



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 10:57 PM UTC

PDB ID : 4FBY / pdb\_00004fby  
Title : fs X-ray diffraction of Photosystem II  
Authors : Kern, J.; Alonso-Mori, R.; Hellmich, J.; Tran, R.; Hattne, J.; Laksmono, H.; Gloeckner, C.; Echols, N.; Sierra, R.G.; Sellberg, J.; Lassalle-Kaiser, B.; Gildea, R.J.; Glatzel, P.; Grosse-Kunstleve, R.W.; Latimer, M.J.; McQueen, T.A.; Difiore, D.; Fry, A.R.; Messerschmidt, M.M.; Miahnahri, A.; Schafer, D.W.; Seibert, M.M.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; White, W.E.; Adams, P.D.; Bogan, M.J.; Boutet, S.; Williams, G.J.; Messinger, J.; Sauter, N.K.; Zouni, A.; Bergmann, U.; Yano, J.; Yachandra, V.K.  
Deposited on : 2012-05-23  
Resolution : 6.56 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)

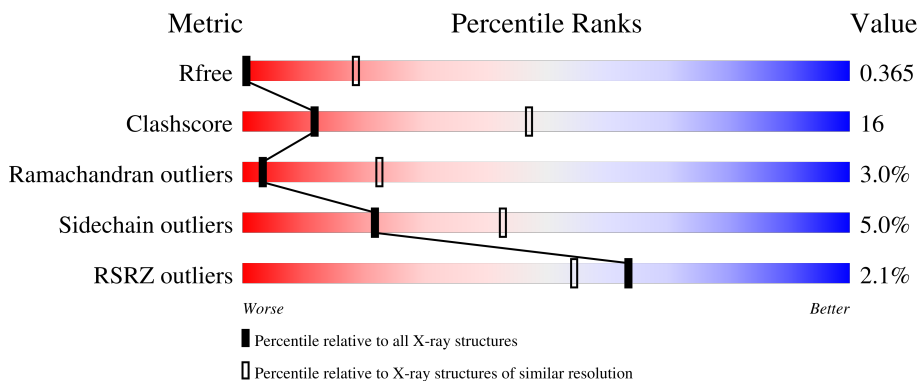
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.56 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))
$R_{free}$	180053	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	G	344	

*Continued on next page...*






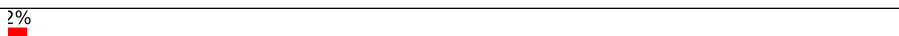
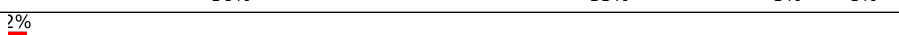
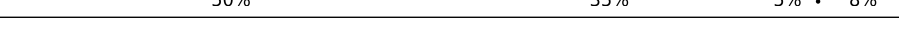
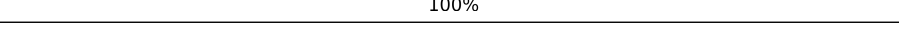

Density-Fitness : 1.0.12  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	510	2% 66% 27% ..
2	N	510	3% 67% 25% ..
3	C	461	% 59% 34% . .
3	P	461	% 59% 34% . .
4	D	352	2% 63% 29% 5% .
4	Q	352	3% 64% 28% 5% .
5	E	83	52% 39% 7% ..
5	R	83	6% 51% 40% 7% ..
6	F	44	45% 34% 20%
6	S	44	50% 30% 20%
7	H	65	3% 63% 29% 6% .
7	W	65	8% 62% 31% 6% .
8	I	38	53% 37% . 8%
8	a	38	55% 34% . 8%
9	J	39	41% 46% 13%
9	b	39	10% 44% 44% 13%
10	K	37	43% 51% 5%
10	c	37	3% 46% 49% 5%
11	L	37	5% 68% 24% 8%
11	d	37	5% 65% 27% 8%
12	M	36	6% 56% 36% . 6%
12	e	36	6% 53% 36% 6% 6%
13	O	246	67% 28% . .
13	f	246	% 68% 28% . .
14	T	32	59% 38% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	g	32	
15	U	104	
15	h	104	
16	V	137	
16	i	137	
17	m	46	
17	y	46	
18	X	40	
18	j	40	
19	Y	28	
19	k	28	
20	Z	62	
20	l	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
21	CLA	A	401	X	-	-	-
21	CLA	A	402	X	-	-	-
21	CLA	A	403	X	-	-	-
21	CLA	A	405	X	-	-	-
21	CLA	B	601	X	-	-	-
21	CLA	B	602	X	-	-	-
21	CLA	B	603	X	-	-	-
21	CLA	B	604	X	-	-	-
21	CLA	B	605	X	-	-	-
21	CLA	B	606	X	-	-	-
21	CLA	B	607	X	-	-	-
21	CLA	B	608	X	-	-	-
21	CLA	B	609	X	-	-	-
21	CLA	B	610	X	-	-	-
21	CLA	B	611	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	612	X	-	-	-
21	CLA	B	613	X	-	-	-
21	CLA	B	614	X	-	-	-
21	CLA	B	615	X	-	-	-
21	CLA	B	616	X	-	-	-
21	CLA	C	501	X	-	-	-
21	CLA	C	502	X	-	-	-
21	CLA	C	503	X	-	-	-
21	CLA	C	504	X	-	-	-
21	CLA	C	505	X	-	-	-
21	CLA	C	506	X	-	-	-
21	CLA	C	507	X	-	-	-
21	CLA	C	508	X	-	-	-
21	CLA	C	509	X	-	-	-
21	CLA	C	510	X	-	-	-
21	CLA	C	511	X	-	-	-
21	CLA	C	512	X	-	-	-
21	CLA	C	513	X	-	-	-
21	CLA	D	401	X	-	-	-
21	CLA	D	403	X	-	-	-
21	CLA	G	402	X	-	-	-
21	CLA	G	403	X	-	-	-
21	CLA	G	404	X	-	-	-
21	CLA	G	406	X	-	-	-
21	CLA	N	605	X	-	-	-
21	CLA	N	606	X	-	-	-
21	CLA	N	607	X	-	-	-
21	CLA	N	608	X	-	-	-
21	CLA	N	609	X	-	-	-
21	CLA	N	610	X	-	-	-
21	CLA	N	611	X	-	-	-
21	CLA	N	612	X	-	-	-
21	CLA	N	613	X	-	-	-
21	CLA	N	614	X	-	-	-
21	CLA	N	615	X	-	-	-
21	CLA	N	616	X	-	-	-
21	CLA	N	617	X	-	-	-
21	CLA	N	618	X	-	-	-
21	CLA	N	619	X	-	-	-
21	CLA	N	620	X	-	-	-
21	CLA	P	501	X	-	-	-
21	CLA	P	502	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	P	503	X	-	-	-
21	CLA	P	504	X	-	-	-
21	CLA	P	505	X	-	-	-
21	CLA	P	506	X	-	-	-
21	CLA	P	507	X	-	-	-
21	CLA	P	508	X	-	-	-
21	CLA	P	509	X	-	-	-
21	CLA	P	510	X	-	-	-
21	CLA	P	511	X	-	-	-
21	CLA	P	512	X	-	-	-
21	CLA	P	513	X	-	-	-
21	CLA	Q	402	X	-	-	-
21	CLA	Q	404	X	-	-	-
24	DGD	A	407	X	-	-	-
24	DGD	B	621	X	-	-	-
24	DGD	B	628	X	-	-	-
24	DGD	C	516	X	-	-	-
24	DGD	C	517	X	-	-	-
24	DGD	C	518	X	-	-	-
24	DGD	D	408	X	-	-	-
24	DGD	G	408	X	-	-	-
24	DGD	N	602	X	-	-	-
24	DGD	P	517	X	-	-	-
24	DGD	P	518	X	-	-	-
24	DGD	P	519	X	-	-	-
24	DGD	Q	409	X	-	-	-
24	DGD	W	102	X	-	-	-
27	LMG	A	410	X	-	-	-
27	LMG	B	622	X	-	-	-
27	LMG	B	623	X	-	-	-
27	LMG	C	519	X	-	-	-
27	LMG	C	520	X	-	-	-
27	LMG	D	406	X	-	-	-
27	LMG	D	407	X	-	-	-
27	LMG	D	412	X	-	-	-
27	LMG	E	102	X	-	-	-
27	LMG	G	411	X	-	-	-
27	LMG	I	102	X	-	-	-
27	LMG	M	101	X	-	-	-
27	LMG	N	622	X	-	-	-
27	LMG	N	623	X	-	-	-
27	LMG	P	520	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
27	LMG	P	521	X	-	-	-
27	LMG	Q	401	X	-	-	-
27	LMG	Q	406	X	-	-	-
27	LMG	Q	407	X	-	-	-
27	LMG	R	102	X	-	-	-
27	LMG	a	102	X	-	-	-
27	LMG	e	102	X	-	-	-

## 2 Entry composition [i](#)

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	G	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- 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	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	N	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

- 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	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	P	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

- 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	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	Q	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

- 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	R	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	S	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	W	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	a	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	b	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			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	c	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	d	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	e	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	f	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	g	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	h	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	i	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	m	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

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

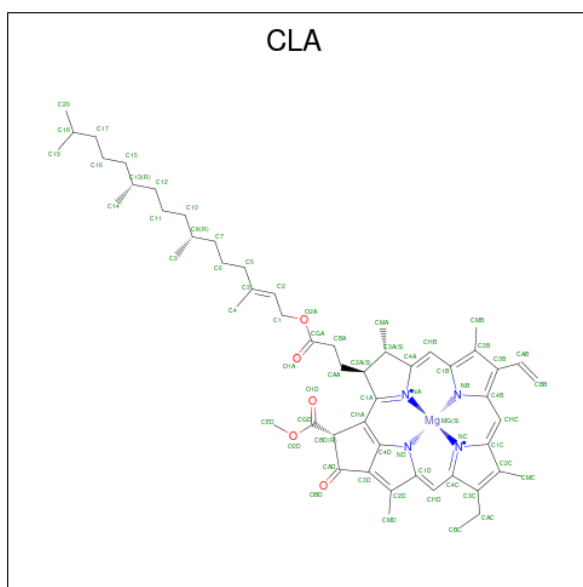
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			
19	k	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	l	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

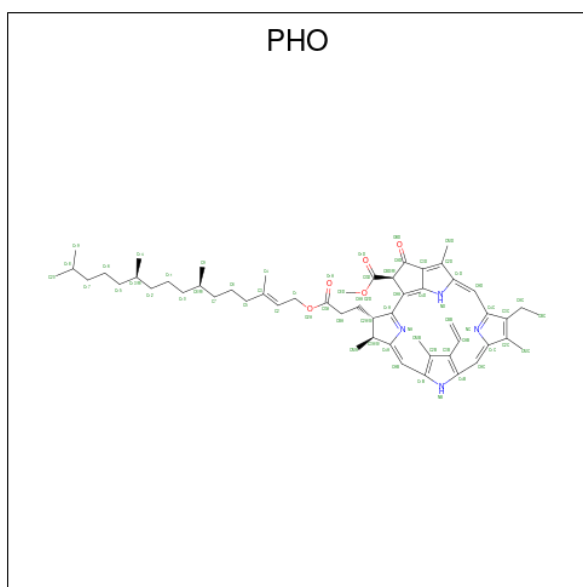
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	N	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

*Continued on next page...*

*Continued from previous page...*

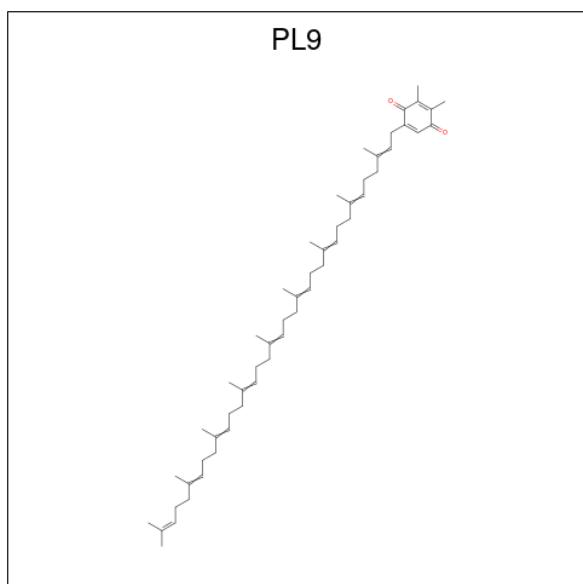
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 22 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



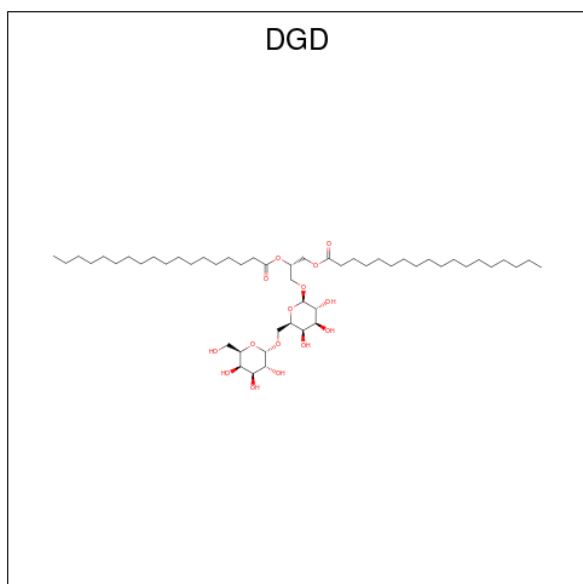
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
22	A	1	64	55	4	5	0	0
22	D	1	64	55	4	5	0	0
22	G	1	64	55	4	5	0	0
22	Q	1	64	55	4	5	0	0

- 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 (CCD ID: 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	G	1	Total	C	O	0	0
			45	43	2		
23	Q	1	Total	C	O	0	0
			55	53	2		
23	b	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



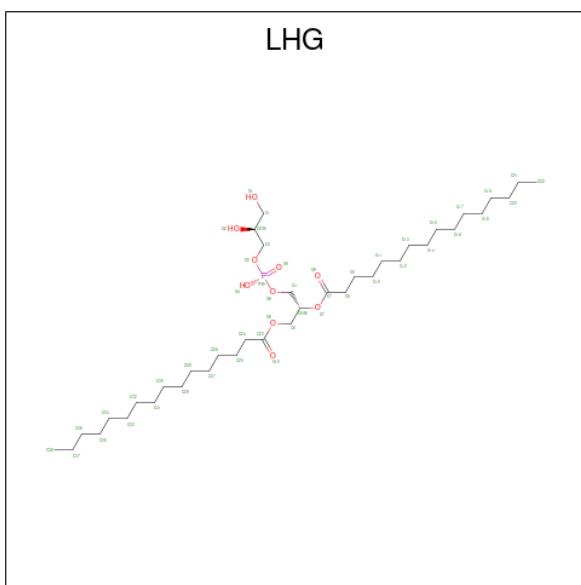
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			56	41	15		
24	B	1	Total	C	O	0	0
			58	43	15		
24	B	1	Total	C	O	0	0
			52	37	15		
24	C	1	Total	C	O	0	0
			53	38	15		
24	C	1	Total	C	O	0	0
			62	47	15		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			66	51	15		
24	D	1	Total	C	O	0	0
			63	48	15		
24	G	1	Total	C	O	0	0
			56	41	15		
24	N	1	Total	C	O	0	0
			52	37	15		
24	P	1	Total	C	O	0	0
			53	38	15		
24	P	1	Total	C	O	0	0
			62	47	15		
24	P	1	Total	C	O	0	0
			66	51	15		
24	Q	1	Total	C	O	0	0
			63	48	15		
24	W	1	Total	C	O	0	0
			58	43	15		

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



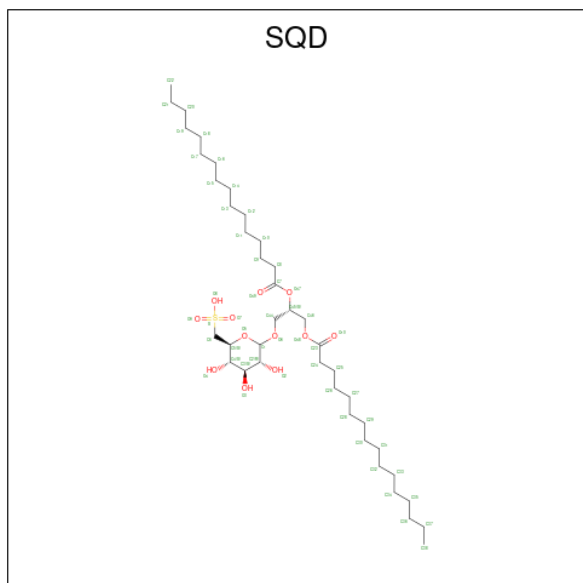
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	P	0	0
			39	28	10	1		
25	A	1	Total	C	O	P	0	0
			37	26	10	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
25	G	1	39	28	10	1	0	0
25	G	1	37	26	10	1	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



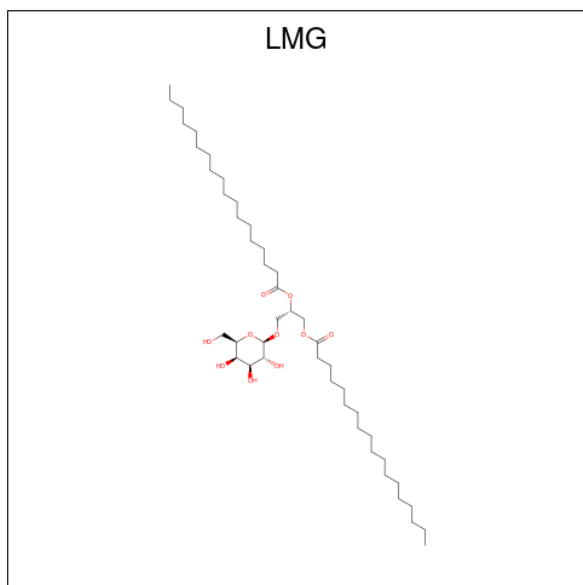
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	A	1	51	38	12	1	0	0
26	A	1	54	41	12	1	0	0
26	B	1	43	30	12	1	0	0
26	B	1	47	34	12	1	0	0
26	F	1	45	32	12	1	0	0
26	G	1	54	41	12	1	0	0
26	G	1	51	38	12	1	0	0
26	N	1	47	34	12	1	0	0
26	Q	1	43	30	12	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	S	1	45	32	12	1	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



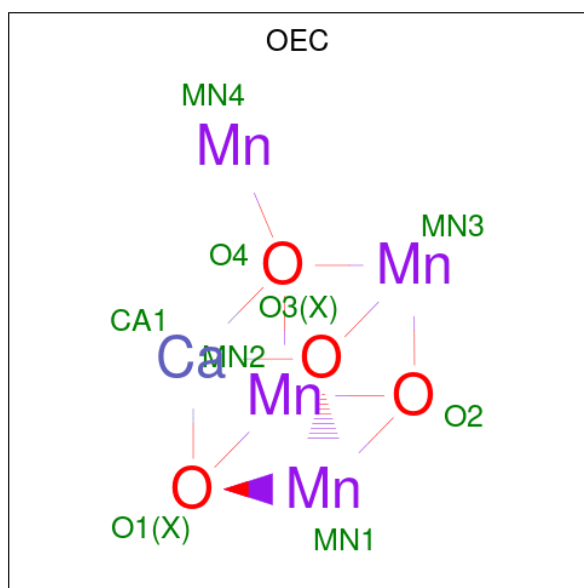
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	1	51	41	10	0	0
27	B	1	49	39	10	0	0
27	B	1	49	39	10	0	0
27	C	1	48	38	10	0	0
27	C	1	45	35	10	0	0
27	D	1	46	36	10	0	0
27	D	1	48	38	10	0	0
27	D	1	42	32	10	0	0
27	E	1	44	34	10	0	0
27	I	1	43	33	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	M	1	Total	C	O	0	0
			42	32	10		
27	G	1	Total	C	O	0	0
			51	41	10		
27	N	1	Total	C	O	0	0
			49	39	10		
27	N	1	Total	C	O	0	0
			49	39	10		
27	P	1	Total	C	O	0	0
			48	38	10		
27	P	1	Total	C	O	0	0
			45	35	10		
27	Q	1	Total	C	O	0	0
			42	32	10		
27	Q	1	Total	C	O	0	0
			48	38	10		
27	Q	1	Total	C	O	0	0
			46	36	10		
27	R	1	Total	C	O	0	0
			44	34	10		
27	a	1	Total	C	O	0	0
			43	33	10		
27	e	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula:  $\text{CaMn}_4\text{O}_4$ ).

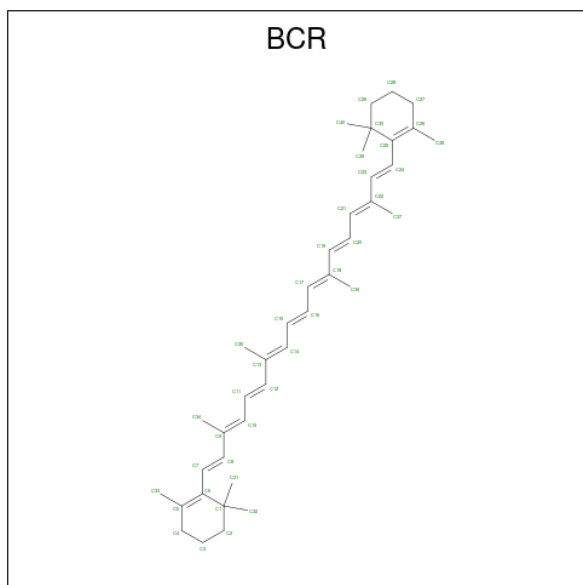


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	0	0
			5	1	4		
28	G	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	1	Total	Fe	0	0
			1	1		
29	G	1	Total	Fe	0	0
			1	1		

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



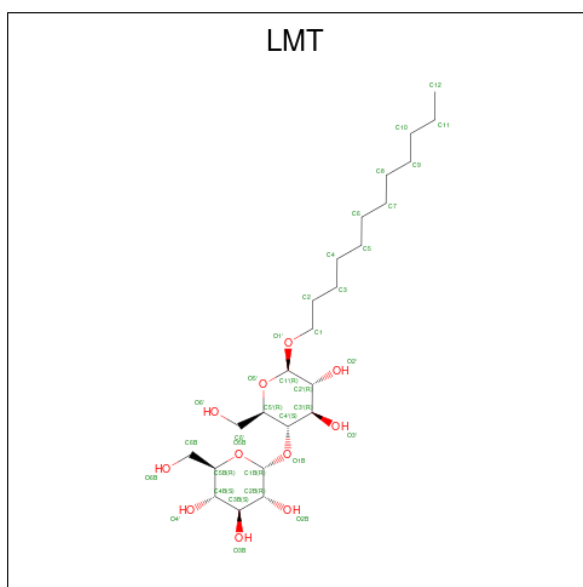
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	C	0	0
			40	40		
30	B	1	Total	C	0	0
			40	40		
30	B	1	Total	C	0	0
			40	40		
30	B	1	Total	C	0	0
			40	40		
30	C	1	Total	C	0	0
			40	40		
30	C	1	Total	C	0	0
			40	40		

*Continued on next page...*

*Continued from previous page...*

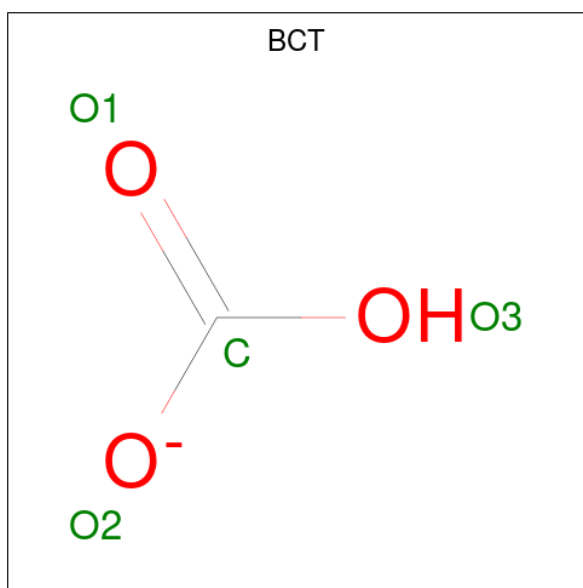
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	D	1	Total C 40 40	0	0
30	H	1	Total C 40 40	0	0
30	I	1	Total C 40 40	0	0
30	J	1	Total C 40 40	0	0
30	K	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	Z	1	Total C 40 40	0	0
30	N	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	S	1	Total C 40 40	0	0
30	W	1	Total C 40 40	0	0
30	a	1	Total C 40 40	0	0
30	b	1	Total C 40 40	0	0
30	c	1	Total C 40 40	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



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	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	Q	1	Total	C	O	0	0
			31	20	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	e	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).

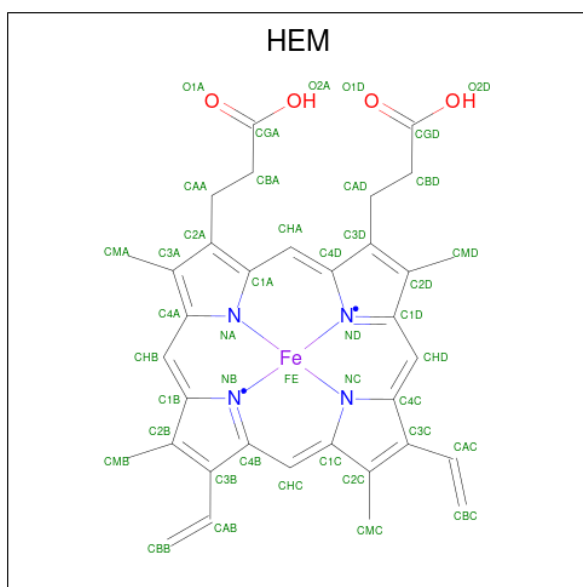


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	D	1	Total C O 4 1 3	0	0
32	Q	1	Total C O 4 1 3	0	0

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total Cl 1 1	0	0
33	G	1	Total Cl 1 1	0	0

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
34	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	i	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

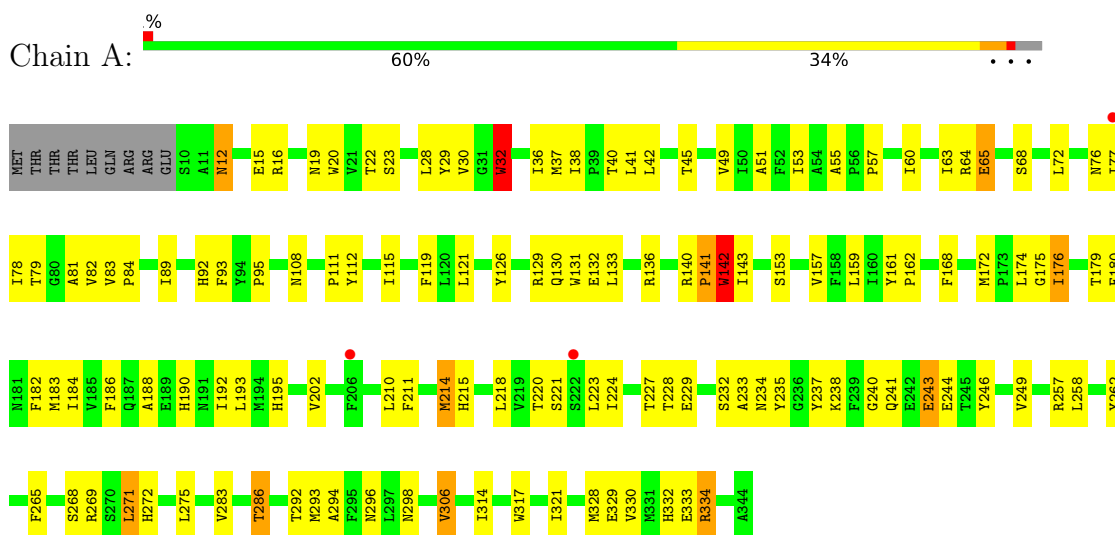
- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total	Ca	0	0
			1	1		
35	f	1	Total	Ca	0	0
			1	1		

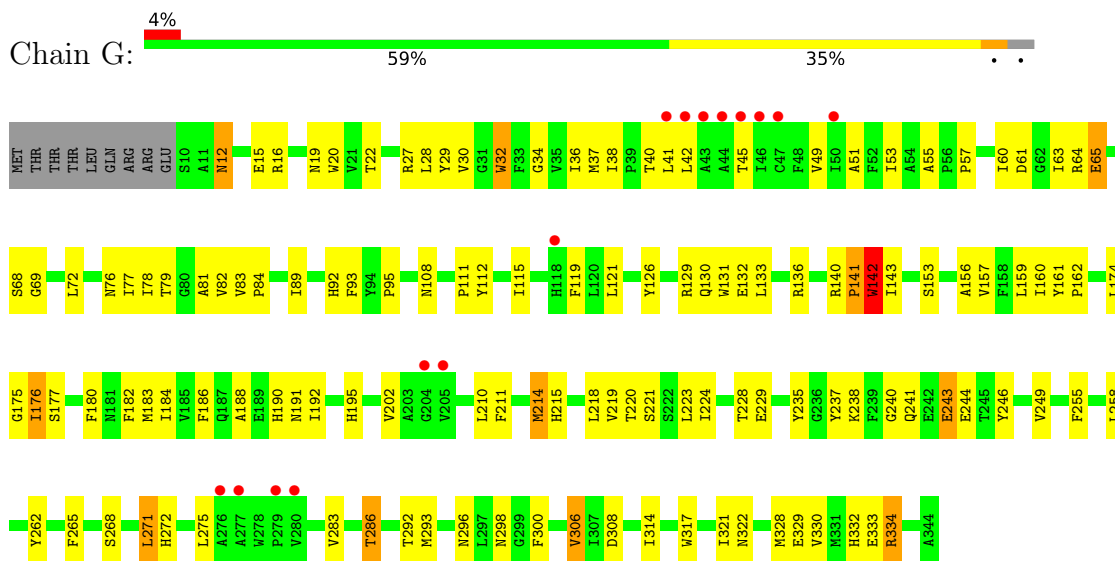
### 3 Residue-property plots i

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

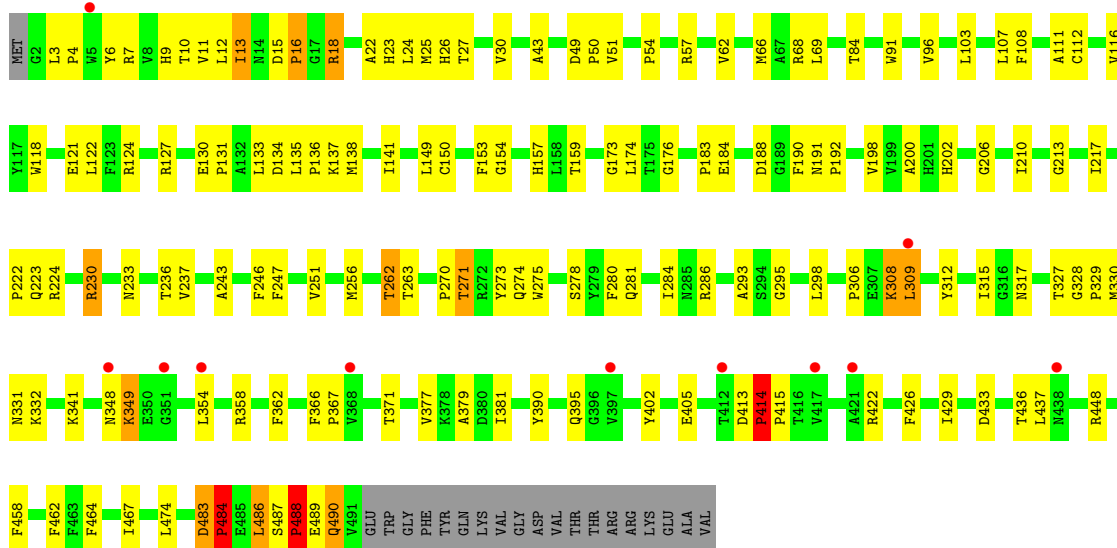


- Molecule 1: Photosystem Q(B) protein 1

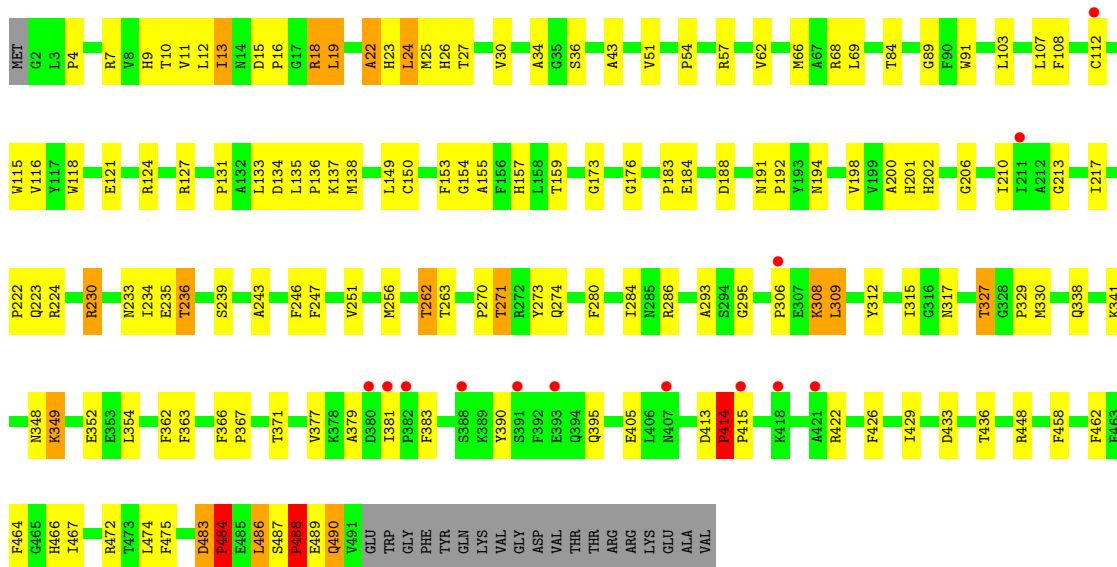


- Molecule 2: Photosystem II core light harvesting protein

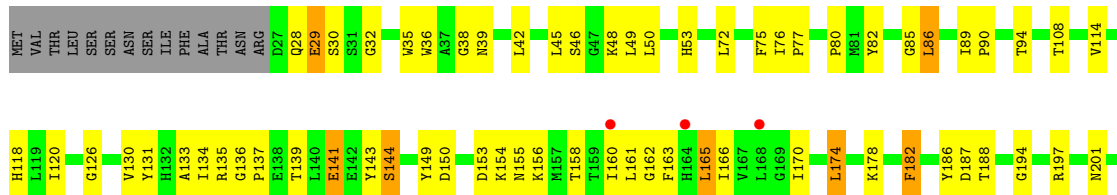


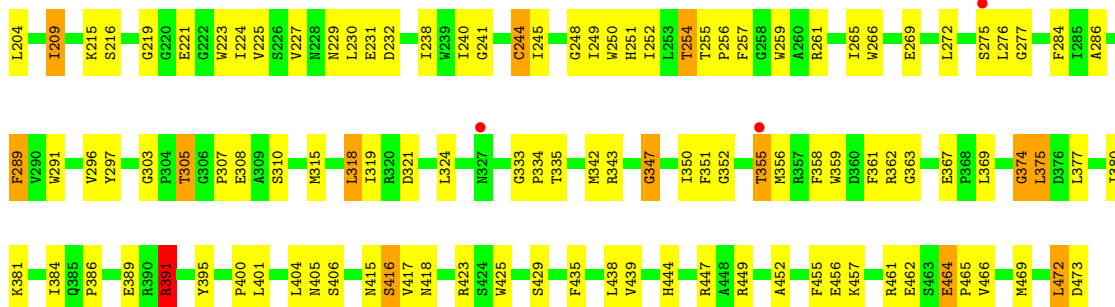


• Molecule 2: Photosystem II core light harvesting protein

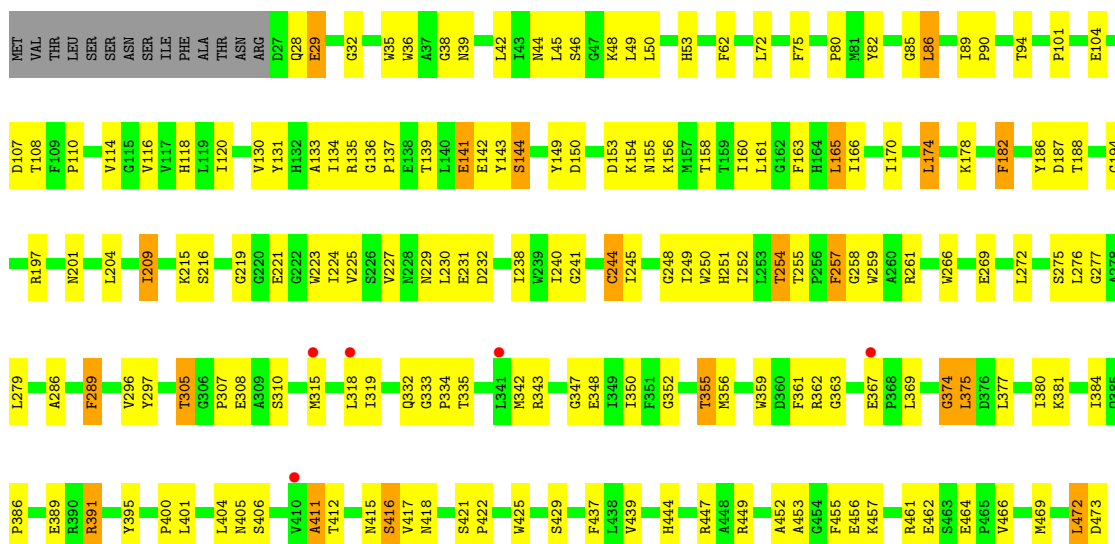


• Molecule 3: Photosystem II CP43 protein

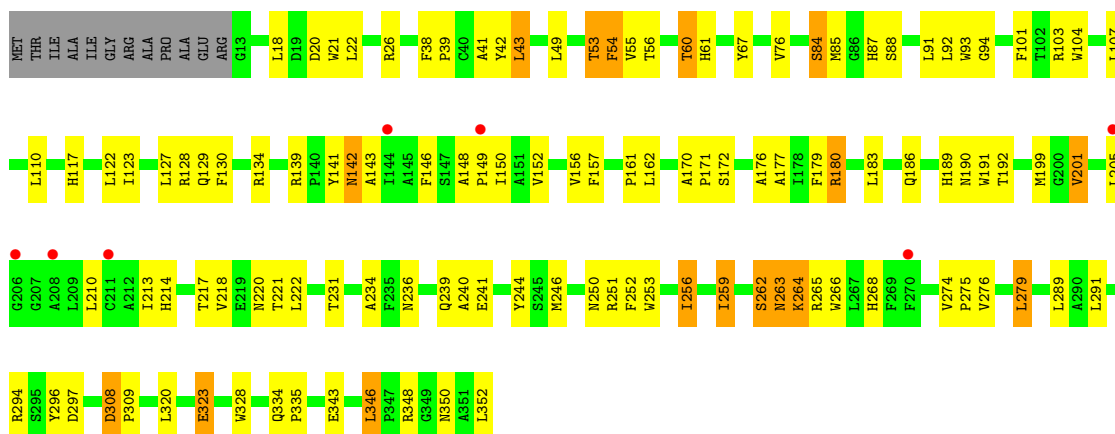




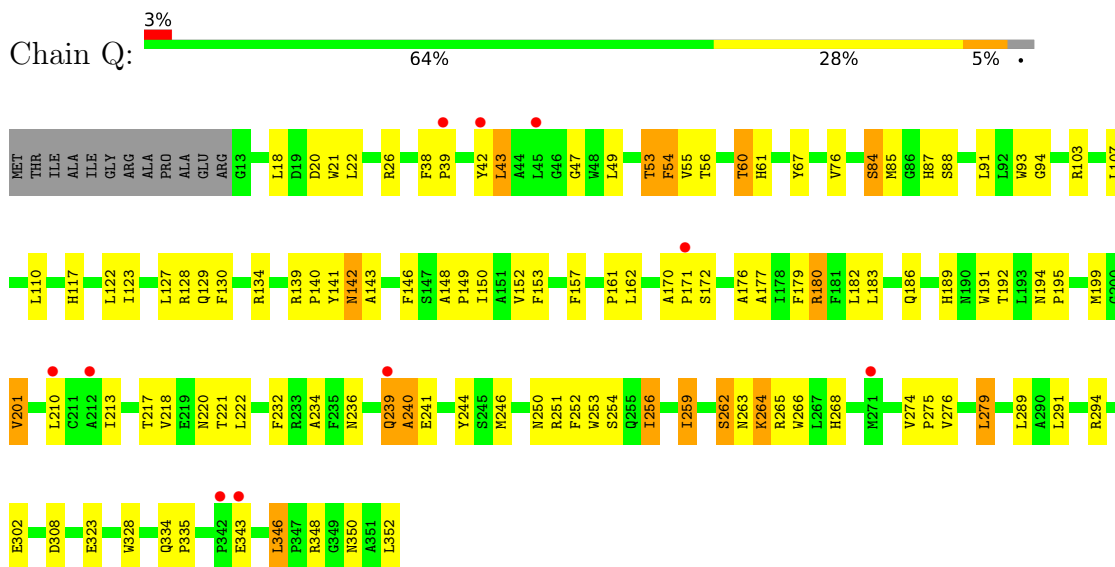
• Molecule 3: Photosystem II CP43 protein



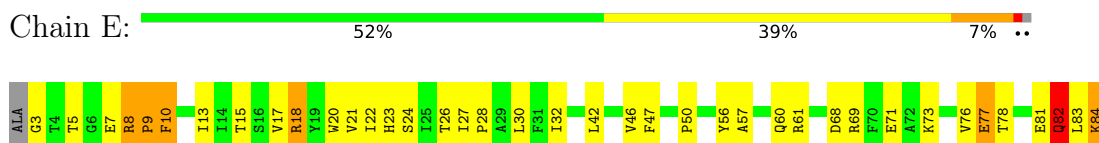
• Molecule 4: Photosystem II D2 protein



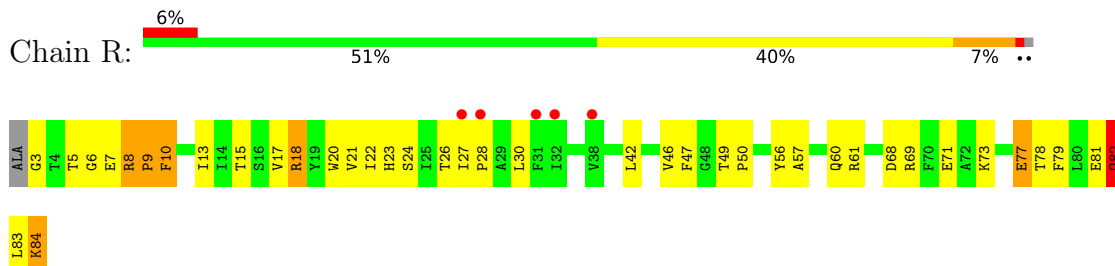
• Molecule 4: Photosystem II D2 protein



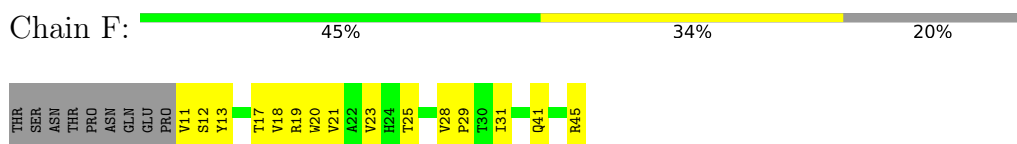
• Molecule 5: Cytochrome b559 subunit alpha



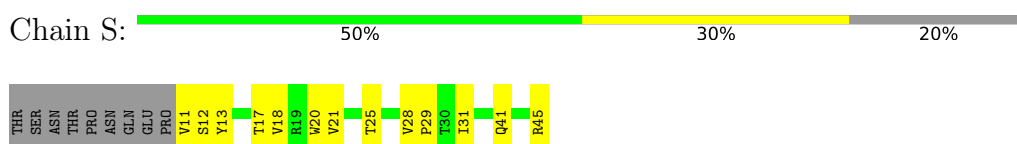
• Molecule 5: Cytochrome b559 subunit alpha



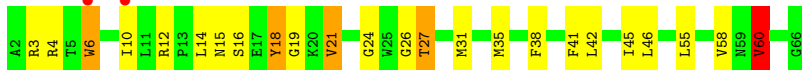
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta



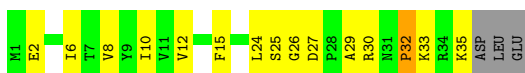
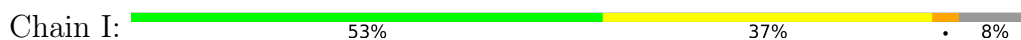
• Molecule 7: Photosystem II reaction center protein H



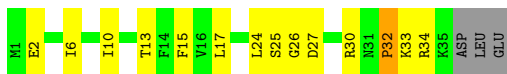
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



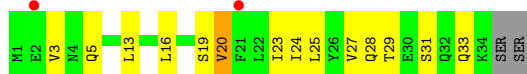
• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



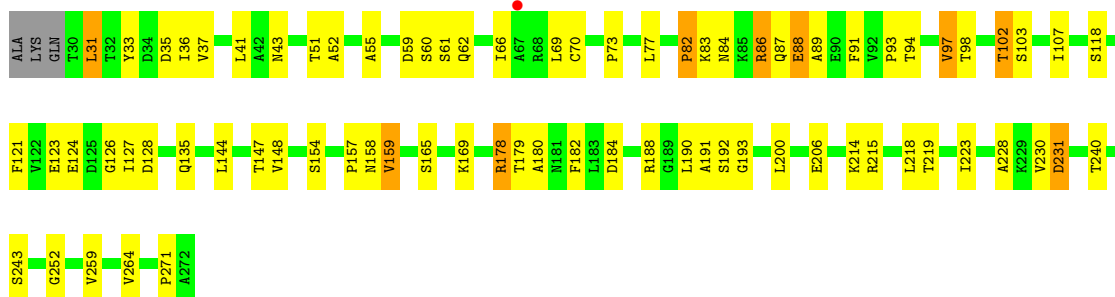
• Molecule 12: Photosystem II reaction center protein M



• Molecule 12: Photosystem II reaction center protein M



• Molecule 13: Photosystem II manganese-stabilizing polypeptide



• Molecule 13: Photosystem II manganese-stabilizing polypeptide



Chain i:  75% 23% ..



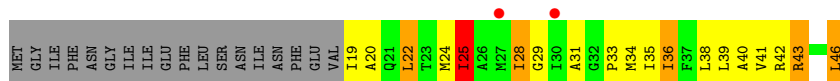
- Molecule 17: Photosystem II reaction center protein ycf12

Chain y:  20% 30% 9% . 39%



- Molecule 17: Photosystem II reaction center protein ycf12

Chain m:  4% 20% 28% 11% . 39%



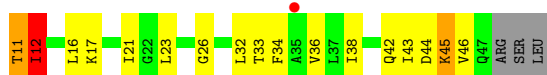
- Molecule 18: Photosystem II reaction center protein X

Chain X:  2% 50% 35% 5% . 8%



- Molecule 18: Photosystem II reaction center protein X

Chain j:  2% 50% 35% 5% . 8%



- 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 k:  93% 7%



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.78Å 227.76Å 308.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.89 – 6.56 85.89 – 6.56	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.89-6.56) 97.9 (85.89-6.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.06 (at 6.72Å)	Xtrriage
Refinement program	PHENIX 1.7.3	Depositor
R, $R_{free}$	0.366 , 0.385 0.343 , 0.365	Depositor DCC
$R_{free}$ test set	897 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.8	Xtrriage
Anisotropy	6.750	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 106.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.14$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.66	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	163.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: BCR, HEM, DGD, CLA, LHG, FE2, PL9, CA, LMT, SQD, CL, BCT, OEC, PHO, LMG

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	0.34	0/2713	0.95	8/3700 (0.2%)
1	G	0.35	0/2713	0.95	6/3700 (0.2%)
2	B	0.35	0/3986	0.95	14/5433 (0.3%)
2	N	0.36	0/3986	0.98	18/5433 (0.3%)
3	C	0.34	0/3556	0.94	10/4842 (0.2%)
3	P	0.34	0/3556	0.94	9/4842 (0.2%)
4	D	0.33	0/2801	0.92	8/3818 (0.2%)
4	Q	0.33	0/2801	0.92	6/3818 (0.2%)
5	E	0.38	0/685	1.01	4/933 (0.4%)
5	R	0.38	0/685	1.03	5/933 (0.5%)
6	F	0.41	0/291	0.80	0/397
6	S	0.37	0/291	0.79	0/397
7	H	0.40	0/520	0.91	0/709
7	W	0.41	0/520	0.91	0/709
8	I	0.34	0/293	0.92	1/395 (0.3%)
8	a	0.35	0/293	0.94	1/395 (0.3%)
9	J	0.36	0/255	1.07	2/346 (0.6%)
9	b	0.36	0/255	1.08	2/346 (0.6%)
10	K	0.46	0/303	0.88	0/416
10	c	0.46	0/303	0.89	0/416
11	L	0.32	0/311	0.90	0/422
11	d	0.32	0/311	0.92	2/422 (0.5%)
12	M	0.39	0/270	0.94	1/367 (0.3%)
12	e	0.40	0/270	0.93	1/367 (0.3%)
13	O	0.34	0/1876	0.87	5/2548 (0.2%)
13	f	0.33	0/1876	0.87	5/2548 (0.2%)
14	T	0.32	0/284	0.90	0/381
14	g	0.32	0/284	0.90	0/381
15	U	0.41	0/785	0.97	4/1064 (0.4%)
15	h	0.41	0/785	1.00	5/1064 (0.5%)
16	V	0.33	0/1081	0.89	6/1468 (0.4%)
16	i	0.33	0/1081	0.89	4/1468 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	m	0.42	0/202	1.03	2/272 (0.7%)
17	y	0.45	0/202	1.01	1/272 (0.4%)
18	X	0.50	0/273	0.91	1/370 (0.3%)
18	j	0.50	0/273	0.95	1/370 (0.3%)
20	Z	0.38	0/490	1.00	2/669 (0.3%)
20	l	0.38	0/490	1.00	2/669 (0.3%)
All	All	0.36	0/41950	0.94	136/57100 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	N	22	ALA	CA-C-N	9.36	134.04	120.38
2	N	22	ALA	C-N-CA	9.36	134.04	120.38
2	N	483	ASP	CA-C-N	8.80	130.84	119.84
2	N	483	ASP	C-N-CA	8.80	130.84	119.84
2	B	483	ASP	CA-C-N	8.59	130.58	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	23	HIS	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	106	0
1	G	2628	0	2524	108	0
2	B	3850	0	3718	108	0
2	N	3850	0	3718	111	0
3	C	3444	0	3365	131	0
3	P	3444	0	3365	131	0
4	D	2706	0	2608	100	0
4	Q	2706	0	2608	103	0
5	E	666	0	651	39	0
5	R	666	0	651	38	0
6	F	282	0	291	13	0
6	S	282	0	291	12	0
7	H	507	0	521	26	0
7	W	507	0	521	26	0
8	I	286	0	308	8	0
8	a	286	0	308	8	0
9	J	249	0	262	18	0
9	b	249	0	262	18	0
10	K	293	0	305	18	0
10	c	293	0	305	21	0
11	L	304	0	316	15	0
11	d	304	0	316	14	0
12	M	267	0	289	17	0
12	e	267	0	289	18	0
13	O	1845	0	1801	48	0
13	f	1845	0	1801	49	1
14	T	275	0	288	13	0
14	g	275	0	288	9	0
15	U	774	0	773	16	0
15	h	774	0	773	16	0
16	V	1060	0	1068	22	0
16	i	1060	0	1068	23	0
17	m	201	0	226	18	0
17	y	201	0	226	17	0
18	X	270	0	299	10	0
18	j	270	0	299	10	0
19	Y	140	0	32	0	0
19	k	140	0	32	1	0
20	Z	479	0	516	21	1
20	l	479	0	516	21	0
21	A	260	0	288	27	0
21	B	1040	0	1152	66	0
21	C	845	0	936	49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	D	130	0	144	11	0
21	G	260	0	288	26	0
21	N	1040	0	1152	65	0
21	P	845	0	936	45	0
21	Q	130	0	144	14	0
22	A	64	0	74	6	0
22	D	64	0	74	5	0
22	G	64	0	74	7	0
22	Q	64	0	74	5	0
23	A	45	0	61	5	0
23	D	55	0	80	6	0
23	G	45	0	61	5	0
23	J	35	0	45	1	0
23	Q	55	0	80	5	0
23	b	35	0	45	2	0
24	A	56	0	70	1	0
24	B	110	0	136	5	0
24	C	181	0	245	17	0
24	D	63	0	87	0	0
24	G	56	0	70	2	0
24	N	52	0	62	4	0
24	P	181	0	245	14	0
24	Q	63	0	87	1	0
24	W	58	0	74	3	0
25	A	76	0	95	4	0
25	G	76	0	95	4	0
26	A	105	0	147	13	0
26	B	90	0	111	10	0
26	F	45	0	54	2	0
26	G	105	0	147	16	0
26	N	47	0	61	7	0
26	Q	43	0	50	3	0
26	S	45	0	54	2	0
27	A	51	0	72	2	0
27	B	98	0	136	2	0
27	C	93	0	126	4	0
27	D	136	0	182	15	0
27	E	44	0	58	2	0
27	G	51	0	72	2	0
27	I	43	0	56	4	0
27	M	42	0	54	4	0
27	N	98	0	136	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	P	93	0	126	4	0
27	Q	136	0	182	15	0
27	R	44	0	58	2	0
27	a	43	0	56	2	0
27	e	42	0	54	3	0
28	A	5	0	0	0	0
28	G	5	0	0	0	0
29	A	1	0	0	0	0
29	G	1	0	0	0	0
30	B	160	0	224	16	0
30	C	80	0	112	16	0
30	D	40	0	56	3	0
30	H	40	0	56	2	0
30	I	40	0	56	5	0
30	J	40	0	56	4	0
30	K	40	0	56	11	0
30	N	40	0	56	4	0
30	P	120	0	168	20	0
30	S	40	0	56	5	0
30	T	120	0	168	17	0
30	W	40	0	56	3	0
30	Z	40	0	56	3	0
30	a	40	0	56	4	0
30	b	40	0	56	3	0
30	c	40	0	56	12	0
31	B	140	0	184	8	0
31	D	31	0	35	0	0
31	I	35	0	46	2	0
31	M	35	0	46	1	0
31	N	140	0	184	9	0
31	Q	31	0	35	0	0
31	a	35	0	46	1	0
31	e	35	0	46	1	0
32	D	4	0	1	0	0
32	Q	4	0	1	0	0
33	D	1	0	0	0	0
33	G	1	0	0	0	0
34	E	43	0	30	7	0
34	R	43	0	30	6	0
34	V	43	0	30	5	0
34	i	43	0	30	4	0
35	O	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	f	1	0	0	0	0
All	All	50232	0	51376	1600	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 1600 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:33:GLN:HB3	12:e:33:GLN:HB3	1.41	1.02
2:N:121:GLU:HG2	7:W:4:ARG:HG2	1.49	0.94
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.50	0.93
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.52	0.92
4:Q:26:ARG:HD3	6:S:18:VAL:HG11	1.54	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:60:PHE:O	13:f:115:SER:OG[3_755]	2.16	0.04

## 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%)	297 (89%)	31 (9%)	5 (2%)	8	40
1	G	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	8	40
2	B	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	4	26
2	N	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	4	26
3	C	445/461 (96%)	375 (84%)	55 (12%)	15 (3%)	3	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	445/461 (96%)	376 (84%)	53 (12%)	16 (4%)	2	20
4	D	338/352 (96%)	292 (86%)	40 (12%)	6 (2%)	6	34
4	Q	338/352 (96%)	291 (86%)	41 (12%)	6 (2%)	6	34
5	E	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	2	19
5	R	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	2	19
6	F	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
6	S	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
7	H	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	9
7	W	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	9
8	I	33/38 (87%)	24 (73%)	7 (21%)	2 (6%)	1	13
8	a	33/38 (87%)	25 (76%)	6 (18%)	2 (6%)	1	13
9	J	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	12
9	b	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	12
10	K	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	14
10	c	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	14
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	d	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	e	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	203 (84%)	27 (11%)	11 (5%)	2	16
13	f	241/246 (98%)	203 (84%)	29 (12%)	9 (4%)	2	19
14	T	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3	21
14	g	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3	21
15	U	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	2	17
15	h	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	2	17
16	V	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	18	56
16	i	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	18	56
17	m	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	10
17	y	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	10
18	X	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	5
18	j	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Z	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	1	16
20	l	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	1	16
All	All	5138/5426 (95%)	4357 (85%)	626 (12%)	155 (3%)	3	22

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO

### 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%)	258 (95%)	13 (5%)	23	44
1	G	271/280 (97%)	258 (95%)	13 (5%)	23	44
2	B	390/407 (96%)	373 (96%)	17 (4%)	25	47
2	N	390/407 (96%)	373 (96%)	17 (4%)	25	47
3	C	347/362 (96%)	334 (96%)	13 (4%)	30	51
3	P	347/362 (96%)	334 (96%)	13 (4%)	30	51
4	D	275/283 (97%)	257 (94%)	18 (6%)	15	37
4	Q	275/283 (97%)	257 (94%)	18 (6%)	15	37
5	E	72/72 (100%)	66 (92%)	6 (8%)	10	30
5	R	72/72 (100%)	66 (92%)	6 (8%)	10	30
6	F	29/38 (76%)	29 (100%)	0	100	100
6	S	29/38 (76%)	29 (100%)	0	100	100
7	H	53/54 (98%)	50 (94%)	3 (6%)	18	40
7	W	53/54 (98%)	49 (92%)	4 (8%)	12	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/35 (91%)	30 (94%)	2 (6%)	16	37
8	a	32/35 (91%)	30 (94%)	2 (6%)	16	37
9	J	24/27 (89%)	23 (96%)	1 (4%)	26	48
9	b	24/27 (89%)	23 (96%)	1 (4%)	26	48
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	36
10	c	30/30 (100%)	28 (93%)	2 (7%)	15	36
11	L	35/35 (100%)	32 (91%)	3 (9%)	10	29
11	d	35/35 (100%)	32 (91%)	3 (9%)	10	29
12	M	31/33 (94%)	30 (97%)	1 (3%)	34	56
12	e	31/33 (94%)	30 (97%)	1 (3%)	34	56
13	O	202/208 (97%)	196 (97%)	6 (3%)	36	57
13	f	202/208 (97%)	196 (97%)	6 (3%)	36	57
14	T	29/29 (100%)	28 (97%)	1 (3%)	32	54
14	g	29/29 (100%)	28 (97%)	1 (3%)	32	54
15	U	84/89 (94%)	81 (96%)	3 (4%)	31	52
15	h	84/89 (94%)	81 (96%)	3 (4%)	31	52
16	V	116/117 (99%)	113 (97%)	3 (3%)	40	62
16	i	116/117 (99%)	113 (97%)	3 (3%)	40	62
17	m	20/37 (54%)	16 (80%)	4 (20%)	1	7
17	y	20/37 (54%)	16 (80%)	4 (20%)	1	7
18	X	30/33 (91%)	25 (83%)	5 (17%)	2	10
18	j	30/33 (91%)	25 (83%)	5 (17%)	2	10
20	Z	52/52 (100%)	47 (90%)	5 (10%)	8	25
20	l	52/52 (100%)	47 (90%)	5 (10%)	8	25
All	All	4244/4442 (96%)	4031 (95%)	213 (5%)	22	43

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	275	LEU
3	P	305	THR
17	m	25	ILE
2	N	11	VAL
2	N	422	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	118	HIS
11	d	8	GLN
4	Q	117	HIS
4	Q	250	ASN
13	f	130	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 182 ligands modelled in this entry, 6 are monoatomic - leaving 176 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
31	LMT	Q	410	-	32,32,36	0.48	0	43,43,47	0.66	1 (2%)
27	LMG	e	102	-	42,42,55	1.04	2 (4%)	50,50,63	1.32	6 (12%)
31	LMT	N	625	-	36,36,36	0.42	0	47,47,47	0.67	1 (2%)
27	LMG	B	622	-	49,49,55	0.94	2 (4%)	57,57,63	1.28	7 (12%)
24	DGD	B	628	-	53,53,67	1.03	3 (5%)	67,67,81	1.51	11 (16%)
24	DGD	P	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.50	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	G	404	-	69,73,73	1.54	15 (21%)	82,113,113	1.94	14 (17%)
25	LHG	G	409	-	38,38,48	1.07	2 (5%)	41,44,54	0.96	3 (7%)
21	CLA	N	619	-	69,73,73	1.52	13 (18%)	82,113,113	1.97	14 (17%)
27	LMG	D	406	-	46,46,55	0.99	2 (4%)	54,54,63	1.34	7 (12%)
27	LMG	A	410	-	51,51,55	0.96	2 (3%)	59,59,63	1.27	4 (6%)
24	DGD	A	407	-	57,57,67	0.99	4 (7%)	71,71,81	1.47	8 (11%)
26	SQD	A	409	-	49,51,54	1.14	3 (6%)	59,62,65	1.38	9 (15%)
23	PL9	J	101	-	35,35,55	1.20	5 (14%)	44,45,69	1.57	8 (18%)
21	CLA	B	606	-	69,73,73	1.55	14 (20%)	82,113,113	1.90	13 (15%)
21	CLA	N	607	-	69,73,73	1.57	16 (23%)	82,113,113	1.90	13 (15%)
21	CLA	N	616	-	69,73,73	1.54	13 (18%)	82,113,113	1.98	11 (13%)
22	PHO	Q	403	-	58,69,69	2.81	12 (20%)	55,99,99	2.59	15 (27%)
26	SQD	A	414	-	52,54,54	1.09	3 (5%)	62,65,65	1.04	3 (4%)
21	CLA	G	402	-	69,73,73	1.55	16 (23%)	82,113,113	1.91	11 (13%)
30	BCR	B	617	-	41,41,41	0.73	0	56,56,56	1.61	11 (19%)
21	CLA	B	611	-	69,73,73	1.55	14 (20%)	82,113,113	1.98	12 (14%)
21	CLA	P	501	-	69,73,73	1.54	14 (20%)	82,113,113	1.95	10 (12%)
27	LMG	P	521	-	45,45,55	1.03	2 (4%)	53,53,63	1.23	5 (9%)
21	CLA	G	406	-	69,73,73	1.53	16 (23%)	82,113,113	1.93	13 (15%)
27	LMG	R	102	-	44,44,55	1.01	2 (4%)	52,52,63	1.12	4 (7%)
26	SQD	Q	408	-	41,43,54	1.28	4 (9%)	51,54,65	1.44	7 (13%)
30	BCR	P	516	-	41,41,41	0.77	0	56,56,56	1.70	13 (23%)
21	CLA	N	614	-	69,73,73	1.56	15 (21%)	82,113,113	1.89	13 (15%)
30	BCR	C	515	-	41,41,41	0.78	0	56,56,56	1.70	11 (19%)
21	CLA	G	403	-	69,73,73	1.55	16 (23%)	82,113,113	1.95	16 (19%)
27	LMG	C	519	-	48,48,55	0.97	2 (4%)	56,56,63	1.30	6 (10%)
32	BCT	Q	411	29	3,3,3	0.71	0	2,3,3	0.09	0
21	CLA	Q	402	-	69,73,73	1.57	13 (18%)	82,113,113	1.89	14 (17%)
30	BCR	Z	101	-	41,41,41	0.68	0	56,56,56	1.63	14 (25%)
24	DGD	P	517	-	54,54,67	1.00	3 (5%)	68,68,81	1.54	10 (14%)
30	BCR	B	618	-	41,41,41	0.72	0	56,56,56	1.91	14 (25%)
27	LMG	N	623	-	49,49,55	0.95	2 (4%)	57,57,63	1.25	8 (14%)
30	BCR	T	102	-	41,41,41	0.71	0	56,56,56	1.88	16 (28%)
24	DGD	P	519	-	67,67,67	0.90	4 (5%)	81,81,81	1.28	7 (8%)
30	BCR	a	101	-	41,41,41	0.70	0	56,56,56	1.60	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	B	602	-	69,73,73	1.55	14 (20%)	82,113,113	1.90	13 (15%)
24	DGD	B	621	-	59,59,67	0.95	3 (5%)	73,73,81	1.39	9 (12%)
21	CLA	B	610	-	69,73,73	1.56	14 (20%)	82,113,113	1.93	13 (15%)
27	LMG	G	411	-	51,51,55	0.96	2 (3%)	59,59,63	1.24	4 (6%)
21	CLA	N	620	-	69,73,73	1.55	13 (18%)	82,113,113	1.94	14 (17%)
21	CLA	C	505	-	69,73,73	1.53	14 (20%)	82,113,113	1.98	10 (12%)
26	SQD	N	601	-	45,47,54	1.21	4 (8%)	55,58,65	1.47	10 (18%)
31	LMT	B	629	-	36,36,36	0.45	0	47,47,47	0.78	1 (2%)
22	PHO	A	404	-	58,69,69	2.77	12 (20%)	55,99,99	2.66	17 (30%)
30	BCR	P	514	-	41,41,41	0.70	0	56,56,56	2.41	17 (30%)
21	CLA	P	513	-	69,73,73	1.55	15 (21%)	82,113,113	1.90	12 (14%)
21	CLA	C	510	-	69,73,73	1.55	15 (21%)	82,113,113	1.91	11 (13%)
21	CLA	N	613	-	69,73,73	1.55	15 (21%)	82,113,113	1.93	10 (12%)
32	BCT	D	410	29	3,3,3	0.71	0	2,3,3	0.06	0
24	DGD	C	518	-	67,67,67	0.93	4 (5%)	81,81,81	1.33	7 (8%)
30	BCR	H	101	-	41,41,41	0.78	0	56,56,56	1.48	10 (17%)
30	BCR	T	103	-	41,41,41	0.70	0	56,56,56	1.64	11 (19%)
22	PHO	G	405	-	58,69,69	2.76	12 (20%)	55,99,99	2.73	17 (30%)
21	CLA	Q	404	-	69,73,73	1.57	15 (21%)	82,113,113	1.95	12 (14%)
21	CLA	A	405	-	69,73,73	1.56	16 (23%)	82,113,113	1.93	13 (15%)
21	CLA	C	507	-	69,73,73	1.56	15 (21%)	82,113,113	1.91	11 (13%)
21	CLA	N	605	-	69,73,73	1.54	15 (21%)	82,113,113	1.94	13 (15%)
31	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.70	1 (2%)
24	DGD	W	102	-	59,59,67	0.96	3 (5%)	73,73,81	1.41	8 (10%)
23	PL9	D	404	-	55,55,55	1.27	8 (14%)	68,69,69	1.64	18 (26%)
21	CLA	N	615	-	69,73,73	1.56	15 (21%)	82,113,113	1.94	13 (15%)
30	BCR	b	102	-	41,41,41	0.80	0	56,56,56	3.18	20 (35%)
21	CLA	N	617	-	69,73,73	1.57	15 (21%)	82,113,113	1.91	9 (10%)
31	LMT	B	630	-	36,36,36	0.39	0	47,47,47	0.63	0
21	CLA	P	509	-	69,73,73	1.55	15 (21%)	82,113,113	1.89	13 (15%)
21	CLA	P	512	-	69,73,73	1.56	14 (20%)	82,113,113	1.93	13 (15%)
21	CLA	B	612	-	69,73,73	1.57	15 (21%)	82,113,113	1.91	12 (14%)
21	CLA	C	512	-	69,73,73	1.54	13 (18%)	82,113,113	1.94	13 (15%)
21	CLA	N	606	-	69,73,73	1.55	15 (21%)	82,113,113	1.94	12 (14%)
21	CLA	N	608	-	69,73,73	1.56	14 (20%)	82,113,113	1.93	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	SQD	G	410	-	49,51,54	1.14	3 (6%)	59,62,65	1.41	9 (15%)
21	CLA	N	611	-	69,73,73	1.57	16 (23%)	82,113,113	1.92	12 (14%)
21	CLA	B	613	-	69,73,73	1.54	15 (21%)	82,113,113	1.91	11 (13%)
30	BCR	W	101	-	41,41,41	0.78	0	56,56,56	1.48	8 (14%)
30	BCR	C	514	-	41,41,41	0.73	0	56,56,56	2.38	17 (30%)
30	BCR	K	101	-	41,41,41	0.81	0	56,56,56	1.64	12 (21%)
21	CLA	P	506	-	69,73,73	1.57	15 (21%)	82,113,113	1.91	13 (15%)
21	CLA	P	505	-	69,73,73	1.56	15 (21%)	82,113,113	1.97	10 (12%)
21	CLA	D	401	-	69,73,73	1.57	14 (20%)	82,113,113	1.90	13 (15%)
26	SQD	B	627	-	45,47,54	1.21	4 (8%)	55,58,65	1.40	8 (14%)
30	BCR	J	102	-	41,41,41	0.81	0	56,56,56	3.15	20 (35%)
31	LMT	D	409	-	32,32,36	0.47	0	43,43,47	0.66	1 (2%)
21	CLA	P	510	-	69,73,73	1.55	15 (21%)	82,113,113	1.92	12 (14%)
21	CLA	B	615	-	69,73,73	1.54	14 (20%)	82,113,113	1.95	13 (15%)
24	DGD	Q	409	-	64,64,67	0.91	2 (3%)	78,78,81	1.33	9 (11%)
31	LMT	N	624	-	36,36,36	0.42	0	47,47,47	0.67	0
27	LMG	Q	406	-	46,46,55	0.99	2 (4%)	54,54,63	1.31	4 (7%)
21	CLA	C	504	-	69,73,73	1.56	15 (21%)	82,113,113	1.90	13 (15%)
26	SQD	B	624	-	41,43,54	1.27	4 (9%)	51,54,65	1.43	7 (13%)
30	BCR	c	101	-	41,41,41	0.80	0	56,56,56	1.59	12 (21%)
31	LMT	N	603	-	36,36,36	0.45	0	47,47,47	0.80	1 (2%)
27	LMG	I	102	-	43,43,55	1.01	2 (4%)	51,51,63	1.32	5 (9%)
27	LMG	N	622	-	49,49,55	0.94	2 (4%)	57,57,63	1.36	7 (12%)
26	SQD	S	102	-	43,45,54	1.25	4 (9%)	53,56,65	1.17	5 (9%)
31	LMT	B	626	-	36,36,36	0.45	0	47,47,47	0.67	1 (2%)
21	CLA	D	403	-	69,73,73	1.56	15 (21%)	82,113,113	1.95	12 (14%)
21	CLA	A	403	-	69,73,73	1.56	17 (24%)	82,113,113	1.90	12 (14%)
21	CLA	A	402	-	69,73,73	1.55	16 (23%)	82,113,113	1.97	14 (17%)
31	LMT	I	103	-	36,36,36	0.48	1 (2%)	47,47,47	0.71	1 (2%)
27	LMG	E	102	-	44,44,55	1.02	2 (4%)	52,52,63	1.11	5 (9%)
31	LMT	B	625	-	36,36,36	0.41	0	47,47,47	0.70	0
21	CLA	C	511	3	69,73,73	1.55	15 (21%)	82,113,113	1.96	13 (15%)
24	DGD	C	516	-	54,54,67	0.99	3 (5%)	68,68,81	1.51	11 (16%)
34	HEM	R	101	5,6	50,50,50	1.84	8 (16%)	67,82,82	1.56	10 (14%)
26	SQD	G	401	-	52,54,54	1.10	3 (5%)	62,65,65	1.02	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	B	605	-	69,73,73	1.55	16 (23%)	82,113,113	1.95	15 (18%)
21	CLA	P	507	-	69,73,73	1.56	15 (21%)	82,113,113	1.90	10 (12%)
30	BCR	N	621	-	41,41,41	0.76	0	56,56,56	1.54	12 (21%)
21	CLA	B	608	-	69,73,73	1.57	15 (21%)	82,113,113	1.90	10 (12%)
27	LMG	D	412	-	42,42,55	1.04	3 (7%)	50,50,63	1.27	5 (10%)
30	BCR	D	405	-	41,41,41	0.73	0	56,56,56	1.74	10 (17%)
30	BCR	B	619	-	41,41,41	0.76	0	56,56,56	1.52	10 (17%)
21	CLA	B	601	-	69,73,73	1.55	14 (20%)	82,113,113	1.97	12 (14%)
21	CLA	C	501	-	69,73,73	1.54	14 (20%)	82,113,113	1.93	11 (13%)
21	CLA	C	509	-	69,73,73	1.57	15 (21%)	82,113,113	1.88	13 (15%)
21	CLA	P	508	-	69,73,73	1.55	16 (23%)	82,113,113	1.96	11 (13%)
21	CLA	N	612	-	69,73,73	1.57	16 (23%)	82,113,113	1.88	11 (13%)
23	PL9	Q	405	-	55,55,55	1.27	8 (14%)	68,69,69	1.66	18 (26%)
25	LHG	G	412	-	36,36,48	1.09	2 (5%)	39,42,54	1.07	2 (5%)
27	LMG	C	520	-	45,45,55	1.04	2 (4%)	53,53,63	1.27	5 (9%)
27	LMG	D	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.28	5 (8%)
21	CLA	C	508	-	69,73,73	1.55	14 (20%)	82,113,113	1.94	12 (14%)
25	LHG	A	408	-	38,38,48	1.07	2 (5%)	41,44,54	0.96	2 (4%)
21	CLA	B	614	-	69,73,73	1.55	13 (18%)	82,113,113	1.87	12 (14%)
25	LHG	A	411	-	36,36,48	1.08	2 (5%)	39,42,54	1.09	2 (5%)
24	DGD	G	408	-	57,57,67	0.98	4 (7%)	71,71,81	1.46	8 (11%)
21	CLA	A	401	-	69,73,73	1.57	16 (23%)	82,113,113	1.88	12 (14%)
27	LMG	B	623	-	49,49,55	0.95	2 (4%)	57,57,63	1.26	8 (14%)
31	LMT	e	101	-	36,36,36	0.41	0	47,47,47	0.66	1 (2%)
23	PL9	b	101	-	35,35,55	1.20	5 (14%)	44,45,69	1.59	9 (20%)
27	LMG	a	102	-	43,43,55	1.01	2 (4%)	51,51,63	1.33	6 (11%)
31	LMT	a	103	-	36,36,36	0.46	0	47,47,47	0.70	1 (2%)
27	LMG	M	101	-	42,42,55	1.03	2 (4%)	50,50,63	1.29	6 (12%)
24	DGD	C	517	-	63,63,67	0.93	3 (4%)	77,77,81	1.49	14 (18%)
22	PHO	D	402	-	58,69,69	2.81	12 (20%)	55,99,99	2.62	16 (29%)
21	CLA	B	607	-	69,73,73	1.57	15 (21%)	82,113,113	1.93	12 (14%)
21	CLA	B	604	-	69,73,73	1.55	13 (18%)	82,113,113	1.93	12 (14%)
30	BCR	S	101	-	41,41,41	0.74	0	56,56,56	1.76	11 (19%)
21	CLA	B	603	-	69,73,73	1.57	16 (23%)	82,113,113	1.93	13 (15%)
34	HEM	V	201	16	50,50,50	1.83	10 (20%)	67,82,82	1.38	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	B	616	-	69,73,73	1.55	15 (21%)	82,113,113	1.94	13 (15%)
21	CLA	P	504	-	69,73,73	1.56	14 (20%)	82,113,113	1.88	12 (14%)
30	BCR	P	515	-	41,41,41	0.69	0	56,56,56	1.58	14 (25%)
34	HEM	E	101	5,6	50,50,50	1.86	8 (16%)	67,82,82	1.55	11 (16%)
21	CLA	B	609	-	69,73,73	1.54	15 (21%)	82,113,113	1.91	10 (12%)
21	CLA	C	513	-	69,73,73	1.55	15 (21%)	82,113,113	1.91	11 (13%)
21	CLA	C	503	-	69,73,73	1.54	15 (21%)	82,113,113	1.93	14 (17%)
21	CLA	C	506	-	69,73,73	1.58	17 (24%)	82,113,113	1.92	13 (15%)
34	HEM	i	201	16	50,50,50	1.85	9 (18%)	67,82,82	1.43	6 (8%)
23	PL9	A	406	-	45,45,55	1.25	7 (15%)	56,57,69	1.70	15 (26%)
27	LMG	Q	401	-	42,42,55	1.04	2 (4%)	50,50,63	1.24	5 (10%)
30	BCR	I	101	-	41,41,41	0.70	0	56,56,56	1.58	13 (23%)
21	CLA	C	502	-	69,73,73	1.55	14 (20%)	82,113,113	1.91	10 (12%)
31	LMT	N	604	-	36,36,36	0.42	0	47,47,47	0.63	1 (2%)
27	LMG	P	520	-	48,48,55	0.96	2 (4%)	56,56,63	1.30	6 (10%)
24	DGD	D	408	-	64,64,67	0.91	2 (3%)	78,78,81	1.33	9 (11%)
21	CLA	P	503	-	69,73,73	1.54	14 (20%)	82,113,113	1.90	14 (17%)
21	CLA	N	610	-	69,73,73	1.54	14 (20%)	82,113,113	1.92	12 (14%)
23	PL9	G	407	-	45,45,55	1.25	7 (15%)	56,57,69	1.71	15 (26%)
27	LMG	Q	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.30	5 (8%)
21	CLA	N	618	-	69,73,73	1.56	14 (20%)	82,113,113	1.85	12 (14%)
21	CLA	P	511	3	69,73,73	1.54	13 (18%)	82,113,113	1.93	12 (14%)
21	CLA	N	609	-	69,73,73	1.55	16 (23%)	82,113,113	1.99	16 (19%)
21	CLA	P	502	-	69,73,73	1.56	14 (20%)	82,113,113	1.93	12 (14%)
24	DGD	N	602	-	53,53,67	1.02	3 (5%)	67,67,81	1.51	10 (14%)
30	BCR	B	620	-	41,41,41	0.73	0	56,56,56	1.62	10 (17%)
30	BCR	T	101	-	41,41,41	0.73	0	56,56,56	1.59	11 (19%)
26	SQD	F	101	-	43,45,54	1.23	3 (6%)	53,56,65	1.17	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	Q	410	-	-	0/17/57/61	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	e	102	-	2/2/8/8	12/37/57/70	0/1/1/1
31	LMT	N	625	-	-	2/21/61/61	0/2/2/2
27	LMG	B	622	-	2/2/8/8	24/44/64/70	0/1/1/1
24	DGD	B	628	-	3/3/13/13	22/41/81/95	0/2/2/2
24	DGD	P	518	-	3/3/13/13	19/51/91/95	0/2/2/2
21	CLA	G	404	-	1/1/15/20	12/39/115/115	-
25	LHG	G	409	-	-	13/43/43/53	-
21	CLA	N	619	-	1/1/15/20	10/39/115/115	-
27	LMG	D	406	-	2/2/8/8	13/41/61/70	0/1/1/1
27	LMG	A	410	-	2/2/8/8	22/46/66/70	0/1/1/1
24	DGD	A	407	-	3/3/13/13	13/45/85/95	0/2/2/2
26	SQD	A	409	-	-	16/46/66/69	0/1/1/1
23	PL9	J	101	-	-	12/29/49/73	0/1/1/1
21	CLA	B	606	-	1/1/15/20	15/39/115/115	-
21	CLA	N	607	-	1/1/15/20	13/39/115/115	-
21	CLA	N	616	-	1/1/15/20	12/39/115/115	-
22	PHO	Q	403	-	-	11/37/103/103	0/5/6/6
26	SQD	A	414	-	-	19/49/69/69	0/1/1/1
21	CLA	G	402	-	1/1/15/20	9/39/115/115	-
30	BCR	B	617	-	-	2/29/63/63	0/2/2/2
21	CLA	B	611	-	1/1/15/20	15/39/115/115	-
21	CLA	P	501	-	1/1/15/20	14/39/115/115	-
27	LMG	P	521	-	2/2/8/8	19/40/60/70	0/1/1/1
21	CLA	G	406	-	1/1/15/20	12/39/115/115	-
27	LMG	R	102	-	2/2/8/8	16/39/59/70	0/1/1/1
26	SQD	Q	408	-	-	10/38/58/69	0/1/1/1
30	BCR	P	516	-	-	8/29/63/63	0/2/2/2
21	CLA	N	614	-	1/1/15/20	19/39/115/115	-
30	BCR	C	515	-	-	8/29/63/63	0/2/2/2
21	CLA	G	403	-	1/1/15/20	14/39/115/115	-
27	LMG	C	519	-	2/2/8/8	20/43/63/70	0/1/1/1
21	CLA	Q	402	-	1/1/15/20	15/39/115/115	-
30	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
24	DGD	P	517	-	3/3/13/13	17/42/82/95	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	B	618	-	-	4/29/63/63	0/2/2/2
27	LMG	N	623	-	2/2/8/8	17/44/64/70	0/1/1/1
30	BCR	T	102	-	-	4/29/63/63	0/2/2/2
24	DGD	P	519	-	3/3/13/13	19/55/95/95	0/2/2/2
30	BCR	a	101	-	-	4/29/63/63	0/2/2/2
21	CLA	B	602	-	1/1/15/20	19/39/115/115	-
24	DGD	B	621	-	3/3/13/13	17/47/87/95	0/2/2/2
21	CLA	B	610	-	1/1/15/20	19/39/115/115	-
27	LMG	G	411	-	2/2/8/8	22/46/66/70	0/1/1/1
21	CLA	N	620	-	1/1/15/20	21/39/115/115	-
21	CLA	C	505	-	1/1/15/20	19/39/115/115	-
26	SQD	N	601	-	-	13/42/62/69	0/1/1/1
31	LMT	B	629	-	-	3/21/61/61	0/2/2/2
22	PHO	A	404	-	-	10/37/103/103	0/5/6/6
30	BCR	P	514	-	-	4/29/63/63	0/2/2/2
21	CLA	P	513	-	1/1/15/20	19/39/115/115	-
21	CLA	C	510	-	1/1/15/20	15/39/115/115	-
21	CLA	N	613	-	1/1/15/20	9/39/115/115	-
24	DGD	C	518	-	3/3/13/13	21/55/95/95	0/2/2/2
30	BCR	H	101	-	-	2/29/63/63	0/2/2/2
30	BCR	T	103	-	-	2/29/63/63	0/2/2/2
22	PHO	G	405	-	-	9/37/103/103	0/5/6/6
21	CLA	Q	404	-	1/1/15/20	7/39/115/115	-
21	CLA	A	405	-	1/1/15/20	13/39/115/115	-
21	CLA	C	507	-	1/1/15/20	13/39/115/115	-
21	CLA	N	605	-	1/1/15/20	20/39/115/115	-
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
24	DGD	W	102	-	3/3/13/13	17/47/87/95	0/2/2/2
23	PL9	D	404	-	-	17/53/73/73	0/1/1/1
21	CLA	N	615	-	1/1/15/20	15/39/115/115	-
30	BCR	b	102	-	-	2/29/63/63	0/2/2/2
21	CLA	N	617	-	1/1/15/20	20/39/115/115	-
31	LMT	B	630	-	-	5/21/61/61	0/2/2/2
21	CLA	P	509	-	1/1/15/20	12/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	P	512	-	1/1/15/20	20/39/115/115	-
21	CLA	B	612	-	1/1/15/20	12/39/115/115	-
21	CLA	C	512	-	1/1/15/20	21/39/115/115	-
21	CLA	N	606	-	1/1/15/20	20/39/115/115	-
21	CLA	N	608	-	1/1/15/20	10/39/115/115	-
26	SQD	G	410	-	-	15/46/66/69	0/1/1/1
21	CLA	N	611	-	1/1/15/20	9/39/115/115	-
21	CLA	B	613	-	1/1/15/20	17/39/115/115	-
30	BCR	W	101	-	-	2/29/63/63	0/2/2/2
30	BCR	C	514	-	-	4/29/63/63	0/2/2/2
30	BCR	K	101	-	-	6/29/63/63	0/2/2/2
21	CLA	P	506	-	1/1/15/20	18/39/115/115	-
21	CLA	P	505	-	1/1/15/20	20/39/115/115	-
21	CLA	D	401	-	1/1/15/20	15/39/115/115	-
26	SQD	B	627	-	-	14/42/62/69	0/1/1/1
30	BCR	J	102	-	-	2/29/63/63	0/2/2/2
31	LMT	D	409	-	-	0/17/57/61	0/2/2/2
21	CLA	P	510	-	1/1/15/20	13/39/115/115	-
21	CLA	B	615	-	1/1/15/20	10/39/115/115	-
24	DGD	Q	409	-	3/3/13/13	34/52/92/95	0/2/2/2
31	LMT	N	624	-	-	3/21/61/61	0/2/2/2
27	LMG	Q	406	-	2/2/8/8	13/41/61/70	0/1/1/1
21	CLA	C	504	-	1/1/15/20	12/39/115/115	-
26	SQD	B	624	-	-	10/38/58/69	0/1/1/1
30	BCR	c	101	-	-	6/29/63/63	0/2/2/2
31	LMT	N	603	-	-	3/21/61/61	0/2/2/2
27	LMG	I	102	-	2/2/8/8	19/38/58/70	0/1/1/1
27	LMG	N	622	-	2/2/8/8	23/44/64/70	0/1/1/1
26	SQD	S	102	-	-	13/40/60/69	0/1/1/1
31	LMT	B	626	-	-	2/21/61/61	0/2/2/2
21	CLA	D	403	-	1/1/15/20	8/39/115/115	-
21	CLA	A	403	-	1/1/15/20	13/39/115/115	-
21	CLA	A	402	-	1/1/15/20	15/39/115/115	-
31	LMT	I	103	-	-	4/21/61/61	0/2/2/2

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	E	102	-	2/2/8/8	15/39/59/70	0/1/1/1
31	LMT	B	625	-	-	3/21/61/61	0/2/2/2
21	CLA	C	511	3	1/1/15/20	16/39/115/115	-
24	DGD	C	516	-	3/3/13/13	19/42/82/95	0/2/2/2
34	HEM	R	101	5,6	-	3/14/54/54	-
26	SQD	G	401	-	-	17/49/69/69	0/1/1/1
21	CLA	B	605	-	1/1/15/20	22/39/115/115	-
21	CLA	P	507	-	1/1/15/20	13/39/115/115	-
30	BCR	N	621	-	-	0/29/63/63	0/2/2/2
21	CLA	B	608	-	1/1/15/20	18/39/115/115	-
27	LMG	D	412	-	2/2/8/8	15/37/57/70	0/1/1/1
30	BCR	D	405	-	-	6/29/63/63	0/2/2/2
30	BCR	B	619	-	-	0/29/63/63	0/2/2/2
21	CLA	B	601	-	1/1/15/20	20/39/115/115	-
21	CLA	C	501	-	1/1/15/20	14/39/115/115	-
21	CLA	C	509	-	1/1/15/20	13/39/115/115	-
21	CLA	P	508	-	1/1/15/20	13/39/115/115	-
21	CLA	N	612	-	1/1/15/20	18/39/115/115	-
27	LMG	C	520	-	2/2/8/8	17/40/60/70	0/1/1/1
23	PL9	Q	405	-	-	17/53/73/73	0/1/1/1
25	LHG	G	412	-	-	13/41/41/53	-
27	LMG	D	407	-	2/2/8/8	20/43/63/70	0/1/1/1
21	CLA	C	508	-	1/1/15/20	13/39/115/115	-
25	LHG	A	408	-	-	12/43/43/53	-
21	CLA	B	614	-	1/1/15/20	18/39/115/115	-
27	LMG	B	623	-	2/2/8/8	15/44/64/70	0/1/1/1
24	DGD	G	408	-	3/3/13/13	13/45/85/95	0/2/2/2
21	CLA	A	401	-	1/1/15/20	9/39/115/115	-
25	LHG	A	411	-	-	12/41/41/53	-
31	LMT	e	101	-	-	0/21/61/61	0/2/2/2
23	PL9	b	101	-	-	11/29/49/73	0/1/1/1
27	LMG	a	102	-	2/2/8/8	20/38/58/70	0/1/1/1
31	LMT	a	103	-	-	4/21/61/61	0/2/2/2
27	LMG	M	101	-	2/2/8/8	14/37/57/70	0/1/1/1
24	DGD	C	517	-	3/3/13/13	18/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PHO	D	402	-	-	13/37/103/103	0/5/6/6
21	CLA	B	607	-	1/1/15/20	10/39/115/115	-
21	CLA	B	604	-	1/1/15/20	10/39/115/115	-
30	BCR	S	101	-	-	6/29/63/63	0/2/2/2
21	CLA	B	603	-	1/1/15/20	15/39/115/115	-
34	HEM	V	201	16	-	3/14/54/54	-
21	CLA	B	616	-	1/1/15/20	21/39/115/115	-
21	CLA	P	504	-	1/1/15/20	12/39/115/115	-
30	BCR	P	515	-	-	4/29/63/63	0/2/2/2
34	HEM	E	101	5,6	-	4/14/54/54	-
21	CLA	B	609	-	1/1/15/20	9/39/115/115	-
21	CLA	C	513	-	1/1/15/20	20/39/115/115	-
21	CLA	C	503	-	1/1/15/20	16/39/115/115	-
21	CLA	C	506	-	1/1/15/20	18/39/115/115	-
34	HEM	i	201	16	-	3/14/54/54	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
27	LMG	Q	401	-	2/2/8/8	16/37/57/70	0/1/1/1
30	BCR	I	101	-	-	4/29/63/63	0/2/2/2
21	CLA	C	502	-	1/1/15/20	11/39/115/115	-
31	LMT	N	604	-	-	5/21/61/61	0/2/2/2
27	LMG	P	520	-	2/2/8/8	20/43/63/70	0/1/1/1
24	DGD	D	408	-	3/3/13/13	33/52/92/95	0/2/2/2
21	CLA	P	503	-	1/1/15/20	16/39/115/115	-
21	CLA	N	610	-	1/1/15/20	15/39/115/115	-
23	PL9	G	407	-	-	18/41/61/73	0/1/1/1
27	LMG	Q	407	-	2/2/8/8	18/43/63/70	0/1/1/1
21	CLA	N	618	-	1/1/15/20	19/39/115/115	-
21	CLA	P	511	3	1/1/15/20	15/39/115/115	-
21	CLA	N	609	-	1/1/15/20	23/39/115/115	-
21	CLA	P	502	-	1/1/15/20	11/39/115/115	-
24	DGD	N	602	-	3/3/13/13	22/41/81/95	0/2/2/2
30	BCR	B	620	-	-	2/29/63/63	0/2/2/2
30	BCR	T	101	-	-	2/29/63/63	0/2/2/2
26	SQD	F	101	-	-	14/40/60/69	0/1/1/1

The worst 5 of 1288 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	402	PHO	C1D-C2D	10.28	1.50	1.39
22	G	405	PHO	C1D-C2D	10.16	1.50	1.39
22	Q	403	PHO	C1D-C2D	10.11	1.50	1.39
22	A	404	PHO	C1D-C2D	10.04	1.50	1.39
22	A	404	PHO	C1B-C2B	9.39	1.49	1.39

The worst 5 of 1695 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	102	BCR	C32-C1-C6	-13.90	88.45	110.24
30	J	102	BCR	C32-C1-C6	-13.83	88.56	110.24
21	C	505	CLA	C4A-NA-C1A	13.12	112.67	106.68
21	P	505	CLA	C4A-NA-C1A	12.97	112.60	106.68
21	B	611	CLA	C4A-NA-C1A	12.70	112.47	106.68

5 of 156 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	401	CLA	ND
21	A	402	CLA	ND
21	A	403	CLA	ND
21	A	405	CLA	ND
21	B	601	CLA	ND

5 of 2177 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	401	CLA	C1A-C2A-CAA-CBA
21	A	401	CLA	C3A-C2A-CAA-CBA
21	A	401	CLA	CBD-CGD-O2D-CED
21	A	402	CLA	C1A-C2A-CAA-CBA
21	A	402	CLA	C1-C2-C3-C4

There are no ring outliers.

165 monomers are involved in 586 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	e	102	LMG	3	0
31	N	625	LMT	1	0
27	B	622	LMG	1	0
24	B	628	DGD	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	P	518	DGD	5	0
21	G	404	CLA	4	0
25	G	409	LHG	1	0
21	N	619	CLA	3	0
27	D	406	LMG	4	0
27	A	410	LMG	2	0
24	A	407	DGD	1	0
26	A	409	SQD	5	0
23	J	101	PL9	1	0
21	B	606	CLA	8	0
21	N	607	CLA	7	0
21	N	616	CLA	8	0
22	Q	403	PHO	5	0
26	A	414	SQD	8	0
21	G	402	CLA	12	0
30	B	617	BCR	8	0
21	B	611	CLA	3	0
21	P	501	CLA	2	0
27	P	521	LMG	4	0
21	G	406	CLA	4	0
27	R	102	LMG	2	0
26	Q	408	SQD	3	0
30	P	516	BCR	3	0
21	N	614	CLA	3	0
30	C	515	BCR	4	0
21	G	403	CLA	8	0
21	Q	402	CLA	10	0
30	Z	101	BCR	3	0
24	P	517	DGD	2	0
30	B	618	BCR	5	0
27	N	623	LMG	1	0
30	T	102	BCR	9	0
24	P	519	DGD	7	0
30	a	101	BCR	4	0
21	B	602	CLA	4	0
24	B	621	DGD	2	0
21	B	610	CLA	4	0
27	G	411	LMG	2	0
21	N	620	CLA	4	0
21	C	505	CLA	7	0
26	N	601	SQD	7	0
31	B	629	LMT	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	404	PHO	6	0
30	P	514	BCR	12	0
21	P	513	CLA	3	0
21	C	510	CLA	2	0
21	N	613	CLA	2	0
24	C	518	DGD	7	0
30	H	101	BCR	2	0
30	T	103	BCR	3	0
22	G	405	PHO	7	0
21	Q	404	CLA	4	0
21	A	405	CLA	3	0
21	C	507	CLA	3	0
31	M	102	LMT	1	0
24	W	102	DGD	3	0
23	D	404	PL9	6	0
21	N	615	CLA	3	0
30	b	102	BCR	3	0
21	N	617	CLA	2	0
31	B	630	LMT	3	0
21	P	509	CLA	5	0
21	P	512	CLA	4	0
21	B	612	CLA	6	0
21	C	512	CLA	3	0
21	N	606	CLA	5	0
21	N	608	CLA	6	0
26	G	410	SQD	7	0
21	N	611	CLA	5	0
21	B	613	CLA	3	0
30	W	101	BCR	3	0
30	C	514	BCR	12	0
30	K	101	BCR	11	0
21	P	506	CLA	1	0
21	P	505	CLA	6	0
21	D	401	CLA	7	0
26	B	627	SQD	5	0
30	J	102	BCR	4	0
21	P	510	CLA	2	0
21	B	615	CLA	3	0
24	Q	409	DGD	1	0
31	N	624	LMT	1	0
27	Q	406	LMG	5	0
21	C	504	CLA	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	624	SQD	5	0
30	c	101	BCR	12	0
31	N	603	LMT	3	0
27	I	102	LMG	4	0
27	N	622	LMG	2	0
26	S	102	SQD	2	0
31	B	626	LMT	1	0
21	D	403	CLA	4	0
21	A	403	CLA	5	0
21	A	402	CLA	8	0
31	I	103	LMT	2	0
27	E	102	LMG	2	0
31	B	625	LMT	1	0
21	C	511	CLA	8	0
24	C	516	DGD	3	0
34	R	101	HEM	6	0
26	G	401	SQD	9	0
21	B	605	CLA	5	0
21	P	507	CLA	3	0
30	N	621	BCR	4	0
21	B	608	CLA	9	0
27	D	412	LMG	2	0
30	D	405	BCR	3	0
30	B	619	BCR	2	0
21	C	501	CLA	5	0
21	C	509	CLA	7	0
21	P	508	CLA	4	0
21	N	612	CLA	6	0
23	Q	405	PL9	5	0
25	G	412	LHG	3	0
27	C	520	LMG	4	0
27	D	407	LMG	9	0
21	C	508	CLA	5	0
25	A	408	LHG	2	0
21	B	614	CLA	7	0
25	A	411	LHG	2	0
24	G	408	DGD	2	0
21	A	401	CLA	12	0
27	B	623	LMG	1	0
31	e	101	LMT	1	0
23	b	101	PL9	2	0
27	a	102	LMG	2	0

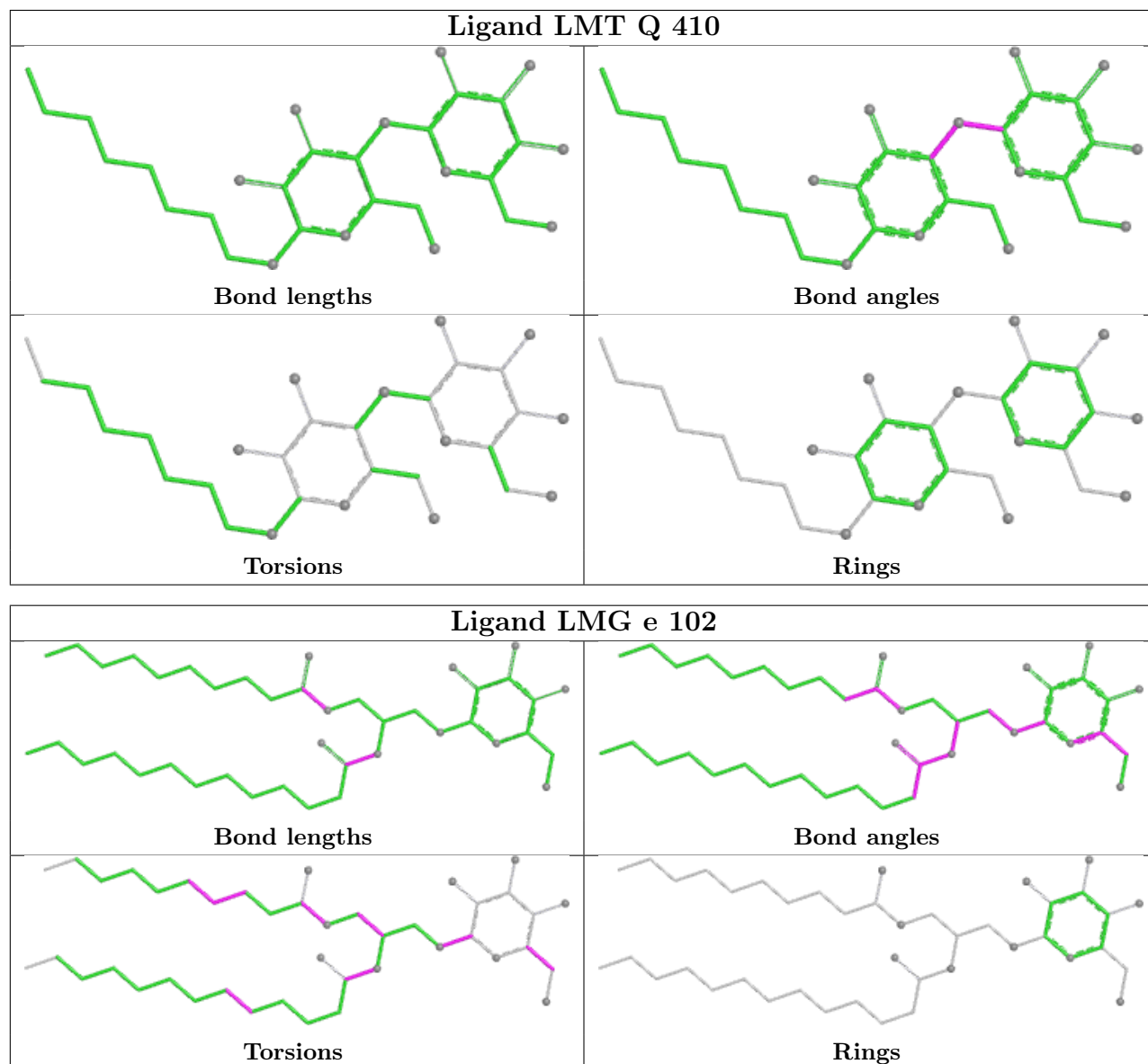
*Continued on next page...*

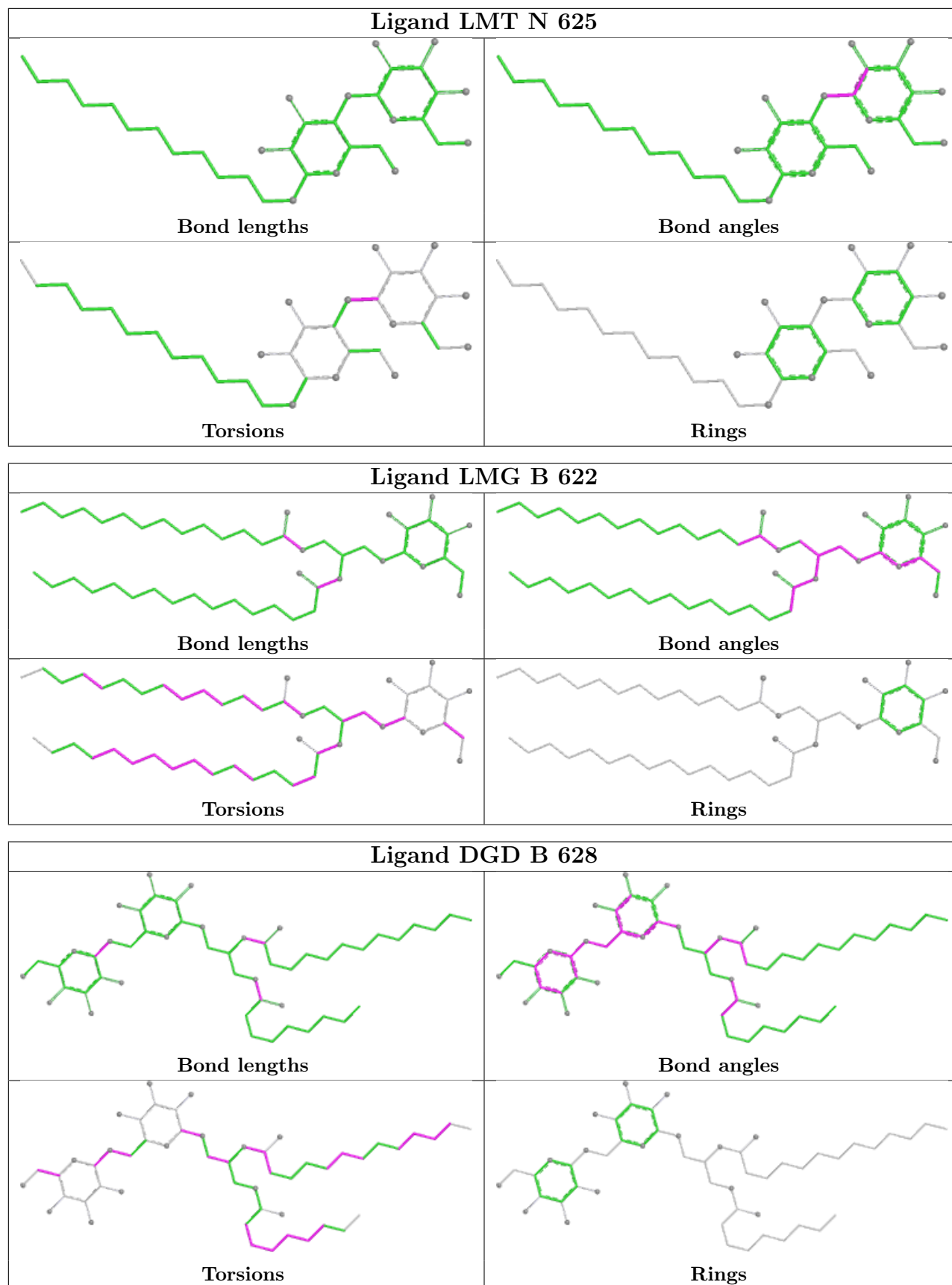
*Continued from previous page...*

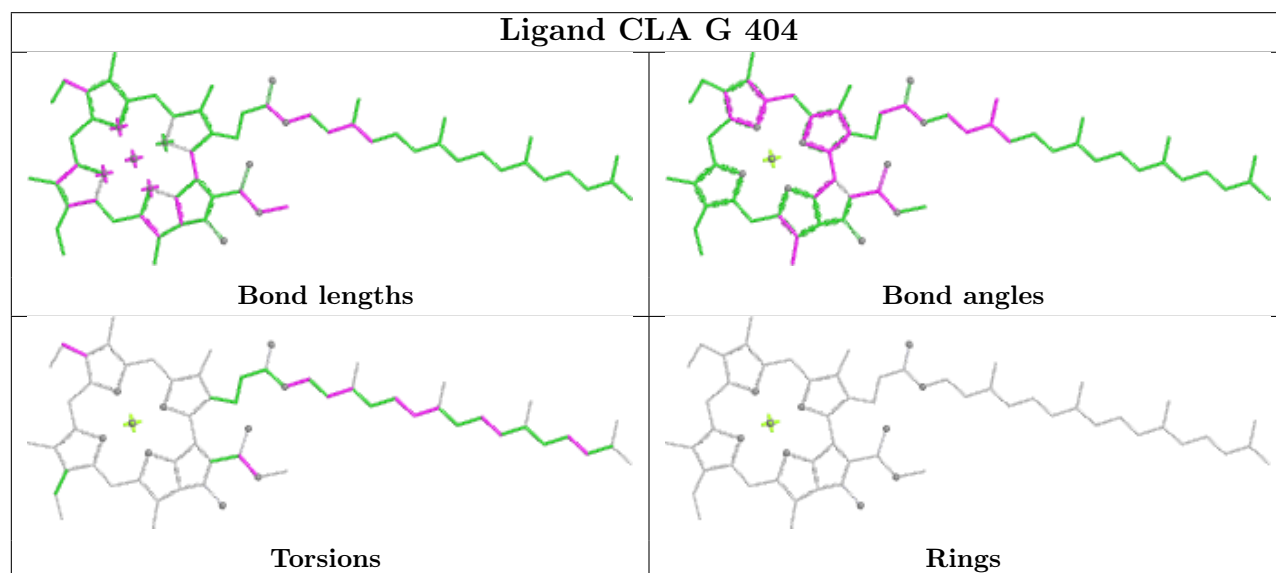
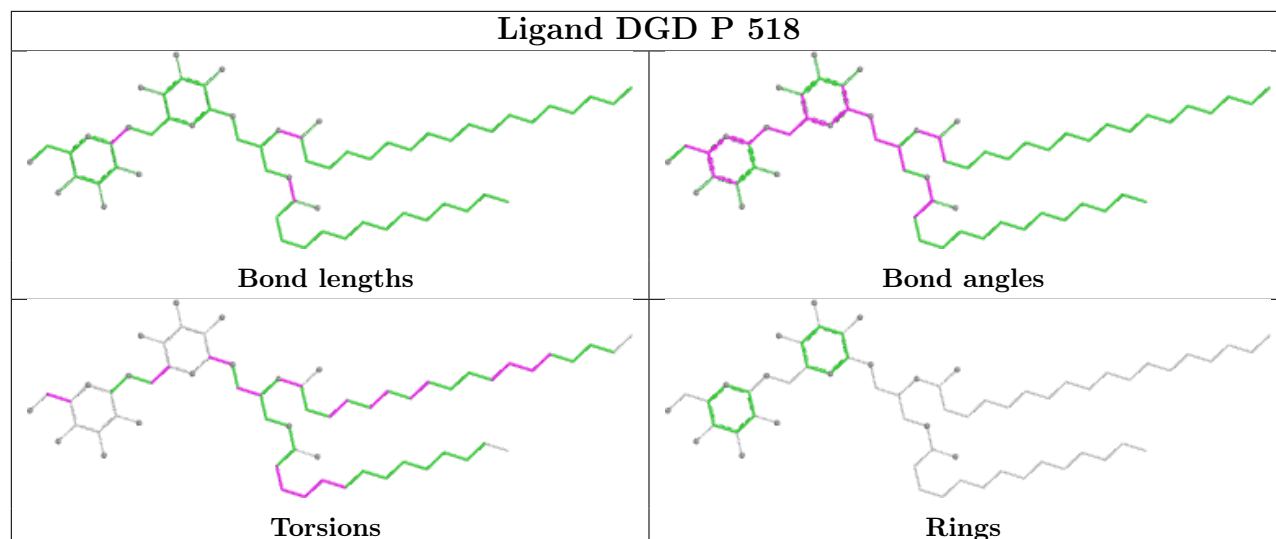
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	103	LMT	1	0
27	M	101	LMG	4	0
24	C	517	DGD	7	0
22	D	402	PHO	5	0
21	B	607	CLA	6	0
21	B	604	CLA	5	0
30	S	101	BCR	5	0
21	B	603	CLA	7	0
34	V	201	HEM	5	0
21	B	616	CLA	6	0
21	P	504	CLA	5	0
30	P	515	BCR	5	0
34	E	101	HEM	7	0
21	B	609	CLA	3	0
21	C	513	CLA	3	0
21	C	503	CLA	6	0
21	C	506	CLA	2	0
34	i	201	HEM	4	0
23	A	406	PL9	5	0
27	Q	401	LMG	2	0
30	I	101	BCR	5	0
21	C	502	CLA	1	0
31	N	604	LMT	4	0
21	P	503	CLA	6	0
21	N	610	CLA	5	0
23	G	407	PL9	5	0
27	Q	407	LMG	8	0
21	N	618	CLA	11	0
21	P	511	CLA	9	0
21	N	609	CLA	7	0
21	P	502	CLA	2	0
24	N	602	DGD	4	0
30	B	620	BCR	2	0
30	T	101	BCR	5	0
26	F	101	SQD	2	0

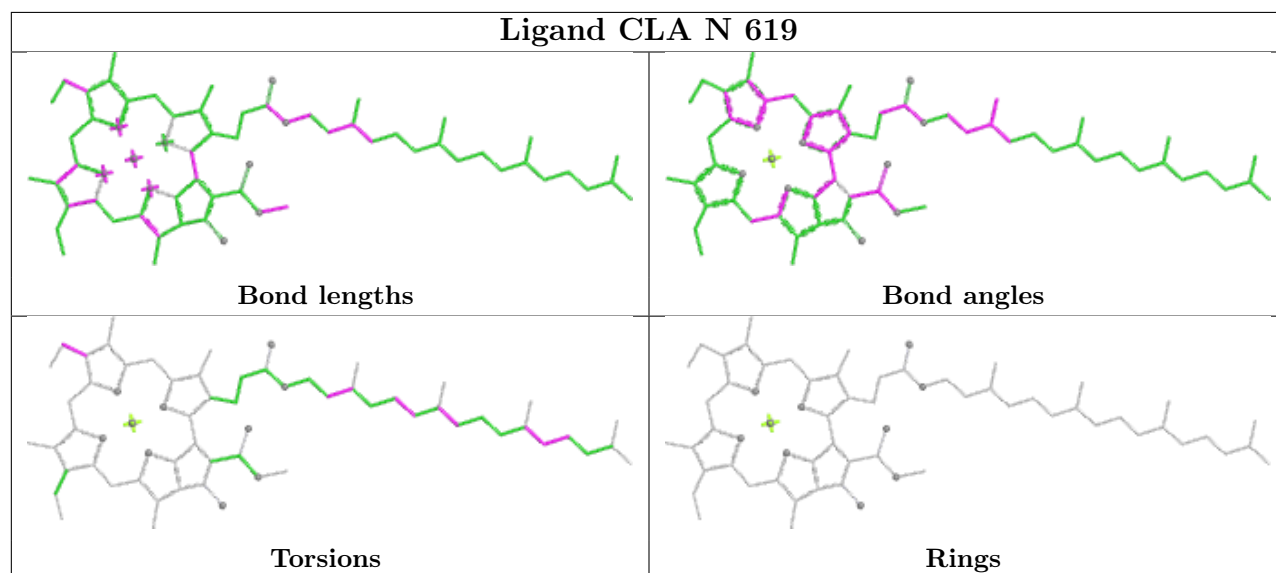
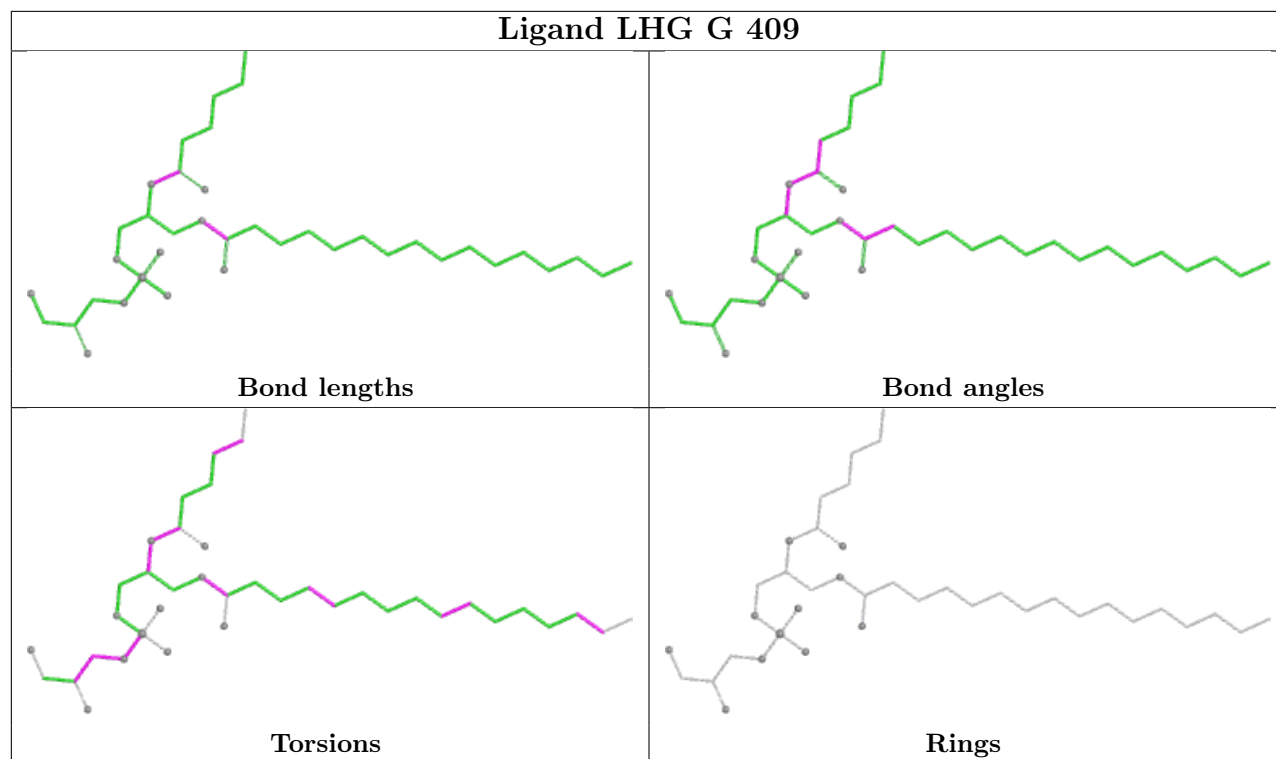
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

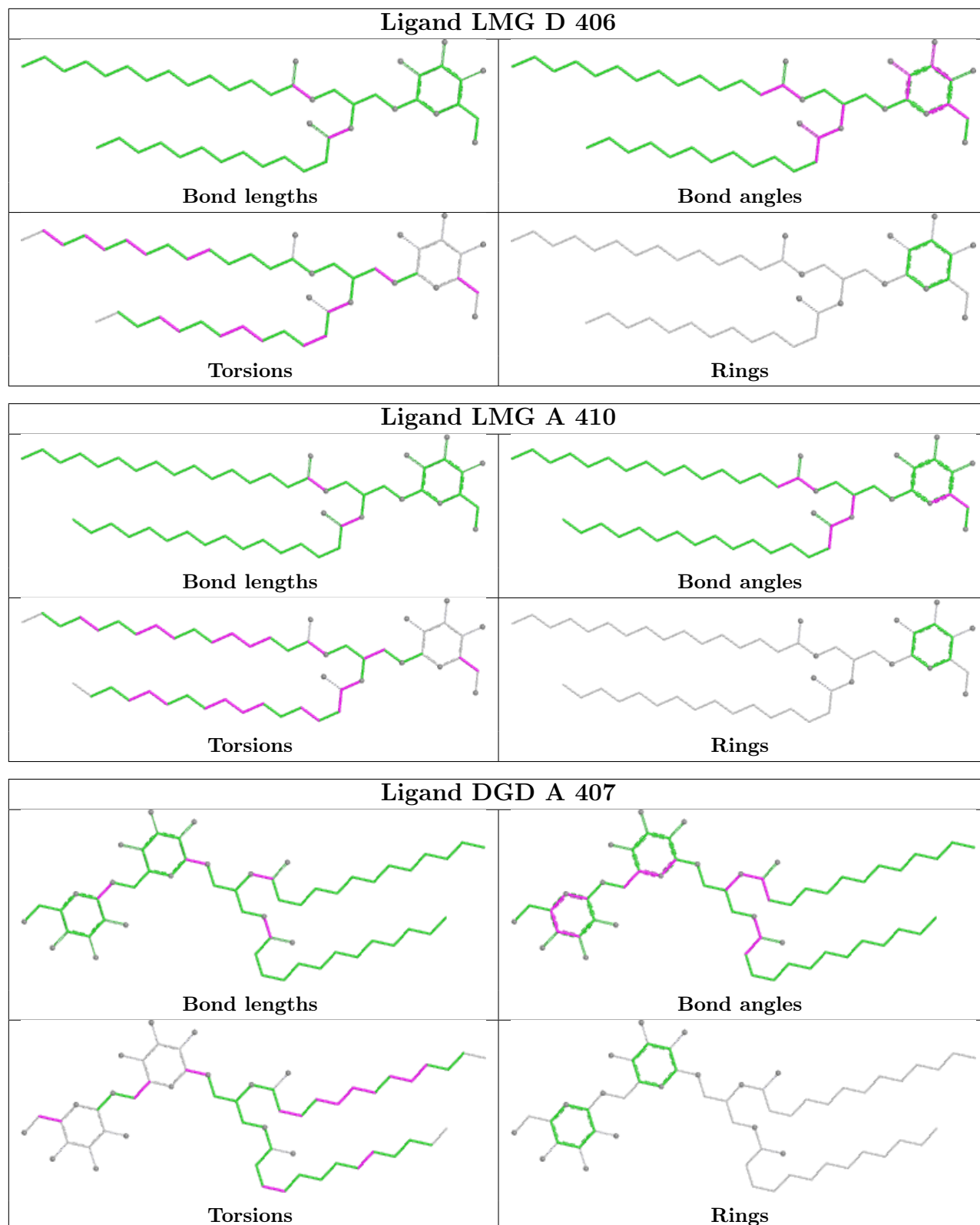
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

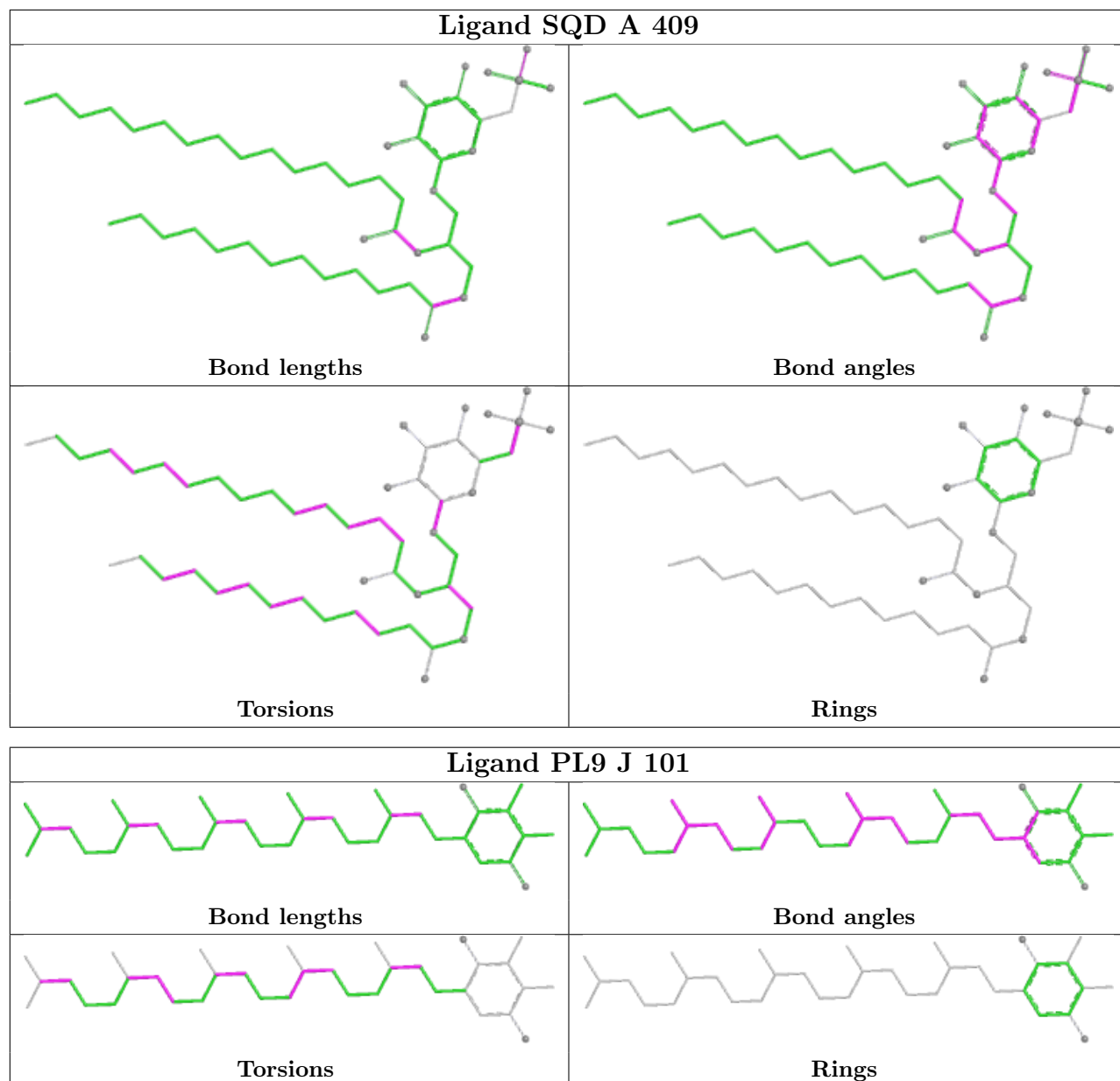


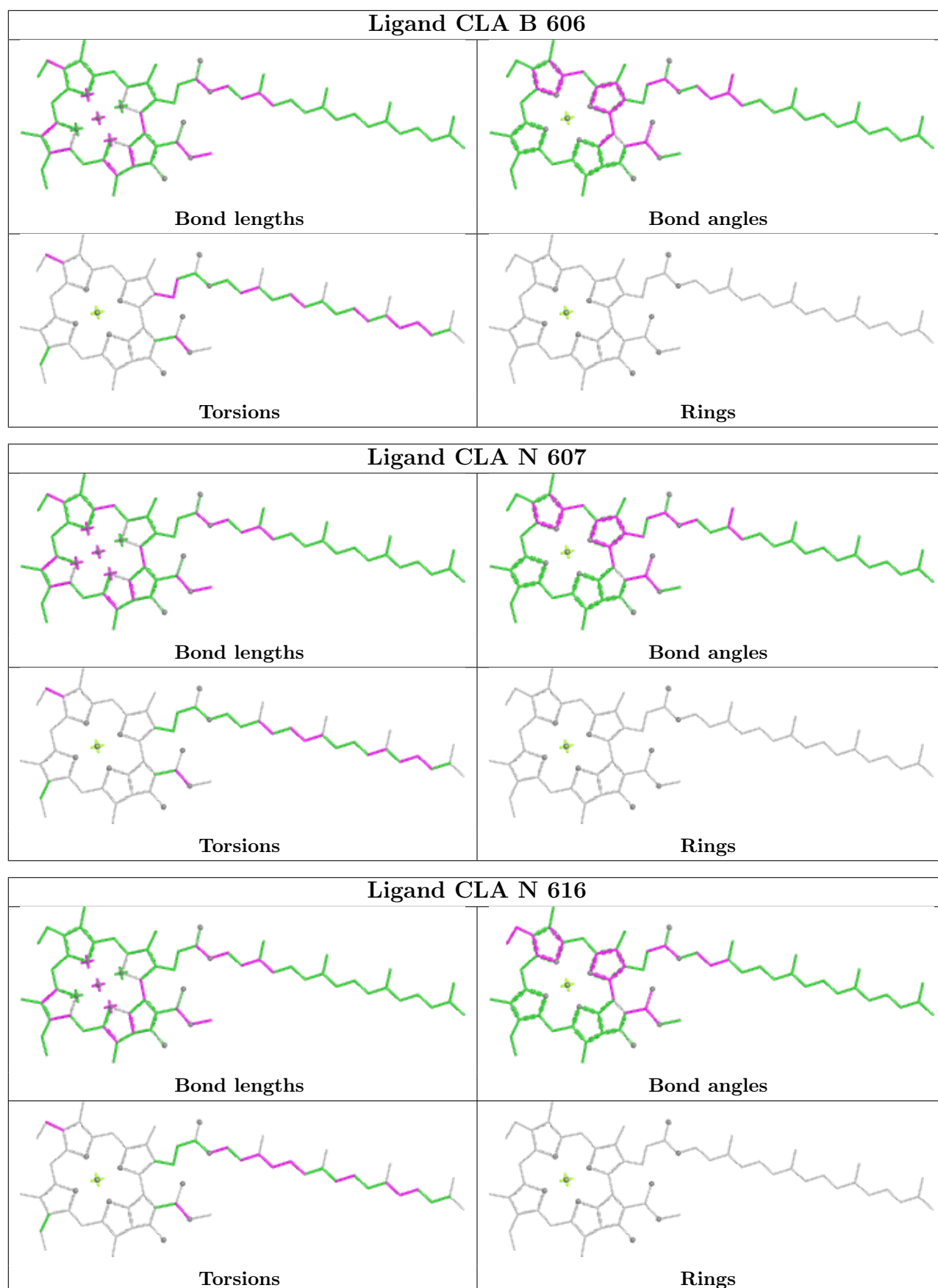


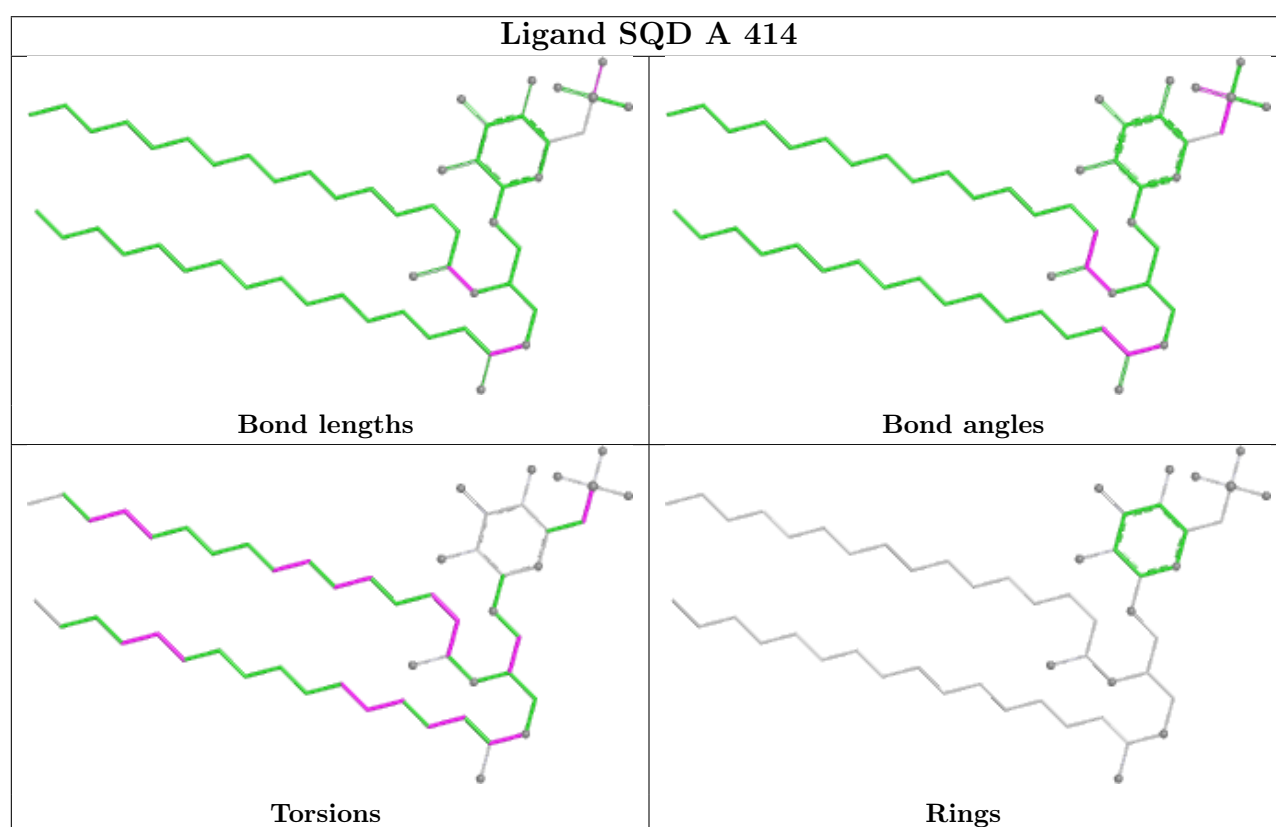
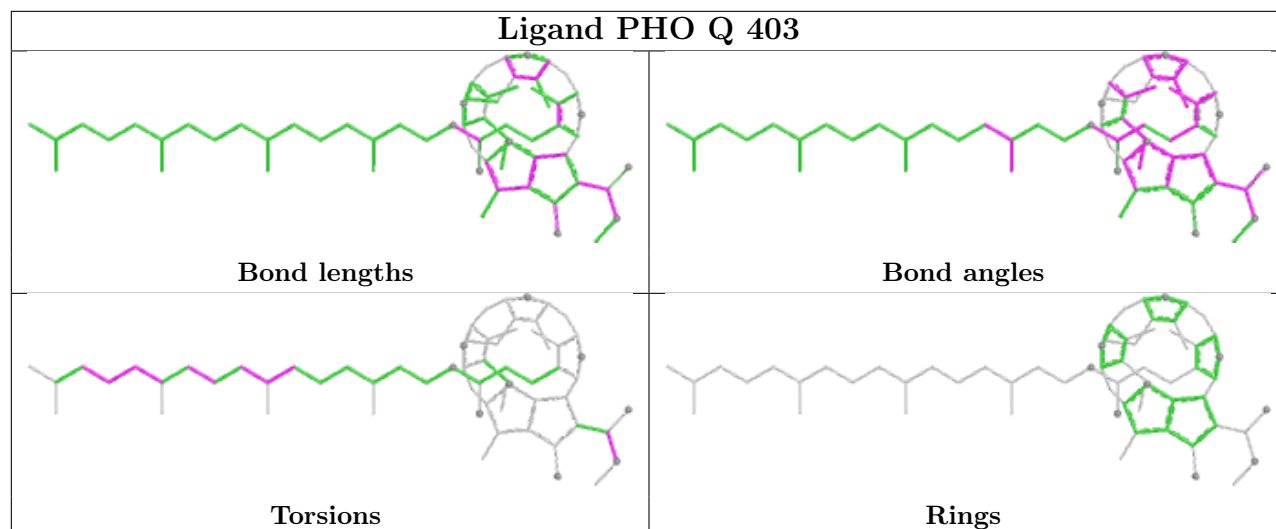


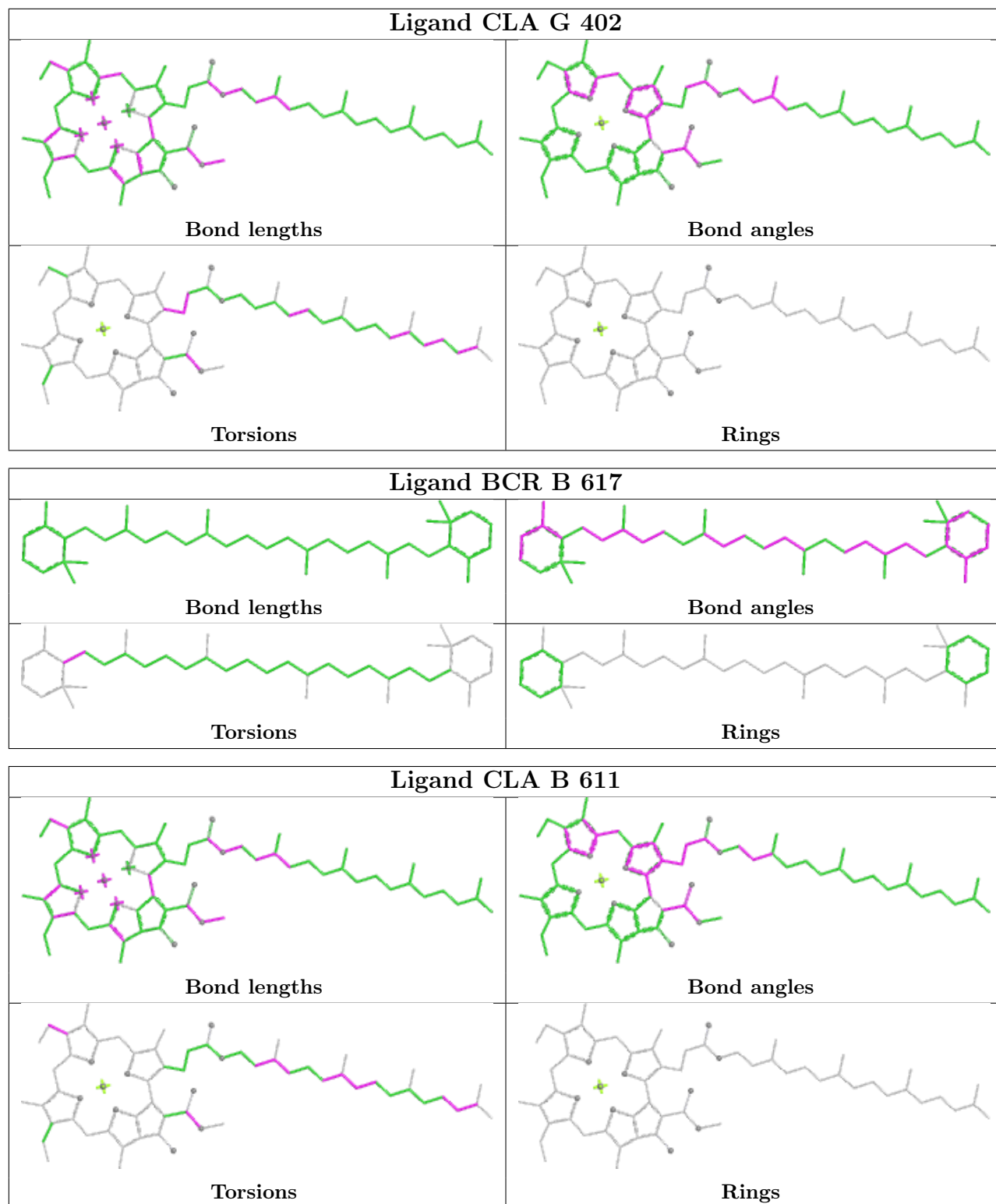


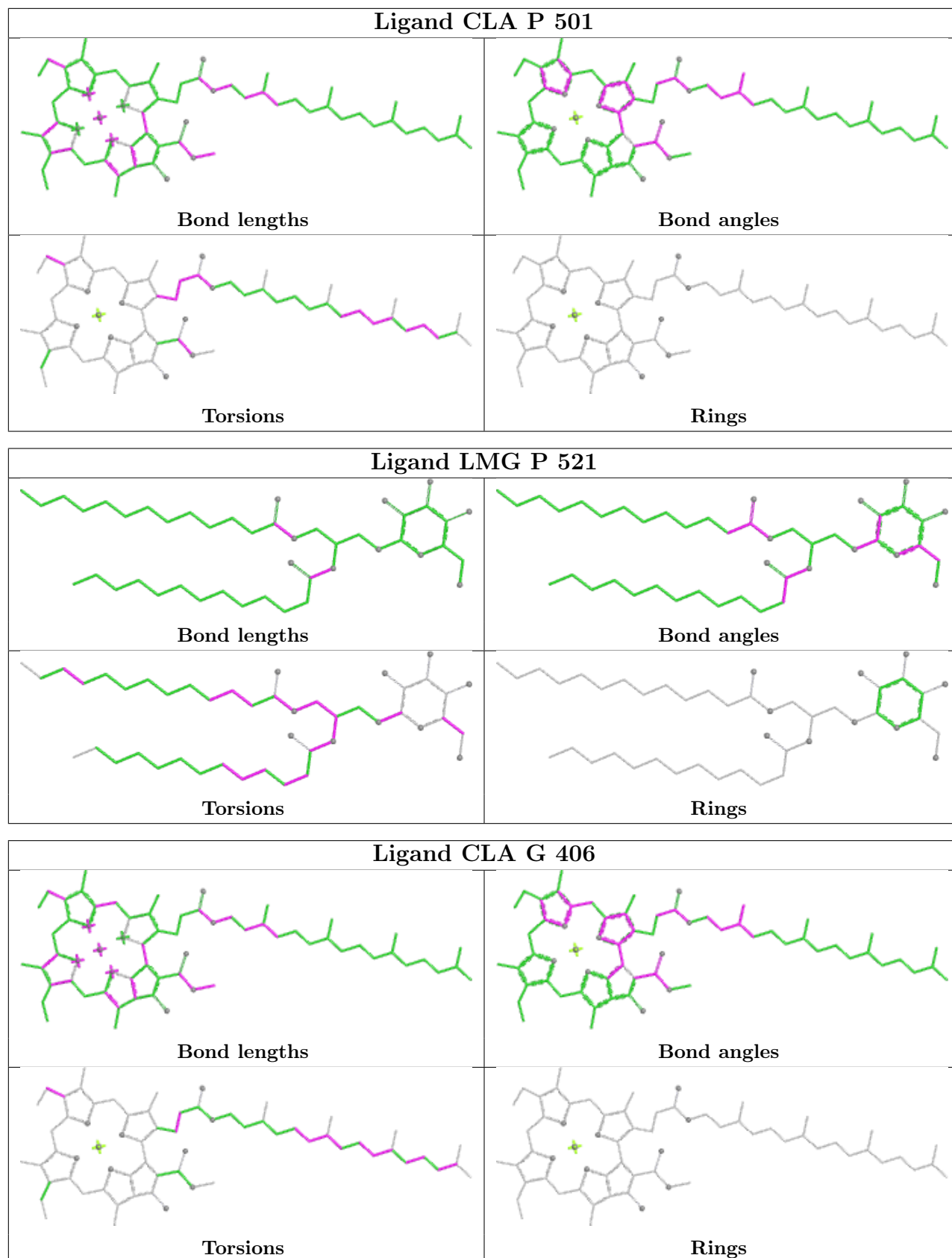


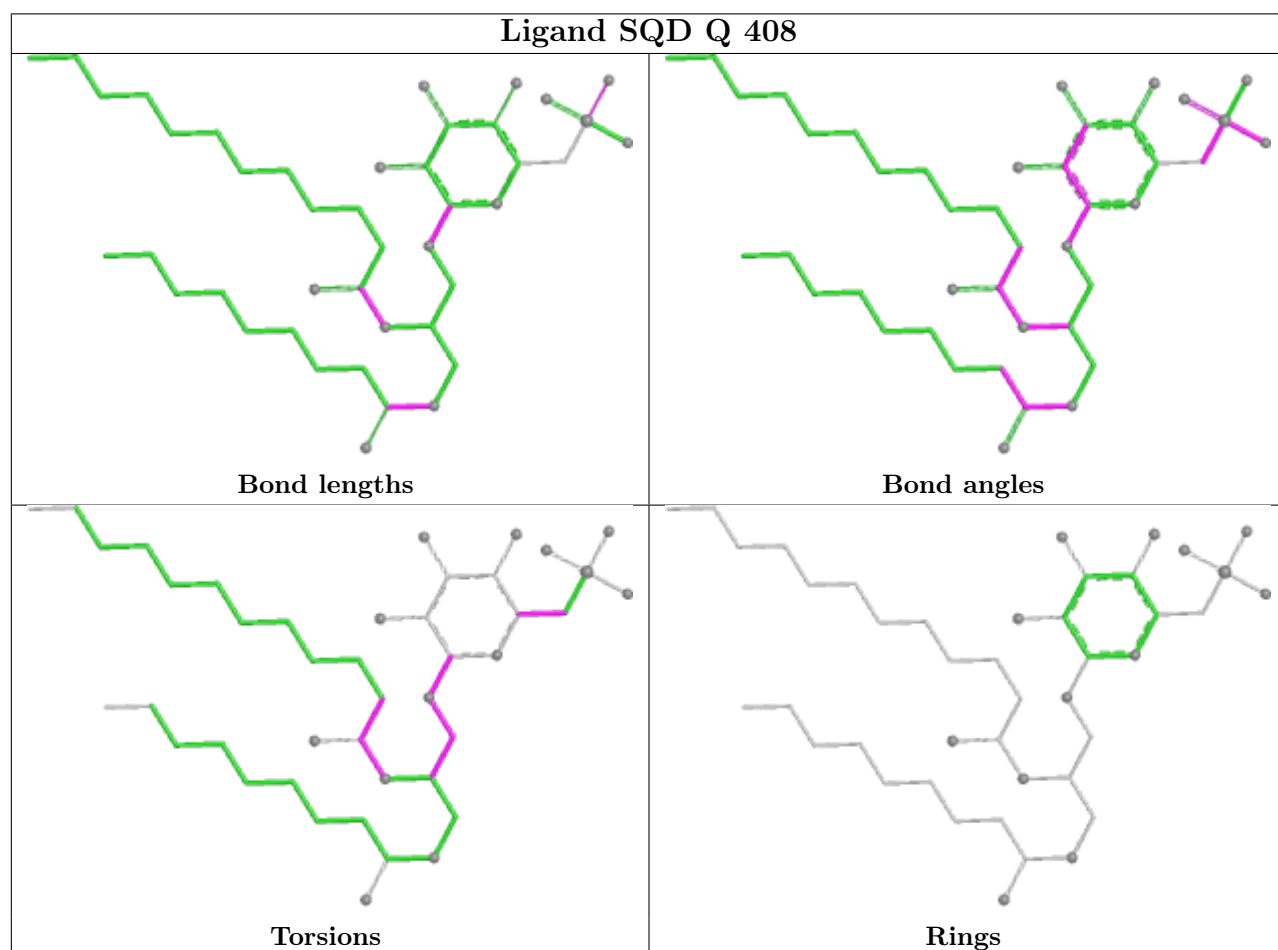
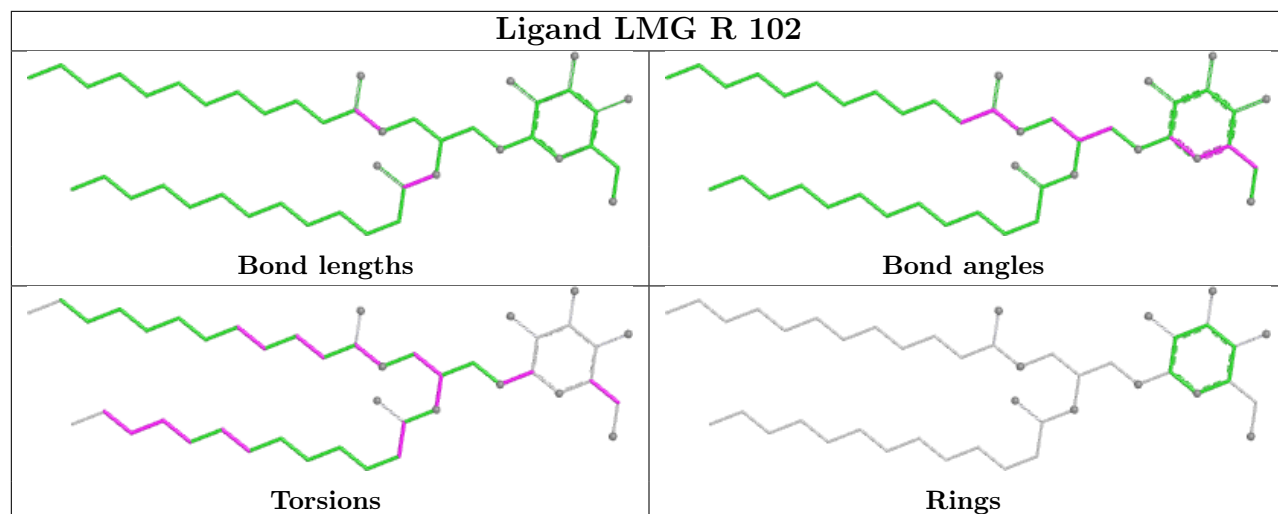


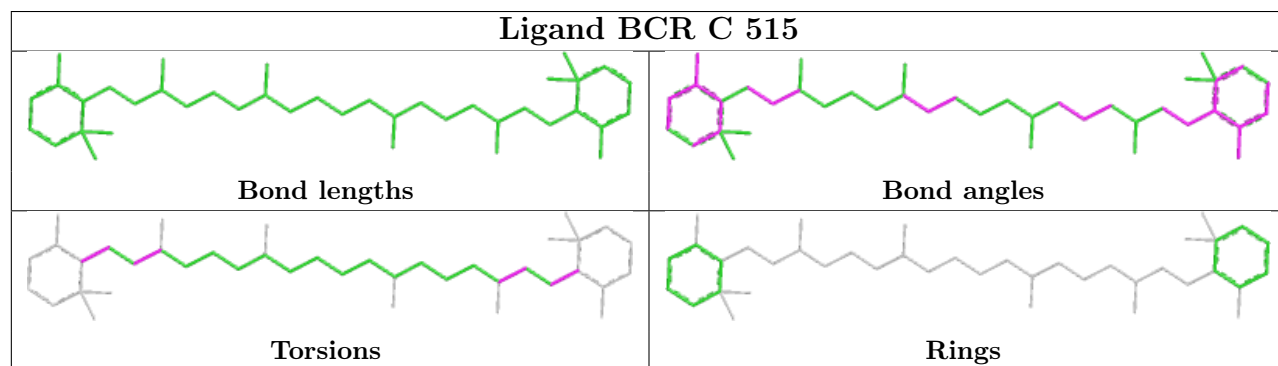
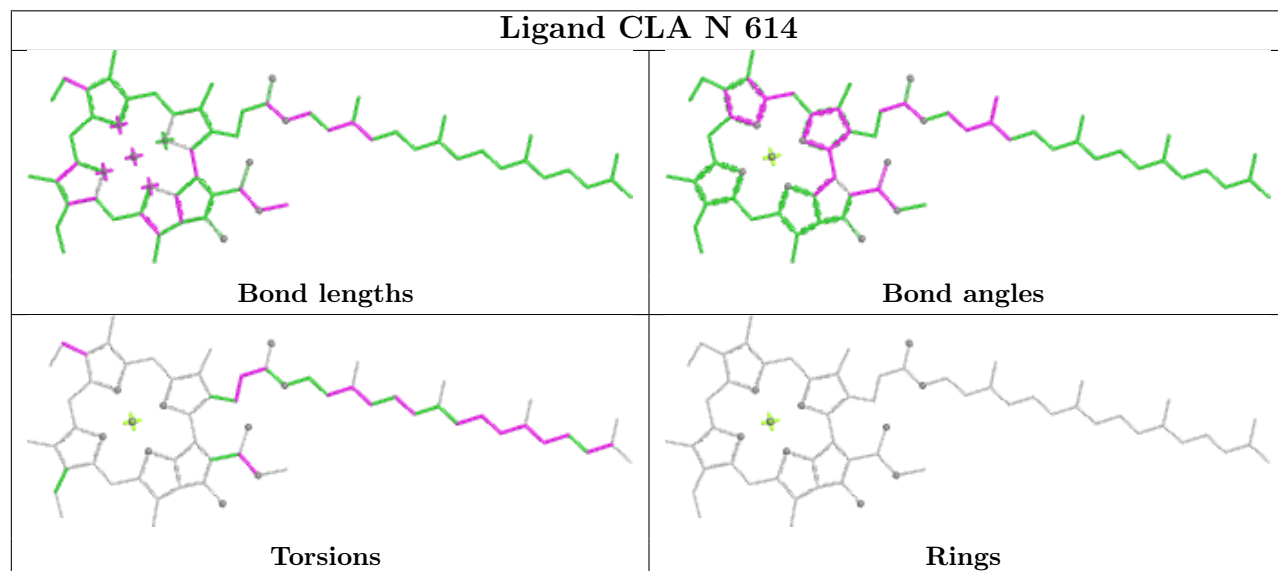
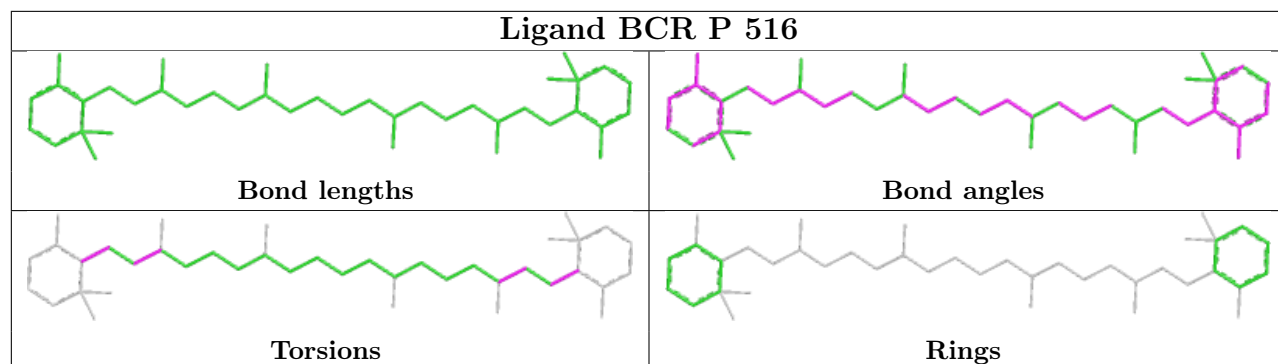


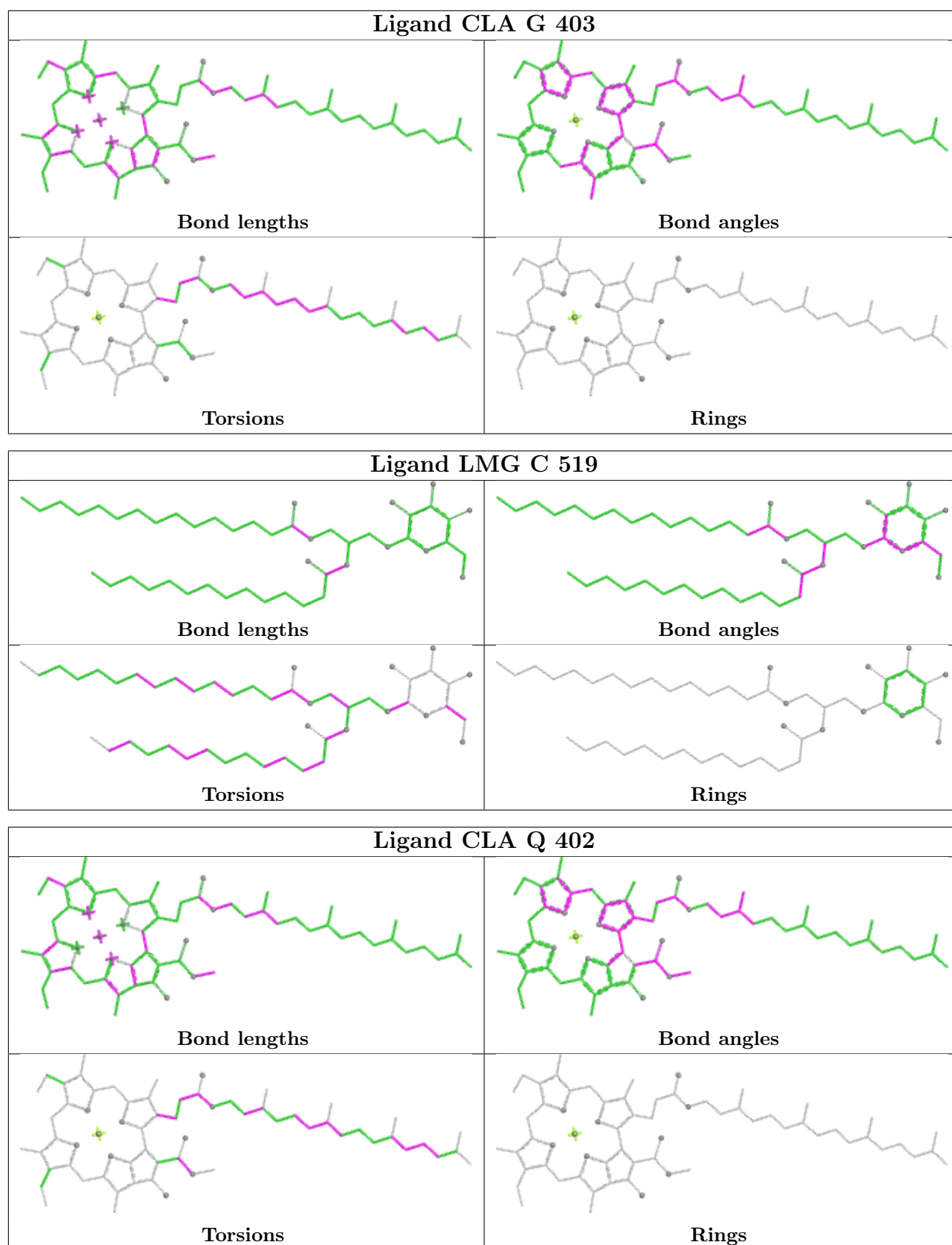


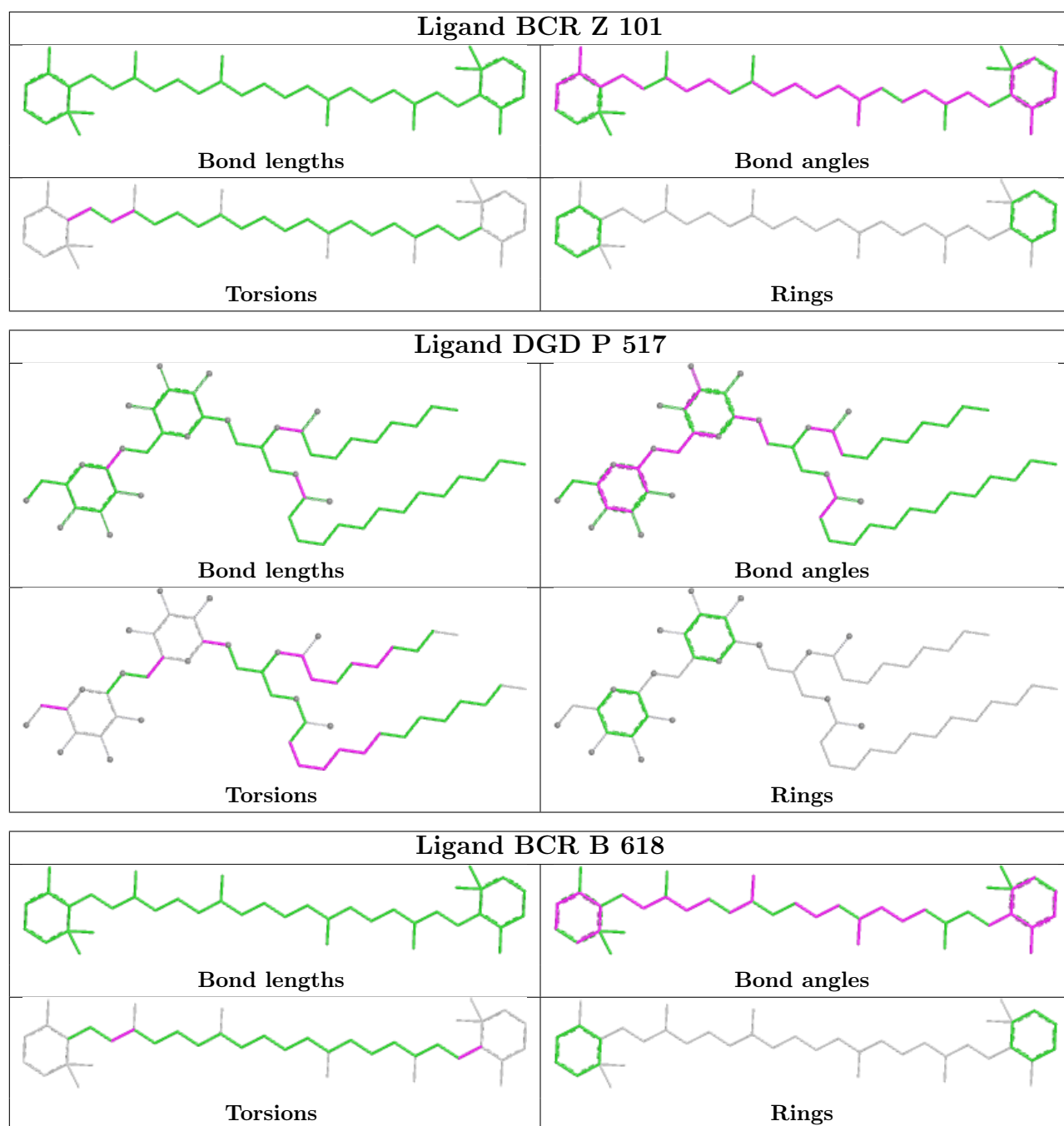


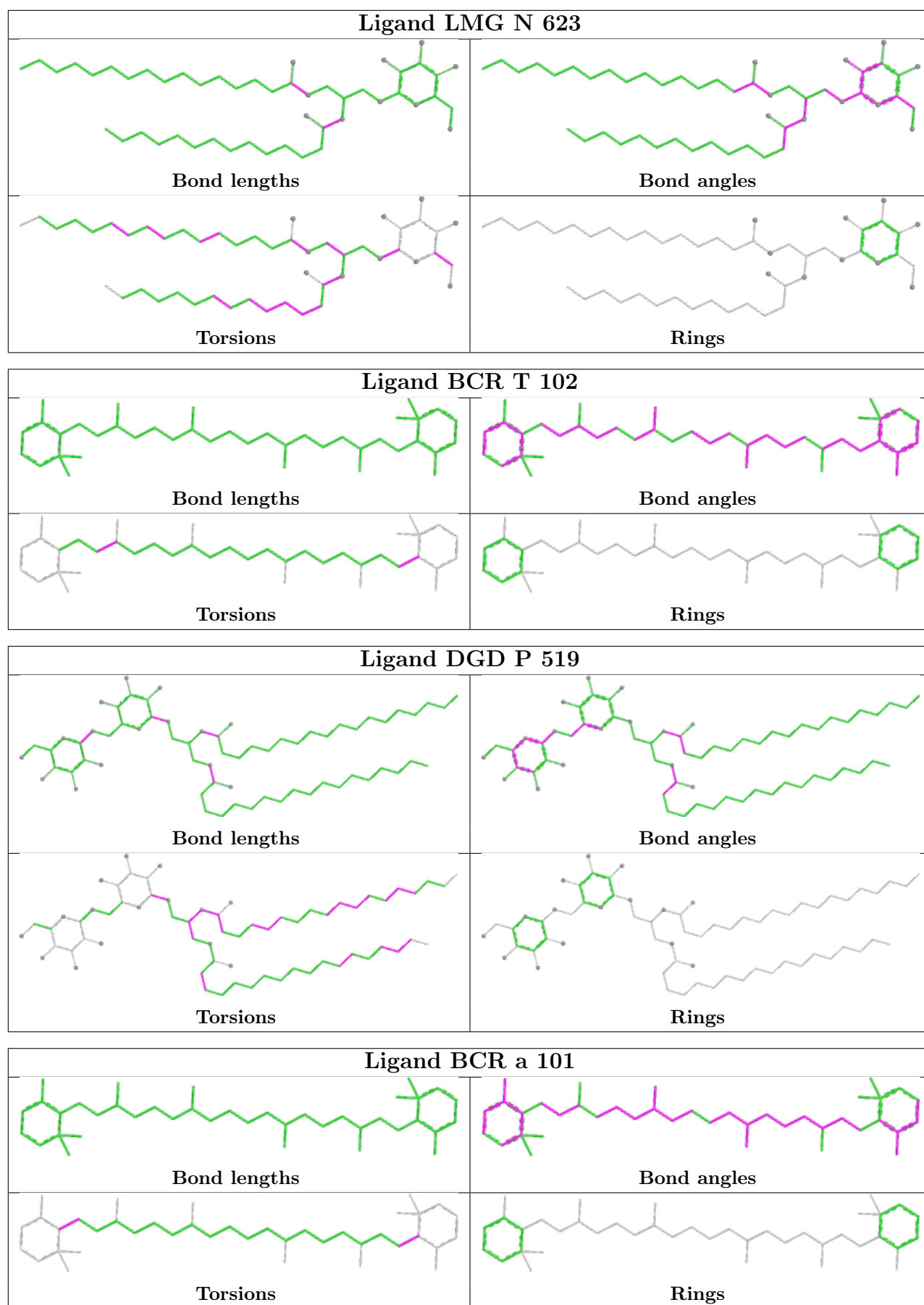


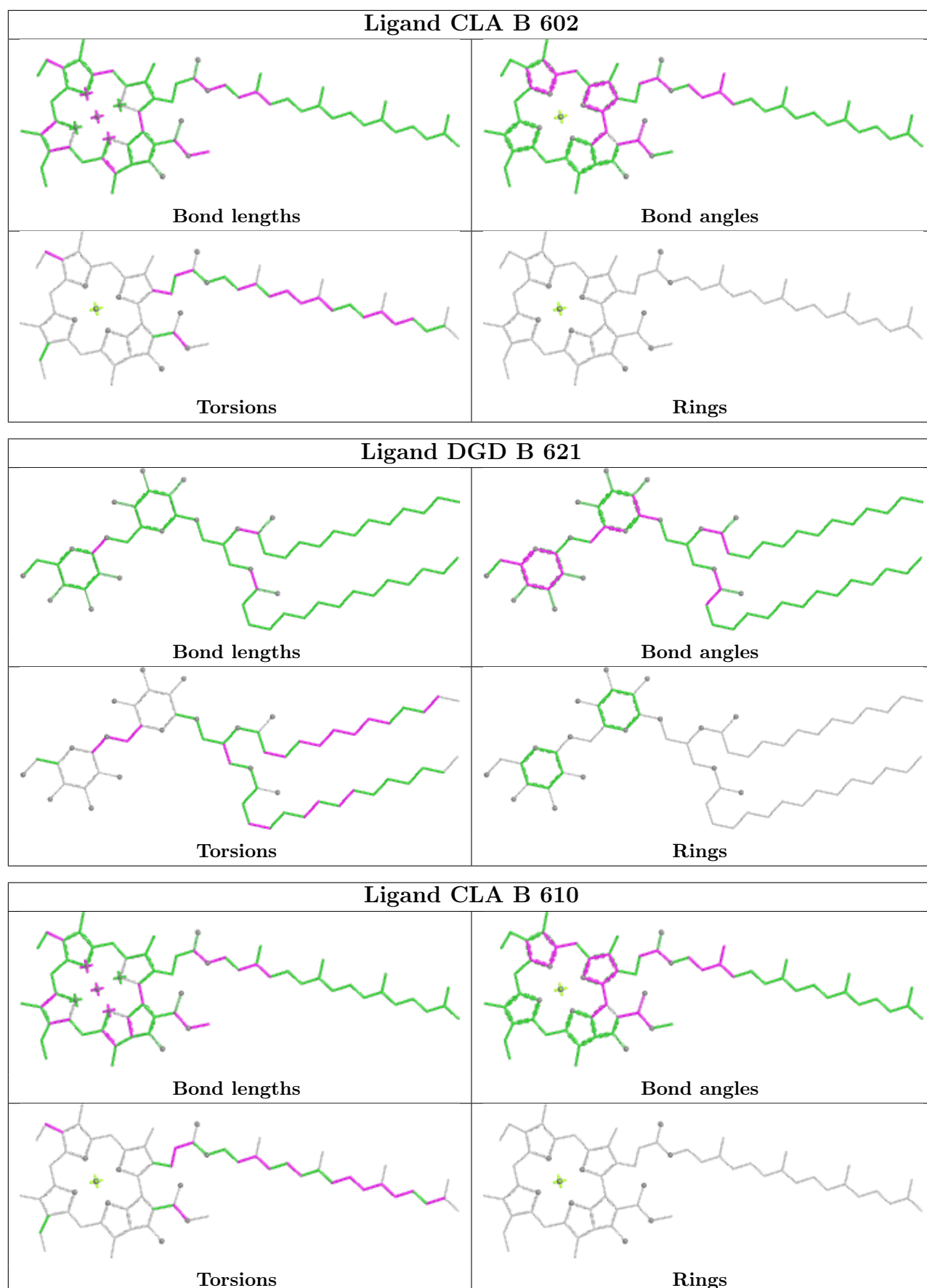


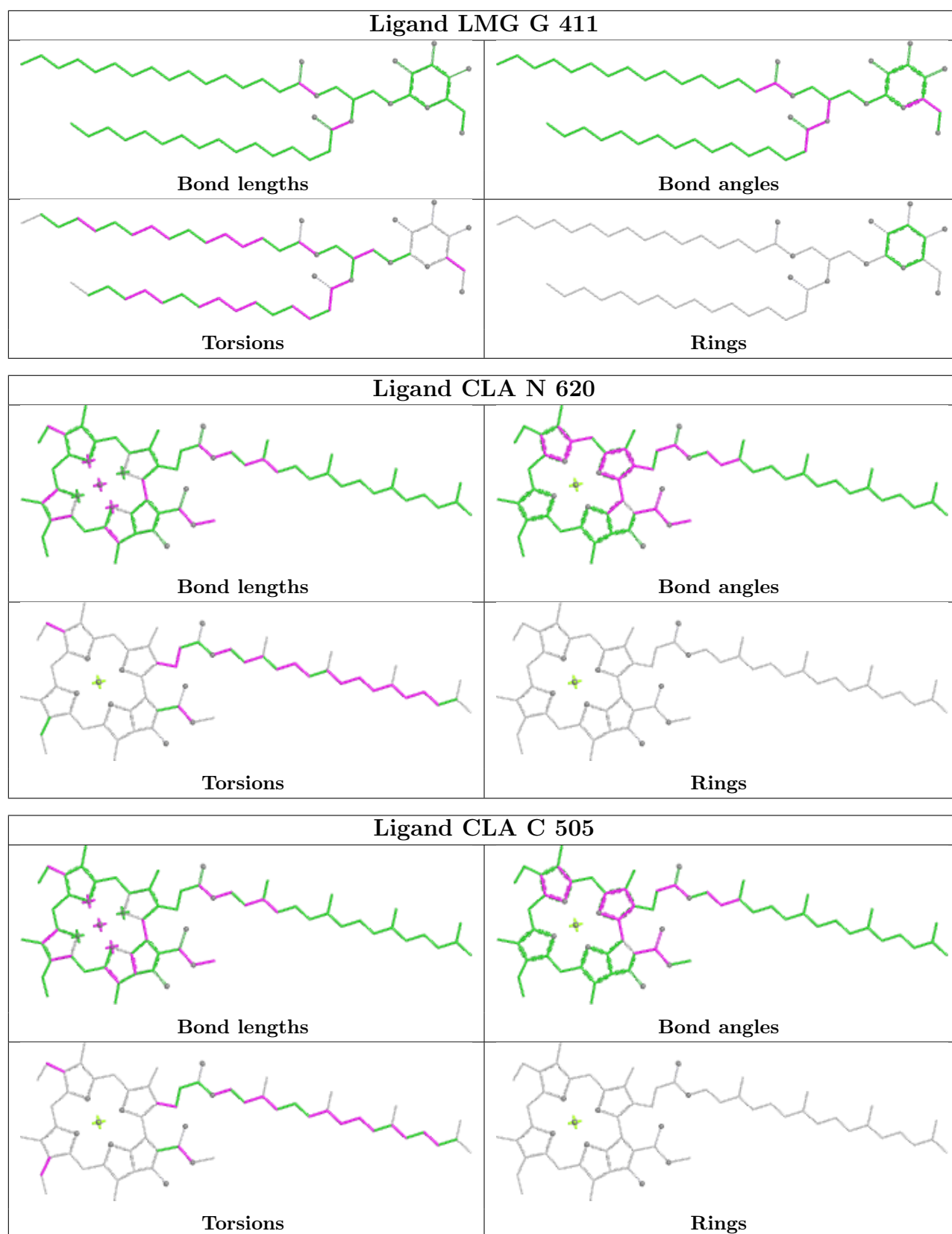


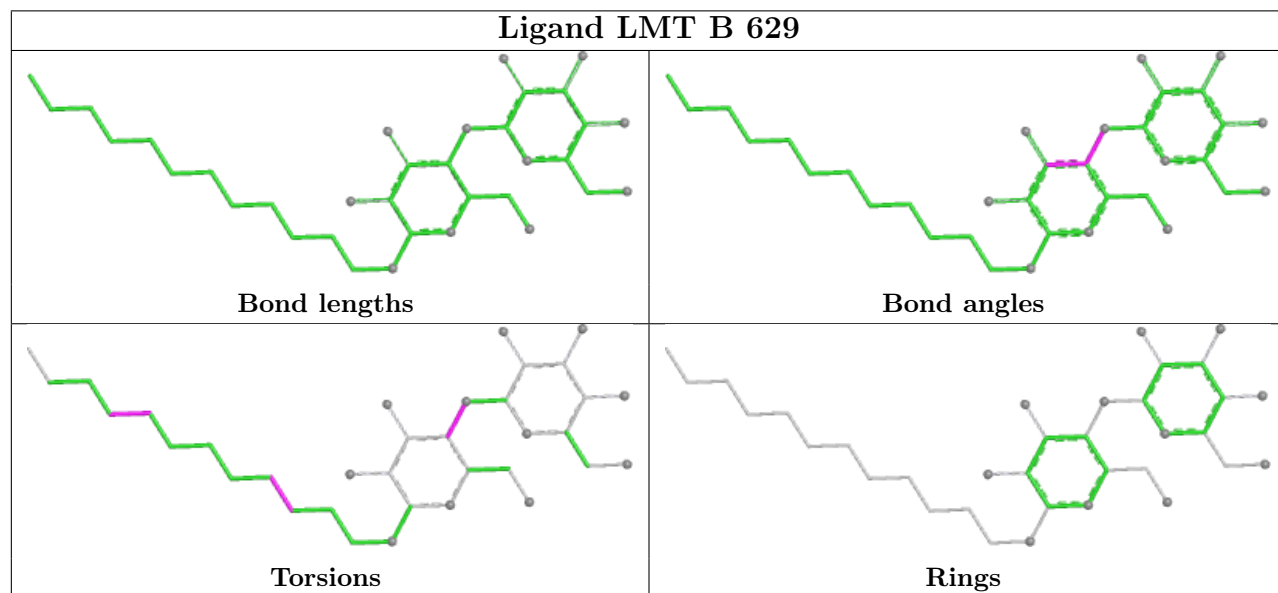
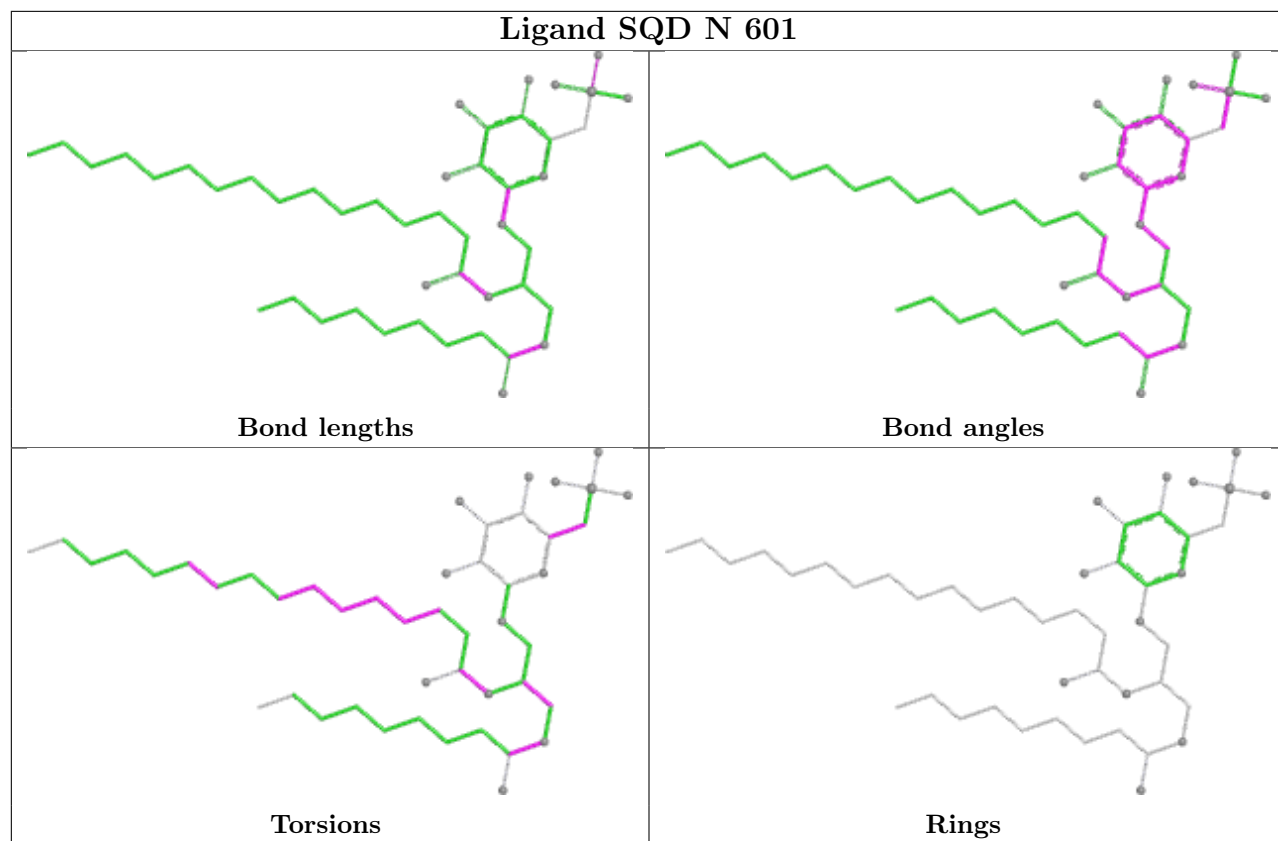


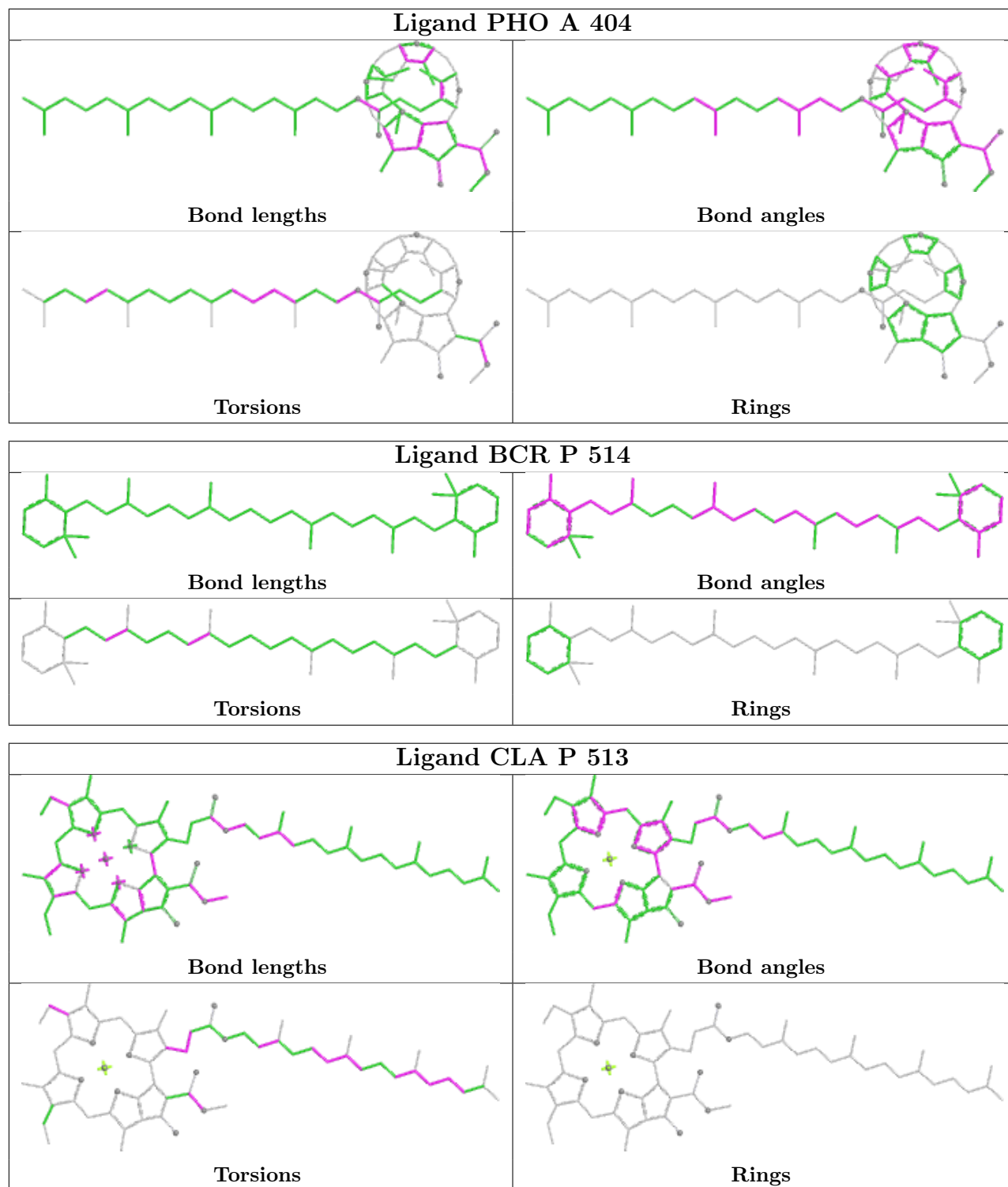


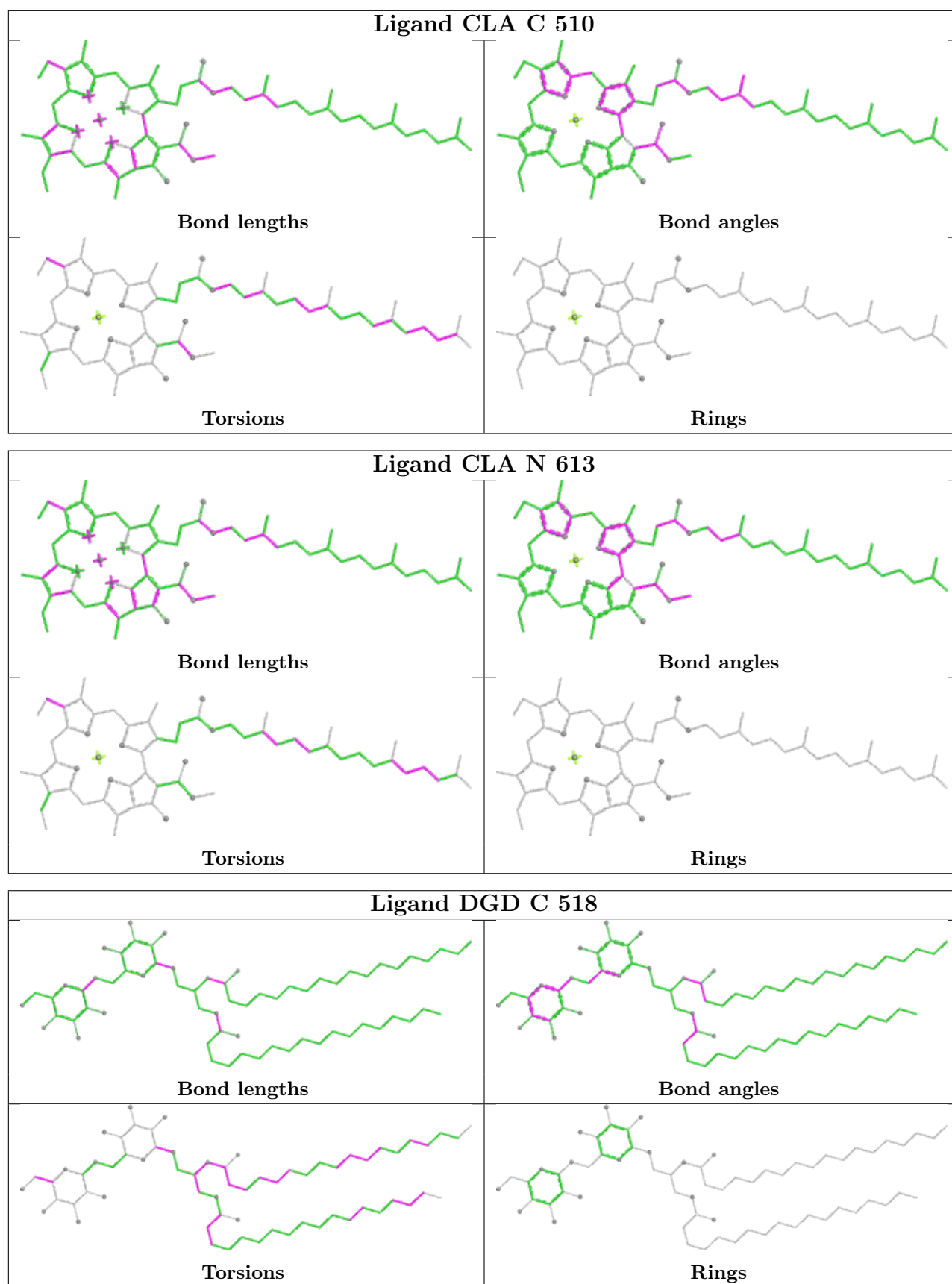


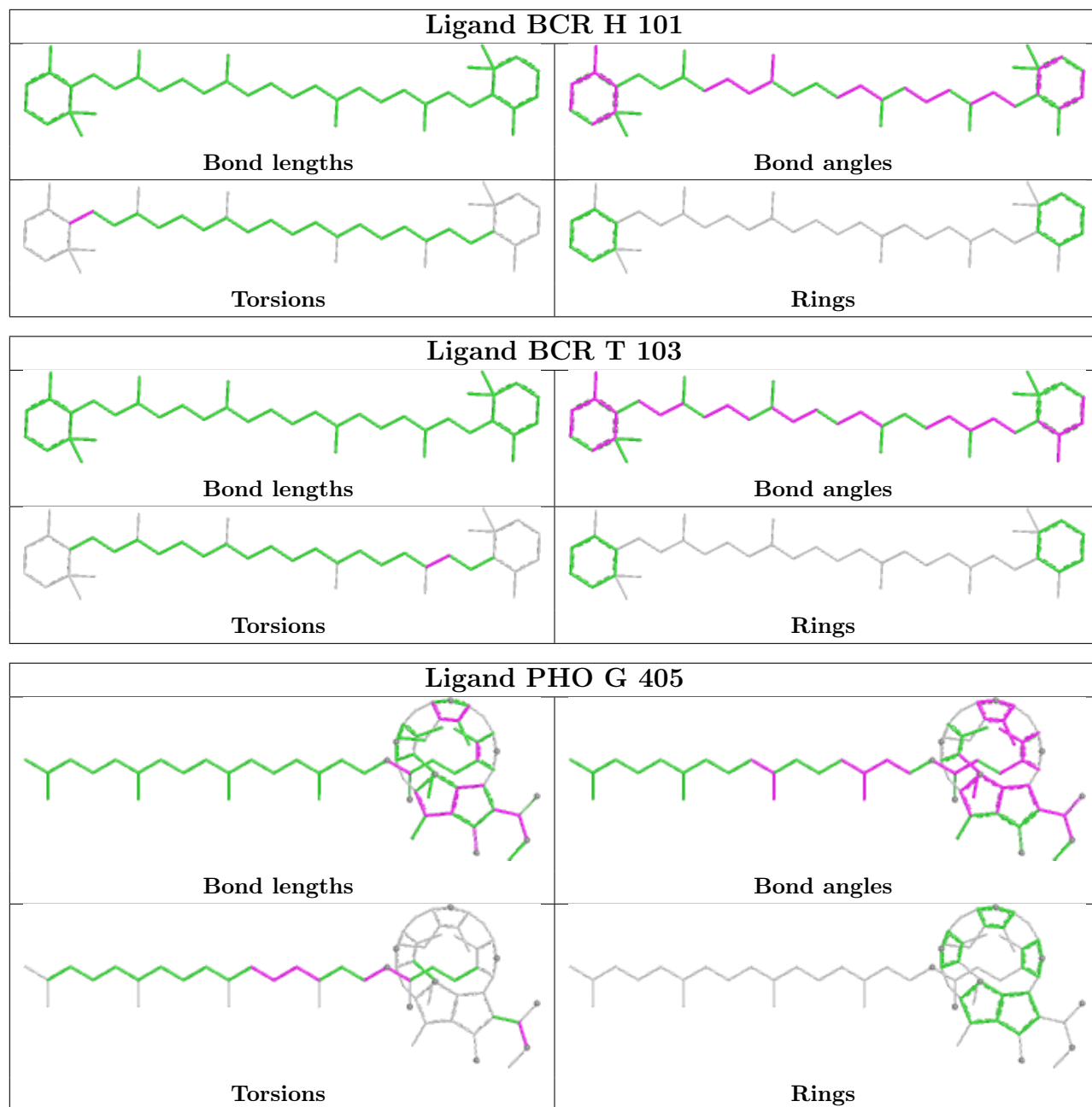


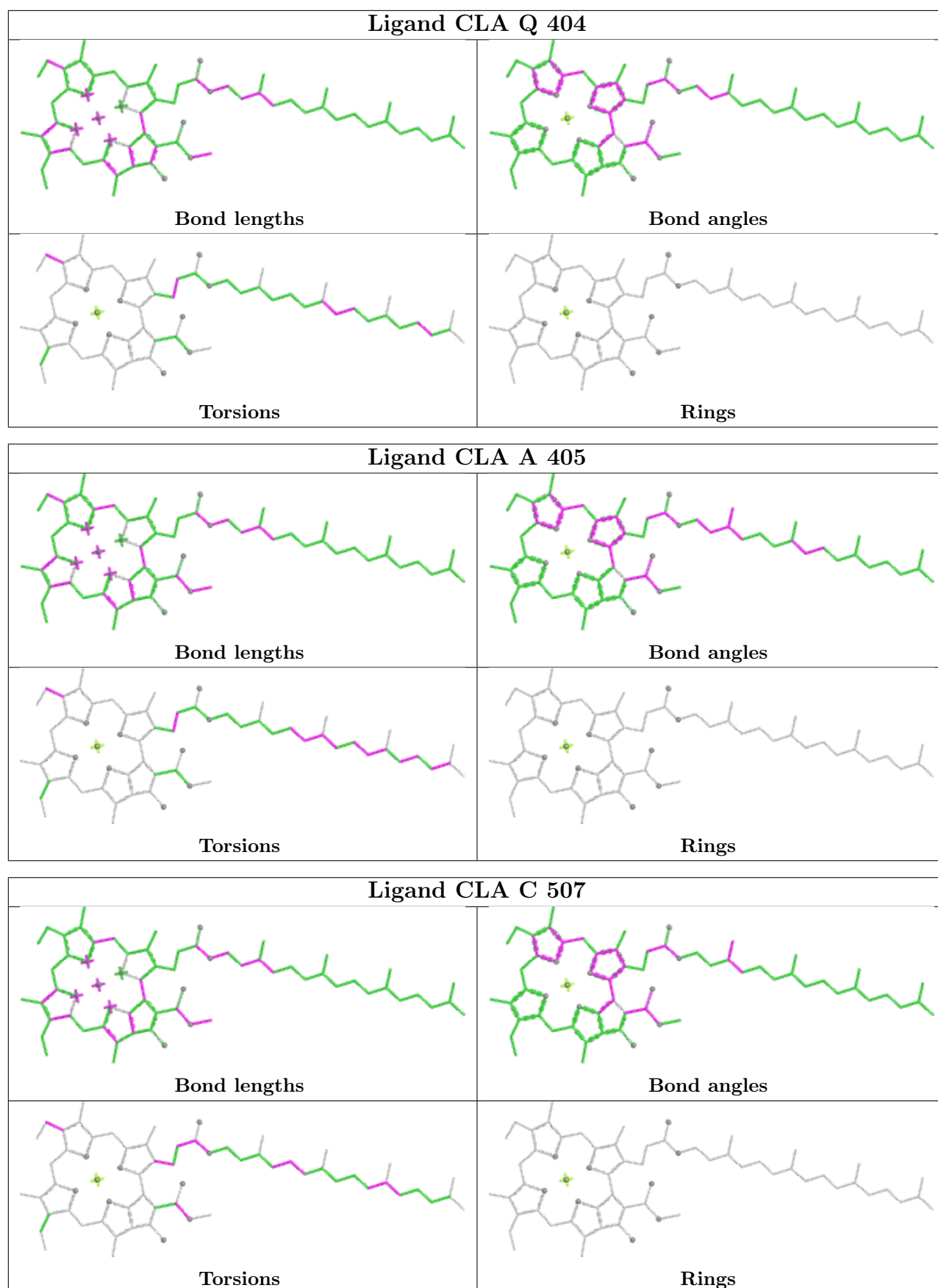


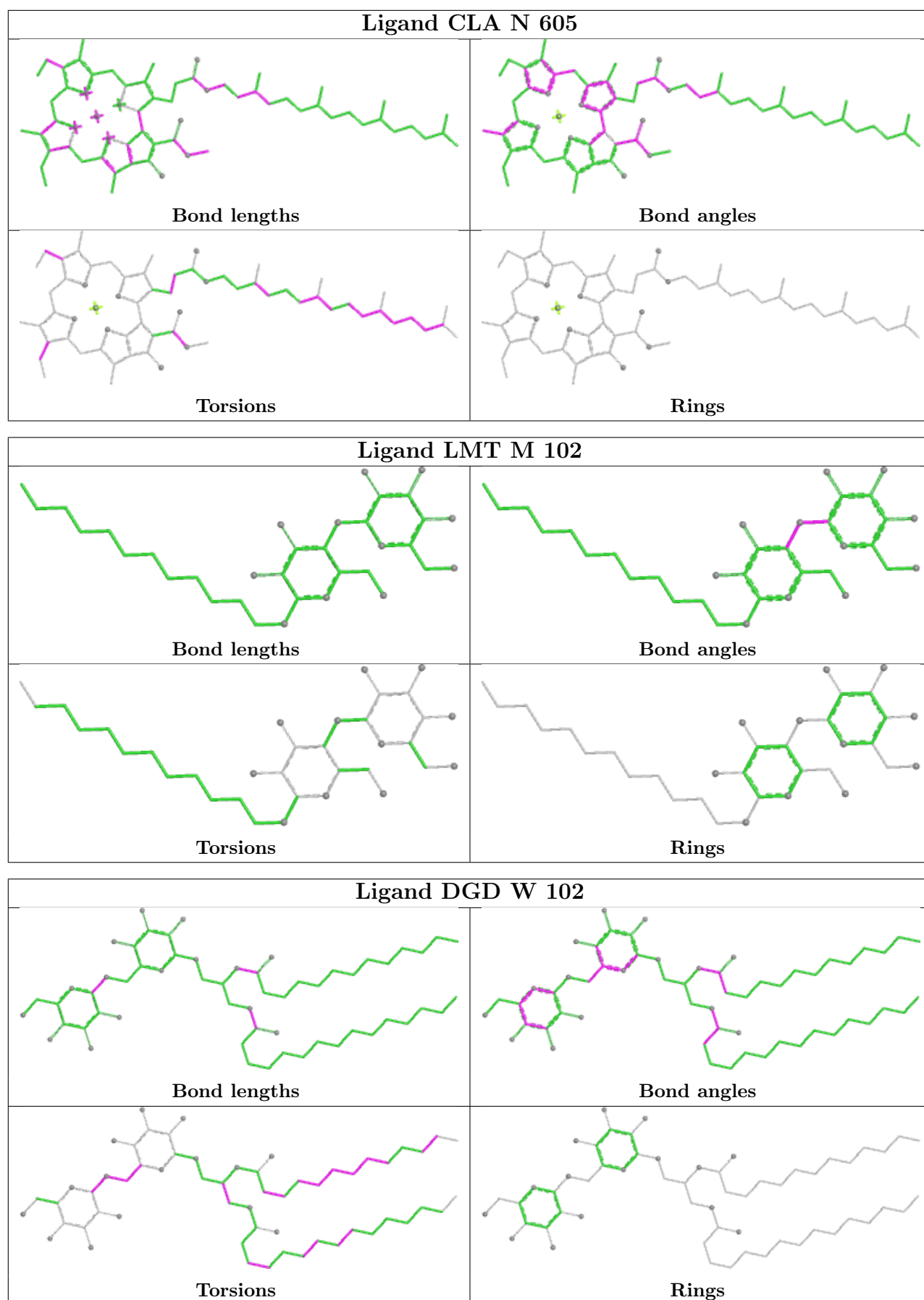


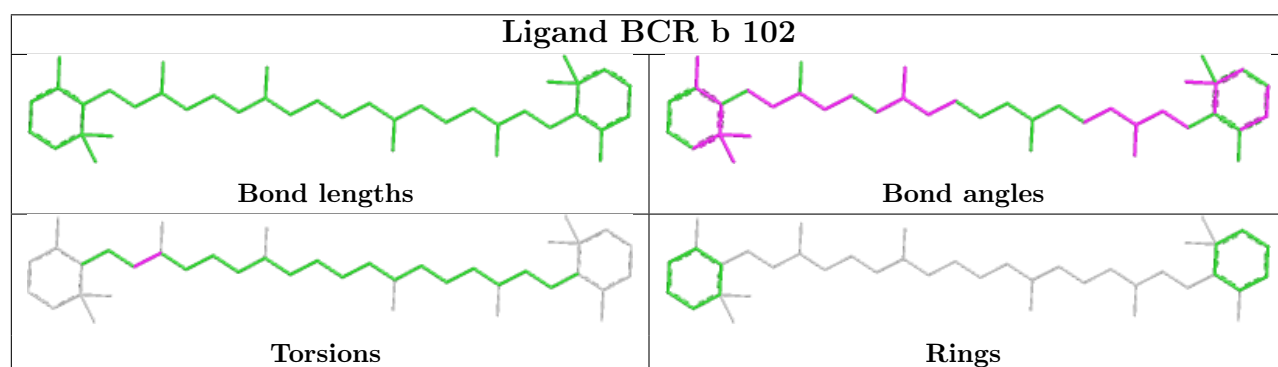
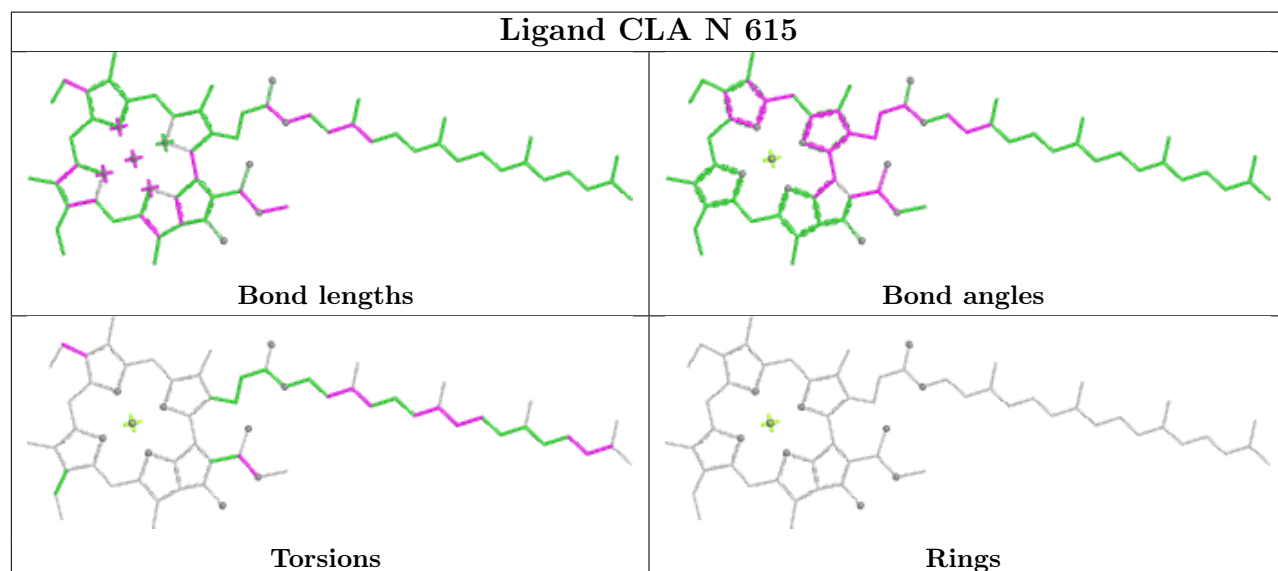
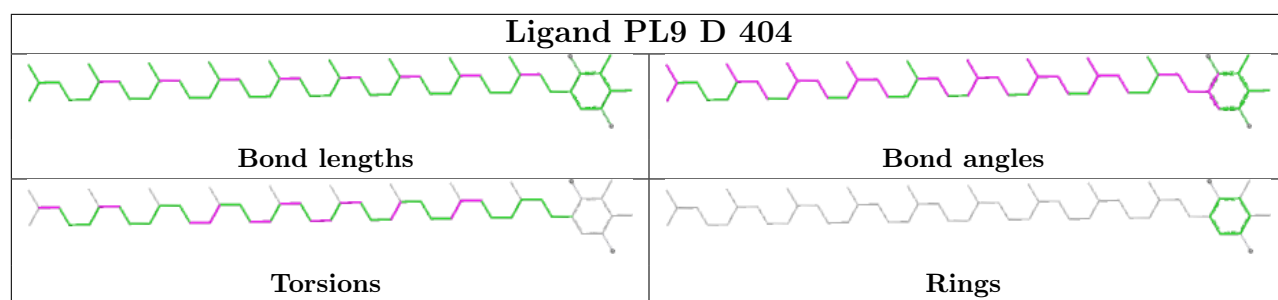


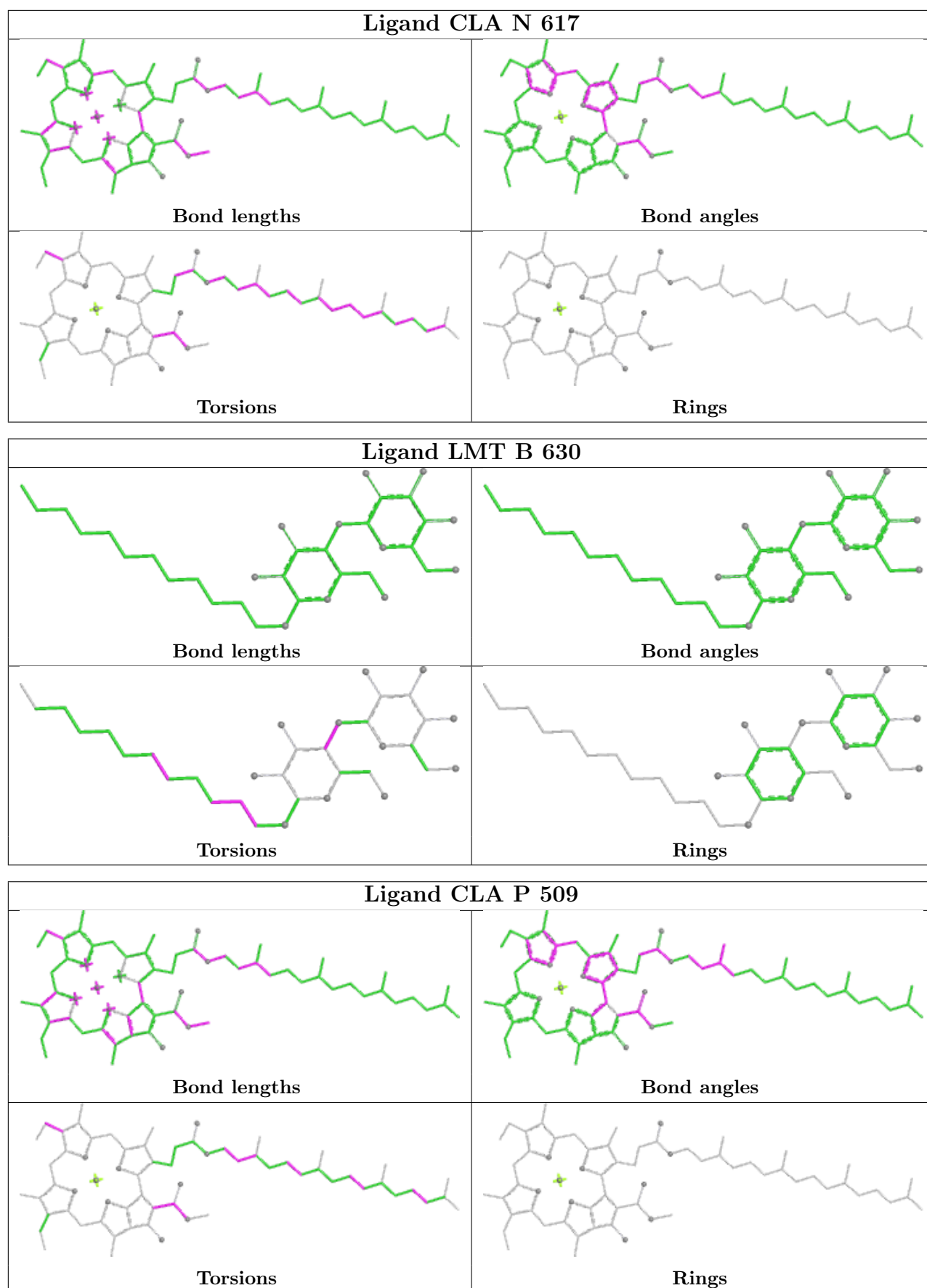


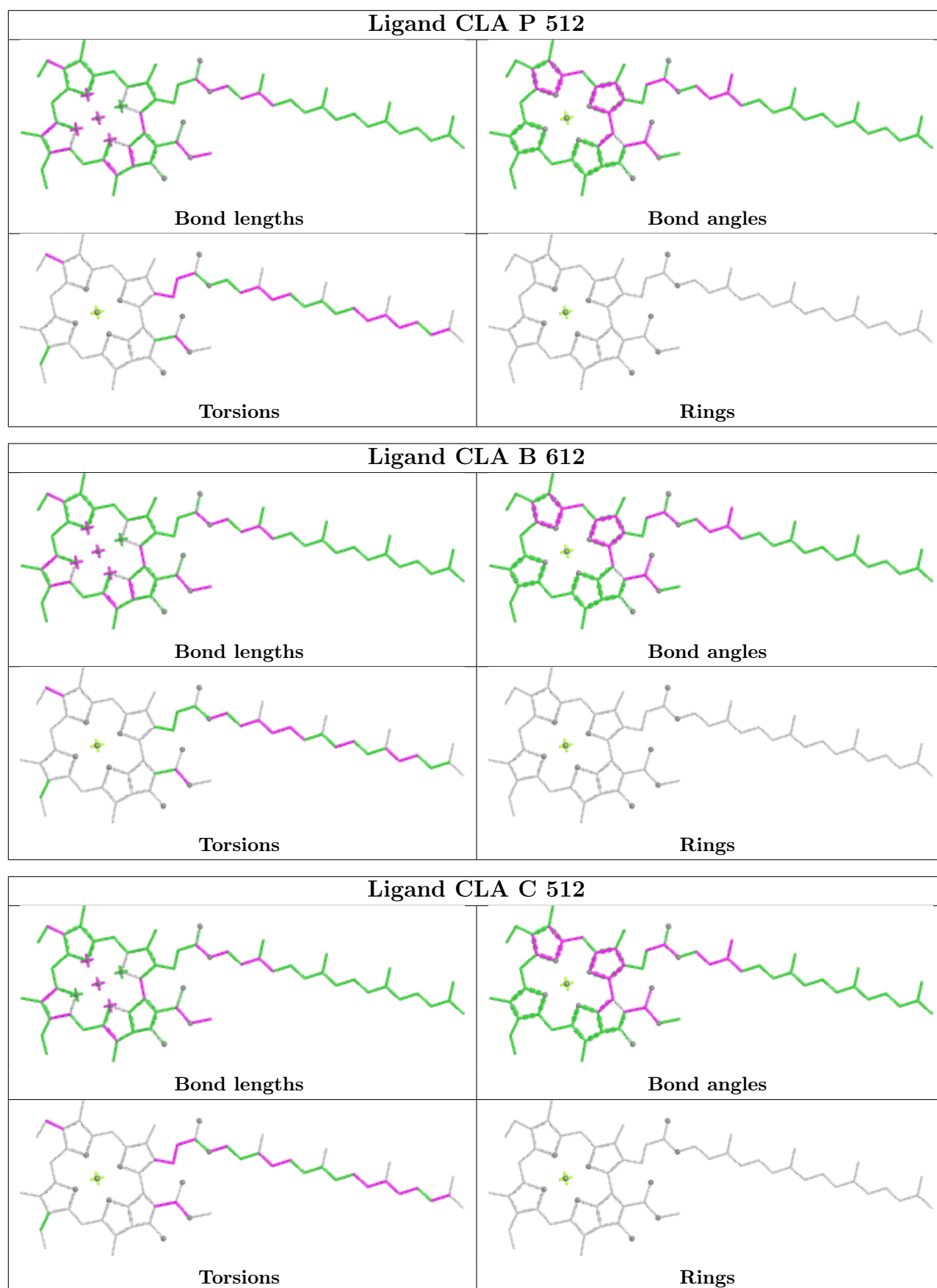


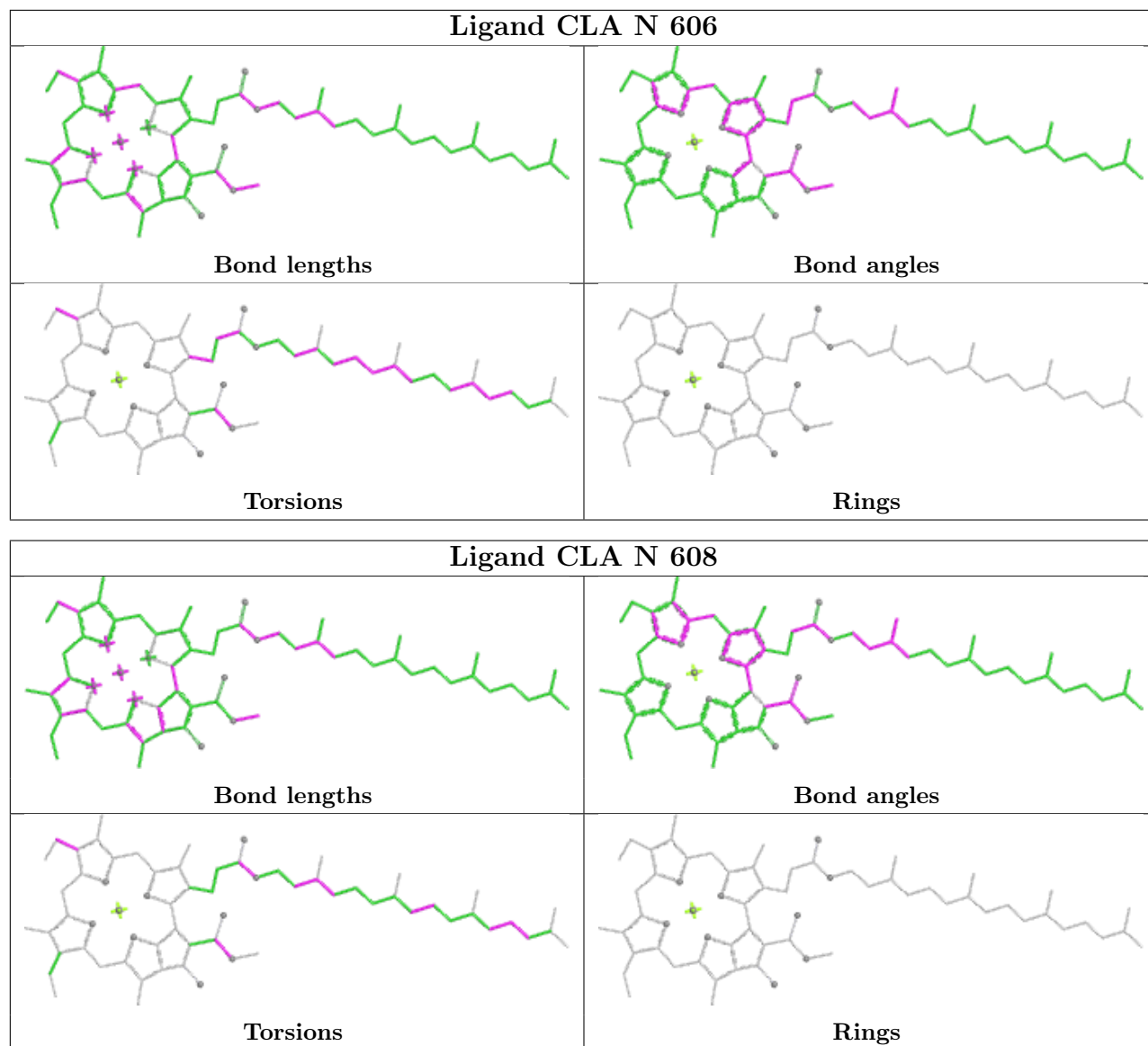


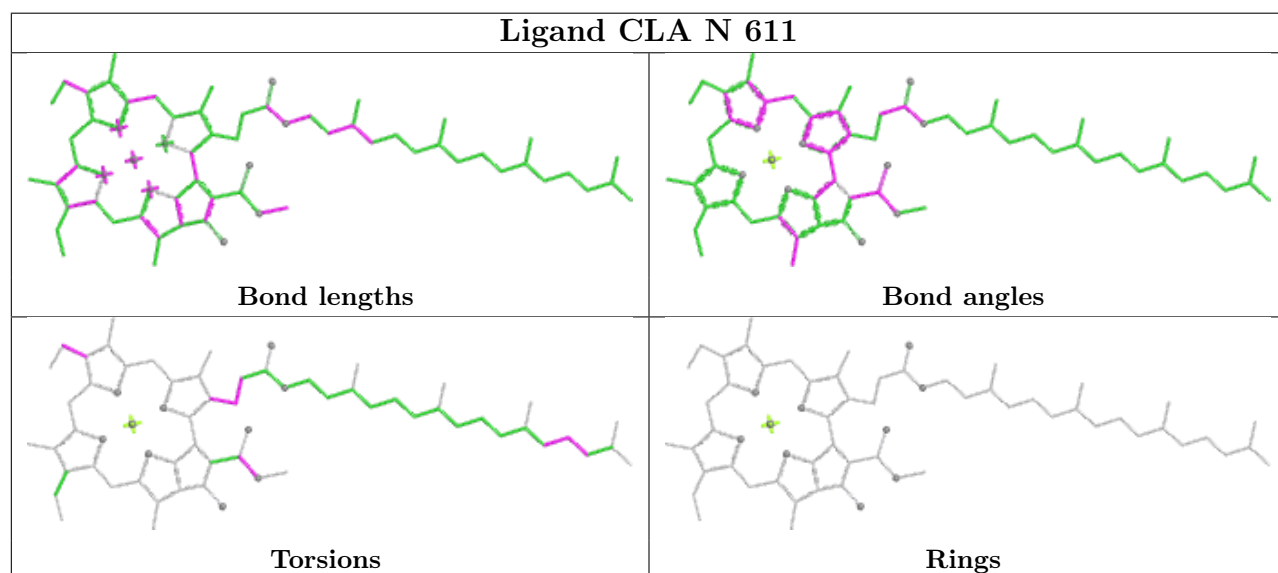
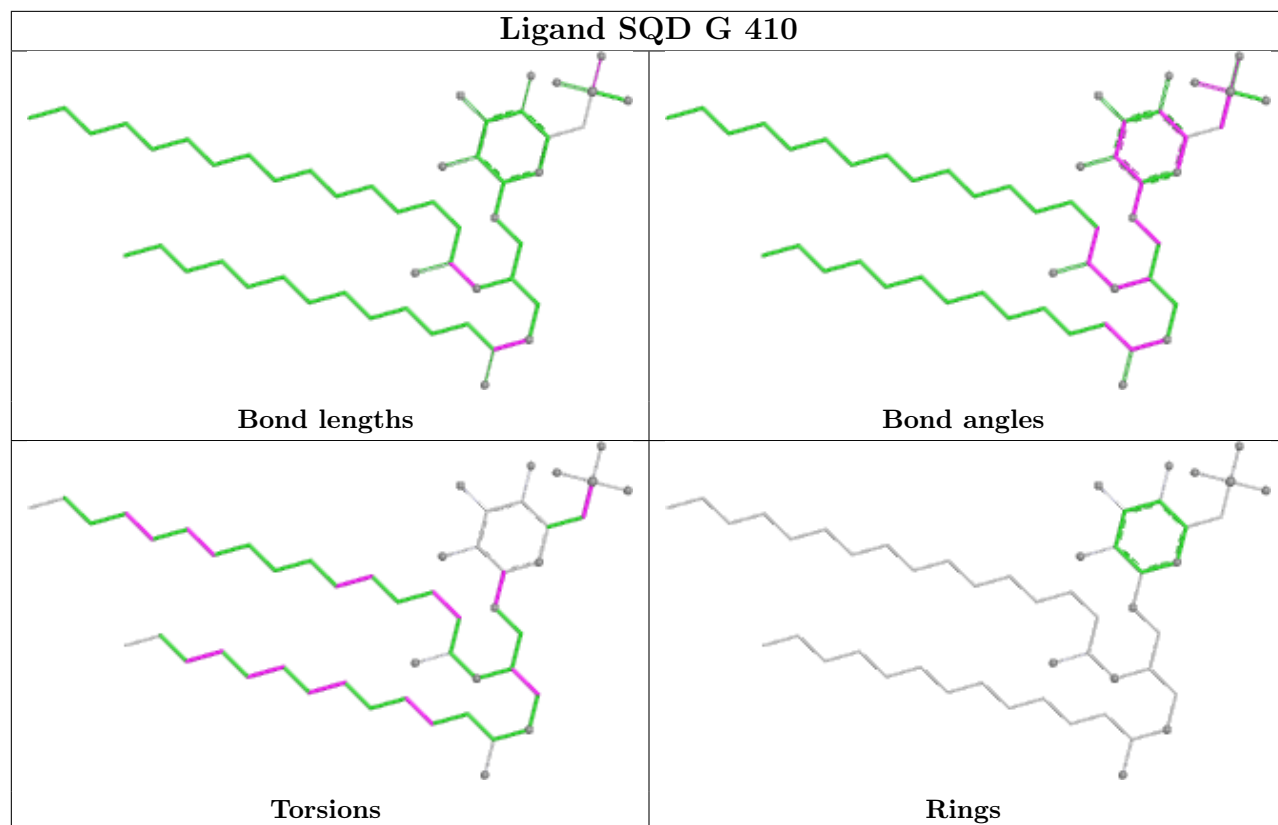


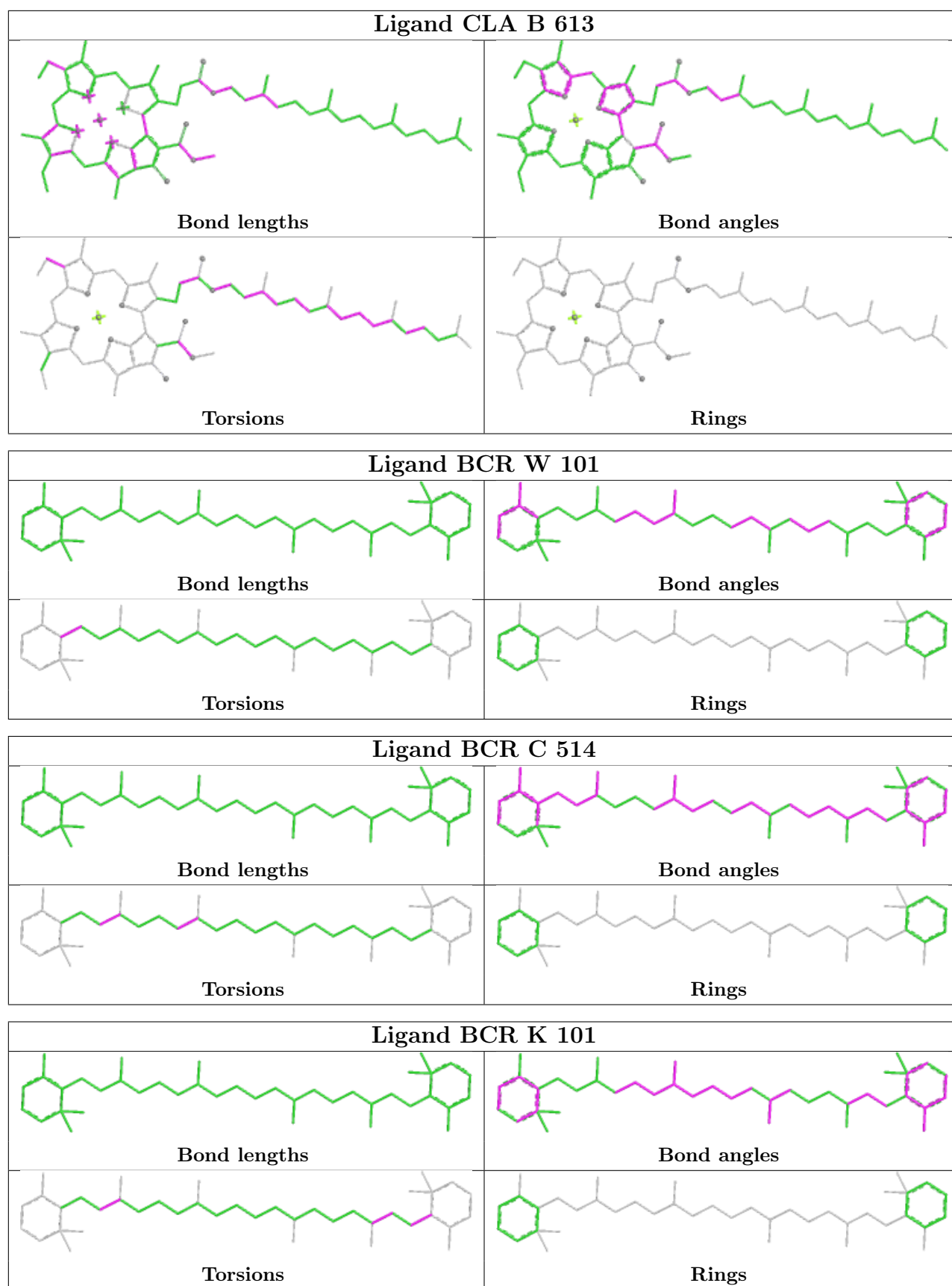


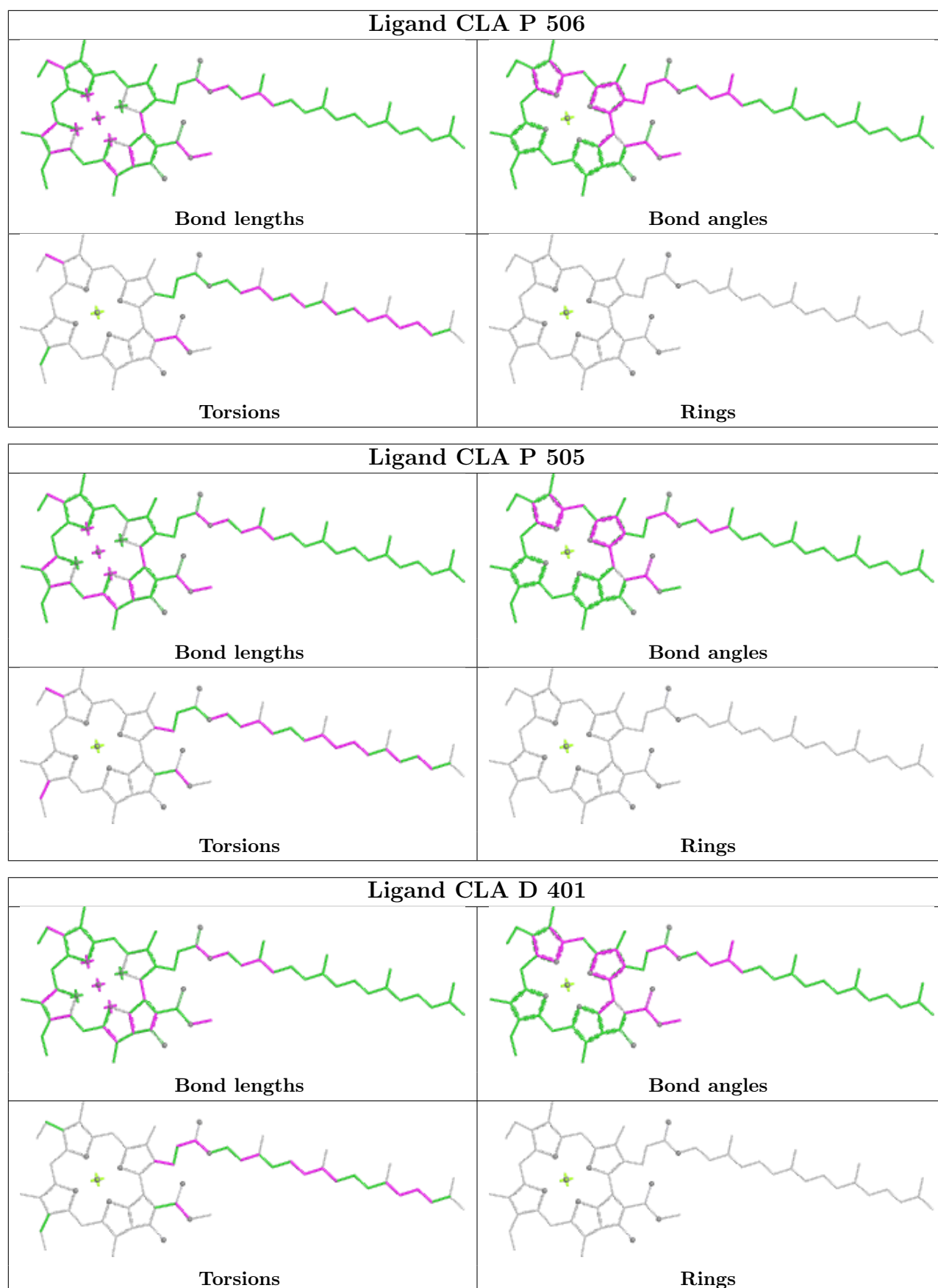


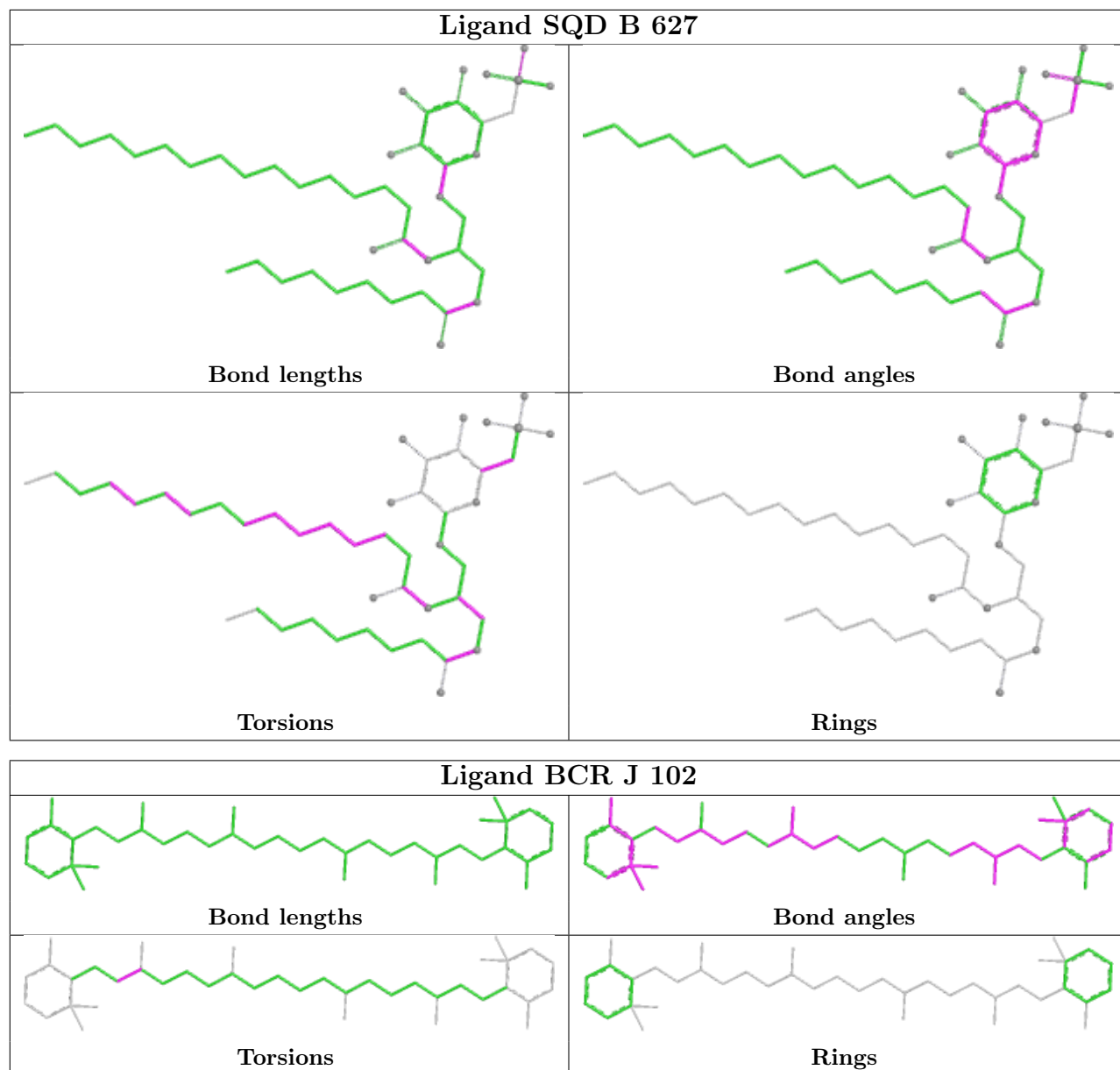


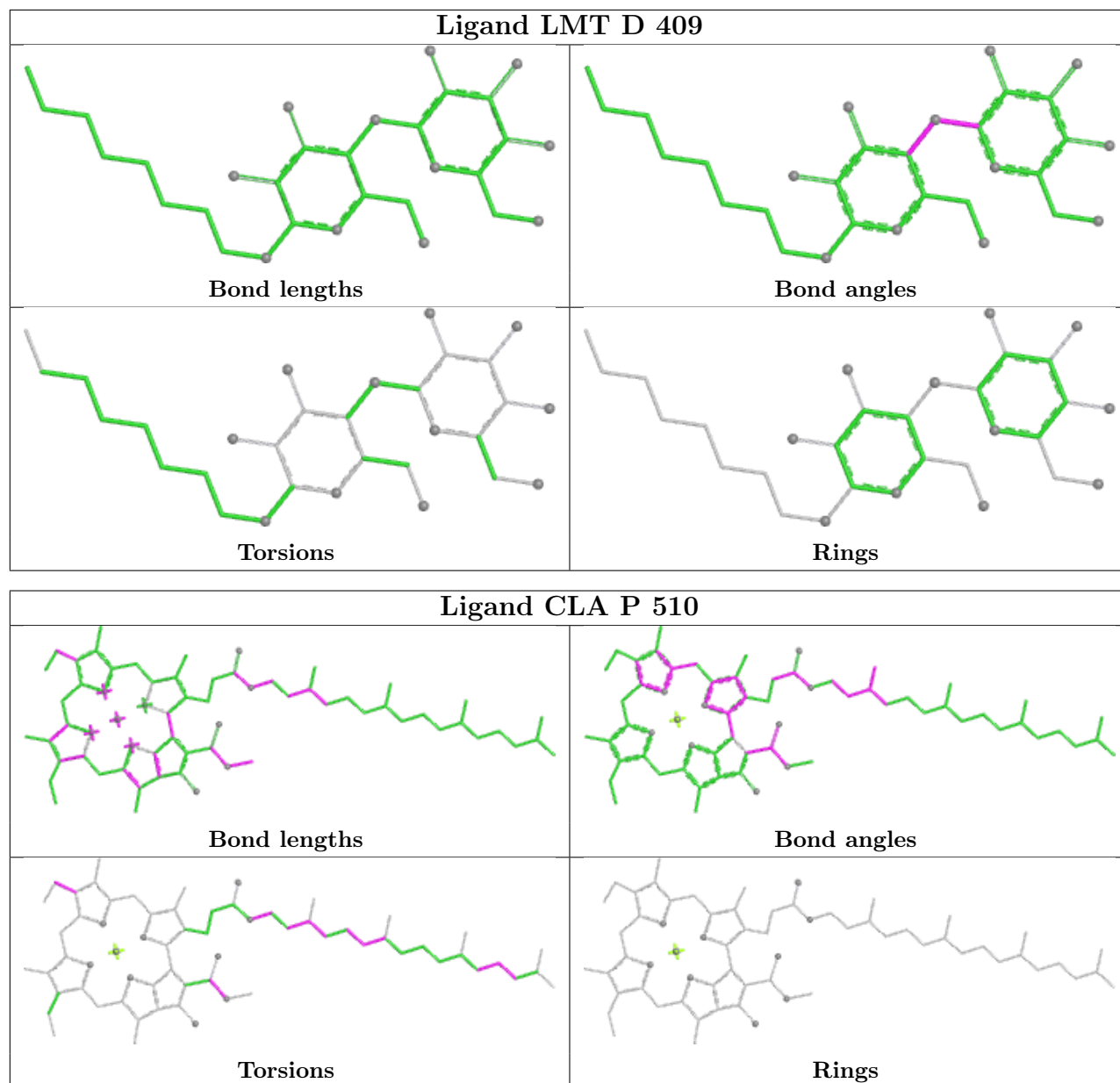


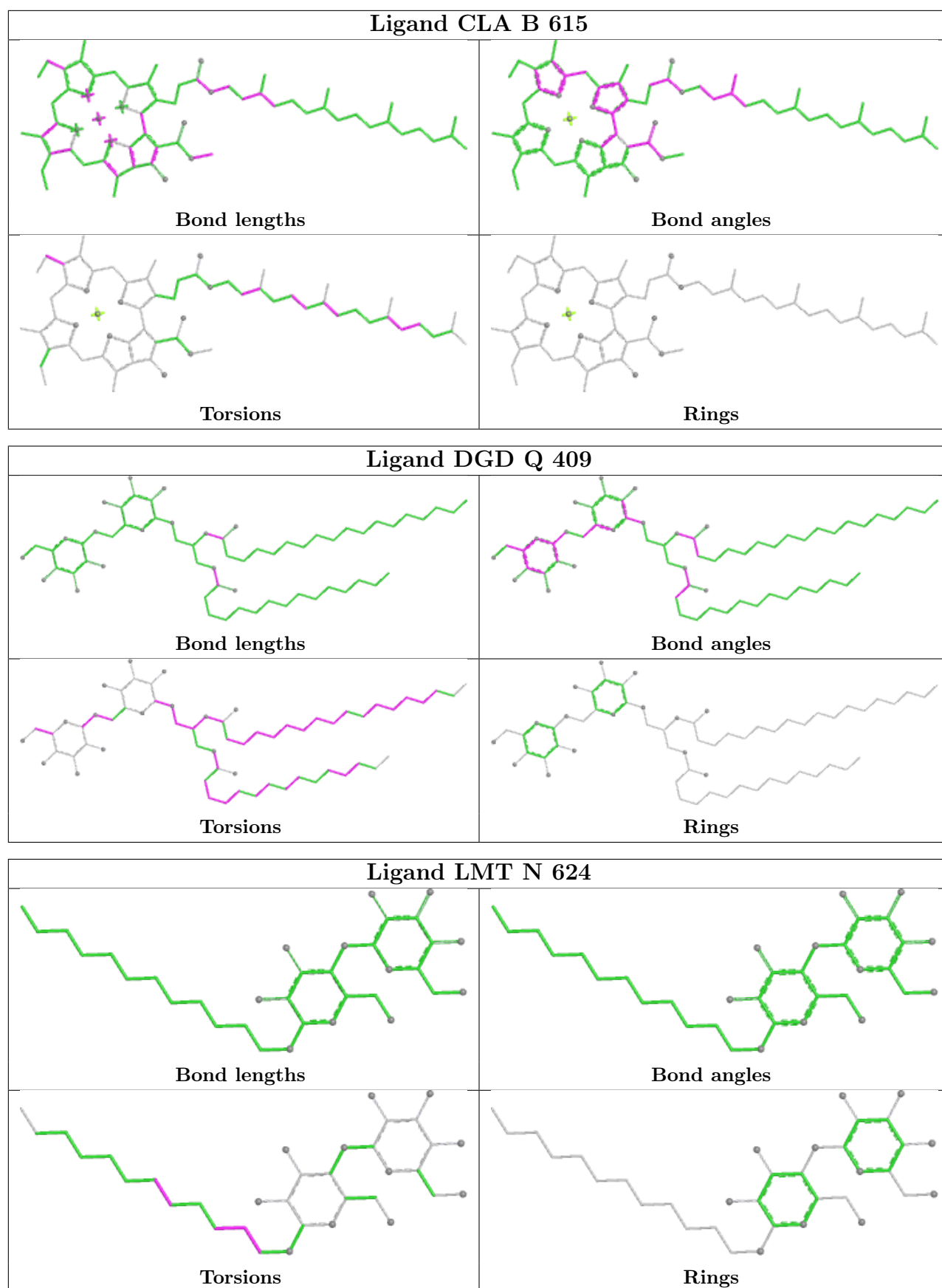


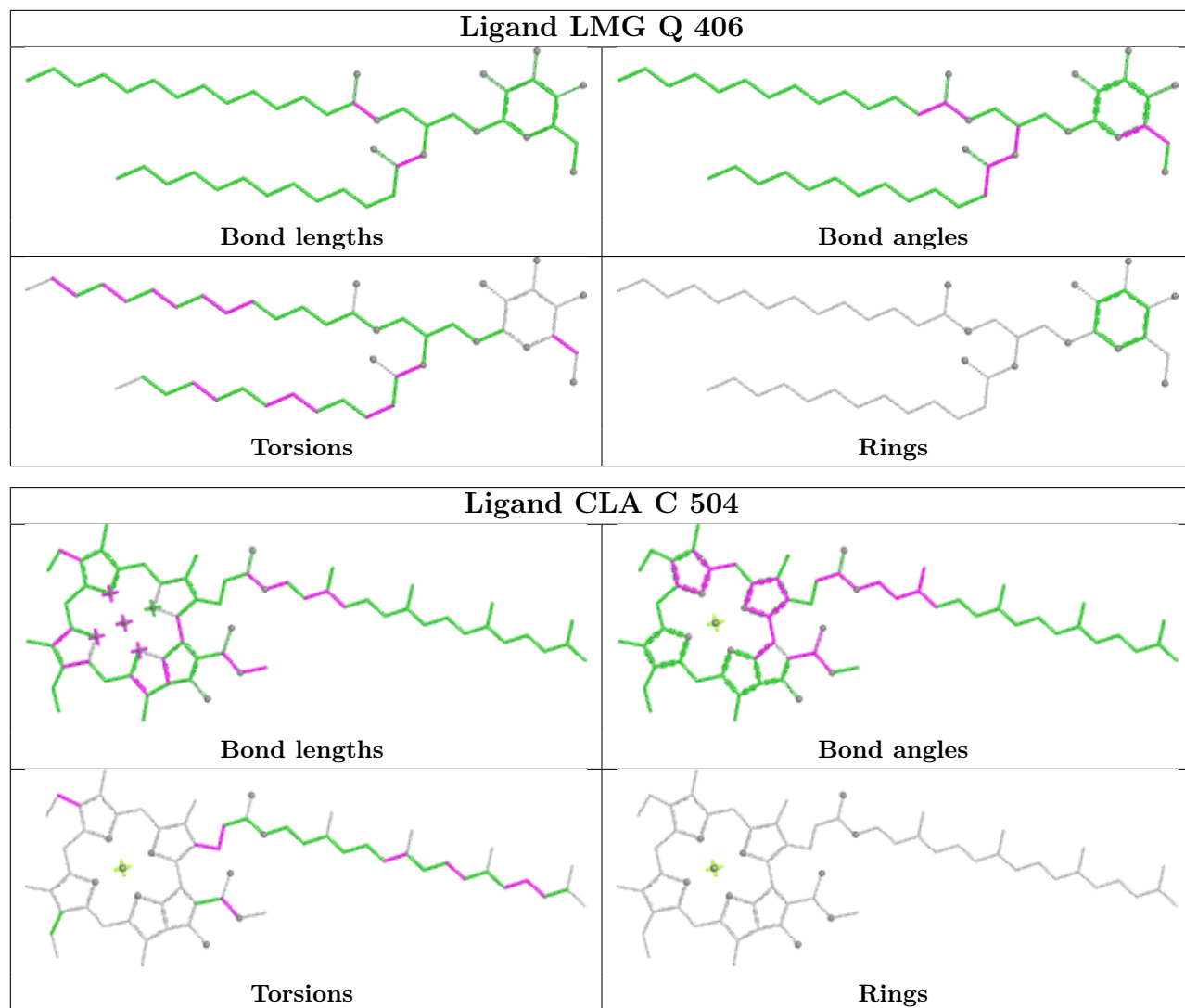


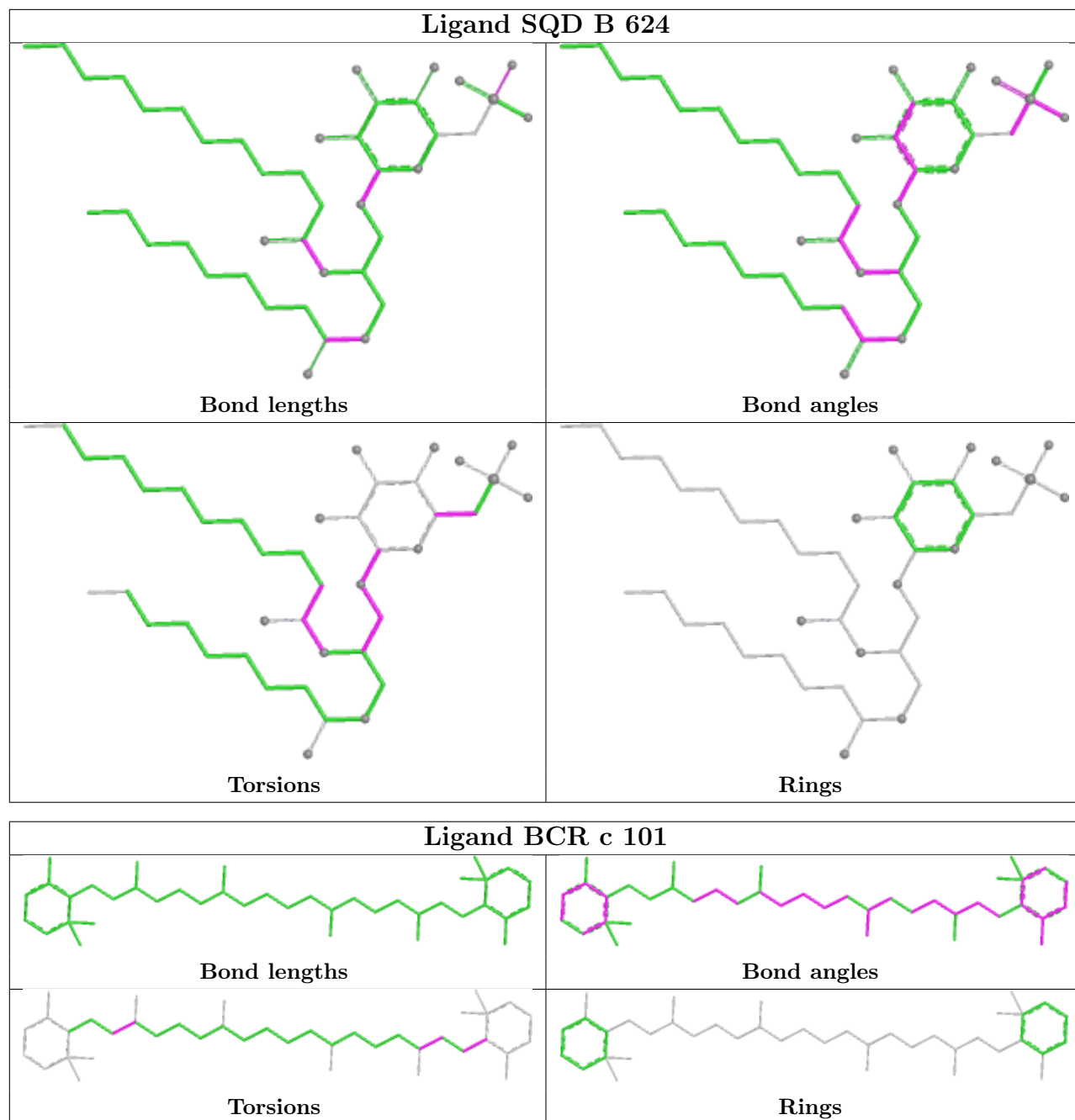


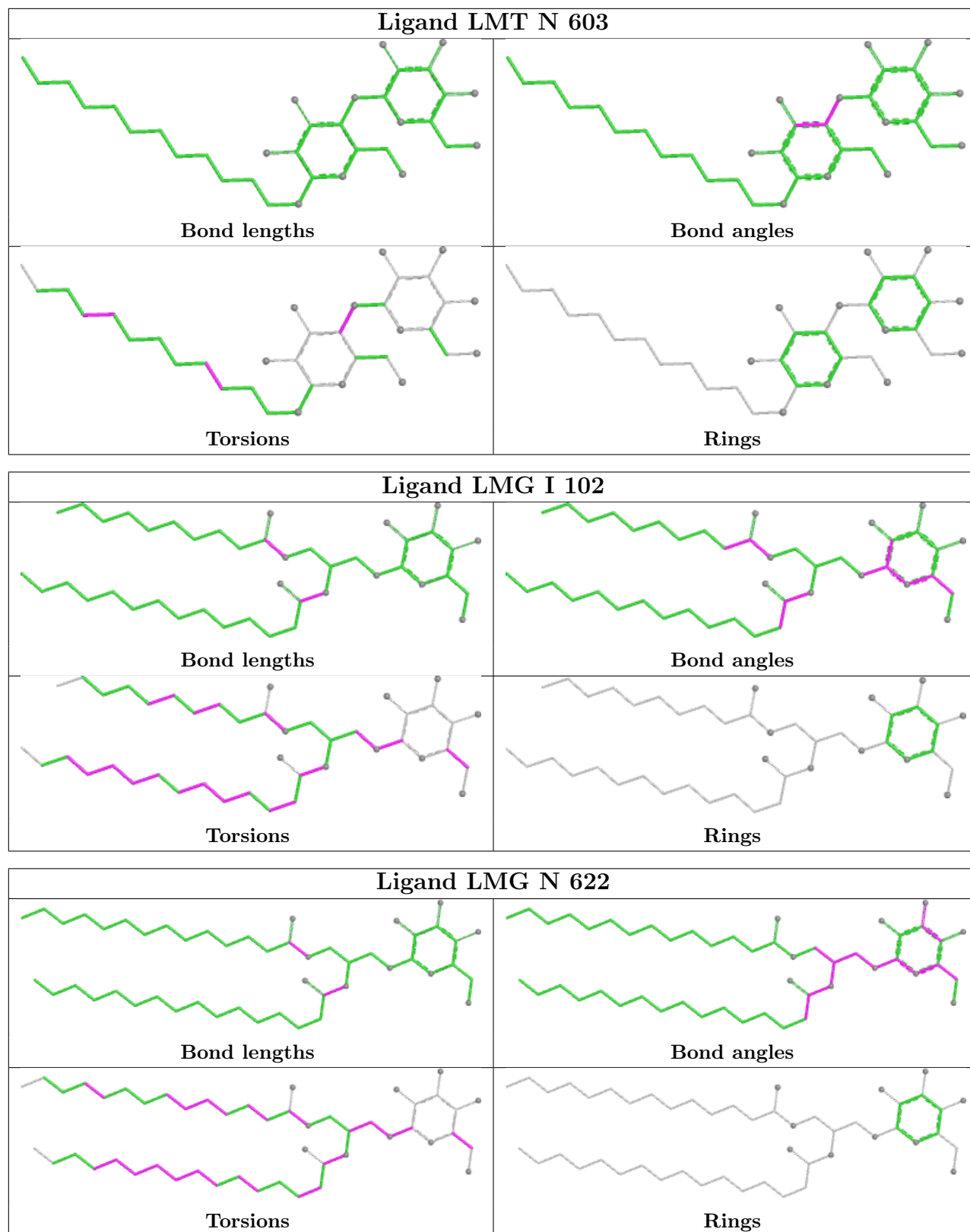


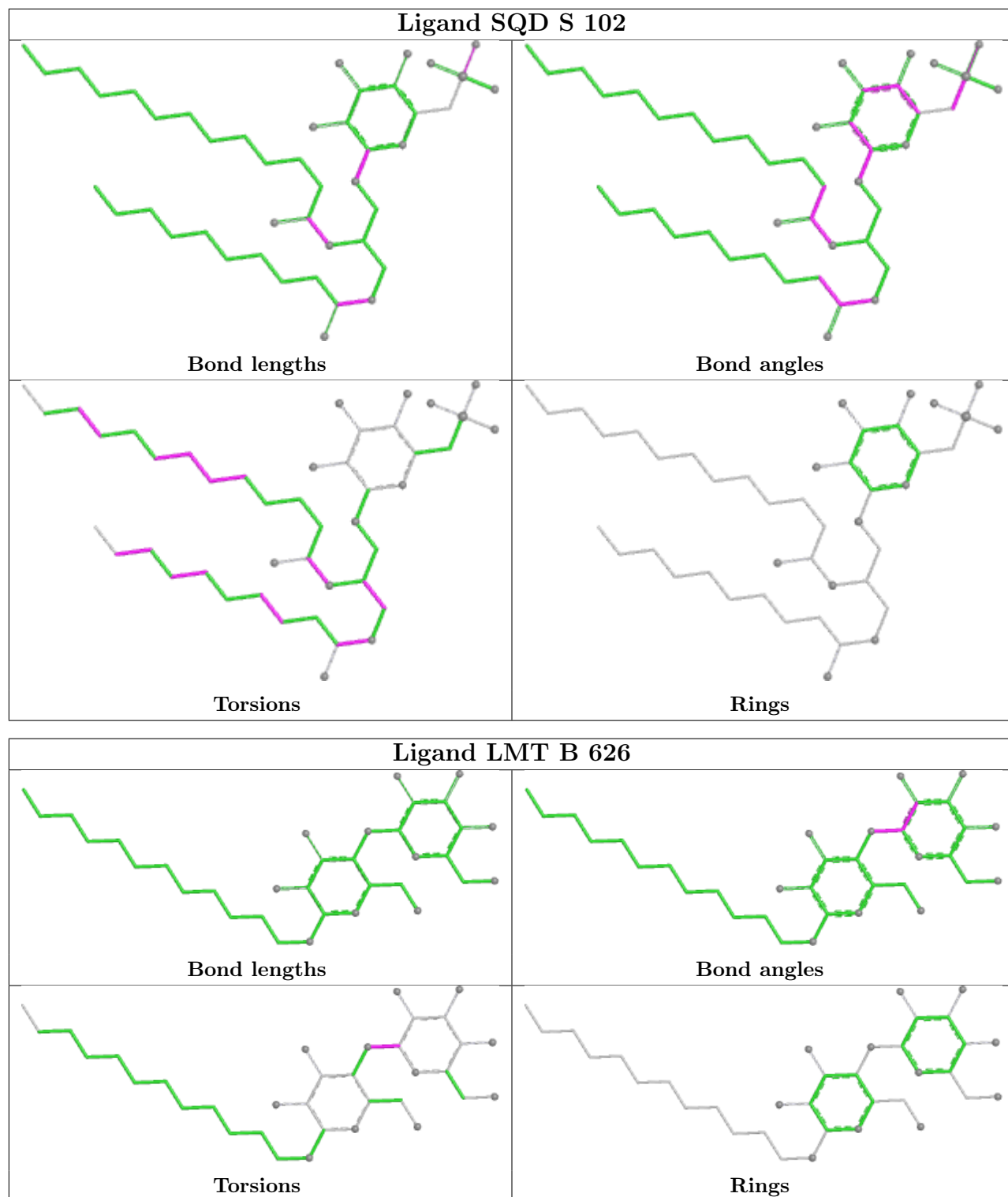


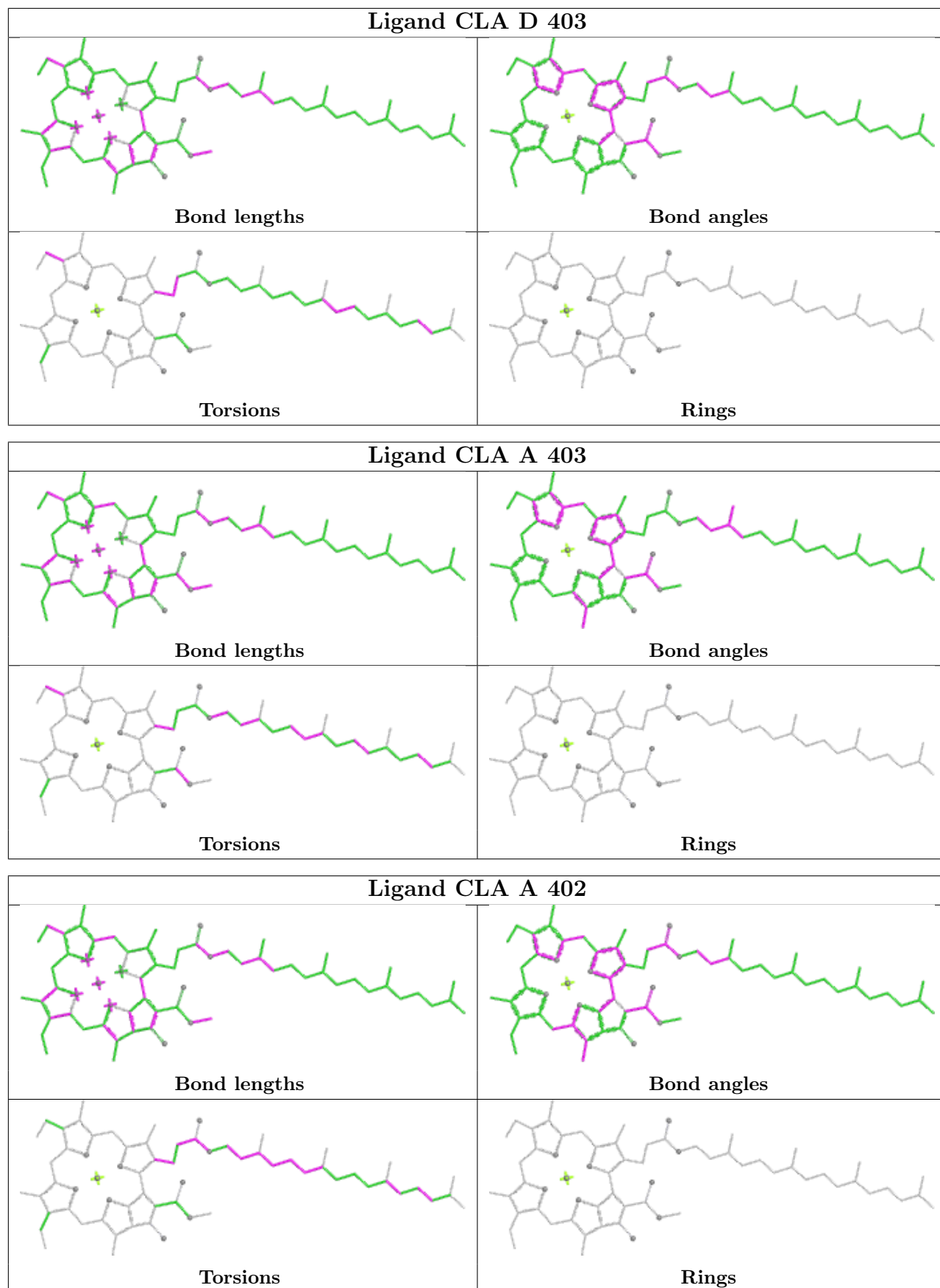


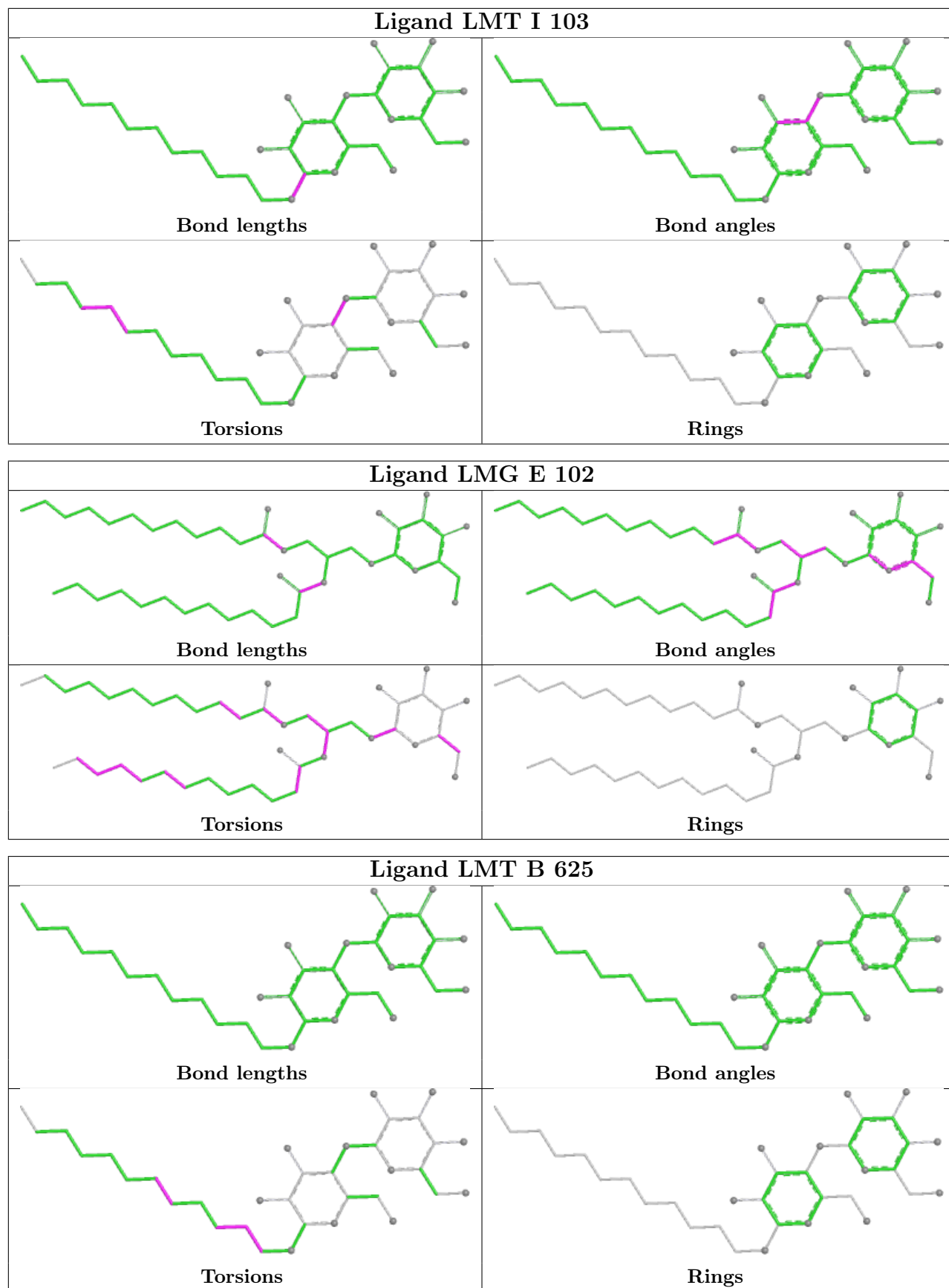


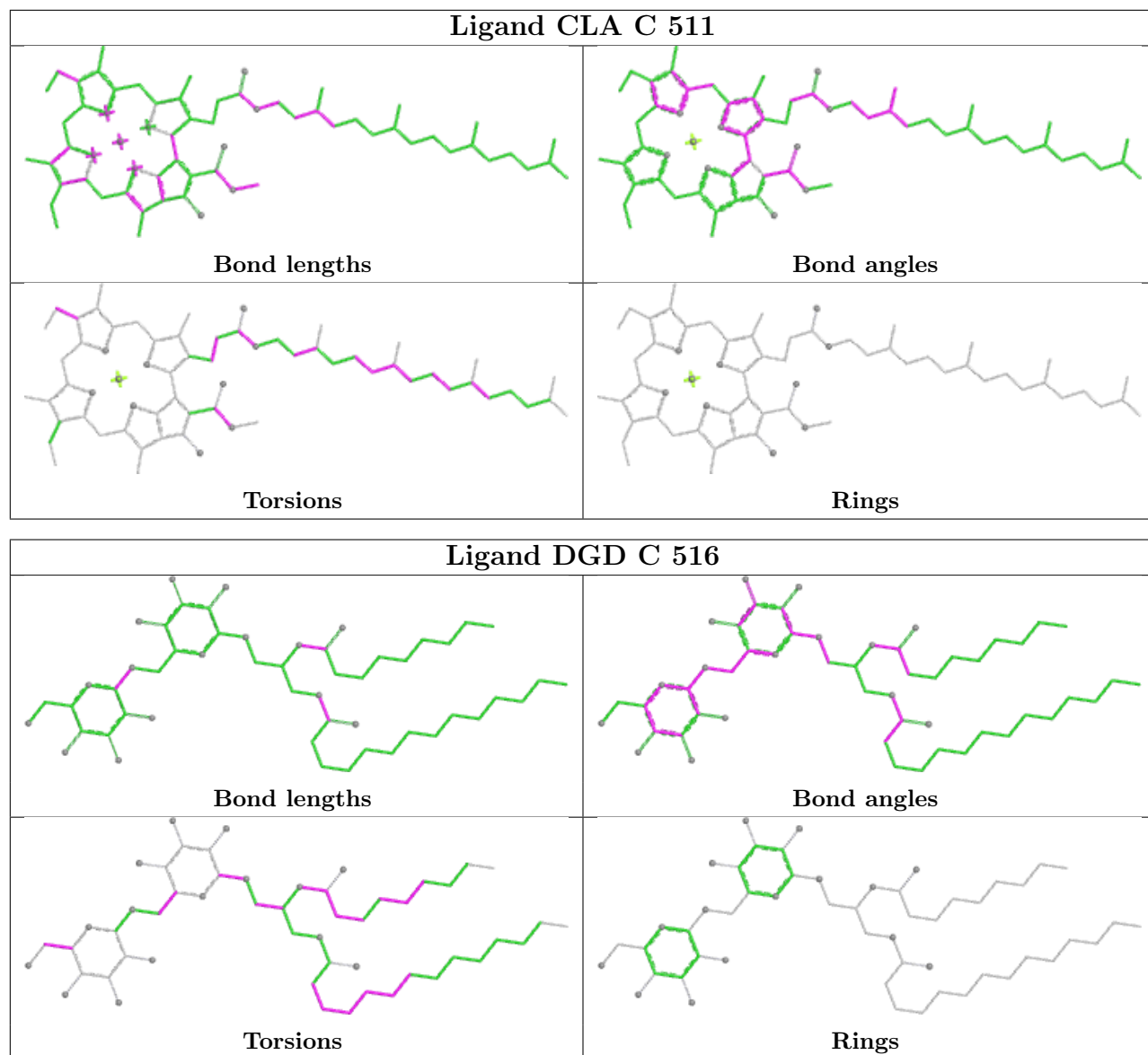


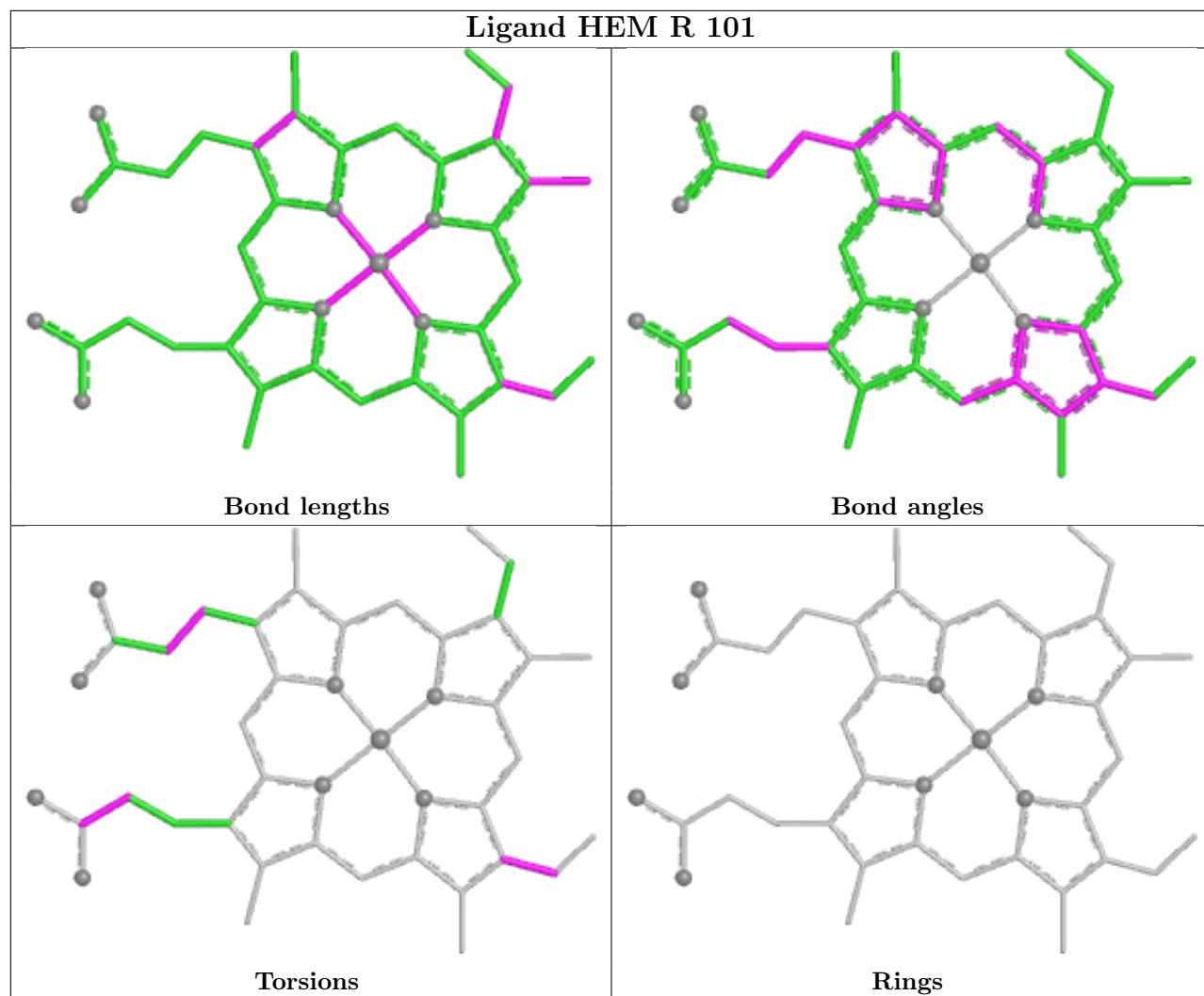


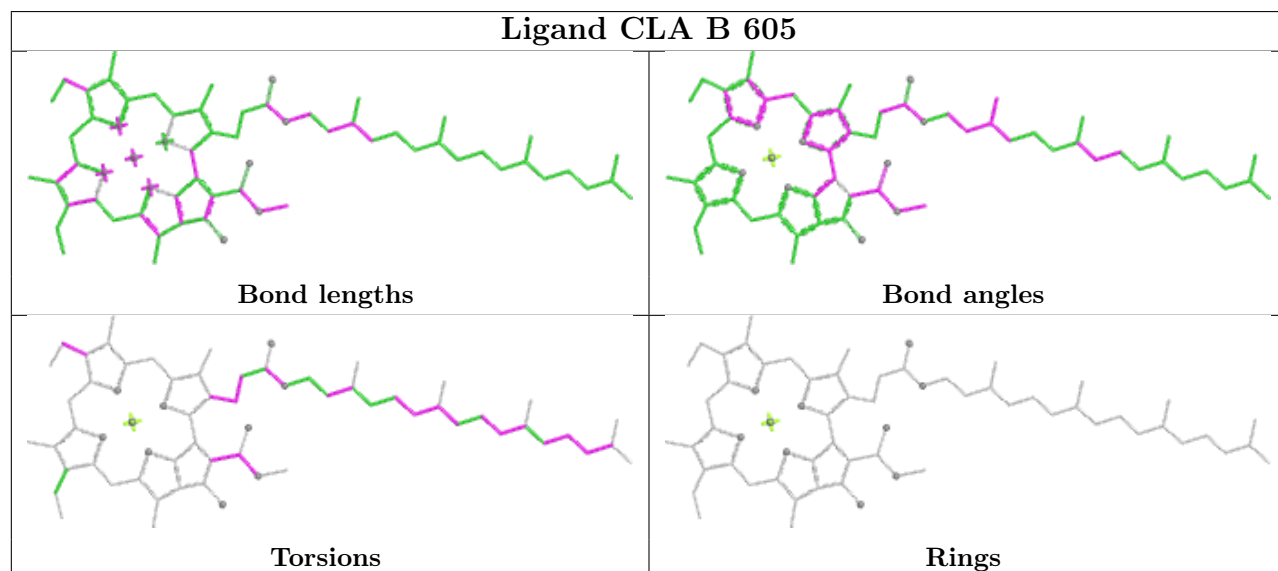
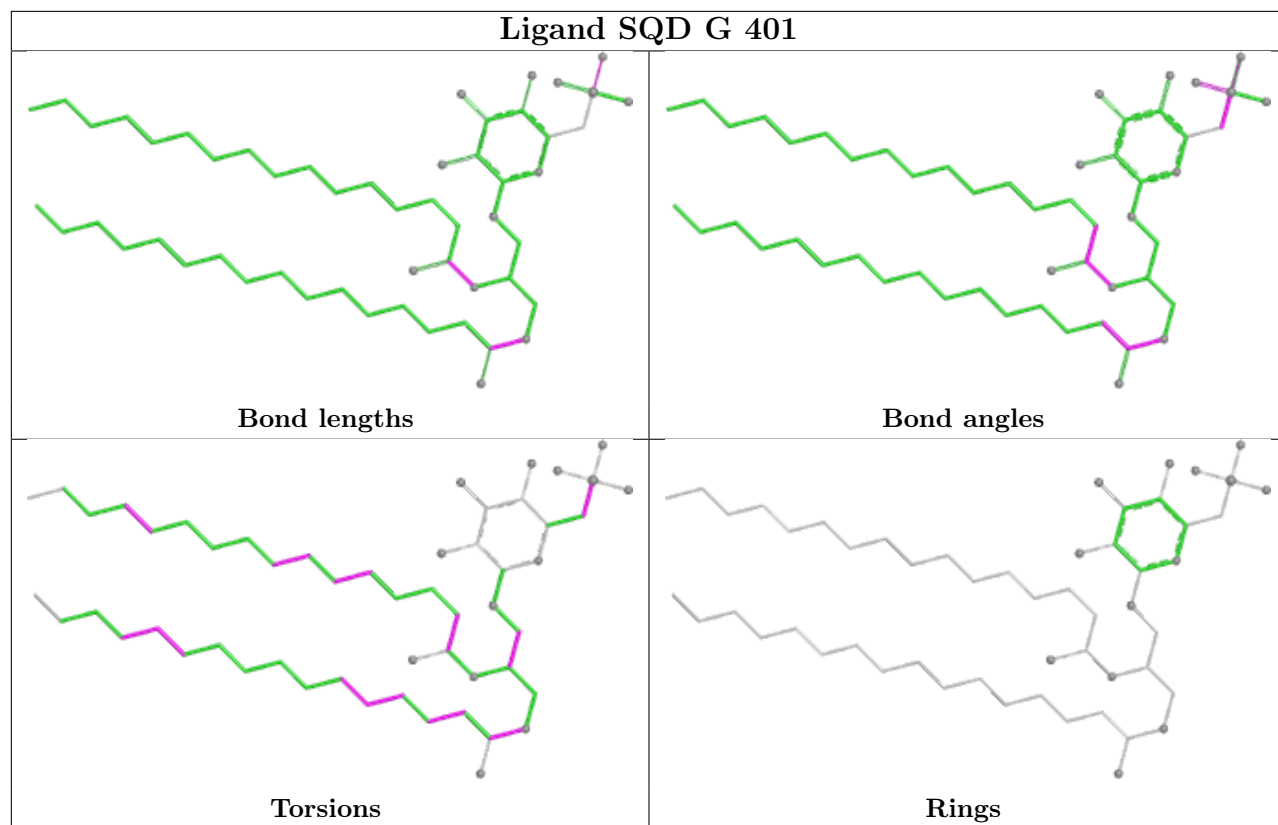


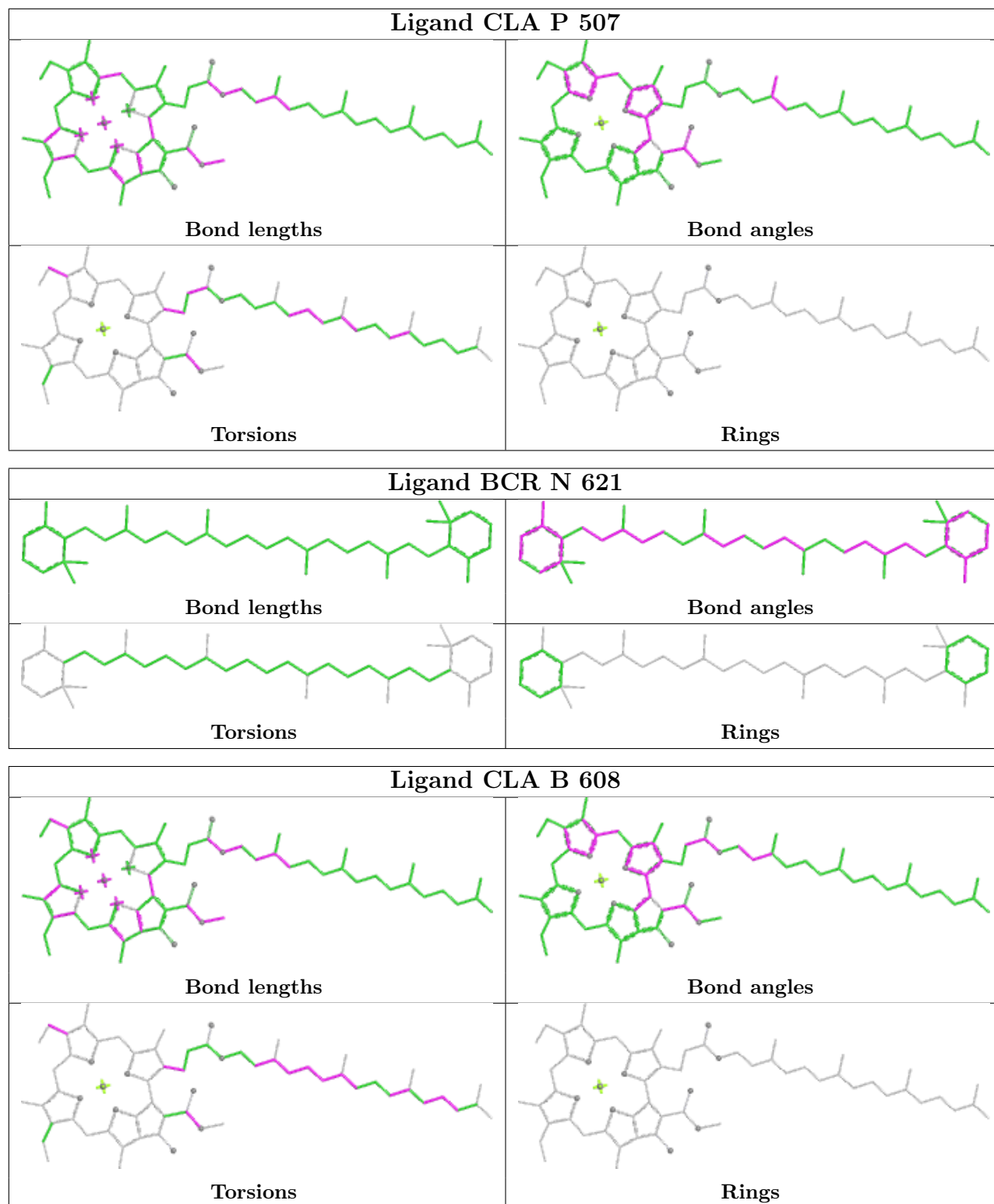


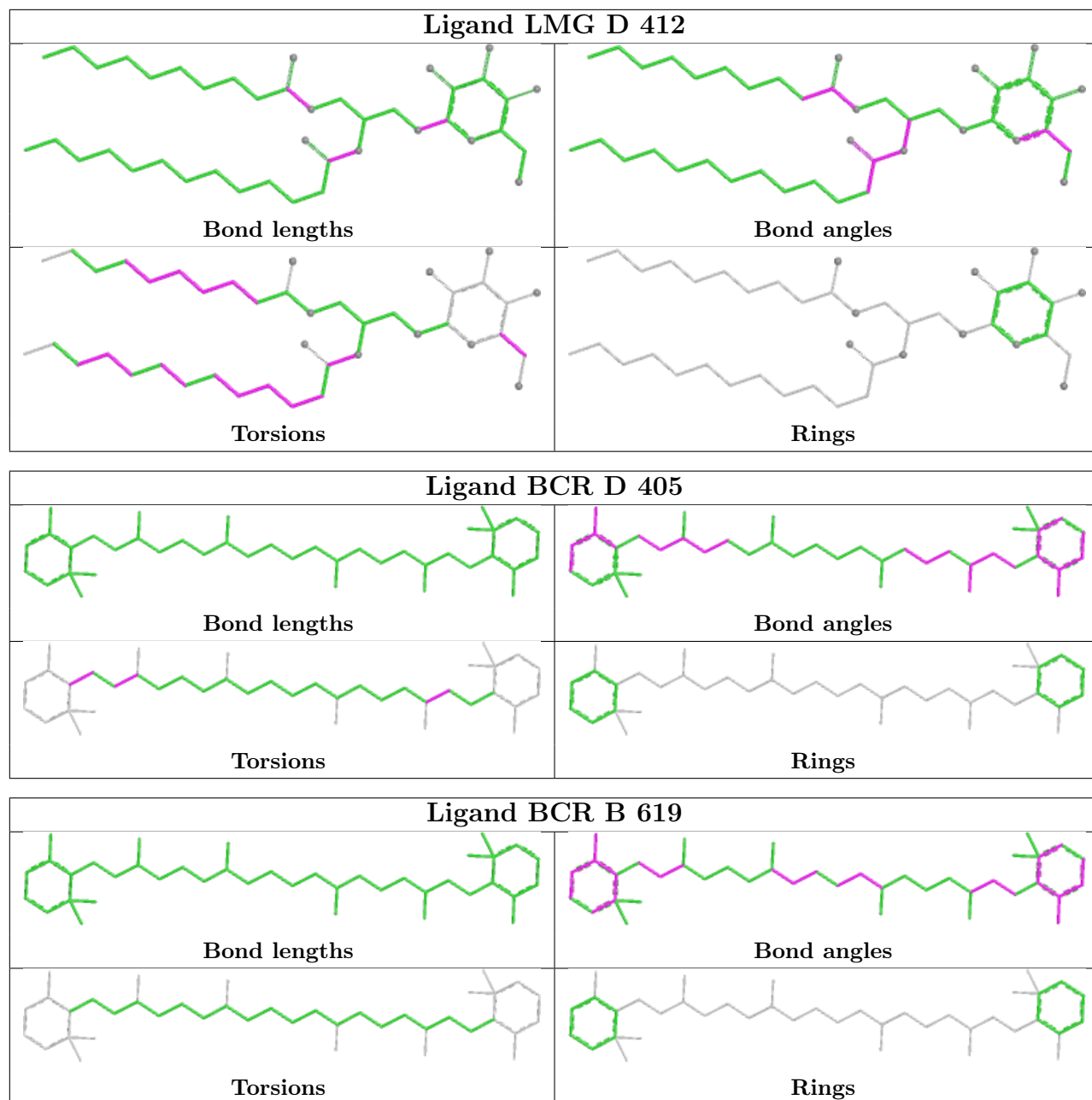


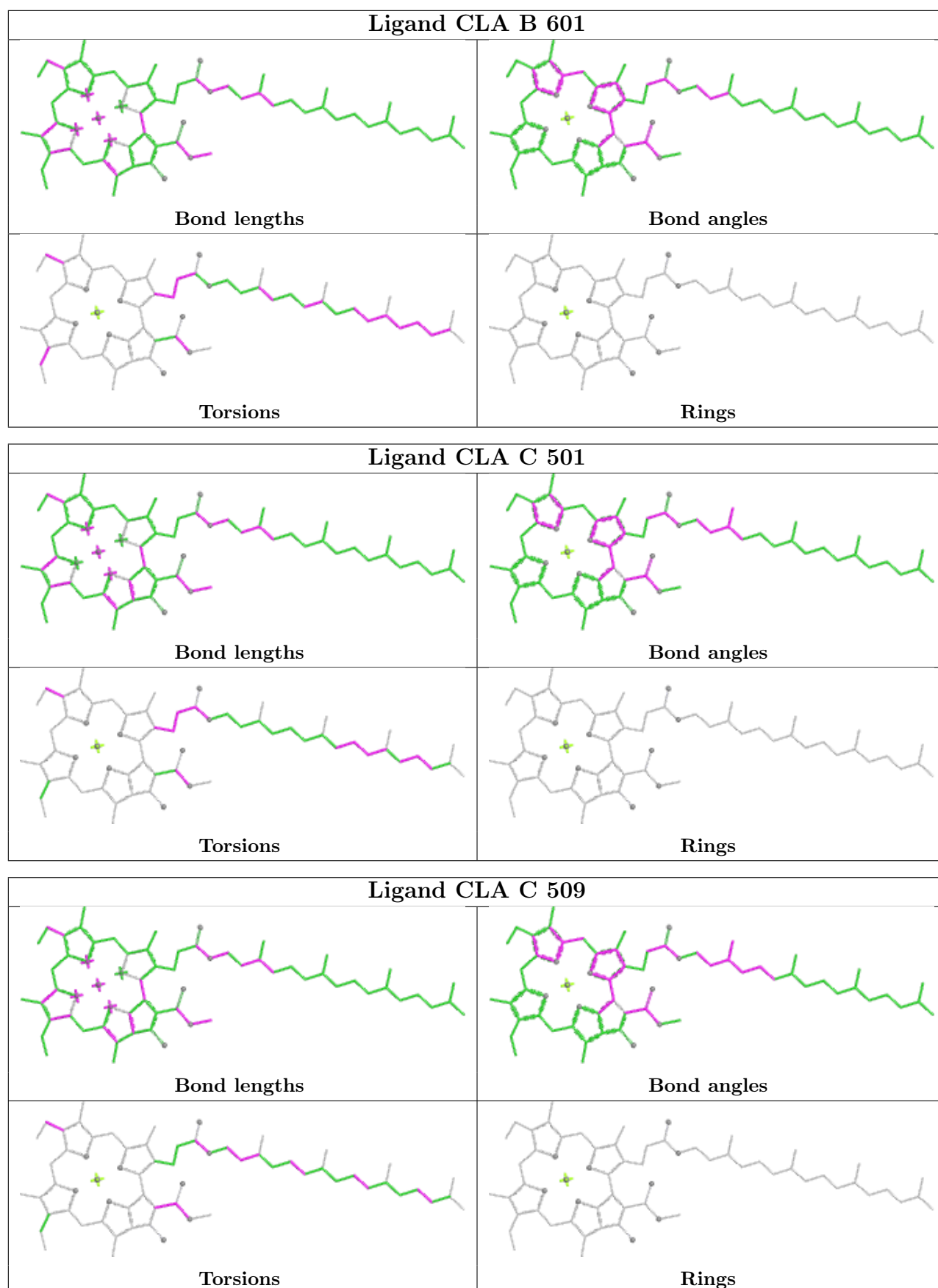


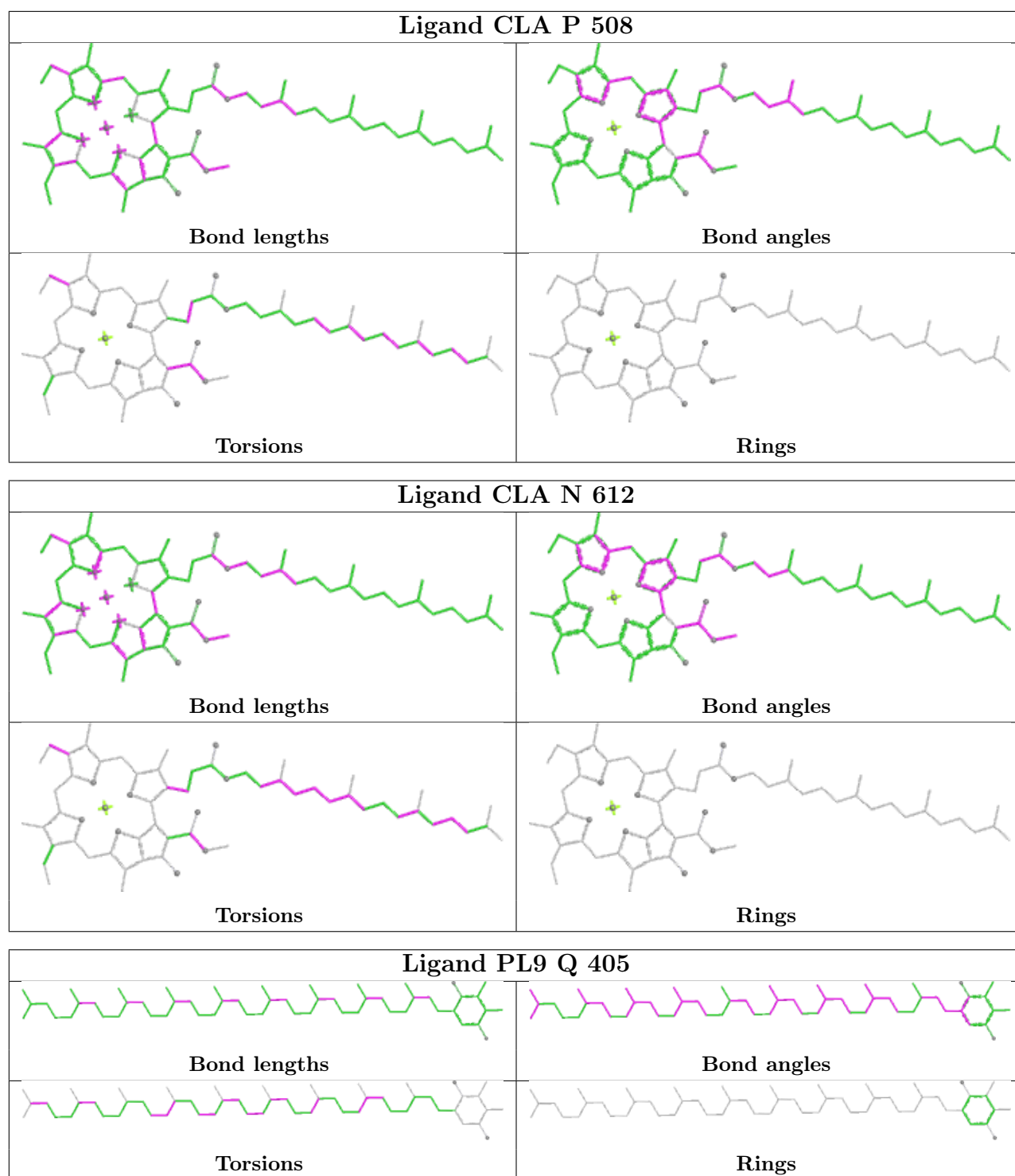


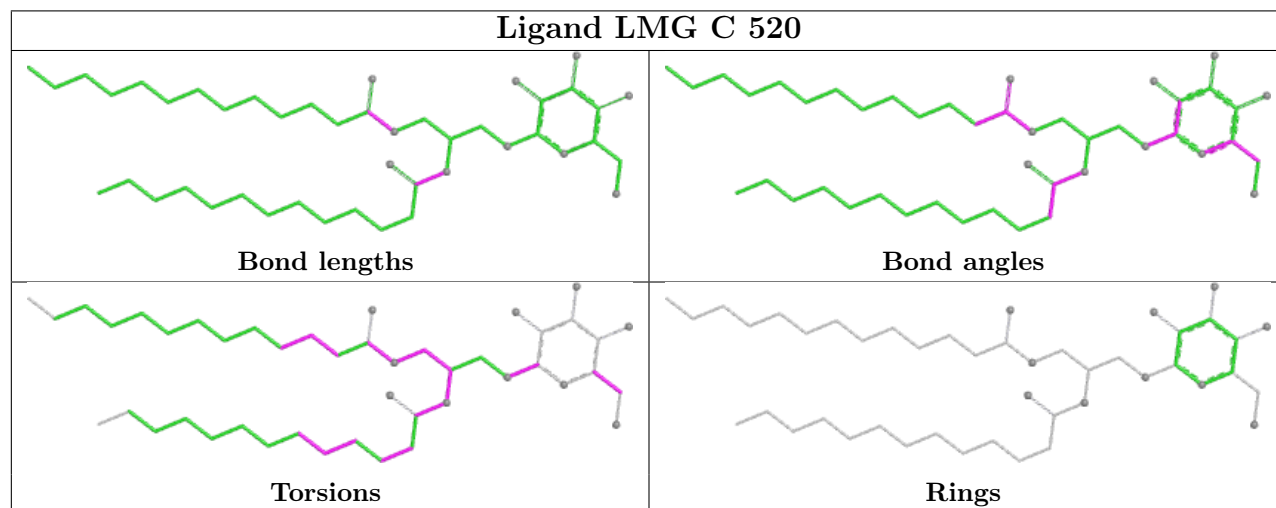
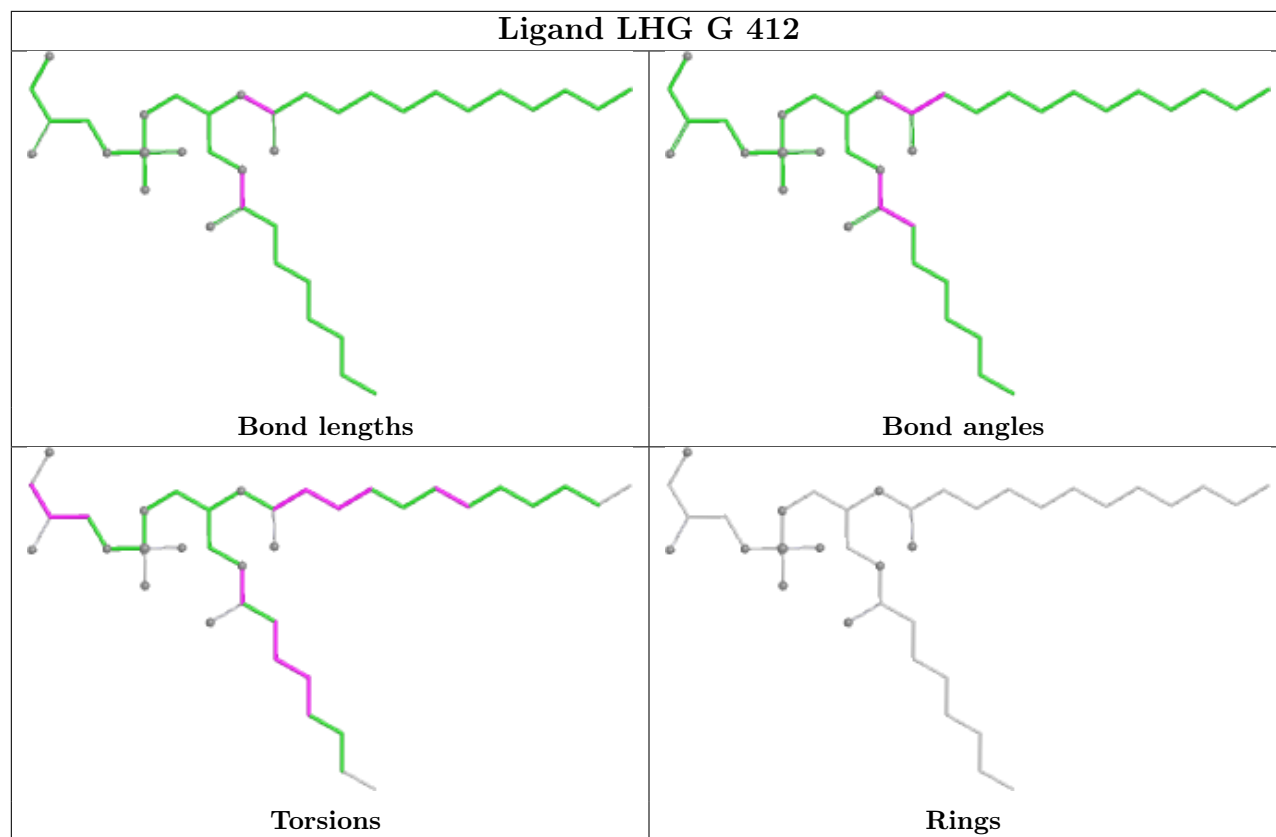


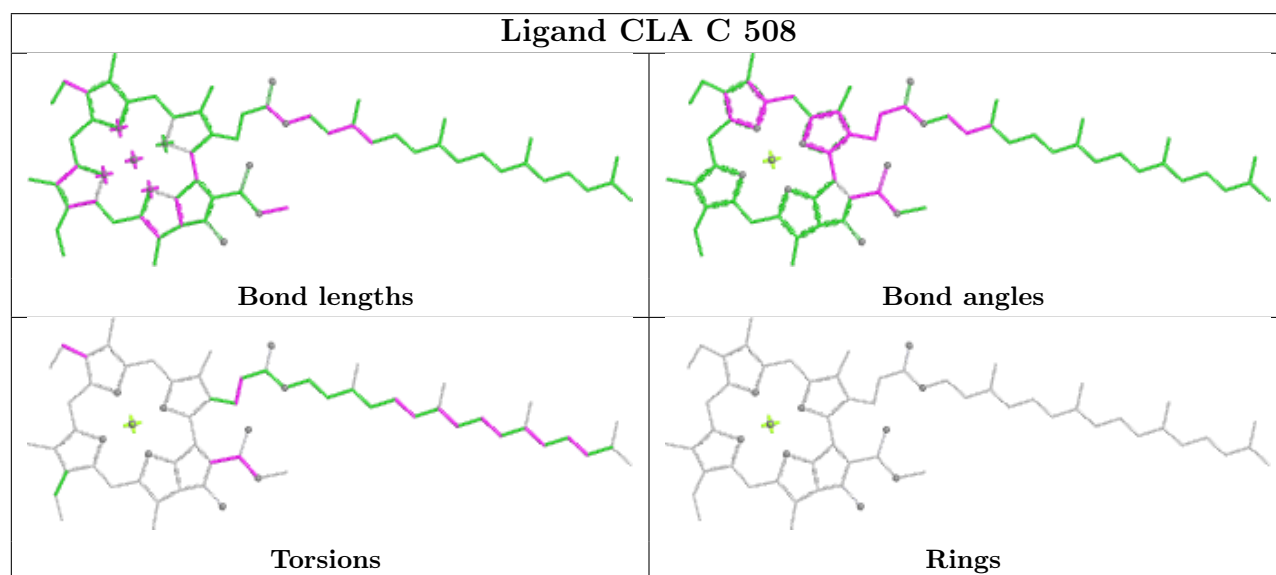
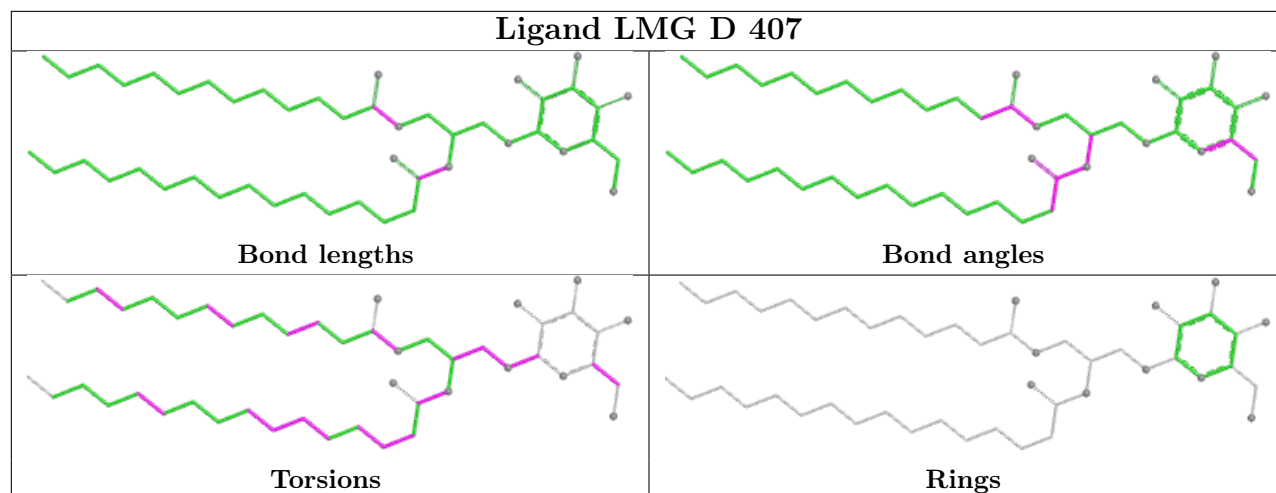


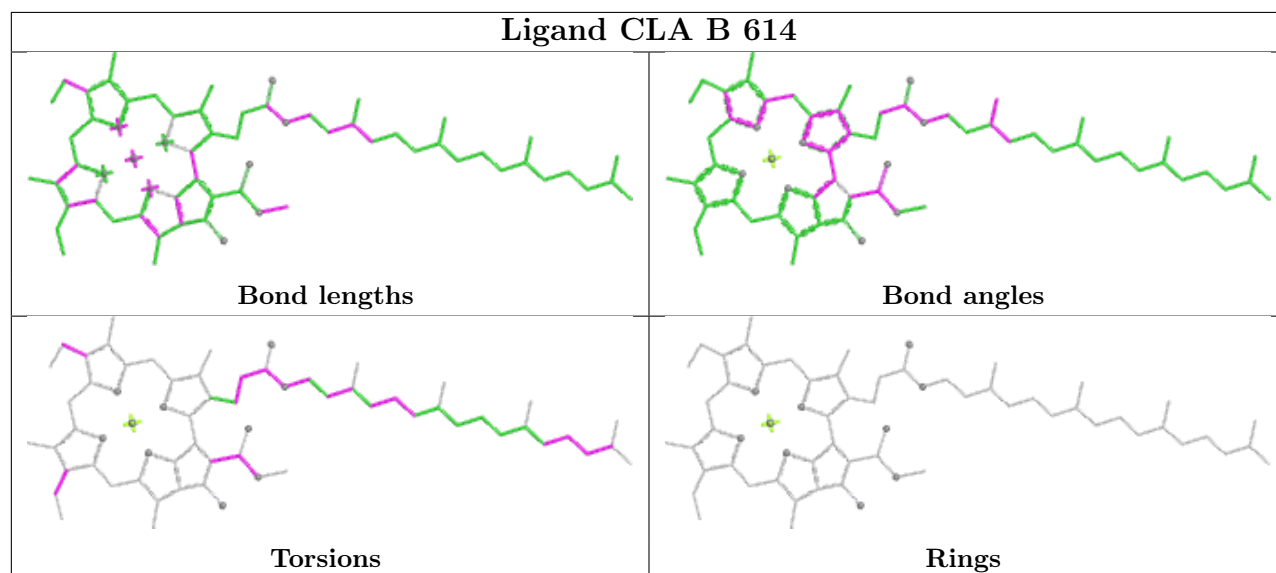
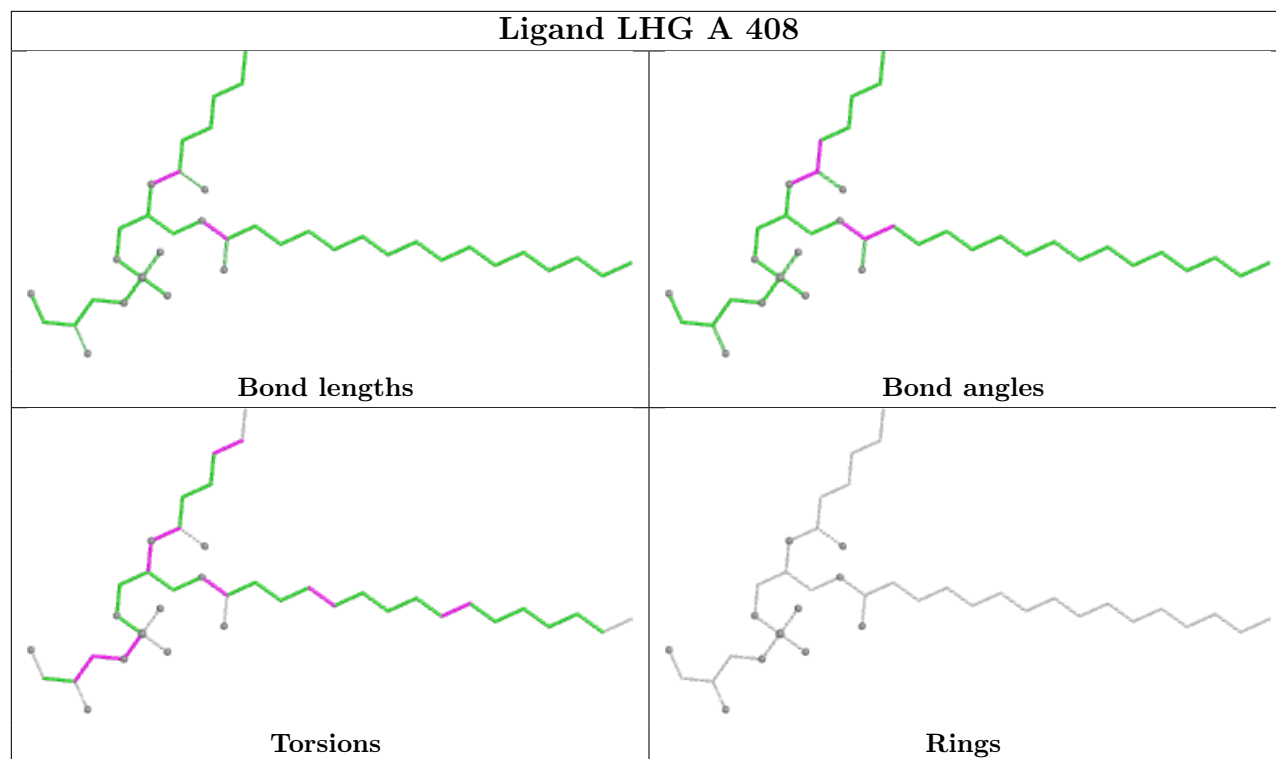


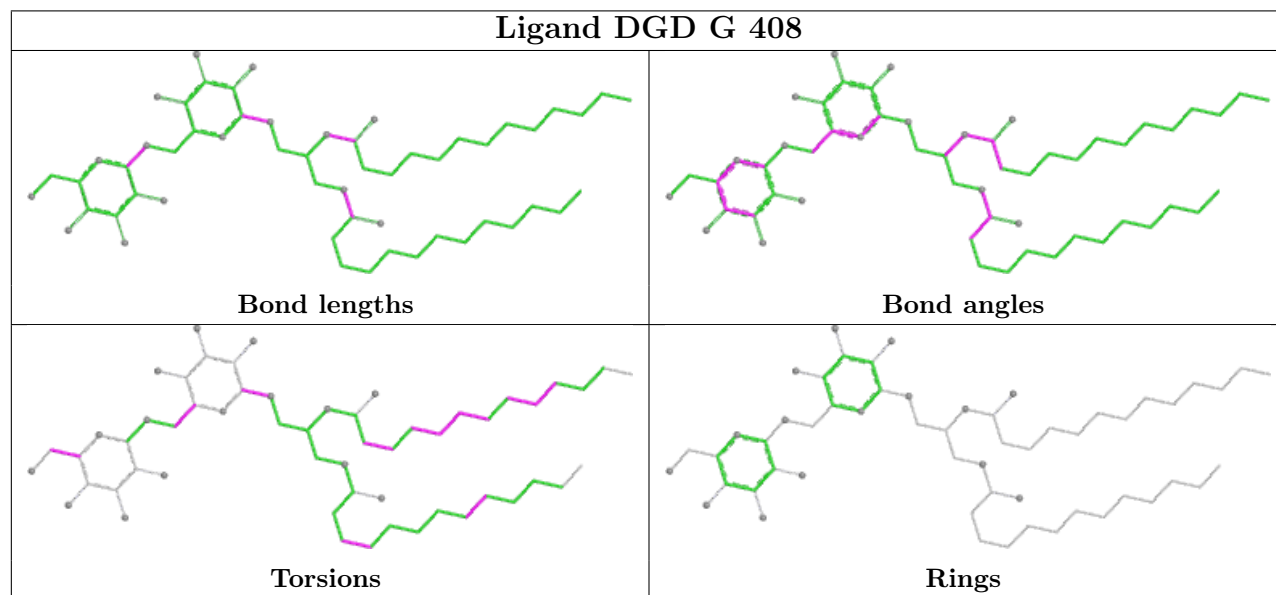
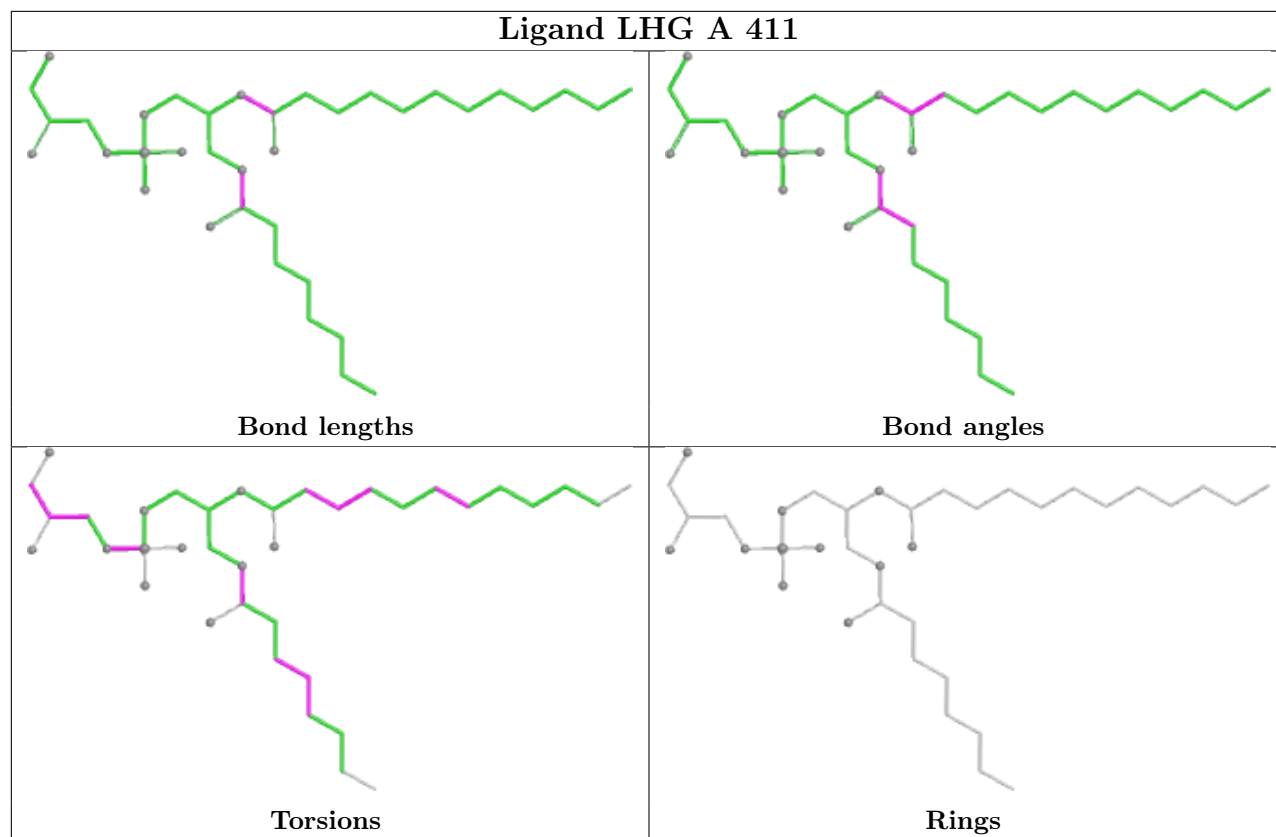


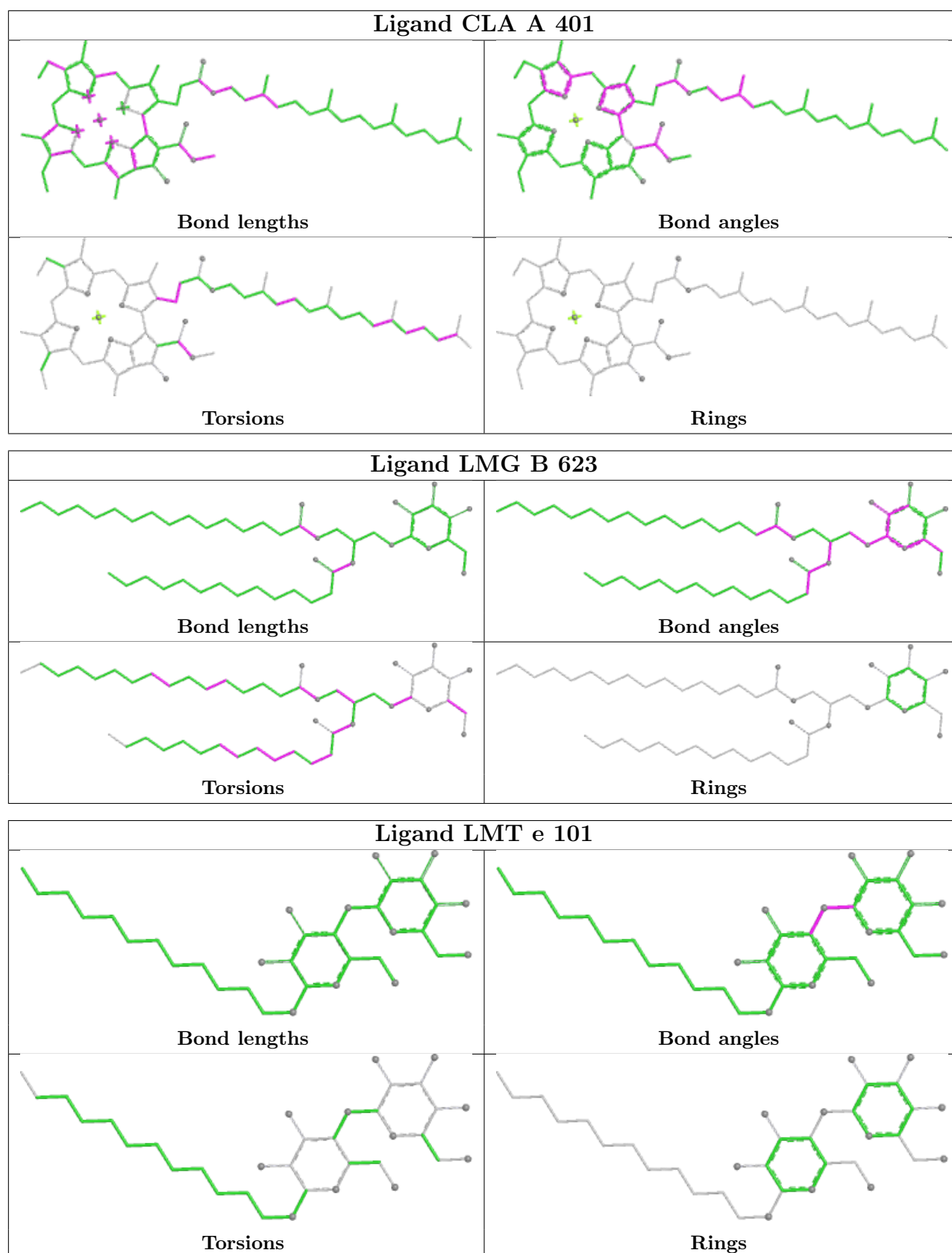


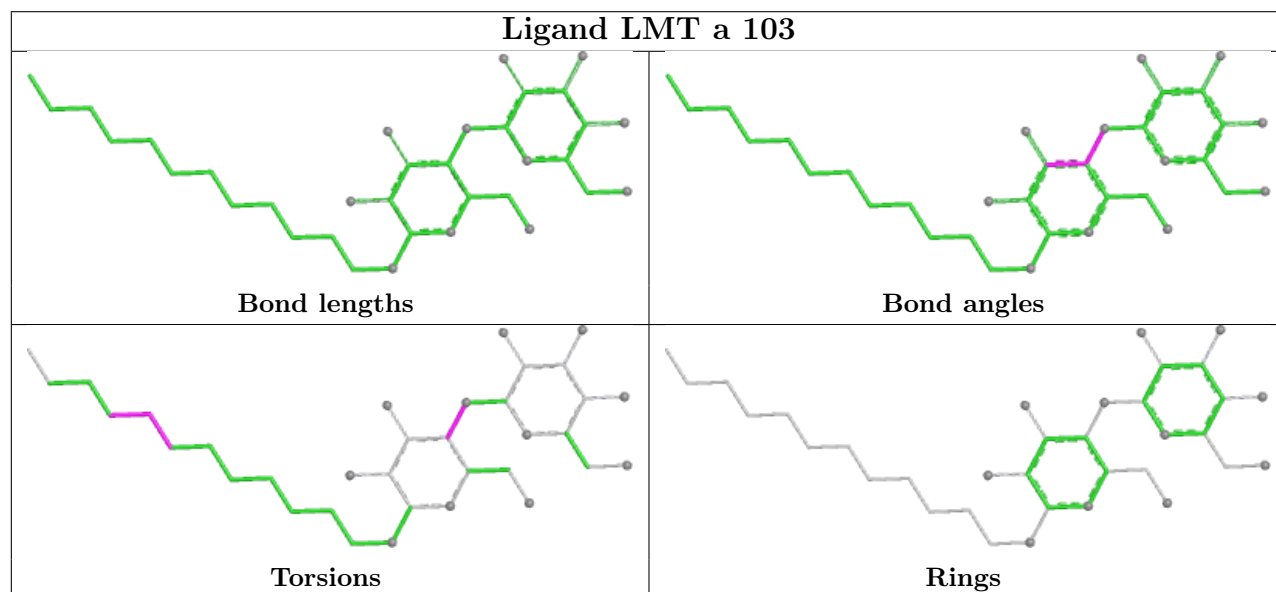
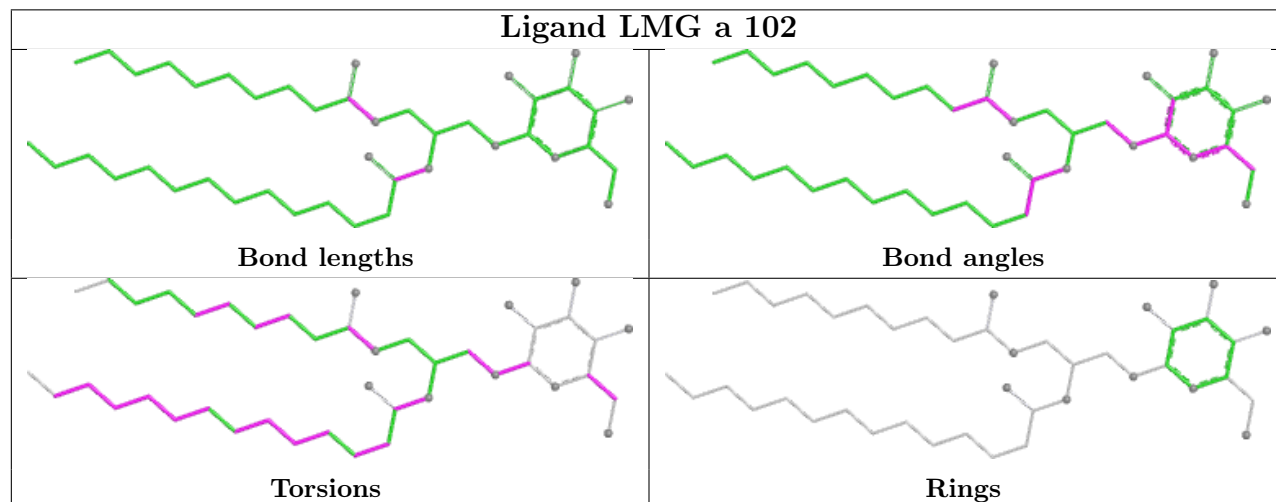
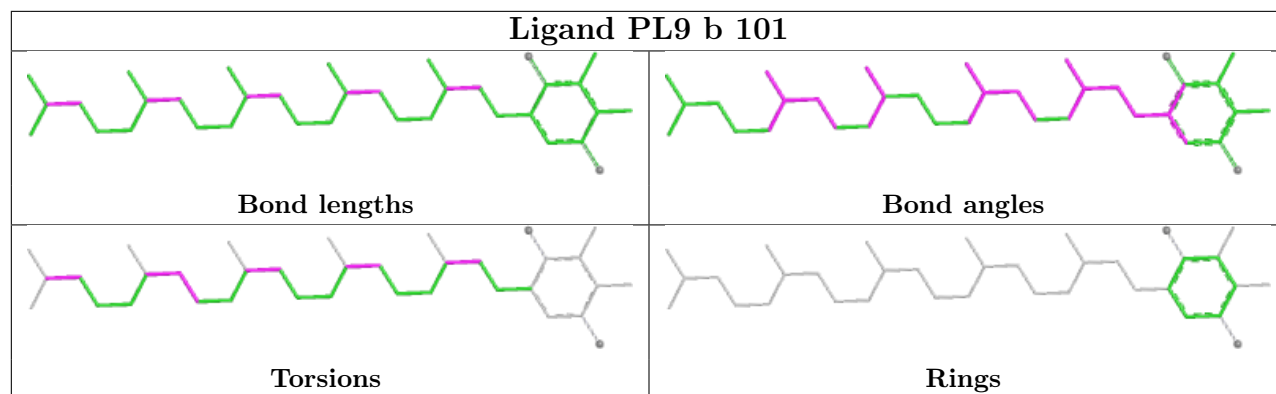


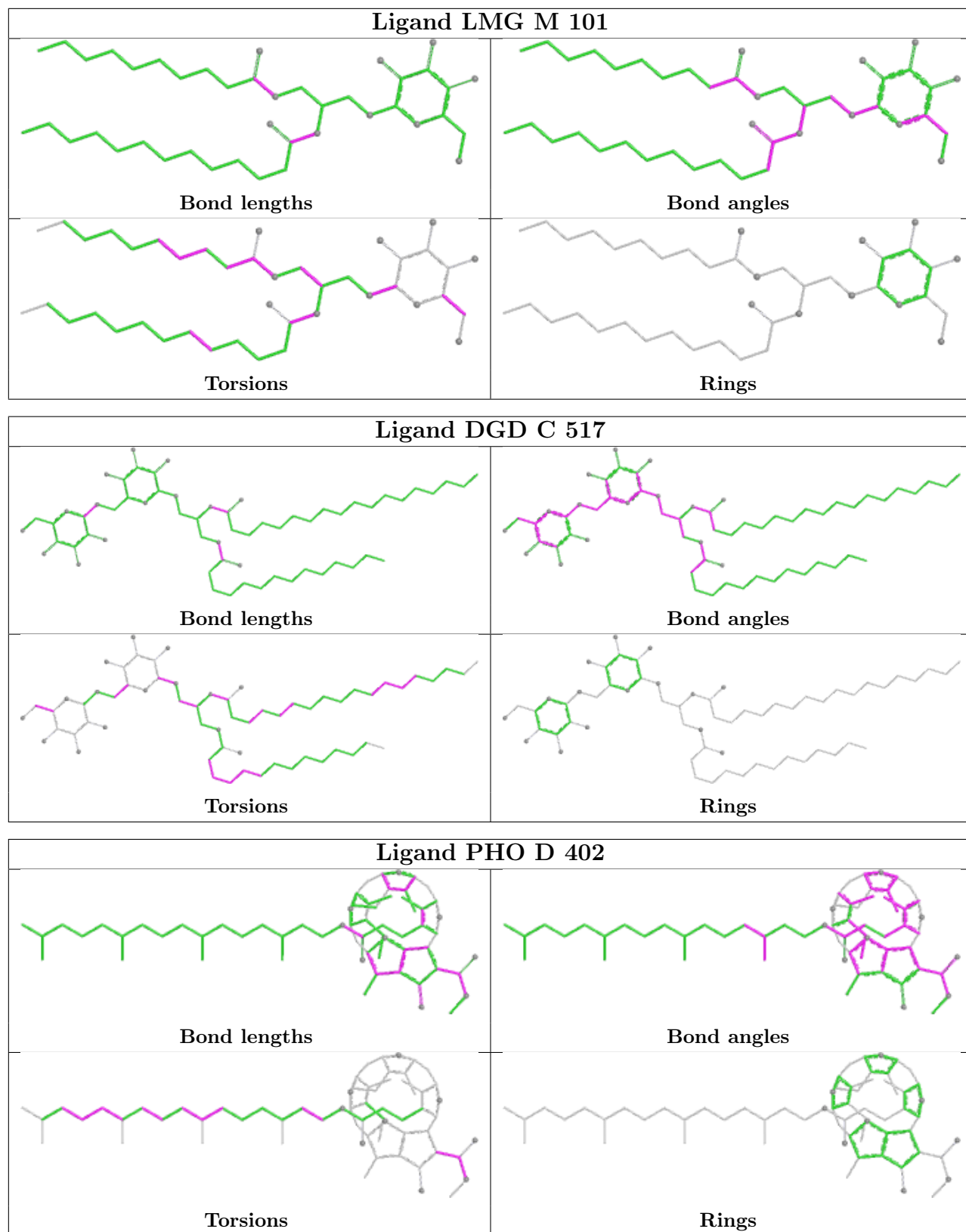


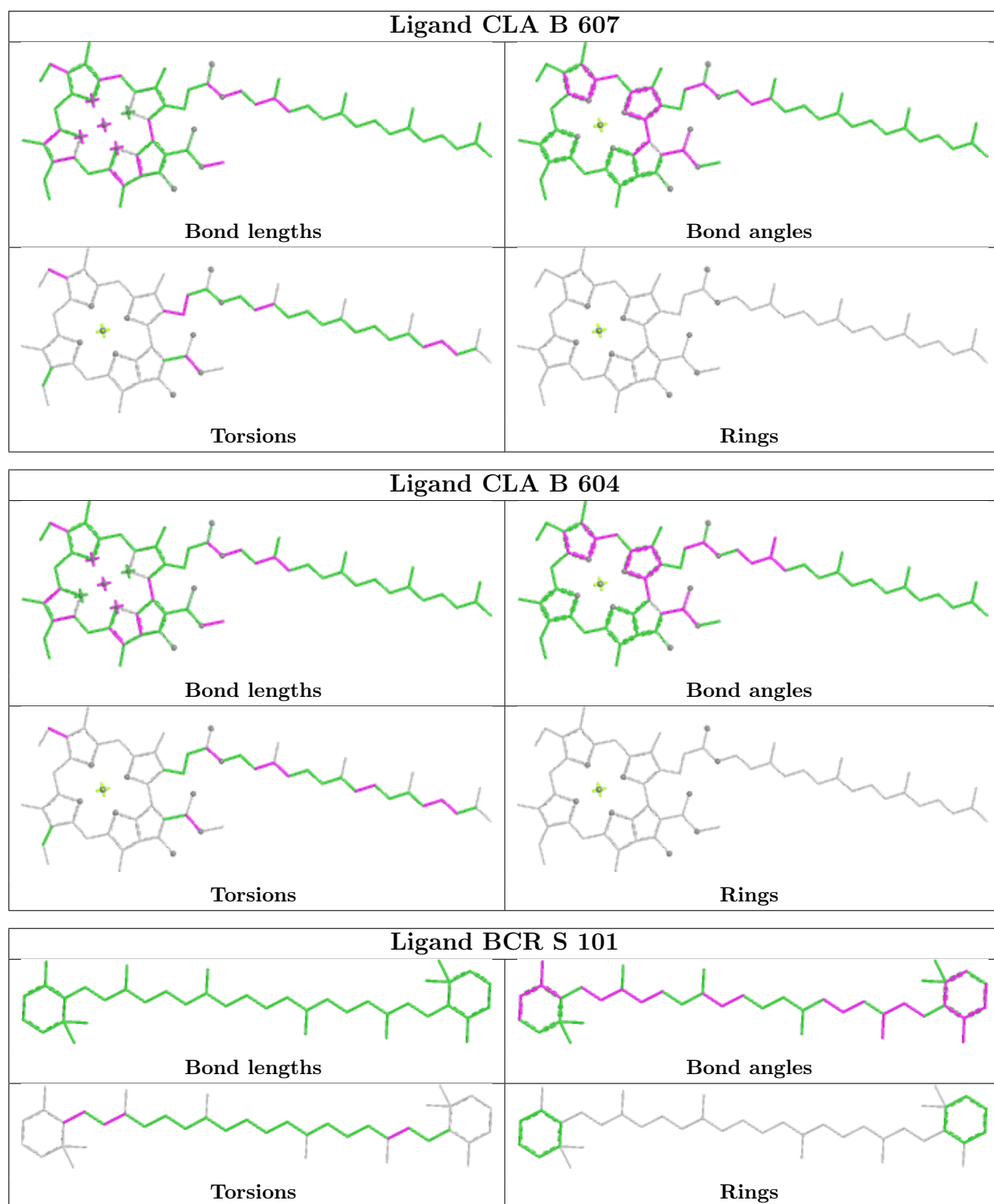


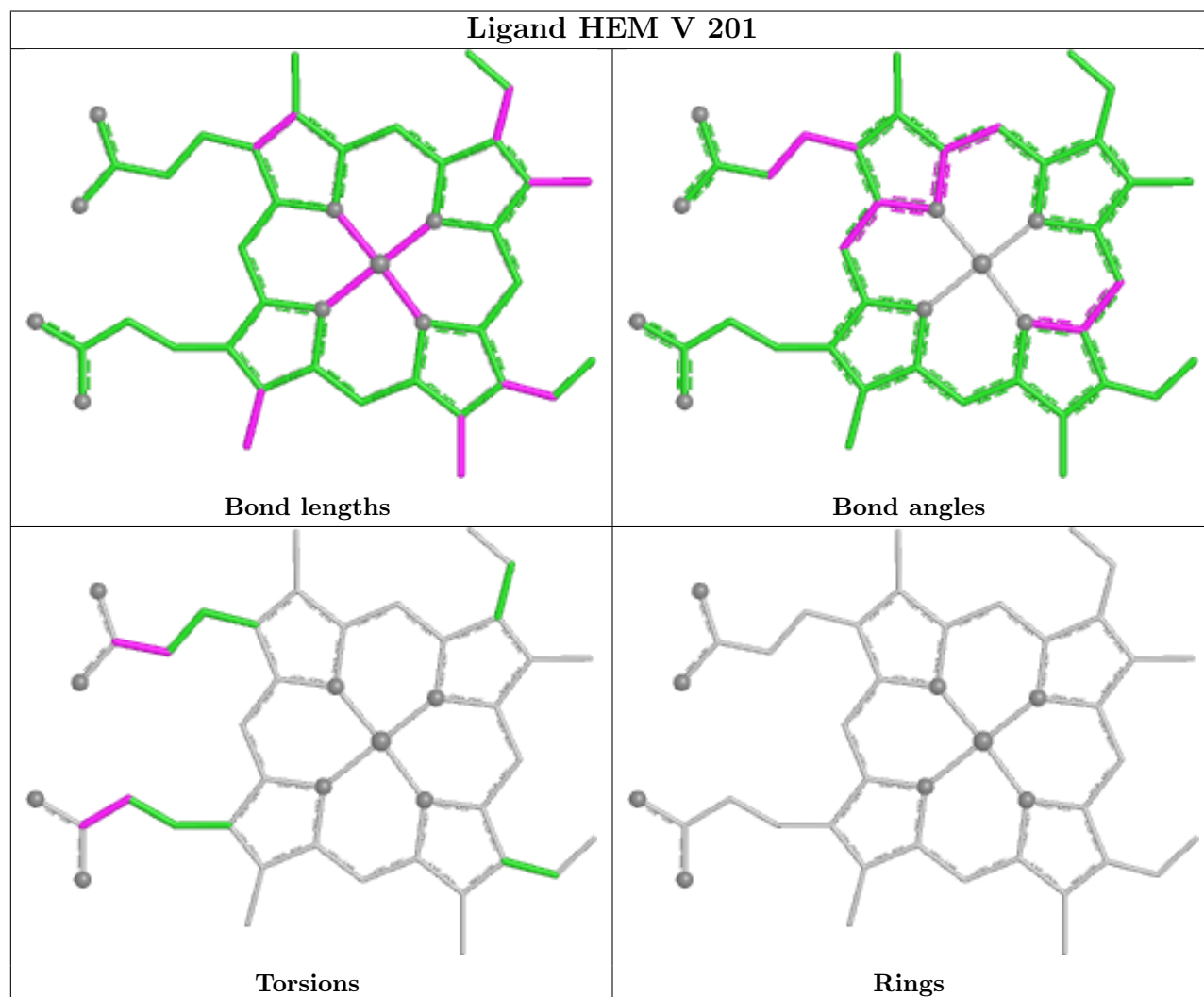
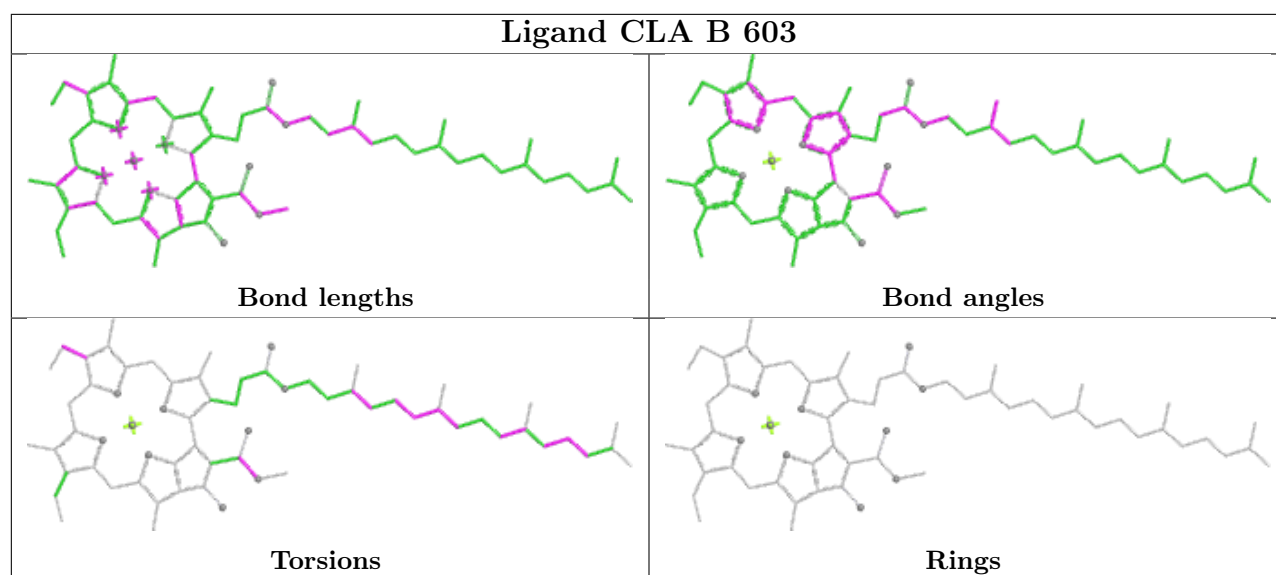


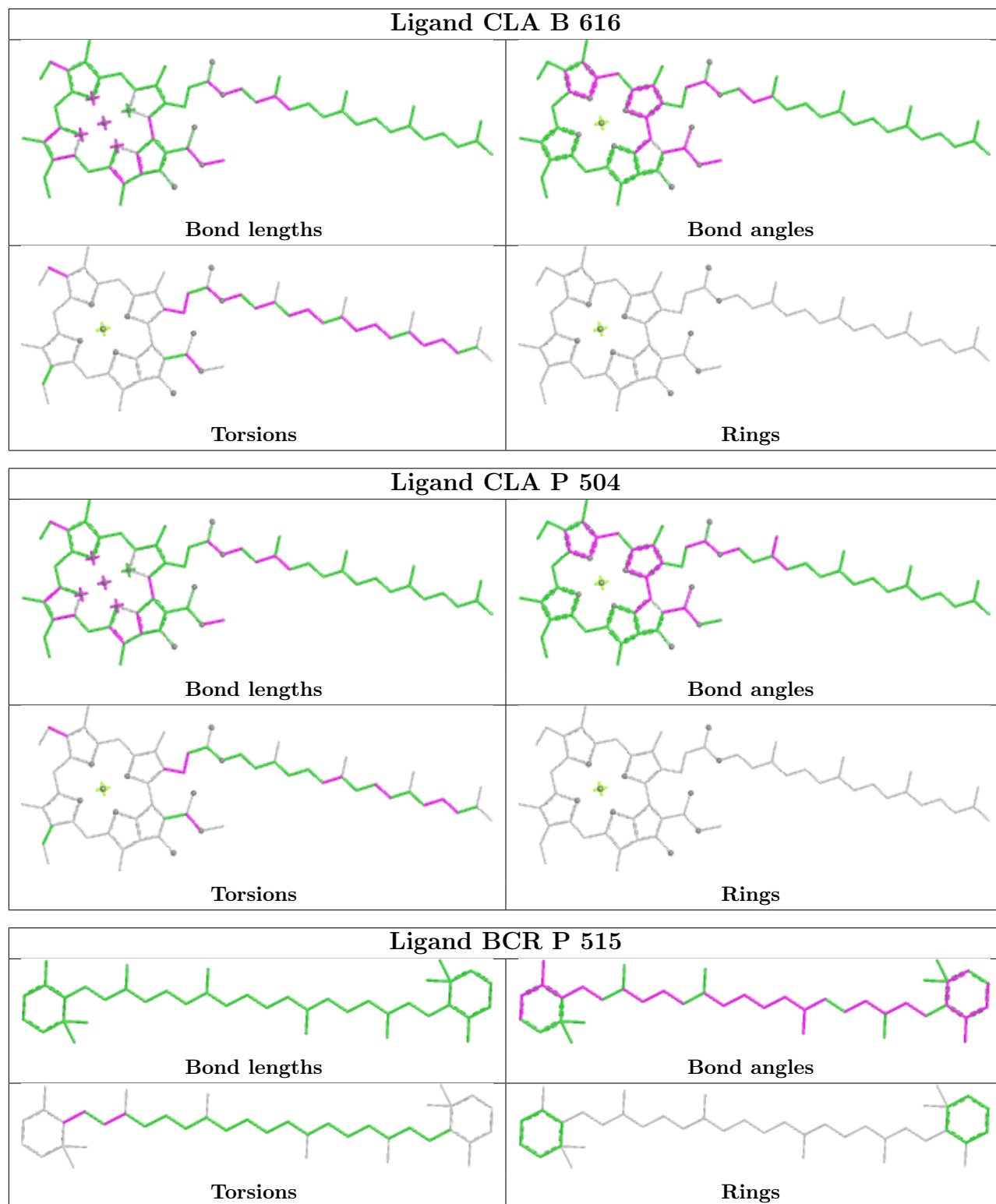


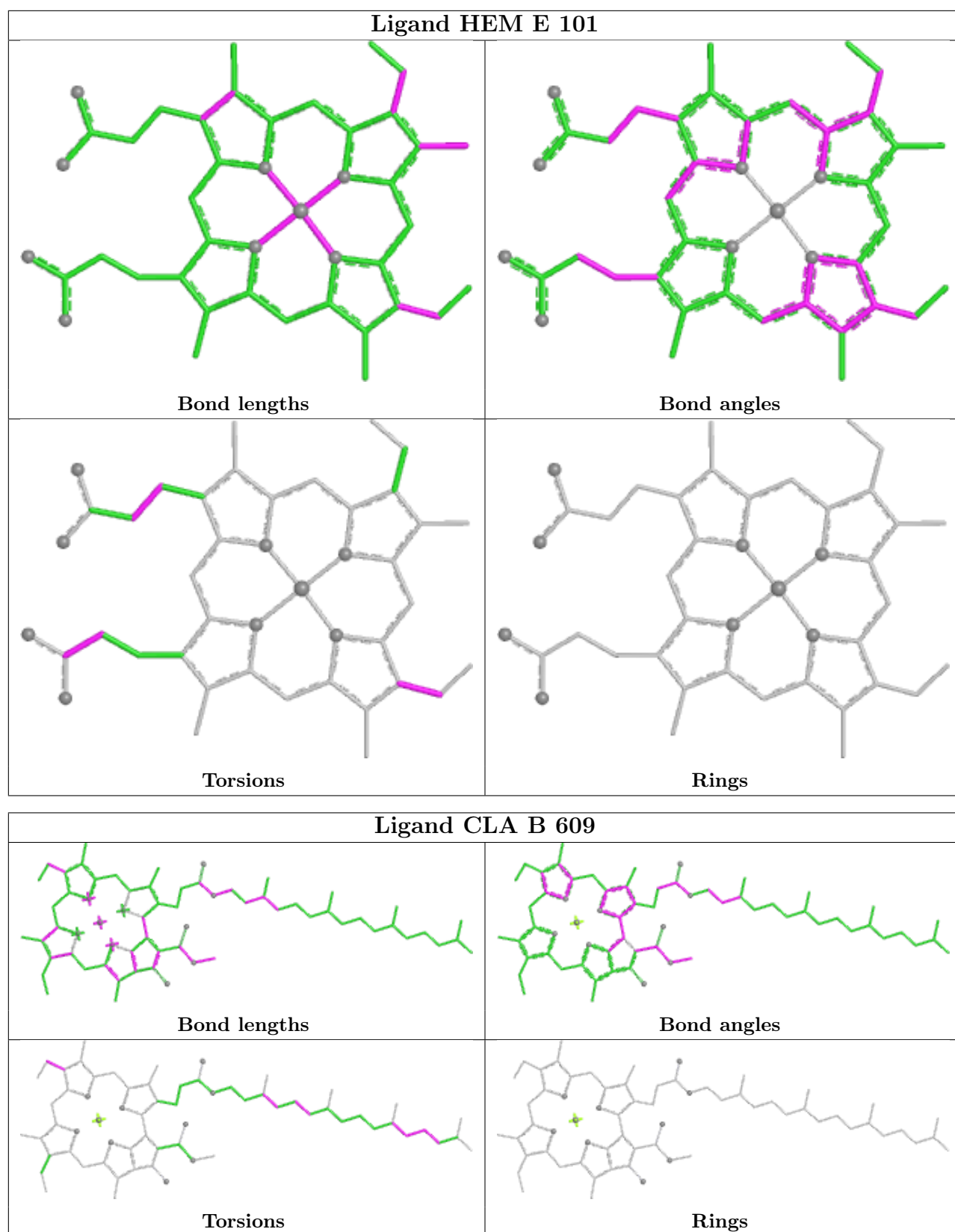


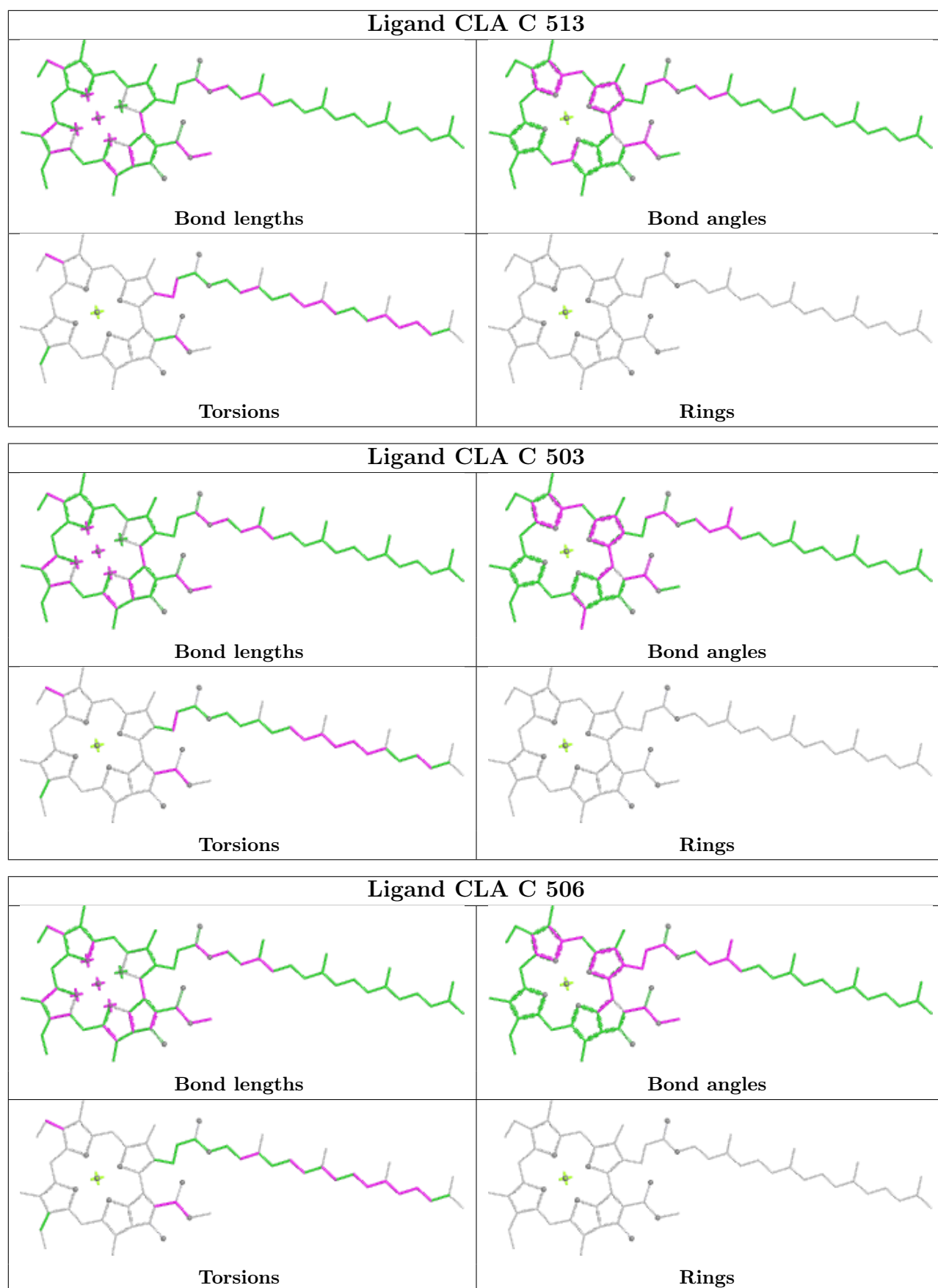


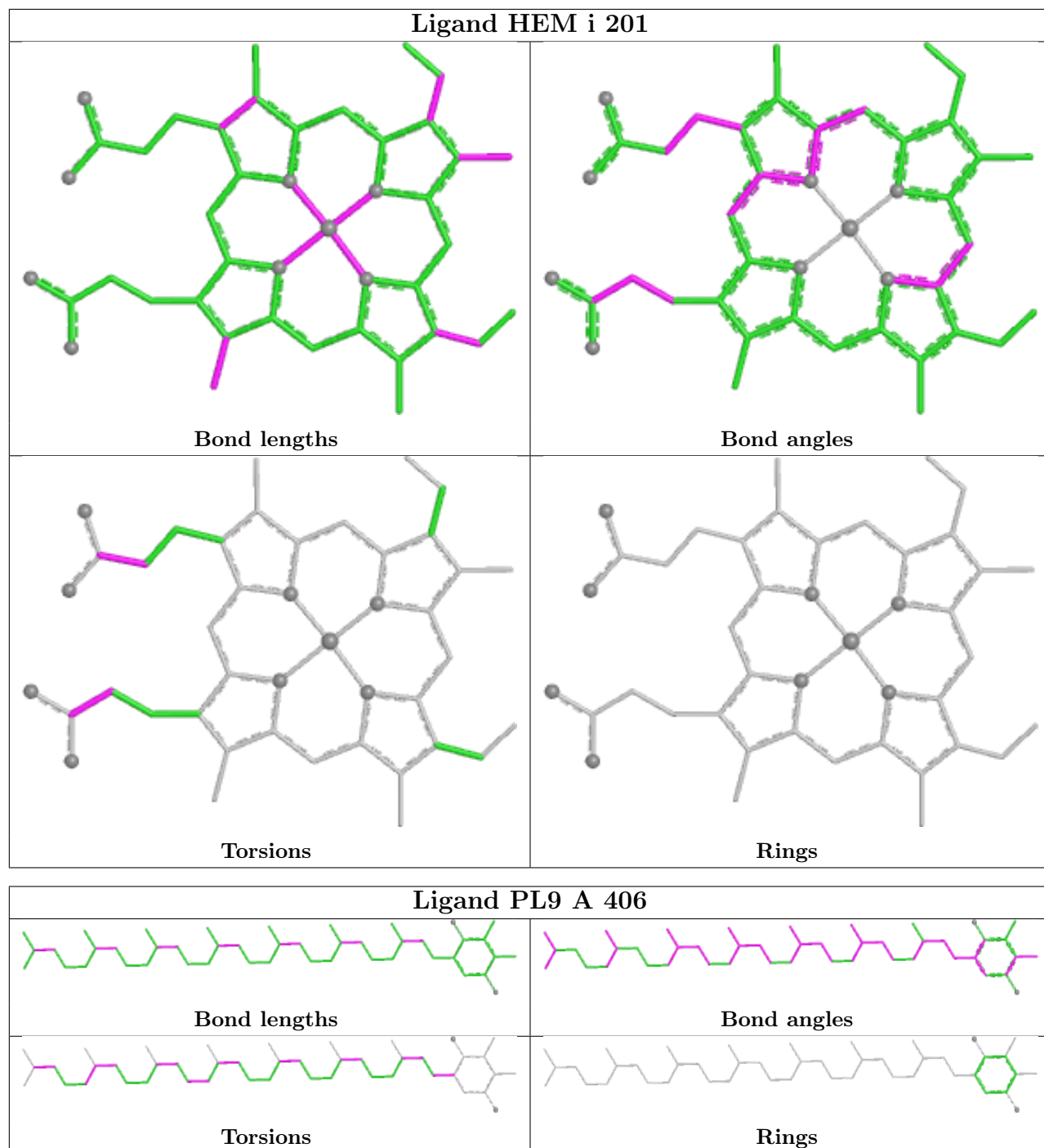


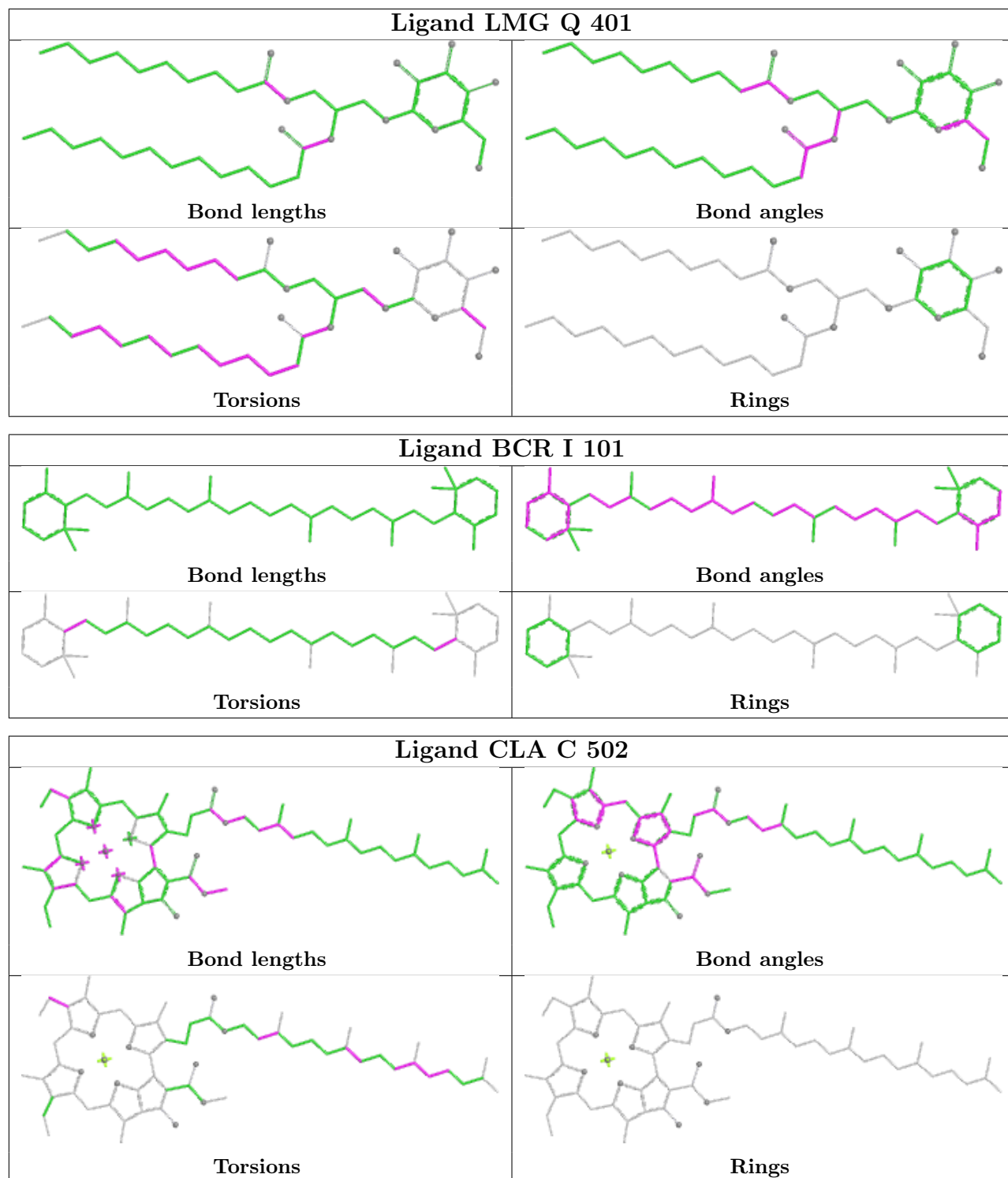


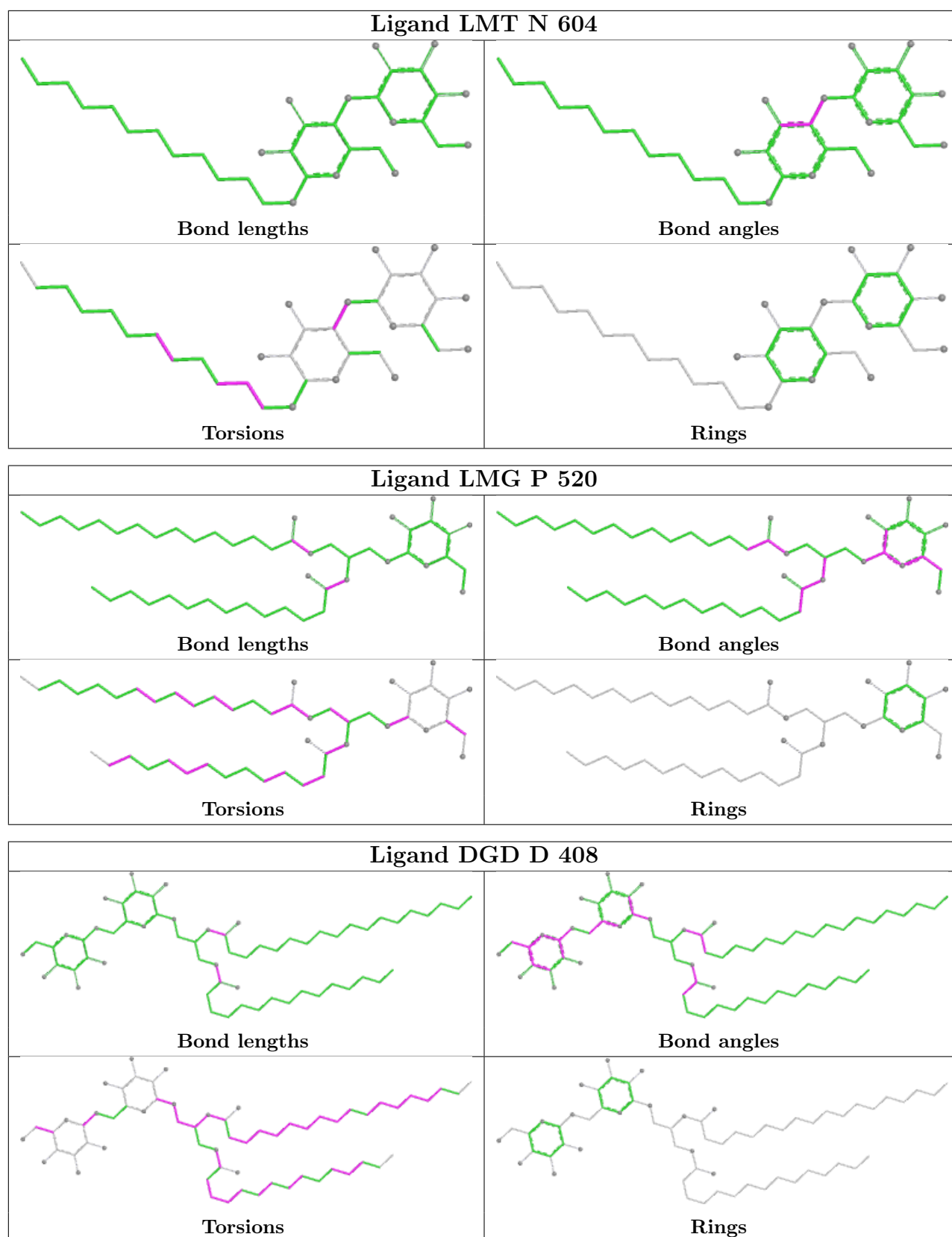


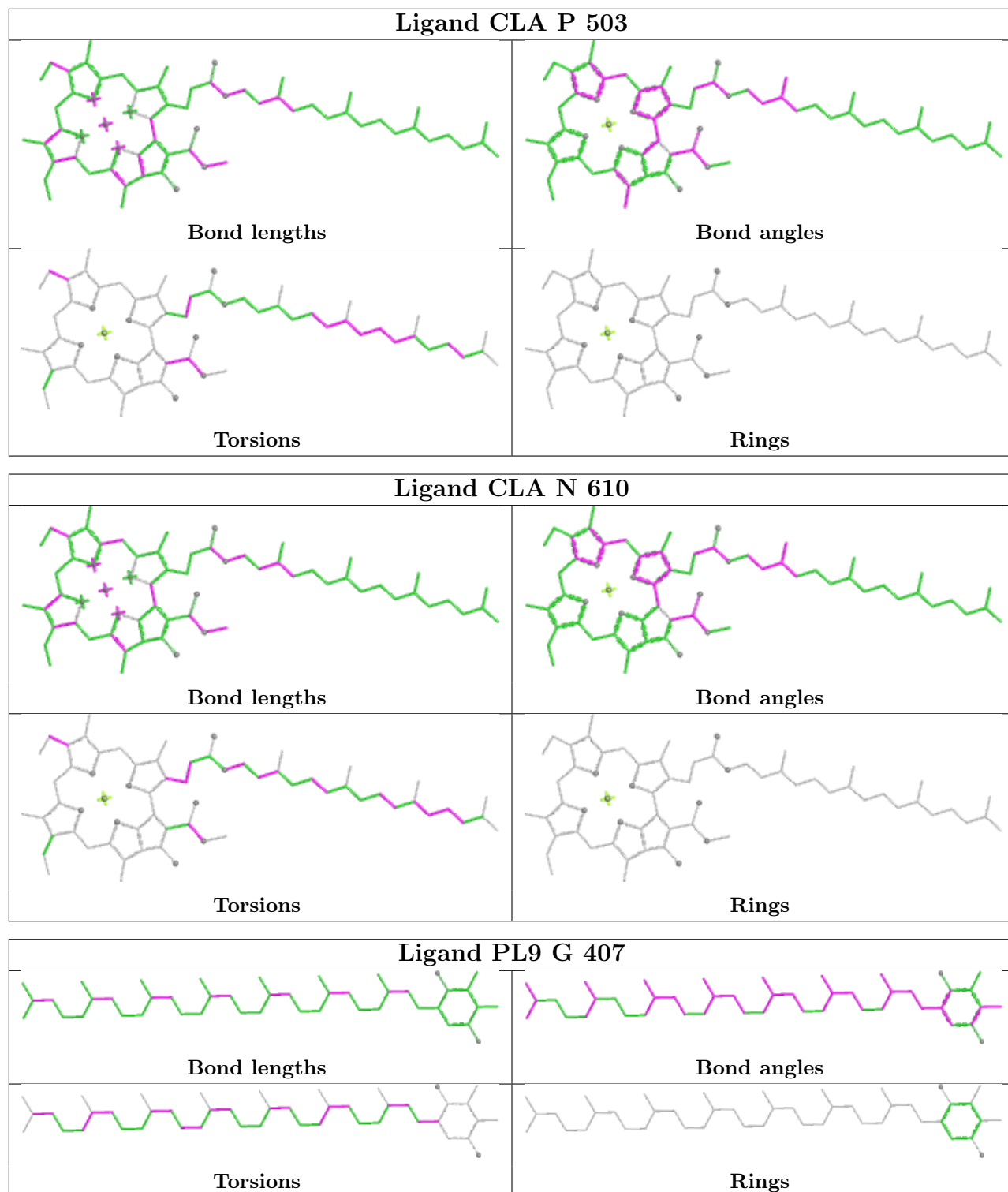


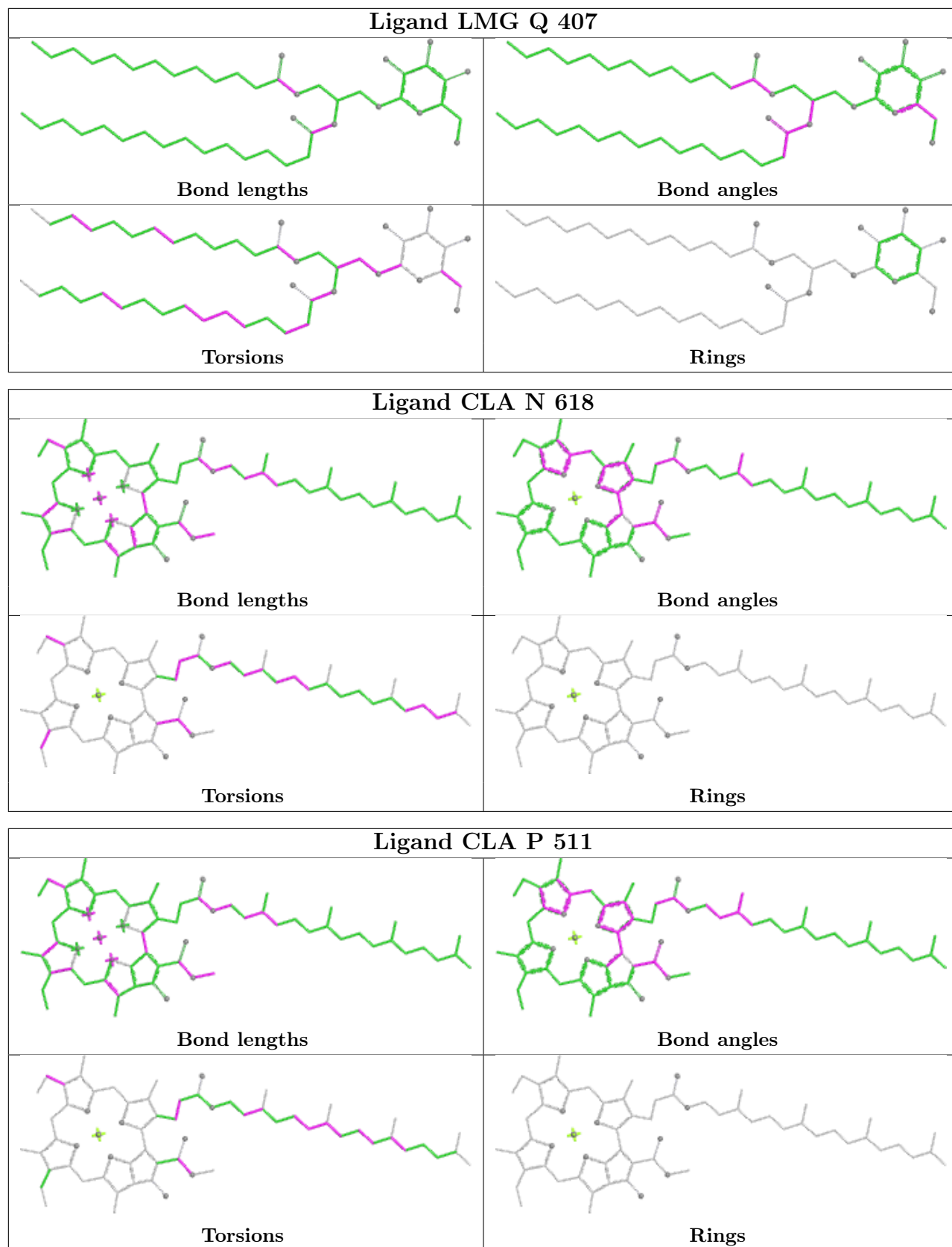


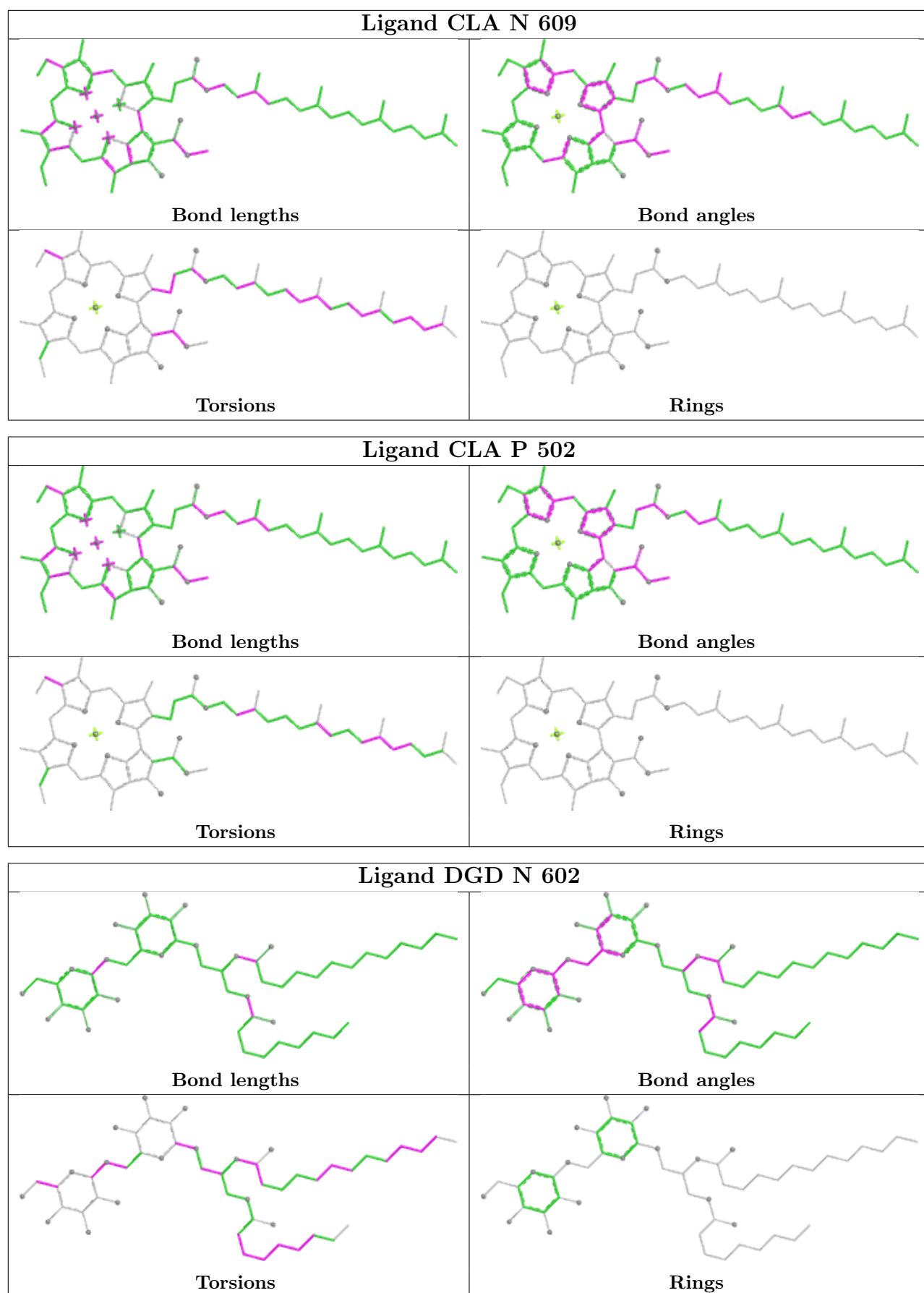


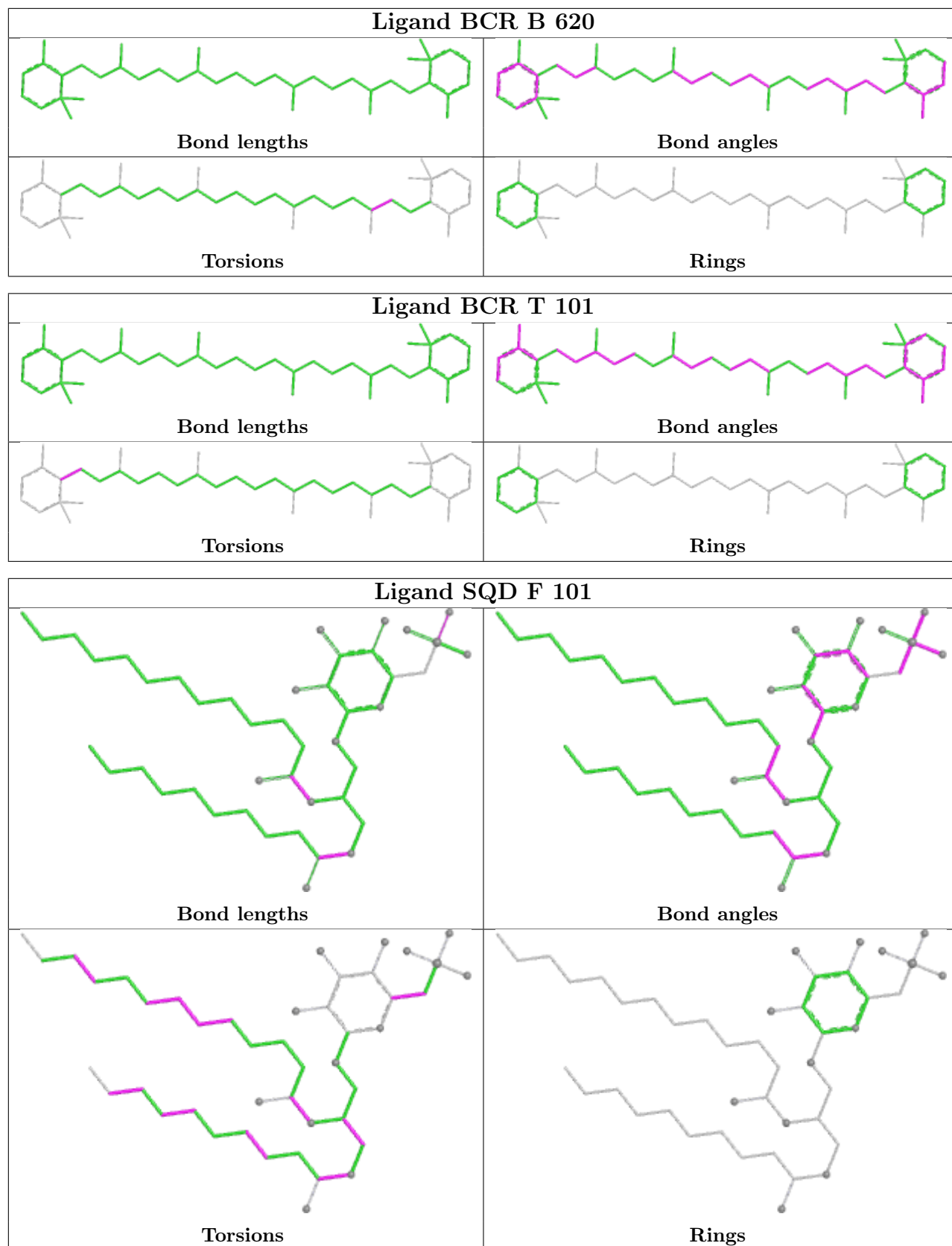












## 5.7 Other polymers [i](#)

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%)	-0.17	3 (0%) 81 70	131, 152, 182, 204	0
1	G	335/344 (97%)	0.06	15 (4%) 38 38	128, 156, 184, 213	0
2	B	490/510 (96%)	-0.17	11 (2%) 62 53	128, 158, 178, 195	0
2	N	490/510 (96%)	-0.07	13 (2%) 56 48	129, 160, 180, 207	0
3	C	447/461 (96%)	-0.14	6 (1%) 75 64	129, 164, 183, 211	0
3	P	447/461 (96%)	-0.07	5 (1%) 78 66	139, 165, 183, 197	0
4	D	340/352 (96%)	-0.15	7 (2%) 63 54	125, 152, 176, 198	0
4	Q	340/352 (96%)	-0.07	10 (2%) 53 47	130, 155, 175, 184	0
5	E	82/83 (98%)	-0.33	0 100 100	148, 171, 188, 198	0
5	R	82/83 (98%)	0.14	5 (6%) 27 32	148, 171, 188, 195	0
6	F	35/44 (79%)	-0.31	0 100 100	140, 168, 185, 199	0
6	S	35/44 (79%)	0.14	0 100 100	148, 165, 187, 188	0
7	H	65/65 (100%)	-0.05	2 (3%) 51 46	154, 172, 189, 195	0
7	W	65/65 (100%)	0.28	5 (7%) 19 26	154, 173, 188, 196	0
8	I	35/38 (92%)	0.09	0 100 100	147, 163, 174, 178	0
8	a	35/38 (92%)	0.07	0 100 100	148, 164, 179, 190	0
9	J	34/39 (87%)	-0.13	0 100 100	155, 165, 183, 189	0
9	b	34/39 (87%)	0.99	4 (11%) 9 17	156, 176, 190, 190	0
10	K	37/37 (100%)	-0.15	0 100 100	158, 170, 181, 185	0
10	c	37/37 (100%)	0.10	1 (2%) 56 48	152, 171, 187, 195	0
11	L	37/37 (100%)	0.15	2 (5%) 31 34	137, 155, 186, 190	0
11	d	37/37 (100%)	0.08	2 (5%) 31 34	143, 158, 194, 201	0
12	M	34/36 (94%)	0.18	2 (5%) 28 32	147, 163, 179, 195	0
12	e	34/36 (94%)	0.16	2 (5%) 28 32	147, 159, 176, 192	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/246 (98%)	-0.06	1 (0%) 88 79	132, 162, 190, 201	0
13	f	243/246 (98%)	-0.08	3 (1%) 76 65	127, 164, 191, 211	0
14	T	32/32 (100%)	-0.23	0 100 100	144, 157, 187, 198	0
14	g	32/32 (100%)	-0.13	0 100 100	145, 158, 179, 198	0
15	U	97/104 (93%)	-0.14	1 (1%) 79 68	136, 154, 173, 177	0
15	h	97/104 (93%)	-0.12	1 (1%) 79 68	140, 154, 165, 174	0
16	V	137/137 (100%)	-0.20	0 100 100	135, 156, 170, 180	0
16	i	137/137 (100%)	-0.15	0 100 100	131, 158, 176, 185	0
17	m	28/46 (60%)	0.85	2 (7%) 22 28	167, 183, 198, 205	0
17	y	28/46 (60%)	0.05	0 100 100	164, 182, 197, 200	0
18	X	37/40 (92%)	0.01	1 (2%) 56 48	158, 173, 188, 190	0
18	j	37/40 (92%)	0.06	1 (2%) 56 48	161, 175, 191, 202	0
19	Y	0/28	-	-	-	-
19	k	0/28	-	-	-	-
20	Z	62/62 (100%)	0.02	2 (3%) 50 45	159, 178, 198, 208	0
20	l	62/62 (100%)	0.08	3 (4%) 35 37	164, 178, 199, 208	0
All	All	5214/5482 (95%)	-0.07	110 (2%) 63 54	125, 161, 185, 213	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	44	ALA	6.2
7	W	30	LEU	5.7
17	m	30	ILE	5.7
2	N	211	ILE	5.3
1	G	43	ALA	5.2

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
33	CL	D	411	1/1	-0.16	0.17	121,121,121,121	0
35	CA	O	301	1/1	0.33	0.13	138,138,138,138	0
31	LMT	Q	410	31/35	0.34	0.17	165,182,193,197	0
31	LMT	I	103	35/35	0.42	0.20	153,189,201,206	0
21	CLA	N	605	65/65	0.47	0.17	170,189,202,205	0
31	LMT	D	409	31/35	0.48	0.11	162,187,202,208	0
31	LMT	N	624	35/35	0.53	0.14	166,201,210,213	0
21	CLA	B	601	65/65	0.53	0.15	167,188,199,203	0
30	BCR	H	101	40/40	0.61	0.19	165,178,188,190	0
30	BCR	b	102	40/40	0.61	0.34	158,178,202,203	0
31	LMT	N	625	35/35	0.63	0.11	165,184,206,216	0
31	LMT	N	604	35/35	0.65	0.12	145,180,209,212	0
31	LMT	B	625	35/35	0.66	0.12	163,196,218,227	0
26	SQD	B	627	47/54	0.68	0.15	143,179,209,227	0
31	LMT	a	103	35/35	0.68	0.13	169,180,206,216	0
27	LMG	C	520	45/55	0.69	0.16	164,178,186,187	0
30	BCR	c	101	40/40	0.69	0.18	151,171,188,190	0
21	CLA	B	604	65/65	0.69	0.15	148,158,172,182	0
33	CL	G	415	1/1	0.70	0.20	122,122,122,122	0
26	SQD	N	601	47/54	0.71	0.17	141,176,198,202	0
21	CLA	C	507	65/65	0.71	0.17	159,172,185,187	0
30	BCR	a	101	40/40	0.73	0.25	139,159,176,181	0
21	CLA	N	607	65/65	0.73	0.14	133,163,170,175	0
22	PHO	A	404	64/64	0.74	0.14	129,151,167,177	0
30	BCR	J	102	40/40	0.74	0.25	167,182,207,208	0
21	CLA	G	406	65/65	0.76	0.16	145,159,181,186	0
31	LMT	B	630	35/35	0.76	0.18	157,169,199,220	0
30	BCR	P	514	40/40	0.77	0.14	139,152,173,175	0
23	PL9	b	101	35/55	0.77	0.28	168,188,199,208	0
21	CLA	C	509	65/65	0.77	0.16	145,170,180,183	0
22	PHO	D	402	64/64	0.77	0.12	135,155,161,168	0
25	LHG	G	412	37/49	0.78	0.20	147,176,193,204	0
30	BCR	T	103	40/40	0.78	0.21	155,168,181,184	0
31	LMT	B	626	35/35	0.79	0.11	163,194,202,213	0
30	BCR	I	101	40/40	0.79	0.22	143,155,171,183	0
27	LMG	I	102	43/55	0.79	0.18	152,184,203,207	0
21	CLA	P	509	65/65	0.80	0.13	152,174,181,184	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMG	P	521	45/55	0.80	0.14	149,175,191,198	0
21	CLA	C	513	65/65	0.80	0.13	173,193,206,213	0
31	LMT	N	603	35/35	0.80	0.16	153,179,189,190	0
21	CLA	N	620	65/65	0.81	0.17	156,175,192,194	0
21	CLA	P	507	65/65	0.81	0.14	162,172,191,194	0
34	HEM	i	201	43/43	0.81	0.15	131,158,169,172	0
31	LMT	B	629	35/35	0.81	0.18	153,166,181,185	0
21	CLA	C	512	65/65	0.82	0.13	173,183,196,199	0
32	BCT	Q	411	4/4	0.82	0.13	164,166,168,173	0
21	CLA	B	609	65/65	0.82	0.14	162,177,185,186	0
30	BCR	B	618	40/40	0.83	0.19	149,162,168,169	0
21	CLA	P	501	65/65	0.83	0.13	149,170,185,188	0
30	BCR	P	516	40/40	0.83	0.18	164,173,180,187	0
30	BCR	S	101	40/40	0.83	0.21	145,159,176,178	0
26	SQD	A	414	54/54	0.83	0.26	139,173,190,200	0
27	LMG	B	623	49/55	0.83	0.19	128,147,164,167	0
30	BCR	W	101	40/40	0.84	0.12	164,176,182,186	0
24	DGD	C	518	66/66	0.84	0.14	139,157,179,185	0
24	DGD	D	408	63/66	0.84	0.18	167,181,198,212	0
27	LMG	a	102	43/55	0.84	0.16	160,179,196,200	0
21	CLA	N	610	65/65	0.84	0.15	152,178,191,194	0
30	BCR	C	514	40/40	0.84	0.13	153,160,171,173	0
24	DGD	B	628	52/66	0.84	0.15	148,173,194,200	0
21	CLA	C	505	65/65	0.85	0.17	147,172,186,188	0
21	CLA	P	513	65/65	0.85	0.13	168,182,207,216	0
27	LMG	D	412	42/55	0.85	0.17	147,178,195,199	0
21	CLA	N	609	65/65	0.85	0.12	148,165,174,178	0
27	LMG	P	520	48/55	0.86	0.29	147,168,177,184	0
30	BCR	T	101	40/40	0.86	0.16	144,167,181,184	0
24	DGD	Q	409	63/66	0.86	0.20	157,183,208,238	0
27	LMG	Q	401	42/55	0.86	0.15	131,168,174,183	0
24	DGD	C	516	53/66	0.86	0.17	141,158,168,170	0
24	DGD	B	621	58/66	0.86	0.14	142,158,168,171	0
27	LMG	D	407	48/55	0.86	0.20	145,159,169,175	0
23	PL9	J	101	35/55	0.86	0.21	177,190,200,204	0
26	SQD	G	401	54/54	0.86	0.19	158,176,209,210	0
21	CLA	B	607	65/65	0.87	0.13	135,152,161,165	0
30	BCR	B	619	40/40	0.87	0.24	140,156,169,178	0
26	SQD	F	101	45/54	0.87	0.17	157,176,196,198	0
24	DGD	A	407	56/66	0.87	0.14	147,171,188,195	0
21	CLA	B	608	65/65	0.87	0.15	147,165,180,186	0
21	CLA	B	605	65/65	0.87	0.11	156,167,176,179	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMG	C	519	48/55	0.87	0.18	132,169,183,188	0
21	CLA	B	610	65/65	0.87	0.11	146,163,174,176	0
24	DGD	C	517	62/66	0.87	0.12	145,169,193,200	0
21	CLA	B	615	65/65	0.87	0.12	162,178,191,194	0
21	CLA	N	616	65/65	0.87	0.10	156,167,181,184	0
31	LMT	e	101	35/35	0.87	0.20	164,176,191,195	0
22	PHO	Q	403	64/64	0.87	0.11	144,155,164,168	0
25	LHG	A	411	37/49	0.87	0.13	156,178,214,232	0
23	PL9	A	406	45/55	0.87	0.18	152,174,185,188	0
21	CLA	D	401	65/65	0.87	0.15	137,149,176,181	0
30	BCR	B	617	40/40	0.87	0.14	151,158,176,180	0
35	CA	f	301	1/1	0.87	0.09	210,210,210,210	0
22	PHO	G	405	64/64	0.88	0.12	131,149,159,162	0
21	CLA	N	608	65/65	0.88	0.12	146,158,176,191	0
21	CLA	N	618	65/65	0.88	0.13	153,171,180,185	0
31	LMT	M	102	35/35	0.88	0.16	134,165,196,205	0
30	BCR	T	102	40/40	0.88	0.18	143,167,176,178	0
21	CLA	P	511	65/65	0.88	0.10	156,174,184,187	0
26	SQD	G	410	51/54	0.88	0.18	161,172,184,190	0
30	BCR	P	515	40/40	0.88	0.13	165,176,185,189	0
27	LMG	Q	407	48/55	0.88	0.13	142,156,168,176	0
23	PL9	Q	405	55/55	0.88	0.13	137,146,166,170	0
27	LMG	B	622	49/55	0.88	0.18	148,163,174,176	0
24	DGD	P	519	66/66	0.88	0.14	142,157,177,186	0
21	CLA	D	403	65/65	0.88	0.13	153,160,181,189	0
21	CLA	C	501	65/65	0.88	0.13	160,174,184,185	0
30	BCR	C	515	40/40	0.88	0.13	139,164,177,180	0
30	BCR	D	405	40/40	0.88	0.14	145,161,176,179	0
21	CLA	P	502	65/65	0.88	0.11	146,161,175,182	0
21	CLA	B	614	65/65	0.89	0.13	157,172,181,184	0
21	CLA	P	505	65/65	0.89	0.15	134,164,180,183	0
26	SQD	B	624	43/54	0.89	0.13	150,181,199,206	0
21	CLA	A	405	65/65	0.89	0.12	144,155,176,187	0
24	DGD	N	602	52/66	0.89	0.13	154,176,204,206	0
27	LMG	N	623	49/55	0.89	0.17	139,152,164,171	0
24	DGD	P	518	62/66	0.89	0.19	144,168,195,200	0
21	CLA	C	506	65/65	0.89	0.15	159,175,202,211	0
21	CLA	G	402	65/65	0.89	0.12	136,148,155,166	0
26	SQD	Q	408	43/54	0.89	0.15	143,180,193,194	0
27	LMG	Q	406	46/55	0.89	0.16	135,162,171,180	0
24	DGD	W	102	58/66	0.89	0.17	145,157,168,172	0
21	CLA	G	403	65/65	0.89	0.12	123,139,149,162	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMG	G	411	51/55	0.90	0.14	152,164,177,178	0
21	CLA	P	503	65/65	0.90	0.11	144,174,187,195	0
21	CLA	P	504	65/65	0.90	0.14	155,169,181,186	0
21	CLA	A	403	65/65	0.90	0.15	142,161,183,185	0
26	SQD	S	102	45/54	0.90	0.14	160,188,201,203	0
21	CLA	N	619	65/65	0.90	0.11	158,180,190,193	0
26	SQD	A	409	51/54	0.90	0.15	156,178,191,194	0
21	CLA	C	511	65/65	0.90	0.12	155,172,181,184	0
21	CLA	P	510	65/65	0.90	0.11	145,161,170,178	0
34	HEM	V	201	43/43	0.90	0.12	139,151,166,173	0
21	CLA	N	614	65/65	0.90	0.11	150,162,173,178	0
21	CLA	P	512	65/65	0.90	0.10	172,184,194,199	0
21	CLA	B	603	65/65	0.90	0.11	147,166,178,179	0
21	CLA	G	404	65/65	0.91	0.12	141,159,179,181	0
21	CLA	N	611	65/65	0.91	0.11	145,156,164,166	0
21	CLA	B	612	65/65	0.91	0.09	152,163,174,176	0
23	PL9	D	404	55/55	0.91	0.15	129,150,158,160	0
25	LHG	A	408	39/49	0.91	0.12	146,167,179,179	0
24	DGD	G	408	56/66	0.91	0.14	163,179,188,193	0
21	CLA	B	616	65/65	0.91	0.13	155,166,199,214	0
27	LMG	R	102	44/55	0.91	0.17	161,177,189,192	0
27	LMG	E	102	44/55	0.91	0.13	168,188,198,203	0
24	DGD	P	517	53/66	0.91	0.14	141,160,173,176	0
21	CLA	N	612	65/65	0.92	0.13	151,164,181,190	0
21	CLA	P	508	65/65	0.92	0.13	157,168,182,193	0
21	CLA	B	611	65/65	0.92	0.11	149,160,167,169	0
21	CLA	B	602	65/65	0.92	0.11	152,172,182,185	0
21	CLA	N	617	65/65	0.92	0.13	149,168,182,188	0
30	BCR	K	101	40/40	0.92	0.14	154,167,176,181	0
27	LMG	e	102	42/55	0.92	0.20	155,166,183,191	0
27	LMG	A	410	51/55	0.92	0.14	138,157,168,171	0
21	CLA	N	606	65/65	0.92	0.10	152,172,178,182	0
30	BCR	N	621	40/40	0.92	0.17	132,154,165,172	0
34	HEM	R	101	43/43	0.92	0.12	164,184,192,199	0
21	CLA	A	401	65/65	0.92	0.11	138,146,156,160	0
30	BCR	B	620	40/40	0.92	0.15	161,168,186,196	0
23	PL9	G	407	45/55	0.92	0.17	148,160,183,188	0
21	CLA	C	510	65/65	0.93	0.09	149,161,171,178	0
21	CLA	A	402	65/65	0.93	0.10	139,147,158,164	0
21	CLA	B	613	65/65	0.93	0.11	148,160,171,175	0
21	CLA	N	613	65/65	0.93	0.10	160,170,177,182	0
34	HEM	E	101	43/43	0.93	0.09	166,179,188,190	0

*Continued on next page...*

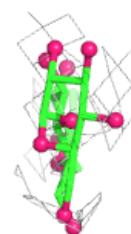
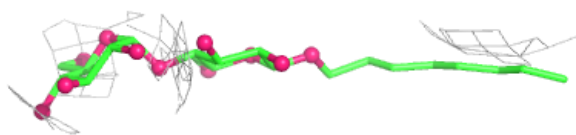
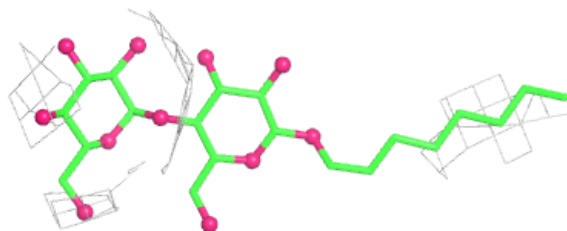
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	BCR	Z	101	40/40	0.93	0.10	163,178,192,197	0
21	CLA	Q	402	65/65	0.93	0.12	136,144,158,169	0
21	CLA	Q	404	65/65	0.93	0.13	152,162,187,194	0
21	CLA	C	503	65/65	0.93	0.10	155,171,181,183	0
21	CLA	C	504	65/65	0.93	0.11	153,172,198,204	0
21	CLA	C	502	65/65	0.94	0.09	142,157,179,185	0
28	OEC	G	413	5/9	0.94	0.14	91,102,115,124	0
21	CLA	N	615	65/65	0.94	0.09	152,158,168,173	0
21	CLA	C	508	65/65	0.94	0.09	154,170,194,203	0
27	LMG	M	101	42/55	0.94	0.15	166,174,184,188	0
27	LMG	D	406	46/55	0.94	0.13	140,153,176,181	0
21	CLA	P	506	65/65	0.94	0.14	159,176,194,202	0
27	LMG	N	622	49/55	0.94	0.16	145,154,172,174	0
32	BCT	D	410	4/4	0.94	0.07	166,167,167,169	0
21	CLA	B	606	65/65	0.95	0.10	156,173,194,204	0
25	LHG	G	409	39/49	0.95	0.11	156,168,188,191	0
29	FE2	A	413	1/1	0.97	0.07	166,166,166,166	0
28	OEC	A	412	5/9	0.99	0.05	122,122,126,129	0
29	FE2	G	414	1/1	0.99	0.07	149,149,149,149	0

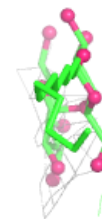
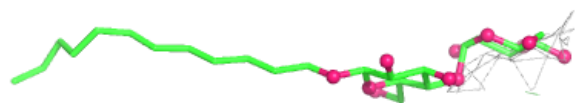
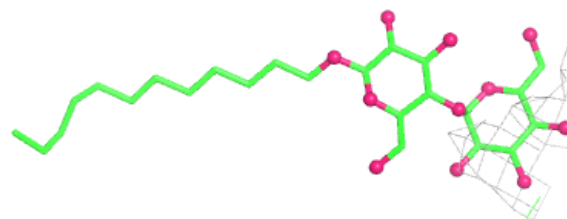
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

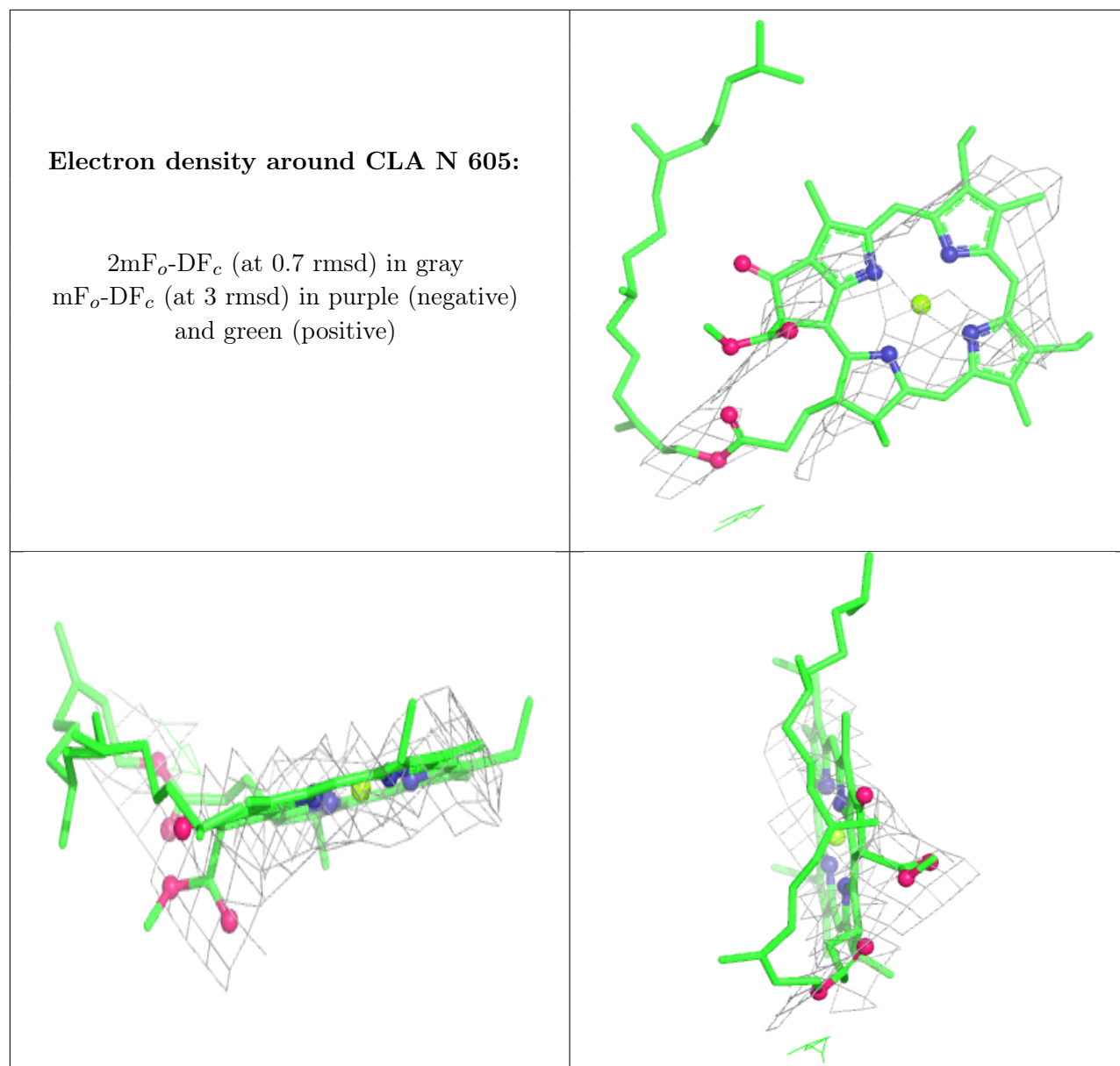
**Electron density around LMT Q 410:**

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

**Electron density around LMT I 103:**

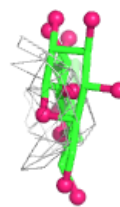
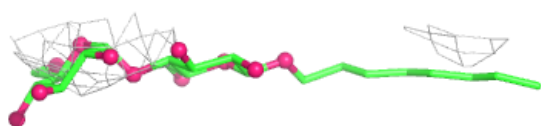
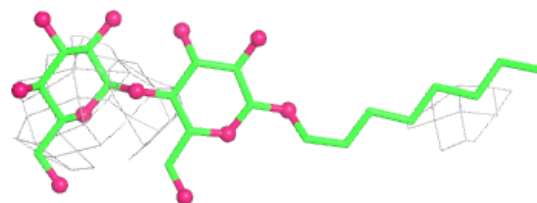
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



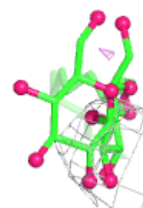
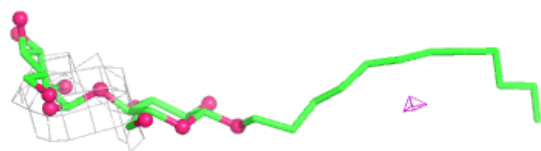
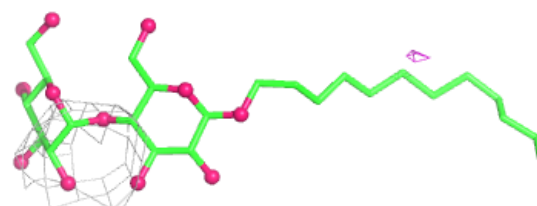


**Electron density around LMT D 409:**

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

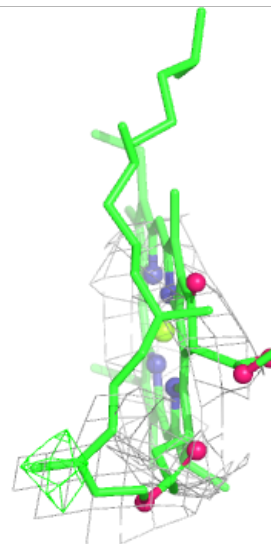
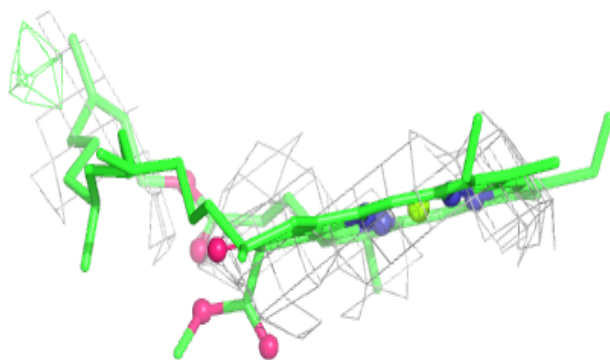
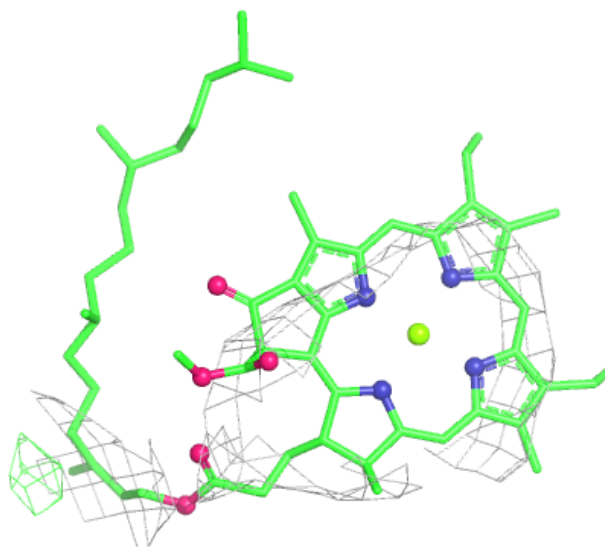
**Electron density around LMT N 624:**

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



**Electron density around CLA B 601:**

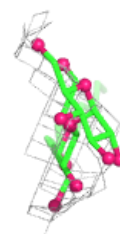
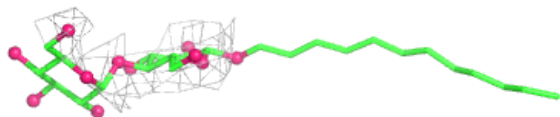
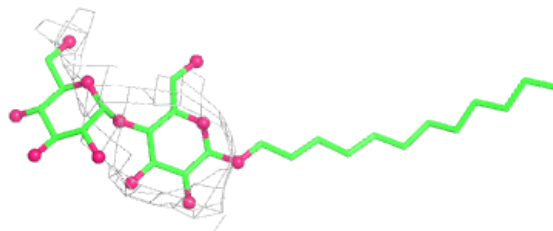
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



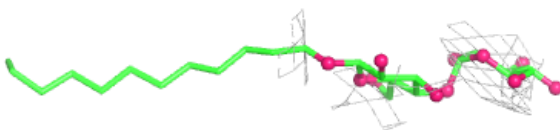
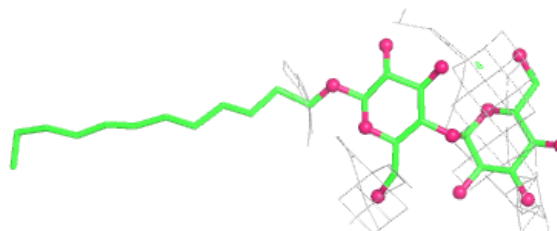
<p><b>Electron density around BCR H 101:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rmsd) in gray <math>mF_o-DF_c</math> (at 3 rmsd) in purple (negative) and green (positive)</p>	
<p><b>Electron density around BCR b 102:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rmsd) in gray <math>mF_o-DF_c</math> (at 3 rmsd) in purple (negative) and green (positive)</p>	

**Electron density around LMT N 625:**

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

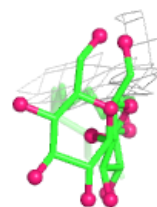
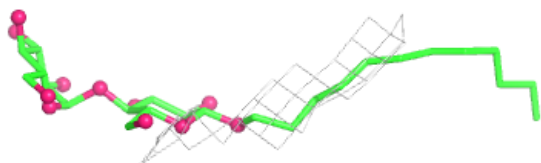
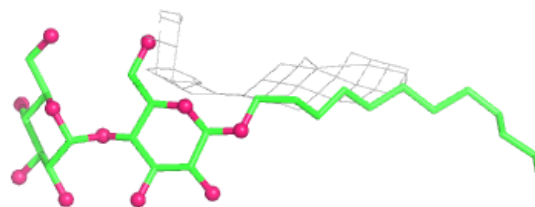
**Electron density around LMT N 604:**

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

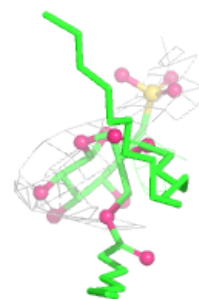
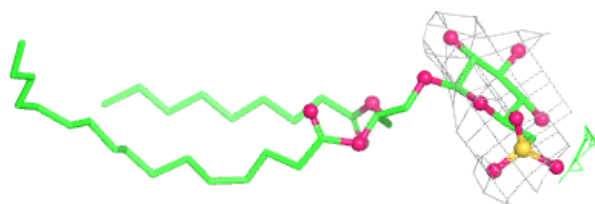
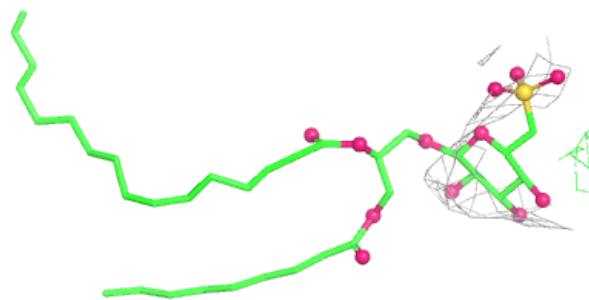


**Electron density around LMT B 625:**

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

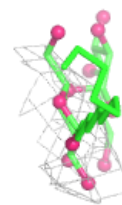
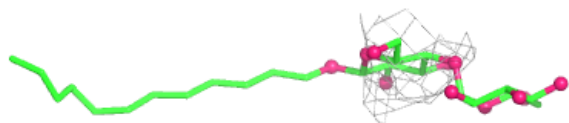
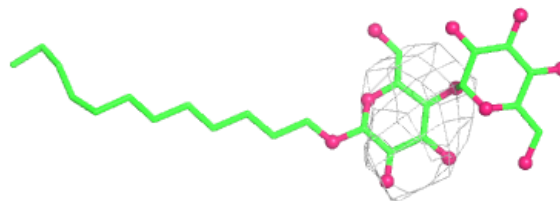
**Electron density around SQD B 627:**

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

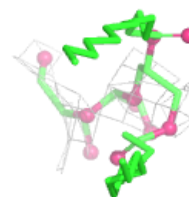
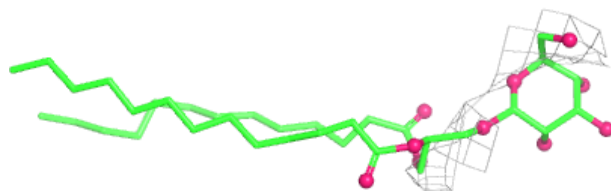
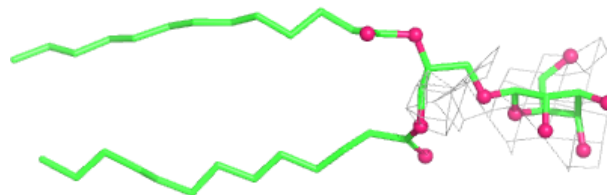


**Electron density around LMT a 103:**

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

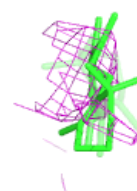
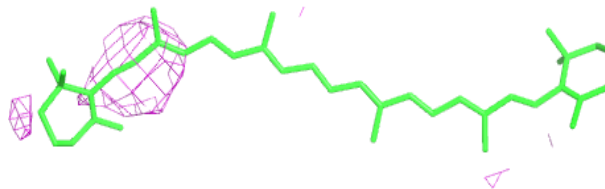
**Electron density around LMG C 520:**

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

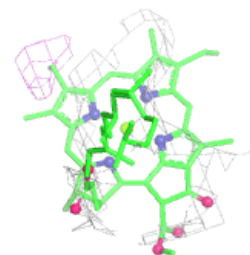
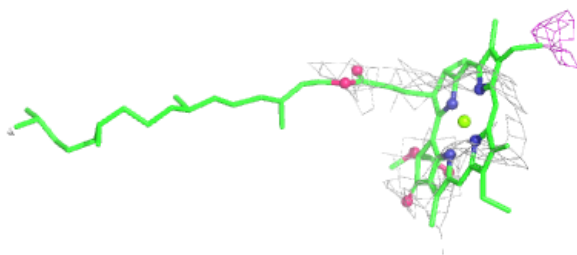
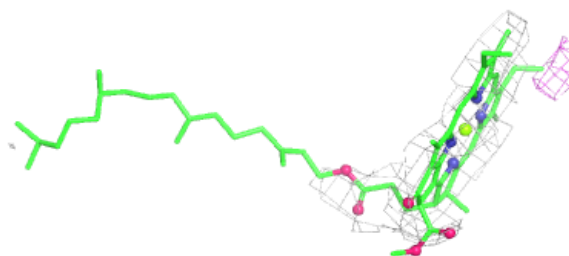


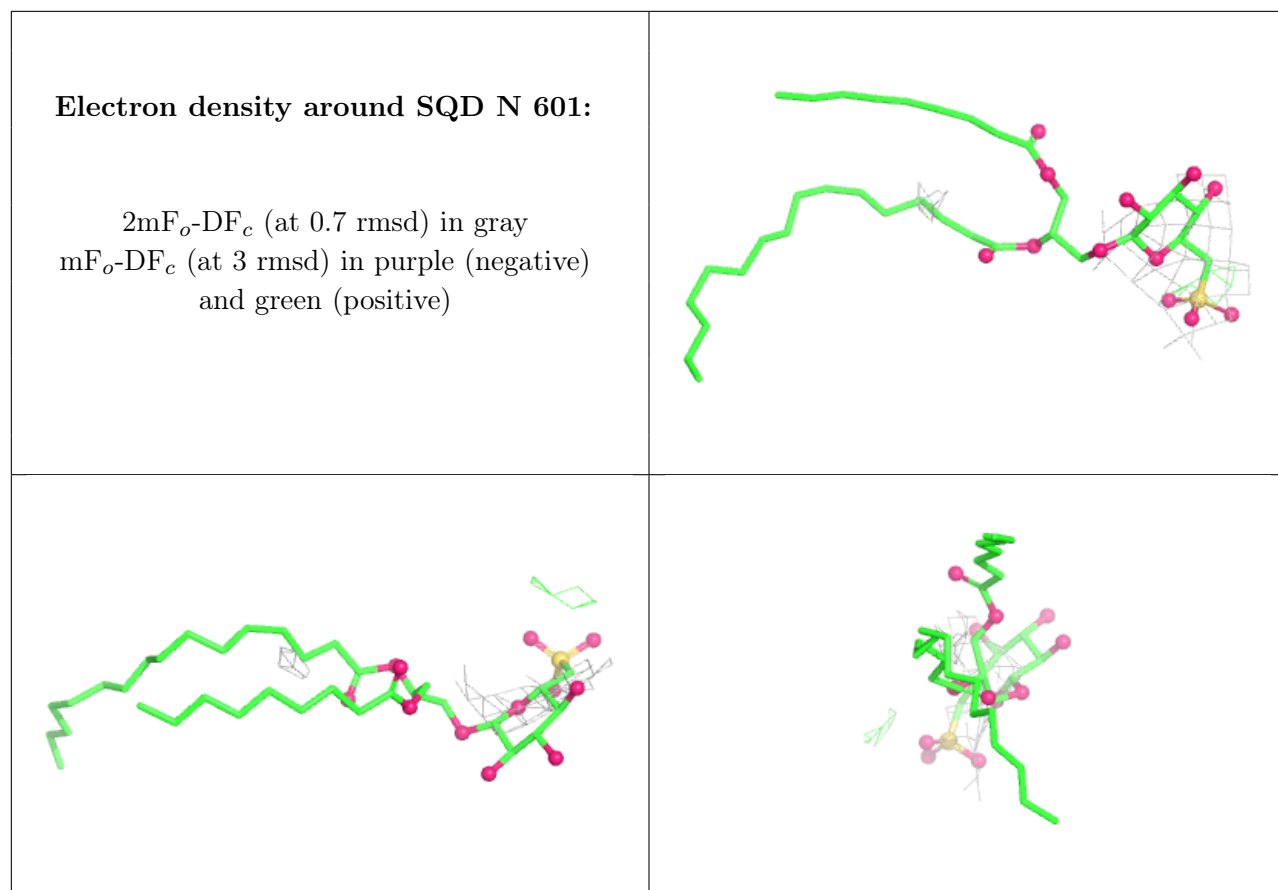
**Electron density around BCR c 101:**

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

**Electron density around CLA B 604:**

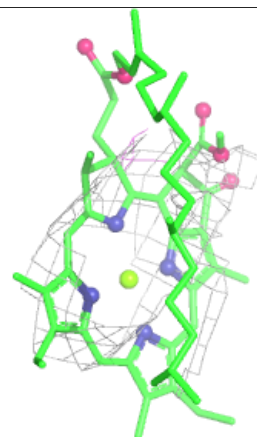
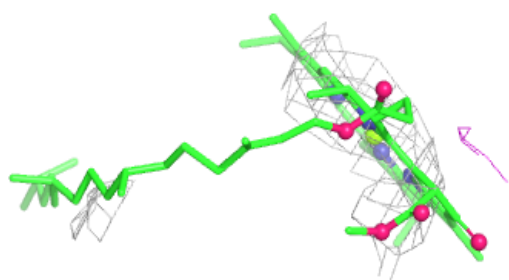
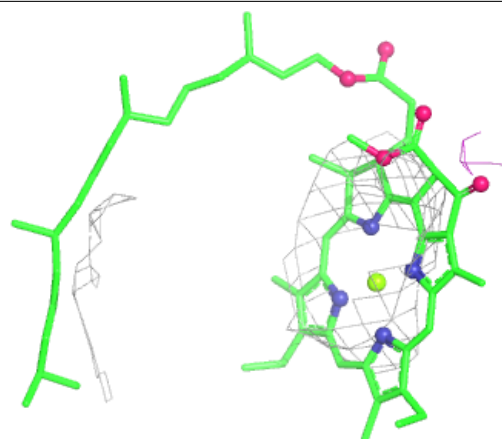
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



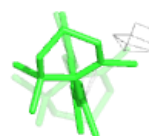


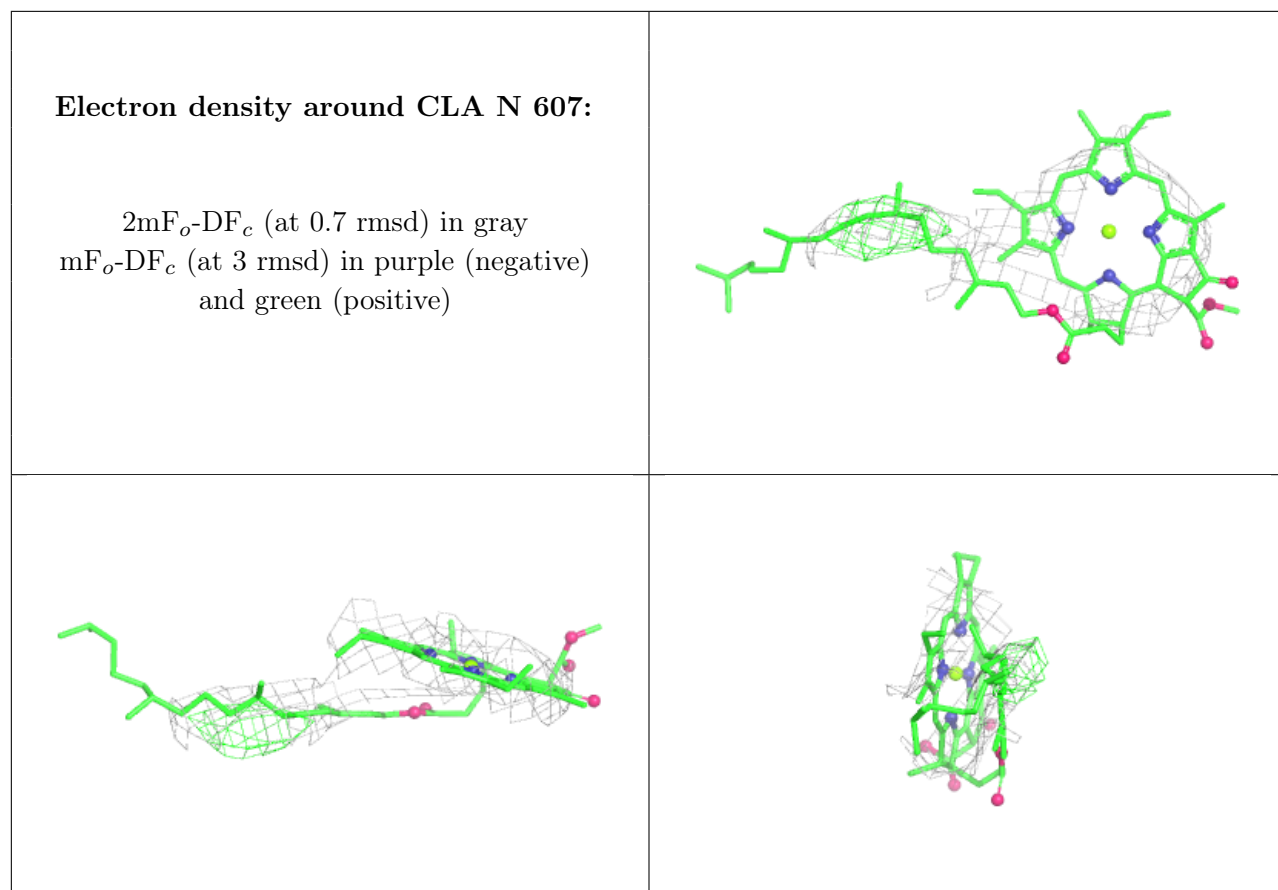
**Electron density around CLA C 507:**

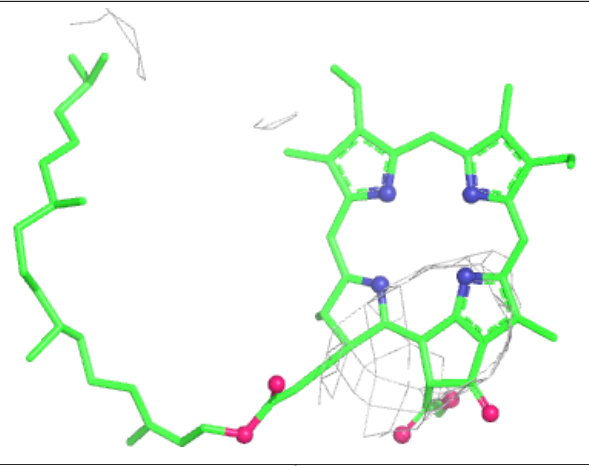
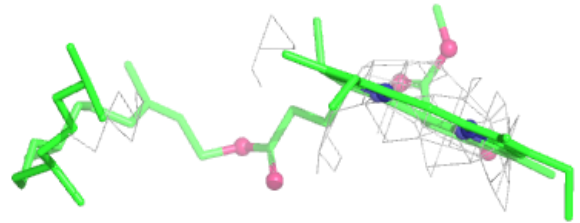

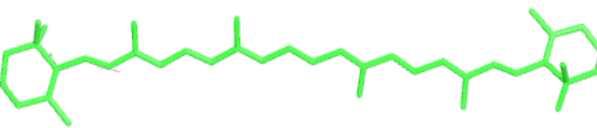
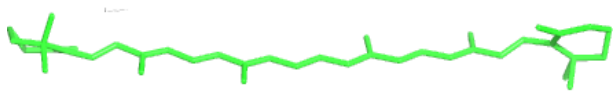

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

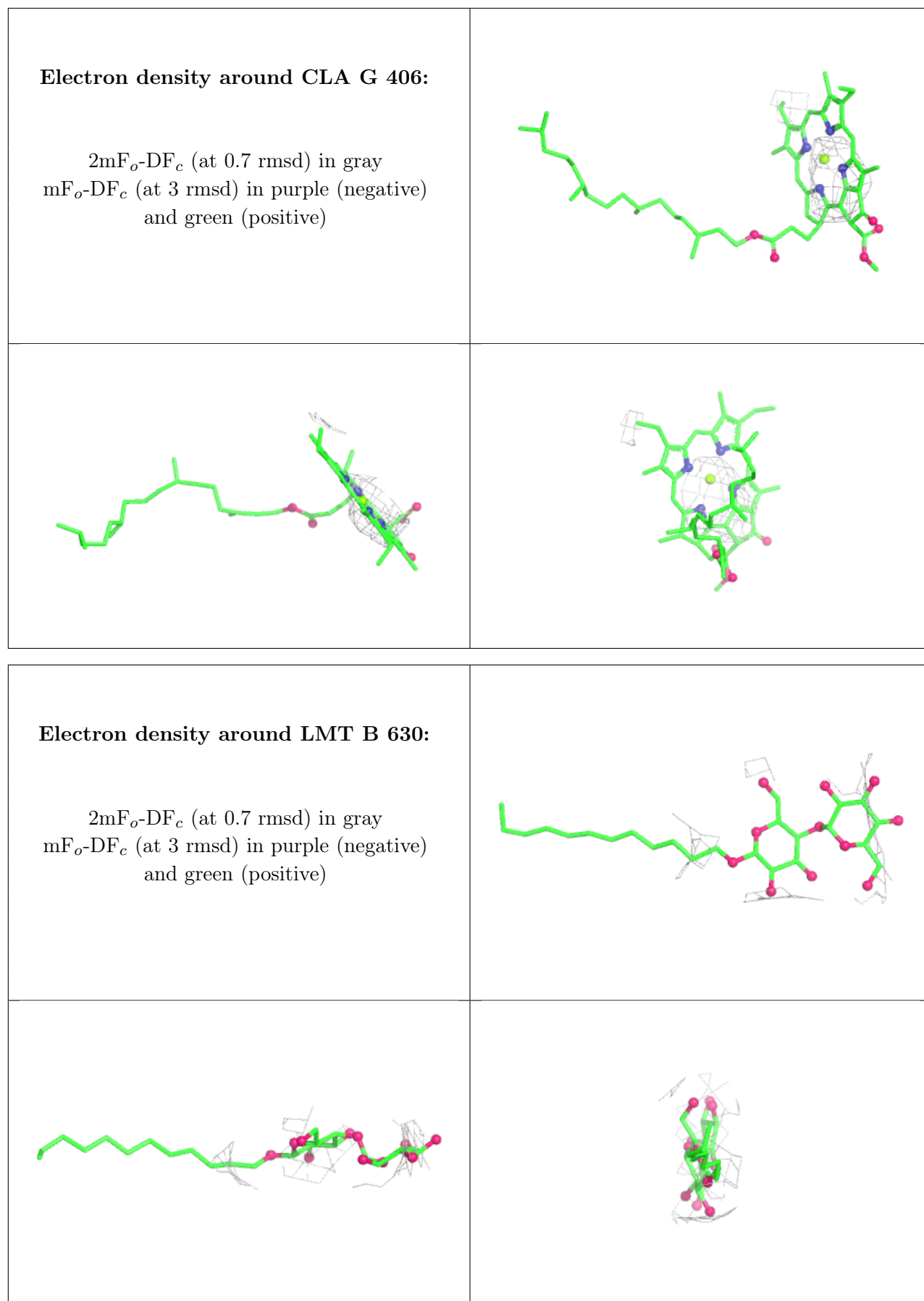
**Electron density around BCR a 101:**

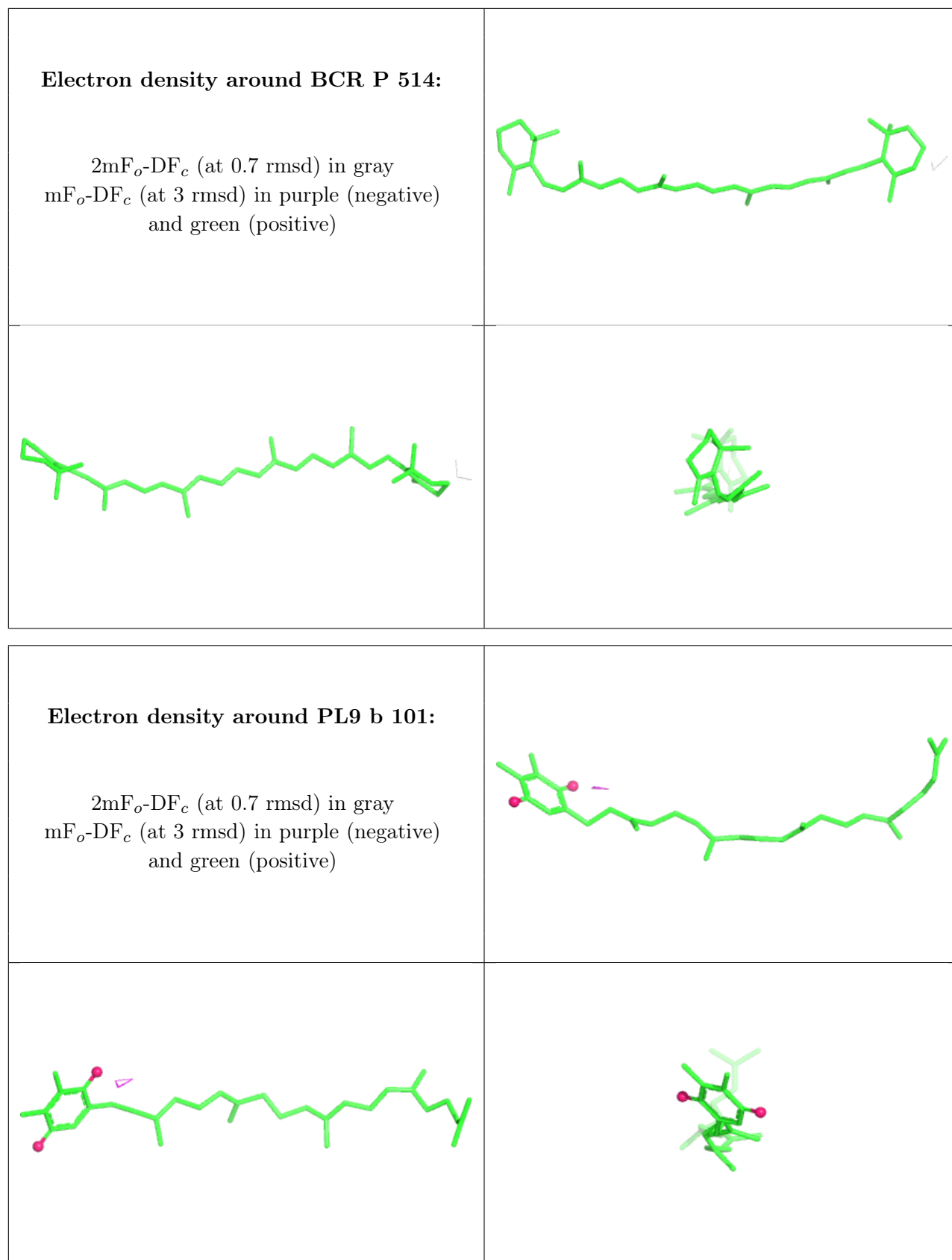
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





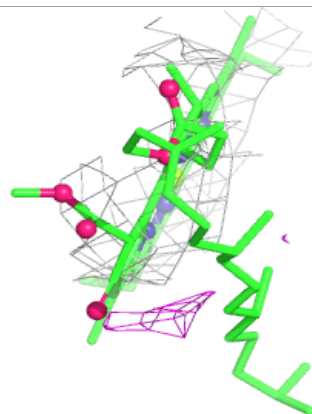
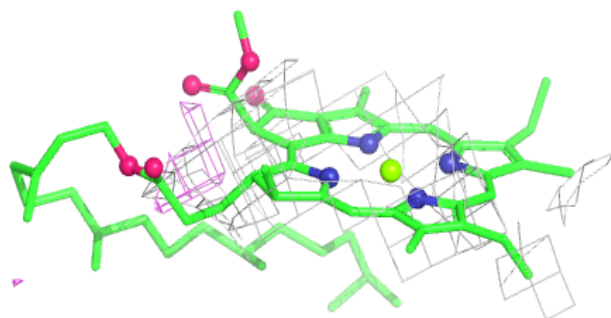
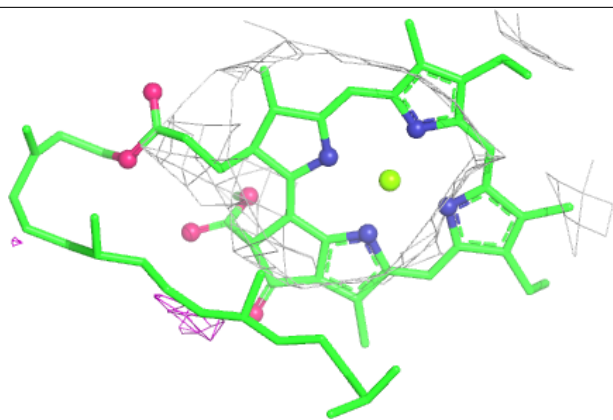
<p><b>Electron density around PHO A 404:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rnsd) in gray <math>mF_o-DF_c</math> (at 3 rnsd) in purple (negative) and green (positive)</p>	
	
<p><b>Electron density around BCR J 102:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rnsd) in gray <math>mF_o-DF_c</math> (at 3 rnsd) in purple (negative) and green (positive)</p>	
	



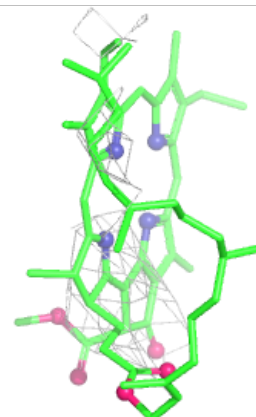
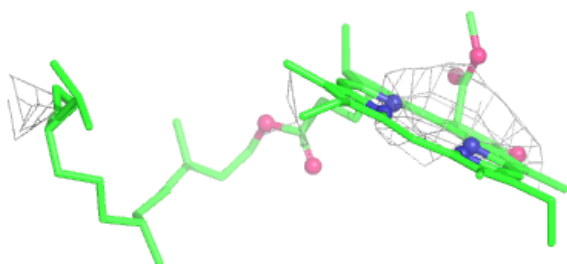
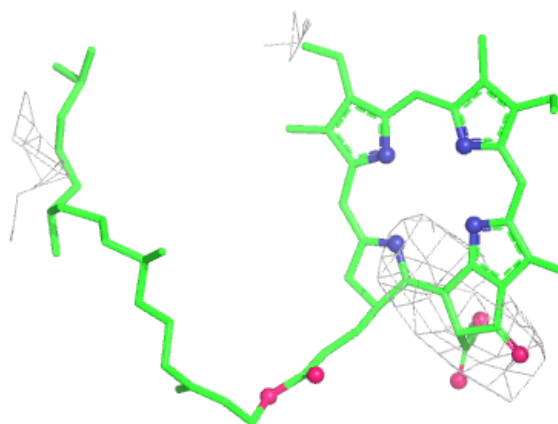


**Electron density around CLA C 509:**

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

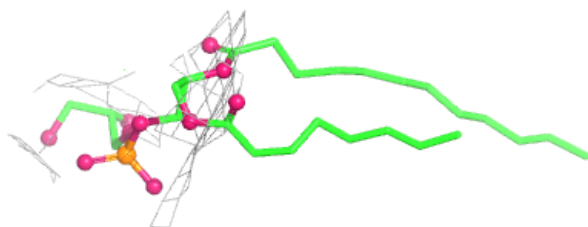
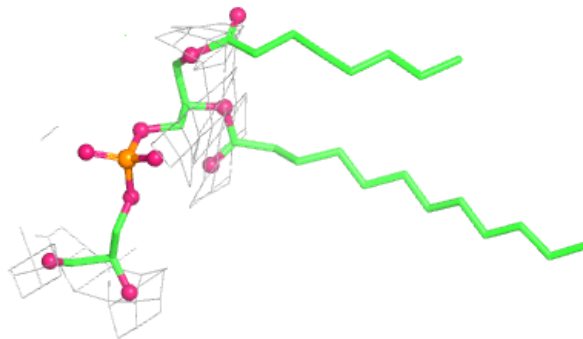
**Electron density around PHO D 402:**

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

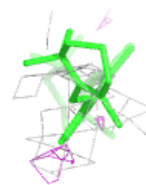
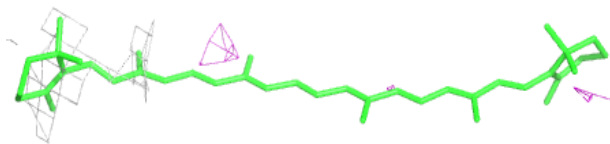
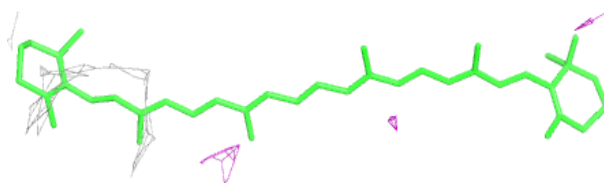


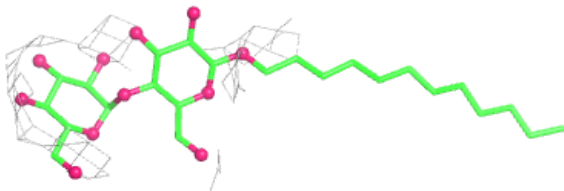
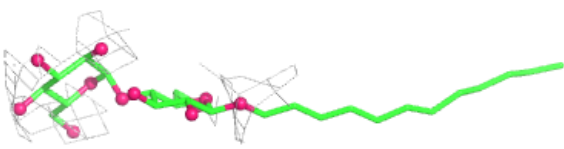
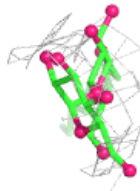
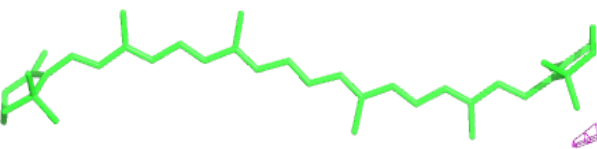

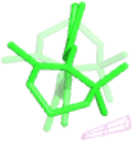
**Electron density around LHG G 412:**

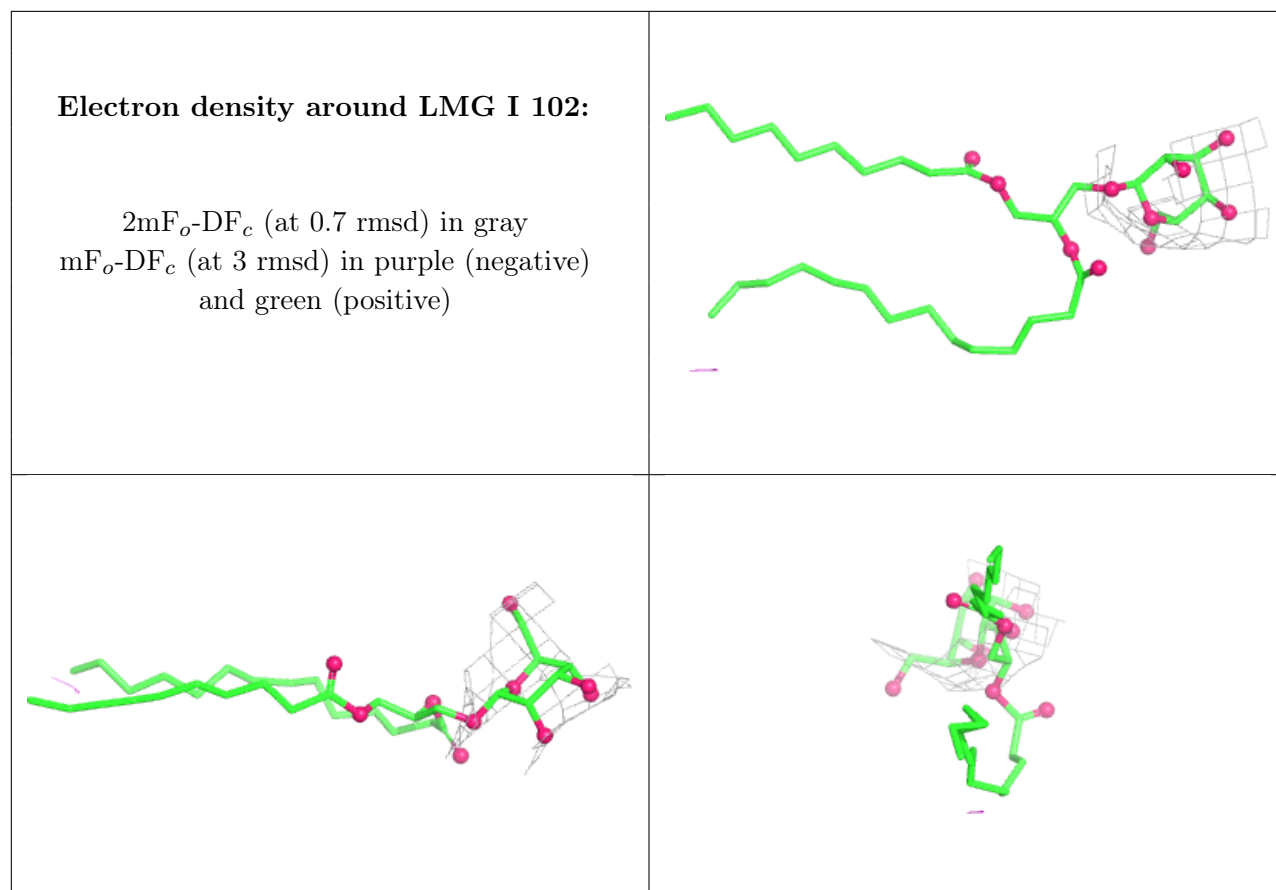
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR T 103:**

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

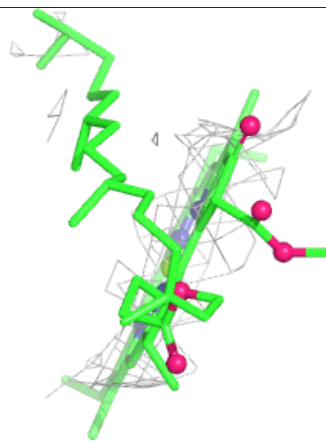
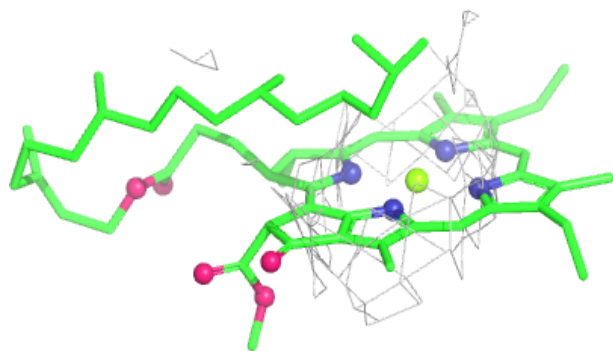
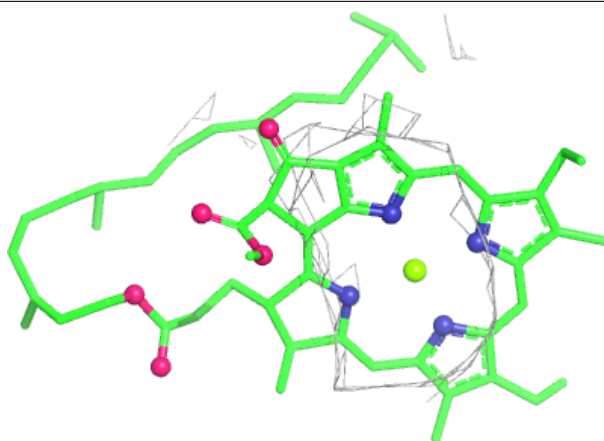


<p><b>Electron density around LMT B 626:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rmsd) in gray <math>mF_o-DF_c</math> (at 3 rmsd) in purple (negative) and green (positive)</p>	
	
<p><b>Electron density around BCR I 101:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rmsd) in gray <math>mF_o-DF_c</math> (at 3 rmsd) in purple (negative) and green (positive)</p>	
	

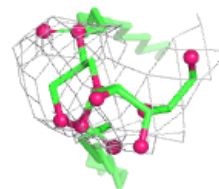
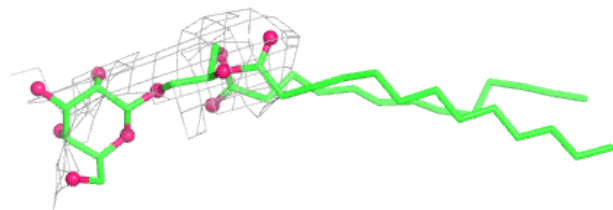
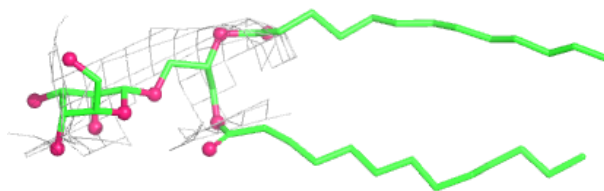


**Electron density around CLA P 509:**

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

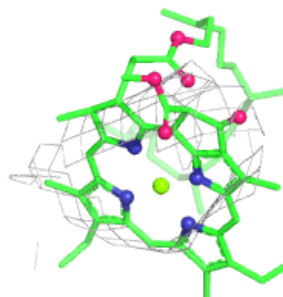
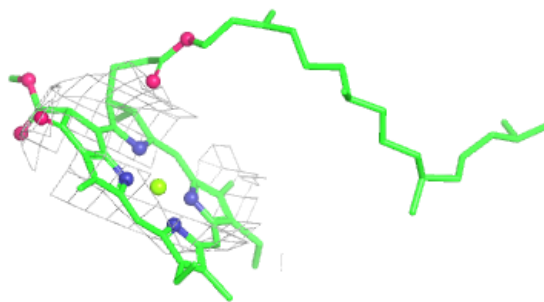
**Electron density around LMG P 521:**

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

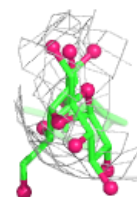
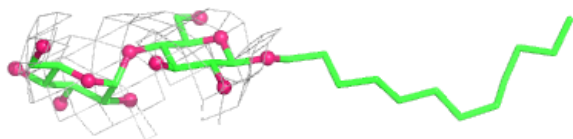
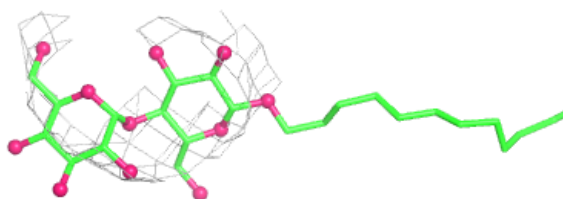


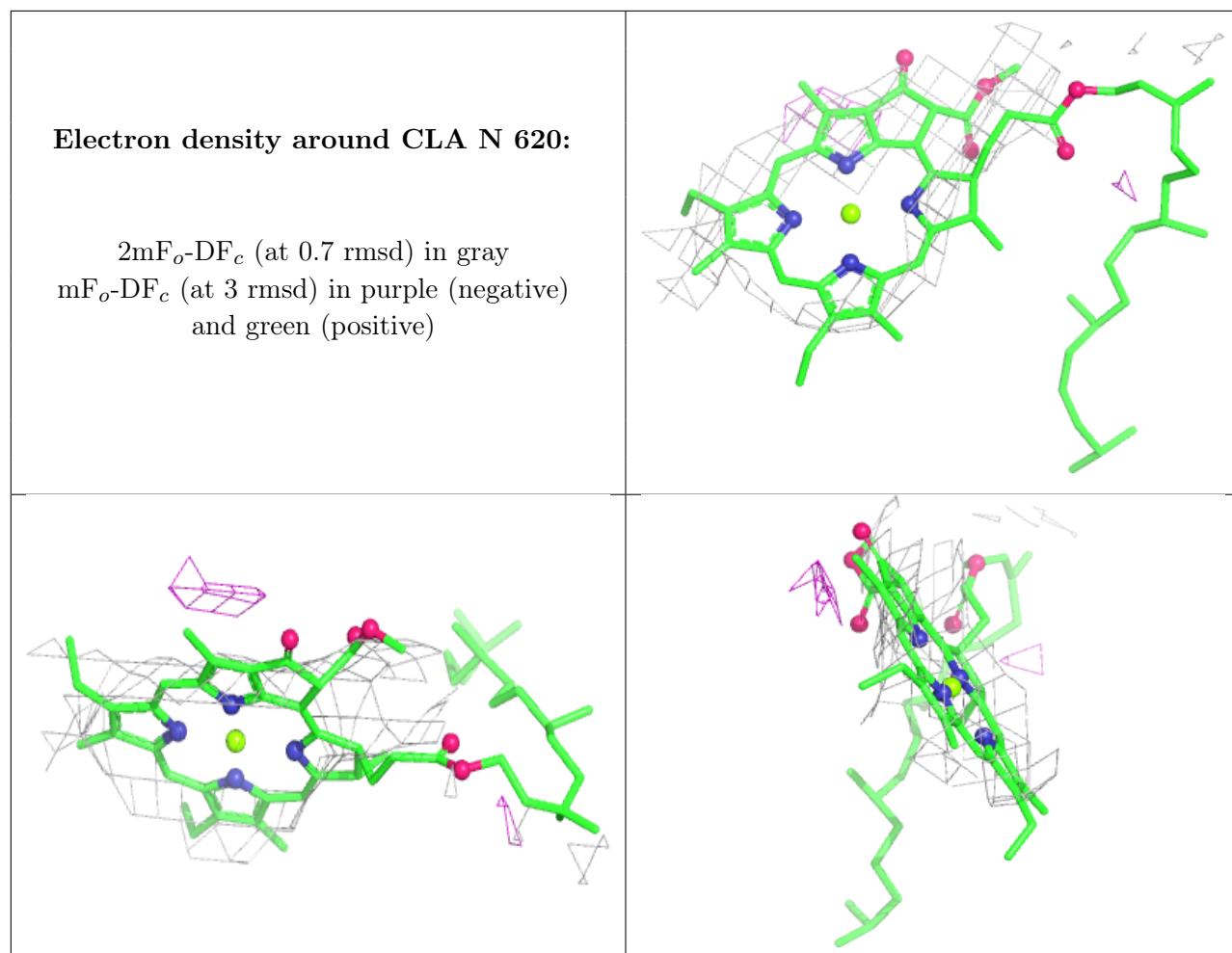
**Electron density around CLA C 513:**

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

**Electron density around LMT N 603:**

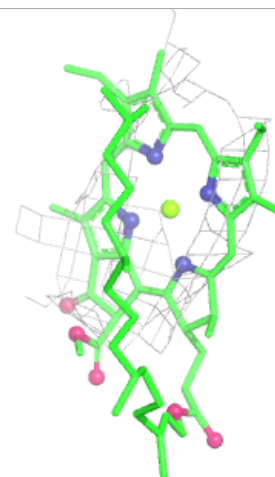
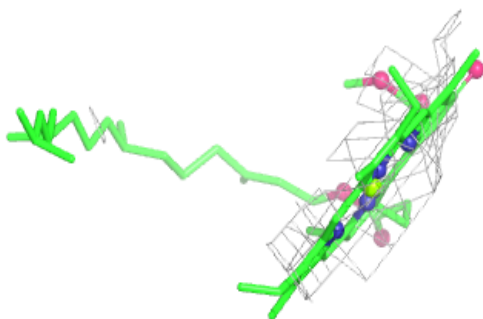
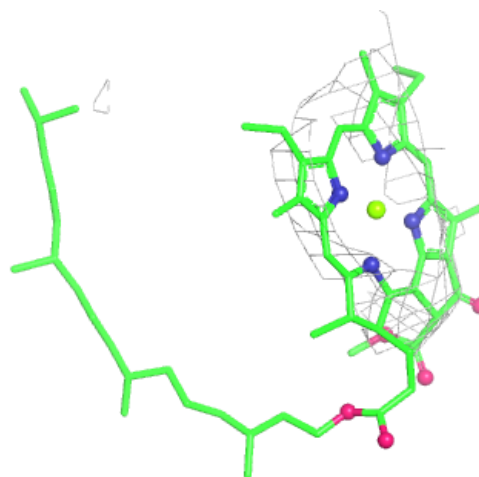
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





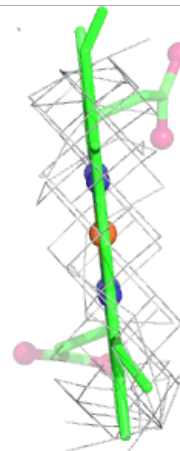
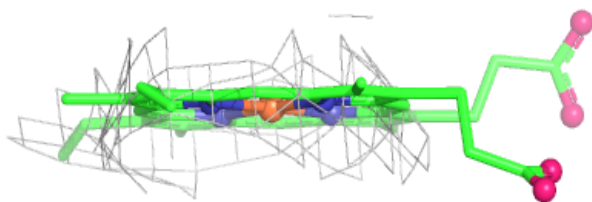
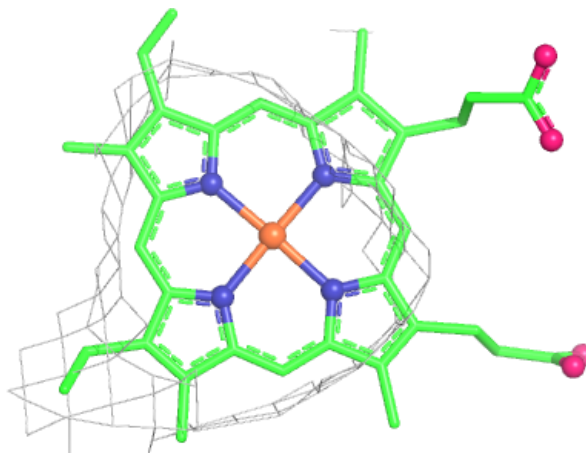
**Electron density around CLA P 507:**

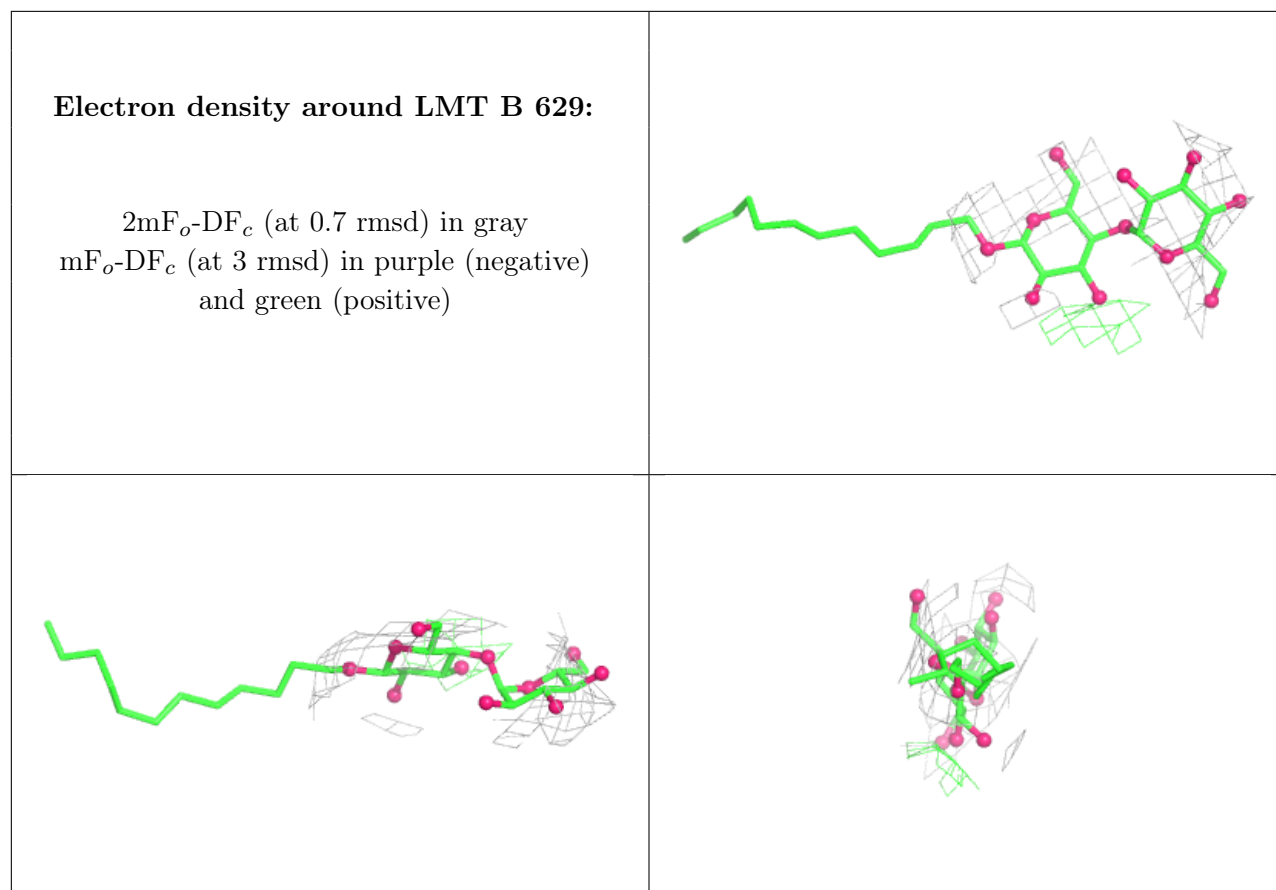
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

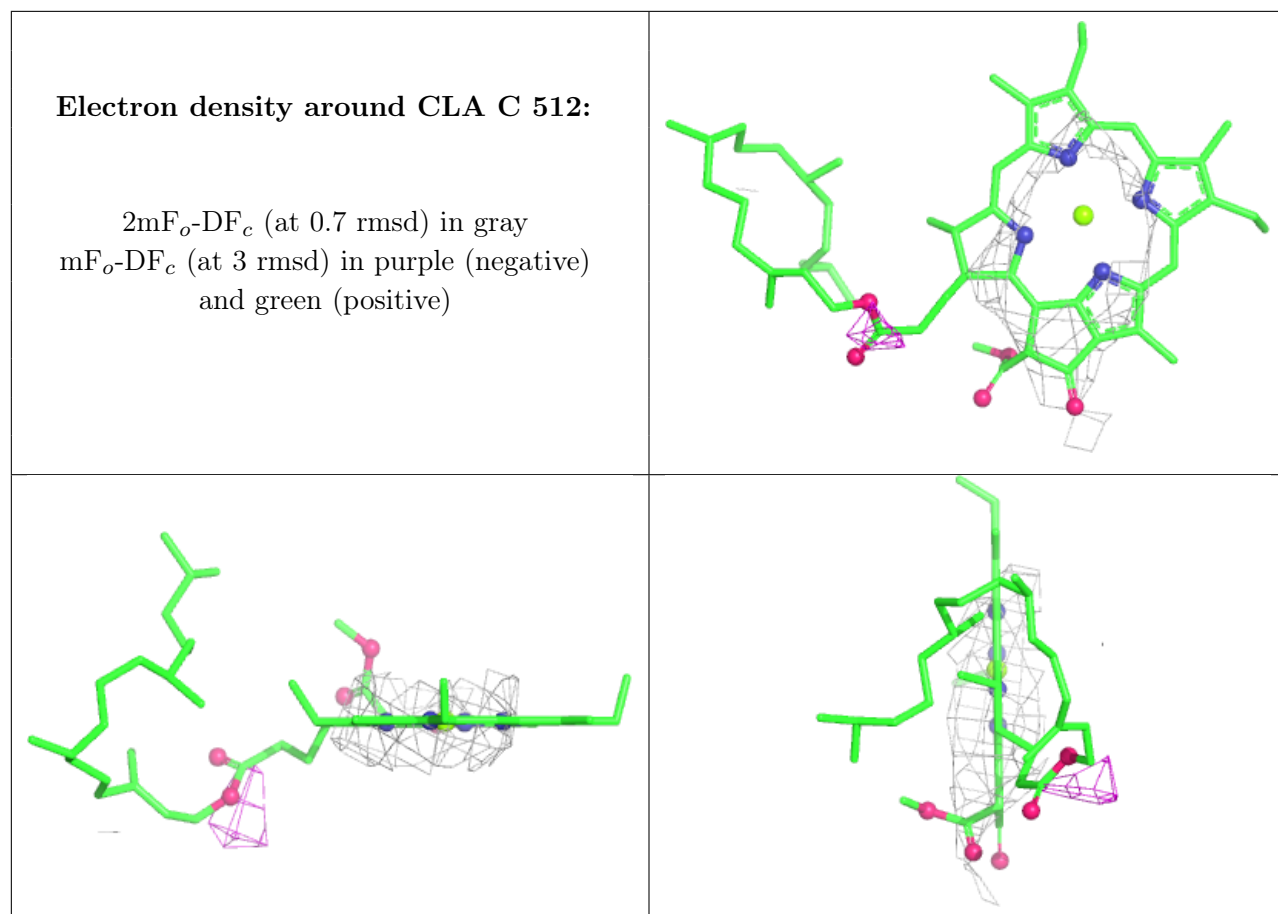


**Electron density around HEM i 201:**

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

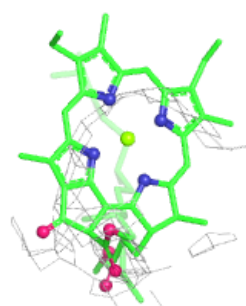
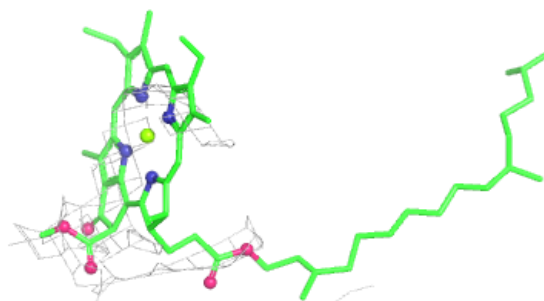




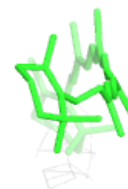
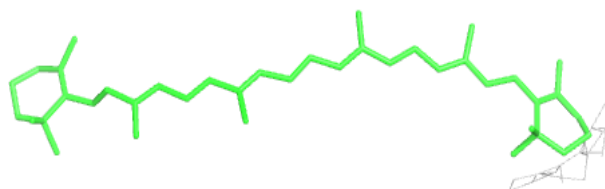


**Electron density around CLA B 609:**

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

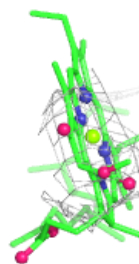
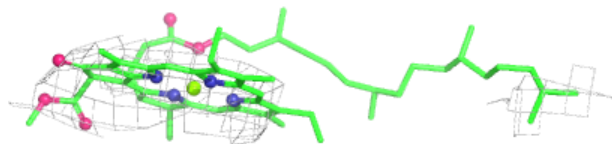
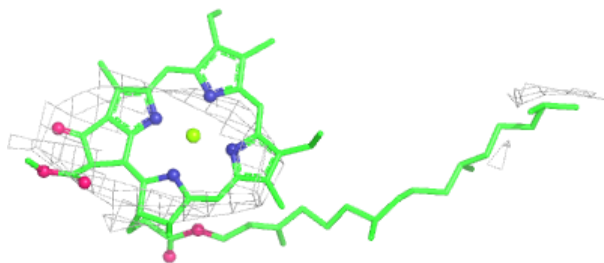
**Electron density around BCR B 618:**

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

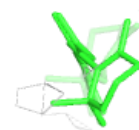
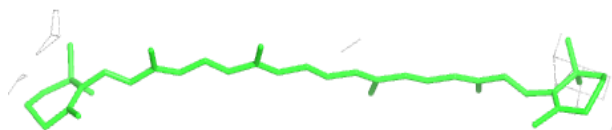
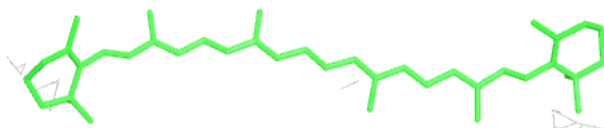


**Electron density around CLA P 501:**

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

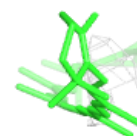
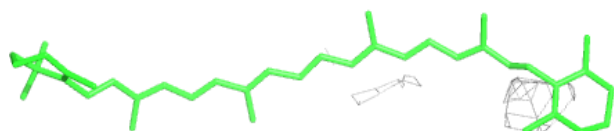
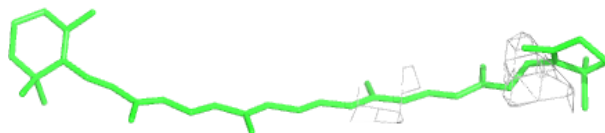
**Electron density around BCR P 516:**

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

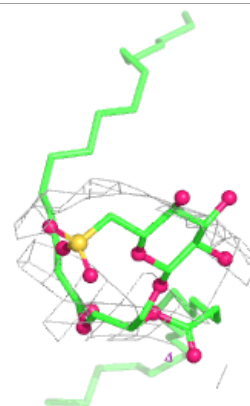
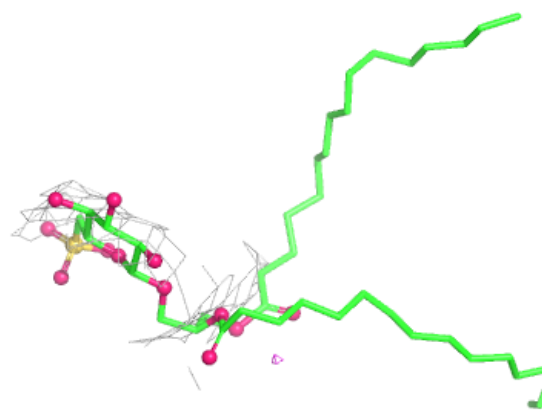


**Electron density around BCR S 101:**

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

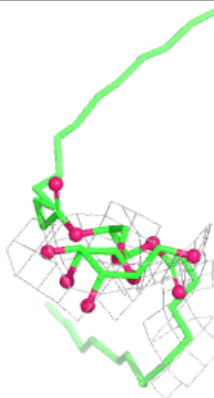
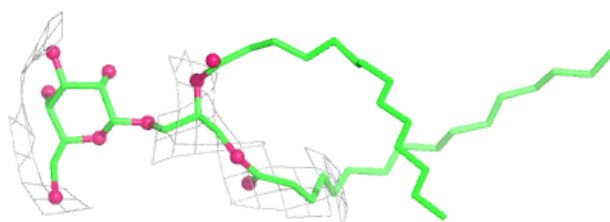
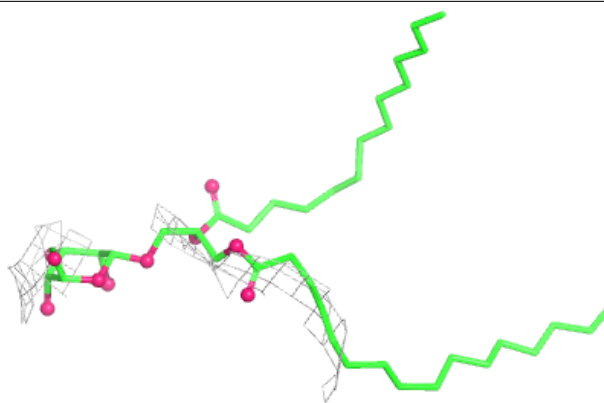
**Electron density around SQD A 414:**

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

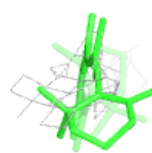
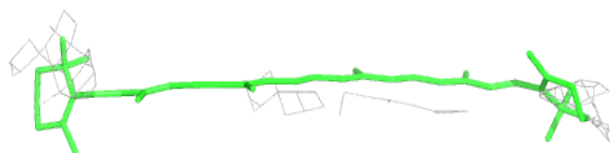
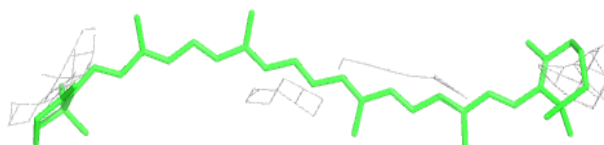


**Electron density around LMG B 623:**

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

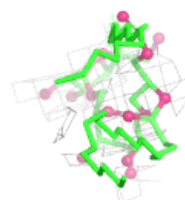
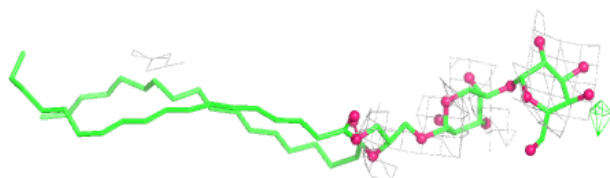
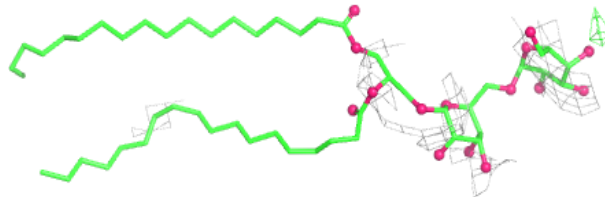
**Electron density around BCR W 101:**

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

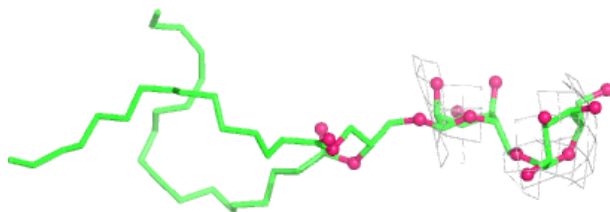
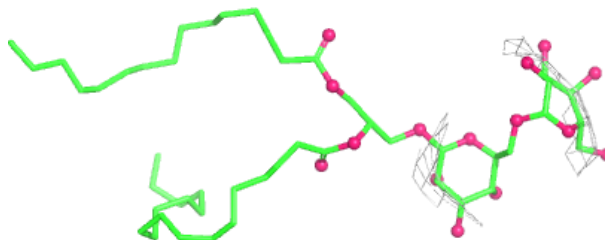


**Electron density around DGD C 518:**

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

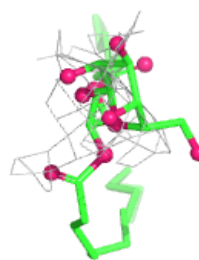
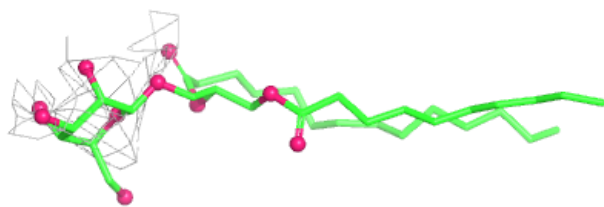
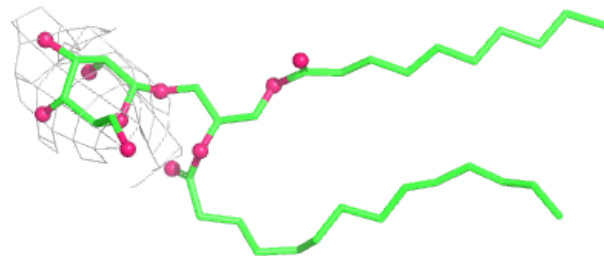
**Electron density around DGD D 408:**

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

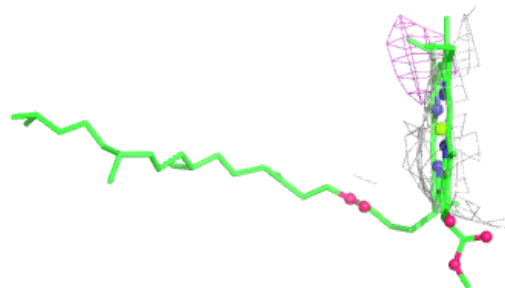


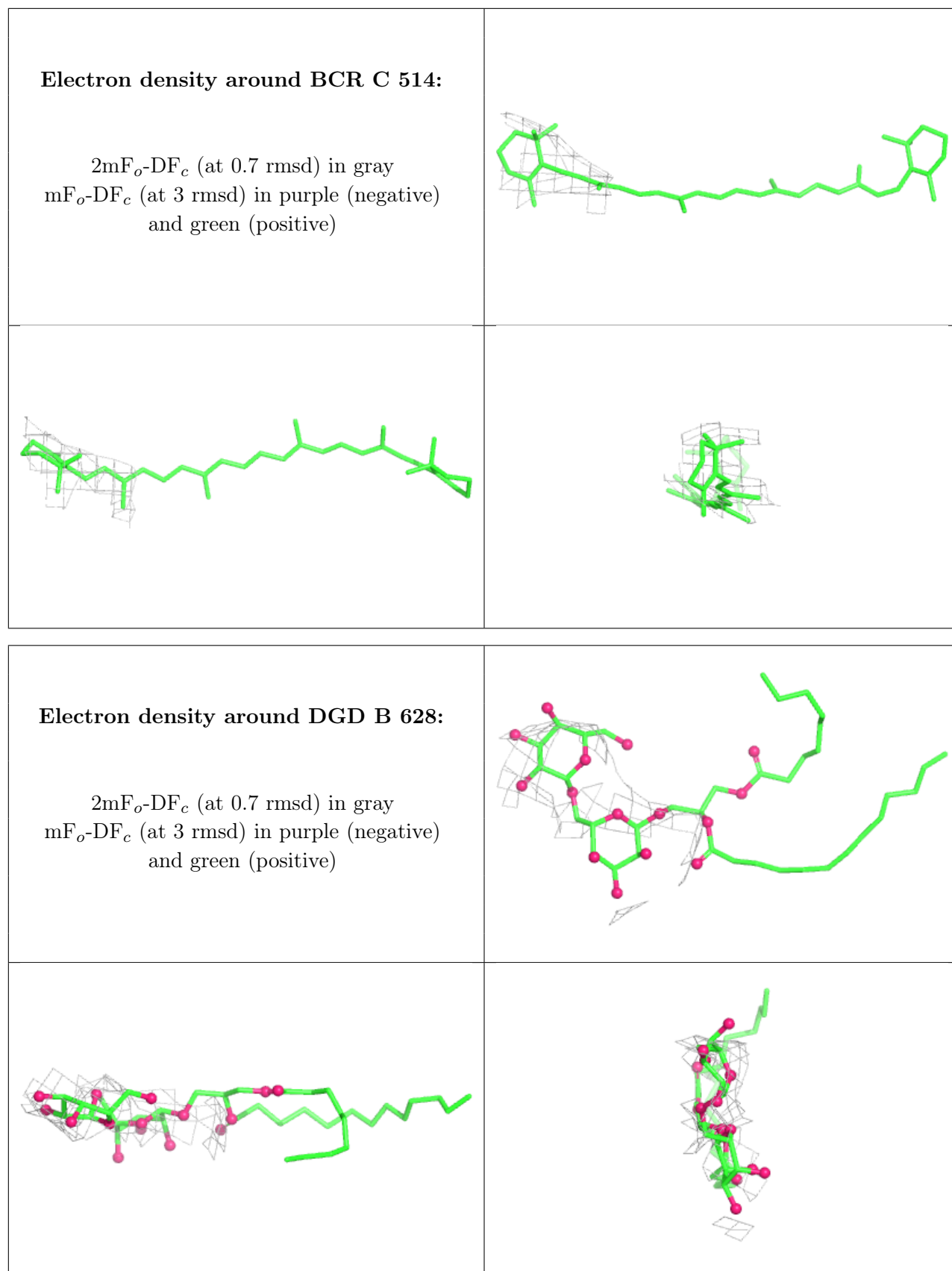
**Electron density around LMG a 102:**

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

**Electron density around CLA N 610:**

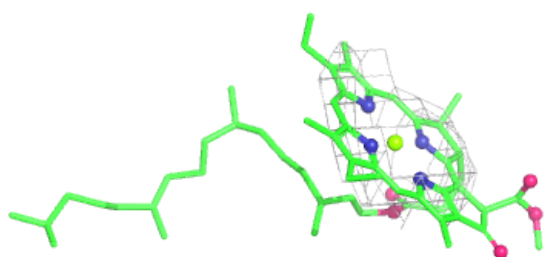
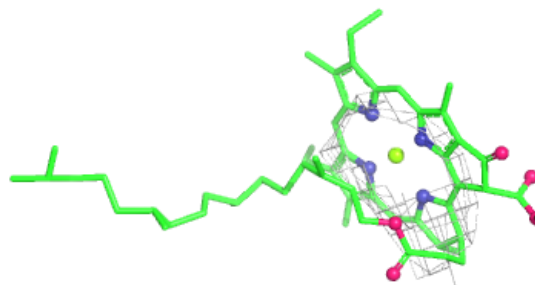
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



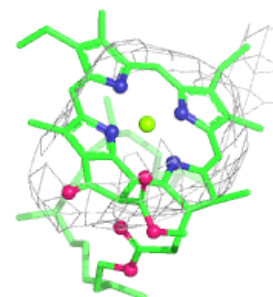
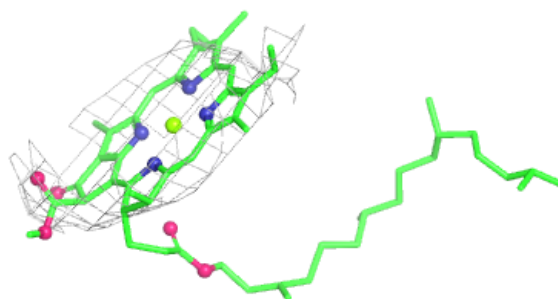


**Electron density around CLA C 505:**

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

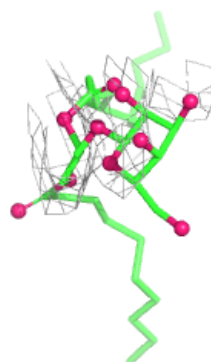
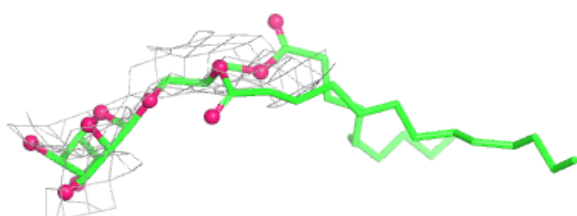
**Electron density around CLA P 513:**

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

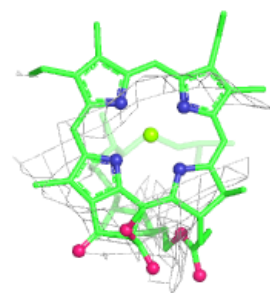
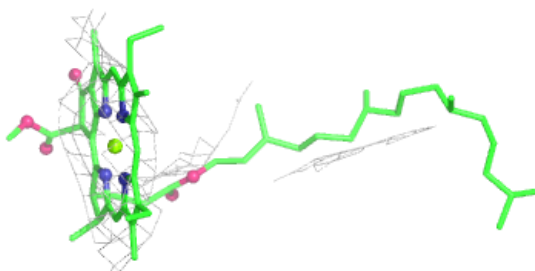
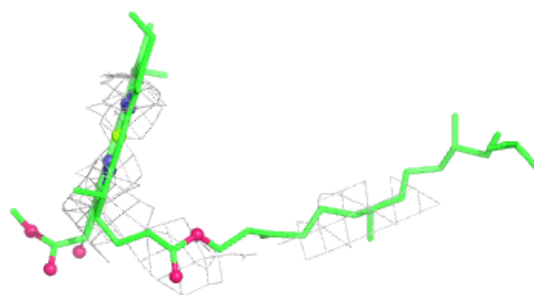


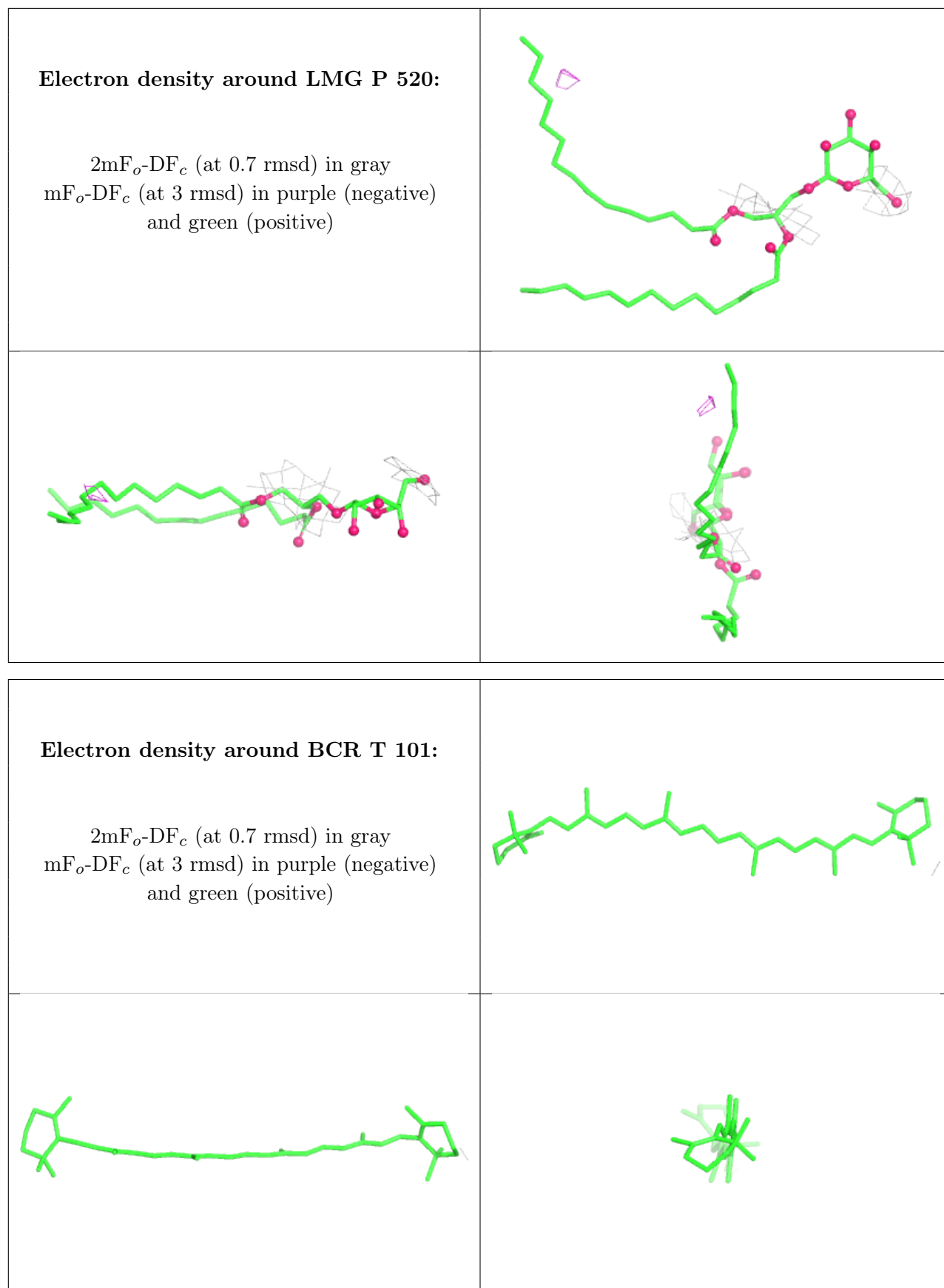
**Electron density around LMG D 412:**

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

**Electron density around CLA N 609:**

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



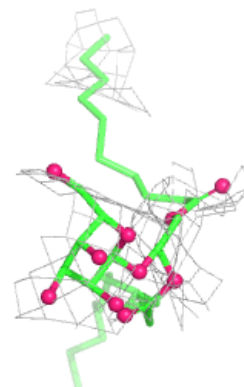
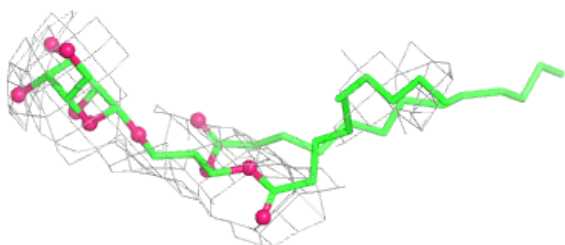
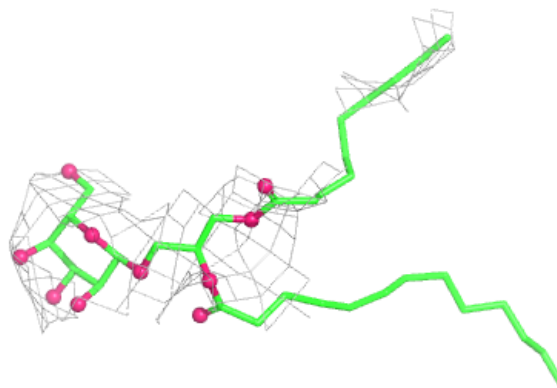


**Electron density around DGD Q 409:**

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

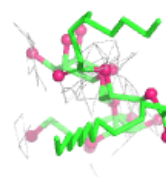
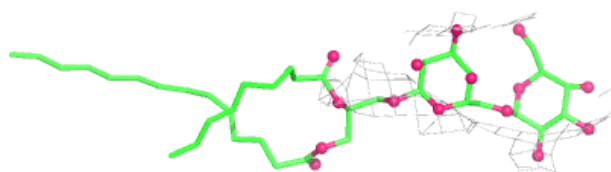
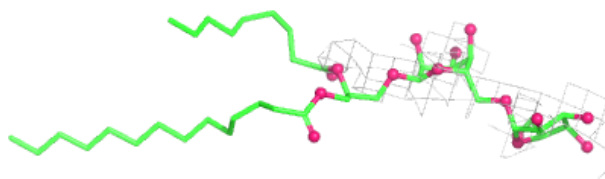
**Electron density around LMG Q 401:**

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

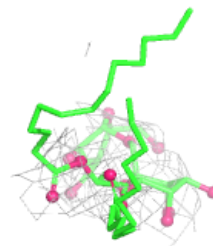
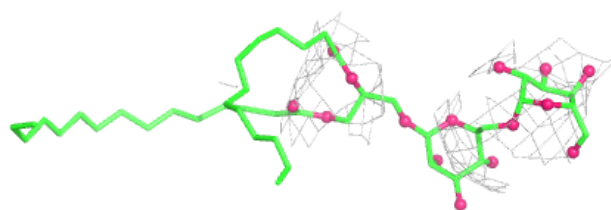
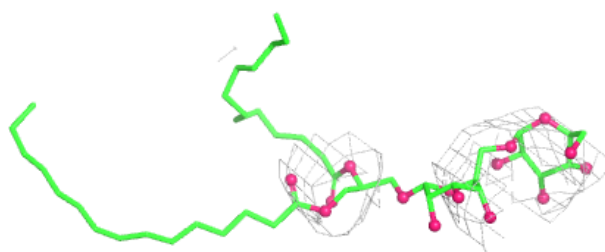


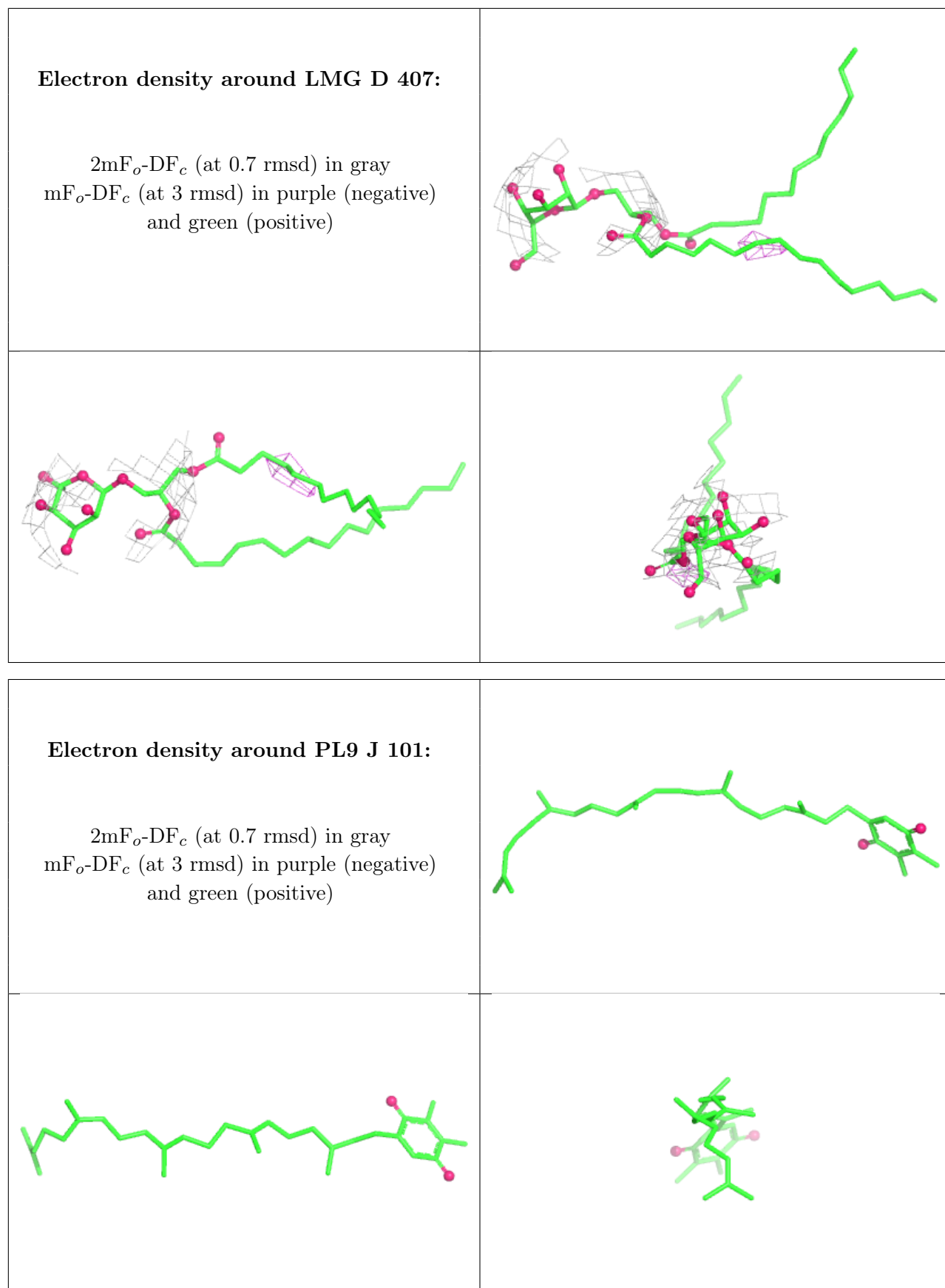
**Electron density around DGD C 516:**

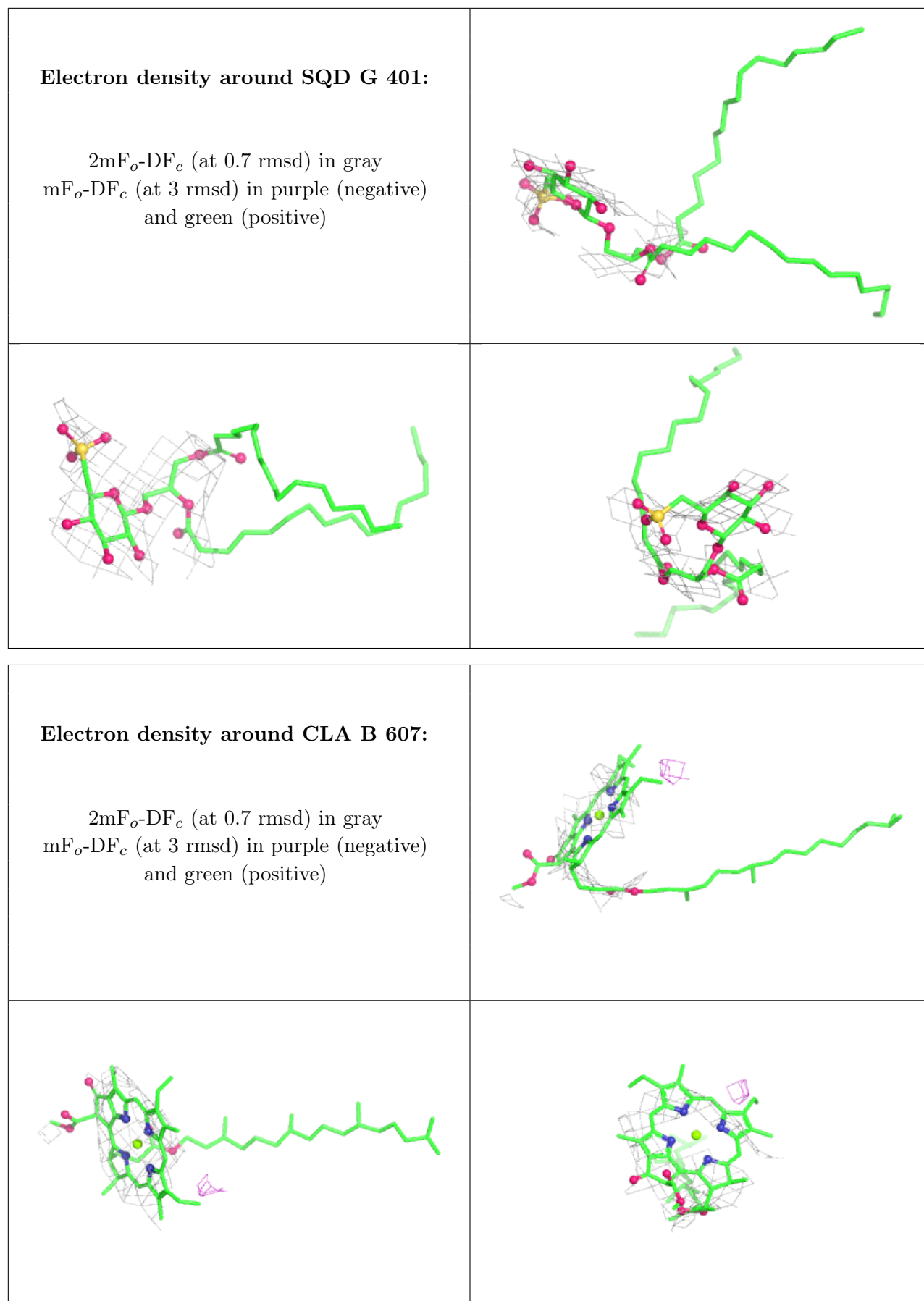
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

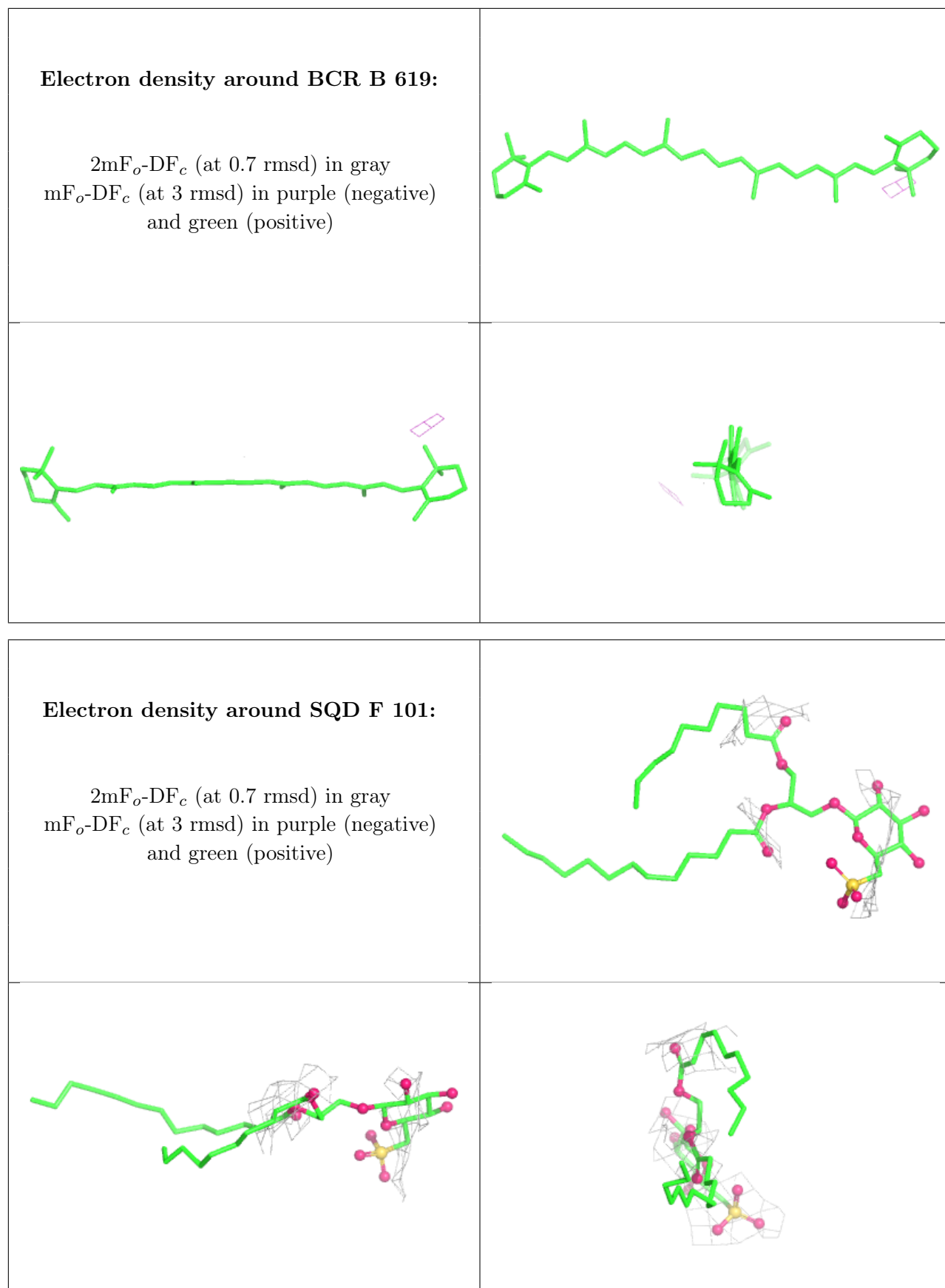
**Electron density around DGD B 621:**

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



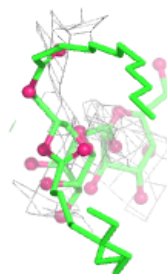
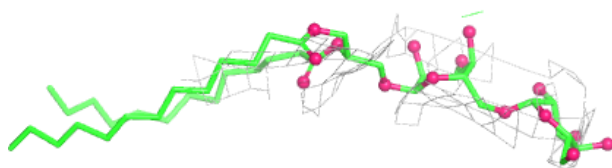




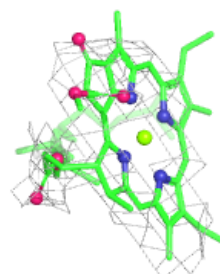
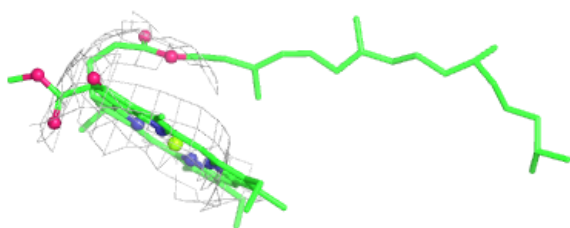
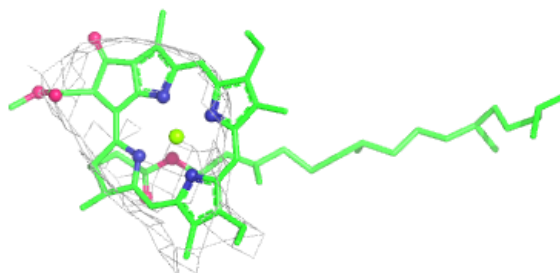


**Electron density around DGD A 407:**

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

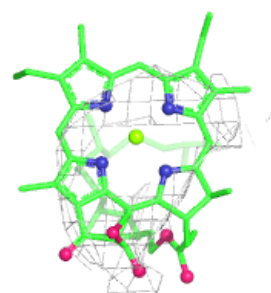
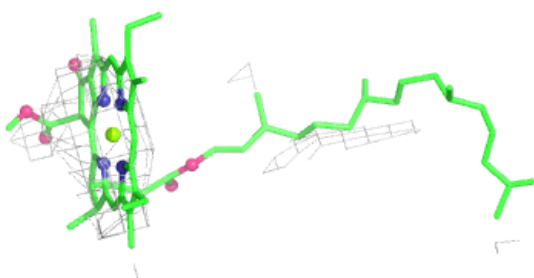
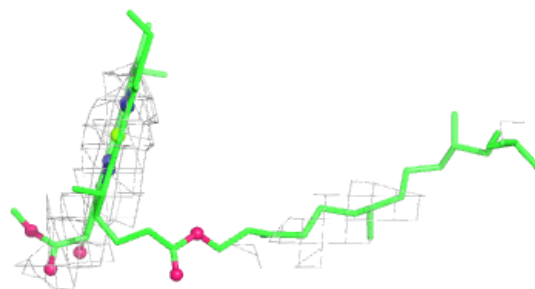
**Electron density around CLA B 608:**

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

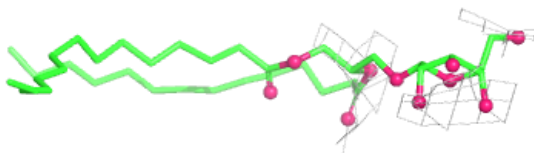
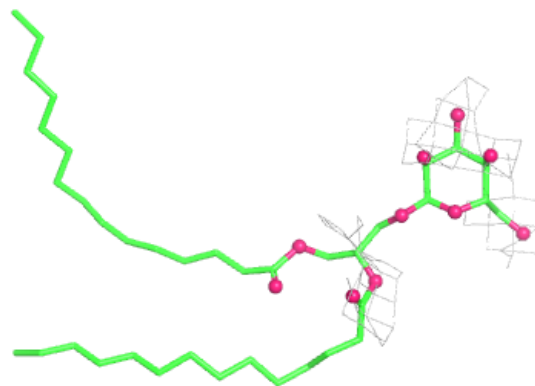


**Electron density around CLA B 605:**

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

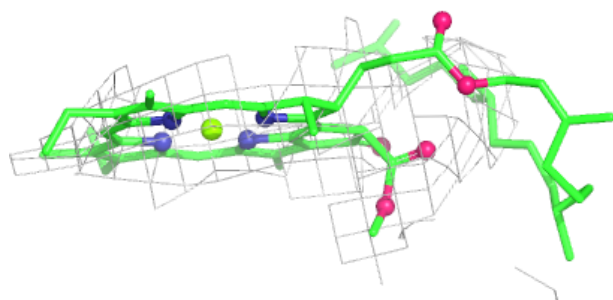
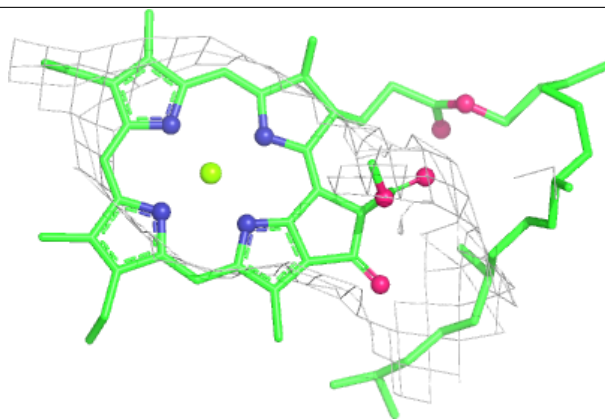
**Electron density around LMG C 519:**

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

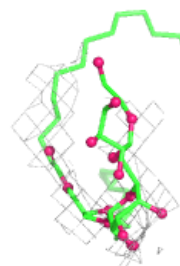
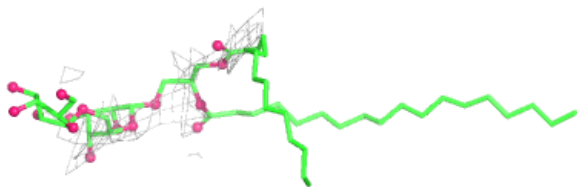


**Electron density around CLA B 610:**

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

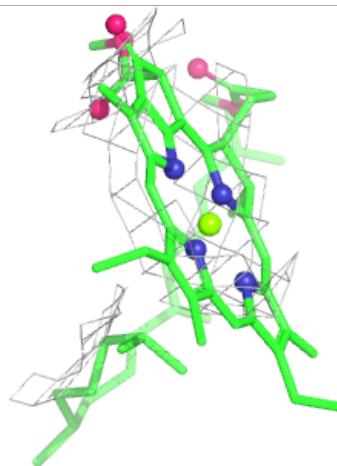
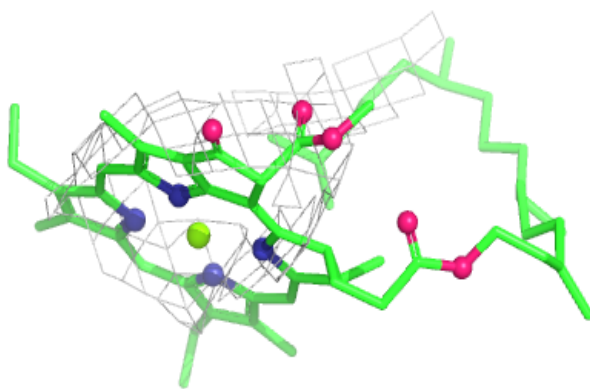
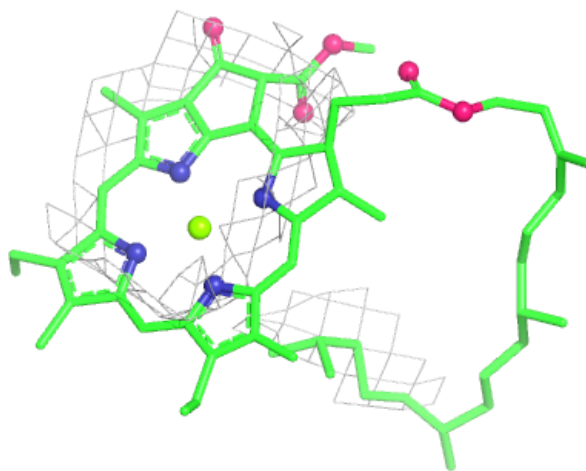
**Electron density around DGD C 517:**

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



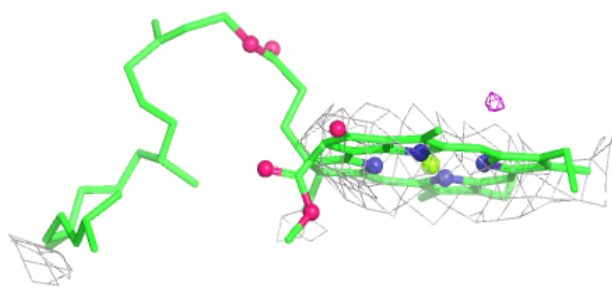
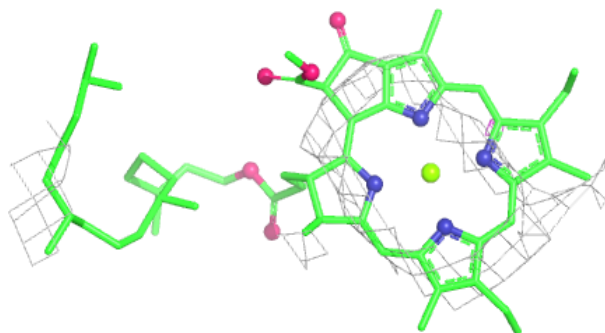
**Electron density around CLA B 615:**

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

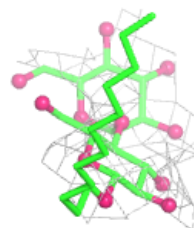
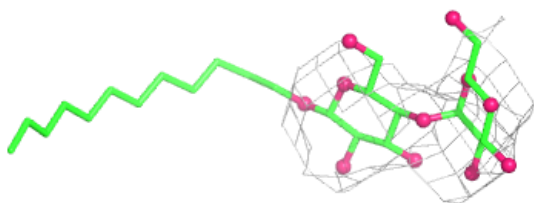
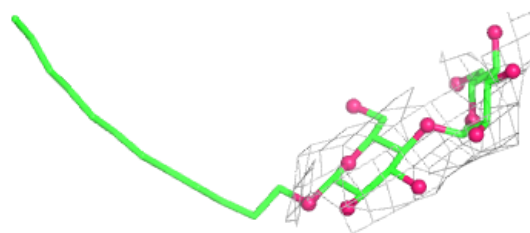


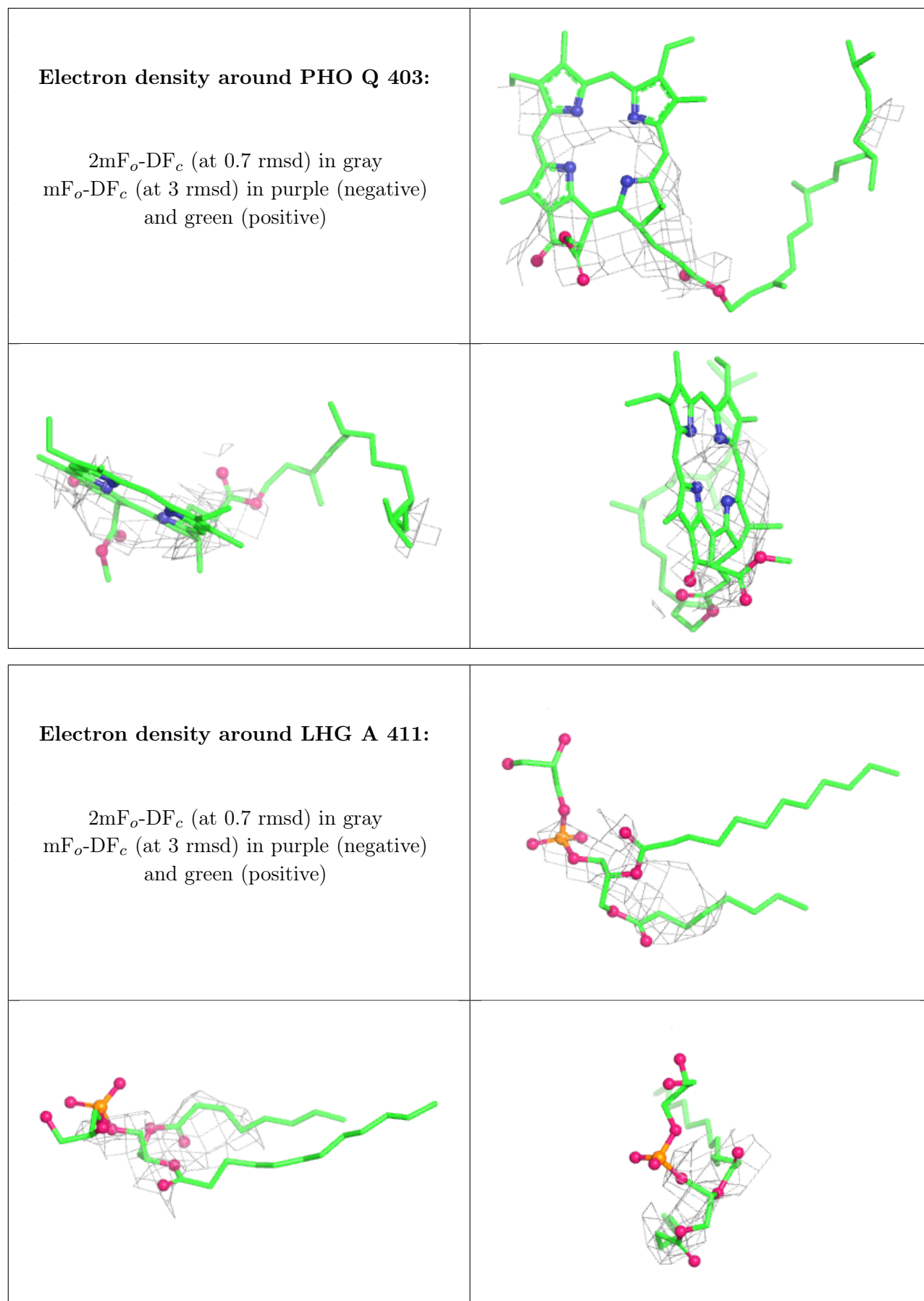
**Electron density around CLA N 616:**

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

**Electron density around LMT e 101:**

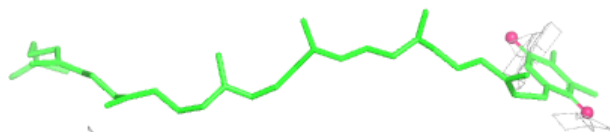
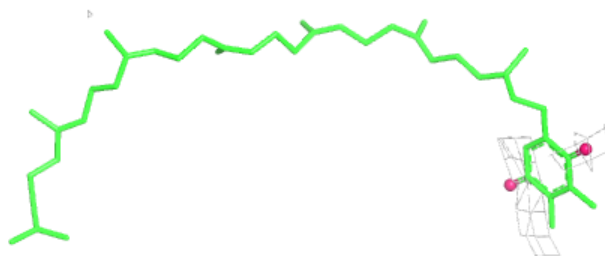
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



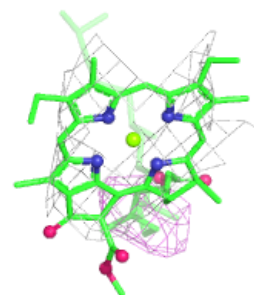
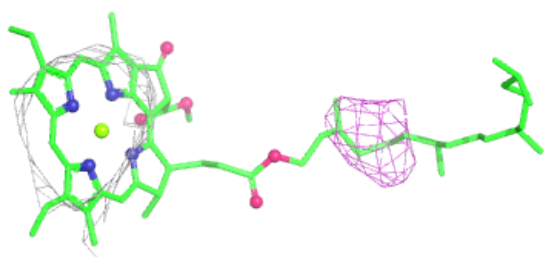
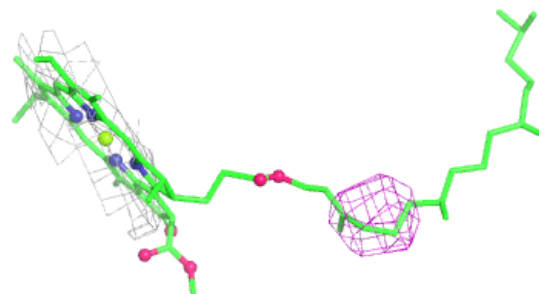


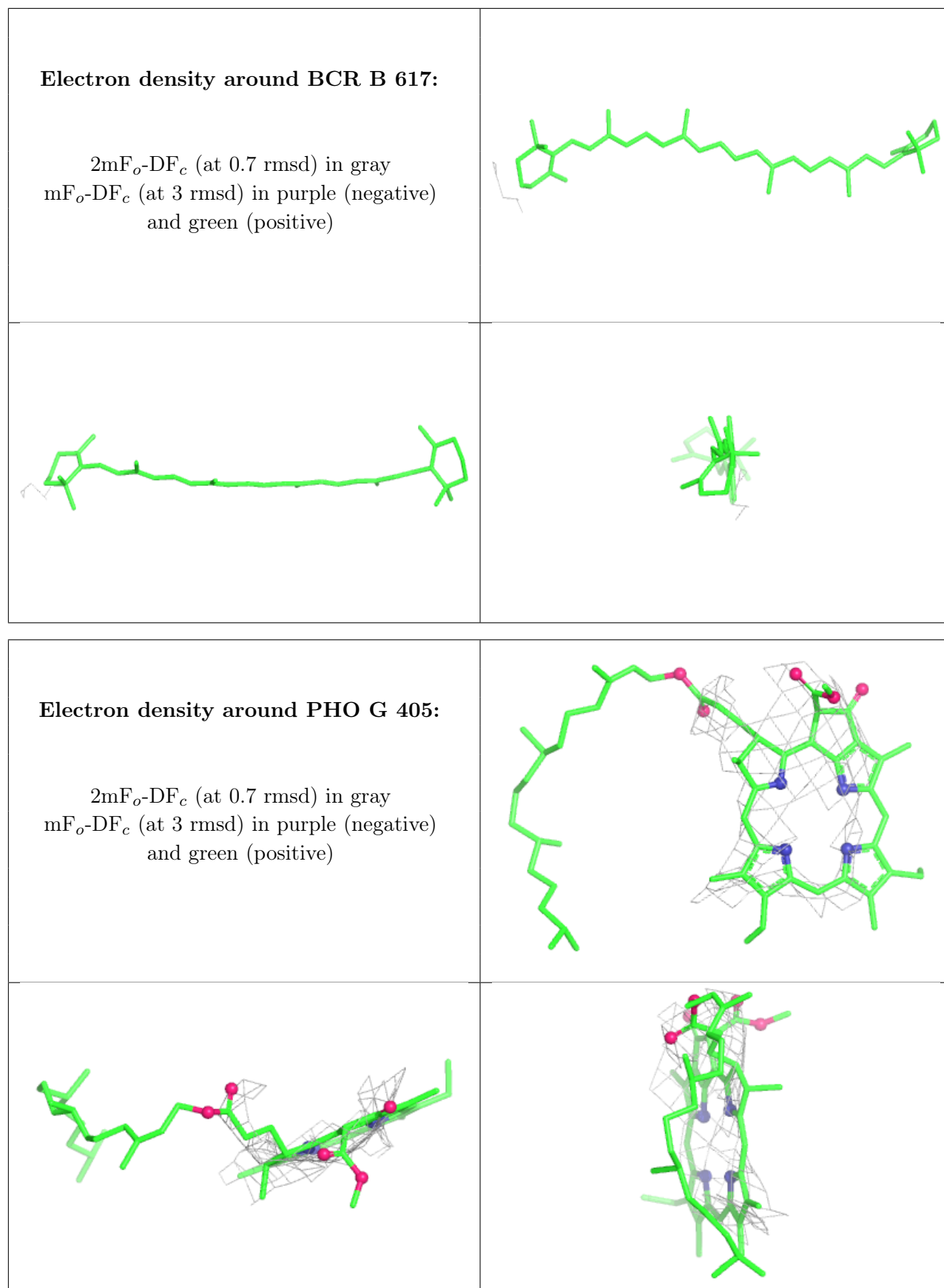
**Electron density around PL9 A 406:**

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

**Electron density around CLA D 401:**

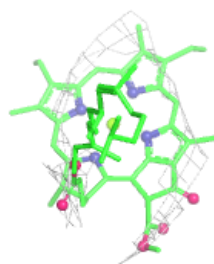
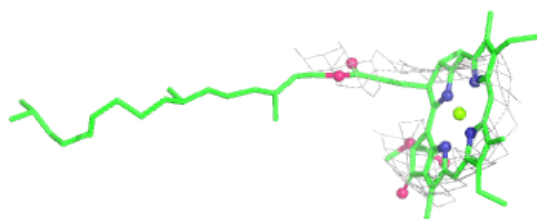
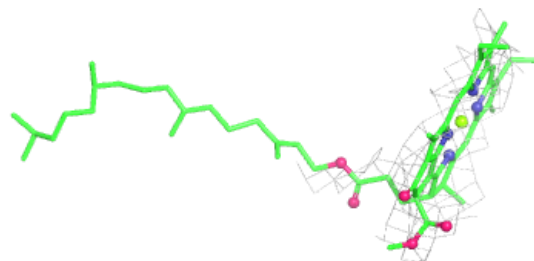
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



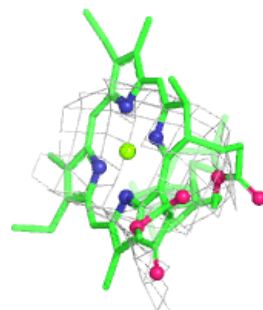
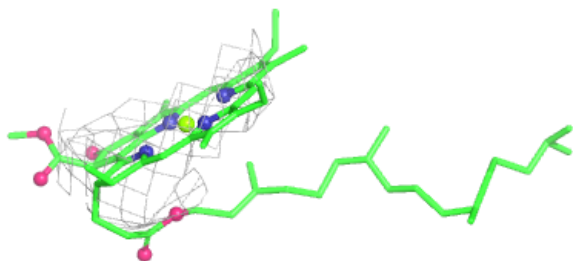
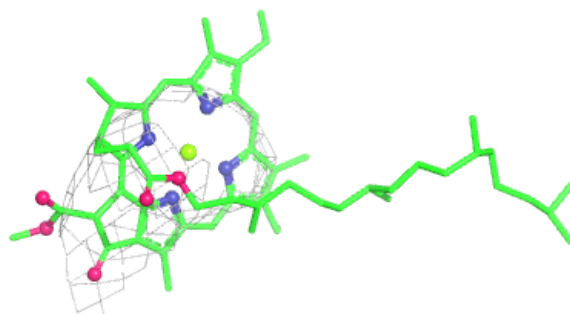


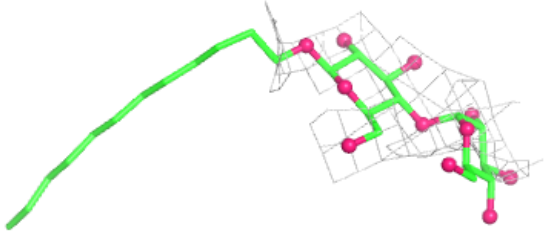
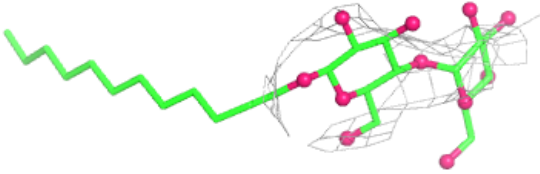
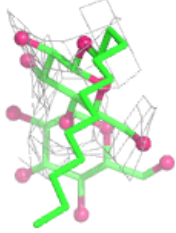
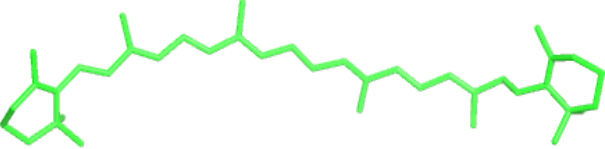

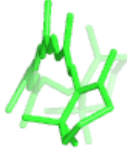
**Electron density around CLA N 608:**

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

**Electron density around CLA N 618:**

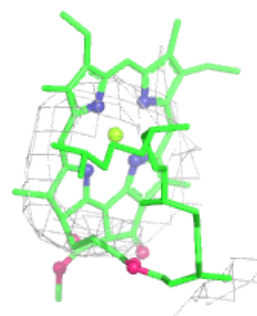
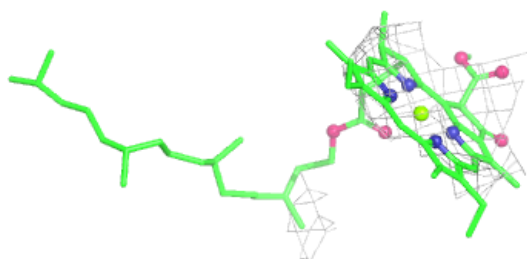
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



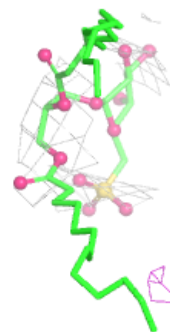
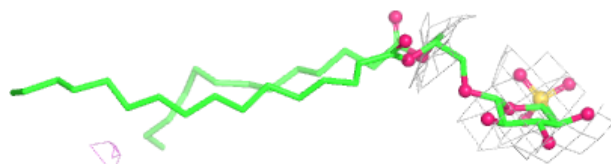
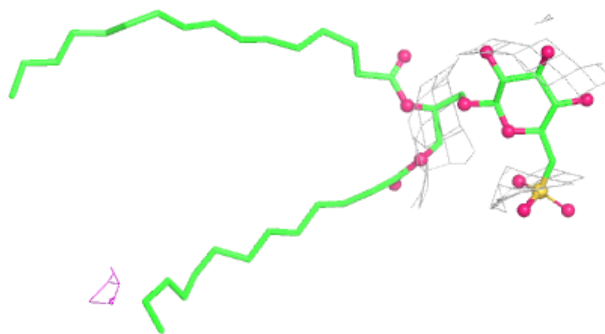
<p><b>Electron density around LMT M 102:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rmsd) in gray <math>mF_o-DF_c</math> (at 3 rmsd) in purple (negative) and green (positive)</p>	 A 3D molecular model of LMT M 102 is shown in stick representation. The atoms are colored: carbon in green, oxygen in red, and nitrogen in blue. The model is overlaid on a gray mesh representing the $2mF_o-DF_c$ electron density map at 0.7 Å resolution. Purple and green mesh regions represent the $mF_o-DF_c$ map at 3 Å resolution, indicating negative and positive density respectively.
 A 3D molecular model of LMT M 102 is shown in stick representation, similar to the top-right panel. It is overlaid on a gray mesh representing the $2mF_o-DF_c$ electron density map at 0.7 Å resolution.	 A 3D molecular model of LMT M 102 is shown in stick representation, similar to the top-right panel. It is overlaid on a purple mesh representing the $mF_o-DF_c$ electron density map at 3 Å resolution, highlighting negative density.
<p><b>Electron density around BCR T 102:</b></p> <p><math>2mF_o-DF_c</math> (at 0.7 rmsd) in gray <math>mF_o-DF_c</math> (at 3 rmsd) in purple (negative) and green (positive)</p>	 A 3D molecular model of BCR T 102 is shown in stick representation. The atoms are colored: carbon in green, oxygen in red, and nitrogen in blue. The model is overlaid on a gray mesh representing the $2mF_o-DF_c$ electron density map at 0.7 Å resolution.
 A 3D molecular model of BCR T 102 is shown in stick representation, similar to the bottom-right panel. It is overlaid on a gray mesh representing the $2mF_o-DF_c$ electron density map at 0.7 Å resolution.	 A 3D molecular model of BCR T 102 is shown in stick representation, similar to the bottom-right panel. It is overlaid on a purple mesh representing the $mF_o-DF_c$ electron density map at 3 Å resolution, highlighting negative density.

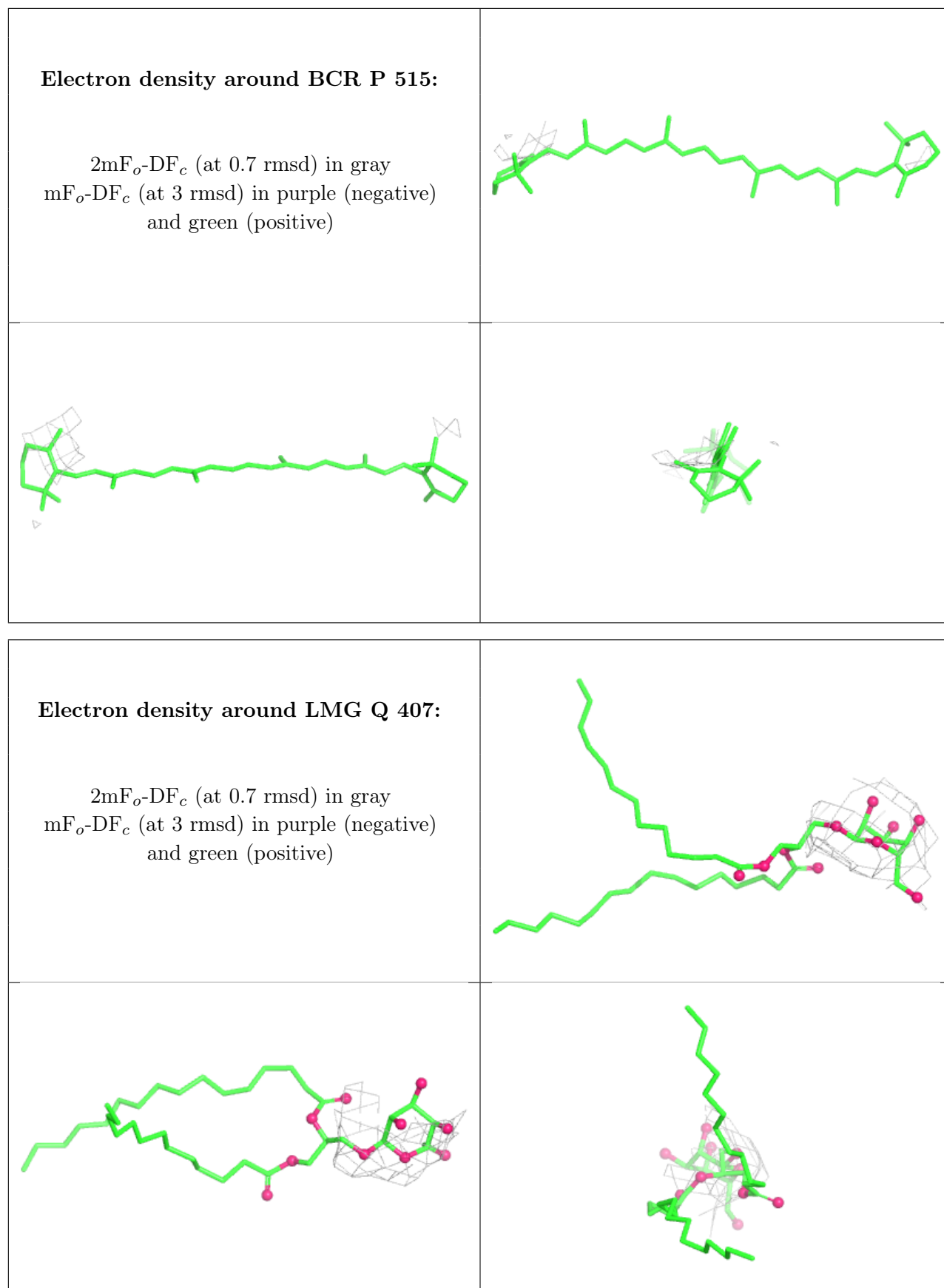
**Electron density around CLA P 511:**

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

**Electron density around SQD G 410:**

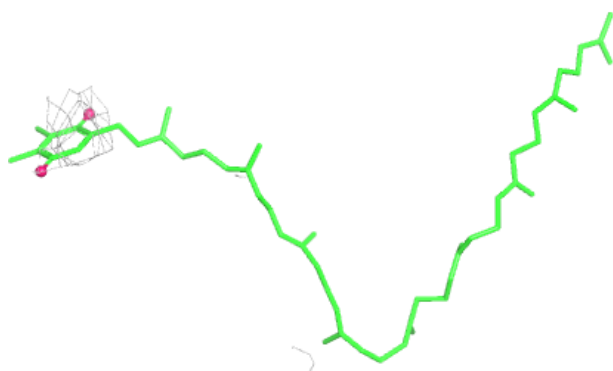
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



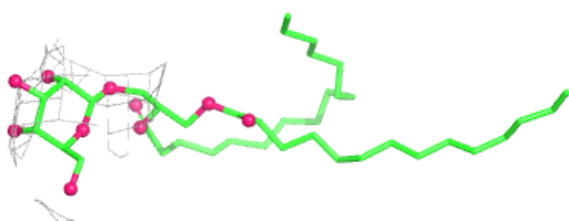
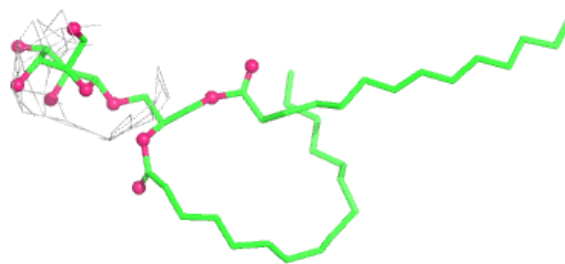


**Electron density around PL9 Q 405:**

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

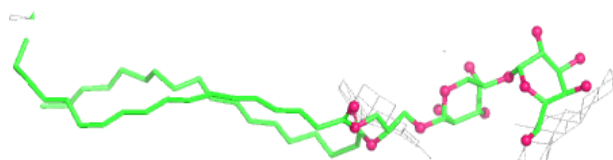
**Electron density around LMG B 622:**

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

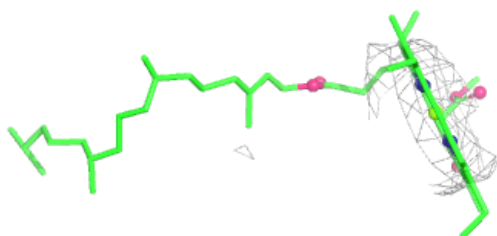
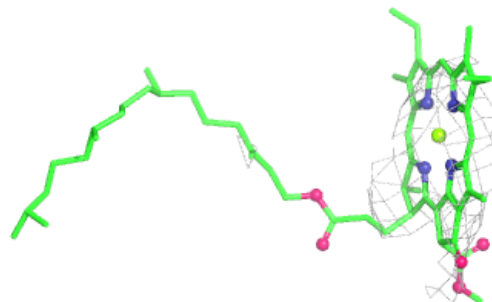


**Electron density around DGD P 519:**

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

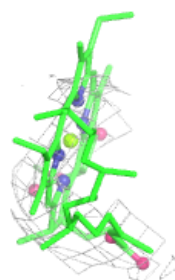
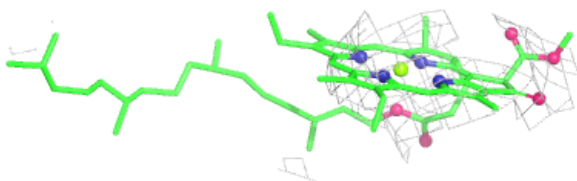
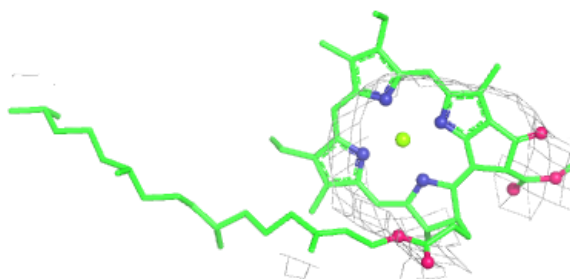
**Electron density around CLA D 403:**

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

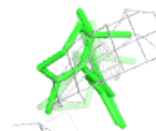
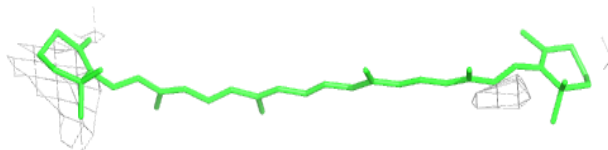


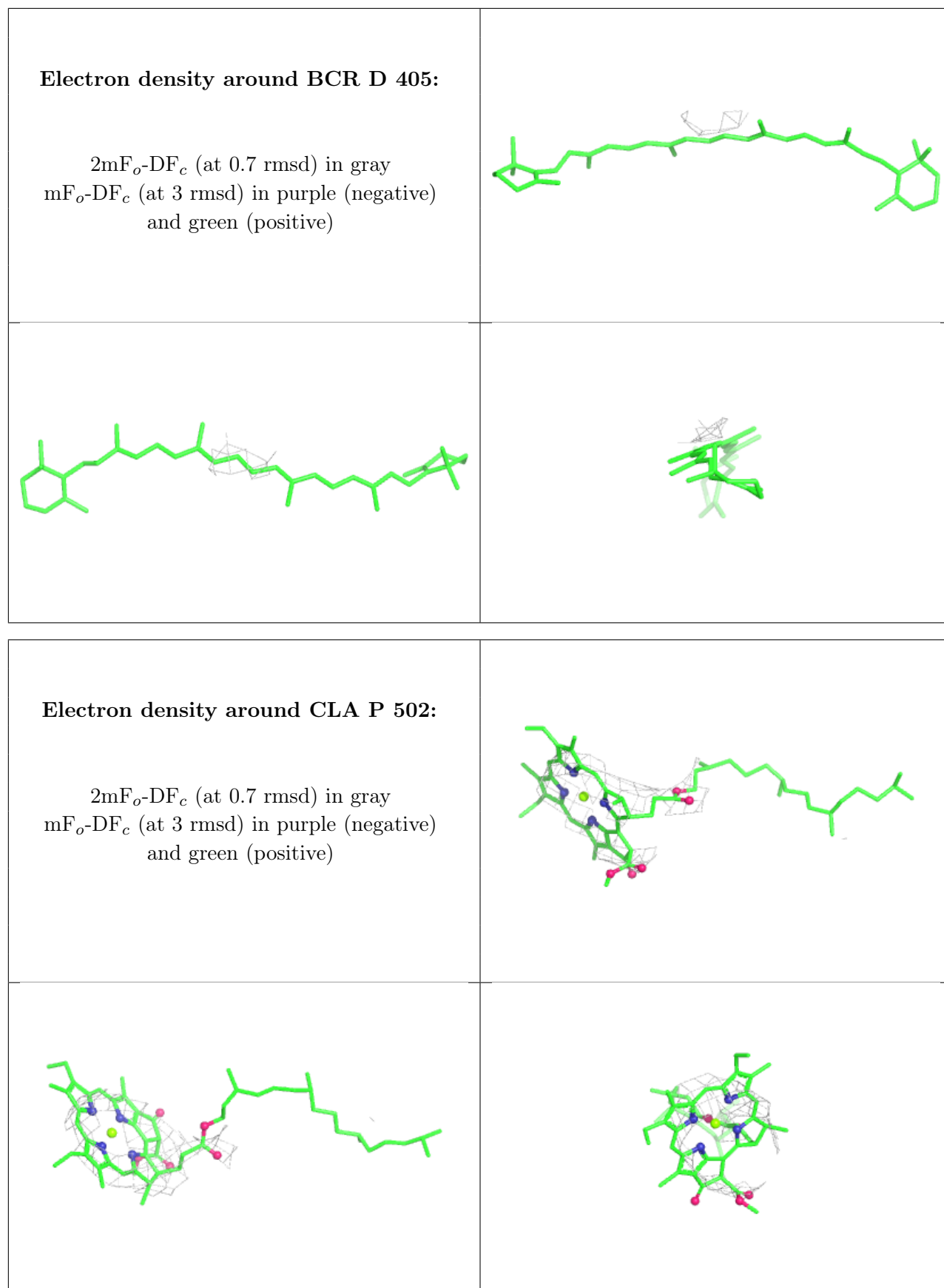
**Electron density around CLA C 501:**

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

**Electron density around BCR C 515:**

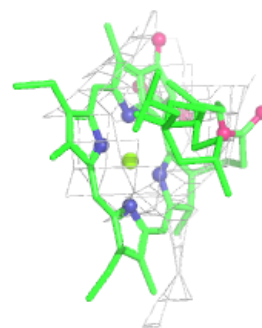
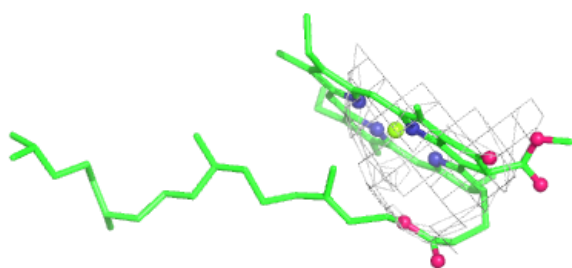
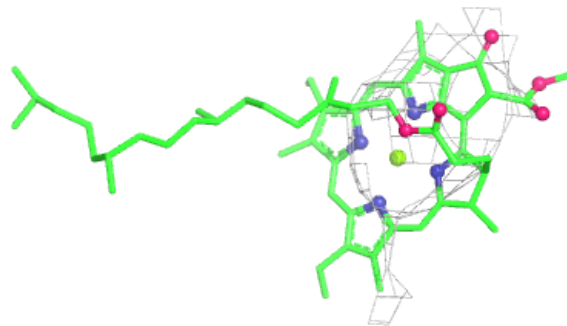
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)



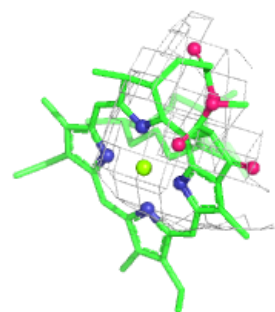
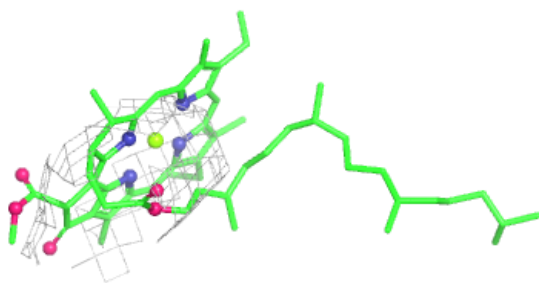
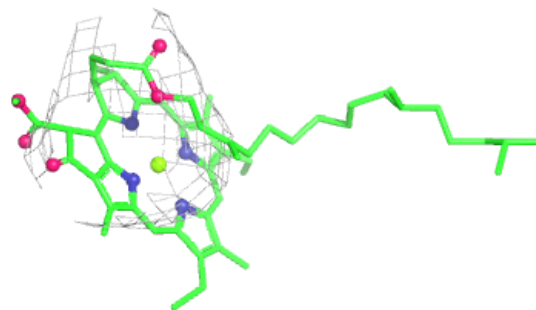


**Electron density around CLA B 614:**

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

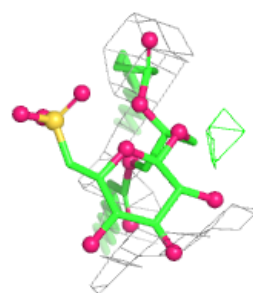
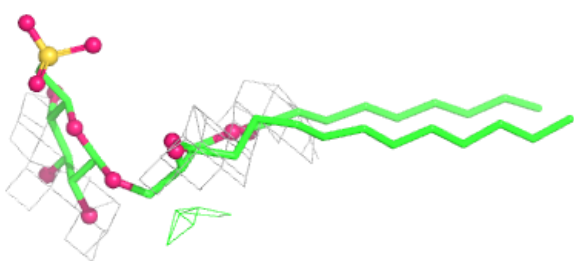
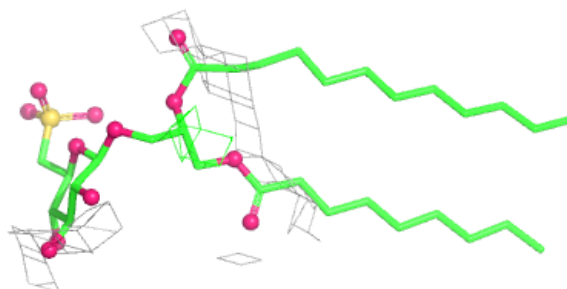
**Electron density around CLA P 505:**

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

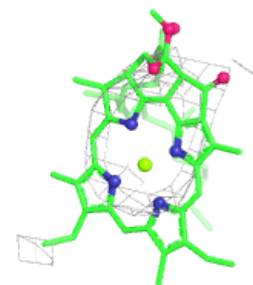
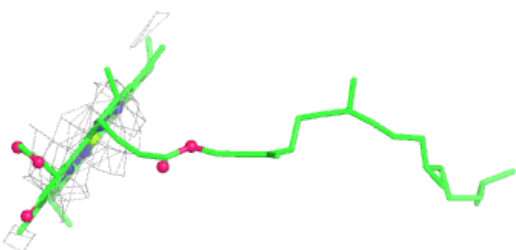
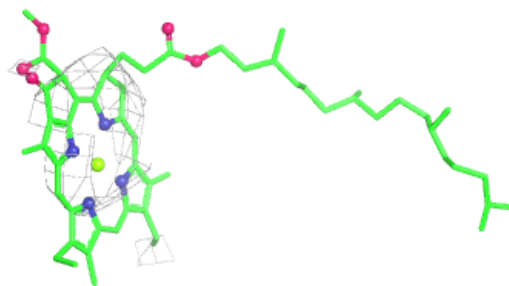


**Electron density around SQD B 624:**

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

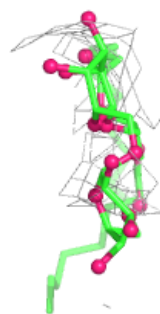
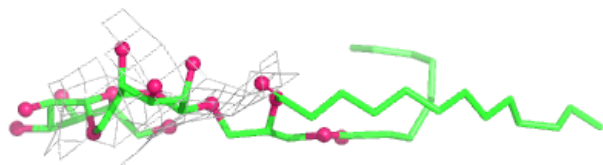
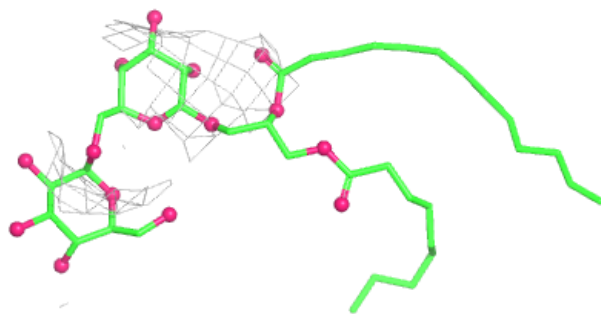
**Electron density around CLA A 405:**

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

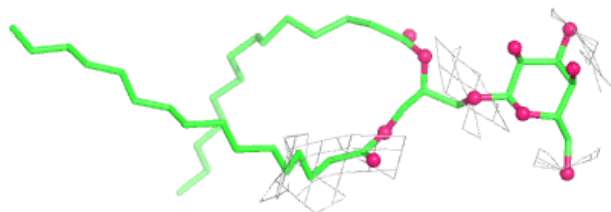
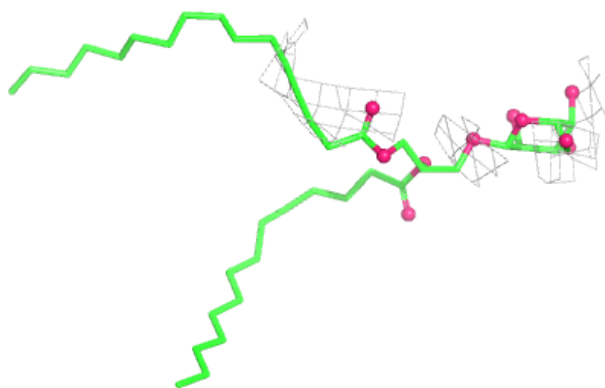


**Electron density around DGD N 602:**

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

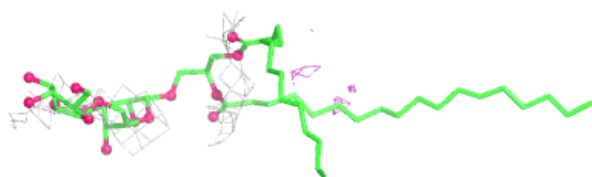
**Electron density around LMG N 623:**

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

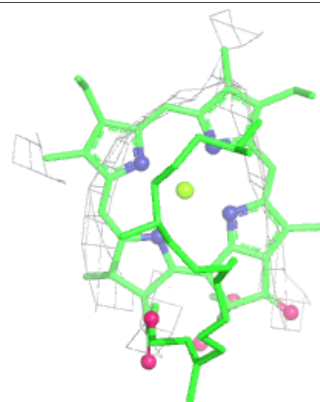
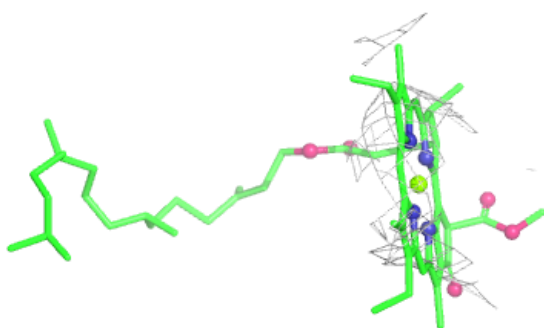
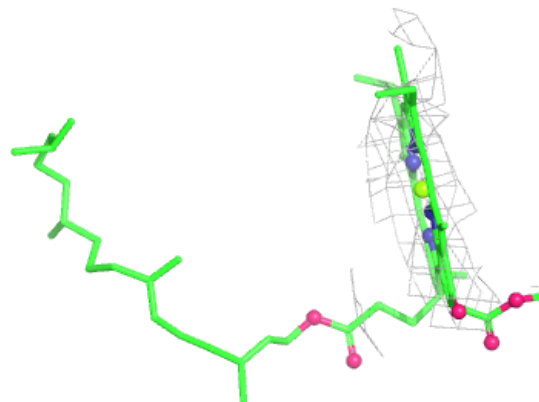


**Electron density around DGD P 518:**

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

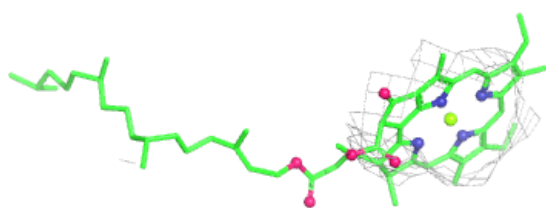
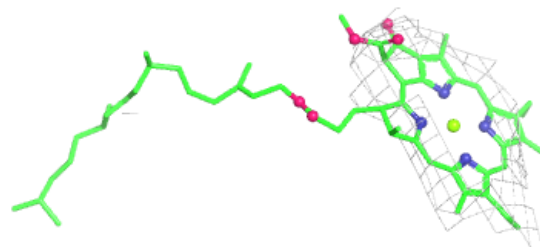
**Electron density around CLA C 506:**

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

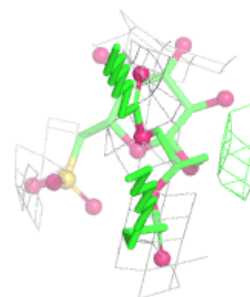
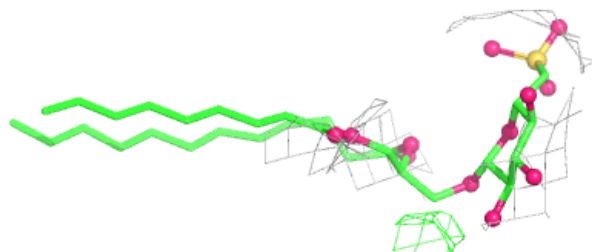
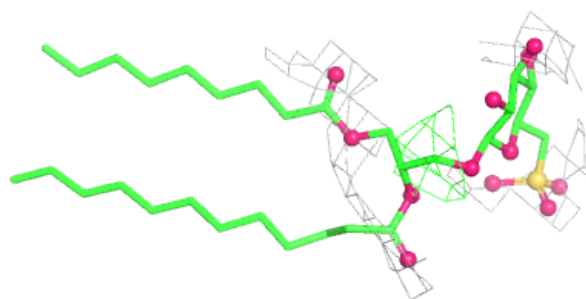


**Electron density around CLA G 402:**

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

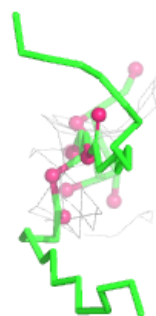
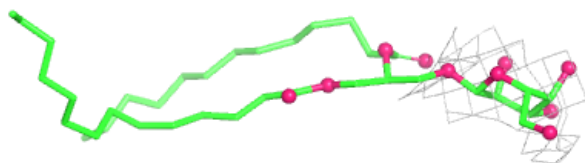
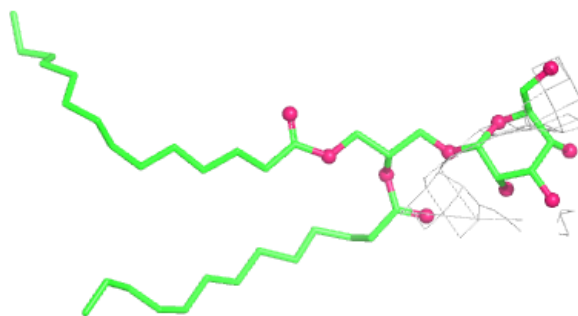
**Electron density around SQD Q 408:**

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

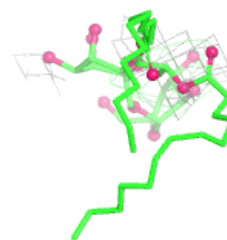
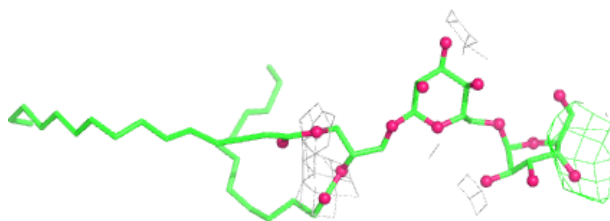


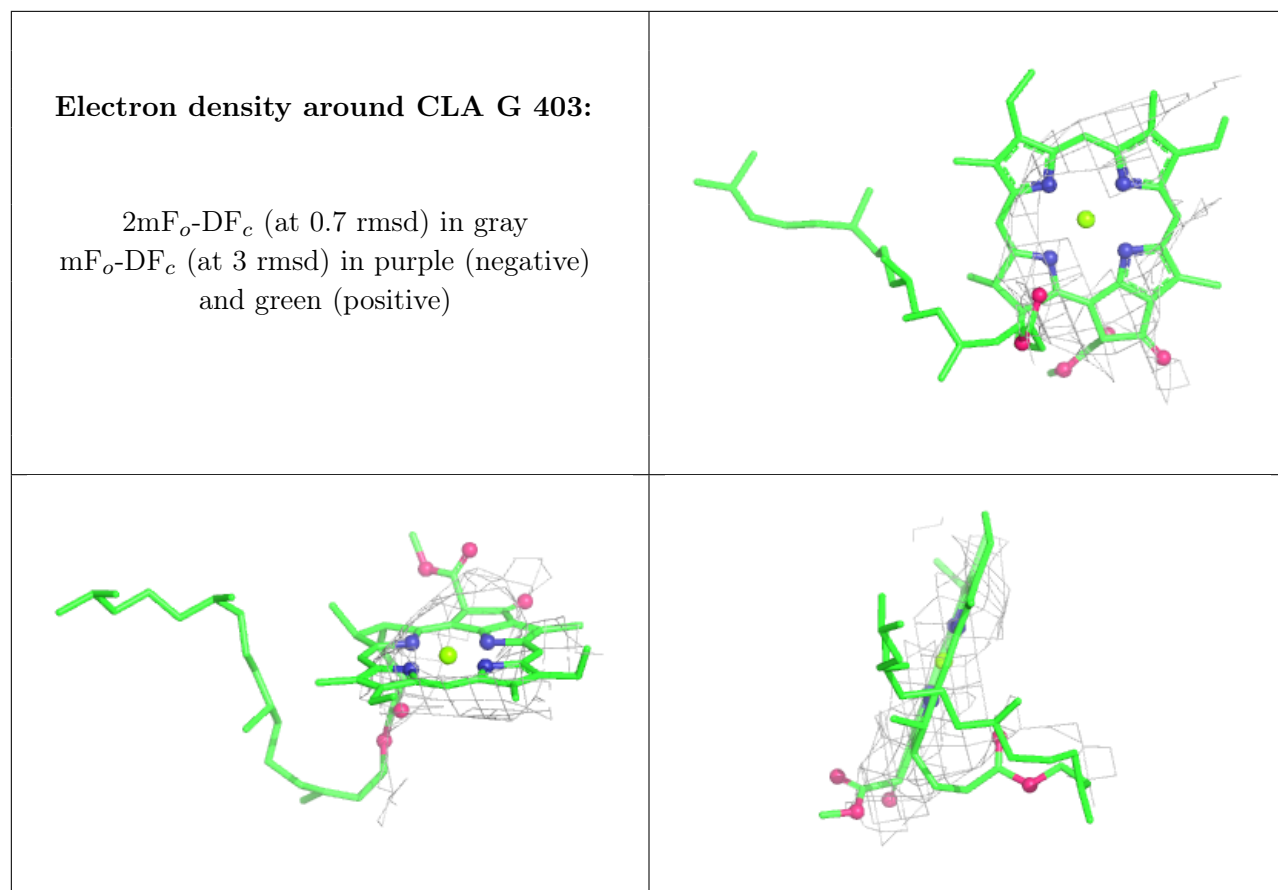
**Electron density around LMG Q 406:**

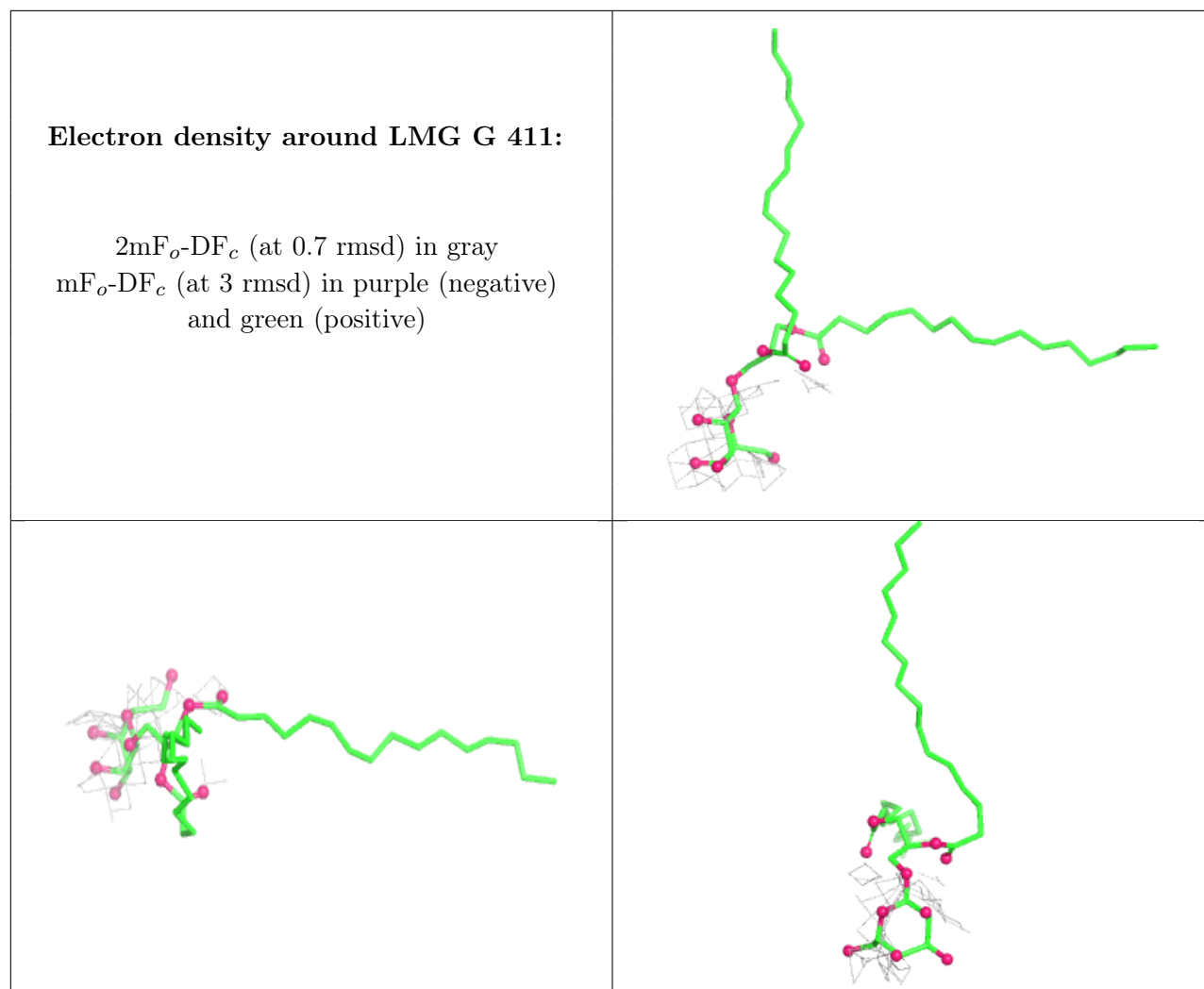
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DGD W 102:**

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

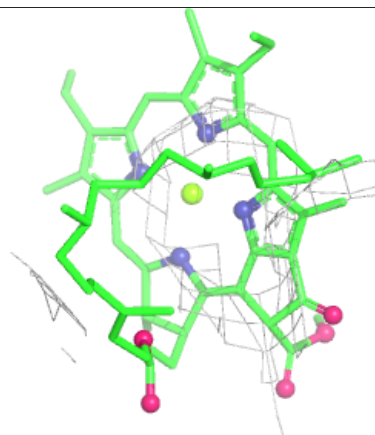
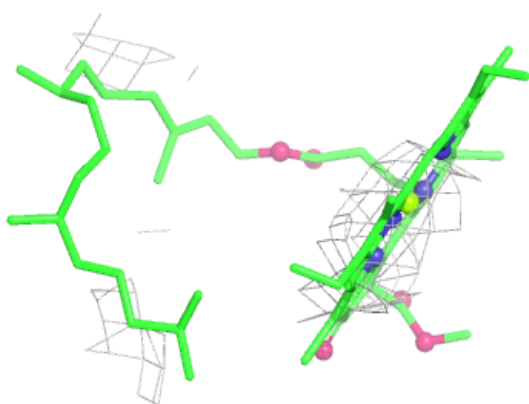
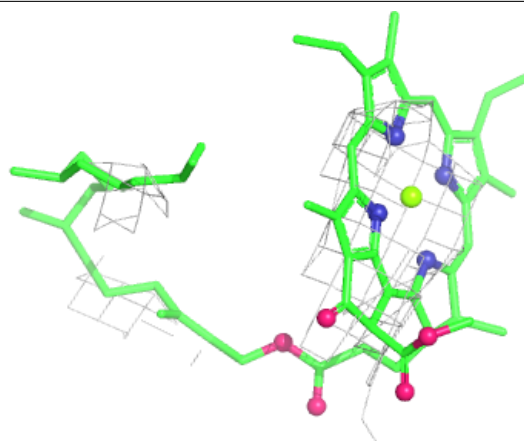






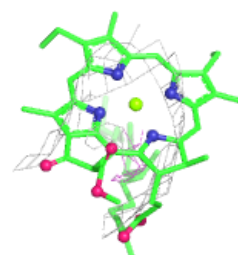
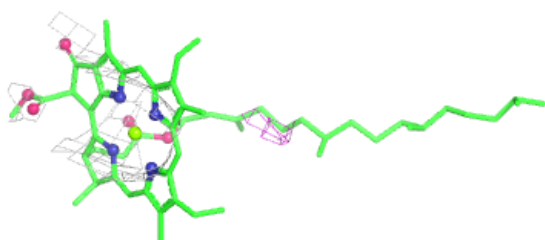
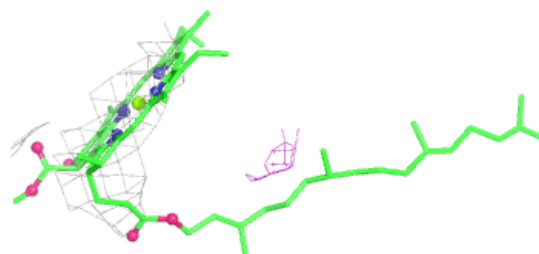
**Electron density around CLA P 503:**

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

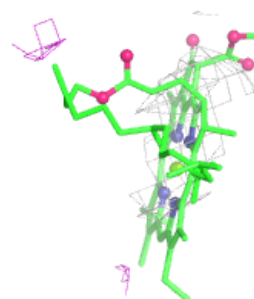
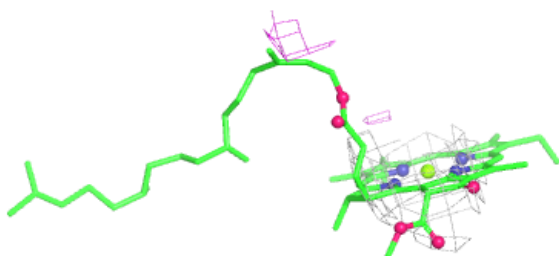
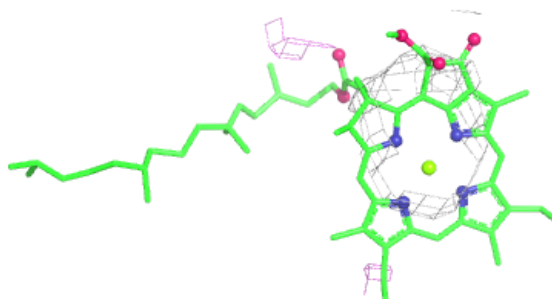


**Electron density around CLA P 504:**

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

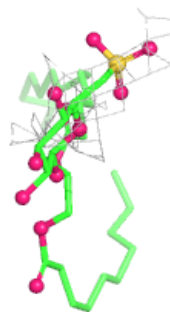
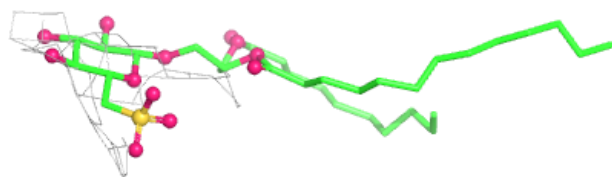
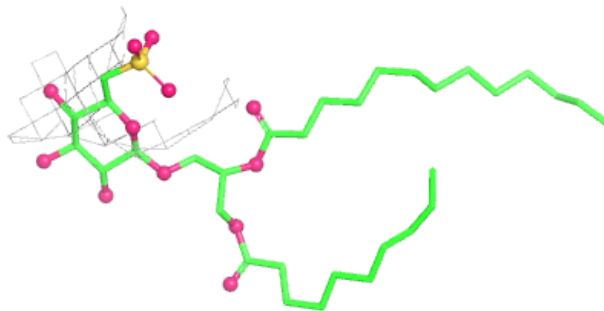
**Electron density around CLA A 403:**

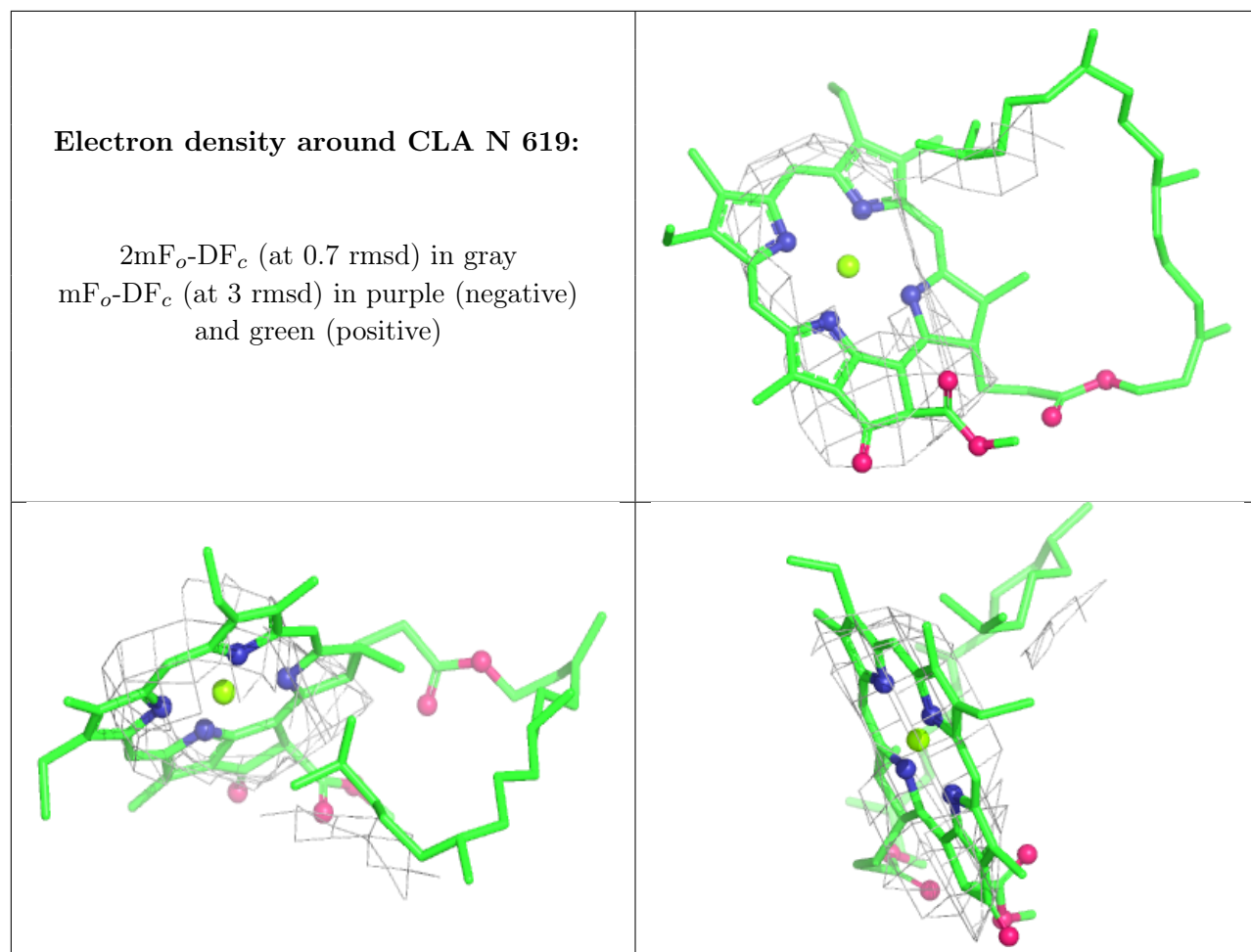
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

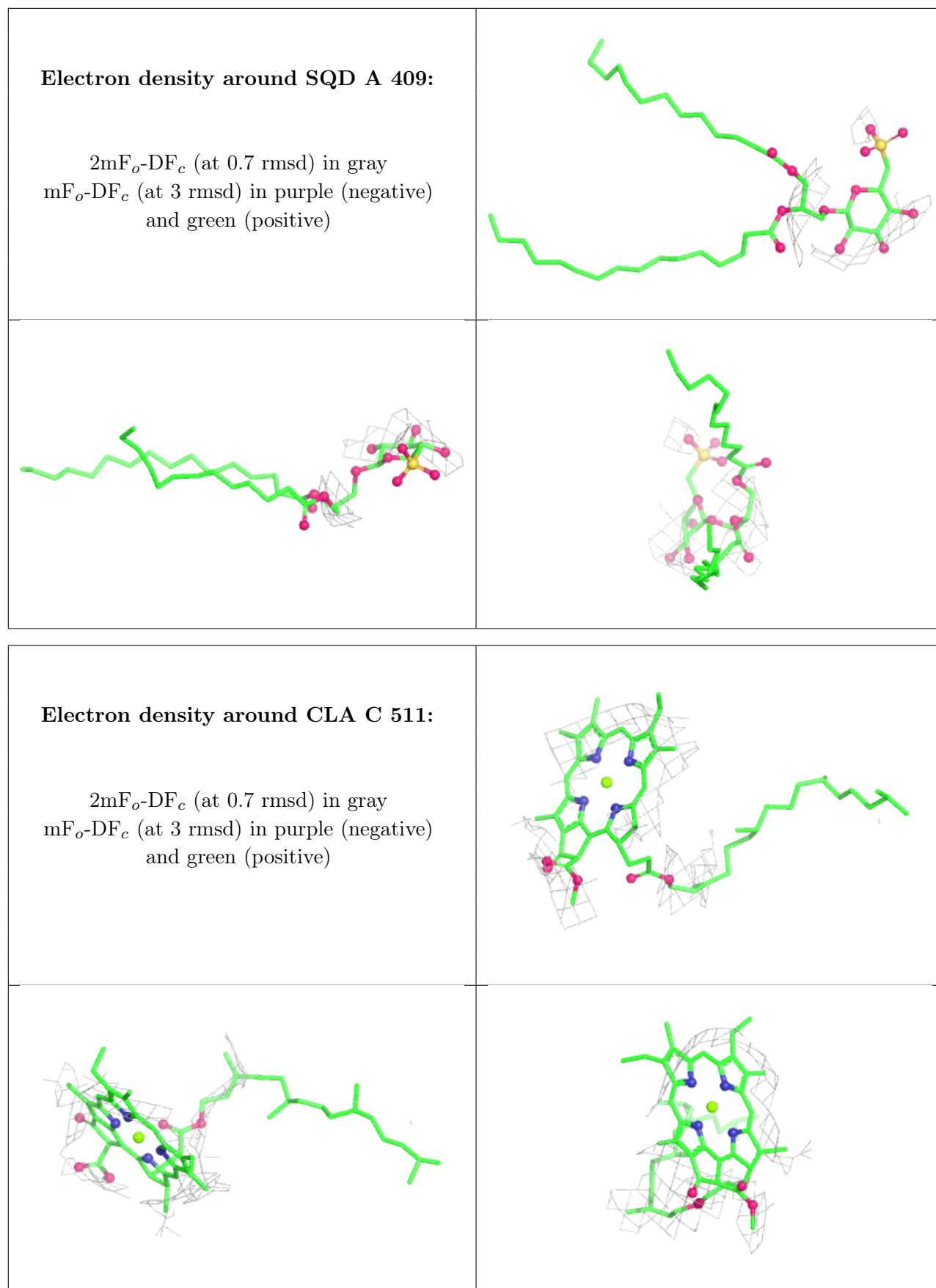


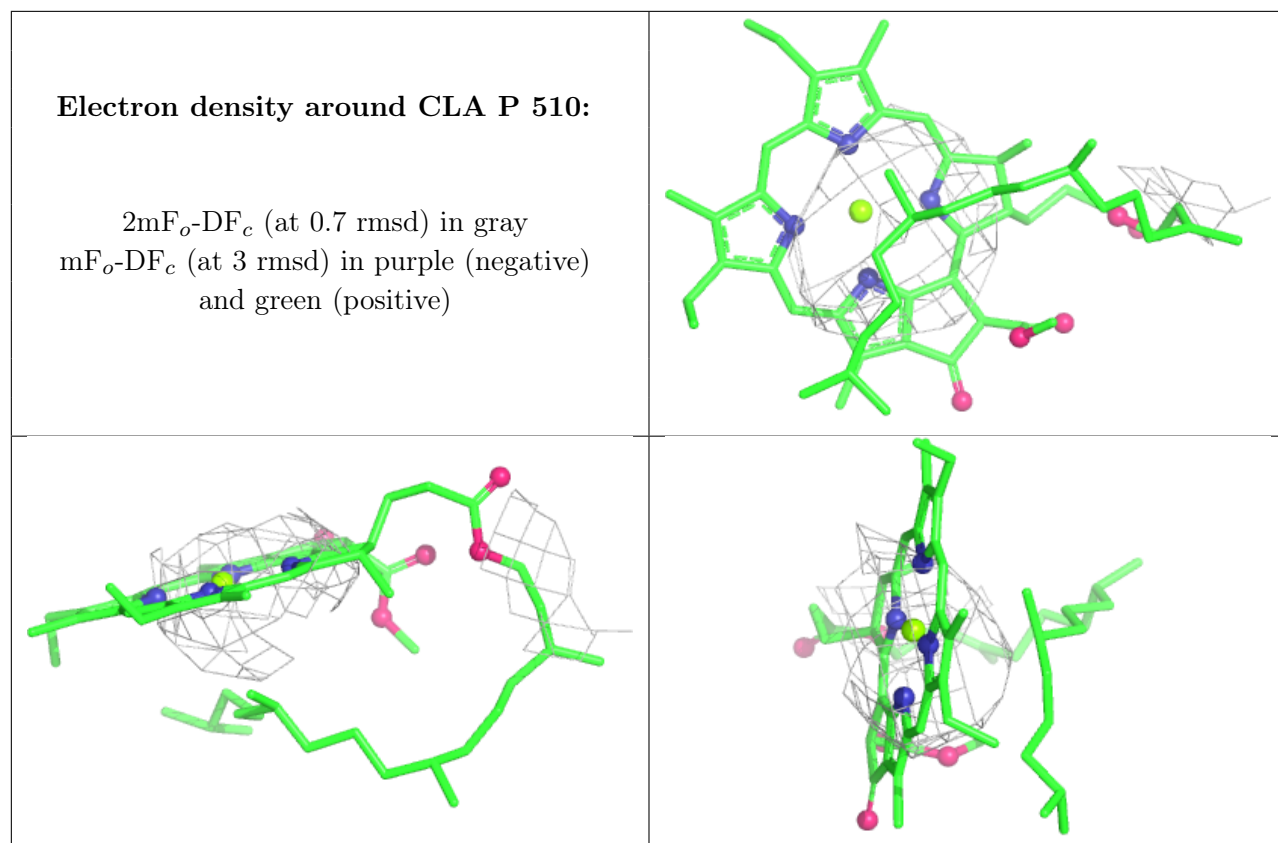
**Electron density around SQD S 102:**

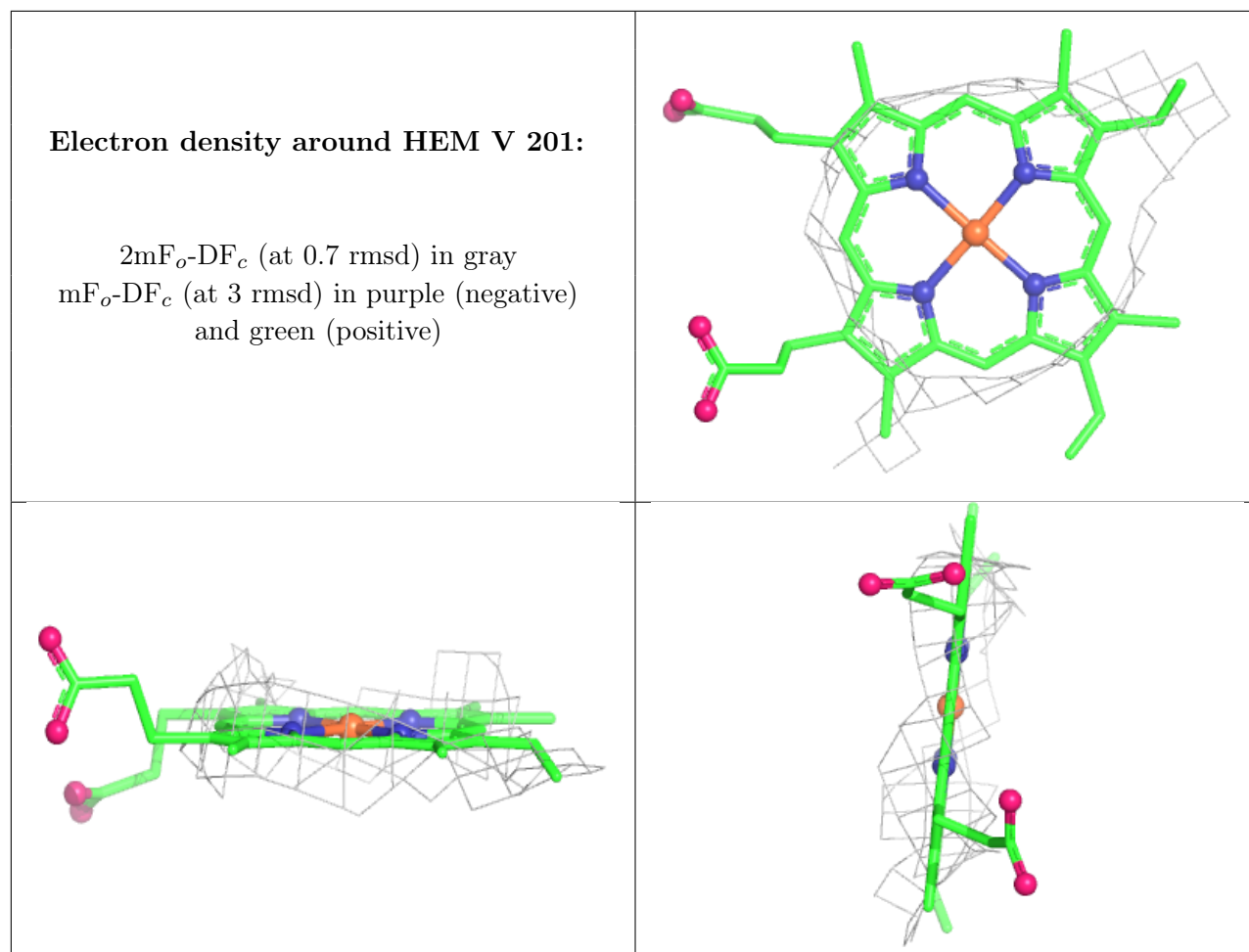
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

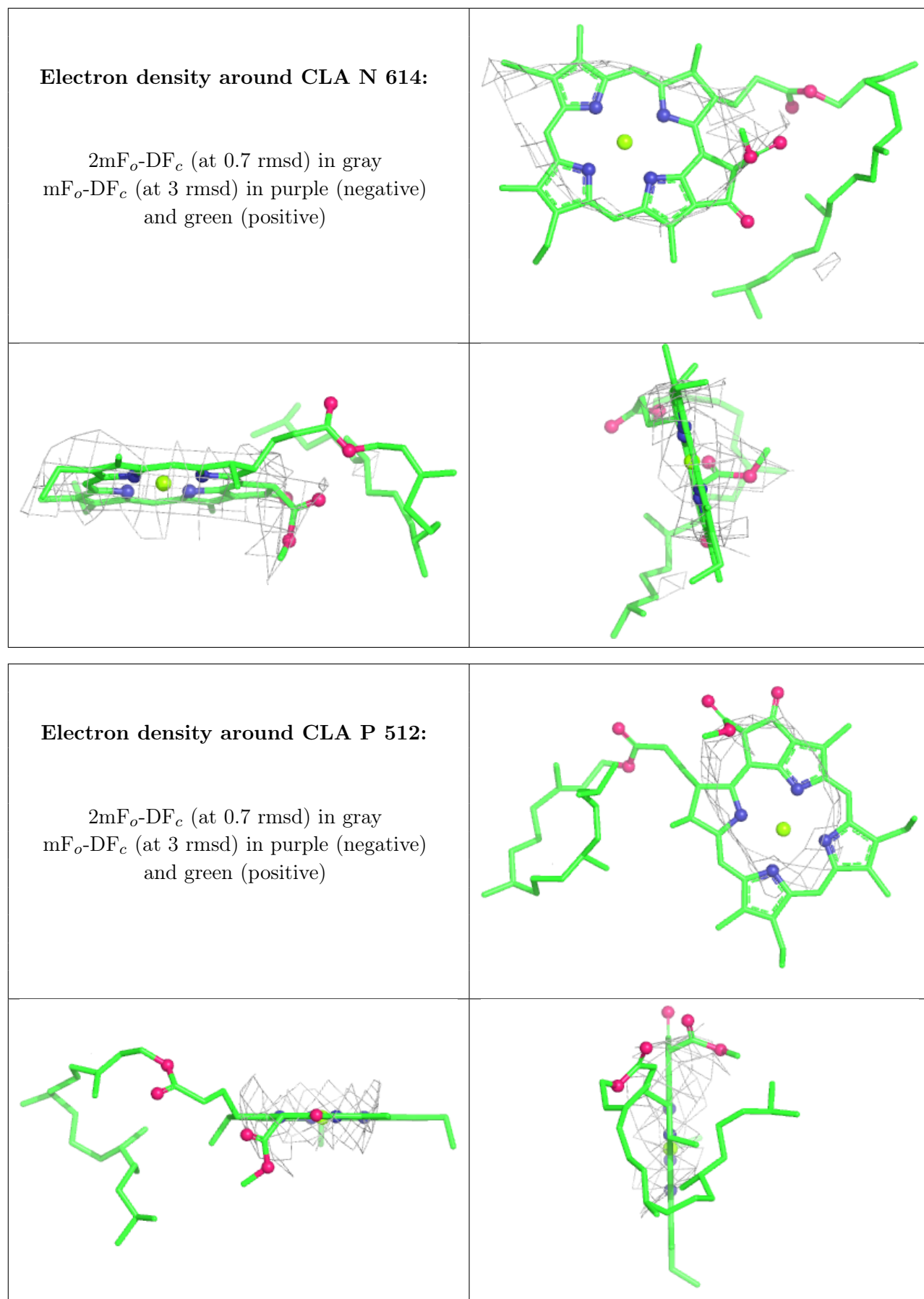






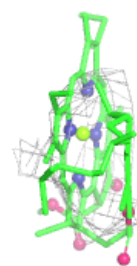
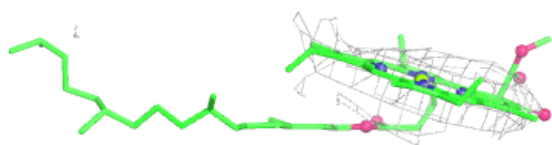
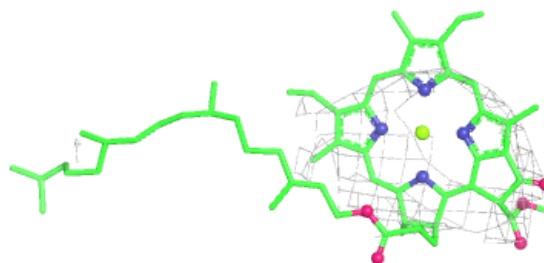




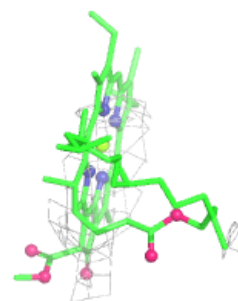
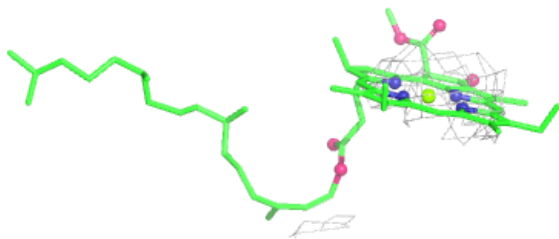
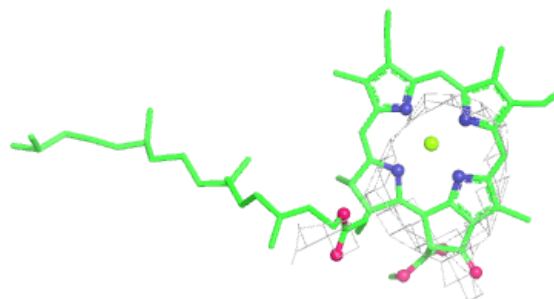


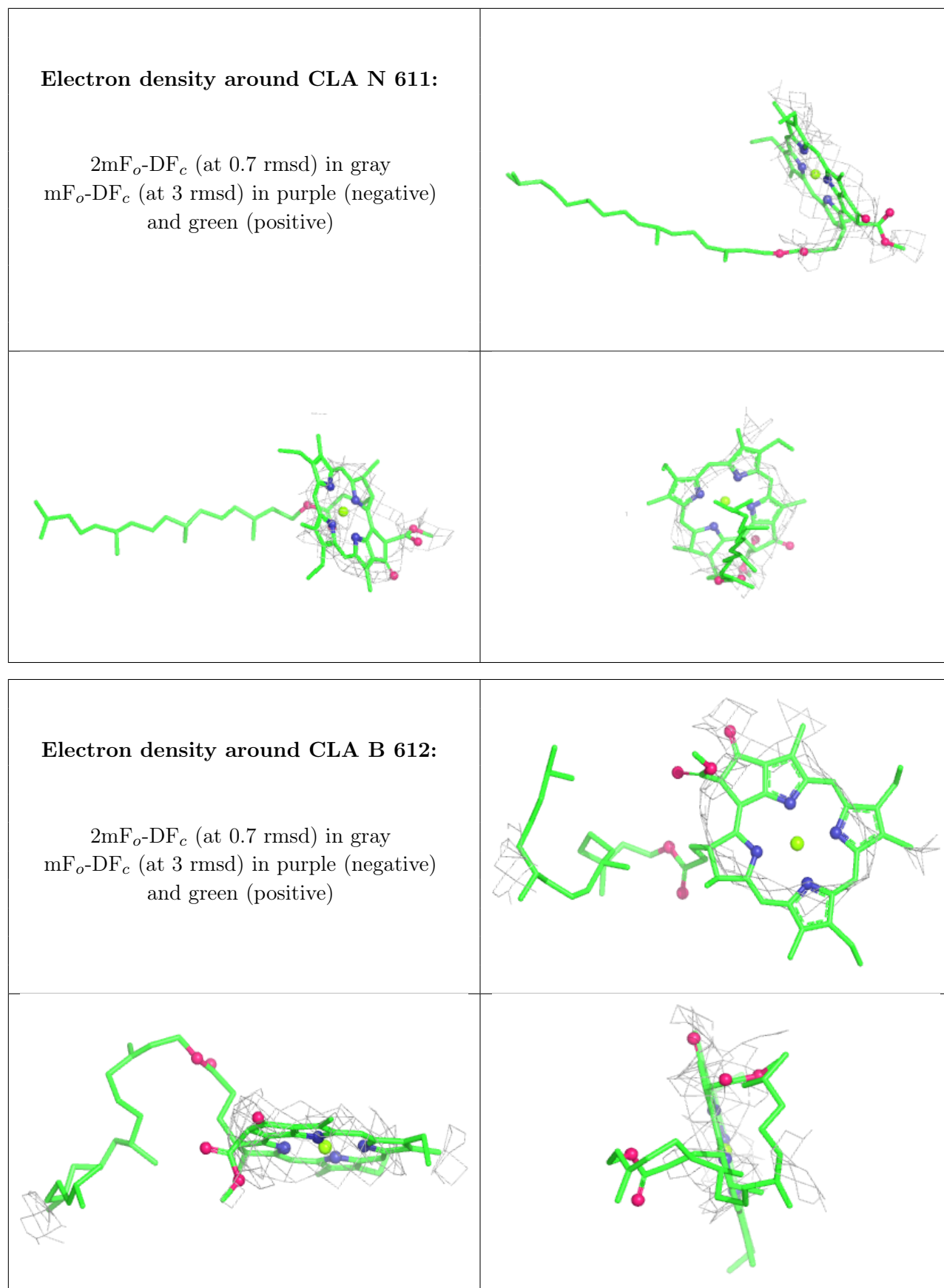
**Electron density around CLA B 603:**

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

**Electron density around CLA G 404:**

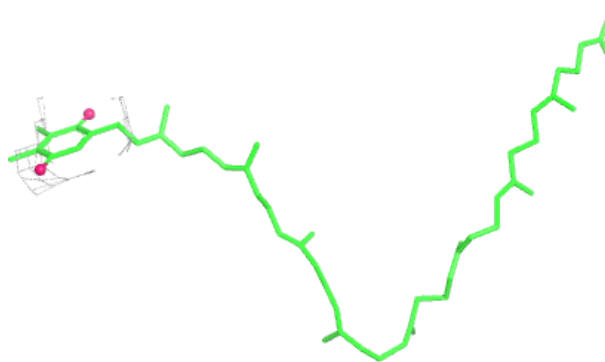
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



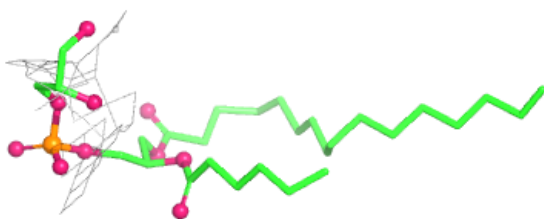


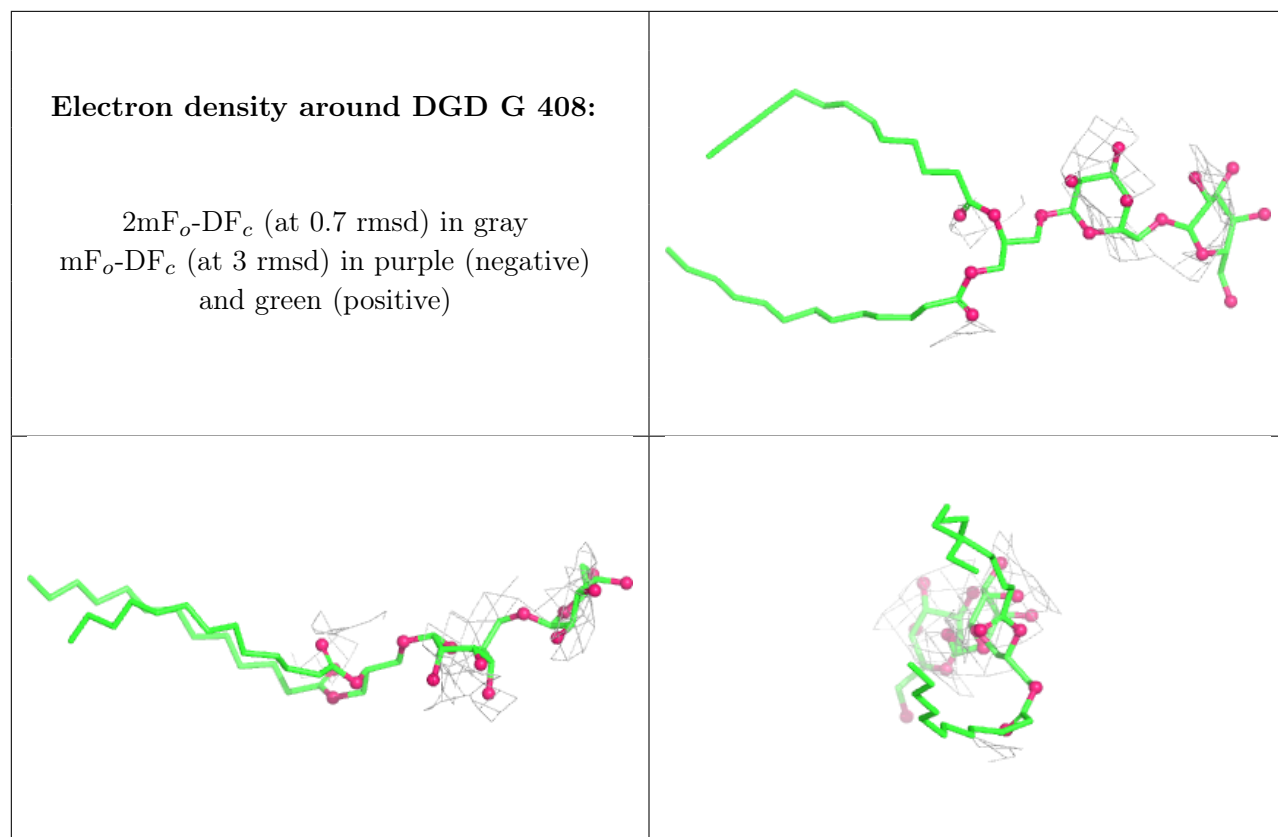
**Electron density around PL9 D 404:**

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

**Electron density around LHG A 408:**

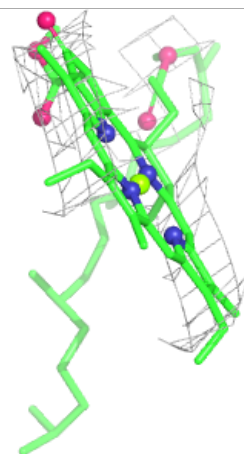
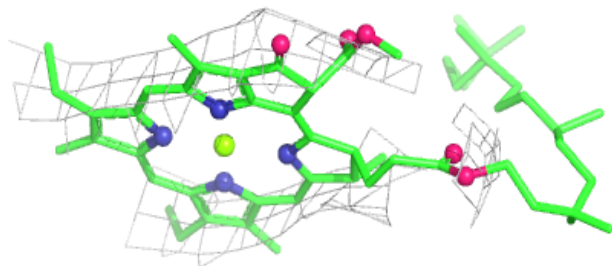
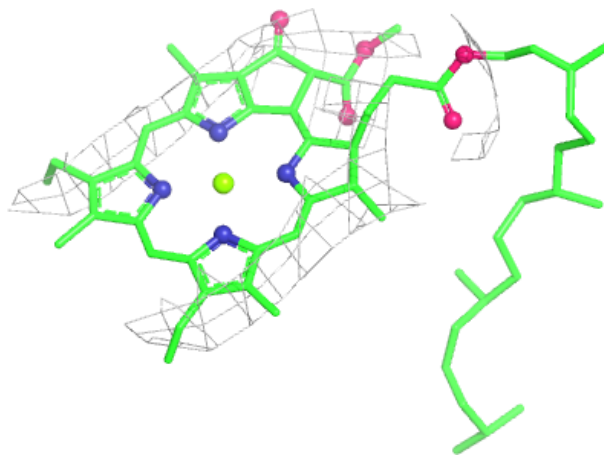
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

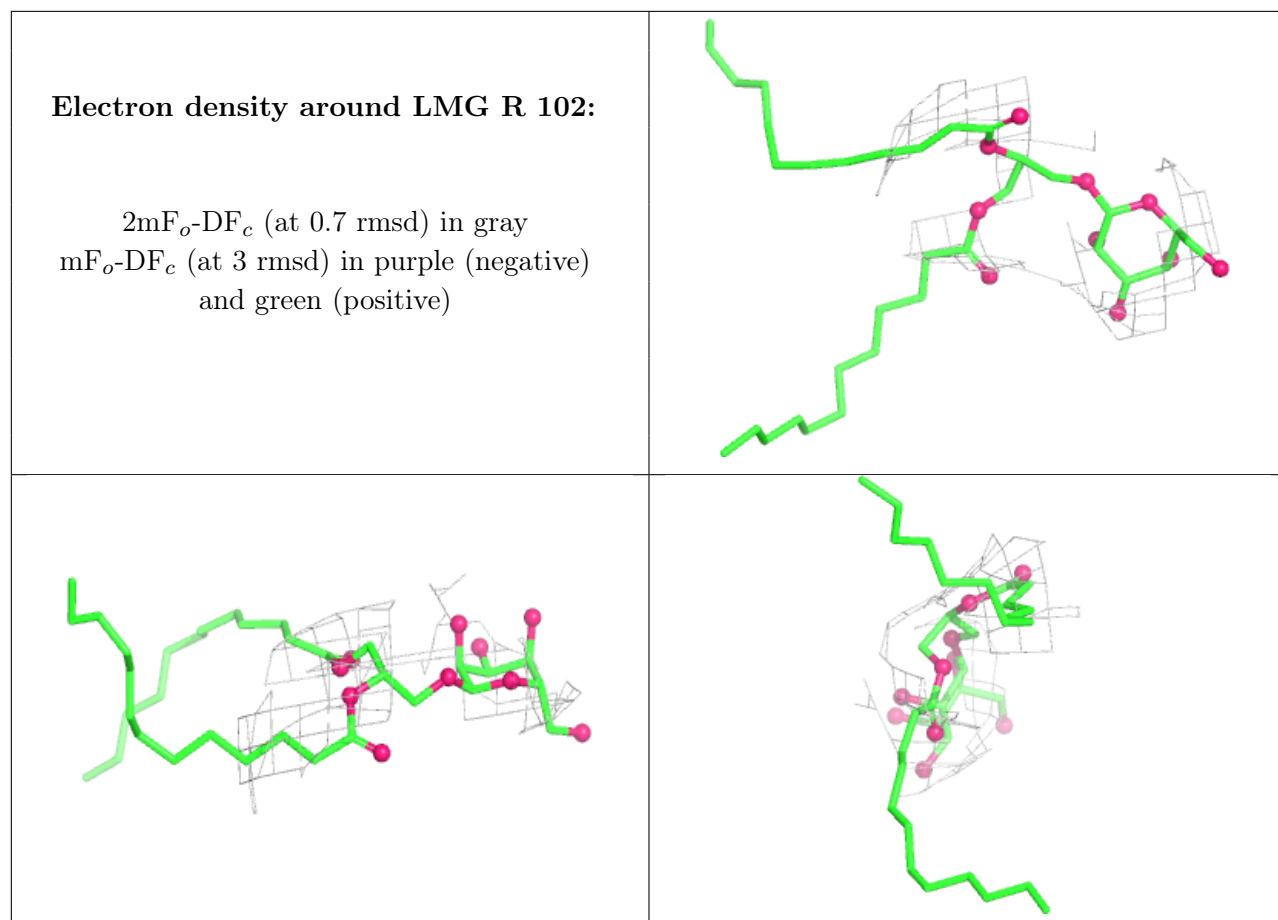


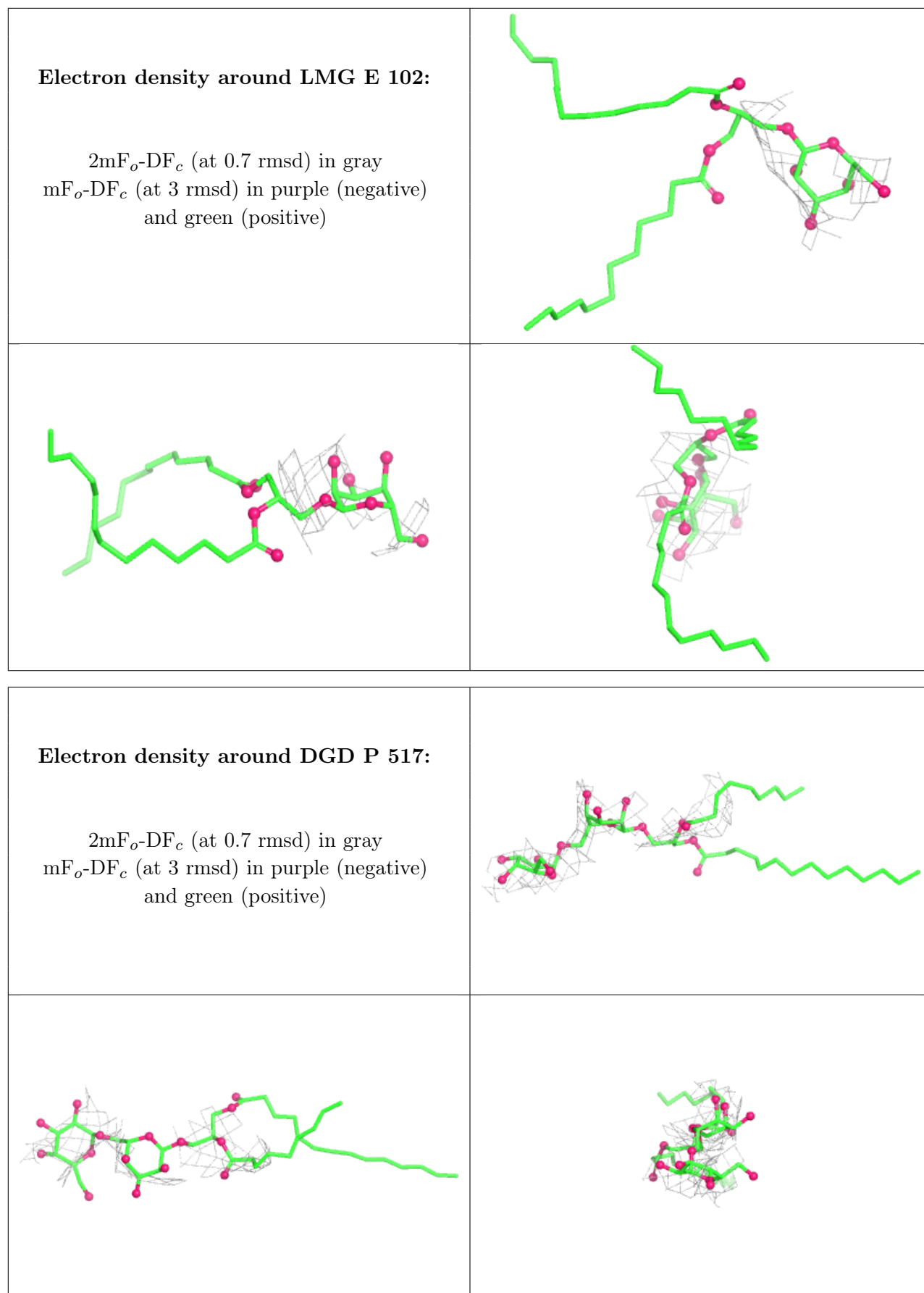


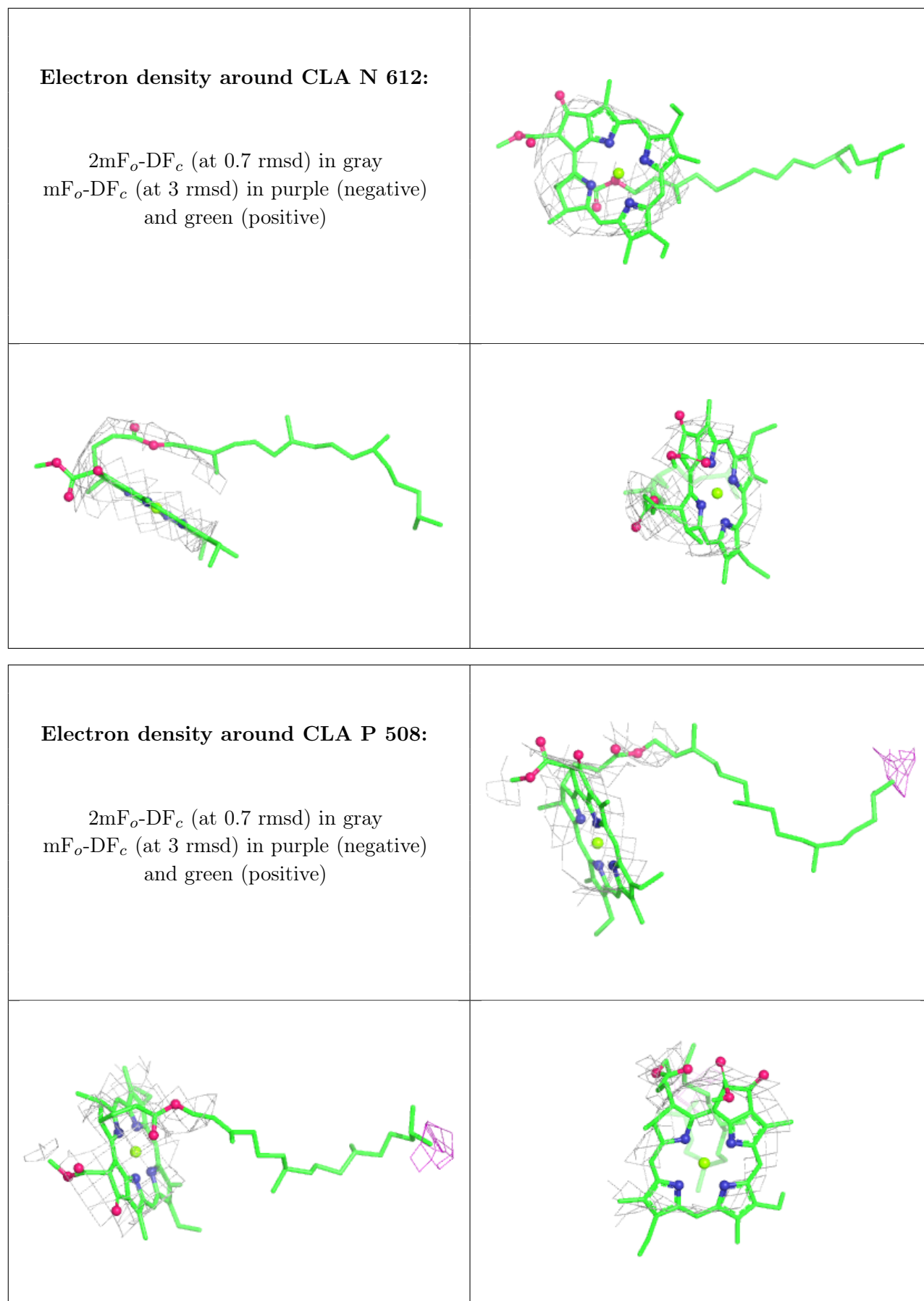
**Electron density around CLA B 616:**

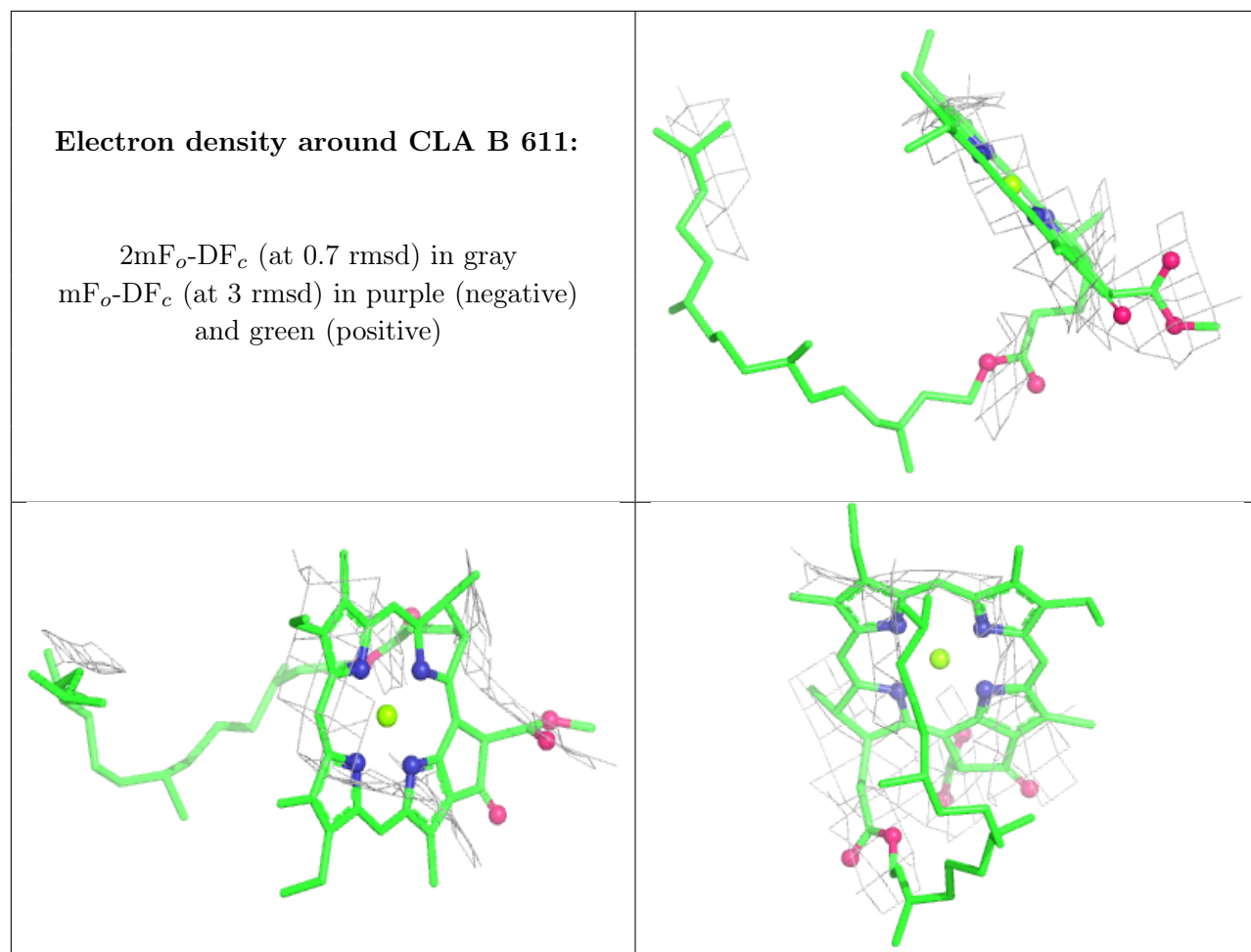
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

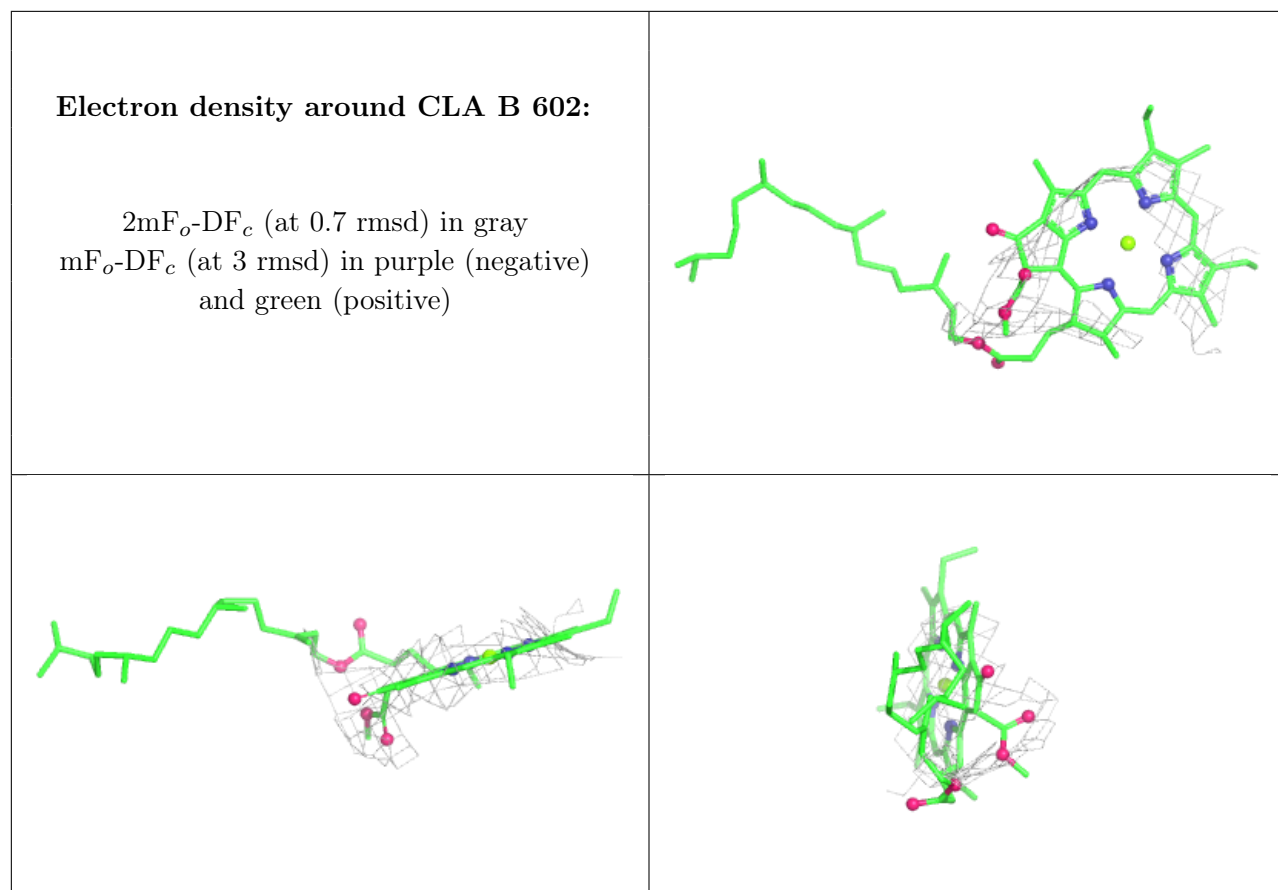


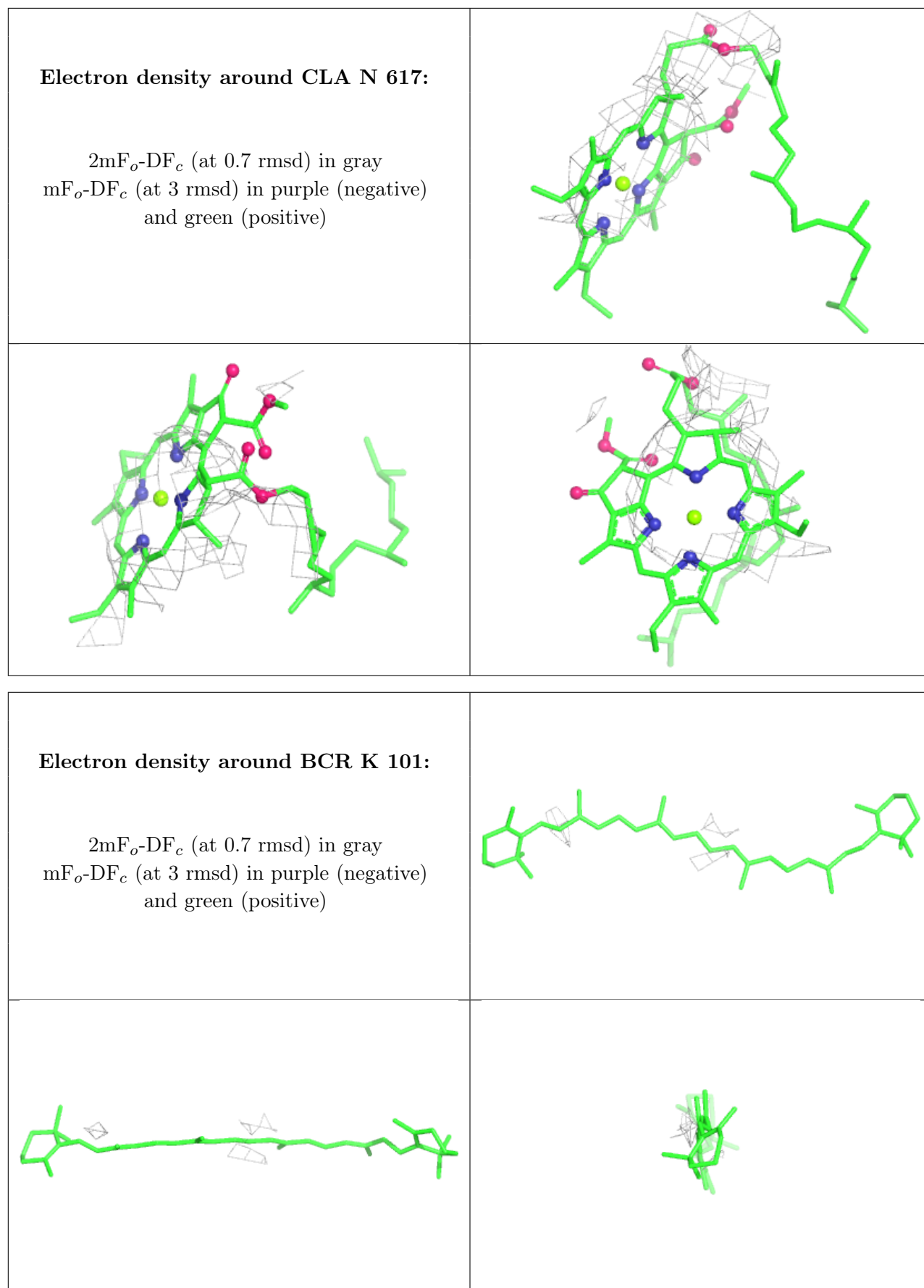


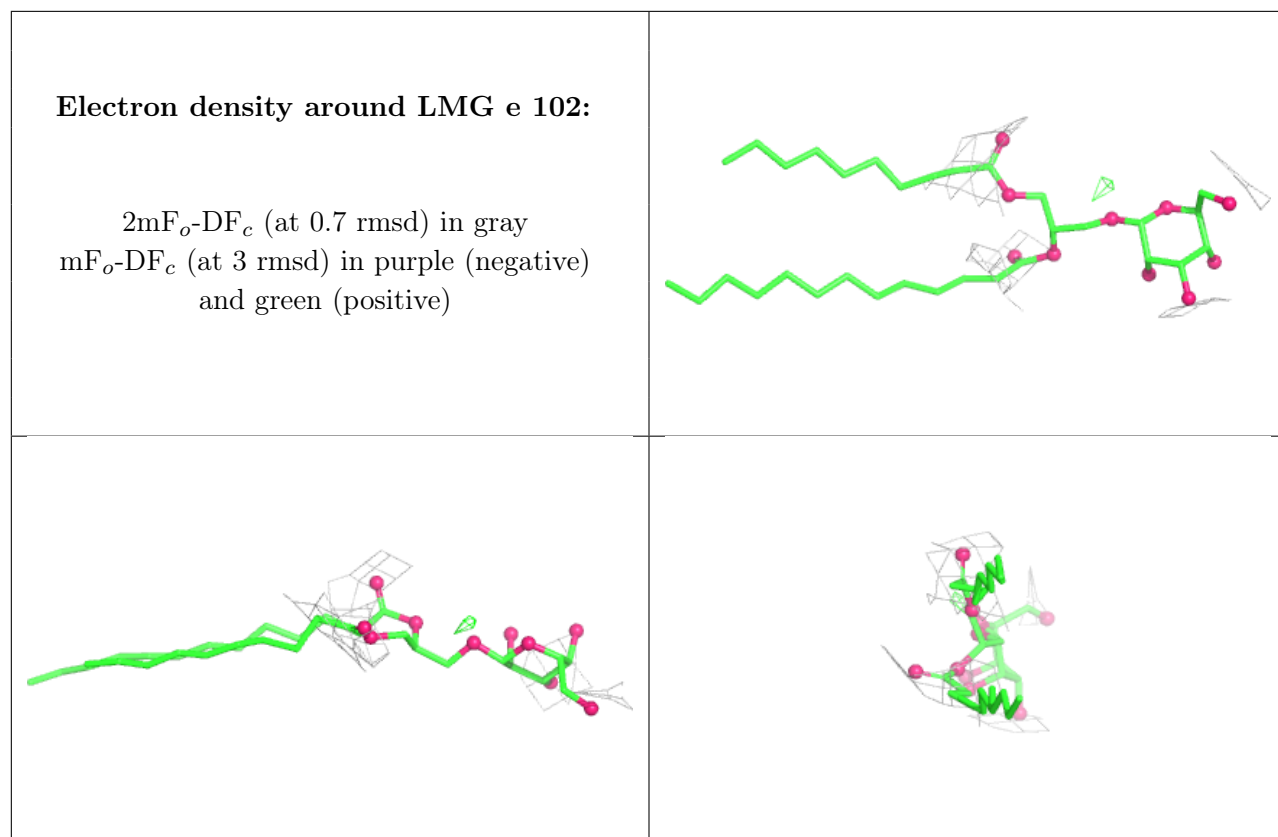






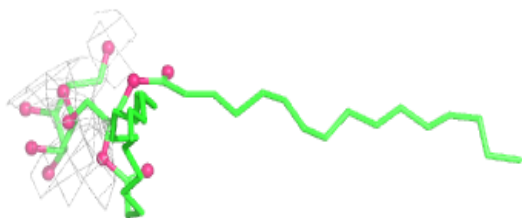
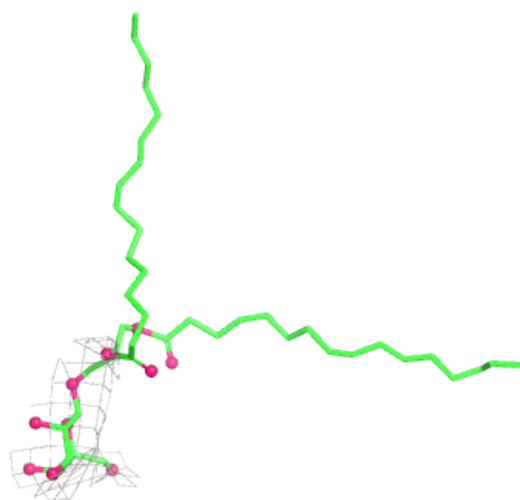


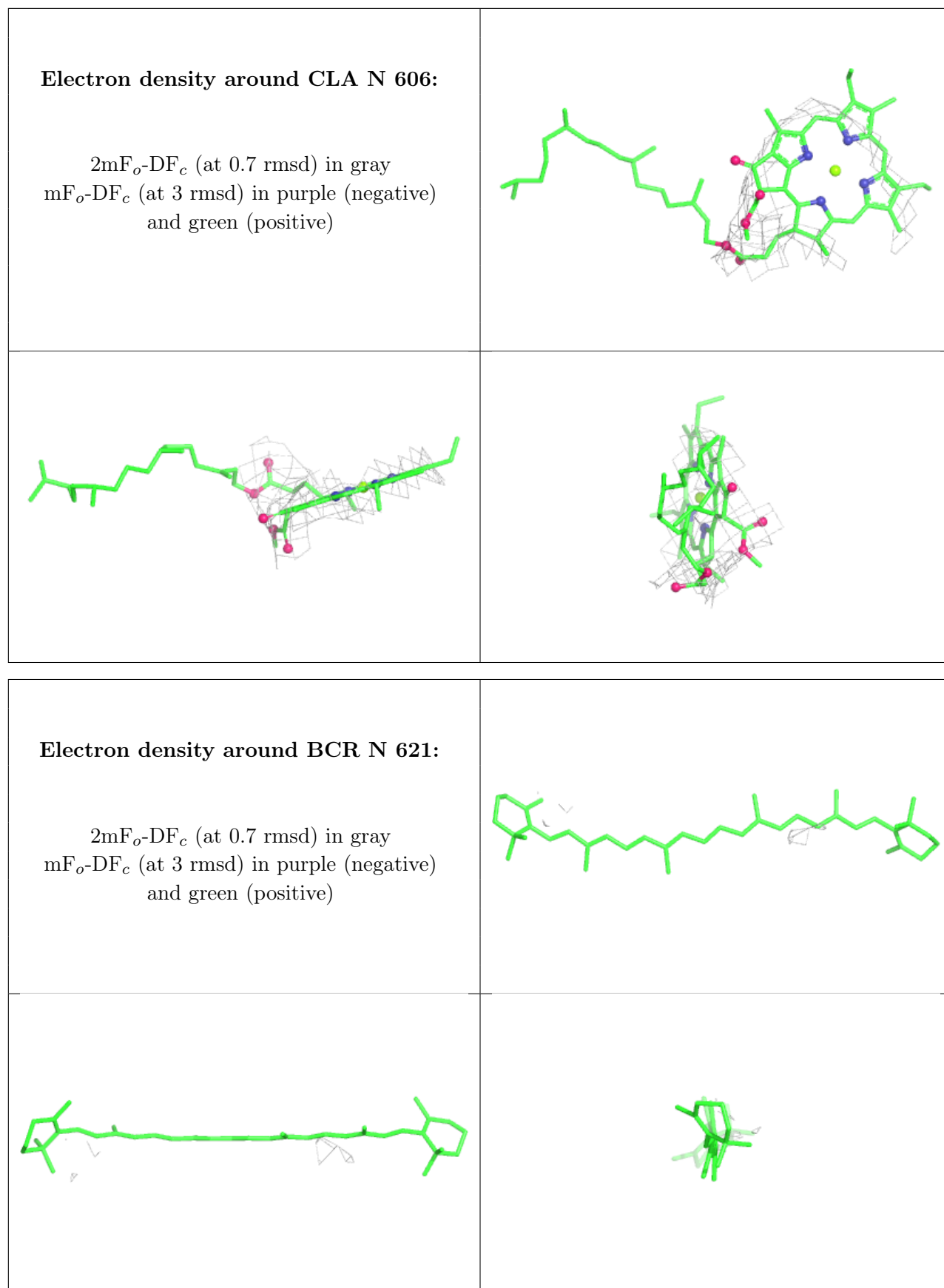


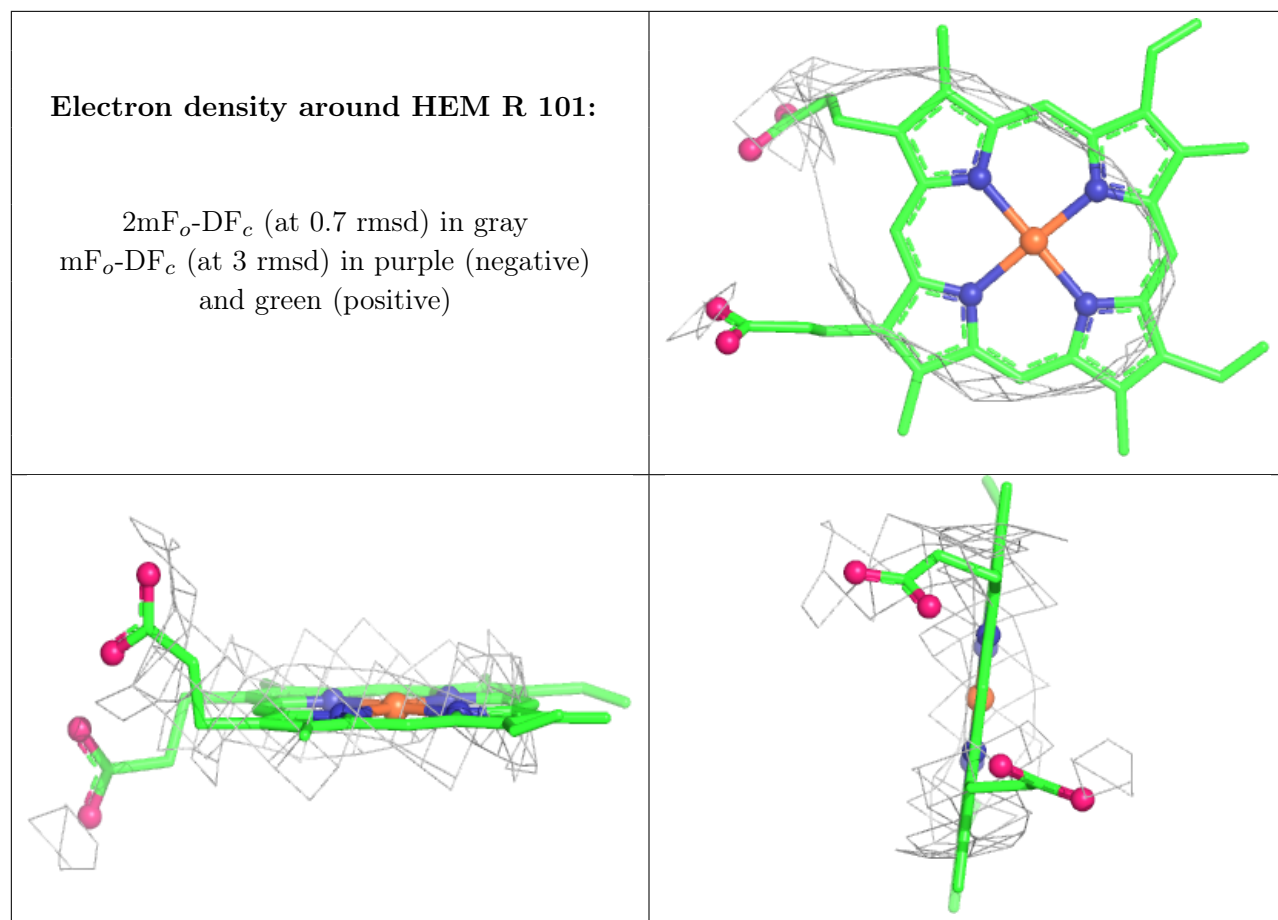


**Electron density around LMG A 410:**

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

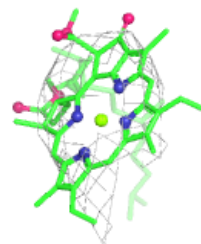
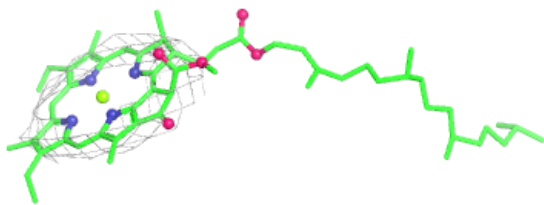
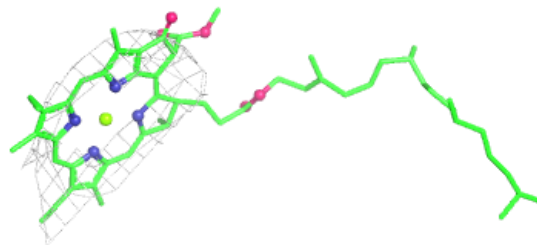




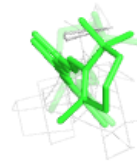
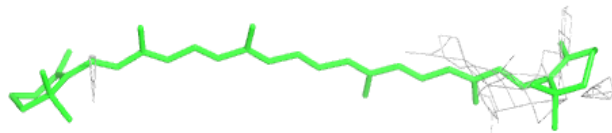
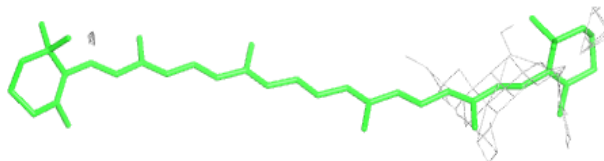


**Electron density around CLA A 401:**

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

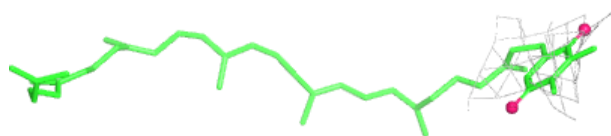
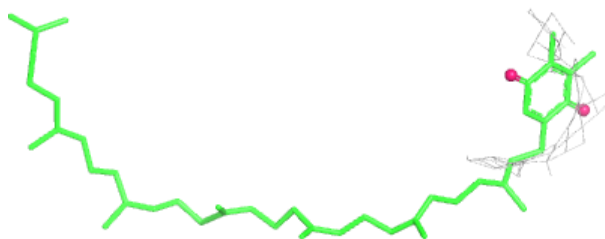
**Electron density around BCR B 620:**

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

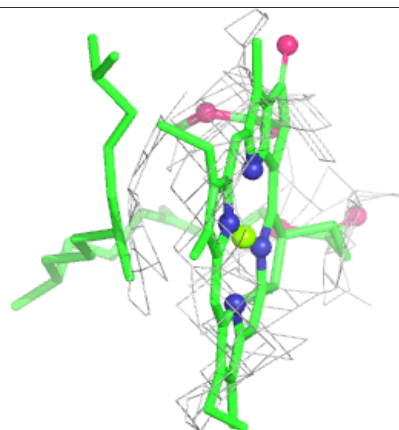
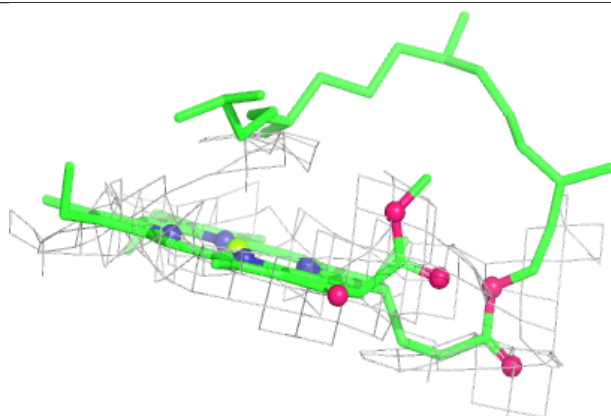
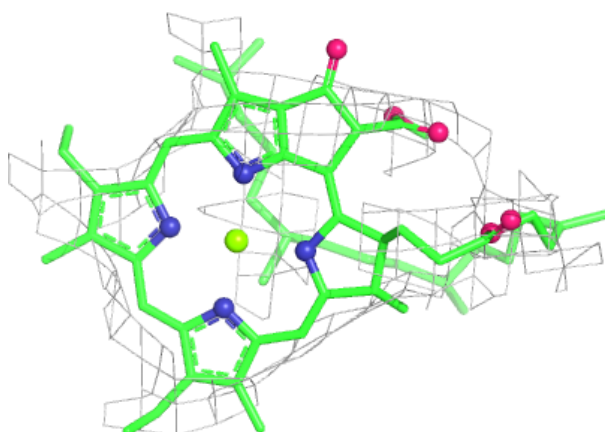


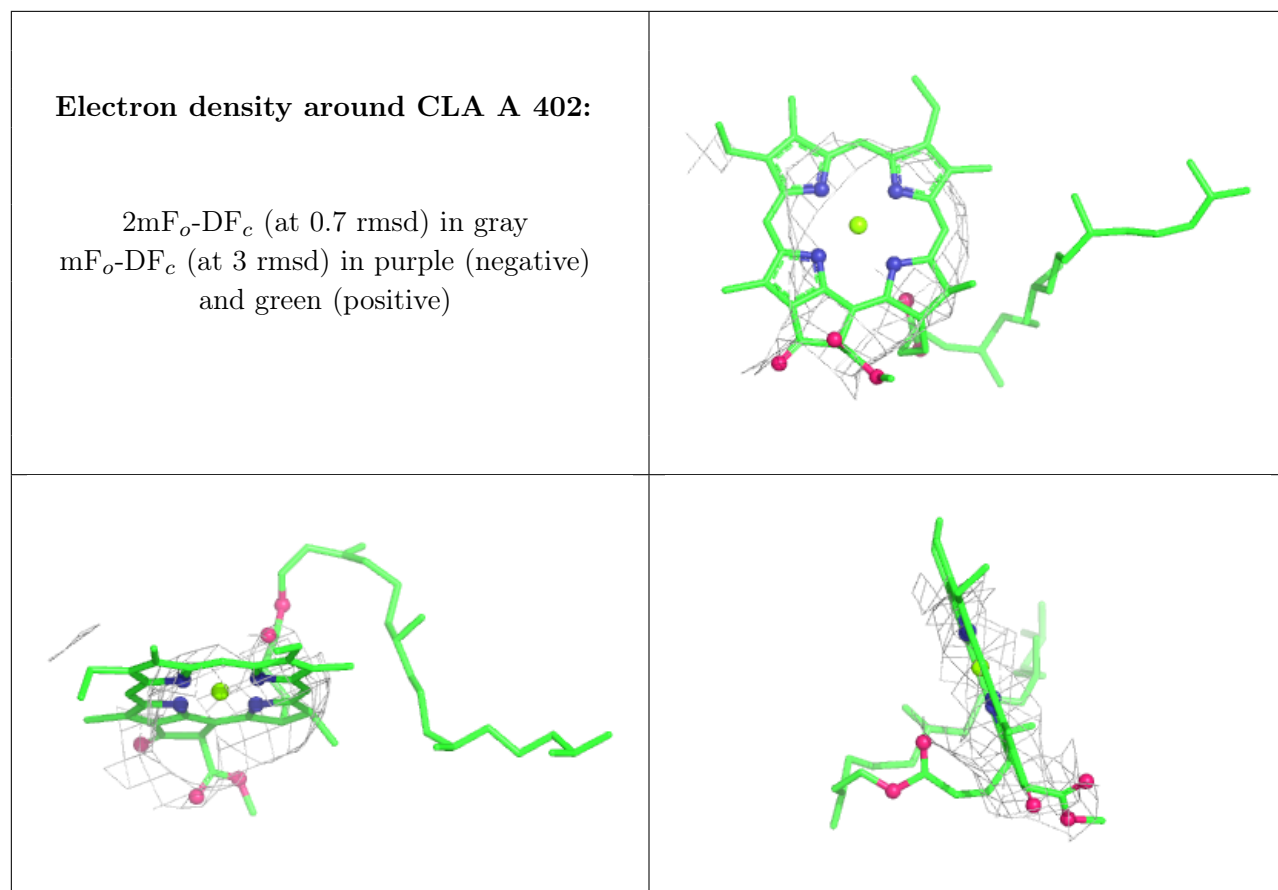
**Electron density around PL9 G 407:**

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

**Electron density around CLA C 510:**

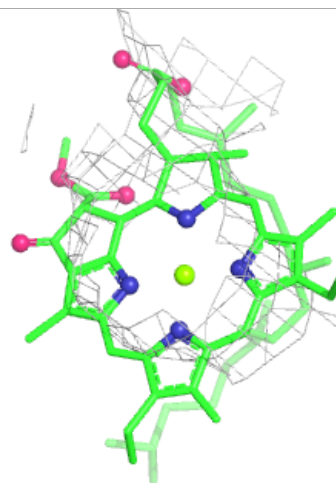
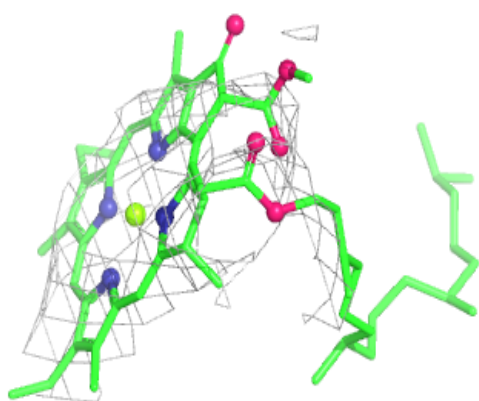
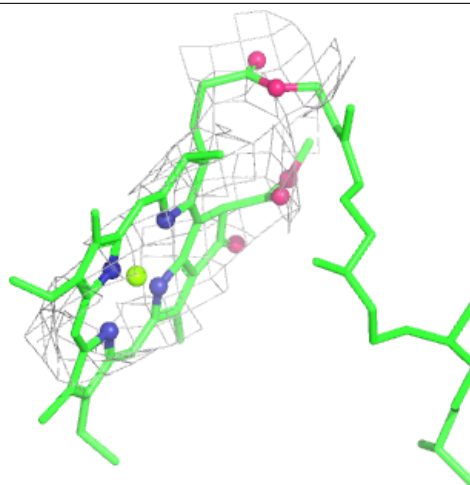
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)

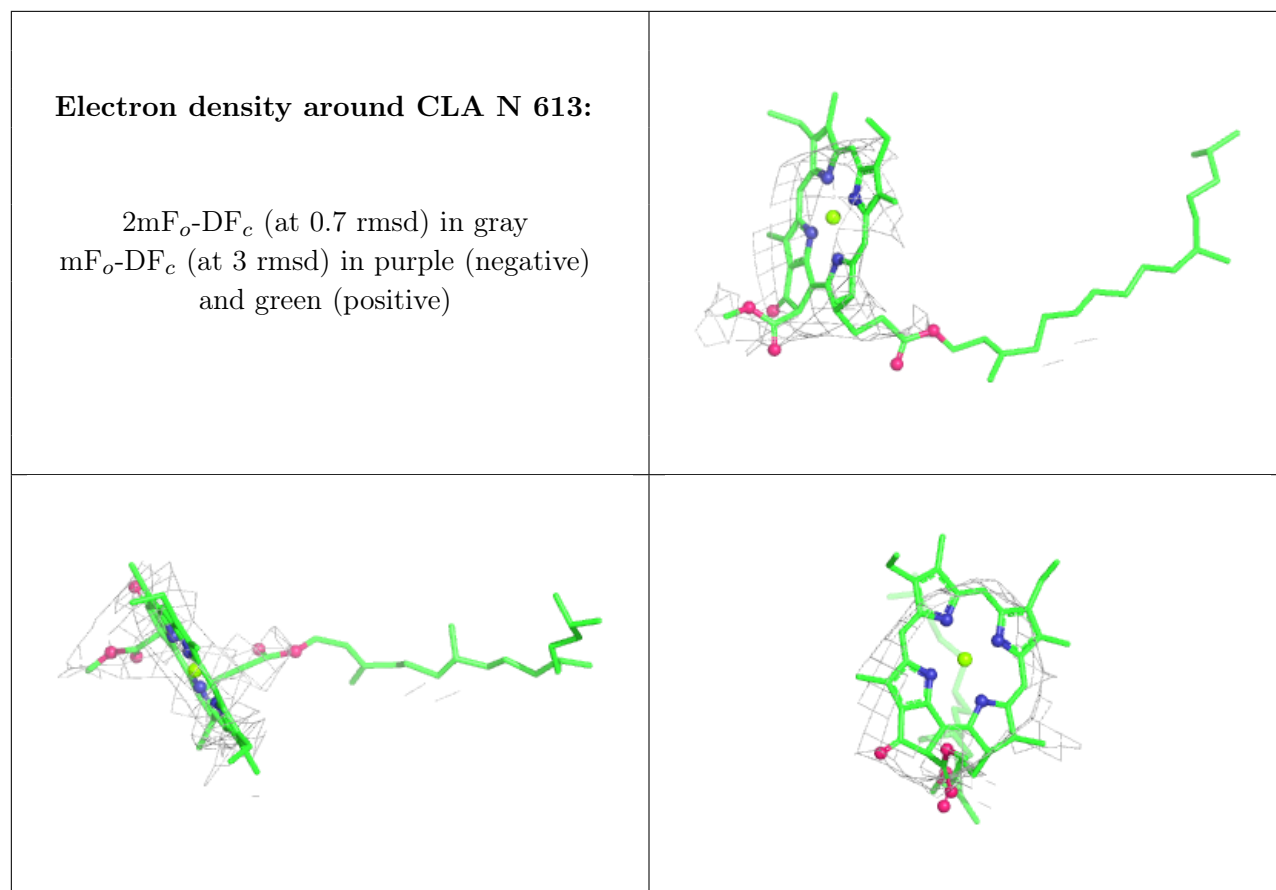


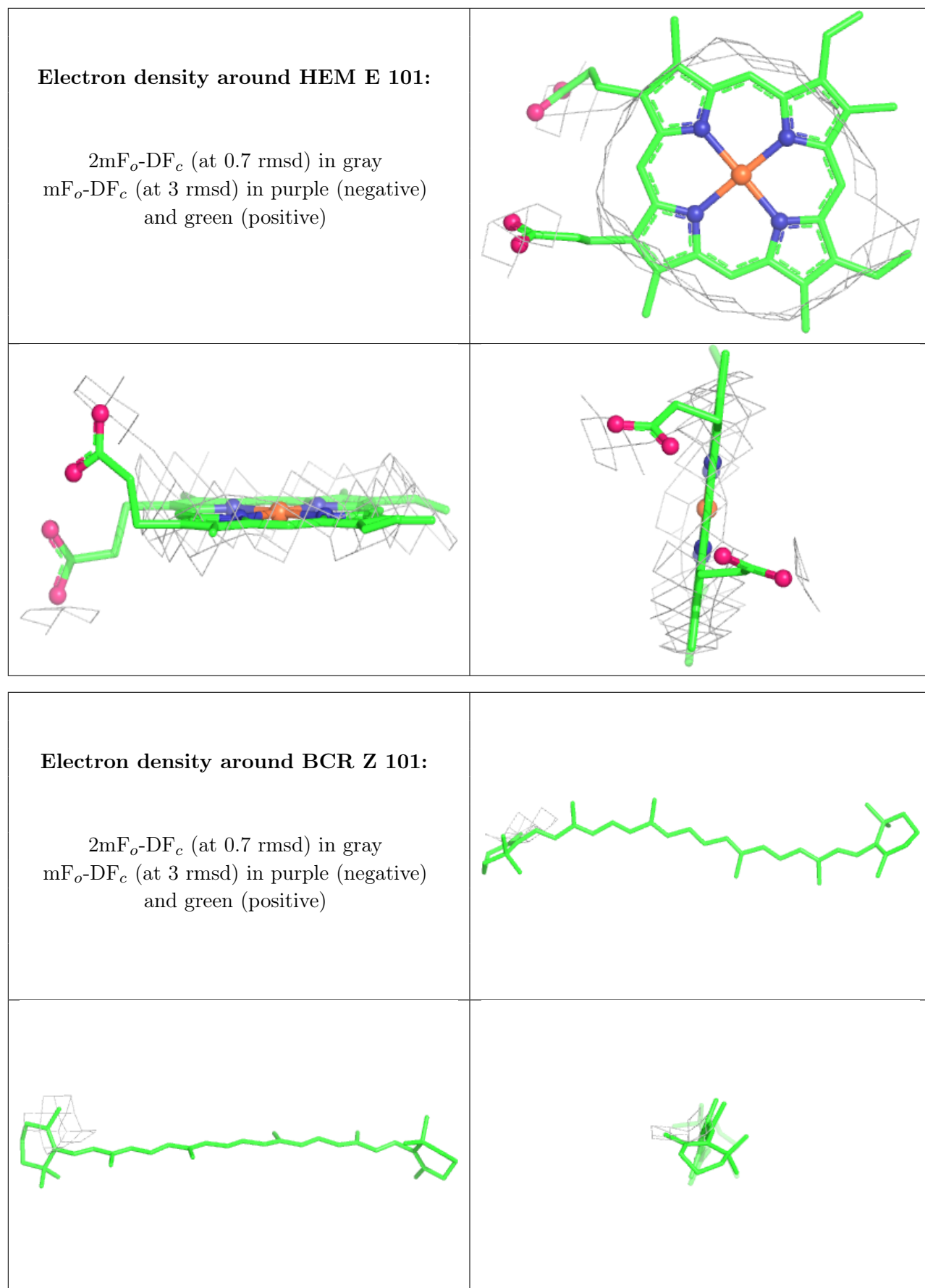


**Electron density around CLA B 613:**

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

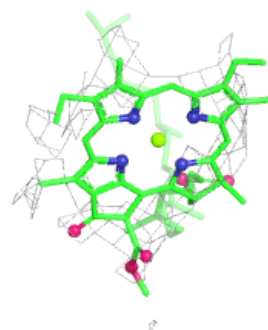
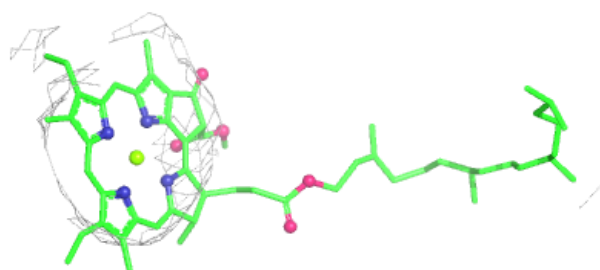
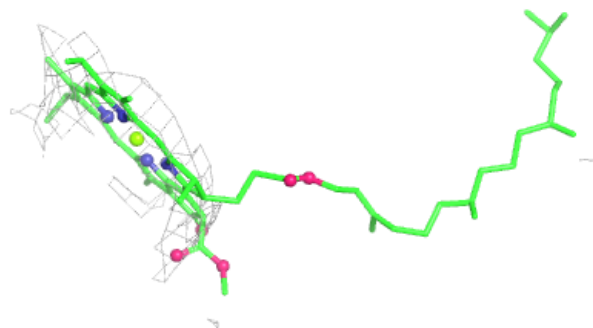




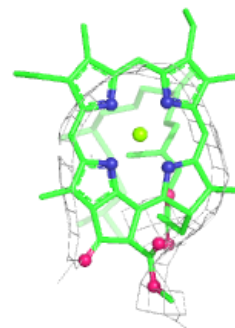
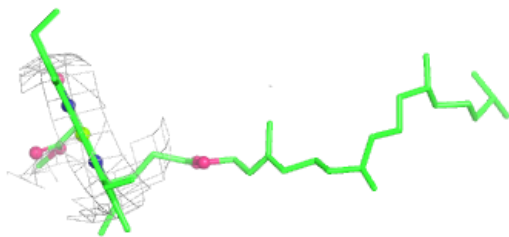
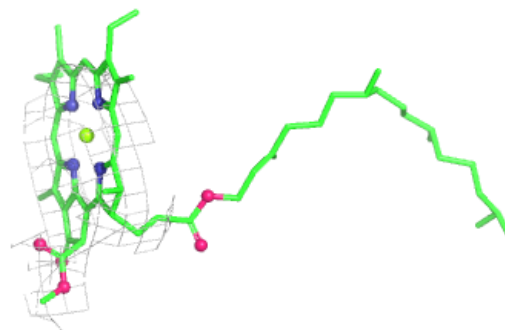


**Electron density around CLA Q 402:**

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

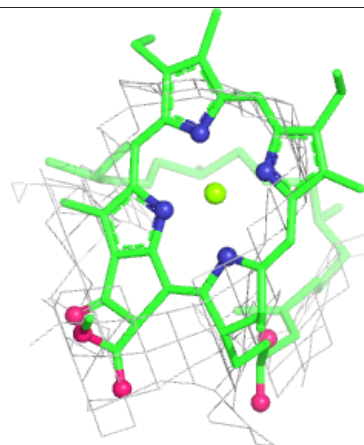
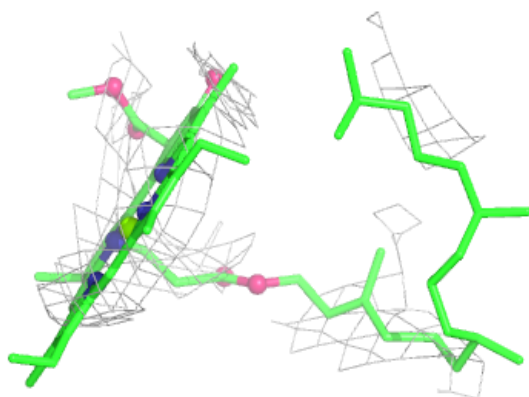
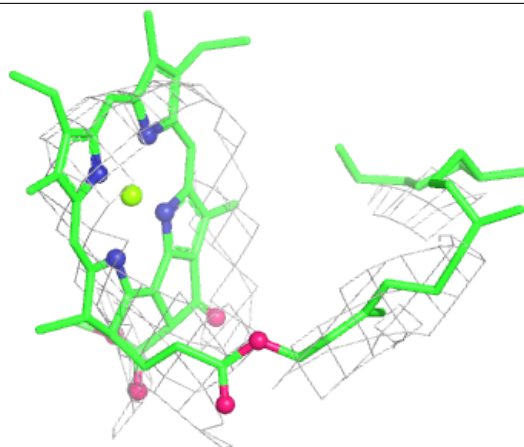
**Electron density around CLA Q 404:**

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



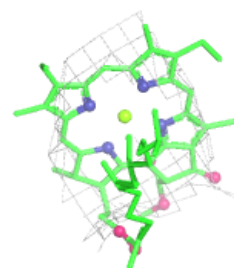
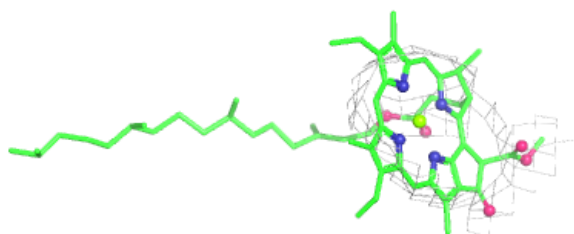
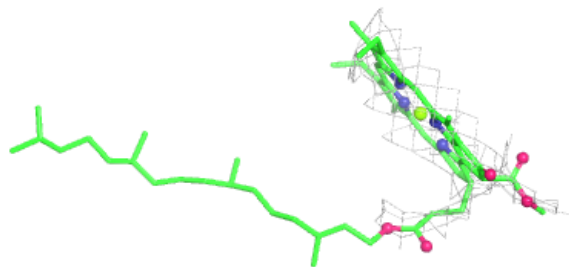
**Electron density around CLA C 503:**

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

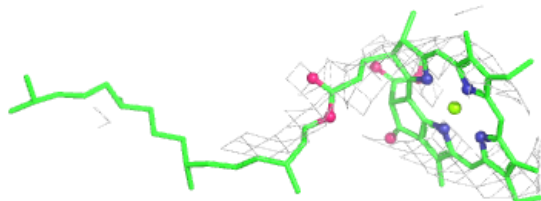
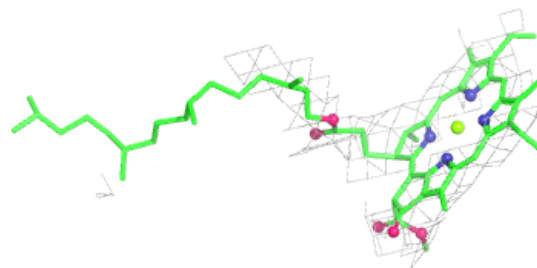


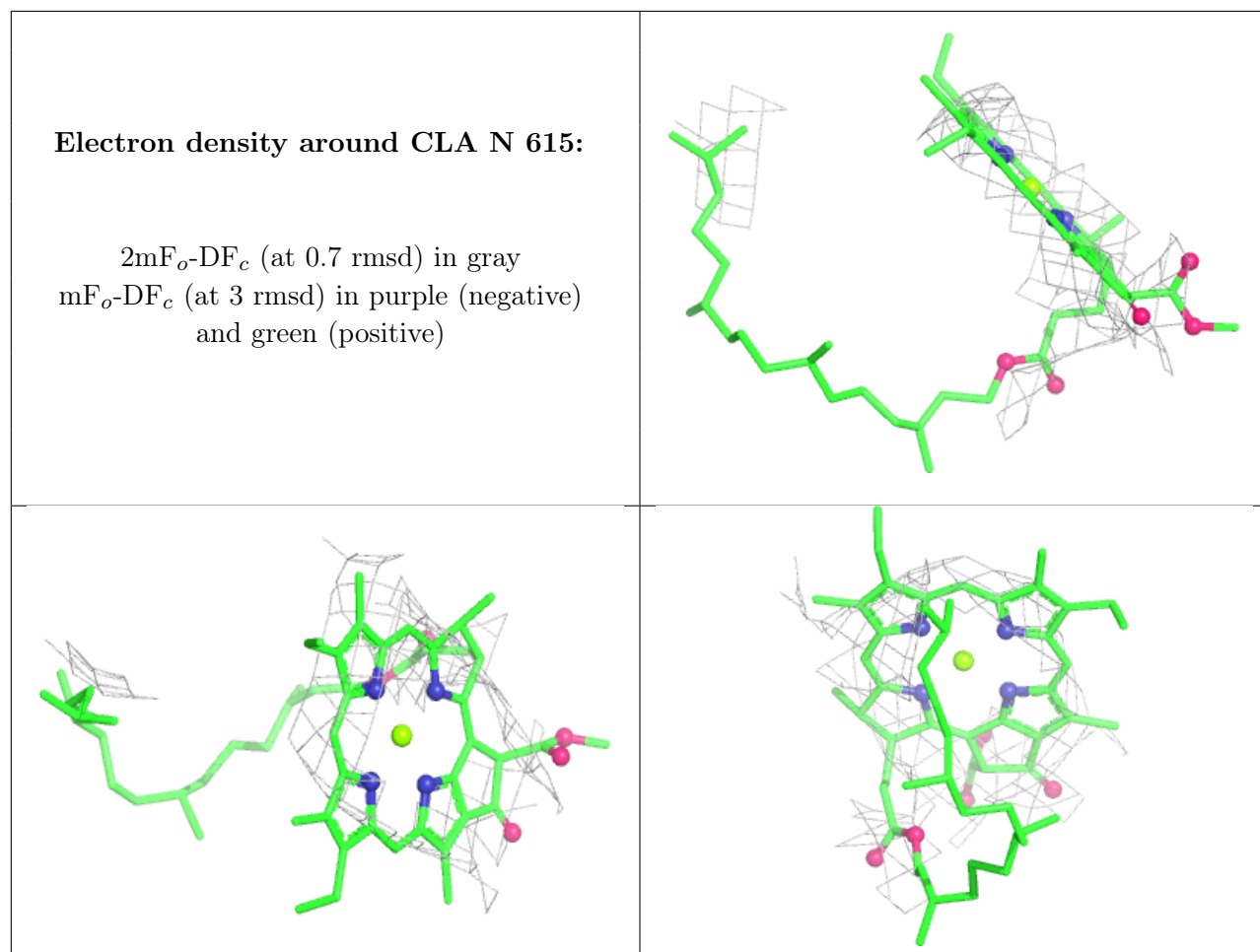
**Electron density around CLA C 504:**

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

**Electron density around CLA C 502:**

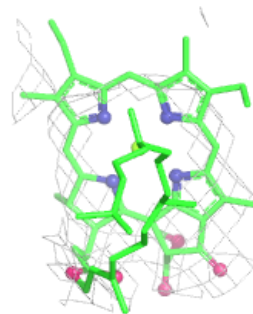
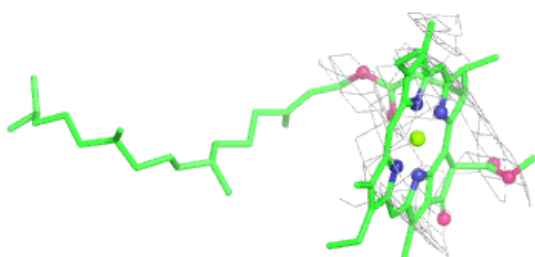
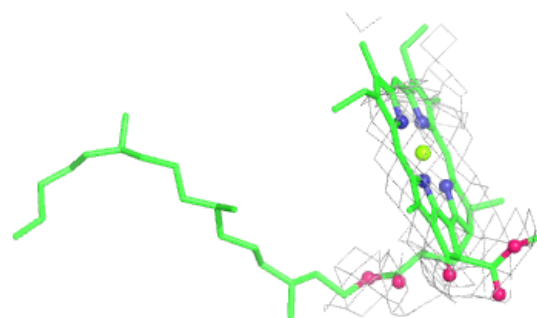
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



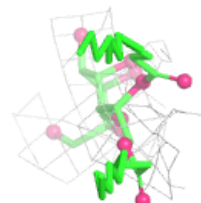
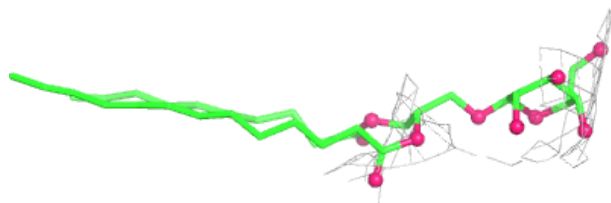
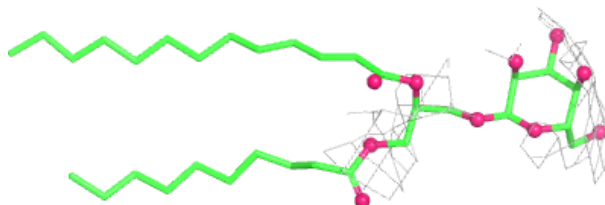


**Electron density around CLA C 508:**

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

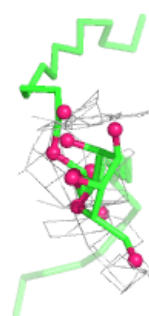
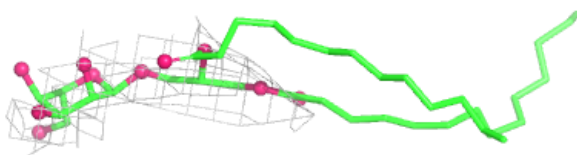
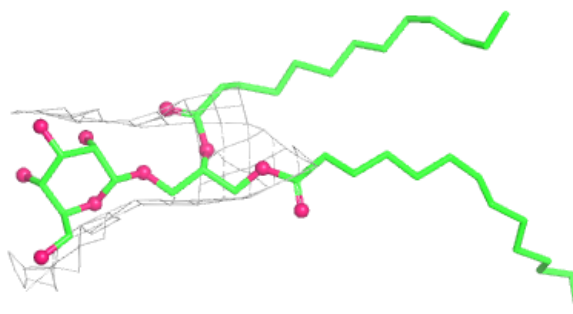
**Electron density around LMG M 101:**

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

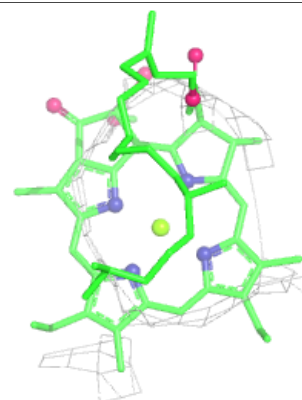
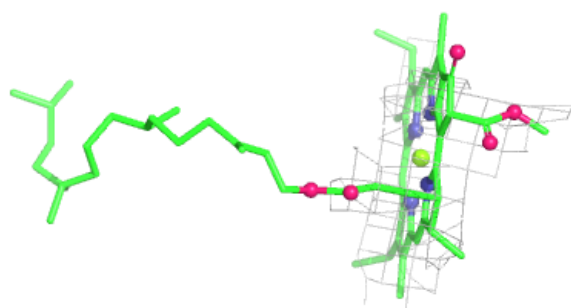


**Electron density around LMG D 406:**

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

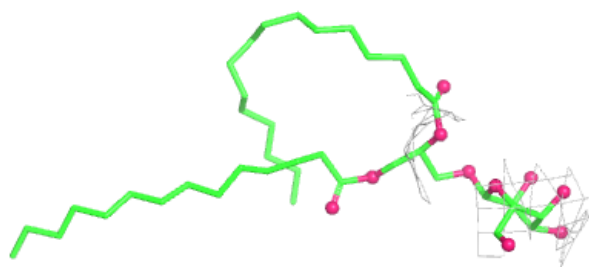
**Electron density around CLA P 506:**

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

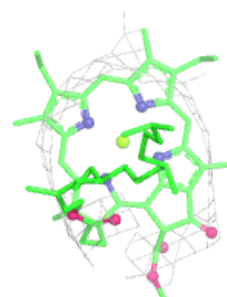
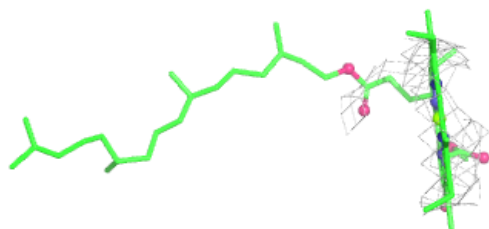
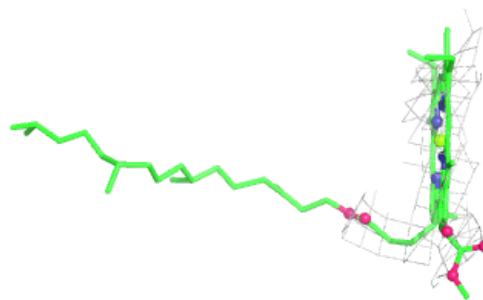


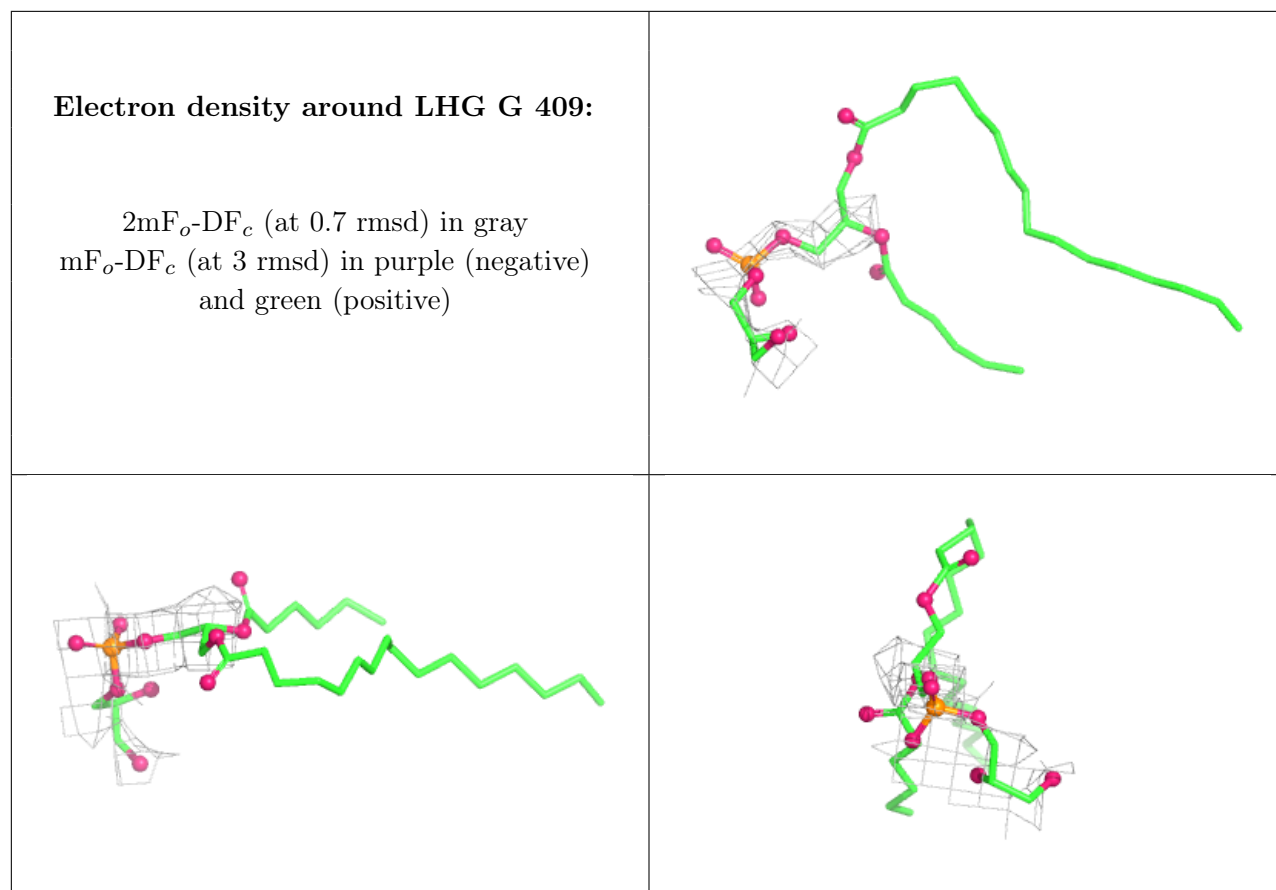
**Electron density around LMG N 622:**

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

**Electron density around CLA 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.