



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2023 – 07:07 AM EDT

PDB ID : 4IXQ
Title : RT fs X-ray diffraction of Photosystem II, dark state
Authors : Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on : 2013-01-27
Resolution : 5.70 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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 : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

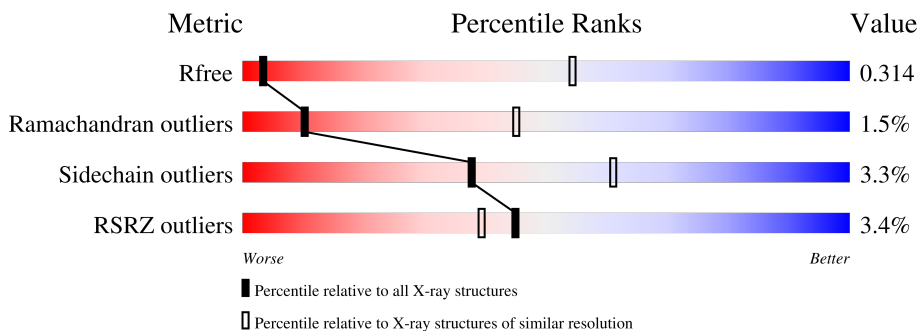
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.70 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	1003 (7.54-3.86)
Ramachandran outliers	138981	1011 (7.54-3.84)
Sidechain outliers	138945	1002 (7.58-3.82)
RSRZ outliers	127900	1002 (7.60-3.78)

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

Mol	Chain	Length	Quality of chain
1	A	360	
1	a	360	
2	B	510	

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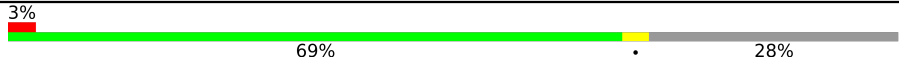
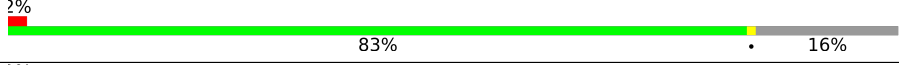



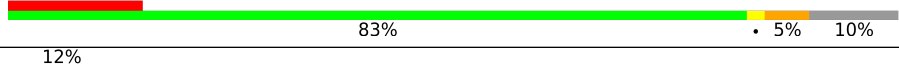

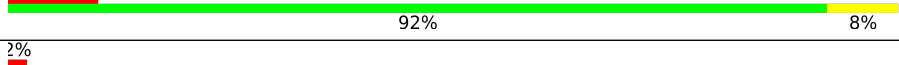
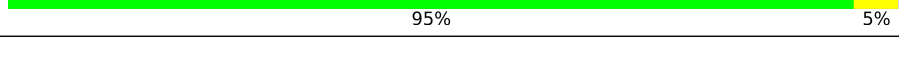
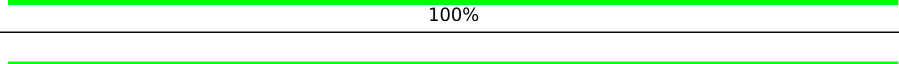
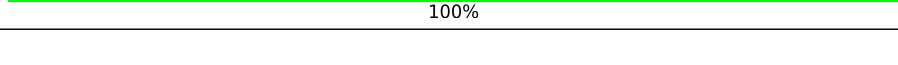
Refmac : 5.8.0158
 CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
2	b	510	3% 93% 5% . .
3	C	461	3% 92% 5% .
3	c	461	5% 92% 5% .
4	D	352	92% 5% .
4	d	352	% 92% 5% .
5	E	84	2% 93% . . .
5	e	84	% 93% . . .
6	F	45	78% 22%
6	f	45	2% 78% 22%
7	H	66	6% 88% 11% .
7	h	66	11% 88% 11% .
8	I	38	87% 5% 8%
8	i	38	87% 5% 8%
9	J	40	80% 5% 15%
9	j	40	80% 5% 15%
10	K	46	76% . 20%
10	k	46	2% 76% . 20%
11	L	37	11% 97% .
11	l	37	97% .
12	M	36	6% 94% 6%
12	m	36	8% 94% 6%
13	O	272	8% 87% . 11%
13	o	272	3% 88% . 11%
14	T	32	12% 94% 6%
14	t	32	94% 6%

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Mol	Chain	Length	Quality of chain
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	G	28	
20	Y	28	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	X
23	CLA	B	601	X	-	-	X
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	X
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	X
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	X
23	CLA	C	502	X	-	-	X
23	CLA	C	503	X	-	-	X
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	X
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	X
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	X
23	CLA	b	604	X	-	-	X
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	X
23	CLA	b	613	X	-	-	X
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	X
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	506	X	-	-	X
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	X
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	X
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	X
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	PL9	A	408	-	-	-	X
25	PL9	J	101	-	-	-	X
25	PL9	j	101	-	-	-	X
27	BCR	A	410	-	-	-	X
27	BCR	B	620	-	-	-	X
27	BCR	C	514	-	-	-	X
27	BCR	C	515	-	-	-	X
27	BCR	D	405	-	-	-	X
27	BCR	H	101	-	-	-	X
27	BCR	J	102	-	-	-	X
27	BCR	K	102	-	-	-	X
27	BCR	Z	101	-	-	-	X
27	BCR	a	412	-	-	-	X
27	BCR	b	621	-	-	-	X
27	BCR	c	514	-	-	-	X
27	BCR	c	515	-	-	-	X
27	BCR	c	516	-	-	-	X
27	BCR	f	102	-	-	-	X
27	BCR	j	102	-	-	-	X
27	BCR	k	102	-	-	-	X
27	BCR	x	101	-	-	-	X
28	DGD	B	621	-	-	-	X
28	DGD	B	626	-	-	-	X
28	DGD	D	410	-	-	-	X
28	DGD	b	602	-	-	-	X
28	DGD	d	408	-	-	-	X
29	LHG	A	415	-	-	-	X
29	LHG	a	417	-	-	-	X
30	SQD	D	409	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	d	407	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	f	103	-	-	-	X
31	LMG	A	418	-	-	-	X
31	LMG	C	520	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	M	101	-	-	-	X
31	LMG	M	102	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	c	520	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	101	-	-	-	X
31	LMG	k	103	-	-	-	X
33	LMT	B	623	-	-	-	X
33	LMT	B	624	-	-	-	X
33	LMT	B	627	-	-	-	X
33	LMT	B	628	-	-	-	X
33	LMT	D	411	-	-	-	X
33	LMT	I	102	-	-	-	X
33	LMT	T	101	-	-	-	X
33	LMT	b	603	-	-	-	X
33	LMT	b	625	-	-	-	X
33	LMT	b	626	-	-	-	X
33	LMT	i	102	-	-	-	X
33	LMT	m	101	-	-	-	X
33	LMT	x	102	-	-	-	X
35	CA	K	101	-	-	-	X
35	CA	o	301	-	-	-	X

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 50232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2627	1720	432	460	15	0	0	0
1	a	335	2627	1720	432	460	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	490	3850	2528	641	668	13	0	0	0
2	b	490	3850	2528	641	668	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	447	3444	2256	576	599	13	0	0	0
3	c	447	3444	2256	576	599	13	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

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

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

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

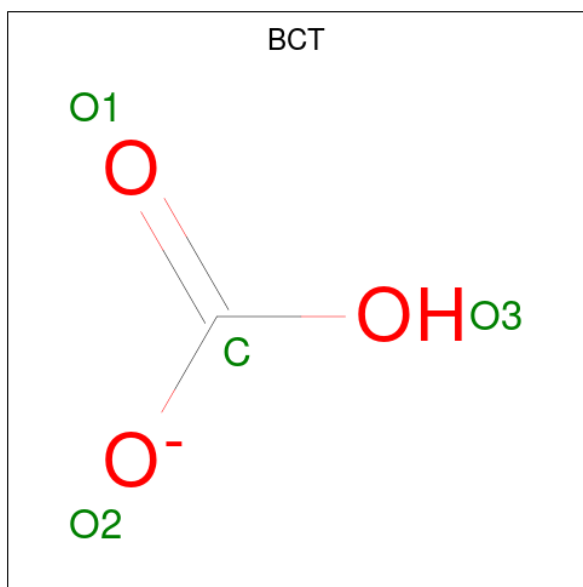
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			
20	G	28	Total	C	N	O	0	0	0
			140	84	28	28			

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

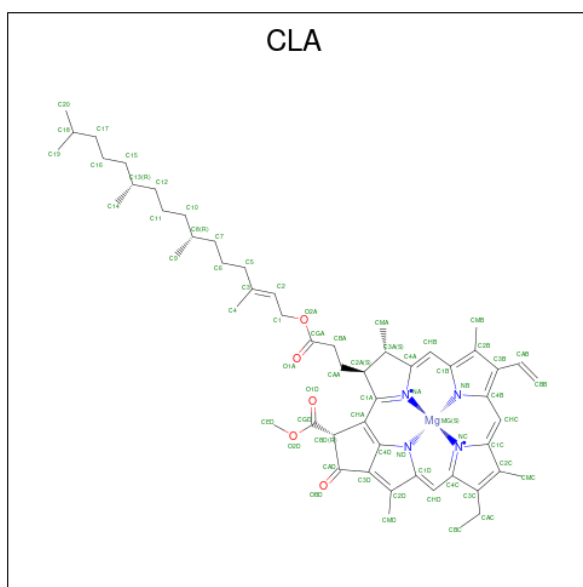
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			4	1	3		
22	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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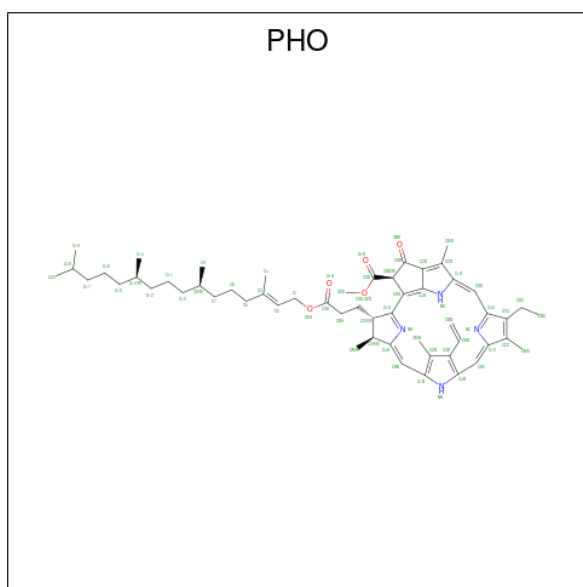
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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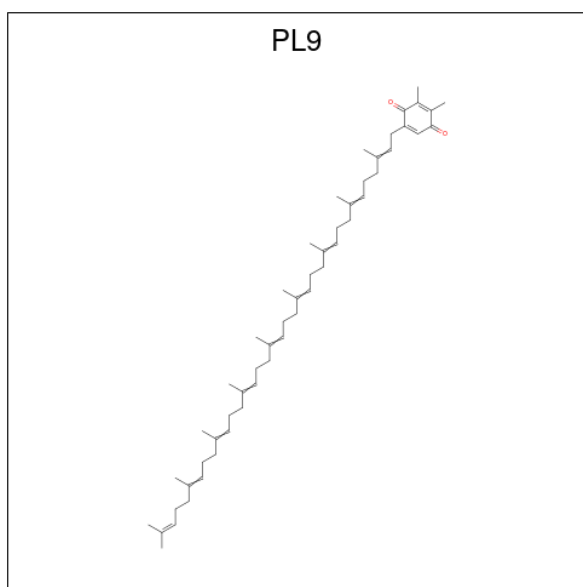
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



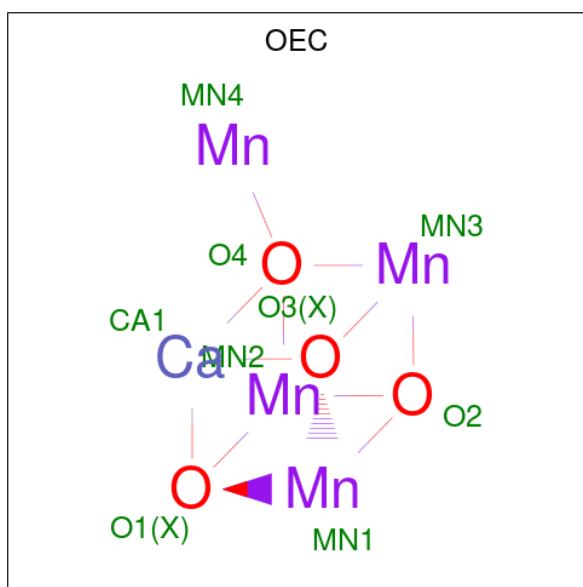
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	64	55	4	5	0	0
24	D	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0

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



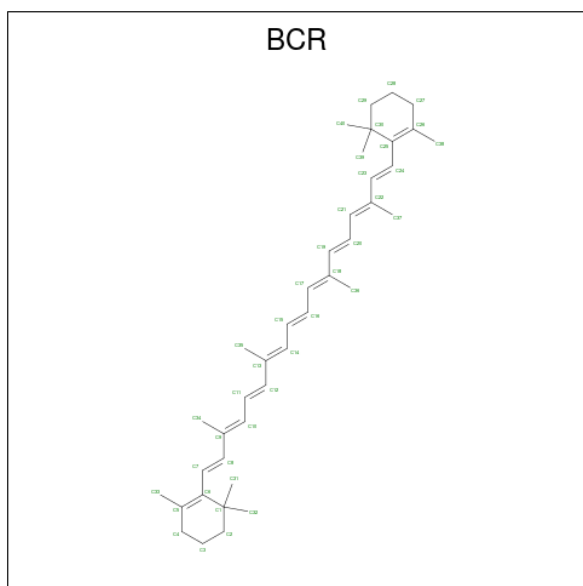
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	J	1	Total	C	O	0	0
			35	33	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			55	53	2		
25	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Ca	Mn		
26	A	1	5	1	4	0	0
26	a	1	5	1	4	0	0

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
27	A	1	40	40	0	0
27	B	1	40	40	0	0

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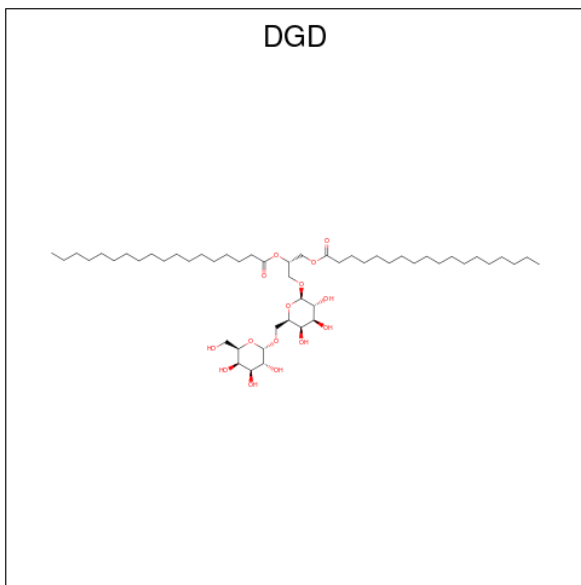
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Z	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	f	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	x	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



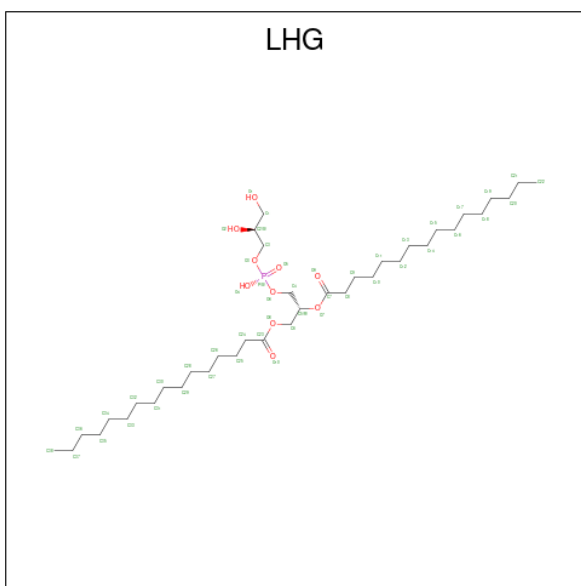
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0
28	B	1	Total C O 58 43 15	0	0
28	B	1	Total C O 52 37 15	0	0
28	C	1	Total C O 53 38 15	0	0
28	C	1	Total C O 62 47 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	D	1	Total C O 63 48 15	0	0
28	a	1	Total C O 56 41 15	0	0
28	b	1	Total C O 52 37 15	0	0
28	b	1	Total C O 58 43 15	0	0

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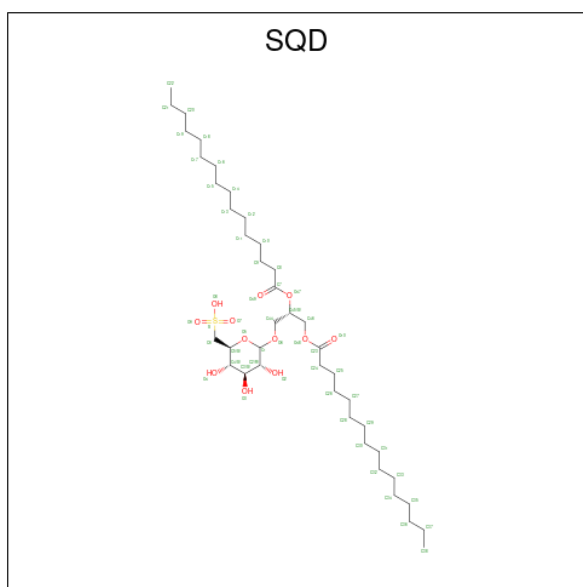
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	c	1	Total	C	O	0	0
			53	38	15		
28	c	1	Total	C	O	0	0
			62	47	15		
28	c	1	Total	C	O	0	0
			66	51	15		
28	d	1	Total	C	O	0	0
			63	48	15		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



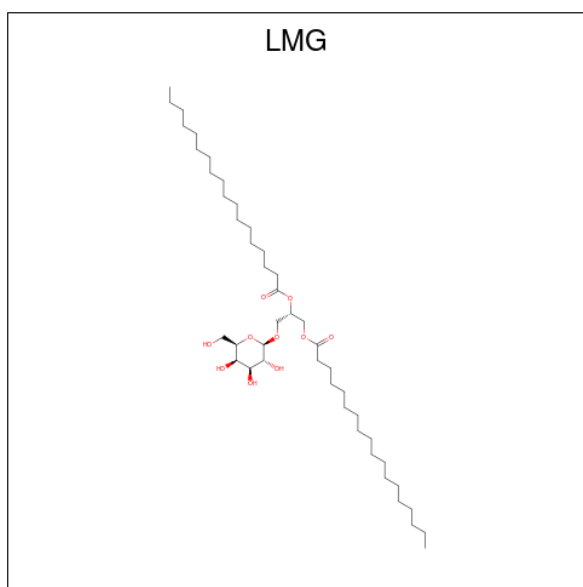
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			39	28	10	1		
29	A	1	Total	C	O	P	0	0
			37	26	10	1		
29	a	1	Total	C	O	P	0	0
			39	28	10	1		
29	a	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
30	A	1	51	38	12	1	0	0
30	A	1	54	41	12	1	0	0
30	B	1	47	34	12	1	0	0
30	D	1	43	30	12	1	0	0
30	F	1	45	32	12	1	0	0
30	a	1	54	41	12	1	0	0
30	a	1	51	38	12	1	0	0
30	b	1	47	34	12	1	0	0
30	d	1	43	30	12	1	0	0
30	f	1	45	32	12	1	0	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			51	41	10		
31	A	1	Total	C	O	0	0
			42	32	10		
31	B	1	Total	C	O	0	0
			49	39	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	C	1	Total	C	O	0	0
			45	35	10		
31	D	1	Total	C	O	0	0
			46	36	10		
31	D	1	Total	C	O	0	0
			49	39	10		
31	D	1	Total	C	O	0	0
			48	38	10		
31	E	1	Total	C	O	0	0
			44	34	10		
31	I	1	Total	C	O	0	0
			43	33	10		
31	M	1	Total	C	O	0	0
			42	32	10		
31	M	1	Total	C	O	0	0
			42	32	10		
31	a	1	Total	C	O	0	0
			42	32	10		
31	a	1	Total	C	O	0	0
			51	41	10		

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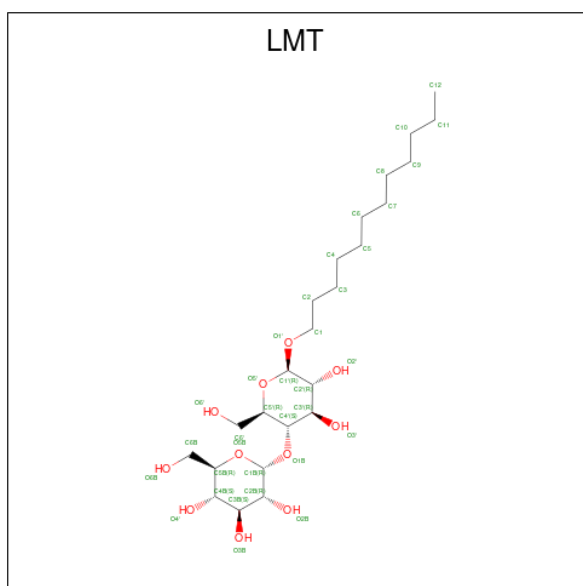
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	b	1	Total	C	O	0	0
			49	39	10		
31	b	1	Total	C	O	0	0
			49	39	10		
31	c	1	Total	C	O	0	0
			45	35	10		
31	d	1	Total	C	O	0	0
			46	36	10		
31	d	1	Total	C	O	0	0
			48	38	10		
31	e	1	Total	C	O	0	0
			44	34	10		
31	i	1	Total	C	O	0	0
			43	33	10		
31	k	1	Total	C	O	0	0
			48	38	10		

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

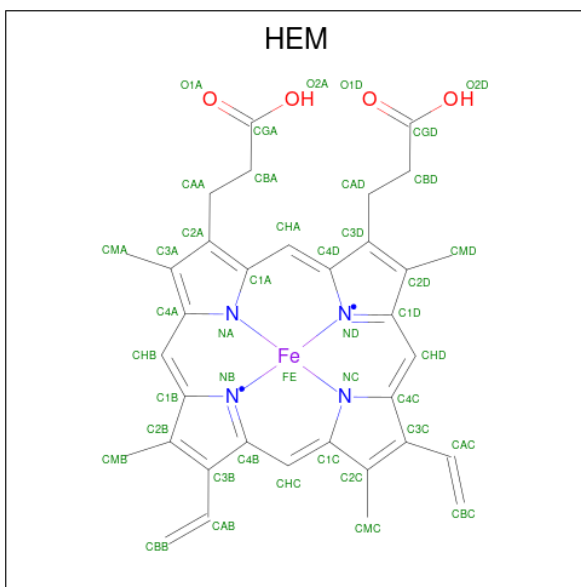
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Cl	0	0
			1	1		
32	d	1	Total	Cl	0	0
			1	1		

- Molecule 33 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	D	1	Total	C	O	0	0
			31	20	11		
33	I	1	Total	C	O	0	0
			35	24	11		
33	M	1	Total	C	O	0	0
			35	24	11		
33	T	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			35	24	11		
33	i	1	Total	C	O	0	0
			35	24	11		
33	m	1	Total	C	O	0	0
			35	24	11		
33	x	1	Total	C	O	0	0
			31	20	11		

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



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

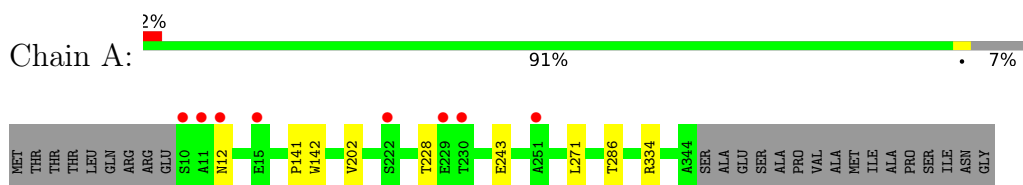
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	K	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	k	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

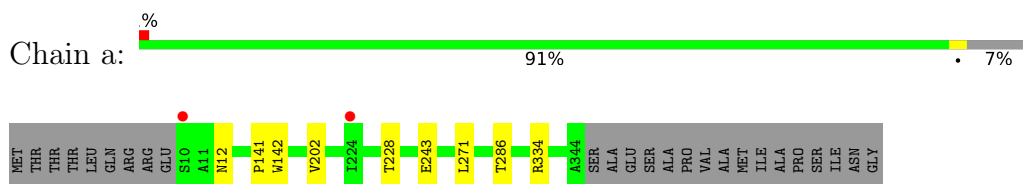
3 Residue-property plots [i](#)

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.

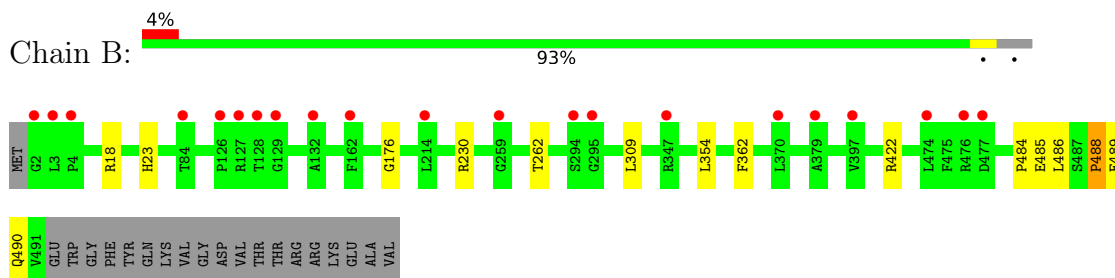
- Molecule 1: Photosystem Q(B) protein 1



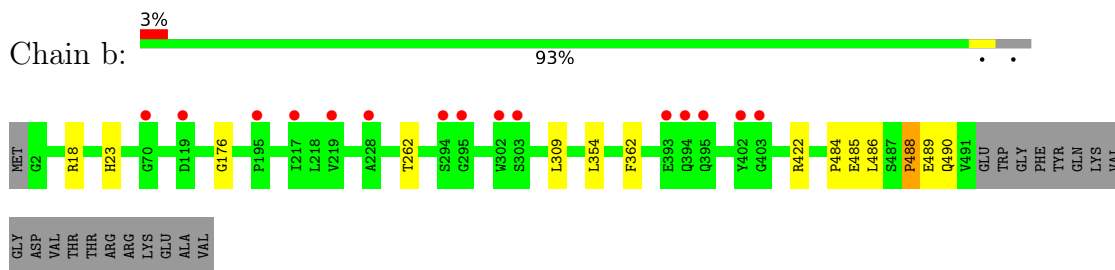
- Molecule 1: Photosystem Q(B) protein 1



- Molecule 2: Photosystem II core light harvesting protein

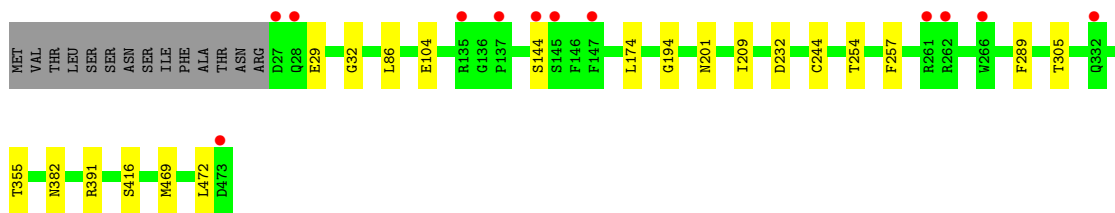


- Molecule 2: Photosystem II core light harvesting protein

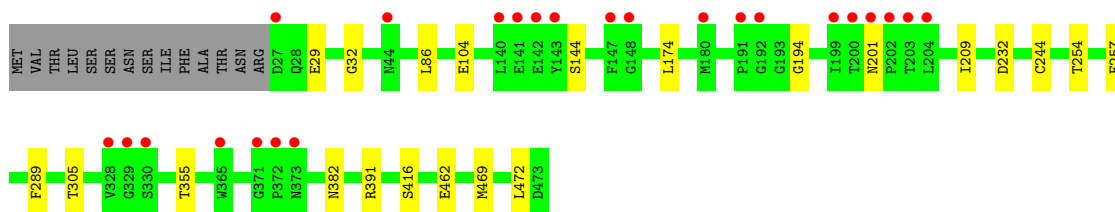
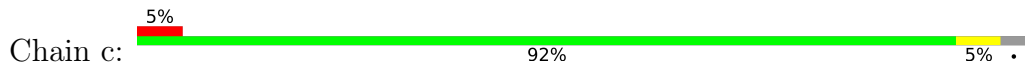


- Molecule 3: Photosystem II CP43 protein





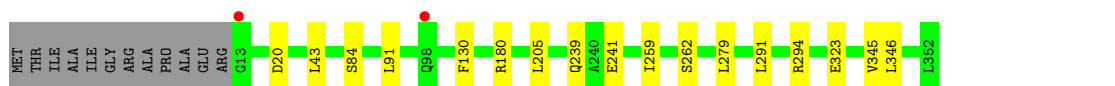
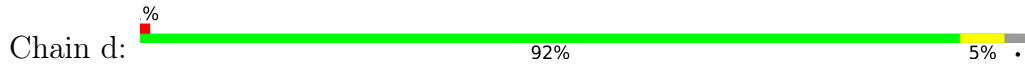
● Molecule 3: Photosystem II CP43 protein



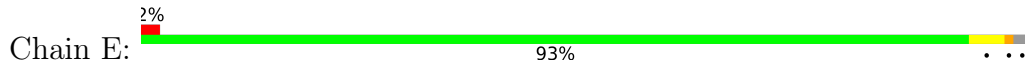
● Molecule 4: Photosystem II D2 protein



● Molecule 4: Photosystem II D2 protein




● Molecule 5: Cytochrome b559 subunit alpha

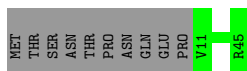


● Molecule 5: Cytochrome b559 subunit alpha




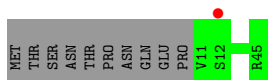
● Molecule 6: Cytochrome b559 subunit beta

Chain F:  78% 22%




- Molecule 6: Cytochrome b559 subunit beta

Chain f:  2% 78% 22%




- Molecule 7: Photosystem II reaction center protein H

Chain H:  6% 88% 11%




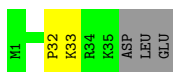
- Molecule 7: Photosystem II reaction center protein H

Chain h:  11% 88% 11%




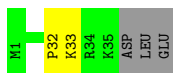
- Molecule 8: Photosystem II reaction center protein I

Chain I:  87% 5% 8%




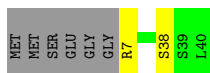
- Molecule 8: Photosystem II reaction center protein I

Chain i:  87% 5% 8%




- Molecule 9: Photosystem II reaction center protein J

Chain J:  80% 5% 15%




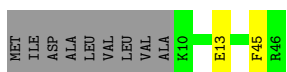
- Molecule 9: Photosystem II reaction center protein J

Chain j:  80% 5% 15%




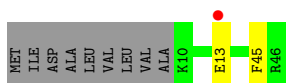
- Molecule 10: Photosystem II reaction center protein K

Chain K:  76% 0% 20%



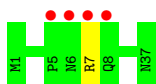
- Molecule 10: Photosystem II reaction center protein K

Chain k:  2% 76% 0% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  11% 97% 0% 0%



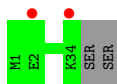
- Molecule 11: Photosystem II reaction center protein L

Chain l:  97% 0% 0%



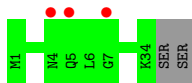
- Molecule 12: Photosystem II reaction center protein M

Chain M:  6% 94% 0% 6%

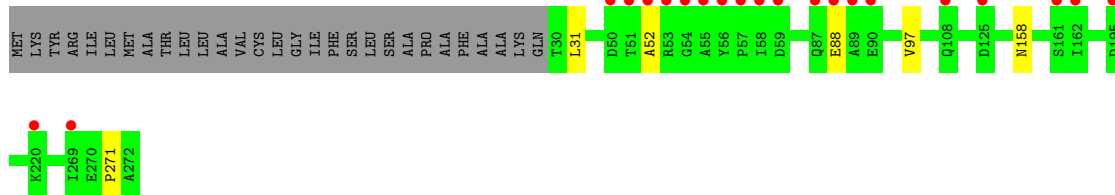
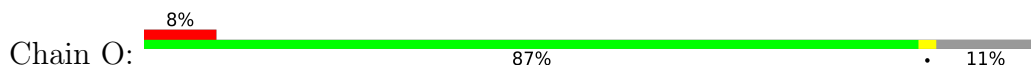


- Molecule 12: Photosystem II reaction center protein M

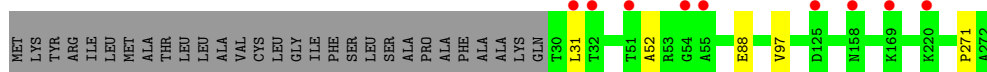
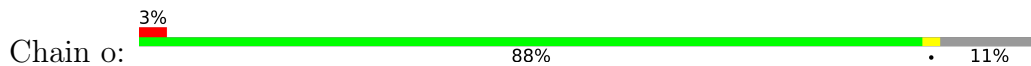
Chain m:  8% 94% 0% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



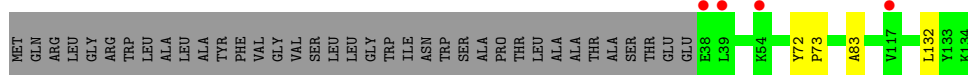
- Molecule 14: Photosystem II reaction center protein T



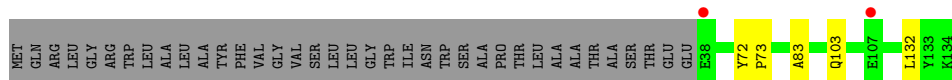
- Molecule 14: Photosystem II reaction center protein T



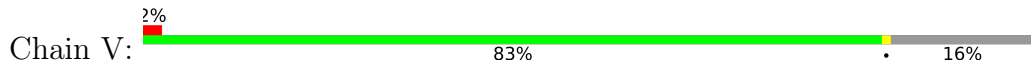
- Molecule 15: Photosystem II 12 kDa extrinsic protein

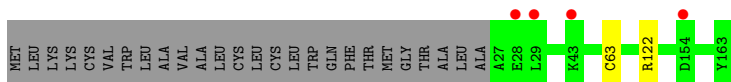


- Molecule 15: Photosystem II 12 kDa extrinsic protein

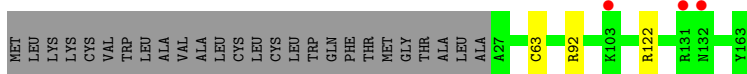
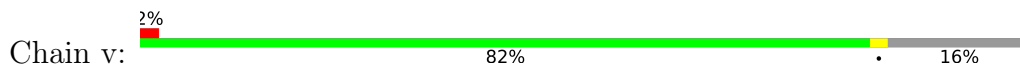


- Molecule 16: Cytochrome c-550

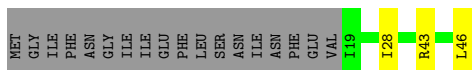




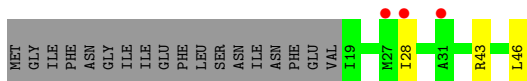
- Molecule 16: Cytochrome c-550



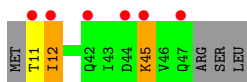
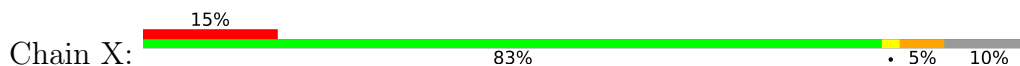
- Molecule 17: Photosystem II reaction center protein ycf12



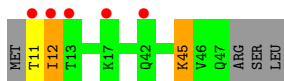
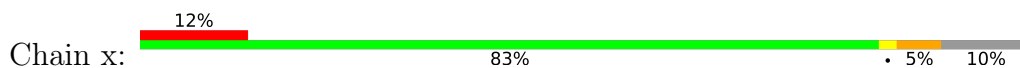
- Molecule 17: Photosystem II reaction center protein ycf12



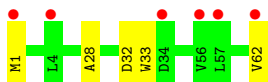
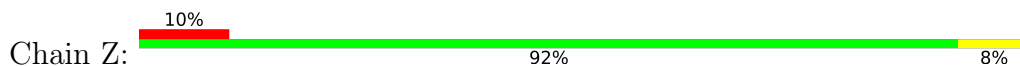
- Molecule 18: Photosystem II reaction center X protein



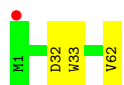
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Y



There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Y



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.86Å 227.51Å 307.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.94 – 5.70 82.94 – 5.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.94-5.70) 98.3 (82.94-5.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 5.76Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.277 , 0.314 0.277 , 0.314	Depositor DCC
R_{free} test set	1325 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtrriage
Anisotropy	3.698	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BCR, SQD, FE2, BCT, CL, HEM, OEC, DGD, CA, LMG, PHO, PL9, LMT, LHG, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/2712	0.48	0/3700
1	a	0.30	0/2712	0.48	0/3700
2	B	0.29	0/3986	0.46	0/5433
2	b	0.29	0/3986	0.46	0/5433
3	C	0.29	0/3556	0.46	0/4842
3	c	0.28	0/3556	0.46	0/4842
4	D	0.28	0/2801	0.46	0/3818
4	d	0.30	0/2801	0.46	0/3818
5	E	0.28	0/685	0.48	0/933
5	e	0.27	0/685	0.46	0/933
6	F	0.26	0/291	0.44	0/397
6	f	0.26	0/291	0.42	0/397
7	H	0.27	0/520	0.50	0/709
7	h	0.28	0/520	0.51	0/709
8	I	0.28	0/293	0.47	0/395
8	i	0.31	0/293	0.49	0/395
9	J	0.25	0/255	0.44	0/346
9	j	0.27	0/255	0.45	0/346
10	K	0.28	0/303	0.53	0/416
10	k	0.29	0/303	0.53	0/416
11	L	0.27	0/311	0.47	0/422
11	l	0.24	0/311	0.45	0/422
12	M	0.41	0/270	0.66	0/367
12	m	0.41	0/270	0.66	0/367
13	O	0.27	0/1876	0.48	0/2548
13	o	0.28	0/1876	0.49	0/2548
14	T	0.35	0/284	0.47	0/381
14	t	0.36	0/284	0.48	0/381
15	U	0.28	0/785	0.49	0/1064
15	u	0.32	0/785	0.55	0/1064
16	V	0.31	0/1081	0.51	0/1468
16	v	0.26	0/1081	0.47	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.24	0/202	0.52	0/272
17	y	0.25	0/202	0.51	0/272
18	X	0.31	0/273	0.49	0/370
18	x	0.31	0/273	0.53	0/370
19	Z	0.29	0/490	0.50	0/669
19	z	0.27	0/490	0.47	0/669
All	All	0.29	0/41948	0.48	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	311 (93%)	18 (5%)	4 (1%)	13	49
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	13	49
2	B	488/510 (96%)	448 (92%)	35 (7%)	5 (1%)	15	54
2	b	488/510 (96%)	448 (92%)	36 (7%)	4 (1%)	19	60
3	C	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	12	48
3	c	445/461 (96%)	405 (91%)	33 (7%)	7 (2%)	9	43
4	D	338/352 (96%)	315 (93%)	20 (6%)	3 (1%)	17	56
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	48
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	20
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	20
8	I	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	4	28
8	i	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	4	28
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	27
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	27
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1	18
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1	18
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	207 (86%)	30 (12%)	4 (2%)	9	42
13	o	241/272 (89%)	209 (87%)	29 (12%)	3 (1%)	13	49
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	26
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	26
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	4	26
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	4	26
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	126 (93%)	9 (7%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	24
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	24
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1	18
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1	18
19	Z	60/62 (97%)	54 (90%)	4 (7%)	2 (3%)	4	26
19	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	42
All	All	5138/5650 (91%)	4681 (91%)	382 (7%)	75 (2%)	10	45

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA

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	A	271/291 (93%)	266 (98%)	5 (2%)	59	77
1	a	271/291 (93%)	266 (98%)	5 (2%)	59	77
2	B	390/407 (96%)	379 (97%)	11 (3%)	43	64
2	b	390/407 (96%)	379 (97%)	11 (3%)	43	64
3	C	347/362 (96%)	332 (96%)	15 (4%)	29	53
3	c	347/362 (96%)	332 (96%)	15 (4%)	29	53
4	D	275/283 (97%)	262 (95%)	13 (5%)	26	51
4	d	275/283 (97%)	260 (94%)	15 (6%)	21	47
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	46
5	e	72/73 (99%)	68 (94%)	4 (6%)	21	46
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	13	38
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	38
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	62
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	62
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	54
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	54
10	K	30/37 (81%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	64
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	76	86
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	86
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	60
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	60
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	83
15	u	84/112 (75%)	82 (98%)	2 (2%)	49	69
16	V	116/138 (84%)	114 (98%)	2 (2%)	60	78
16	v	116/138 (84%)	113 (97%)	3 (3%)	46	66
17	g	20/37 (54%)	18 (90%)	2 (10%)	7	26
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	26
18	X	30/34 (88%)	27 (90%)	3 (10%)	7	26
18	x	30/34 (88%)	27 (90%)	3 (10%)	7	26
19	Z	52/52 (100%)	49 (94%)	3 (6%)	20	45
19	z	52/52 (100%)	50 (96%)	2 (4%)	33	57
All	All	4244/4616 (92%)	4103 (97%)	141 (3%)	38	61

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	18	ARG
7	h	27	THR
15	u	132	LEU
7	H	27	THR
5	E	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	201	HIS

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Mol	Chain	Res	Type
4	d	142	ASN
2	B	409	GLN
4	D	117	HIS
4	D	332	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 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	k	103	-	48,48,55	1.15	6 (12%)	56,56,63	1.28	6 (10%)
24	PHO	D	402	-	51,69,69	1.03	5 (9%)	47,99,99	1.10	4 (8%)
23	CLA	C	506	-	65,73,73	1.53	5 (7%)	76,113,113	1.48	9 (11%)
33	LMT	B	627	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
34	HEM	f	101	6,5	41,50,50	1.93	5 (12%)	45,82,82	1.78	9 (20%)
23	CLA	B	610	-	65,73,73	1.51	5 (7%)	76,113,113	1.43	8 (10%)
23	CLA	b	613	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	8 (10%)
23	CLA	c	502	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	6 (7%)
28	DGD	D	410	-	64,64,67	1.15	8 (12%)	78,78,81	1.39	8 (10%)
29	LHG	a	414	-	38,38,48	1.09	2 (5%)	41,44,54	0.96	2 (4%)
23	CLA	c	513	-	65,73,73	1.50	5 (7%)	76,113,113	1.44	9 (11%)
23	CLA	d	402	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	8 (10%)
33	LMT	I	102	-	36,36,36	0.42	0	47,47,47	0.68	1 (2%)
28	DGD	c	518	-	63,63,67	1.23	9 (14%)	77,77,81	1.25	7 (9%)
23	CLA	a	404	-	65,73,73	1.54	6 (9%)	76,113,113	1.42	9 (11%)
30	SQD	a	401	-	53,54,54	0.98	5 (9%)	62,65,65	1.59	11 (17%)
23	CLA	c	512	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
27	BCR	H	101	-	41,41,41	0.73	0	56,56,56	1.72	15 (26%)
24	PHO	a	407	-	51,69,69	1.02	4 (7%)	47,99,99	1.18	5 (10%)
27	BCR	b	621	-	41,41,41	0.75	0	56,56,56	2.18	18 (32%)
23	CLA	a	405	-	65,73,73	1.49	5 (7%)	76,113,113	1.46	9 (11%)
23	CLA	D	401	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
23	CLA	a	406	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	8 (10%)
23	CLA	B	608	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
30	SQD	D	409	-	42,43,54	1.11	4 (9%)	51,54,65	2.02	10 (19%)
23	CLA	C	513	-	65,73,73	1.51	5 (7%)	76,113,113	1.42	8 (10%)
25	PL9	D	404	-	55,55,55	1.22	8 (14%)	68,69,69	1.70	20 (29%)
27	BCR	Z	101	-	41,41,41	0.67	0	56,56,56	1.88	15 (26%)
23	CLA	A	407	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	6 (7%)
31	LMG	C	520	-	45,45,55	1.21	7 (15%)	53,53,63	1.44	8 (15%)
23	CLA	B	602	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	6 (7%)
31	LMG	d	406	-	48,48,55	1.16	8 (16%)	56,56,63	1.38	7 (12%)
27	BCR	j	102	-	41,41,41	0.73	0	56,56,56	3.35	24 (42%)
23	CLA	C	511	3	65,73,73	1.51	5 (7%)	76,113,113	1.47	8 (10%)
27	BCR	T	103	-	41,41,41	0.70	0	56,56,56	2.26	17 (30%)
33	LMT	D	411	-	32,32,36	0.48	0	43,43,47	0.71	1 (2%)
31	LMG	E	101	-	44,44,55	1.23	8 (18%)	52,52,63	1.36	8 (15%)
23	CLA	b	604	-	65,73,73	1.53	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	B	606	-	65,73,73	1.48	5 (7%)	76,113,113	1.35	6 (7%)
29	LHG	A	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.07	2 (5%)
27	BCR	K	102	-	41,41,41	0.73	0	56,56,56	1.85	12 (21%)
31	LMG	d	405	-	46,46,55	1.20	7 (15%)	54,54,63	1.38	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	615	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)
30	SQD	b	601	-	46,47,54	1.04	5 (10%)	55,58,65	1.61	9 (16%)
31	LMG	B	622	-	49,49,55	1.19	8 (16%)	57,57,63	1.38	9 (15%)
29	LHG	a	417	-	36,36,48	1.08	2 (5%)	39,42,54	1.07	2 (5%)
33	LMT	B	624	-	36,36,36	0.44	0	47,47,47	0.70	1 (2%)
33	LMT	m	101	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)
23	CLA	B	601	-	65,73,73	1.56	6 (9%)	76,113,113	1.36	8 (10%)
28	DGD	C	516	-	54,54,67	1.26	6 (11%)	68,68,81	1.29	9 (13%)
23	CLA	c	509	-	65,73,73	1.52	5 (7%)	76,113,113	1.41	8 (10%)
27	BCR	f	102	-	41,41,41	0.69	0	56,56,56	2.17	19 (33%)
23	CLA	B	604	-	65,73,73	1.49	7 (10%)	76,113,113	1.35	8 (10%)
31	LMG	b	624	-	49,49,55	1.17	7 (14%)	57,57,63	1.39	9 (15%)
23	CLA	c	511	-	65,73,73	1.55	5 (7%)	76,113,113	1.42	7 (9%)
23	CLA	A	403	-	65,73,73	1.53	6 (9%)	76,113,113	1.41	7 (9%)
27	BCR	C	514	-	41,41,41	0.75	0	56,56,56	2.40	20 (35%)
28	DGD	C	518	-	67,67,67	1.16	7 (10%)	81,81,81	1.47	9 (11%)
28	DGD	d	408	-	64,64,67	1.13	7 (10%)	78,78,81	1.41	9 (11%)
31	LMG	D	406	-	46,46,55	1.17	6 (13%)	54,54,63	1.37	6 (11%)
23	CLA	c	506	-	65,73,73	1.53	6 (9%)	76,113,113	1.45	8 (10%)
31	LMG	D	407	-	49,49,55	1.19	7 (14%)	57,57,63	1.26	8 (14%)
33	LMT	M	103	-	36,36,36	0.41	0	47,47,47	0.68	1 (2%)
27	BCR	c	516	-	41,41,41	0.70	0	56,56,56	1.94	15 (26%)
23	CLA	b	616	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
28	DGD	b	622	-	59,59,67	1.25	9 (15%)	73,73,81	1.18	7 (9%)
33	LMT	T	101	-	36,36,36	0.41	0	47,47,47	0.85	1 (2%)
28	DGD	c	519	-	67,67,67	1.16	7 (10%)	81,81,81	1.46	10 (12%)
30	SQD	F	102	-	44,45,54	1.05	5 (11%)	53,56,65	1.69	10 (18%)
23	CLA	b	607	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	9 (11%)
31	LMG	e	101	-	44,44,55	1.23	8 (18%)	52,52,63	1.30	8 (15%)
23	CLA	D	403	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	10 (13%)
28	DGD	c	517	-	54,54,67	1.27	7 (12%)	68,68,81	1.27	8 (11%)
23	CLA	b	614	-	65,73,73	1.55	6 (9%)	76,113,113	1.36	8 (10%)
33	LMT	b	603	-	36,36,36	0.40	0	47,47,47	0.61	0
23	CLA	d	403	-	65,73,73	1.52	5 (7%)	76,113,113	1.35	6 (7%)
27	BCR	B	618	-	41,41,41	0.71	0	56,56,56	2.27	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	A	410	-	41,41,41	0.76	0	56,56,56	1.98	15 (26%)
23	CLA	b	609	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	8 (10%)
23	CLA	B	605	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
23	CLA	c	508	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	7 (9%)
23	CLA	a	409	-	65,73,73	1.51	5 (7%)	76,113,113	1.40	8 (10%)
33	LMT	B	623	-	36,36,36	0.41	0	47,47,47	0.73	0
23	CLA	C	503	-	65,73,73	1.53	6 (9%)	76,113,113	1.35	8 (10%)
23	CLA	B	612	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
23	CLA	C	509	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	9 (11%)
23	CLA	B	616	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	6 (7%)
30	SQD	d	407	-	42,43,54	1.14	4 (9%)	51,54,65	2.03	10 (19%)
27	BCR	T	102	-	41,41,41	0.75	0	56,56,56	1.93	13 (23%)
31	LMG	a	402	-	42,42,55	1.24	6 (14%)	50,50,63	1.49	8 (16%)
23	CLA	b	605	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	6 (7%)
23	CLA	C	510	-	65,73,73	1.53	6 (9%)	76,113,113	1.36	7 (9%)
25	PL9	A	408	-	45,45,55	1.28	7 (15%)	56,57,69	1.58	14 (25%)
30	SQD	B	625	-	46,47,54	1.04	5 (10%)	55,58,65	1.58	10 (18%)
31	LMG	a	416	-	51,51,55	1.15	6 (11%)	59,59,63	1.43	5 (8%)
23	CLA	A	404	-	65,73,73	1.51	6 (9%)	76,113,113	1.40	9 (11%)
23	CLA	c	503	-	65,73,73	1.52	5 (7%)	76,113,113	1.35	8 (10%)
27	BCR	B	617	-	41,41,41	0.74	0	56,56,56	1.94	14 (25%)
23	CLA	B	607	-	65,73,73	1.50	6 (9%)	76,113,113	1.47	9 (11%)
27	BCR	B	619	-	41,41,41	0.67	0	56,56,56	1.89	15 (26%)
31	LMG	M	102	-	42,42,55	1.29	7 (16%)	50,50,63	1.48	7 (14%)
23	CLA	C	501	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
27	BCR	D	405	-	41,41,41	0.69	0	56,56,56	2.23	20 (35%)
31	LMG	I	101	-	43,43,55	1.28	8 (18%)	51,51,63	1.35	7 (13%)
27	BCR	c	515	-	41,41,41	0.66	0	56,56,56	1.80	15 (26%)
33	LMT	x	102	-	32,32,36	0.49	1 (3%)	43,43,47	0.66	1 (2%)
27	BCR	k	102	-	41,41,41	0.72	0	56,56,56	1.90	16 (28%)
23	CLA	b	608	-	65,73,73	1.52	7 (10%)	76,113,113	1.39	6 (7%)
23	CLA	C	505	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
34	HEM	F	101	6,5	41,50,50	1.94	5 (12%)	45,82,82	1.76	9 (20%)
23	CLA	b	617	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	6 (7%)
31	LMG	M	101	-	42,42,55	1.32	7 (16%)	50,50,63	1.51	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	508	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
23	CLA	b	619	-	65,73,73	1.50	5 (7%)	76,113,113	1.31	6 (7%)
25	PL9	d	404	-	55,55,55	1.25	9 (16%)	68,69,69	1.68	16 (23%)
27	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.98	16 (28%)
33	LMT	i	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.64	0
28	DGD	C	517	-	63,63,67	1.22	10 (15%)	77,77,81	1.23	7 (9%)
23	CLA	c	505	-	65,73,73	1.54	6 (9%)	76,113,113	1.50	9 (11%)
23	CLA	B	609	-	65,73,73	1.51	5 (7%)	76,113,113	1.41	8 (10%)
23	CLA	b	618	-	65,73,73	1.48	5 (7%)	76,113,113	1.44	9 (11%)
27	BCR	J	102	-	41,41,41	0.71	0	56,56,56	3.35	25 (44%)
30	SQD	A	417	-	53,54,54	1.02	5 (9%)	62,65,65	1.58	11 (17%)
23	CLA	C	512	-	65,73,73	1.51	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	c	504	-	65,73,73	1.54	6 (9%)	76,113,113	1.50	9 (11%)
23	CLA	c	507	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
28	DGD	B	621	-	59,59,67	1.28	9 (15%)	73,73,81	1.15	6 (8%)
34	HEM	v	201	16	41,50,50	2.06	8 (19%)	45,82,82	1.73	5 (11%)
27	BCR	c	514	-	41,41,41	0.72	0	56,56,56	2.44	18 (32%)
33	LMT	b	625	-	36,36,36	0.40	0	47,47,47	0.75	1 (2%)
23	CLA	B	613	-	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
25	PL9	a	410	-	45,45,55	1.23	7 (15%)	56,57,69	1.66	12 (21%)
30	SQD	f	103	-	44,45,54	1.04	5 (11%)	53,56,65	1.66	11 (20%)
24	PHO	A	406	-	51,69,69	1.02	4 (7%)	47,99,99	1.19	4 (8%)
33	LMT	B	628	-	36,36,36	0.46	0	47,47,47	0.63	0
28	DGD	b	602	-	53,53,67	1.26	7 (13%)	67,67,81	1.39	9 (13%)
31	LMG	D	408	-	48,48,55	1.21	8 (16%)	56,56,63	1.38	7 (12%)
23	CLA	B	611	-	65,73,73	1.49	6 (9%)	76,113,113	1.46	7 (9%)
30	SQD	a	415	-	50,51,54	1.01	5 (10%)	59,62,65	1.56	10 (16%)
31	LMG	A	414	-	51,51,55	1.17	6 (11%)	59,59,63	1.36	5 (8%)
34	HEM	V	201	16	41,50,50	2.00	7 (17%)	45,82,82	1.42	4 (8%)
23	CLA	b	610	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	9 (11%)
31	LMG	i	101	-	43,43,55	1.28	7 (16%)	51,51,63	1.32	8 (15%)
23	CLA	B	603	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	9 (11%)
25	PL9	J	101	-	35,35,55	1.19	5 (14%)	44,45,69	1.59	8 (18%)
23	CLA	b	611	-	65,73,73	1.52	6 (9%)	76,113,113	1.48	9 (11%)
27	BCR	B	620	-	41,41,41	0.73	0	56,56,56	2.13	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCT	d	401	21	2,3,3	0.45	0	2,3,3	0.15	0
23	CLA	C	507	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
30	SQD	A	413	-	50,51,54	0.98	6 (12%)	59,62,65	1.55	9 (15%)
25	PL9	j	101	-	35,35,55	1.18	5 (14%)	44,45,69	1.60	9 (20%)
29	LHG	A	412	-	38,38,48	1.06	2 (5%)	41,44,54	0.98	2 (4%)
23	CLA	A	405	-	65,73,73	1.49	5 (7%)	76,113,113	1.29	8 (10%)
22	BCT	A	402	21	2,3,3	0.45	0	2,3,3	0.09	0
28	DGD	a	413	-	57,57,67	1.23	8 (14%)	71,71,81	1.60	13 (18%)
23	CLA	b	615	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
27	BCR	x	101	-	41,41,41	0.71	0	56,56,56	1.72	16 (28%)
27	BCR	b	620	-	41,41,41	0.67	0	56,56,56	1.94	15 (26%)
31	LMG	C	519	-	48,48,55	1.15	6 (12%)	56,56,63	1.36	7 (12%)
23	CLA	B	614	-	65,73,73	1.51	5 (7%)	76,113,113	1.31	6 (7%)
23	CLA	b	612	-	65,73,73	1.53	5 (7%)	76,113,113	1.31	7 (9%)
24	PHO	a	408	-	51,69,69	0.98	3 (5%)	47,99,99	1.11	3 (6%)
23	CLA	C	504	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
28	DGD	A	411	-	57,57,67	1.24	8 (14%)	71,71,81	1.64	13 (18%)
31	LMG	A	418	-	42,42,55	1.24	6 (14%)	50,50,63	1.54	11 (22%)
33	LMT	b	626	-	36,36,36	0.44	0	47,47,47	0.67	1 (2%)
23	CLA	b	606	-	65,73,73	1.47	5 (7%)	76,113,113	1.35	8 (10%)
27	BCR	a	412	-	41,41,41	0.72	0	56,56,56	1.90	15 (26%)
31	LMG	b	623	-	49,49,55	1.22	7 (14%)	57,57,63	1.35	7 (12%)
31	LMG	c	520	-	45,45,55	1.22	7 (15%)	53,53,63	1.41	8 (15%)
23	CLA	C	502	-	65,73,73	1.50	7 (10%)	76,113,113	1.42	7 (9%)
28	DGD	B	626	-	53,53,67	1.25	8 (15%)	67,67,81	1.40	9 (13%)
23	CLA	c	501	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	9 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	k	103	-	-	17/43/63/70	0/1/1/1
24	PHO	D	402	-	-	10/37/103/103	0/5/6/6
23	CLA	C	506	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	B	627	-	-	3/21/61/61	0/2/2/2
34	HEM	f	101	6,5	-	2/12/54/54	-
23	CLA	B	610	-	1/1/15/20	18/37/115/115	-
23	CLA	b	613	-	1/1/15/20	17/37/115/115	-
23	CLA	c	502	-	1/1/15/20	12/37/115/115	-
23	CLA	c	510	-	1/1/15/20	16/37/115/115	-
28	DGD	D	410	-	-	31/52/92/95	0/2/2/2
29	LHG	a	414	-	-	18/43/43/53	-
23	CLA	c	513	-	1/1/15/20	21/37/115/115	-
23	CLA	d	402	-	1/1/15/20	11/37/115/115	-
33	LMT	I	102	-	-	3/21/61/61	0/2/2/2
28	DGD	c	518	-	-	22/51/91/95	0/2/2/2
23	CLA	a	404	-	1/1/15/20	8/37/115/115	-
30	SQD	a	401	-	-	17/49/69/69	0/1/1/1
23	CLA	c	512	-	1/1/15/20	18/37/115/115	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
24	PHO	a	407	-	-	12/37/103/103	0/5/6/6
27	BCR	b	621	-	-	3/29/63/63	0/2/2/2
23	CLA	a	405	-	1/1/15/20	16/37/115/115	-
23	CLA	D	401	-	1/1/15/20	13/37/115/115	-
23	CLA	a	406	-	1/1/15/20	10/37/115/115	-
23	CLA	B	608	-	1/1/15/20	13/37/115/115	-
30	SQD	D	409	-	-	11/38/58/69	0/1/1/1
23	CLA	C	513	-	1/1/15/20	17/37/115/115	-
25	PL9	D	404	-	-	13/53/73/73	0/1/1/1
27	BCR	Z	101	-	-	2/29/63/63	0/2/2/2
23	CLA	A	407	-	1/1/15/20	8/37/115/115	-
31	LMG	C	520	-	-	19/40/60/70	0/1/1/1
23	CLA	B	602	-	1/1/15/20	17/37/115/115	-
31	LMG	d	406	-	-	20/43/63/70	0/1/1/1
27	BCR	j	102	-	-	6/29/63/63	0/2/2/2
23	CLA	C	511	3	1/1/15/20	15/37/115/115	-
27	BCR	T	103	-	-	9/29/63/63	0/2/2/2
33	LMT	D	411	-	-	0/17/57/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	E	101	-	-	18/39/59/70	0/1/1/1
23	CLA	b	604	-	1/1/15/20	15/37/115/115	-
23	CLA	B	606	-	1/1/15/20	11/37/115/115	-
29	LHG	A	415	-	-	12/41/41/53	-
27	BCR	K	102	-	-	8/29/63/63	0/2/2/2
31	LMG	d	405	-	-	10/41/61/70	0/1/1/1
23	CLA	B	615	-	1/1/15/20	10/37/115/115	-
30	SQD	b	601	-	-	13/42/62/69	0/1/1/1
31	LMG	B	622	-	-	15/44/64/70	0/1/1/1
29	LHG	a	417	-	-	13/41/41/53	-
33	LMT	B	624	-	-	2/21/61/61	0/2/2/2
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
23	CLA	B	601	-	1/1/15/20	16/37/115/115	-
28	DGD	C	516	-	-	19/42/82/95	0/2/2/2
23	CLA	c	509	-	1/1/15/20	16/37/115/115	-
27	BCR	f	102	-	-	6/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/15/20	8/37/115/115	-
31	LMG	b	624	-	-	15/44/64/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	15/37/115/115	-
23	CLA	A	403	-	1/1/15/20	8/37/115/115	-
27	BCR	C	514	-	-	7/29/63/63	0/2/2/2
28	DGD	C	518	-	-	23/55/95/95	0/2/2/2
28	DGD	d	408	-	-	29/52/92/95	0/2/2/2
31	LMG	D	406	-	-	11/41/61/70	0/1/1/1
23	CLA	c	506	-	1/1/15/20	16/37/115/115	-
31	LMG	D	407	-	-	23/44/64/70	0/1/1/1
33	LMT	M	103	-	-	0/21/61/61	0/2/2/2
27	BCR	c	516	-	-	8/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/15/20	16/37/115/115	-
28	DGD	b	622	-	-	19/47/87/95	0/2/2/2
33	LMT	T	101	-	-	3/21/61/61	0/2/2/2
28	DGD	c	519	-	-	21/55/95/95	0/2/2/2
30	SQD	F	102	-	-	16/40/60/69	0/1/1/1
23	CLA	b	607	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	e	101	-	-	18/39/59/70	0/1/1/1
23	CLA	D	403	-	1/1/15/20	7/37/115/115	-
28	DGD	c	517	-	-	20/42/82/95	0/2/2/2
23	CLA	b	614	-	1/1/15/20	9/37/115/115	-
33	LMT	b	603	-	-	3/21/61/61	0/2/2/2
23	CLA	d	403	-	1/1/15/20	8/37/115/115	-
27	BCR	B	618	-	-	9/29/63/63	0/2/2/2
27	BCR	A	410	-	-	0/29/63/63	0/2/2/2
23	CLA	b	609	-	1/1/15/20	12/37/115/115	-
23	CLA	B	605	-	1/1/15/20	15/37/115/115	-
23	CLA	c	508	-	1/1/15/20	14/37/115/115	-
23	CLA	a	409	-	1/1/15/20	7/37/115/115	-
33	LMT	B	623	-	-	2/21/61/61	0/2/2/2
23	CLA	C	503	-	1/1/15/20	15/37/115/115	-
23	CLA	B	612	-	1/1/15/20	11/37/115/115	-
23	CLA	C	509	-	1/1/15/20	16/37/115/115	-
23	CLA	B	616	-	1/1/15/20	19/37/115/115	-
30	SQD	d	407	-	-	12/38/58/69	0/1/1/1
27	BCR	T	102	-	-	2/29/63/63	0/2/2/2
31	LMG	a	402	-	-	16/37/57/70	0/1/1/1
23	CLA	b	605	-	1/1/15/20	20/37/115/115	-
23	CLA	C	510	-	1/1/15/20	16/37/115/115	-
25	PL9	A	408	-	-	22/41/61/73	0/1/1/1
30	SQD	B	625	-	-	14/42/62/69	0/1/1/1
31	LMG	a	416	-	-	21/46/66/70	0/1/1/1
23	CLA	A	404	-	1/1/15/20	15/37/115/115	-
23	CLA	c	503	-	1/1/15/20	14/37/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	607	-	1/1/15/20	9/37/115/115	-
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	LMG	M	102	-	-	17/37/57/70	0/1/1/1
23	CLA	C	501	-	1/1/15/20	13/37/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
31	LMG	I	101	-	-	20/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
33	LMT	x	102	-	-	0/17/57/61	0/2/2/2
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
23	CLA	b	608	-	1/1/15/20	15/37/115/115	-
23	CLA	C	505	-	1/1/15/20	18/37/115/115	-
34	HEM	F	101	6,5	-	2/12/54/54	-
23	CLA	b	617	-	1/1/15/20	17/37/115/115	-
31	LMG	M	101	-	-	15/37/57/70	0/1/1/1
23	CLA	C	508	-	1/1/15/20	14/37/115/115	-
23	CLA	b	619	-	1/1/15/20	19/37/115/115	-
25	PL9	d	404	-	-	13/53/73/73	0/1/1/1
27	BCR	C	515	-	-	7/29/63/63	0/2/2/2
33	LMT	i	102	-	-	3/21/61/61	0/2/2/2
28	DGD	C	517	-	-	21/51/91/95	0/2/2/2
23	CLA	c	505	-	1/1/15/20	18/37/115/115	-
23	CLA	B	609	-	1/1/15/20	11/37/115/115	-
23	CLA	b	618	-	1/1/15/20	8/37/115/115	-
27	BCR	J	102	-	-	3/29/63/63	0/2/2/2
30	SQD	A	417	-	-	17/49/69/69	0/1/1/1
23	CLA	C	512	-	1/1/15/20	18/37/115/115	-
23	CLA	c	504	-	1/1/15/20	12/37/115/115	-
23	CLA	c	507	-	1/1/15/20	14/37/115/115	-
28	DGD	B	621	-	-	19/47/87/95	0/2/2/2
34	HEM	v	201	16	-	3/12/54/54	-
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
33	LMT	b	625	-	-	2/21/61/61	0/2/2/2
23	CLA	B	613	-	1/1/15/20	15/37/115/115	-
25	PL9	a	410	-	-	22/41/61/73	0/1/1/1
30	SQD	f	103	-	-	15/40/60/69	0/1/1/1
24	PHO	A	406	-	-	12/37/103/103	0/5/6/6
33	LMT	B	628	-	-	3/21/61/61	0/2/2/2
28	DGD	b	602	-	-	18/41/81/95	0/2/2/2
31	LMG	D	408	-	-	21/43/63/70	0/1/1/1
23	CLA	B	611	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	a	415	-	-	19/46/66/69	0/1/1/1
31	LMG	A	414	-	-	21/46/66/70	0/1/1/1
34	HEM	V	201	16	-	3/12/54/54	-
23	CLA	b	610	-	1/1/15/20	9/37/115/115	-
31	LMG	i	101	-	-	18/38/58/70	0/1/1/1
23	CLA	B	603	-	1/1/15/20	15/37/115/115	-
25	PL9	J	101	-	-	12/29/49/73	0/1/1/1
23	CLA	b	611	-	1/1/15/20	16/37/115/115	-
27	BCR	B	620	-	-	2/29/63/63	0/2/2/2
23	CLA	C	507	-	1/1/15/20	12/37/115/115	-
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
25	PL9	j	101	-	-	13/29/49/73	0/1/1/1
29	LHG	A	412	-	-	18/43/43/53	-
23	CLA	A	405	-	1/1/15/20	11/37/115/115	-
28	DGD	a	413	-	-	11/45/85/95	0/2/2/2
23	CLA	b	615	-	1/1/15/20	12/37/115/115	-
27	BCR	x	101	-	-	3/29/63/63	0/2/2/2
27	BCR	b	620	-	-	0/29/63/63	0/2/2/2
31	LMG	C	519	-	-	16/43/63/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	17/37/115/115	-
23	CLA	b	612	-	-	11/37/115/115	-
24	PHO	a	408	-	-	12/37/103/103	0/5/6/6
23	CLA	C	504	-	1/1/15/20	10/37/115/115	-
28	DGD	A	411	-	-	11/45/85/95	0/2/2/2
31	LMG	A	418	-	-	15/37/57/70	0/1/1/1
33	LMT	b	626	-	-	2/21/61/61	0/2/2/2
23	CLA	b	606	-	1/1/15/20	15/37/115/115	-
27	BCR	a	412	-	-	3/29/63/63	0/2/2/2
31	LMG	b	623	-	-	23/44/64/70	0/1/1/1
31	LMG	c	520	-	-	21/40/60/70	0/1/1/1
23	CLA	C	502	-	1/1/15/20	9/37/115/115	-
28	DGD	B	626	-	-	17/41/81/95	0/2/2/2
23	CLA	c	501	-	1/1/15/20	13/37/115/115	-

The worst 5 of 792 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3D-C2D	8.45	1.54	1.36
23	c	504	CLA	C4B-NB	8.24	1.42	1.35
34	F	101	HEM	C3D-C2D	8.14	1.54	1.36
34	V	201	HEM	C3D-C2D	8.06	1.53	1.36
23	a	404	CLA	C4B-NB	7.99	1.42	1.35

The worst 5 of 1465 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	102	BCR	C32-C1-C6	-13.60	88.24	110.30
27	j	102	BCR	C32-C1-C6	-13.52	88.37	110.30
27	j	102	BCR	C32-C1-C31	-8.60	82.13	108.53
27	B	618	BCR	C7-C8-C9	-8.58	113.28	126.23
27	J	102	BCR	C32-C1-C31	-8.52	82.39	108.53

5 of 69 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND

5 of 2114 torsion outliers are listed below:

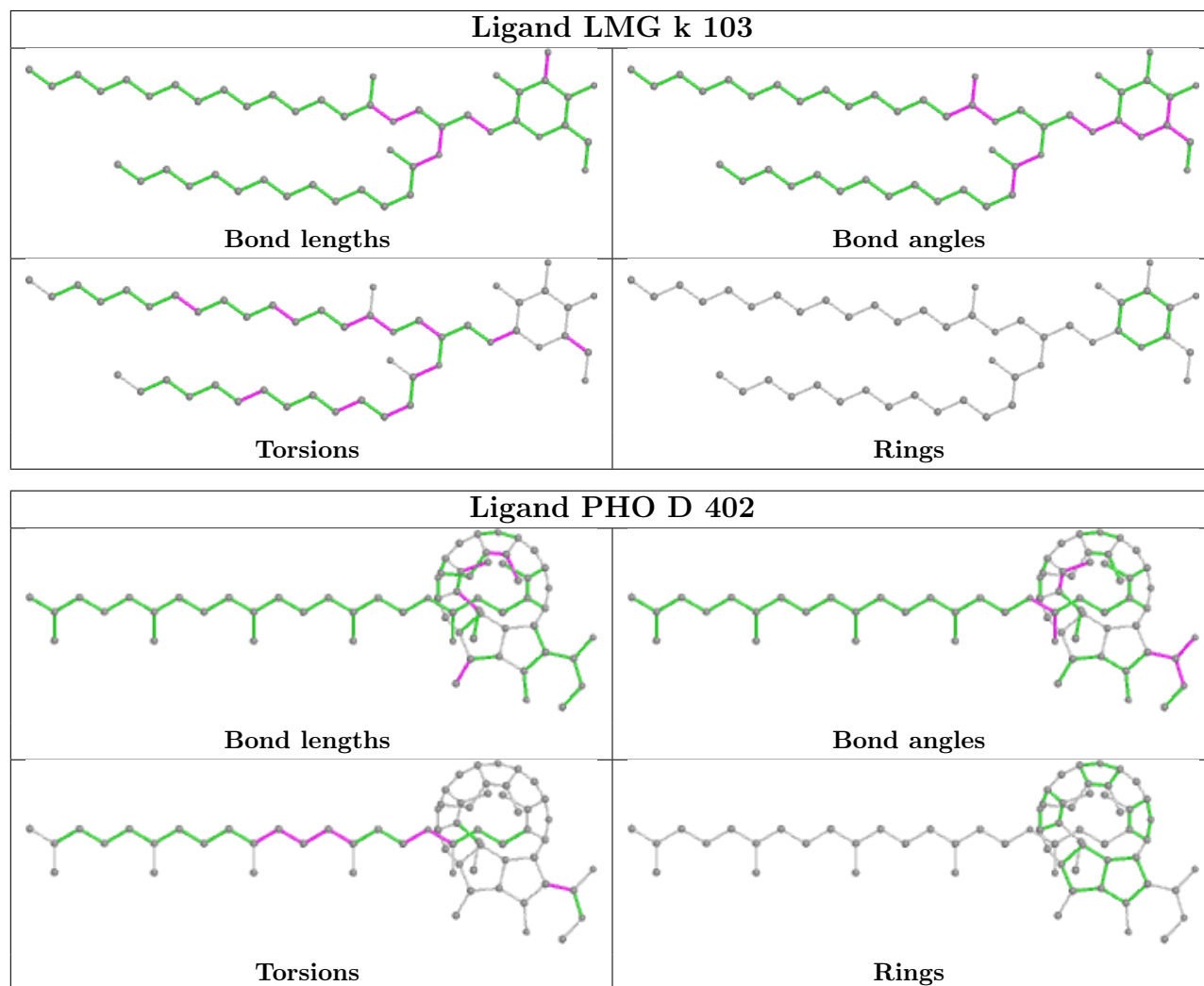
Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-C2A-CAA-CBA
23	A	404	CLA	C3A-C2A-CAA-CBA
23	A	404	CLA	CHA-CBD-CGD-O1D
23	A	404	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CBD-CGD-O2D-CED

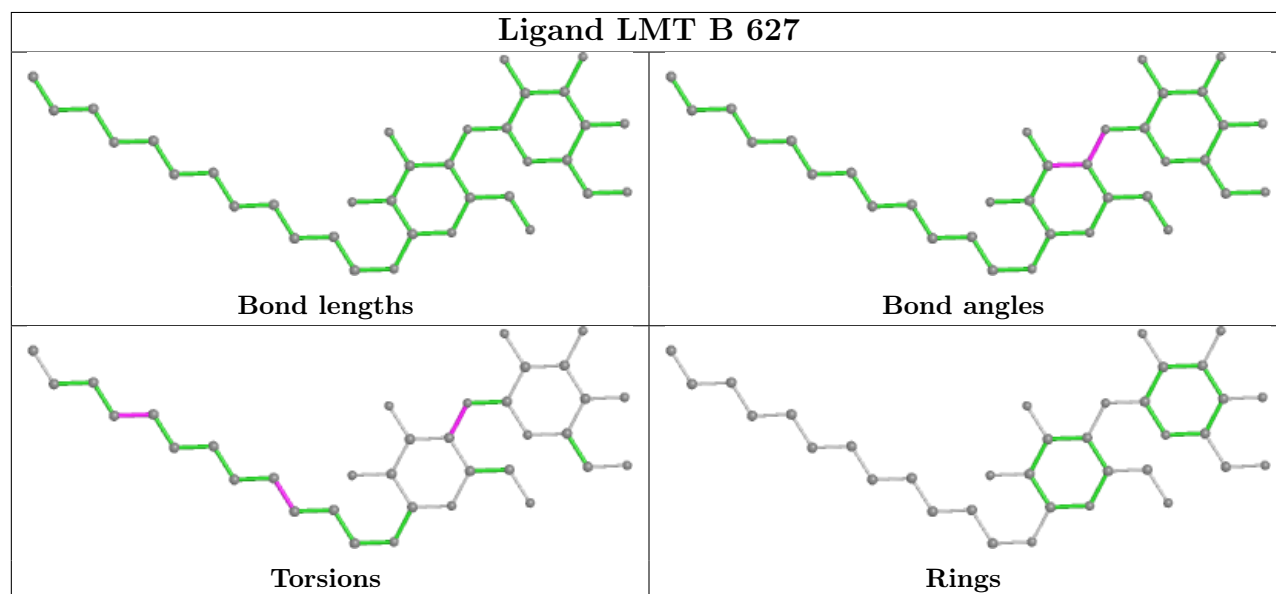
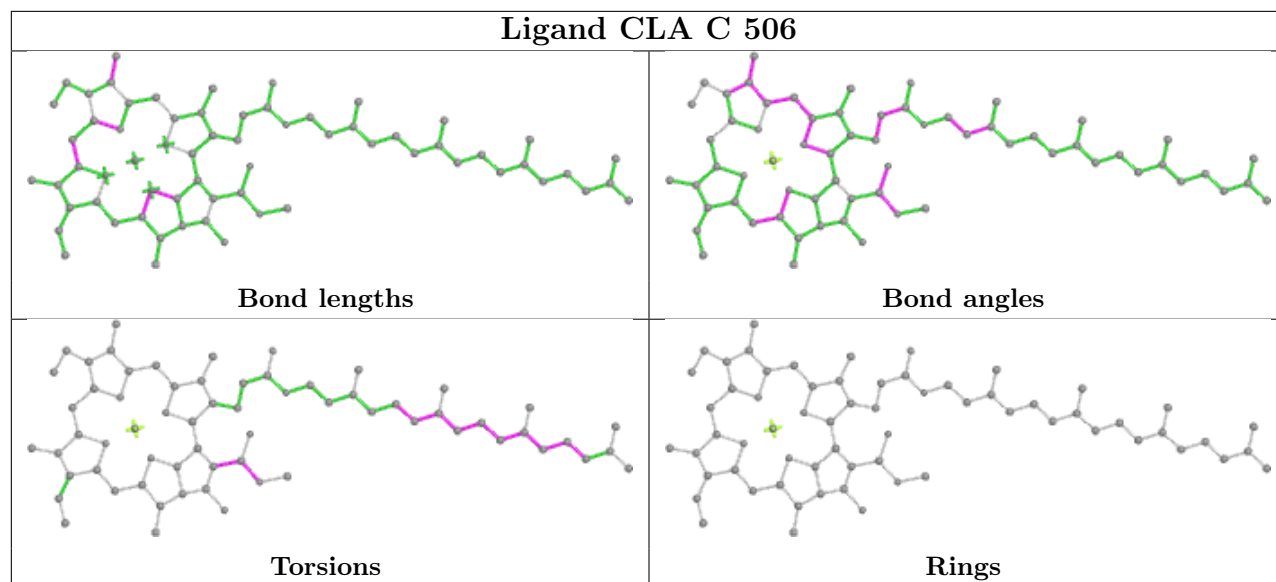
There are no ring outliers.

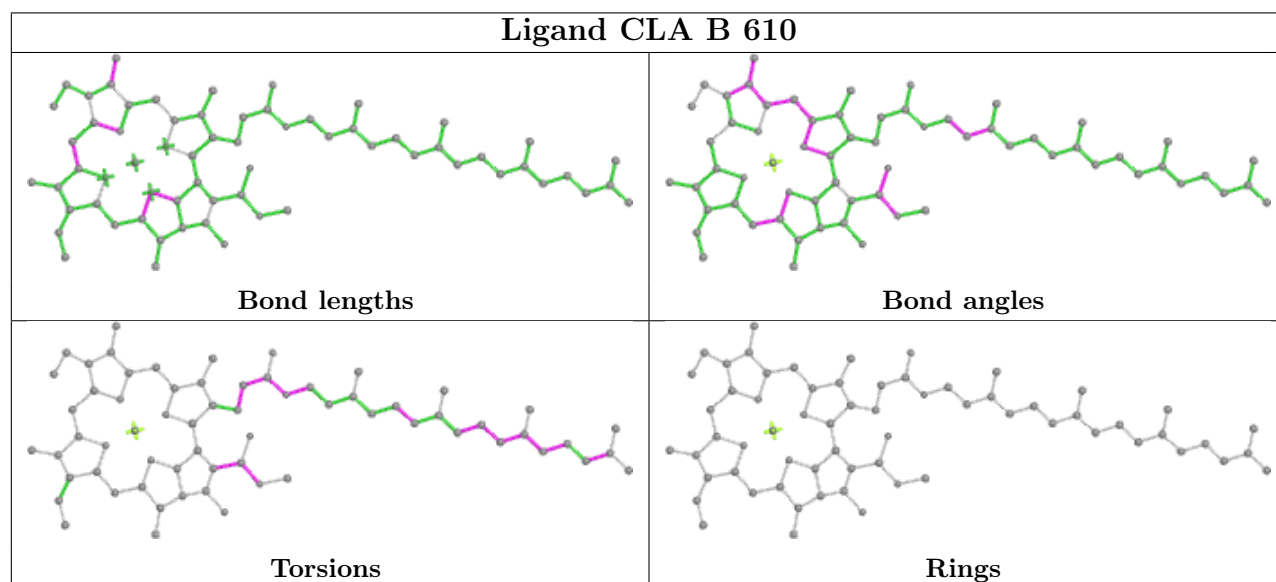
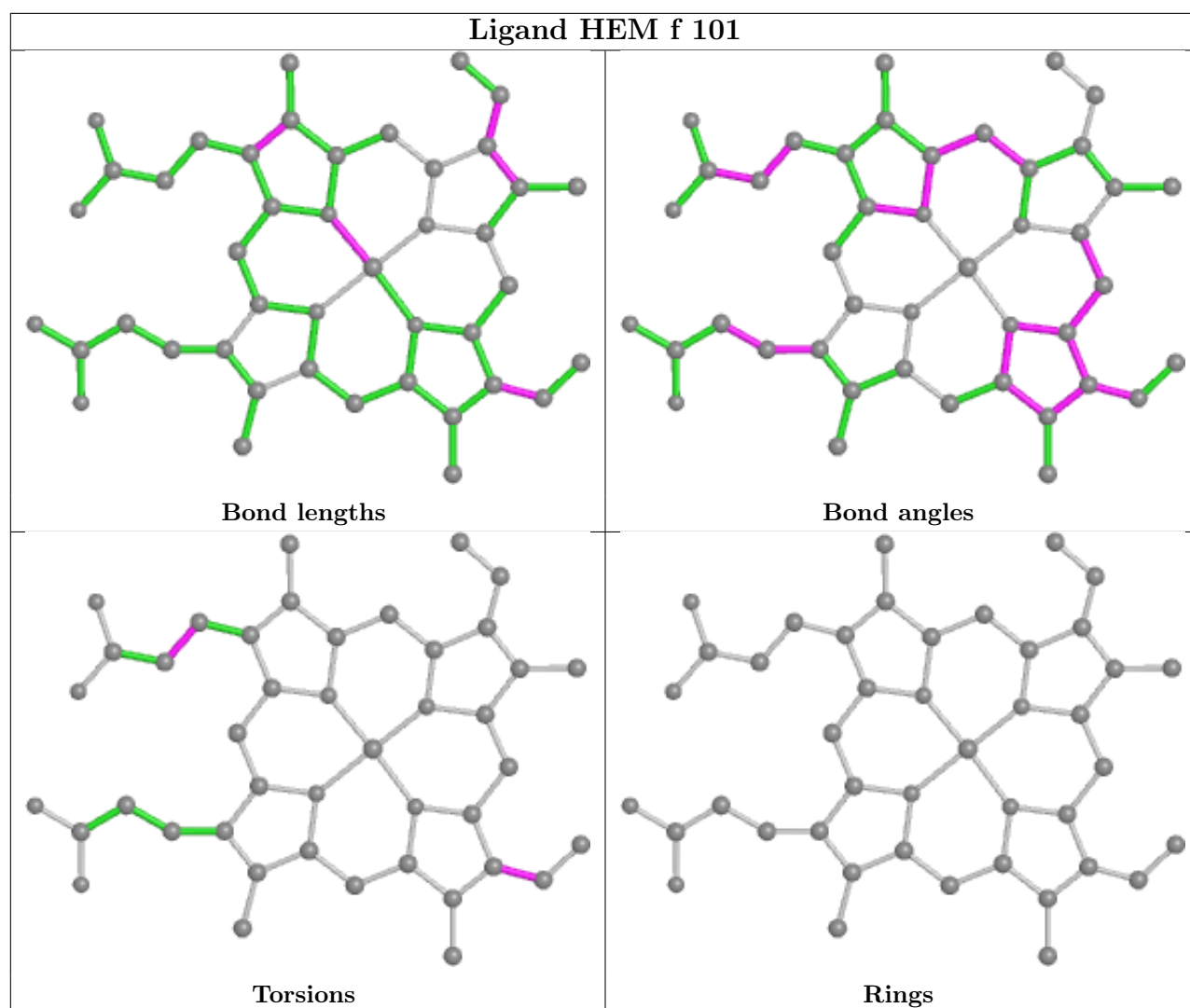
No monomer is involved in short contacts.

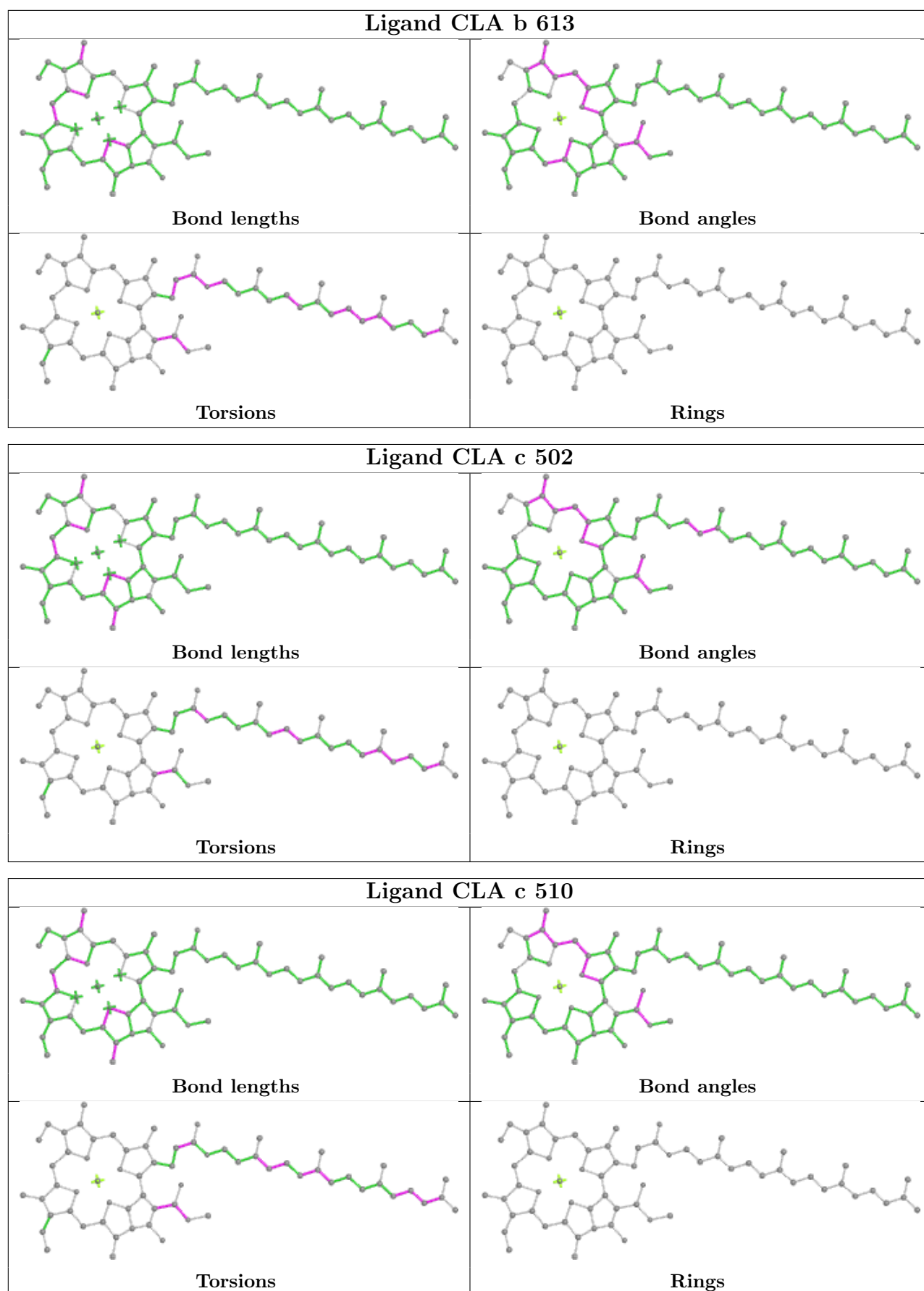
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

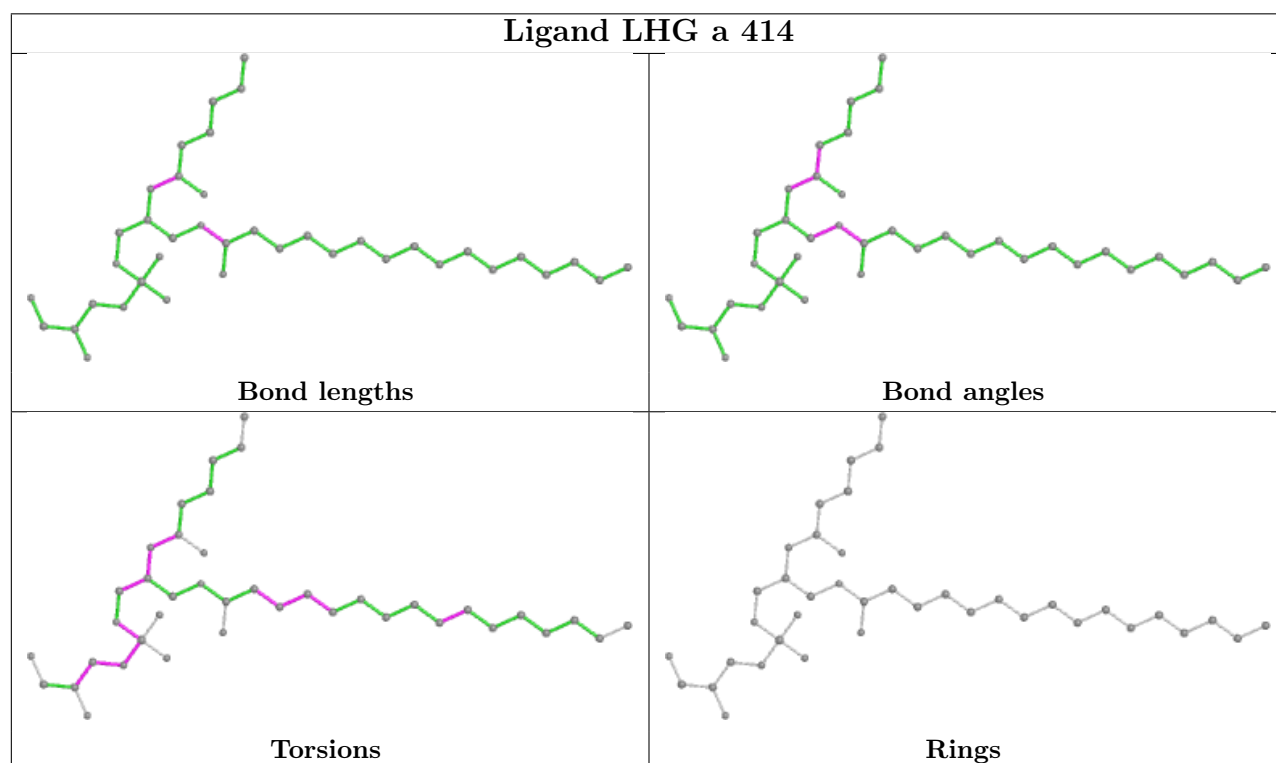
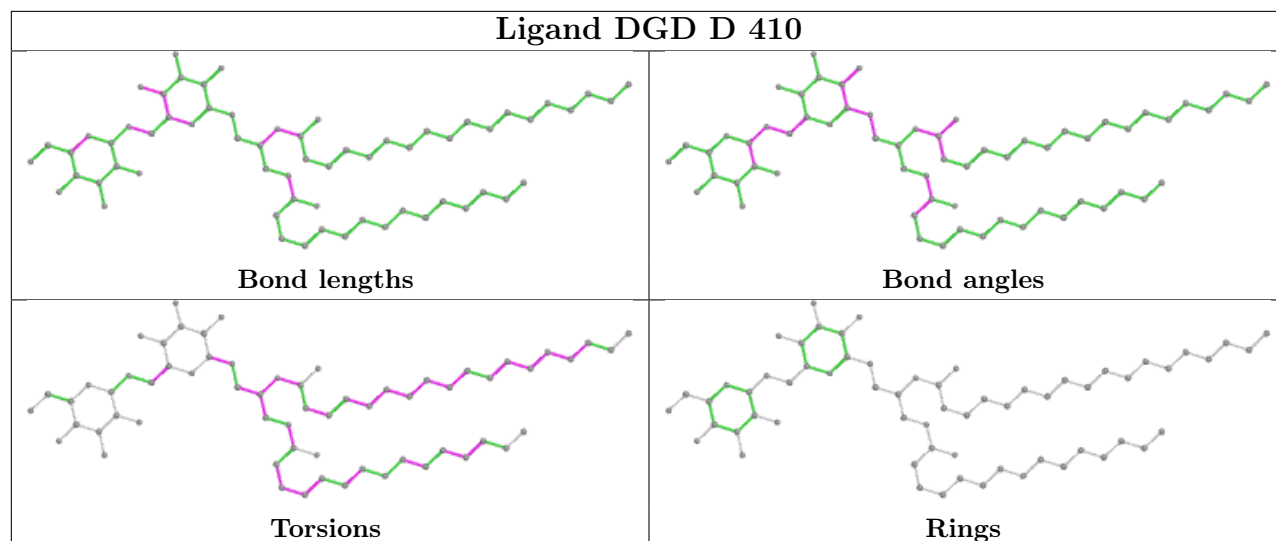
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

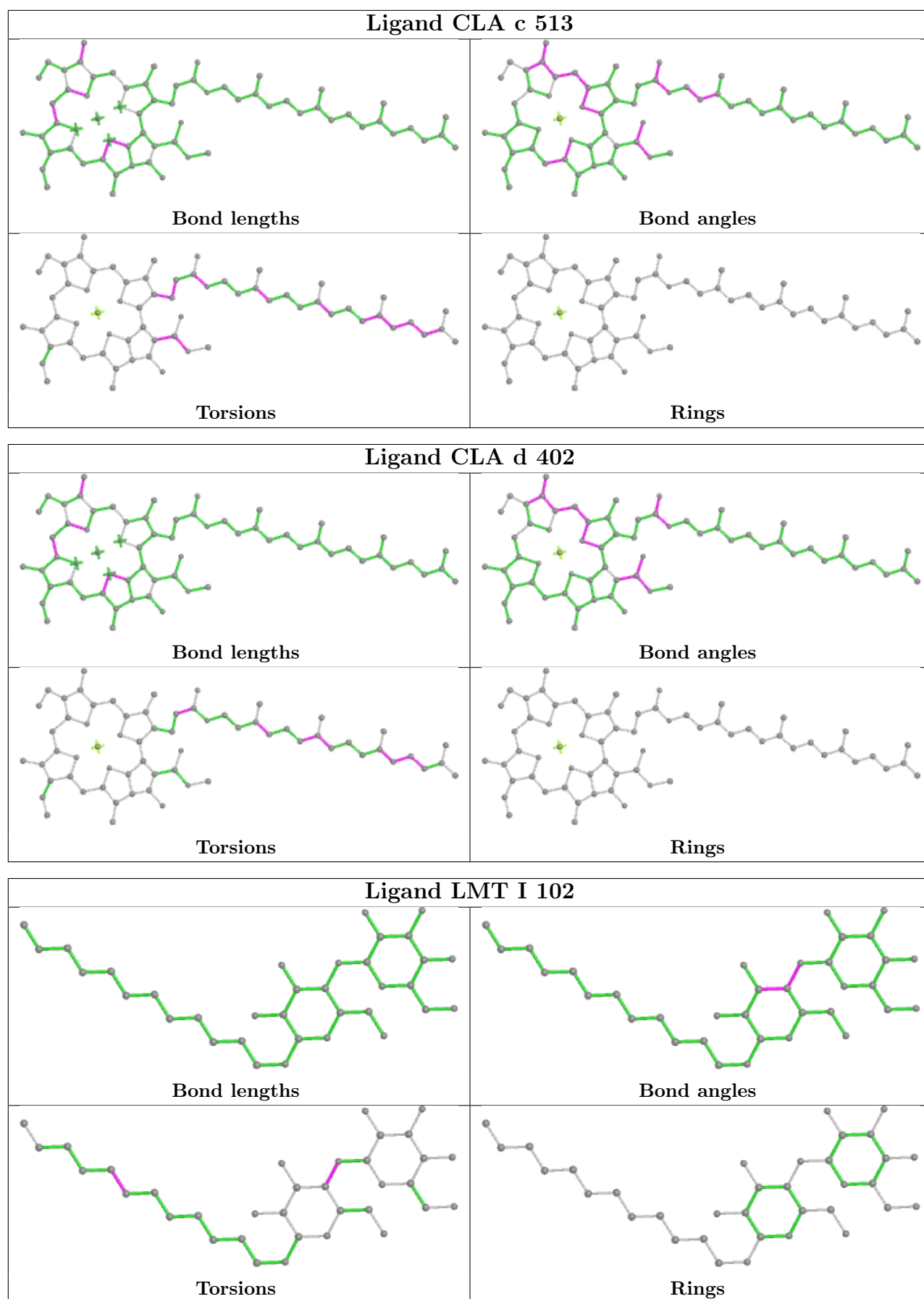


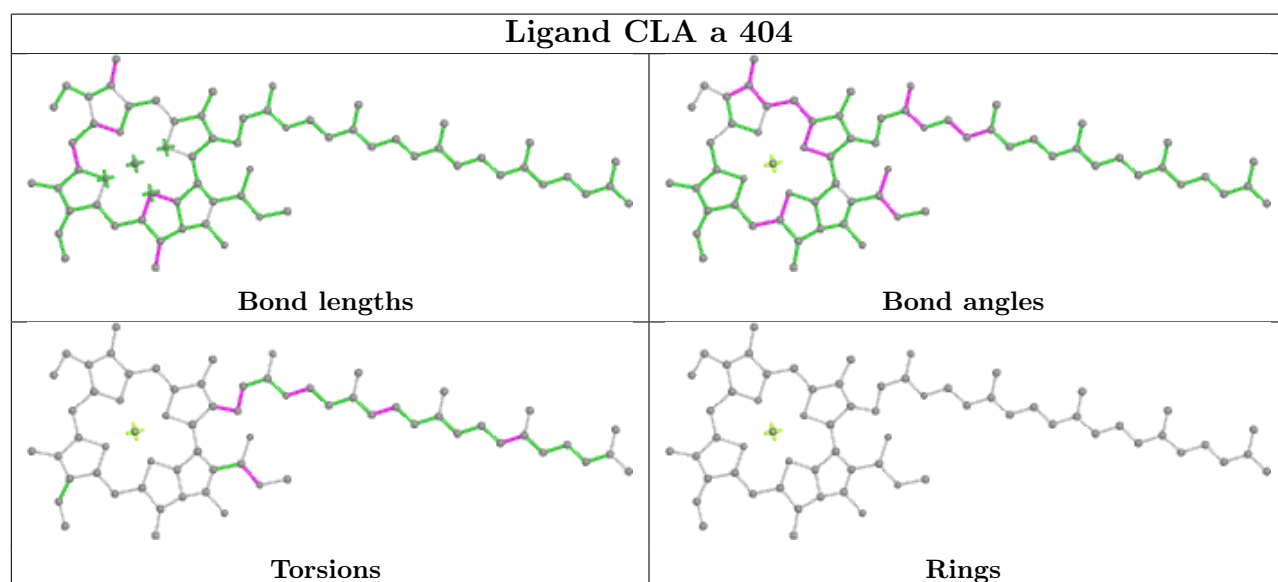
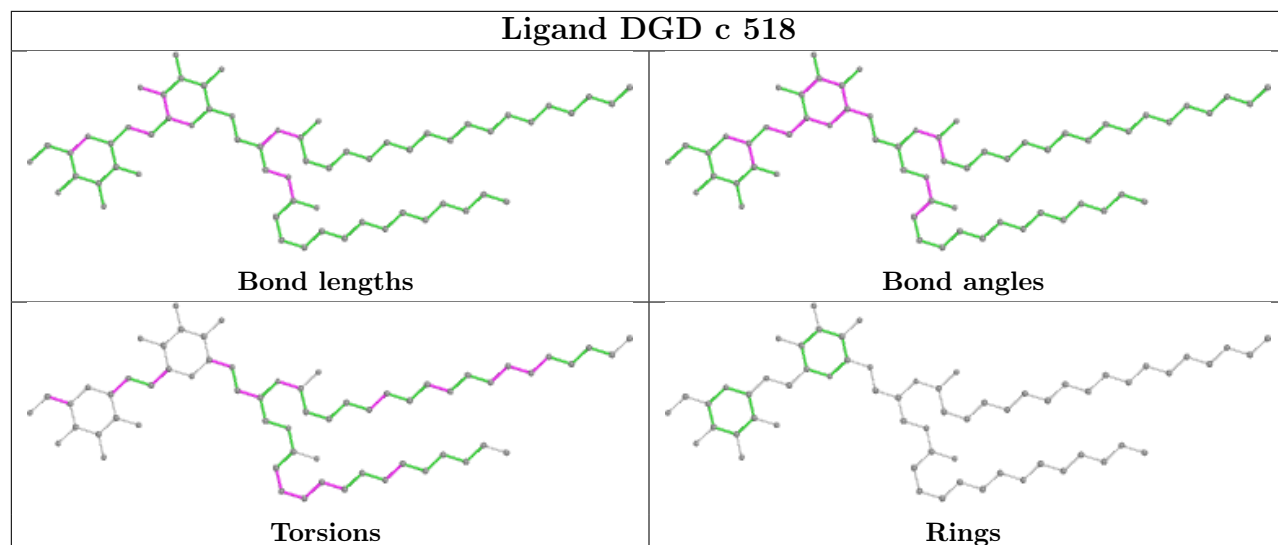


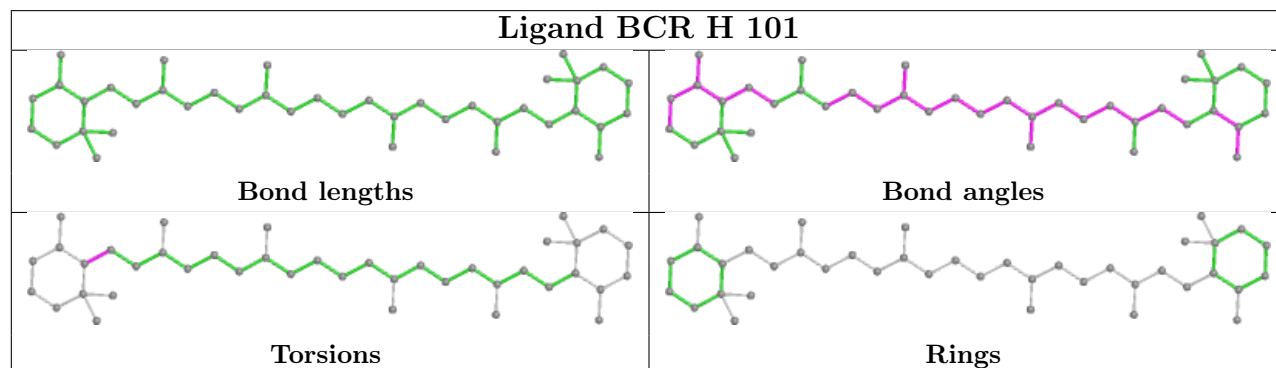
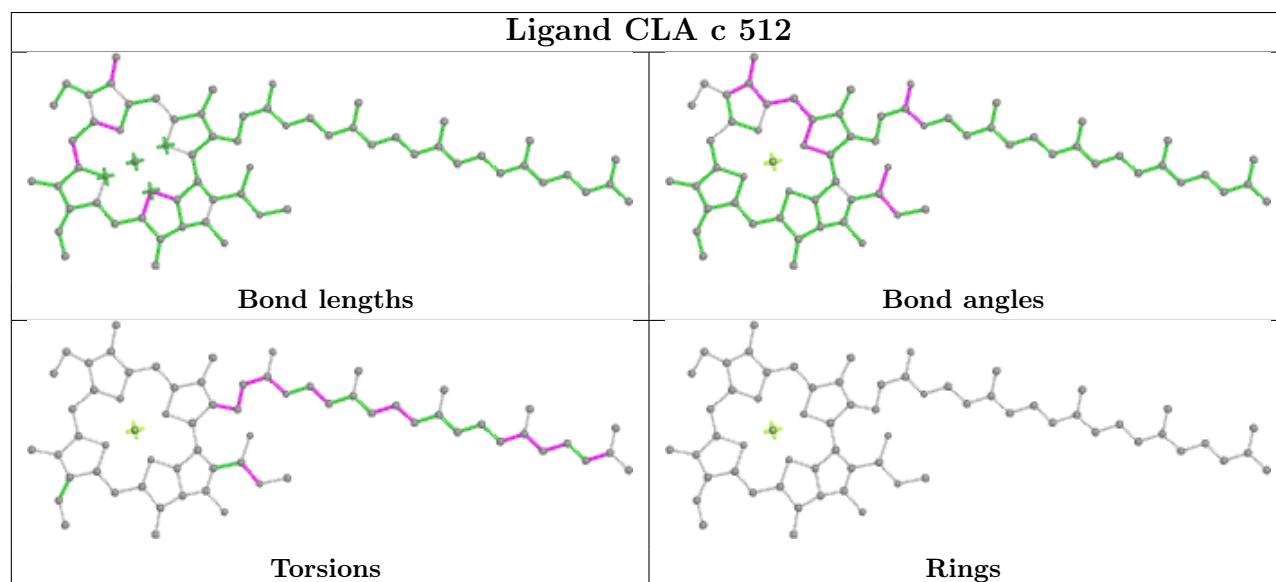
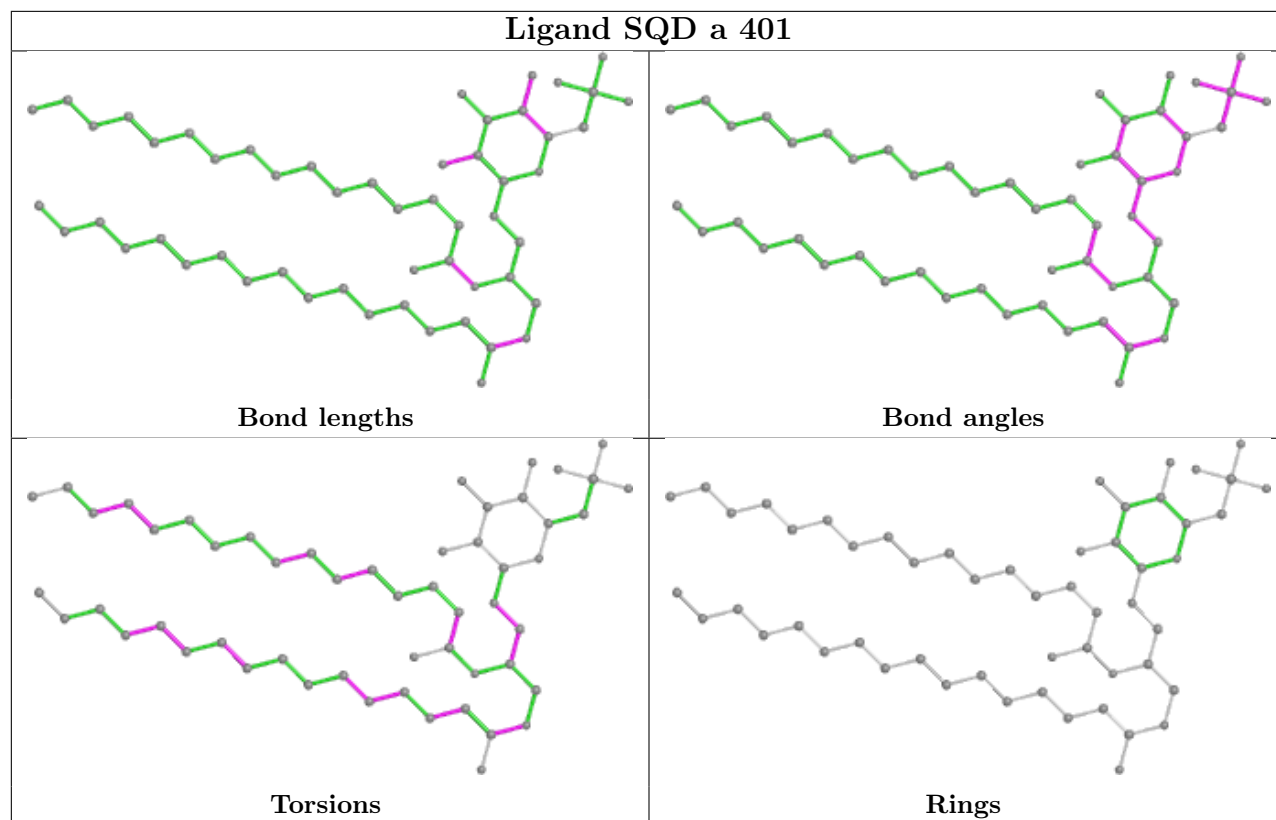


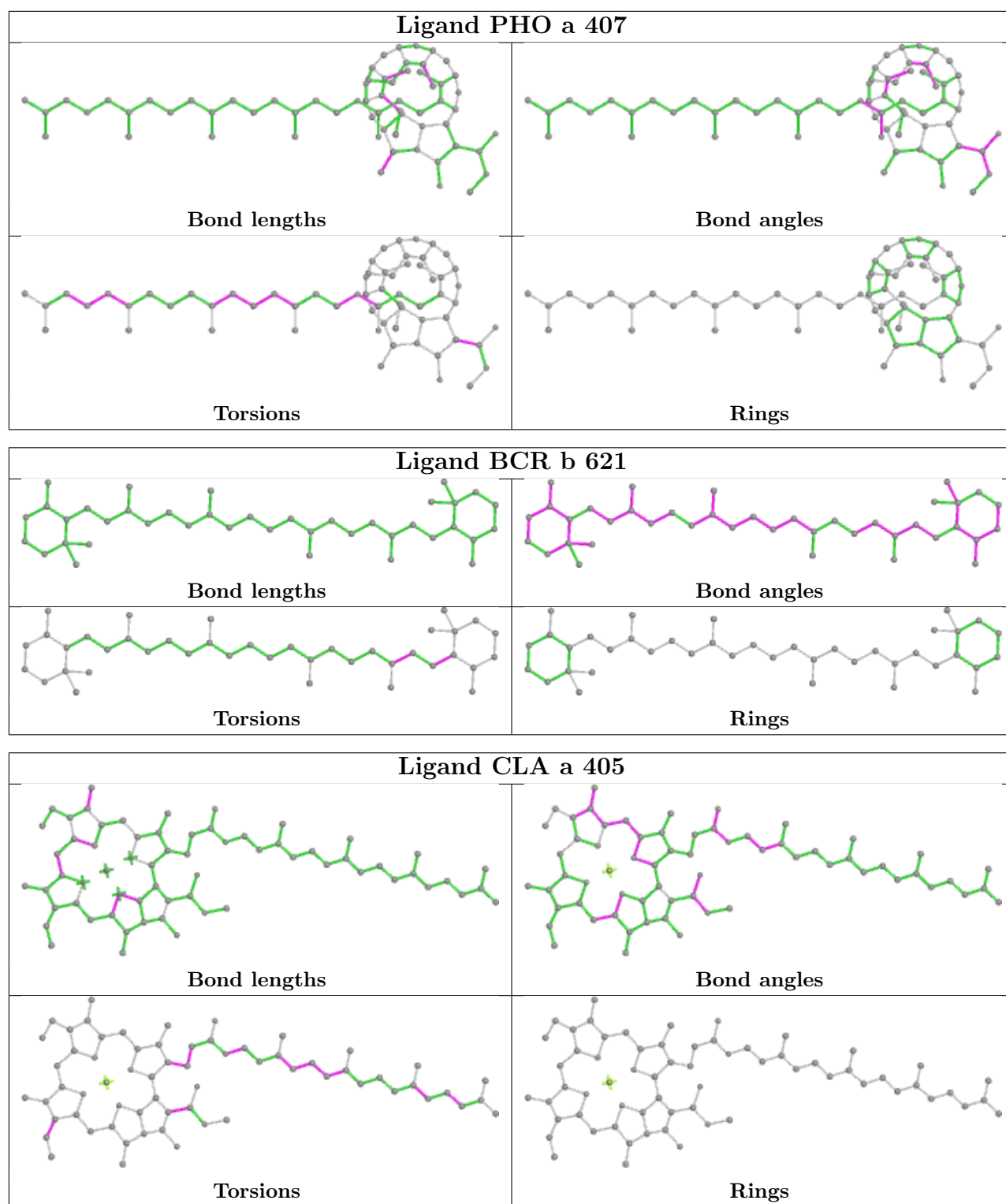


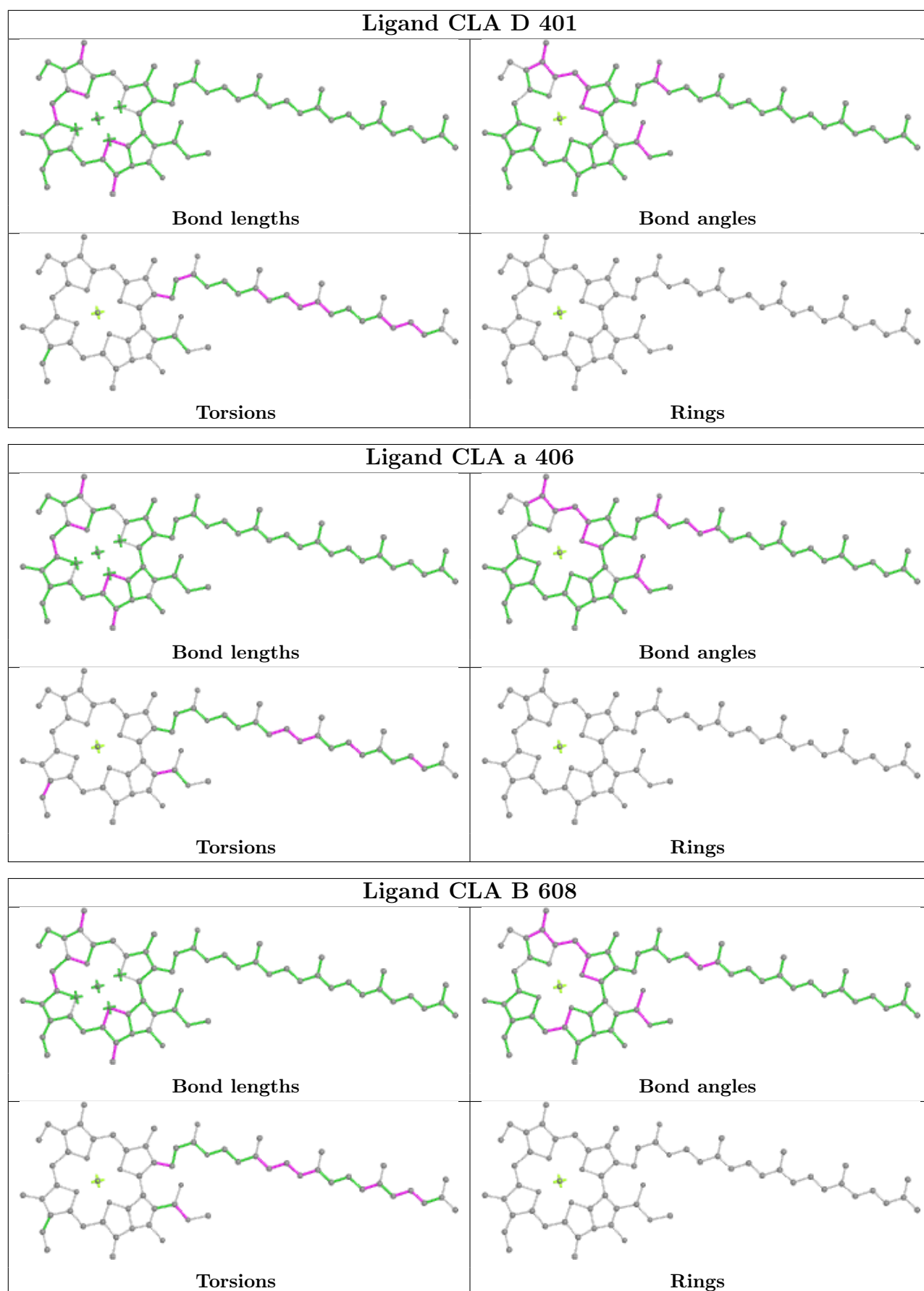


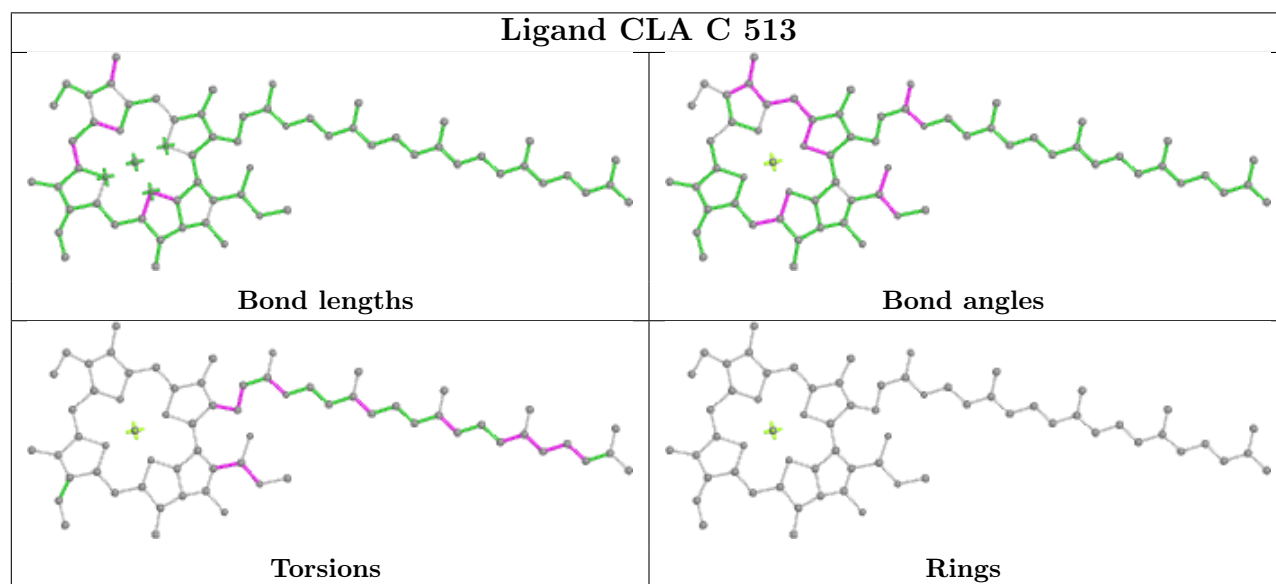
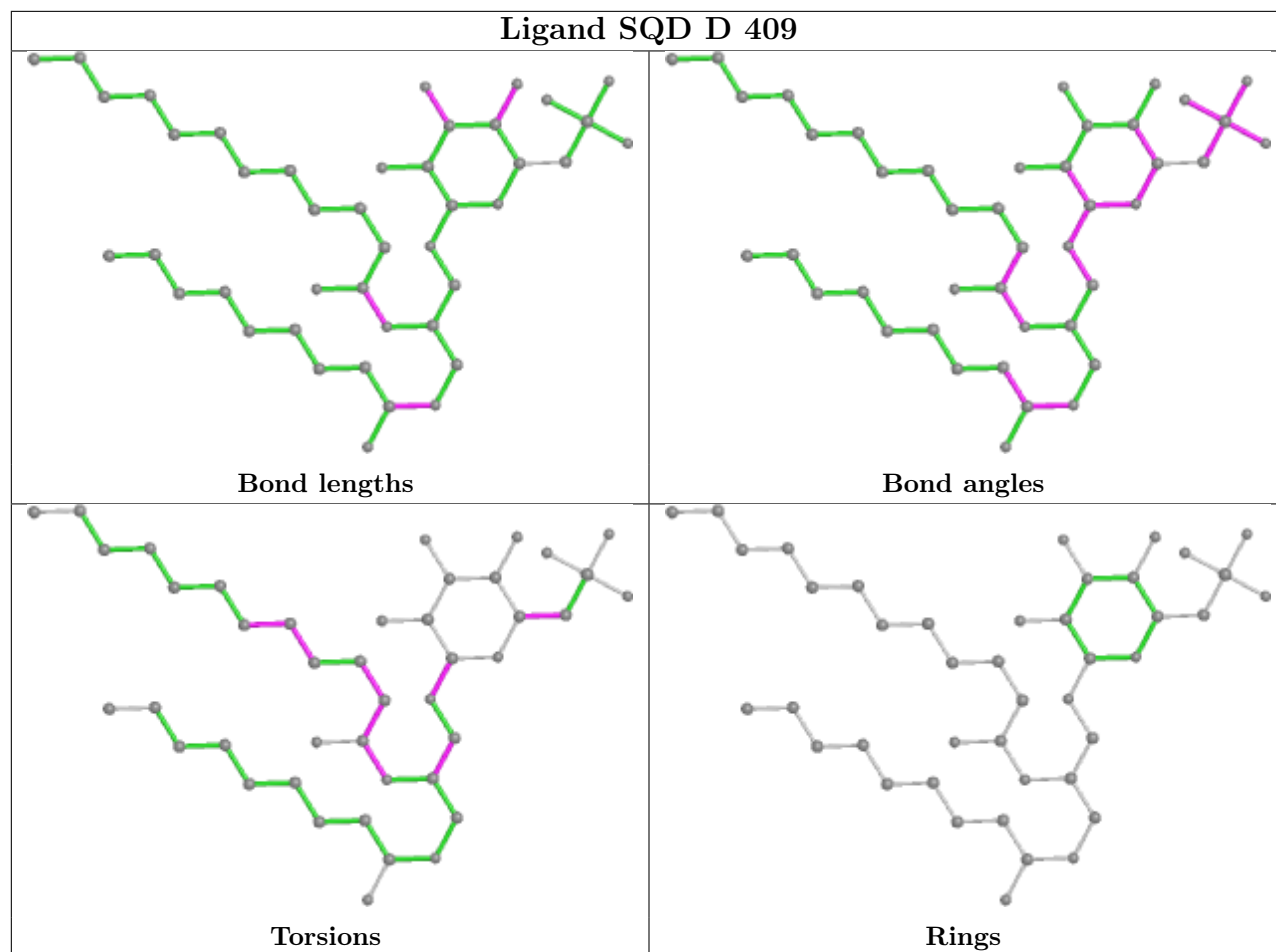


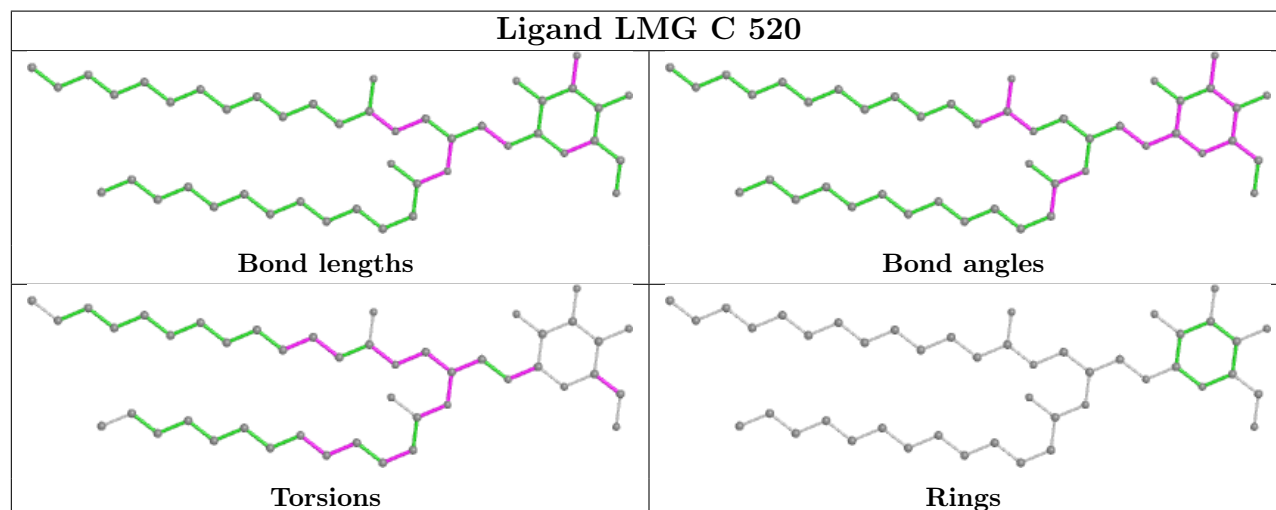
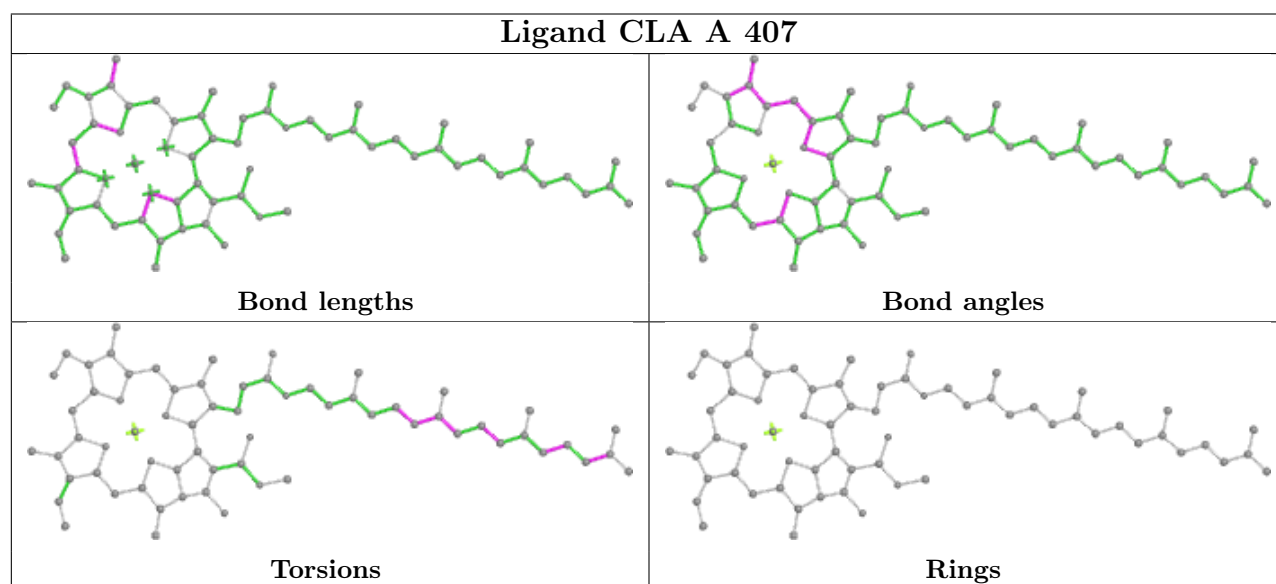
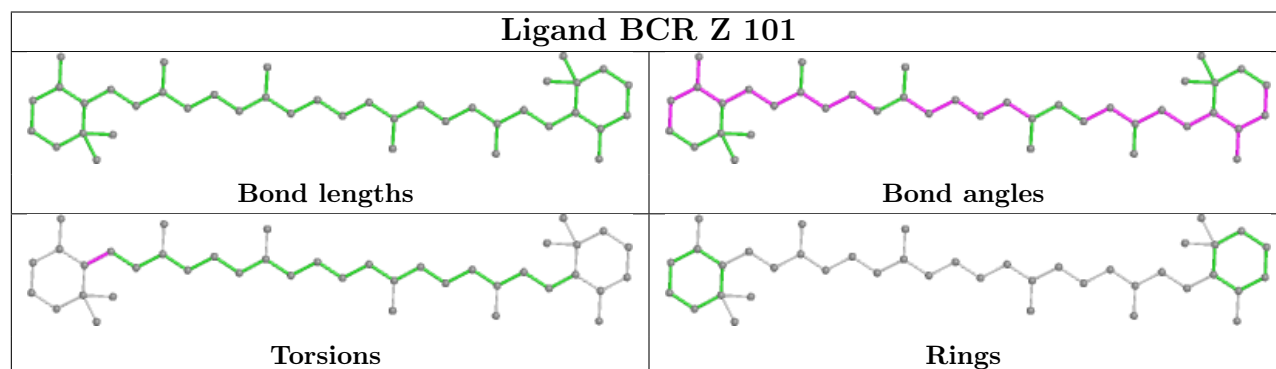
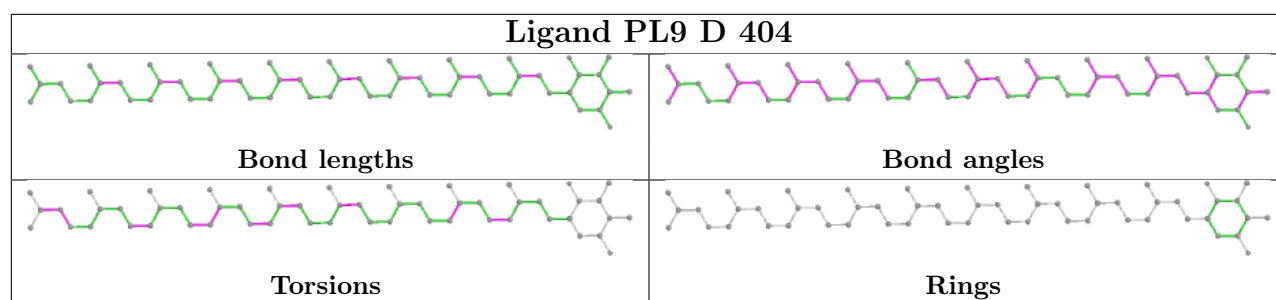


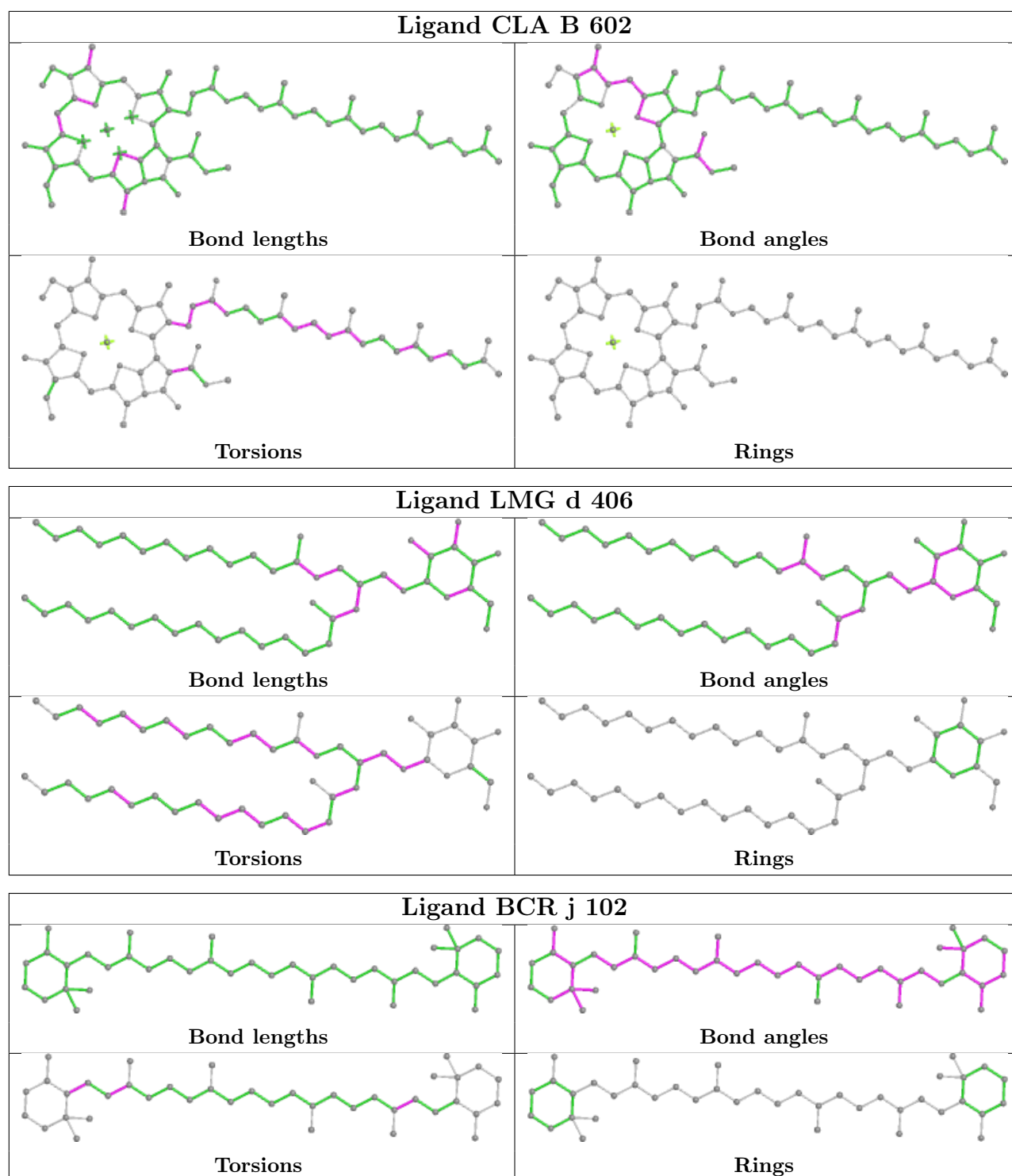


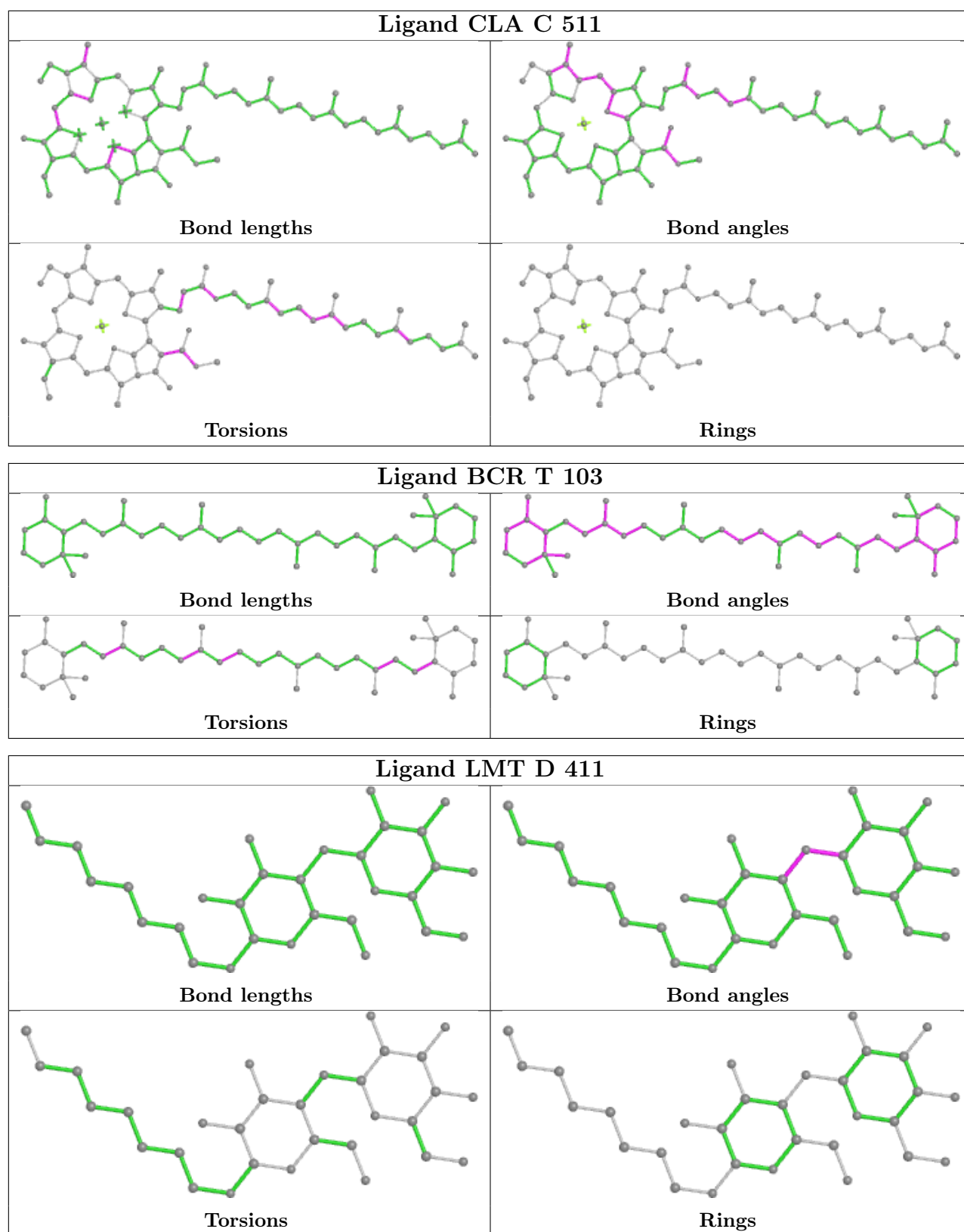


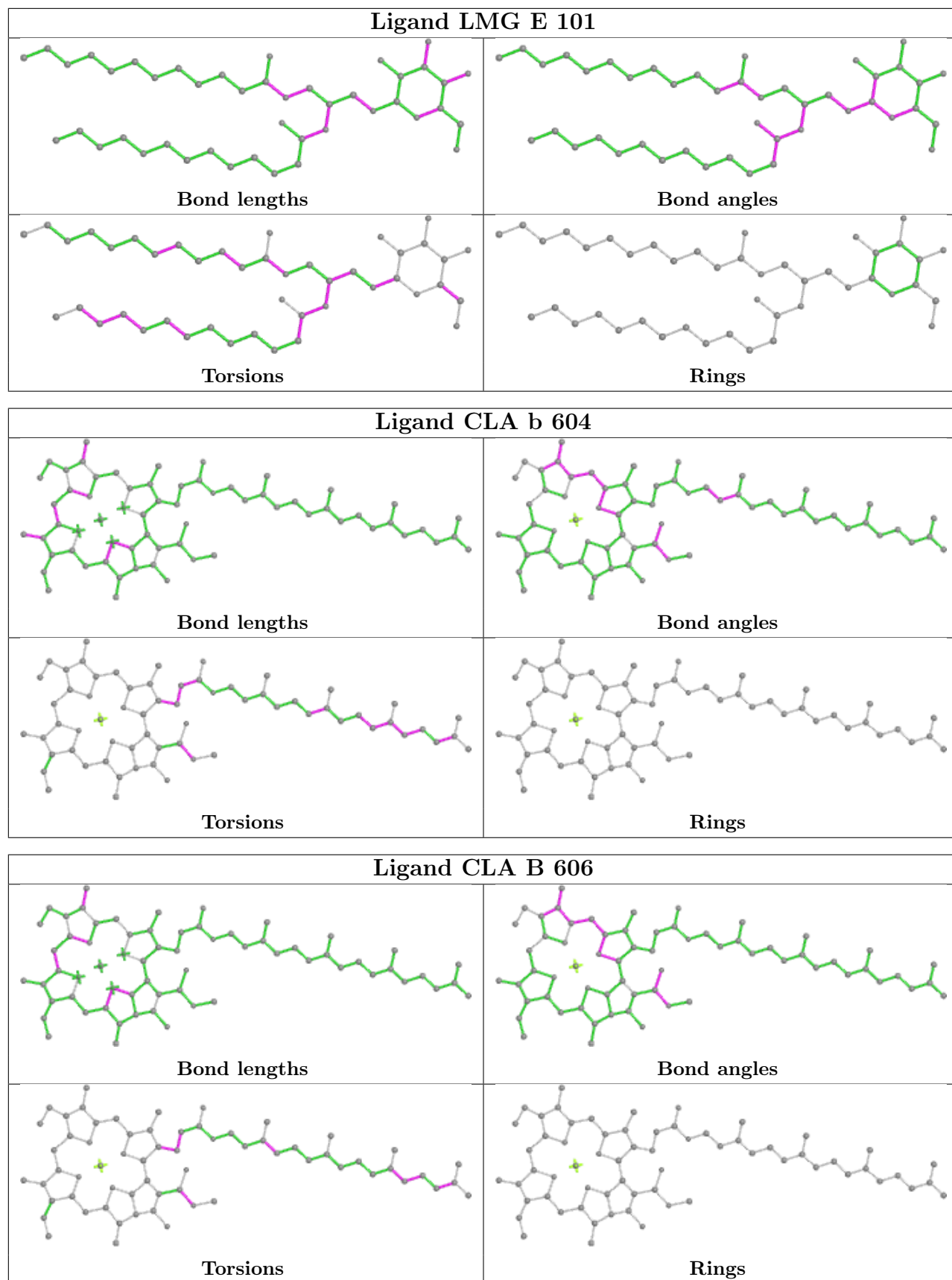


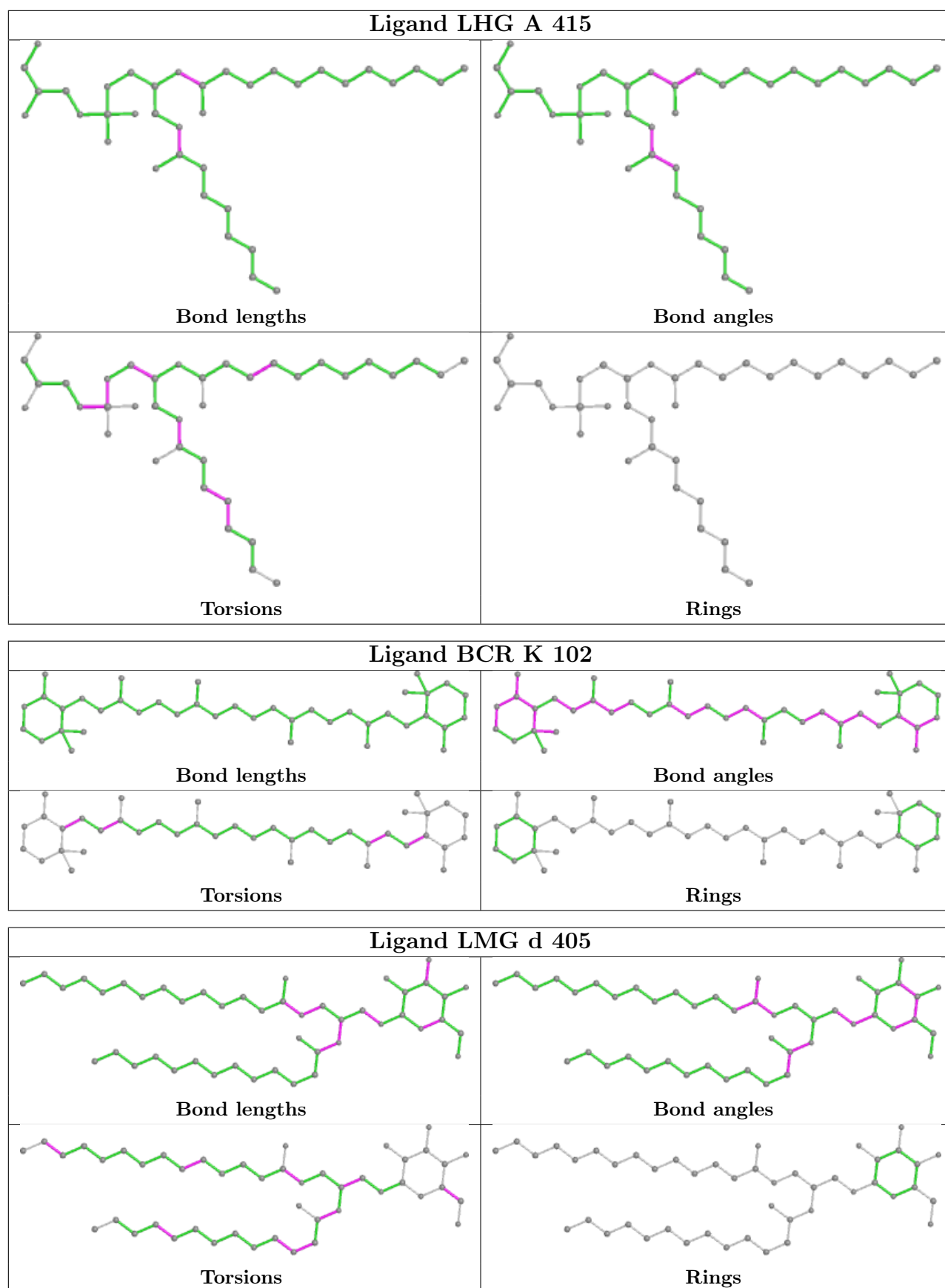


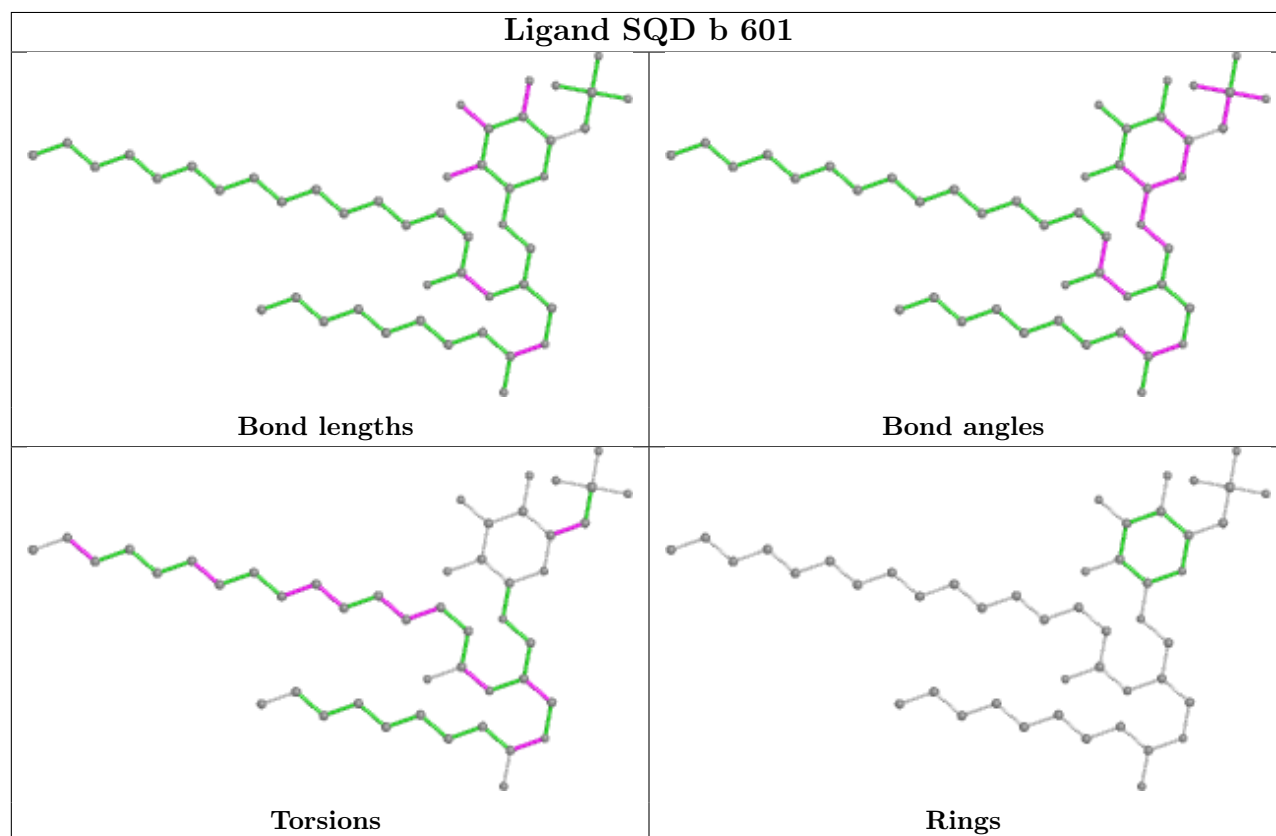
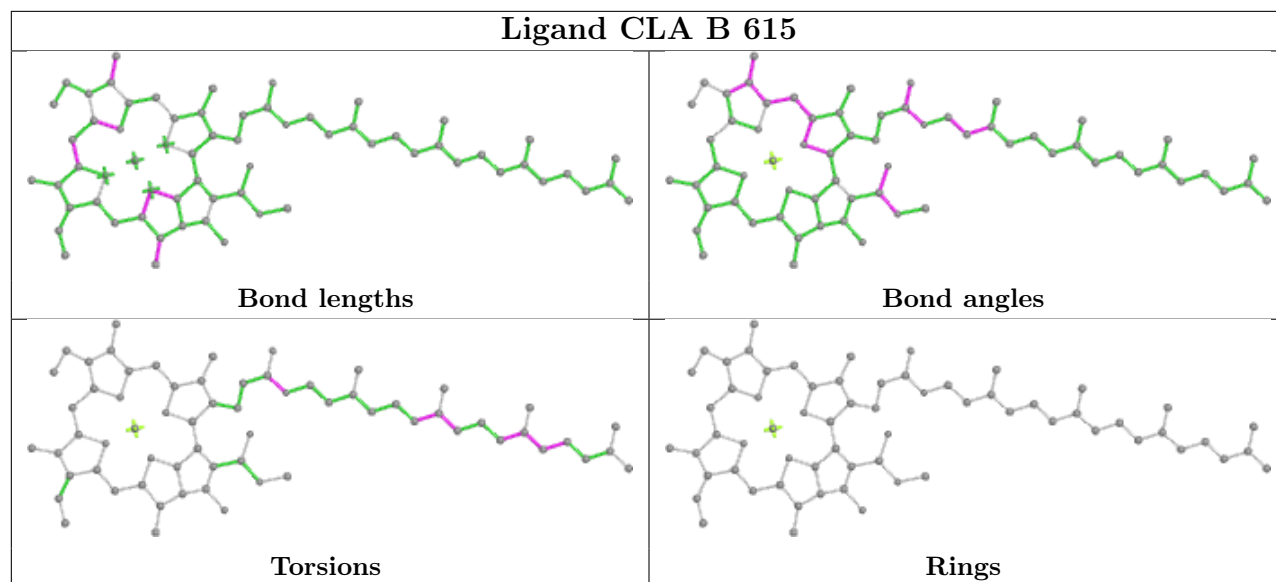


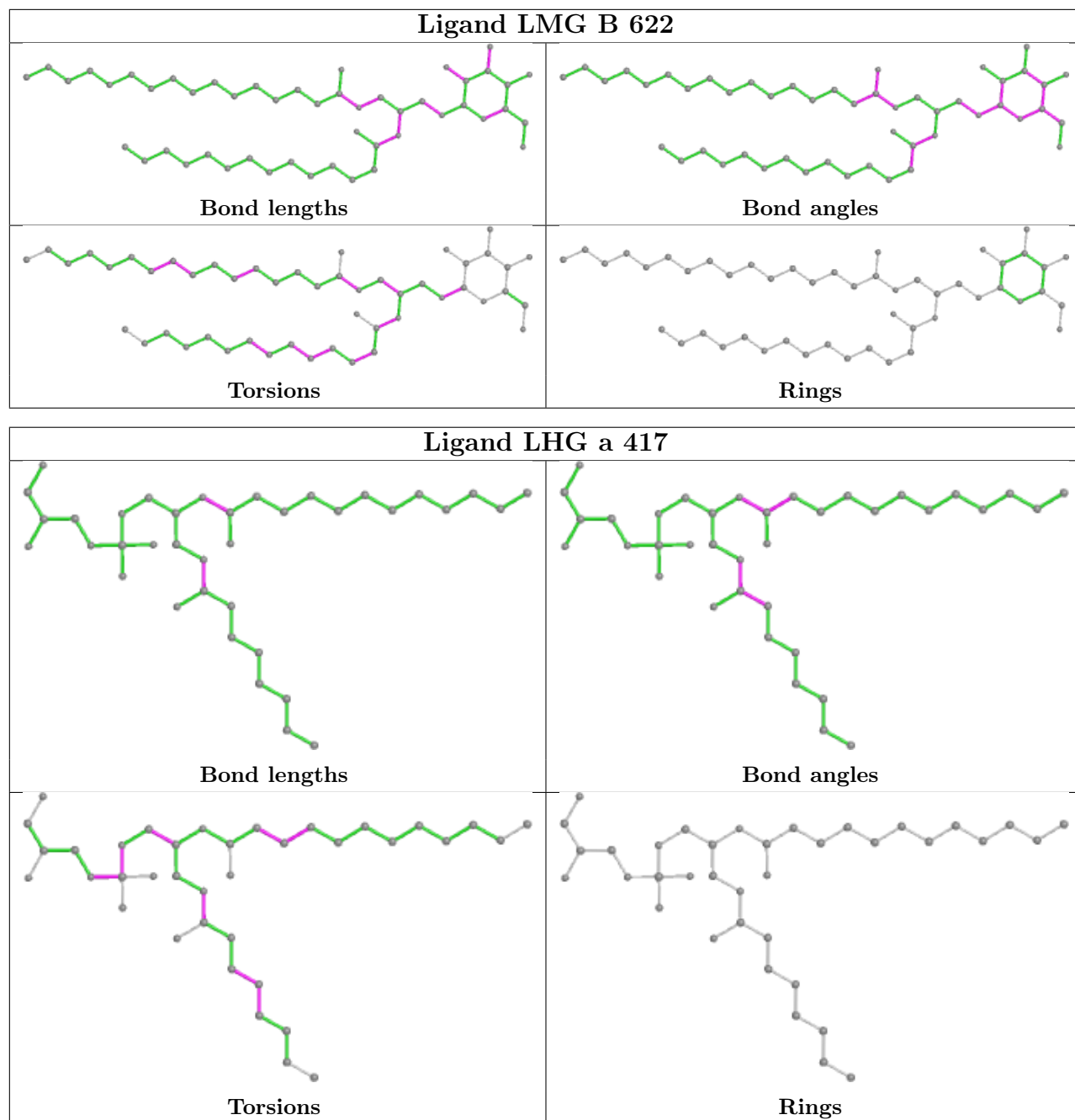


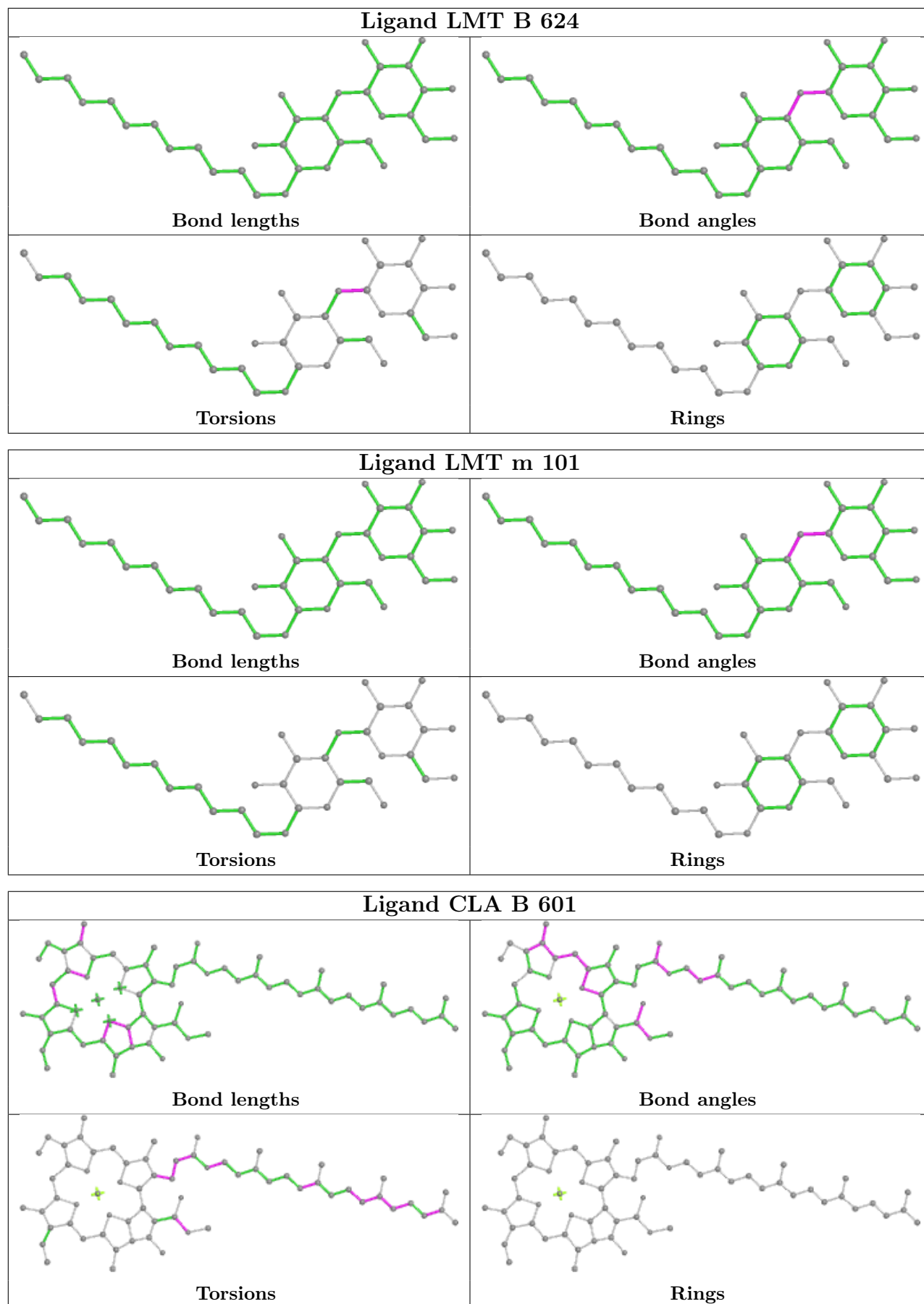


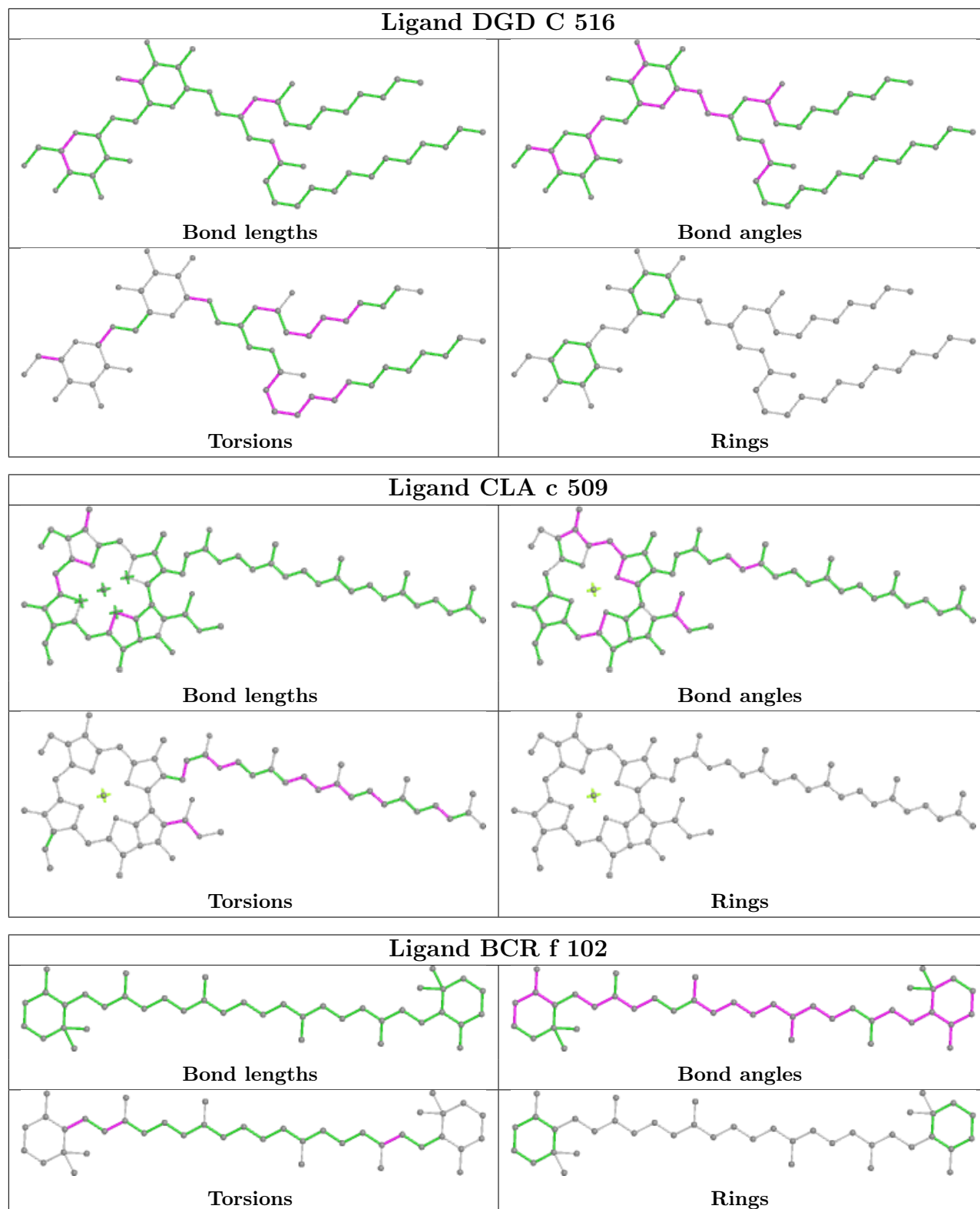


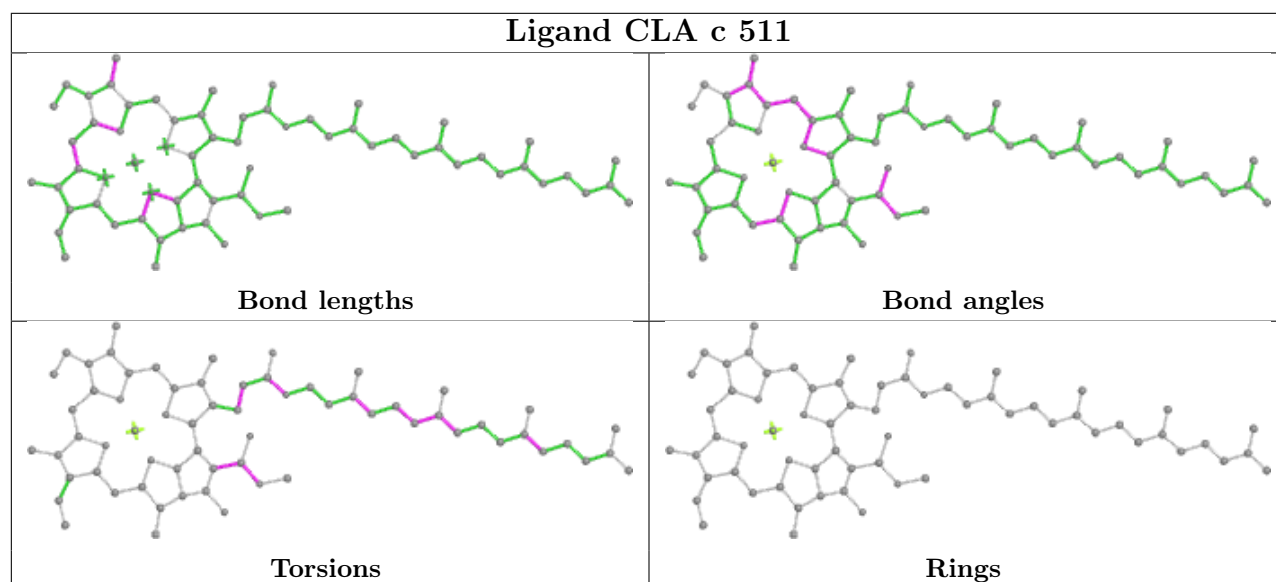
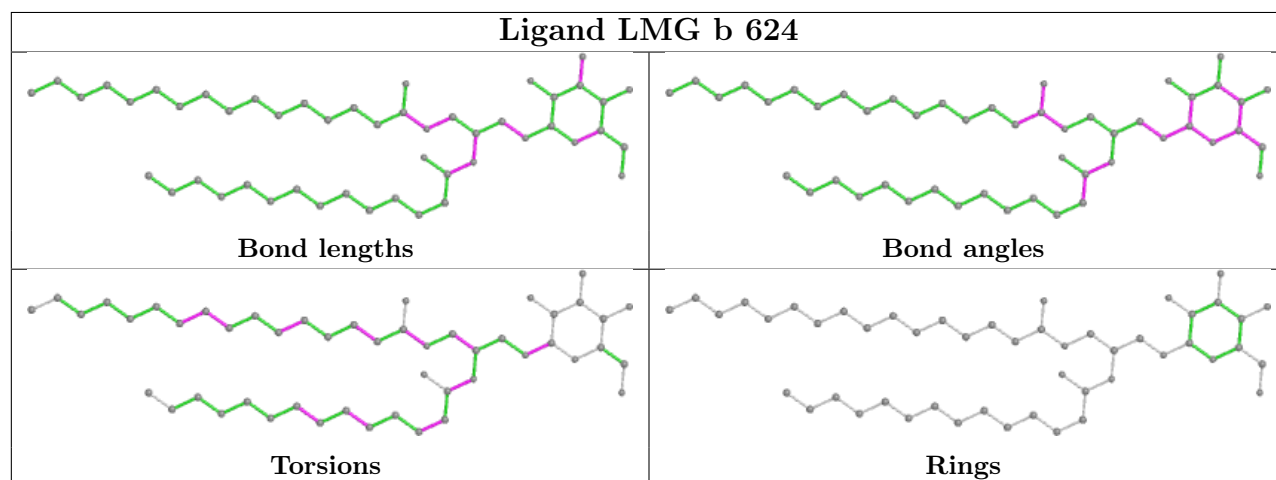
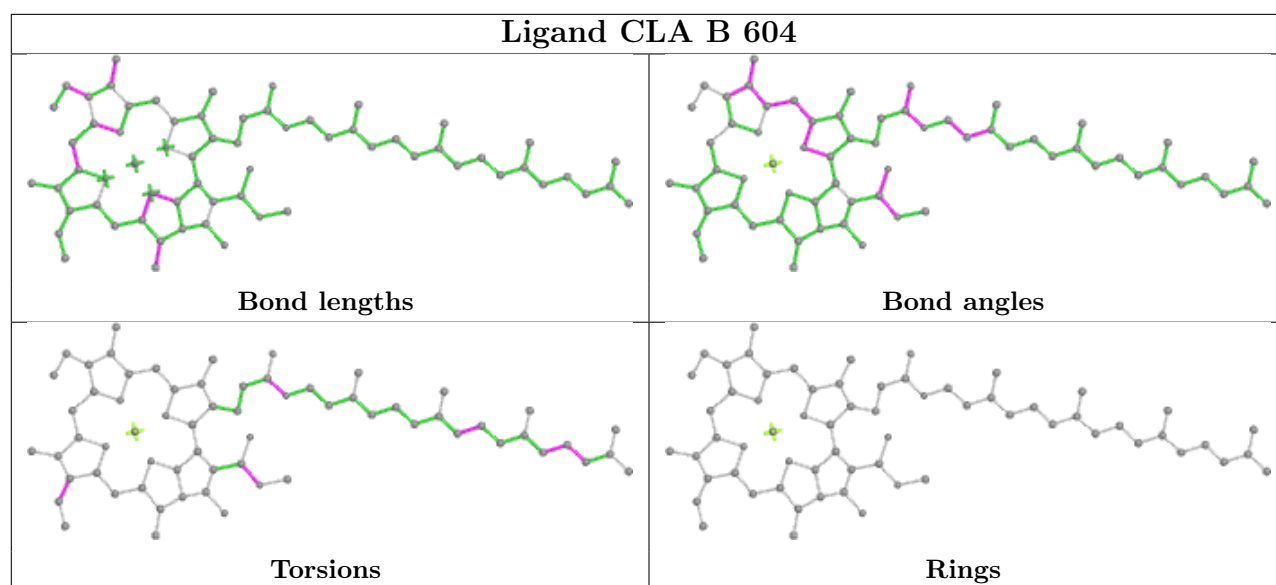


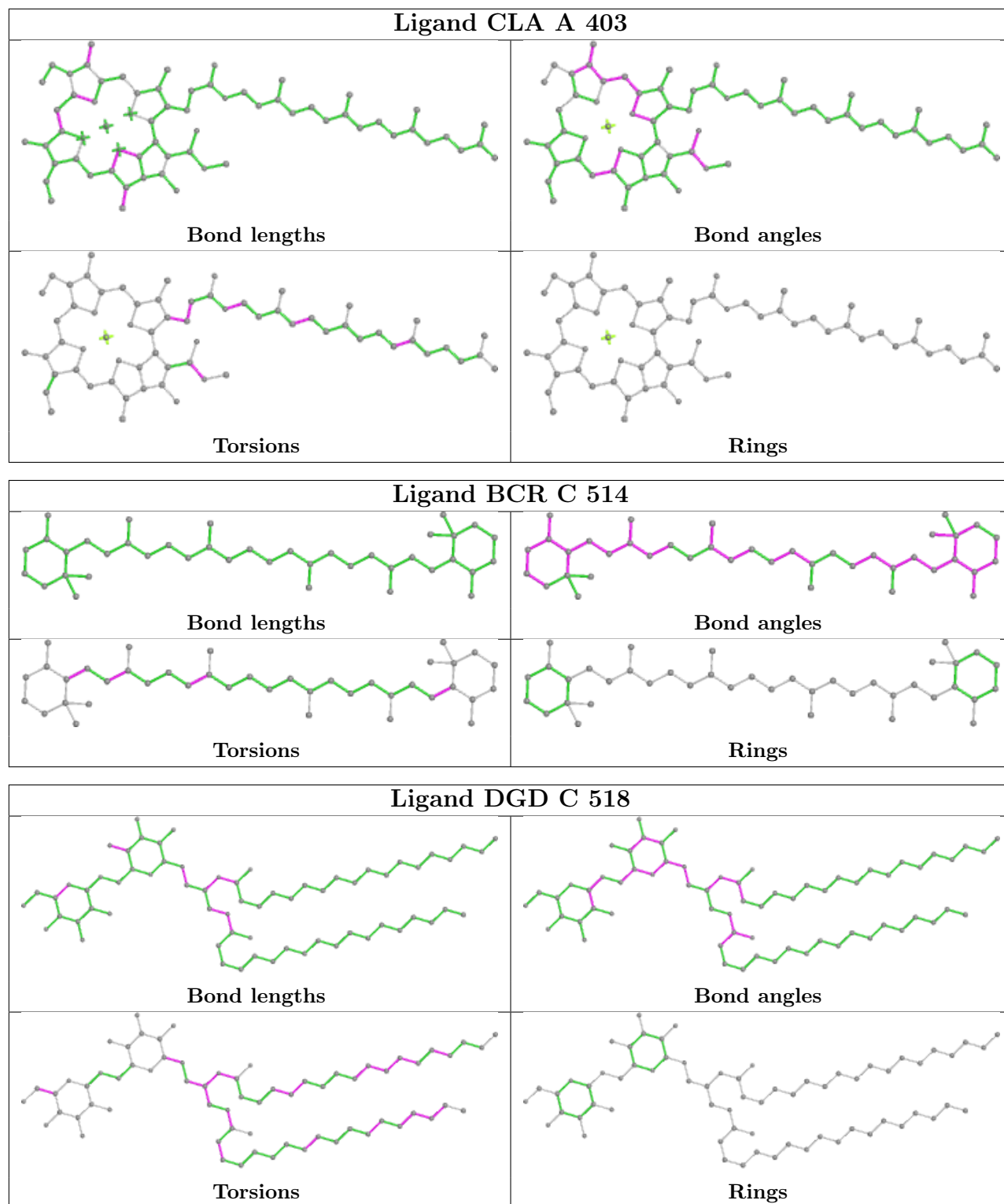


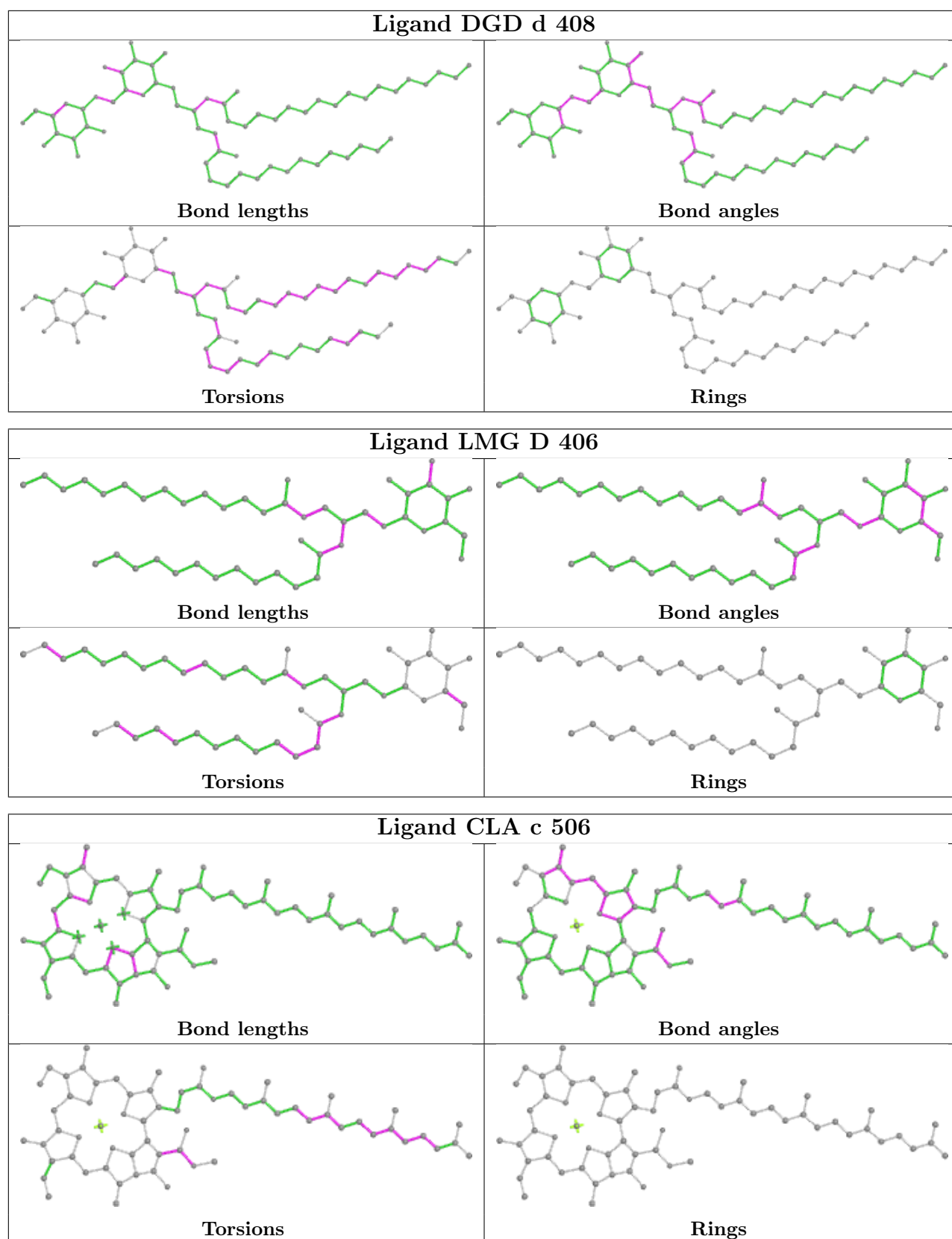


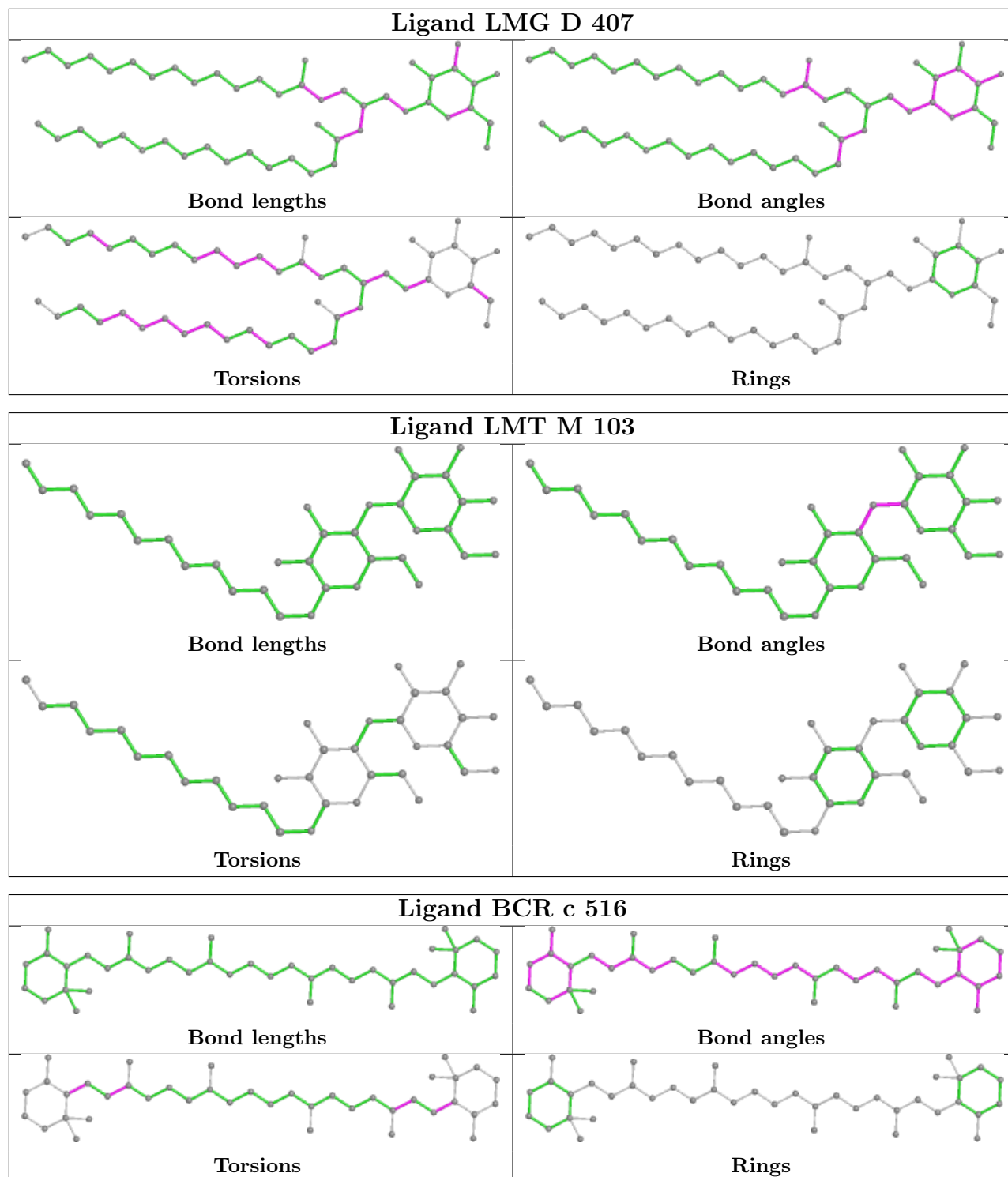


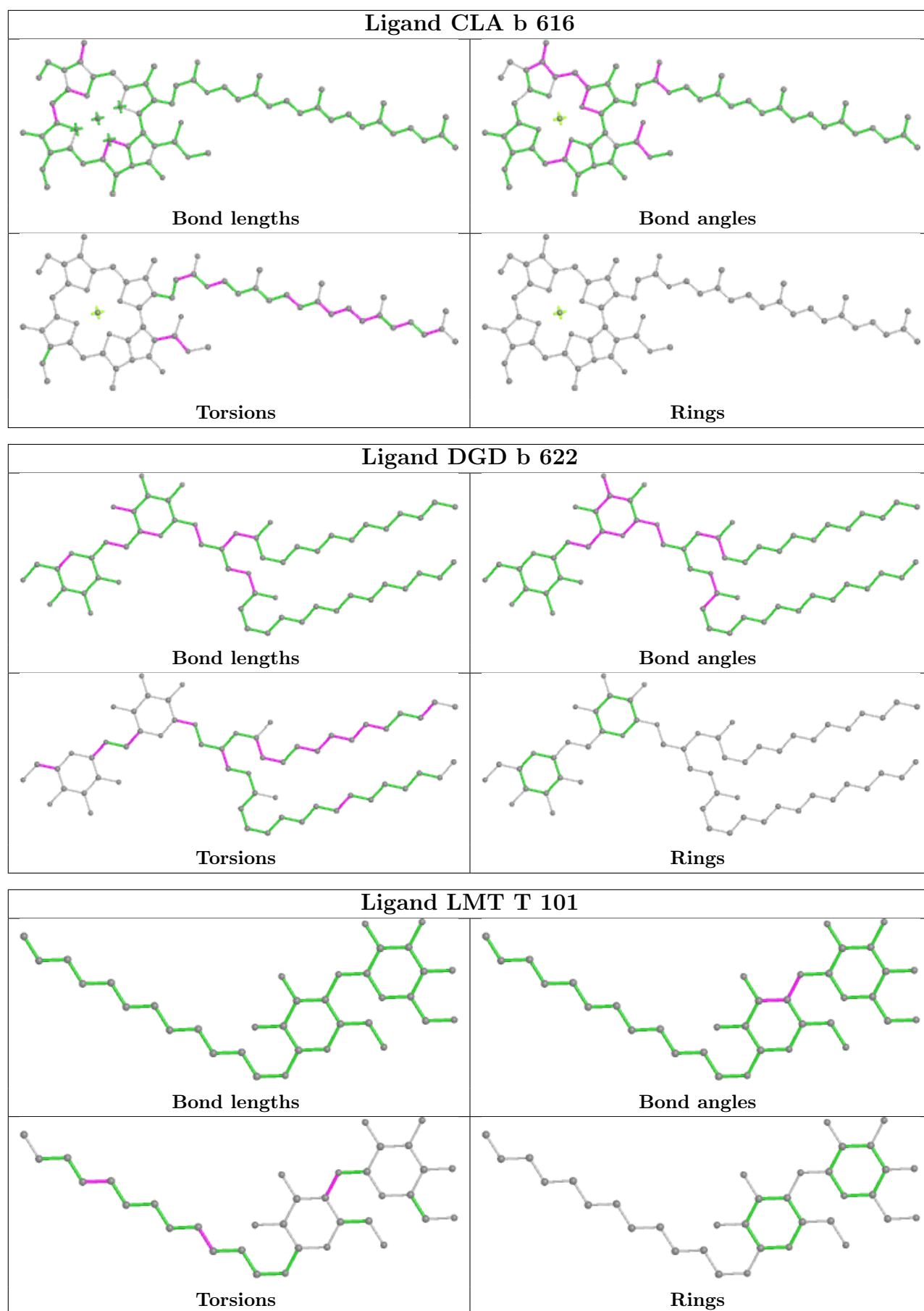


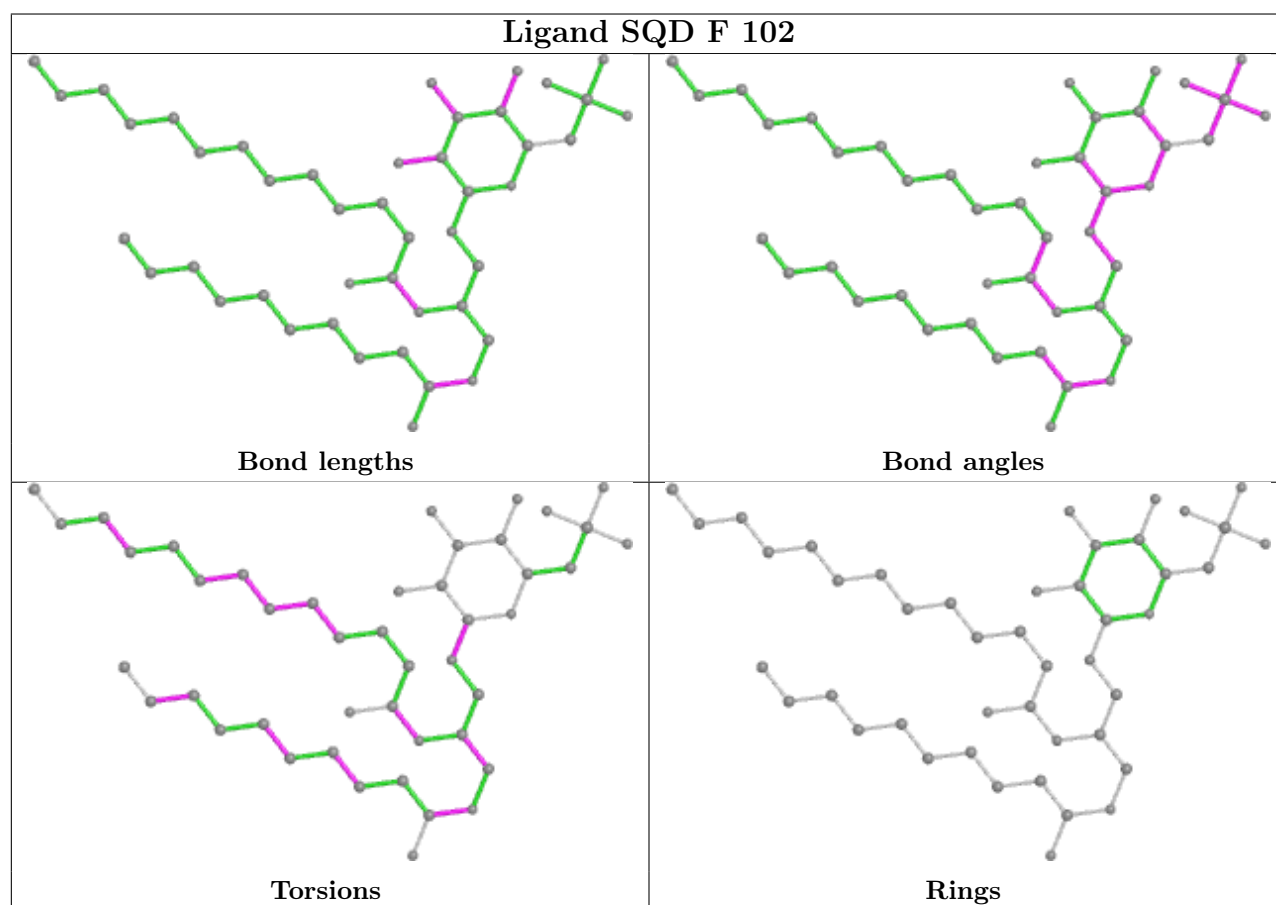
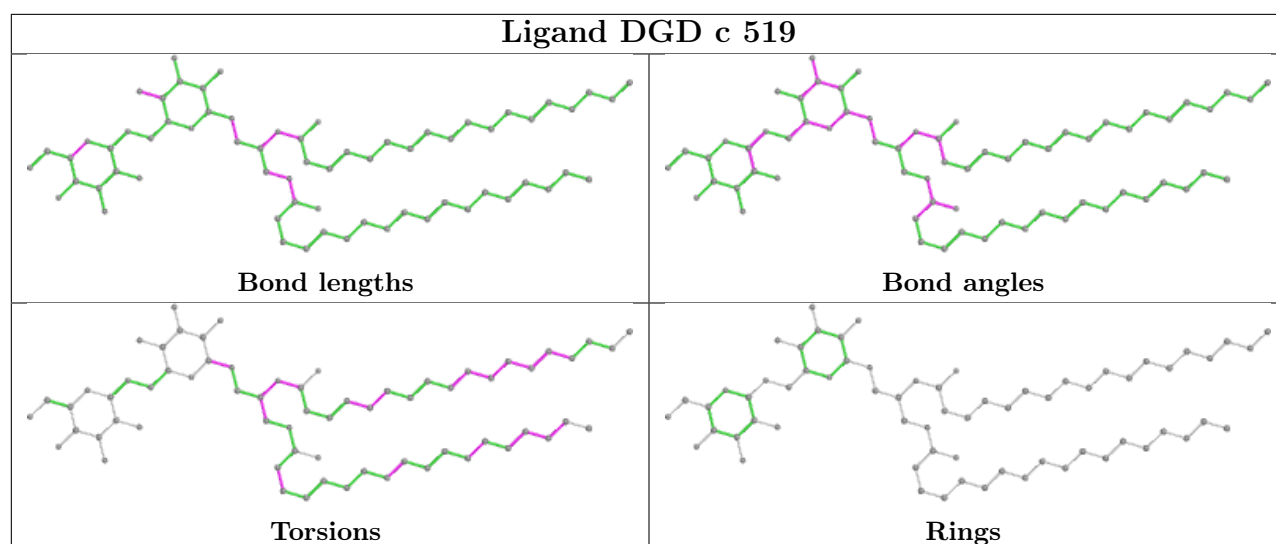


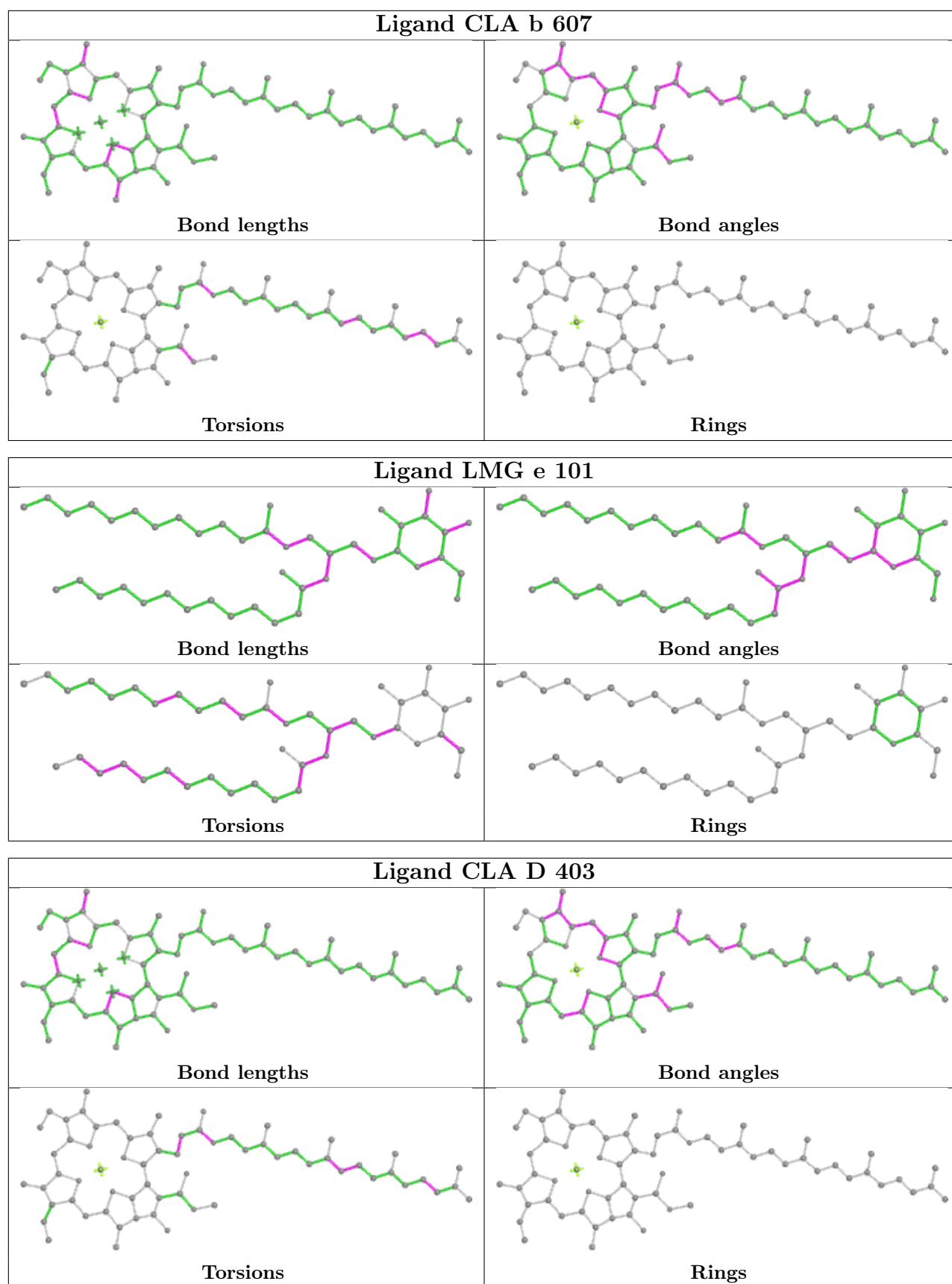


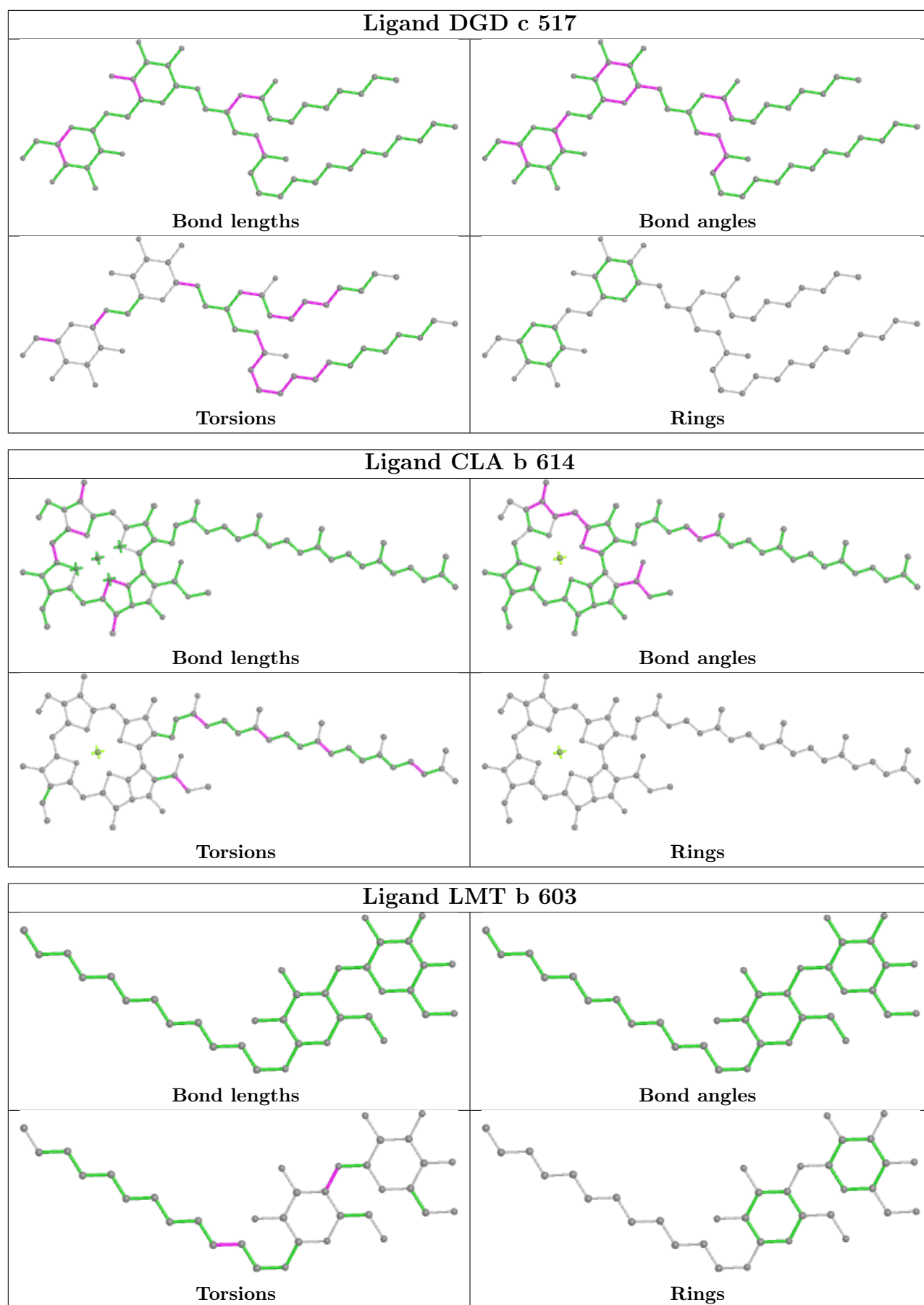


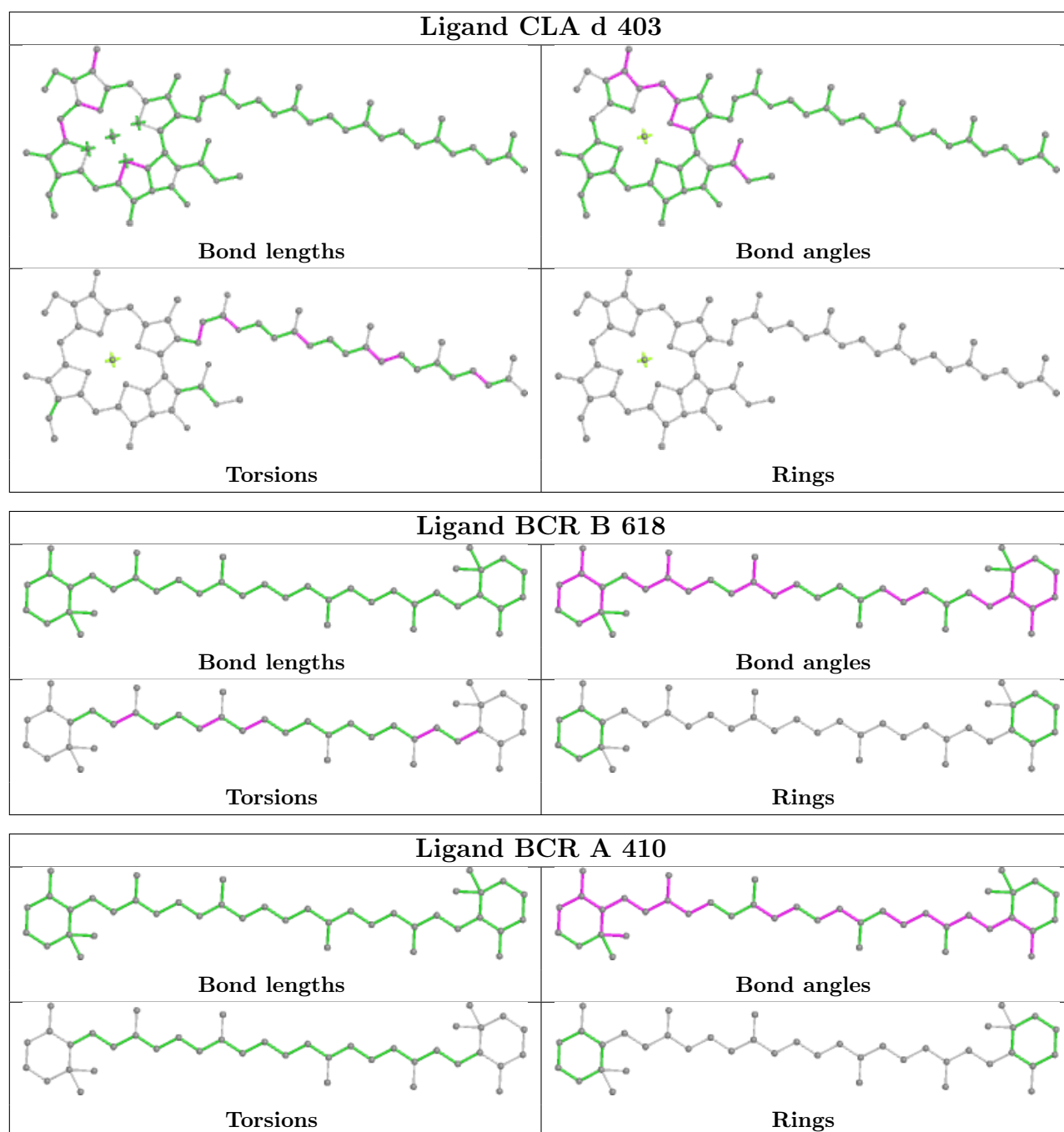


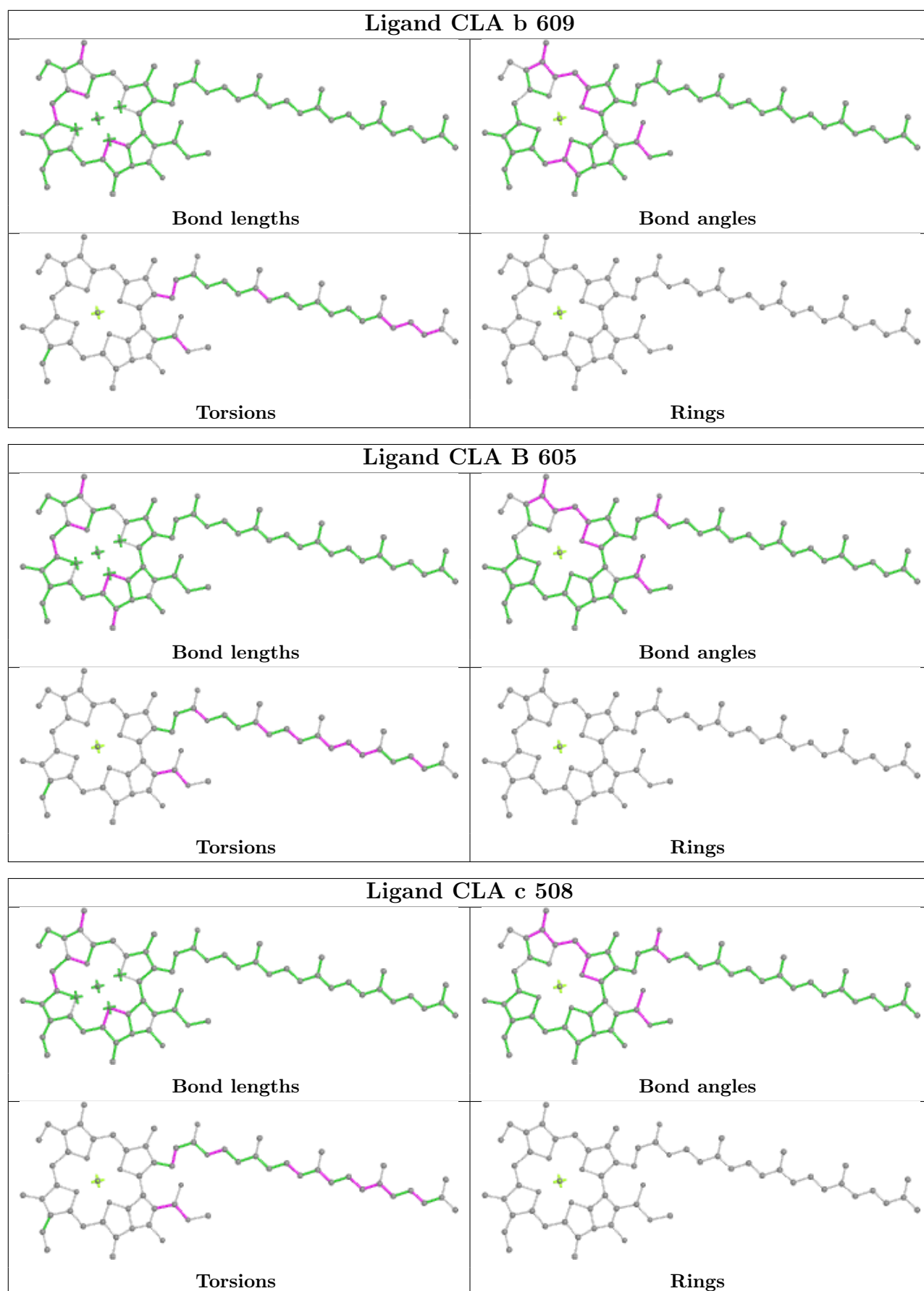


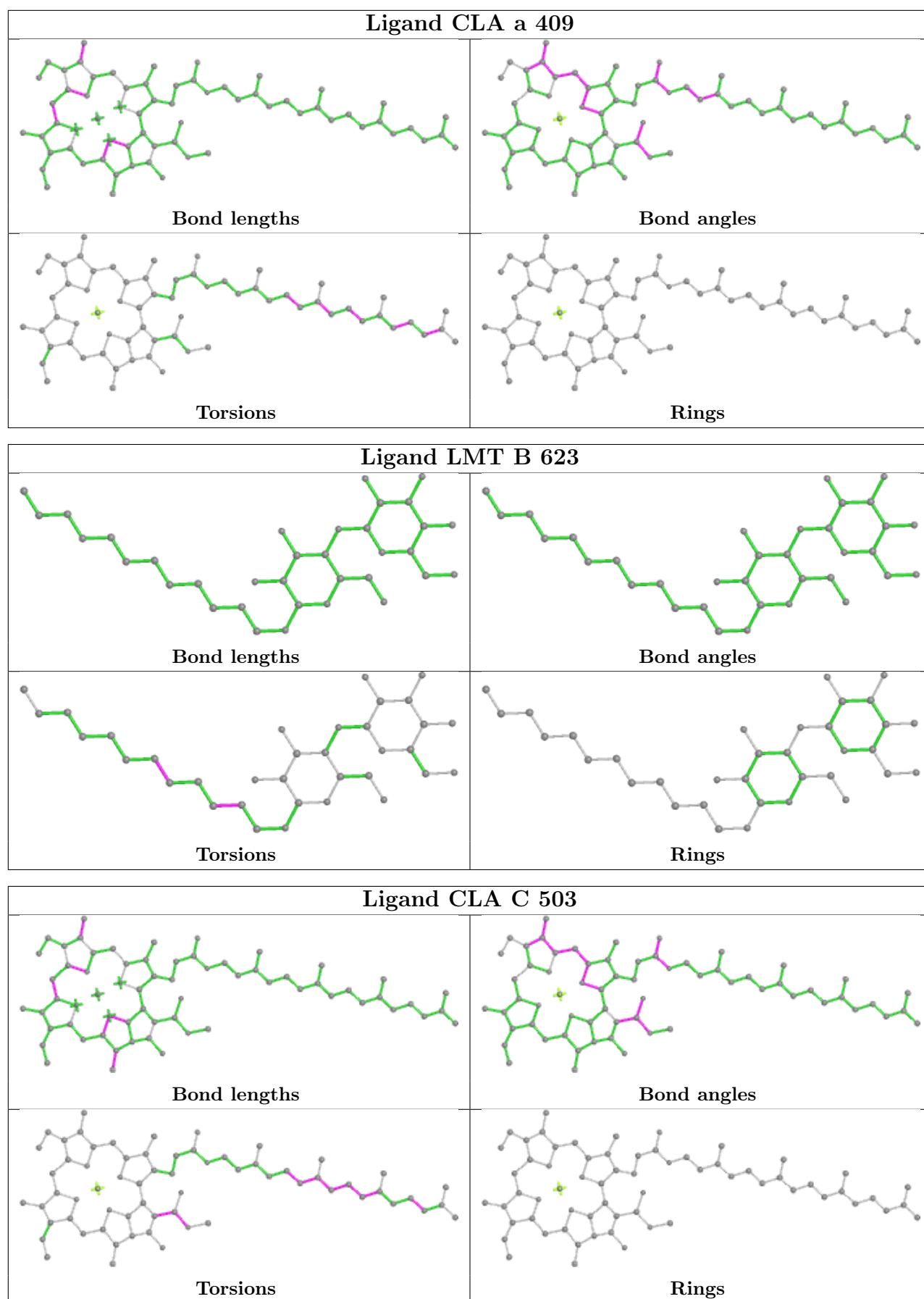


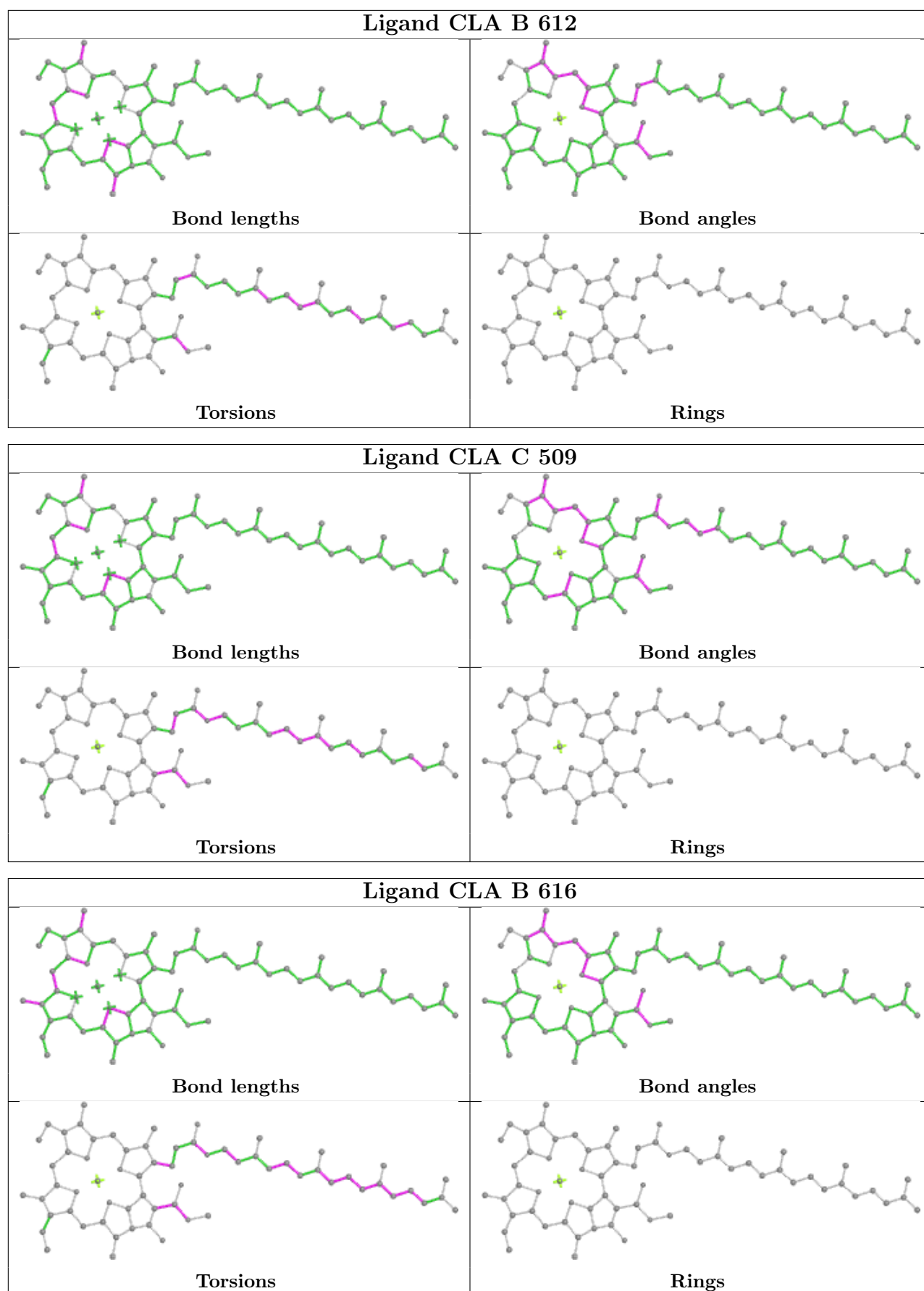


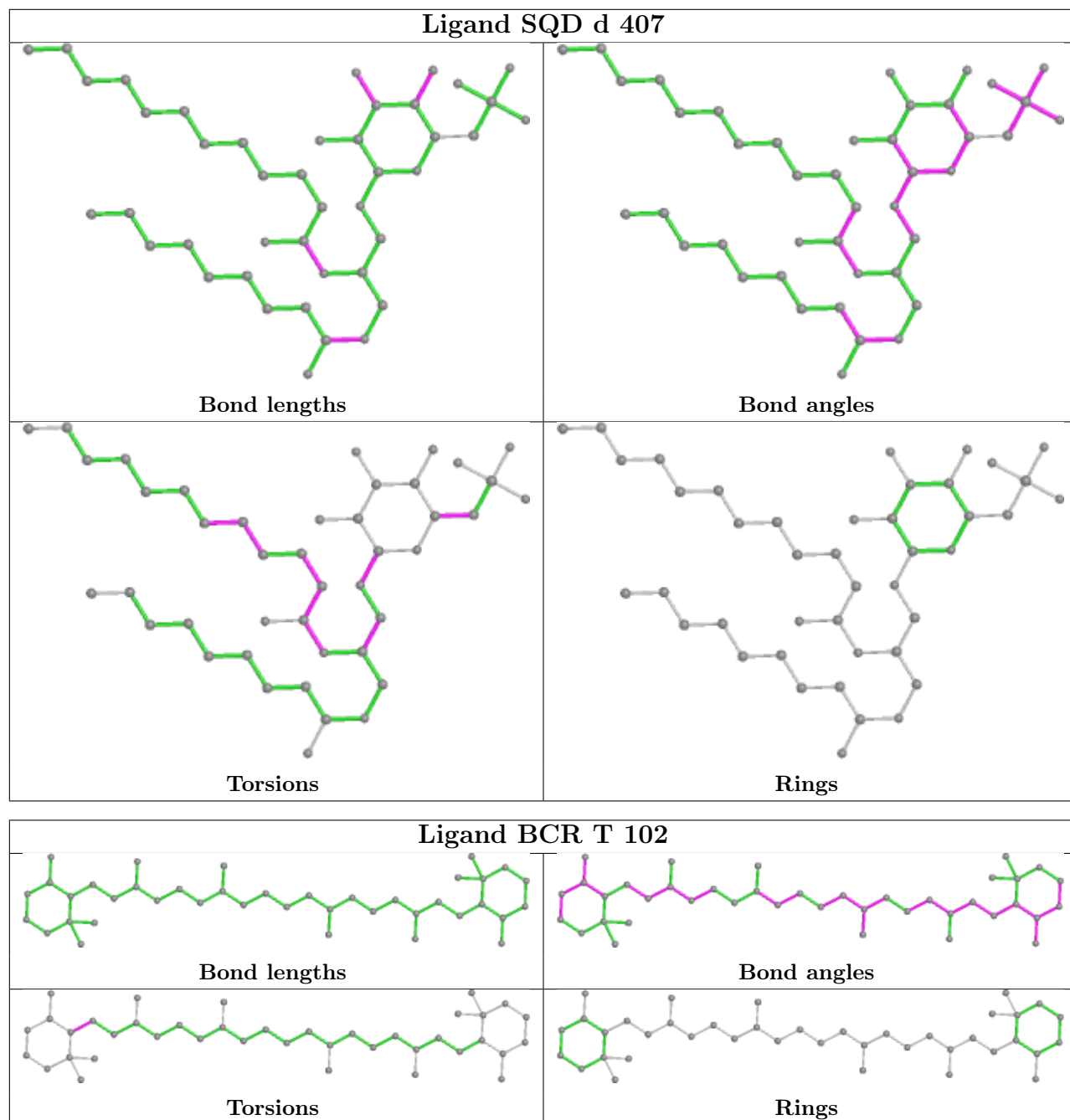


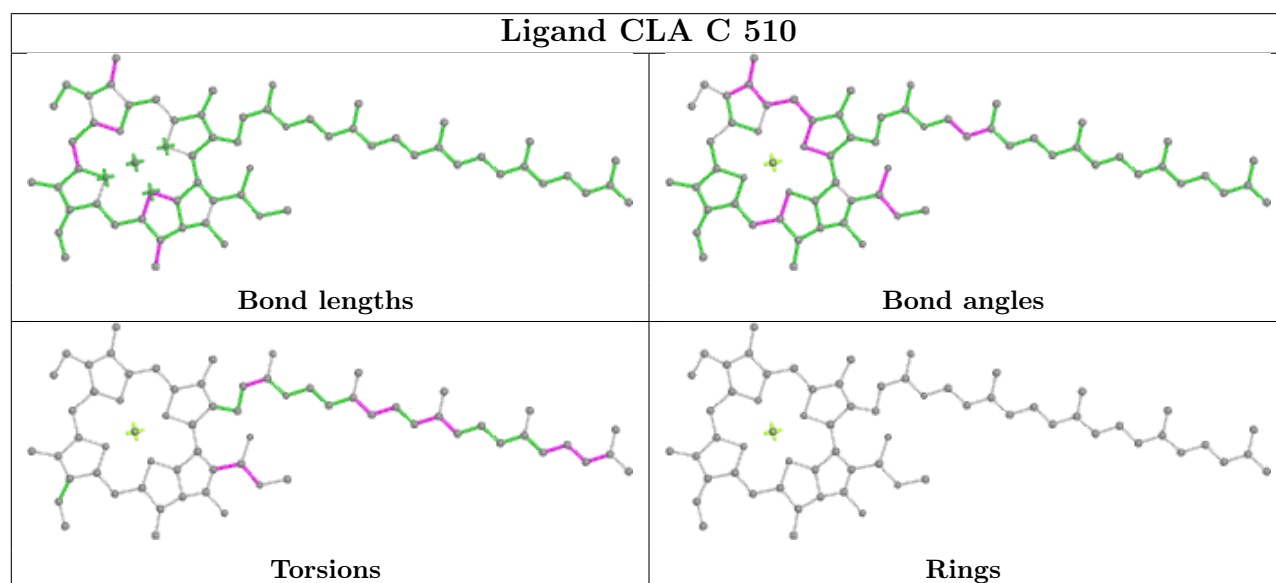
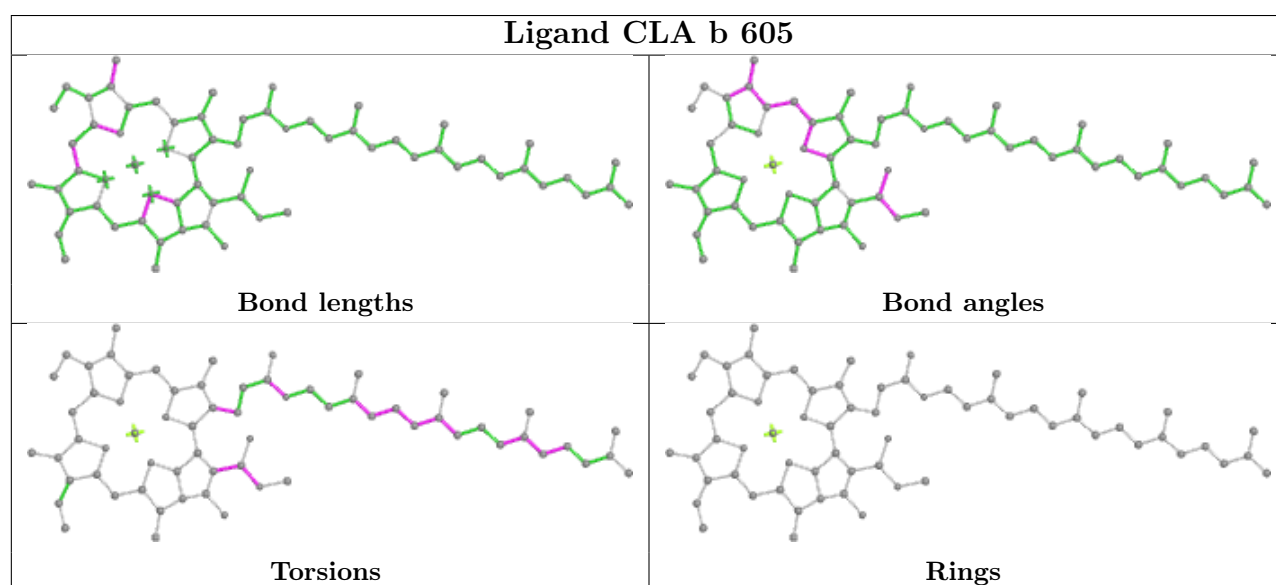
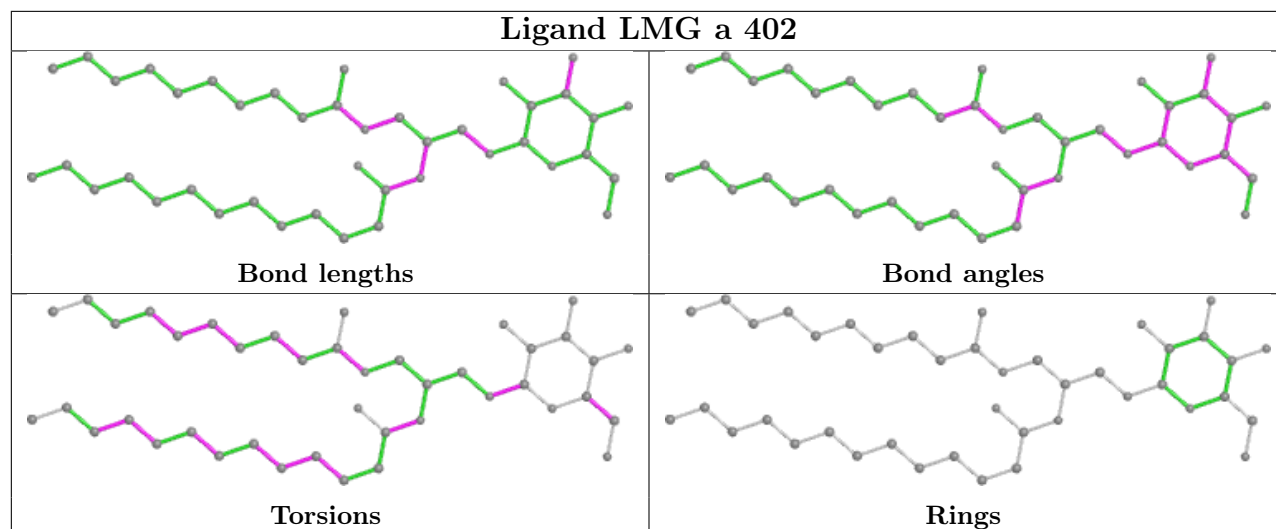


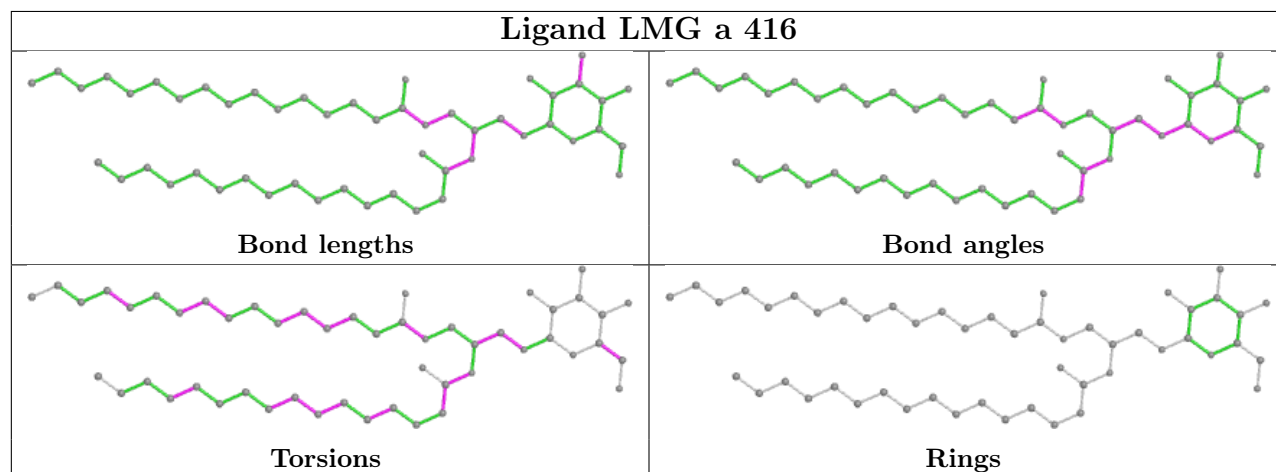
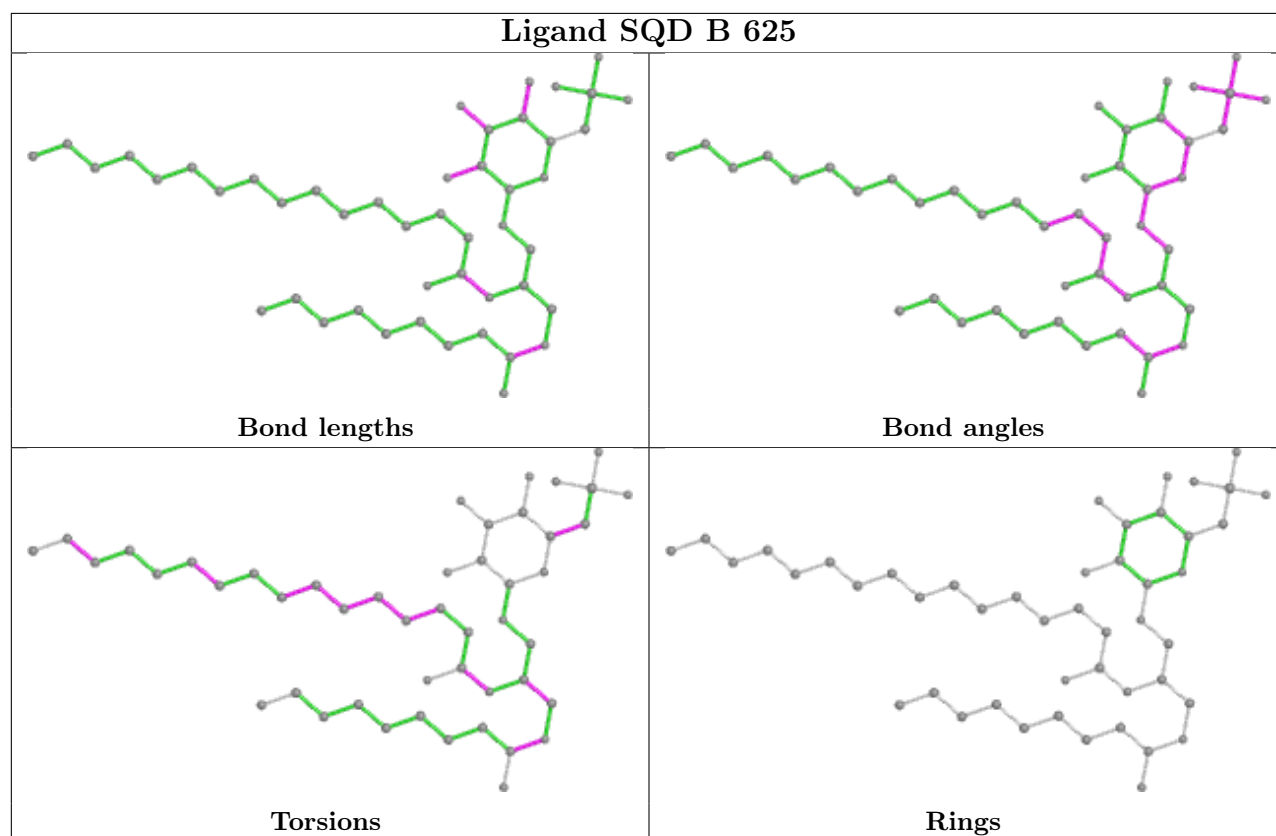
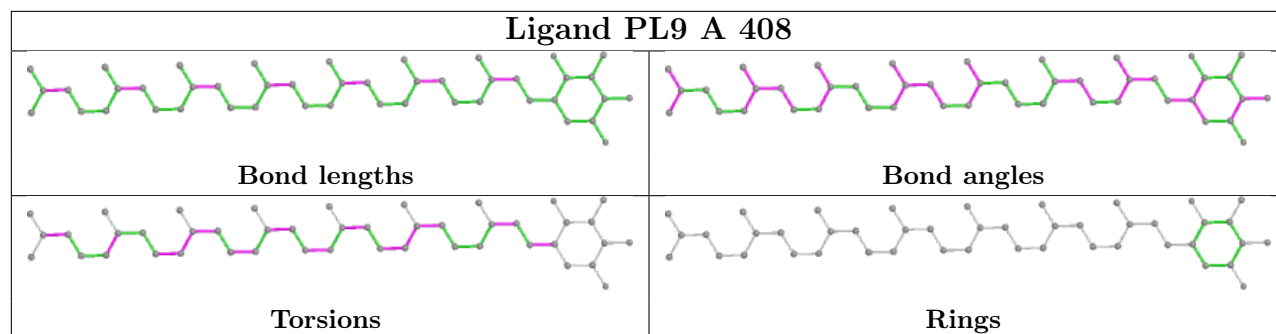


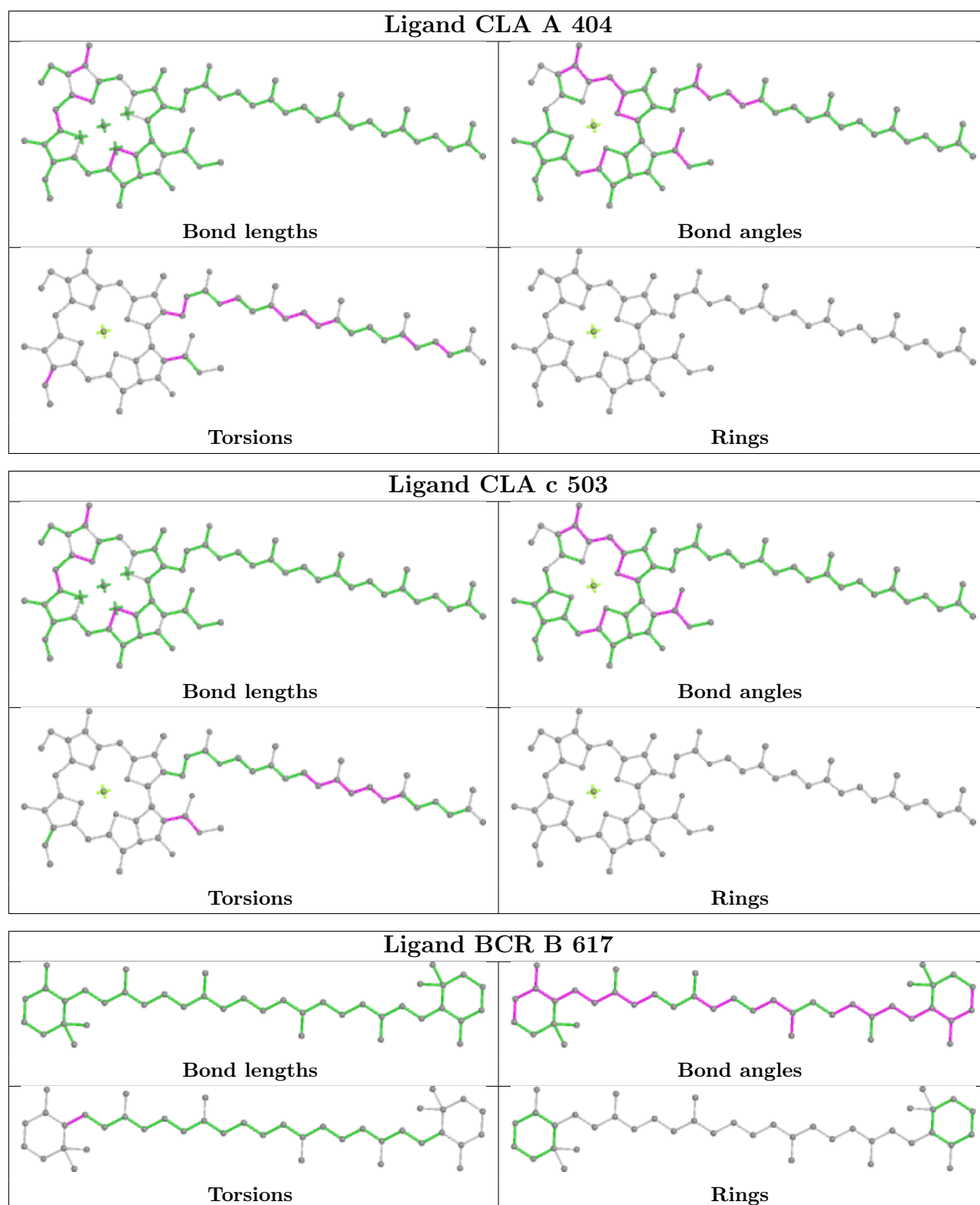


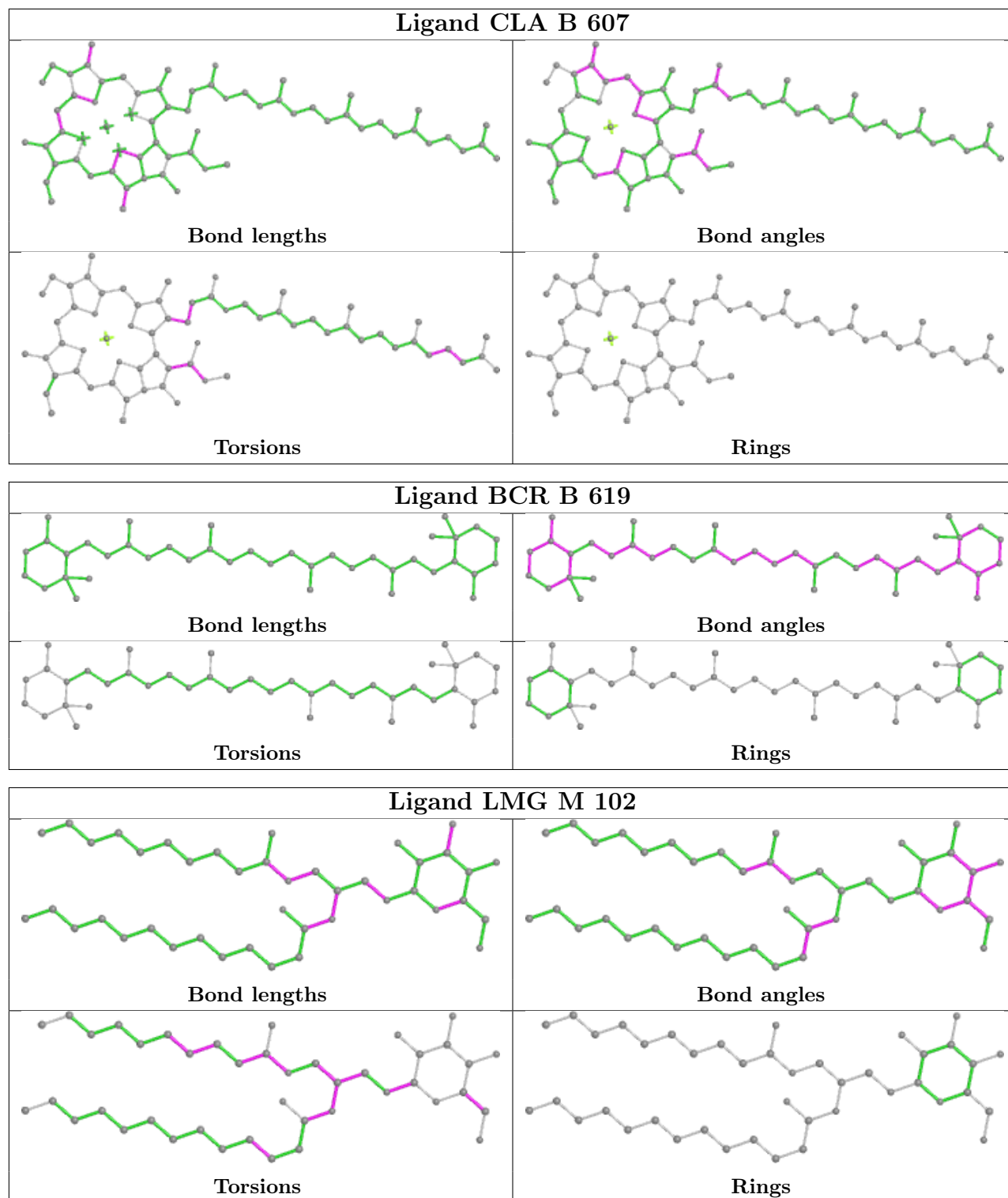


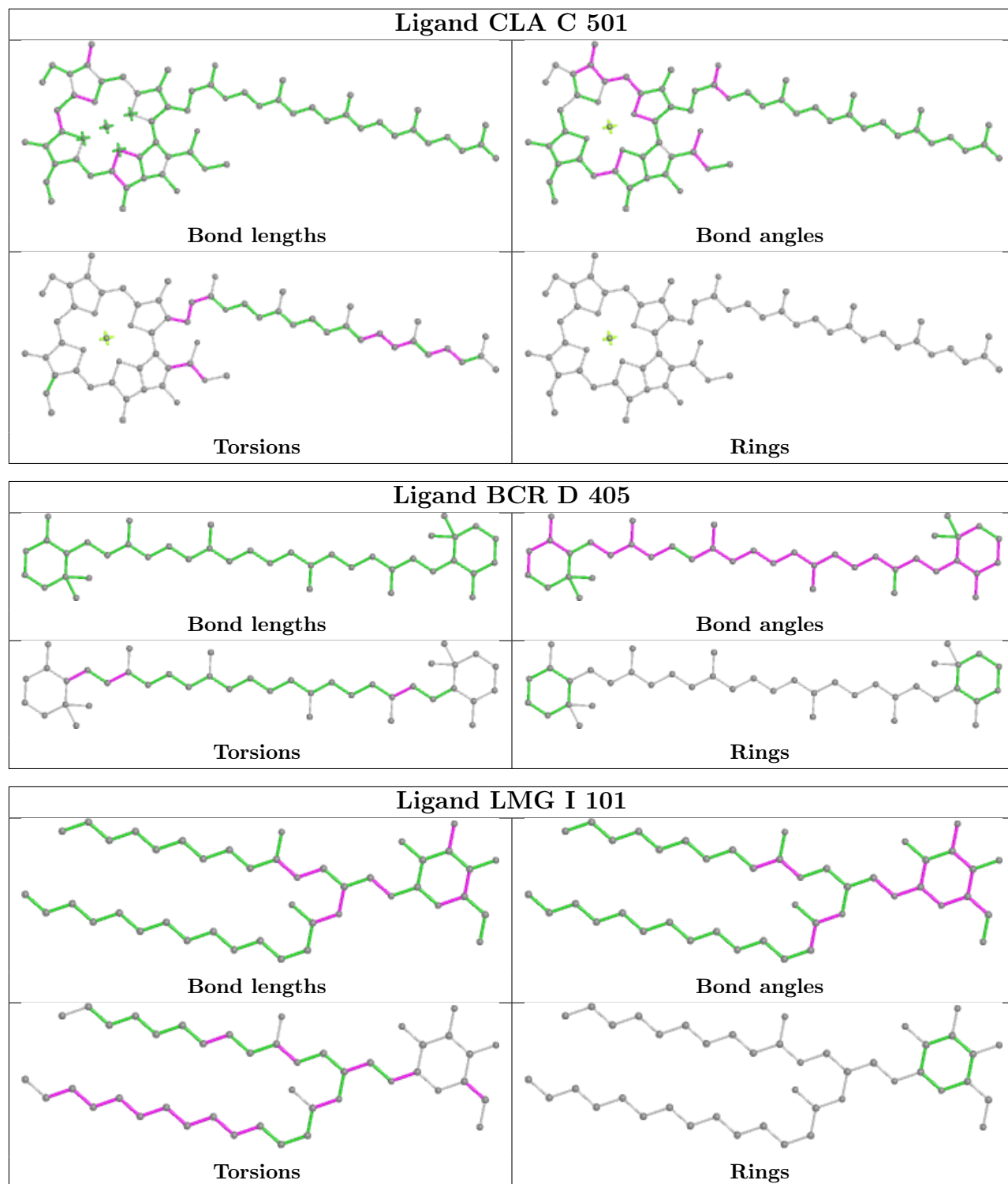


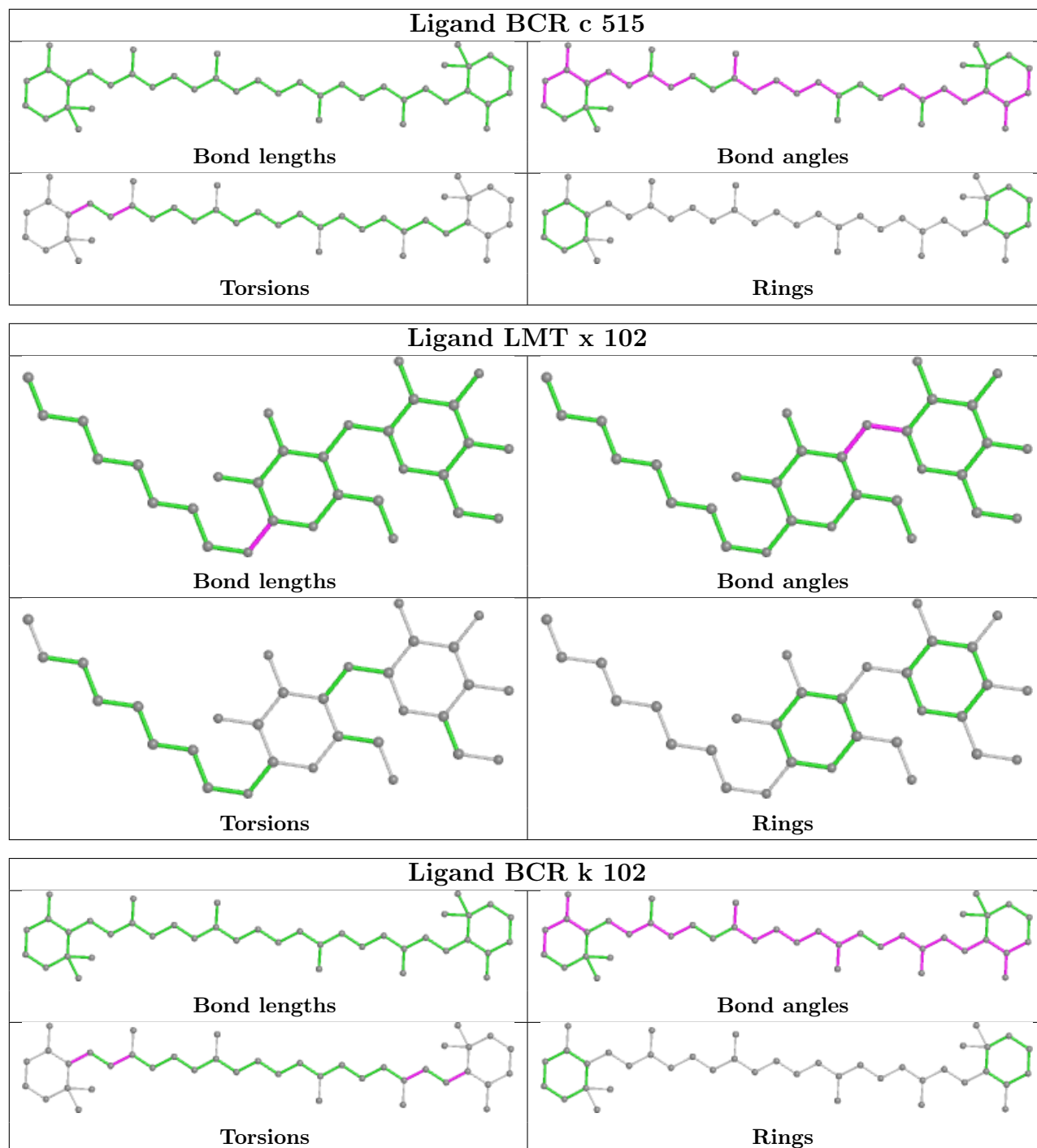


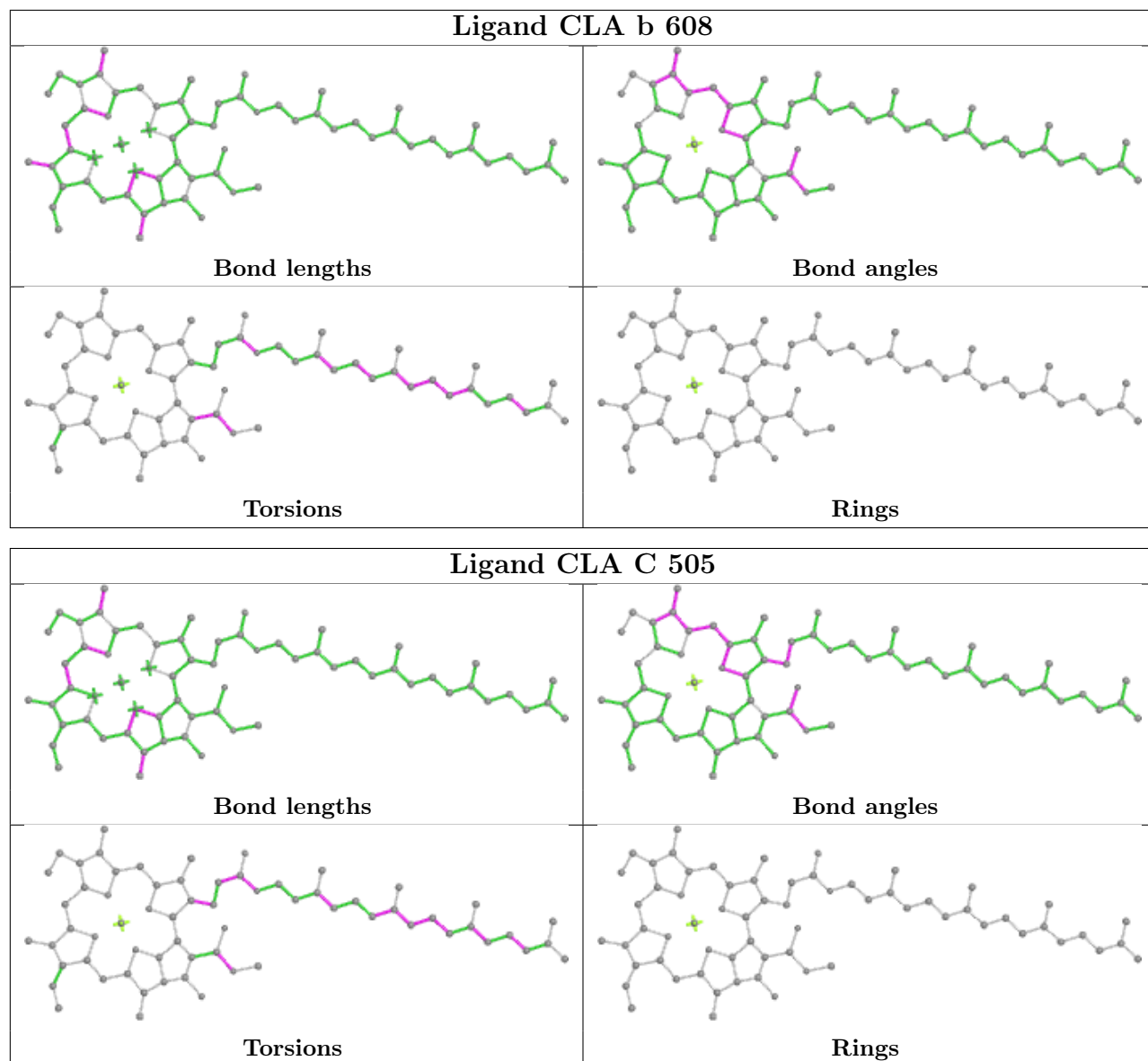


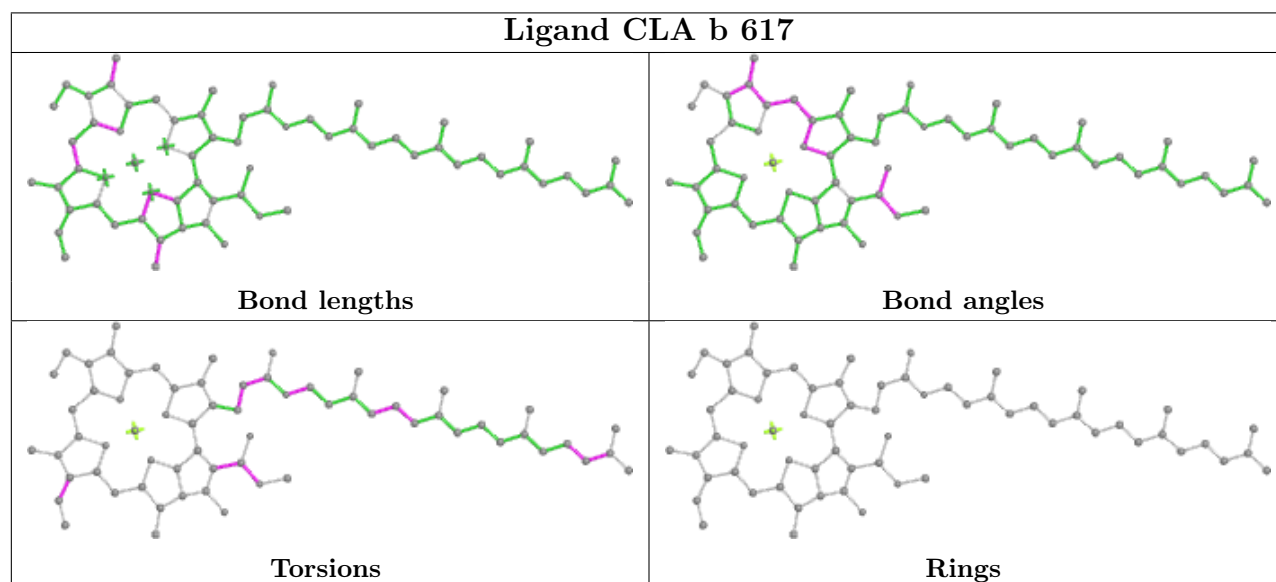
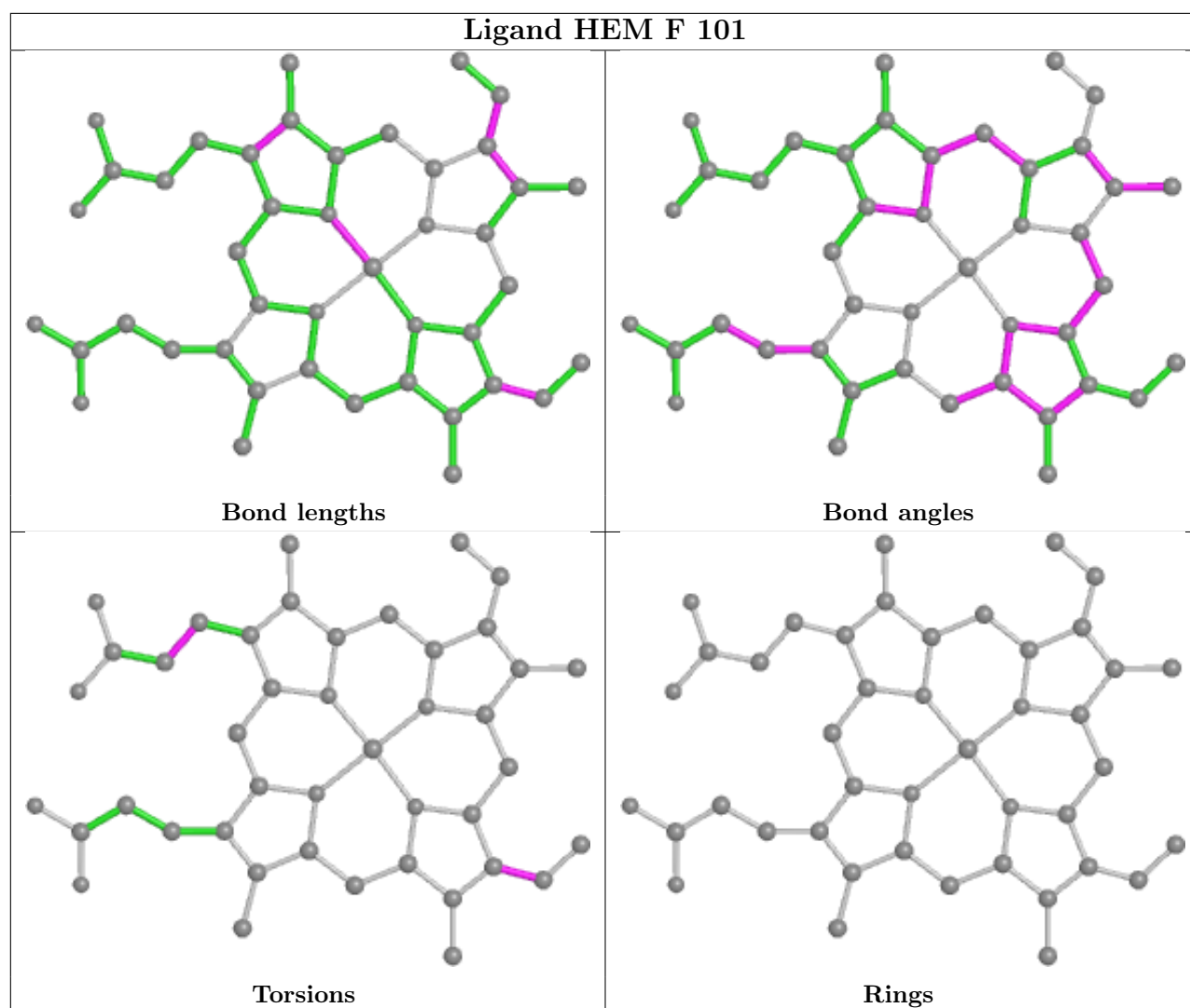


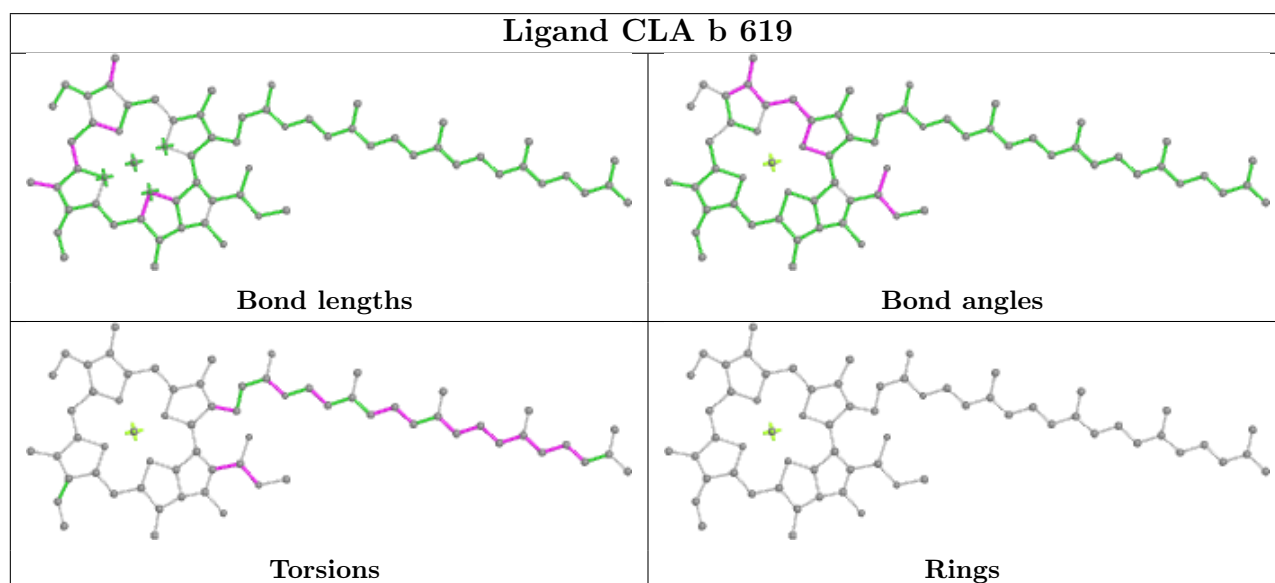
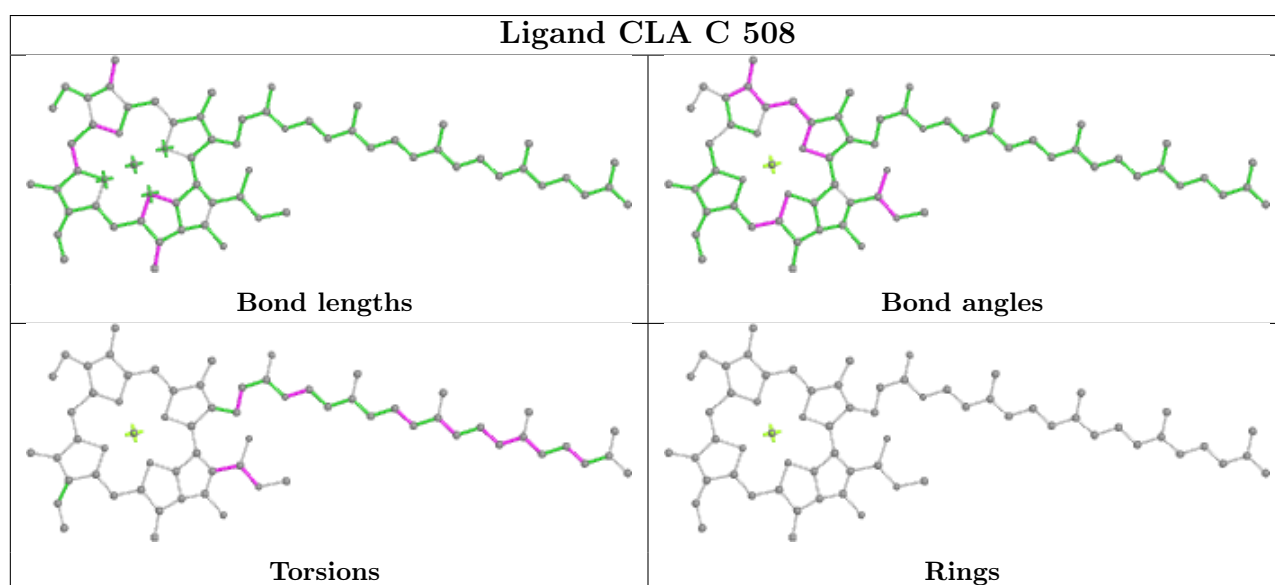
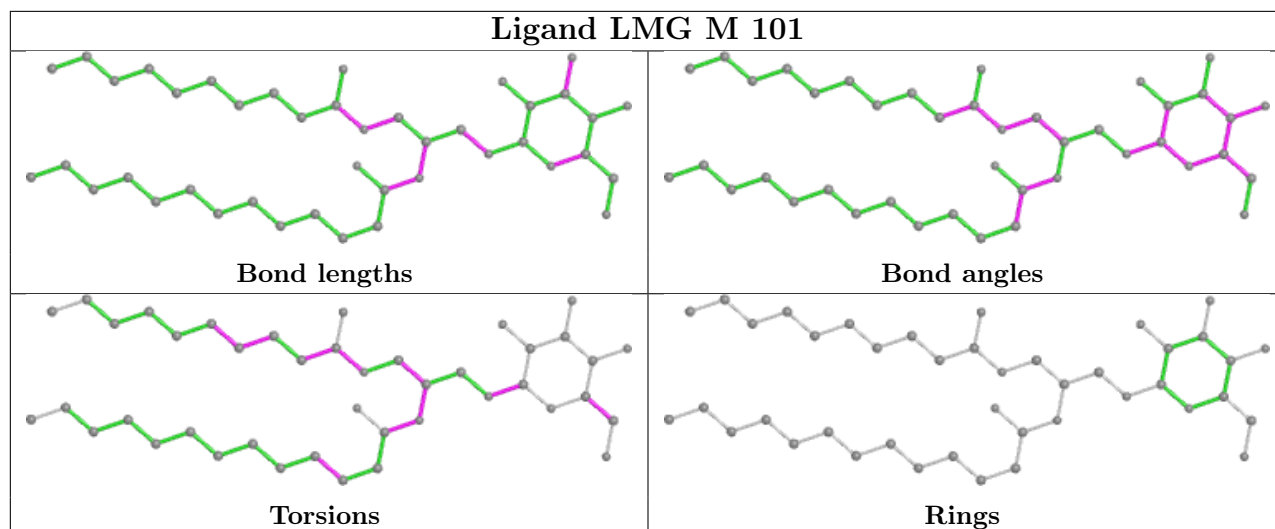


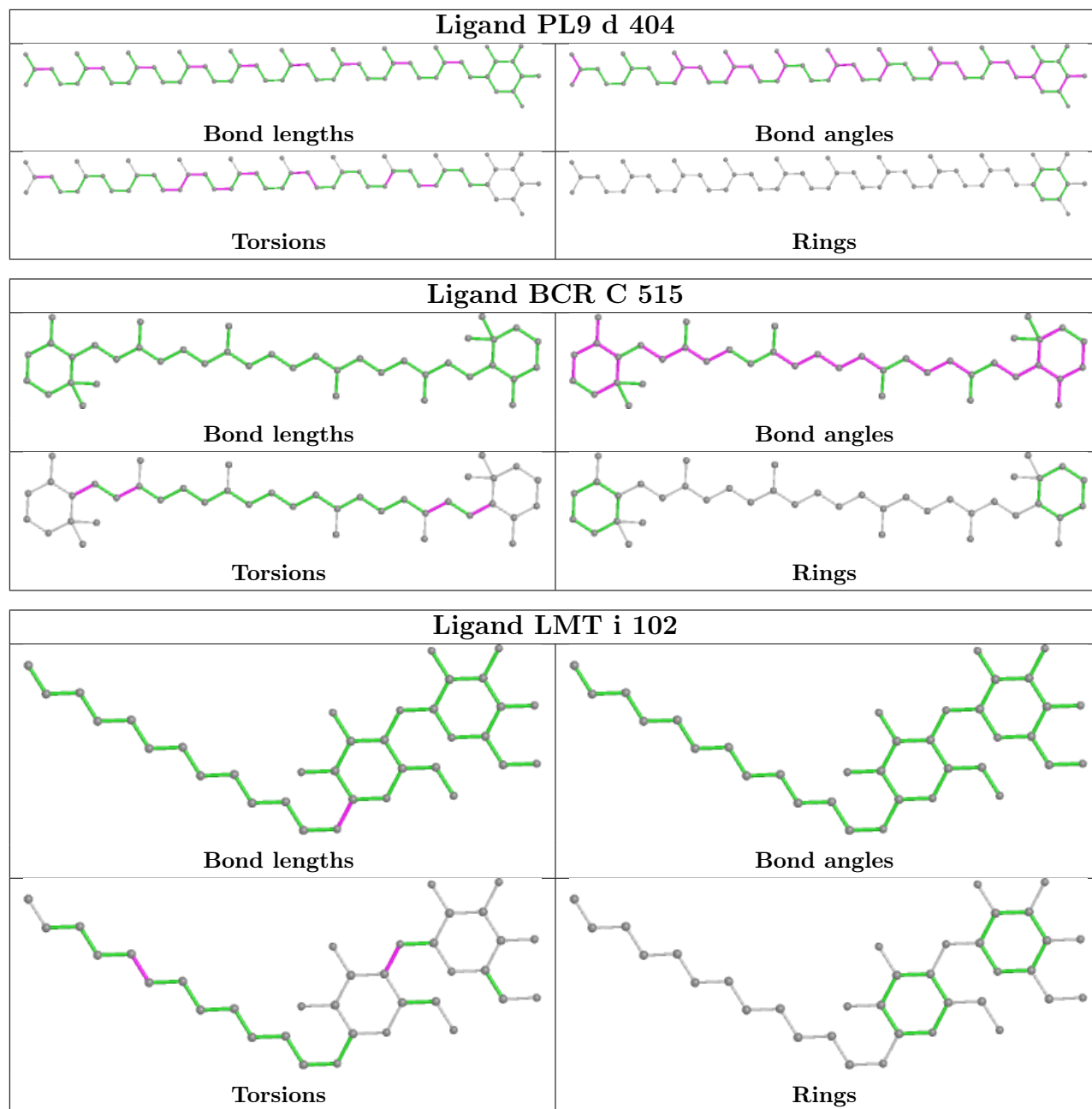


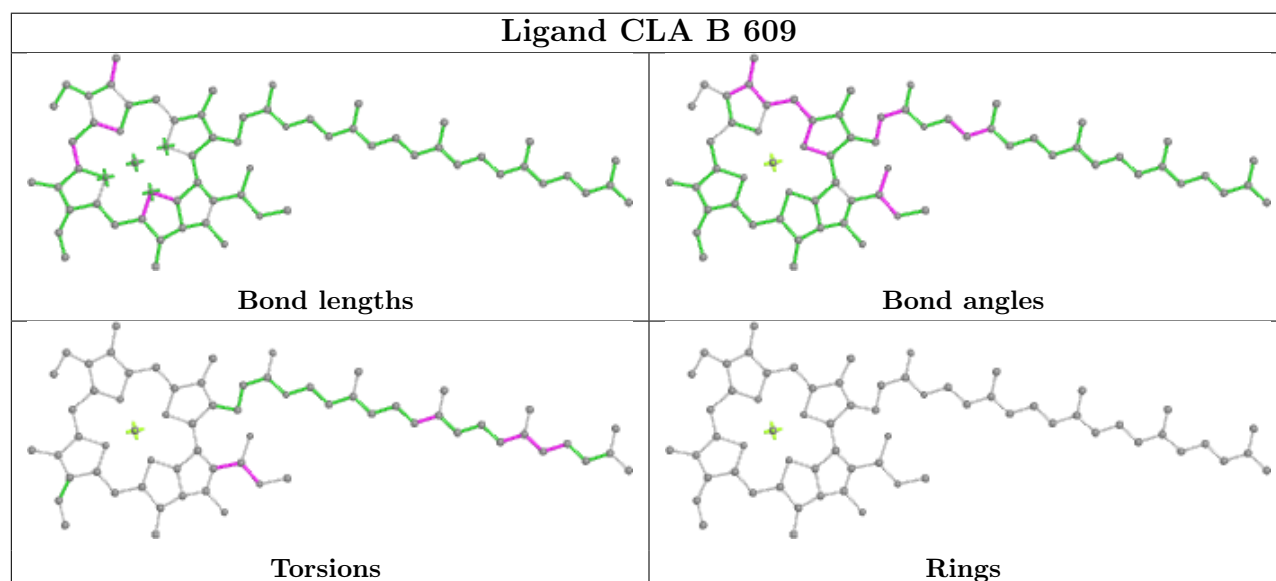
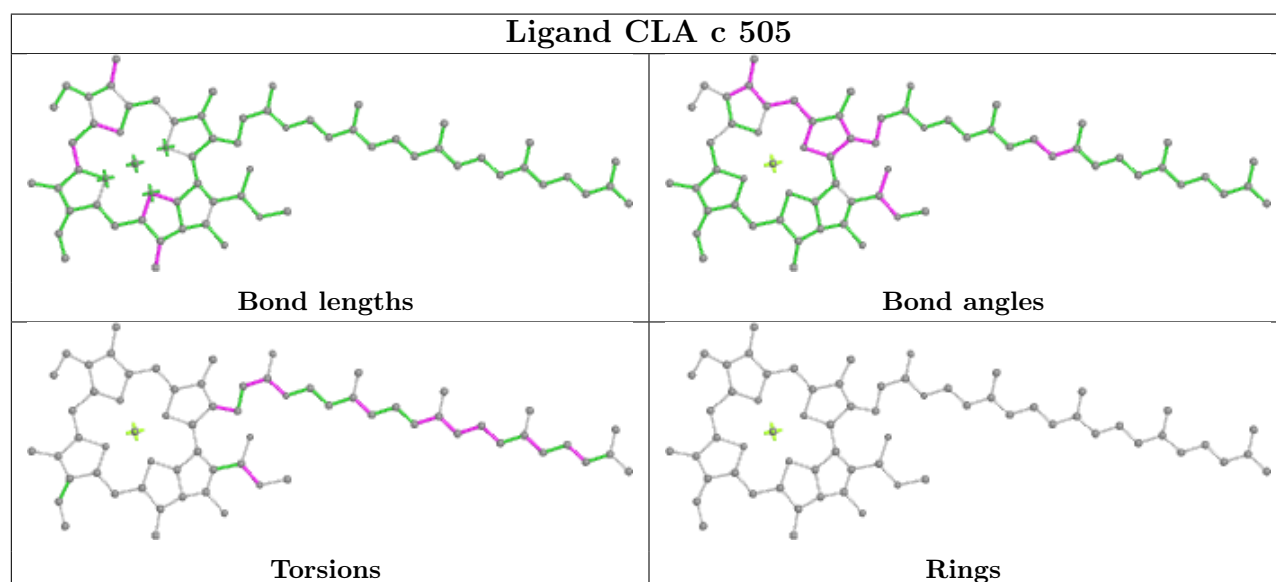
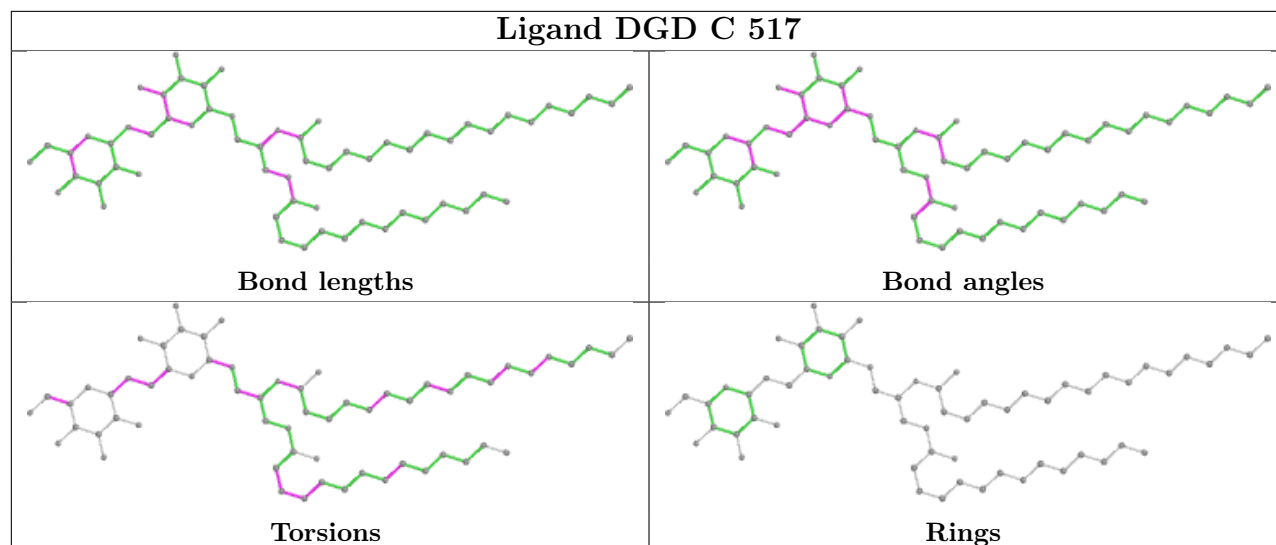


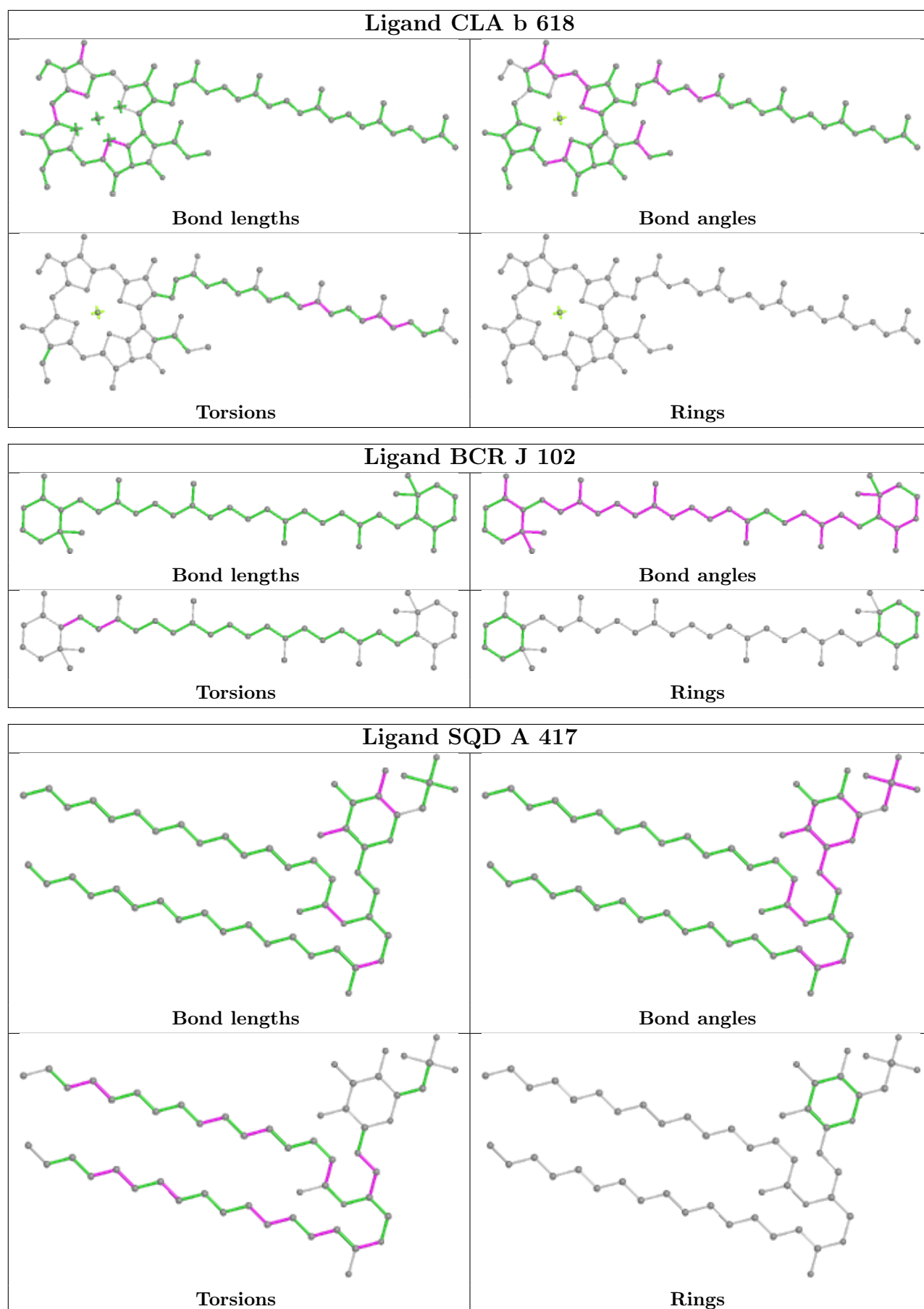


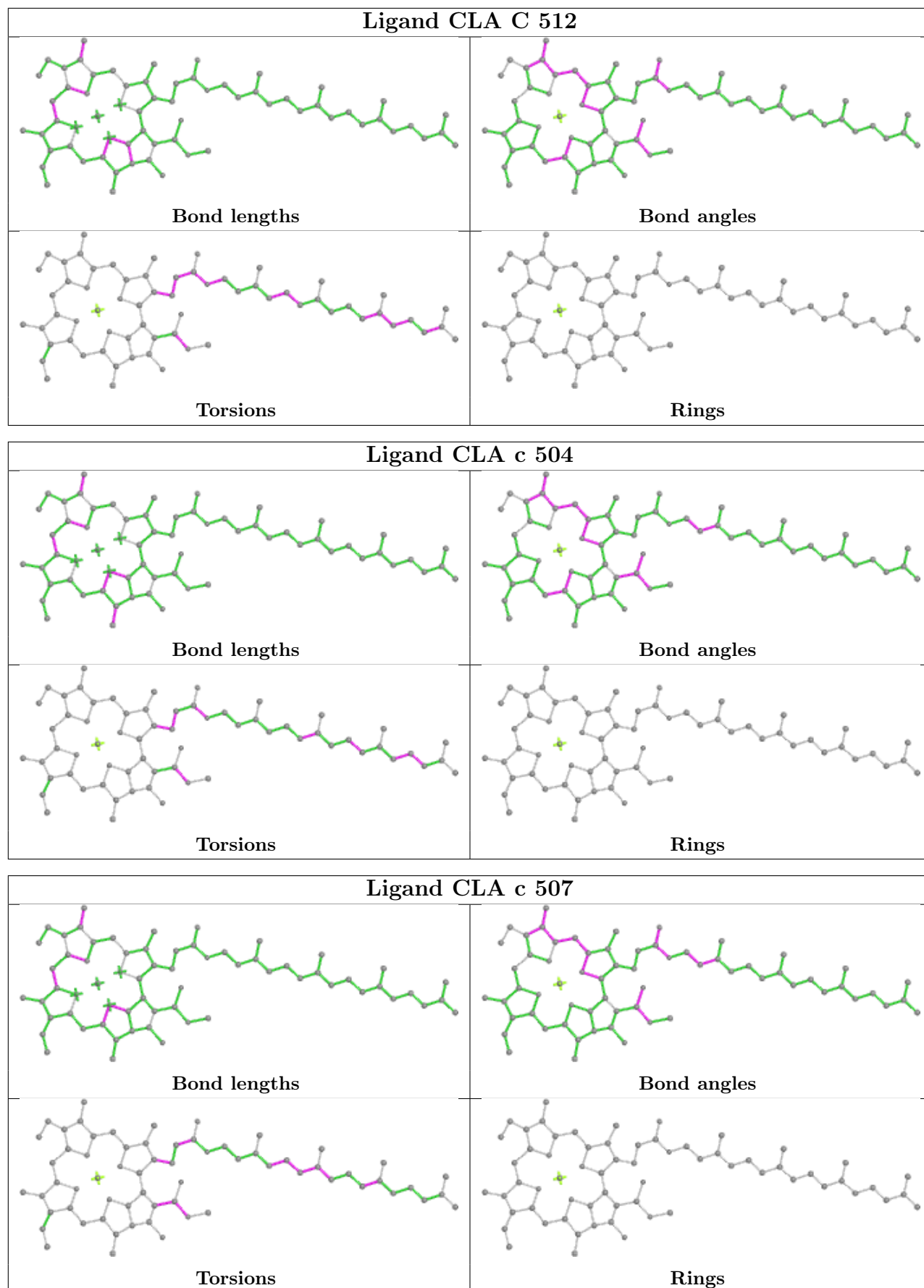


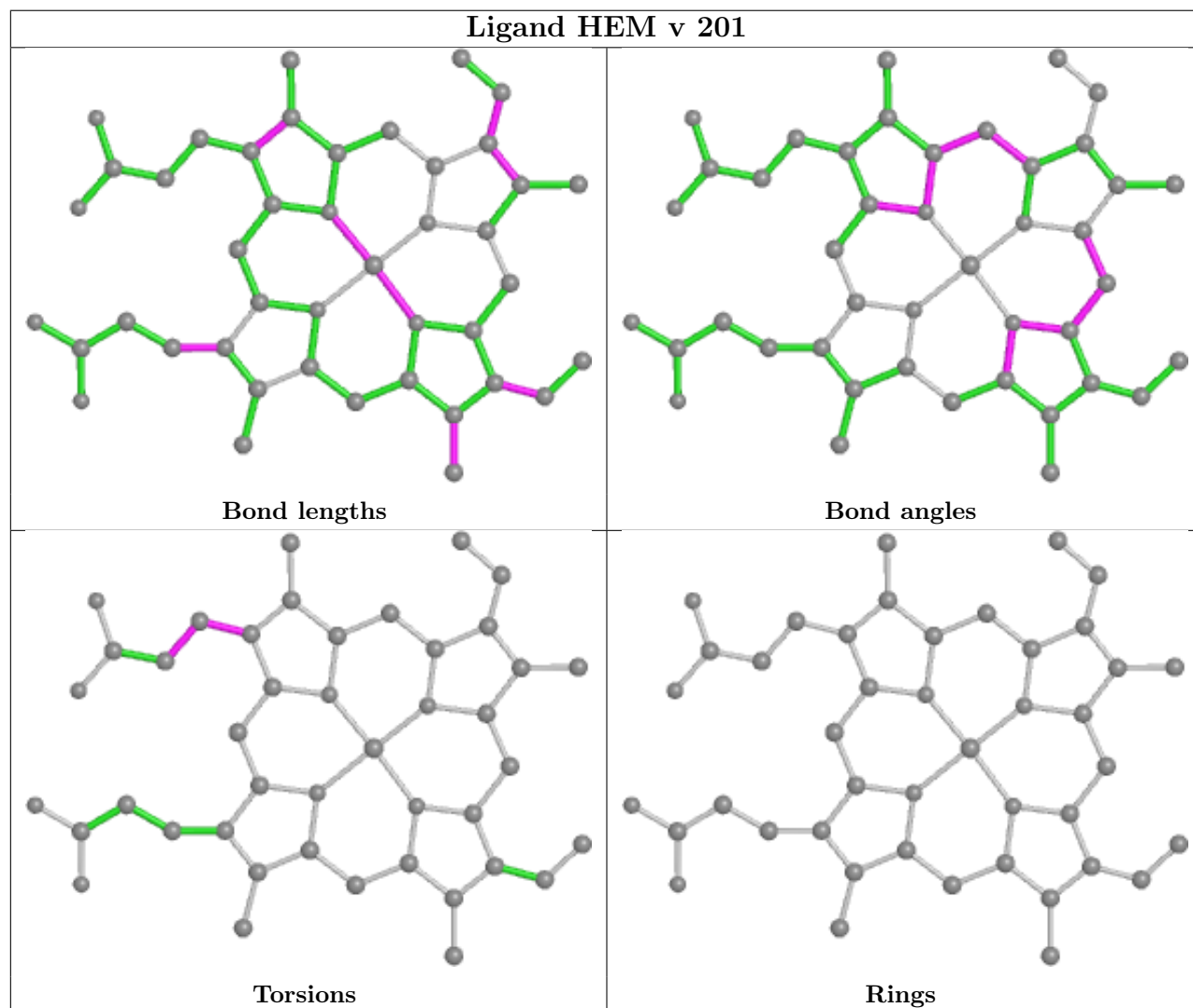
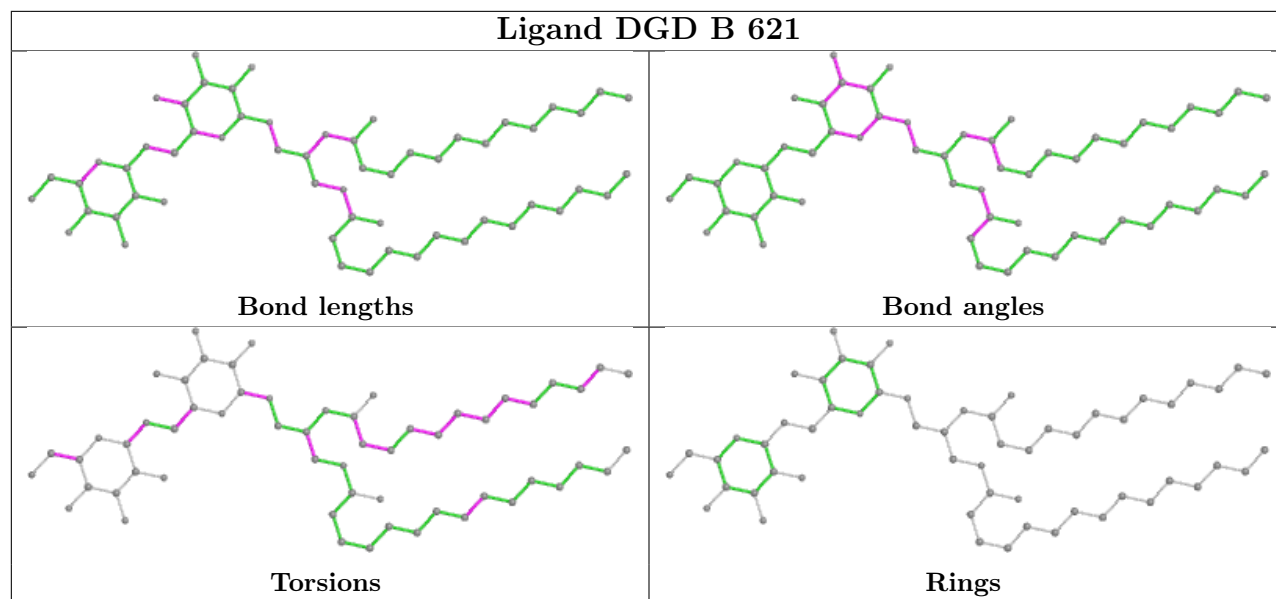


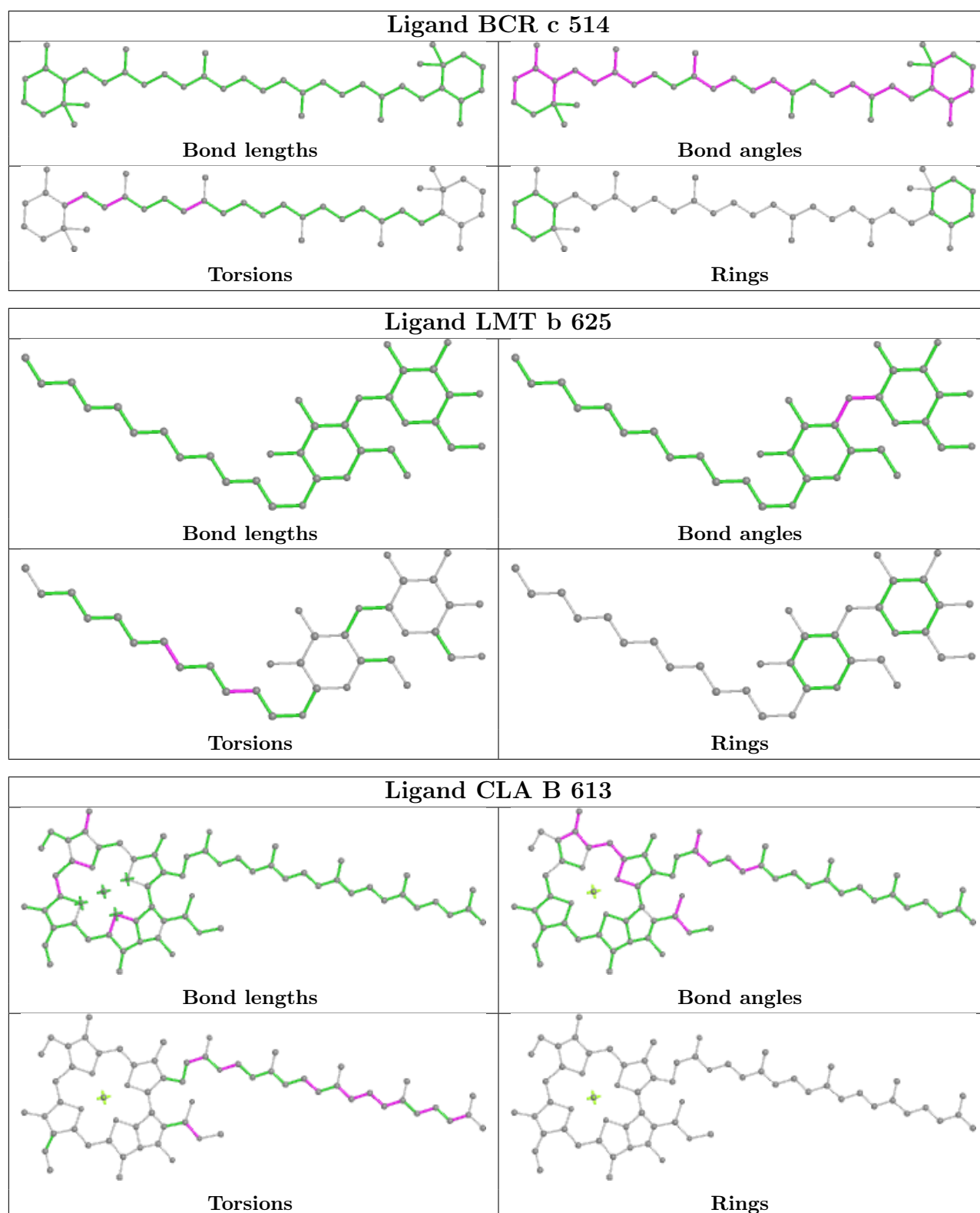


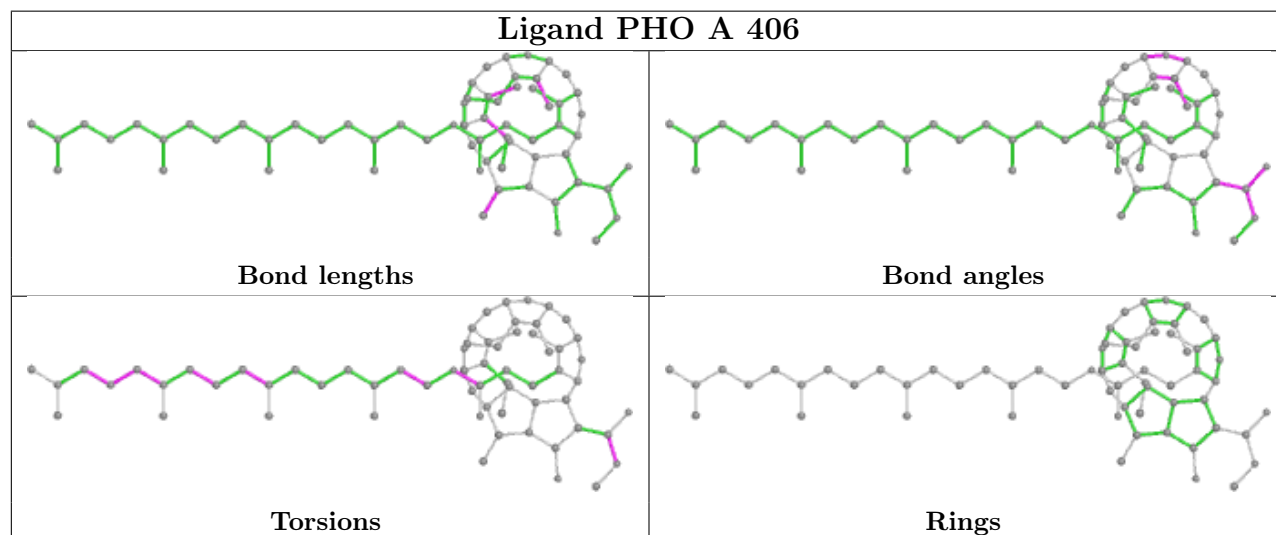
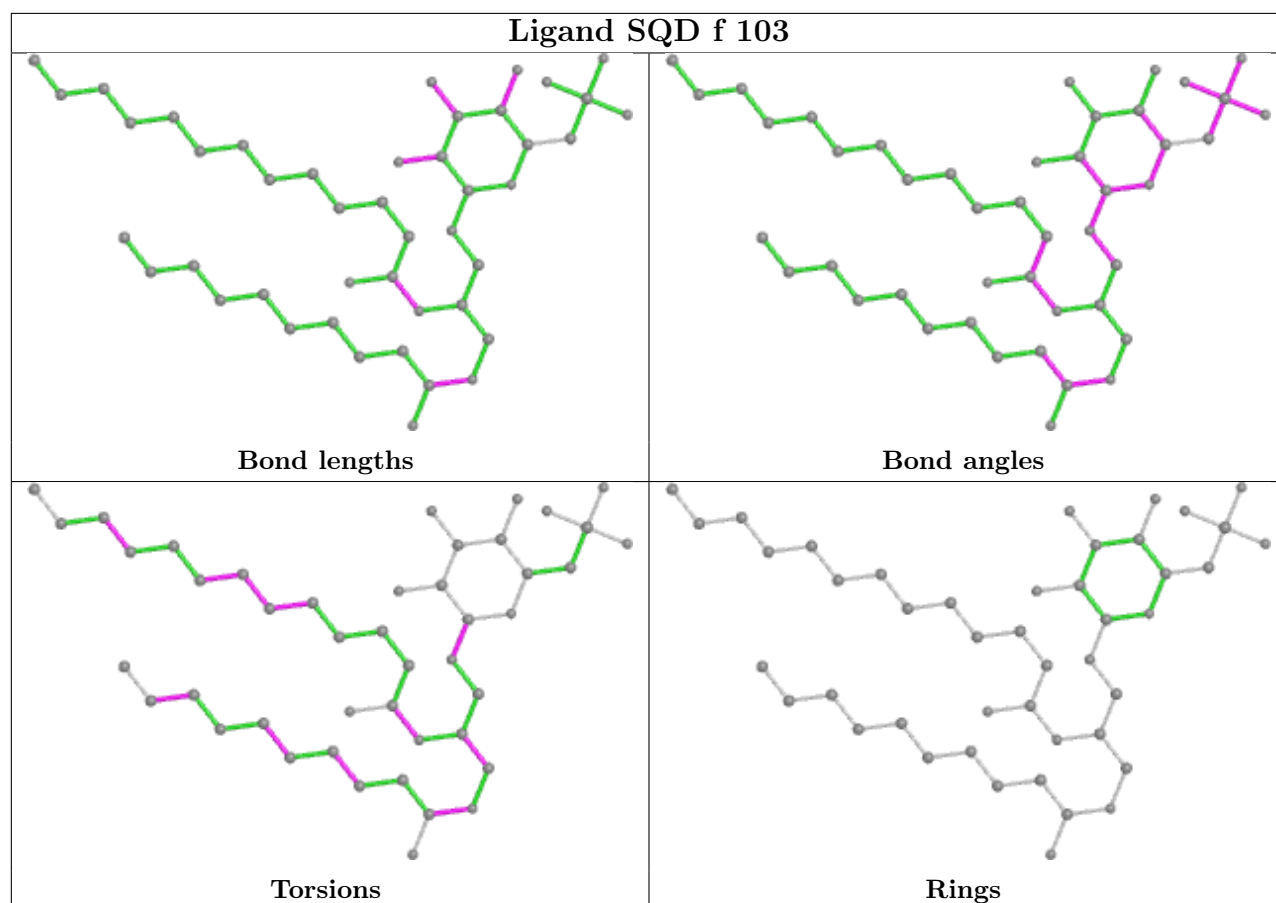
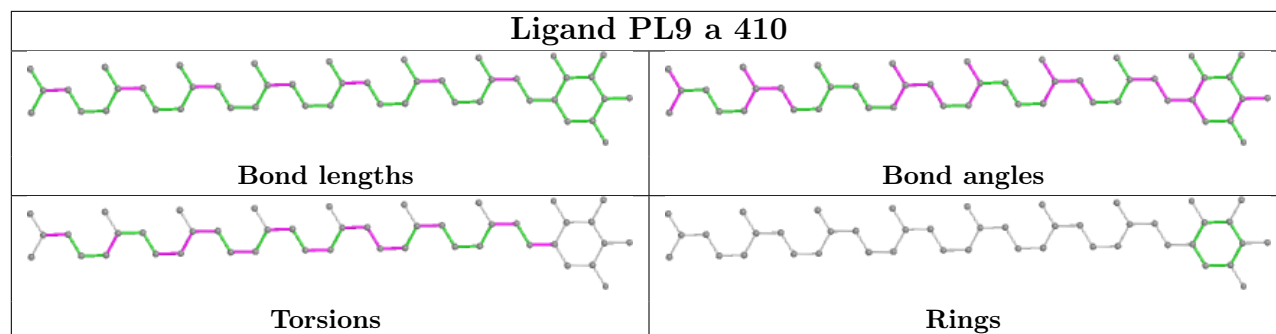


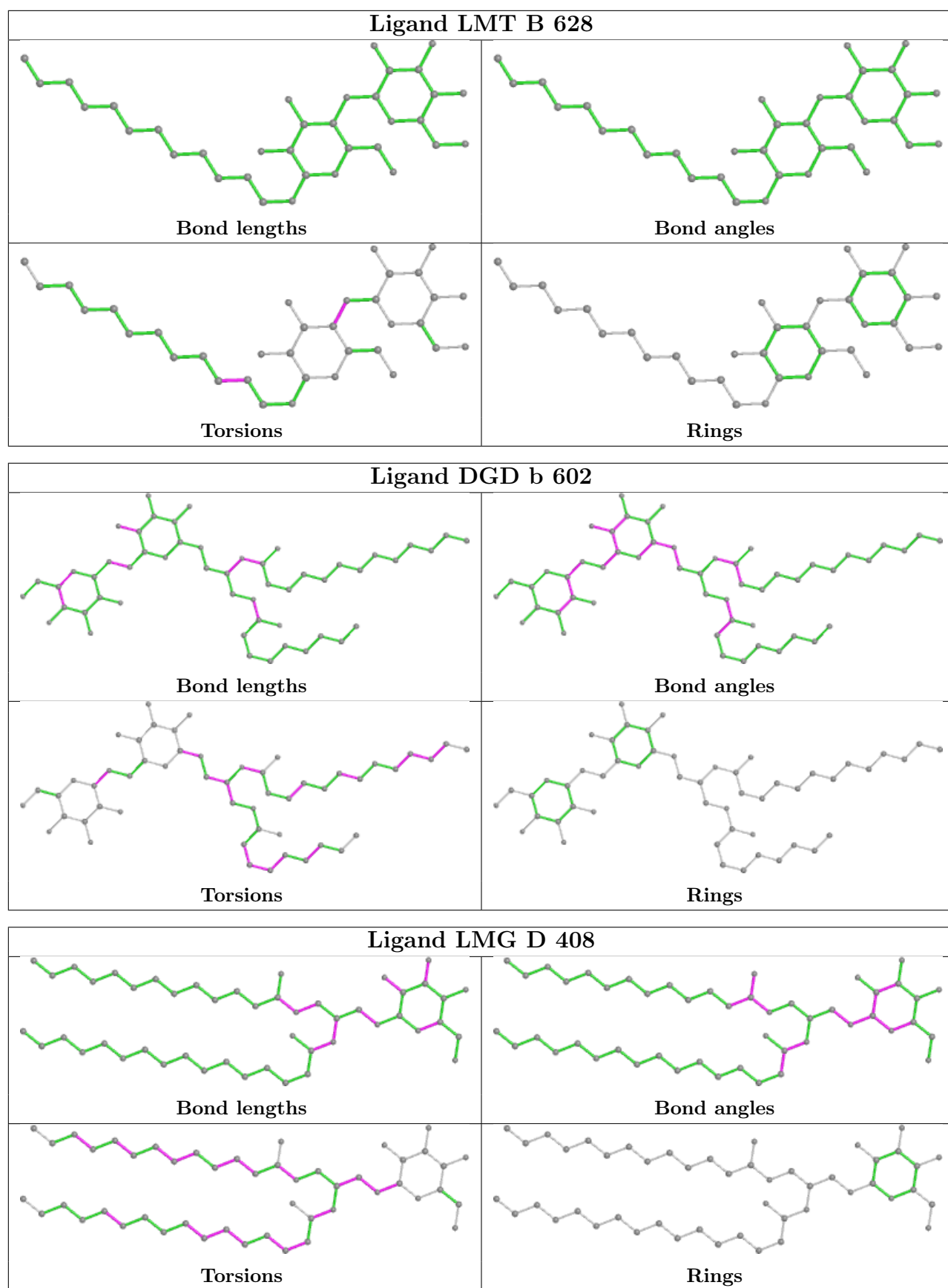


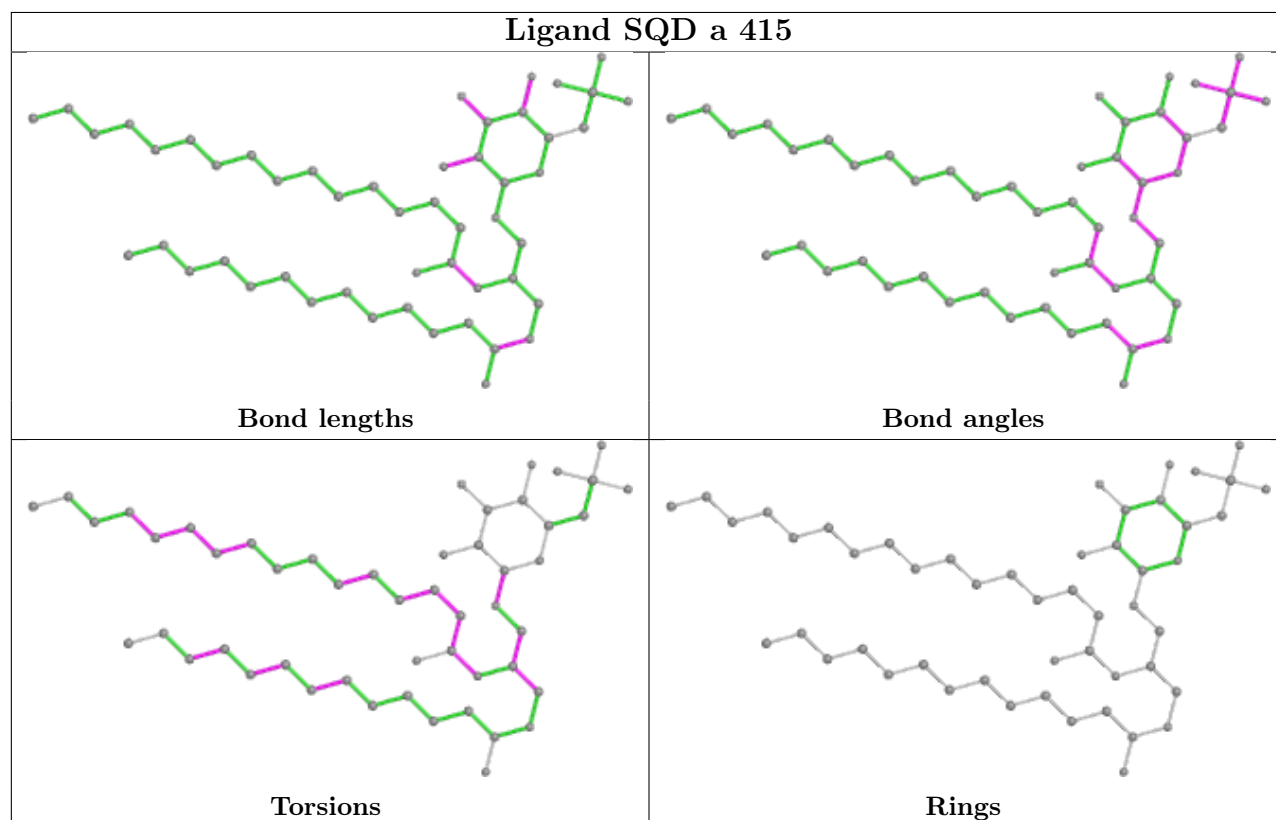
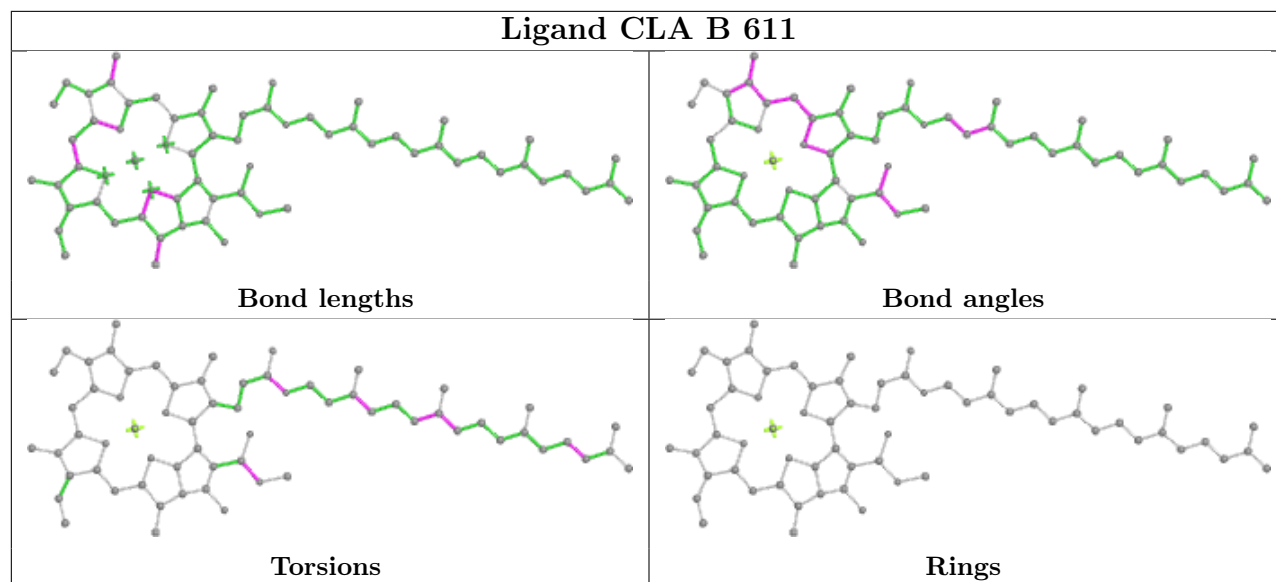


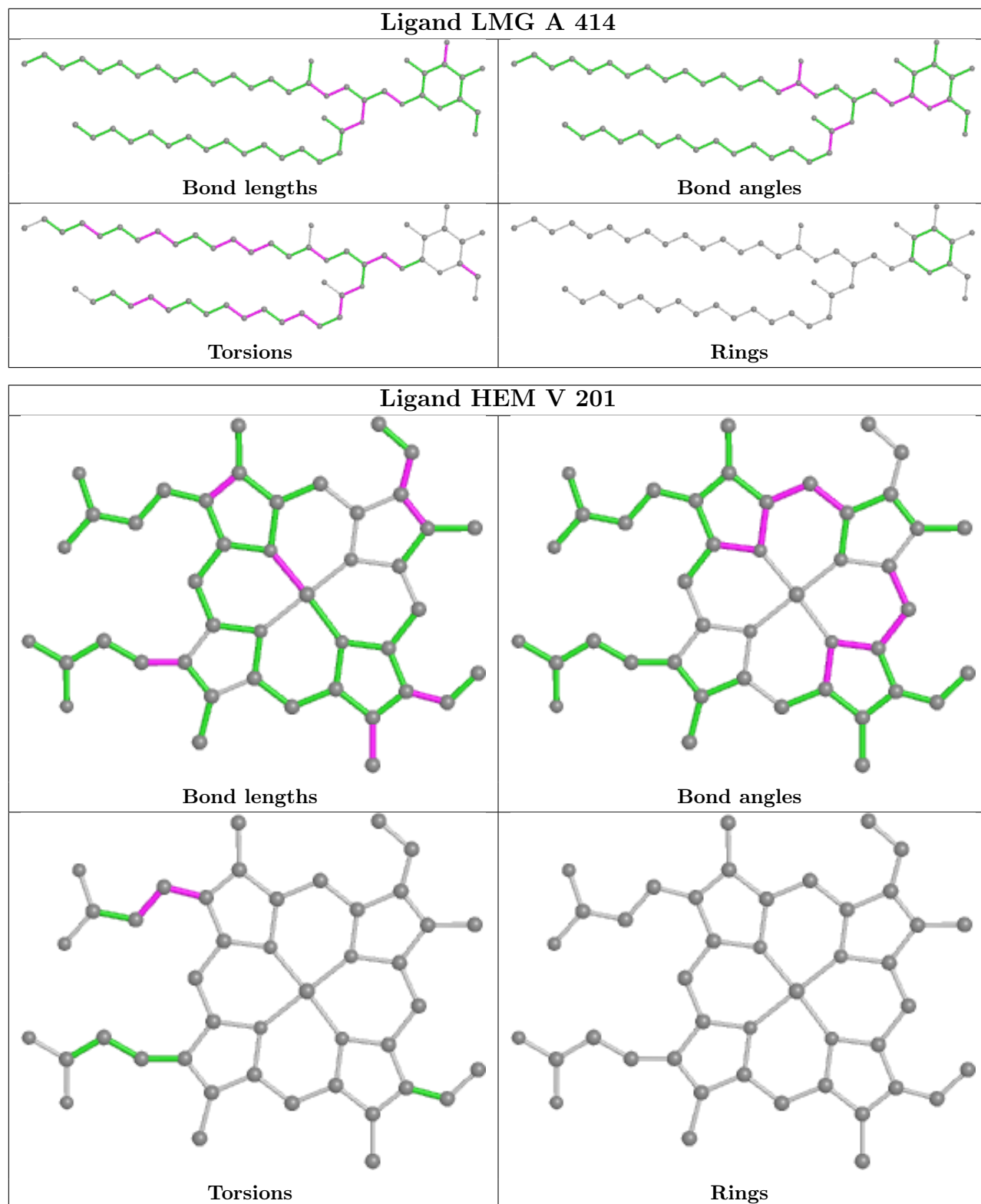


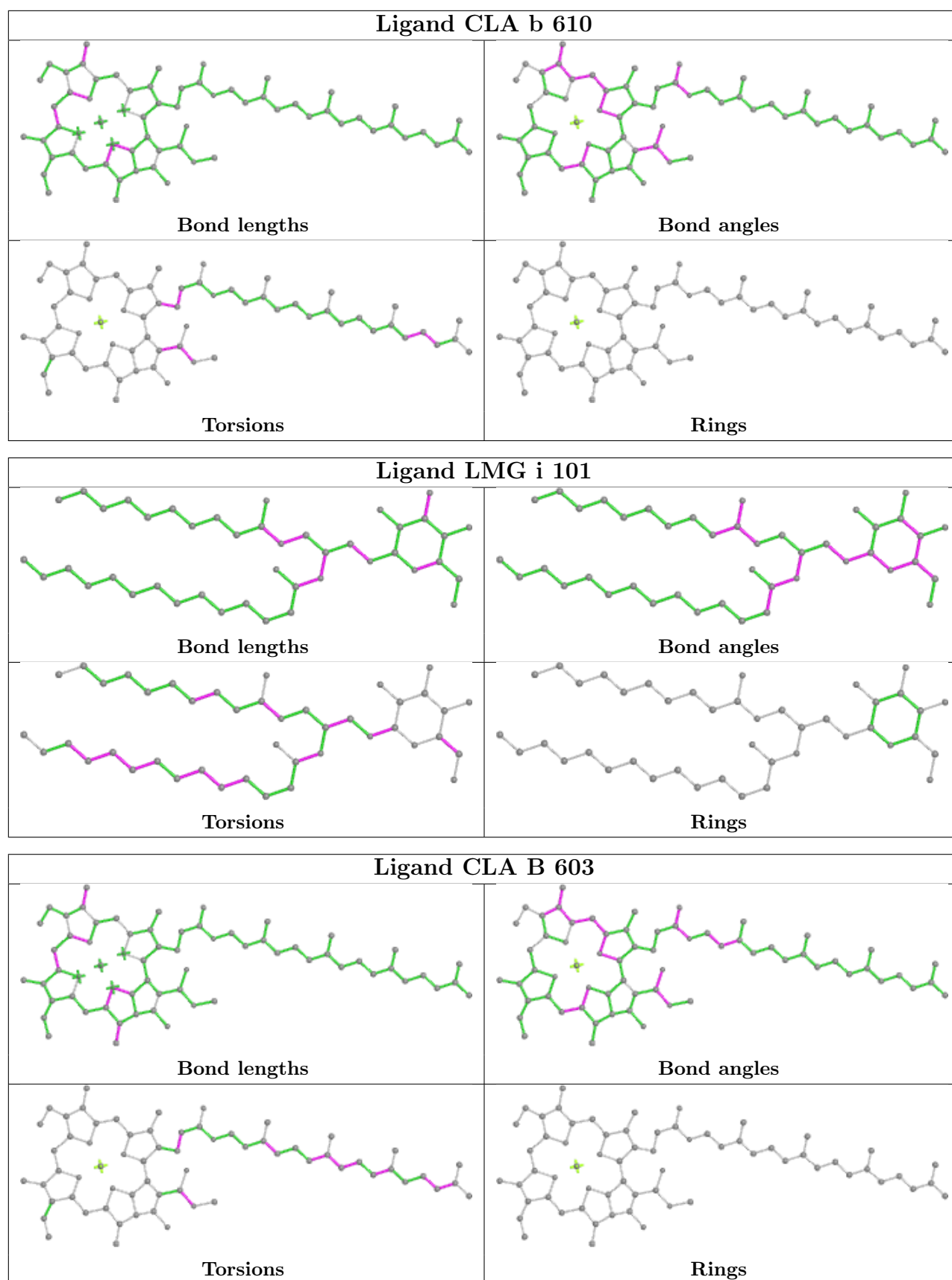


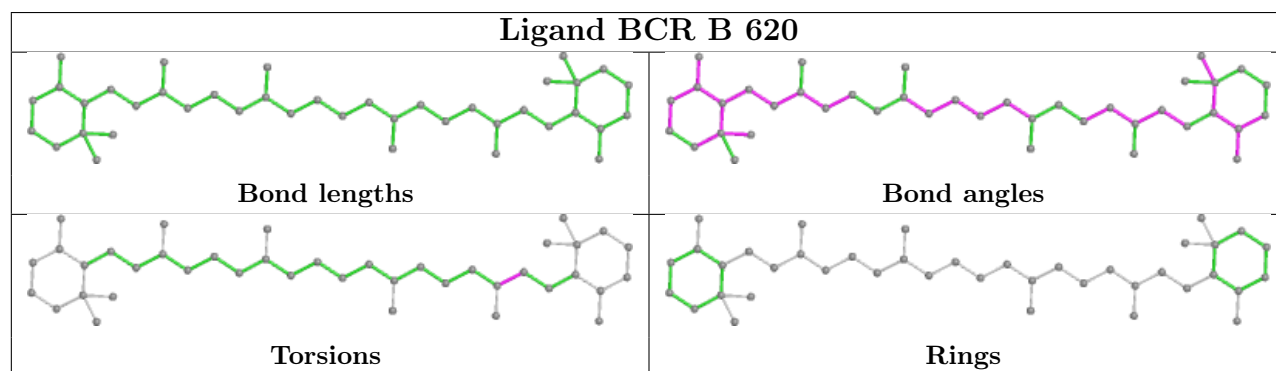
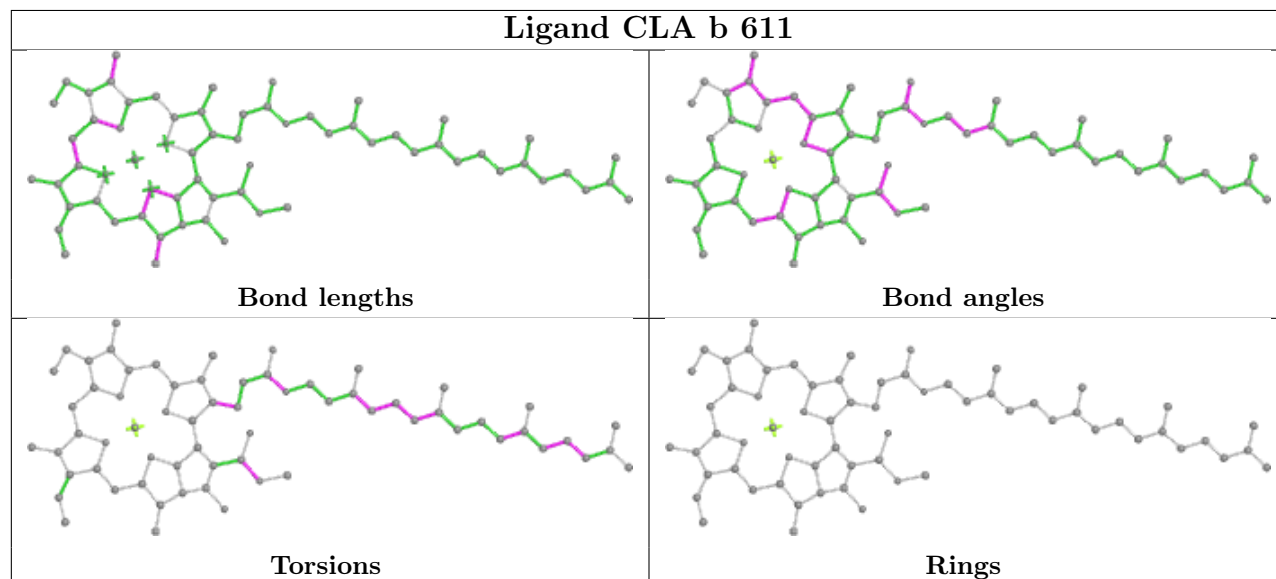
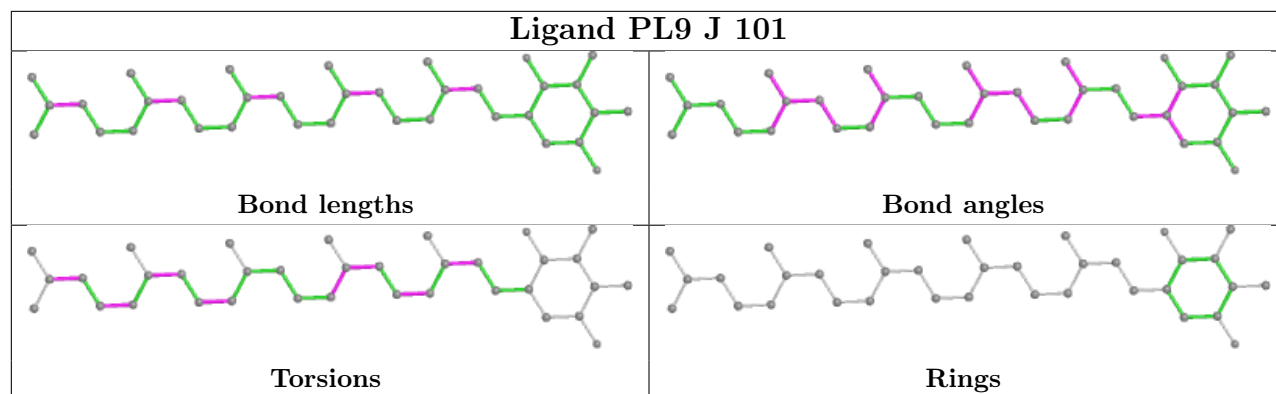


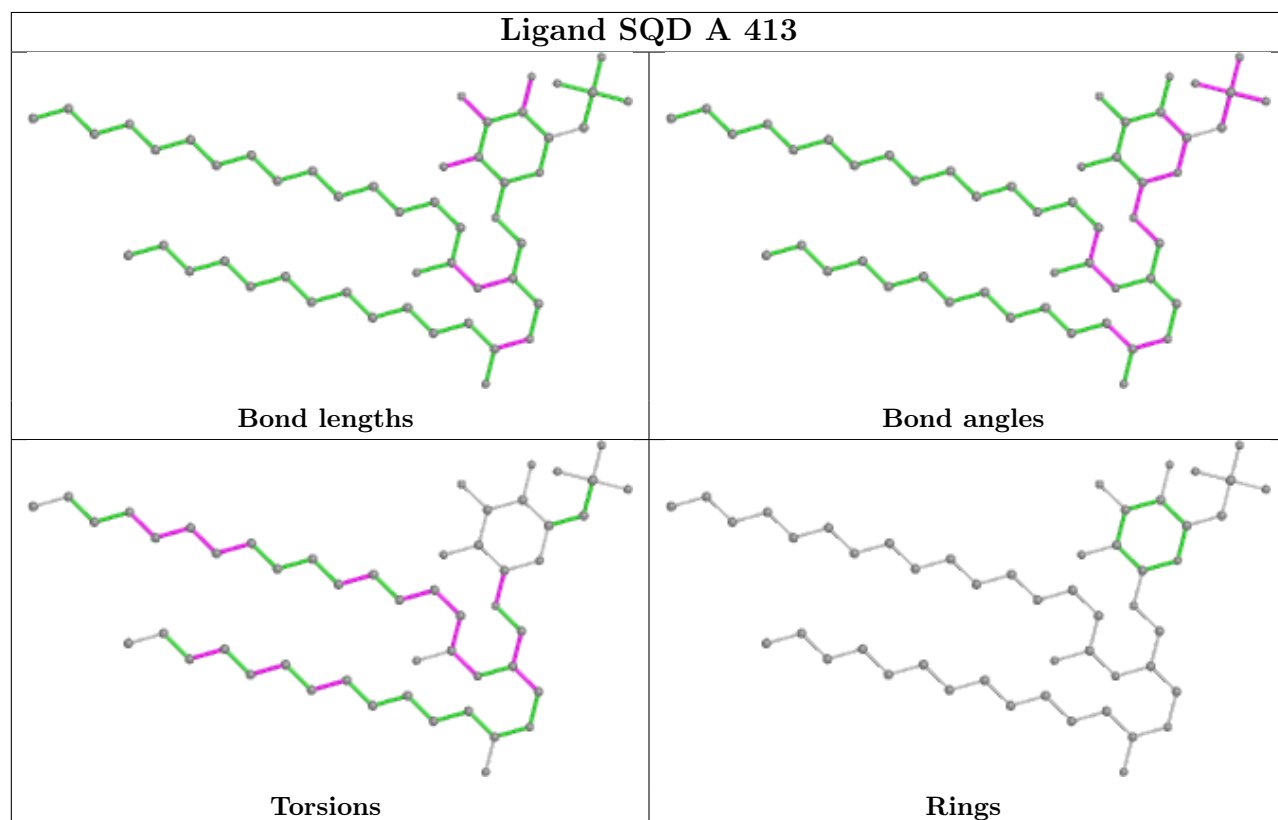
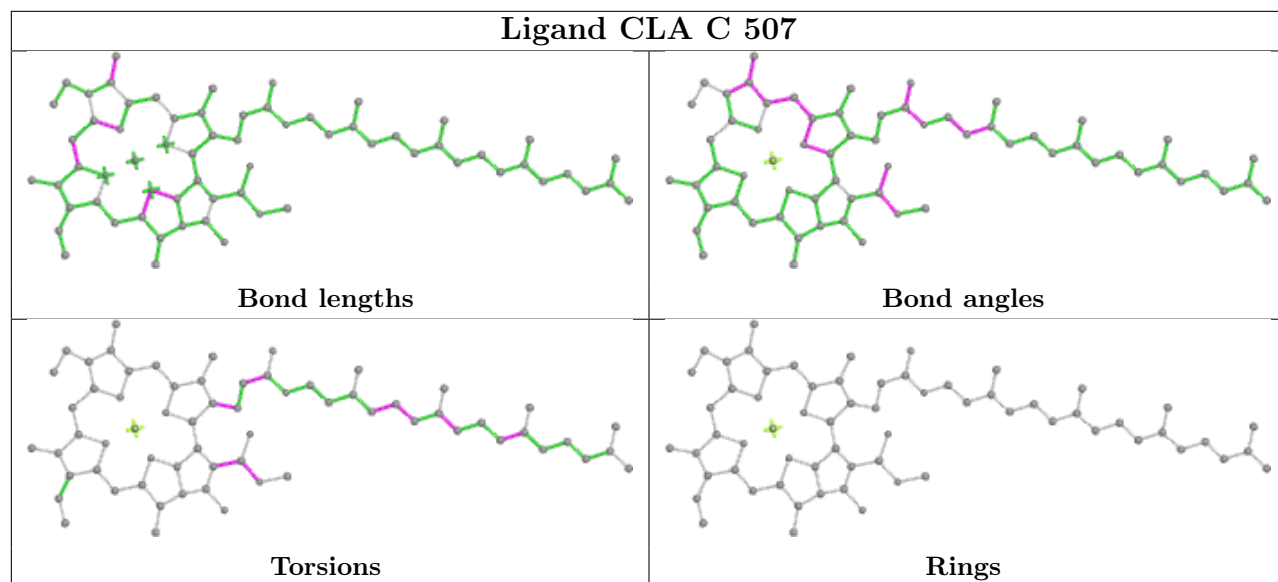


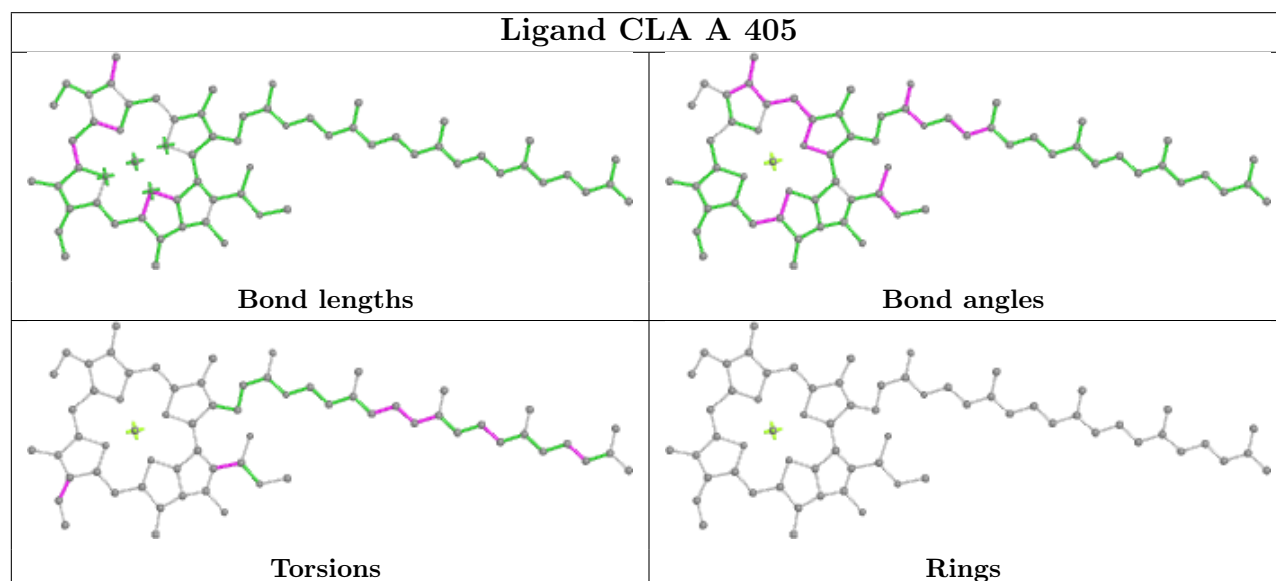
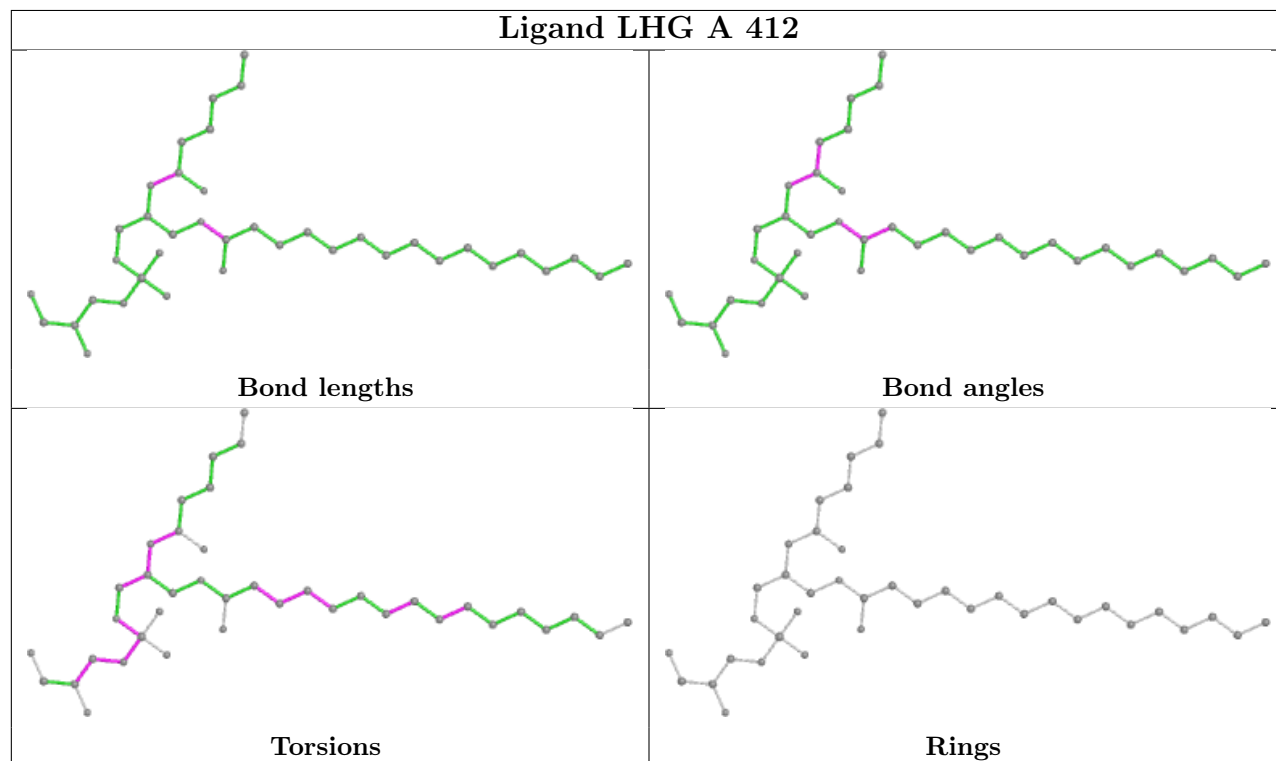
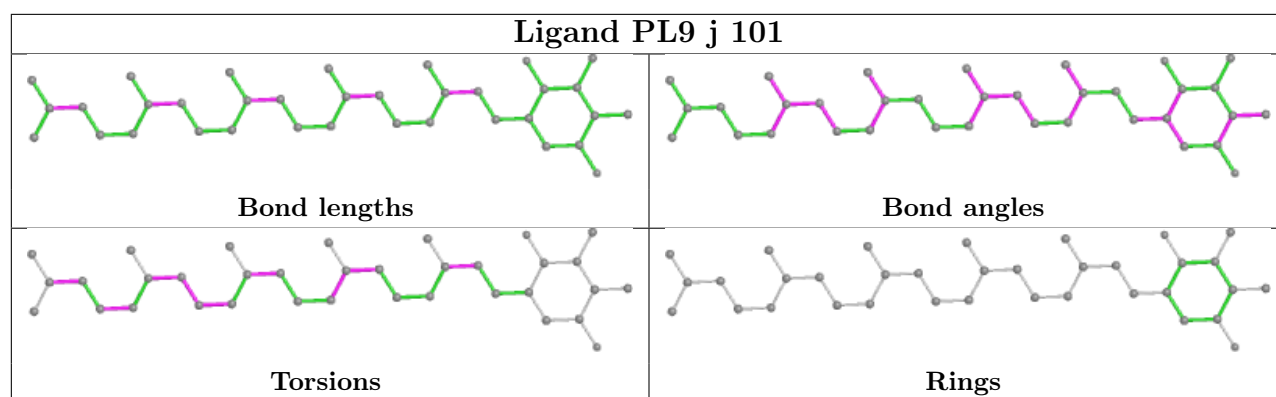


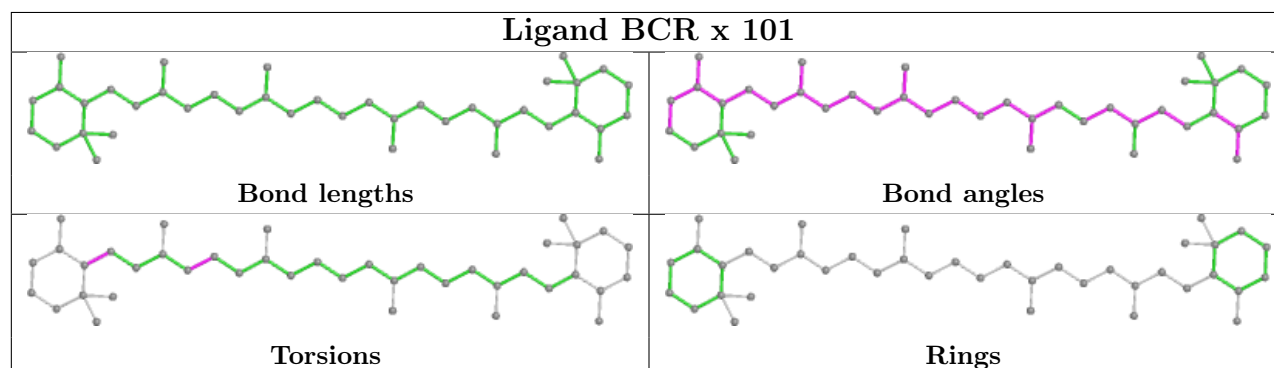
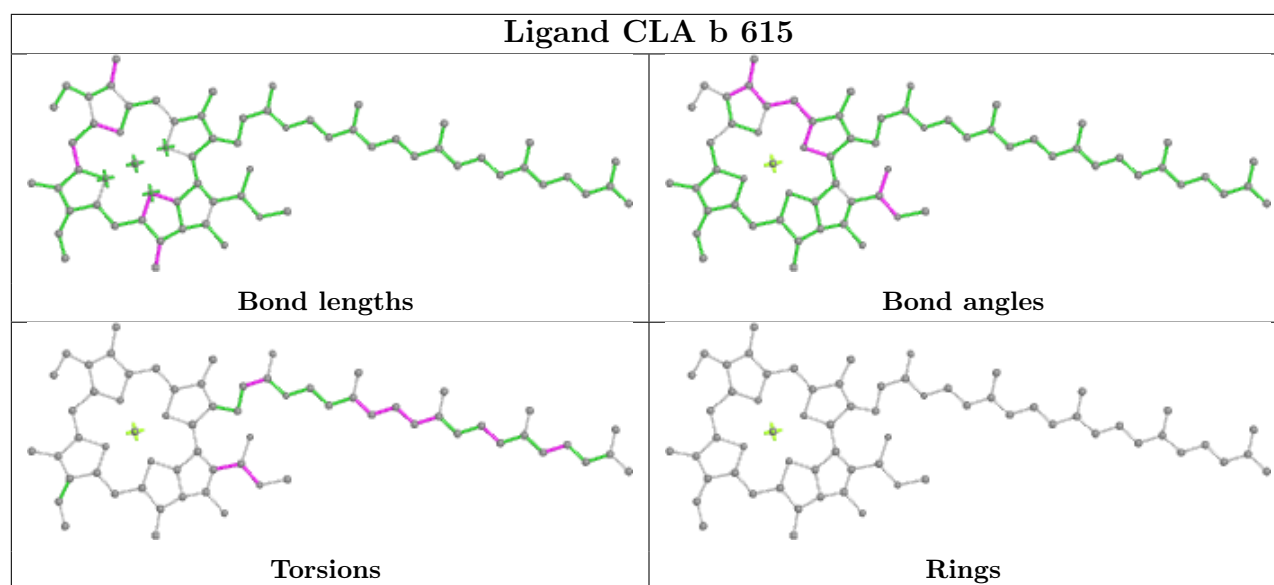
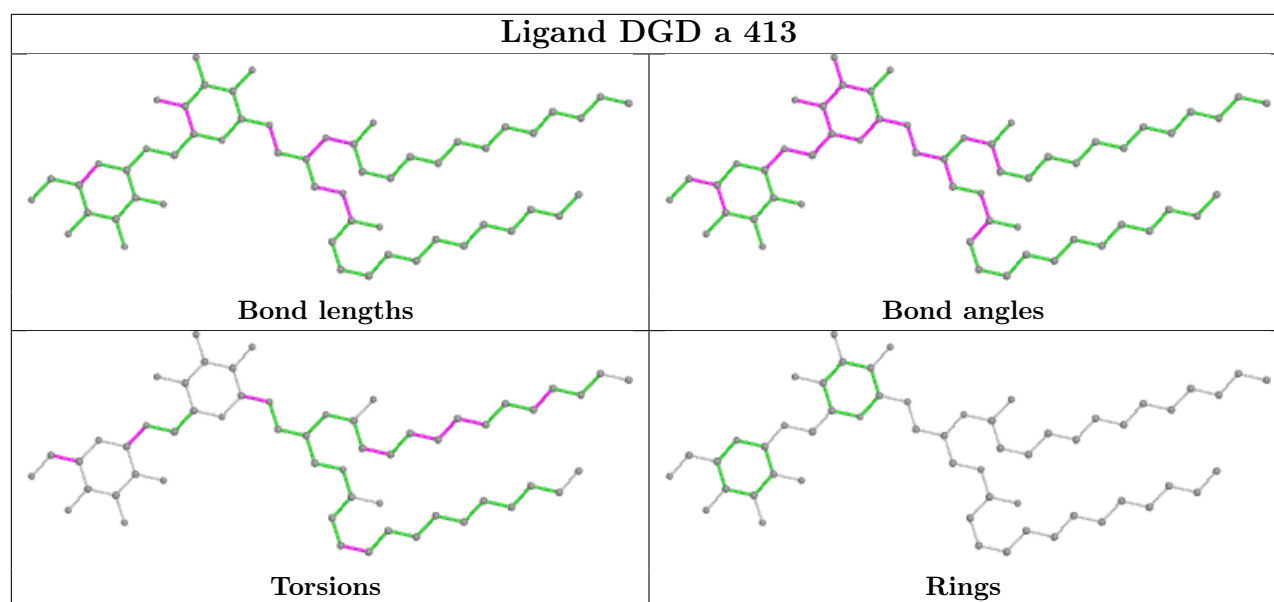


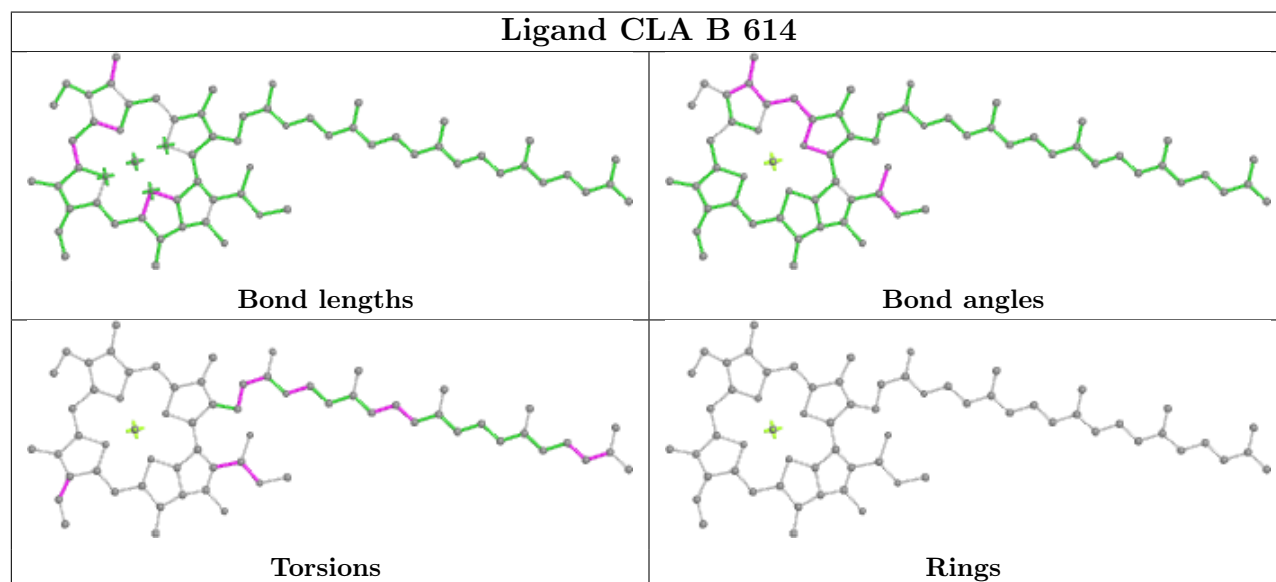
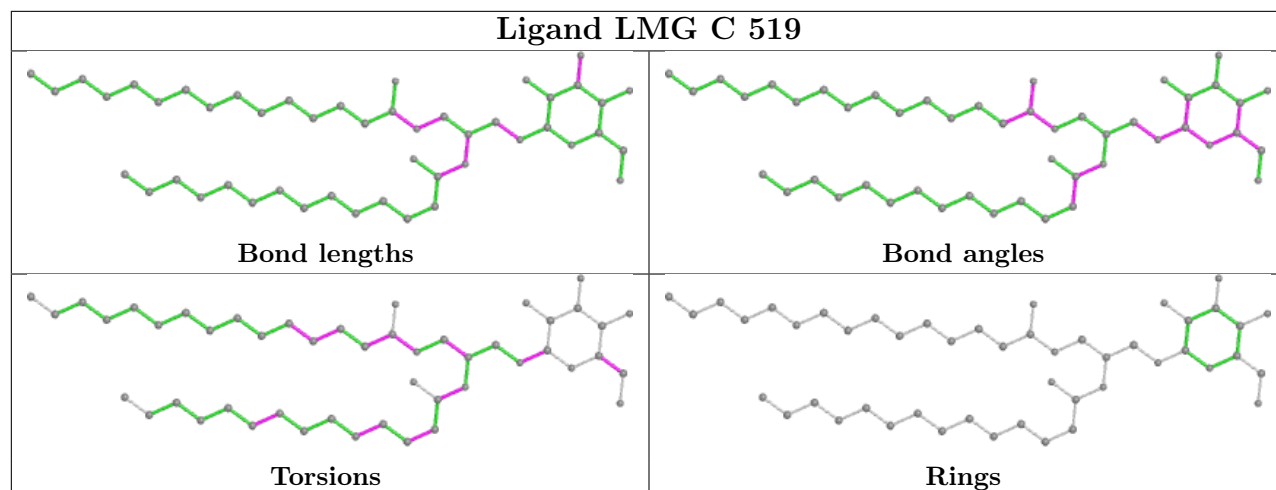
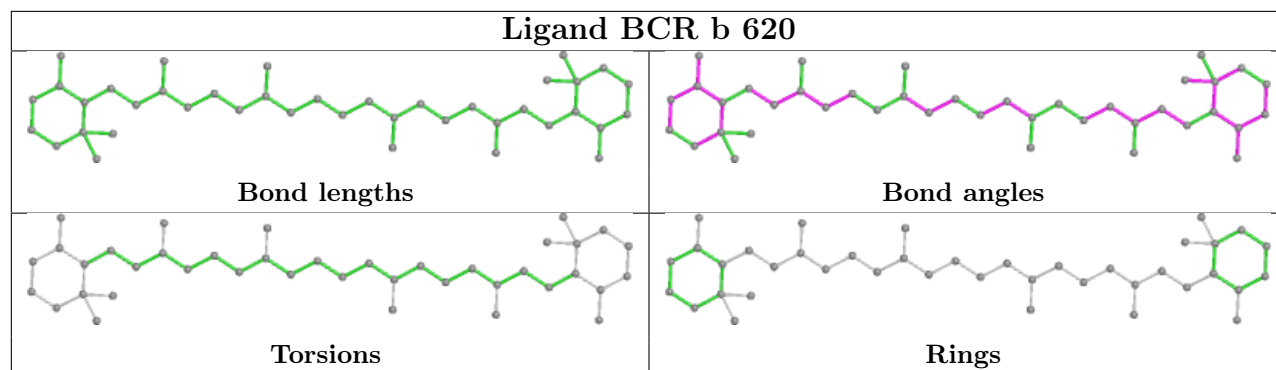


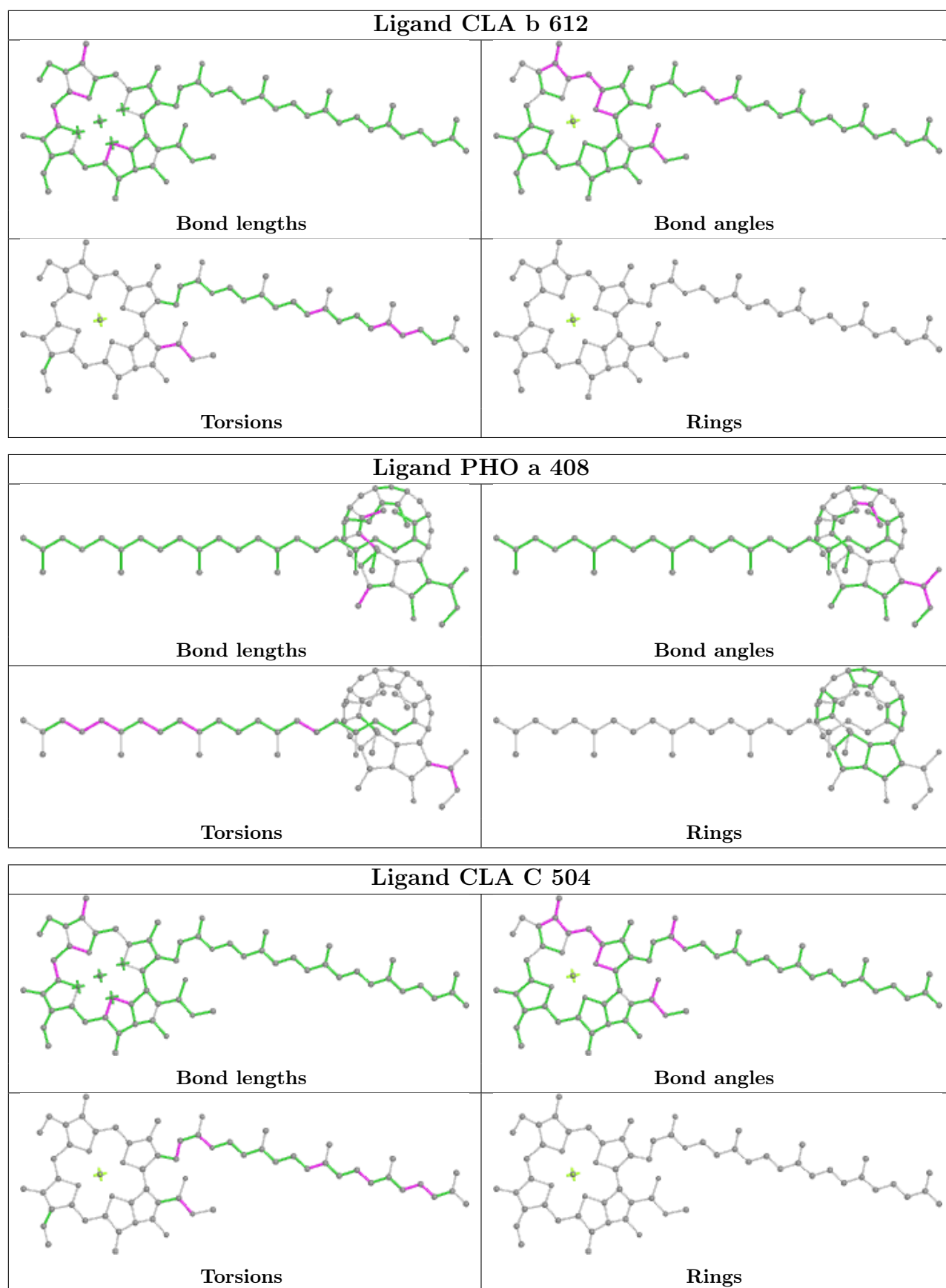


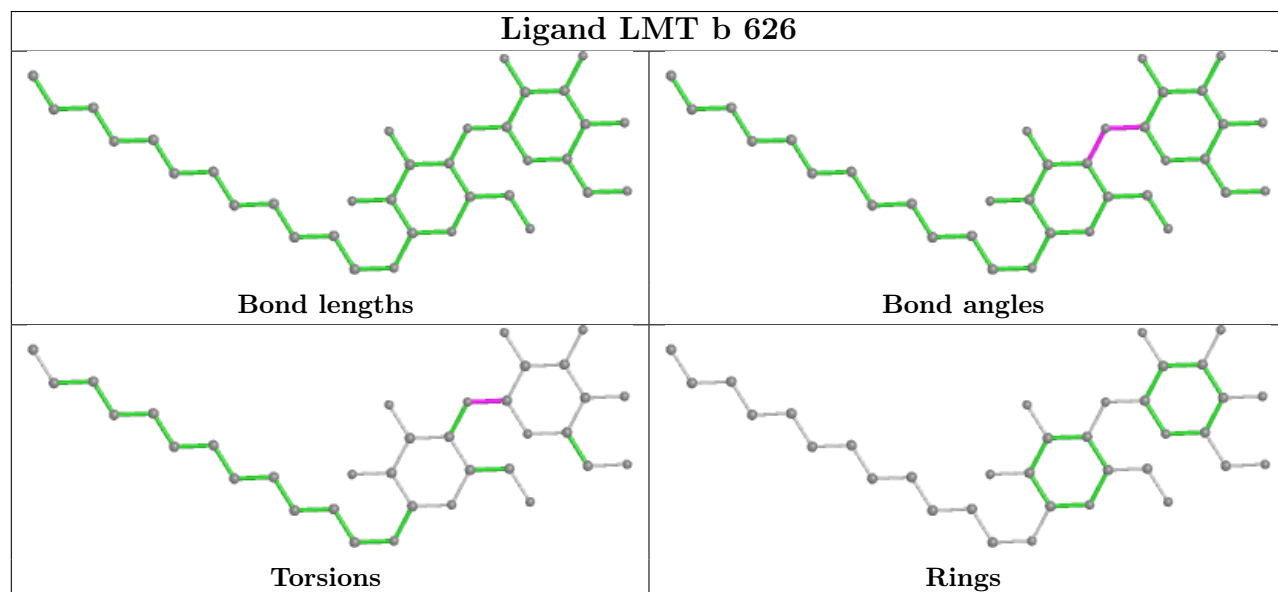
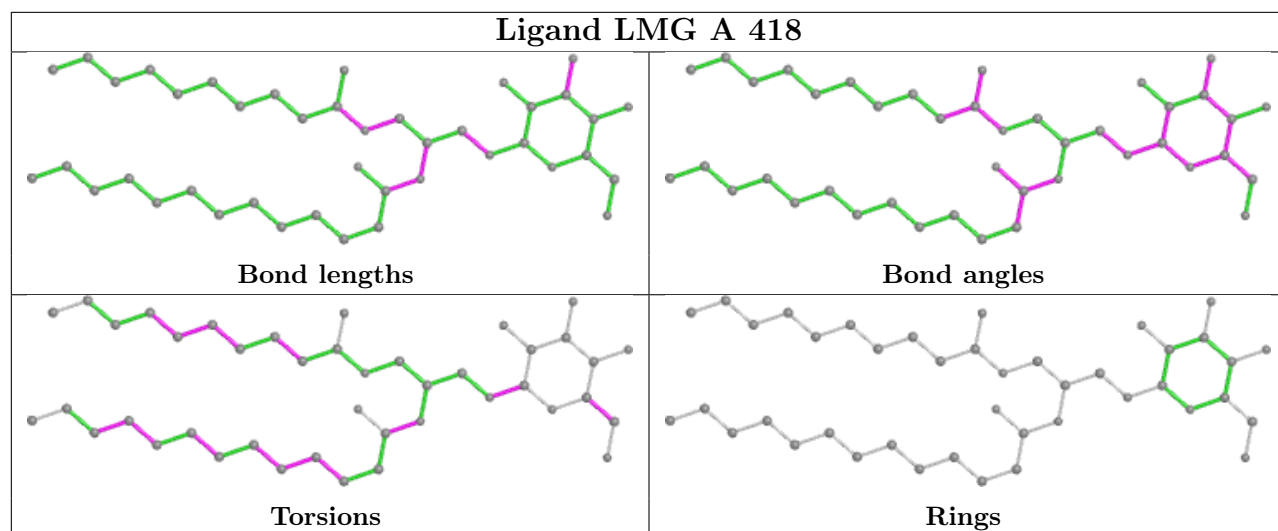
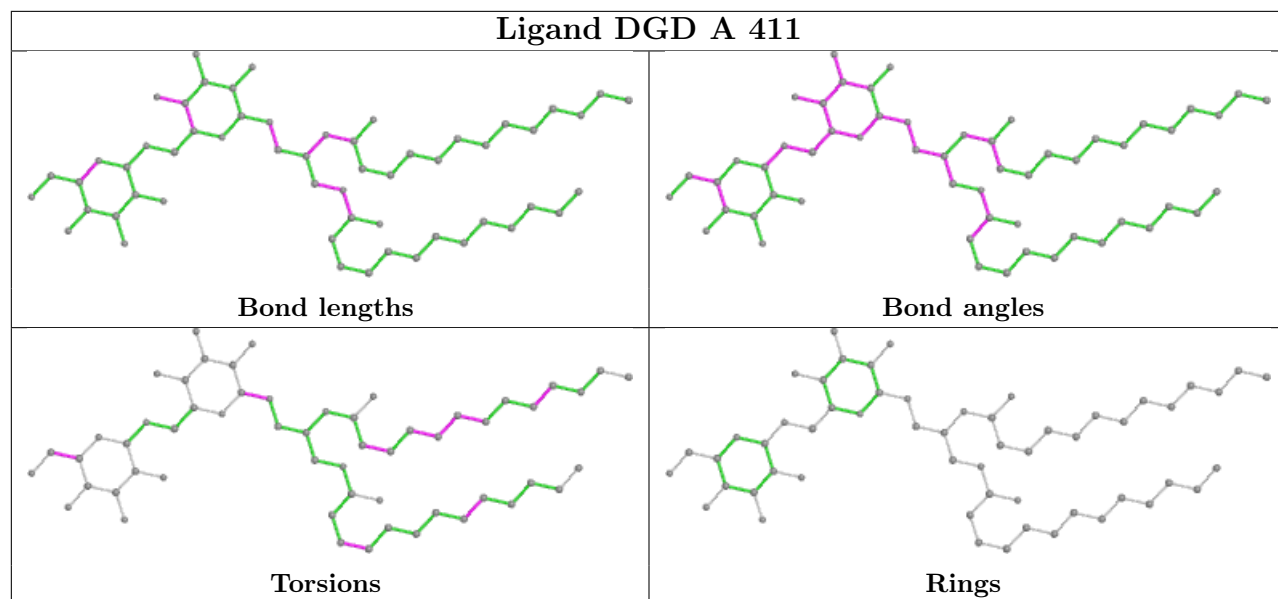


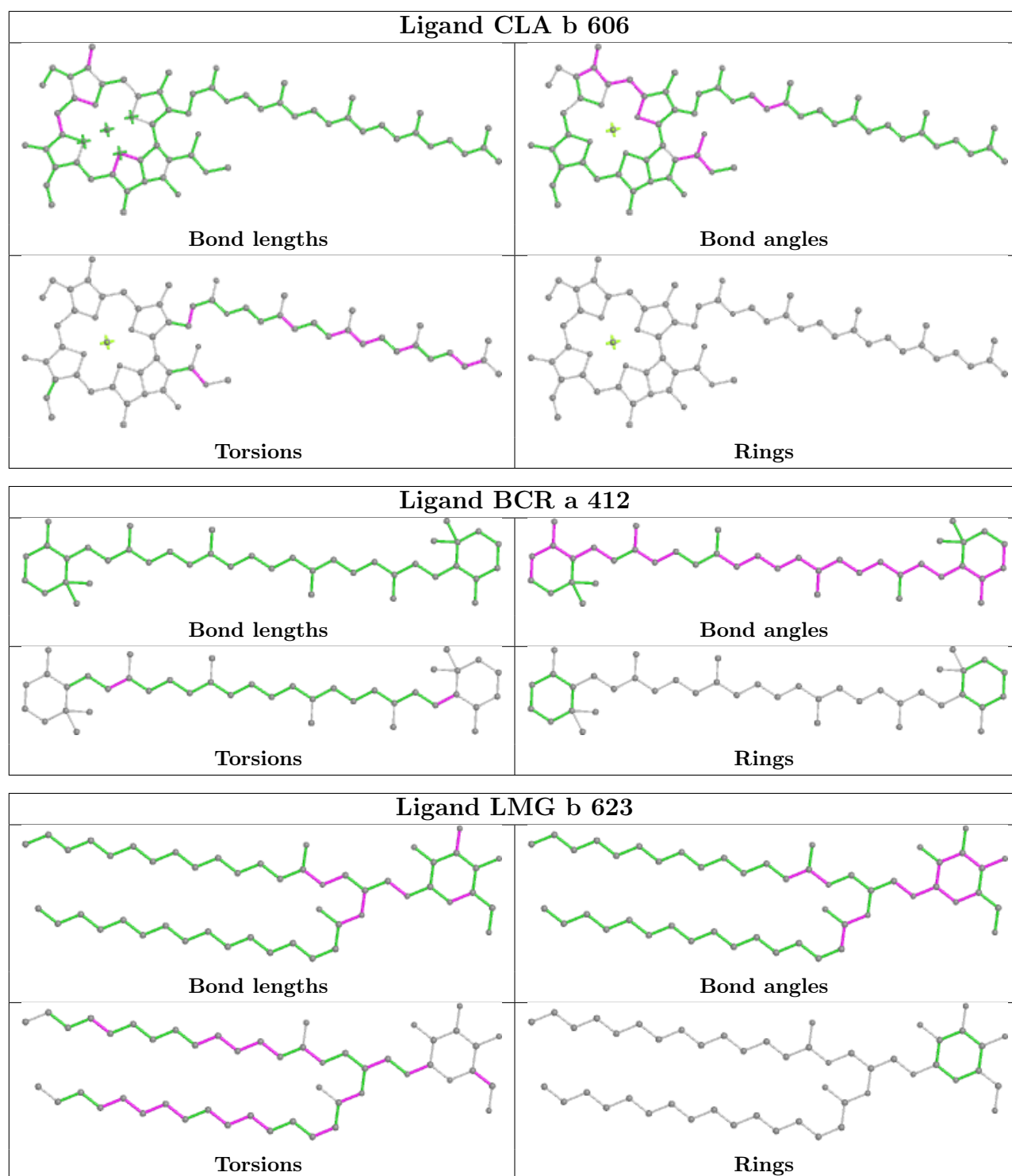


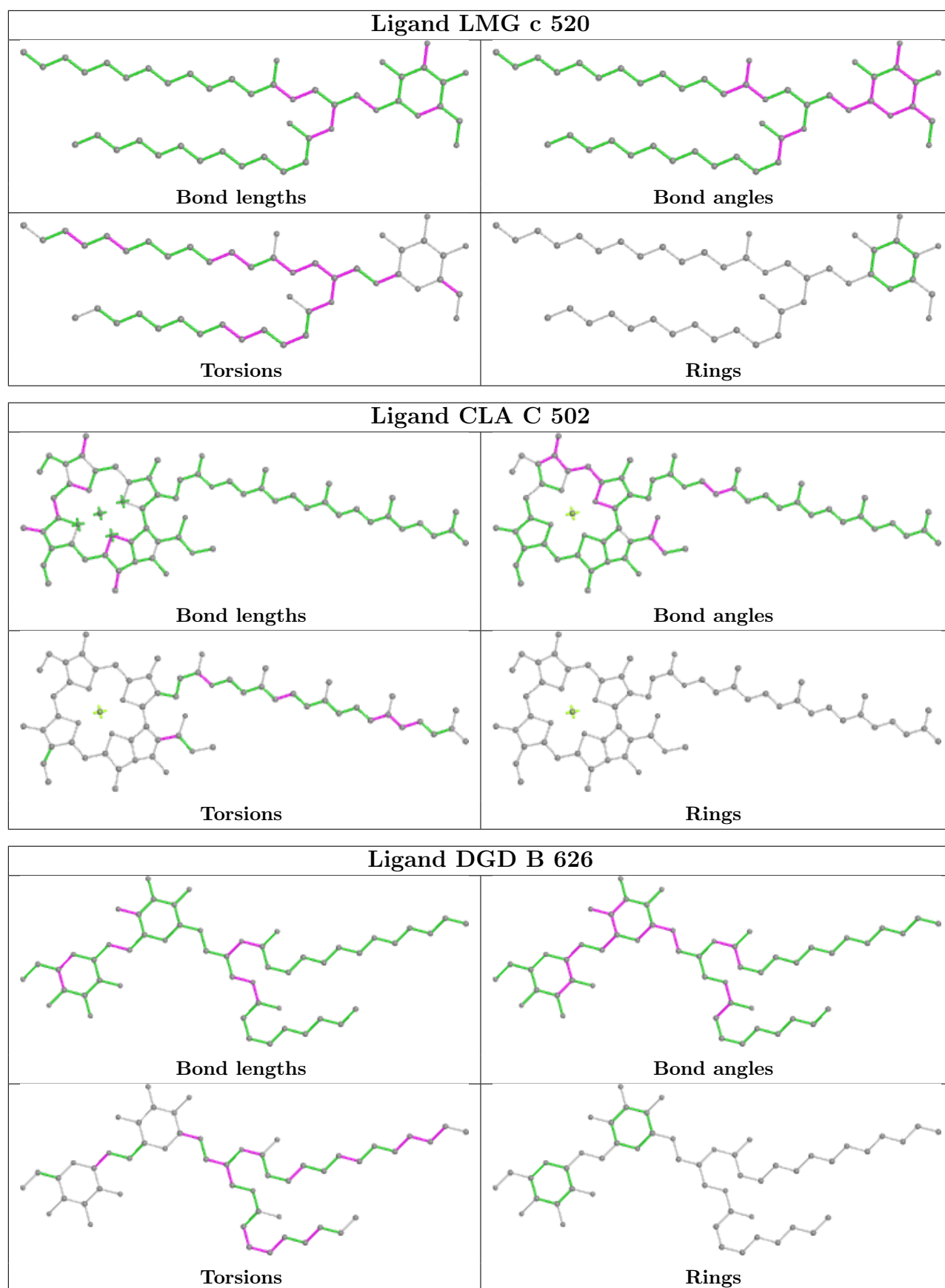


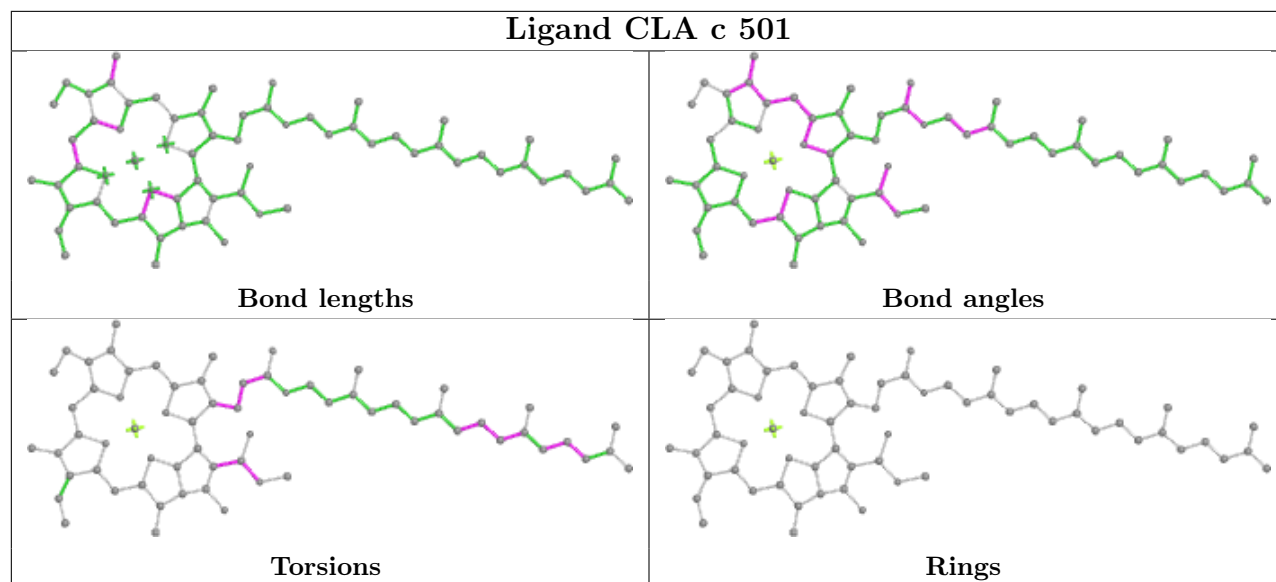












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	335/360 (93%)	0.03	8 (2%) 59 51	44, 65, 104, 152	0
1	a	335/360 (93%)	-0.18	2 (0%) 89 83	46, 65, 104, 153	0
2	B	490/510 (96%)	0.22	21 (4%) 35 32	46, 70, 103, 156	0
2	b	490/510 (96%)	0.21	15 (3%) 49 41	43, 70, 103, 160	0
3	C	447/461 (96%)	0.01	12 (2%) 54 47	52, 79, 105, 133	0
3	c	447/461 (96%)	0.14	24 (5%) 25 25	56, 81, 106, 135	0
4	D	340/352 (96%)	-0.13	1 (0%) 94 90	44, 66, 102, 139	0
4	d	340/352 (96%)	-0.10	2 (0%) 89 83	43, 66, 102, 135	0
5	E	82/84 (97%)	0.08	2 (2%) 59 51	68, 92, 123, 132	0
5	e	82/84 (97%)	-0.14	1 (1%) 79 70	70, 92, 123, 127	0
6	F	35/45 (77%)	-0.30	0 100 100	67, 84, 119, 143	0
6	f	35/45 (77%)	-0.21	1 (2%) 51 44	72, 83, 121, 141	0
7	H	65/66 (98%)	0.39	4 (6%) 20 19	74, 93, 119, 145	0
7	h	65/66 (98%)	0.63	7 (10%) 5 8	73, 94, 119, 148	0
8	I	35/38 (92%)	0.18	0 100 100	65, 80, 106, 120	0
8	i	35/38 (92%)	-0.08	0 100 100	68, 80, 105, 120	0
9	J	34/40 (85%)	-0.24	0 100 100	72, 85, 95, 112	0
9	j	34/40 (85%)	-0.06	0 100 100	77, 87, 96, 115	0
10	K	37/46 (80%)	-0.15	0 100 100	76, 88, 99, 125	0
10	k	37/46 (80%)	0.41	1 (2%) 54 47	73, 89, 104, 126	0
11	L	37/37 (100%)	0.35	4 (10%) 5 8	50, 63, 126, 156	0
11	l	37/37 (100%)	0.05	0 100 100	51, 63, 127, 155	0
12	M	34/36 (94%)	0.14	2 (5%) 22 21	53, 69, 107, 165	0
12	m	34/36 (94%)	0.21	3 (8%) 10 11	55, 69, 109, 163	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.54	21 (8%) 10 11	49, 79, 122, 167	0
13	o	243/272 (89%)	0.44	9 (3%) 41 36	49, 79, 121, 167	0
14	T	32/32 (100%)	0.22	4 (12%) 3 7	57, 69, 159, 169	0
14	t	32/32 (100%)	-0.08	0 100 100	56, 67, 158, 170	0
15	U	97/134 (72%)	0.57	4 (4%) 37 33	56, 70, 90, 112	0
15	u	97/134 (72%)	0.52	2 (2%) 63 55	56, 70, 89, 111	0
16	V	137/163 (84%)	0.02	4 (2%) 51 44	55, 71, 85, 100	0
16	v	137/163 (84%)	0.43	3 (2%) 62 54	58, 71, 86, 96	0
17	g	28/46 (60%)	0.85	3 (10%) 6 8	96, 108, 125, 129	0
17	y	28/46 (60%)	0.03	0 100 100	92, 108, 128, 129	0
18	X	37/41 (90%)	0.84	6 (16%) 1 4	77, 92, 120, 140	0
18	x	37/41 (90%)	0.76	5 (13%) 3 5	75, 90, 124, 145	0
19	Z	62/62 (100%)	0.83	6 (9%) 7 9	87, 103, 170, 186	0
19	z	62/62 (100%)	0.36	1 (1%) 72 63	88, 104, 169, 184	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.15	178 (3%) 45 39	43, 75, 115, 186	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.2
16	v	132	ASN	5.2
1	A	10	SER	4.6
1	A	11	ALA	4.6
7	h	66	GLY	4.2

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, 95th 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 ²)	Q<0.9
31	LMG	C	520	45/55	0.27	1.27	80,119,142,171	0
25	PL9	J	101	35/55	0.30	0.52	119,157,183,185	0
25	PL9	j	101	35/55	0.34	0.46	120,159,178,180	0
33	LMT	i	102	35/35	0.35	1.16	99,136,146,150	0
33	LMT	I	102	35/35	0.39	0.94	94,136,147,149	0
35	CA	K	101	1/1	0.42	0.51	72,72,72,72	0
33	LMT	B	623	35/35	0.45	0.86	76,136,170,172	0
31	LMG	E	101	44/55	0.49	0.62	85,123,134,138	0
27	BCR	j	102	40/40	0.50	0.51	107,125,176,178	0
27	BCR	J	102	40/40	0.51	0.41	109,129,176,177	0
31	LMG	c	520	45/55	0.54	1.18	82,119,140,168	0
33	LMT	b	626	35/35	0.54	1.07	99,143,152,153	0
33	LMT	x	102	31/35	0.55	0.68	79,130,156,157	0
28	DGD	d	408	63/66	0.56	0.65	104,127,184,187	0
28	DGD	D	410	63/66	0.56	0.74	104,127,181,188	0
33	LMT	B	627	35/35	0.57	0.57	71,122,138,140	0
23	CLA	b	604	65/65	0.58	0.88	93,108,130,134	0
27	BCR	D	405	40/40	0.58	0.57	65,80,101,108	0
33	LMT	D	411	31/35	0.59	1.00	82,132,156,156	0
23	CLA	B	601	65/65	0.59	0.90	94,108,129,134	0
27	BCR	B	620	40/40	0.60	0.80	77,87,92,92	0
33	LMT	T	101	35/35	0.60	0.57	63,115,136,143	0
28	DGD	b	602	52/66	0.61	0.57	81,104,177,178	0
29	LHG	A	415	37/49	0.63	0.41	108,137,192,202	0
29	LHG	a	417	37/49	0.63	0.43	111,134,197,206	0
33	LMT	B	624	35/35	0.64	0.64	91,142,154,155	0
31	LMG	A	418	42/55	0.64	0.43	76,107,120,142	0
31	LMG	a	402	42/55	0.64	0.52	76,105,121,142	0
27	BCR	A	410	40/40	0.65	0.46	53,68,81,91	0
33	LMT	b	603	35/35	0.65	0.52	76,131,155,156	0
27	BCR	H	101	40/40	0.66	1.12	82,95,131,132	0
30	SQD	d	407	43/54	0.66	0.86	73,107,144,149	0
31	LMG	I	101	43/55	0.67	0.70	87,115,159,171	0
31	LMG	M	102	42/55	0.67	0.44	70,109,133,139	0
31	LMG	i	101	43/55	0.67	0.69	85,120,158,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	LMT	B	628	35/35	0.67	0.49	72,137,162,163	0
27	BCR	B	618	40/40	0.68	0.35	68,80,90,92	0
31	LMG	C	519	48/55	0.68	0.38	86,99,110,116	0
23	CLA	c	513	65/65	0.68	0.93	94,107,138,149	0
28	DGD	C	518	66/66	0.69	0.36	58,72,106,121	0
27	BCR	b	621	40/40	0.69	0.67	72,83,92,94	0
30	SQD	F	102	45/54	0.69	0.69	86,129,153,154	0
27	BCR	c	516	40/40	0.69	0.80	76,86,93,103	0
23	CLA	C	506	65/65	0.69	0.46	75,91,123,134	0
27	BCR	x	101	40/40	0.70	0.72	81,97,129,130	0
23	CLA	B	614	65/65	0.70	0.42	64,83,124,132	0
31	LMG	e	101	44/55	0.70	0.42	85,122,133,140	0
27	BCR	C	515	40/40	0.70	0.57	76,87,95,98	0
35	CA	o	301	1/1	0.70	0.41	106,106,106,106	0
27	BCR	a	412	40/40	0.71	0.44	51,71,82,84	0
28	DGD	B	626	52/66	0.71	0.46	77,104,179,183	0
27	BCR	k	102	40/40	0.71	0.80	69,85,106,109	0
28	DGD	A	411	56/66	0.72	0.40	79,100,145,149	0
23	CLA	b	619	65/65	0.72	0.62	78,99,142,147	0
23	CLA	C	502	65/65	0.72	0.49	62,72,104,112	0
25	PL9	A	408	45/55	0.72	0.46	84,103,119,127	0
30	SQD	D	409	43/54	0.72	0.58	72,103,147,151	0
30	SQD	b	601	47/54	0.73	0.38	86,99,139,146	0
31	LMG	M	101	42/55	0.73	0.40	78,110,135,144	0
25	PL9	d	404	55/55	0.73	0.31	48,65,76,86	0
30	SQD	f	103	45/54	0.73	0.67	88,129,148,155	0
27	BCR	K	102	40/40	0.73	0.76	74,85,102,103	0
27	BCR	f	102	40/40	0.73	0.45	64,83,107,110	0
23	CLA	C	507	65/65	0.73	0.59	77,92,101,105	0
31	LMG	k	103	48/55	0.73	0.43	80,100,118,120	0
32	CL	A	416	1/1	0.73	0.38	49,49,49,49	0
31	LMG	D	407	49/55	0.73	0.36	59,80,109,117	0
30	SQD	a	401	54/54	0.73	0.45	75,116,152,156	0
28	DGD	a	413	56/66	0.74	0.39	74,101,145,149	0
23	CLA	a	409	65/65	0.74	0.58	55,69,129,134	0
30	SQD	a	415	51/54	0.74	0.38	81,102,128,134	0
33	LMT	b	625	35/35	0.75	0.58	78,139,172,176	0
27	BCR	Z	101	40/40	0.75	0.90	81,93,117,118	0
23	CLA	C	503	65/65	0.76	0.51	76,88,99,101	0
28	DGD	c	519	66/66	0.76	0.34	61,72,104,113	0
25	PL9	a	410	45/55	0.76	0.35	82,98,119,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	502	65/65	0.76	0.52	67,75,101,107	0
23	CLA	C	513	65/65	0.76	0.84	93,108,142,149	0
30	SQD	A	413	51/54	0.76	0.34	81,95,126,130	0
33	LMT	m	101	35/35	0.76	0.51	71,95,109,109	0
30	SQD	B	625	47/54	0.76	0.38	73,102,139,146	0
31	LMG	a	416	51/55	0.76	0.33	61,80,92,99	0
23	CLA	b	613	65/65	0.76	0.66	71,81,88,91	0
27	BCR	c	515	40/40	0.77	1.10	83,95,112,115	0
28	DGD	B	621	58/66	0.77	0.45	51,69,99,106	0
27	BCR	T	103	40/40	0.77	0.32	69,79,87,95	0
31	LMG	b	624	49/55	0.77	0.29	56,76,88,91	0
27	BCR	c	514	40/40	0.77	0.85	66,80,89,91	0
30	SQD	A	417	54/54	0.77	0.37	81,116,146,153	0
33	LMT	M	103	35/35	0.78	0.35	68,98,108,115	0
27	BCR	C	514	40/40	0.78	0.83	70,80,86,90	0
23	CLA	A	407	65/65	0.78	0.49	57,69,128,131	0
23	CLA	c	509	65/65	0.78	0.60	73,82,91,98	0
35	CA	O	301	1/1	0.78	0.30	123,123,123,123	0
23	CLA	c	511	65/65	0.78	0.61	72,91,102,106	0
23	CLA	C	501	65/65	0.79	0.49	66,80,90,95	0
27	BCR	B	617	40/40	0.79	0.28	64,73,79,80	0
23	CLA	c	506	65/65	0.79	0.45	79,94,122,126	0
27	BCR	b	620	40/40	0.79	0.30	59,72,79,80	0
24	PHO	A	406	64/64	0.79	0.39	57,69,74,76	0
23	CLA	b	611	65/65	0.79	0.47	63,76,96,100	0
29	LHG	A	412	39/49	0.80	0.33	61,80,92,94	0
25	PL9	D	404	55/55	0.80	0.30	47,59,70,74	0
23	CLA	B	606	65/65	0.80	0.59	68,84,111,123	0
23	CLA	B	610	65/65	0.80	0.73	68,82,87,91	0
24	PHO	a	408	64/64	0.80	0.36	58,71,81,87	0
23	CLA	C	504	65/65	0.80	0.36	67,83,133,136	0
28	DGD	C	517	62/66	0.80	0.33	61,84,132,147	0
31	LMG	B	622	49/55	0.80	0.31	50,74,85,91	0
23	CLA	B	616	65/65	0.81	0.61	75,93,144,150	0
23	CLA	C	509	65/65	0.81	0.73	65,81,95,98	0
23	CLA	b	618	65/65	0.81	0.56	78,97,109,116	0
27	BCR	B	619	40/40	0.81	0.27	62,76,82,84	0
23	CLA	c	512	65/65	0.81	0.96	90,102,148,154	0
23	CLA	C	511	65/65	0.81	0.49	73,90,100,109	0
23	CLA	d	403	65/65	0.81	0.57	72,88,124,128	0
23	CLA	b	609	65/65	0.81	0.58	71,86,111,121	0
23	CLA	D	403	65/65	0.82	0.85	73,85,121,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	609	65/65	0.82	0.81	73,89,105,112	0
28	DGD	b	622	58/66	0.82	0.34	57,71,97,102	0
28	DGD	c	518	62/66	0.82	0.33	65,86,138,143	0
29	LHG	a	414	39/49	0.82	0.36	62,79,91,94	0
23	CLA	C	512	65/65	0.83	0.93	83,101,147,151	0
24	PHO	D	402	64/64	0.83	0.30	48,61,71,77	0
24	PHO	a	407	64/64	0.83	0.32	52,62,71,76	0
23	CLA	b	607	65/65	0.83	0.39	62,67,112,117	0
23	CLA	c	507	65/65	0.83	0.65	84,94,102,109	0
23	CLA	b	612	65/65	0.83	0.66	69,89,104,106	0
31	LMG	d	405	46/55	0.83	0.33	65,71,116,128	0
23	CLA	b	605	65/65	0.84	0.44	73,87,96,98	0
23	CLA	b	606	65/65	0.84	0.61	69,79,93,100	0
31	LMG	d	406	48/55	0.84	0.26	56,71,86,120	0
23	CLA	b	617	65/65	0.84	0.31	67,82,130,135	0
23	CLA	a	406	65/65	0.84	0.29	53,70,143,149	0
23	CLA	b	608	65/65	0.84	0.45	58,76,85,89	0
23	CLA	C	505	65/65	0.84	0.34	69,77,84,88	0
23	CLA	B	604	65/65	0.84	0.44	55,66,109,121	0
31	LMG	D	408	48/55	0.85	0.27	52,73,83,120	0
23	CLA	c	505	65/65	0.85	0.30	66,78,83,86	0
23	CLA	B	605	65/65	0.85	0.60	58,77,87,92	0
23	CLA	C	508	65/65	0.85	0.31	70,84,123,140	0
23	CLA	B	608	65/65	0.85	0.61	62,74,94,97	0
23	CLA	C	510	65/65	0.85	0.32	63,73,85,93	0
27	BCR	T	102	40/40	0.85	0.27	66,73,83,85	0
23	CLA	a	405	65/65	0.85	0.33	40,54,65,72	0
23	CLA	A	405	65/65	0.86	0.27	48,69,139,145	0
31	LMG	A	414	51/55	0.86	0.27	61,74,88,96	0
28	DGD	c	517	53/66	0.86	0.28	58,75,98,102	0
23	CLA	d	402	65/65	0.86	0.30	49,59,79,91	0
23	CLA	c	504	65/65	0.86	0.28	69,82,132,136	0
23	CLA	b	610	65/65	0.86	0.31	52,64,82,88	0
31	LMG	D	406	46/55	0.86	0.29	55,74,116,125	0
23	CLA	c	501	65/65	0.86	0.63	68,81,89,95	0
34	HEM	F	101	43/43	0.87	0.44	92,104,127,128	0
23	CLA	b	614	65/65	0.87	0.34	57,71,79,93	0
23	CLA	b	615	65/65	0.87	0.33	62,72,83,94	0
23	CLA	B	615	65/65	0.87	0.63	82,94,108,116	0
22	BCT	d	401	4/4	0.88	0.26	77,80,82,85	0
23	CLA	B	602	65/65	0.88	0.53	68,87,96,99	0
23	CLA	c	503	65/65	0.88	0.80	73,89,97,103	0

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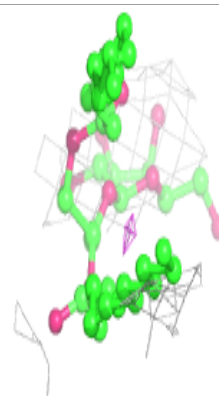
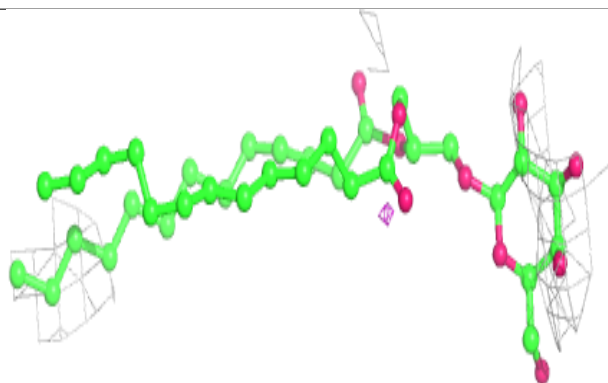
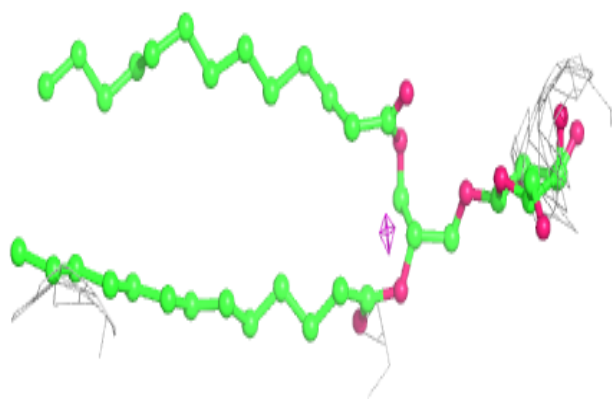
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	603	65/65	0.88	0.69	65,80,91,105	0
23	CLA	B	611	65/65	0.88	0.32	65,73,80,81	0
35	CA	k	101	1/1	0.88	0.21	94,94,94,94	0
23	CLA	B	612	65/65	0.88	0.40	56,69,84,87	0
23	CLA	c	508	65/65	0.89	0.30	73,84,120,134	0
23	CLA	A	403	65/65	0.89	0.27	47,58,67,68	0
32	CL	d	409	1/1	0.89	0.25	49,49,49,49	0
34	HEM	v	201	43/43	0.89	0.46	61,68,75,78	0
23	CLA	c	510	65/65	0.90	0.33	66,74,85,87	0
23	CLA	B	607	65/65	0.90	0.25	56,64,84,91	0
23	CLA	B	613	65/65	0.90	0.27	44,63,88,92	0
34	HEM	V	201	43/43	0.90	0.35	46,65,74,79	0
34	HEM	f	101	43/43	0.90	0.38	77,103,125,130	0
23	CLA	a	404	65/65	0.91	0.35	44,58,65,73	0
31	LMG	b	623	49/55	0.91	0.25	57,80,96,113	0
23	CLA	D	401	65/65	0.91	0.26	47,58,85,99	0
23	CLA	A	404	65/65	0.92	0.33	39,54,66,70	0
28	DGD	C	516	53/66	0.92	0.25	58,75,97,102	0
22	BCT	A	402	4/4	0.92	0.43	84,88,89,93	0
23	CLA	b	616	65/65	0.93	0.32	54,68,90,92	0
21	FE2	A	401	1/1	0.94	0.15	60,60,60,60	0
26	OEC	a	411	5/9	0.94	0.39	35,44,62,62	0
26	OEC	A	409	5/9	0.96	0.43	35,44,46,62	0
21	FE2	a	403	1/1	0.97	0.13	70,70,70,70	0

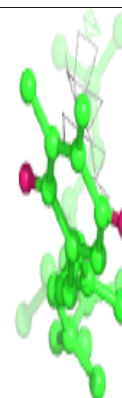
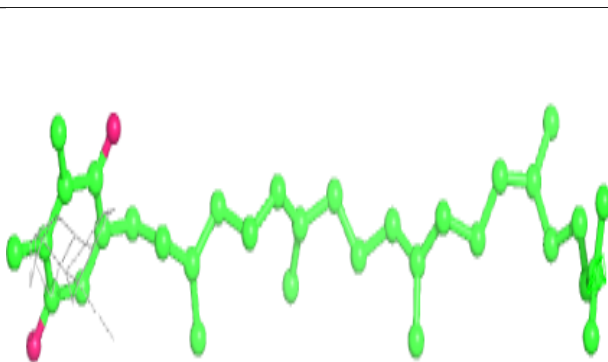
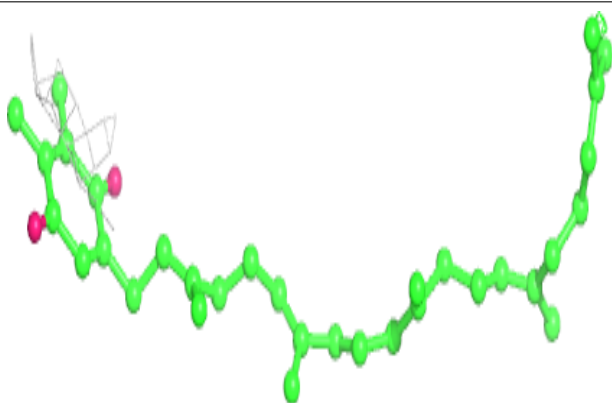
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMG C 520:

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

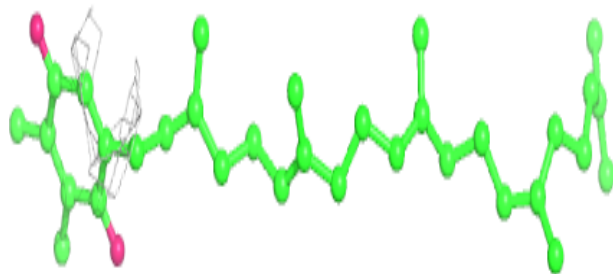
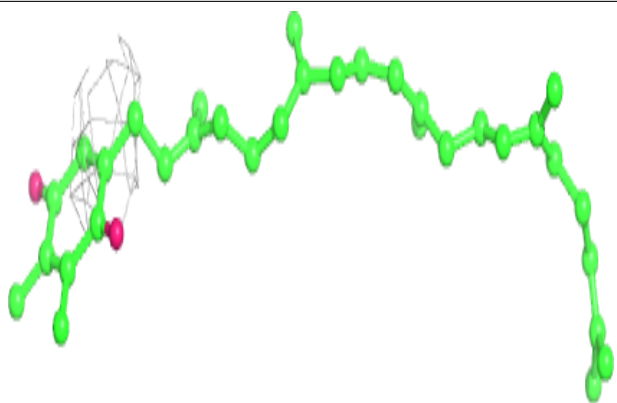
**Electron density around PL9 J 101:**

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

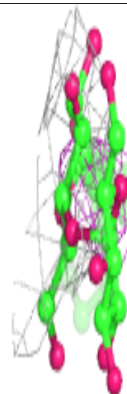
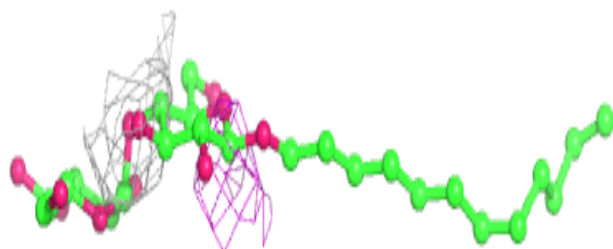
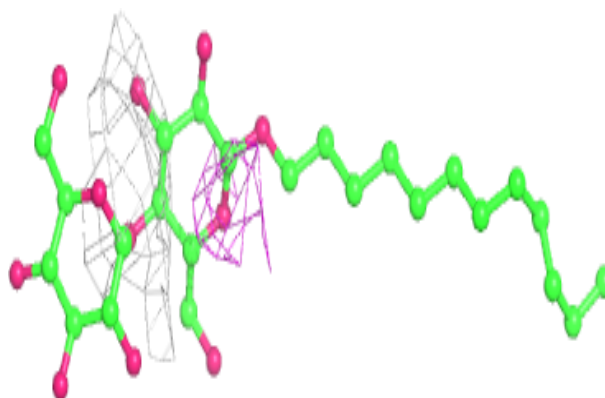


Electron density around PL9 j 101:

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

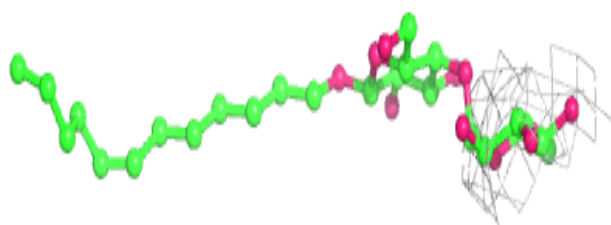
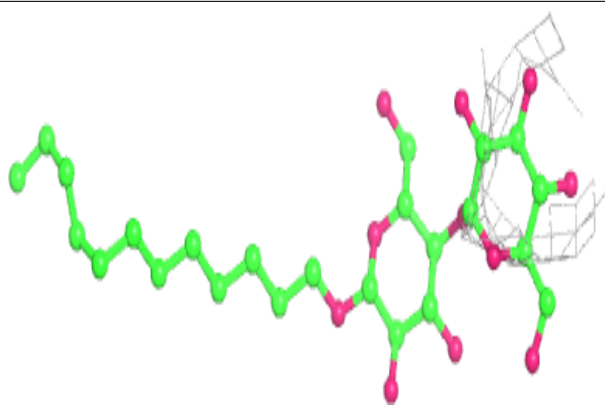
**Electron density around LMT i 102:**

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

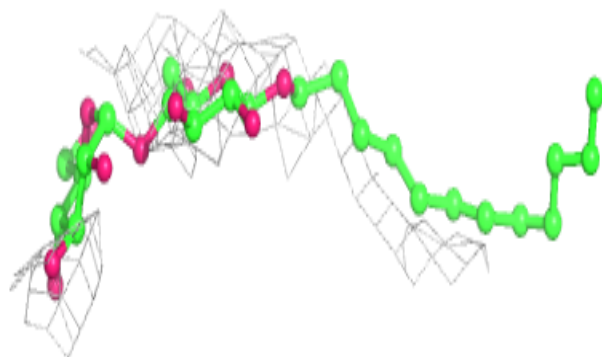
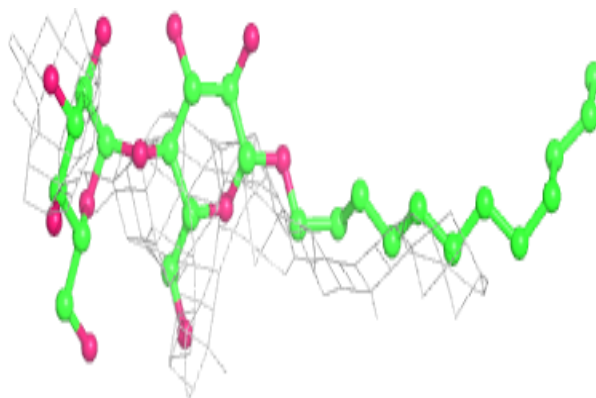


Electron density around LMT I 102:

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

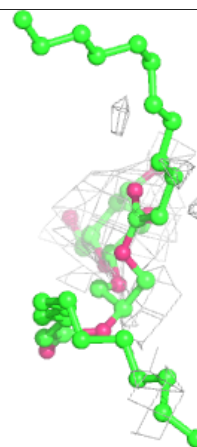
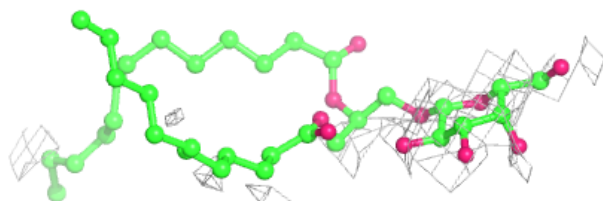
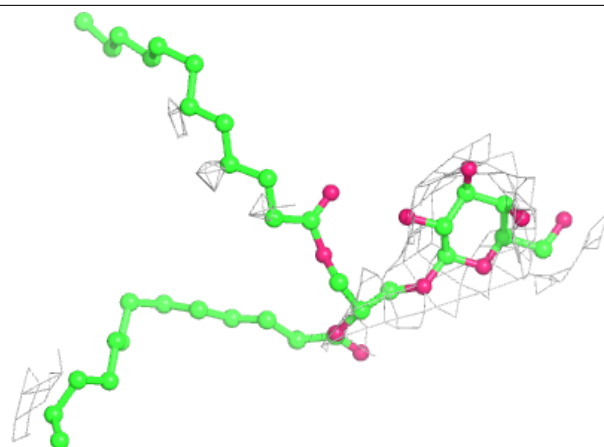
**Electron density around LMT B 623:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

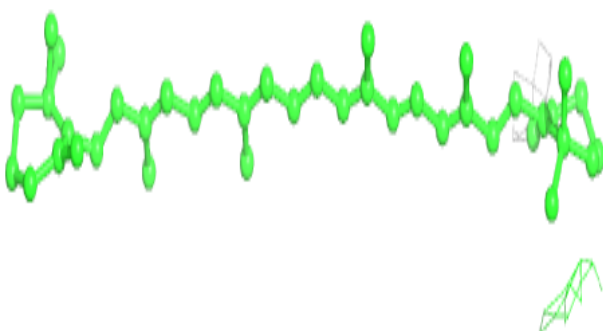
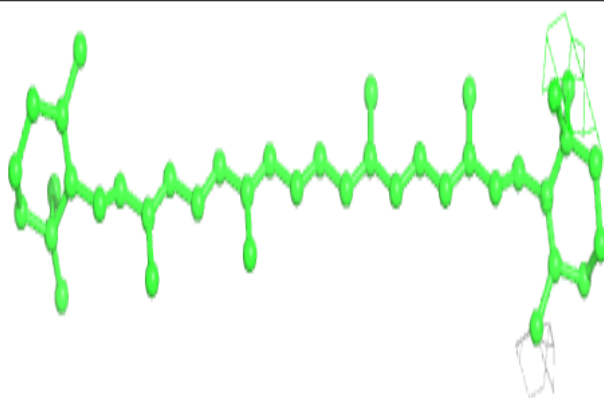


Electron density around LMG E 101:

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

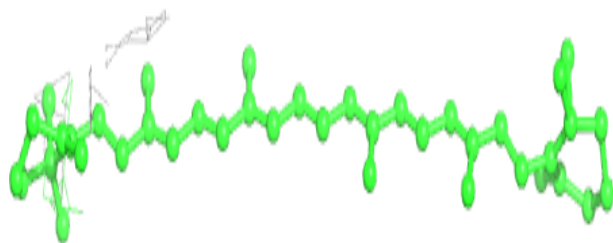
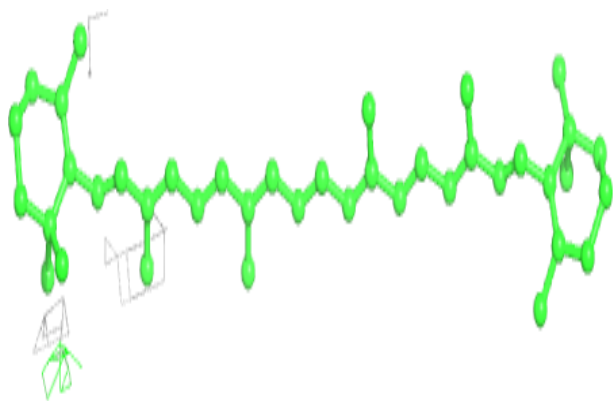
**Electron density around BCR j 102:**

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

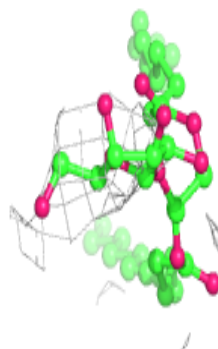
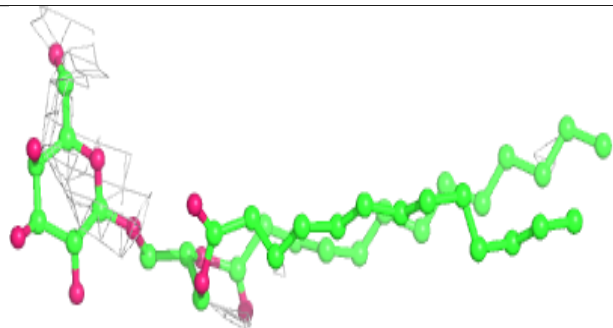
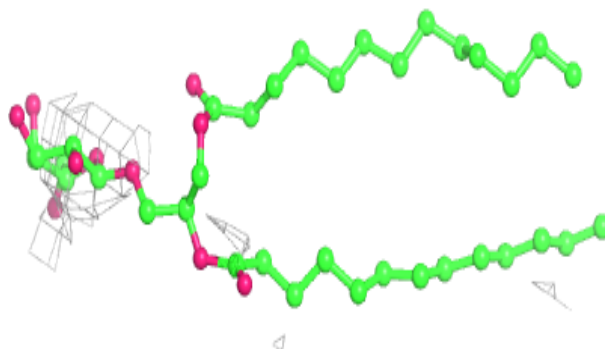


Electron density around BCR J 102:

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

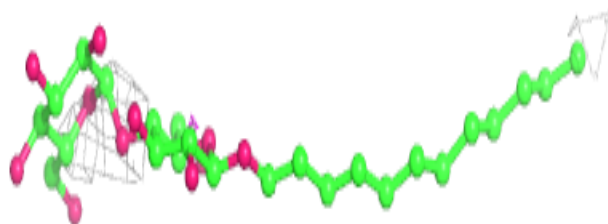
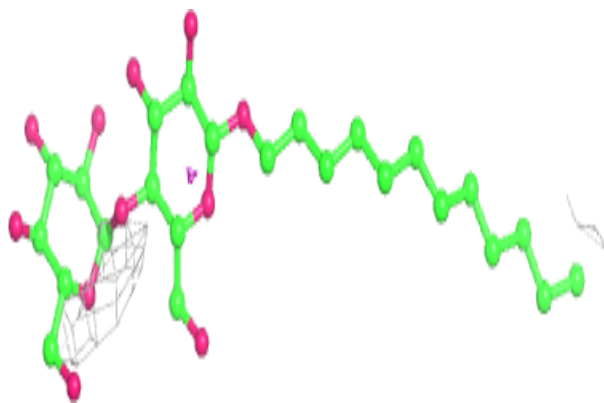
**Electron density around LMG c 520:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

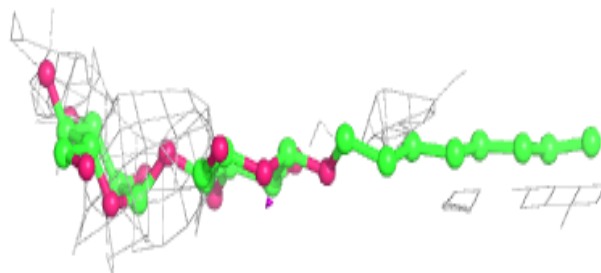
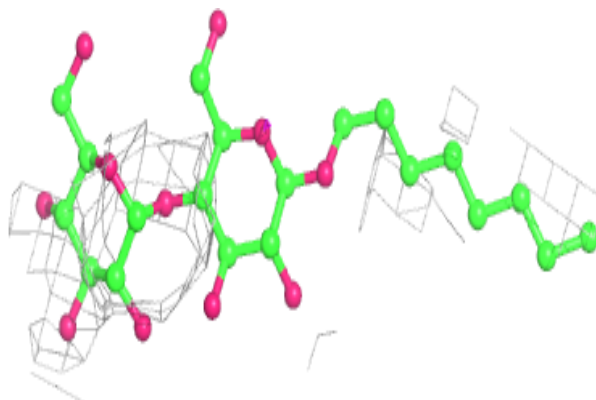


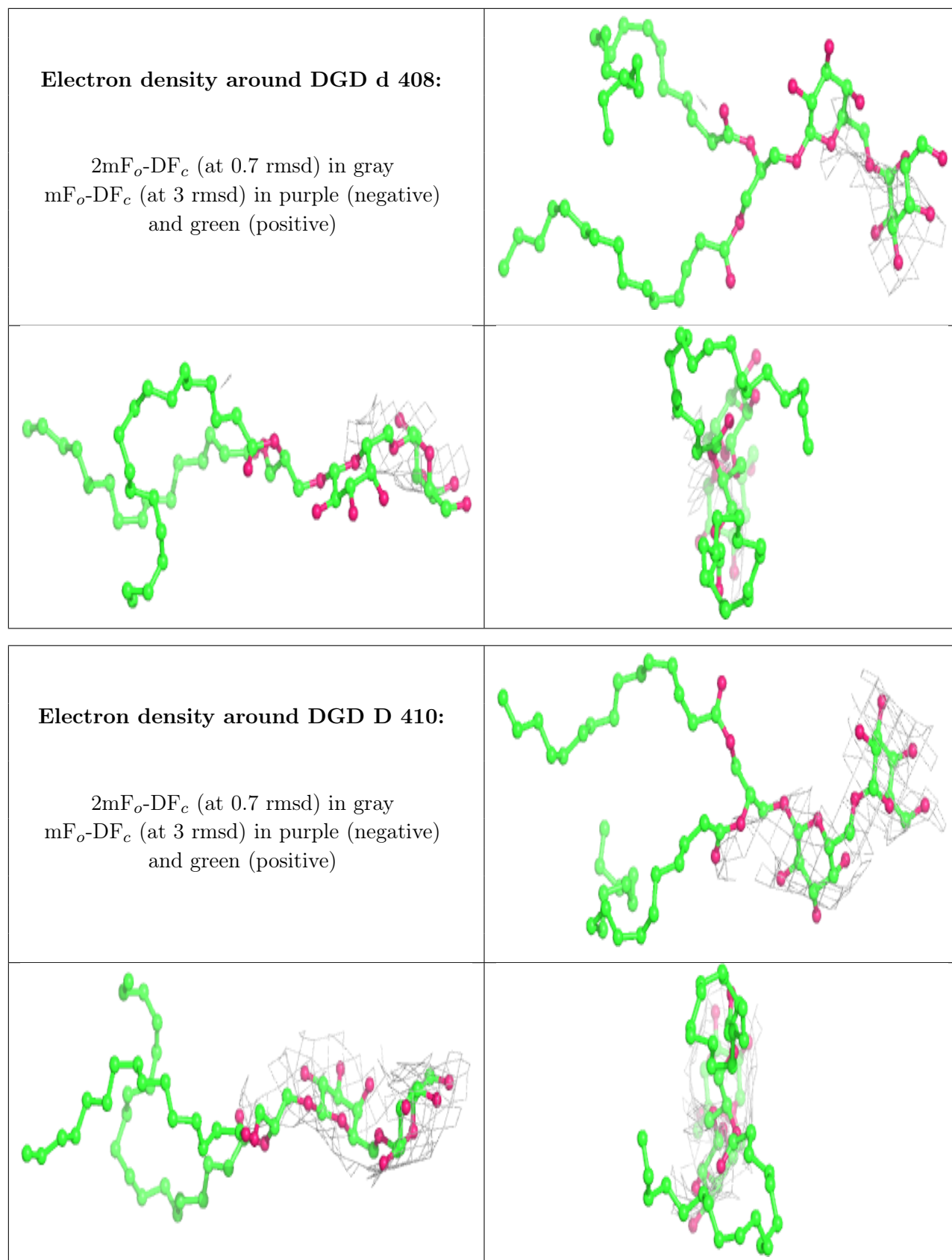
Electron density around LMT b 626:

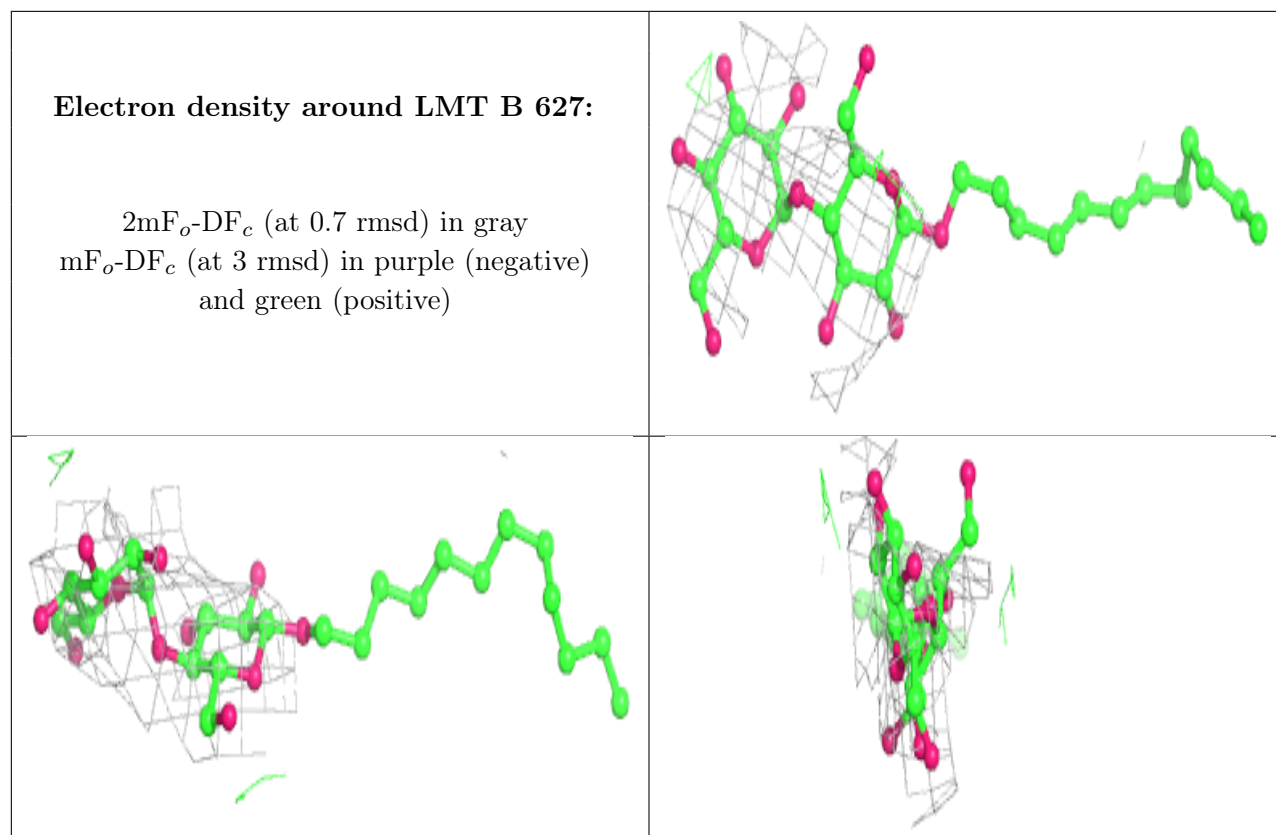
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMT x 102:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

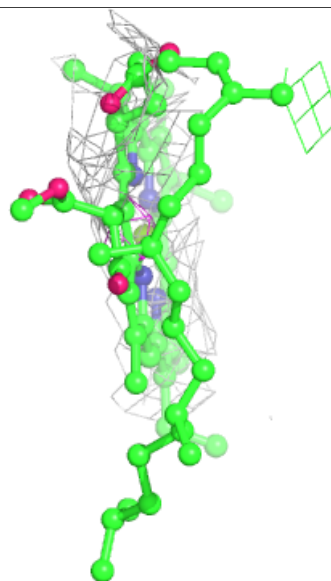
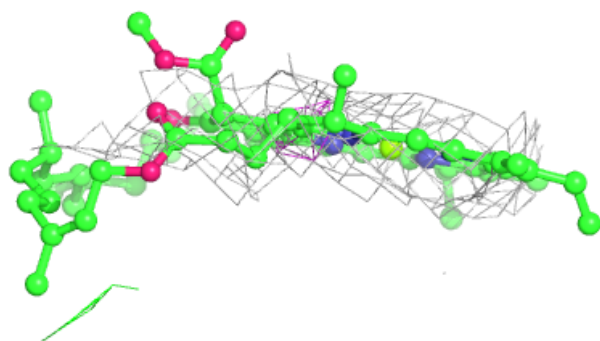
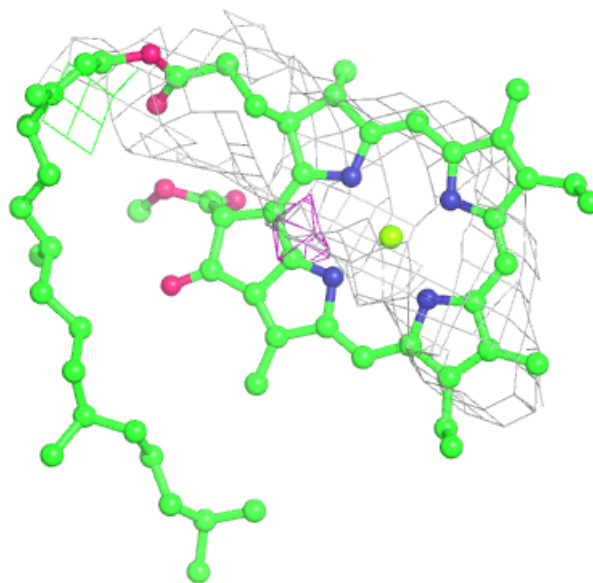


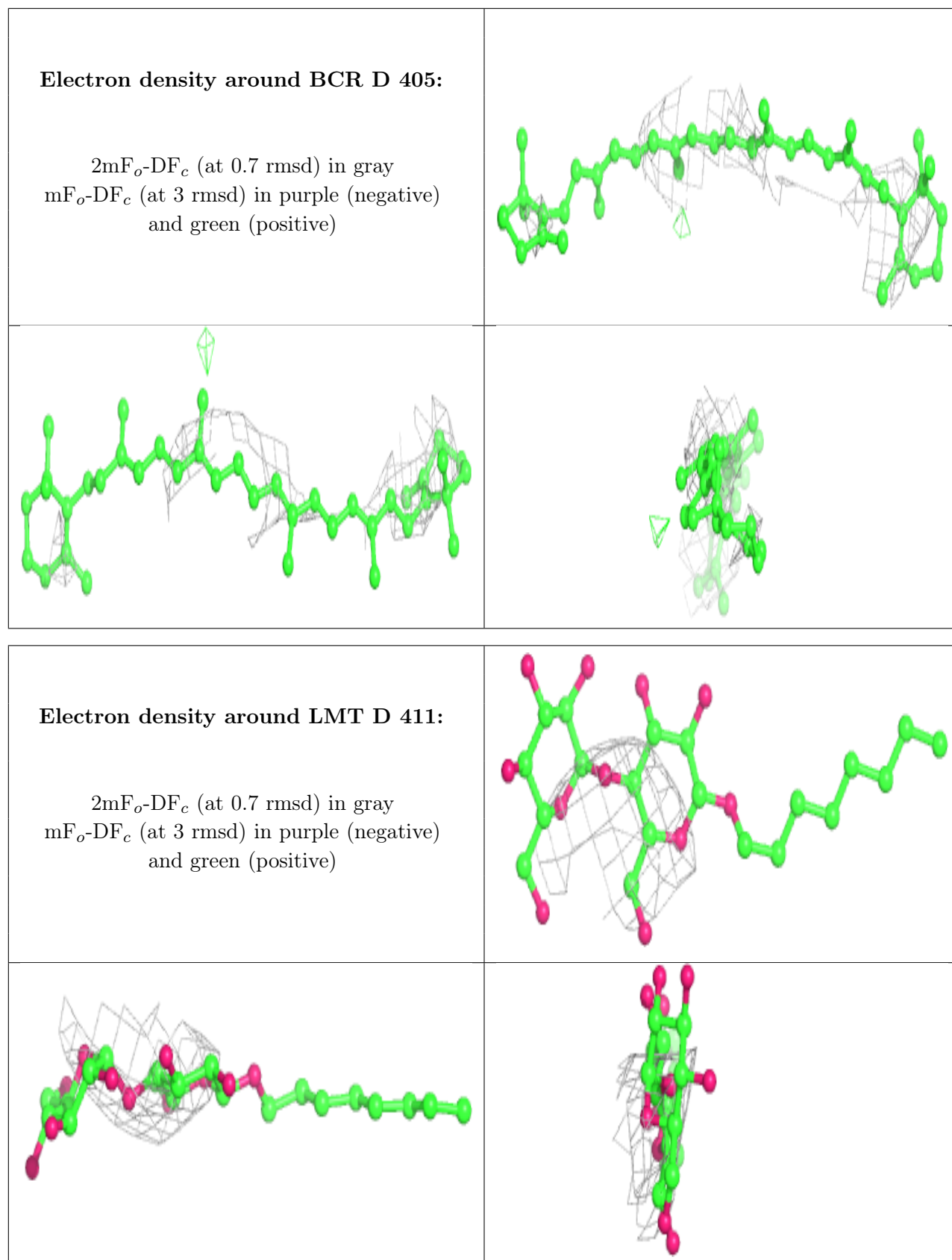




Electron density around CLA b 604:

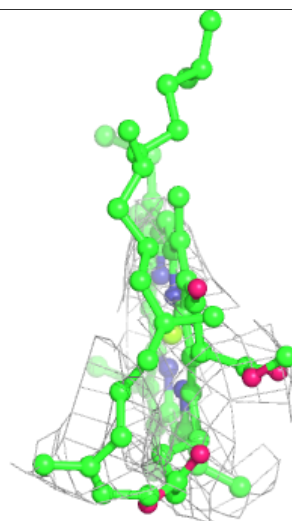
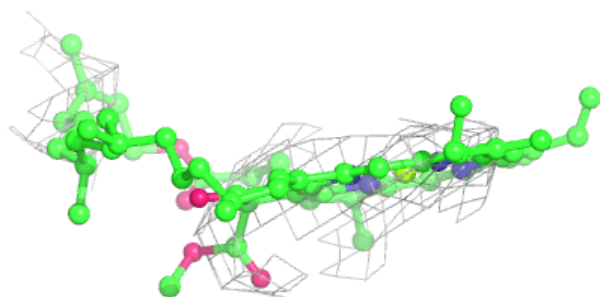
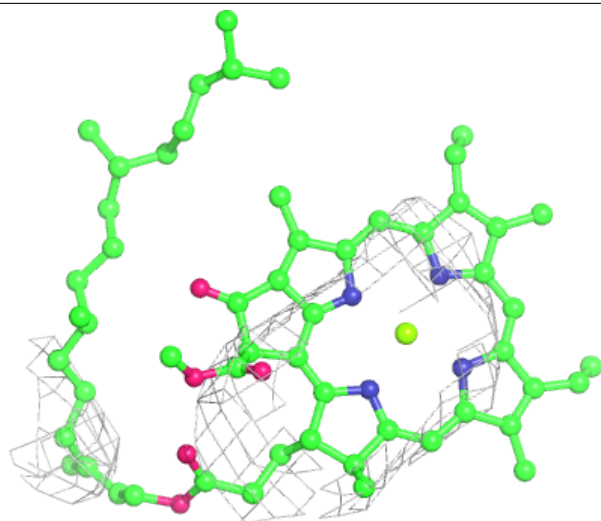
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

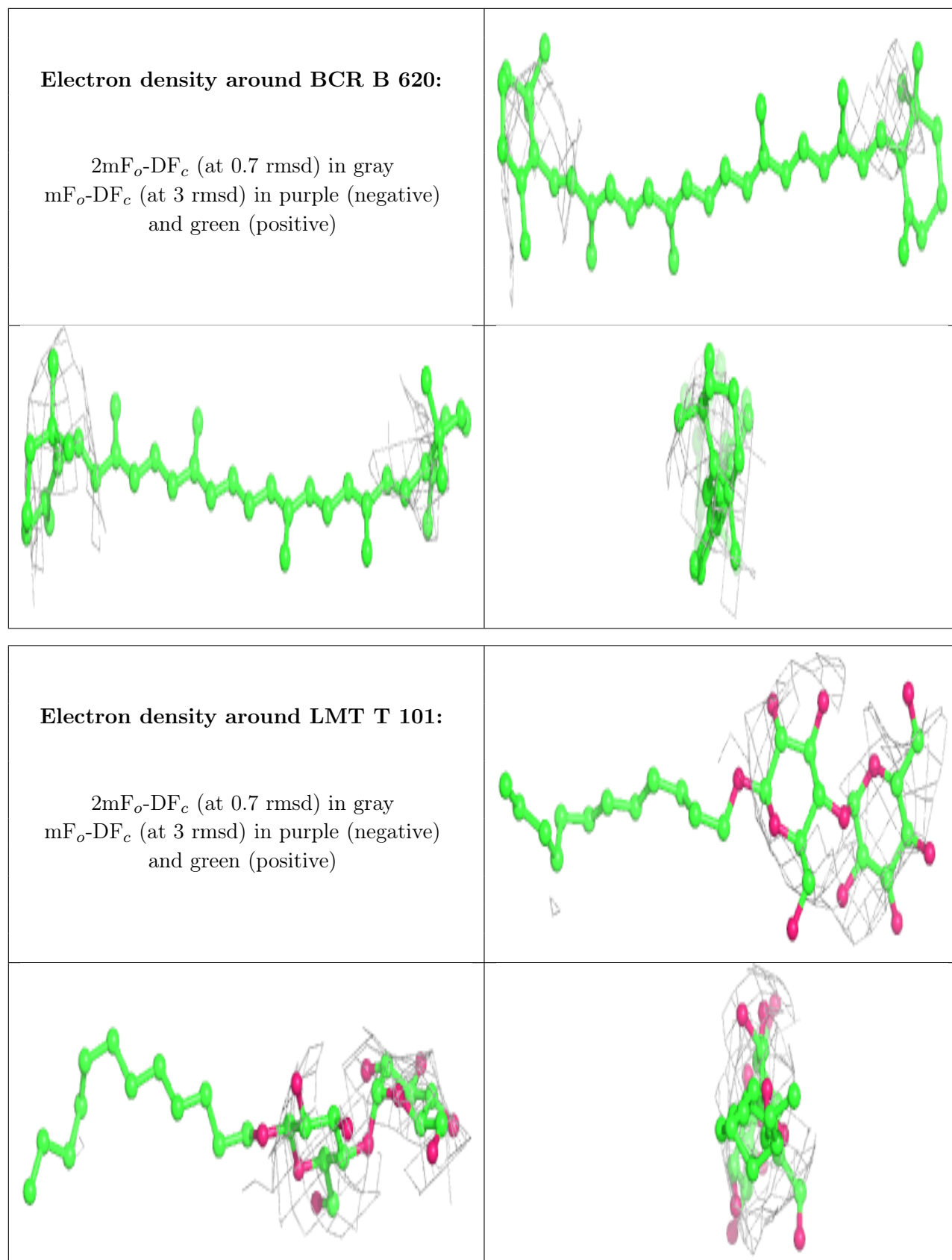


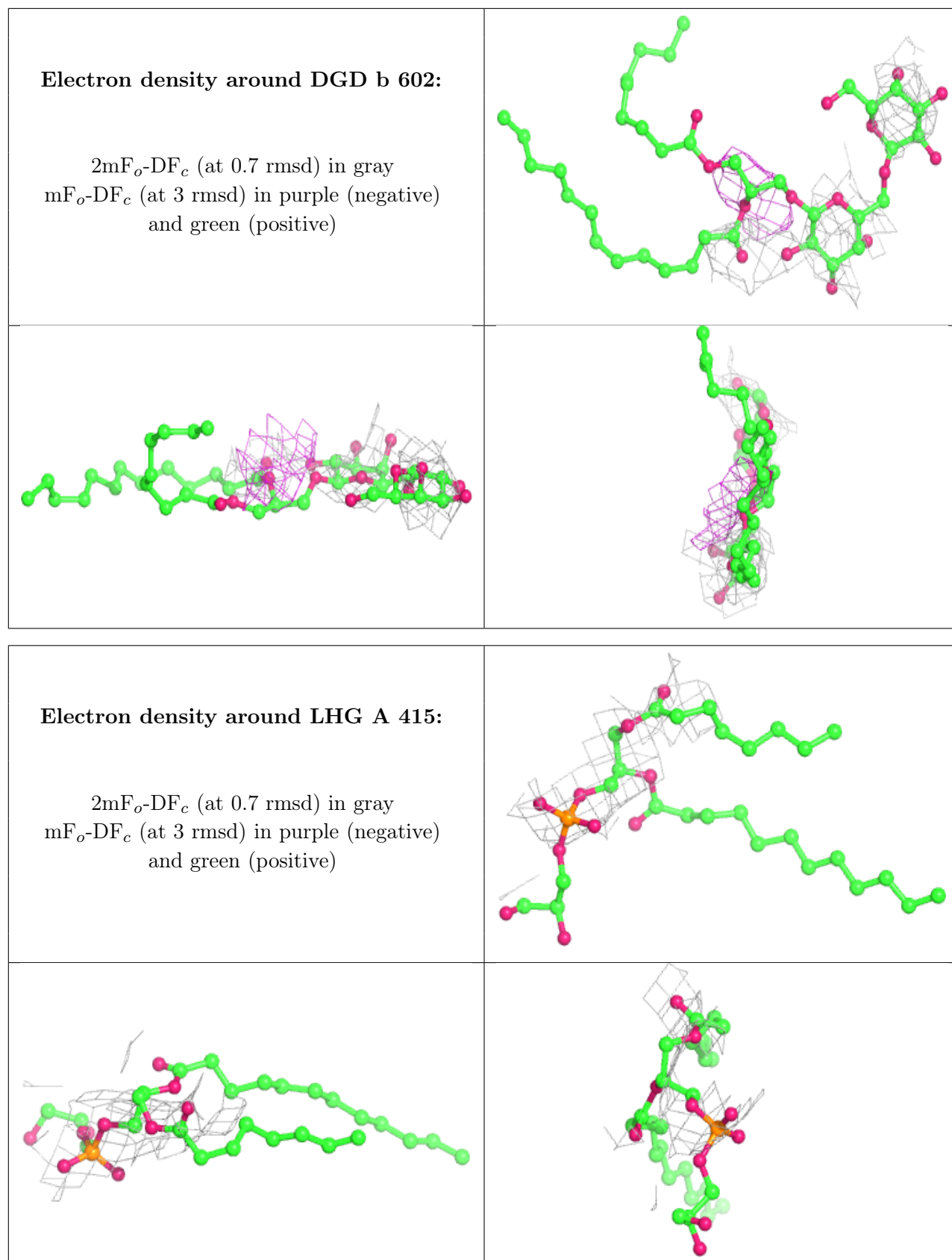


Electron density around CLA B 601:

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

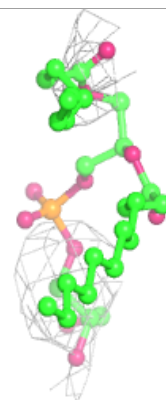
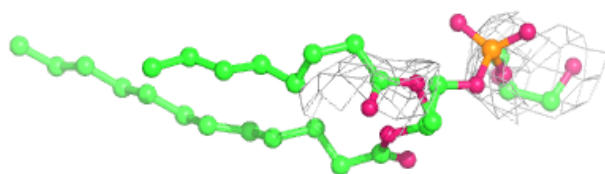
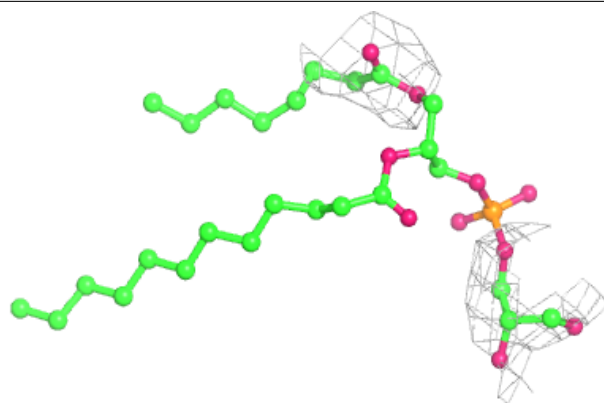




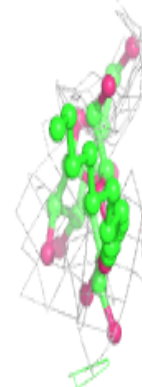
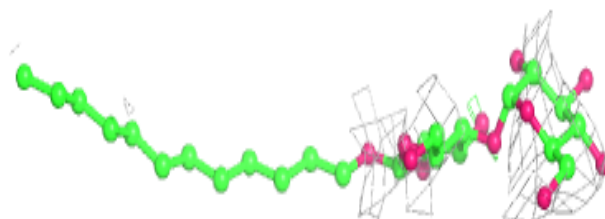
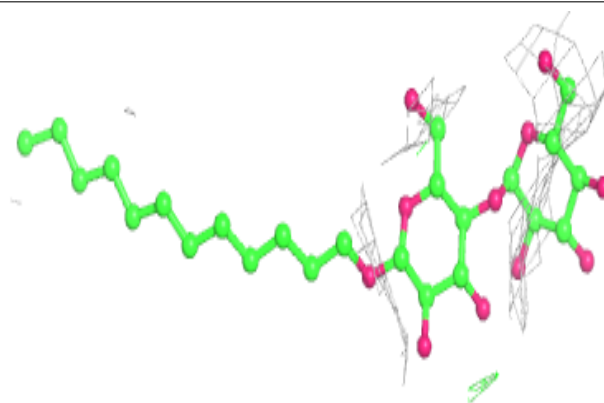


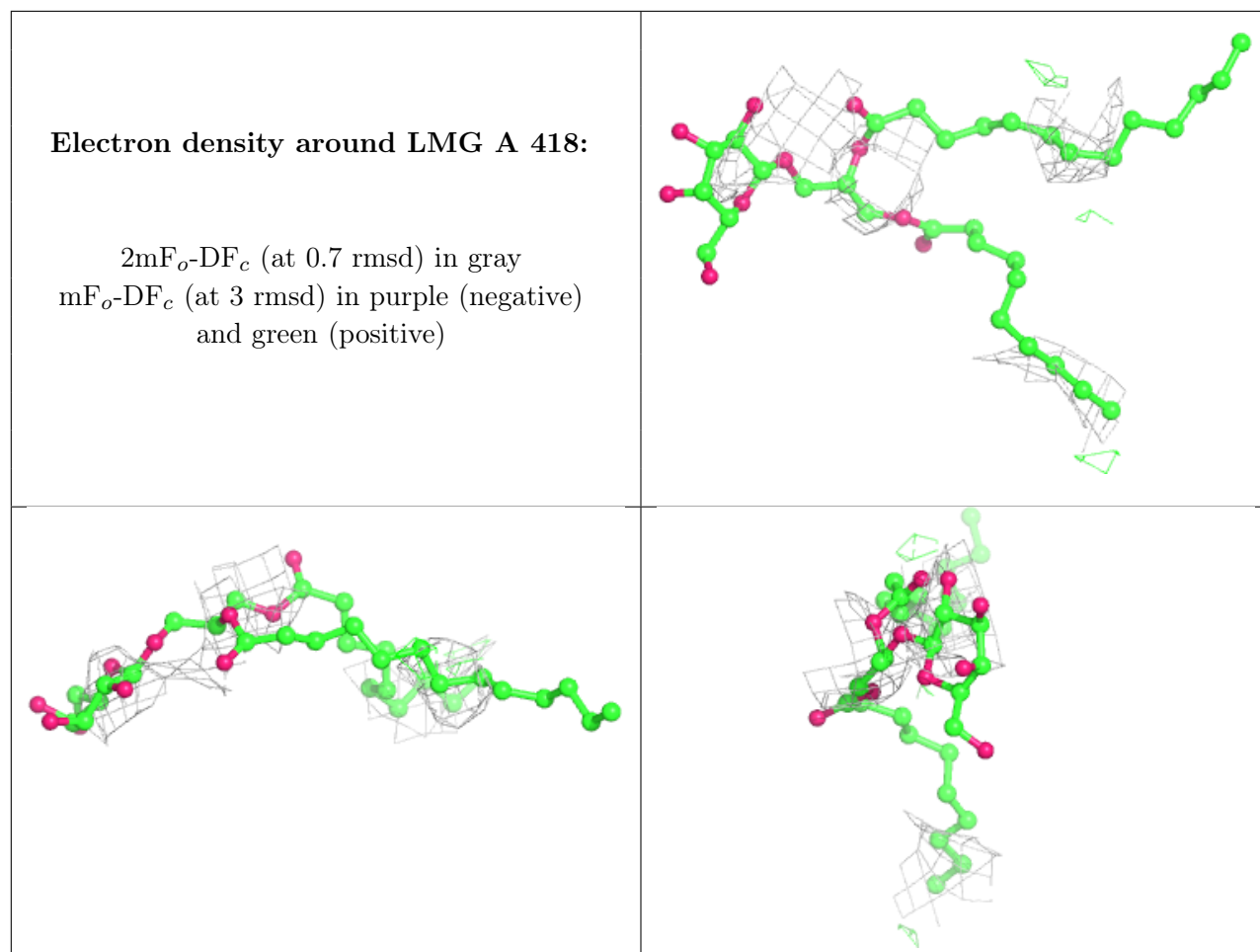
Electron density around LHG a 417:

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

**Electron density around LMT B 624:**

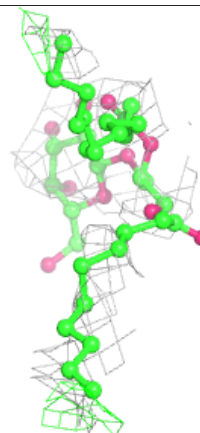
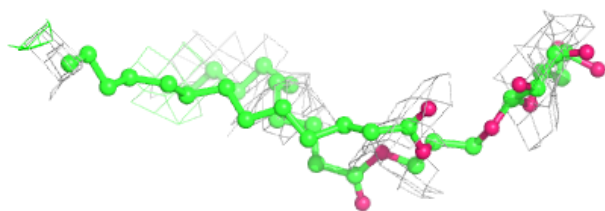
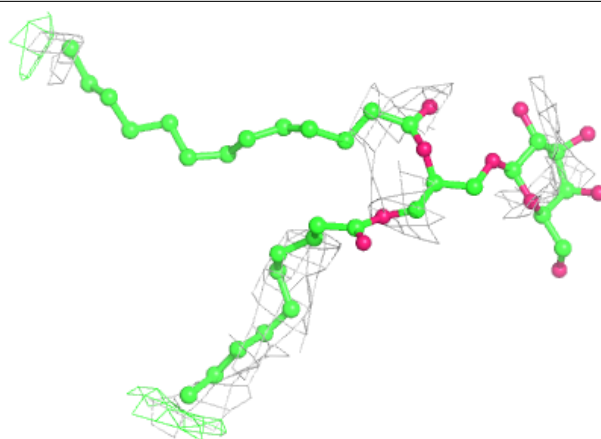
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



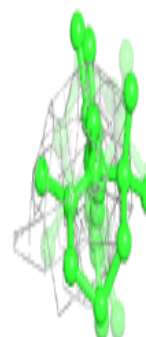
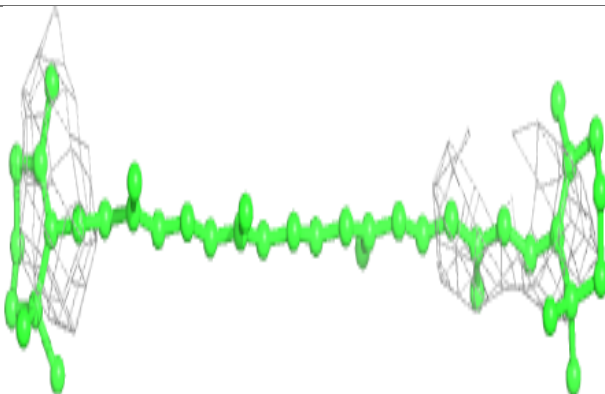
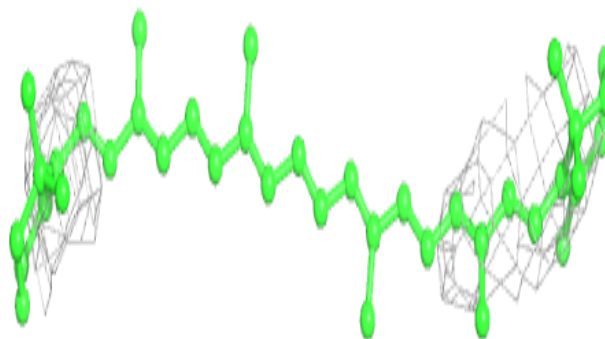


Electron density around LMG a 402:

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

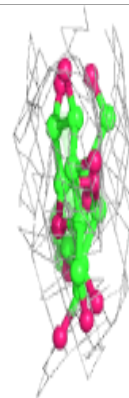
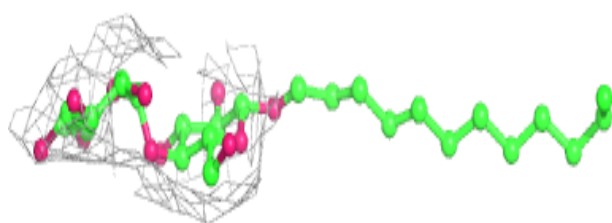
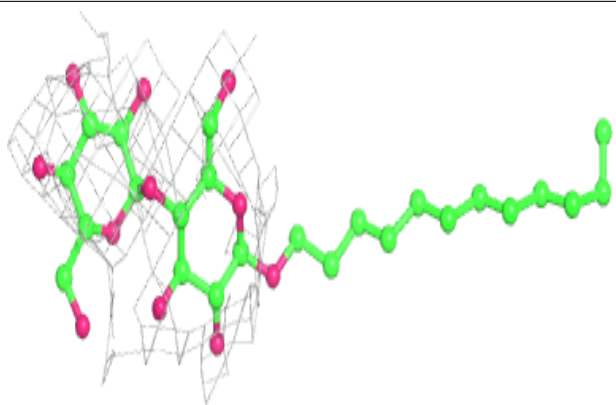
**Electron density around BCR A 410:**

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

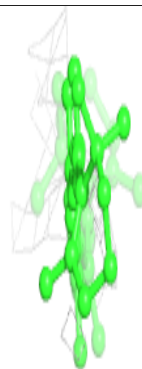
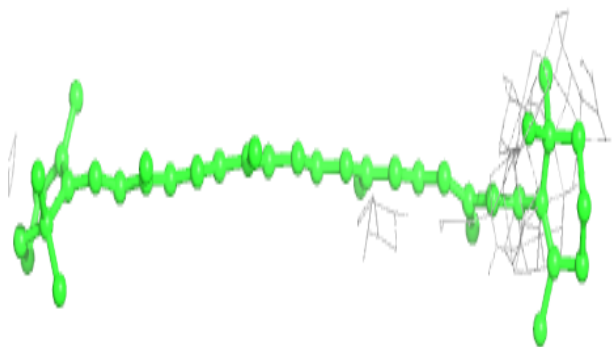
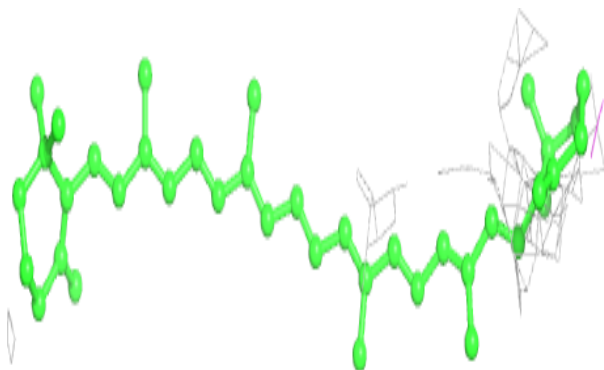


Electron density around LMT b 603:

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

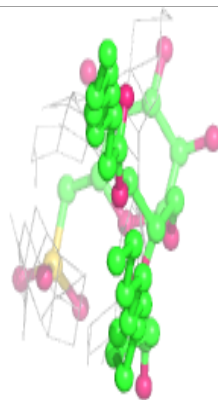
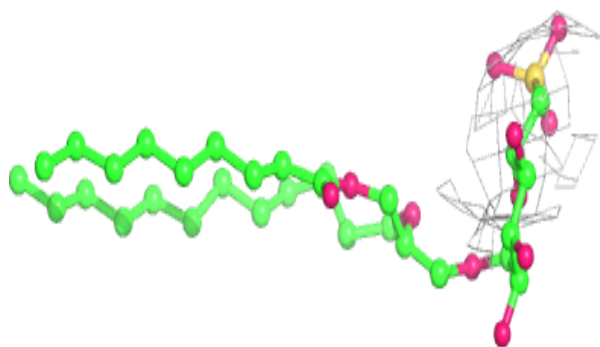
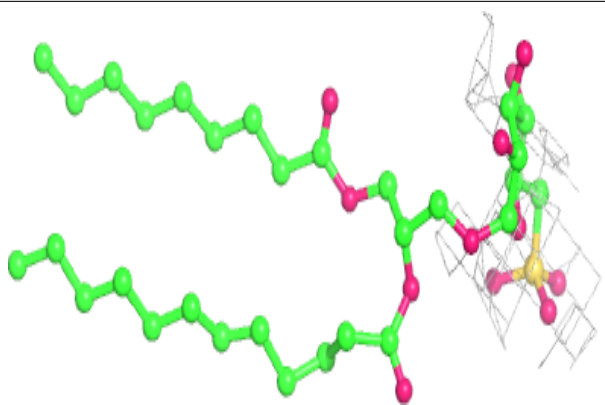
**Electron density around BCR H 101:**

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

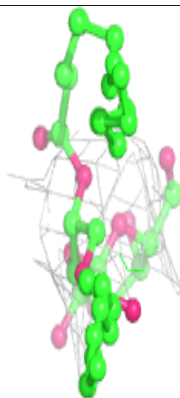
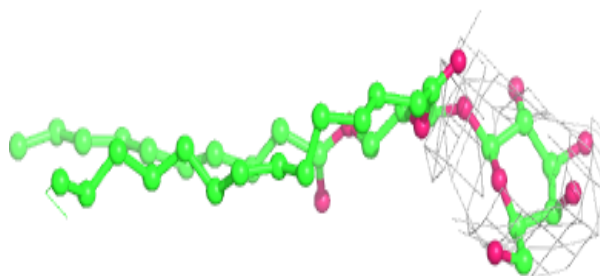
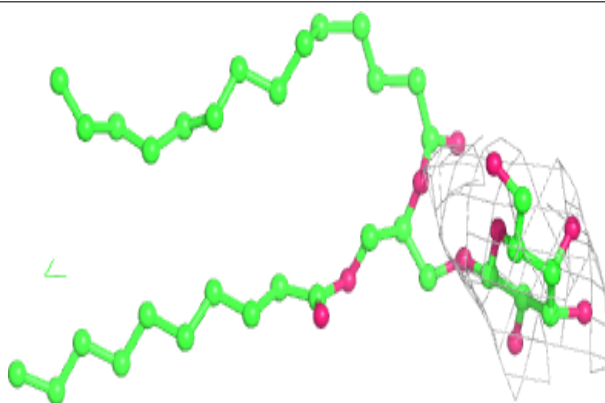


Electron density around SQD d 407:

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

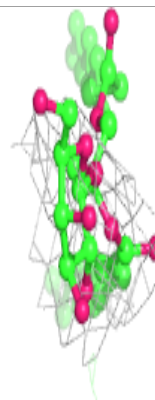
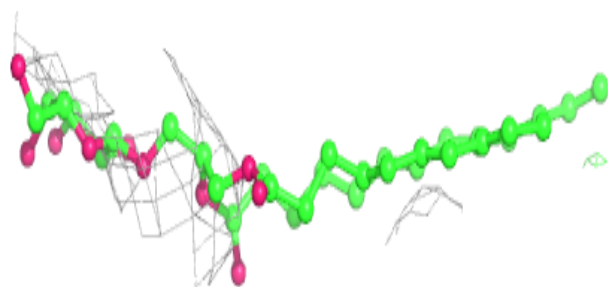
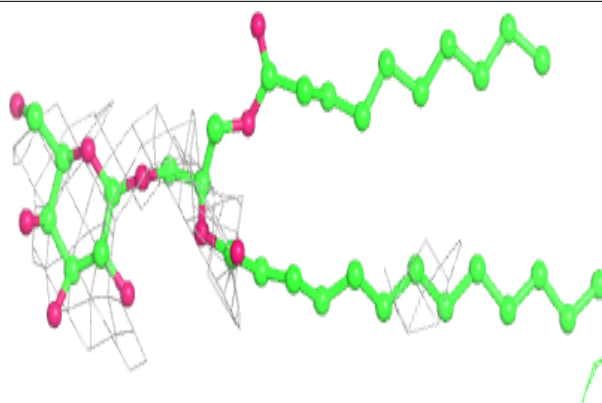
**Electron density around LMG I 101:**

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

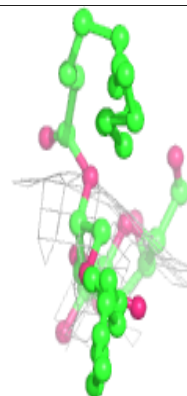
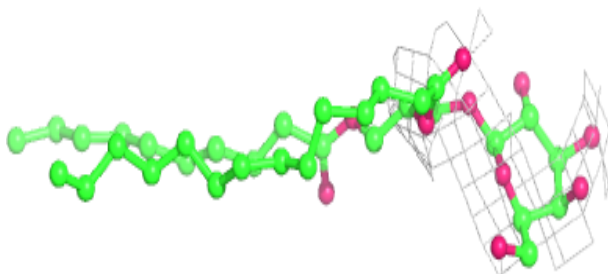
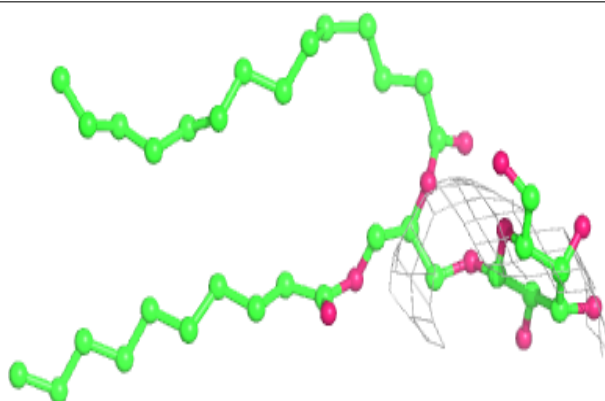


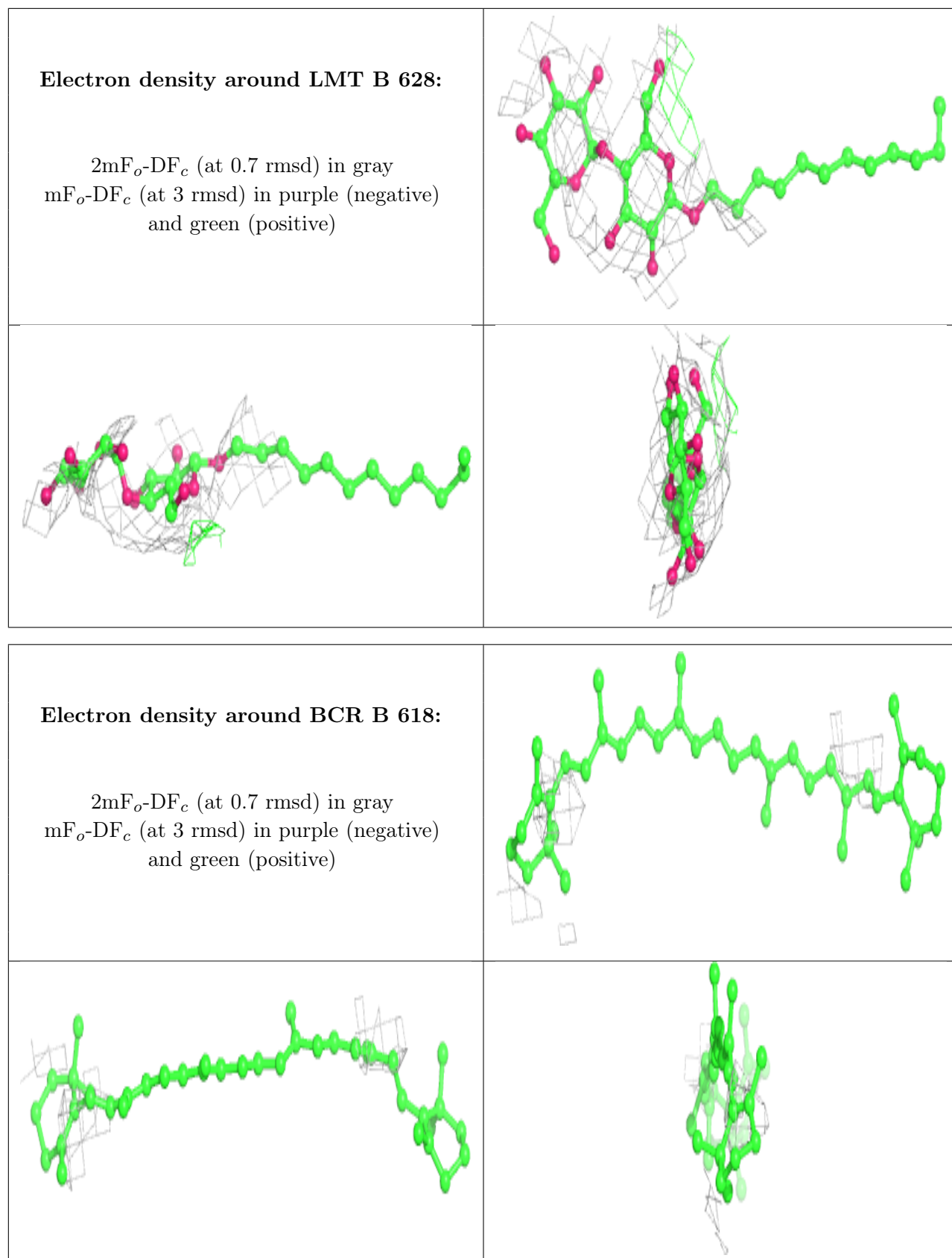
Electron density around LMG M 102:

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

**Electron density around LMG i 101:**

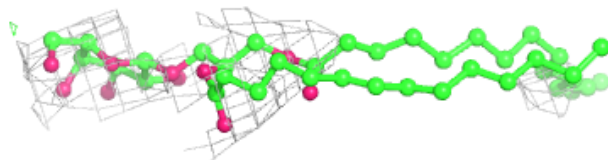
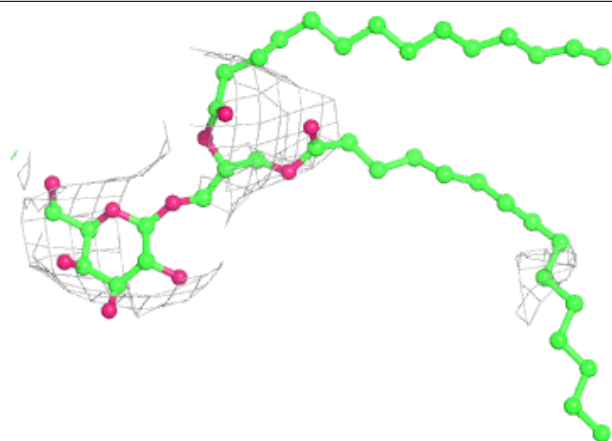
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



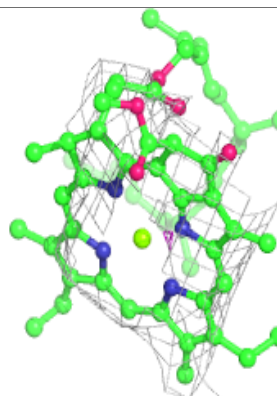
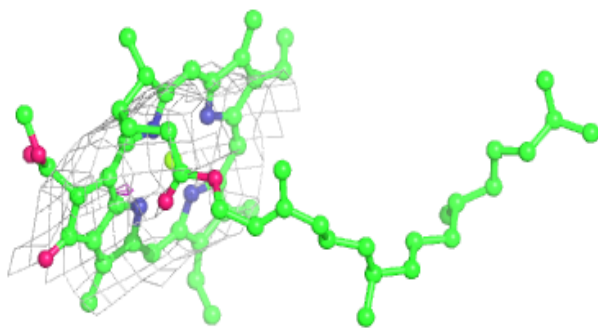
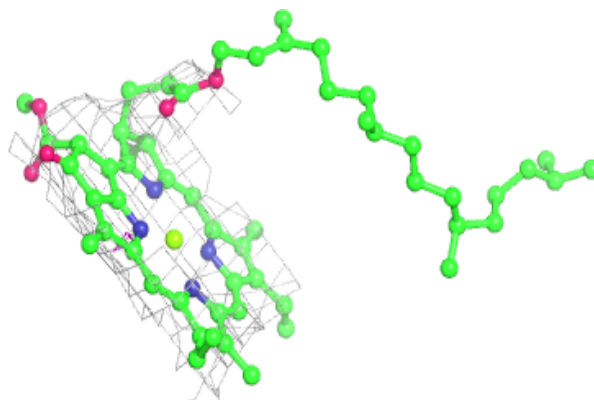


Electron density around LMG C 519:

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

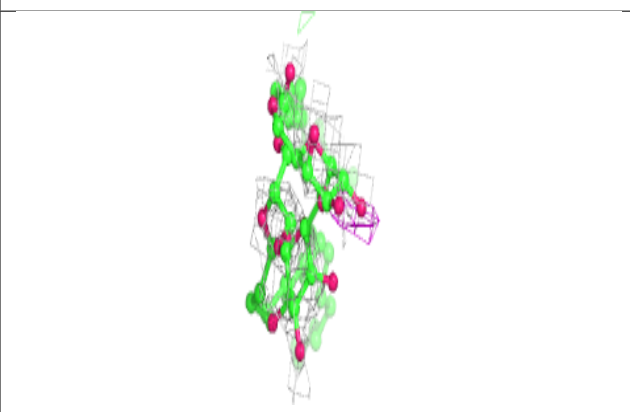
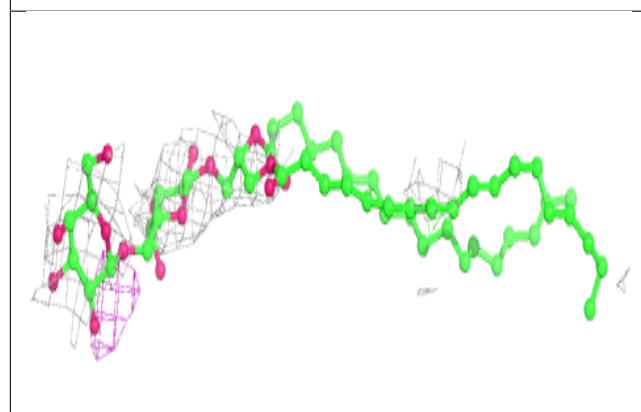
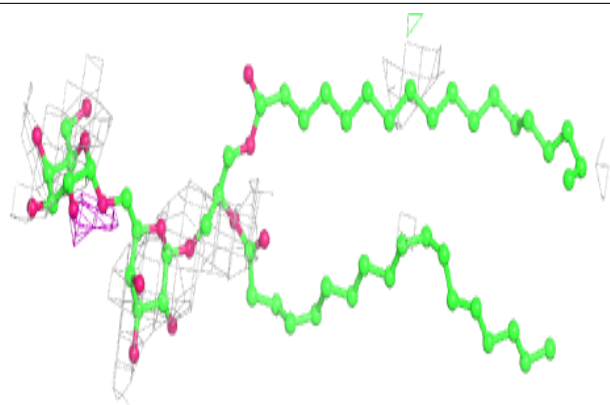
**Electron density around CLA c 513:**

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

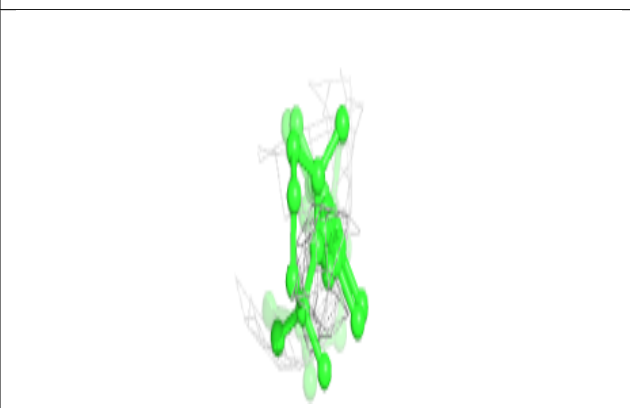
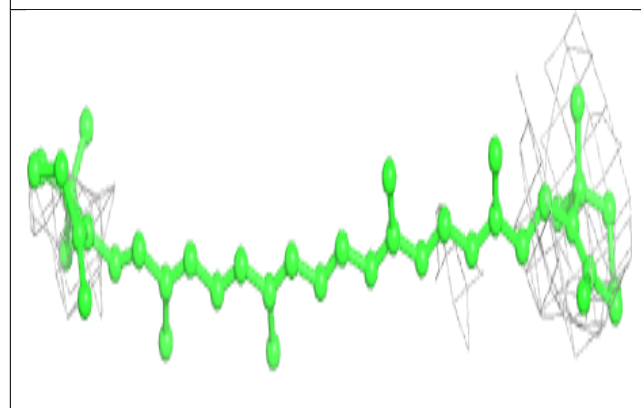
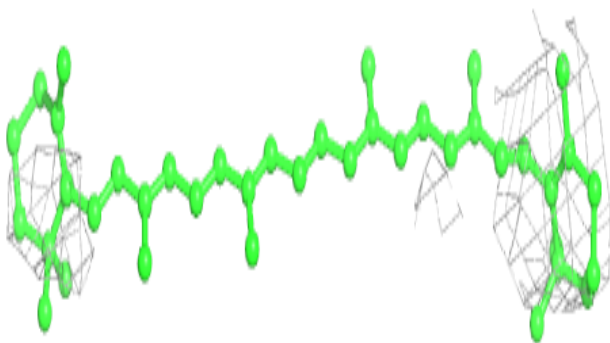


Electron density around DGD C 518:

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

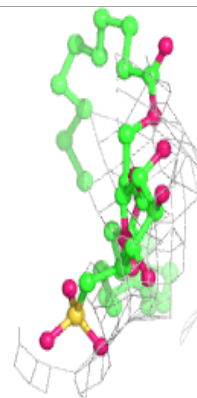
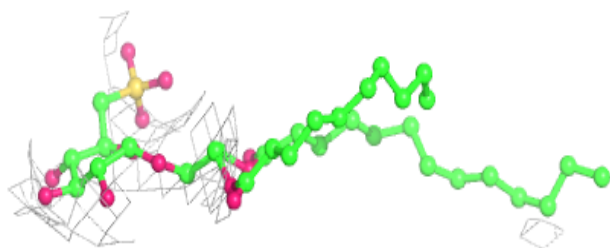
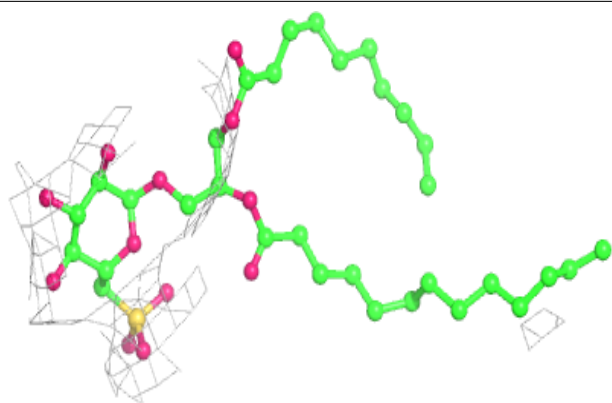
**Electron density around BCR b 621:**

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

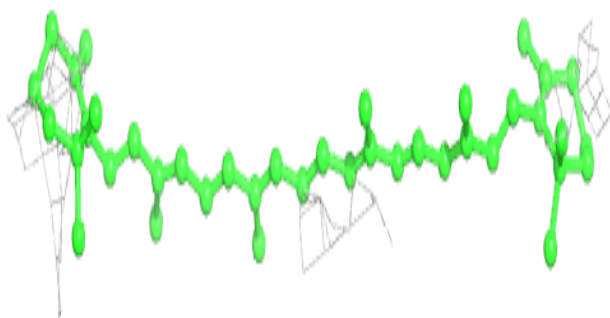
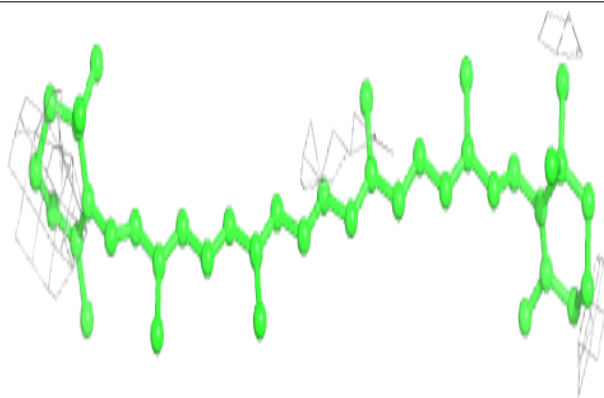


Electron density around SQD F 102:

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

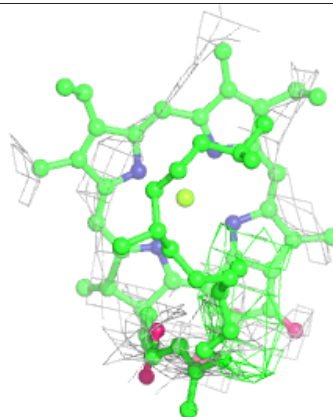
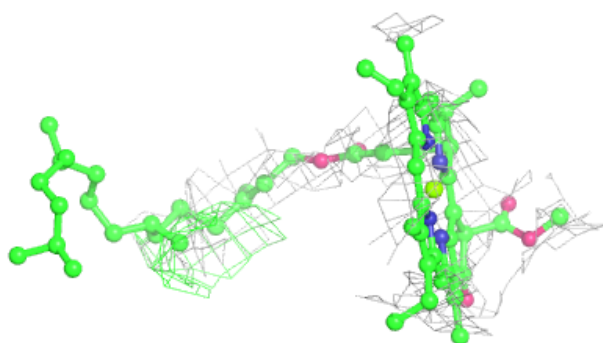
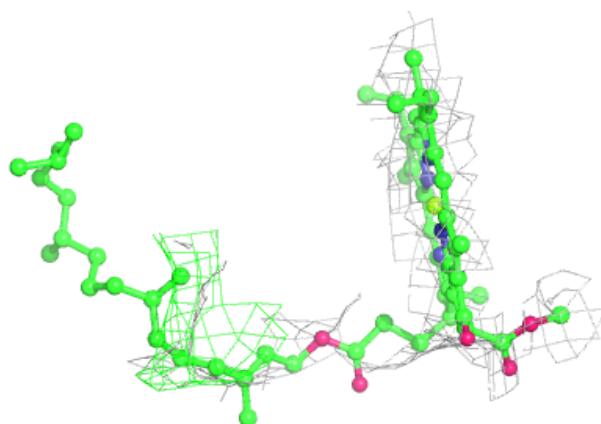
**Electron density around BCR c 516:**

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

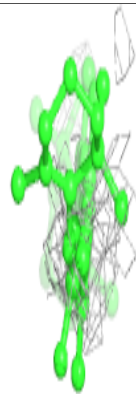
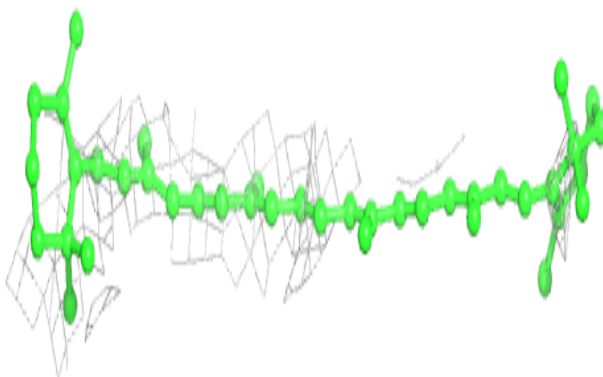
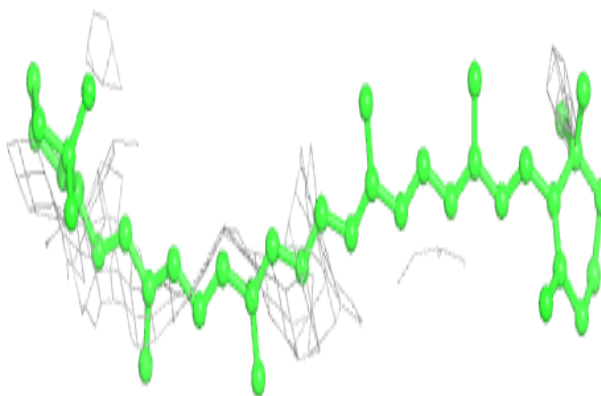


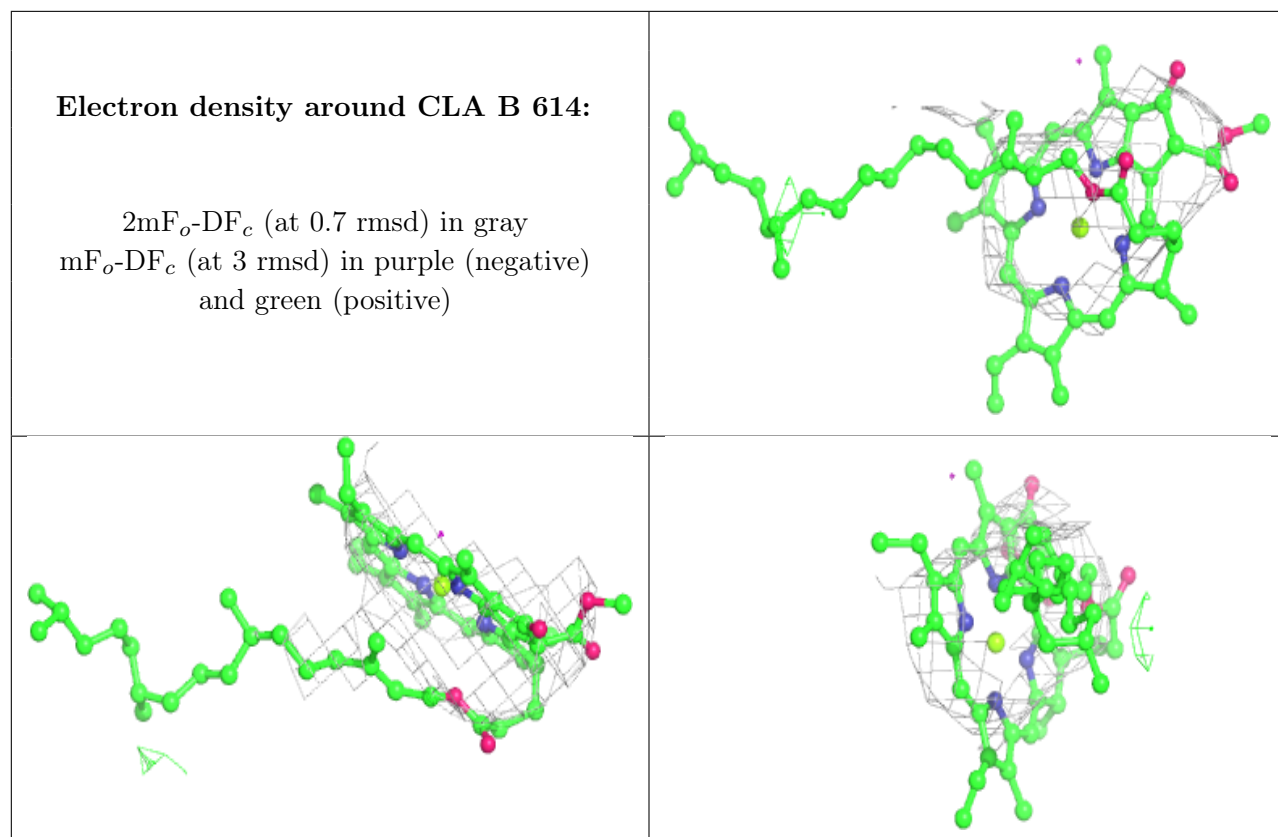
Electron density around CLA C 506:

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

**Electron density around BCR x 101:**

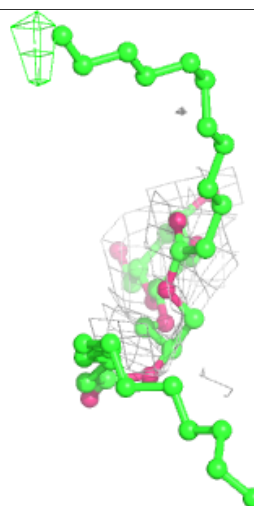
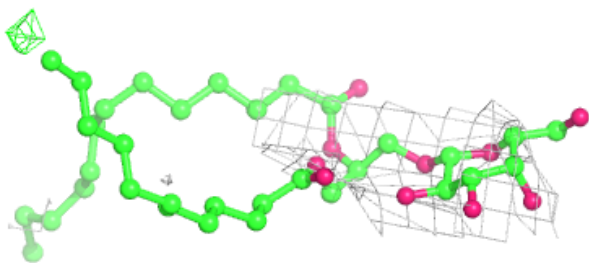
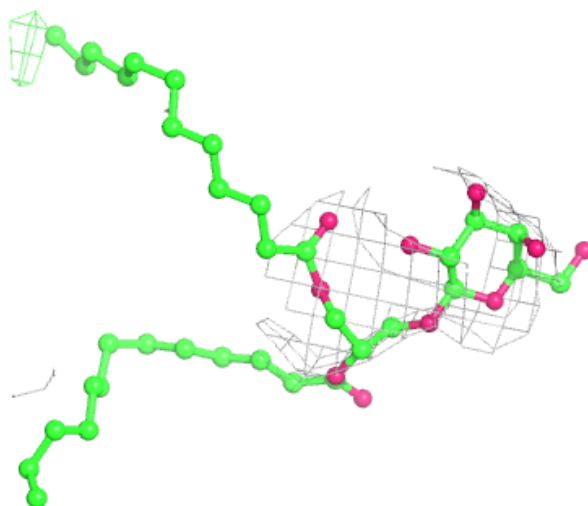
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

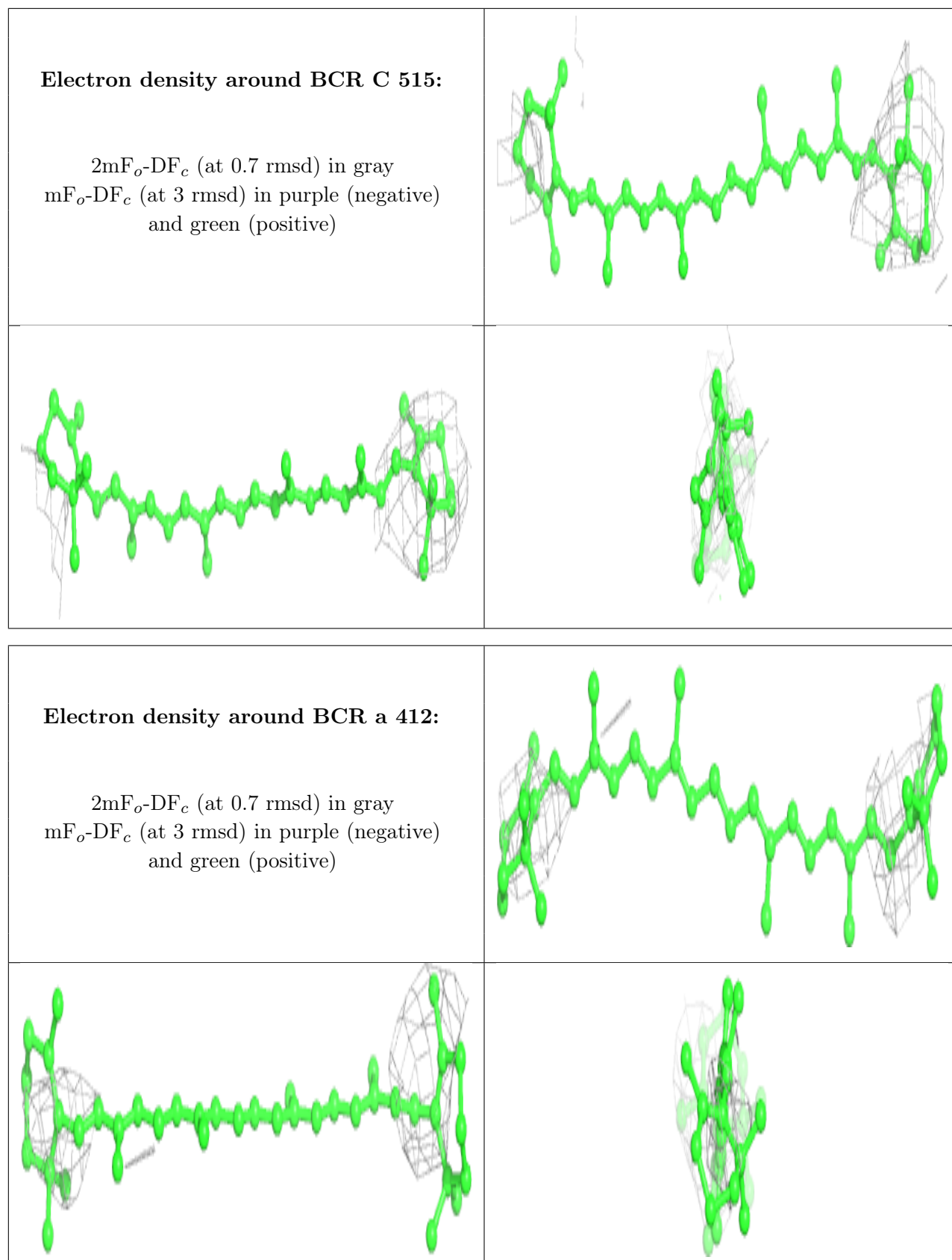




Electron density around LMG e 101:

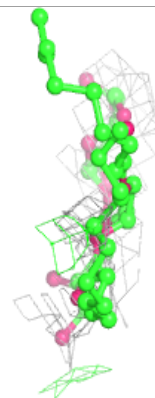
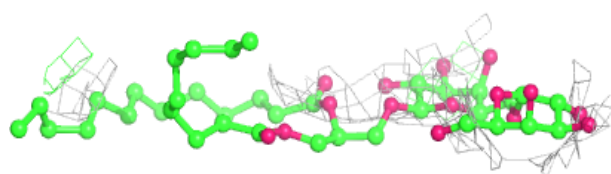
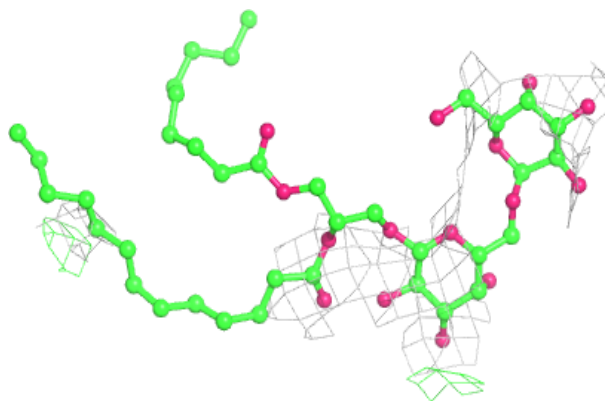
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



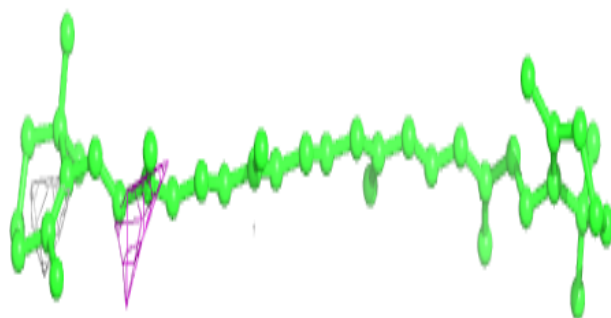
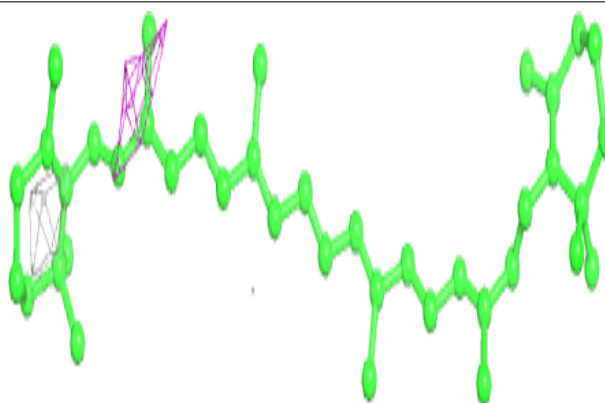


Electron density around DGD B 626:

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

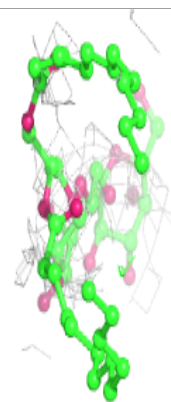
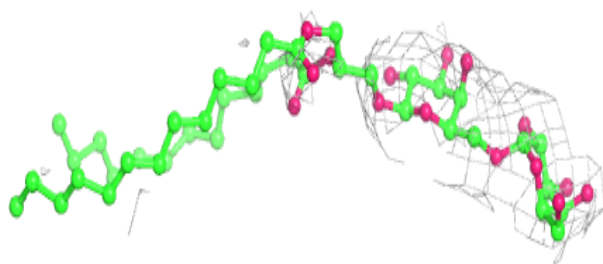
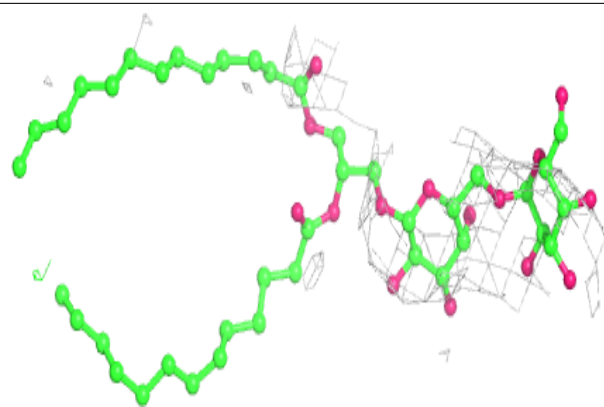
**Electron density around BCR k 102:**

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

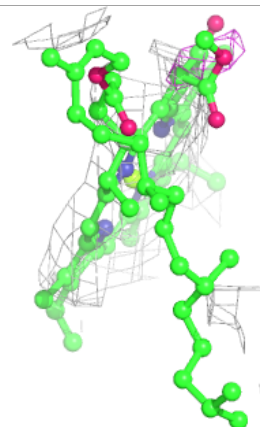
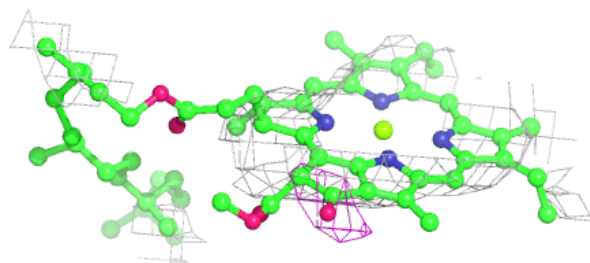
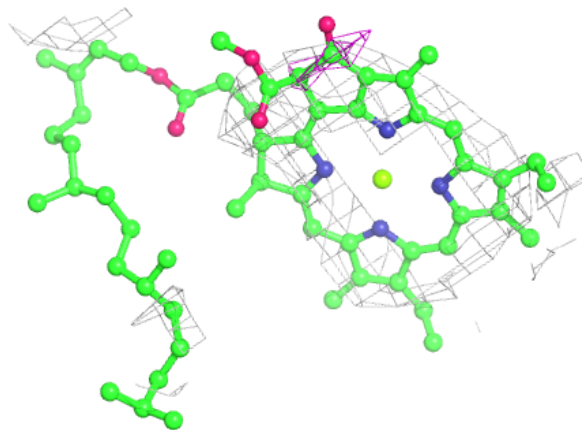


Electron density around DGD A 411:

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

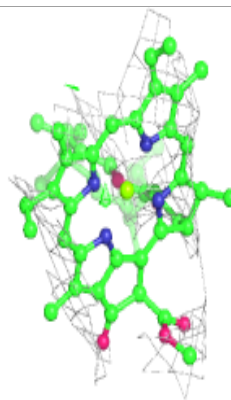
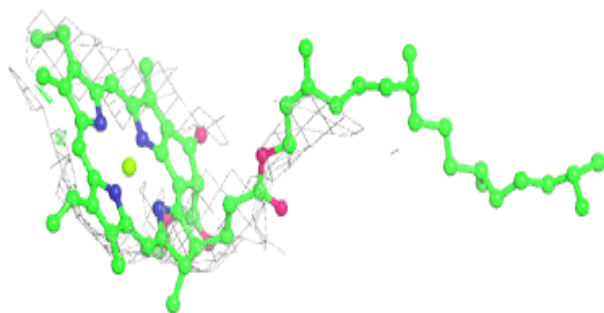
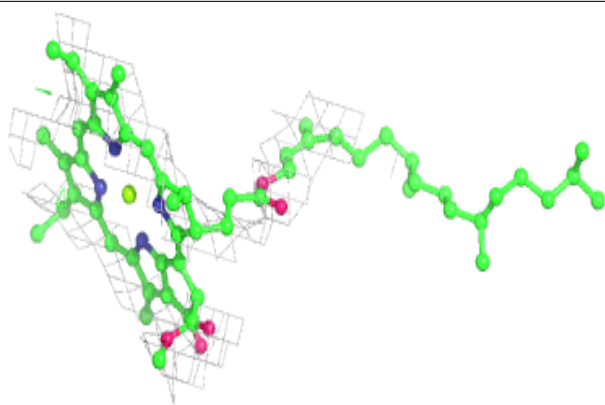
**Electron density around CLA b 619:**

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

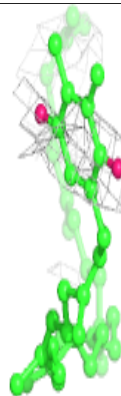
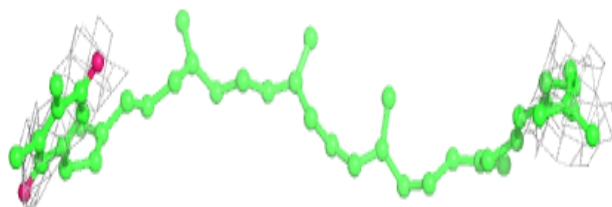
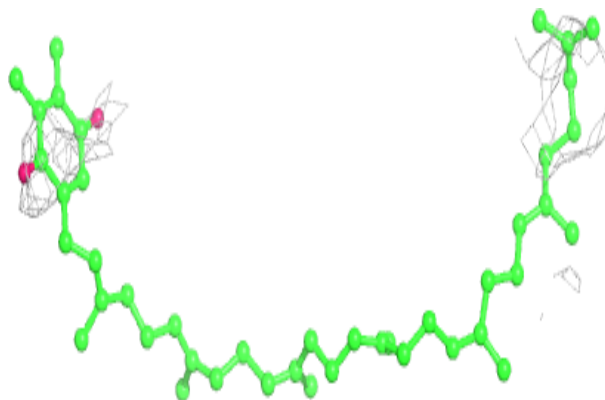


Electron density around CLA C 502:

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

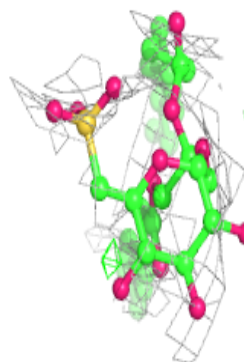
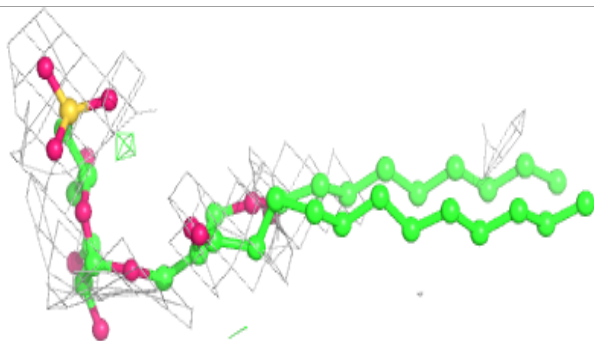
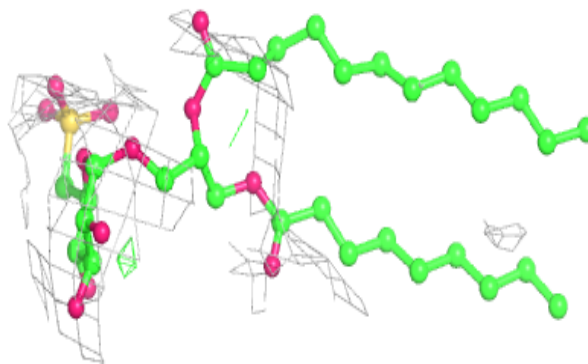
**Electron density around PL9 A 408:**

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

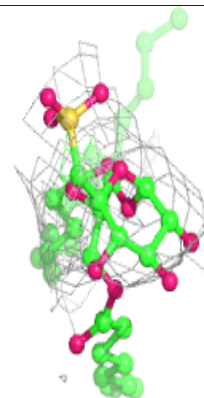
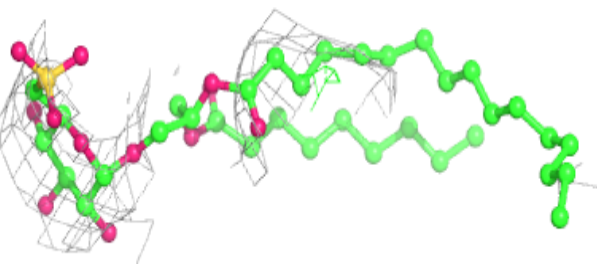
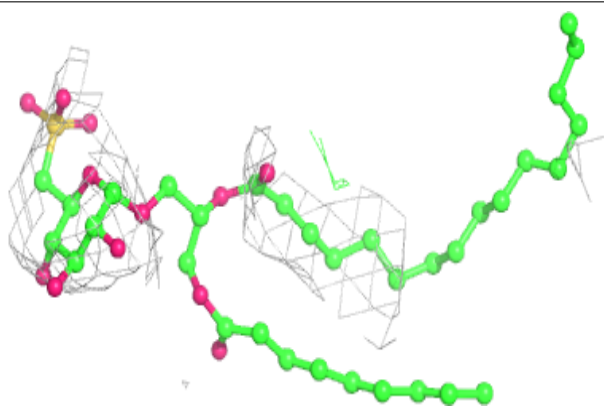


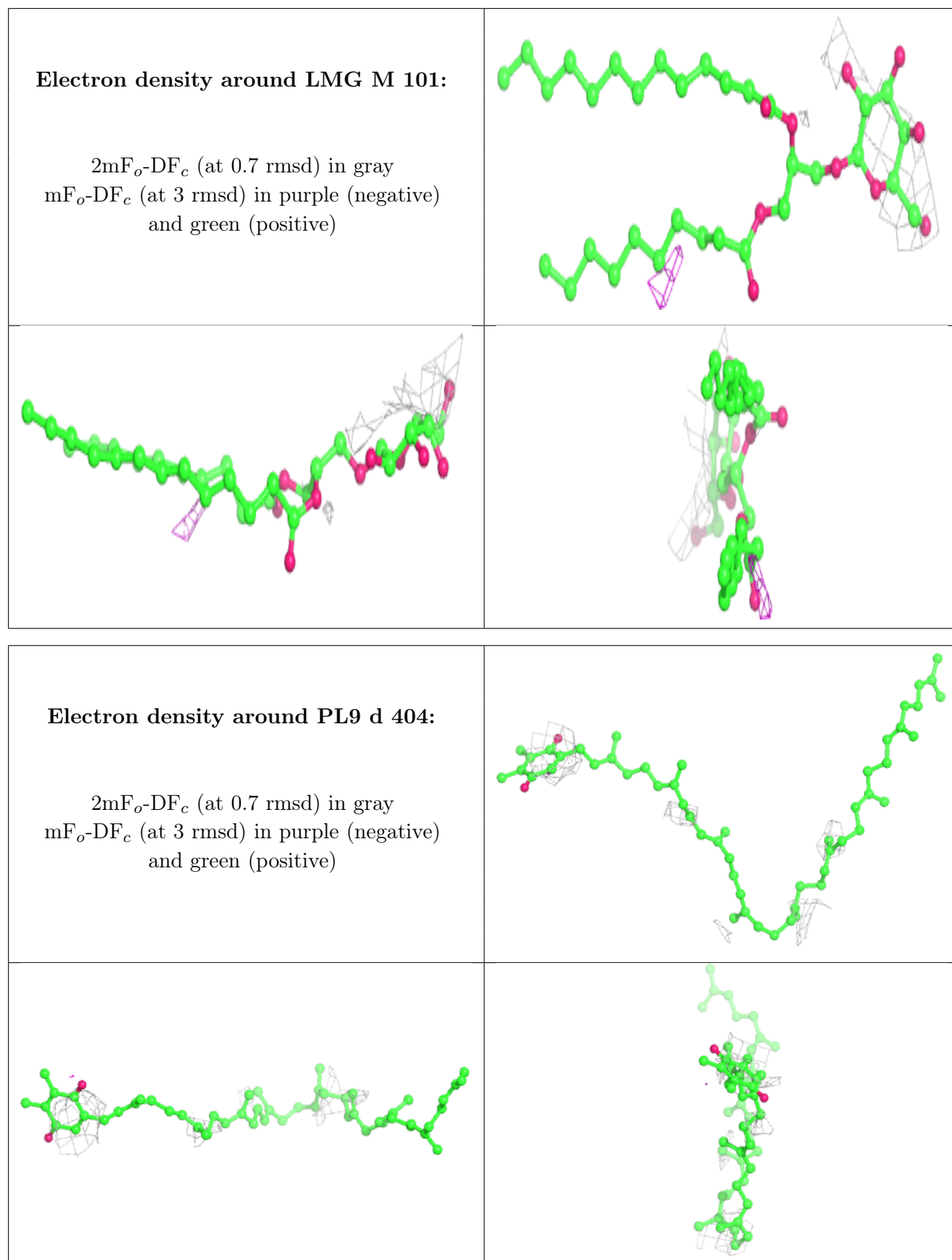
Electron density around SQD D 409:

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

**Electron density around SQD b 601:**

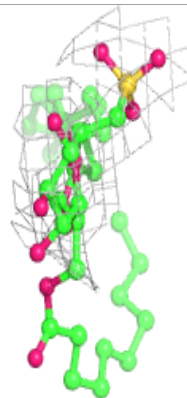
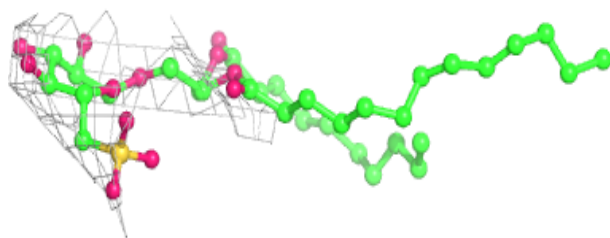
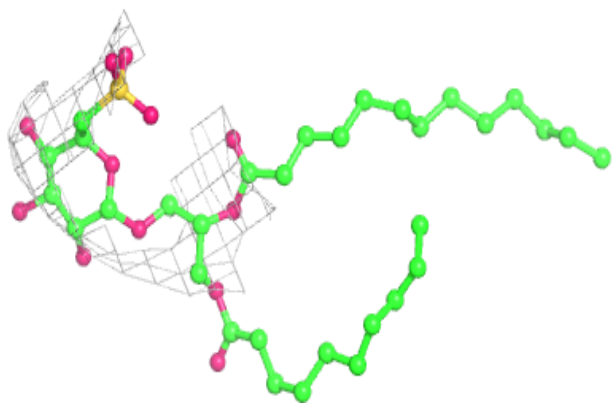
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



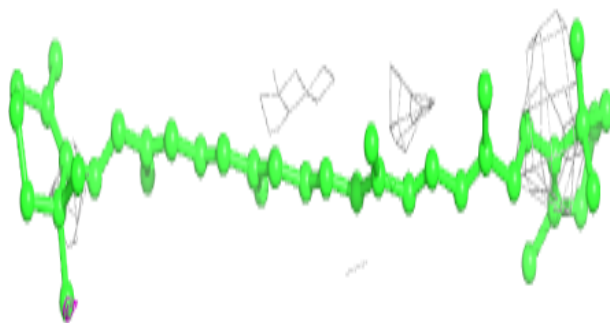
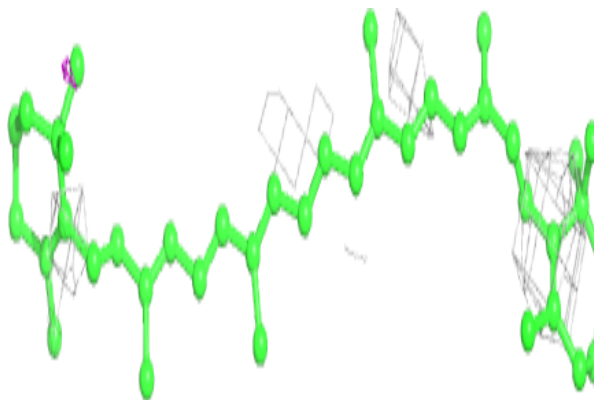


Electron density around SQD f 103:

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

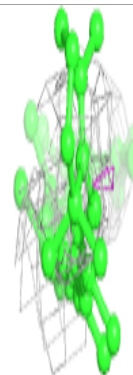
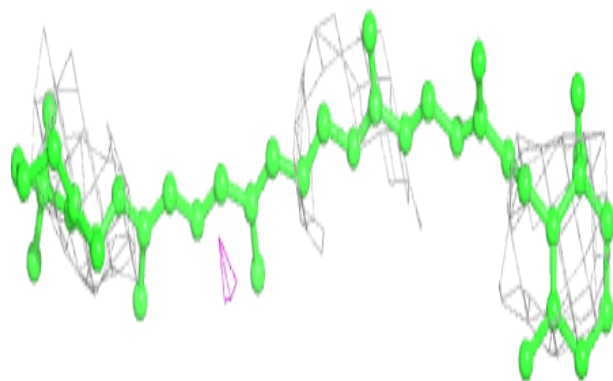
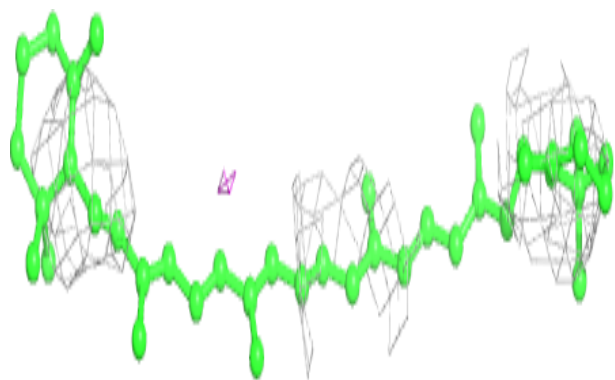
**Electron density around BCR K 102:**

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



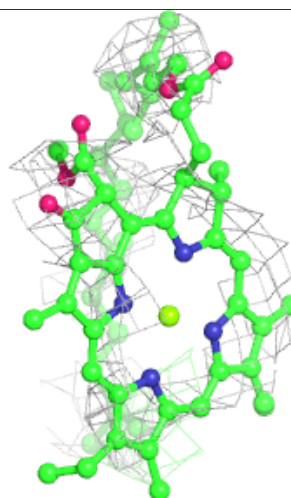
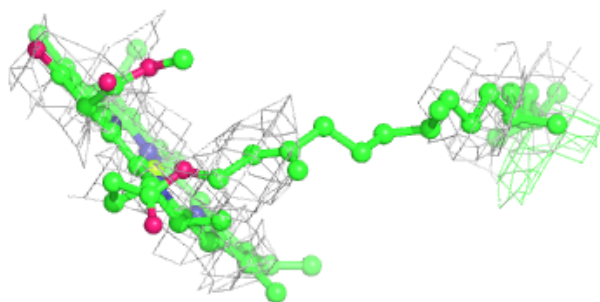
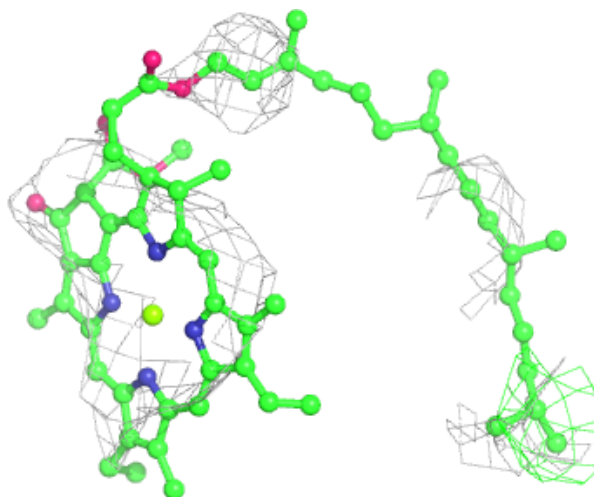
Electron density around BCR f 102:

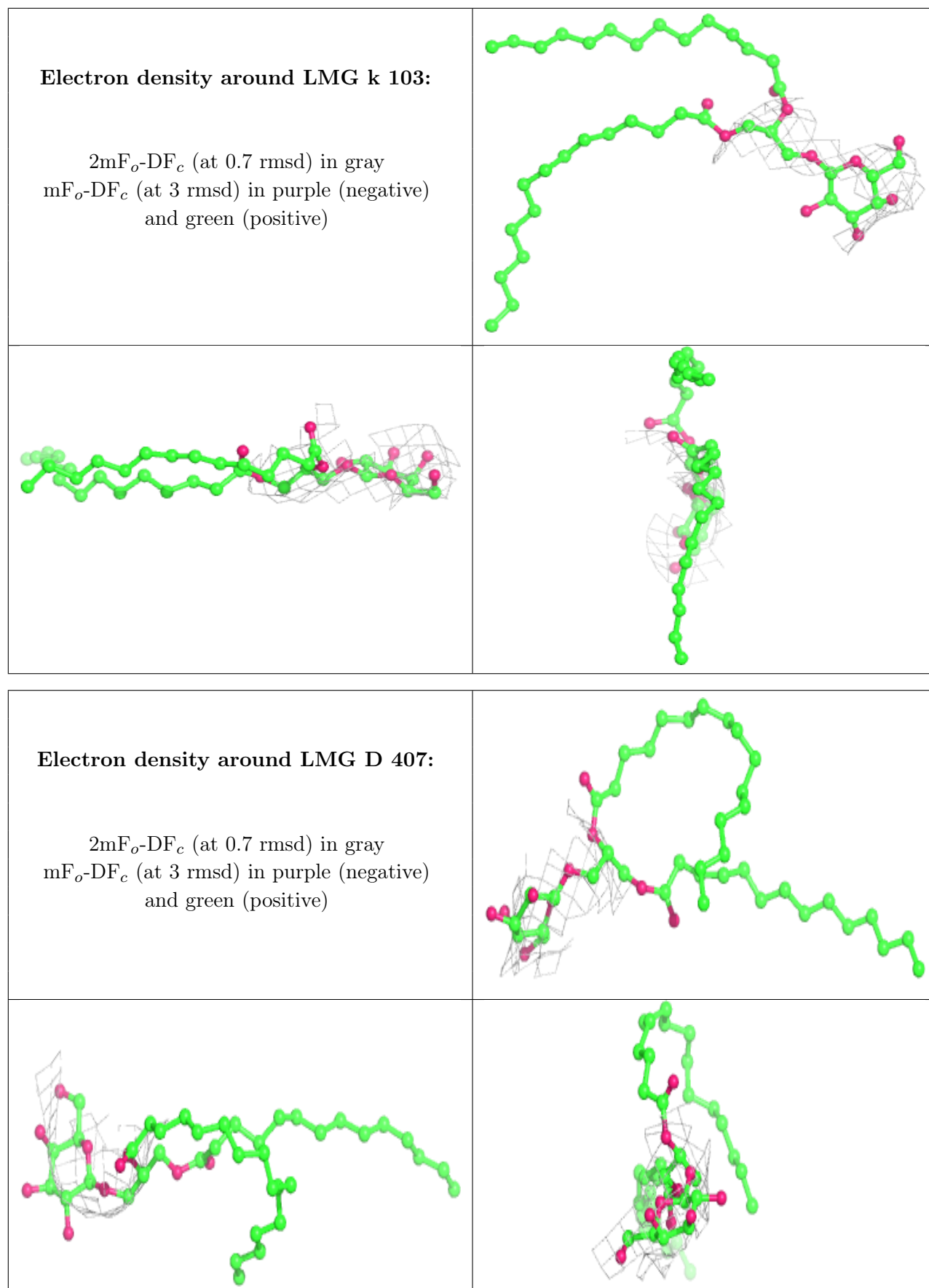
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 507:

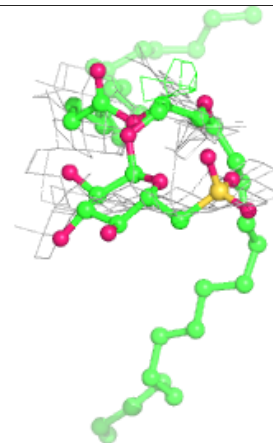
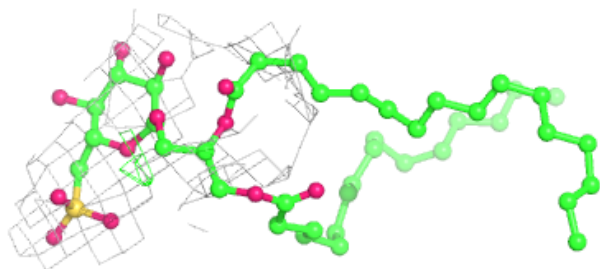
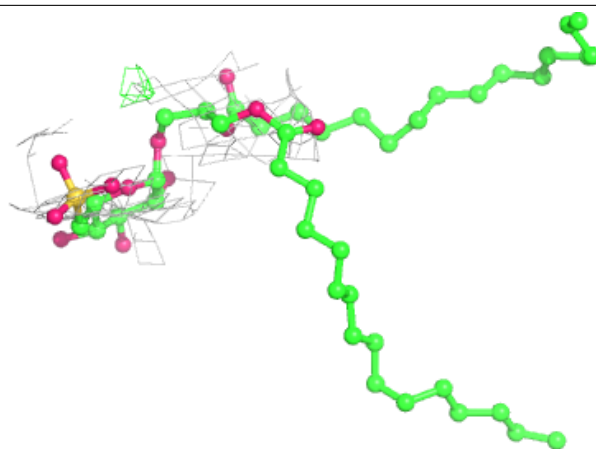
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



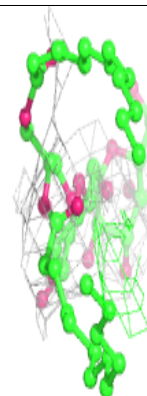
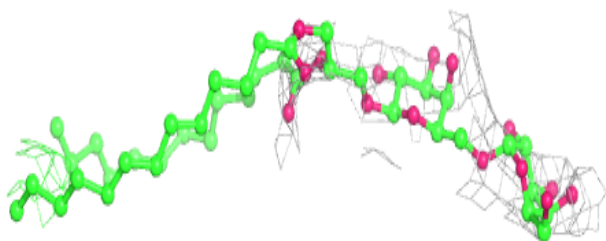
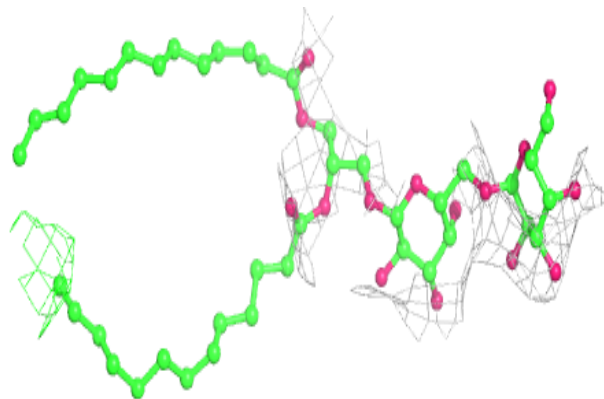


Electron density around SQD a 401:

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

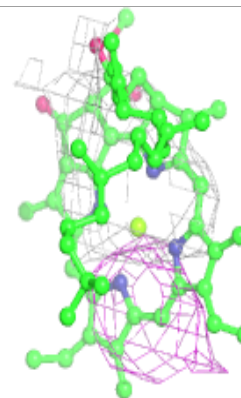
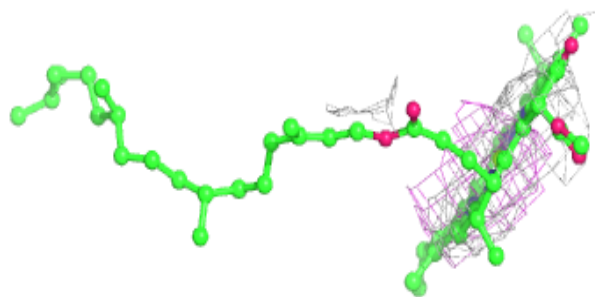
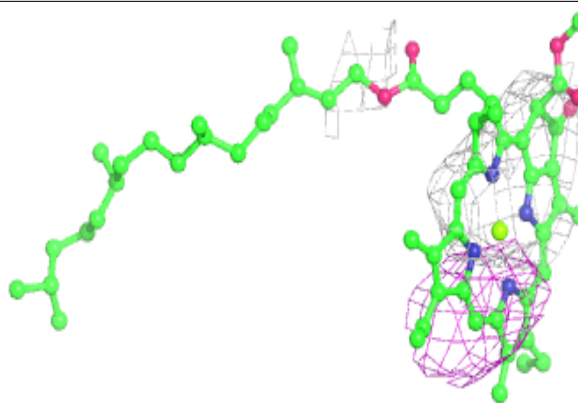
**Electron density around DGD a 413:**

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

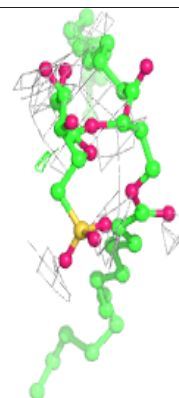
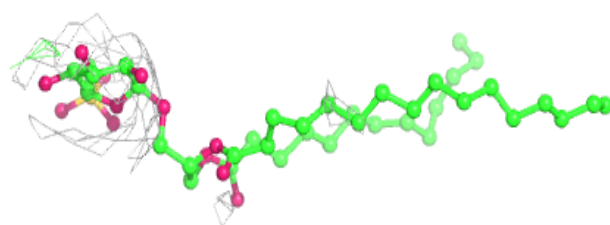
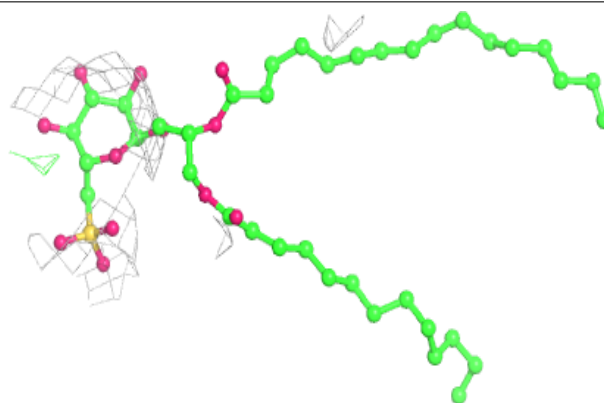


Electron density around CLA a 409:

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

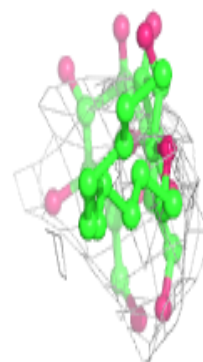
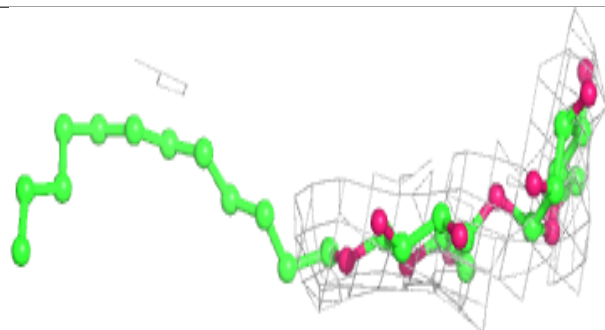
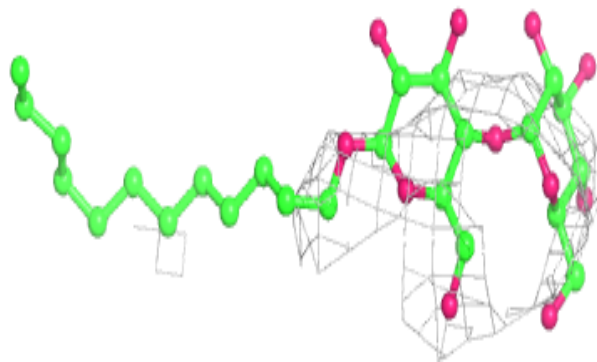
**Electron density around SQD a 415:**

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

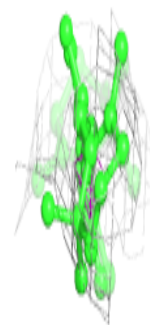
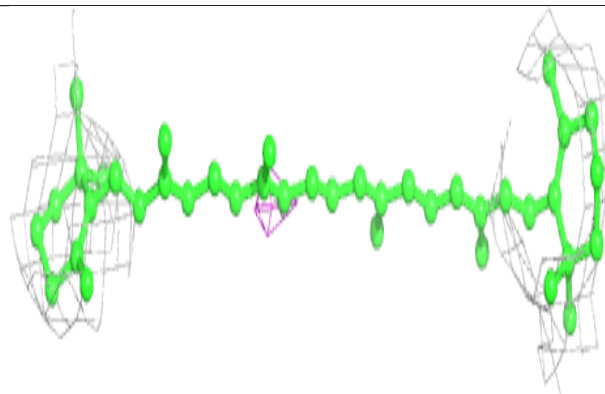
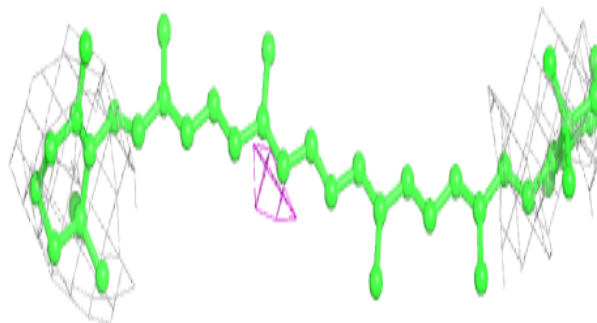


Electron density around LMT b 625:

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

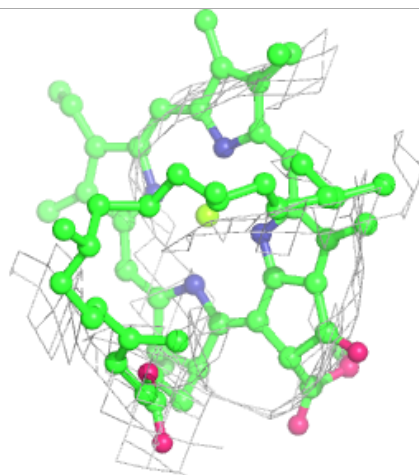
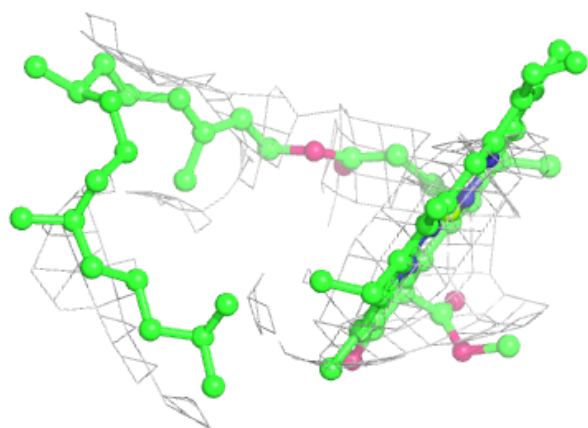
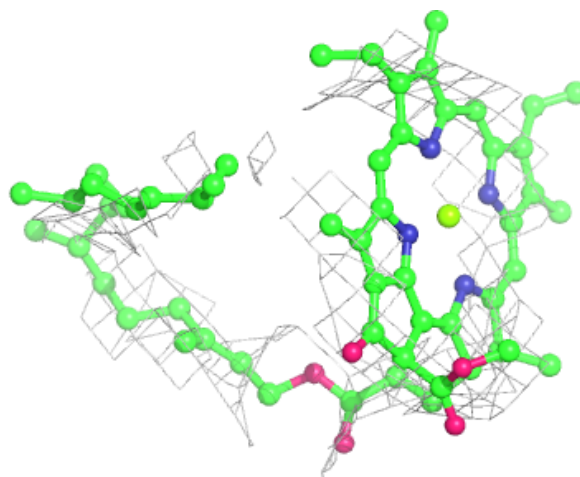
**Electron density around BCR Z 101:**

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



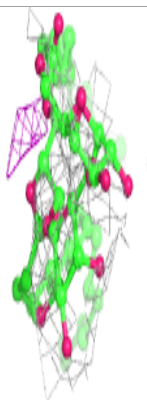
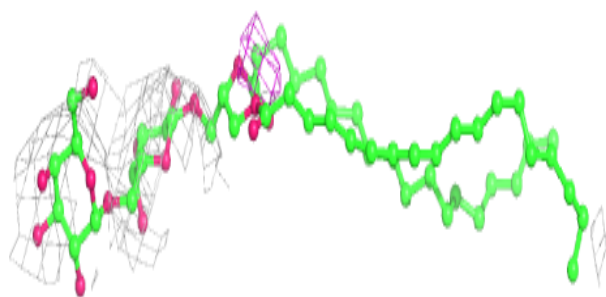
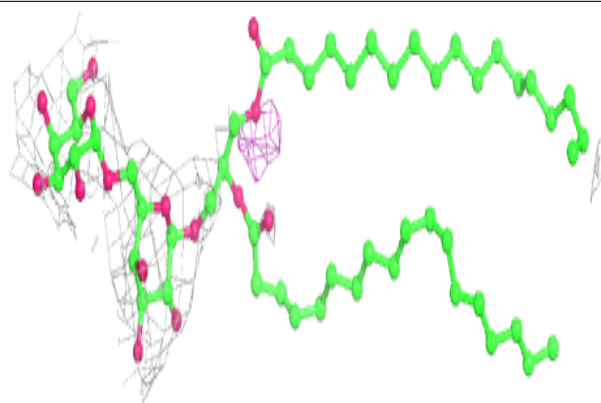
Electron density around CLA C 503:

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

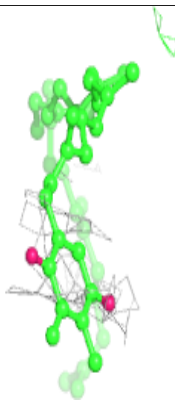
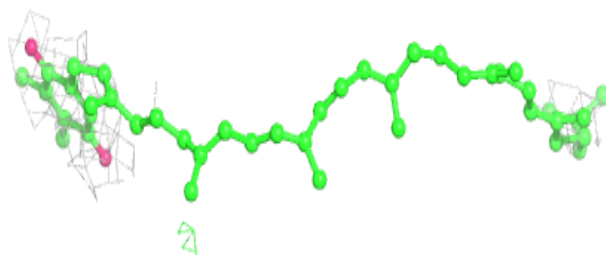
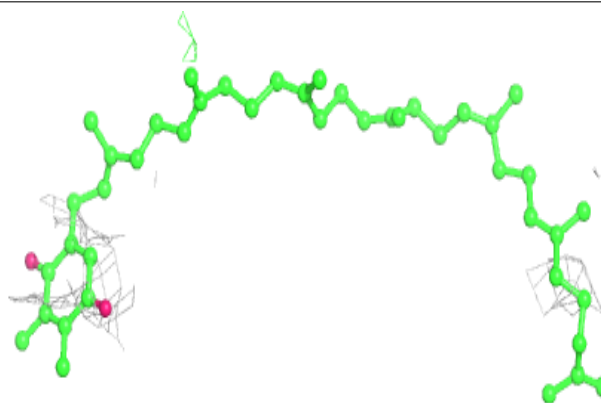


Electron density around DGD c 519:

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

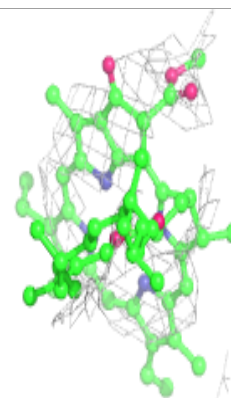
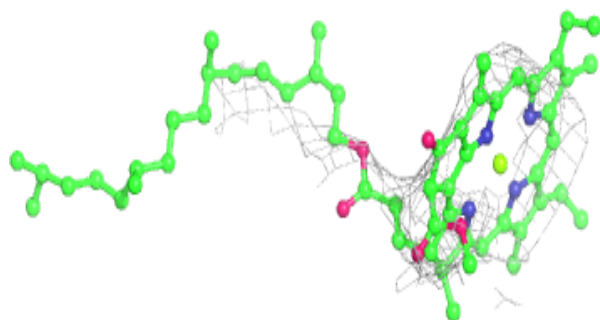
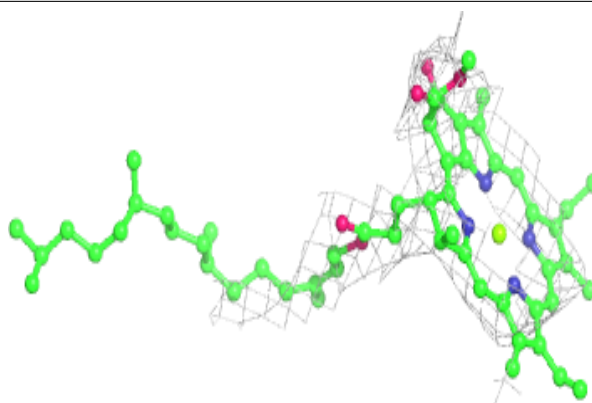
**Electron density around PL9 a 410:**

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

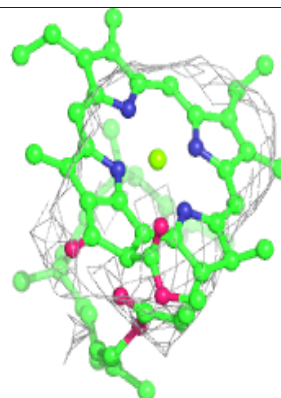
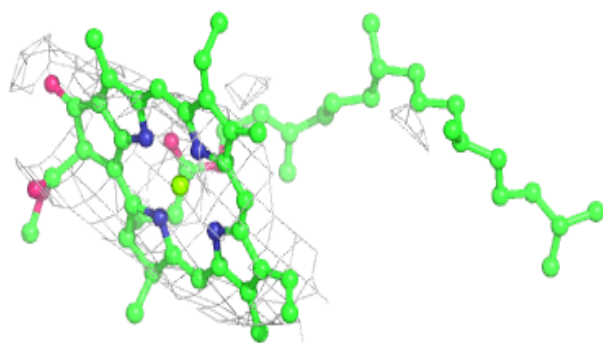
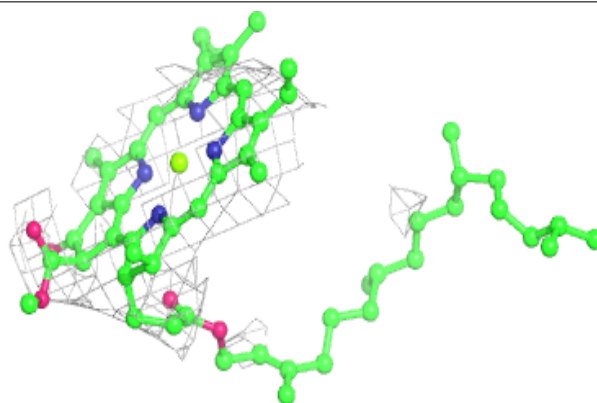


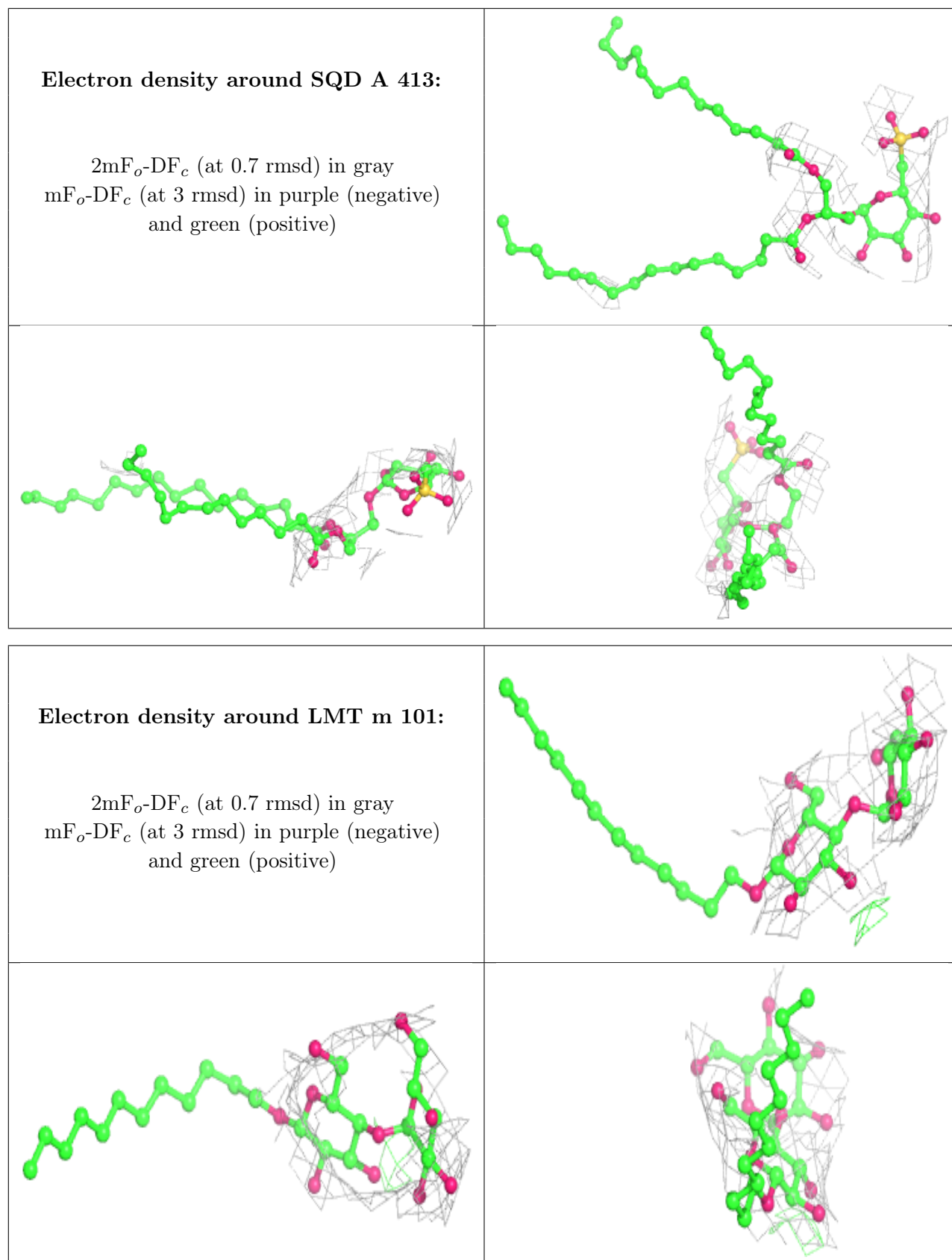
Electron density around CLA c 502:

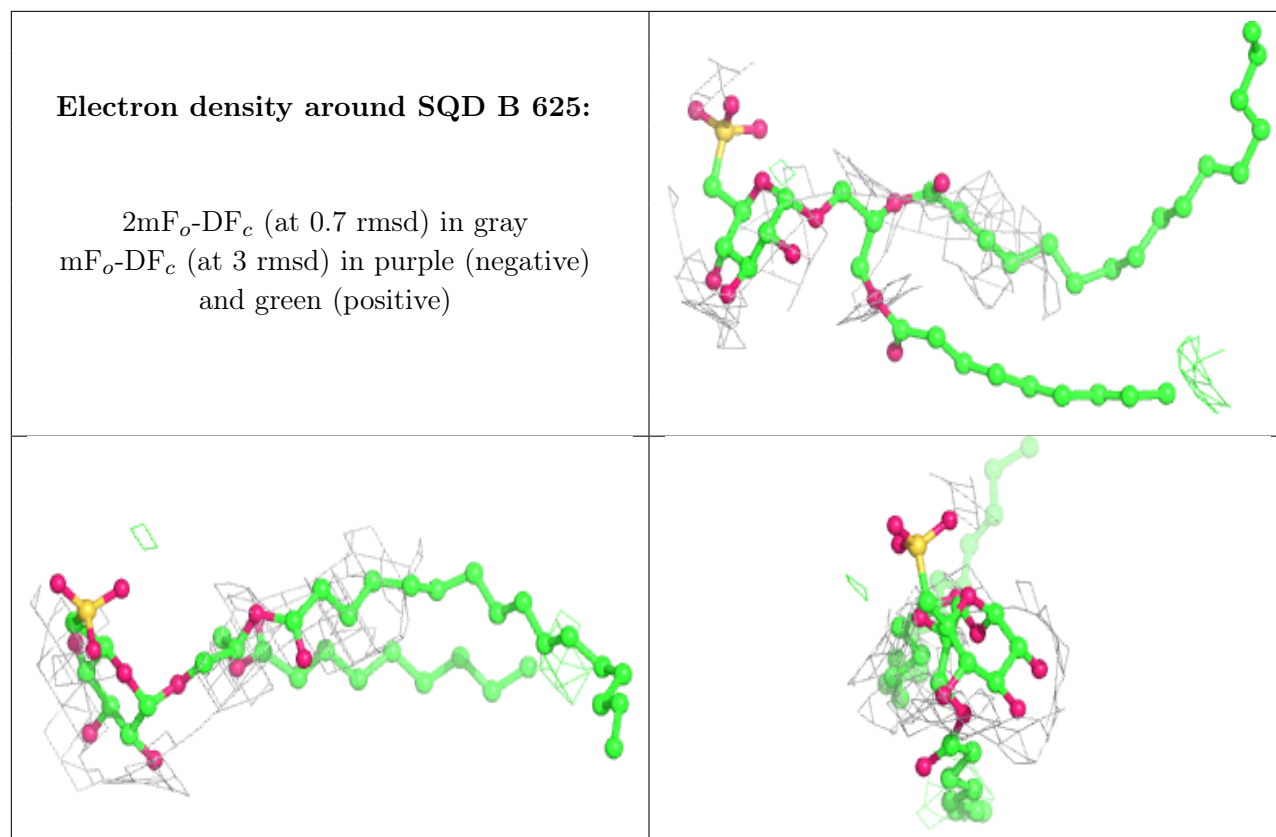
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA C 513:**

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

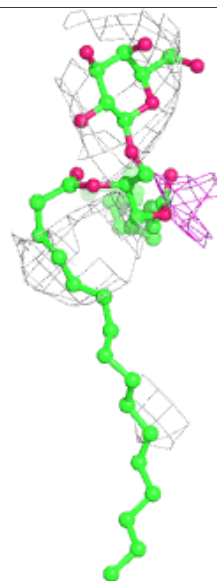
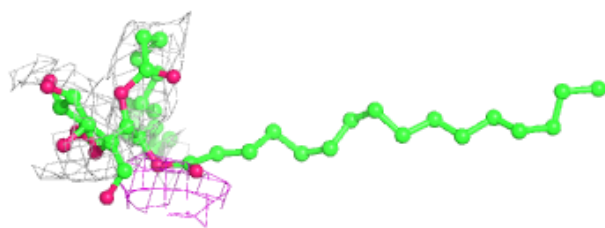
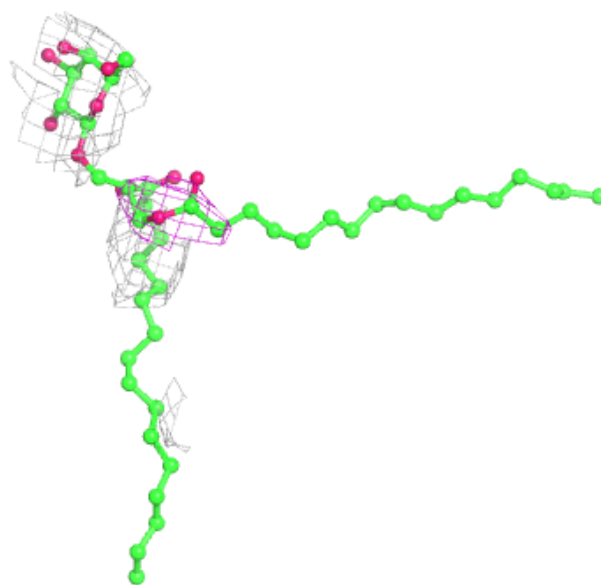






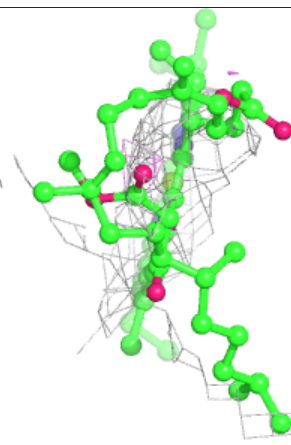
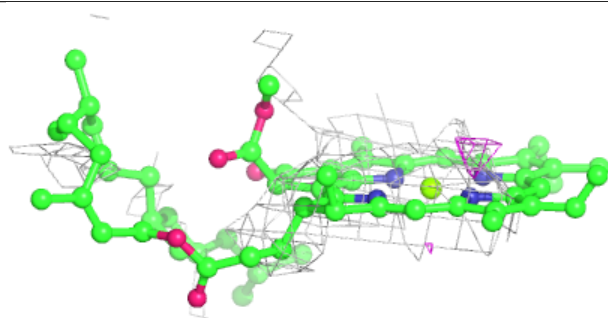
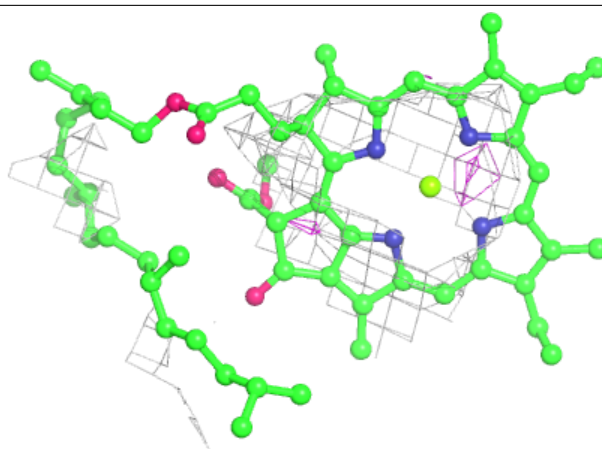
Electron density around LMG a 416:

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

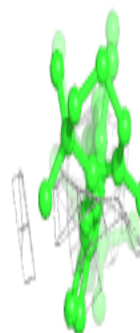
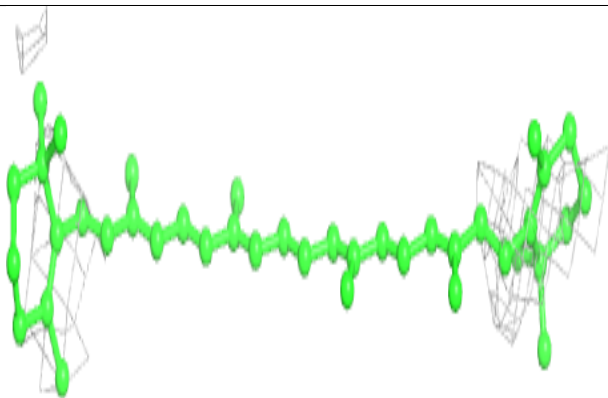
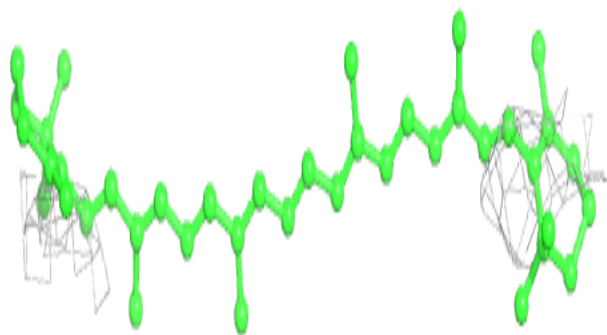


Electron density around CLA b 613:

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

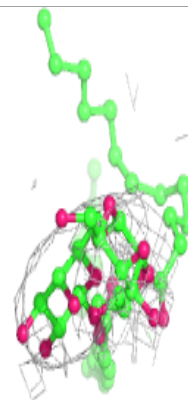
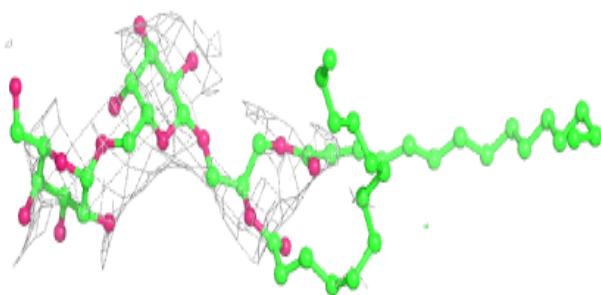
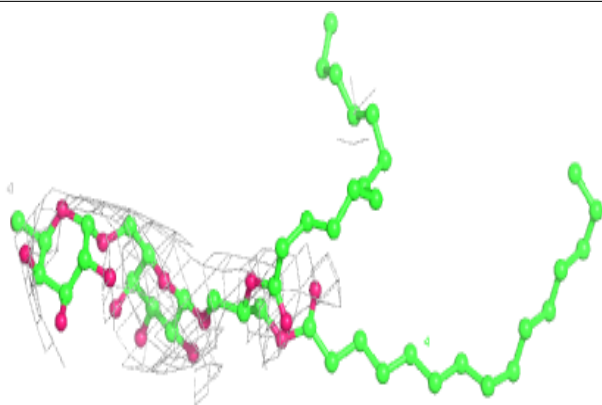
**Electron density around BCR c 515:**

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

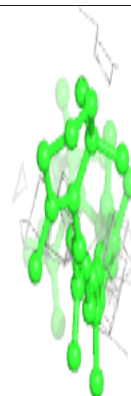
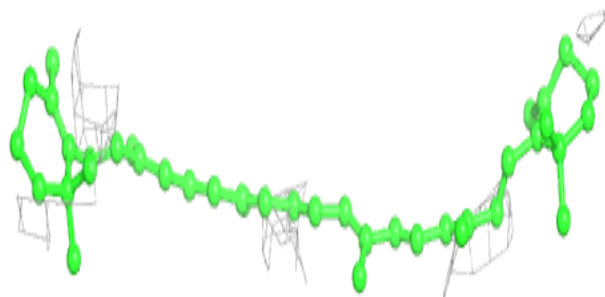
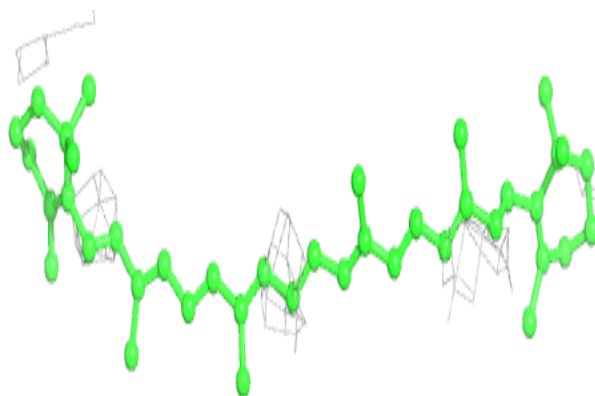


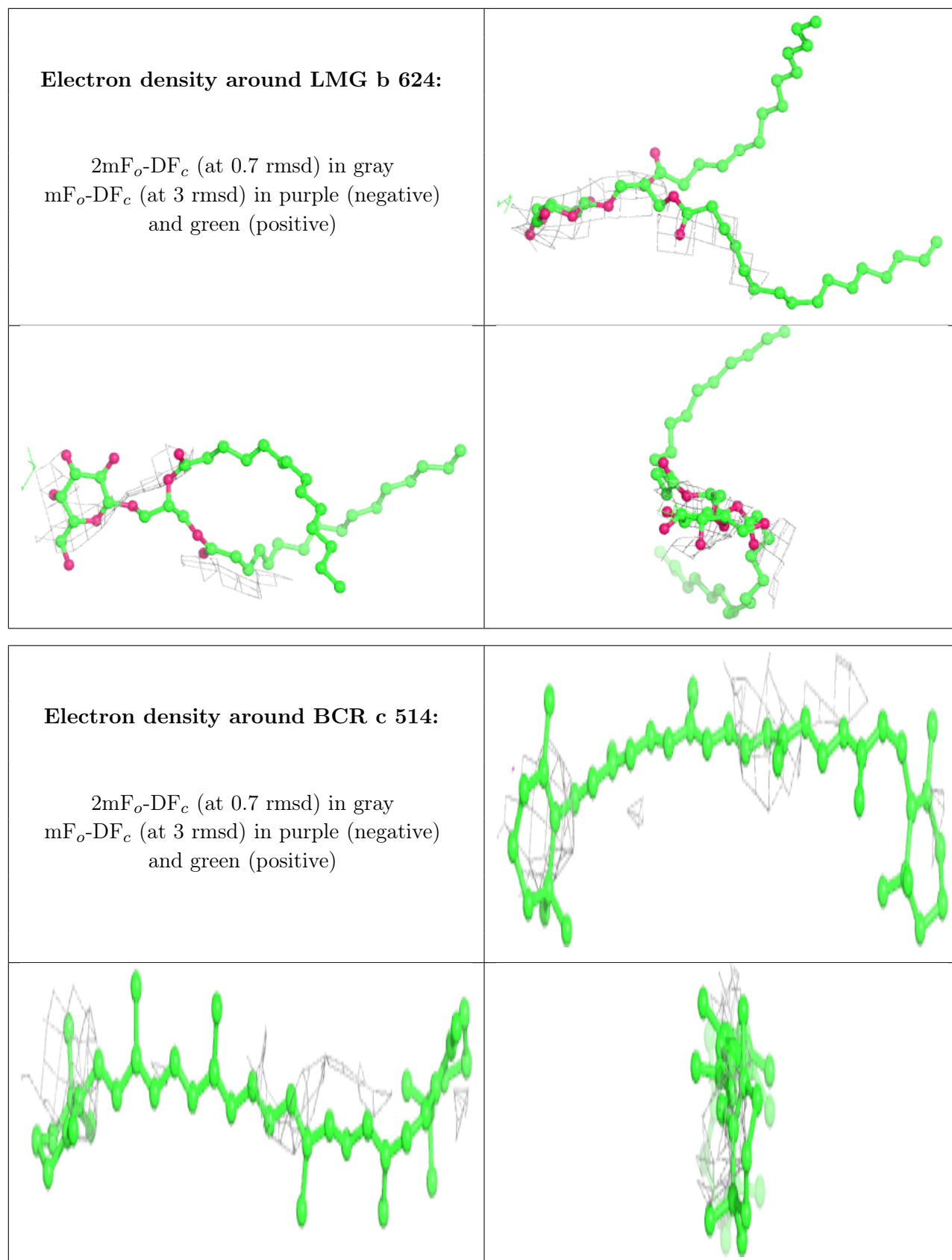
Electron density around DGD B 621:

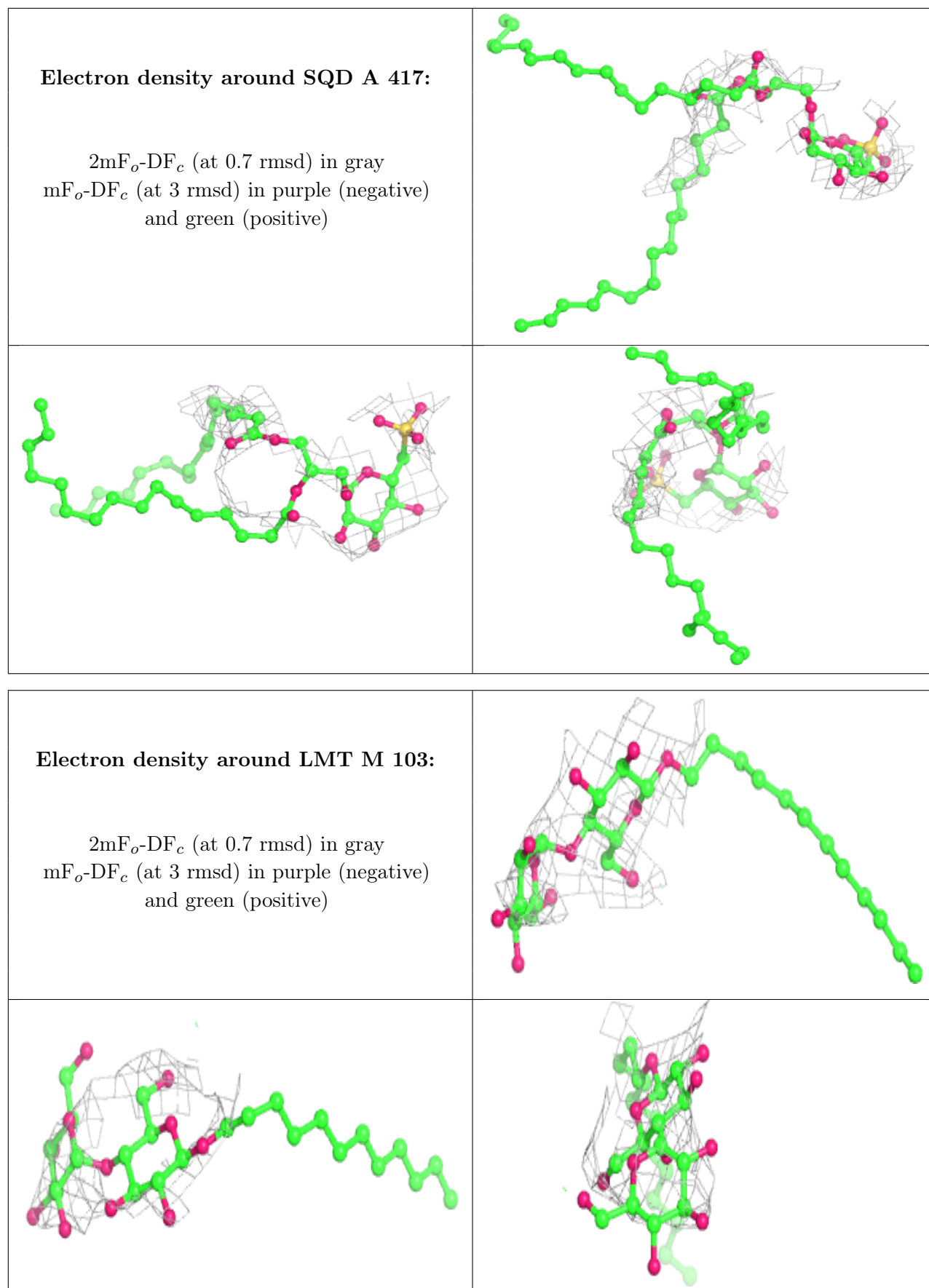
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

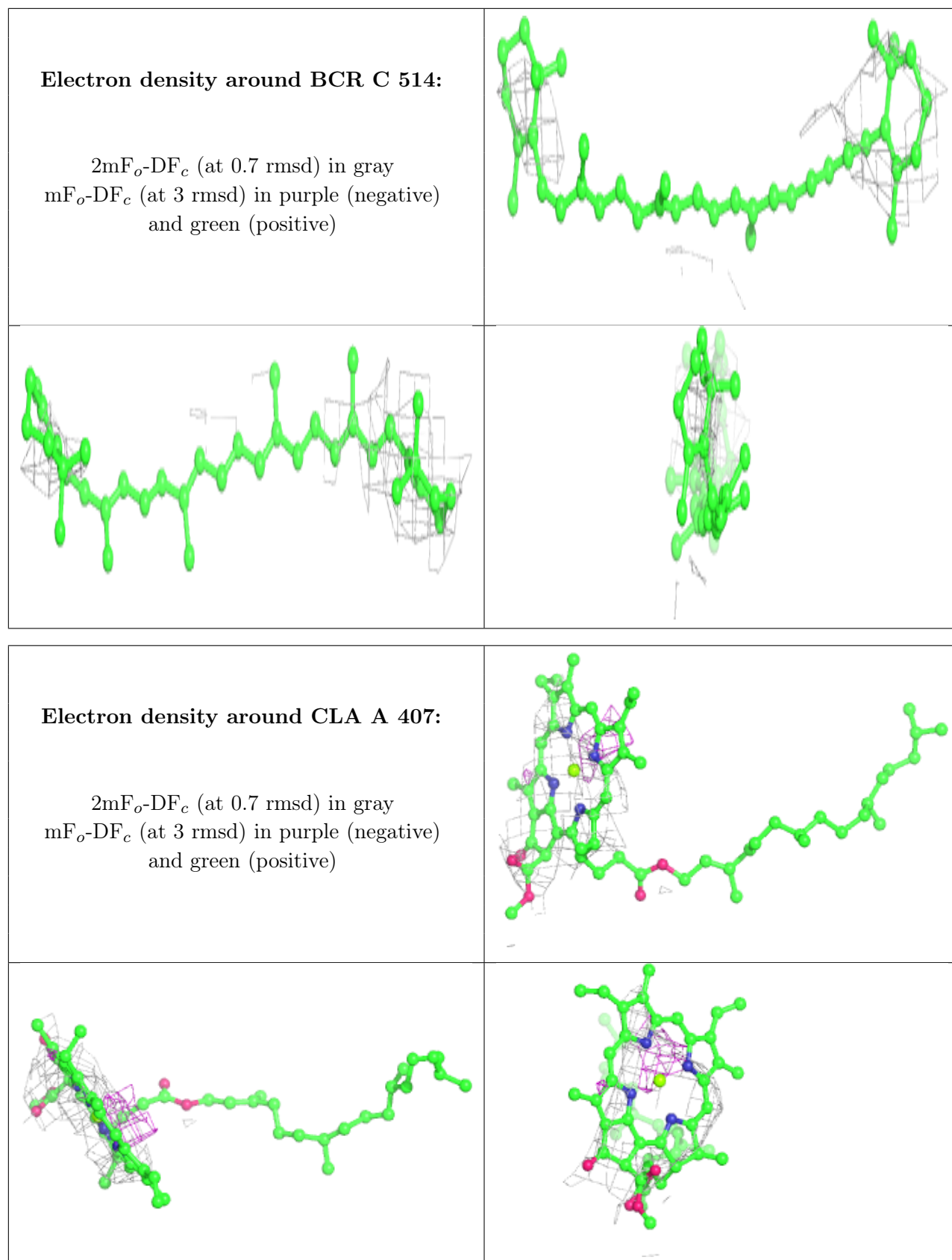
**Electron density around BCR T 103:**

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



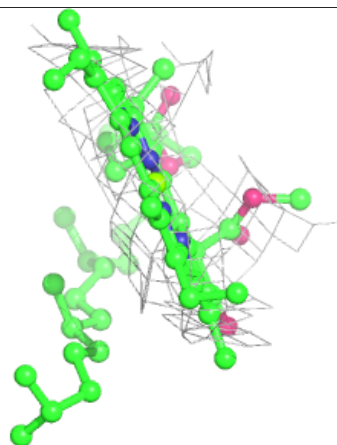
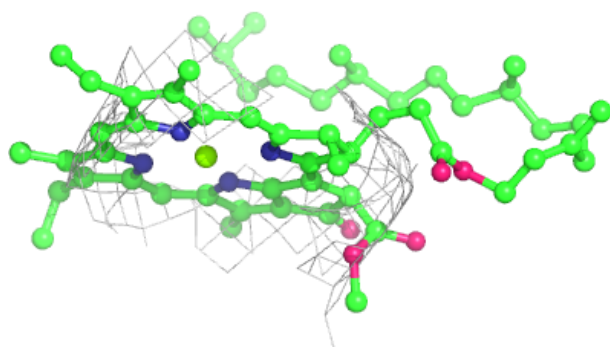
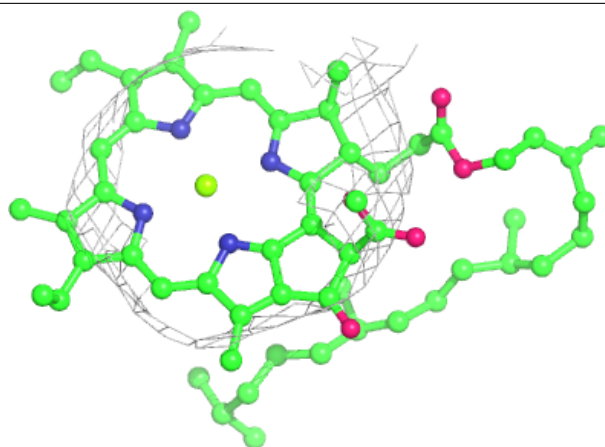




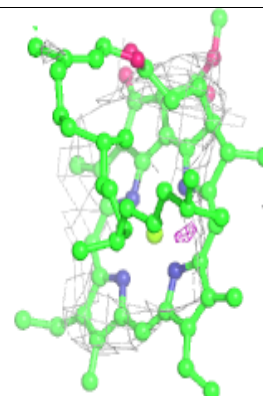
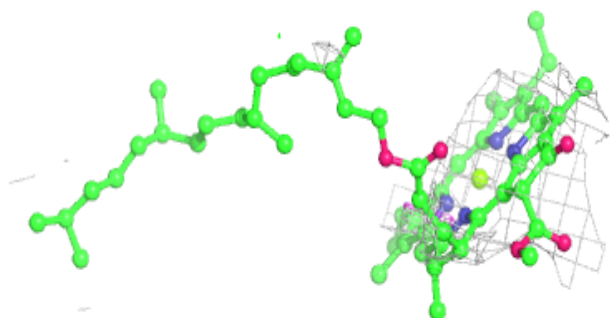
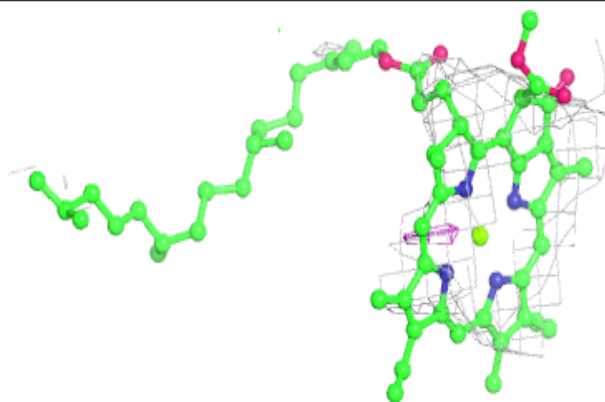


Electron density around CLA c 509:

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

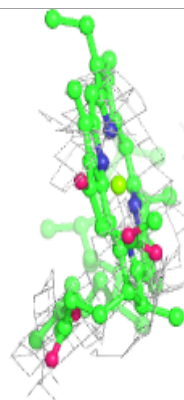
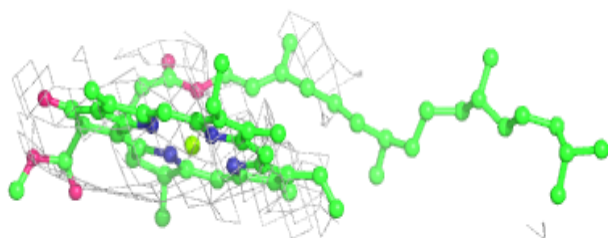
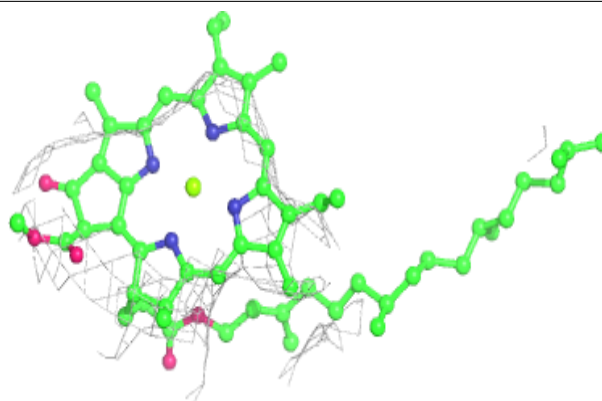
**Electron density around CLA c 511:**

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

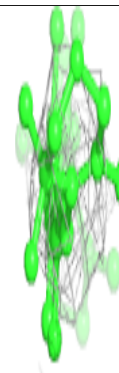
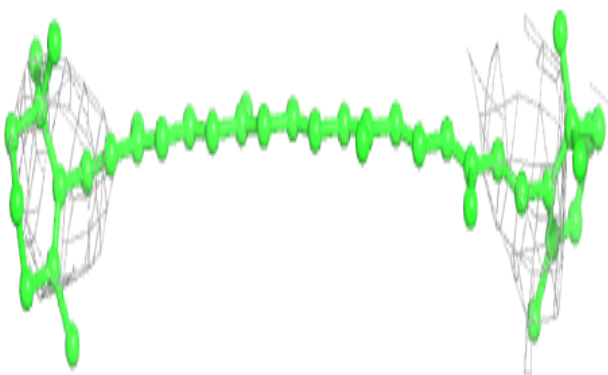
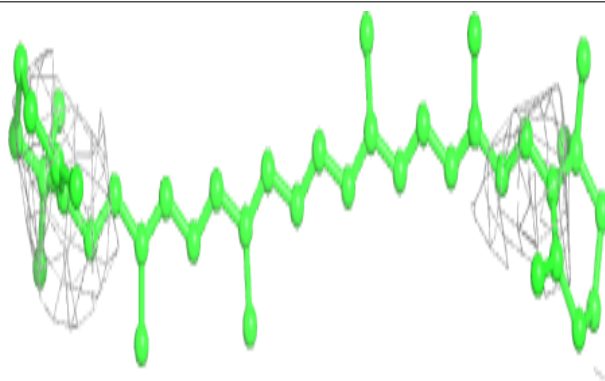


Electron density around CLA C 501:

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

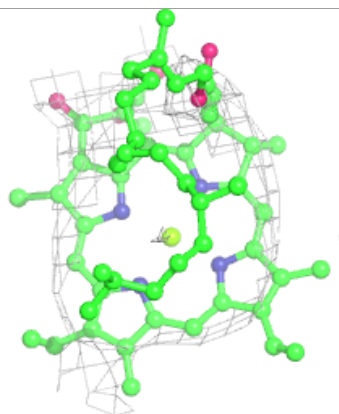
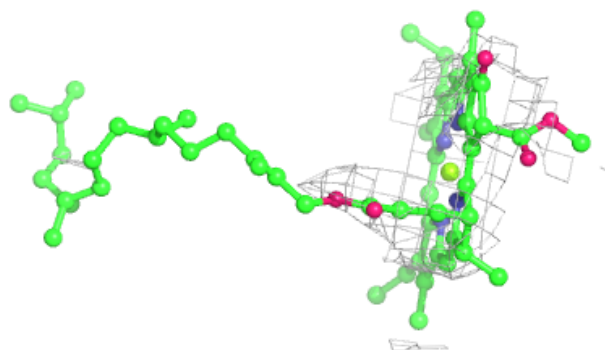
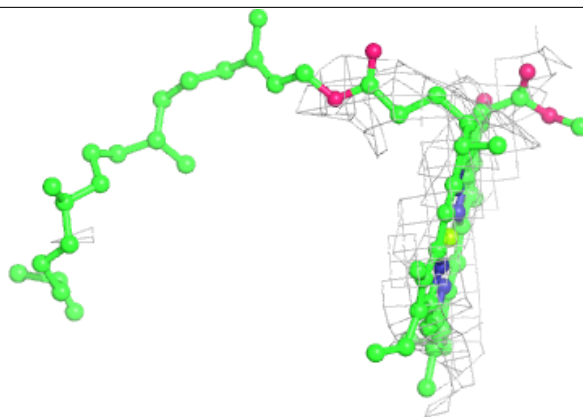
**Electron density around BCR B 617:**

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

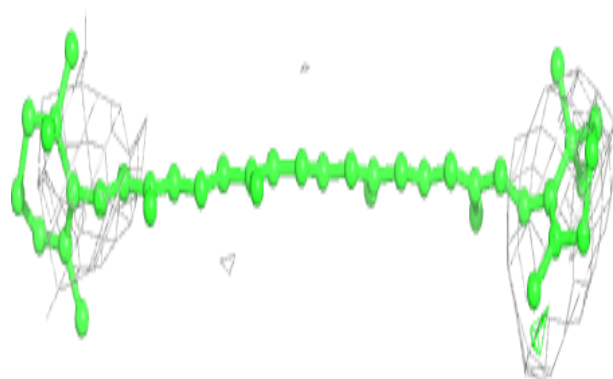
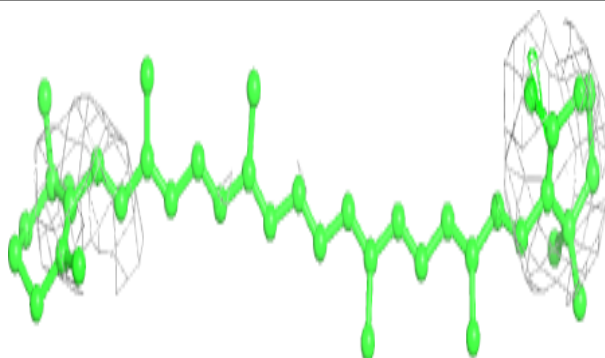


Electron density around CLA c 506:

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

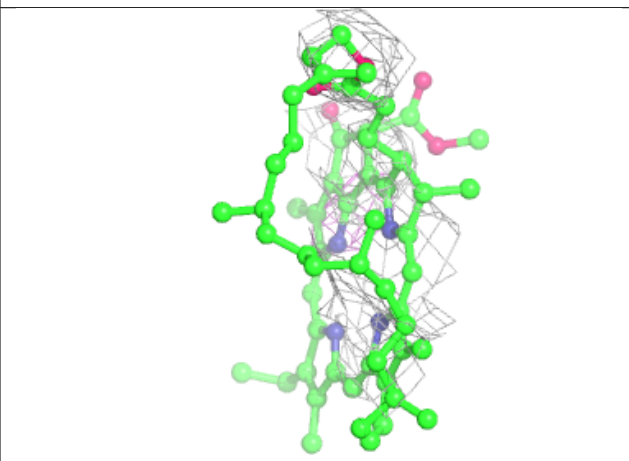
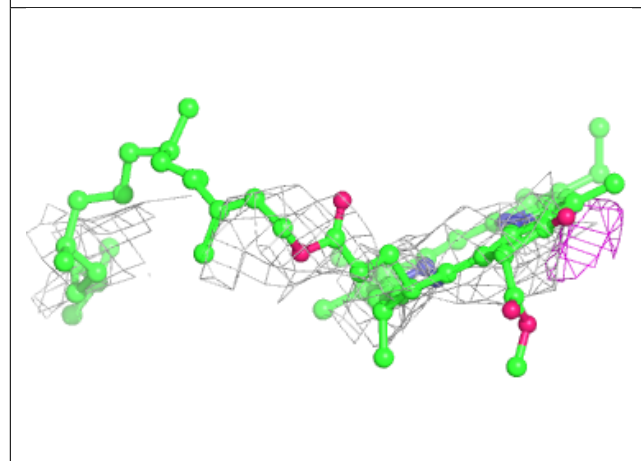
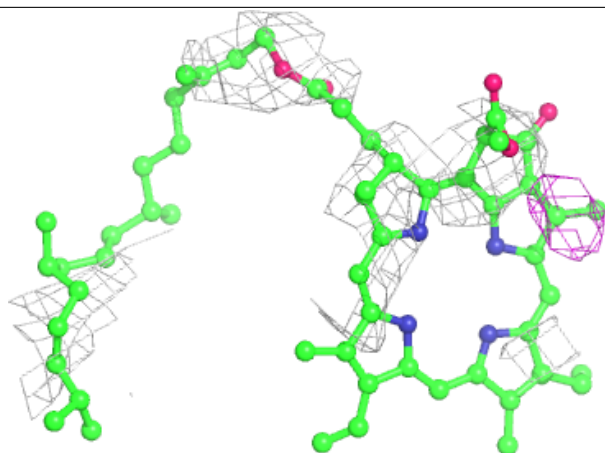
**Electron density around BCR b 620:**

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

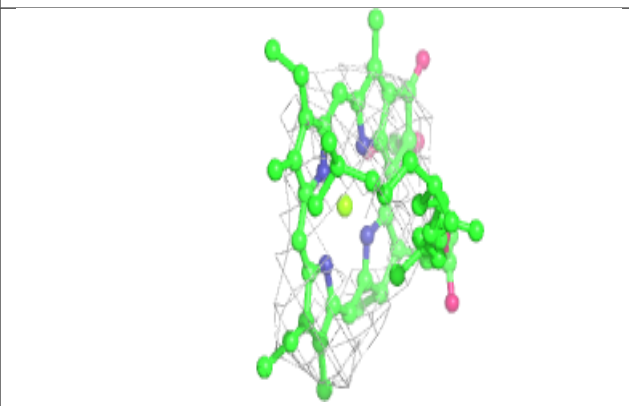
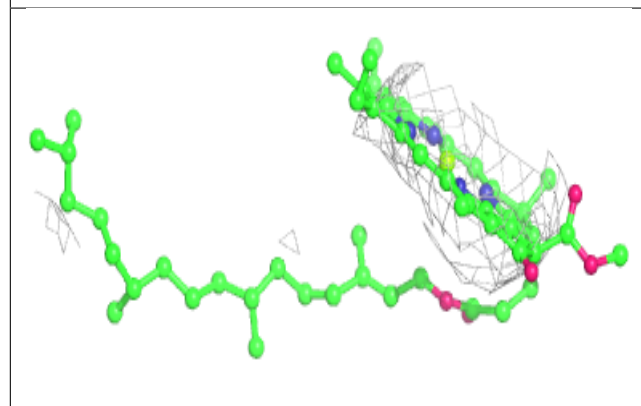
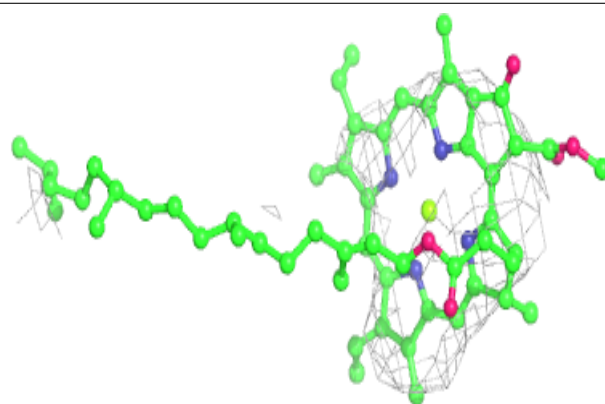


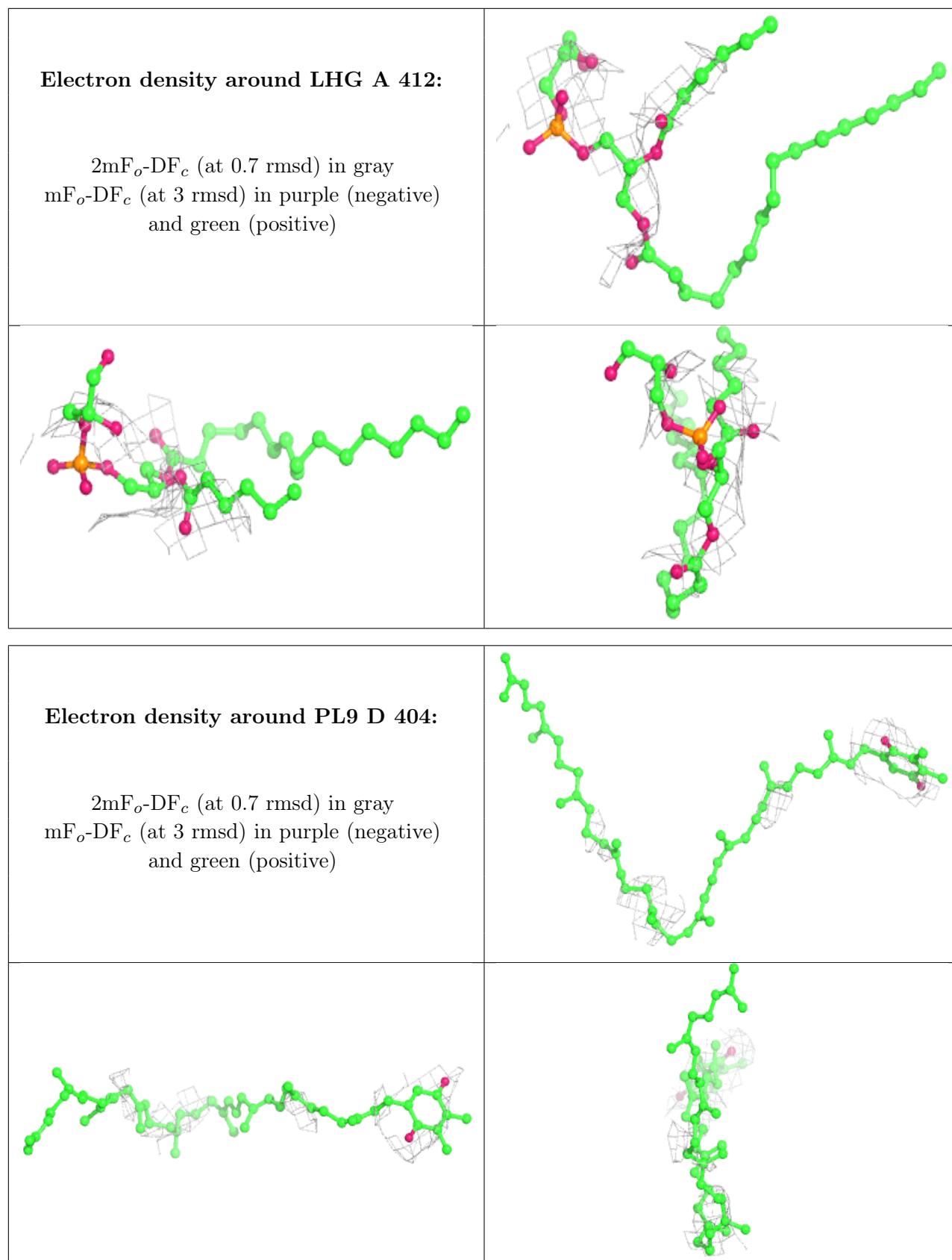
Electron density around PHO A 406:

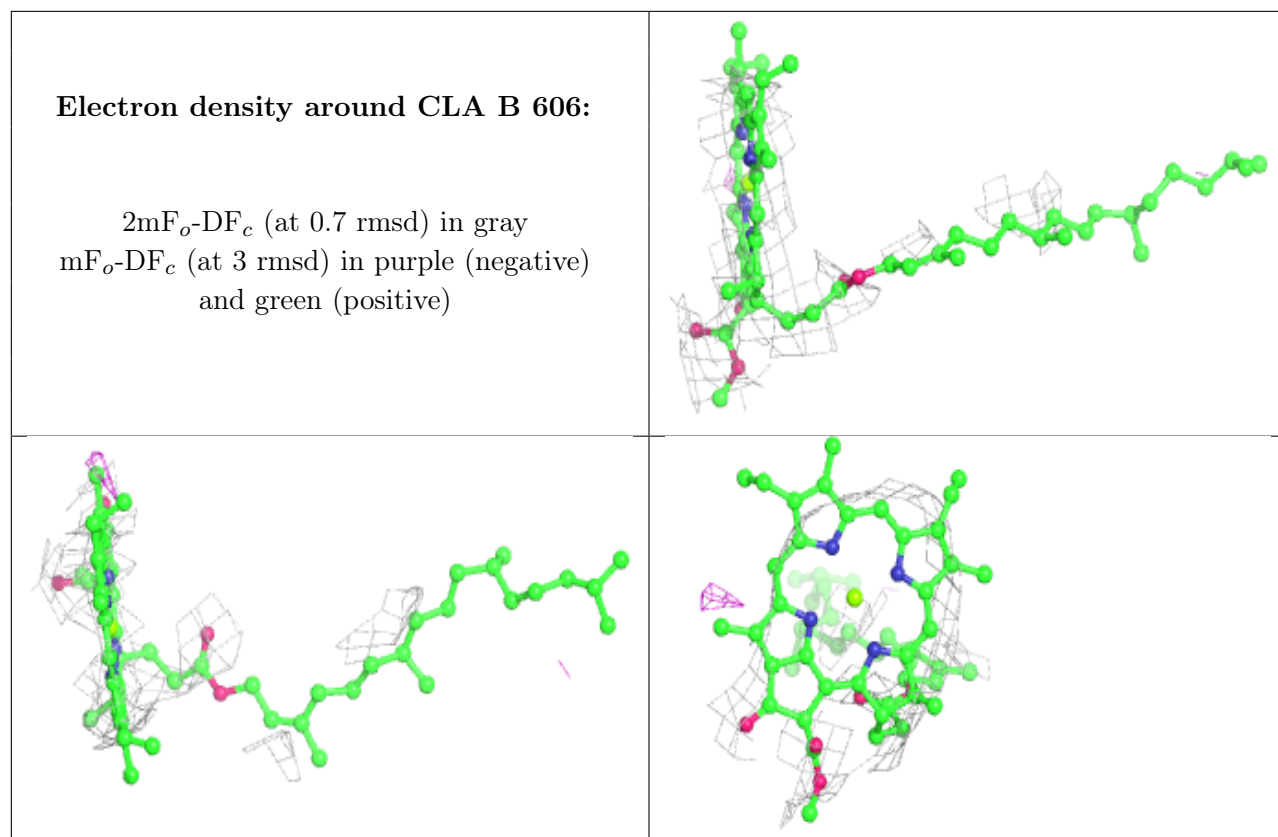
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA b 611:**

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

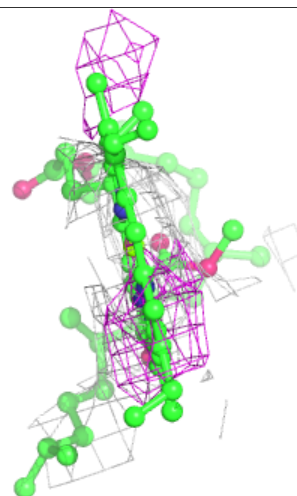
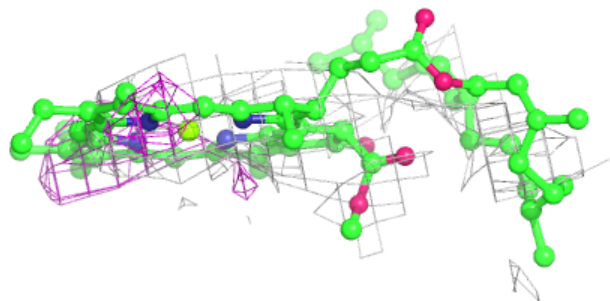
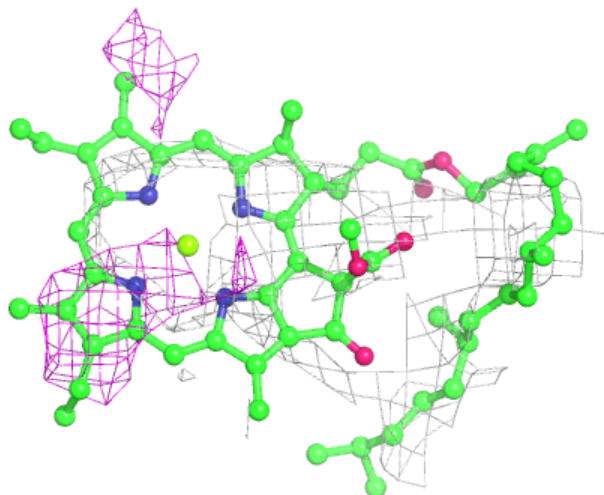






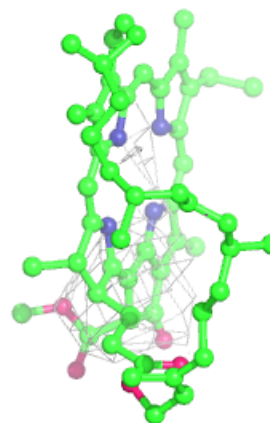
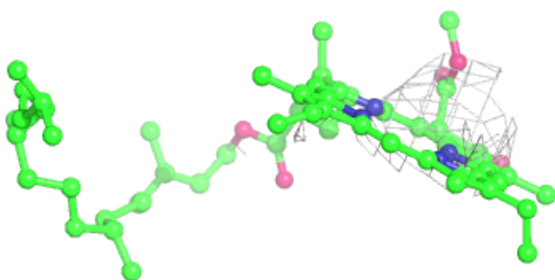
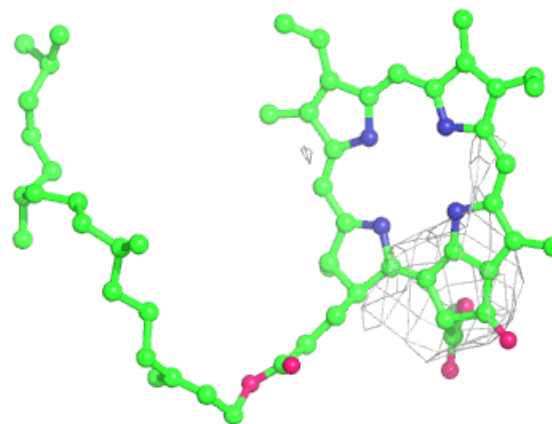
Electron density around CLA B 610:

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

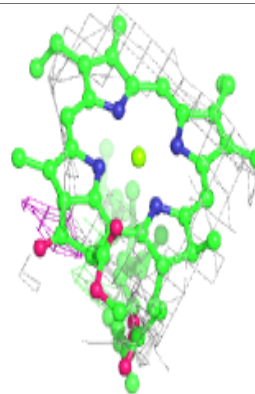
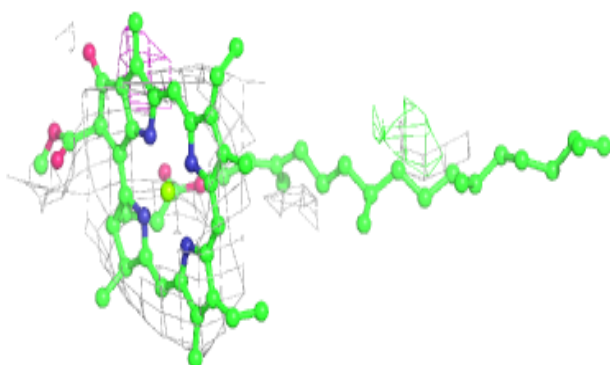
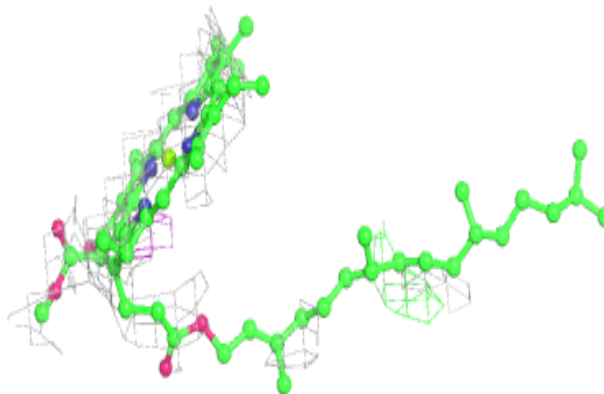


Electron density around PHO a 408:

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

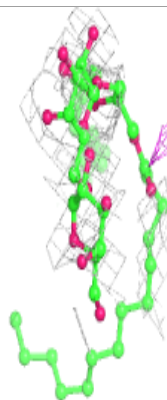
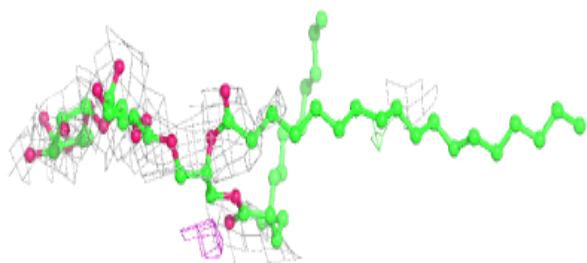
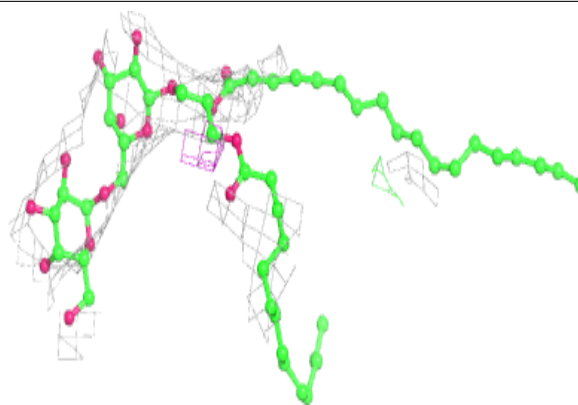
**Electron density around CLA C 504:**

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

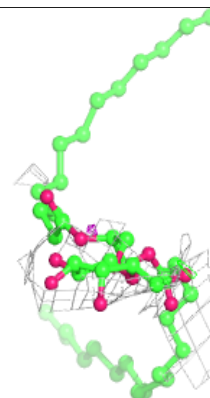
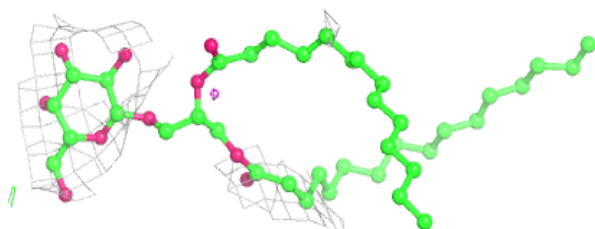
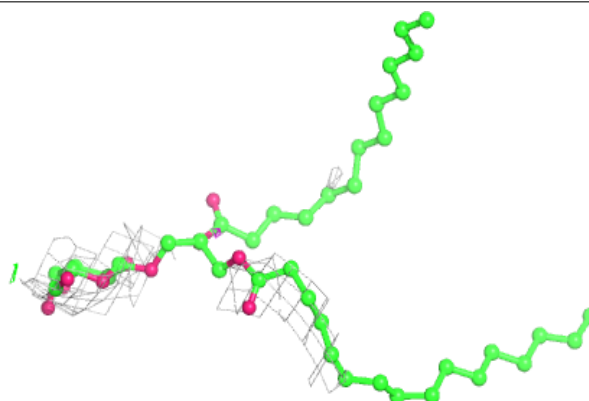


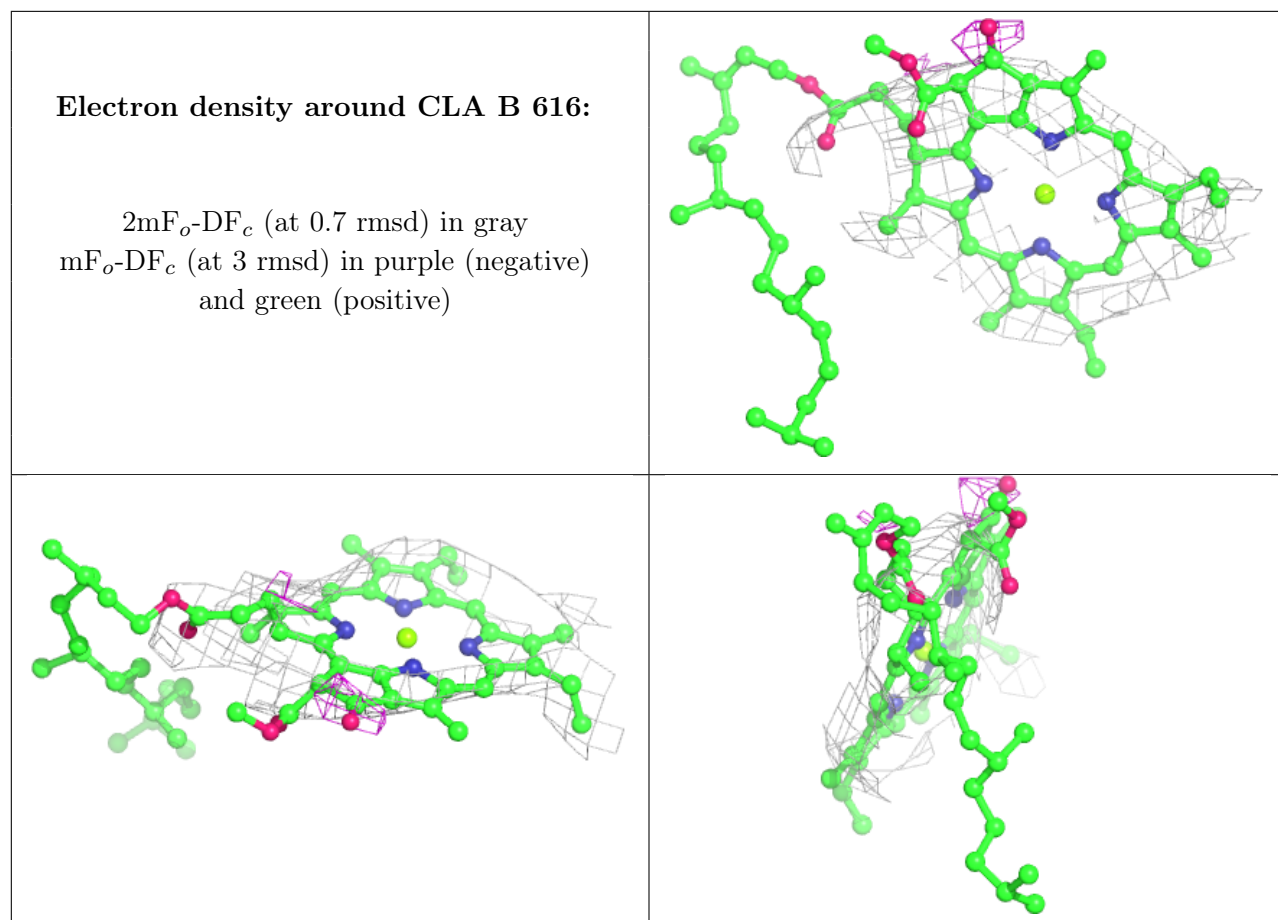
Electron density around DGD C 517:

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

**Electron density around LMG B 622:**

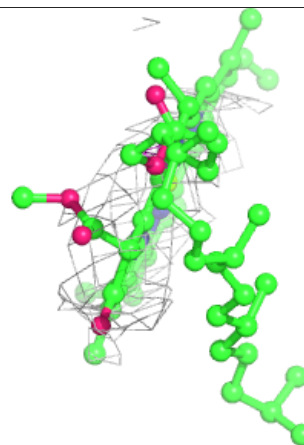
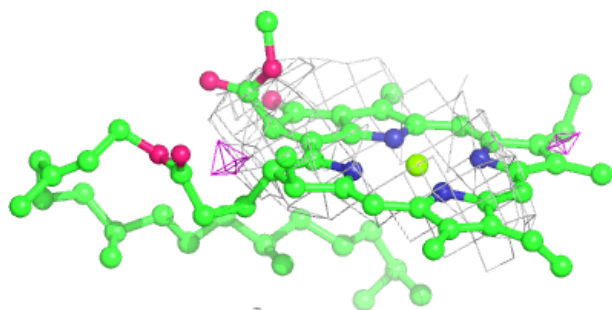
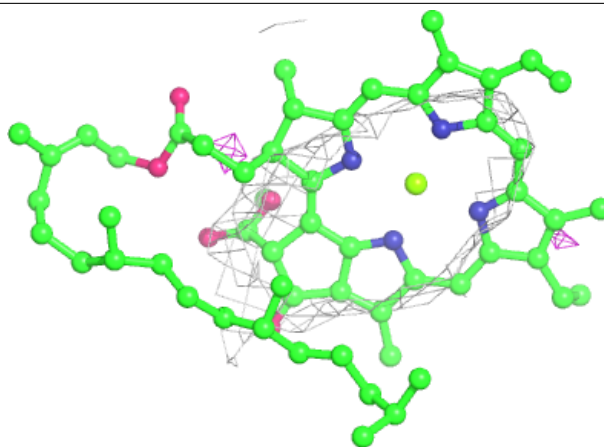
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





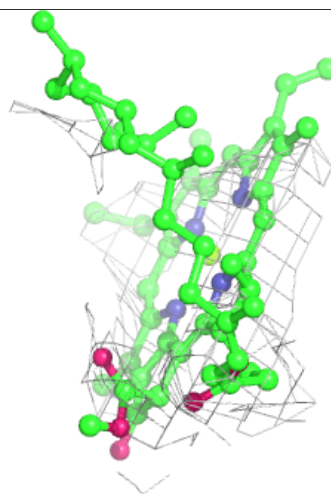
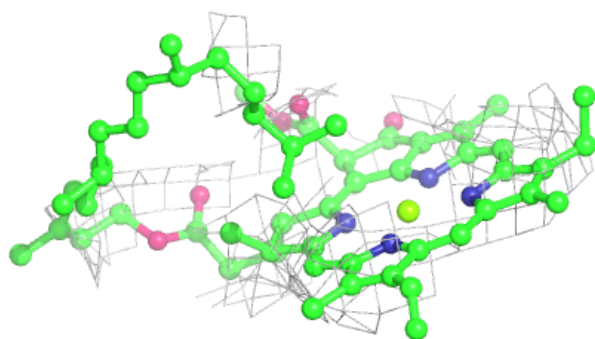
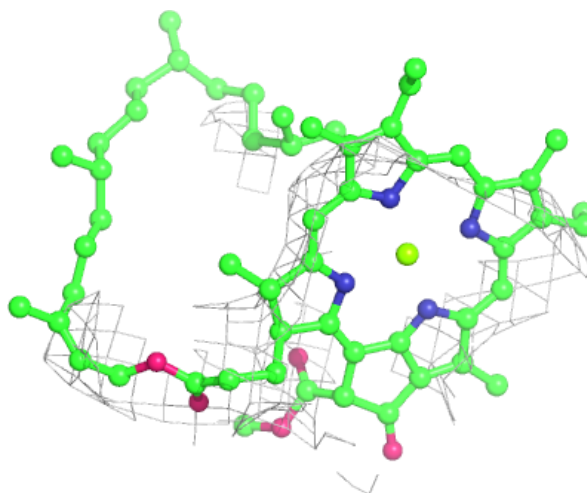
Electron density around CLA C 509:

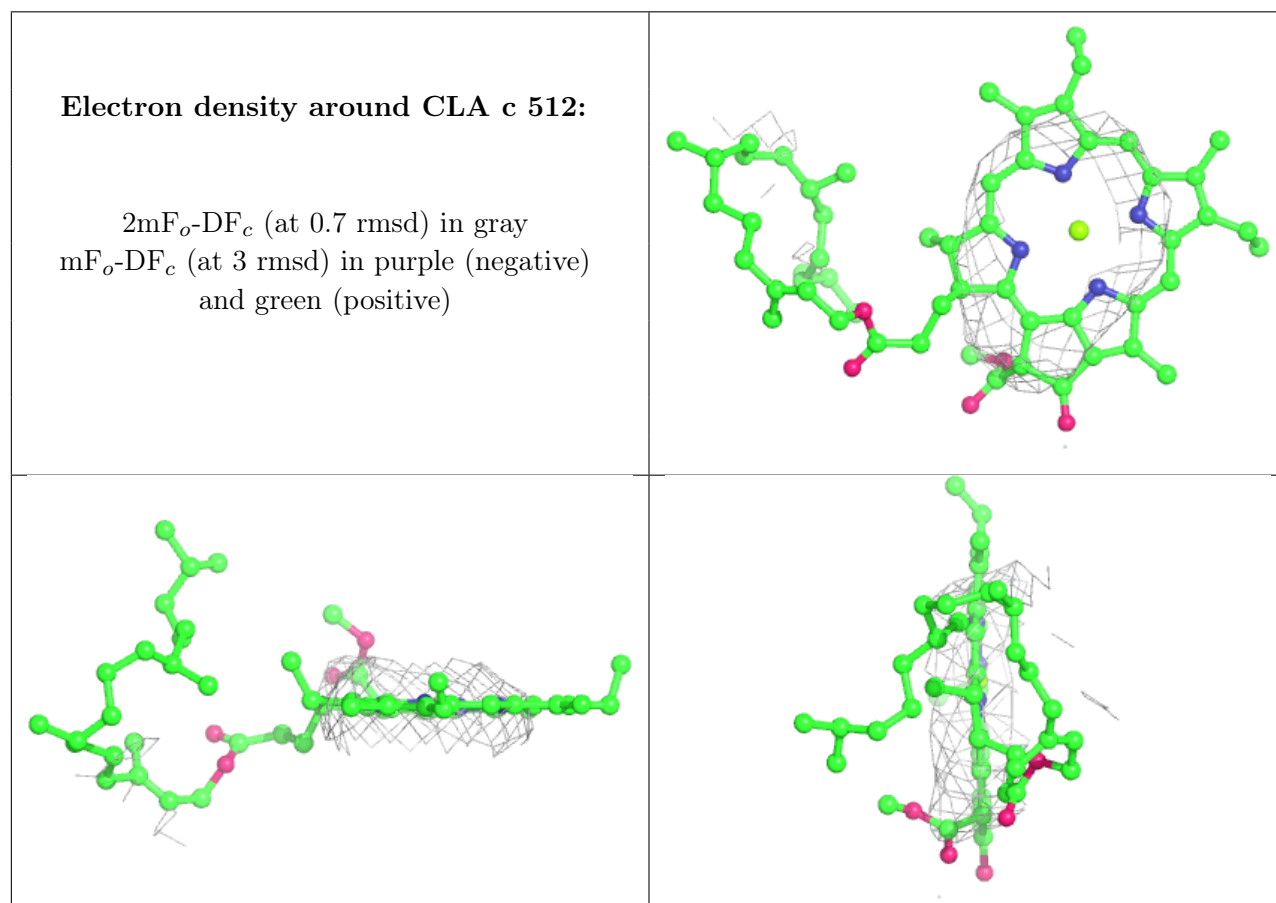
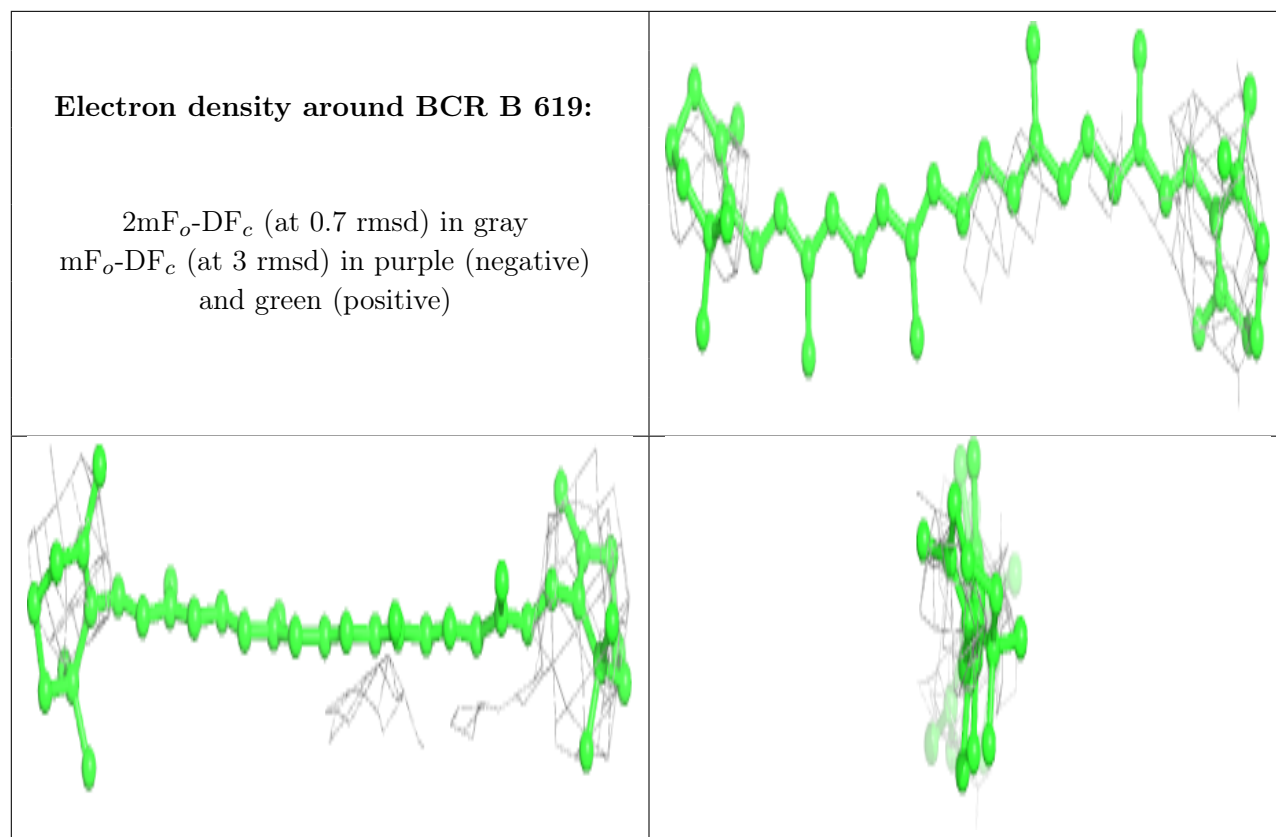
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 618:

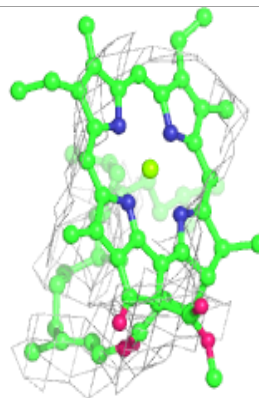
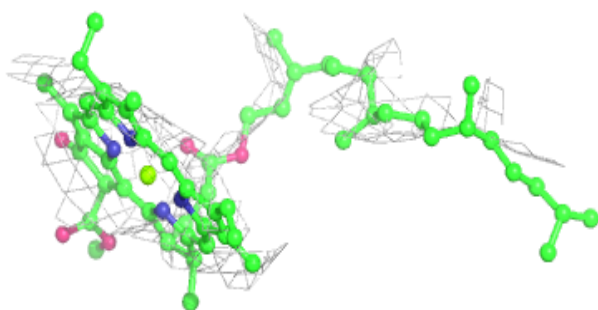
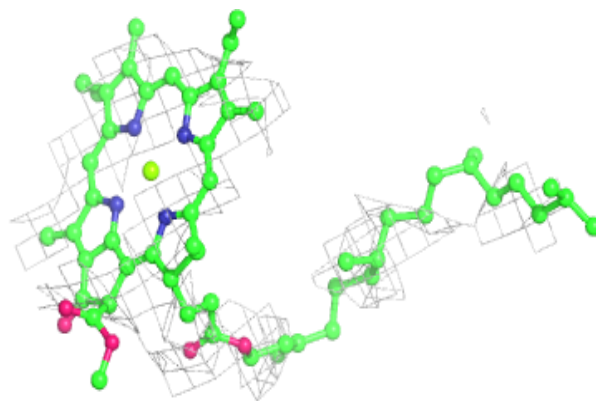
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



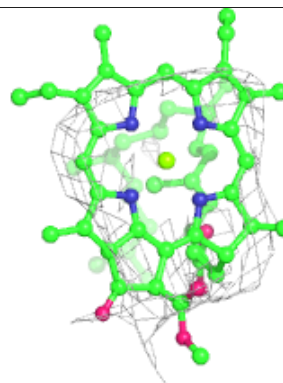
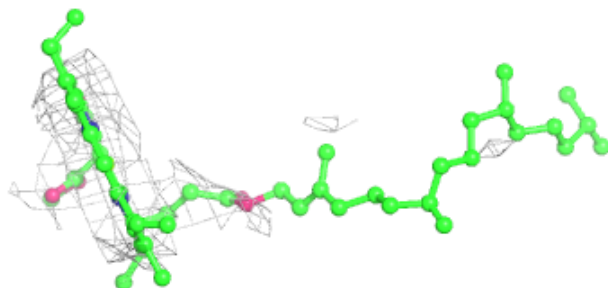
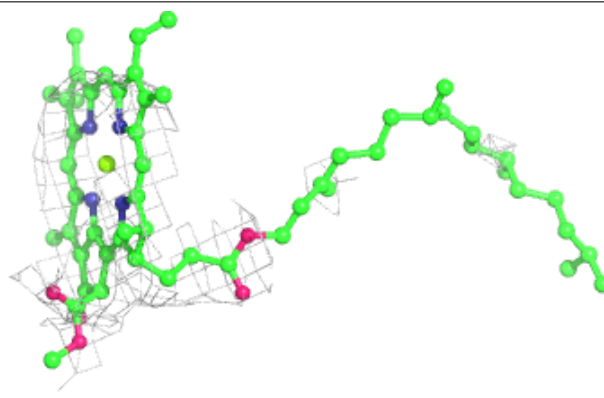


Electron density around CLA C 511:

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

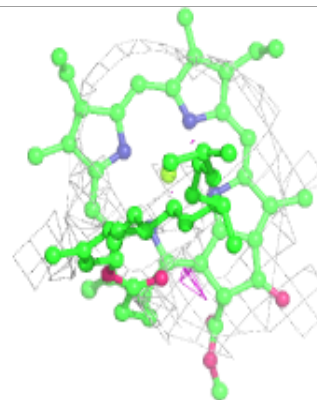
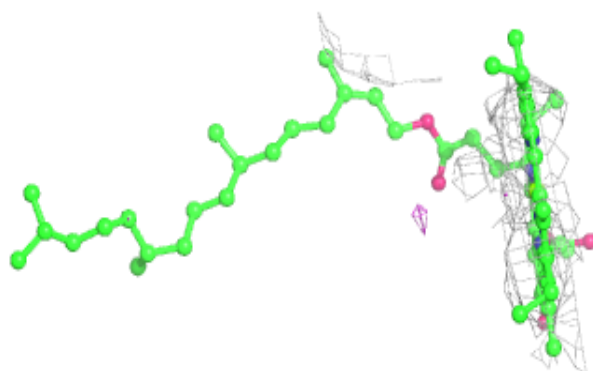
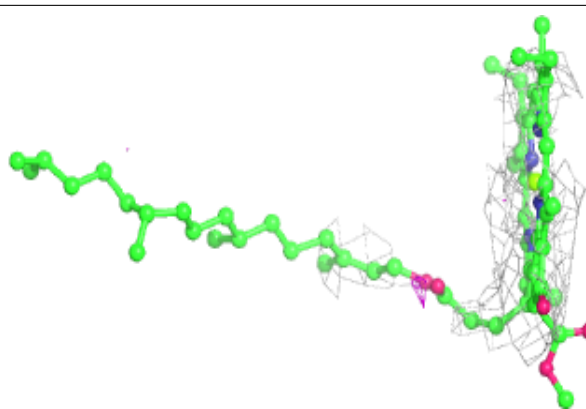
**Electron density around CLA d 403:**

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

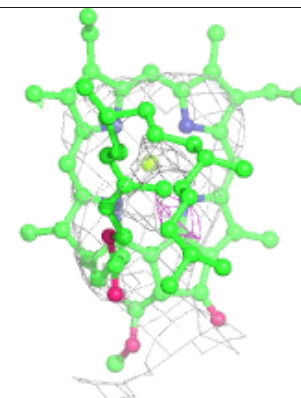
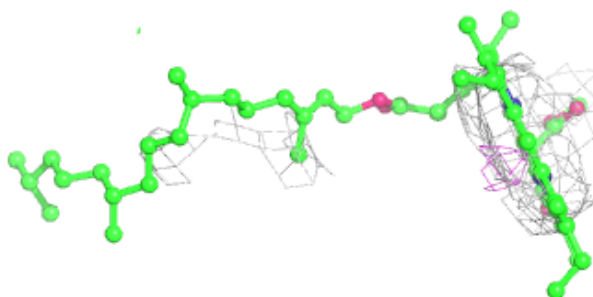
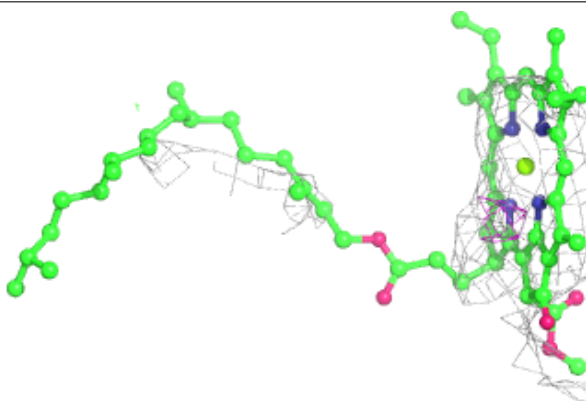


Electron density around CLA b 609:

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

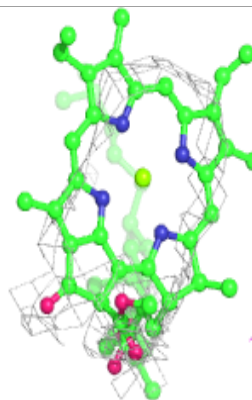
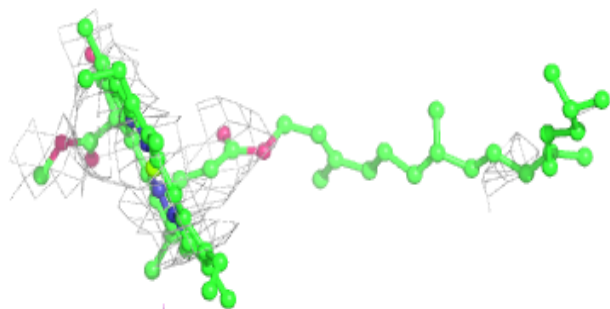
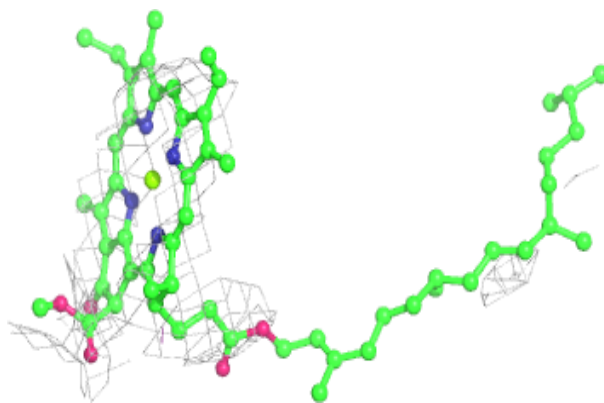
**Electron density around CLA D 403:**

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

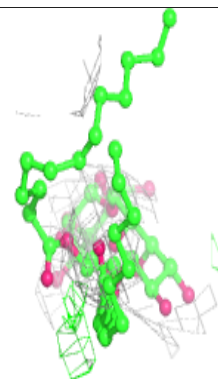
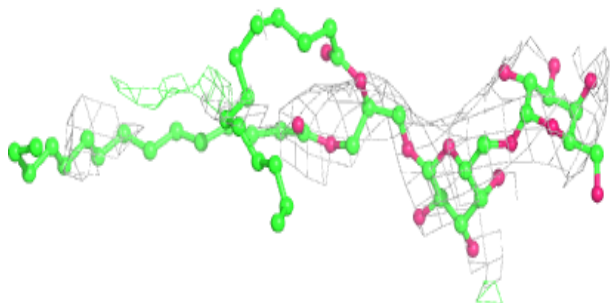
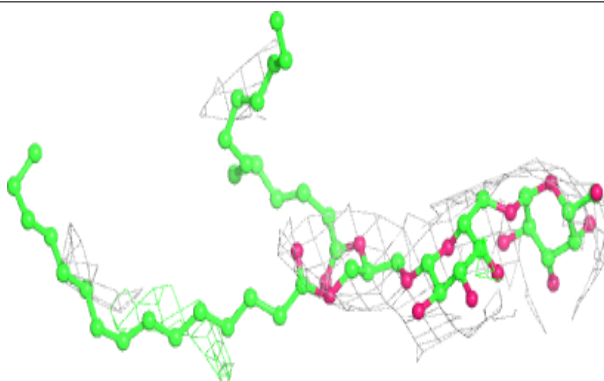


Electron density around CLA B 609:

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

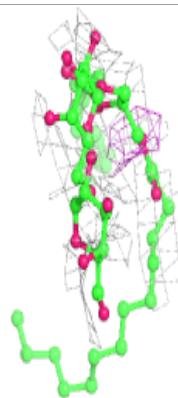
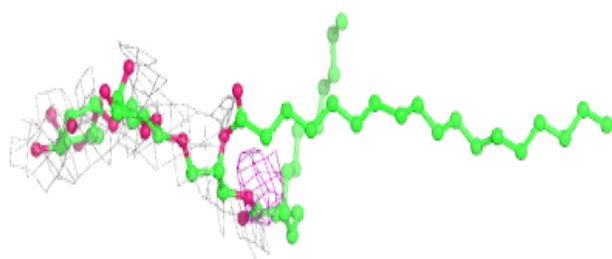
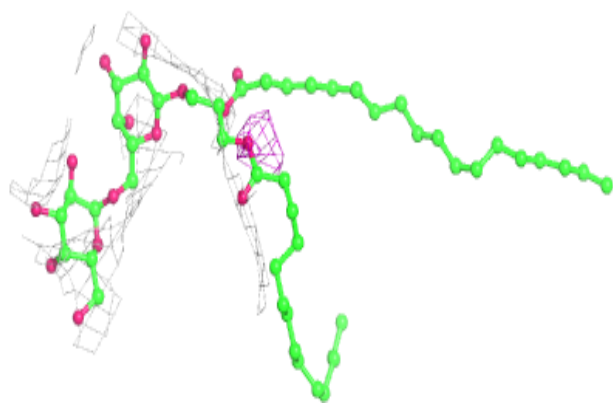
**Electron density around DGD b 622:**

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

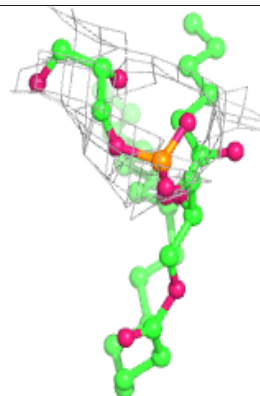
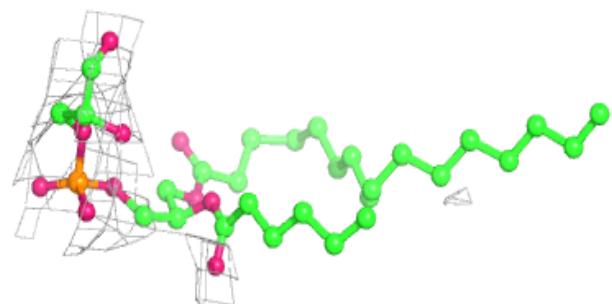
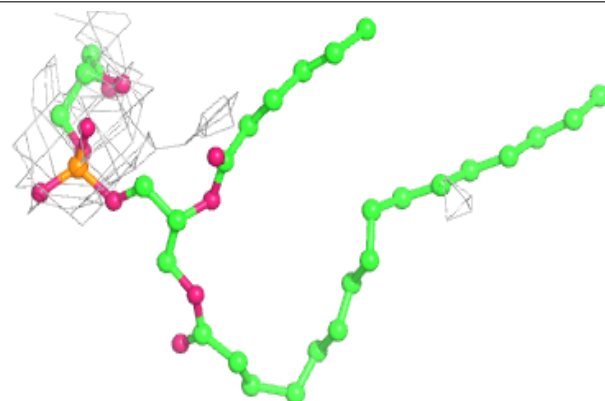


Electron density around DGD c 518:

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

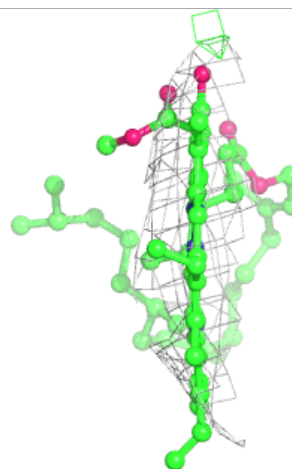
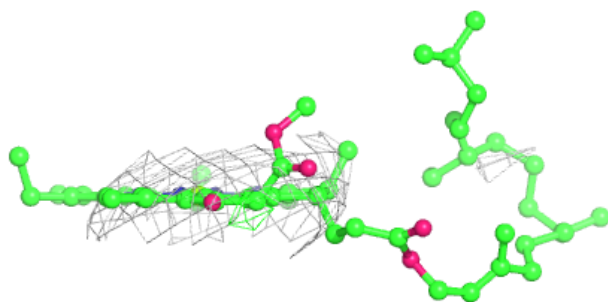
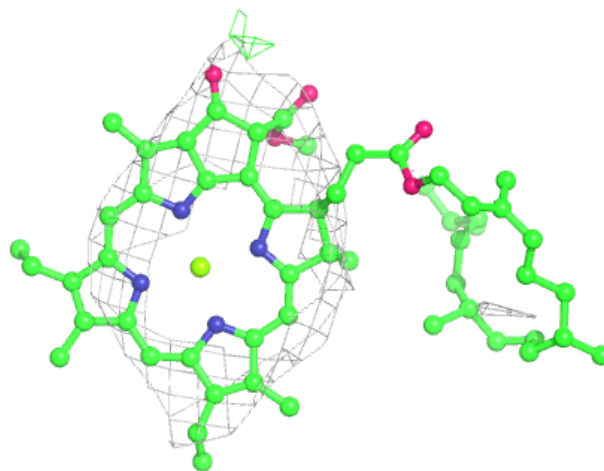
**Electron density around LHG a 414:**

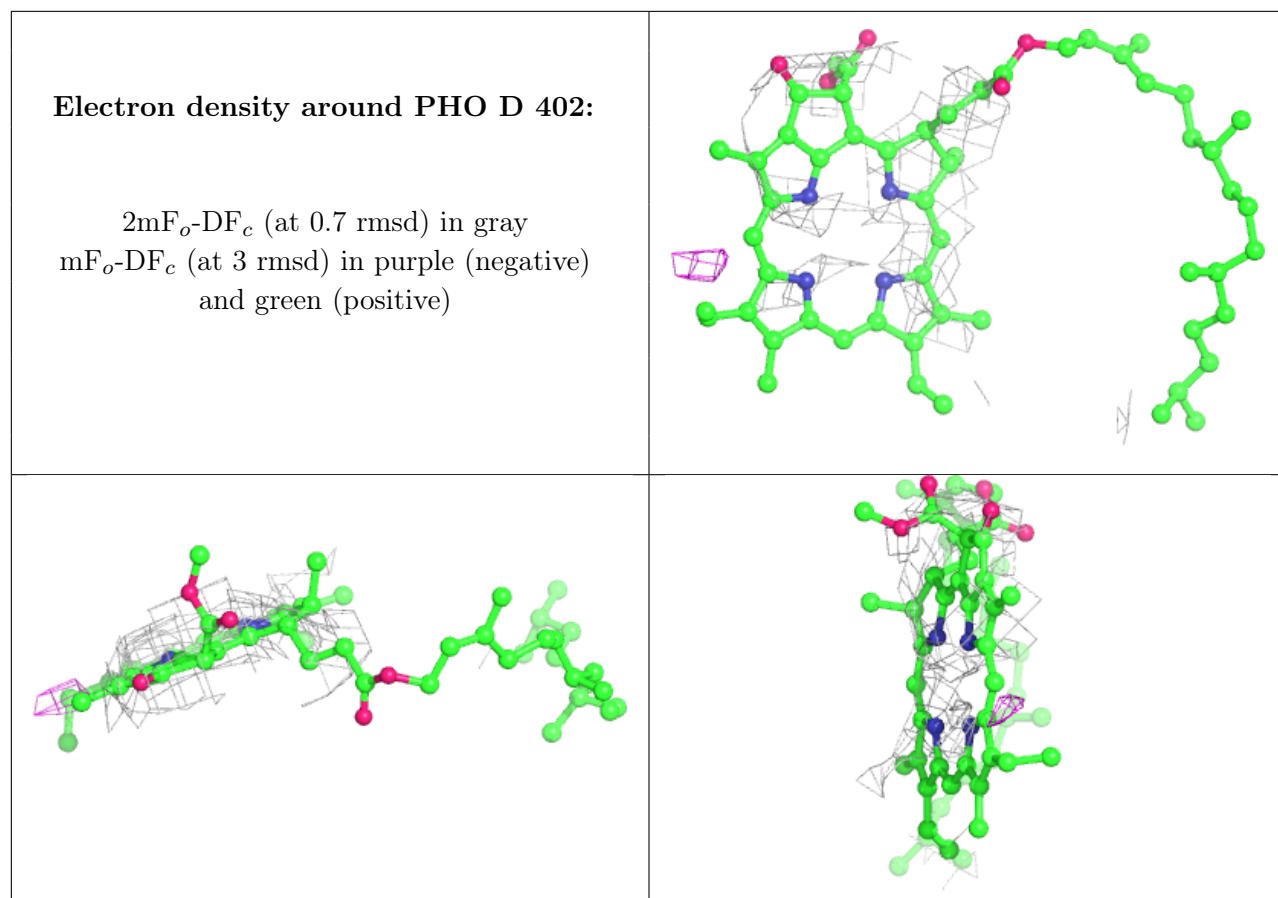
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 512:

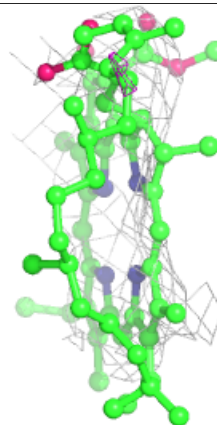
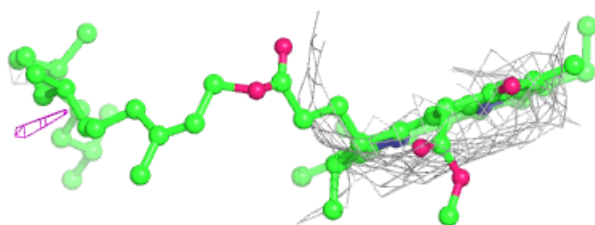
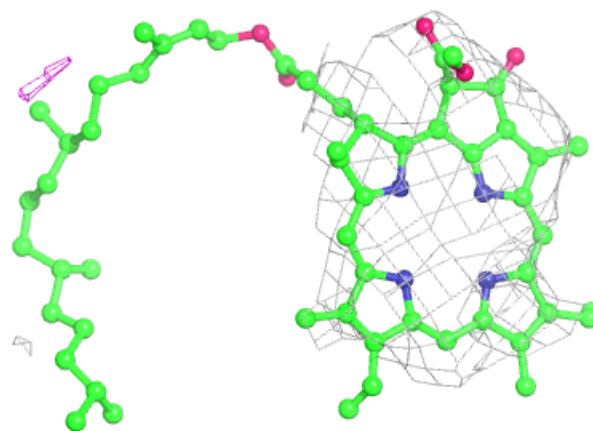
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



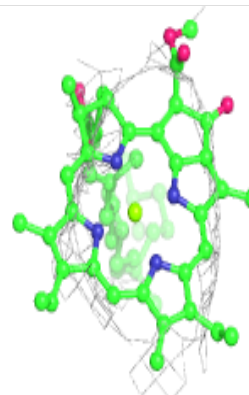
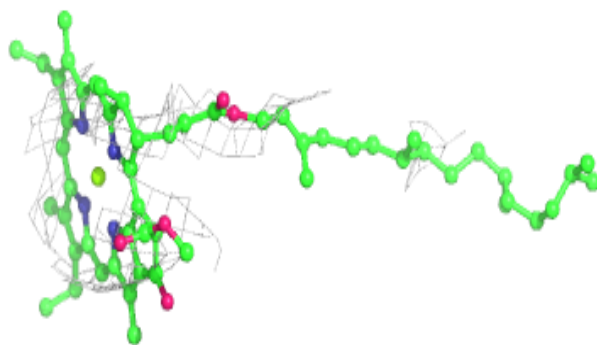
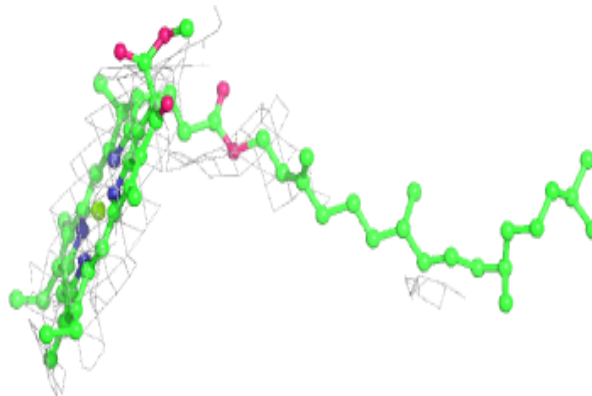


Electron density around PHO a 407:

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

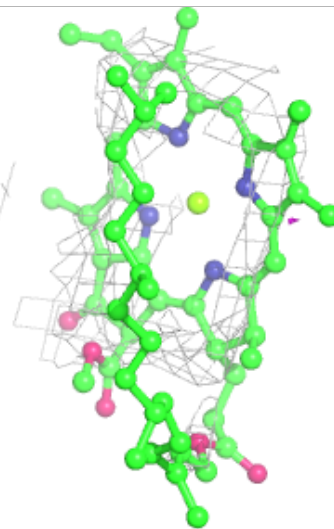
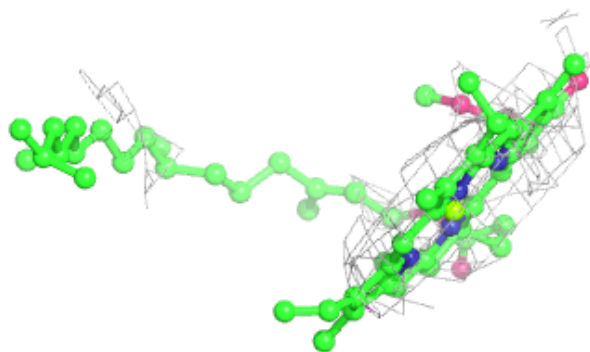
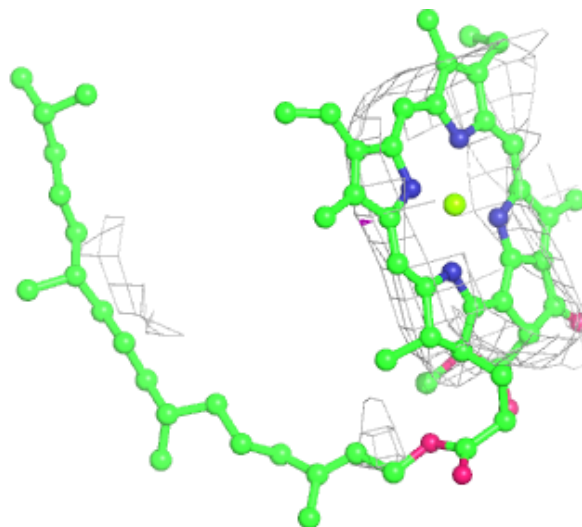
**Electron density around CLA b 607:**

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



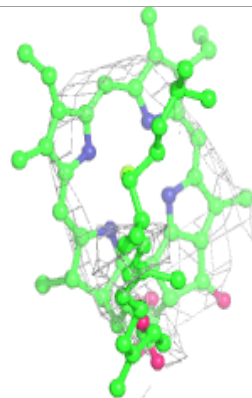
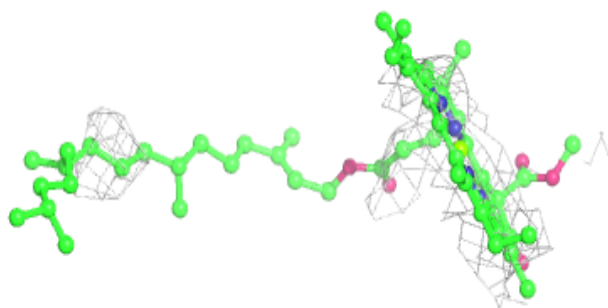
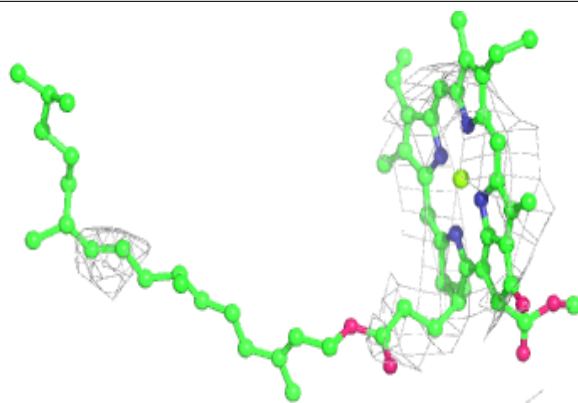
Electron density around CLA c 507:

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

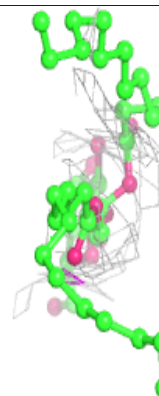
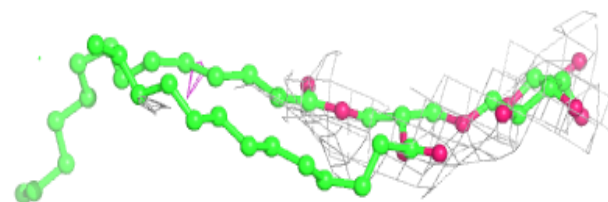
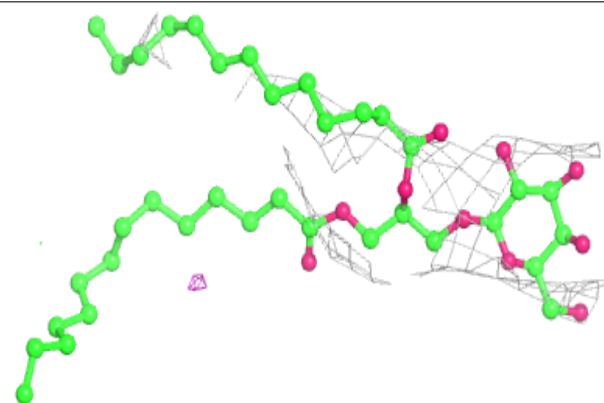


Electron density around CLA b 612:

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

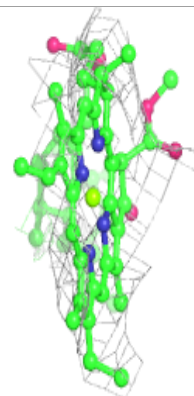
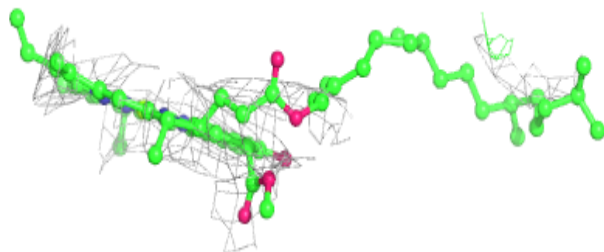
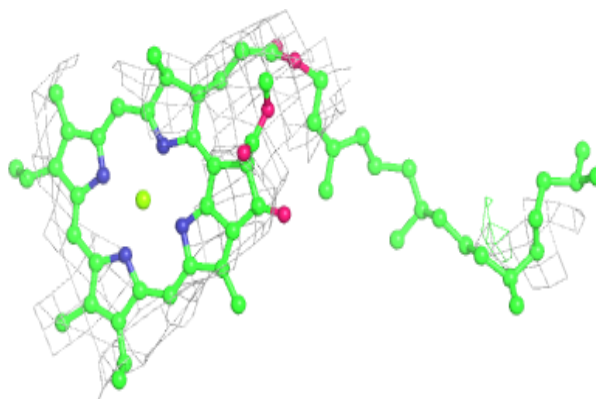
**Electron density around LMG d 405:**

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

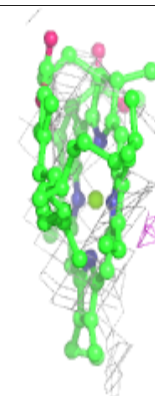
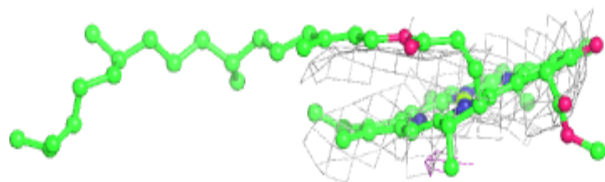
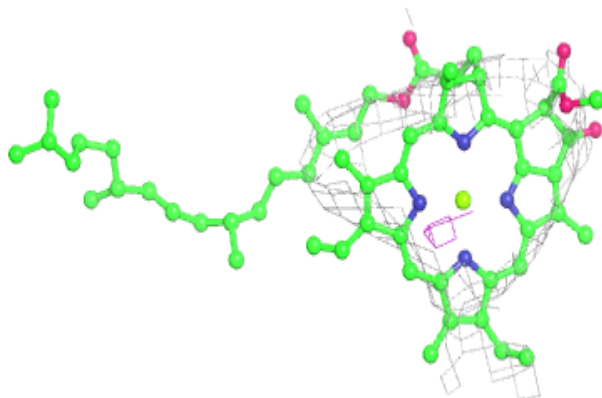


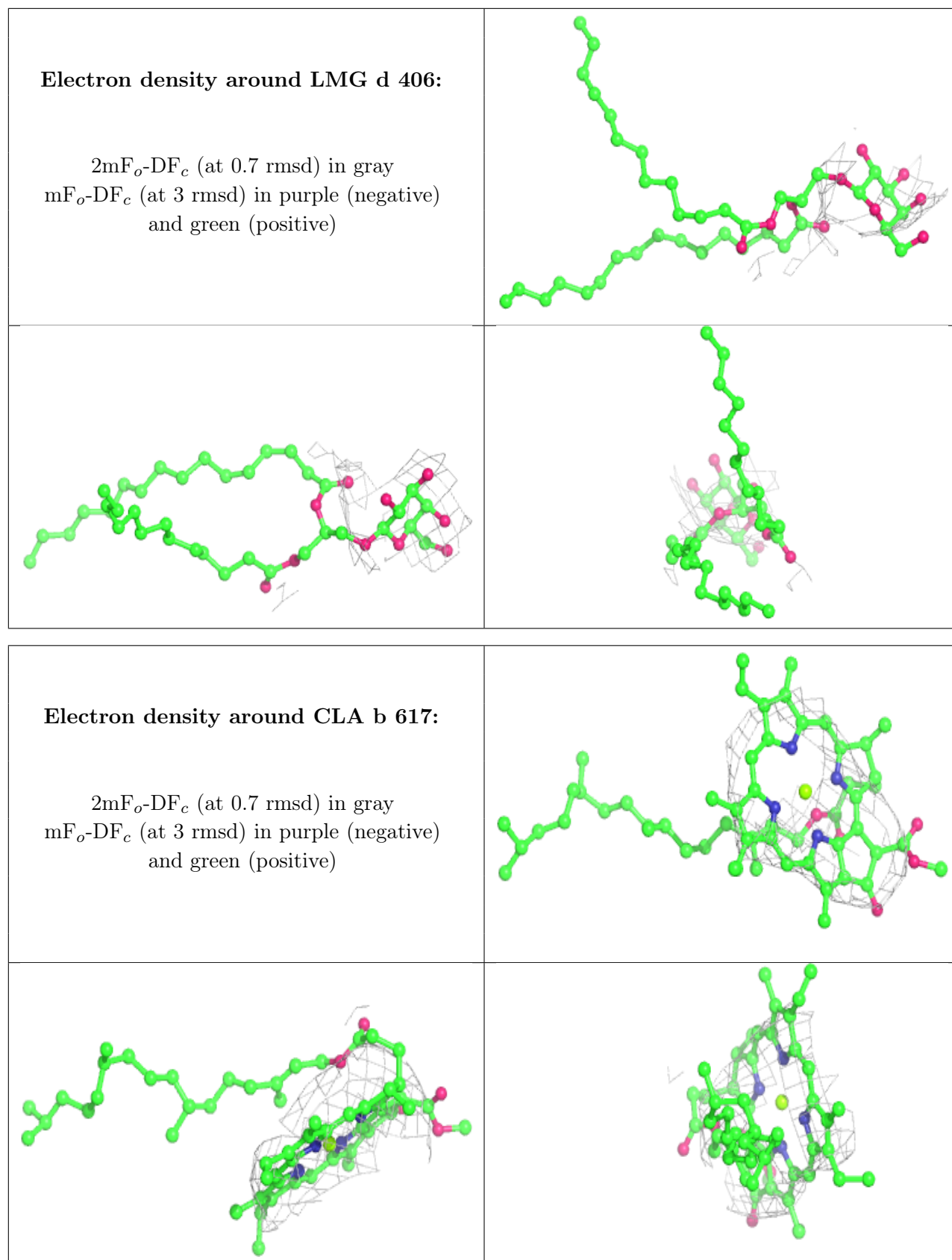
Electron density around CLA b 605:

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

**Electron density around CLA b 606:**

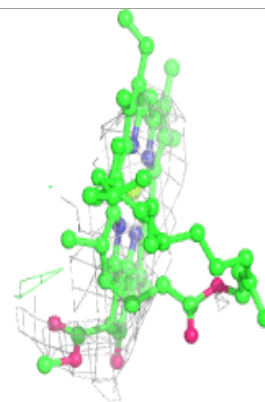
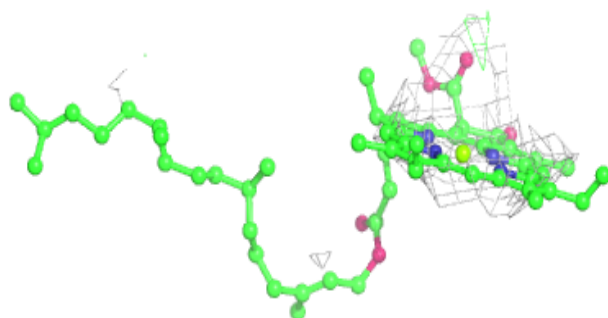
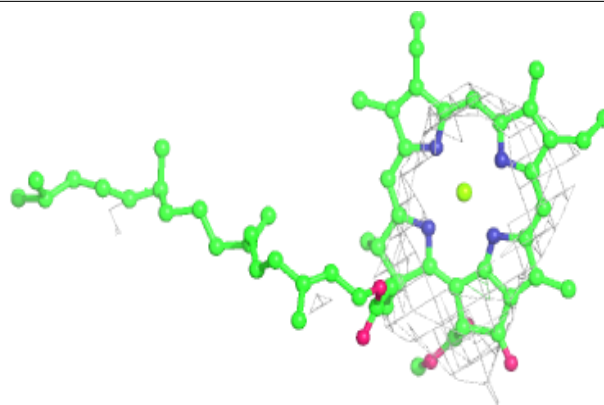
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



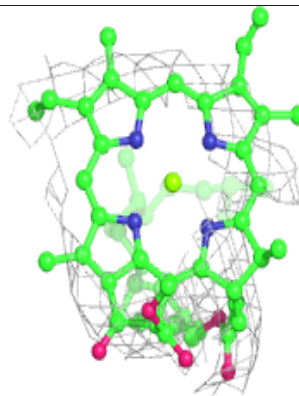
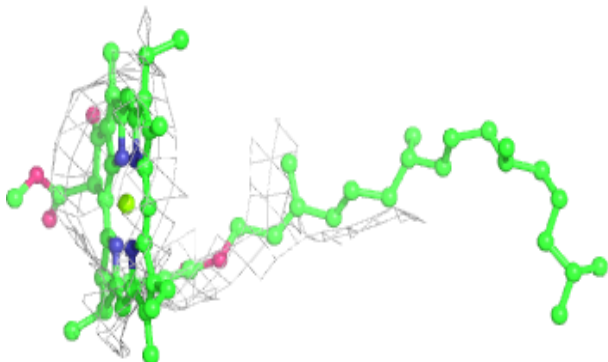
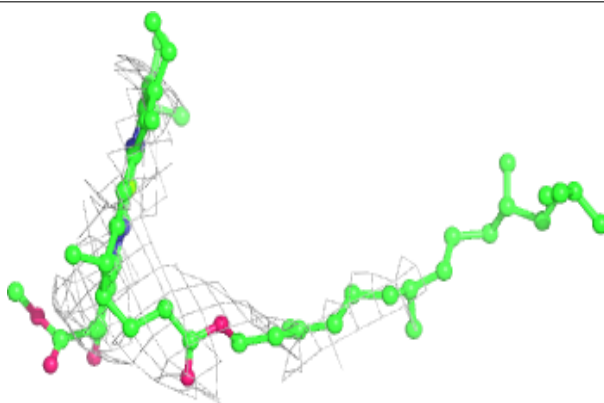


Electron density around CLA a 406:

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

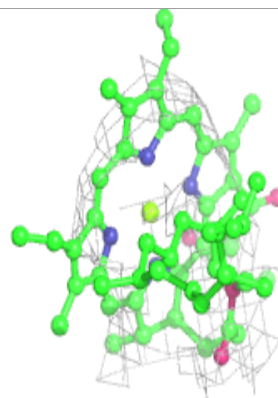
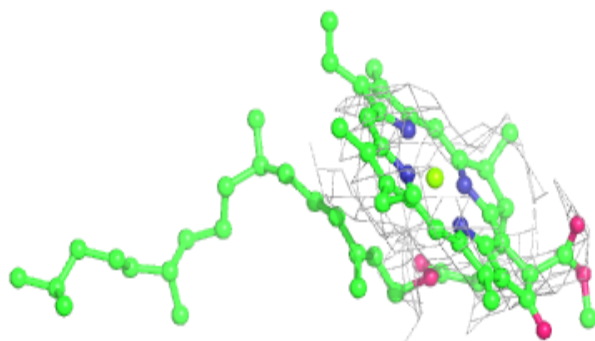
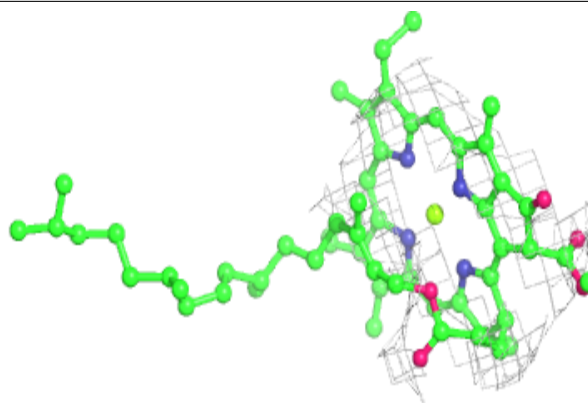
**Electron density around CLA b 608:**

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

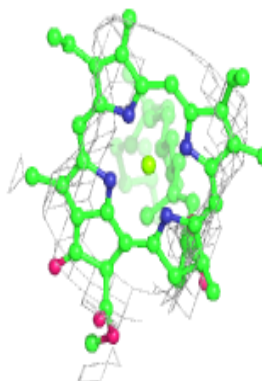
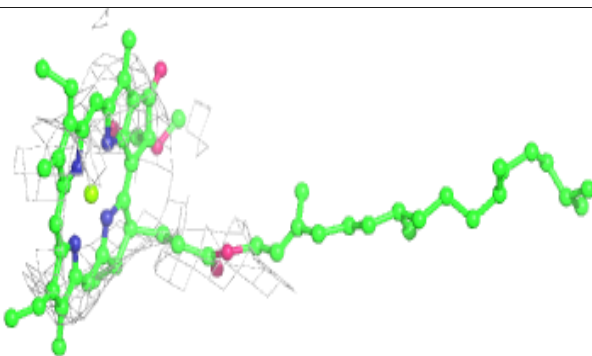
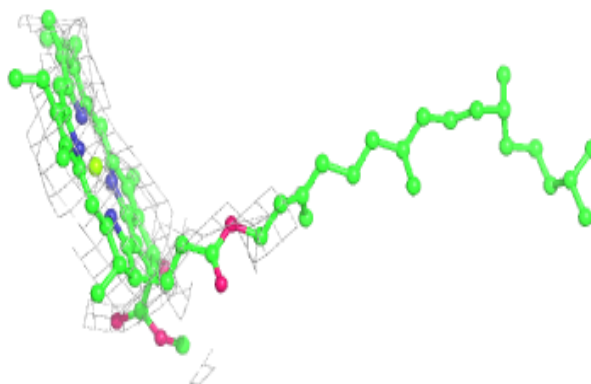


Electron density around CLA C 505:

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

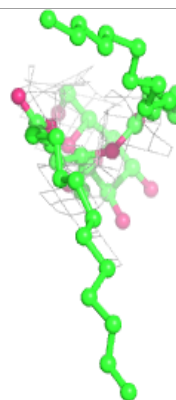
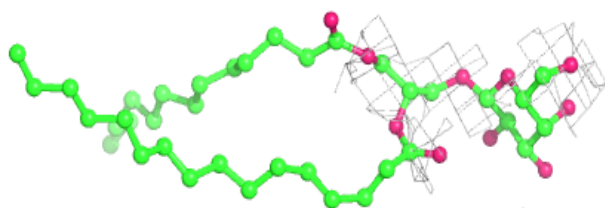
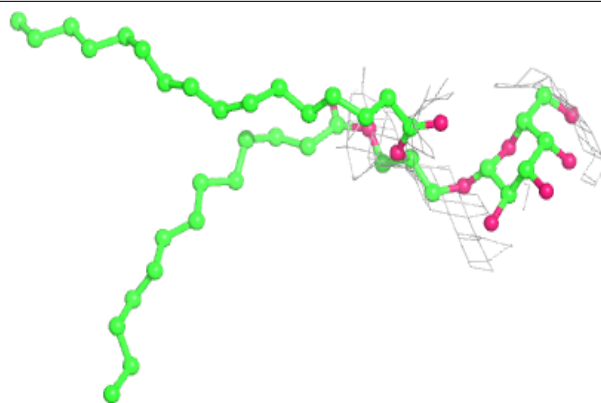
**Electron density around CLA B 604:**

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

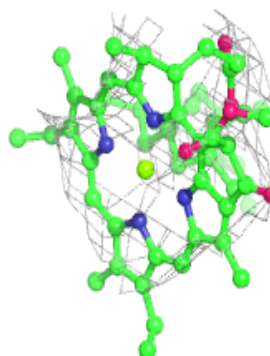
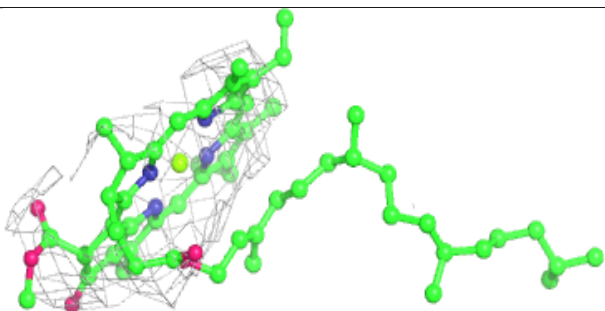
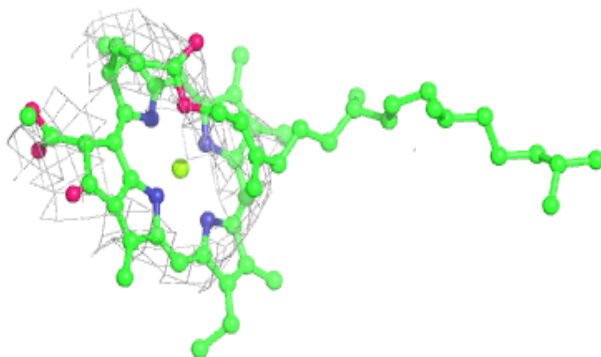


Electron density around LMG D 408:

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

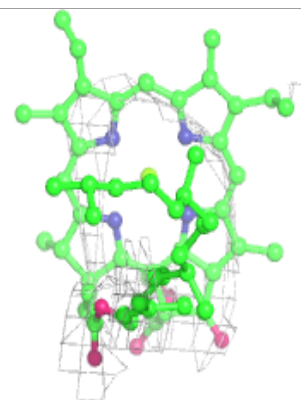
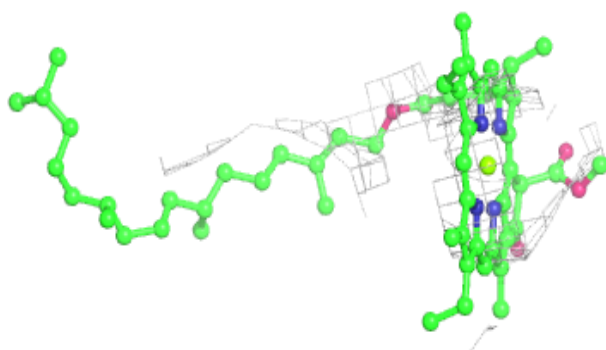
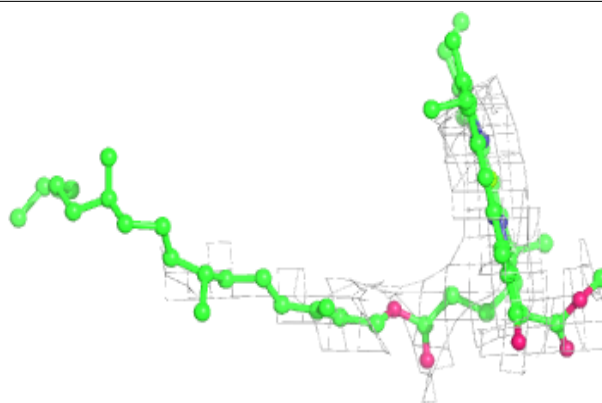
**Electron density around CLA c 505:**

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

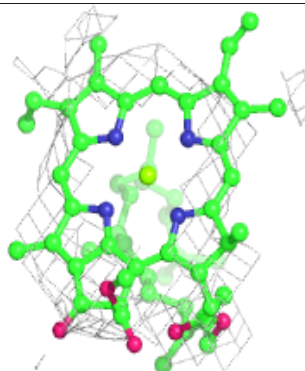
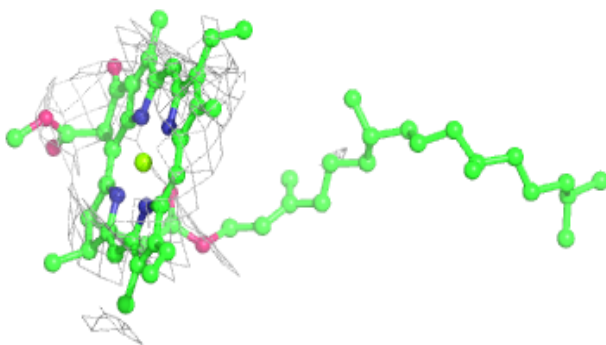
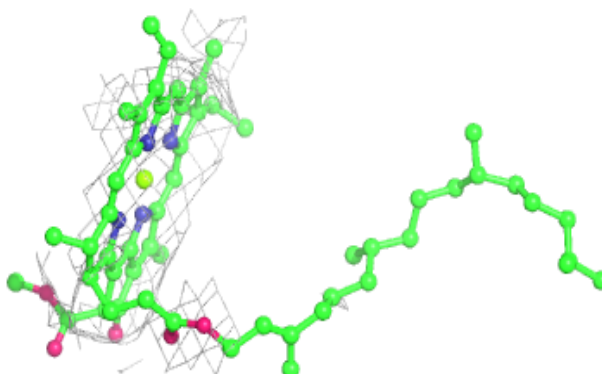


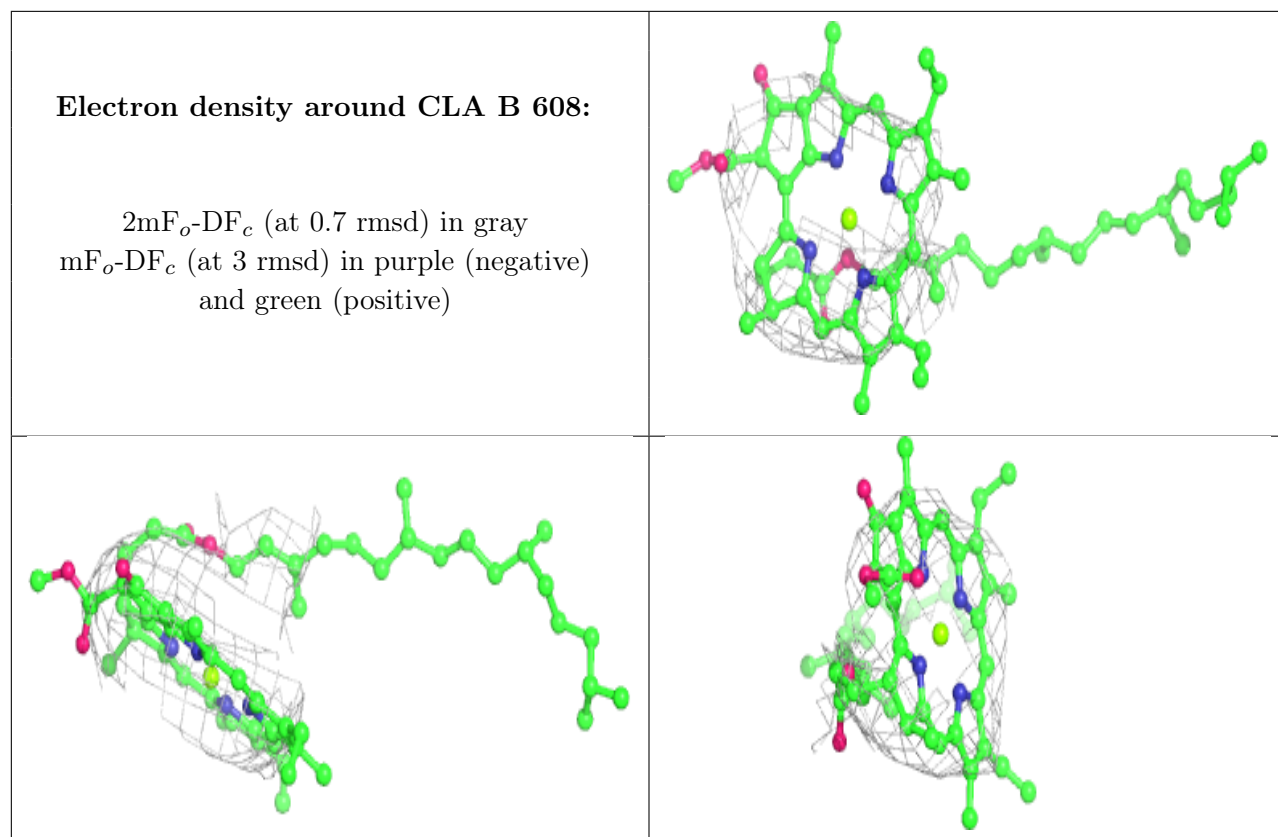
Electron density around CLA B 605:

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

**Electron density around CLA C 508:**

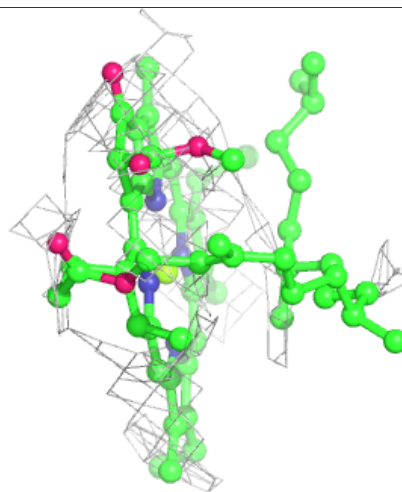
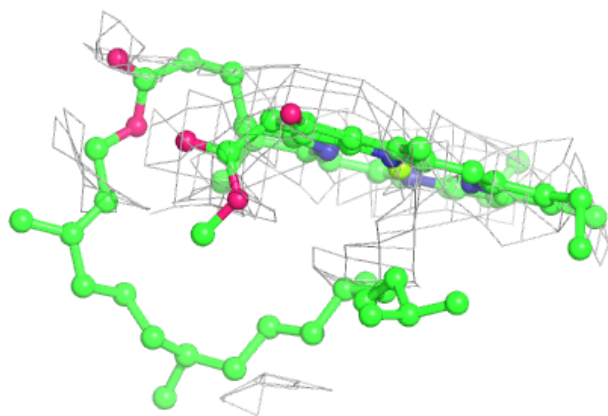
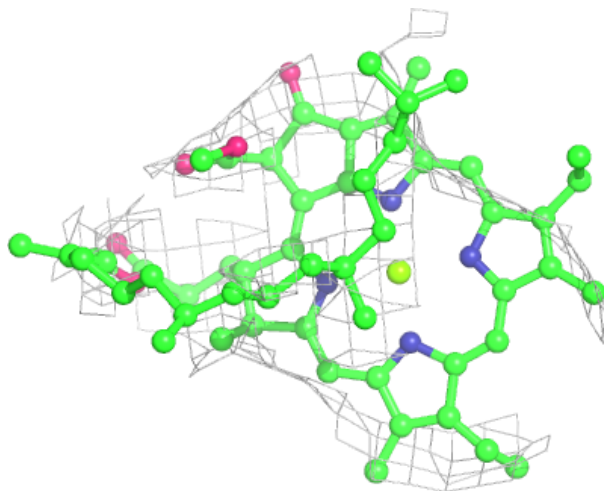
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

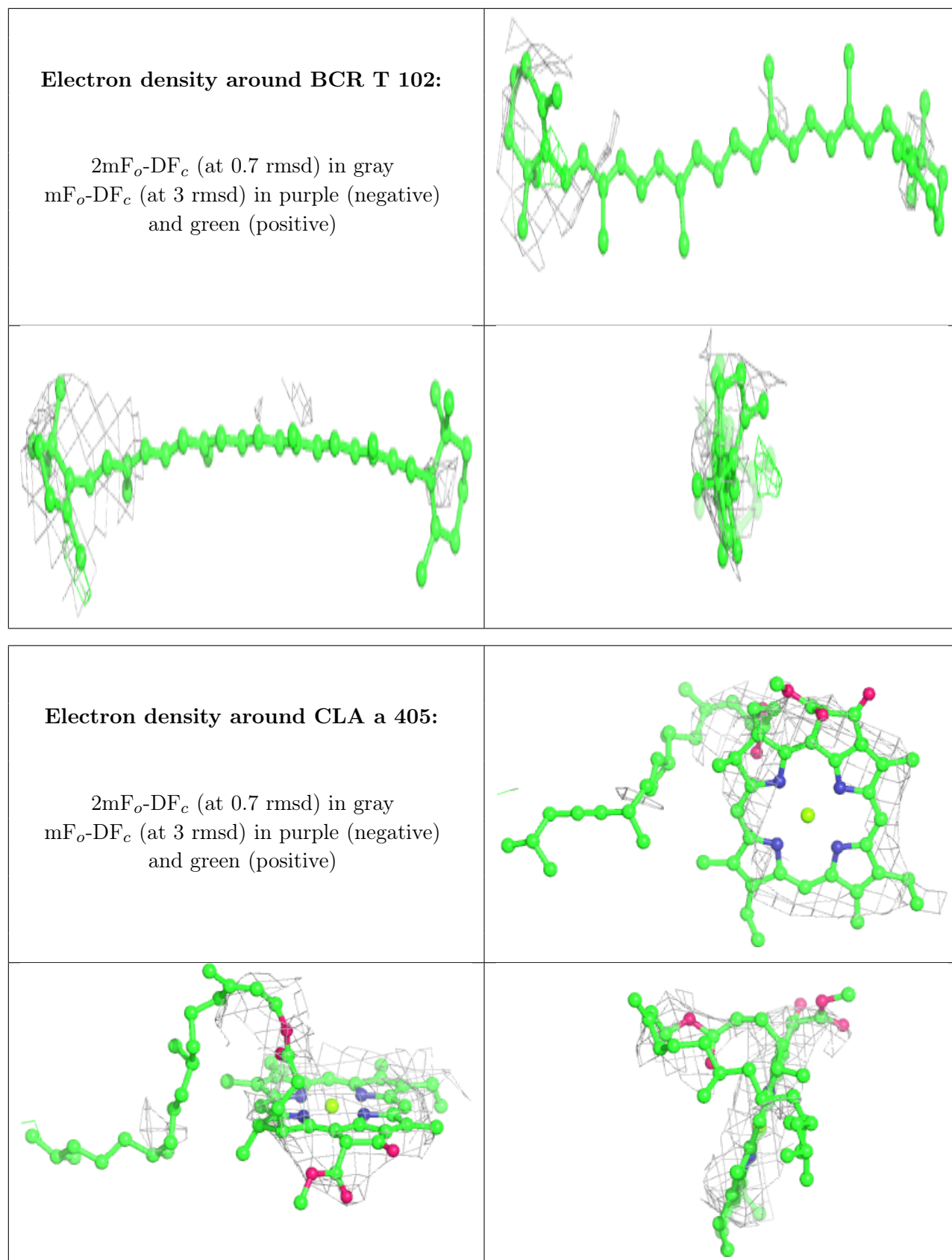


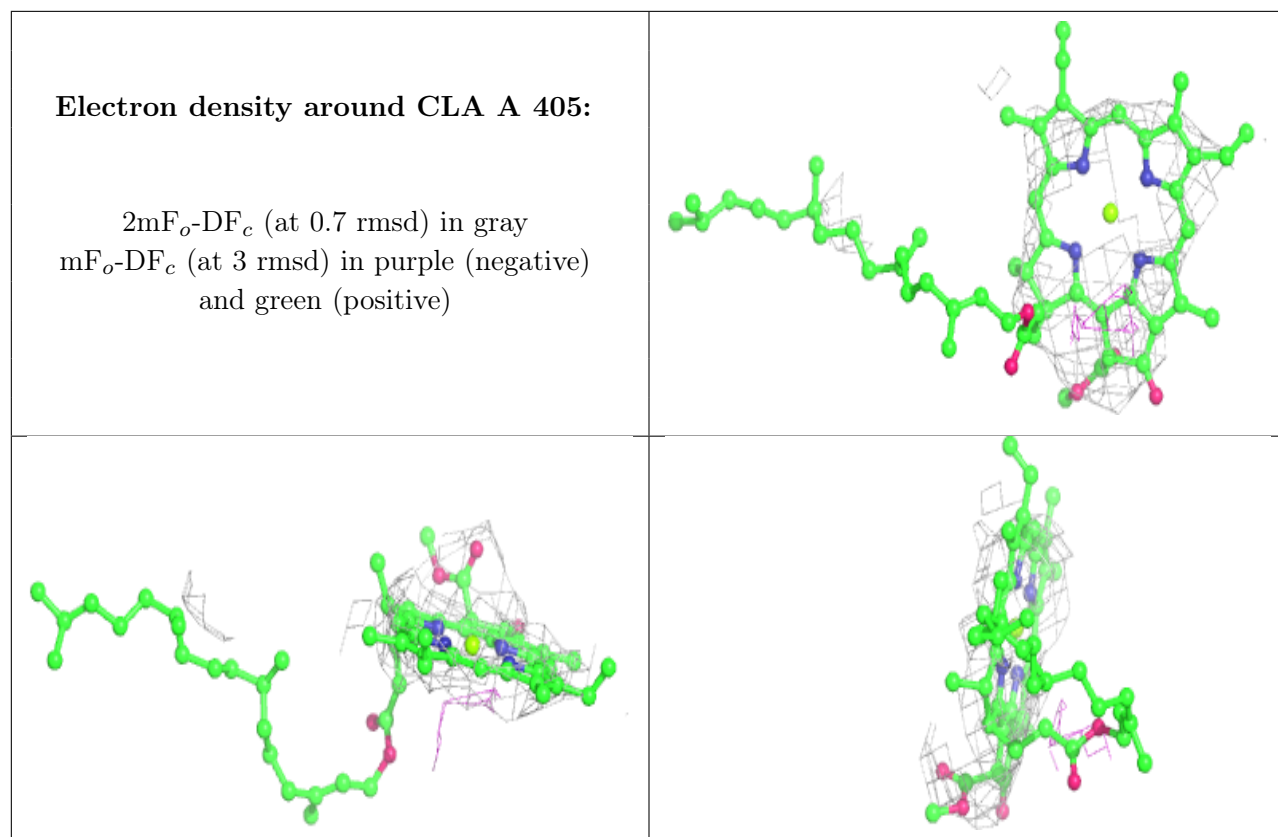


Electron density around CLA C 510:

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

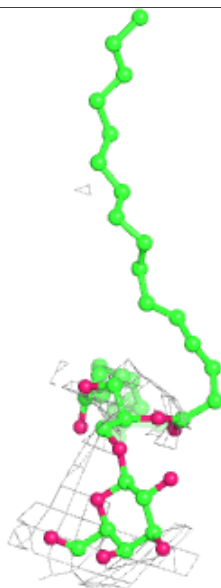
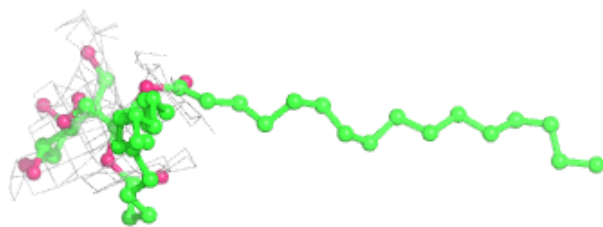
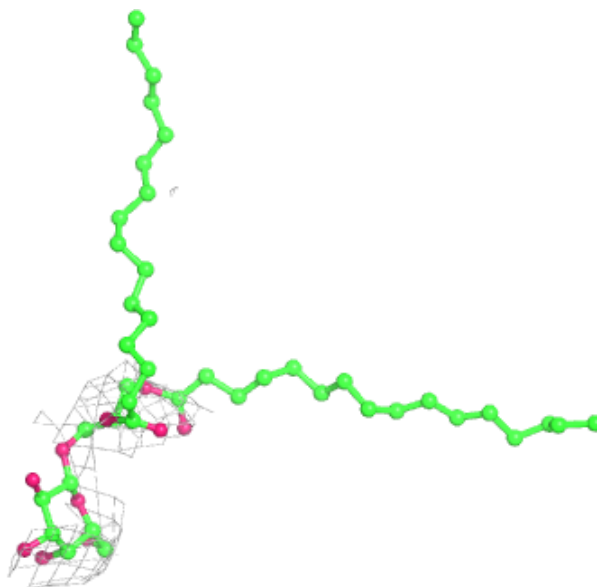






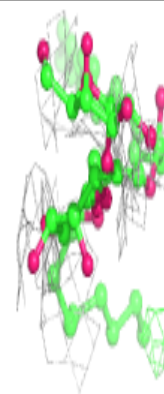
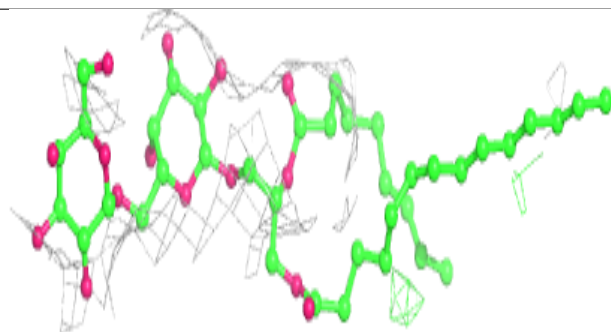
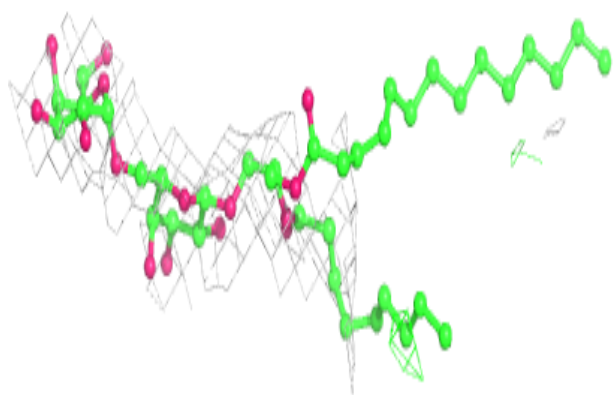
Electron density around LMG A 414:

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

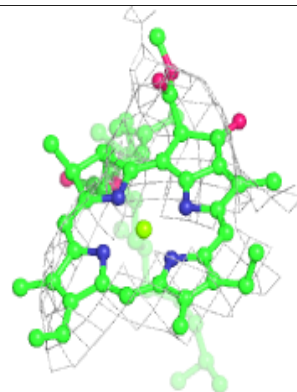
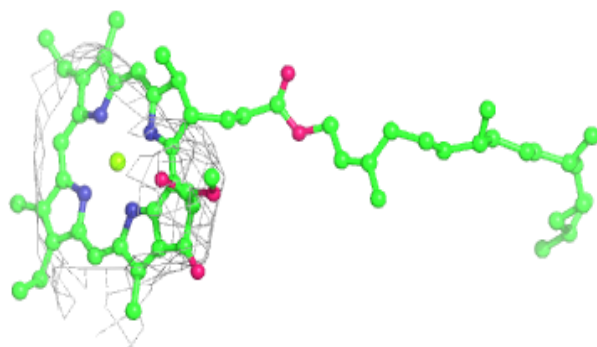
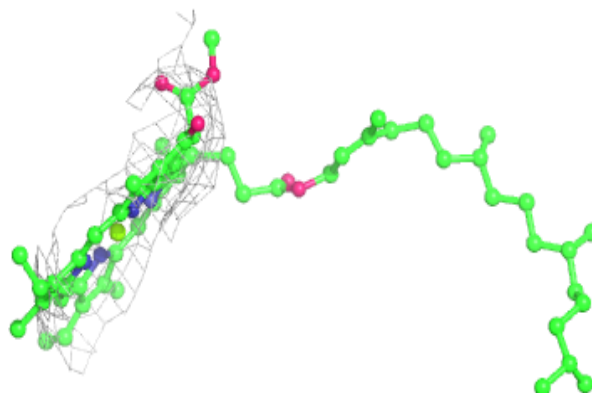


Electron density around DGD c 517:

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

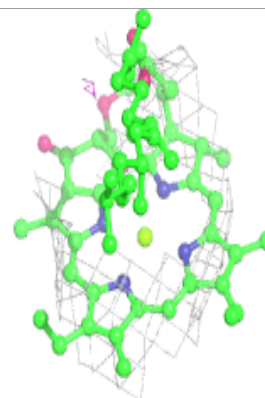
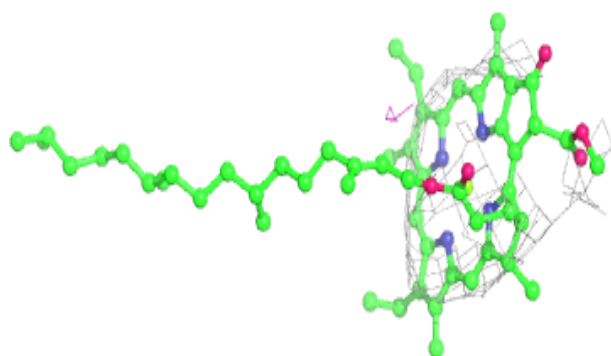
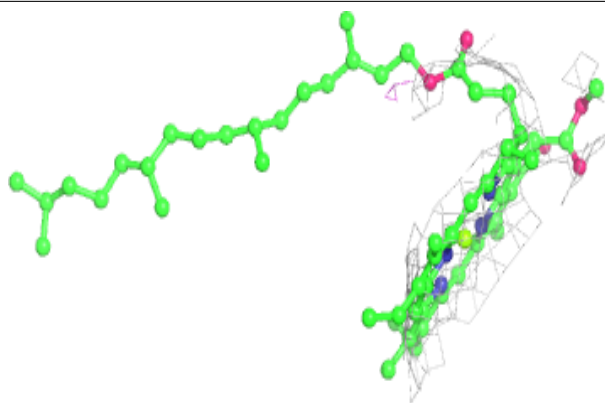
**Electron density around CLA d 402:**

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

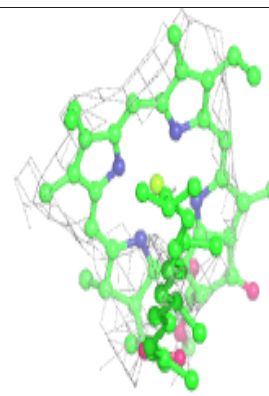
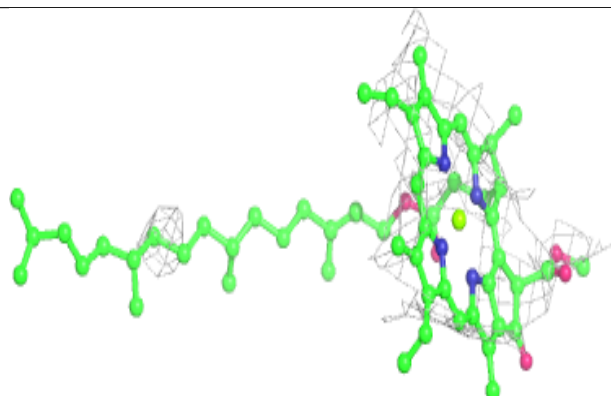
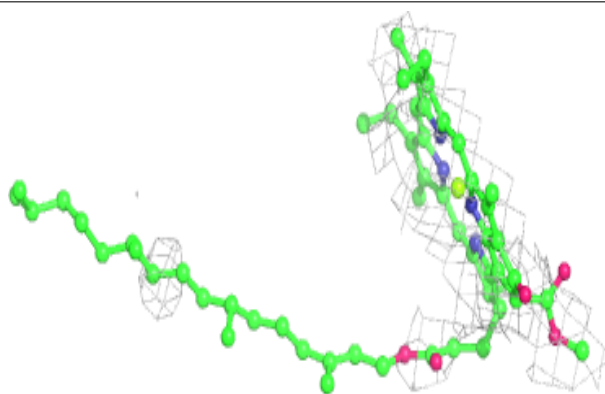


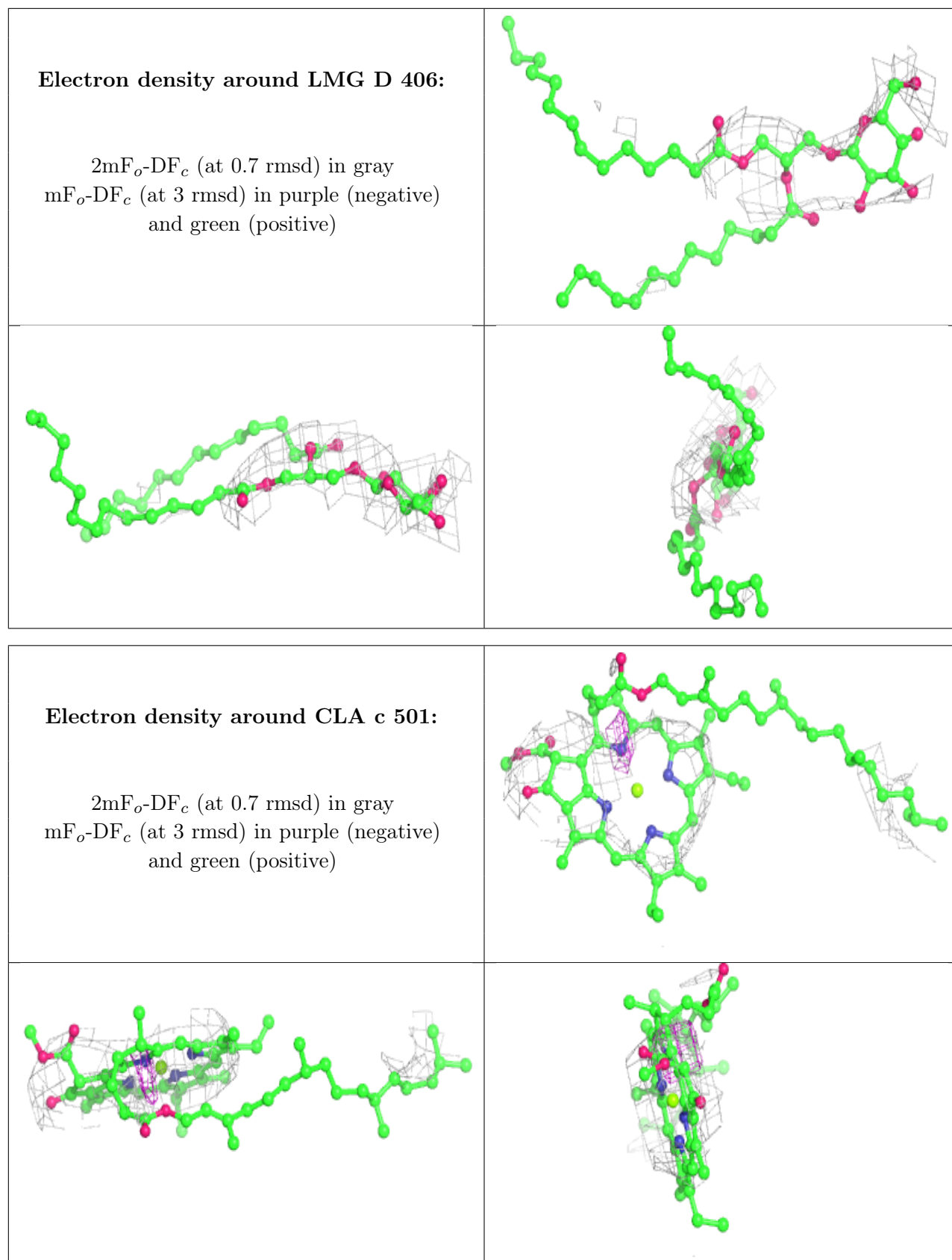
Electron density around CLA c 504:

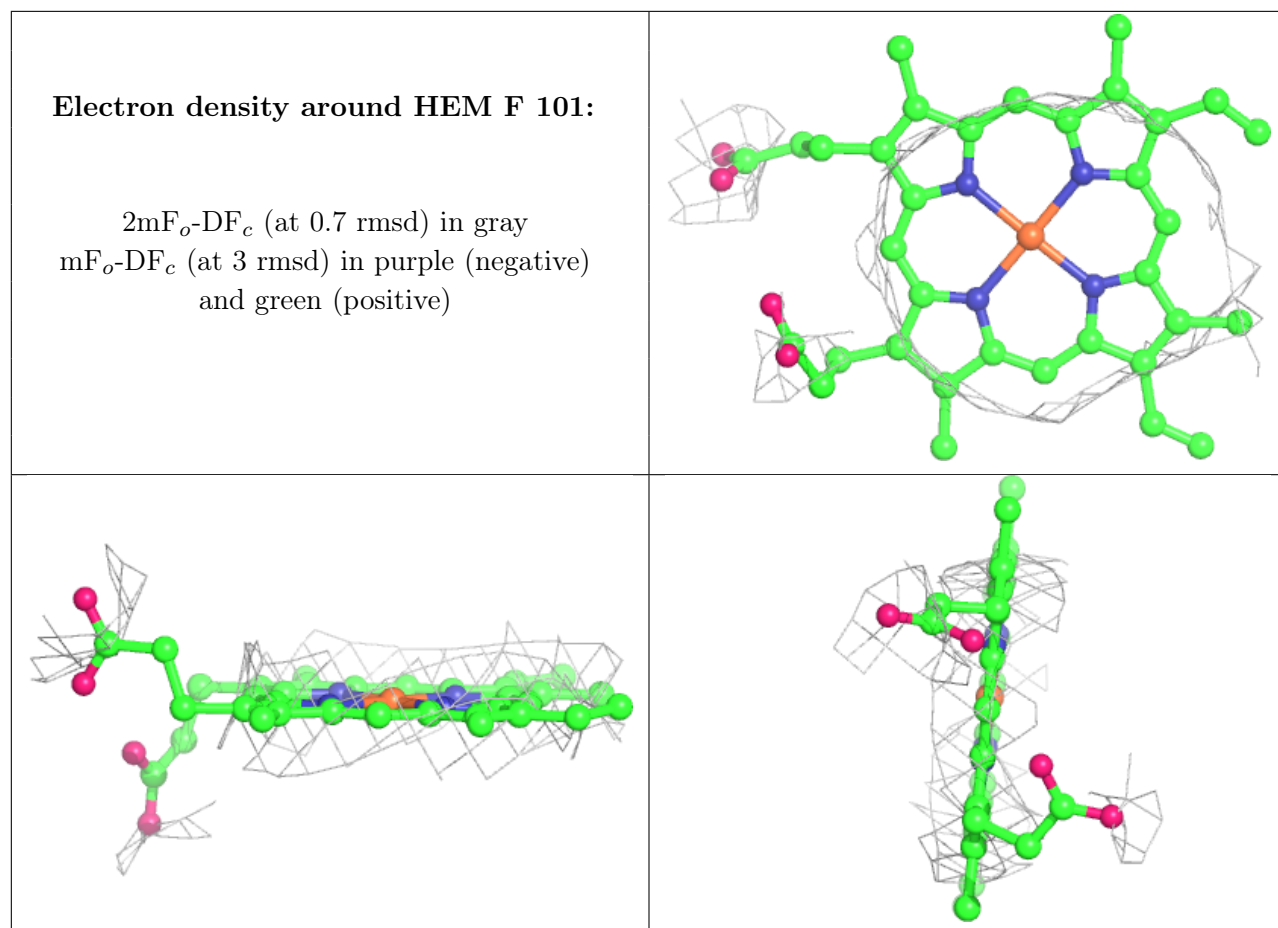
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA b 610:**

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

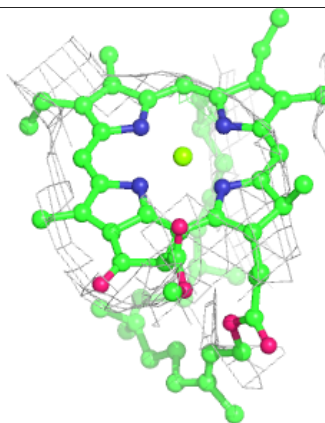
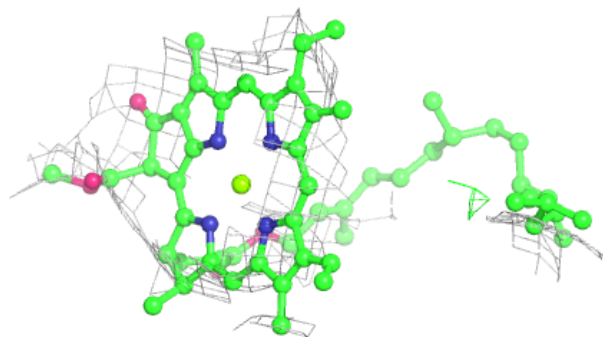
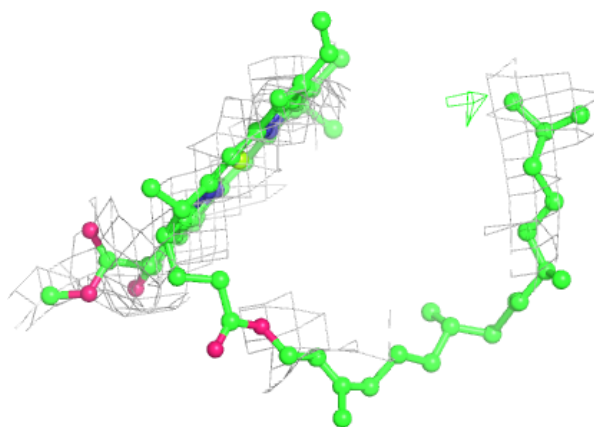




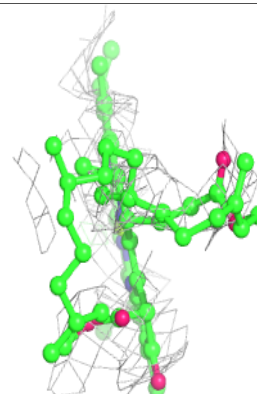
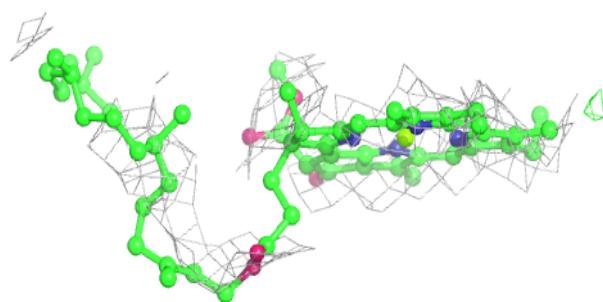
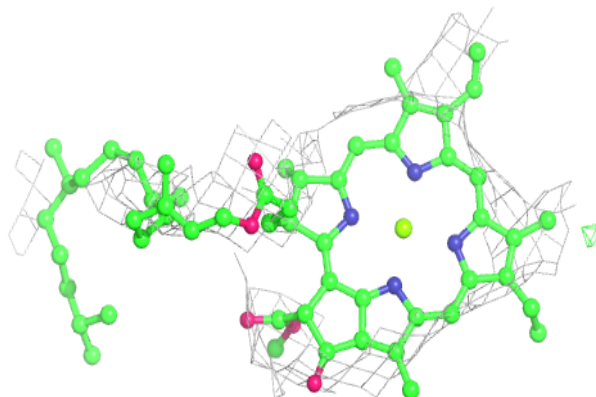


Electron density around CLA b 614:

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

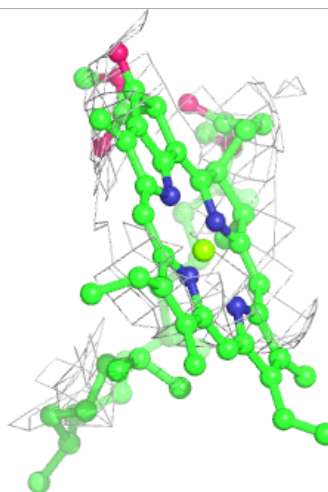
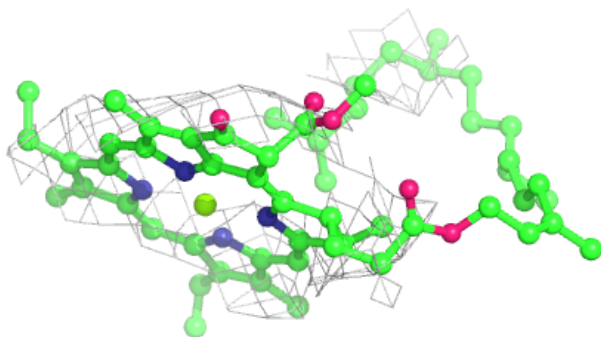
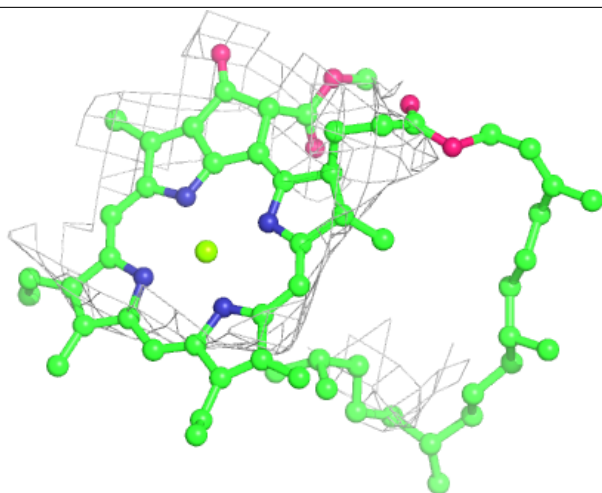
**Electron density around CLA b 615:**

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



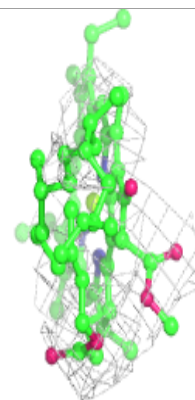
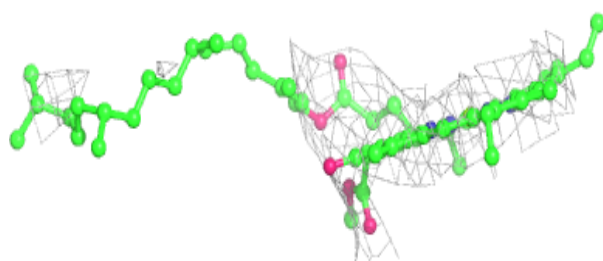
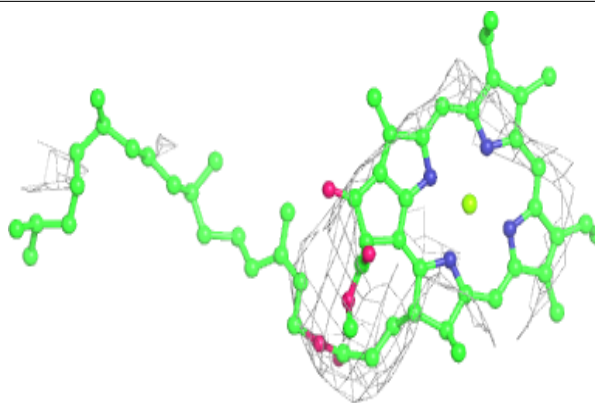
Electron density around CLA B 615:

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

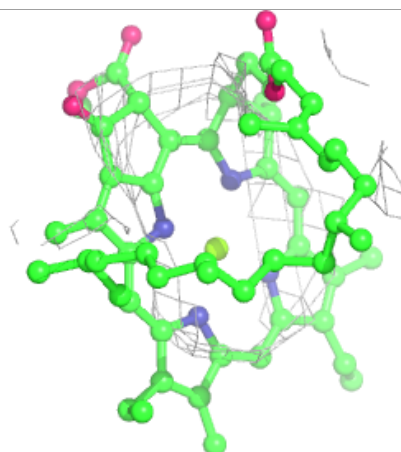
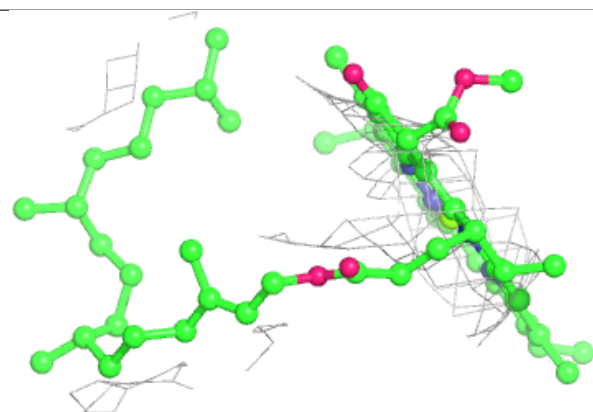
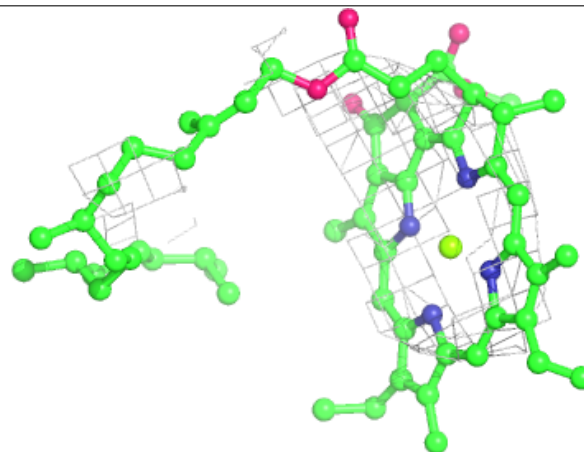


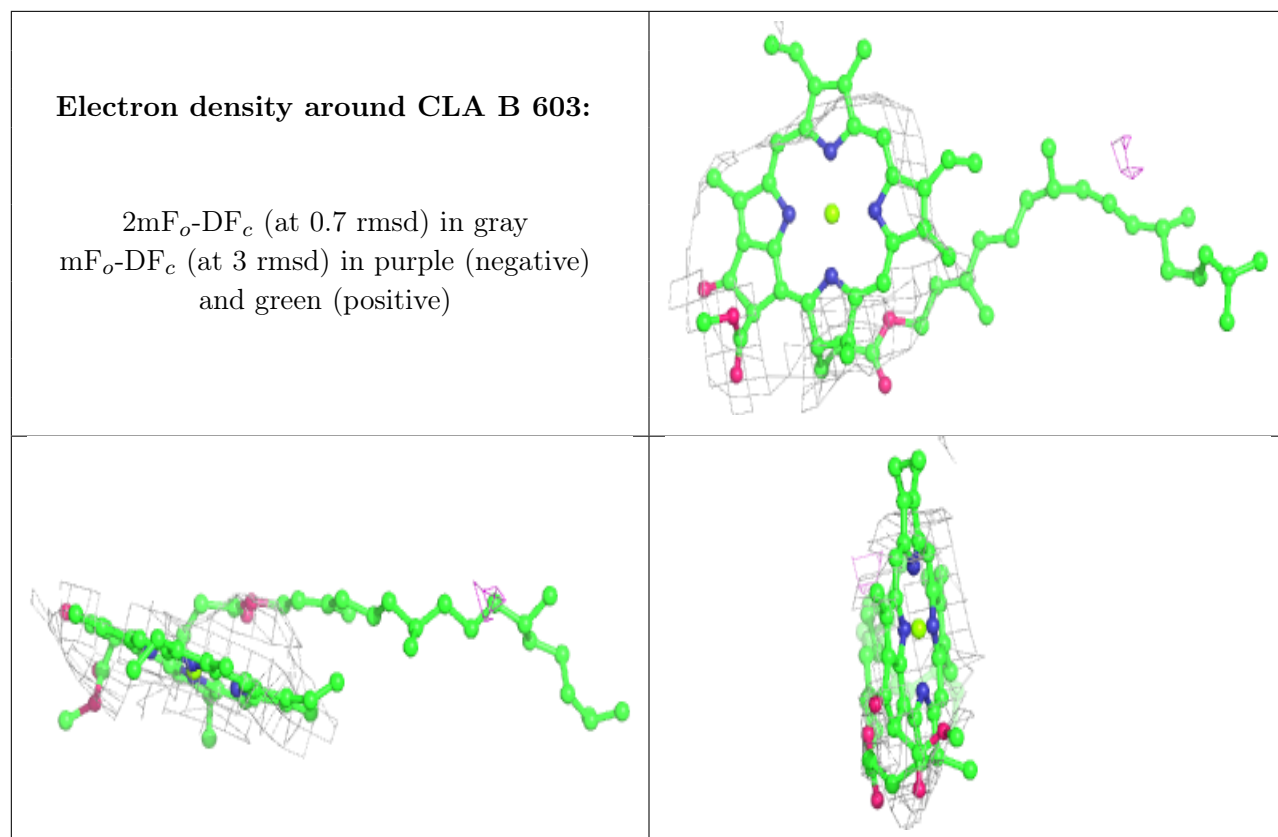
Electron density around CLA B 602:

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

**Electron density around CLA c 503:**

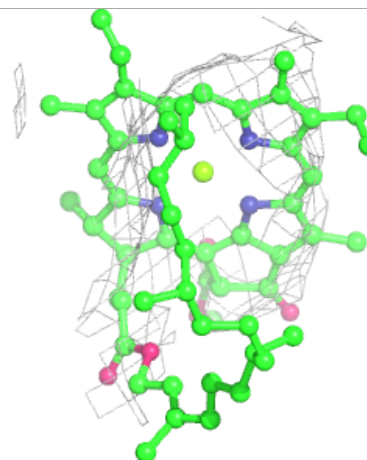
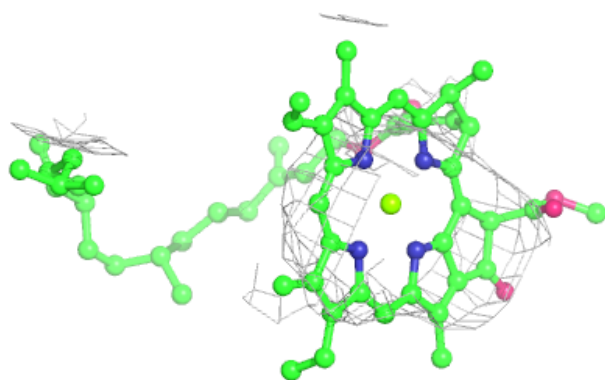
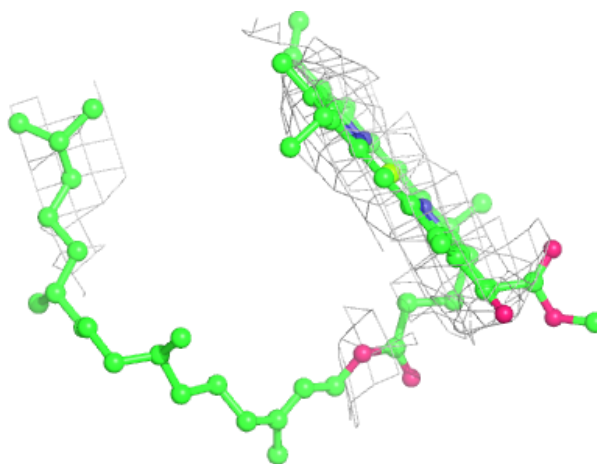
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





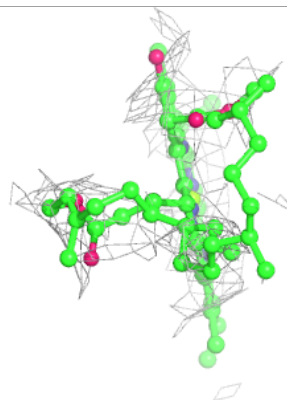
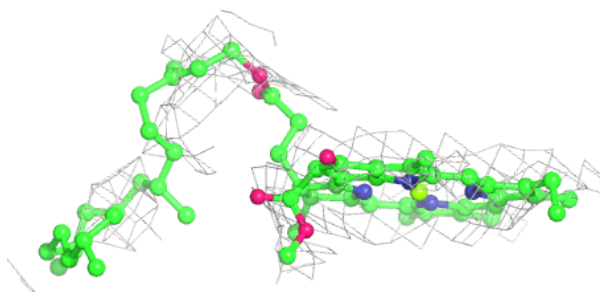
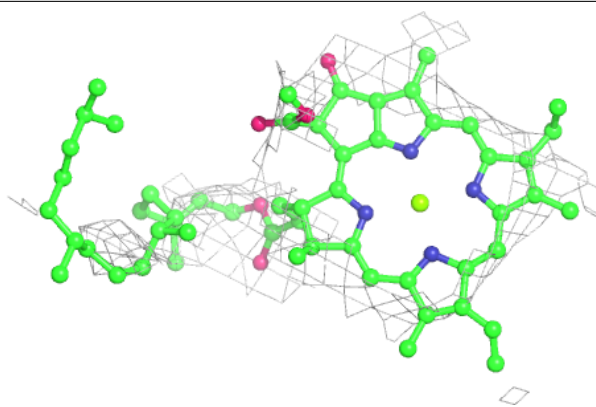
Electron density around CLA B 611:

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

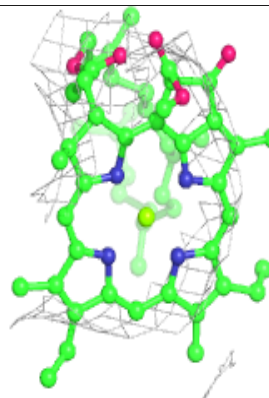
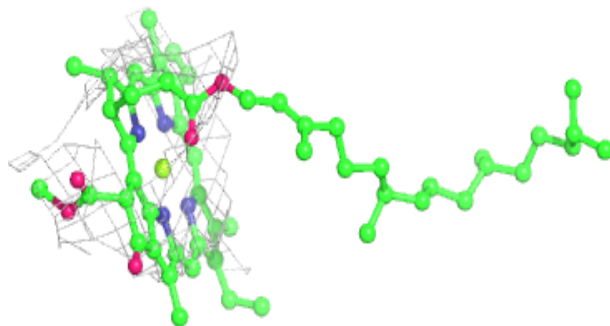
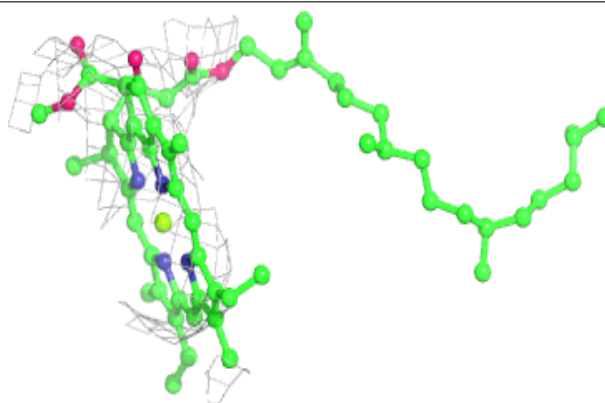


Electron density around CLA B 612:

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

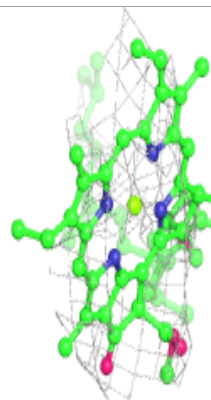
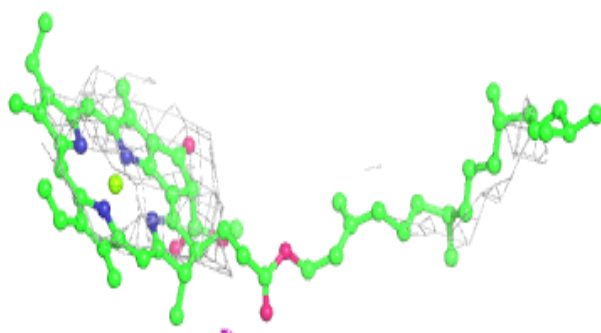
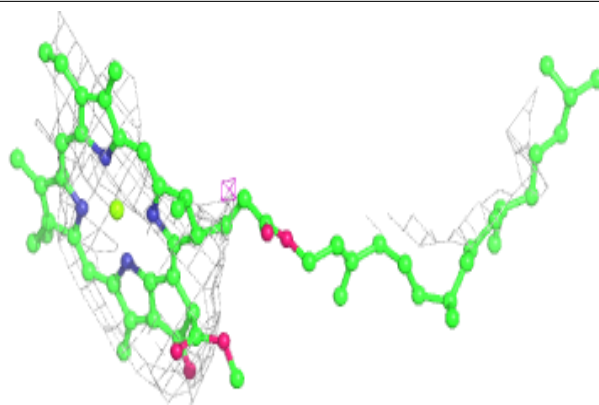
**Electron density around CLA c 508:**

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

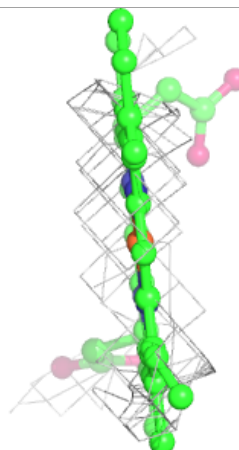
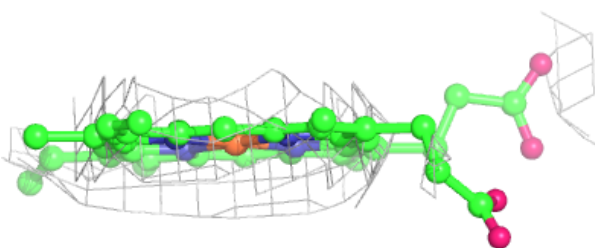
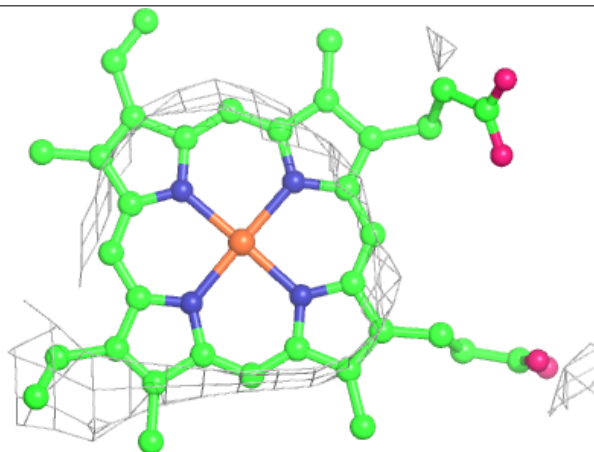


Electron density around CLA A 403:

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

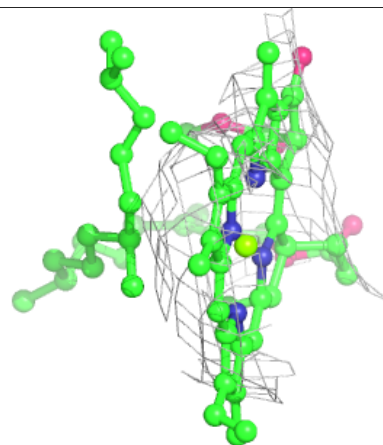
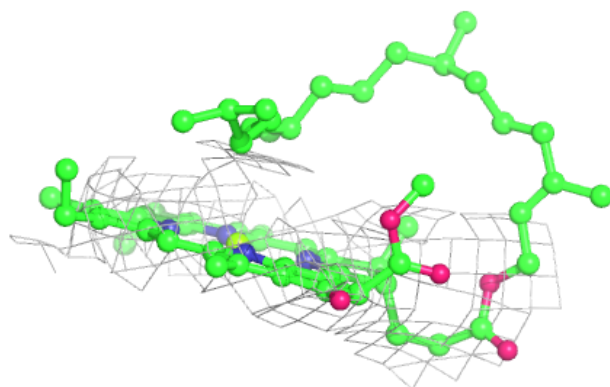
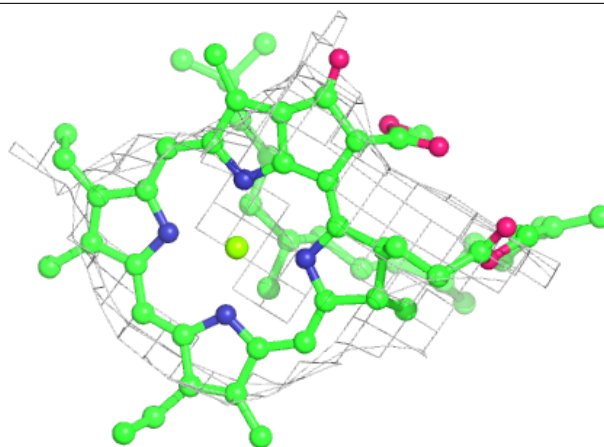
**Electron density around HEM v 201:**

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

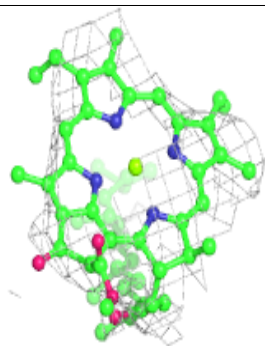
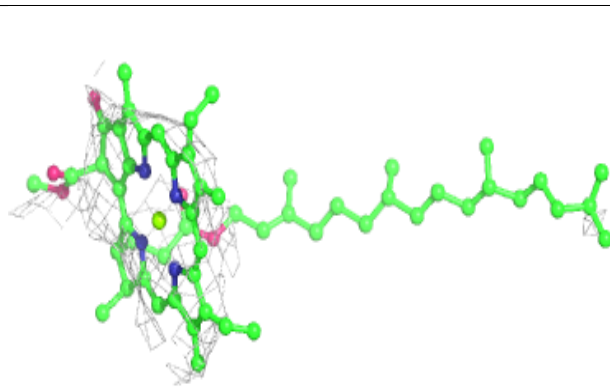
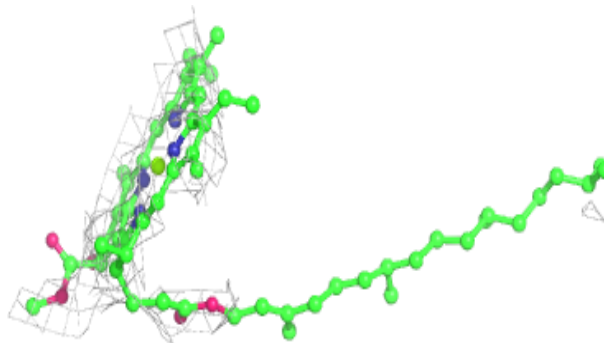


Electron density around CLA c 510:

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

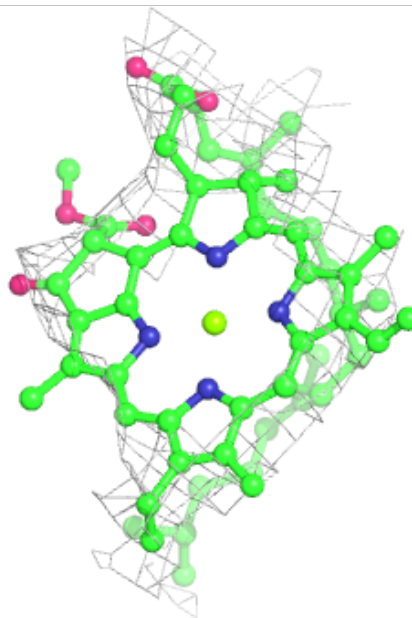
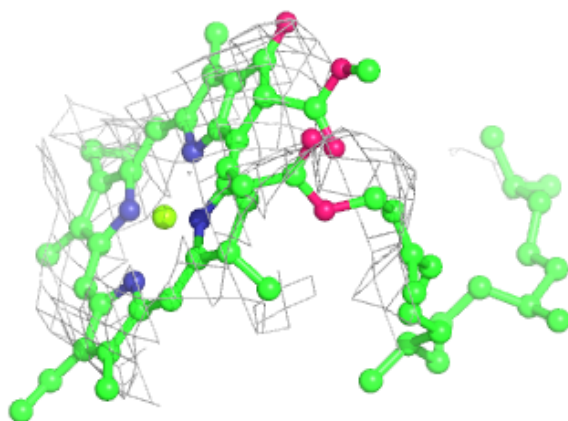
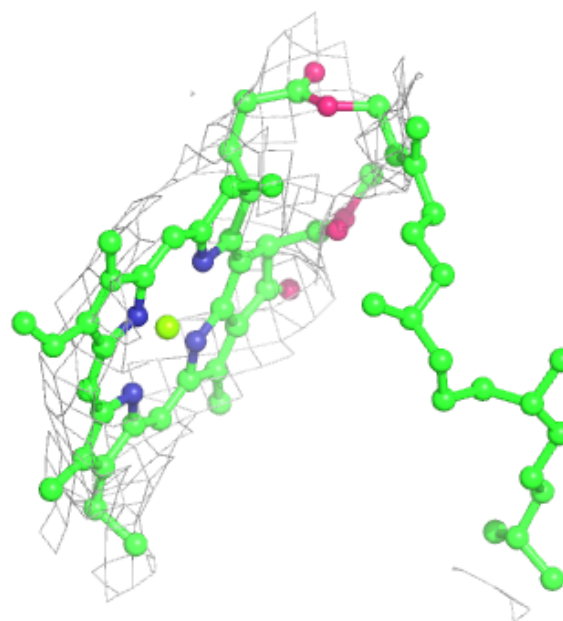
**Electron density around CLA B 607:**

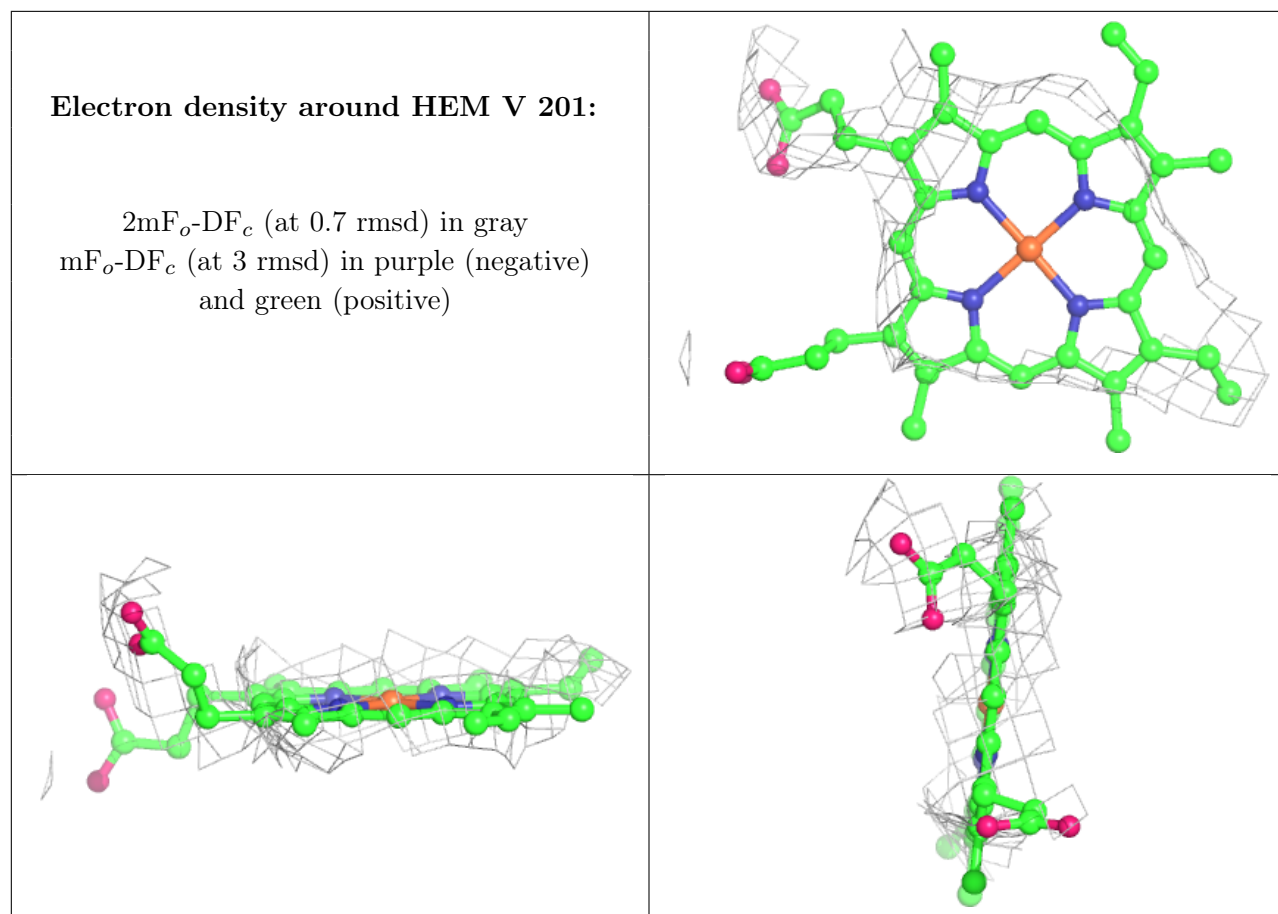
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 613:

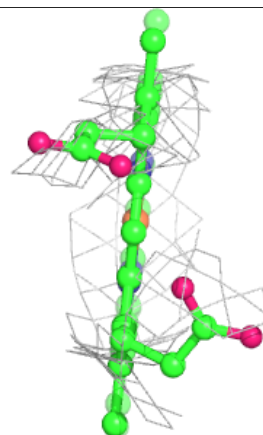
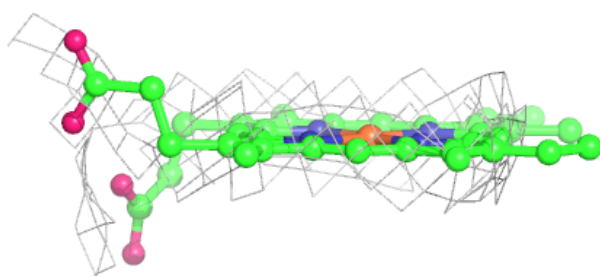
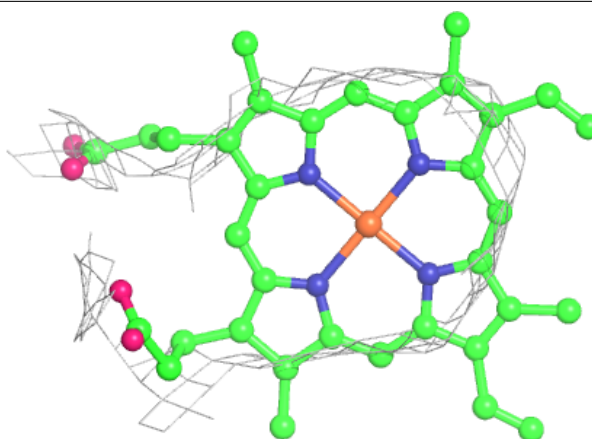
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



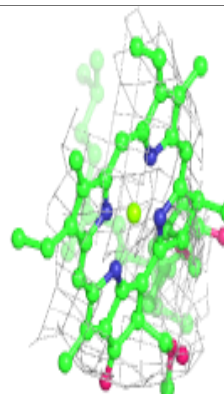
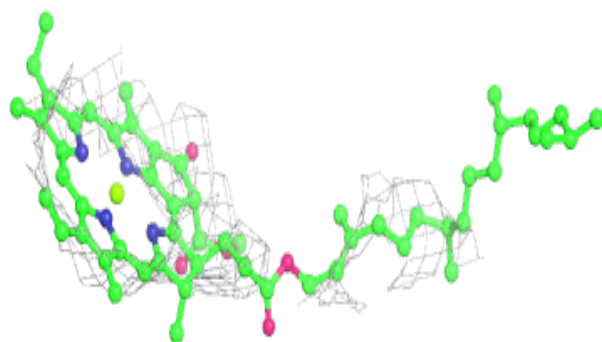
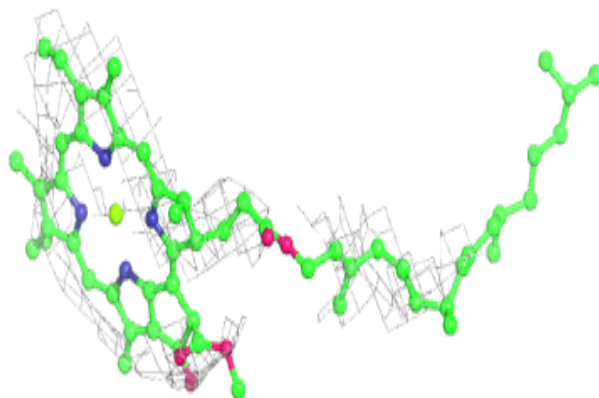


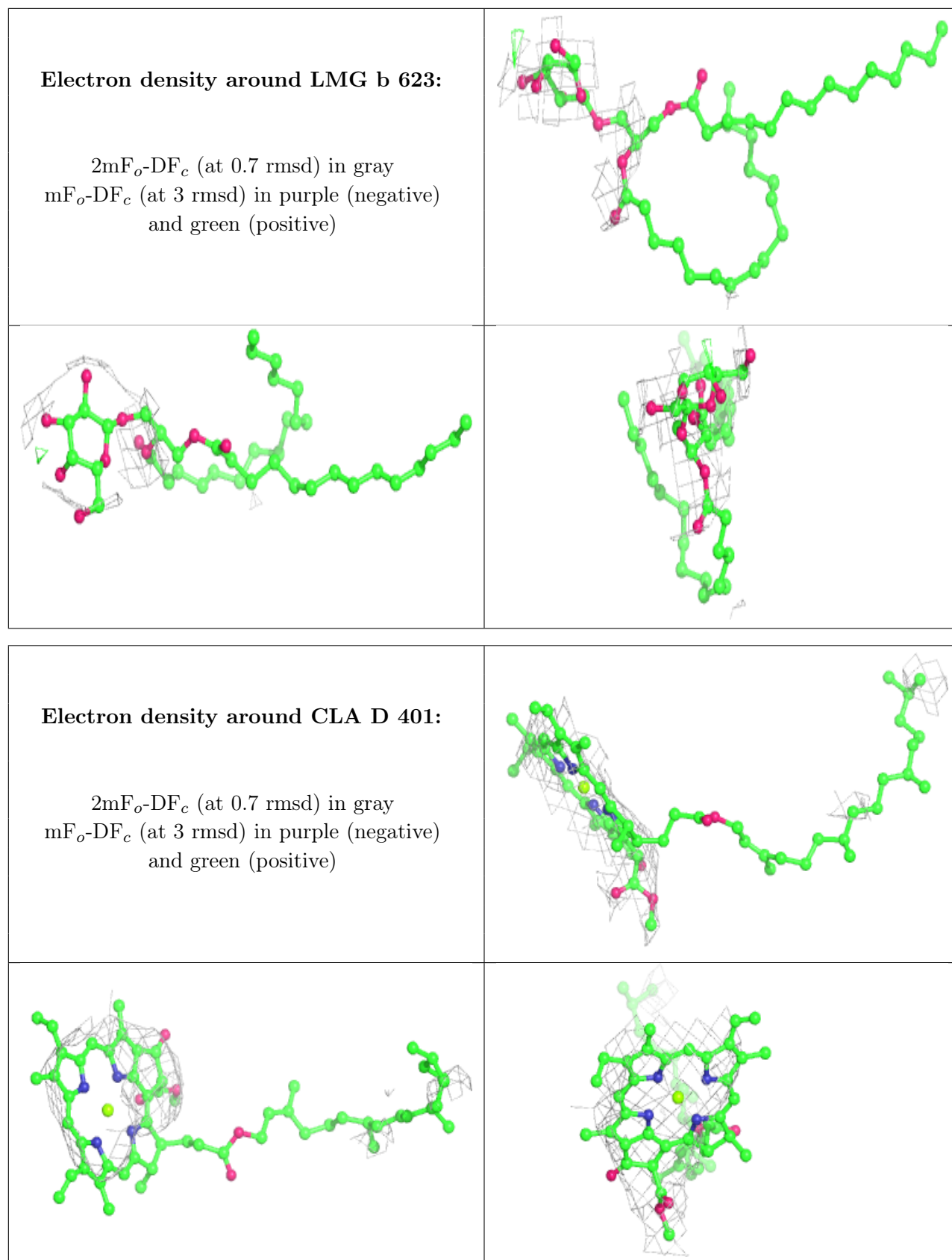
Electron density around HEM f 101:

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

**Electron density around CLA a 404:**

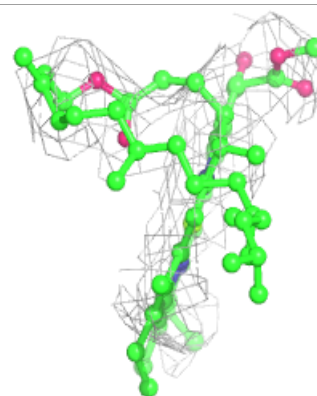
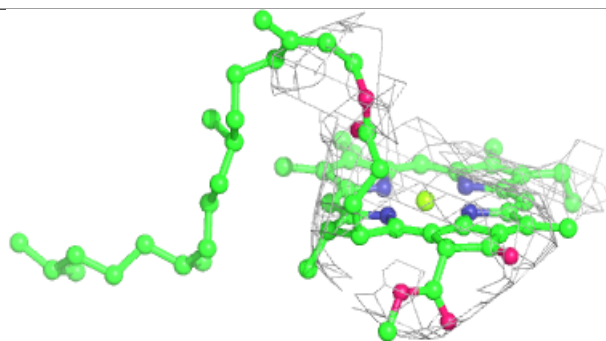
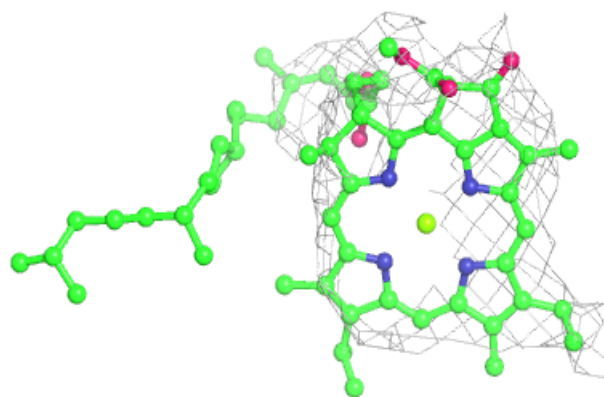
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



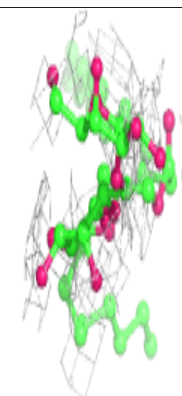
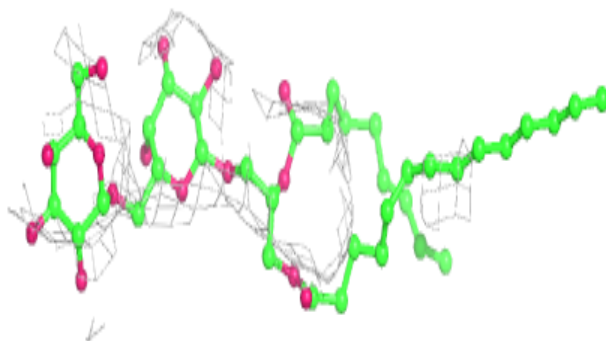
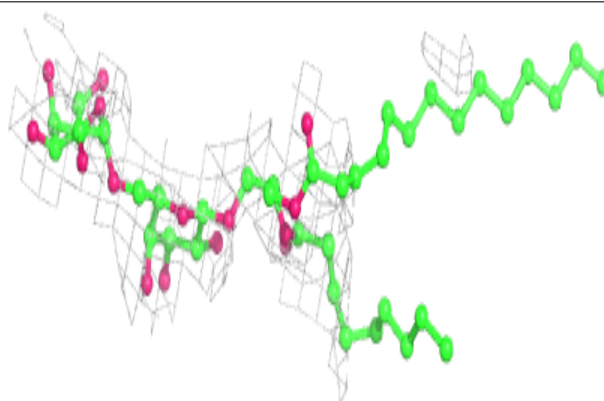


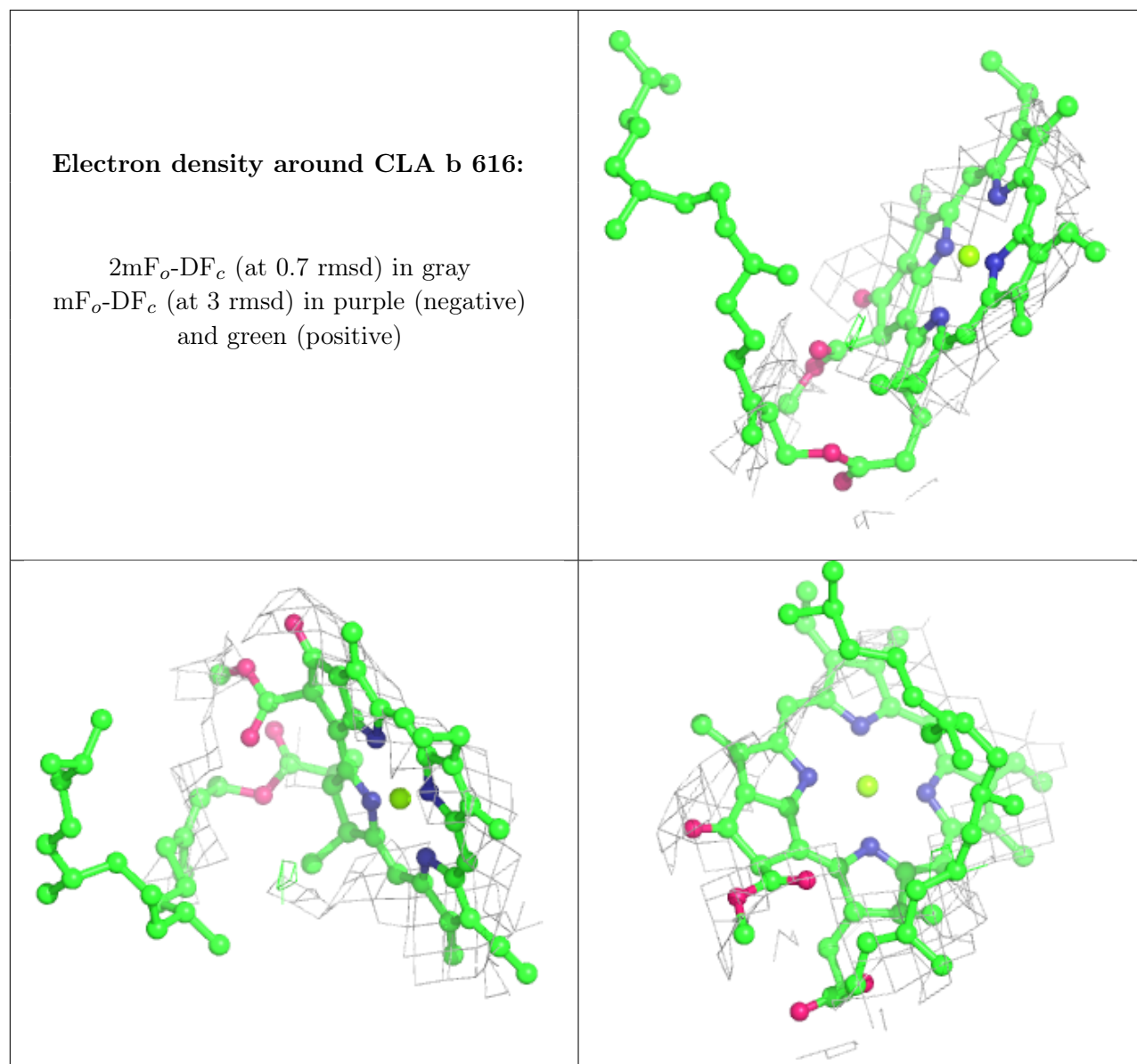
Electron density around CLA A 404:

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

**Electron density around DGD C 516:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.