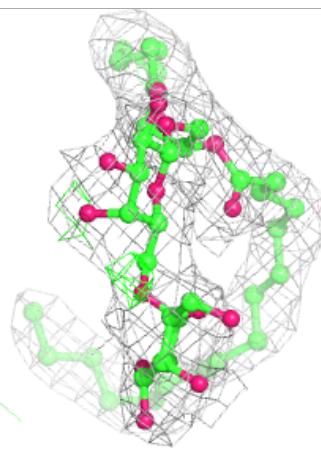
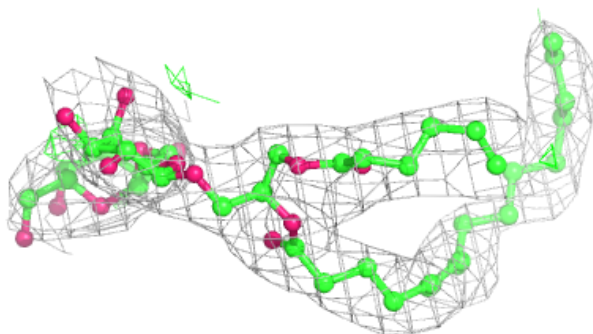
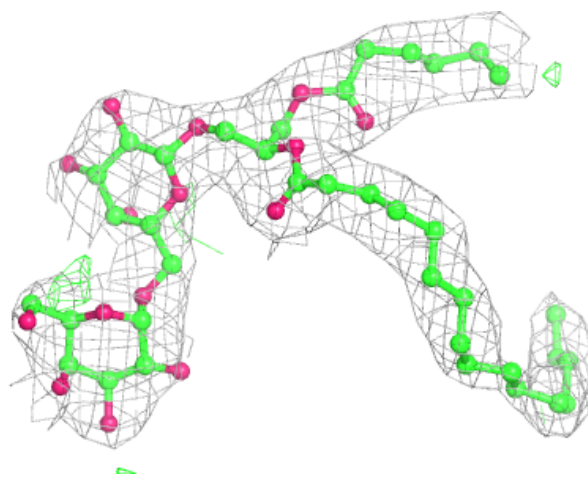






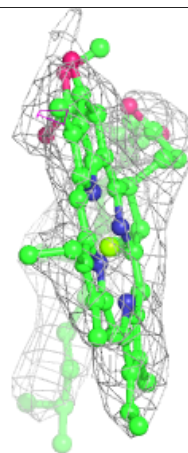
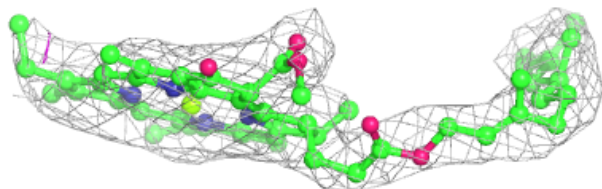
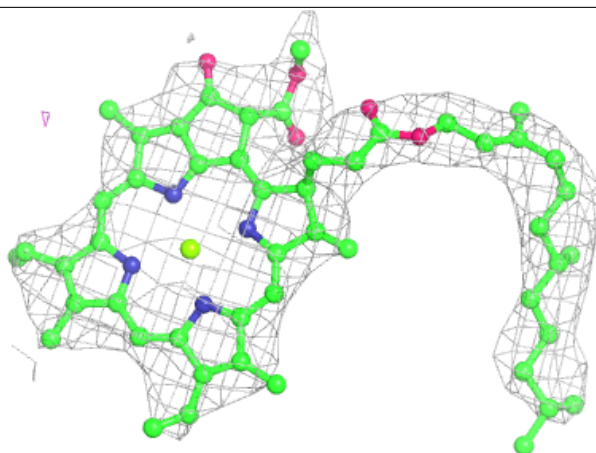
**Electron density around DGD C1 515:**

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

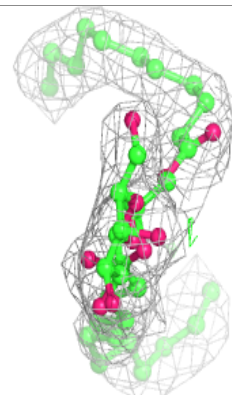
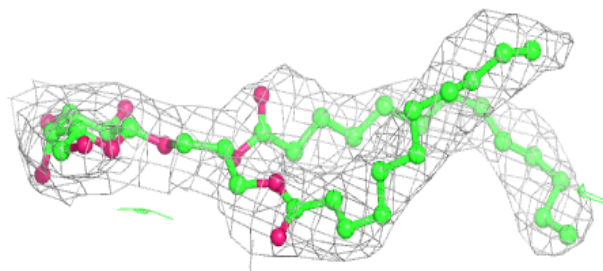
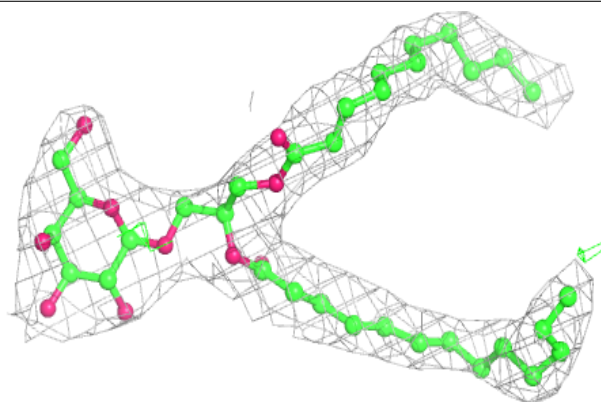


**Electron density around CLA B2 618:**

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

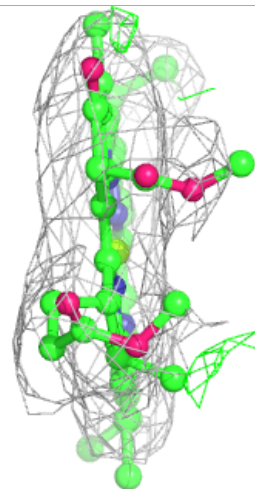
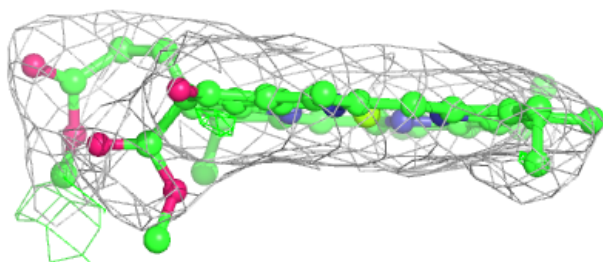
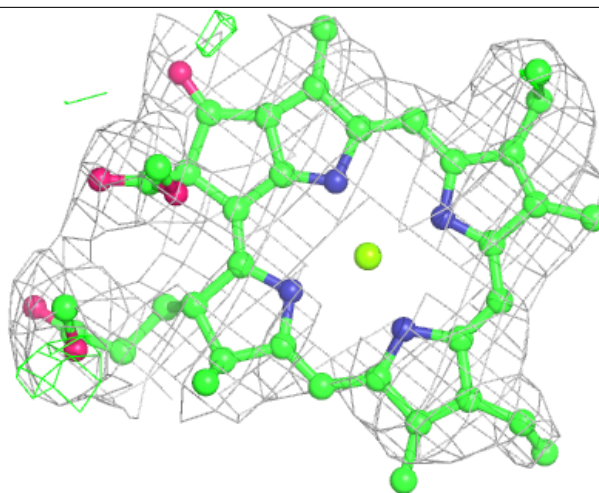
**Electron density around LMG A1 410:**

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



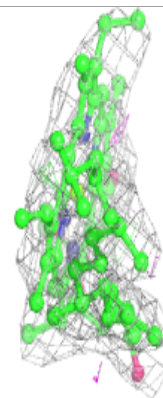
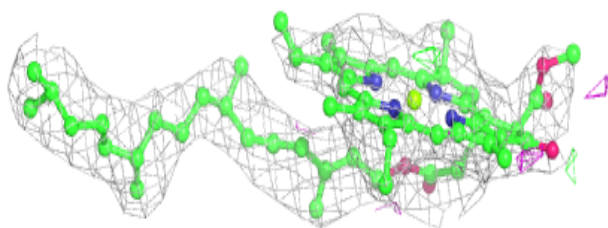
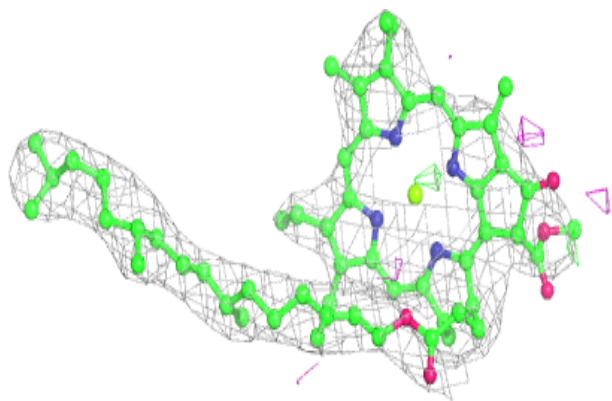
**Electron density around CLA C2 516:**

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

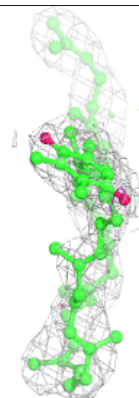
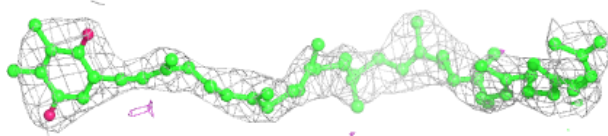
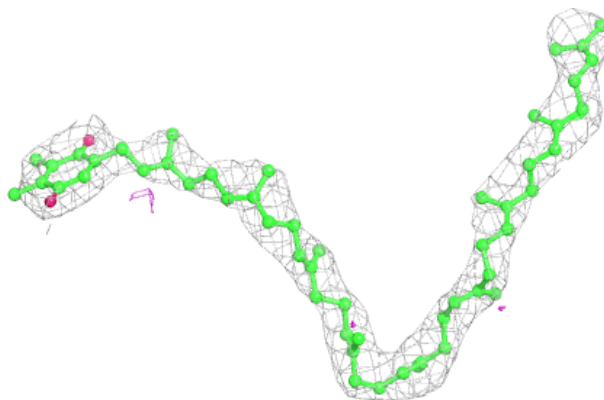


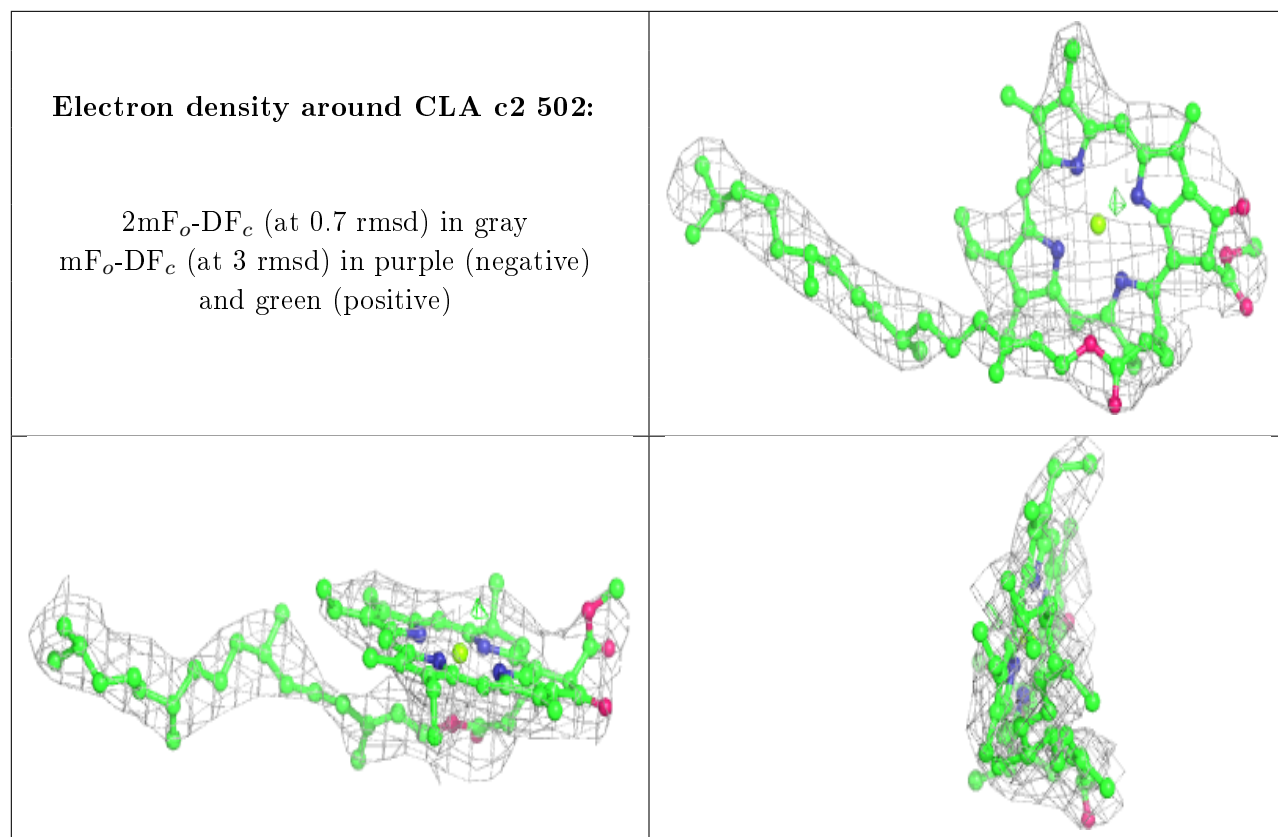
**Electron density around CLA C1 502:**

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

**Electron density around PL9 D2 408:**

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

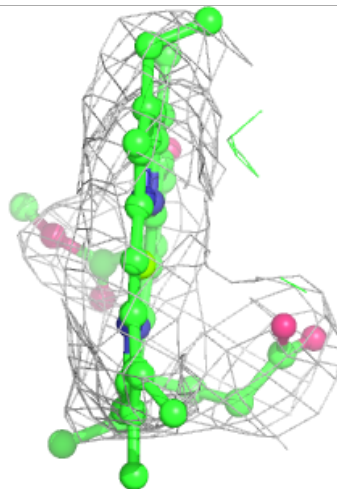
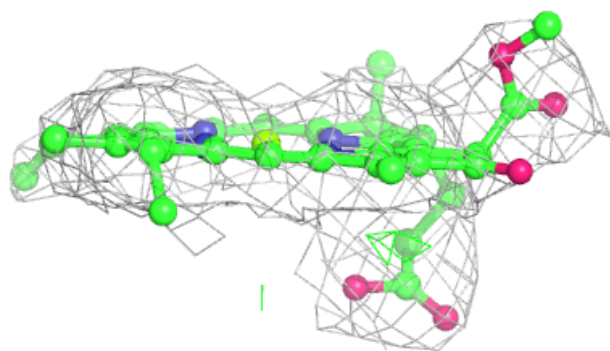
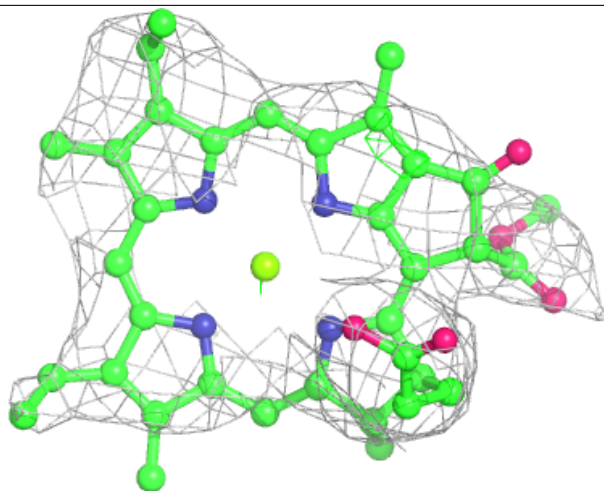






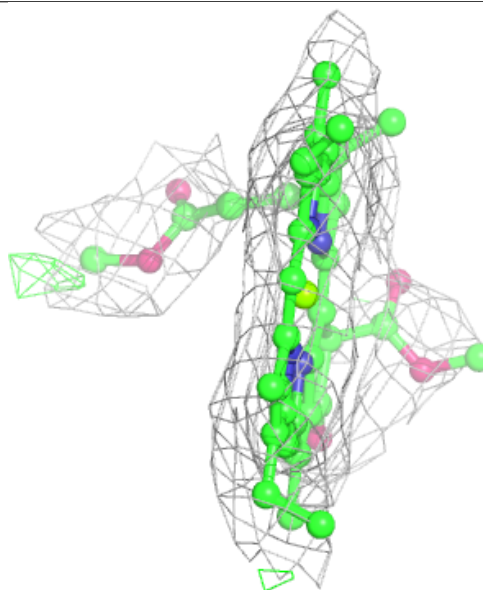
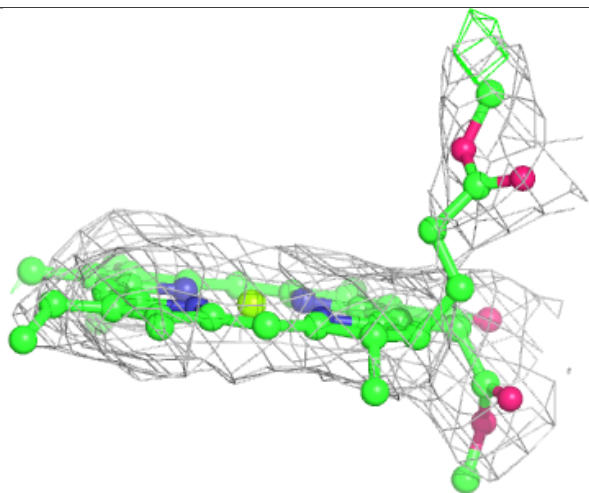
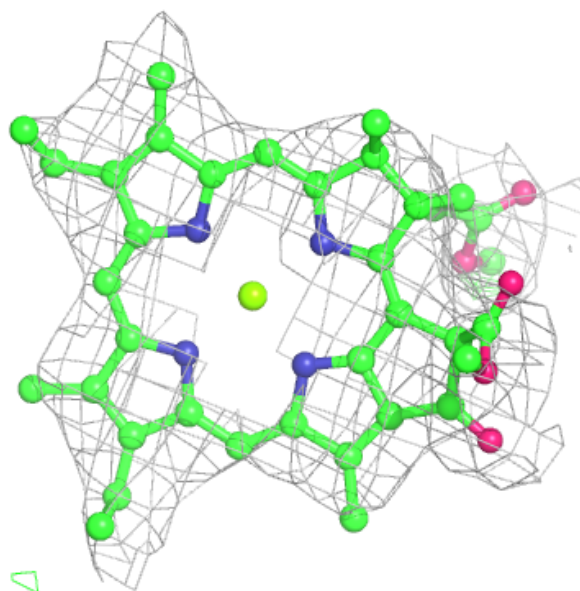
**Electron density around CLA C2 507:**

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



**Electron density around CLA C2 504:**

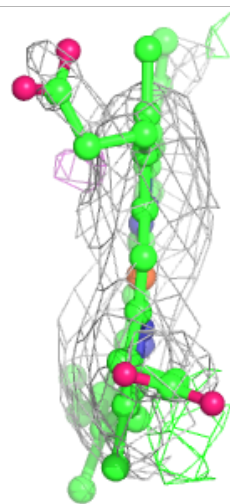
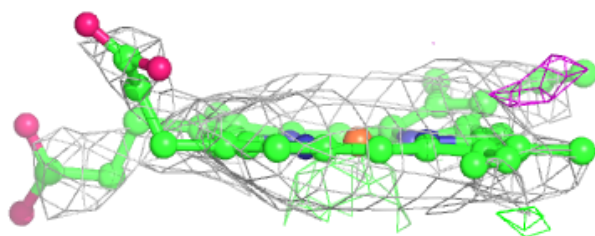
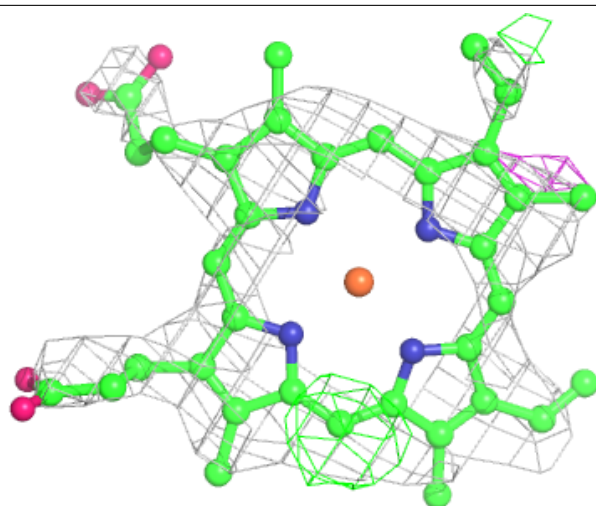
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





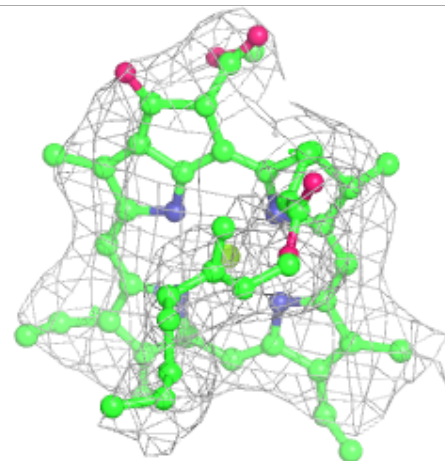
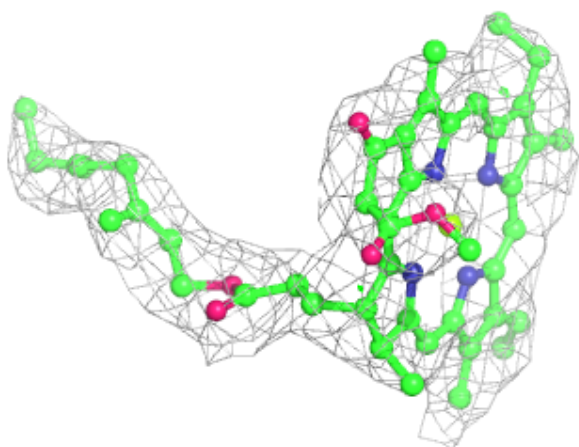
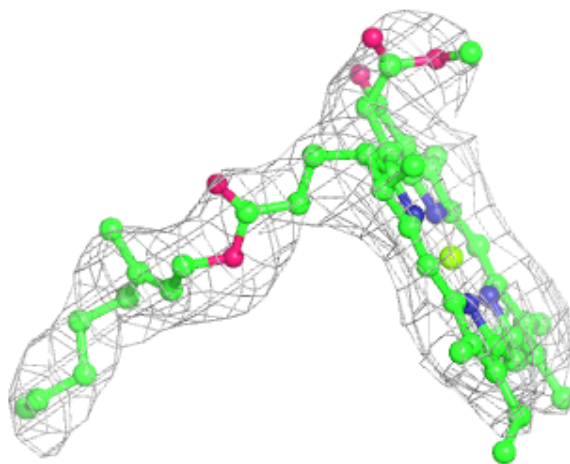
**Electron density around HEM V2 201:**

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



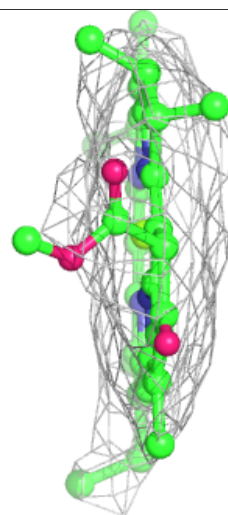
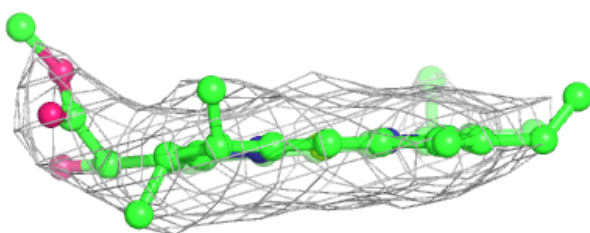
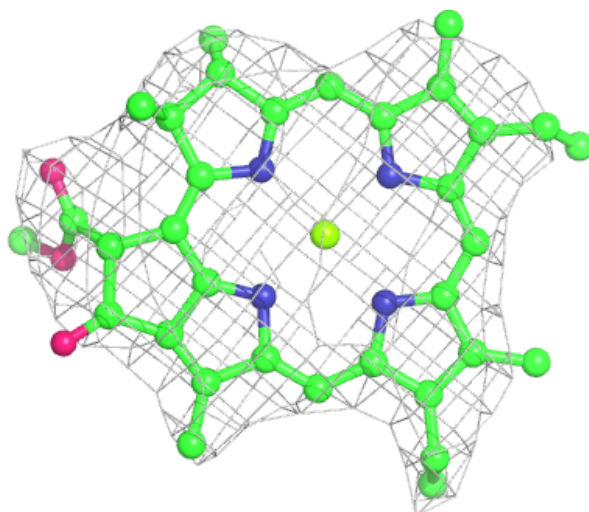
**Electron density around CLA c2 507:**

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



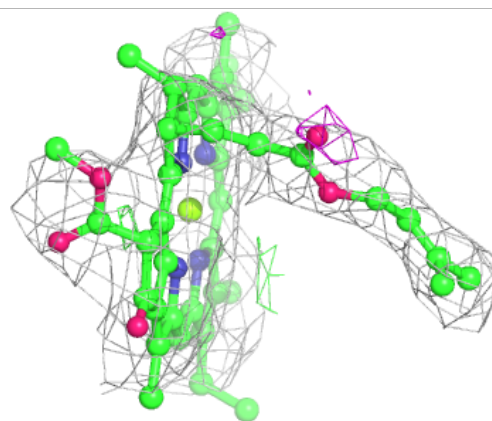
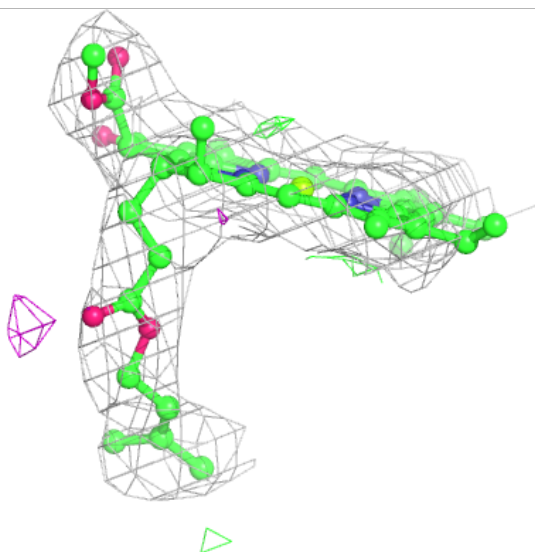
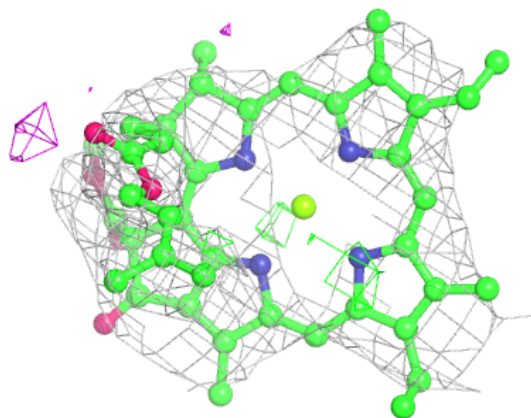
**Electron density around CLA B2 604:**

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



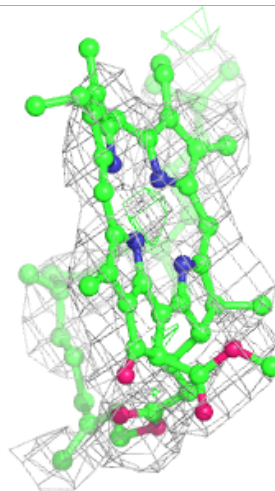
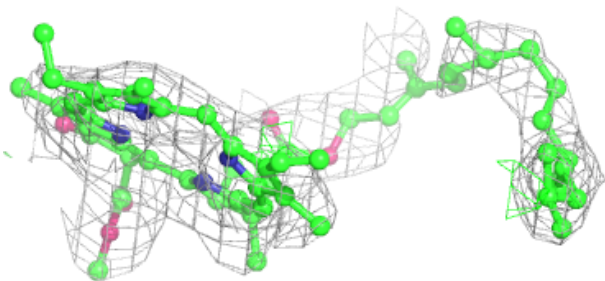
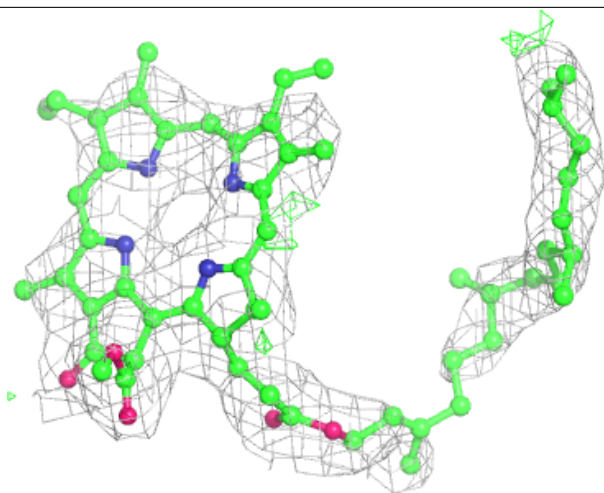
**Electron density around CLA C2 511:**

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



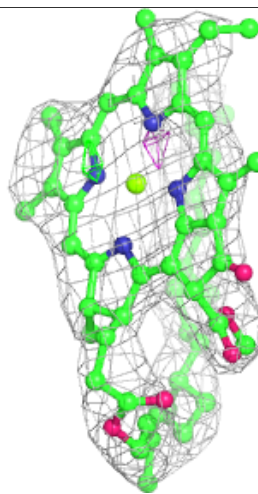
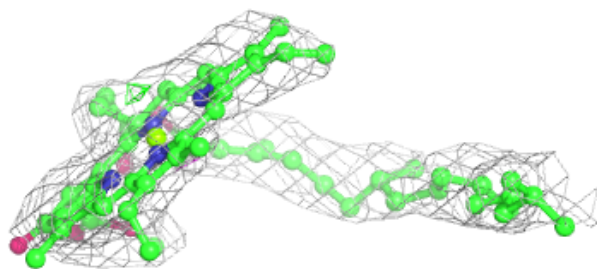
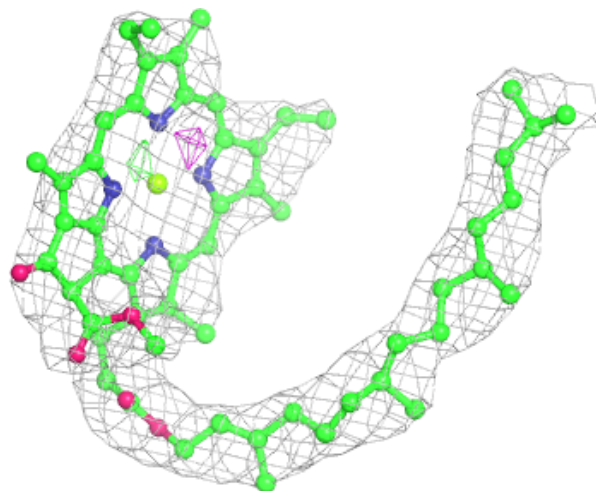
**Electron density around PHO D2 407:**

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



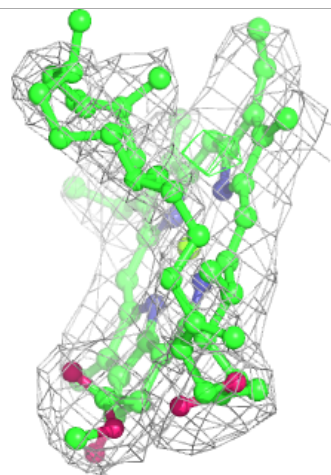
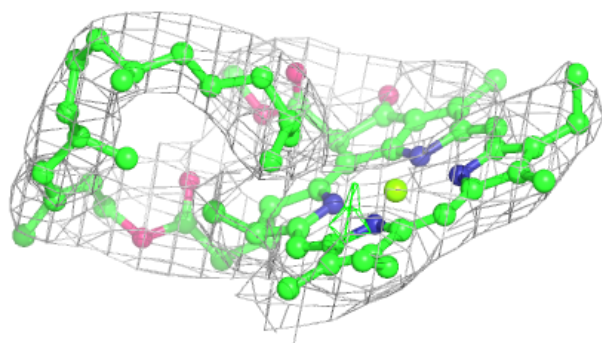
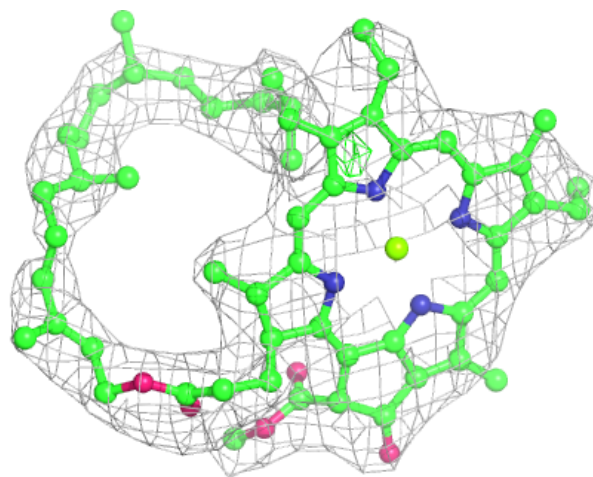
**Electron density around CLA c1 509:**

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



**Electron density around CLA B1 617:**

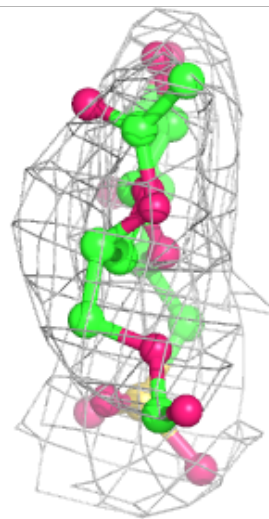
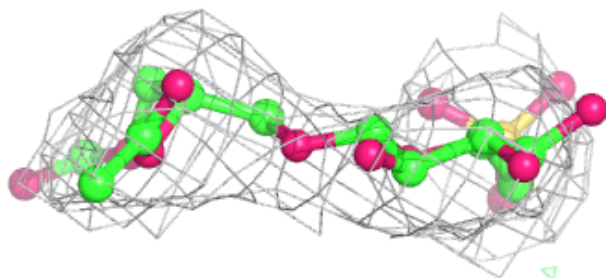
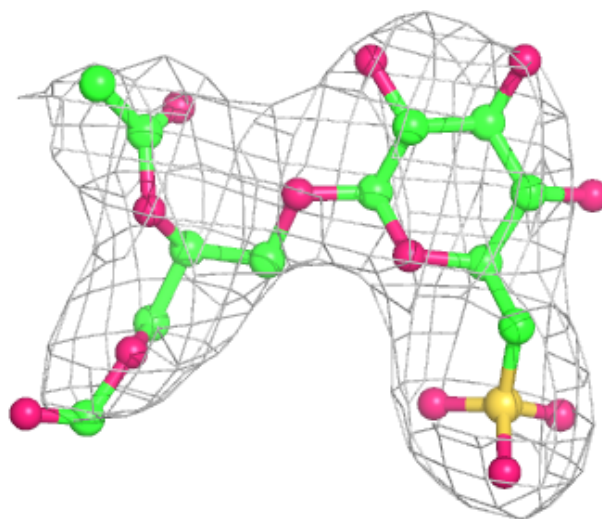
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



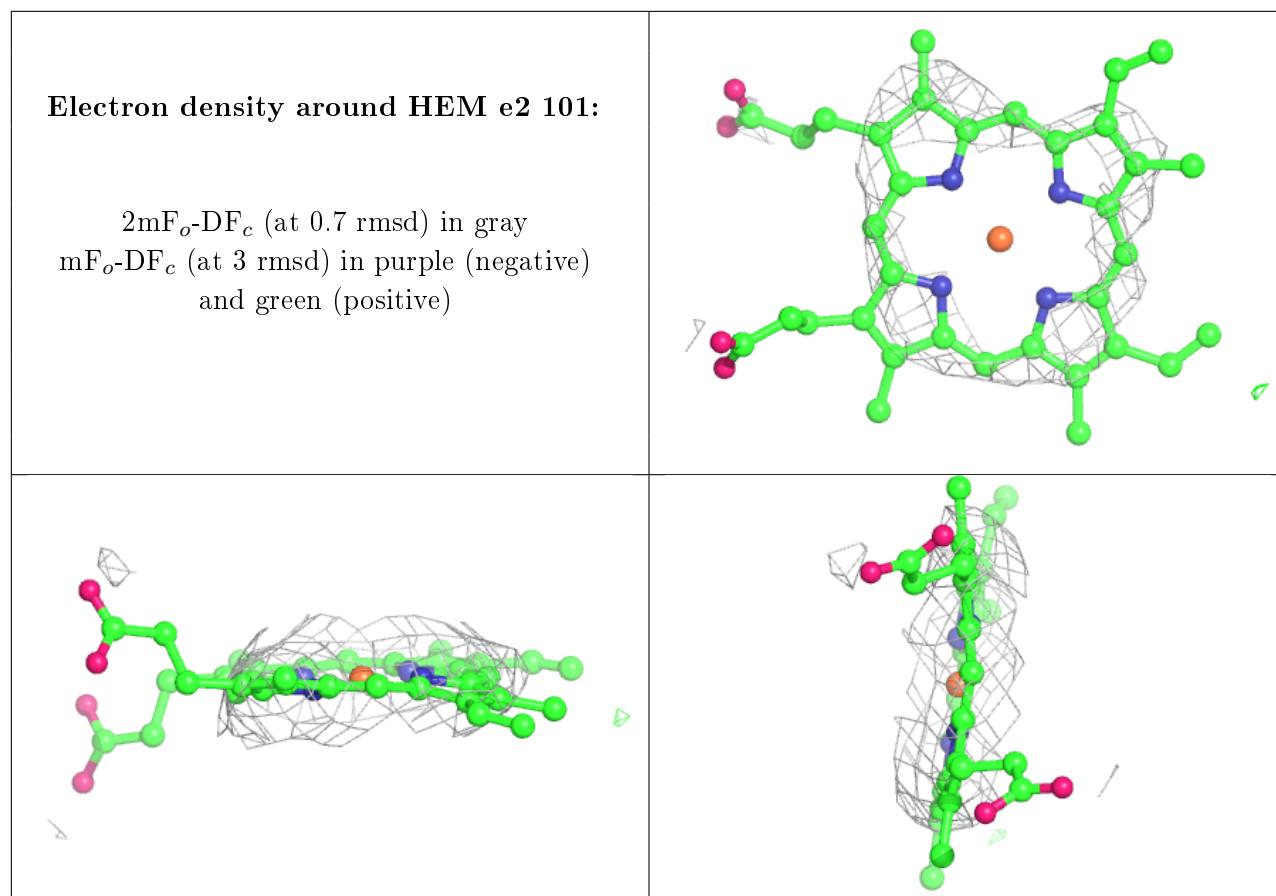


**Electron density around SQD D2 402:**

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

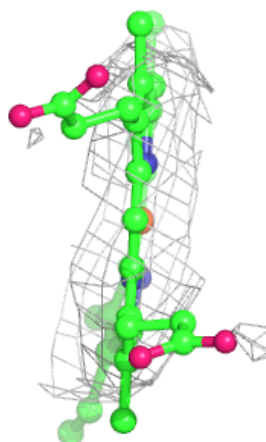
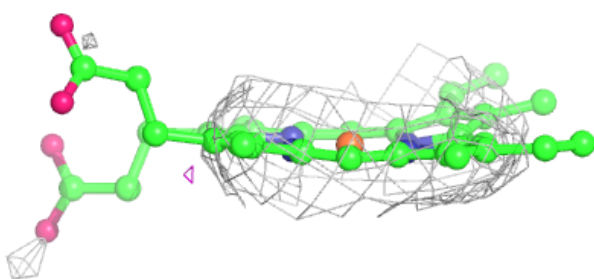
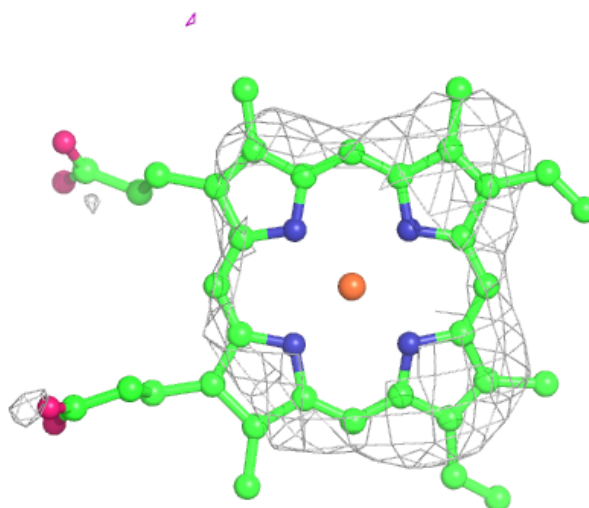






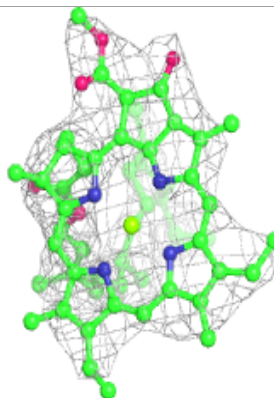
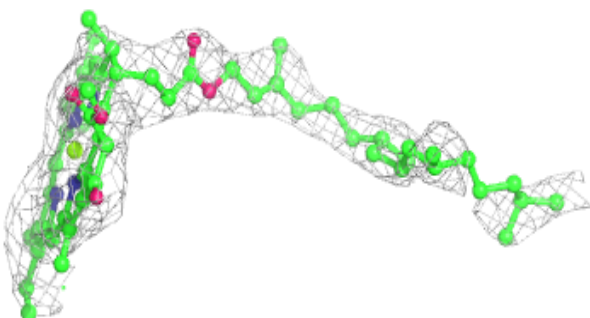
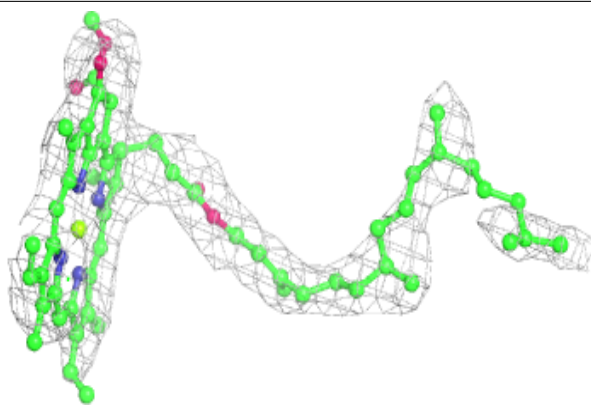
**Electron density around HEM E1 101:**

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

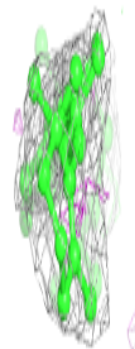
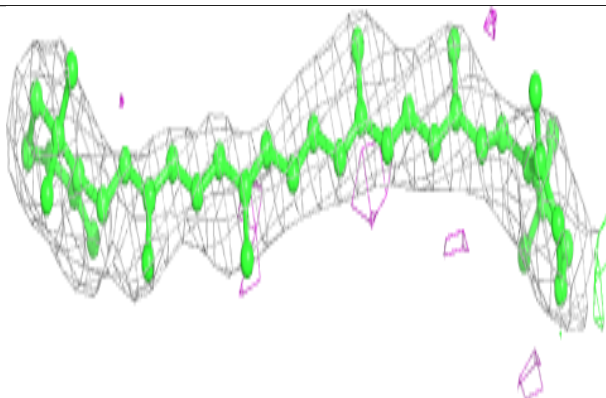
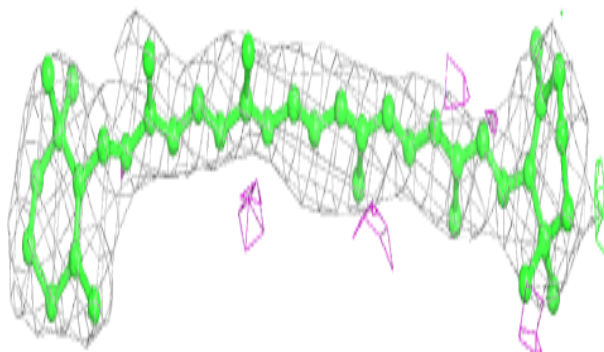


**Electron density around CLA B1 609:**

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

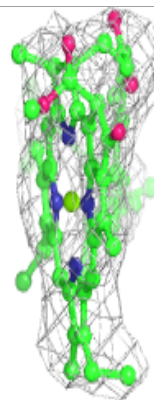
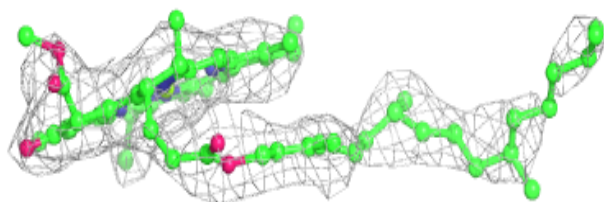
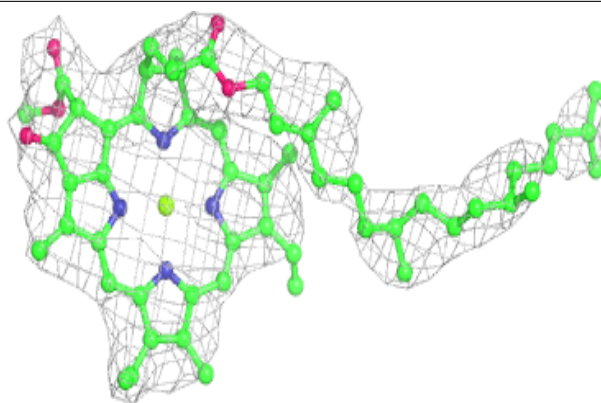
**Electron density around BCR B2 603:**

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

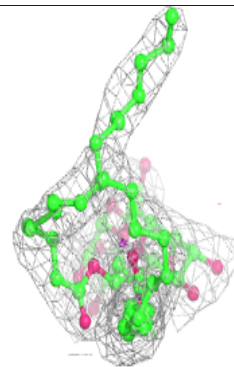
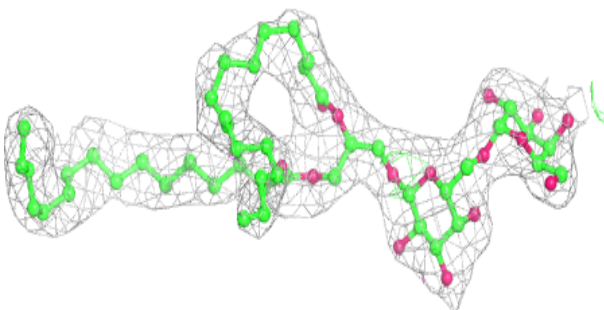
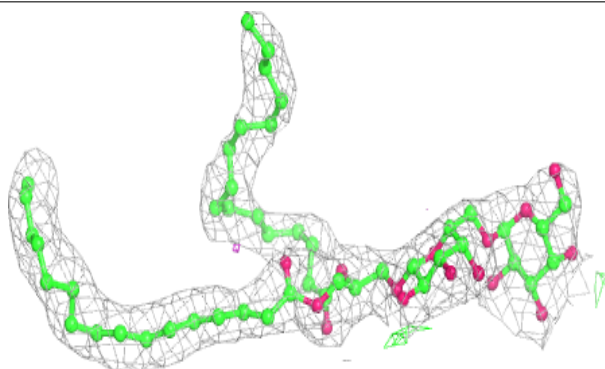


**Electron density around CLA B2 606:**

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

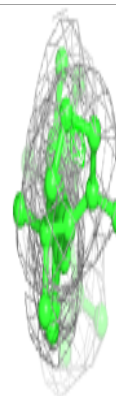
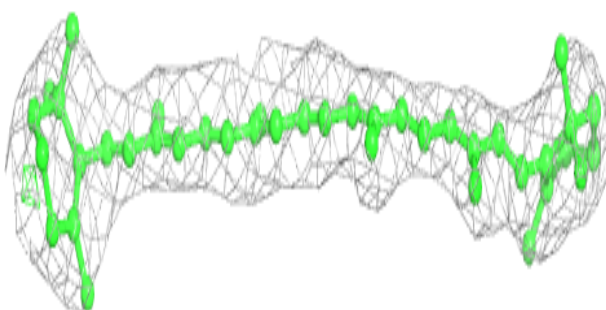
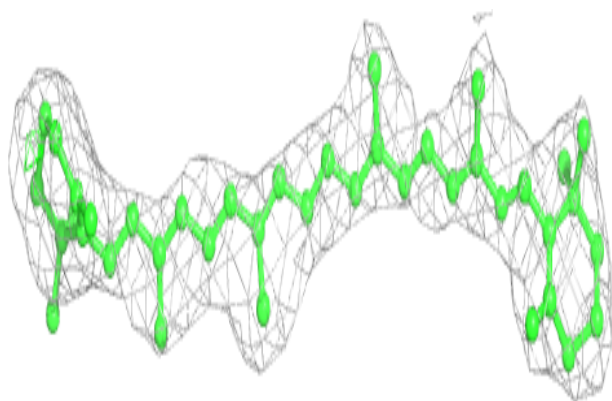
**Electron density around DGD h1 101:**

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

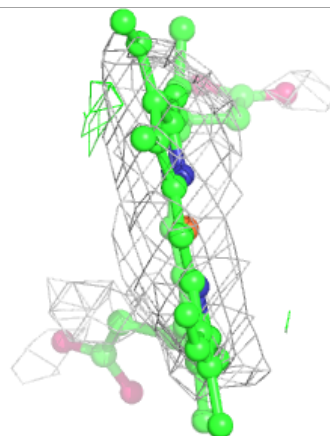
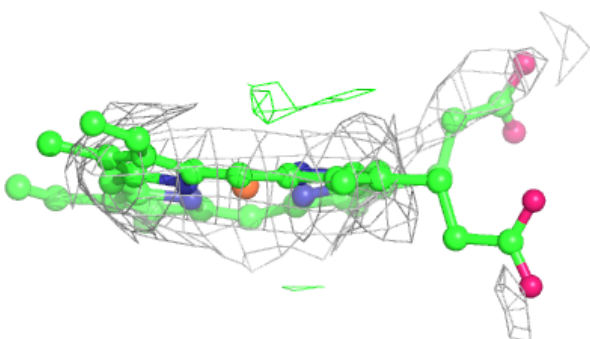
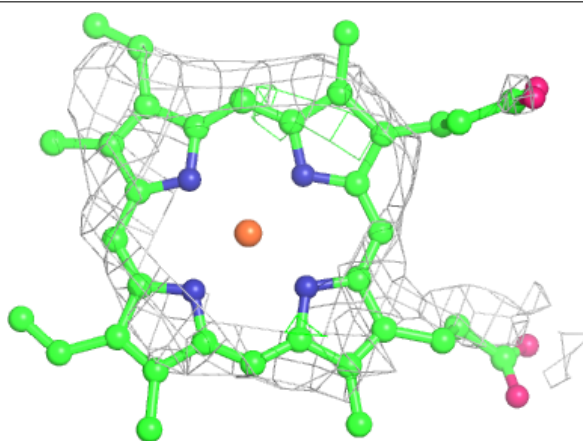


**Electron density around BCR b2 601:**

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

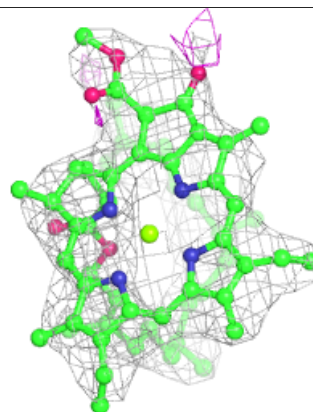
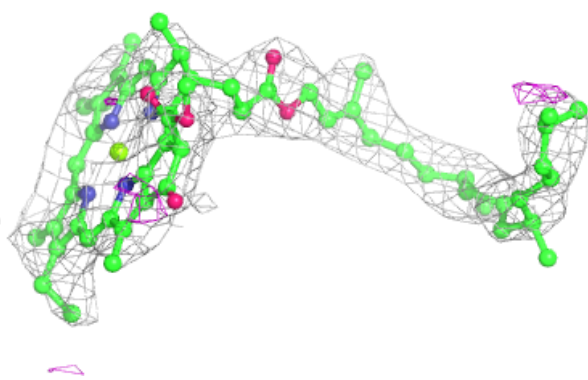
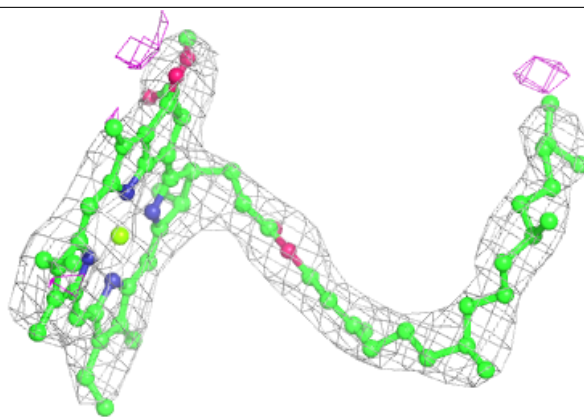
**Electron density around HEM E2 101:**

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



**Electron density around CLA B2 609:**

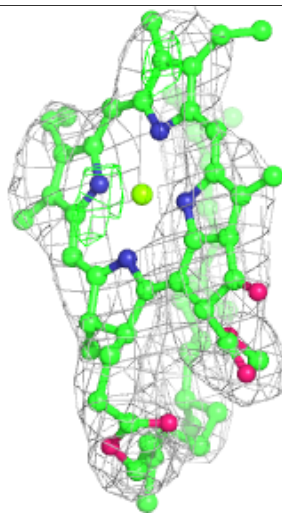
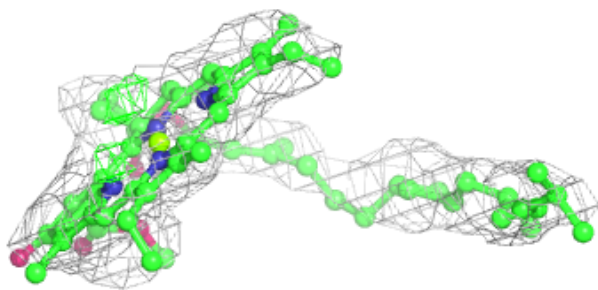
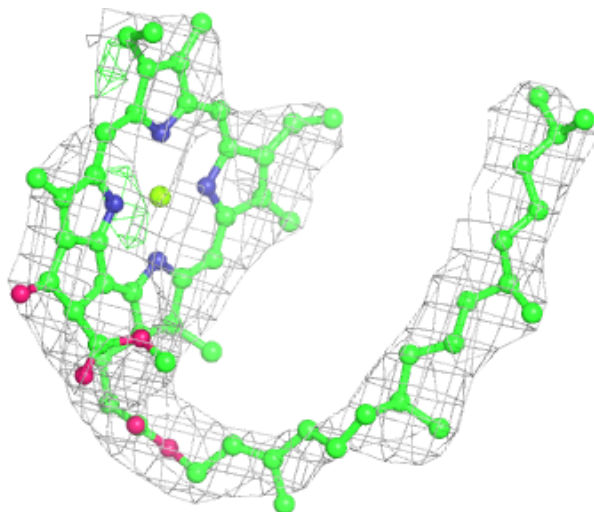
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





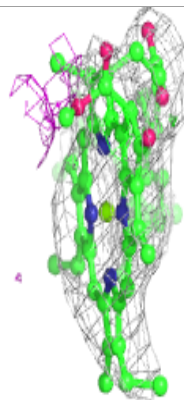
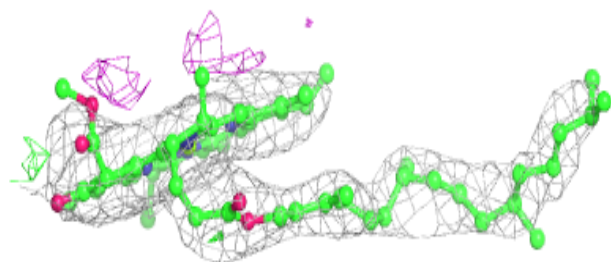
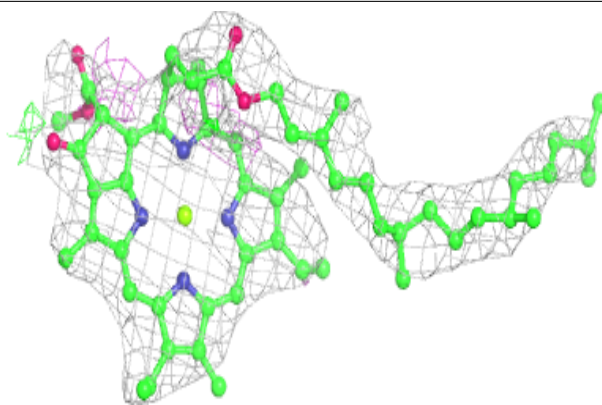
**Electron density around CLA c2 508:**

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



**Electron density around CLA b2 606:**

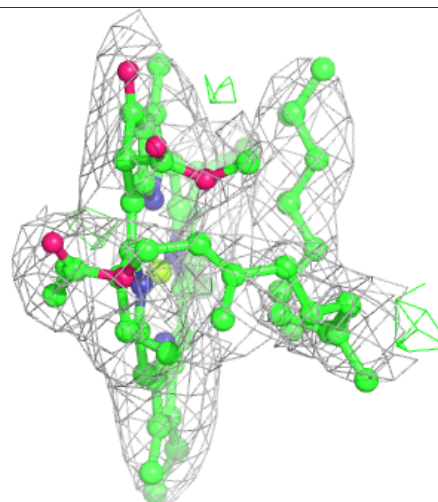
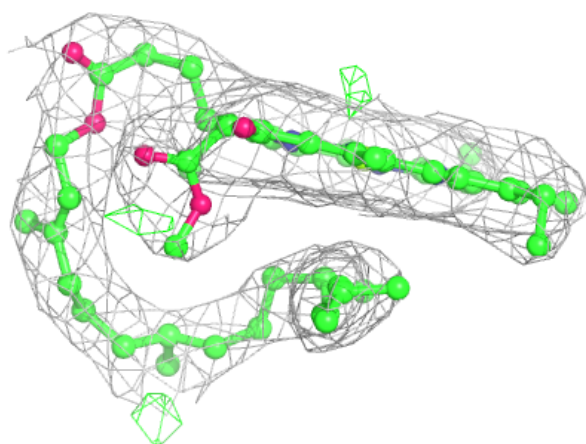
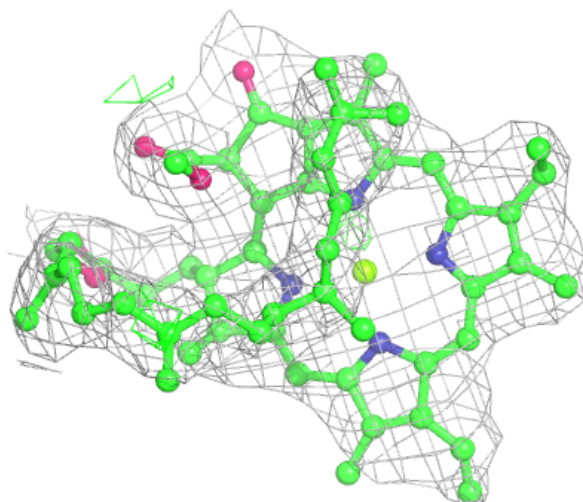
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





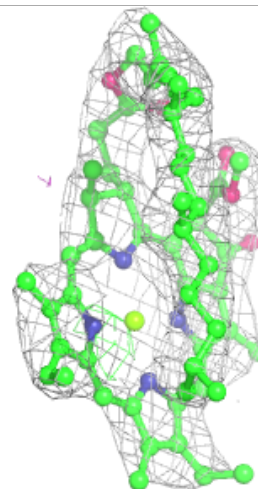
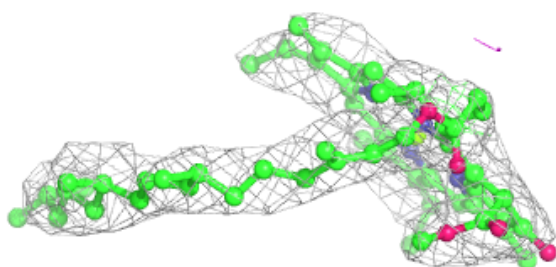
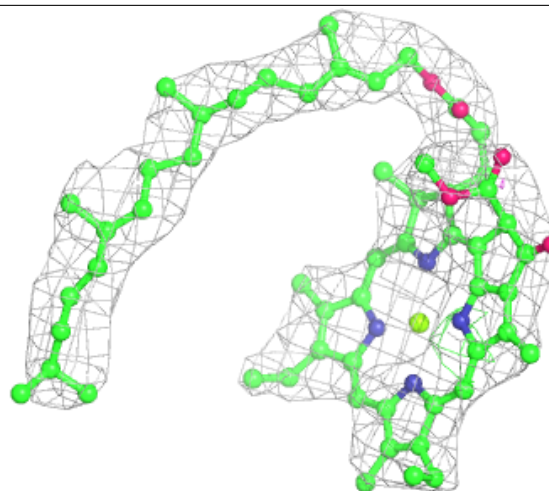
**Electron density around CLA C1 511:**

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



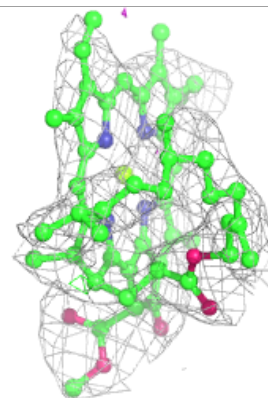
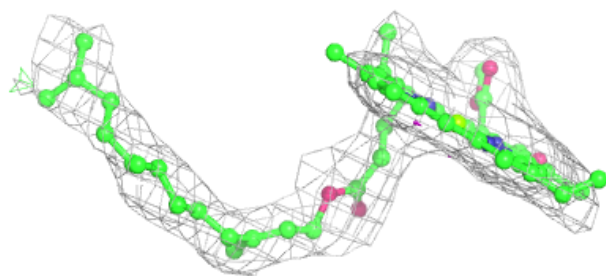
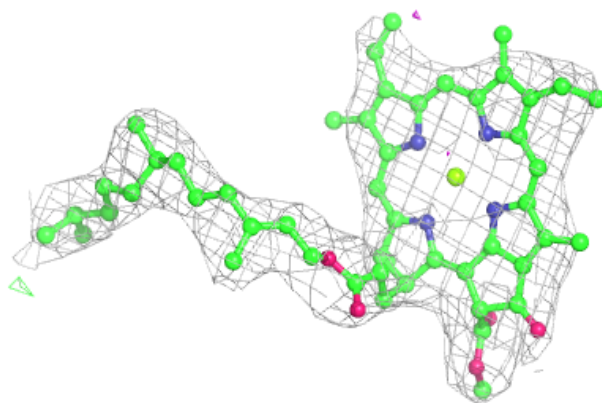
**Electron density around CLA C1 508:**

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

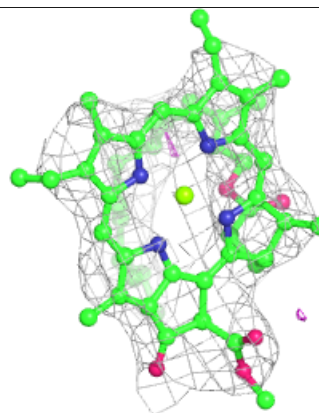
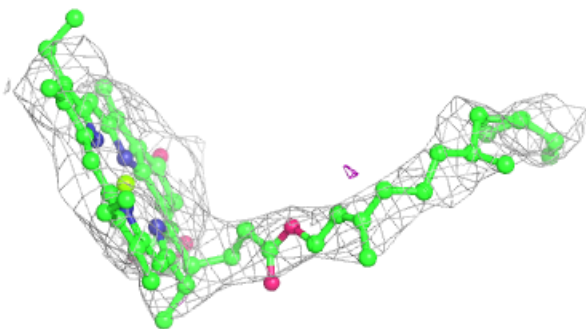
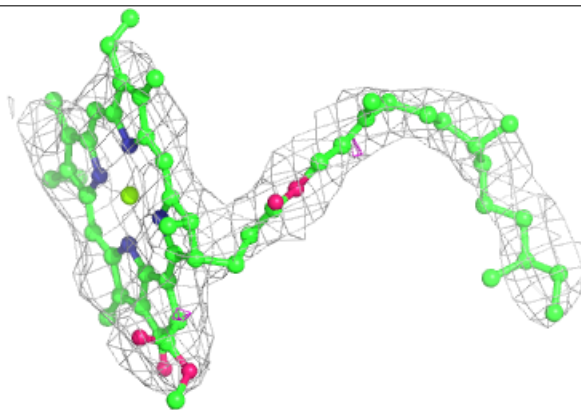


**Electron density around CLA a1 404:**

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

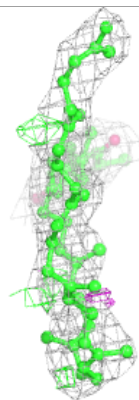
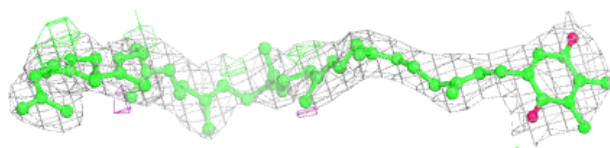
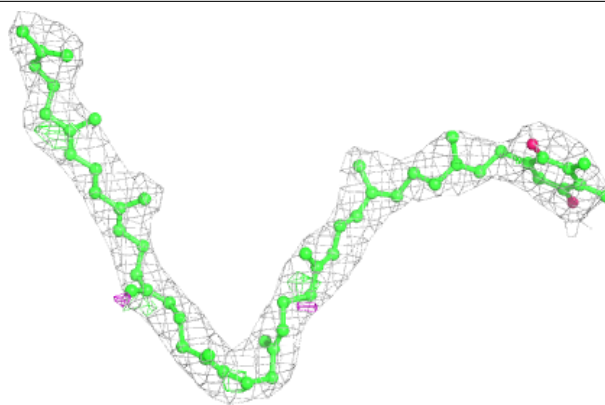
**Electron density around CLA b2 609:**

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

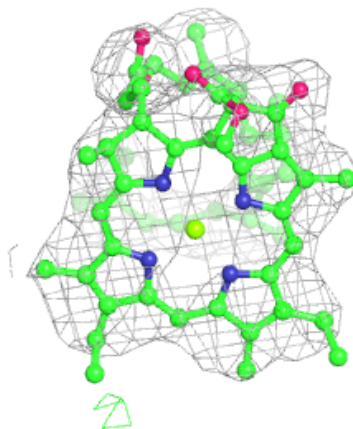
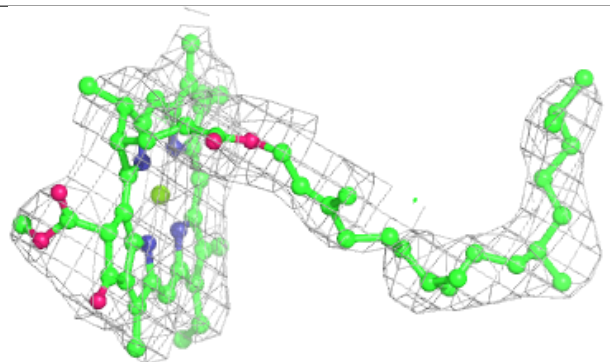
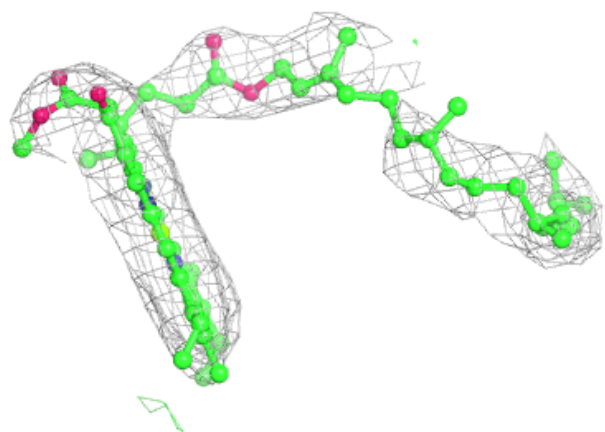


**Electron density around PL9 d1 409:**

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

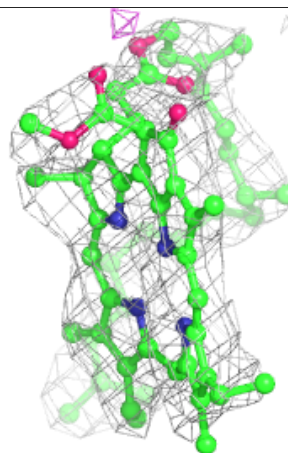
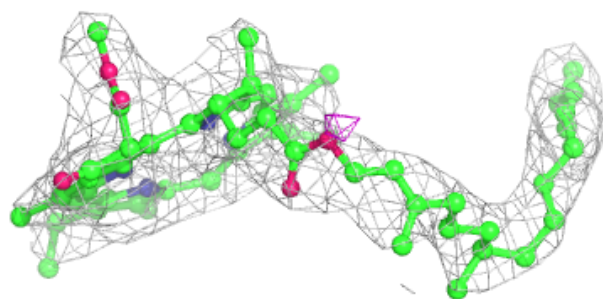
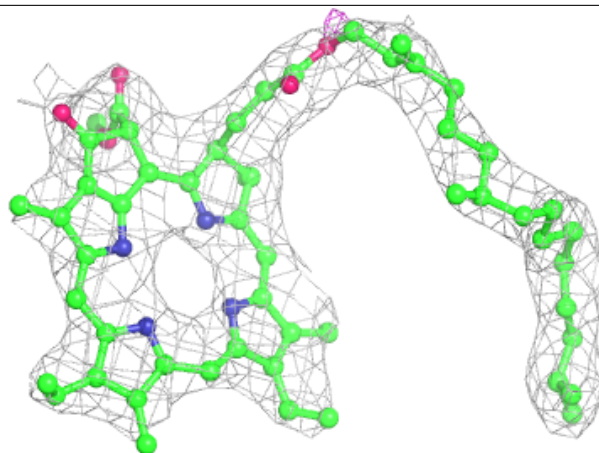
**Electron density around CLA C1 507:**

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

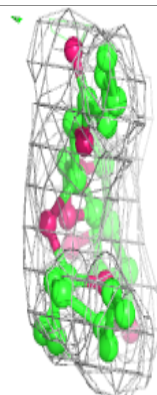
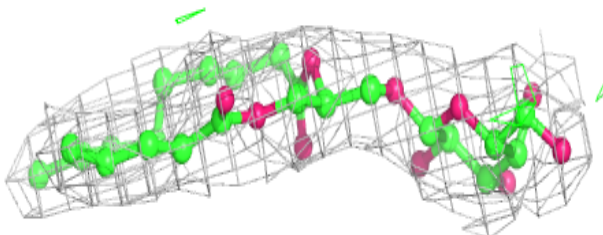
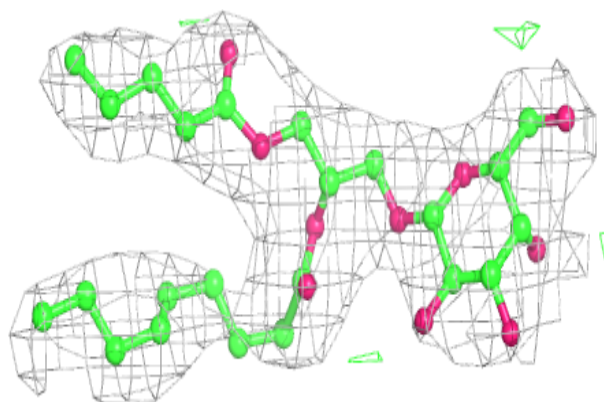


**Electron density around PHO D1 407:**

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

**Electron density around LMG d1 408:**

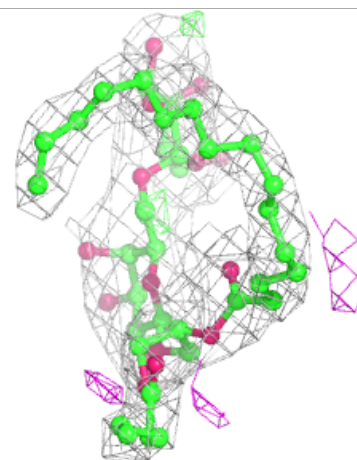
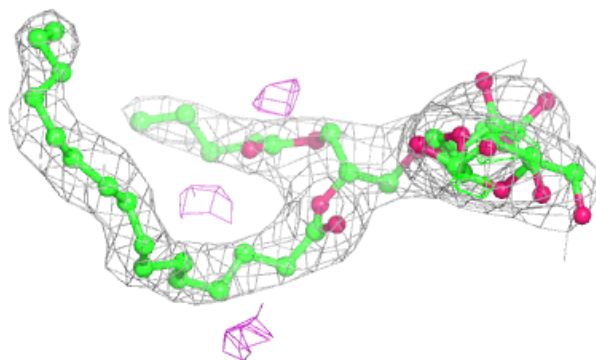
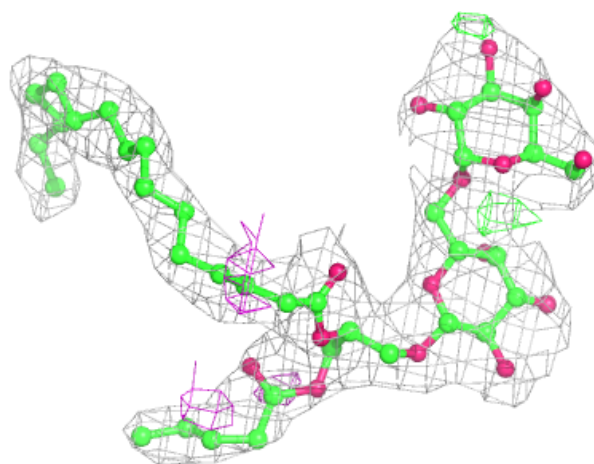
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





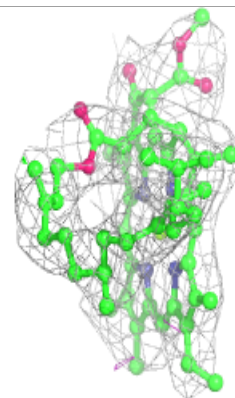
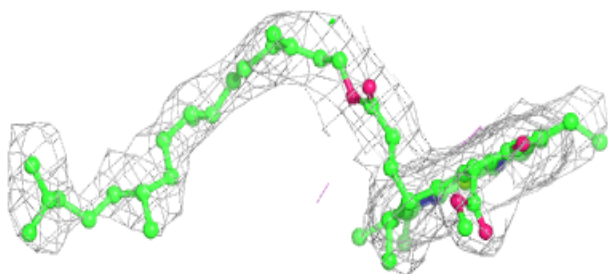
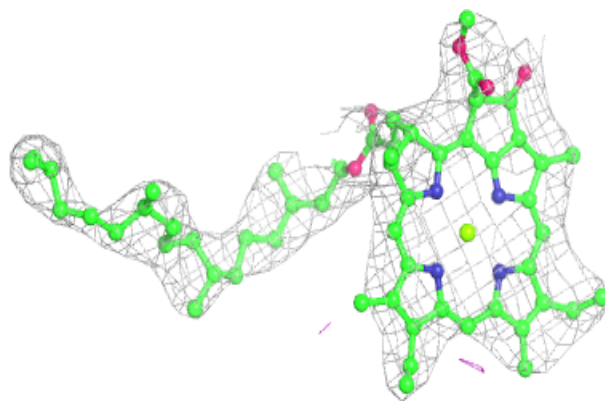
**Electron density around DGD c1 514:**

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

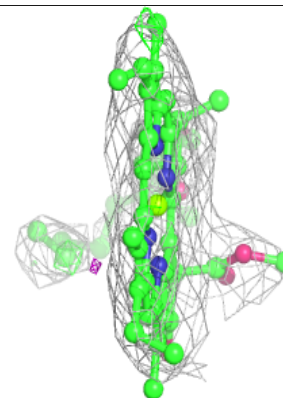
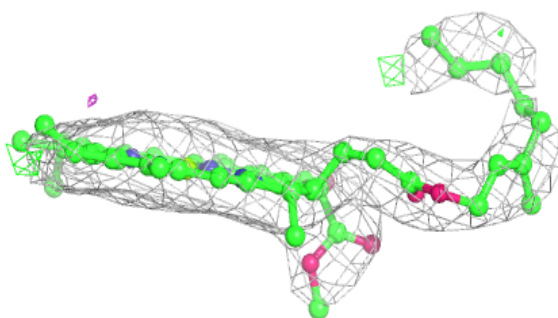
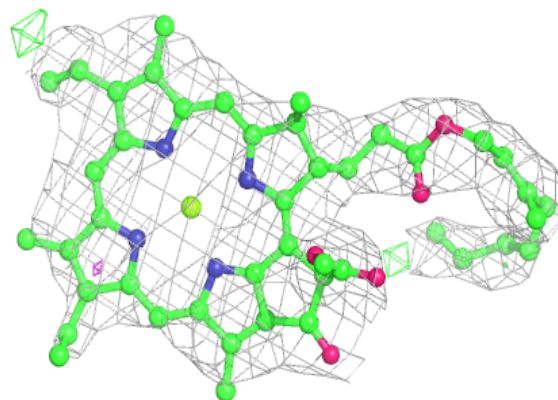


**Electron density around CLA a2 405:**

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

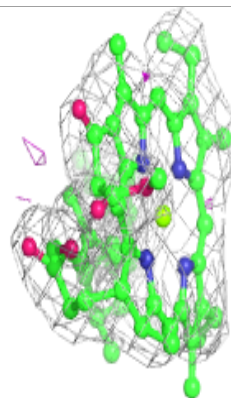
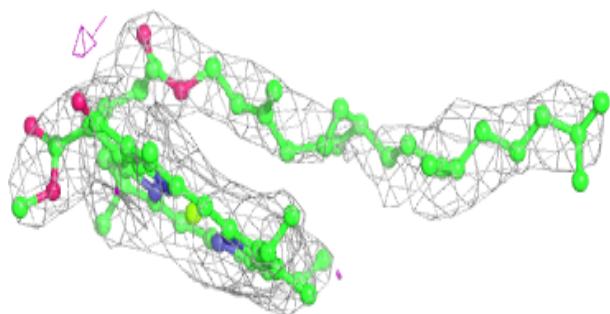
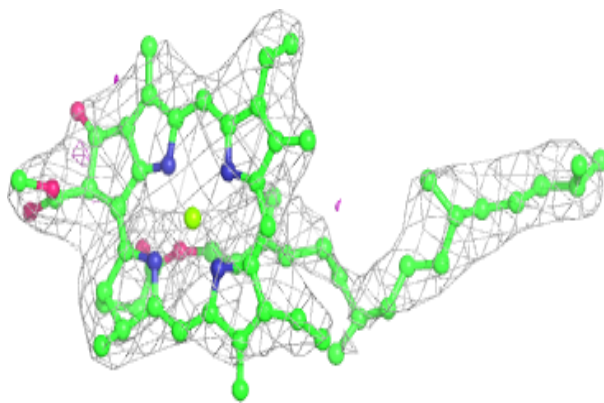
**Electron density around CLA c2 510:**

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

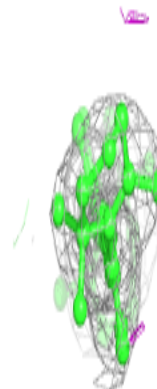
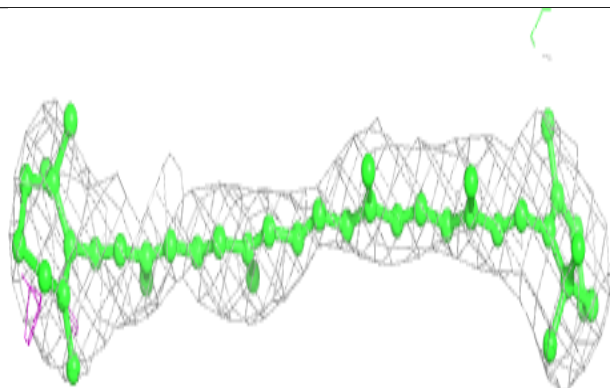
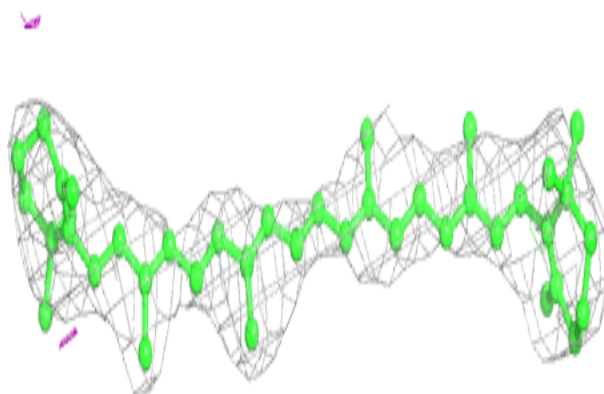


**Electron density around CLA C1 506:**

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

**Electron density around BCR A2 401:**

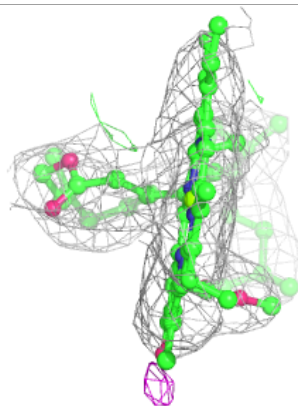
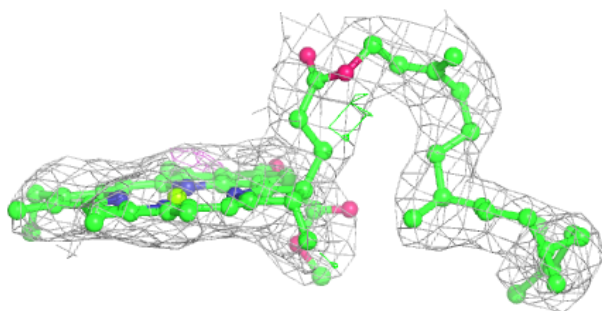
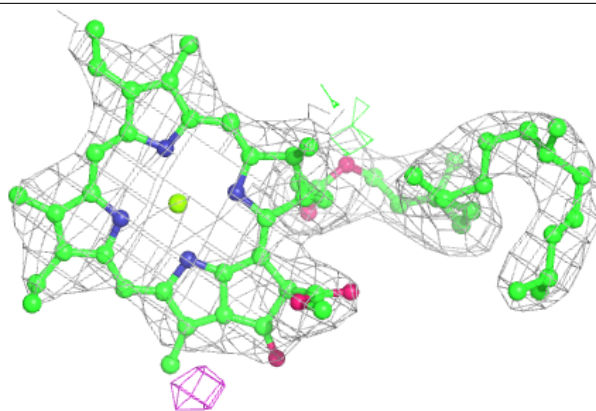
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



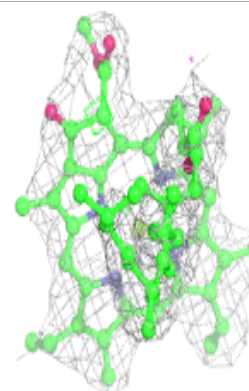
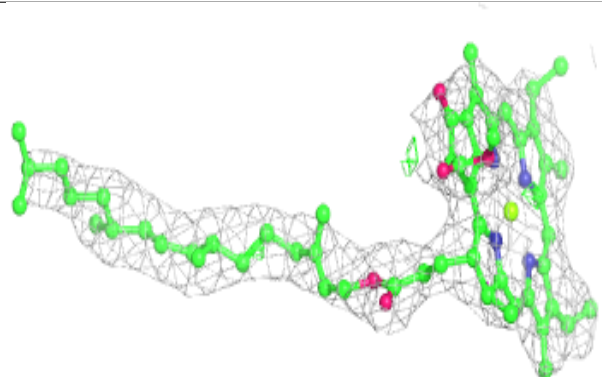
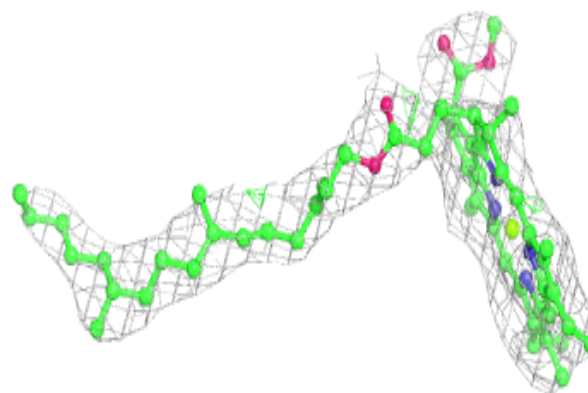


**Electron density around CLA B2 614:**

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

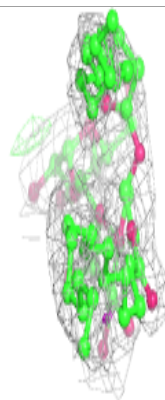
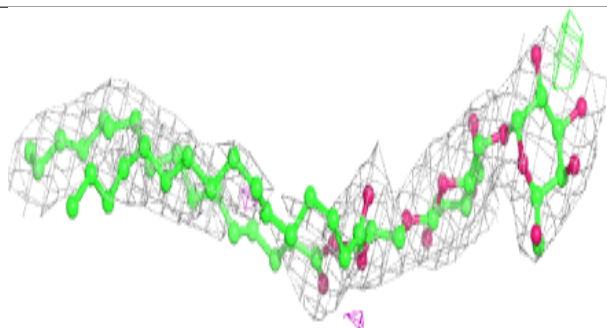
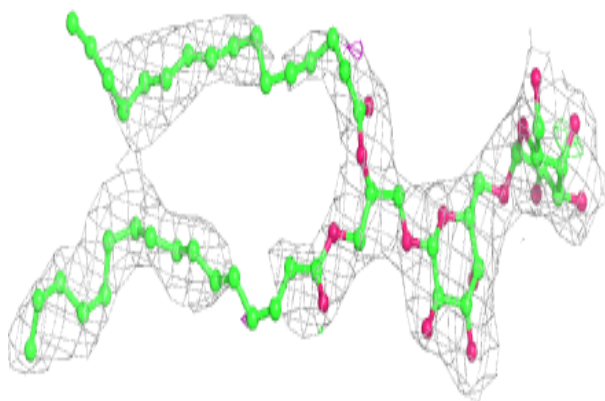
**Electron density around CLA B2 607:**

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

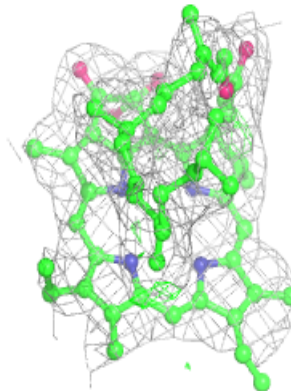
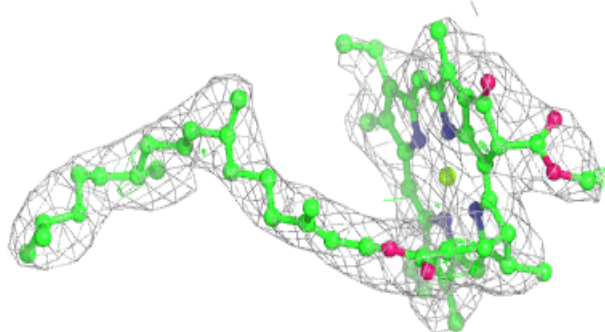
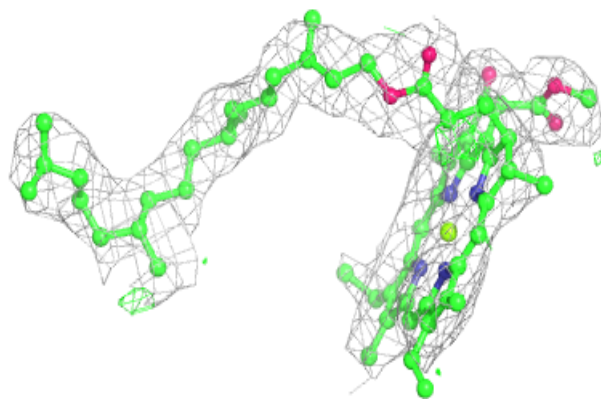


**Electron density around DGD c1 520:**

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

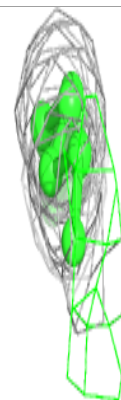
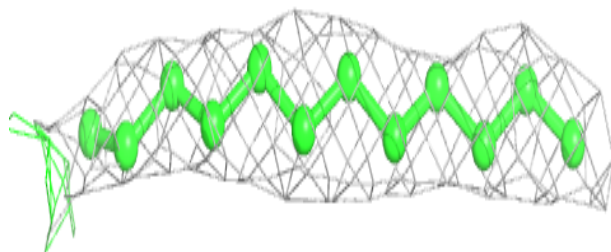
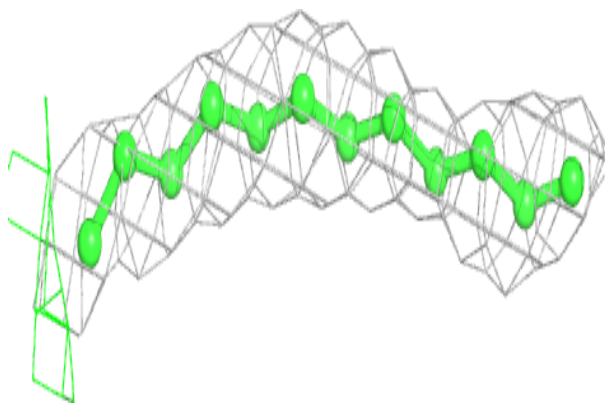
**Electron density around CLA c1 510:**

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

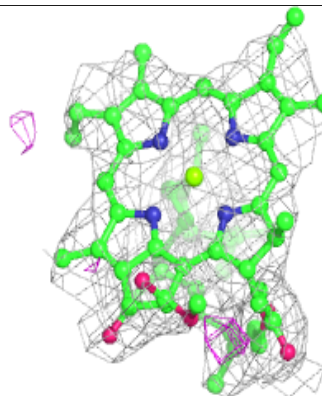
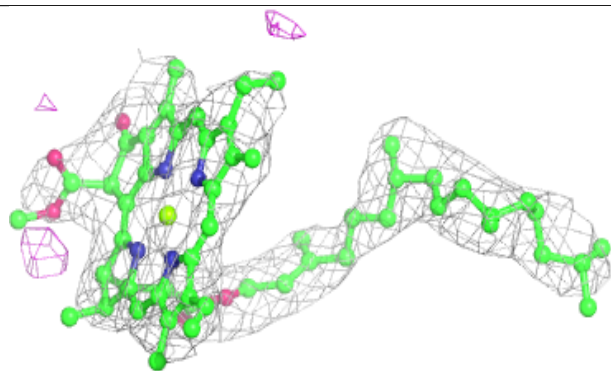
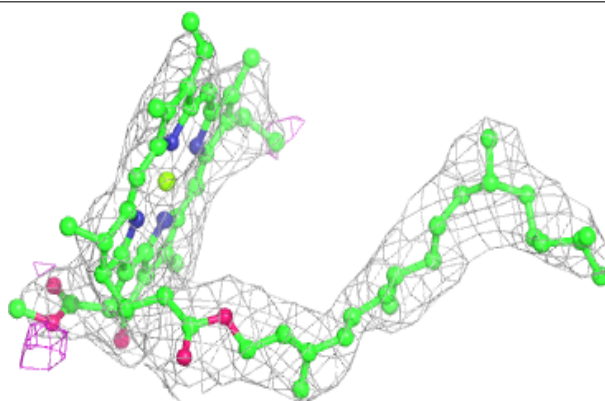


**Electron density around LMT L1 102:**

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

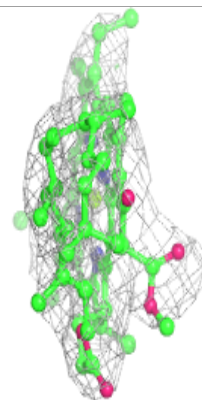
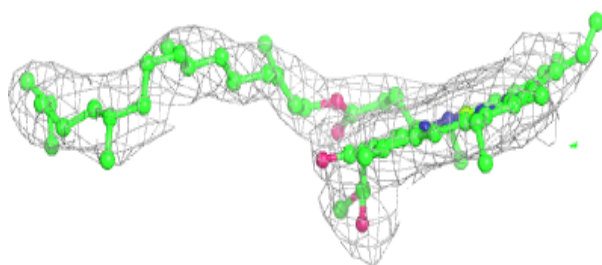
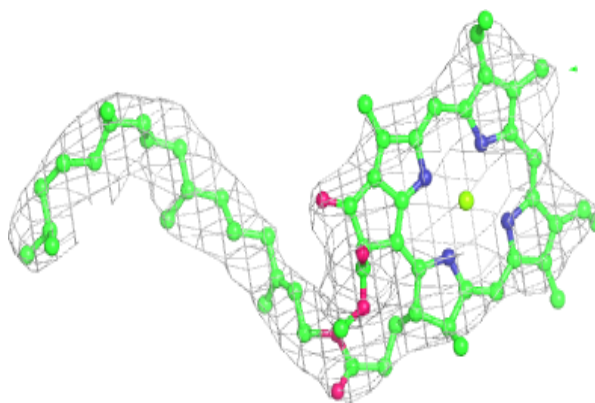
**Electron density around CLA c2 509:**

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

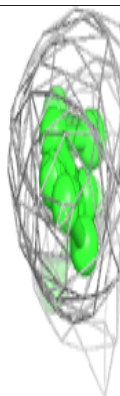
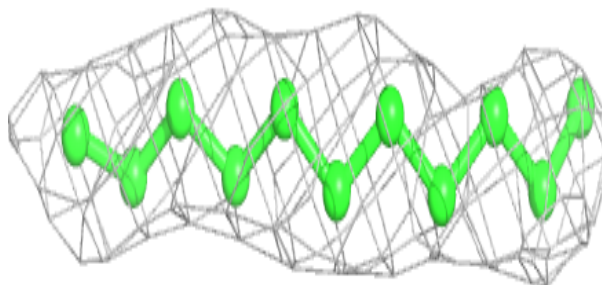
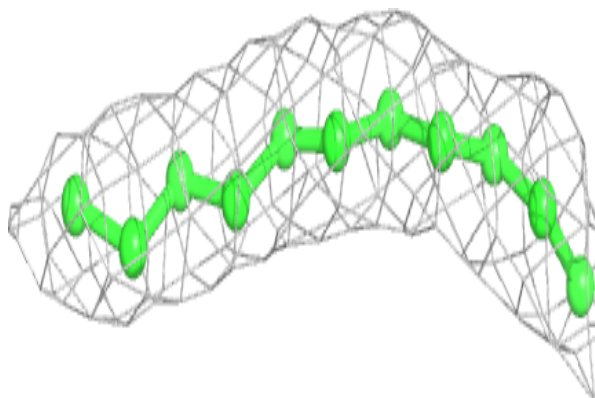


**Electron density around CLA B2 605:**

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

**Electron density around LMT M1 102:**

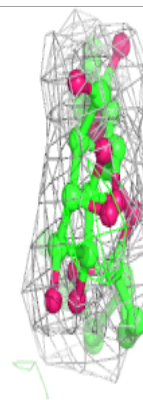
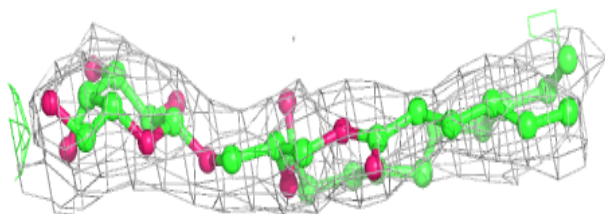
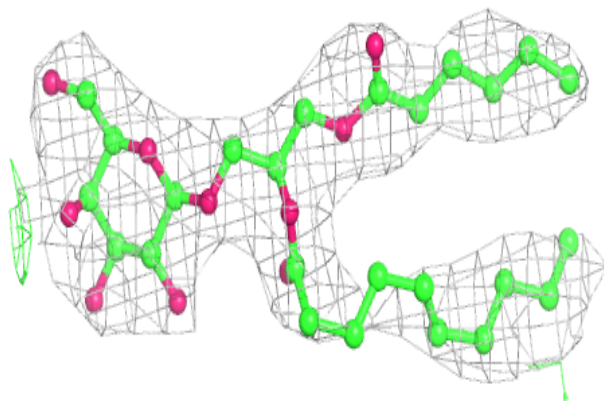
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



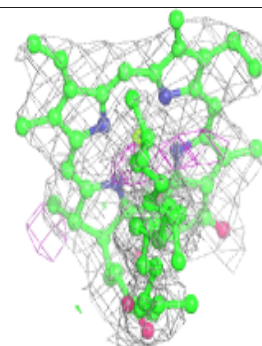
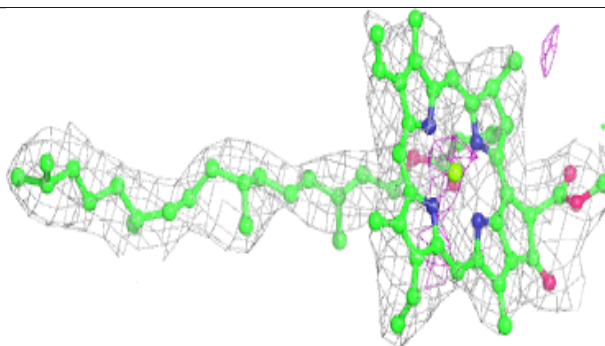
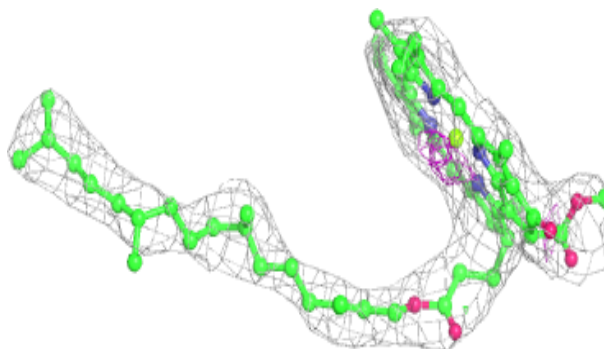


**Electron density around LMG D1 406:**

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

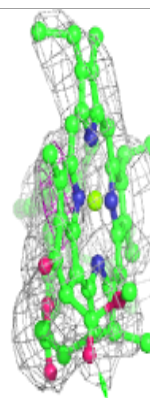
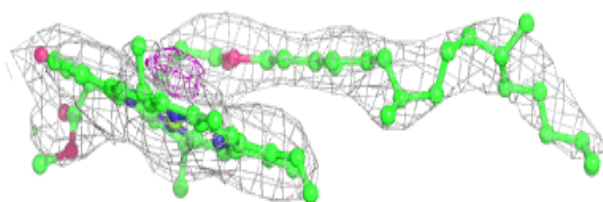
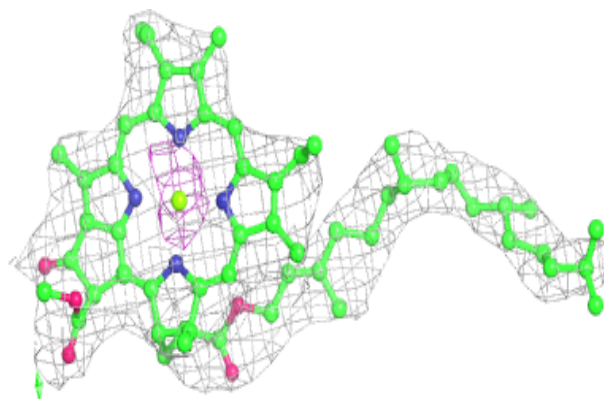
**Electron density around CLA c1 506:**

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

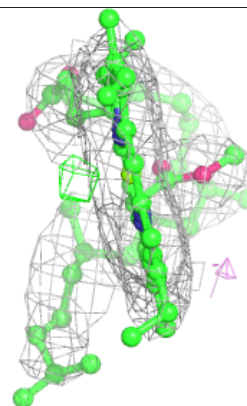
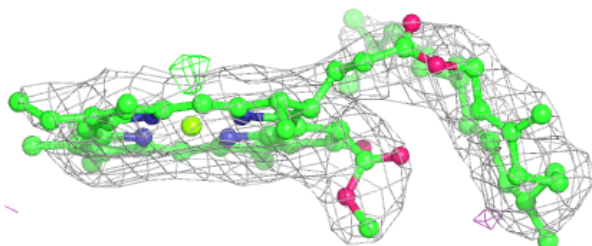
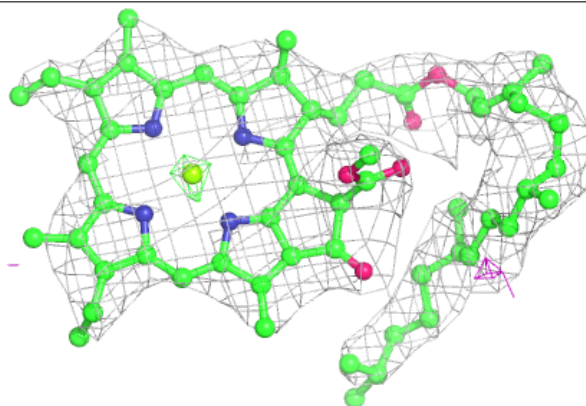


**Electron density around CLA B1 606:**

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

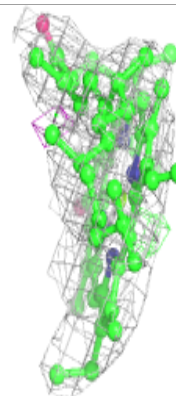
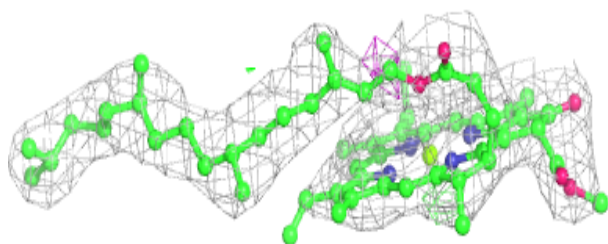
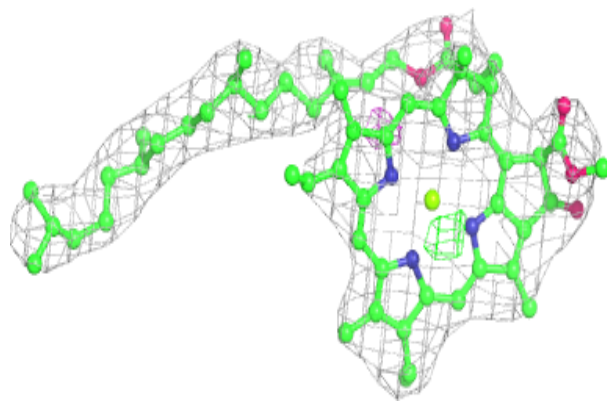
**Electron density around CLA B2 612:**

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



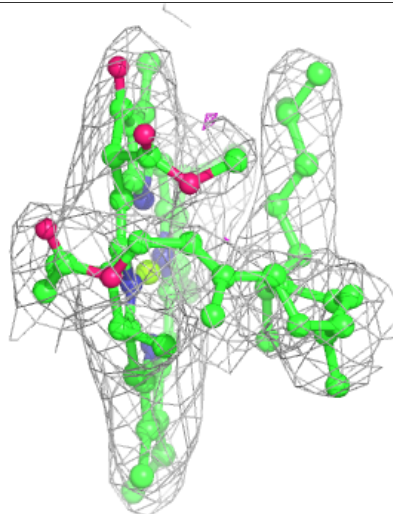
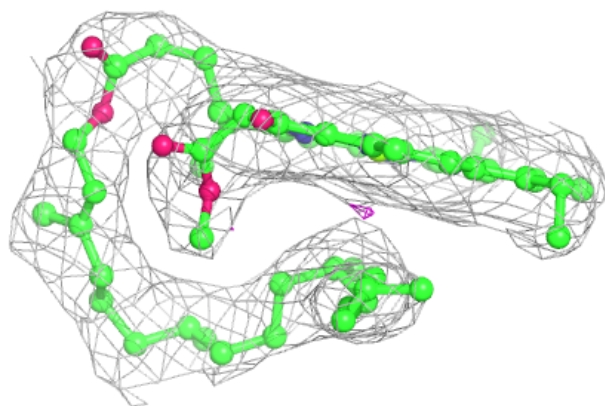
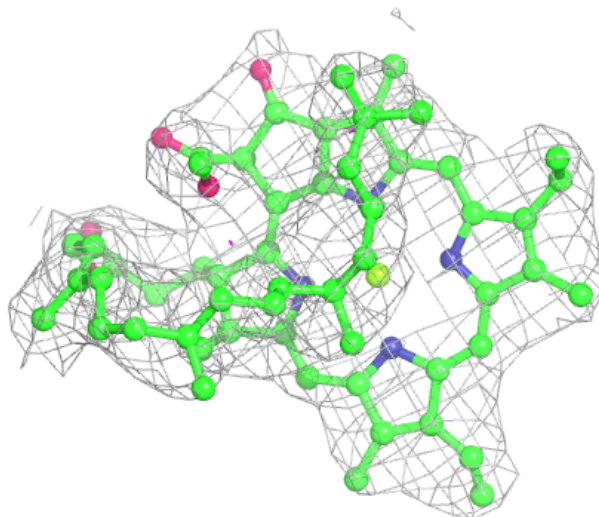
**Electron density around CLA c1 503:**

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

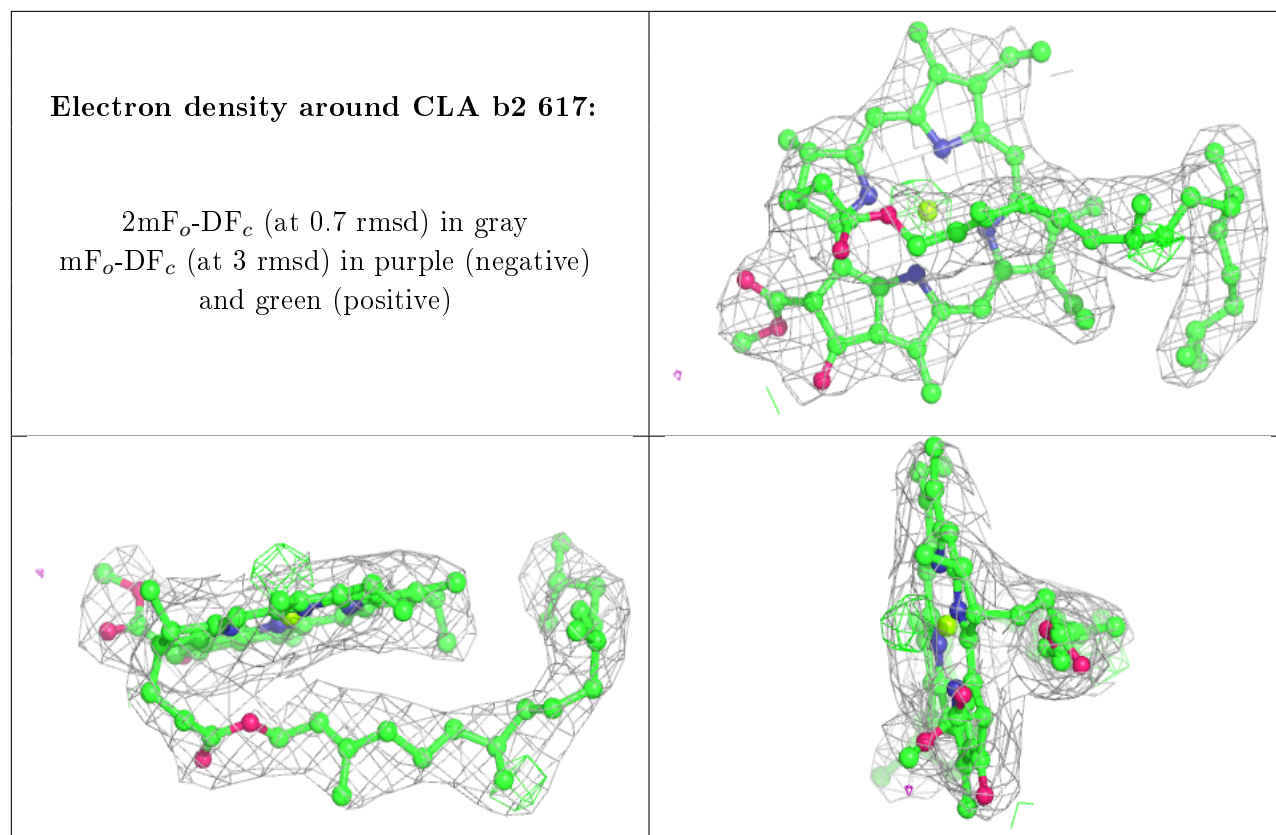


**Electron density around CLA c2 511:**

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

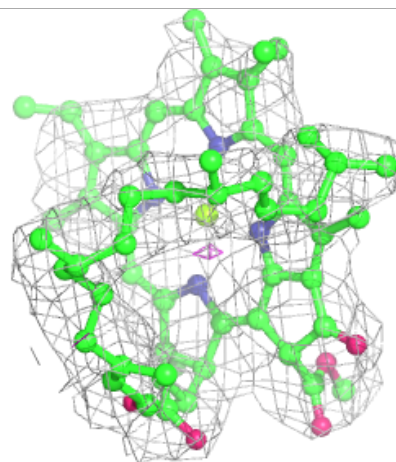
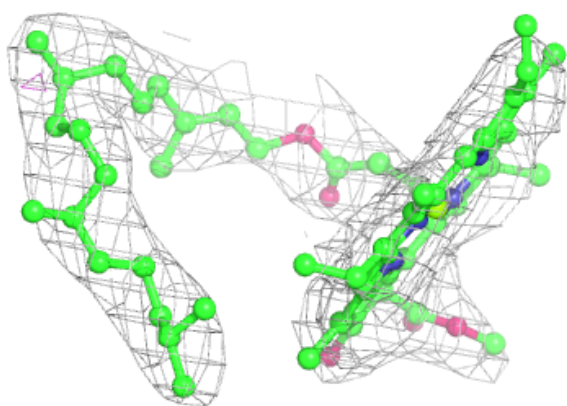
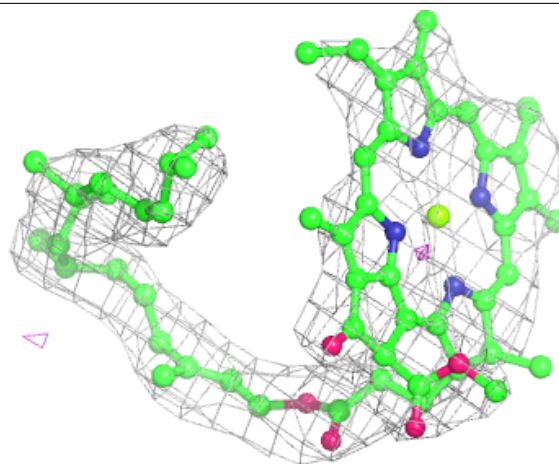






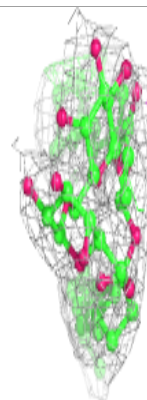
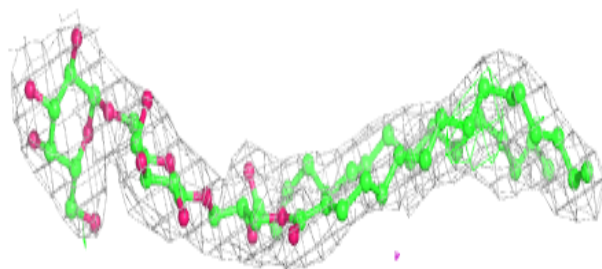
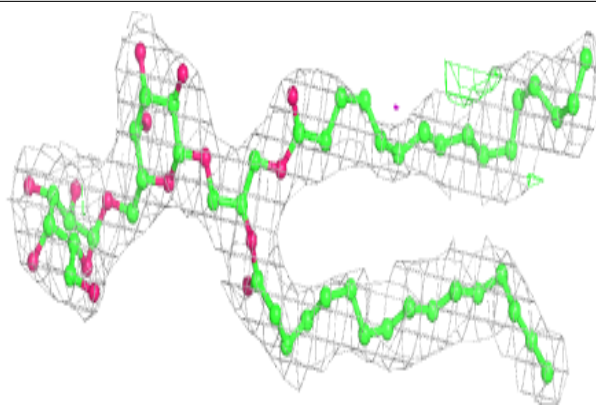
**Electron density around CLA c1 505:**

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



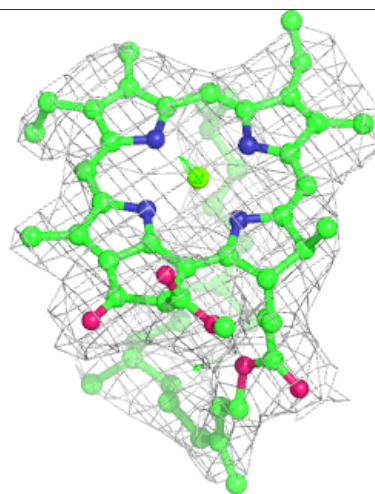
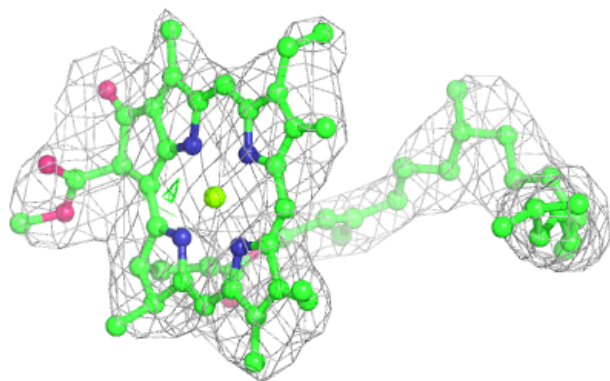
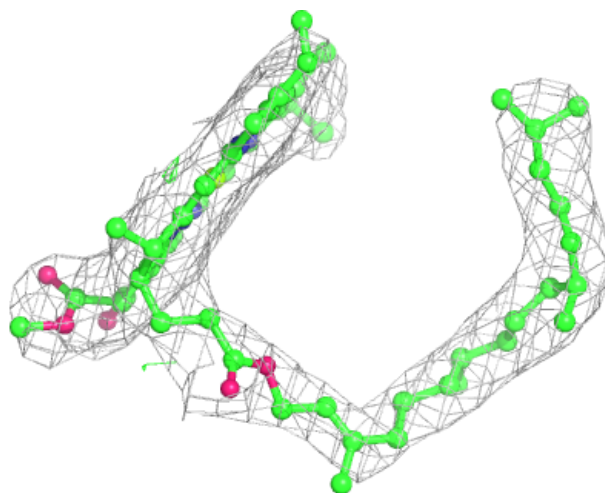
**Electron density around DGD c2 517:**

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



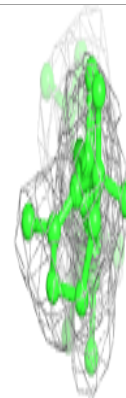
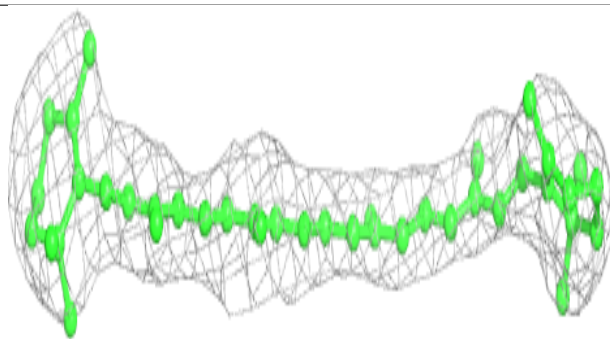
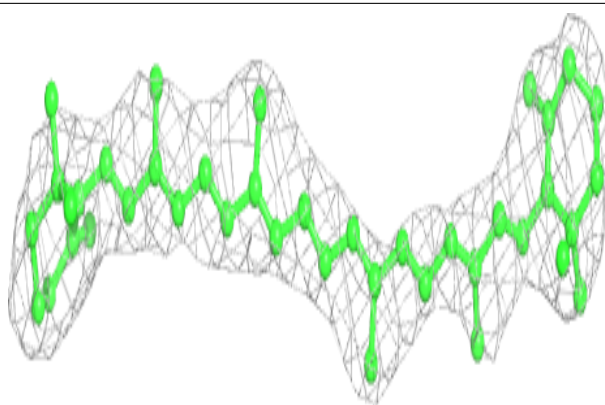
**Electron density around CLA b2 612:**

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

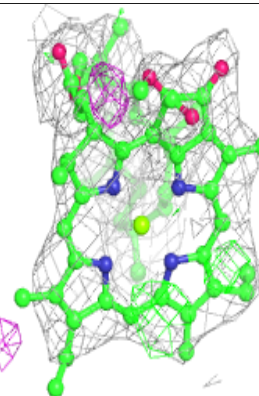
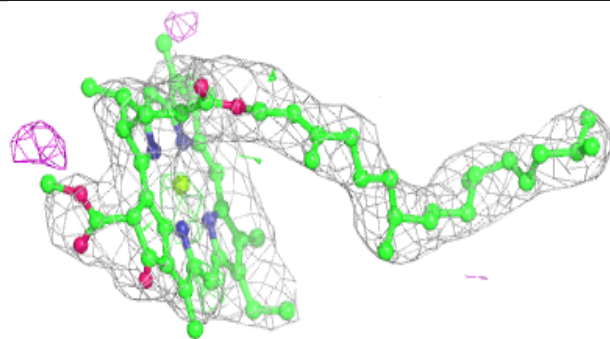
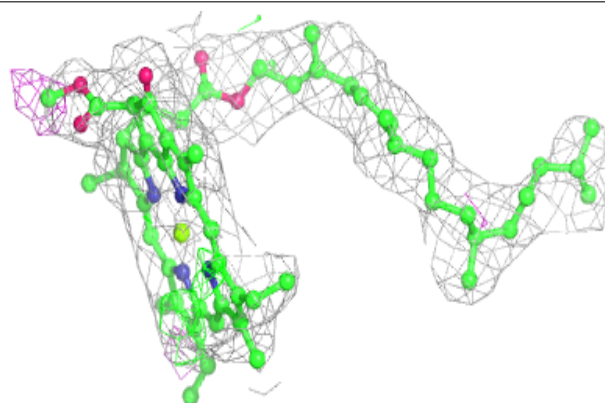


**Electron density around BCR B1 601:**

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

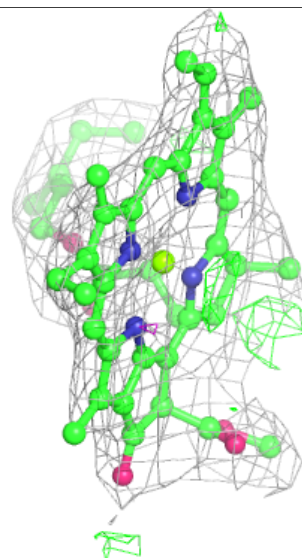
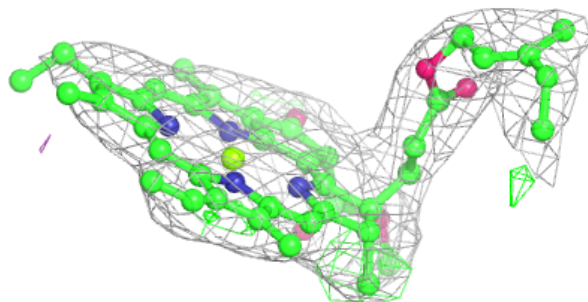
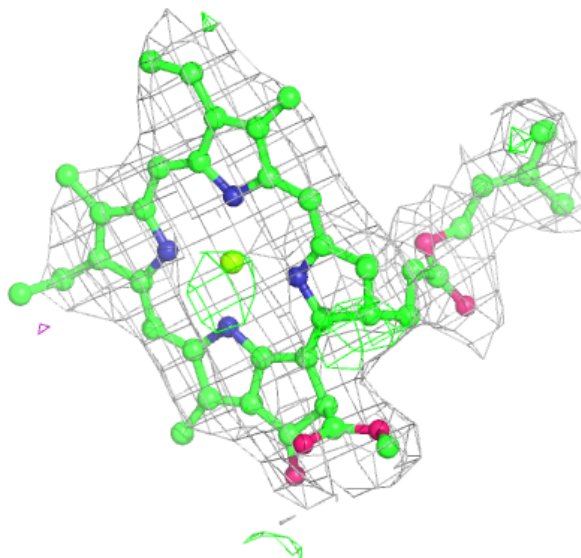
**Electron density around CLA C1 509:**

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



**Electron density around CLA A2 404:**

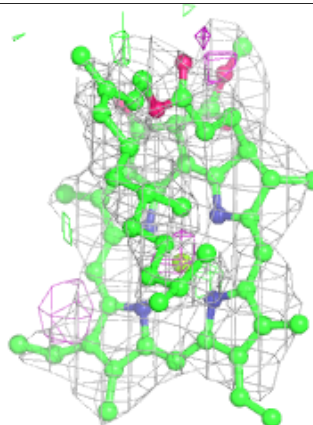
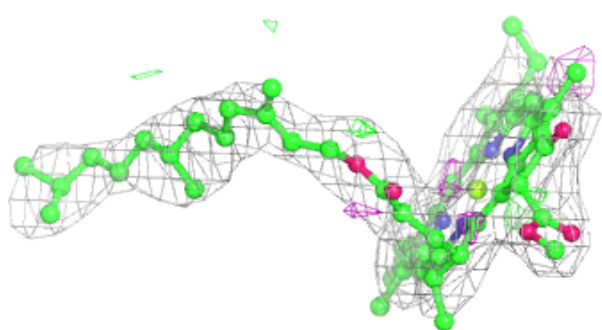
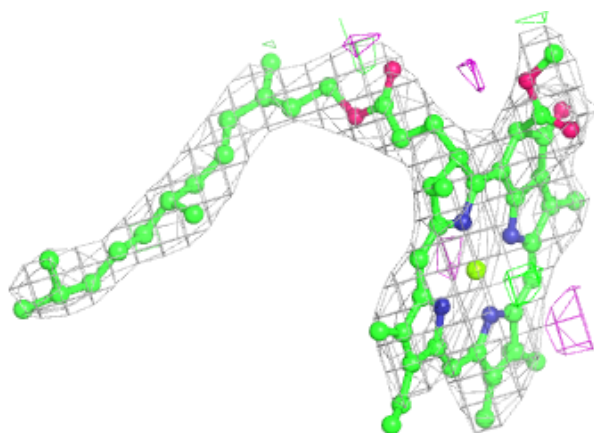
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



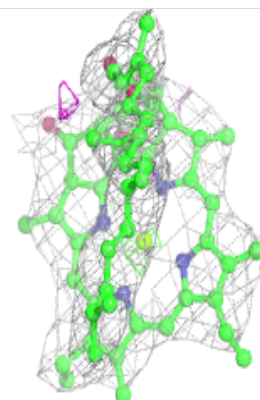
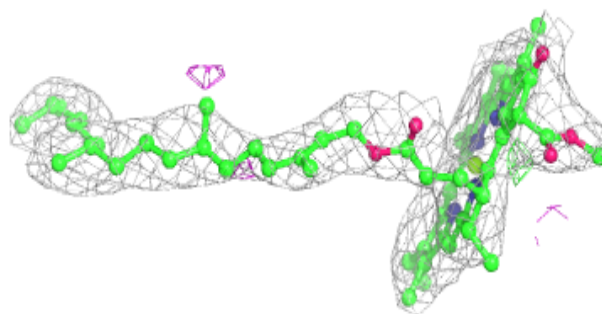
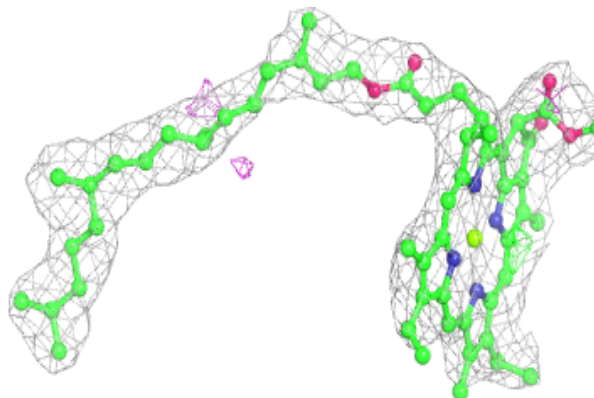


**Electron density around CLA c1 513:**

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

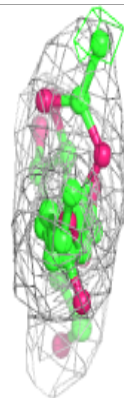
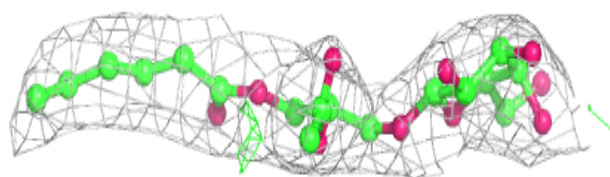
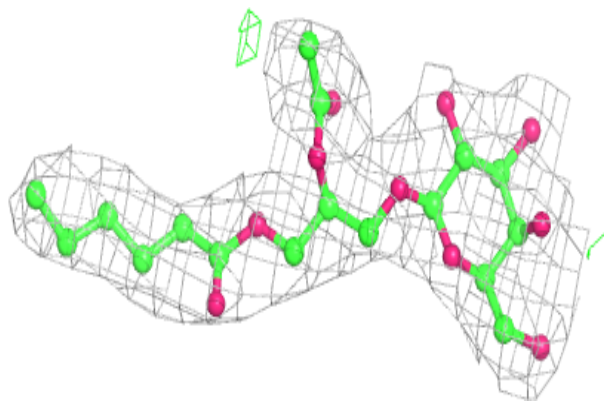
**Electron density around CLA b1 611:**

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

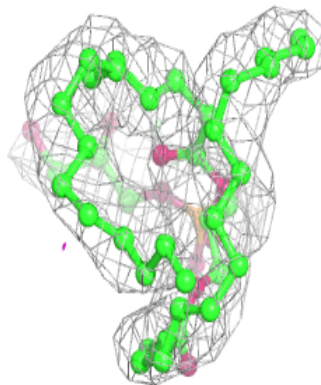
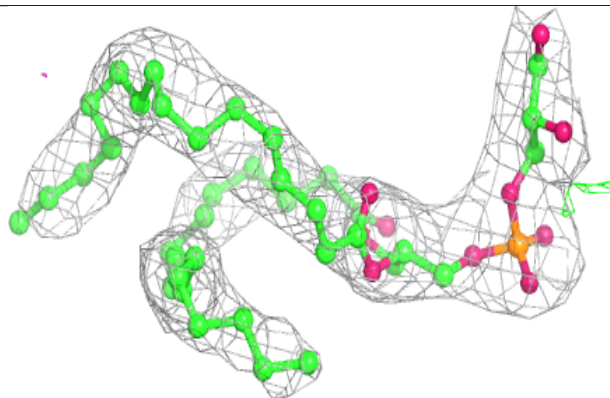
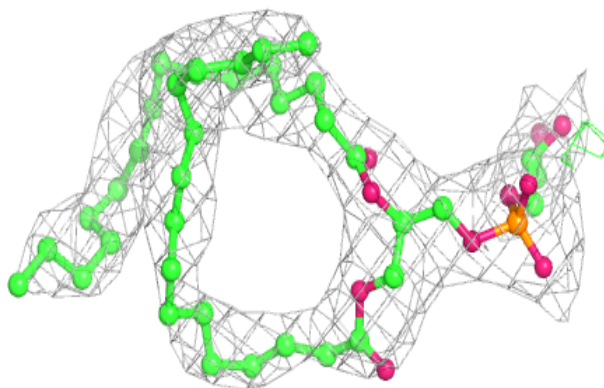


**Electron density around LMG d2 407:**

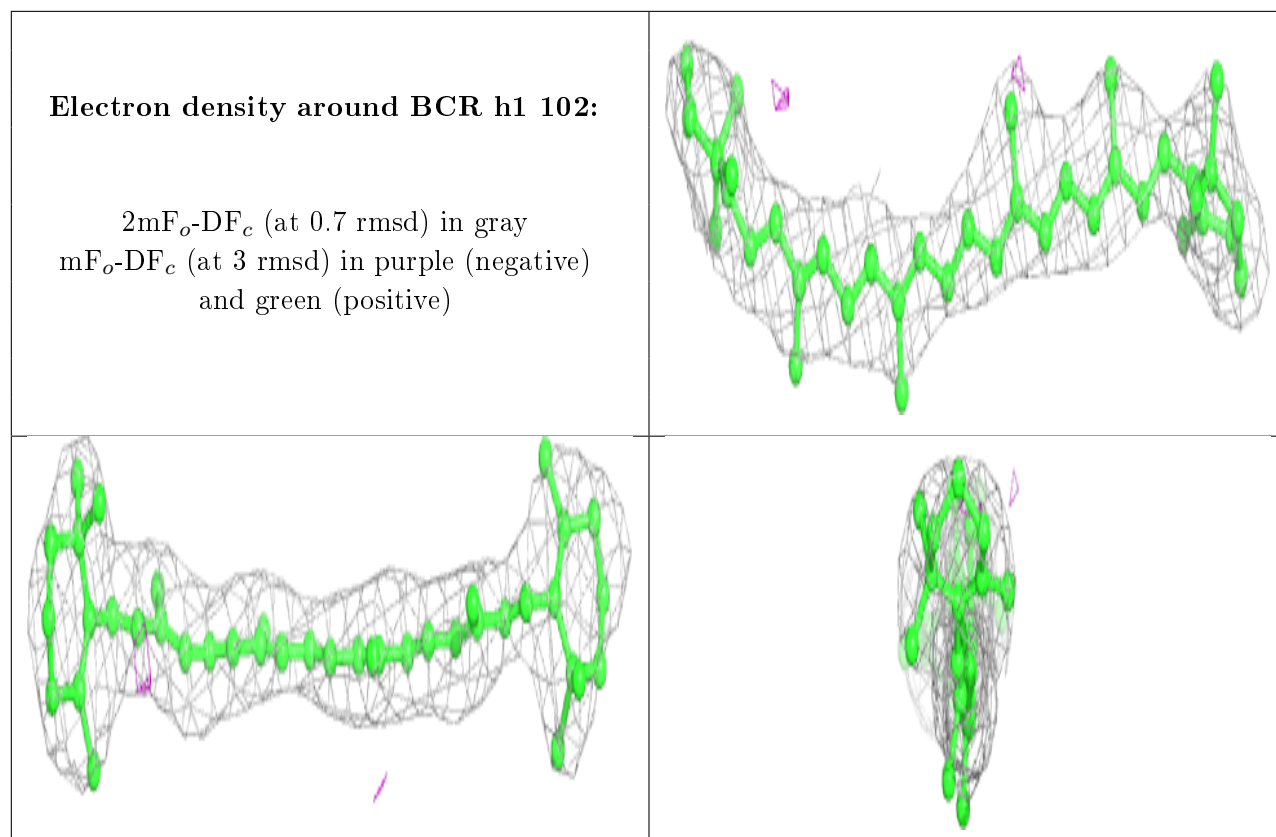
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LHG B1 621:**

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

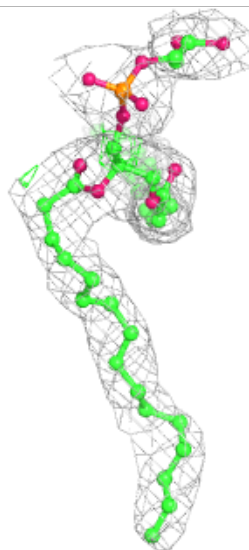
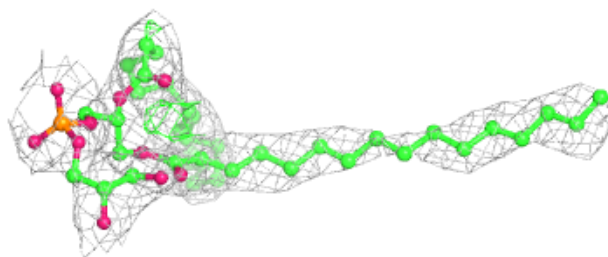
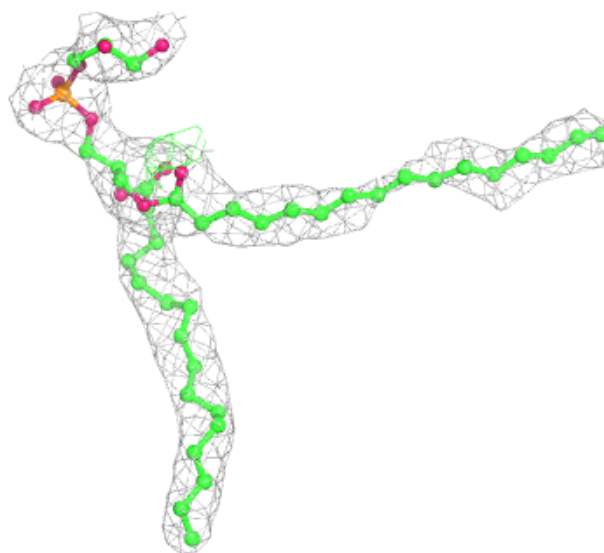


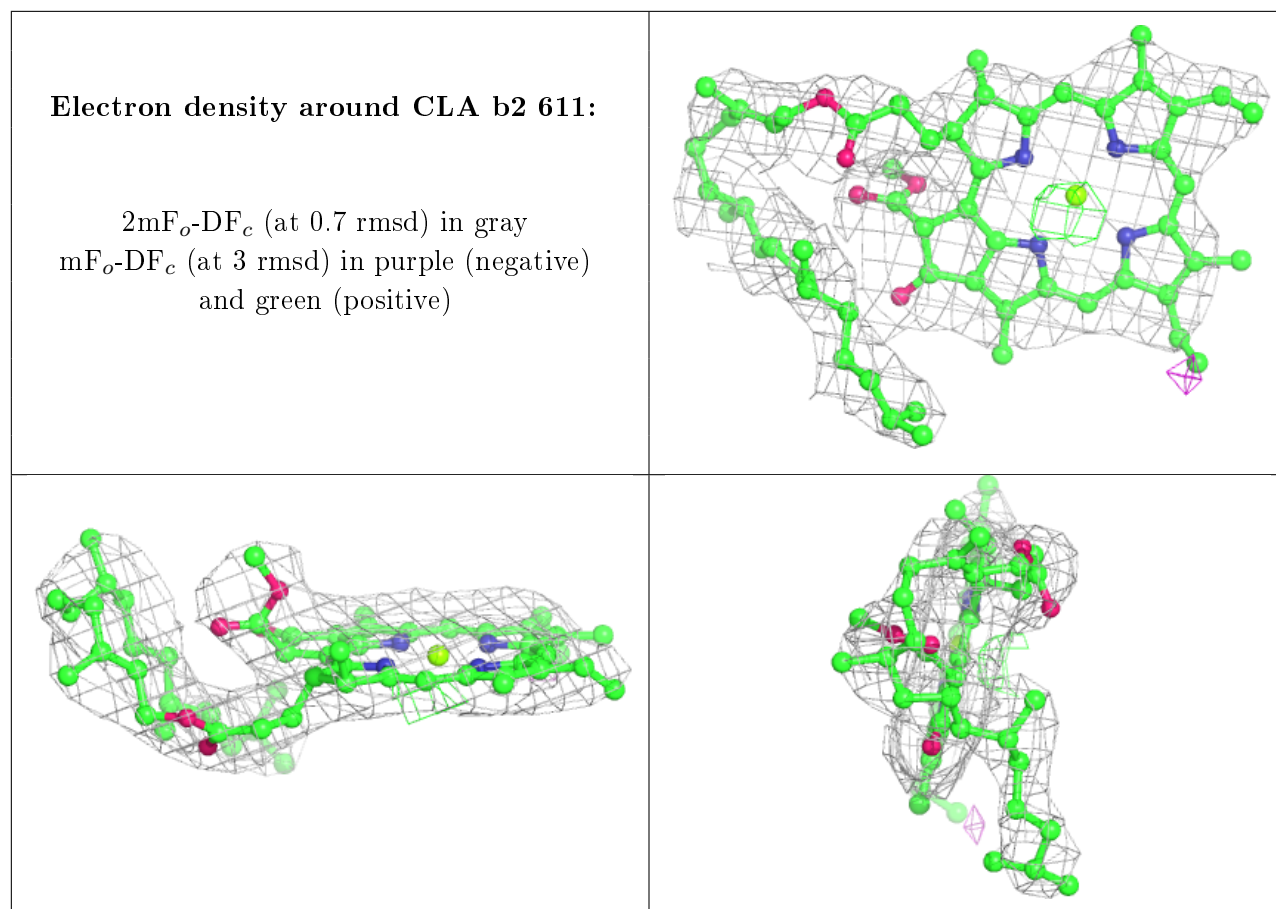




**Electron density around LHG L2 101:**

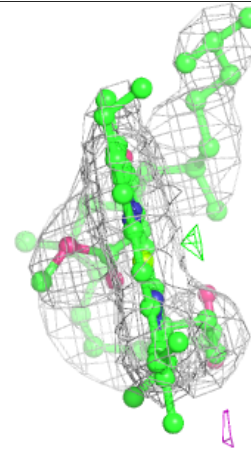
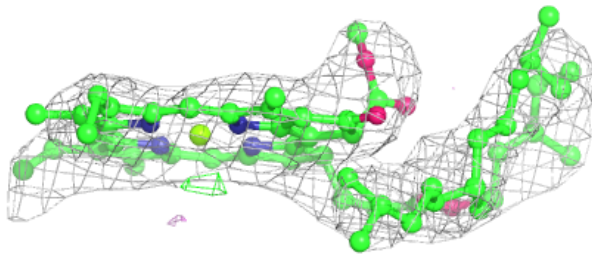
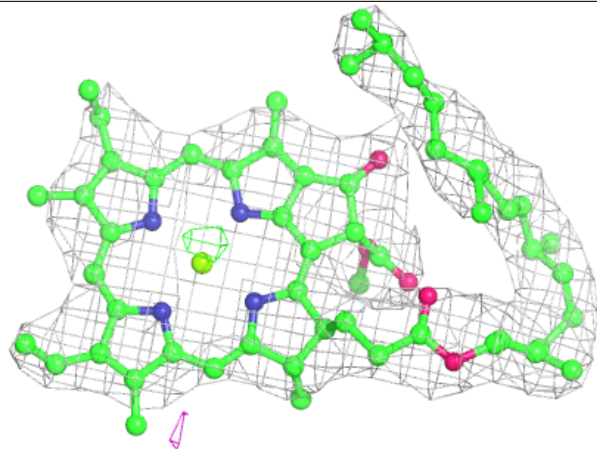
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



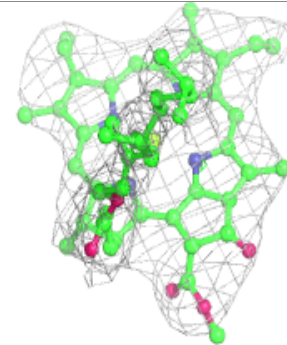
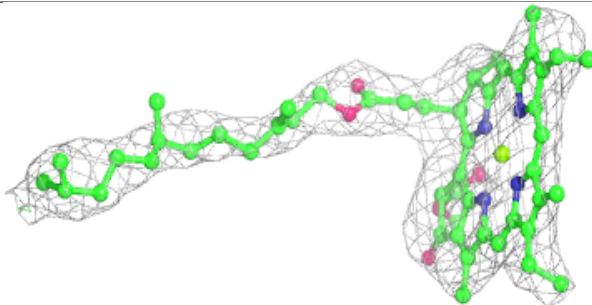
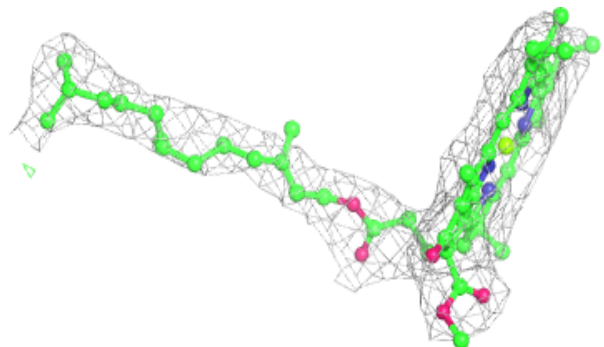


**Electron density around CLA B1 612:**

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

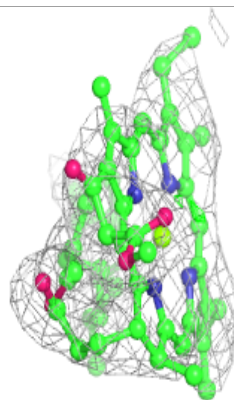
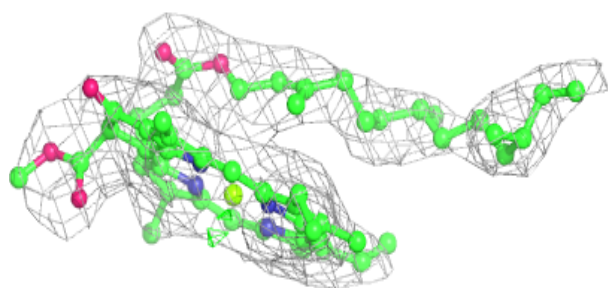
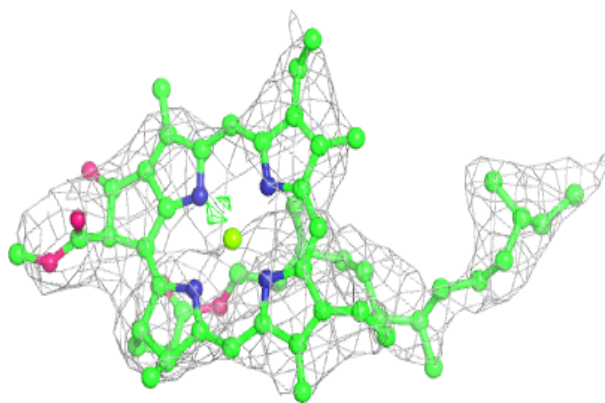
**Electron density around CLA B1 607:**

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



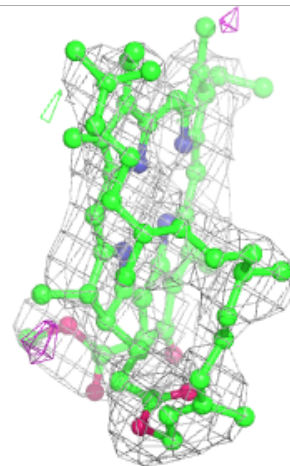
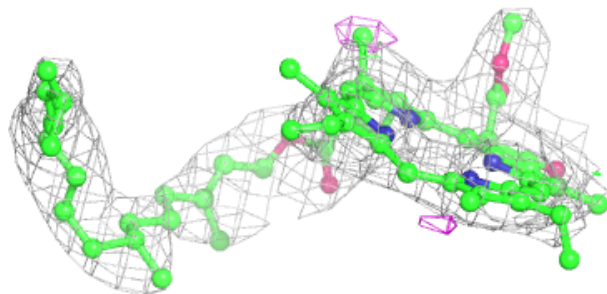
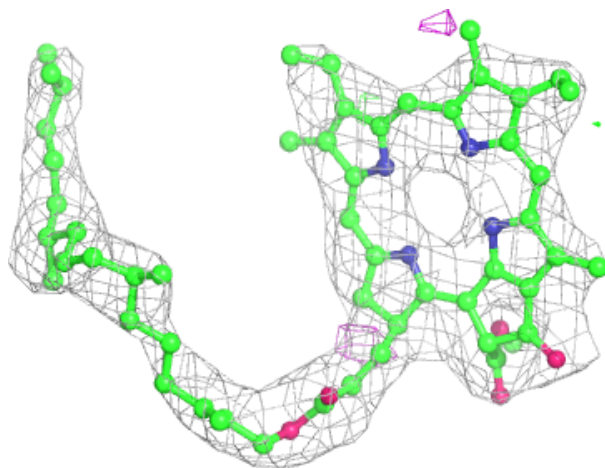
**Electron density around CLA c2 506:**

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



**Electron density around PHO d2 408:**

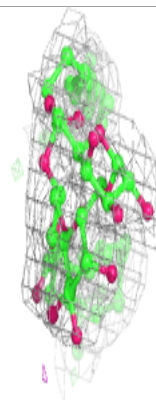
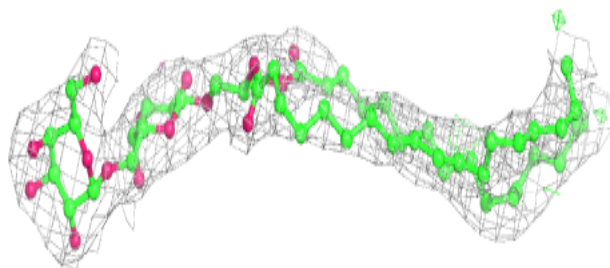
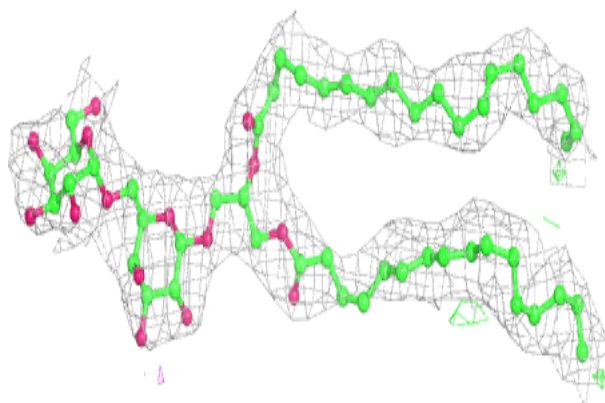
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



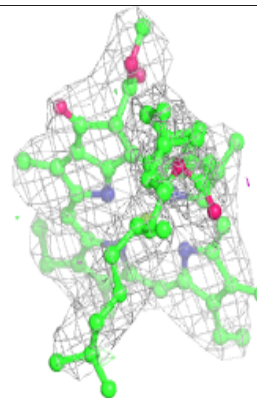
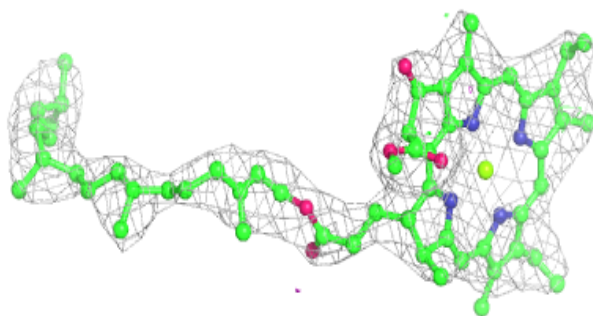
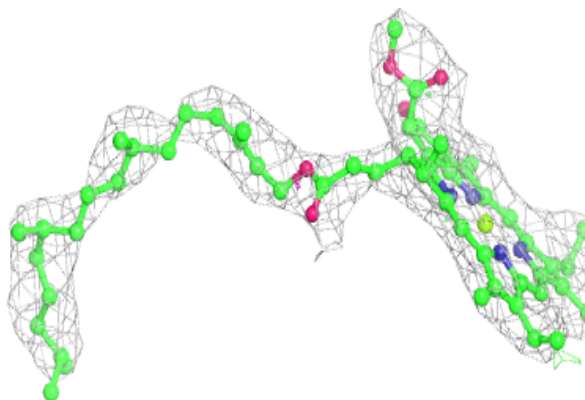


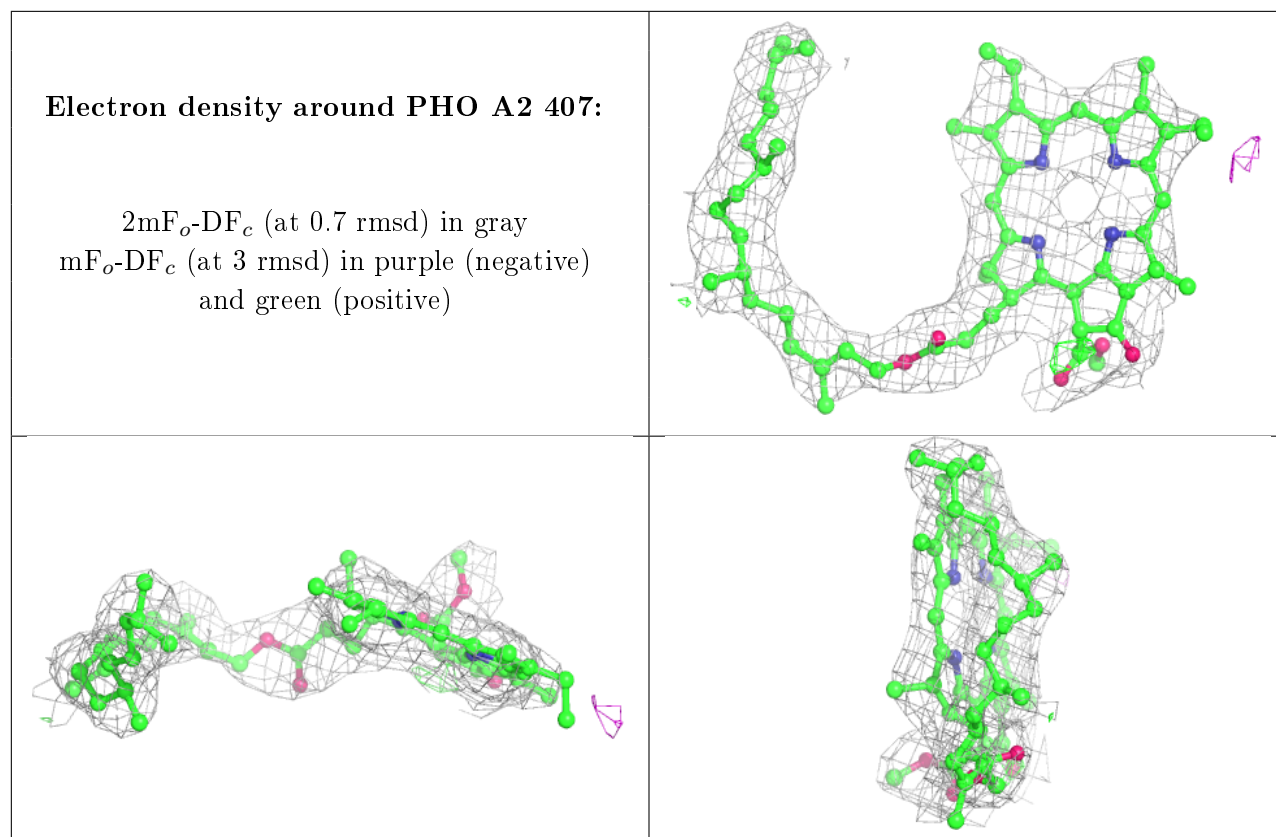
**Electron density around DGD C1 517:**

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

**Electron density around CLA d2 405:**

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

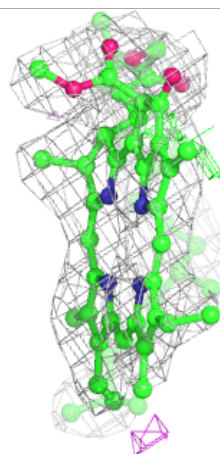
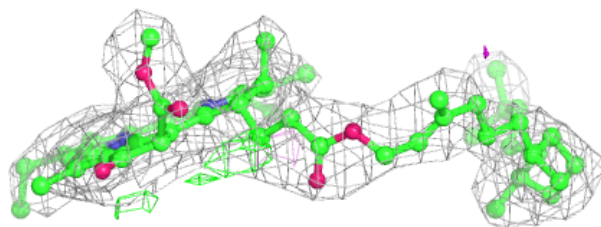
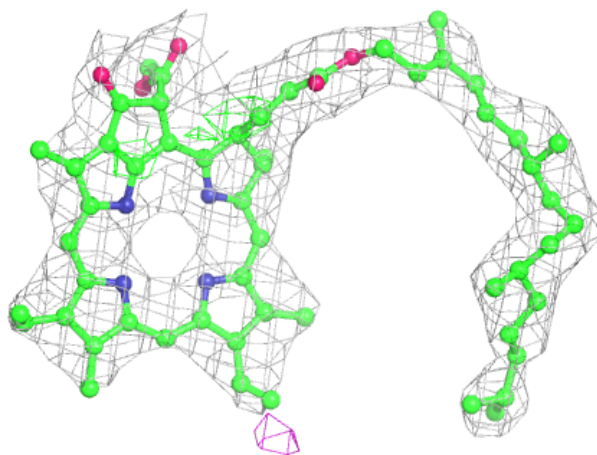






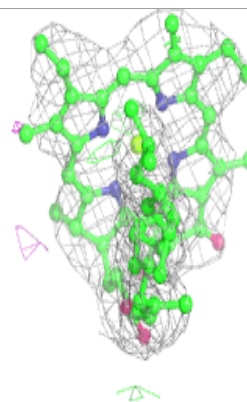
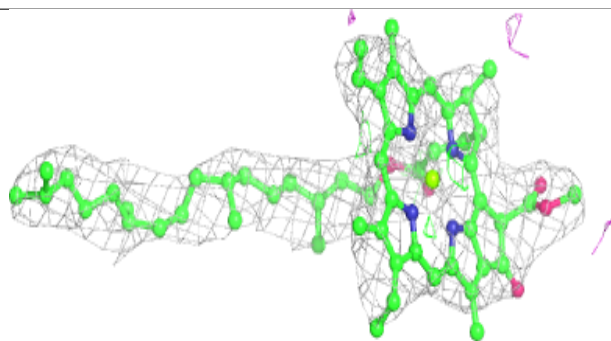
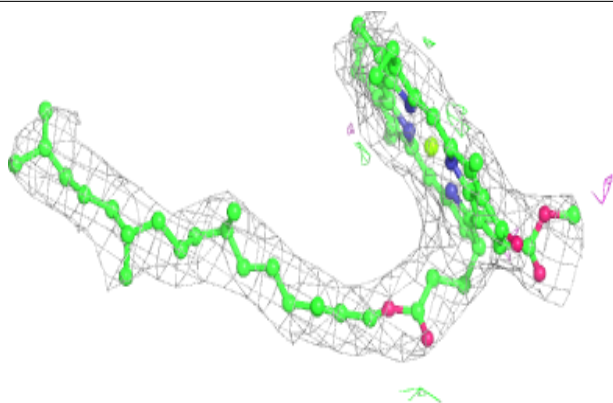
**Electron density around PHO a2 416:**

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

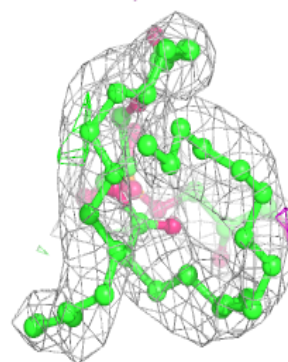
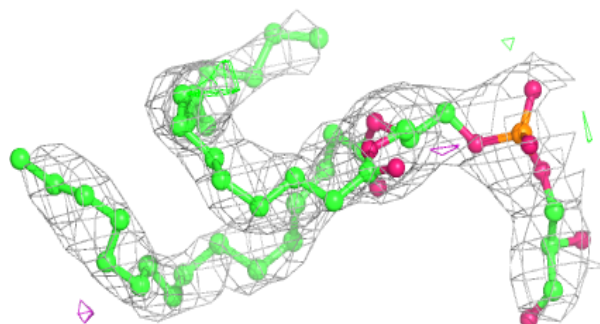
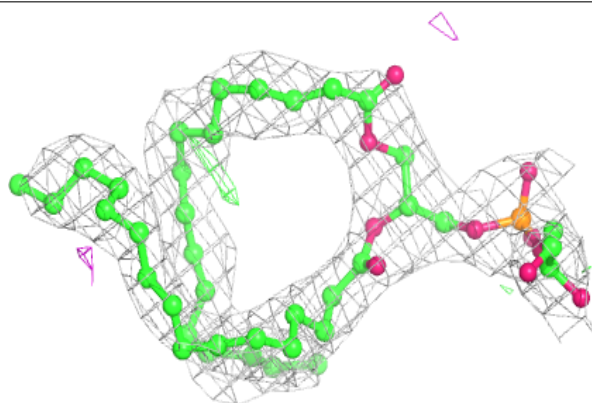


**Electron density around CLA c2 505:**

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

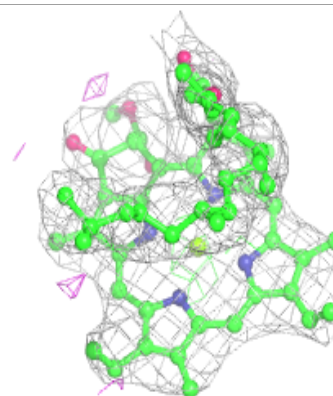
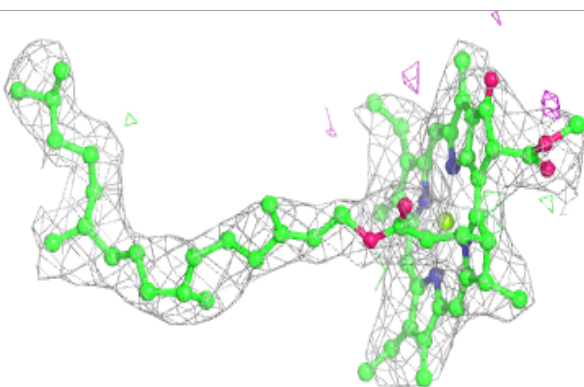
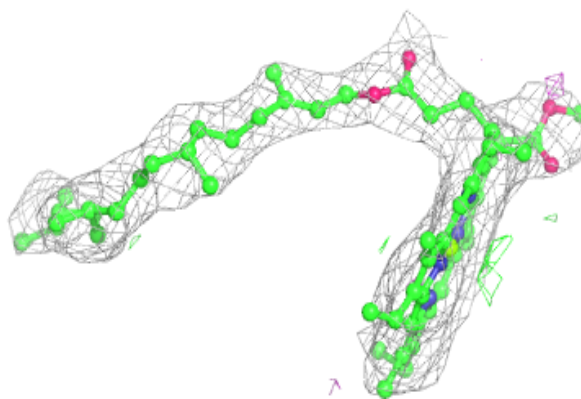
**Electron density around LHG d2 403:**

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

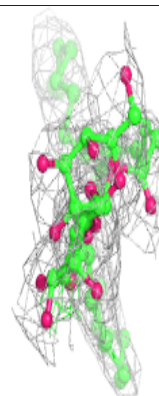
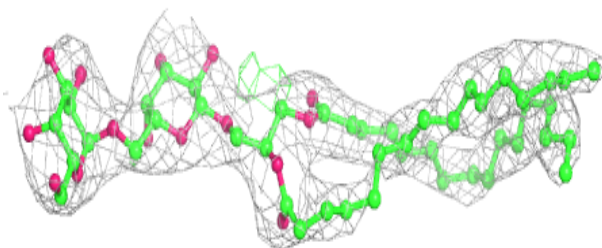
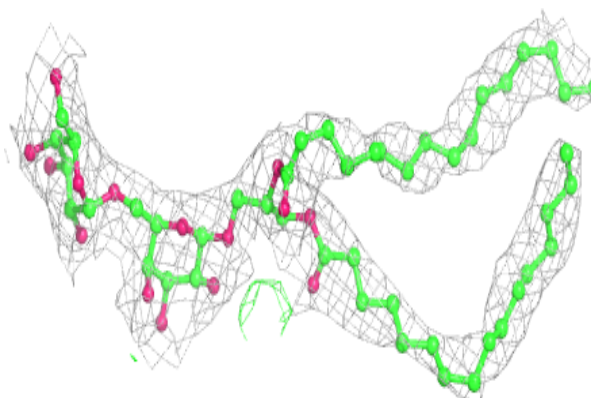


**Electron density around CLA B2 619:**

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

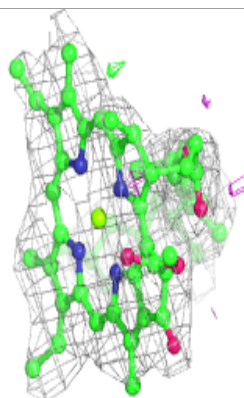
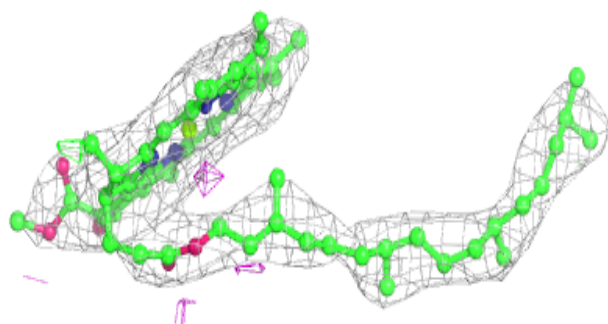
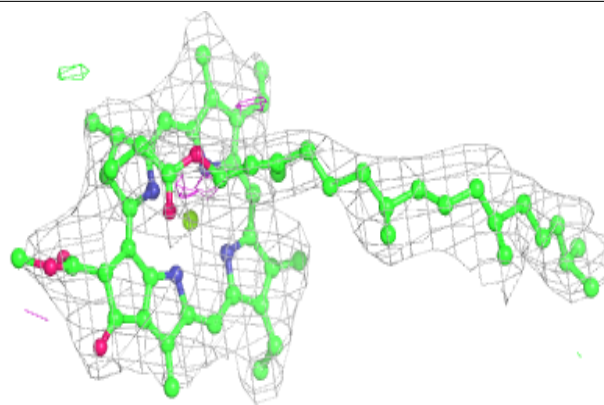
**Electron density around DGD c1 518:**

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

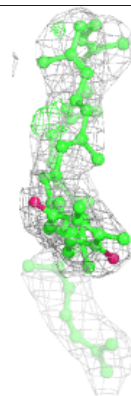
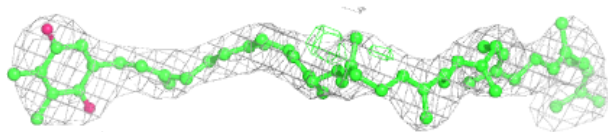
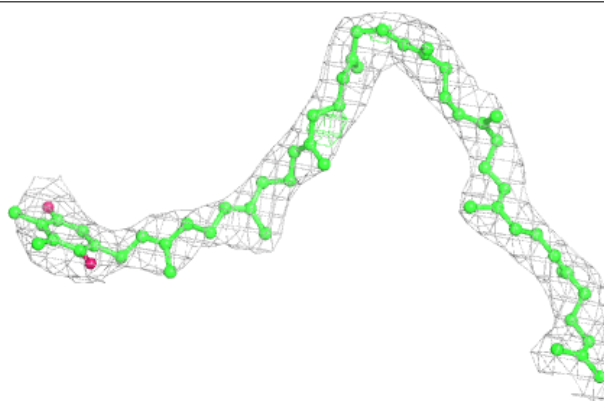


**Electron density around CLA b2 624:**

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

**Electron density around PL9 D1 408:**

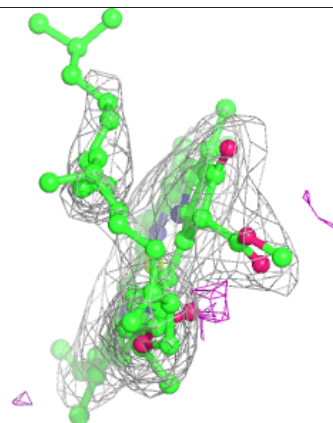
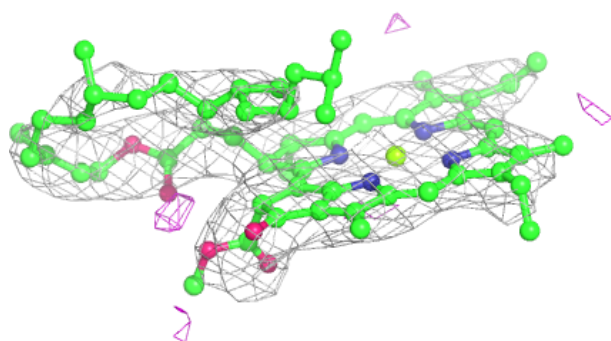
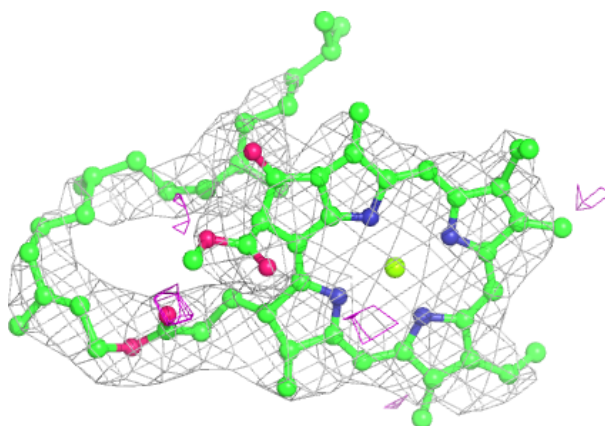
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



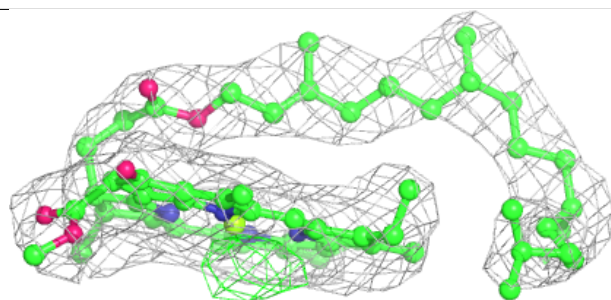
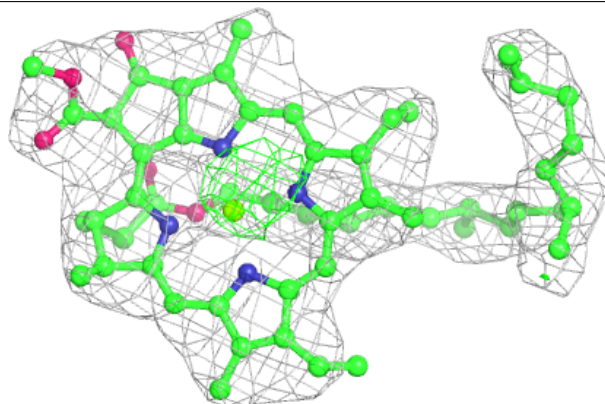


**Electron density around CLA C1 510:**

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

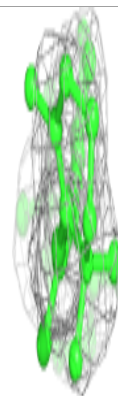
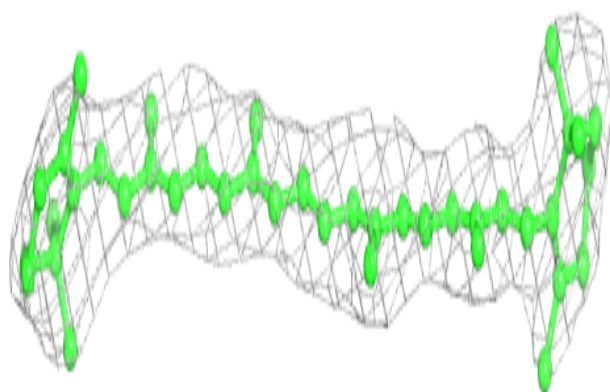
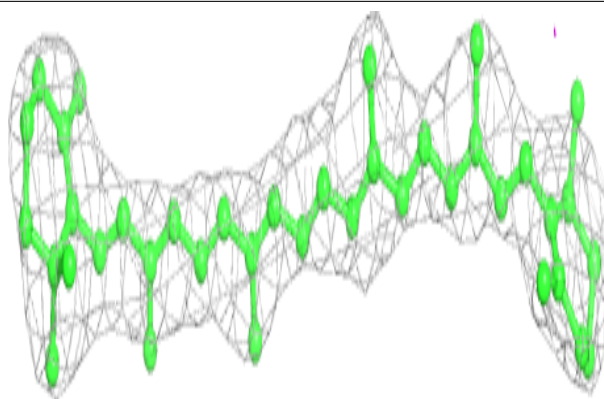
**Electron density around CLA b1 616:**

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

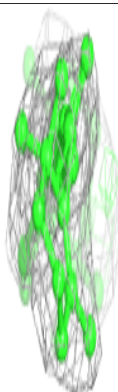
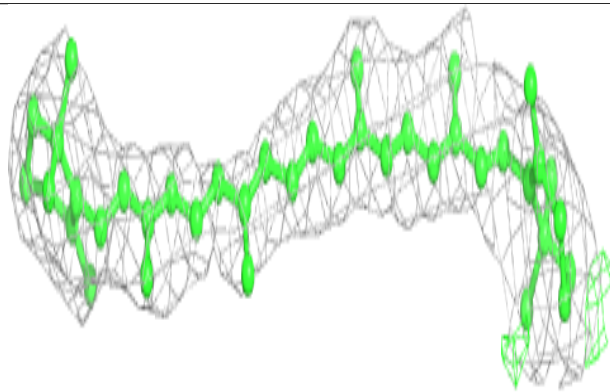
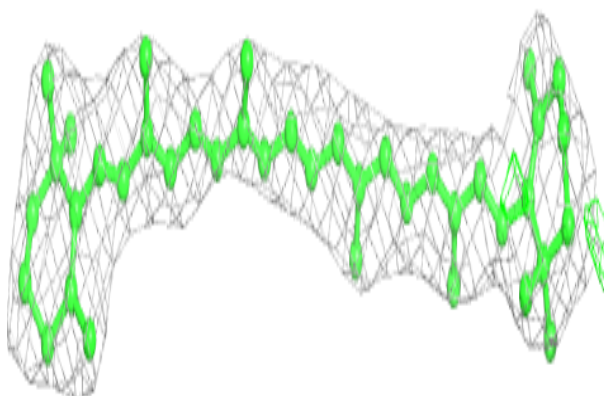


**Electron density around BCR a1 401:**

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

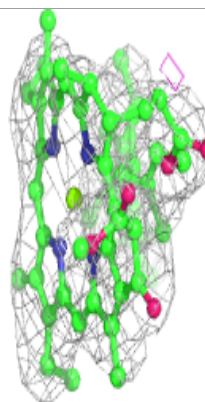
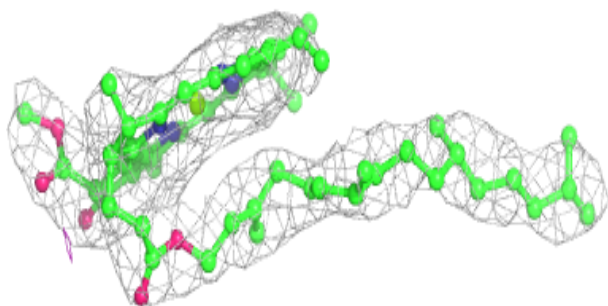
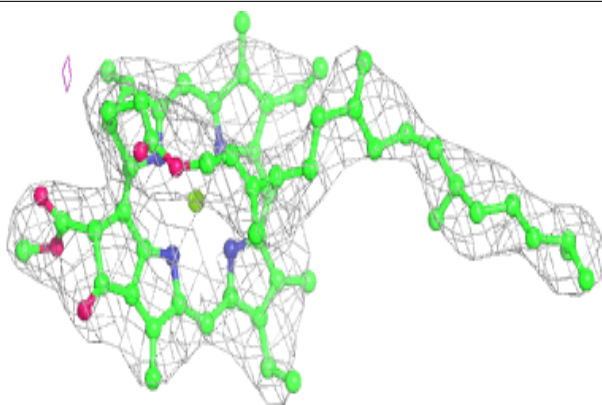
**Electron density around BCR B1 603:**

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

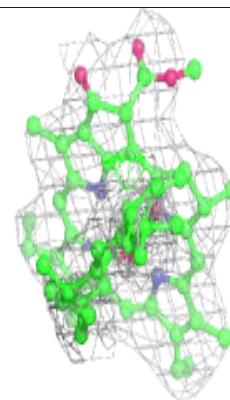
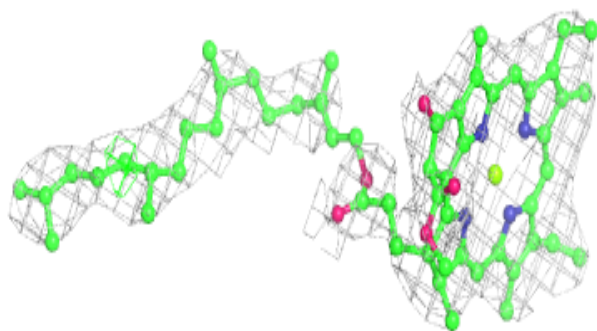
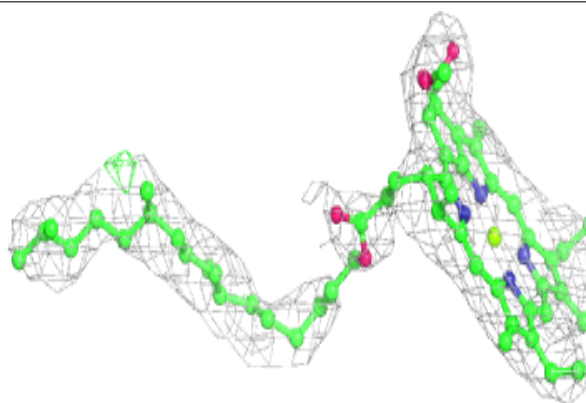


**Electron density around CLA c1 507:**

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

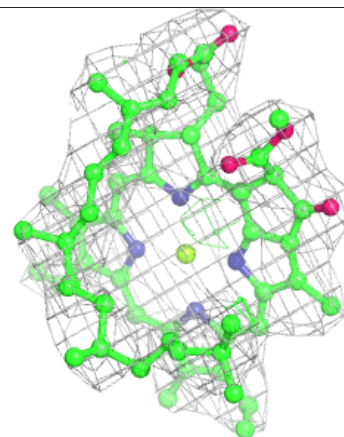
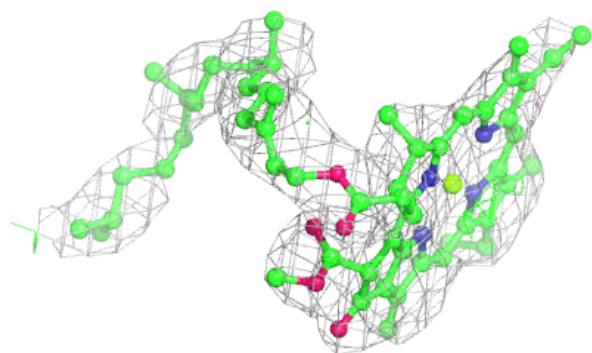
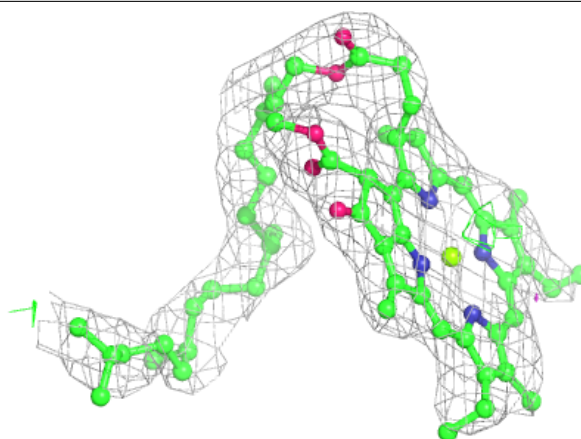
**Electron density around CLA c2 503:**

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



**Electron density around CLA B2 615:**

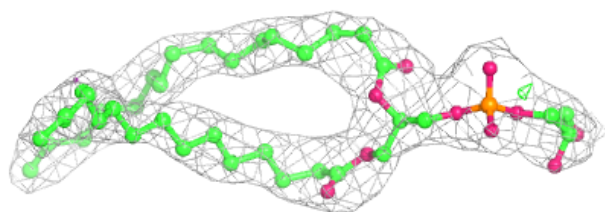
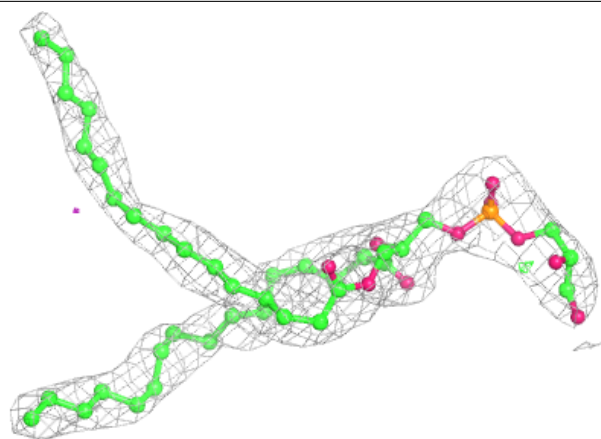
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



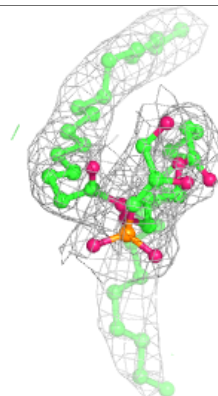
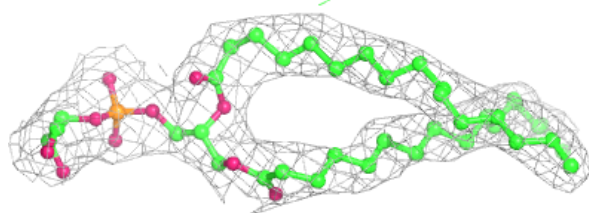
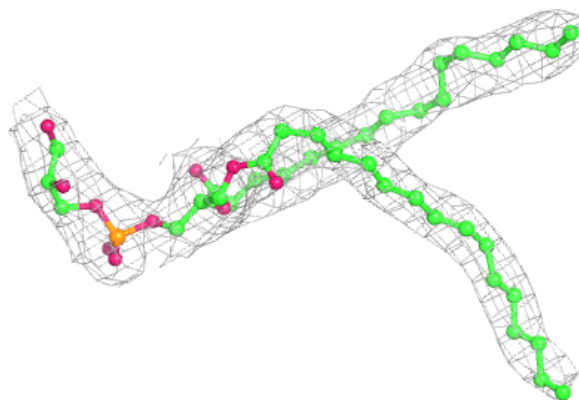


**Electron density around LHG D2 405:**

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

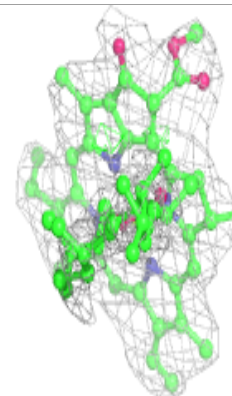
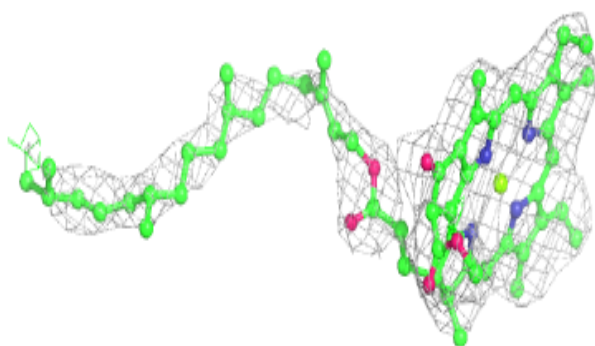
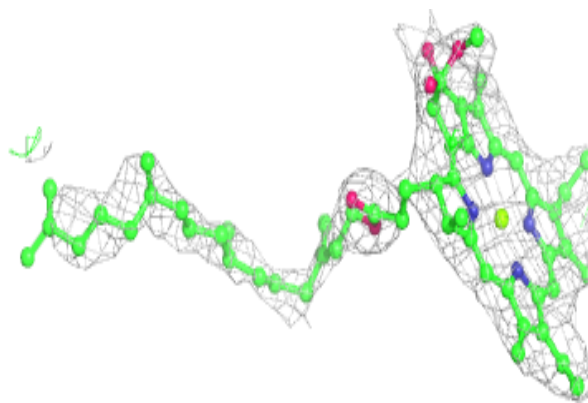
**Electron density around LHG d2 406:**

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

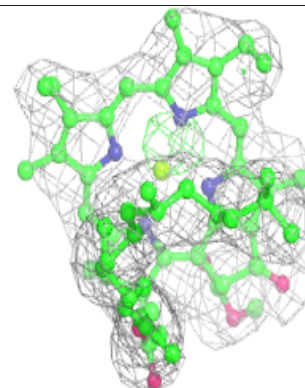
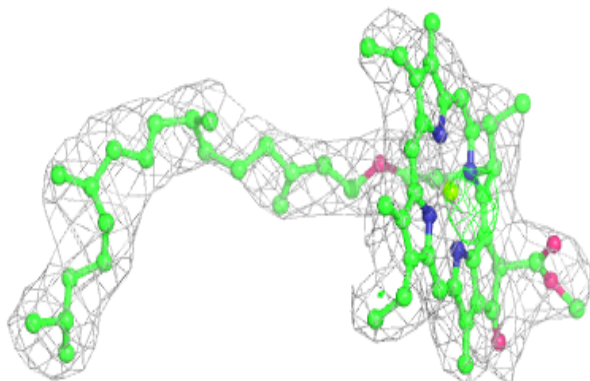
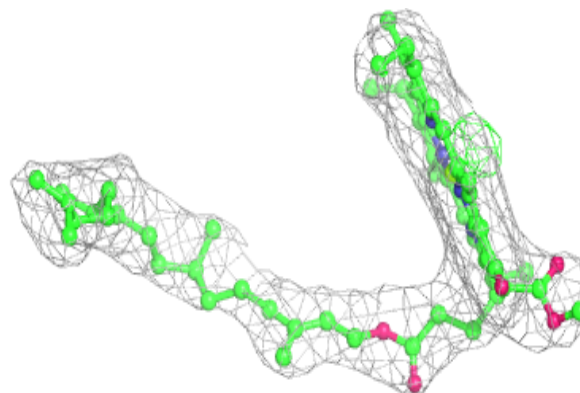


**Electron density around CLA c1 504:**

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

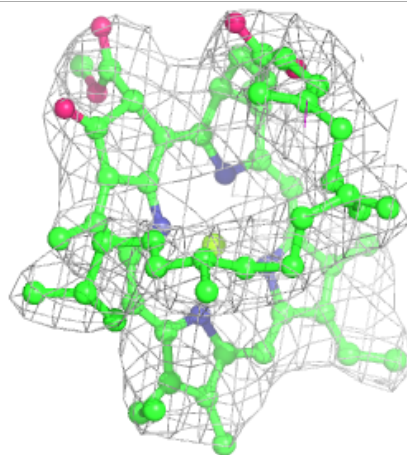
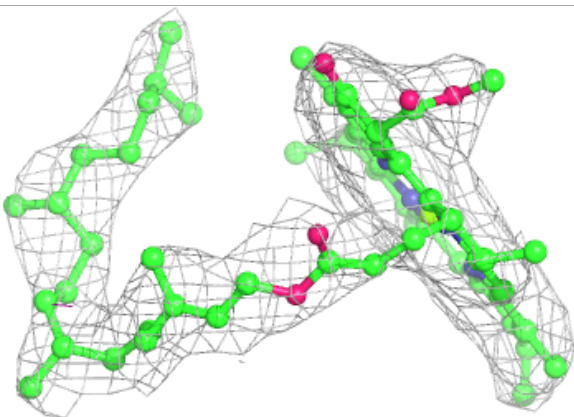
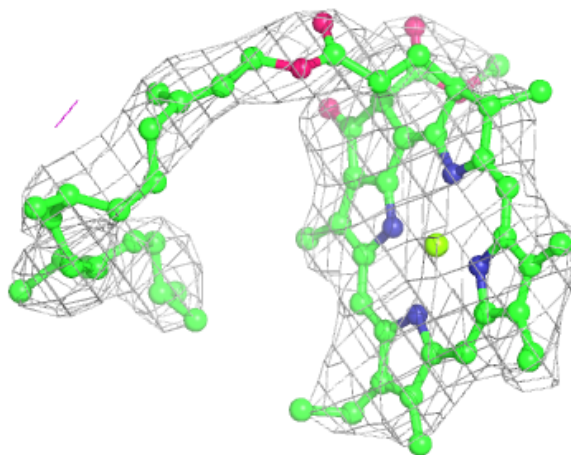
**Electron density around CLA B1 619:**

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



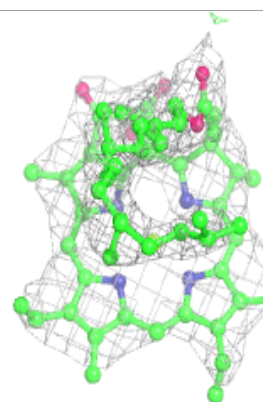
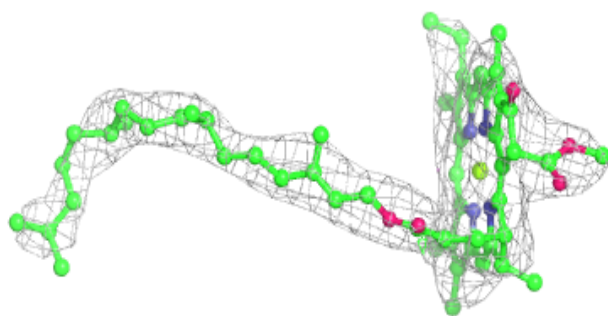
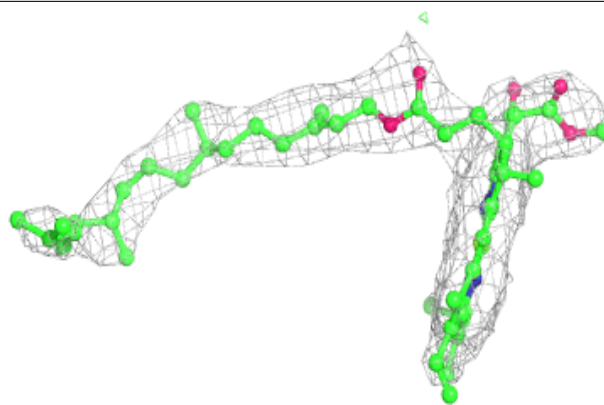
**Electron density around CLA C1 504:**

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

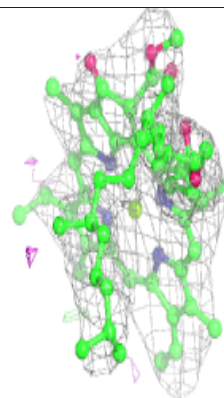
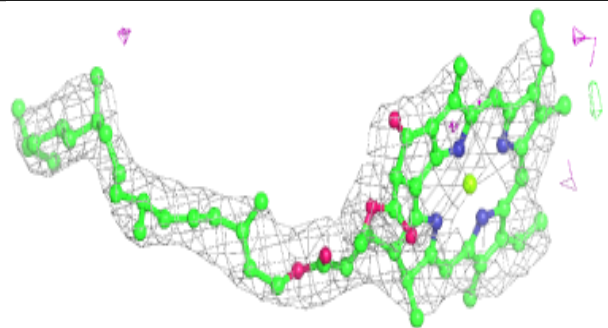
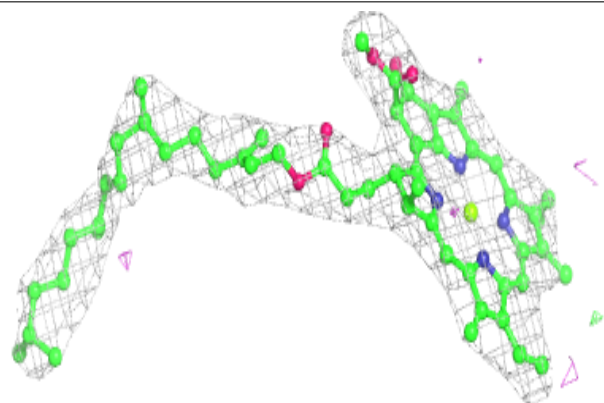


**Electron density around CLA b2 608:**

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

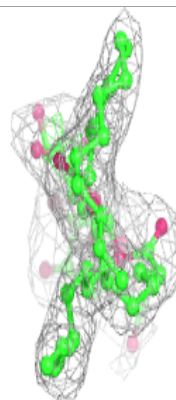
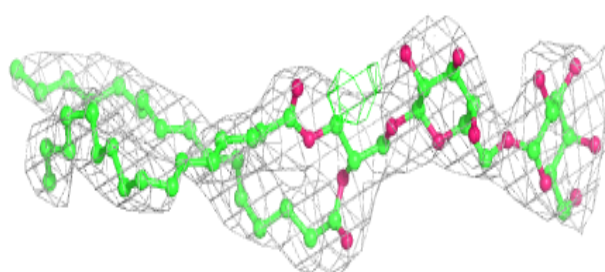
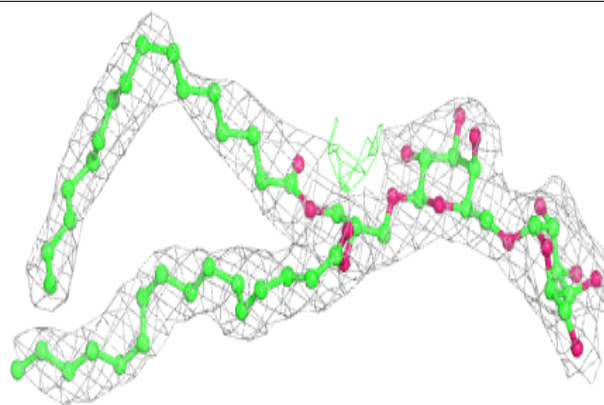
**Electron density around CLA A2 402:**

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

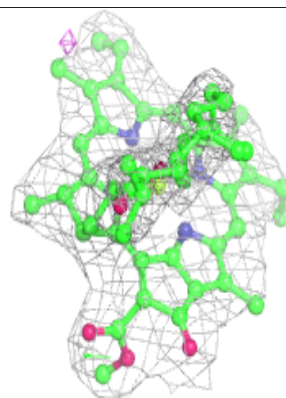
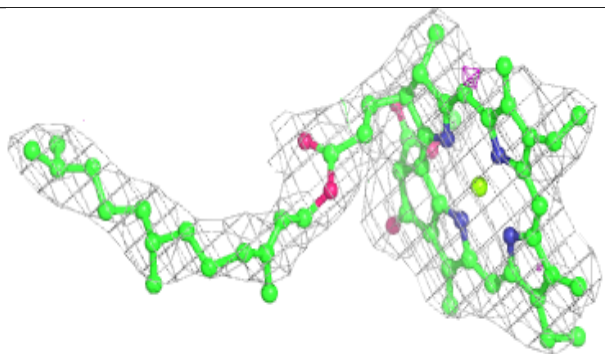
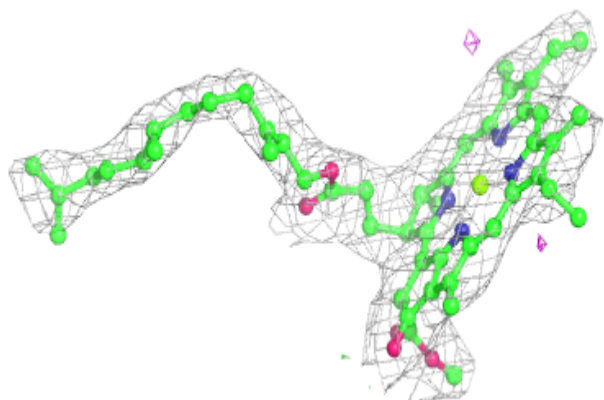


**Electron density around DGD c2 514:**

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

**Electron density around CLA C1 503:**

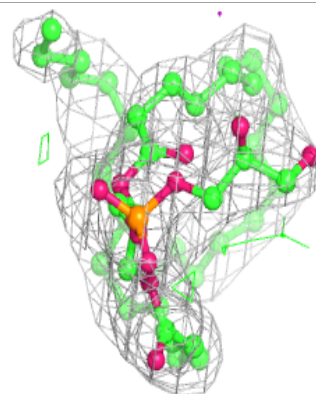
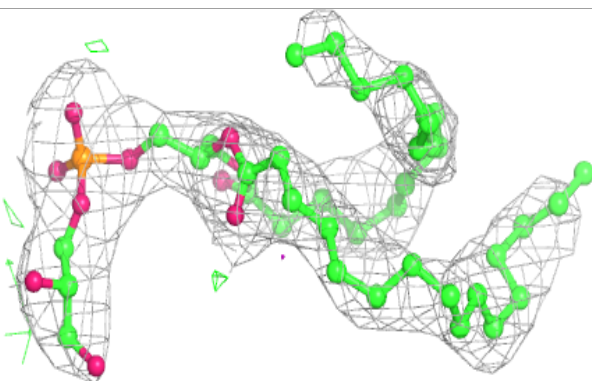
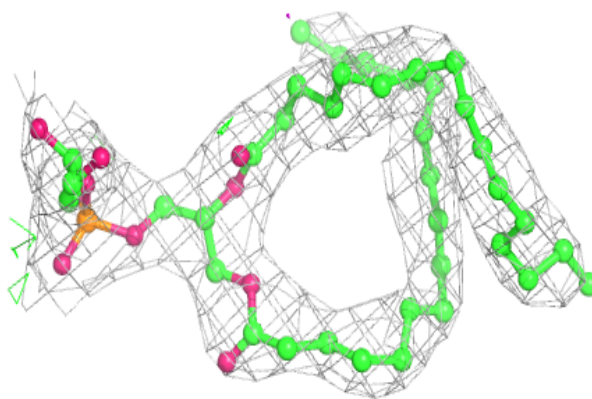
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



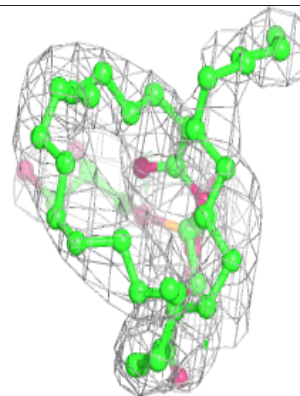
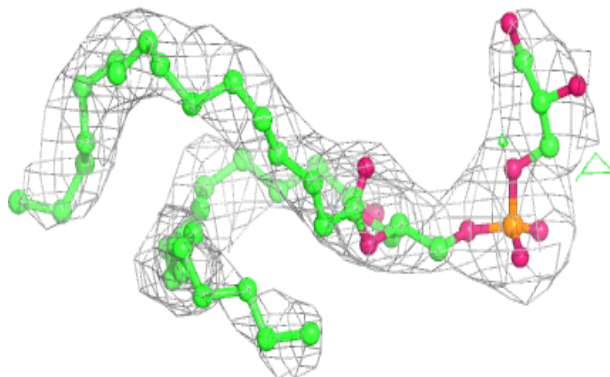
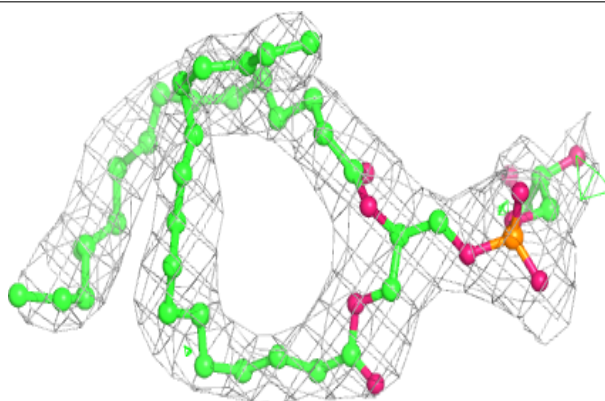


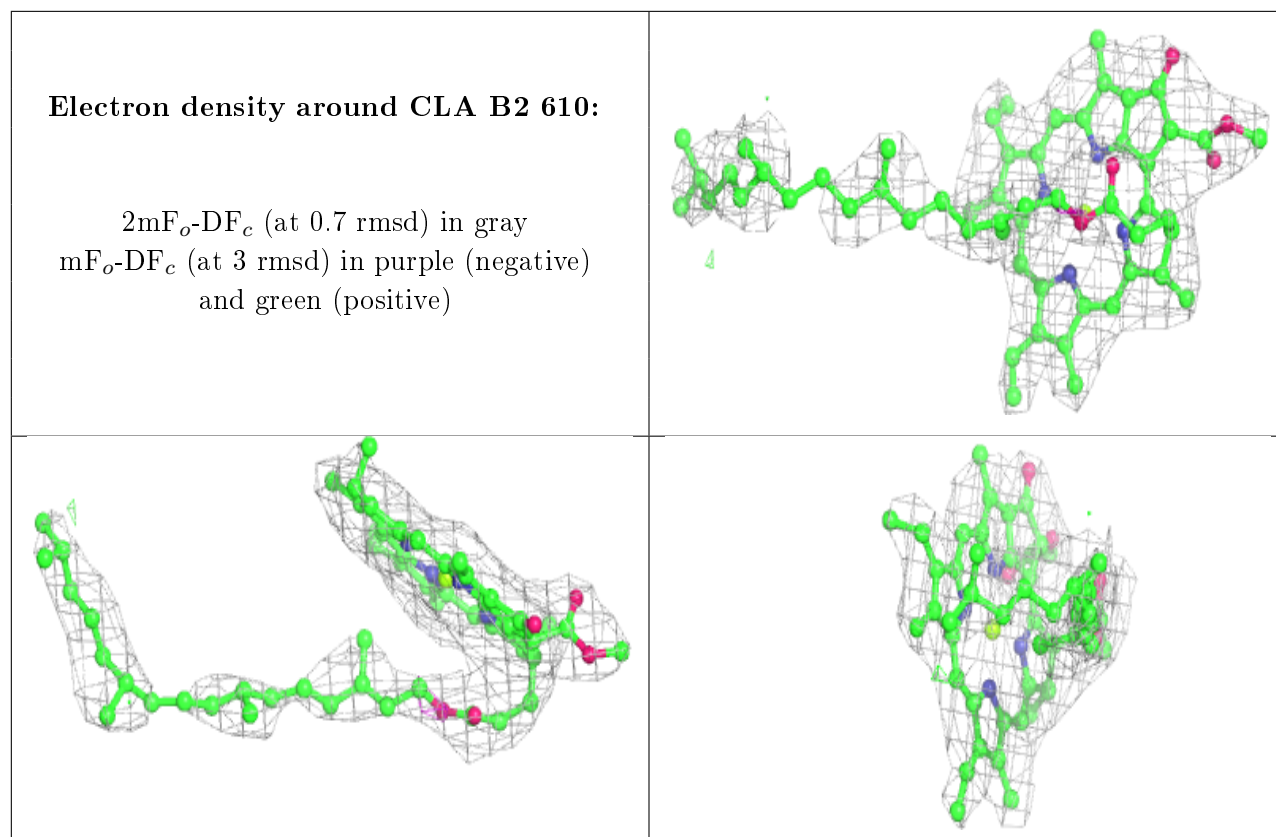
**Electron density around LHG D2 403:**

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

**Electron density around LHG b1 622:**

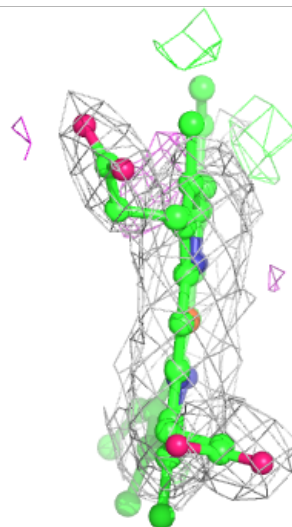
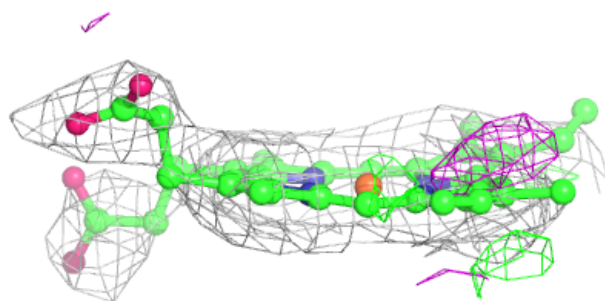
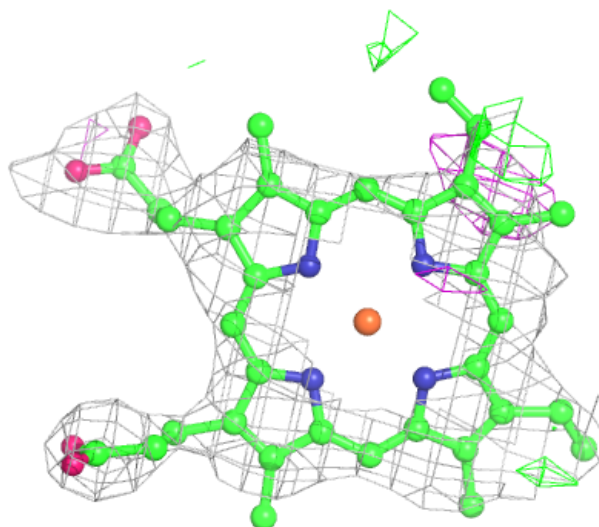
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM v1 201:**

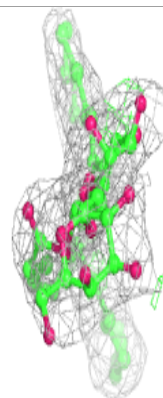
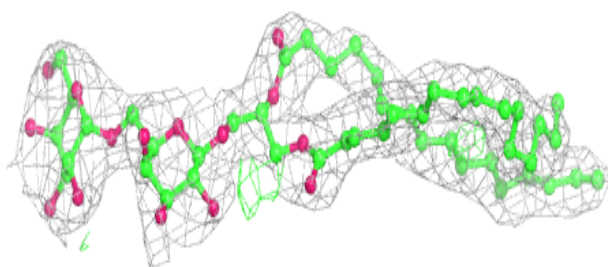
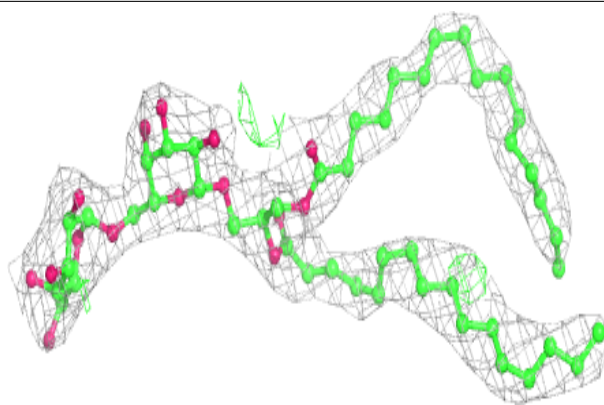
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



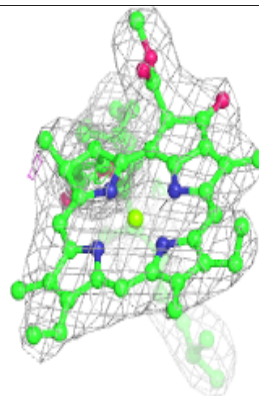
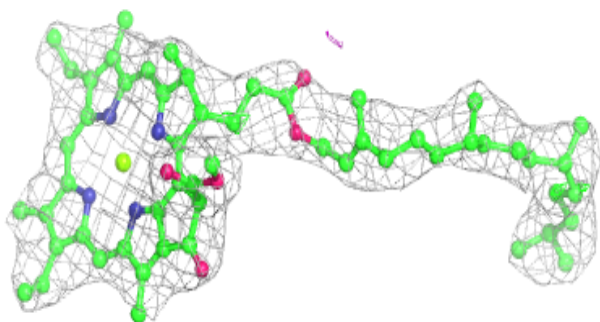
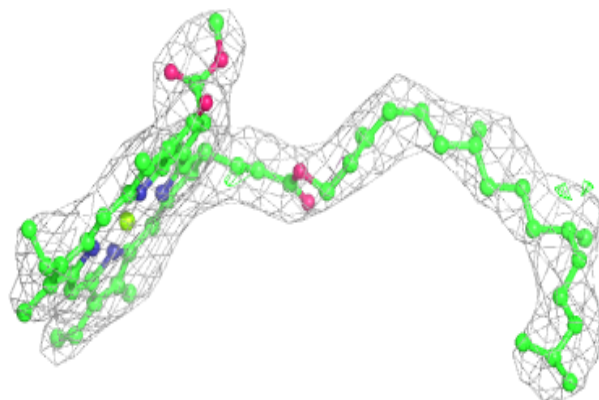


**Electron density around DGD C1 516:**

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

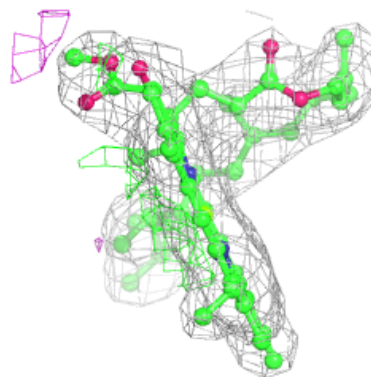
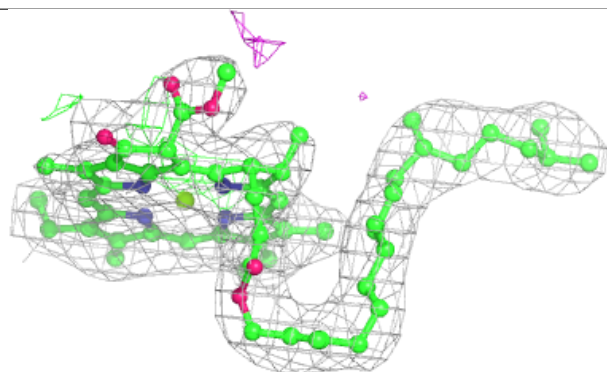
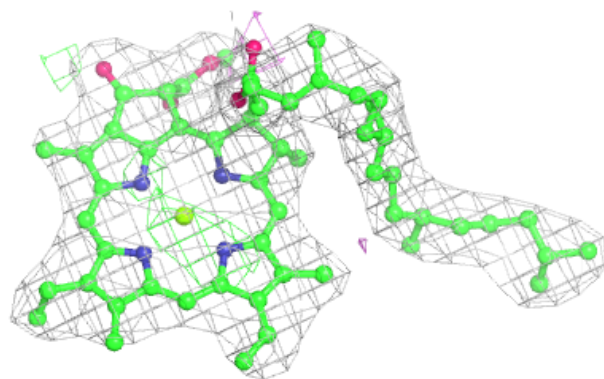
**Electron density around CLA d1 401:**

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

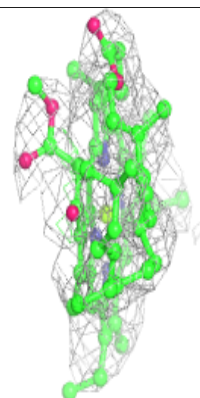
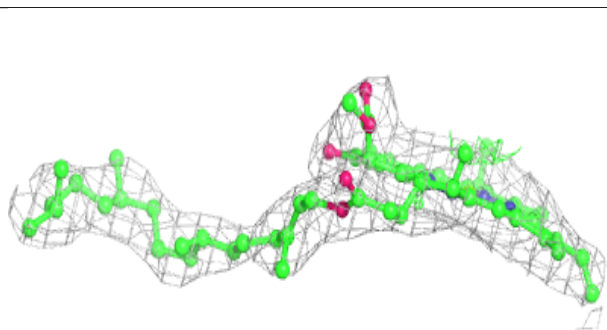
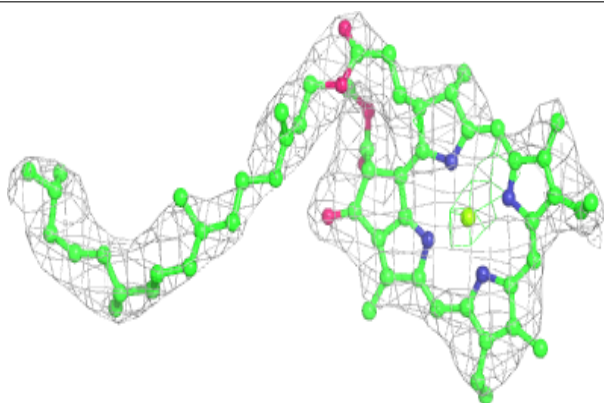


**Electron density around CLA d1 404:**

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

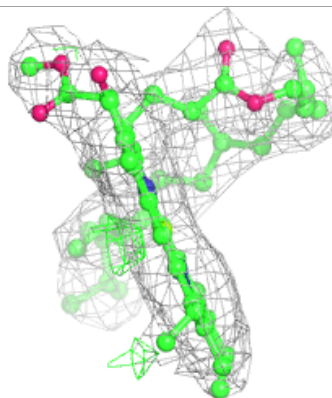
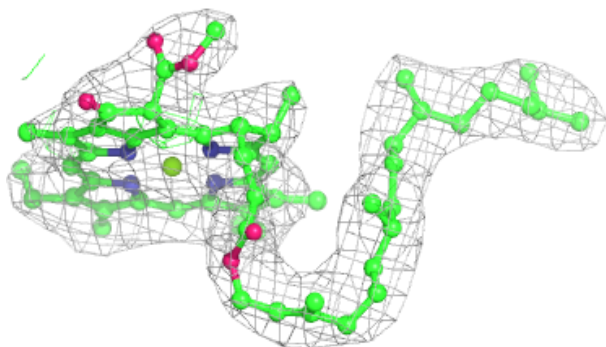
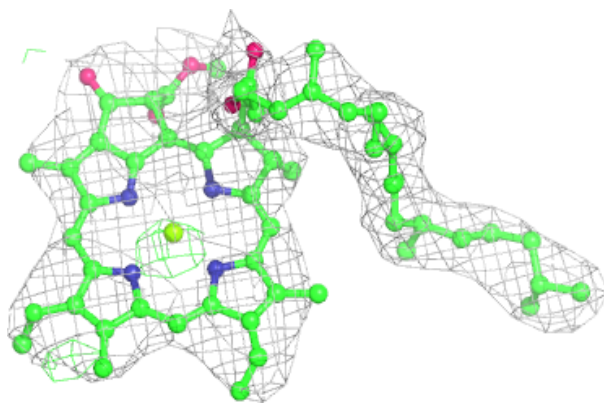
**Electron density around CLA B1 605:**

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

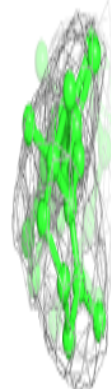
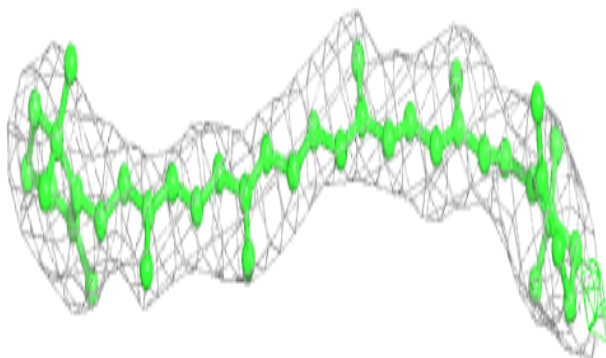
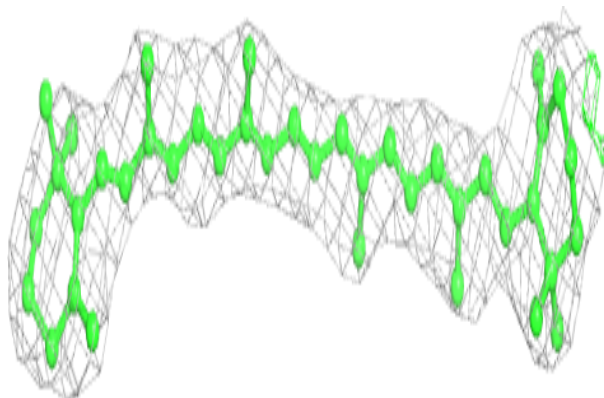


**Electron density around CLA D2 406:**

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

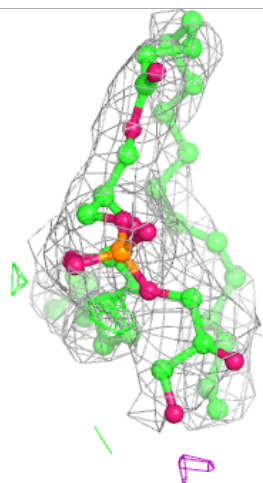
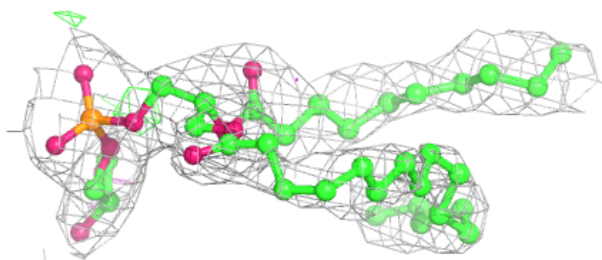
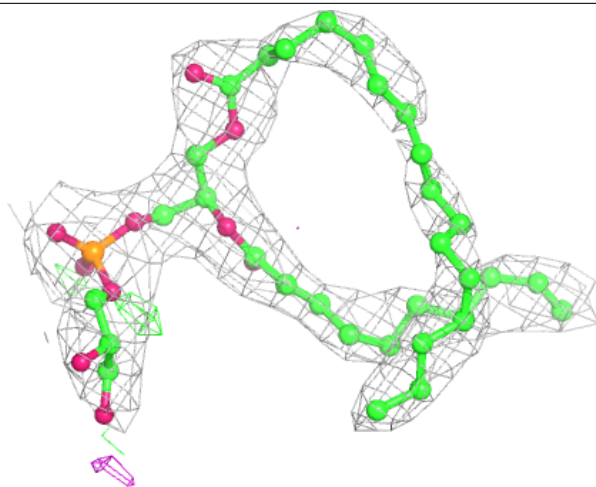
**Electron density around BCR b1 603:**

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



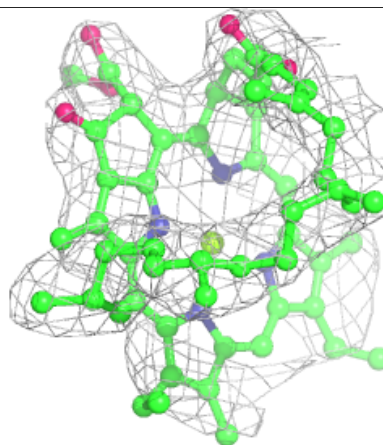
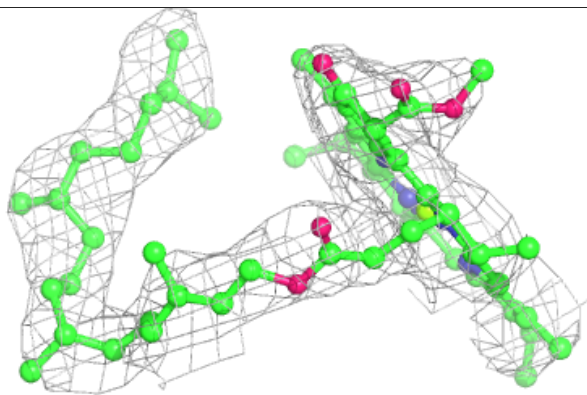
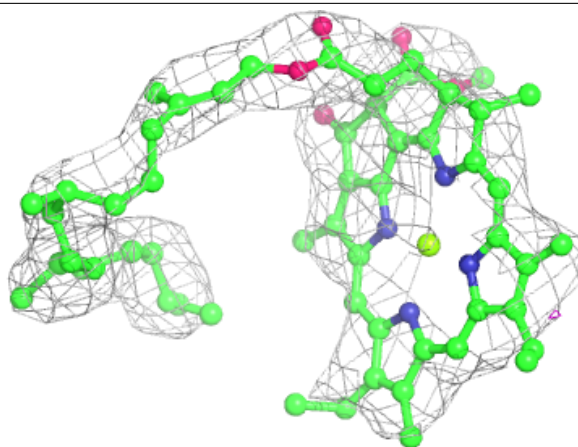
**Electron density around LHG a1 407:**

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



**Electron density around CLA c2 504:**

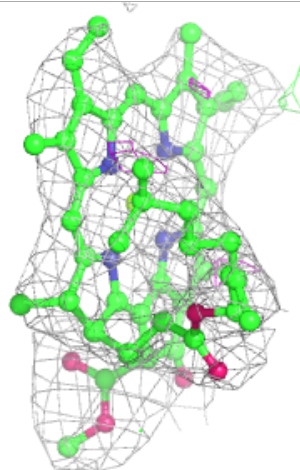
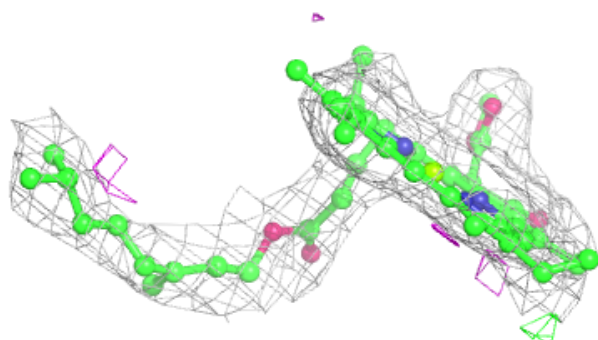
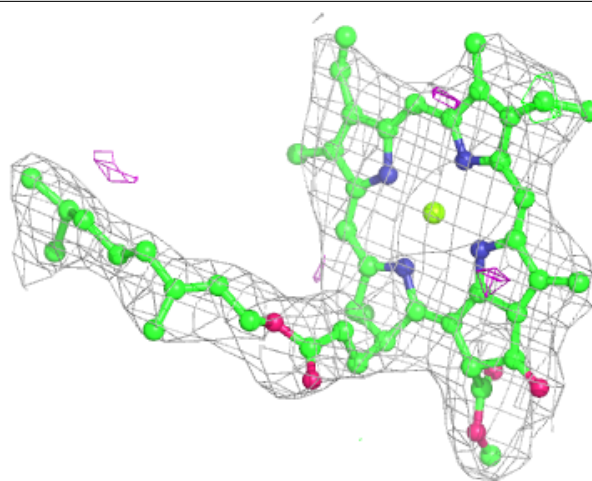
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

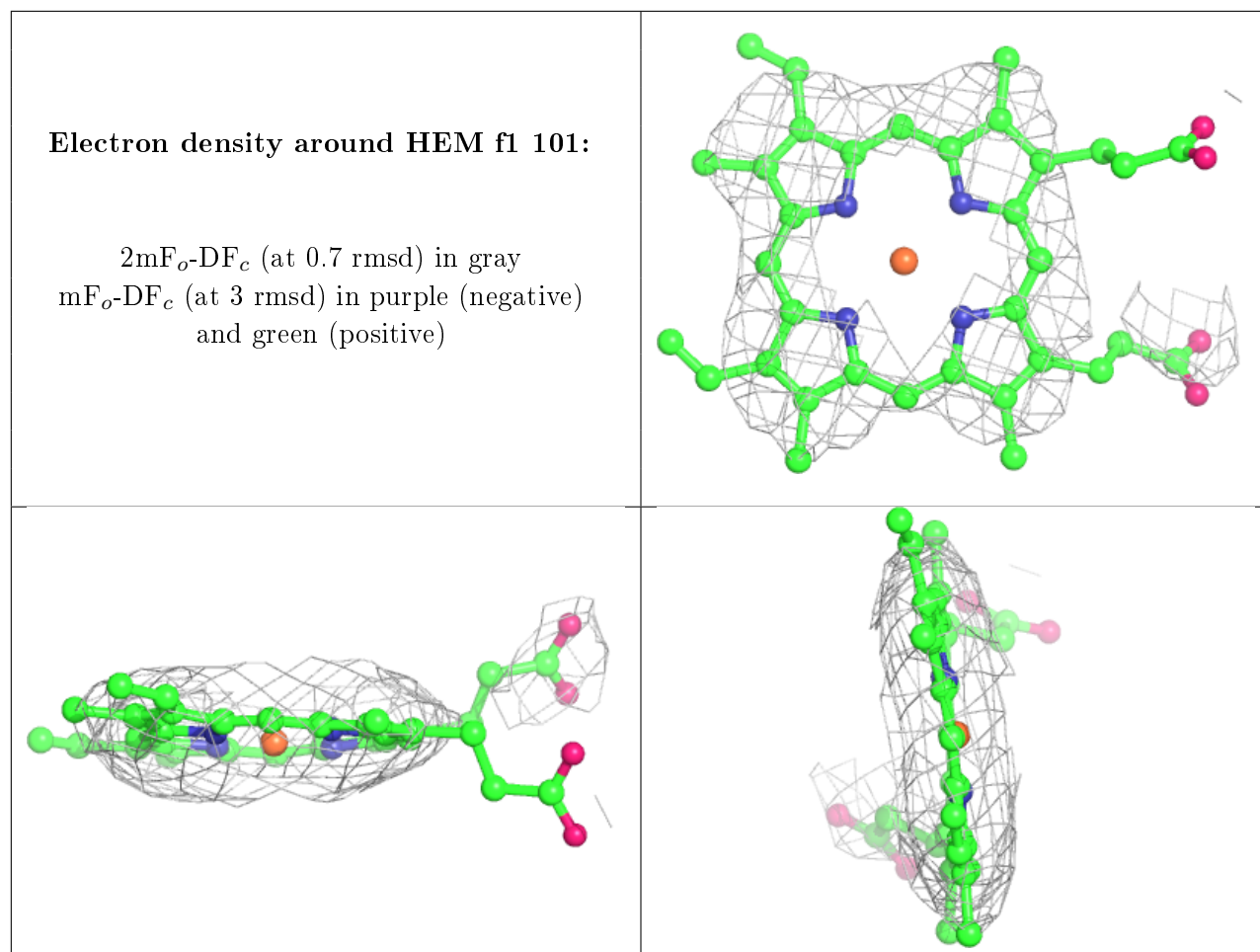


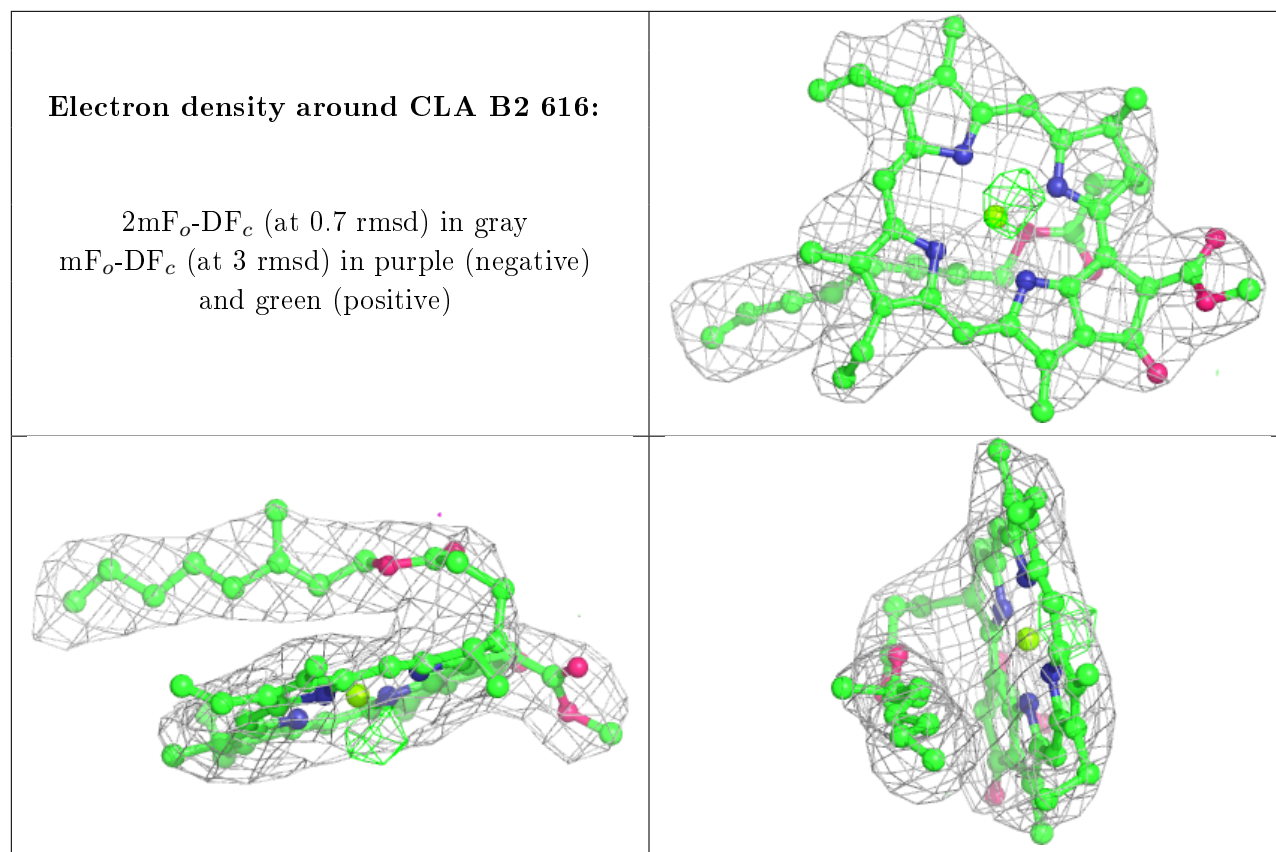


**Electron density around CLA A1 405:**

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



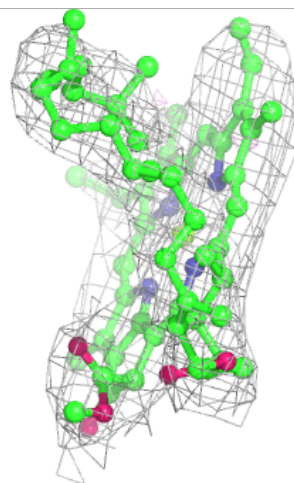
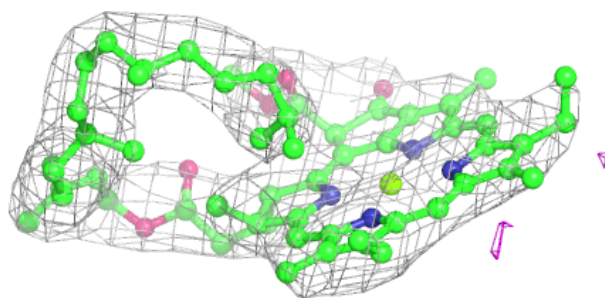
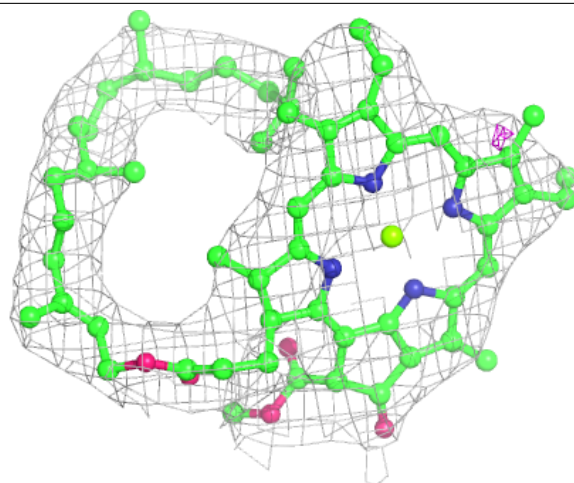






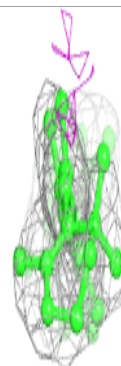
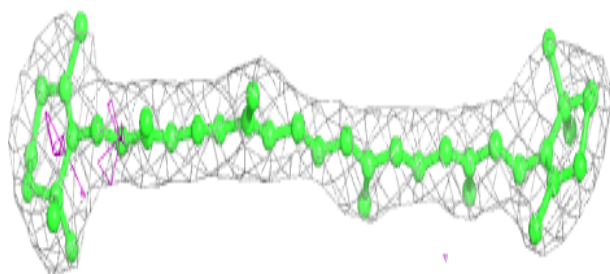
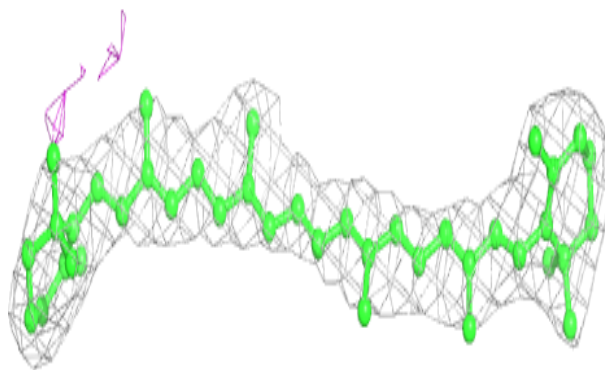
**Electron density around CLA B2 617:**

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

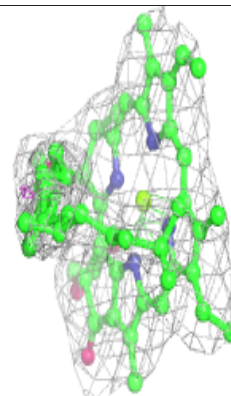
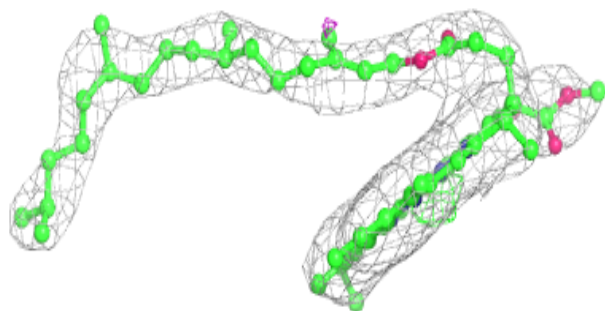
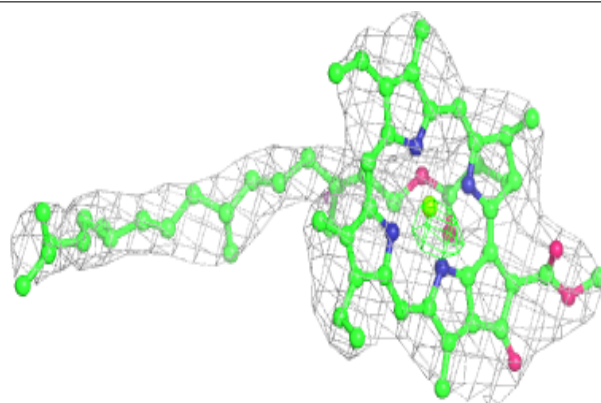


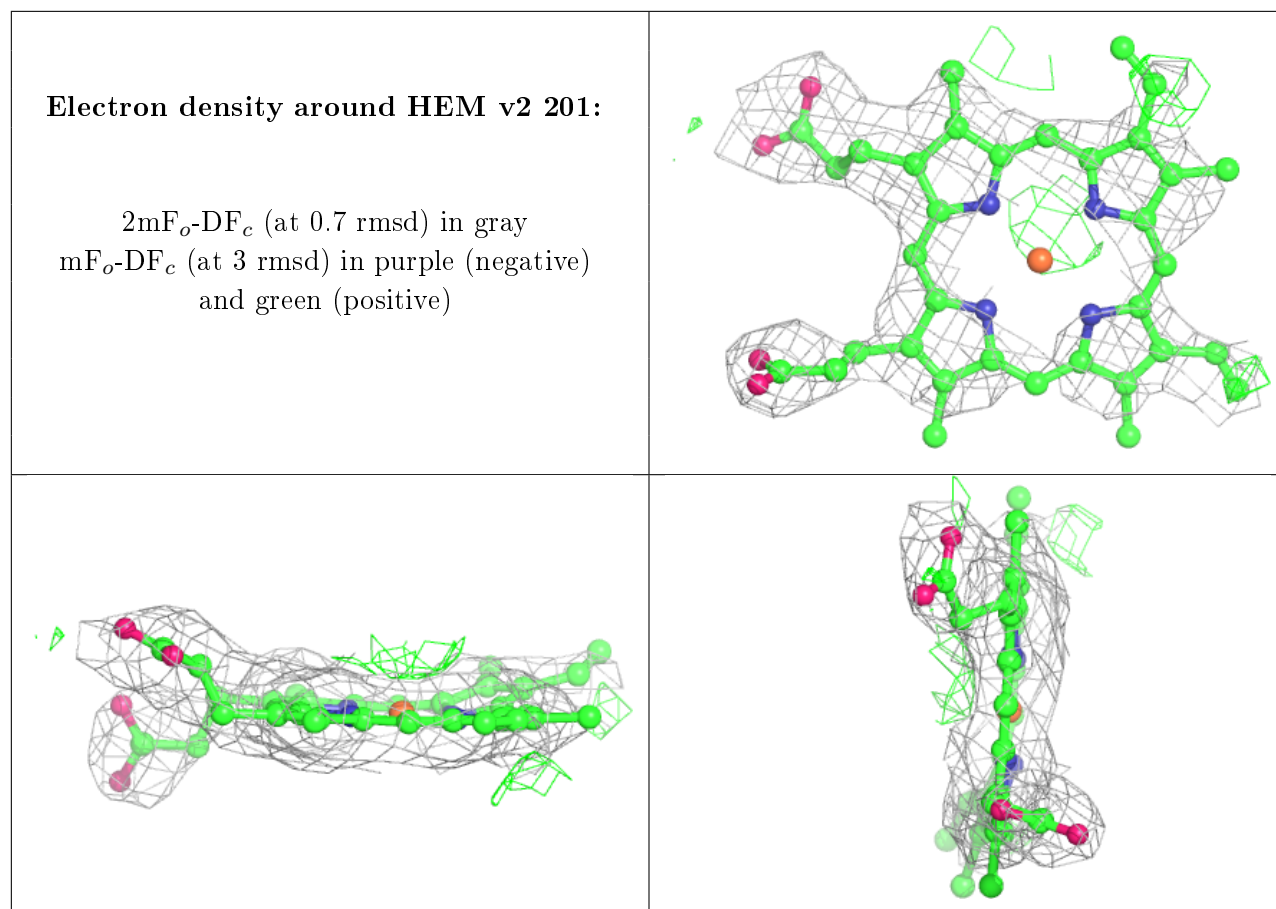
**Electron density around BCR a2 402:**

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

**Electron density around CLA B1 610:**

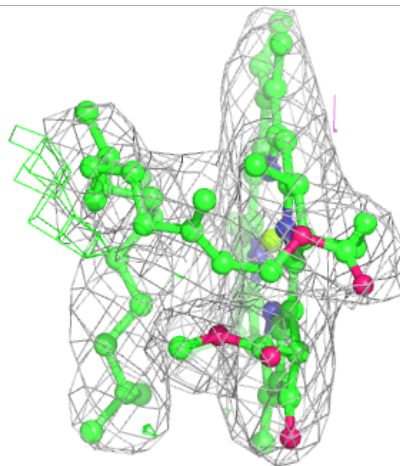
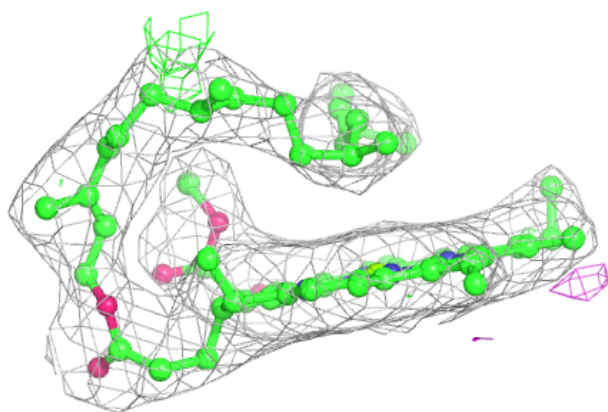
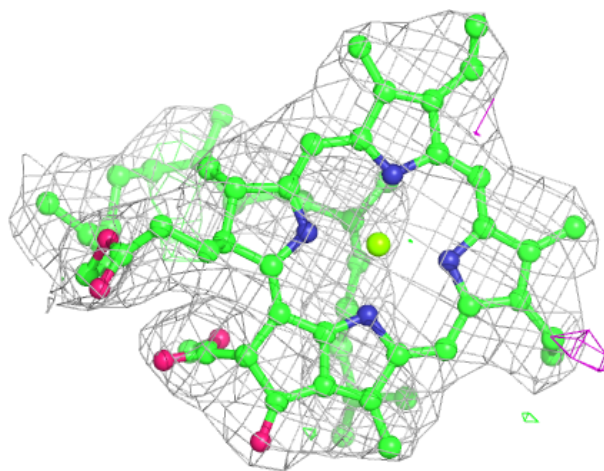
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





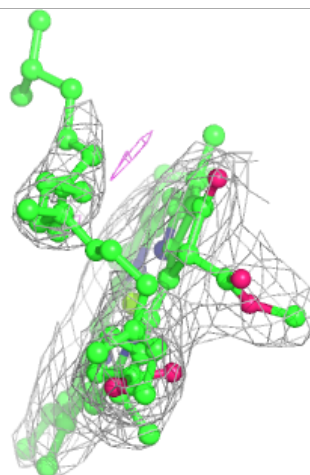
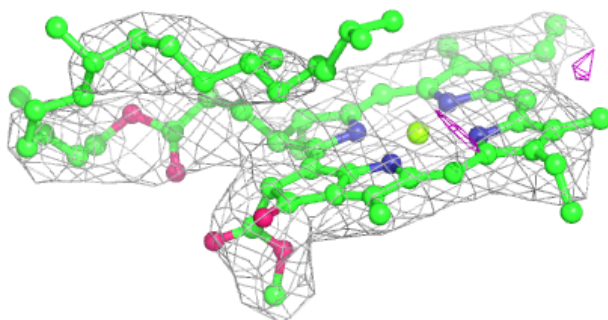
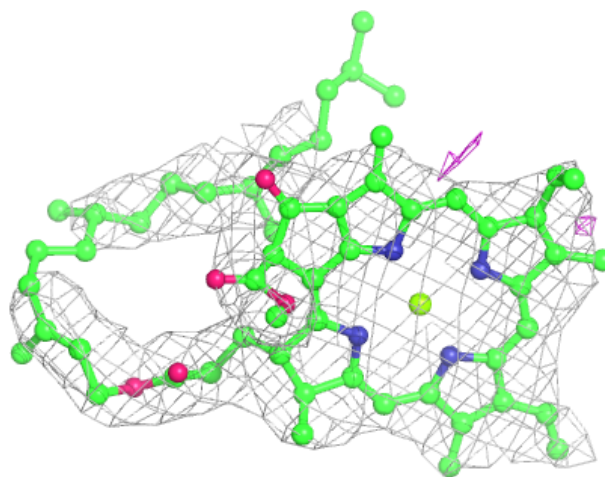
**Electron density around CLA c1 512:**

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



**Electron density around CLA c1 511:**

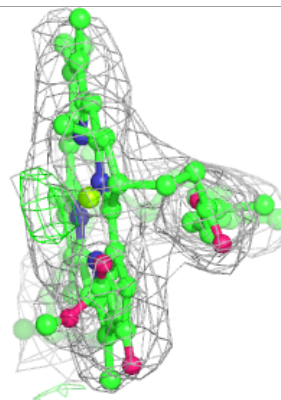
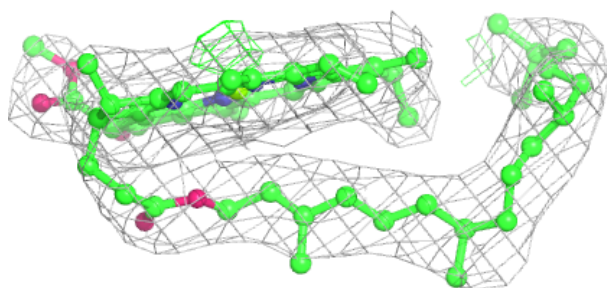
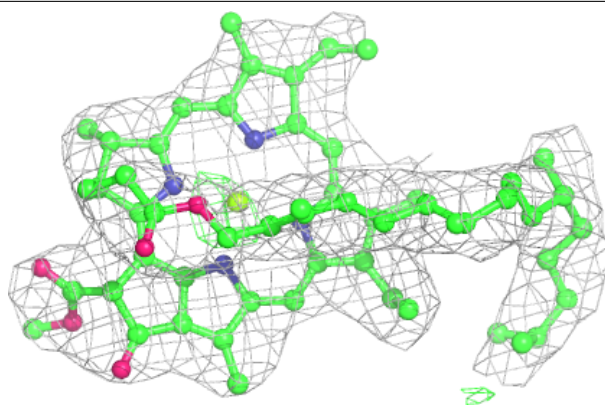
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



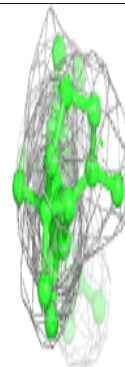
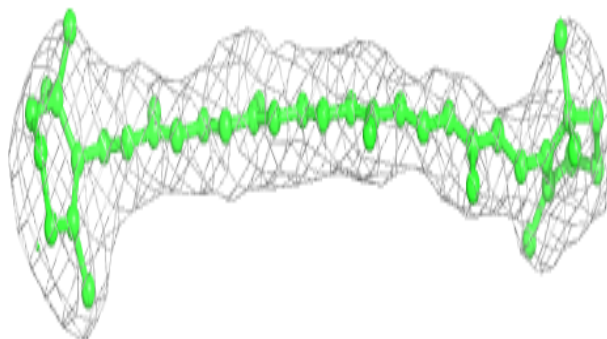
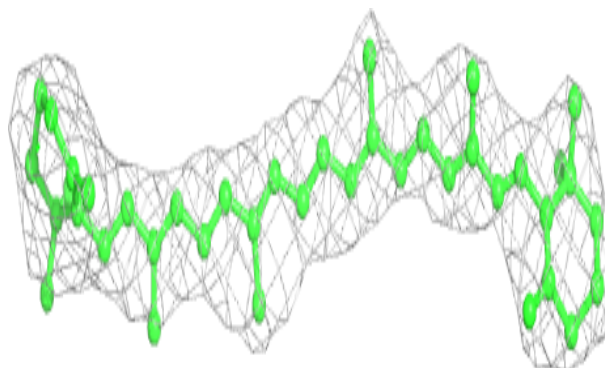


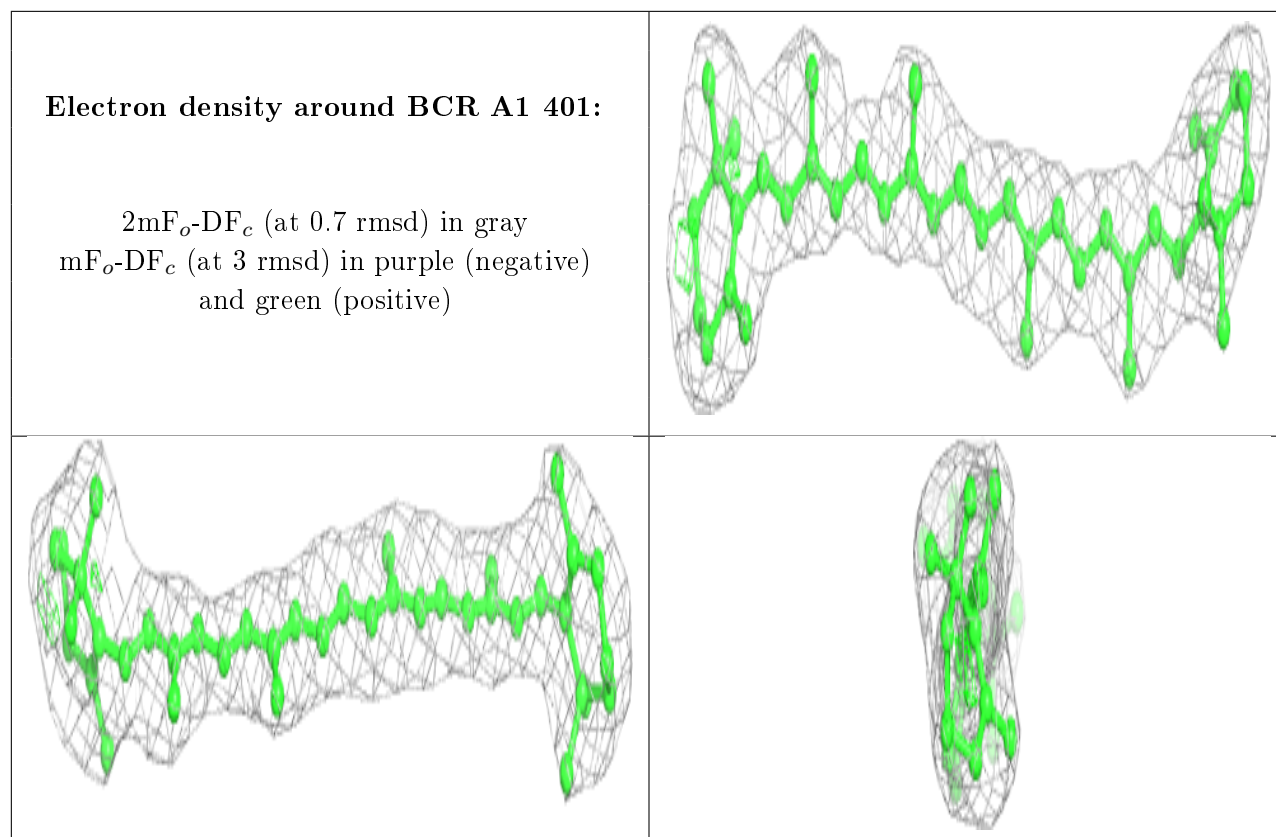
**Electron density around CLA B1 616:**

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

**Electron density around BCR B2 601:**

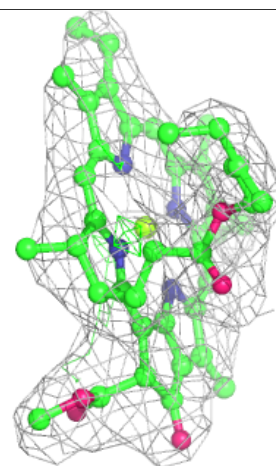
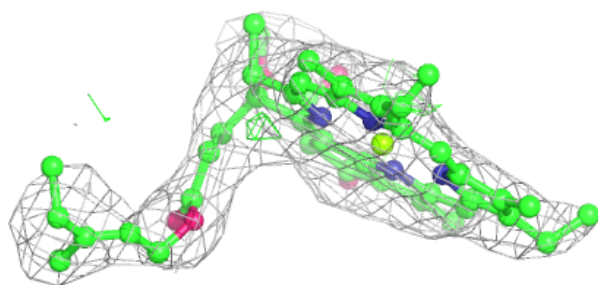
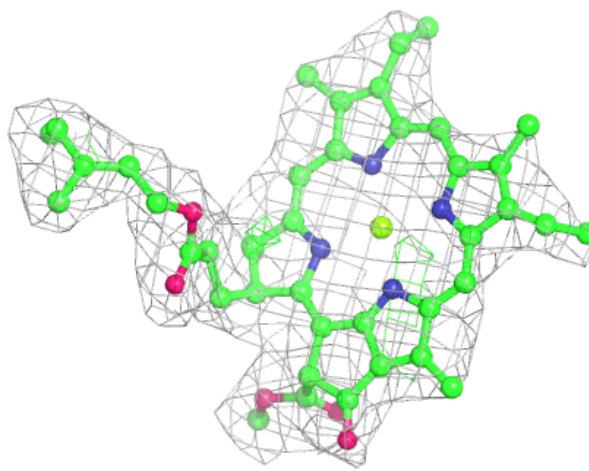
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A1 404:**

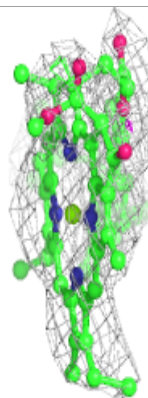
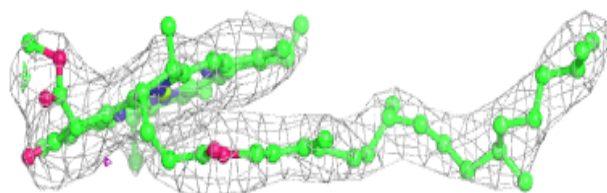
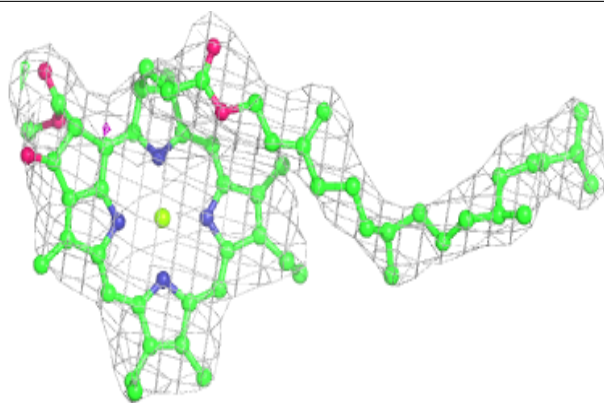
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



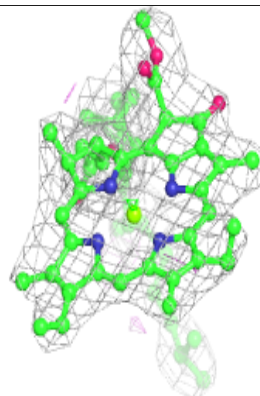
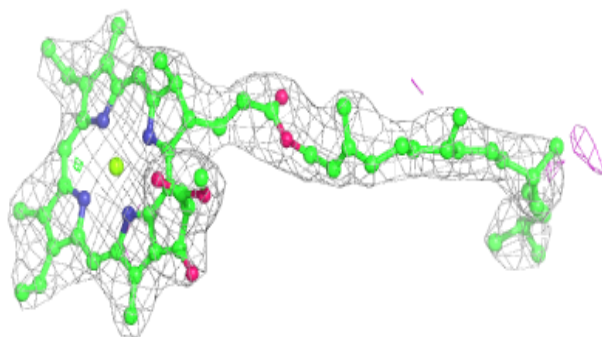
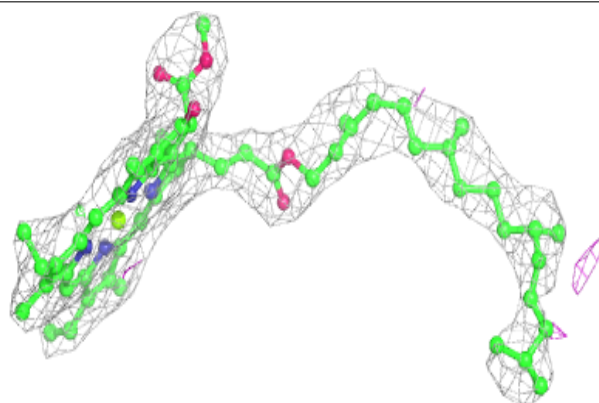


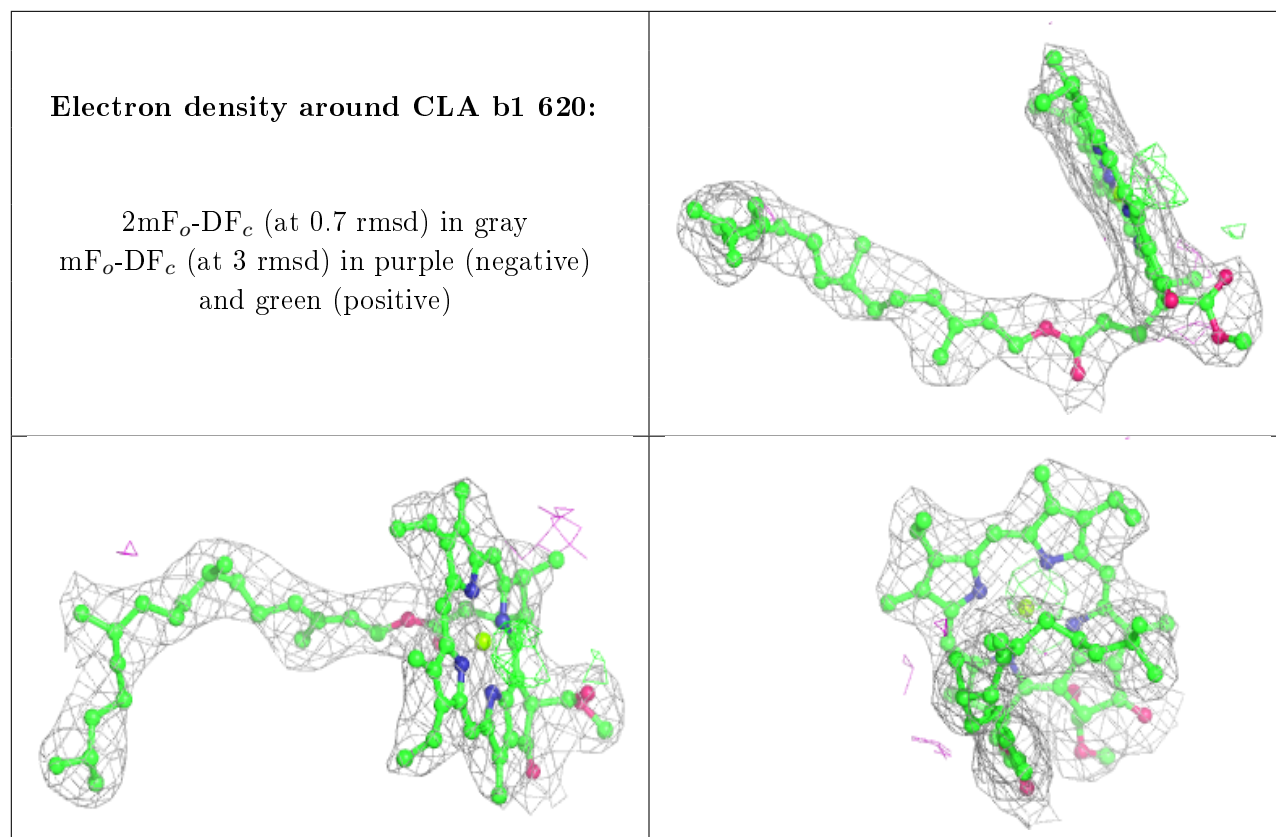
**Electron density around CLA b1 606:**

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

**Electron density around CLA D1 402:**

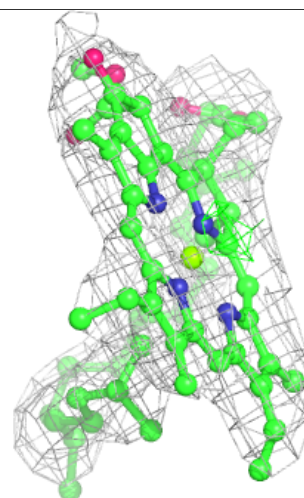
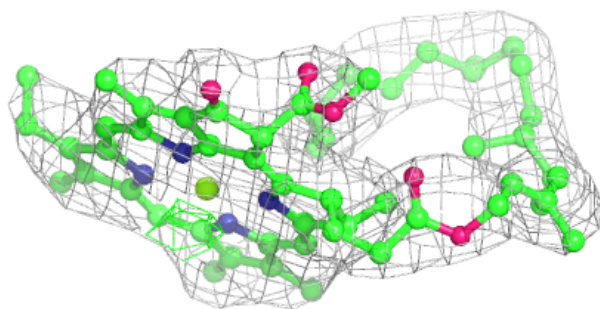
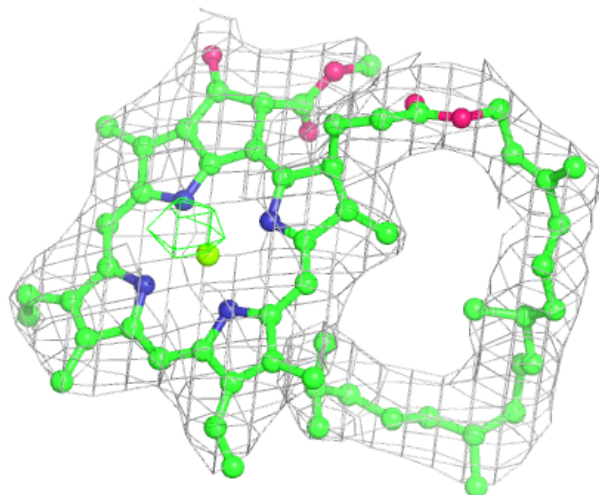
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





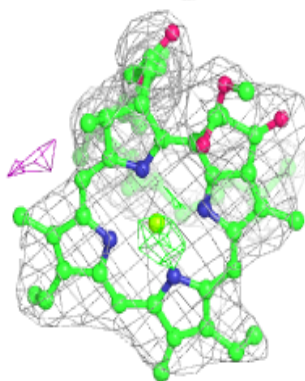
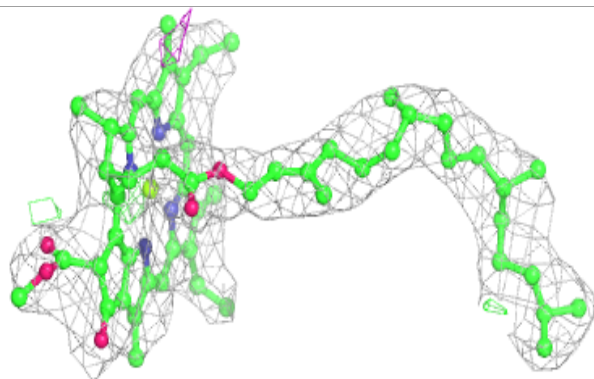
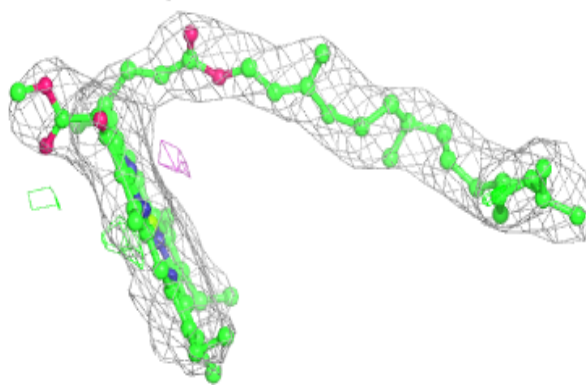
**Electron density around CLA b1 617:**

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

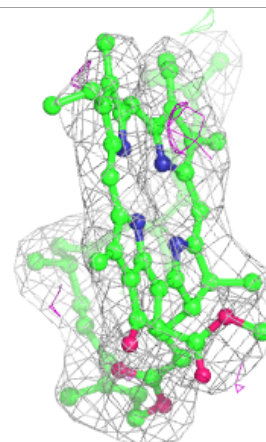
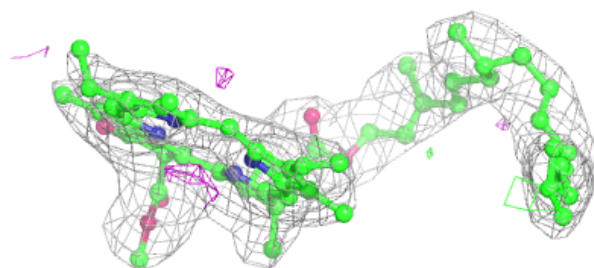
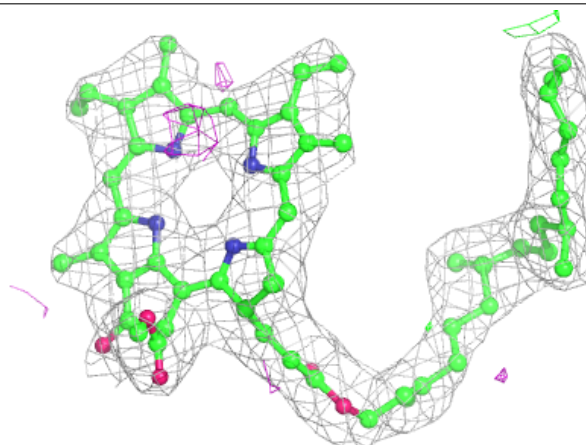


**Electron density around CLA b2 620:**

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

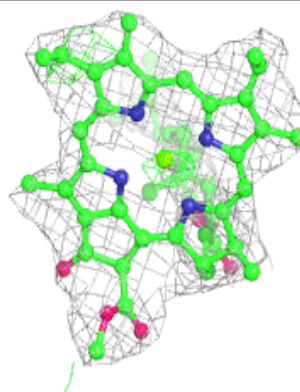
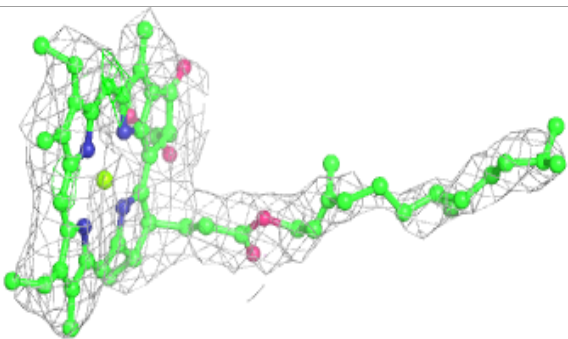
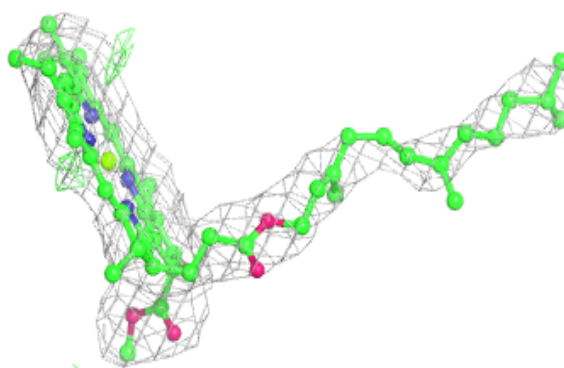
**Electron density around PHO d1 403:**

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

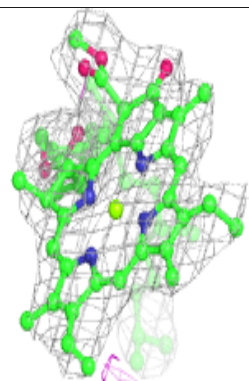
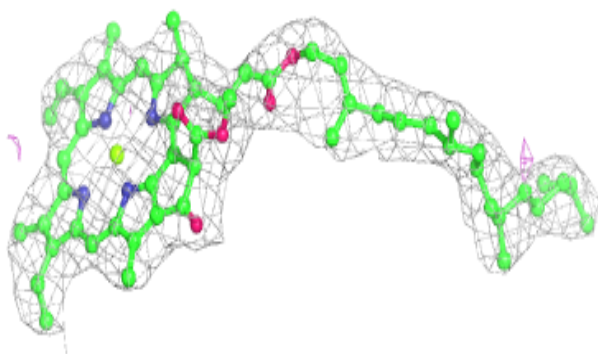
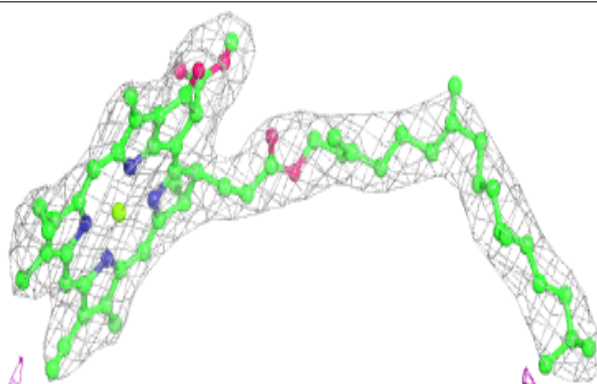


**Electron density around CLA b2 616:**

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

**Electron density around CLA a1 403:**

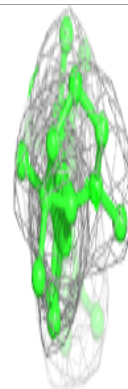
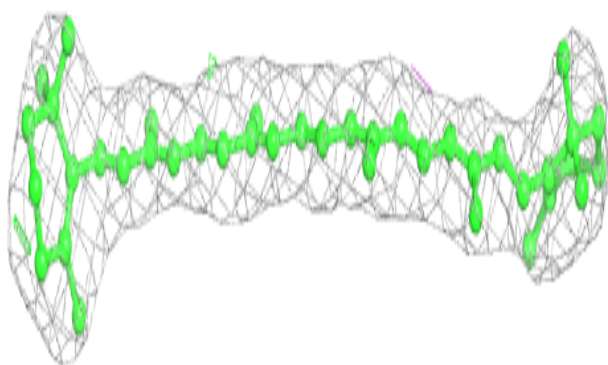
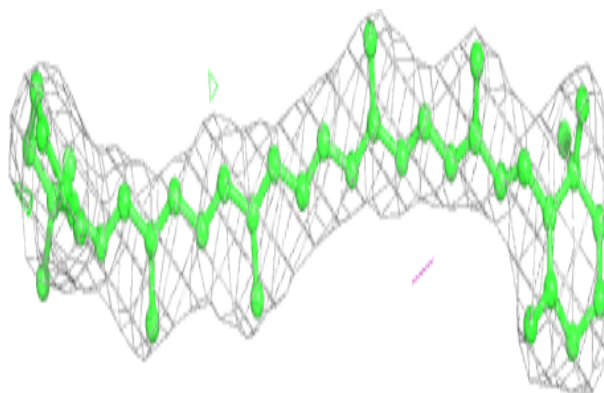
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



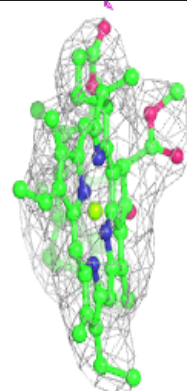
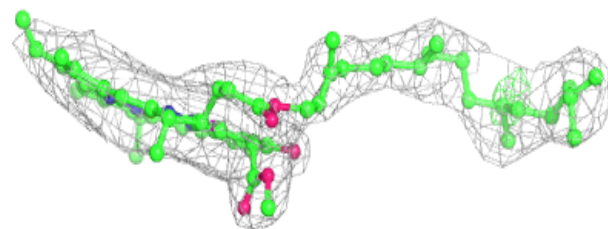
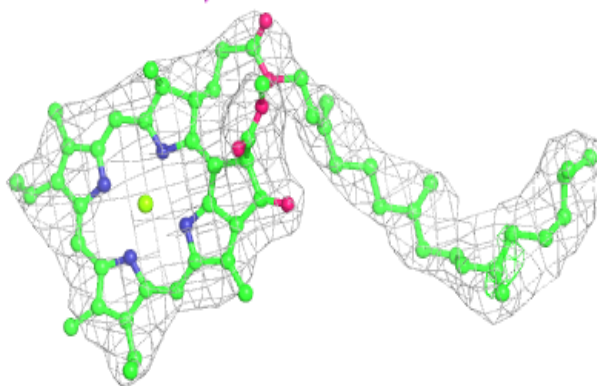


**Electron density around BCR b1 601:**

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

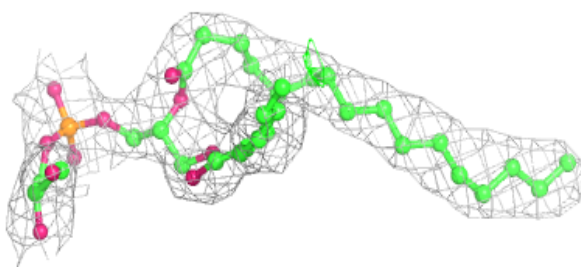
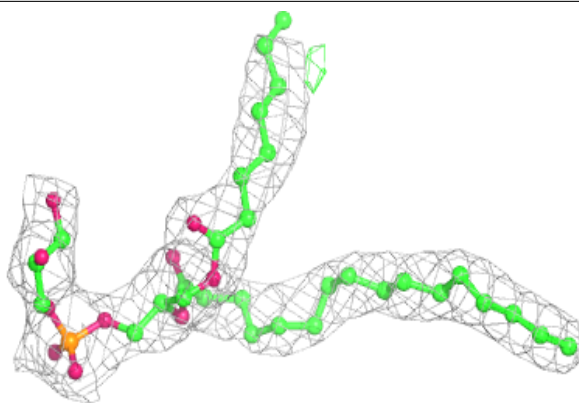
**Electron density around CLA b1 605:**

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

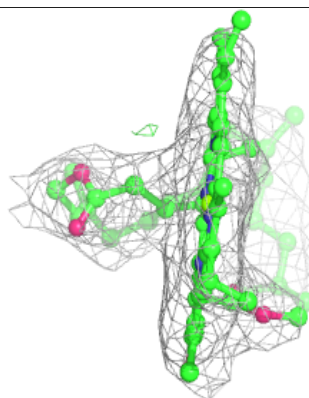
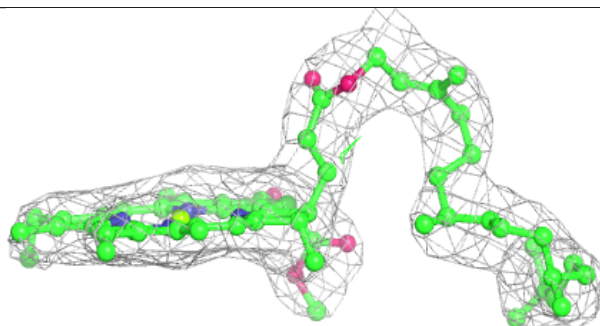
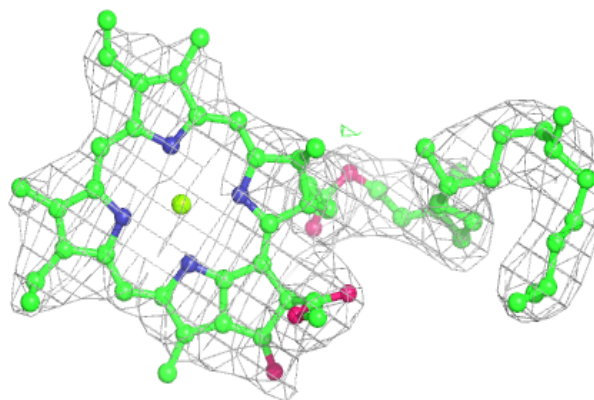


**Electron density around LHG L1 101:**

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

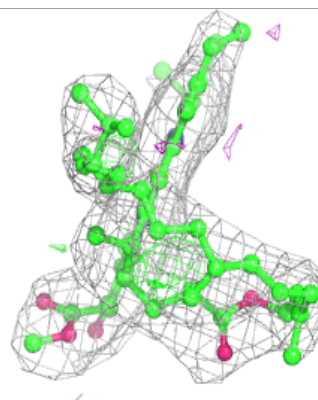
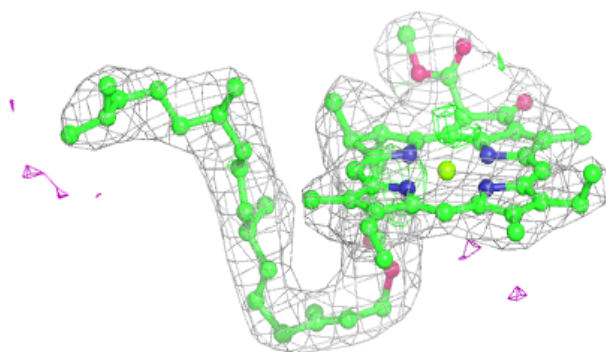
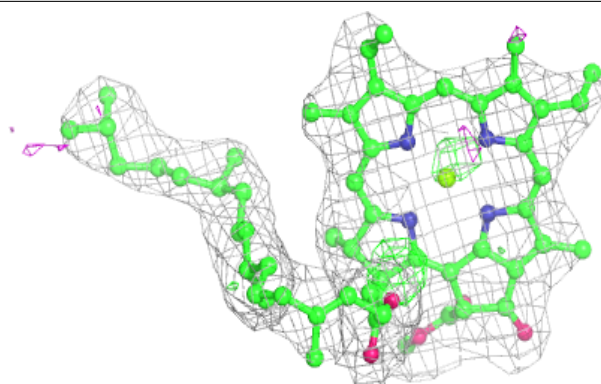
**Electron density around CLA b2 614:**

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

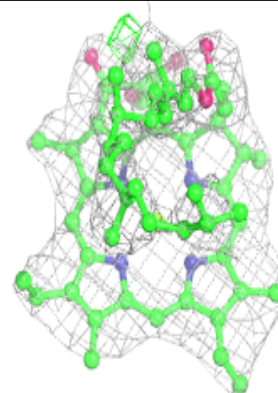
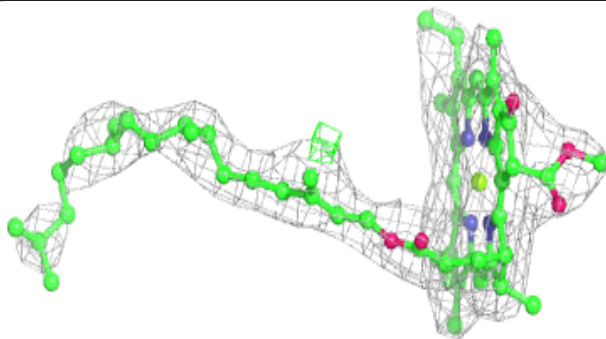
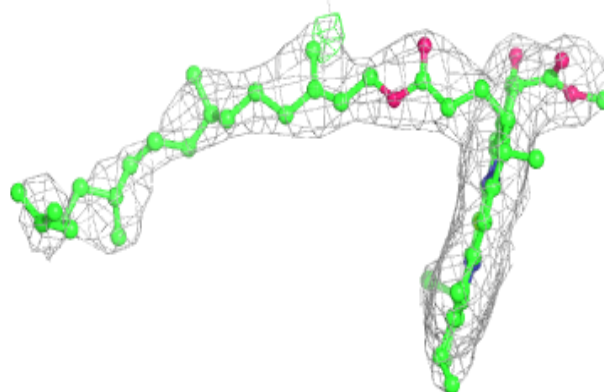


**Electron density around CLA d2 402:**

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

**Electron density around CLA B2 608:**

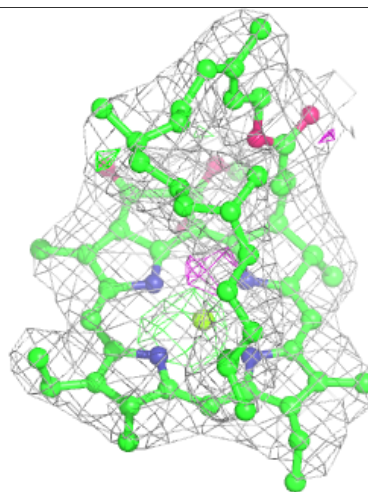
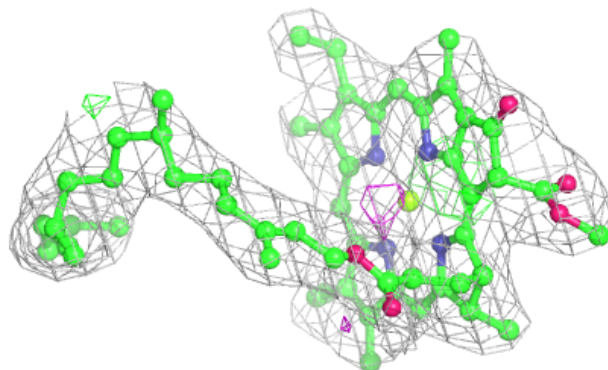
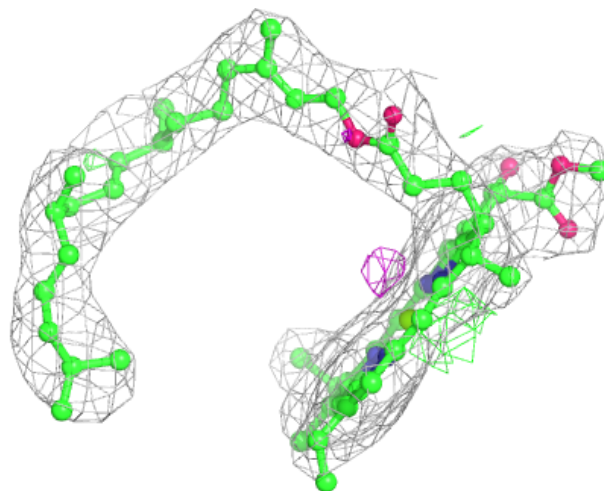
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





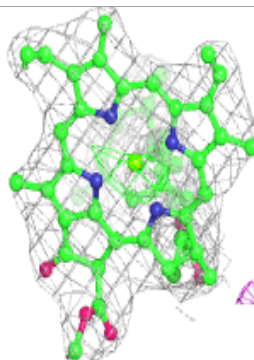
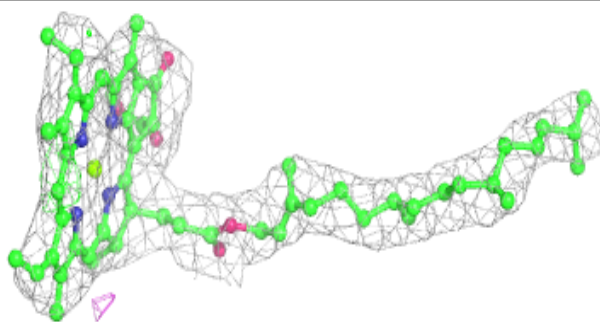
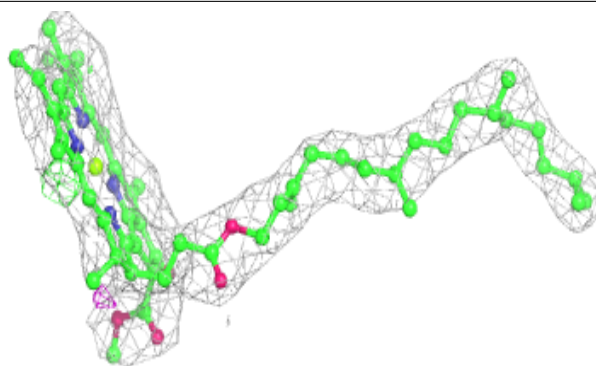
**Electron density around CLA b1 613:**

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

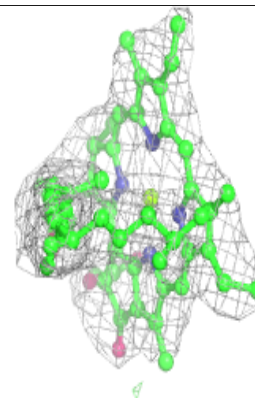
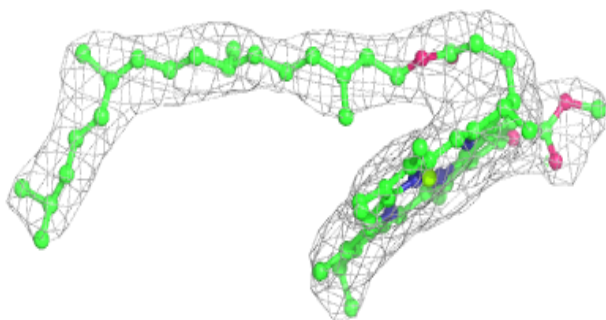
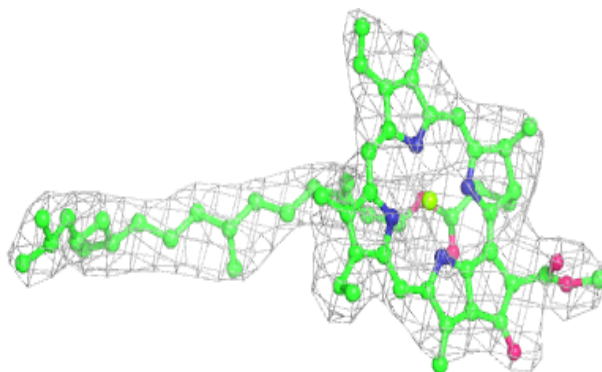


**Electron density around CLA b1 607:**

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

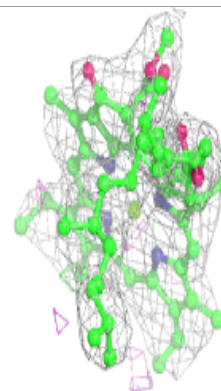
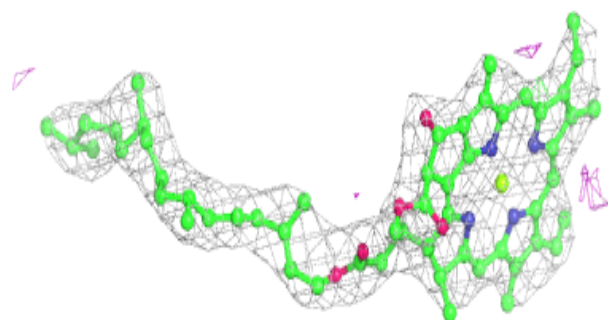
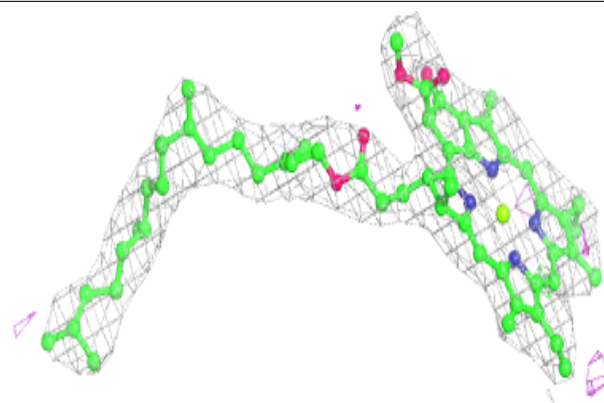
**Electron density around CLA b1 610:**

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

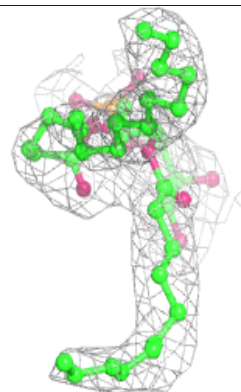
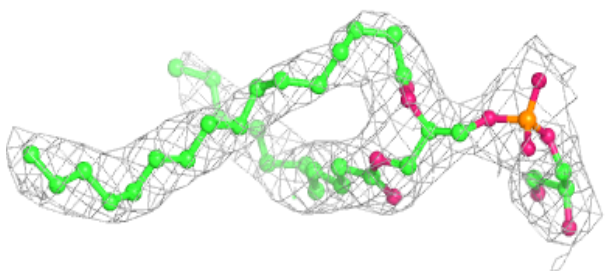
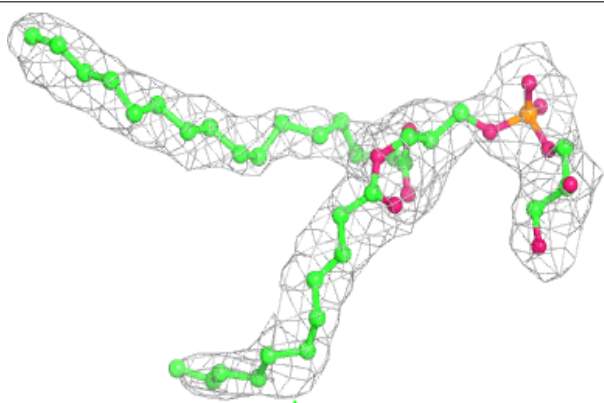


**Electron density around CLA a2 404:**

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

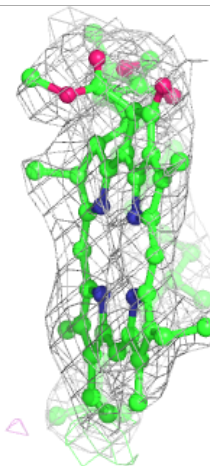
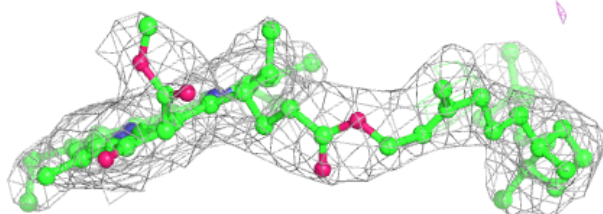
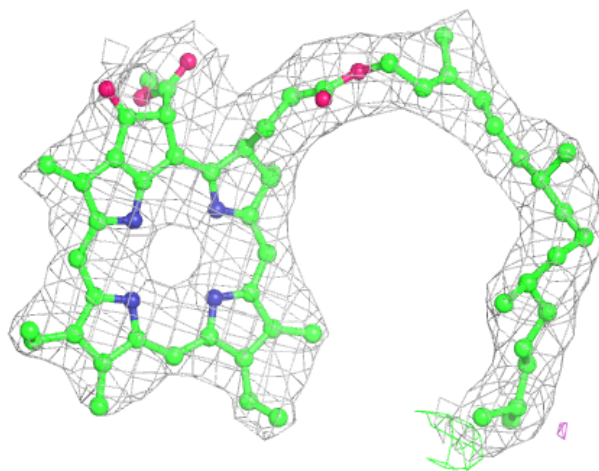
**Electron density around LHG 12 101:**

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



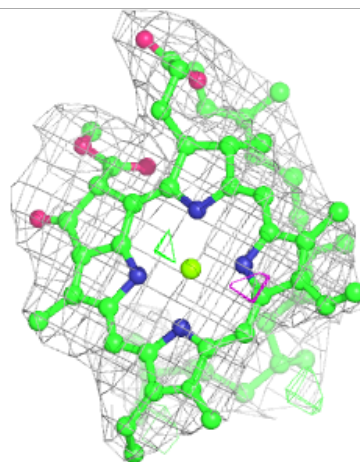
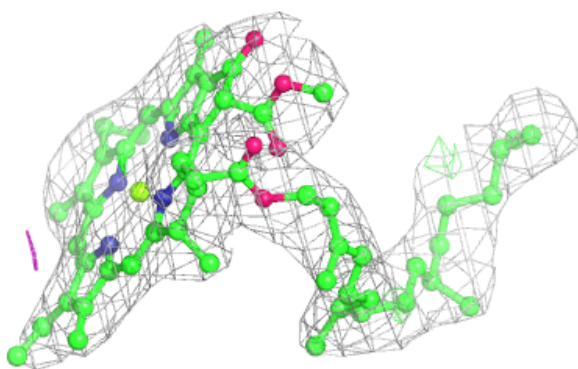
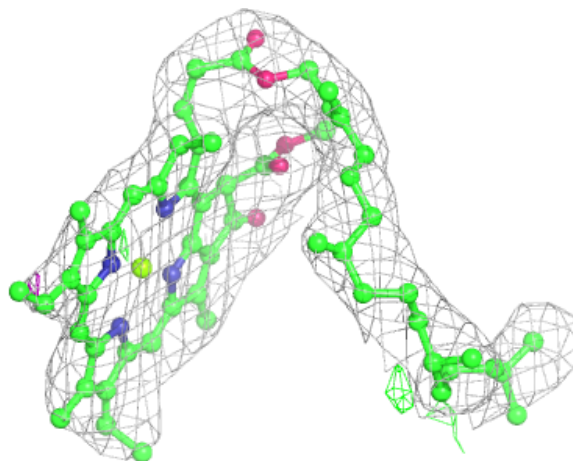
**Electron density around PHO a1 411:**

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



**Electron density around CLA B1 615:**

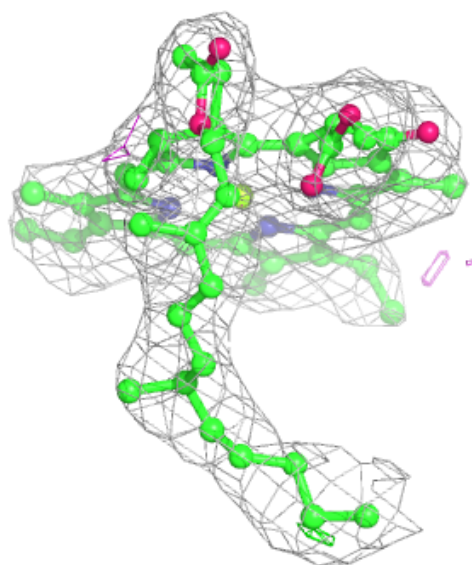
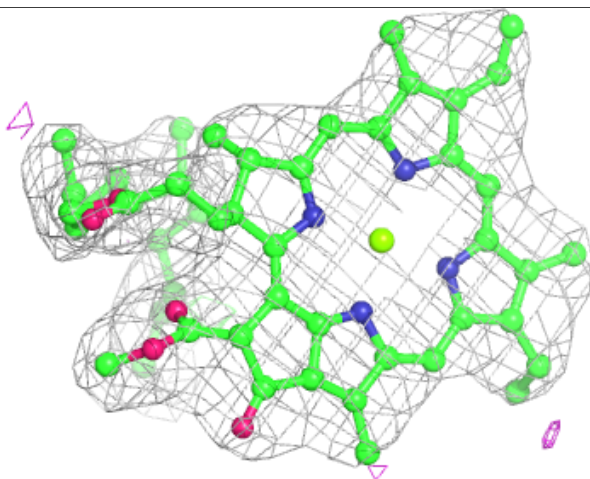
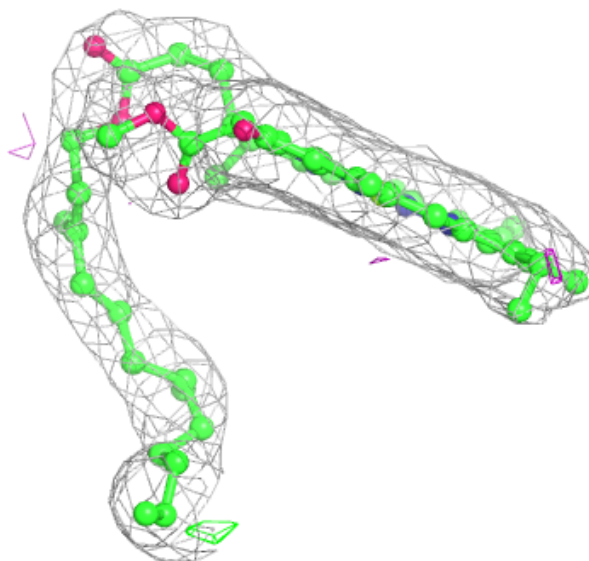
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





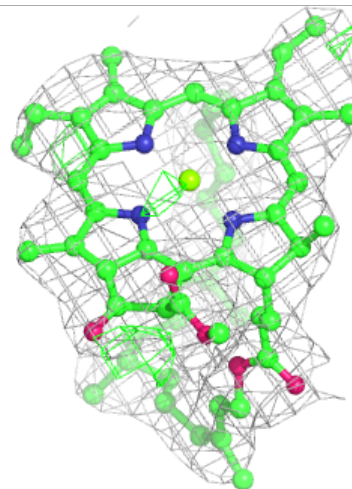
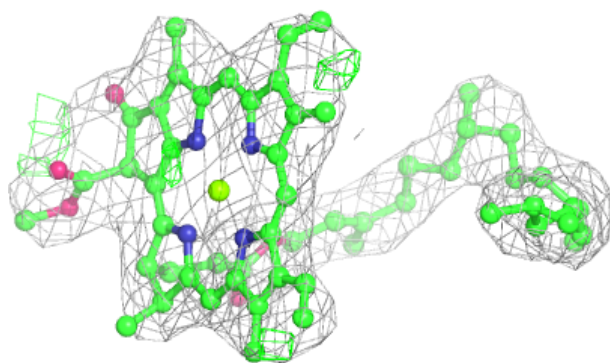
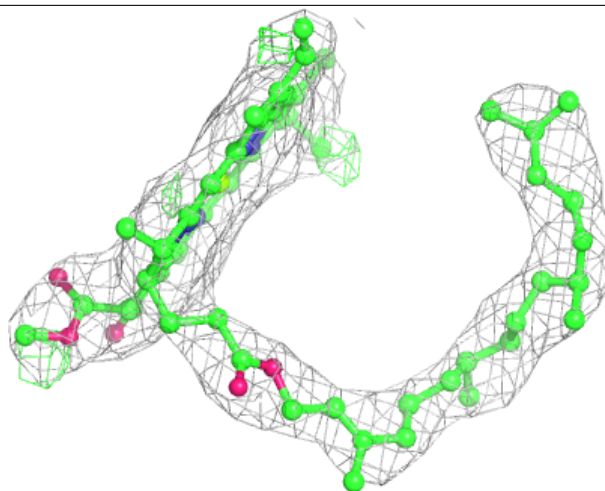
**Electron density around CLA b1 615:**

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



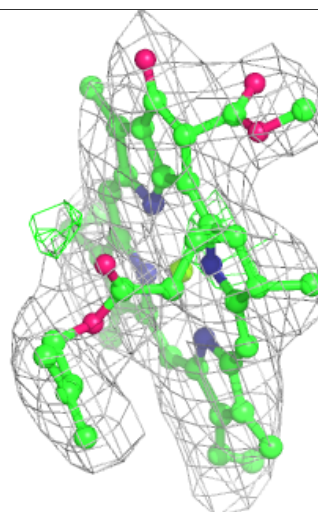
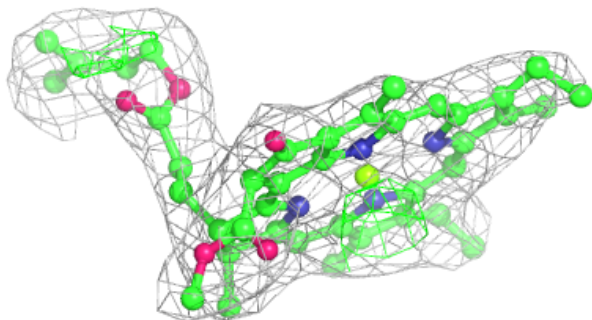
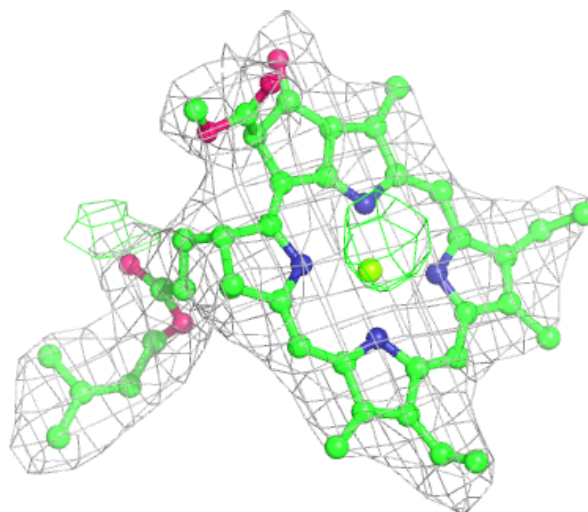
**Electron density around CLA B2 613:**

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

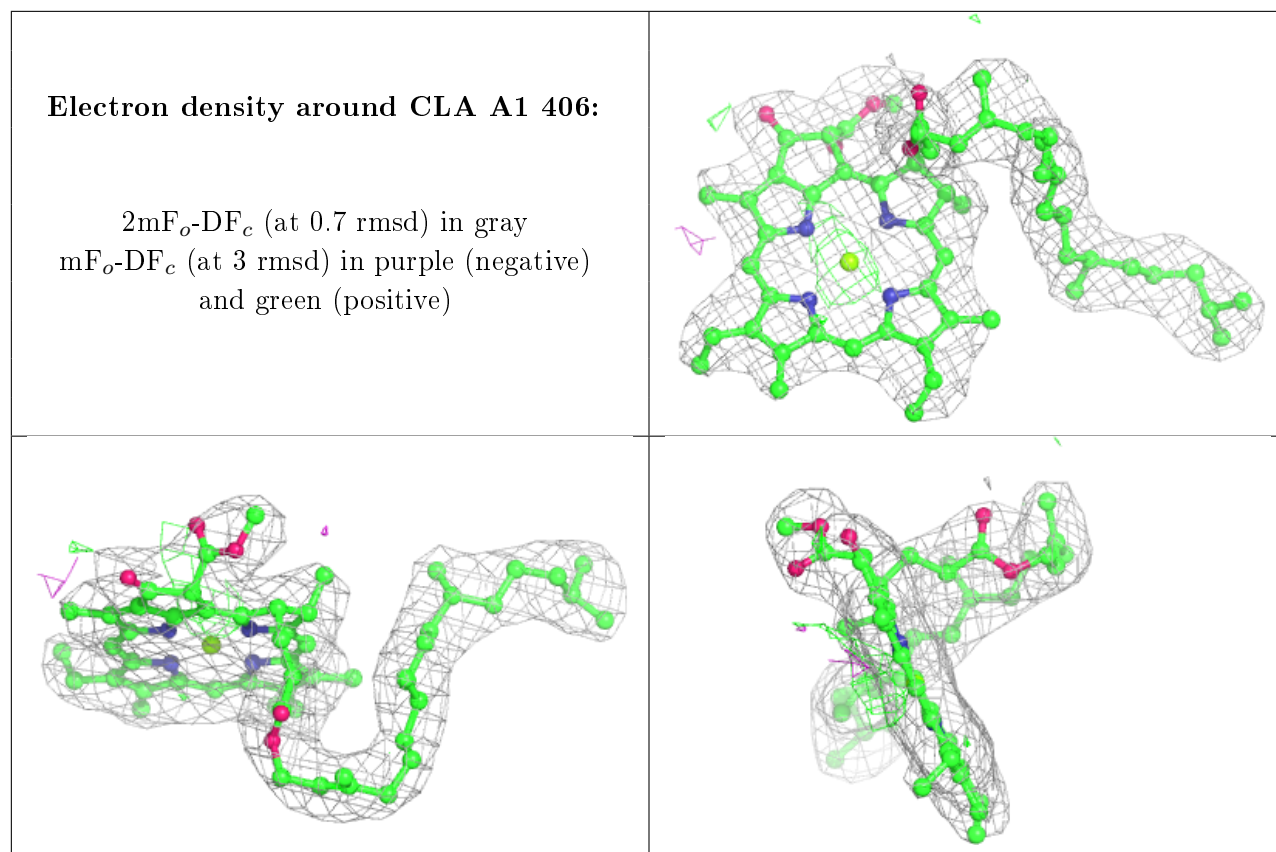


**Electron density around CLA a1 405:**

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

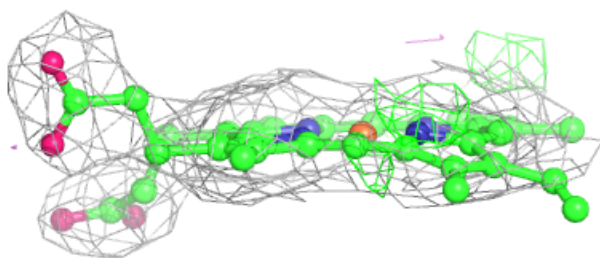
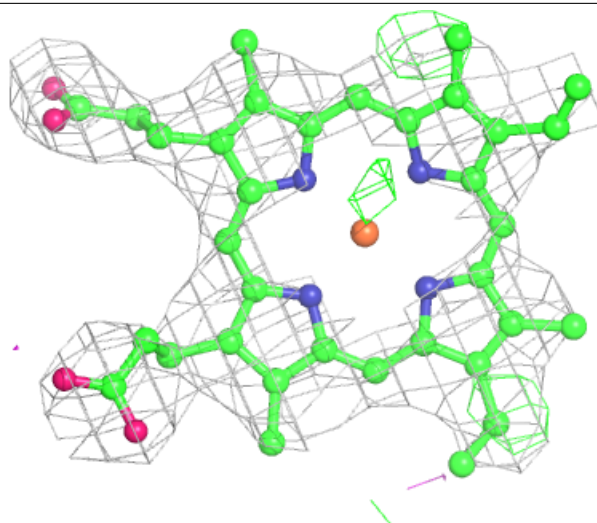






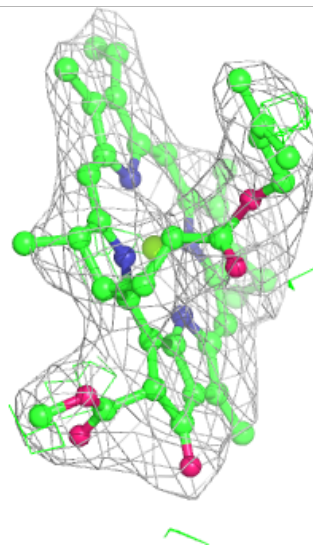
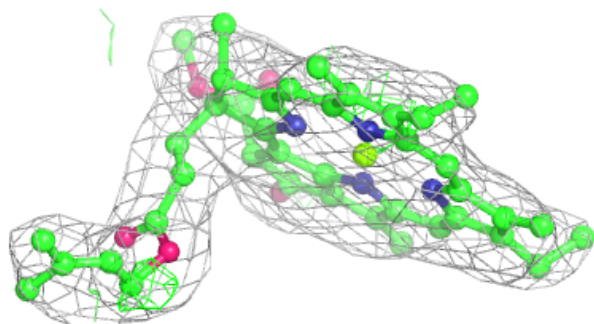
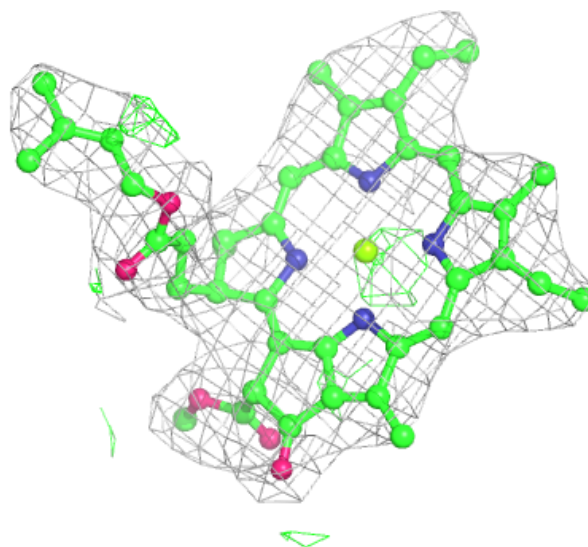
**Electron density around HEM V1 201:**

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



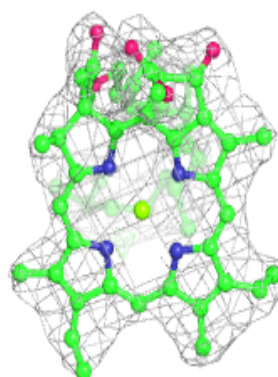
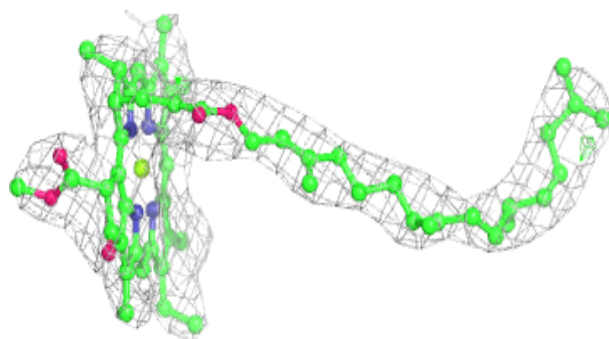
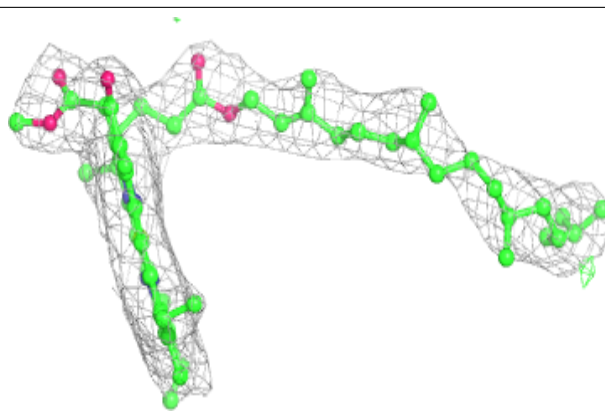
**Electron density around CLA a2 413:**

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

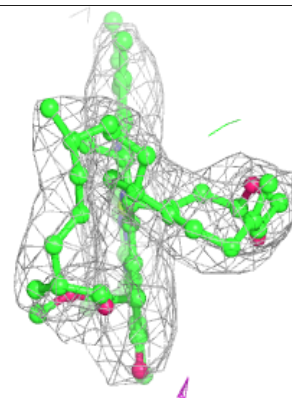
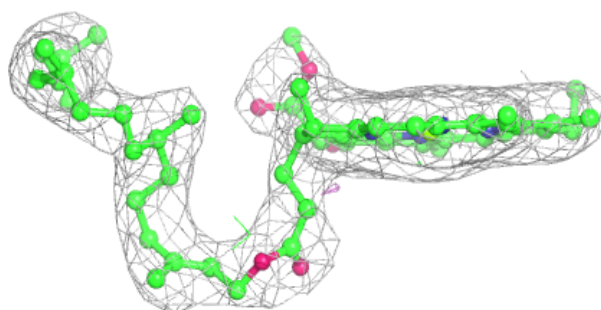
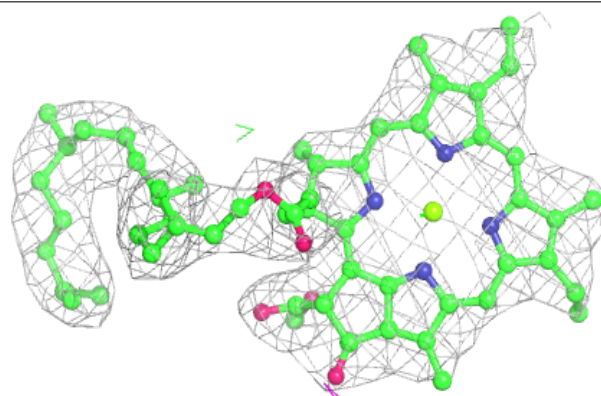


**Electron density around CLA b1 608:**

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

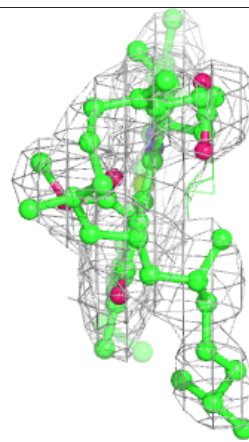
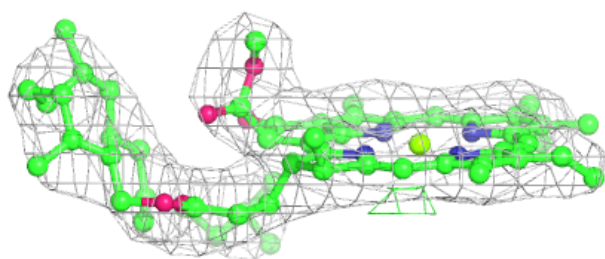
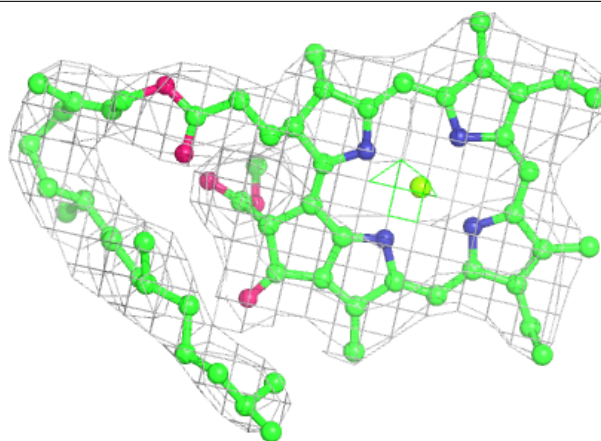
**Electron density around CLA b1 614:**

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



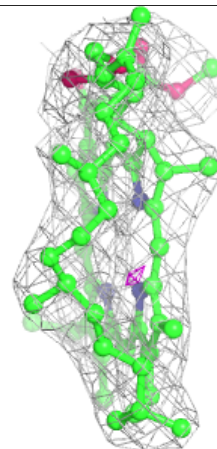
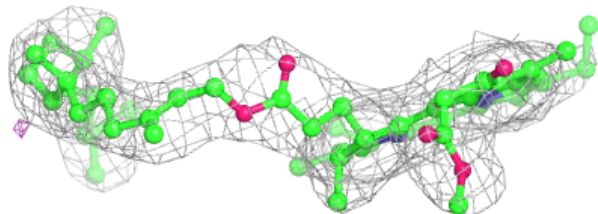
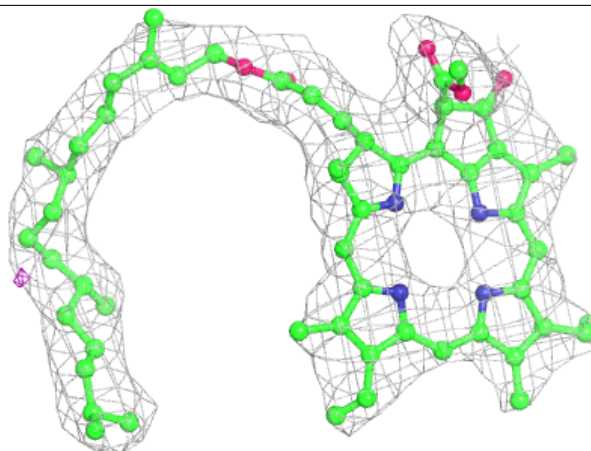
**Electron density around CLA b1 612:**

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



**Electron density around PHO A1 408:**

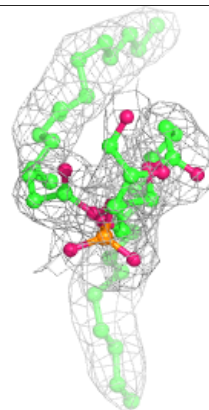
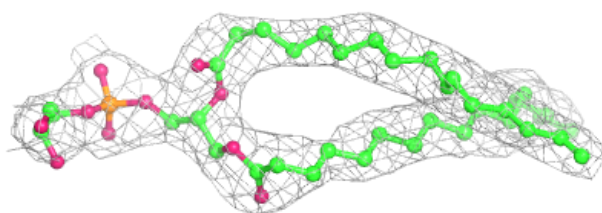
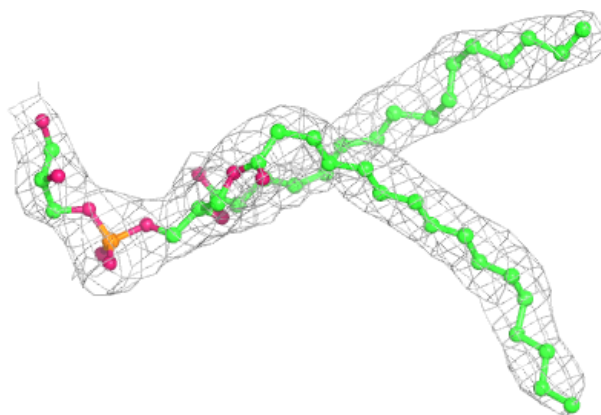
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



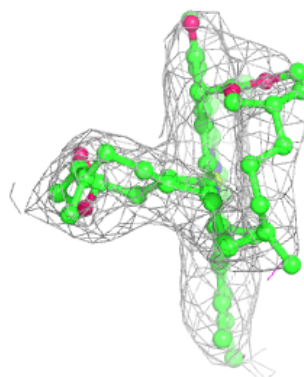
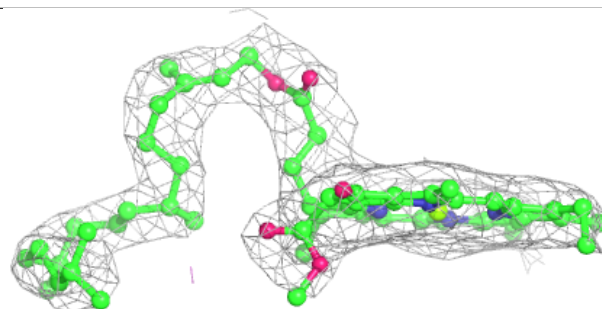
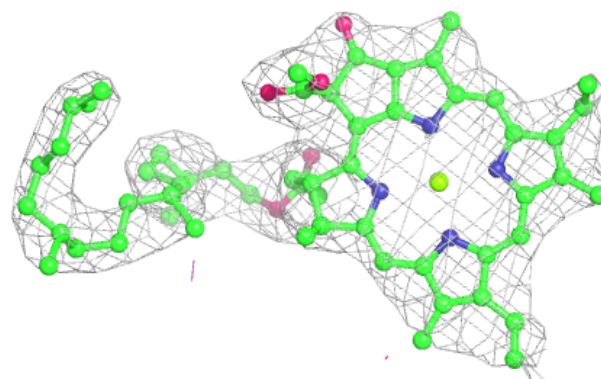


**Electron density around LHG D1 405:**

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

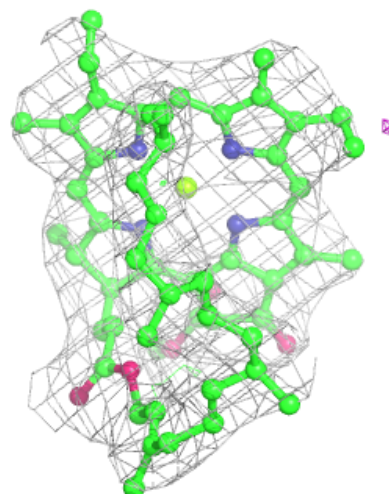
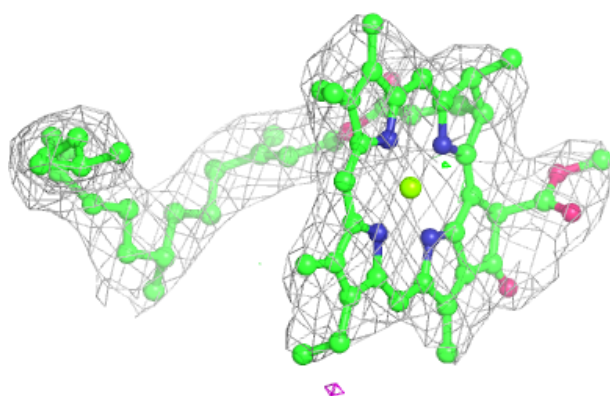
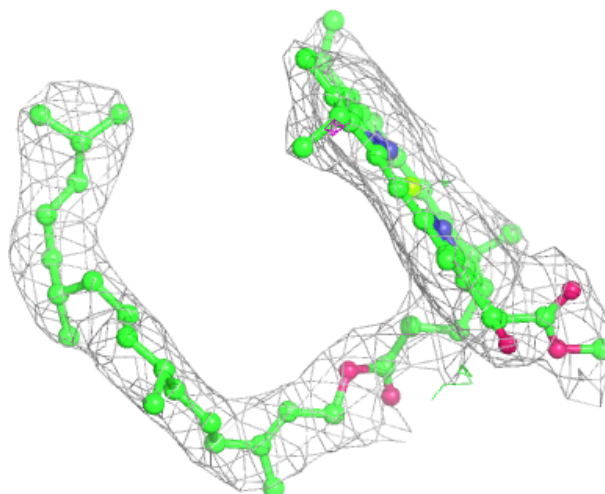
**Electron density around CLA B1 614:**

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



**Electron density around CLA B1 613:**

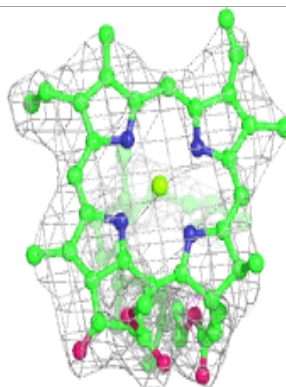
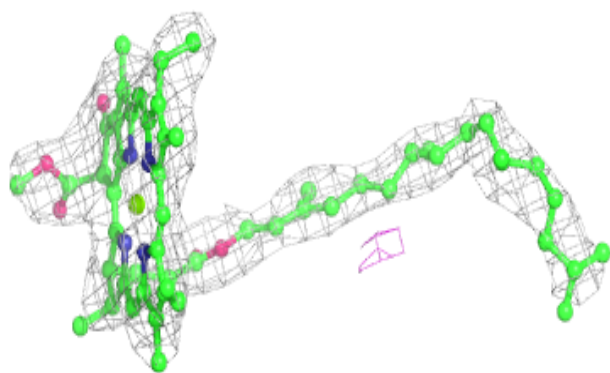
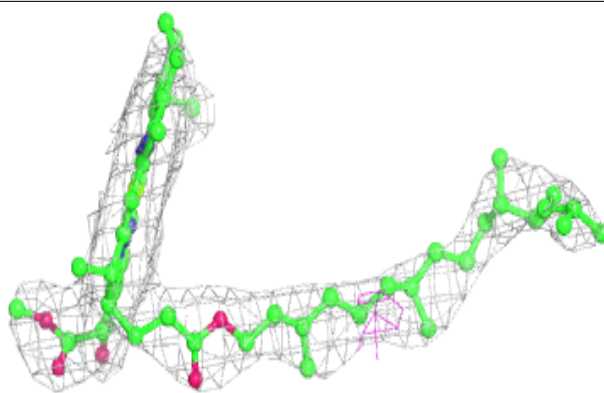
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



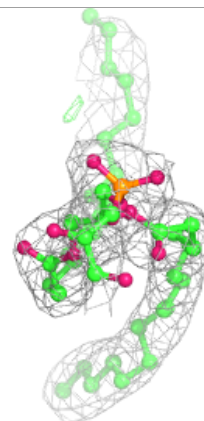
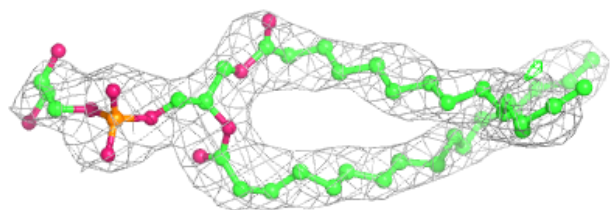
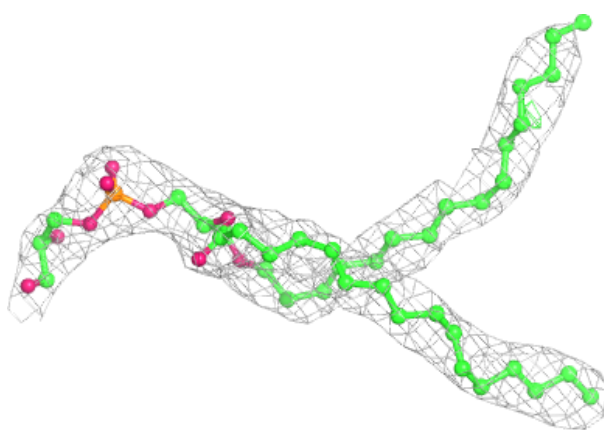


**Electron density around CLA B1 608:**

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

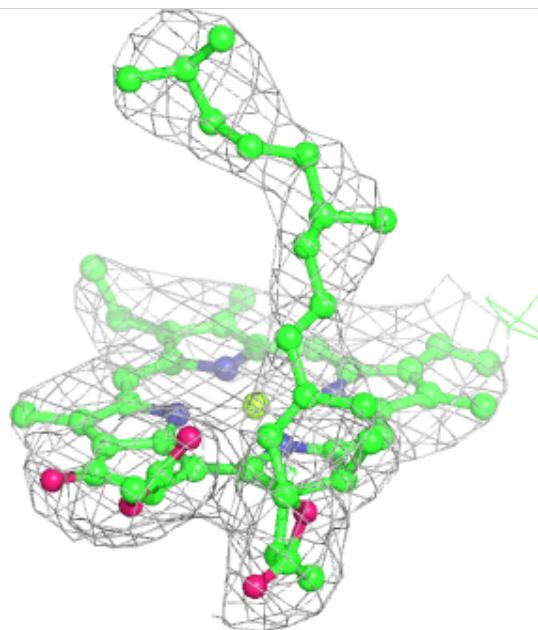
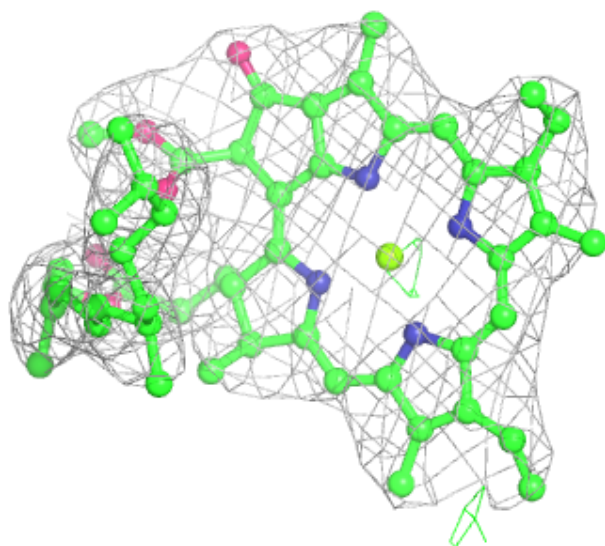
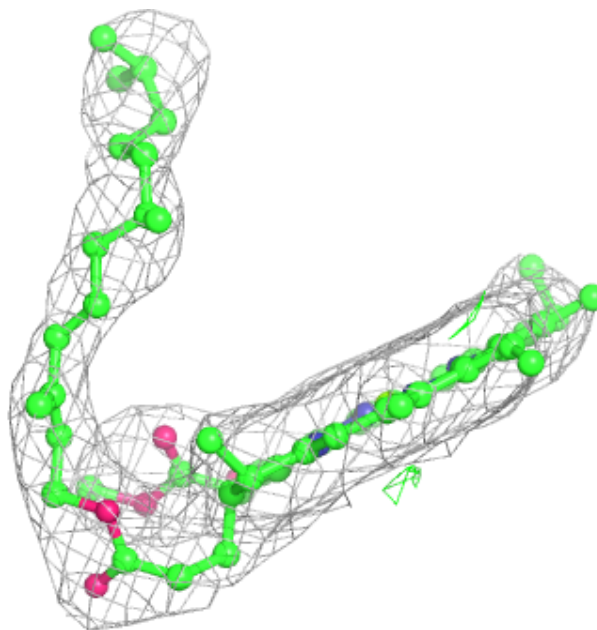
**Electron density around LHG d1 407:**

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



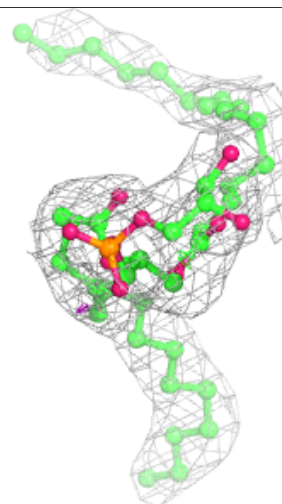
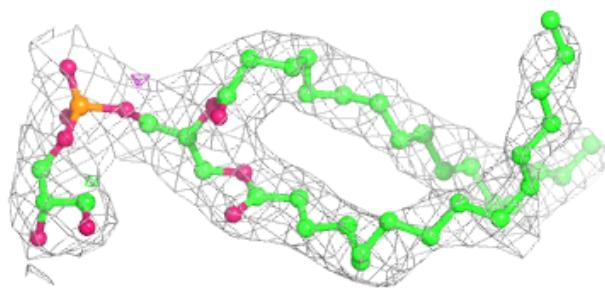
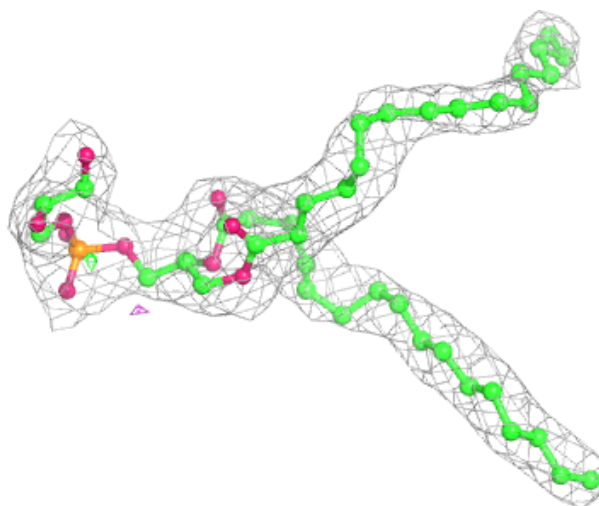
**Electron density around CLA b2 615:**

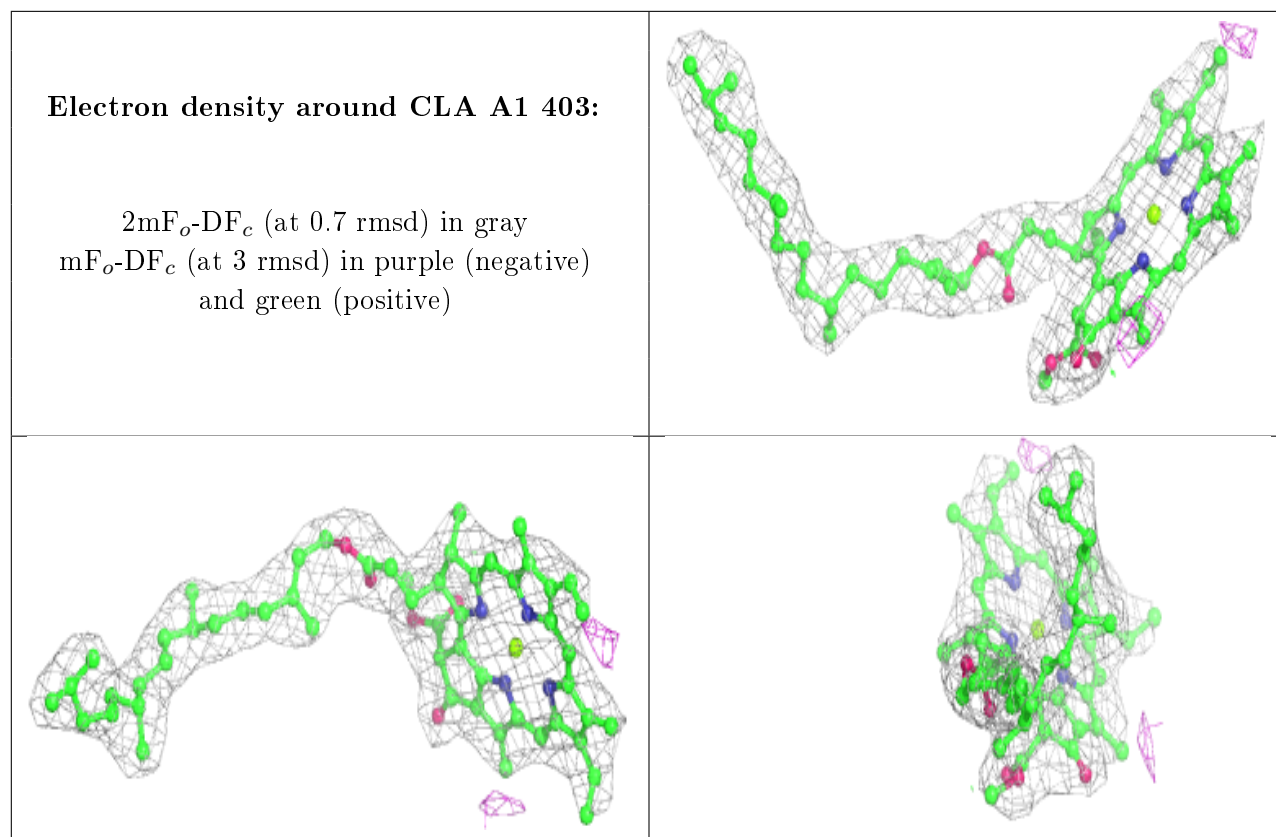
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG II 102:**

$2mF_o-DF_c$  (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.