



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2023 – 12:11 AM EDT

PDB ID : 4TNJ  
Title : RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 4.5 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 : 4.50 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1

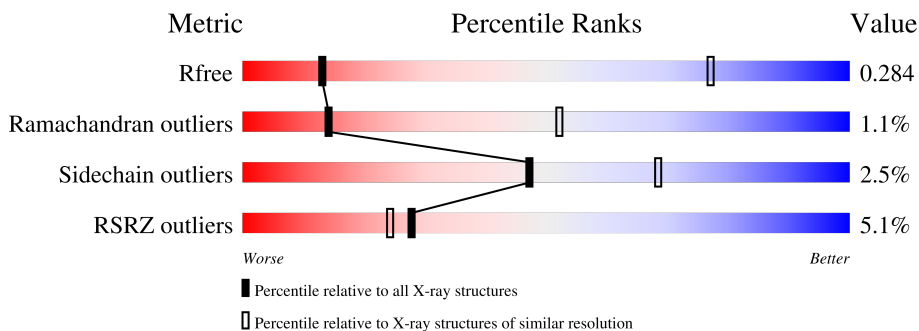
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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	1055 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	

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buster-report : 1.1.7 (2018)  
 Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
 Refmac : 5.8.0158  
 CCP4 : 7.0.044 (Gargrove)  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.35.1

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

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Mol	Chain	Length	Quality of chain
14	t	32	
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	-	-	-
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	X
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	-	-	-
22	CLA	C	520	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	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	X
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-
22	CLA	h	101	X	-	-	X
23	PL9	A	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	C	521	-	-	-	X
24	BCR	D	411	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	J	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	514	-	-	-	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	a	411	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	408	-	-	-	X
26	LHG	C	519	-	-	-	X
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	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	a	413	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	i	101	-	-	-	X
27	LMG	m	101	-	-	-	X
28	CL	A	411	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	d	402	-	-	-	X
31	LMT	B	622	-	-	-	X
31	LMT	B	623	-	-	-	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	604	-	-	-	X
31	LMT	b	626	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	409	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	d	401	-	-	-	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			

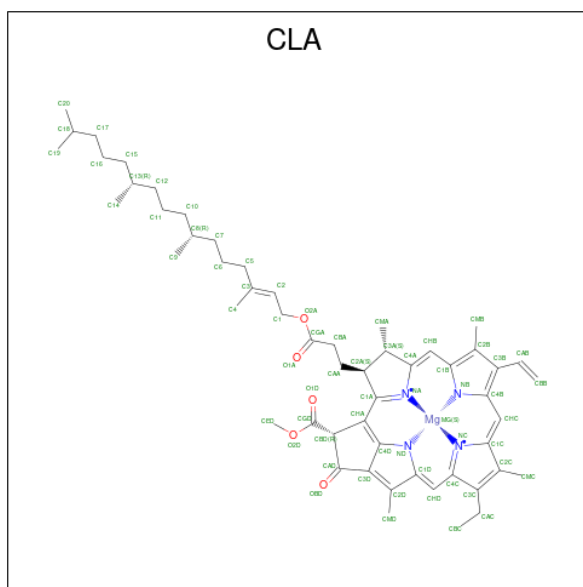
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	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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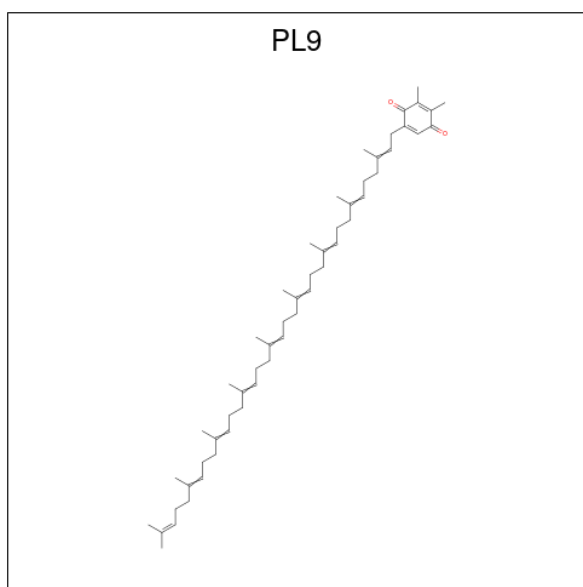
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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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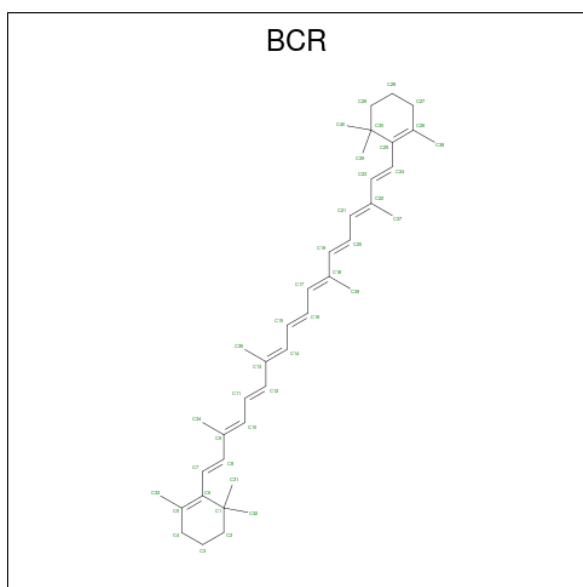
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



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: C<sub>40</sub>H<sub>56</sub>).



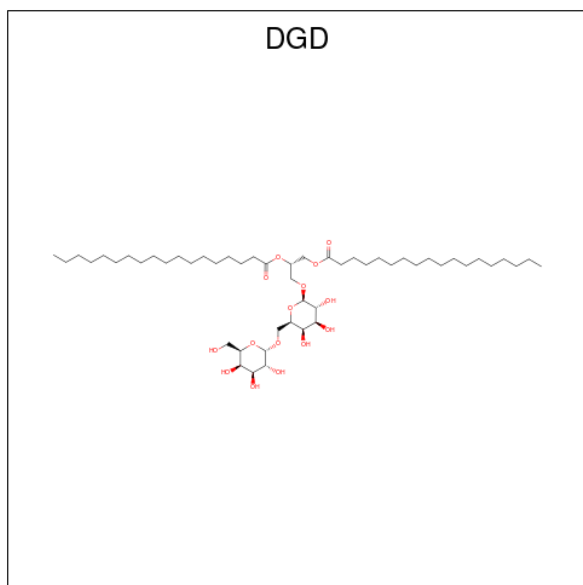
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total 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 (DGD) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



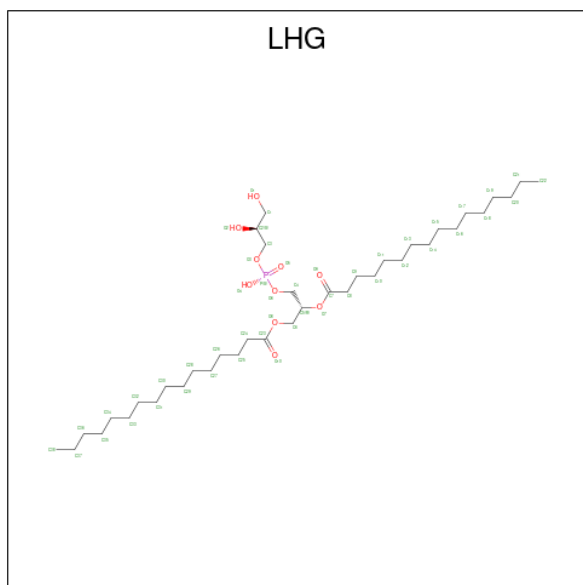
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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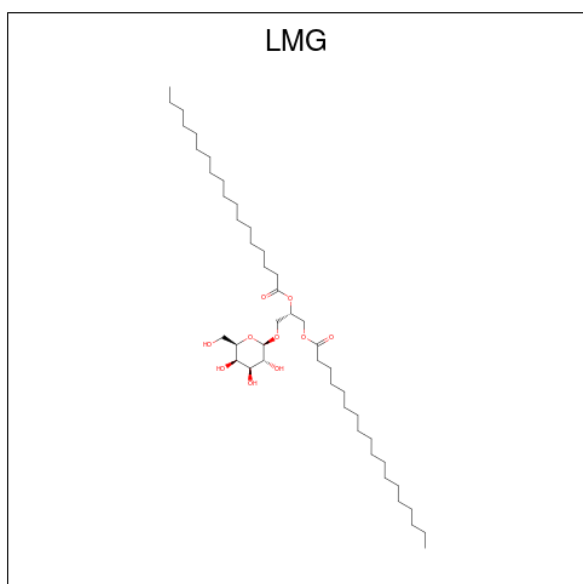
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total	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: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



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:  $C_{45}H_{86}O_{10}$ ).



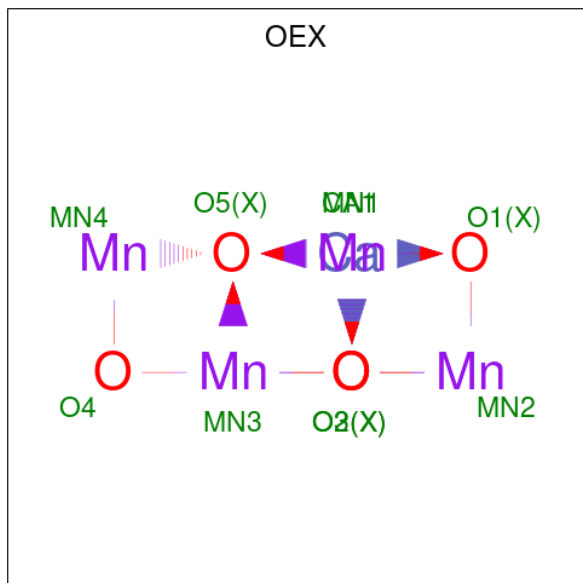


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	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	a	1	Total	C	O	0	0
			51	41	10		
27	b	1	Total	C	O	0	0
			49	39	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
			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		

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

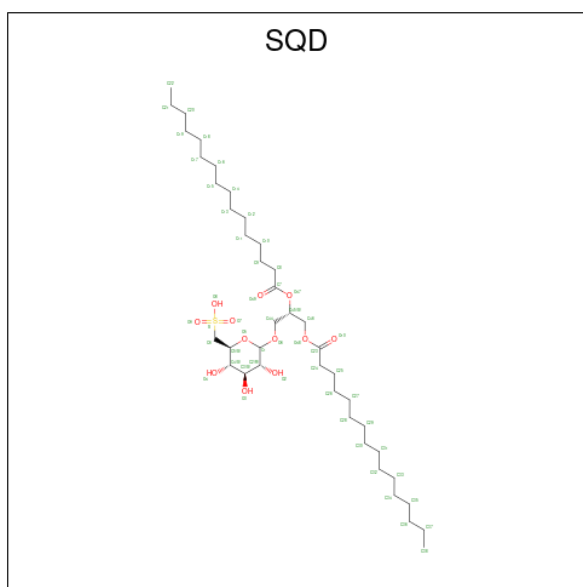
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Cl 1 1	0	0
28	a	1	Total Cl 1 1	0	0

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn<sub>4</sub>O<sub>5</sub>).



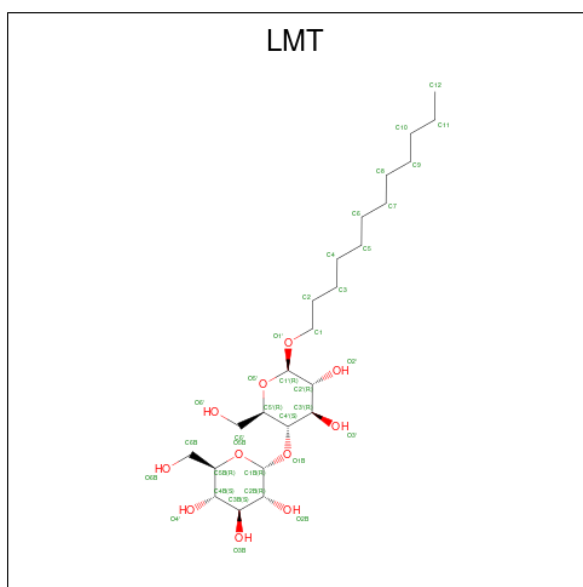
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Ca Mn O 10 1 4 5	0	0
29	a	1	Total Ca Mn O 10 1 4 5	0	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



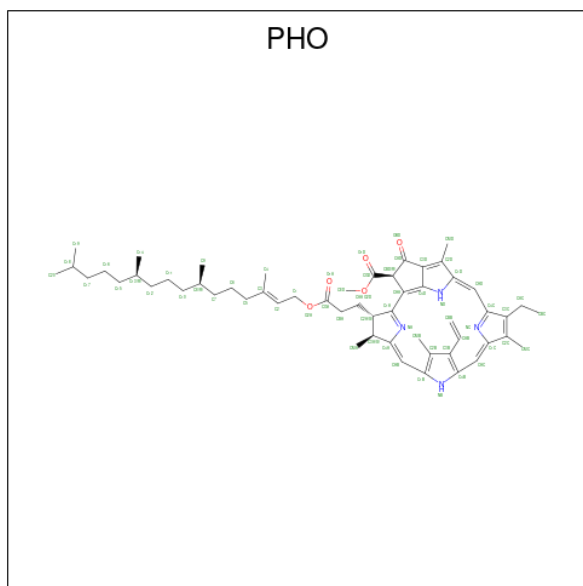
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			S
30	A	1	51	38	12	1	0	0
30	A	1	54	41	12	1	0	0
30	B	1	47	34	12	1	0	0
30	D	1	43	30	12	1	0	0
30	F	1	45	32	12	1	0	0
30	a	1	54	41	12	1	0	0
30	a	1	51	38	12	1	0	0
30	b	1	47	34	12	1	0	0
30	d	1	43	30	12	1	0	0
30	f	1	45	32	12	1	0	0

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



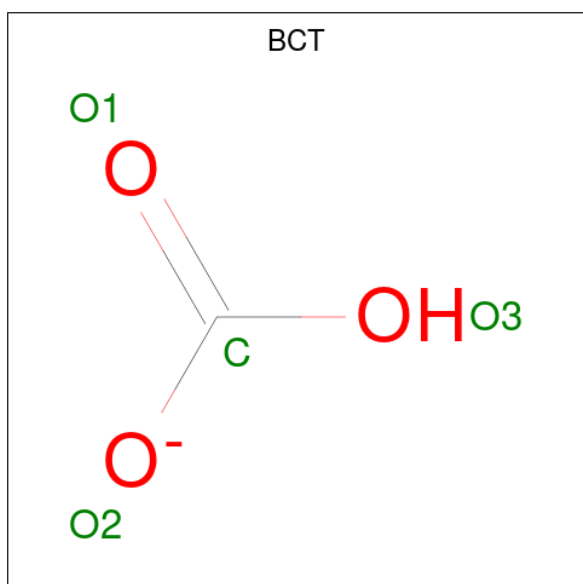
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	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:  $CHO_3$ ).





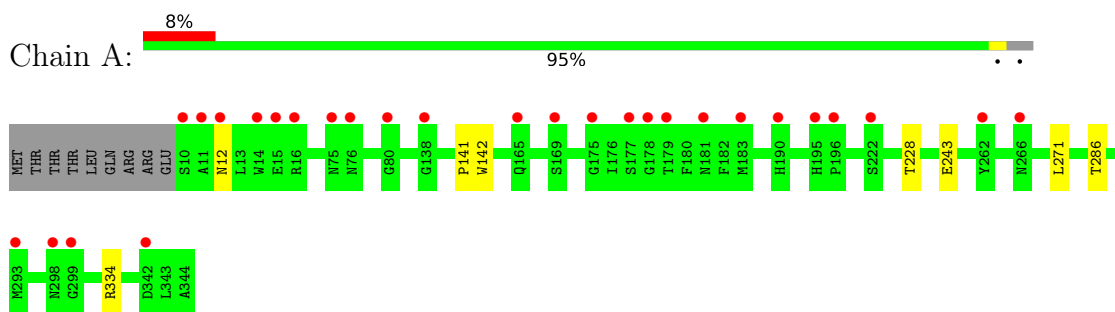
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
35	o	1	Total	Ca	0	0
			1	1		

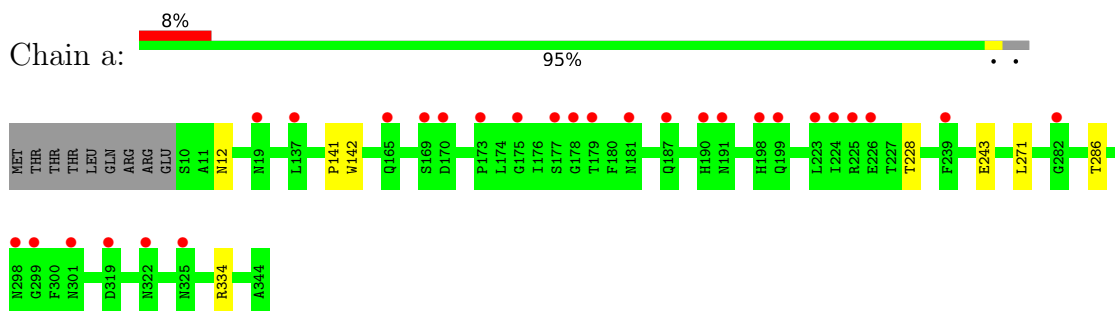
### 3 Residue-property plots [i](#)

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.

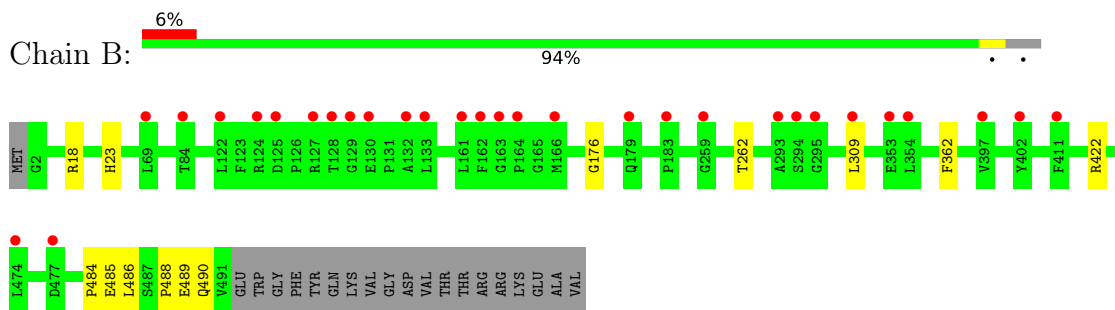
- Molecule 1: Photosystem Q(B) protein 1



- Molecule 1: Photosystem Q(B) protein 1



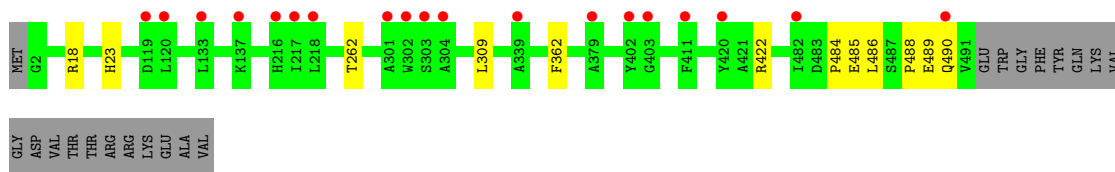
- Molecule 2: Photosystem II core light harvesting protein



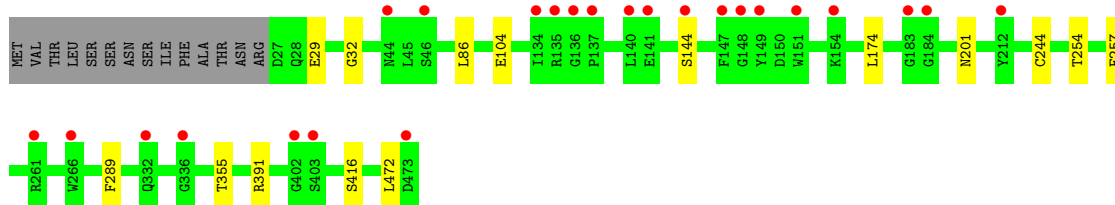
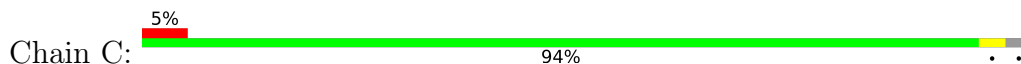
- Molecule 2: Photosystem II core light harvesting protein



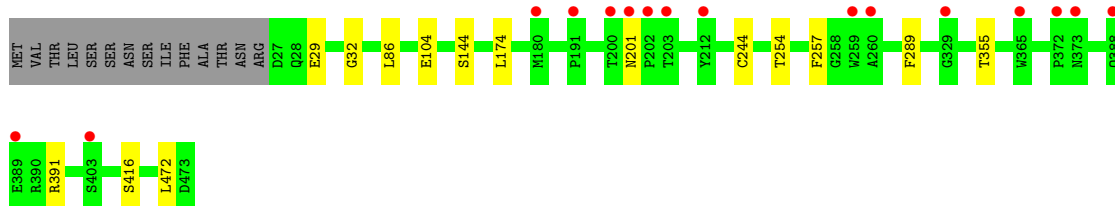




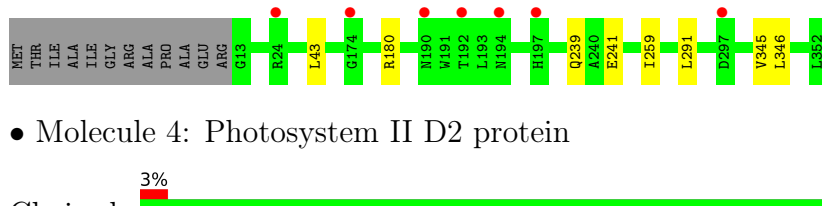
● Molecule 3: Photosystem II CP43 protein



● Molecule 3: Photosystem II CP43 protein



● Molecule 4: Photosystem II D2 protein



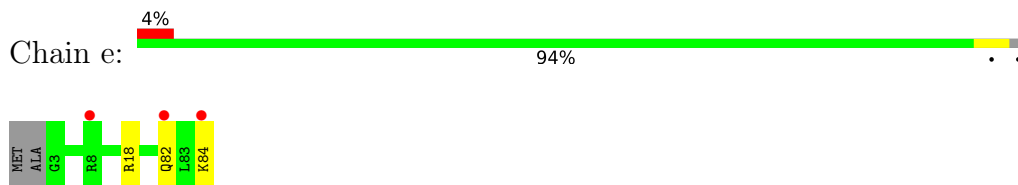
● Molecule 4: Photosystem II D2 protein



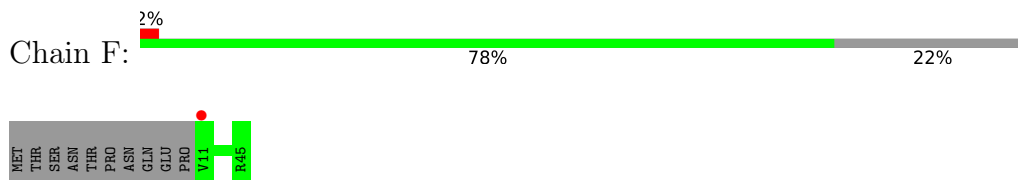
● Molecule 5: Cytochrome b559 subunit alpha



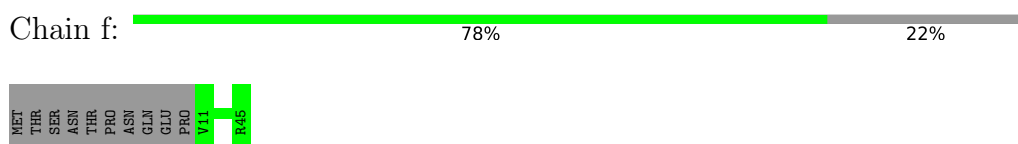
- Molecule 5: Cytochrome b559 subunit alpha



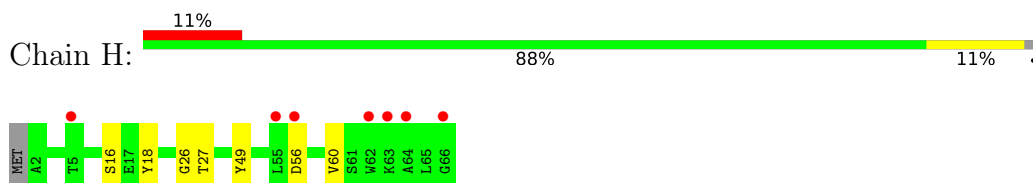
- Molecule 6: Cytochrome b559 subunit beta



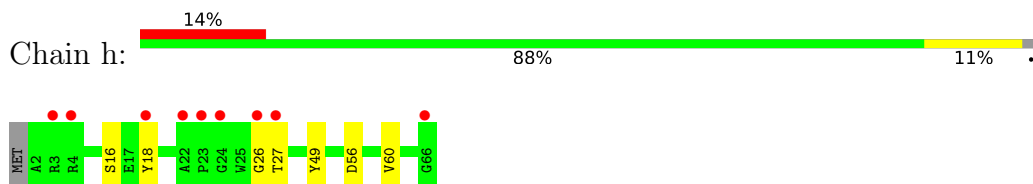
- Molecule 6: Cytochrome b559 subunit beta



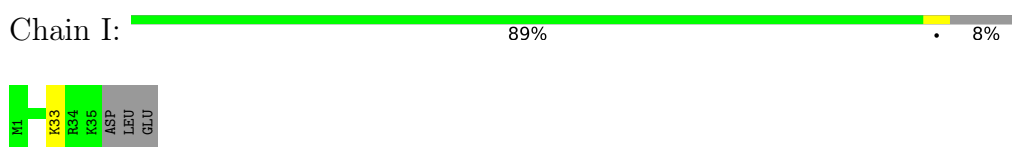
- Molecule 7: Photosystem II reaction center protein H



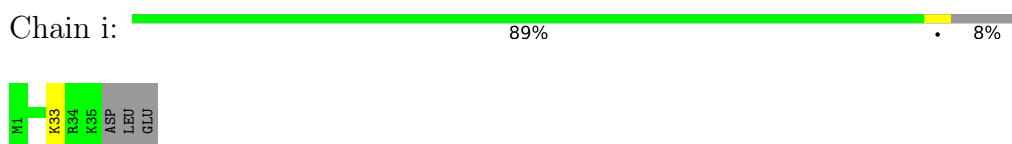
- Molecule 7: Photosystem II reaction center protein H




- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I




- Molecule 9: Photosystem II reaction center protein J

Chain J:  80% 5% 15%




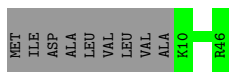
- Molecule 9: Photosystem II reaction center protein J

Chain j:  80% 5% 15%




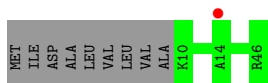
- Molecule 10: Photosystem II reaction center protein K

Chain K:  80% 20%



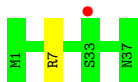
- Molecule 10: Photosystem II reaction center protein K

Chain k:  2% 80% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  3% 97%



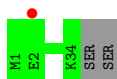
- Molecule 11: Photosystem II reaction center protein L

Chain l:  97%

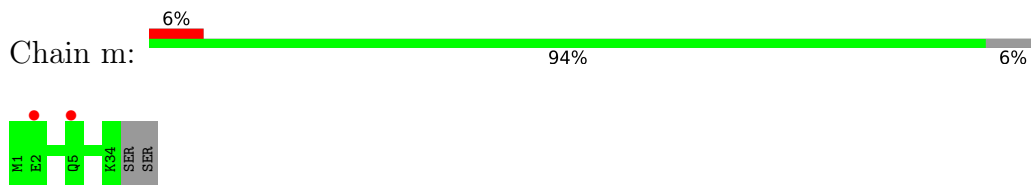


- Molecule 12: Photosystem II reaction center protein M

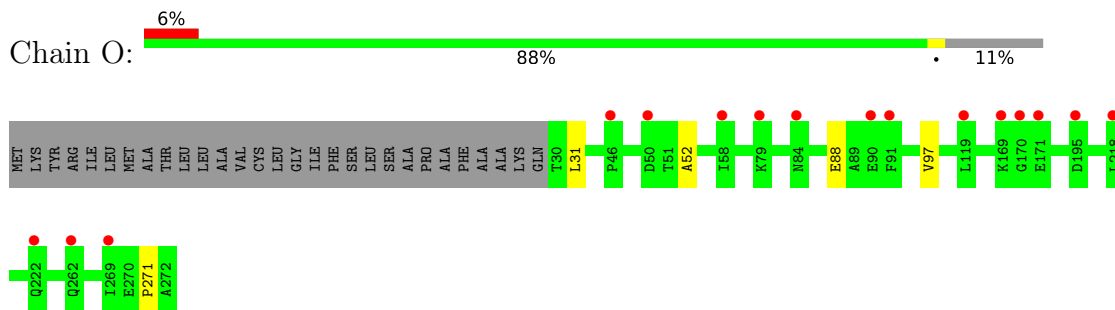
Chain M:  3% 94% 6%



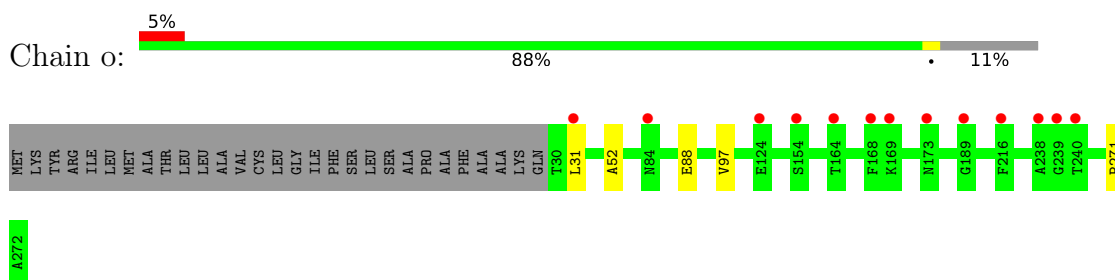
- Molecule 12: Photosystem II reaction center protein M



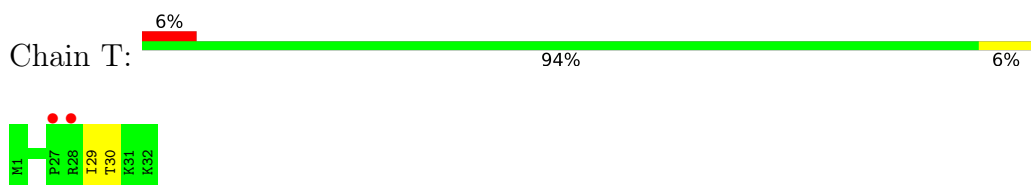
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



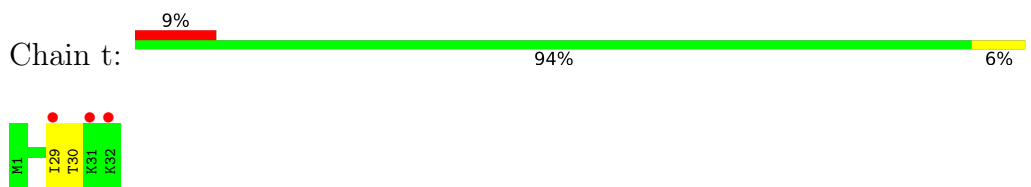
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



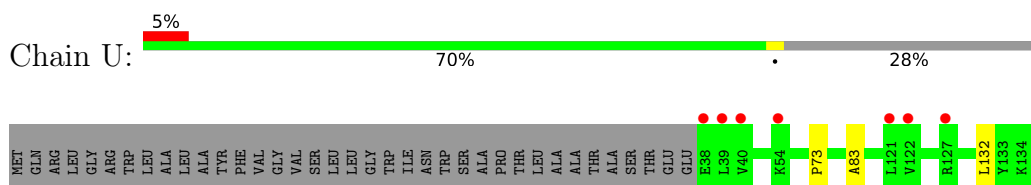
- Molecule 14: Photosystem II reaction center protein T



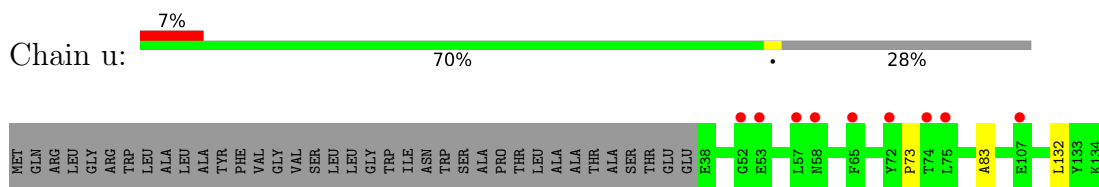
- Molecule 14: Photosystem II reaction center protein T



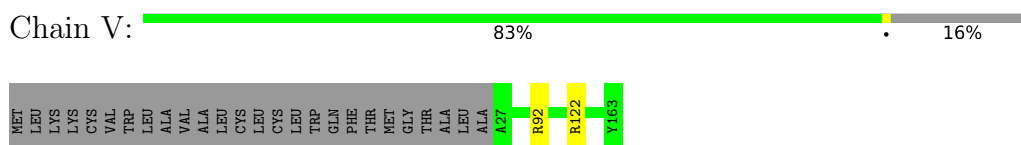
- Molecule 15: Photosystem II 12 kDa extrinsic protein



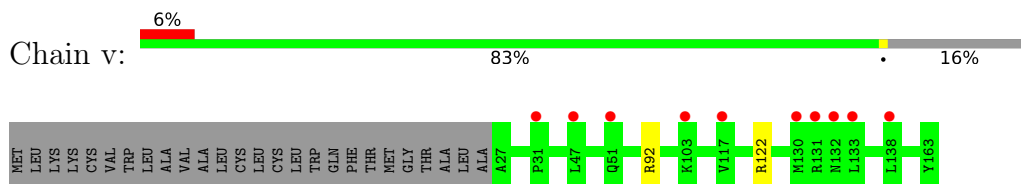
- Molecule 15: Photosystem II 12 kDa extrinsic protein



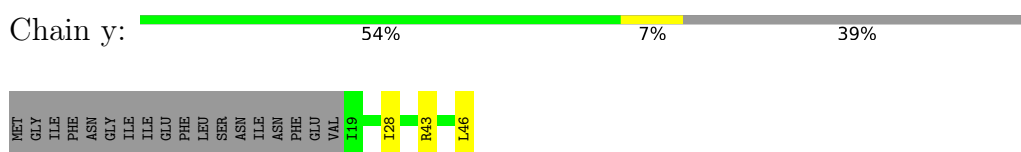
- Molecule 16: Cytochrome c-550



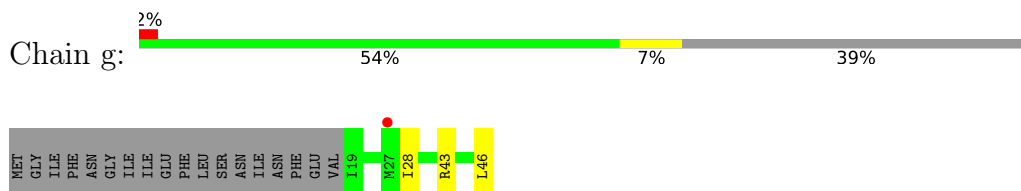
- Molecule 16: Cytochrome c-550



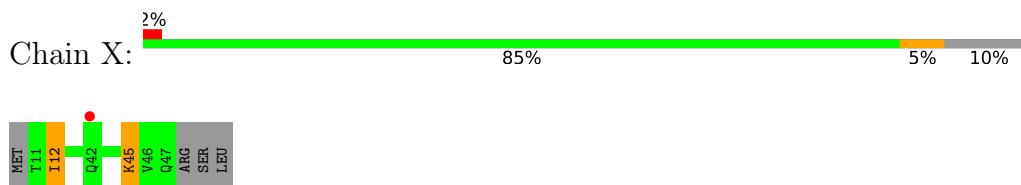
- Molecule 17: Photosystem II reaction center protein Ycf12



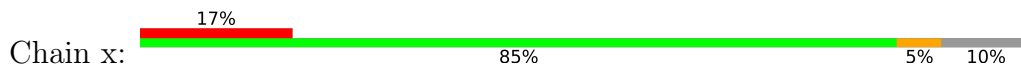
- Molecule 17: Photosystem II reaction center protein Ycf12

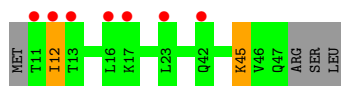


- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein





- Molecule 19: Photosystem II reaction center protein Y

Chain Y: 100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

Chain G: 100%

There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 2% 95% 5%



- Molecule 20: Photosystem II reaction center protein Z

Chain z: 8% 95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.30Å 228.71Å 307.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 4.50 72.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.97-4.50) 96.8 (72.97-4.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 4.46Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, $R_{free}$	0.276 , 0.284 0.277 , 0.284	Depositor DCC
$R_{free}$ test set	2668 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	153.6	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 115.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.16$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	174.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.25	0/293	0.43	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.22	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	0.24	0/270	0.44	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.25	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.44	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	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.26	0/273	0.44	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.25	0/490	0.44	0/669
All	All	0.23	0/41950	0.42	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%)	310 (93%)	19 (6%)	4 (1%)	13	50
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
2	B	488/510 (96%)	450 (92%)	34 (7%)	4 (1%)	19	60
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	25	65
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
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%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	31
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	31
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	30
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	30
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	39
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	39
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	27
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	27
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%)	4673 (91%)	410 (8%)	55 (1%)	14	52

5 of 55 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
1	a	12	ASN

### 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	62
3	c	347/362 (96%)	336 (97%)	11 (3%)	39	62
4	D	275/283 (97%)	268 (98%)	7 (2%)	47	68
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	40
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	40
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	63
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	63
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	55
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	55
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	61
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	61
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	43
18	x	30/34 (88%)	28 (93%)	2 (7%)	16	43
20	Z	52/52 (100%)	50 (96%)	2 (4%)	33	58
20	z	52/52 (100%)	50 (96%)	2 (4%)	33	58
All	All	4244/4594 (92%)	4140 (98%)	104 (2%)	47	68

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	23	HIS
3	c	254	THR
17	g	46	LEU
2	b	309	LEU
3	c	29	GLU

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

Mol	Chain	Res	Type
3	C	118	HIS

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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$
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
27	LMG	C	522	-	48,48,55	0.77	0	56,56,63	1.31	5 (8%)
26	LHG	c	519	-	36,36,48	0.73	2 (5%)	39,42,54	1.26	4 (10%)
24	BCR	b	621	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
31	LMT	b	627	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
24	BCR	C	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	9 (16%)
22	CLA	c	505	-	65,73,73	1.52	5 (7%)	76,113,113	1.40	6 (7%)
22	CLA	b	619	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	7 (9%)
22	CLA	C	512	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	402	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
24	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	9 (16%)
27	LMG	A	410	-	51,51,55	0.74	0	59,59,63	1.36	5 (8%)
25	DGD	A	408	-	57,57,67	0.93	0	71,71,81	1.41	7 (9%)
22	CLA	a	404	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	8 (10%)
27	LMG	a	402	-	42,42,55	0.84	0	50,50,63	1.25	3 (6%)
30	SQD	a	415	-	50,51,54	0.97	4 (8%)	59,62,65	1.74	10 (16%)
22	CLA	c	506	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	7 (9%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.31	5 (8%)
24	BCR	g	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
22	CLA	b	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	8 (10%)
22	CLA	c	508	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
24	BCR	b	623	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
25	DGD	C	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.44	12 (15%)
30	SQD	f	103	-	44,45,54	1.04	4 (9%)	53,56,65	1.63	11 (20%)
30	SQD	F	102	-	44,45,54	1.04	5 (11%)	53,56,65	1.64	10 (18%)
31	LMT	B	627	-	36,36,36	1.13	5 (13%)	47,47,47	0.95	1 (2%)
22	CLA	a	408	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	6 (7%)
22	CLA	C	504	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	7 (9%)
29	OEX	A	412	3,1	0,15,15	-	-	-	-	-
23	PL9	A	406	-	45,45,55	0.98	4 (8%)	56,57,69	1.56	10 (17%)
22	CLA	a	406	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	c	509	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	8 (10%)
25	DGD	c	516	-	63,63,67	0.92	1 (1%)	77,77,81	1.45	12 (15%)
25	DGD	B	620	-	59,59,67	0.90	1 (1%)	73,73,81	1.34	8 (10%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.28	6 (8%)
30	SQD	D	403	-	42,43,54	1.04	3 (7%)	51,54,65	1.78	10 (19%)
25	DGD	D	409	-	64,64,67	0.91	0	78,78,81	1.33	9 (11%)
27	LMG	i	101	-	43,43,55	0.82	0	51,51,63	1.27	6 (11%)
22	CLA	b	618	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	8 (10%)
25	DGD	b	601	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
24	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
27	LMG	d	407	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
22	CLA	b	614	-	65,73,73	1.55	6 (9%)	76,113,113	1.39	6 (7%)
25	DGD	b	624	-	59,59,67	0.91	1 (1%)	73,73,81	1.33	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	a	410	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	7 (12%)
27	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.30	4 (7%)
24	BCR	C	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	9 (16%)
22	CLA	c	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
27	LMG	b	628	-	49,49,55	0.76	0	57,57,63	1.31	4 (7%)
32	PHO	D	402	-	51,69,69	1.01	3 (5%)	47,99,99	1.10	4 (8%)
32	PHO	D	401	-	51,69,69	1.01	4 (7%)	47,99,99	1.11	5 (10%)
22	CLA	c	520	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
22	CLA	C	505	-	65,73,73	1.52	5 (7%)	76,113,113	1.40	7 (9%)
27	LMG	B	624	-	49,49,55	0.76	0	57,57,63	1.32	5 (8%)
27	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
22	CLA	B	614	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
24	BCR	y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	7 (12%)
30	SQD	d	402	-	42,43,54	1.05	3 (7%)	51,54,65	1.79	10 (19%)
31	LMT	I	102	-	36,36,36	1.11	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	D	405	-	65,73,73	1.51	5 (7%)	76,113,113	1.32	7 (9%)
23	PL9	d	406	-	55,55,55	1.02	2 (3%)	68,69,69	1.53	14 (20%)
31	LMT	d	409	-	32,32,36	1.18	5 (15%)	43,43,47	0.98	2 (4%)
22	CLA	C	510	3	65,73,73	1.50	5 (7%)	76,113,113	1.43	7 (9%)
22	CLA	b	617	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	6 (7%)
31	LMT	b	626	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	1 (2%)
24	BCR	f	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	5 (8%)
22	CLA	B	602	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
22	CLA	C	506	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	7 (9%)
22	CLA	A	403	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
22	CLA	c	503	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
22	CLA	B	611	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
26	LHG	a	412	-	38,38,48	0.68	1 (2%)	41,44,54	1.19	3 (7%)
27	LMG	M	101	-	42,42,55	0.86	0	50,50,63	1.24	4 (8%)
27	LMG	d	410	-	46,46,55	0.80	1 (2%)	54,54,63	1.31	4 (7%)
22	CLA	b	613	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
22	CLA	d	405	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	8 (10%)
22	CLA	C	507	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
24	BCR	D	411	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	7 (12%)
22	CLA	B	601	-	65,73,73	1.53	5 (7%)	76,113,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	404	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	6 (7%)
24	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.35	10 (17%)
22	CLA	B	615	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
27	LMG	b	625	-	49,49,55	0.78	1 (2%)	57,57,63	1.31	6 (10%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
30	SQD	A	414	-	53,54,54	0.96	5 (9%)	62,65,65	1.57	9 (14%)
31	LMT	B	622	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	1 (2%)
31	LMT	B	628	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	1 (2%)
24	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.58	12 (21%)
22	CLA	C	509	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
30	SQD	b	602	-	46,47,54	1.02	4 (8%)	55,58,65	1.79	10 (18%)
31	LMT	M	102	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	b	610	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	8 (10%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.30	5 (9%)
33	BCT	D	404	21	2,3,3	1.24	0	2,3,3	4.17	1 (50%)
31	LMT	B	623	-	36,36,36	1.10	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	b	615	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
31	LMT	b	603	-	36,36,36	1.13	5 (13%)	47,47,47	0.94	1 (2%)
22	CLA	b	607	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	9 (11%)
30	SQD	A	413	-	50,51,54	0.97	4 (8%)	59,62,65	1.72	10 (16%)
22	CLA	B	607	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
22	CLA	B	606	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	9 (11%)
24	BCR	H	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	3 (5%)
26	LHG	A	409	-	38,38,48	0.69	0	41,44,54	1.18	3 (7%)
22	CLA	B	610	-	65,73,73	1.54	6 (9%)	76,113,113	1.39	7 (9%)
22	CLA	c	511	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)
22	CLA	b	612	-	65,73,73	1.52	5 (7%)	76,113,113	1.31	7 (9%)
27	LMG	D	412	-	46,46,55	0.79	1 (2%)	54,54,63	1.31	4 (7%)
22	CLA	C	520	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
22	CLA	d	404	-	65,73,73	1.52	5 (7%)	76,113,113	1.34	7 (9%)
22	CLA	a	405	-	65,73,73	1.51	5 (7%)	76,113,113	1.42	8 (10%)
27	LMG	C	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
24	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	7 (12%)
23	PL9	D	407	-	55,55,55	1.03	3 (5%)	68,69,69	1.52	13 (19%)
22	CLA	B	604	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LHG	C	519	-	36,36,48	0.71	0	39,42,54	1.25	4 (10%)
23	PL9	a	409	-	45,45,55	1.02	3 (6%)	56,57,69	1.55	10 (17%)
22	CLA	h	101	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	6 (7%)
25	DGD	d	408	-	64,64,67	0.92	2 (3%)	78,78,81	1.34	9 (11%)
22	CLA	c	512	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	8 (10%)
25	DGD	C	517	-	67,67,67	0.88	1 (1%)	81,81,81	1.41	10 (12%)
34	HEM	V	201	16	41,50,50	2.03	8 (19%)	45,82,82	1.56	4 (8%)
22	CLA	D	406	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	8 (10%)
22	CLA	C	503	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	6 (7%)
22	CLA	B	612	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
22	CLA	b	611	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	6 (7%)
22	CLA	b	605	-	65,73,73	1.53	5 (7%)	76,113,113	1.37	6 (7%)
25	DGD	c	517	-	67,67,67	0.88	0	81,81,81	1.40	10 (12%)
34	HEM	v	201	16	41,50,50	2.03	9 (21%)	45,82,82	1.59	4 (8%)
22	CLA	B	603	-	65,73,73	1.49	6 (9%)	76,113,113	1.43	9 (11%)
23	PL9	J	101	-	35,35,55	1.02	1 (2%)	44,45,69	1.56	7 (15%)
27	LMG	a	413	-	51,51,55	0.74	1 (1%)	59,59,63	1.34	7 (11%)
22	CLA	C	511	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
24	BCR	c	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	8 (14%)
23	PL9	j	101	-	35,35,55	1.00	1 (2%)	44,45,69	1.56	7 (15%)
33	BCT	d	403	21	2,3,3	1.24	0	2,3,3	4.15	1 (50%)
24	BCR	C	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	10 (17%)
22	CLA	b	608	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
22	CLA	C	508	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
24	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
32	PHO	d	401	-	51,69,69	1.01	4 (7%)	47,99,99	1.12	5 (10%)
31	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.02	1 (2%)
22	CLA	c	507	-	65,73,73	1.50	5 (7%)	76,113,113	1.43	9 (11%)
24	BCR	x	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	2 (3%)
24	BCR	b	620	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	B	613	-	65,73,73	1.49	5 (7%)	76,113,113	1.36	6 (7%)
22	CLA	B	608	-	65,73,73	1.52	5 (7%)	76,113,113	1.33	7 (9%)
30	SQD	a	401	-	53,54,54	0.96	4 (7%)	62,65,65	1.56	9 (14%)
22	CLA	C	502	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
31	LMT	i	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	D	410	-	32,32,36	1.18	5 (15%)	43,43,47	1.00	2 (4%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.26	4 (7%)
22	CLA	c	504	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	8 (14%)
31	LMT	M	103	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	2 (4%)
22	CLA	A	405	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	6 (7%)
24	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	6 (10%)
22	CLA	B	609	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	7 (9%)
30	SQD	B	626	-	46,47,54	1.02	4 (8%)	55,58,65	1.77	10 (18%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	6 (10%)
25	DGD	a	411	-	57,57,67	0.94	1 (1%)	71,71,81	1.39	7 (9%)
34	HEM	f	101	5,6	41,50,50	1.96	6 (14%)	45,82,82	1.70	6 (13%)
25	DGD	C	515	-	54,54,67	0.98	2 (3%)	68,68,81	1.27	6 (8%)
27	LMG	m	101	-	42,42,55	0.85	0	50,50,63	1.24	4 (8%)
22	CLA	H	101	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)
22	CLA	c	502	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
24	BCR	B	616	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	8 (14%)
27	LMG	A	415	-	42,42,55	0.83	0	50,50,63	1.25	4 (8%)
32	PHO	a	407	-	51,69,69	1.01	3 (5%)	47,99,99	1.09	4 (8%)
22	CLA	b	616	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
22	CLA	b	606	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
34	HEM	F	101	5,6	41,50,50	1.97	6 (14%)	45,82,82	1.69	6 (13%)
24	BCR	j	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.57	12 (21%)
22	CLA	C	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
22	CLA	B	605	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
22	CLA	c	510	3	65,73,73	1.51	5 (7%)	76,113,113	1.41	7 (9%)
29	OEX	a	414	3,1	0,15,15	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
27	LMG	C	522	-	-	20/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	c	519	-	-	17/41/41/53	-
24	BCR	b	621	-	-	9/29/63/63	0/2/2/2
31	LMT	b	627	-	-	2/21/61/61	0/2/2/2
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	c	505	-	1/1/15/20	17/37/115/115	-
22	CLA	b	619	-	1/1/15/20	19/37/115/115	-
22	CLA	C	512	-	1/1/15/20	17/37/115/115	-
22	CLA	A	402	-	1/1/15/20	8/37/115/115	-
24	BCR	b	622	-	-	3/29/63/63	0/2/2/2
27	LMG	A	410	-	-	26/46/66/70	0/1/1/1
25	DGD	A	408	-	-	15/45/85/95	0/2/2/2
22	CLA	a	404	-	1/1/15/20	8/37/115/115	-
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
30	SQD	a	415	-	-	18/46/66/69	0/1/1/1
22	CLA	c	506	-	1/1/15/20	13/37/115/115	-
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
24	BCR	g	101	-	-	6/29/63/63	0/2/2/2
22	CLA	b	609	-	1/1/15/20	15/37/115/115	-
22	CLA	c	508	-	1/1/15/20	15/37/115/115	-
24	BCR	b	623	-	-	4/29/63/63	0/2/2/2
25	DGD	C	516	-	-	20/51/91/95	0/2/2/2
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
30	SQD	F	102	-	-	10/40/60/69	0/1/1/1
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
22	CLA	a	408	-	1/1/15/20	8/37/115/115	-
22	CLA	C	504	-	1/1/15/20	19/37/115/115	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
22	CLA	a	406	-	1/1/15/20	9/37/115/115	-
22	CLA	c	509	-	1/1/15/20	16/37/115/115	-
25	DGD	c	516	-	-	20/51/91/95	0/2/2/2
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2
25	DGD	c	515	-	-	20/42/82/95	0/2/2/2
30	SQD	D	403	-	-	13/38/58/69	0/1/1/1
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	i	101	-	-	18/38/58/70	0/1/1/1
22	CLA	b	618	-	1/1/15/20	9/37/115/115	-
25	DGD	b	601	-	-	18/41/81/95	0/2/2/2
24	BCR	B	617	-	-	9/29/63/63	0/2/2/2
27	LMG	d	407	-	-	20/43/63/70	0/1/1/1
22	CLA	b	614	-	1/1/15/20	9/37/115/115	-
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
27	LMG	E	101	-	-	18/39/59/70	0/1/1/1
24	BCR	C	521	-	-	6/29/63/63	0/2/2/2
22	CLA	c	501	-	1/1/15/20	13/37/115/115	-
27	LMG	b	628	-	-	24/44/64/70	0/1/1/1
32	PHO	D	402	-	-	12/37/103/103	0/5/6/6
32	PHO	D	401	-	-	12/37/103/103	0/5/6/6
22	CLA	c	520	-	1/1/15/20	10/37/115/115	-
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
27	LMG	B	624	-	-	24/44/64/70	0/1/1/1
27	LMG	c	518	-	-	21/40/60/70	0/1/1/1
22	CLA	B	614	-	1/1/15/20	10/37/115/115	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
30	SQD	d	402	-	-	13/38/58/69	0/1/1/1
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
22	CLA	D	405	-	1/1/15/20	14/37/115/115	-
23	PL9	d	406	-	-	11/53/73/73	0/1/1/1
31	LMT	d	409	-	-	0/17/57/61	0/2/2/2
22	CLA	C	510	3	1/1/15/20	15/37/115/115	-
22	CLA	b	617	-	1/1/15/20	15/37/115/115	-
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
24	BCR	f	102	-	-	7/29/63/63	0/2/2/2
22	CLA	B	602	-	1/1/15/20	15/37/115/115	-
22	CLA	C	506	-	1/1/15/20	13/37/115/115	-
22	CLA	A	403	-	1/1/15/20	14/37/115/115	-
22	CLA	c	503	-	1/1/15/20	14/37/115/115	-
22	CLA	B	611	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	a	412	-	-	12/43/43/53	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
27	LMG	d	410	-	-	15/41/61/70	0/1/1/1
22	CLA	b	613	-	1/1/15/20	18/37/115/115	-
22	CLA	d	405	-	1/1/15/20	6/37/115/115	-
22	CLA	C	507	-	1/1/15/20	15/37/115/115	-
24	BCR	D	411	-	-	6/29/63/63	0/2/2/2
22	CLA	B	601	-	1/1/15/20	16/37/115/115	-
22	CLA	A	404	-	1/1/15/20	10/37/115/115	-
24	BCR	c	513	-	-	6/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/15/20	18/37/115/115	-
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
27	LMG	D	408	-	-	21/43/63/70	0/1/1/1
30	SQD	A	414	-	-	11/49/69/69	0/1/1/1
31	LMT	B	622	-	-	3/21/61/61	0/2/2/2
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
22	CLA	C	509	-	1/1/15/20	16/37/115/115	-
30	SQD	b	602	-	-	15/42/62/69	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
22	CLA	b	610	-	1/1/15/20	9/37/115/115	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
31	LMT	B	623	-	-	4/21/61/61	0/2/2/2
22	CLA	b	615	-	1/1/15/20	13/37/115/115	-
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	b	607	-	1/1/15/20	7/37/115/115	-
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
22	CLA	B	607	-	1/1/15/20	12/37/115/115	-
22	CLA	B	606	-	1/1/15/20	9/37/115/115	-
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
26	LHG	A	409	-	-	14/43/43/53	-
22	CLA	B	610	-	1/1/15/20	10/37/115/115	-
22	CLA	c	511	-	1/1/15/20	19/37/115/115	-
22	CLA	b	612	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	D	412	-	-	14/41/61/70	0/1/1/1
22	CLA	C	520	-	1/1/15/20	12/37/115/115	-
22	CLA	d	404	-	1/1/15/20	12/37/115/115	-
22	CLA	a	405	-	1/1/15/20	14/37/115/115	-
27	LMG	C	518	-	-	21/40/60/70	0/1/1/1
24	BCR	c	521	-	-	6/29/63/63	0/2/2/2
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
22	CLA	B	604	-	1/1/15/20	14/37/115/115	-
26	LHG	C	519	-	-	16/41/41/53	-
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
22	CLA	h	101	-	1/1/15/20	19/37/115/115	-
25	DGD	d	408	-	-	35/52/92/95	0/2/2/2
22	CLA	c	512	-	1/1/15/20	21/37/115/115	-
25	DGD	C	517	-	-	22/55/95/95	0/2/2/2
34	HEM	V	201	16	-	4/12/54/54	-
22	CLA	D	406	-	-	6/37/115/115	-
22	CLA	C	503	-	1/1/15/20	15/37/115/115	-
22	CLA	B	612	-	1/1/15/20	15/37/115/115	-
22	CLA	b	611	-	1/1/15/20	12/37/115/115	-
22	CLA	b	605	-	1/1/15/20	14/37/115/115	-
25	DGD	c	517	-	-	21/55/95/95	0/2/2/2
34	HEM	v	201	16	-	4/12/54/54	-
22	CLA	B	603	-	1/1/15/20	7/37/115/115	-
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
27	LMG	a	413	-	-	25/46/66/70	0/1/1/1
22	CLA	C	511	-	1/1/15/20	19/37/115/115	-
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/15/20	15/37/115/115	-
22	CLA	C	508	-	1/1/15/20	16/37/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
32	PHO	d	401	-	-	11/37/103/103	0/5/6/6
31	LMT	b	604	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	507	-	1/1/15/20	14/37/115/115	-
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
22	CLA	B	613	-	1/1/15/20	16/37/115/115	-
22	CLA	B	608	-	1/1/15/20	11/37/115/115	-
30	SQD	a	401	-	-	13/49/69/69	0/1/1/1
22	CLA	C	502	-	1/1/15/20	9/37/115/115	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
27	LMG	I	101	-	-	17/38/58/70	0/1/1/1
22	CLA	c	504	-	1/1/15/20	19/37/115/115	-
24	BCR	B	618	-	-	3/29/63/63	0/2/2/2
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	A	405	-	1/1/15/20	8/37/115/115	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
22	CLA	B	609	-	1/1/15/20	18/37/115/115	-
30	SQD	B	626	-	-	13/42/62/69	0/1/1/1
27	LMG	B	621	-	-	16/44/64/70	0/1/1/1
25	DGD	a	411	-	-	14/45/85/95	0/2/2/2
34	HEM	f	101	5,6	-	2/12/54/54	-
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
27	LMG	m	101	-	-	17/37/57/70	0/1/1/1
22	CLA	H	101	-	1/1/15/20	19/37/115/115	-
22	CLA	c	502	-	1/1/15/20	11/37/115/115	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
32	PHO	a	407	-	-	12/37/103/103	0/5/6/6
22	CLA	b	616	-	1/1/15/20	15/37/115/115	-
22	CLA	b	606	-	1/1/15/20	13/37/115/115	-
34	HEM	F	101	5,6	-	2/12/54/54	-
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/15/20	15/37/115/115	-
22	CLA	B	605	-	1/1/15/20	12/37/115/115	-
22	CLA	c	510	3	1/1/15/20	17/37/115/115	-

The worst 5 of 615 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	8.29	1.54	1.36
34	F	101	HEM	C3D-C2D	8.05	1.53	1.36
34	f	101	HEM	C3D-C2D	7.98	1.53	1.36
22	A	402	CLA	C4B-NB	7.79	1.42	1.35

The worst 5 of 1150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.20	109.94	106.71
22	c	504	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	C	510	CLA	C4A-NA-C1A	7.11	109.90	106.71
22	B	603	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	B	611	CLA	C4A-NA-C1A	7.06	109.88	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 2140 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

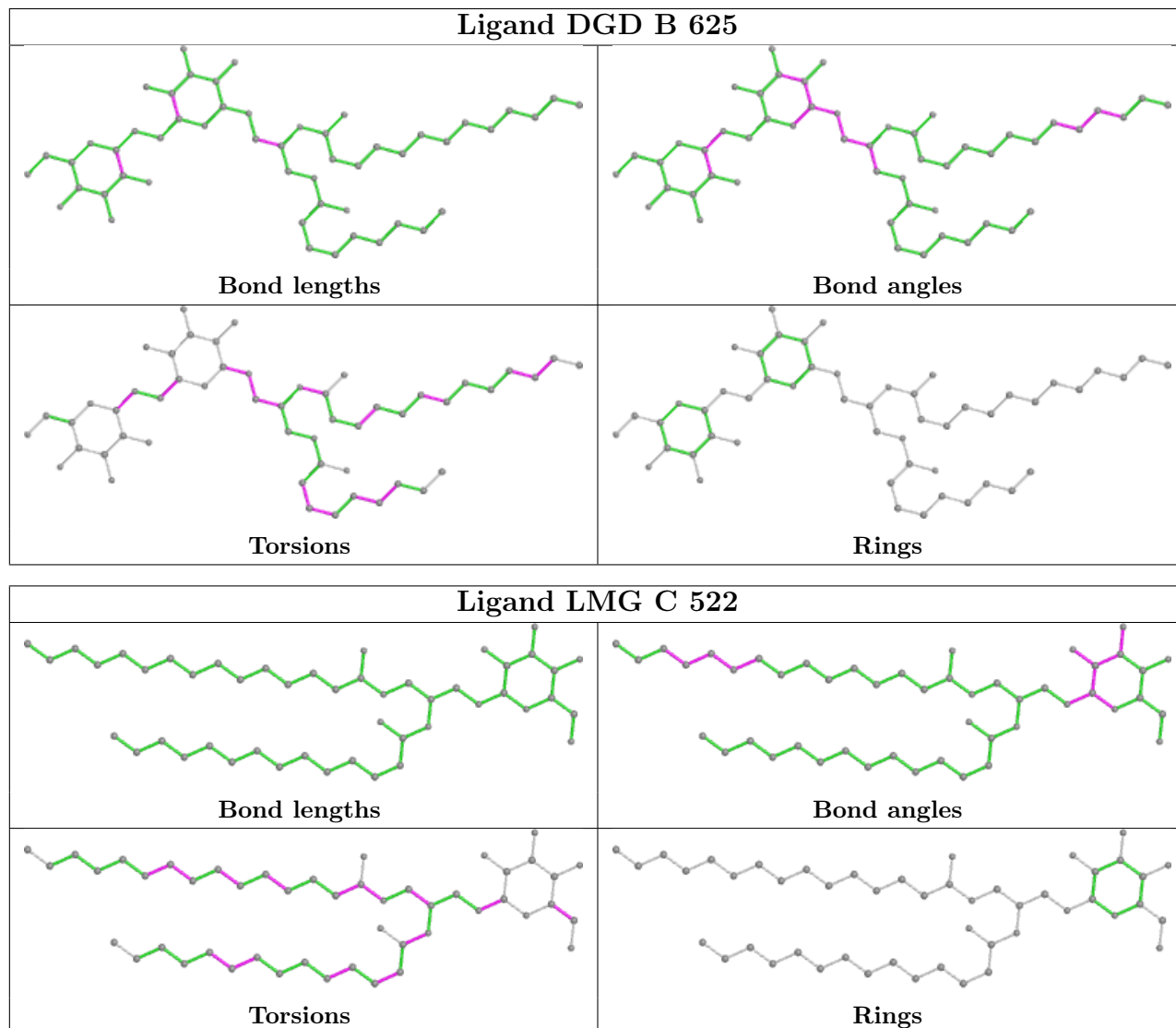
There are no ring outliers.

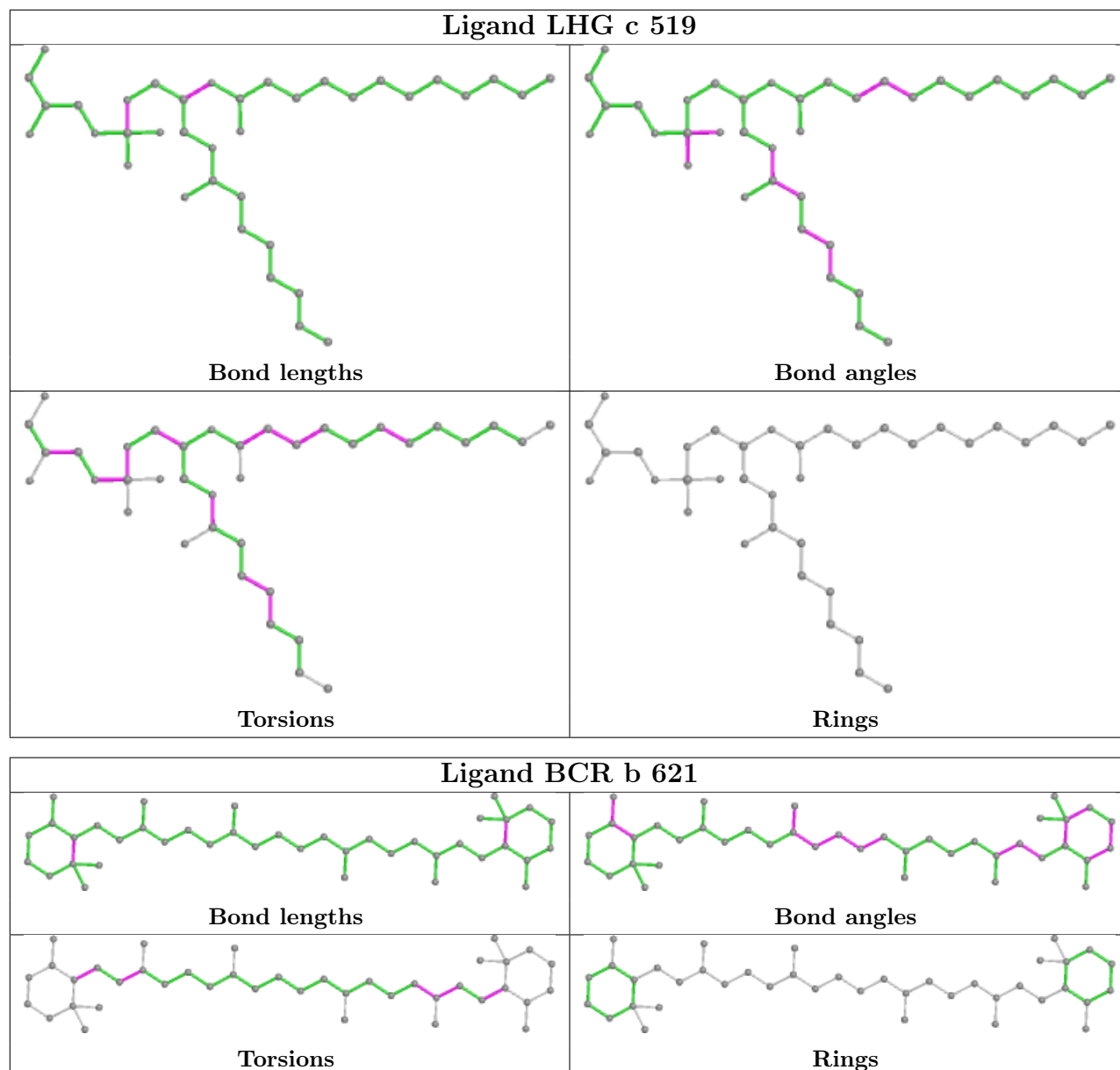
No monomer is involved in short contacts.

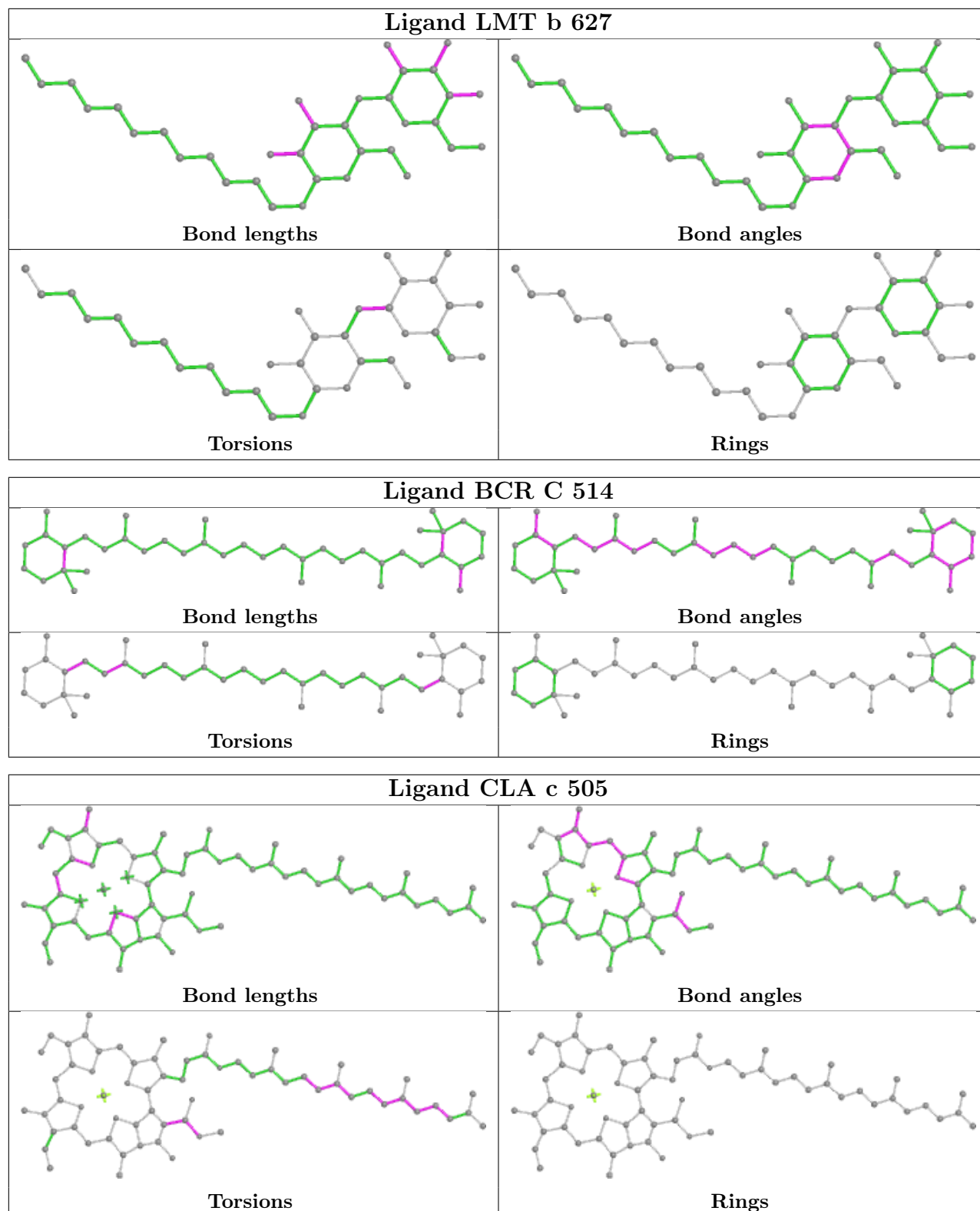
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

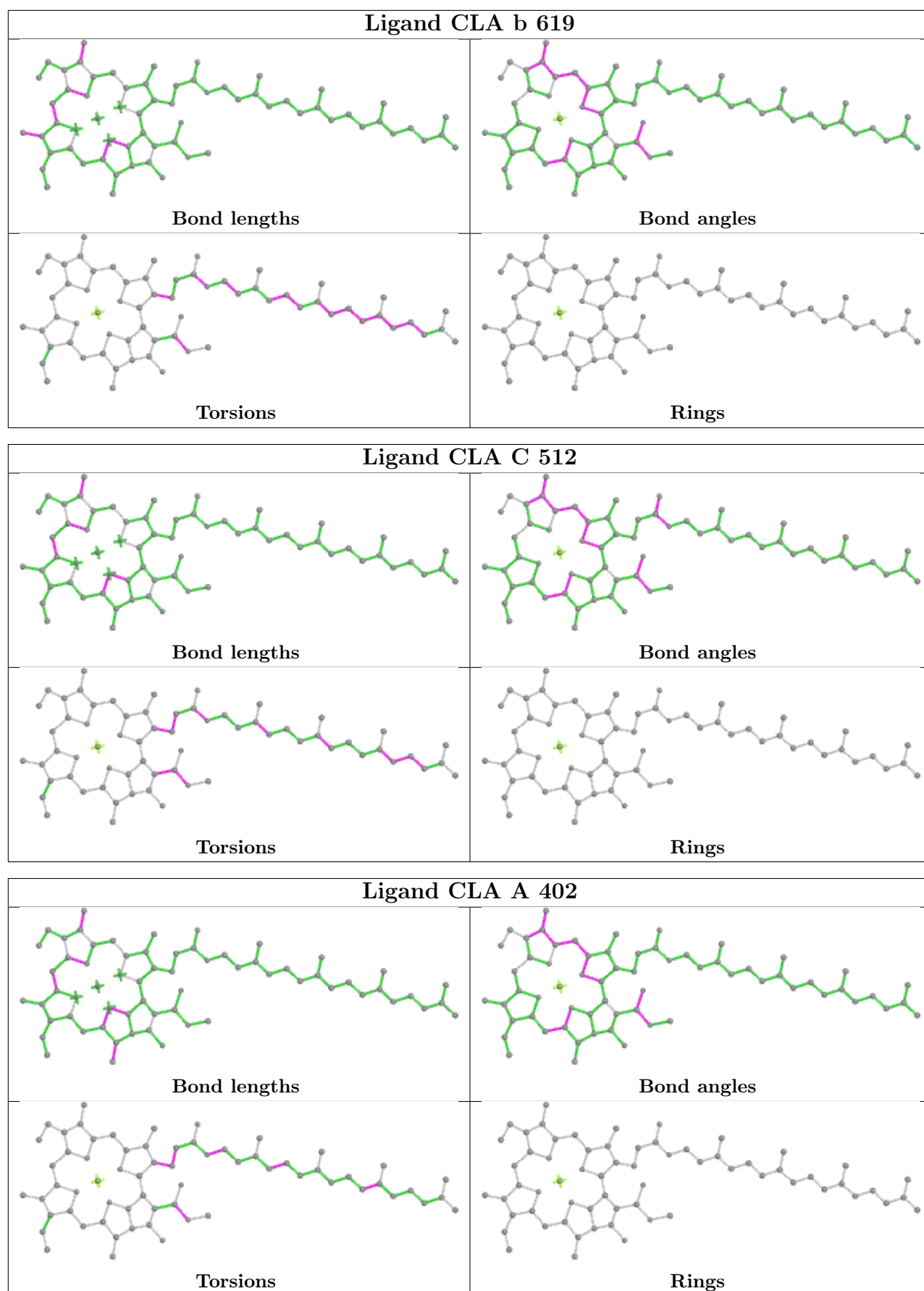


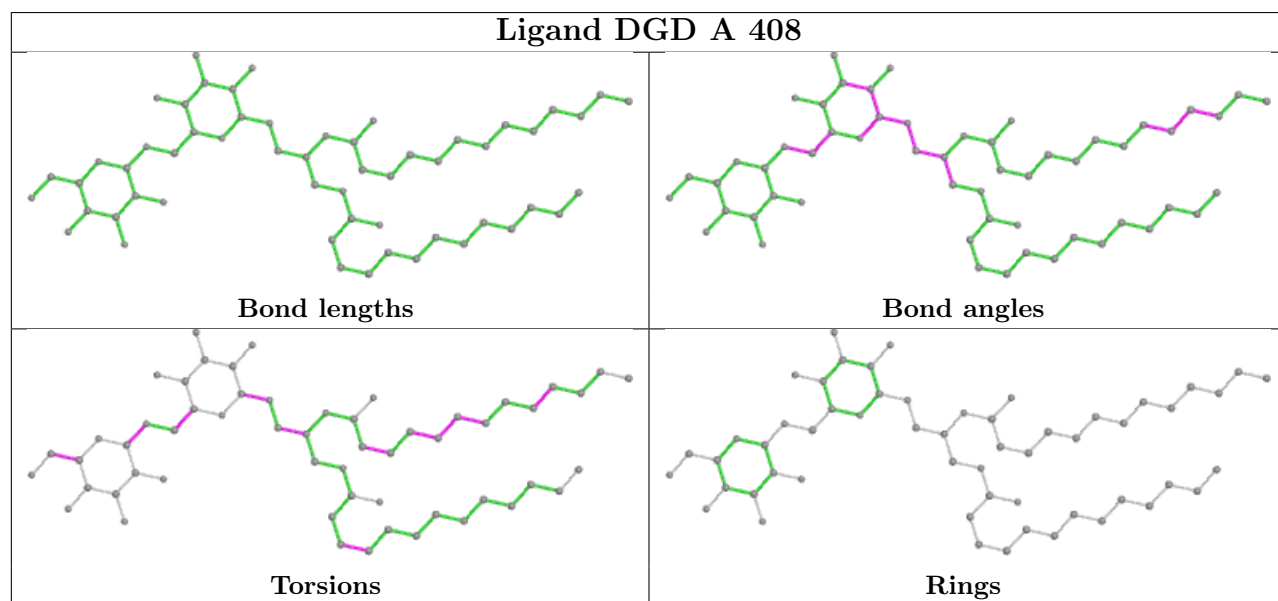
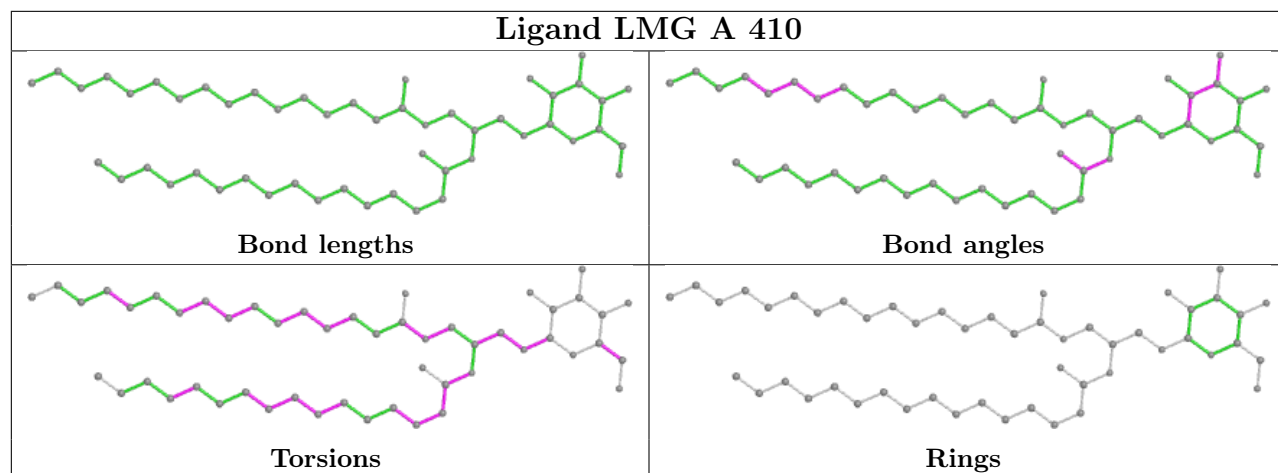
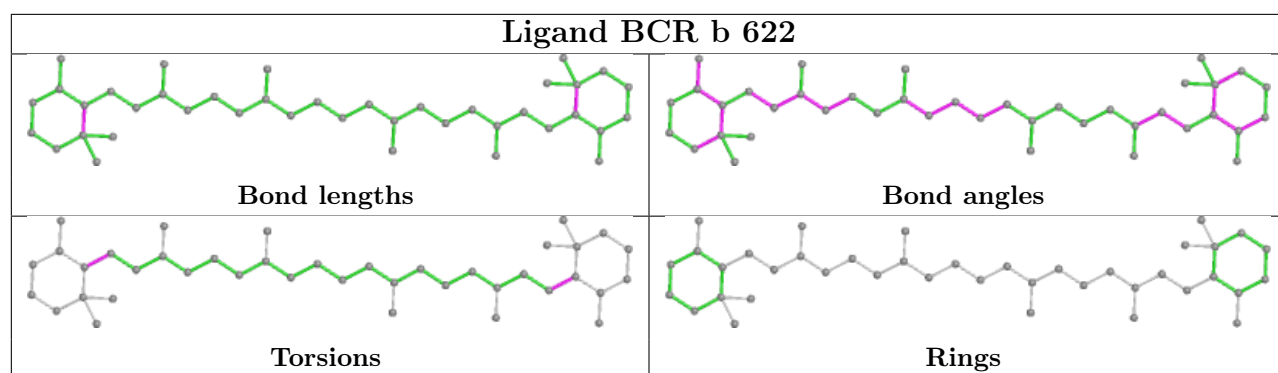
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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

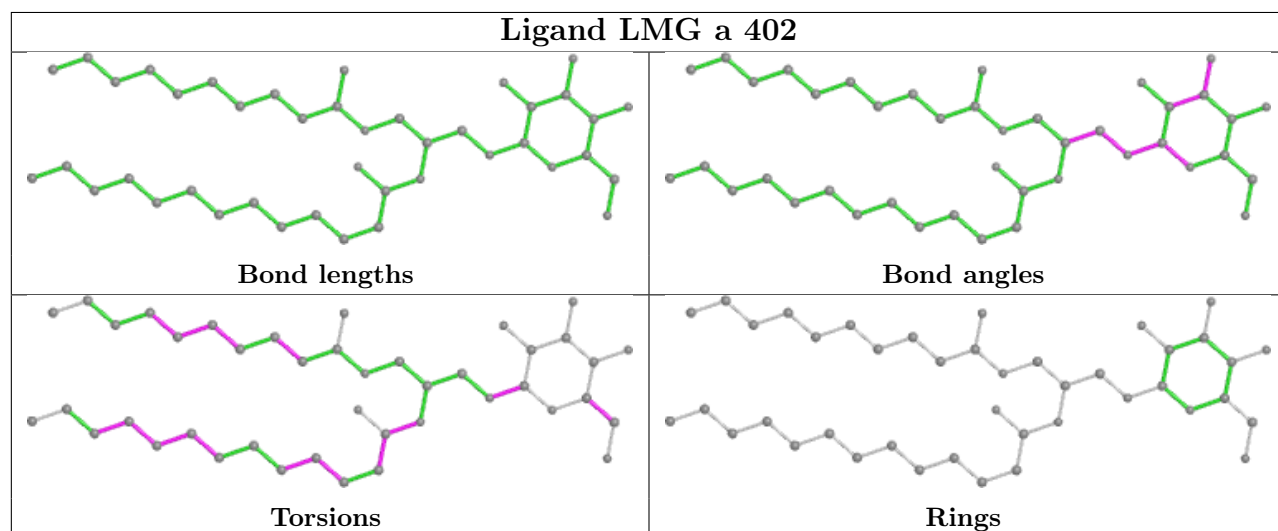
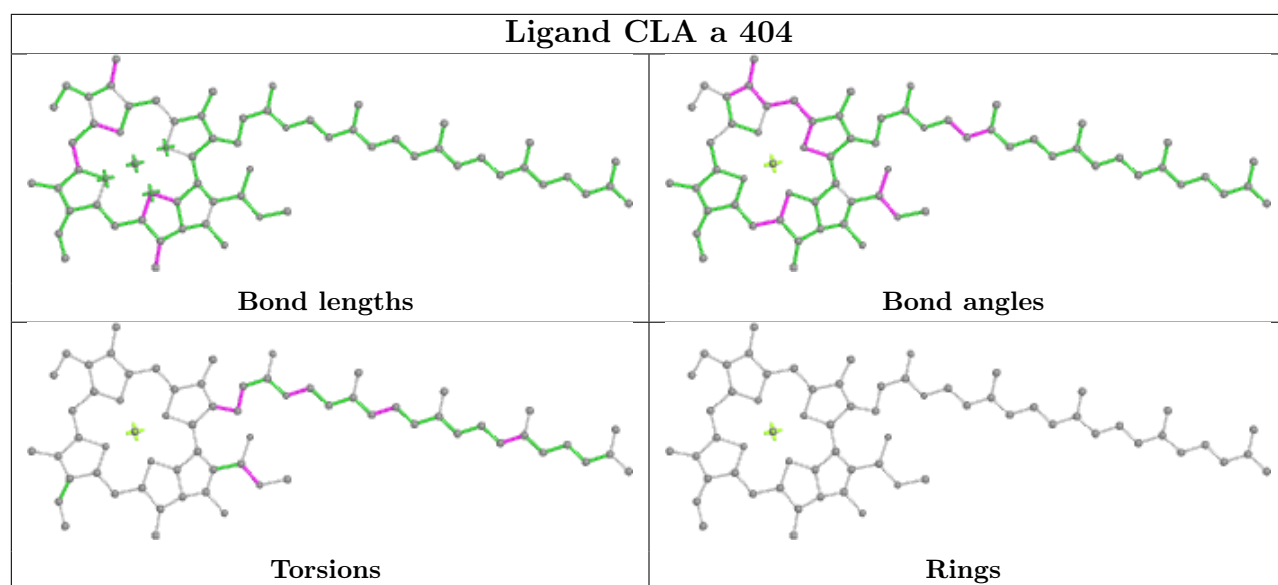


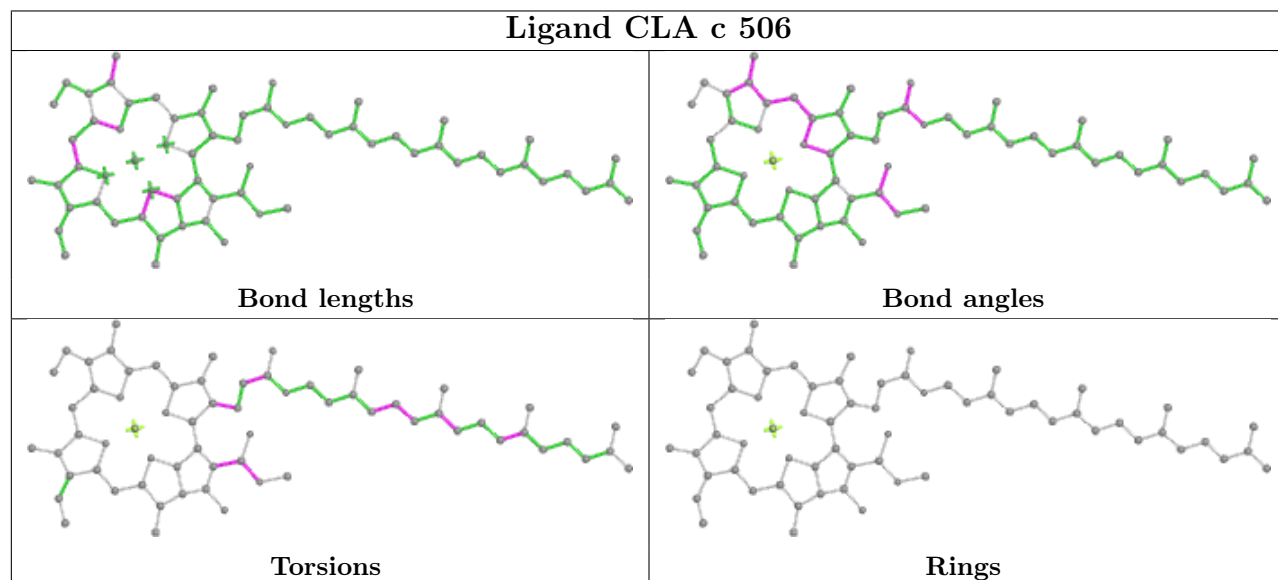
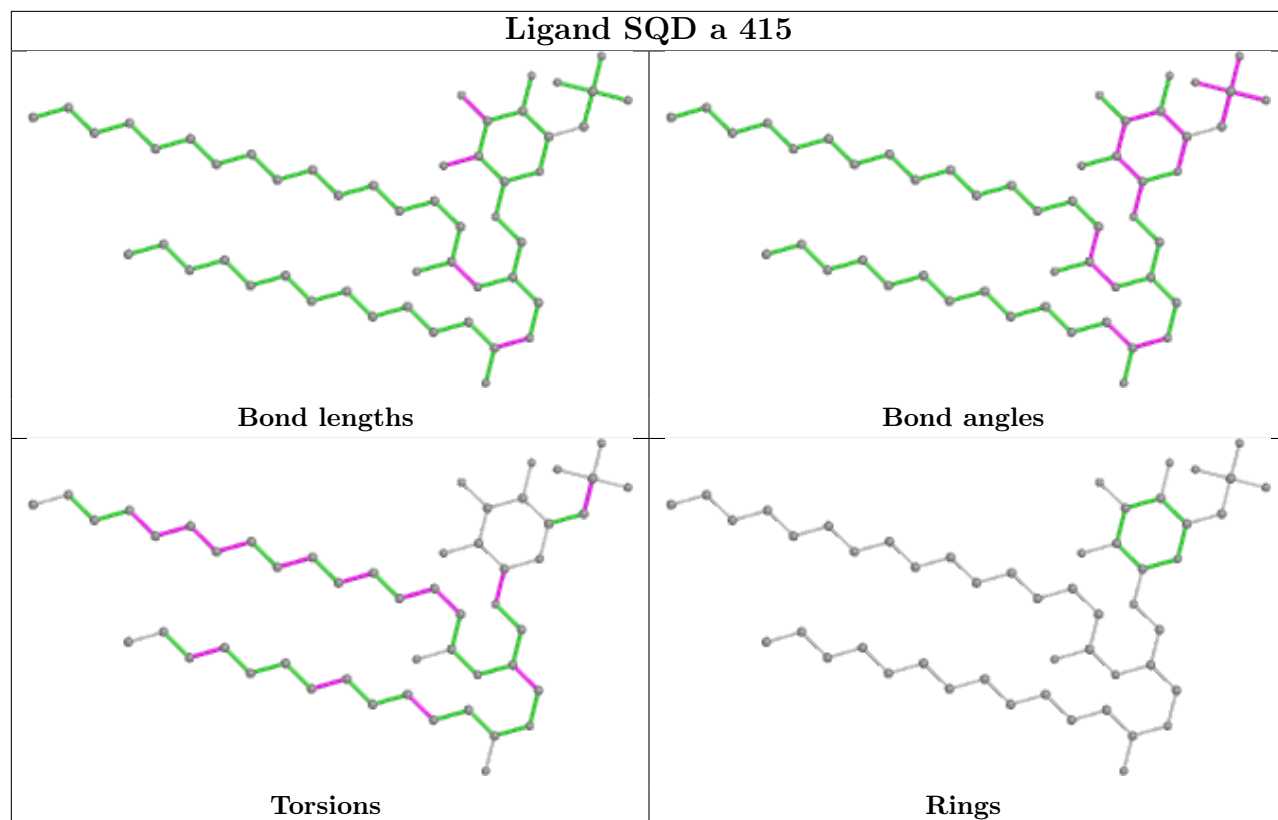


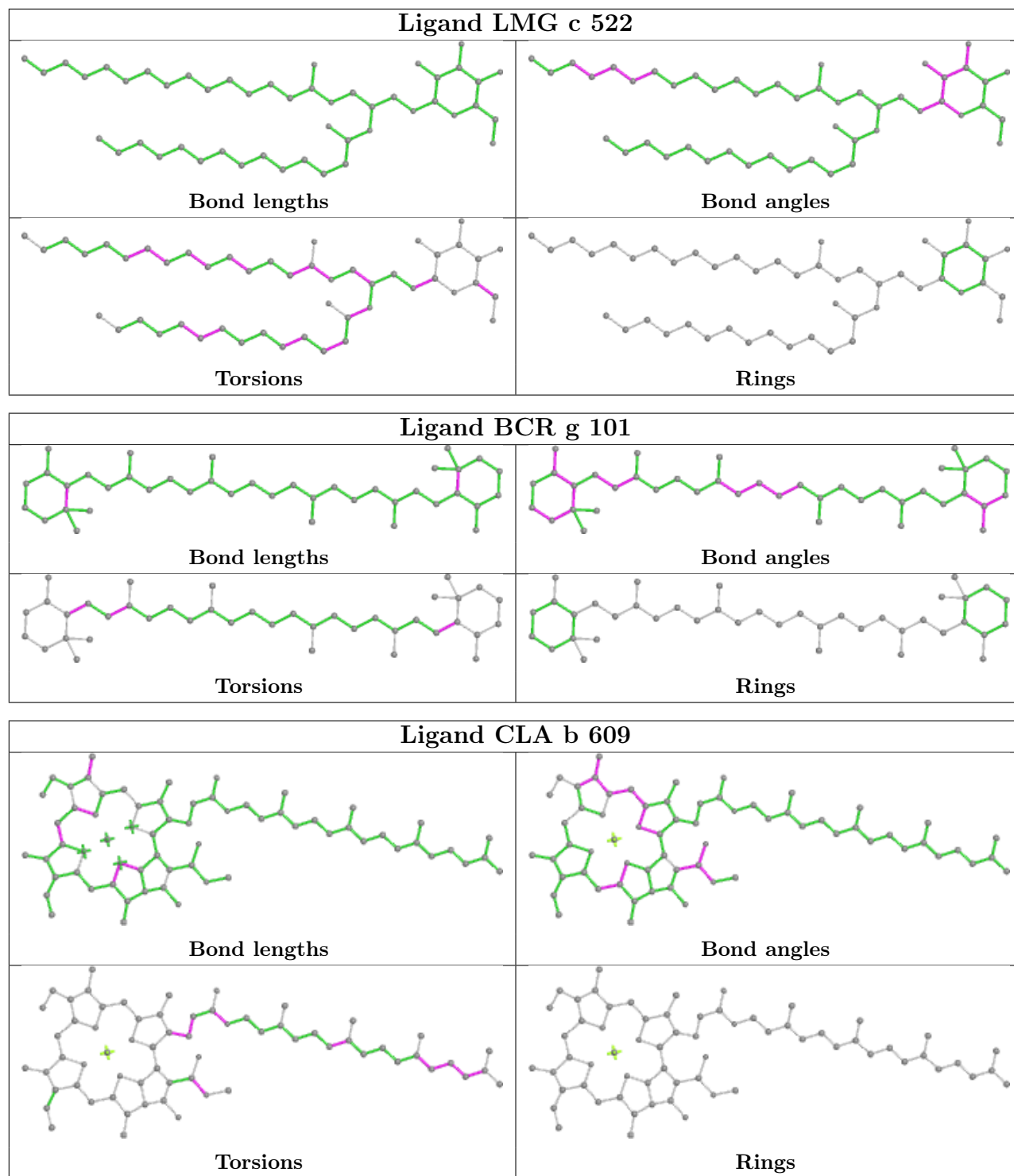




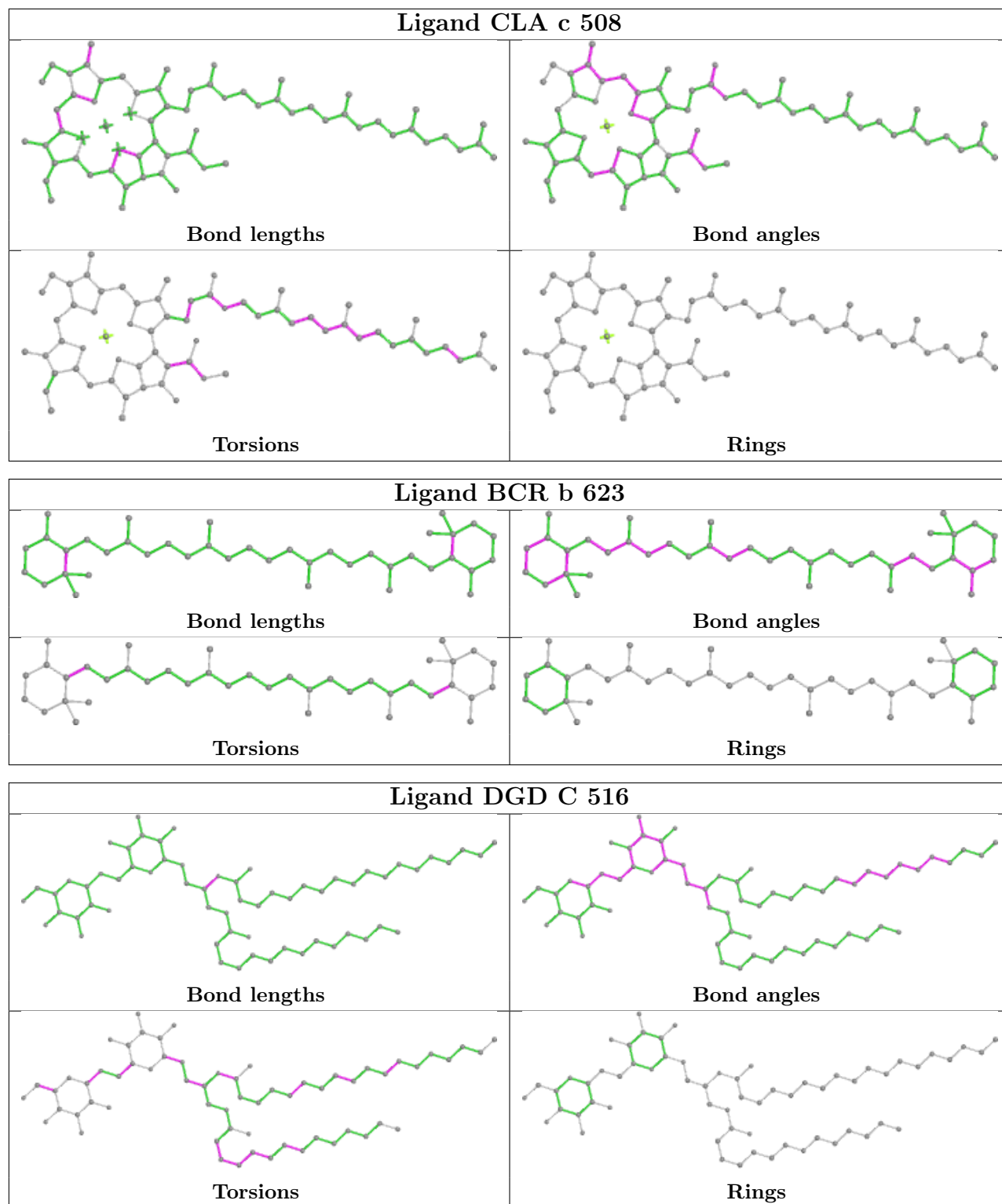


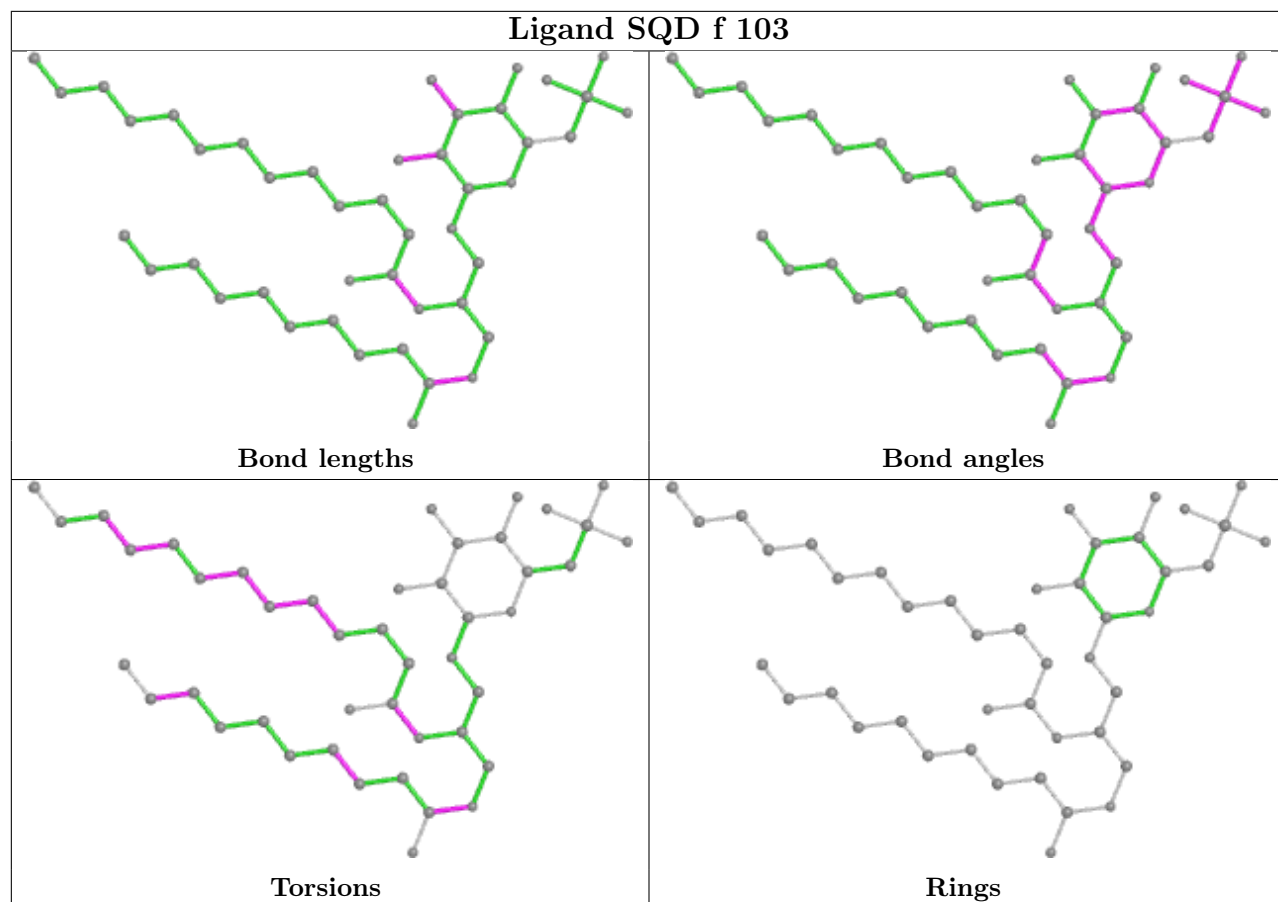


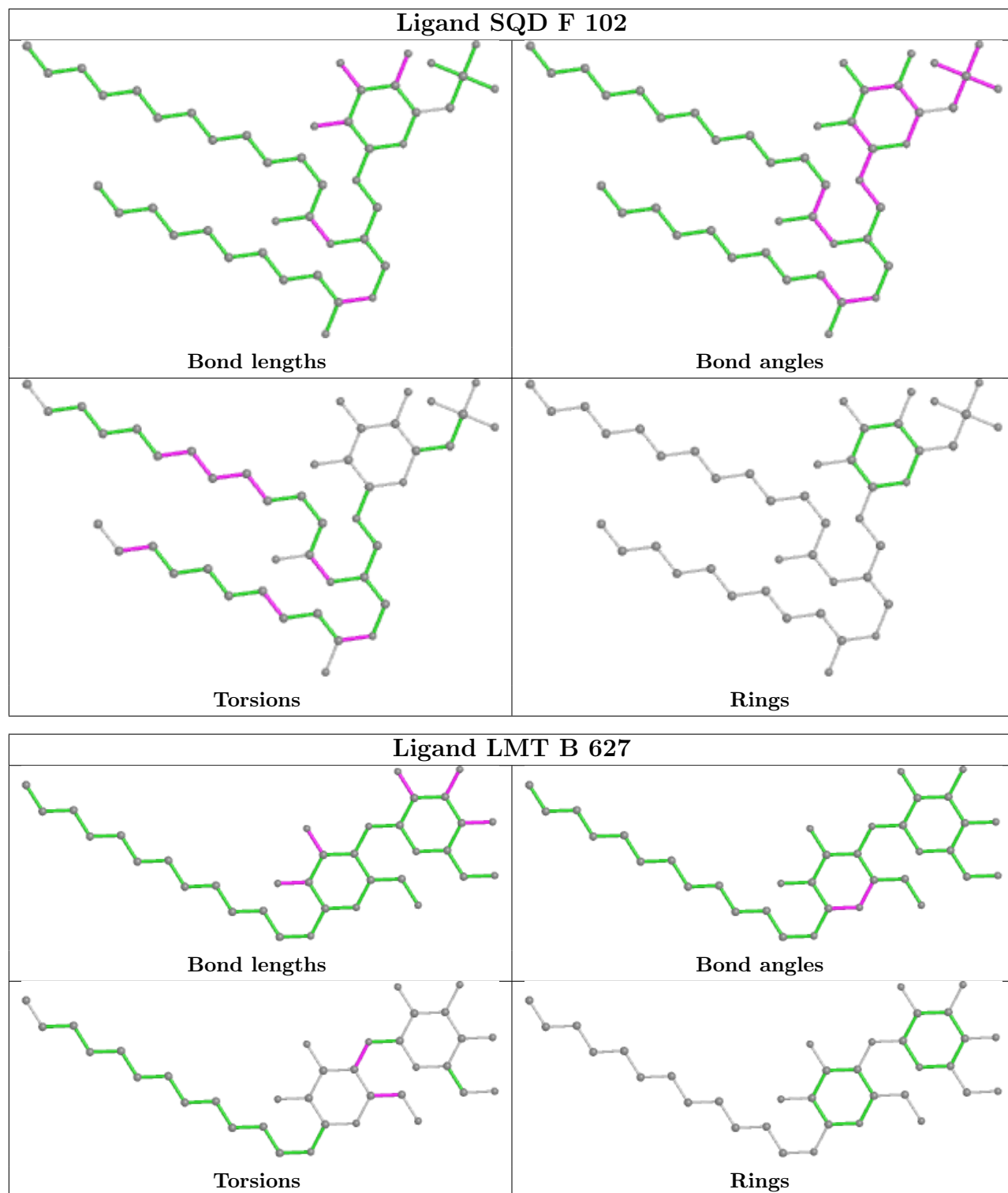


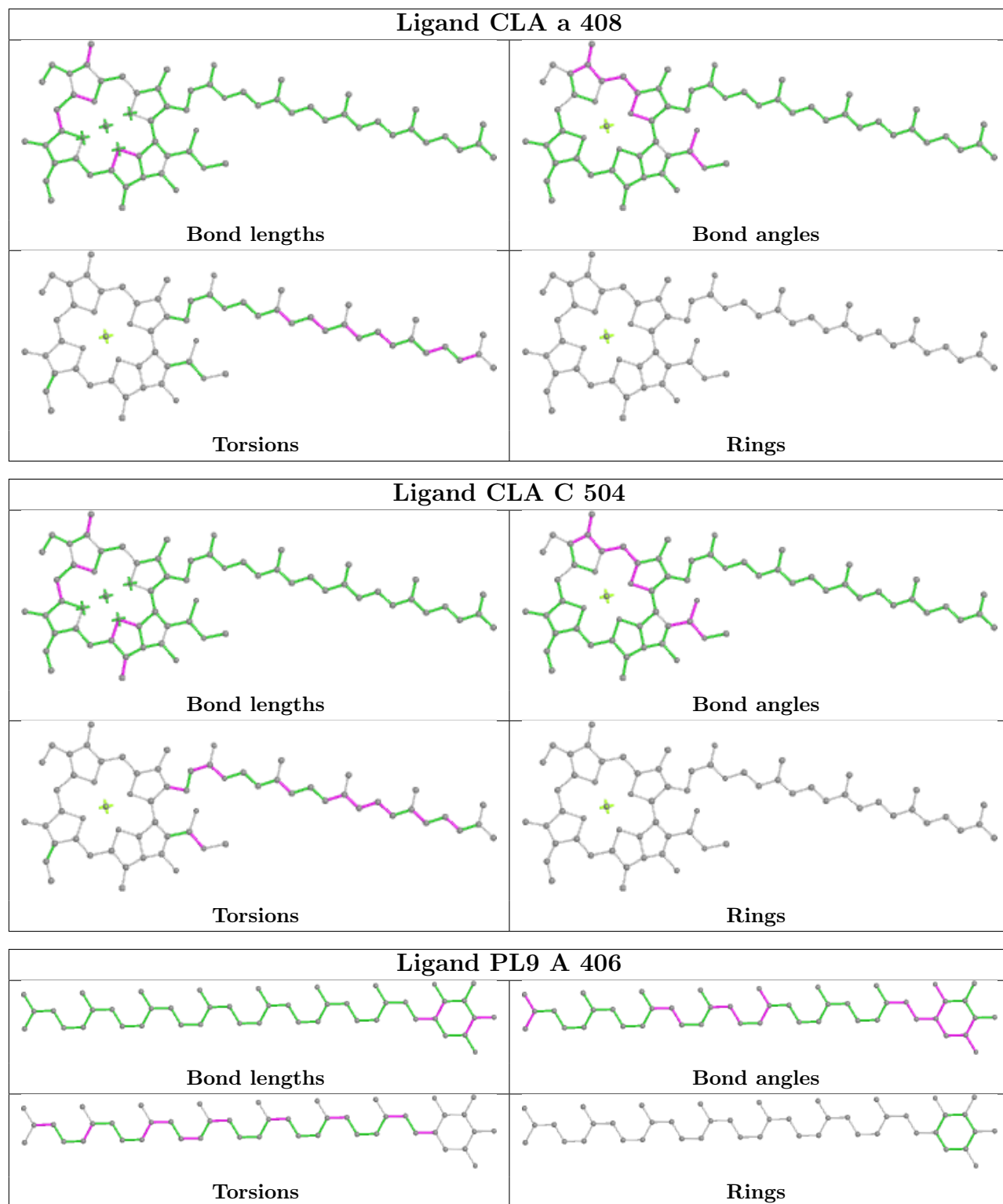


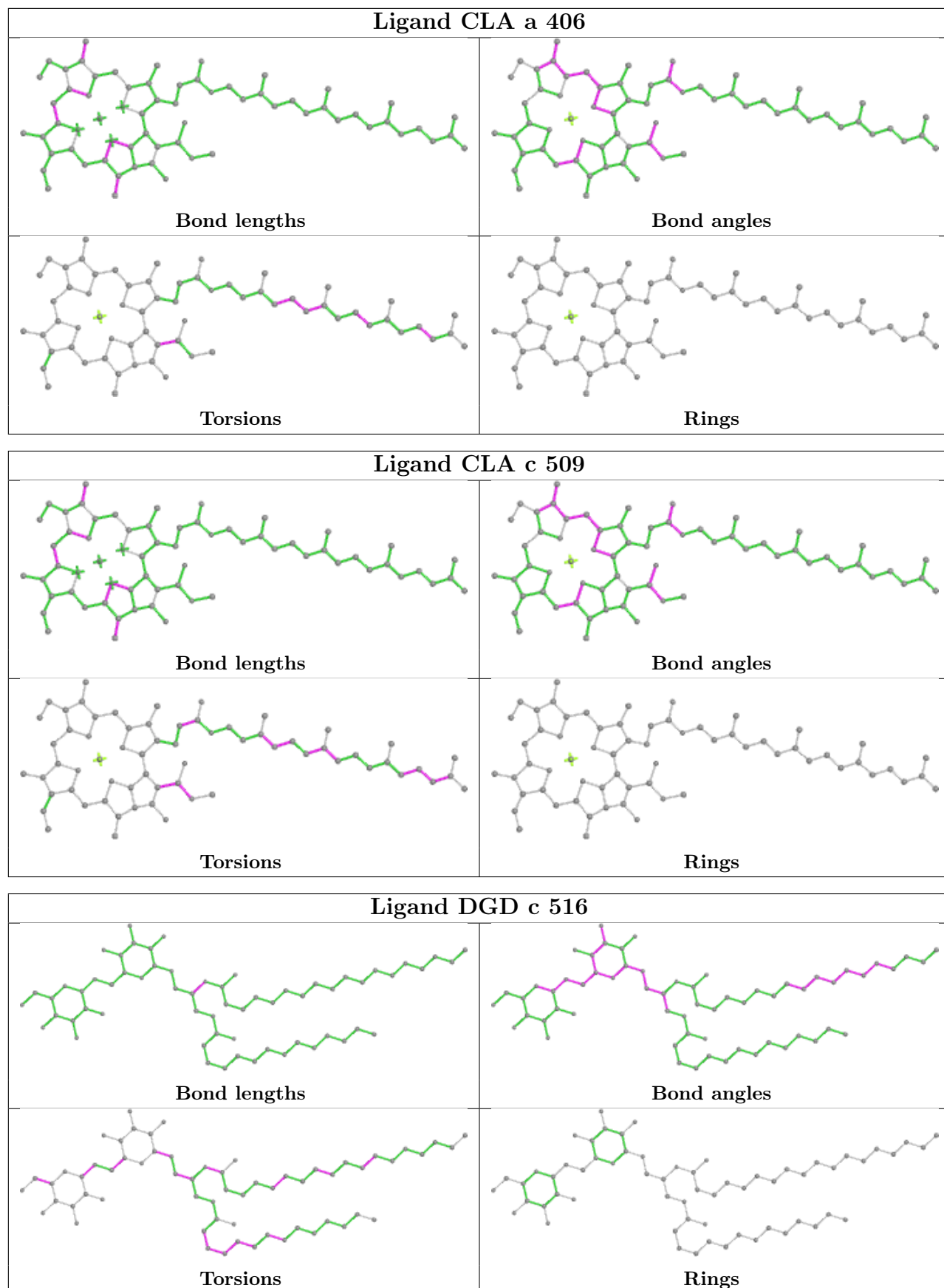


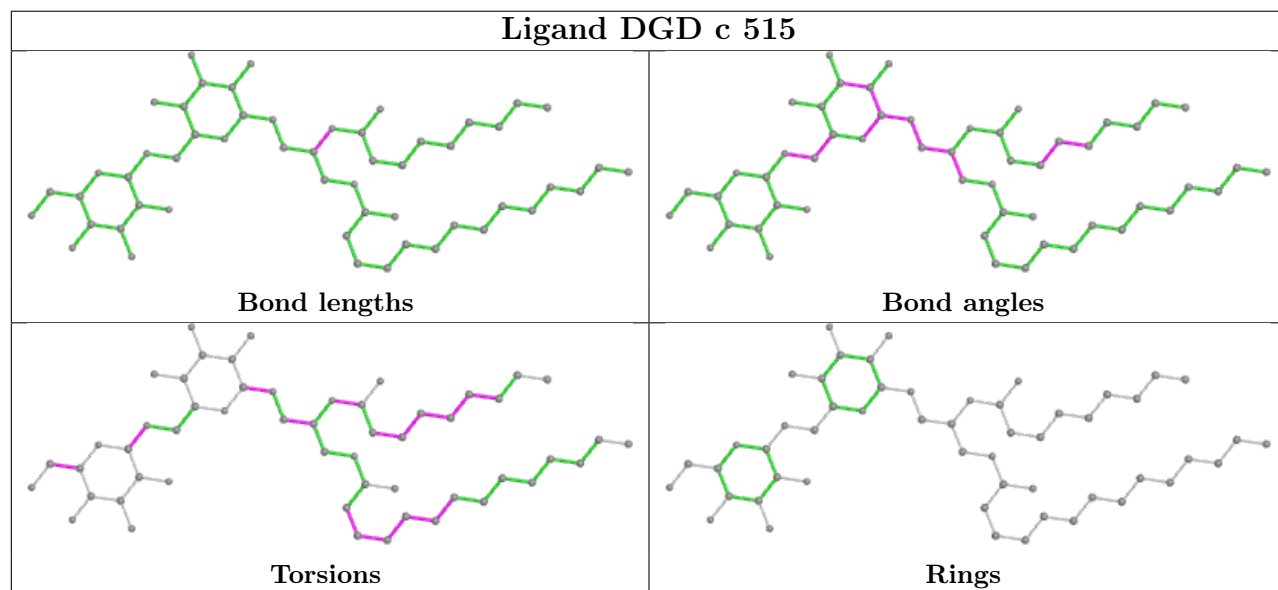
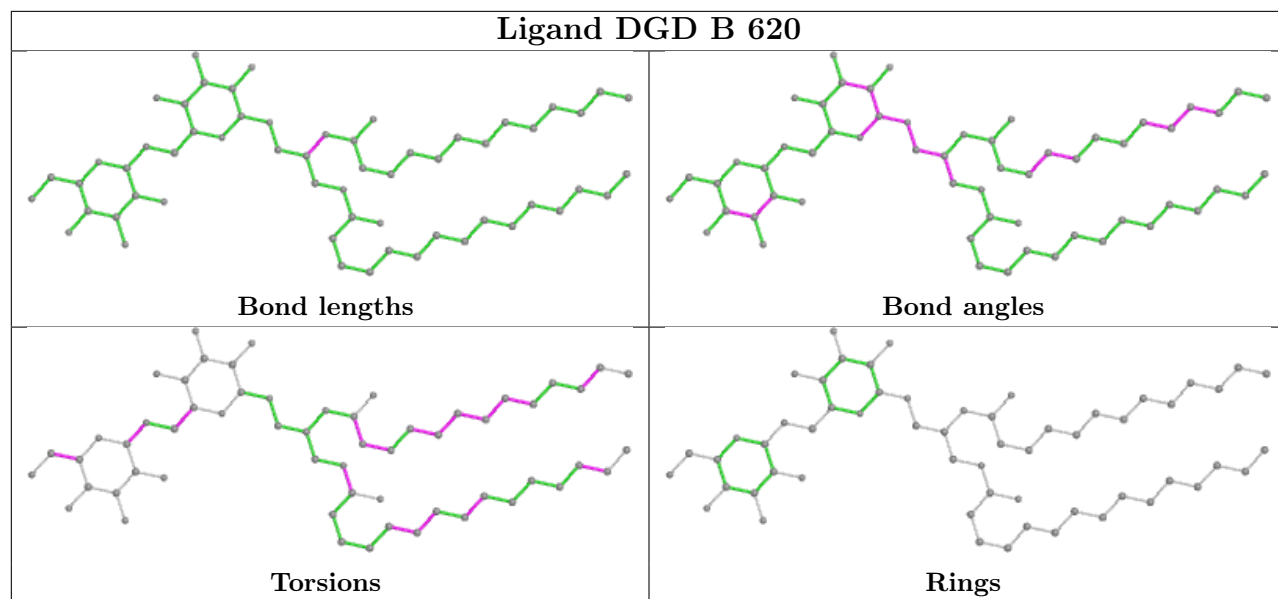


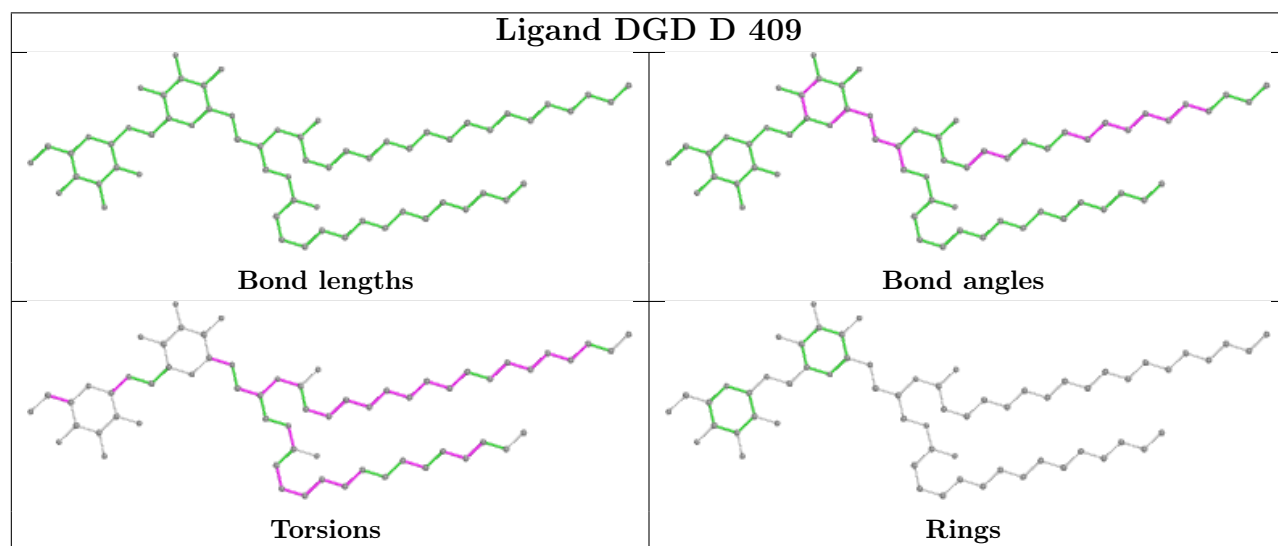
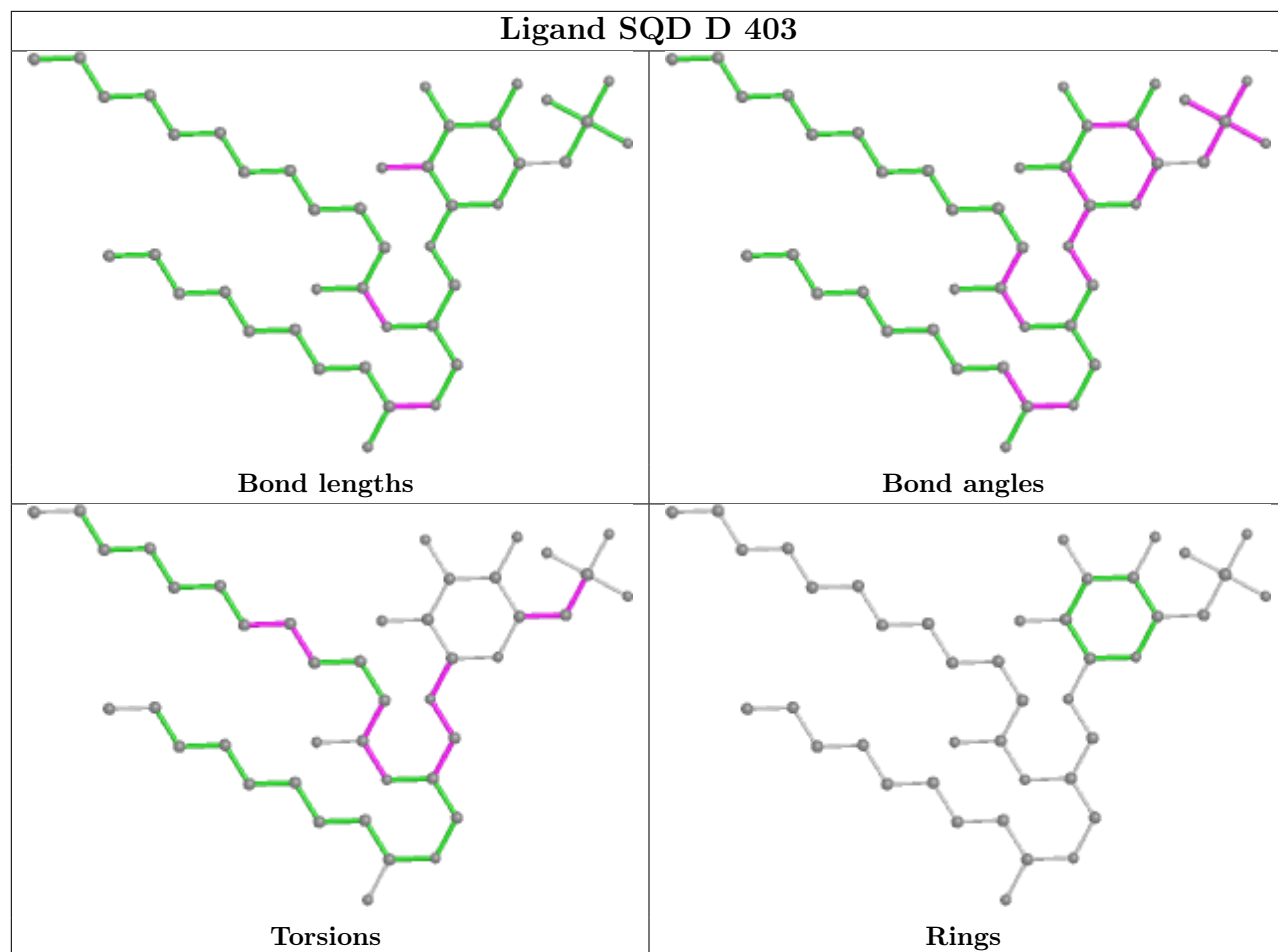


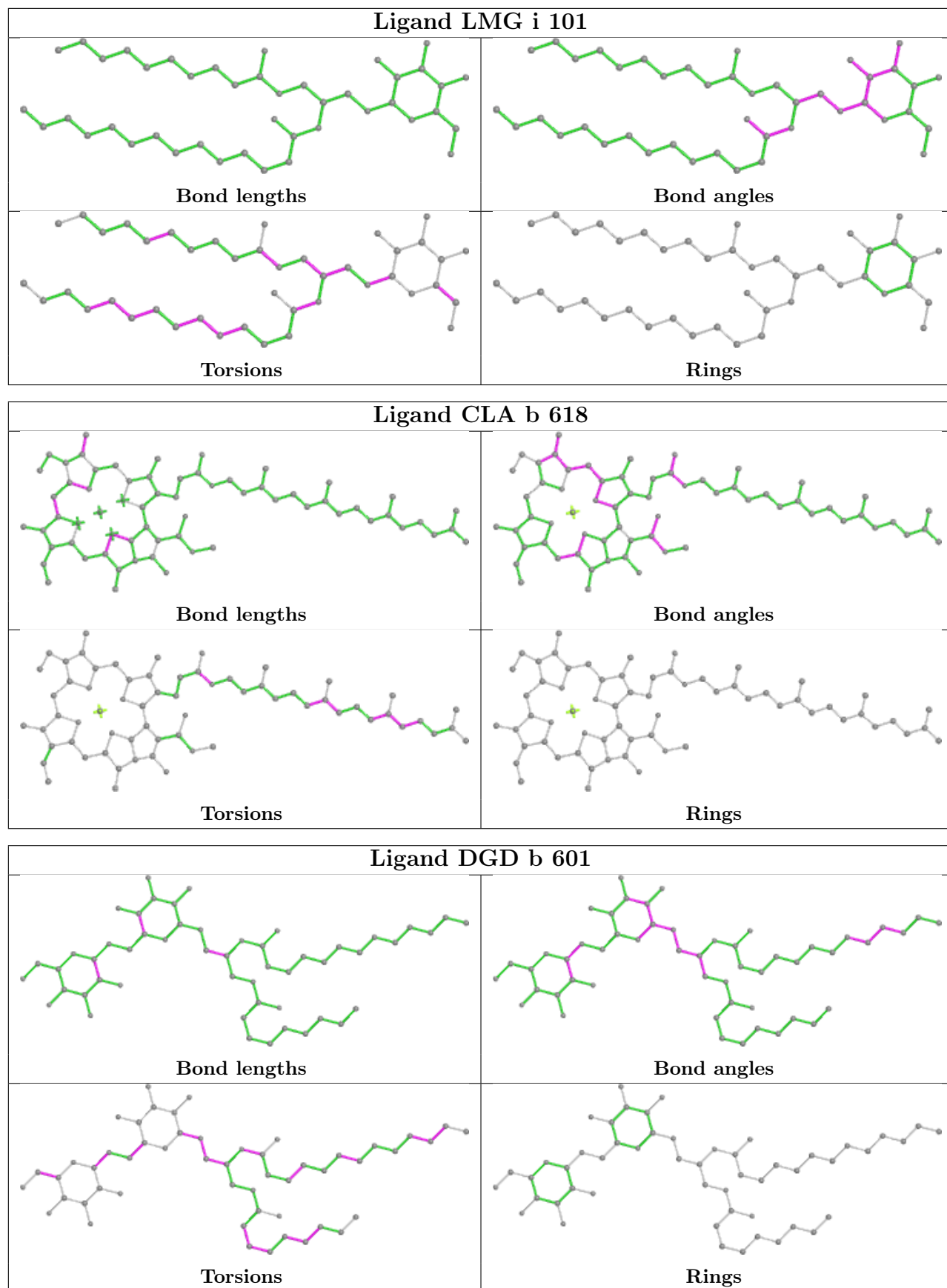




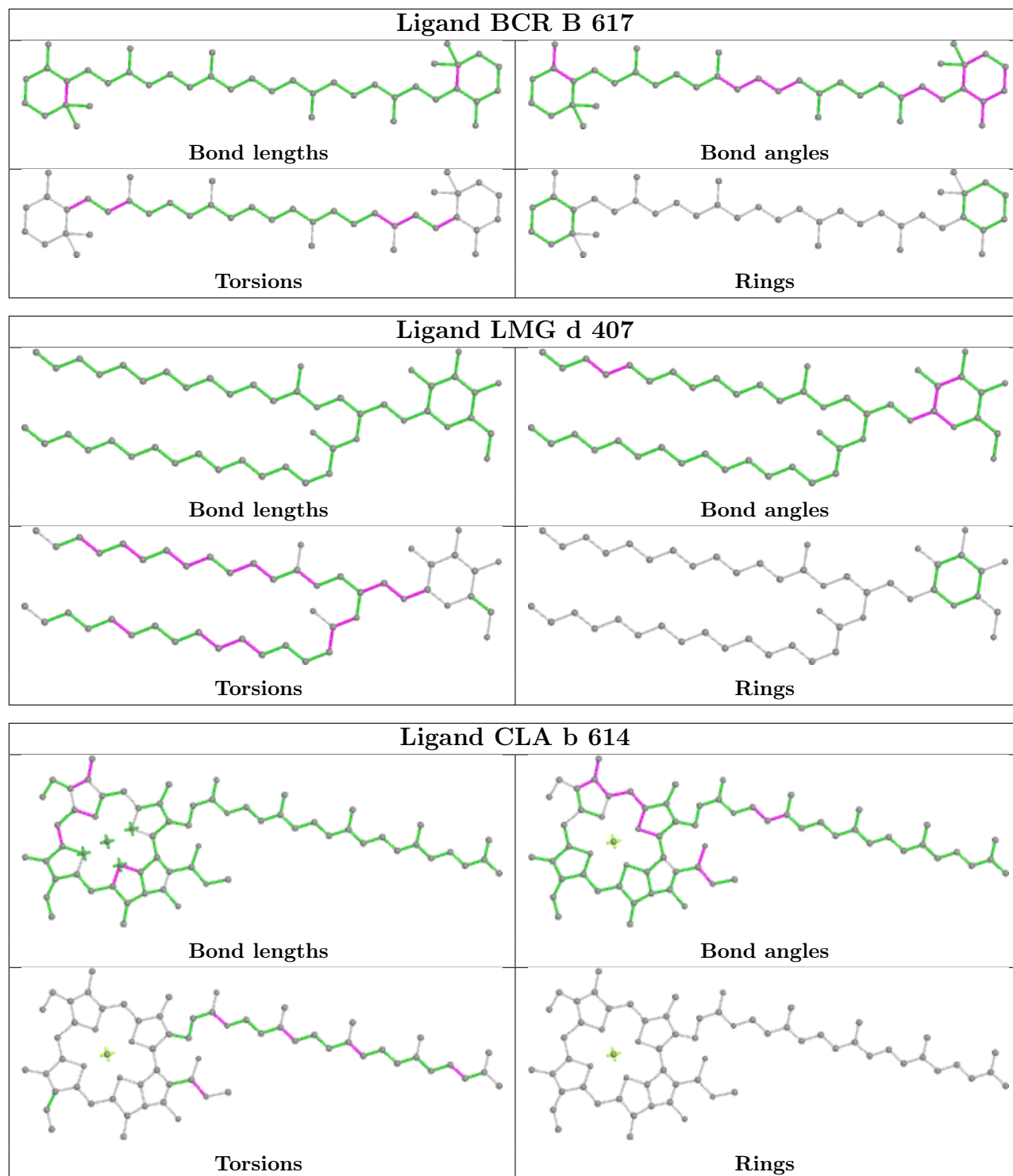


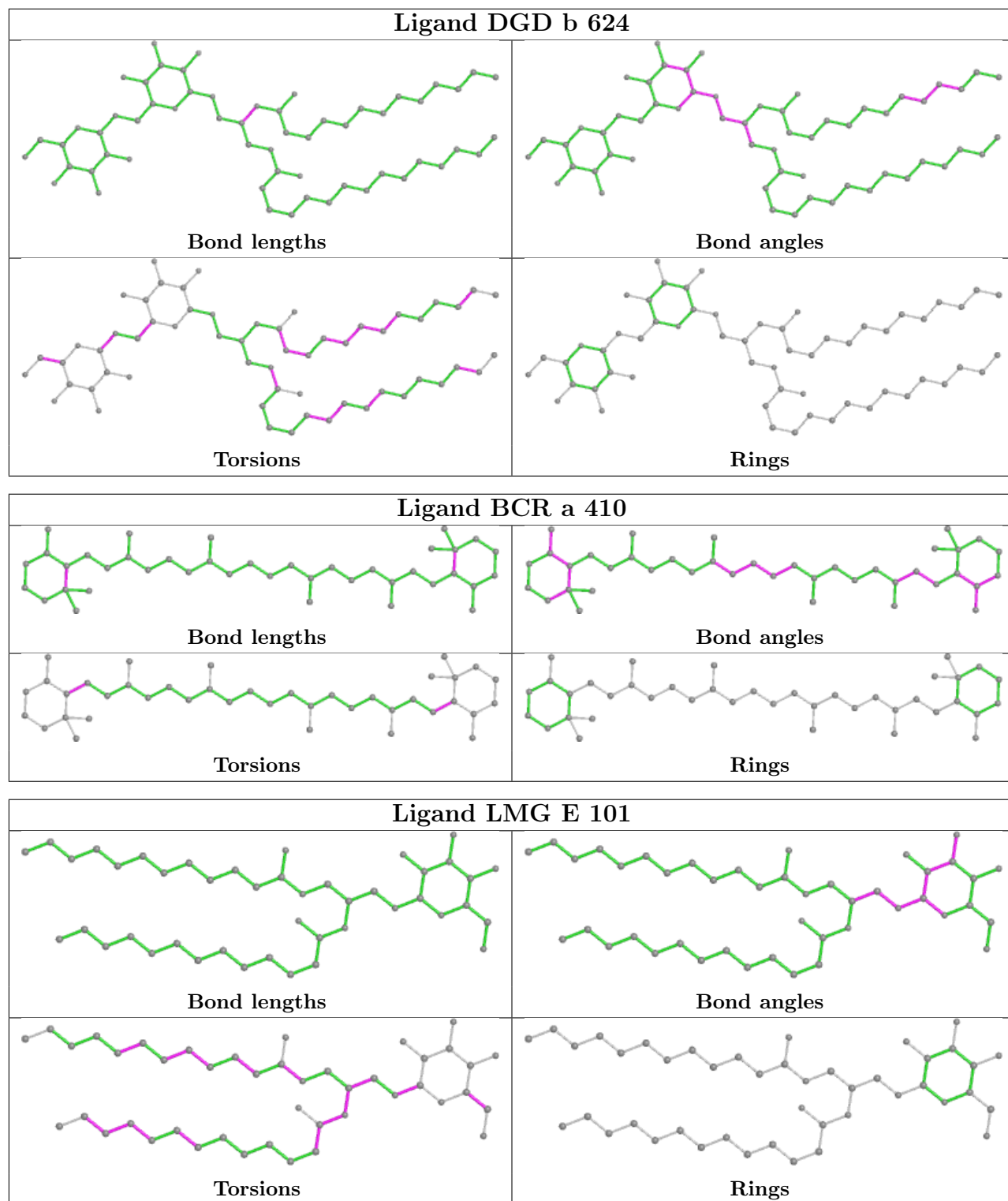


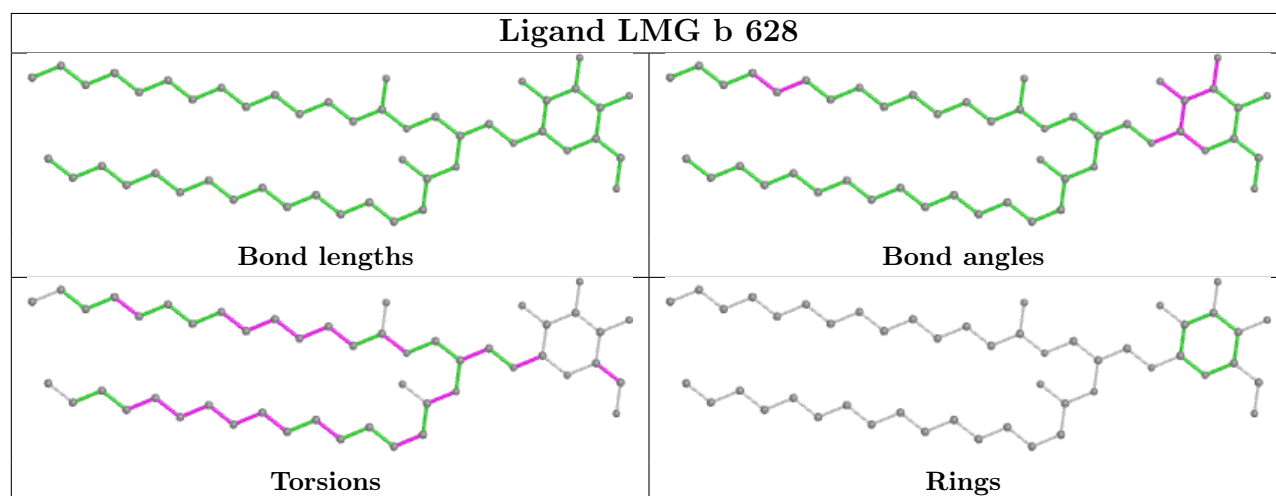
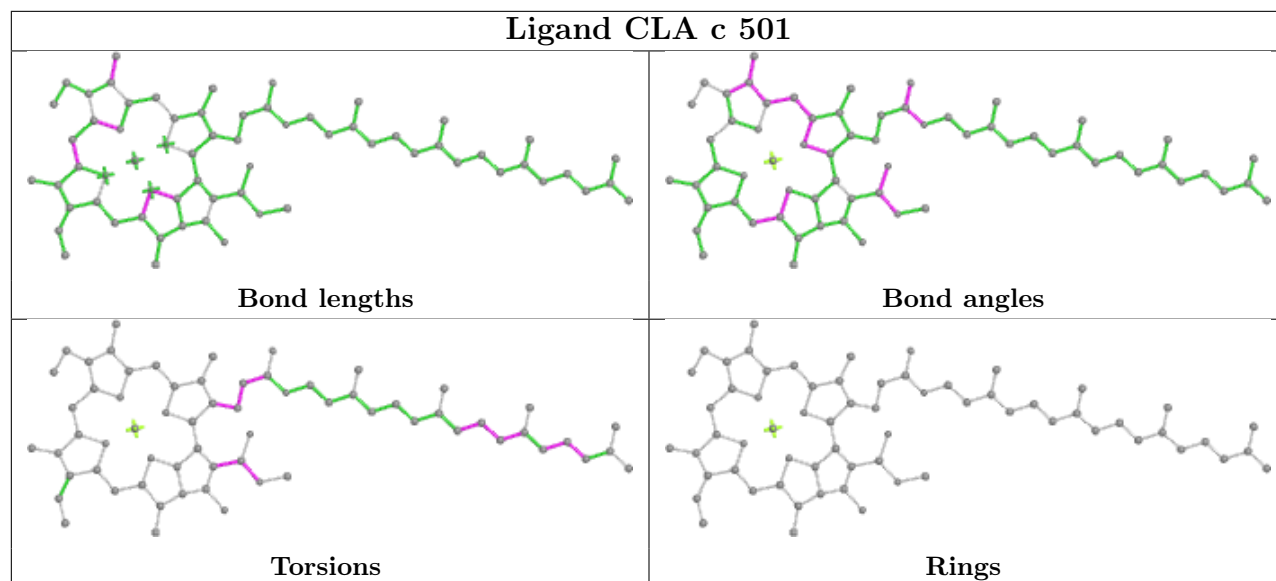
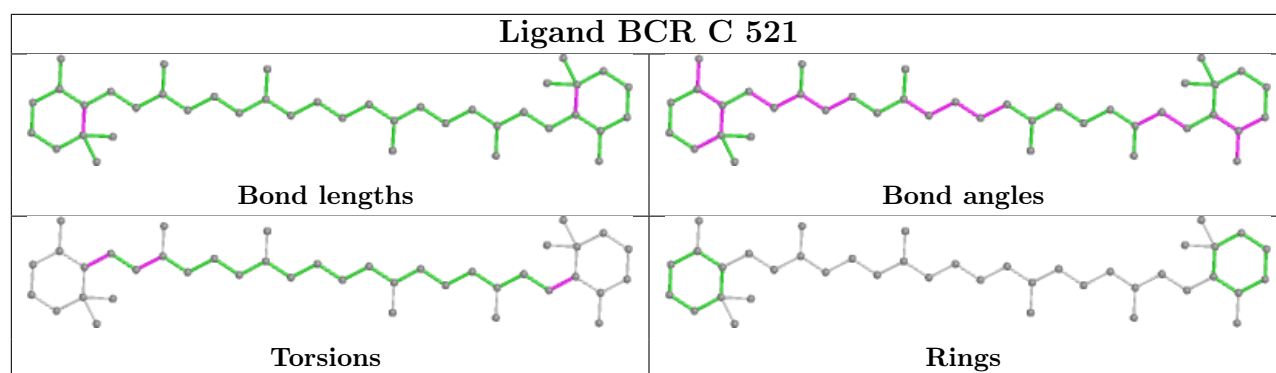


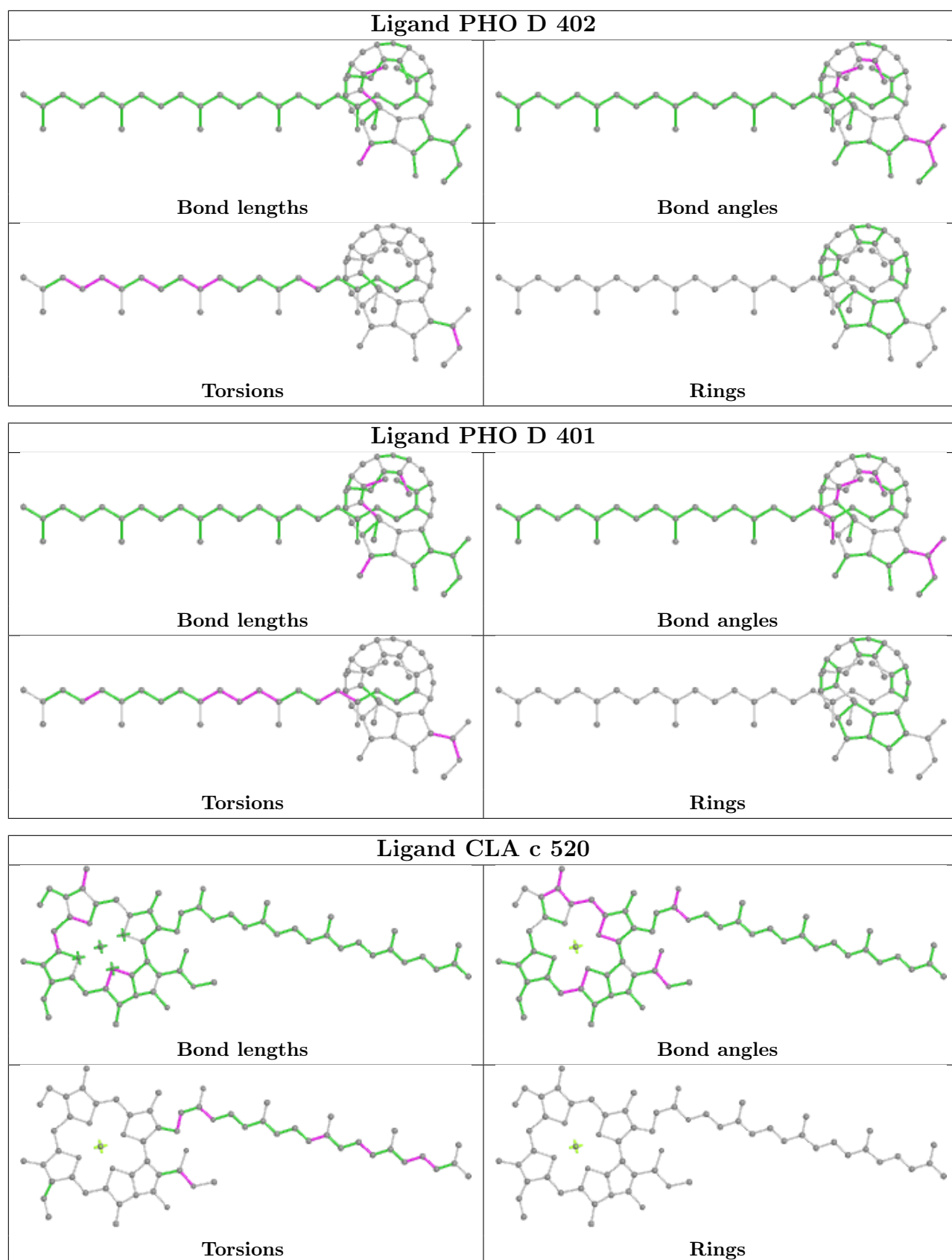


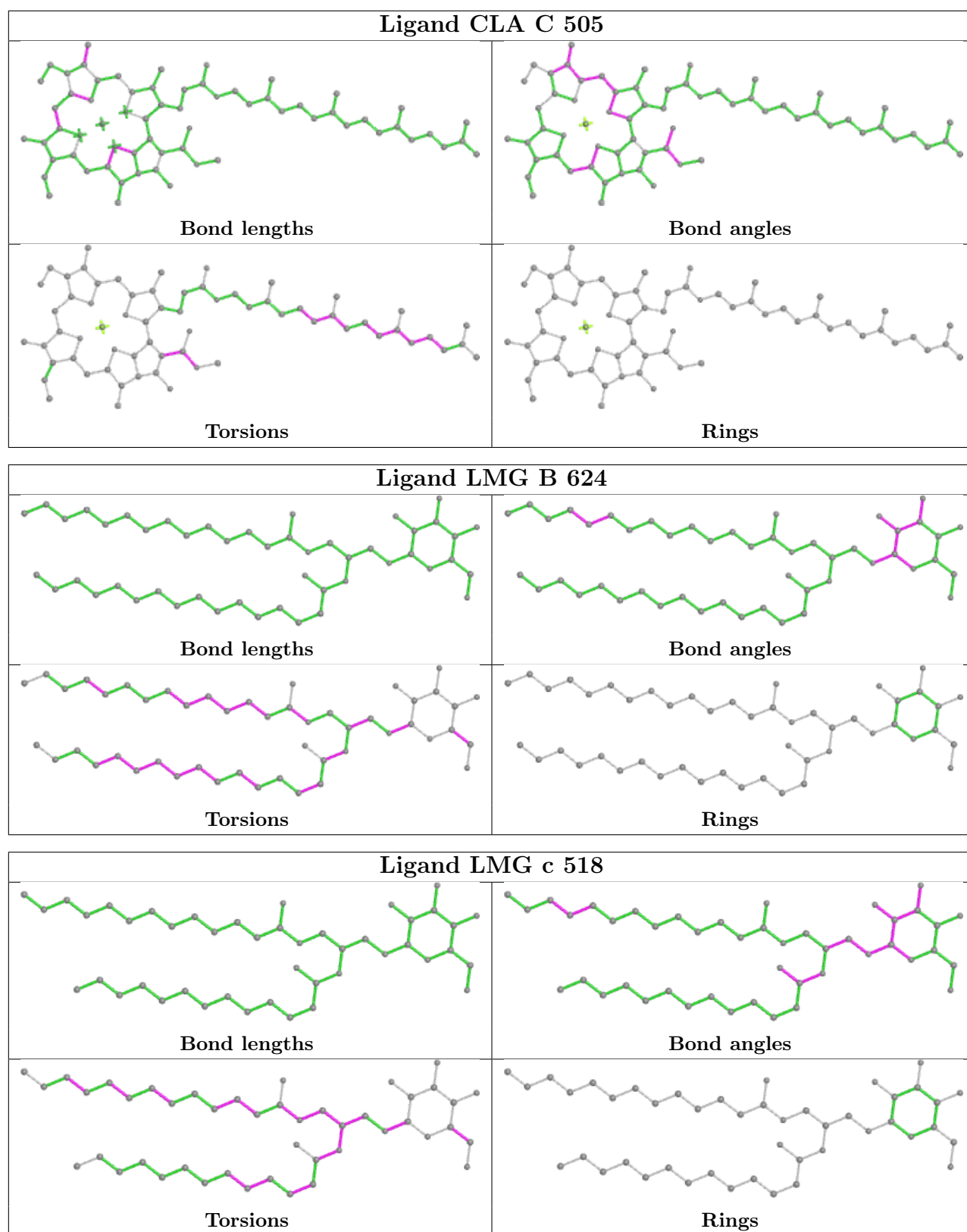


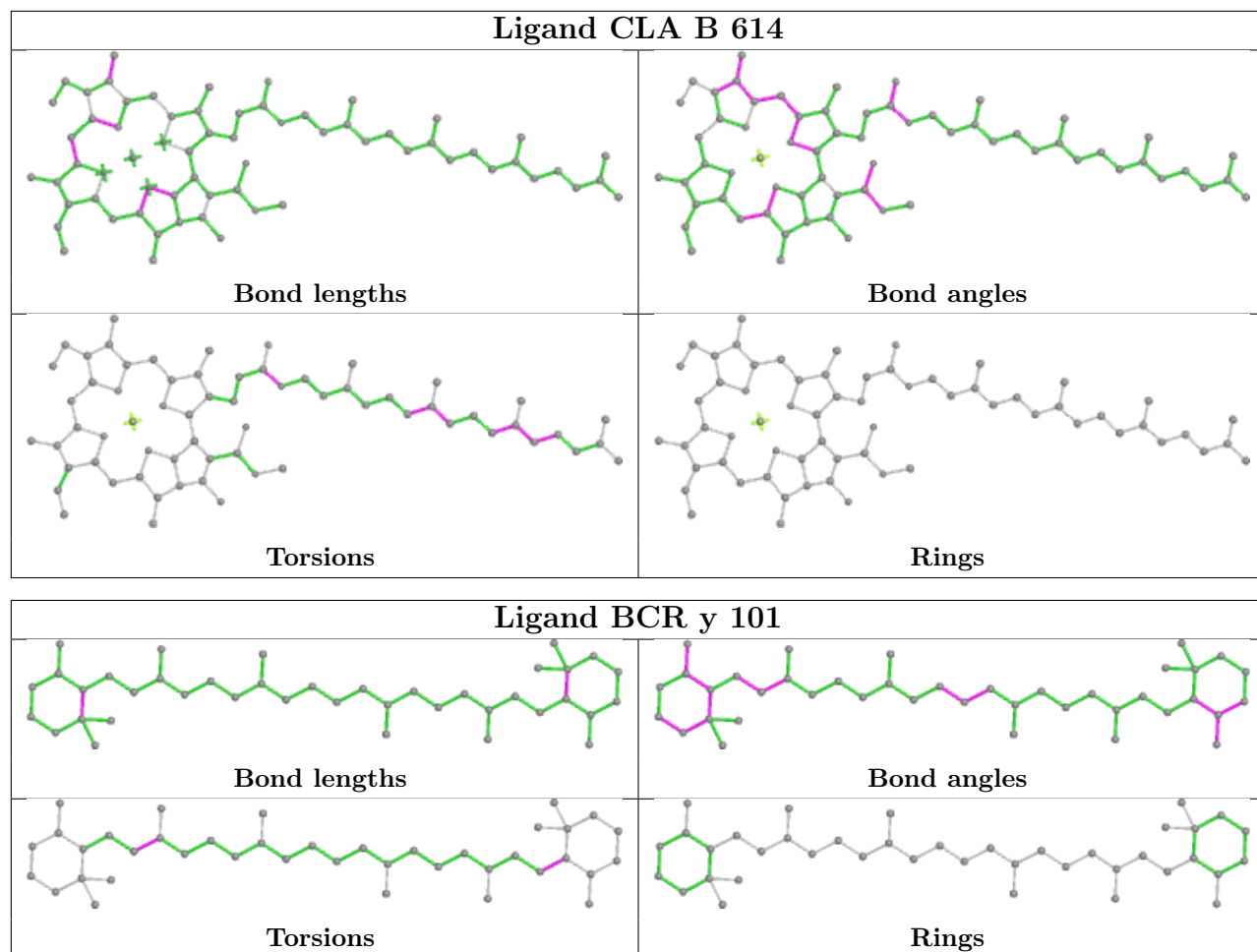


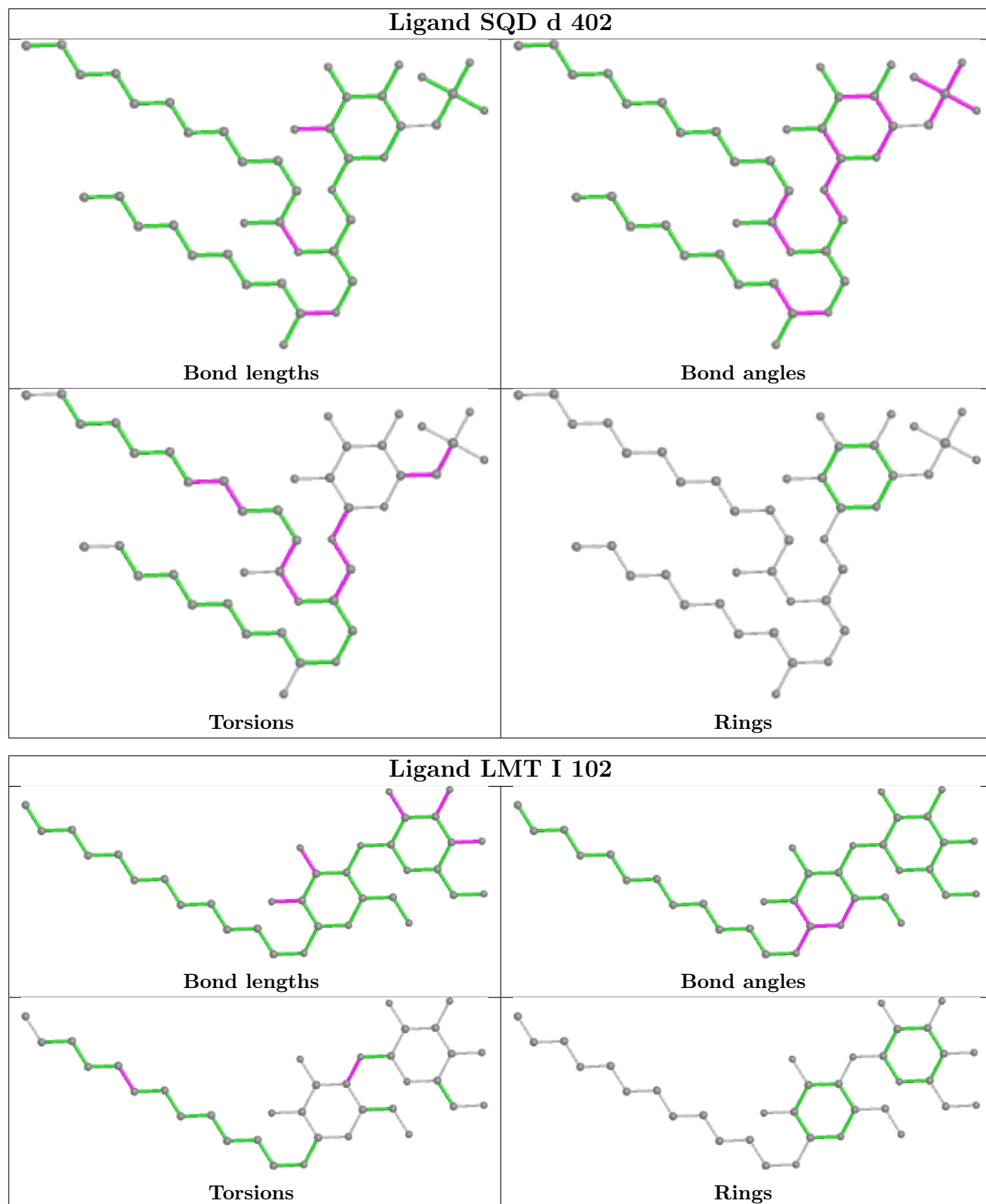


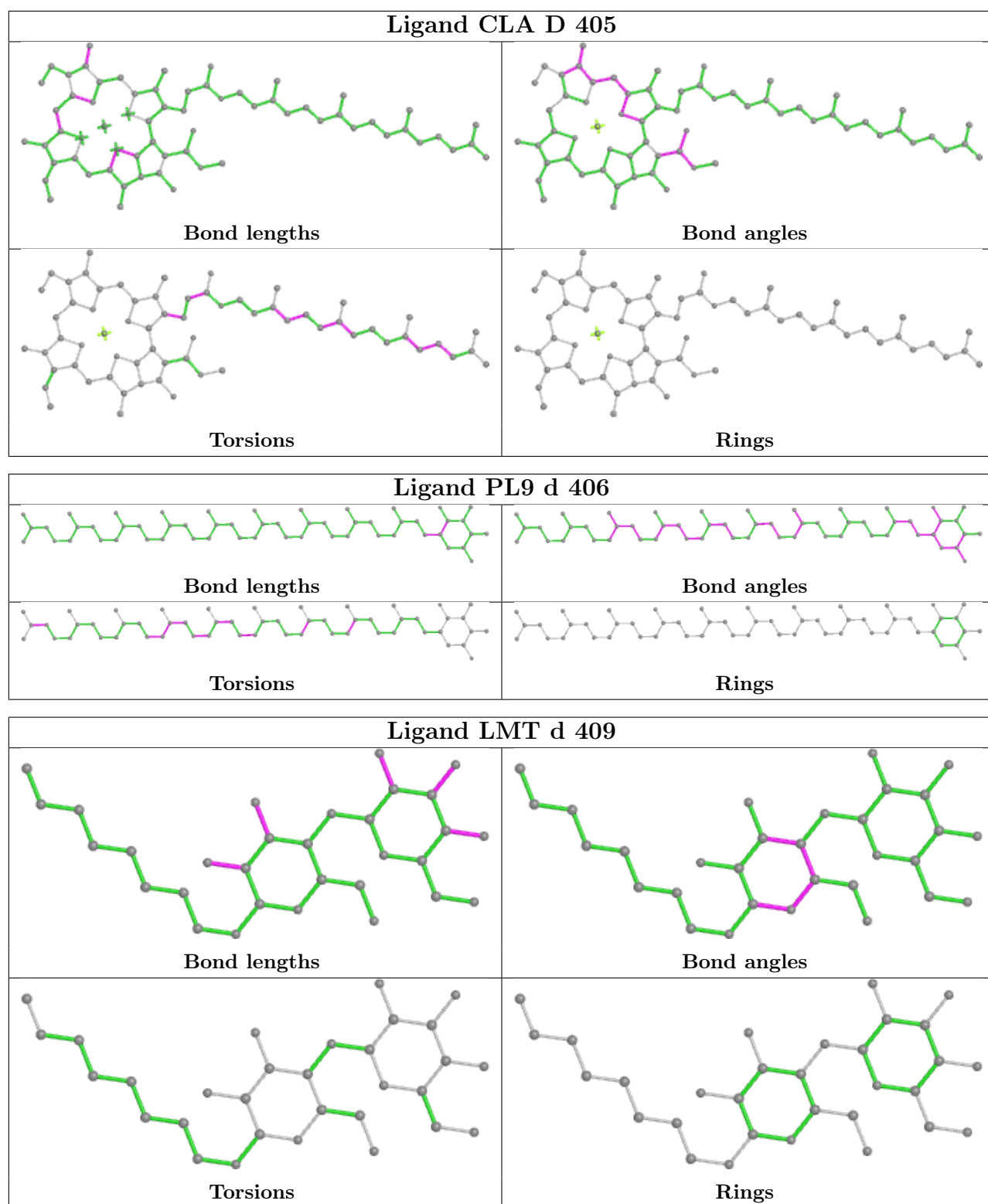




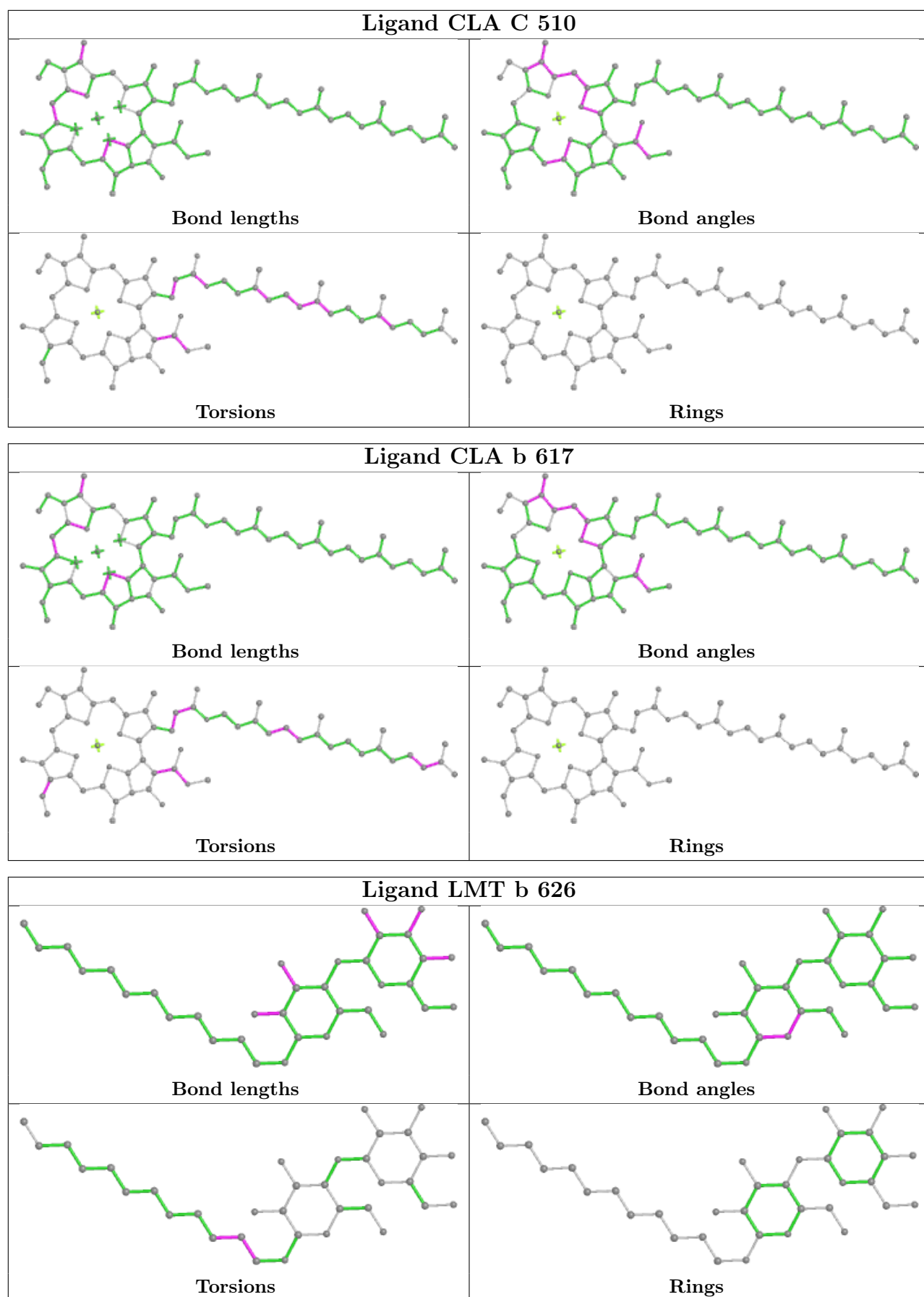


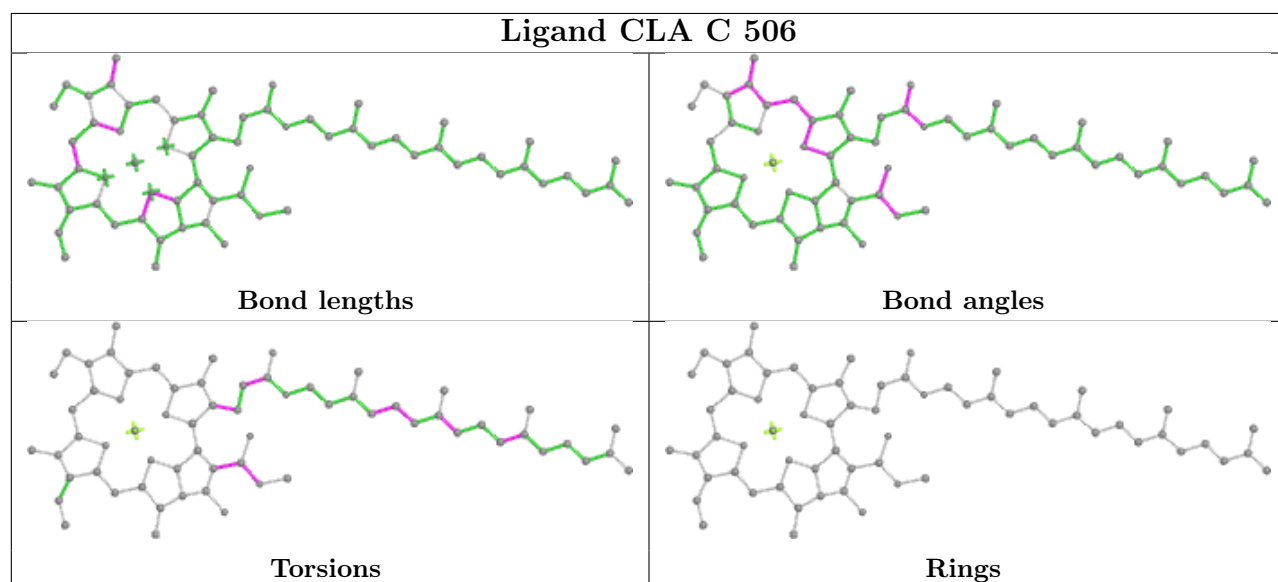
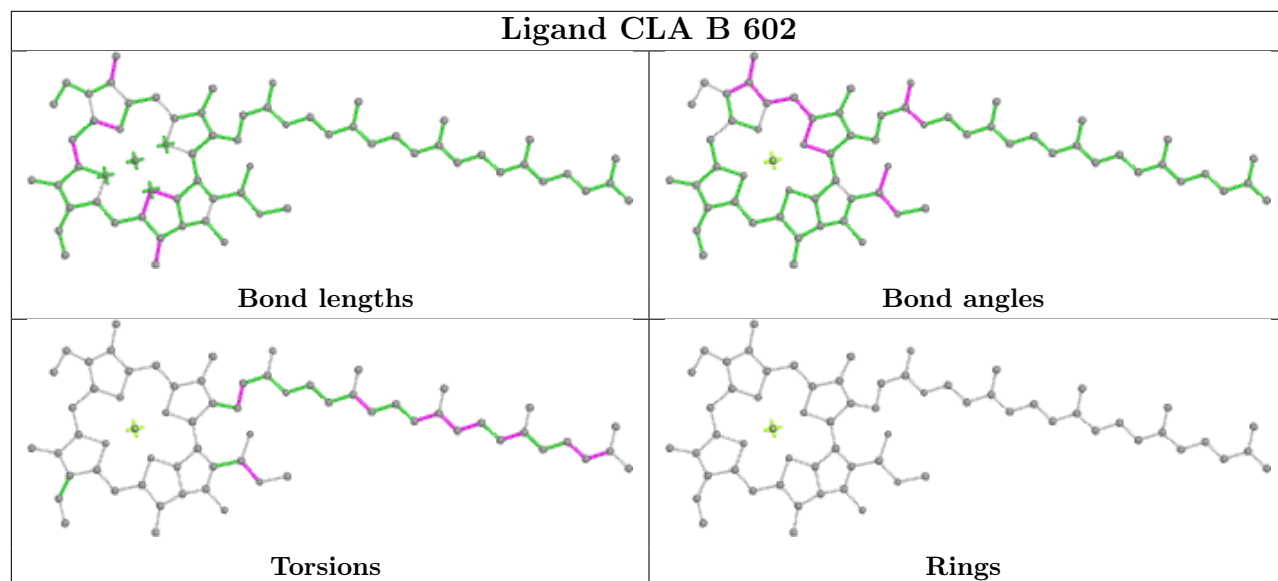
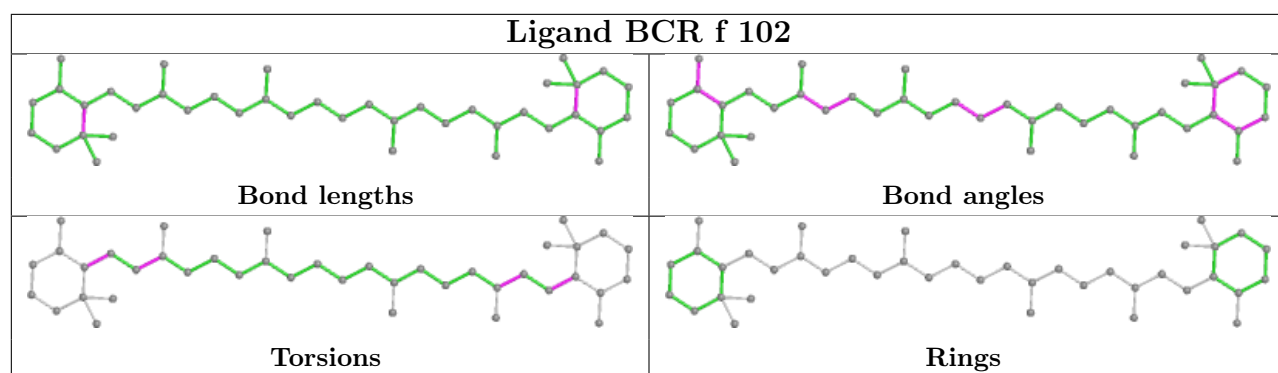


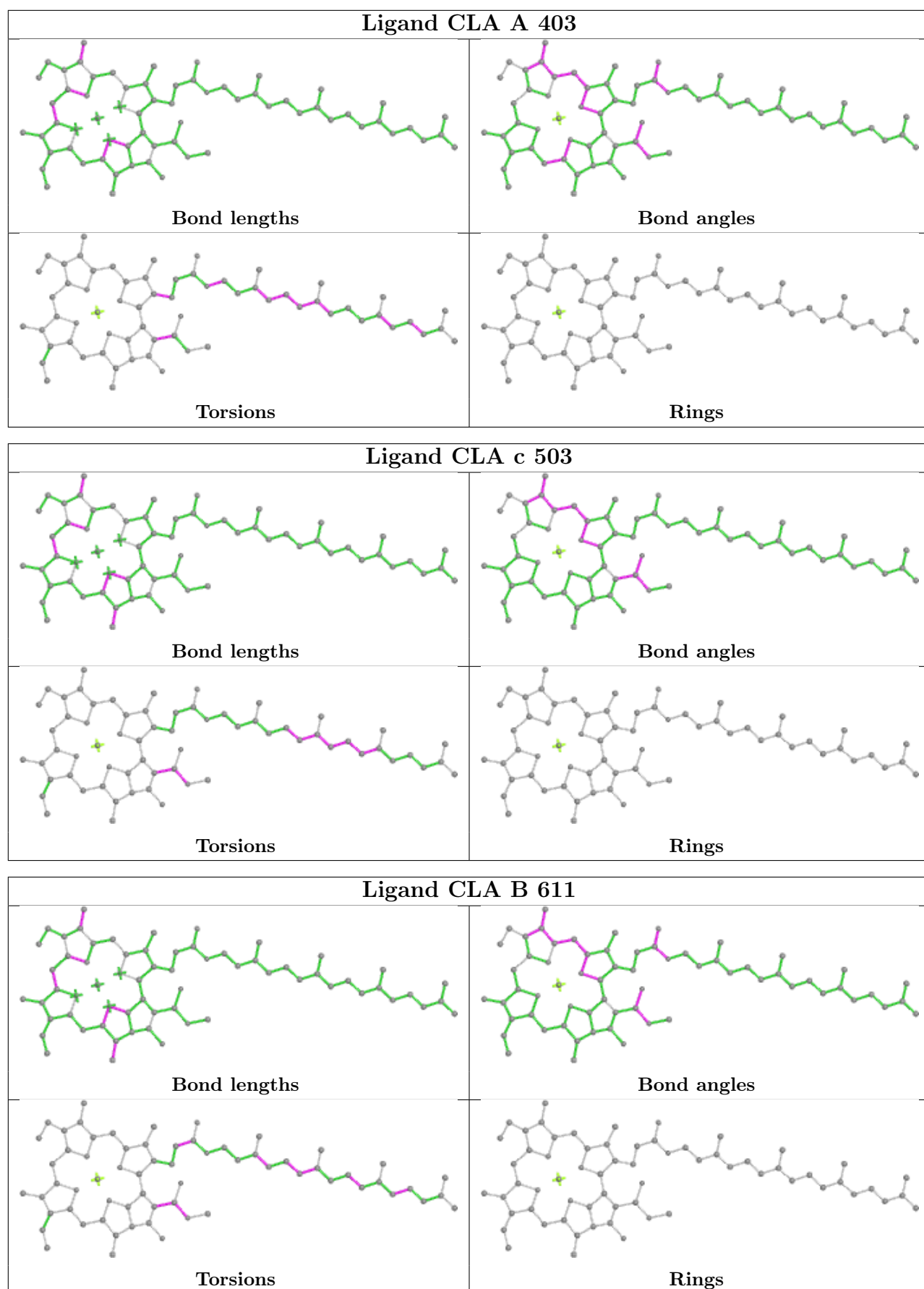


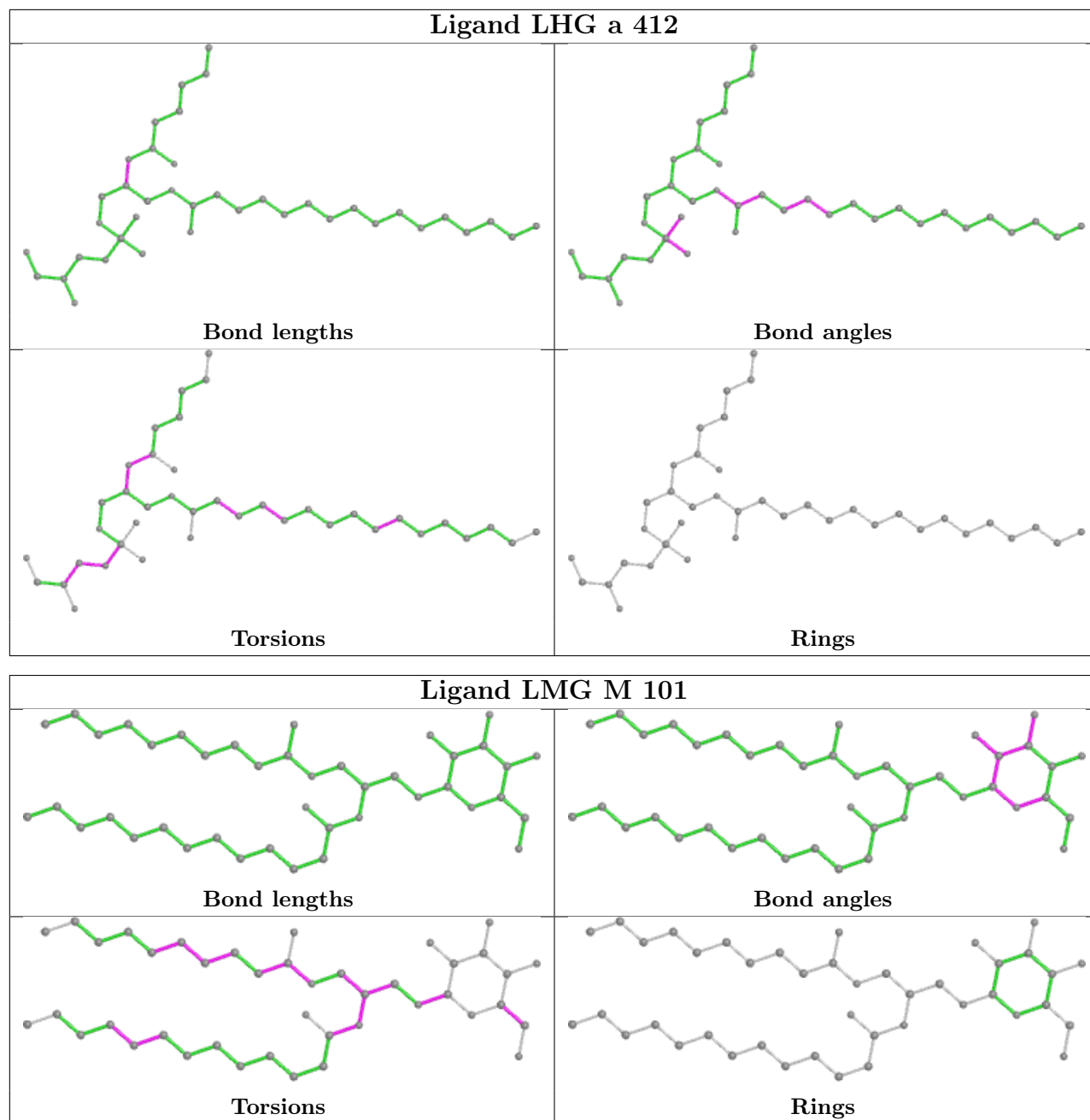


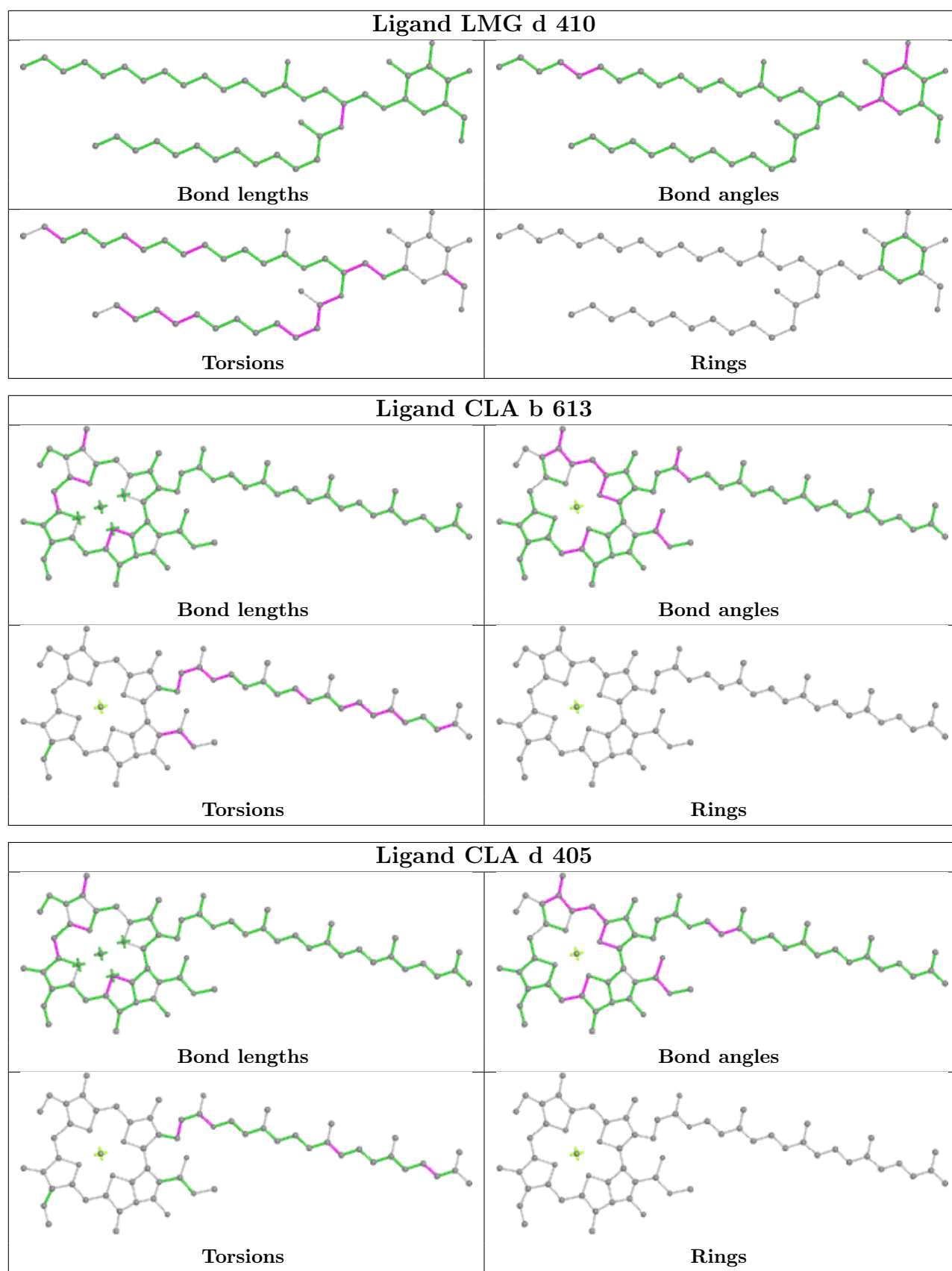


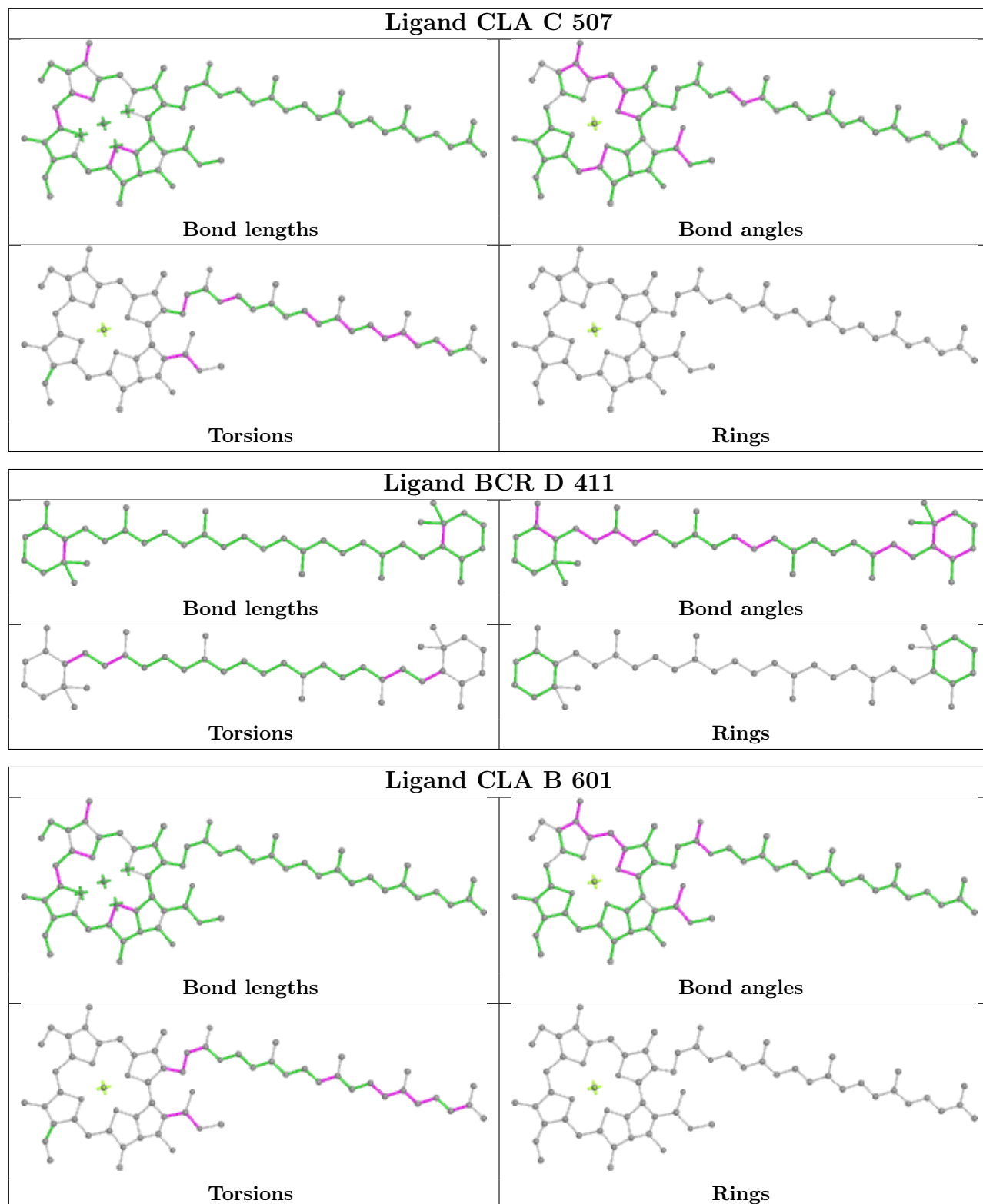


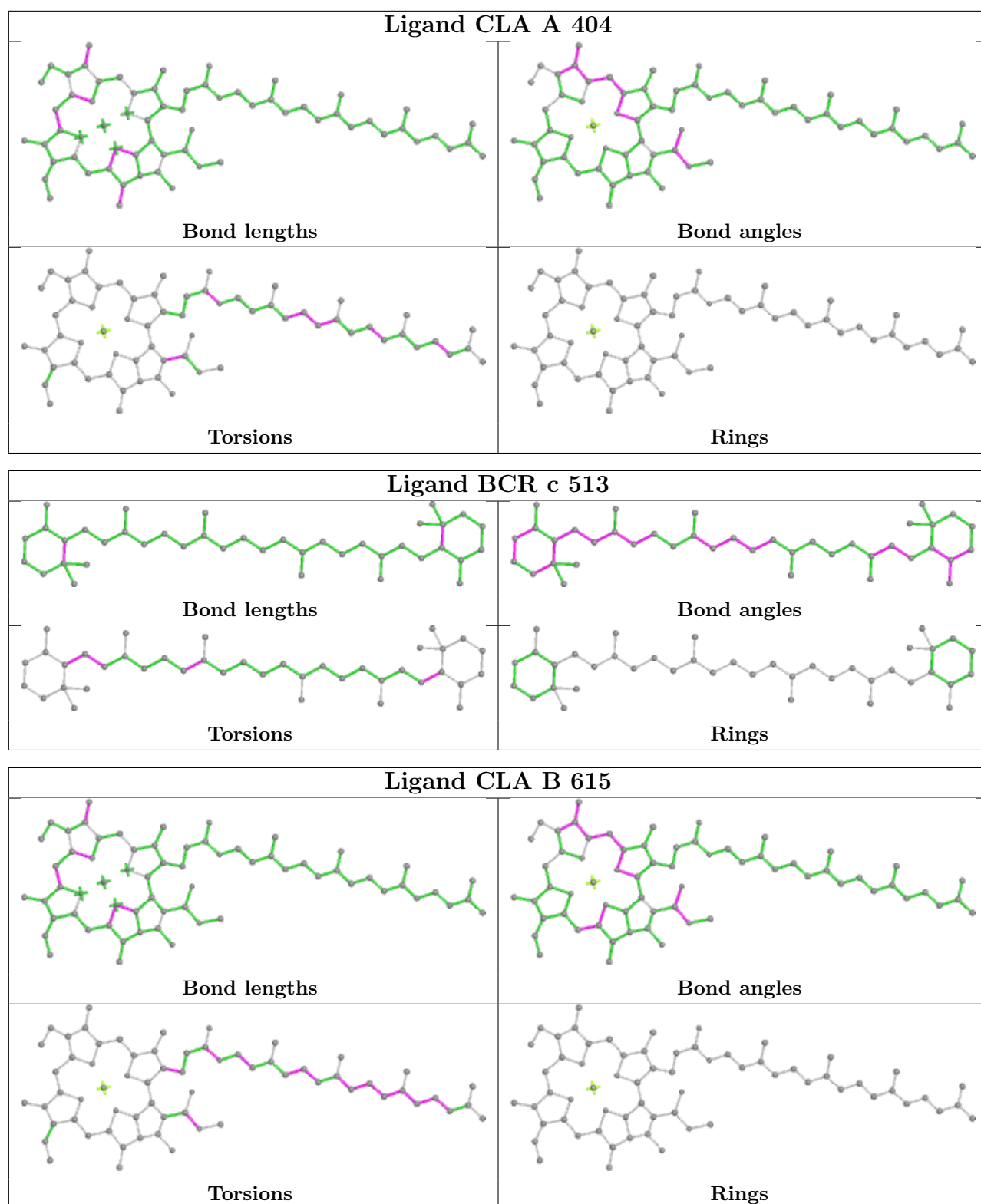


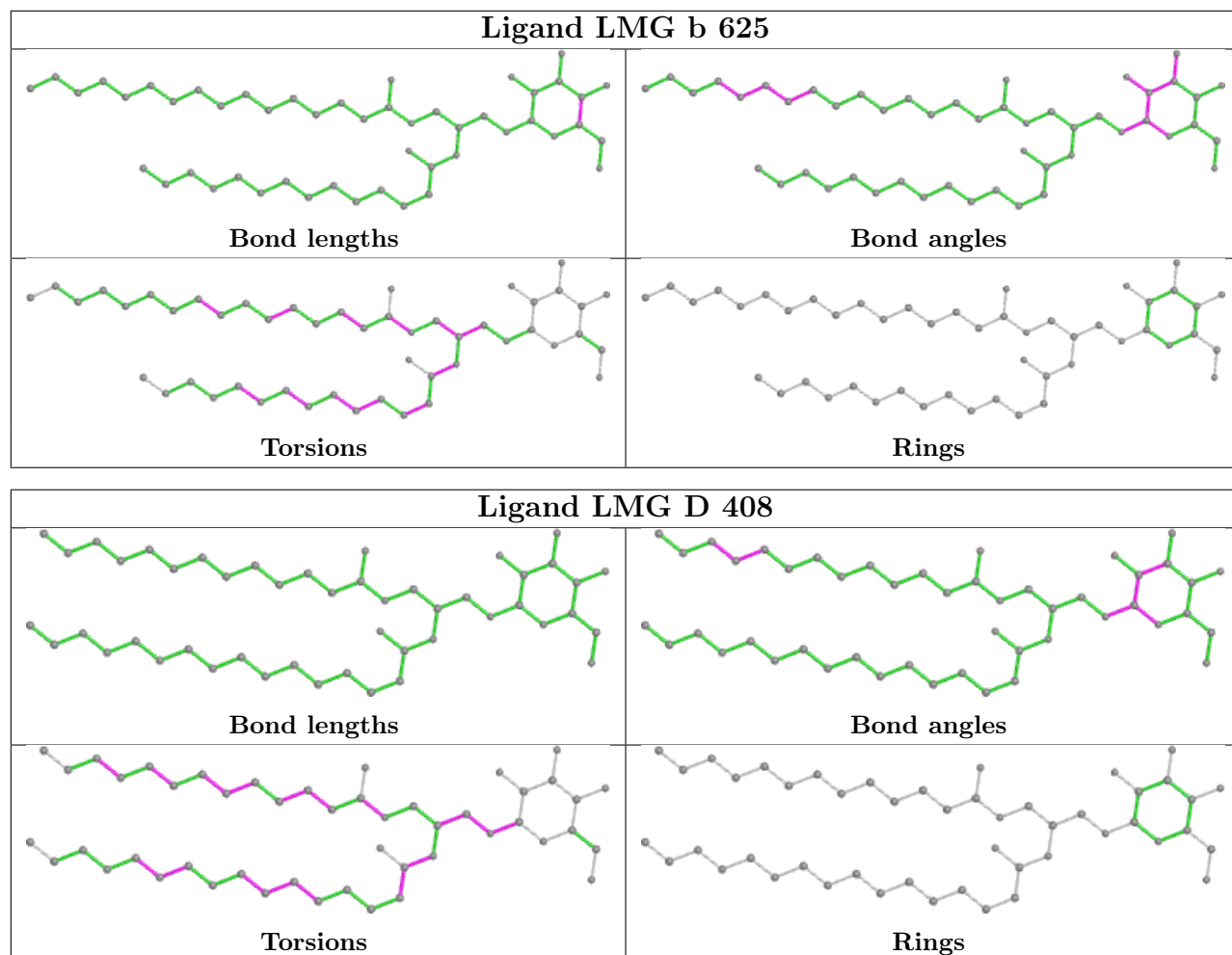




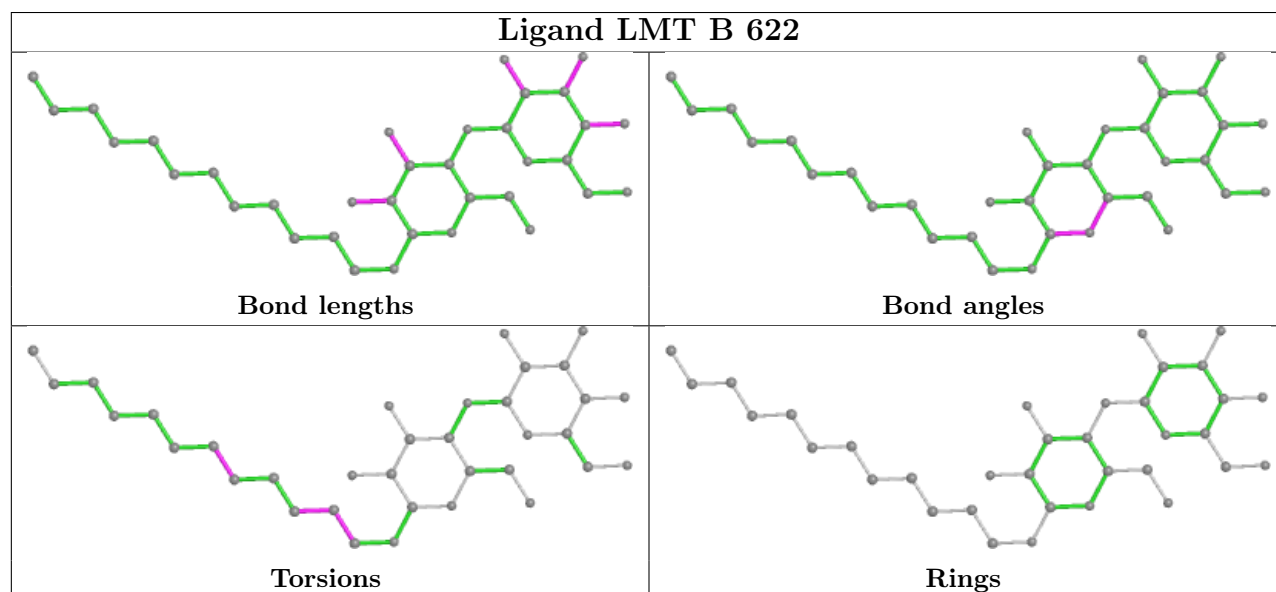
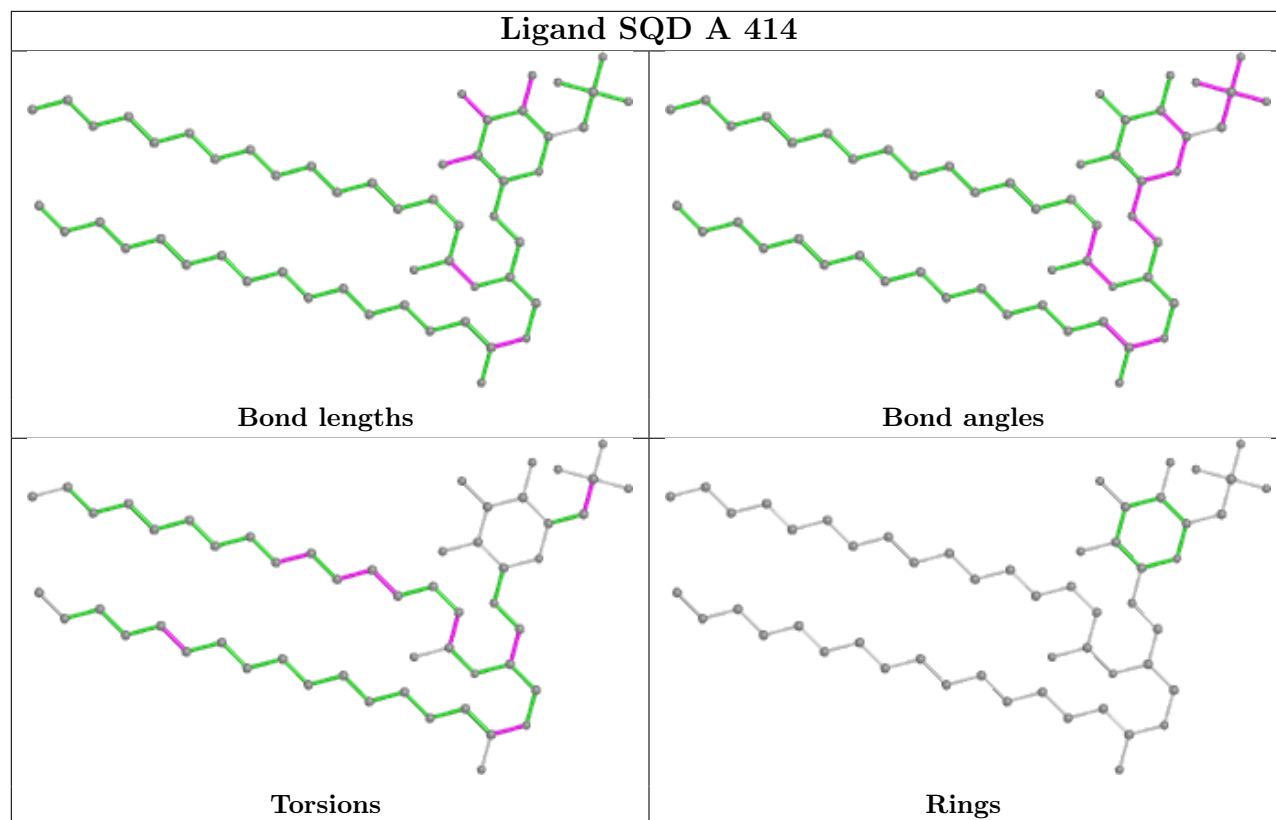


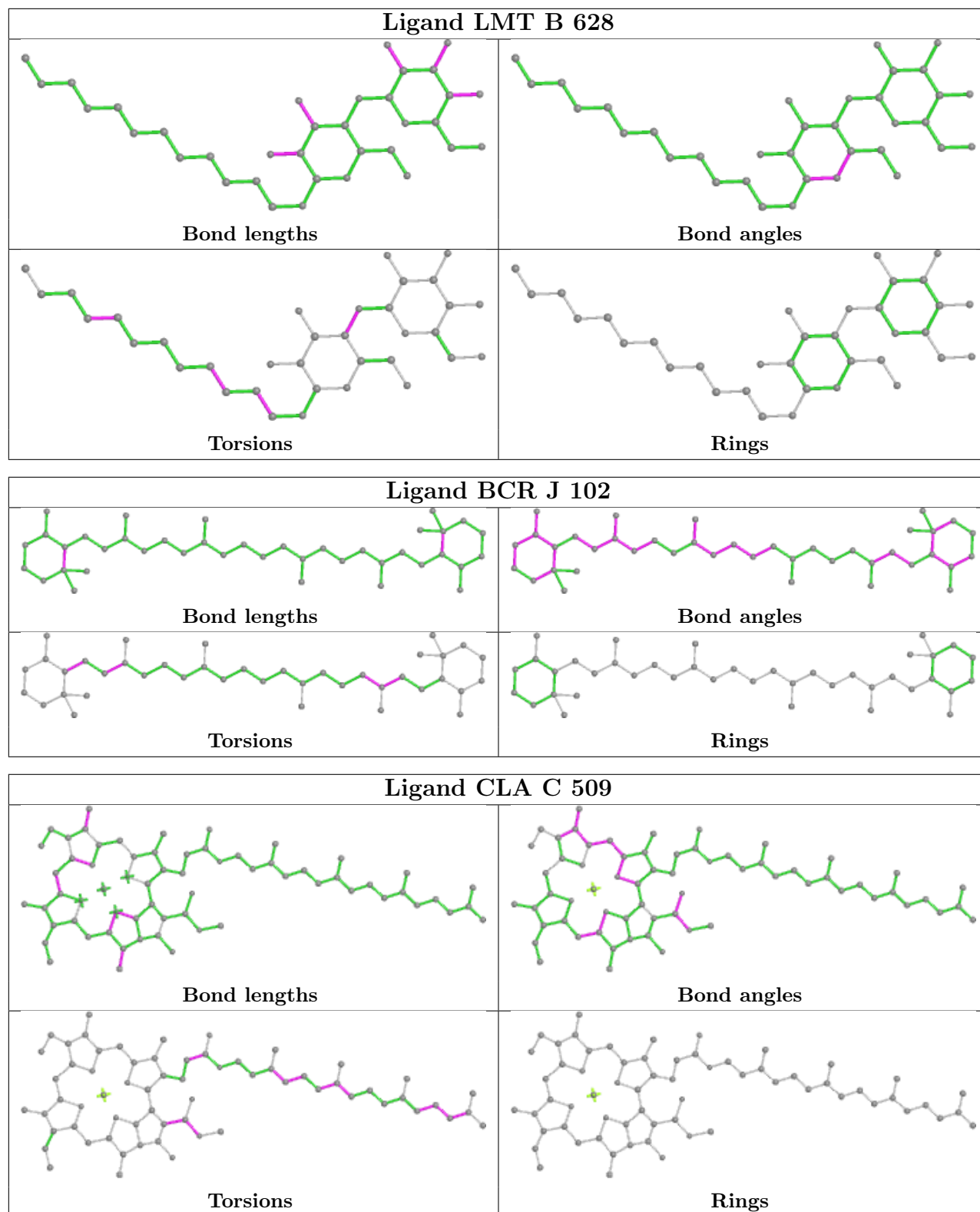


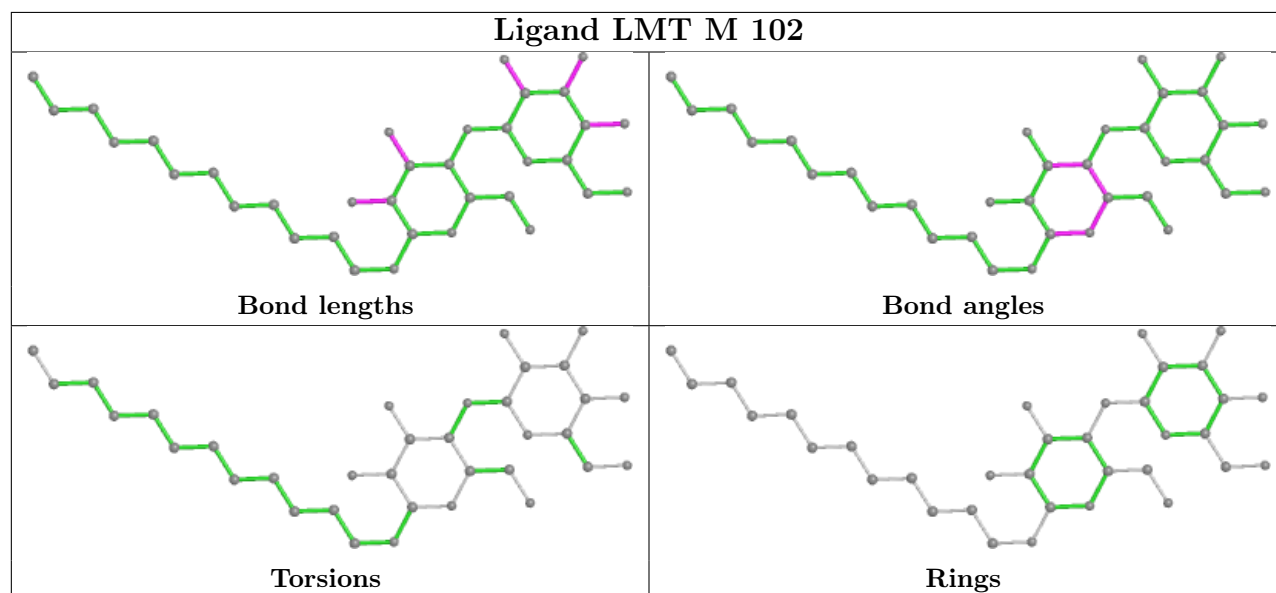
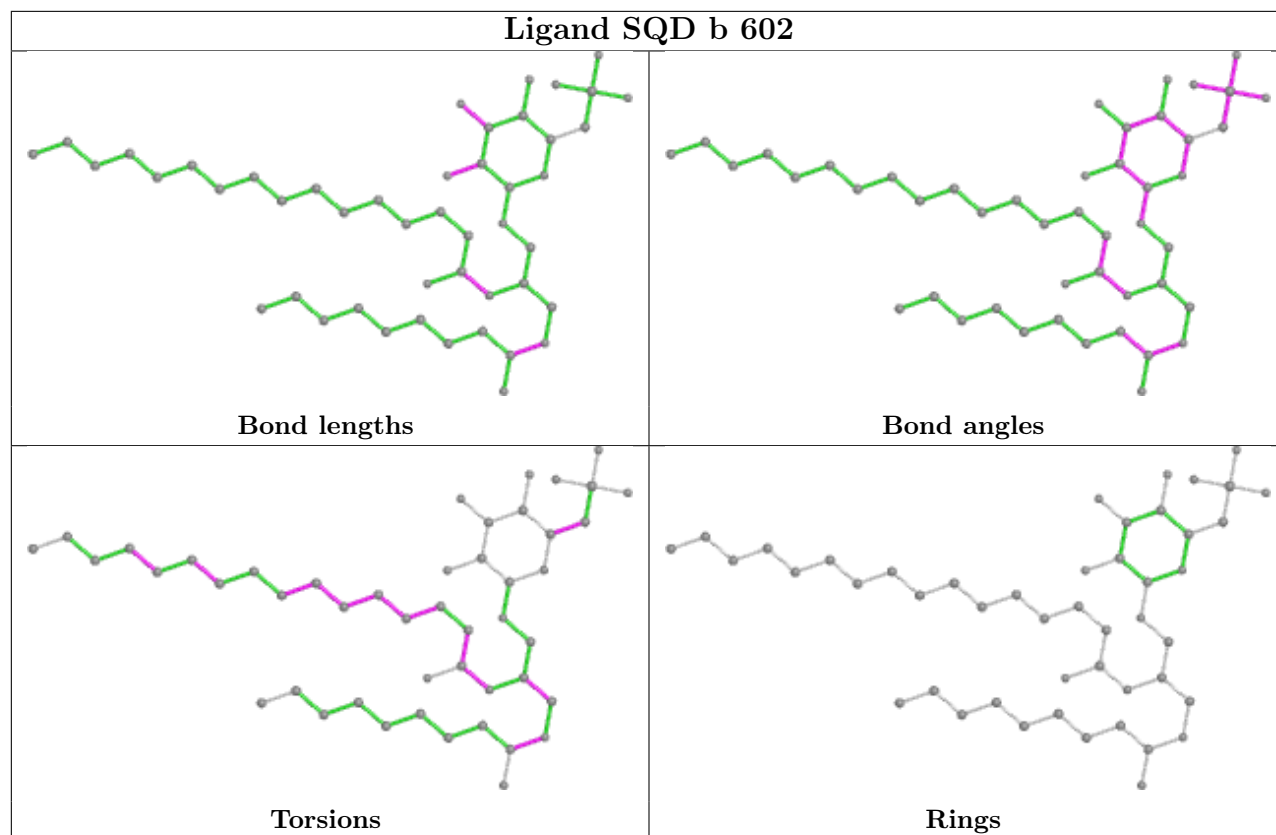


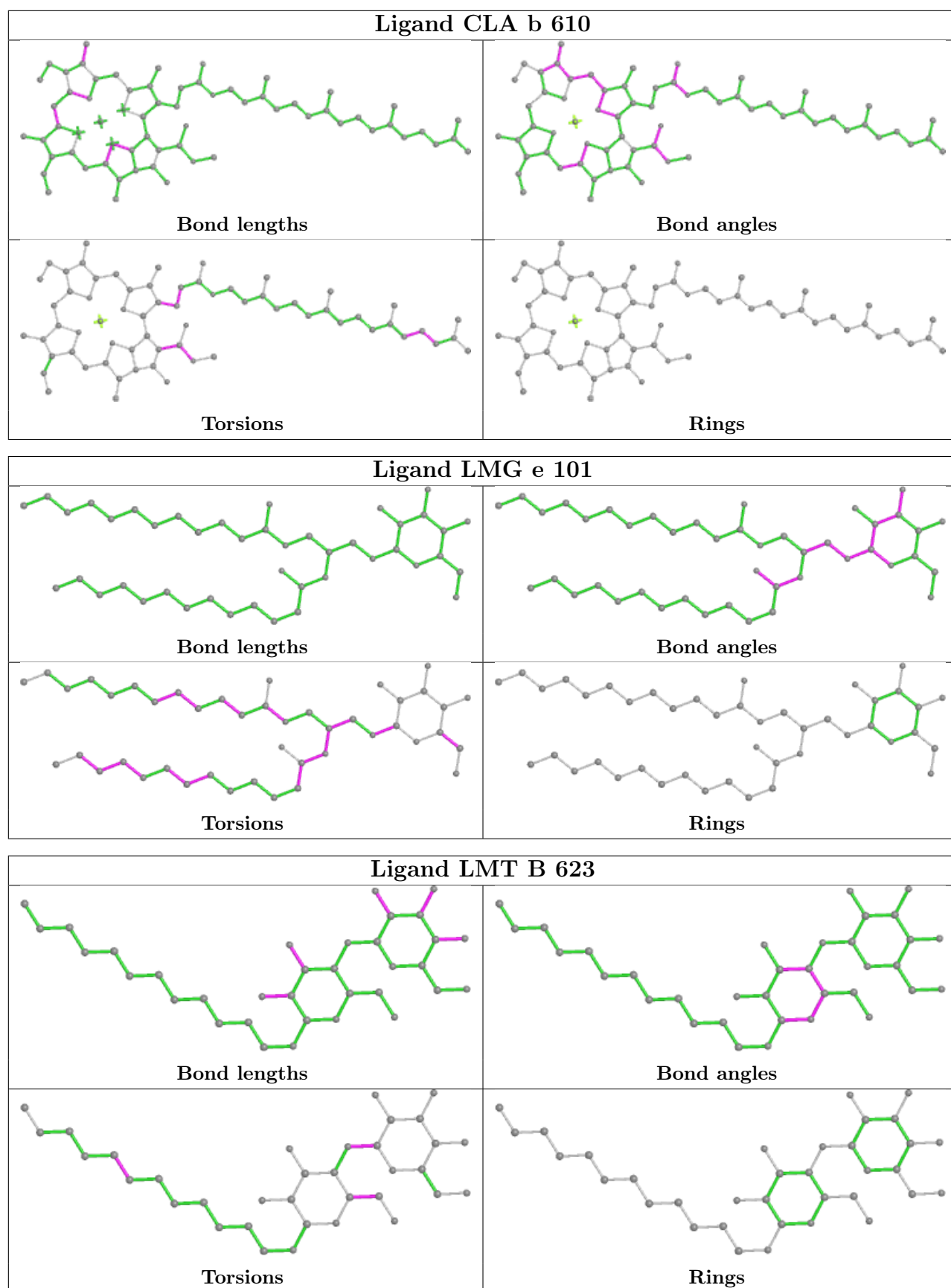


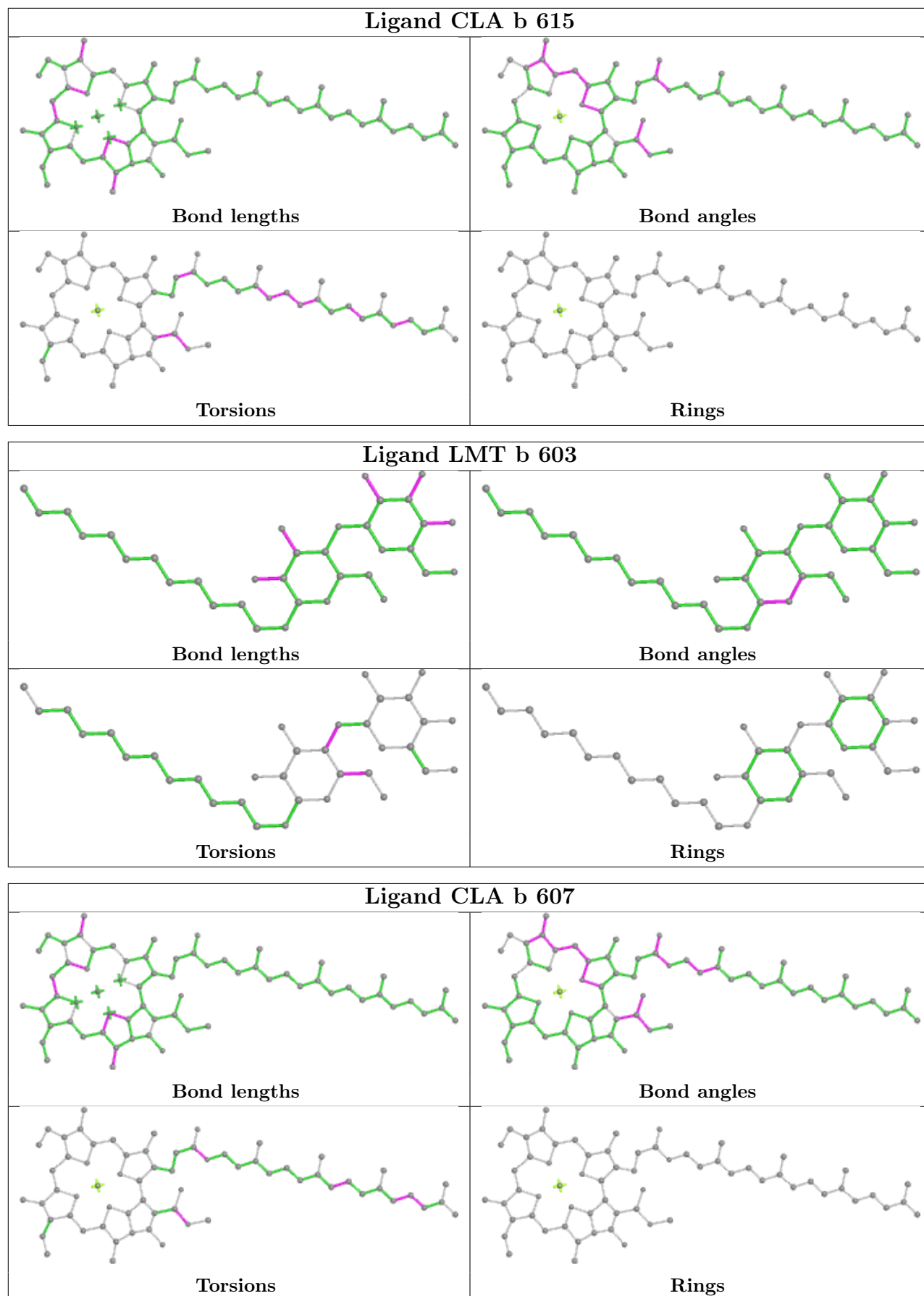


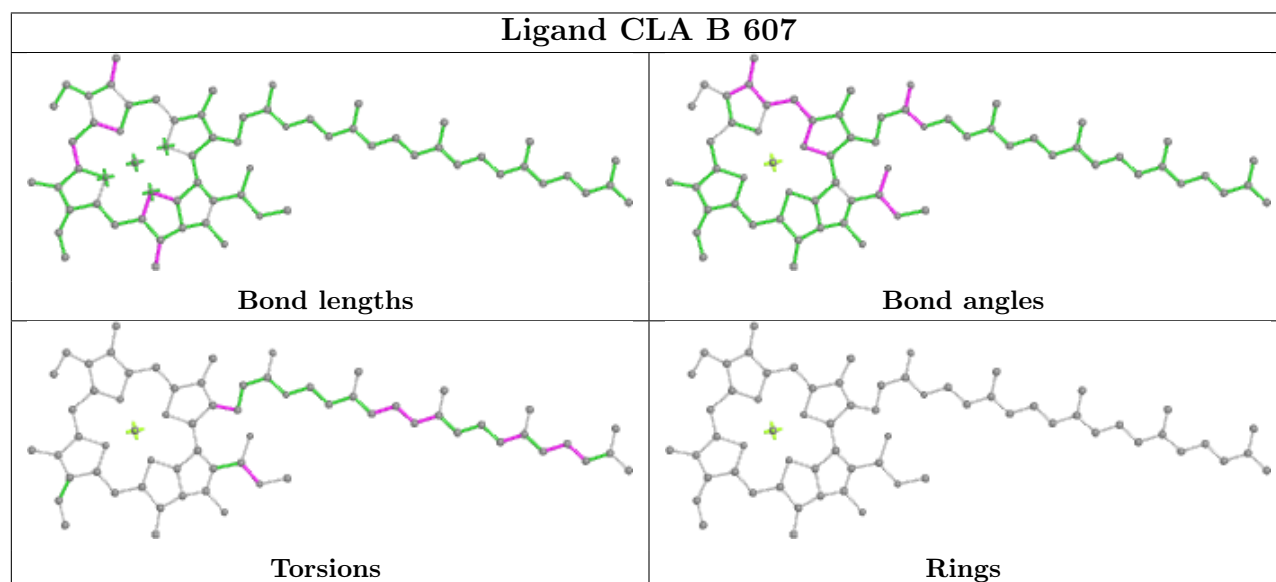
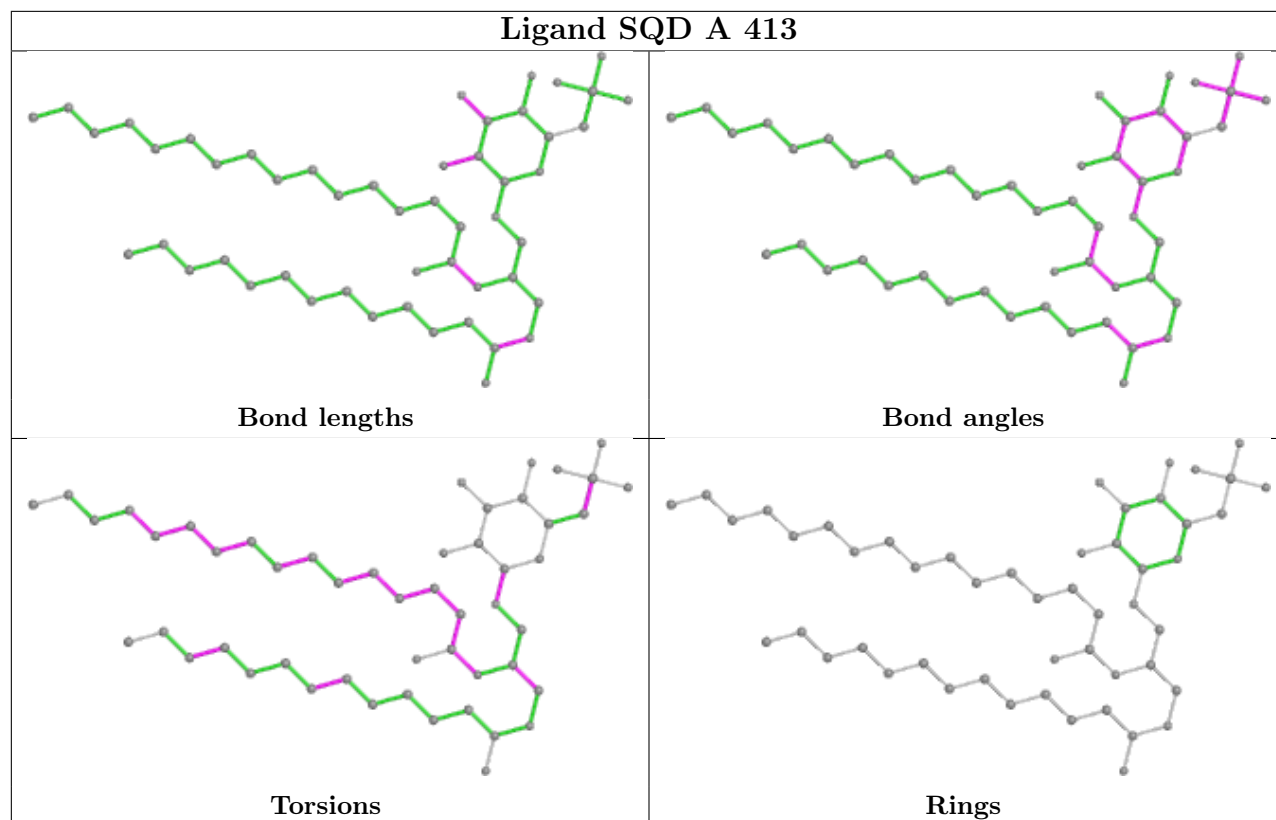


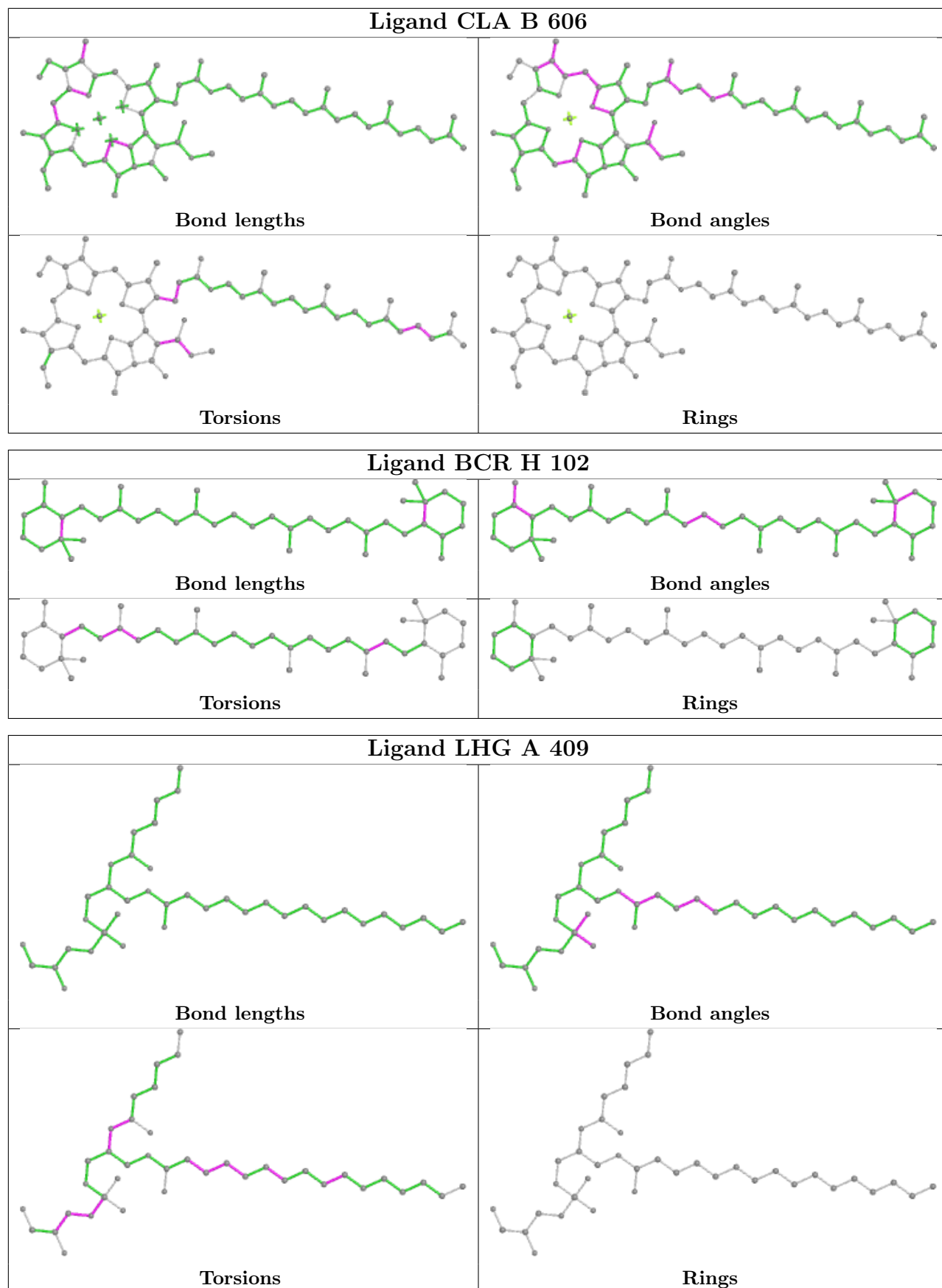


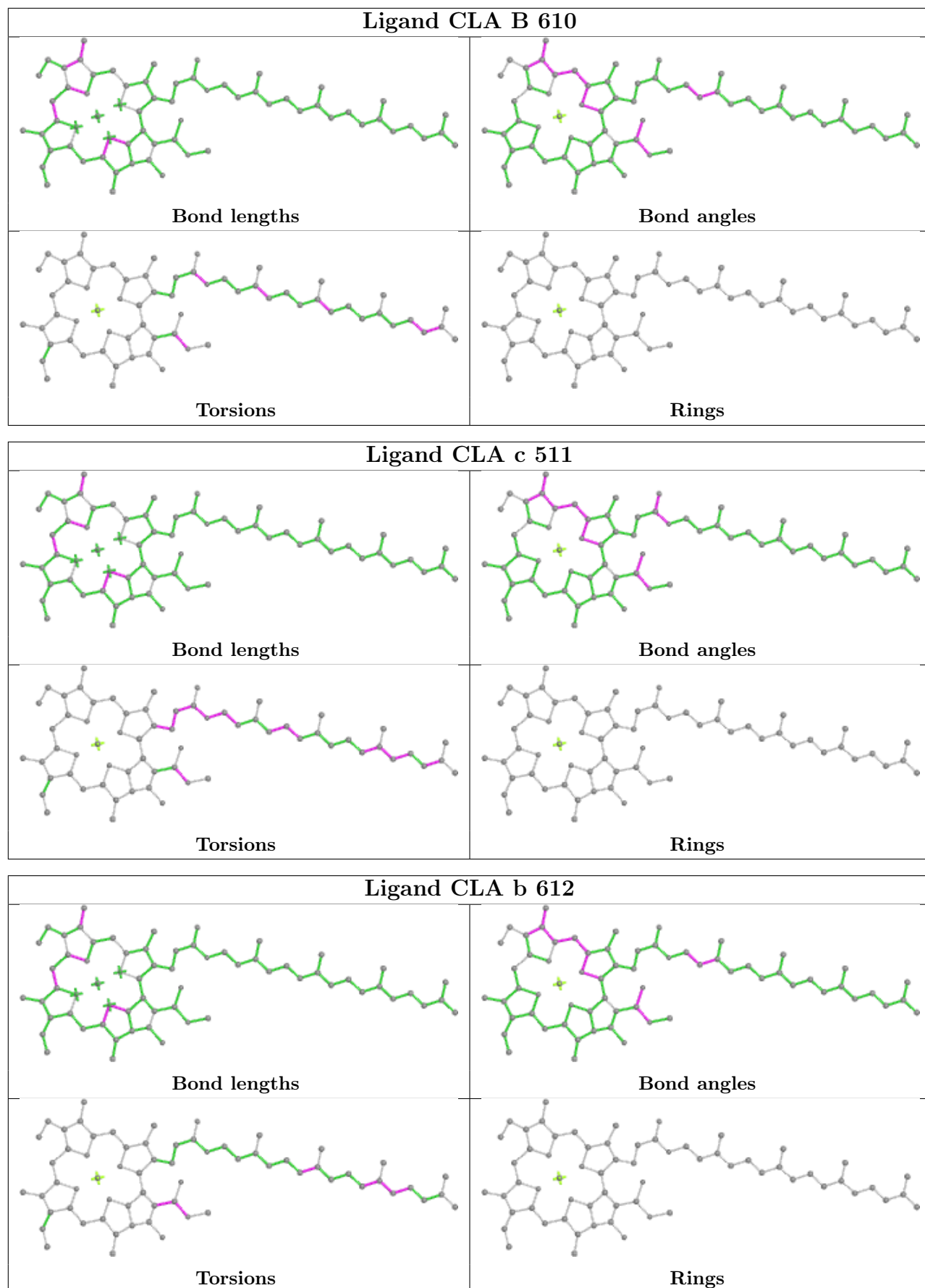




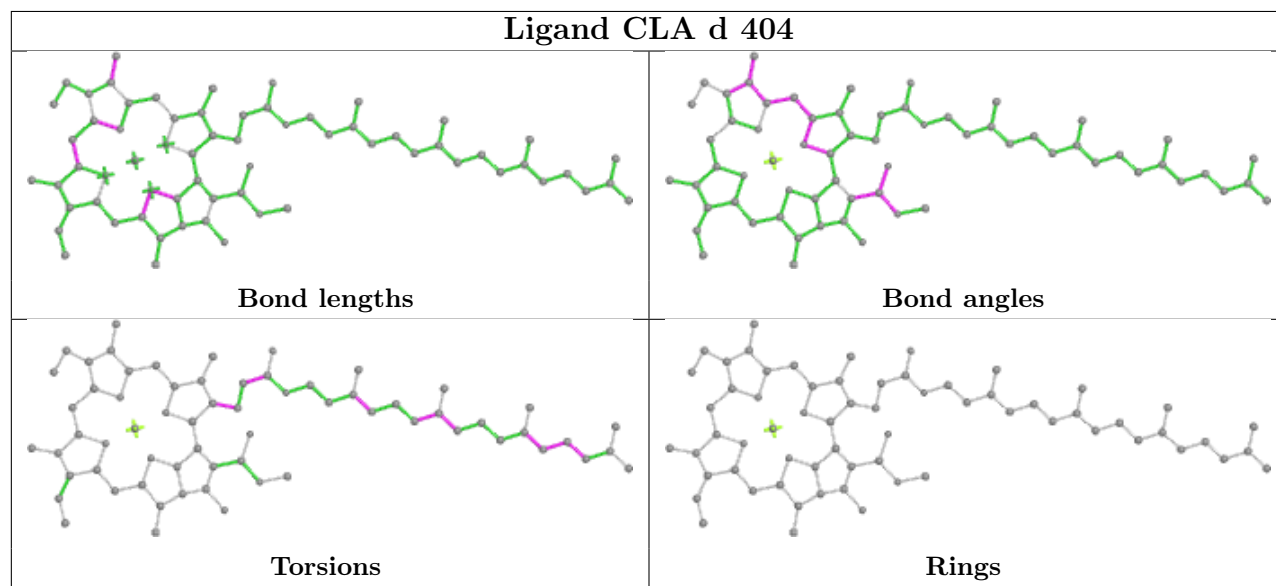
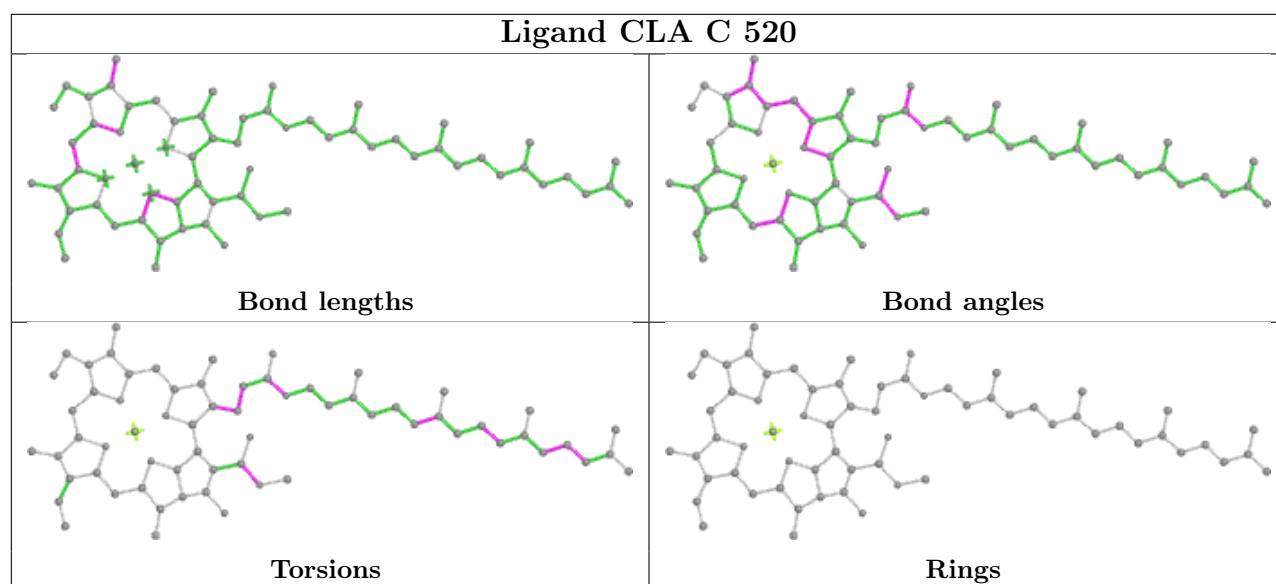
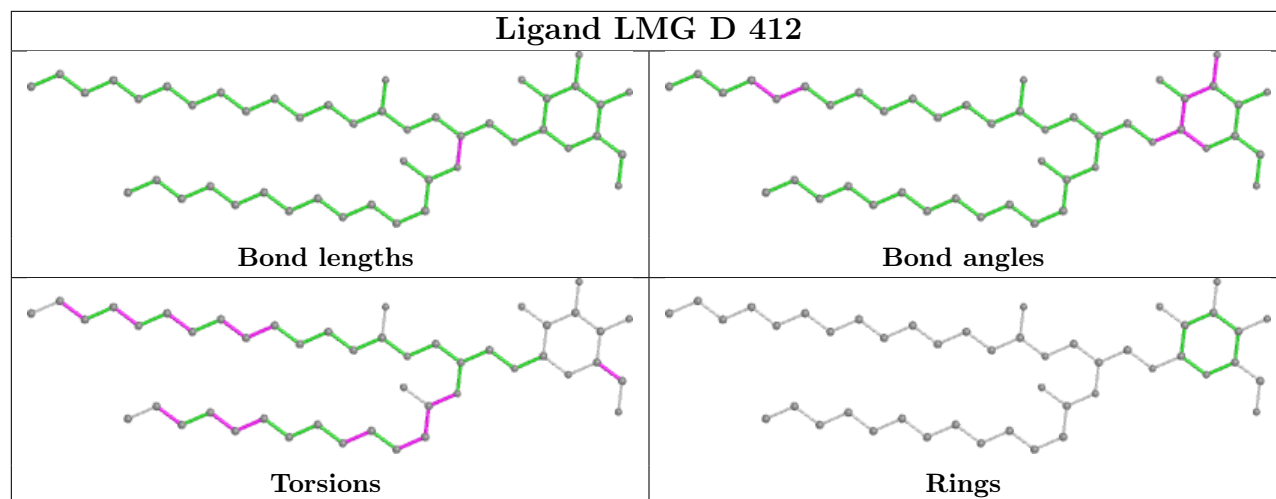


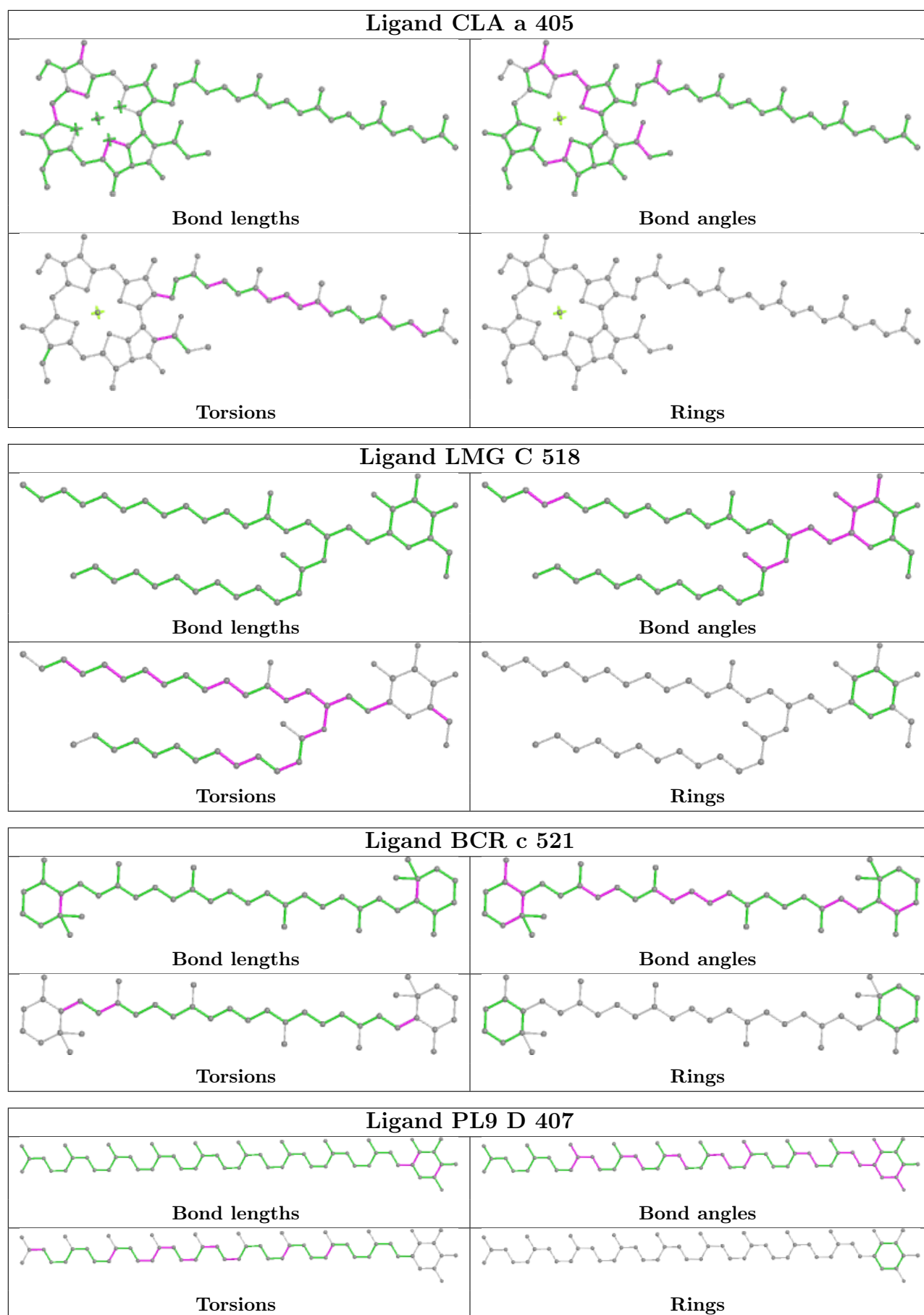


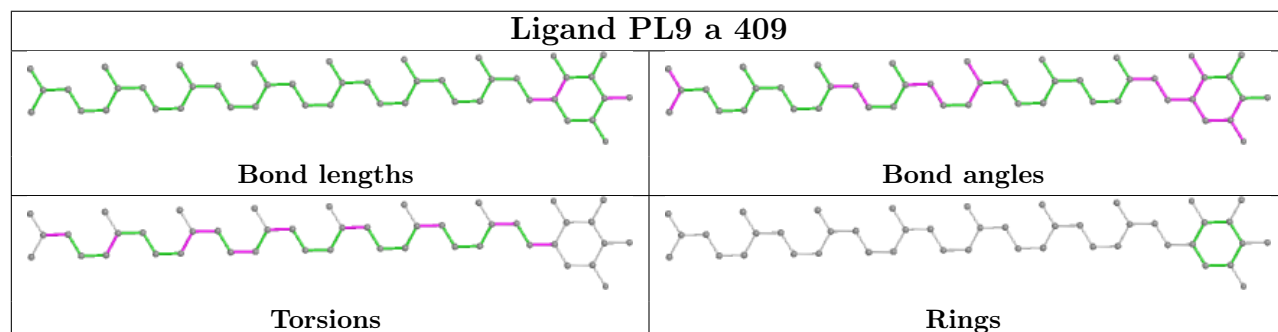
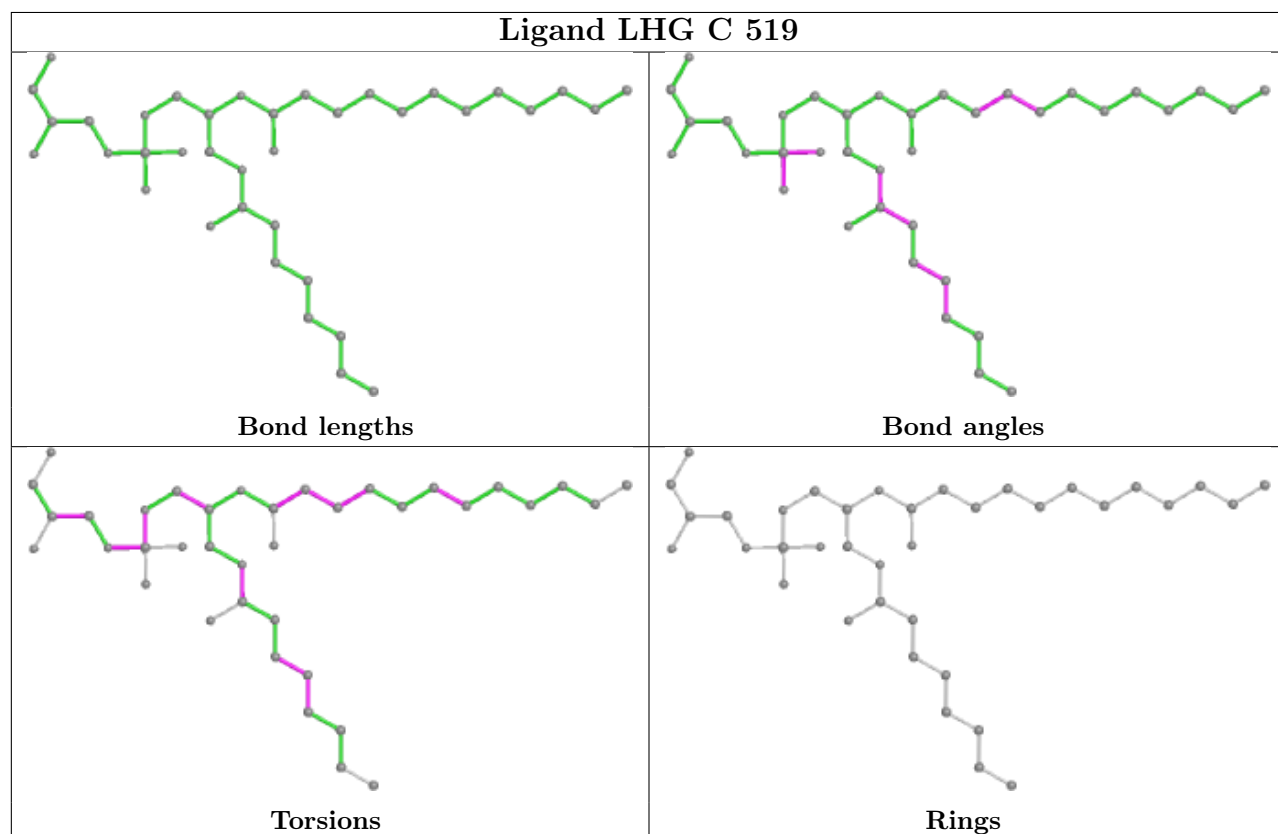
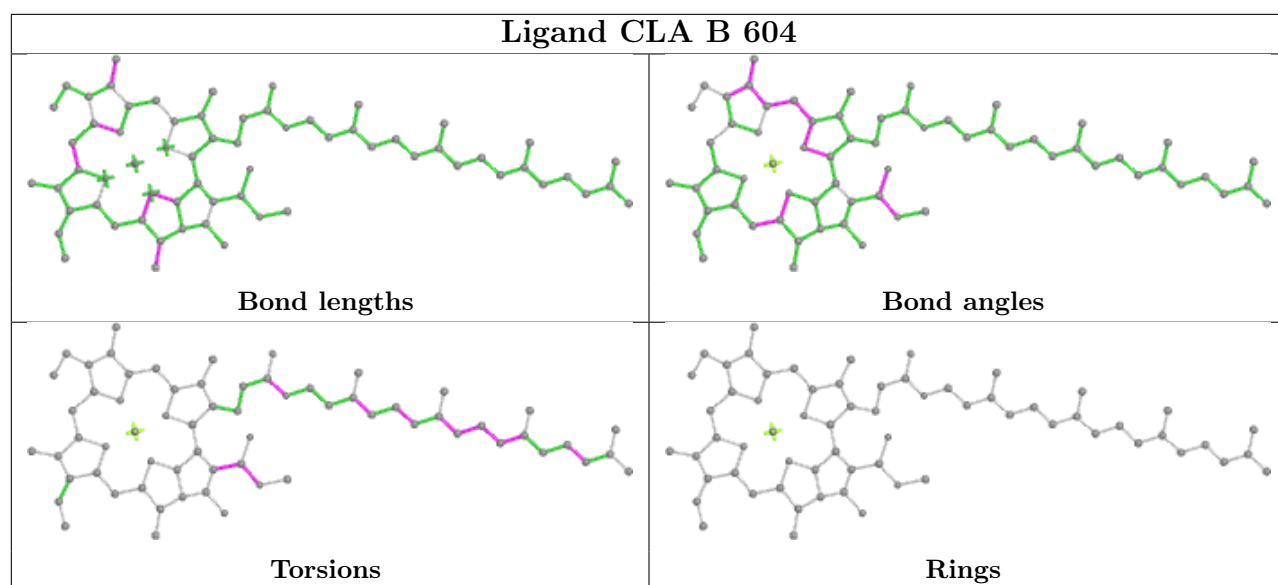


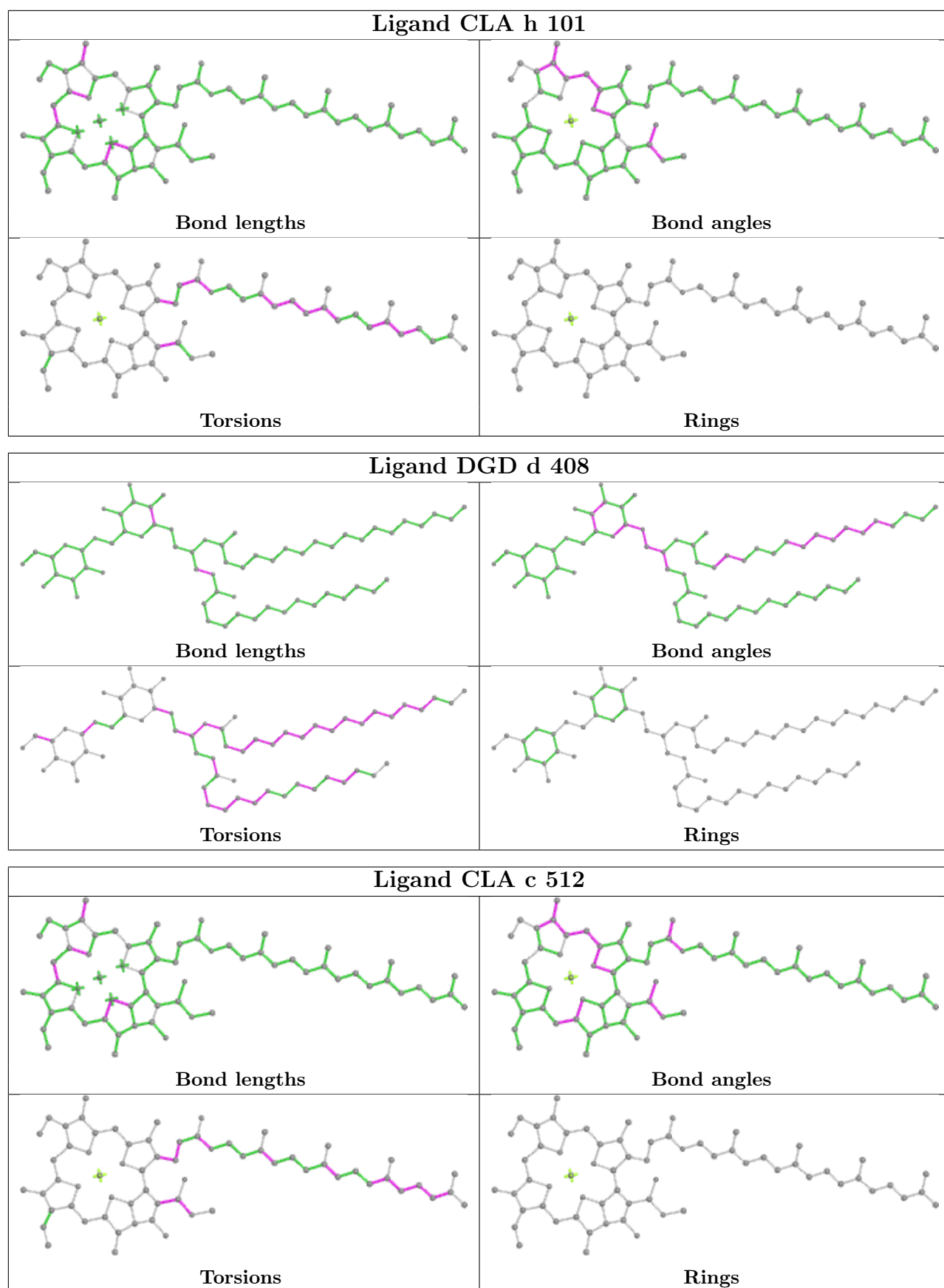


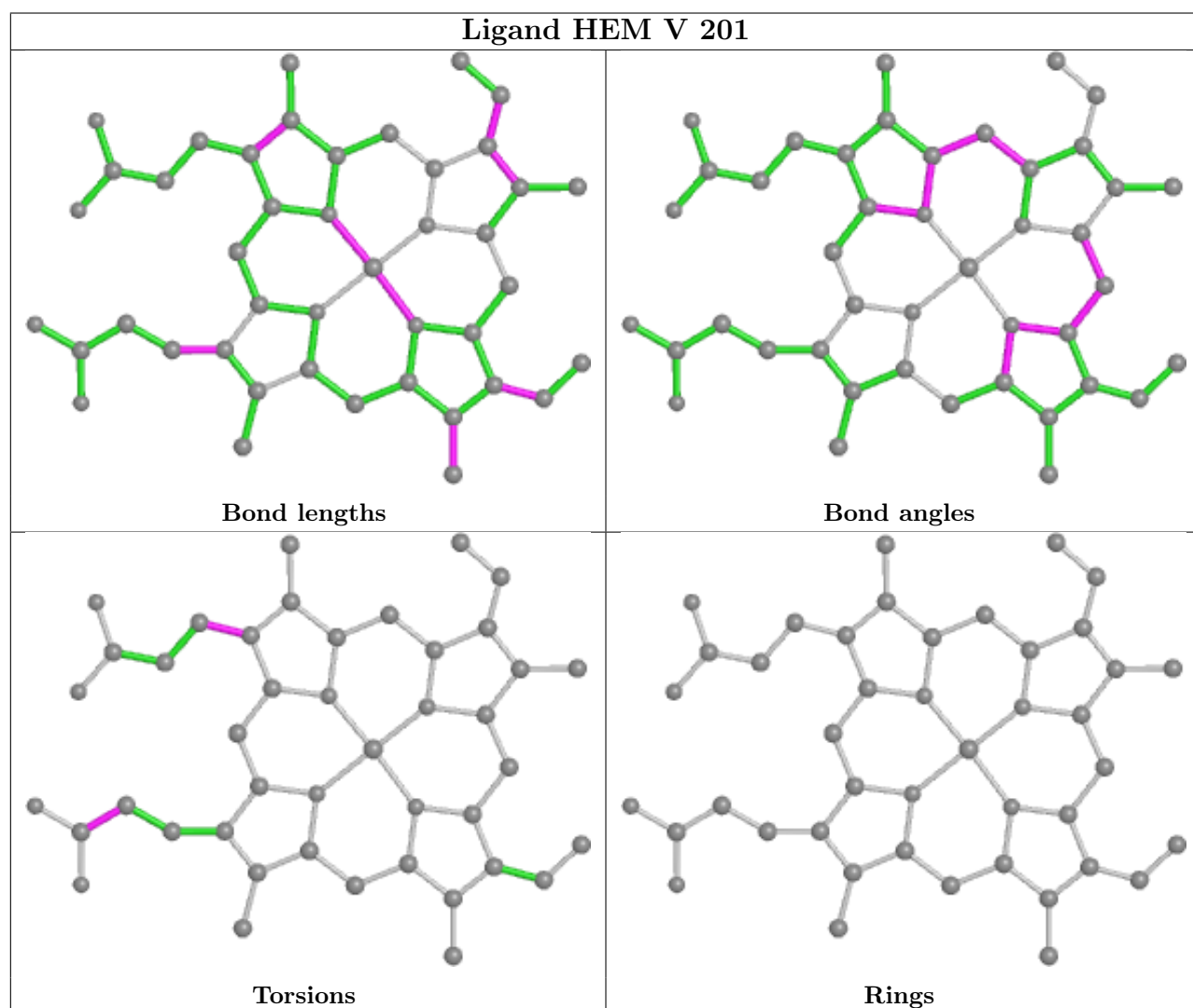
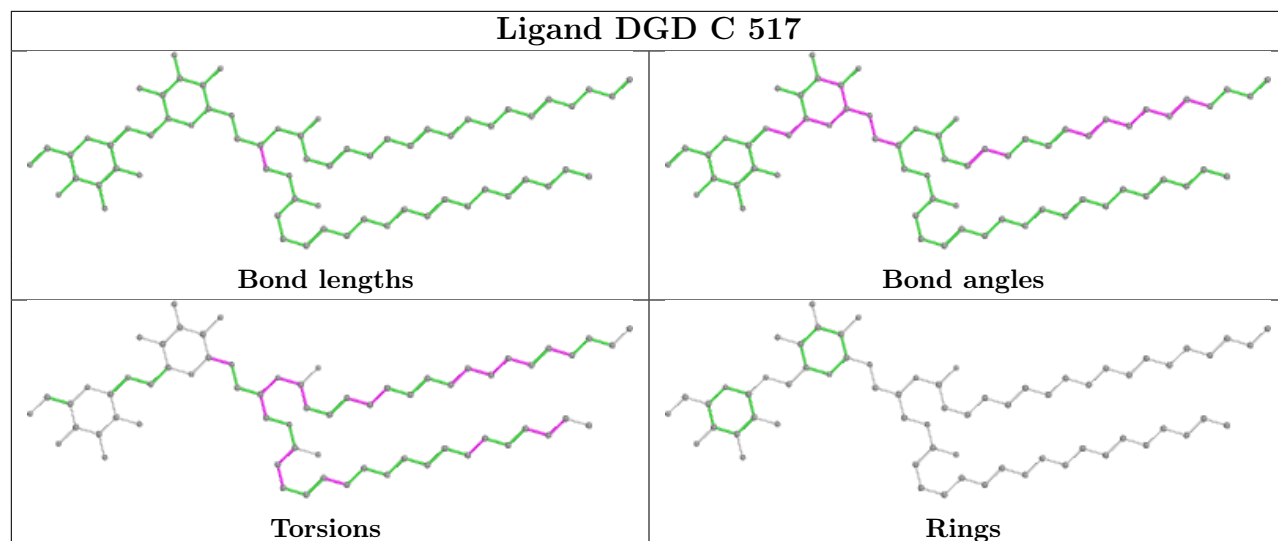


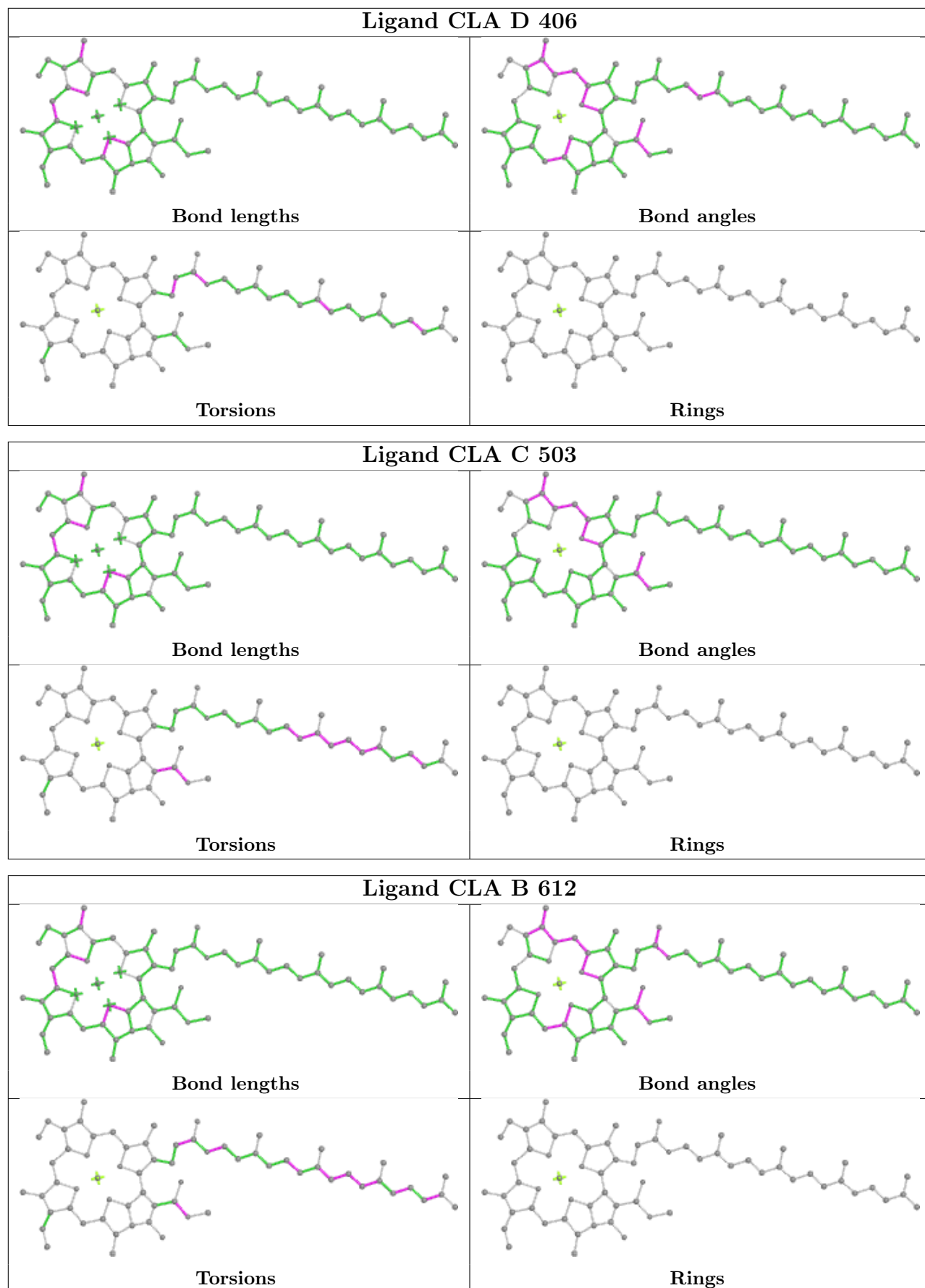


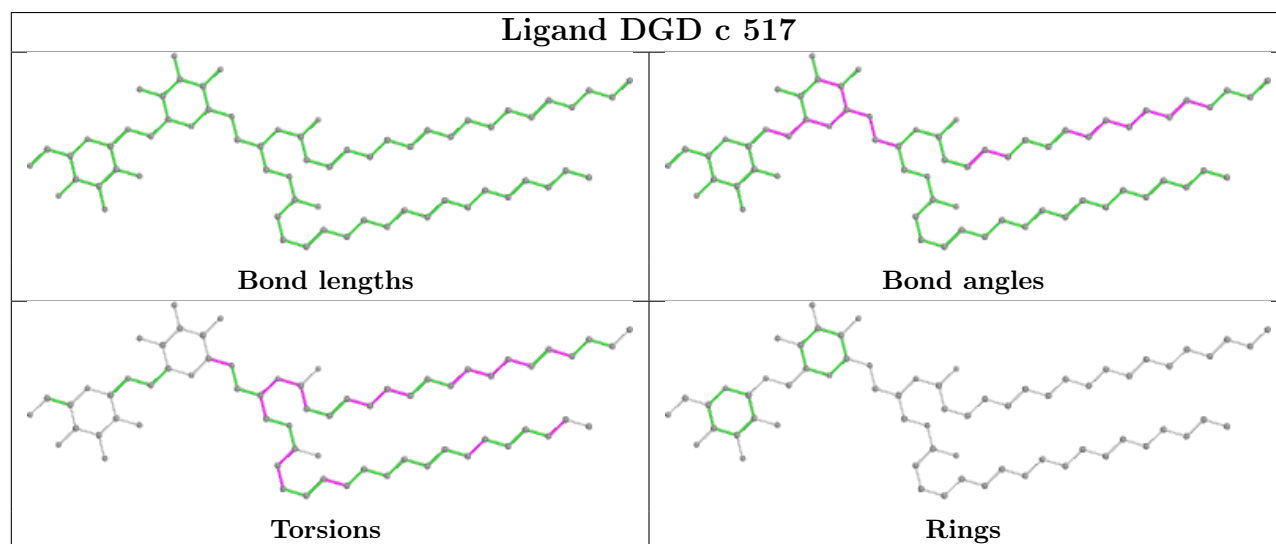
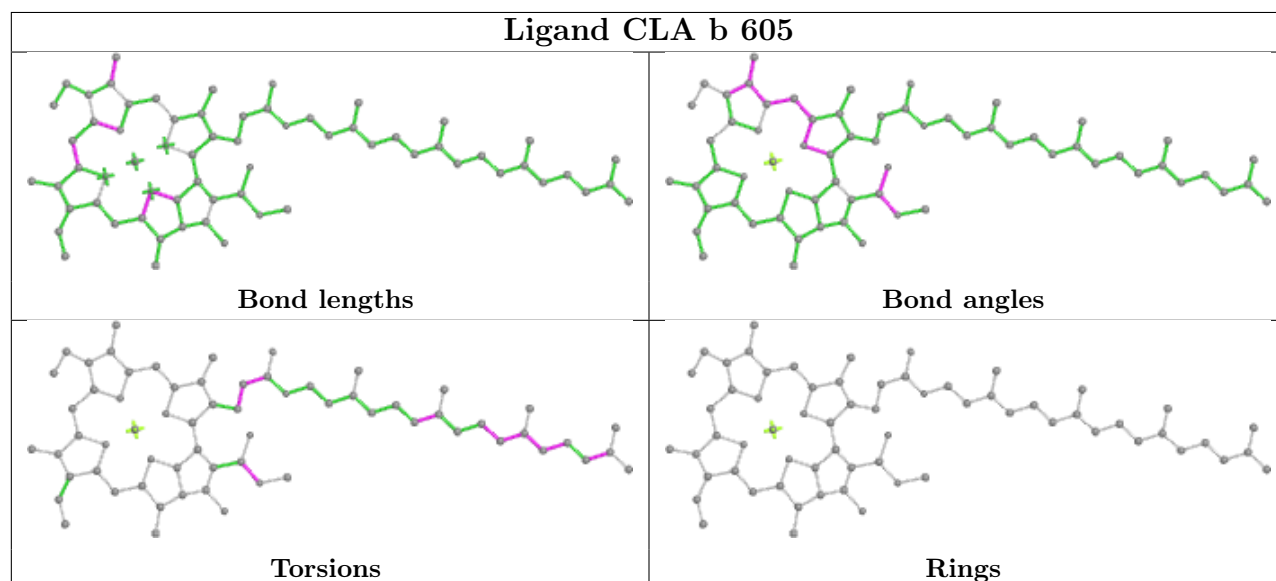
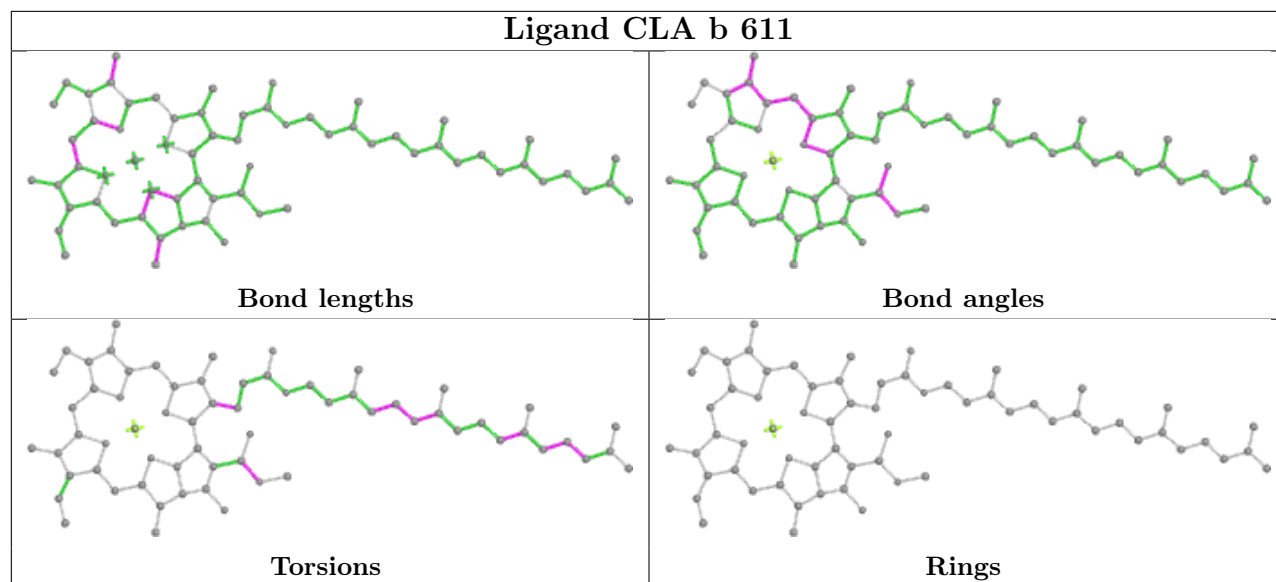


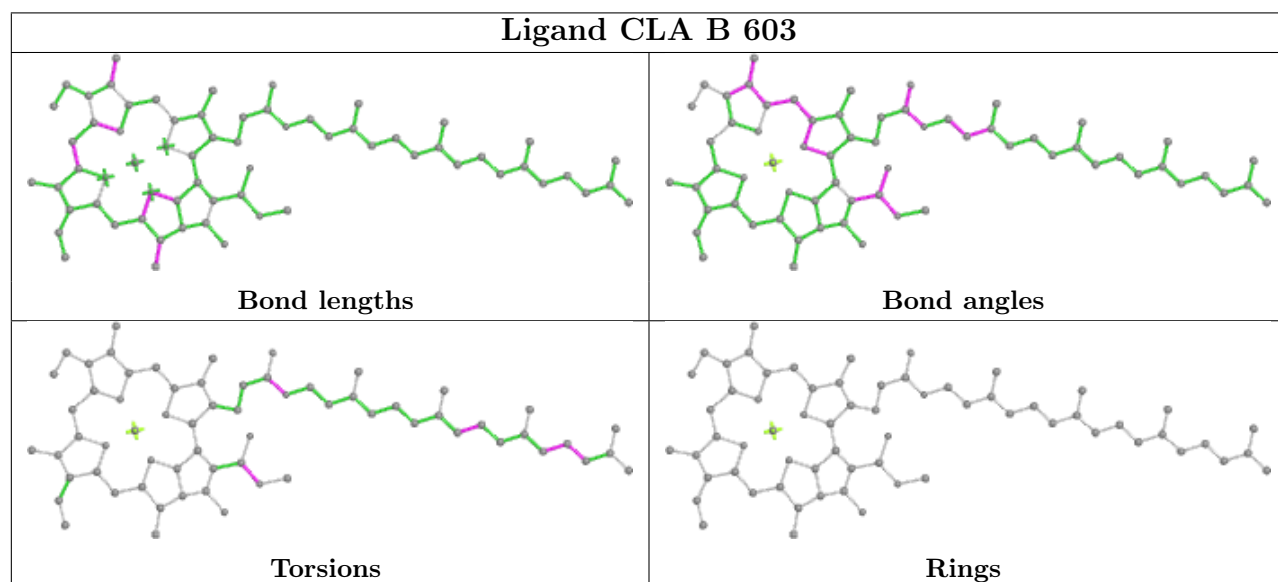
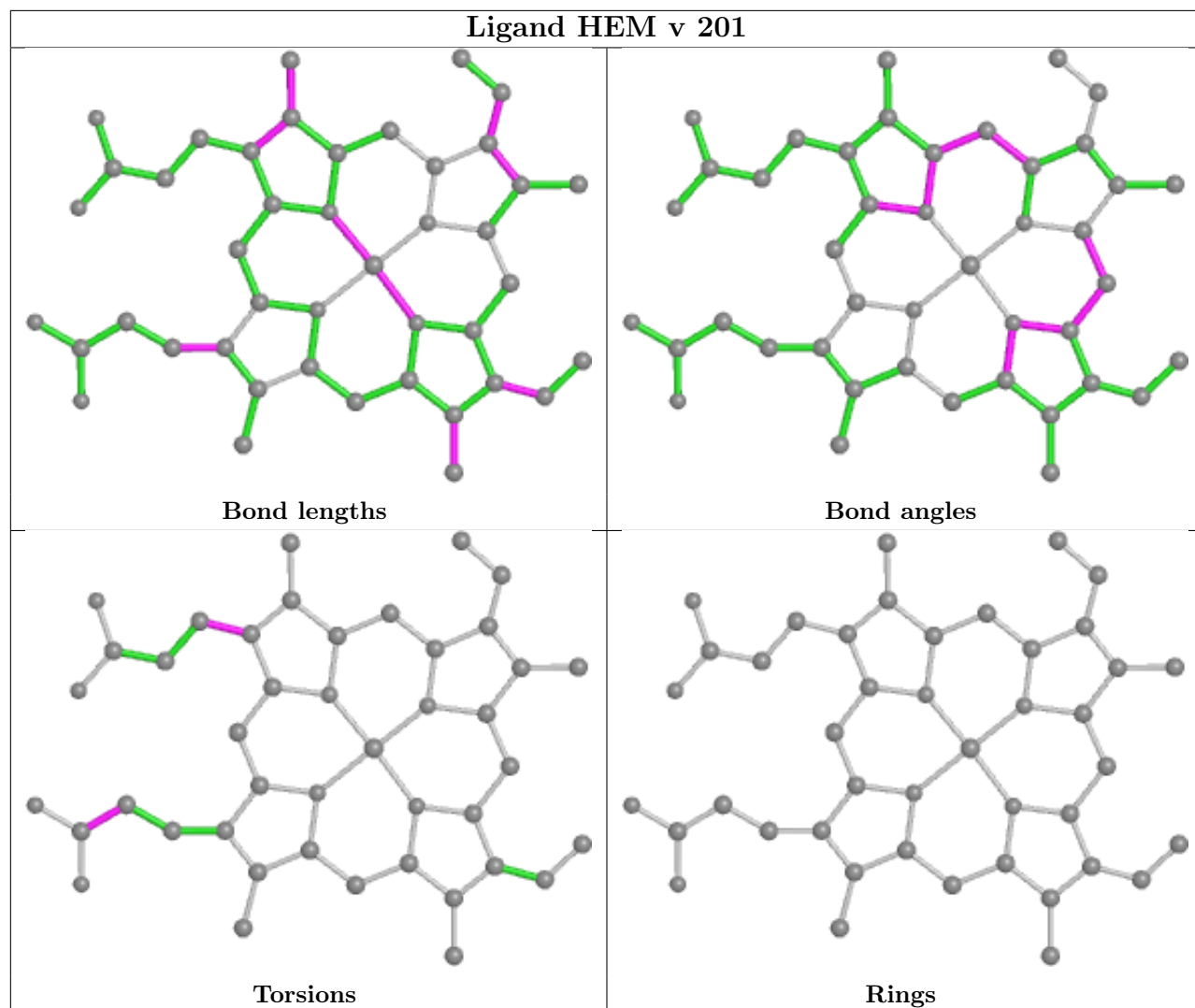




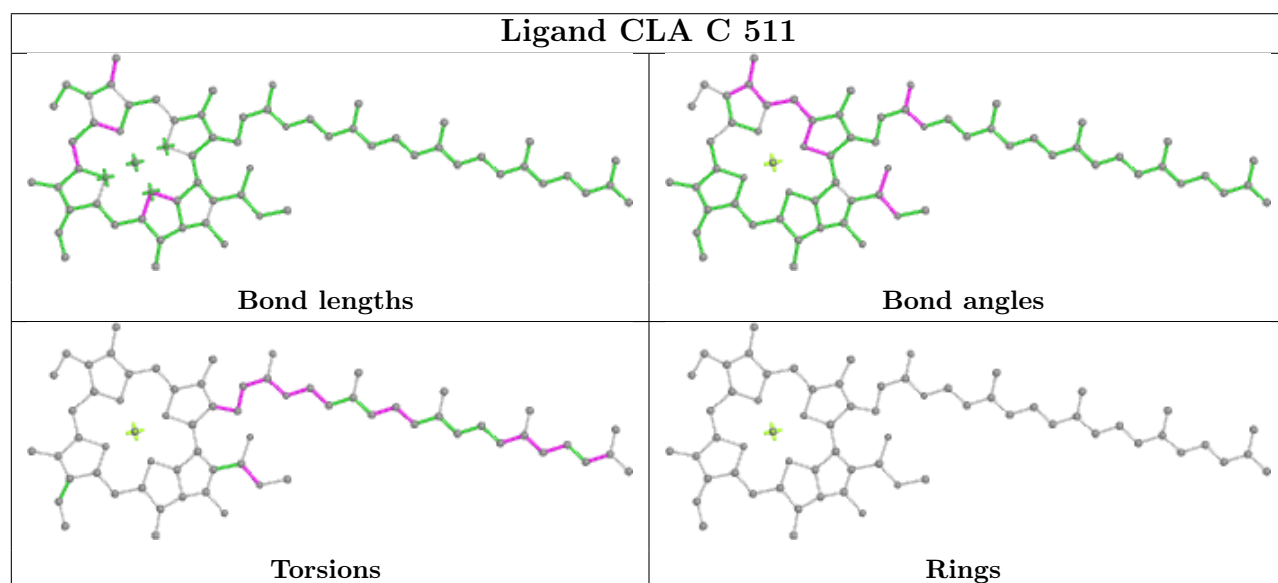
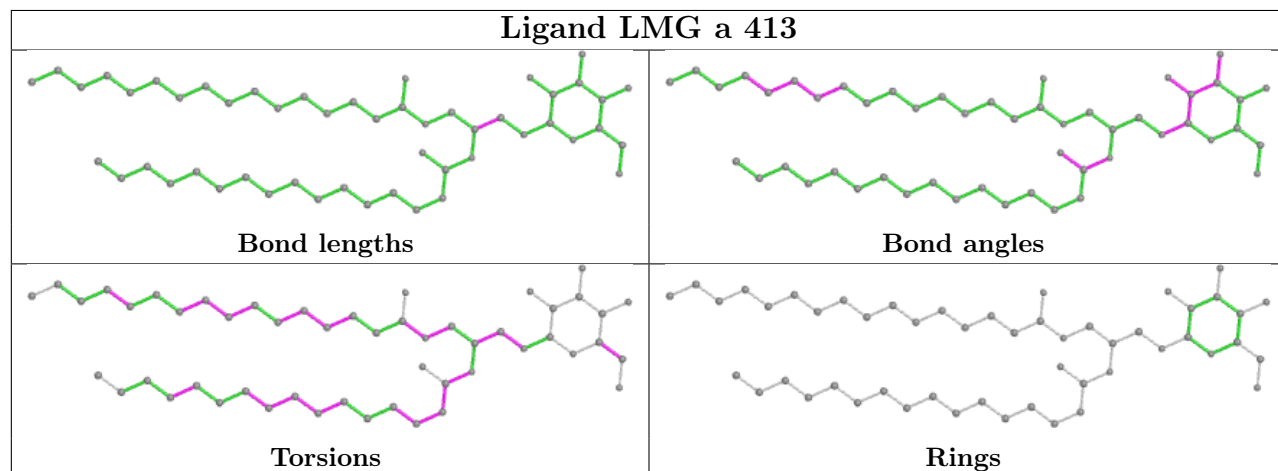
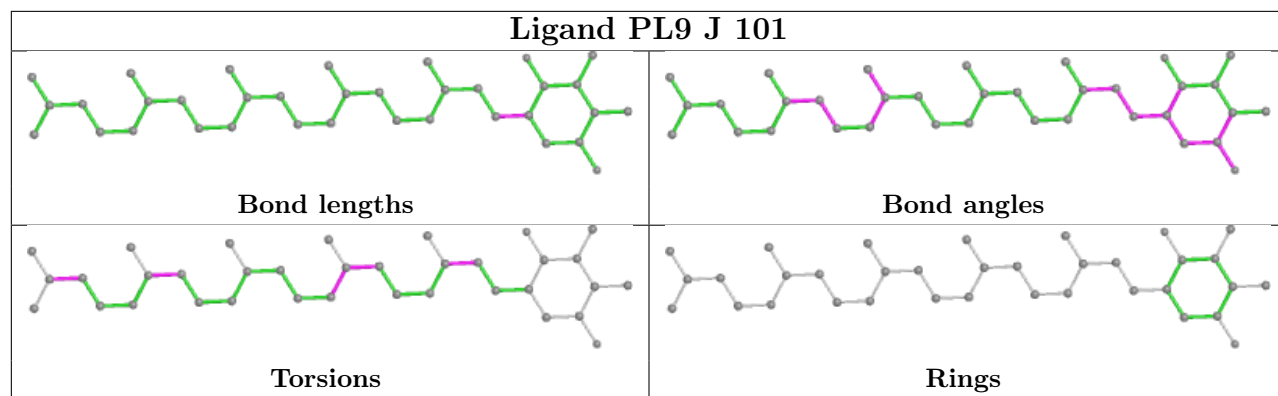


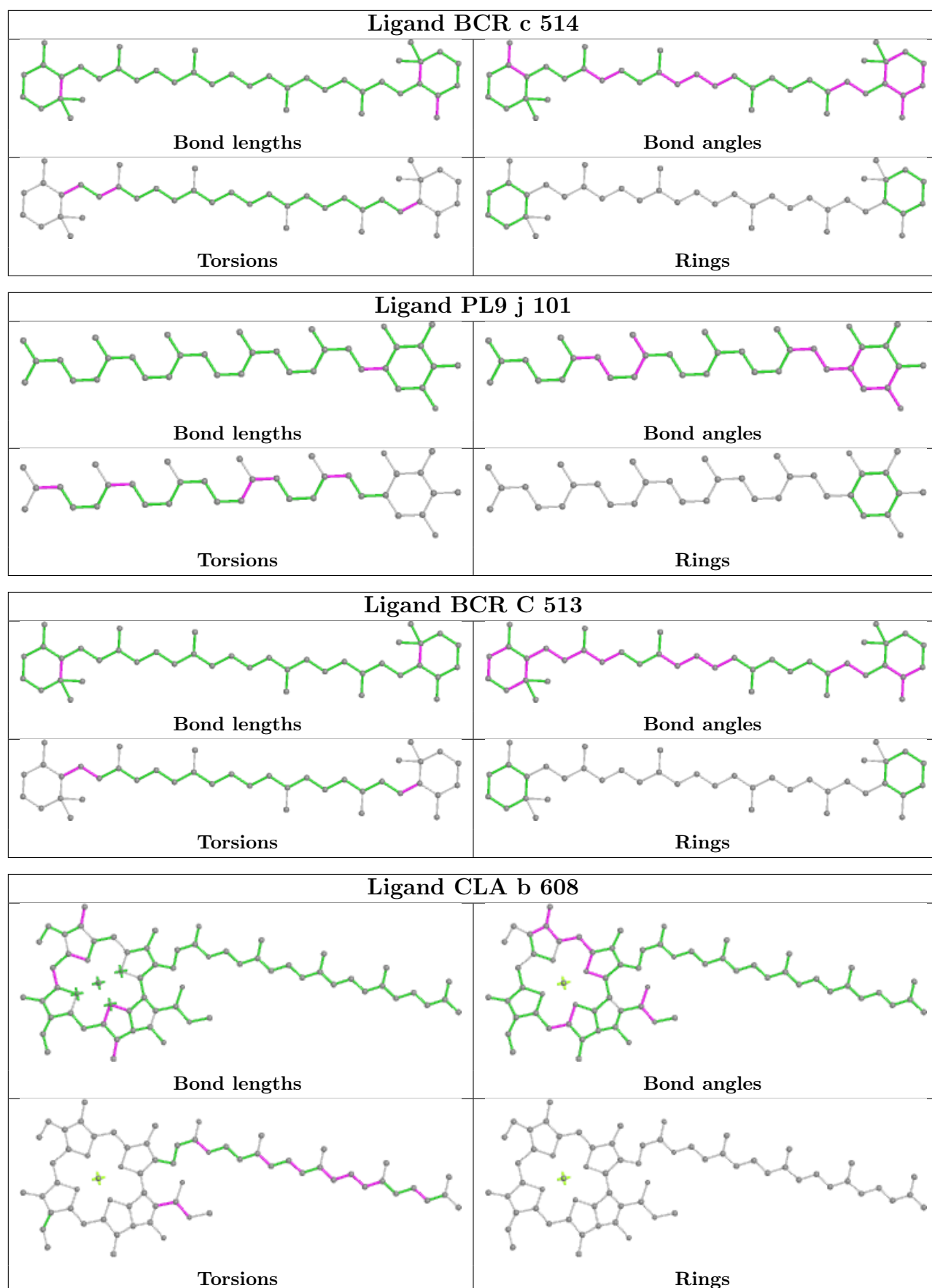


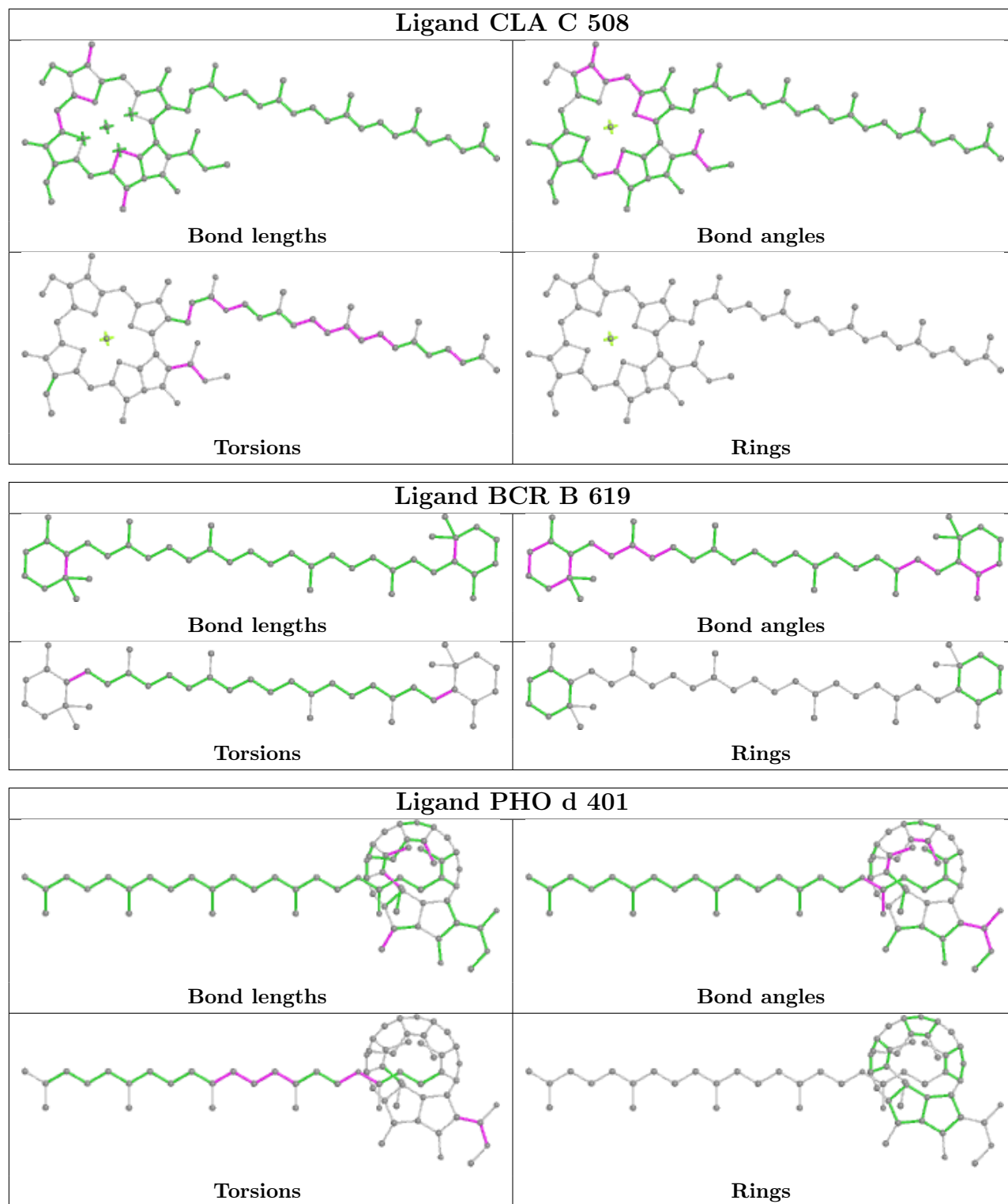


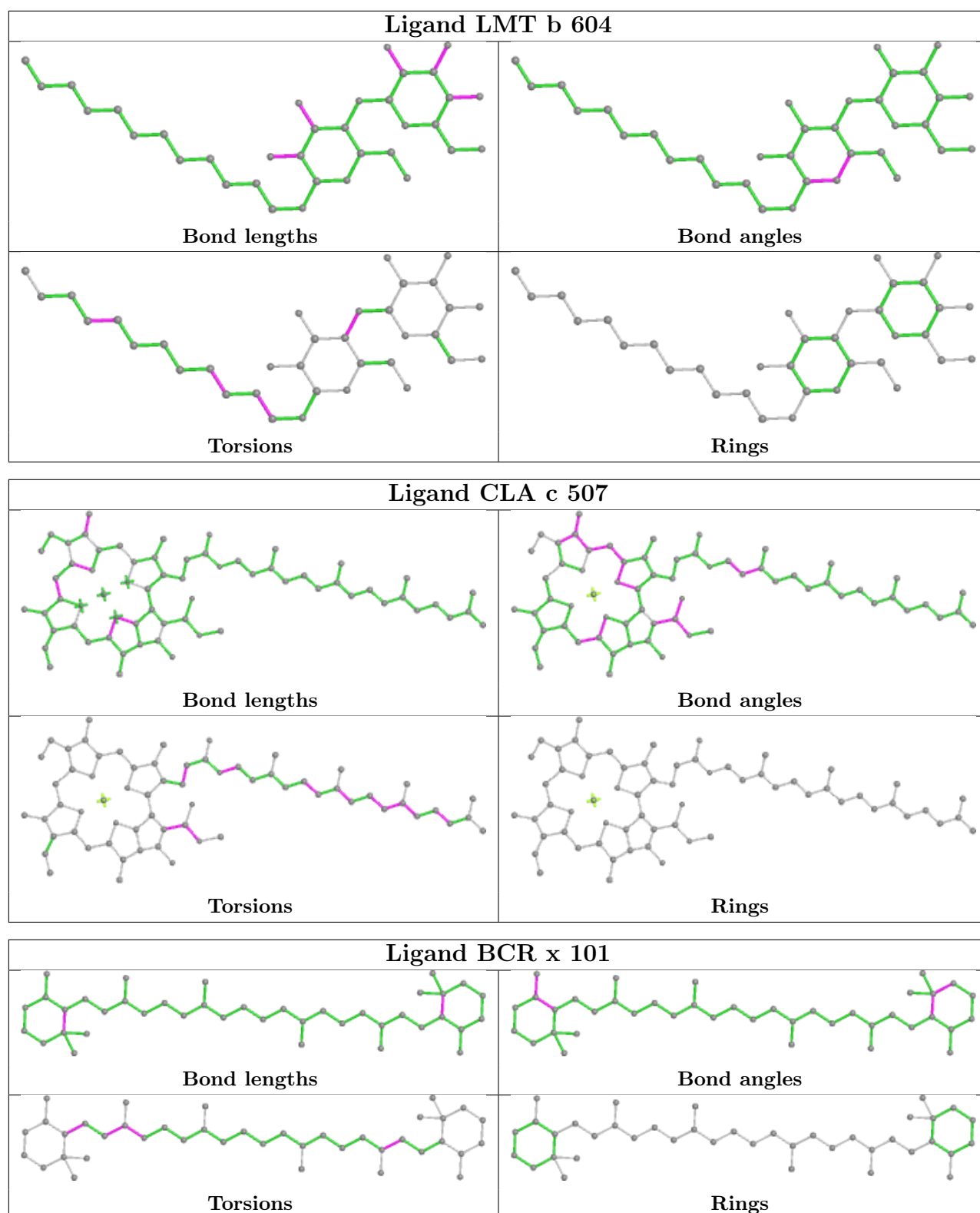


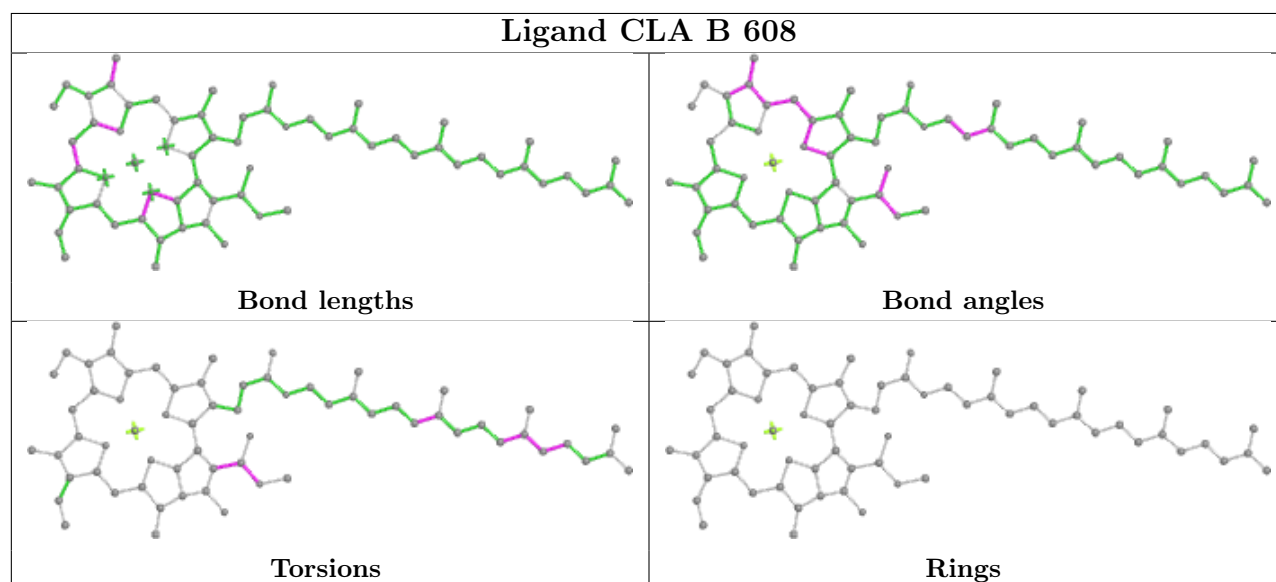
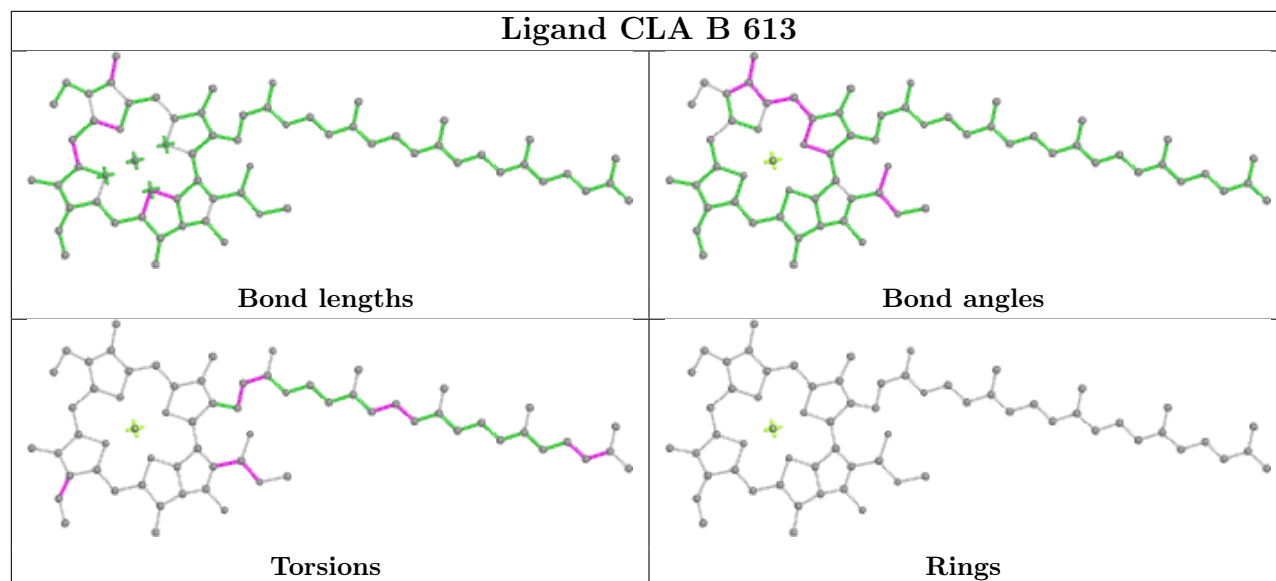
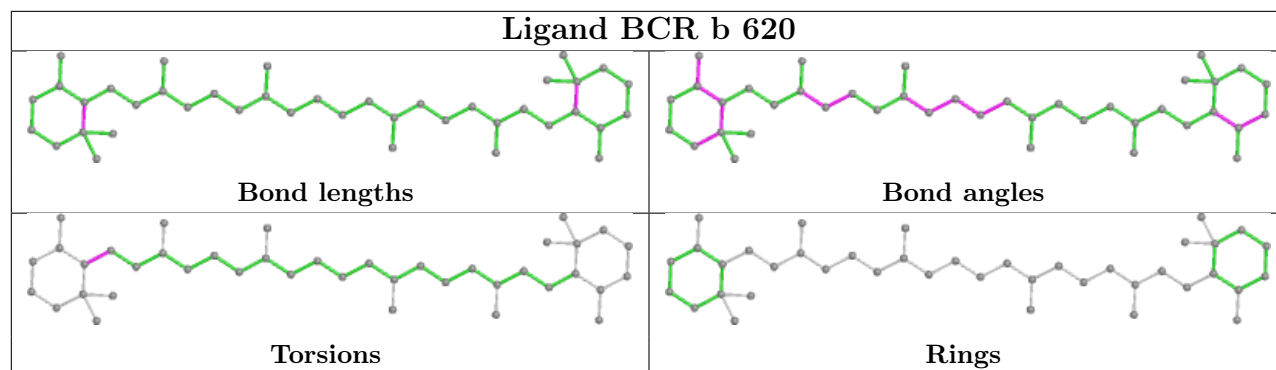


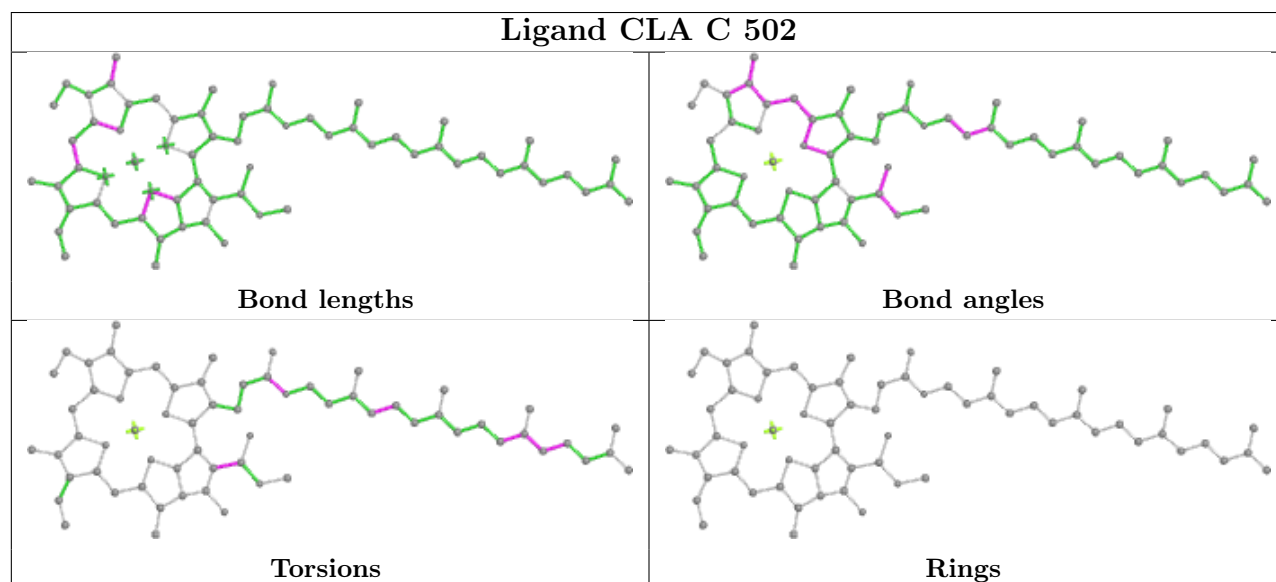
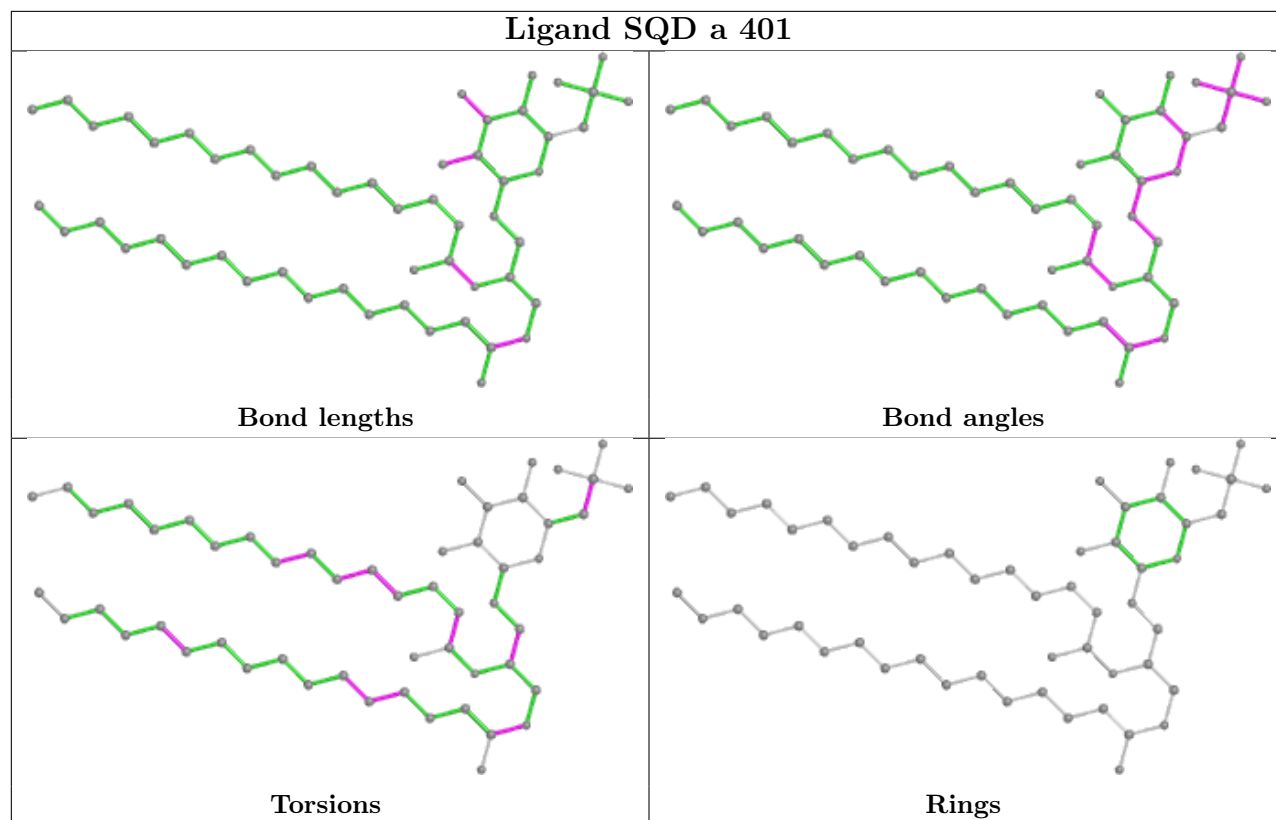


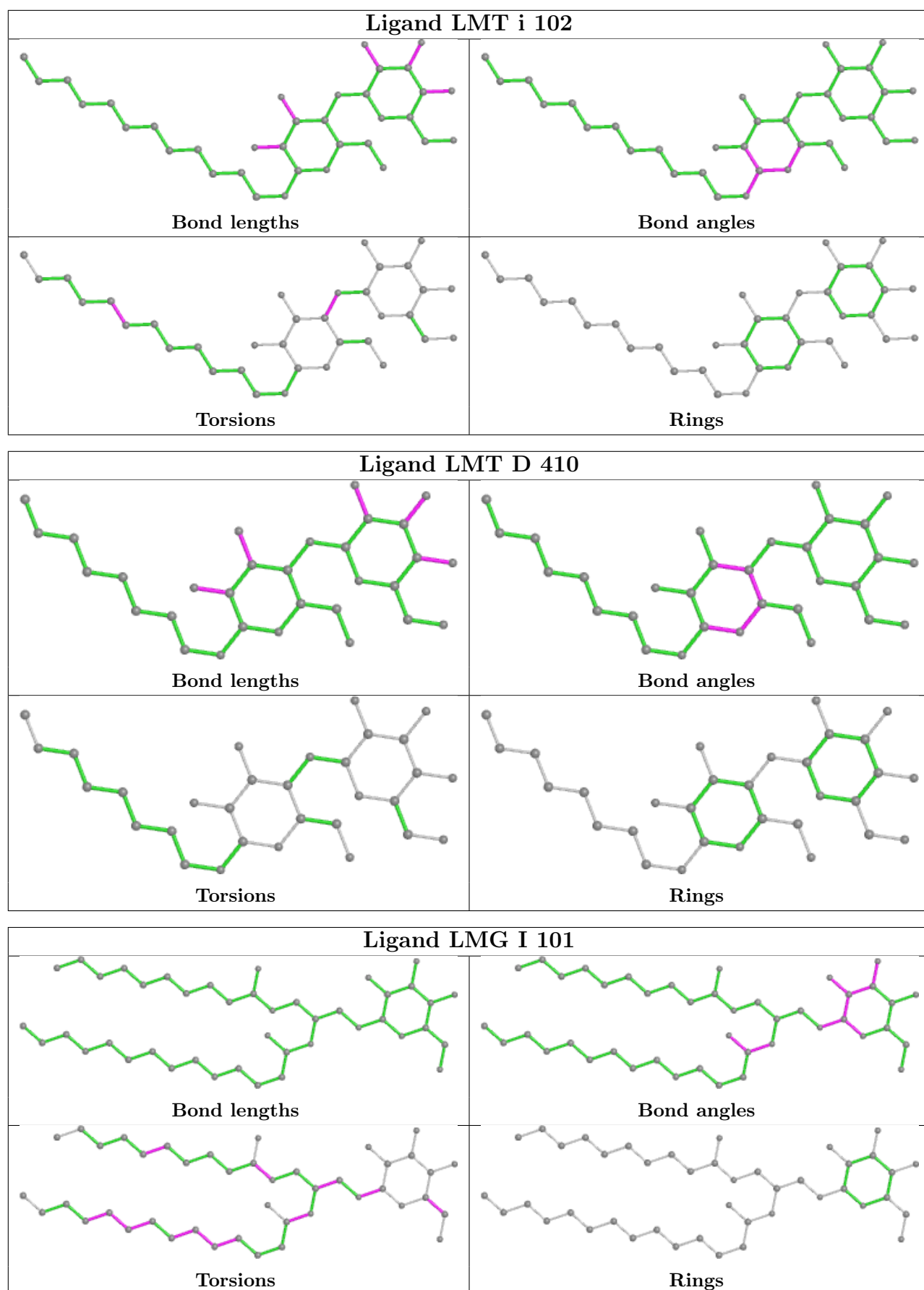


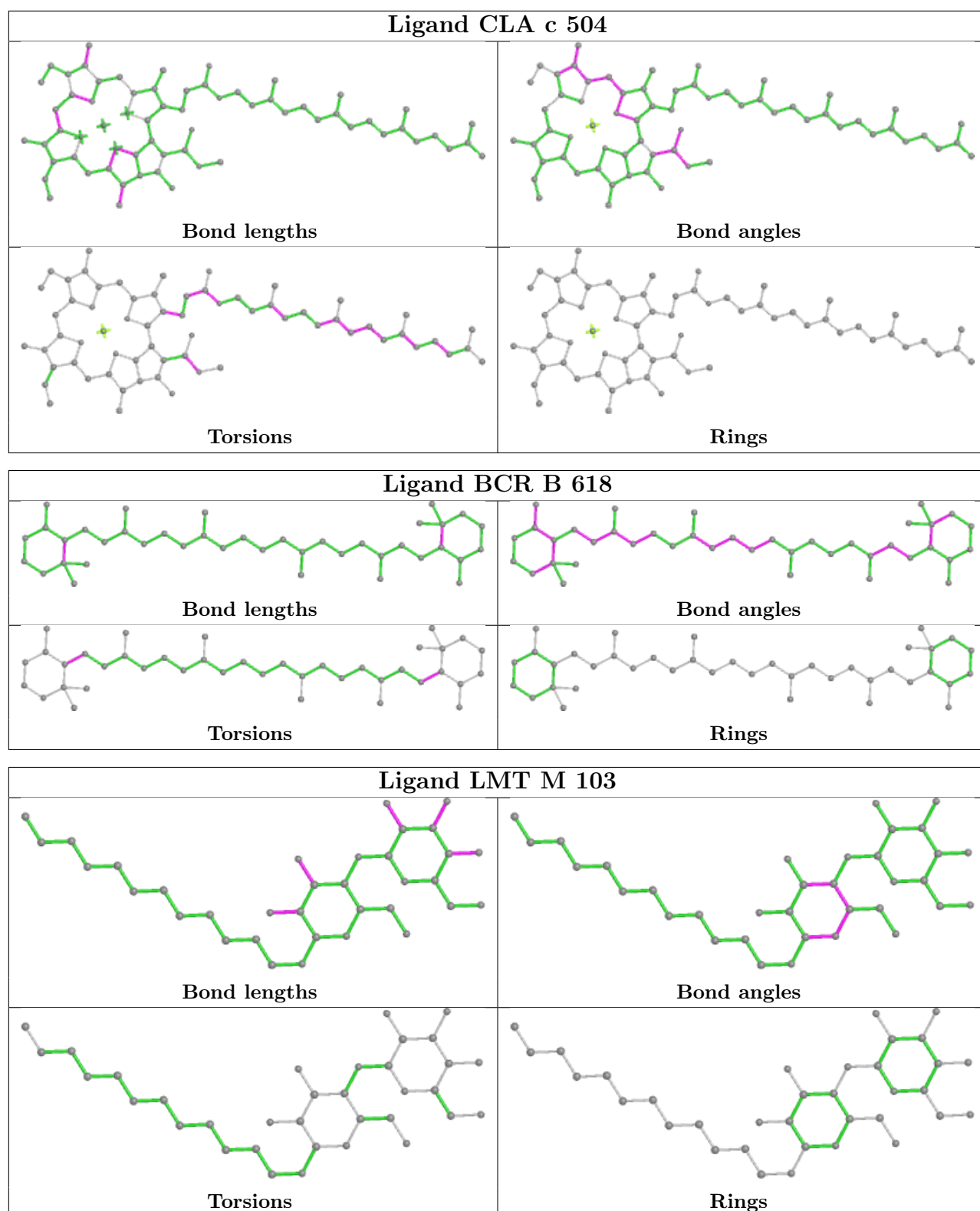




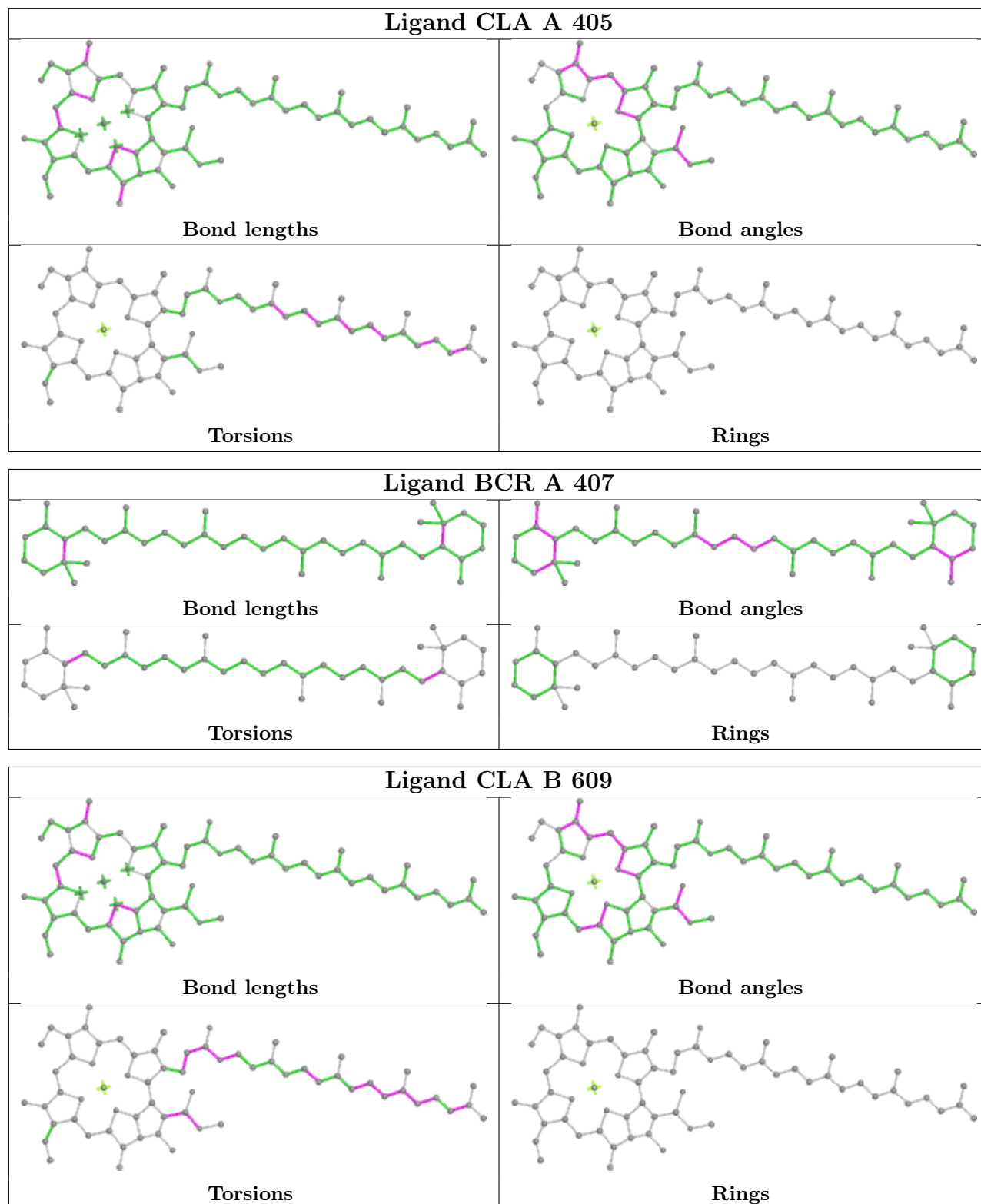


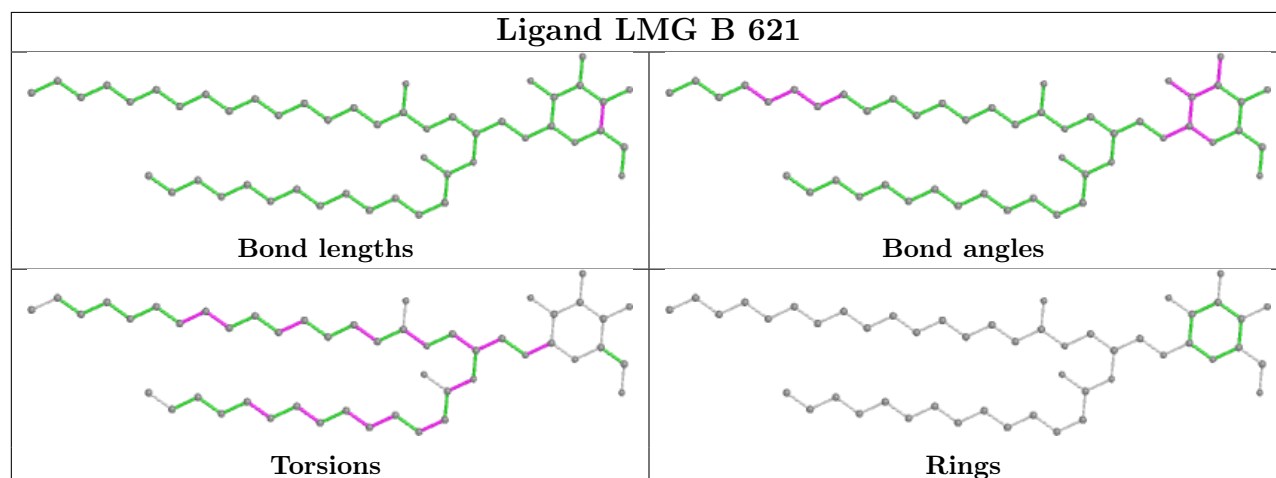
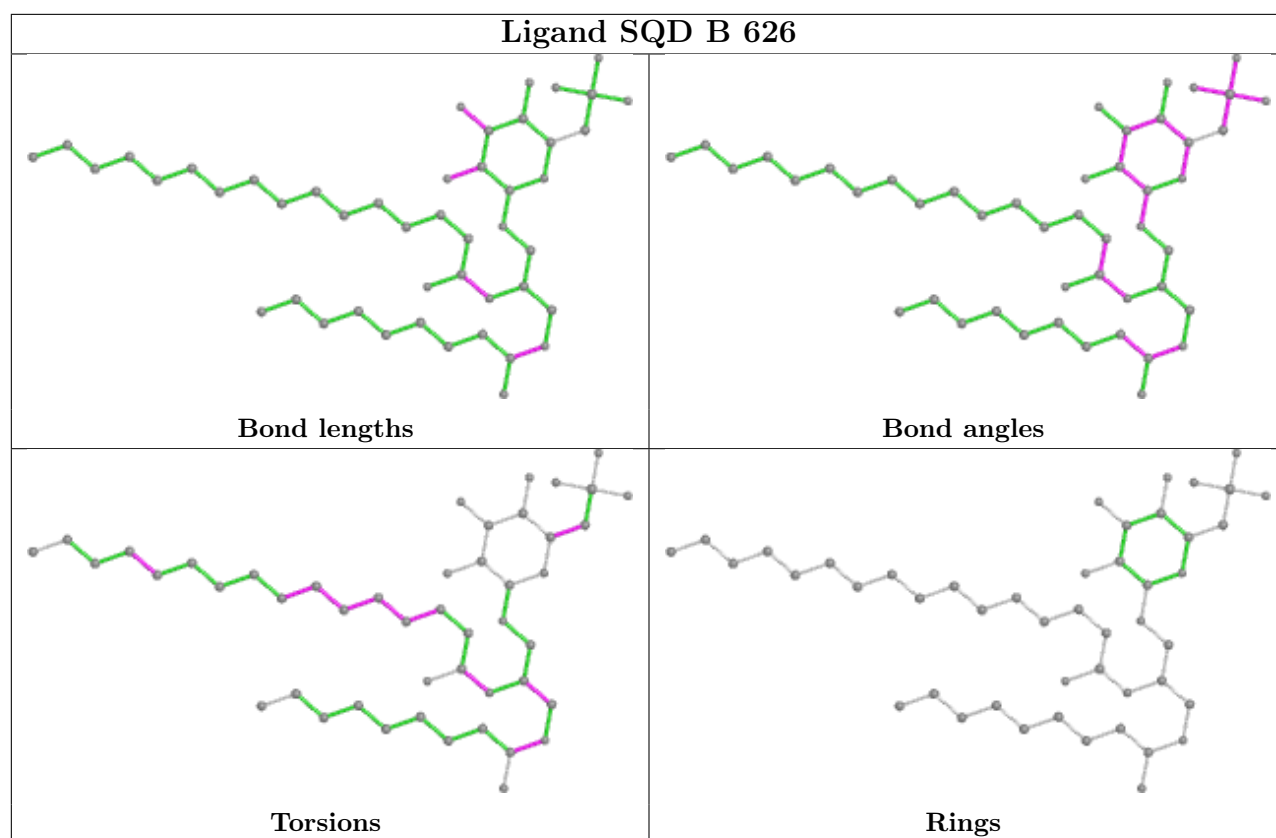


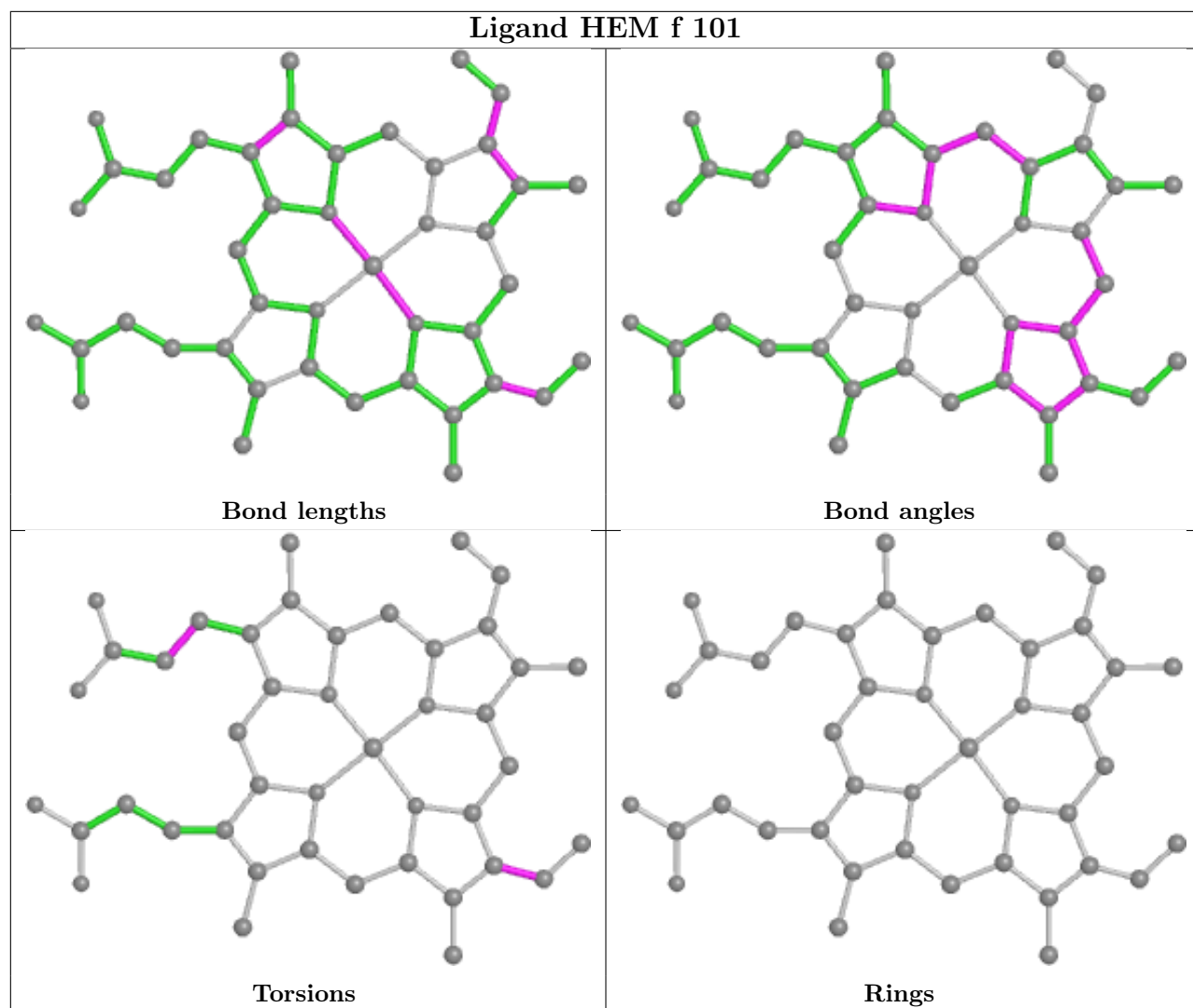
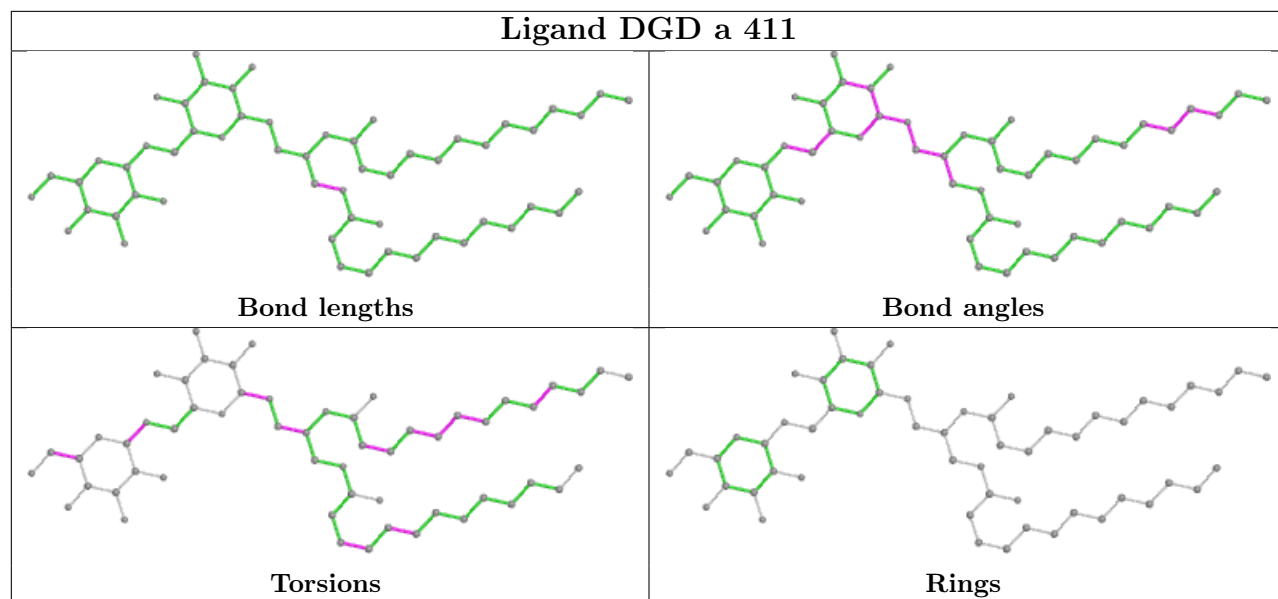


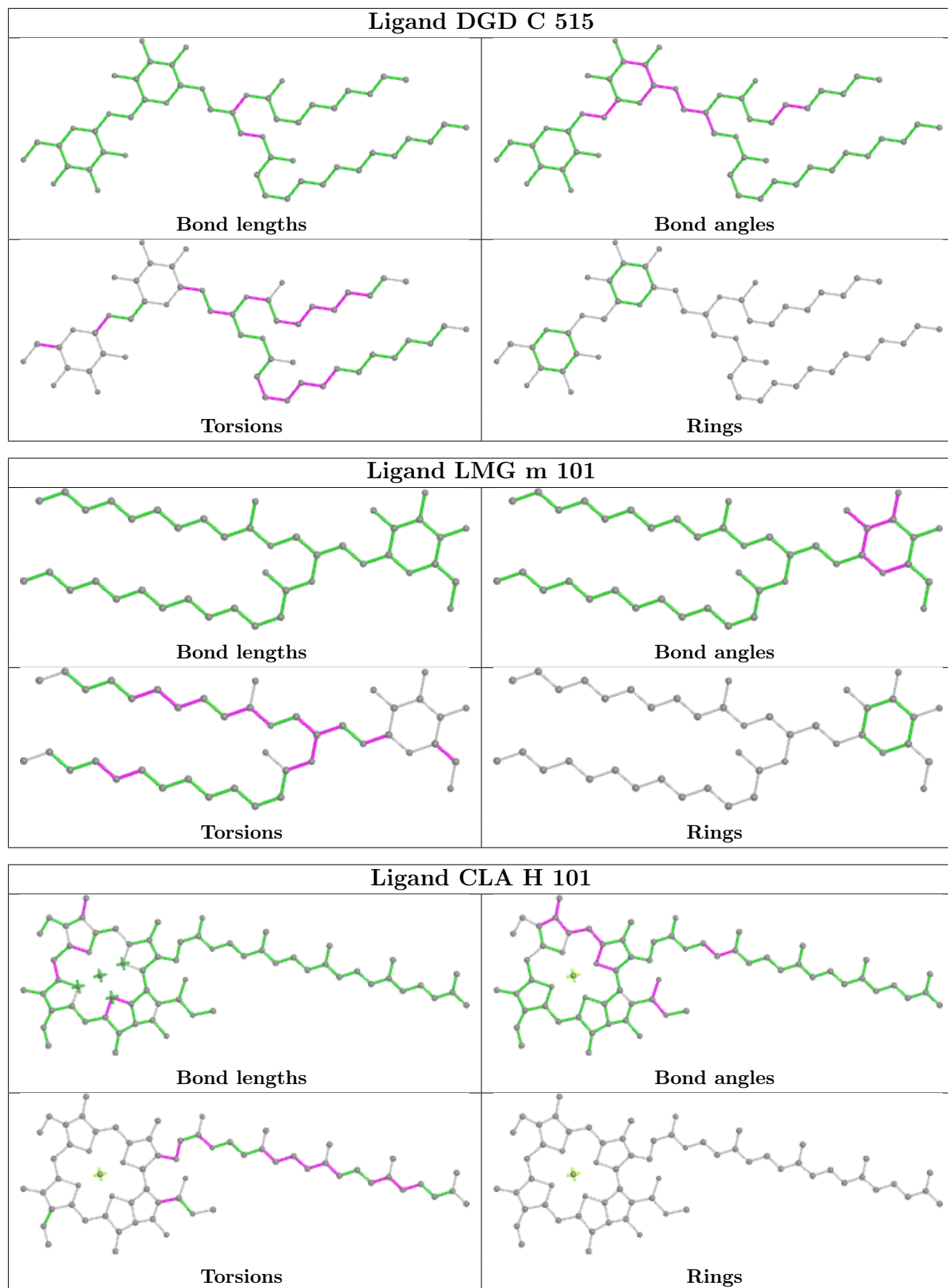


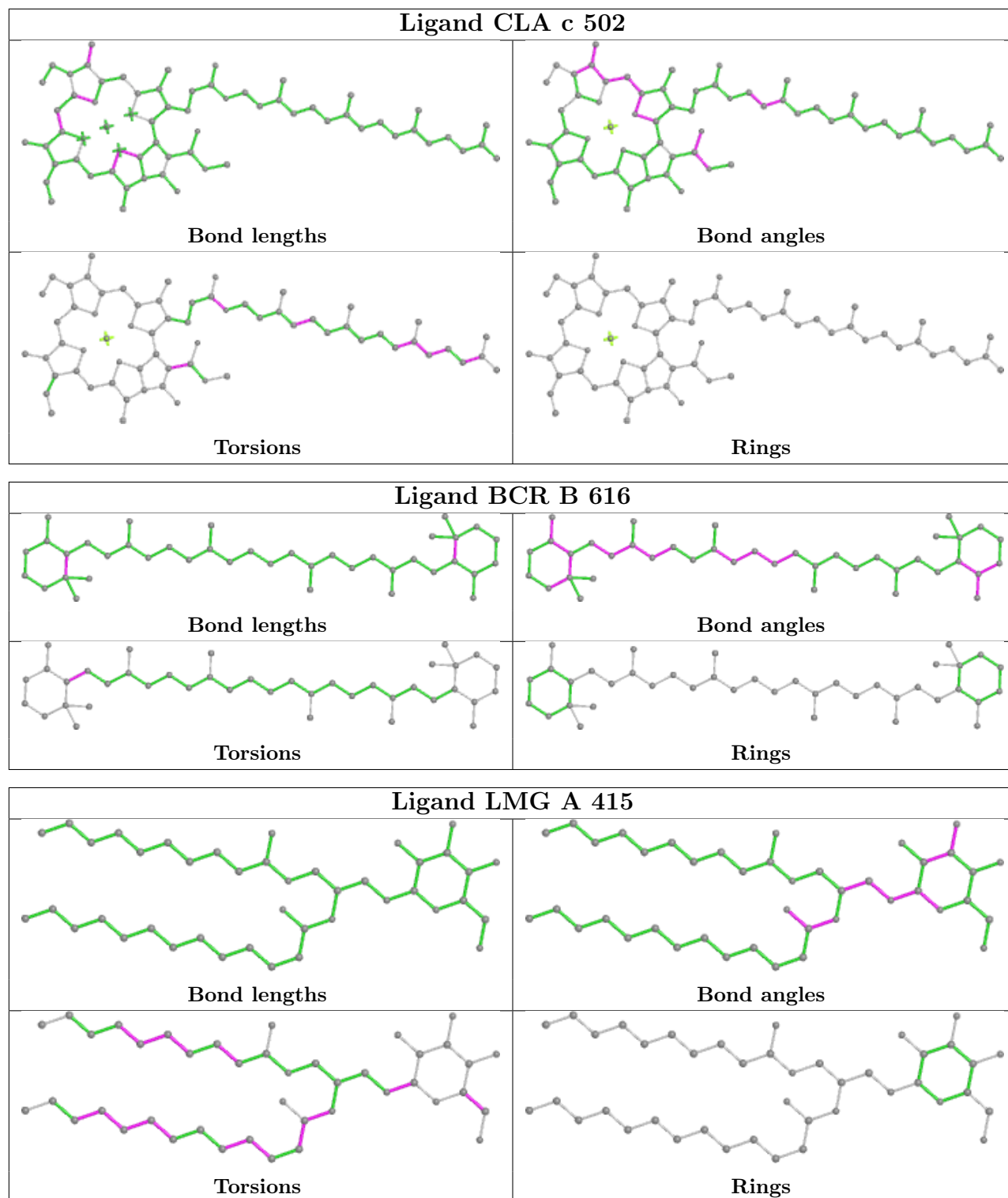


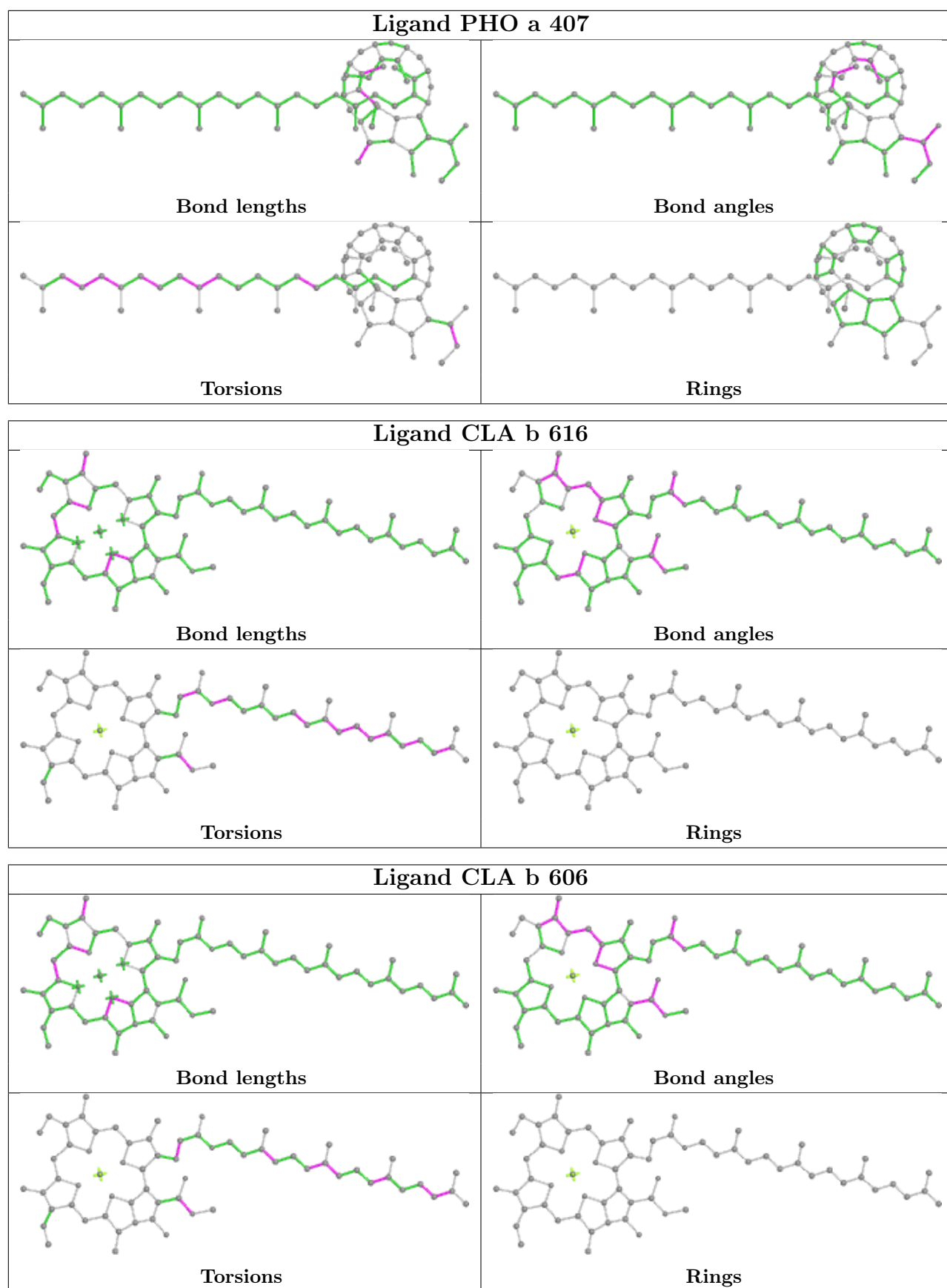


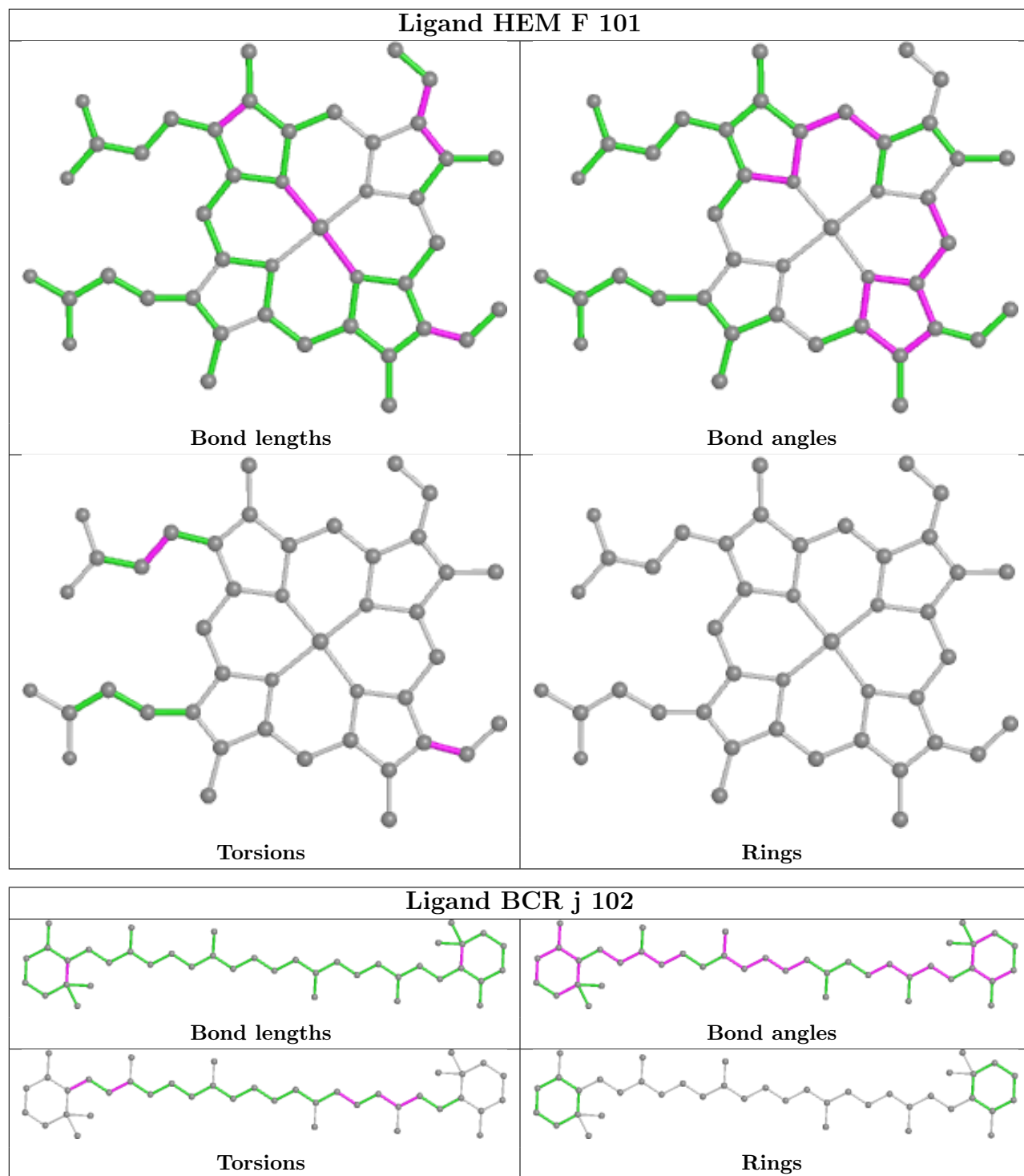


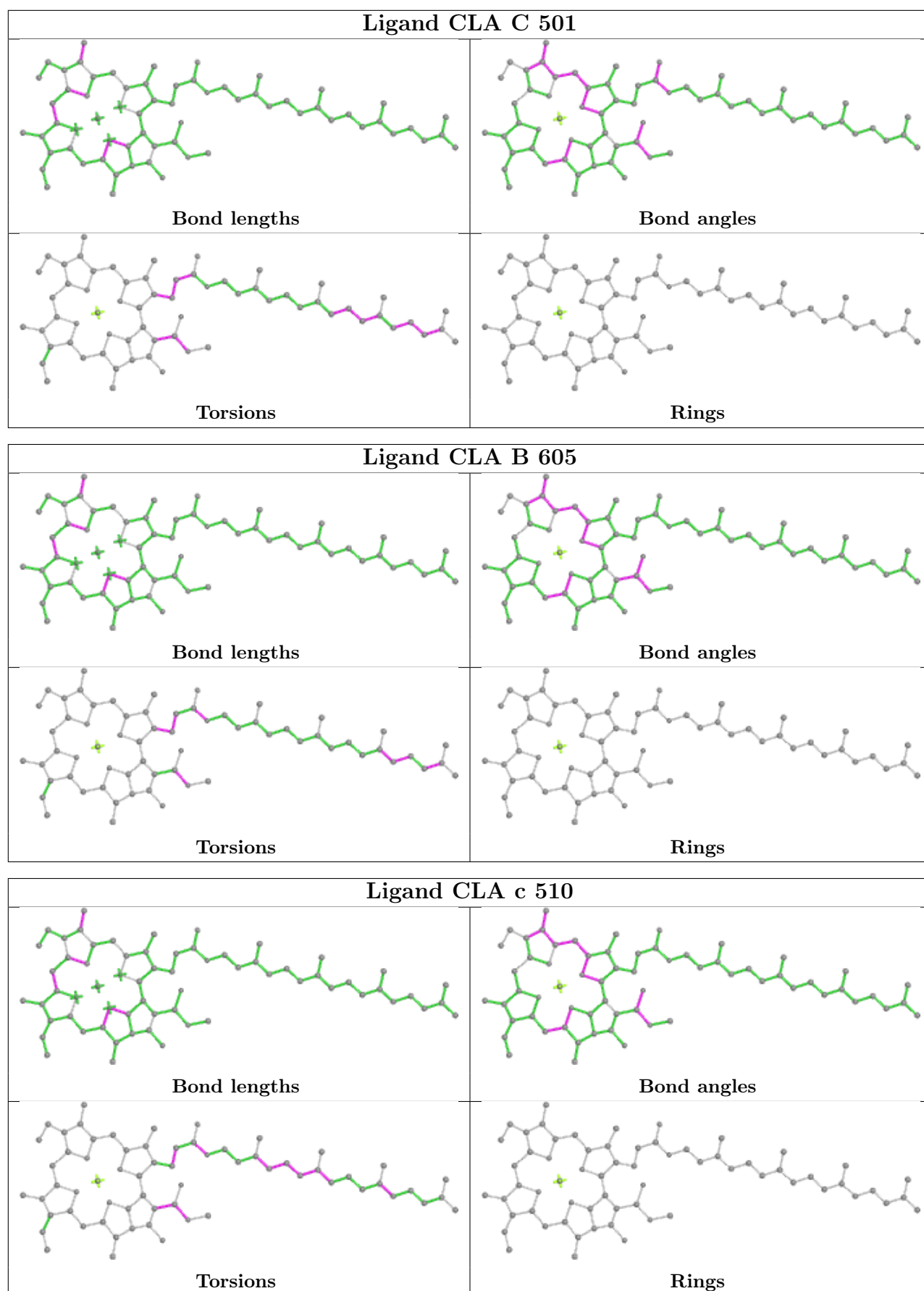














## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	335/344 (97%)	0.43	28 (8%) 11 10	172, 174, 175, 176	0
1	a	335/344 (97%)	0.45	28 (8%) 11 10	172, 174, 175, 176	0
2	B	490/510 (96%)	0.22	30 (6%) 21 17	172, 174, 175, 176	0
2	b	490/510 (96%)	0.27	19 (3%) 39 31	172, 174, 175, 176	0
3	C	447/461 (96%)	0.25	24 (5%) 25 22	172, 174, 175, 176	0
3	c	447/461 (96%)	0.13	16 (3%) 42 35	173, 174, 175, 176	0
4	D	340/352 (96%)	0.17	7 (2%) 63 54	171, 174, 175, 176	0
4	d	340/352 (96%)	0.17	11 (3%) 47 38	172, 174, 175, 175	0
5	E	82/84 (97%)	-0.07	1 (1%) 79 70	172, 174, 175, 175	0
5	e	82/84 (97%)	0.03	3 (3%) 41 33	173, 174, 175, 177	0
6	F	35/45 (77%)	-0.14	1 (2%) 51 41	173, 174, 175, 175	0
6	f	35/45 (77%)	-0.45	0 100 100	174, 174, 175, 176	0
7	H	65/66 (98%)	0.42	7 (10%) 5 6	173, 174, 175, 176	0
7	h	65/66 (98%)	0.71	9 (13%) 2 3	173, 174, 175, 176	0
8	I	35/38 (92%)	0.24	0 100 100	173, 174, 175, 176	0
8	i	35/38 (92%)	-0.12	0 100 100	173, 174, 175, 176	0
9	J	34/40 (85%)	-0.11	0 100 100	173, 174, 175, 175	0
9	j	34/40 (85%)	-0.43	0 100 100	173, 174, 175, 175	0
10	K	37/46 (80%)	-0.31	0 100 100	173, 174, 175, 175	0
10	k	37/46 (80%)	0.15	1 (2%) 54 45	174, 174, 175, 176	0
11	L	37/37 (100%)	0.35	1 (2%) 54 45	172, 174, 175, 175	0
11	l	37/37 (100%)	0.16	0 100 100	173, 174, 175, 176	0
12	M	34/36 (94%)	0.21	1 (2%) 51 41	172, 174, 174, 176	0
12	m	34/36 (94%)	0.11	2 (5%) 22 19	173, 173, 174, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	0.47	16 (6%) 18 15	172, 174, 175, 176	0
13	o	243/272 (89%)	0.47	13 (5%) 26 23	172, 174, 175, 176	0
14	T	32/32 (100%)	0.27	2 (6%) 20 16	173, 174, 176, 176	0
14	t	32/32 (100%)	0.34	3 (9%) 8 8	173, 174, 175, 176	0
15	U	97/134 (72%)	0.46	7 (7%) 15 13	172, 174, 174, 175	0
15	u	97/134 (72%)	0.63	9 (9%) 8 8	173, 174, 175, 175	0
16	V	137/163 (84%)	0.05	0 100 100	172, 174, 175, 175	0
16	v	137/163 (84%)	0.49	10 (7%) 15 12	173, 174, 175, 176	0
17	g	28/46 (60%)	0.32	1 (3%) 42 35	174, 175, 176, 176	0
17	y	28/46 (60%)	-0.06	0 100 100	173, 174, 176, 176	0
18	X	37/41 (90%)	0.31	1 (2%) 54 45	173, 174, 175, 176	0
18	x	37/41 (90%)	0.84	7 (18%) 1 2	173, 174, 175, 175	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.26	1 (1%) 72 62	173, 174, 175, 176	0
20	z	62/62 (100%)	0.88	5 (8%) 12 11	173, 175, 176, 176	0
All	All	5214/5674 (91%)	0.27	264 (5%) 28 24	171, 174, 175, 177	0

The worst 5 of 264 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.6
1	a	224	ILE	5.2
5	e	84	LYS	5.0
15	U	38	GLU	4.9
3	C	135	ARG	4.6

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
35	CA	o	301	1/1	0.32	0.68	180,180,180,180	0
31	LMT	I	102	35/35	0.40	0.94	173,175,176,178	0
23	PL9	J	101	35/55	0.43	0.54	172,175,176,176	0
23	PL9	j	101	35/55	0.49	0.37	173,175,175,176	0
24	BCR	J	102	40/40	0.50	0.44	172,174,176,177	0
31	LMT	i	102	35/35	0.52	1.29	173,175,176,177	0
35	CA	O	301	1/1	0.53	0.38	177,177,177,177	0
31	LMT	d	409	31/35	0.53	0.66	172,175,177,177	0
31	LMT	b	627	35/35	0.54	1.22	173,175,177,177	0
31	LMT	b	626	35/35	0.59	0.69	172,175,176,177	0
22	CLA	b	605	65/65	0.61	1.14	172,175,176,176	0
27	LMG	A	415	42/55	0.62	0.53	171,174,176,177	0
27	LMG	C	518	45/55	0.62	1.09	171,174,175,175	0
22	CLA	B	601	65/65	0.62	0.85	172,175,176,177	0
24	BCR	j	102	40/40	0.63	0.34	173,175,177,178	0
27	LMG	E	101	44/55	0.63	0.56	170,174,176,177	0
24	BCR	f	102	40/40	0.63	0.47	171,173,175,175	0
31	LMT	D	410	31/35	0.64	0.93	174,175,176,176	0
24	BCR	g	101	40/40	0.64	0.78	173,174,175,175	0
27	LMG	a	402	42/55	0.65	0.49	171,174,176,176	0
26	LHG	C	519	37/49	0.65	0.48	172,174,179,183	0
22	CLA	b	619	65/65	0.65	0.77	172,174,175,175	0
25	DGD	d	408	63/66	0.66	0.77	172,175,177,178	0
27	LMG	I	101	43/55	0.66	1.04	172,174,177,177	0
22	CLA	c	502	65/65	0.66	0.54	173,174,175,175	0
31	LMT	B	628	35/35	0.66	0.46	172,174,177,178	0
24	BCR	D	411	40/40	0.67	0.44	171,173,174,175	0
24	BCR	c	514	40/40	0.67	0.71	172,173,175,175	0
31	LMT	B	622	35/35	0.67	0.88	171,175,177,177	0
23	PL9	D	407	55/55	0.68	0.39	171,173,174,175	0
23	PL9	d	406	55/55	0.68	0.39	172,173,175,175	0
24	BCR	H	102	40/40	0.69	0.94	173,174,175,176	0
27	LMG	a	413	51/55	0.69	0.42	172,173,175,176	0
23	PL9	A	406	45/55	0.69	0.43	172,174,175,175	0
22	CLA	C	502	65/65	0.70	0.53	173,174,174,175	0
25	DGD	D	409	63/66	0.70	0.81	172,174,176,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	LMT	b	604	35/35	0.70	0.47	172,174,176,176	0
27	LMG	c	518	45/55	0.71	1.01	172,174,176,176	0
25	DGD	A	408	56/66	0.71	0.45	172,174,175,176	0
24	BCR	x	101	40/40	0.71	0.86	173,174,175,175	0
32	PHO	d	401	64/64	0.72	0.42	172,173,174,174	0
24	BCR	B	616	40/40	0.72	0.43	172,173,174,175	0
25	DGD	b	601	52/66	0.72	0.47	172,174,176,177	0
25	DGD	a	411	56/66	0.73	0.44	173,174,175,176	0
24	BCR	a	410	40/40	0.73	0.68	172,173,174,175	0
30	SQD	A	413	51/54	0.73	0.37	172,174,175,176	0
27	LMG	M	101	42/55	0.73	0.53	173,174,176,176	0
27	LMG	C	522	48/55	0.73	0.36	172,174,174,175	0
22	CLA	a	408	65/65	0.74	0.82	173,174,175,175	0
27	LMG	i	101	43/55	0.74	0.80	172,174,177,178	0
26	LHG	c	519	37/49	0.74	0.35	172,174,178,181	0
24	BCR	B	617	40/40	0.75	0.44	172,173,174,174	0
27	LMG	e	101	44/55	0.75	0.39	171,174,175,176	0
30	SQD	d	402	43/54	0.75	0.83	172,174,176,178	0
22	CLA	B	613	65/65	0.76	0.46	172,174,174,175	0
31	LMT	B	627	35/35	0.76	0.55	172,175,177,177	0
23	PL9	a	409	45/55	0.76	0.38	171,173,174,175	0
28	CL	A	411	1/1	0.76	0.42	172,172,172,172	0
25	DGD	B	625	52/66	0.76	0.56	172,175,177,177	0
31	LMT	M	103	35/35	0.76	0.47	172,173,175,176	0
25	DGD	b	624	58/66	0.76	0.40	171,173,174,175	0
31	LMT	M	102	35/35	0.77	0.46	172,174,175,175	0
22	CLA	C	506	65/65	0.77	0.73	172,174,175,175	0
25	DGD	C	517	66/66	0.77	0.34	172,173,174,175	0
24	BCR	y	101	40/40	0.77	1.00	173,173,174,175	0
35	CA	k	101	1/1	0.77	0.20	172,172,172,172	0
22	CLA	C	507	65/65	0.77	0.40	173,174,175,177	0
27	LMG	b	625	49/55	0.78	0.34	172,174,175,175	0
27	LMG	D	412	46/55	0.78	0.40	172,174,175,175	0
22	CLA	h	101	65/65	0.78	0.53	171,174,175,175	0
24	BCR	b	622	40/40	0.78	0.36	171,172,173,173	0
27	LMG	m	101	42/55	0.78	0.45	170,174,175,175	0
27	LMG	B	624	49/55	0.78	0.31	171,173,174,175	0
24	BCR	C	514	40/40	0.78	0.83	172,173,175,175	0
22	CLA	c	512	65/65	0.78	0.68	172,174,176,176	0
24	BCR	A	407	40/40	0.79	0.48	171,173,174,174	0
30	SQD	B	626	47/54	0.79	0.46	170,174,176,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	SQD	F	102	45/54	0.79	0.69	172,175,177,178	0
32	PHO	D	402	64/64	0.79	0.37	171,173,175,175	0
22	CLA	C	505	65/65	0.79	0.45	172,174,175,176	0
24	BCR	C	521	40/40	0.79	0.82	172,174,175,176	0
31	LMT	B	623	35/35	0.79	0.50	173,174,177,177	0
27	LMG	A	410	51/55	0.79	0.35	171,173,174,175	0
30	SQD	b	602	47/54	0.80	0.38	171,174,176,178	0
25	DGD	c	517	66/66	0.80	0.35	172,173,175,176	0
24	BCR	B	619	40/40	0.80	0.83	172,173,174,175	0
24	BCR	b	623	40/40	0.80	0.76	171,173,174,174	0
22	CLA	b	609	65/65	0.81	0.55	172,174,175,175	0
31	LMT	b	603	35/35	0.81	0.44	172,174,175,176	0
22	CLA	b	613	65/65	0.81	0.67	172,174,175,175	0
35	CA	K	101	1/1	0.81	0.35	177,177,177,177	0
24	BCR	c	521	40/40	0.81	1.26	172,174,175,175	0
27	LMG	c	522	48/55	0.81	0.29	172,174,175,176	0
22	CLA	B	603	65/65	0.81	0.49	171,173,175,175	0
30	SQD	D	403	43/54	0.82	0.41	172,174,177,180	0
22	CLA	b	607	65/65	0.82	0.43	172,173,175,176	0
22	CLA	c	503	65/65	0.82	0.57	172,174,175,175	0
22	CLA	b	617	65/65	0.82	0.45	173,173,175,176	0
22	CLA	b	618	65/65	0.82	0.66	172,174,175,175	0
22	CLA	C	520	65/65	0.82	0.33	172,174,175,176	0
25	DGD	C	515	53/66	0.83	0.36	172,173,174,174	0
22	CLA	a	405	65/65	0.83	0.58	170,172,174,175	0
26	LHG	a	412	39/49	0.83	0.28	171,174,176,177	0
22	CLA	C	510	65/65	0.83	0.46	172,173,175,175	0
24	BCR	B	618	40/40	0.83	0.32	171,172,174,174	0
24	BCR	c	513	40/40	0.83	0.87	172,173,175,175	0
22	CLA	C	512	65/65	0.83	0.88	172,174,176,177	0
22	CLA	A	405	65/65	0.83	0.62	172,174,175,176	0
22	CLA	c	508	65/65	0.84	0.56	172,174,175,175	0
22	CLA	C	504	65/65	0.84	0.41	171,173,175,175	0
25	DGD	B	620	58/66	0.84	0.33	171,173,175,176	0
32	PHO	D	401	64/64	0.84	0.40	171,173,174,175	0
30	SQD	a	401	54/54	0.84	0.58	172,174,176,178	0
22	CLA	d	404	65/65	0.84	0.45	172,173,174,174	0
22	CLA	B	610	65/65	0.84	0.34	172,174,174,175	0
30	SQD	f	103	45/54	0.84	0.52	172,174,176,178	0
25	DGD	C	516	62/66	0.84	0.29	171,174,175,176	0
22	CLA	b	612	65/65	0.84	0.66	171,174,175,176	0
30	SQD	A	414	54/54	0.85	0.40	171,174,176,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	BCR	b	621	40/40	0.85	0.33	171,173,174,174	0
26	LHG	A	409	39/49	0.85	0.28	172,173,175,176	0
22	CLA	a	406	65/65	0.85	0.36	172,174,175,176	0
22	CLA	c	505	65/65	0.85	0.45	172,174,175,175	0
30	SQD	a	415	51/54	0.85	0.29	173,174,175,176	0
22	CLA	B	607	65/65	0.85	0.42	172,174,174,175	0
22	CLA	C	509	65/65	0.85	0.34	173,173,174,174	0
22	CLA	c	501	65/65	0.85	0.45	172,174,175,175	0
22	CLA	b	606	65/65	0.85	0.61	172,173,174,174	0
27	LMG	d	407	48/55	0.86	0.28	171,173,175,175	0
22	CLA	C	503	65/65	0.86	0.41	172,174,175,176	0
25	DGD	c	515	53/66	0.86	0.36	171,174,175,177	0
22	CLA	B	605	65/65	0.86	0.72	172,173,175,176	0
21	FE2	a	403	1/1	0.86	0.18	175,175,175,175	0
24	BCR	C	513	40/40	0.86	0.77	172,173,174,174	0
22	CLA	c	506	65/65	0.86	0.55	173,174,175,175	0
32	PHO	a	407	64/64	0.86	0.26	173,174,175,175	0
22	CLA	B	615	65/65	0.86	0.66	172,174,175,175	0
22	CLA	c	510	65/65	0.86	0.53	173,174,175,176	0
22	CLA	H	101	65/65	0.86	0.35	172,174,175,175	0
22	CLA	B	609	65/65	0.86	0.53	172,174,175,175	0
22	CLA	d	405	65/65	0.86	0.45	172,174,175,175	0
22	CLA	A	404	65/65	0.87	0.47	170,173,174,175	0
22	CLA	c	520	65/65	0.87	0.36	173,174,174,175	0
22	CLA	B	604	65/65	0.87	0.67	172,173,175,175	0
25	DGD	c	516	62/66	0.87	0.30	172,174,175,175	0
22	CLA	C	501	65/65	0.87	0.40	172,174,174,175	0
22	CLA	C	508	65/65	0.87	0.86	172,174,175,175	0
22	CLA	c	509	65/65	0.87	0.32	172,173,175,175	0
27	LMG	D	408	48/55	0.87	0.28	170,173,175,175	0
22	CLA	D	406	65/65	0.87	0.64	172,174,175,176	0
22	CLA	a	404	65/65	0.88	0.54	172,173,174,176	0
34	HEM	V	201	43/43	0.88	0.45	172,173,175,175	0
22	CLA	b	608	65/65	0.88	0.51	172,173,175,176	0
22	CLA	b	614	65/65	0.88	0.30	172,173,174,175	0
22	CLA	B	606	65/65	0.88	0.34	172,173,174,175	0
27	LMG	B	621	49/55	0.88	0.26	172,173,174,174	0
22	CLA	D	405	65/65	0.89	0.36	172,173,174,175	0
22	CLA	c	511	65/65	0.89	0.62	172,174,175,176	0
22	CLA	c	504	65/65	0.89	0.33	172,174,175,175	0
22	CLA	B	614	65/65	0.89	0.62	172,174,175,175	0
22	CLA	b	610	65/65	0.90	0.33	172,173,175,175	0

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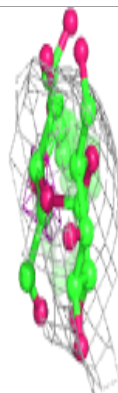
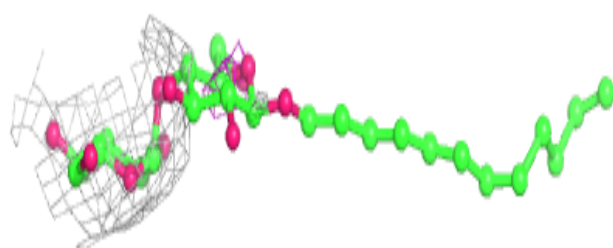
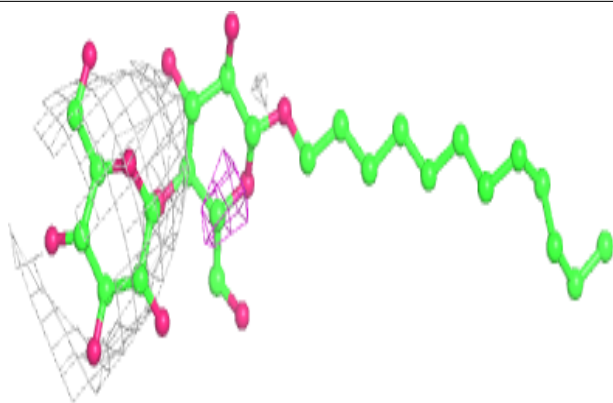
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	BCR	b	620	40/40	0.90	0.32	172,173,174,175	0
34	HEM	v	201	43/43	0.90	0.55	171,174,175,175	0
22	CLA	A	402	65/65	0.90	0.42	172,173,174,175	0
22	CLA	C	511	65/65	0.90	0.92	172,174,175,175	0
22	CLA	B	608	65/65	0.90	0.50	172,174,175,175	0
22	CLA	B	612	65/65	0.90	0.28	171,173,175,175	0
28	CL	a	416	1/1	0.91	0.33	173,173,173,173	0
22	CLA	c	507	65/65	0.91	0.24	172,174,175,176	0
33	BCT	d	403	4/4	0.91	0.92	174,174,175,176	0
34	HEM	F	101	43/43	0.91	0.48	173,174,175,176	0
27	LMG	d	410	46/55	0.91	0.23	172,173,175,175	0
21	FE2	A	401	1/1	0.92	0.18	170,170,170,170	0
22	CLA	B	602	65/65	0.92	0.52	171,173,174,175	0
22	CLA	B	611	65/65	0.92	0.36	171,173,174,174	0
22	CLA	b	615	65/65	0.92	0.40	172,173,174,175	0
22	CLA	b	611	65/65	0.92	0.31	172,174,175,175	0
29	OEX	A	412	10/10	0.93	0.42	165,169,172,173	0
27	LMG	b	628	49/55	0.93	0.23	172,174,175,175	0
34	HEM	f	101	43/43	0.93	0.34	173,174,175,175	0
22	CLA	A	403	65/65	0.93	0.54	171,173,174,175	0
33	BCT	D	404	4/4	0.95	0.25	173,174,174,174	0
22	CLA	b	616	65/65	0.95	0.29	171,173,174,175	0
29	OEX	a	414	10/10	0.96	0.45	168,171,173,177	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.

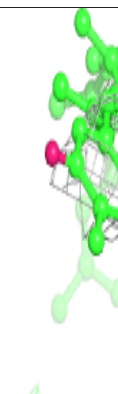
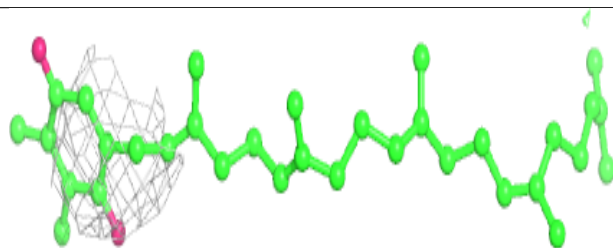
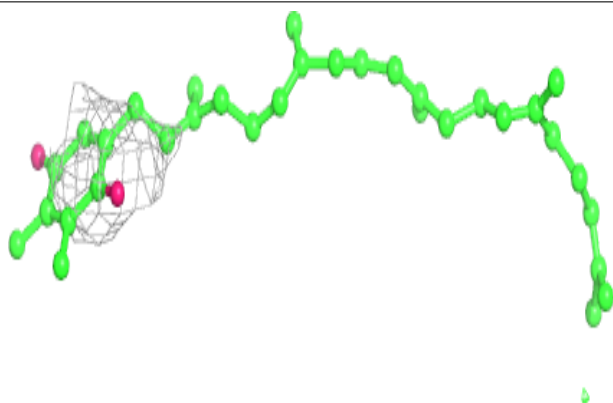


**Electron density around LMT I 102:**

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

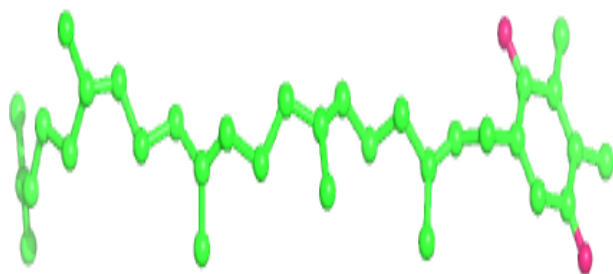
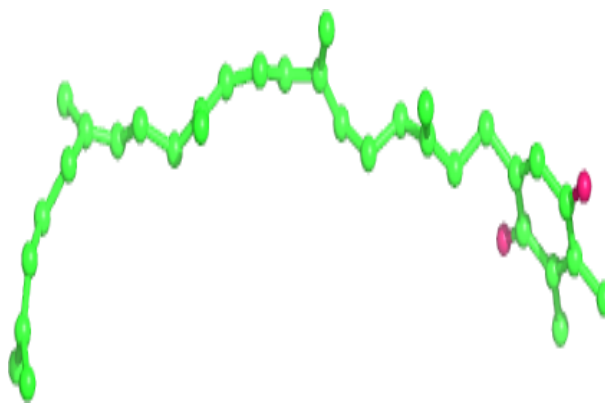
**Electron density around PL9 J 101:**

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

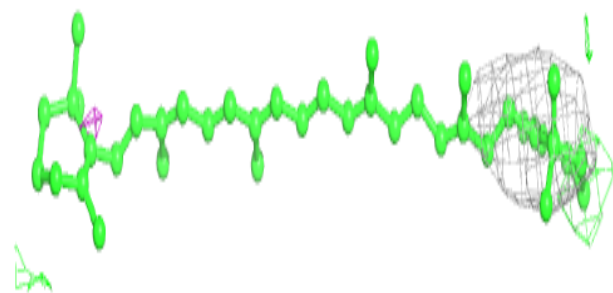
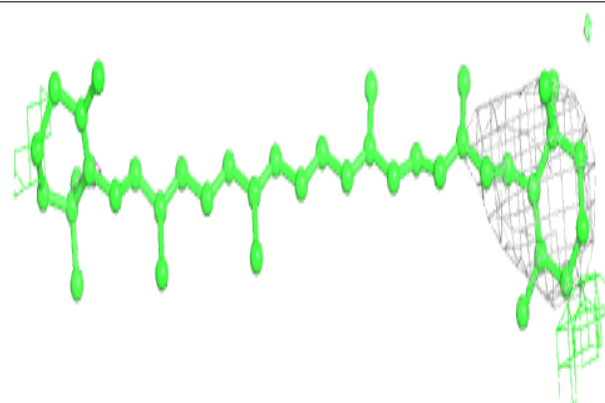


**Electron density around PL9 j 101:**

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

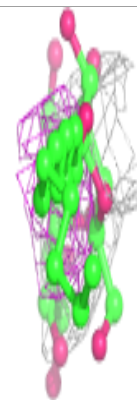
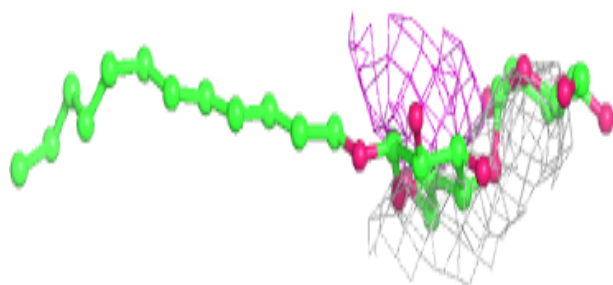
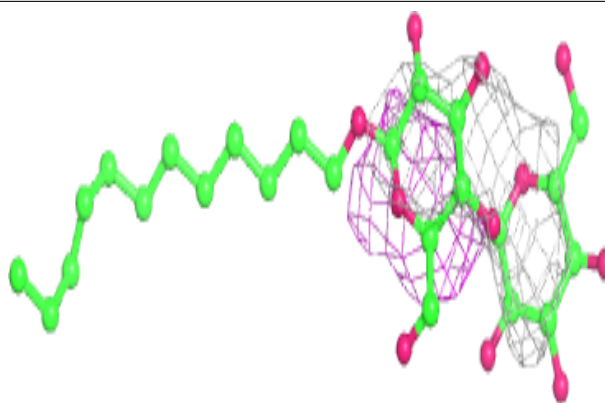
**Electron density around BCR J 102:**

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

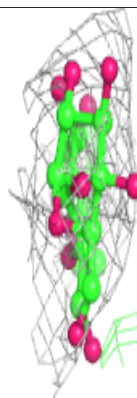
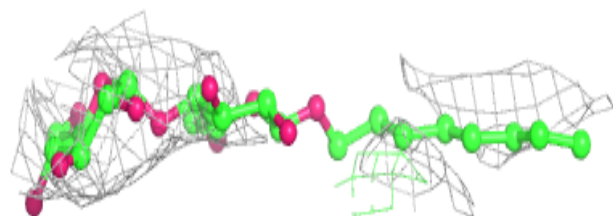
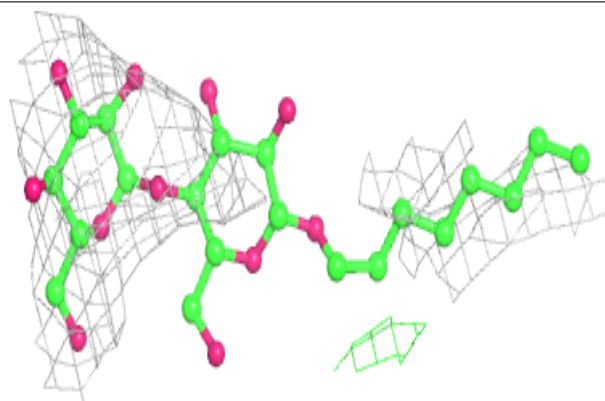


**Electron density around LMT i 102:**

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

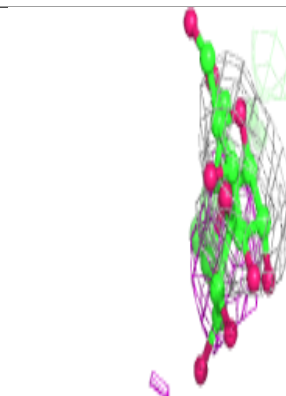
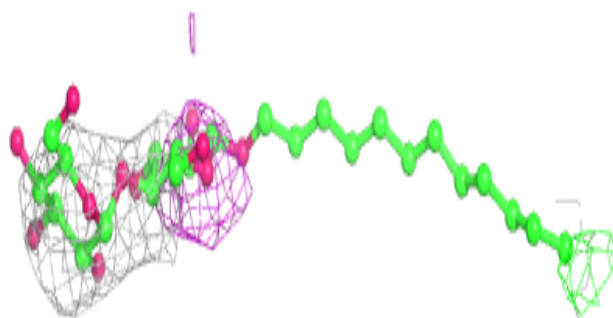
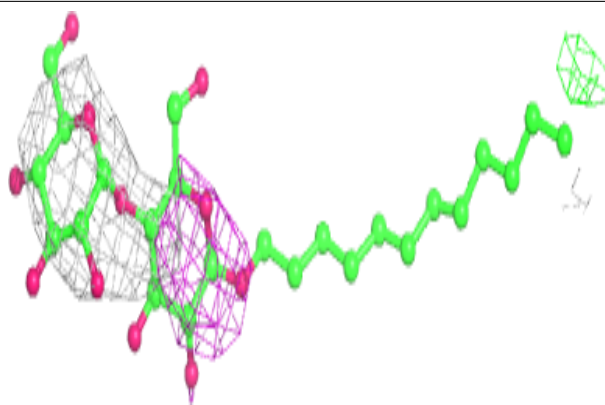
**Electron density around LMT d 409:**

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

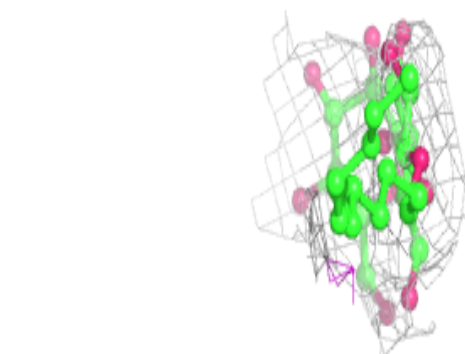
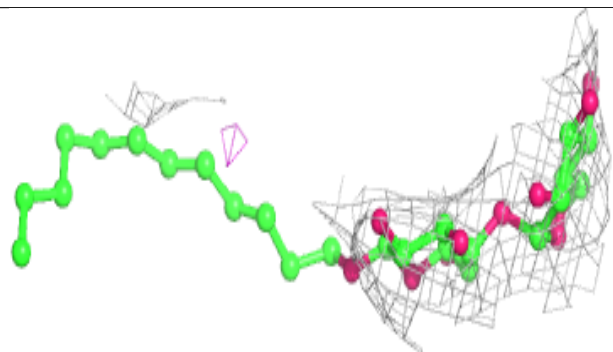
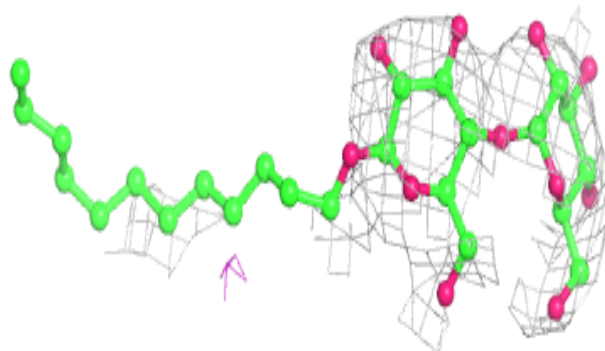


**Electron density around LMT b 627:**

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

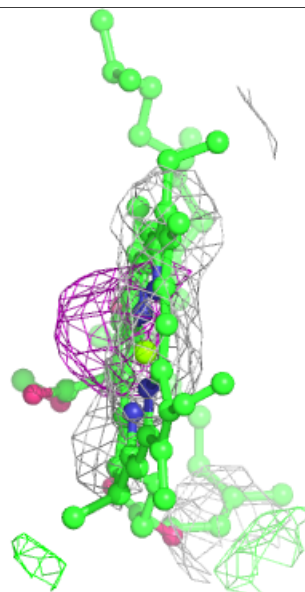
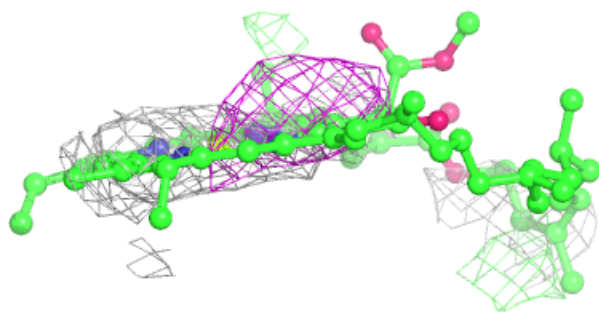
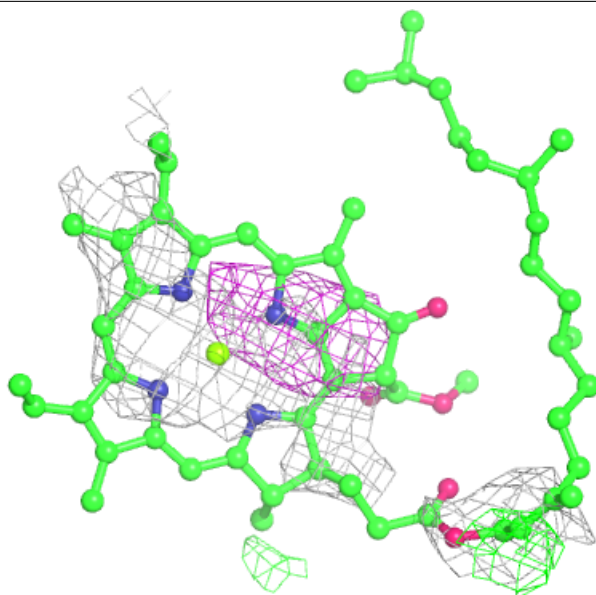
**Electron density around LMT b 626:**

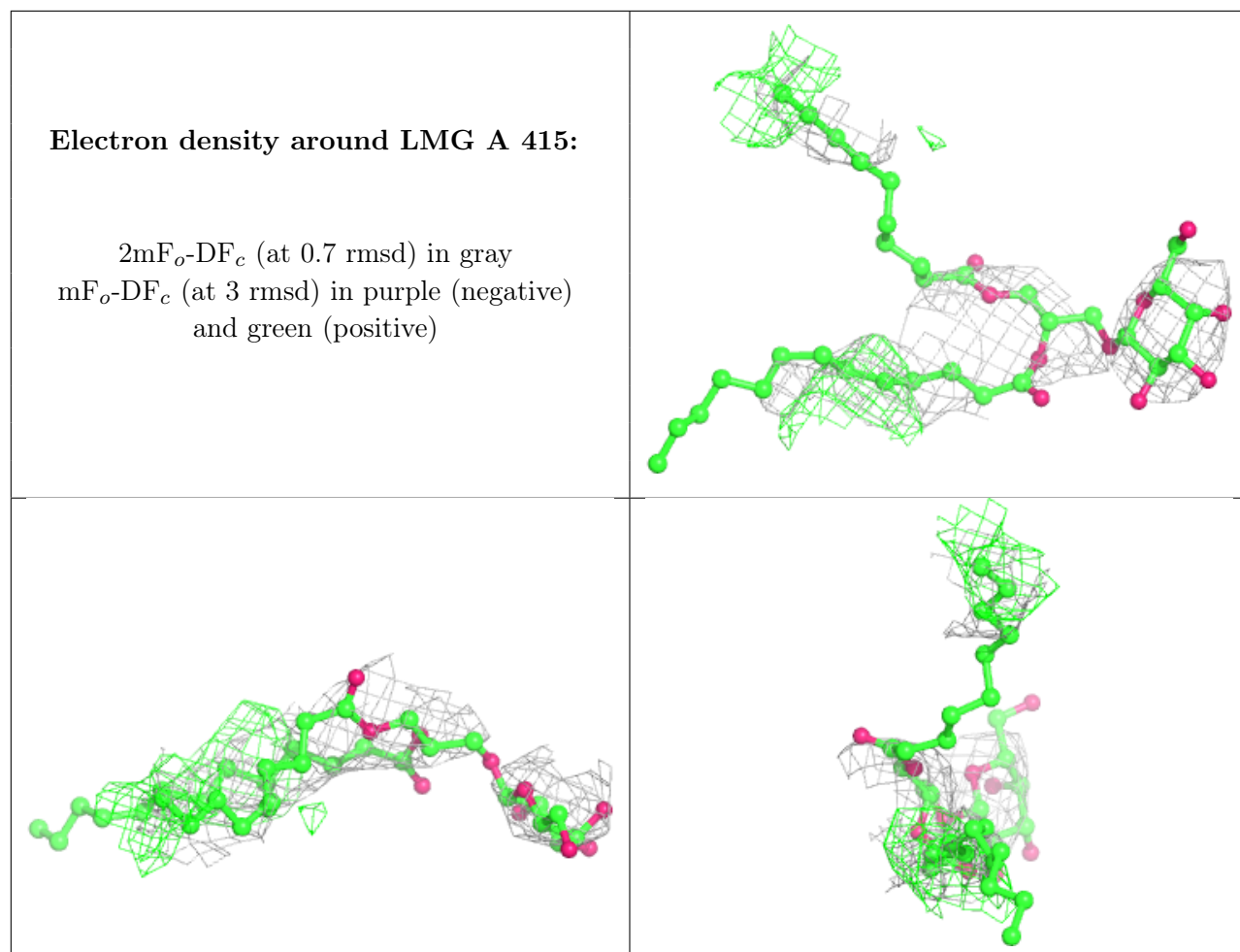
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

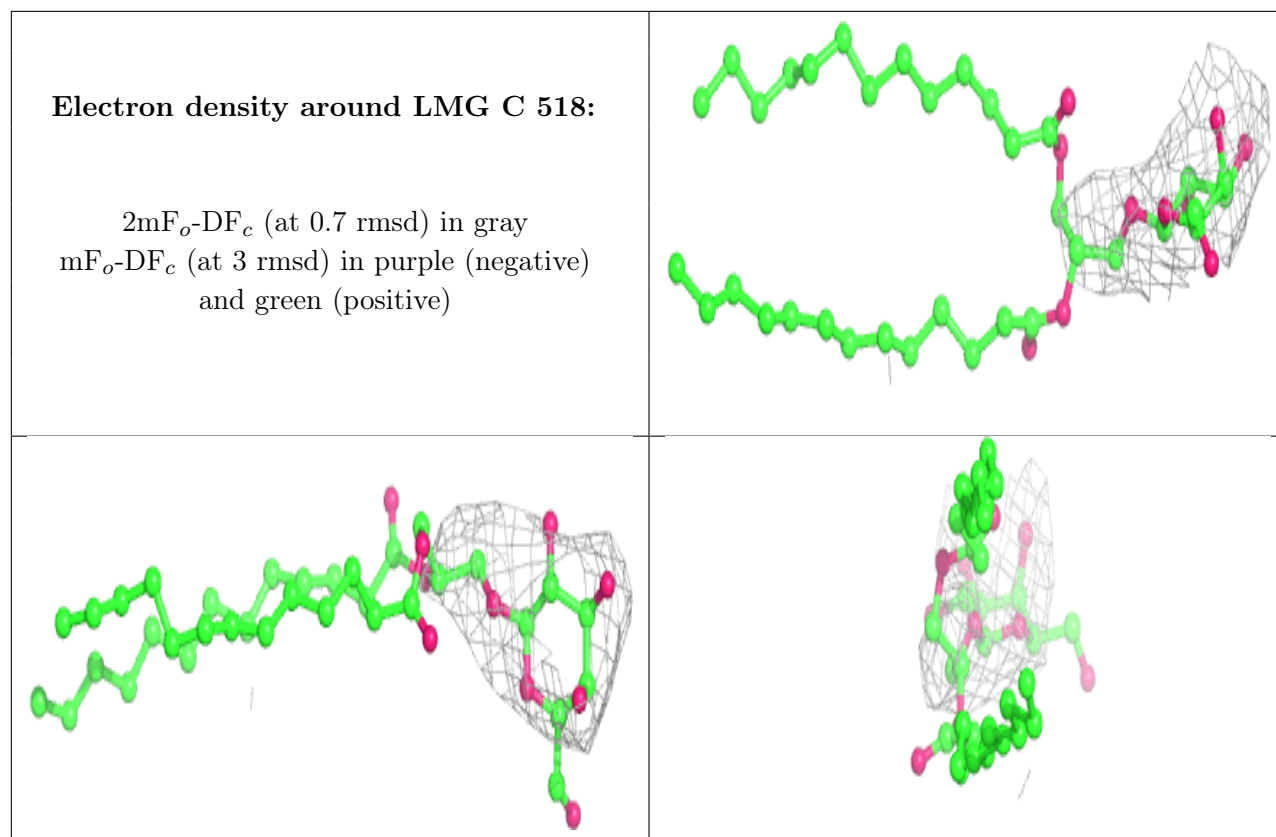


**Electron density around CLA b 605:**

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



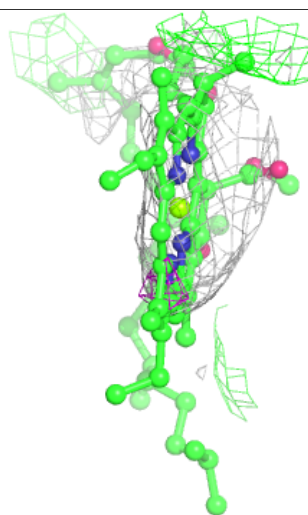
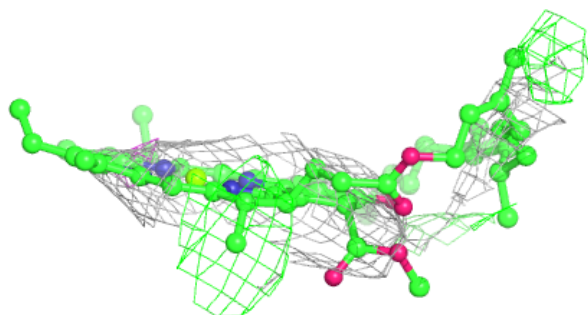
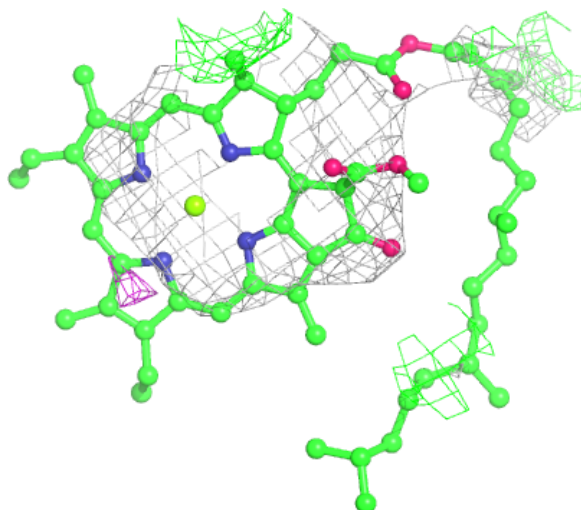






**Electron density around CLA B 601:**

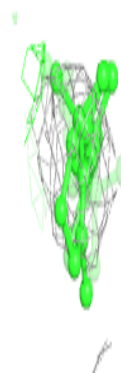
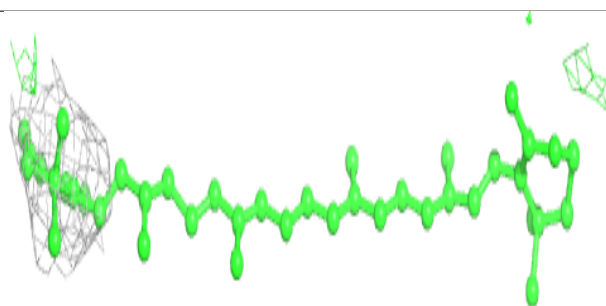
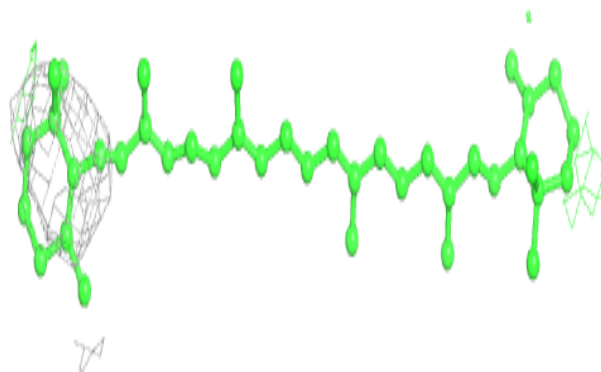
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





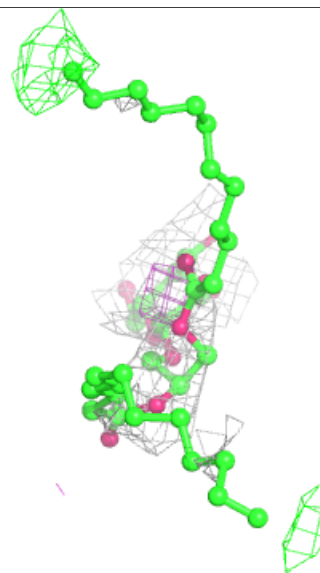
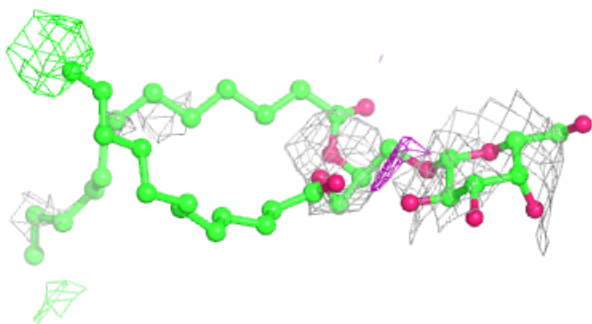
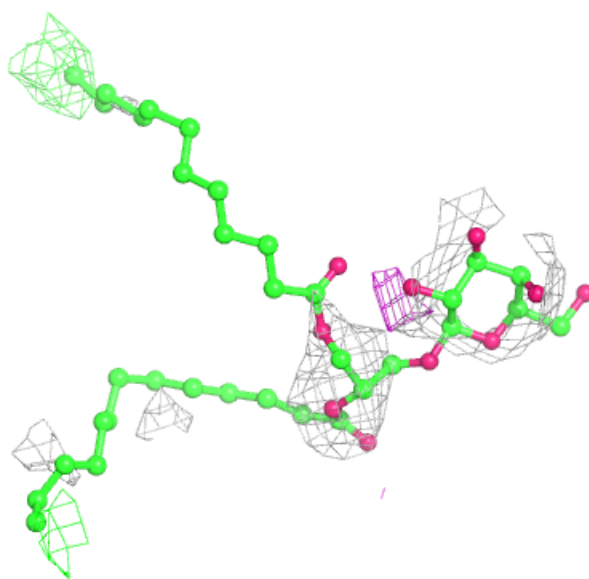
**Electron density around BCR j 102:**

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



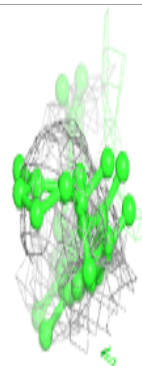
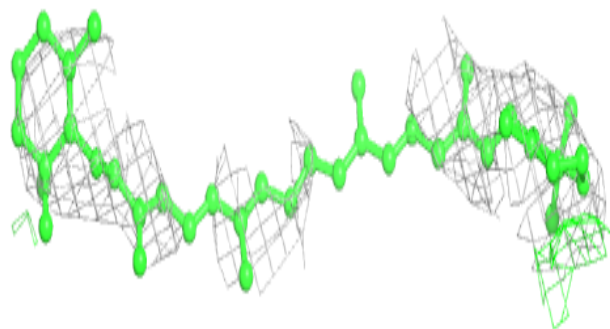
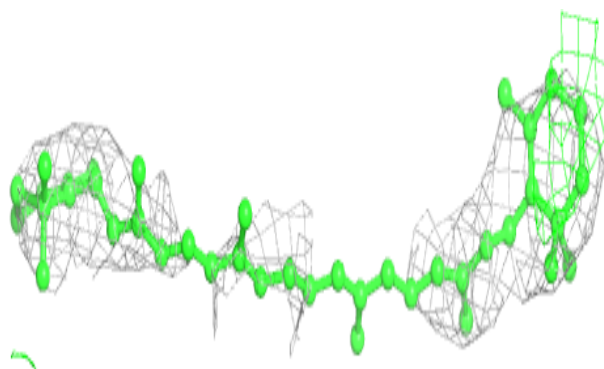
**Electron density around LMG E 101:**

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

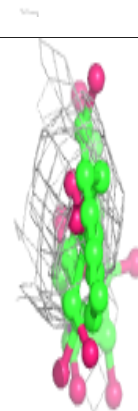
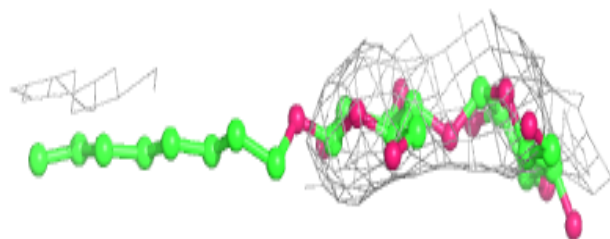
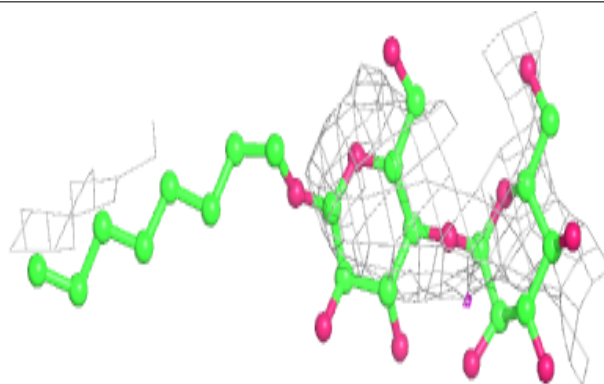


**Electron density around BCR f 102:**

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

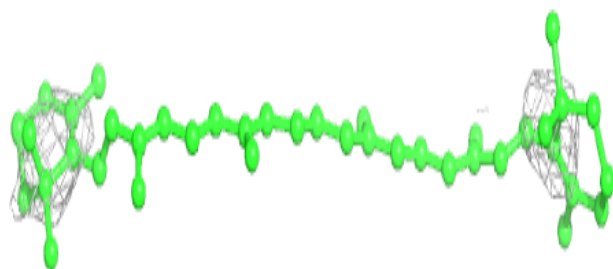
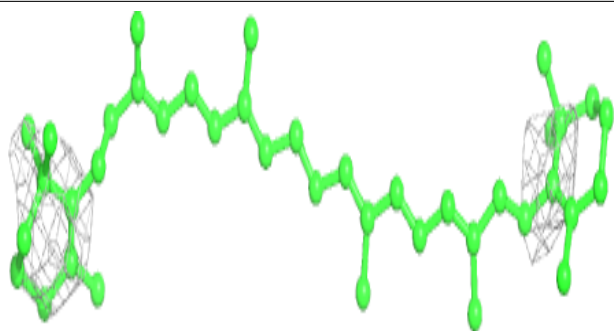
**Electron density around LMT D 410:**

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

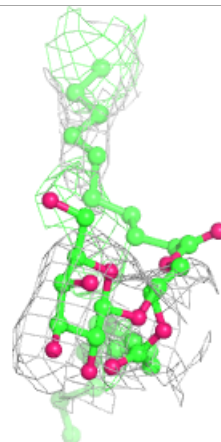
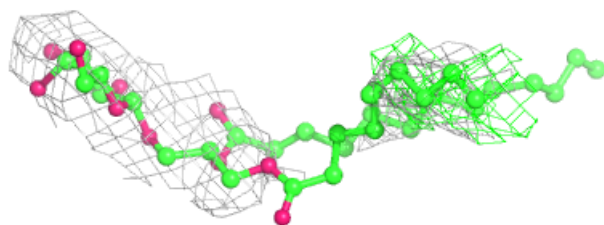
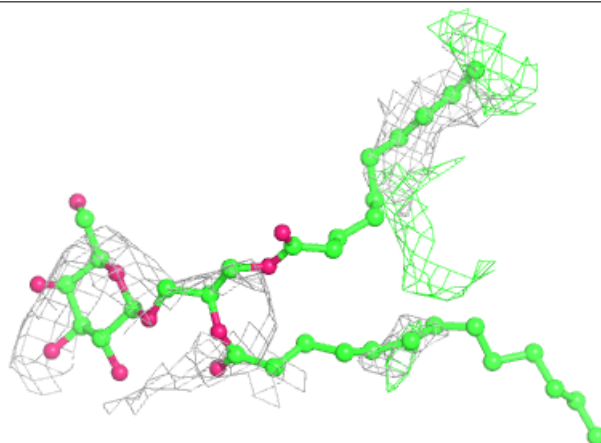


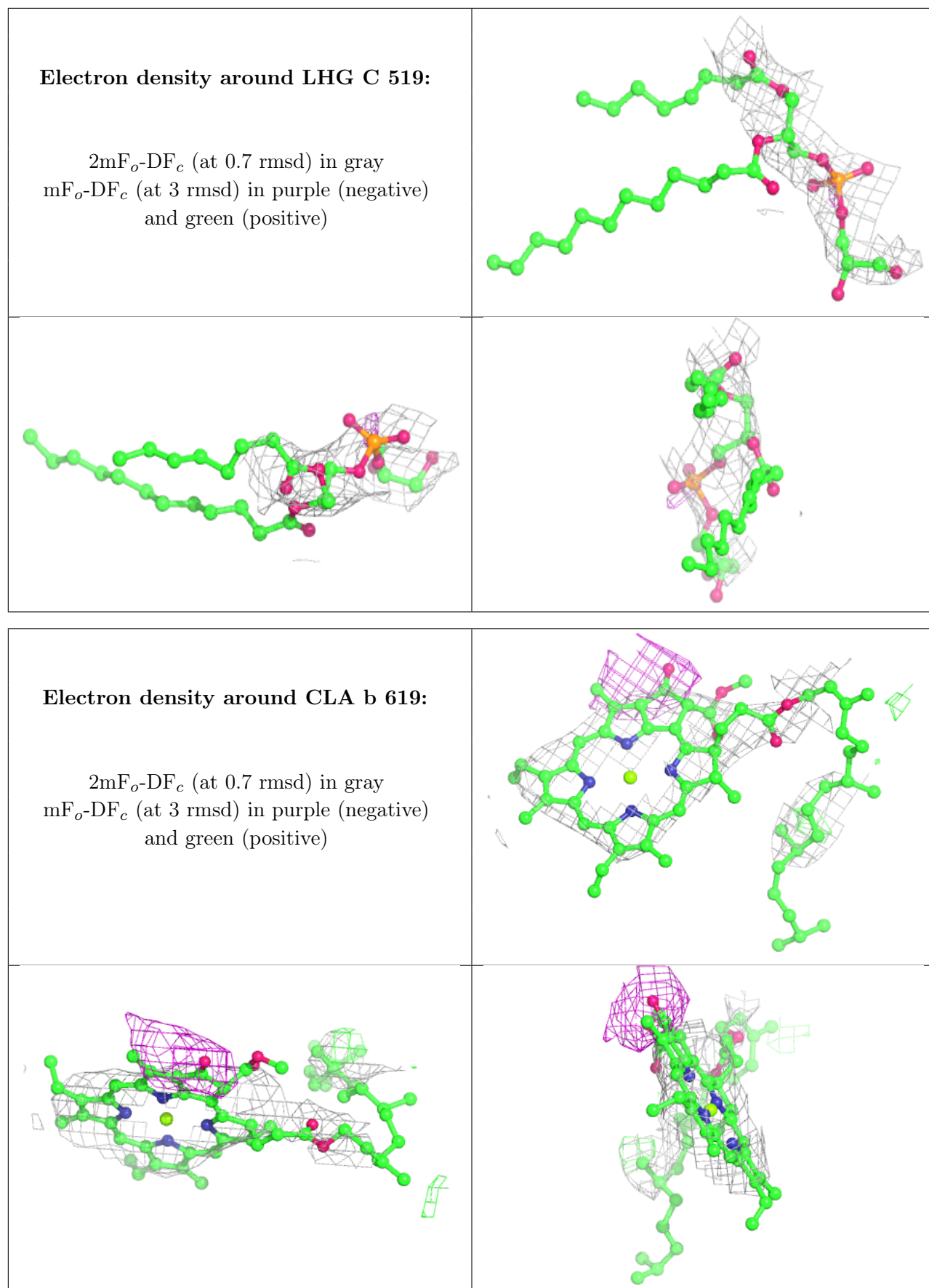
**Electron density around BCR g 101:**

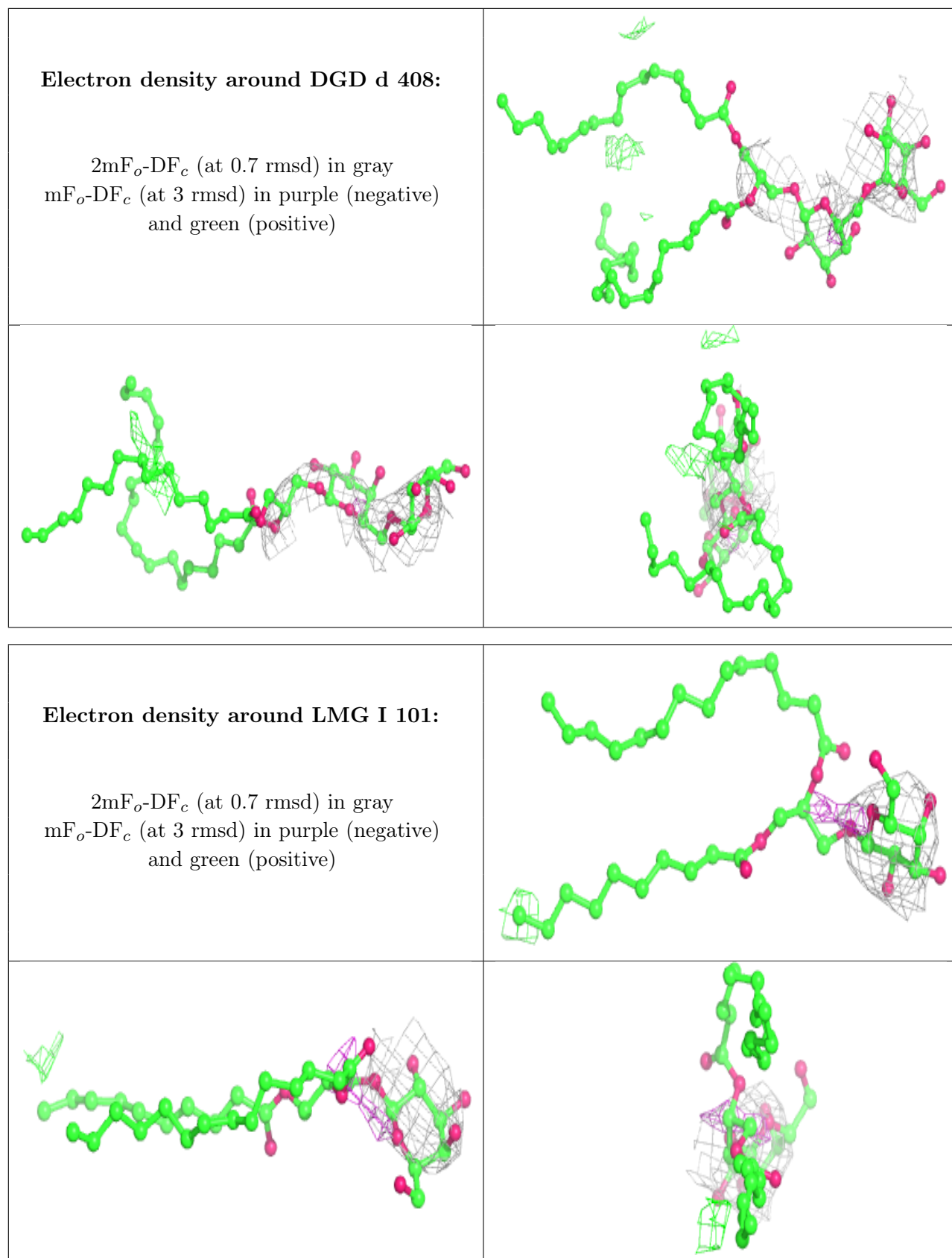
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)

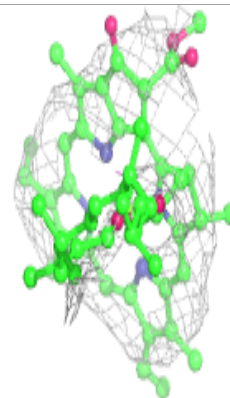
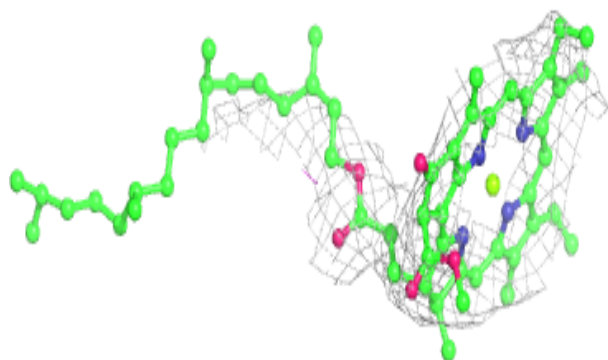
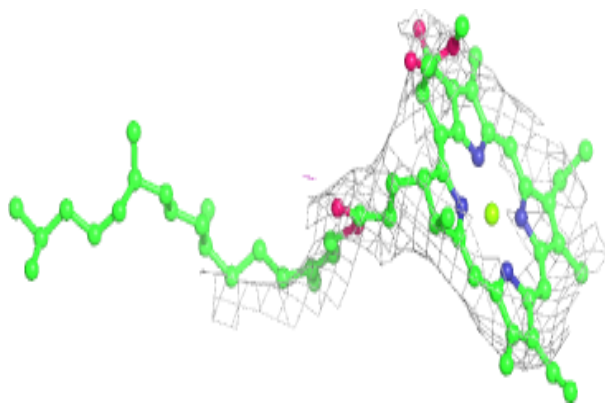




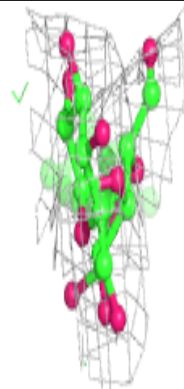
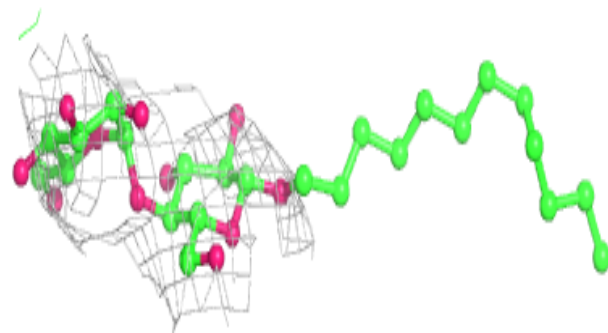
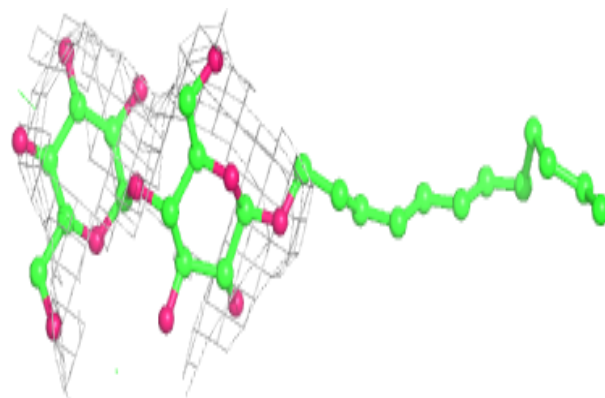


**Electron density around CLA c 502:**

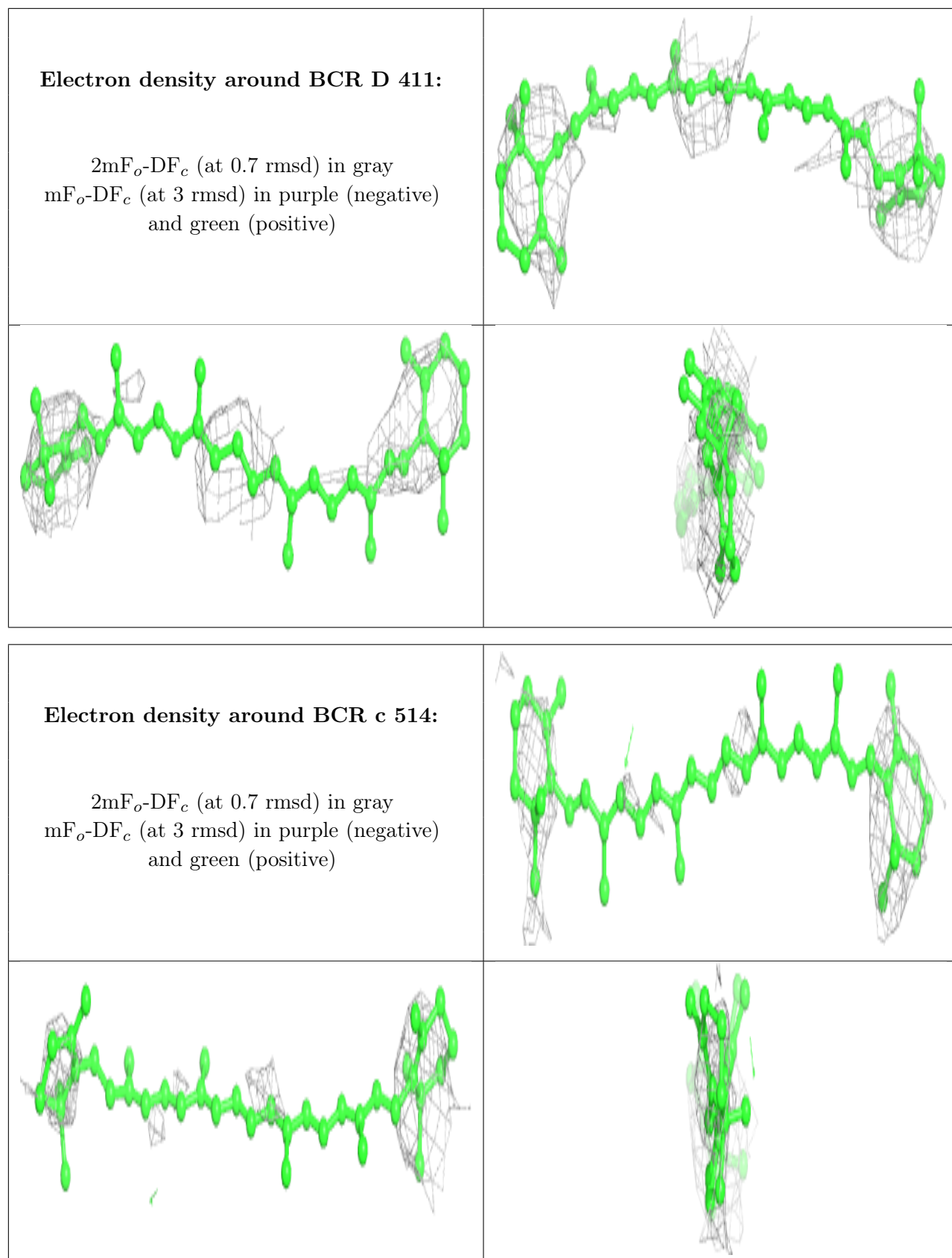
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMT B 628:**

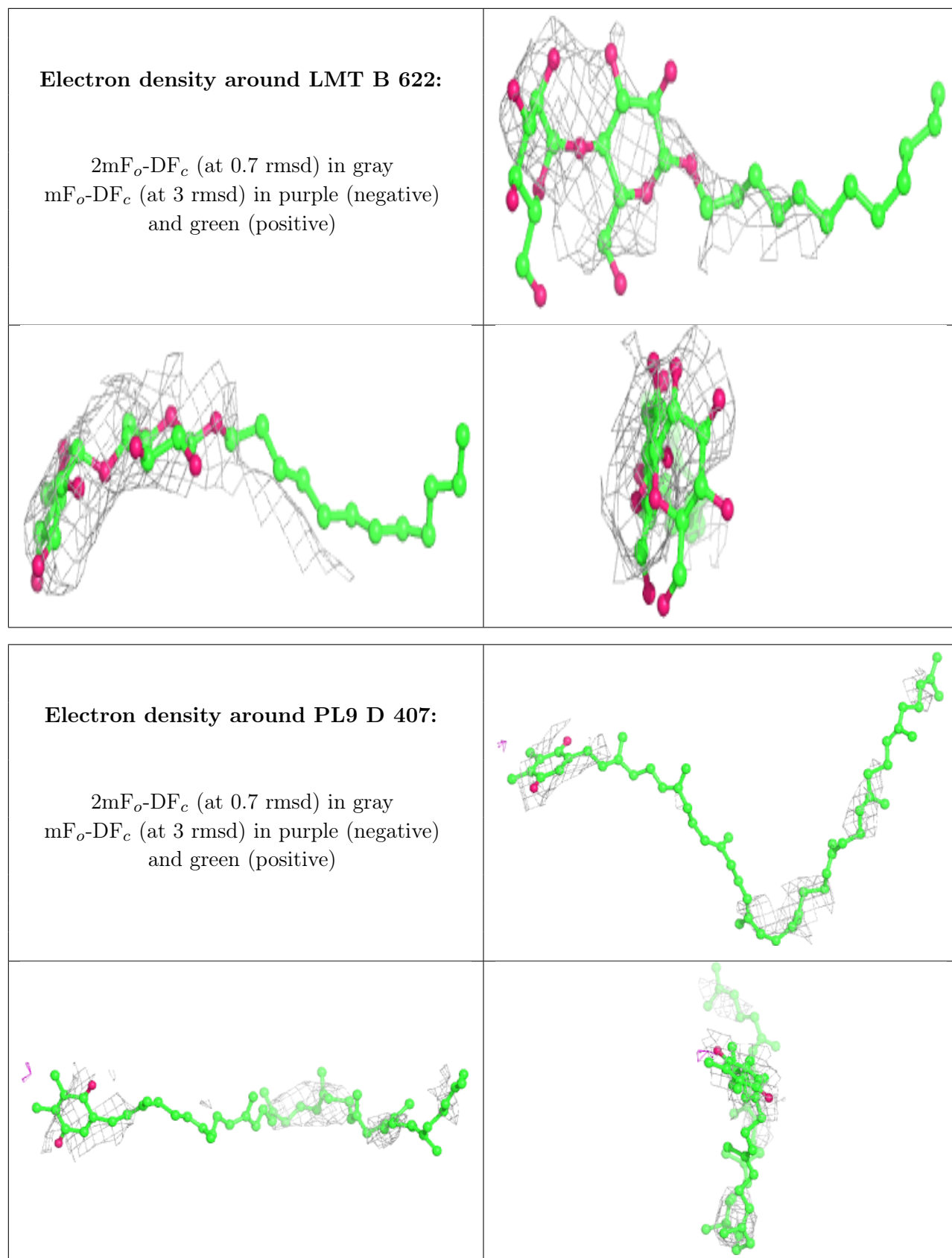
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





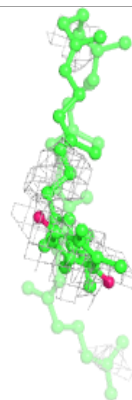
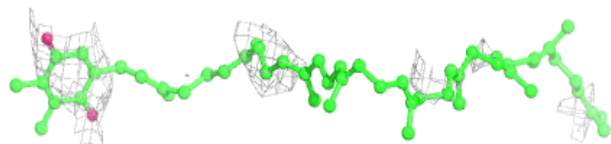
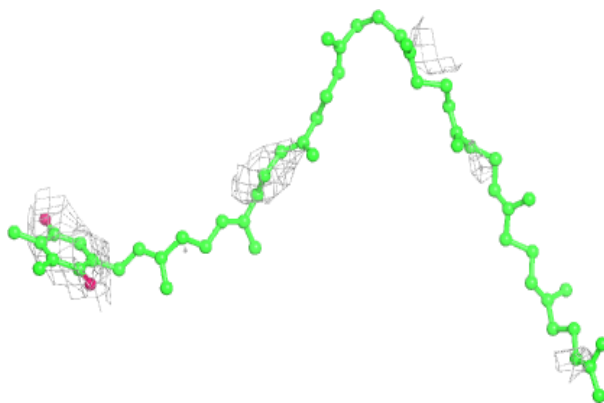




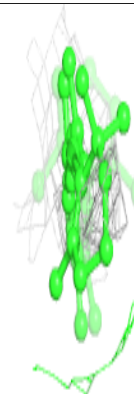
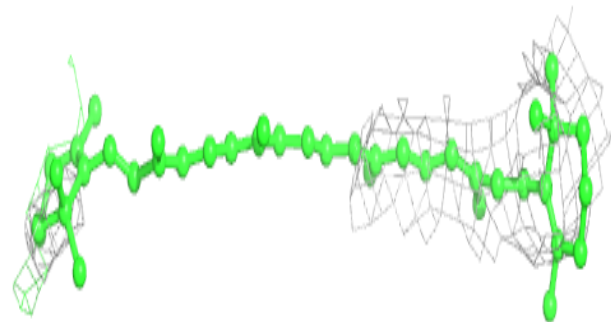
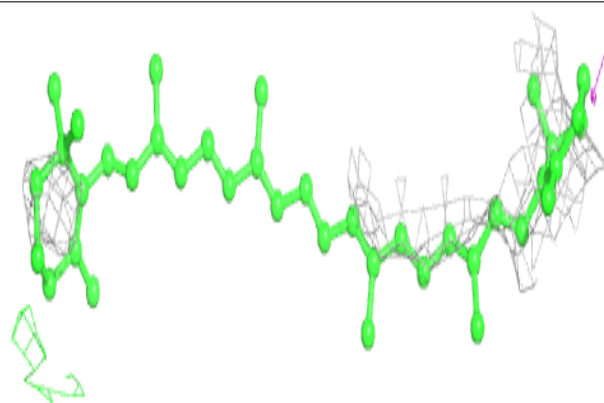


**Electron density around PL9 d 406:**

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

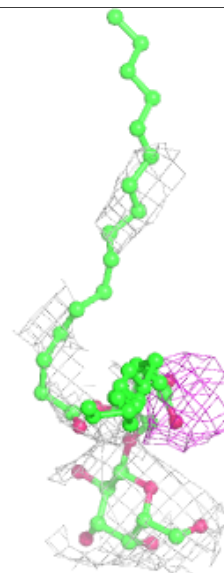
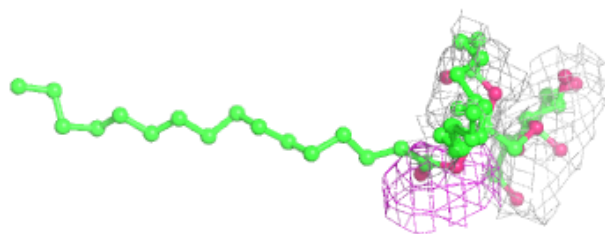
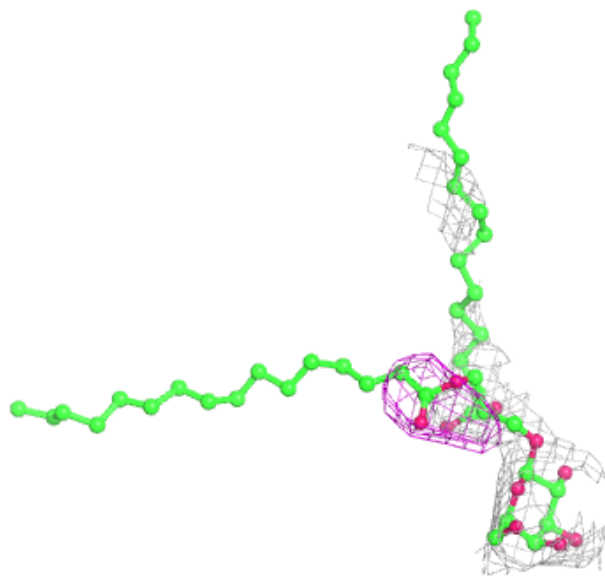
**Electron density around BCR H 102:**

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



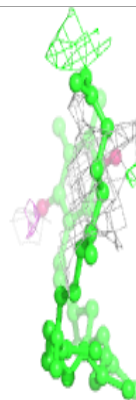
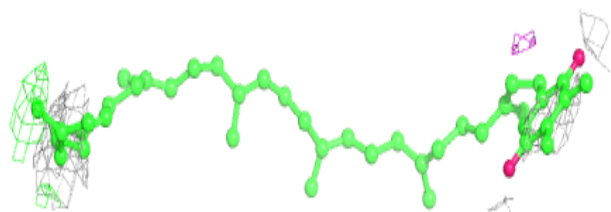
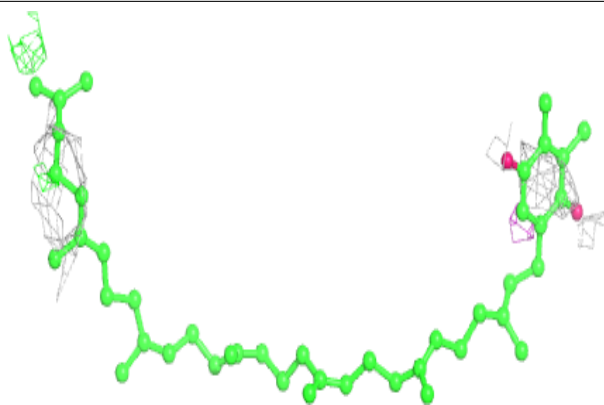
**Electron density around LMG a 413:**

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

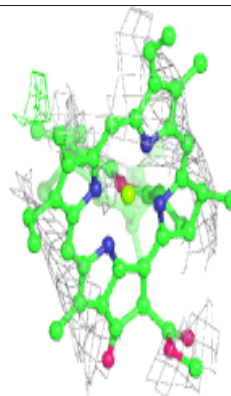
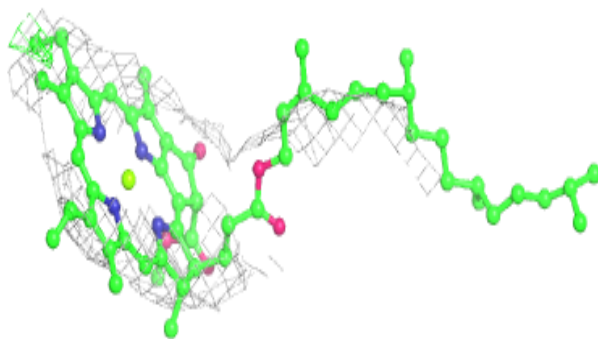
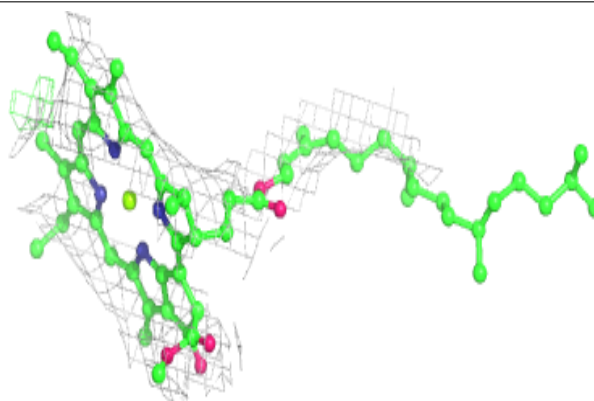


**Electron density around PL9 A 406:**

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

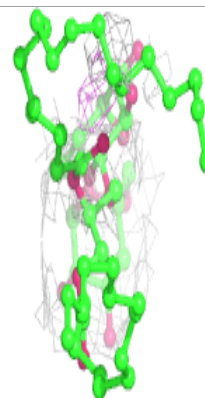
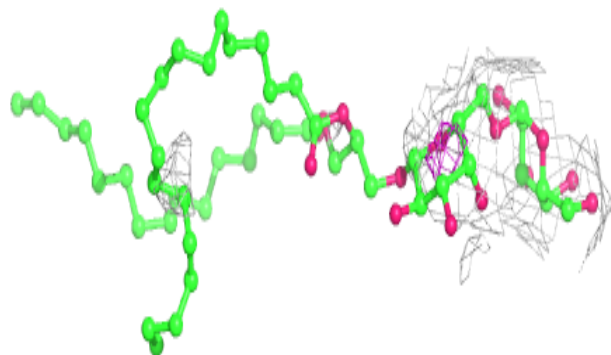
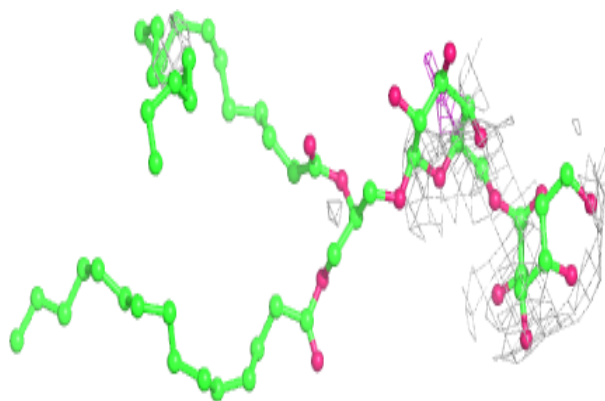
**Electron density around CLA C 502:**

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

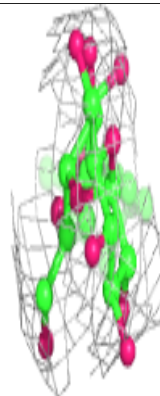
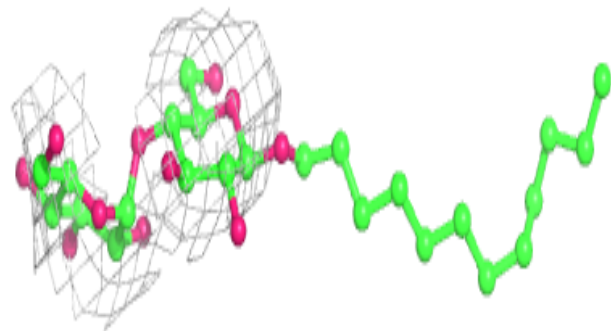
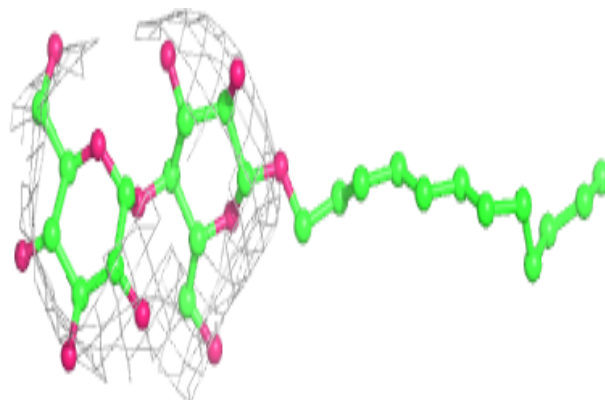


**Electron density around DGD D 409:**

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

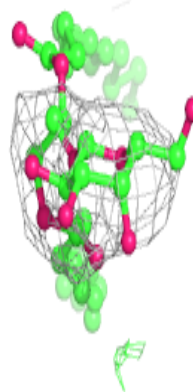
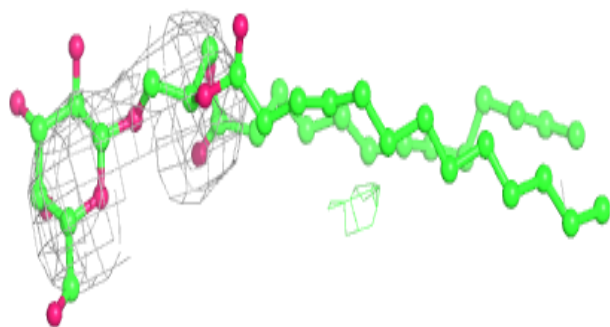
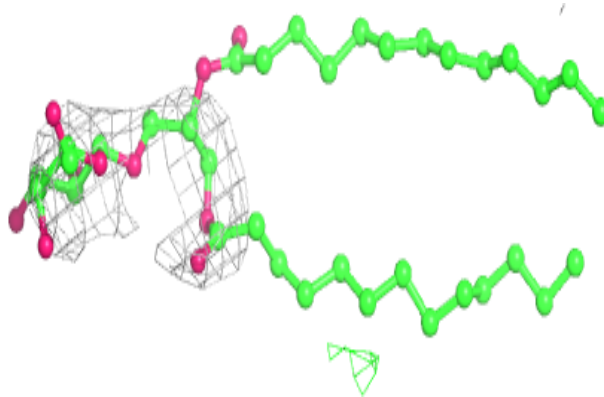
**Electron density around LMT b 604:**

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

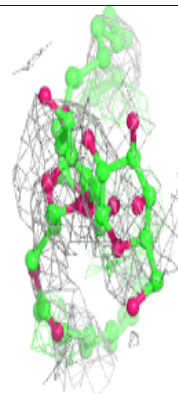
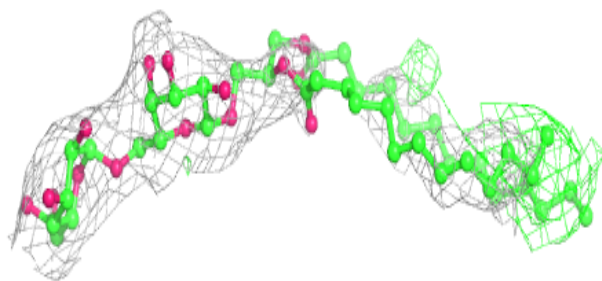
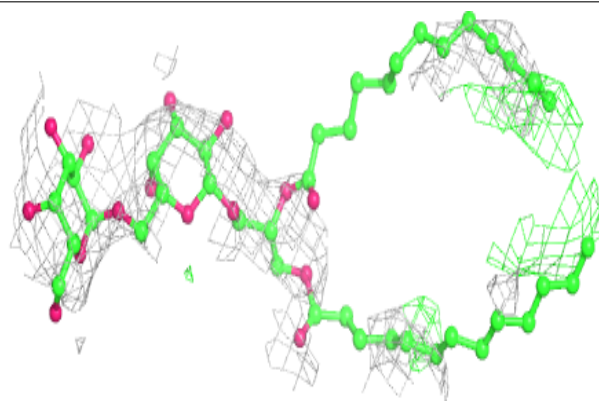


**Electron density around LMG c 518:**

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

**Electron density around DGD A 408:**

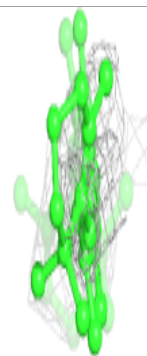
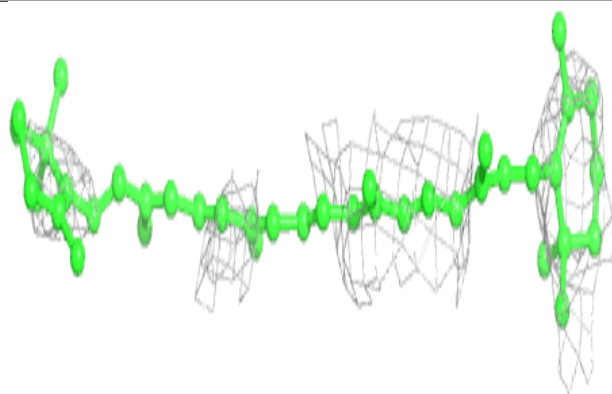
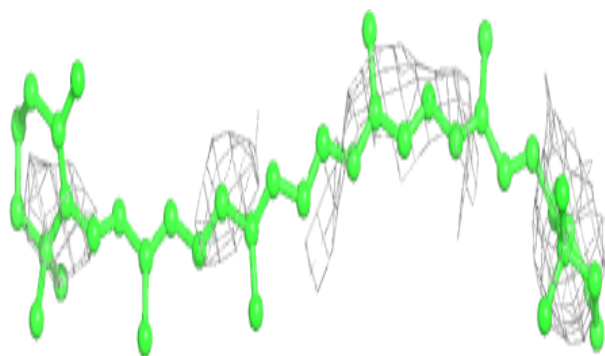
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



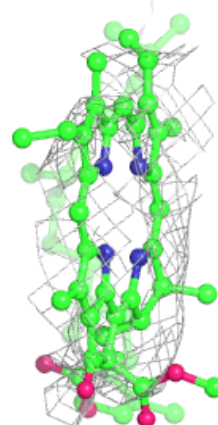
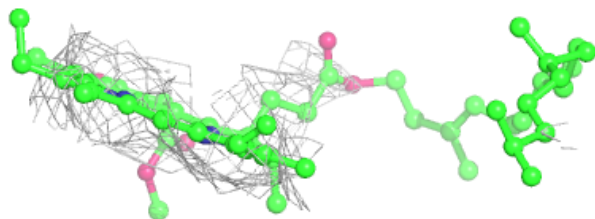
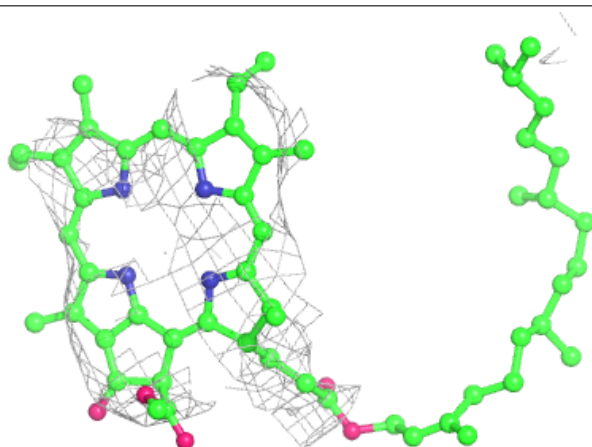


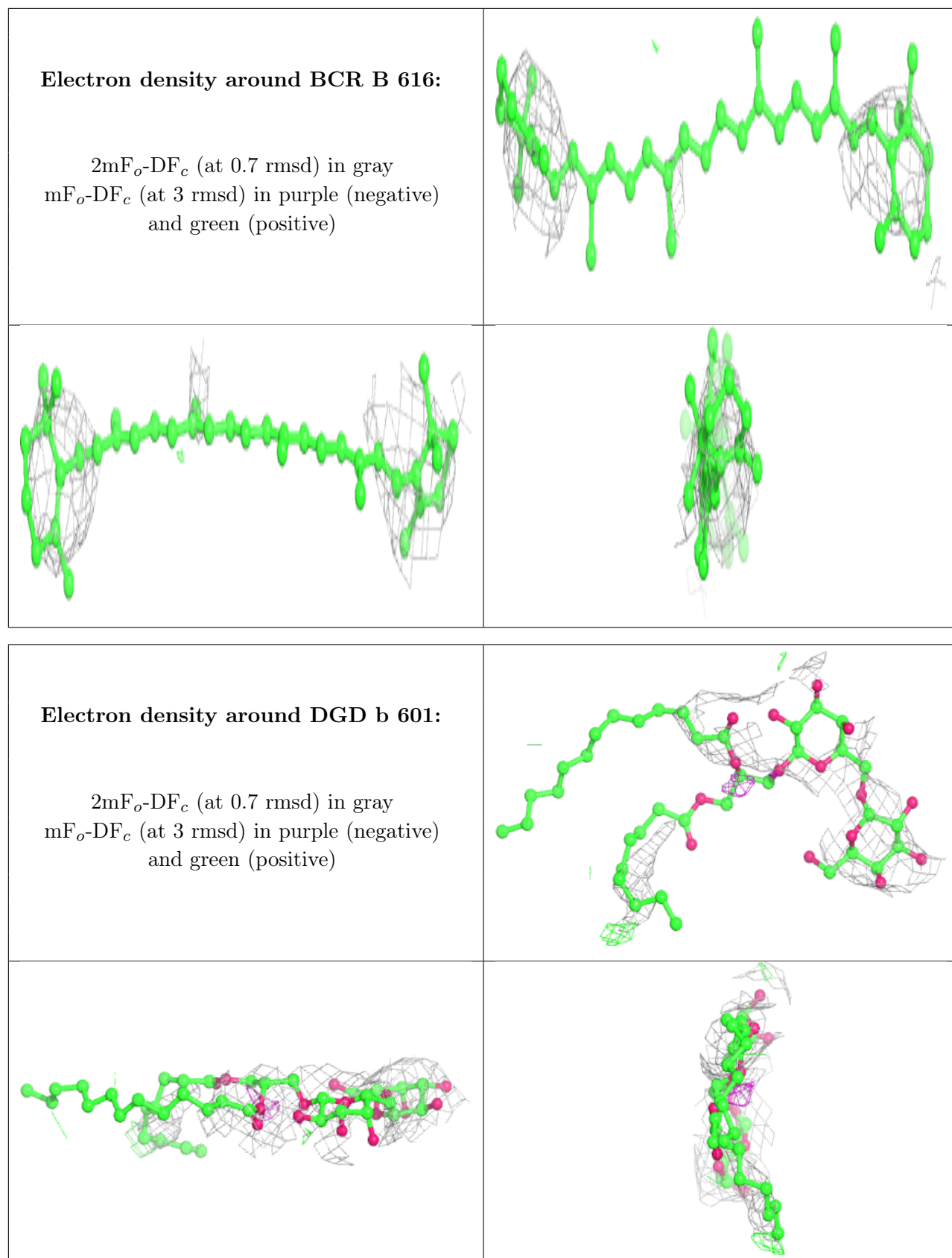
**Electron density around BCR x 101:**

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

**Electron density around PHO d 401:**

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

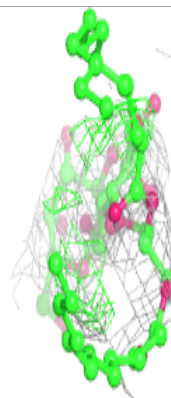
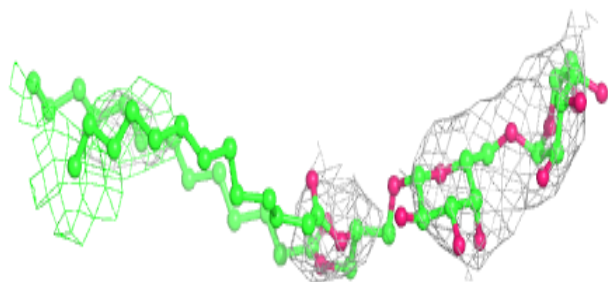
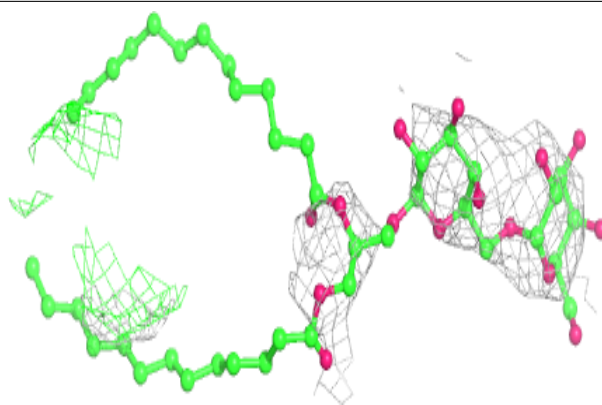




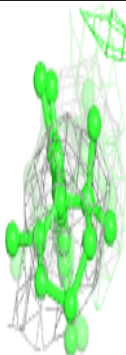
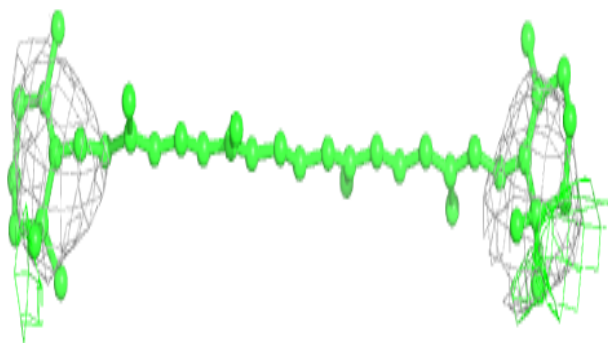
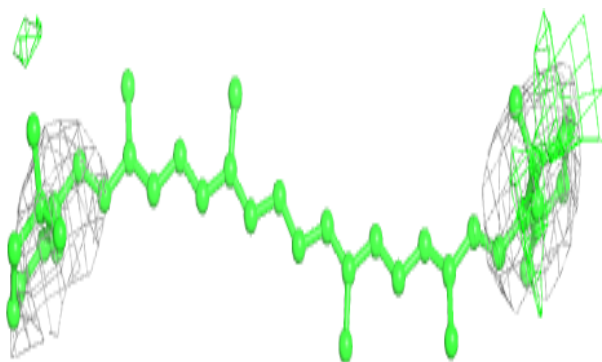


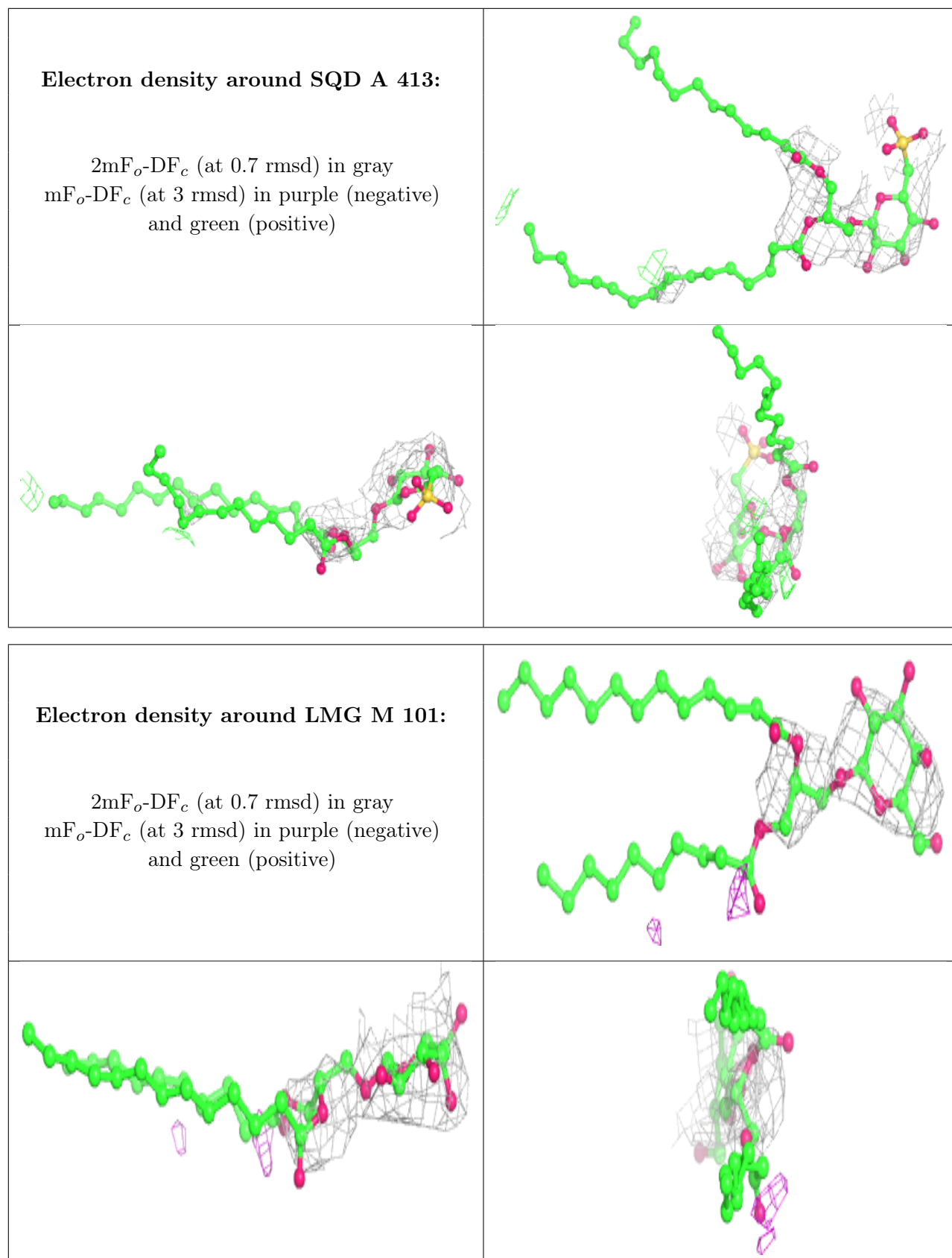
**Electron density around DGD a 411:**

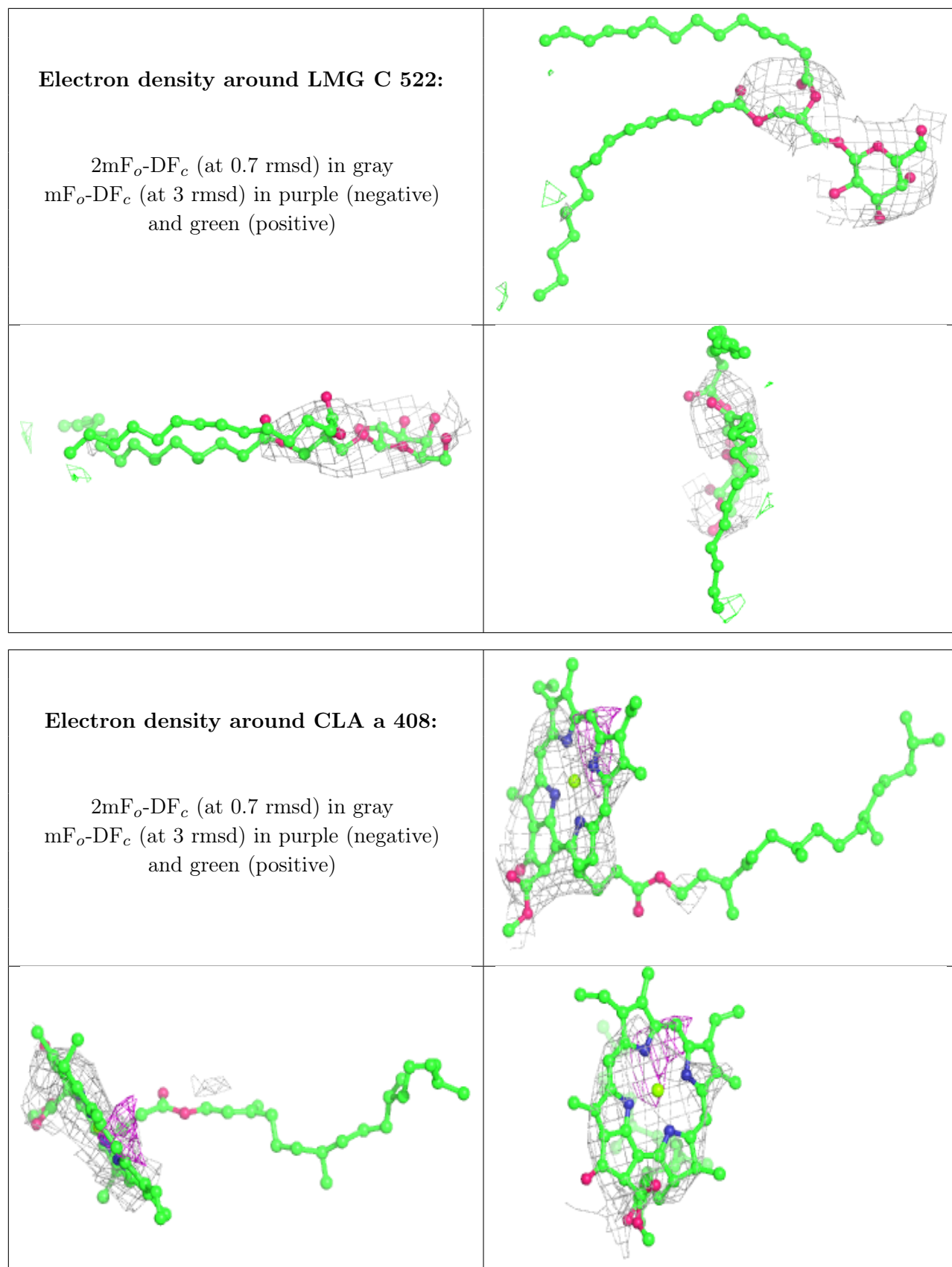
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

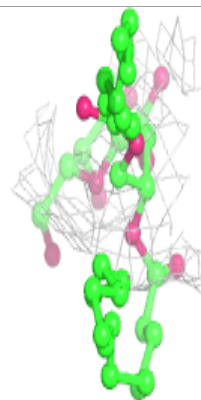
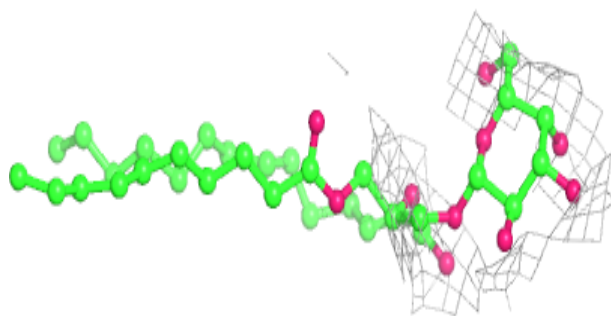
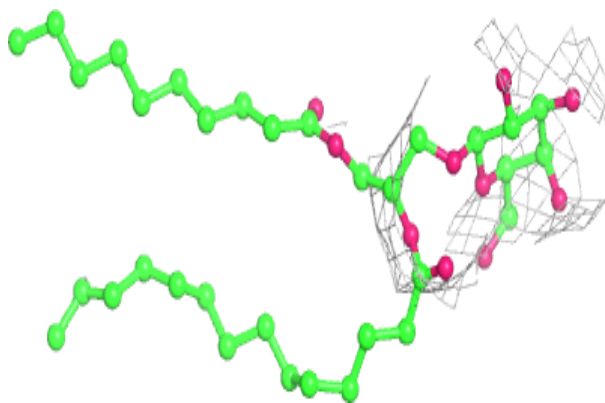




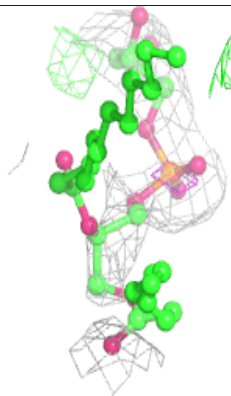
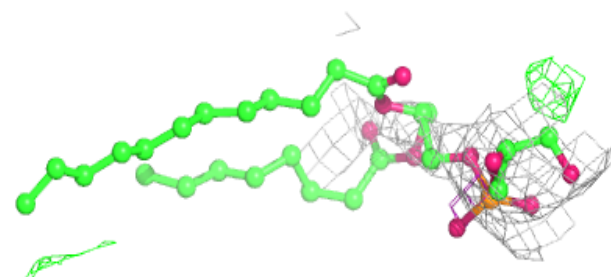
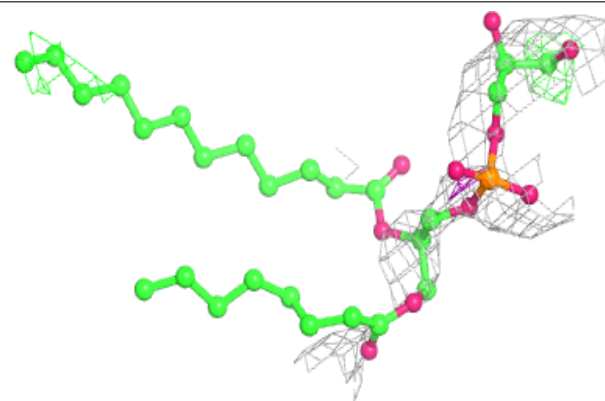


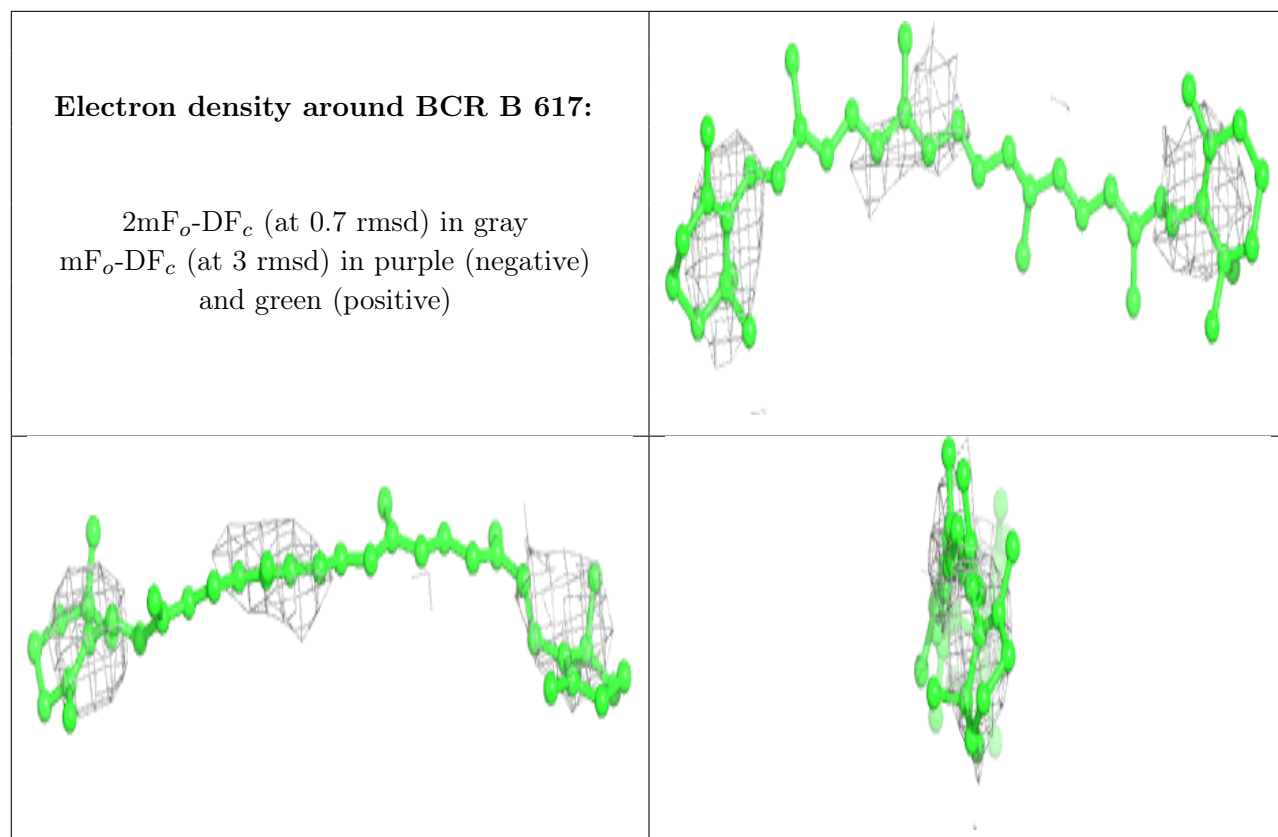
**Electron density around LMG i 101:**

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

**Electron density around LHG c 519:**

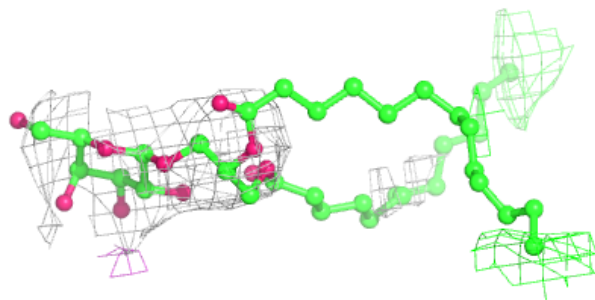
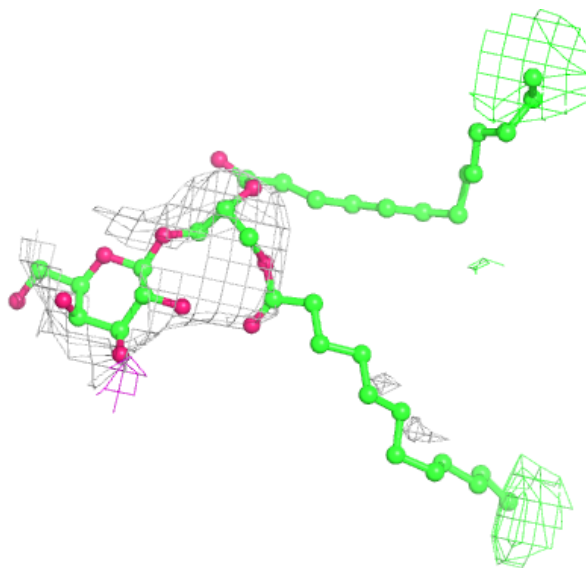
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





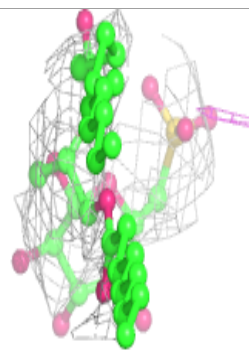
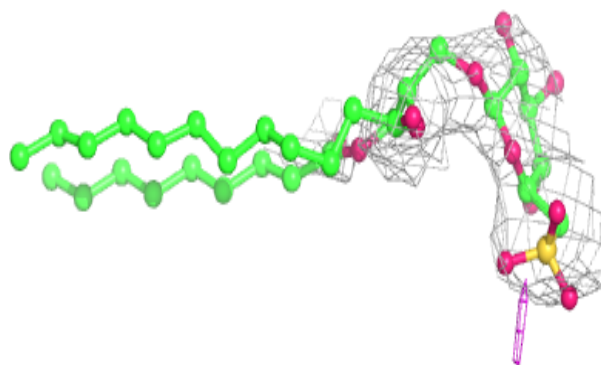
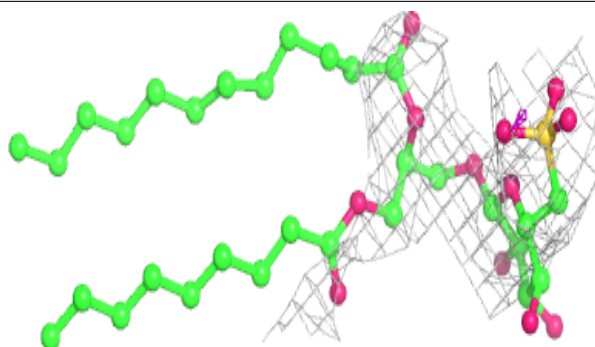
**Electron density around LMG e 101:**

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

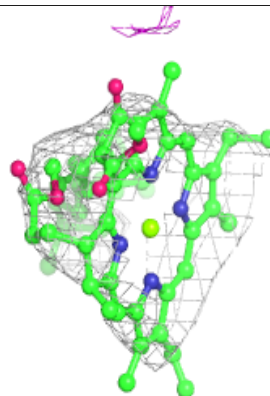
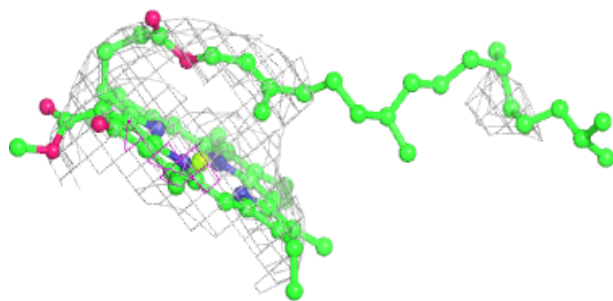
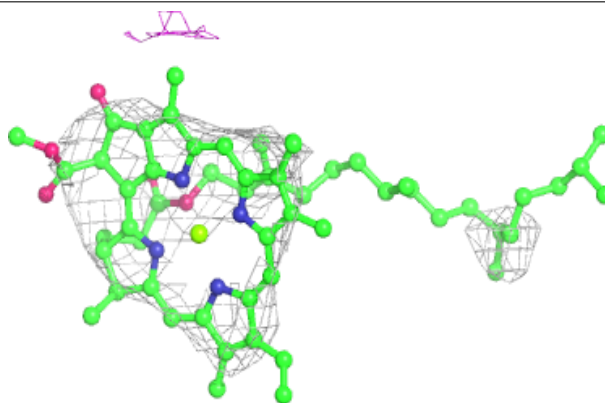


**Electron density around SQD d 402:**

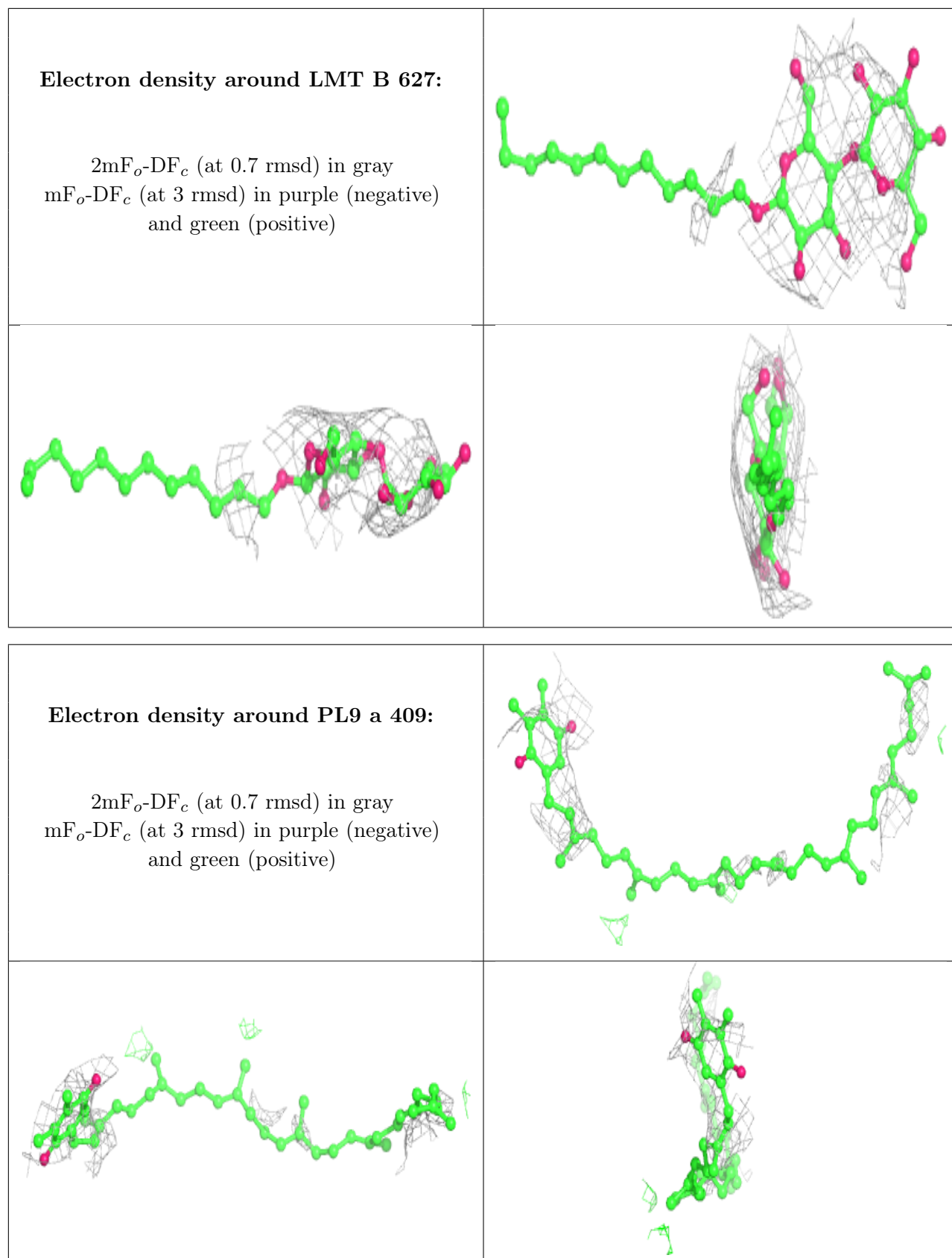
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)



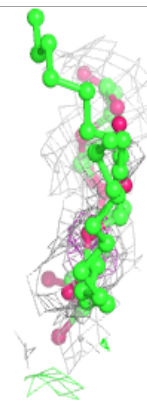
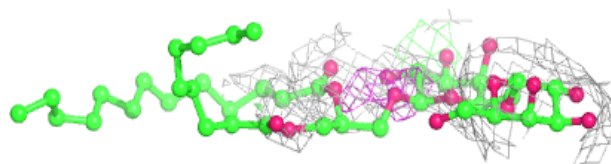
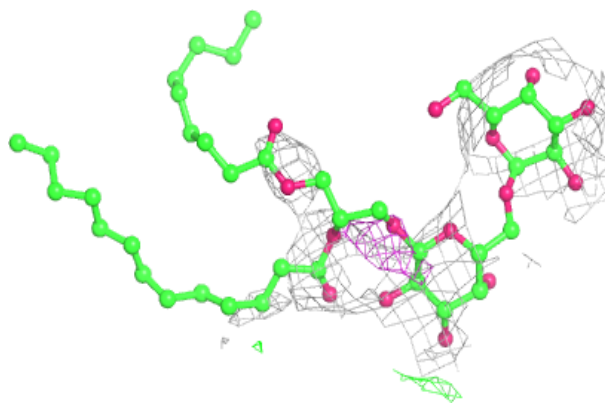




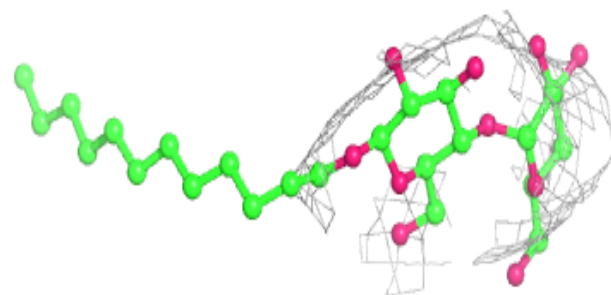
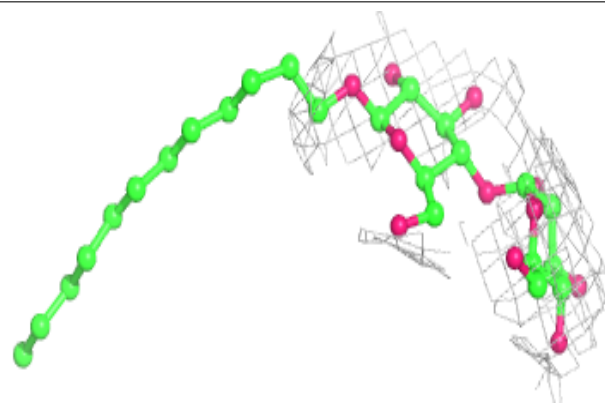


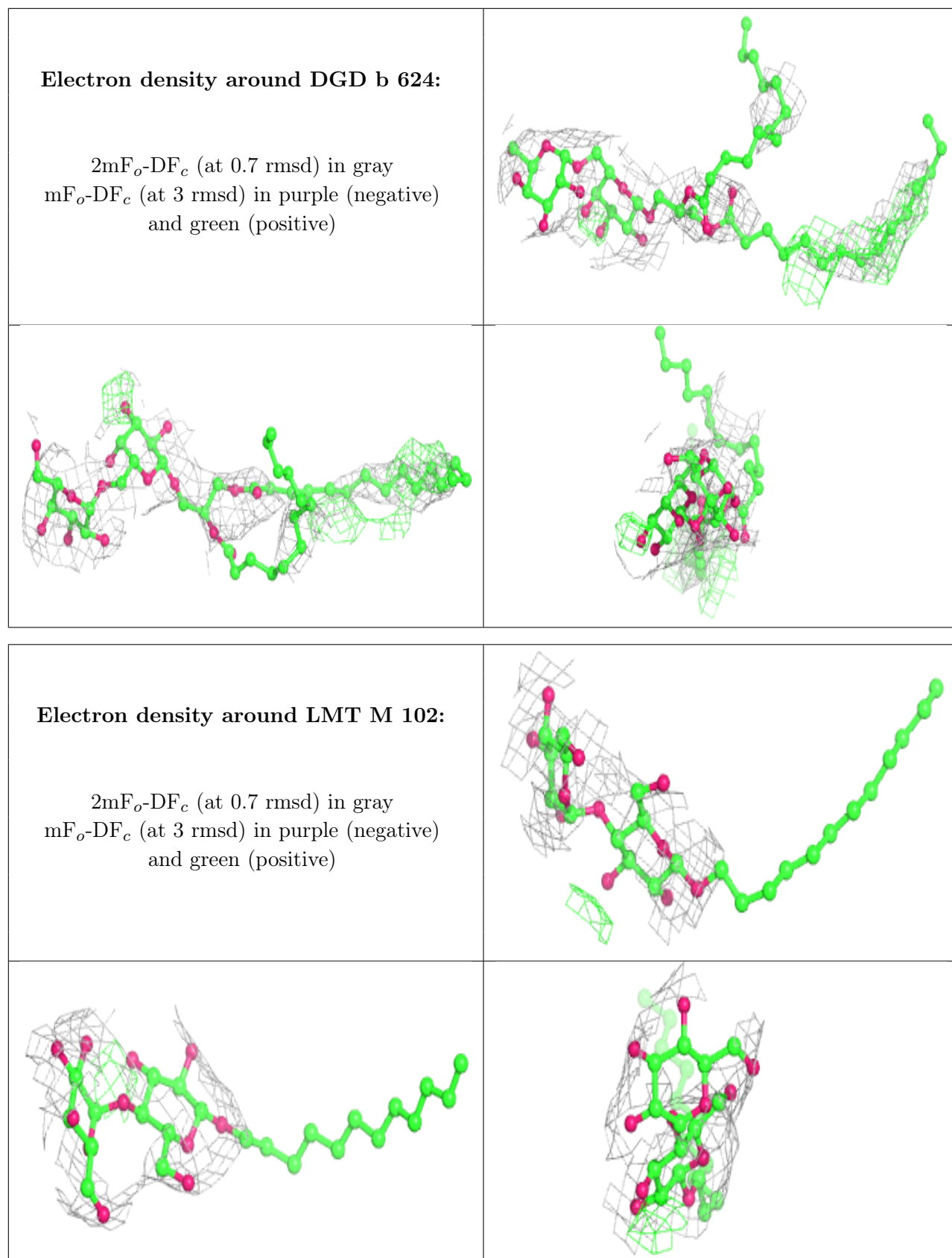
**Electron density around DGD B 625:**

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

**Electron density around LMT M 103:**

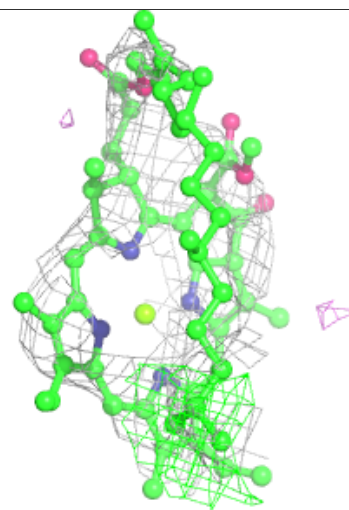
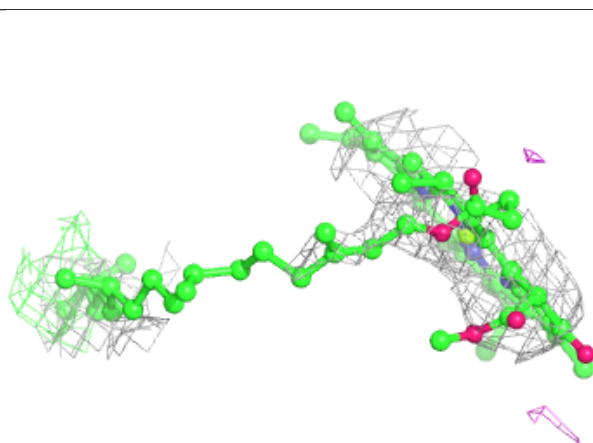
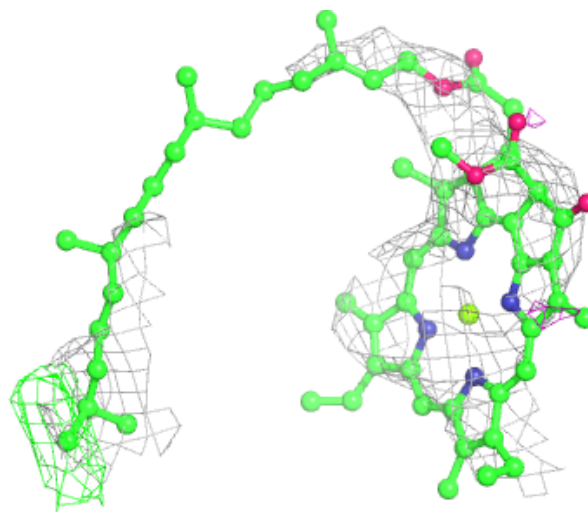
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





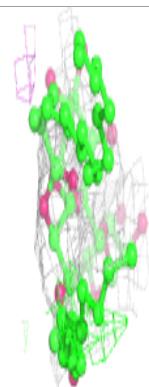
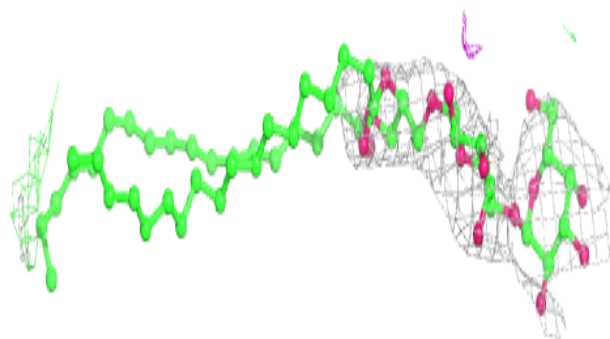
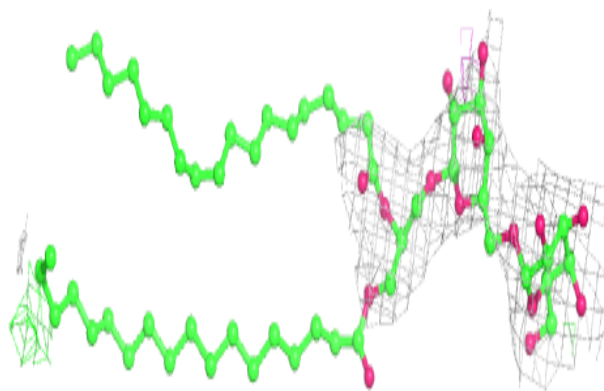
**Electron density around CLA C 506:**

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

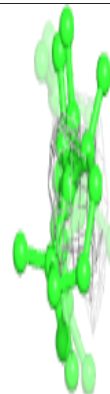
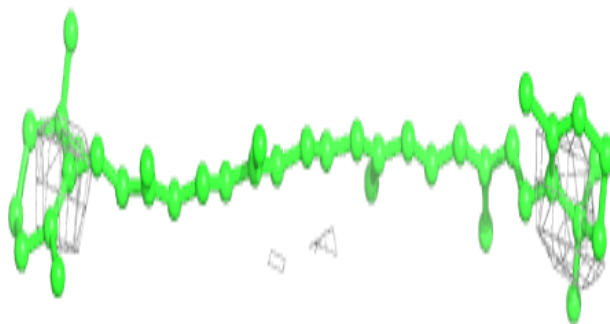
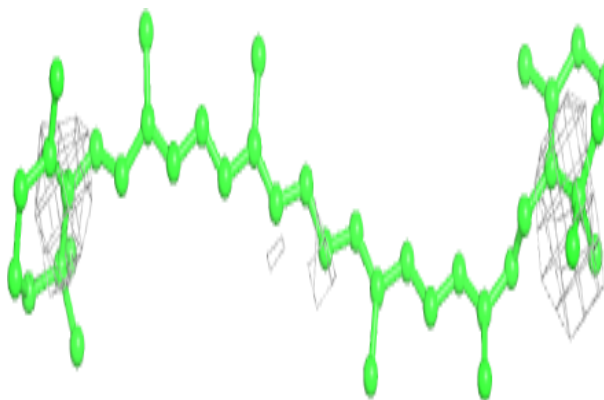


**Electron density around DGD C 517:**

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

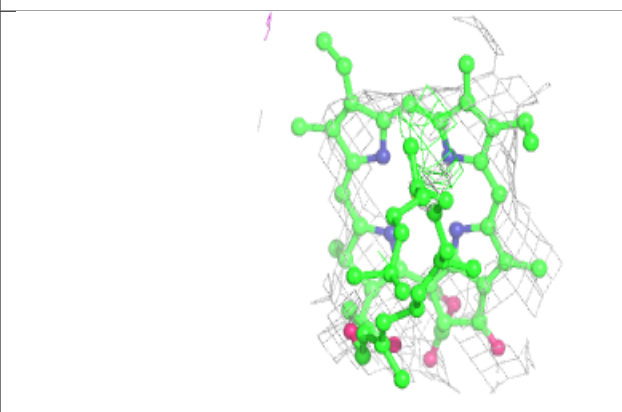
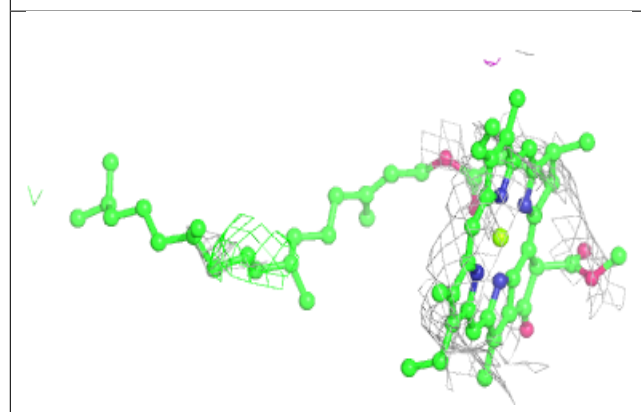
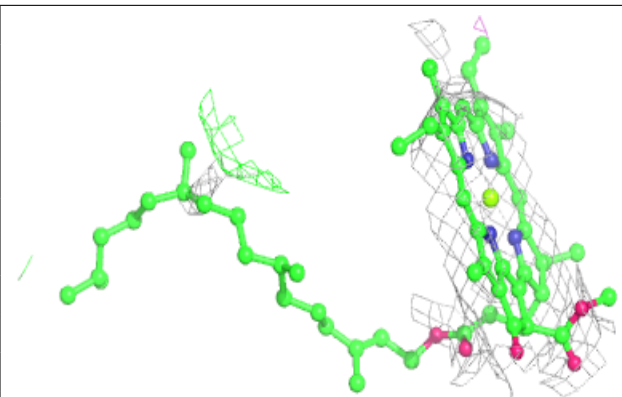
**Electron density around BCR y 101:**

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

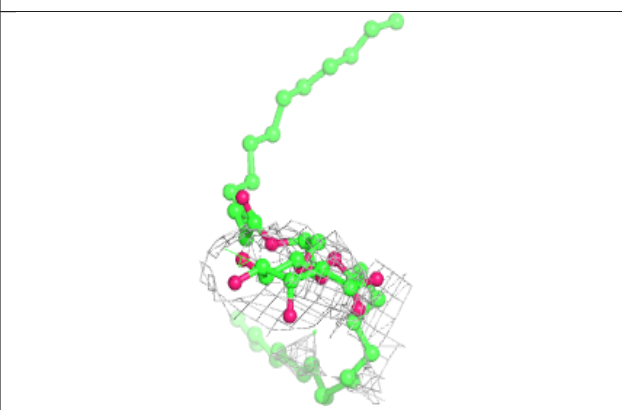
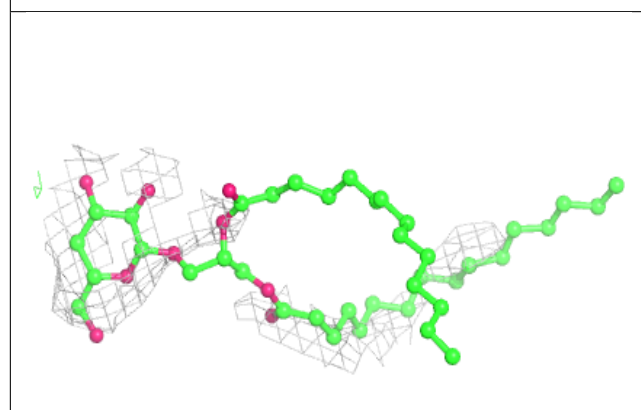
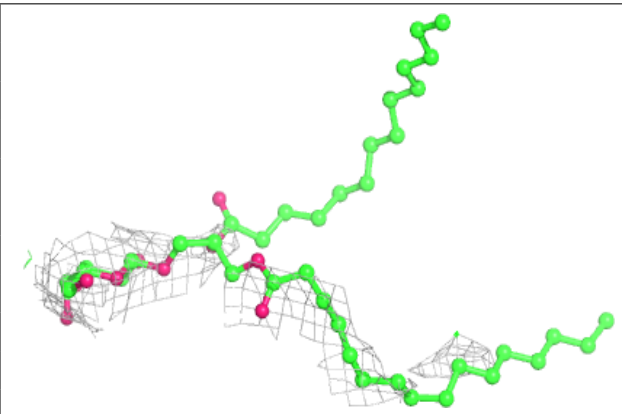


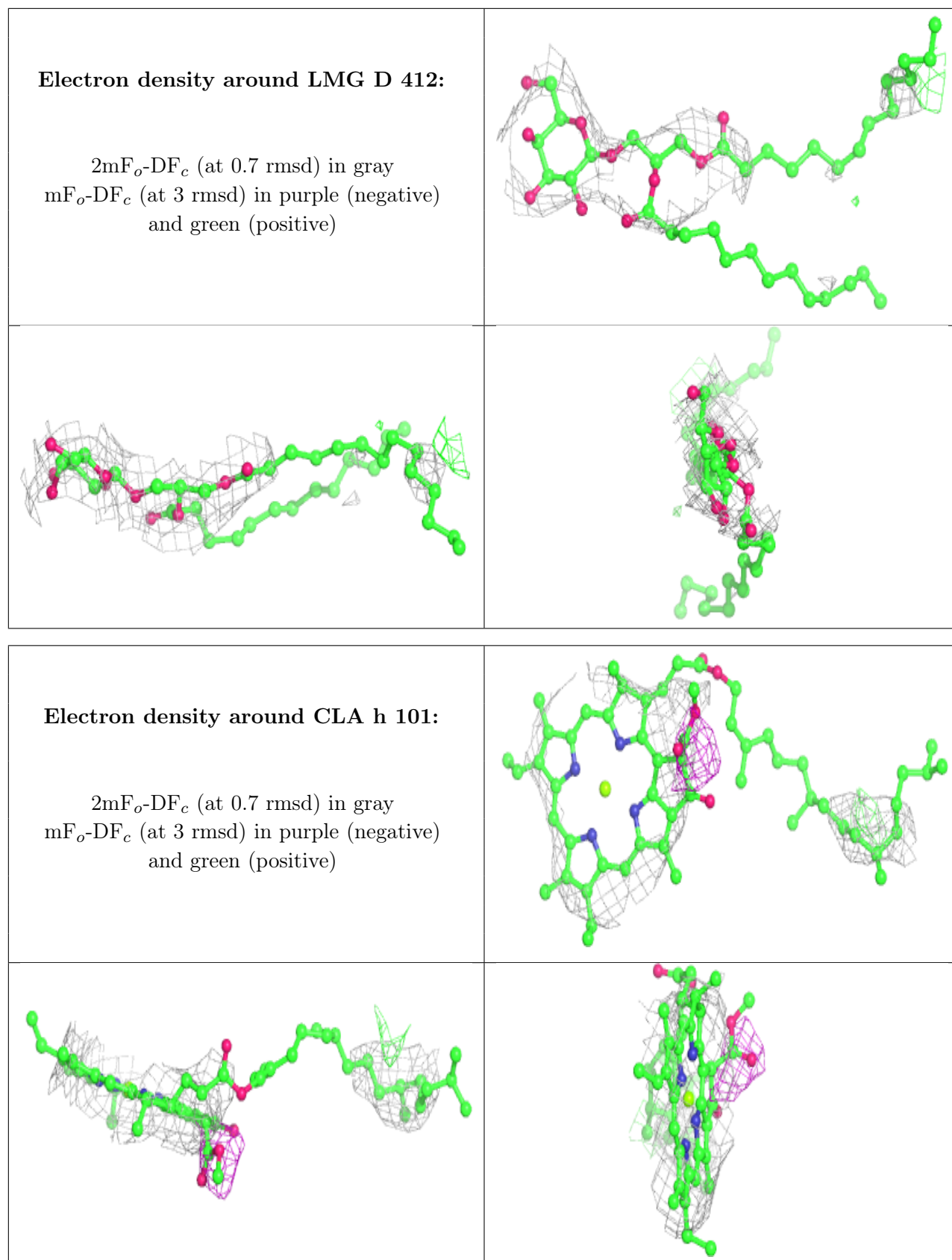
**Electron density around CLA C 507:**

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

**Electron density around LMG b 625:**

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

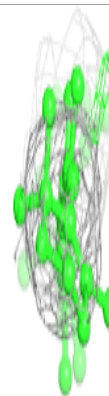
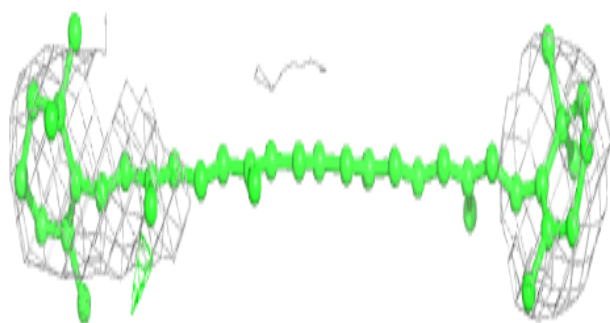
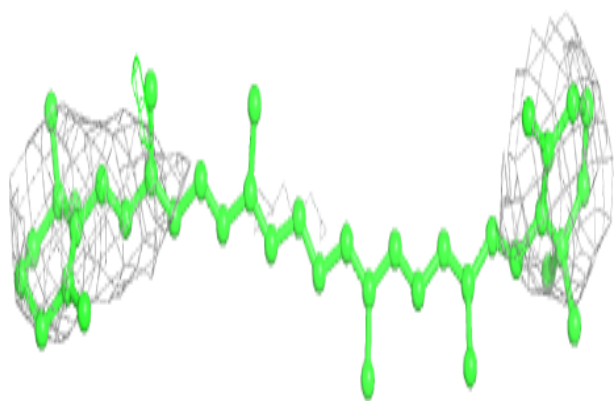




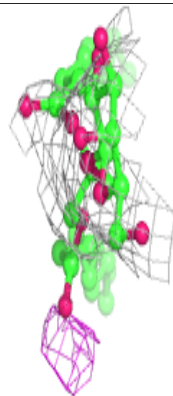
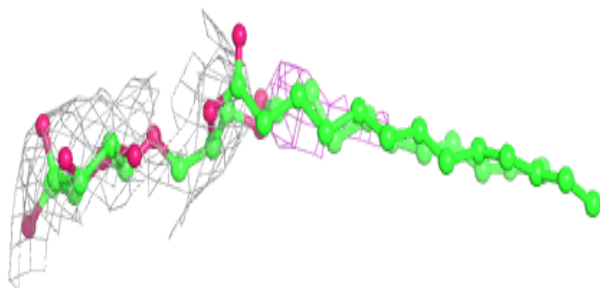
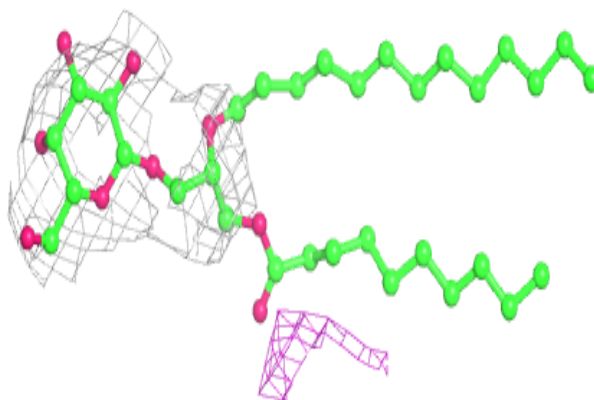


**Electron density around BCR b 622:**

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

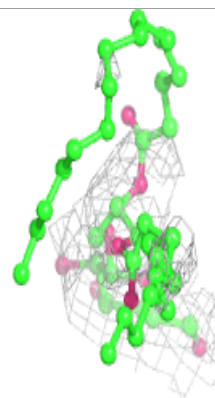
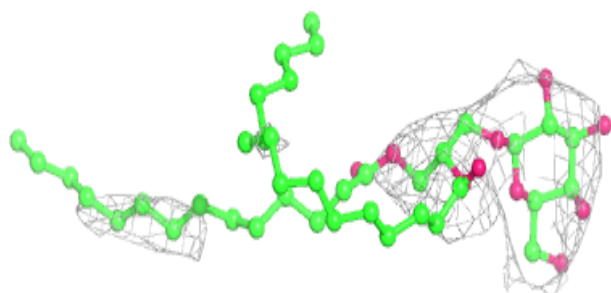
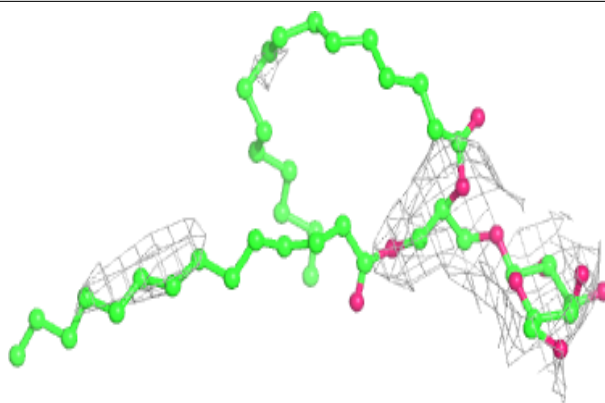
**Electron density around LMG m 101:**

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

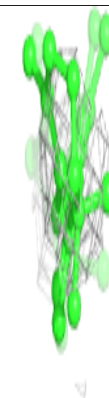
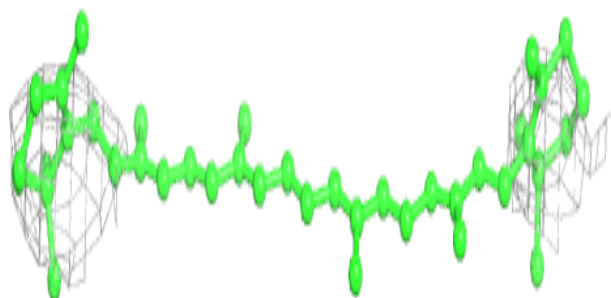
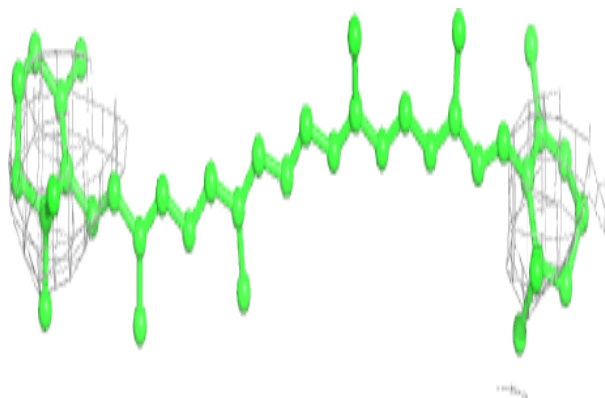


**Electron density around LMG B 624:**

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

**Electron density around BCR C 514:**

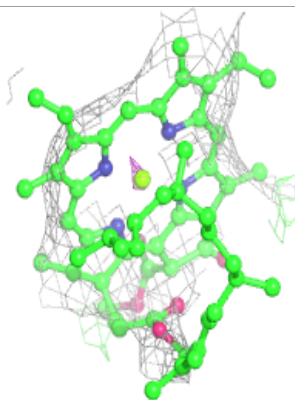
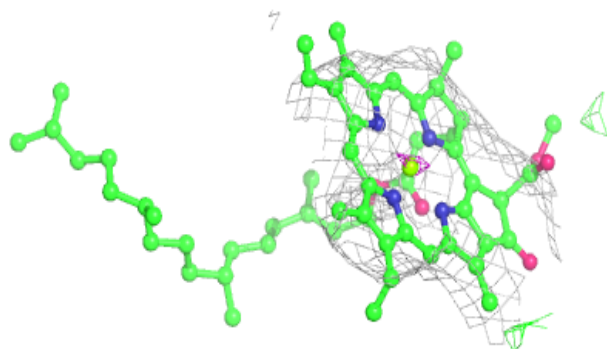
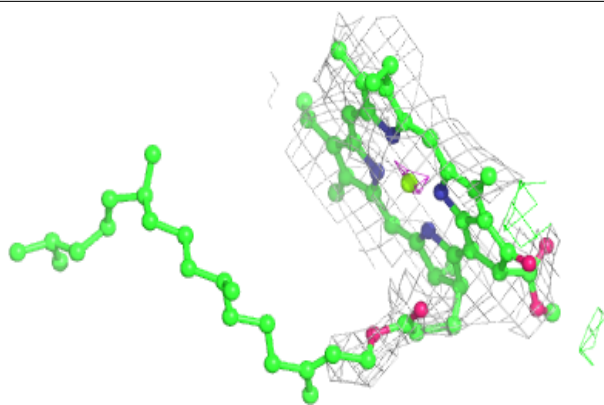
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



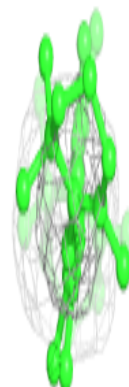
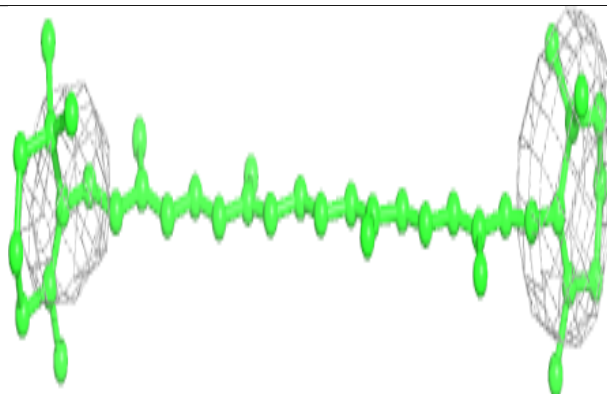
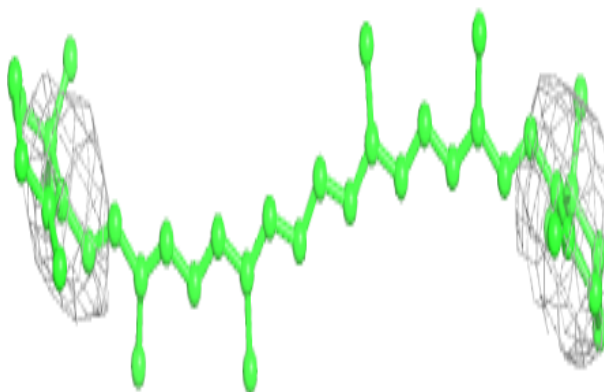


**Electron density around CLA c 512:**

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

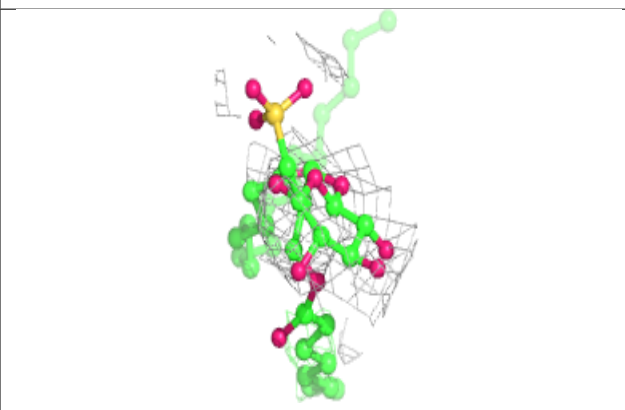
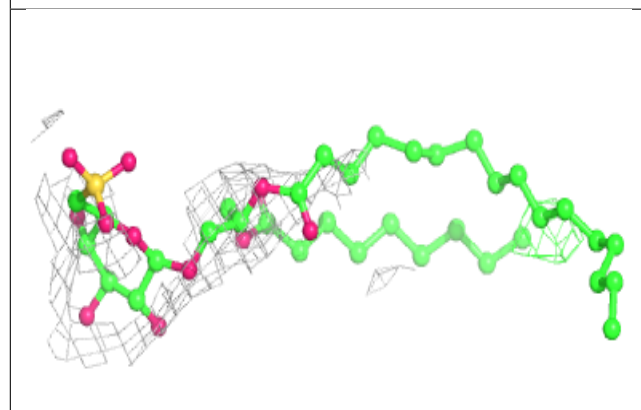
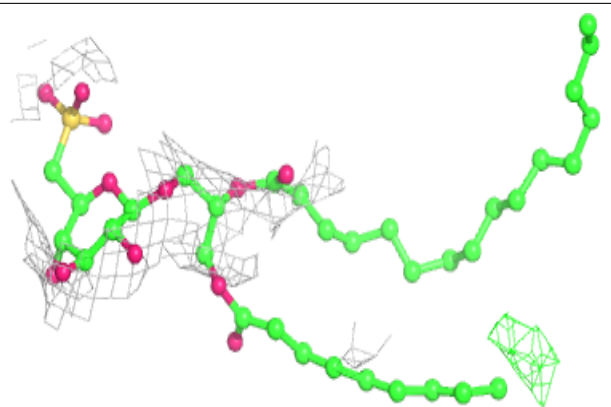
**Electron density around BCR A 407:**

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

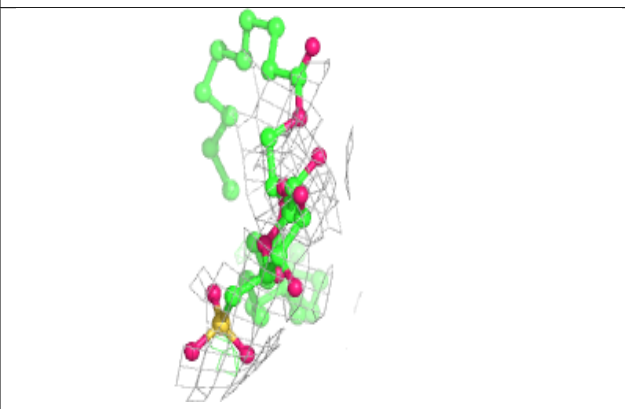
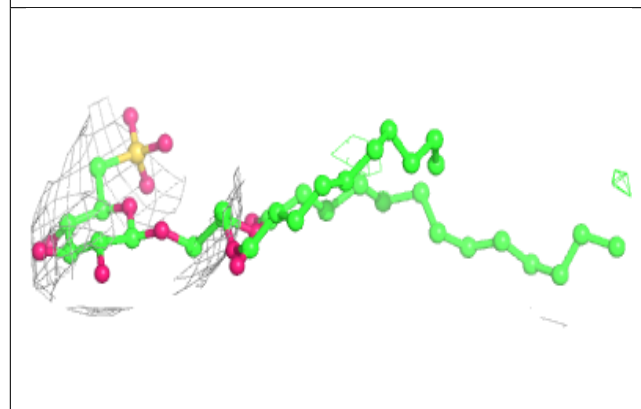
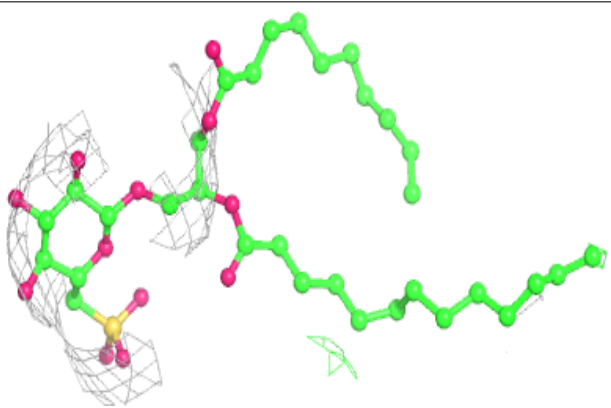


**Electron density around SQD B 626:**

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

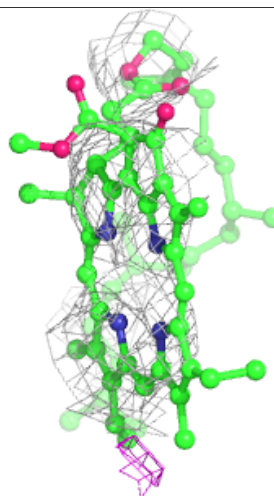
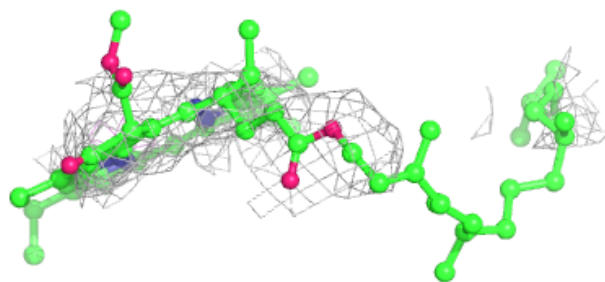
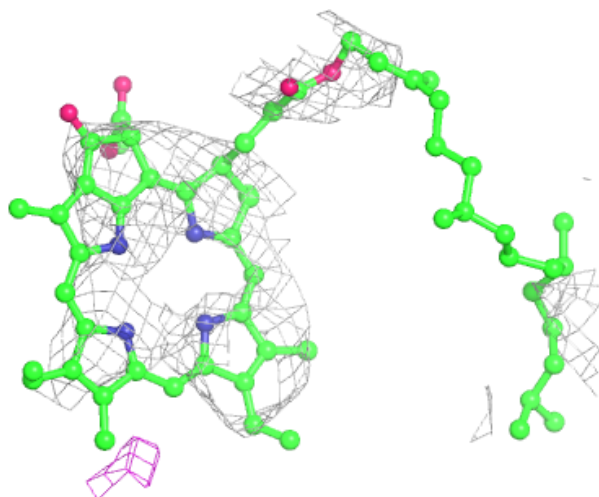
**Electron density around SQD F 102:**

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



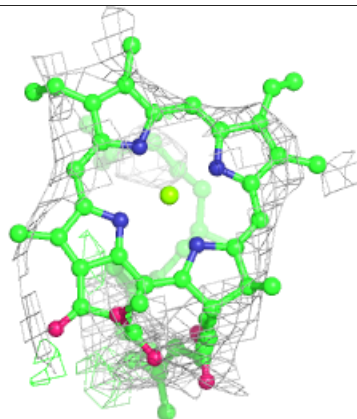
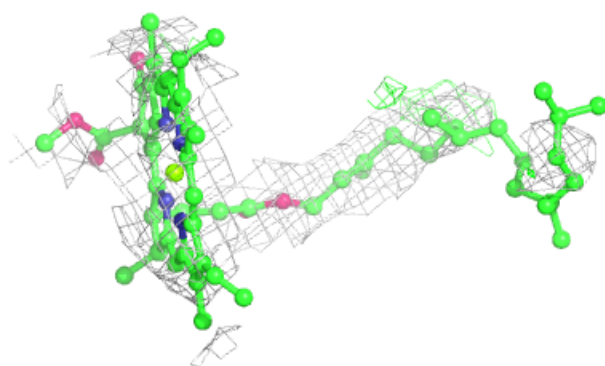
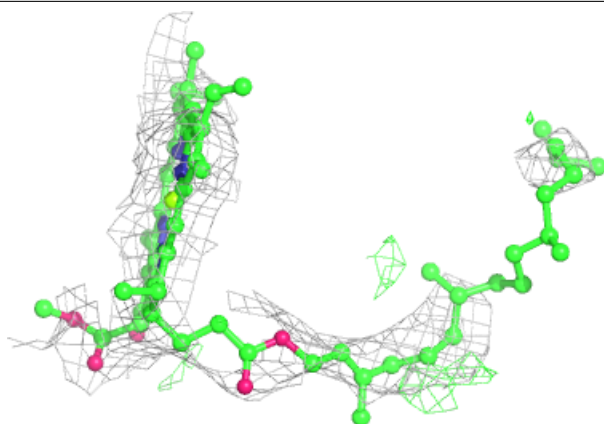
**Electron density around PHO D 402:**

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

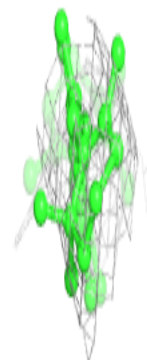
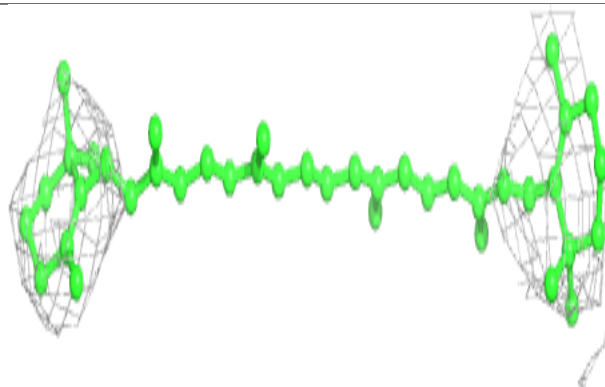
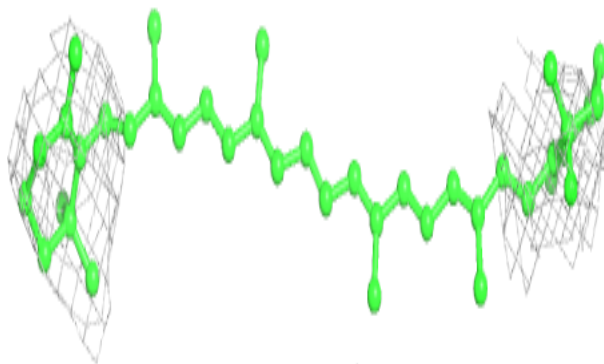


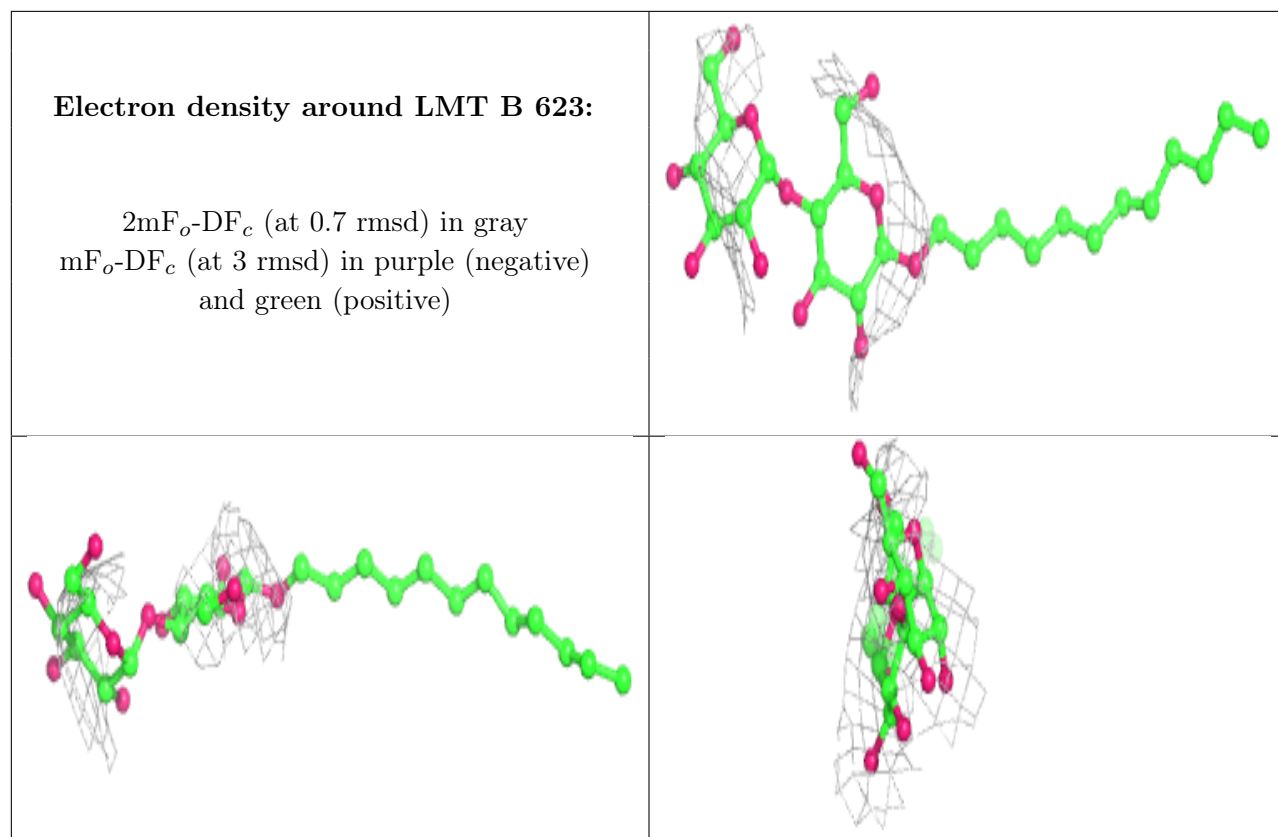
**Electron density around CLA C 505:**

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

**Electron density around BCR C 521:**

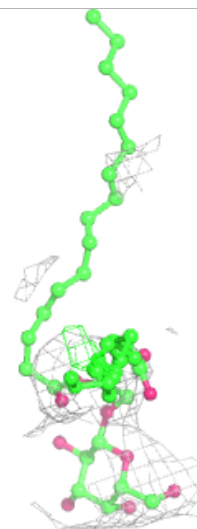
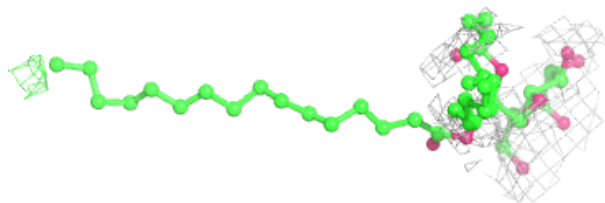
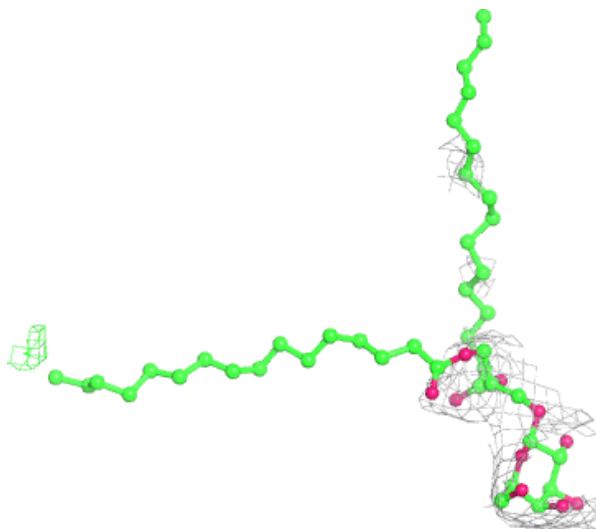
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





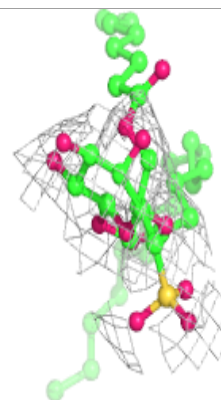
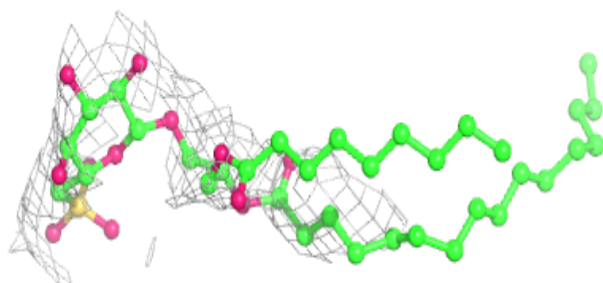
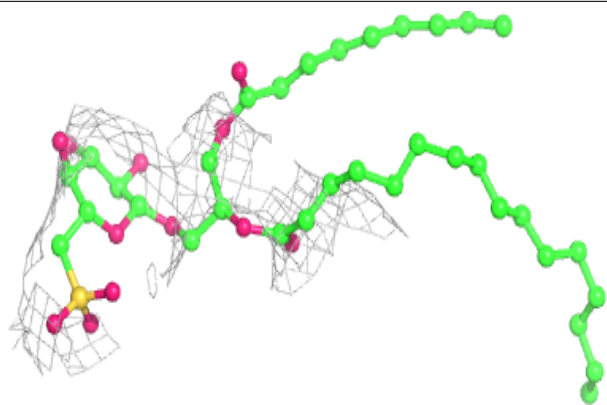
**Electron density around LMG A 410:**

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

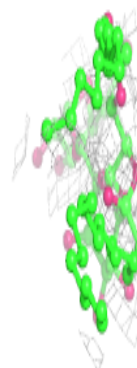
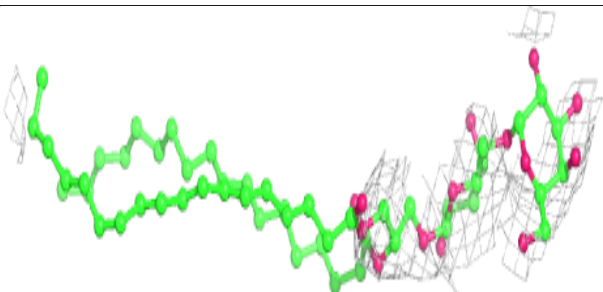
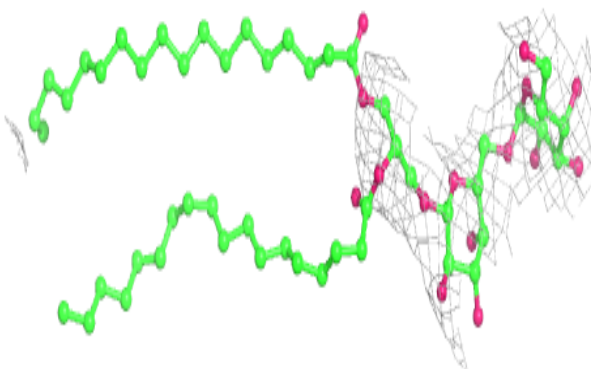


**Electron density around SQD b 602:**

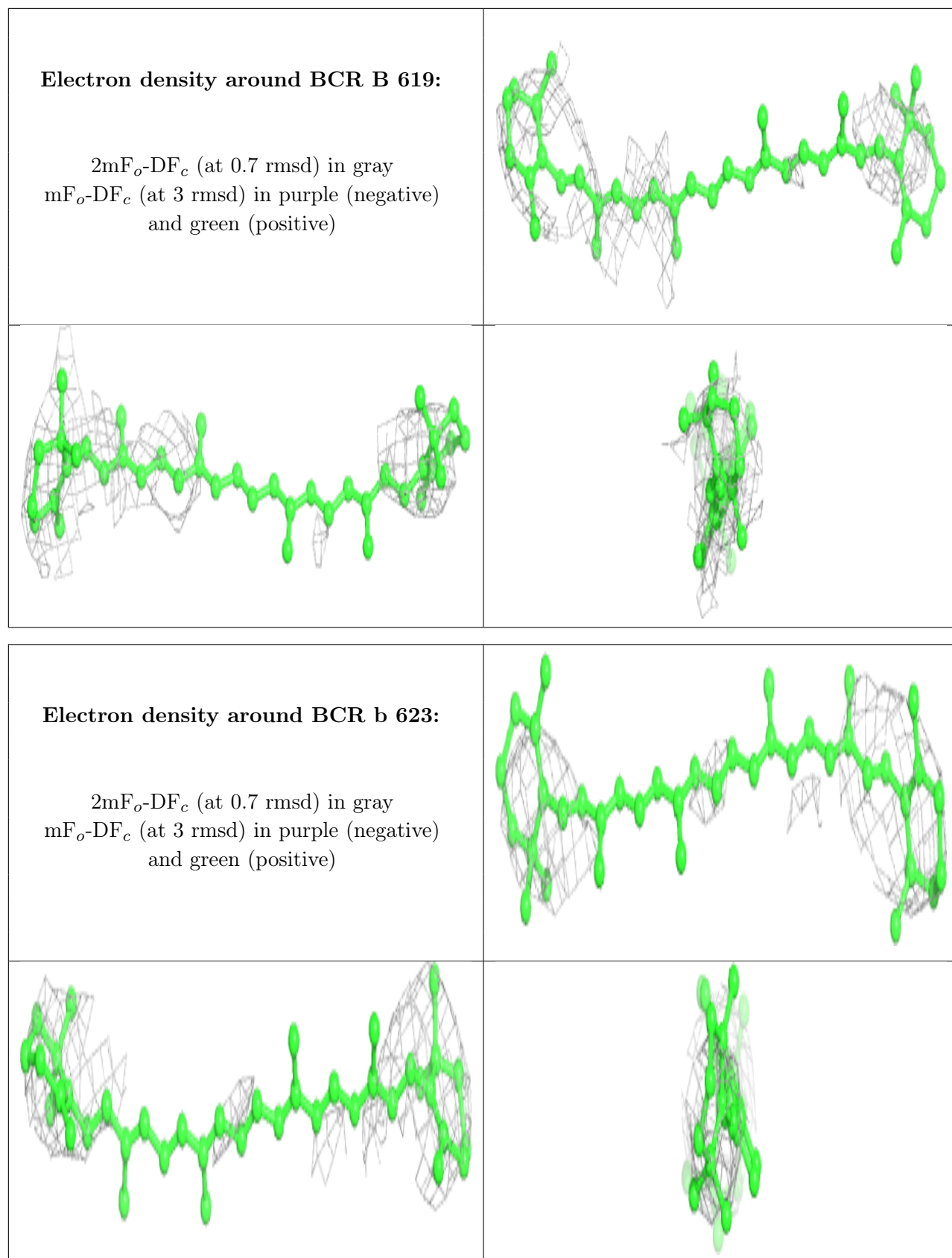
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)



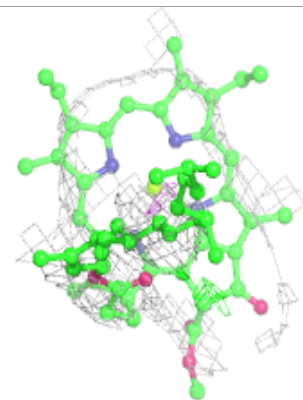
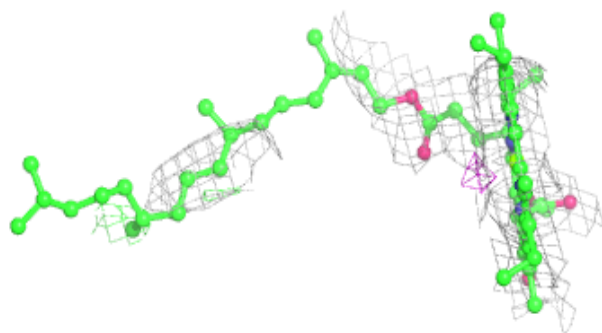
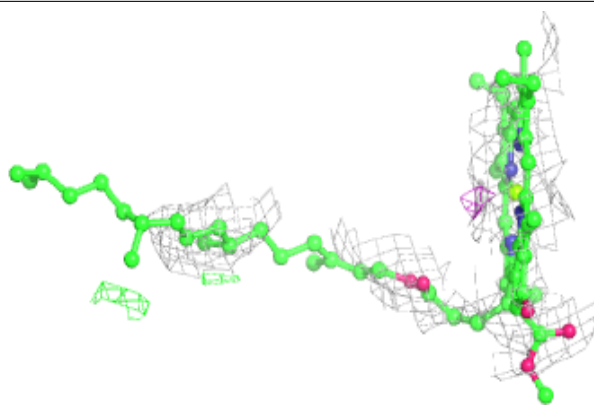




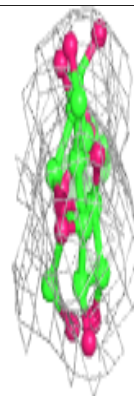
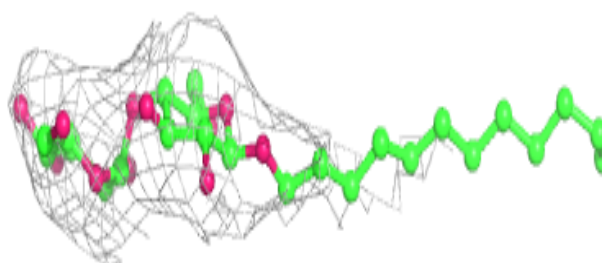
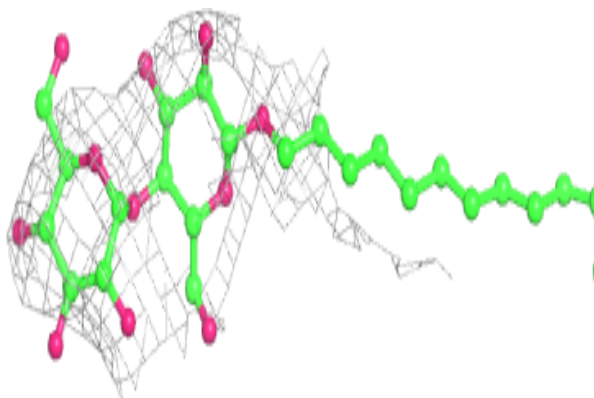


**Electron density around CLA b 609:**

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

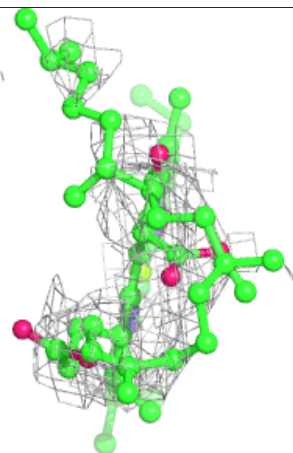
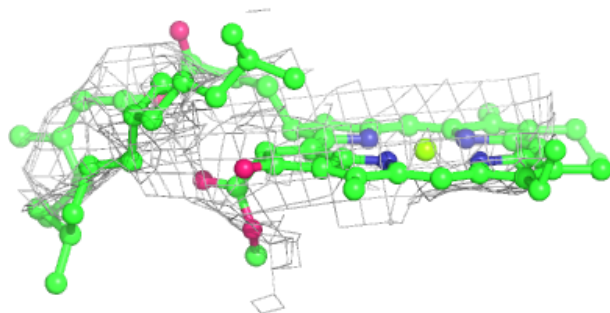
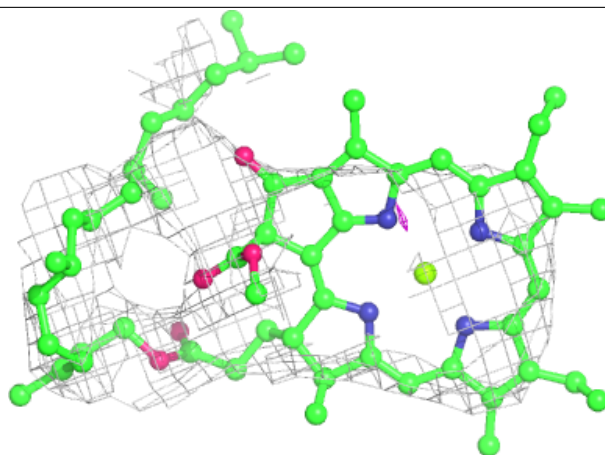
**Electron density around LMT b 603:**

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

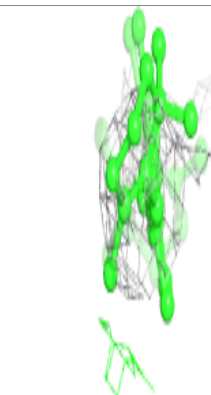
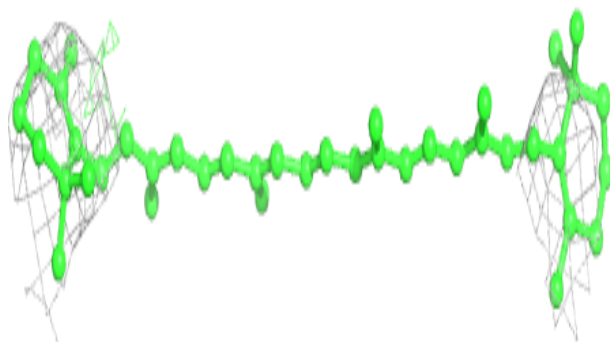
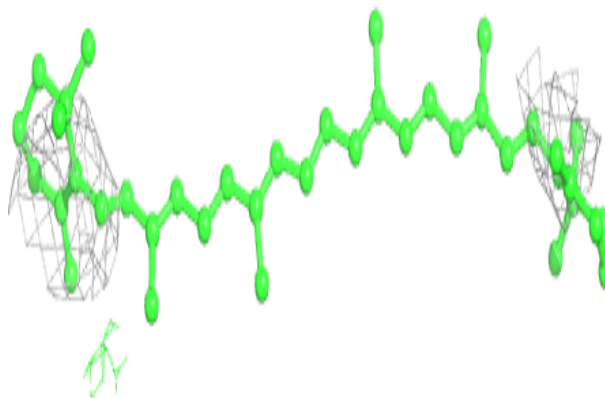


**Electron density around CLA b 613:**

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

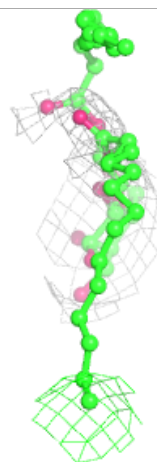
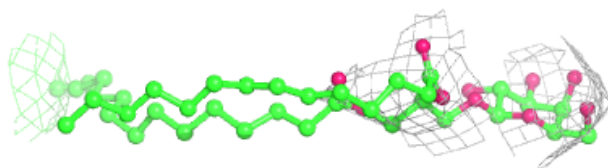
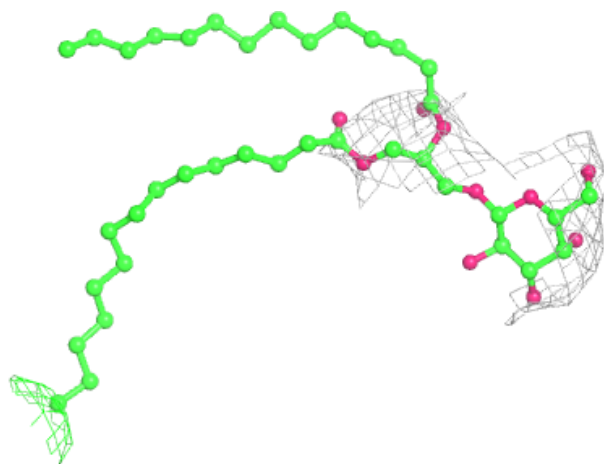
**Electron density around BCR c 521:**

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



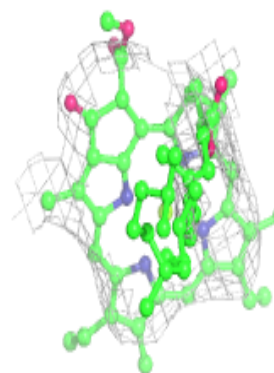
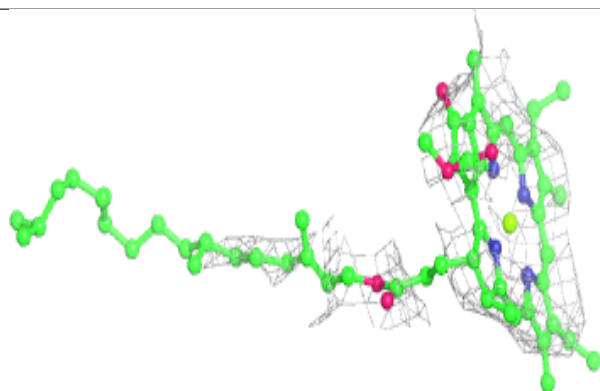
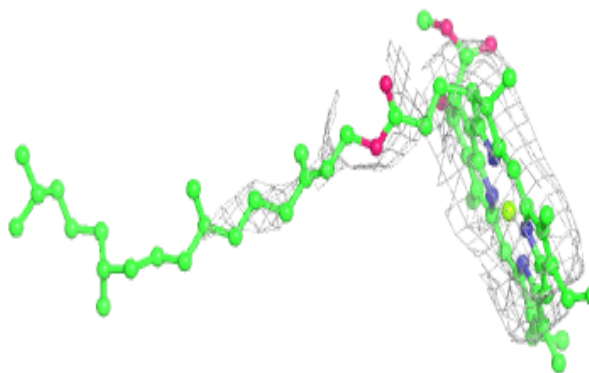
**Electron density around LMG c 522:**

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

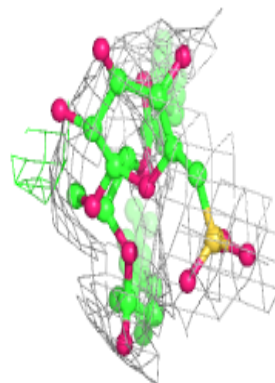
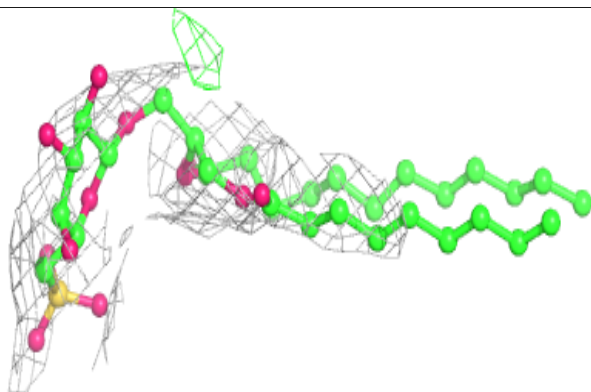
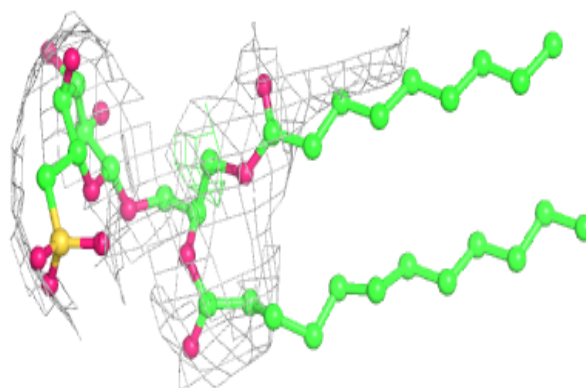


**Electron density around CLA B 603:**

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

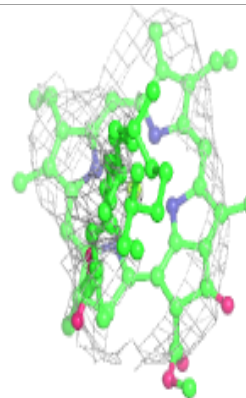
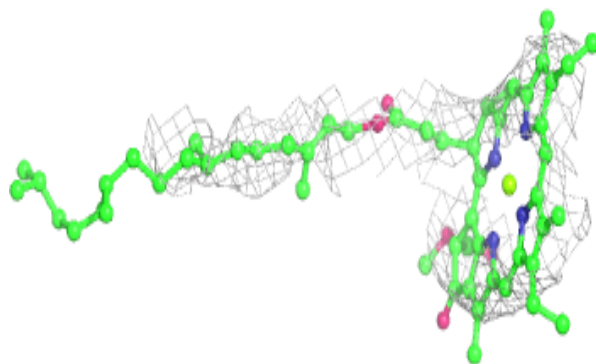
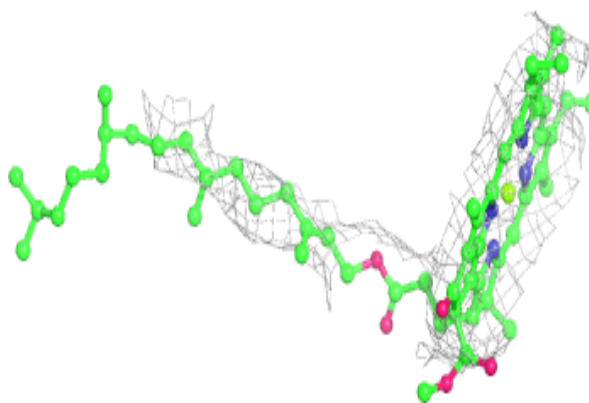
**Electron density around SQD D 403:**

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



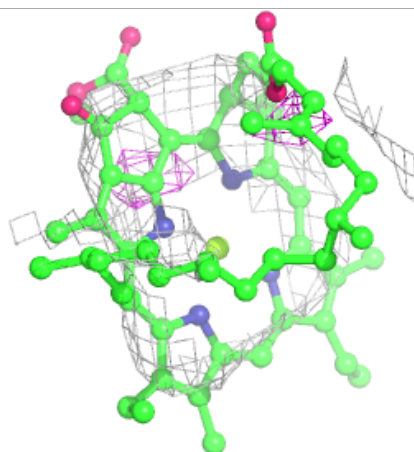
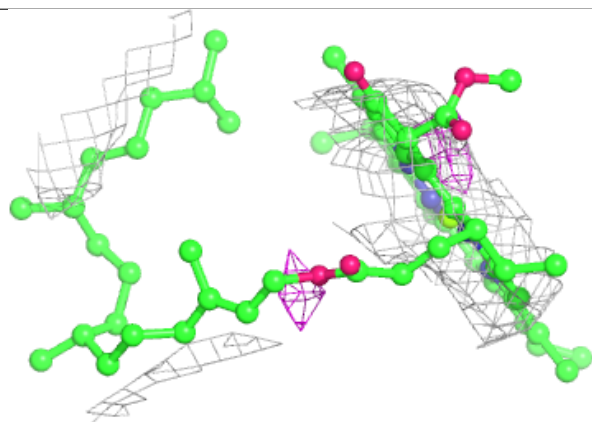
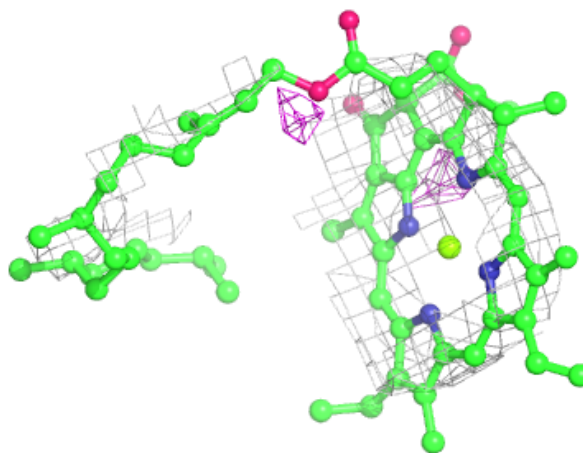
**Electron density around CLA b 607:**

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



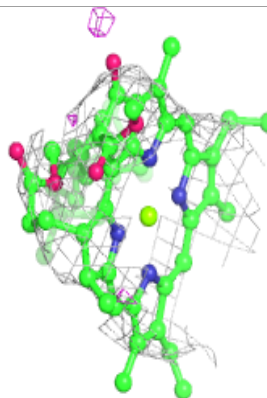
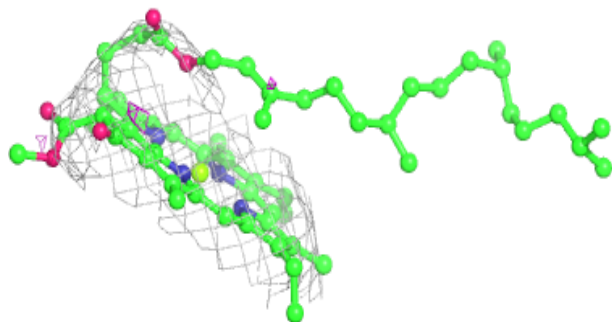
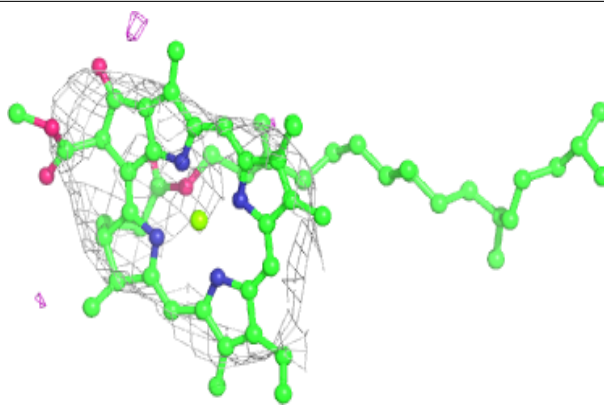
**Electron density around CLA c 503:**

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



**Electron density around CLA b 617:**

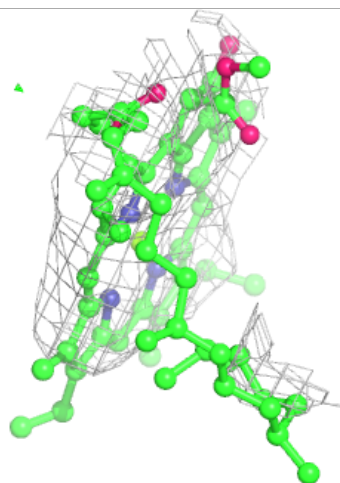
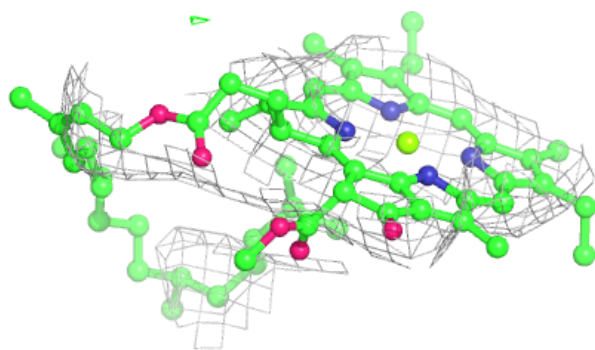
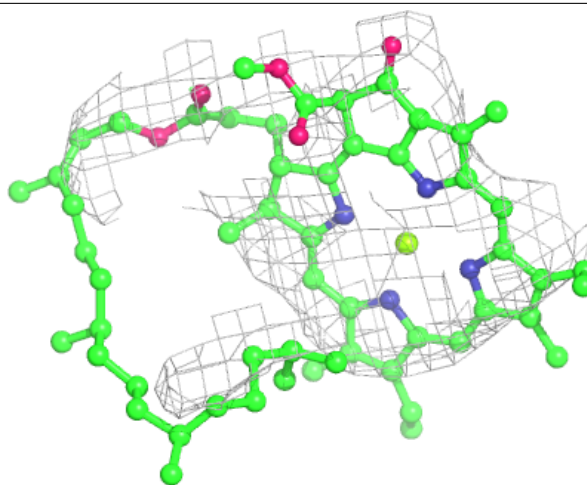
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA b 618:**

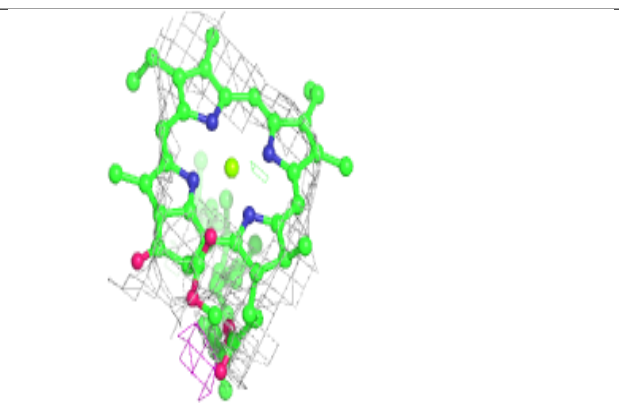
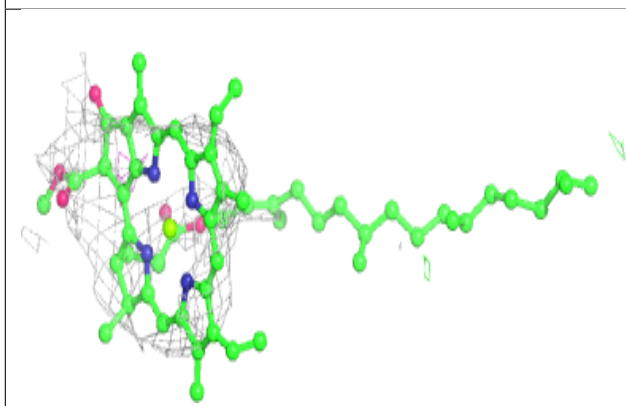
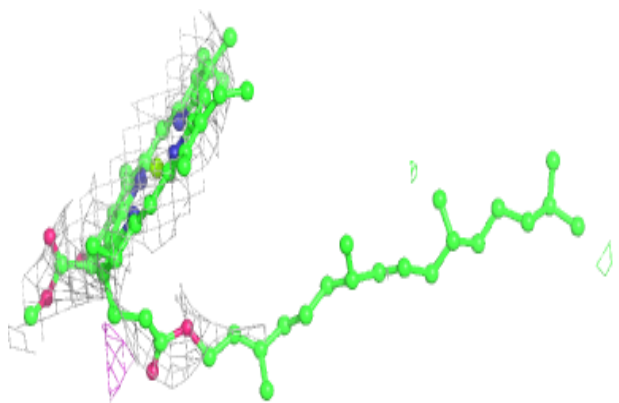
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



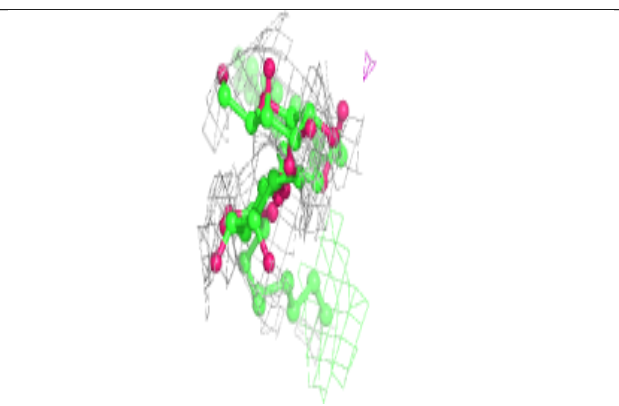
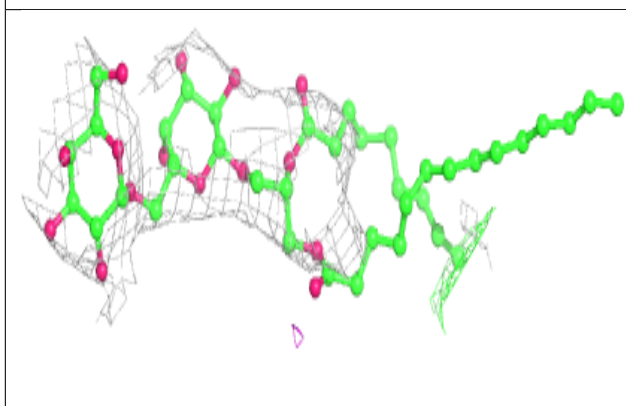
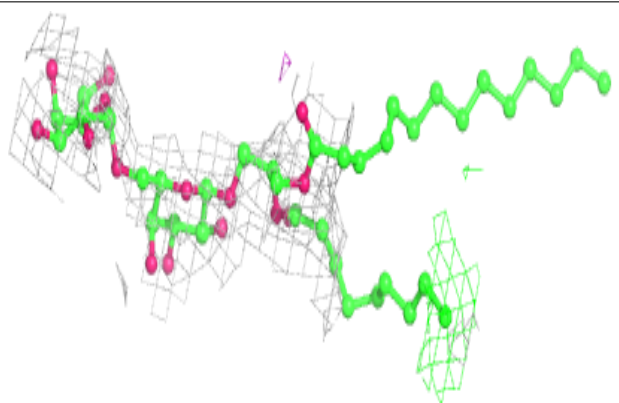


**Electron density around CLA C 520:**

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

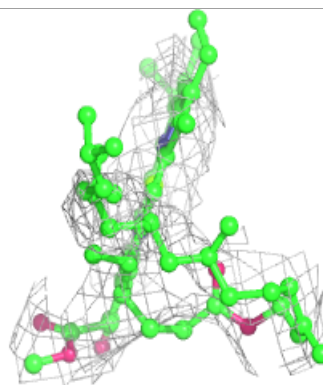
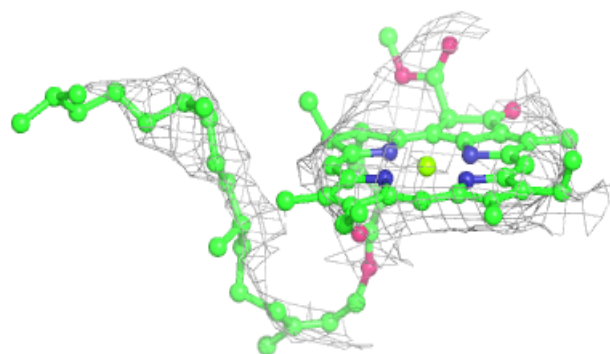
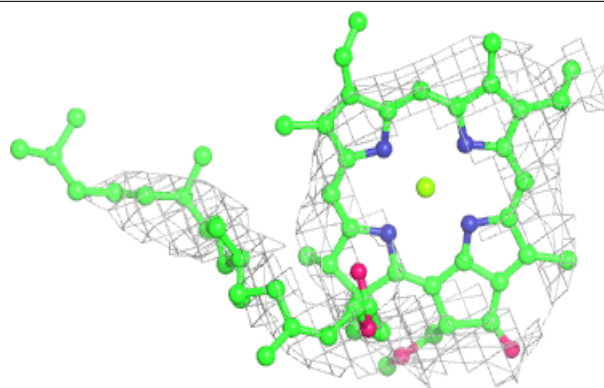
**Electron density around DGD C 515:**

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

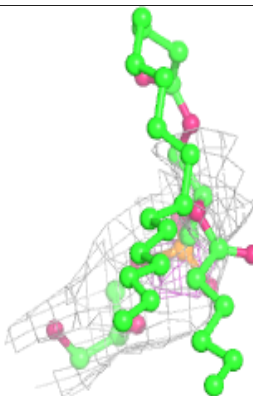
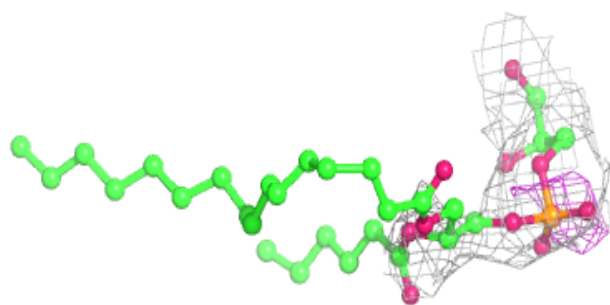
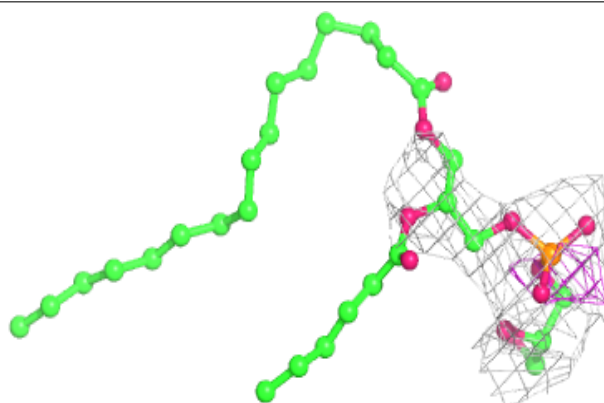


**Electron density around CLA a 405:**

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

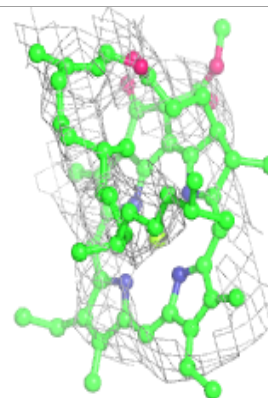
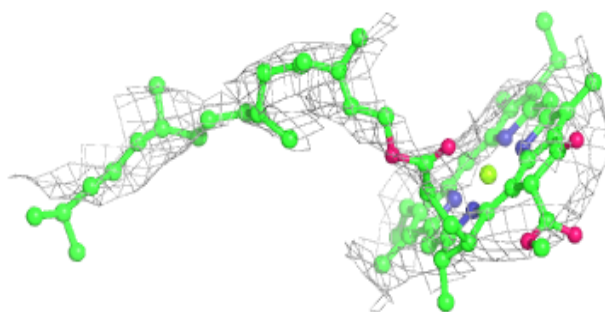
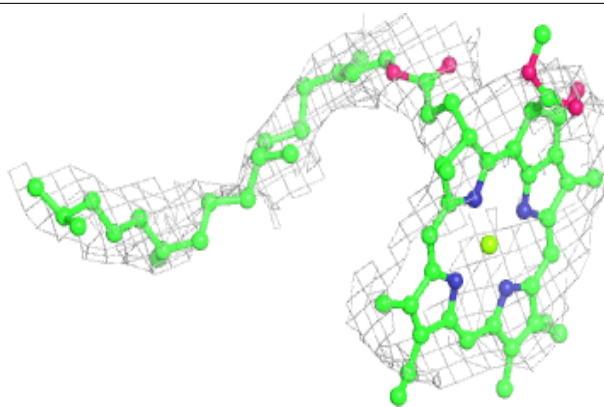
**Electron density around LHG a 412:**

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

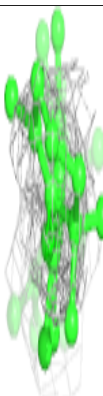
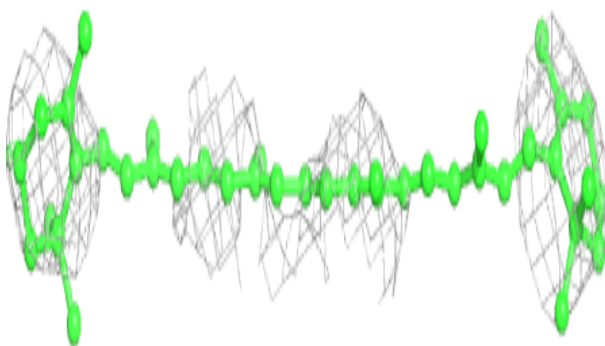
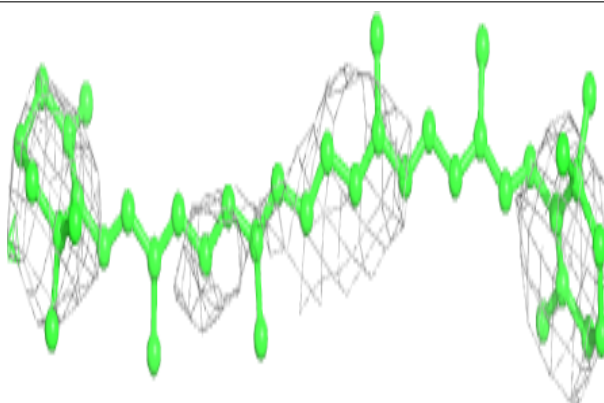


**Electron density around CLA C 510:**

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

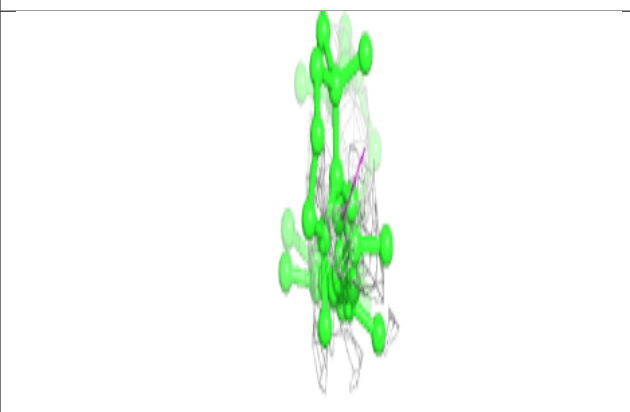
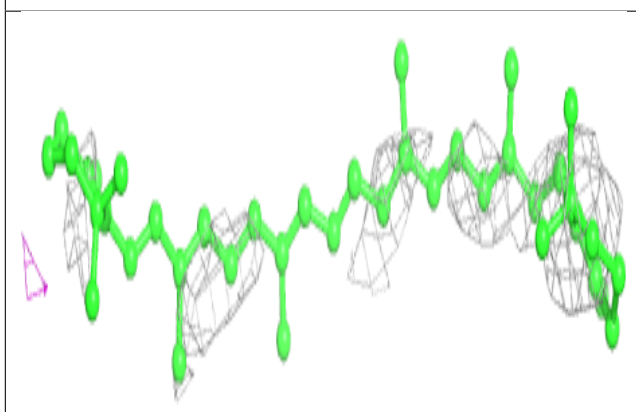
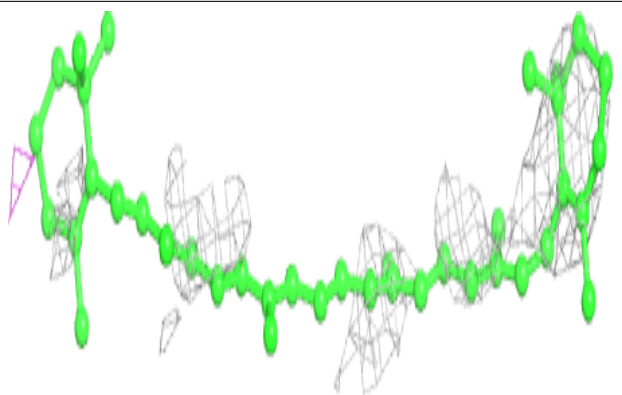
**Electron density around BCR B 618:**

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

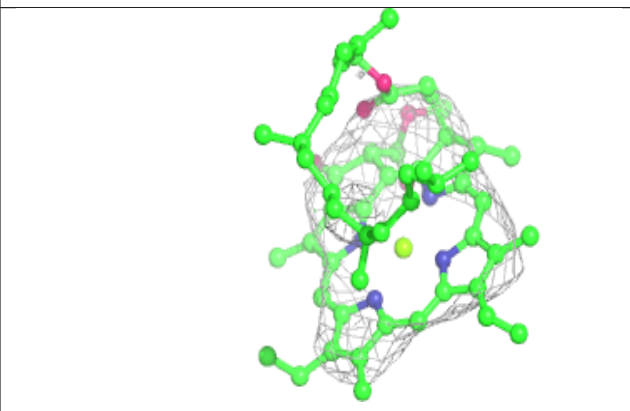
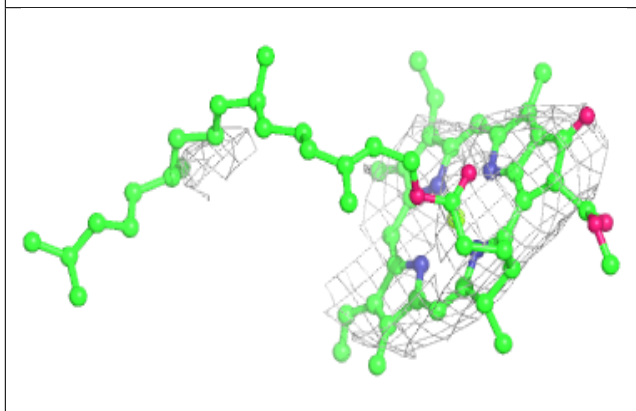
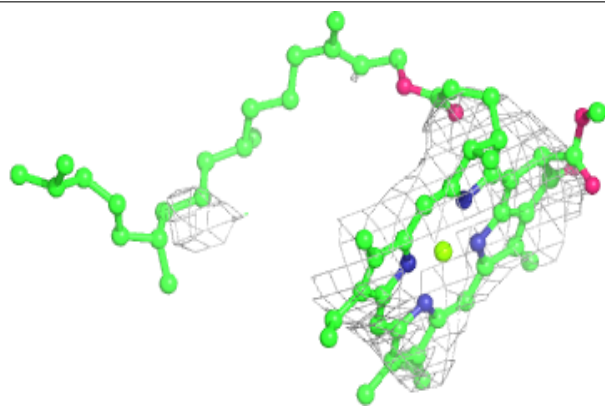


**Electron density around BCR c 513:**

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

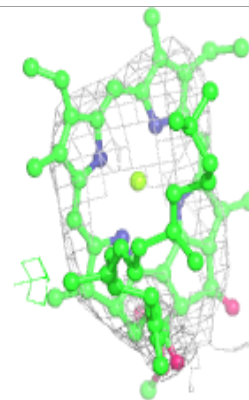
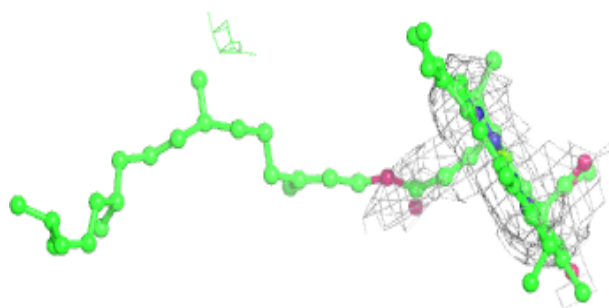
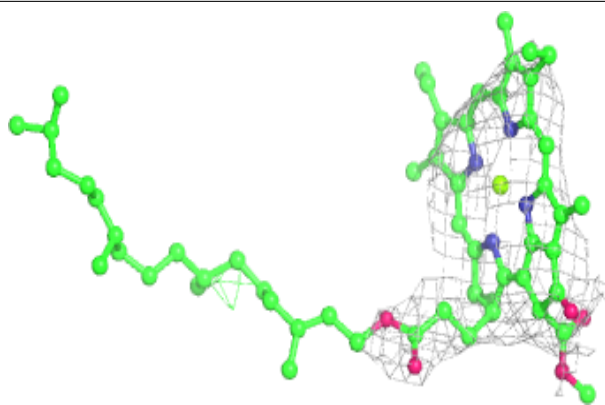
**Electron density around CLA C 512:**

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

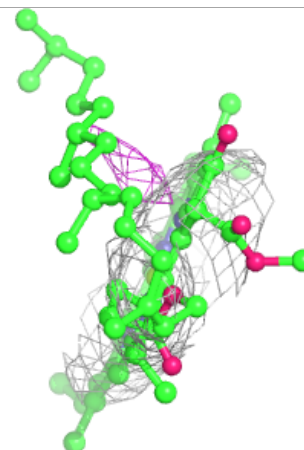
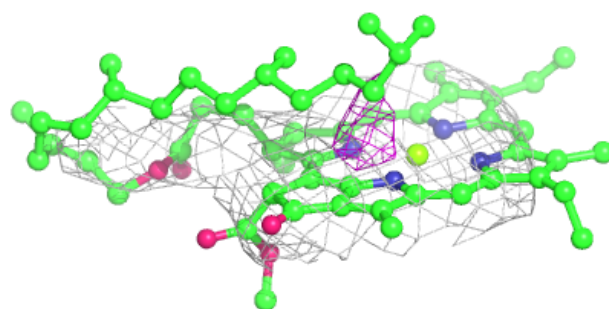
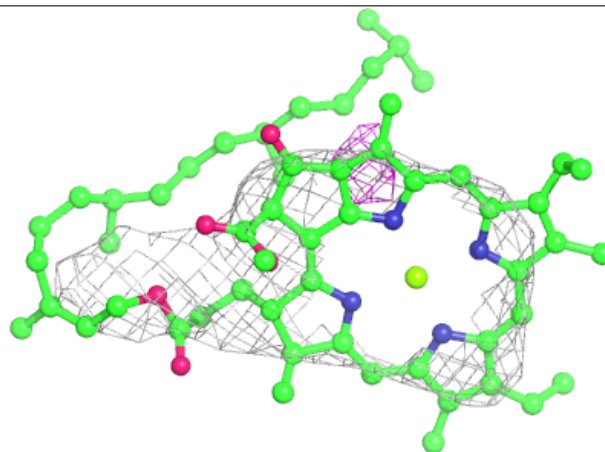


**Electron density around CLA A 405:**

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

**Electron density around CLA c 508:**

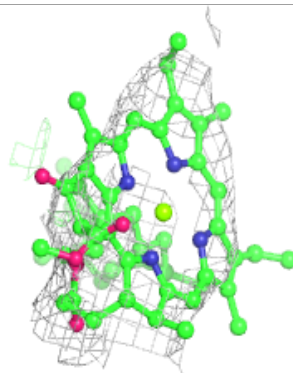
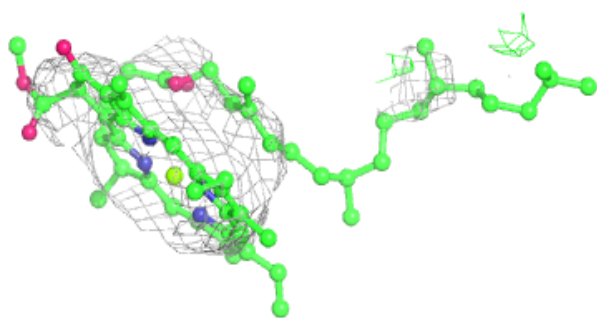
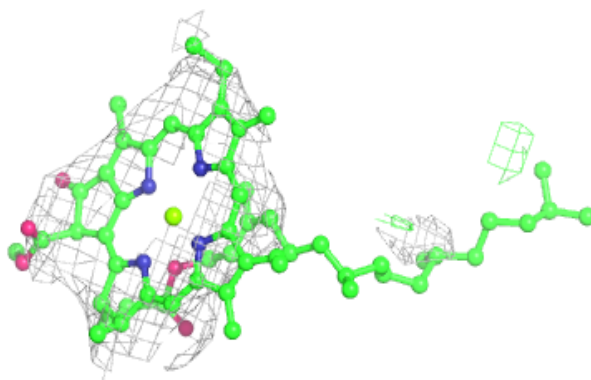
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



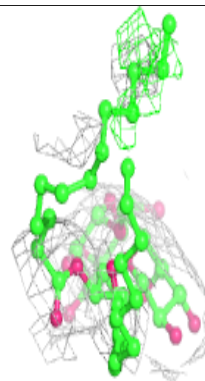
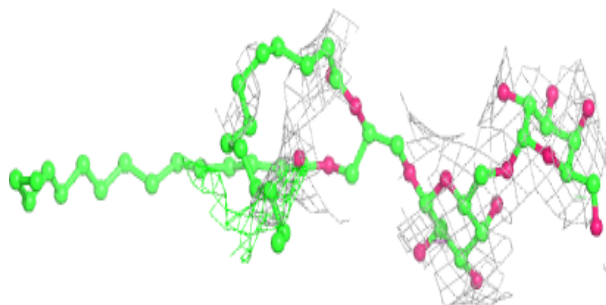
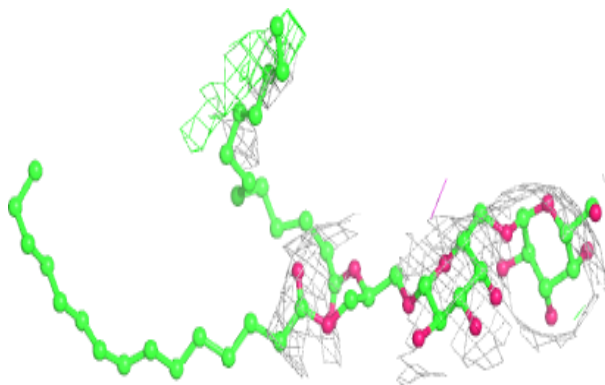


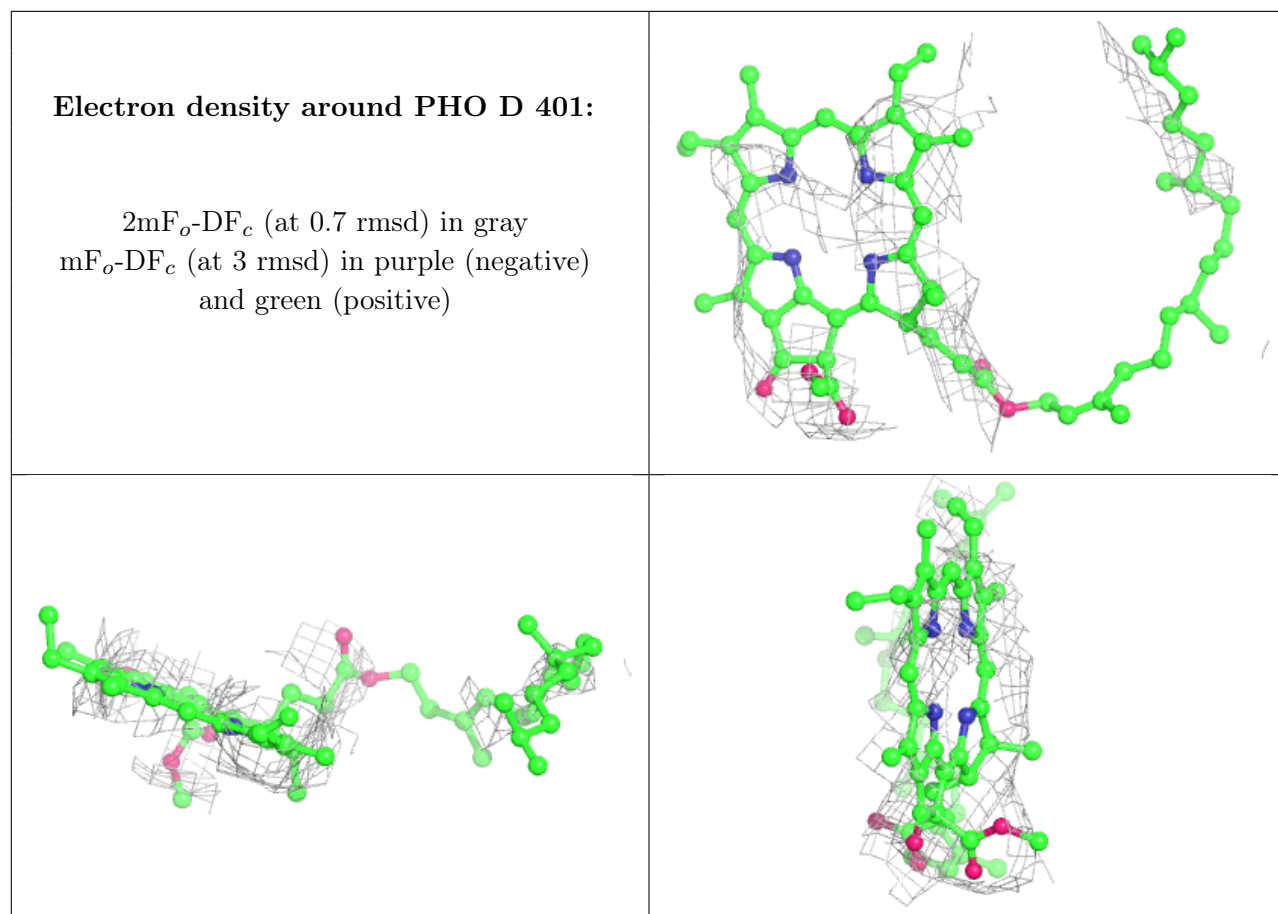
**Electron density around CLA C 504:**

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

**Electron density around DGD B 620:**

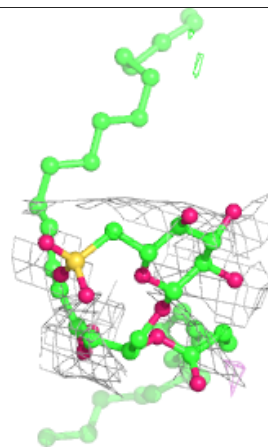
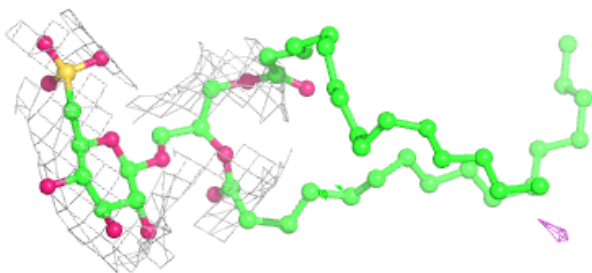
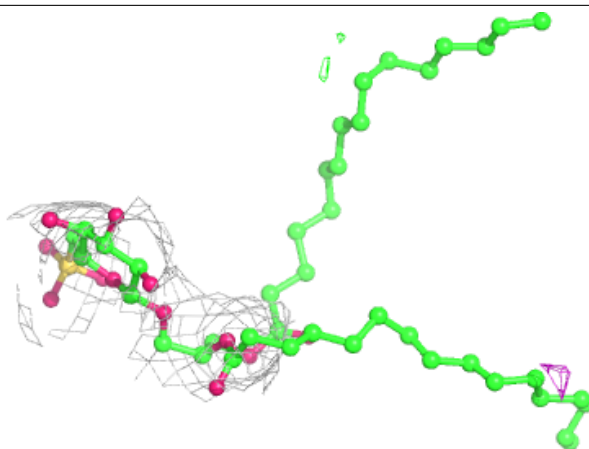
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



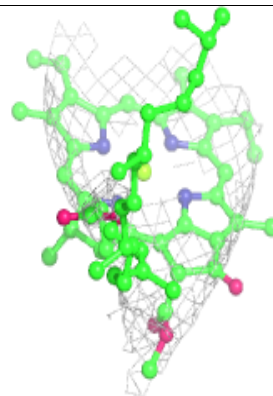
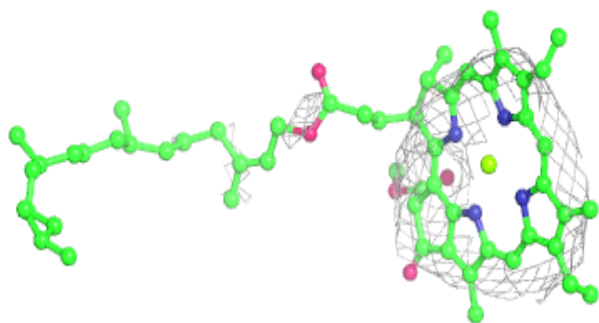
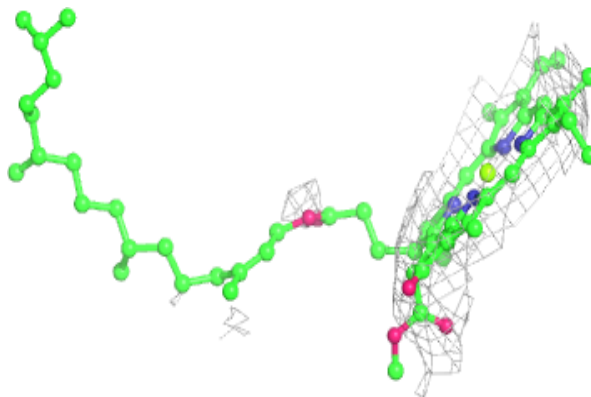


**Electron density around SQD a 401:**

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

**Electron density around CLA d 404:**

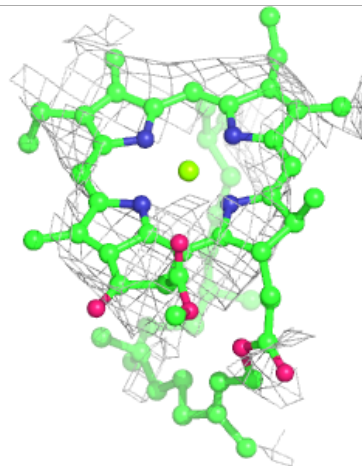
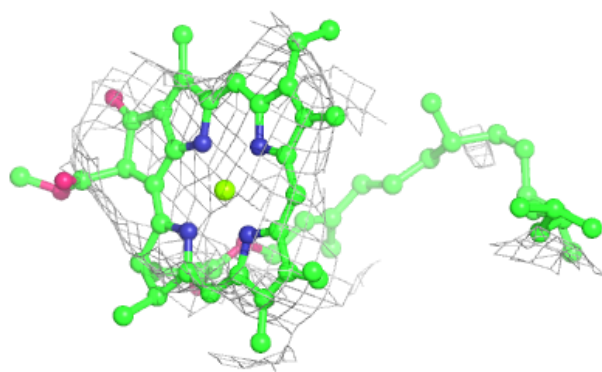
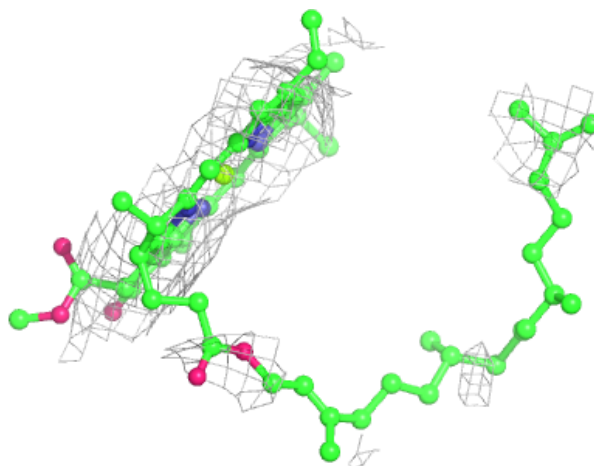
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)





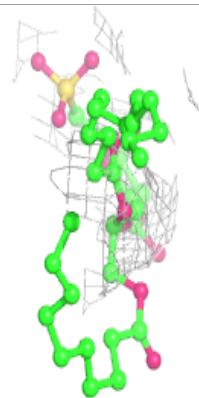
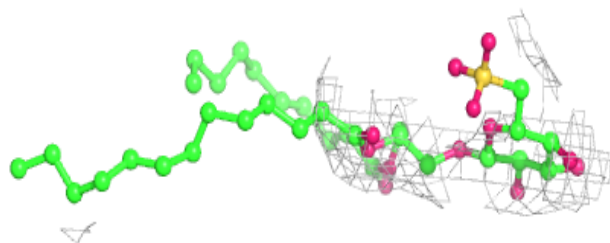
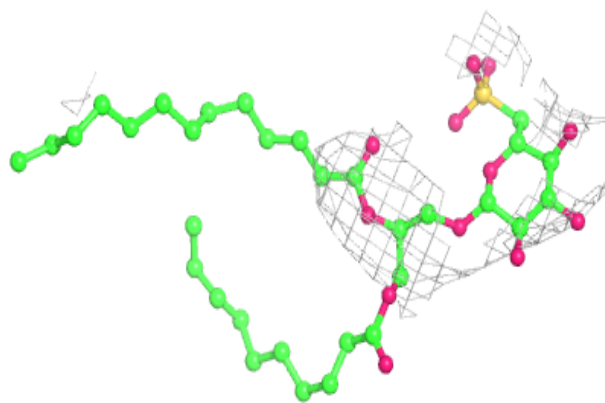
**Electron density around CLA B 610:**

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

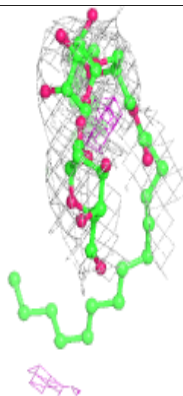
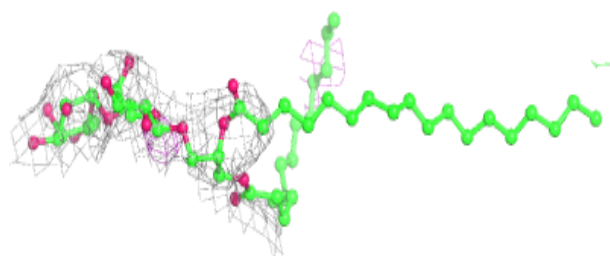
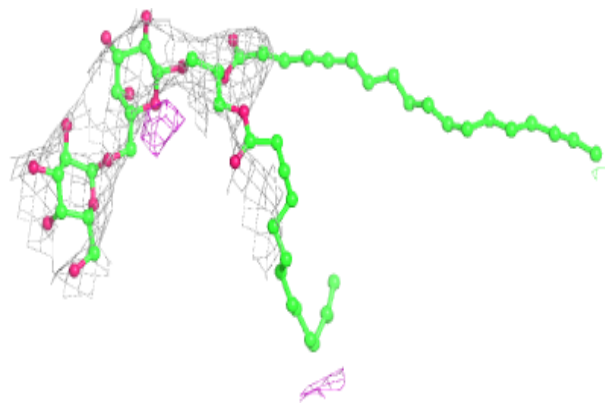


**Electron density around SQD f 103:**

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

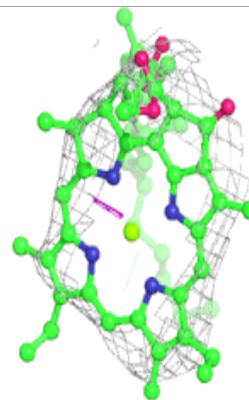
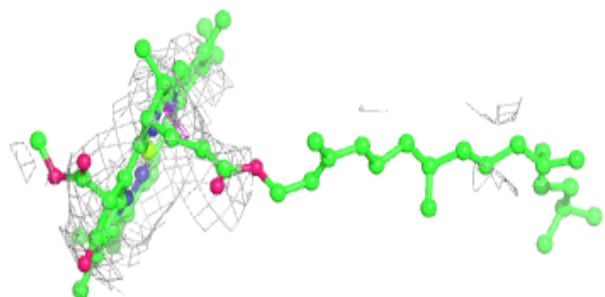
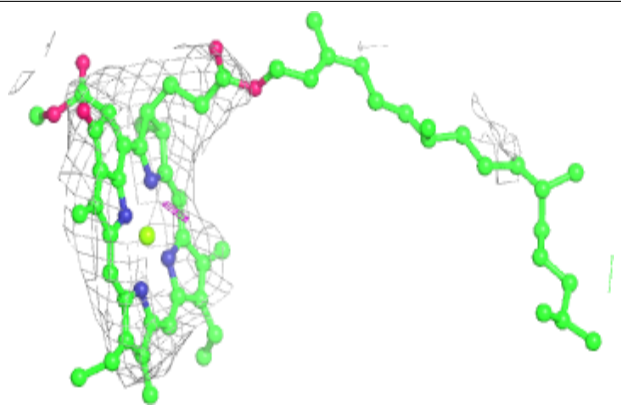
**Electron density around DGD C 516:**

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

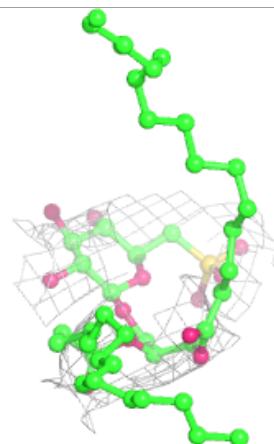
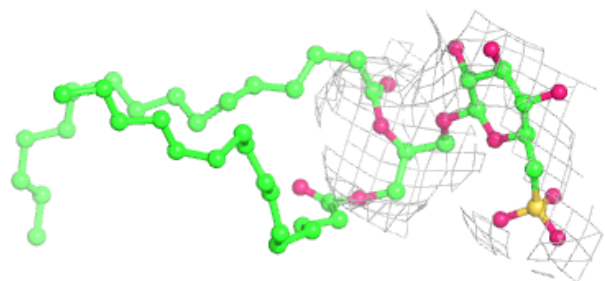
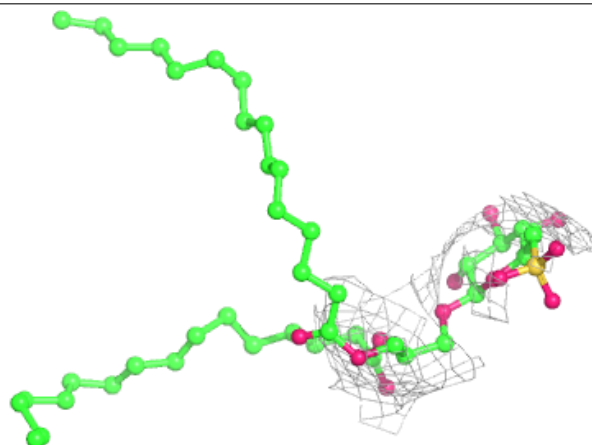


**Electron density around CLA b 612:**

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

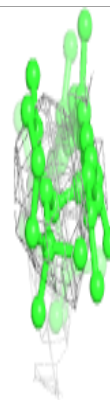
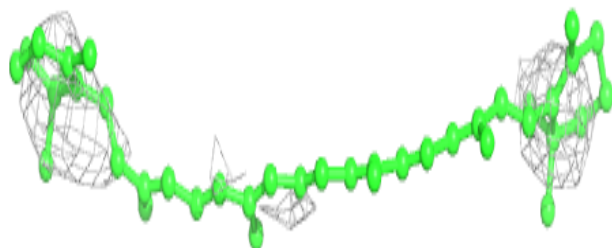
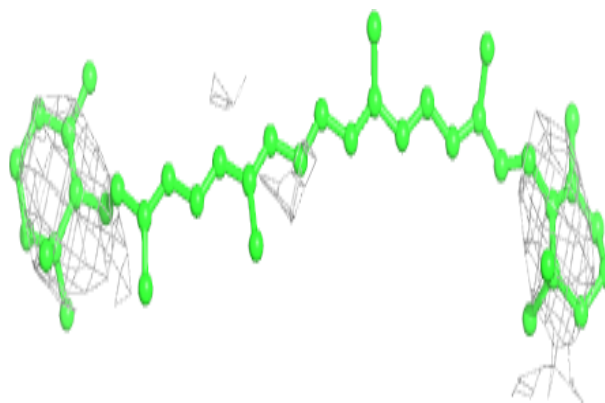
**Electron density around SQD A 414:**

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

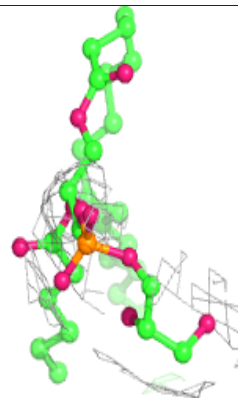
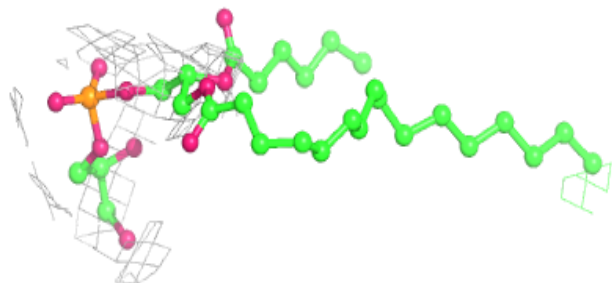
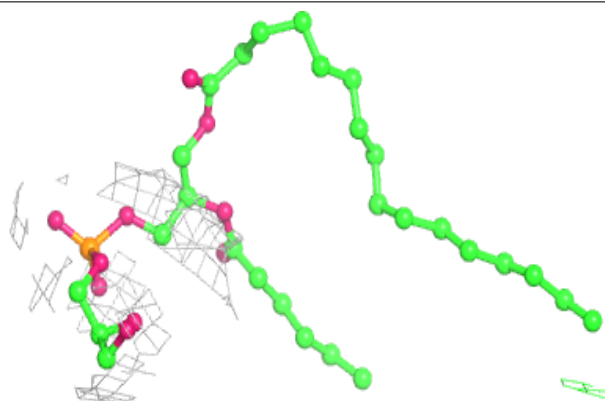


**Electron density around BCR b 621:**

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

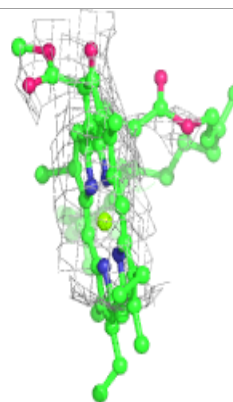
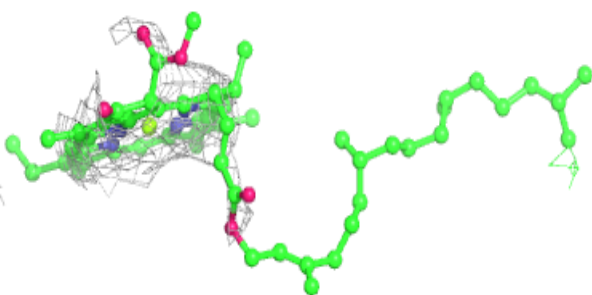
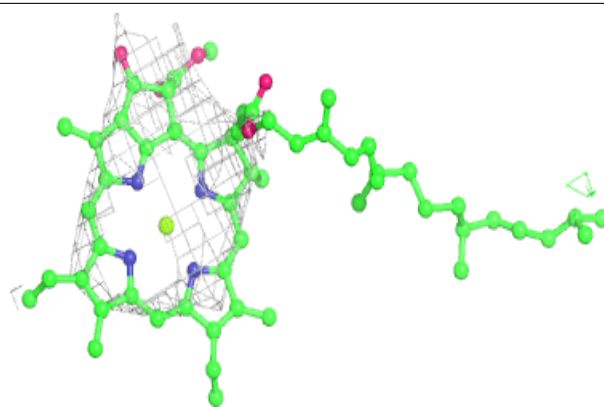
**Electron density around LHG A 409:**

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

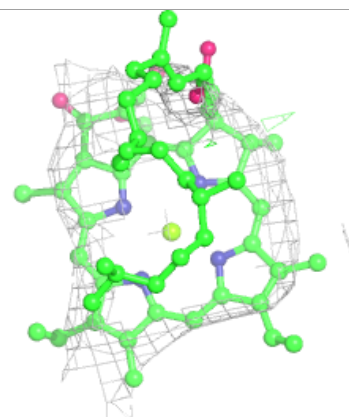
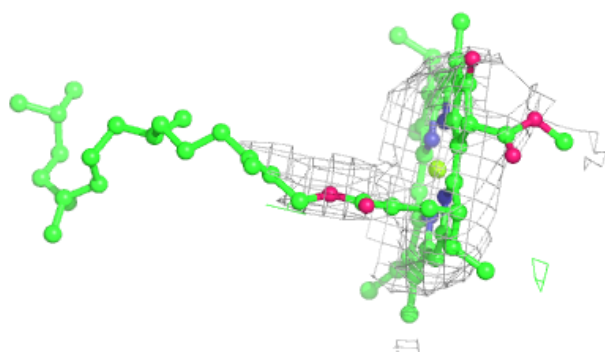
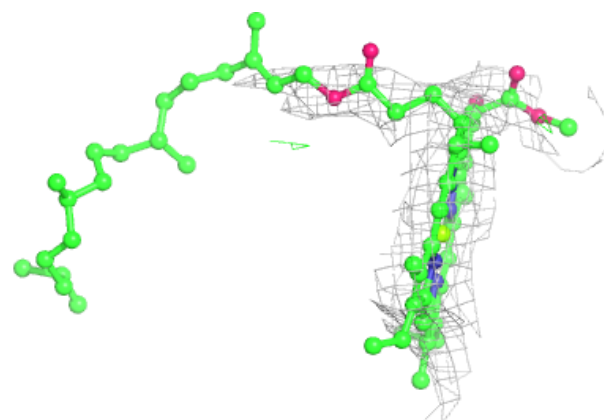


**Electron density around CLA a 406:**

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

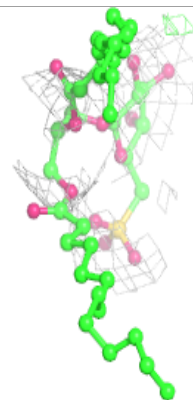
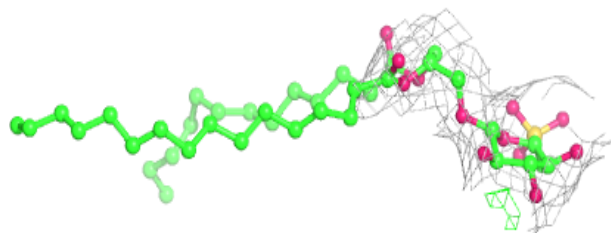
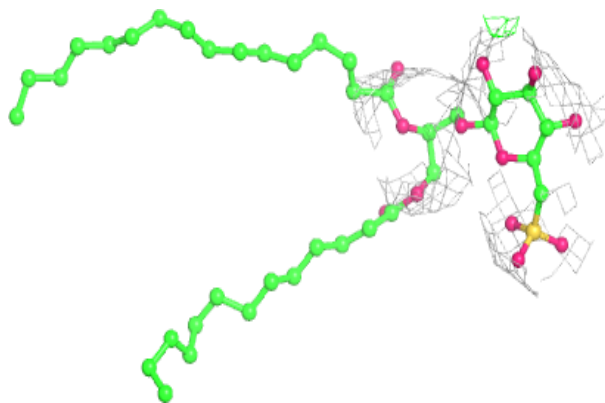
**Electron density around CLA c 505:**

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

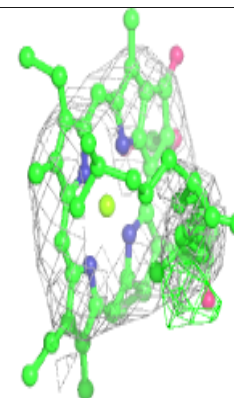
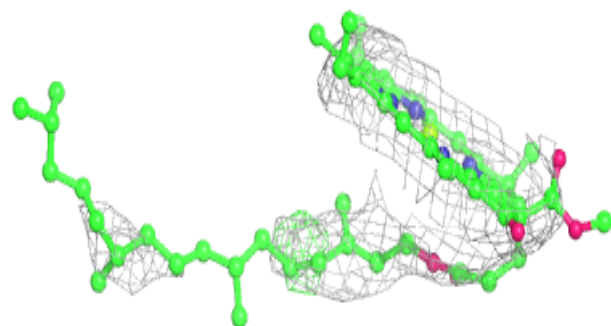
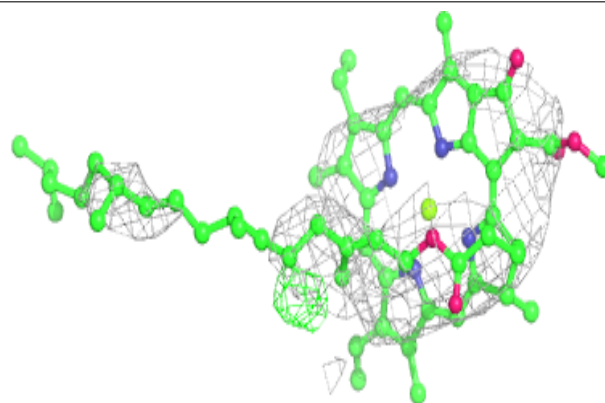


**Electron density around SQD a 415:**

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

**Electron density around CLA B 607:**

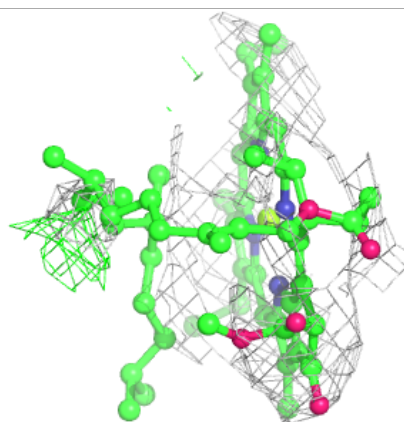
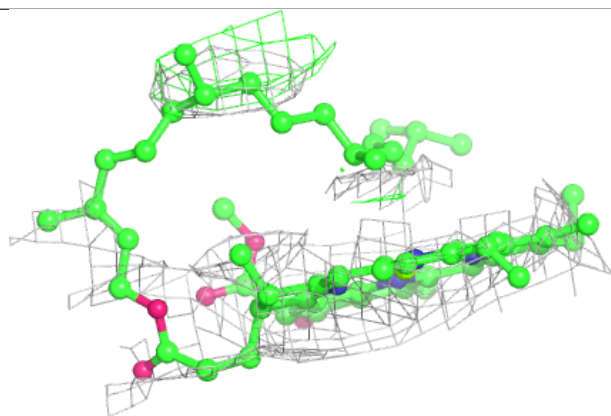
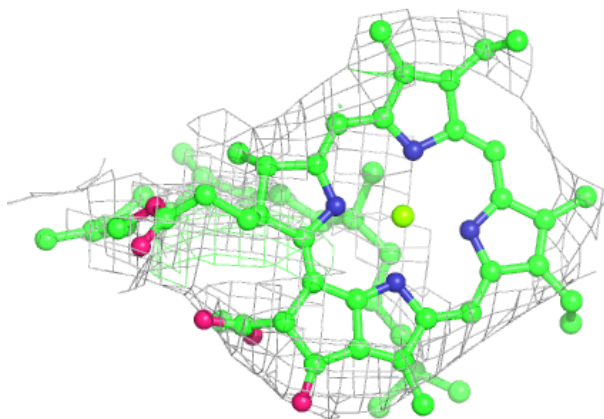
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)





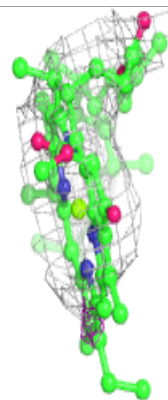
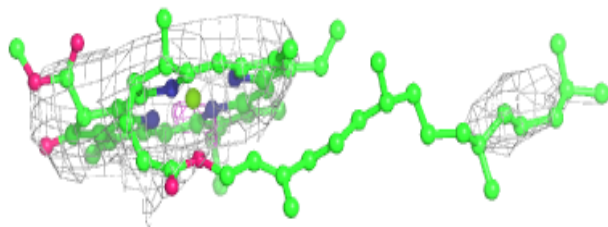
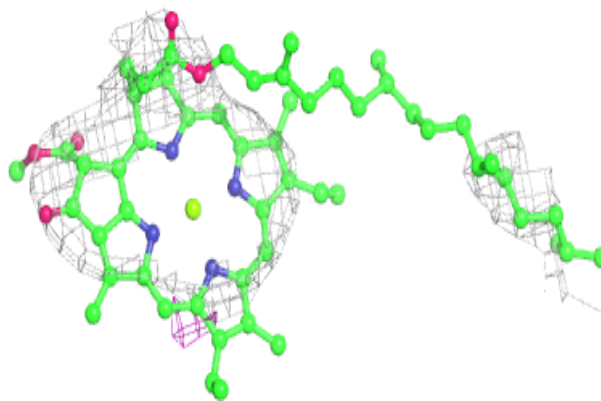
**Electron density around CLA C 509:**

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

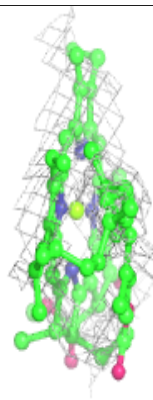
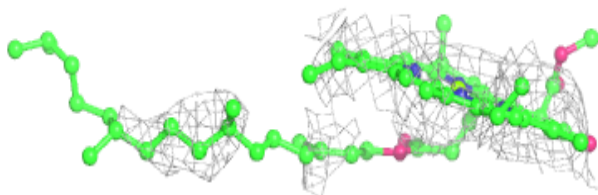
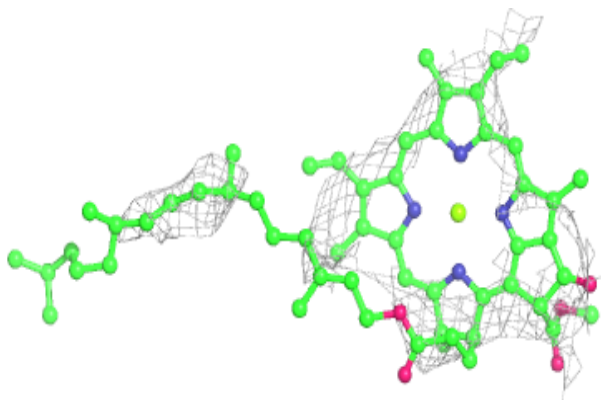


**Electron density around CLA c 501:**

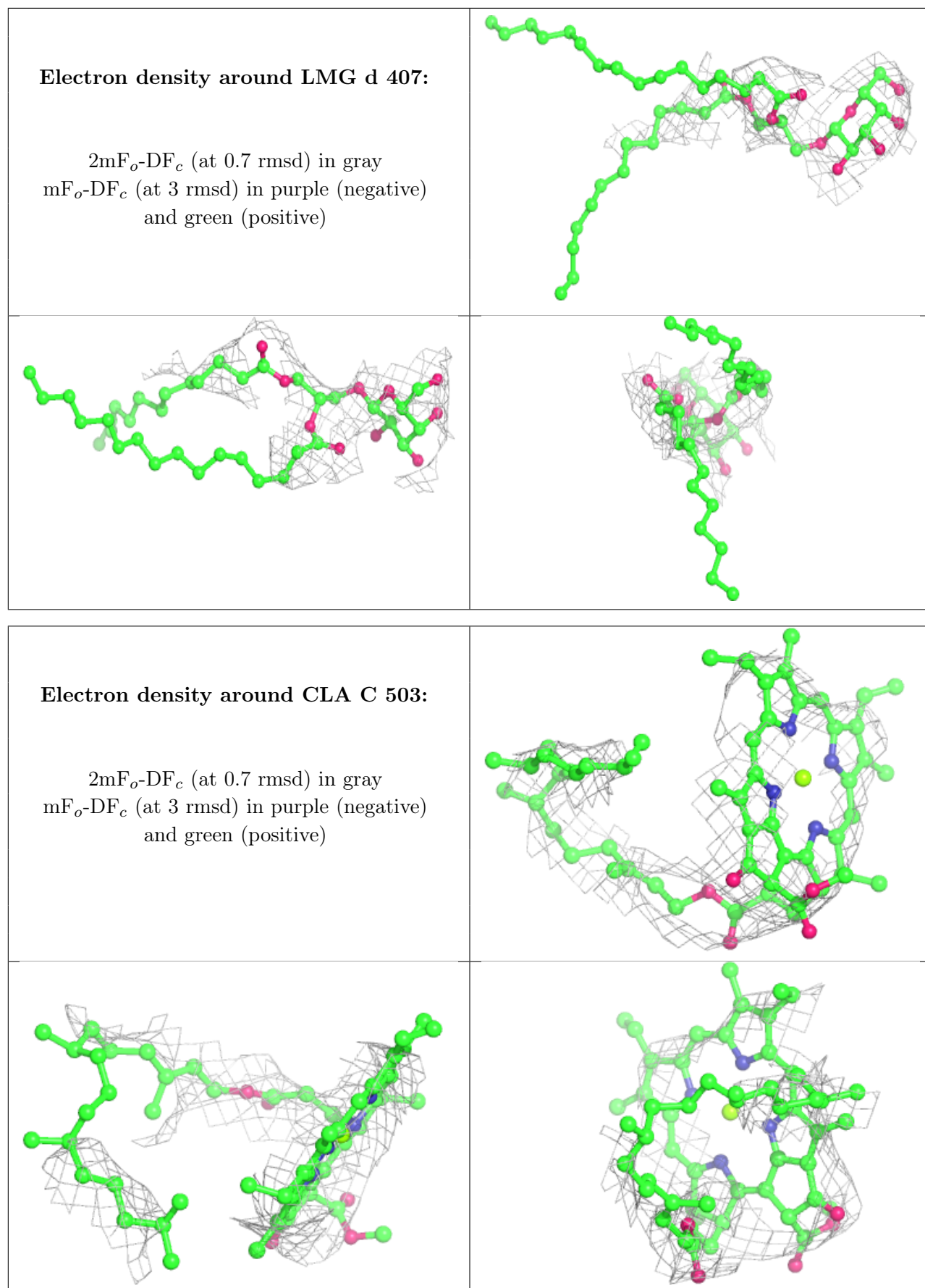
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA b 606:**

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

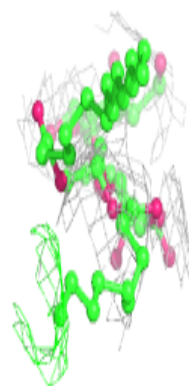
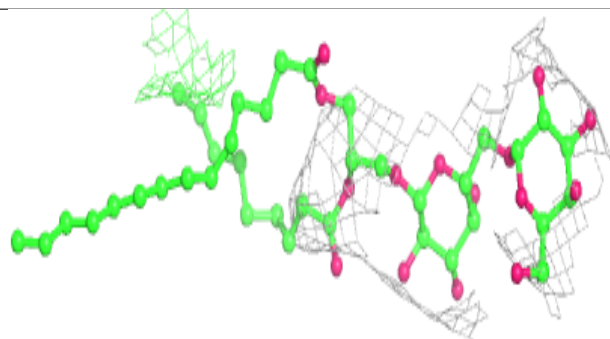
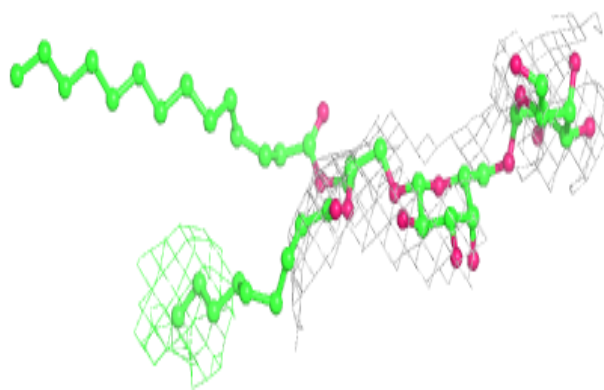




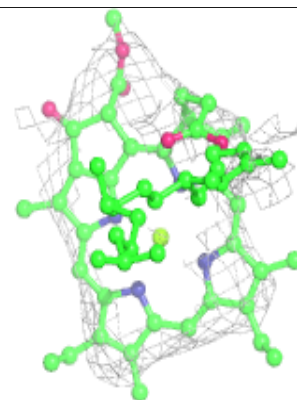
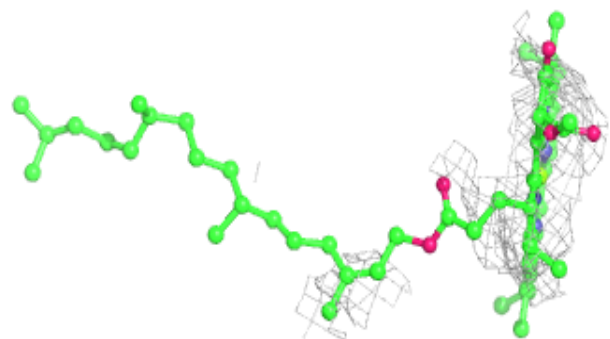
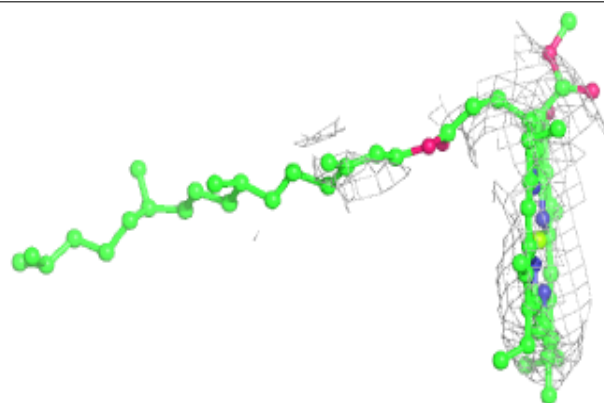


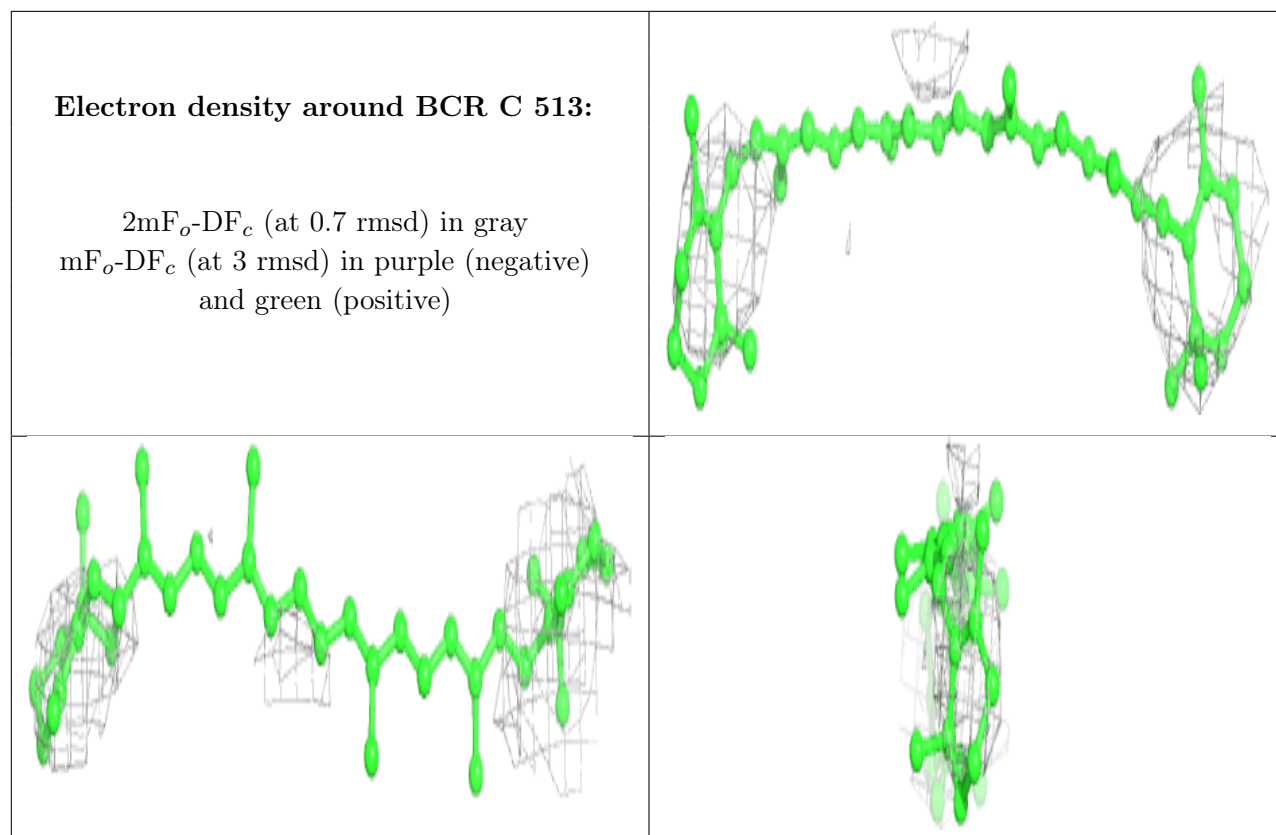
**Electron density around DGD c 515:**

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

**Electron density around CLA B 605:**

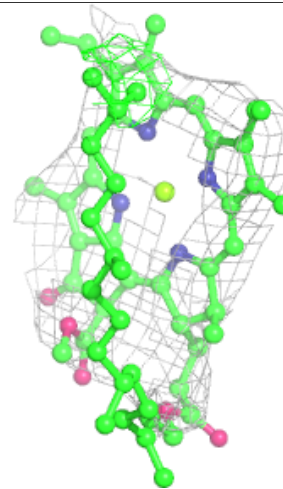
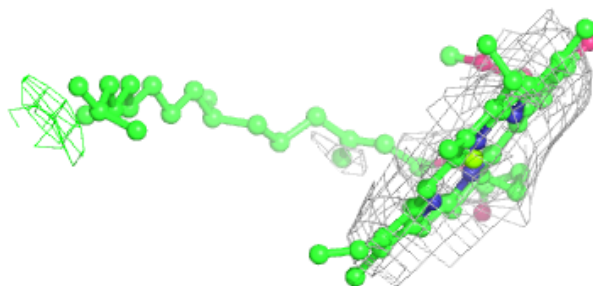
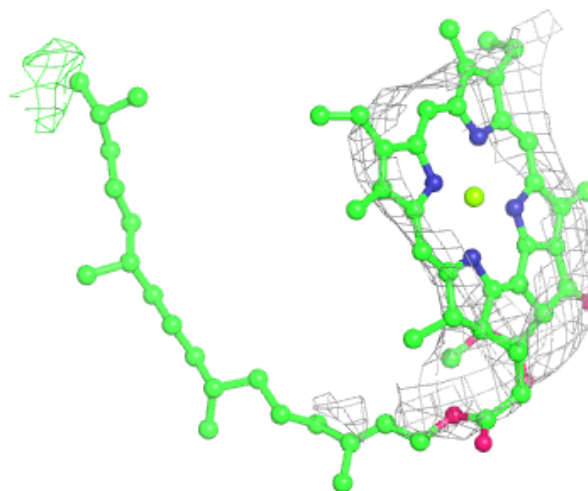
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





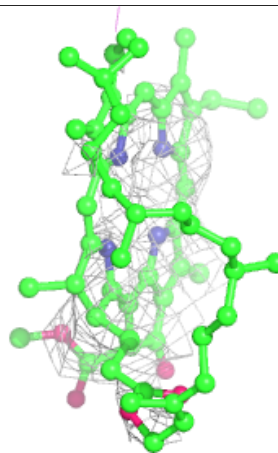
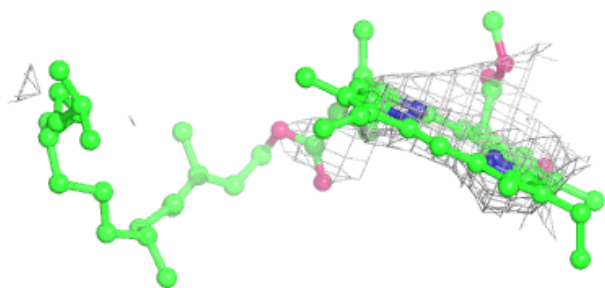
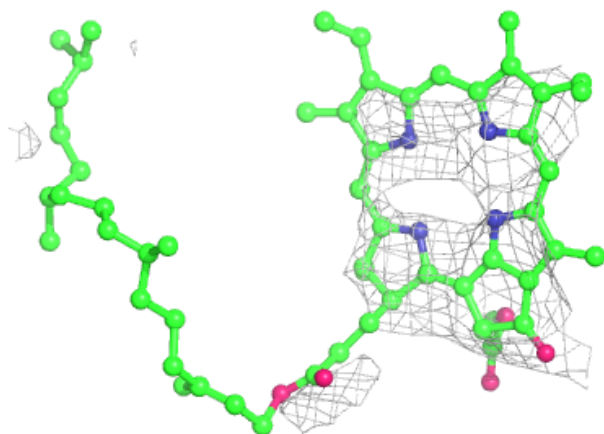
**Electron density around CLA c 506:**

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



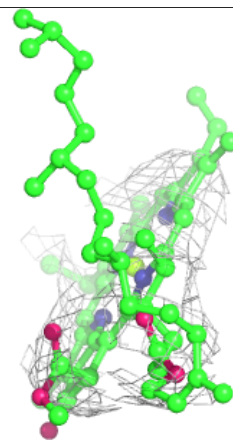
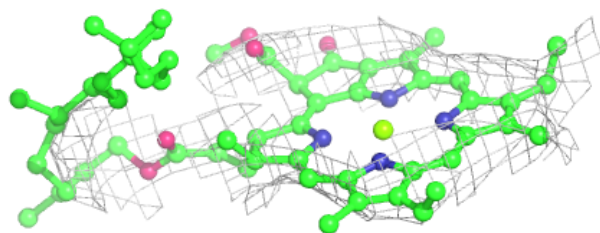
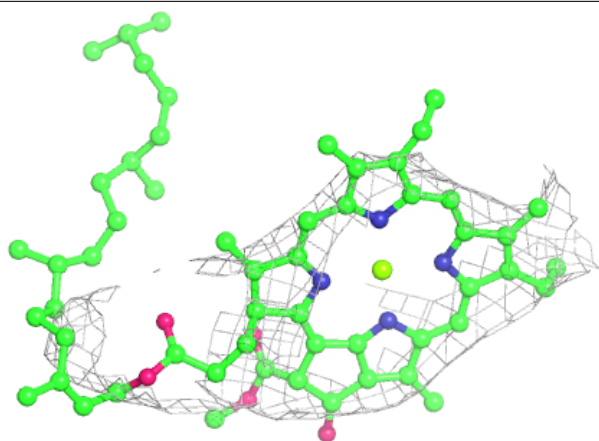
**Electron density around PHO a 407:**

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

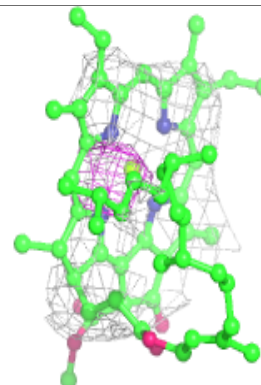
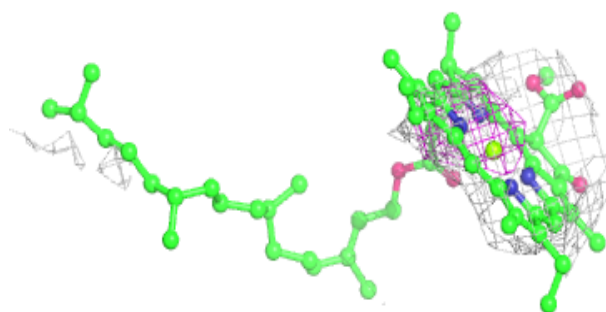
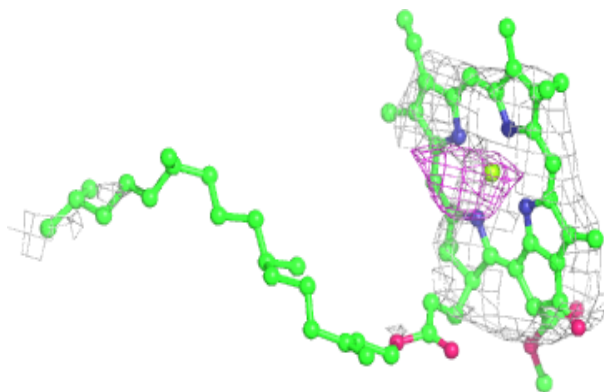


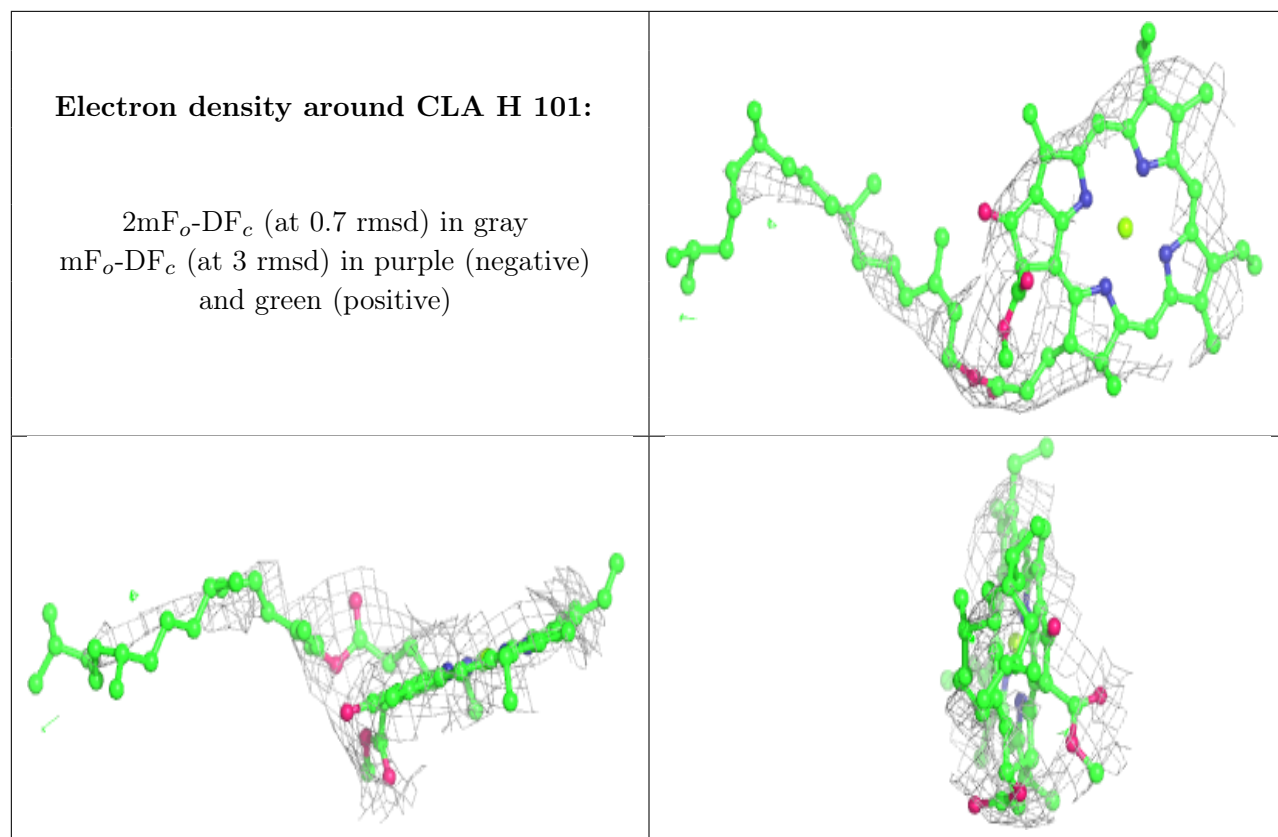
**Electron density around CLA B 615:**

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

**Electron density around CLA c 510:**

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

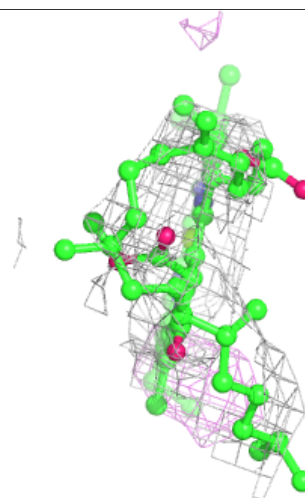
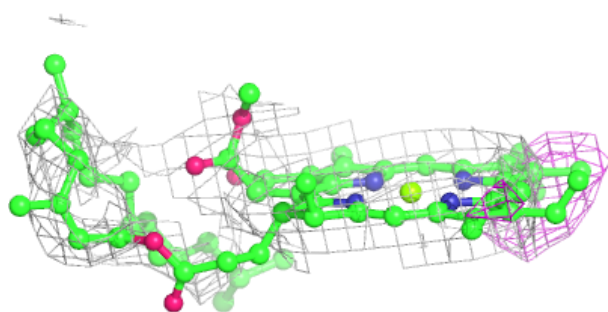
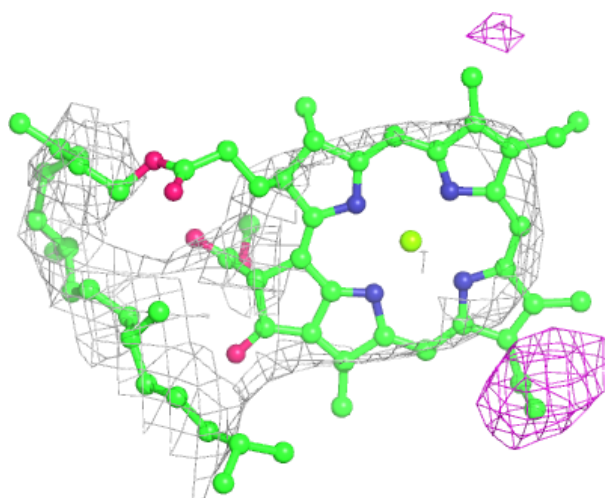






**Electron density around CLA B 609:**

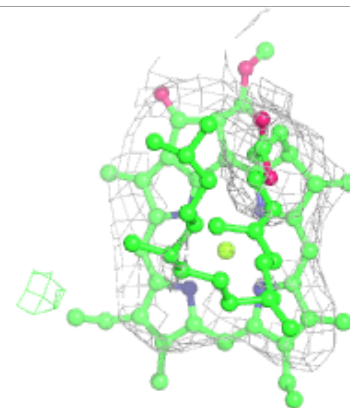
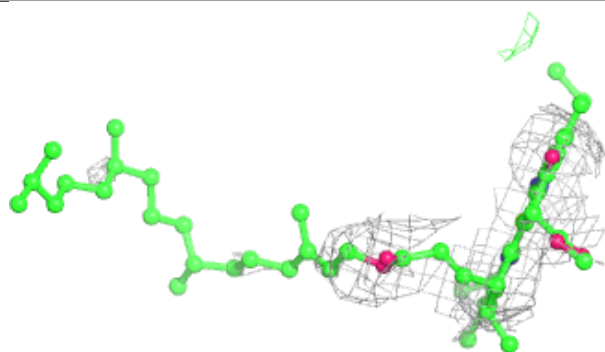
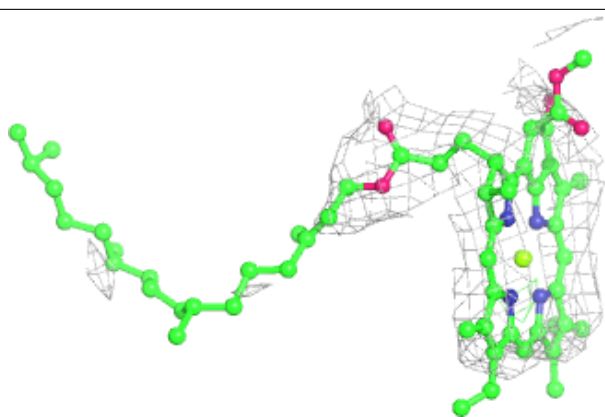
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



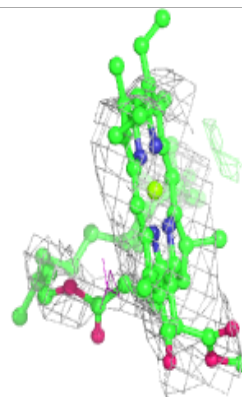
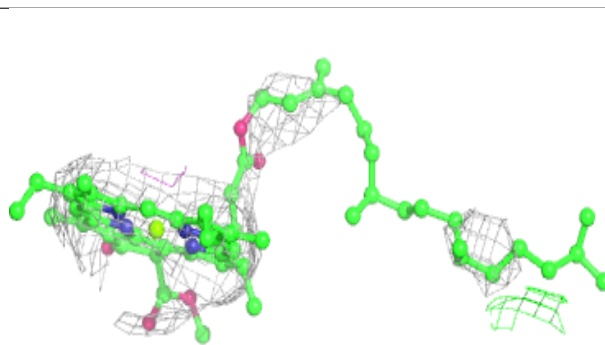
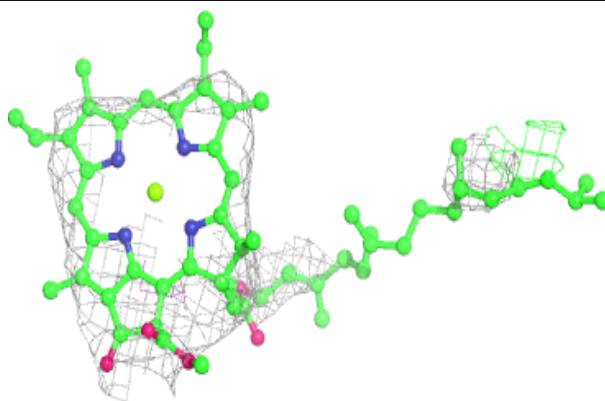


**Electron density around CLA d 405:**

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

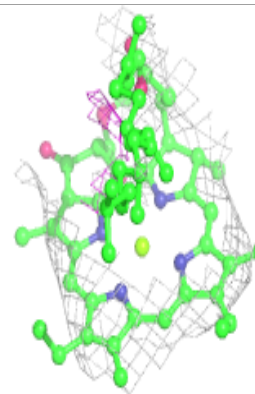
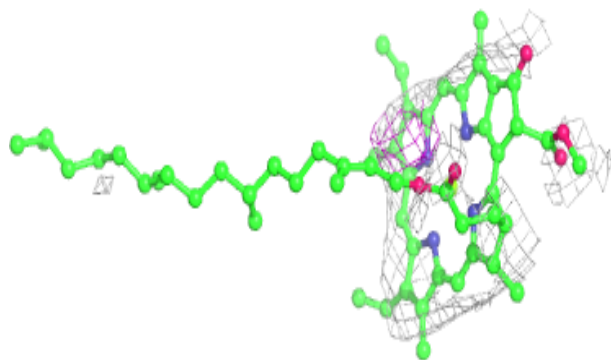
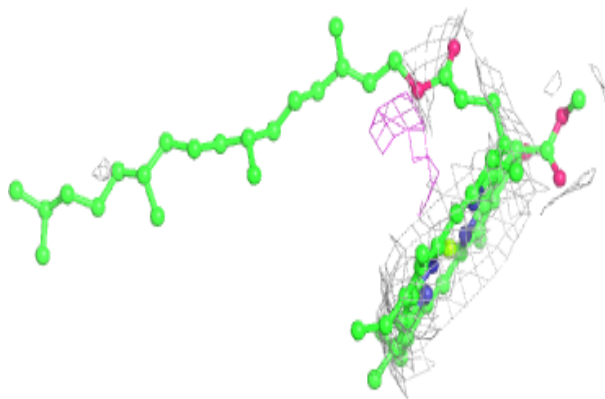
**Electron density around CLA A 404:**

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

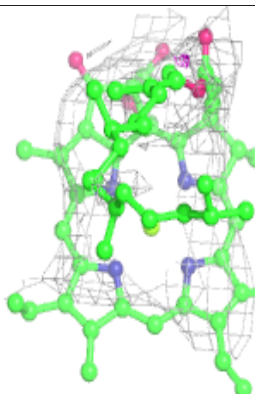
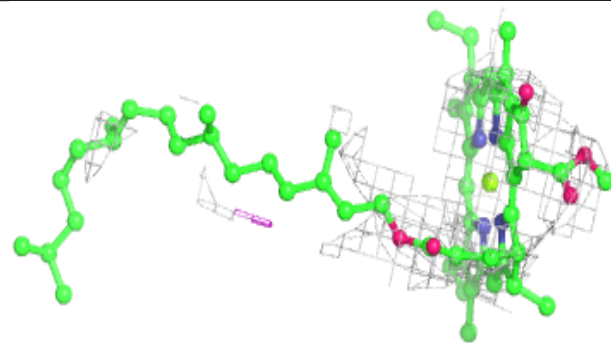
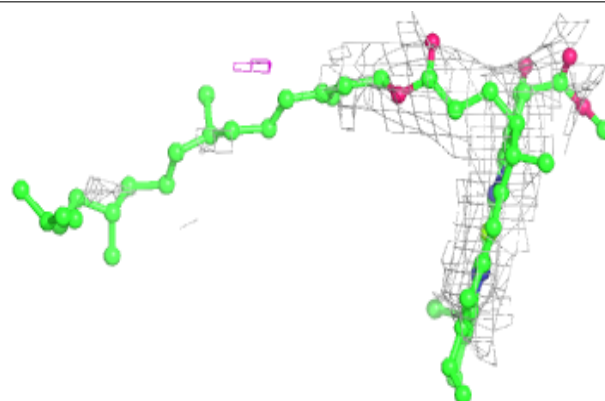


**Electron density around CLA c 520:**

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

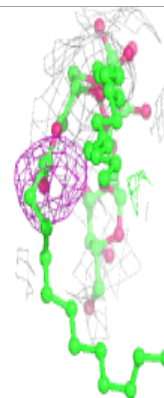
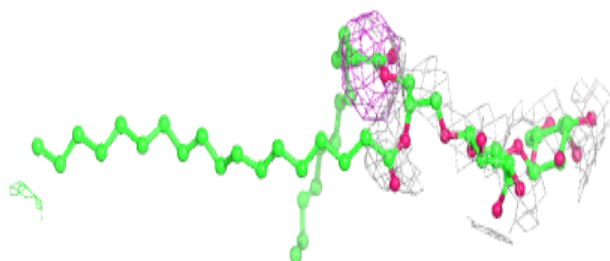
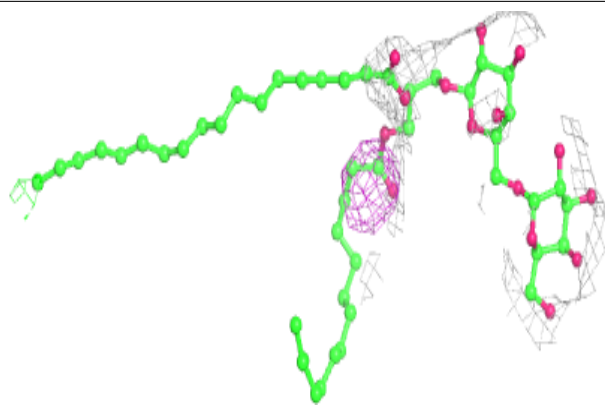
**Electron density around CLA B 604:**

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

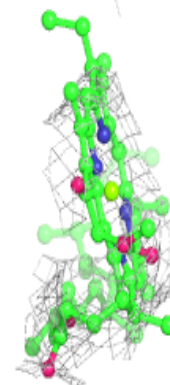
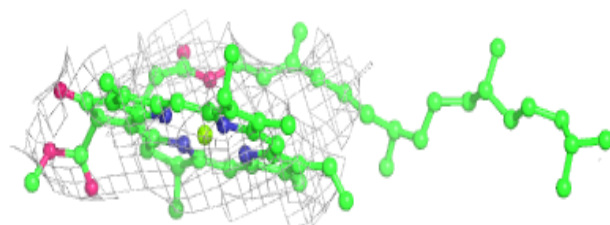
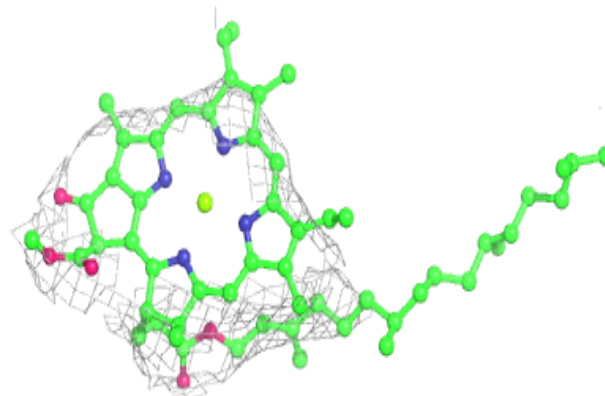


**Electron density around DGD c 516:**

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

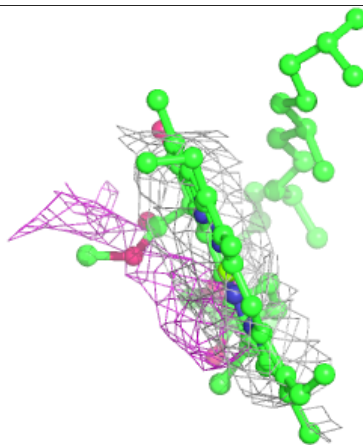
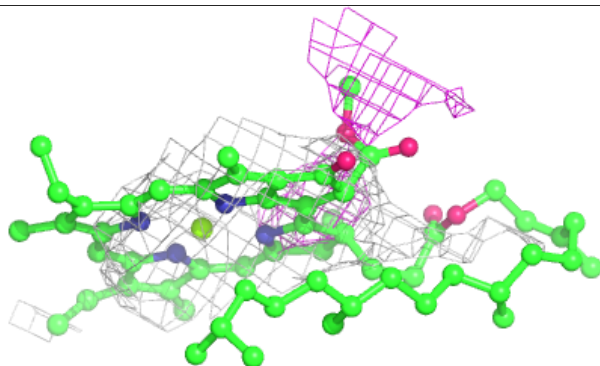
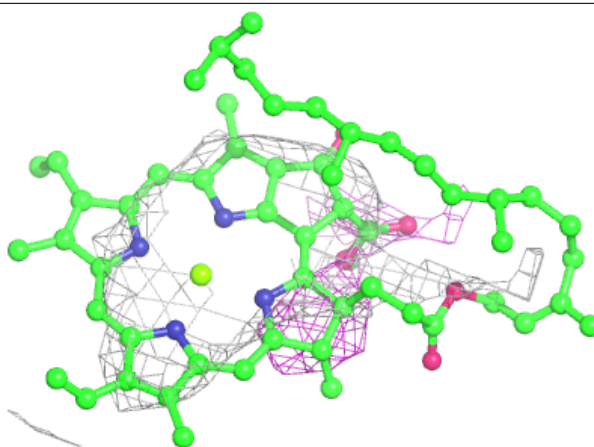
**Electron density around CLA C 501:**

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



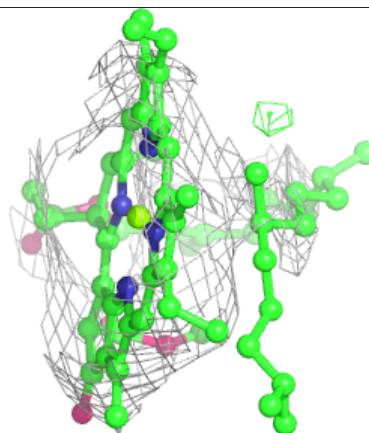
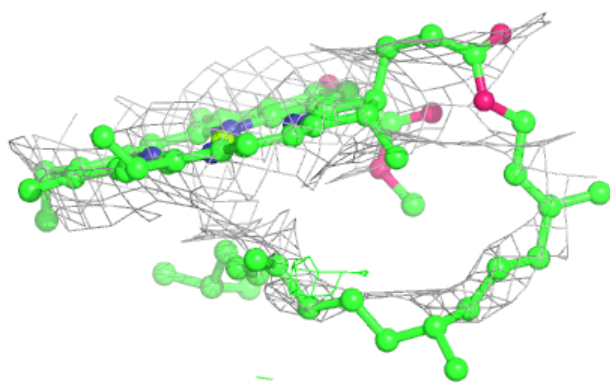
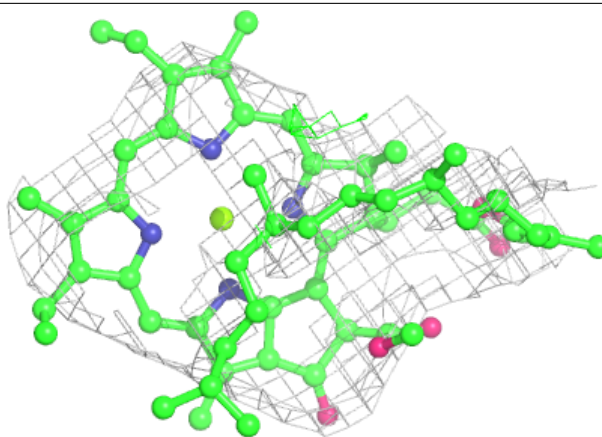
**Electron density around CLA C 508:**

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

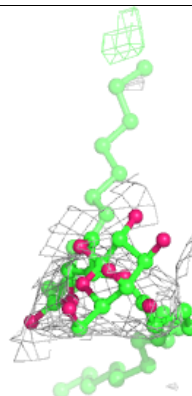
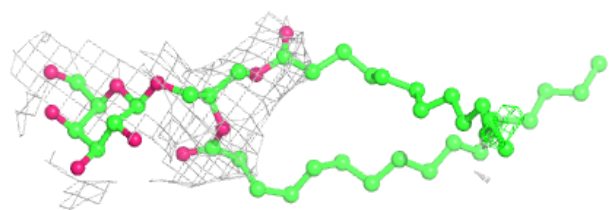
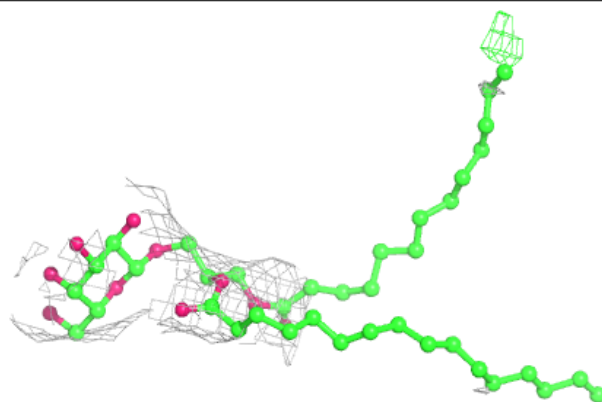


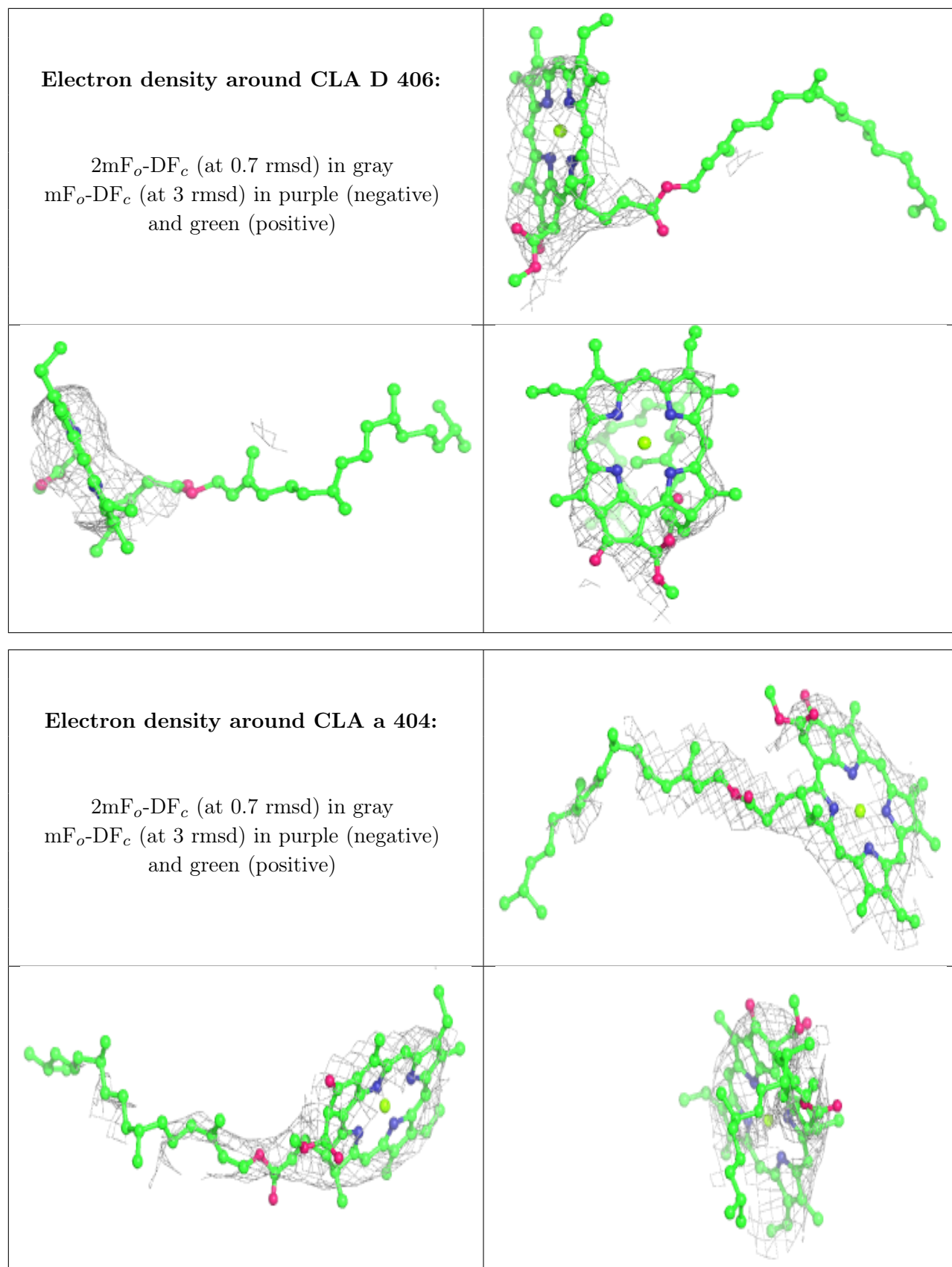
**Electron density around CLA c 509:**

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

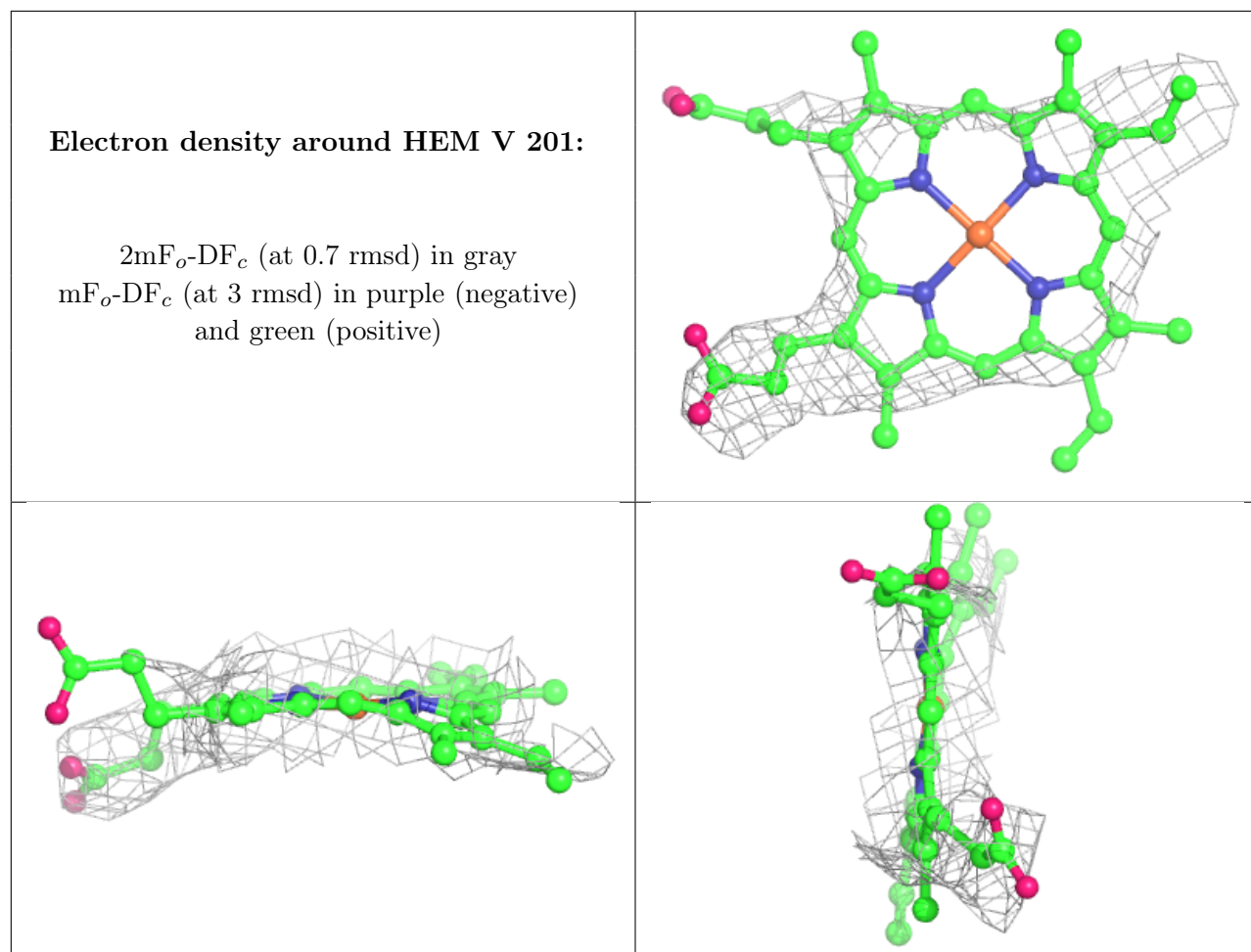
**Electron density around LMG D 408:**

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



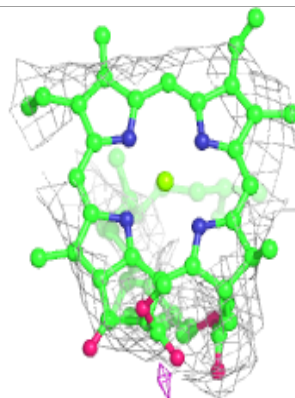
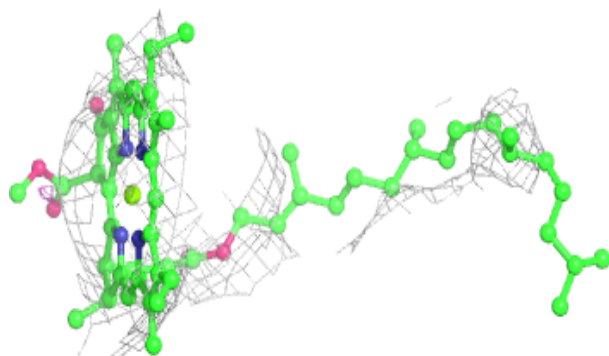
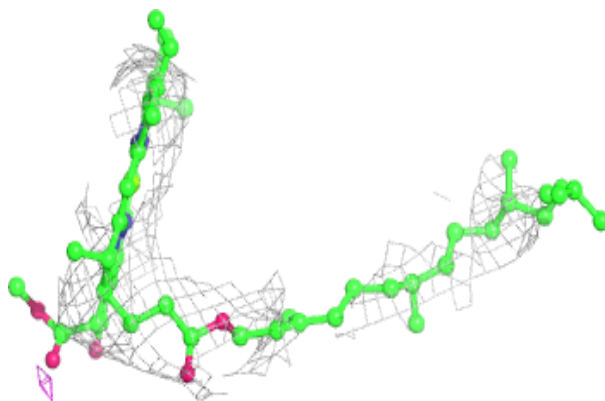






**Electron density around CLA b 608:**

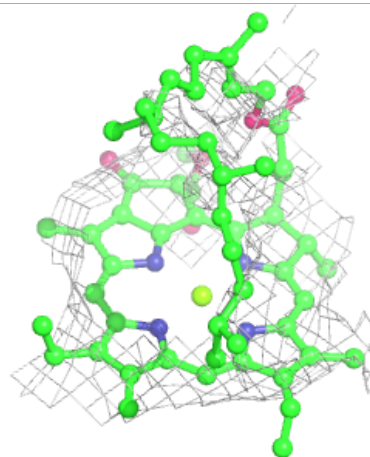
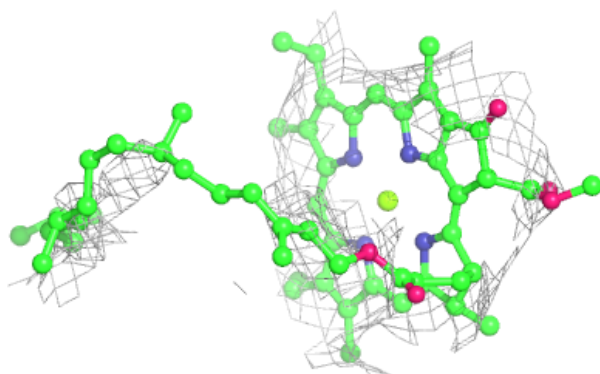
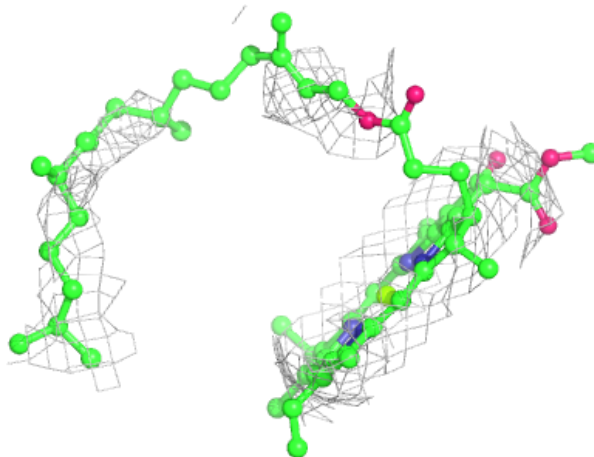
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





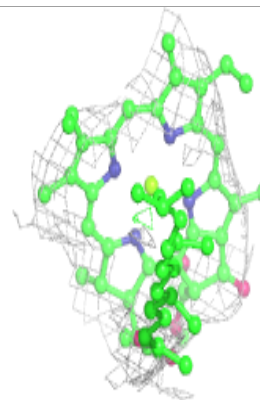
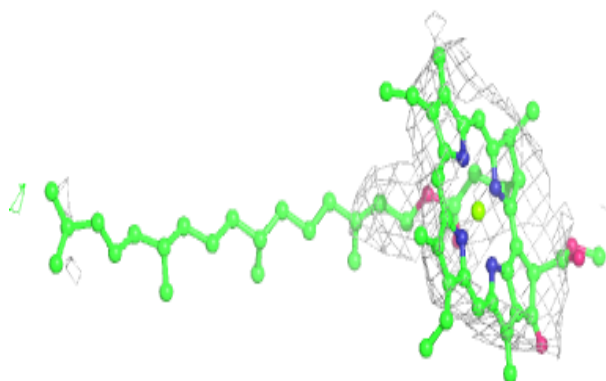
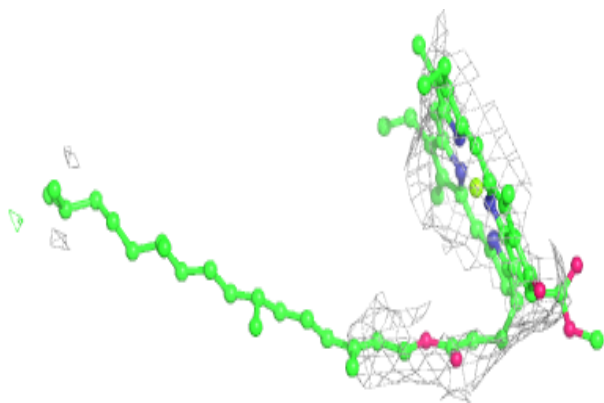
**Electron density around CLA b 614:**

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

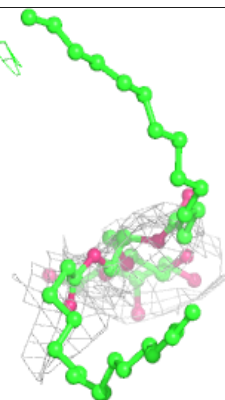
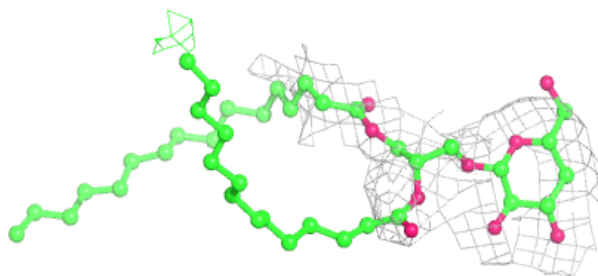
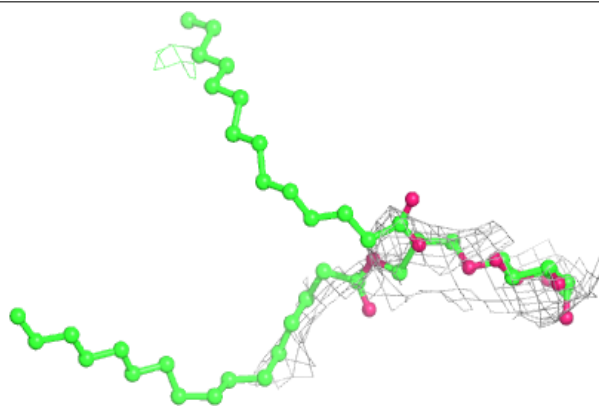


**Electron density around CLA B 606:**

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

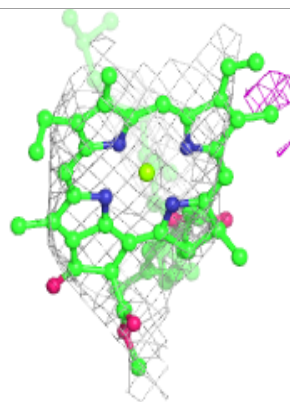
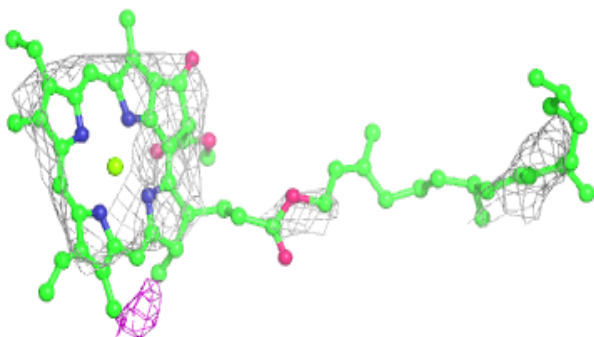
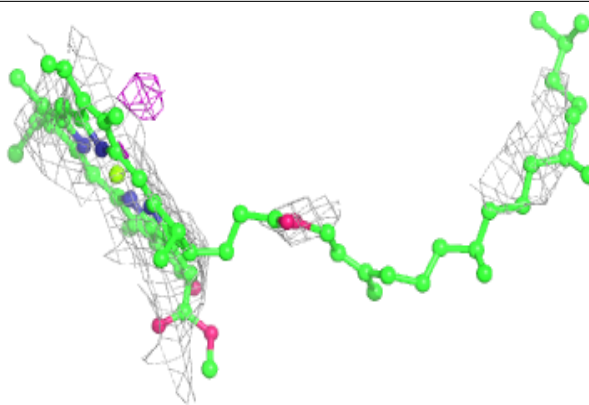
**Electron density around LMG B 621:**

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

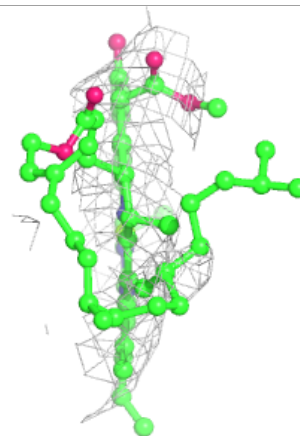
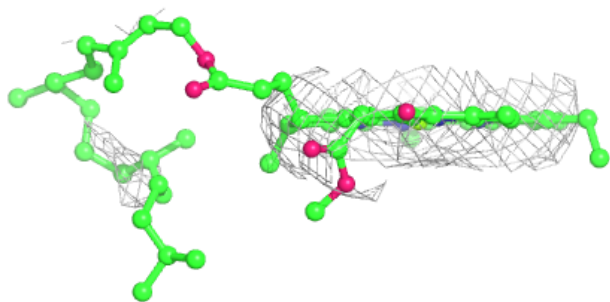
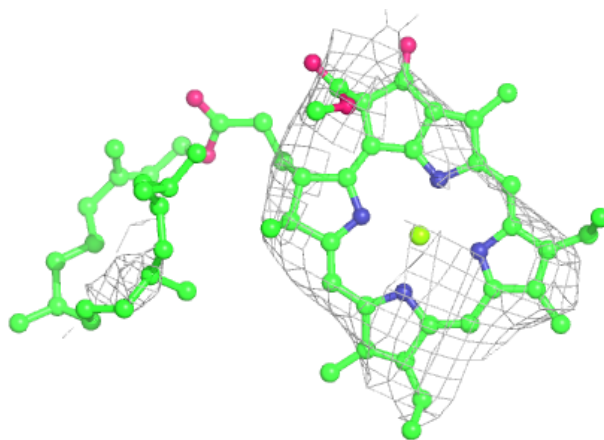


**Electron density around CLA D 405:**

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

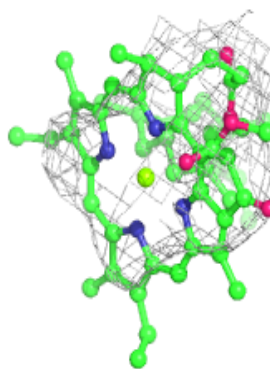
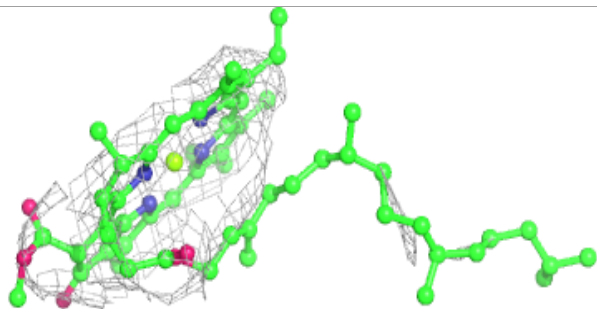
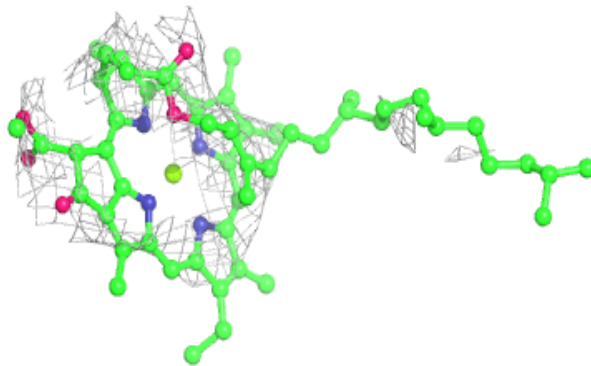
**Electron density around CLA c 511:**

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



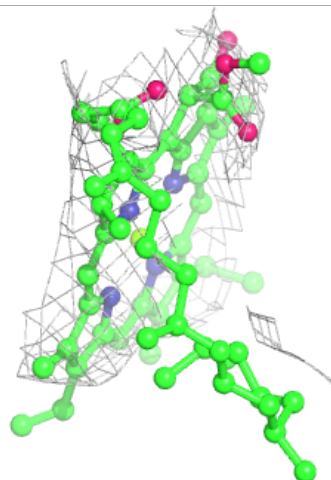
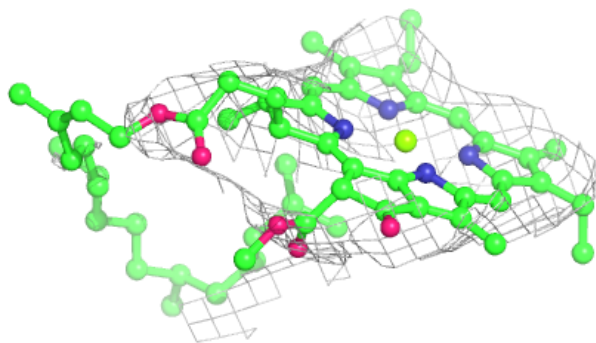
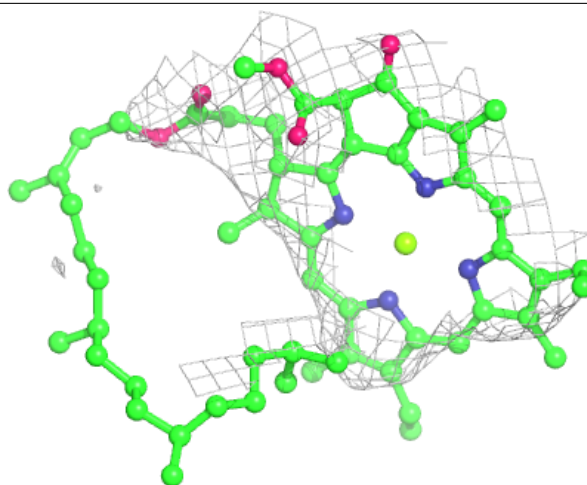
**Electron density around CLA c 504:**

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



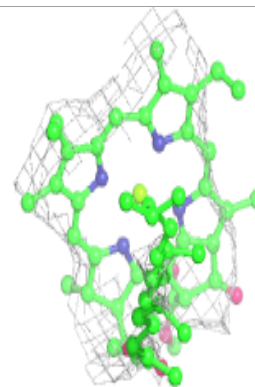
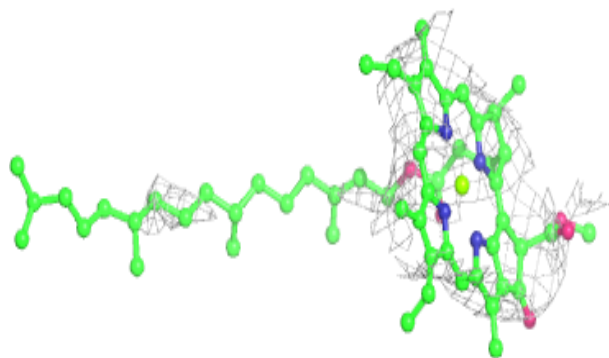
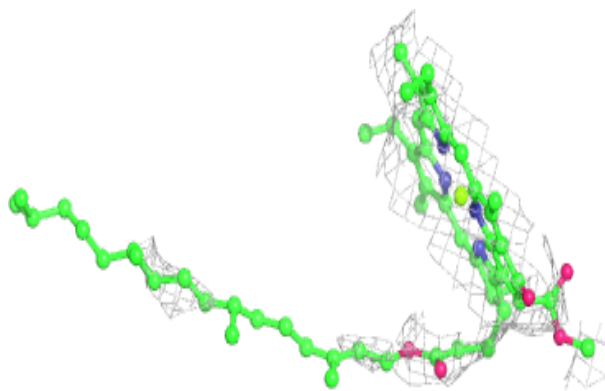
**Electron density around CLA B 614:**

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

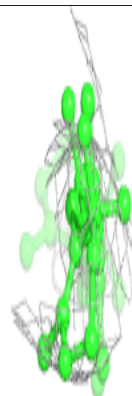
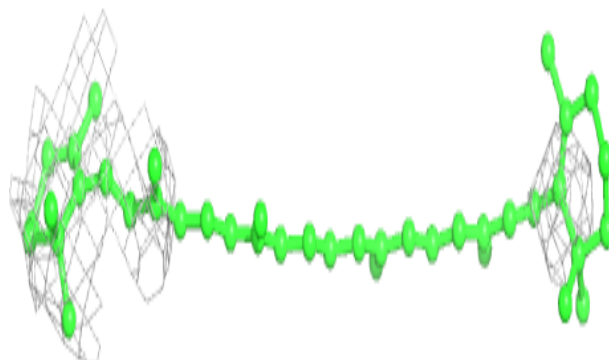
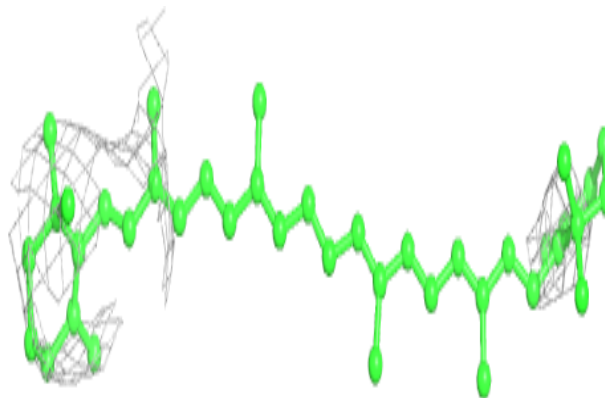


**Electron density around CLA b 610:**

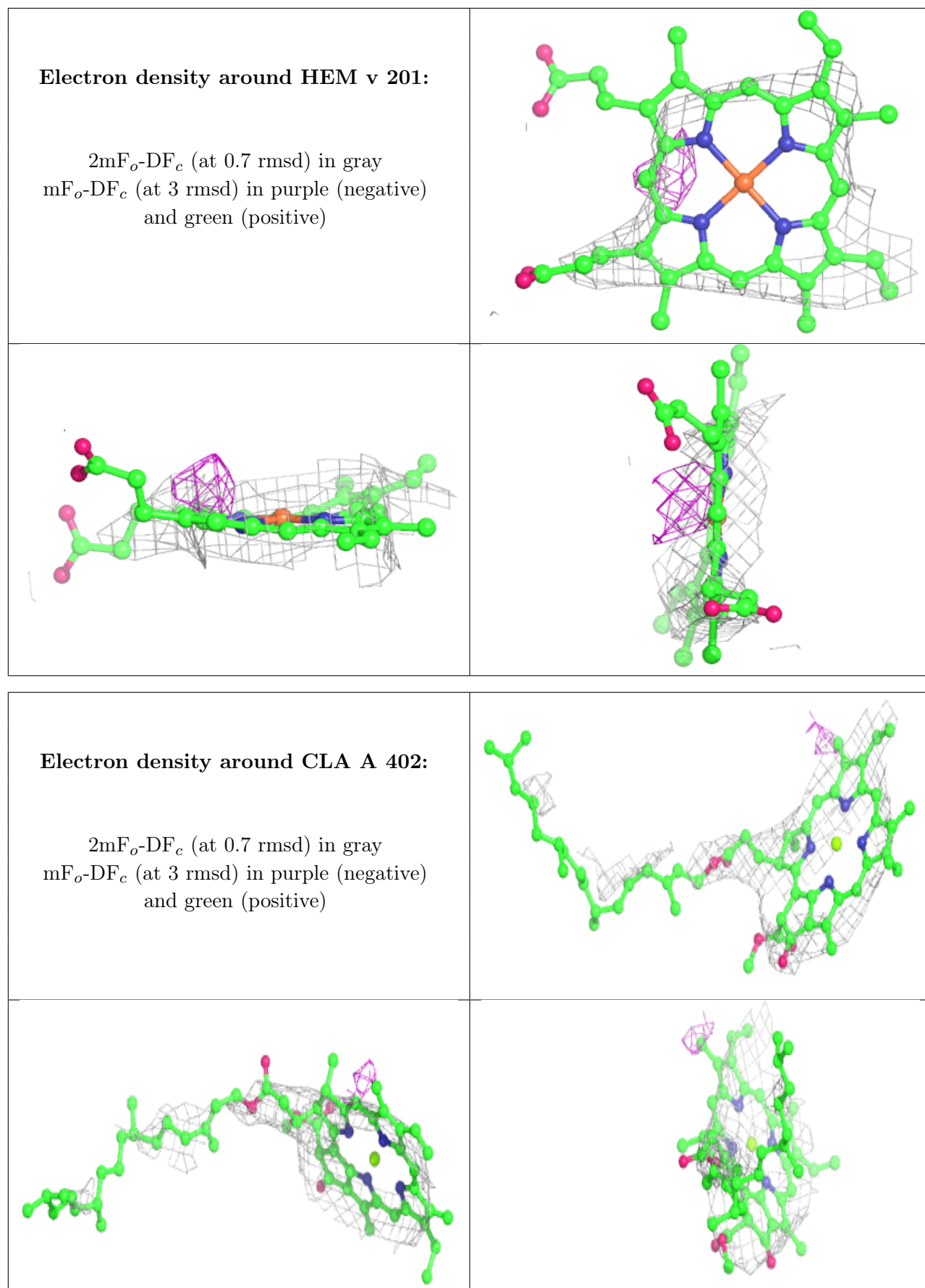
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

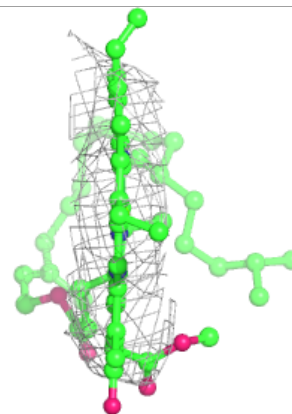
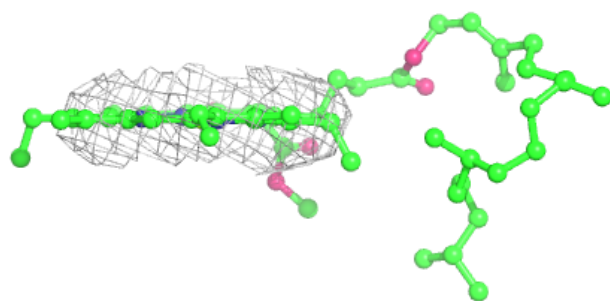
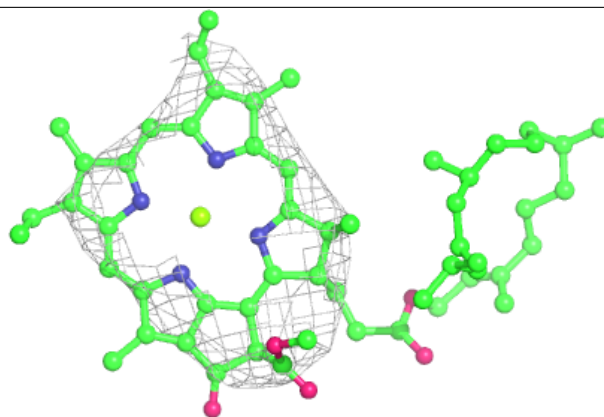




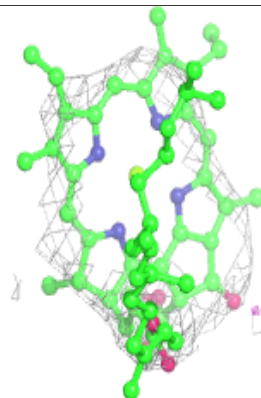
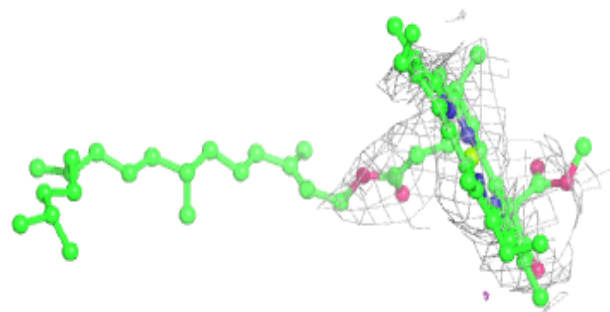
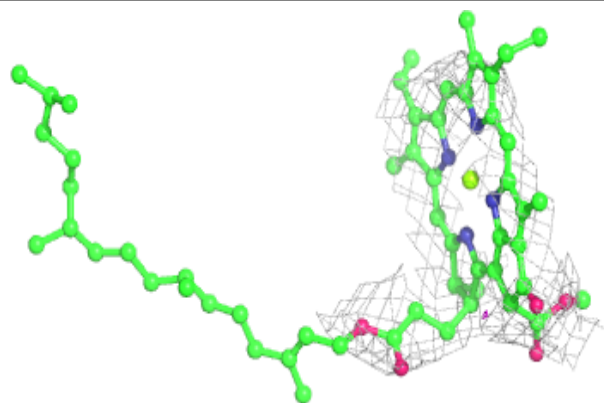


**Electron density around CLA C 511:**

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

**Electron density around CLA B 608:**

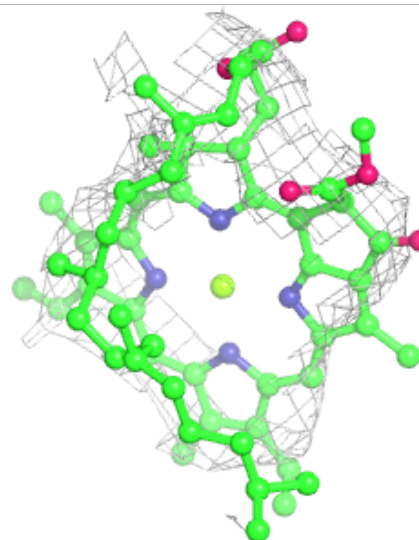
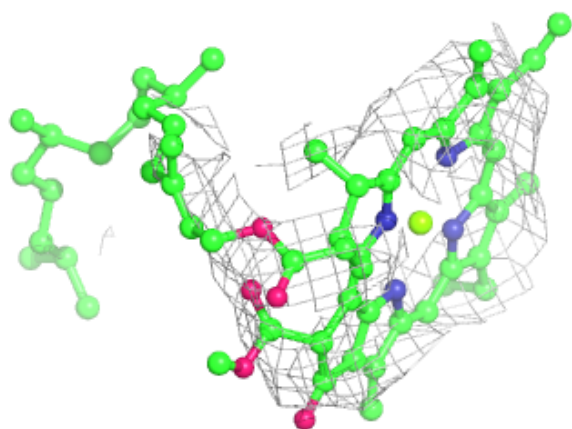
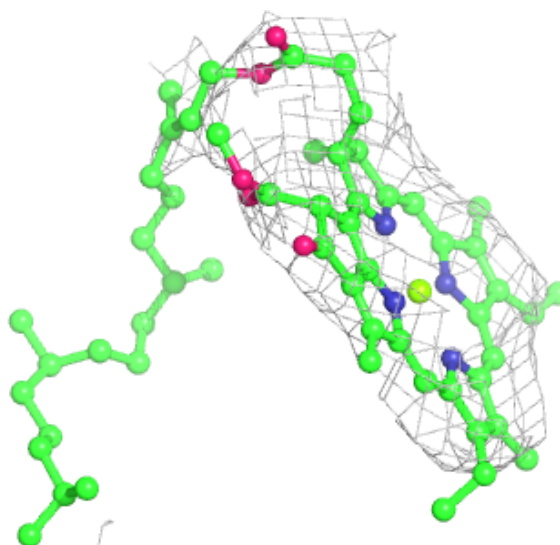
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





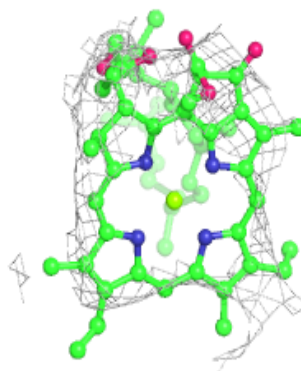
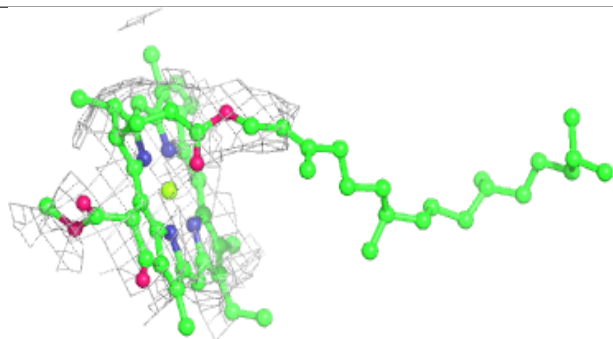
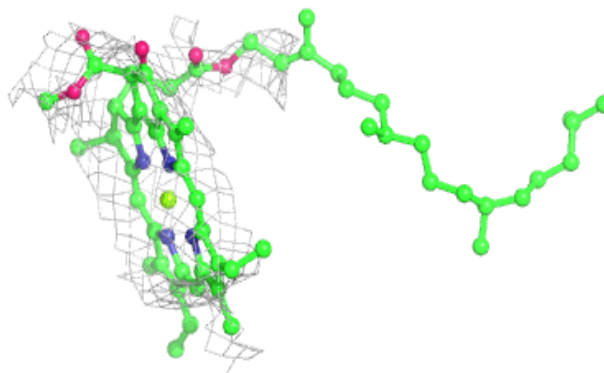
**Electron density around CLA B 612:**

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

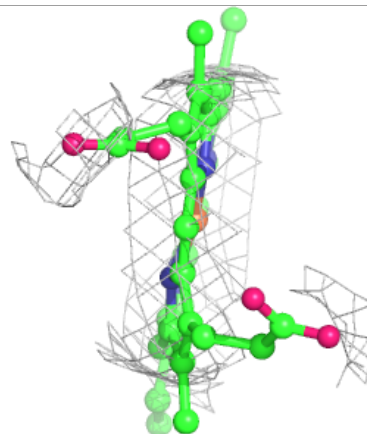
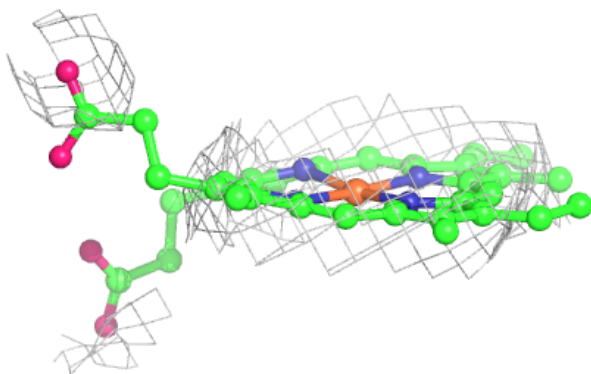
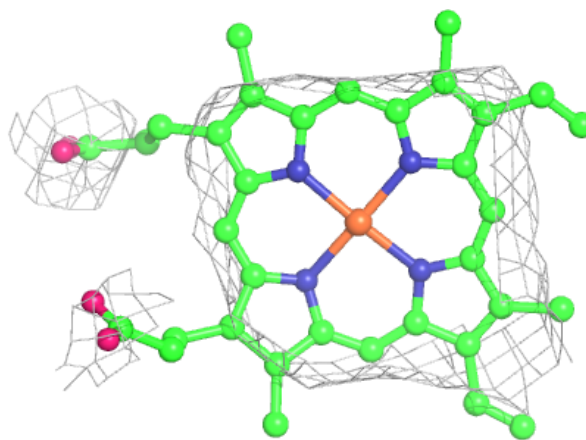


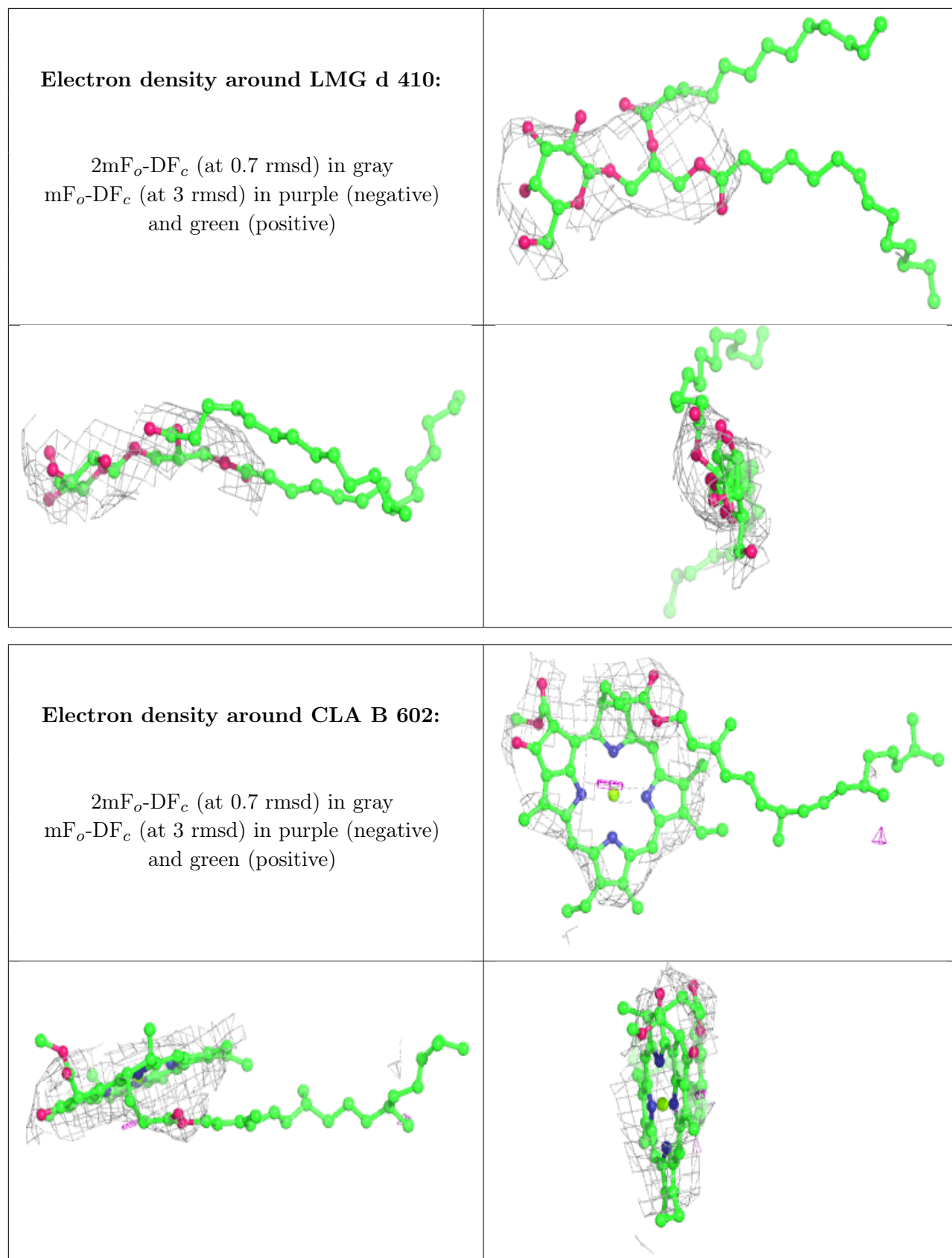
**Electron density around CLA c 507:**

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

**Electron density around HEM F 101:**

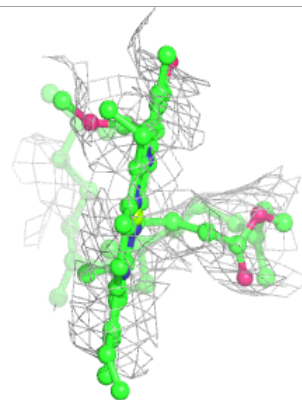
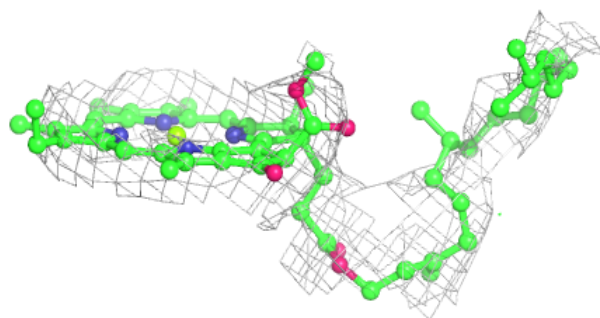
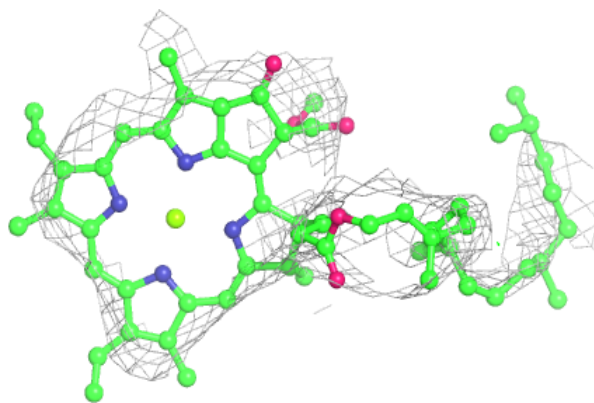
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



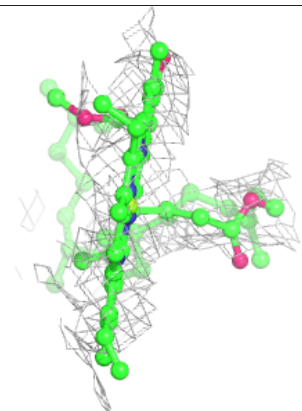
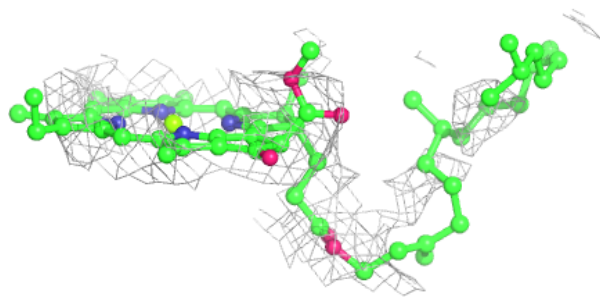
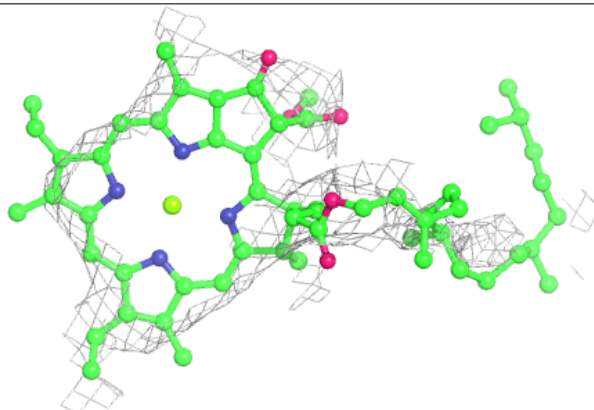


**Electron density around CLA B 611:**

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

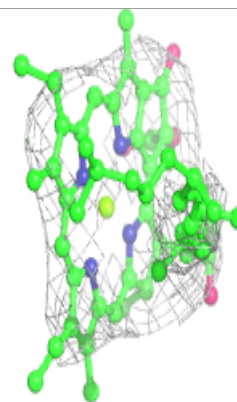
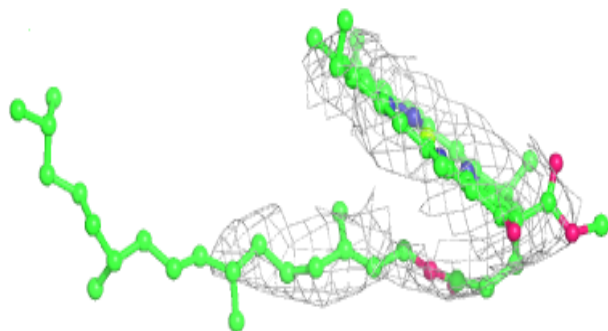
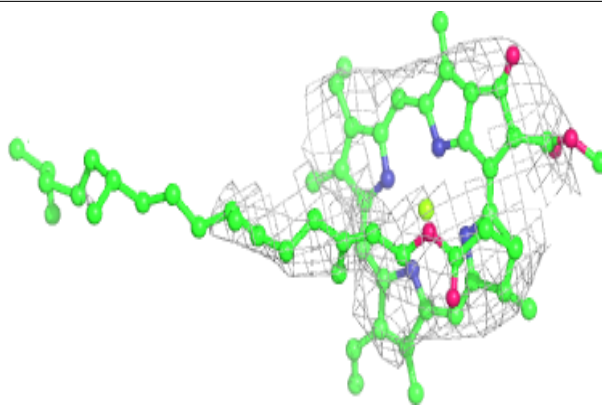
**Electron density around CLA b 615:**

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

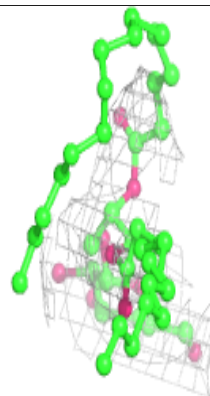
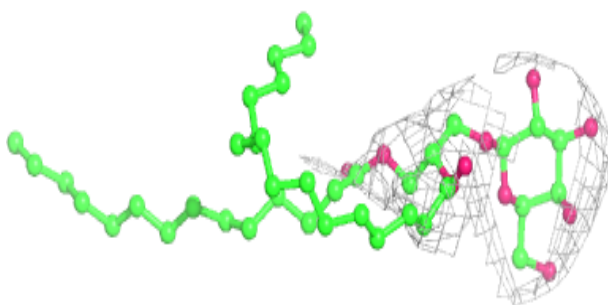
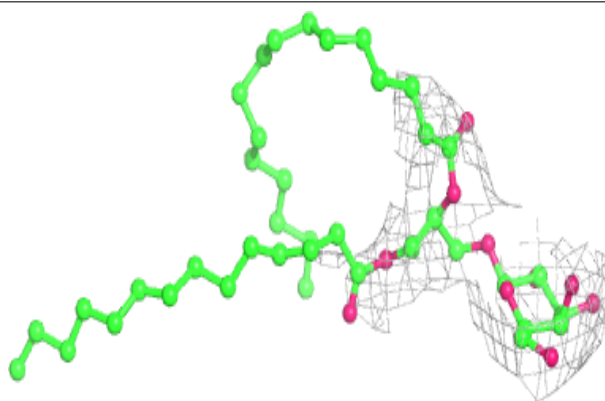


**Electron density around CLA b 611:**

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

**Electron density around LMG b 628:**

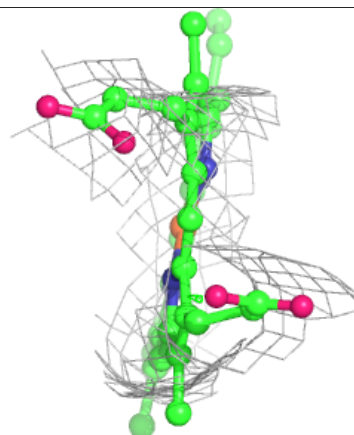
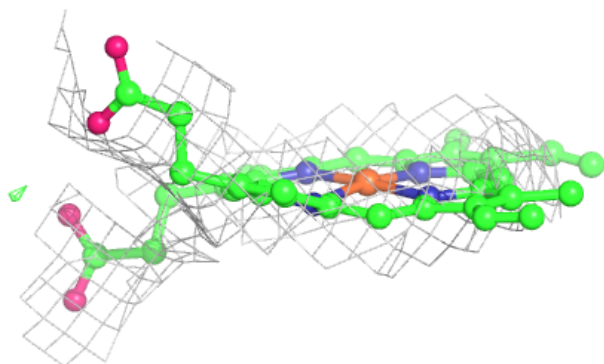
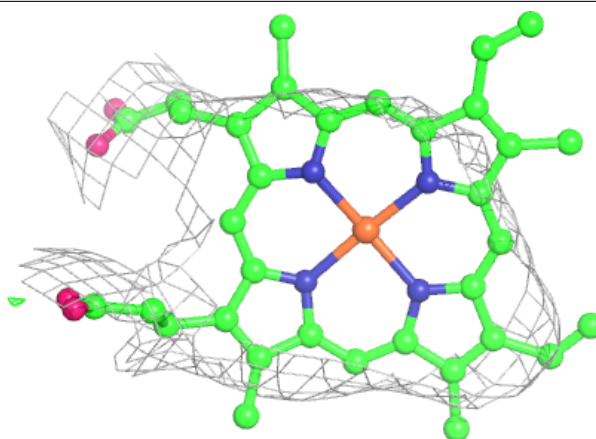
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



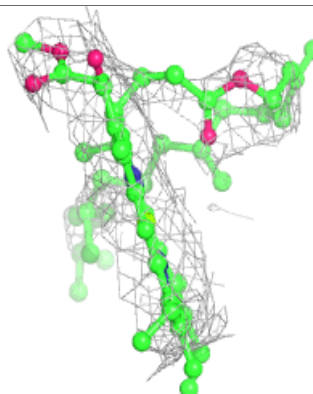
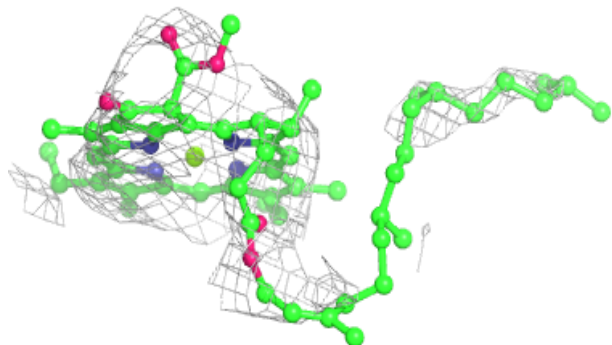
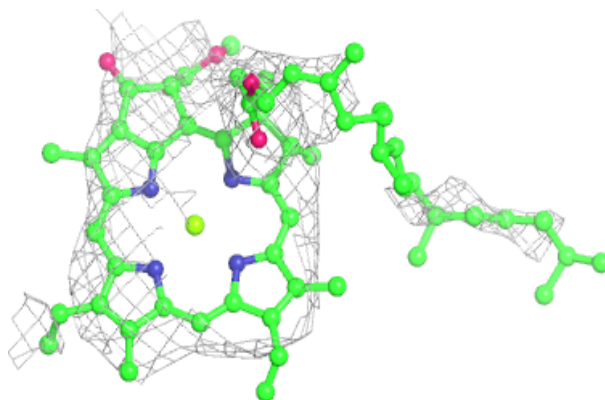


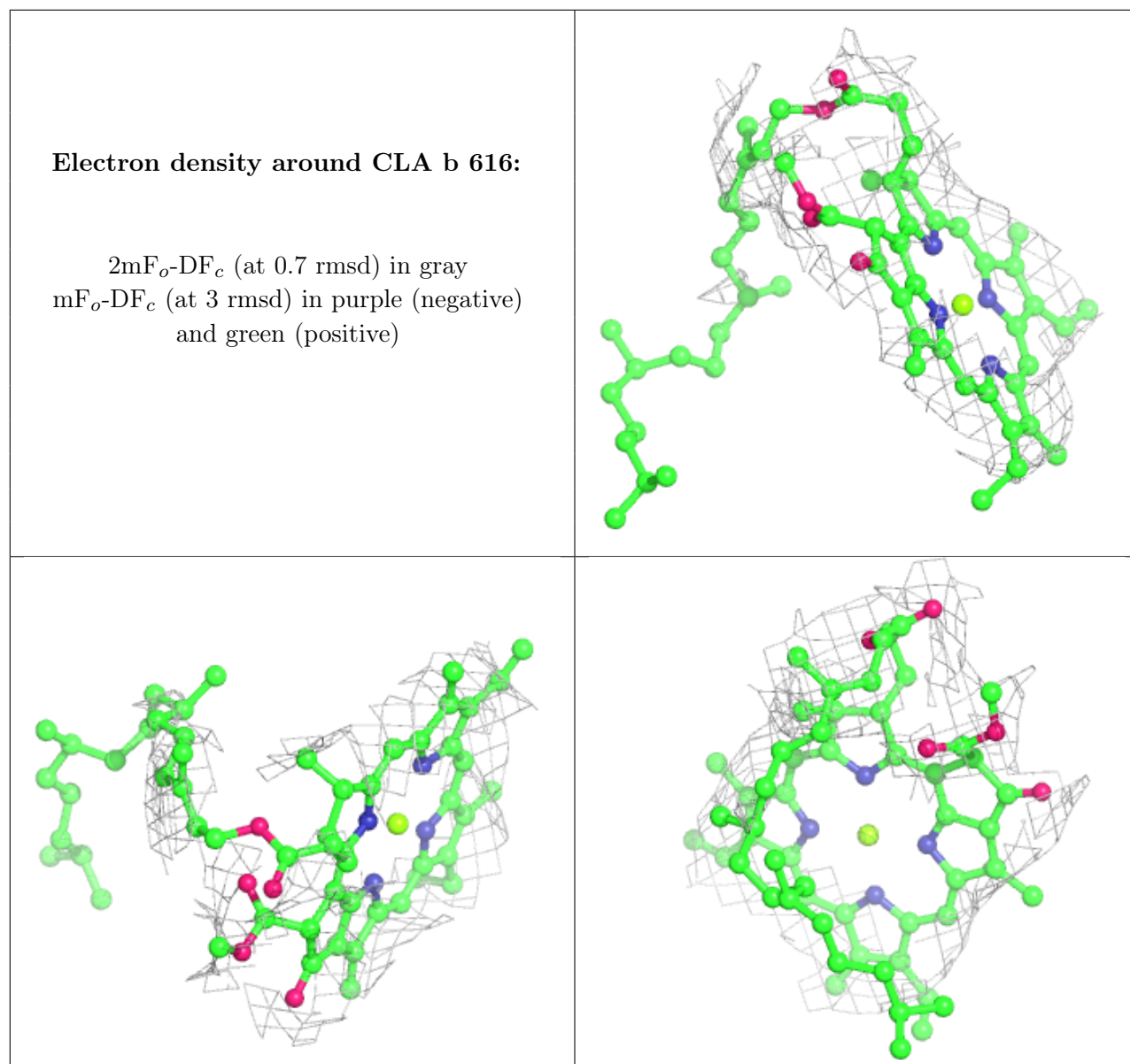
**Electron density around HEM f 101:**

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

**Electron density around CLA A 403:**

$2mF_o-DF_c$  (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.