



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2023 – 09:31 PM EDT

PDB ID : 4TNH
Title : RT XFEL structure of Photosystem II in the dark state at 4.9 Å resolution
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2014-06-04
Resolution : 4.90 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)

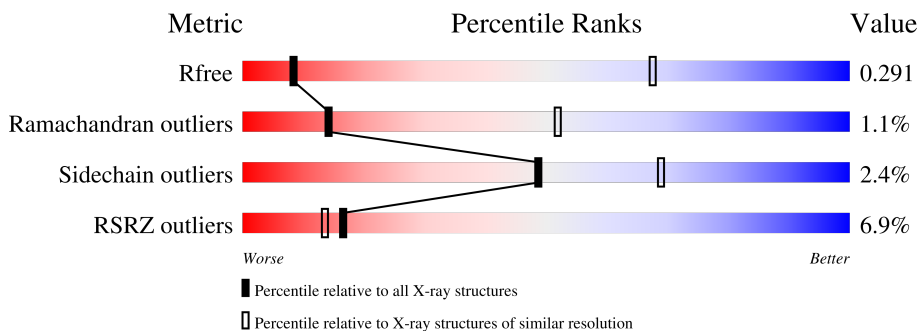
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.90 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	1134 (6.00-3.80)
Ramachandran outliers	138981	1140 (6.00-3.80)
Sidechain outliers	138945	1117 (6.00-3.80)
RSRZ outliers	127900	1005 (6.00-3.72)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	

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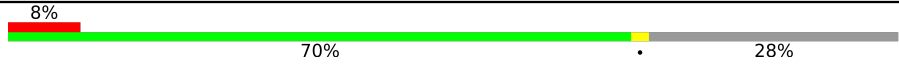

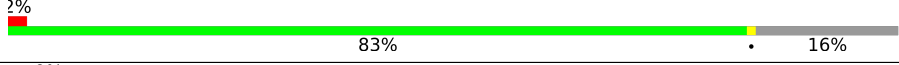



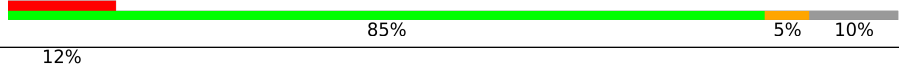

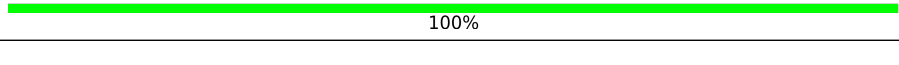
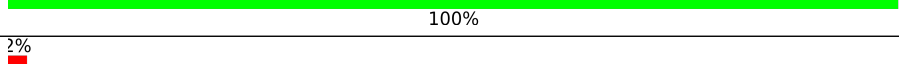
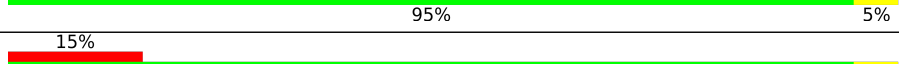
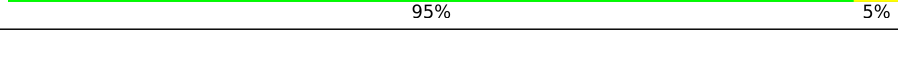
Refmac : 5.8.0158
 CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
2	b	510	7% 94% ..
3	C	461	8% 94% ..
3	c	461	5% 93% ..
4	D	352	5% 95% ..
4	d	352	5% 94% ..
5	E	84	% 94% ..
5	e	84	2% 94% ..
6	F	45	78% 22%
6	f	45	78% 22%
7	H	66	14% 88% 11% .
7	h	66	18% 88% 11% .
8	I	38	11% 89% . 8%
8	i	38	89% . 8%
9	J	40	5% 80% 5% 15%
9	j	40	80% 5% 15%
10	K	46	80% 20%
10	k	46	4% 80% 20%
11	L	37	5% 97% .
11	l	37	3% 97% .
12	M	36	11% 94% 6%
12	m	36	6% 94% 6%
13	O	272	8% 88% . 11%
13	o	272	6% 88% . 11%
14	T	32	9% 94% 6%
14	t	32	9% 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	G	28	
19	Y	28	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	X
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	X
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	X
22	CLA	C	520	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	X
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	X
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	X
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	h	101	X	-	-	-
23	PL9	A	406	-	-	-	X
23	PL9	D	406	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	d	406	-	-	-	X
23	PL9	j	101	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	F	102	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	513	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	521	-	-	-	X
24	BCR	f	102	-	-	-	X
24	BCR	g	101	-	-	-	X
24	BCR	x	101	-	-	-	X
24	BCR	y	101	-	-	-	X
25	DGD	A	408	-	-	-	X
25	DGD	B	625	-	-	-	X
25	DGD	D	409	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	d	409	-	-	-	X
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	D	411	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	I	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	d	408	-	-	-	X
27	LMG	e	101	-	-	-	X
27	LMG	i	101	-	-	-	X
27	LMG	l	101	-	-	-	X
27	LMG	m	101	-	-	-	X
30	SQD	B	622	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	F	103	-	-	-	X
30	SQD	d	402	-	-	-	X
31	LMT	B	623	-	-	-	X
31	LMT	B	624	-	-	-	X
31	LMT	B	627	-	-	-	X
31	LMT	B	628	-	-	-	X
31	LMT	D	410	-	-	-	X
31	LMT	I	102	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	M	103	-	-	-	X
31	LMT	b	603	-	-	-	X
31	LMT	b	604	-	-	-	X
31	LMT	b	626	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	410	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	d	401	-	-	-	X
33	BCT	d	403	-	-	-	X
35	CA	o	301	-	-	-	X

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 50244 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	2628	1720	432	461	15	0	0	0
1	a	335	2628	1720	432	461	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
			Total	C	N	O			
10	k	37	293	204	43	46	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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 Y.

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

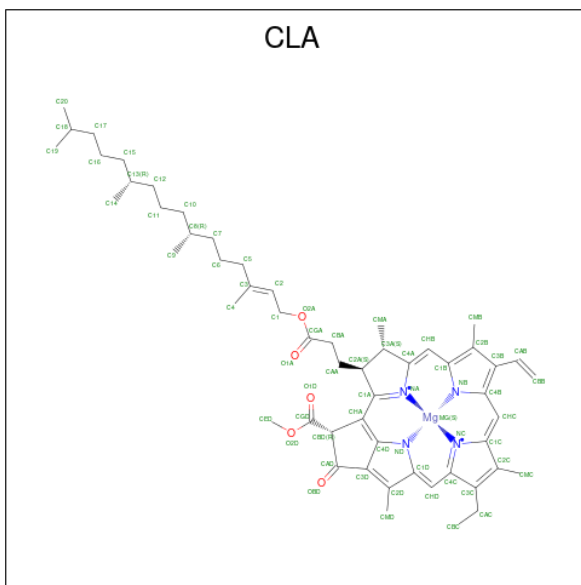
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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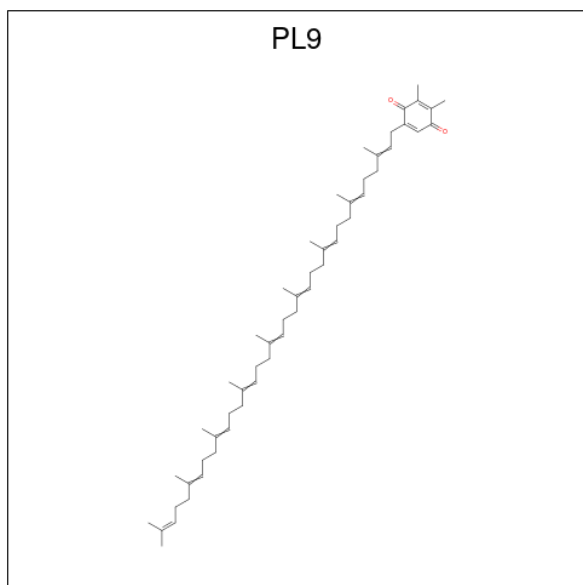
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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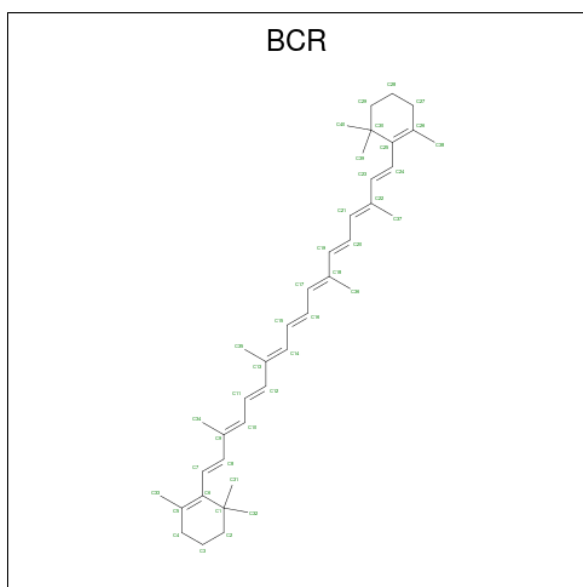
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 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: C₅₃H₈₀O₂).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



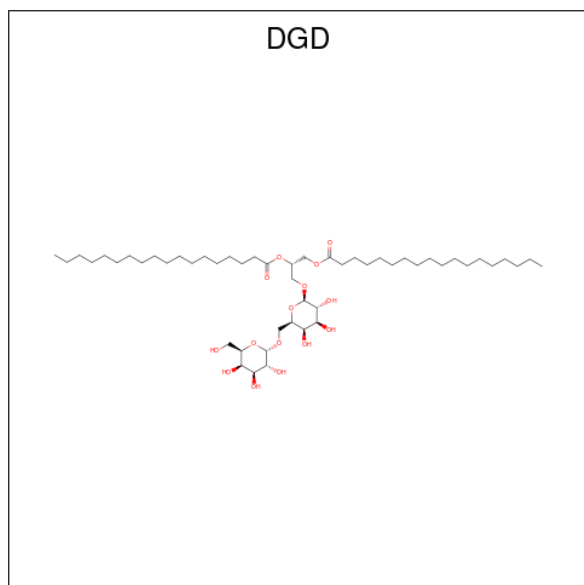
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



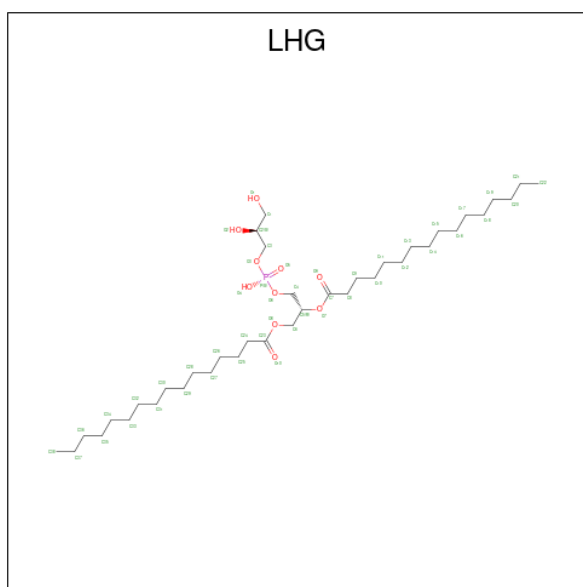
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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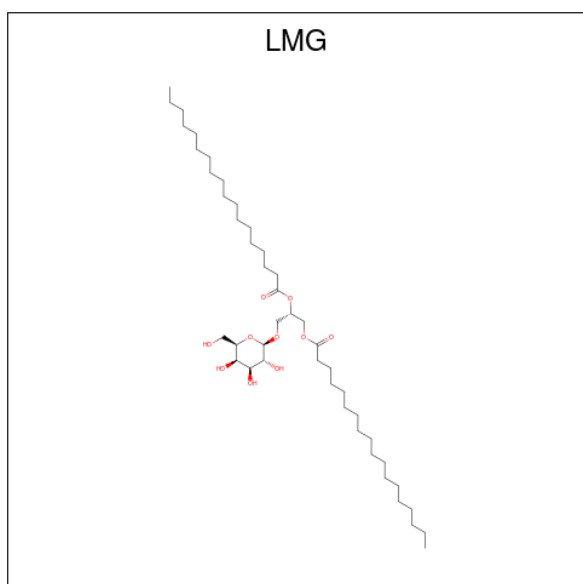
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

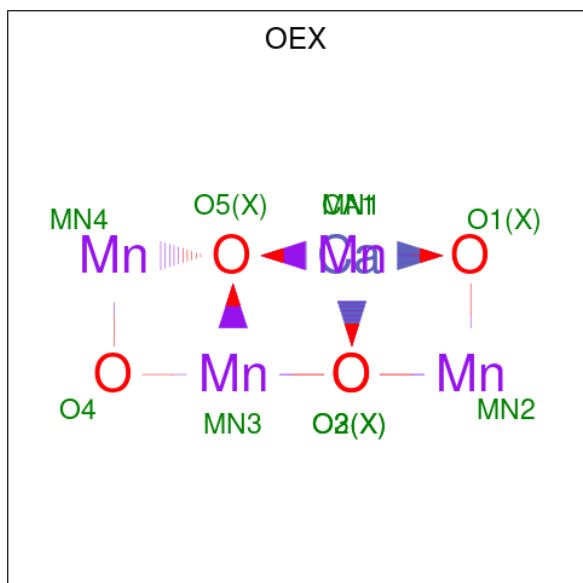


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	E	1	Total	C	O	0	0
			44	34	10		
27	I	1	Total	C	O	0	0
			43	33	10		
27	M	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			42	32	10		
27	b	1	Total	C	O	0	0
			49	39	10		
27	c	1	Total	C	O	0	0
			45	35	10		
27	c	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			49	39	10		
27	d	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			46	36	10		
27	e	1	Total	C	O	0	0
			44	34	10		
27	i	1	Total	C	O	0	0
			43	33	10		
27	l	1	Total	C	O	0	0
			51	41	10		
27	m	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

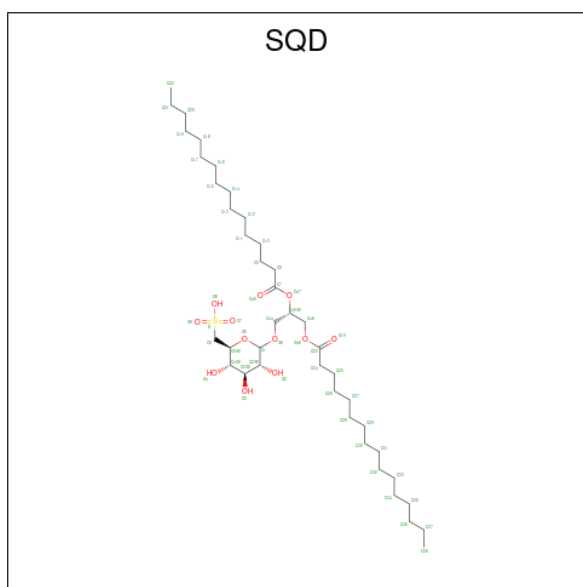
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Cl 1 1	0	0
28	a	1	Total Cl 1 1	0	0

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



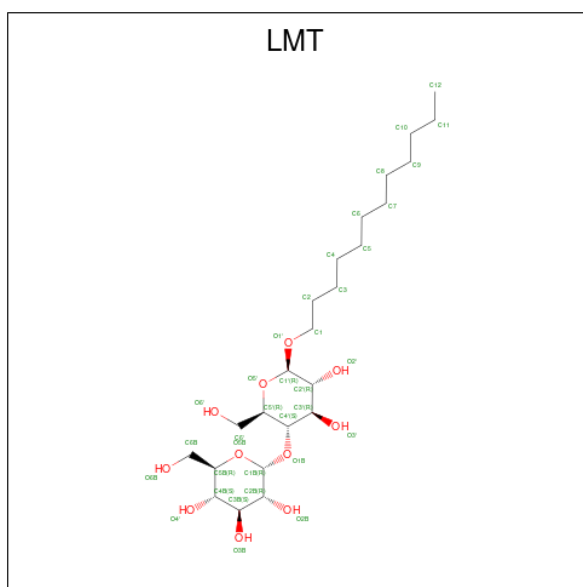
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Ca Mn O 10 1 4 5	0	0
29	a	1	Total Ca Mn O 10 1 4 5	0	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



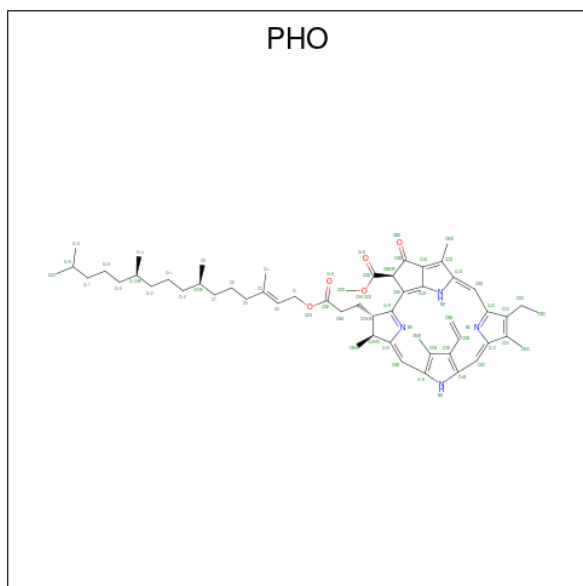
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
30	A	1	51	38	12	1	0	0
30	A	1	54	41	12	1	0	0
30	B	1	43	30	12	1	0	0
30	B	1	47	34	12	1	0	0
30	F	1	45	32	12	1	0	0
30	a	1	54	41	12	1	0	0
30	a	1	51	38	12	1	0	0
30	b	1	47	34	12	1	0	0
30	d	1	43	30	12	1	0	0
30	f	1	45	32	12	1	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



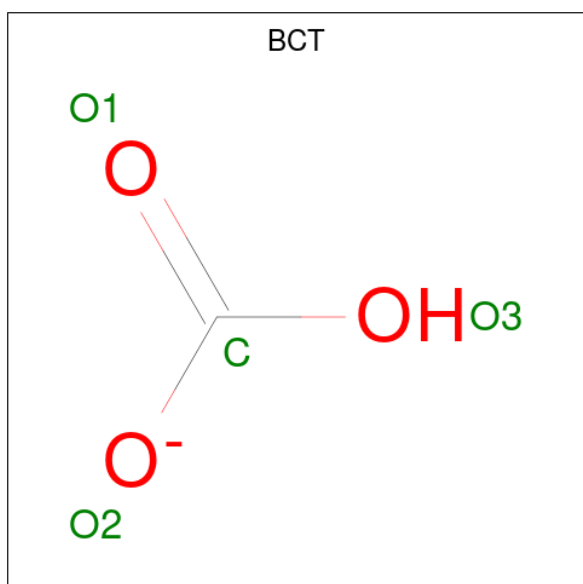
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total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

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



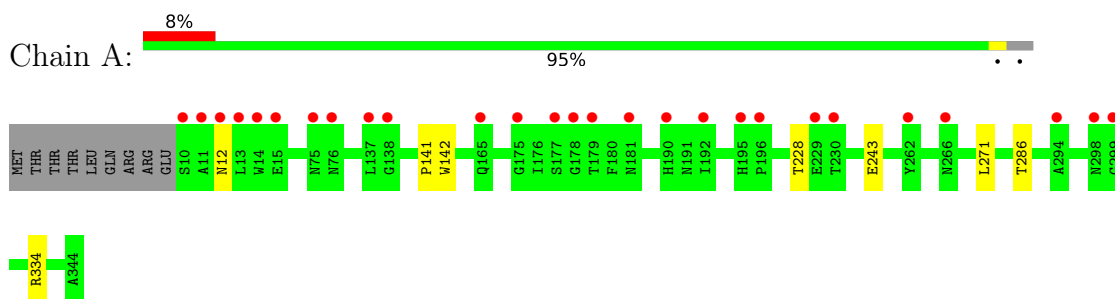
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total	Ca	0	0
			1	1		

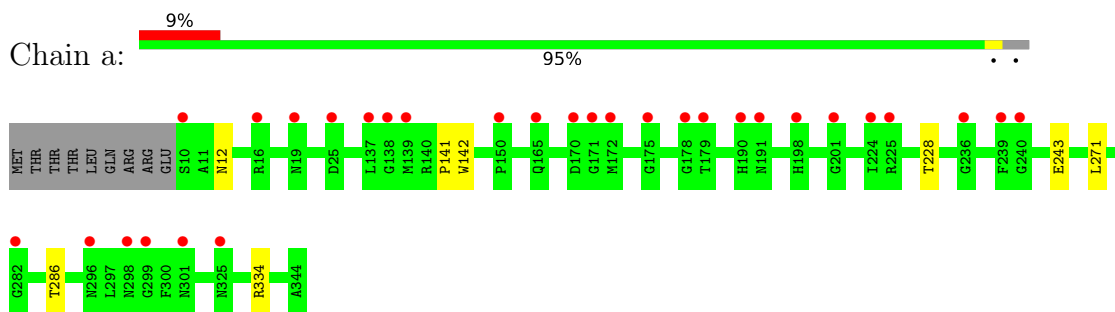
3 Residue-property plots [i](#)

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.

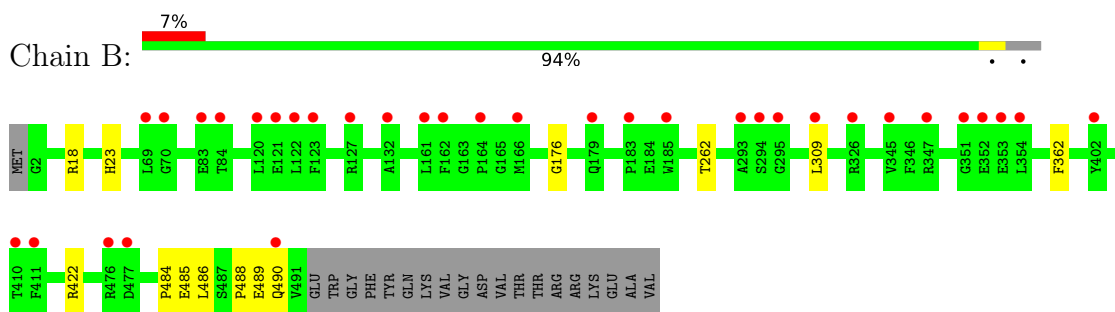
- Molecule 1: Photosystem Q(B) protein 1



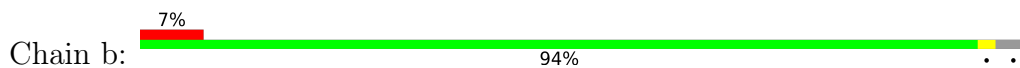
- Molecule 1: Photosystem Q(B) protein 1

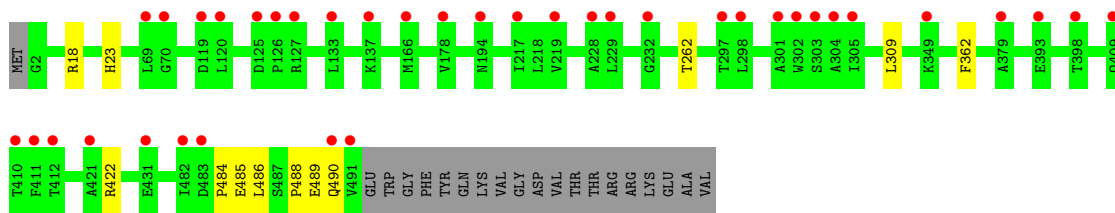


- Molecule 2: Photosystem II core light harvesting protein

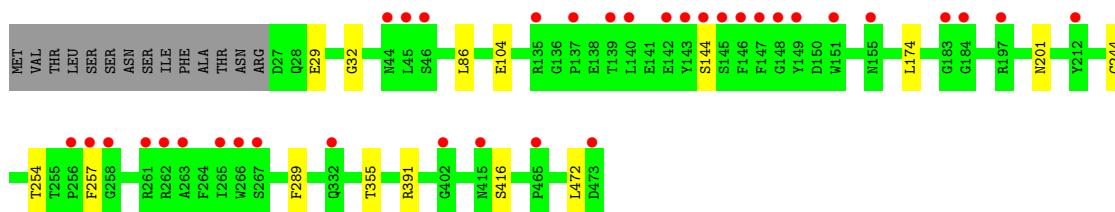


- Molecule 2: Photosystem II core light harvesting protein

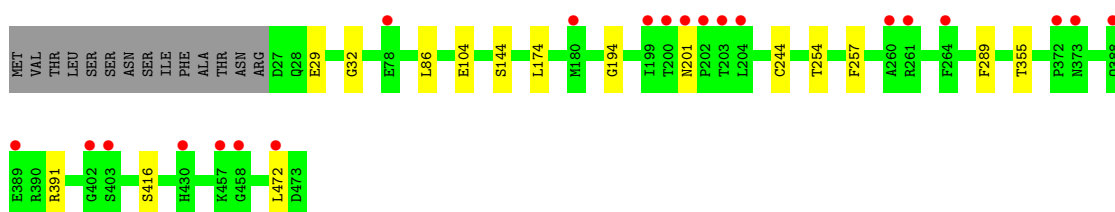
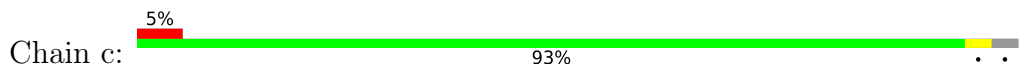




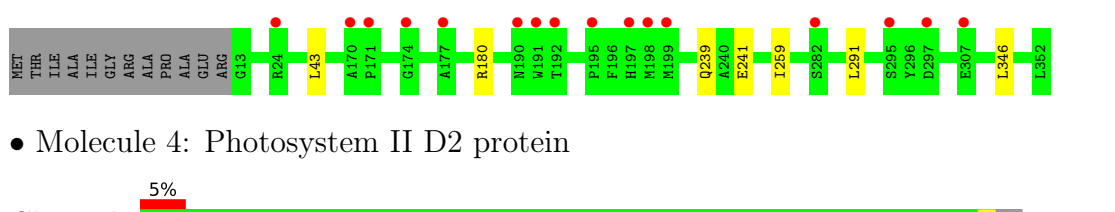
• Molecule 3: Photosystem II CP43 protein



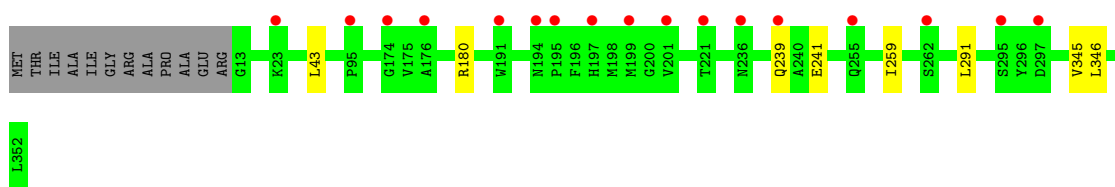
• Molecule 3: Photosystem II CP43 protein



• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein

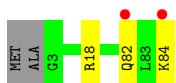


• Molecule 5: Cytochrome b559 subunit alpha

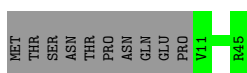
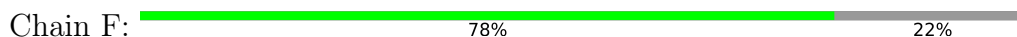




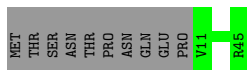
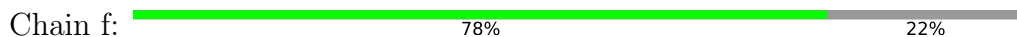
- Molecule 5: Cytochrome b559 subunit alpha



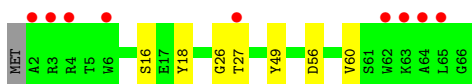
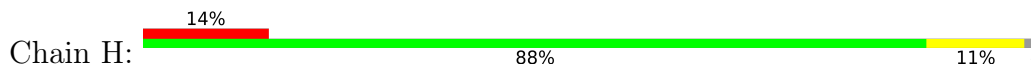
- Molecule 6: Cytochrome b559 subunit beta



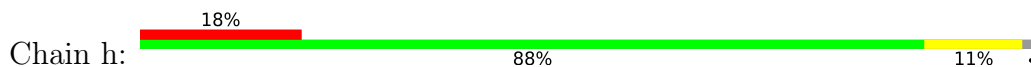
- Molecule 6: Cytochrome b559 subunit beta



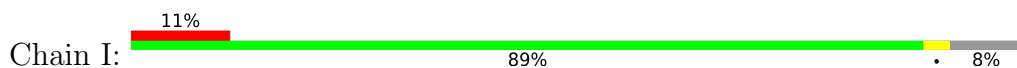
- Molecule 7: Photosystem II reaction center protein H




- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I




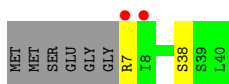
- Molecule 8: Photosystem II reaction center protein I

Chain i:  89% 8%




- Molecule 9: Photosystem II reaction center protein J

Chain J:  5% 80% 5% 15%




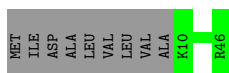
- Molecule 9: Photosystem II reaction center protein J

Chain j:  80% 5% 15%




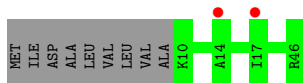
- Molecule 10: Photosystem II reaction center protein K

Chain K:  80% 20%



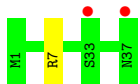
- Molecule 10: Photosystem II reaction center protein K

Chain k:  4% 80% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  5% 97%

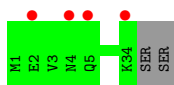


- Molecule 11: Photosystem II reaction center protein L

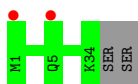
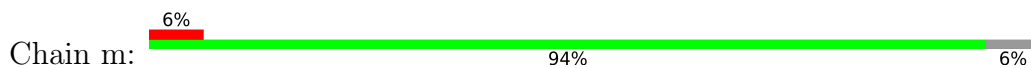
Chain l:  3% 97%



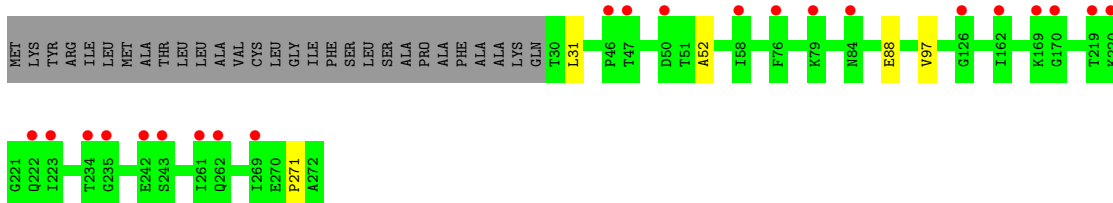
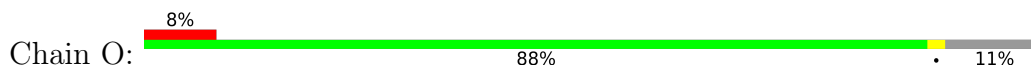
- Molecule 12: Photosystem II reaction center protein M



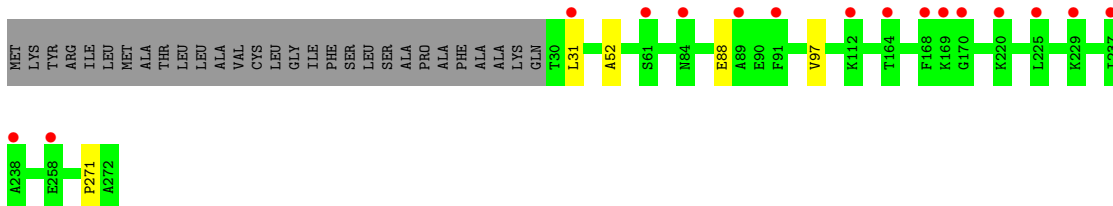
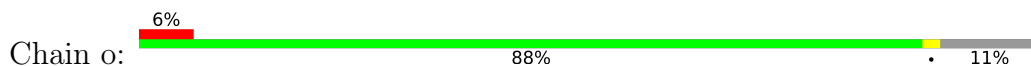
- Molecule 12: Photosystem II reaction center protein M



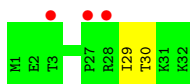
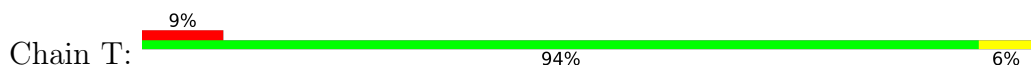
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



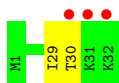
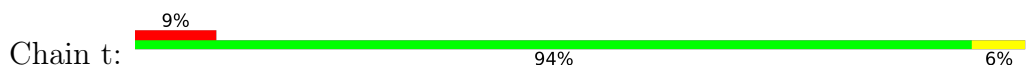
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

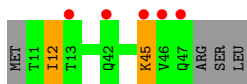


- Molecule 14: Photosystem II reaction center protein T

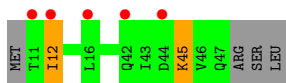
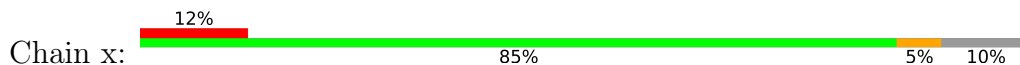


- Molecule 14: Photosystem II reaction center protein T





- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Y



There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

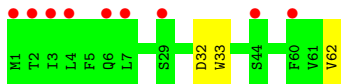


There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.88Å 229.03Å 307.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 4.90 72.93 – 4.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (72.93-4.90) 97.8 (72.93-4.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 4.87Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.281 , 0.292 0.283 , 0.291	Depositor DCC
R_{free} test set	2096 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	173.1	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 153.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	206.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: DGD, BCR, HEM, OEX, PL9, LMG, CLA, LHG, BCT, CA, CL, SQD, LMT, FE2, PHO

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	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.23	0/3556	0.41	0/4842
3	c	0.23	0/3556	0.41	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.43	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.46	0/709
7	h	0.23	0/520	0.46	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.21	0/255	0.40	0/346
9	j	0.21	0/255	0.40	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.49	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.44	0/367
12	m	0.23	0/270	0.43	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.24	0/284	0.40	0/381
14	t	0.24	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.43	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.21	0/202	0.46	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.24	0/490	0.44	0/669
All	All	0.23	0/41950	0.41	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	333/344 (97%)	312 (94%)	17 (5%)	4 (1%)	13	50
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	19	60
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	25	65
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	17	56
3	c	445/461 (96%)	405 (91%)	35 (8%)	5 (1%)	14	52
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	48
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	30
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	30
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
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%)	208 (86%)	30 (12%)	3 (1%)	13	50
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	13	50
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	29
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	29
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	38
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	38
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	26
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	26
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	20
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	20
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	43
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	43
All	All	5138/5618 (92%)	4678 (91%)	404 (8%)	56 (1%)	14	52

5 of 56 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	271/280 (97%)	267 (98%)	4 (2%)	65	80
1	a	271/280 (97%)	267 (98%)	4 (2%)	65	80
2	B	390/407 (96%)	381 (98%)	9 (2%)	50	70
2	b	390/407 (96%)	381 (98%)	9 (2%)	50	70
3	C	347/362 (96%)	336 (97%)	11 (3%)	39	61
3	c	347/362 (96%)	336 (97%)	11 (3%)	39	61
4	D	275/283 (97%)	269 (98%)	6 (2%)	52	71
4	d	275/283 (97%)	268 (98%)	7 (2%)	47	68
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	65
5	e	72/73 (99%)	70 (97%)	2 (3%)	43	65
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	39
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	39
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	84
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	84
16	V	116/138 (84%)	114 (98%)	2 (2%)	60	78
16	v	116/138 (84%)	114 (98%)	2 (2%)	60	78
17	g	20/37 (54%)	18 (90%)	2 (10%)	7	28
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	28
18	X	30/34 (88%)	28 (93%)	2 (7%)	16	42
18	x	30/34 (88%)	28 (93%)	2 (7%)	16	42
20	Z	52/52 (100%)	50 (96%)	2 (4%)	33	57
20	z	52/52 (100%)	50 (96%)	2 (4%)	33	57
All	All	4244/4594 (92%)	4141 (98%)	103 (2%)	49	69

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	262	THR
3	c	289	PHE
18	x	12	ILE
2	b	362	PHE
3	c	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN

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Mol	Chain	Res	Type
4	D	117	HIS
4	d	117	HIS

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$
22	CLA	c	506	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	8 (10%)
24	BCR	y	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.27	7 (12%)
23	PL9	j	101	-	35,35,55	1.00	2 (5%)	44,45,69	1.58	7 (15%)
22	CLA	c	505	-	65,73,73	1.52	5 (7%)	76,113,113	1.41	7 (9%)
30	SQD	a	401	-	53,54,54	0.95	4 (7%)	62,65,65	1.55	9 (14%)
31	LMT	B	627	-	36,36,36	1.14	5 (13%)	47,47,47	0.96	1 (2%)
25	DGD	c	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.44	11 (14%)
22	CLA	B	603	-	65,73,73	1.49	6 (9%)	76,113,113	1.43	9 (11%)
22	CLA	B	605	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	504	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	7 (9%)
22	CLA	c	512	-	65,73,73	1.52	5 (7%)	76,113,113	1.39	8 (10%)
24	BCR	c	514	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
22	CLA	d	405	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	8 (10%)
22	CLA	H	101	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
25	DGD	B	625	-	53,53,67	1.07	3 (5%)	67,67,81	1.30	7 (10%)
30	SQD	B	622	-	42,43,54	1.05	3 (7%)	51,54,65	1.76	11 (21%)
25	DGD	C	516	-	63,63,67	0.91	2 (3%)	77,77,81	1.44	12 (15%)
22	CLA	b	607	-	65,73,73	1.50	6 (9%)	76,113,113	1.42	9 (11%)
22	CLA	b	619	-	65,73,73	1.51	7 (10%)	76,113,113	1.33	8 (10%)
22	CLA	C	506	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	7 (9%)
25	DGD	b	601	-	53,53,67	1.05	3 (5%)	67,67,81	1.32	7 (10%)
27	LMG	E	101	-	44,44,55	0.76	0	52,52,63	1.28	4 (7%)
22	CLA	B	613	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
24	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
22	CLA	c	520	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	8 (10%)
24	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.58	13 (23%)
24	BCR	b	621	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	8 (14%)
30	SQD	a	415	-	50,51,54	0.96	4 (8%)	59,62,65	1.75	10 (16%)
22	CLA	B	614	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
22	CLA	c	508	-	65,73,73	1.52	5 (7%)	76,113,113	1.34	8 (10%)
26	LHG	C	519	-	36,36,48	0.70	0	39,42,54	1.26	4 (10%)
22	CLA	C	511	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)
22	CLA	C	508	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
31	LMT	i	102	-	36,36,36	1.11	4 (11%)	47,47,47	1.00	2 (4%)
22	CLA	C	502	-	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
22	CLA	c	507	-	65,73,73	1.50	5 (7%)	76,113,113	1.43	9 (11%)
27	LMG	C	518	-	45,45,55	0.77	0	53,53,63	1.29	6 (11%)
31	LMT	I	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	2 (4%)
24	BCR	a	410	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	7 (12%)
27	LMG	i	101	-	43,43,55	0.82	0	51,51,63	1.26	5 (9%)
24	BCR	x	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	4 (7%)
22	CLA	c	511	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
22	CLA	C	510	3	65,73,73	1.50	5 (7%)	76,113,113	1.42	8 (10%)
22	CLA	c	502	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
22	CLA	a	408	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	6 (7%)
22	CLA	D	405	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
22	CLA	B	611	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
32	PHO	D	401	-	51,69,69	1.01	4 (7%)	47,99,99	1.11	5 (10%)
31	LMT	B	624	-	36,36,36	1.12	4 (11%)	47,47,47	1.00	2 (4%)
27	LMG	C	521	-	48,48,55	0.77	0	56,56,63	1.30	6 (10%)
31	LMT	D	410	-	32,32,36	1.20	5 (15%)	43,43,47	0.99	2 (4%)
31	LMT	b	603	-	36,36,36	1.14	5 (13%)	47,47,47	0.95	1 (2%)
22	CLA	b	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	8 (10%)
22	CLA	a	404	-	65,73,73	1.52	6 (9%)	76,113,113	1.36	8 (10%)
25	DGD	b	624	-	59,59,67	0.91	1 (1%)	73,73,81	1.34	6 (8%)
24	BCR	K	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	8 (14%)
22	CLA	B	601	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	7 (9%)
22	CLA	A	404	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	6 (7%)
26	LHG	a	412	-	38,38,48	0.69	1 (2%)	41,44,54	1.20	3 (7%)
22	CLA	b	616	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	7 (9%)
27	LMG	M	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.22	4 (8%)
30	SQD	b	602	-	46,47,54	1.01	4 (8%)	55,58,65	1.77	10 (18%)
27	LMG	d	411	-	46,46,55	0.78	1 (2%)	54,54,63	1.30	5 (9%)
22	CLA	b	608	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	7 (9%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
24	BCR	H	102	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	4 (7%)
22	CLA	C	507	-	65,73,73	1.50	5 (7%)	76,113,113	1.42	8 (10%)
23	PL9	D	406	-	55,55,55	1.06	3 (5%)	68,69,69	1.51	12 (17%)
30	SQD	d	402	-	42,43,54	1.05	3 (7%)	51,54,65	1.77	11 (21%)
27	LMG	d	408	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
22	CLA	c	510	3	65,73,73	1.51	5 (7%)	76,113,113	1.39	7 (9%)
22	CLA	B	610	-	65,73,73	1.55	7 (10%)	76,113,113	1.44	6 (7%)
31	LMT	d	410	-	32,32,36	1.19	5 (15%)	43,43,47	0.99	2 (4%)
22	CLA	C	520	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
27	LMG	D	411	-	46,46,55	0.76	1 (2%)	54,54,63	1.30	5 (9%)
25	DGD	c	517	-	67,67,67	0.88	0	81,81,81	1.40	10 (12%)
31	LMT	B	623	-	36,36,36	1.13	5 (13%)	47,47,47	0.97	1 (2%)
22	CLA	B	607	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	V	201	16	41,50,50	2.03	8 (19%)	45,82,82	1.57	4 (8%)
22	CLA	A	402	-	65,73,73	1.51	6 (9%)	76,113,113	1.35	8 (10%)
24	BCR	C	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	8 (14%)
22	CLA	C	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
22	CLA	h	101	-	65,73,73	1.50	5 (7%)	76,113,113	1.34	6 (7%)
22	CLA	d	404	-	65,73,73	1.51	5 (7%)	76,113,113	1.32	8 (10%)
26	LHG	c	519	-	36,36,48	0.73	1 (2%)	39,42,54	1.25	4 (10%)
23	PL9	a	409	-	45,45,55	1.07	3 (6%)	56,57,69	1.57	10 (17%)
22	CLA	b	610	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
22	CLA	c	504	-	65,73,73	1.51	6 (9%)	76,113,113	1.41	7 (9%)
25	DGD	c	515	-	54,54,67	0.96	1 (1%)	68,68,81	1.27	6 (8%)
22	CLA	a	406	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)
27	LMG	m	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.24	4 (8%)
22	CLA	B	606	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	9 (11%)
31	LMT	B	628	-	36,36,36	1.15	5 (13%)	47,47,47	1.04	1 (2%)
25	DGD	C	515	-	54,54,67	0.97	2 (3%)	68,68,81	1.26	6 (8%)
22	CLA	C	509	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
27	LMG	d	407	-	49,49,55	0.77	0	57,57,63	1.30	4 (7%)
24	BCR	B	616	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
24	BCR	b	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
26	LHG	A	409	-	38,38,48	0.69	1 (2%)	41,44,54	1.19	3 (7%)
22	CLA	C	503	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	7 (9%)
22	CLA	C	512	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
22	CLA	c	509	-	65,73,73	1.52	6 (9%)	76,113,113	1.34	8 (10%)
24	BCR	j	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.57	13 (23%)
22	CLA	b	611	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	6 (7%)
22	CLA	b	618	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	8 (10%)
22	CLA	b	617	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	6 (7%)
24	BCR	c	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	8 (14%)
22	CLA	b	606	-	65,73,73	1.49	5 (7%)	76,113,113	1.35	7 (9%)
23	PL9	J	101	-	35,35,55	1.04	2 (5%)	44,45,69	1.57	7 (15%)
27	LMG	A	415	-	42,42,55	0.83	0	50,50,63	1.25	4 (8%)
24	BCR	B	617	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	9 (16%)
31	LMT	M	102	-	36,36,36	1.16	6 (16%)	47,47,47	0.99	2 (4%)
23	PL9	d	406	-	55,55,55	1.05	2 (3%)	68,69,69	1.53	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	OEX	a	414	3,1	0,15,15	-	-	-		
30	SQD	F	103	-	44,45,54	1.03	4 (9%)	53,56,65	1.65	10 (18%)
30	SQD	A	413	-	50,51,54	0.96	3 (6%)	59,62,65	1.75	10 (16%)
24	BCR	F	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
27	LMG	I	101	-	43,43,55	0.81	0	51,51,63	1.26	4 (7%)
31	LMT	b	626	-	36,36,36	1.13	5 (13%)	47,47,47	0.96	1 (2%)
34	HEM	v	201	16	41,50,50	2.03	7 (17%)	45,82,82	1.62	4 (8%)
22	CLA	C	505	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	7 (9%)
22	CLA	B	602	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	7 (9%)
24	BCR	b	623	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	9 (16%)
22	CLA	B	604	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	7 (9%)
22	CLA	B	612	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
25	DGD	C	517	-	67,67,67	0.89	2 (2%)	81,81,81	1.40	10 (12%)
24	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	10 (17%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.29	5 (8%)
29	OEX	A	412	3,1	0,15,15	-	-	-		
22	CLA	B	608	-	65,73,73	1.53	5 (7%)	76,113,113	1.34	7 (9%)
24	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	8 (14%)
24	BCR	g	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.29	8 (14%)
22	CLA	b	615	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
30	SQD	B	626	-	46,47,54	1.02	4 (8%)	55,58,65	1.77	10 (18%)
32	PHO	D	402	-	51,69,69	1.01	3 (5%)	47,99,99	1.12	4 (8%)
33	BCT	D	403	21	2,3,3	1.23	0	2,3,3	4.21	2 (100%)
34	HEM	f	101	6,5	41,50,50	1.96	6 (14%)	45,82,82	1.71	6 (13%)
27	LMG	A	410	-	51,51,55	0.75	0	59,59,63	1.36	7 (11%)
32	PHO	a	407	-	51,69,69	1.01	3 (5%)	47,99,99	1.10	4 (8%)
22	CLA	a	405	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
31	LMT	b	627	-	36,36,36	1.11	4 (11%)	47,47,47	1.00	2 (4%)
31	LMT	M	103	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
22	CLA	b	612	-	65,73,73	1.52	5 (7%)	76,113,113	1.32	6 (7%)
23	PL9	A	406	-	45,45,55	1.00	3 (6%)	56,57,69	1.57	10 (17%)
22	CLA	A	405	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	6 (7%)
22	CLA	b	605	-	65,73,73	1.54	5 (7%)	76,113,113	1.37	7 (9%)
24	BCR	C	513	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
24	BCR	f	102	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DGD	D	409	-	64,64,67	0.92	0	78,78,81	1.33	9 (11%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
30	SQD	f	103	-	44,45,54	1.03	4 (9%)	53,56,65	1.65	10 (18%)
30	SQD	A	414	-	53,54,54	0.96	4 (7%)	62,65,65	1.56	9 (14%)
32	PHO	d	401	-	51,69,69	1.01	4 (7%)	47,99,99	1.13	5 (10%)
22	CLA	B	609	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	7 (9%)
34	HEM	F	101	6,5	41,50,50	1.96	6 (14%)	45,82,82	1.70	7 (15%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.38	8 (14%)
27	LMG	D	407	-	49,49,55	0.76	0	57,57,63	1.31	4 (7%)
27	LMG	l	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.34	6 (10%)
24	BCR	c	513	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	9 (16%)
22	CLA	A	403	-	65,73,73	1.50	5 (7%)	76,113,113	1.42	8 (10%)
25	DGD	A	408	-	57,57,67	0.92	0	71,71,81	1.41	8 (11%)
22	CLA	c	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
25	DGD	B	620	-	59,59,67	0.92	1 (1%)	73,73,81	1.33	8 (10%)
31	LMT	b	604	-	36,36,36	1.15	5 (13%)	47,47,47	1.03	1 (2%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	6 (10%)
22	CLA	c	503	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	7 (9%)
22	CLA	D	404	-	65,73,73	1.51	5 (7%)	76,113,113	1.31	7 (9%)
22	CLA	b	614	-	65,73,73	1.55	7 (10%)	76,113,113	1.43	6 (7%)
25	DGD	d	409	-	64,64,67	0.93	1 (1%)	78,78,81	1.34	9 (11%)
22	CLA	b	613	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
27	LMG	a	402	-	42,42,55	0.83	0	50,50,63	1.25	3 (6%)
22	CLA	B	615	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
33	BCT	d	403	21	2,3,3	1.24	0	2,3,3	4.20	2 (100%)
27	LMG	e	101	-	44,44,55	0.76	0	52,52,63	1.29	4 (7%)
25	DGD	a	411	-	57,57,67	0.92	1 (1%)	71,71,81	1.40	7 (9%)

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
22	CLA	c	506	-	1/1/15/20	13/37/115/115	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
22	CLA	c	505	-	1/1/15/20	17/37/115/115	-
30	SQD	a	401	-	-	14/49/69/69	0/1/1/1
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
25	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	B	603	-	1/1/15/20	8/37/115/115	-
22	CLA	B	605	-	1/1/15/20	12/37/115/115	-
22	CLA	C	504	-	1/1/15/20	19/37/115/115	-
22	CLA	c	512	-	1/1/15/20	18/37/115/115	-
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
22	CLA	d	405	-	-	6/37/115/115	-
22	CLA	H	101	-	1/1/15/20	18/37/115/115	-
25	DGD	B	625	-	-	19/41/81/95	0/2/2/2
30	SQD	B	622	-	-	14/38/58/69	0/1/1/1
25	DGD	C	516	-	-	20/51/91/95	0/2/2/2
22	CLA	b	607	-	1/1/15/20	7/37/115/115	-
22	CLA	b	619	-	1/1/15/20	19/37/115/115	-
22	CLA	C	506	-	1/1/15/20	13/37/115/115	-
25	DGD	b	601	-	-	19/41/81/95	0/2/2/2
27	LMG	E	101	-	-	17/39/59/70	0/1/1/1
22	CLA	B	613	-	1/1/15/20	16/37/115/115	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
22	CLA	c	520	-	1/1/15/20	10/37/115/115	-
24	BCR	J	102	-	-	7/29/63/63	0/2/2/2
24	BCR	b	621	-	-	8/29/63/63	0/2/2/2
30	SQD	a	415	-	-	19/46/66/69	0/1/1/1
22	CLA	B	614	-	1/1/15/20	10/37/115/115	-
22	CLA	c	508	-	1/1/15/20	14/37/115/115	-
26	LHG	C	519	-	-	16/41/41/53	-
22	CLA	C	511	-	1/1/15/20	19/37/115/115	-
22	CLA	C	508	-	1/1/15/20	16/37/115/115	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
22	CLA	C	502	-	1/1/15/20	11/37/115/115	-
22	CLA	c	507	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	C	518	-	-	22/40/60/70	0/1/1/1
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
27	LMG	i	101	-	-	18/38/58/70	0/1/1/1
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
22	CLA	c	511	-	1/1/15/20	19/37/115/115	-
22	CLA	C	510	3	1/1/15/20	17/37/115/115	-
22	CLA	c	502	-	1/1/15/20	11/37/115/115	-
27	LMG	c	518	-	-	22/40/60/70	0/1/1/1
22	CLA	a	408	-	1/1/15/20	8/37/115/115	-
22	CLA	D	405	-	1/1/15/20	6/37/115/115	-
22	CLA	B	611	-	1/1/15/20	12/37/115/115	-
32	PHO	D	401	-	-	11/37/103/103	0/5/6/6
31	LMT	B	624	-	-	3/21/61/61	0/2/2/2
27	LMG	C	521	-	-	20/43/63/70	0/1/1/1
31	LMT	D	410	-	-	2/17/57/61	0/2/2/2
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	b	609	-	1/1/15/20	14/37/115/115	-
22	CLA	a	404	-	1/1/15/20	8/37/115/115	-
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	B	601	-	1/1/15/20	14/37/115/115	-
22	CLA	A	404	-	1/1/15/20	8/37/115/115	-
26	LHG	a	412	-	-	12/43/43/53	-
22	CLA	b	616	-	1/1/15/20	15/37/115/115	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
30	SQD	b	602	-	-	13/42/62/69	0/1/1/1
27	LMG	d	411	-	-	15/41/61/70	0/1/1/1
22	CLA	b	608	-	1/1/15/20	15/37/115/115	-
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
22	CLA	C	507	-	1/1/15/20	14/37/115/115	-
23	PL9	D	406	-	-	12/53/73/73	0/1/1/1
30	SQD	d	402	-	-	14/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	d	408	-	-	20/43/63/70	0/1/1/1
22	CLA	c	510	3	1/1/15/20	17/37/115/115	-
22	CLA	B	610	-	1/1/15/20	9/37/115/115	-
31	LMT	d	410	-	-	0/17/57/61	0/2/2/2
22	CLA	C	520	-	1/1/15/20	12/37/115/115	-
27	LMG	D	411	-	-	15/41/61/70	0/1/1/1
25	DGD	c	517	-	-	20/55/95/95	0/2/2/2
31	LMT	B	623	-	-	3/21/61/61	0/2/2/2
22	CLA	B	607	-	1/1/15/20	12/37/115/115	-
34	HEM	V	201	16	-	4/12/54/54	-
22	CLA	A	402	-	1/1/15/20	8/37/115/115	-
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/15/20	14/37/115/115	-
22	CLA	h	101	-	1/1/15/20	19/37/115/115	-
22	CLA	d	404	-	1/1/15/20	12/37/115/115	-
26	LHG	c	519	-	-	17/41/41/53	-
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
22	CLA	b	610	-	1/1/15/20	8/37/115/115	-
22	CLA	c	504	-	1/1/15/20	19/37/115/115	-
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
22	CLA	a	406	-	1/1/15/20	8/37/115/115	-
27	LMG	m	101	-	-	16/37/57/70	0/1/1/1
22	CLA	B	606	-	1/1/15/20	8/37/115/115	-
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
22	CLA	C	509	-	1/1/15/20	16/37/115/115	-
27	LMG	d	407	-	-	24/44/64/70	0/1/1/1
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
26	LHG	A	409	-	-	12/43/43/53	-
22	CLA	C	503	-	1/1/15/20	15/37/115/115	-
22	CLA	C	512	-	1/1/15/20	19/37/115/115	-
22	CLA	c	509	-	1/1/15/20	16/37/115/115	-
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	611	-	1/1/15/20	12/37/115/115	-
22	CLA	b	618	-	1/1/15/20	10/37/115/115	-
22	CLA	b	617	-	1/1/15/20	16/37/115/115	-
24	BCR	c	521	-	-	6/29/63/63	0/2/2/2
22	CLA	b	606	-	1/1/15/20	14/37/115/115	-
23	PL9	J	101	-	-	9/29/49/73	0/1/1/1
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
23	PL9	d	406	-	-	12/53/73/73	0/1/1/1
30	SQD	F	103	-	-	12/40/60/69	0/1/1/1
30	SQD	A	413	-	-	19/46/66/69	0/1/1/1
24	BCR	F	102	-	-	6/29/63/63	0/2/2/2
27	LMG	I	101	-	-	18/38/58/70	0/1/1/1
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
34	HEM	v	201	16	-	4/12/54/54	-
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
22	CLA	B	602	-	1/1/15/20	14/37/115/115	-
24	BCR	b	623	-	-	5/29/63/63	0/2/2/2
22	CLA	B	604	-	1/1/15/20	14/37/115/115	-
22	CLA	B	612	-	1/1/15/20	15/37/115/115	-
25	DGD	C	517	-	-	20/55/95/95	0/2/2/2
24	BCR	b	622	-	-	3/29/63/63	0/2/2/2
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
22	CLA	B	608	-	1/1/15/20	11/37/115/115	-
24	BCR	B	619	-	-	5/29/63/63	0/2/2/2
24	BCR	g	101	-	-	6/29/63/63	0/2/2/2
22	CLA	b	615	-	1/1/15/20	12/37/115/115	-
30	SQD	B	626	-	-	14/42/62/69	0/1/1/1
32	PHO	D	402	-	-	12/37/103/103	0/5/6/6
34	HEM	f	101	6,5	-	2/12/54/54	-
27	LMG	A	410	-	-	28/46/66/70	0/1/1/1
32	PHO	a	407	-	-	12/37/103/103	0/5/6/6
22	CLA	a	405	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	b	627	-	-	3/21/61/61	0/2/2/2
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	b	612	-	1/1/15/20	11/37/115/115	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
22	CLA	A	405	-	1/1/15/20	8/37/115/115	-
22	CLA	b	605	-	1/1/15/20	15/37/115/115	-
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
24	BCR	f	102	-	-	6/29/63/63	0/2/2/2
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2
27	LMG	D	408	-	-	22/43/63/70	0/1/1/1
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
30	SQD	A	414	-	-	12/49/69/69	0/1/1/1
32	PHO	d	401	-	-	11/37/103/103	0/5/6/6
22	CLA	B	609	-	1/1/15/20	18/37/115/115	-
34	HEM	F	101	6,5	-	2/12/54/54	-
24	BCR	B	618	-	-	3/29/63/63	0/2/2/2
27	LMG	D	407	-	-	24/44/64/70	0/1/1/1
27	LMG	l	101	-	-	25/46/66/70	0/1/1/1
24	BCR	c	513	-	-	5/29/63/63	0/2/2/2
22	CLA	A	403	-	1/1/15/20	14/37/115/115	-
25	DGD	A	408	-	-	14/45/85/95	0/2/2/2
22	CLA	c	501	-	1/1/15/20	13/37/115/115	-
25	DGD	B	620	-	-	18/47/87/95	0/2/2/2
31	LMT	b	604	-	-	5/21/61/61	0/2/2/2
27	LMG	B	621	-	-	14/44/64/70	0/1/1/1
22	CLA	c	503	-	1/1/15/20	15/37/115/115	-
22	CLA	D	404	-	1/1/15/20	13/37/115/115	-
22	CLA	b	614	-	1/1/15/20	9/37/115/115	-
25	DGD	d	409	-	-	34/52/92/95	0/2/2/2
22	CLA	b	613	-	1/1/15/20	18/37/115/115	-
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
22	CLA	B	615	-	1/1/15/20	18/37/115/115	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
25	DGD	a	411	-	-	13/45/85/95	0/2/2/2

The worst 5 of 611 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3D-C2D	8.30	1.54	1.36
34	V	201	HEM	C3D-C2D	8.27	1.54	1.36
34	f	101	HEM	C3D-C2D	8.03	1.53	1.36
34	F	101	HEM	C3D-C2D	8.03	1.53	1.36
22	A	402	CLA	C4B-NB	7.82	1.42	1.35

The worst 5 of 1165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.31	109.99	106.71
22	B	611	CLA	C4A-NA-C1A	7.26	109.97	106.71
22	c	504	CLA	C4A-NA-C1A	7.25	109.97	106.71
22	b	615	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	B	603	CLA	C4A-NA-C1A	7.12	109.91	106.71

5 of 69 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	404	CLA	ND
22	A	405	CLA	ND
22	B	601	CLA	ND

5 of 2136 torsion outliers are listed below:

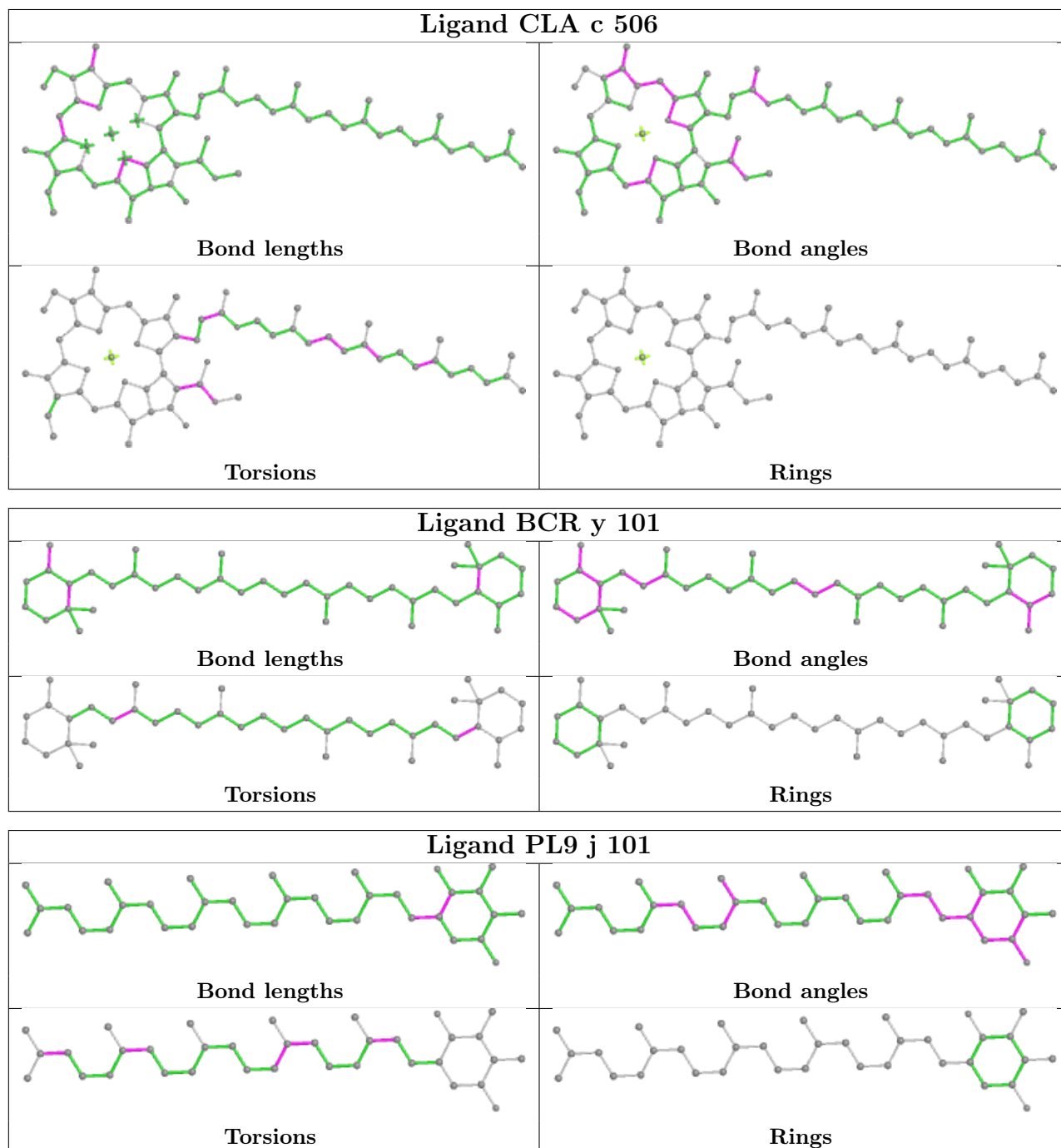
Mol	Chain	Res	Type	Atoms
22	A	402	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D

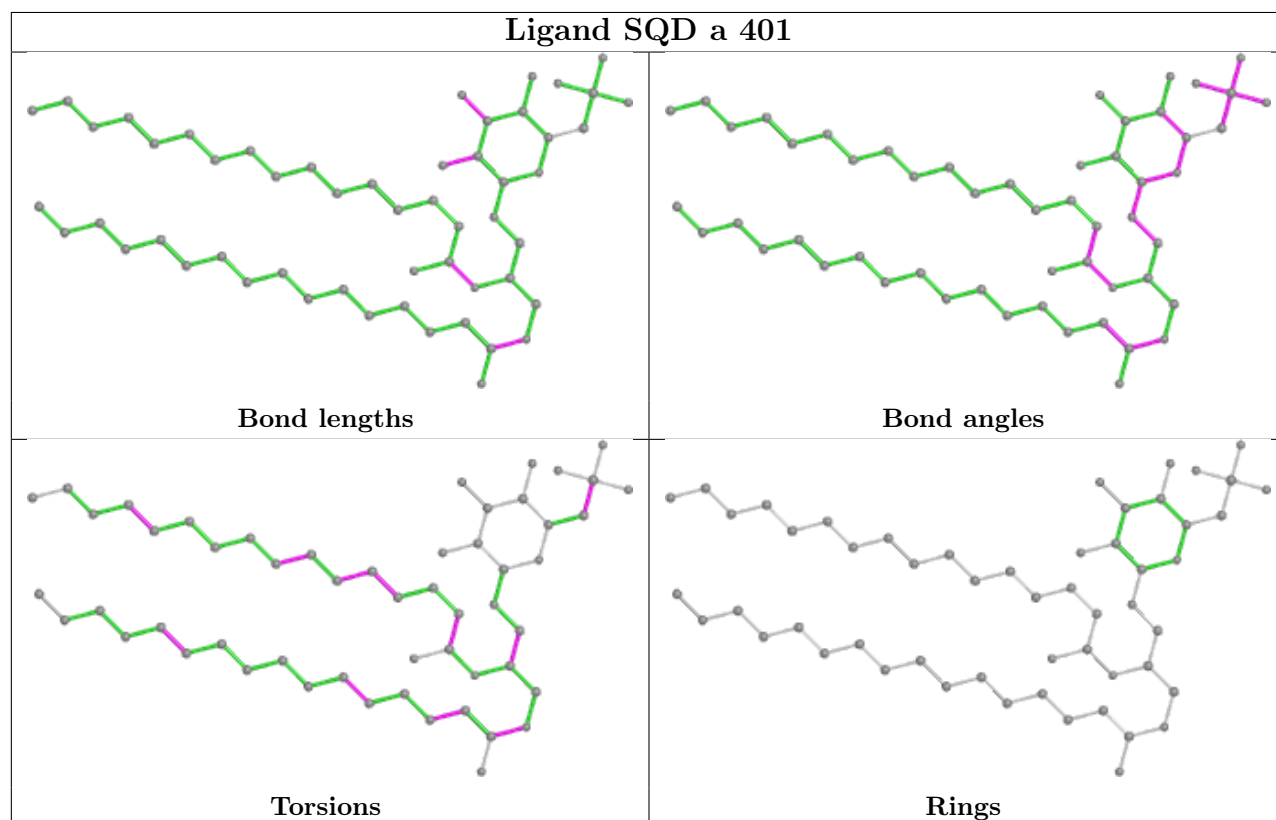
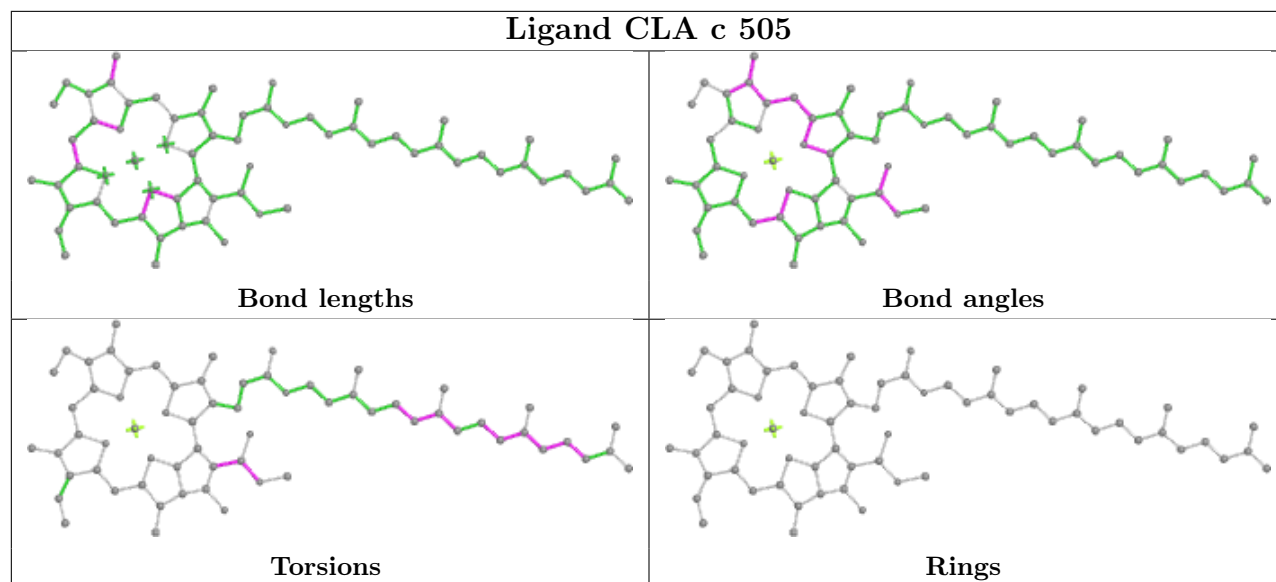
There are no ring outliers.

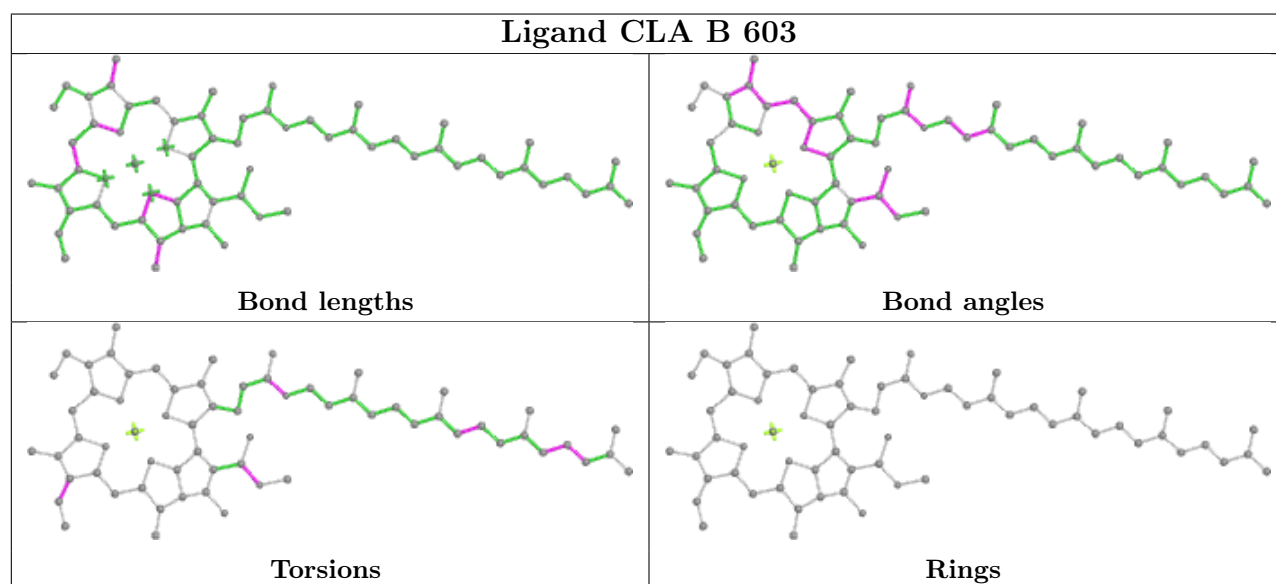
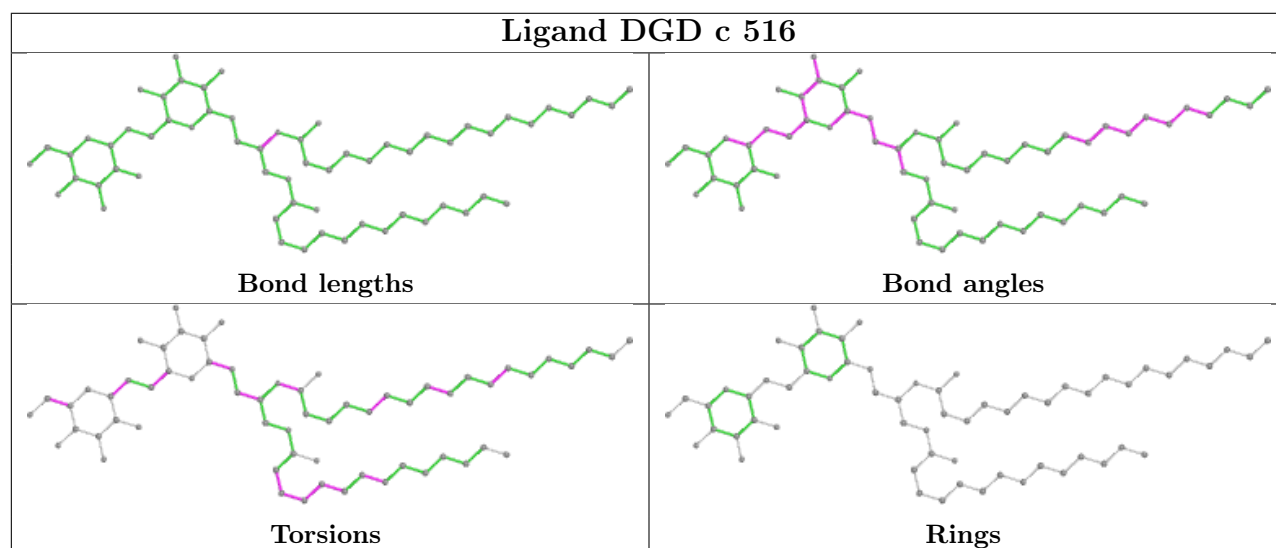
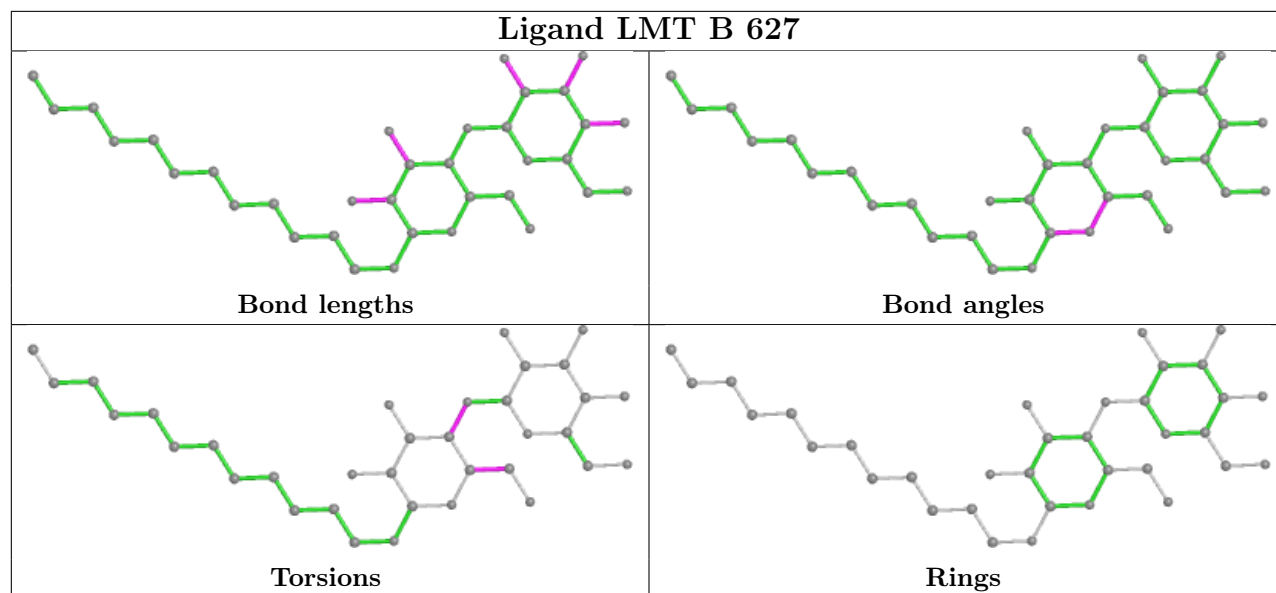
No monomer is involved in short contacts.

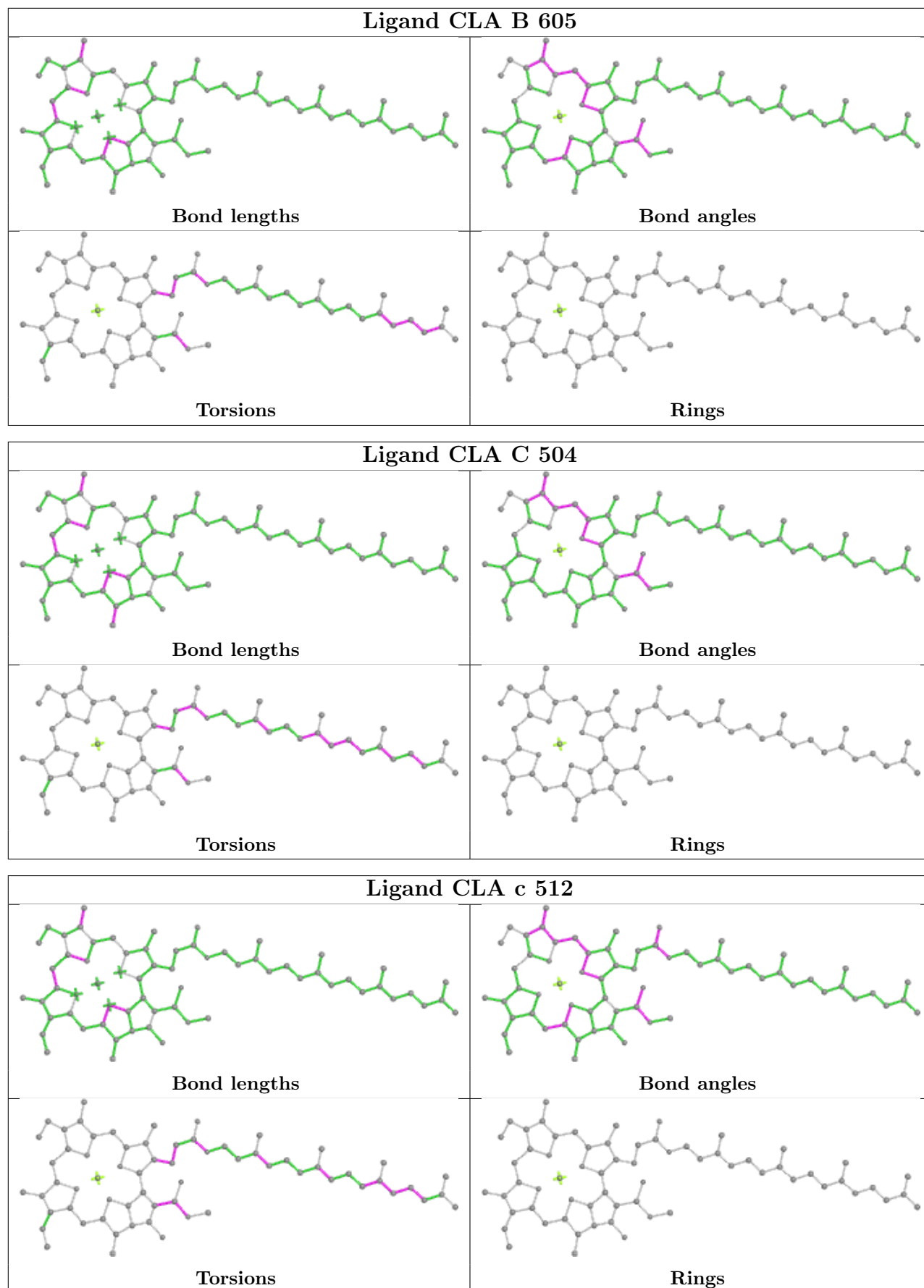
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

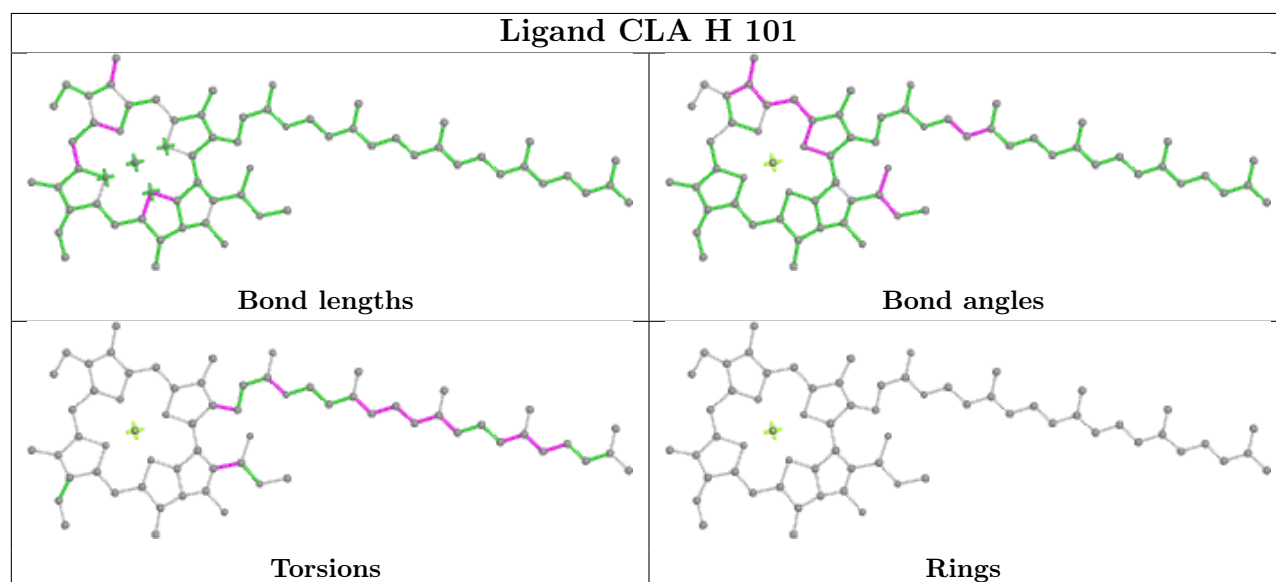
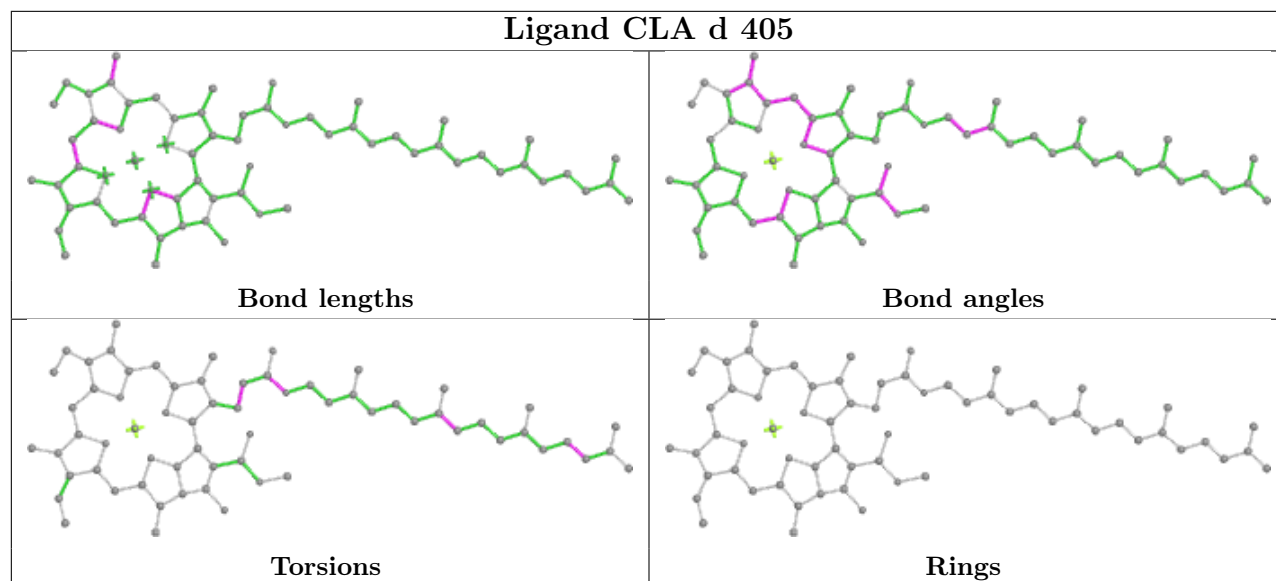
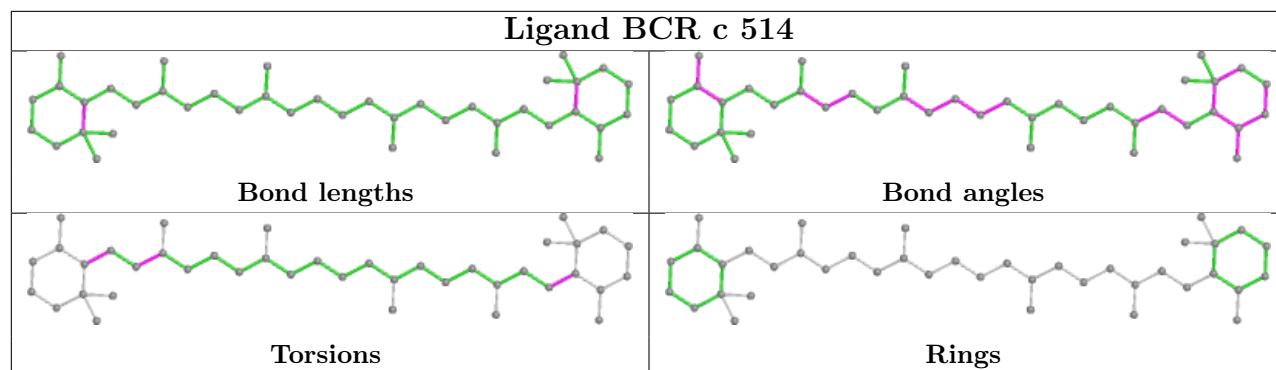
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

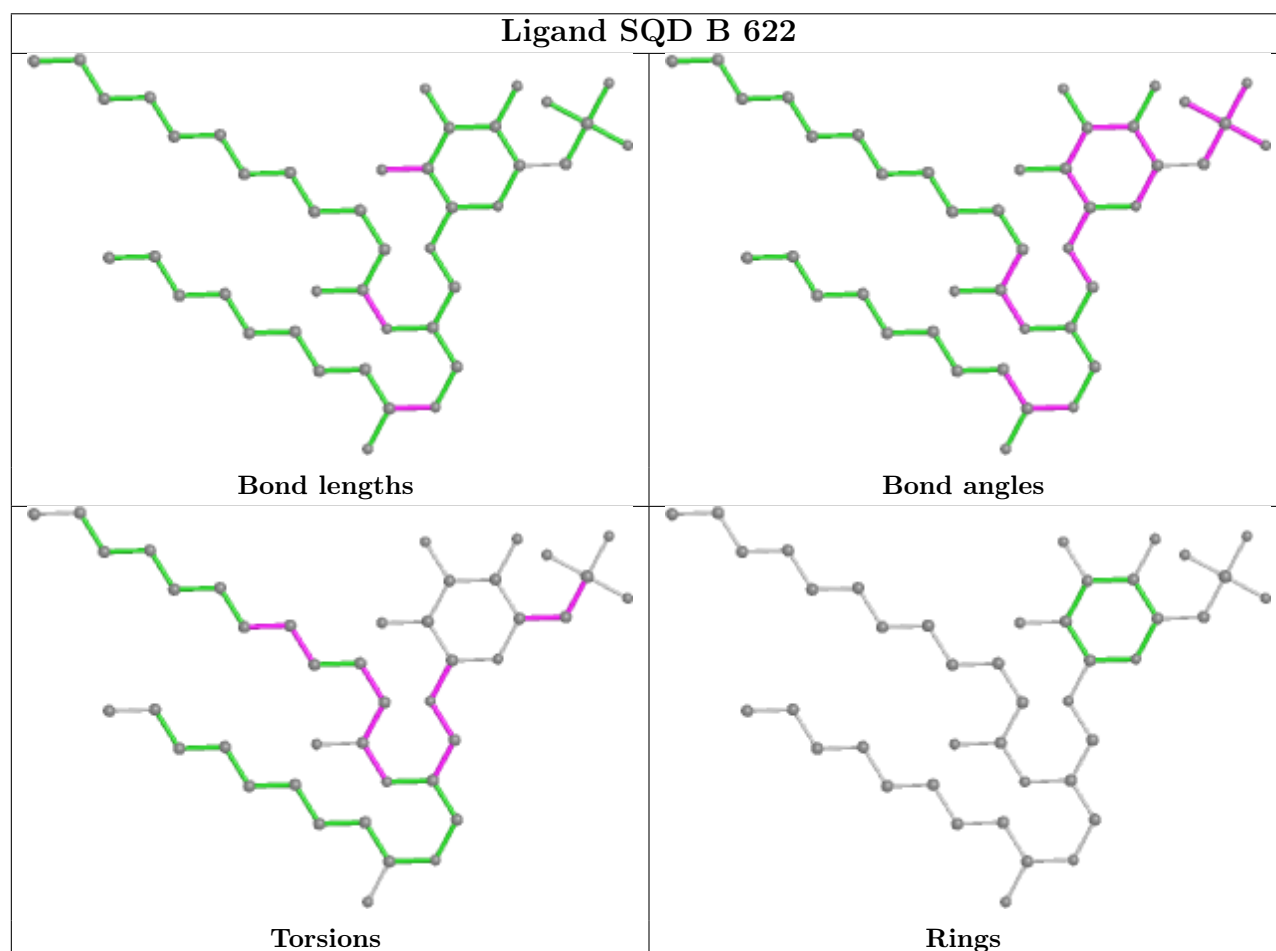
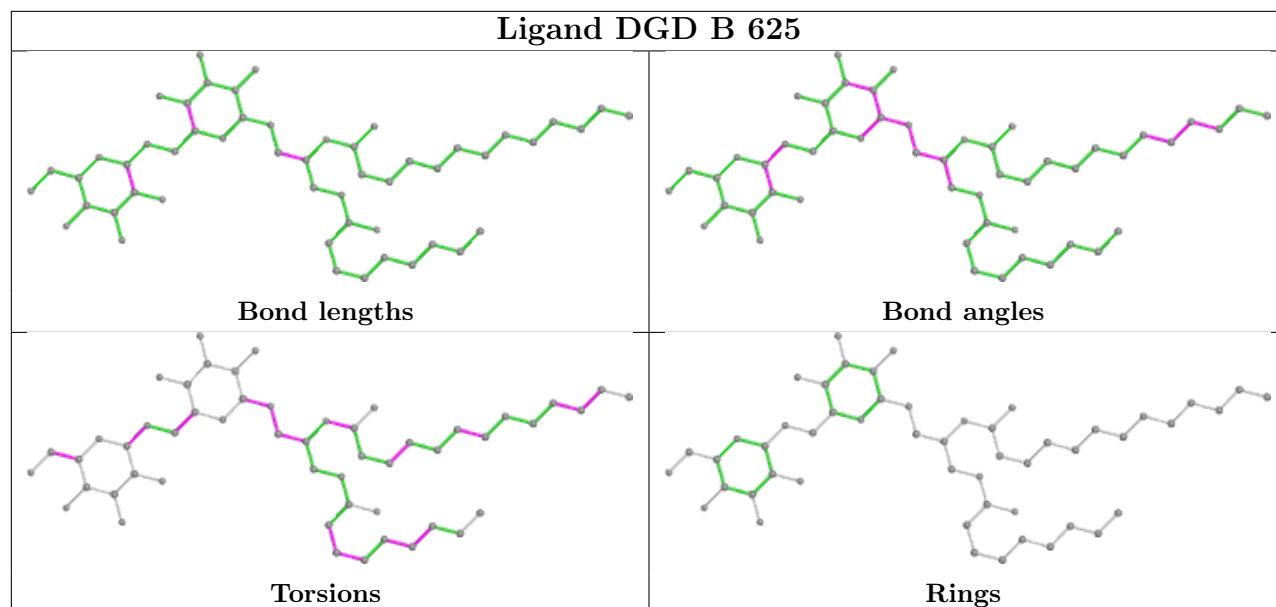


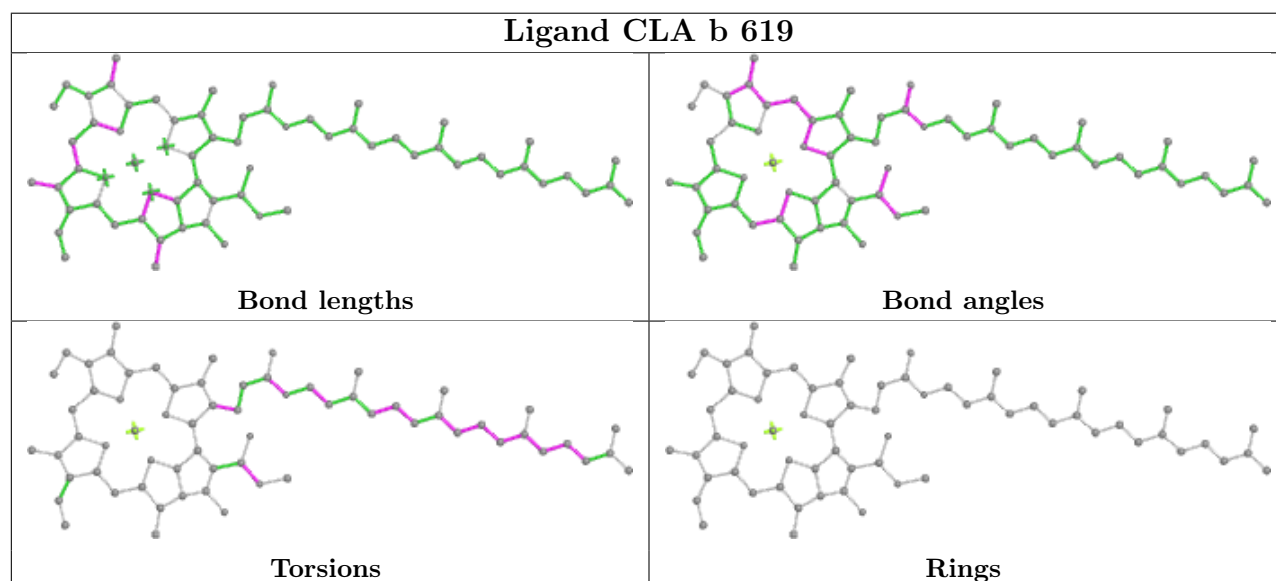
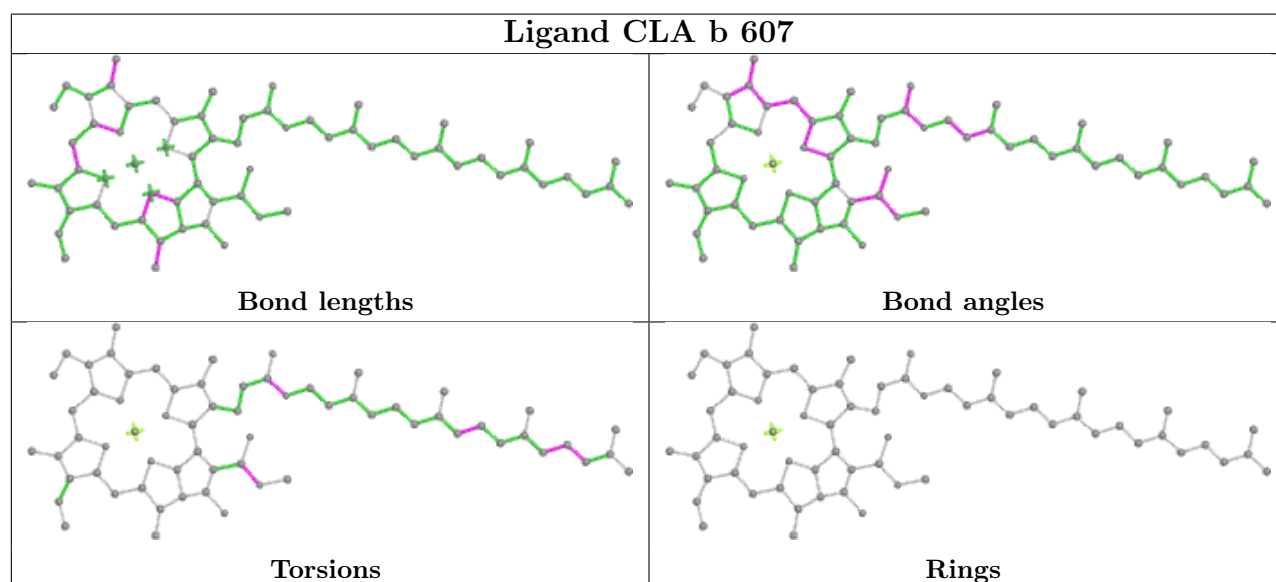
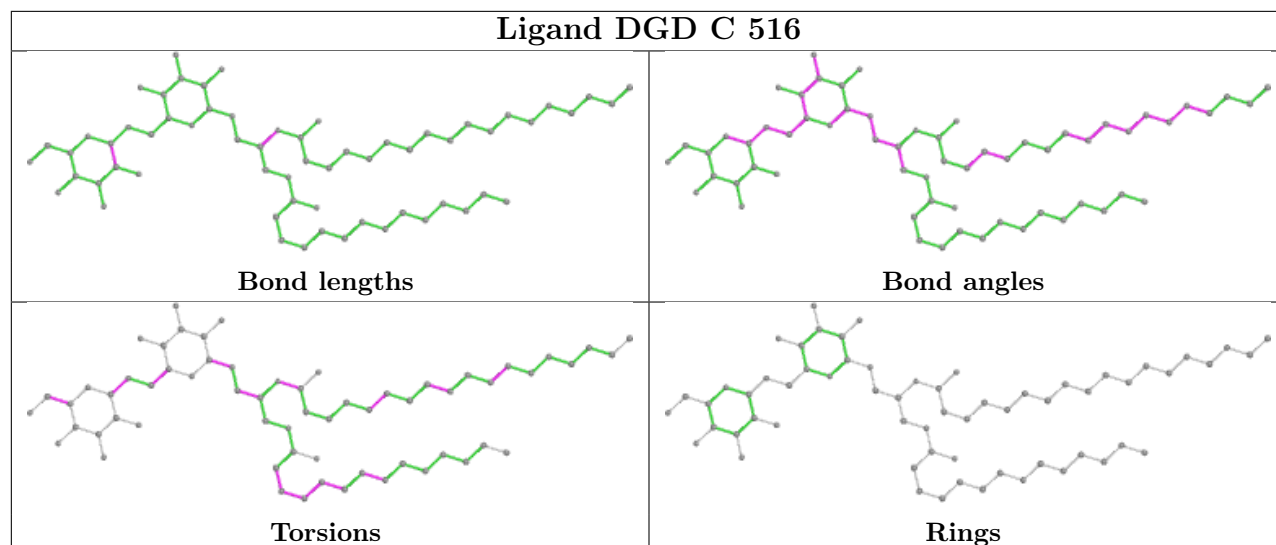


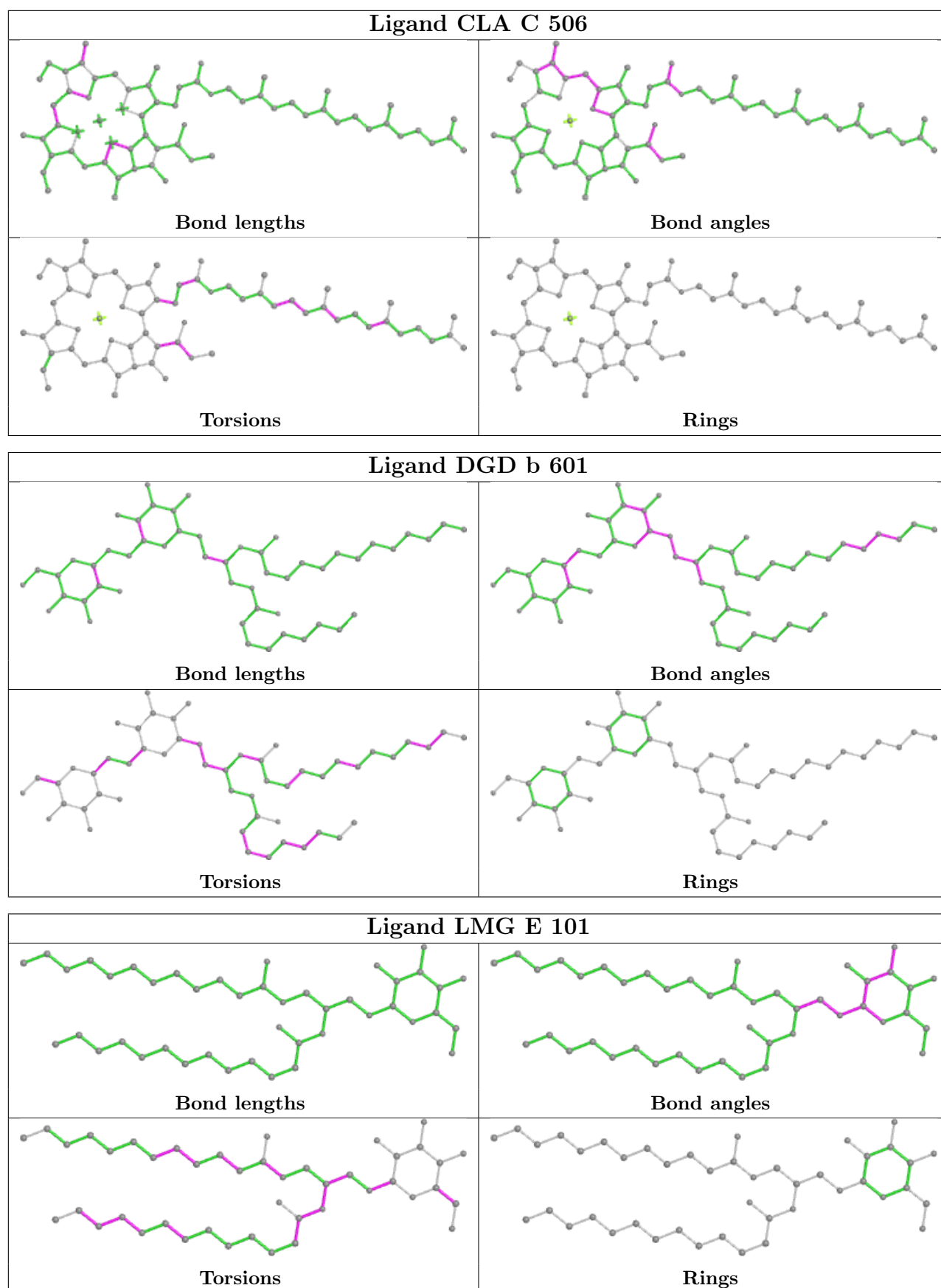


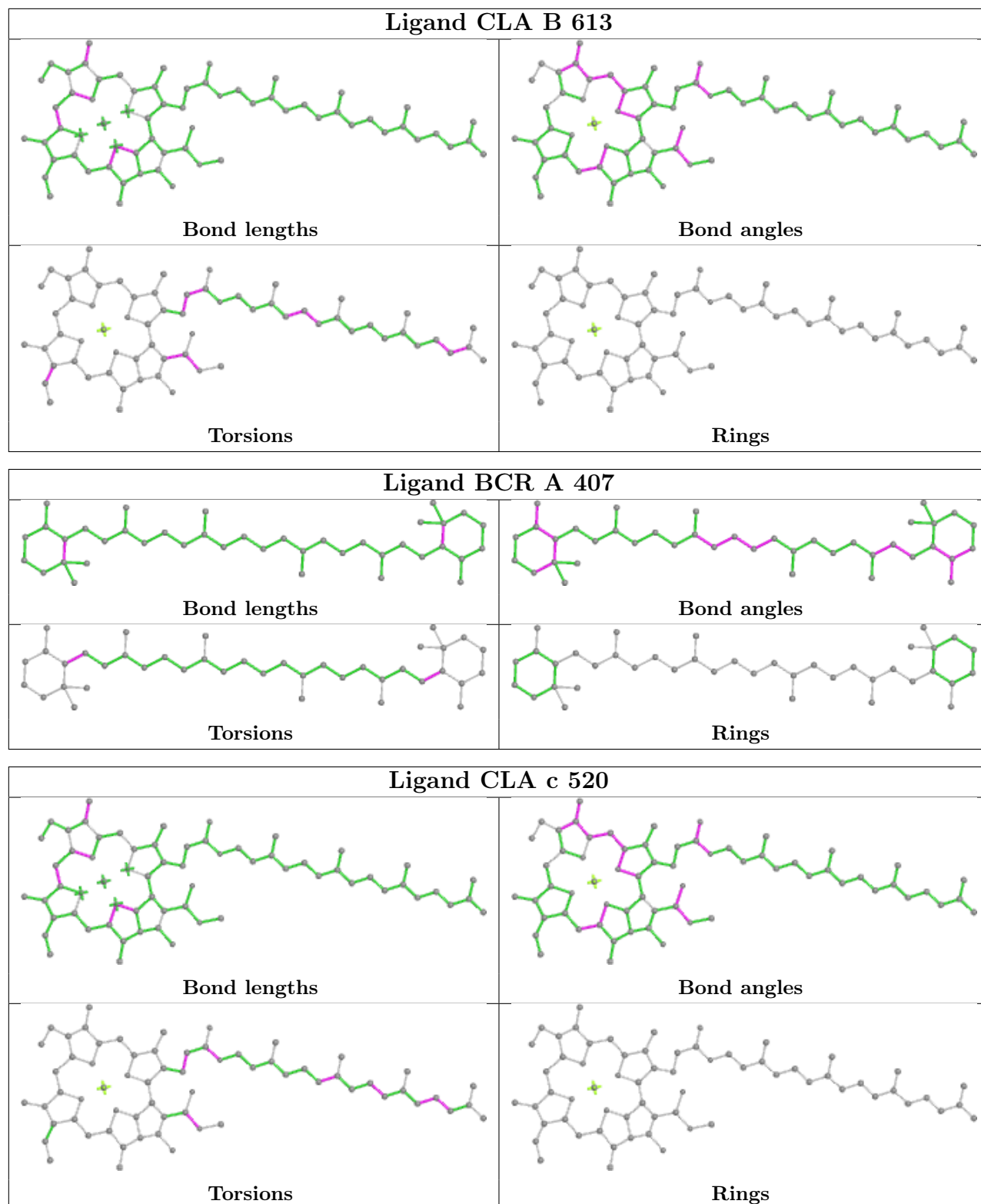


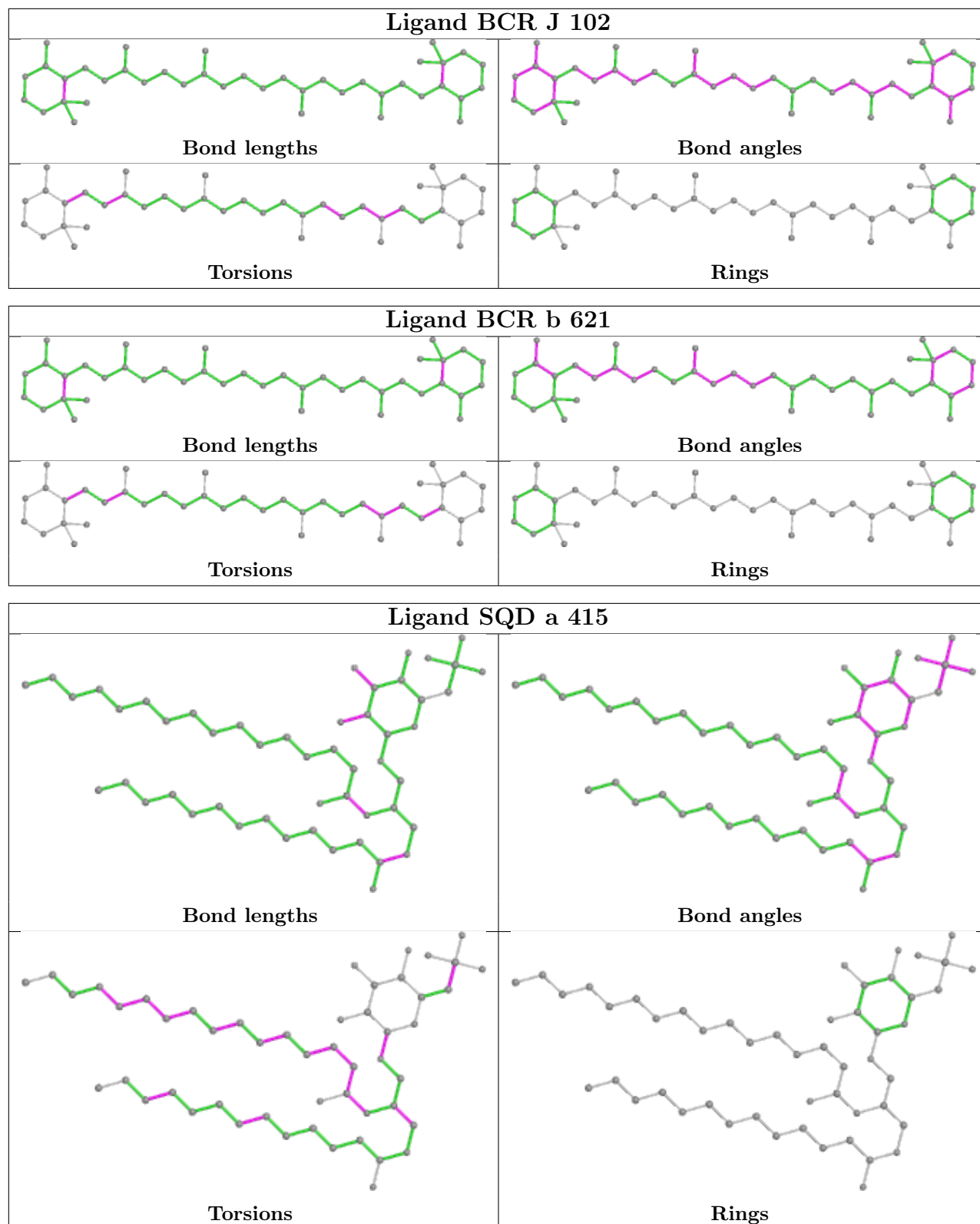


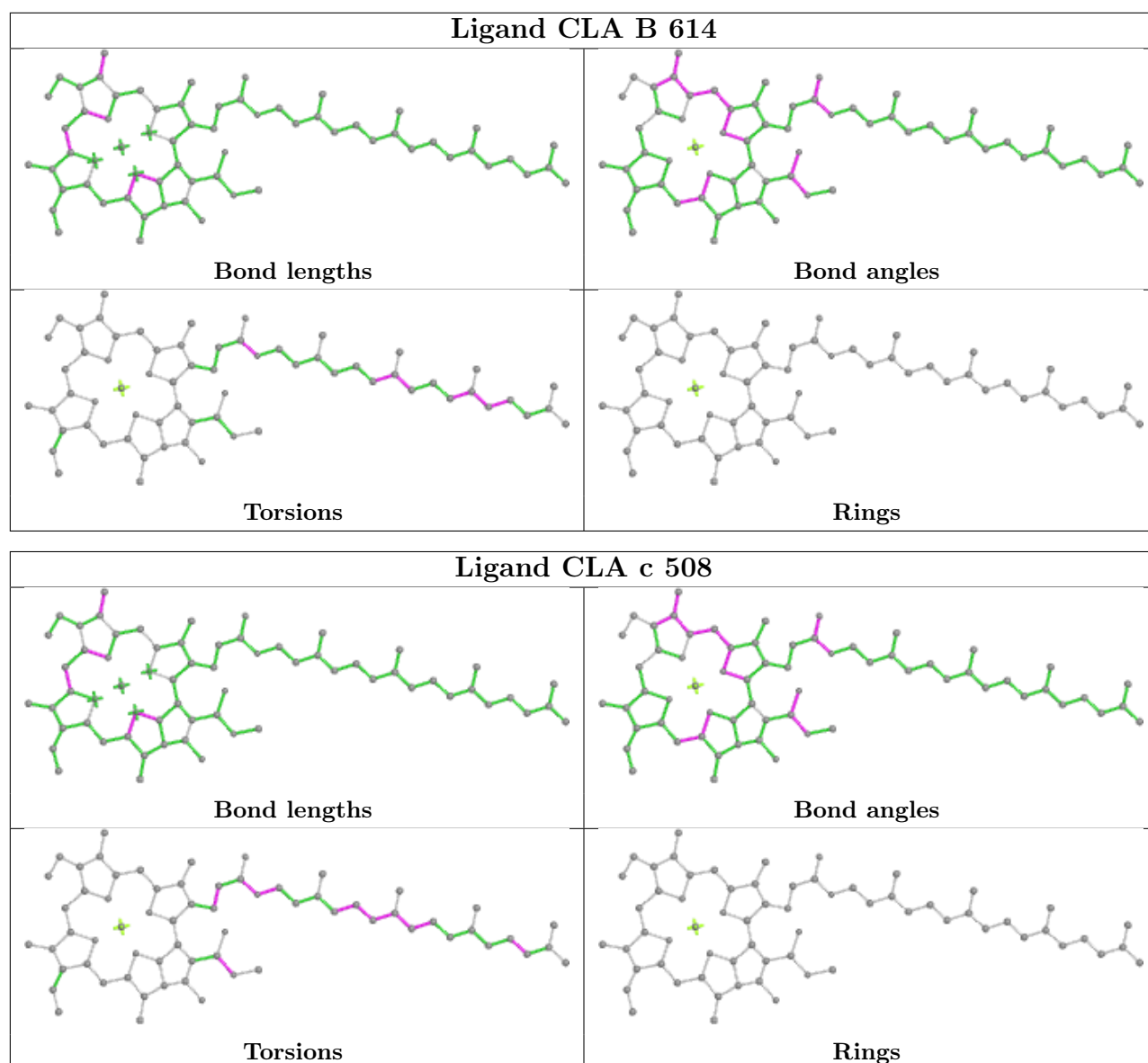


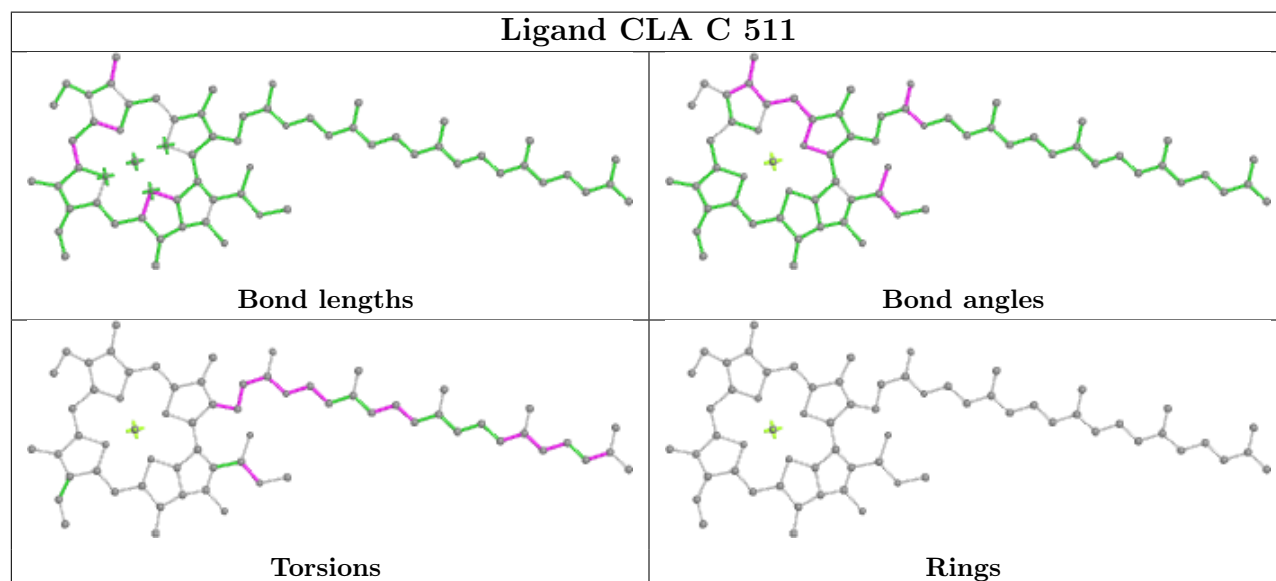
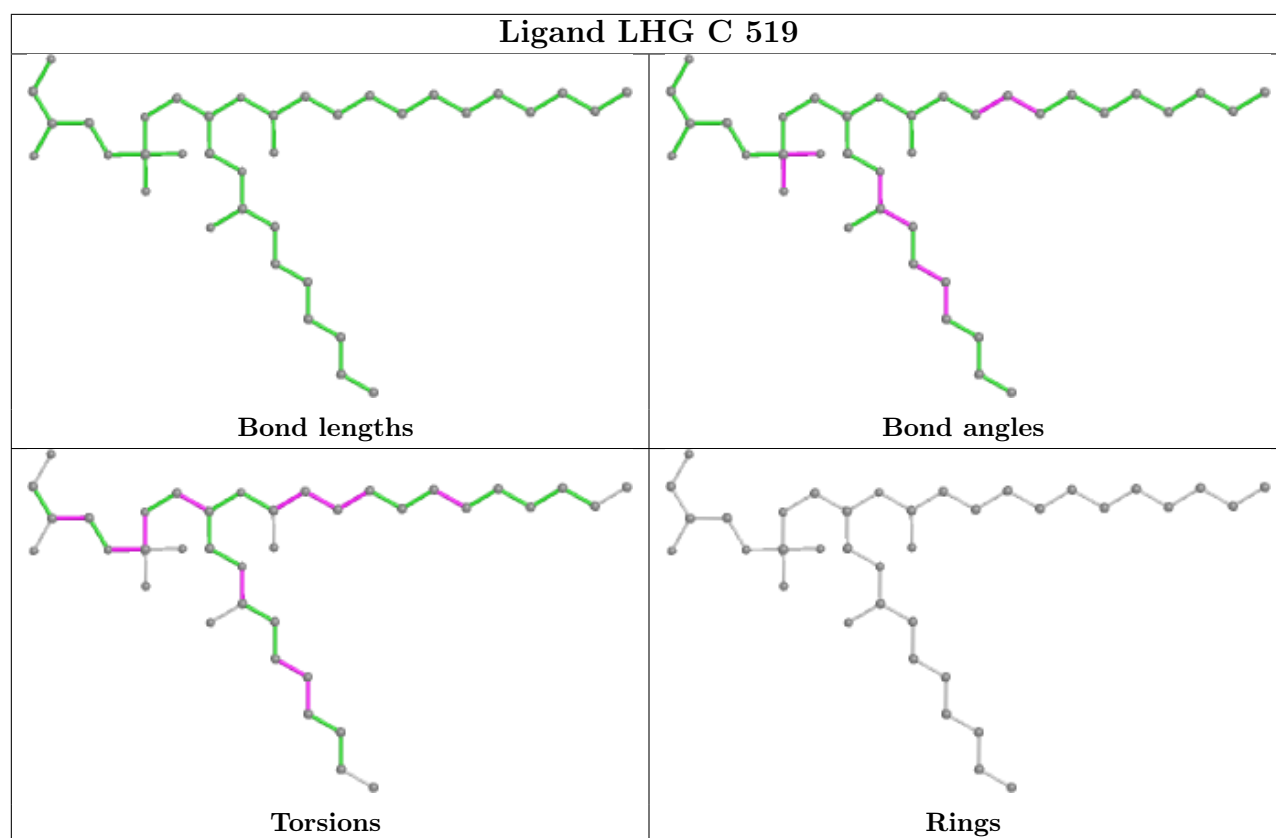


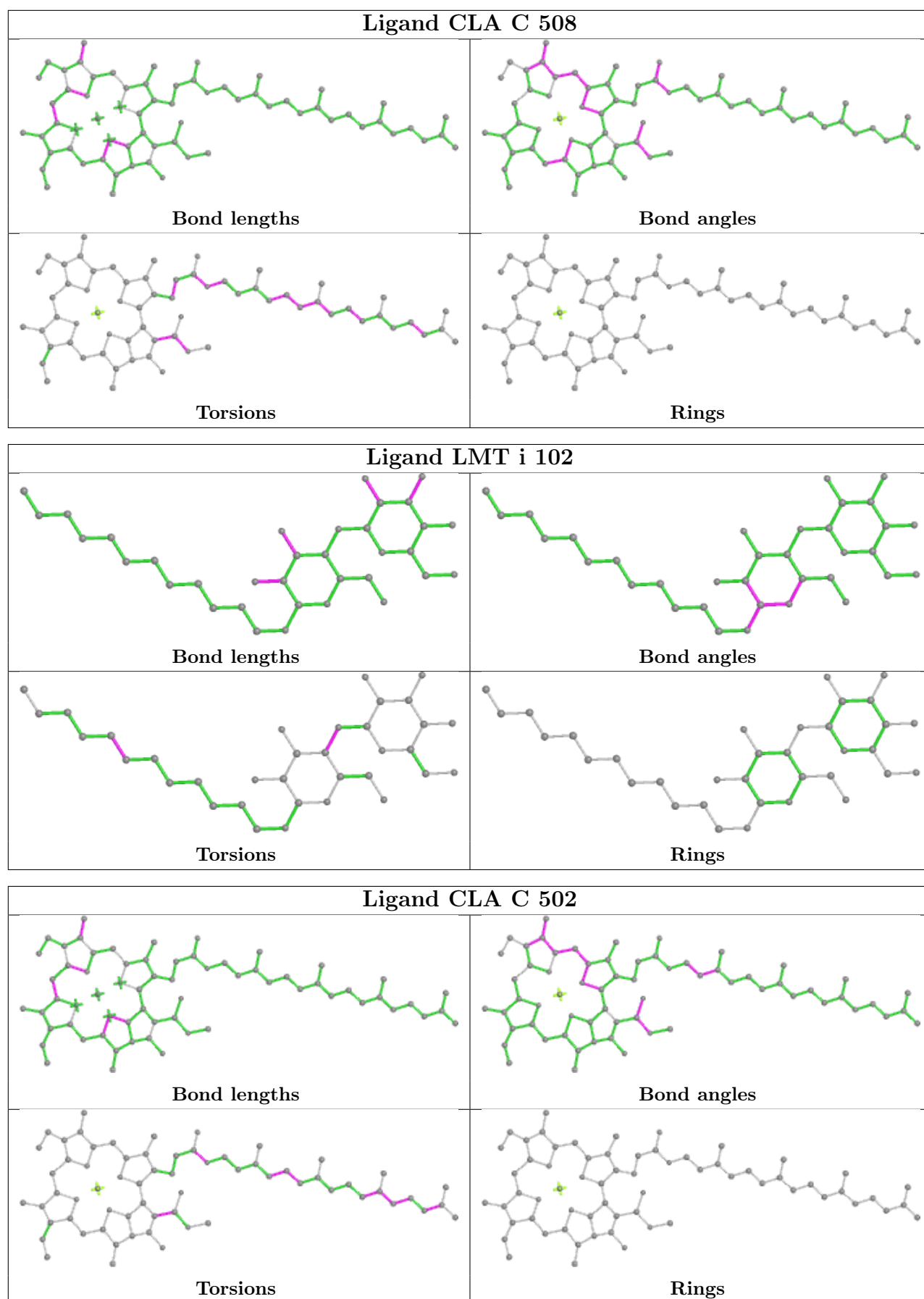


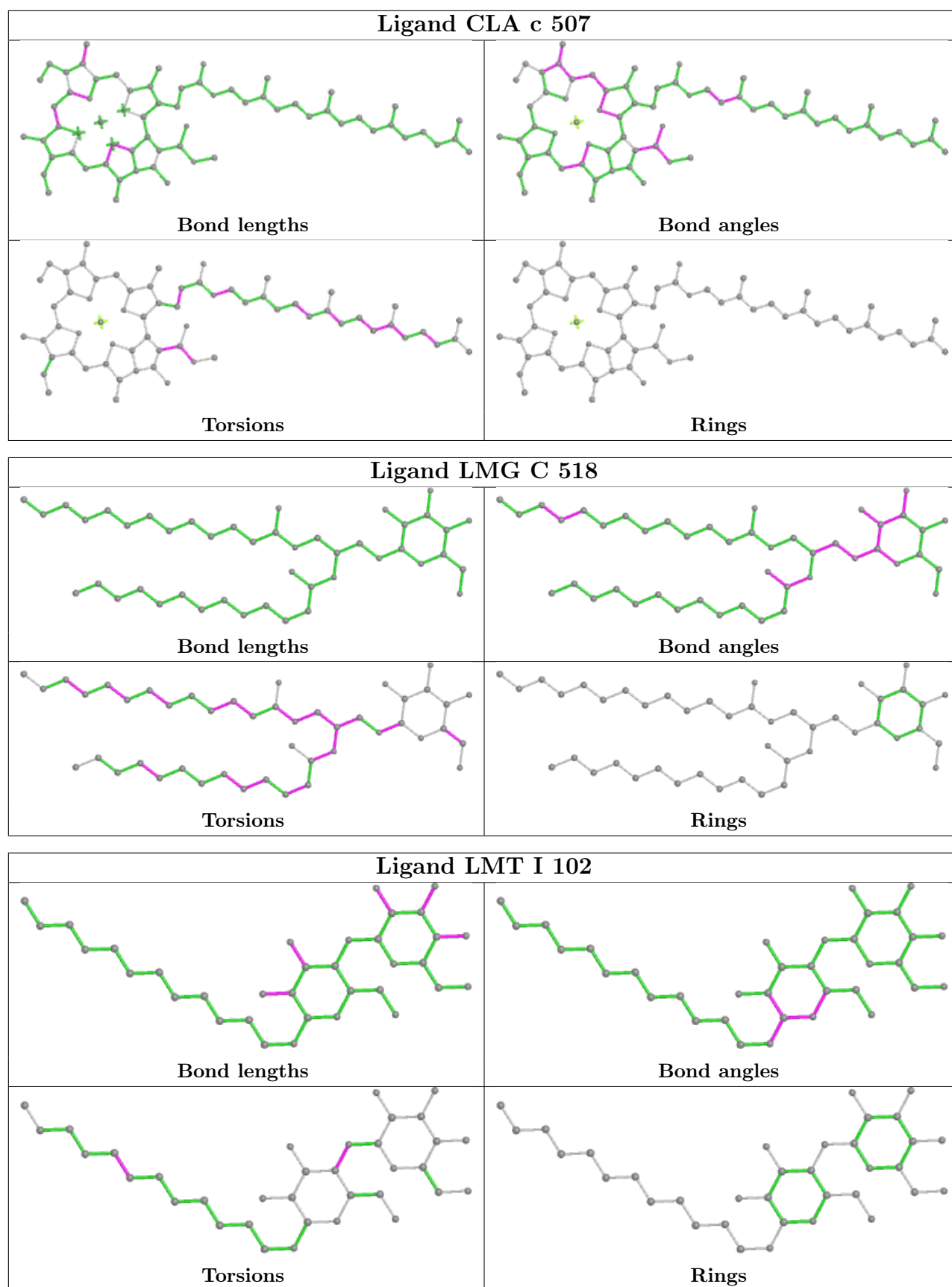


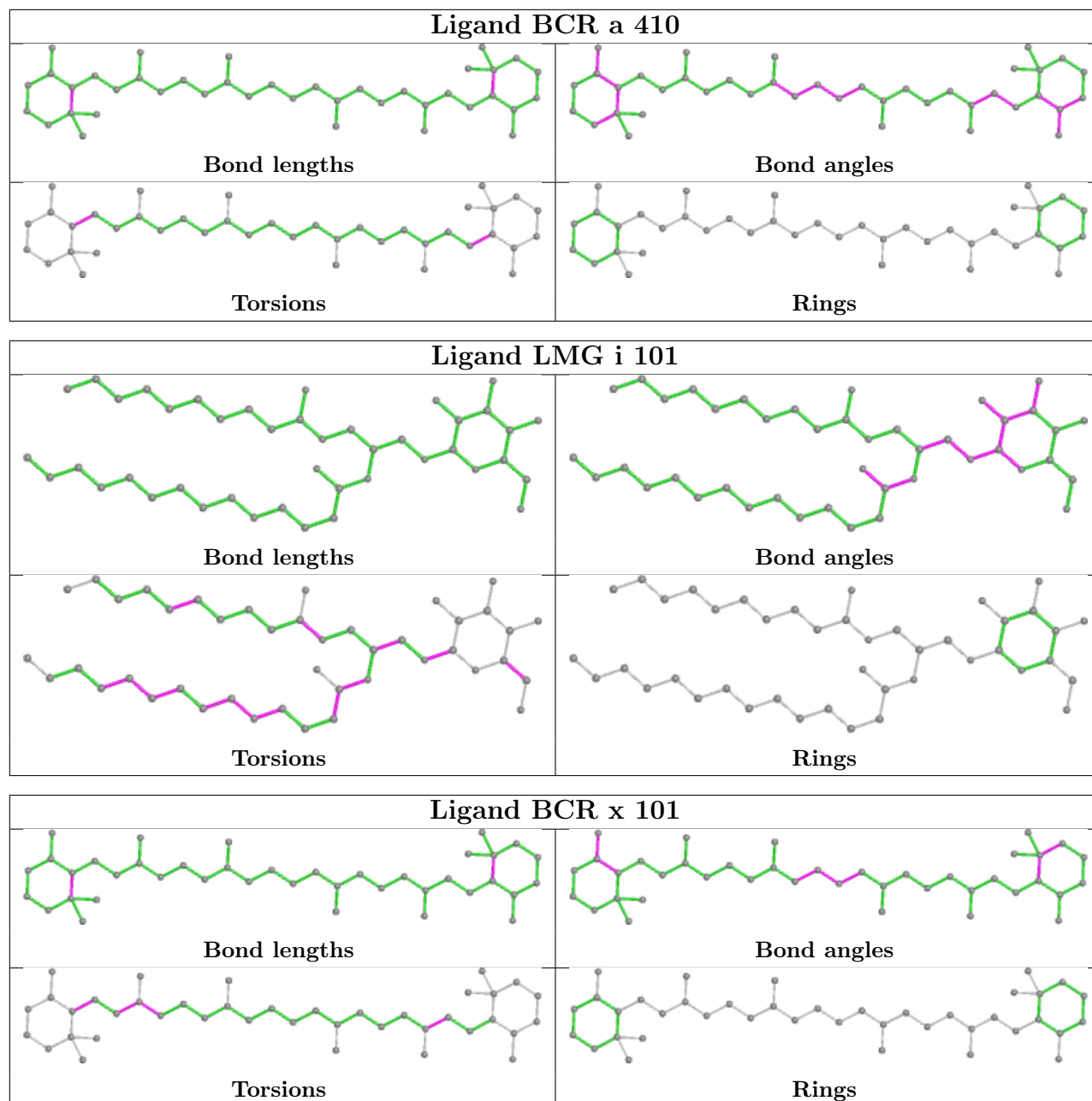


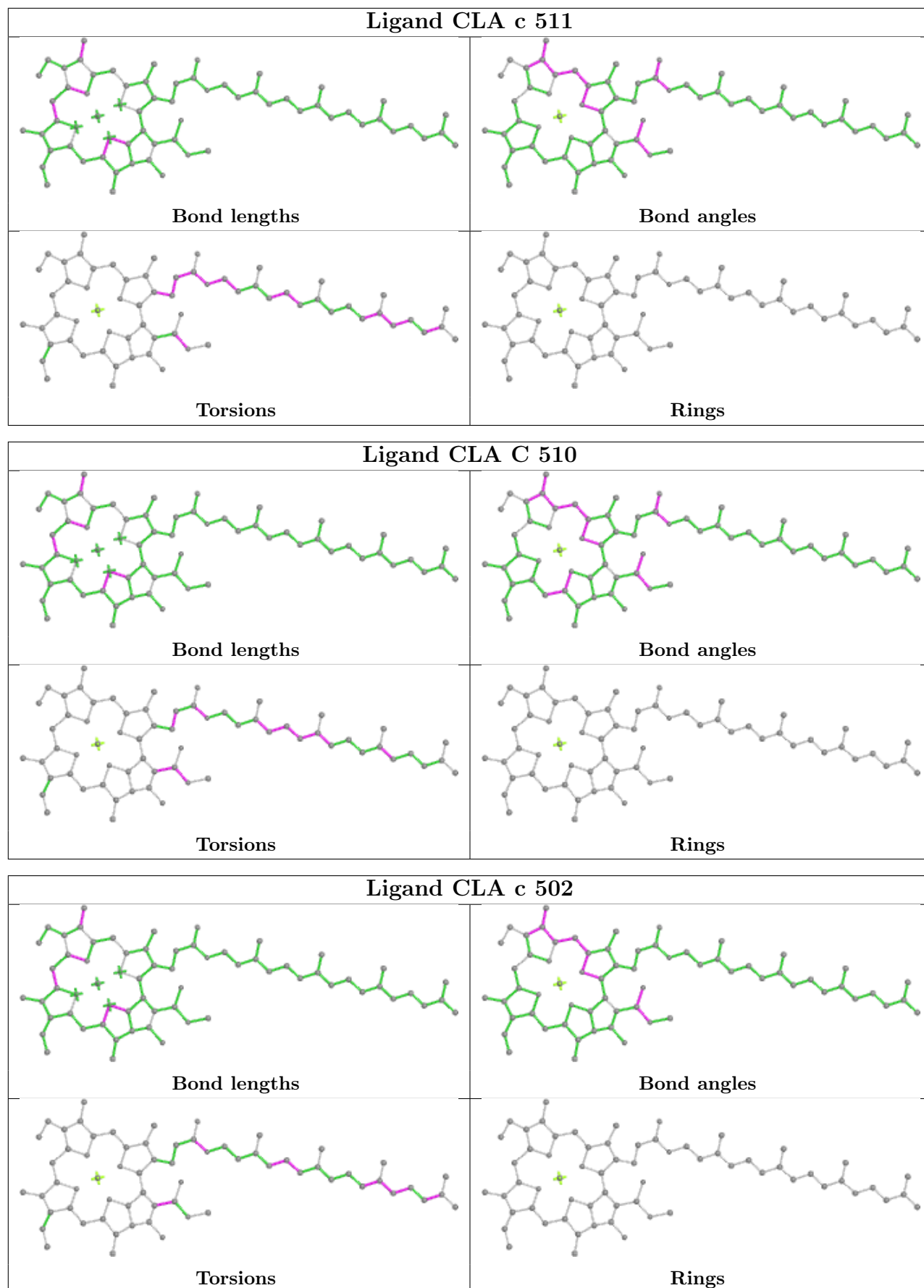


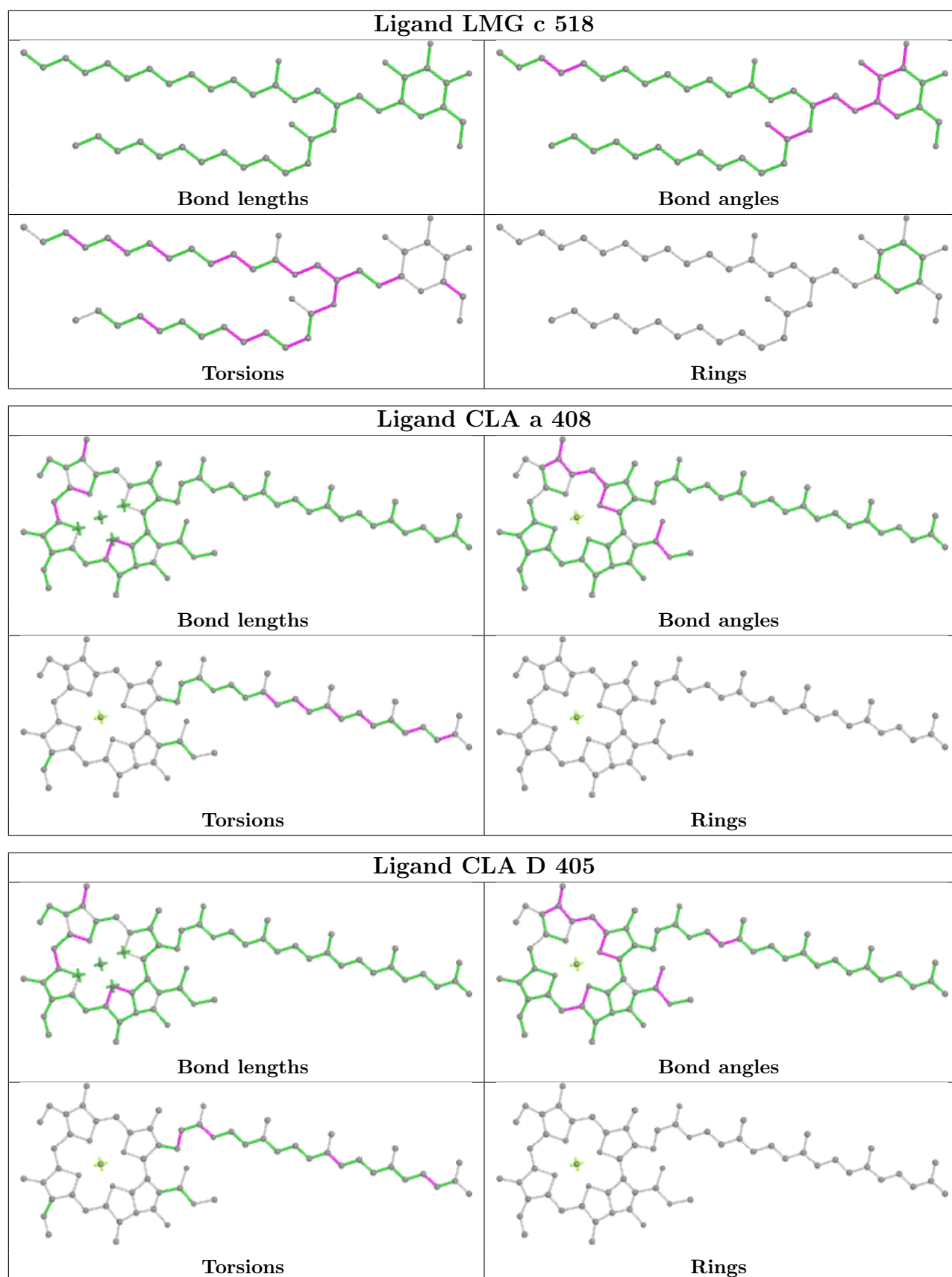


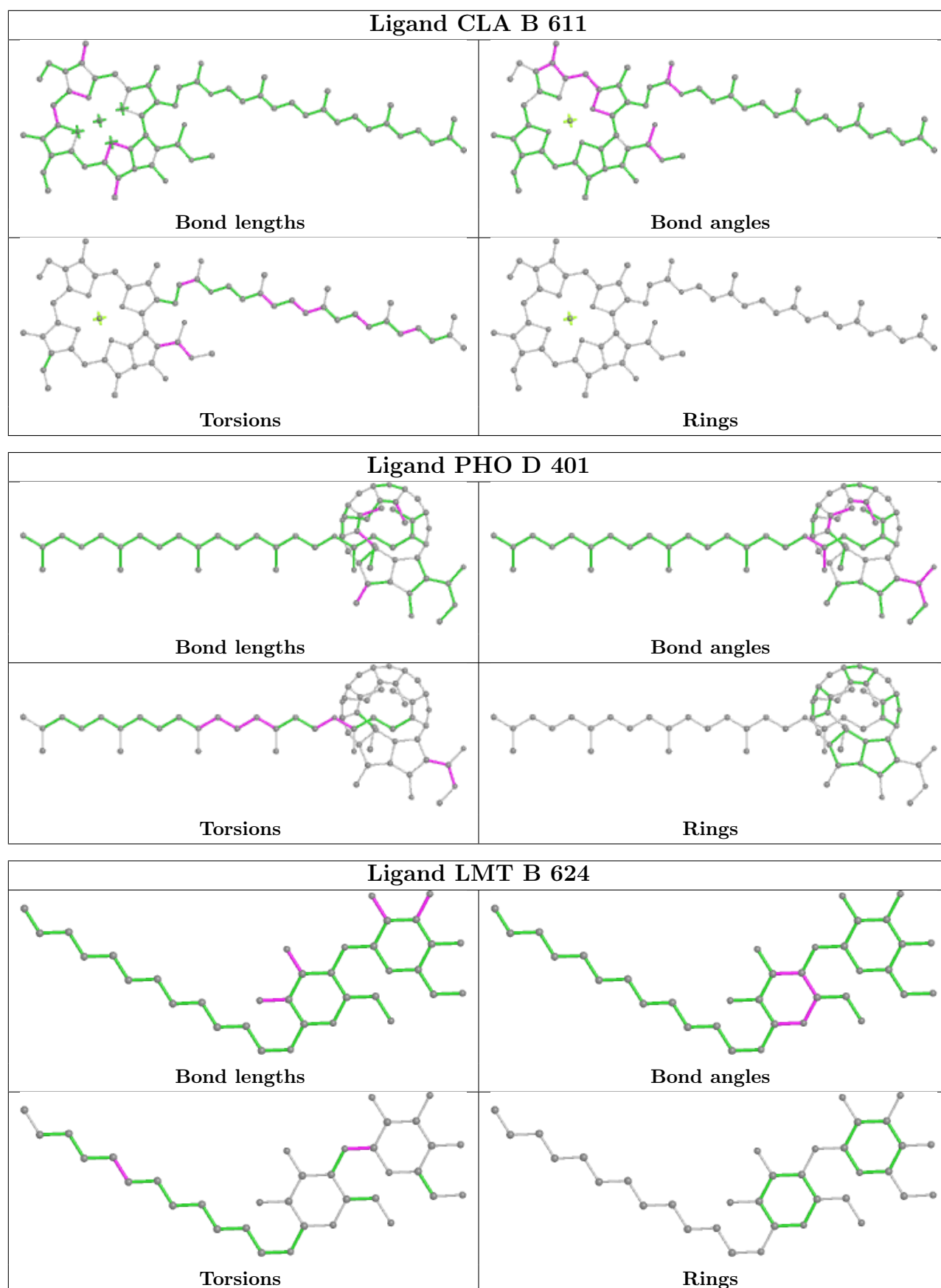


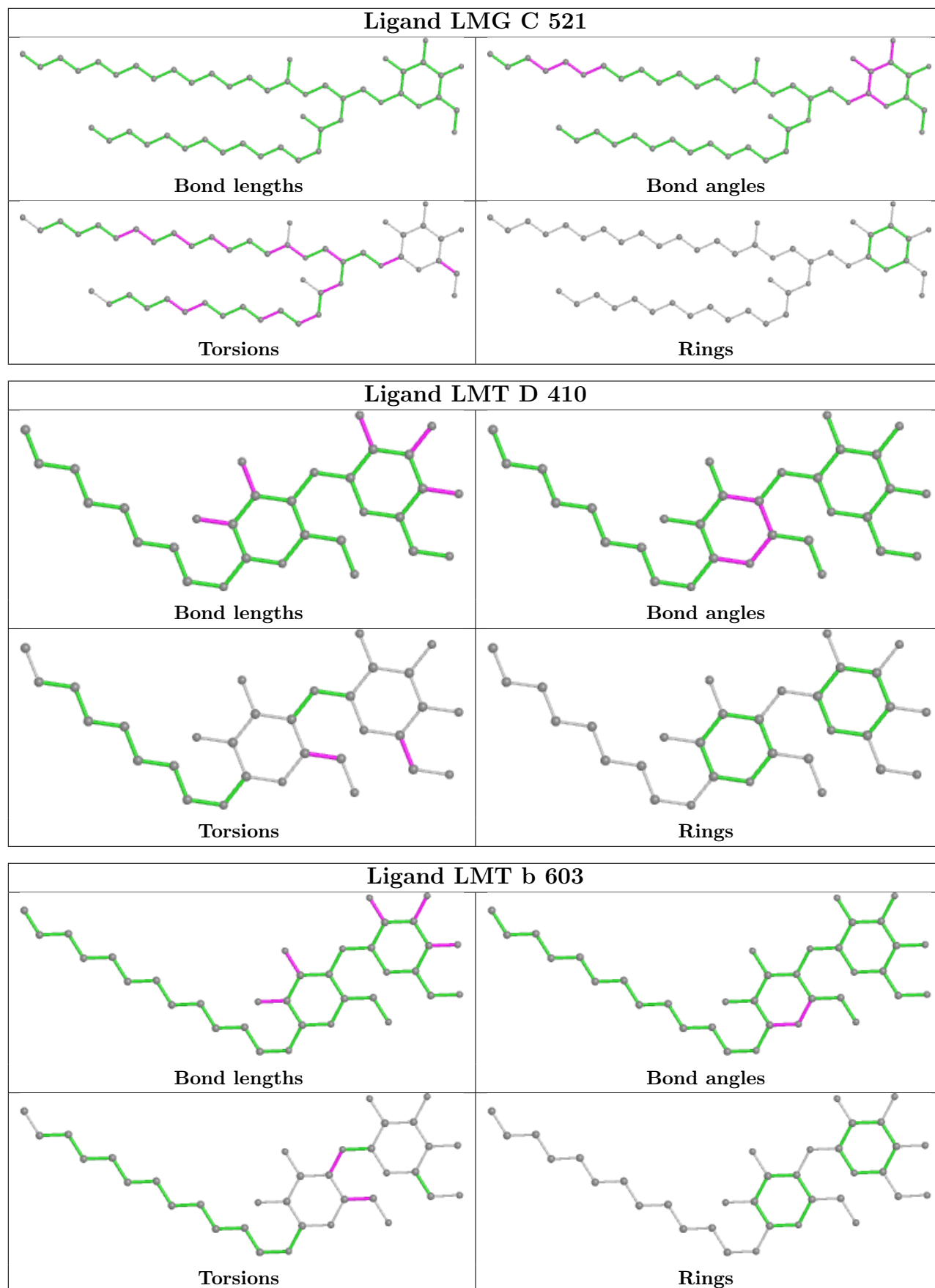


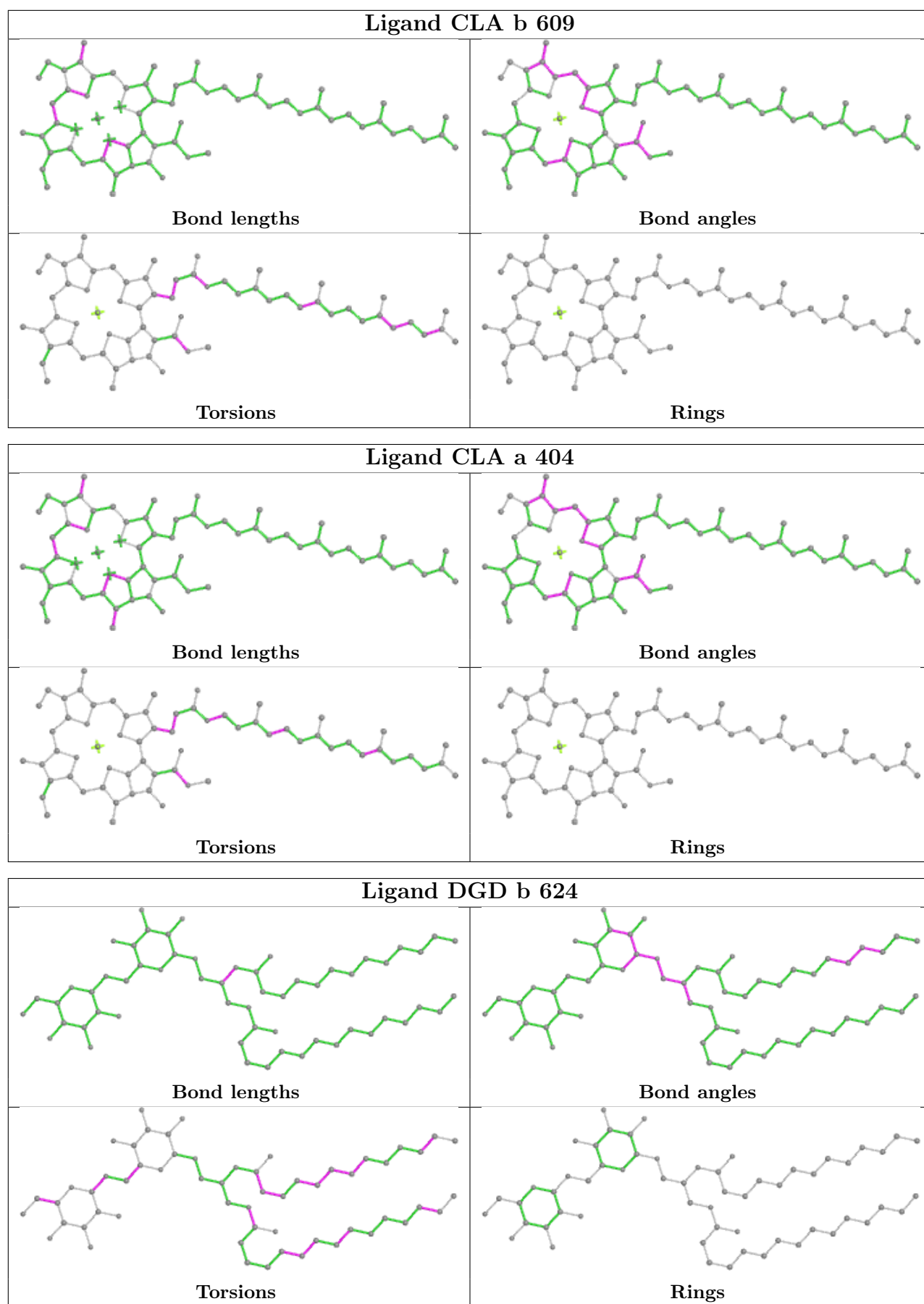


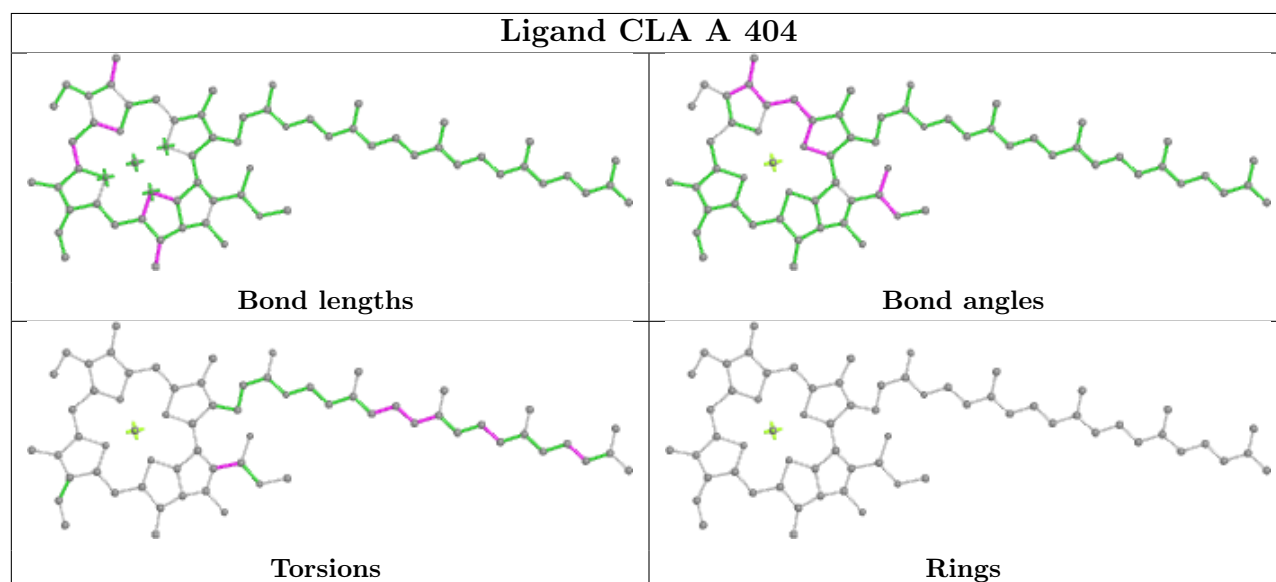
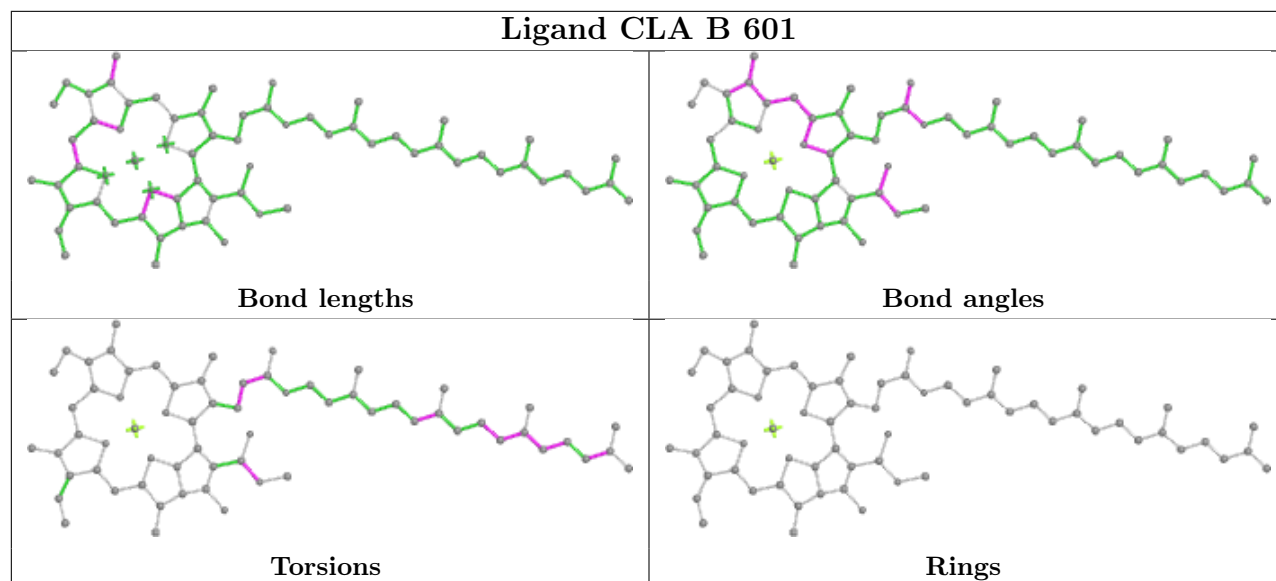
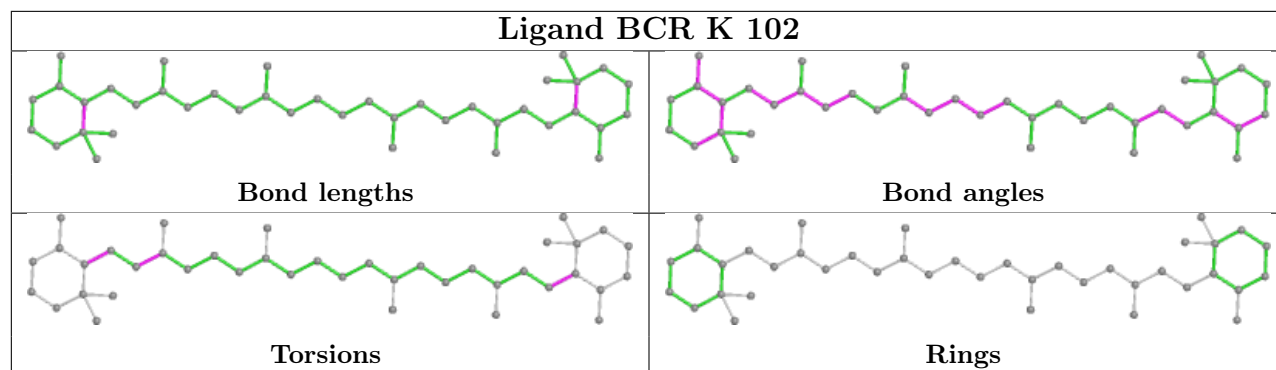


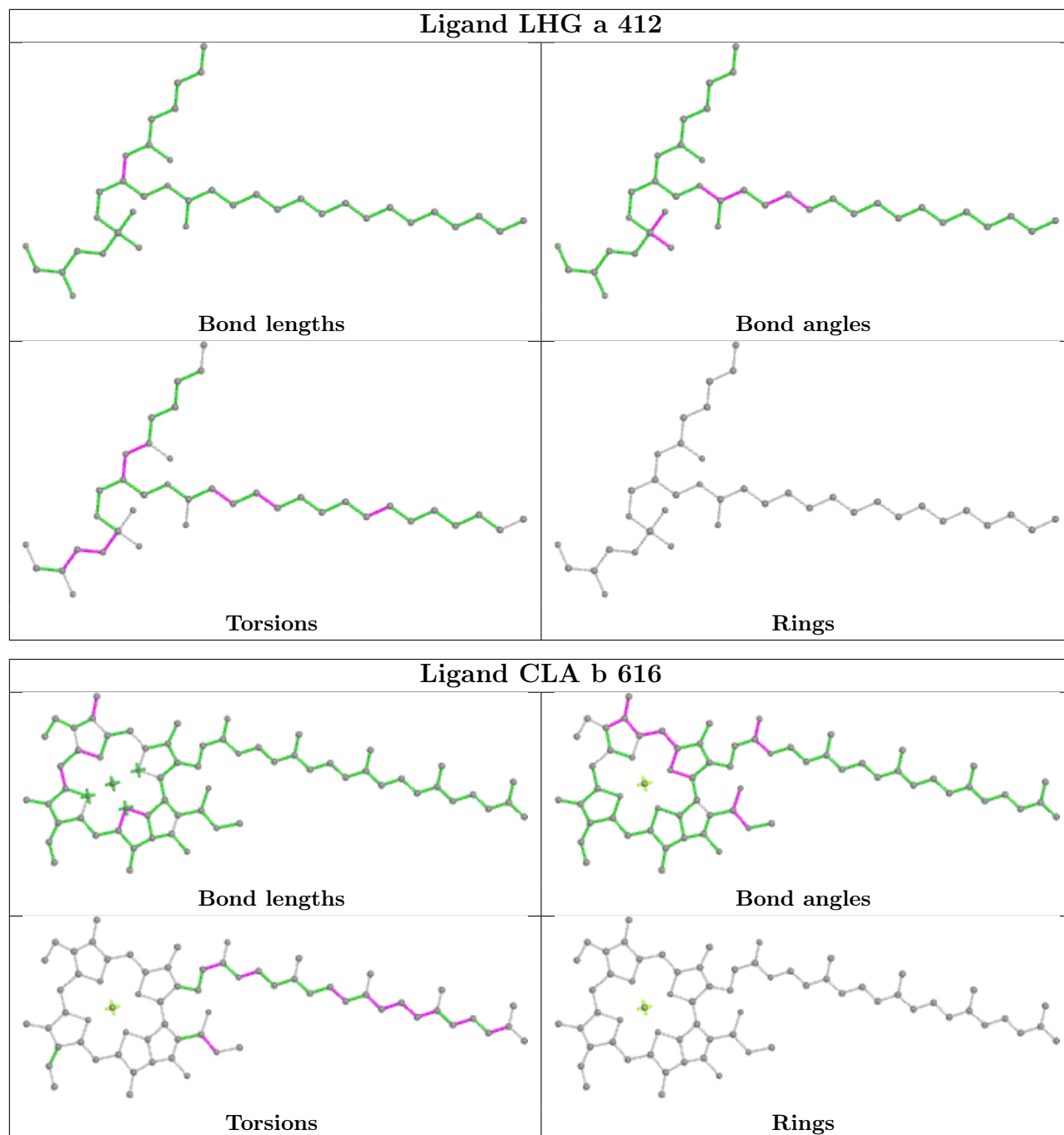


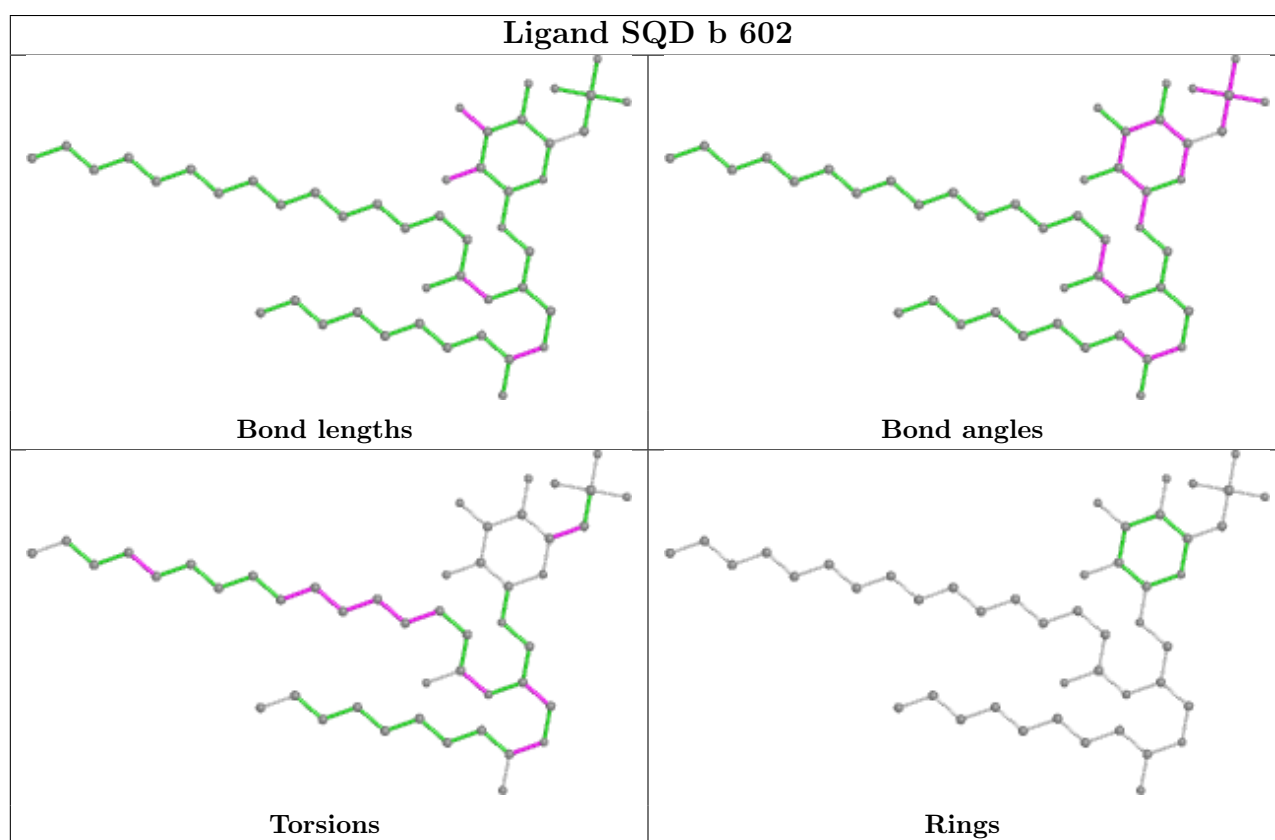
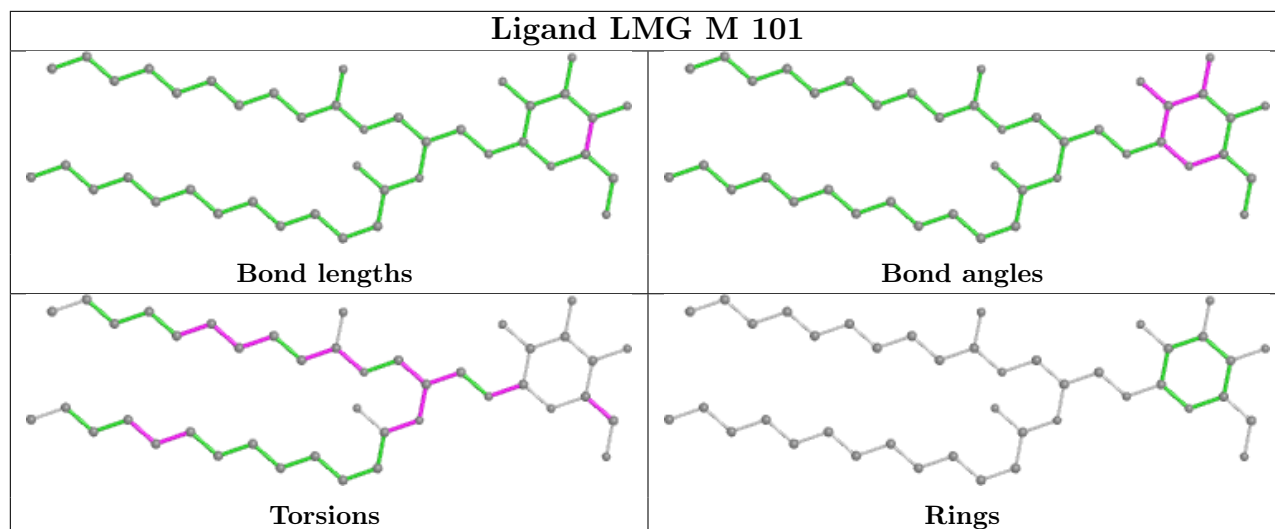


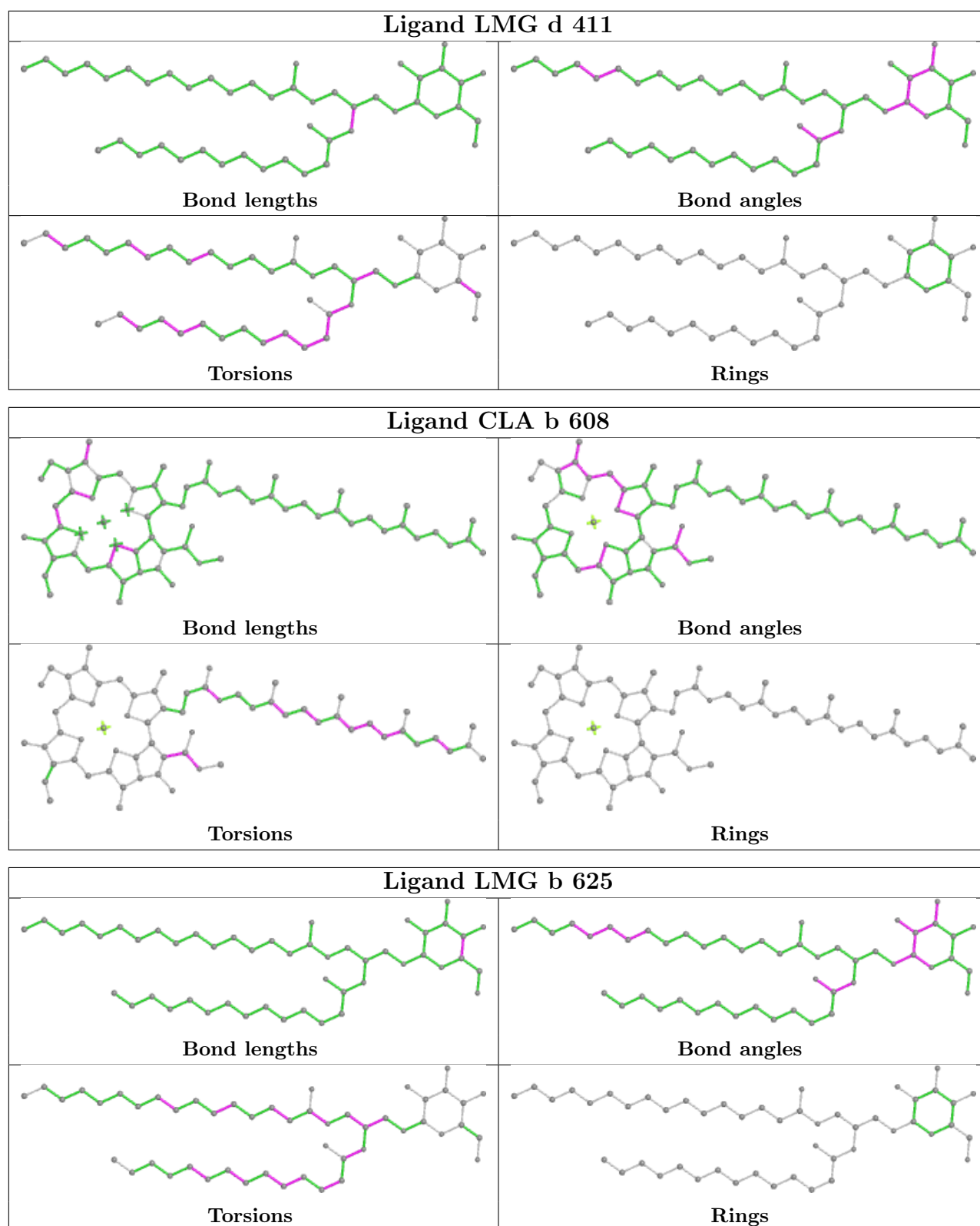


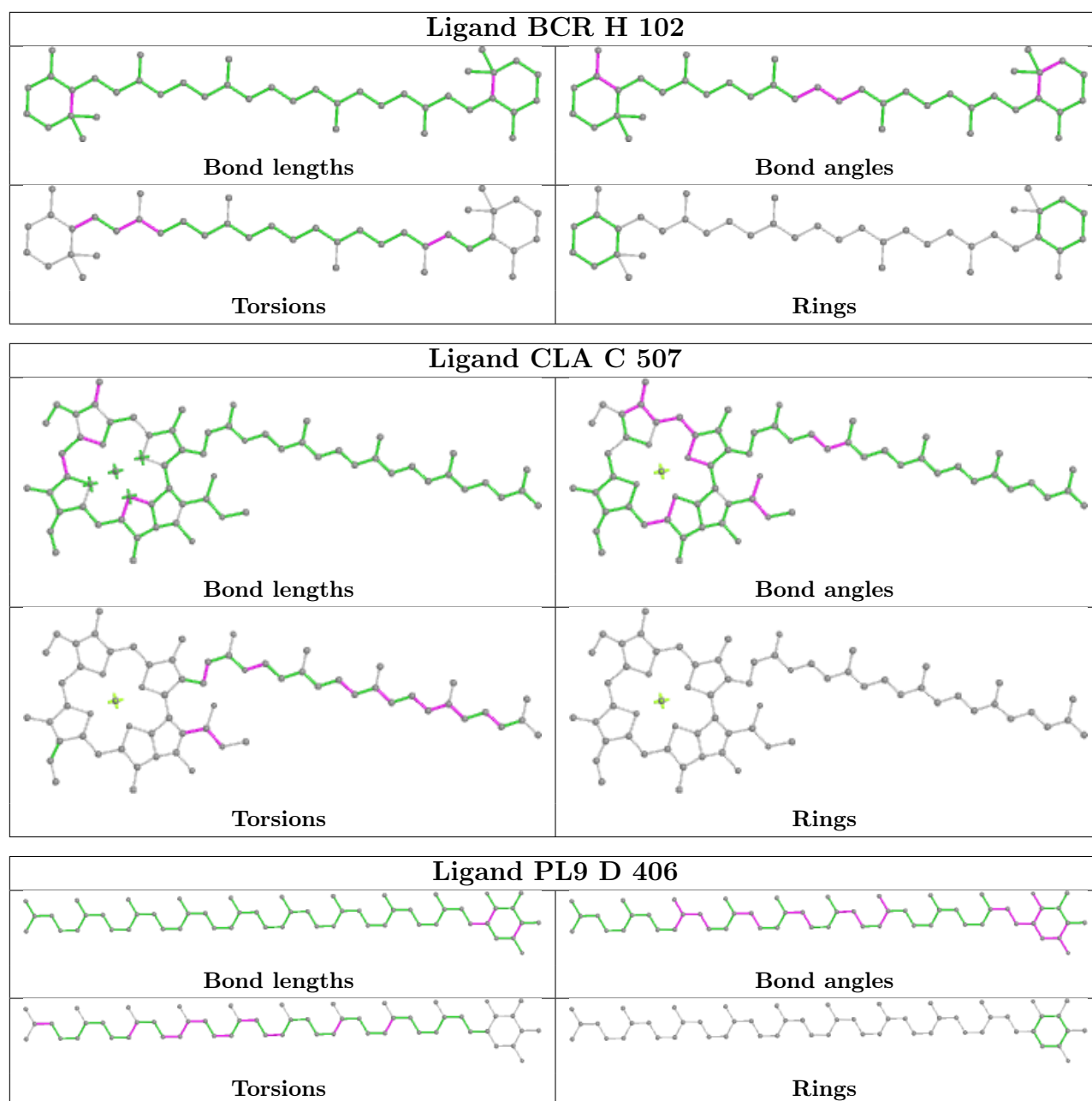


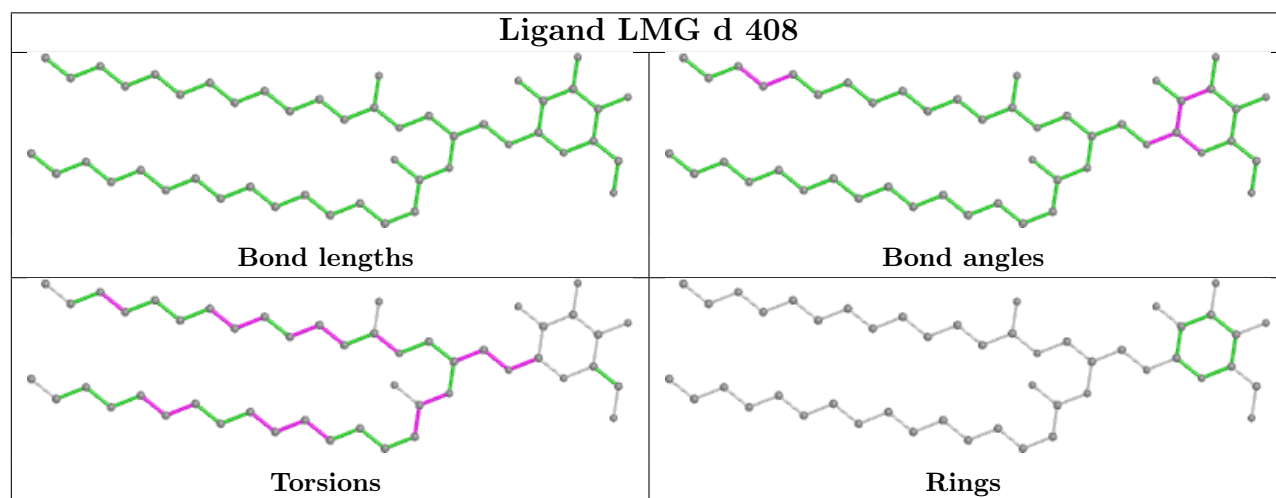
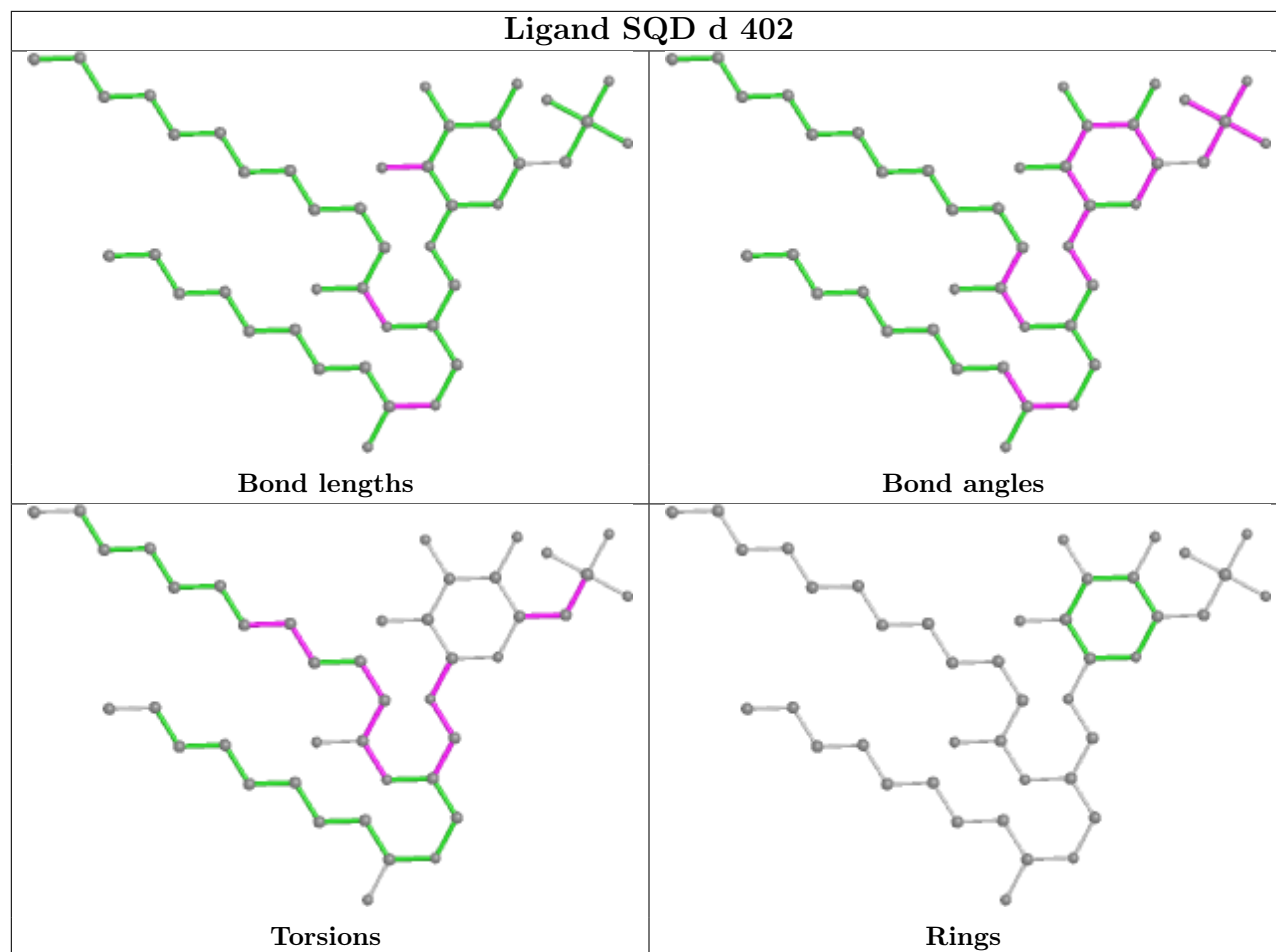


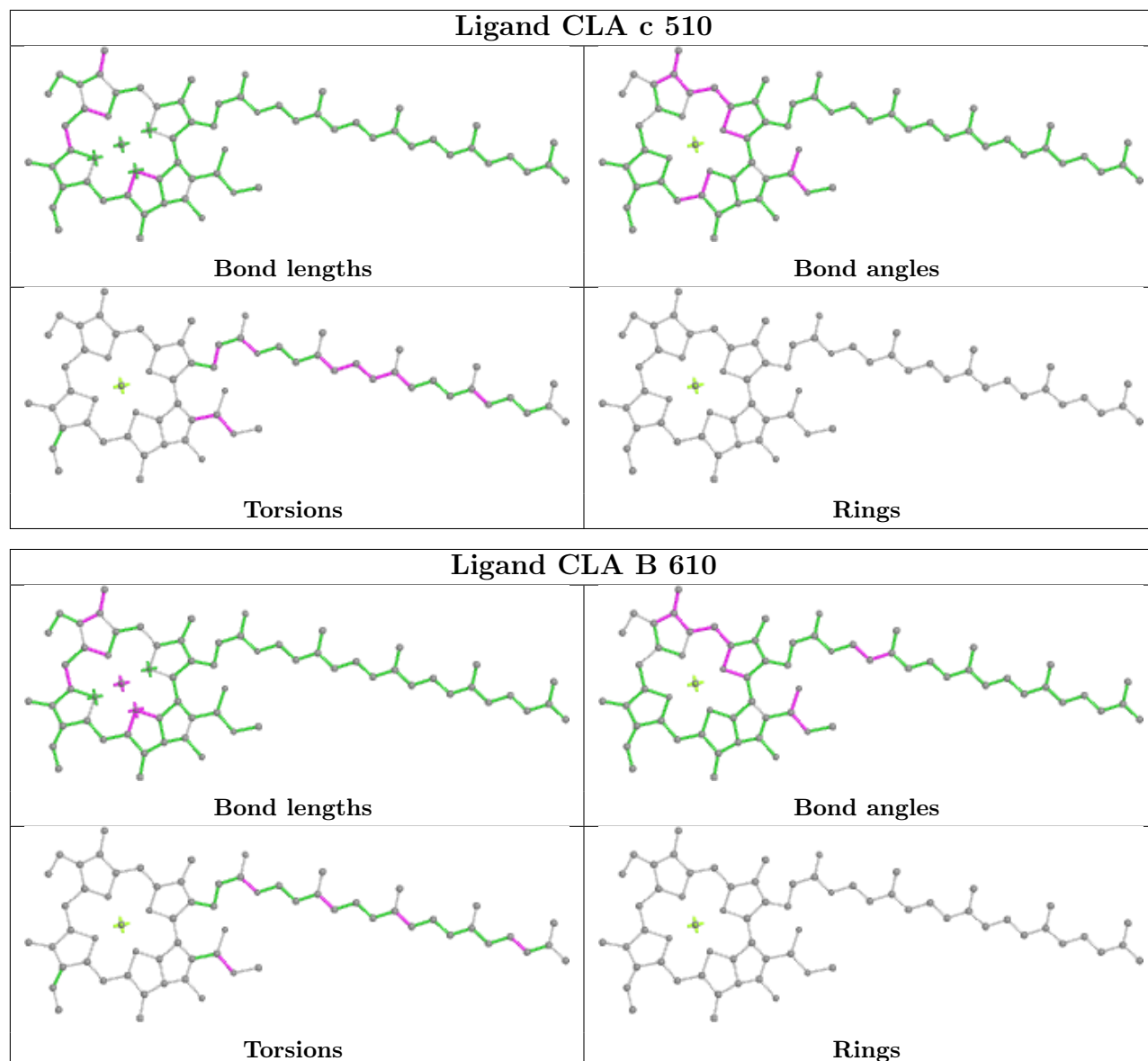


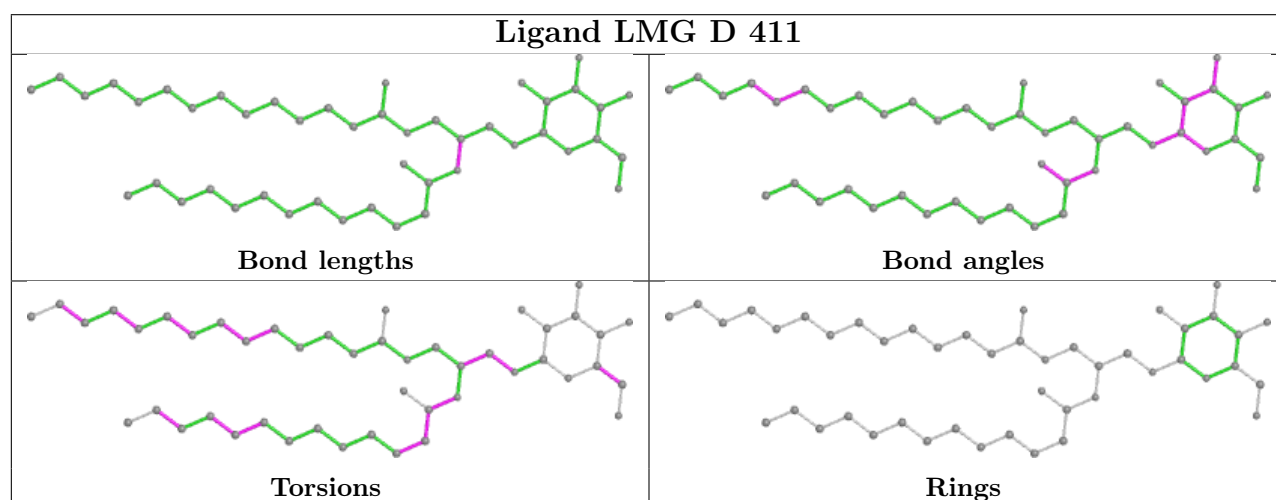
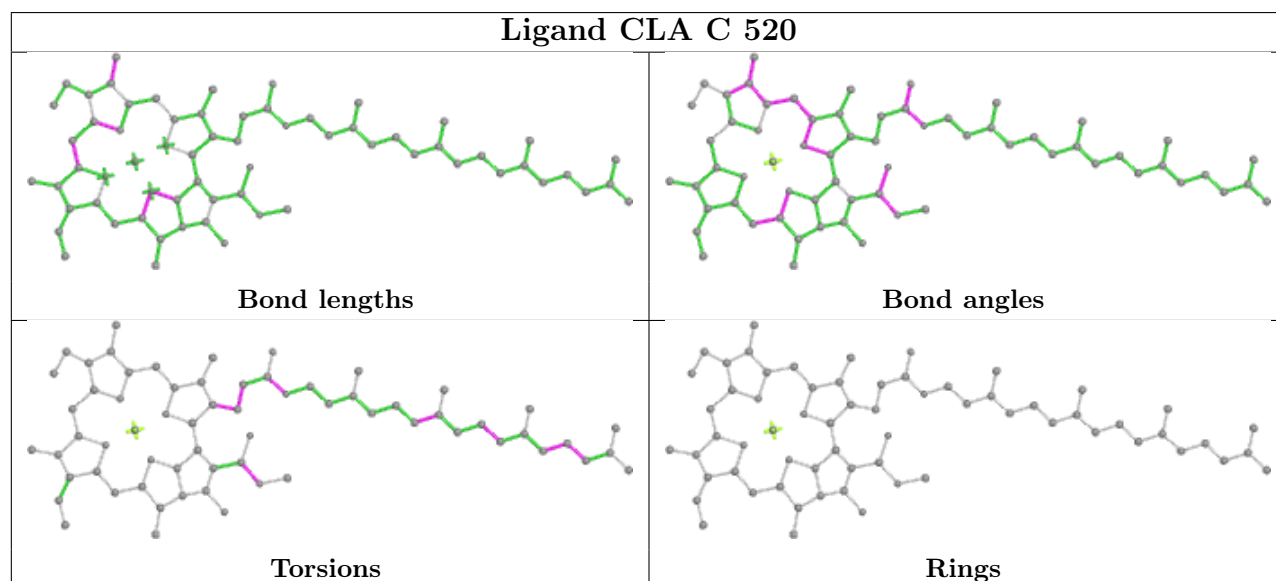
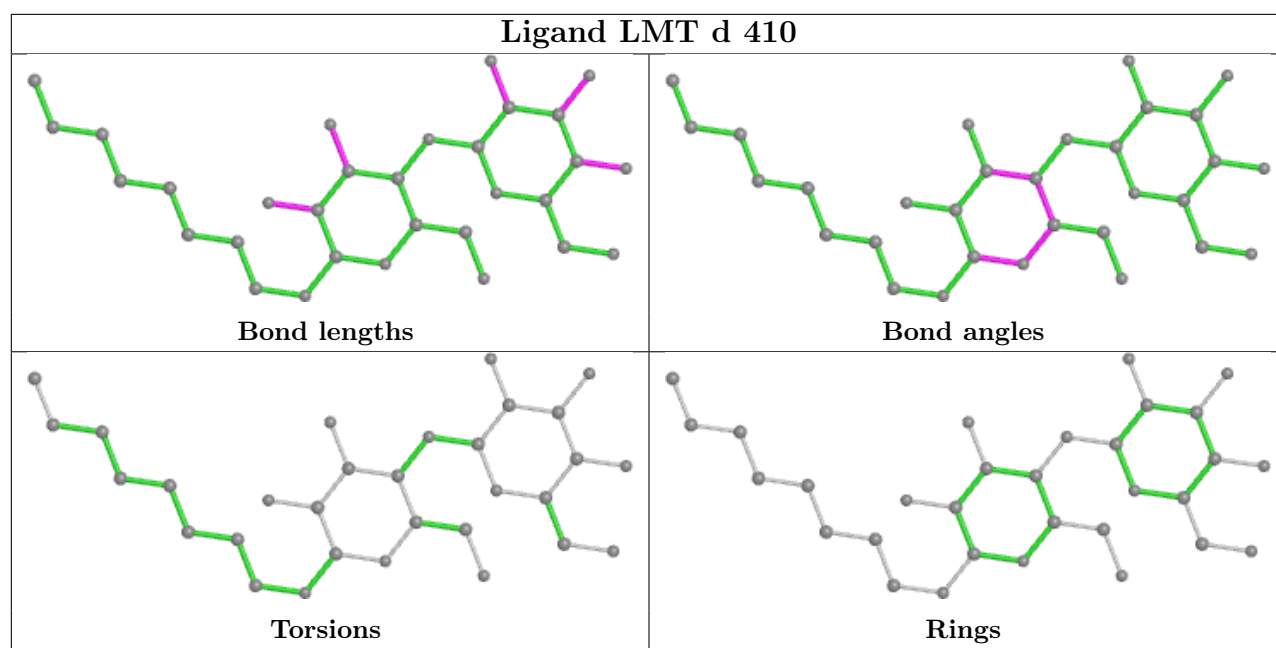


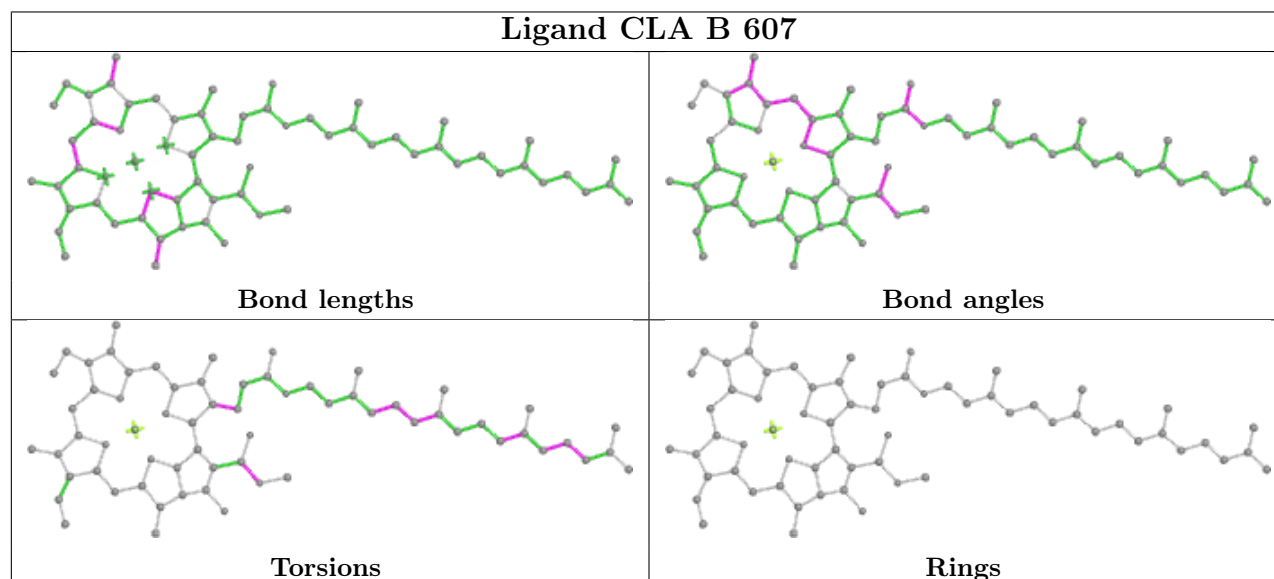
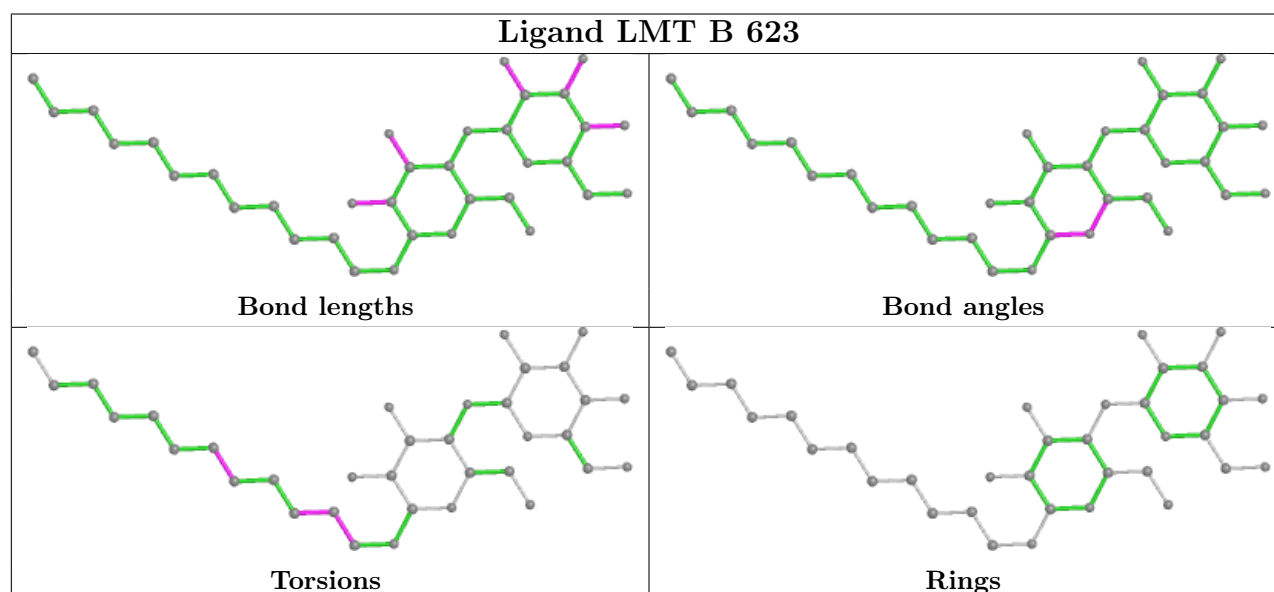
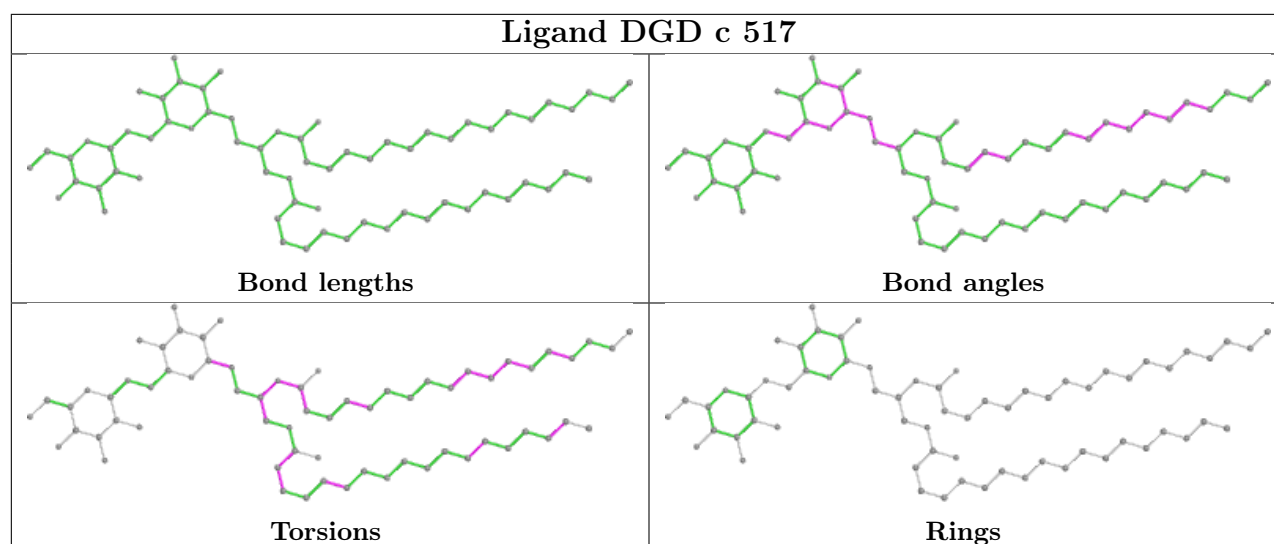


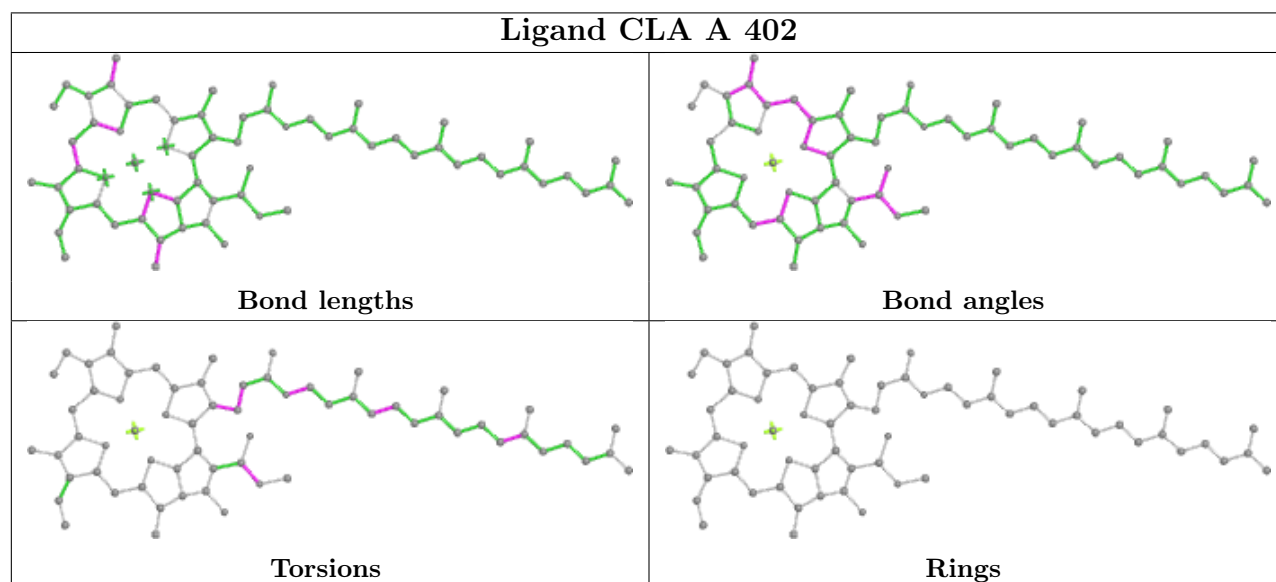
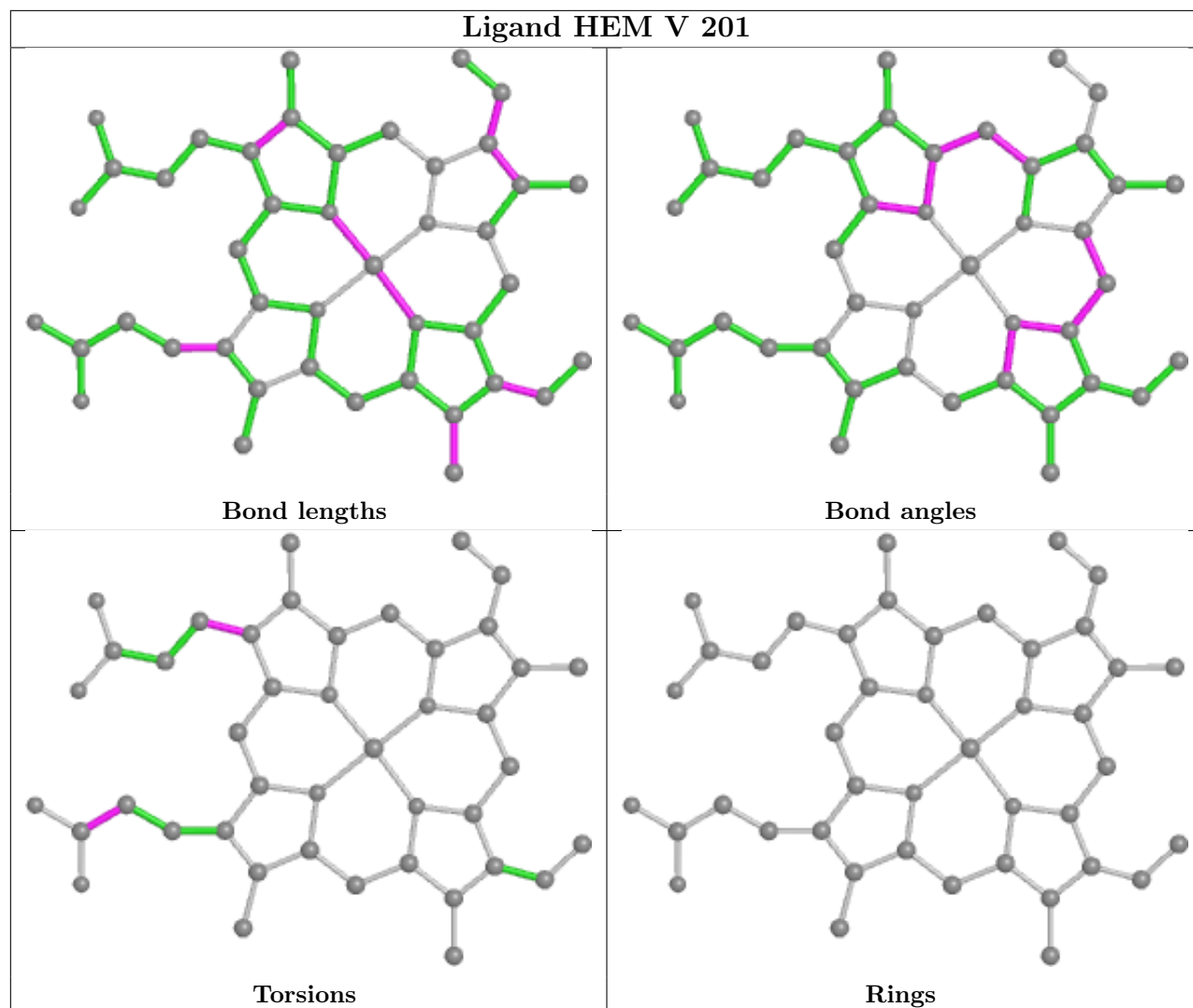


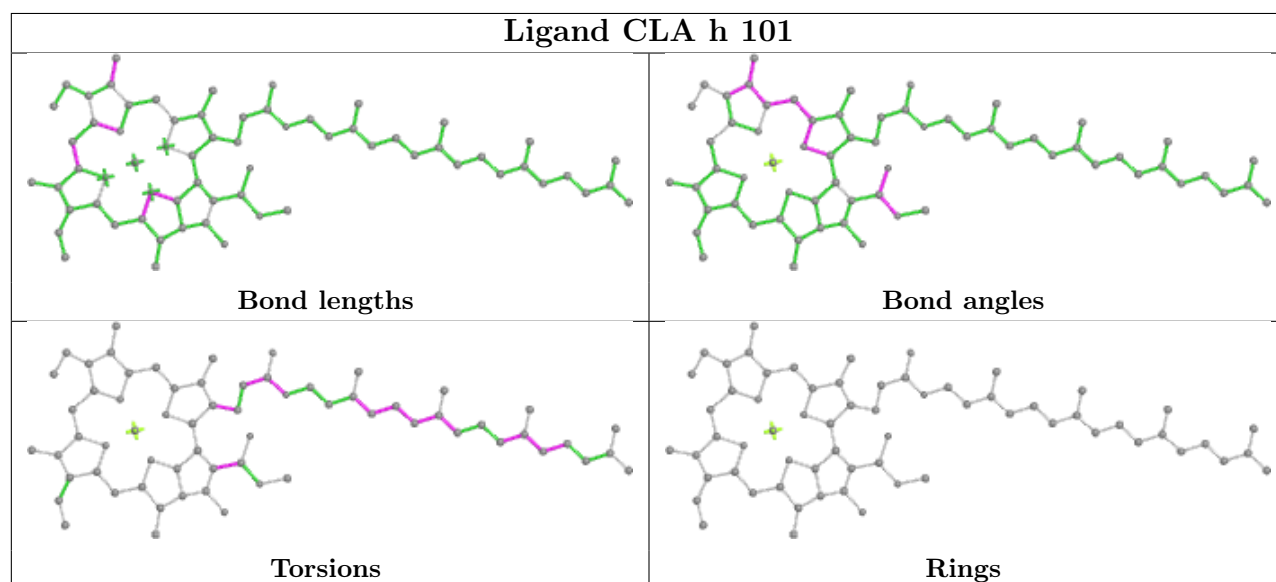
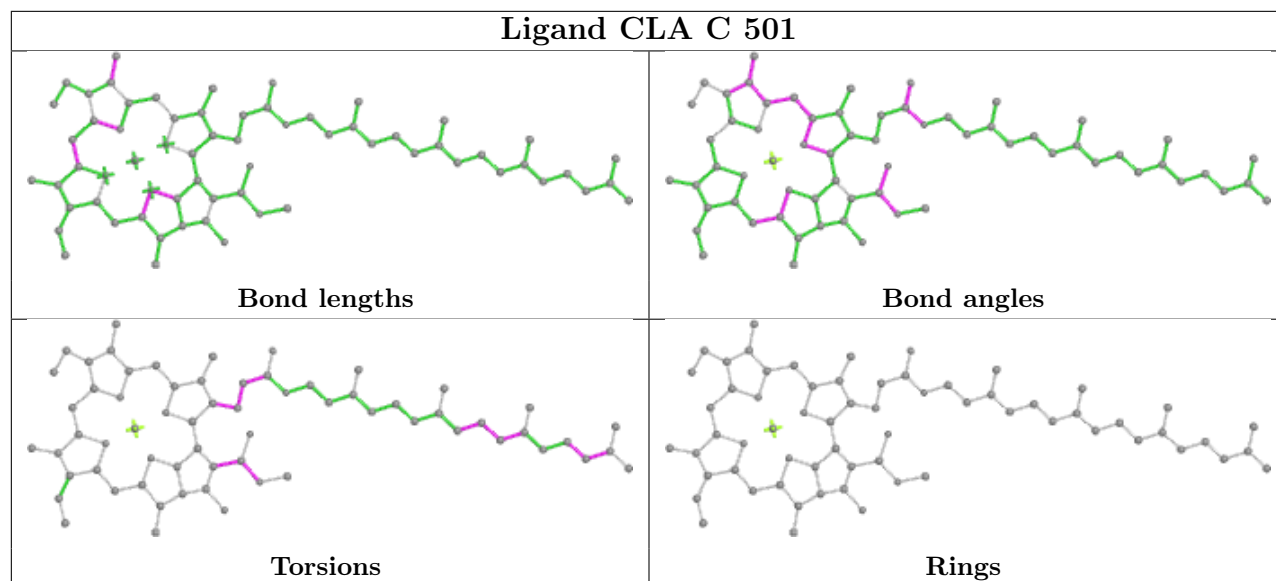
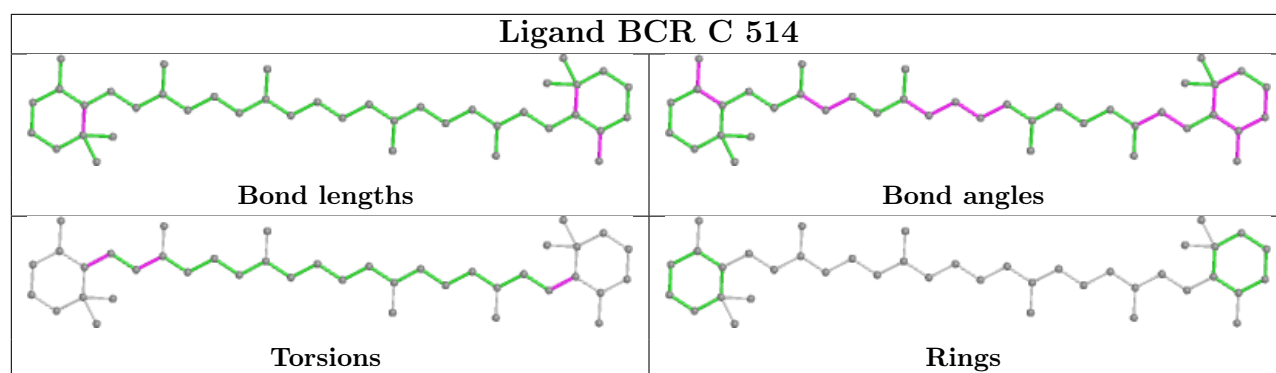


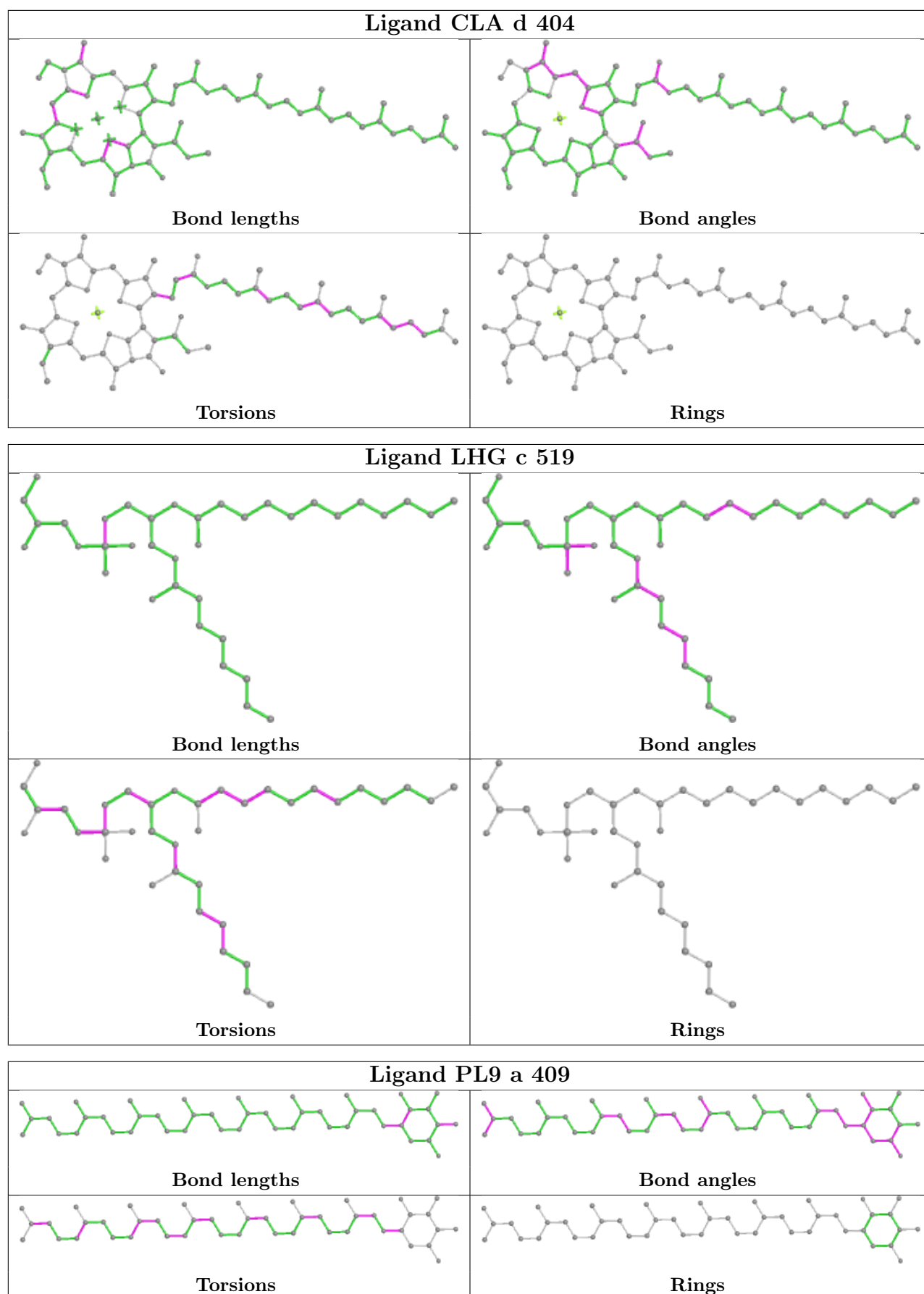


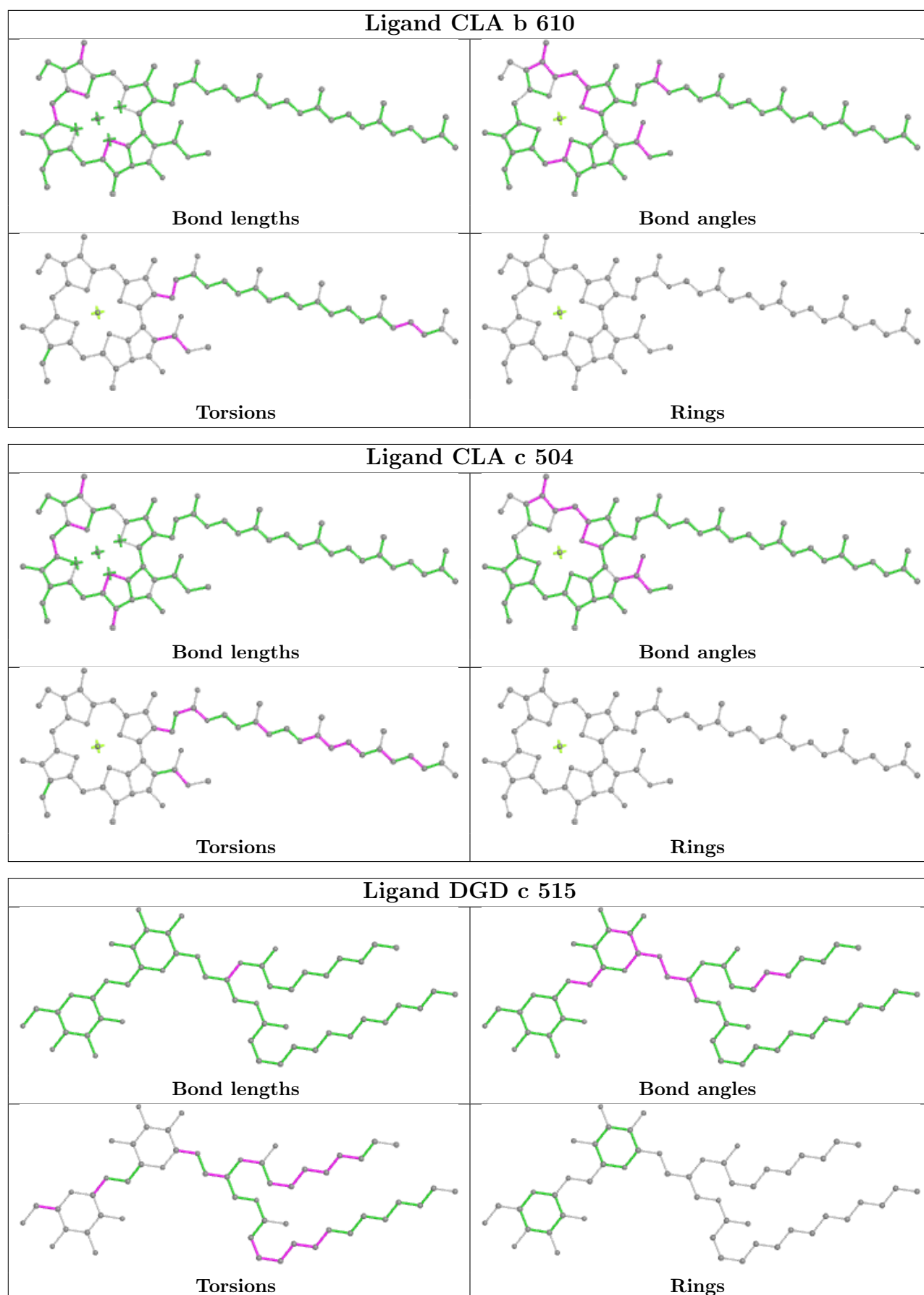


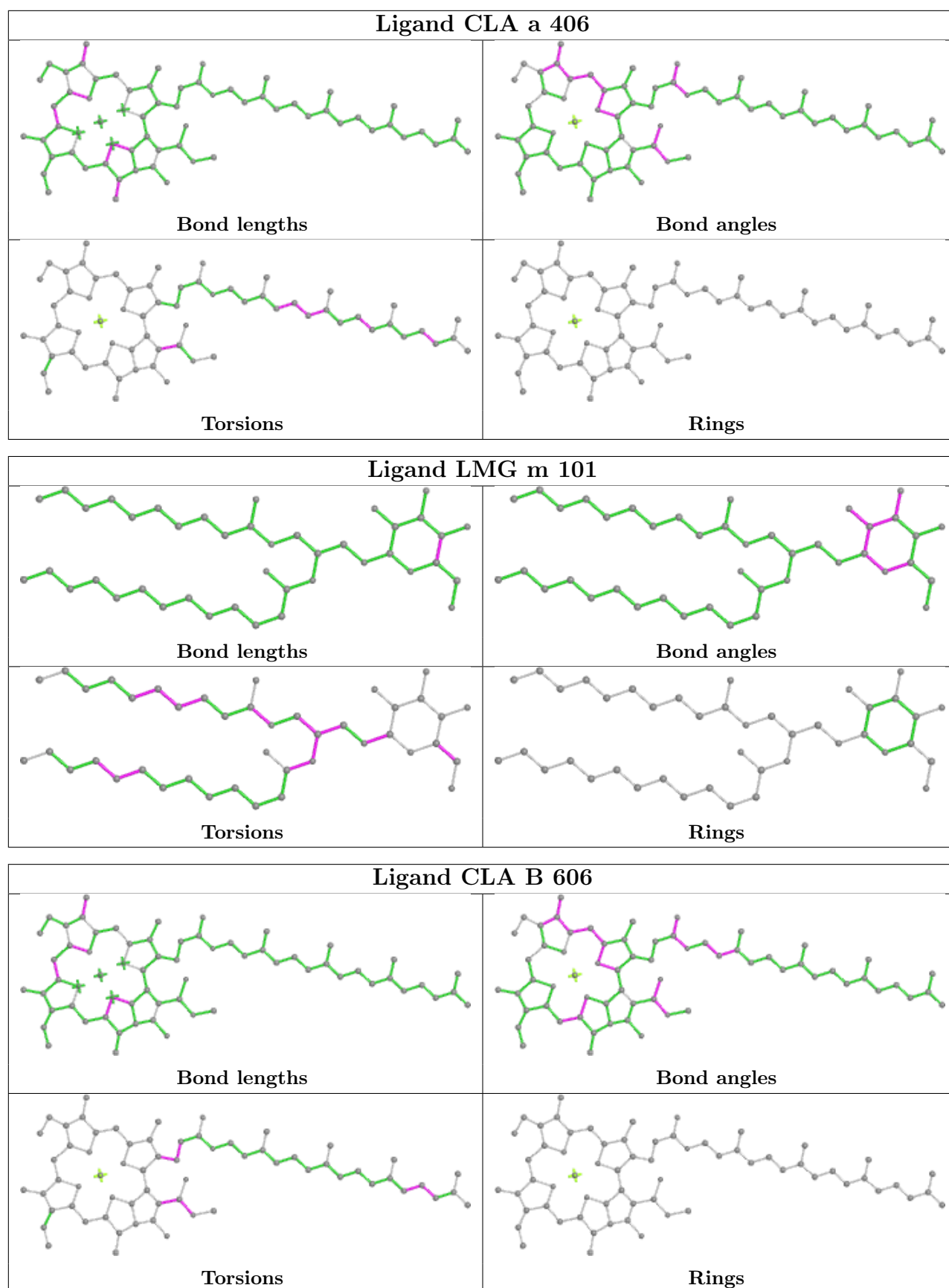


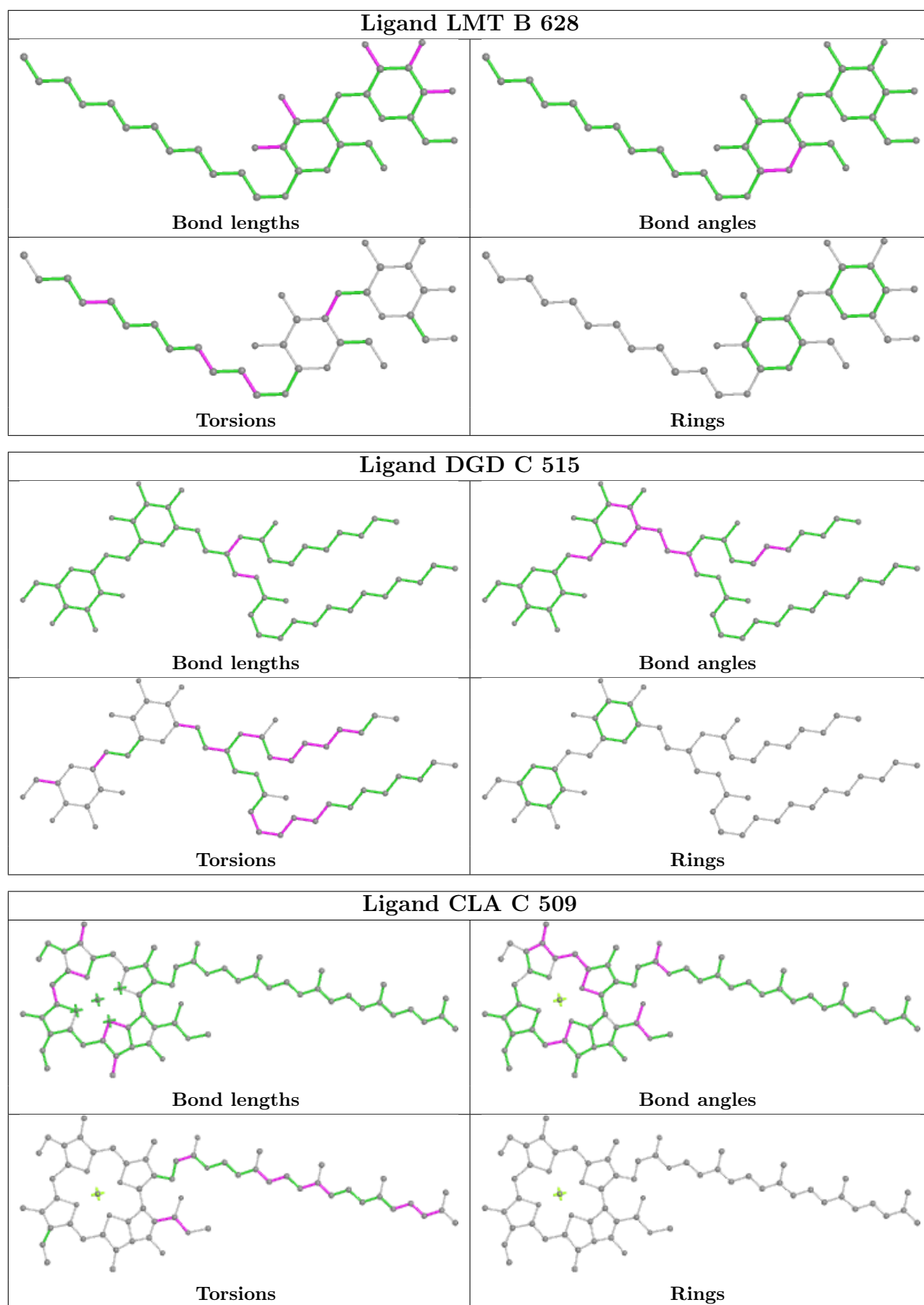


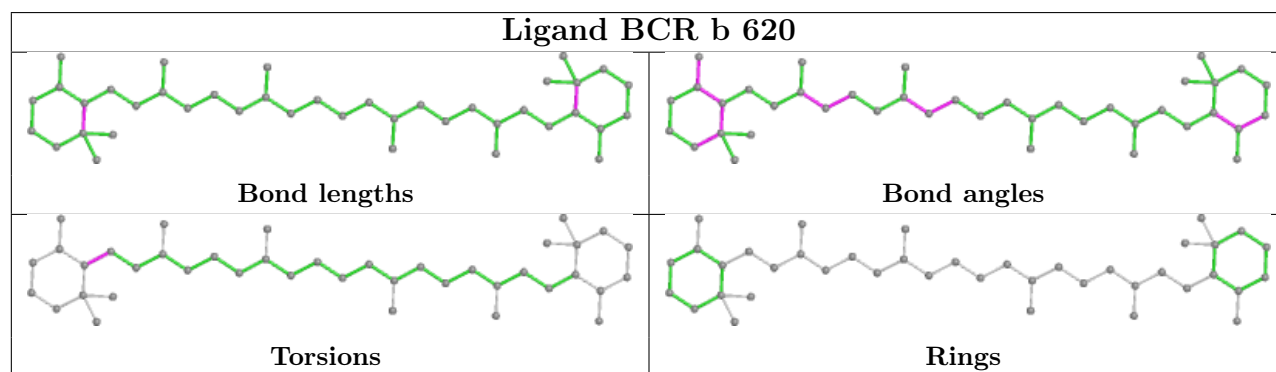
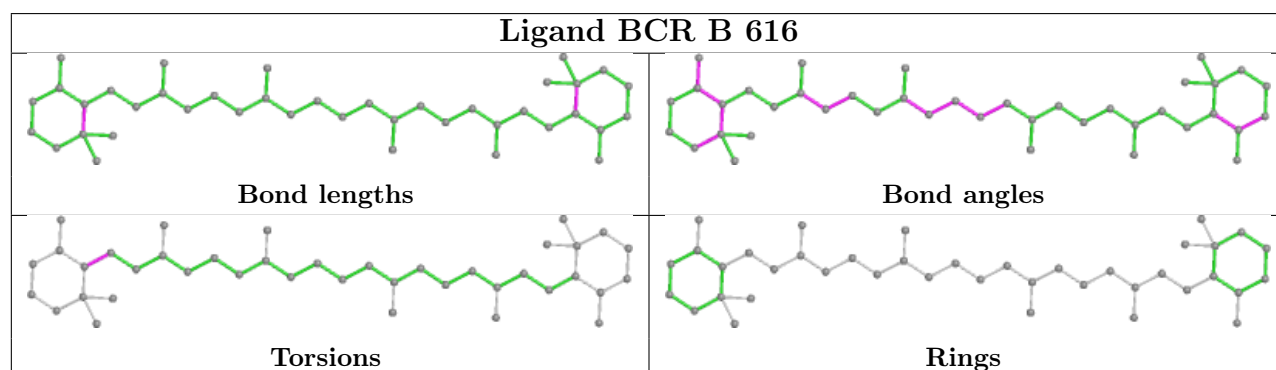
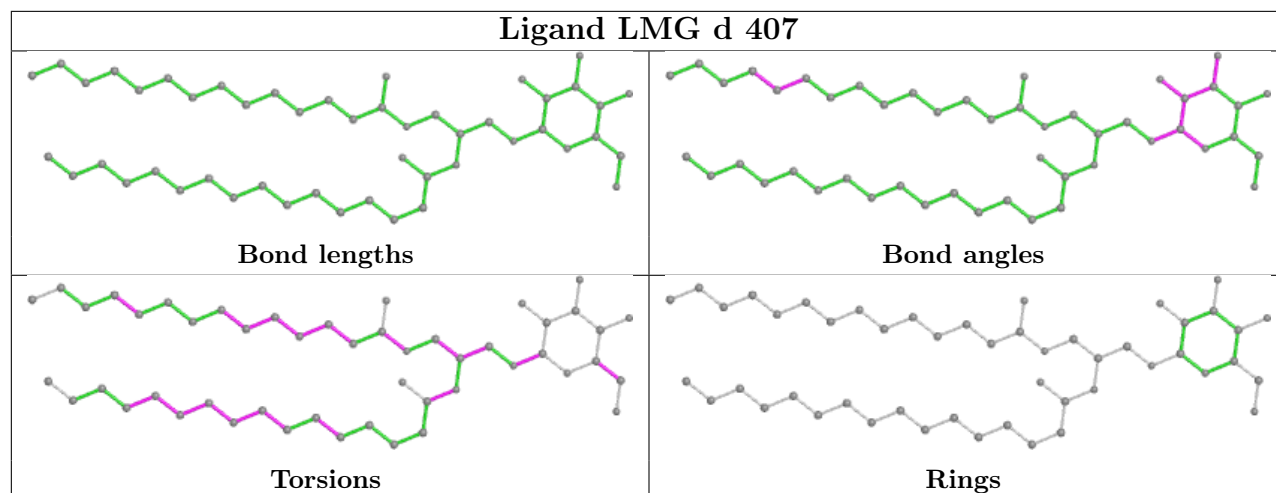


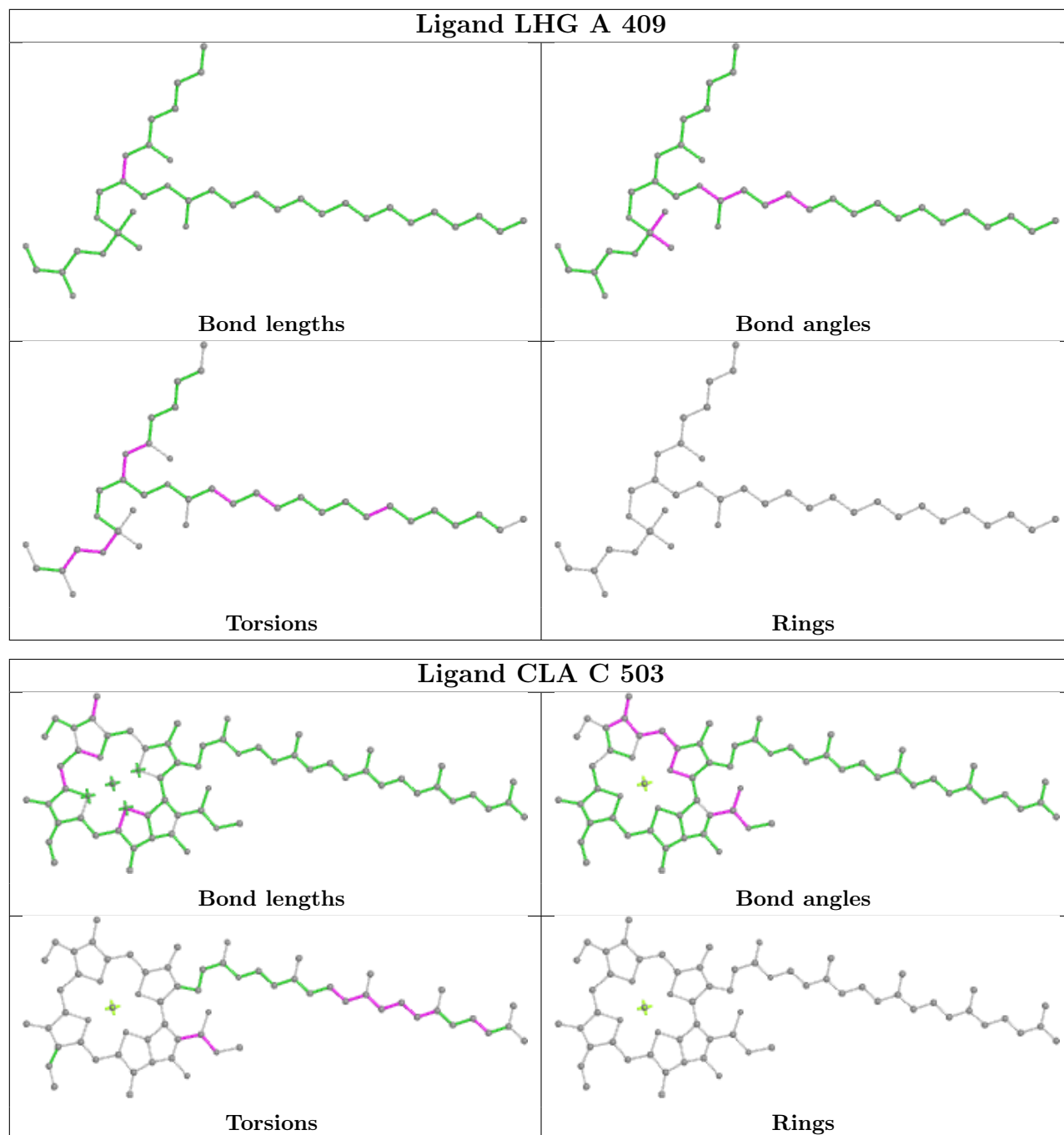


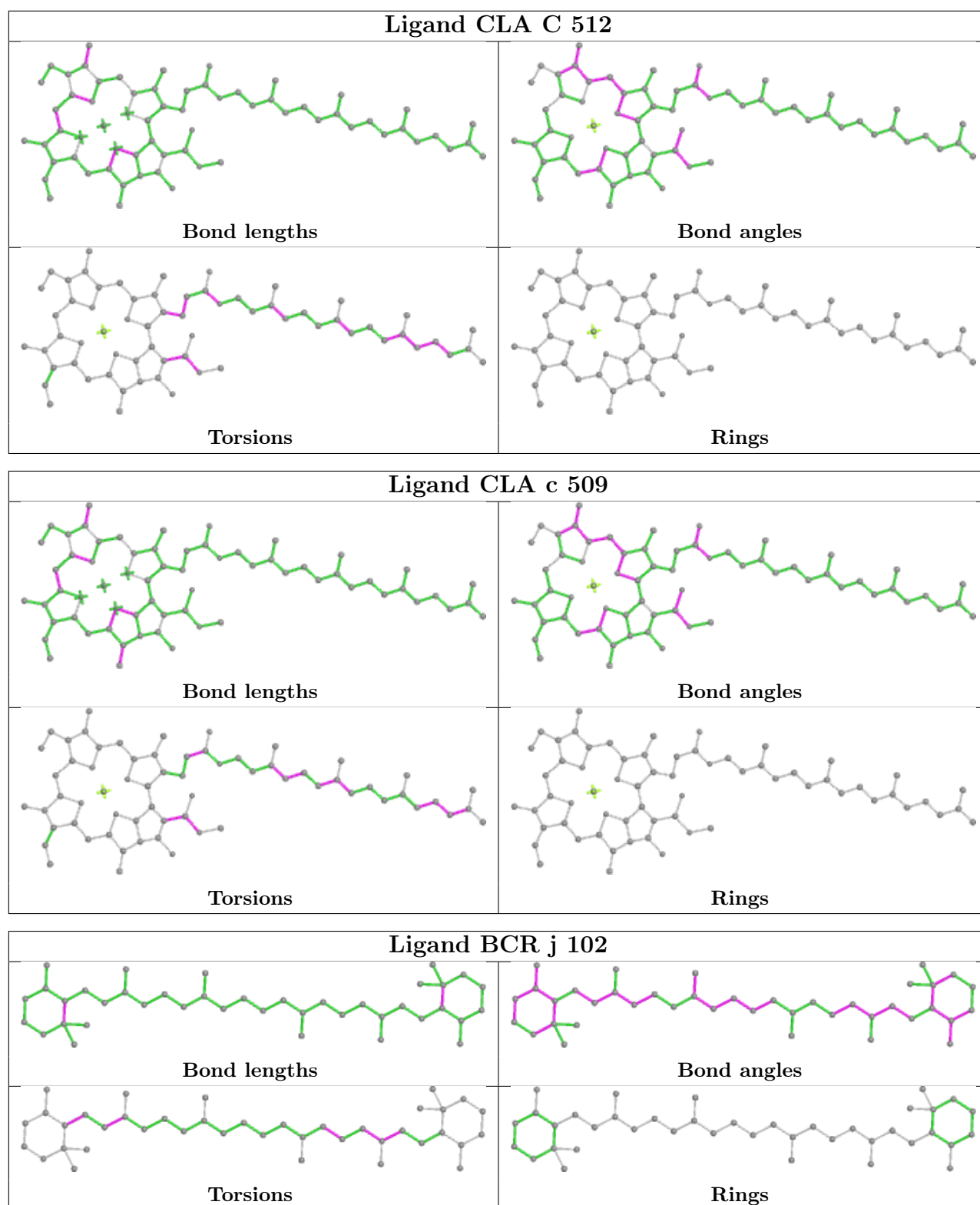


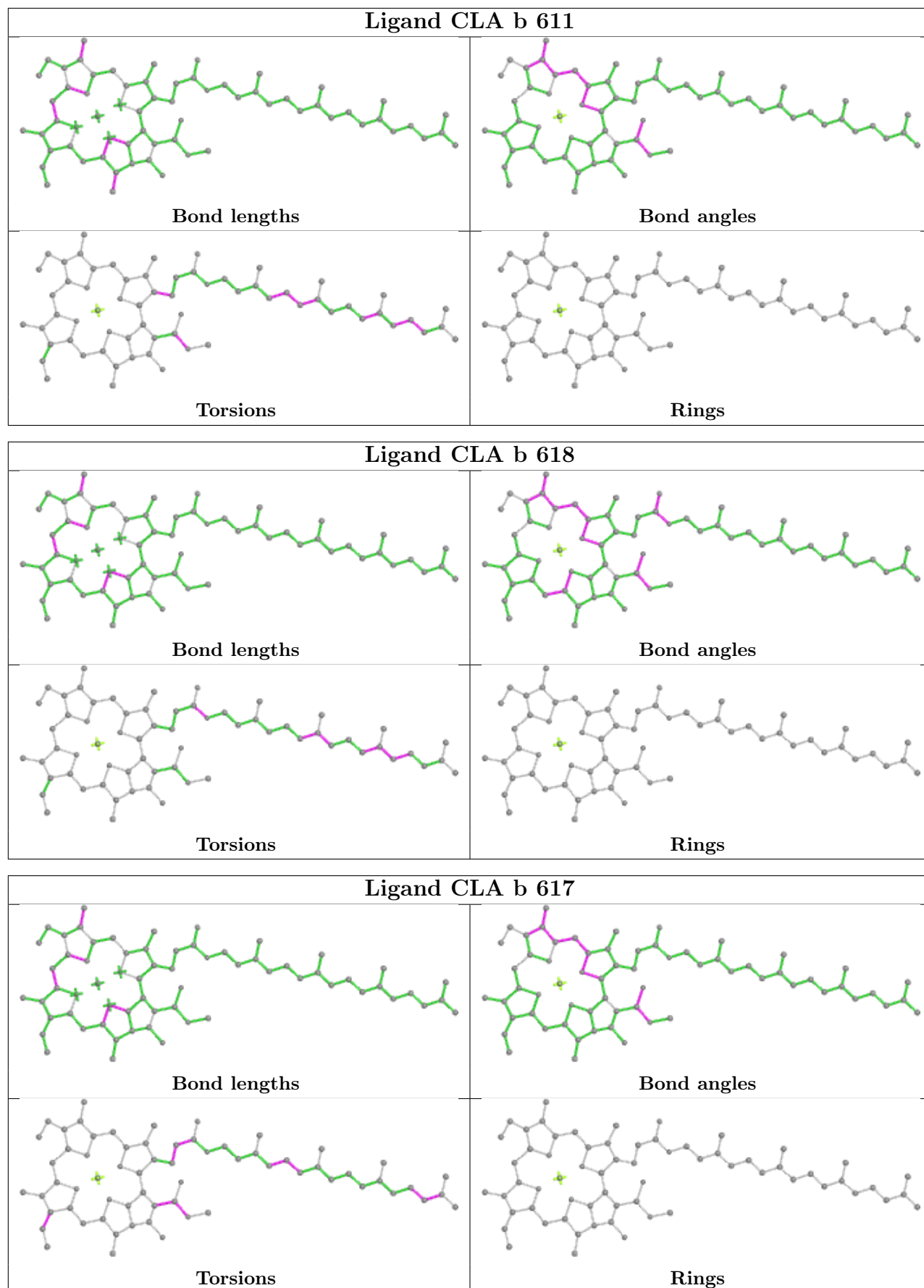


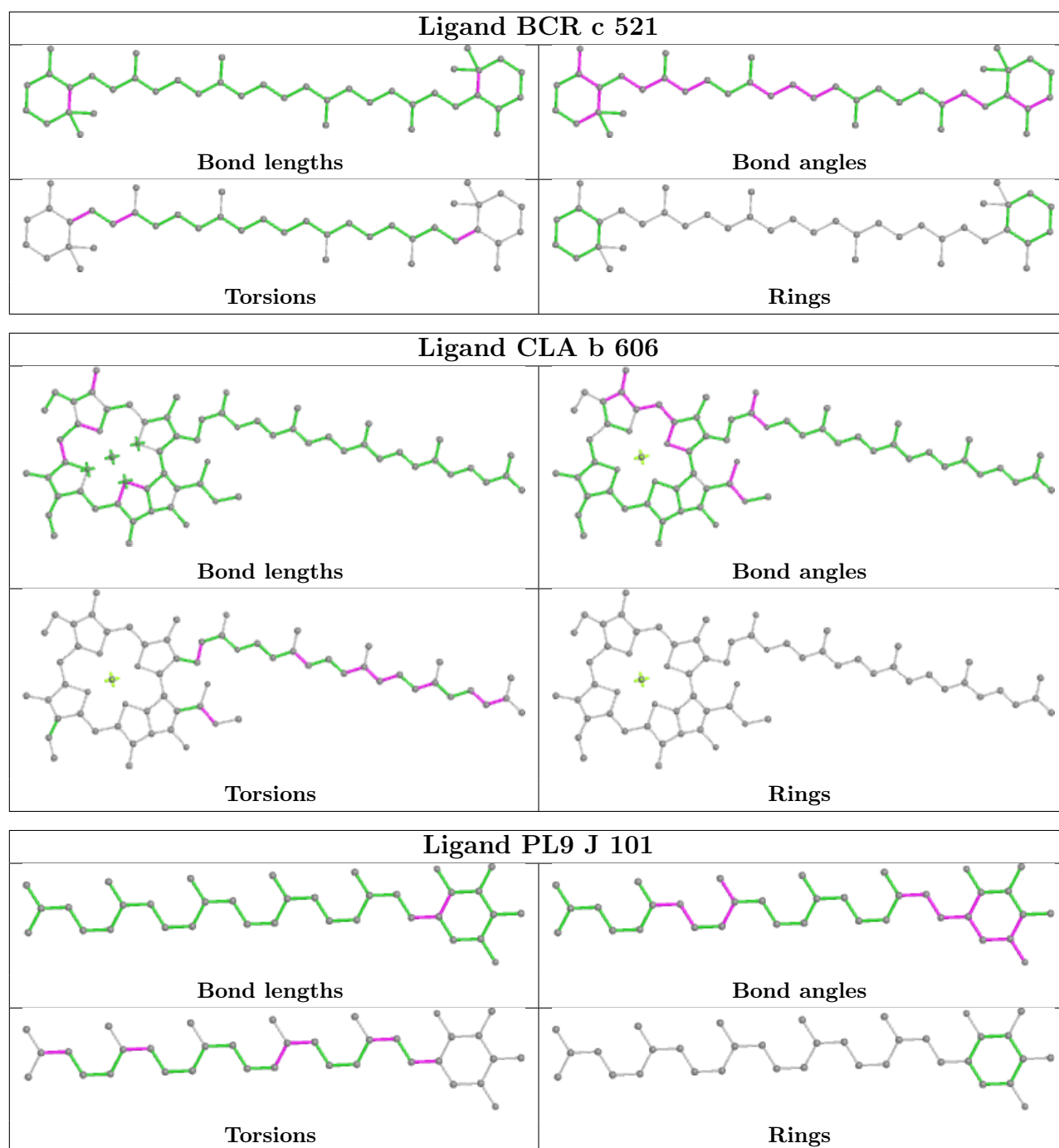


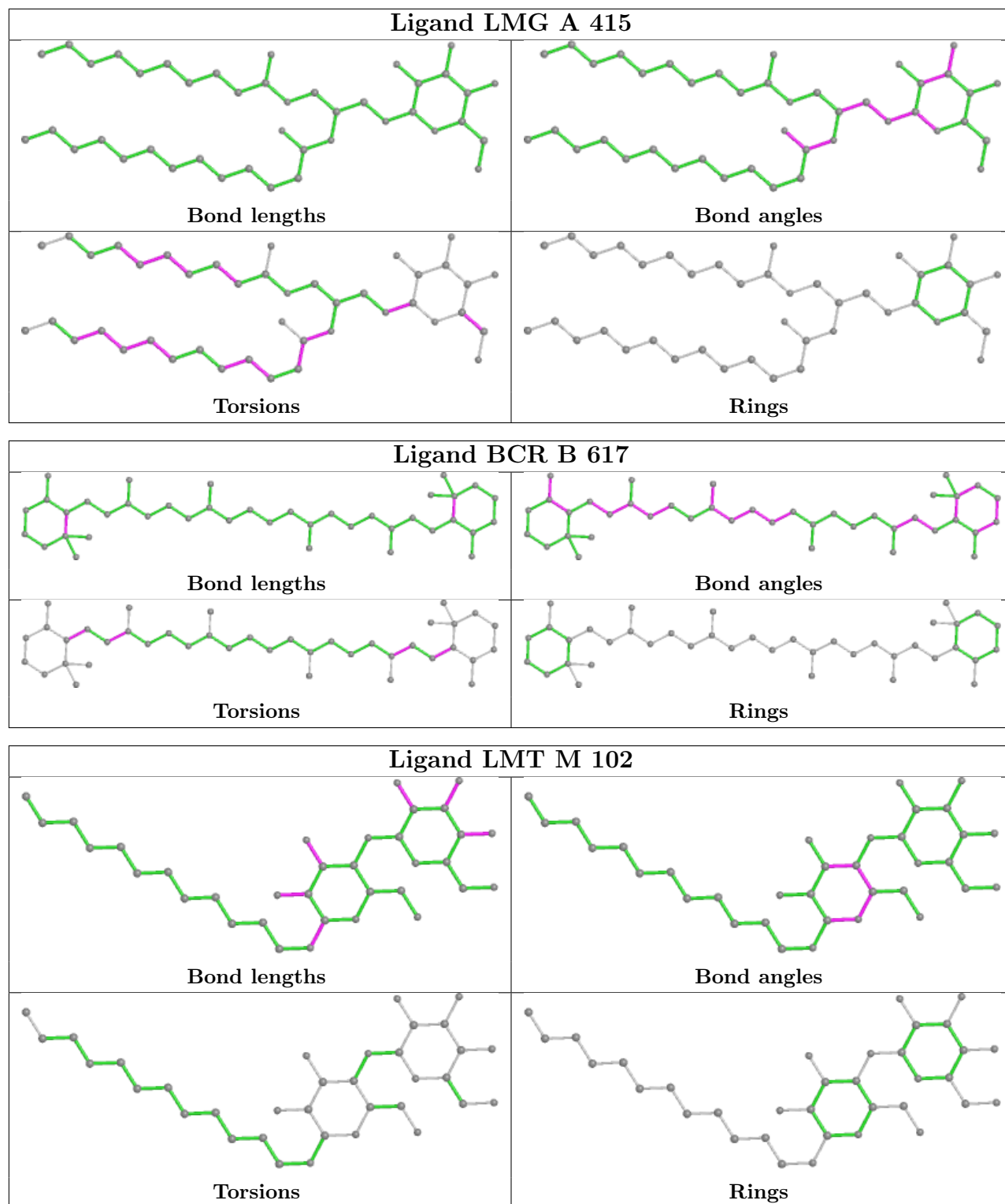


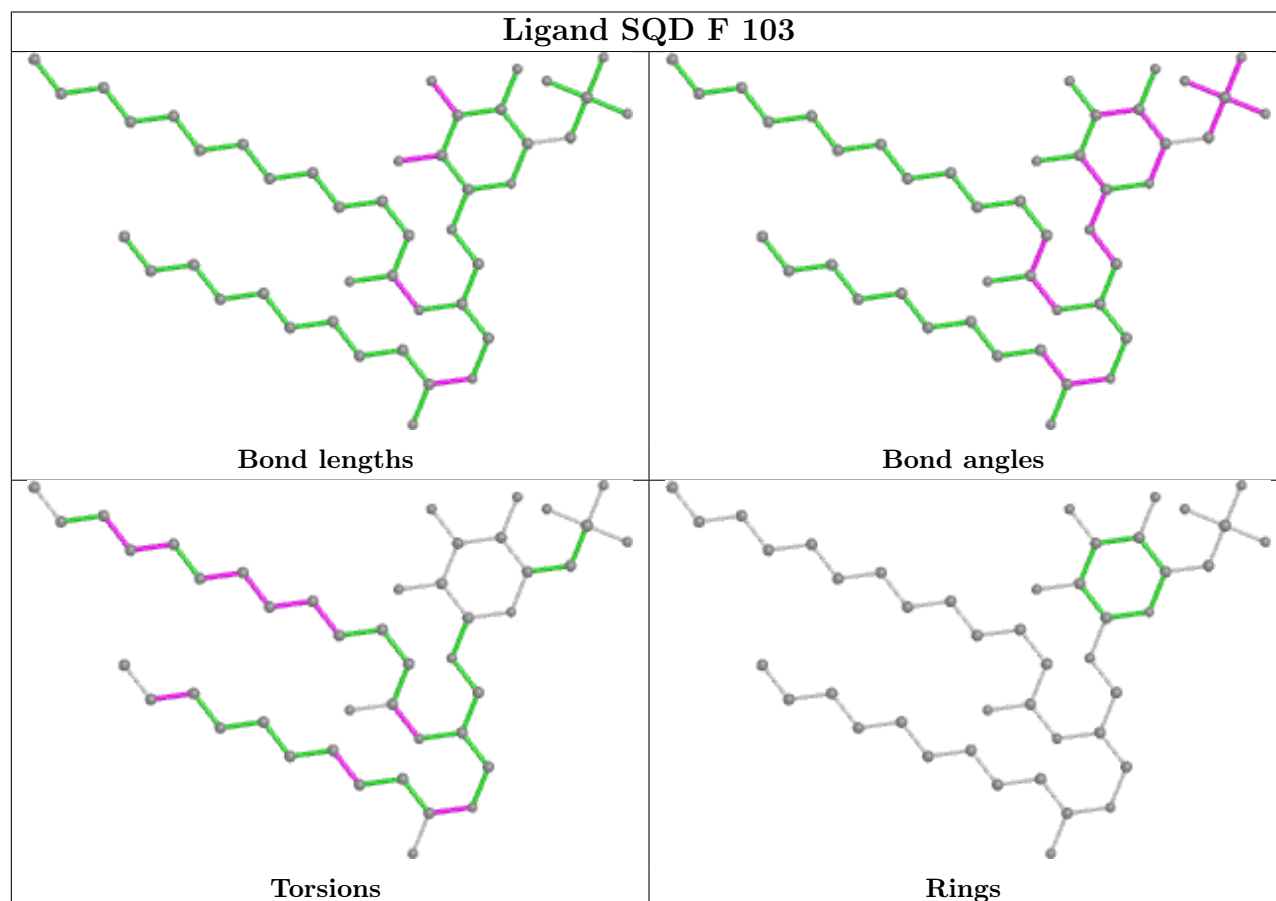
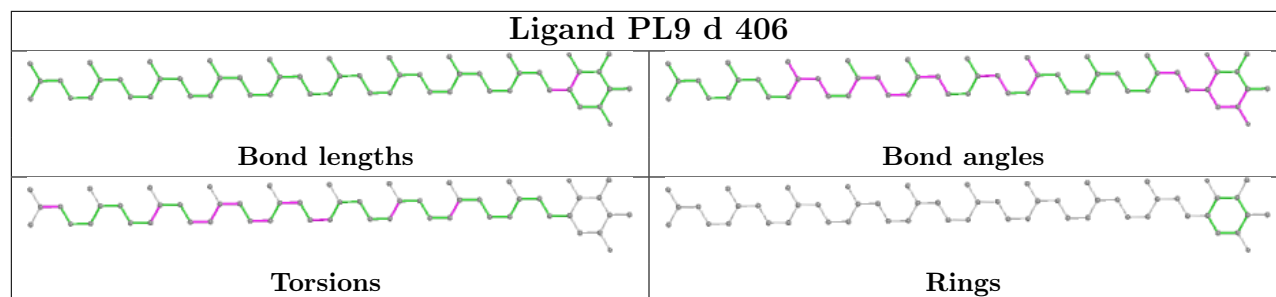


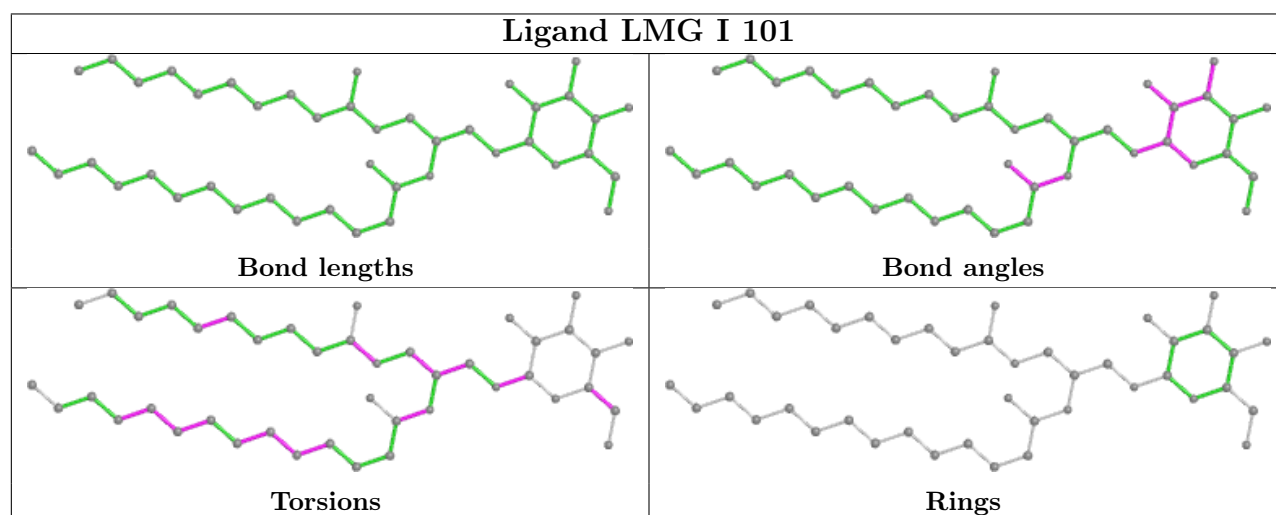
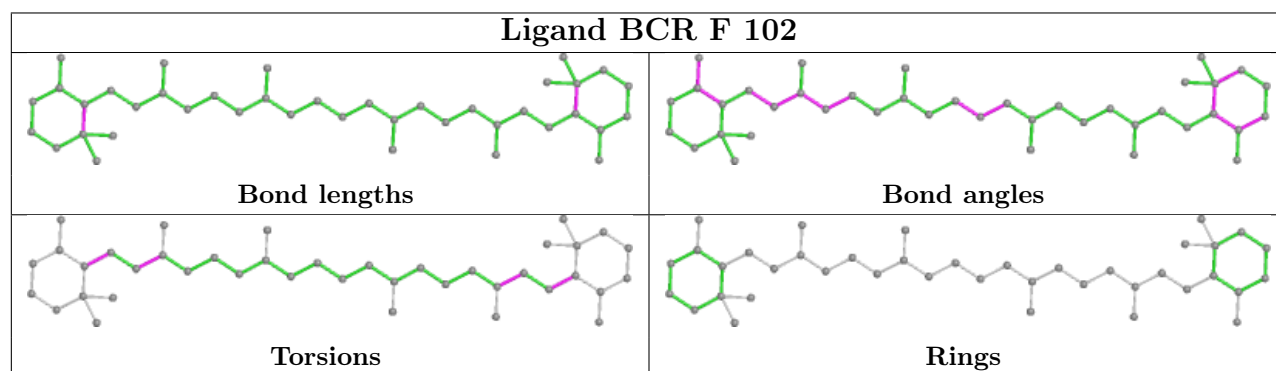
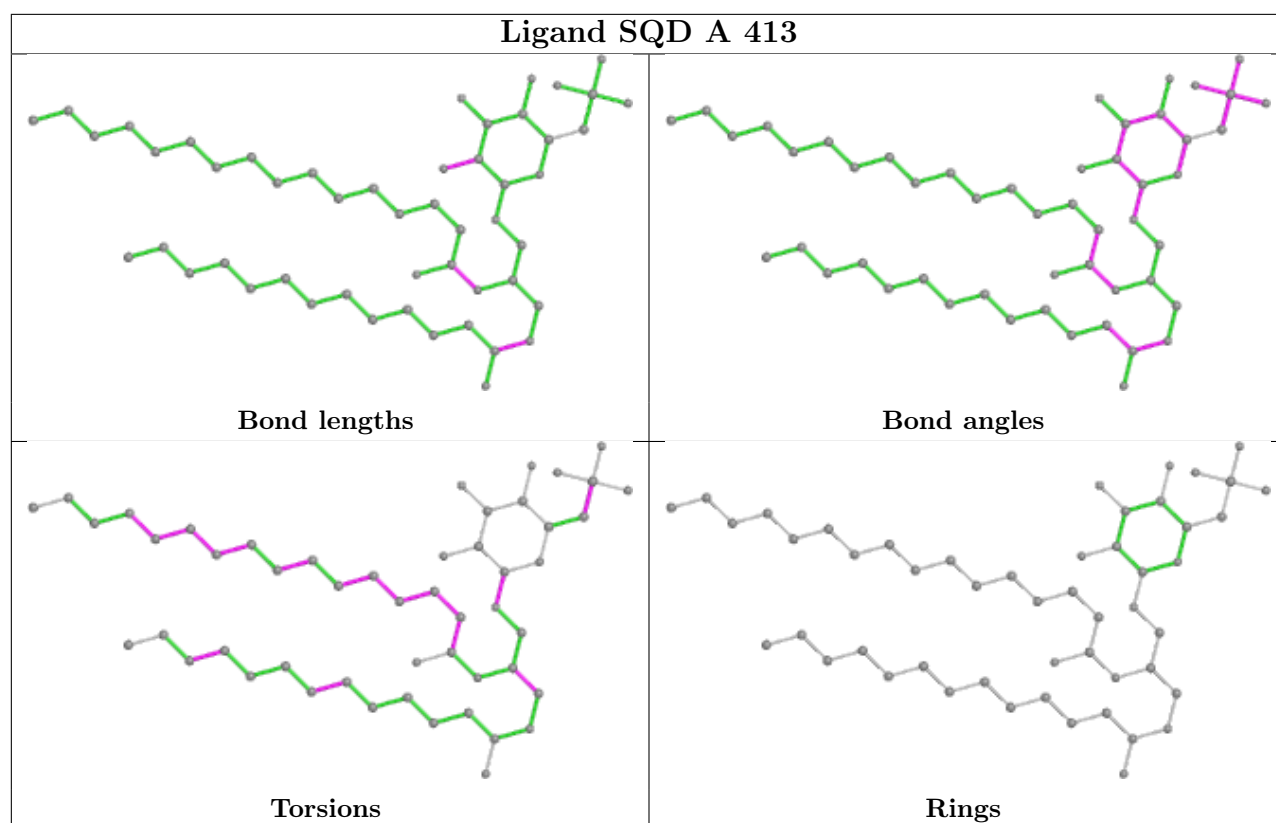


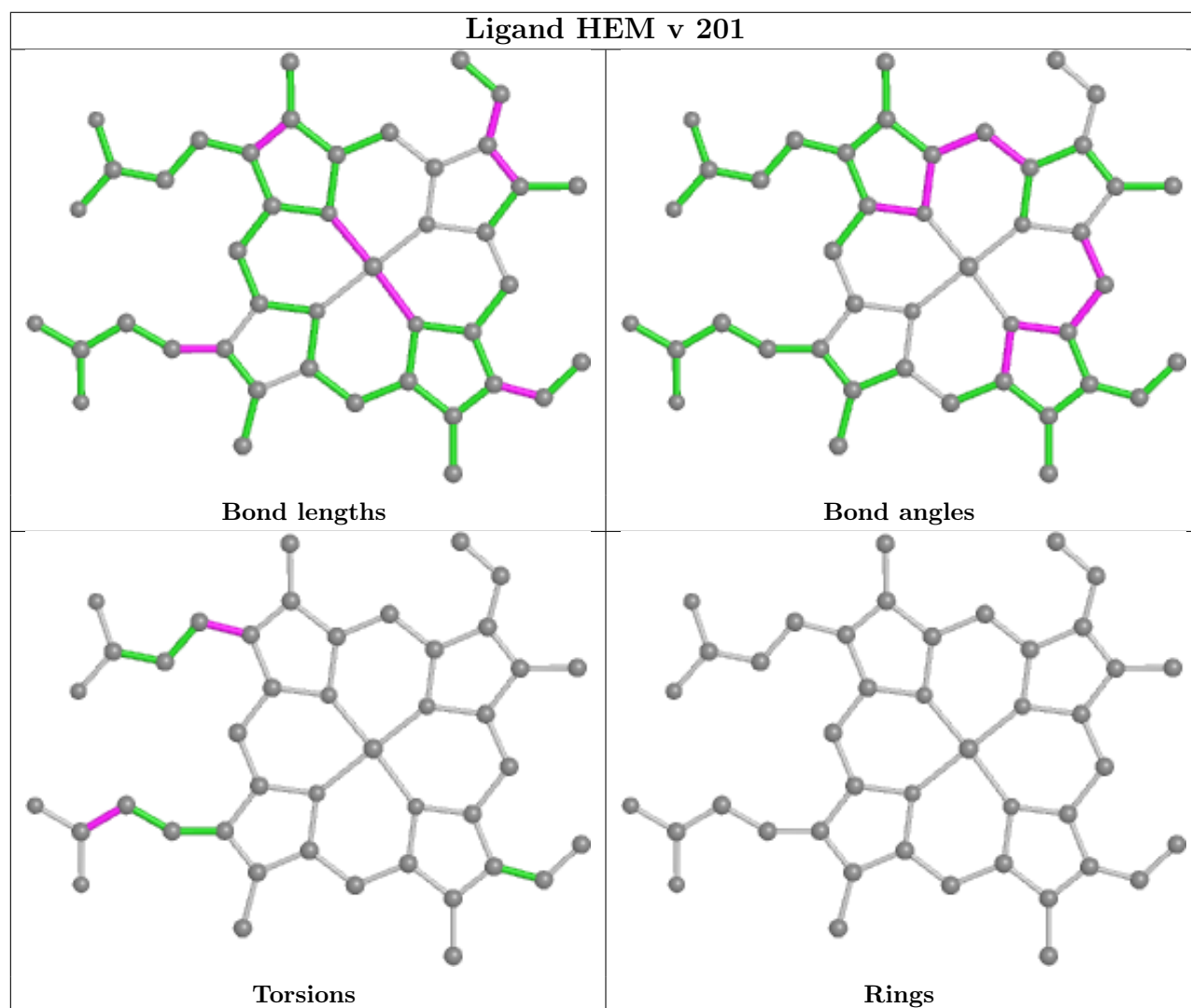
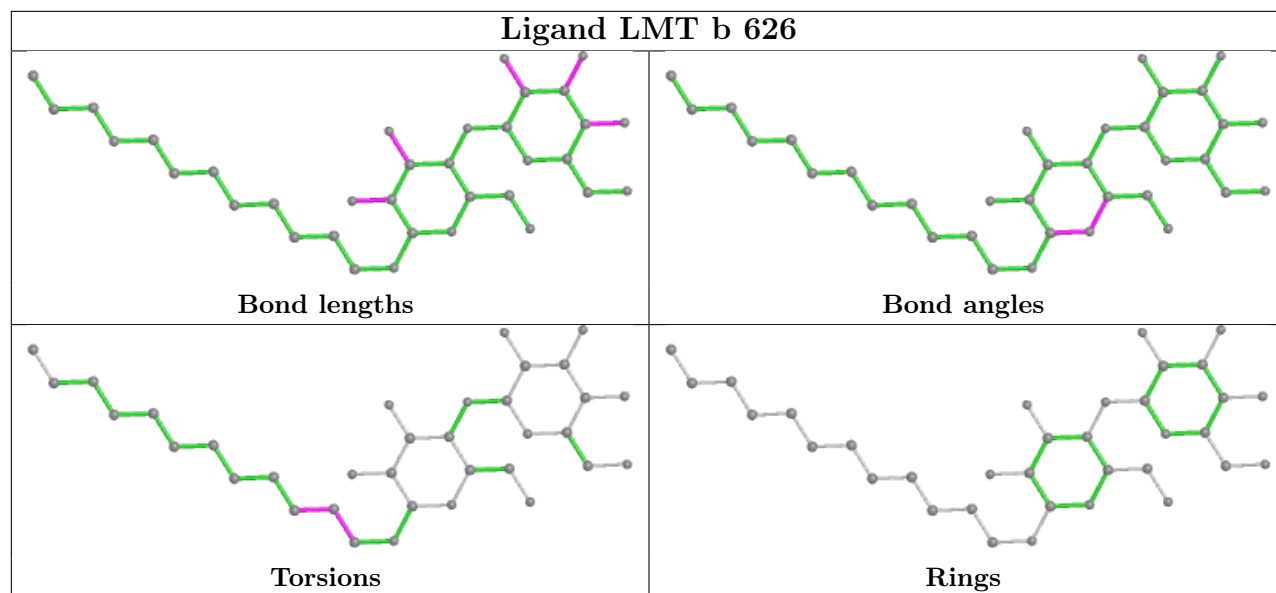


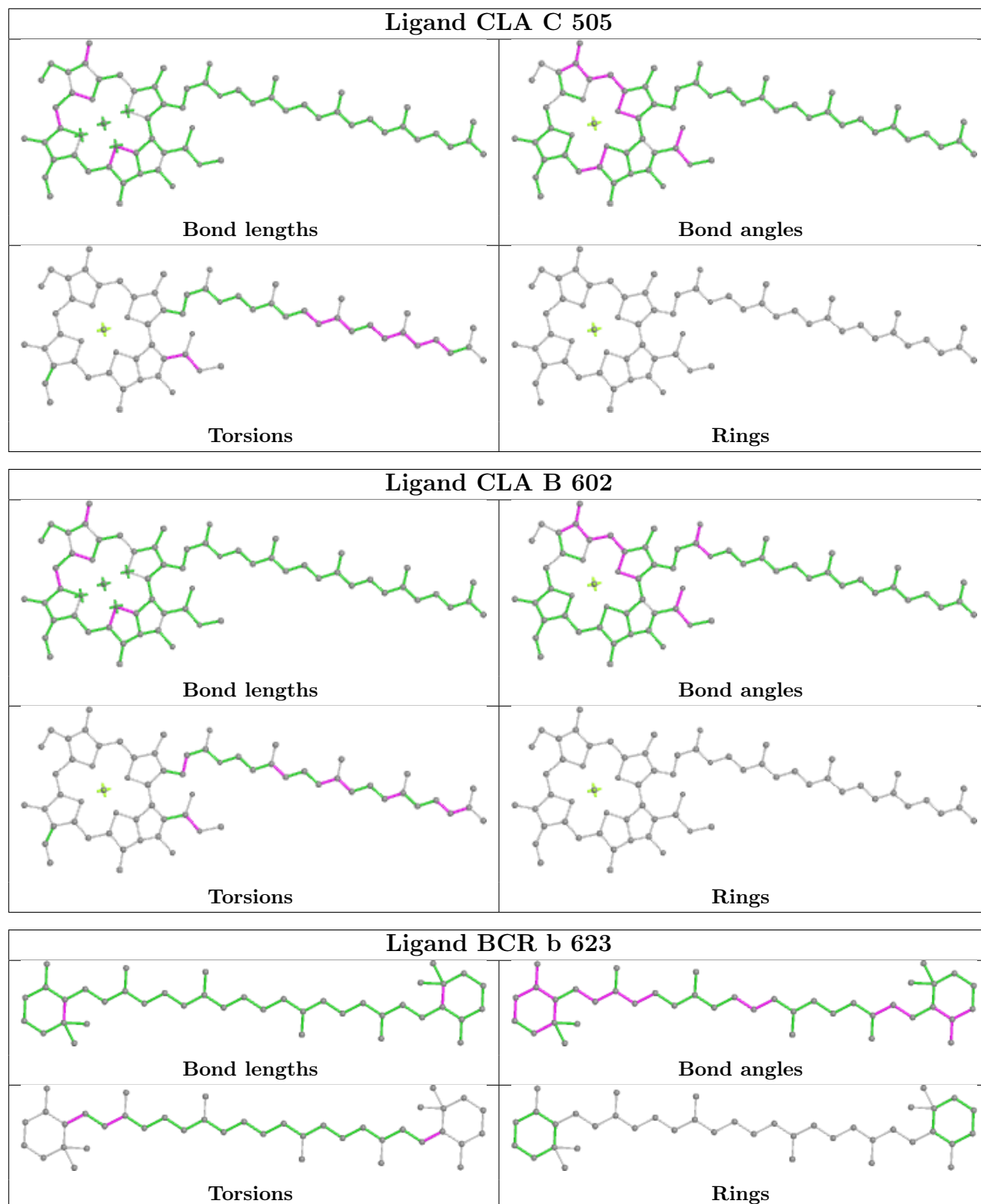


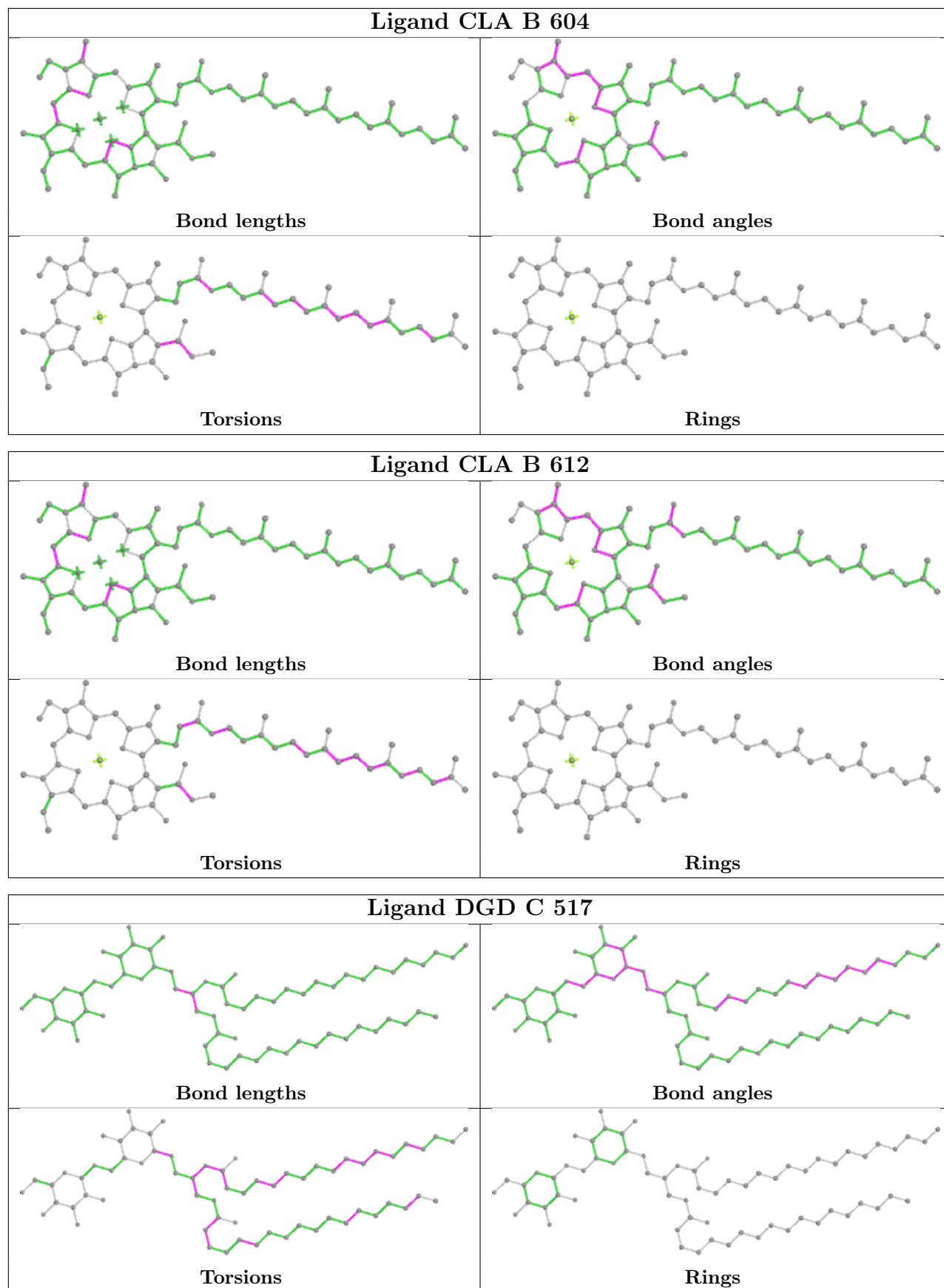


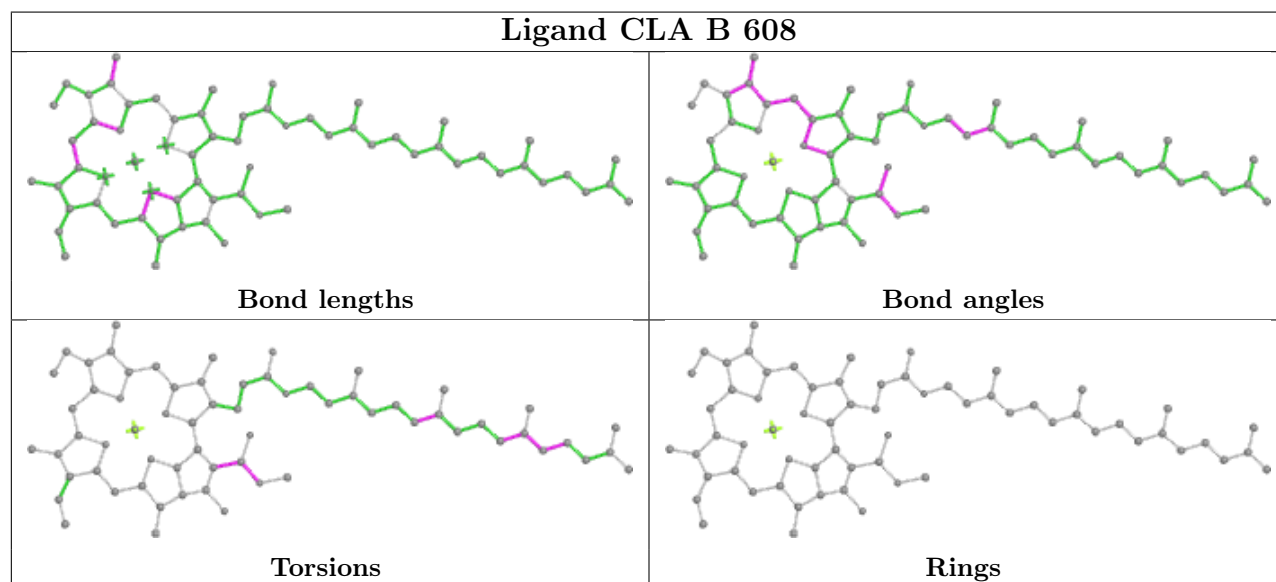
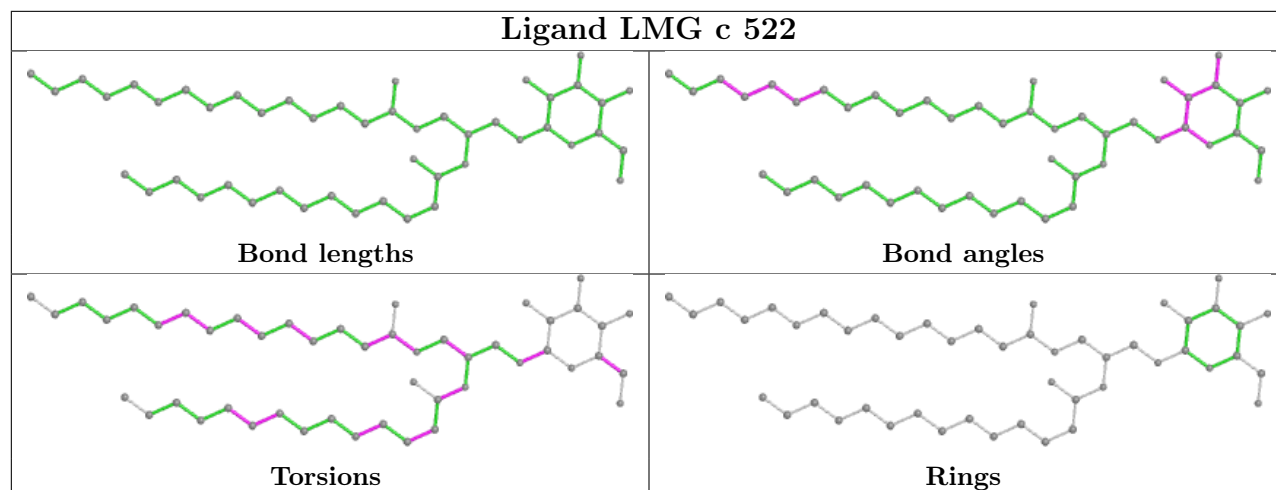
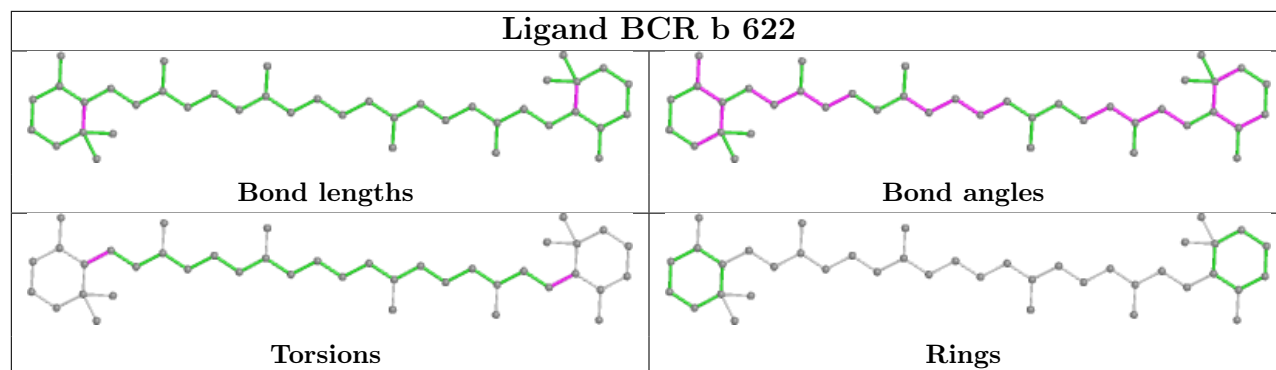


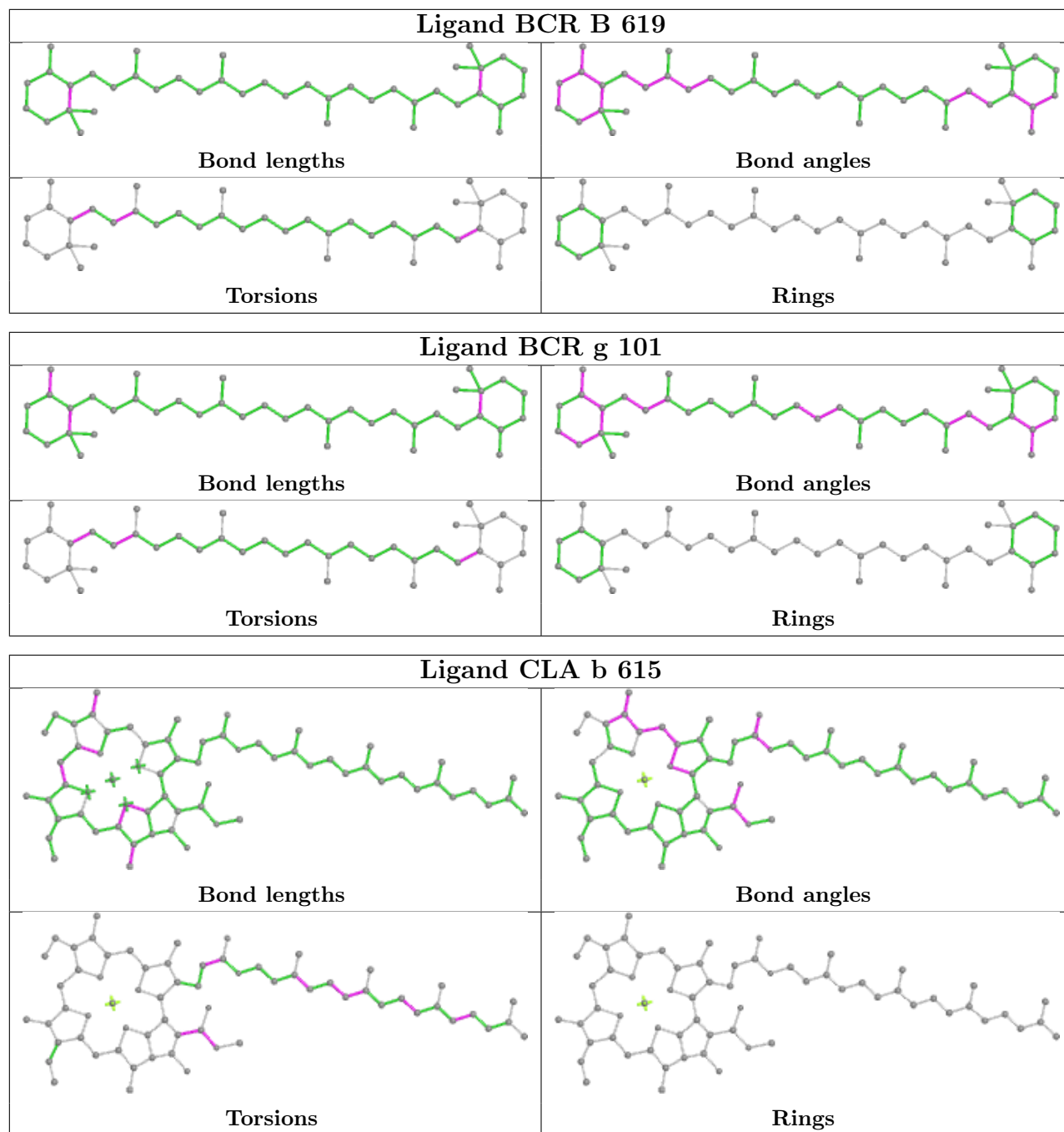


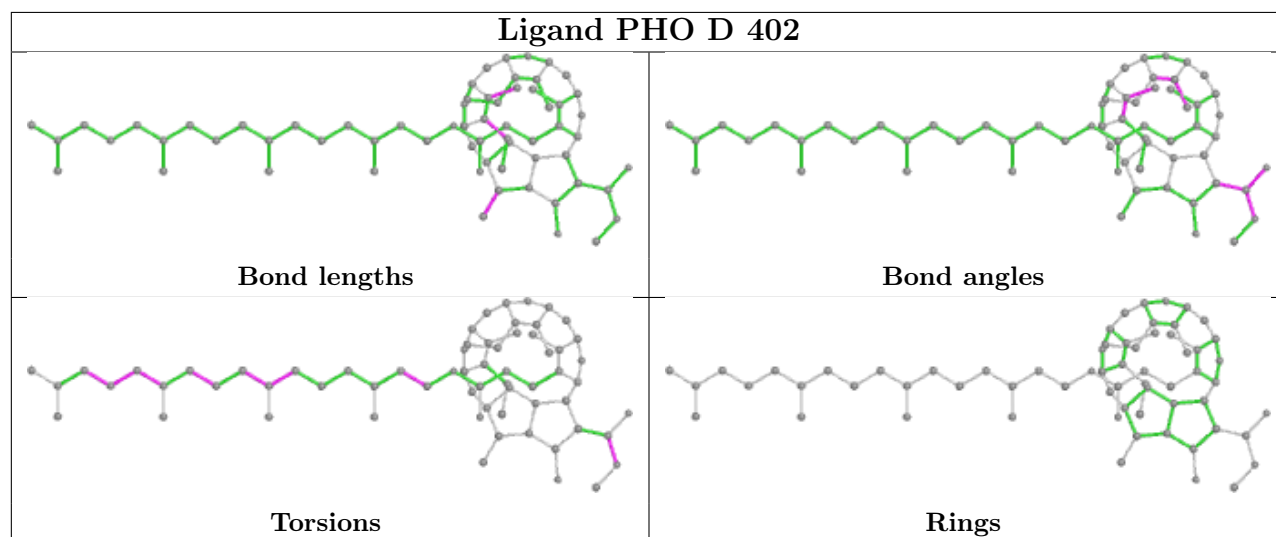
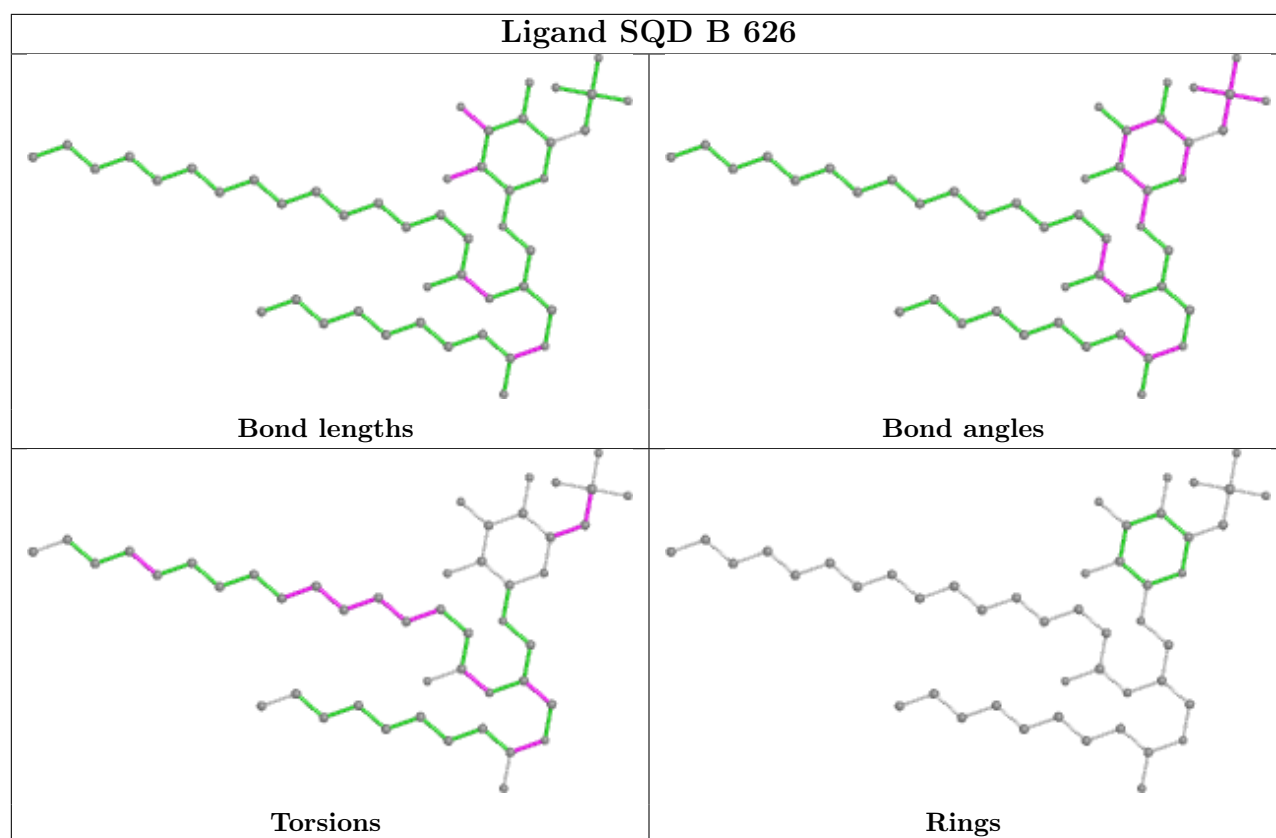


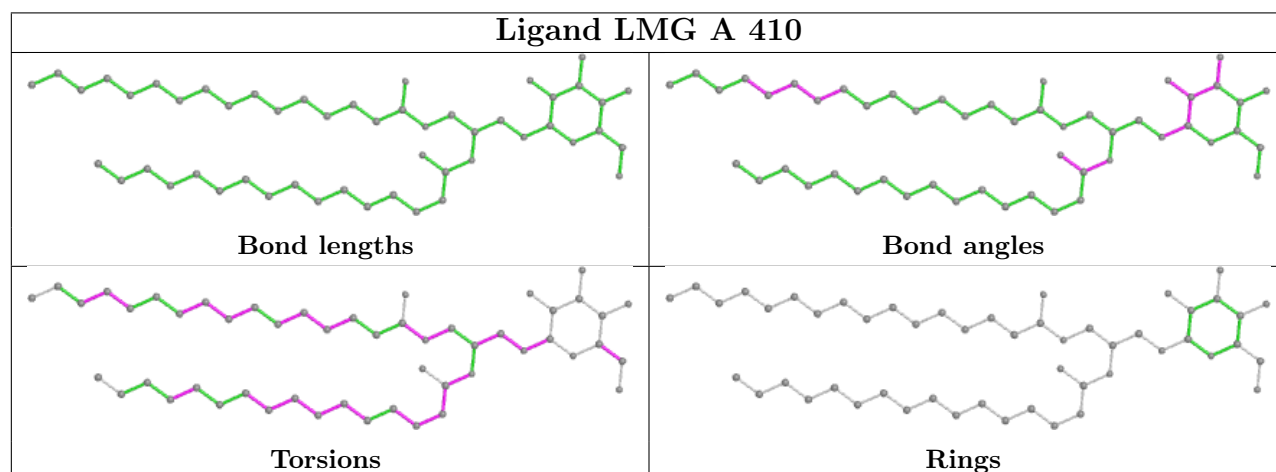
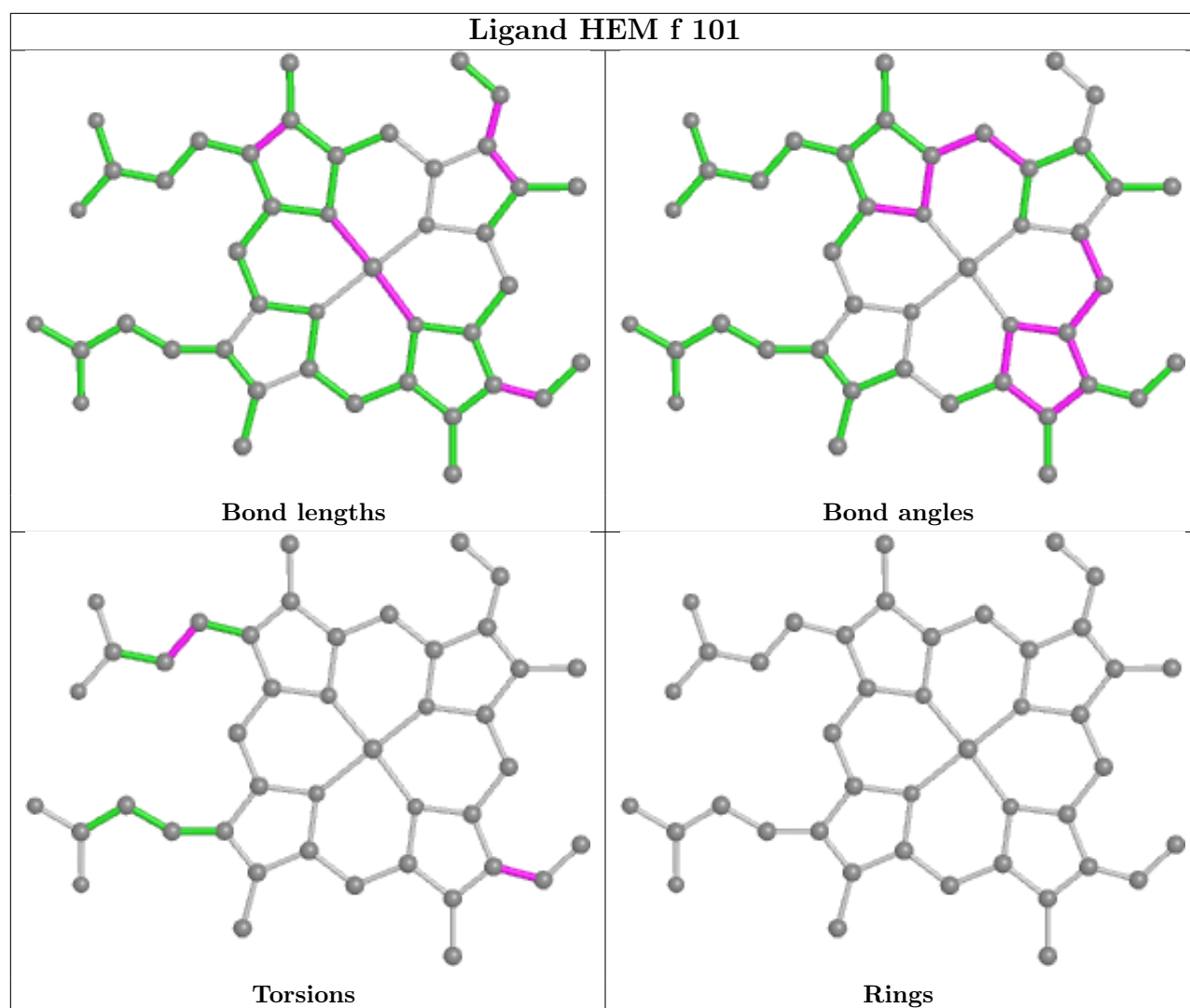


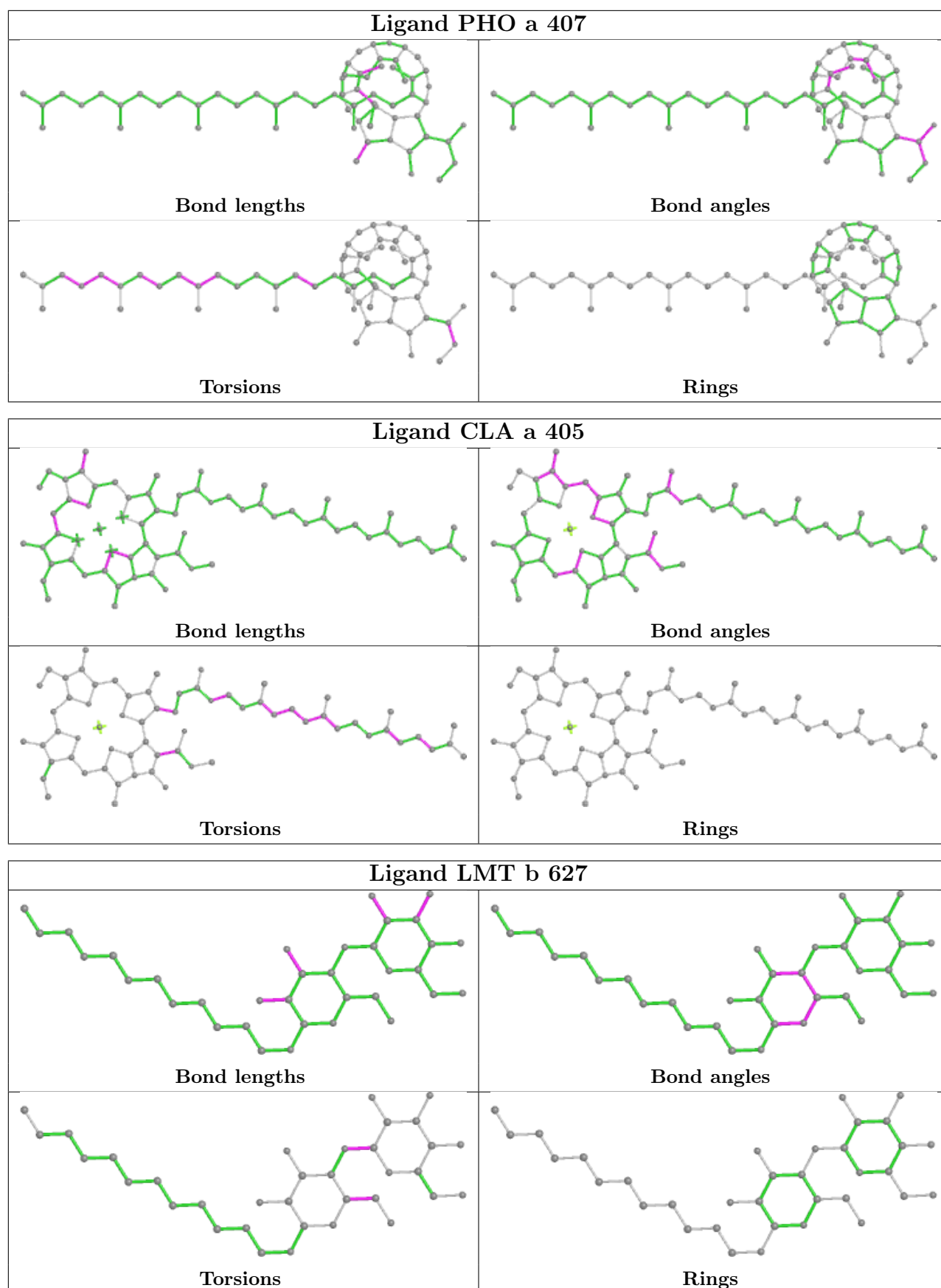


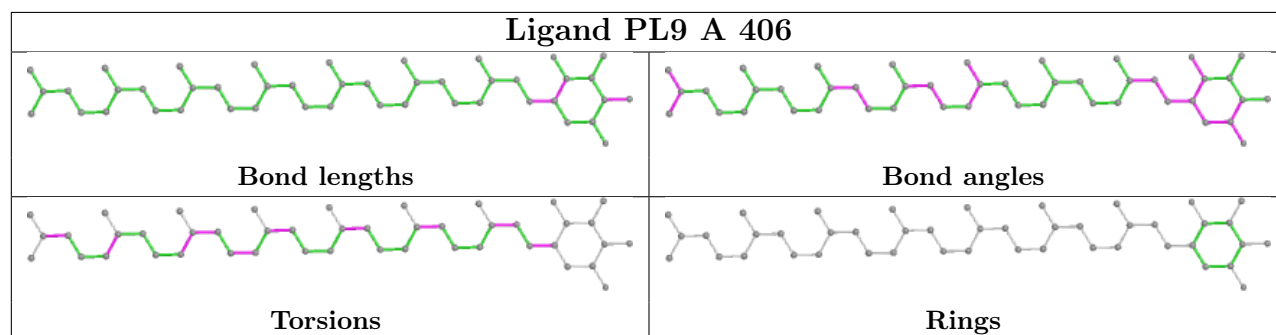
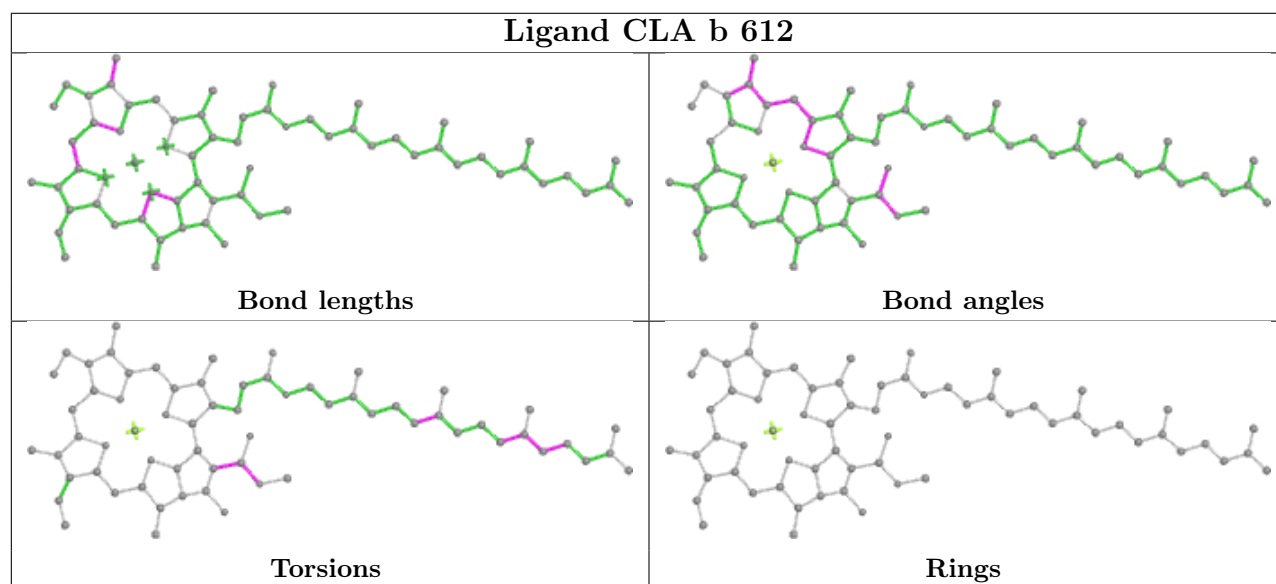
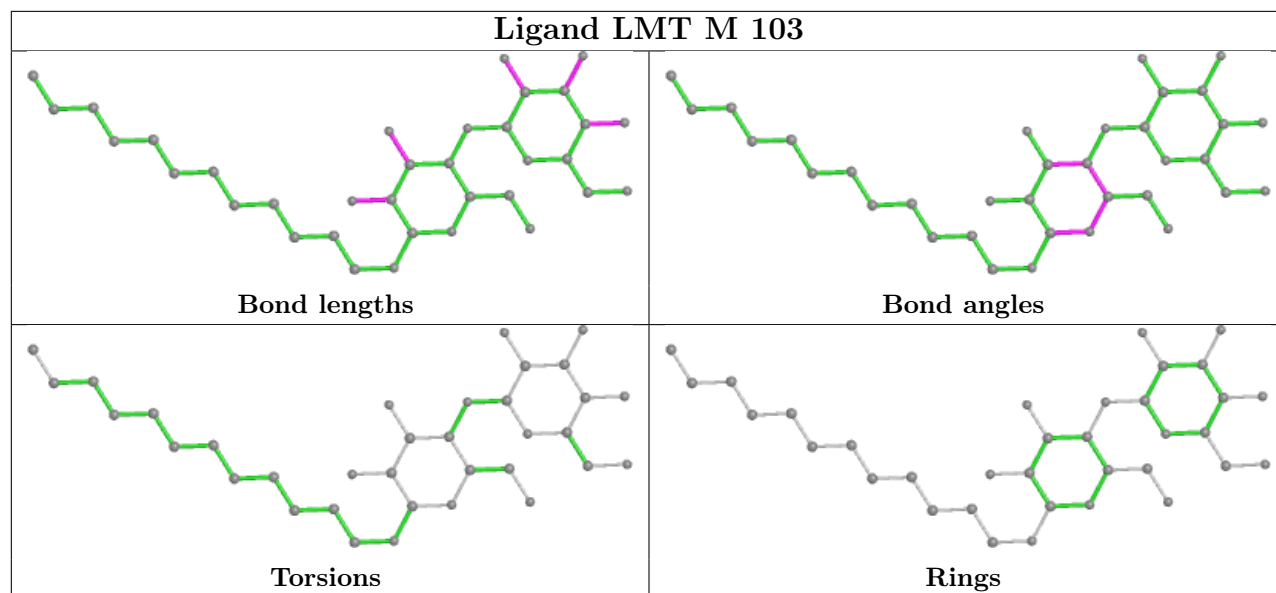


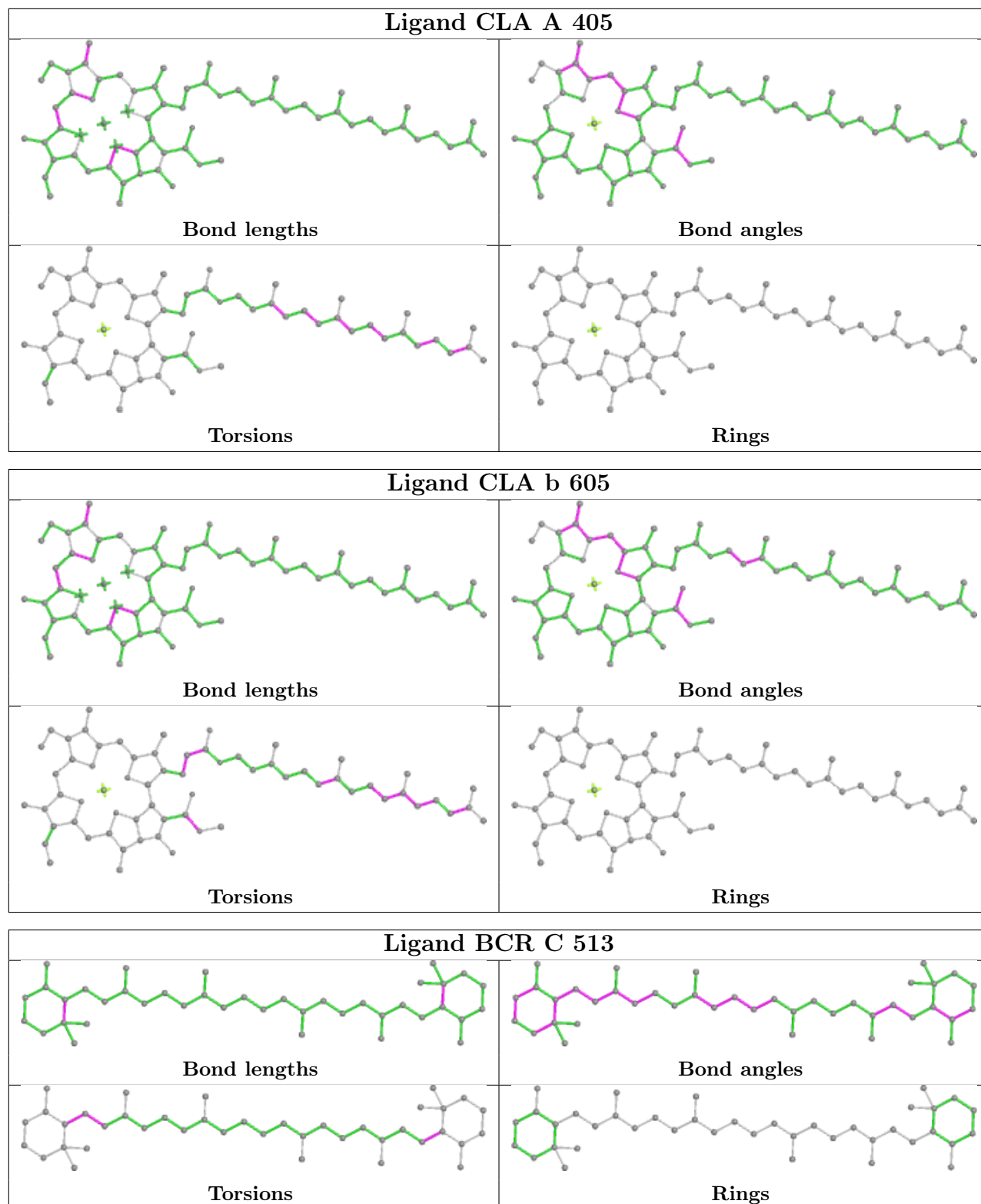


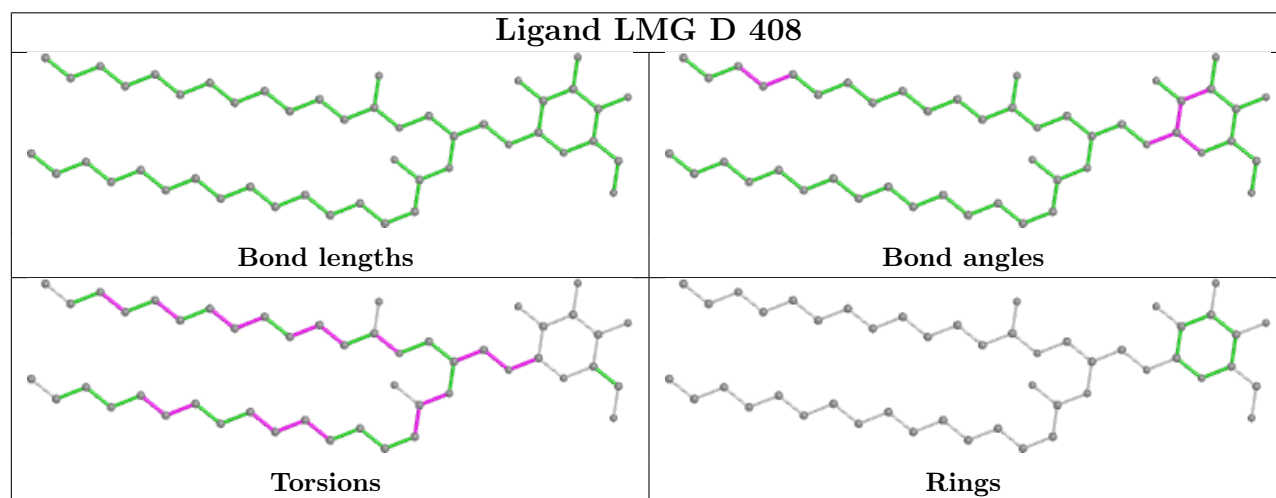
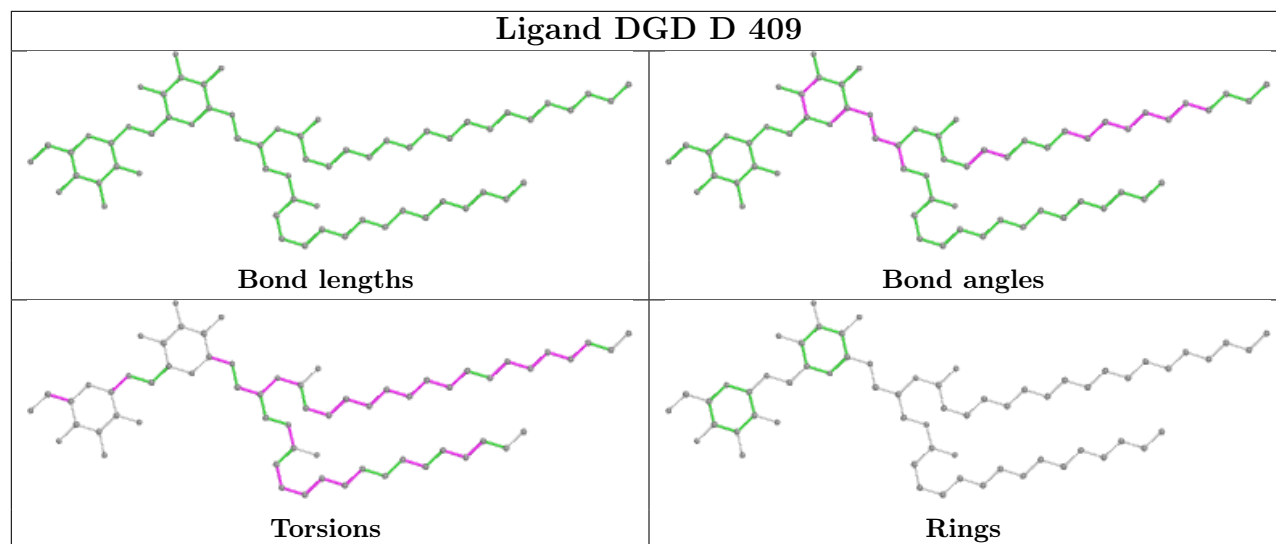
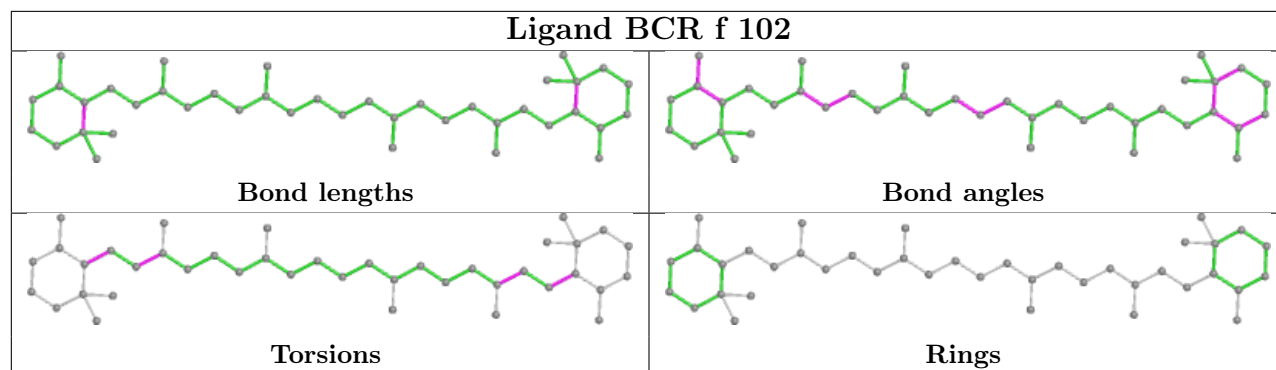


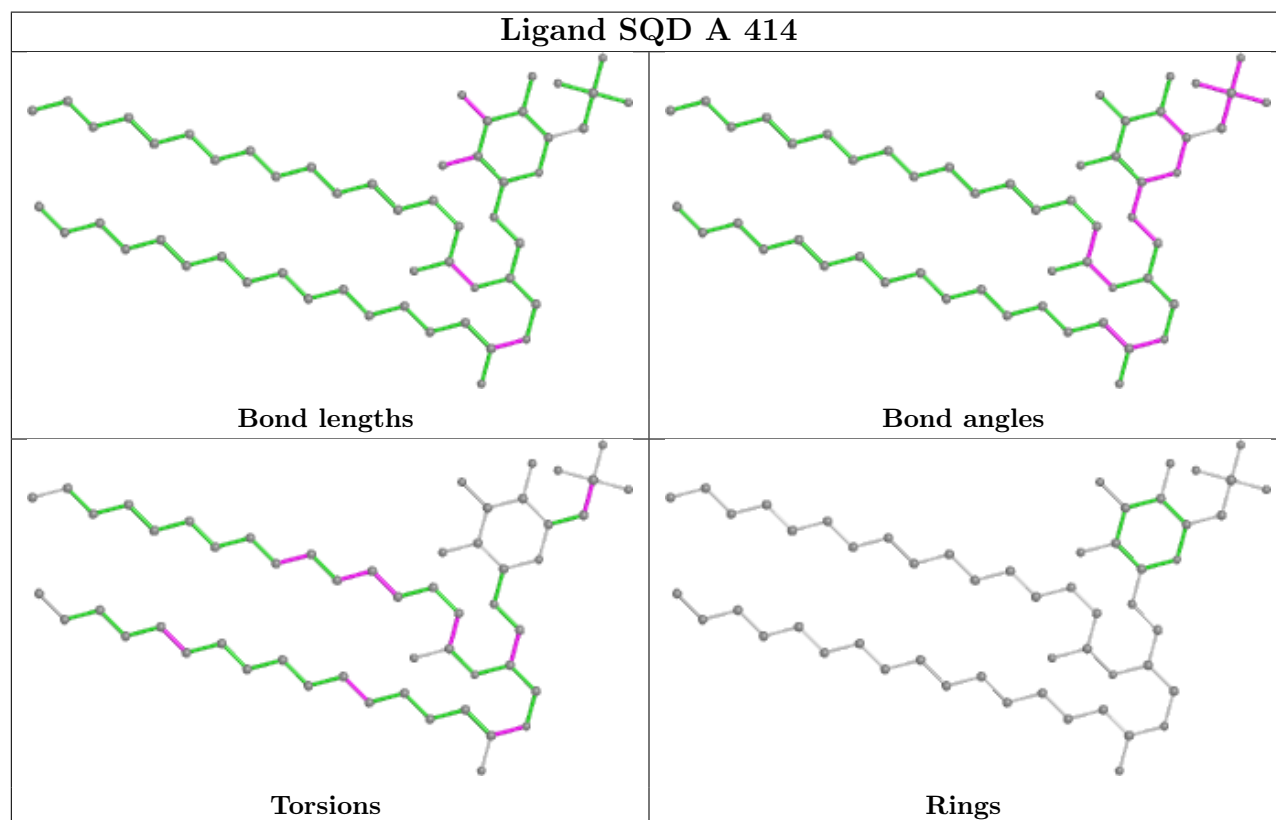
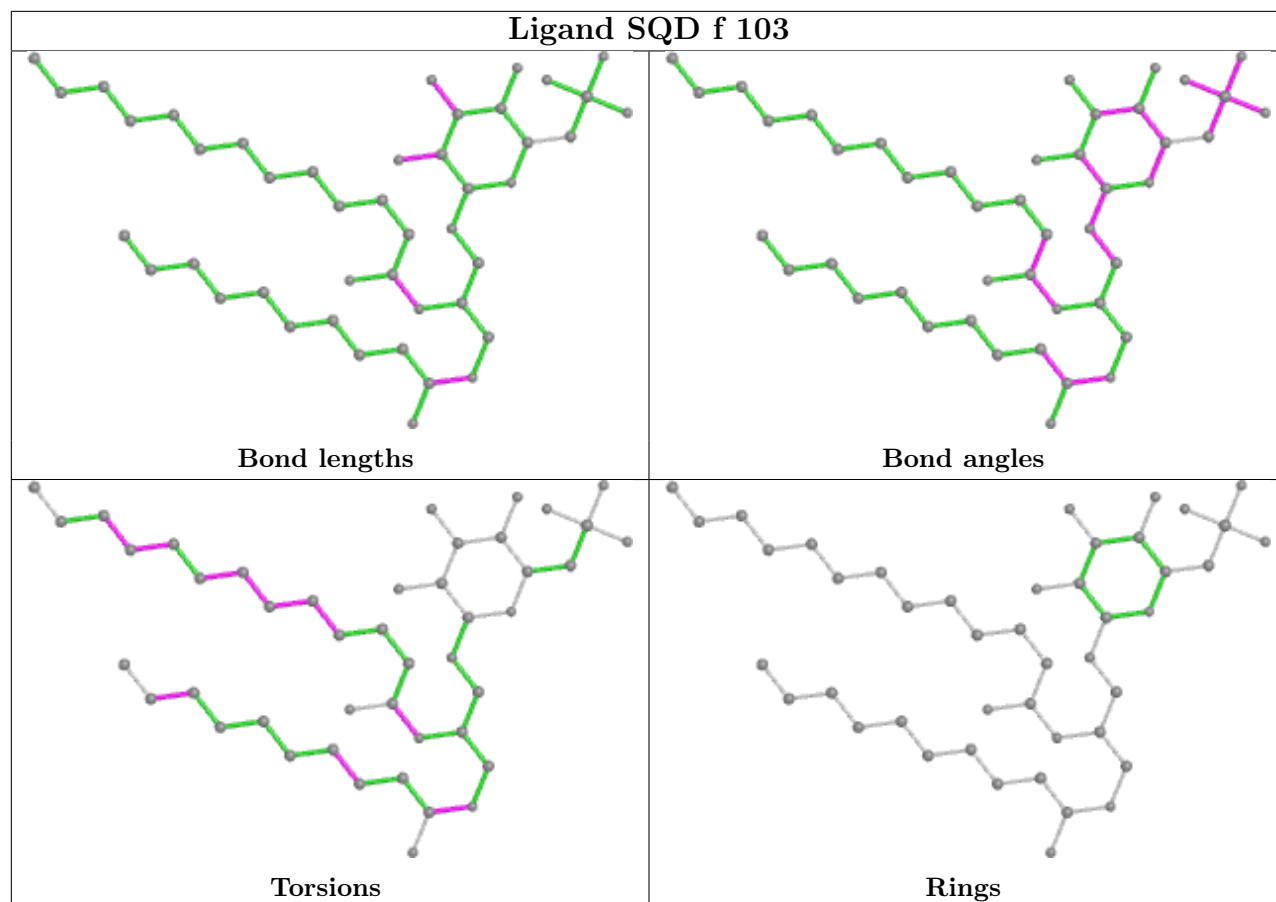


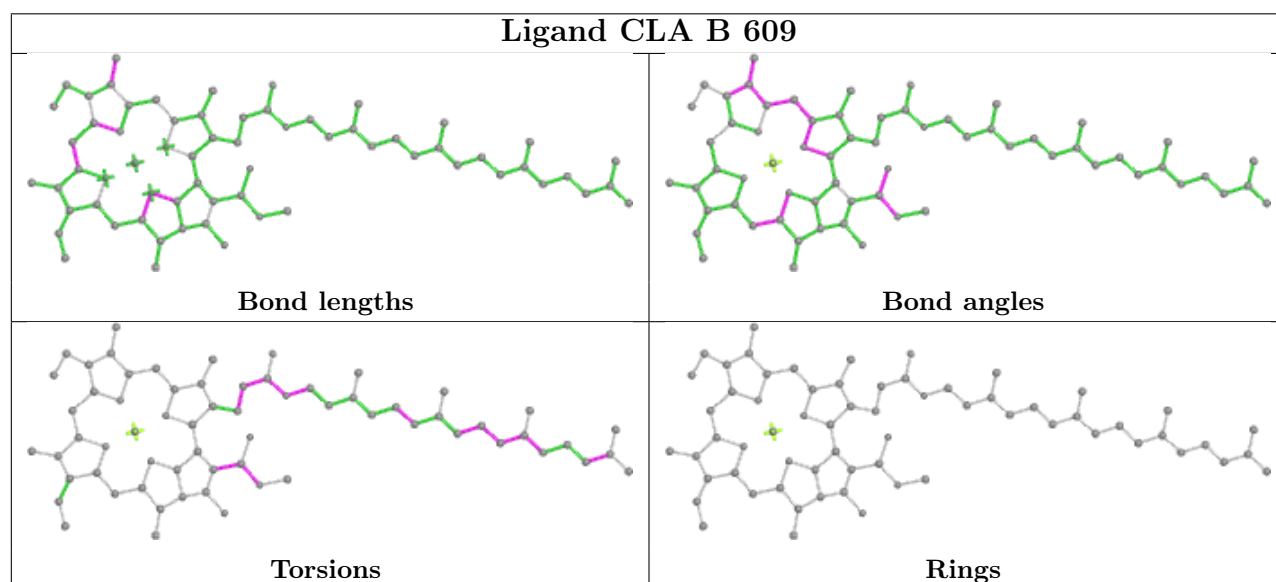
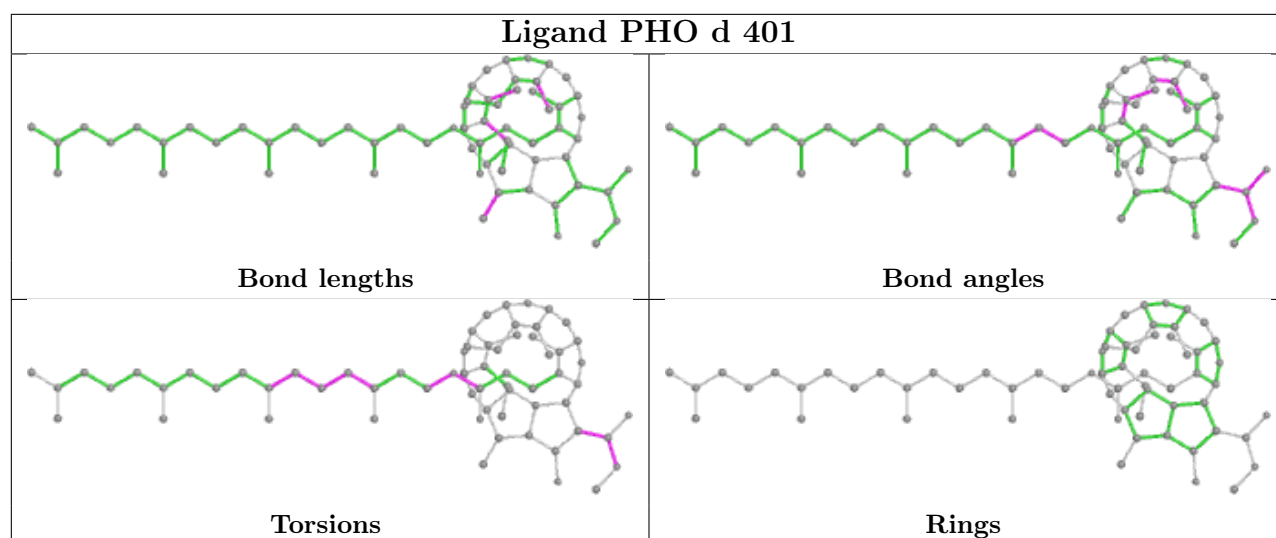


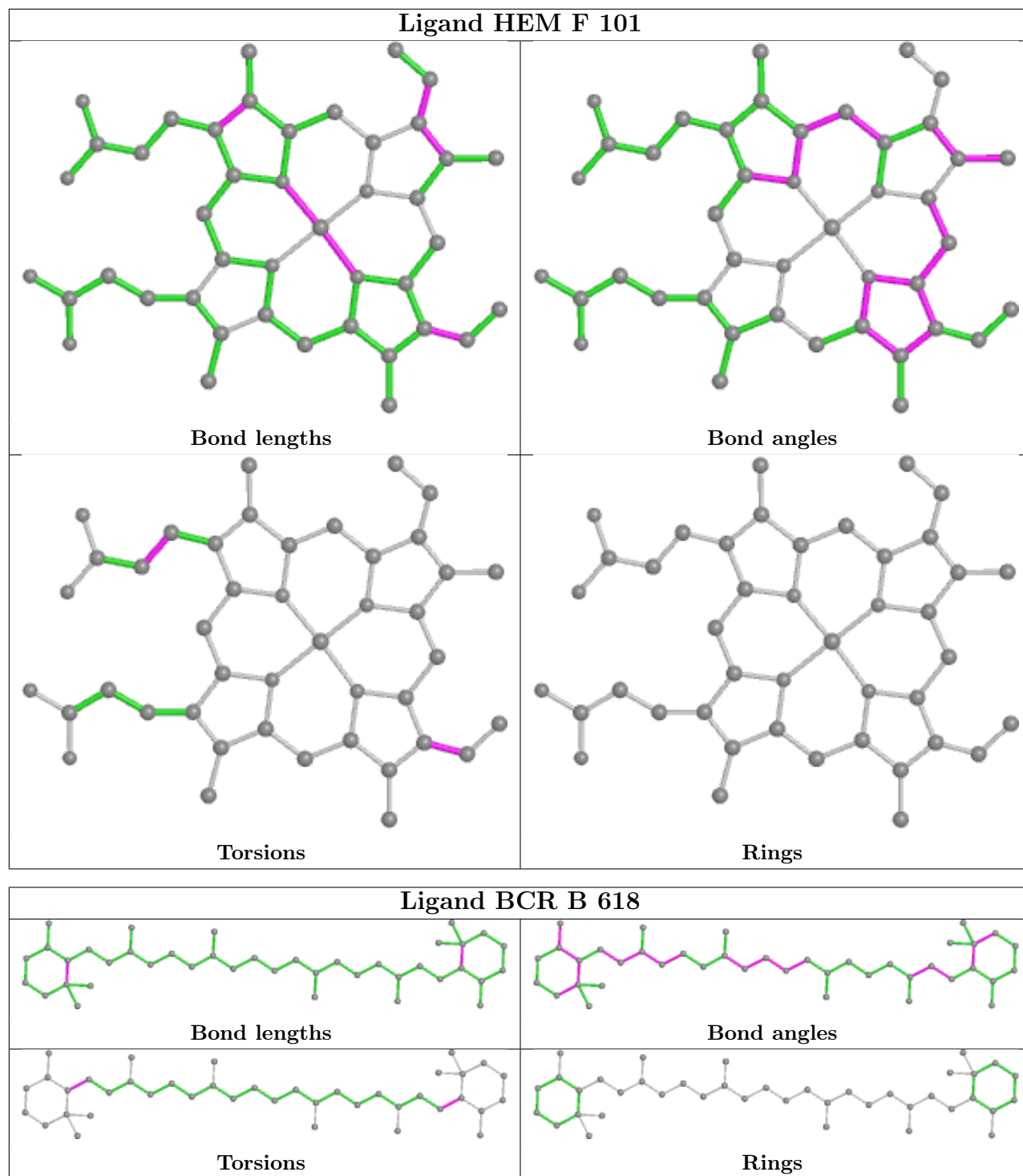


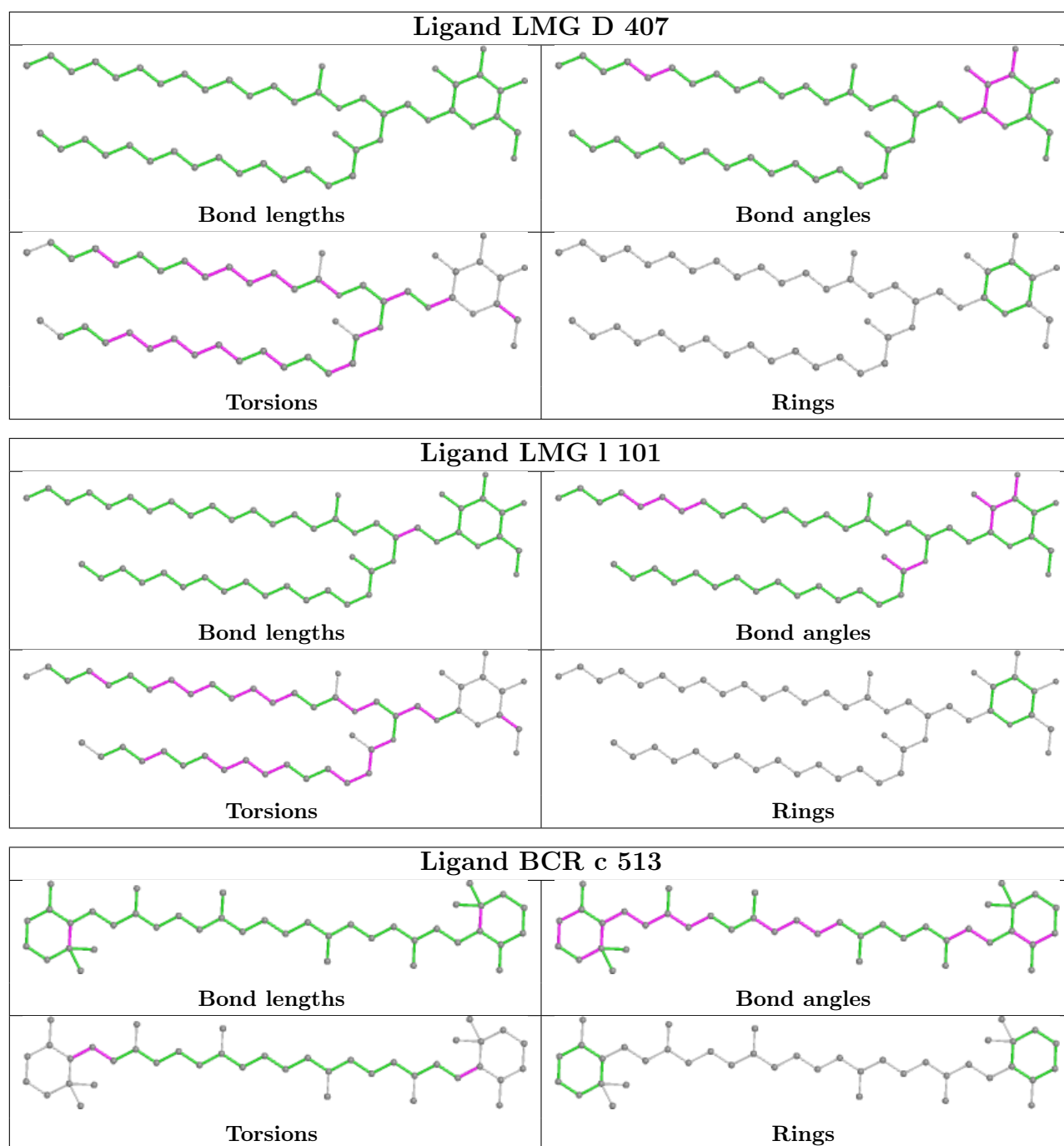


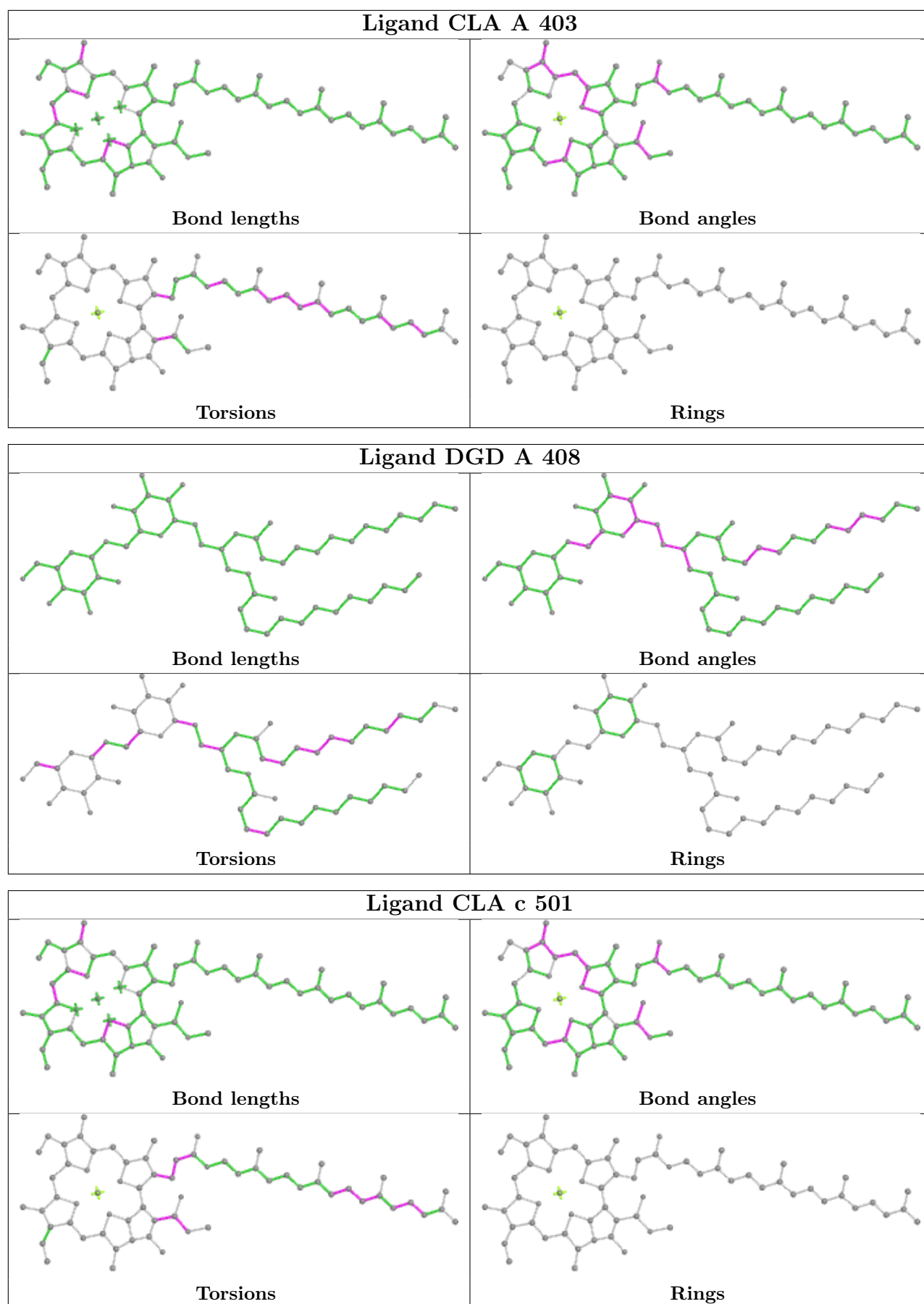


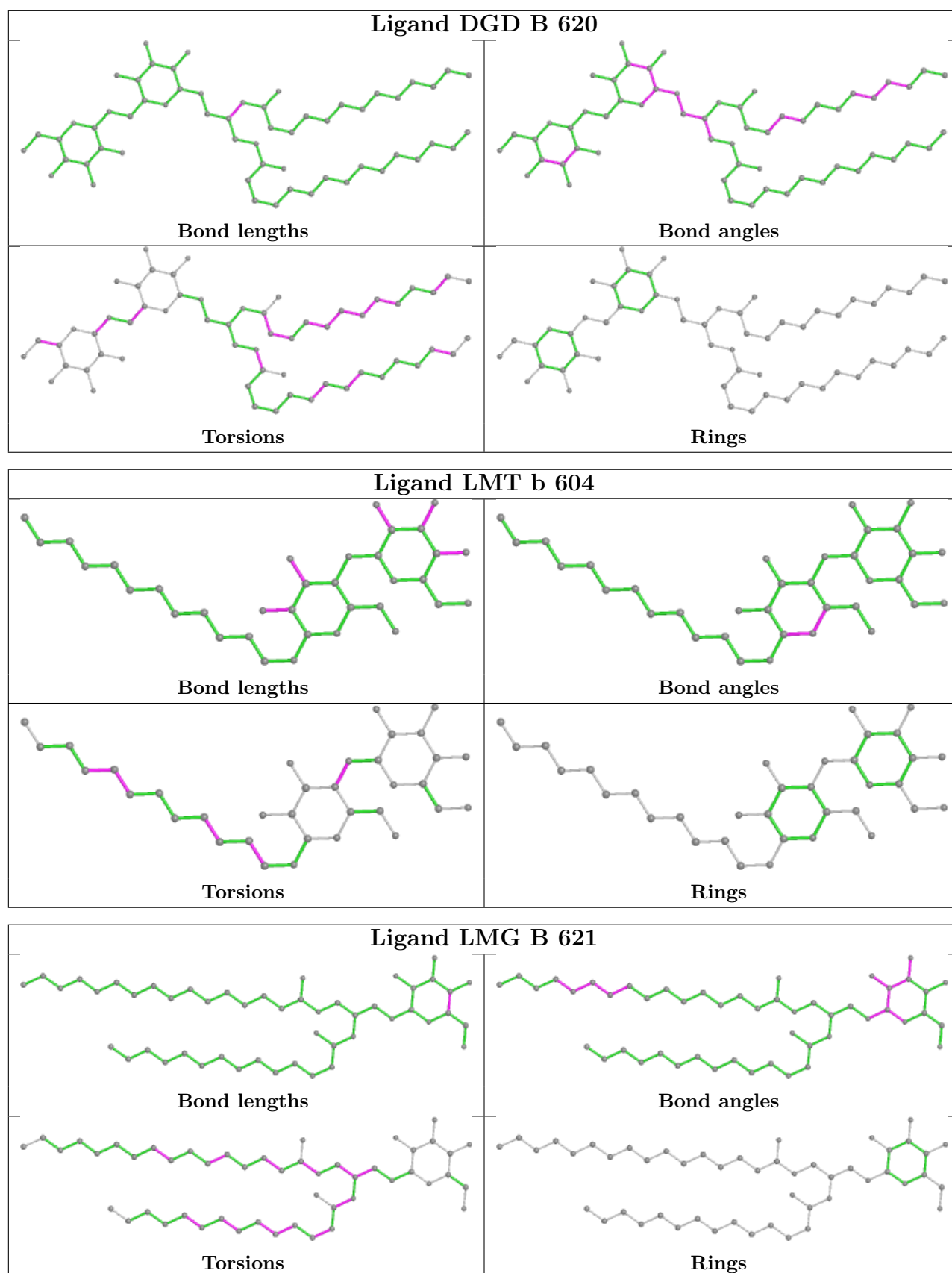


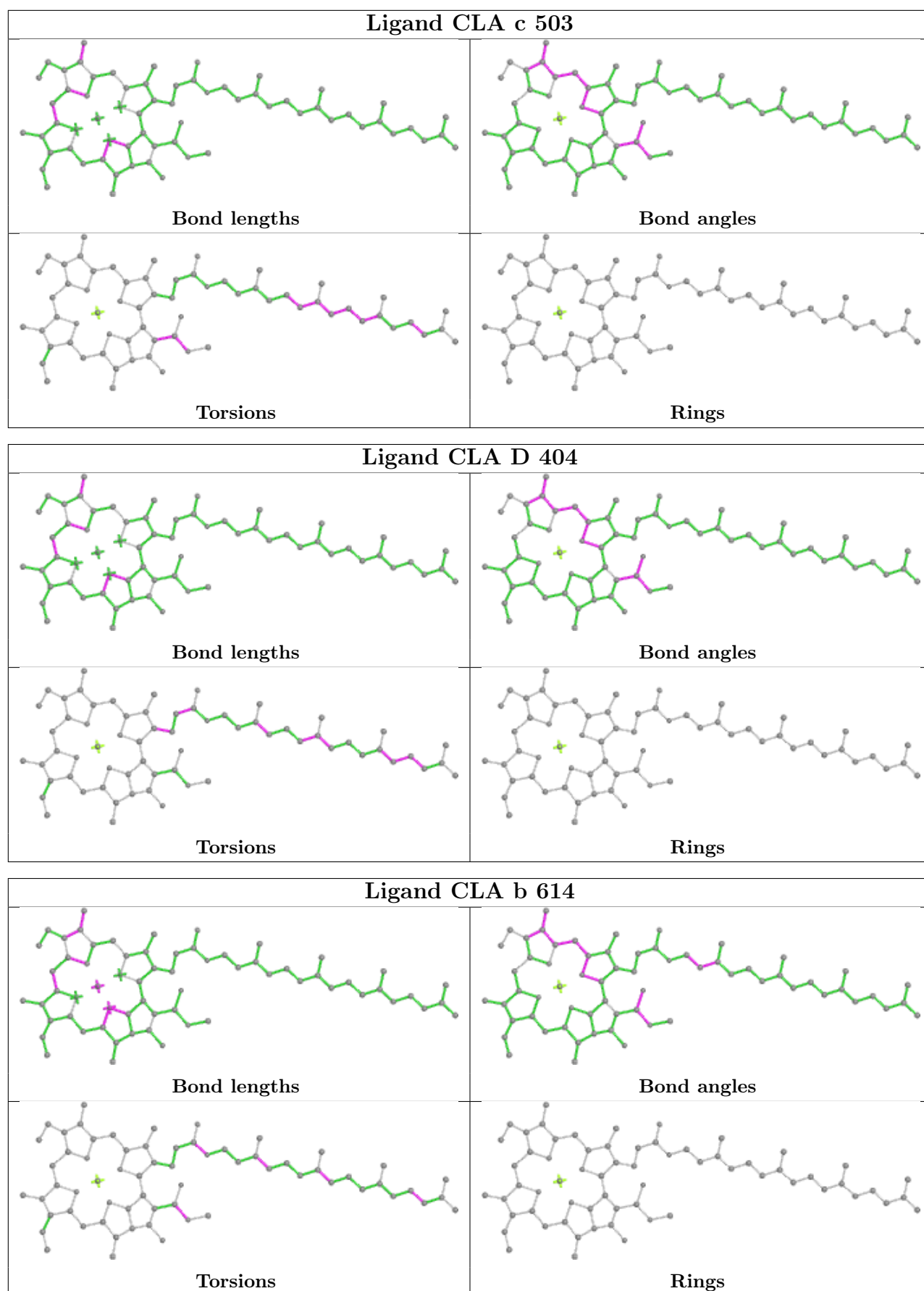


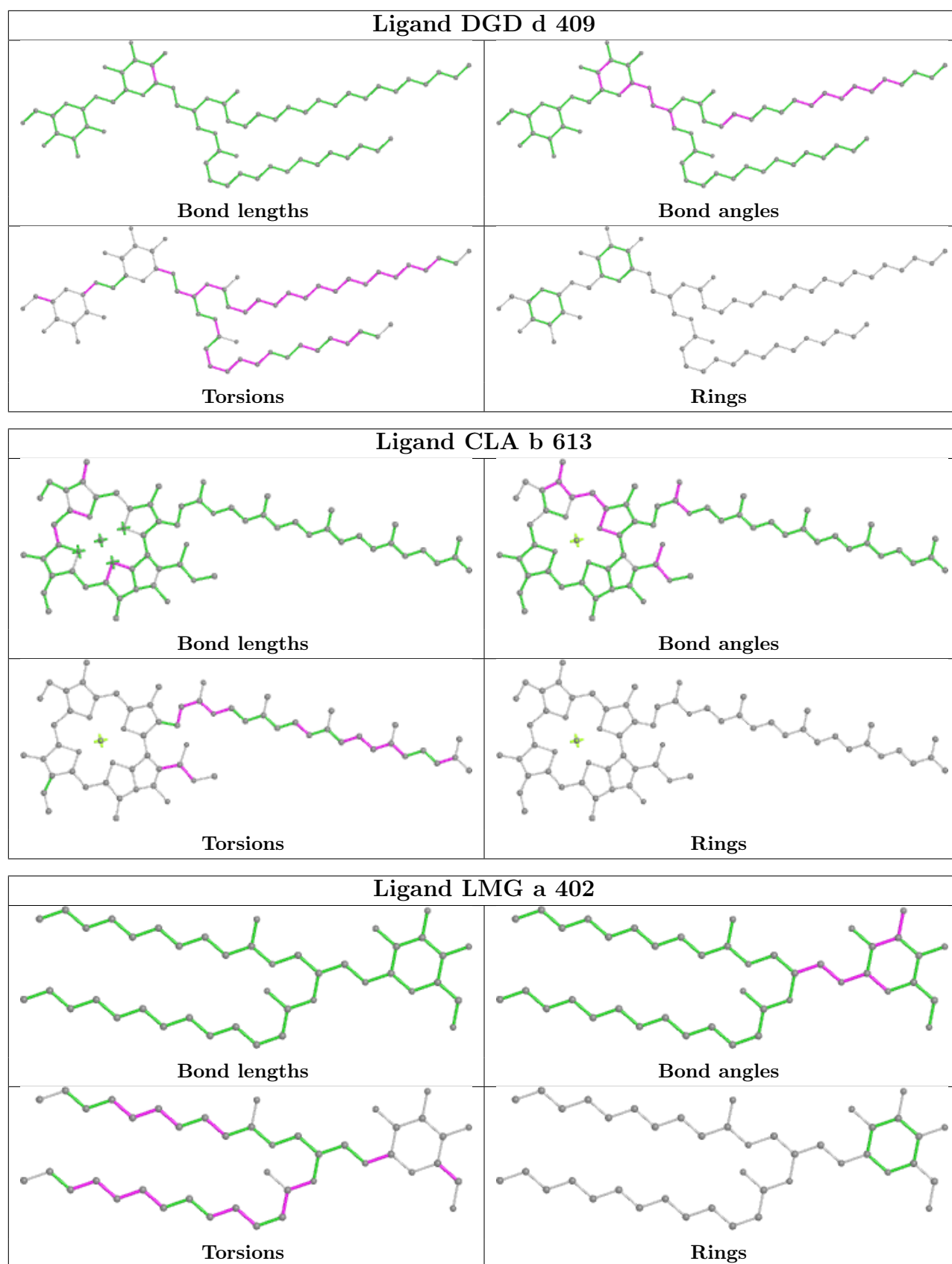


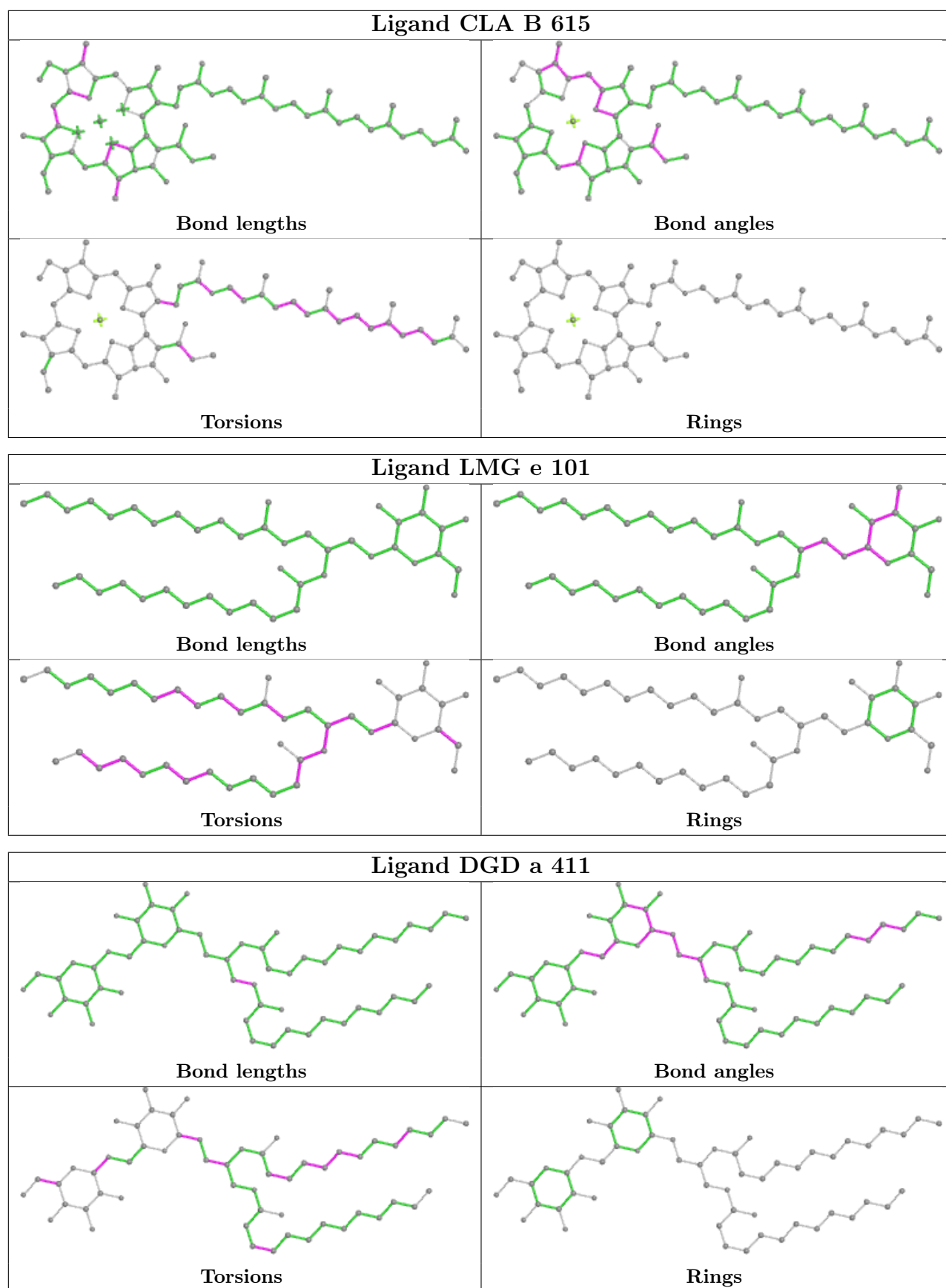












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	335/344 (97%)	0.52	27 (8%) 12 11	205, 207, 208, 208	0
1	a	335/344 (97%)	0.54	30 (8%) 9 9	204, 207, 208, 209	0
2	B	490/510 (96%)	0.33	34 (6%) 16 13	205, 207, 208, 208	0
2	b	490/510 (96%)	0.42	38 (7%) 13 11	205, 207, 208, 209	0
3	C	447/461 (96%)	0.37	35 (7%) 13 11	205, 207, 208, 209	0
3	c	447/461 (96%)	0.20	21 (4%) 31 27	206, 207, 208, 209	0
4	D	340/352 (96%)	0.36	16 (4%) 31 27	204, 207, 208, 209	0
4	d	340/352 (96%)	0.34	17 (5%) 28 25	204, 207, 208, 208	0
5	E	82/84 (97%)	0.22	1 (1%) 79 70	205, 207, 208, 208	0
5	e	82/84 (97%)	0.10	2 (2%) 59 49	206, 207, 208, 208	0
6	F	35/45 (77%)	-0.02	0 100 100	206, 207, 208, 208	0
6	f	35/45 (77%)	-0.39	0 100 100	206, 207, 208, 208	0
7	H	65/66 (98%)	0.45	9 (13%) 2 4	206, 207, 208, 209	0
7	h	65/66 (98%)	0.77	12 (18%) 1 2	206, 207, 208, 208	0
8	I	35/38 (92%)	0.54	4 (11%) 5 6	206, 207, 208, 208	0
8	i	35/38 (92%)	-0.09	0 100 100	206, 207, 208, 208	0
9	J	34/40 (85%)	0.08	2 (5%) 22 19	205, 207, 207, 208	0
9	j	34/40 (85%)	-0.44	0 100 100	206, 207, 208, 209	0
10	K	37/46 (80%)	-0.11	0 100 100	206, 207, 208, 208	0
10	k	37/46 (80%)	0.32	2 (5%) 25 22	206, 207, 208, 209	0
11	L	37/37 (100%)	0.56	2 (5%) 25 22	205, 207, 208, 208	0
11	l	37/37 (100%)	0.21	1 (2%) 54 45	206, 207, 208, 209	0
12	M	34/36 (94%)	0.58	4 (11%) 4 6	205, 206, 207, 208	0
12	m	34/36 (94%)	0.27	2 (5%) 22 19	205, 207, 207, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.64	22 (9%) 9 8	205, 207, 208, 209	0
13	o	243/272 (89%)	0.62	16 (6%) 18 15	205, 207, 208, 209	0
14	T	32/32 (100%)	0.23	3 (9%) 8 8	206, 207, 208, 209	0
14	t	32/32 (100%)	0.49	3 (9%) 8 8	205, 206, 208, 208	0
15	U	97/134 (72%)	0.86	11 (11%) 5 6	205, 207, 208, 208	0
15	u	97/134 (72%)	0.67	8 (8%) 11 10	205, 207, 208, 208	0
16	V	137/163 (84%)	0.24	3 (2%) 62 52	205, 207, 208, 208	0
16	v	137/163 (84%)	0.70	14 (10%) 6 7	206, 207, 208, 208	0
17	g	28/46 (60%)	0.18	0 100 100	206, 207, 208, 209	0
17	y	28/46 (60%)	-0.04	0 100 100	206, 207, 208, 208	0
18	X	37/41 (90%)	0.71	5 (13%) 3 4	205, 207, 208, 209	0
18	x	37/41 (90%)	0.96	5 (13%) 3 4	206, 207, 208, 208	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.22	1 (1%) 72 62	205, 207, 208, 209	0
20	z	62/62 (100%)	0.84	9 (14%) 2 3	206, 207, 208, 209	0
All	All	5214/5674 (91%)	0.41	359 (6%) 16 13	204, 207, 208, 209	0

The worst 5 of 359 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	84	LYS	7.3
18	x	11	THR	6.7
13	o	169	LYS	6.3
5	e	84	LYS	5.2
18	x	42	GLN	5.2

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
23	PL9	J	101	35/55	0.24	0.59	204,207,208,209	0
23	PL9	j	101	35/55	0.26	0.53	205,208,209,209	0
31	LMT	i	102	35/35	0.29	1.67	206,208,209,210	0
27	LMG	E	101	44/55	0.37	0.77	204,207,209,210	0
31	LMT	I	102	35/35	0.39	0.88	205,207,209,210	0
35	CA	O	301	1/1	0.45	0.28	207,207,207,207	0
23	PL9	A	406	45/55	0.49	0.54	205,206,207,208	0
35	CA	K	101	1/1	0.51	0.37	210,210,210,210	0
24	BCR	J	102	40/40	0.52	0.38	205,207,208,209	0
22	CLA	b	605	65/65	0.52	1.06	205,208,209,209	0
35	CA	o	301	1/1	0.52	1.13	209,209,209,209	0
22	CLA	c	502	65/65	0.54	0.65	205,207,208,208	0
23	PL9	D	406	55/55	0.55	0.45	204,206,207,207	0
31	LMT	d	410	31/35	0.56	0.76	206,208,209,210	0
25	DGD	A	408	56/66	0.57	0.56	206,207,209,210	0
24	BCR	g	101	40/40	0.57	0.76	204,206,207,207	0
27	LMG	a	402	42/55	0.57	0.47	204,207,209,209	0
35	CA	k	101	1/1	0.58	0.23	204,204,204,204	0
24	BCR	F	102	40/40	0.60	0.51	205,206,207,208	0
24	BCR	B	616	40/40	0.60	0.52	205,206,207,207	0
27	LMG	C	518	45/55	0.60	1.02	205,206,208,208	0
24	BCR	f	102	40/40	0.60	0.47	206,206,207,208	0
24	BCR	x	101	40/40	0.61	0.84	205,207,208,208	0
31	LMT	b	626	35/35	0.61	0.61	205,208,210,210	0
22	CLA	B	601	65/65	0.61	0.93	206,207,208,209	0
27	LMG	A	415	42/55	0.61	0.46	204,207,208,209	0
23	PL9	d	406	55/55	0.62	0.43	204,206,207,208	0
27	LMG	I	101	43/55	0.64	1.00	204,207,209,210	0
31	LMT	B	623	35/35	0.64	0.77	205,208,209,210	0
30	SQD	d	402	43/54	0.65	1.12	205,207,209,211	0
26	LHG	c	519	37/49	0.65	0.36	205,207,211,214	0
31	LMT	b	603	35/35	0.66	0.58	205,207,208,209	0
24	BCR	j	102	40/40	0.67	0.30	206,207,209,209	0
24	BCR	C	514	40/40	0.67	0.77	205,206,207,207	0
31	LMT	B	628	35/35	0.67	0.54	204,207,209,209	0
27	LMG	c	518	45/55	0.67	0.97	206,207,208,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LMG	l	101	51/55	0.67	0.42	205,206,208,208	0
30	SQD	B	626	47/54	0.67	0.59	204,207,209,211	0
24	BCR	b	623	40/40	0.68	0.83	204,206,207,207	0
22	CLA	b	619	65/65	0.68	0.79	205,207,208,209	0
25	DGD	C	517	66/66	0.68	0.34	205,206,207,208	0
30	SQD	F	103	45/54	0.68	0.82	205,207,209,210	0
31	LMT	M	102	35/35	0.69	0.42	205,207,208,209	0
27	LMG	C	521	48/55	0.69	0.37	204,206,207,208	0
31	LMT	b	604	35/35	0.69	0.45	205,207,209,209	0
25	DGD	D	409	63/66	0.69	0.79	205,208,209,211	0
24	BCR	H	102	40/40	0.69	1.06	206,207,208,208	0
25	DGD	B	625	52/66	0.70	0.63	205,208,210,210	0
27	LMG	M	101	42/55	0.70	0.51	205,207,209,210	0
25	DGD	a	411	56/66	0.70	0.39	205,207,209,209	0
25	DGD	d	409	63/66	0.70	0.74	205,208,210,211	0
22	CLA	B	613	65/65	0.70	0.49	205,206,207,208	0
31	LMT	b	627	35/35	0.70	1.20	205,208,210,210	0
24	BCR	c	514	40/40	0.71	0.85	205,206,207,208	0
24	BCR	B	617	40/40	0.71	0.43	204,206,207,208	0
27	LMG	e	101	44/55	0.71	0.47	204,207,208,209	0
27	LMG	m	101	42/55	0.72	0.57	203,207,208,209	0
32	PHO	d	401	64/64	0.72	0.42	204,206,207,207	0
27	LMG	d	408	48/55	0.72	0.41	204,206,207,208	0
31	LMT	D	410	31/35	0.72	0.81	206,208,208,209	0
26	LHG	C	519	37/49	0.72	0.38	204,207,210,212	0
23	PL9	a	409	45/55	0.72	0.37	204,206,207,208	0
22	CLA	c	512	65/65	0.73	0.75	205,207,208,208	0
24	BCR	B	619	40/40	0.73	1.02	205,206,207,207	0
22	CLA	b	613	65/65	0.73	0.83	205,207,208,209	0
32	PHO	D	402	64/64	0.74	0.36	205,206,207,208	0
30	SQD	A	413	51/54	0.74	0.35	205,207,208,208	0
22	CLA	C	505	65/65	0.74	0.60	205,206,207,208	0
24	BCR	y	101	40/40	0.74	0.81	205,206,207,207	0
22	CLA	c	510	65/65	0.74	0.57	206,207,208,209	0
22	CLA	C	502	65/65	0.74	0.51	205,206,207,208	0
27	LMG	i	101	43/55	0.75	0.84	205,207,209,209	0
22	CLA	a	408	65/65	0.75	0.80	205,206,207,209	0
22	CLA	C	506	65/65	0.75	0.83	204,207,207,208	0
22	CLA	C	512	65/65	0.75	0.94	205,207,208,209	0
27	LMG	D	407	49/55	0.76	0.30	205,206,207,208	0
31	LMT	B	627	35/35	0.76	0.56	205,207,209,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	LMT	B	624	35/35	0.77	0.56	205,207,210,210	0
24	BCR	b	621	40/40	0.77	0.34	204,206,207,207	0
22	CLA	b	617	65/65	0.77	0.42	205,206,208,209	0
24	BCR	c	513	40/40	0.77	0.96	204,206,207,208	0
25	DGD	c	517	66/66	0.77	0.30	204,206,207,208	0
22	CLA	c	503	65/65	0.77	0.62	205,207,208,208	0
30	SQD	b	602	47/54	0.77	0.38	205,207,209,212	0
27	LMG	D	411	46/55	0.77	0.40	205,206,207,208	0
24	BCR	a	410	40/40	0.77	0.70	205,206,207,207	0
24	BCR	A	407	40/40	0.78	0.53	205,206,207,208	0
22	CLA	C	520	65/65	0.78	0.34	205,207,208,209	0
33	BCT	d	403	4/4	0.78	0.96	207,207,207,208	0
25	DGD	b	601	52/66	0.78	0.46	204,207,208,209	0
30	SQD	B	622	43/54	0.78	0.45	205,207,209,212	0
22	CLA	A	405	65/65	0.78	0.67	204,206,208,208	0
31	LMT	M	103	35/35	0.78	0.42	205,206,208,210	0
21	FE2	a	403	1/1	0.79	0.27	211,211,211,211	0
22	CLA	c	508	65/65	0.79	0.53	205,207,208,208	0
27	LMG	A	410	51/55	0.79	0.33	204,206,207,208	0
27	LMG	c	522	48/55	0.79	0.30	205,206,207,208	0
24	BCR	K	102	40/40	0.79	0.90	204,207,208,209	0
24	BCR	c	521	40/40	0.79	1.36	205,207,208,209	0
22	CLA	a	405	65/65	0.80	0.63	202,206,207,208	0
30	SQD	a	415	51/54	0.80	0.31	205,206,208,208	0
27	LMG	b	625	49/55	0.80	0.28	205,206,207,208	0
22	CLA	a	406	65/65	0.80	0.38	205,207,208,209	0
22	CLA	B	603	65/65	0.80	0.52	204,206,207,208	0
22	CLA	c	505	65/65	0.81	0.60	204,206,208,208	0
24	BCR	b	622	40/40	0.81	0.31	204,206,207,207	0
22	CLA	C	504	65/65	0.81	0.41	205,206,207,207	0
26	LHG	a	412	39/49	0.81	0.28	205,207,208,210	0
22	CLA	c	504	65/65	0.81	0.36	205,207,208,208	0
32	PHO	a	407	64/64	0.81	0.29	205,207,207,208	0
32	PHO	D	401	64/64	0.82	0.34	203,206,207,208	0
22	CLA	b	618	65/65	0.82	0.70	205,207,208,208	0
22	CLA	d	404	65/65	0.82	0.41	204,206,207,207	0
28	CL	a	413	1/1	0.82	0.18	204,204,204,204	0
25	DGD	C	516	62/66	0.82	0.28	204,206,208,208	0
22	CLA	d	405	65/65	0.82	0.54	204,206,207,208	0
22	CLA	B	605	65/65	0.82	0.82	205,206,207,208	0
22	CLA	C	508	65/65	0.82	0.86	205,206,207,208	0
22	CLA	H	101	65/65	0.82	0.41	205,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	C	510	65/65	0.83	0.46	205,206,207,208	0
22	CLA	b	606	65/65	0.83	0.77	205,206,207,207	0
22	CLA	b	607	65/65	0.83	0.51	205,206,207,209	0
22	CLA	B	608	65/65	0.83	0.69	205,207,208,209	0
22	CLA	a	404	65/65	0.83	0.57	205,206,207,208	0
25	DGD	b	624	58/66	0.83	0.34	205,206,207,208	0
22	CLA	B	607	65/65	0.84	0.44	205,206,207,209	0
22	CLA	B	615	65/65	0.84	0.84	205,206,208,208	0
30	SQD	A	414	54/54	0.84	0.37	204,207,208,210	0
22	CLA	C	511	65/65	0.84	1.06	205,207,208,208	0
24	BCR	B	618	40/40	0.85	0.30	204,205,207,207	0
22	CLA	c	501	65/65	0.85	0.61	205,207,208,209	0
22	CLA	D	405	65/65	0.85	0.68	205,206,207,207	0
30	SQD	f	103	45/54	0.85	0.60	205,207,208,210	0
22	CLA	h	101	65/65	0.85	0.57	204,207,208,209	0
22	CLA	c	509	65/65	0.85	0.39	204,206,208,209	0
22	CLA	b	612	65/65	0.85	0.59	205,206,207,209	0
22	CLA	B	614	65/65	0.85	0.87	205,206,207,208	0
30	SQD	a	401	54/54	0.85	0.46	205,207,209,211	0
22	CLA	C	509	65/65	0.86	0.36	205,206,207,208	0
22	CLA	A	404	65/65	0.86	0.40	204,206,207,208	0
22	CLA	b	608	65/65	0.86	0.60	205,206,207,208	0
25	DGD	c	515	53/66	0.86	0.41	205,207,208,209	0
22	CLA	b	609	65/65	0.86	0.64	205,207,208,209	0
22	CLA	b	610	65/65	0.86	0.29	205,206,207,208	0
22	CLA	b	611	65/65	0.86	0.43	205,206,207,208	0
22	CLA	c	506	65/65	0.86	0.75	206,207,208,208	0
22	CLA	B	610	65/65	0.86	0.34	205,206,207,207	0
25	DGD	B	620	58/66	0.86	0.30	203,206,208,209	0
22	CLA	B	604	65/65	0.86	0.63	205,207,208,208	0
27	LMG	B	621	49/55	0.86	0.26	204,206,207,208	0
34	HEM	v	201	43/43	0.86	0.75	205,207,207,208	0
22	CLA	C	507	65/65	0.86	0.32	205,206,208,210	0
28	CL	A	411	1/1	0.86	0.25	207,207,207,207	0
22	CLA	c	511	65/65	0.86	0.72	205,207,208,209	0
22	CLA	C	503	65/65	0.86	0.44	205,207,207,208	0
34	HEM	V	201	43/43	0.87	0.52	203,206,207,208	0
22	CLA	B	609	65/65	0.87	0.62	205,206,208,208	0
25	DGD	C	515	53/66	0.87	0.28	204,206,207,208	0
27	LMG	d	411	46/55	0.88	0.29	204,206,207,208	0
22	CLA	c	507	65/65	0.88	0.33	205,207,208,208	0
22	CLA	A	403	65/65	0.88	0.62	204,206,207,207	0

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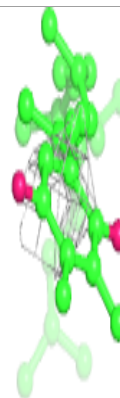
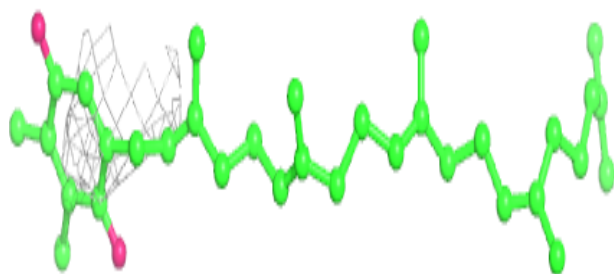
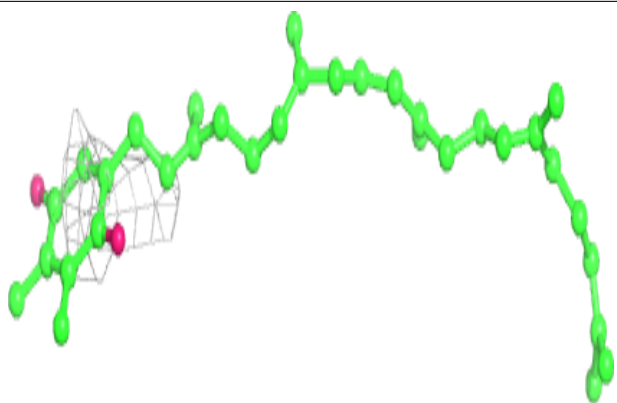
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CLA	B	611	65/65	0.88	0.43	204,206,207,208	0
22	CLA	b	615	65/65	0.88	0.35	205,206,207,208	0
25	DGD	c	516	62/66	0.88	0.26	205,207,208,209	0
26	LHG	A	409	39/49	0.89	0.26	205,206,208,209	0
34	HEM	F	101	43/43	0.89	0.61	205,207,208,209	0
22	CLA	c	520	65/65	0.89	0.29	205,207,207,208	0
22	CLA	A	402	65/65	0.89	0.47	205,206,207,208	0
21	FE2	A	401	1/1	0.89	0.17	206,206,206,206	0
27	LMG	D	408	48/55	0.89	0.25	202,206,208,208	0
24	BCR	C	513	40/40	0.89	0.82	205,206,207,208	0
22	CLA	B	606	65/65	0.89	0.31	205,206,207,208	0
22	CLA	D	404	65/65	0.90	0.39	203,206,207,208	0
22	CLA	b	614	65/65	0.90	0.31	205,206,207,208	0
22	CLA	B	612	65/65	0.90	0.28	204,206,207,207	0
22	CLA	C	501	65/65	0.90	0.44	205,206,207,208	0
24	BCR	b	620	40/40	0.91	0.30	205,206,207,208	0
22	CLA	B	602	65/65	0.92	0.47	204,206,208,209	0
27	LMG	d	407	49/55	0.92	0.23	205,206,207,207	0
34	HEM	f	101	43/43	0.93	0.32	206,207,207,208	0
33	BCT	D	403	4/4	0.93	0.44	206,206,206,206	0
22	CLA	b	616	65/65	0.94	0.33	204,206,208,209	0
29	OEX	A	412	10/10	0.95	0.43	198,204,206,206	0
29	OEX	a	414	10/10	0.95	0.48	198,203,205,207	0

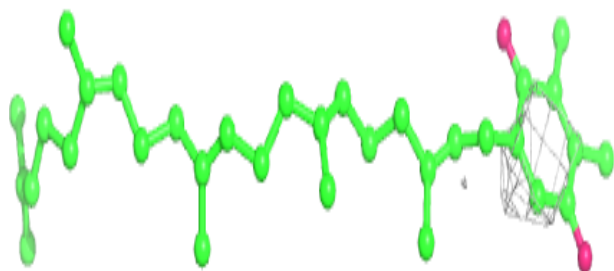
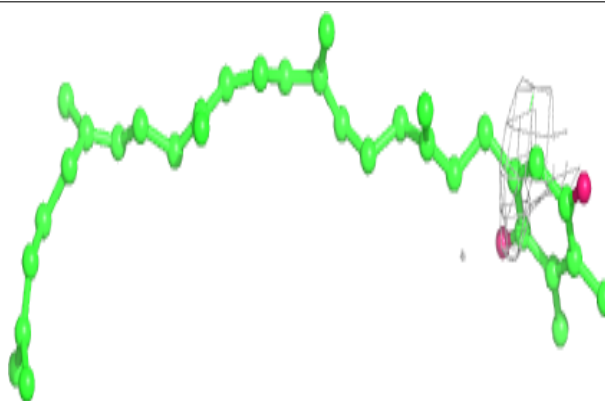
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PL9 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)

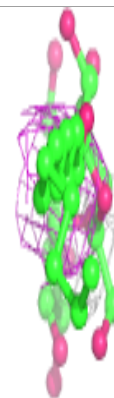
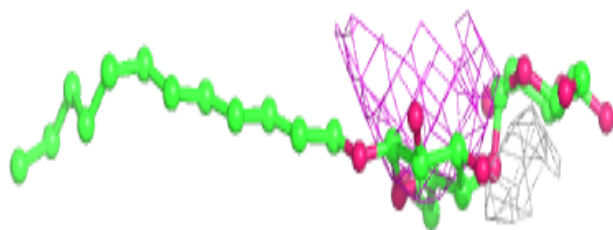
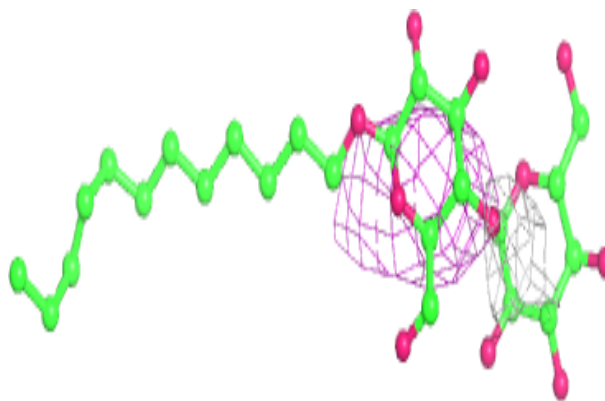
**Electron density around PL9 j 101:**

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



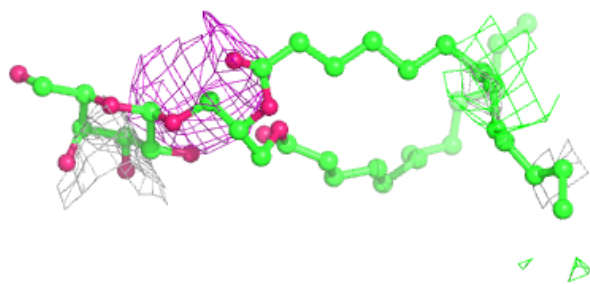
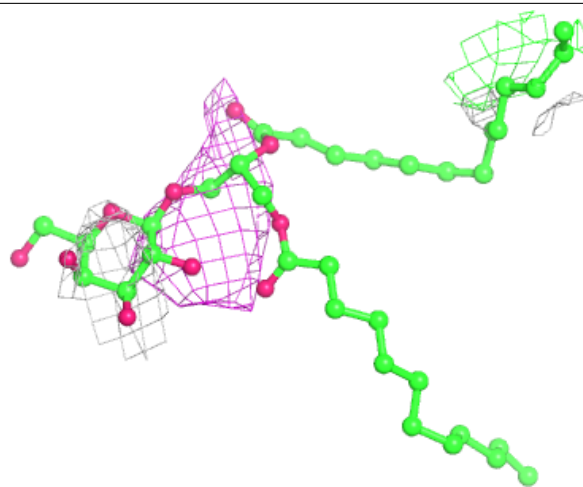
Electron density around LMT i 102:

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



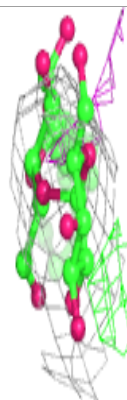
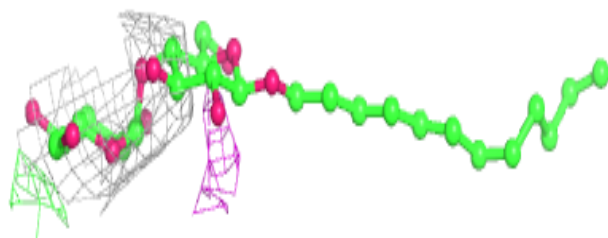
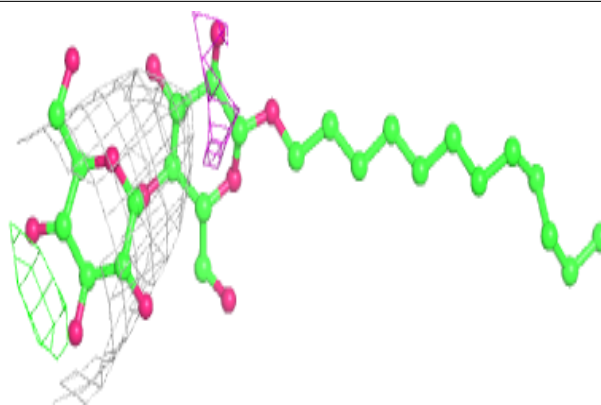
Electron density around LMG E 101:

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

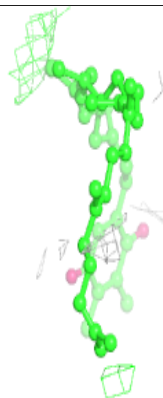
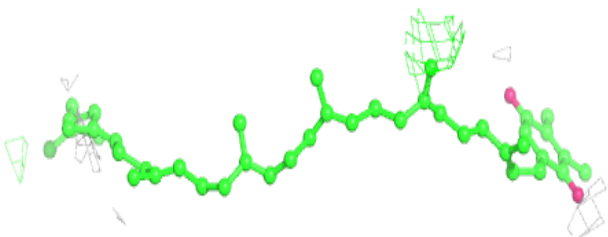
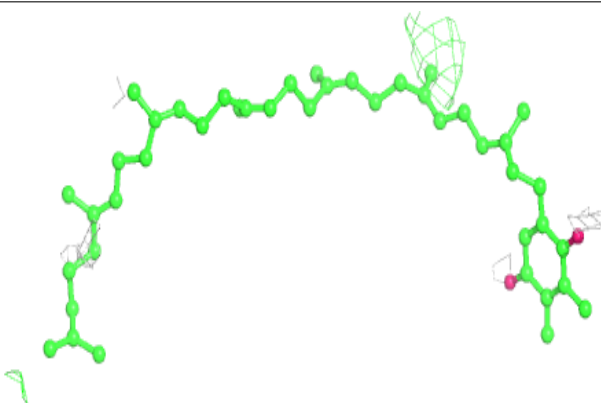


Electron density around LMT I 102:

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

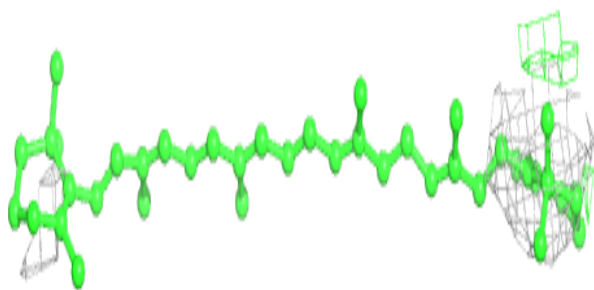
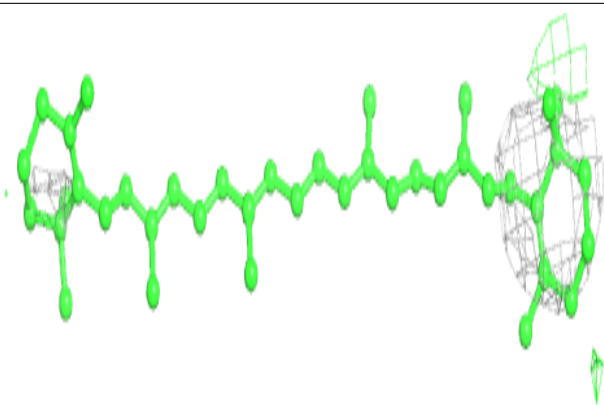
**Electron density around PL9 A 406:**

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



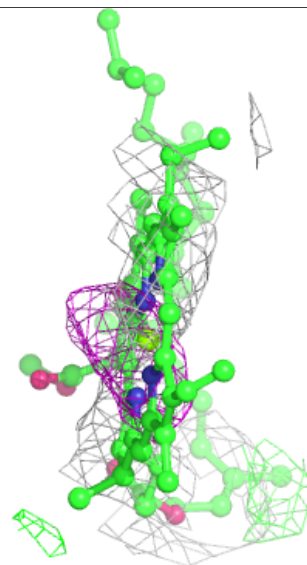
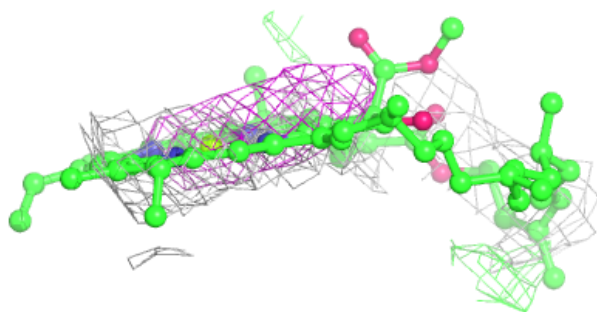
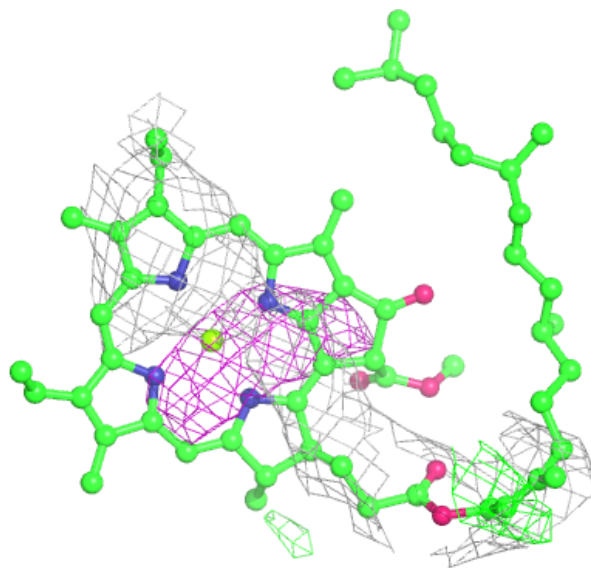
Electron density around BCR J 102:

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



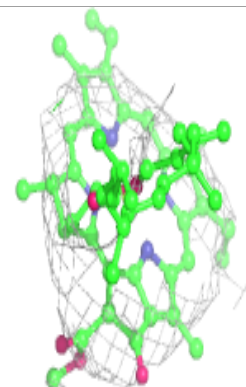
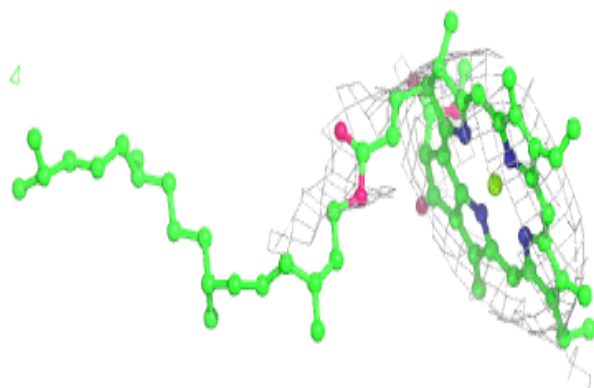
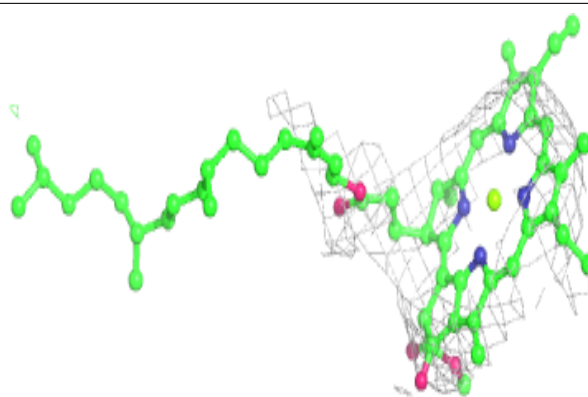
Electron density around CLA b 605:

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

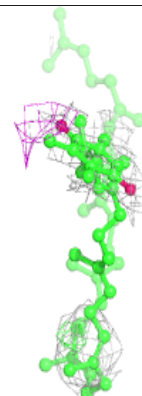
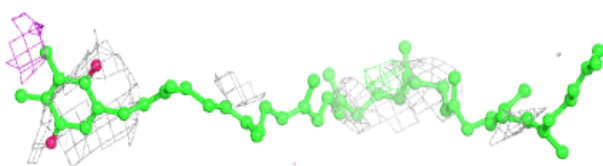
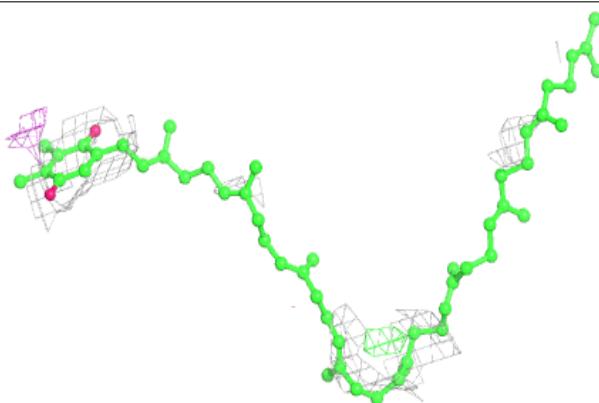


Electron density around CLA c 502:

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

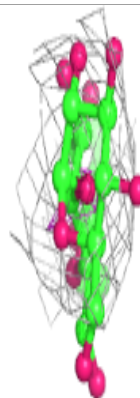
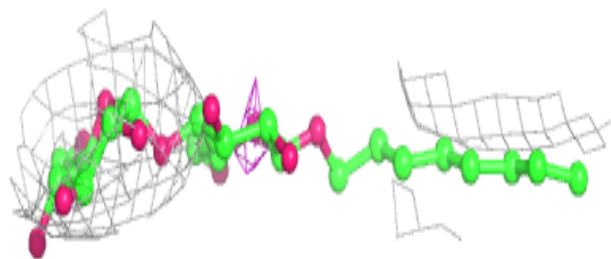
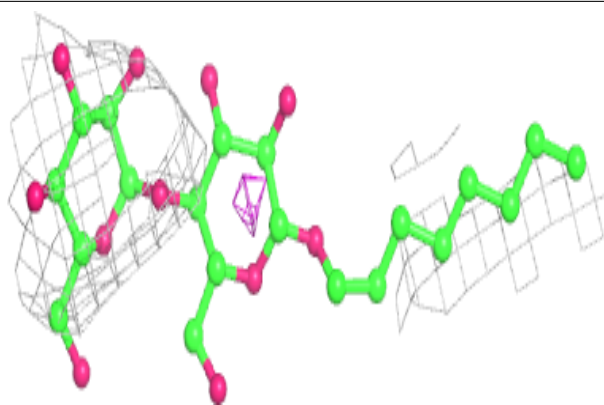
**Electron density around PL9 D 406:**

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

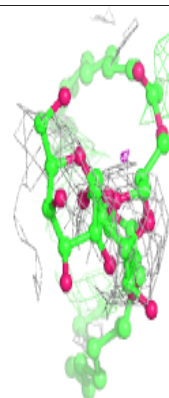
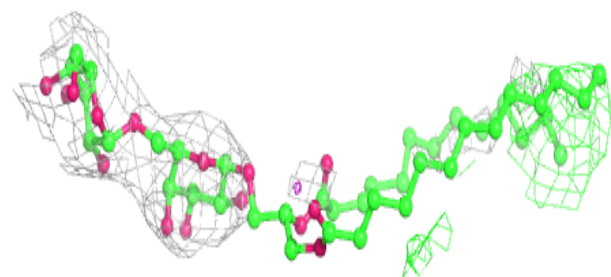
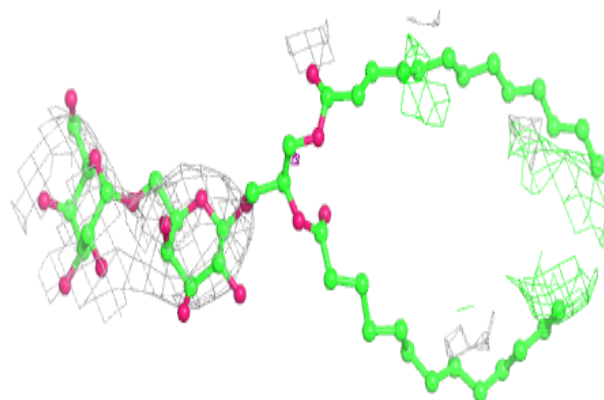


Electron density around LMT d 410:

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

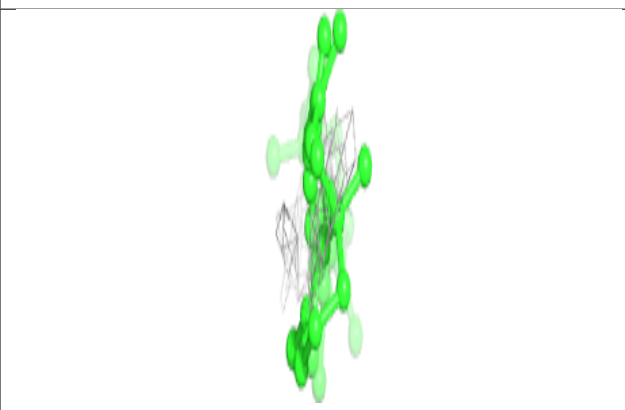
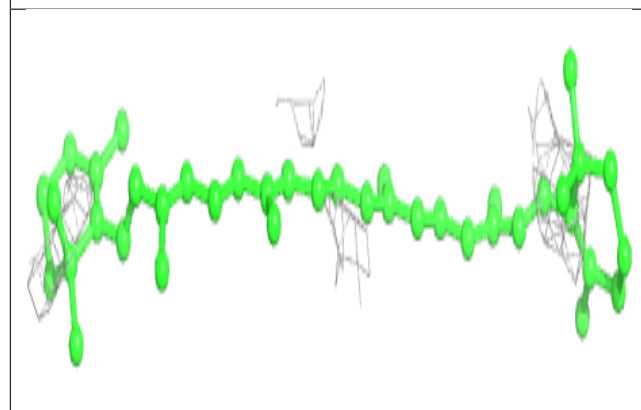
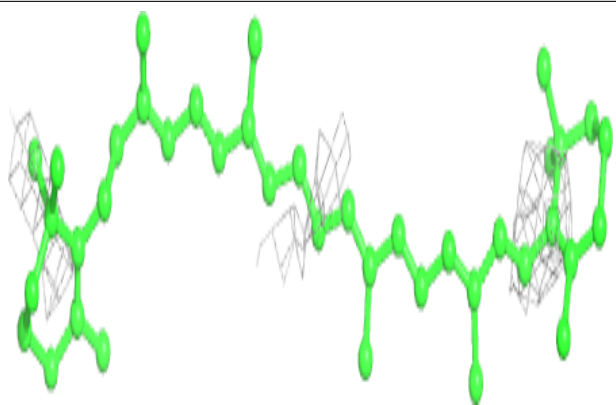
**Electron density around DGD A 408:**

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

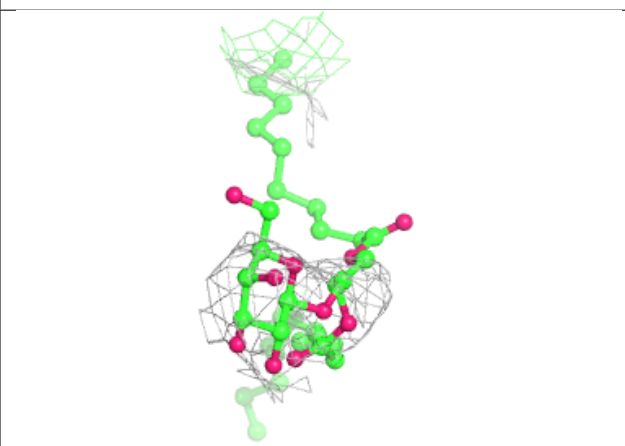
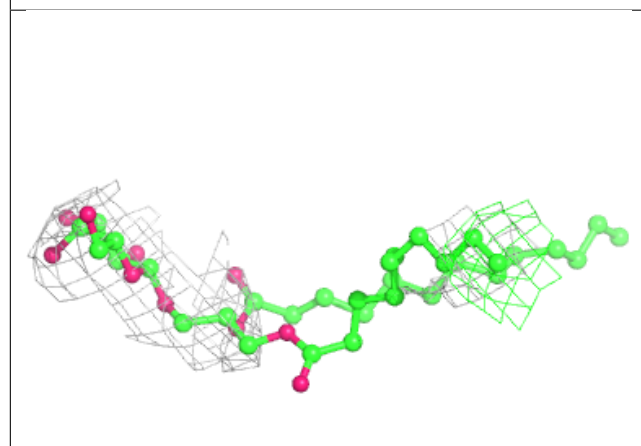
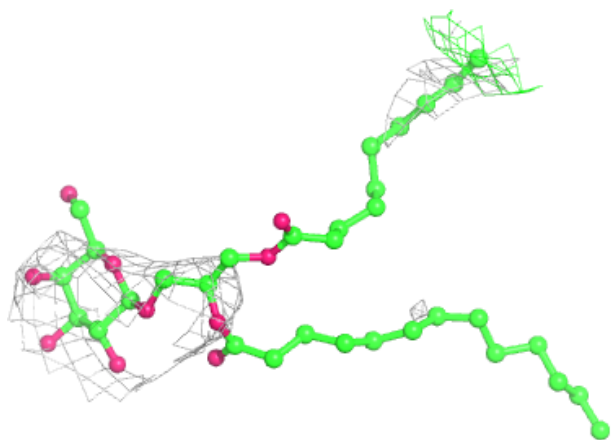


Electron density around BCR g 101:

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

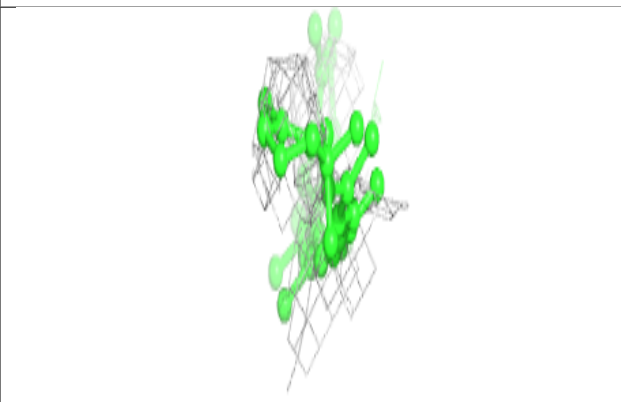
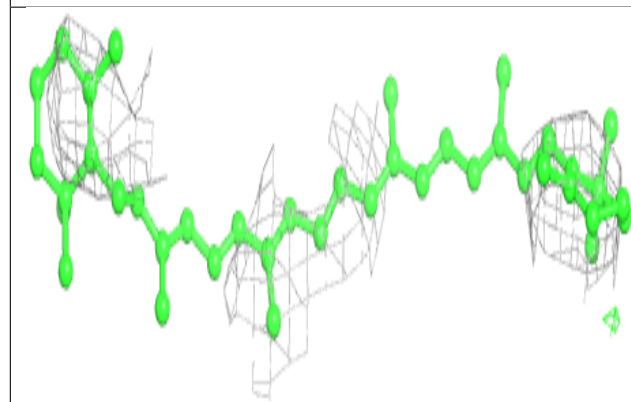
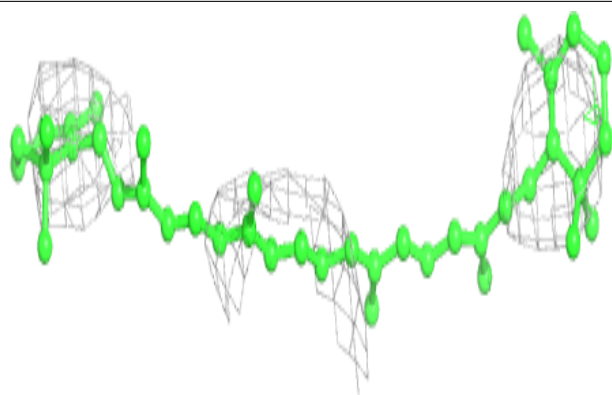
**Electron density around LMG a 402:**

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

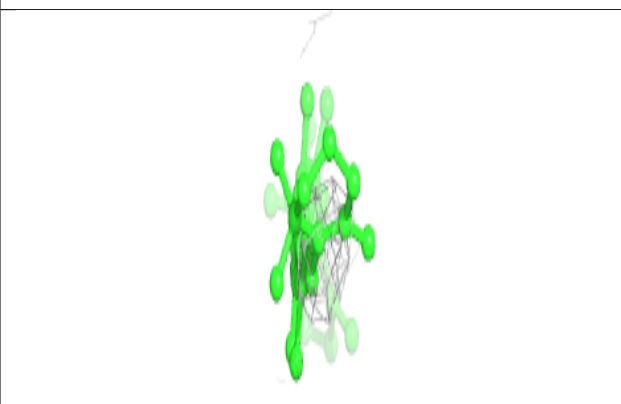
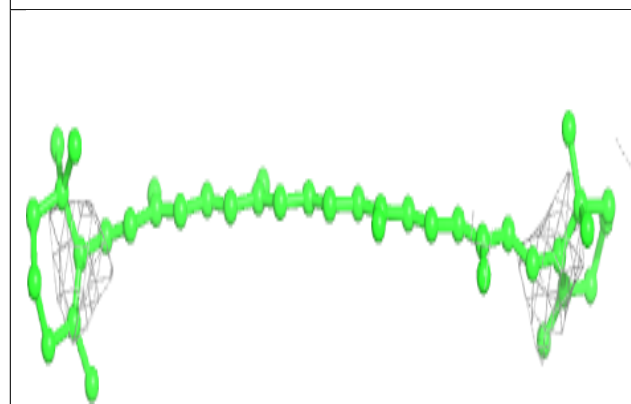
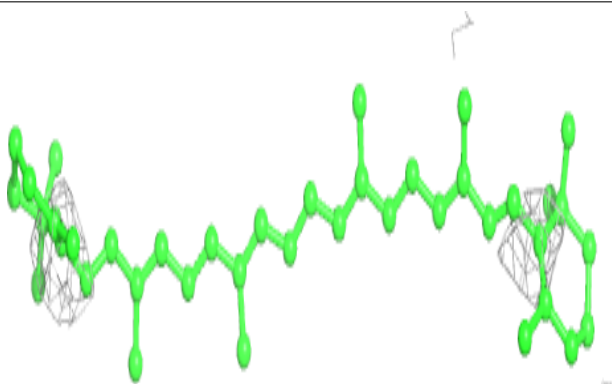


Electron density around BCR F 102:

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

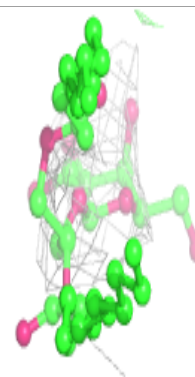
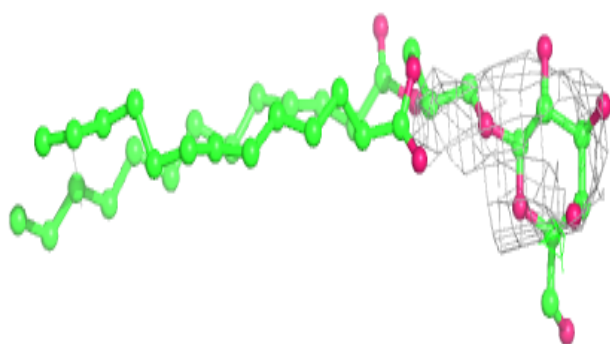
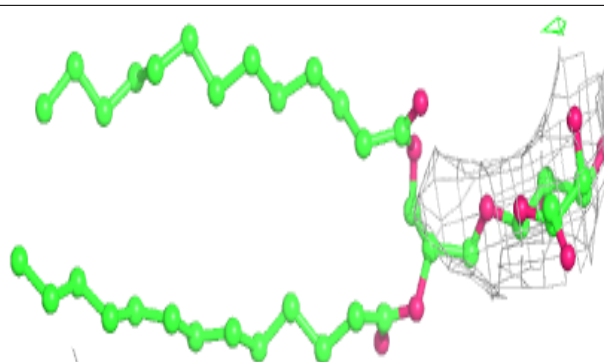
**Electron density around BCR B 616:**

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

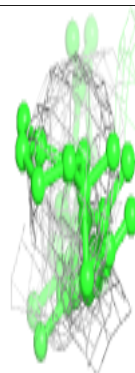
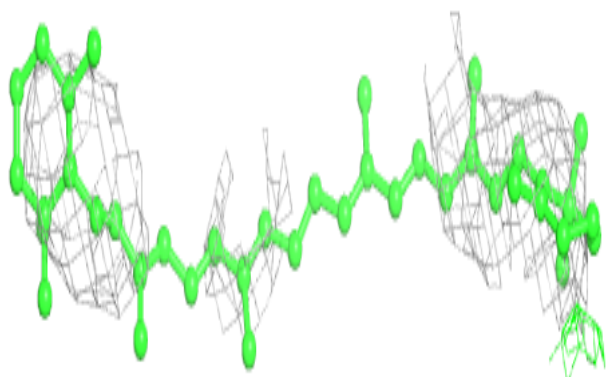
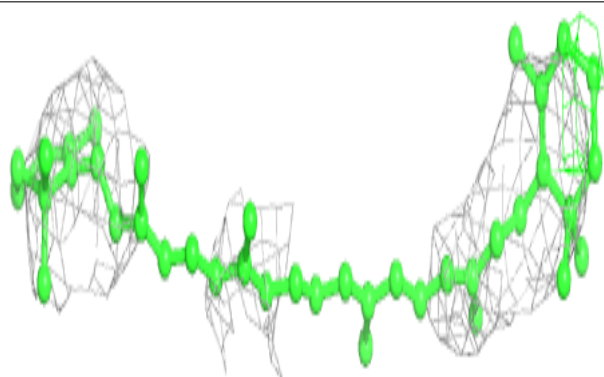


Electron density around LMG C 518:

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

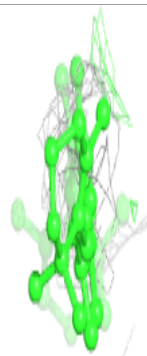
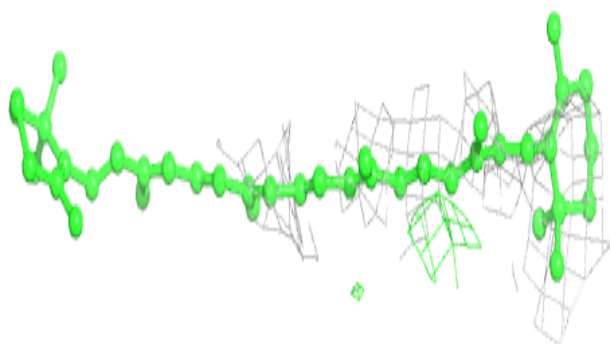
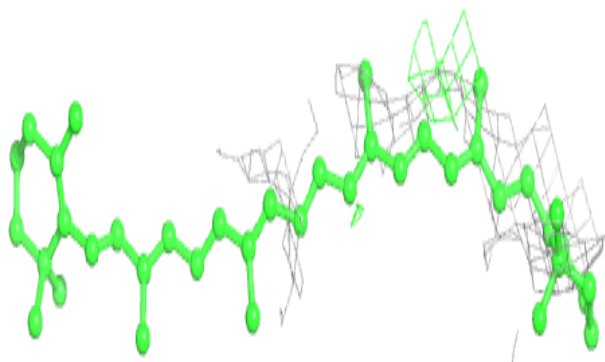
**Electron density around BCR f 102:**

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

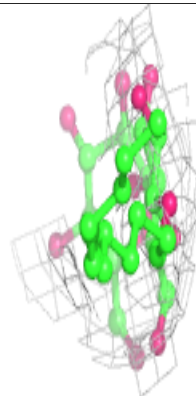
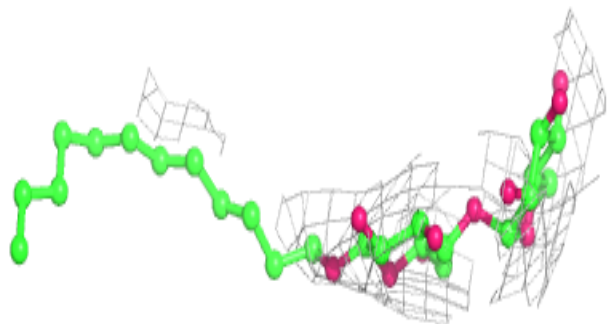
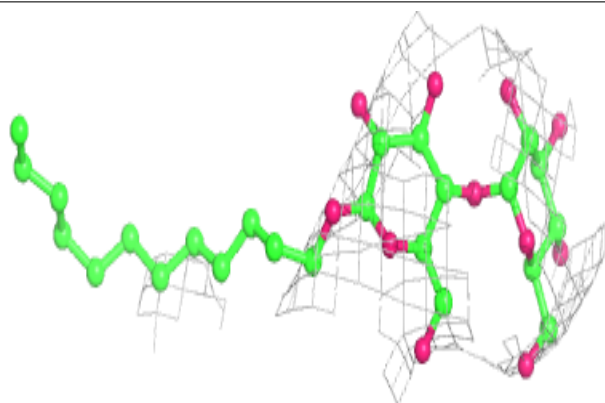


Electron density around BCR x 101:

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

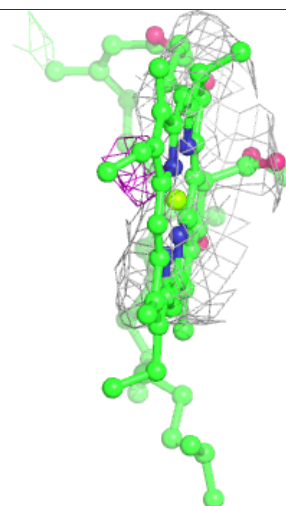
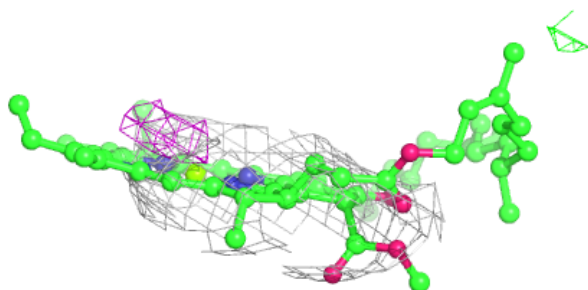
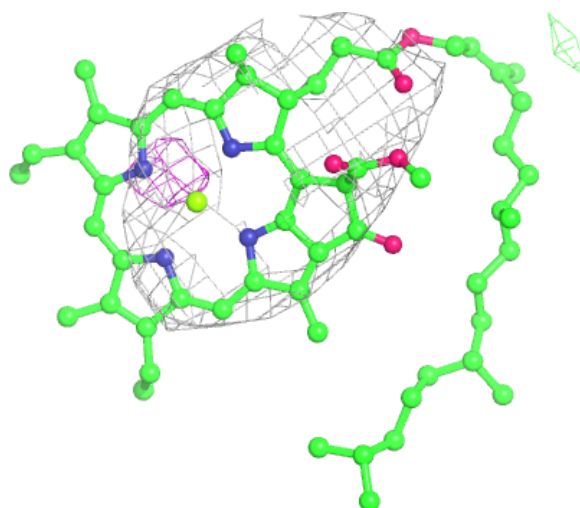
**Electron density around LMT b 626:**

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



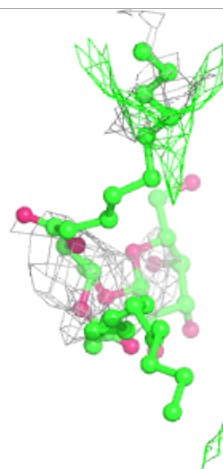
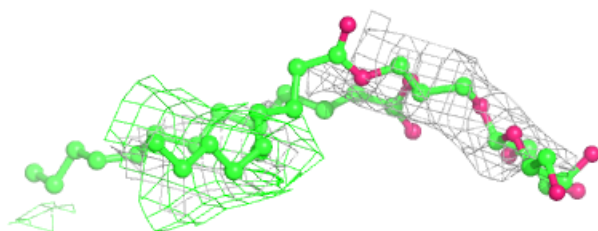
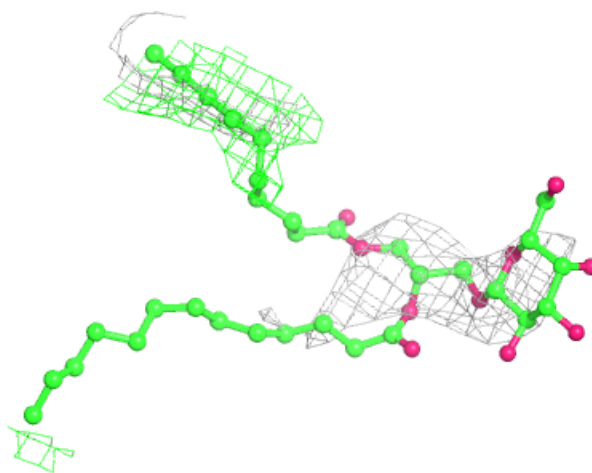
Electron density around CLA B 601:

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



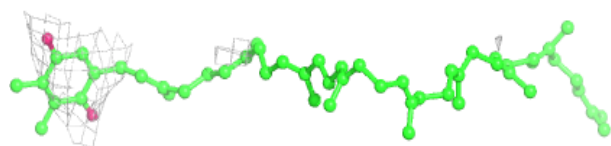
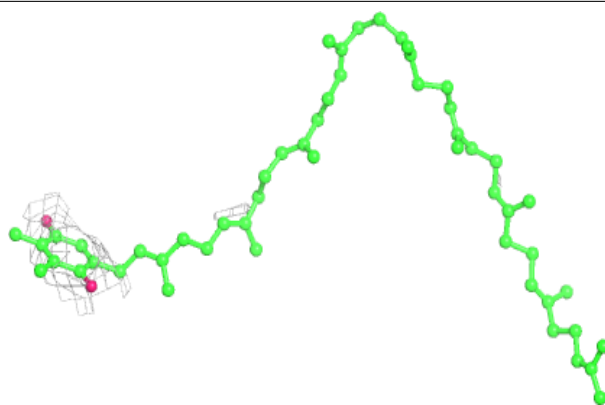
Electron density around LMG A 415:

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

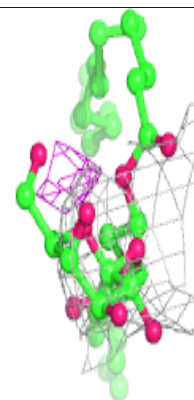
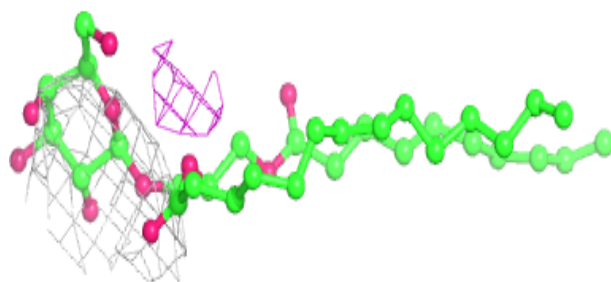
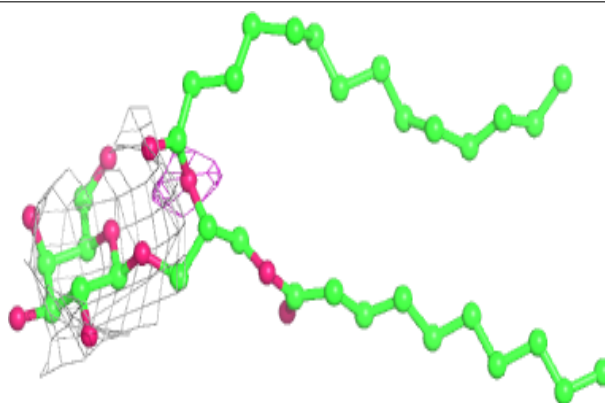


Electron density around PL9 d 406:

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

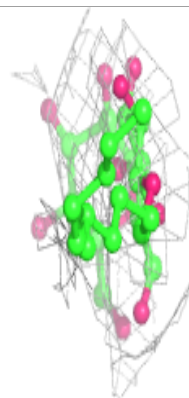
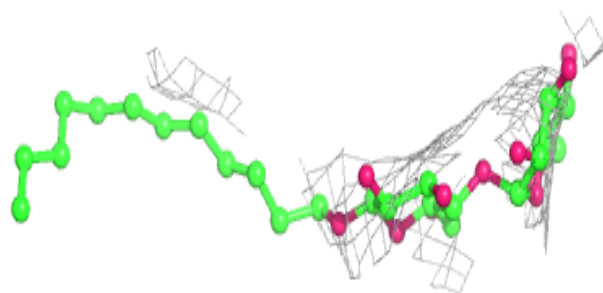
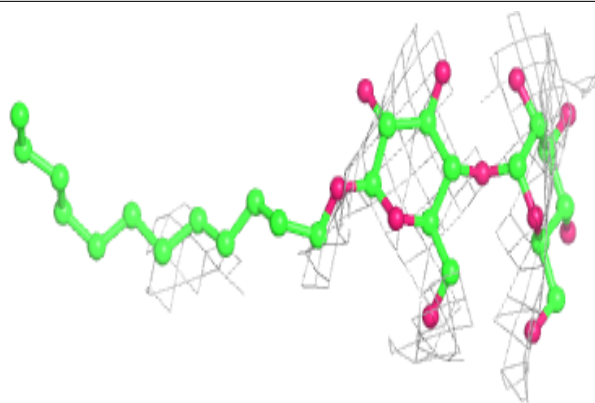
**Electron density around LMG I 101:**

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

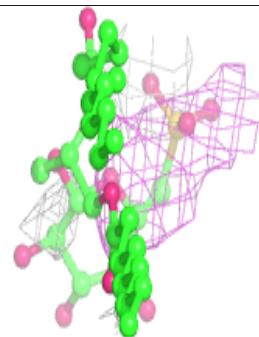
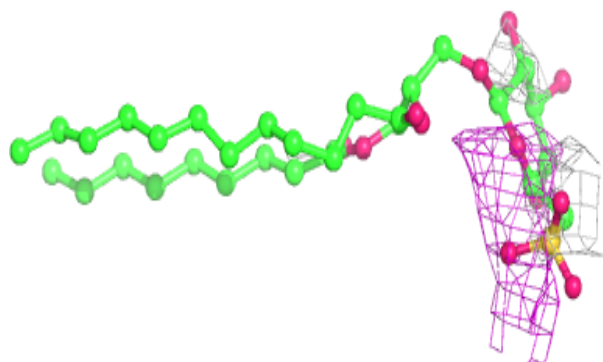
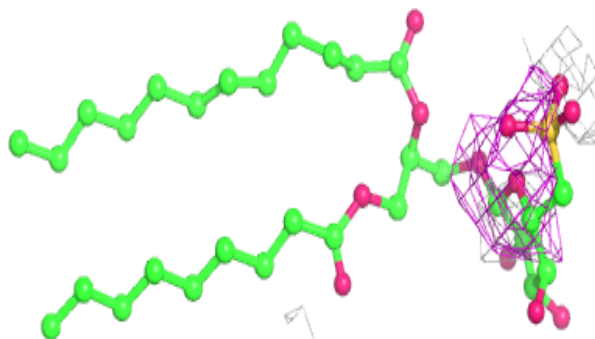


Electron density around LMT B 623:

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

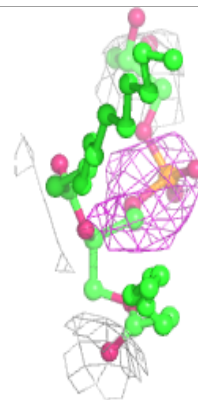
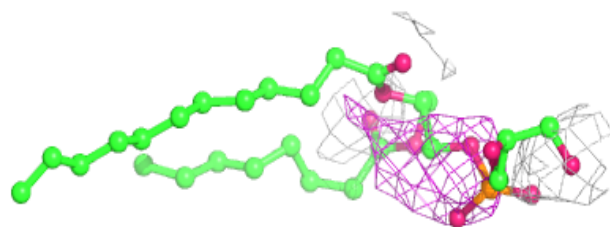
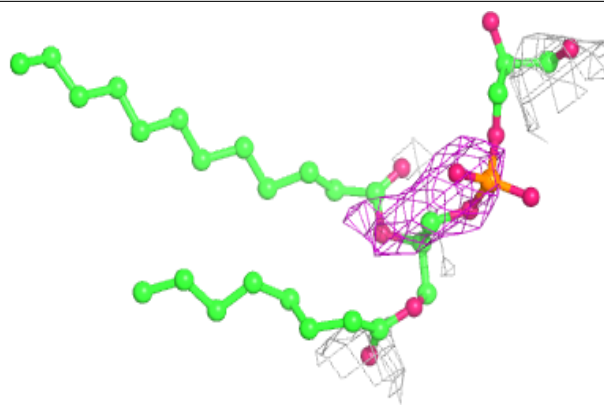
**Electron density around SQD d 402:**

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

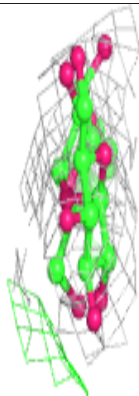
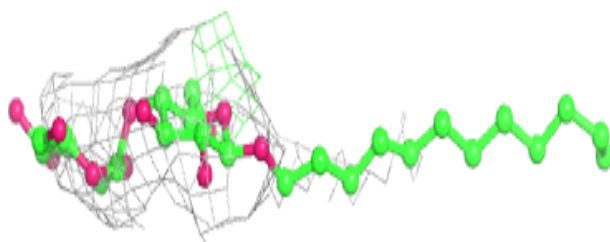
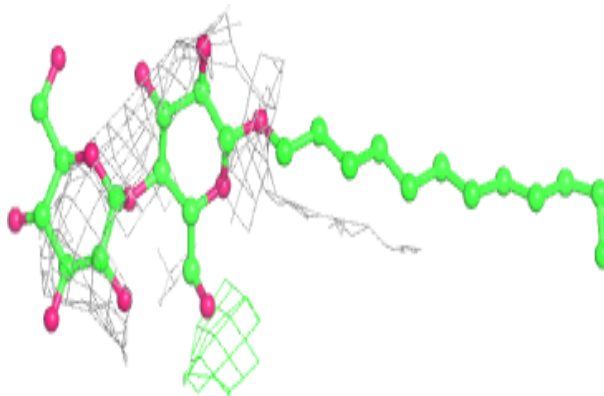


Electron density around LHG c 519:

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

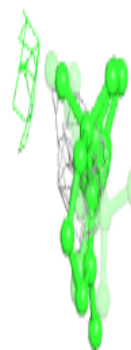
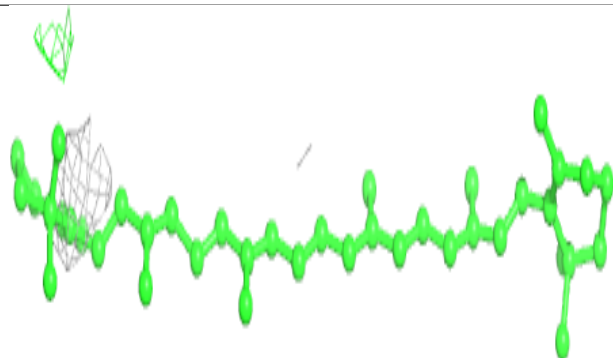
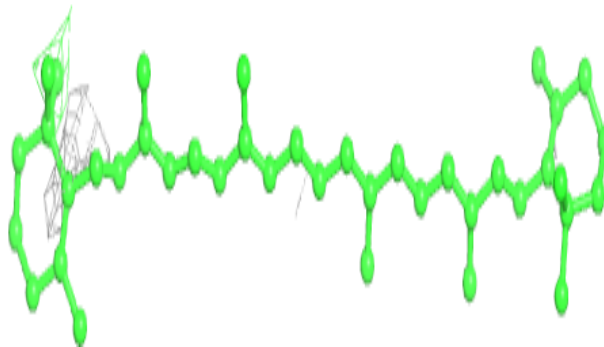
**Electron density around LMT b 603:**

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

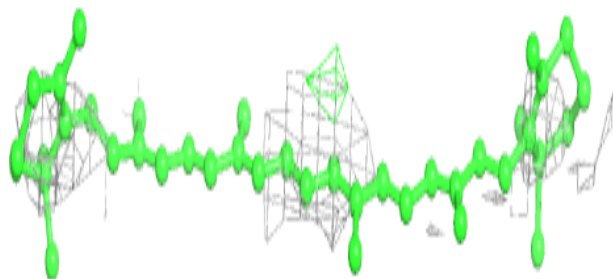
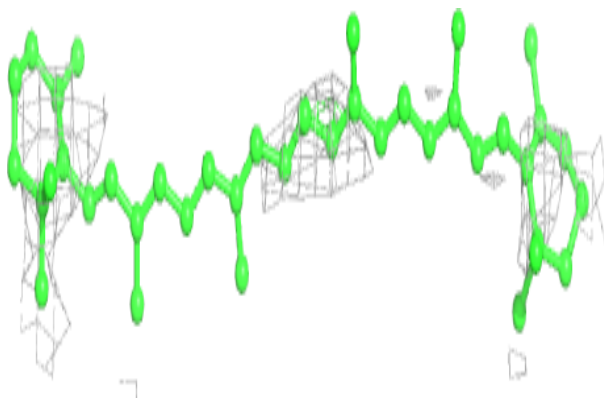


Electron density around BCR j 102:

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

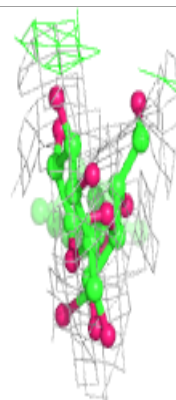
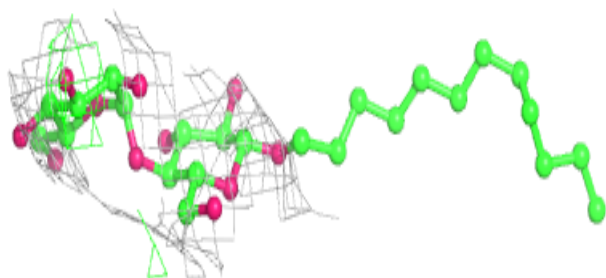
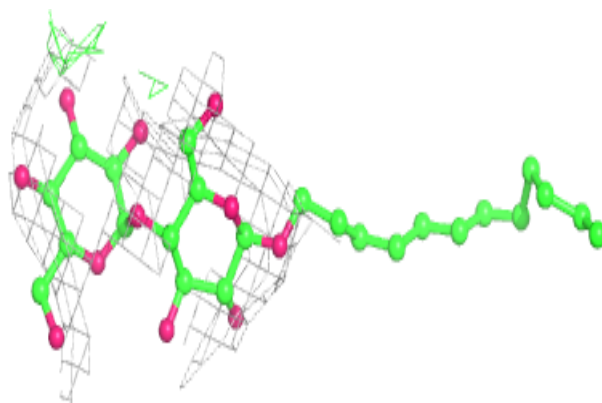
**Electron density around BCR C 514:**

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

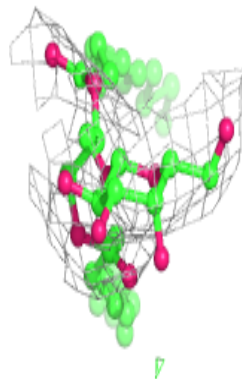
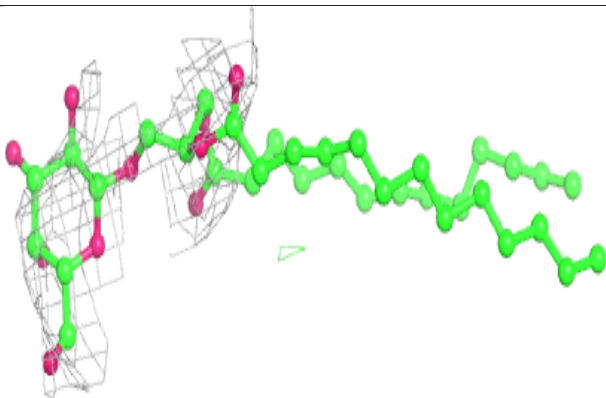
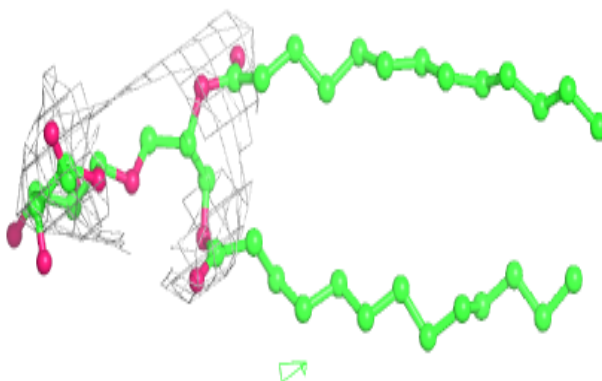


Electron density around LMT B 628:

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

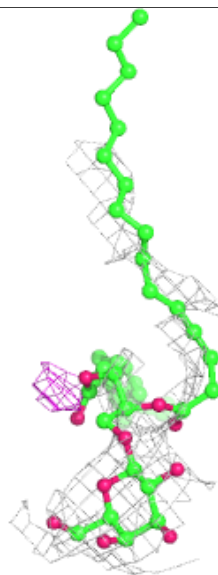
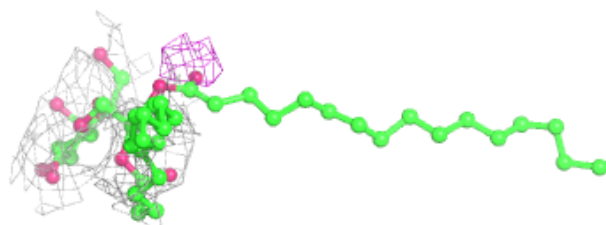
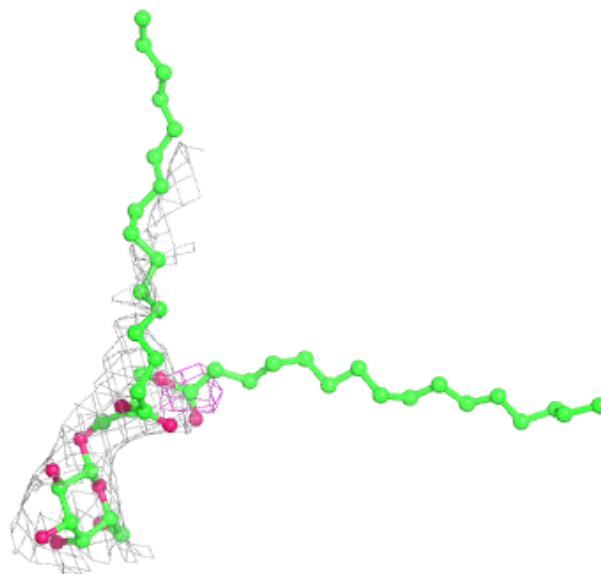
**Electron density around LMG c 518:**

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



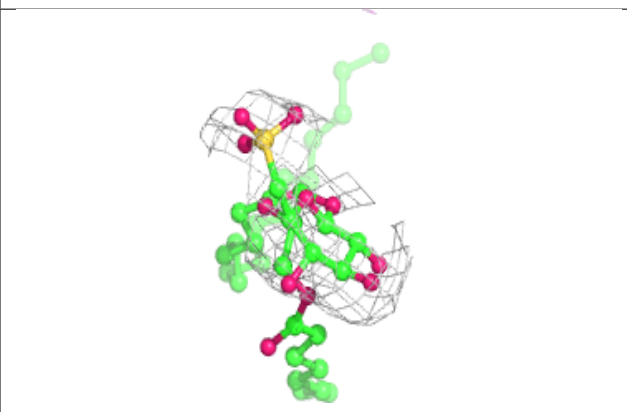
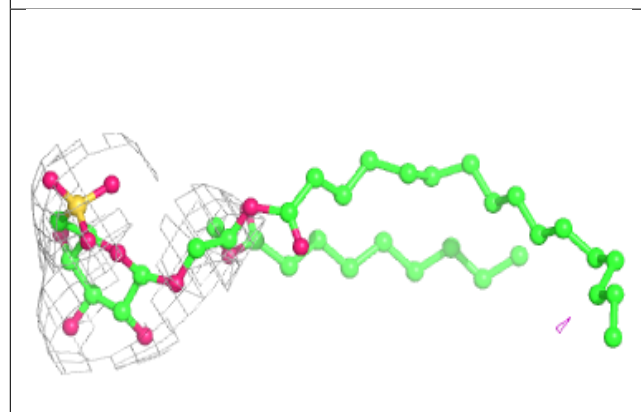
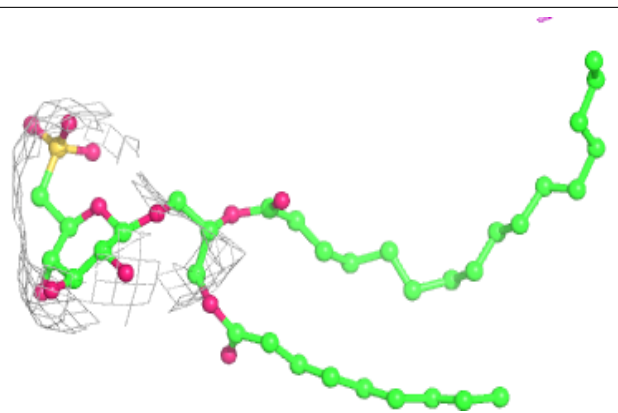
Electron density around LMG 1 101:

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

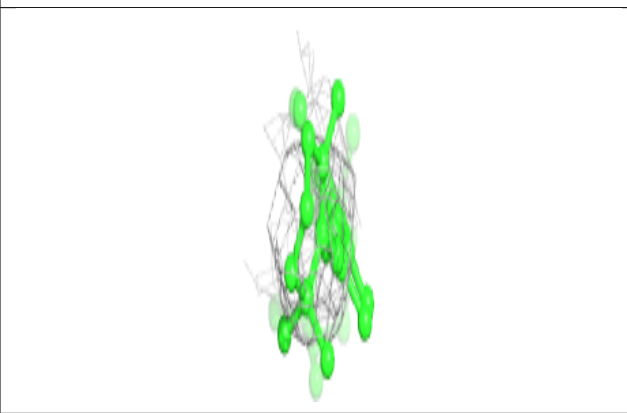
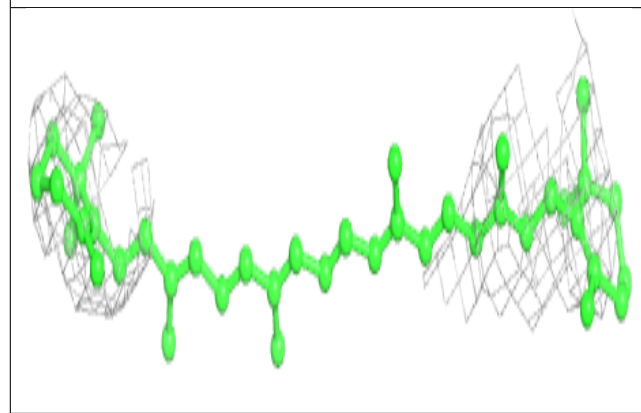
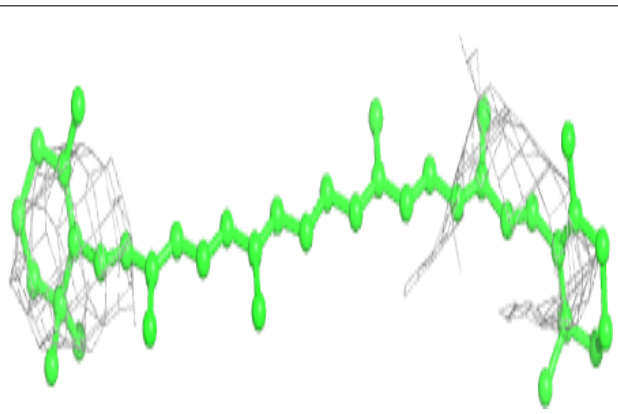


Electron density around SQD B 626:

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

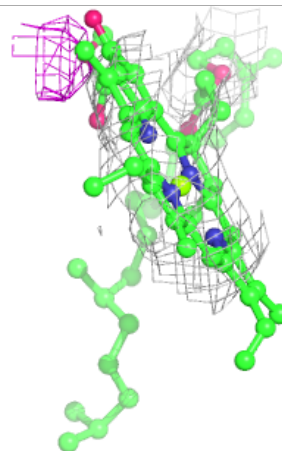
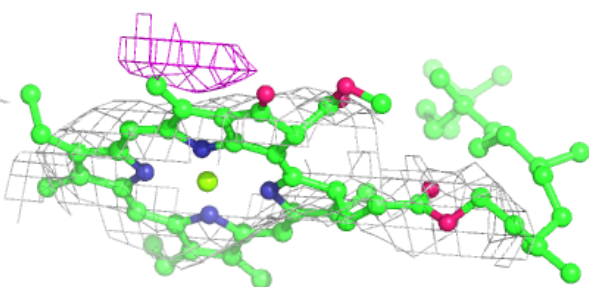
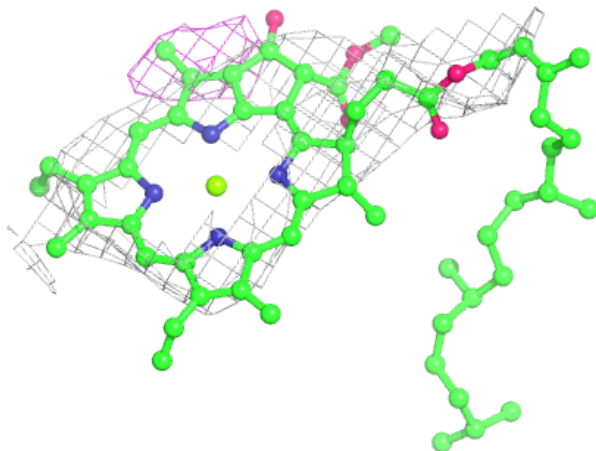
**Electron density around BCR b 623:**

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



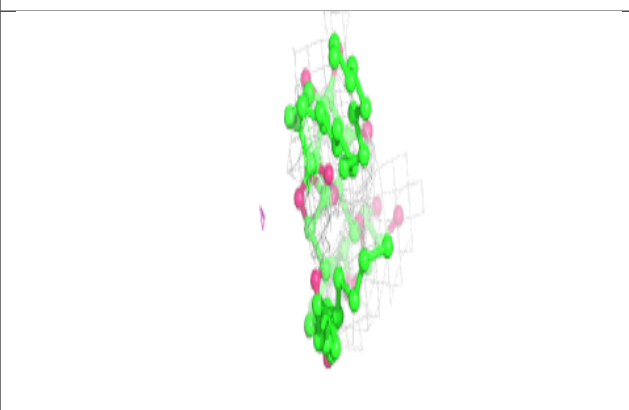
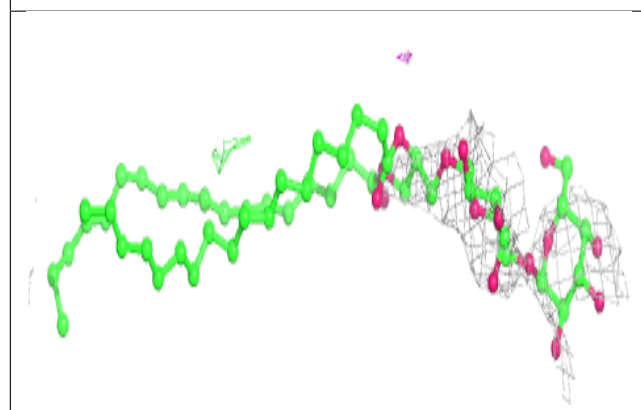
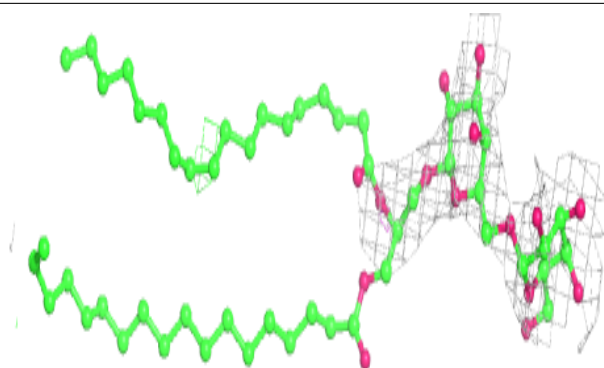
Electron density around CLA b 619:

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

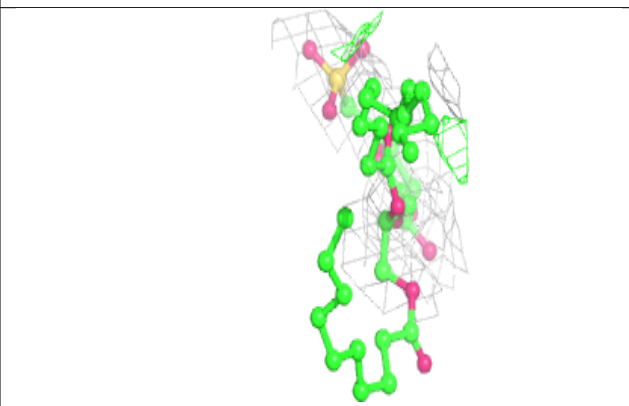
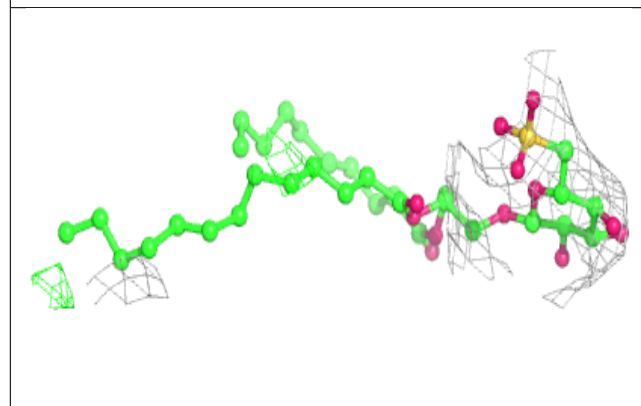
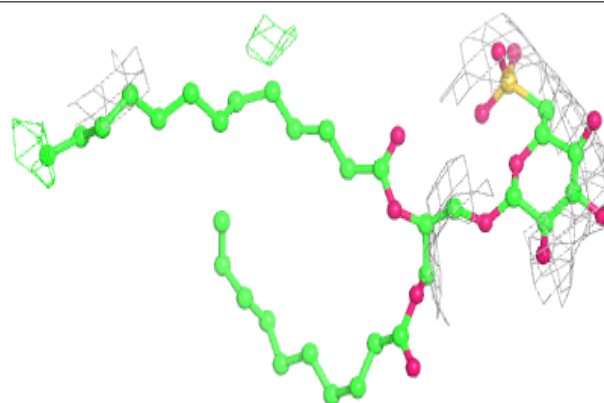


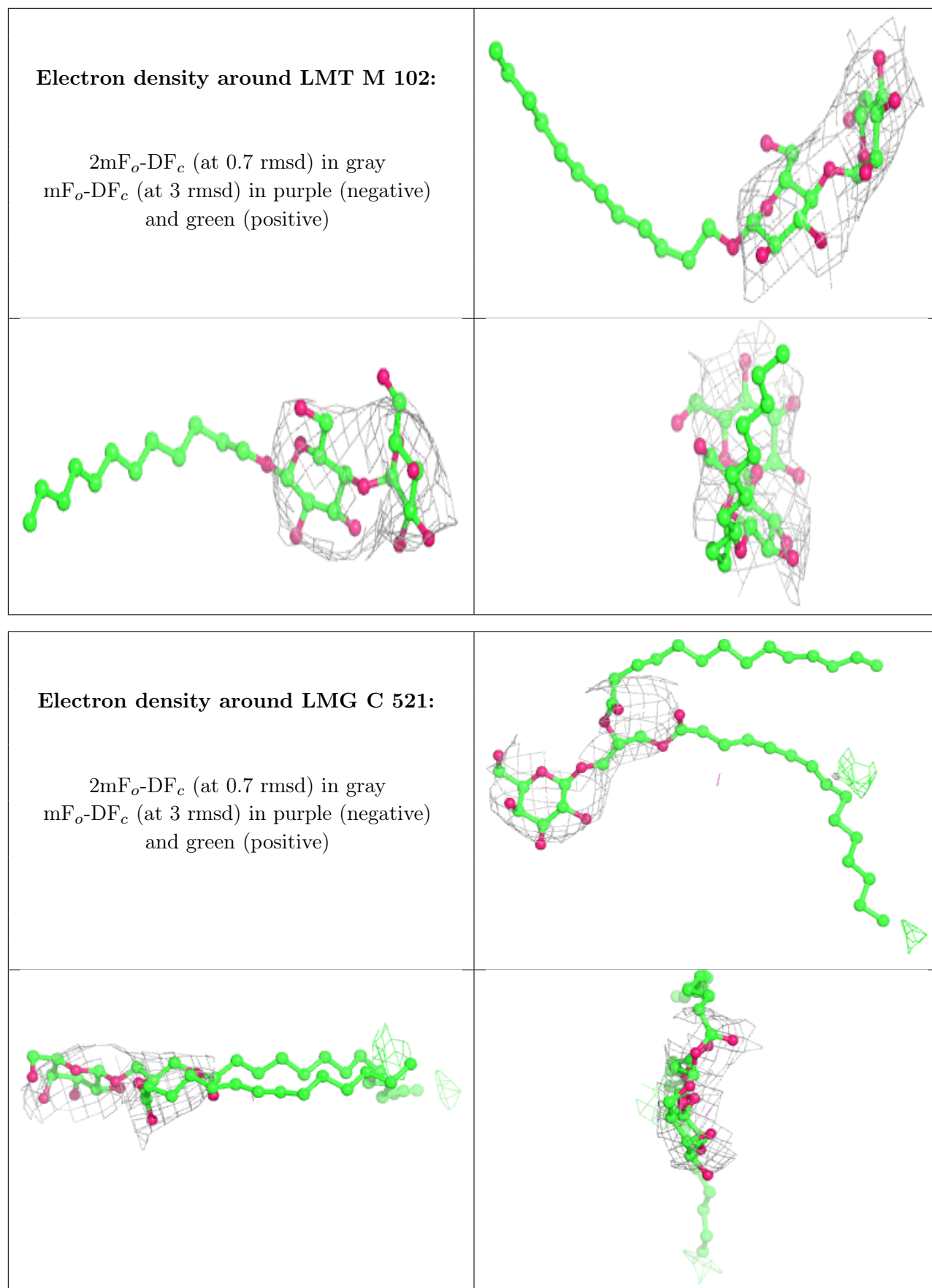
Electron density around DGD C 517:

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

**Electron density around SQD F 103:**

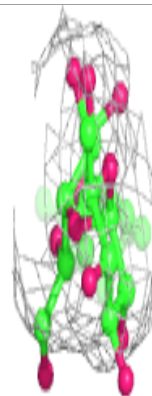
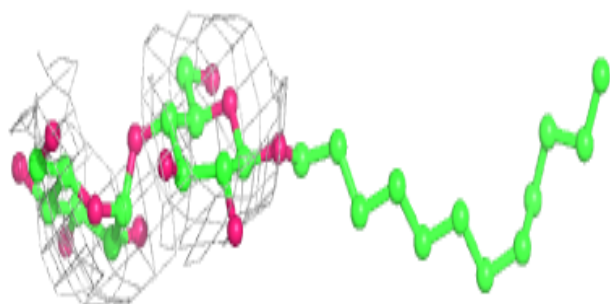
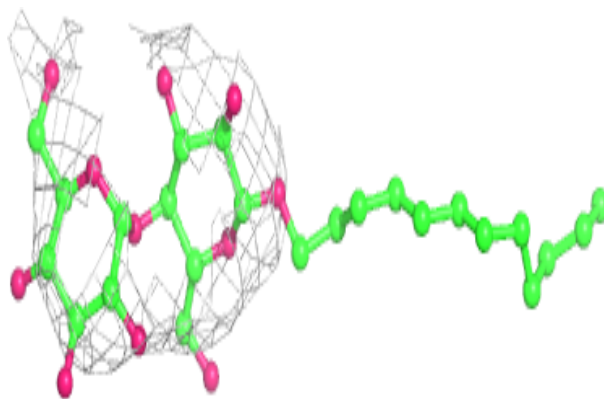
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



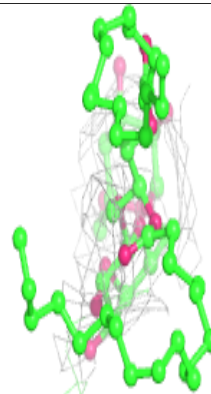
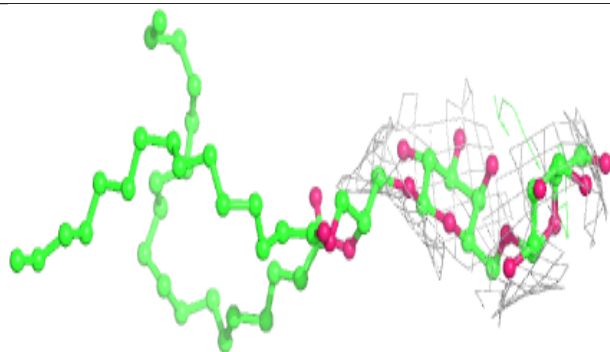
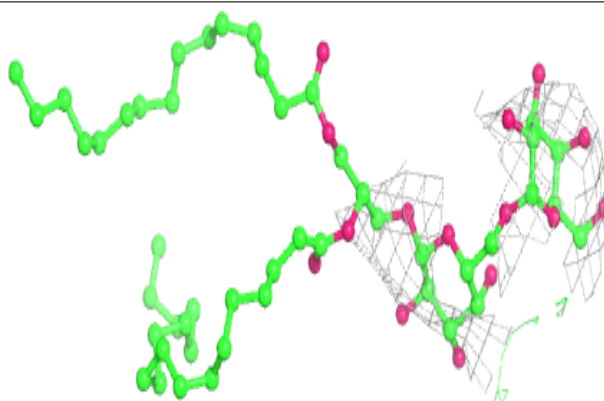


Electron density around LMT b 604:

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

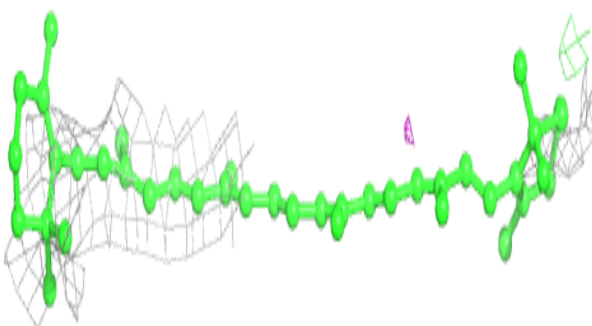
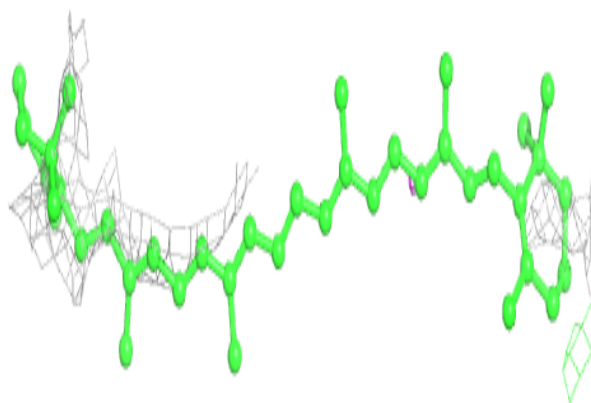
**Electron density around DGD D 409:**

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

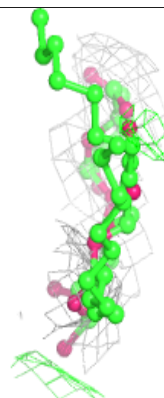
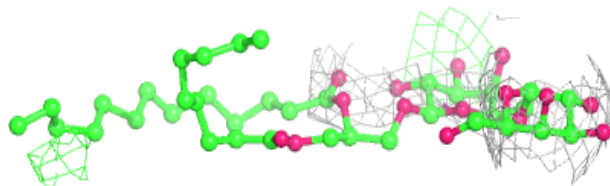
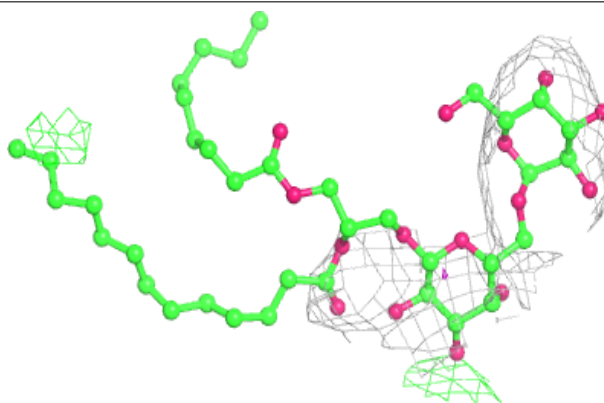


Electron density around BCR H 102:

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

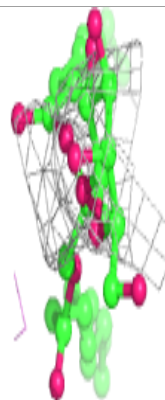
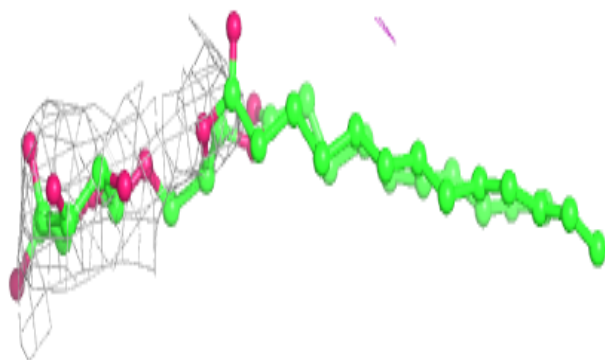
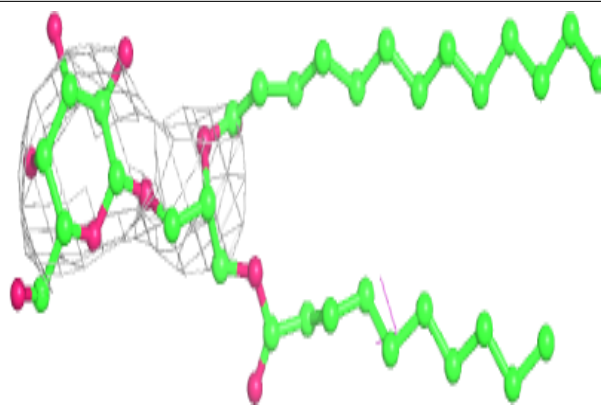
**Electron density around DGD B 625:**

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

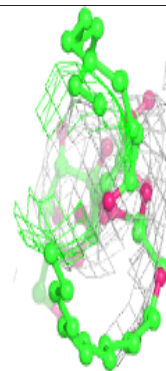
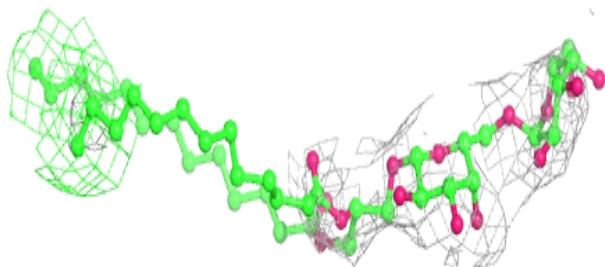
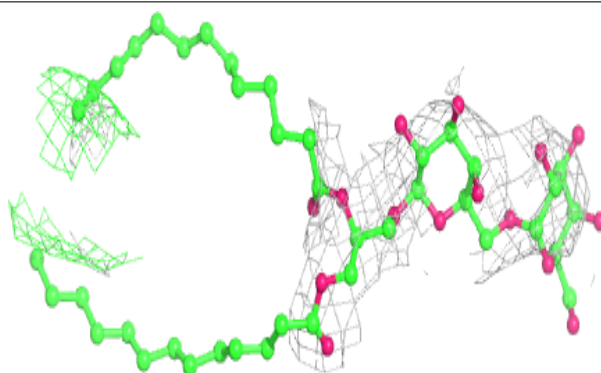


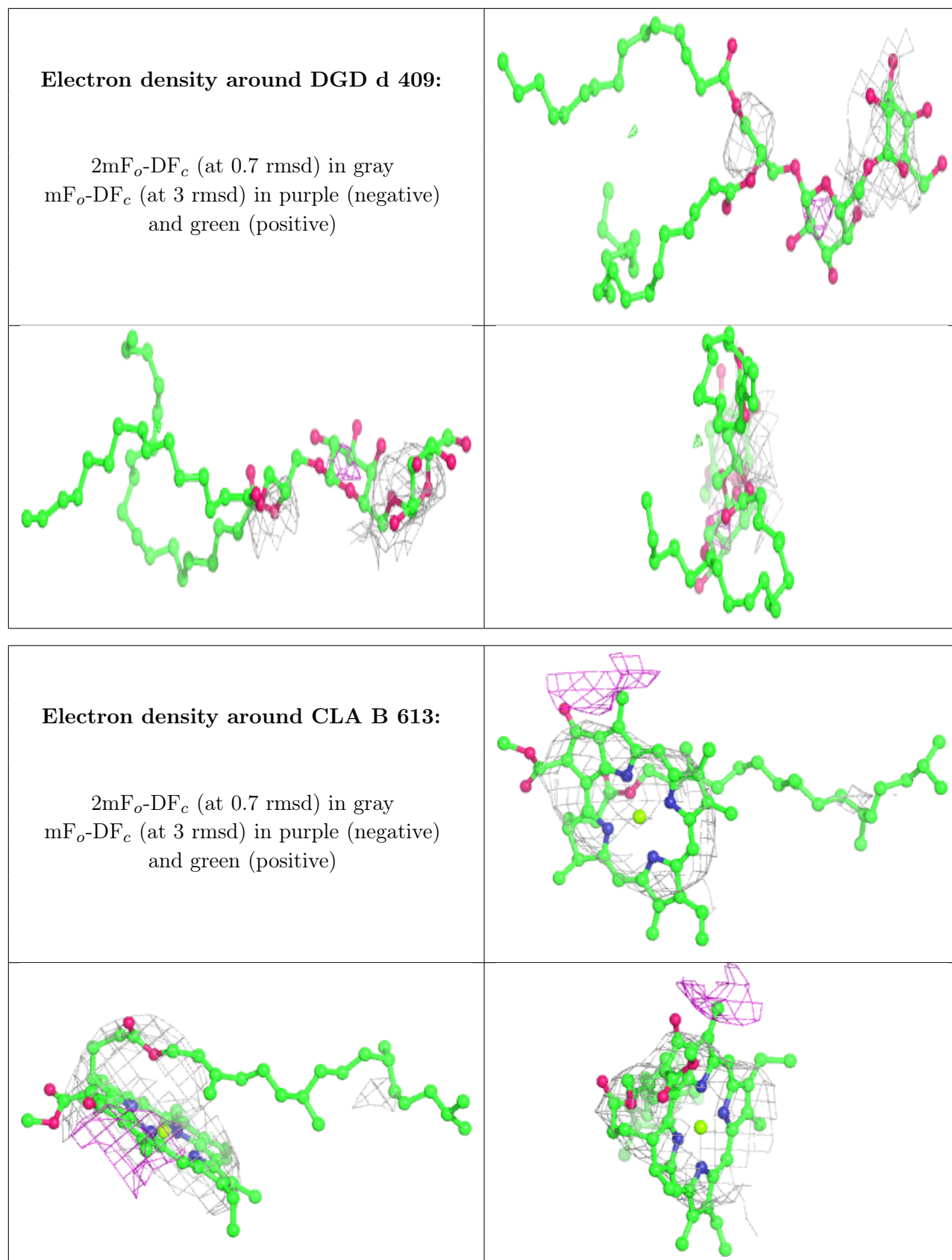
Electron density around LMG M 101:

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

**Electron density around DGD a 411:**

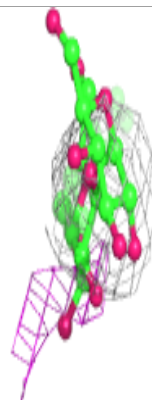
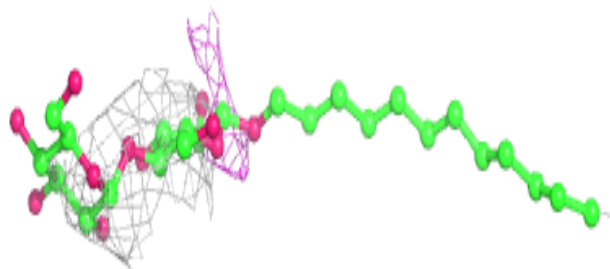
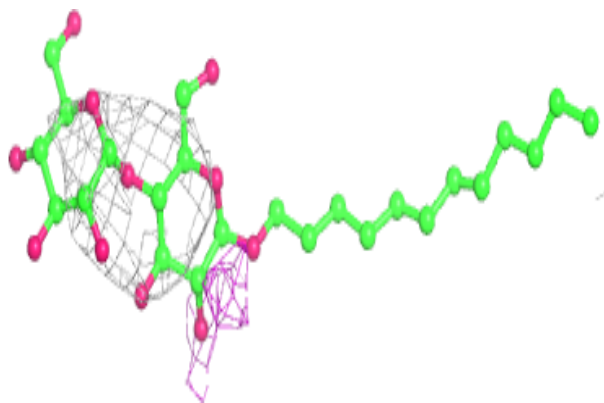
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



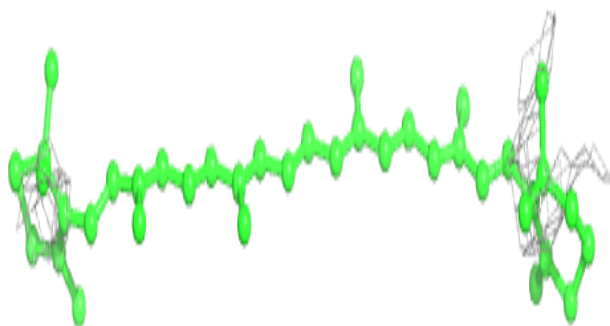
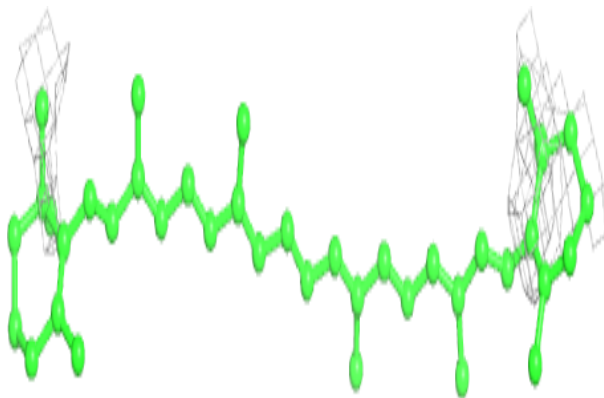


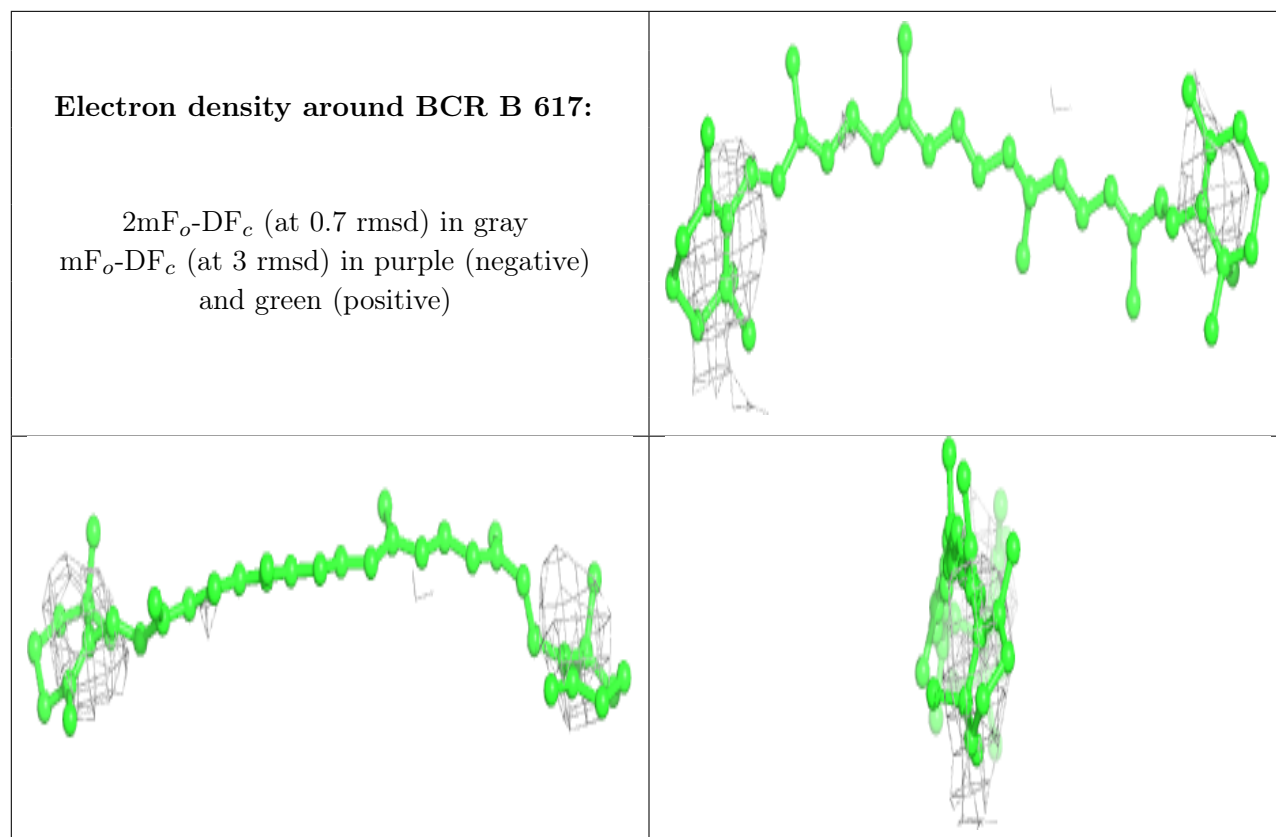
Electron density around LMT b 627:

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

**Electron density around BCR c 514:**

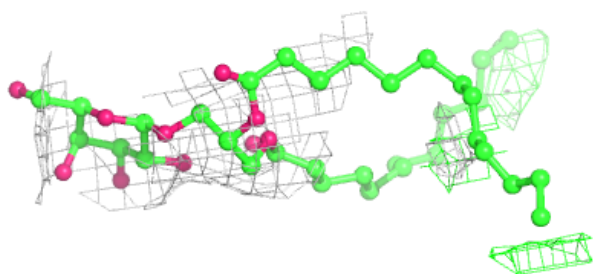
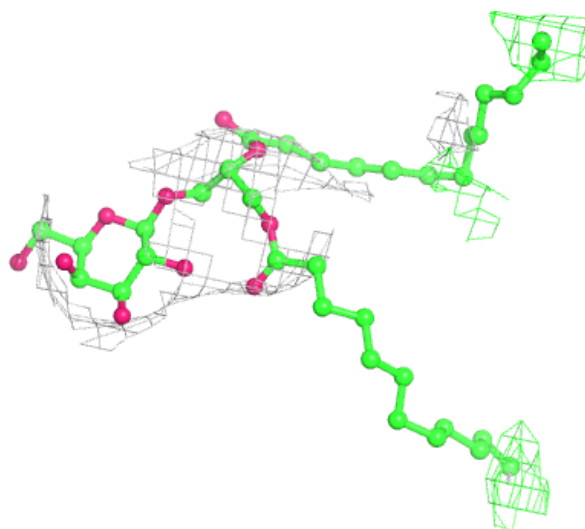
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

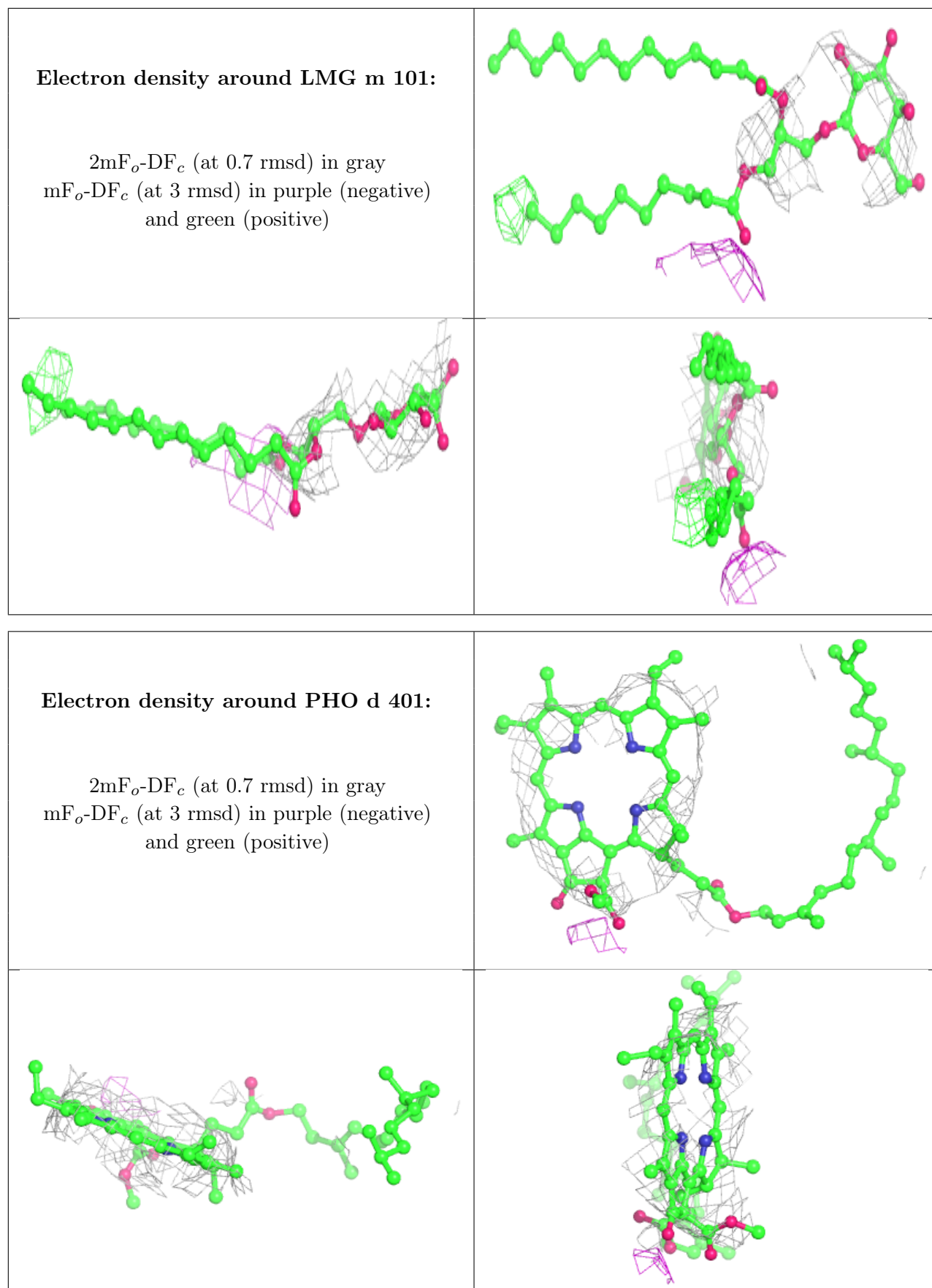


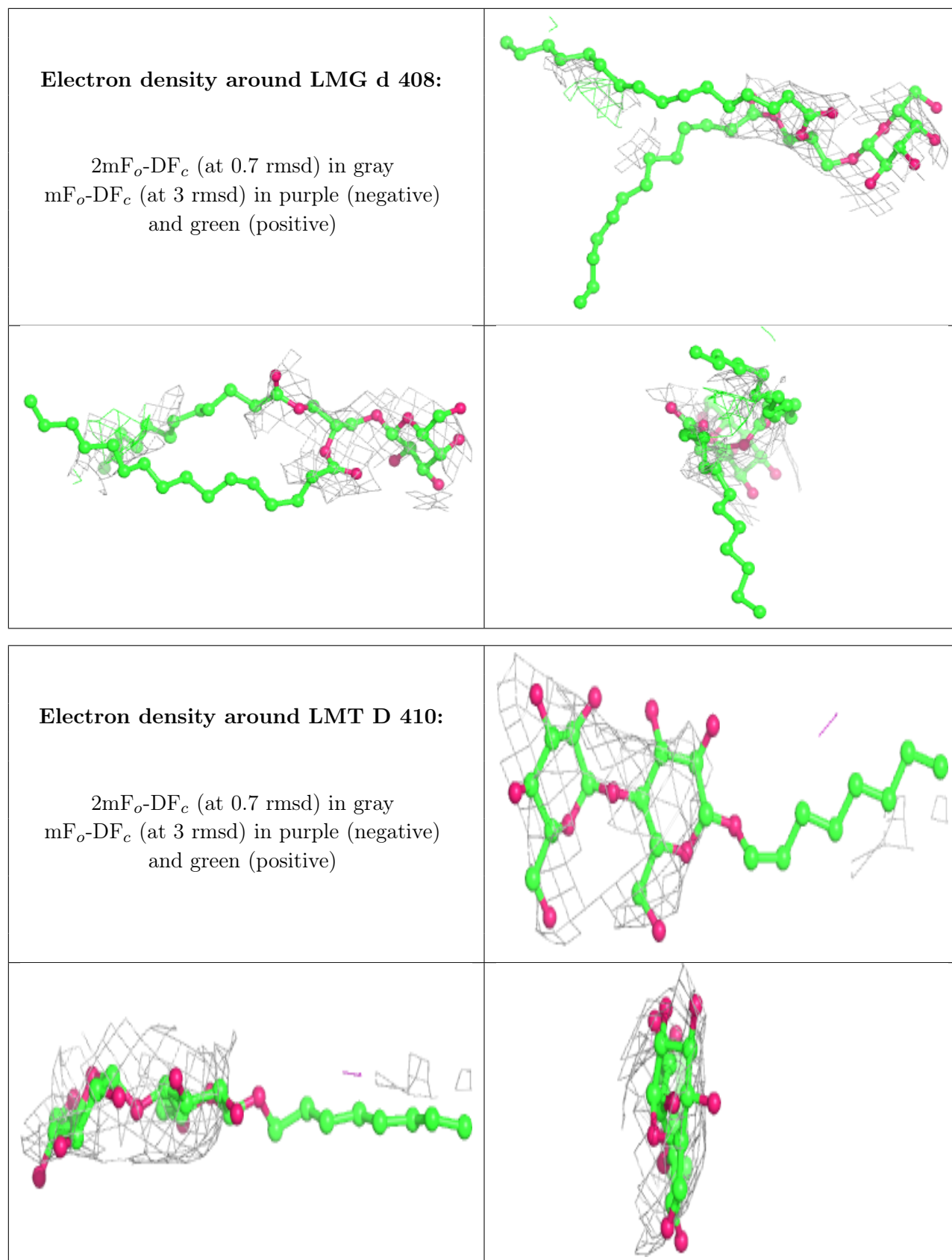


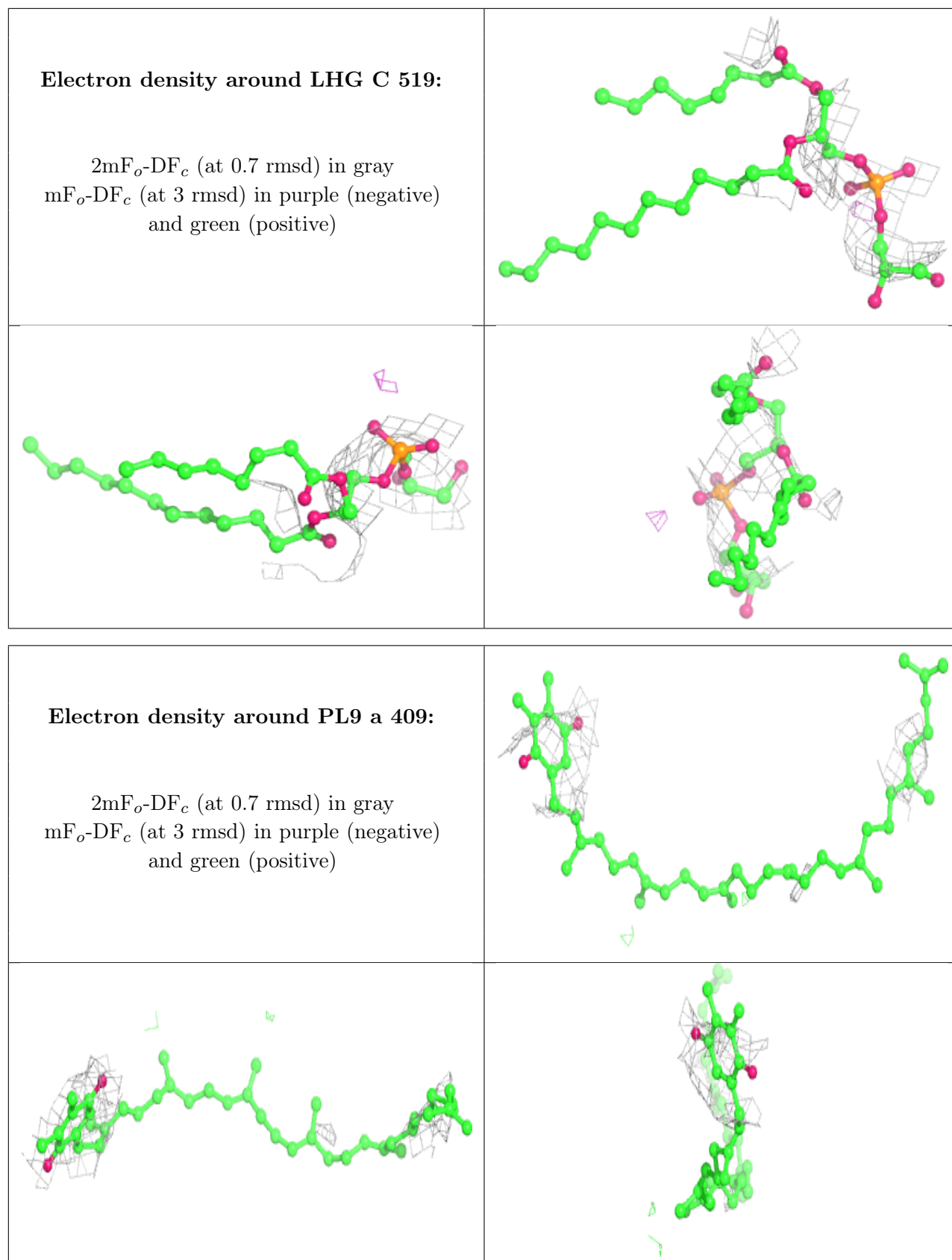
Electron density around LMG e 101:

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



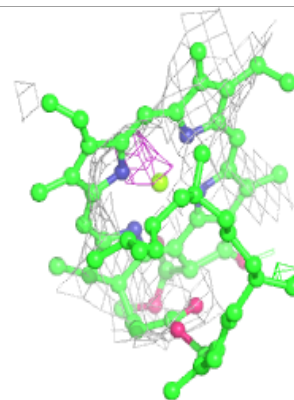
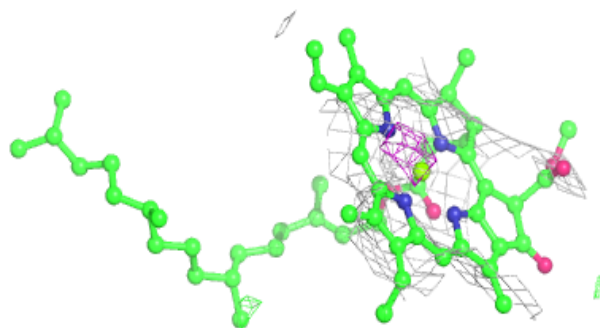
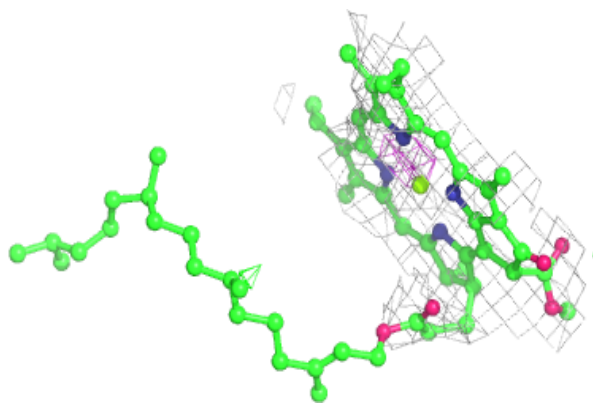




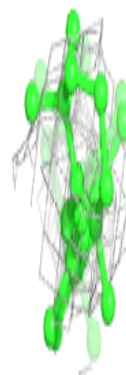
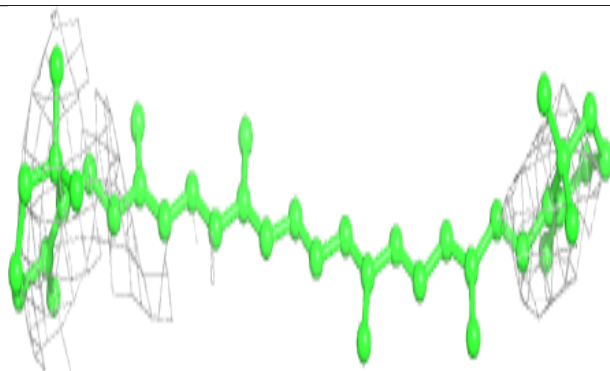
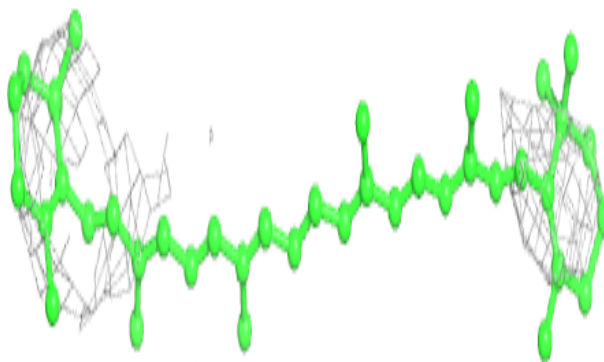


Electron density around CLA c 512:

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

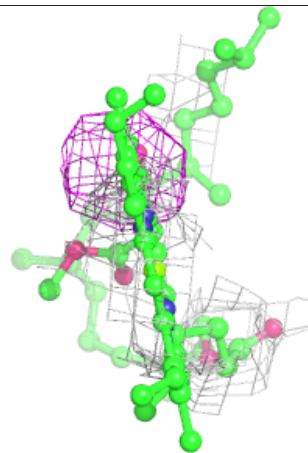
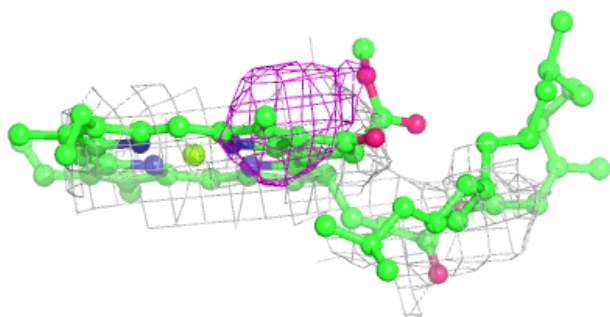
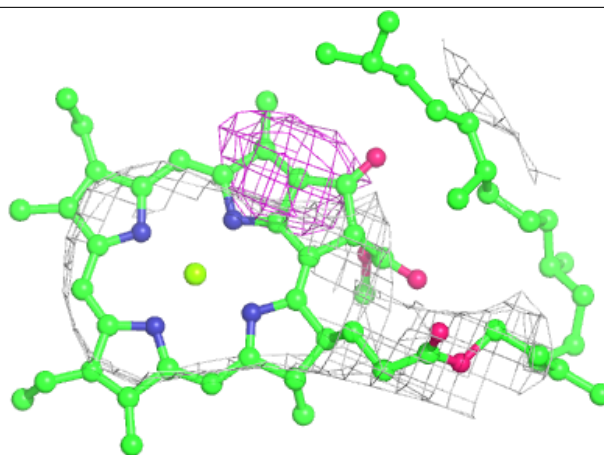
**Electron density around BCR B 619:**

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



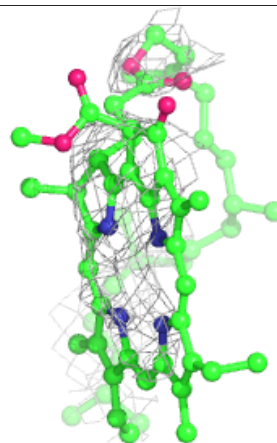
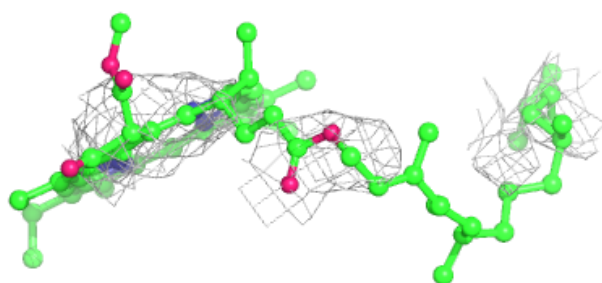
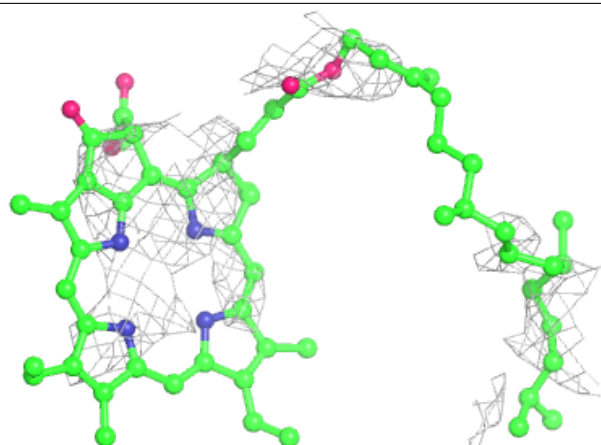
Electron density around CLA b 613:

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

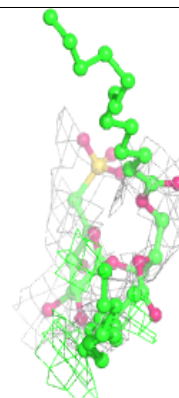
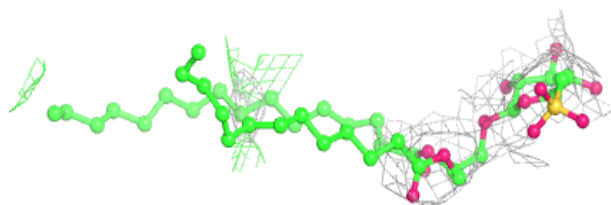
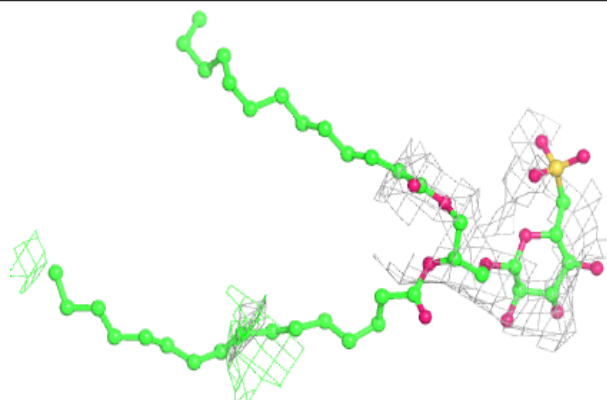


Electron density around PHO D 402:

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

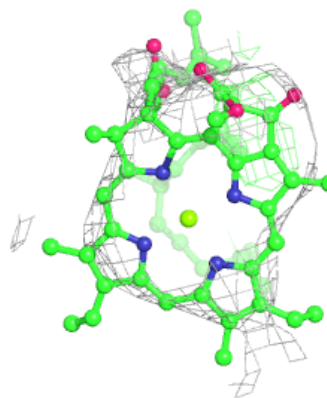
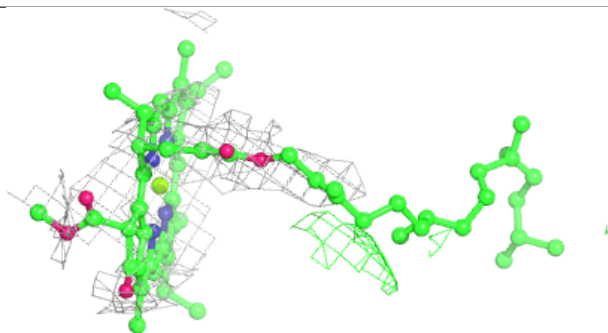
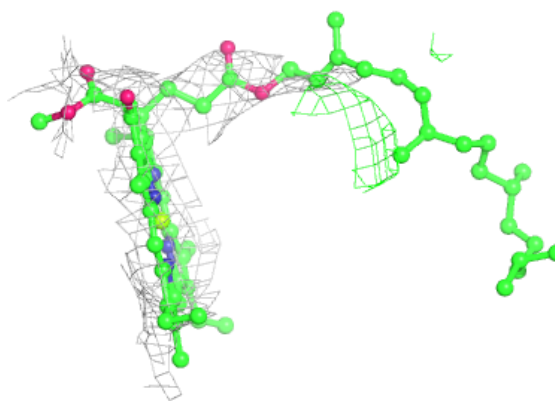
**Electron density around SQD A 413:**

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

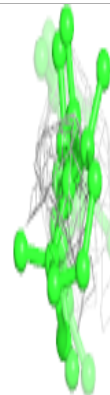
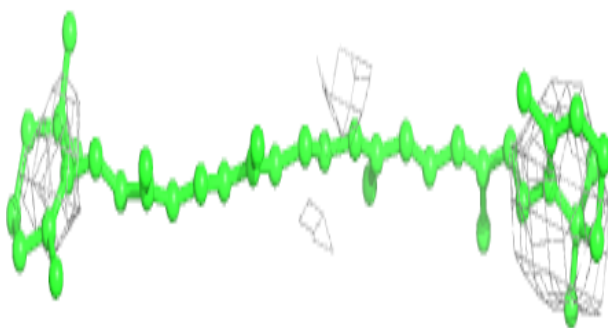
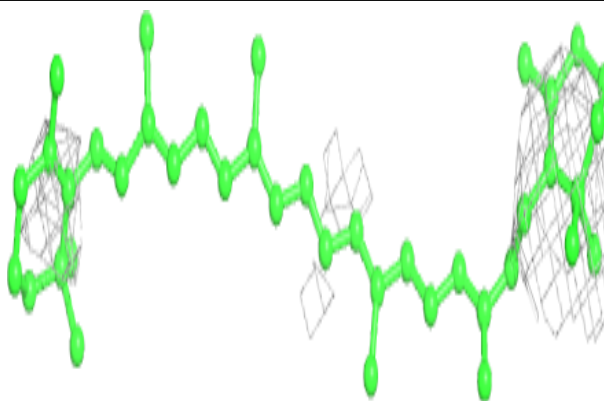


Electron density around CLA C 505:

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

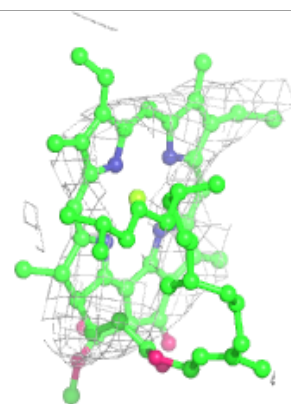
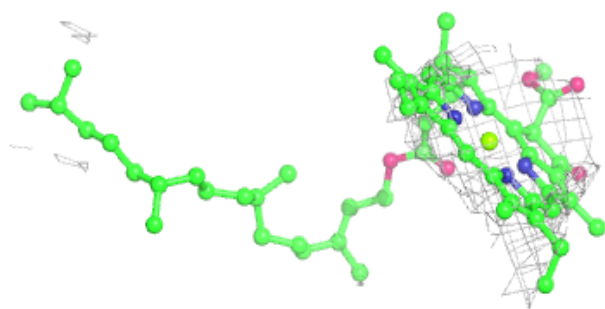
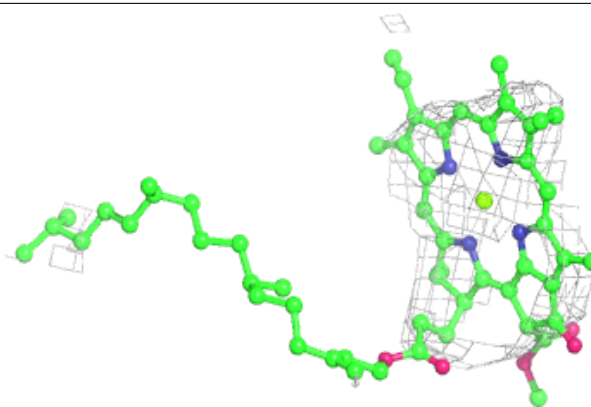
**Electron density around BCR y 101:**

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

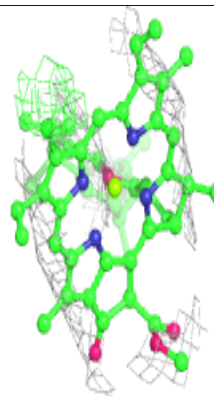
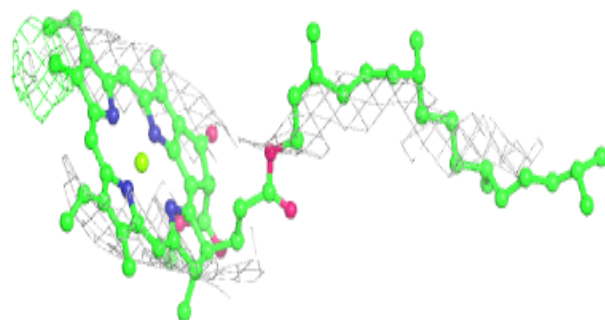
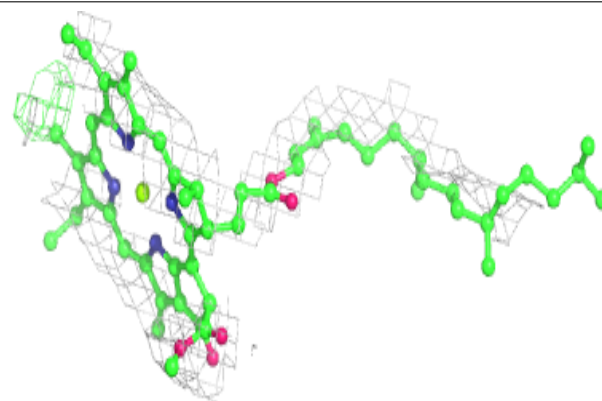


Electron density around CLA c 510:

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

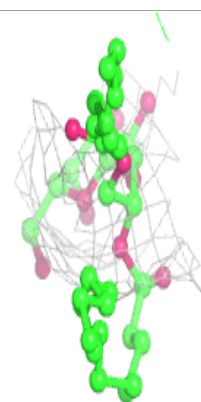
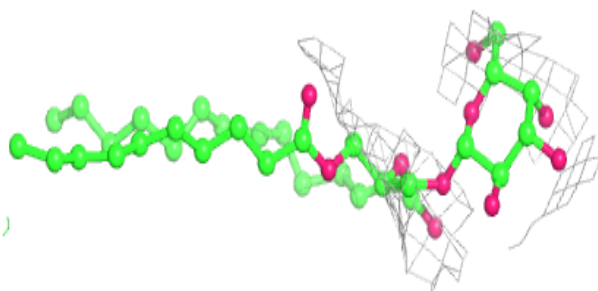
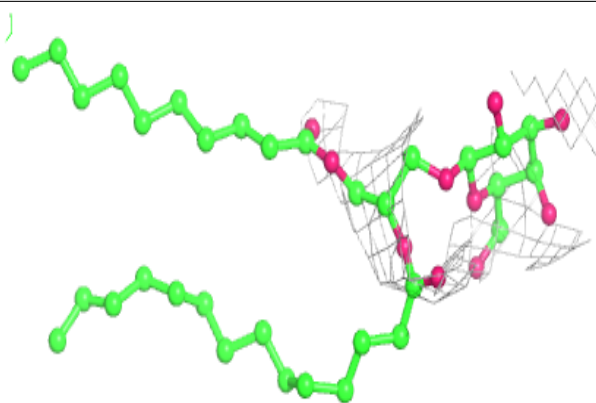
**Electron density around CLA C 502:**

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

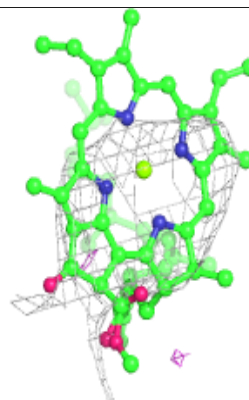
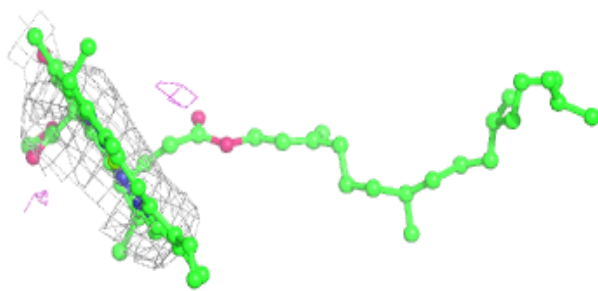
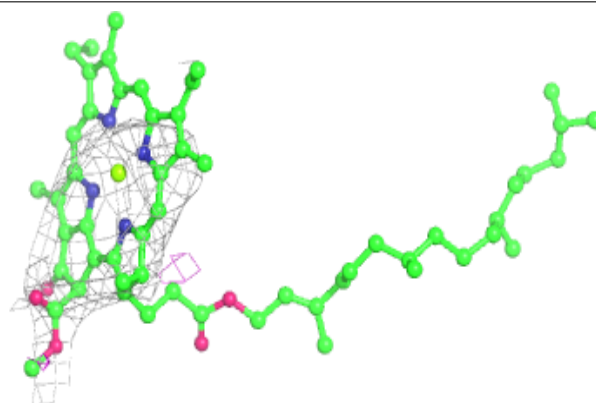


Electron density around LMG i 101:

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

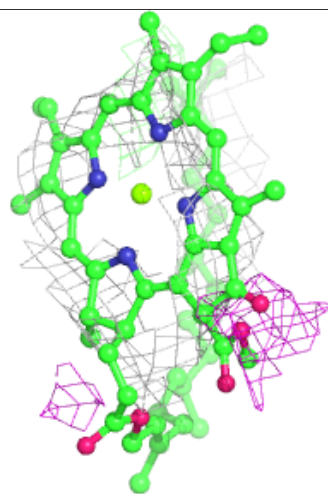
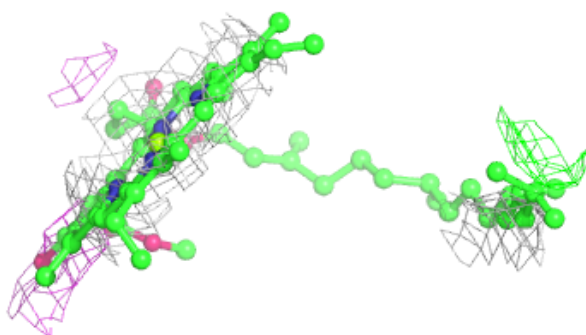
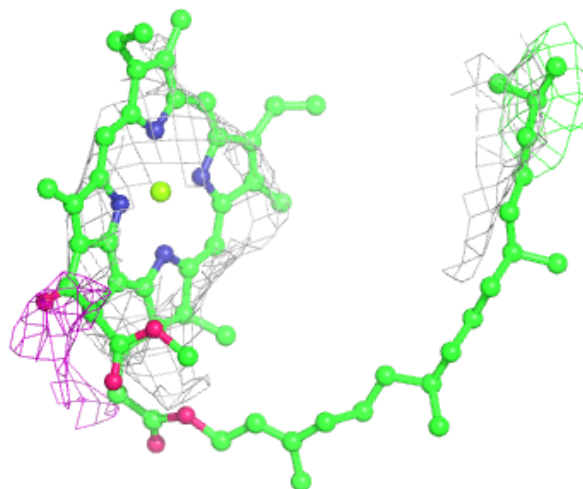
**Electron density around CLA a 408:**

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



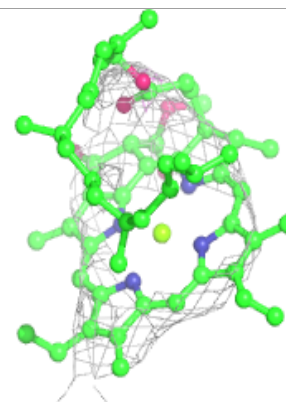
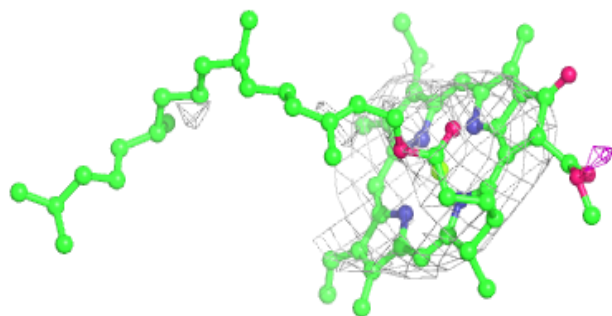
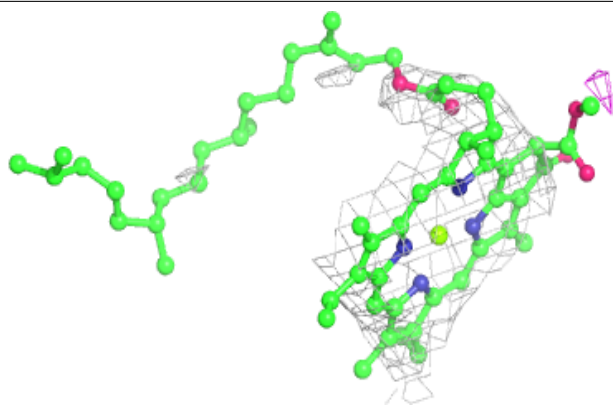
Electron density around CLA C 506:

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

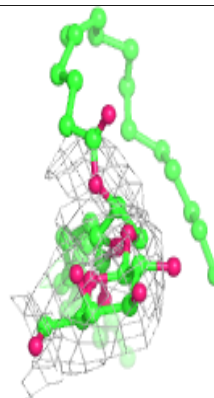
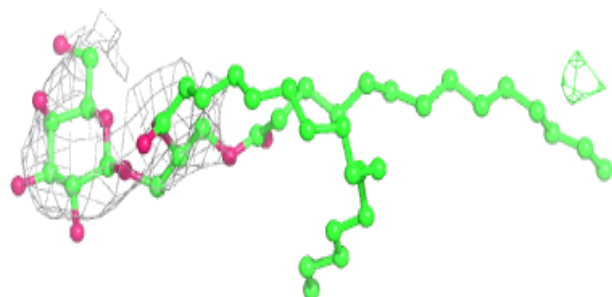
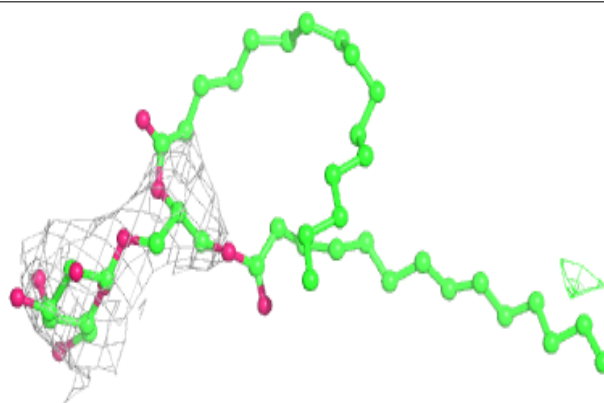


Electron density around CLA C 512:

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

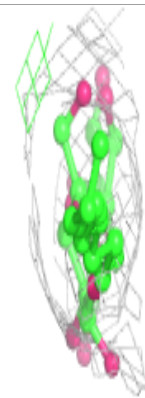
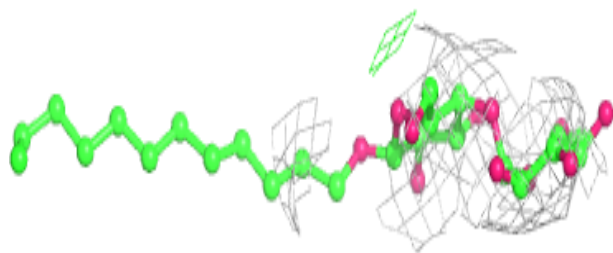
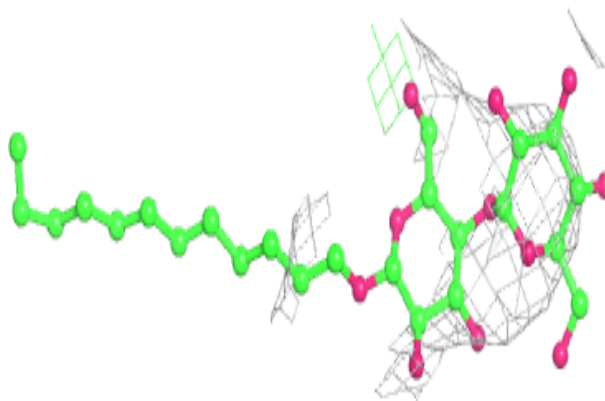
**Electron density around LMG D 407:**

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

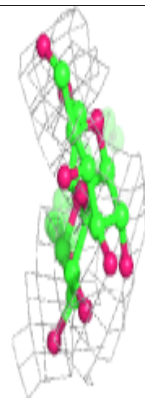
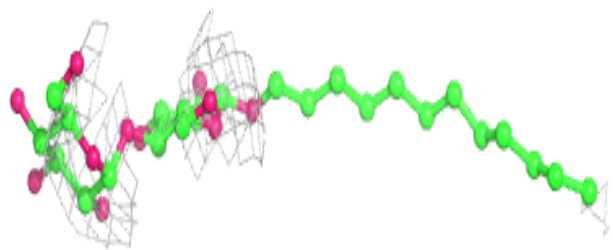
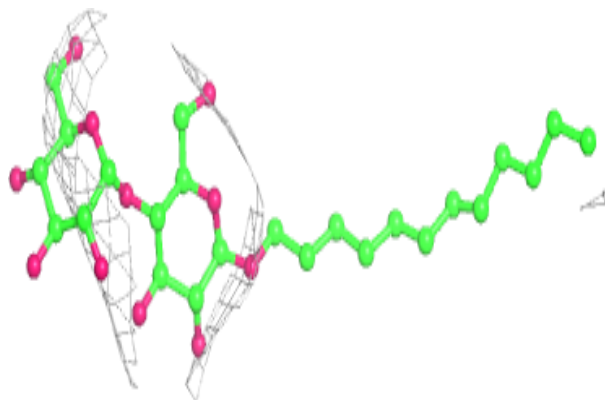


Electron density around LMT B 627:

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

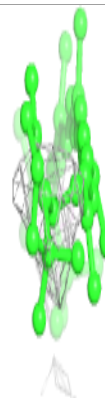
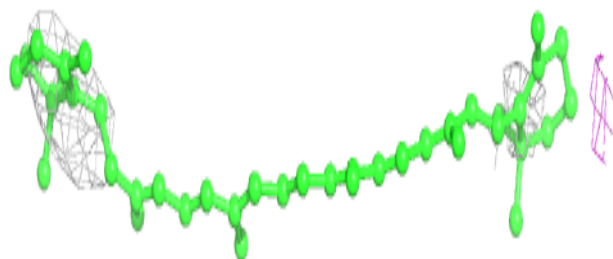
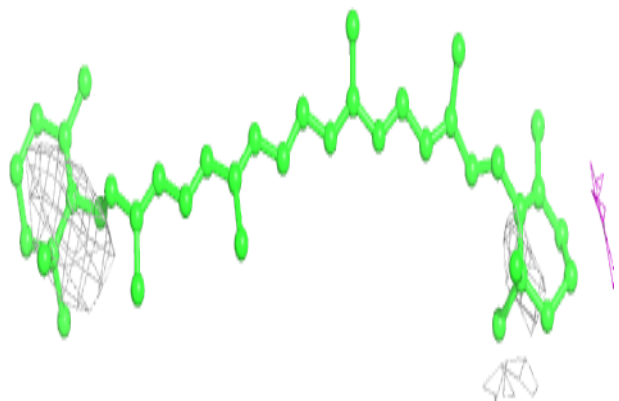
**Electron density around LMT B 624:**

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

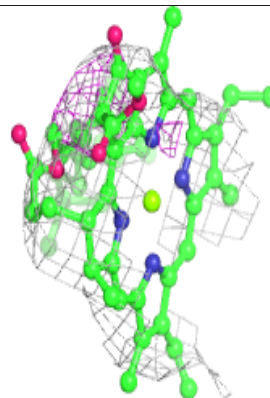
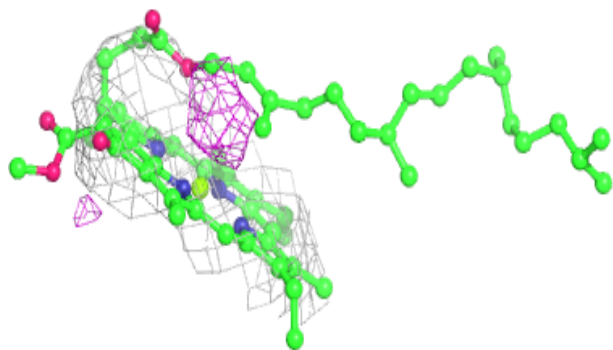
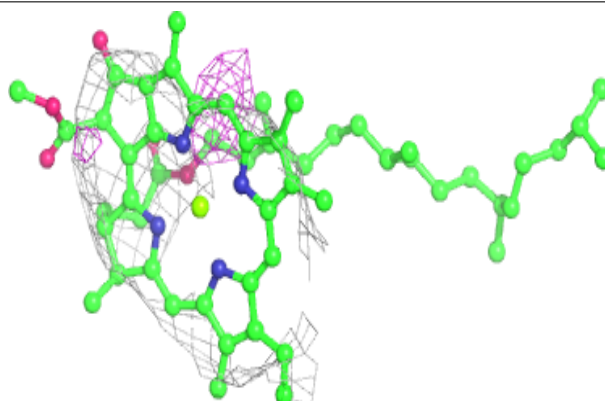


Electron density around BCR b 621:

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

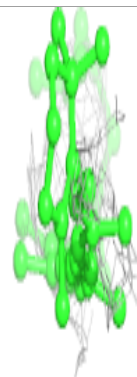
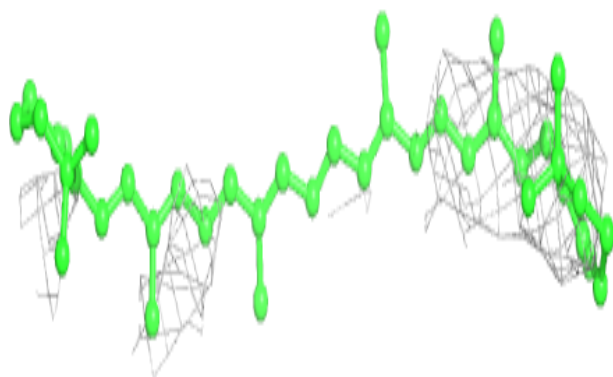
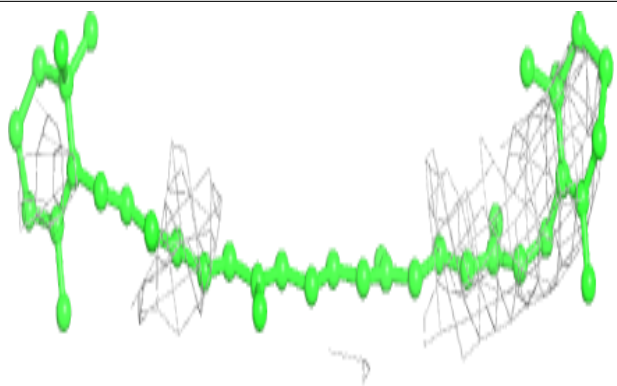
**Electron density around CLA b 617:**

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

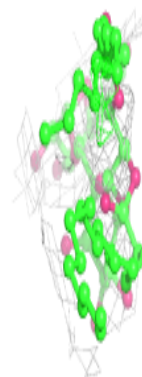
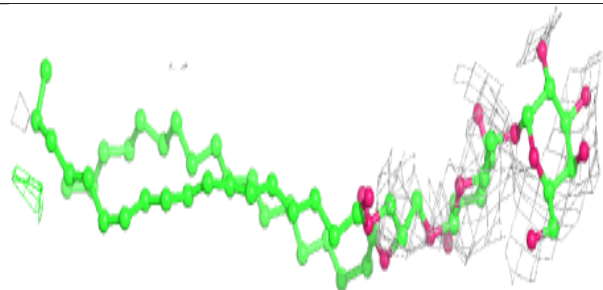
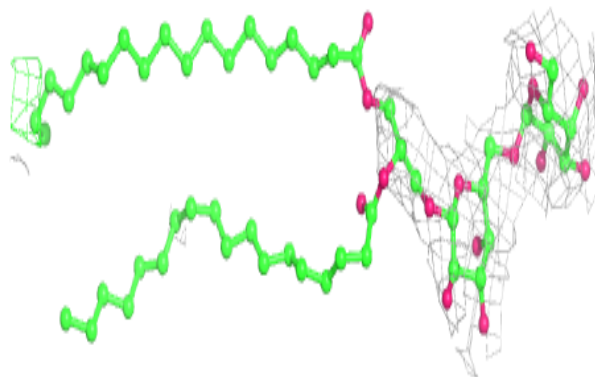


Electron density around BCR c 513:

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

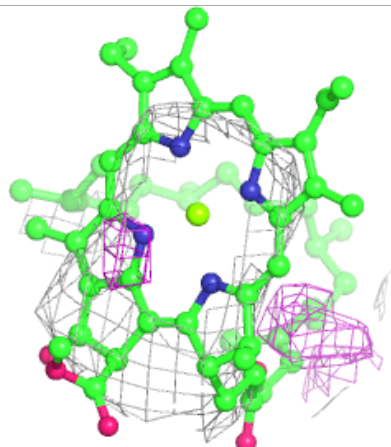
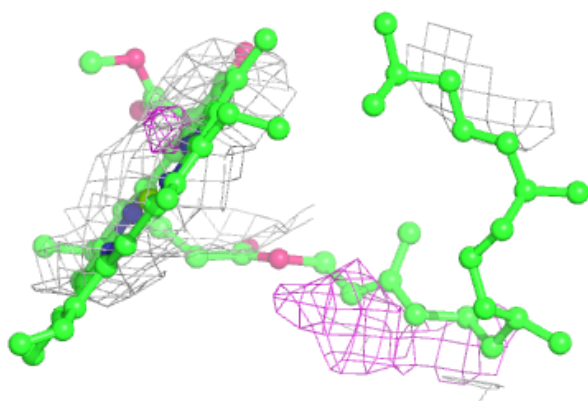
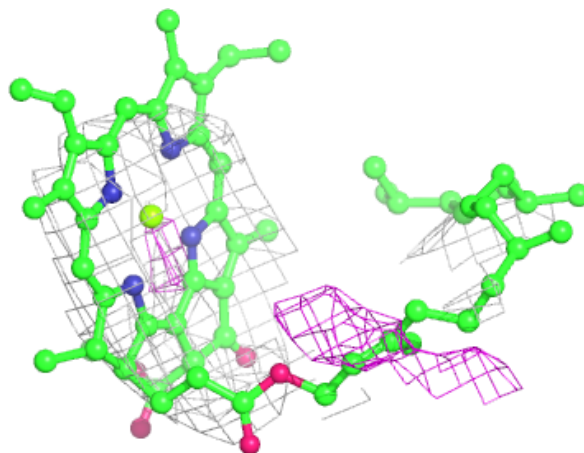
**Electron density around DGD c 517:**

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

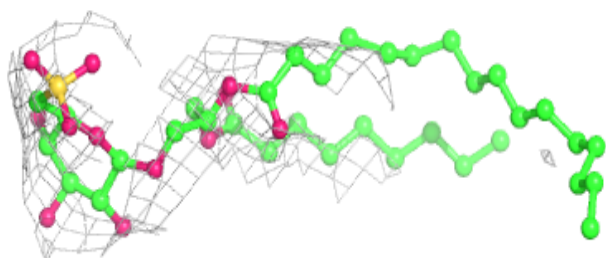
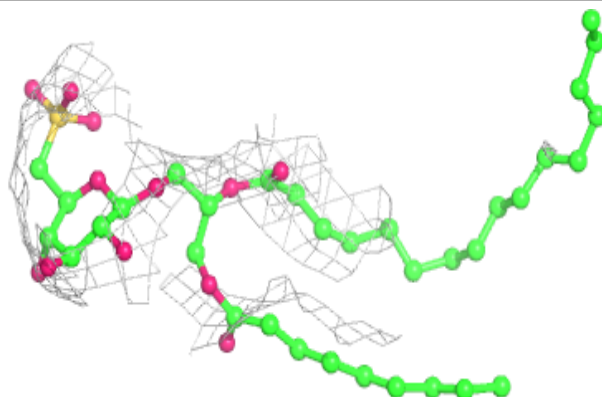


Electron density around CLA c 503:

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

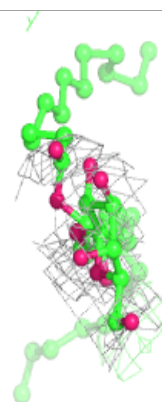
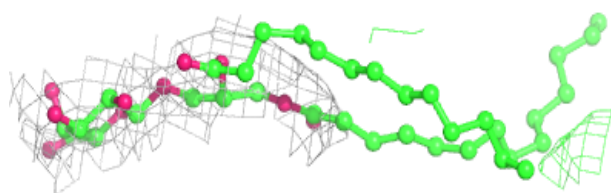
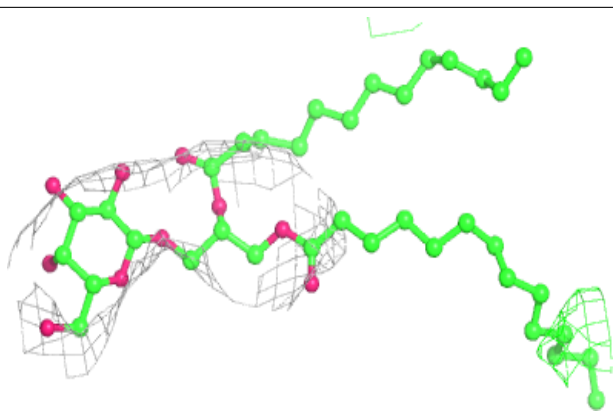
**Electron density around SQD b 602:**

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

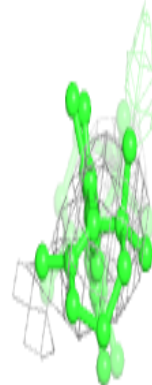
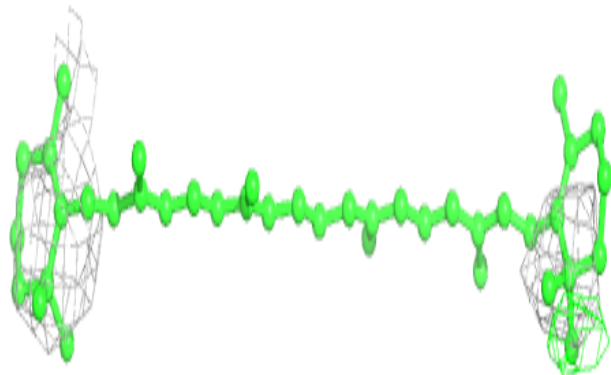
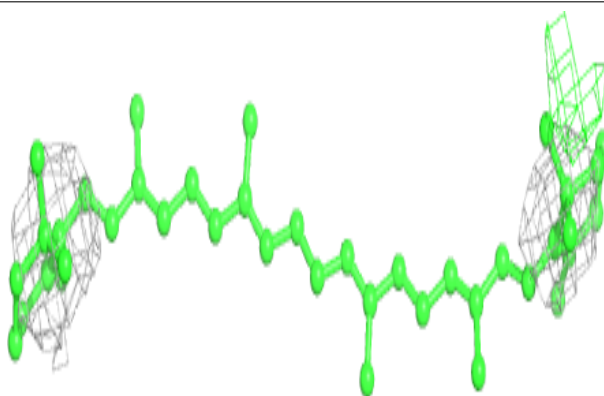


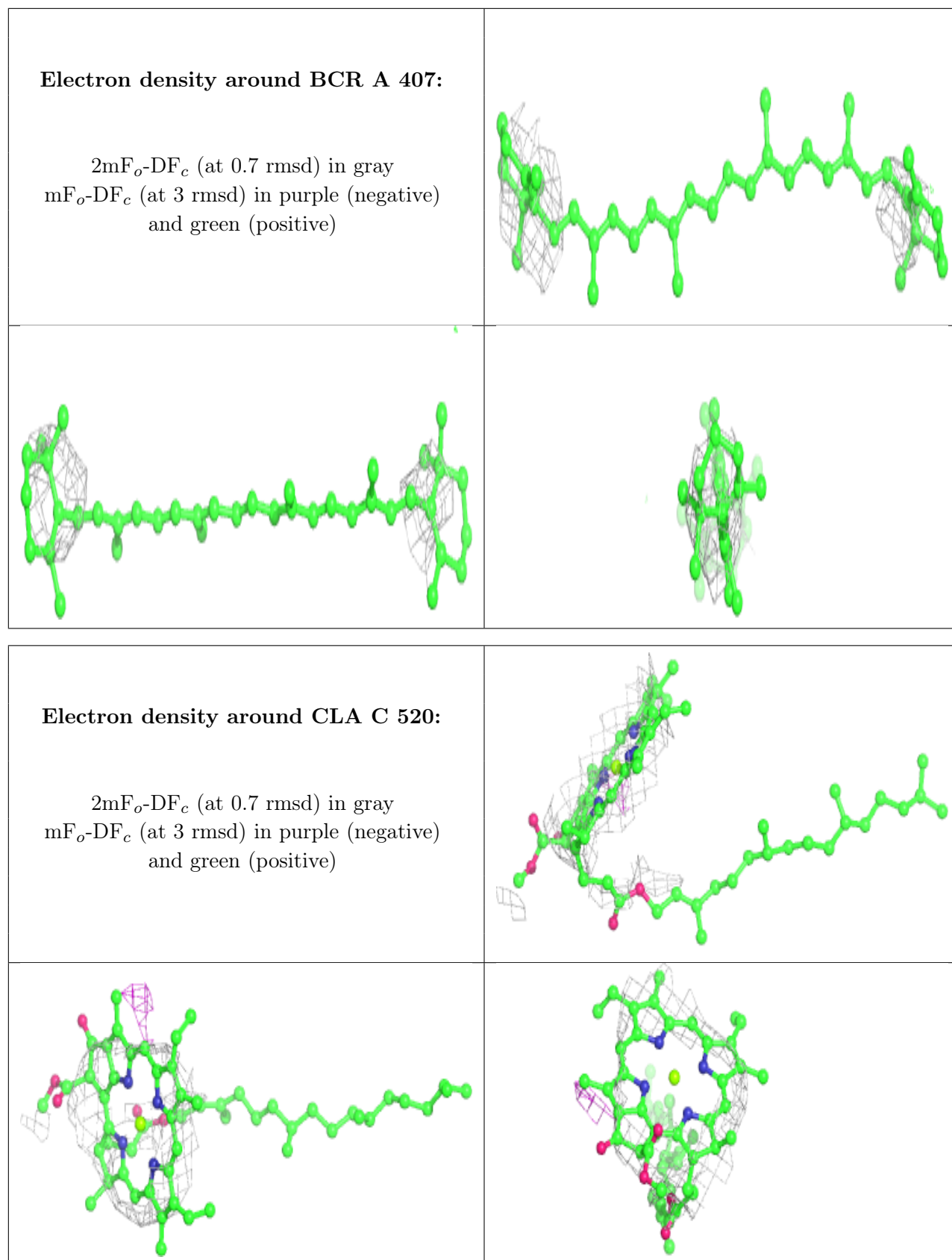
Electron density around LMG D 411:

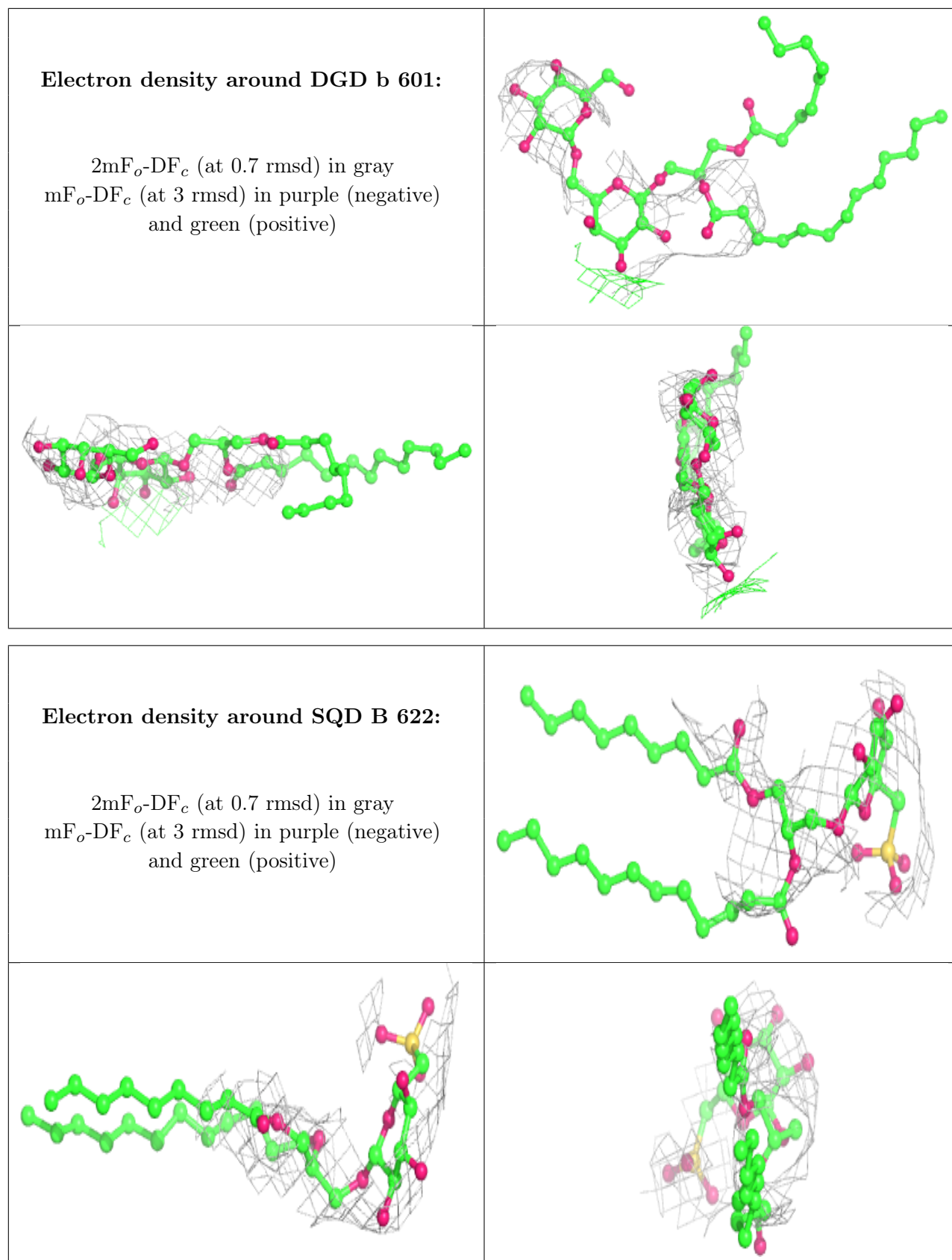
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

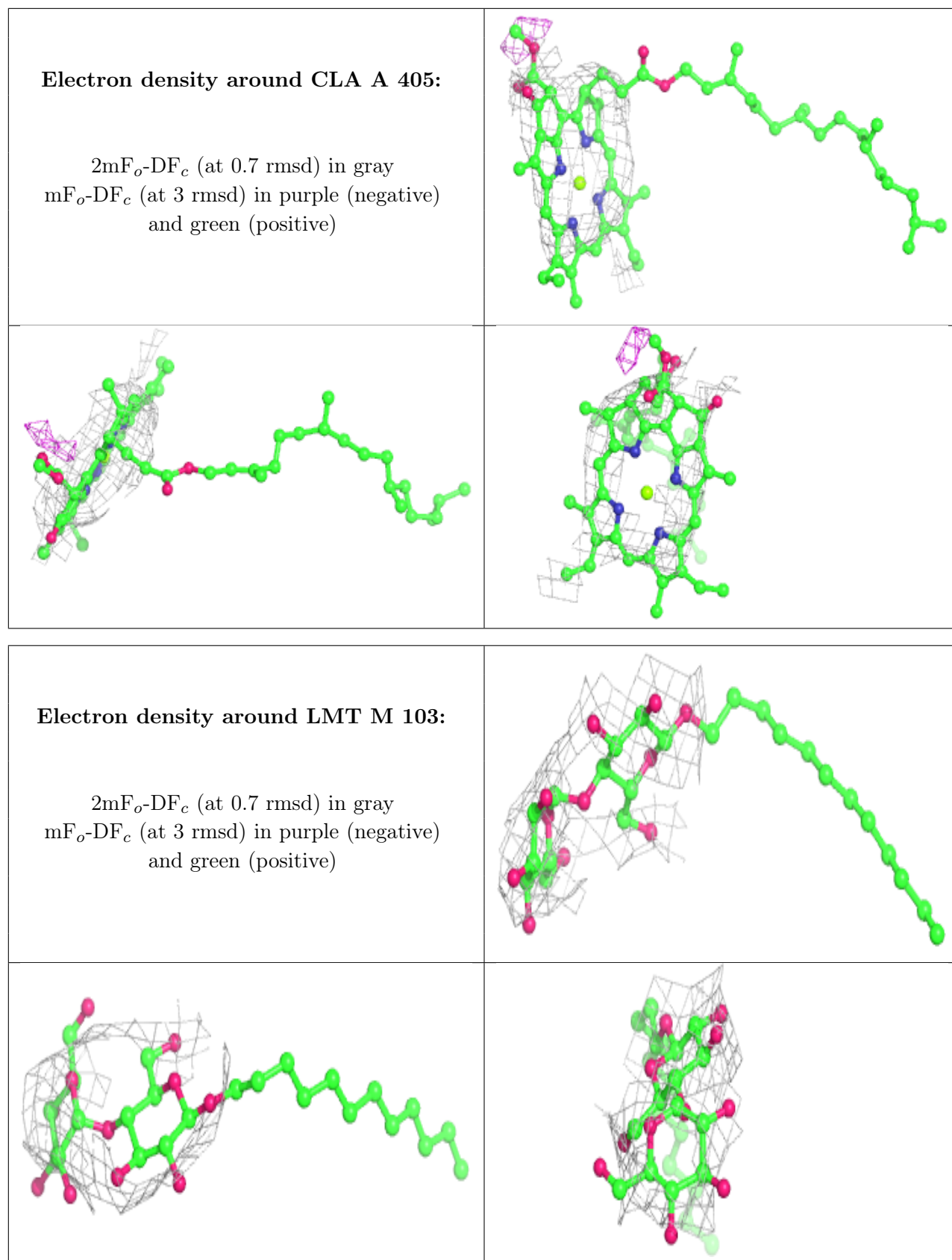
**Electron density around BCR a 410:**

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



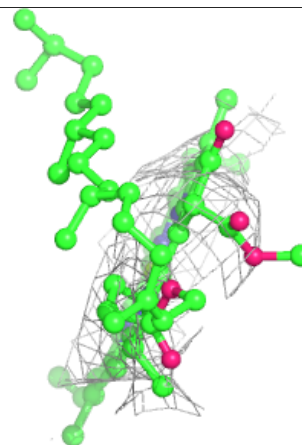
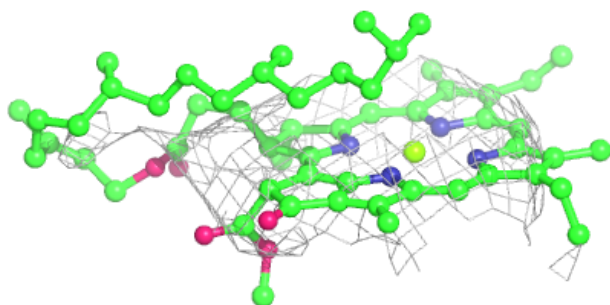
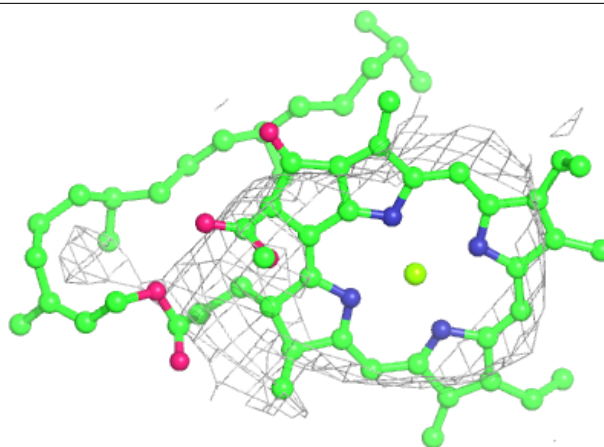


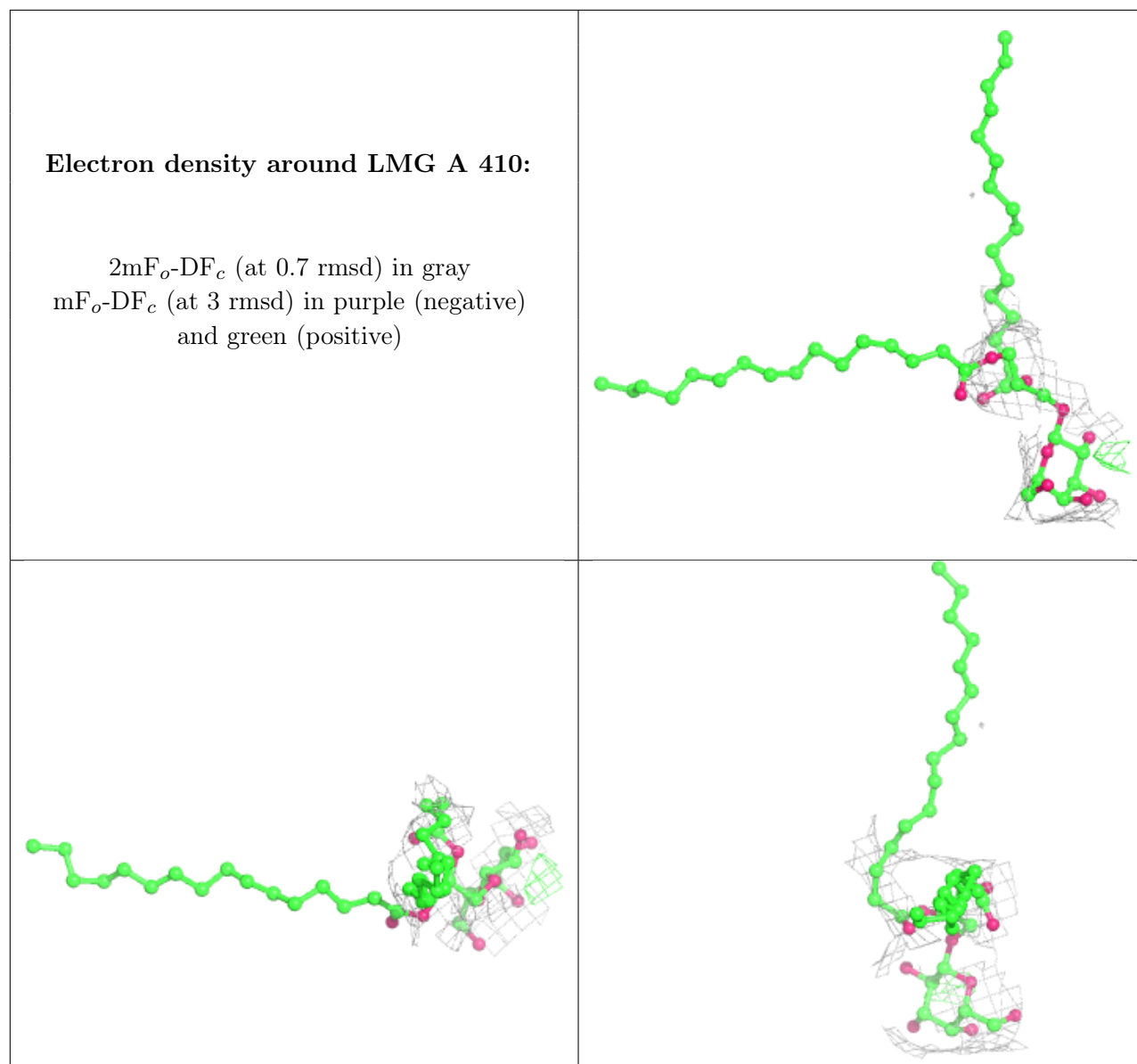




Electron density around CLA c 508:

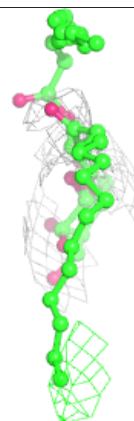
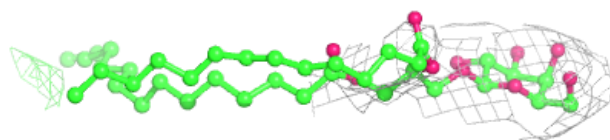
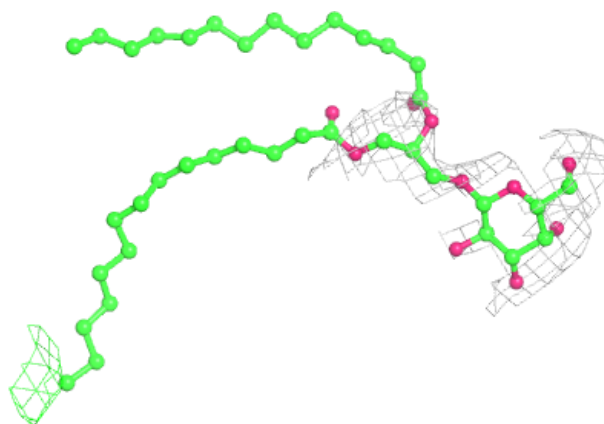
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



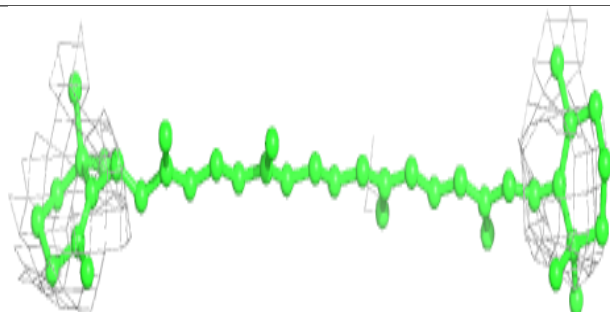
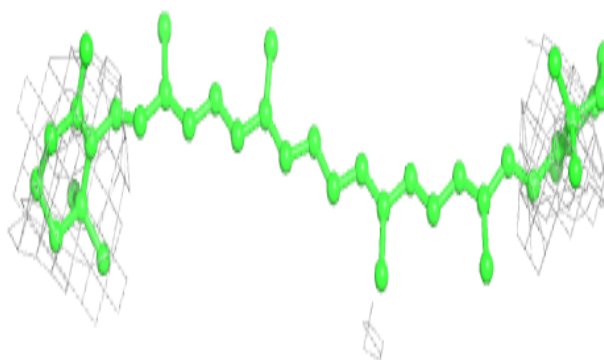


Electron density around LMG c 522:

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

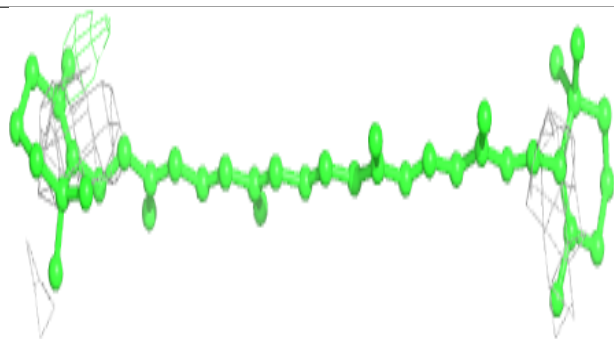
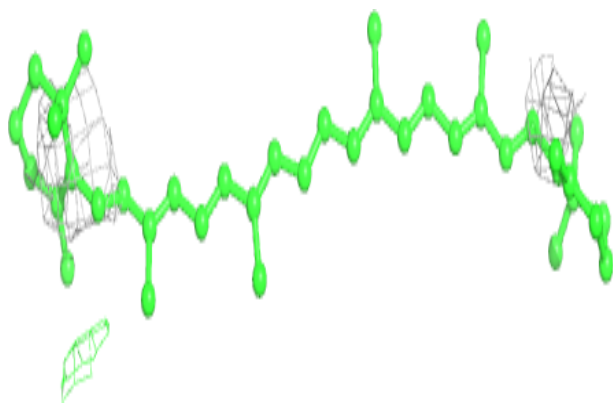
**Electron density around BCR K 102:**

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

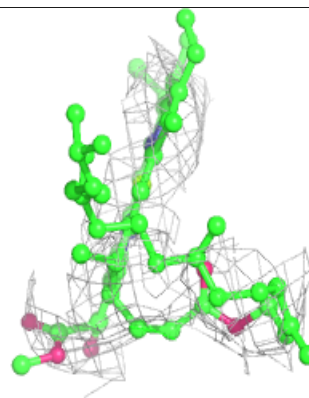
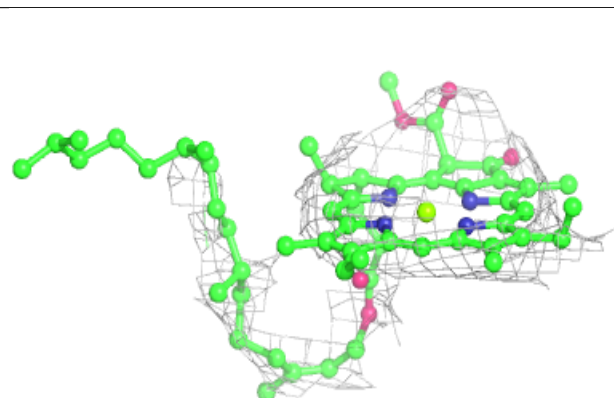
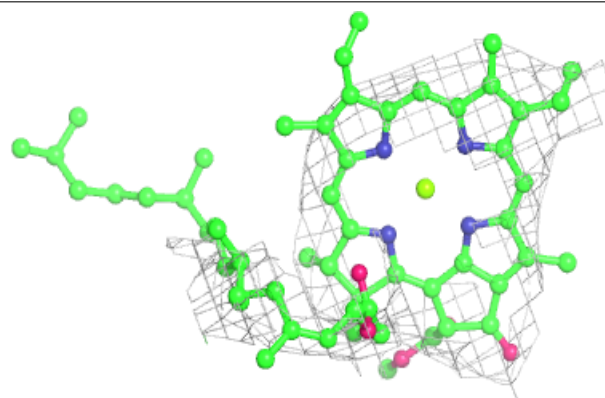


Electron density around BCR c 521:

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

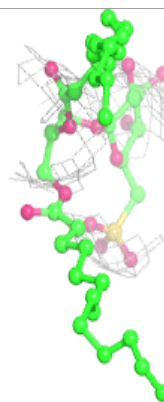
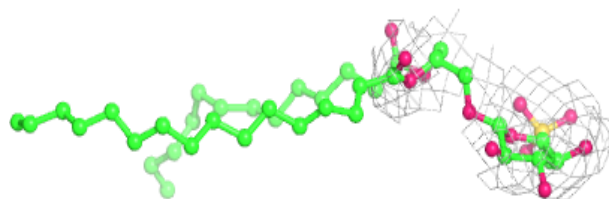
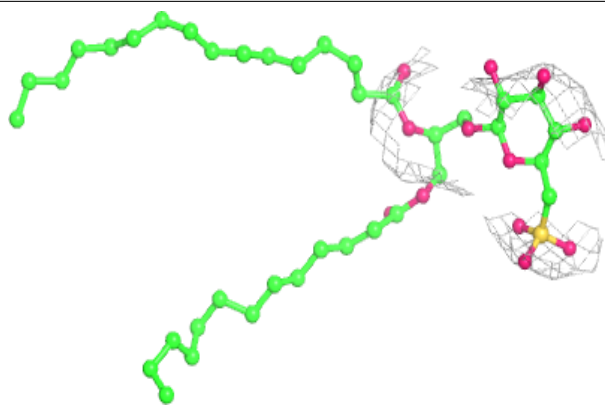
**Electron density around CLA a 405:**

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

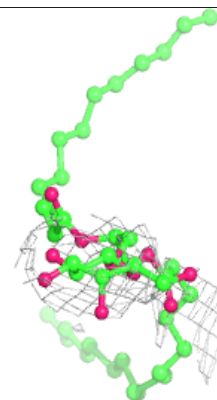
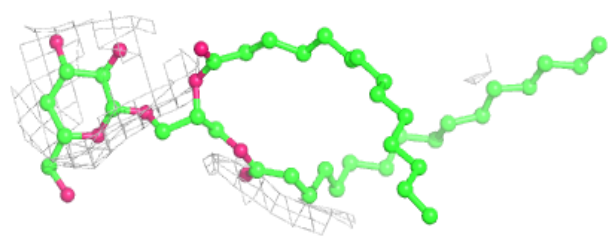
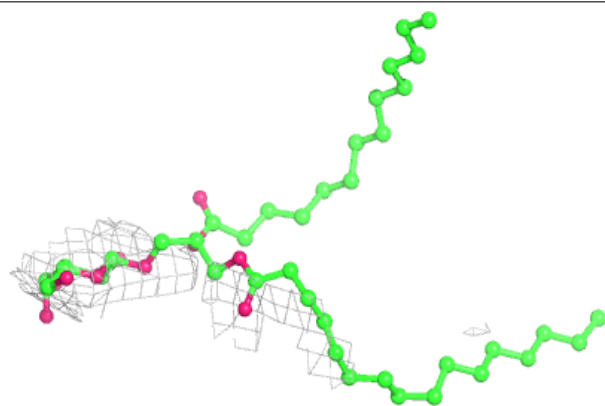


Electron density around SQD a 415:

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

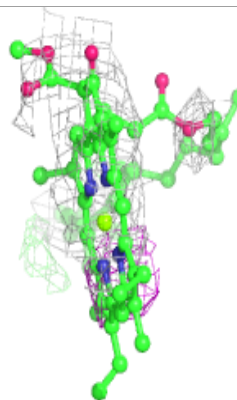
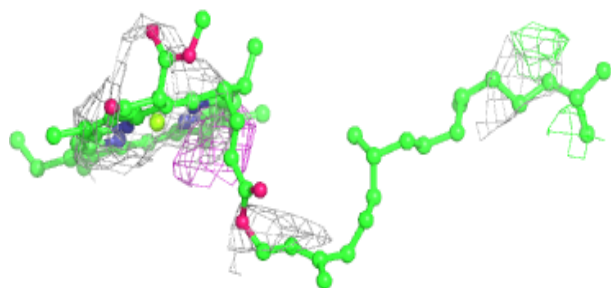
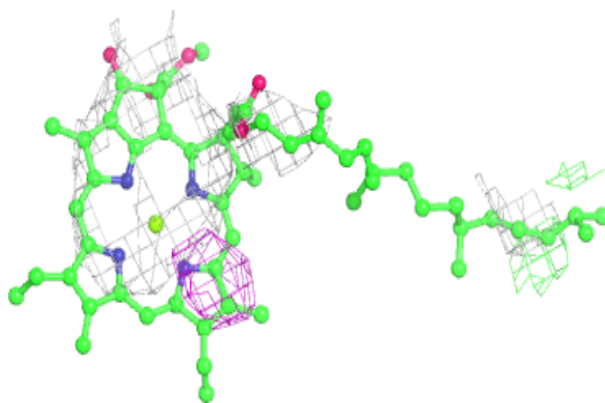
**Electron density around LMG b 625:**

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

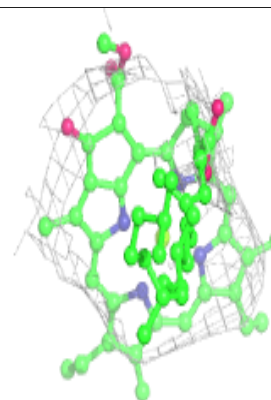
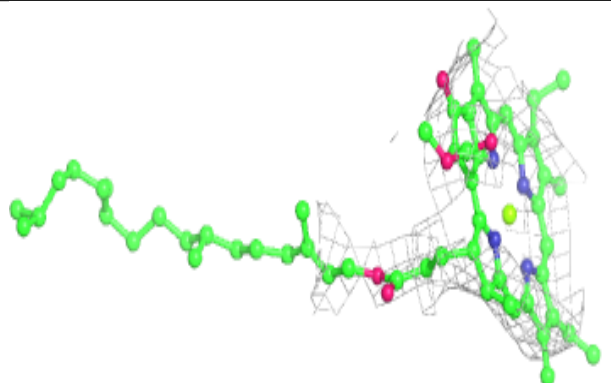
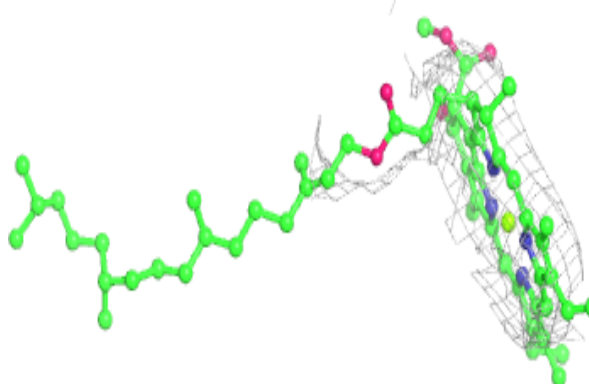


Electron density around CLA a 406:

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

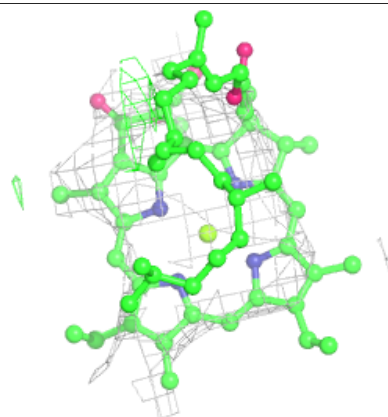
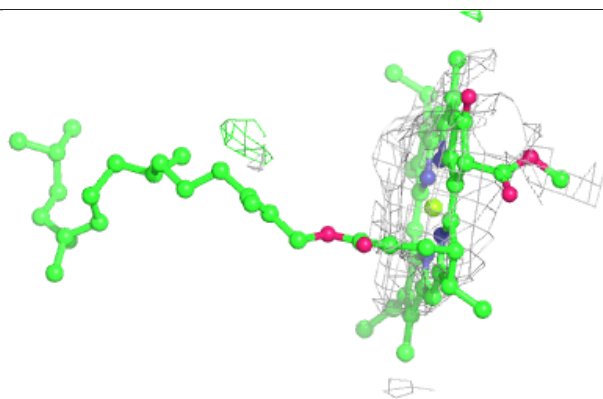
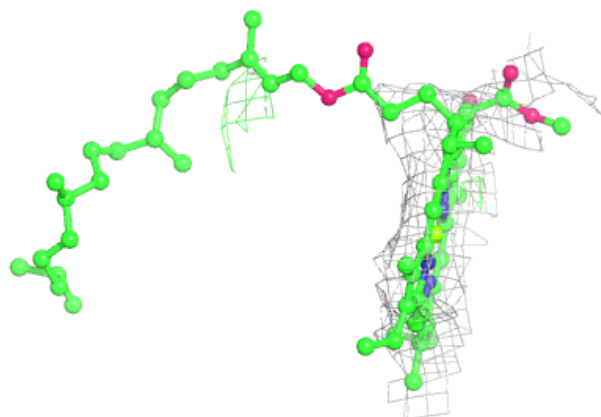
**Electron density around CLA B 603:**

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

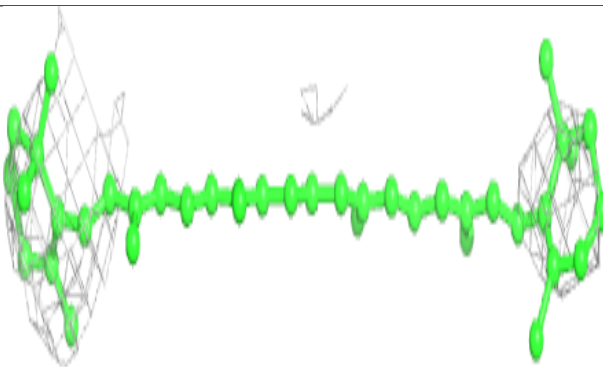
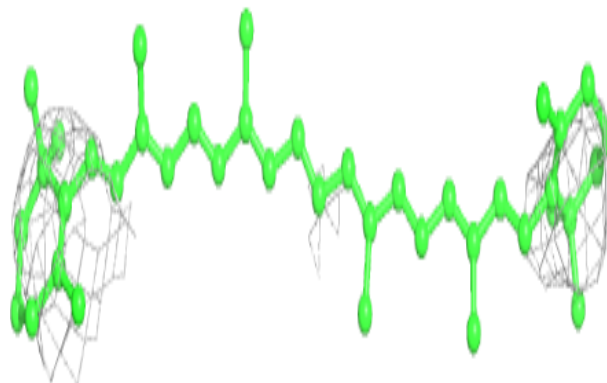


Electron density around CLA c 505:

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

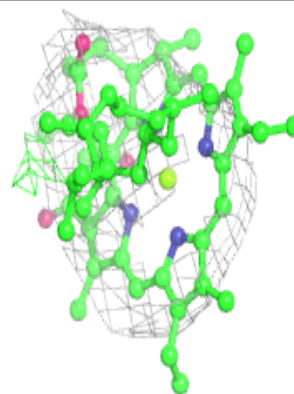
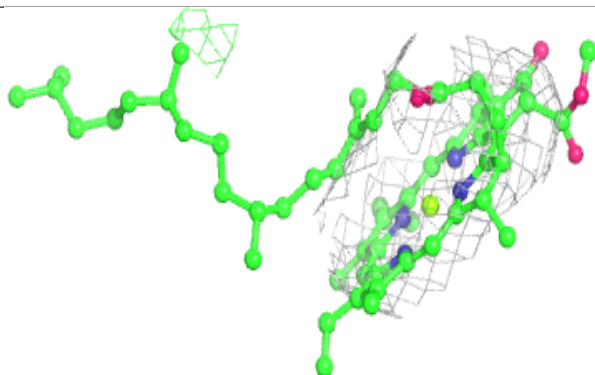
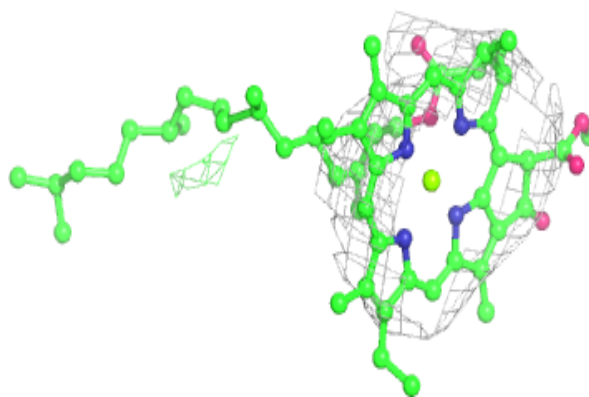
**Electron density around BCR b 622:**

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

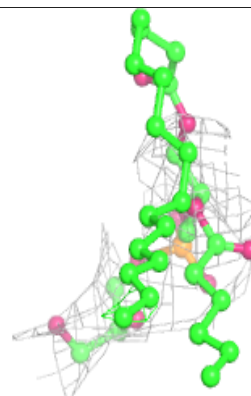
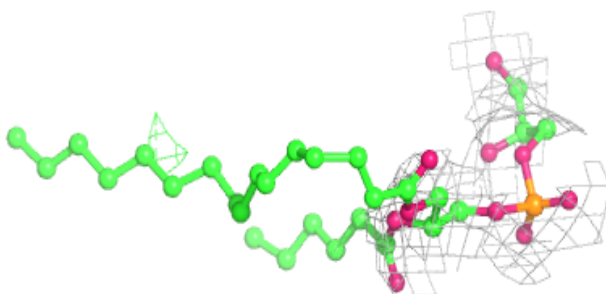
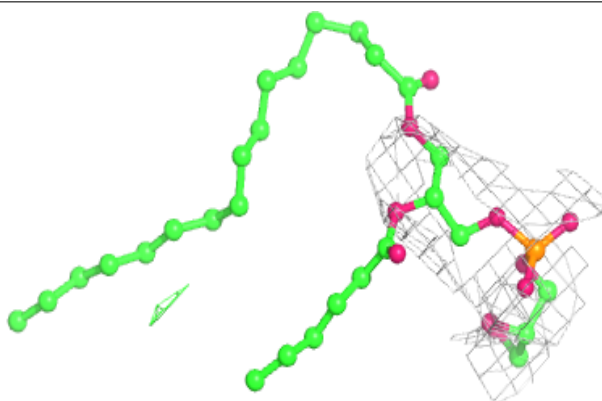


Electron density around CLA C 504:

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

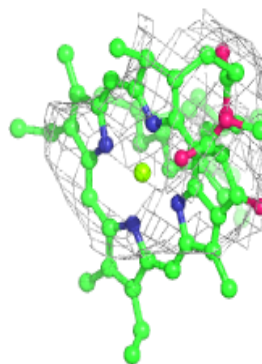
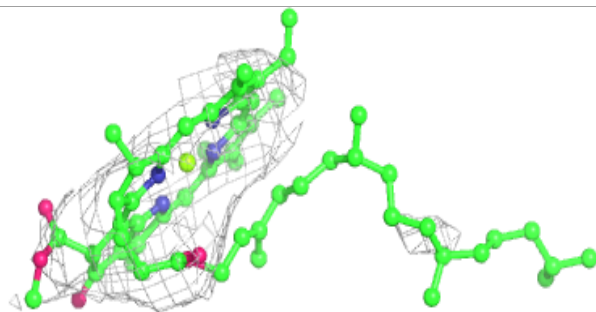
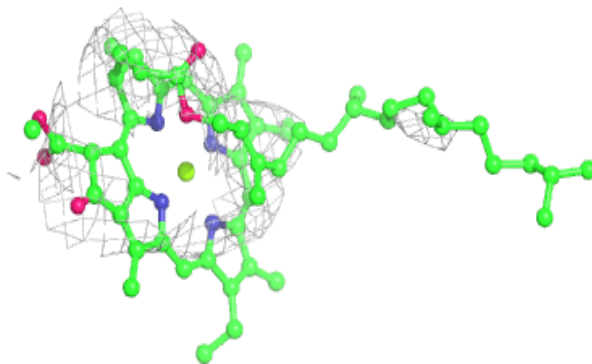
**Electron density around LHG a 412:**

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



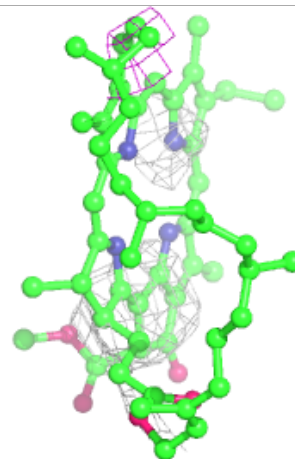
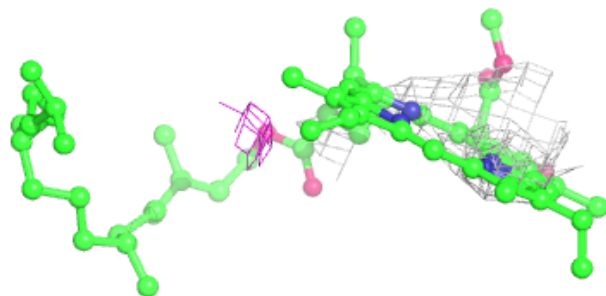
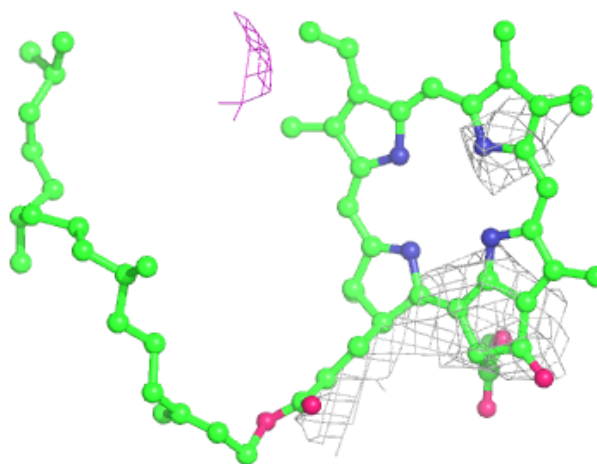
Electron density around CLA c 504:

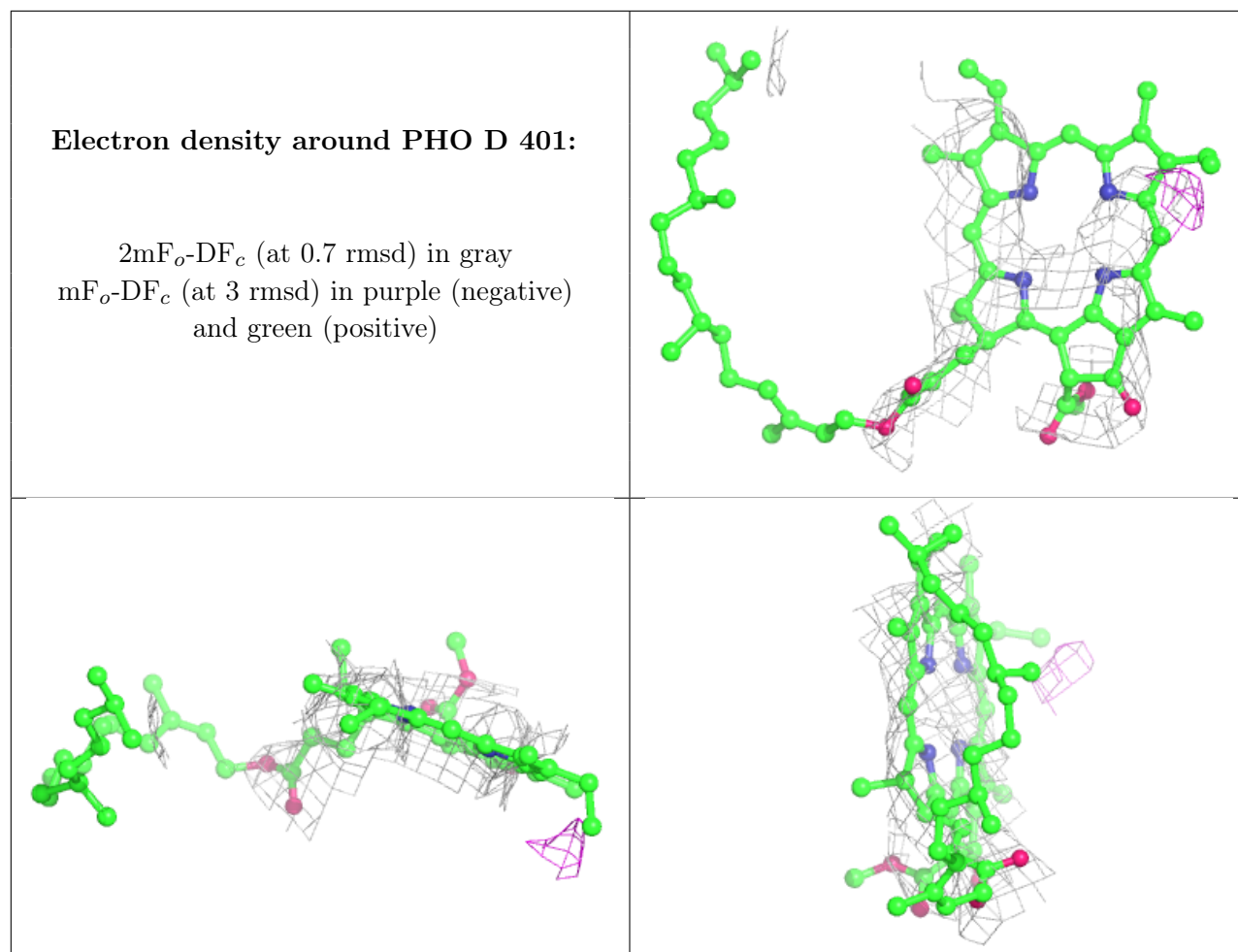
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO a 407:

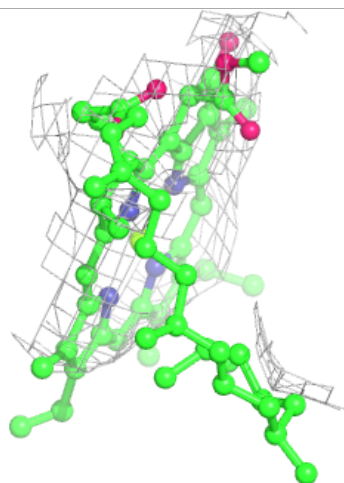
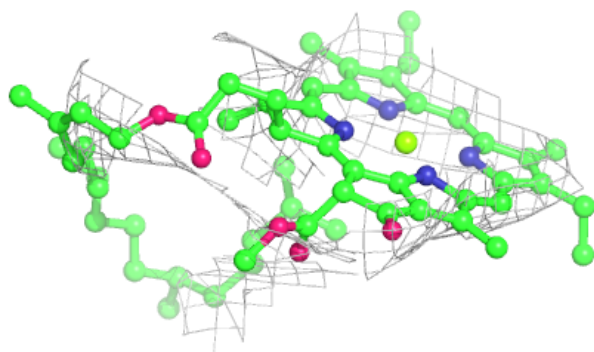
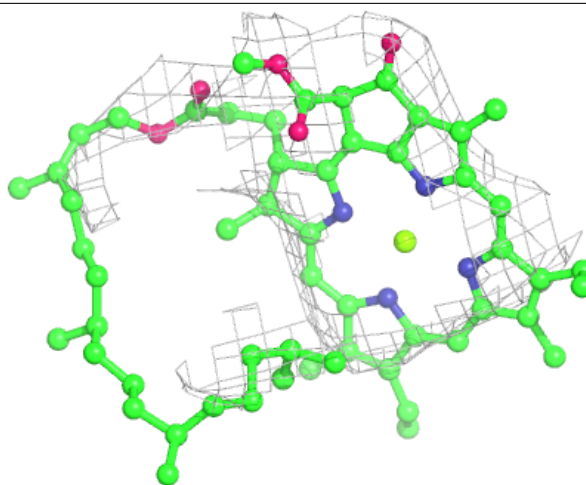
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





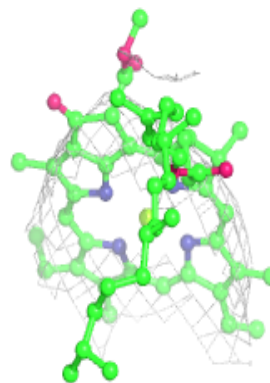
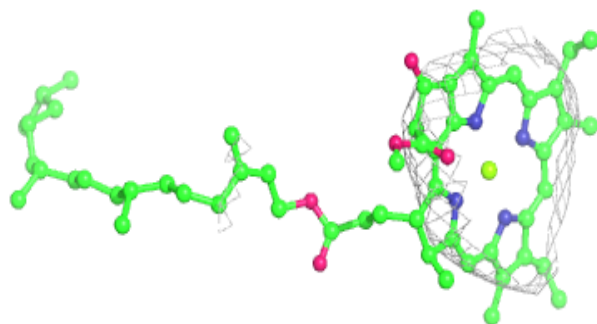
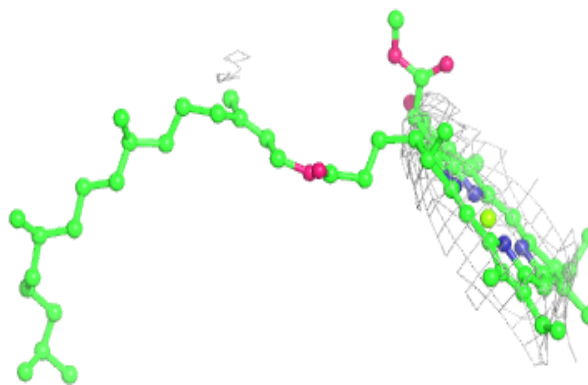
Electron density around CLA b 618:

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

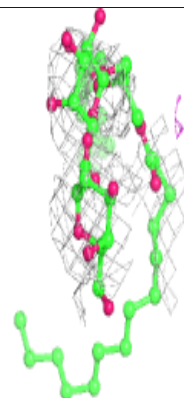
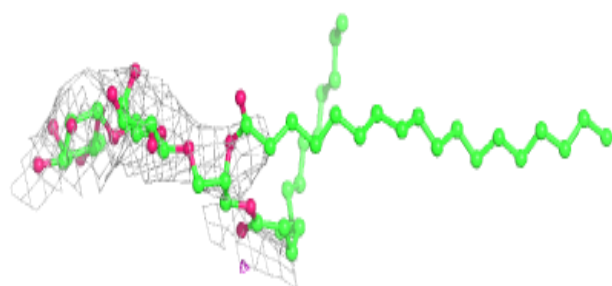
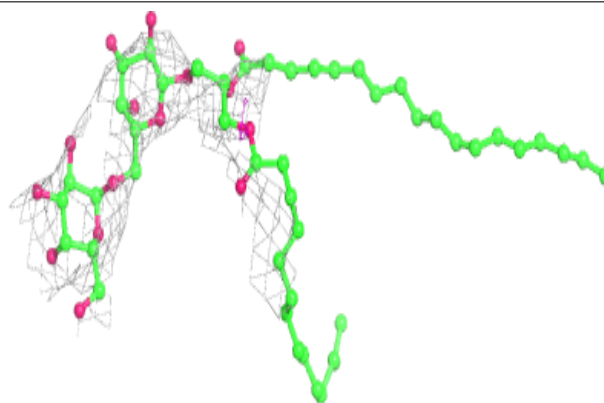


Electron density around CLA d 404:

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

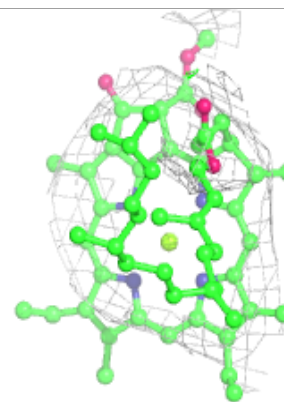
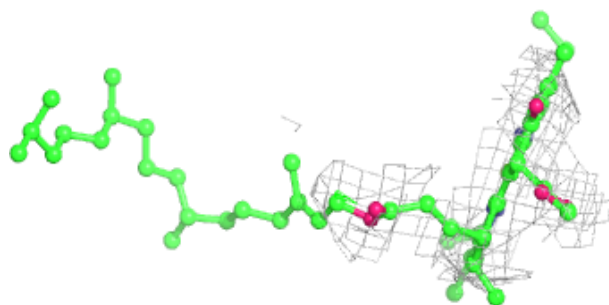
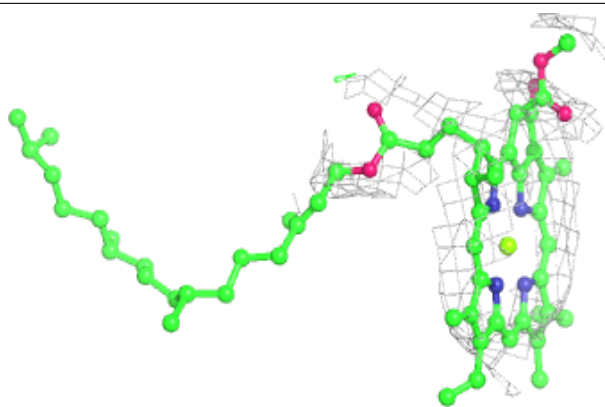
**Electron density around DGD C 516:**

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

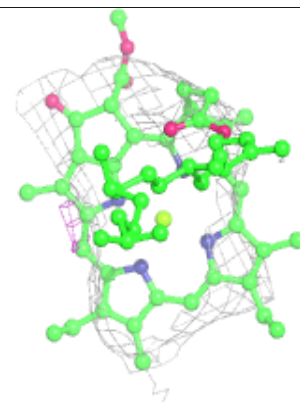
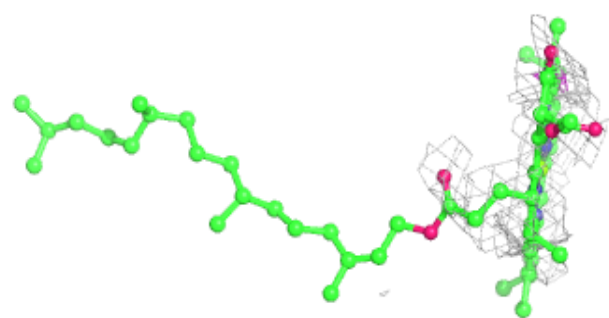
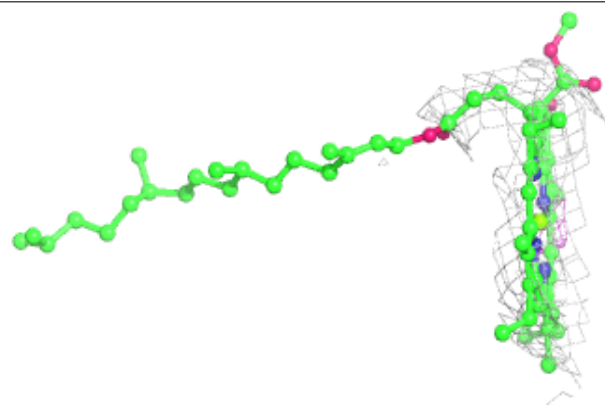


Electron density around CLA d 405:

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

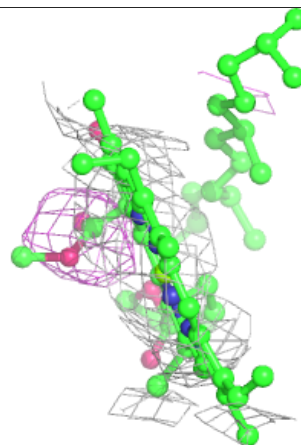
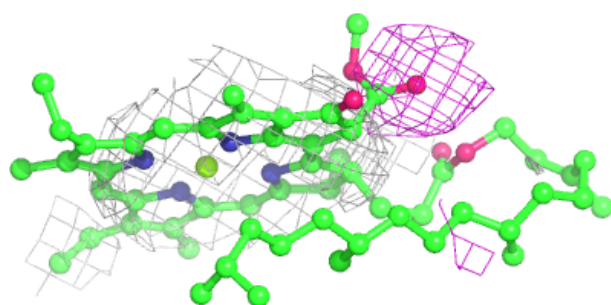
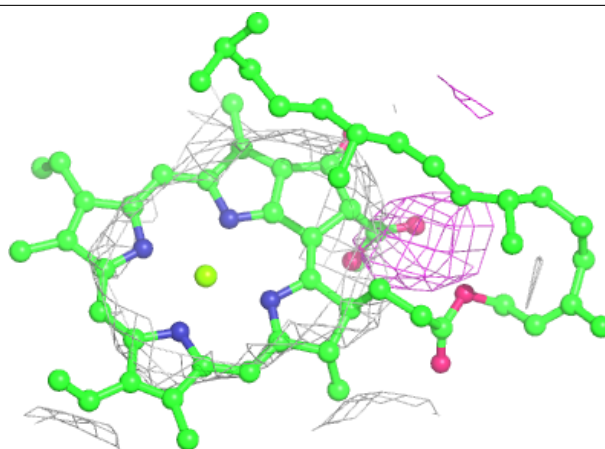
**Electron density around CLA B 605:**

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

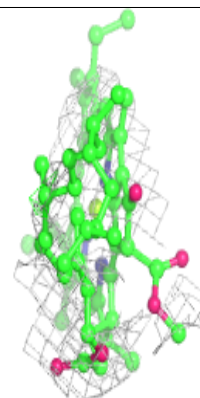
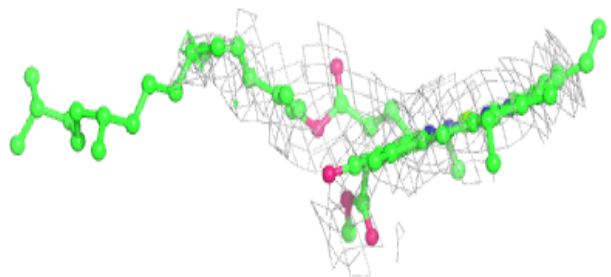
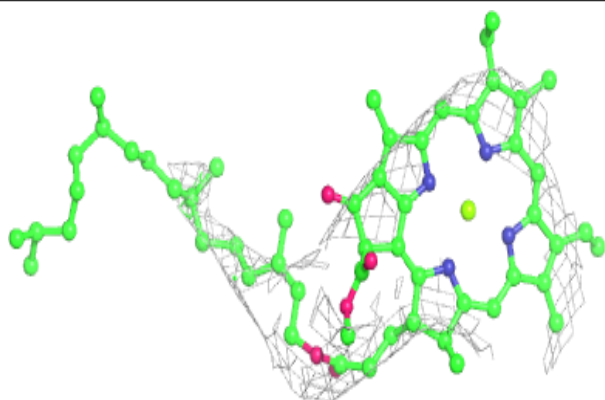


Electron density around CLA C 508:

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

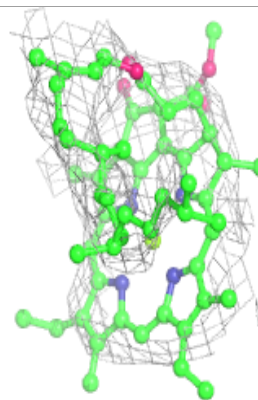
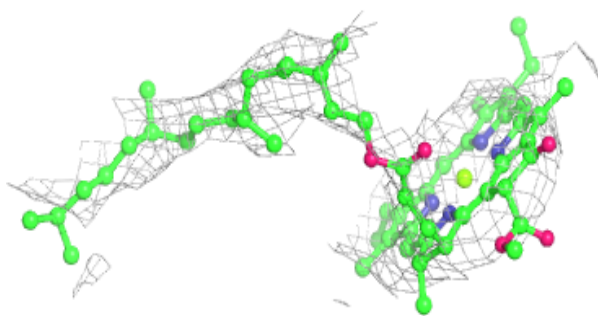
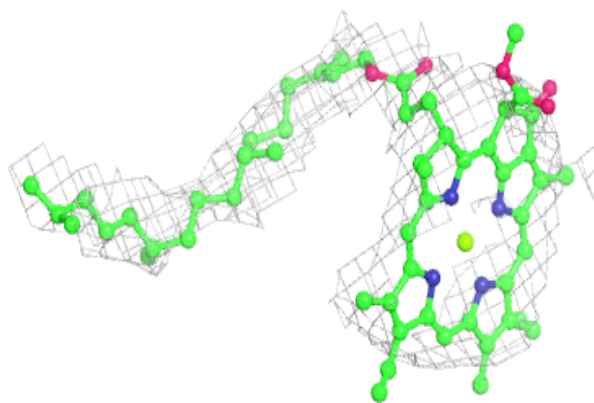
**Electron density around CLA H 101:**

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

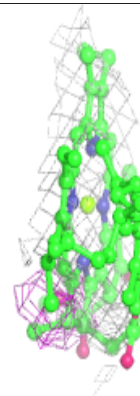
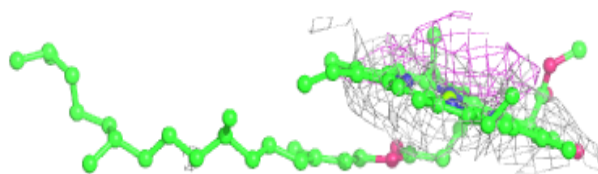
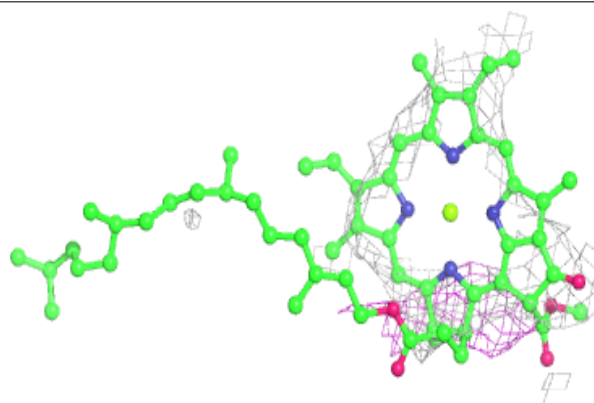


Electron density around CLA C 510:

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

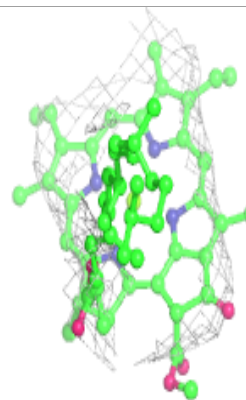
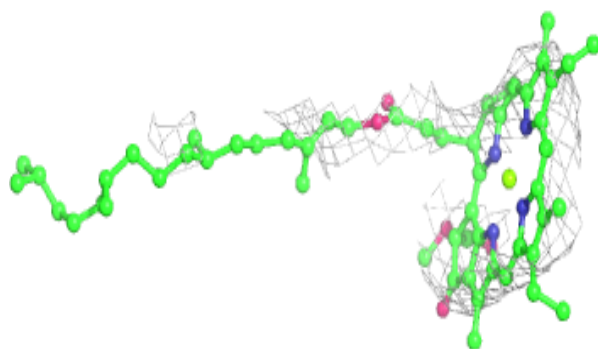
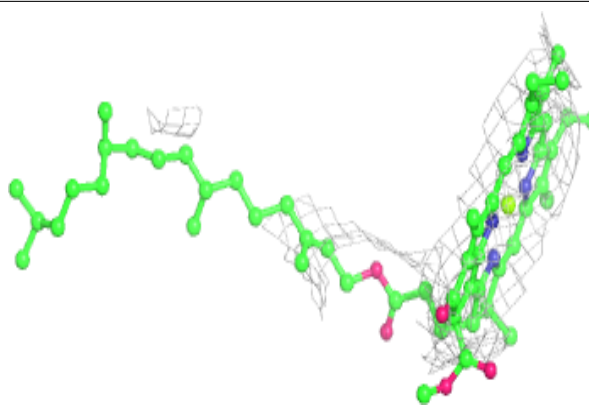
**Electron density around CLA b 606:**

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

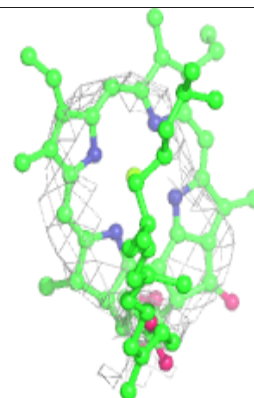
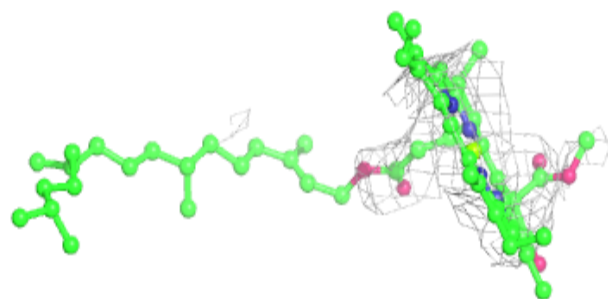
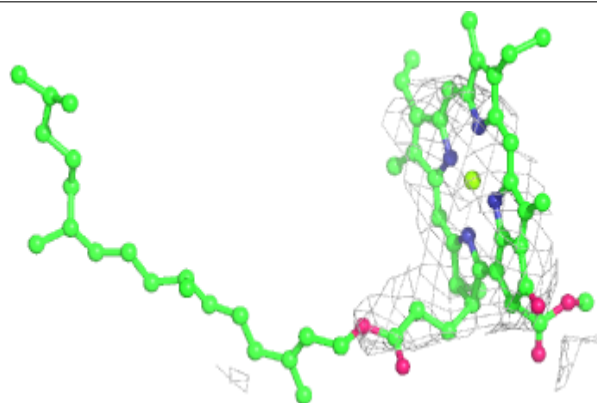


Electron density around CLA b 607:

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

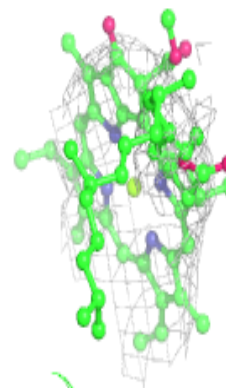
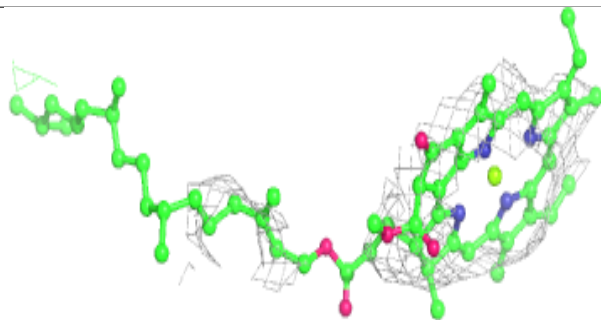
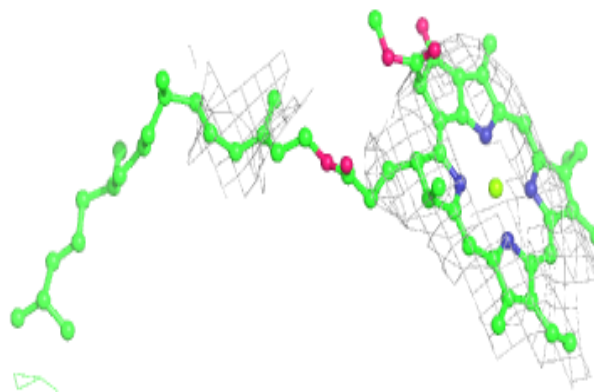
**Electron density around CLA B 608:**

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

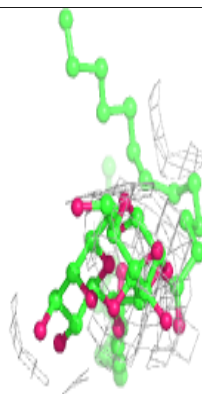
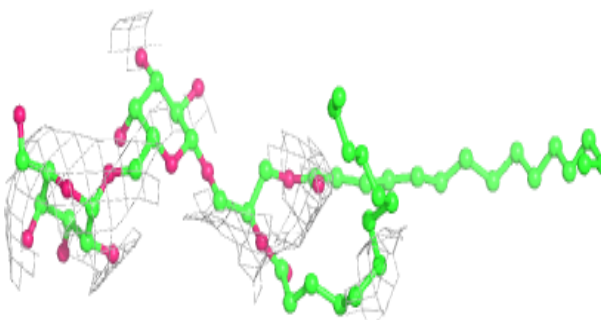
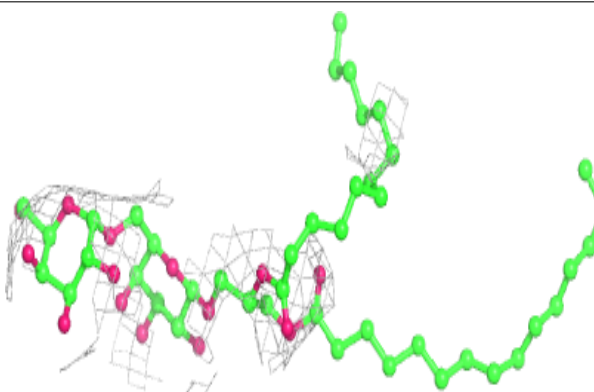


Electron density around CLA a 404:

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

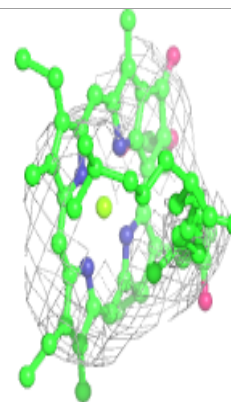
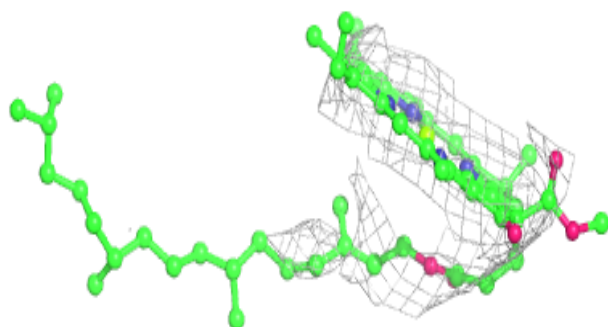
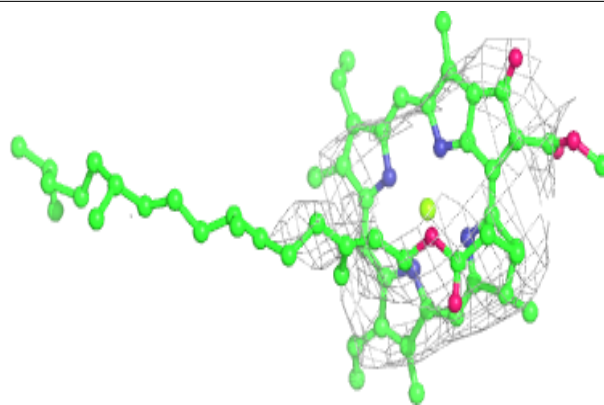
**Electron density around DGD b 624:**

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

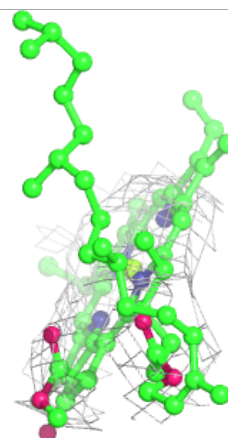
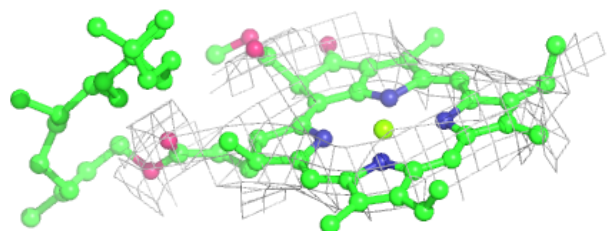
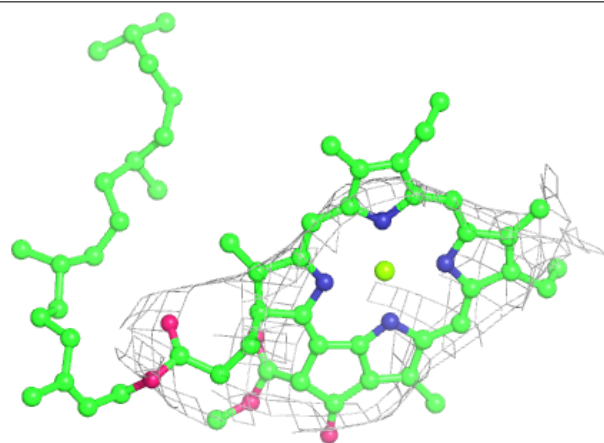


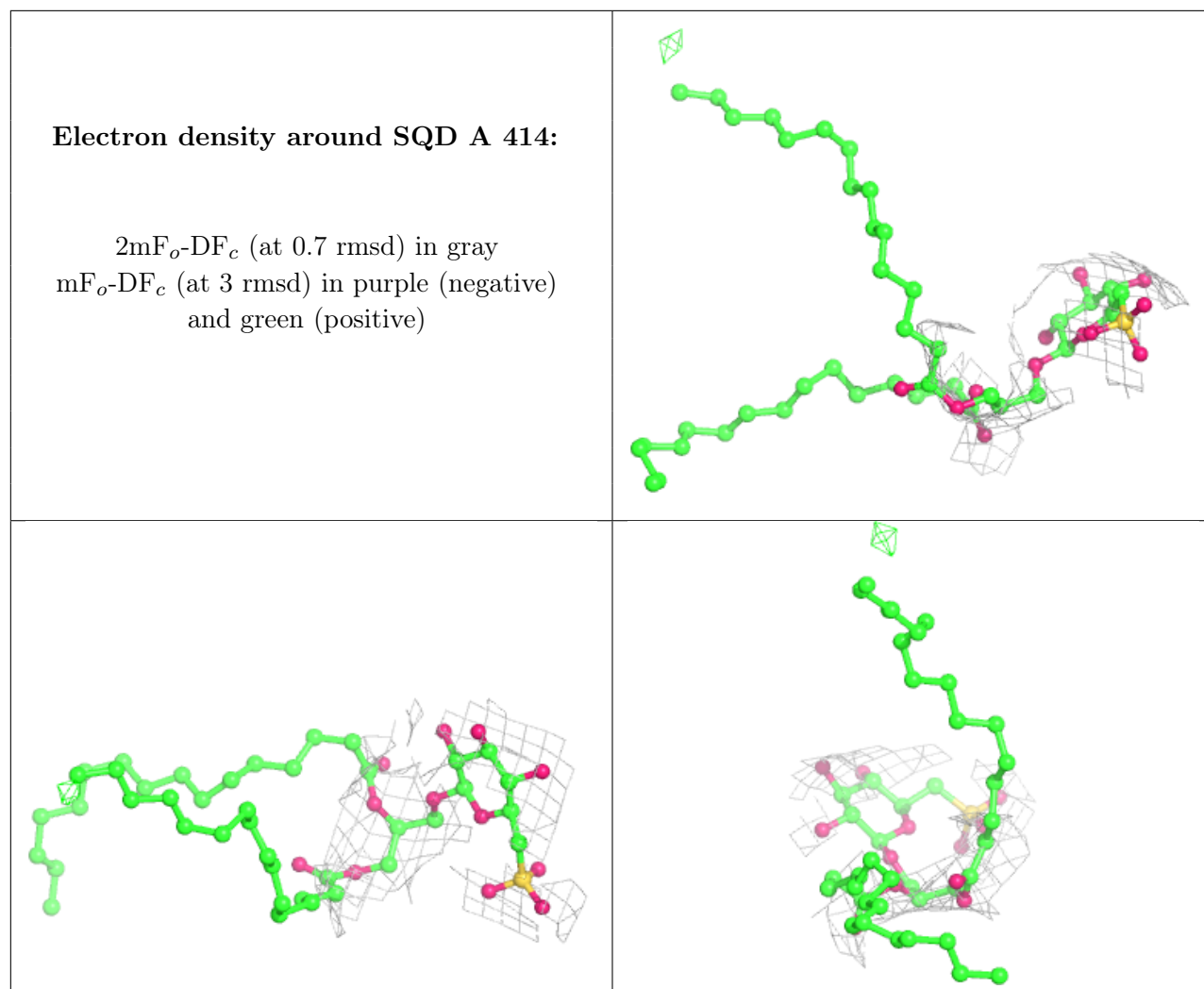
Electron density around CLA B 607:

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

**Electron density around CLA B 615:**

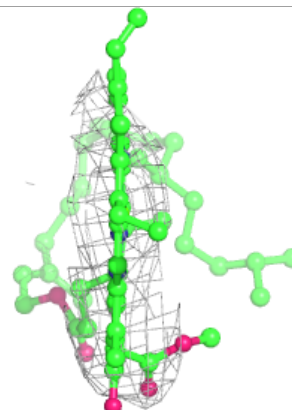
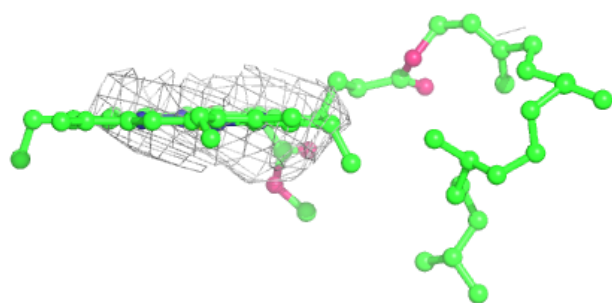
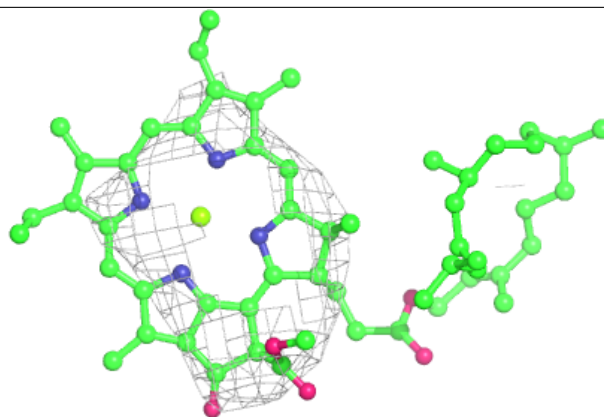
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



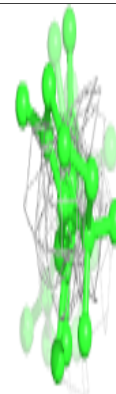
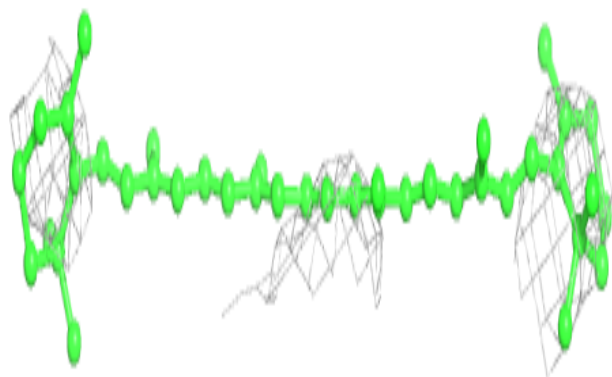
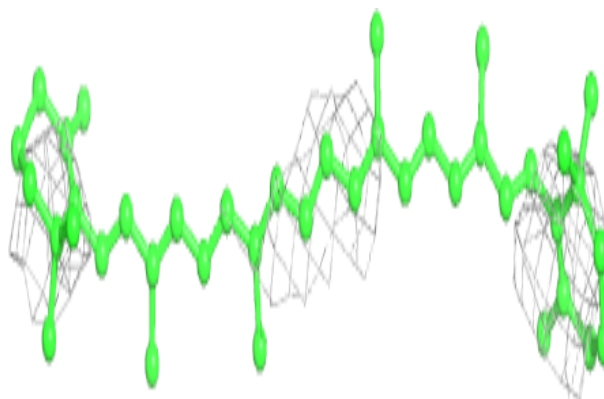


Electron density around CLA C 511:

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

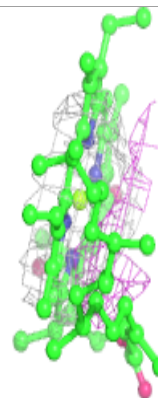
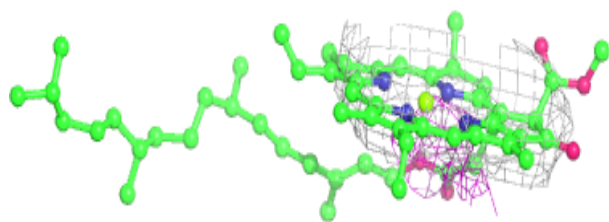
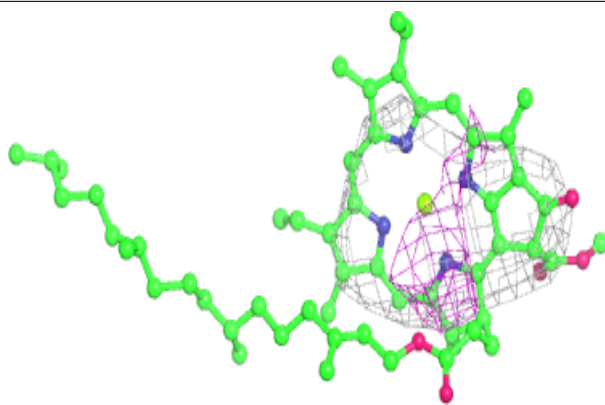
**Electron density around BCR B 618:**

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

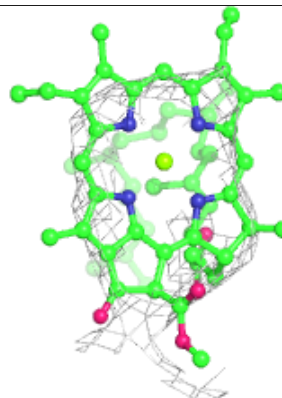
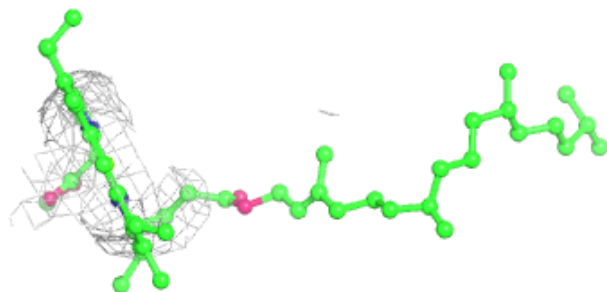
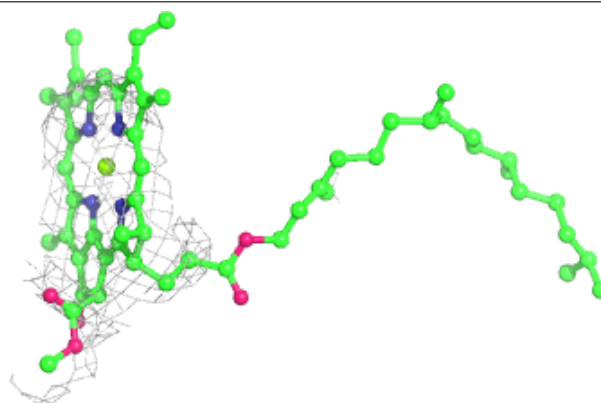


Electron density around CLA c 501:

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

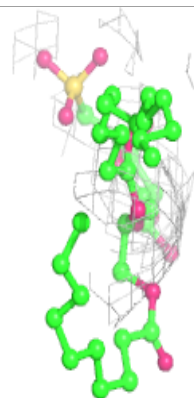
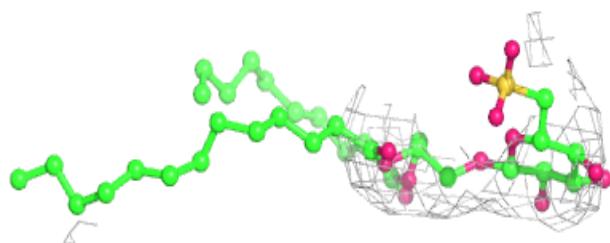
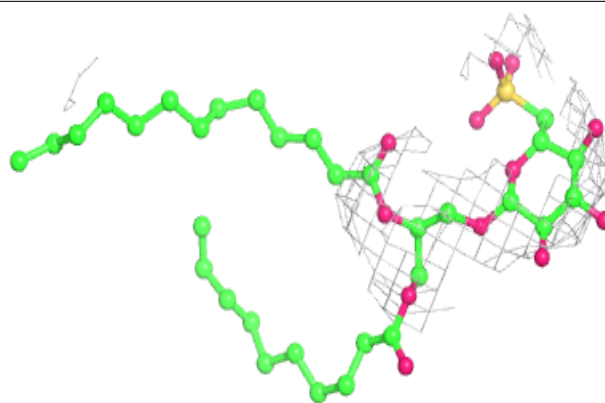
**Electron density around CLA D 405:**

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

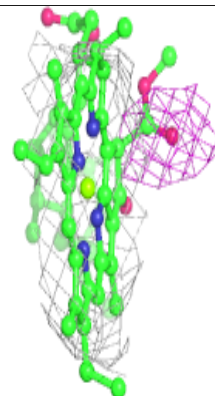
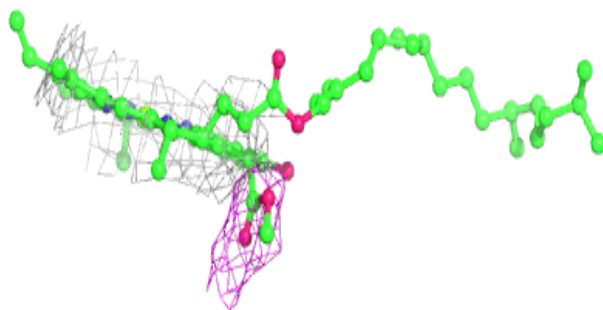
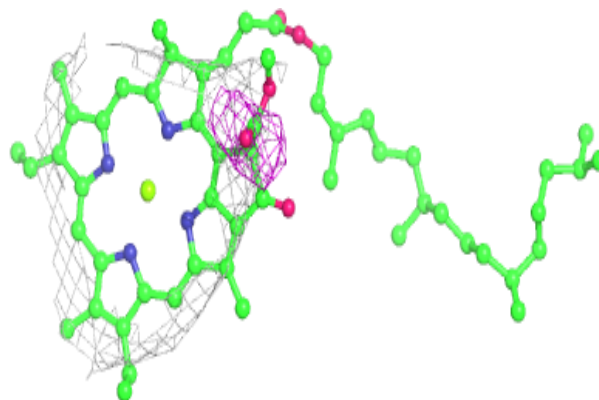


Electron density around SQD f 103:

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

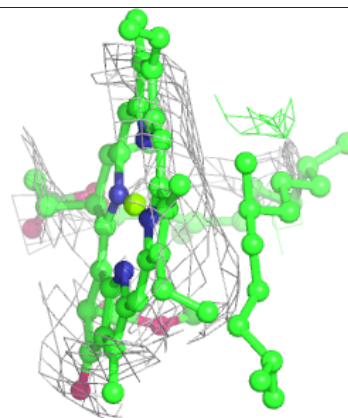
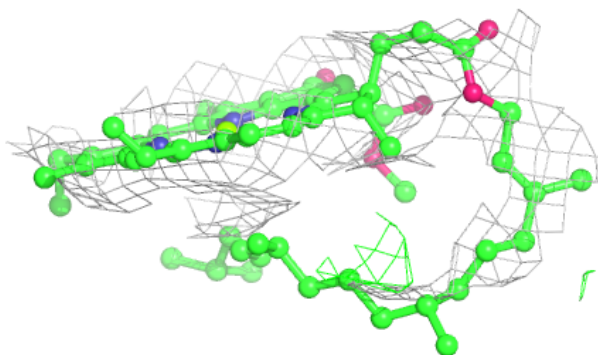
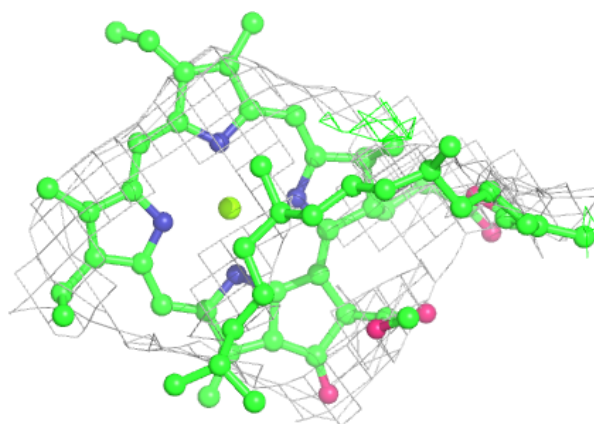
**Electron density around CLA h 101:**

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

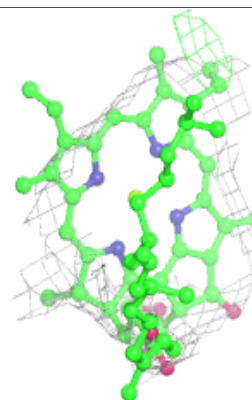
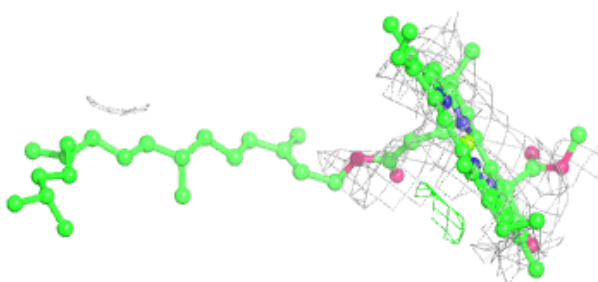
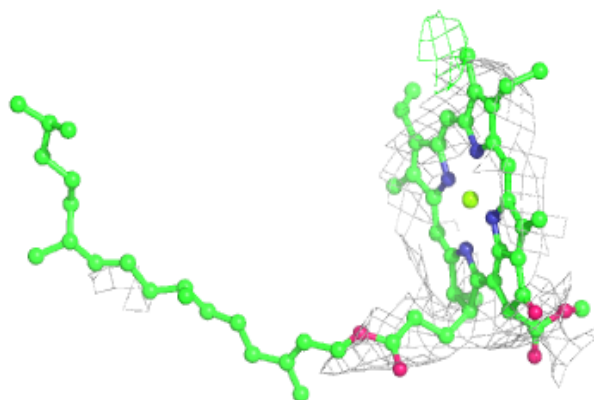


Electron density around CLA c 509:

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

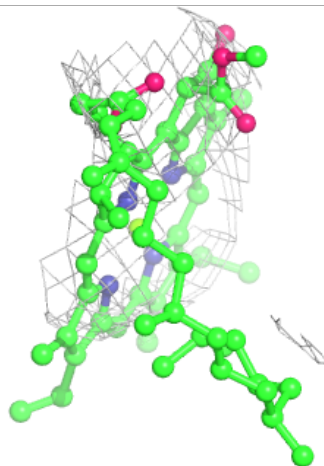
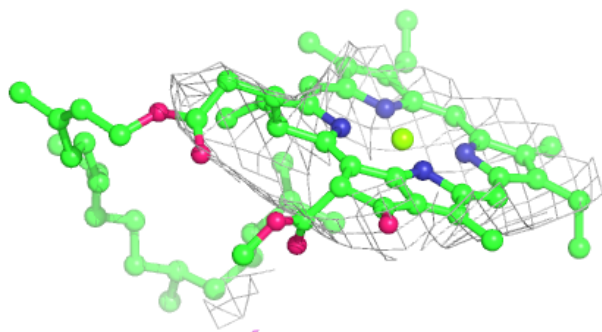
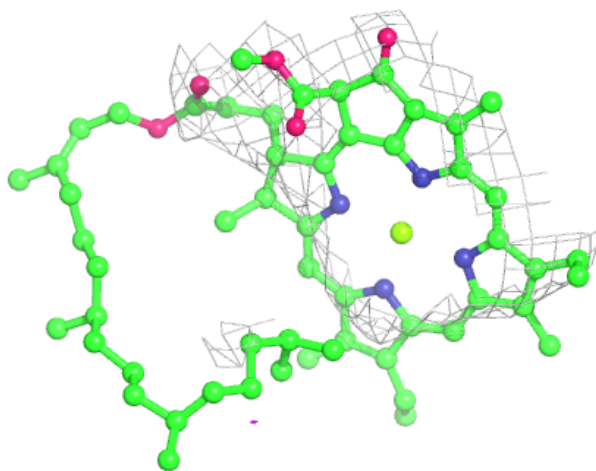
**Electron density around CLA b 612:**

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



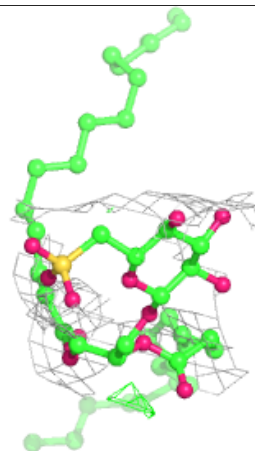
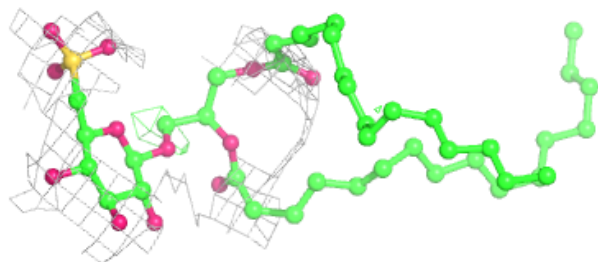
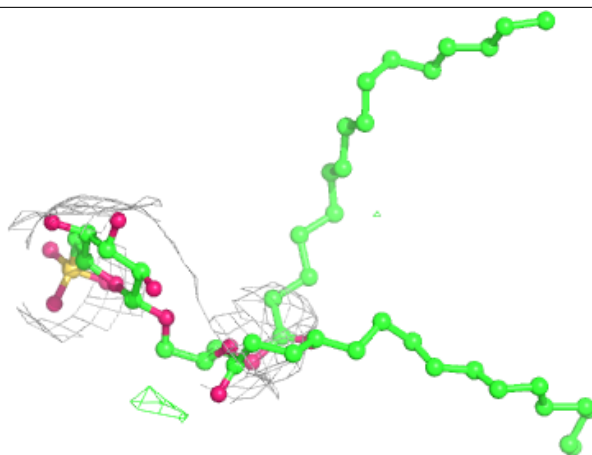
Electron density around CLA B 614:

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



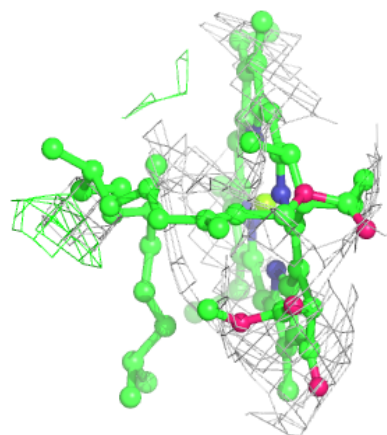
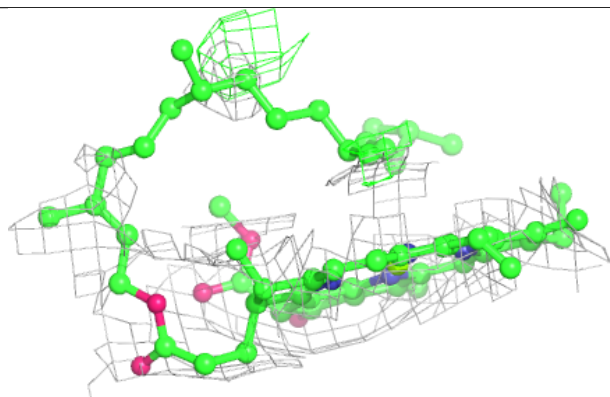
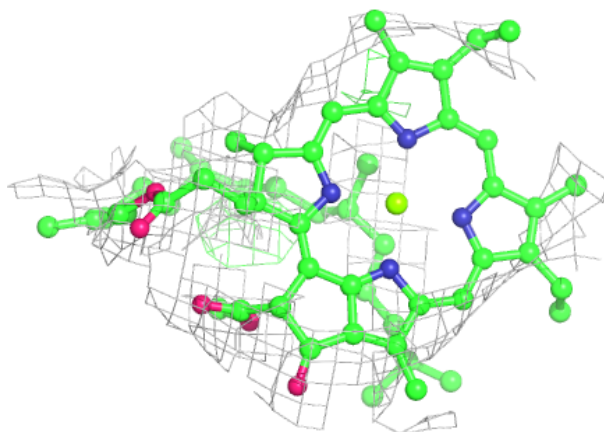
Electron density around SQD a 401:

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

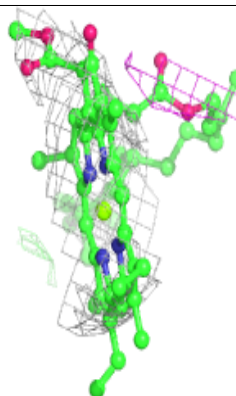
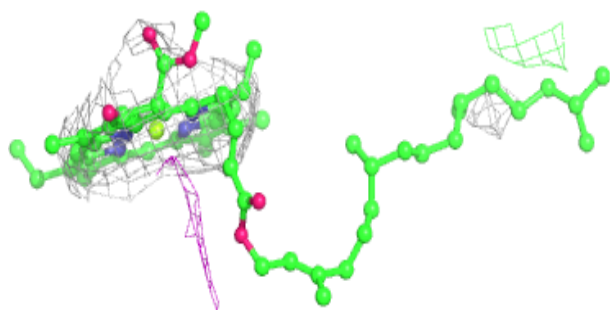
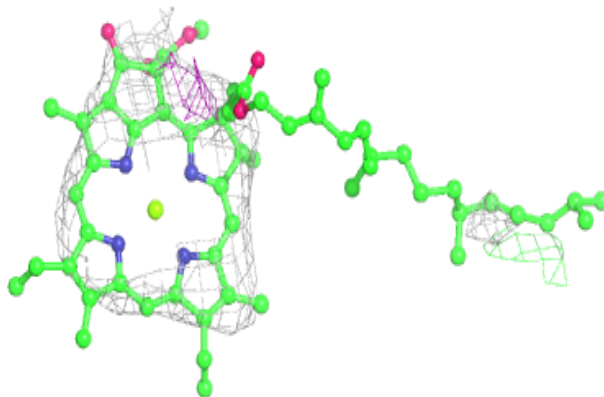


Electron density around CLA C 509:

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

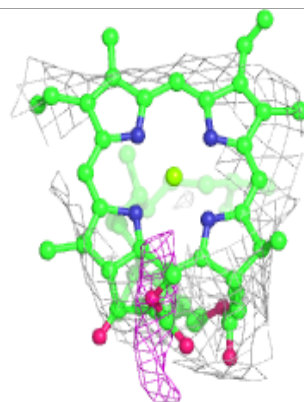
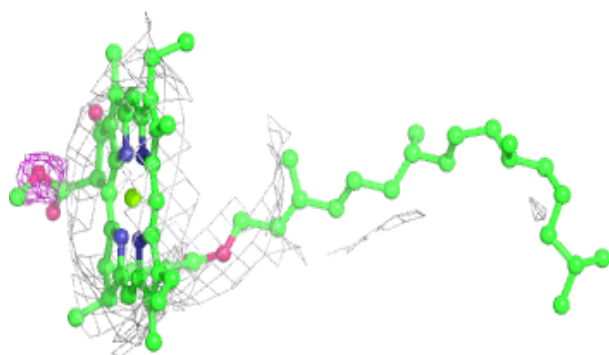
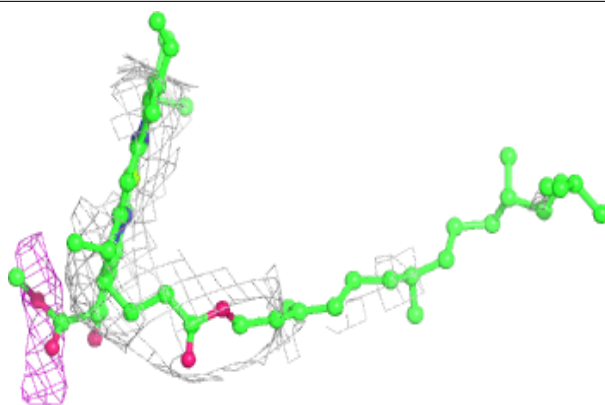
**Electron density around CLA A 404:**

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

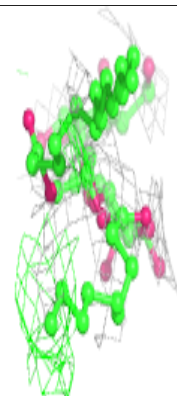
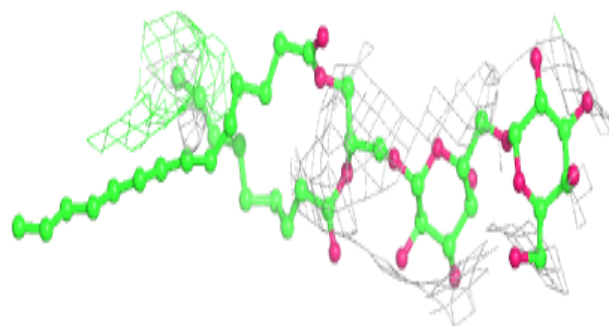
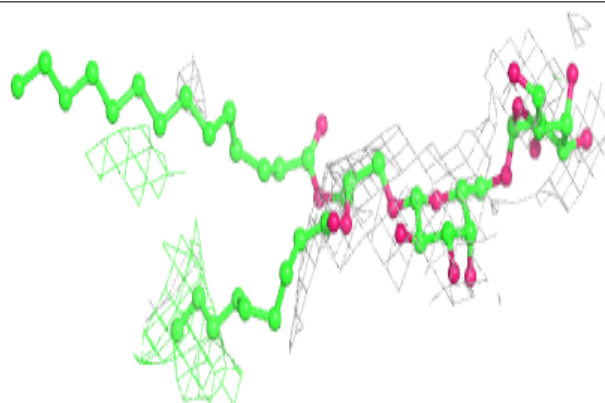


Electron density around CLA b 608:

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

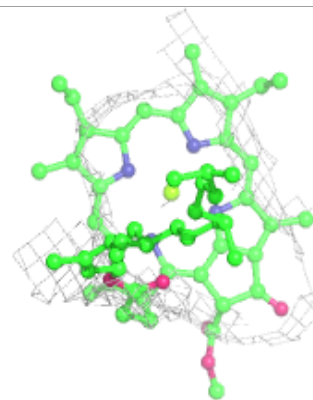
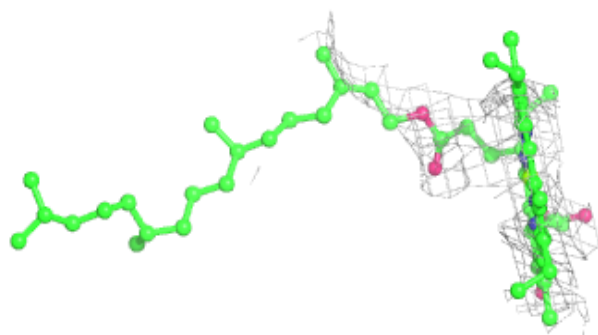
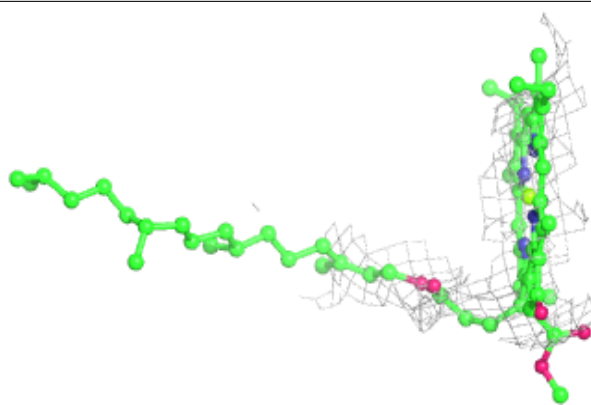
**Electron density around DGD c 515:**

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

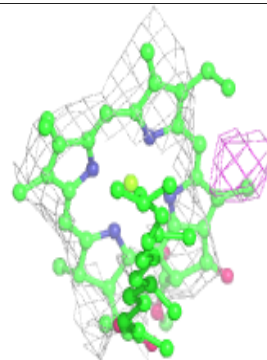
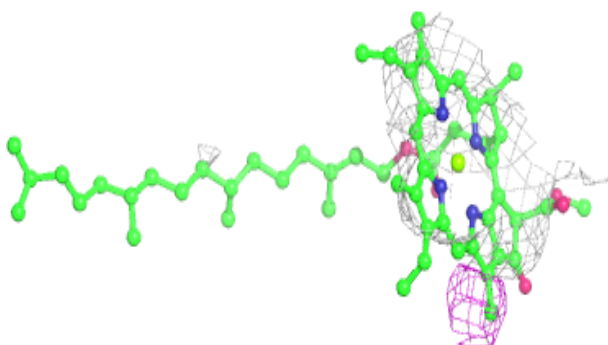
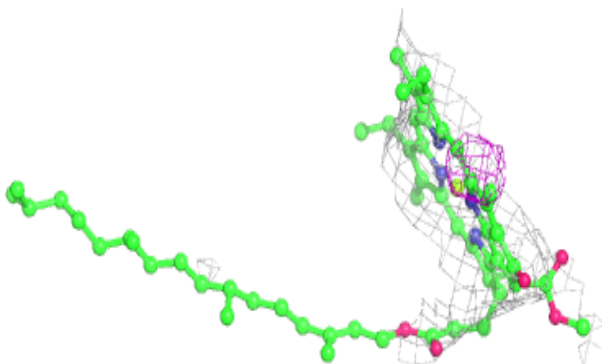


Electron density around CLA b 609:

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

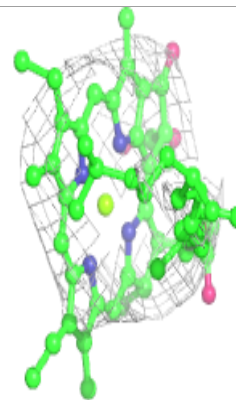
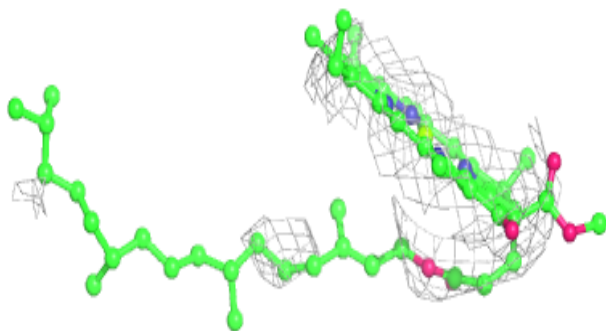
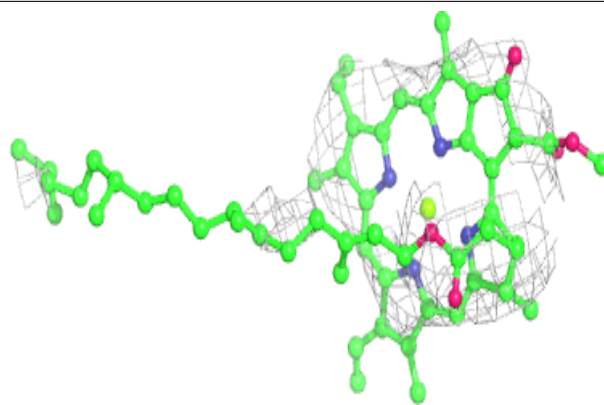
**Electron density around CLA b 610:**

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



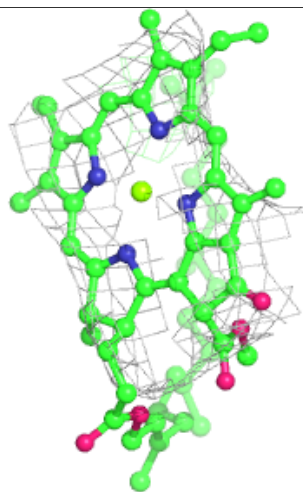
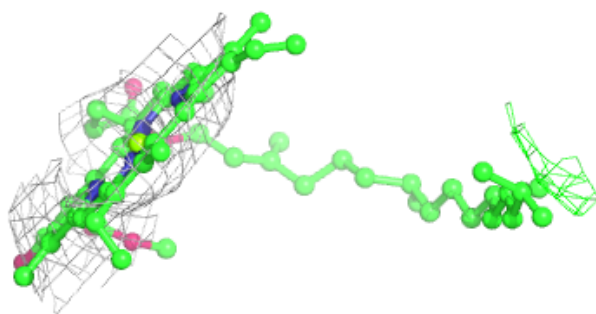
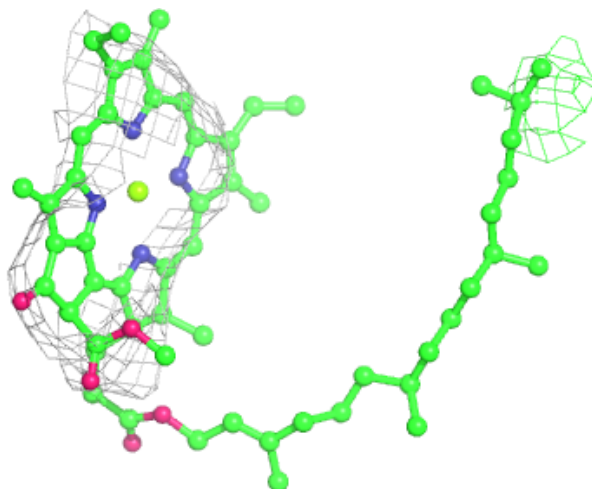
Electron density around CLA b 611:

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



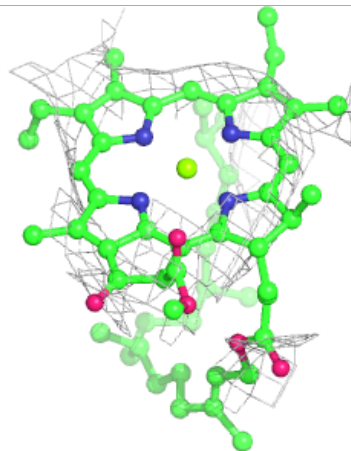
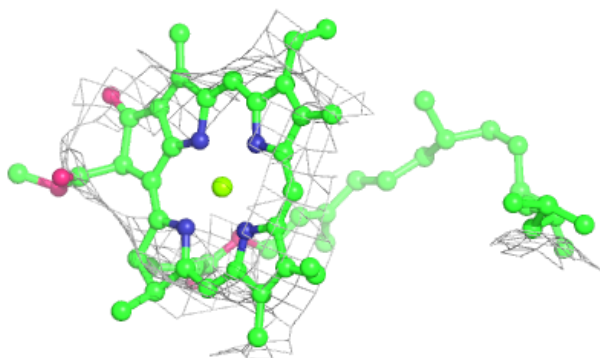
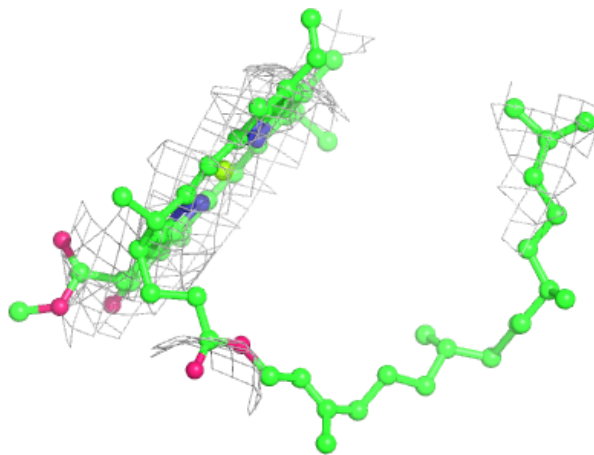
Electron density around CLA c 506:

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



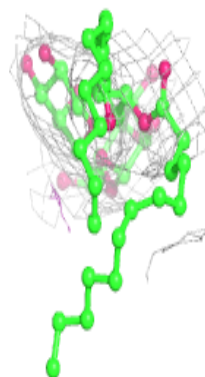
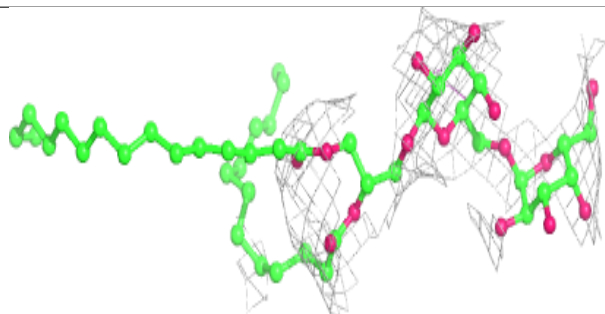
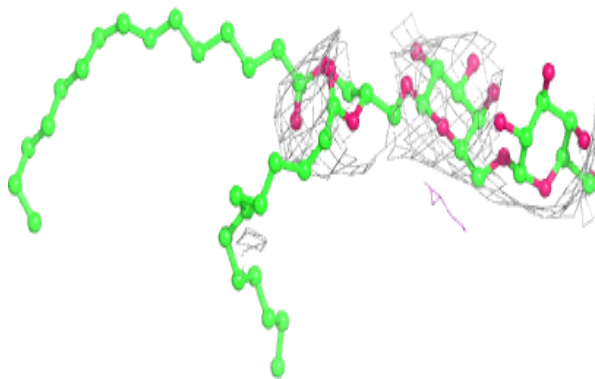
Electron density around CLA B 610:

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

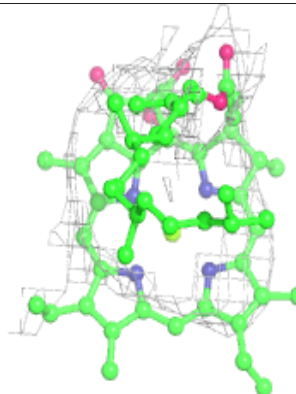
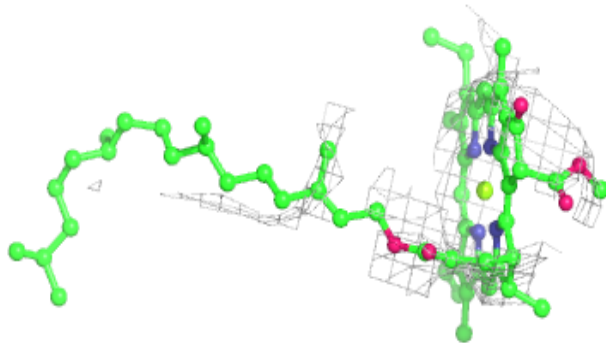


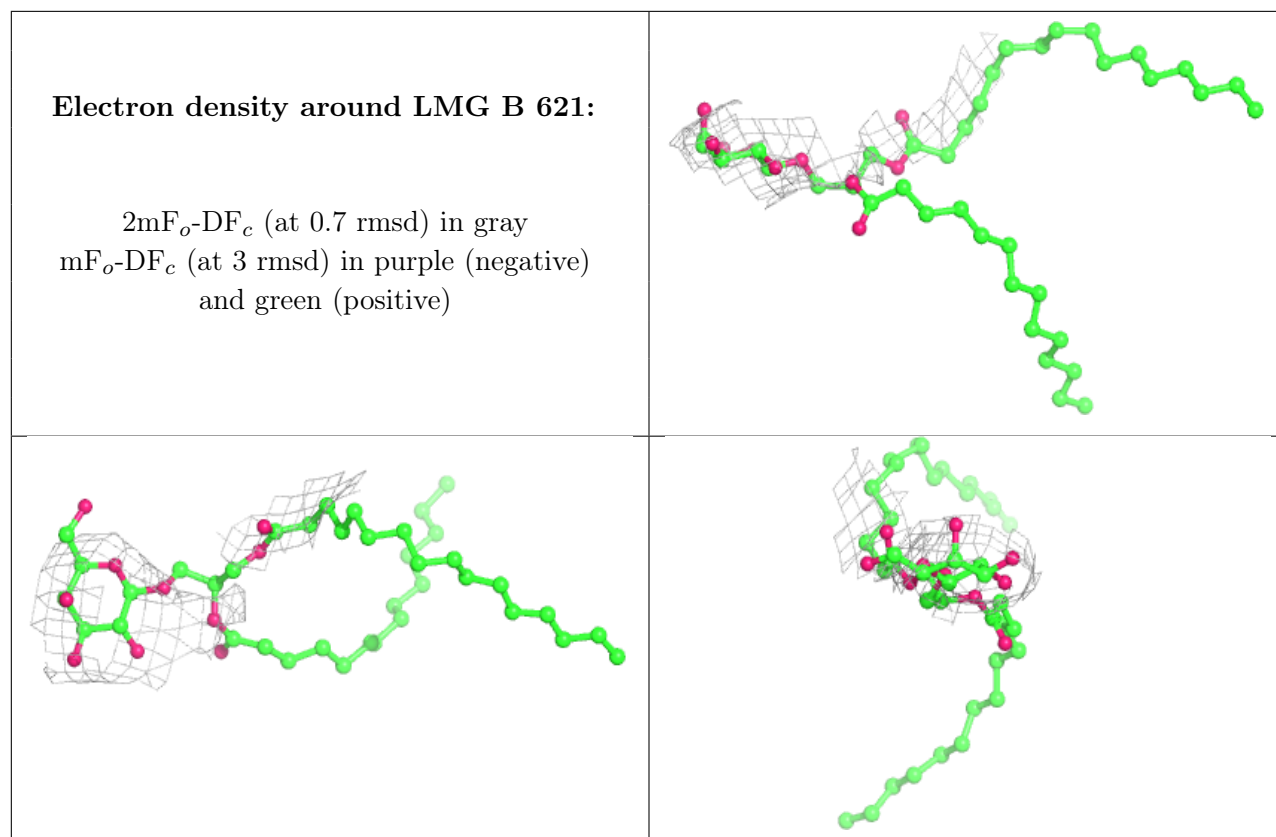
Electron density around DGD B 620:

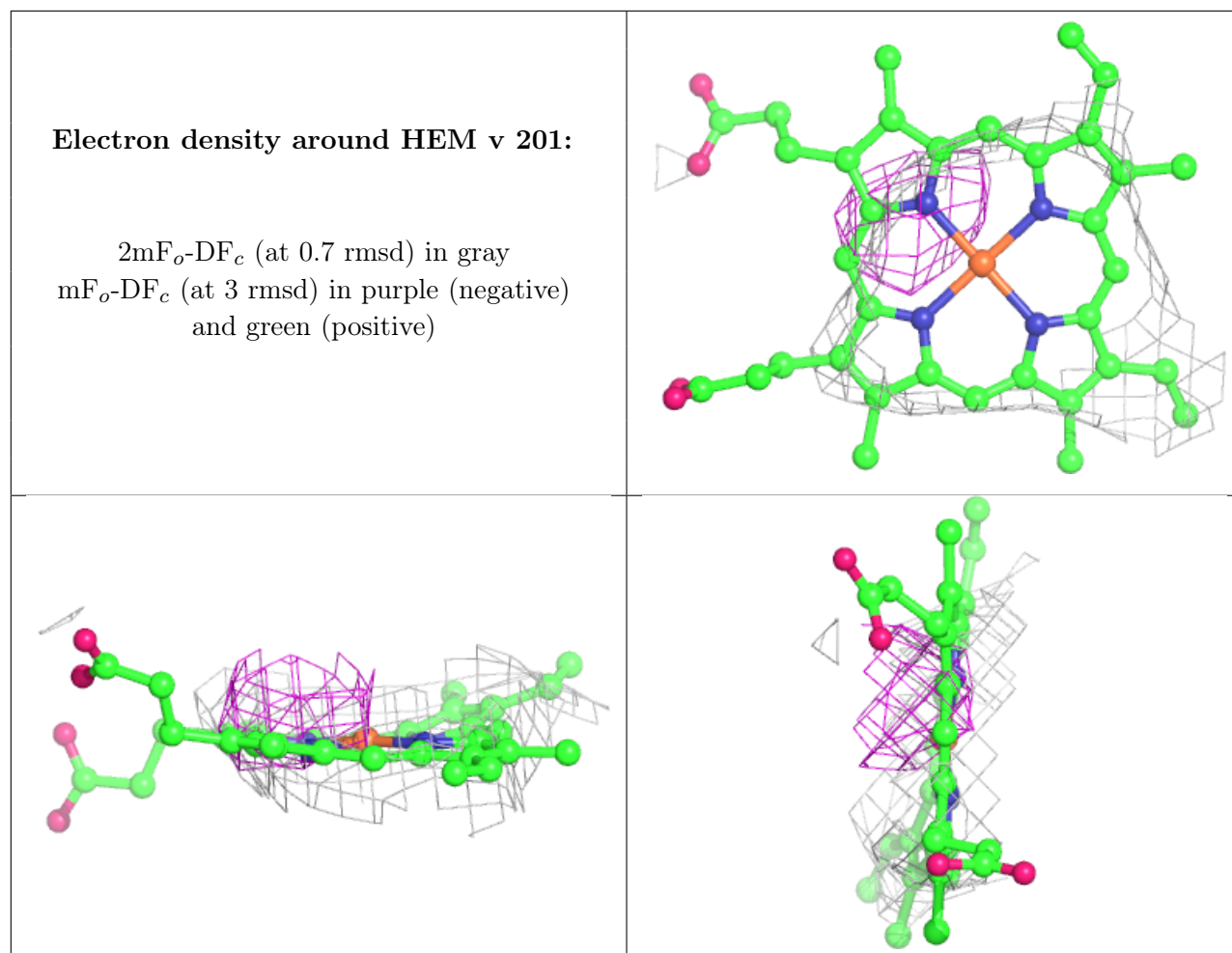
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA B 604:**

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

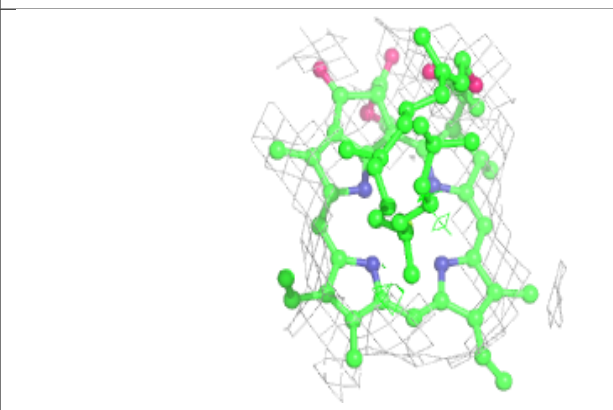
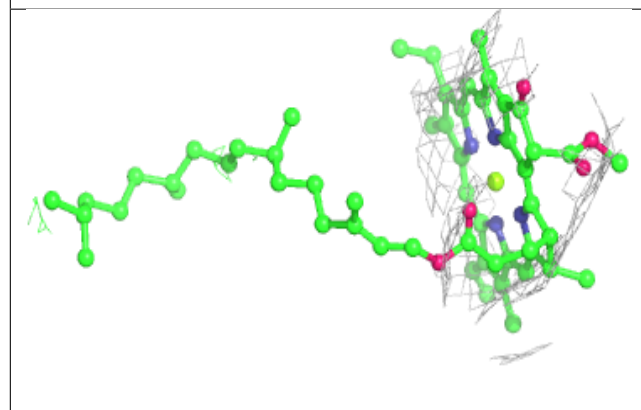
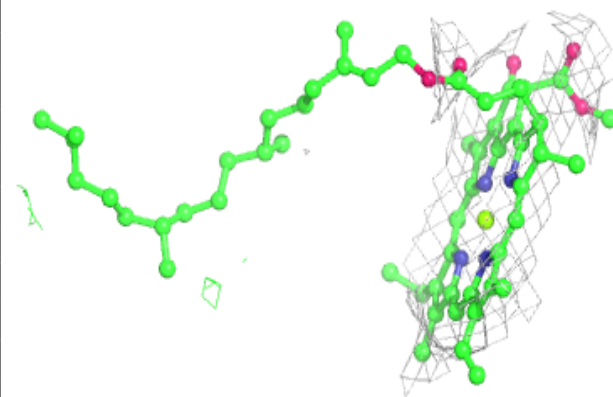




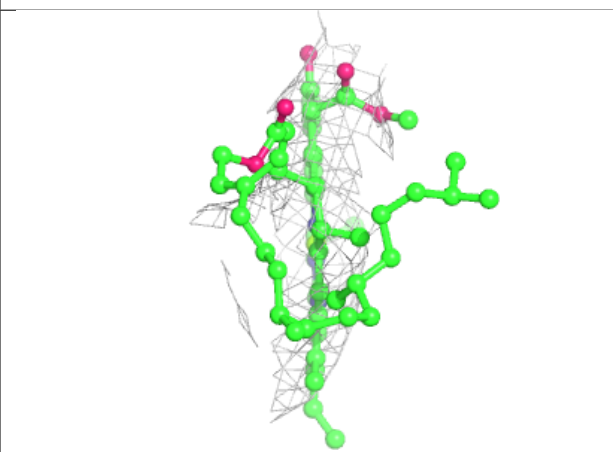
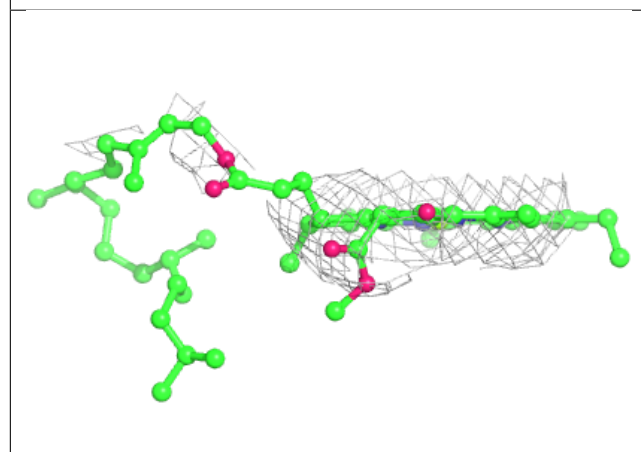
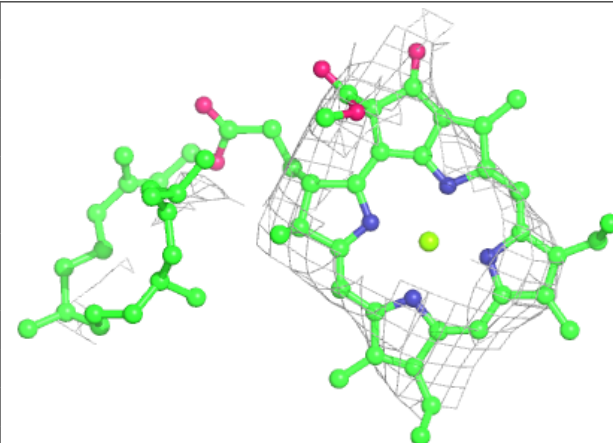


Electron density around CLA C 507:

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

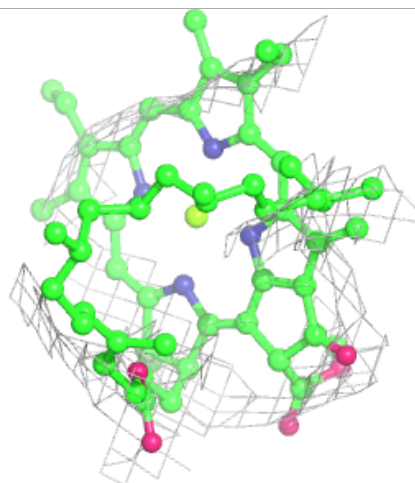
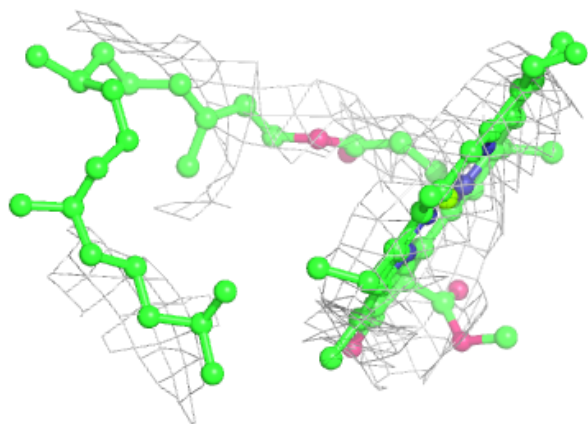
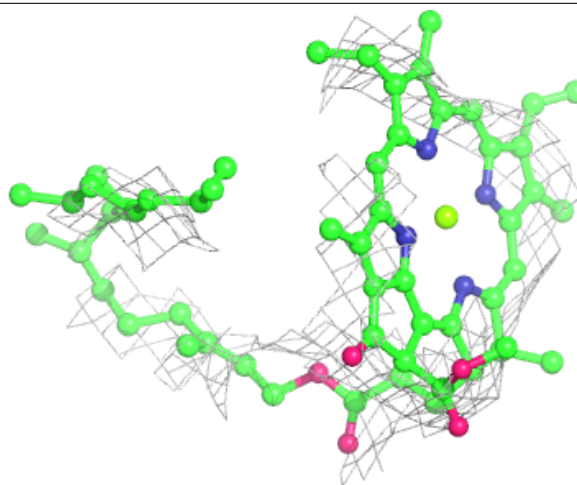
**Electron density around CLA c 511:**

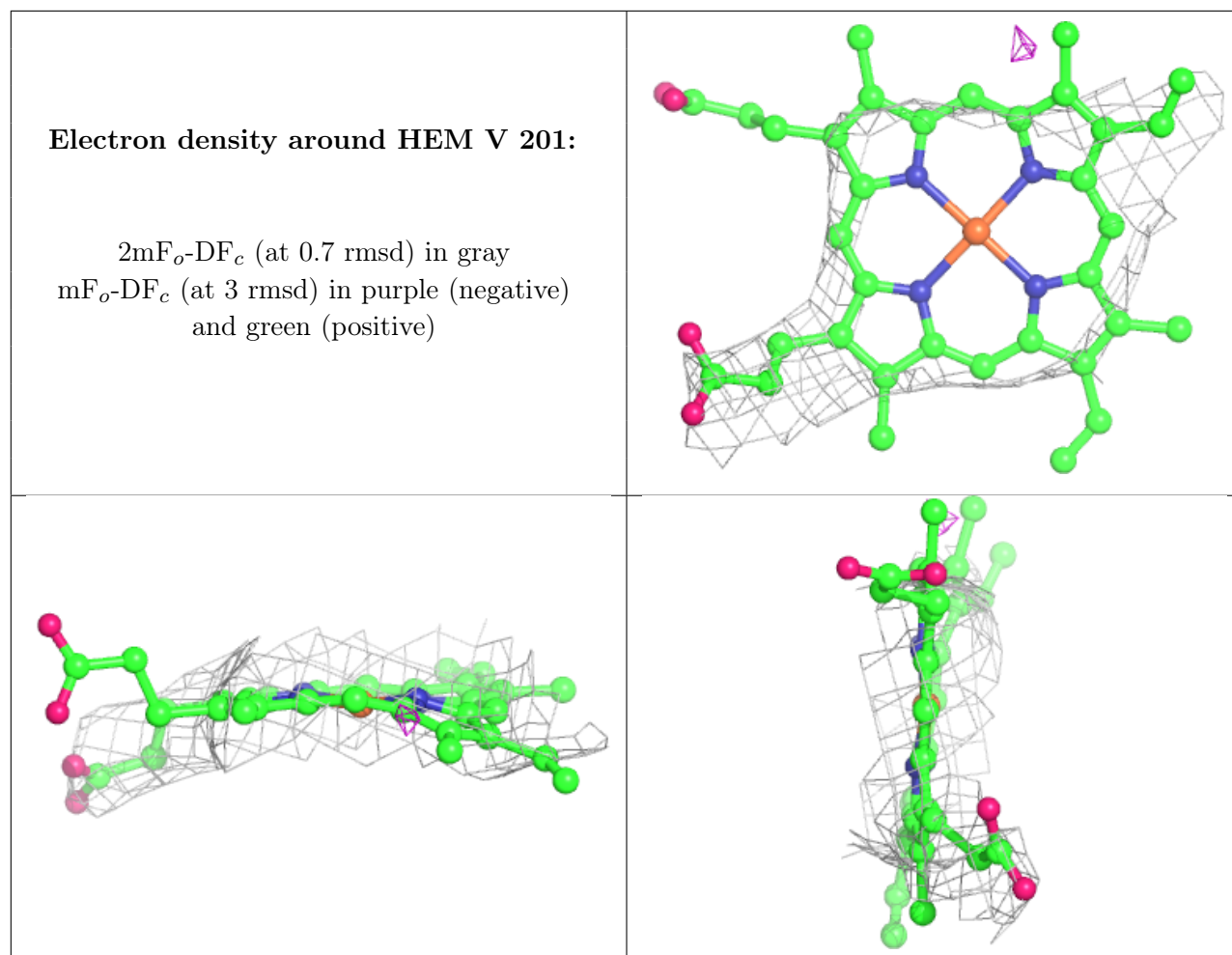
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 503:

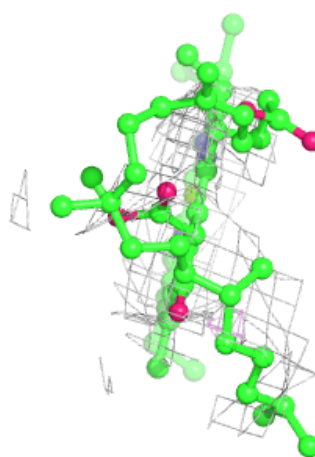
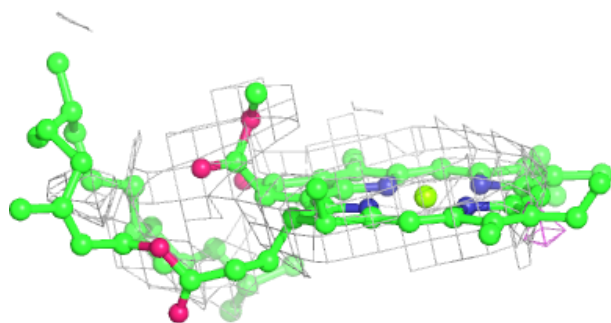
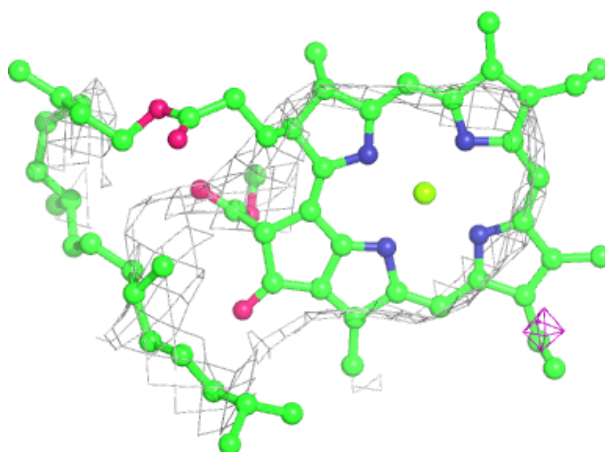
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





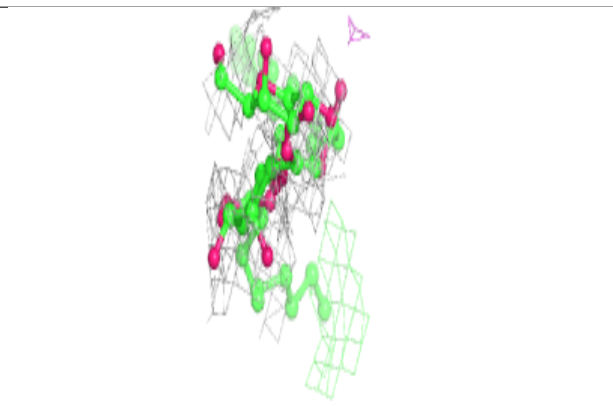
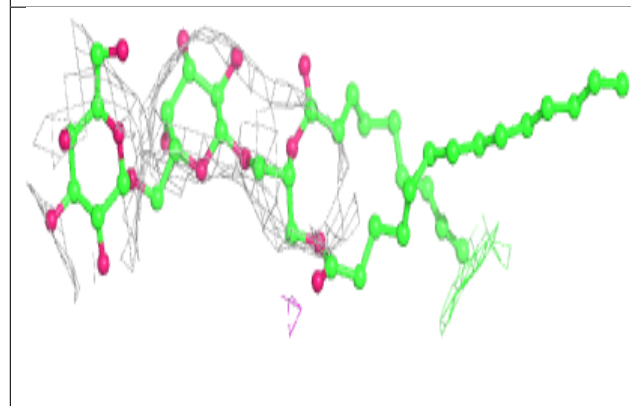
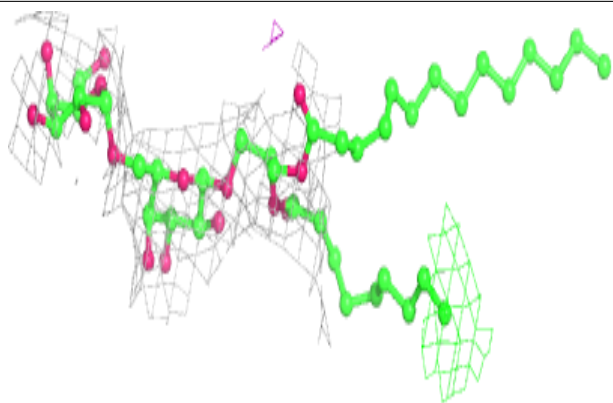
Electron density around CLA B 609:

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

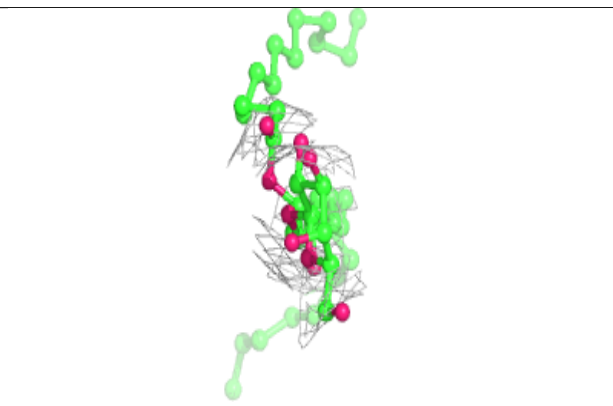
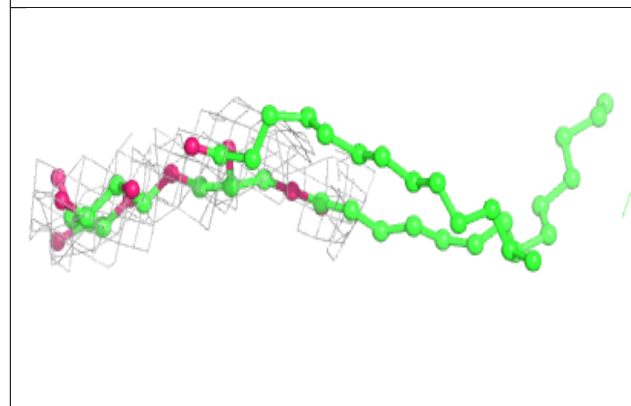
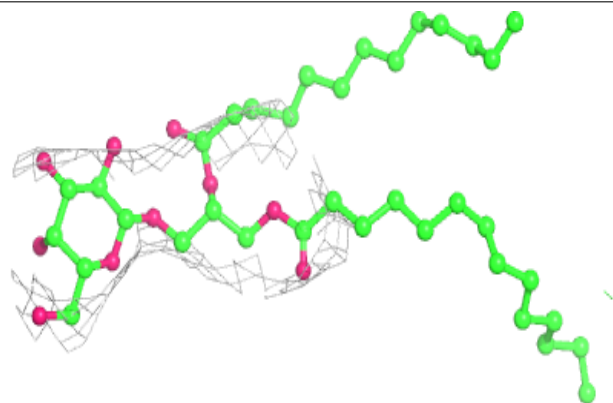


Electron density around DGD C 515:

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

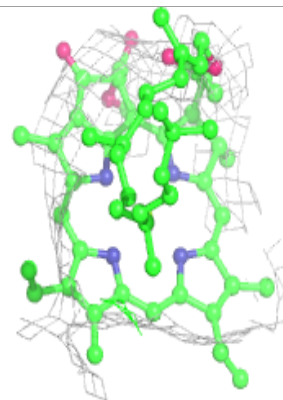
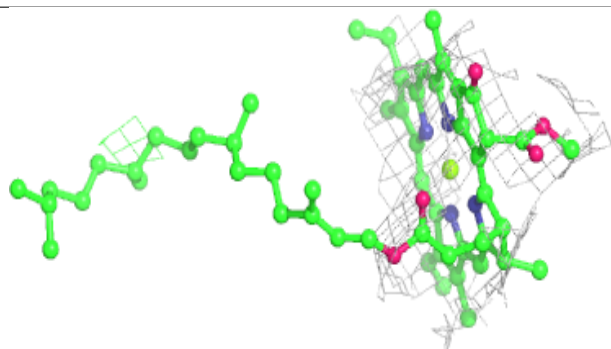
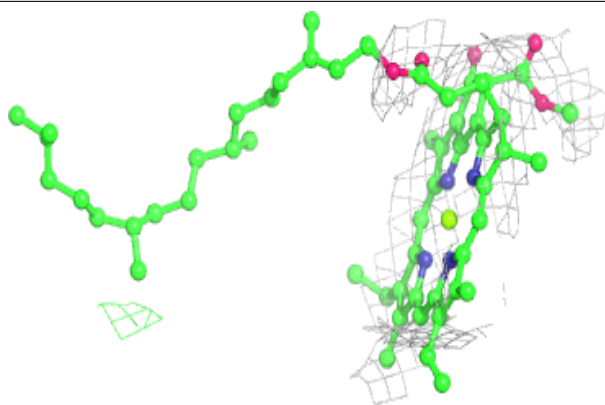
**Electron density around LMG d 411:**

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

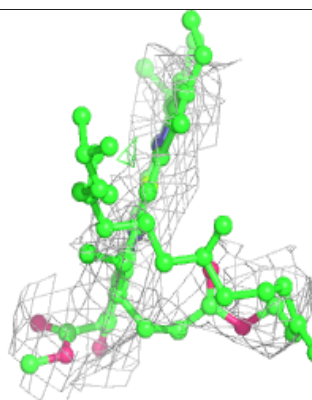
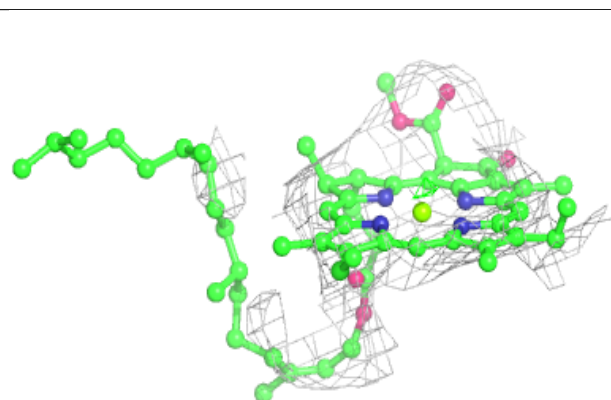
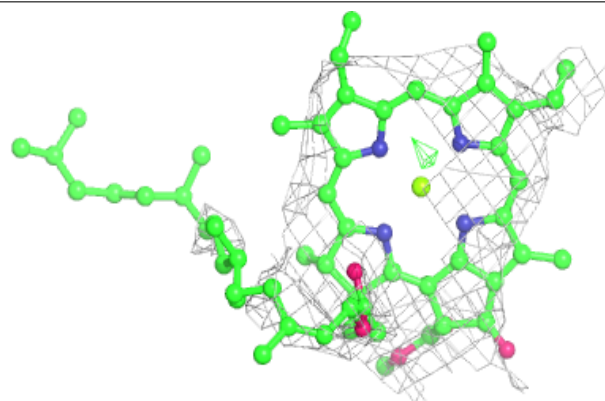


Electron density around CLA c 507:

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

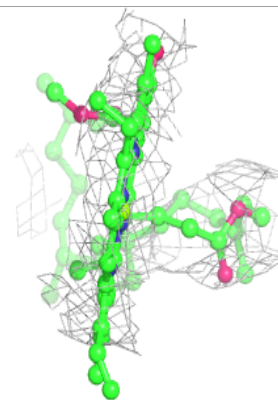
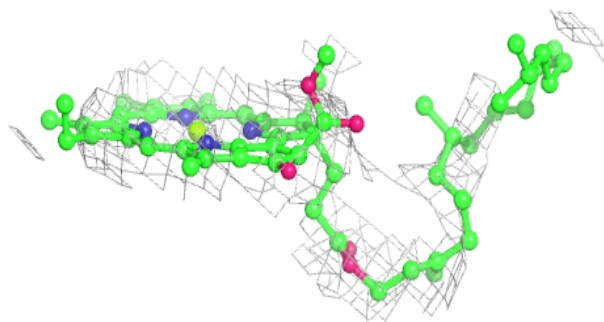
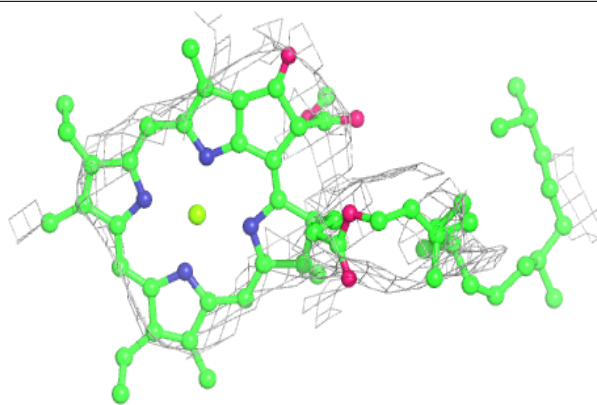
**Electron density around CLA A 403:**

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

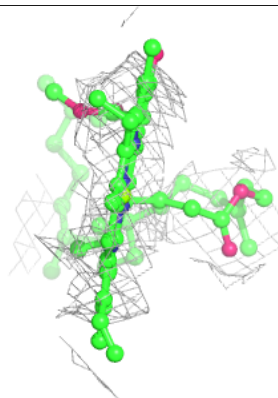
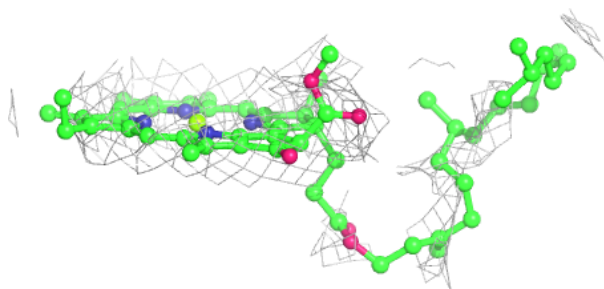
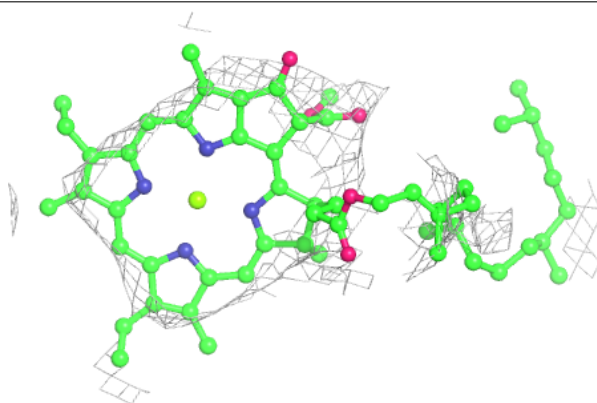


Electron density around CLA B 611:

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

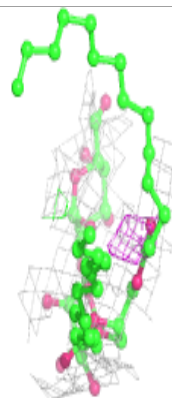
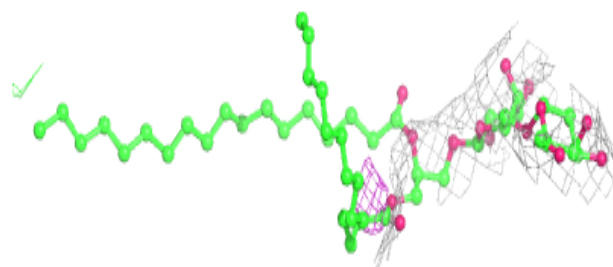
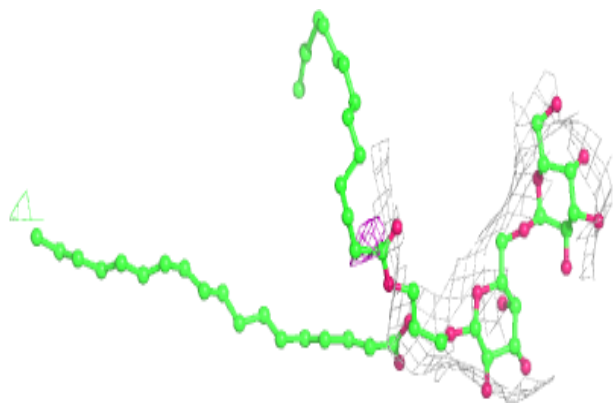
**Electron density around CLA b 615:**

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

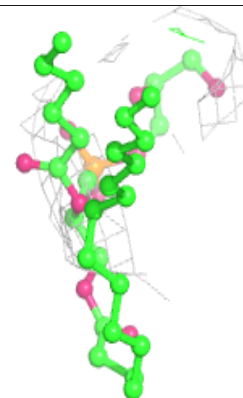
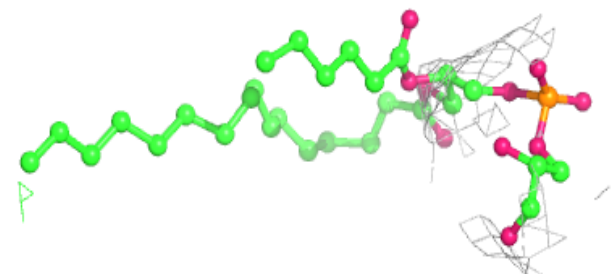
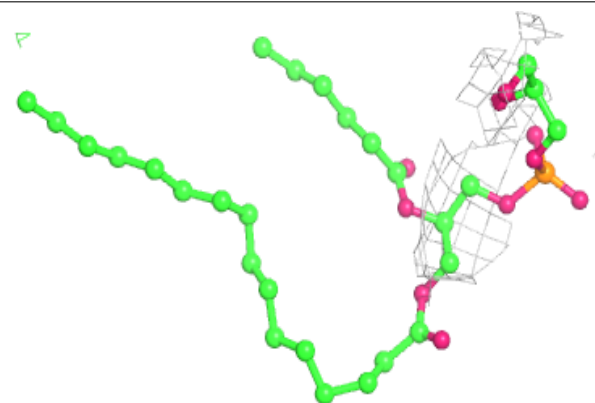


Electron density around DGD c 516:

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

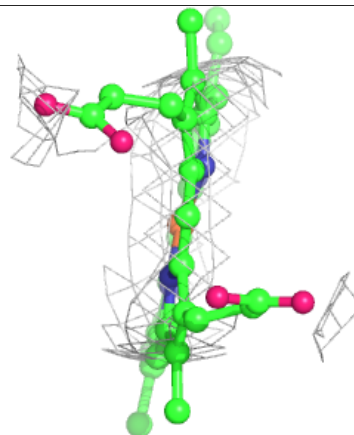
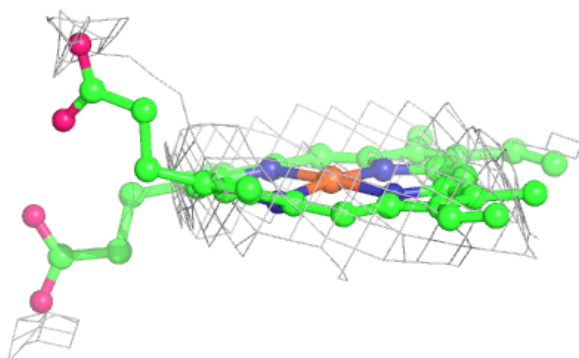
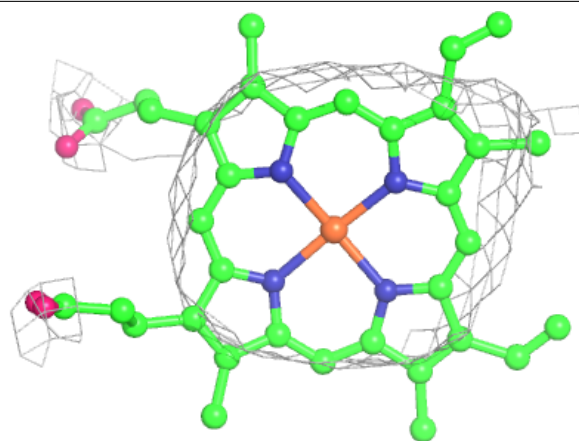
**Electron density around LHG A 409:**

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

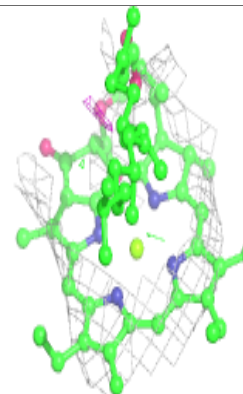
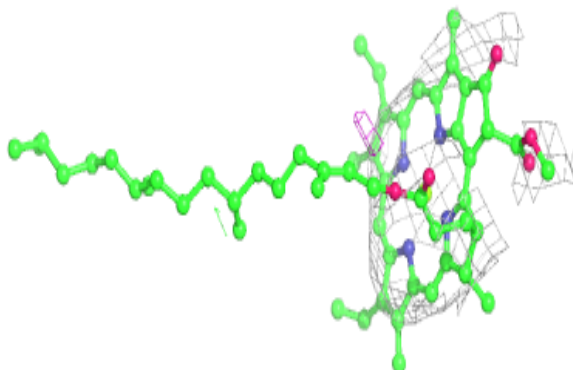
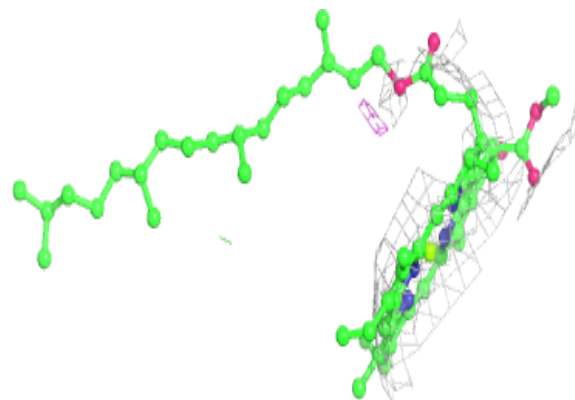


Electron density around HEM F 101:

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

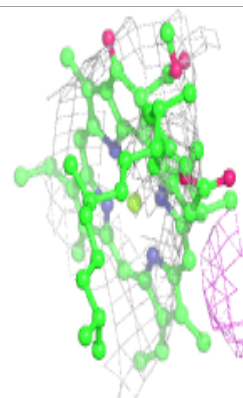
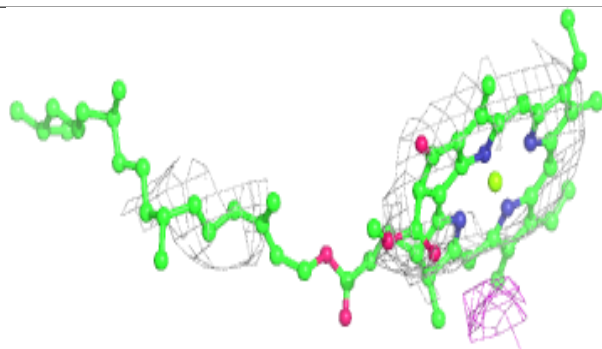
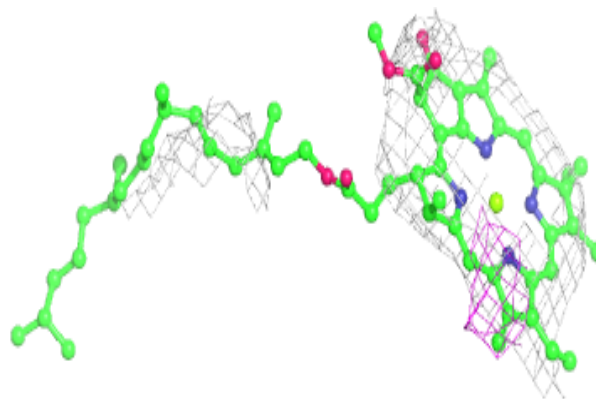
**Electron density around CLA c 520:**

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

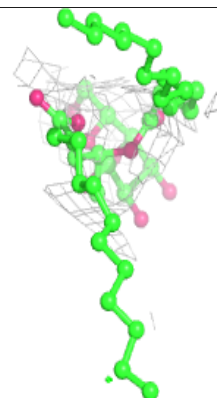
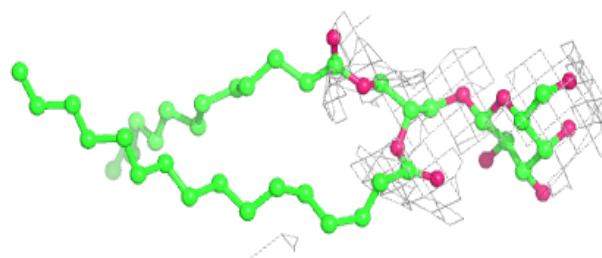
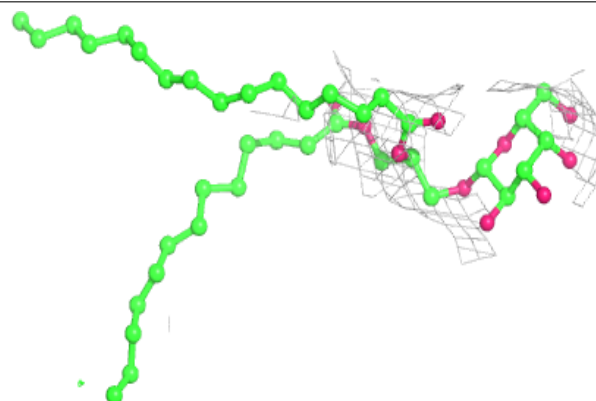


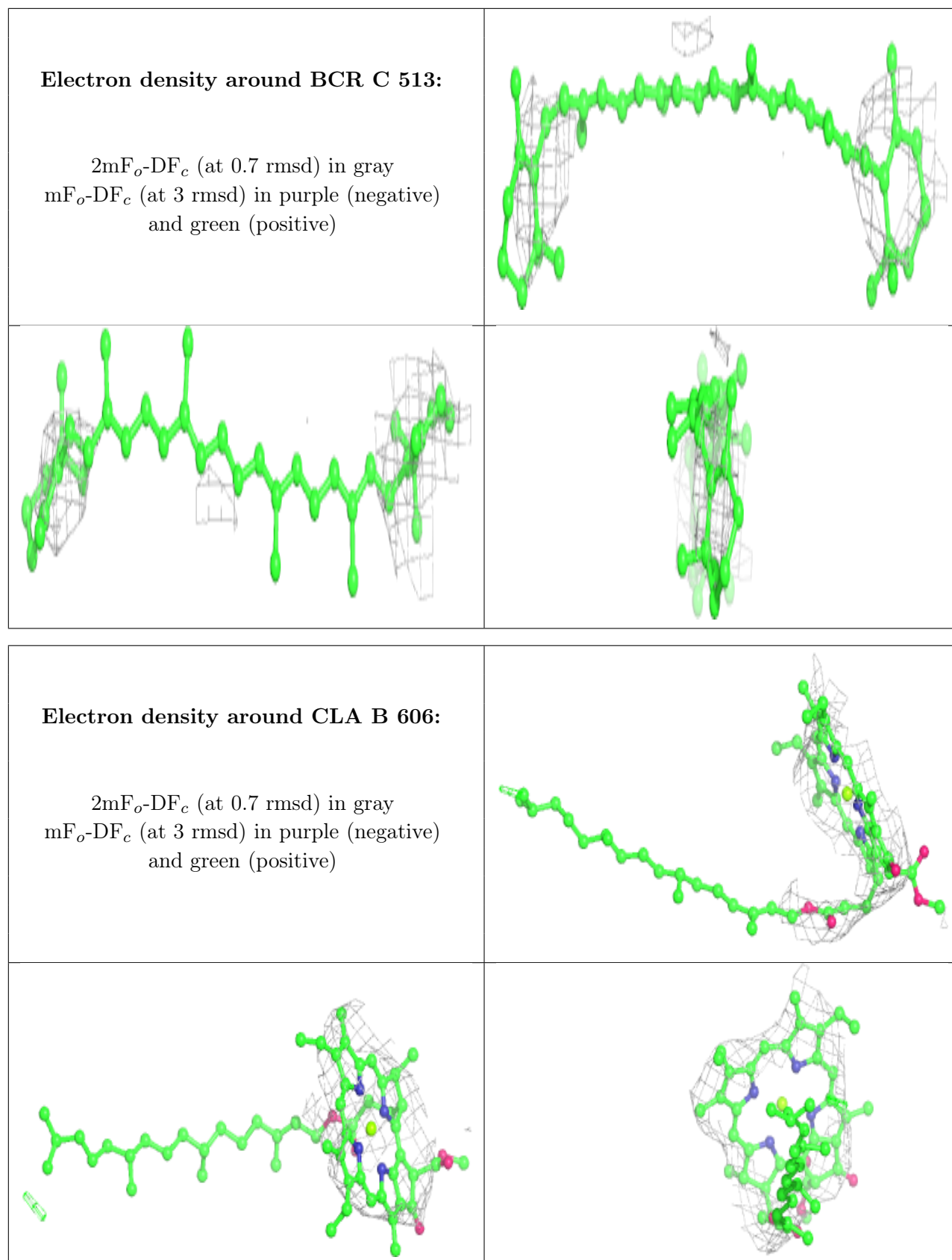
Electron density around CLA A 402:

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

**Electron density around LMG D 408:**

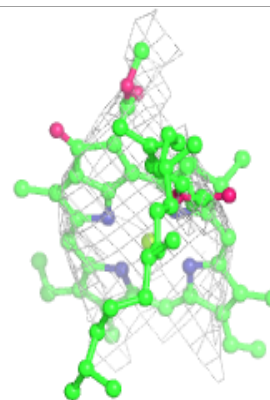
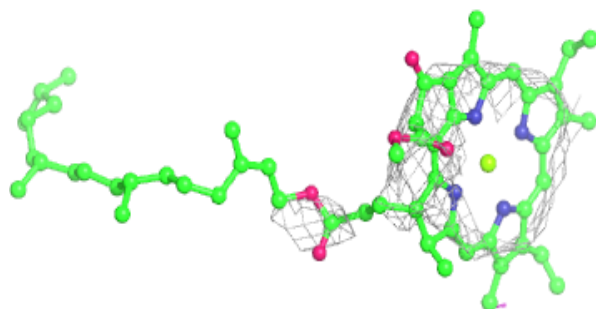
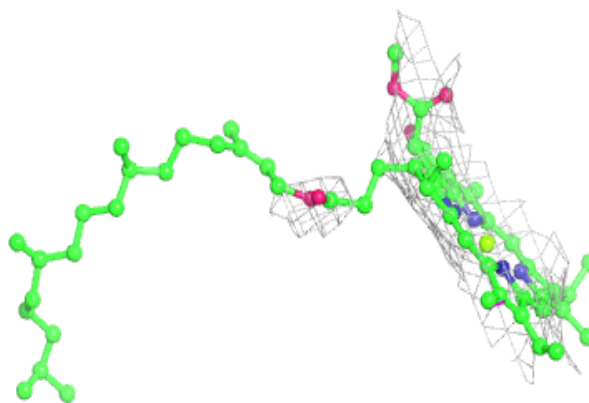
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



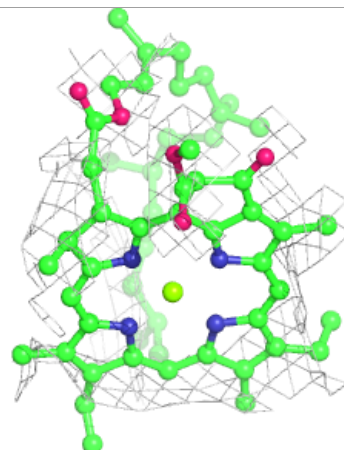
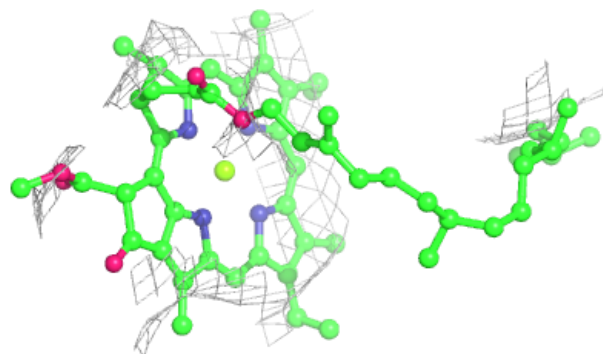
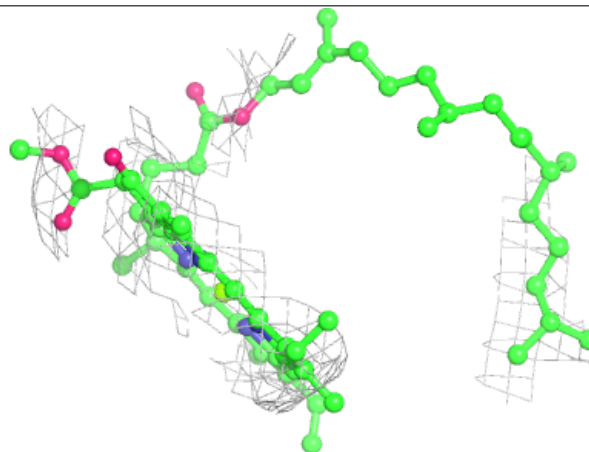


Electron density around CLA D 404:

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

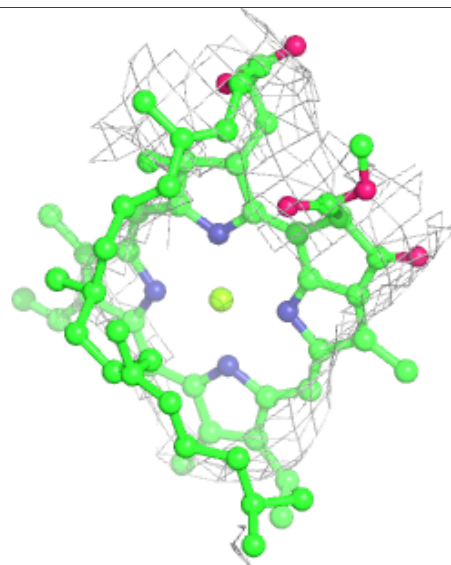
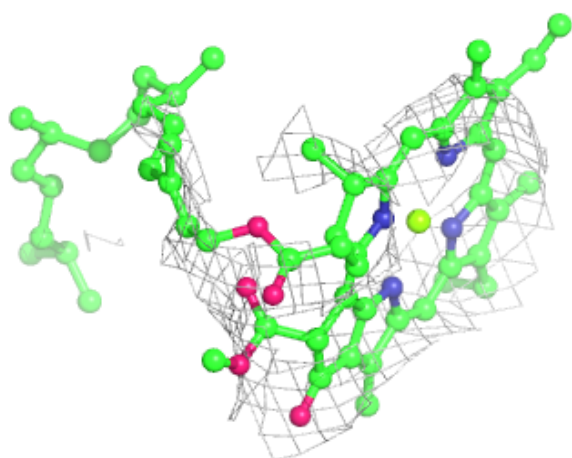
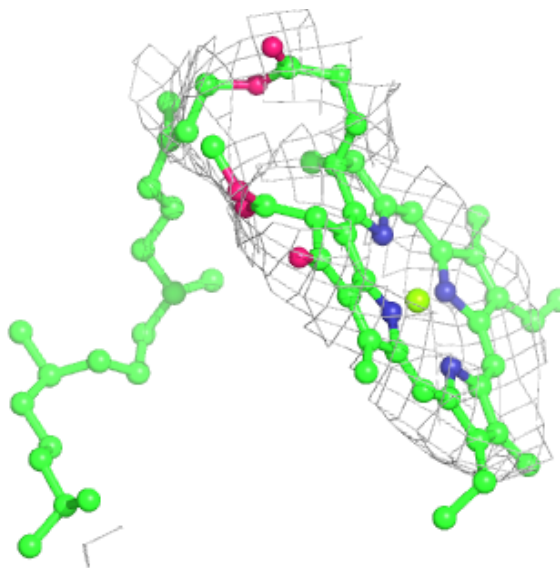
**Electron density around CLA b 614:**

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



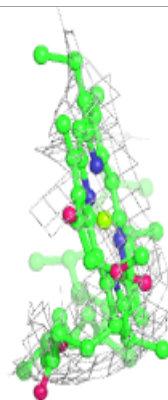
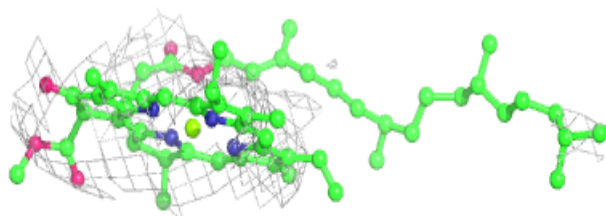
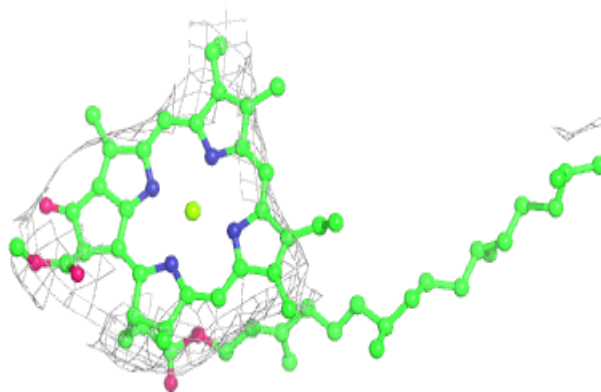
Electron density around CLA B 612:

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

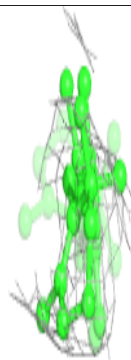
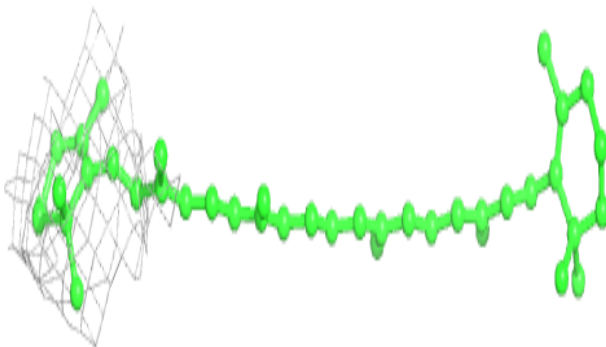
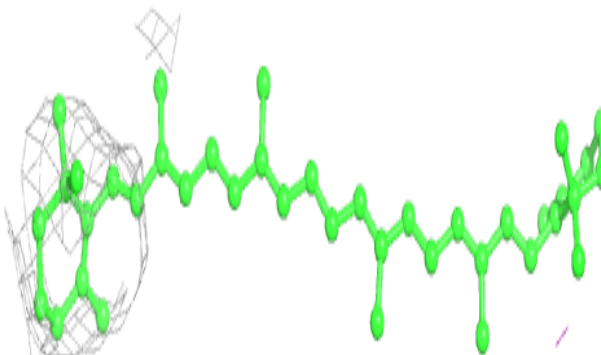


Electron density around CLA C 501:

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

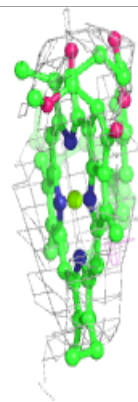
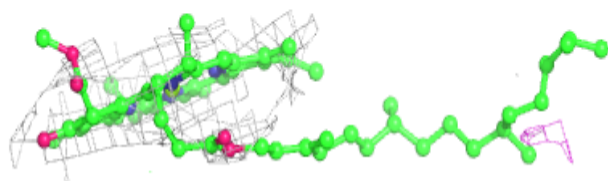
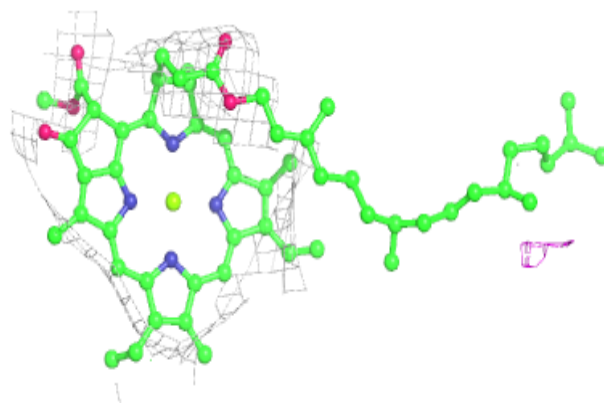
**Electron density around BCR b 620:**

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

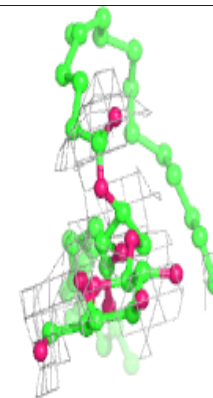
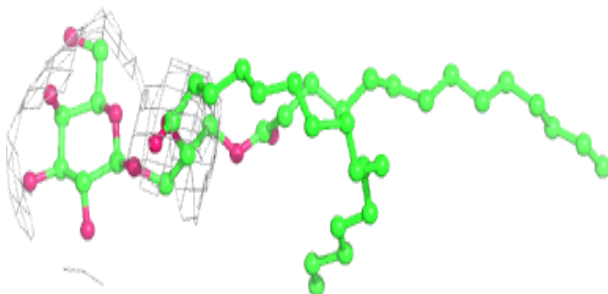
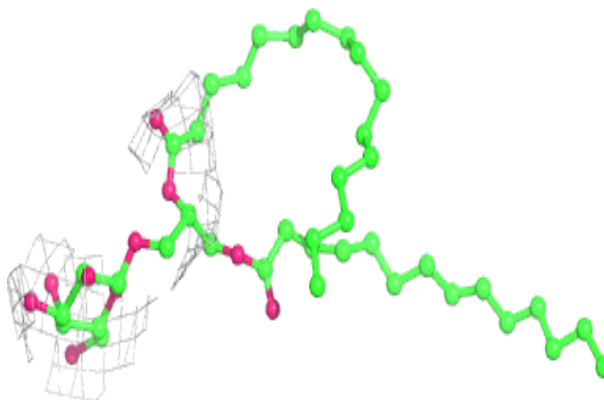


Electron density around CLA B 602:

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

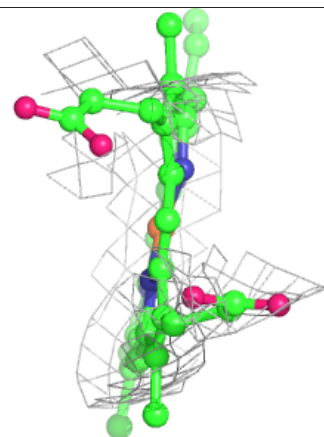
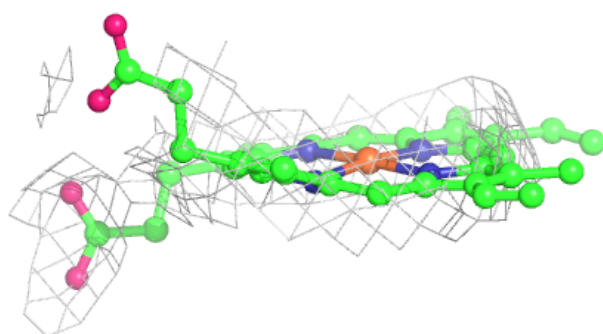
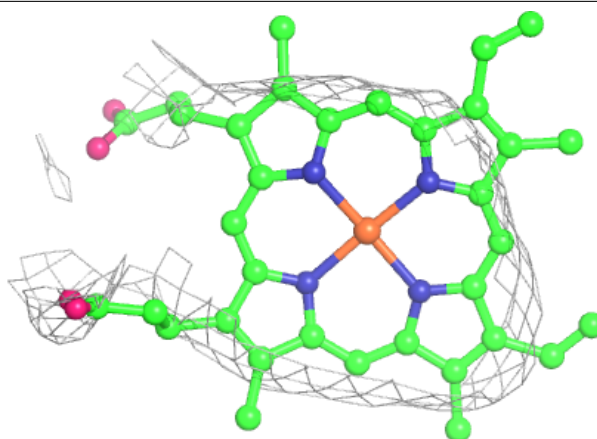
**Electron density around LMG d 407:**

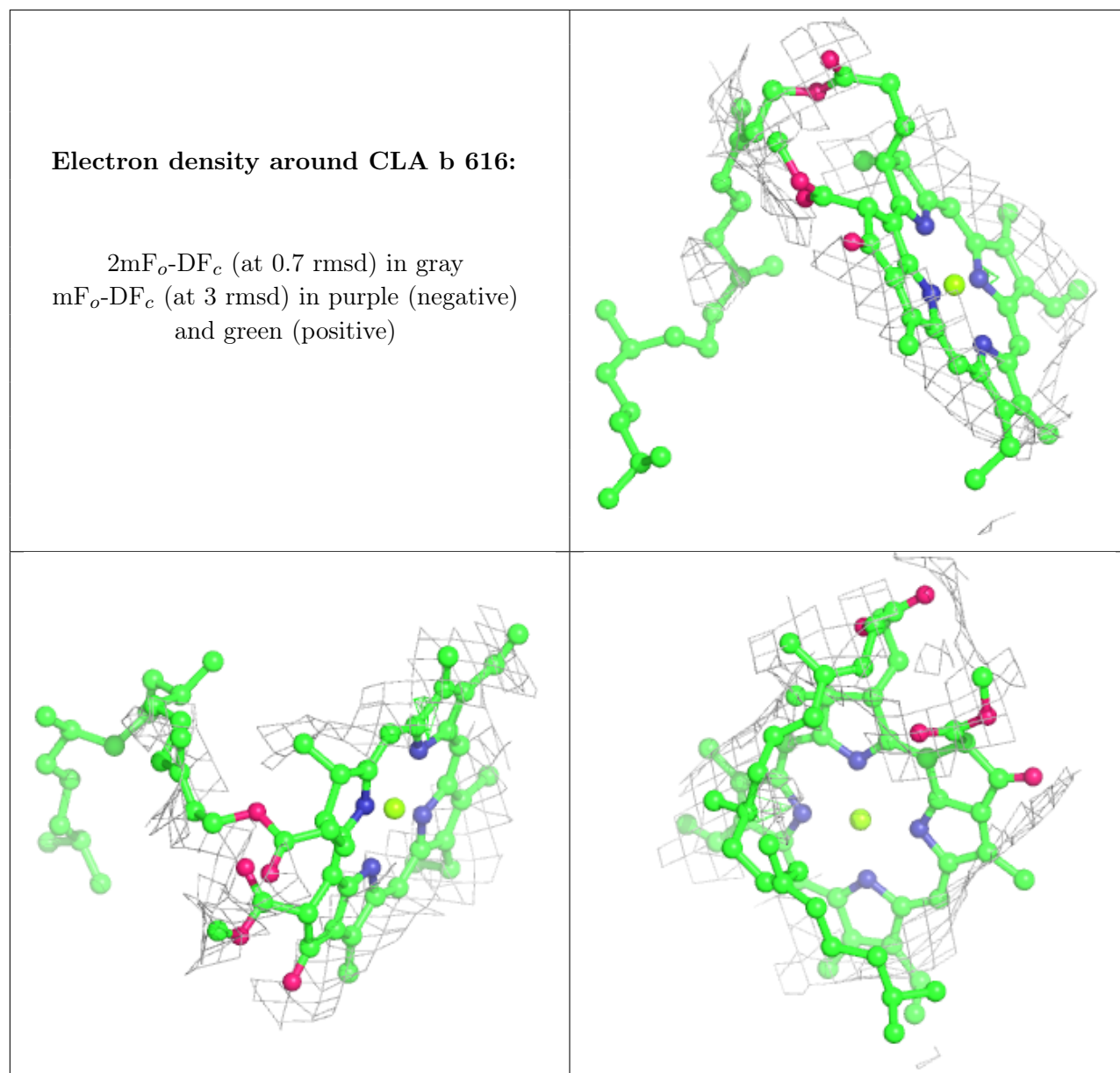
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





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

There are no such residues in this entry.