



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2024 – 11:18 AM JST

PDB ID : 4UB8
Title : Native structure of photosystem II (dataset-2) by a femtosecond X-ray laser
Authors : Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on : 2014-08-12
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

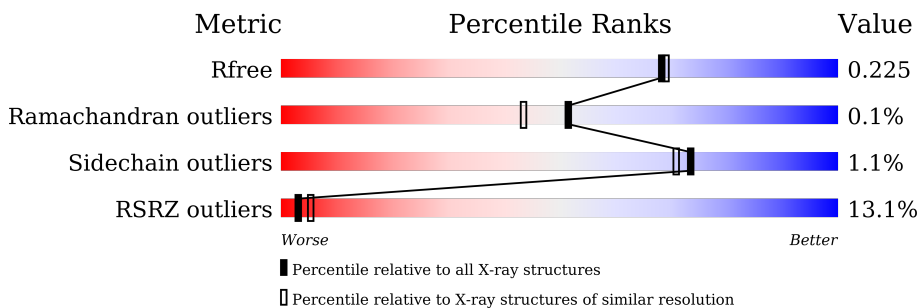
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	344	 13% 97%
1	a	344	 17% 97%
2	B	505	 8% 99%
2	b	505	 10% 99%
3	C	455	 6% 98%
3	c	455	 8% 99%
4	D	342	 18% 100%

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Mol	Chain	Length	Quality of chain
4	d	342	11% 99%
5	E	84	18% 96%
5	e	84	18% 95%
6	F	44	14% 75% 23%
6	f	44	9% 70% 27%
7	H	65	5% 97%
7	h	65	9% 98%
8	I	38	13% 97%
8	i	38	13% 92% 8%
9	J	39	21% 97%
9	j	39	8% 97%
10	K	37	95% 5%
10	k	37	22% 95% 5%
11	L	37	30% 97%
11	l	37	16% 97%
12	M	36	17% 94% 6%
12	m	36	14% 89% 6% 6%
13	O	244	9% 99%
13	o	244	21% 99%
14	T	31	13% 90% 6%
14	t	31	6% 90% 6%
15	U	104	5% 92% 7%
15	u	104	93% 7%
16	V	137	99%
16	v	137	9% 99%

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Mol	Chain	Length	Quality of chain
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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
24	CLA	A	405	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	404	X	-	-	-
28	GOL	B	635	-	-	-	X
29	UNL	J	103	-	-	-	X
29	UNL	k	102	-	-	-	X
30	LMT	a	417	-	-	-	X
36	DGD	D	407	-	-	-	X
36	DGD	d	407	-	-	-	X

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 53958 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 2631	C 1725	N 431	O 460	S 15	0	3	0
1	a	334	Total 2634	C 1727	N 431	O 461	S 15	0	4	0

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	Total 4023	C 2642	N 667	O 701	S 13	0	10	0
2	b	504	Total 4028	C 2645	N 668	O 702	S 13	0	11	0

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3506	C 2296	N 584	O 613	S 13	0	5	0
3	c	455	Total 3544	C 2323	N 589	O 619	S 13	0	6	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	342	Total 2726	C 1805	N 445	O 464	S 12	0	0	0
4	d	341	Total 2720	C 1802	N 444	O 462	S 12	0	1	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	0	0
			662	432	107	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	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	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			282	188	43	49	2			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	309	207	48	53	1	0	1	0
11	l	37	309	207	48	53	1	0	1	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	274	184	40	49	1	0	1	0
12	m	34	269	179	40	49	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	1883	1178	315	385	5	0	4	0
13	o	243	1879	1175	315	384	5	0	3	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	30	264	185	36	41	2	0	1	0
14	t	30	264	185	36	41	2	0	1	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	S	0	1	0
			292	196	46	50				
18	x	39	Total	C	N	O	S	0	0	0
			287	191	46	50				

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

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

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

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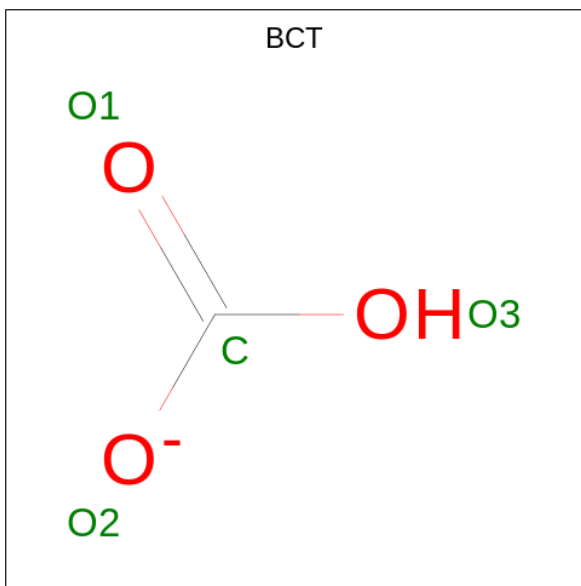
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

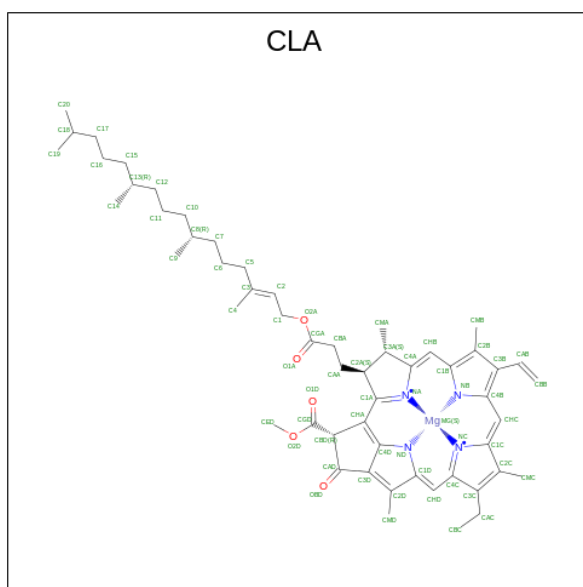
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	V	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	u	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	1	3		
23	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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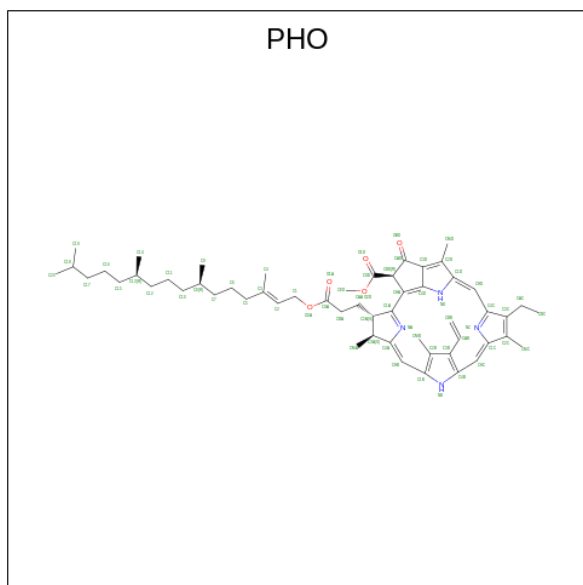
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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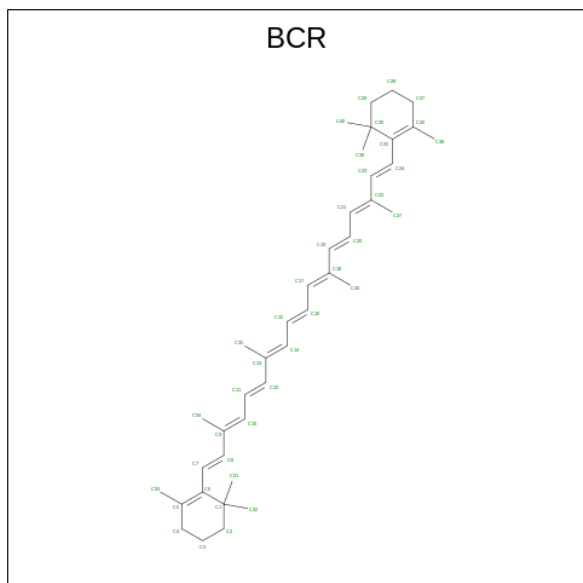
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



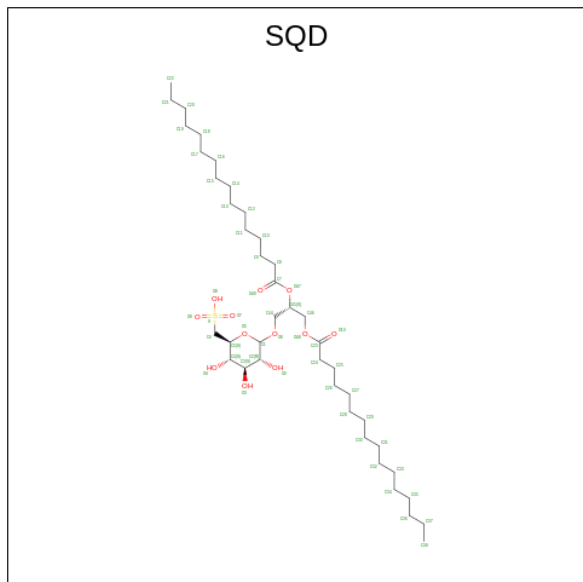
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
25	A	1	64	55	4	5	0	0
25	A	1	64	55	4	5	0	0
25	a	1	64	55	4	5	0	0
25	d	1	64	55	4	5	0	0

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
27	A	1	54	41	12	1	0	0
27	F	1	43	30	12	1	0	0
27	a	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	b	1	54	41	12	1	0	0
27	f	1	43	30	12	1	0	0
27	l	1	54	41	12	1	0	0

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	F	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total 6	C 3	O 3	0	0
28	T	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	f	1	Total 6	C 3	O 3	0	0
28	t	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0

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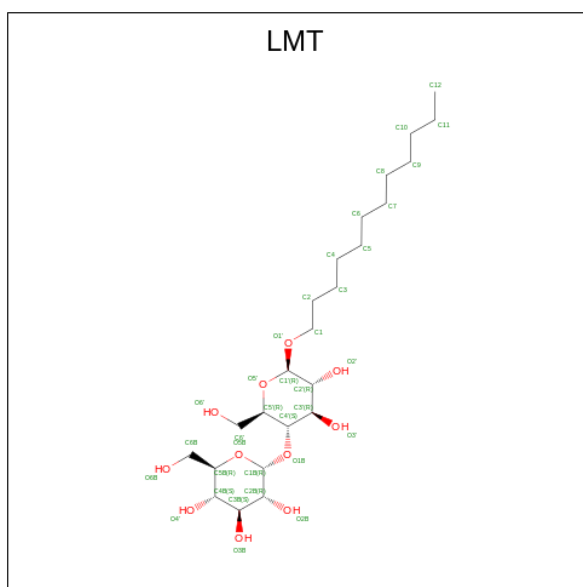
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

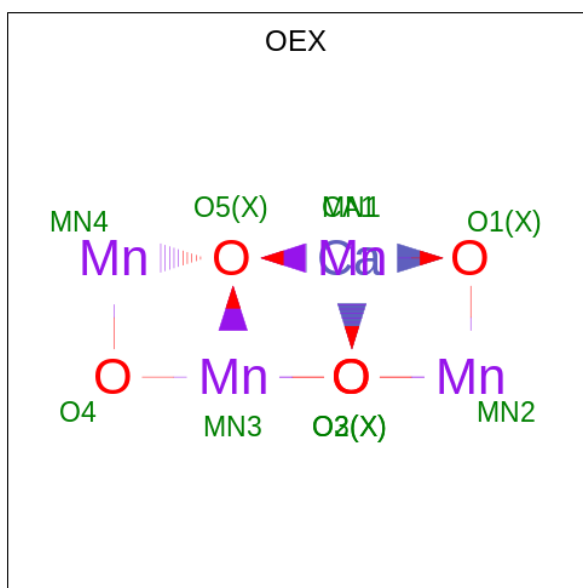
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			28	23	5		
29	B	1	Total	C	O	0	0
			33	28	5		
29	C	1	Total	C	O	0	0
			34	29	5		
29	D	2	Total	C	O	0	0
			57	51	6		
29	I	1	Total	C	O	0	0
			40	35	5		
29	J	1	Total	C		0	0
			10	10			
29	M	1	Total	C		0	0
			10	10			
29	X	1	Total	C		0	0
			10	10			
29	a	1	Total	C	O	0	0
			30	25	5		
29	b	1	Total	C	O	0	0
			33	28	5		
29	d	2	Total	C	O	0	0
			53	47	6		
29	i	1	Total	C	O	0	0
			40	35	5		
29	j	1	Total	C		0	0
			10	10			
29	k	2	Total	C	O	0	0
			42	37	5		
29	m	1	Total	C		0	0
			10	10			
29	x	1	Total	C		0	0
			10	10			

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



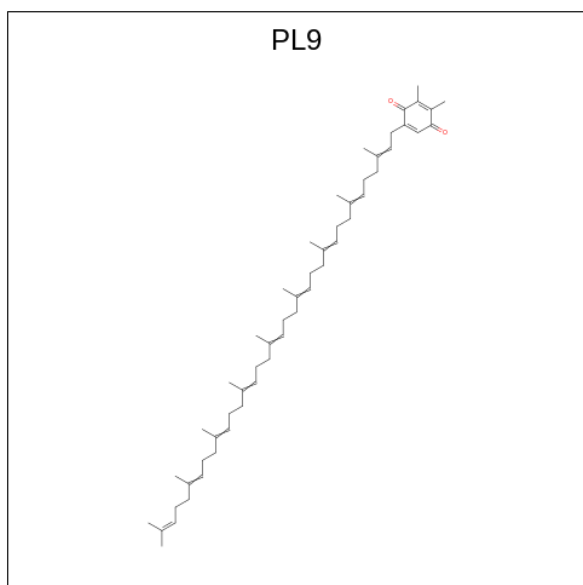
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			33	22	11		
30	B	1	Total	C	O	0	0
			25	19	6		
30	D	1	Total	C	O	0	0
			35	24	11		
30	E	1	Total	C	O	0	0
			35	24	11		
30	I	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	b	1	Total	C	O	0	0
			25	19	6		
30	f	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).

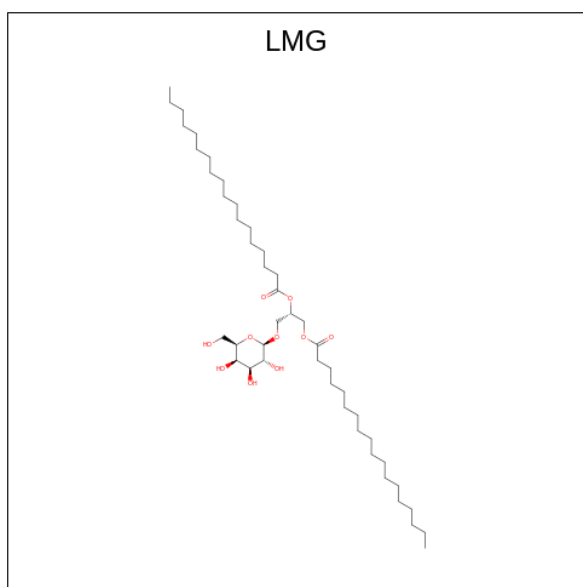


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			55	53	2		
32	D	1	Total	C	O	0	0
			55	53	2		
32	a	1	Total	C	O	0	0
			55	53	2		
32	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

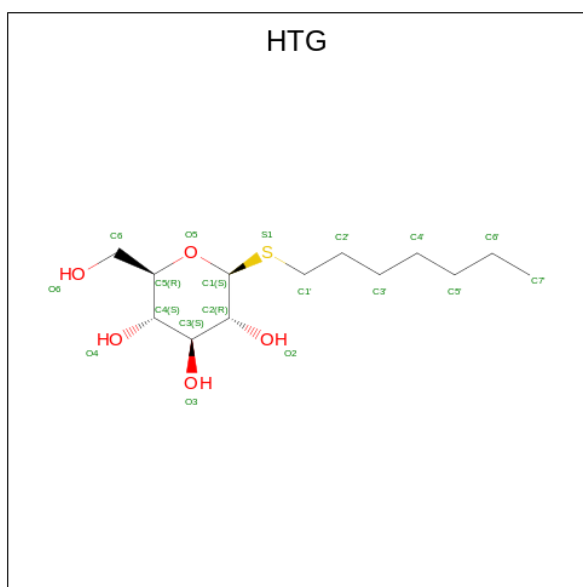
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		
33	F	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		
33	c	1	Total	Ca	0	0
			1	1		
33	f	1	Total	Ca	0	0
			1	1		
33	o	1	Total	Ca	0	0
			1	1		

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	b	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



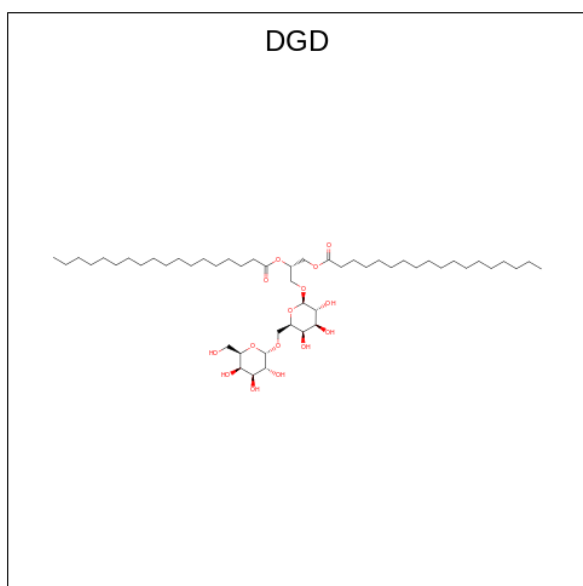
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	B	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	C	1	19	13	5	1	0	0
35	D	1	16	10	5	1	0	0
35	O	1	19	13	5	1	0	0
35	V	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0
35	b	1	19	13	5	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



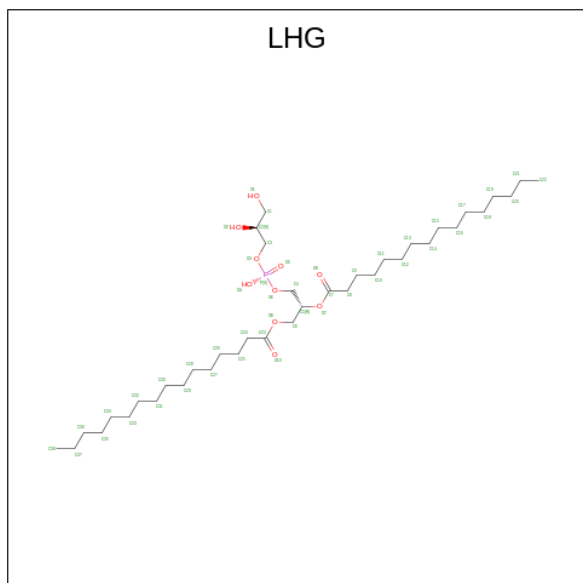
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	D	1	Total	C	O	0	0
			62	47	15		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	d	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



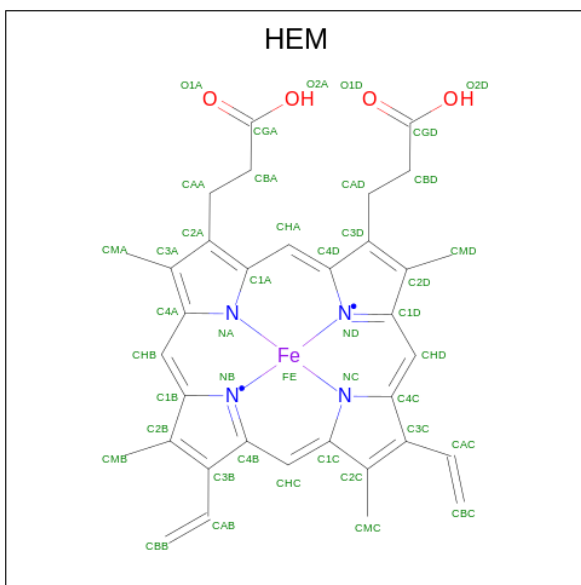
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	e	1	Total	C	O	P	0	0
			42	31	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	1	1	Total	C	O	P	0	0
			49	38	10	1		

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

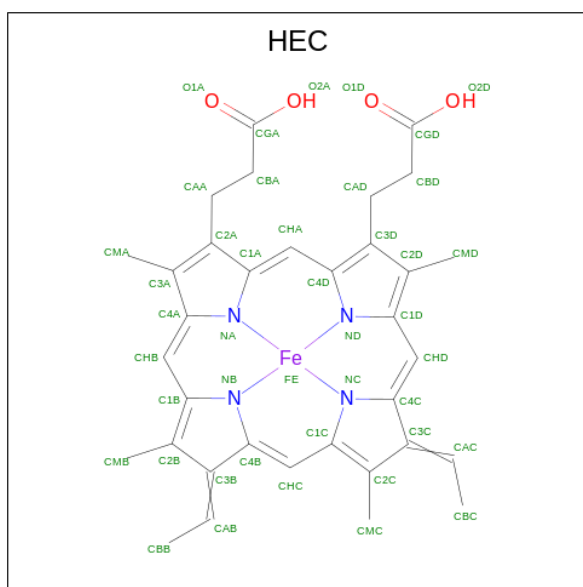


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg	0	0
			1	1		
39	j	1	Total	Mg	0	0
			1	1		

- Molecule 40 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	146	Total	O	0	3
			149	149		
41	B	277	Total	O	0	3
			280	280		
41	C	206	Total	O	0	3
			209	209		
41	D	157	Total	O	0	4
			161	161		
41	E	28	Total	O	0	0
			28	28		
41	F	7	Total	O	0	0
			7	7		
41	H	39	Total	O	0	1
			40	40		
41	I	8	Total	O	0	0
			8	8		
41	J	12	Total	O	0	0
			12	12		
41	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	12	Total O 12 12	0	0
41	M	15	Total O 15 15	0	0
41	O	164	Total O 165 165	0	1
41	T	12	Total O 13 13	0	1
41	U	75	Total O 76 76	0	1
41	V	111	Total O 111 111	0	0
41	Y	1	Total O 1 1	0	0
41	X	8	Total O 8 8	0	0
41	a	151	Total O 151 151	0	0
41	b	247	Total O 249 249	0	2
41	c	187	Total O 189 189	0	2
41	d	136	Total O 139 139	0	3
41	e	15	Total O 15 15	0	0
41	f	7	Total O 7 7	0	0
41	h	36	Total O 36 36	0	0
41	i	5	Total O 5 5	0	0
41	j	7	Total O 7 7	0	0
41	k	3	Total O 3 3	0	0
41	l	10	Total O 10 10	0	0
41	m	12	Total O 12 12	0	0
41	o	137	Total O 137 137	0	0

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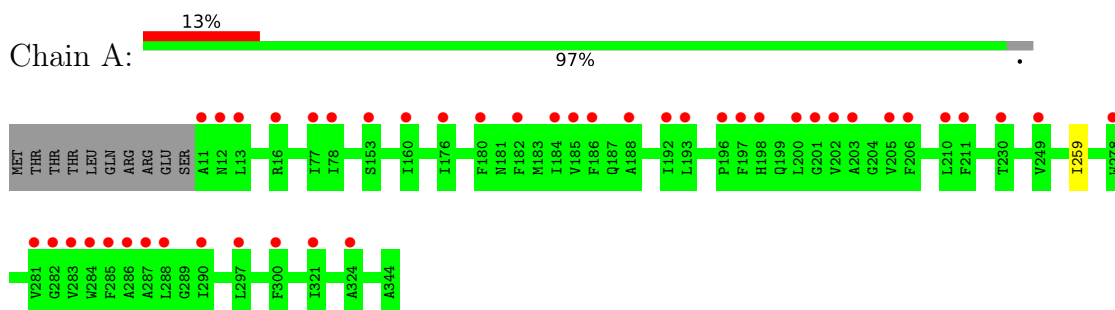
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	t	10	Total O 10 10	0	0
41	u	89	Total O 89 89	0	0
41	v	80	Total O 80 80	0	0
41	y	4	Total O 4 4	0	0
41	x	5	Total O 5 5	0	0

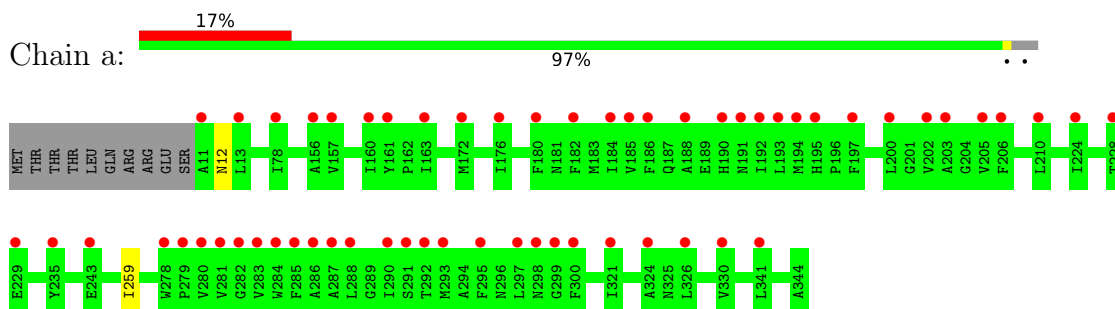
3 Residue-property plots [i](#)

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.

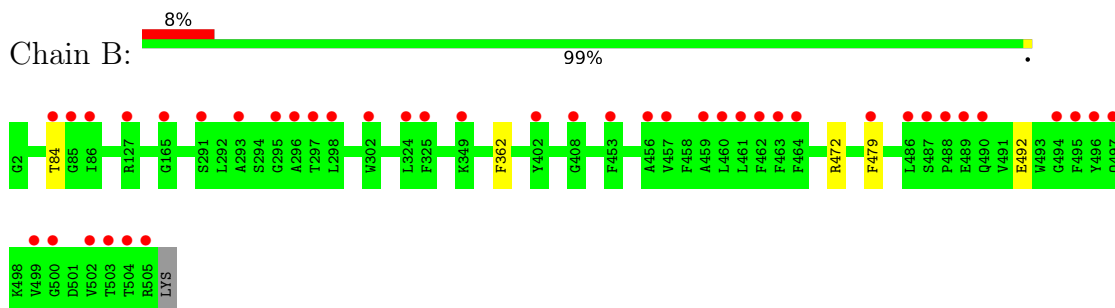
- Molecule 1: Photosystem Q(B) protein



- Molecule 1: Photosystem Q(B) protein

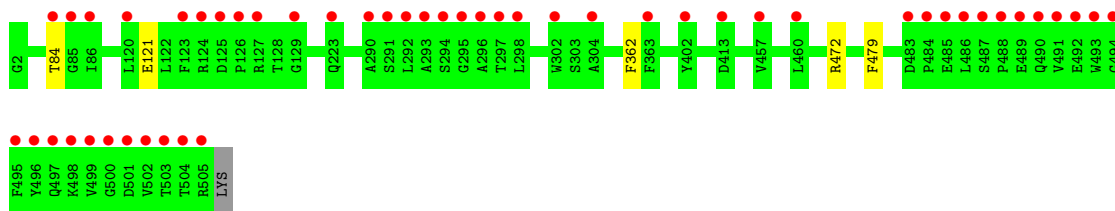


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

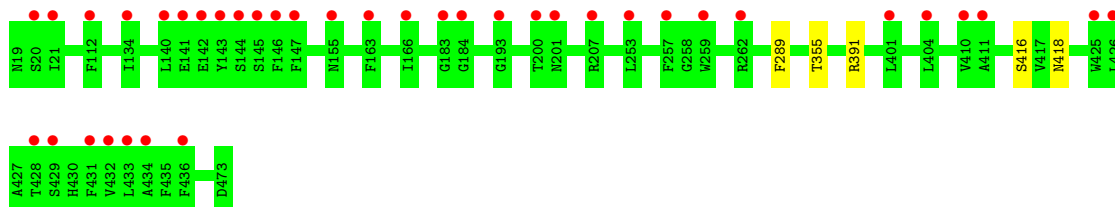




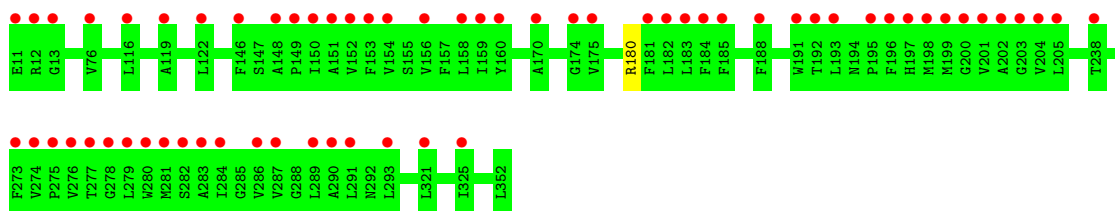
- Molecule 3: Photosystem II 44 kDa reaction center protein



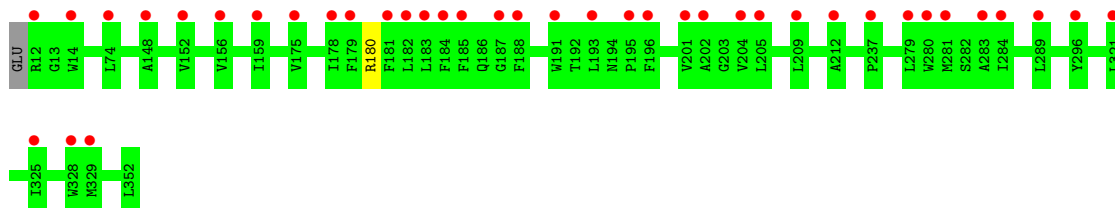
- Molecule 3: Photosystem II 44 kDa reaction center protein



- Molecule 4: Photosystem II D2 protein

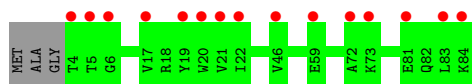


- Molecule 4: Photosystem II D2 protein

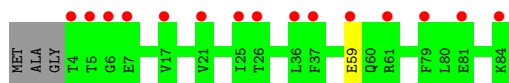
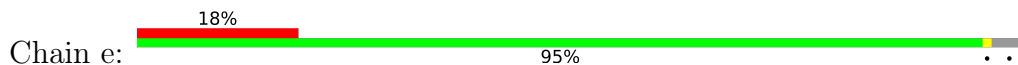


- Molecule 5: Cytochrome b559 subunit alpha

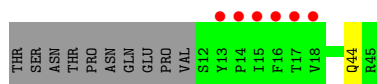
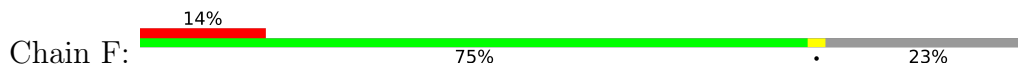




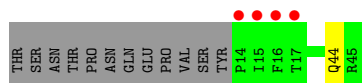
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



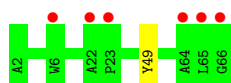
- Molecule 6: Cytochrome b559 subunit beta



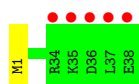
- Molecule 7: Photosystem II reaction center protein H



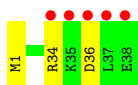
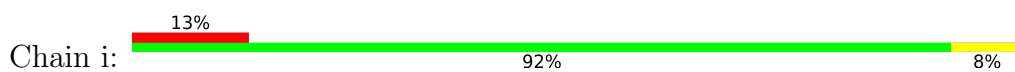
- Molecule 7: Photosystem II reaction center protein H



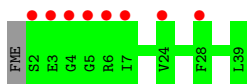
- Molecule 8: Photosystem II reaction center protein I



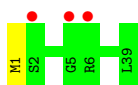
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



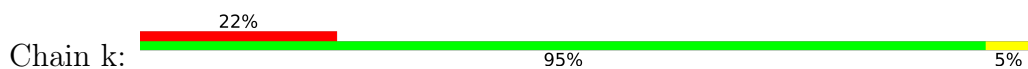
- Molecule 9: Photosystem II reaction center protein J



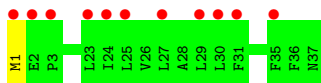
- Molecule 10: Photosystem II reaction center protein K



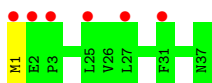
- Molecule 10: Photosystem II reaction center protein K



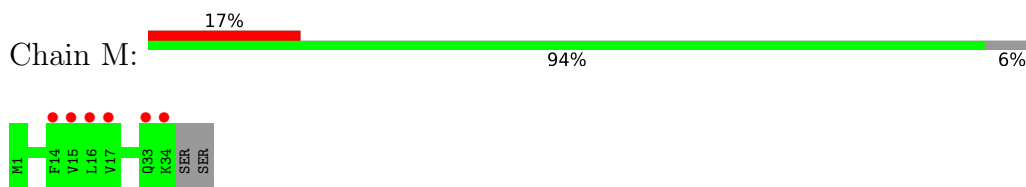
- Molecule 11: Photosystem II reaction center protein L



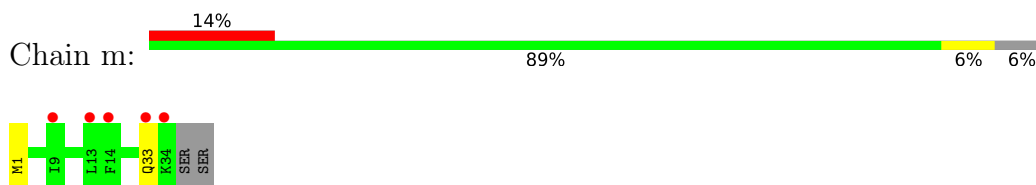
- Molecule 11: Photosystem II reaction center protein L



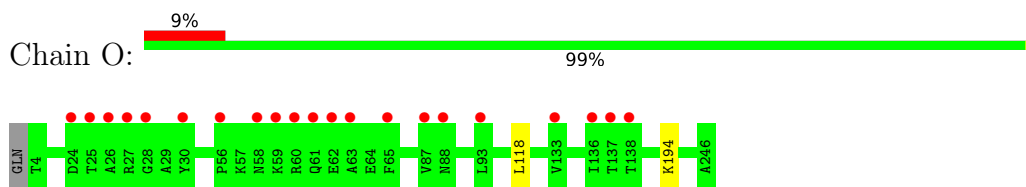
- Molecule 12: Photosystem II reaction center protein M



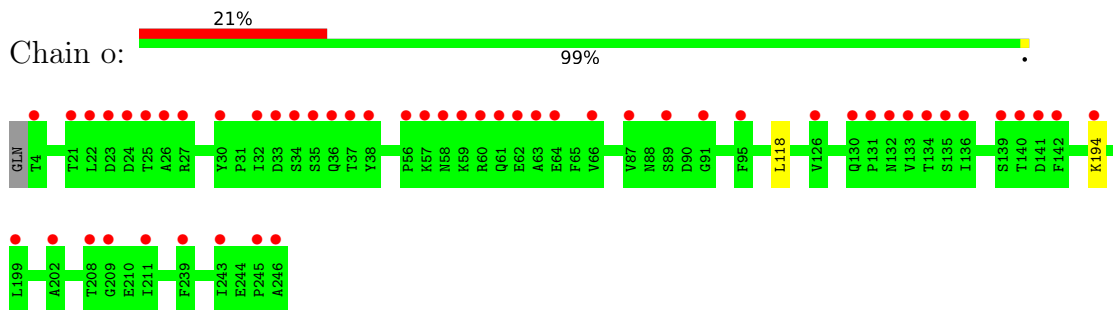
- Molecule 12: Photosystem II reaction center protein M



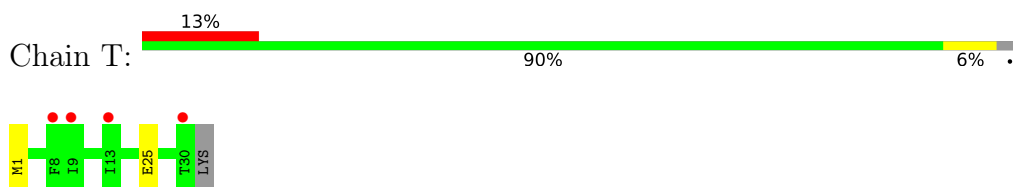
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



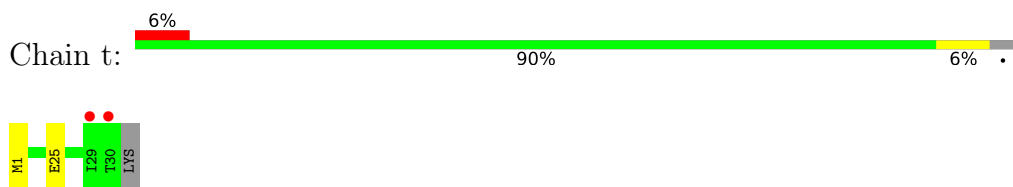
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



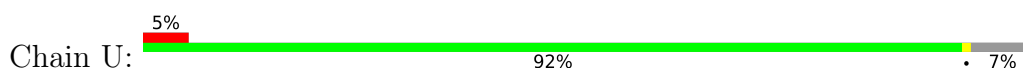
- Molecule 14: Photosystem II reaction center protein T



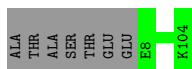
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



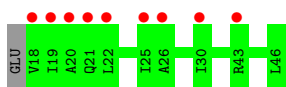
- Molecule 16: Cytochrome c-550



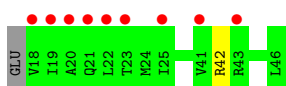
- Molecule 16: Cytochrome c-550



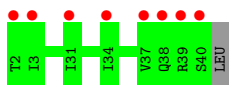
- Molecule 17: Photosystem II reaction center protein Ycf12



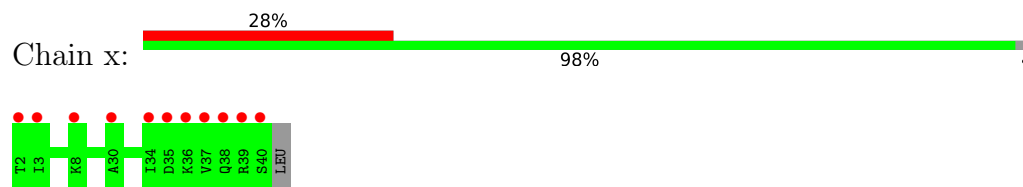
- Molecule 17: Photosystem II reaction center protein Ycf12



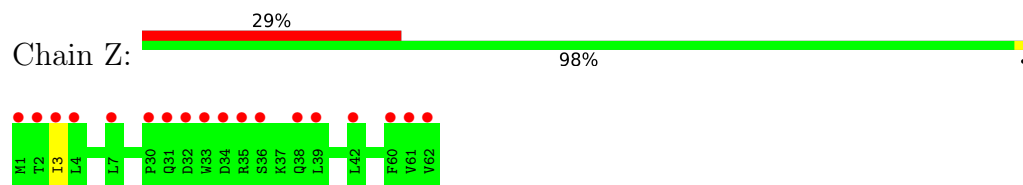
- Molecule 18: Photosystem II reaction center protein X



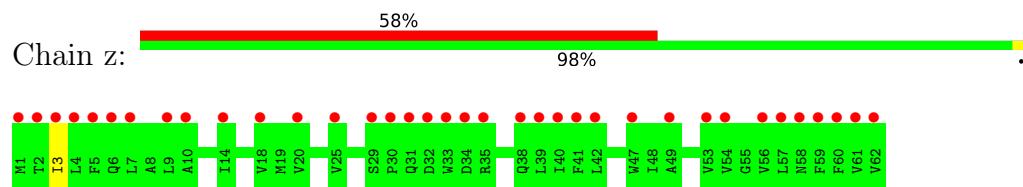
- Molecule 18: Photosystem II reaction center protein X



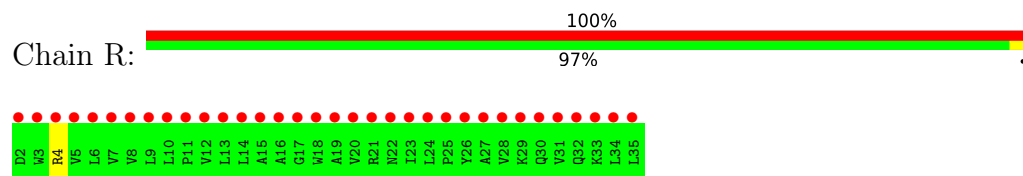
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.81Å 230.00Å 288.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.90 – 1.95 61.90 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.90-1.95) 85.6 (61.90-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.08 (at 1.94Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.225 0.187 , 0.225	Depositor DCC
R_{free} test set	29342 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtrriage
Anisotropy	0.602	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53958	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.53	0/2725	0.59	0/3716
1	a	0.55	0/2731	0.58	0/3724
2	B	0.49	0/4193	0.56	0/5712
2	b	0.47	0/4201	0.55	0/5723
3	C	0.46	0/3634	0.54	0/4947
3	c	0.46	0/3676	0.54	0/5004
4	D	0.53	0/2821	0.56	0/3844
4	d	0.52	0/2818	0.55	0/3840
5	E	0.36	0/693	0.52	0/944
5	e	0.33	0/681	0.52	0/928
6	F	0.39	0/284	0.48	0/387
6	f	0.37	0/265	0.51	0/360
7	H	0.40	0/535	0.53	0/728
7	h	0.35	0/524	0.50	0/713
8	I	0.38	0/311	0.51	0/419
8	i	0.40	0/311	0.50	0/419
9	J	0.37	0/278	0.46	0/376
9	j	0.38	0/278	0.48	0/376
10	K	0.36	0/303	0.48	0/416
10	k	0.36	0/303	0.51	0/416
11	L	0.48	0/319	0.49	0/433
11	l	0.49	0/319	0.50	0/433
12	M	0.43	0/270	0.58	0/368
12	m	0.47	0/262	0.58	0/357
13	O	0.41	0/1926	0.56	0/2611
13	o	0.40	0/1919	0.57	0/2601
14	T	0.54	0/266	0.56	0/362
14	t	0.54	0/266	0.56	0/362
15	U	0.44	0/785	0.55	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.45	0/1096	0.54	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.41	0/1085	0.53	0/1473
17	Y	0.29	0/216	0.46	0/289
17	y	0.28	0/216	0.46	0/289
18	X	0.34	0/298	0.44	0/403
18	x	0.34	0/290	0.48	0/392
19	Z	0.31	0/490	0.43	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.24	0/279	0.38	0/383
All	All	0.46	0/43142	0.55	0/58701

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	41	30
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	41	30
2	B	512/505 (101%)	507 (99%)	5 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	454/455 (100%)	445 (98%)	7 (2%)	2 (0%)	34	22
3	c	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	34	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	1
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	242 (99%)	3 (1%)	0	100	100
13	o	244/244 (100%)	238 (98%)	6 (2%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	29/31 (94%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5279/5382 (98%)	5168 (98%)	104 (2%)	7 (0%)	51	43

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	i	36	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	272 (100%)	0	100	100
1	a	273/279 (98%)	272 (100%)	1 (0%)	91	90
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	68
2	b	413/403 (102%)	408 (99%)	5 (1%)	71	68
3	C	357/356 (100%)	352 (99%)	5 (1%)	67	62
3	c	362/356 (102%)	358 (99%)	4 (1%)	73	71
4	D	277/277 (100%)	276 (100%)	1 (0%)	91	90
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	90
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	72/73 (99%)	71 (99%)	1 (1%)	67	62
6	F	28/38 (74%)	27 (96%)	1 (4%)	35	23
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	21
7	H	55/54 (102%)	52 (94%)	3 (6%)	21	9
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	31
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	5
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	5
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	33
11	l	36/35 (103%)	35 (97%)	1 (3%)	43	33
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	26
13	O	210/207 (101%)	208 (99%)	2 (1%)	76	74
13	o	209/207 (101%)	207 (99%)	2 (1%)	76	74
14	T	27/27 (100%)	25 (93%)	2 (7%)	13	4
14	t	27/27 (100%)	25 (93%)	2 (7%)	13	4
15	U	84/89 (94%)	83 (99%)	1 (1%)	71	68
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	80
16	v	117/117 (100%)	116 (99%)	1 (1%)	78	77
17	Y	22/23 (96%)	22 (100%)	0	100	100
17	y	22/23 (96%)	21 (96%)	1 (4%)	27	15
18	X	33/33 (100%)	33 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	50
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	50
20	R	29/29 (100%)	28 (97%)	1 (3%)	37	25
All	All	4383/4399 (100%)	4331 (99%)	52 (1%)	73	68

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	121	GLU
3	c	418	ASN
16	v	86	GLN

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Mol	Chain	Res	Type
2	b	362	PHE
3	c	289	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	497	GLN
13	o	109	GLN
19	z	6	GLN
15	u	81	HIS
19	Z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	2.28	4 (57%)
9	FME	j	1	9	8,9,10	0.63	0	7,9,11	1.32	1 (14%)
12	FME	M	1	12	8,9,10	0.63	0	7,9,11	1.32	0
12	FME	m	1	12	8,9,10	0.69	0	7,9,11	1.05	1 (14%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.32	2 (28%)
8	FME	i	1	8	8,9,10	0.62	0	7,9,11	1.17	1 (14%)
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.73	3 (42%)

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
14	FME	t	1	14	-	2/7/9/11	-
9	FME	j	1	9	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	3.68	116.36	109.73
14	t	1	FME	O-C-CA	-3.00	116.92	124.78
14	T	1	FME	O-C-CA	-2.78	117.48	124.78
14	T	1	FME	C-CA-N	2.35	113.97	109.73
14	T	1	FME	CA-N-CN	-2.29	119.31	122.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
9	j	1	FME	O1-CN-N-CA
9	j	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 252 ligands modelled in this entry, 17 are monoatomic and 19 are unknown - leaving 216 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
24	CLA	c	506	41	65,73,73	2.04	16 (24%)	76,113,113	2.75	27 (35%)
24	CLA	B	610	-	65,73,73	2.00	15 (23%)	76,113,113	2.85	27 (35%)
28	GOL	a	412	-	5,5,5	0.34	0	5,5,5	0.57	0
28	GOL	c	527	-	5,5,5	0.41	0	5,5,5	0.31	0
28	GOL	B	629	-	5,5,5	0.32	0	5,5,5	0.39	0
24	CLA	c	512	-	65,73,73	2.05	15 (23%)	76,113,113	2.71	29 (38%)
28	GOL	A	412	-	5,5,5	0.26	0	5,5,5	0.68	0
24	CLA	c	505	-	65,73,73	2.02	16 (24%)	76,113,113	2.80	26 (34%)
24	CLA	C	510	-	65,73,73	2.14	16 (24%)	76,113,113	2.71	28 (36%)
28	GOL	t	102	-	5,5,5	0.34	0	5,5,5	0.30	0
24	CLA	c	510	-	65,73,73	2.11	16 (24%)	76,113,113	2.76	29 (38%)
28	GOL	B	633	-	5,5,5	0.30	0	5,5,5	0.66	0
24	CLA	a	407	41	65,73,73	2.06	16 (24%)	76,113,113	2.77	29 (38%)
26	BCR	A	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	7 (12%)
26	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	11 (19%)
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.29	0
30	LMT	M	101	-	36,36,36	0.57	1 (2%)	47,47,47	0.84	0
24	CLA	C	506	-	65,73,73	2.06	16 (24%)	76,113,113	2.57	23 (30%)
24	CLA	C	511	-	65,73,73	2.09	16 (24%)	76,113,113	2.70	28 (36%)
24	CLA	B	614	-	65,73,73	2.06	15 (23%)	76,113,113	2.70	31 (40%)
27	SQD	A	416	-	53,54,54	1.05	3 (5%)	62,65,65	1.15	7 (11%)
24	CLA	b	613	-	65,73,73	2.09	16 (24%)	76,113,113	2.74	30 (39%)
24	CLA	b	618	-	65,73,73	2.05	16 (24%)	76,113,113	2.80	25 (32%)
24	CLA	c	503	-	65,73,73	2.06	16 (24%)	76,113,113	2.77	28 (36%)
26	BCR	b	622	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	4 (7%)
26	BCR	c	526	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	503	-	65,73,73	2.08	16 (24%)	76,113,113	2.66	27 (35%)
30	LMT	m	102	-	36,36,36	0.49	0	47,47,47	0.99	2 (4%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.14	5 (8%)
30	LMT	B	634	-	25,25,36	0.49	0	30,30,47	0.71	0
24	CLA	C	509	-	65,73,73	2.10	16 (24%)	76,113,113	2.75	26 (34%)
26	BCR	k	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.33	5 (8%)
24	CLA	c	514	-	65,73,73	2.03	16 (24%)	76,113,113	2.81	29 (38%)
26	BCR	c	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.41	9 (16%)
30	LMT	E	102	-	36,36,36	0.46	0	47,47,47	0.75	0
24	CLA	c	504	-	65,73,73	2.00	16 (24%)	76,113,113	2.63	25 (32%)
34	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.44	7 (15%)
35	HTG	O	303	-	19,19,19	1.07	1 (5%)	23,24,24	0.93	1 (4%)
24	CLA	B	606	-	65,73,73	1.99	16 (24%)	76,113,113	2.87	28 (36%)
24	CLA	b	612	41	65,73,73	1.97	15 (23%)	76,113,113	2.72	28 (36%)
28	GOL	B	626	-	5,5,5	0.29	0	5,5,5	0.48	0
24	CLA	b	611	-	65,73,73	2.03	16 (24%)	76,113,113	2.80	29 (38%)
24	CLA	B	607	-	65,73,73	2.06	16 (24%)	76,113,113	2.85	28 (36%)
40	HEC	v	202	16	32,50,50	1.49	4 (12%)	24,82,82	1.34	4 (16%)
32	PL9	A	419	-	55,55,55	0.63	1 (1%)	68,69,69	1.85	19 (27%)
34	LMG	c	520	-	51,51,55	0.95	2 (3%)	59,59,63	0.92	2 (3%)
28	GOL	C	525	-	5,5,5	0.33	0	5,5,5	0.72	0
28	GOL	b	631	-	5,5,5	0.34	0	5,5,5	0.45	0
24	CLA	B	615	-	65,73,73	1.98	17 (26%)	76,113,113	2.96	28 (36%)
25	PHO	A	408	-	51,69,69	1.87	8 (15%)	47,99,99	1.80	10 (21%)
26	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	11 (19%)
28	GOL	c	525	-	5,5,5	0.36	0	5,5,5	0.58	0
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.39	0
24	CLA	B	608	41	65,73,73	2.02	16 (24%)	76,113,113	2.70	30 (39%)
24	CLA	b	606	41	65,73,73	2.10	16 (24%)	76,113,113	2.74	24 (31%)
28	GOL	b	632	-	5,5,5	0.44	0	5,5,5	0.52	0
30	LMT	I	102	-	36,36,36	0.45	0	47,47,47	1.18	4 (8%)
36	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.06	4 (5%)
27	SQD	a	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.60	11 (17%)
28	GOL	F	103	33	5,5,5	0.36	0	5,5,5	0.37	0
32	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.85	18 (26%)
24	CLA	b	607	-	65,73,73	2.08	16 (24%)	76,113,113	2.84	32 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	514	-	65,73,73	2.02	16 (24%)	76,113,113	2.73	27 (35%)
34	LMG	b	625	-	51,51,55	0.90	2 (3%)	59,59,63	1.03	4 (6%)
35	HTG	V	204	-	19,19,19	1.00	2 (10%)	23,24,24	1.33	3 (13%)
26	BCR	B	620	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	13 (23%)
25	PHO	A	407	-	51,69,69	1.88	7 (13%)	47,99,99	1.69	9 (19%)
24	CLA	A	406	41	65,73,73	2.10	15 (23%)	76,113,113	2.75	31 (40%)
28	GOL	f	104	33	5,5,5	0.35	0	5,5,5	0.24	0
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.04	3 (6%)
26	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.00	3 (5%)
24	CLA	d	401	41	65,73,73	2.04	13 (20%)	76,113,113	2.71	28 (36%)
24	CLA	b	617	-	65,73,73	2.03	17 (26%)	76,113,113	2.64	27 (35%)
24	CLA	B	602	41	65,73,73	2.09	16 (24%)	76,113,113	2.77	28 (36%)
24	CLA	b	621	-	65,73,73	2.10	17 (26%)	76,113,113	2.70	27 (35%)
27	SQD	A	411	-	53,54,54	0.97	3 (5%)	62,65,65	1.58	11 (17%)
24	CLA	B	605	-	65,73,73	1.98	18 (27%)	76,113,113	2.88	26 (34%)
35	HTG	d	411	-	16,16,19	1.21	2 (12%)	20,21,24	1.55	1 (5%)
37	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	5 (9%)
26	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.25	5 (8%)
38	HEM	E	103	6,5	41,50,50	1.31	5 (12%)	45,82,82	1.94	14 (31%)
35	HTG	c	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
28	GOL	v	205	-	5,5,5	0.35	0	5,5,5	0.46	0
30	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.86	0
35	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	1.28	2 (8%)
26	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.39	8 (14%)
24	CLA	b	608	-	65,73,73	2.07	16 (24%)	76,113,113	2.86	30 (39%)
26	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	8 (14%)
35	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.50	2 (8%)
24	CLA	A	405	-	65,73,73	2.08	17 (26%)	76,113,113	2.74	29 (38%)
24	CLA	c	513	3	65,73,73	2.04	15 (23%)	76,113,113	2.68	26 (34%)
26	BCR	d	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	13 (23%)
28	GOL	V	208	-	5,5,5	0.37	0	5,5,5	0.27	0
35	HTG	b	603	-	19,19,19	1.07	2 (10%)	23,24,24	1.28	1 (4%)
27	SQD	a	402	-	53,54,54	1.03	3 (5%)	62,65,65	1.19	6 (9%)
30	LMT	b	626	-	25,25,36	0.50	0	30,30,47	0.64	0
37	LHG	D	409	-	48,48,48	0.85	2 (4%)	51,54,54	1.08	5 (9%)
37	LHG	l	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	D	402	-	36,36,36	0.48	0	47,47,47	1.01	3 (6%)
24	CLA	A	409	-	65,73,73	2.03	16 (24%)	76,113,113	2.77	29 (38%)
32	PL9	d	406	-	55,55,55	0.71	1 (1%)	68,69,69	1.55	14 (20%)
28	GOL	c	524	-	5,5,5	0.32	0	5,5,5	0.37	0
24	CLA	B	604	-	65,73,73	2.07	16 (24%)	76,113,113	2.81	31 (40%)
36	DGD	D	407	-	63,63,67	0.96	4 (6%)	77,77,81	1.30	9 (11%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.33	8 (14%)
24	CLA	C	504	-	65,73,73	2.09	16 (24%)	76,113,113	2.75	26 (34%)
23	BCT	A	404	21	2,3,3	0.65	0	2,3,3	0.87	0
24	CLA	B	612	-	65,73,73	2.07	16 (24%)	76,113,113	2.81	25 (32%)
24	CLA	D	404	-	65,73,73	2.02	15 (23%)	76,113,113	2.76	29 (38%)
24	CLA	C	507	-	65,73,73	2.06	16 (24%)	76,113,113	2.70	29 (38%)
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.71	0
36	DGD	d	407	-	63,63,67	0.94	3 (4%)	77,77,81	1.04	6 (7%)
30	LMT	a	417	-	36,36,36	0.44	0	47,47,47	0.84	2 (4%)
31	OEX	a	415	1,41,3	0,15,15	-	-	-	-	-
28	GOL	V	207	-	5,5,5	0.37	0	5,5,5	0.46	0
24	CLA	C	505	41	65,73,73	2.06	16 (24%)	76,113,113	2.75	26 (34%)
36	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	0.97	3 (3%)
38	HEM	e	102	6,5	41,50,50	1.32	6 (14%)	45,82,82	1.91	11 (24%)
28	GOL	T	103	-	5,5,5	0.41	0	5,5,5	0.24	0
35	HTG	b	628	-	19,19,19	1.10	2 (10%)	23,24,24	1.83	3 (13%)
30	LMT	b	602	-	25,25,36	0.46	0	30,30,47	1.26	3 (10%)
37	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.09	3 (6%)
26	BCR	t	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	8 (14%)
28	GOL	T	101	-	5,5,5	0.45	0	5,5,5	0.31	0
23	BCT	a	418	21	2,3,3	0.60	0	2,3,3	0.82	0
34	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.11	5 (8%)
36	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	3 (3%)
35	HTG	B	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.89	4 (17%)
40	HEC	V	203	16	32,50,50	1.38	4 (12%)	24,82,82	1.55	4 (16%)
24	CLA	B	611	41	65,73,73	2.05	16 (24%)	76,113,113	2.75	29 (38%)
28	GOL	B	635	-	5,5,5	0.40	0	5,5,5	0.25	0
30	LMT	A	417	-	34,34,36	0.38	0	45,45,47	1.06	3 (6%)
24	CLA	B	603	-	65,73,73	2.05	18 (27%)	76,113,113	2.83	29 (38%)
36	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.02	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	609	-	65,73,73	2.11	16 (24%)	76,113,113	2.71	28 (36%)
24	CLA	C	502	-	65,73,73	2.00	16 (24%)	76,113,113	2.65	25 (32%)
24	CLA	c	508	-	65,73,73	2.05	17 (26%)	76,113,113	2.67	31 (40%)
36	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.09	6 (7%)
27	SQD	b	601	-	53,54,54	1.02	3 (5%)	62,65,65	1.63	10 (16%)
28	GOL	b	630	-	5,5,5	0.34	0	5,5,5	0.16	0
24	CLA	c	509	41	65,73,73	2.01	15 (23%)	76,113,113	2.74	25 (32%)
26	BCR	b	624	-	41,41,41	0.99	1 (2%)	56,56,56	1.25	8 (14%)
24	CLA	b	609	-	65,73,73	2.09	18 (27%)	76,113,113	2.80	26 (34%)
34	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.17	4 (8%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	7 (9%)
27	SQD	F	101	-	42,43,54	1.12	3 (7%)	51,54,65	1.55	9 (17%)
34	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
24	CLA	B	613	-	65,73,73	2.06	17 (26%)	76,113,113	2.61	24 (31%)
24	CLA	D	403	-	65,73,73	2.05	17 (26%)	76,113,113	2.80	27 (35%)
26	BCR	a	410	-	41,41,41	1.14	1 (2%)	56,56,56	1.35	8 (14%)
37	LHG	d	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.97	3 (5%)
27	SQD	f	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.44	7 (13%)
24	CLA	B	617	-	65,73,73	2.04	16 (24%)	76,113,113	2.72	26 (34%)
24	CLA	c	515	-	65,73,73	2.08	17 (26%)	76,113,113	2.73	29 (38%)
34	LMG	c	501	-	51,51,55	0.88	2 (3%)	59,59,63	1.25	6 (10%)
35	HTG	B	631	-	19,19,19	1.03	2 (10%)	23,24,24	1.44	2 (8%)
34	LMG	C	501	-	51,51,55	0.97	2 (3%)	59,59,63	1.10	3 (5%)
24	CLA	b	615	41	65,73,73	2.06	16 (24%)	76,113,113	2.66	27 (35%)
24	CLA	c	507	-	65,73,73	2.00	16 (24%)	76,113,113	2.58	21 (27%)
26	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	5 (8%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.03	3 (15%)
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.39	0
24	CLA	c	511	-	65,73,73	2.17	16 (24%)	76,113,113	2.72	26 (34%)
30	LMT	m	103	-	36,36,36	0.56	1 (2%)	47,47,47	1.05	4 (8%)
24	CLA	b	616	-	65,73,73	2.04	16 (24%)	76,113,113	2.79	27 (35%)
32	PL9	D	406	-	55,55,55	0.77	2 (3%)	68,69,69	1.50	16 (23%)
35	HTG	B	623	-	19,19,19	0.88	1 (5%)	23,24,24	1.25	3 (13%)
24	CLA	b	620	-	65,73,73	2.07	16 (24%)	76,113,113	2.76	25 (32%)
31	OEX	A	418	1,41,3	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	402	-	65,73,73	2.07	17 (26%)	76,113,113	2.78	27 (35%)
28	GOL	A	413	-	5,5,5	0.43	0	5,5,5	0.62	0
35	HTG	b	627	-	19,19,19	0.86	1 (5%)	23,24,24	1.35	4 (17%)
37	LHG	D	408	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
34	LMG	J	101	39	51,51,55	0.84	2 (3%)	59,59,63	1.01	4 (6%)
28	GOL	V	201	-	5,5,5	0.38	0	5,5,5	0.43	0
26	BCR	B	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.24	5 (8%)
24	CLA	b	614	-	65,73,73	2.09	15 (23%)	76,113,113	2.77	28 (36%)
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	0.89	3 (3%)
24	CLA	C	512	3	65,73,73	2.01	16 (24%)	76,113,113	2.75	24 (31%)
35	HTG	B	630	-	19,19,19	0.97	2 (10%)	23,24,24	1.31	1 (4%)
35	HTG	B	622	-	19,19,19	1.20	1 (5%)	23,24,24	1.43	3 (13%)
37	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	5 (9%)
28	GOL	V	206	-	5,5,5	0.37	0	5,5,5	0.46	0
28	GOL	v	203	-	5,5,5	0.27	0	5,5,5	0.49	0
24	CLA	a	409	-	65,73,73	2.03	16 (24%)	76,113,113	2.72	28 (36%)
30	LMT	a	401	-	36,36,36	0.45	0	47,47,47	0.97	3 (6%)
34	LMG	c	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	5 (8%)
28	GOL	v	204	-	5,5,5	0.32	0	5,5,5	0.37	0
36	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.90	3 (3%)
24	CLA	C	508	41	65,73,73	2.07	16 (24%)	76,113,113	2.76	28 (36%)
34	LMG	j	101	39	51,51,55	0.93	3 (5%)	59,59,63	0.98	3 (5%)
24	CLA	B	616	-	65,73,73	2.03	17 (26%)	76,113,113	2.70	28 (36%)
24	CLA	b	619	-	65,73,73	2.02	16 (24%)	76,113,113	2.82	29 (38%)
28	GOL	C	524	-	5,5,5	0.34	0	5,5,5	0.89	0
24	CLA	D	401	41	65,73,73	2.08	16 (24%)	76,113,113	2.73	31 (40%)
25	PHO	d	403	-	51,69,69	1.87	7 (13%)	47,99,99	1.93	11 (23%)
26	BCR	b	623	-	41,41,41	1.08	1 (2%)	56,56,56	1.13	5 (8%)
24	CLA	d	404	-	65,73,73	2.04	18 (27%)	76,113,113	2.80	27 (35%)
25	PHO	a	408	-	51,69,69	1.83	7 (13%)	47,99,99	1.75	8 (17%)
37	LHG	d	408	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	5 (9%)
28	GOL	B	625	-	5,5,5	0.31	0	5,5,5	0.56	0
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	10 (17%)
24	CLA	b	610	-	65,73,73	1.99	16 (24%)	76,113,113	2.91	28 (36%)
28	GOL	A	414	-	5,5,5	0.41	0	5,5,5	0.20	0
30	LMT	f	102	-	36,36,36	0.47	0	47,47,47	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	D	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.70	12 (21%)
24	CLA	a	406	-	65,73,73	2.07	16 (24%)	76,113,113	2.73	28 (36%)
27	SQD	l	101	-	53,54,54	1.00	3 (5%)	62,65,65	1.40	9 (14%)
28	GOL	B	628	-	5,5,5	0.40	0	5,5,5	0.29	0
35	HTG	C	523	-	19,19,19	1.02	2 (10%)	23,24,24	1.77	5 (21%)
28	GOL	a	413	-	5,5,5	0.43	0	5,5,5	0.27	0
35	HTG	b	604	-	19,19,19	1.02	2 (10%)	23,24,24	1.10	2 (8%)
37	LHG	D	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.94	3 (5%)
28	GOL	O	302	-	5,5,5	0.36	0	5,5,5	0.35	0
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.30	0
24	CLA	C	513	-	65,73,73	2.04	16 (24%)	76,113,113	2.73	31 (40%)

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
24	CLA	c	506	41	1/1/15/20	6/37/115/115	-
24	CLA	B	610	-	1/1/15/20	3/37/115/115	-
28	GOL	a	412	-	-	2/4/4/4	-
28	GOL	c	527	-	-	2/4/4/4	-
28	GOL	B	629	-	-	0/4/4/4	-
24	CLA	c	512	-	1/1/15/20	7/37/115/115	-
28	GOL	A	412	-	-	2/4/4/4	-
24	CLA	c	505	-	1/1/15/20	4/37/115/115	-
24	CLA	C	510	-	1/1/15/20	4/37/115/115	-
28	GOL	t	102	-	-	0/4/4/4	-
24	CLA	c	510	-	1/1/15/20	2/37/115/115	-
28	GOL	B	633	-	-	0/4/4/4	-
24	CLA	a	407	41	-	3/37/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
28	GOL	b	629	-	-	2/4/4/4	-
30	LMT	M	101	-	-	8/21/61/61	0/2/2/2
24	CLA	C	506	-	1/1/15/20	5/37/115/115	-
24	CLA	C	511	-	1/1/15/20	8/37/115/115	-
24	CLA	B	614	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	416	-	-	17/49/69/69	0/1/1/1
24	CLA	b	613	-	-	2/37/115/115	-
24	CLA	b	618	-	1/1/15/20	6/37/115/115	-
24	CLA	c	503	-	1/1/15/20	3/37/115/115	-
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
26	BCR	c	526	-	-	1/29/63/63	0/2/2/2
24	CLA	C	503	-	-	8/37/115/115	-
30	LMT	m	102	-	-	3/21/61/61	0/2/2/2
34	LMG	C	521	-	-	14/46/66/70	0/1/1/1
30	LMT	B	634	-	-	5/17/37/61	0/1/1/2
24	CLA	C	509	-	-	3/37/115/115	-
26	BCR	k	103	-	-	1/29/63/63	0/2/2/2
24	CLA	c	514	-	1/1/15/20	12/37/115/115	-
26	BCR	c	516	-	-	4/29/63/63	0/2/2/2
30	LMT	E	102	-	-	9/21/61/61	0/2/2/2
24	CLA	c	504	-	1/1/15/20	3/37/115/115	-
34	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
35	HTG	O	303	-	-	2/10/30/30	0/1/1/1
24	CLA	B	606	-	1/1/15/20	3/37/115/115	-
24	CLA	b	612	41	1/1/15/20	3/37/115/115	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	b	611	-	1/1/15/20	8/37/115/115	-
24	CLA	B	607	-	1/1/15/20	4/37/115/115	-
40	HEC	v	202	16	-	2/10/54/54	-
32	PL9	A	419	-	-	8/53/73/73	0/1/1/1
34	LMG	c	520	-	-	5/46/66/70	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	-
28	GOL	b	631	-	-	2/4/4/4	-
24	CLA	B	615	-	1/1/15/20	14/37/115/115	-
25	PHO	A	408	-	-	1/37/103/103	0/5/6/6
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	GOL	c	525	-	-	1/4/4/4	-
28	GOL	v	201	-	-	0/4/4/4	-
24	CLA	B	608	41	1/1/15/20	5/37/115/115	-
24	CLA	b	606	41	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	b	632	-	-	2/4/4/4	-
30	LMT	I	102	-	-	10/21/61/61	0/2/2/2
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
27	SQD	a	411	-	-	9/49/69/69	0/1/1/1
28	GOL	F	103	33	-	2/4/4/4	-
32	PL9	a	416	-	-	17/53/73/73	0/1/1/1
24	CLA	b	607	-	1/1/15/20	3/37/115/115	-
24	CLA	C	514	-	-	3/37/115/115	-
34	LMG	b	625	-	-	18/46/66/70	0/1/1/1
35	HTG	V	204	-	-	3/10/30/30	0/1/1/1
26	BCR	B	620	-	-	5/29/63/63	0/2/2/2
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
24	CLA	A	406	41	-	5/37/115/115	-
28	GOL	f	104	33	-	3/4/4/4	-
37	LHG	e	101	-	-	18/46/46/53	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	d	401	41	1/1/15/20	7/37/115/115	-
24	CLA	b	617	-	1/1/15/20	3/37/115/115	-
24	CLA	B	602	41	1/1/15/20	15/37/115/115	-
24	CLA	b	621	-	1/1/15/20	10/37/115/115	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
24	CLA	B	605	-	1/1/15/20	4/37/115/115	-
35	HTG	d	411	-	-	2/7/27/30	0/1/1/1
37	LHG	L	101	-	-	12/53/53/53	-
26	BCR	H	101	-	-	1/29/63/63	0/2/2/2
38	HEM	E	103	6,5	-	2/12/54/54	-
35	HTG	c	523	-	-	1/10/30/30	0/1/1/1
28	GOL	v	205	-	-	2/4/4/4	-
30	LMT	M	102	-	-	5/21/61/61	0/2/2/2
35	HTG	C	522	-	-	2/10/30/30	0/1/1/1
26	BCR	C	516	-	-	3/29/63/63	0/2/2/2
24	CLA	b	608	-	1/1/15/20	7/37/115/115	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
35	HTG	c	522	-	-	1/10/30/30	0/1/1/1
24	CLA	A	405	-	1/1/15/20	1/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	513	3	1/1/15/20	5/37/115/115	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
28	GOL	V	208	-	-	2/4/4/4	-
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
30	LMT	b	626	-	-	6/17/37/61	0/1/1/2
37	LHG	D	409	-	-	9/53/53/53	-
37	LHG	l	102	-	-	18/53/53/53	-
30	LMT	D	402	-	-	9/21/61/61	0/2/2/2
24	CLA	A	409	-	-	11/37/115/115	-
32	PL9	d	406	-	-	3/53/73/73	0/1/1/1
28	GOL	c	524	-	-	0/4/4/4	-
24	CLA	B	604	-	1/1/15/20	3/37/115/115	-
36	DGD	D	407	-	-	17/51/91/95	0/2/2/2
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	504	-	-	4/37/115/115	-
24	CLA	B	612	-	-	3/37/115/115	-
24	CLA	D	404	-	1/1/15/20	5/37/115/115	-
24	CLA	C	507	-	1/1/15/20	8/37/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
36	DGD	d	407	-	-	20/51/91/95	0/2/2/2
30	LMT	a	417	-	-	2/21/61/61	0/2/2/2
28	GOL	V	207	-	-	0/4/4/4	-
24	CLA	C	505	41	1/1/15/20	4/37/115/115	-
36	DGD	c	519	-	-	12/51/91/95	0/2/2/2
38	HEM	e	102	6,5	-	4/12/54/54	-
28	GOL	T	103	-	-	3/4/4/4	-
35	HTG	b	628	-	-	2/10/30/30	0/1/1/1
30	LMT	b	602	-	-	7/17/37/61	0/1/1/2
37	LHG	E	101	-	-	20/46/46/53	-
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
28	GOL	T	101	-	-	2/4/4/4	-
34	LMG	C	520	-	-	13/46/66/70	0/1/1/1
36	DGD	c	518	-	-	15/51/91/95	0/2/2/2
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	V	203	16	-	2/10/54/54	-
24	CLA	B	611	41	1/1/15/20	3/37/115/115	-
28	GOL	B	635	-	-	2/4/4/4	-
30	LMT	A	417	-	-	3/19/59/61	0/2/2/2
24	CLA	B	603	-	1/1/15/20	7/37/115/115	-
36	DGD	C	518	-	-	19/51/91/95	0/2/2/2
24	CLA	C	502	-	1/1/15/20	9/37/115/115	-
24	CLA	B	609	-	-	1/37/115/115	-
24	CLA	c	508	-	1/1/15/20	8/37/115/115	-
36	DGD	c	517	-	-	12/51/91/95	0/2/2/2
27	SQD	b	601	-	-	20/49/69/69	0/1/1/1
28	GOL	b	630	-	-	0/4/4/4	-
24	CLA	c	509	41	1/1/15/20	3/37/115/115	-
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
24	CLA	b	609	-	1/1/15/20	3/37/115/115	-
34	LMG	z	101	-	-	13/34/54/70	0/1/1/1
36	DGD	h	102	-	-	9/51/91/95	0/2/2/2
27	SQD	F	101	-	-	12/38/58/69	0/1/1/1
34	LMG	B	621	-	-	7/46/66/70	0/1/1/1
24	CLA	B	613	-	1/1/15/20	2/37/115/115	-
24	CLA	D	403	-	1/1/15/20	2/37/115/115	-
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
37	LHG	d	410	-	-	13/53/53/53	-
27	SQD	f	101	-	-	16/38/58/69	0/1/1/1
24	CLA	B	617	-	1/1/15/20	9/37/115/115	-
24	CLA	c	515	-	-	4/37/115/115	-
34	LMG	c	501	-	-	14/46/66/70	0/1/1/1
35	HTG	B	631	-	-	1/10/30/30	0/1/1/1
34	LMG	C	501	-	-	16/46/66/70	0/1/1/1
24	CLA	b	615	41	1/1/15/20	6/37/115/115	-
24	CLA	c	507	-	1/1/15/20	3/37/115/115	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
28	GOL	b	633	-	-	2/4/4/4	-
24	CLA	c	511	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	m	103	-	-	6/21/61/61	0/2/2/2
24	CLA	b	616	-	1/1/15/20	2/37/115/115	-
32	PL9	D	406	-	-	1/53/73/73	0/1/1/1
35	HTG	B	623	-	-	5/10/30/30	0/1/1/1
24	CLA	b	620	-	1/1/15/20	4/37/115/115	-
24	CLA	d	402	-	1/1/15/20	1/37/115/115	-
28	GOL	A	413	-	-	2/4/4/4	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
37	LHG	D	408	-	-	9/53/53/53	-
34	LMG	J	101	39	-	9/46/66/70	0/1/1/1
28	GOL	V	201	-	-	0/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	b	614	-	1/1/15/20	3/37/115/115	-
36	DGD	C	519	-	-	5/51/91/95	0/2/2/2
24	CLA	C	512	3	1/1/15/20	1/37/115/115	-
35	HTG	B	630	-	-	1/10/30/30	0/1/1/1
35	HTG	B	622	-	-	1/10/30/30	0/1/1/1
37	LHG	d	409	-	-	11/53/53/53	-
28	GOL	V	206	-	-	2/4/4/4	-
28	GOL	v	203	-	-	4/4/4/4	-
24	CLA	a	409	-	1/1/15/20	11/37/115/115	-
30	LMT	a	401	-	-	9/21/61/61	0/2/2/2
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
28	GOL	v	204	-	-	2/4/4/4	-
36	DGD	H	102	-	-	11/51/91/95	0/2/2/2
24	CLA	C	508	41	1/1/15/20	11/37/115/115	-
34	LMG	j	101	39	-	12/46/66/70	0/1/1/1
24	CLA	B	616	-	1/1/15/20	8/37/115/115	-
24	CLA	b	619	-	1/1/15/20	14/37/115/115	-
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	D	401	41	1/1/15/20	5/37/115/115	-
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
24	CLA	d	404	-	1/1/15/20	6/37/115/115	-
25	PHO	a	408	-	-	2/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	d	408	-	-	9/53/53/53	-
28	GOL	B	625	-	-	2/4/4/4	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
24	CLA	b	610	-	1/1/15/20	5/37/115/115	-
28	GOL	A	414	-	-	2/4/4/4	-
30	LMT	f	102	-	-	7/21/61/61	0/2/2/2
26	BCR	D	405	-	-	6/29/63/63	0/2/2/2
24	CLA	a	406	-	1/1/15/20	3/37/115/115	-
27	SQD	l	101	-	-	20/49/69/69	0/1/1/1
28	GOL	B	628	-	-	2/4/4/4	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
28	GOL	a	413	-	-	4/4/4/4	-
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
37	LHG	D	410	-	-	14/53/53/53	-
28	GOL	O	302	-	-	2/4/4/4	-
28	GOL	V	205	-	-	4/4/4/4	-
24	CLA	C	513	-	1/1/15/20	10/37/115/115	-

The worst 5 of 1329 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	PHO	C3B-C2B	6.65	1.49	1.40
24	c	511	CLA	C3B-C2B	6.62	1.49	1.40
24	B	617	CLA	C3B-C2B	6.61	1.49	1.40
24	C	511	CLA	C3B-C2B	6.55	1.49	1.40
25	A	408	PHO	C3B-C2B	6.51	1.49	1.40

The worst 5 of 2520 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C1D-ND-C4D	-10.22	99.08	106.33
24	b	610	CLA	C1D-ND-C4D	-10.12	99.15	106.33
24	B	610	CLA	C1D-ND-C4D	-10.04	99.20	106.33
24	A	409	CLA	C1D-ND-C4D	-9.95	99.27	106.33
24	B	606	CLA	C1D-ND-C4D	-9.75	99.41	106.33

5 of 59 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND

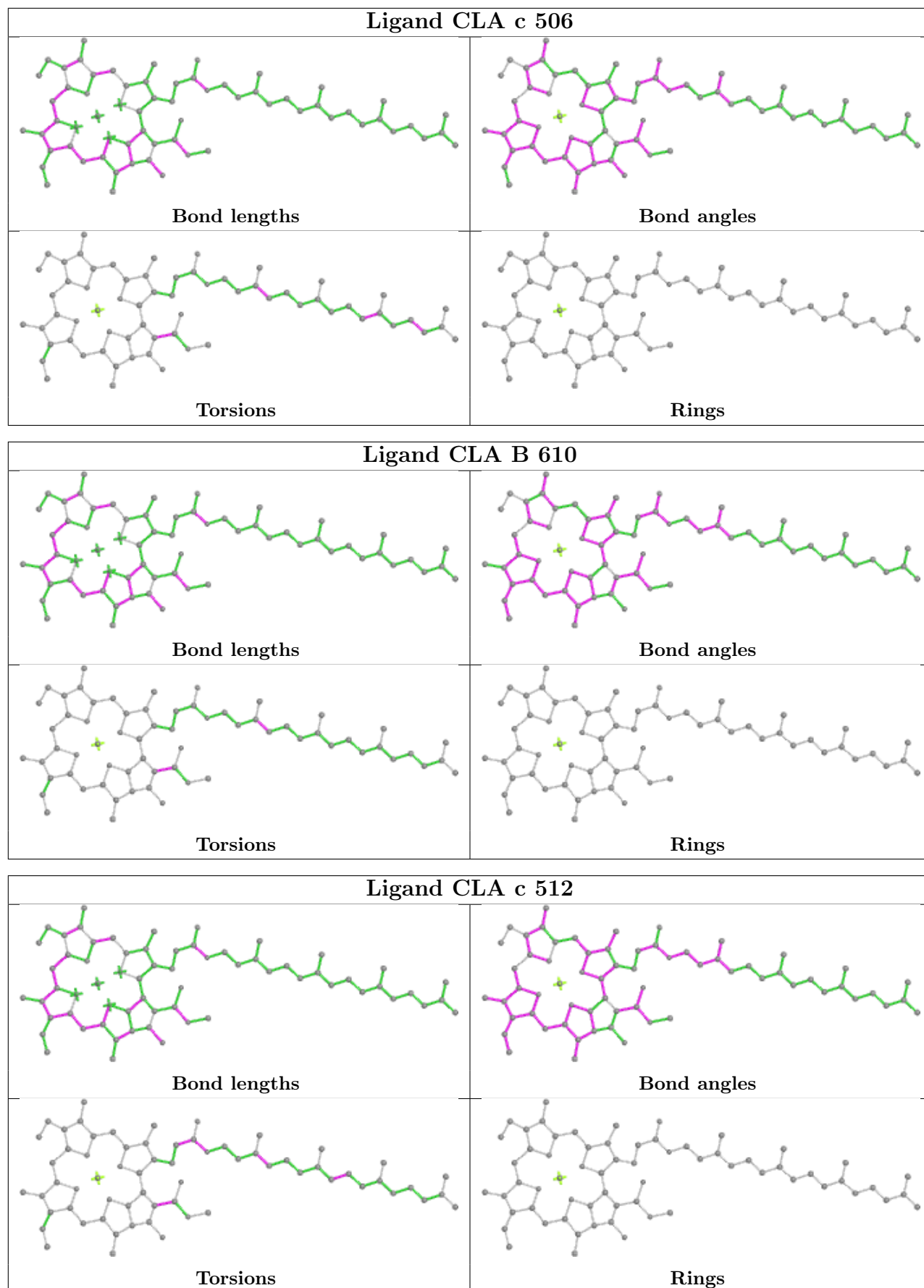
5 of 1188 torsion outliers are listed below:

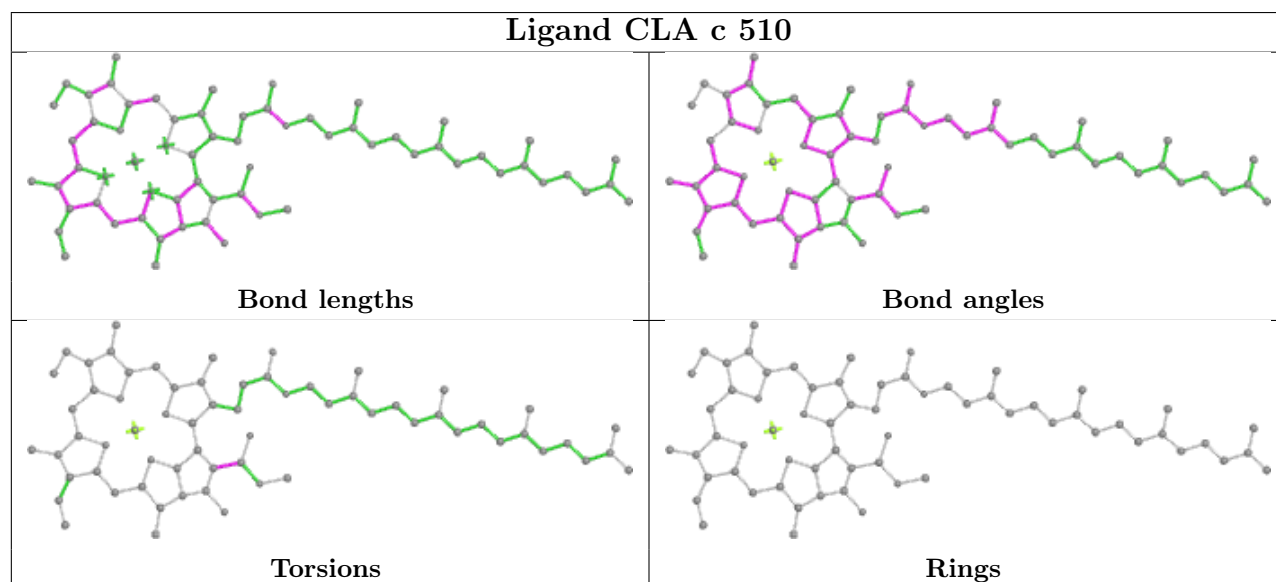
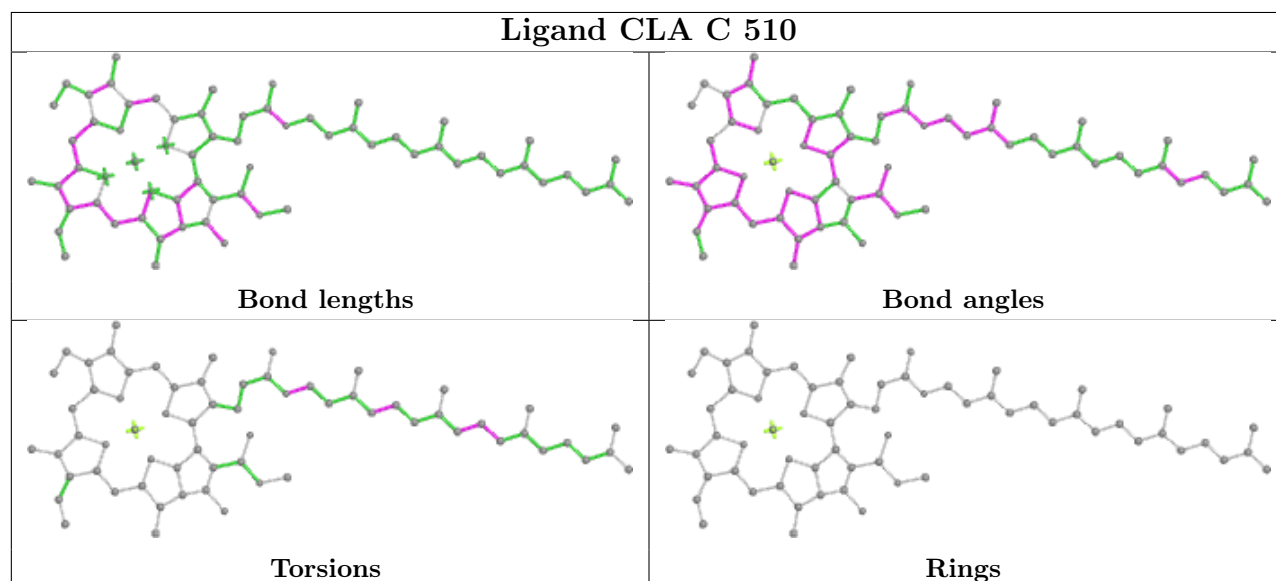
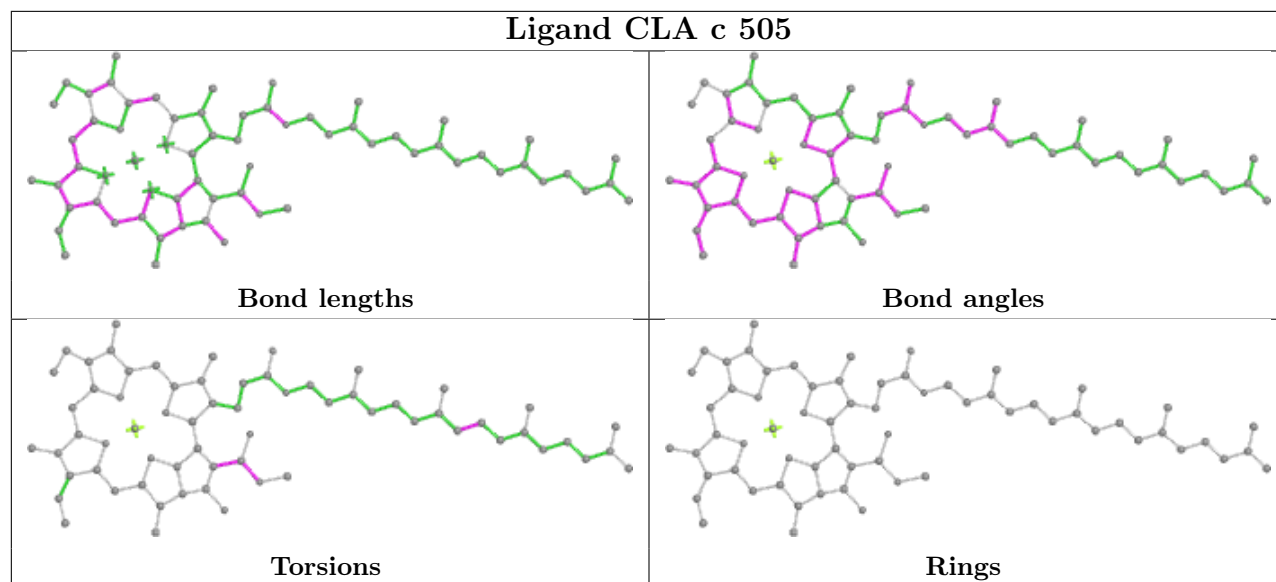
Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D

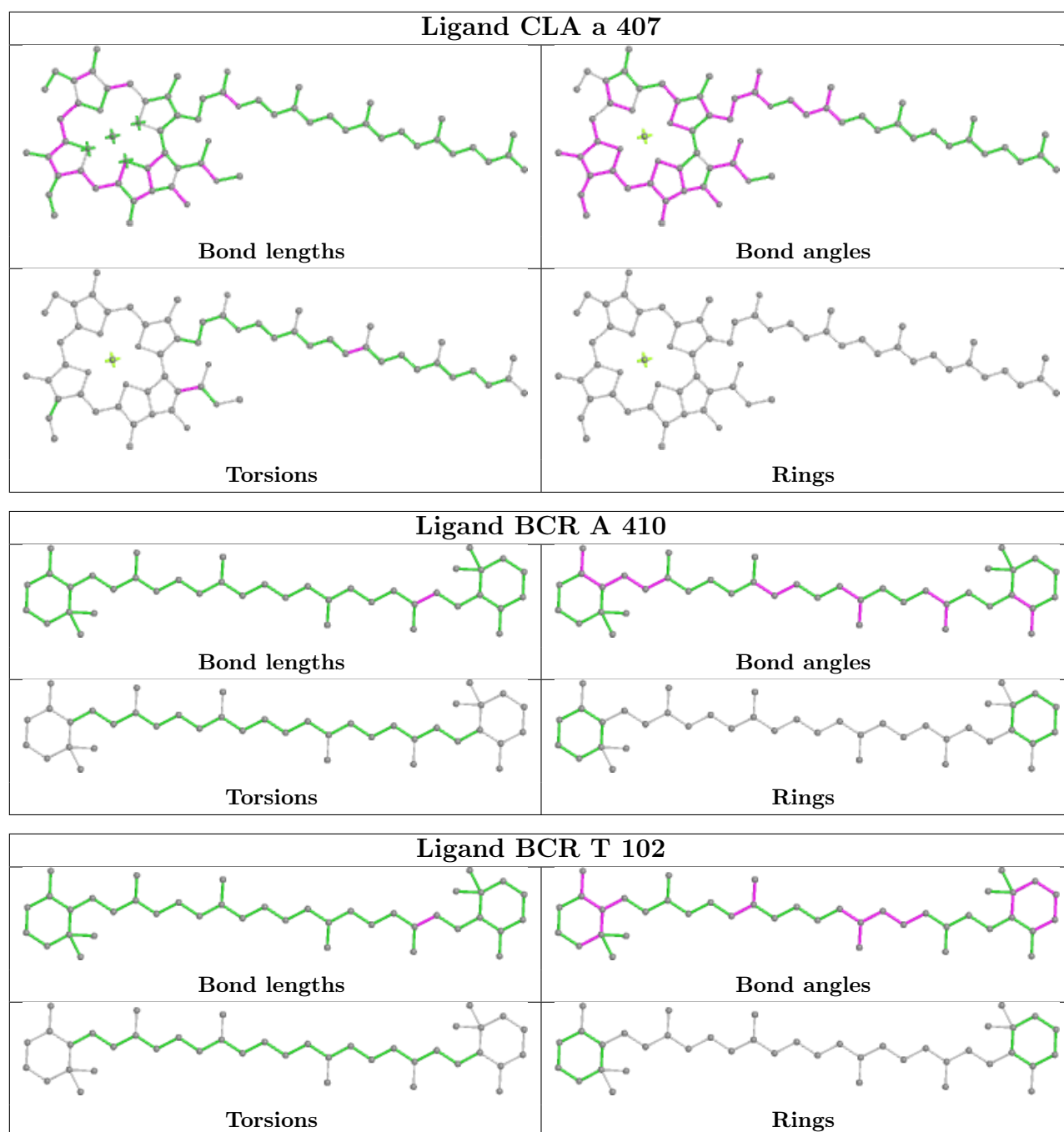
There are no ring outliers.

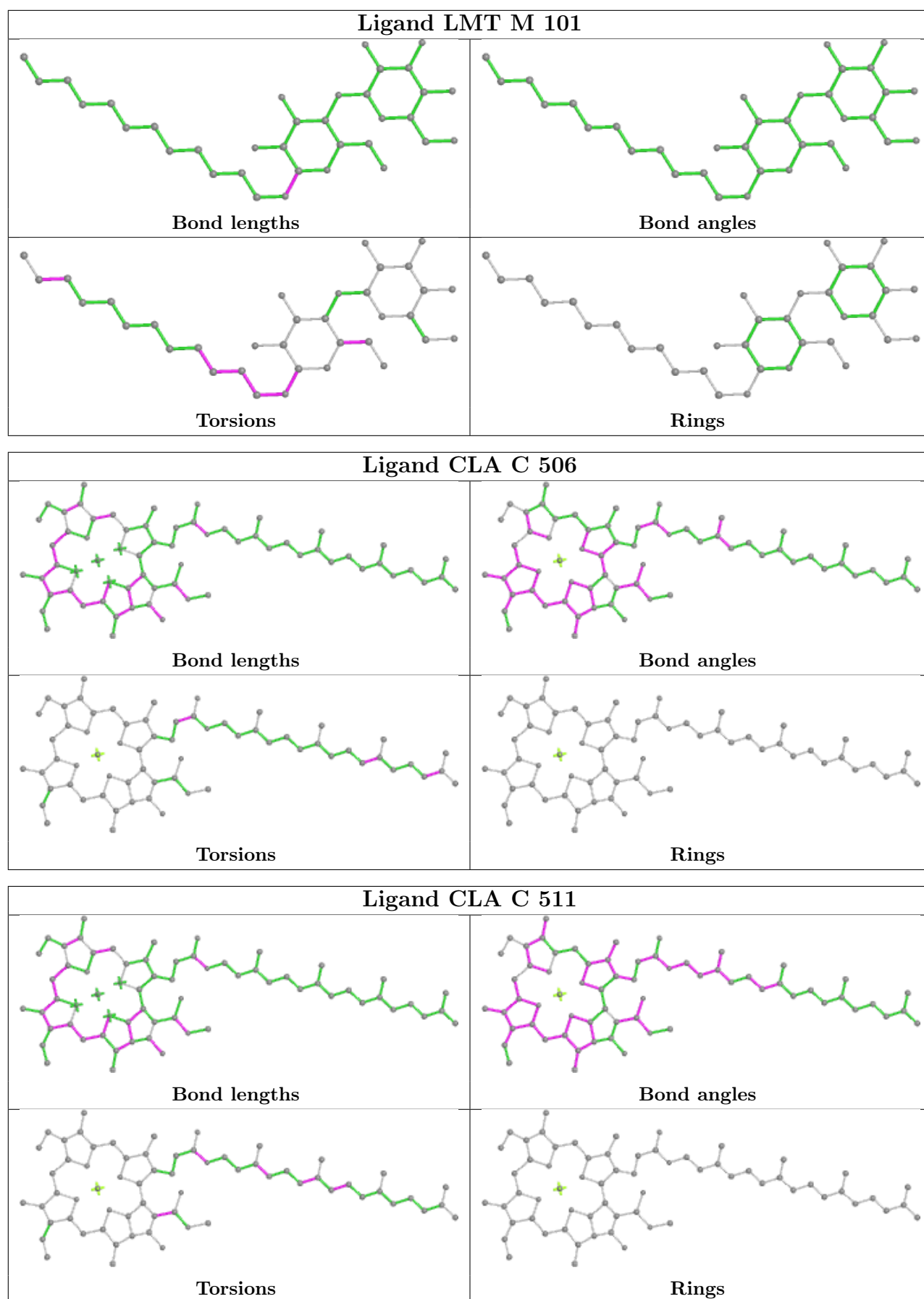
No monomer is involved in short contacts.

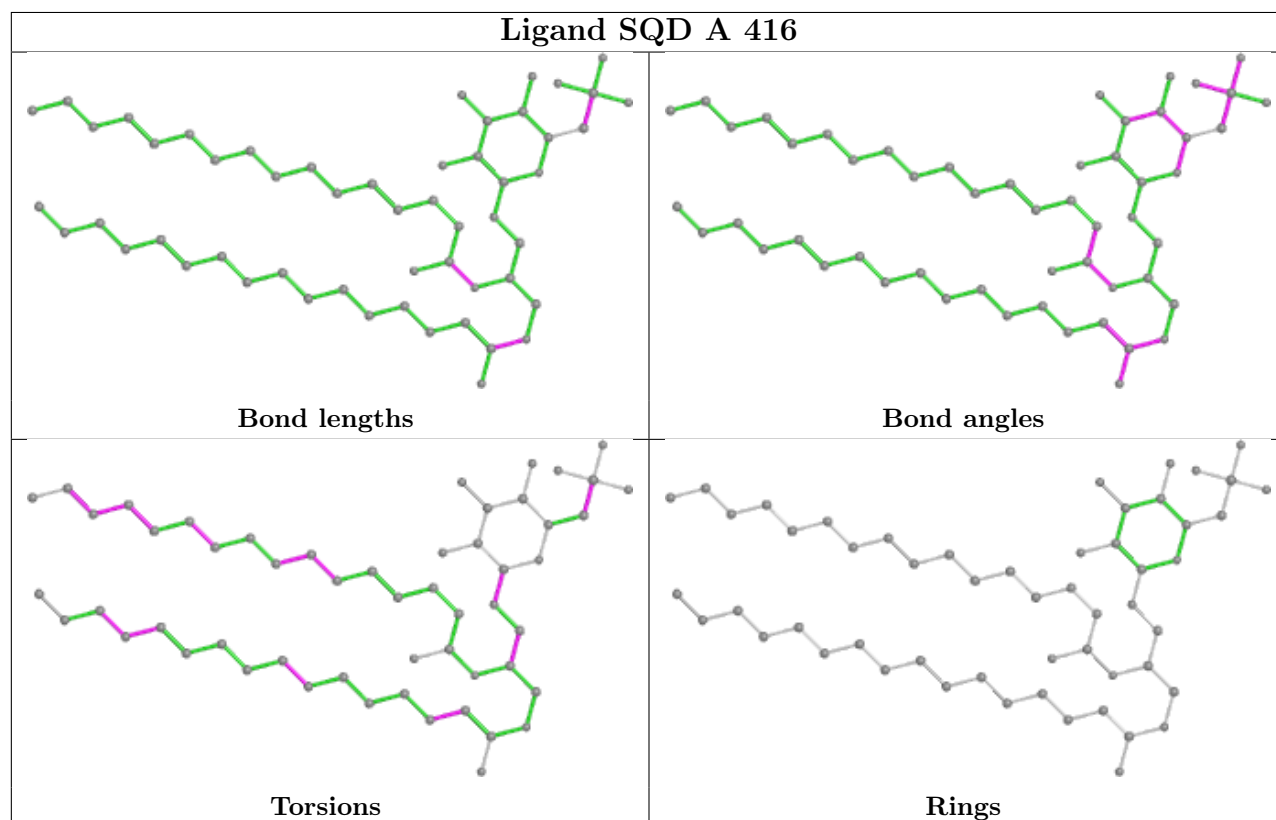
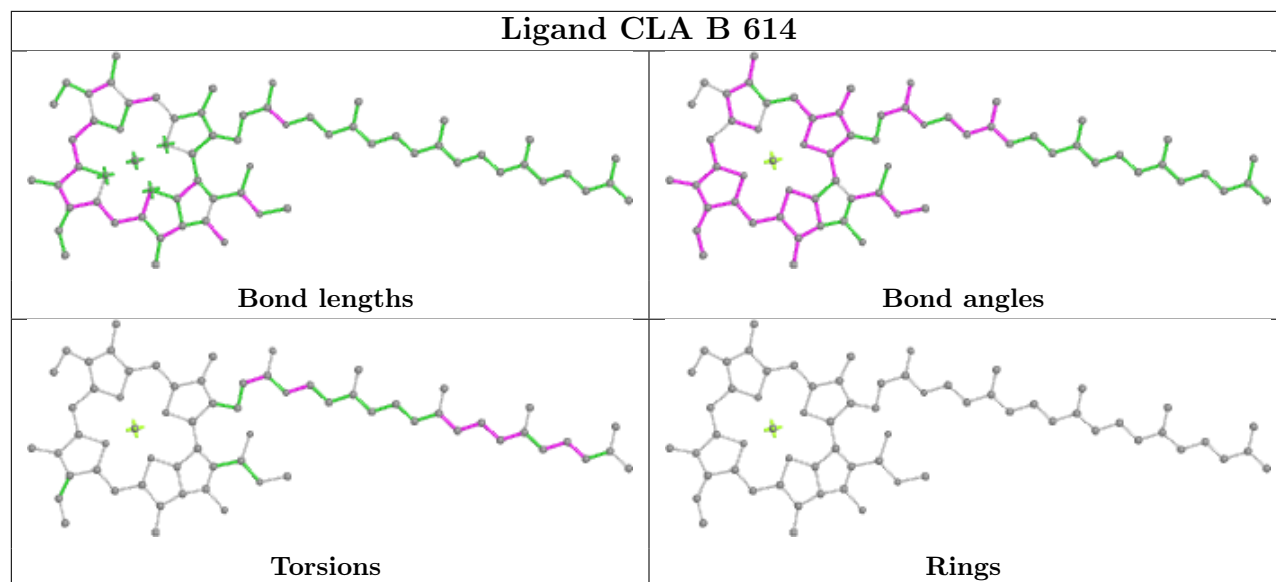
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

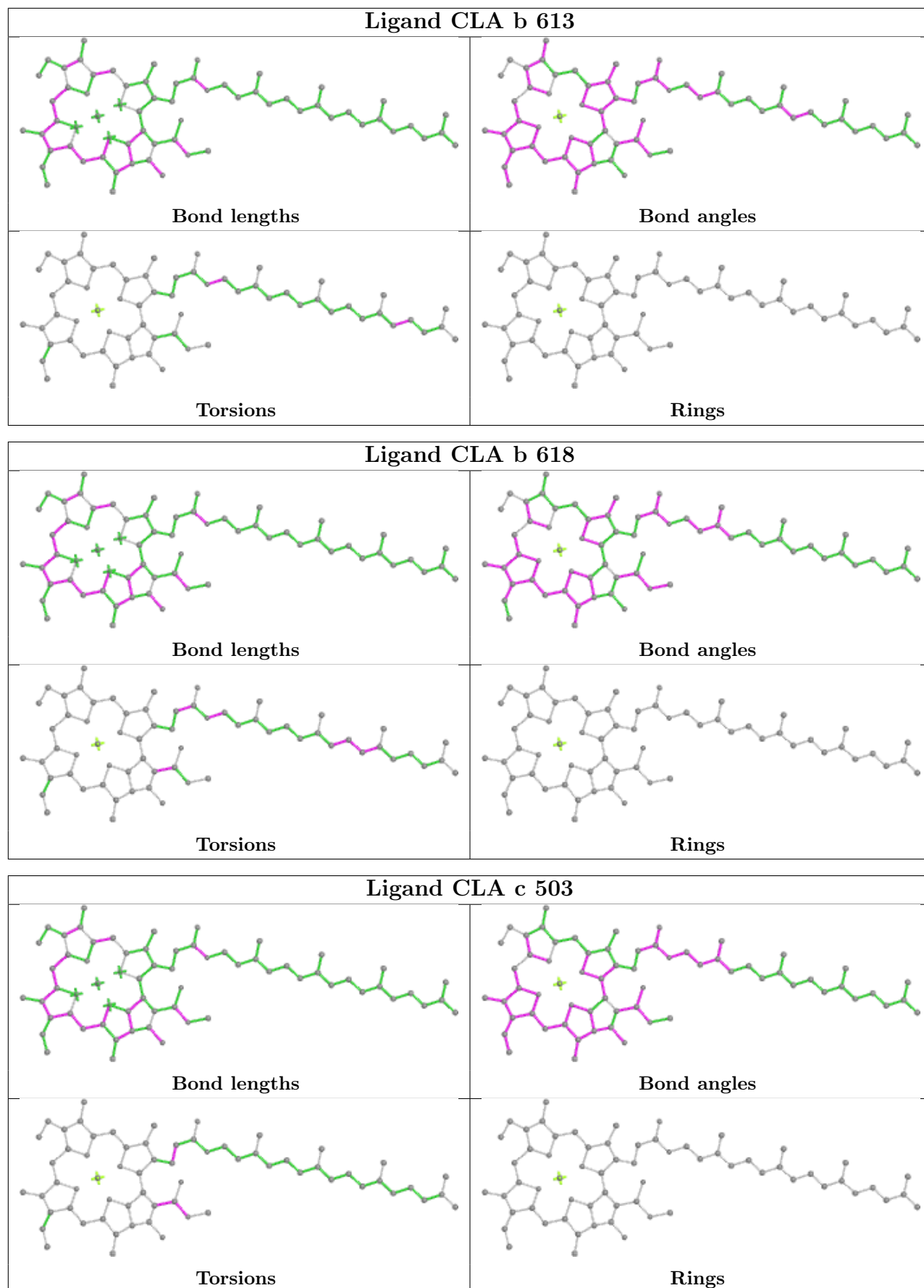


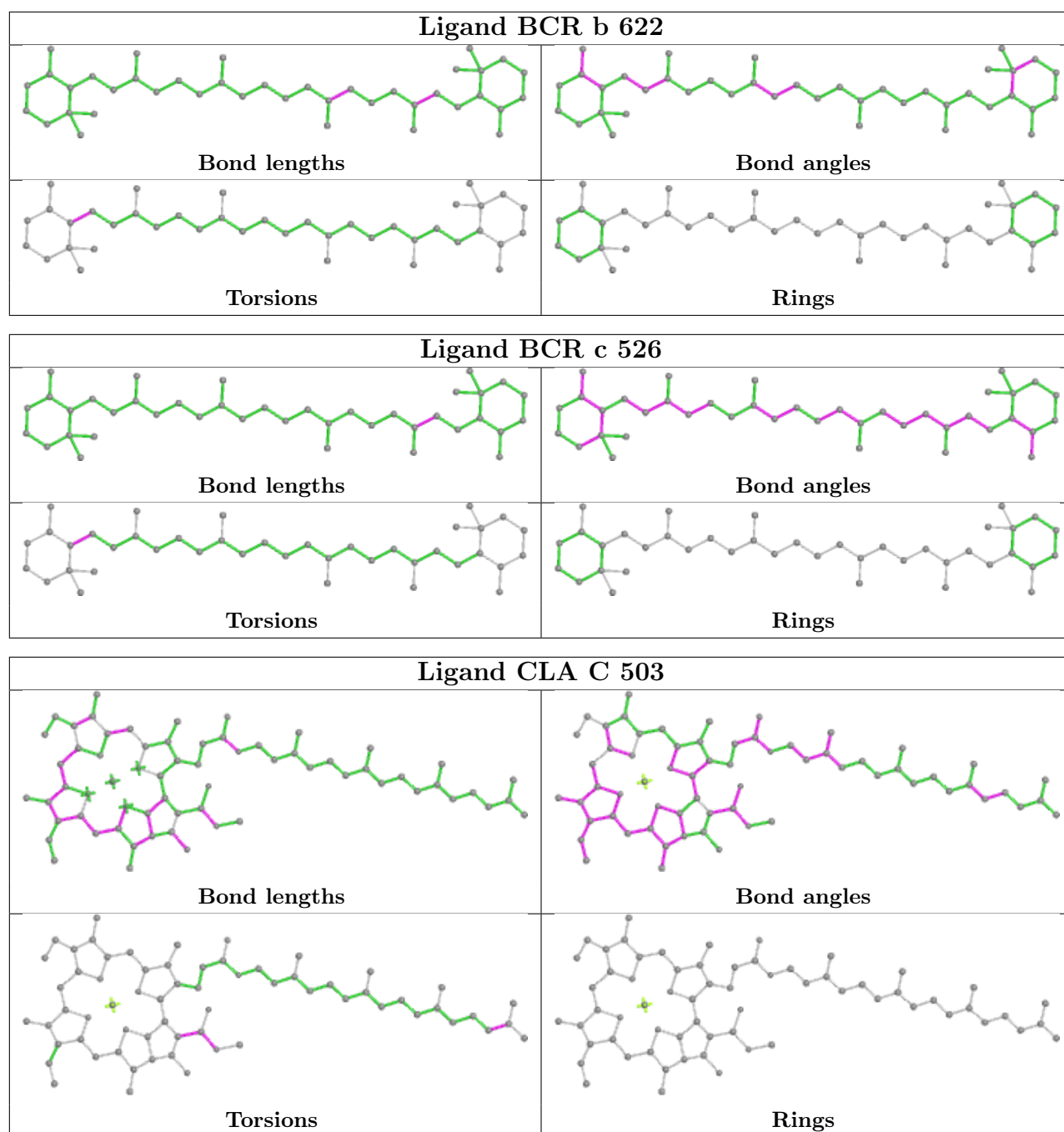


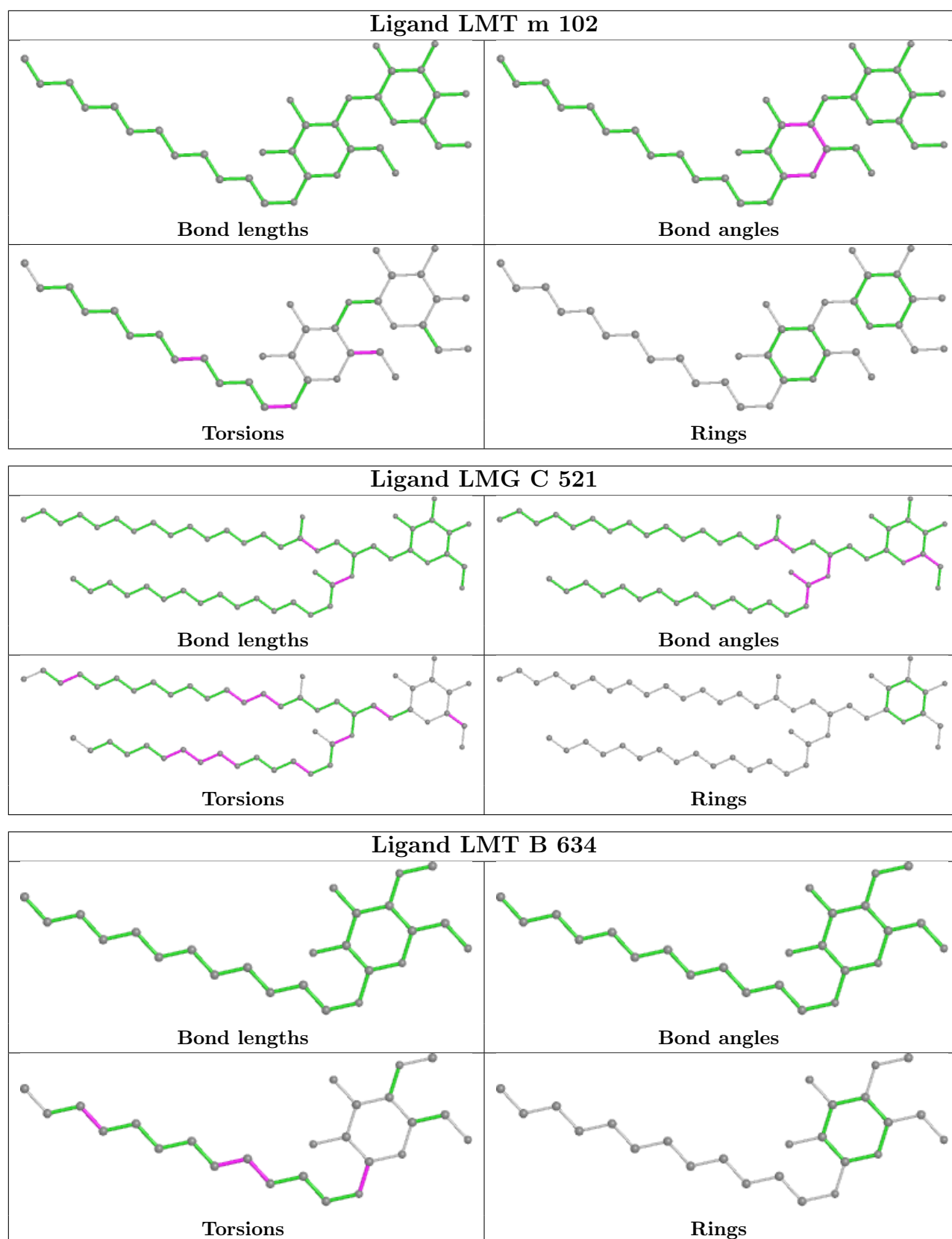


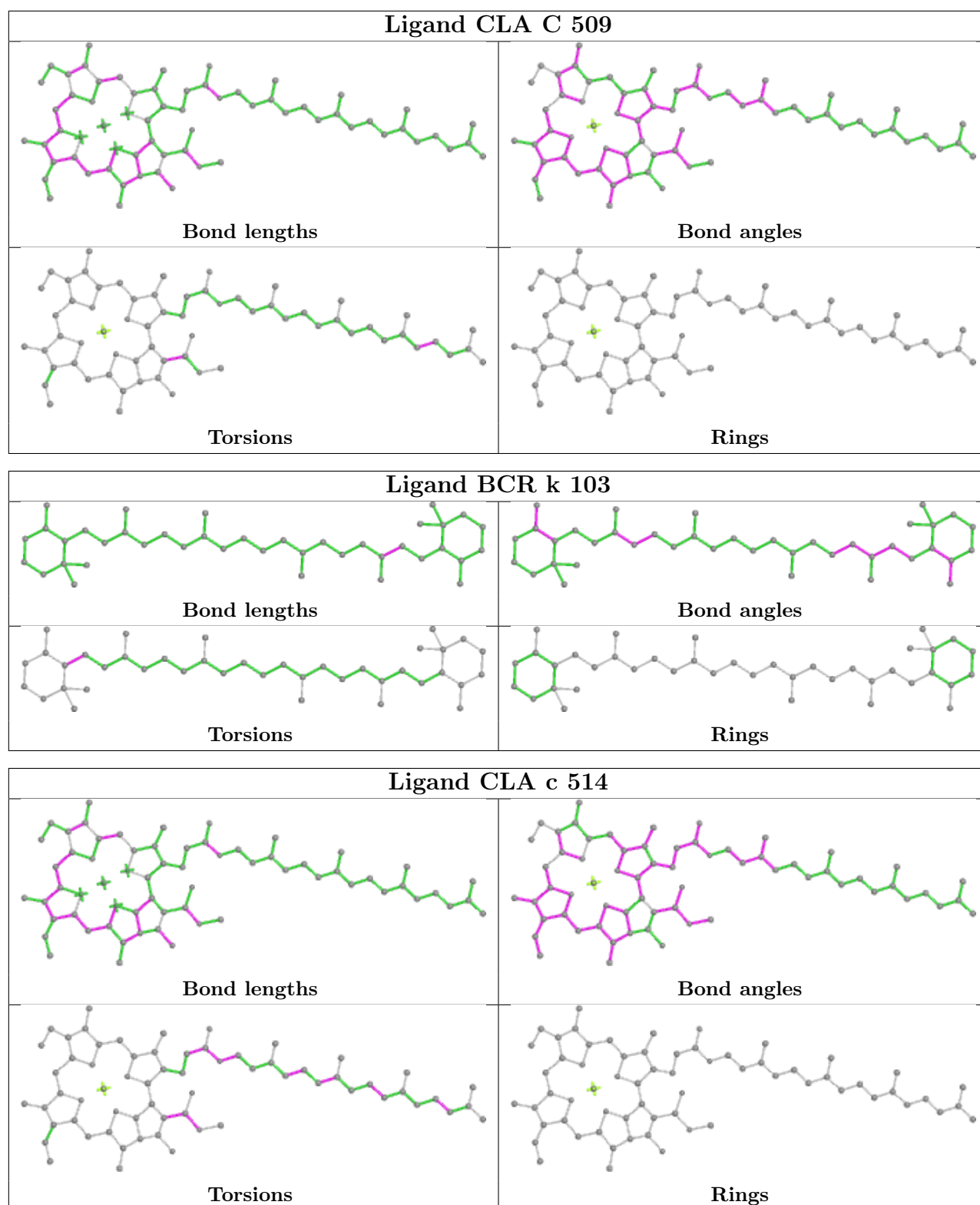


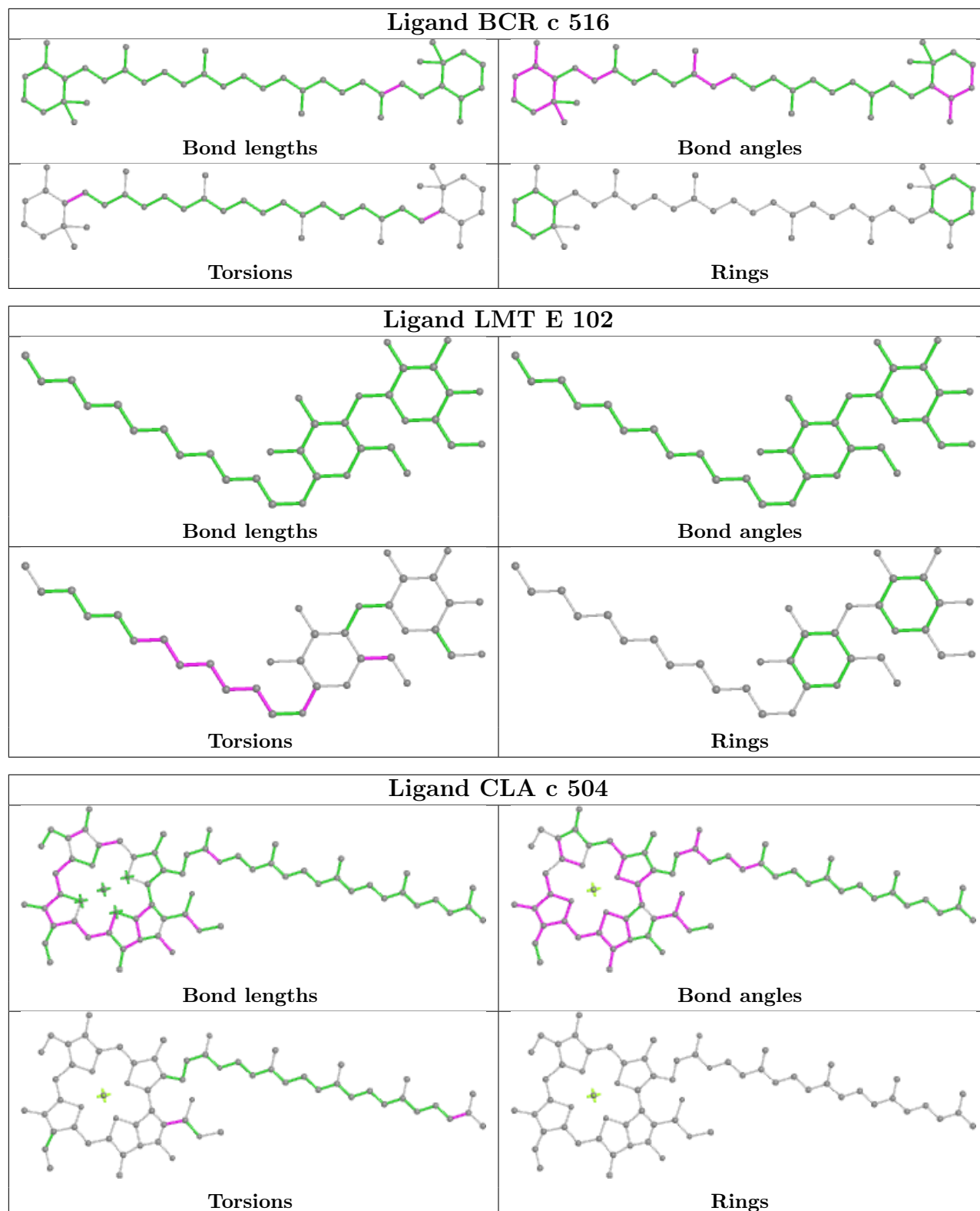


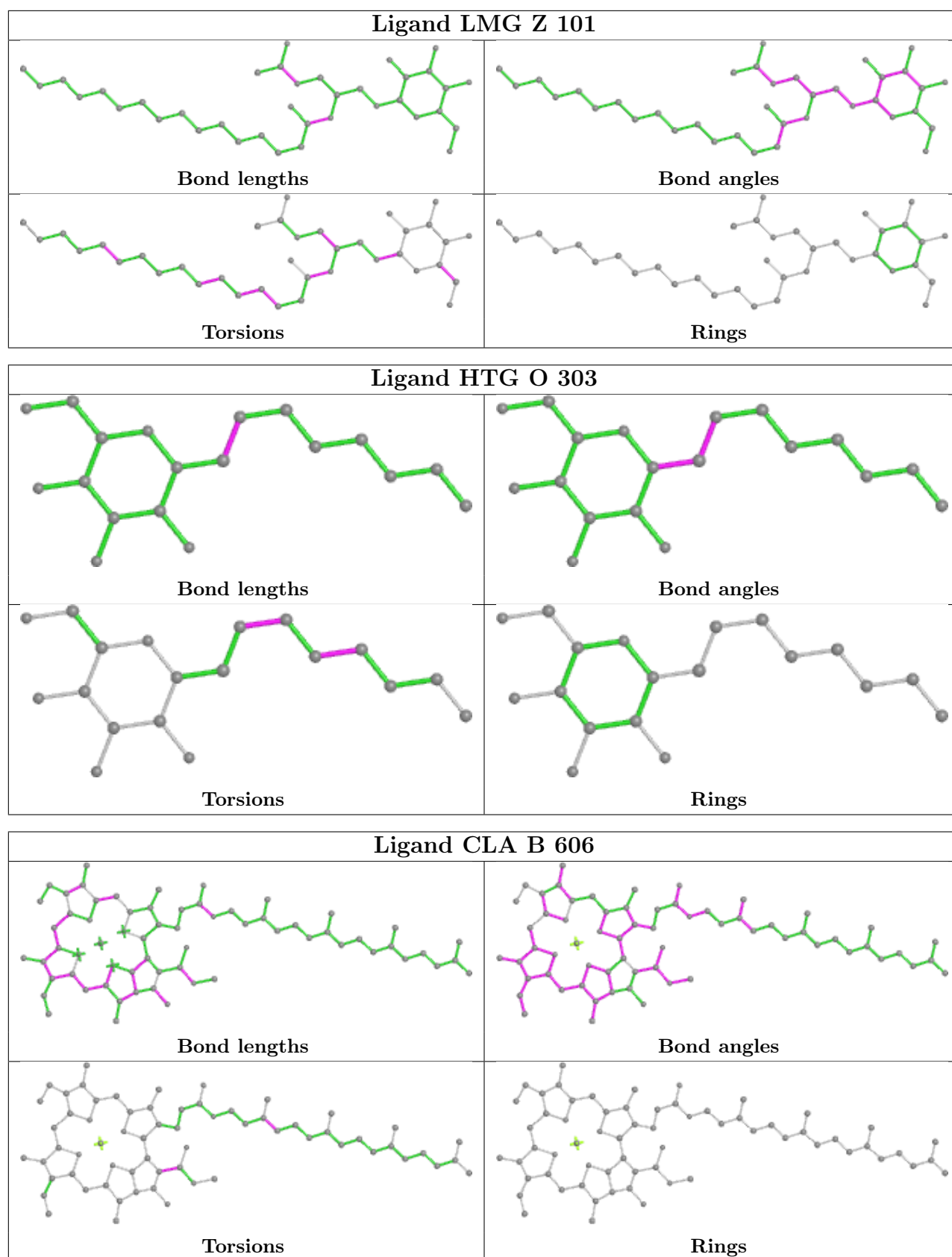


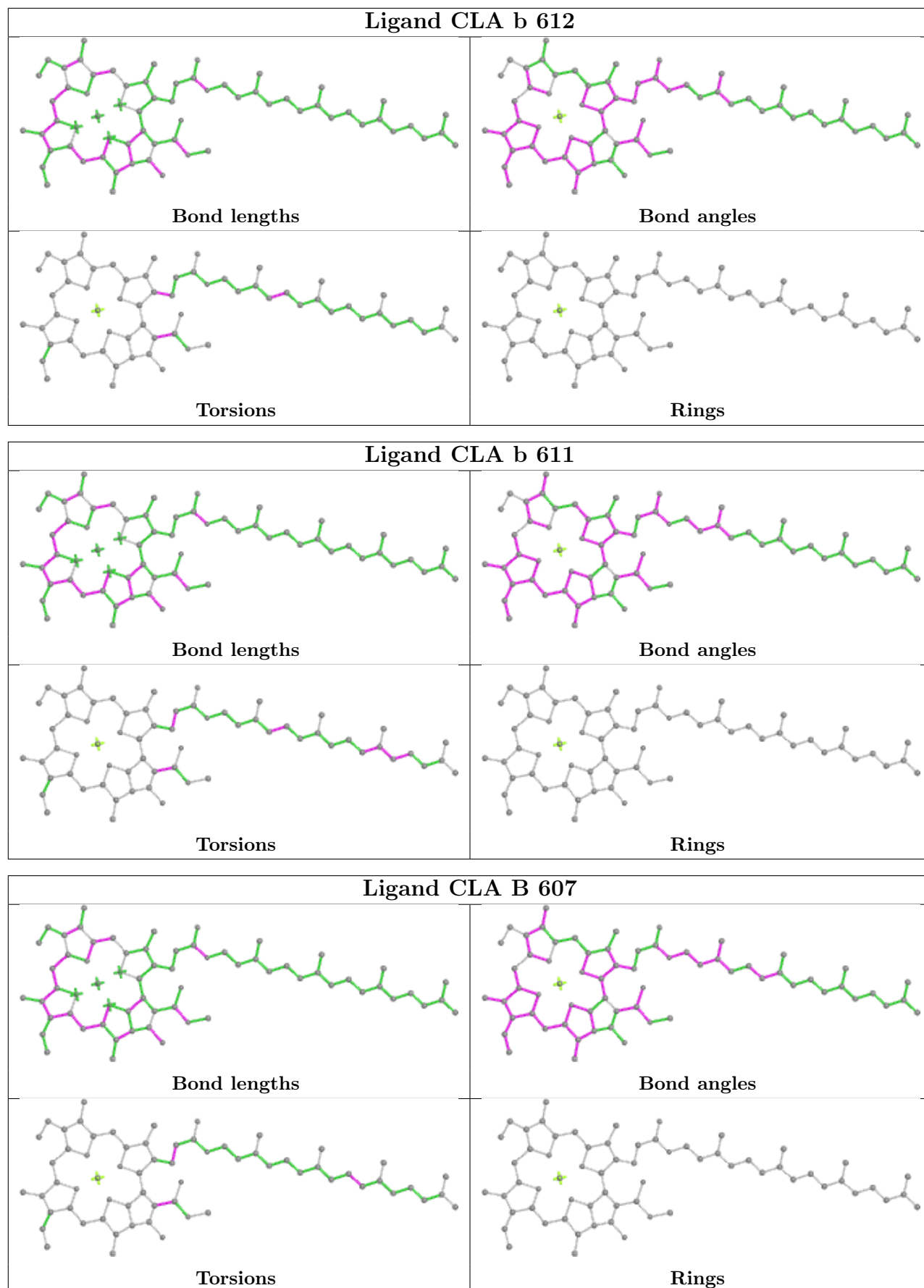


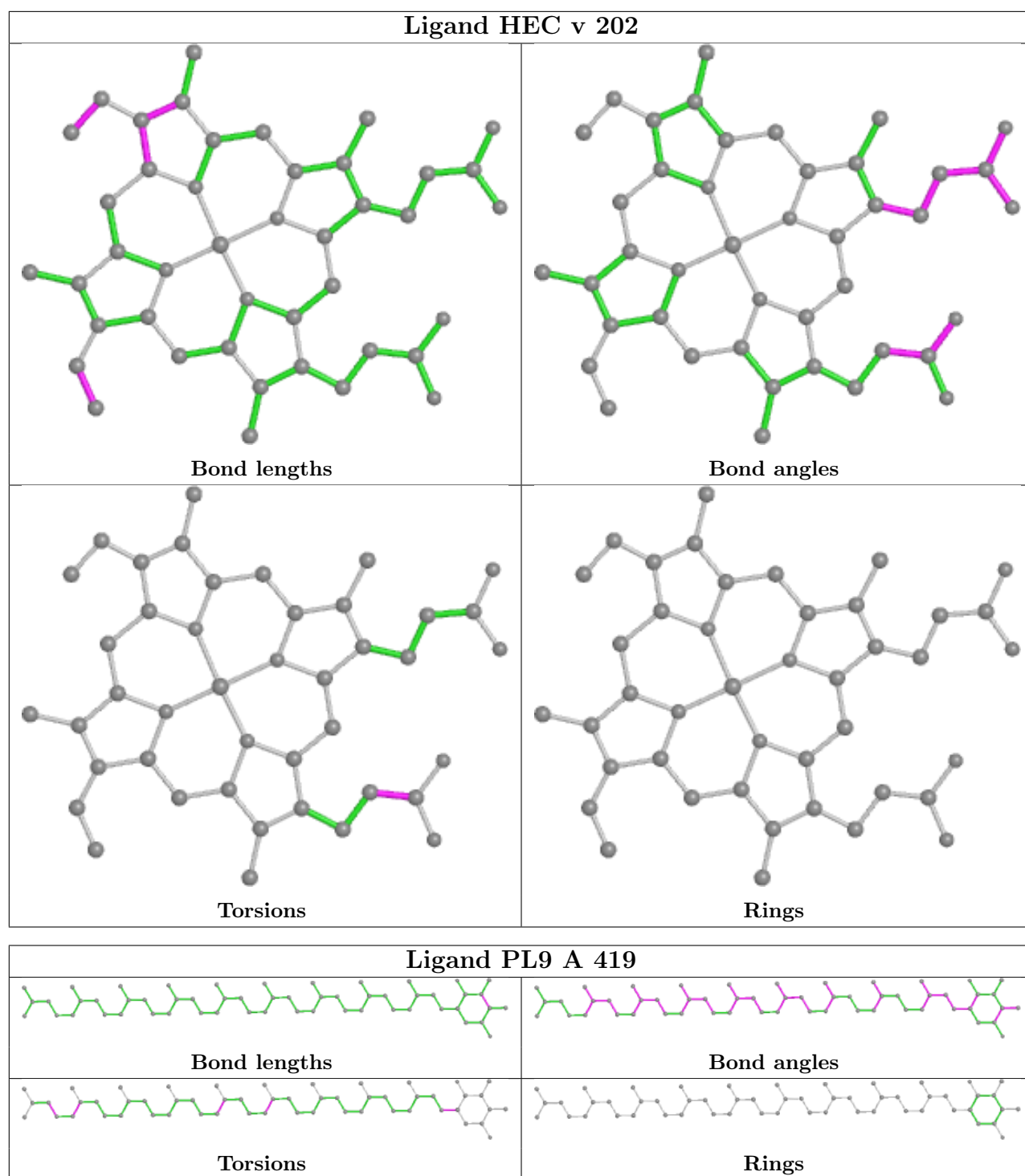


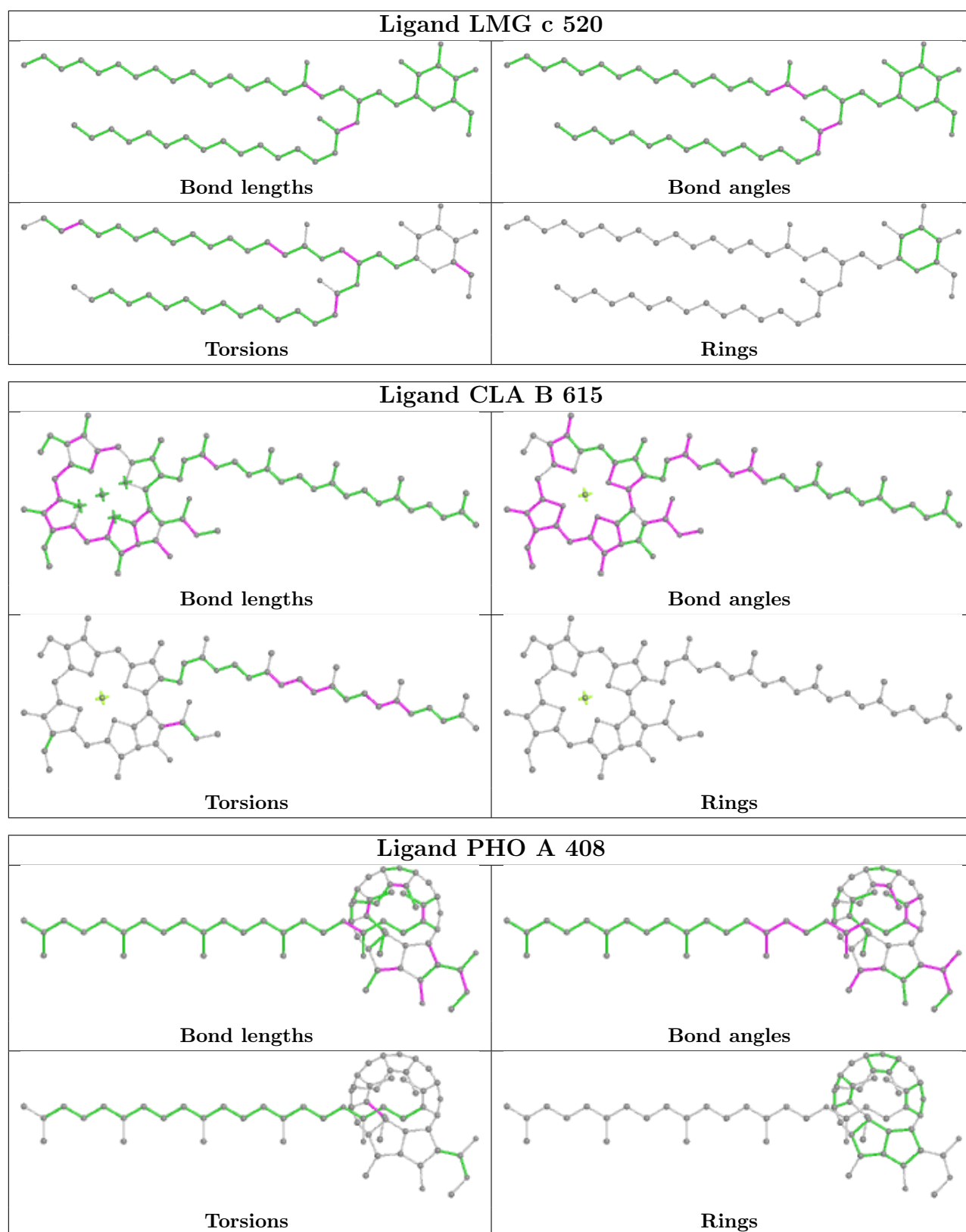


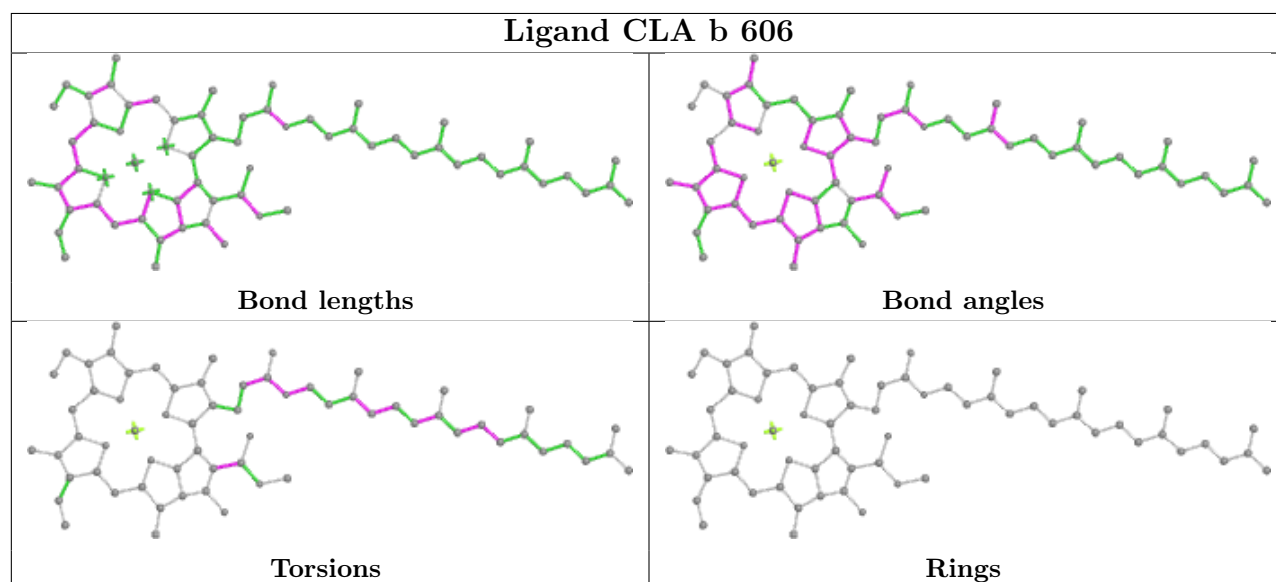
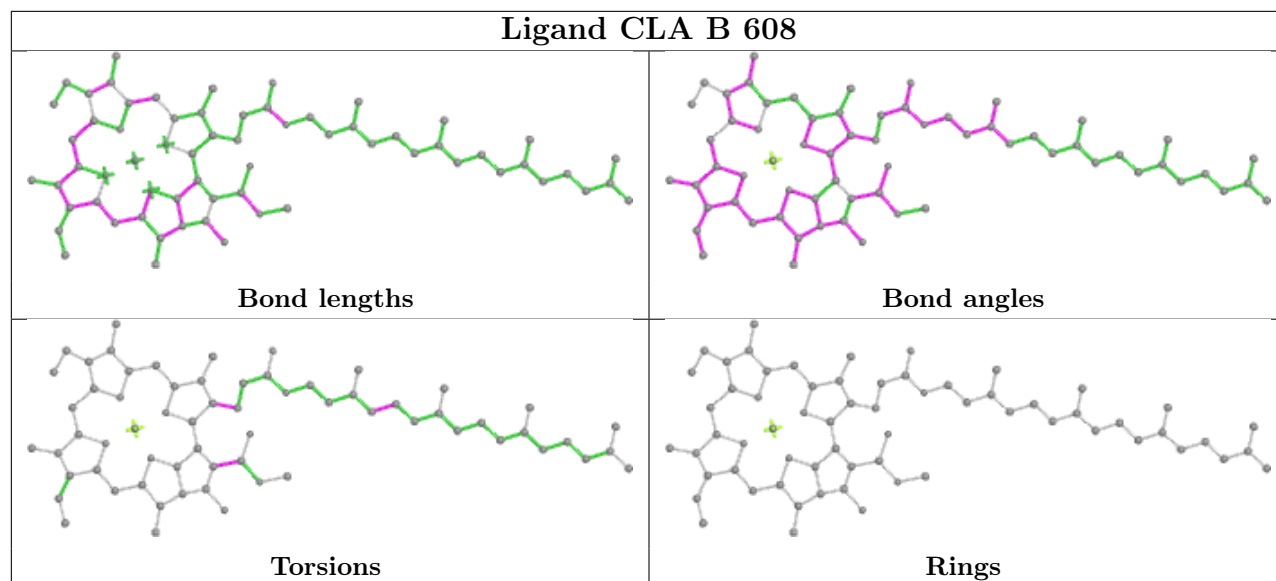
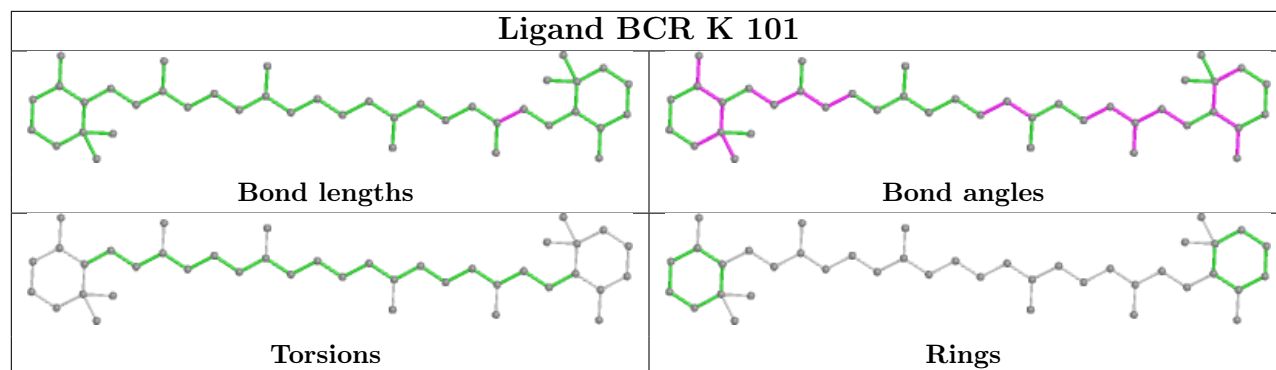


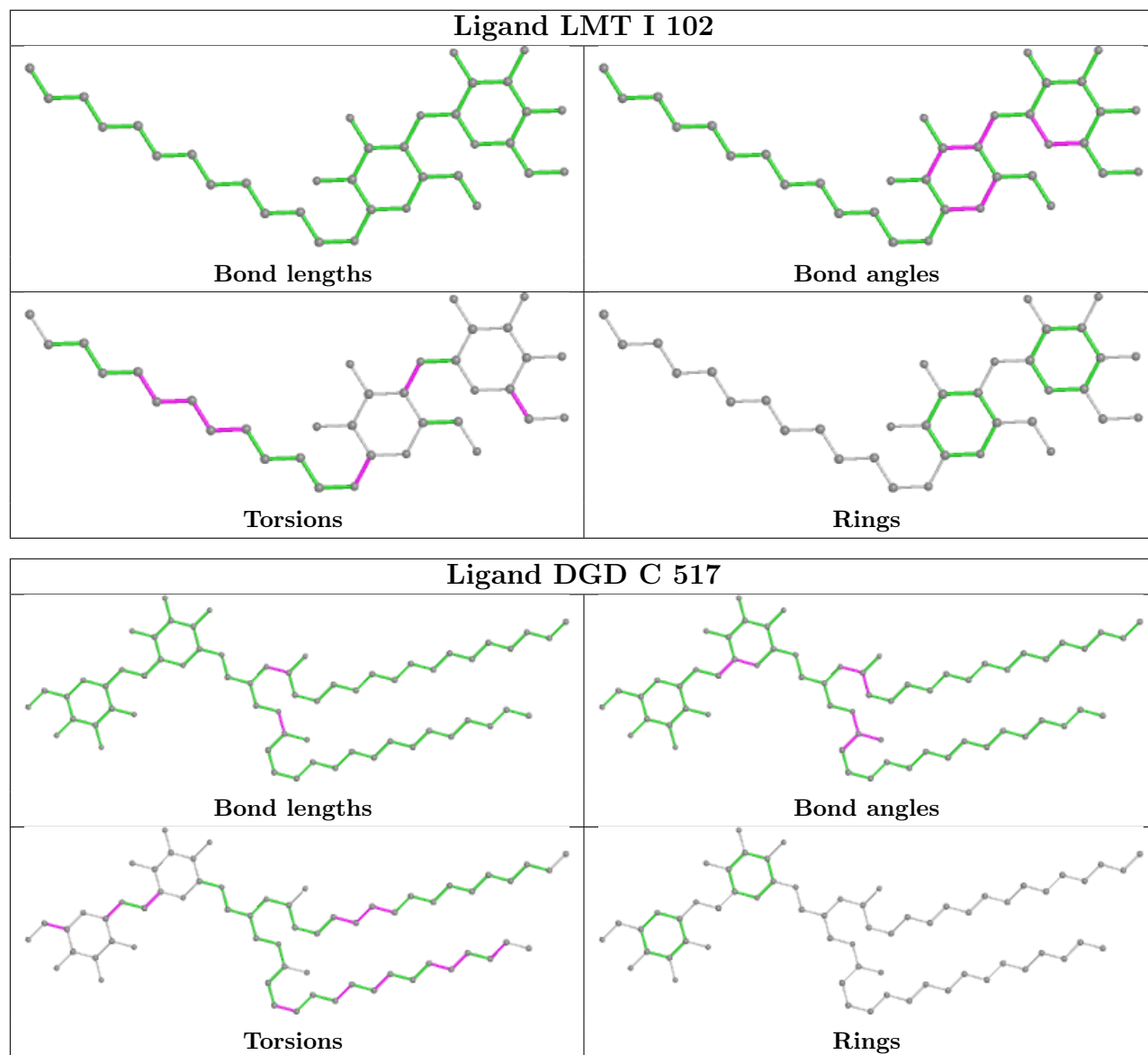


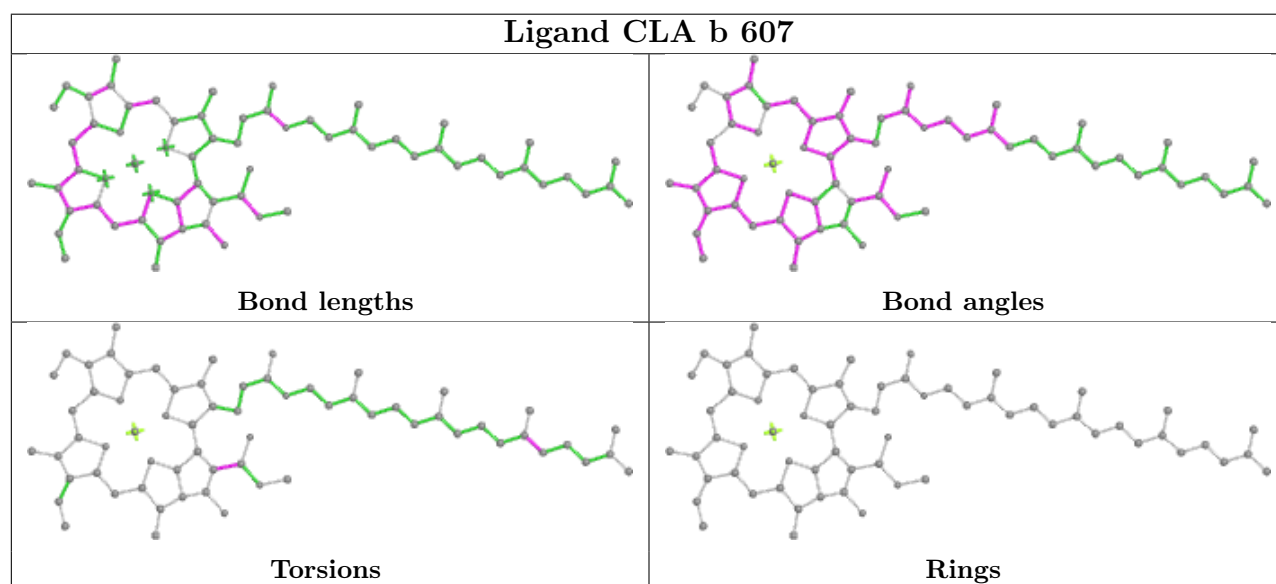
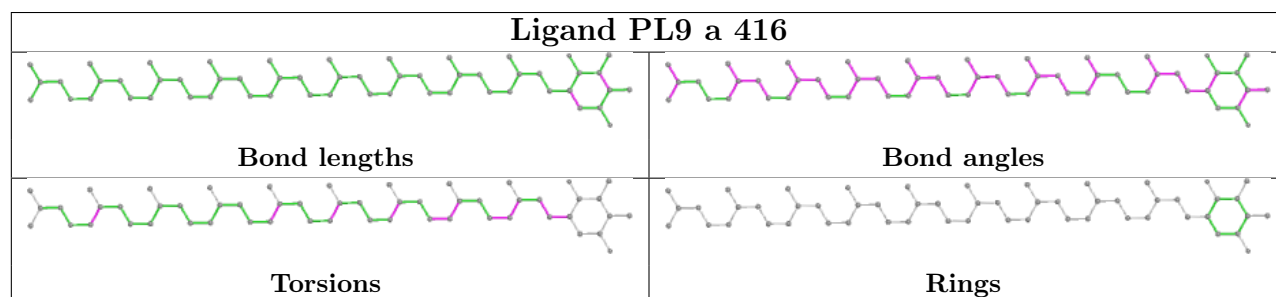
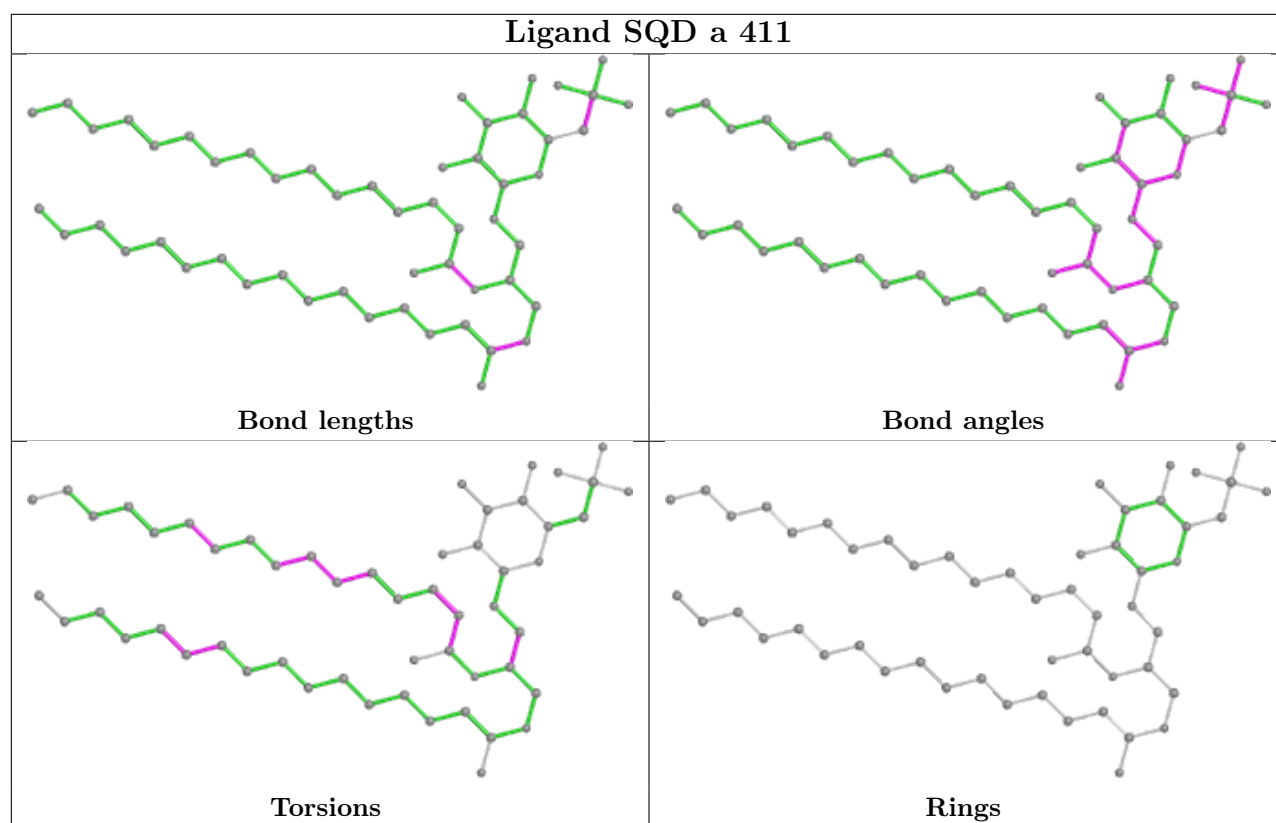


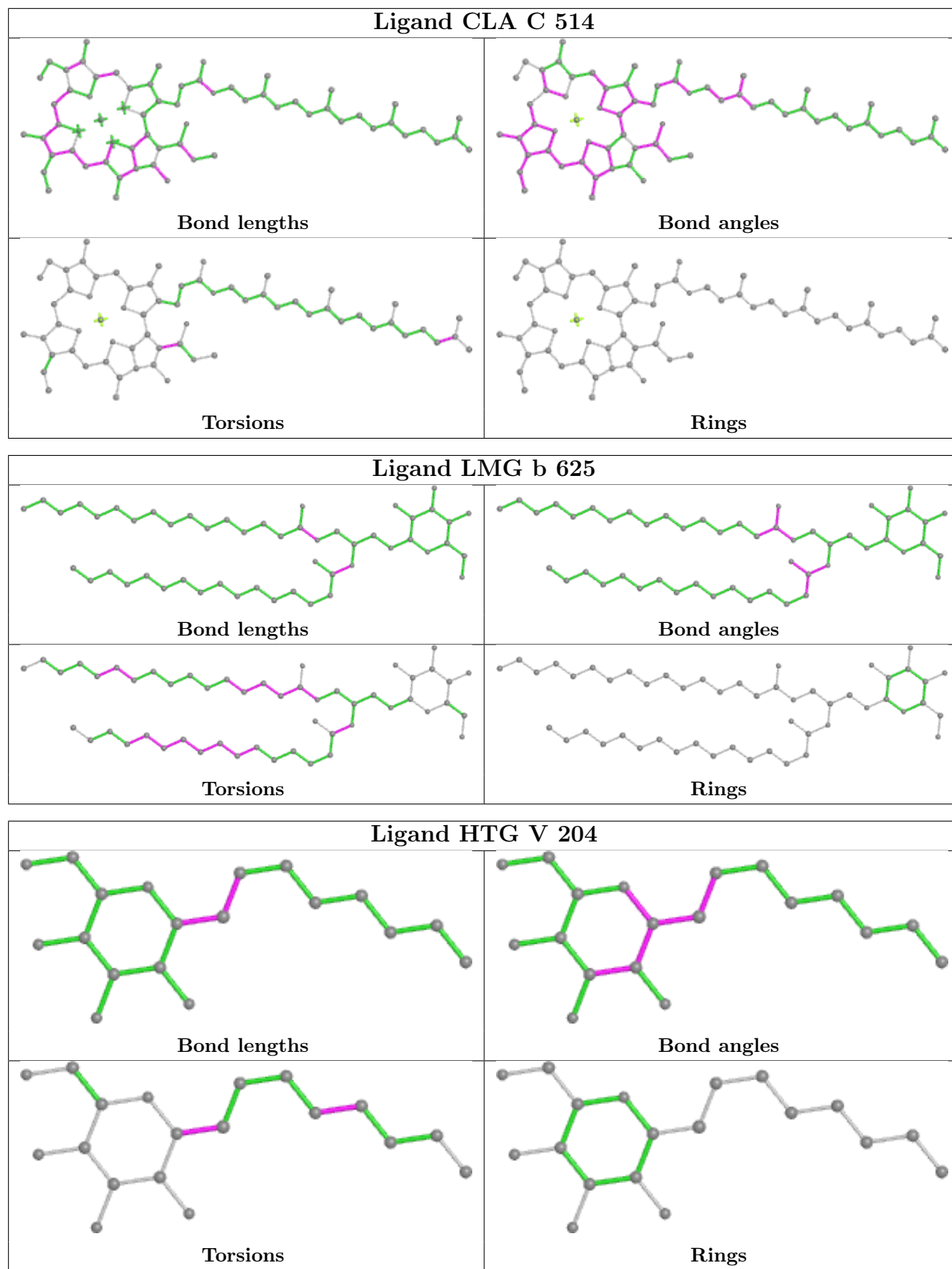


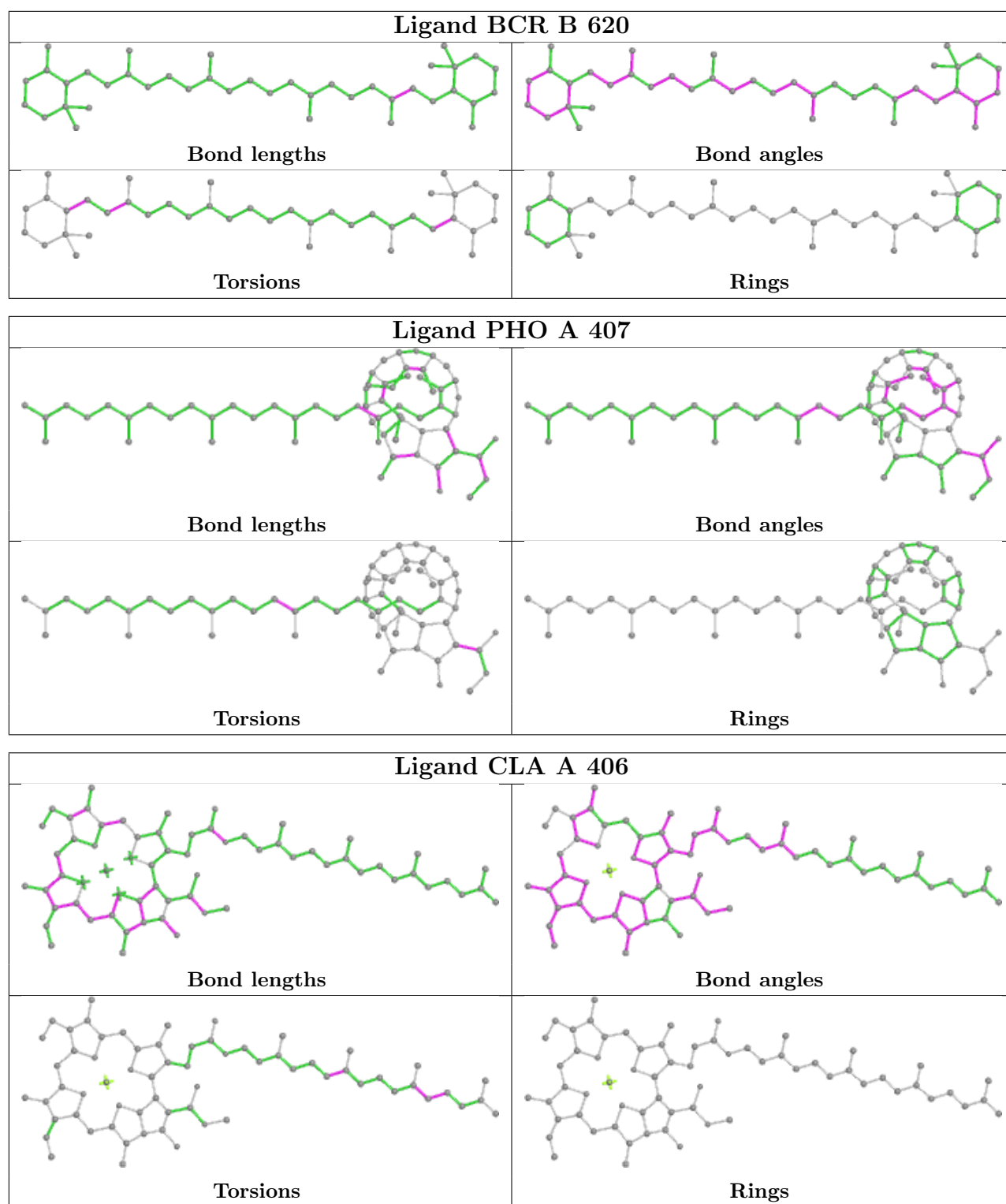


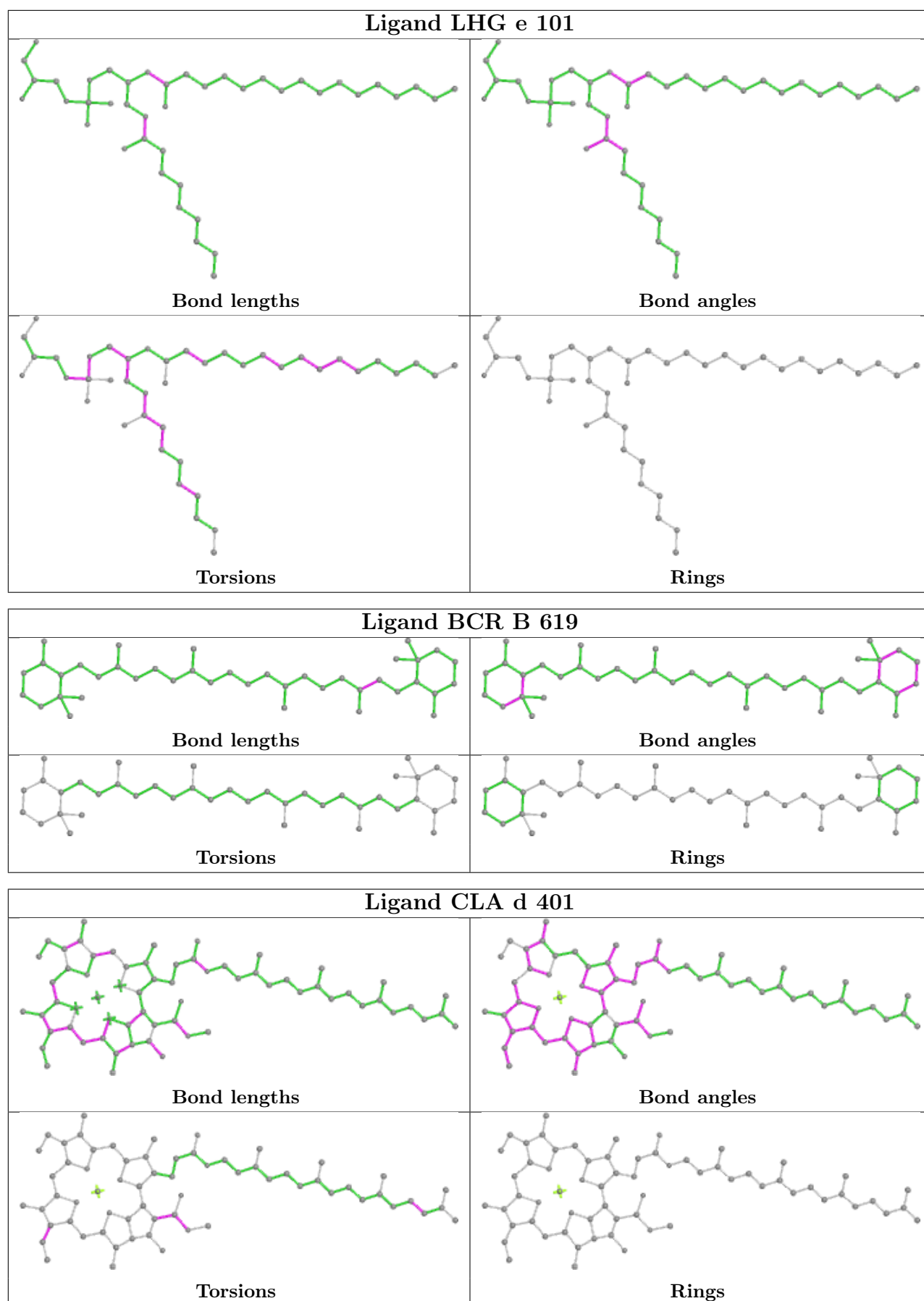


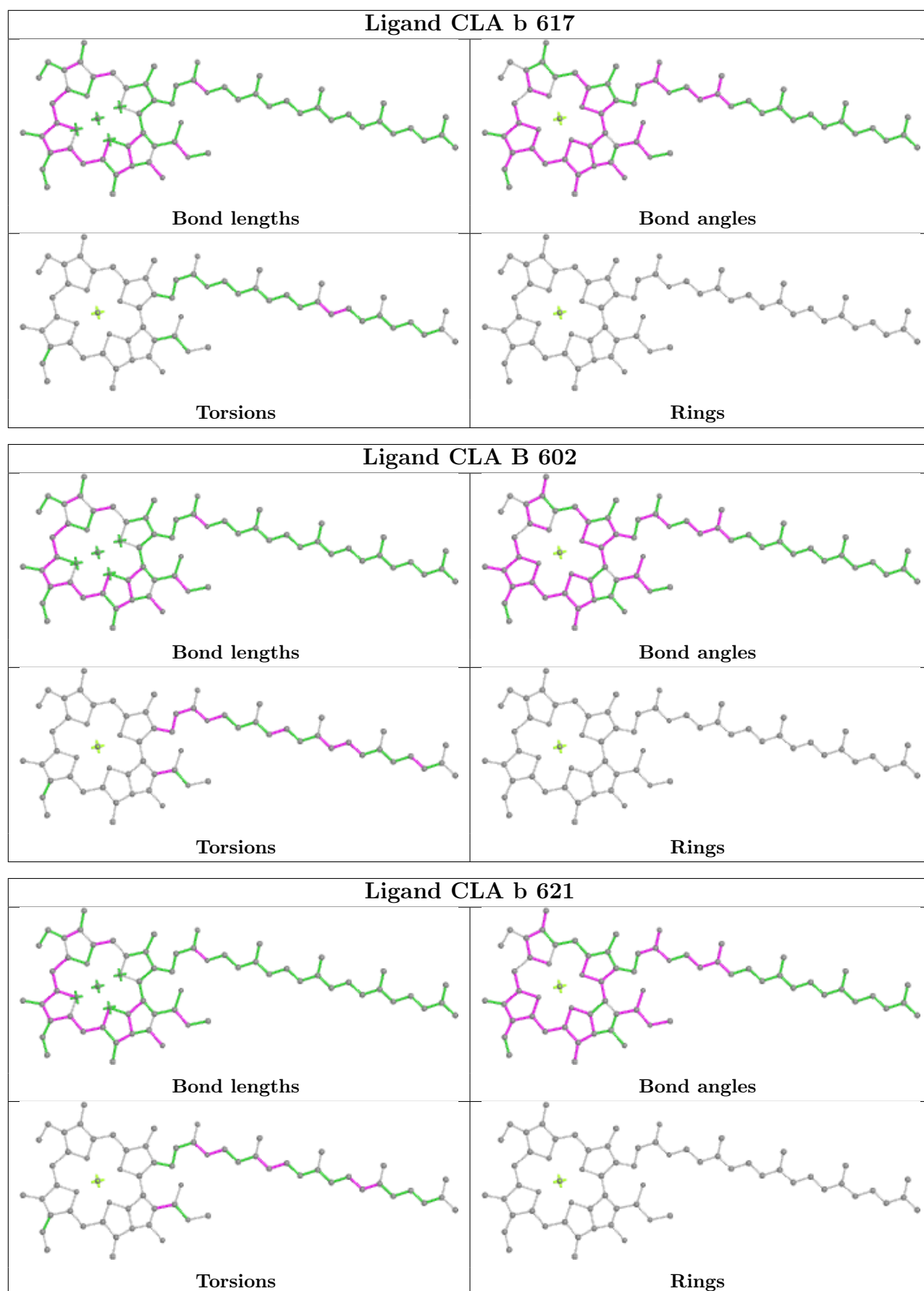


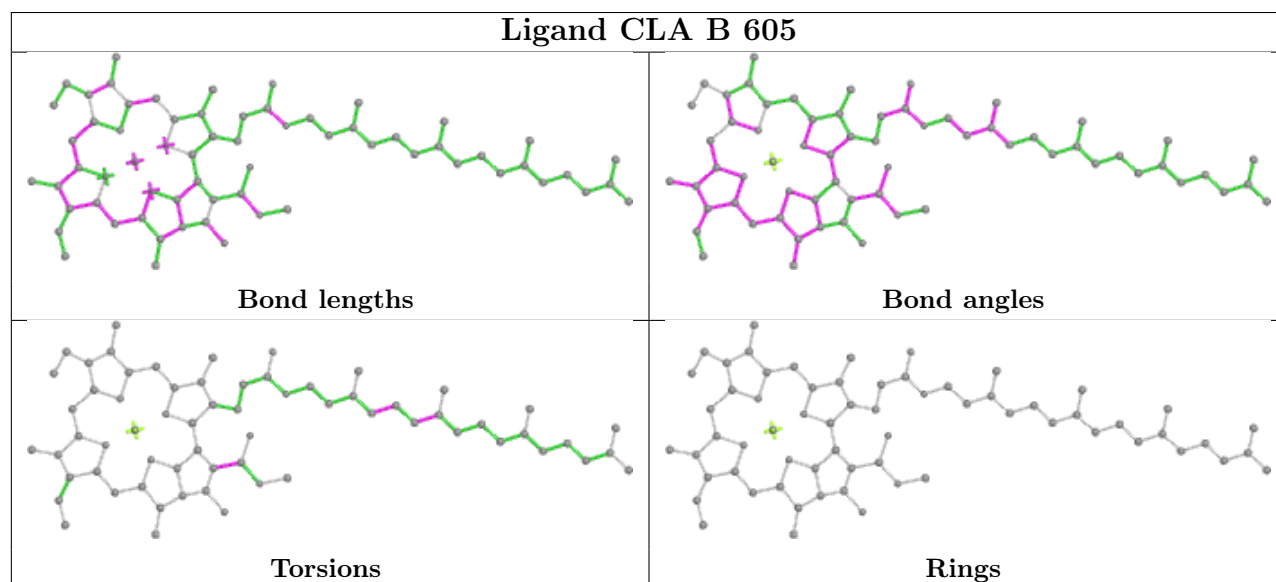
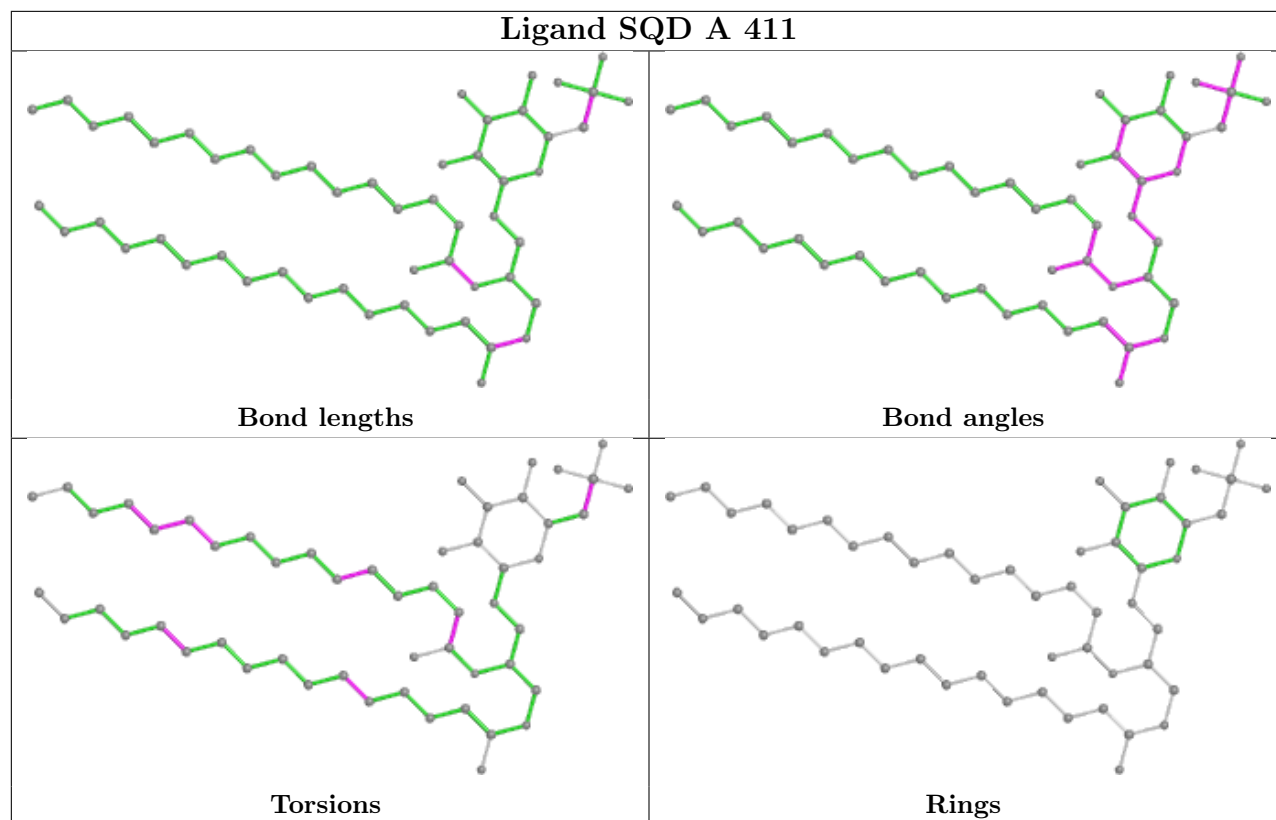


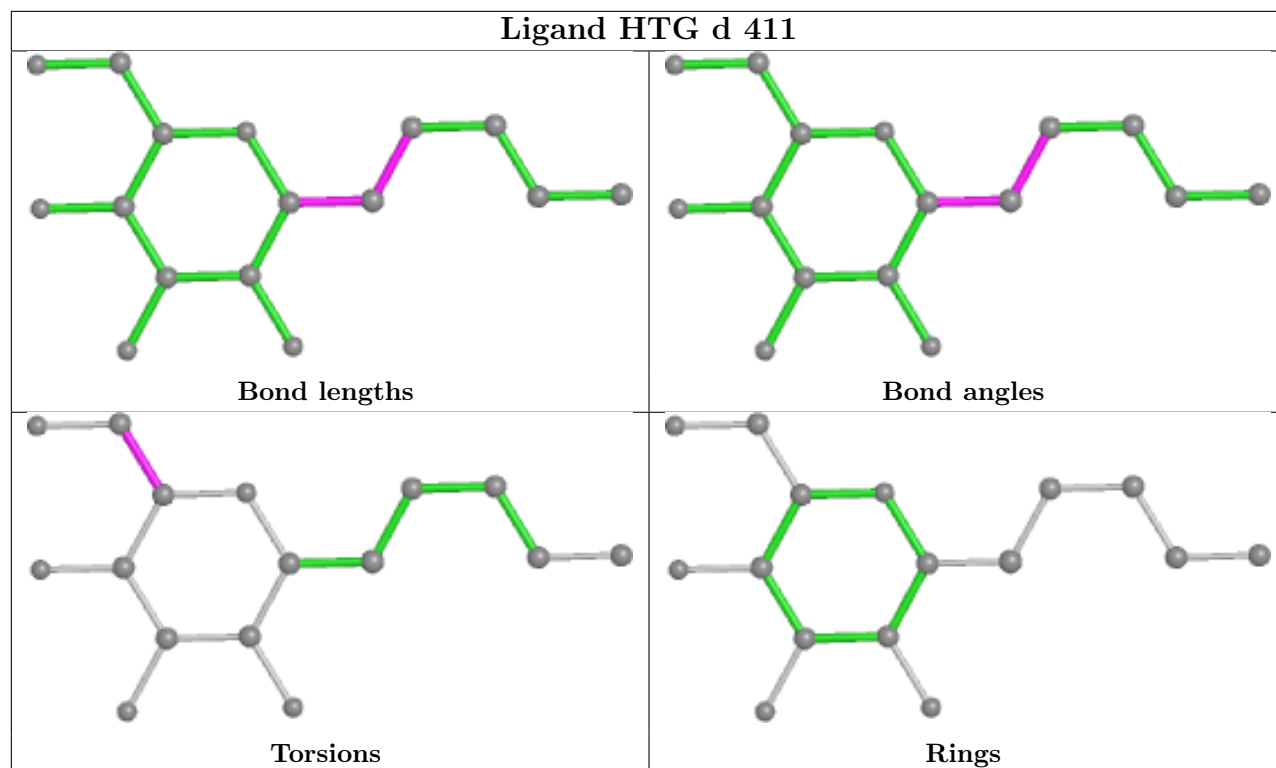


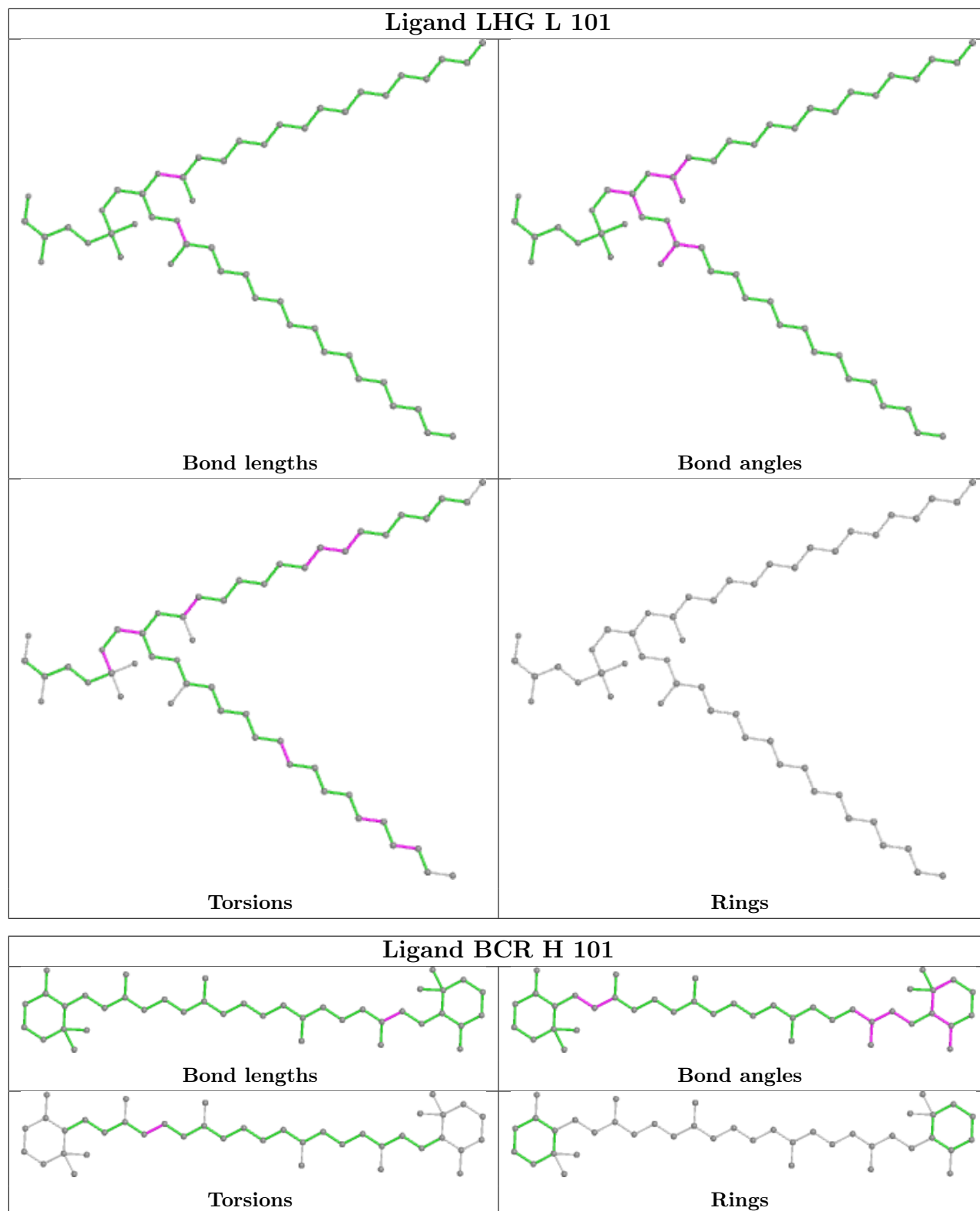


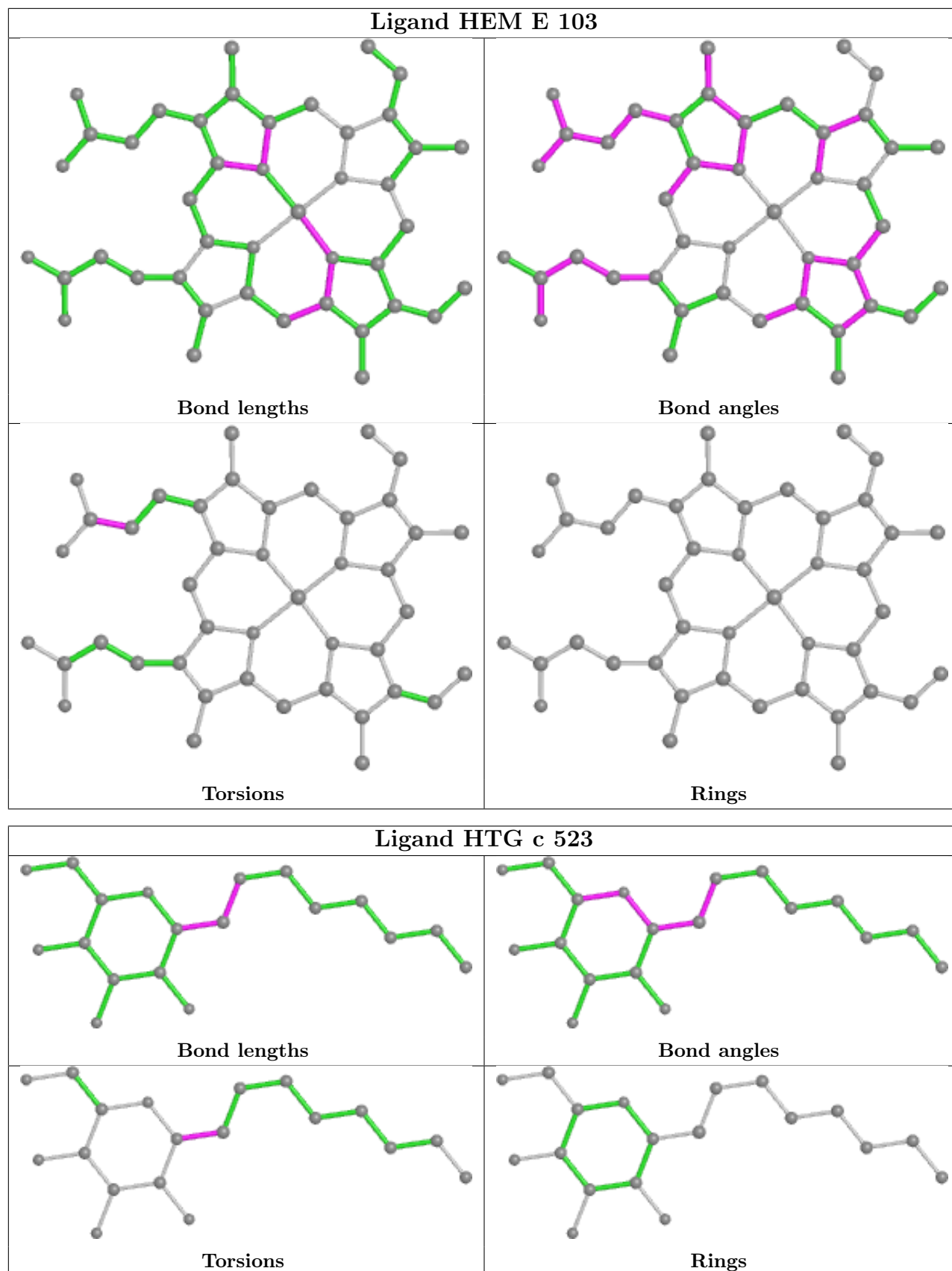


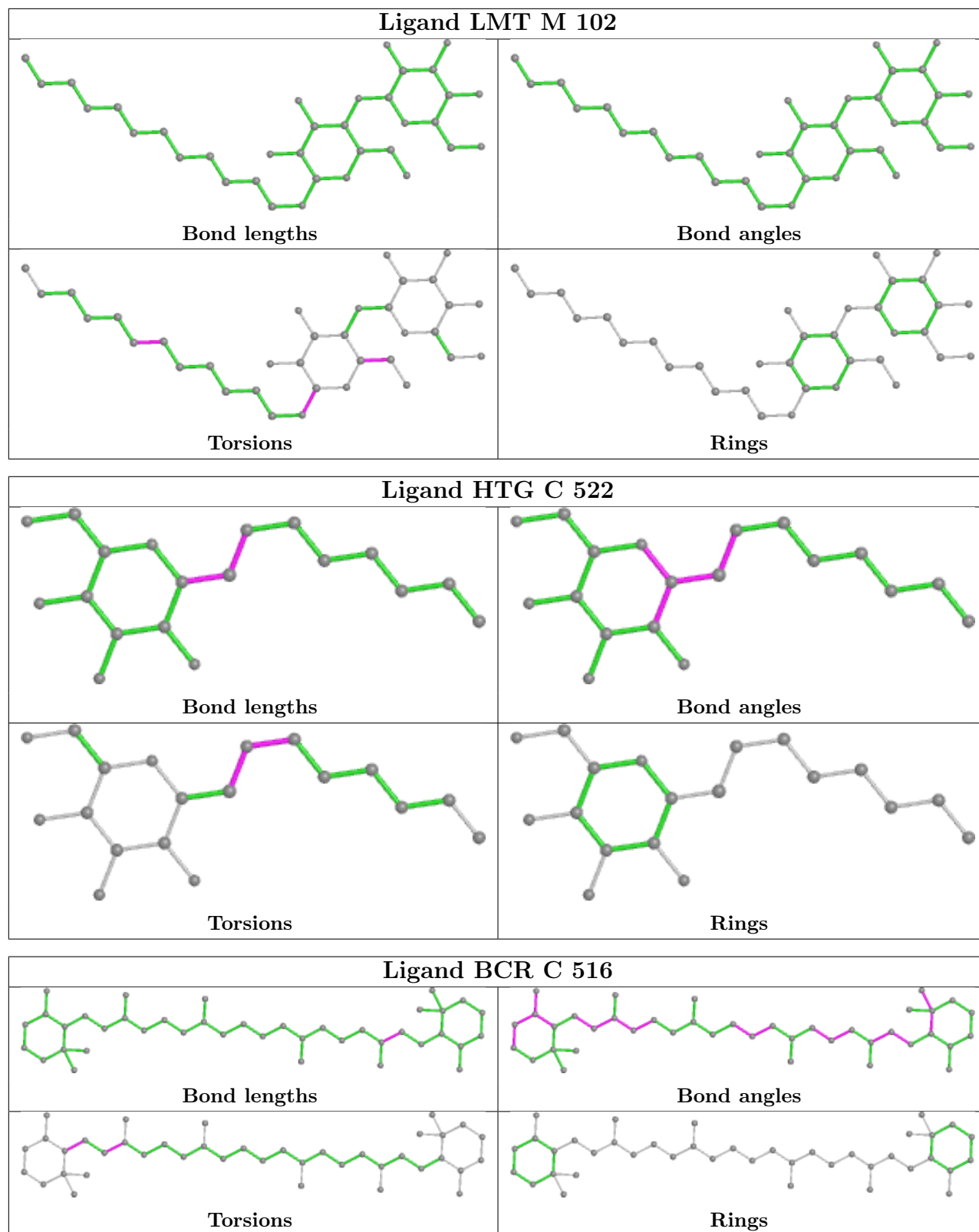


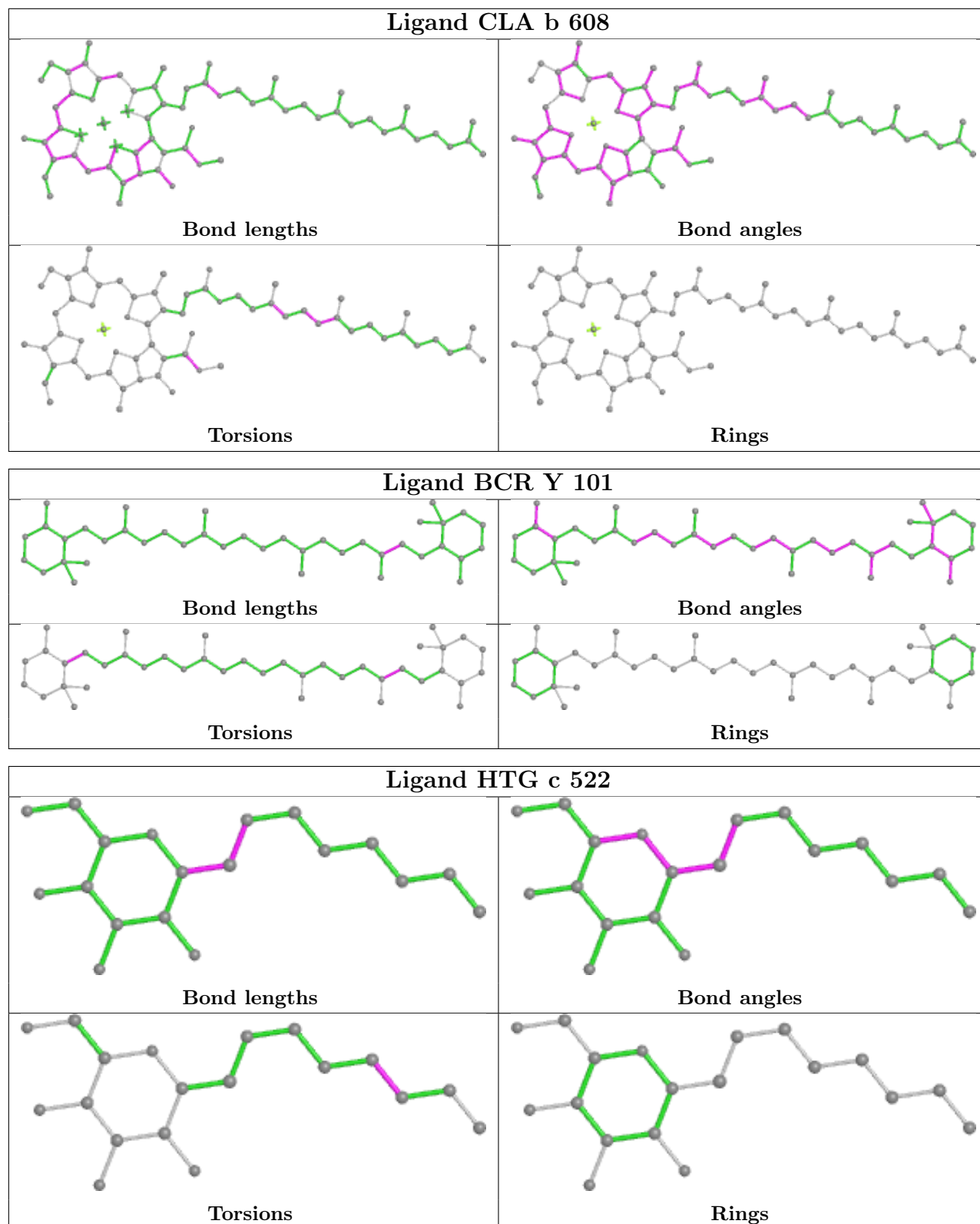


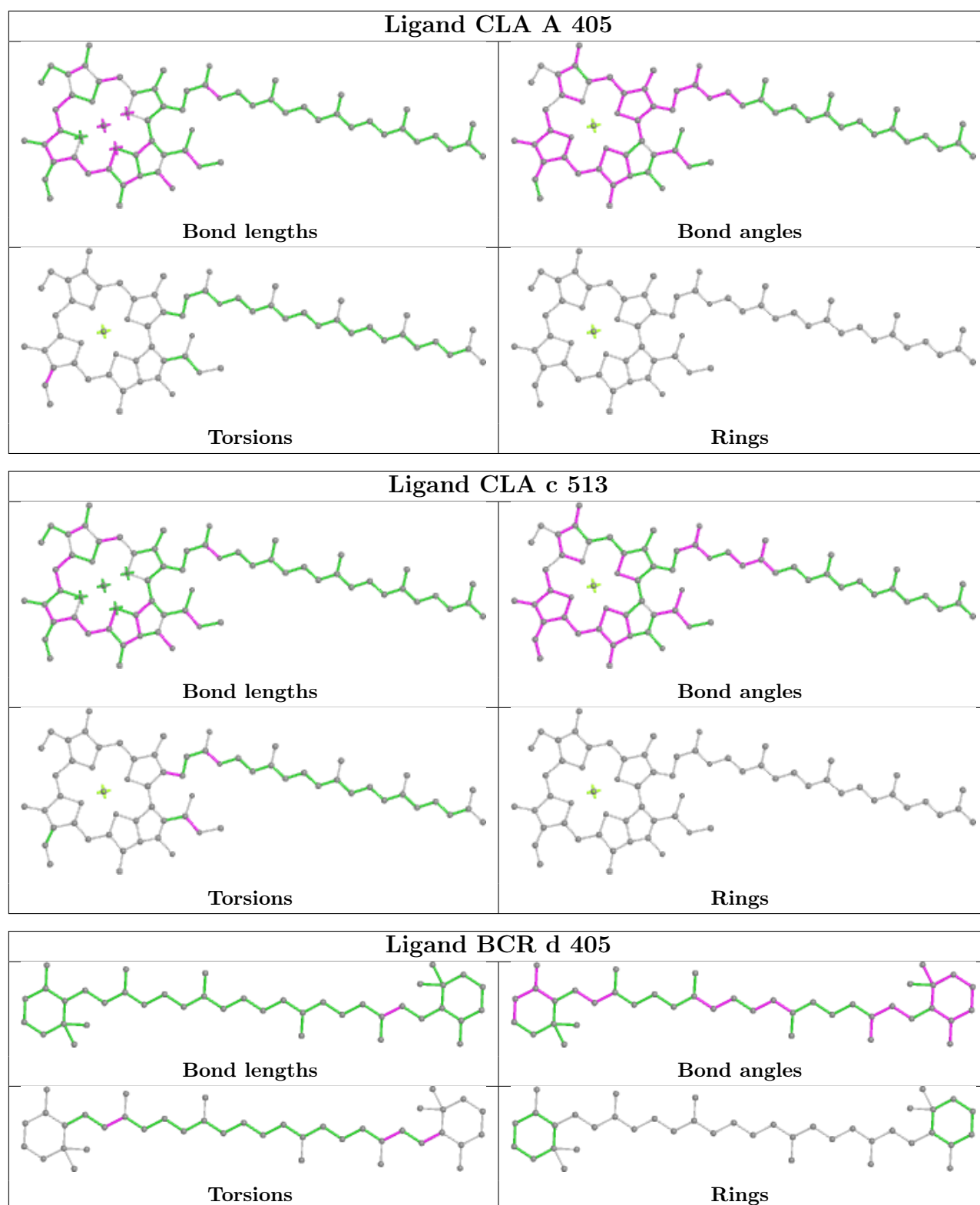


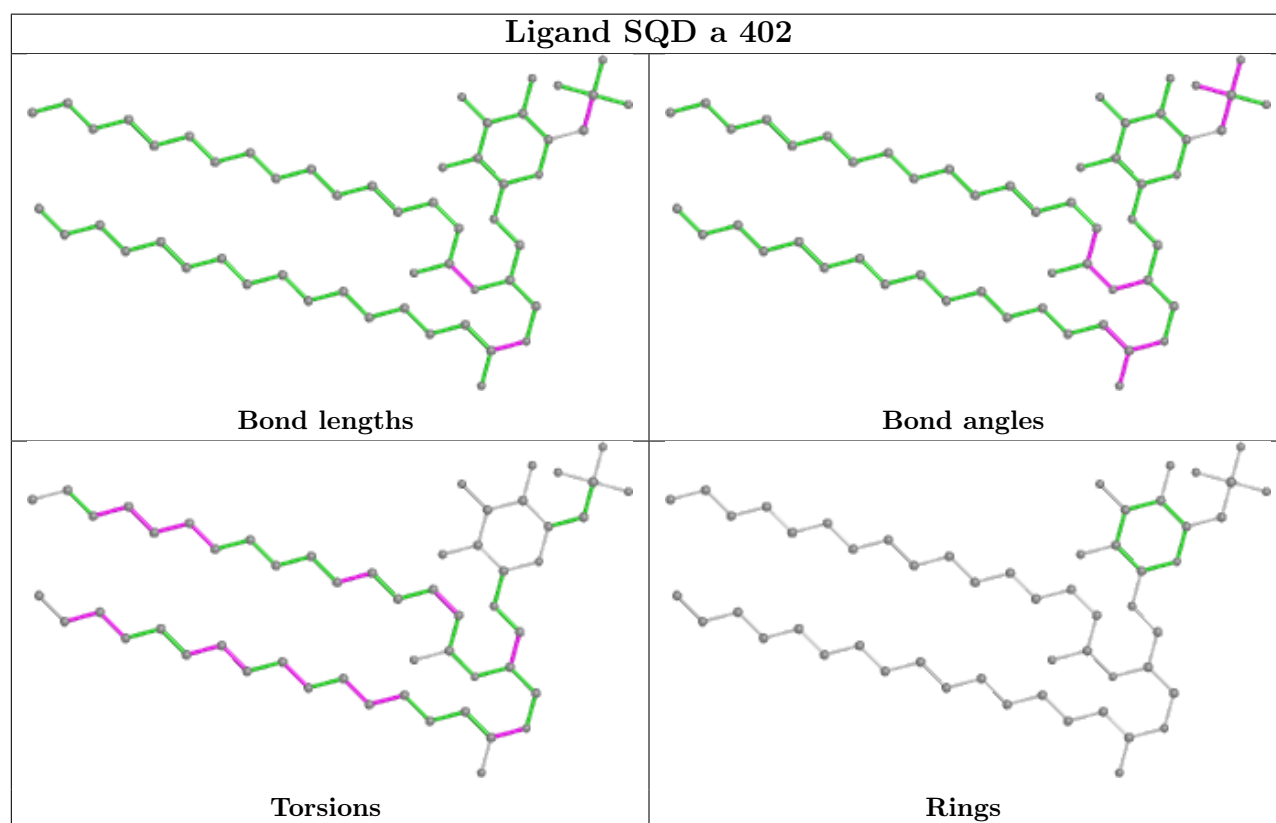
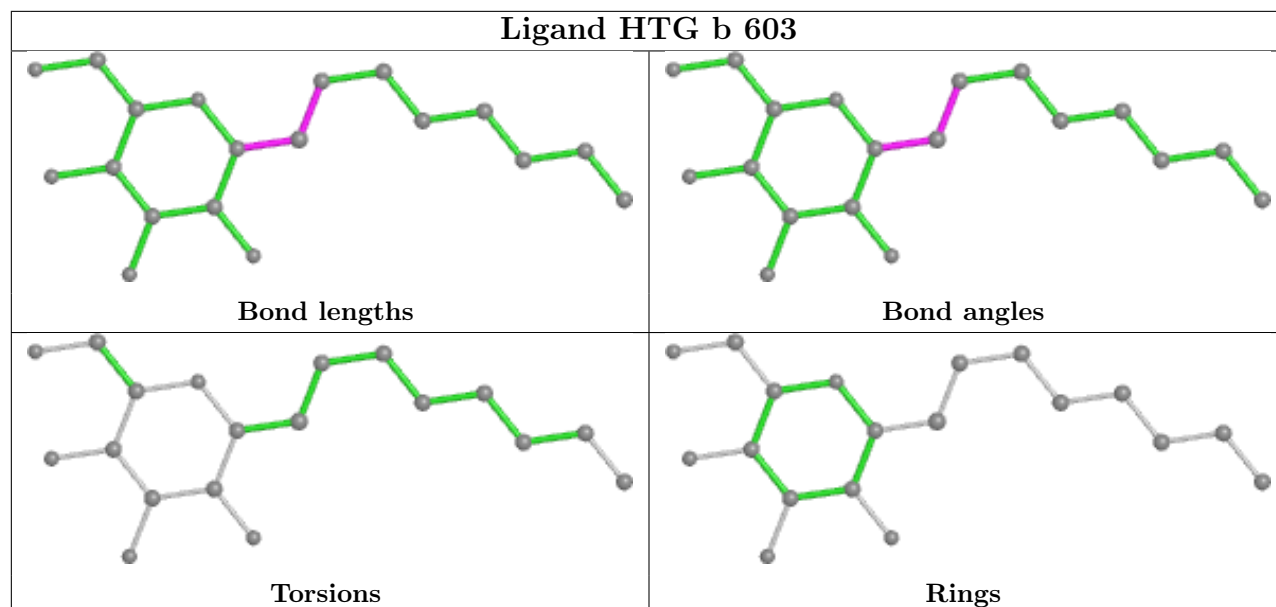


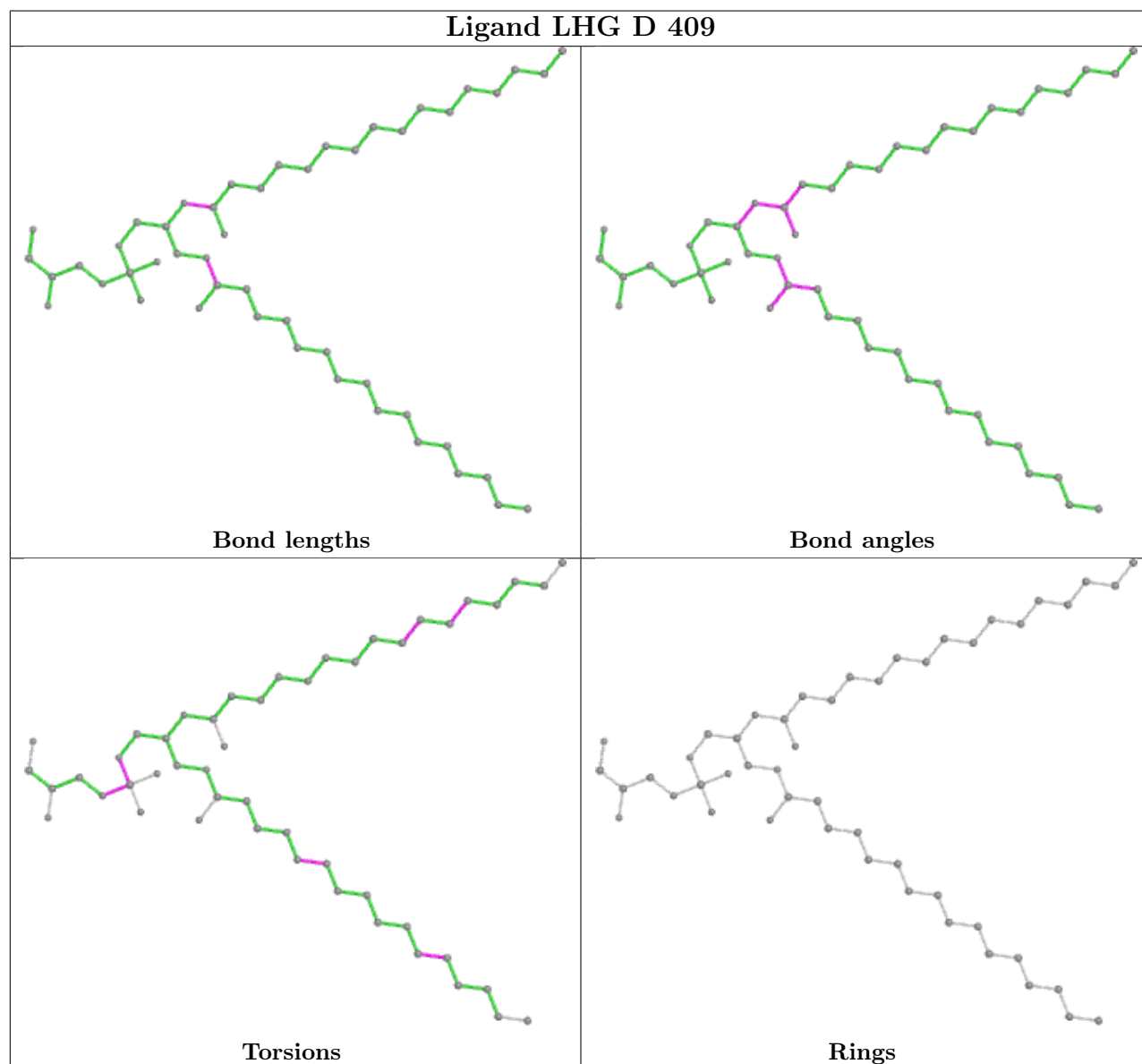
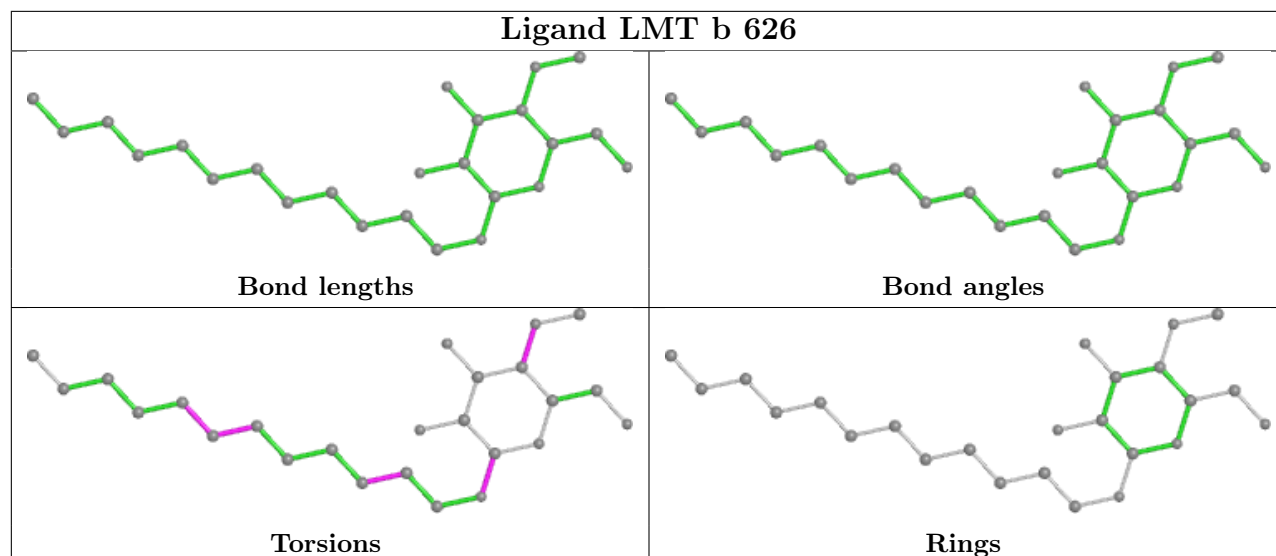


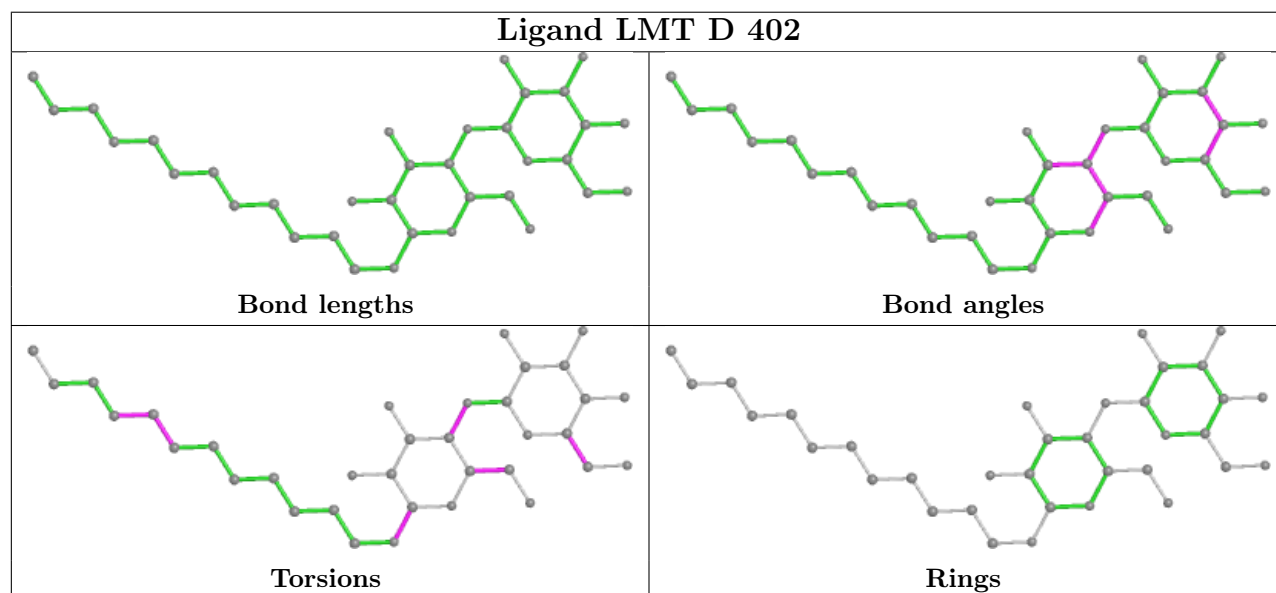
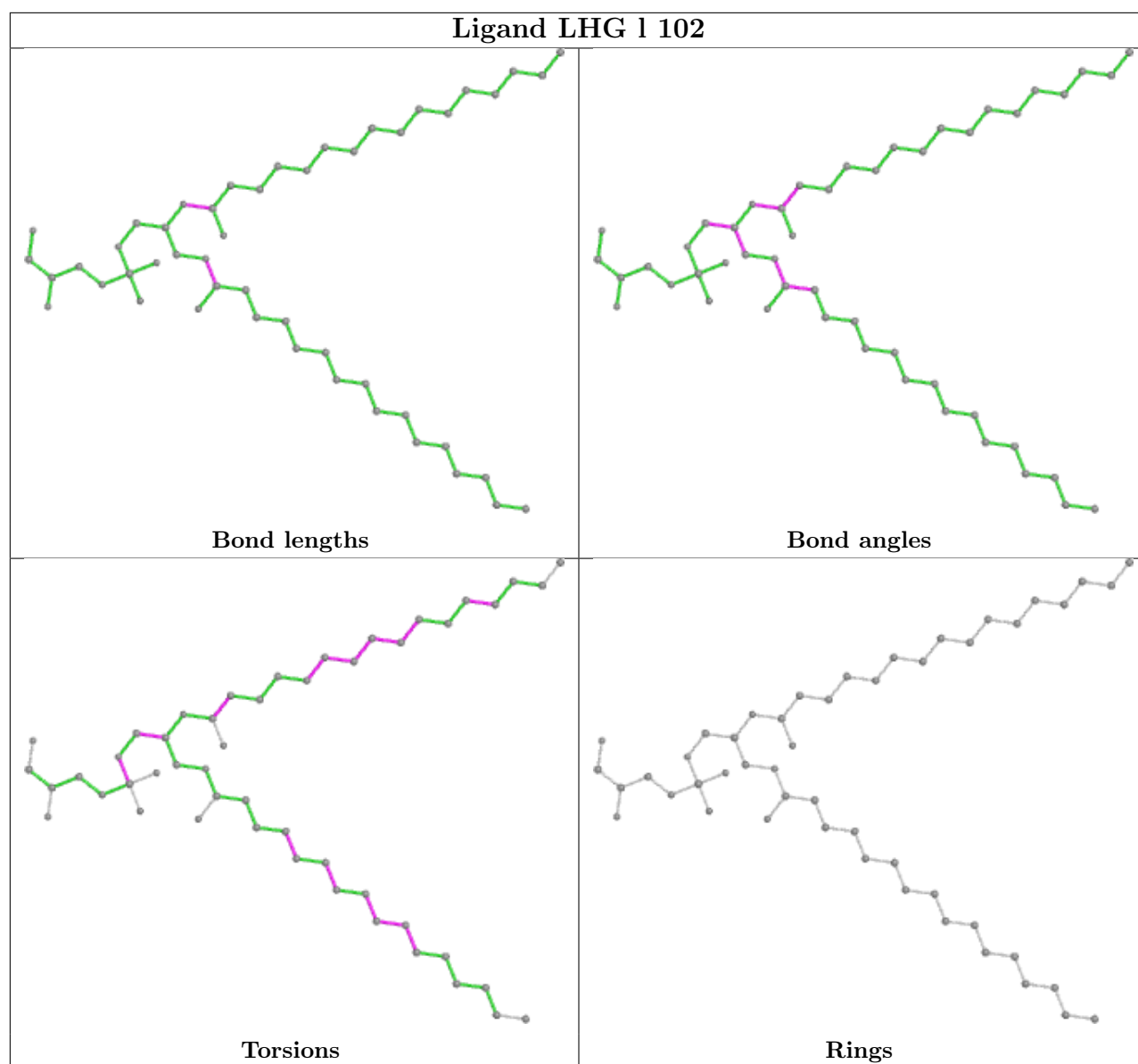


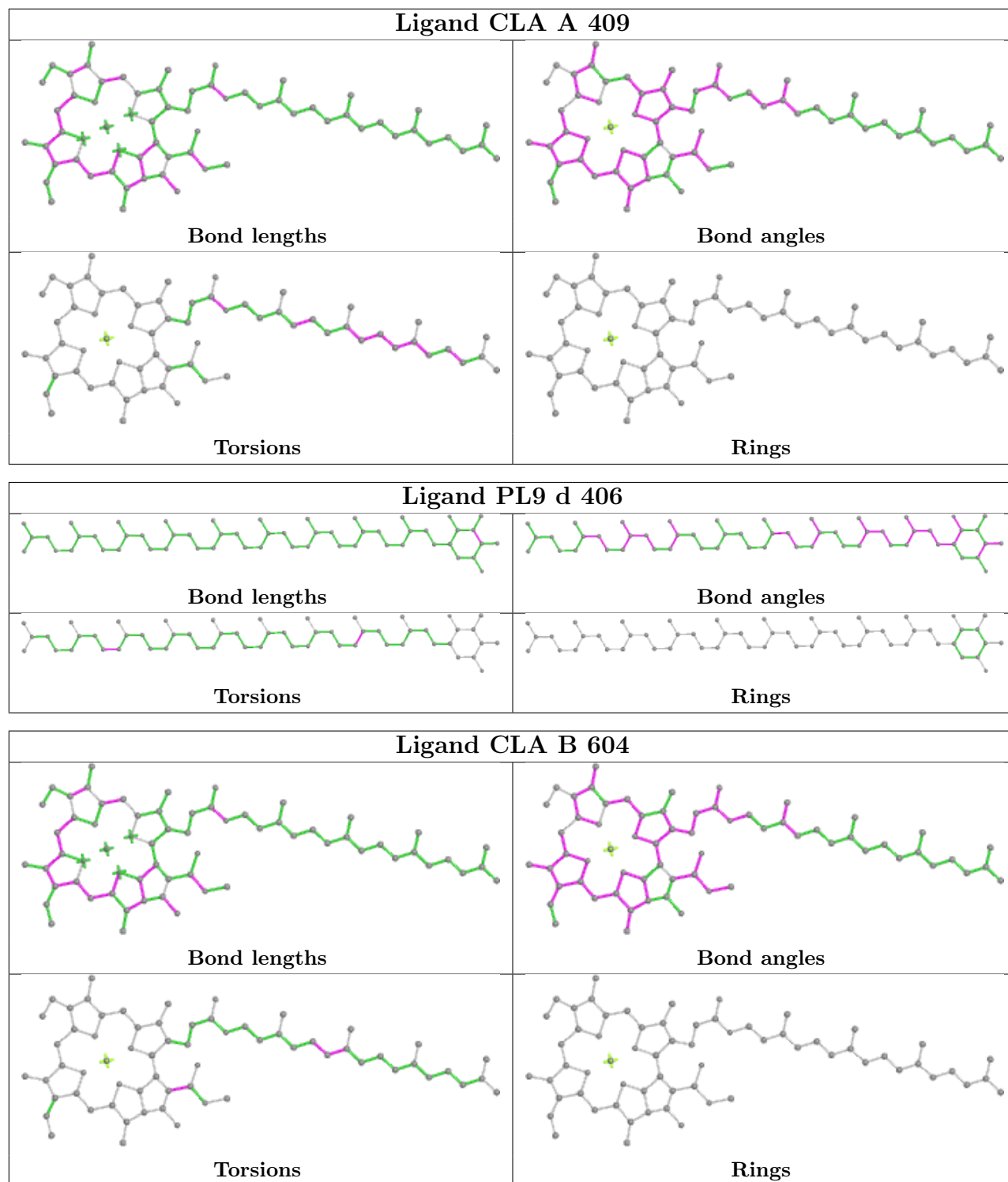


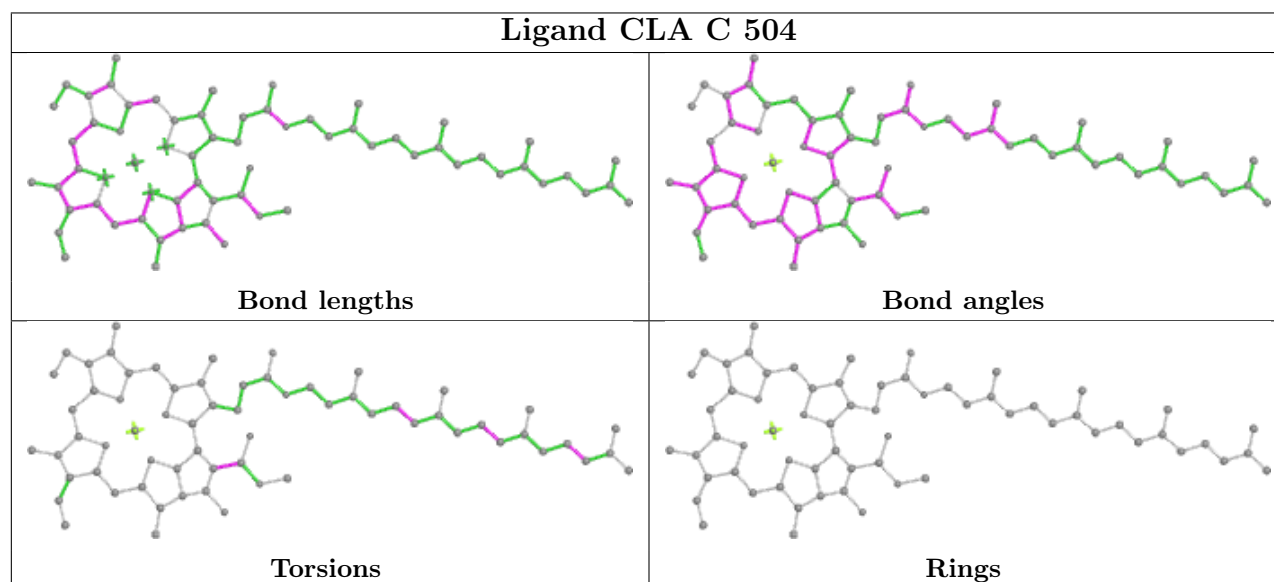
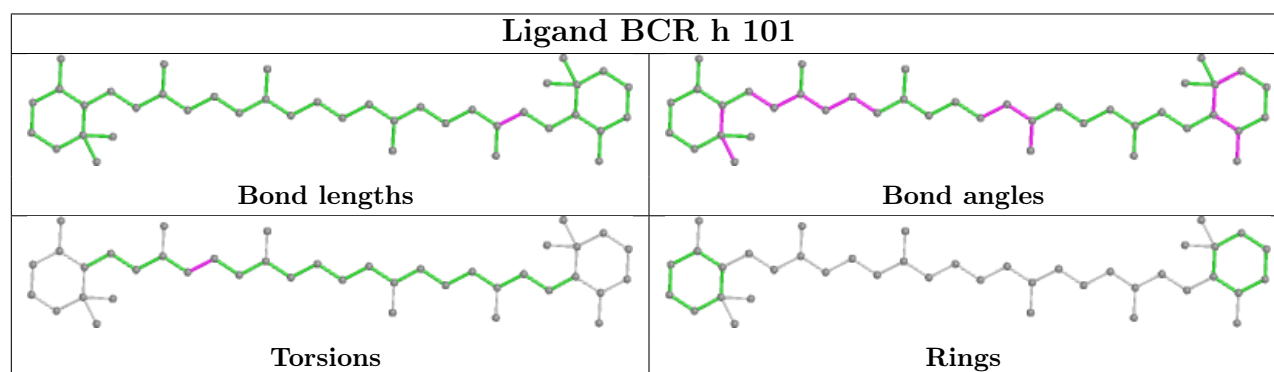
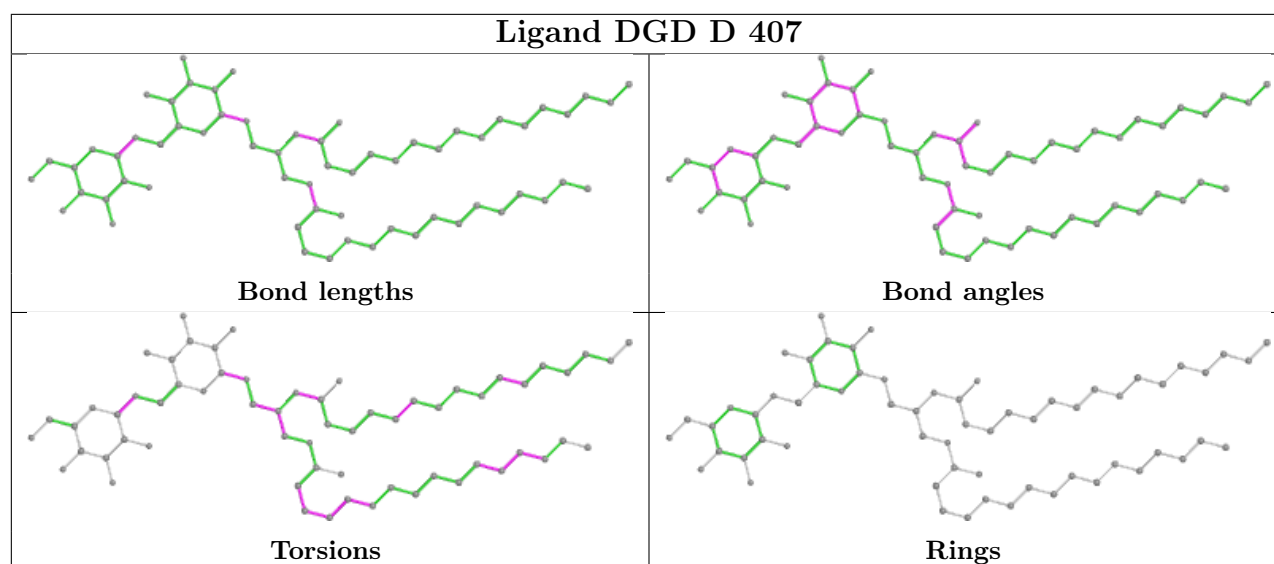


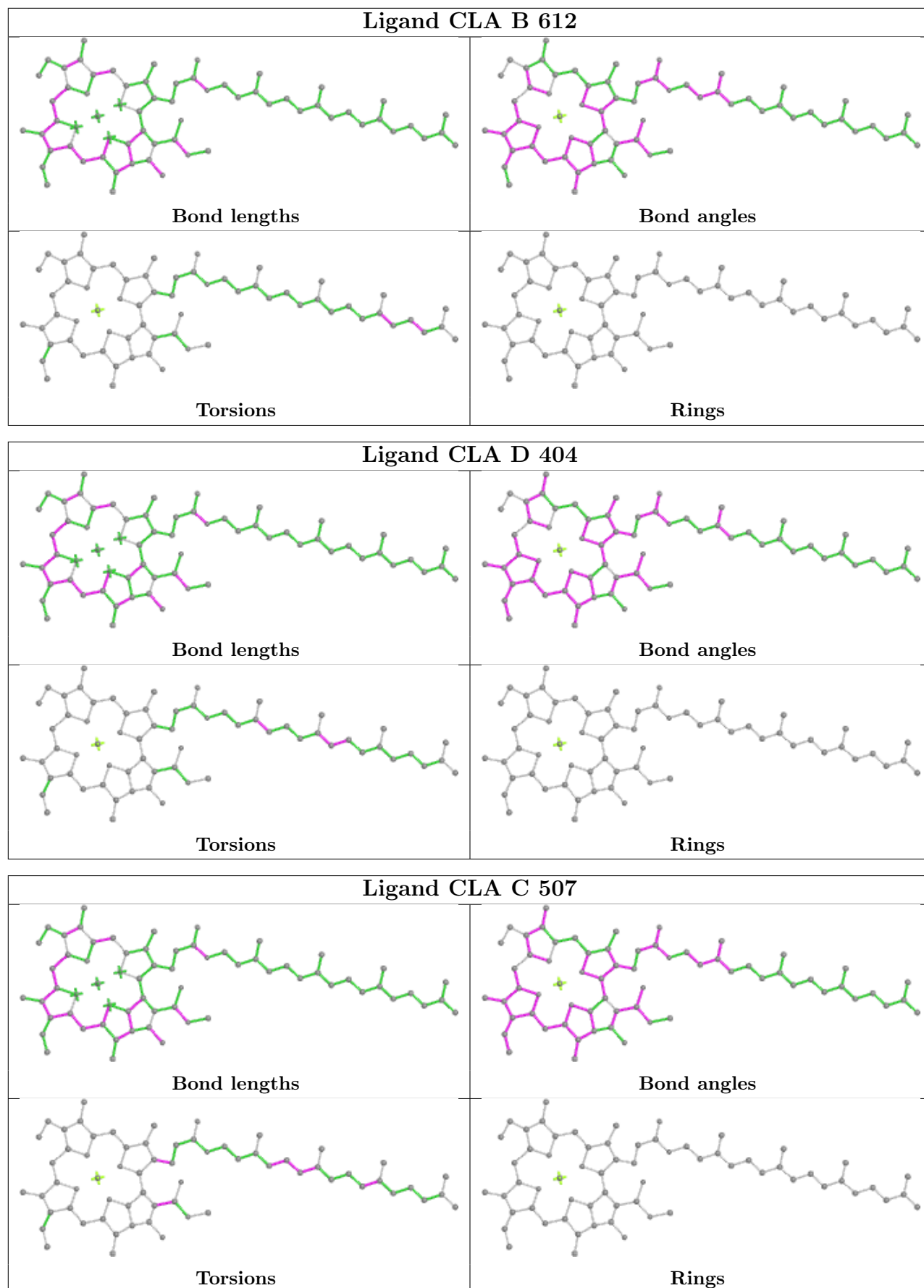


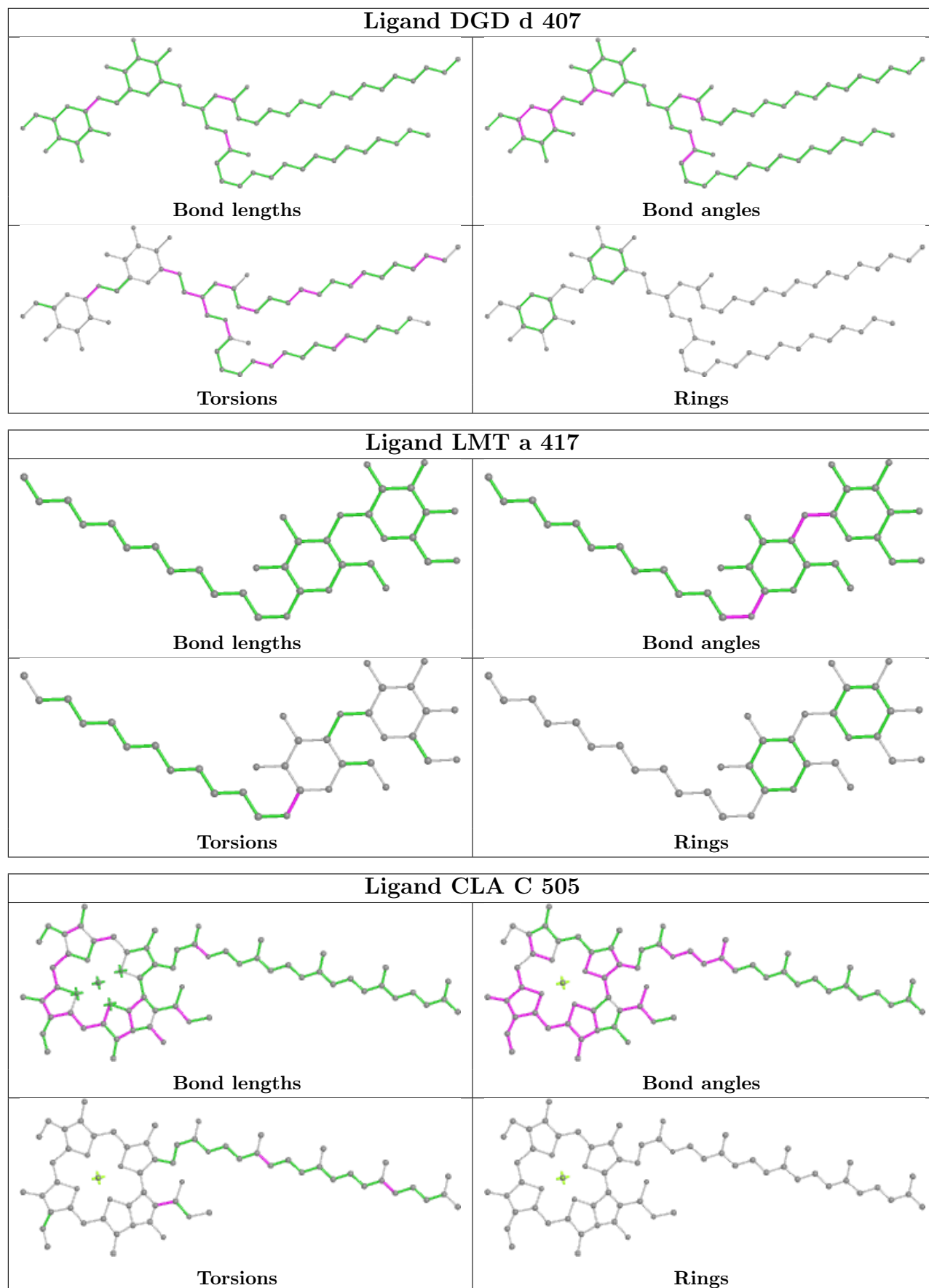


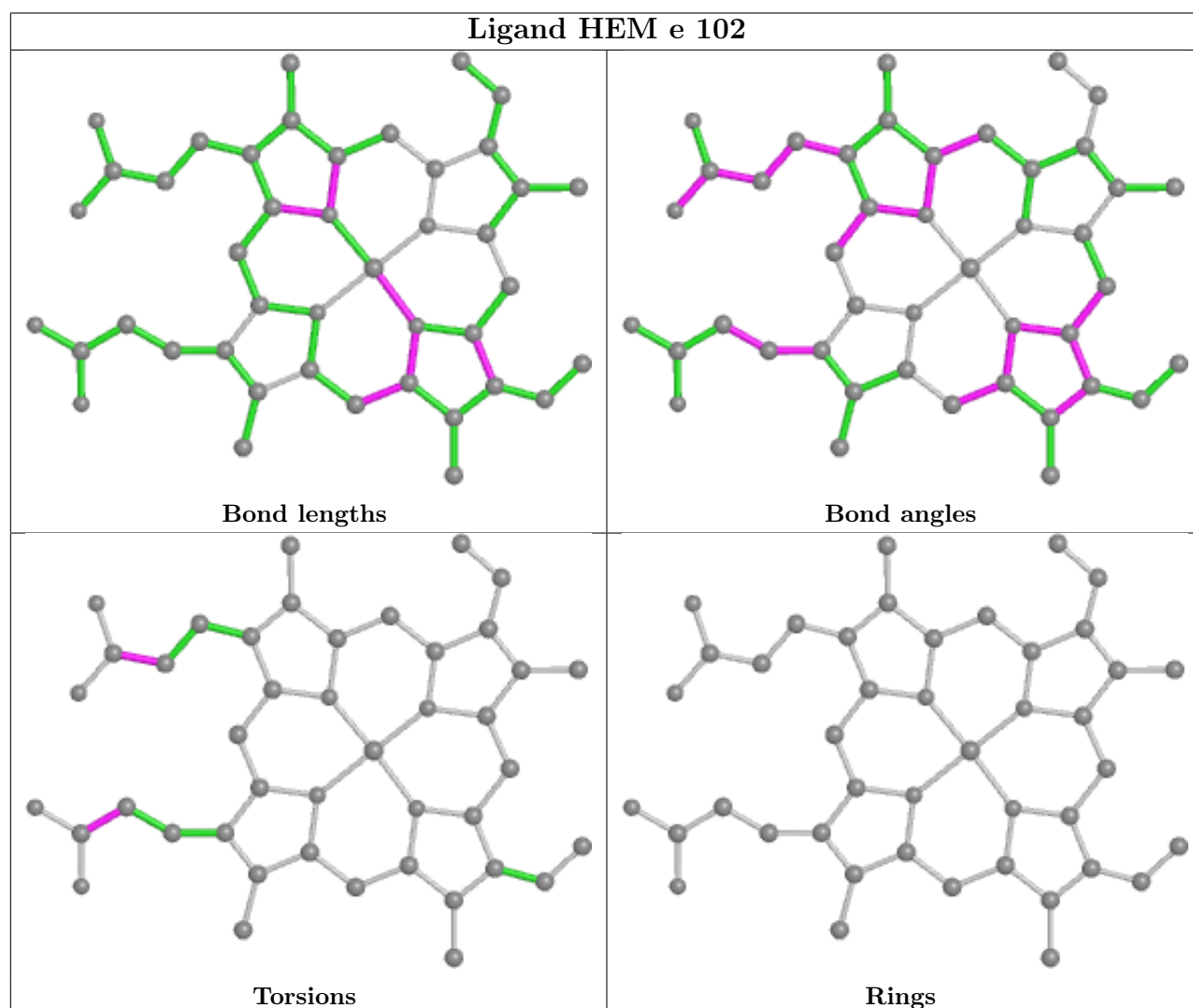
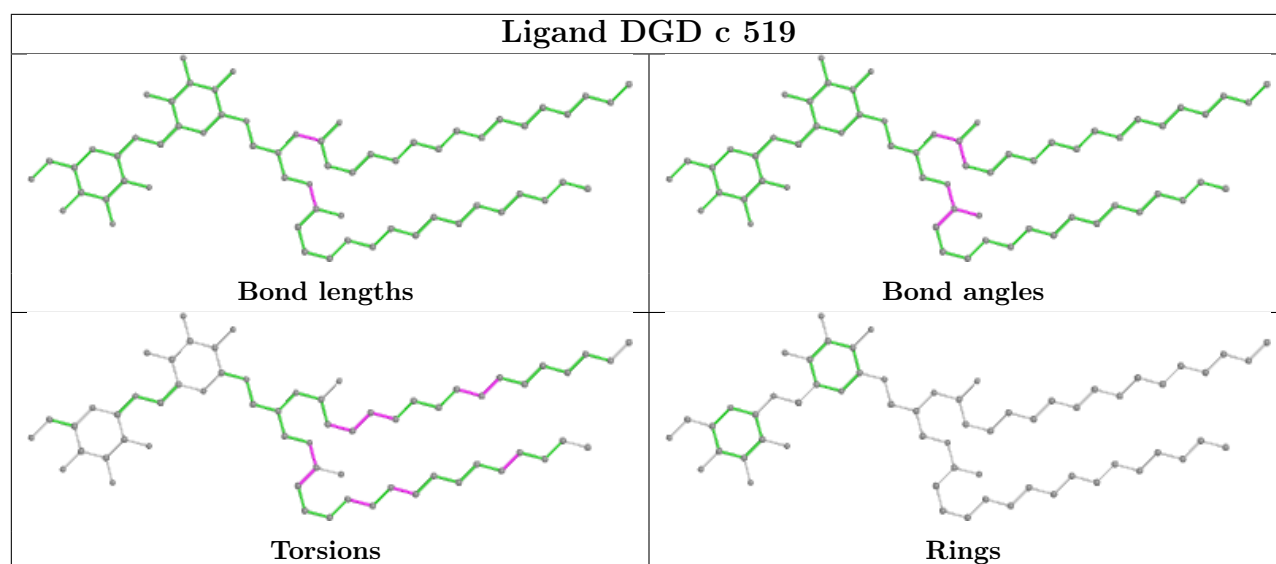


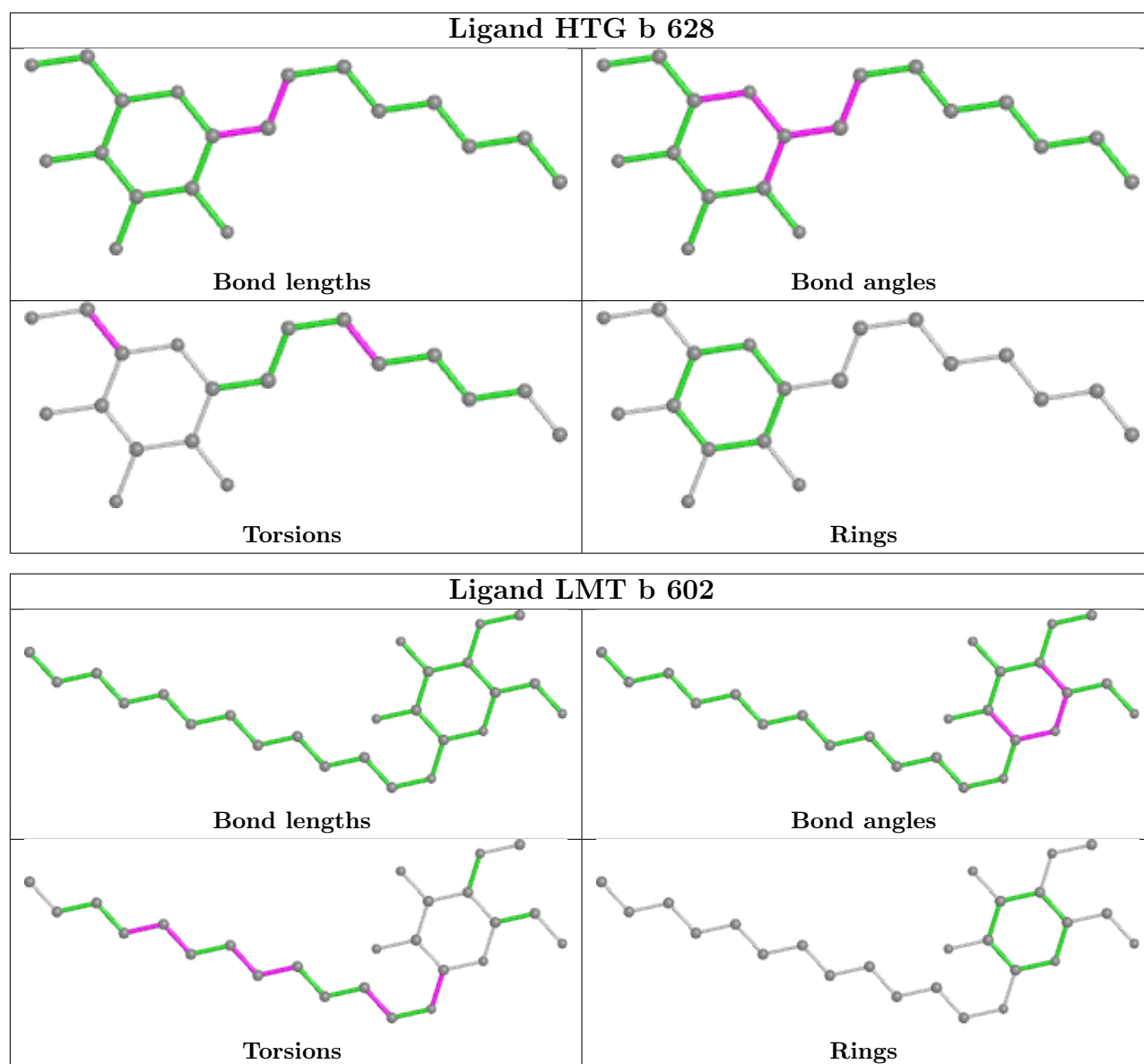


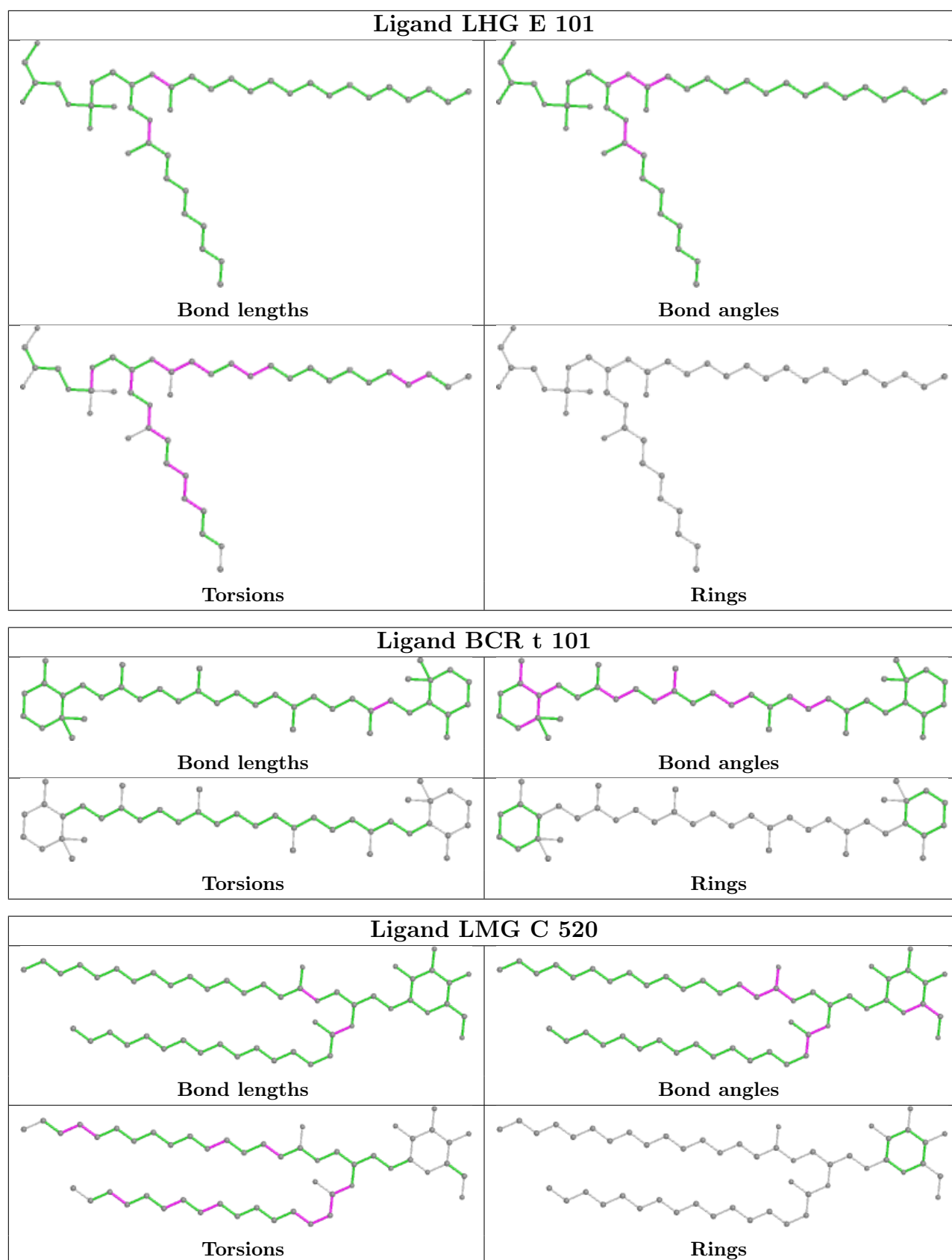


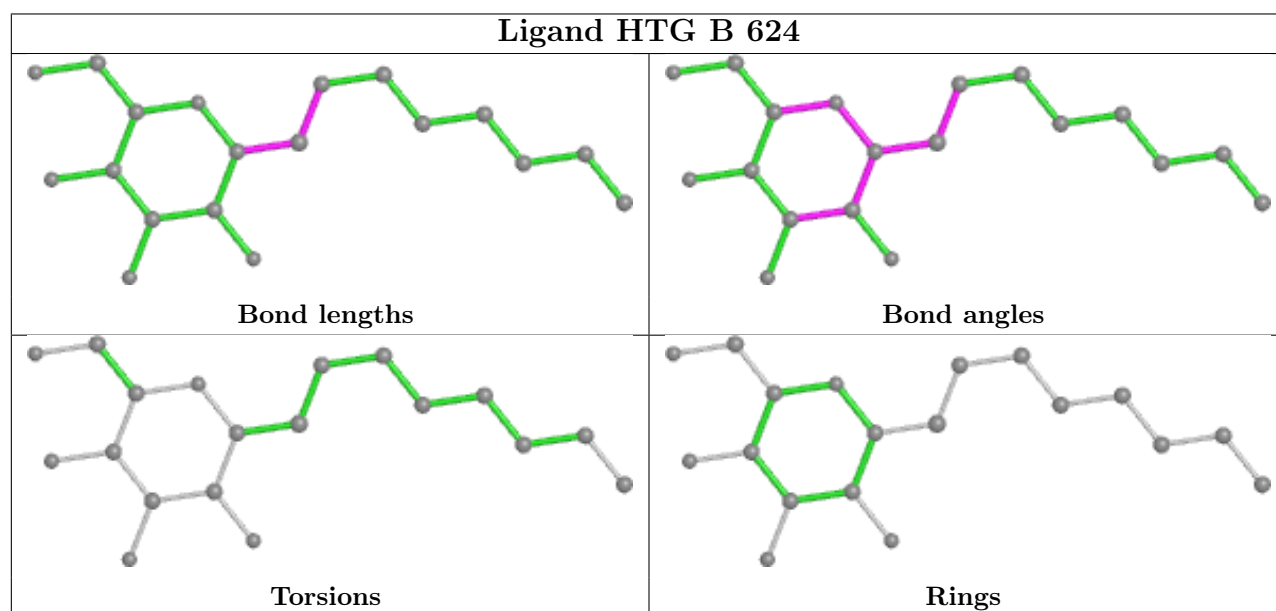
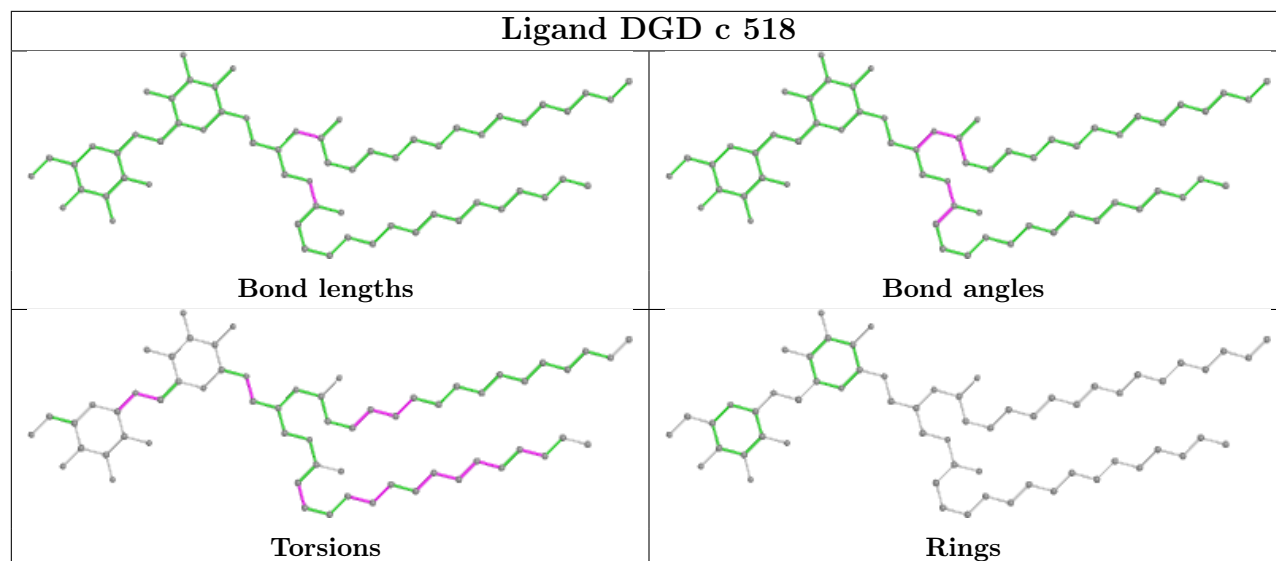


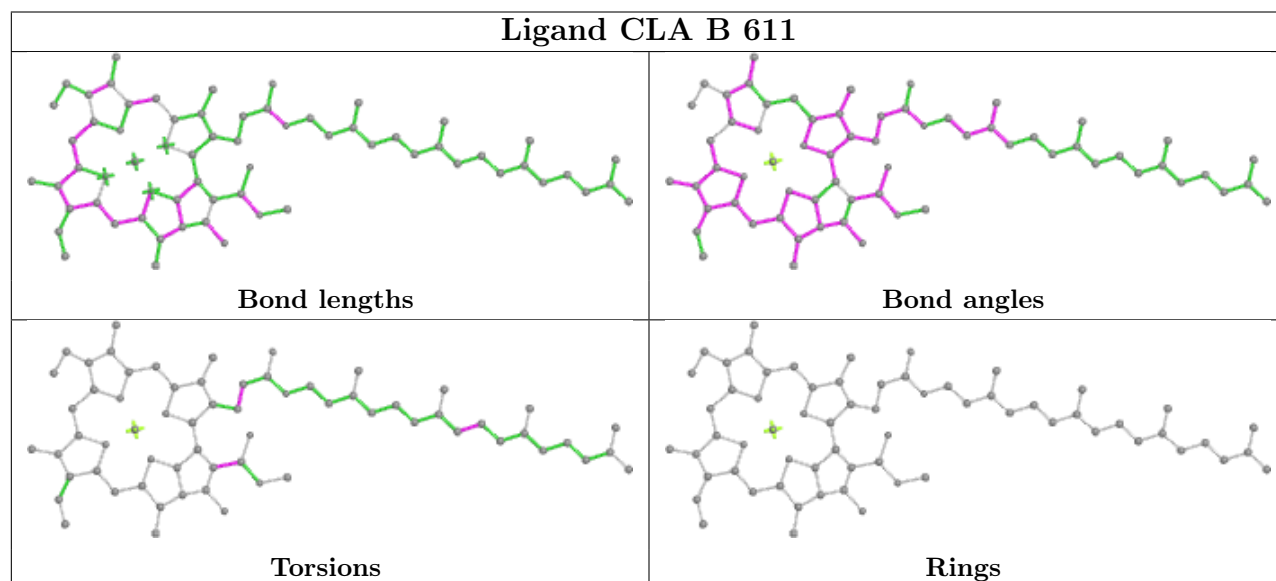
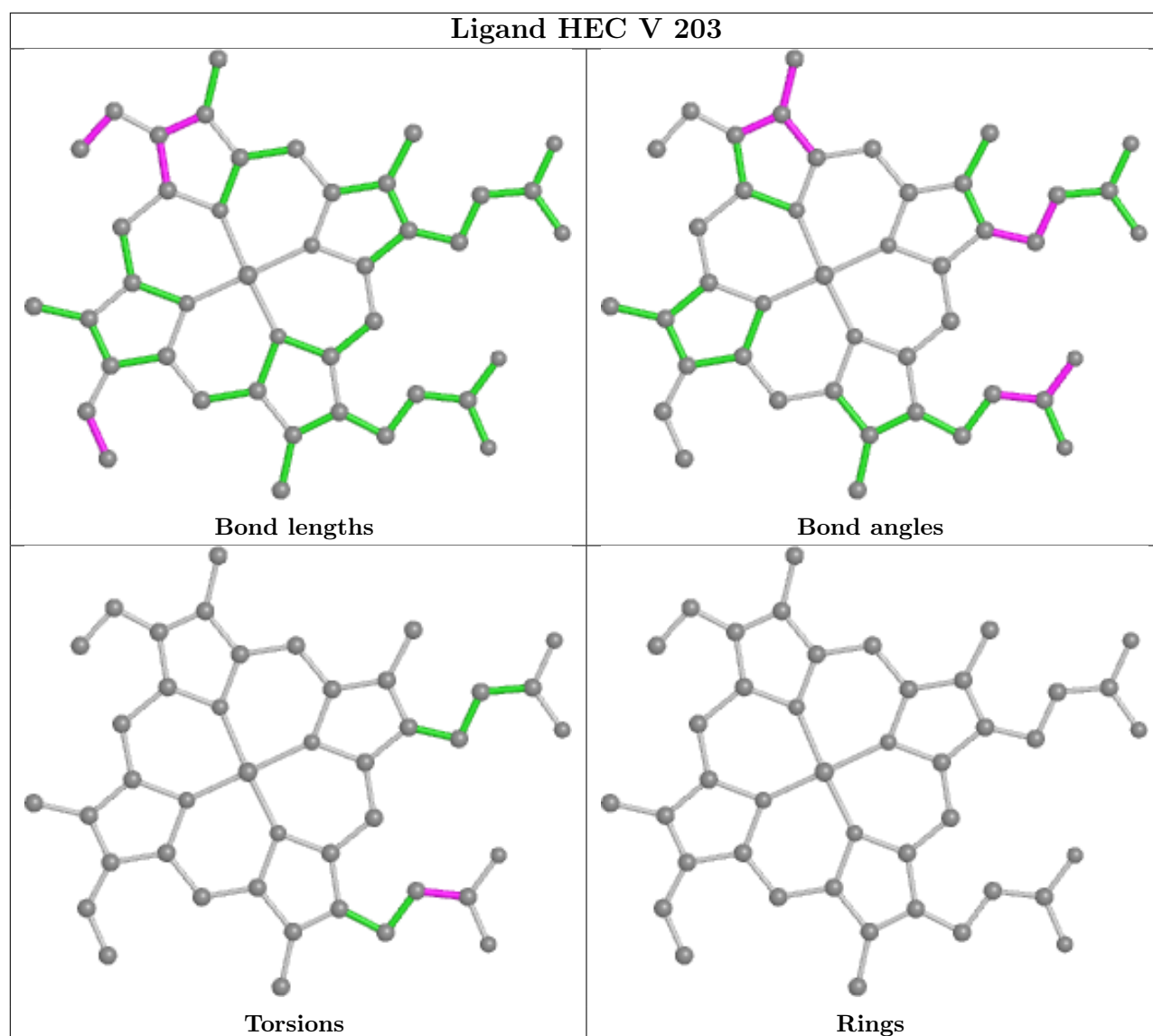


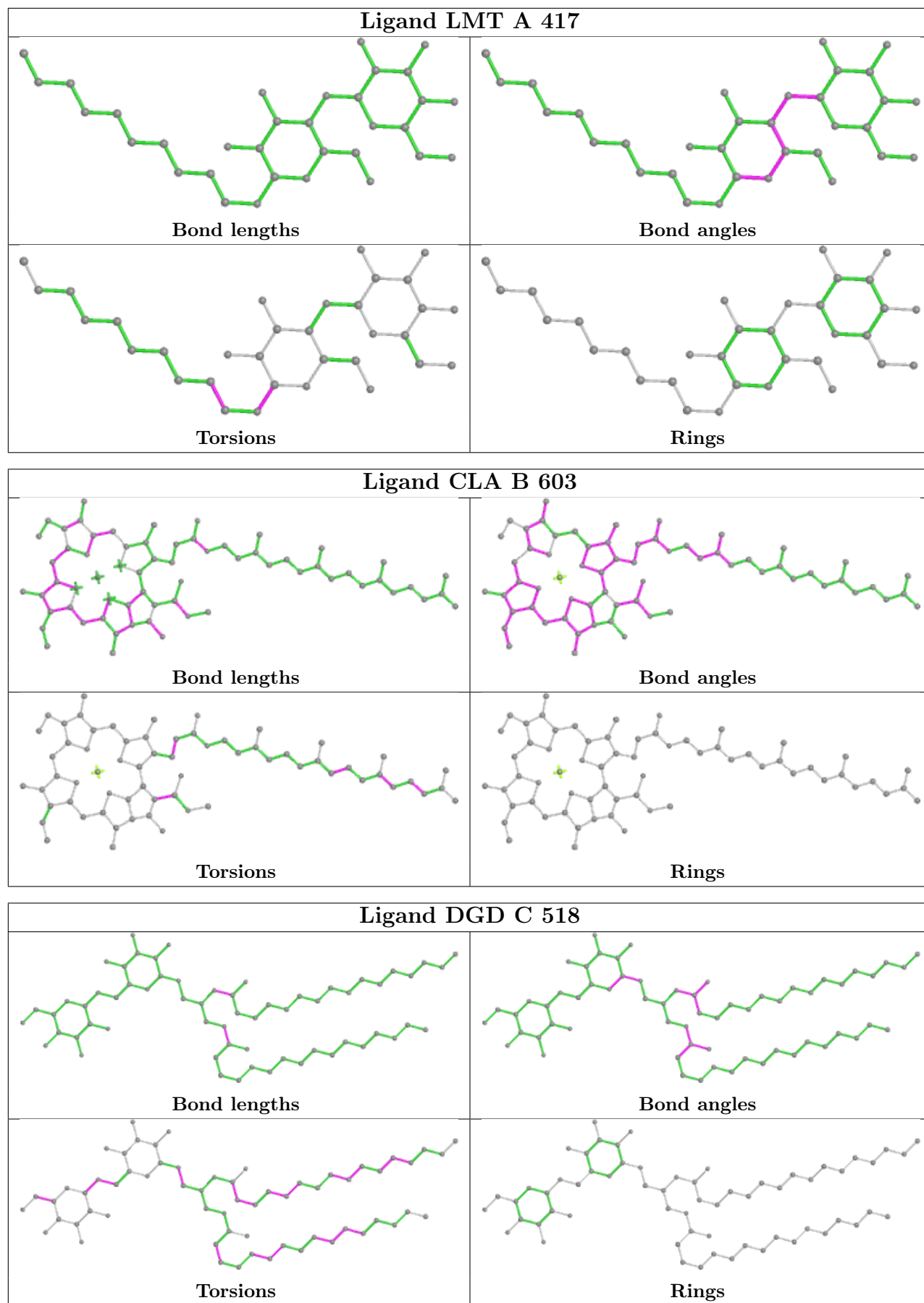


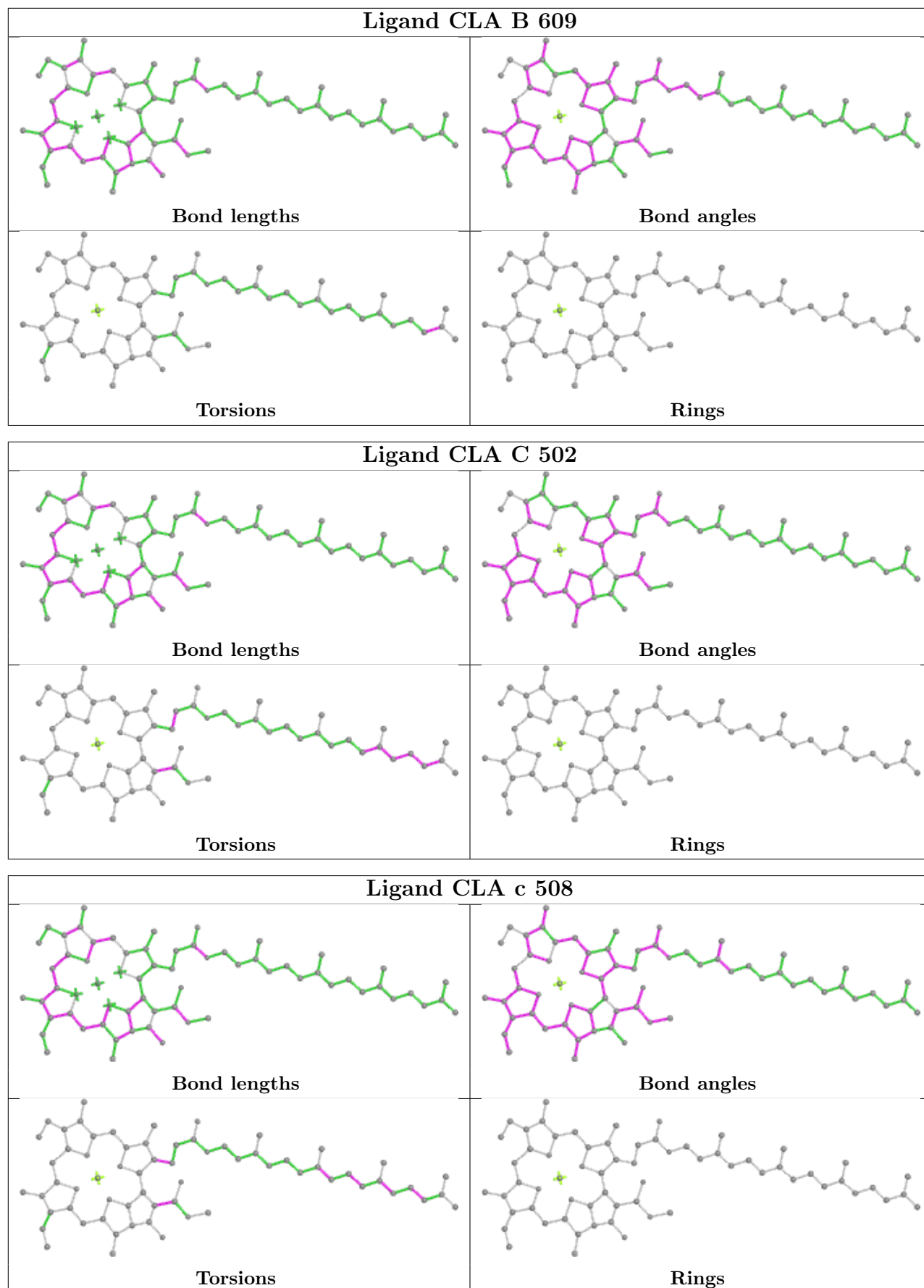


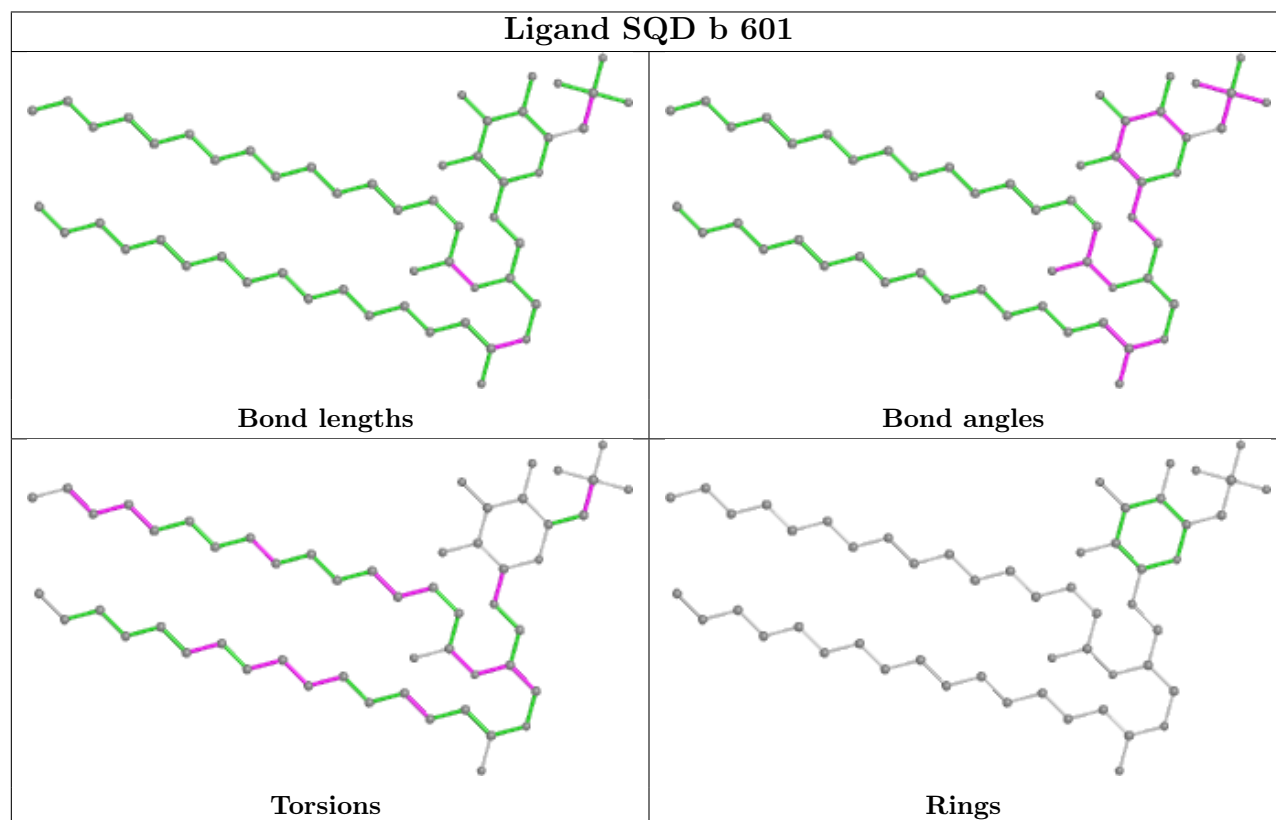
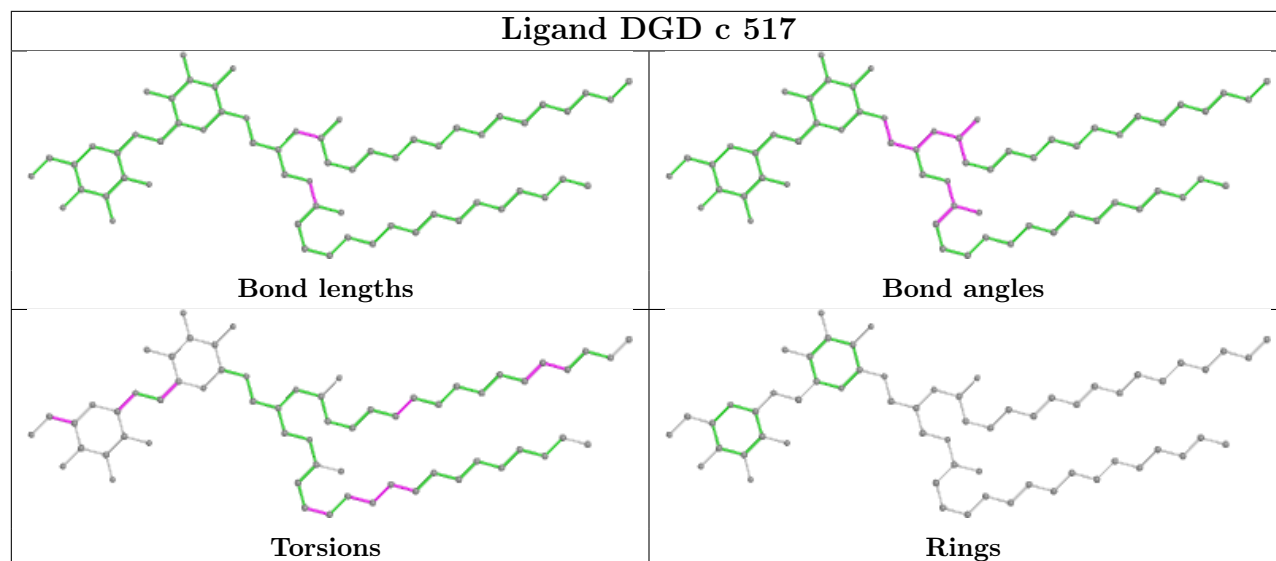


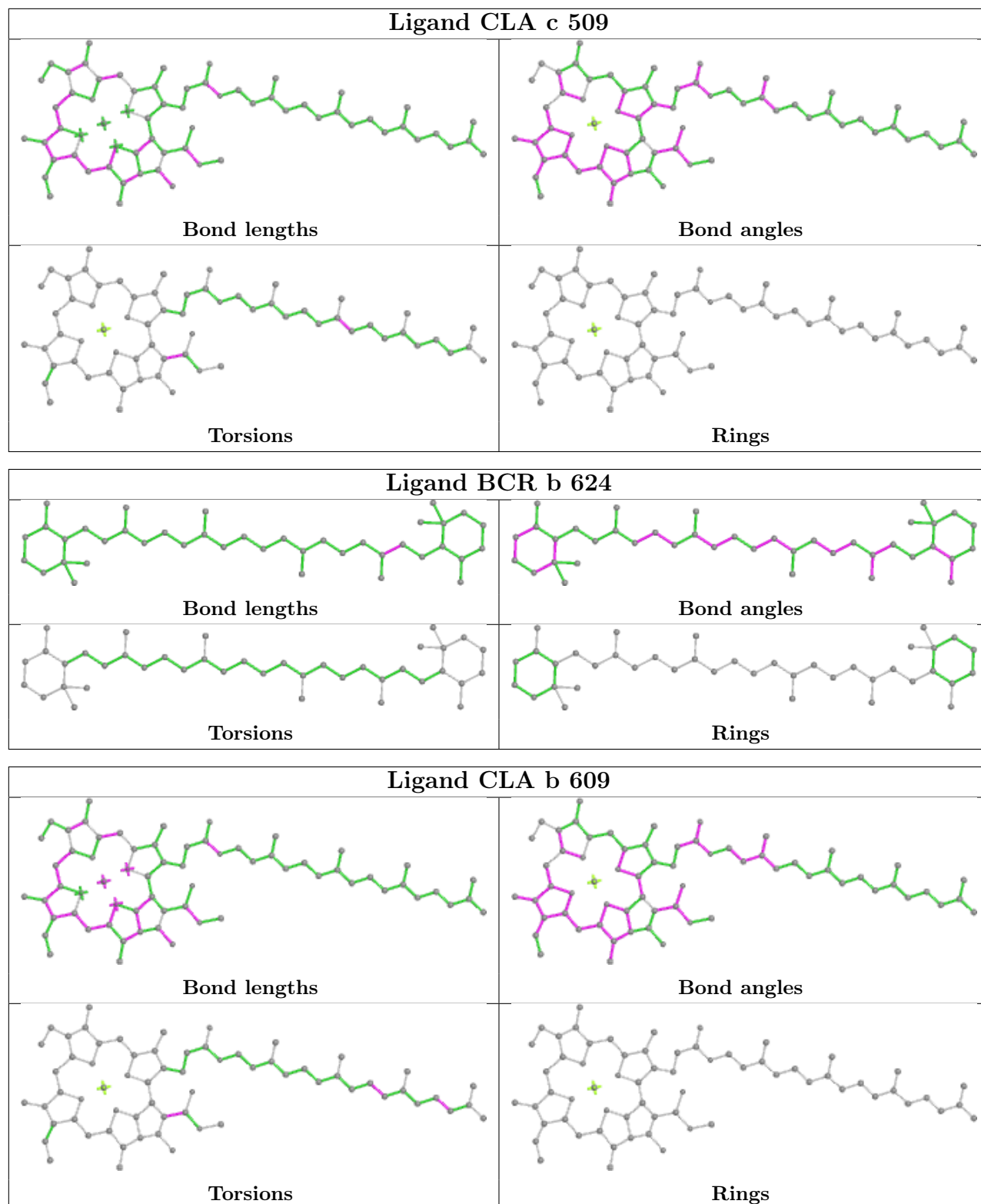


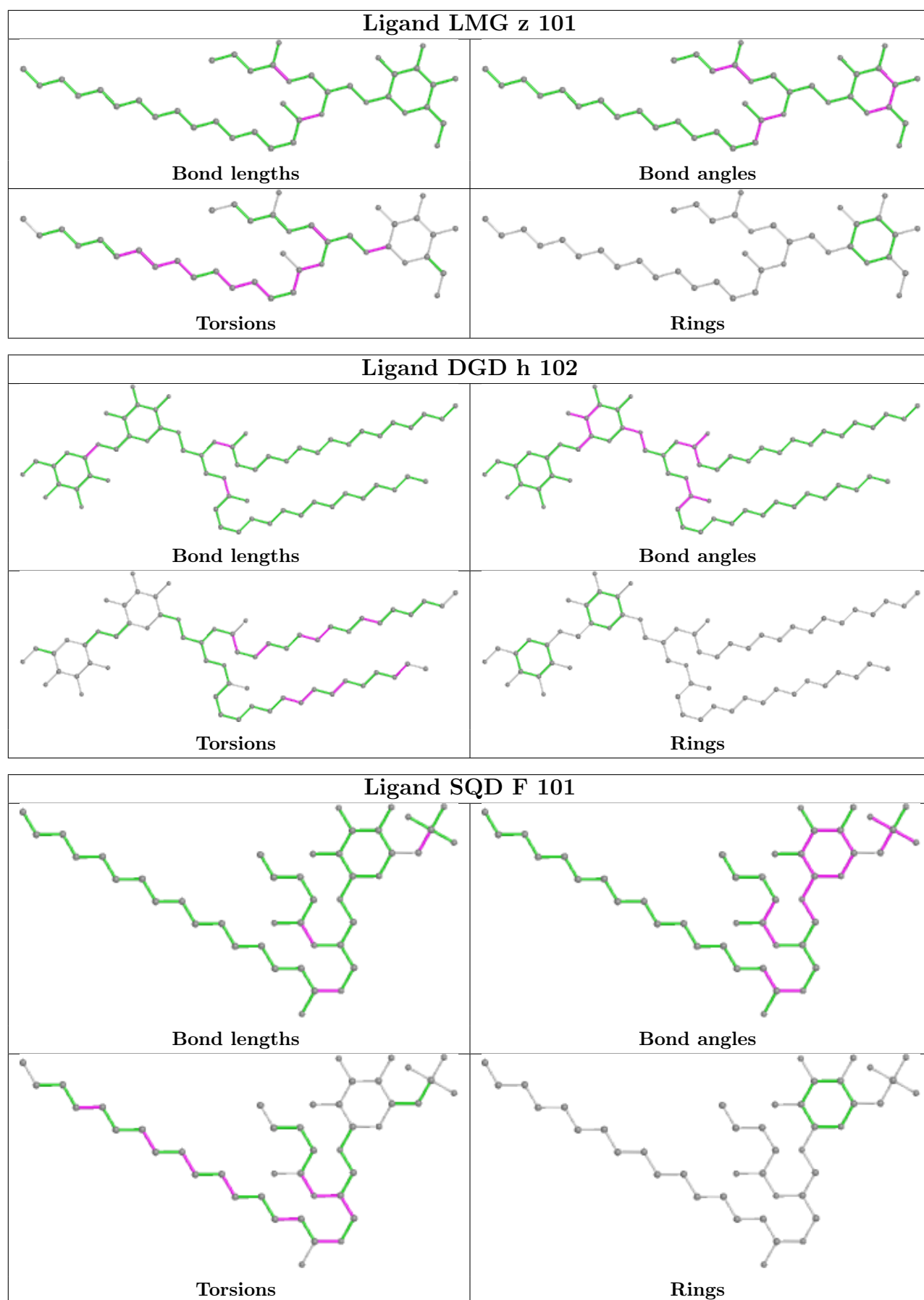


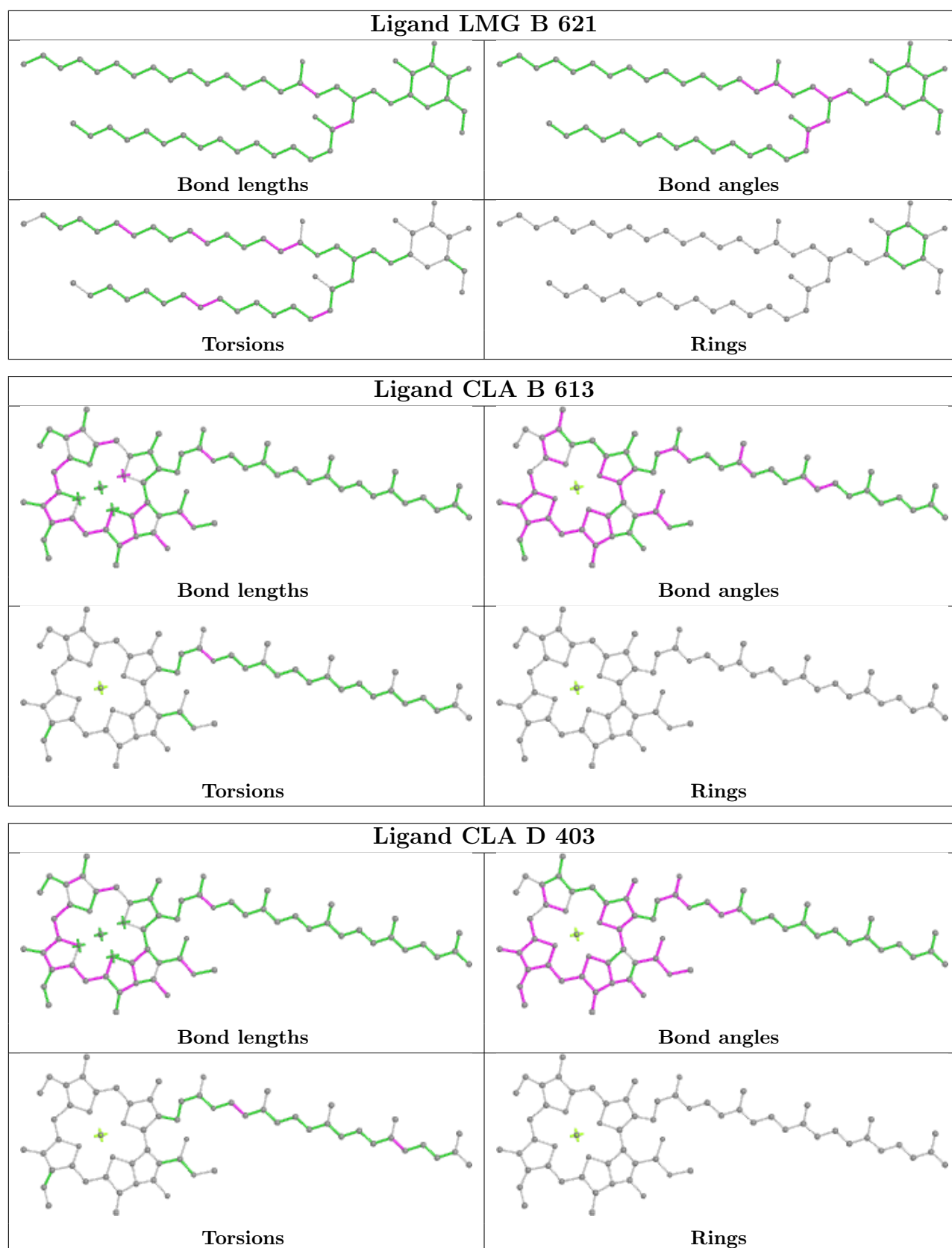


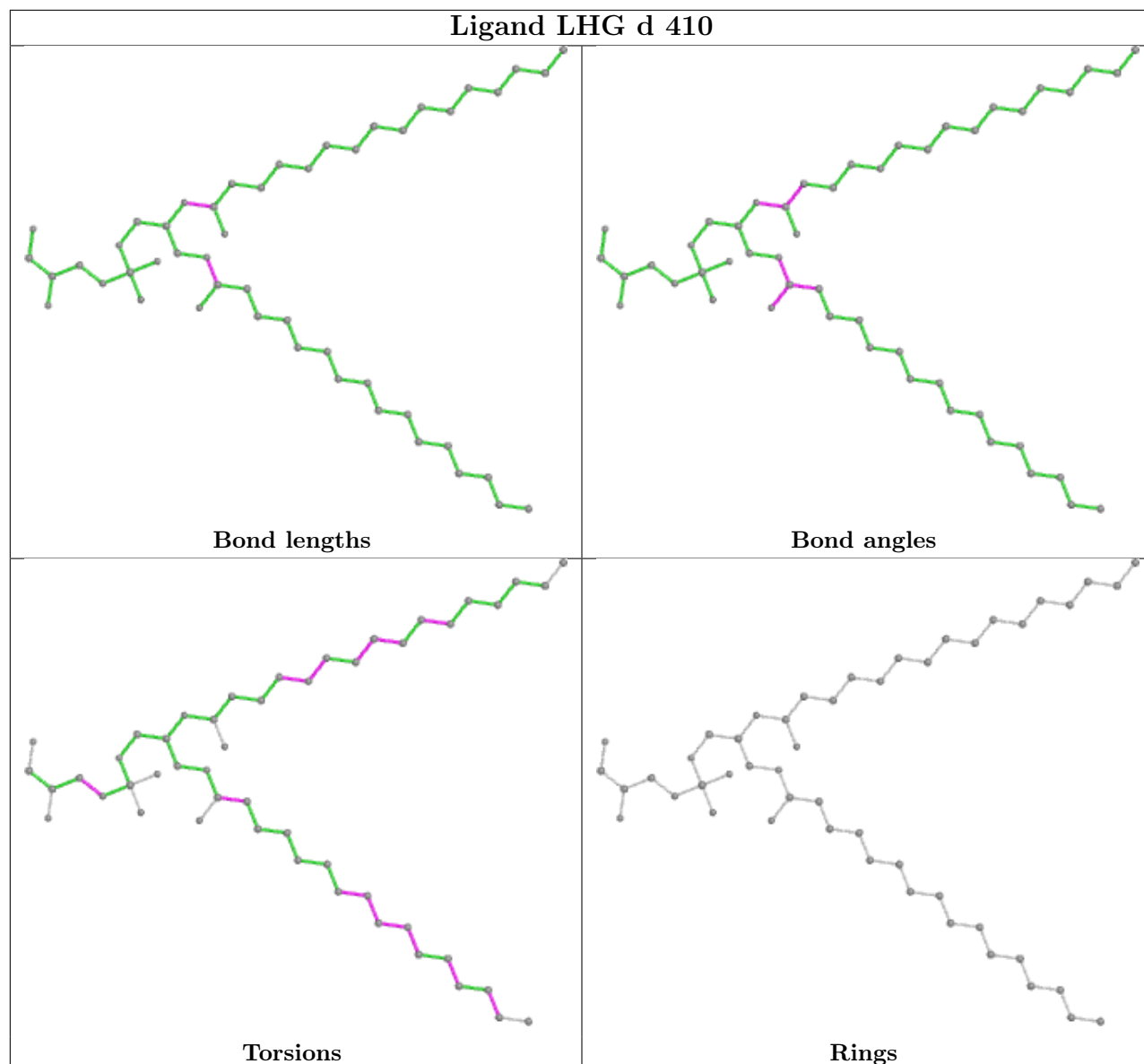
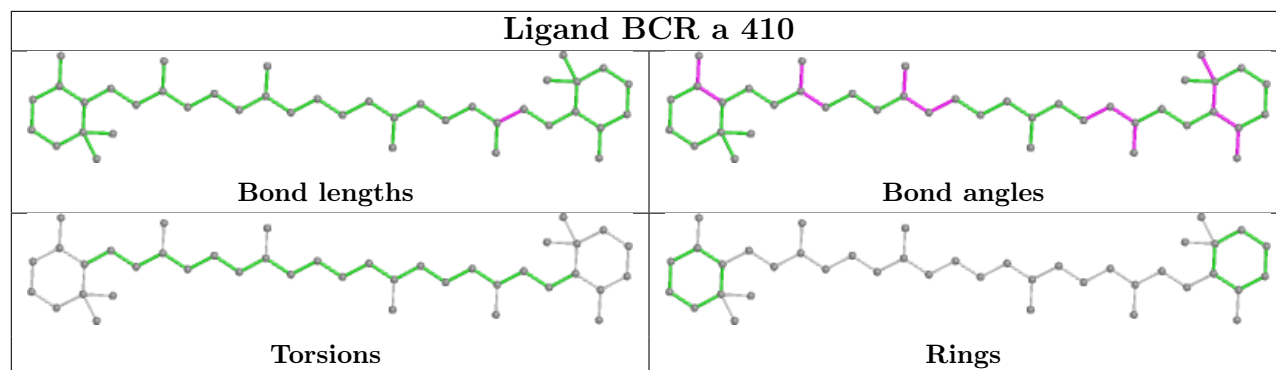


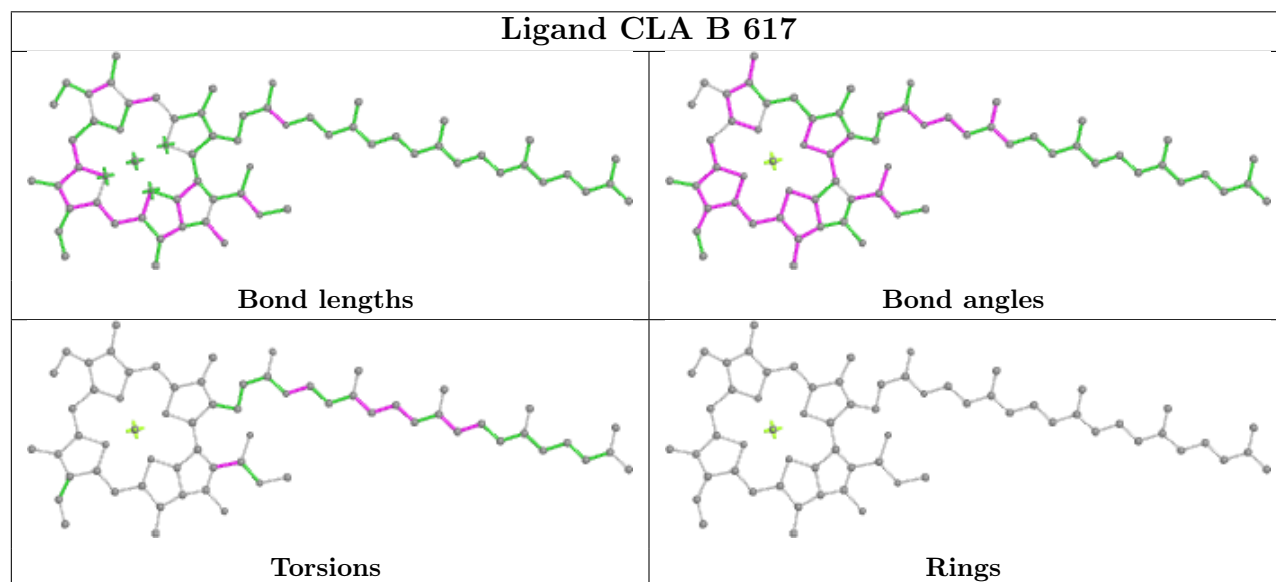
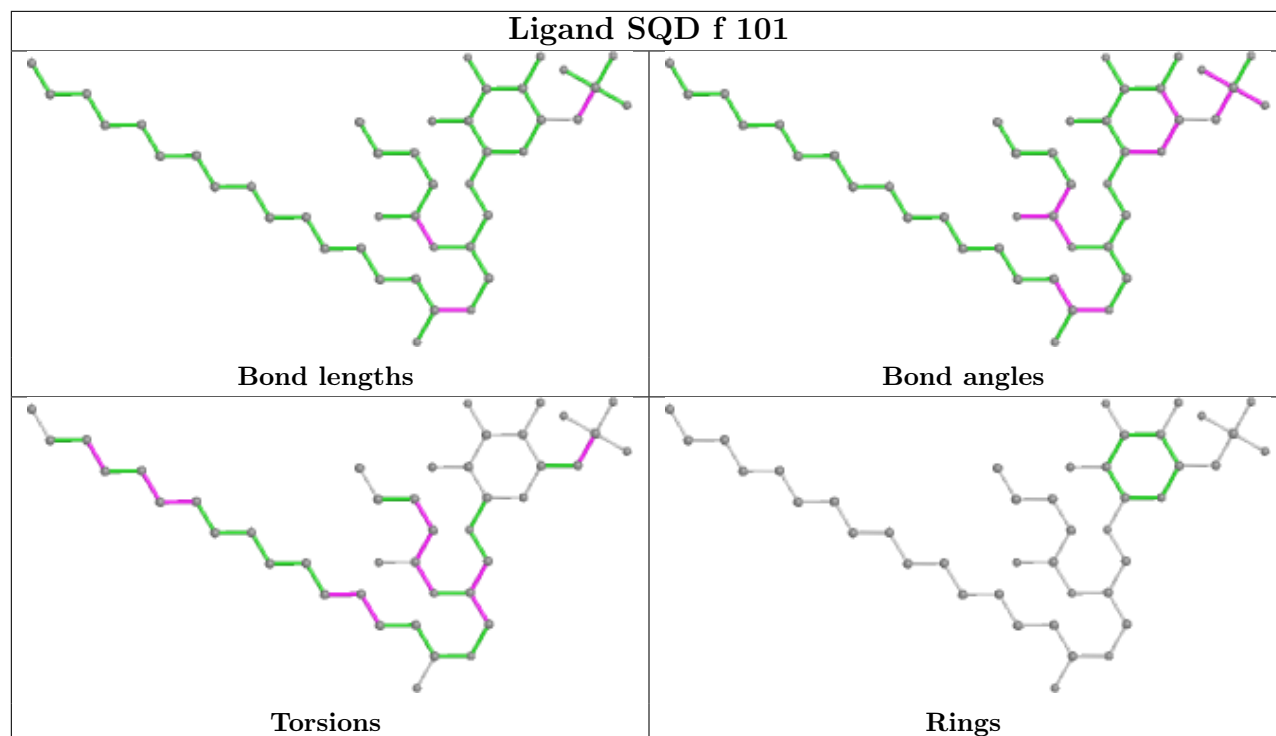


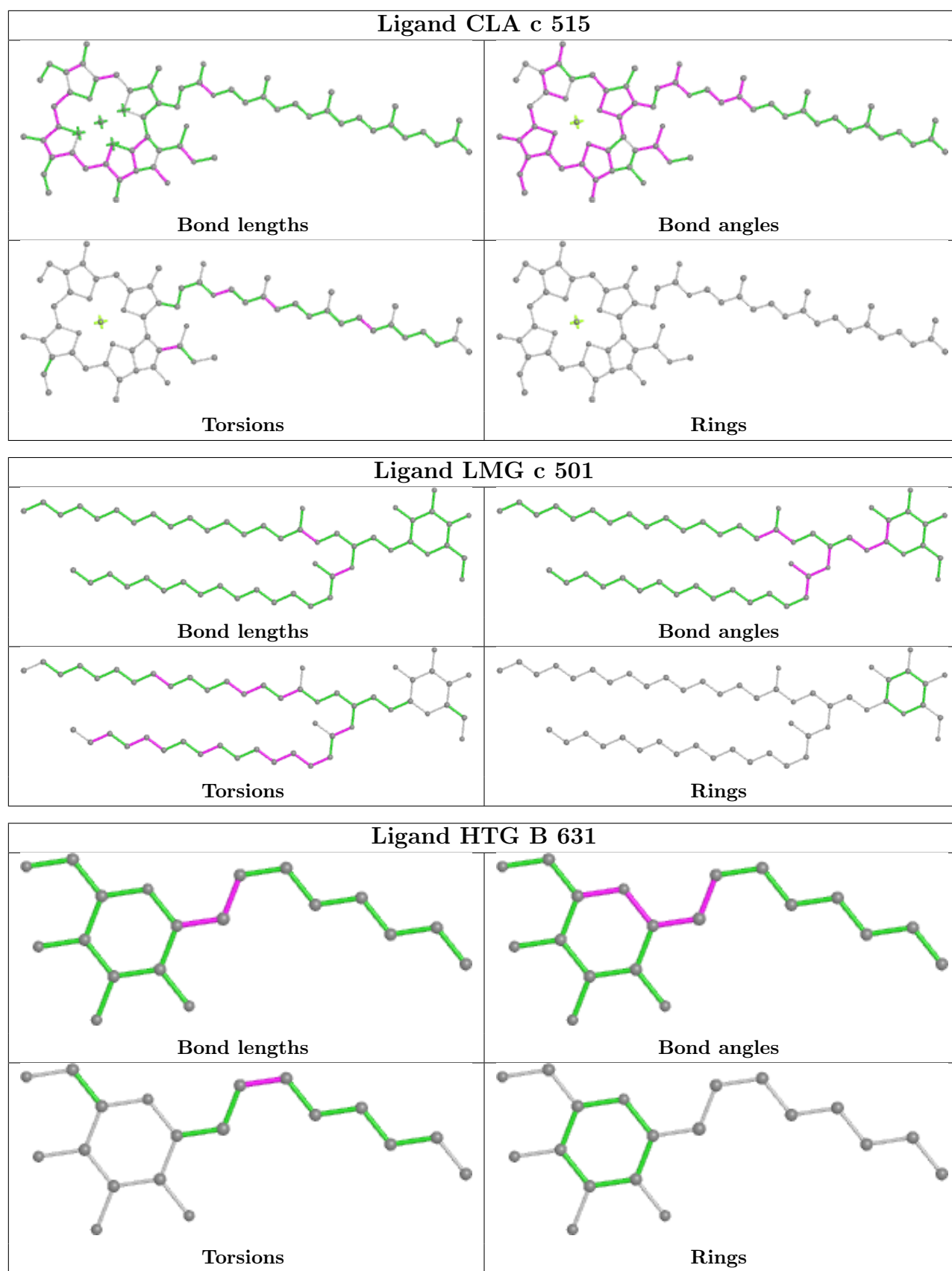


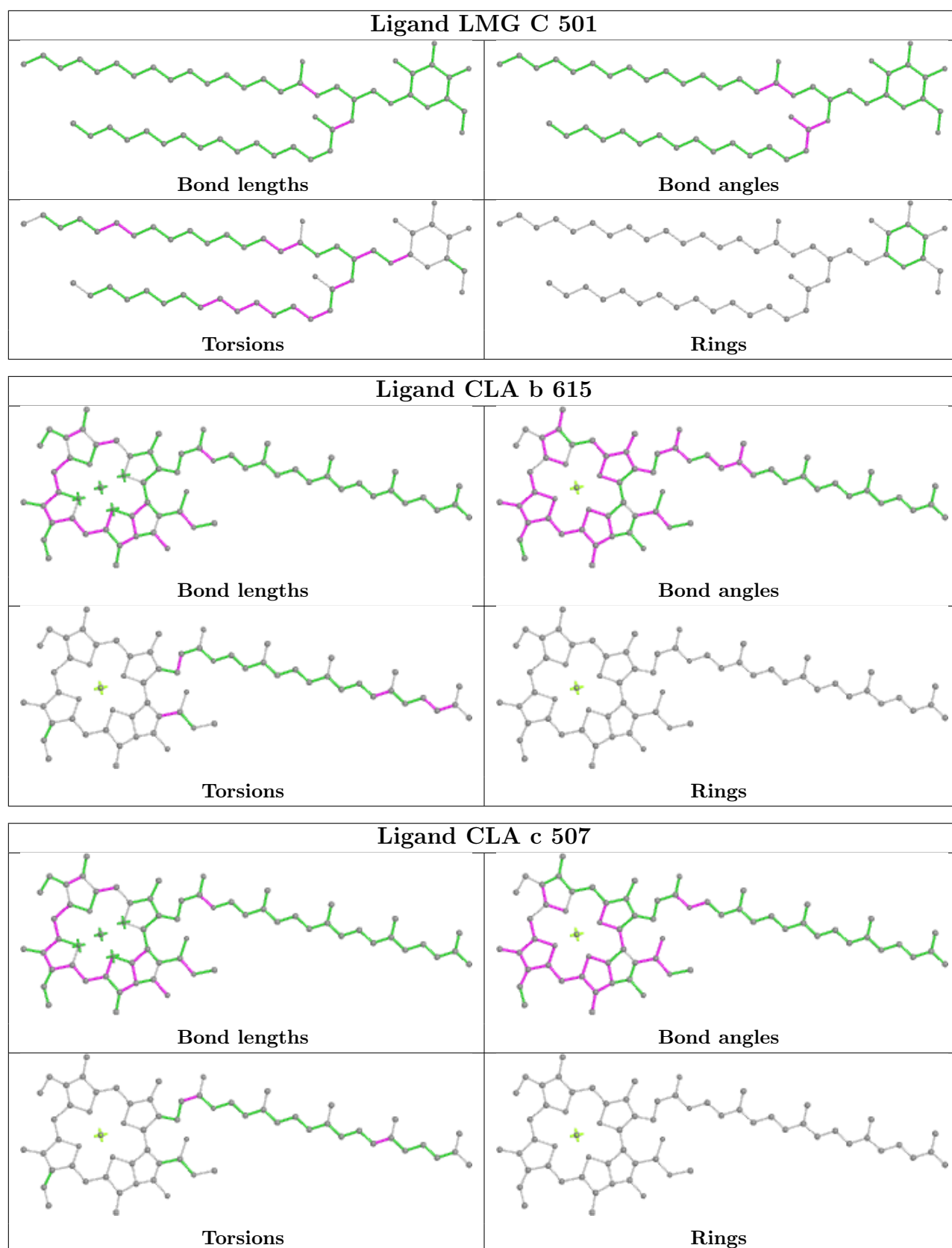


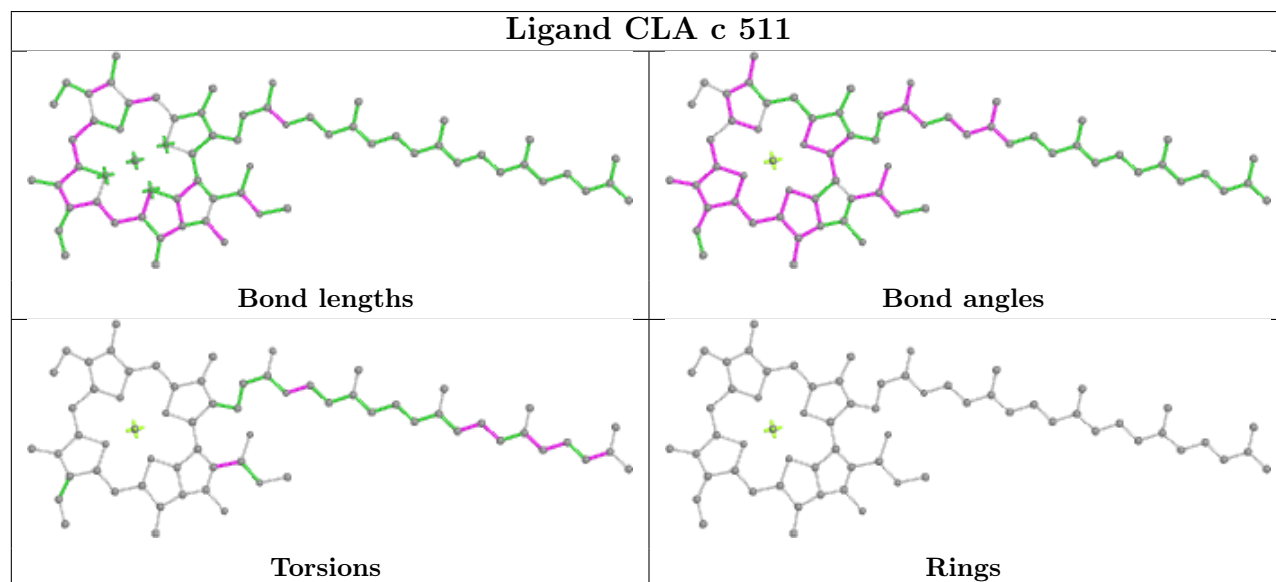
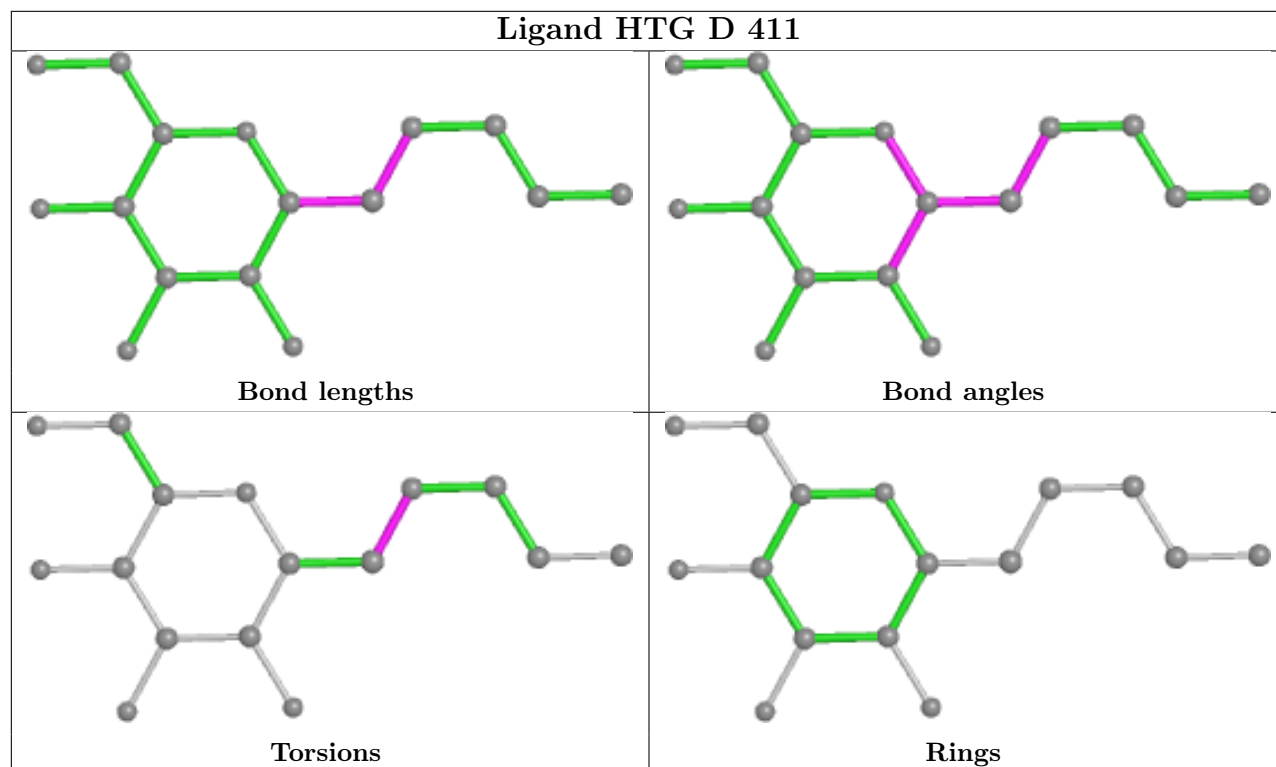
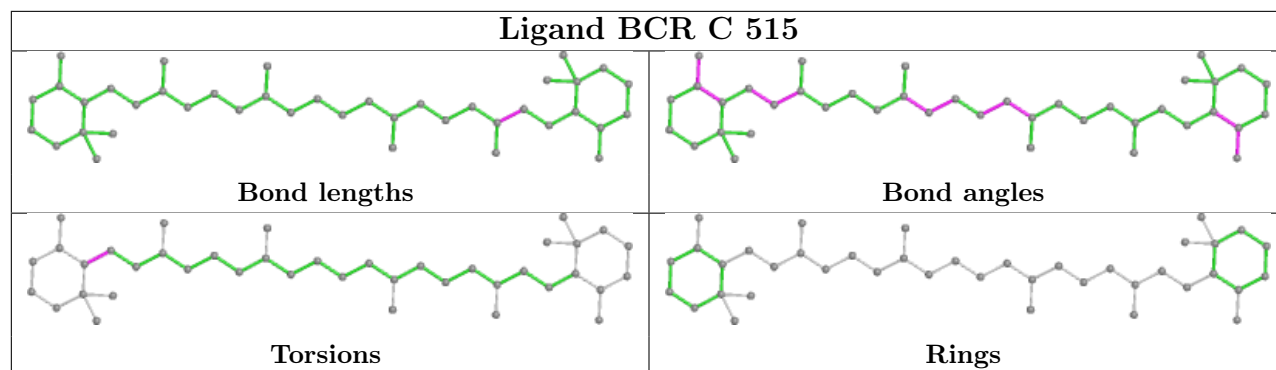


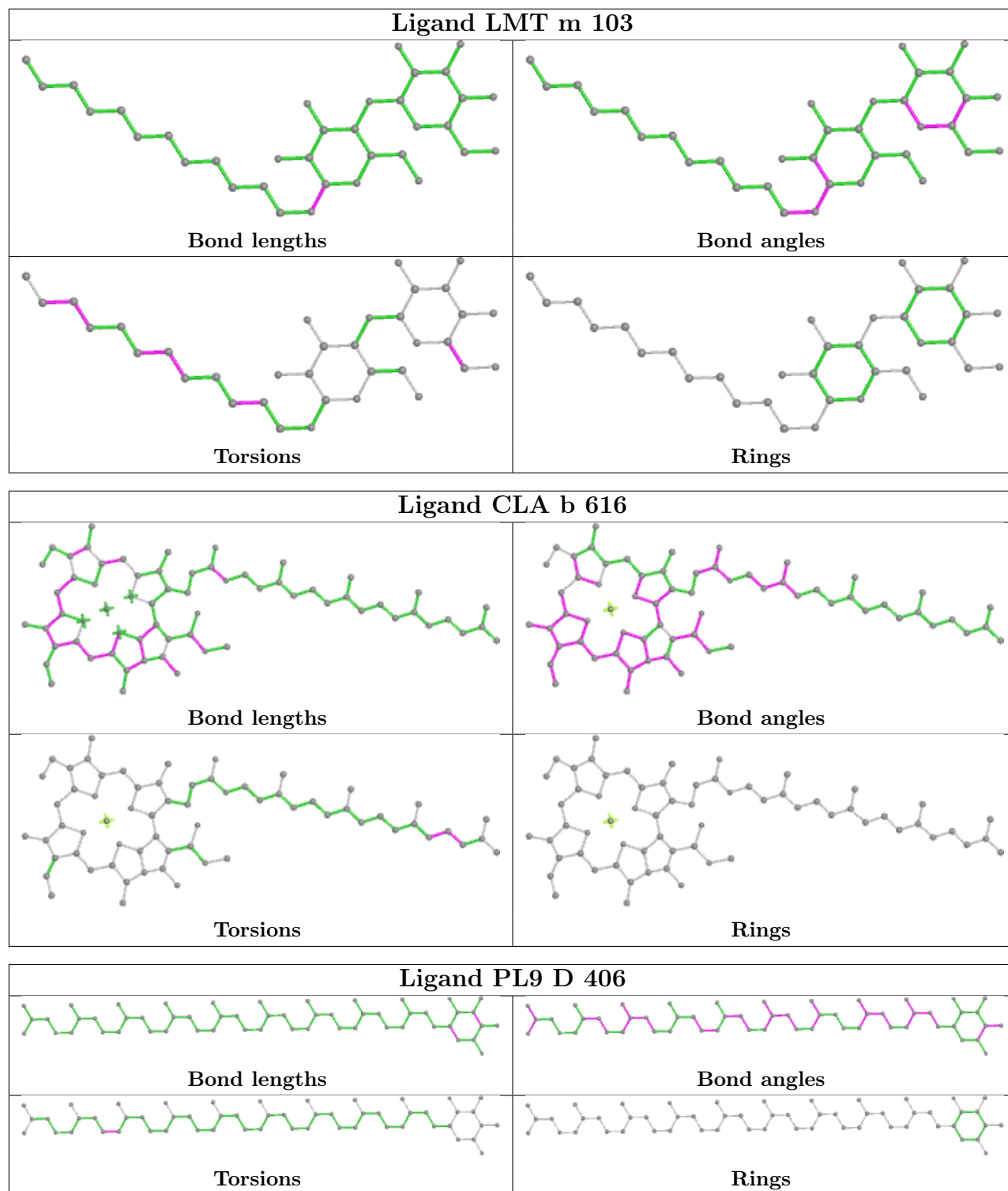


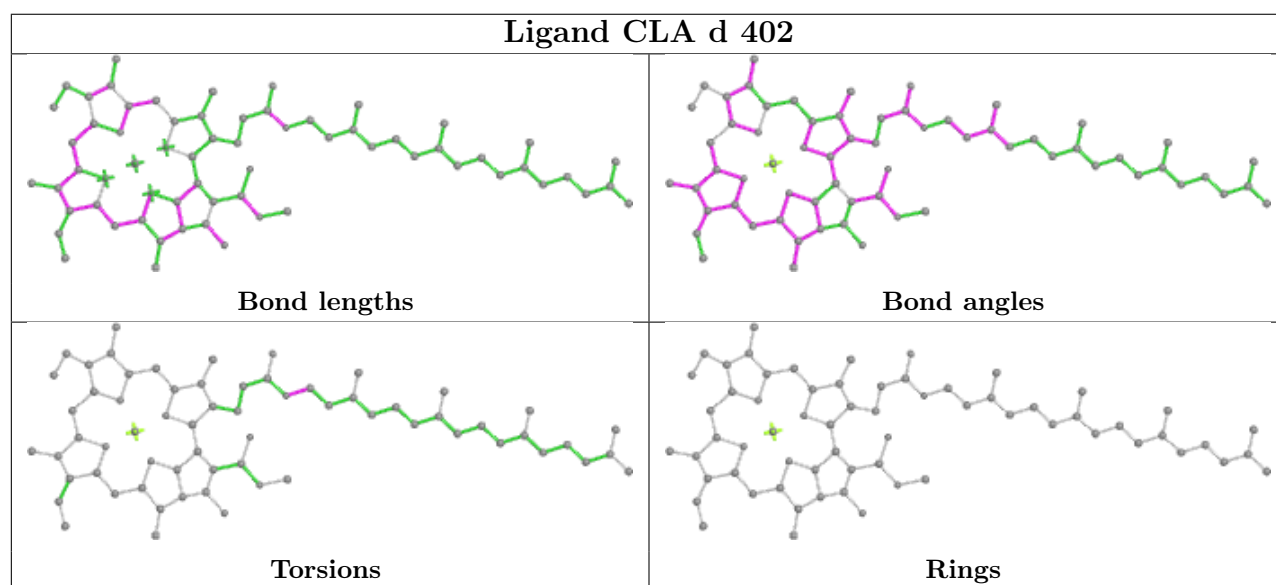
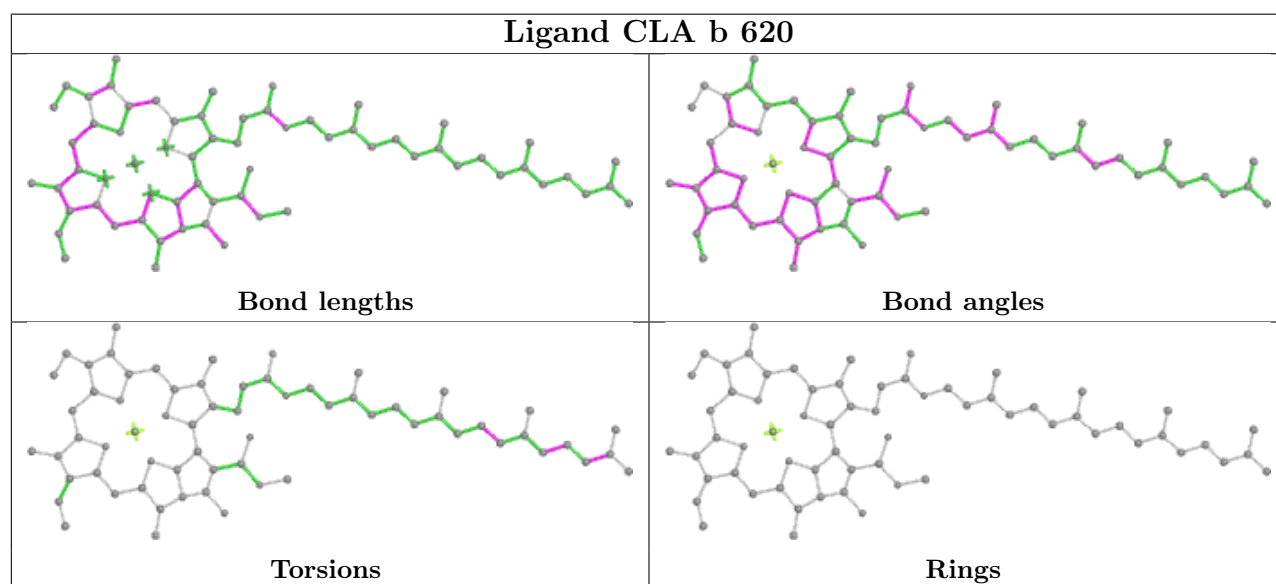
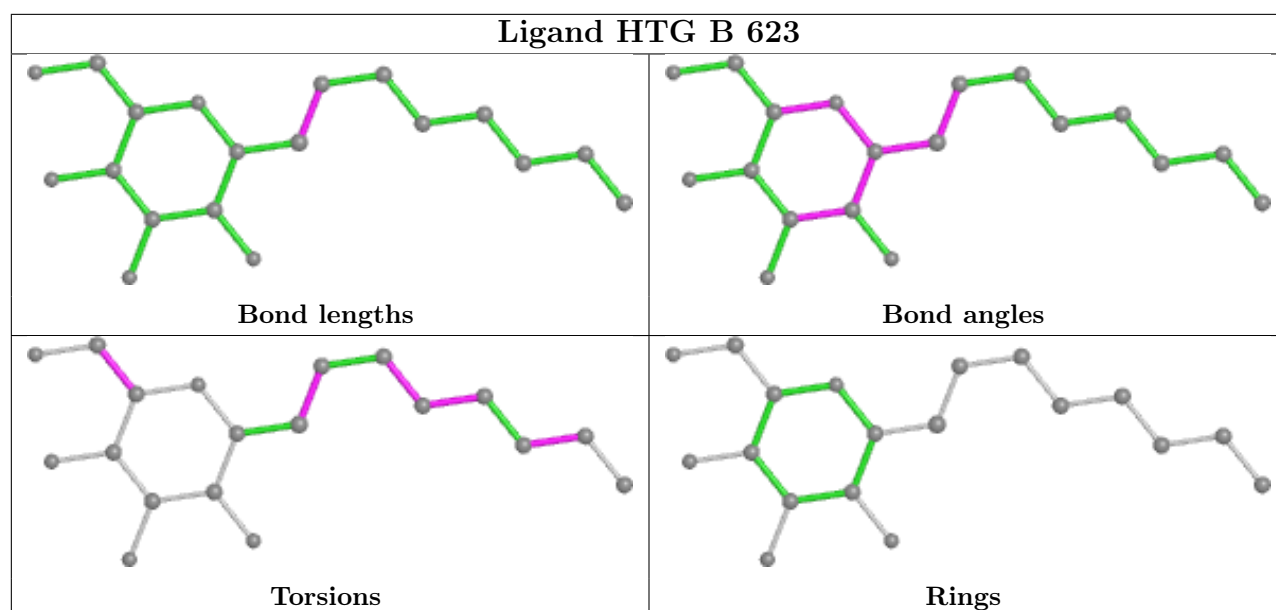


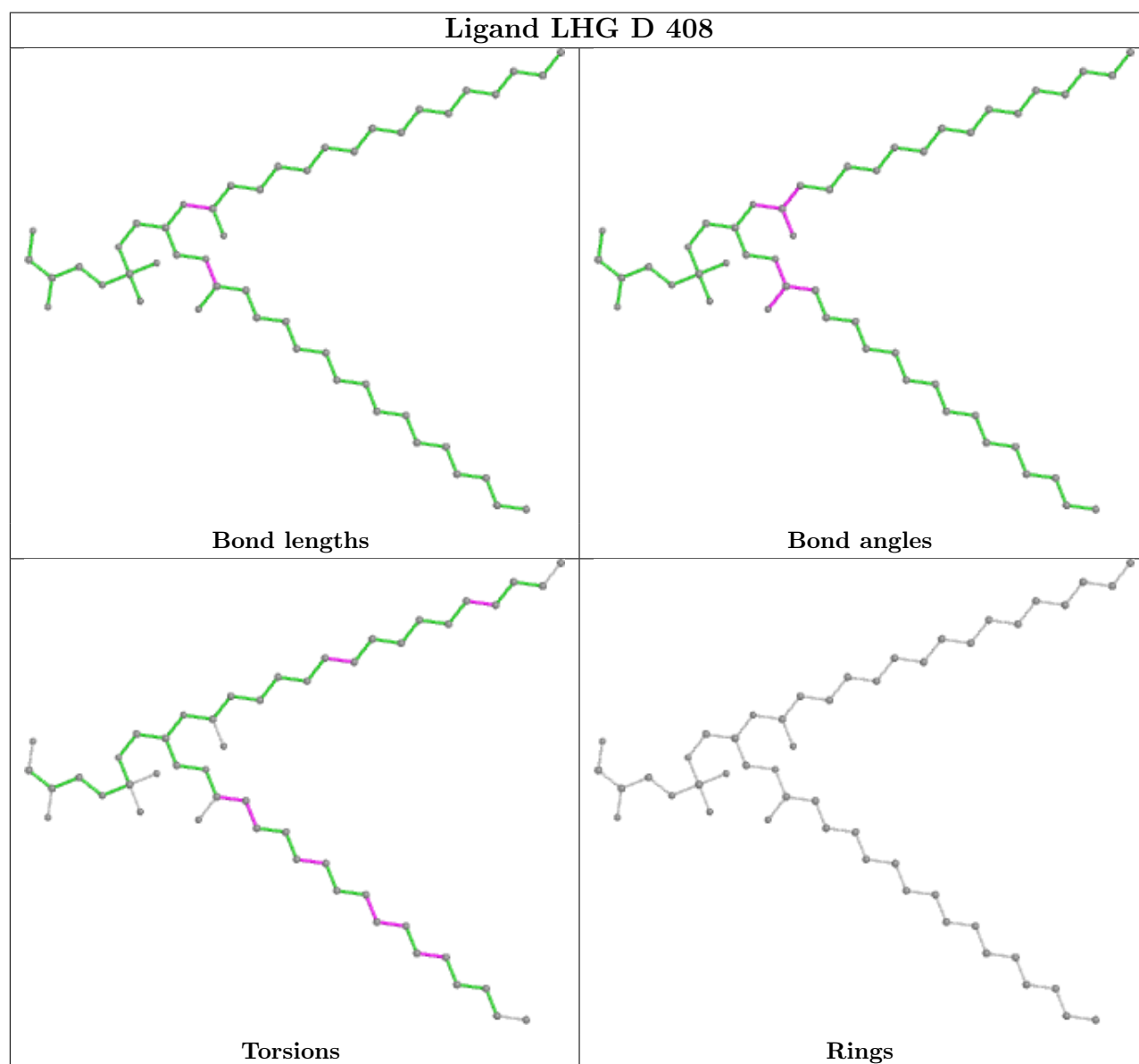
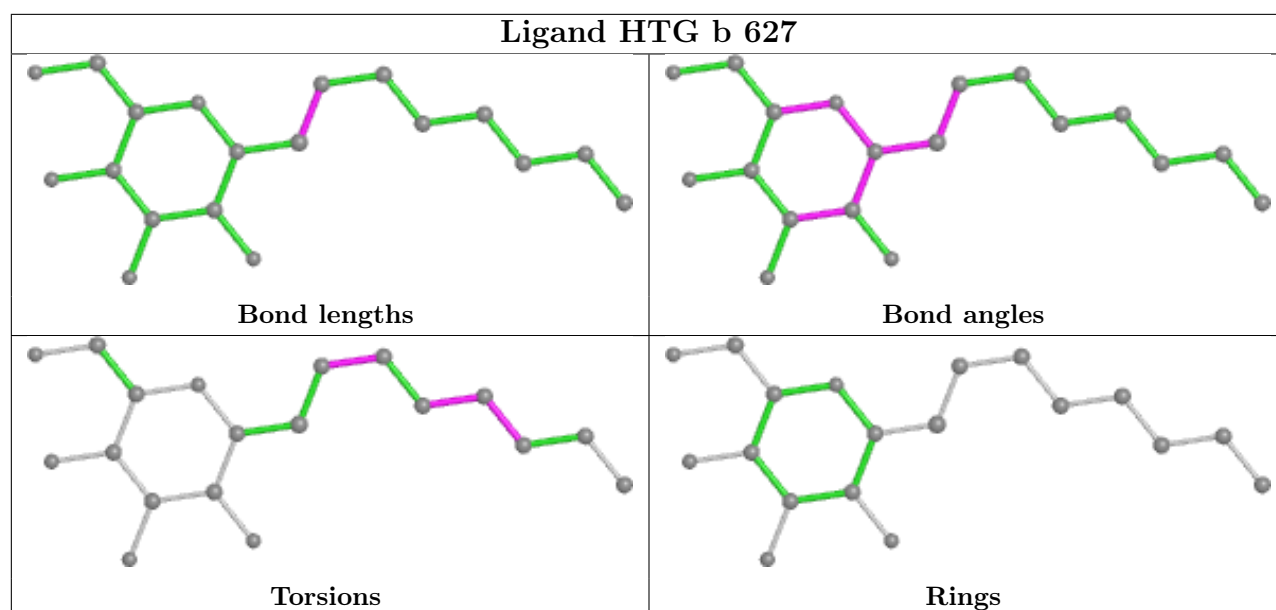


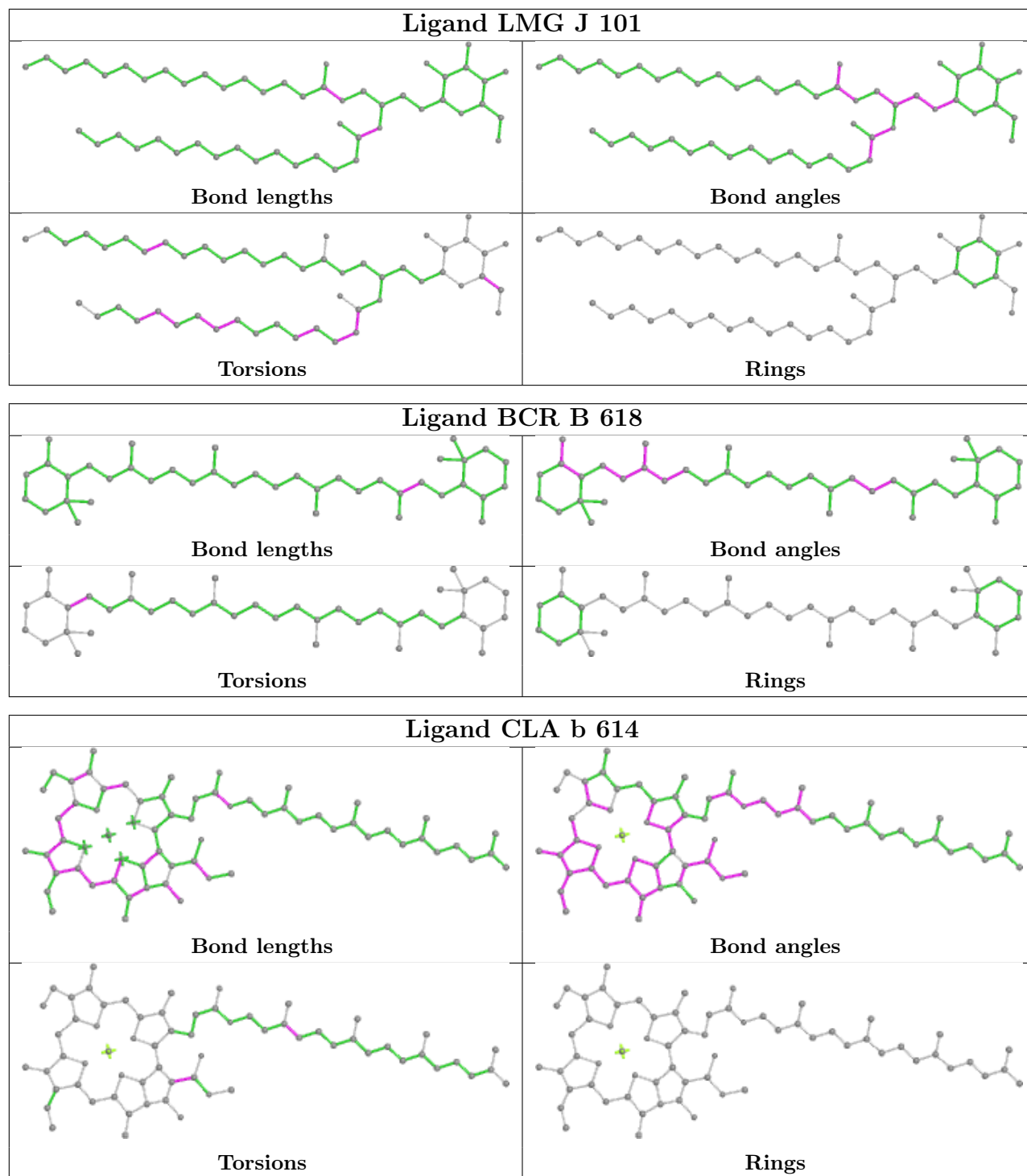


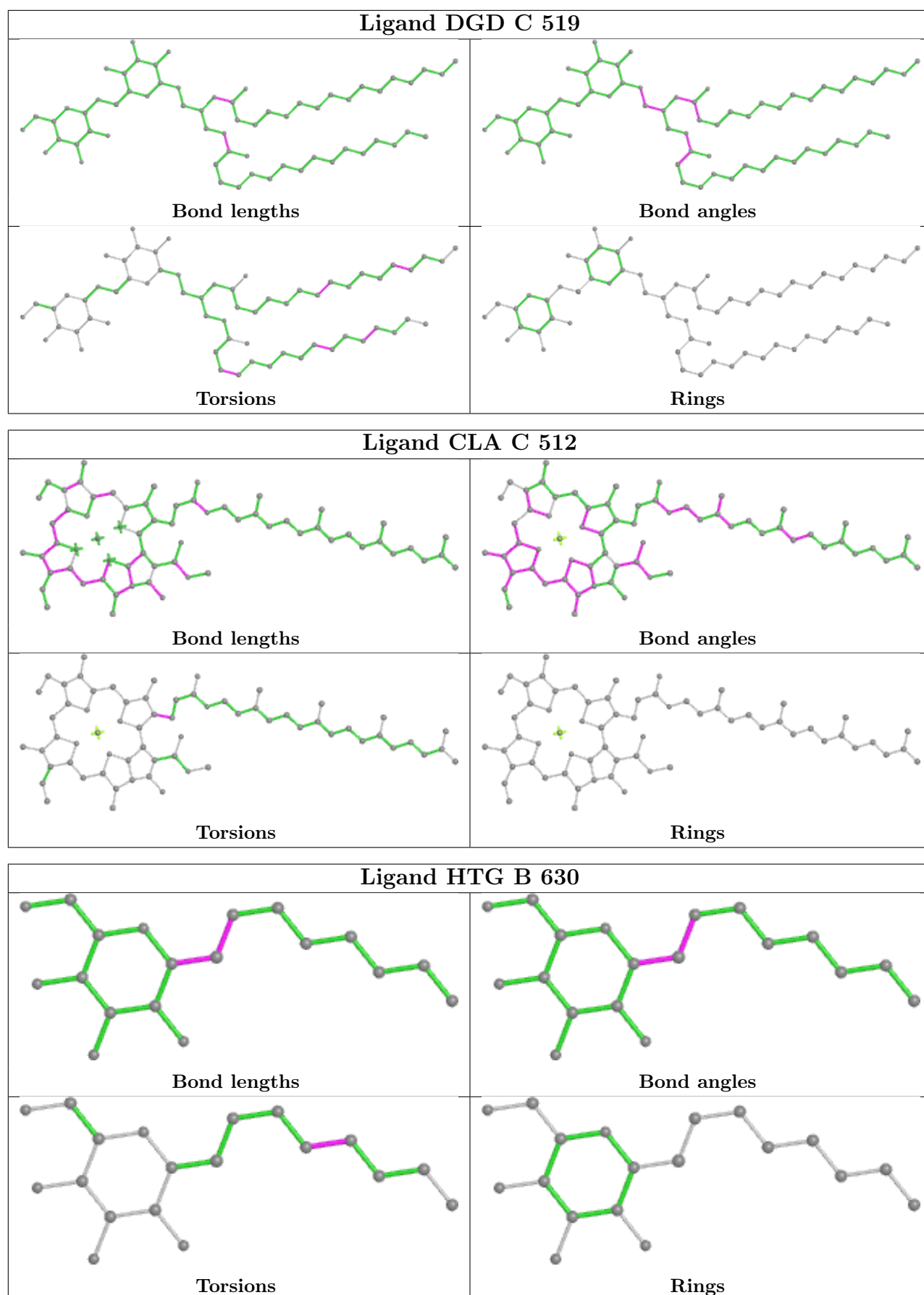


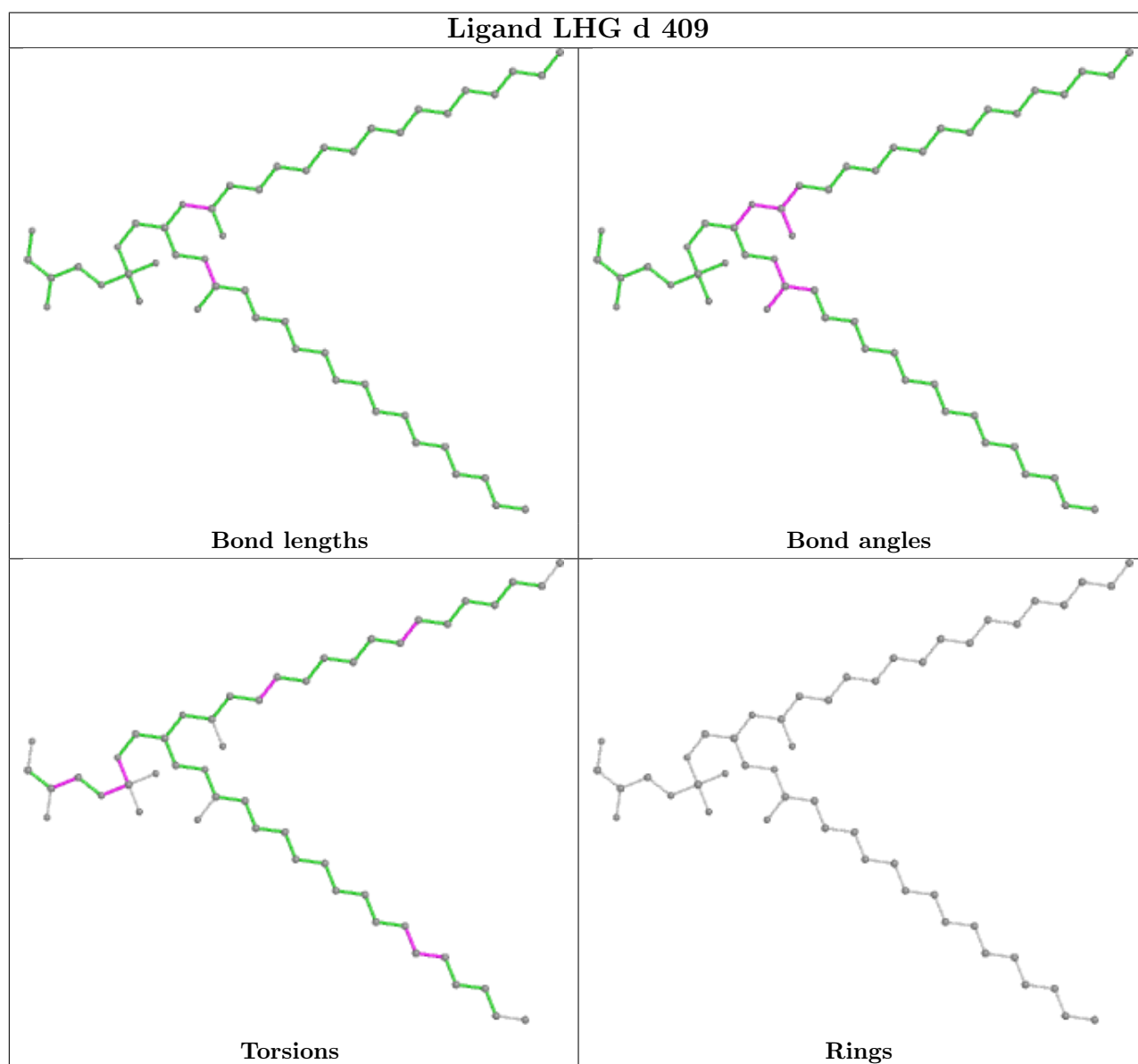
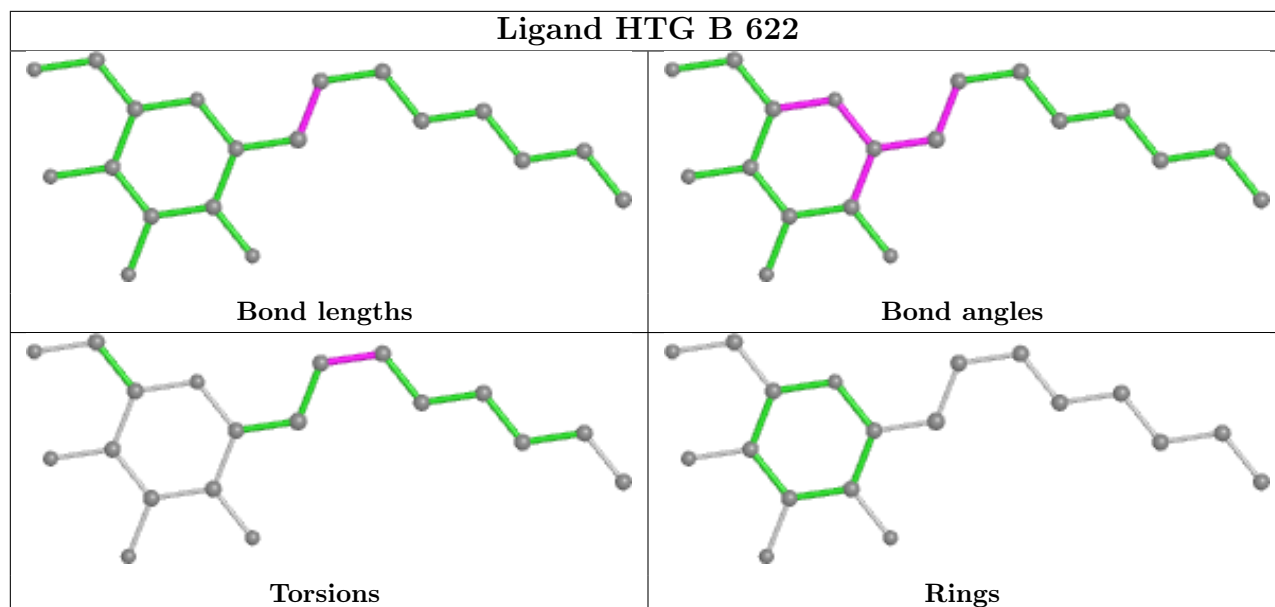


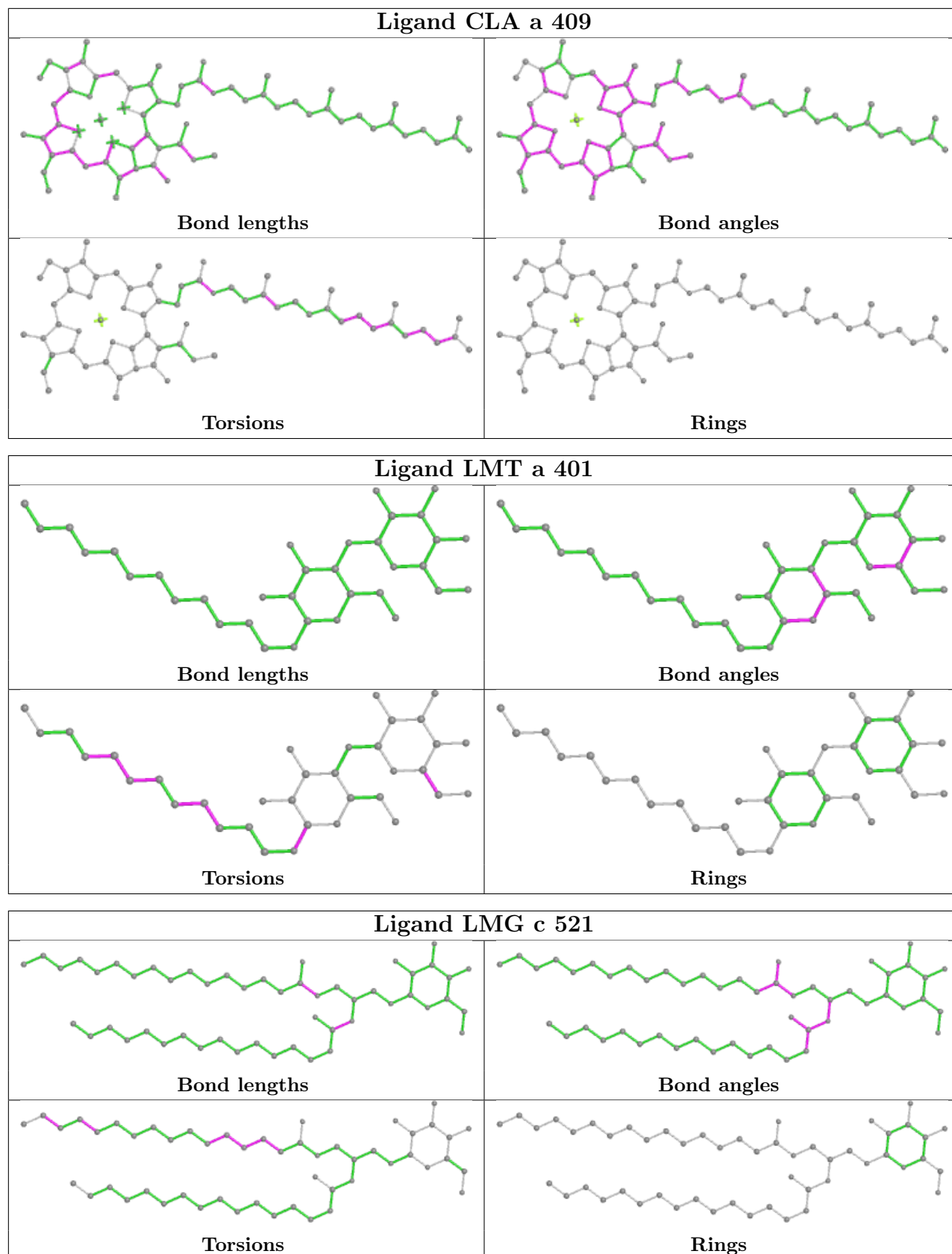


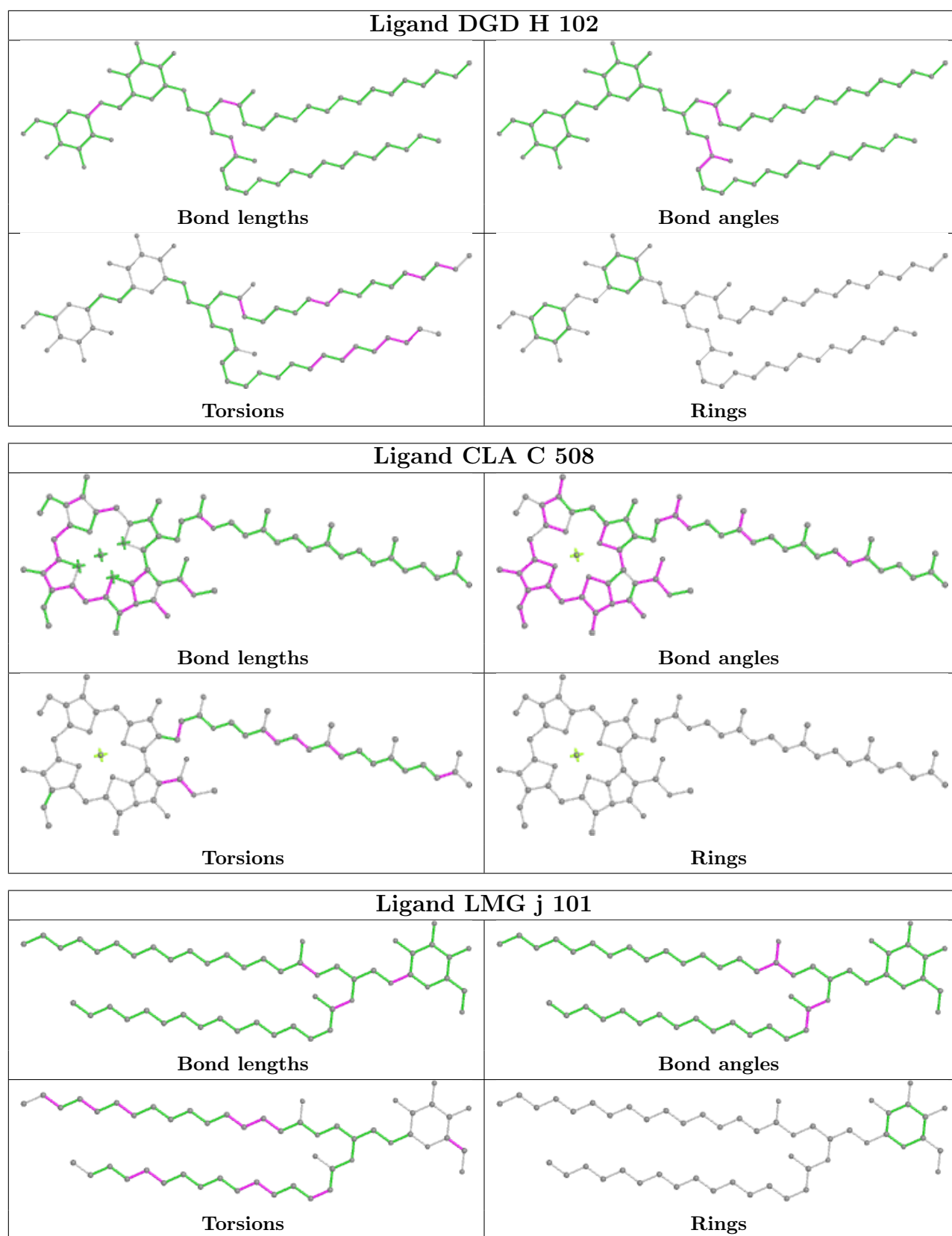


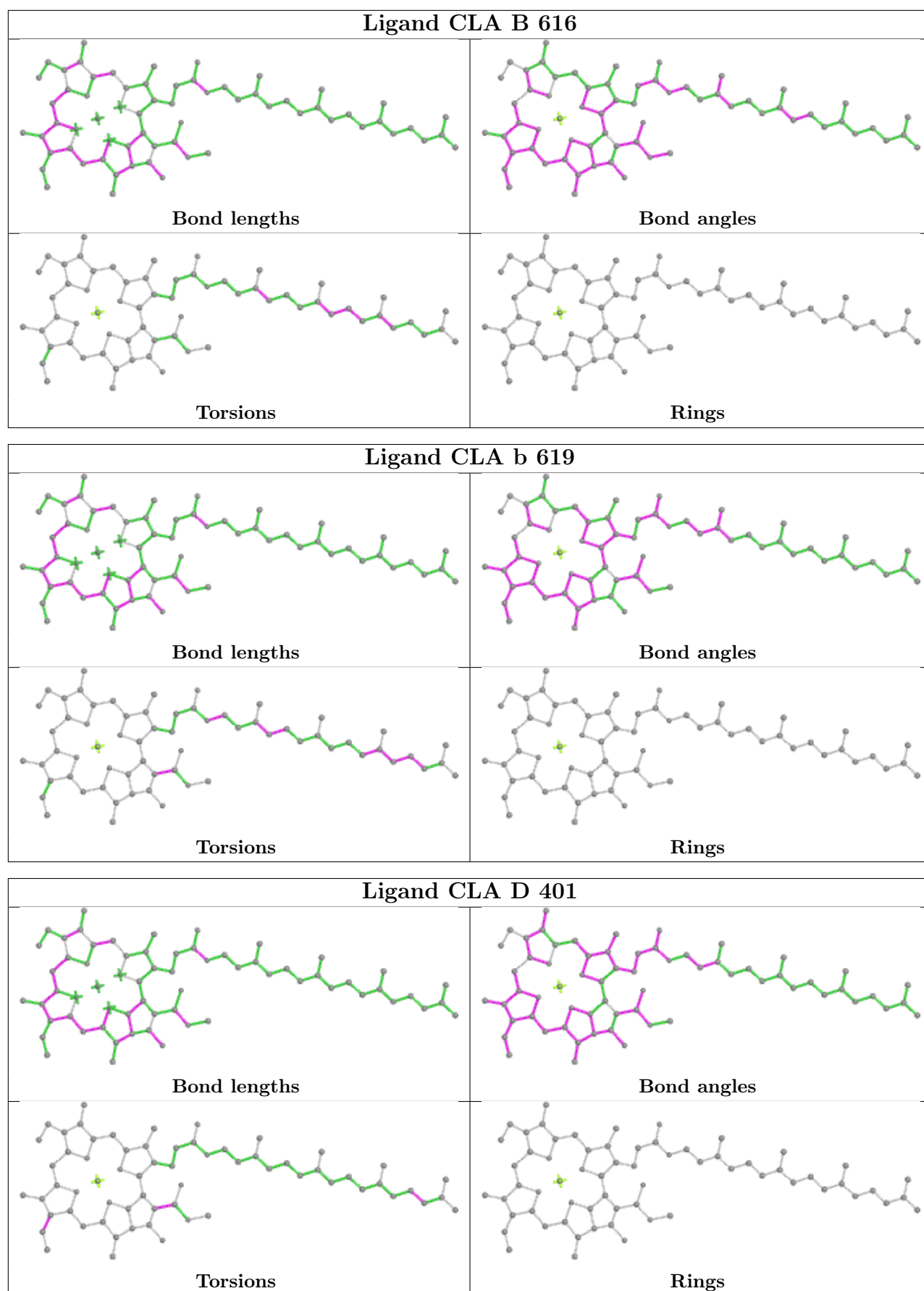


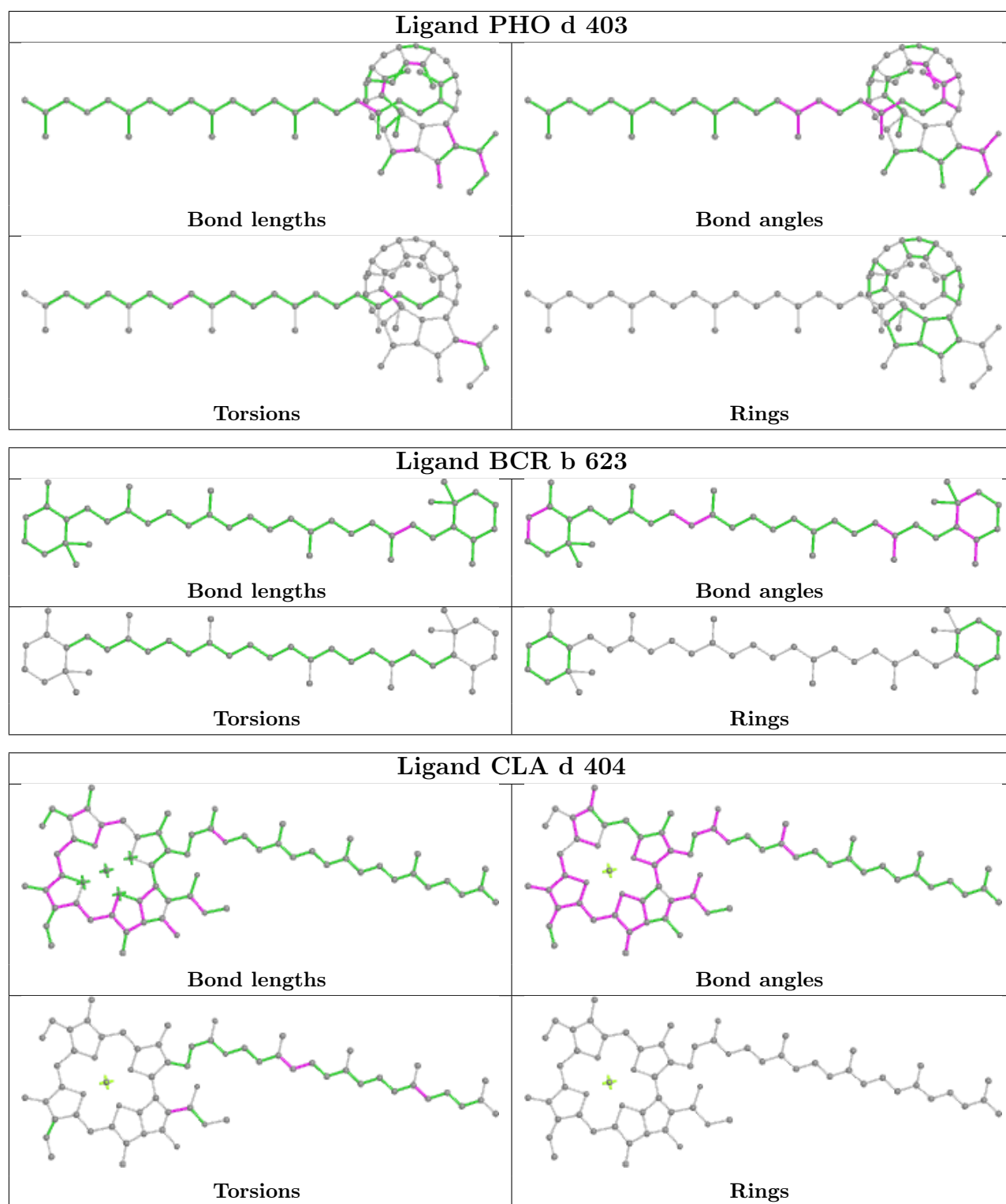


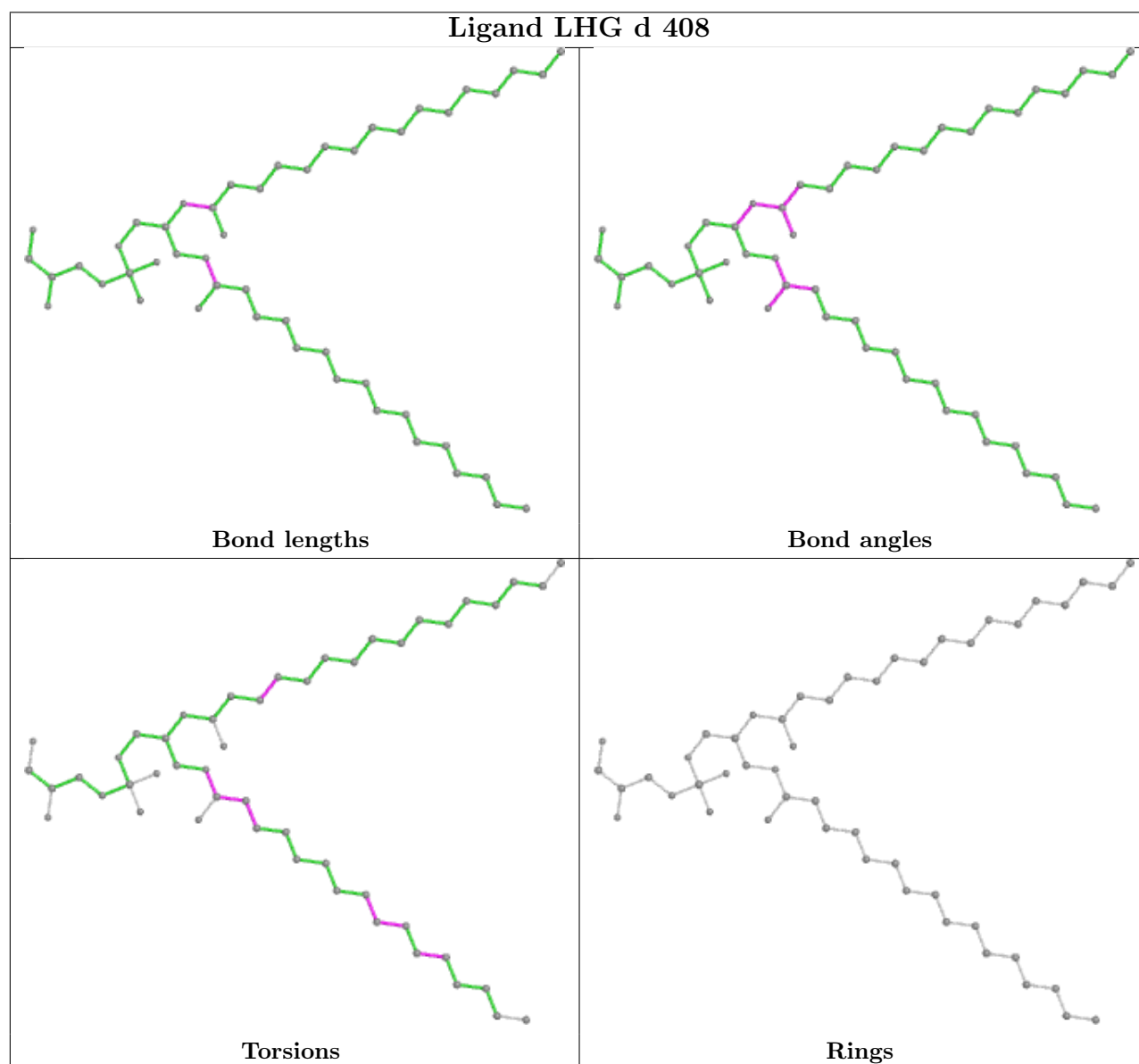
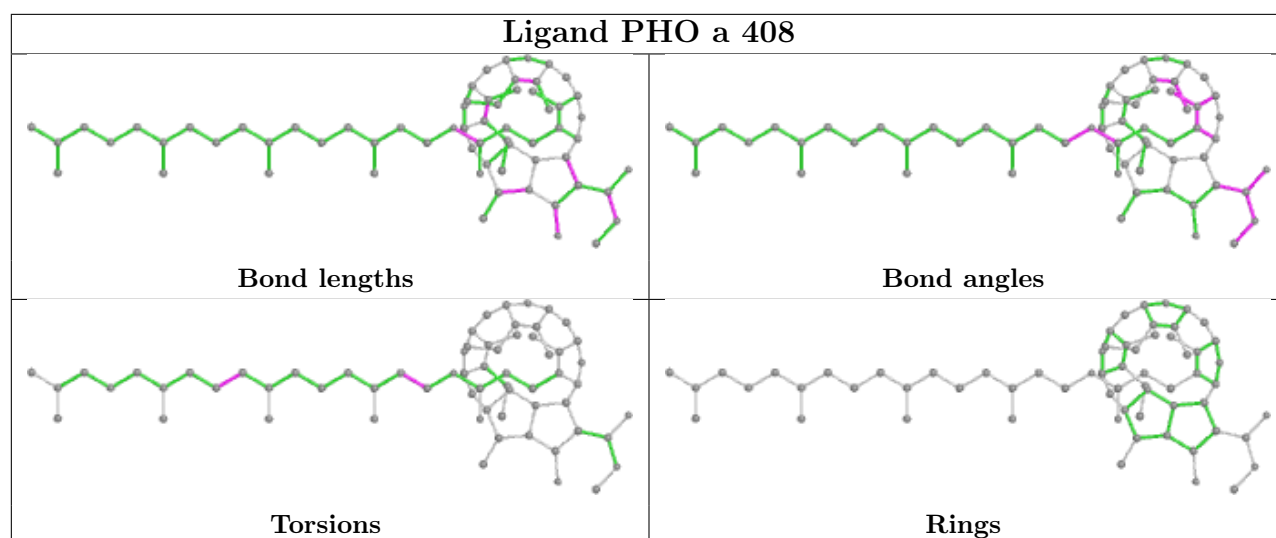


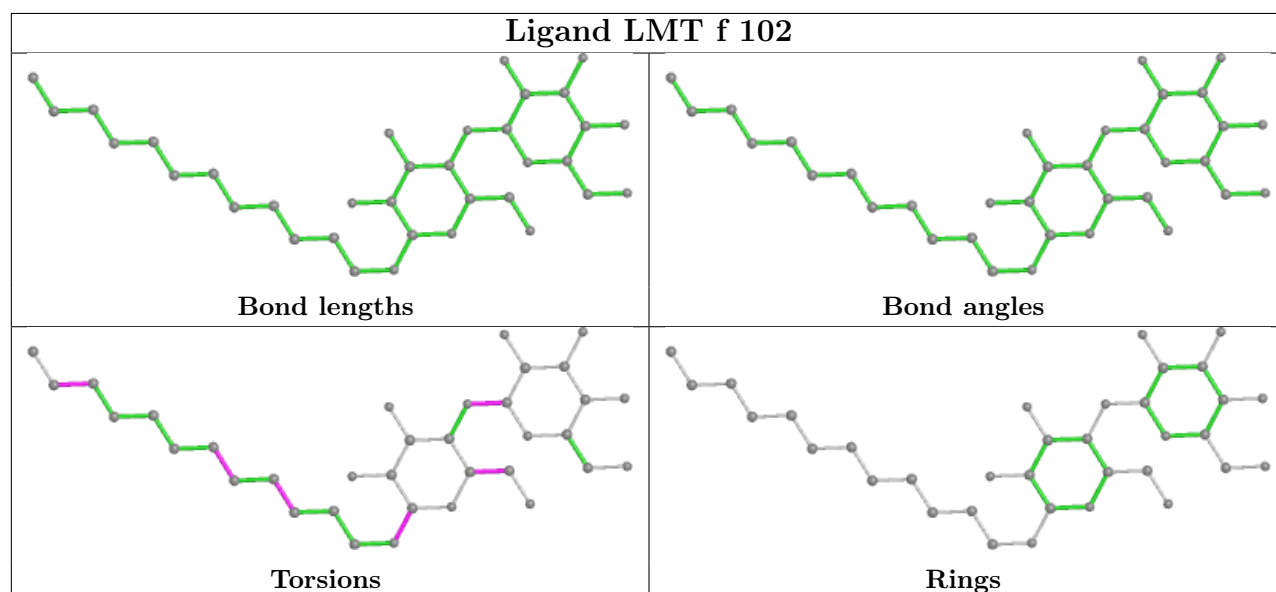
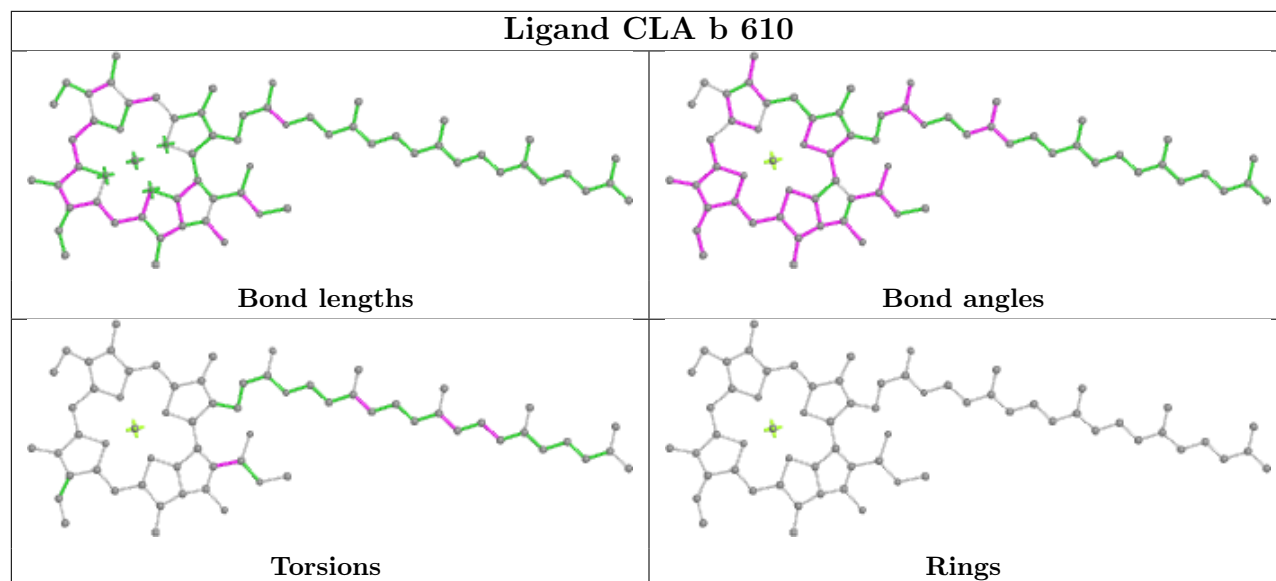
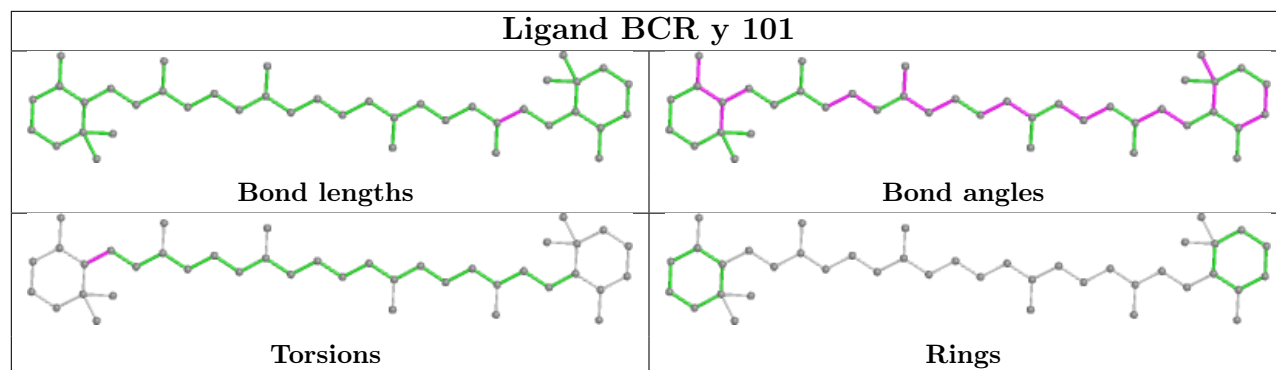


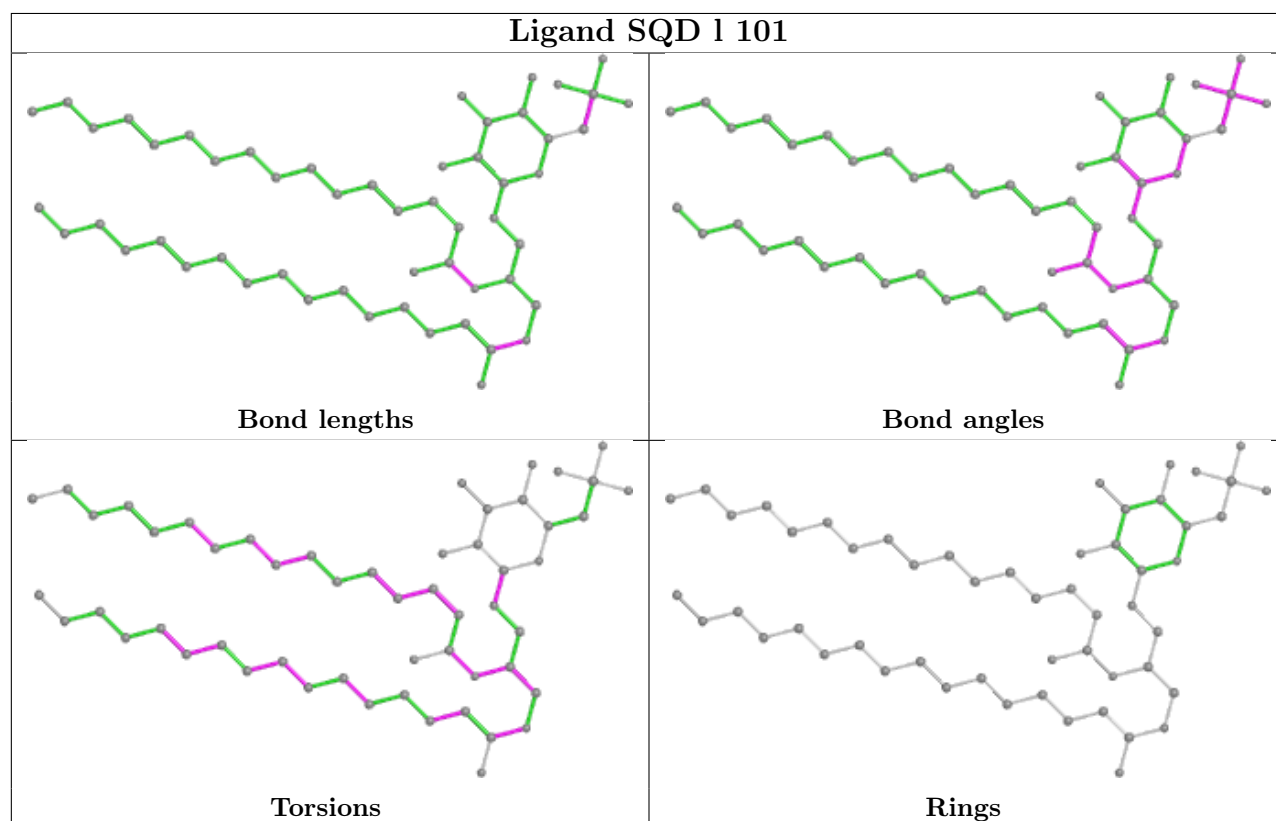
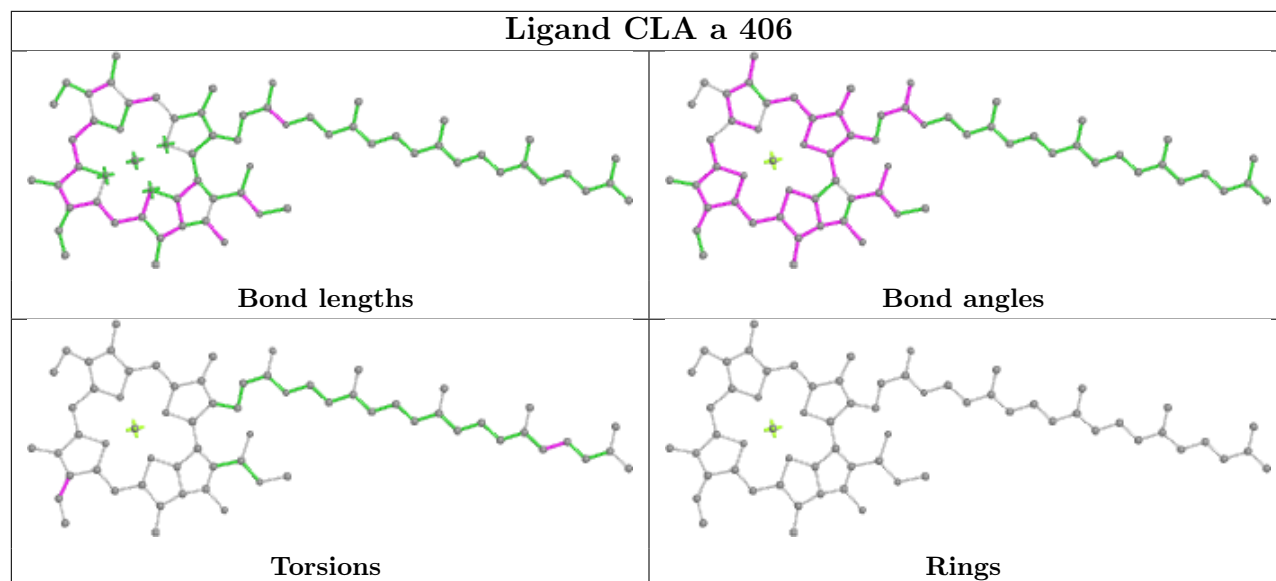
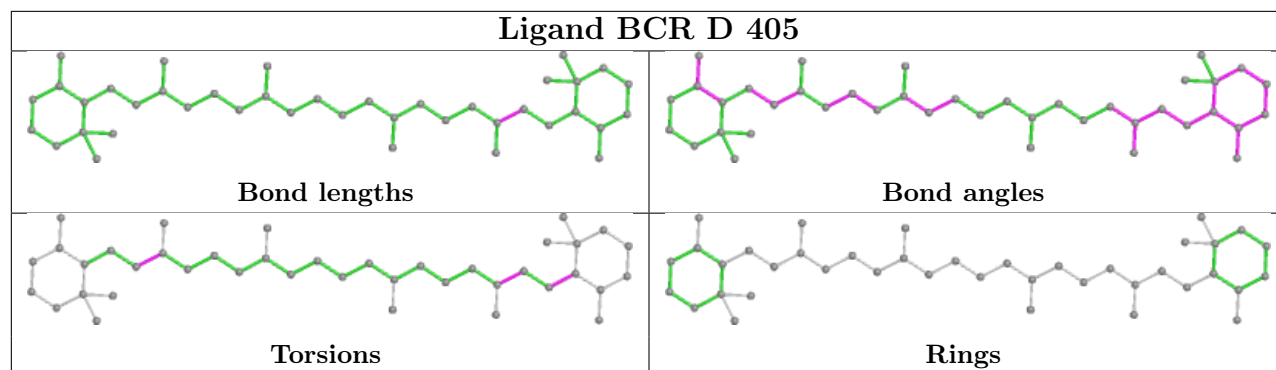


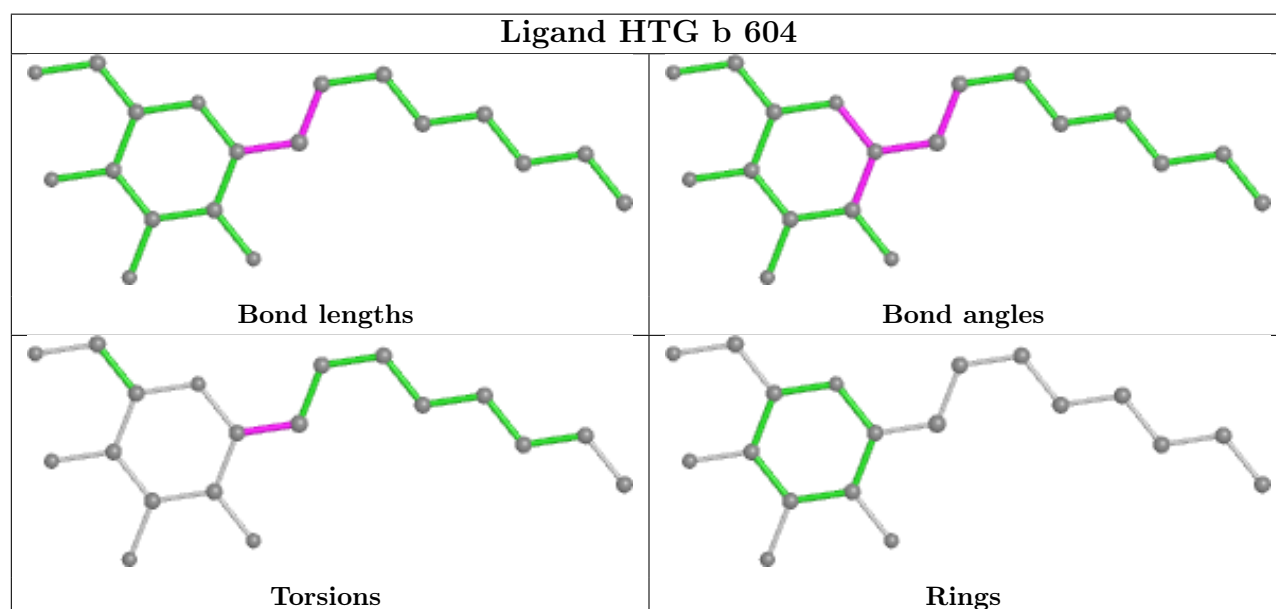
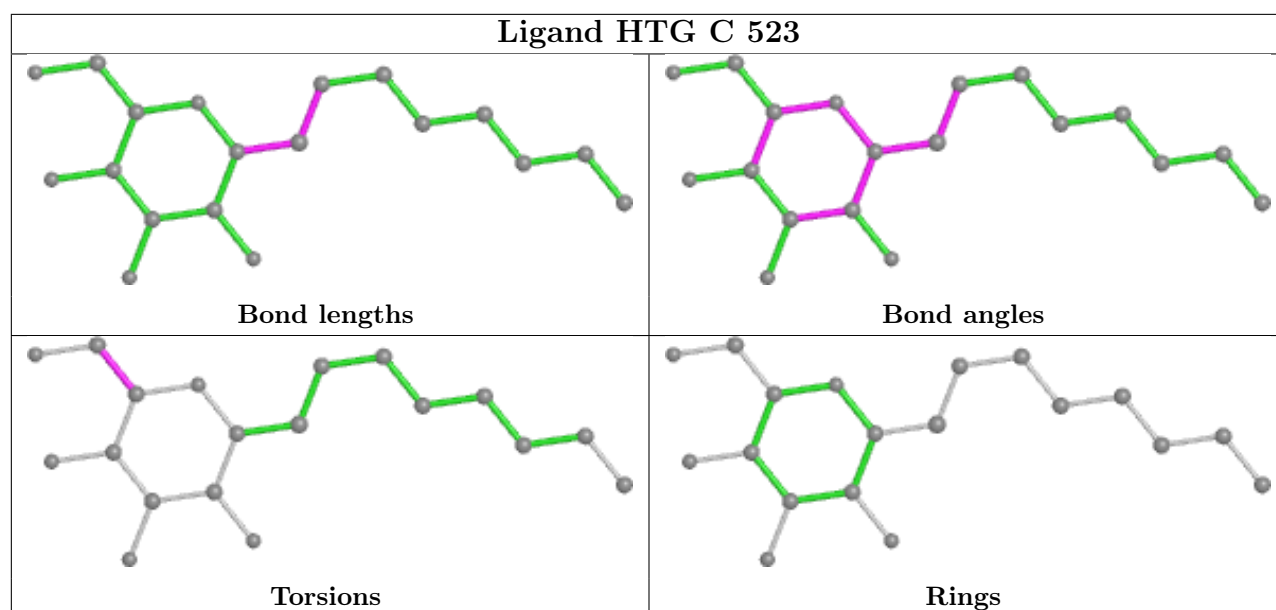


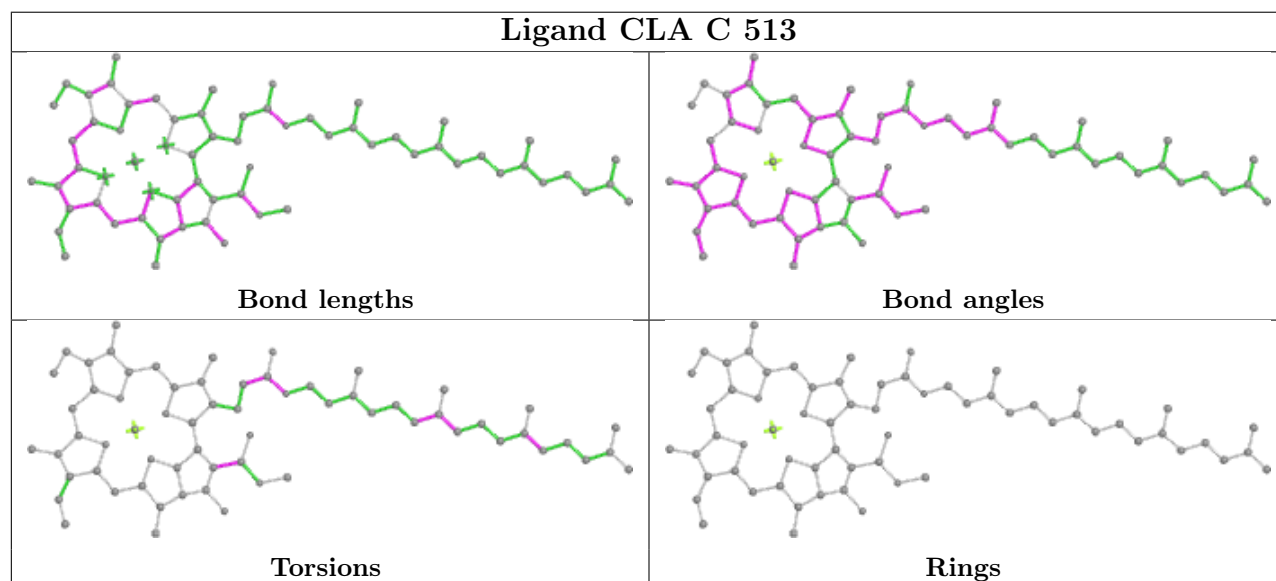
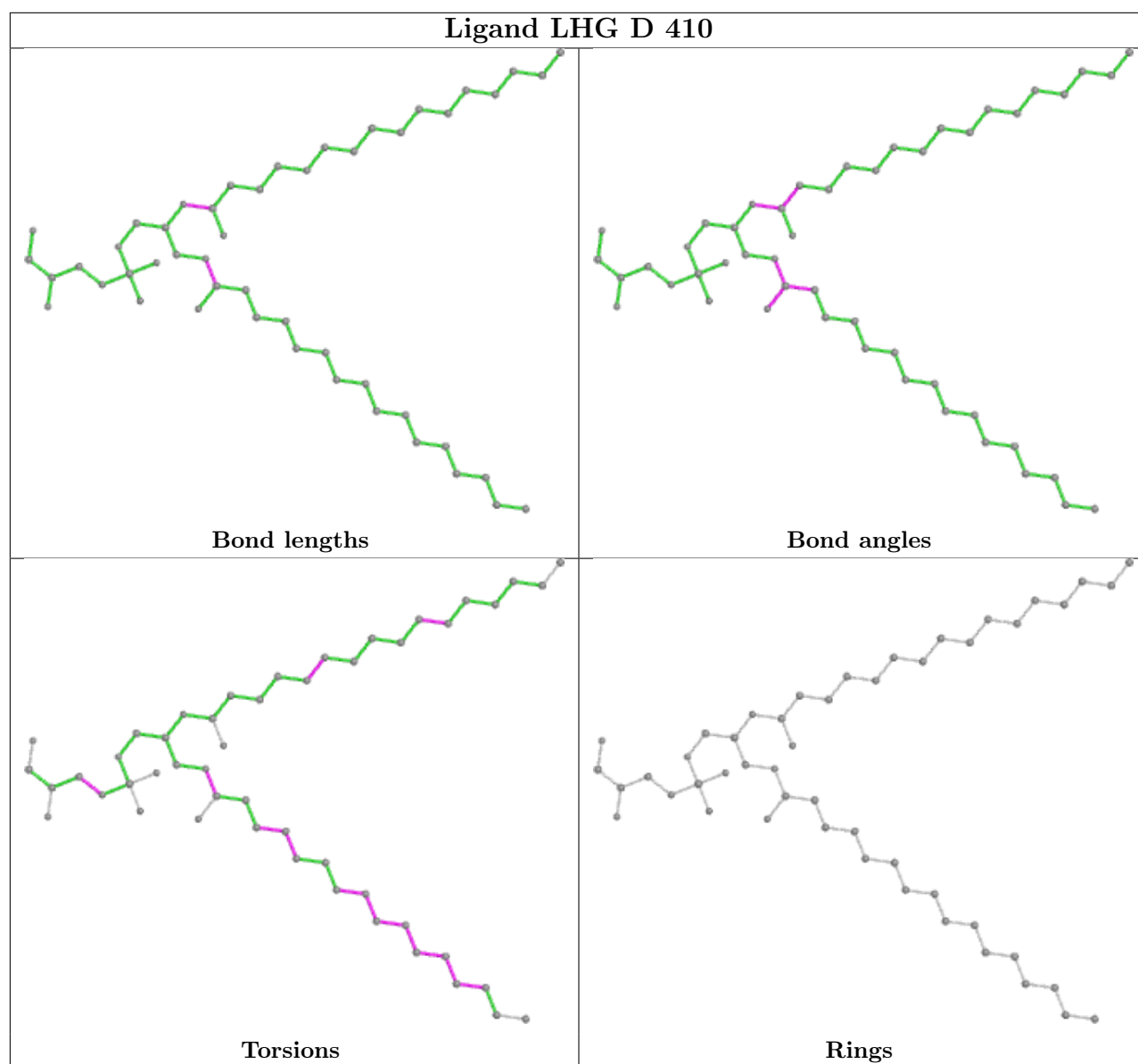












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	0.67	44 (13%) 3 5	16, 23, 42, 79	0
1	a	334/344 (97%)	0.83	59 (17%) 1 1	17, 25, 48, 82	0
2	B	504/505 (99%)	0.27	42 (8%) 11 17	18, 27, 52, 90	0
2	b	504/505 (99%)	0.46	50 (9%) 7 12	19, 29, 60, 108	0
3	C	451/455 (99%)	0.24	28 (6%) 20 29	20, 32, 49, 89	0
3	c	455/455 (100%)	0.43	38 (8%) 11 17	23, 35, 50, 87	0
4	D	342/342 (100%)	0.88	63 (18%) 1 1	15, 24, 40, 114	0
4	d	341/342 (99%)	0.59	39 (11%) 5 8	18, 26, 42, 90	0
5	E	81/84 (96%)	1.20	15 (18%) 1 1	27, 40, 68, 97	0
5	e	81/84 (96%)	1.09	15 (18%) 1 1	32, 45, 77, 97	0
6	F	34/44 (77%)	0.35	6 (17%) 1 1	26, 35, 56, 64	0
6	f	32/44 (72%)	0.40	4 (12%) 3 6	31, 37, 84, 99	0
7	H	65/65 (100%)	0.34	3 (4%) 32 42	24, 34, 52, 97	0
7	h	65/65 (100%)	0.55	6 (9%) 9 14	28, 37, 58, 113	0
8	I	37/38 (97%)	0.83	5 (13%) 3 5	30, 34, 91, 101	0
8	i	37/38 (97%)	0.73	5 (13%) 3 5	29, 34, 79, 102	0
9	J	38/39 (97%)	0.73	8 (21%) 1 1	26, 38, 85, 109	0
9	j	38/39 (97%)	0.25	3 (7%) 12 19	30, 41, 84, 85	0
10	K	37/37 (100%)	0.16	0 100 100	31, 38, 55, 64	0
10	k	37/37 (100%)	0.86	8 (21%) 0 1	33, 42, 56, 66	0
11	L	37/37 (100%)	1.17	11 (29%) 0 0	16, 20, 66, 91	0
11	l	37/37 (100%)	1.04	6 (16%) 1 2	17, 21, 61, 91	0
12	M	33/36 (91%)	0.89	6 (18%) 1 1	18, 23, 44, 100	0
12	m	33/36 (91%)	0.76	5 (15%) 2 3	19, 23, 44, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.38	21 (8%) 10 16	16, 34, 65, 113	0
13	o	243/244 (99%)	0.89	52 (21%) 0 1	18, 35, 75, 122	0
14	T	29/31 (93%)	0.98	4 (13%) 2 4	17, 23, 48, 85	0
14	t	29/31 (93%)	0.55	2 (6%) 16 25	17, 23, 49, 85	0
15	U	97/104 (93%)	0.26	5 (5%) 27 37	22, 33, 53, 85	0
15	u	97/104 (93%)	-0.11	0 100 100	25, 34, 51, 85	0
16	V	137/137 (100%)	-0.03	0 100 100	23, 33, 54, 70	0
16	v	137/137 (100%)	0.49	13 (9%) 8 13	26, 38, 57, 72	0
17	Y	29/30 (96%)	2.05	9 (31%) 0 0	38, 50, 91, 107	0
17	y	29/30 (96%)	1.91	9 (31%) 0 0	40, 54, 91, 107	0
18	X	39/40 (97%)	0.77	8 (20%) 1 1	32, 42, 80, 92	0
18	x	39/40 (97%)	1.59	11 (28%) 0 0	35, 45, 93, 96	0
19	Z	62/62 (100%)	1.28	18 (29%) 0 0	40, 52, 87, 98	0
19	z	62/62 (100%)	2.95	36 (58%) 0 0	44, 53, 87, 98	0
20	R	34/34 (100%)	9.29	34 (100%) 0 0	69, 93, 111, 118	0
All	All	5293/5382 (98%)	0.65	691 (13%) 3 5	15, 31, 63, 122	0

The worst 5 of 691 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	18.4
20	R	6	LEU	14.1
20	R	14	LEU	13.2
20	R	31	VAL	13.0
20	R	20	VAL	12.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	FME	j	1	10/11	0.76	0.35	53,71,94,136	0
12	FME	m	1	10/11	0.93	0.15	25,31,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.95	0.11	13,22,33,65	0
14	FME	T	1	10/11	0.96	0.15	21,27,45,56	0
12	FME	M	1	10/11	0.96	0.14	23,34,56,61	0
8	FME	i	1	10/11	0.97	0.15	23,34,37,42	0
8	FME	I	1	10/11	0.97	0.11	22,34,37,40	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
28	GOL	B	635	6/6	0.22	0.43	82,91,97,98	0
36	DGD	D	407	62/66	0.51	0.49	44,89,114,119	0
29	UNL	k	102	10/-	0.58	0.61	54,83,94,102	0
36	DGD	d	407	62/66	0.59	0.44	41,88,117,122	0
29	UNL	j	103	10/-	0.60	0.32	44,61,67,73	0
30	LMT	f	102	35/35	0.60	0.36	56,83,109,113	0
30	LMT	E	102	35/35	0.61	0.34	43,81,105,107	0
35	HTG	b	628	19/19	0.61	0.31	48,90,106,124	0
29	UNL	A	415	28/-	0.62	0.30	55,65,84,90	0
34	LMG	Z	101	37/55	0.62	0.32	32,81,104,105	0
35	HTG	b	604	19/19	0.62	0.19	50,80,106,112	0
29	UNL	a	414	30/-	0.64	0.28	45,65,86,89	0
30	LMT	m	103	35/35	0.65	0.27	30,60,86,90	0
29	UNL	C	526	34/-	0.65	0.34	46,71,82,84	0
29	UNL	b	634	33/-	0.65	0.26	42,71,112,116	0
30	LMT	M	101	35/35	0.66	0.28	35,60,79,85	0
33	CA	b	605	1/1	0.67	0.14	95,95,95,95	0
35	HTG	d	411	16/19	0.67	0.27	54,73,84,87	0
28	GOL	O	302	6/6	0.68	0.18	52,61,64,70	0
27	SQD	l	101	54/54	0.68	0.25	31,67,98,101	0
32	PL9	A	419	55/55	0.69	0.29	38,66,87,92	0
30	LMT	b	626	25/35	0.69	0.29	33,67,110,115	0
28	GOL	T	103	6/6	0.69	0.31	63,76,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	LMT	D	402	35/35	0.69	0.25	32,75,96,97	0
35	HTG	D	411	16/19	0.70	0.24	38,100,111,113	0
29	UNL	k	101	32/-	0.70	0.38	42,75,105,108	0
30	LMT	m	102	35/35	0.70	0.22	16,51,73,79	0
37	LHG	E	101	42/49	0.70	0.25	38,73,93,103	0
35	HTG	B	624	19/19	0.71	0.36	38,95,102,121	0
29	UNL	J	103	10/-	0.71	0.44	38,53,73,75	0
34	LMG	z	101	39/55	0.72	0.39	47,74,94,101	0
27	SQD	b	601	54/54	0.73	0.23	36,58,91,95	0
29	UNL	i	101	40/-	0.73	0.24	36,64,96,108	0
29	UNL	B	632	33/-	0.74	0.24	32,70,105,113	0
37	LHG	e	101	42/49	0.74	0.23	49,87,117,128	0
28	GOL	v	203	6/6	0.75	0.29	50,69,71,78	0
30	LMT	I	102	35/35	0.75	0.34	59,81,95,100	0
32	PL9	a	416	55/55	0.75	0.27	50,76,94,95	0
29	UNL	I	101	40/-	0.76	0.29	27,63,114,119	0
33	CA	B	601	1/1	0.76	0.09	79,79,79,79	0
35	HTG	B	631	19/19	0.76	0.21	25,84,104,120	0
35	HTG	C	523	19/19	0.76	0.28	46,75,97,109	0
27	SQD	a	402	54/54	0.76	0.23	34,61,79,100	0
29	UNL	x	101	10/-	0.76	0.17	35,44,57,58	0
30	LMT	a	417	35/35	0.77	0.41	52,76,90,94	0
34	LMG	C	520	51/55	0.77	0.28	26,61,82,87	0
28	GOL	t	102	6/6	0.77	0.33	29,60,65,69	0
34	LMG	c	521	51/55	0.77	0.28	35,79,91,98	0
28	GOL	A	414	6/6	0.78	0.19	40,60,69,70	0
30	LMT	B	634	25/35	0.78	0.27	32,63,105,111	0
30	LMT	M	102	35/35	0.78	0.20	22,50,66,76	0
30	LMT	b	602	25/35	0.79	0.30	22,63,102,106	0
34	LMG	C	521	51/55	0.79	0.23	31,74,90,96	0
29	UNL	d	413	36/-	0.80	0.19	35,58,94,99	0
34	LMG	c	501	51/55	0.80	0.21	39,60,77,85	0
27	SQD	A	416	54/54	0.80	0.18	28,52,75,76	0
28	GOL	V	205	6/6	0.80	0.39	37,54,59,72	0
28	GOL	a	413	6/6	0.80	0.22	38,67,69,71	0
29	UNL	D	413	40/-	0.81	0.20	33,55,105,108	0
28	GOL	b	632	6/6	0.81	0.29	40,46,68,69	0
30	LMT	a	401	35/35	0.82	0.19	28,61,79,86	0
35	HTG	c	523	19/19	0.83	0.32	60,84,93,98	0
27	SQD	f	101	43/54	0.83	0.30	55,82,109,117	0
34	LMG	B	621	51/55	0.83	0.25	20,35,52,64	0
28	GOL	v	204	6/6	0.84	0.20	47,64,70,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	LMG	c	520	51/55	0.84	0.22	33,63,86,88	0
29	UNL	d	412	17/-	0.84	0.16	31,48,79,85	0
34	LMG	C	501	51/55	0.84	0.19	37,54,74,82	0
28	GOL	B	627	6/6	0.85	0.22	31,35,43,44	0
29	UNL	M	103	10/-	0.85	0.18	34,42,59,64	0
35	HTG	B	623	19/19	0.85	0.16	29,42,64,71	0
29	UNL	X	101	10/-	0.85	0.15	29,37,41,42	0
30	LMT	A	417	33/35	0.85	0.19	27,65,78,85	0
35	HTG	c	522	19/19	0.86	0.17	63,69,80,85	0
35	HTG	B	630	19/19	0.86	0.17	30,54,78,81	0
24	CLA	c	515	65/65	0.86	0.27	37,51,79,88	0
28	GOL	A	413	6/6	0.86	0.19	35,38,41,42	0
36	DGD	H	102	62/66	0.86	0.19	20,29,42,58	0
28	GOL	V	208	6/6	0.86	0.26	41,56,62,63	0
26	BCR	k	103	40/40	0.86	0.17	32,40,48,52	0
29	UNL	m	101	10/-	0.86	0.26	37,51,60,62	0
28	GOL	V	206	6/6	0.87	0.20	21,38,44,48	0
26	BCR	h	101	40/40	0.87	0.12	27,35,46,49	0
36	DGD	h	102	62/66	0.87	0.17	23,35,52,69	0
26	BCR	d	405	40/40	0.87	0.16	29,35,63,64	0
34	LMG	b	625	51/55	0.87	0.28	24,39,59,71	0
35	HTG	V	204	19/19	0.88	0.26	40,65,99,175	0
28	GOL	C	524	6/6	0.88	0.21	39,45,57,60	0
26	BCR	H	101	40/40	0.88	0.13	21,32,48,52	0
33	CA	F	102	1/1	0.88	0.14	72,72,72,72	0
28	GOL	B	628	6/6	0.88	0.22	35,46,67,70	0
27	SQD	F	101	43/54	0.88	0.30	39,70,96,105	0
28	GOL	T	101	6/6	0.89	0.18	35,60,64,65	0
28	GOL	c	527	6/6	0.89	0.21	36,57,61,63	0
33	CA	f	103	1/1	0.89	0.12	72,72,72,72	0
35	HTG	b	627	19/19	0.89	0.23	27,44,80,80	0
24	CLA	b	614	65/65	0.89	0.12	24,31,41,50	0
32	PL9	d	406	55/55	0.89	0.21	16,23,35,47	0
37	LHG	d	408	49/49	0.89	0.23	26,34,46,50	0
24	CLA	c	505	65/65	0.89	0.13	29,35,46,60	0
28	GOL	B	626	6/6	0.90	0.21	32,37,40,59	0
26	BCR	Y	101	40/40	0.90	0.12	28,35,49,50	0
26	BCR	c	526	40/40	0.90	0.16	39,48,59,63	0
34	LMG	j	101	51/55	0.90	0.19	26,39,70,82	0
28	GOL	b	631	6/6	0.90	0.11	39,46,48,60	0
27	SQD	a	411	54/54	0.90	0.22	32,56,75,78	0
28	GOL	c	525	6/6	0.90	0.24	43,46,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	c	514	65/65	0.90	0.18	34,43,67,76	0
36	DGD	c	518	62/66	0.90	0.19	24,35,79,94	0
24	CLA	C	509	65/65	0.90	0.16	21,29,78,80	0
26	BCR	B	619	40/40	0.90	0.17	17,25,44,46	0
37	LHG	D	408	49/49	0.90	0.25	16,31,43,54	0
27	SQD	A	411	54/54	0.90	0.21	26,51,71,78	0
24	CLA	c	506	65/65	0.90	0.17	26,33,51,61	0
35	HTG	b	603	19/19	0.90	0.14	34,44,64,67	0
37	LHG	l	102	49/49	0.90	0.19	19,30,48,57	0
24	CLA	B	610	65/65	0.91	0.12	19,26,36,40	0
28	GOL	F	103	6/6	0.91	0.18	52,59,65,68	0
26	BCR	T	102	40/40	0.91	0.16	14,28,36,42	0
24	CLA	B	603	65/65	0.91	0.12	18,25,32,38	0
26	BCR	b	622	40/40	0.91	0.18	16,26,33,36	0
26	BCR	b	623	40/40	0.91	0.21	15,27,40,46	0
29	UNL	D	412	17/-	0.91	0.16	24,45,74,78	0
32	PL9	D	406	55/55	0.91	0.24	14,23,36,43	0
26	BCR	c	516	40/40	0.91	0.12	29,36,47,57	0
24	CLA	c	507	65/65	0.91	0.12	22,31,52,62	0
28	GOL	a	412	6/6	0.91	0.16	22,37,41,45	0
24	CLA	c	513	65/65	0.91	0.13	30,39,50,54	0
24	CLA	C	514	65/65	0.91	0.16	32,42,69,72	0
35	HTG	C	522	19/19	0.91	0.18	53,65,89,95	0
24	CLA	B	604	65/65	0.91	0.12	18,25,32,40	0
24	CLA	b	620	65/65	0.91	0.12	22,31,51,74	0
26	BCR	D	405	40/40	0.91	0.14	22,31,61,77	0
28	GOL	b	630	6/6	0.92	0.16	37,48,50,52	0
24	CLA	b	607	65/65	0.92	0.12	23,30,38,41	0
28	GOL	B	625	6/6	0.92	0.14	28,43,48,55	0
24	CLA	B	612	65/65	0.92	0.17	15,21,37,41	0
26	BCR	C	515	40/40	0.92	0.11	31,42,49,53	0
28	GOL	f	104	6/6	0.92	0.22	45,51,59,61	0
26	BCR	t	101	40/40	0.92	0.12	15,24,45,49	0
28	GOL	B	633	6/6	0.92	0.10	27,36,40,41	0
26	BCR	y	101	40/40	0.92	0.12	31,40,53,60	0
24	CLA	B	615	65/65	0.92	0.14	15,24,67,78	0
24	CLA	b	621	65/65	0.92	0.15	21,35,82,84	0
24	CLA	C	504	65/65	0.92	0.11	24,33,42,48	0
34	LMG	J	101	51/55	0.92	0.22	20,37,78,86	0
36	DGD	C	518	62/66	0.92	0.23	22,32,76,92	0
24	CLA	C	505	65/65	0.92	0.21	22,29,59,77	0
24	CLA	C	507	65/65	0.92	0.16	28,42,81,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	GOL	V	201	6/6	0.92	0.11	27,29,40,41	0
36	DGD	c	519	62/66	0.92	0.20	26,34,65,72	0
24	CLA	c	509	65/65	0.92	0.12	27,34,49,58	0
26	BCR	b	624	40/40	0.92	0.10	20,32,46,52	0
24	CLA	B	608	65/65	0.92	0.18	13,20,31,35	0
28	GOL	A	412	6/6	0.92	0.10	29,31,34,37	0
35	HTG	B	622	19/19	0.92	0.11	26,30,44,56	0
24	CLA	B	602	65/65	0.92	0.16	24,39,82,104	0
28	GOL	b	629	6/6	0.92	0.13	32,40,48,57	0
28	GOL	v	201	6/6	0.93	0.13	31,40,49,50	0
24	CLA	b	612	65/65	0.93	0.21	14,23,30,36	0
24	CLA	c	510	65/65	0.93	0.16	24,31,70,87	0
28	GOL	v	205	6/6	0.93	0.17	25,39,52,58	0
24	CLA	c	512	65/65	0.93	0.17	26,32,44,59	0
24	CLA	C	511	65/65	0.93	0.15	23,29,41,62	0
36	DGD	C	519	62/66	0.93	0.23	20,30,58,63	0
24	CLA	b	616	65/65	0.93	0.13	18,26,38,52	0
24	CLA	b	619	65/65	0.93	0.14	15,25,72,77	0
36	DGD	c	517	62/66	0.93	0.17	23,32,68,76	0
26	BCR	B	618	40/40	0.93	0.16	15,23,33,41	0
24	CLA	C	512	65/65	0.93	0.11	26,32,41,48	0
24	CLA	C	513	65/65	0.93	0.12	29,42,67,74	0
24	CLA	c	503	65/65	0.93	0.11	29,34,45,54	0
24	CLA	B	607	65/65	0.93	0.11	18,26,51,75	0
26	BCR	K	101	40/40	0.93	0.12	27,33,42,47	0
37	LHG	L	101	49/49	0.93	0.23	15,29,47,58	0
24	CLA	b	606	65/65	0.93	0.18	30,46,82,98	0
37	LHG	d	409	49/49	0.93	0.14	17,26,39,55	0
24	CLA	C	502	65/65	0.93	0.11	25,32,47,58	0
24	CLA	c	508	65/65	0.93	0.12	30,41,65,70	0
33	CA	o	301	1/1	0.94	0.07	62,62,62,62	0
24	CLA	a	407	65/65	0.94	0.26	19,25,72,79	0
24	CLA	a	409	65/65	0.94	0.12	20,27,83,88	0
26	BCR	C	516	40/40	0.94	0.09	25,34,43,46	0
24	CLA	C	508	65/65	0.94	0.11	25,35,48,57	0
24	CLA	c	504	65/65	0.94	0.14	26,32,45,55	0
24	CLA	B	605	65/65	0.94	0.14	15,22,51,63	0
36	DGD	C	517	62/66	0.94	0.14	22,33,75,83	0
28	GOL	V	207	6/6	0.94	0.21	35,38,41,44	0
24	CLA	b	608	65/65	0.94	0.10	22,29,38,42	0
24	CLA	b	611	65/65	0.94	0.10	19,31,58,74	0
26	BCR	a	410	40/40	0.94	0.09	16,24,31,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	C	503	65/65	0.94	0.12	22,28,40,51	0
24	CLA	b	613	65/65	0.94	0.11	22,29,38,42	0
24	CLA	A	405	65/65	0.94	0.26	15,18,26,50	0
24	CLA	b	615	65/65	0.94	0.11	21,28,39,46	0
24	CLA	B	614	65/65	0.94	0.17	14,22,45,52	0
24	CLA	b	617	65/65	0.94	0.11	18,26,36,50	0
37	LHG	D	409	49/49	0.94	0.18	17,27,48,60	0
37	LHG	D	410	49/49	0.94	0.18	20,33,91,95	0
28	GOL	B	629	6/6	0.94	0.25	24,40,61,78	0
24	CLA	b	618	65/65	0.94	0.18	15,23,48,56	0
24	CLA	d	404	65/65	0.94	0.12	27,34,74,81	0
25	PHO	d	403	64/64	0.94	0.20	20,25,34,38	0
37	LHG	d	410	49/49	0.94	0.18	23,35,85,104	0
35	HTG	O	303	19/19	0.94	0.09	24,32,47,48	0
22	CL	u	201	1/1	0.94	0.05	63,63,63,63	0
38	HEM	e	102	43/43	0.94	0.18	38,48,65,84	0
26	BCR	A	410	40/40	0.95	0.10	16,26,33,35	0
24	CLA	B	611	65/65	0.95	0.12	19,26,36,39	0
24	CLA	C	506	65/65	0.95	0.10	21,29,45,53	0
26	BCR	B	620	40/40	0.95	0.10	22,29,42,47	0
24	CLA	A	409	65/65	0.95	0.12	18,27,83,92	0
24	CLA	b	609	65/65	0.95	0.15	16,25,56,66	0
24	CLA	b	610	65/65	0.95	0.11	18,24,37,42	0
24	CLA	B	613	65/65	0.95	0.11	15,23,32,35	0
24	CLA	B	606	65/65	0.95	0.09	16,22,34,38	0
24	CLA	C	510	65/65	0.95	0.11	25,32,51,57	0
23	BCT	a	418	4/4	0.95	0.17	30,33,42,44	0
24	CLA	c	511	65/65	0.95	0.10	29,36,49,55	0
24	CLA	B	616	65/65	0.95	0.11	19,28,48,60	0
24	CLA	B	617	65/65	0.95	0.17	19,28,88,91	0
28	GOL	b	633	6/6	0.95	0.29	32,54,63,71	0
22	CL	V	202	1/1	0.95	0.05	63,63,63,63	0
24	CLA	D	404	65/65	0.95	0.12	21,28,73,84	0
24	CLA	B	609	65/65	0.95	0.14	17,22,32,36	0
25	PHO	A	407	64/64	0.95	0.18	15,18,23,28	0
25	PHO	A	408	64/64	0.95	0.26	16,22,30,32	0
25	PHO	a	408	64/64	0.95	0.18	16,21,29,37	0
28	GOL	C	525	6/6	0.95	0.13	20,24,26,27	0
24	CLA	A	406	65/65	0.95	0.26	15,19,84,88	0
24	CLA	a	406	65/65	0.96	0.24	17,20,35,51	0
24	CLA	D	401	65/65	0.96	0.24	13,18,30,32	0
24	CLA	D	403	65/65	0.96	0.28	14,19,36,42	0

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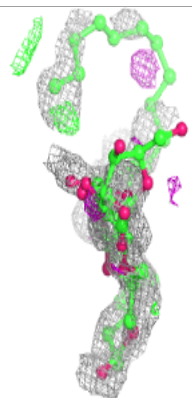
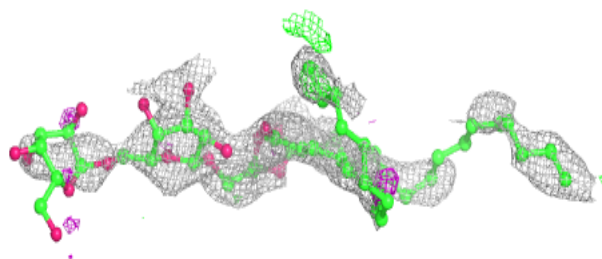
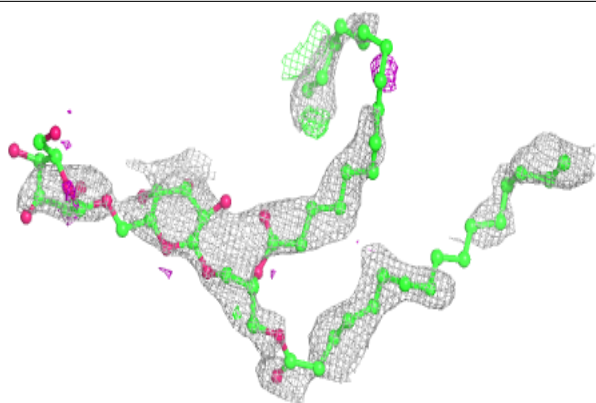
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	CA	c	502	1/1	0.96	0.04	44,44,44,44	0
23	BCT	A	404	4/4	0.96	0.10	27,30,39,40	0
24	CLA	d	401	65/65	0.96	0.21	16,19,26,42	0
38	HEM	E	103	43/43	0.96	0.17	27,38,50,56	0
24	CLA	d	402	65/65	0.96	0.24	18,22,38,46	0
33	CA	O	301	1/1	0.97	0.05	56,56,56,56	0
39	MG	J	102	1/1	0.97	0.04	28,28,28,28	0
40	HEC	V	203	43/43	0.97	0.08	23,26,31,36	0
40	HEC	v	202	43/43	0.97	0.10	29,33,40,48	0
39	MG	j	102	1/1	0.98	0.16	34,34,34,34	0
22	CL	A	403	1/1	0.98	0.07	23,23,23,23	0
28	GOL	c	524	6/6	0.98	0.15	25,28,30,34	0
21	FE2	A	401	1/1	0.99	0.10	27,27,27,27	0
21	FE2	a	403	1/1	0.99	0.11	30,30,30,30	0
22	CL	a	405	1/1	0.99	0.12	26,26,26,26	0
22	CL	A	402	1/1	0.99	0.10	19,19,19,19	0
31	OEX	A	418	10/10	0.99	0.09	16,23,28,32	0
31	OEX	a	415	10/10	0.99	0.11	20,24,35,37	0
22	CL	a	404	1/1	1.00	0.10	20,20,20,20	0

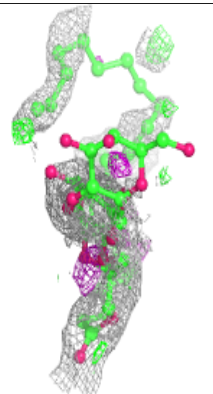
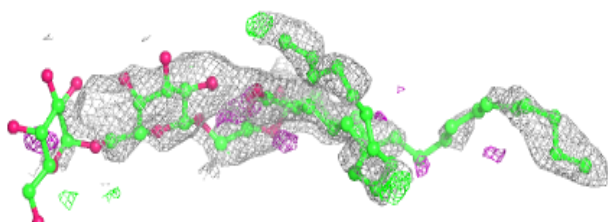
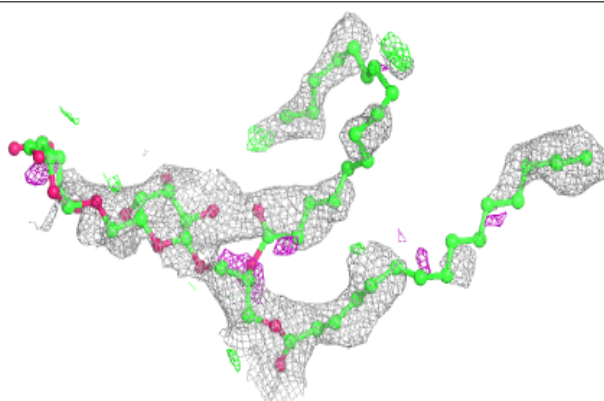
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD D 407:

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

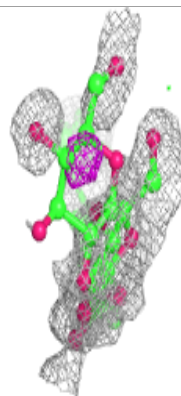
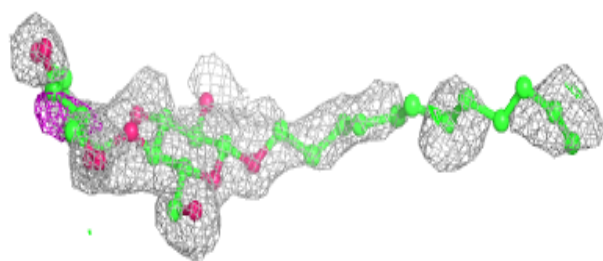
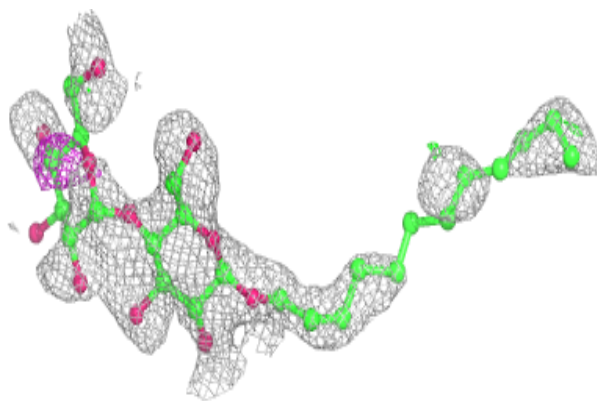
**Electron density around DGD d 407:**

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

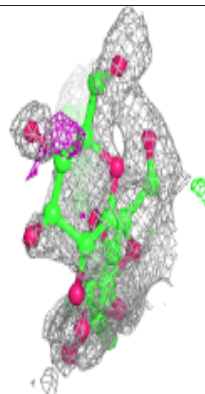
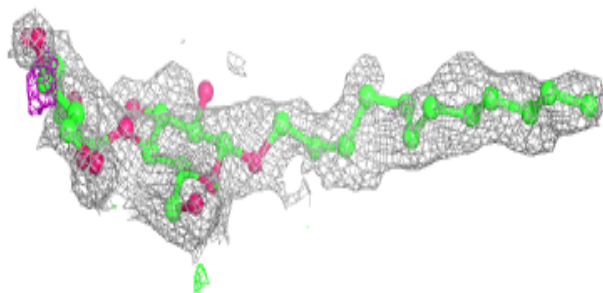
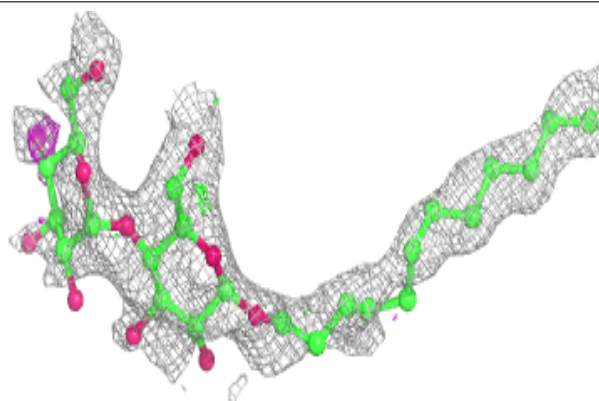


Electron density around LMT f 102:

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

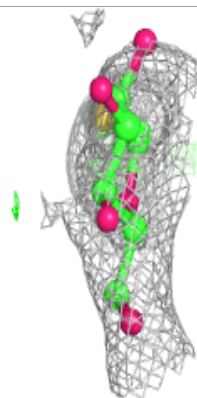
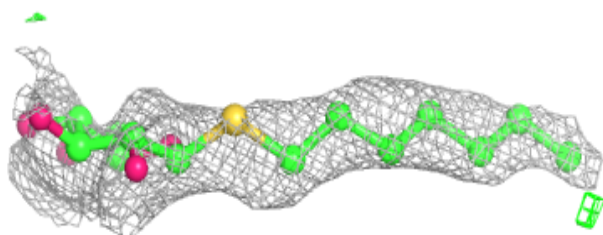
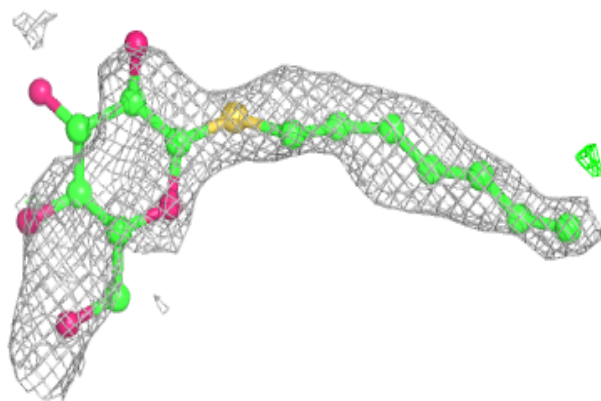
**Electron density around LMT E 102:**

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

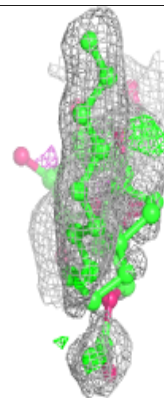
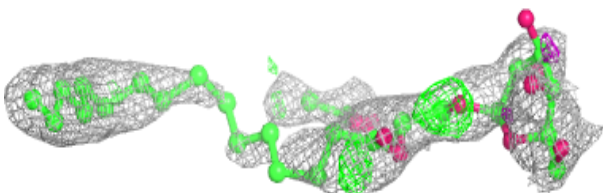
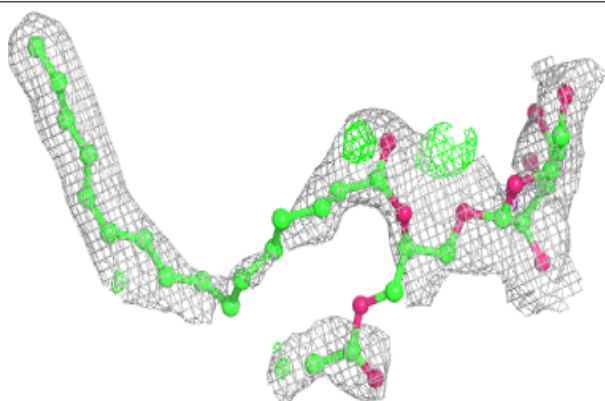


Electron density around HTG b 628:

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

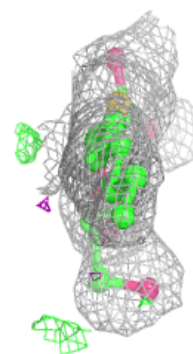
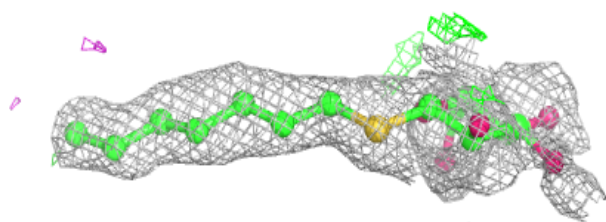
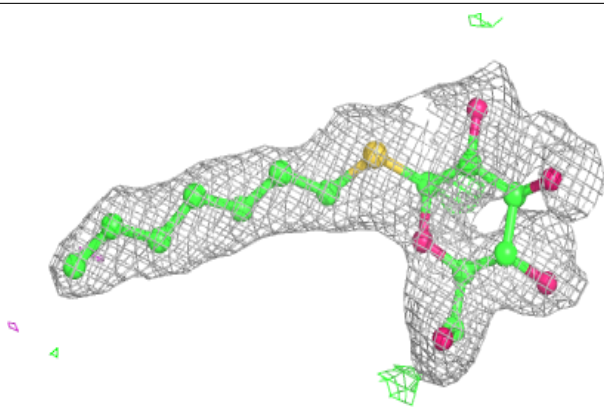
**Electron density around LMG Z 101:**

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

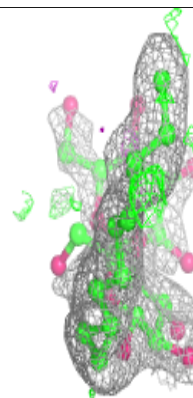
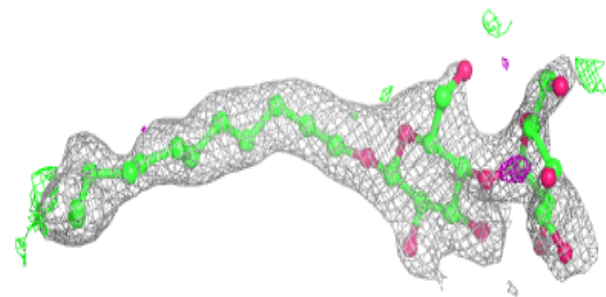
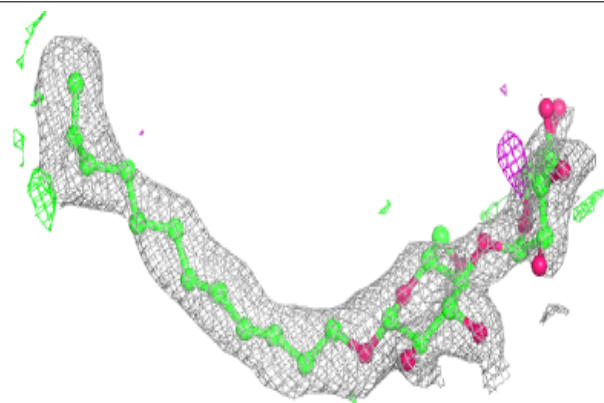


Electron density around HTG b 604:

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

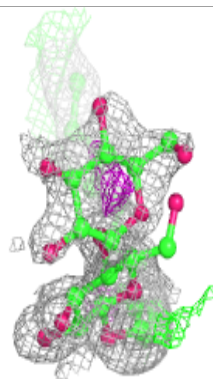
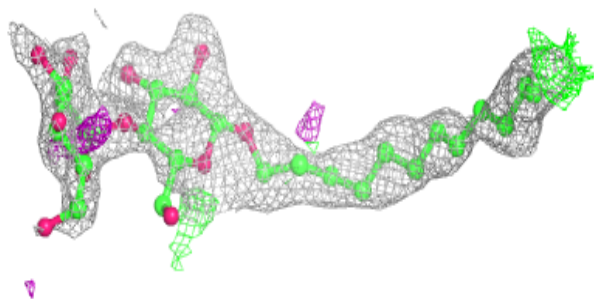
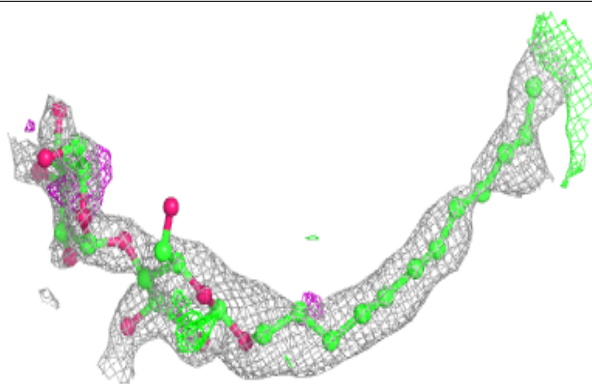
**Electron density around LMT m 103:**

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

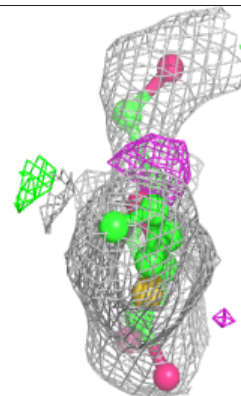
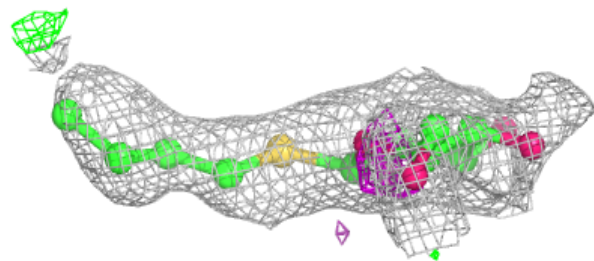
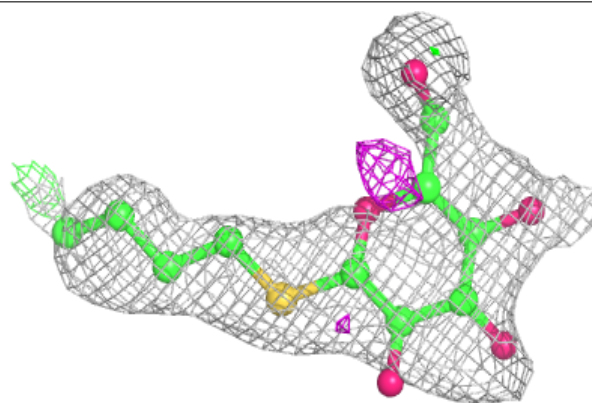


Electron density around LMT M 101:

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

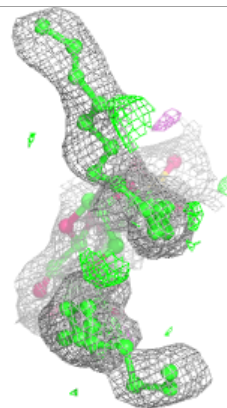
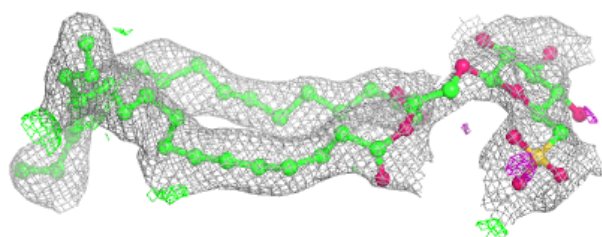
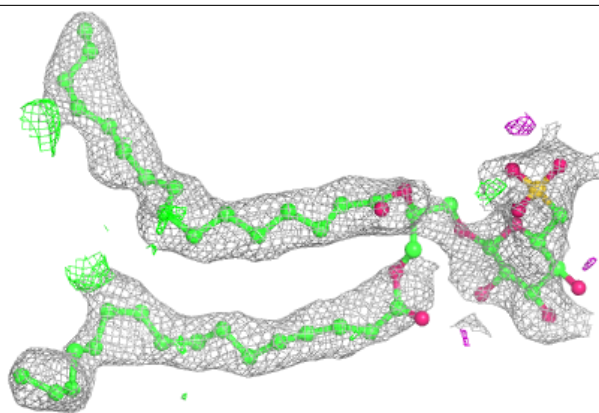
**Electron density around HTG d 411:**

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

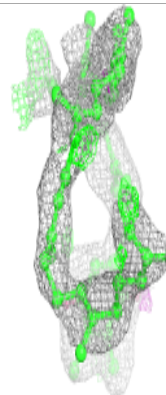
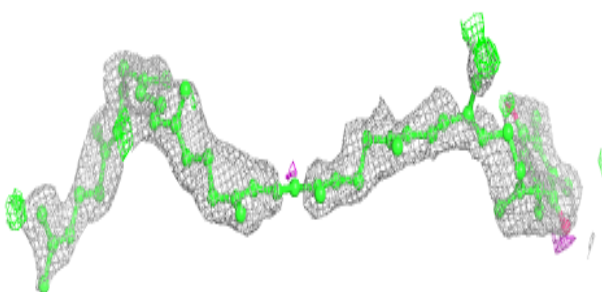
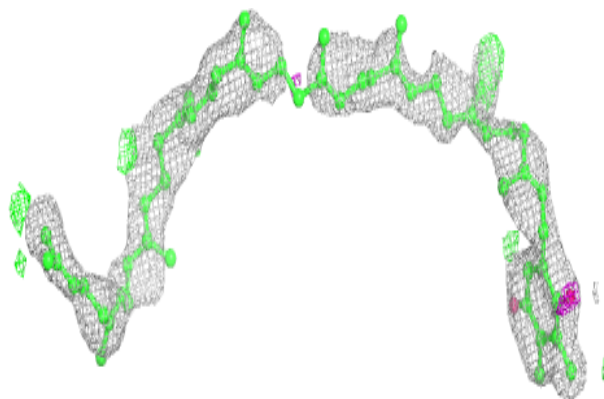


Electron density around SQD 1 101:

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

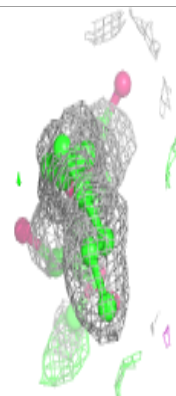
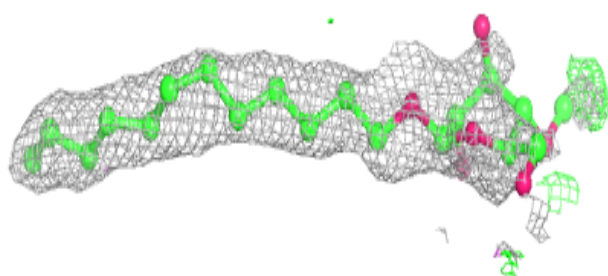
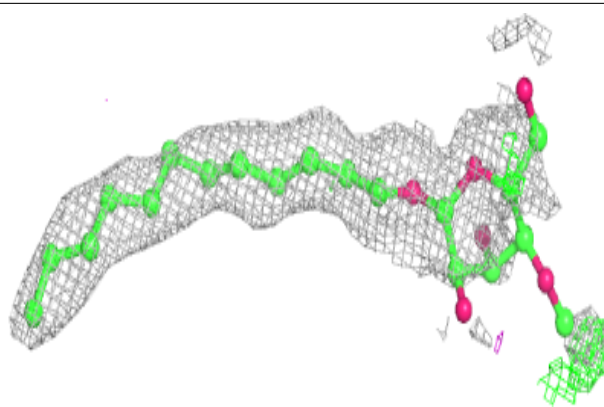
**Electron density around PL9 A 419:**

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

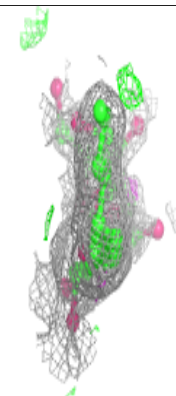
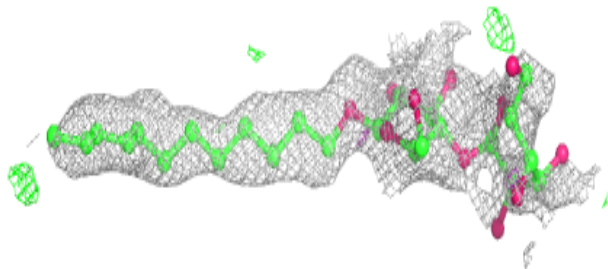
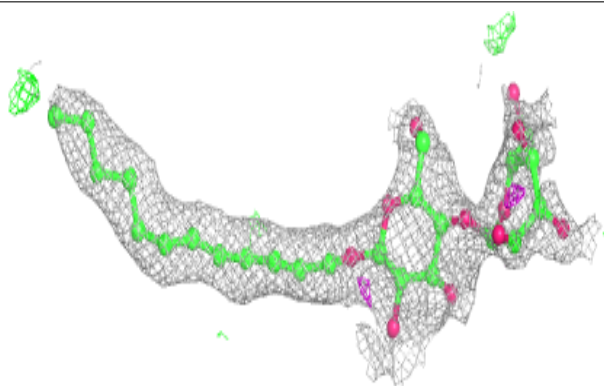


Electron density around LMT b 626:

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

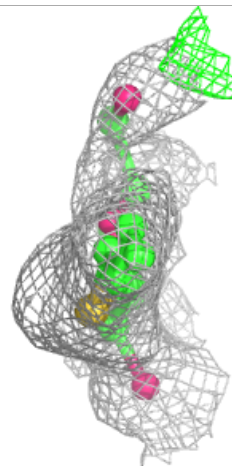
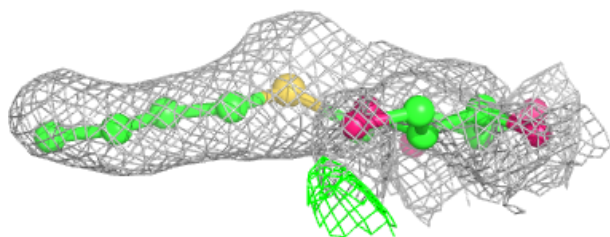
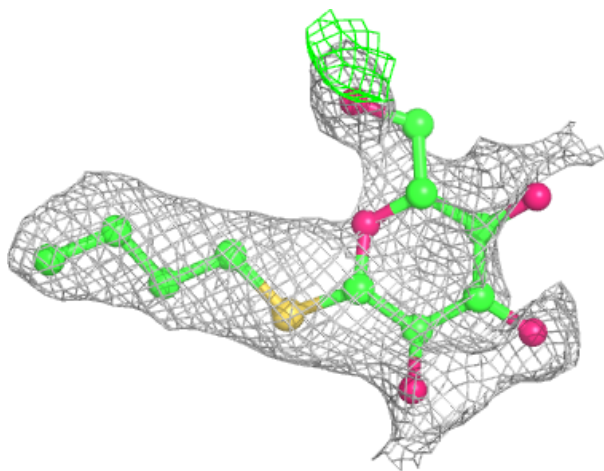
**Electron density around LMT D 402:**

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



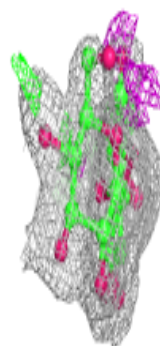
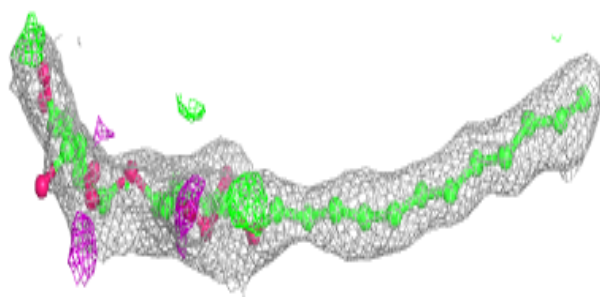
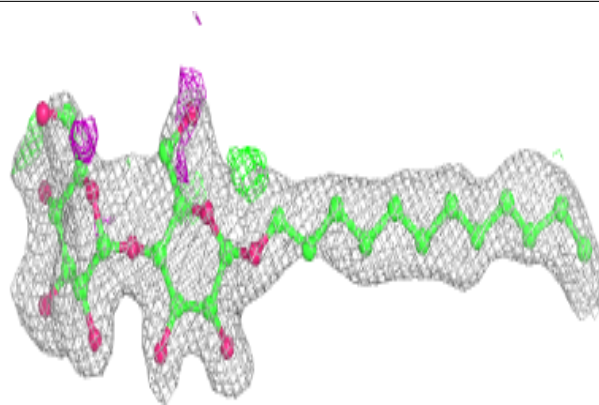
Electron density around HTG D 411:

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

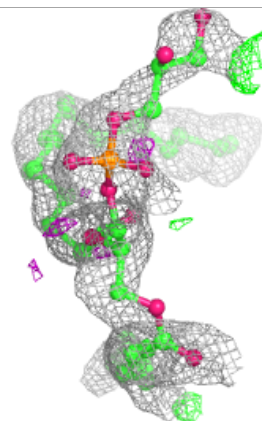
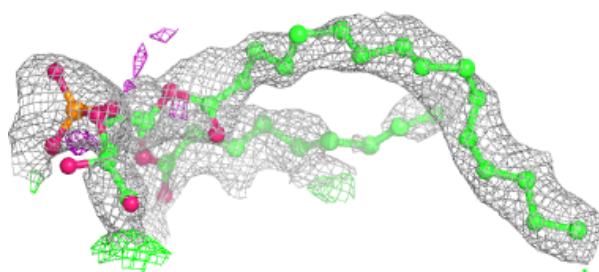
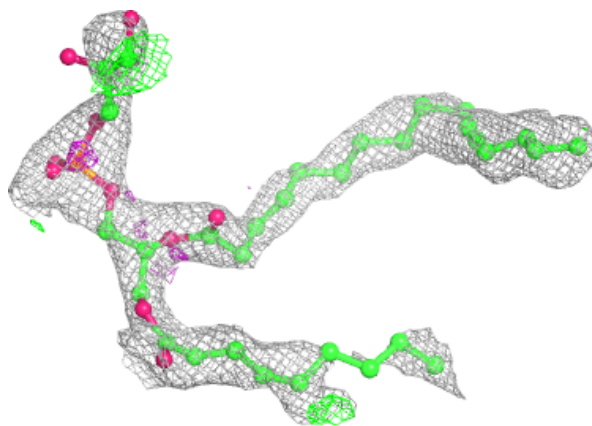


Electron density around LMT m 102:

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

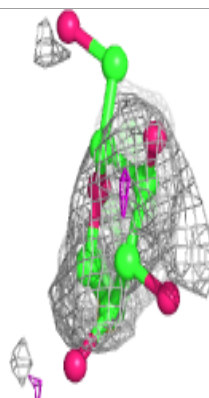
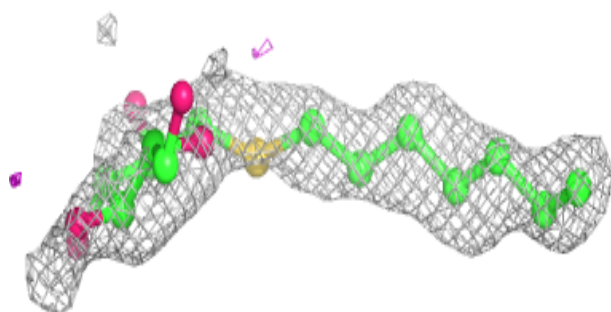
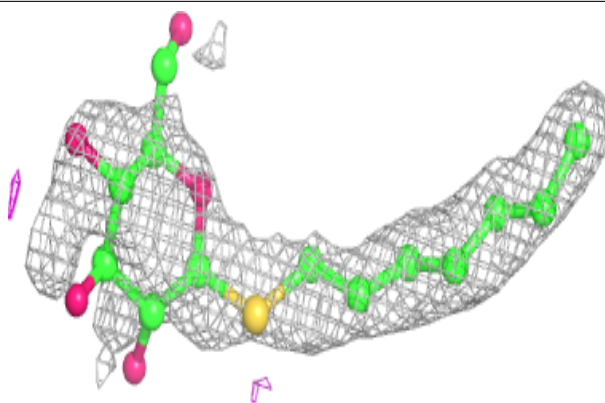
**Electron density around LHG E 101:**

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

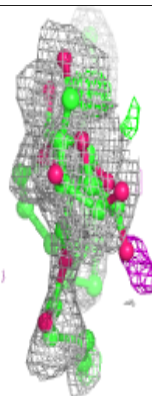
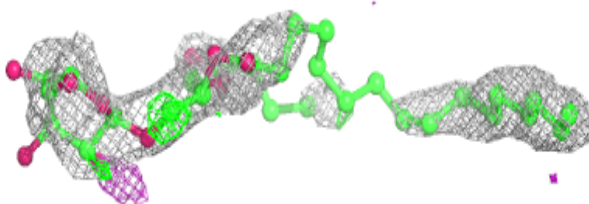
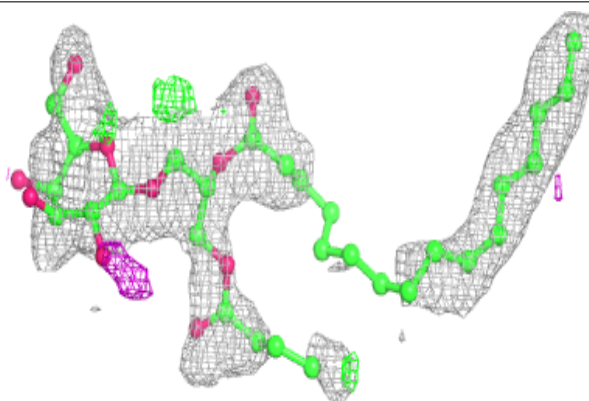


Electron density around HTG B 624:

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

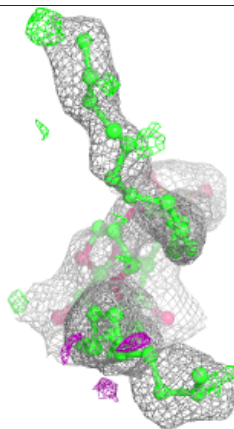
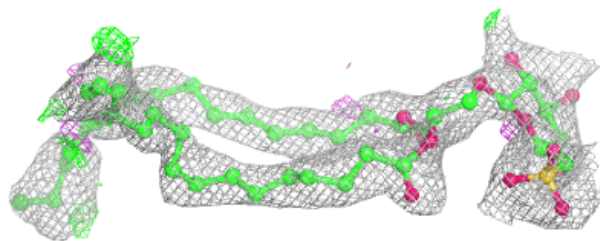
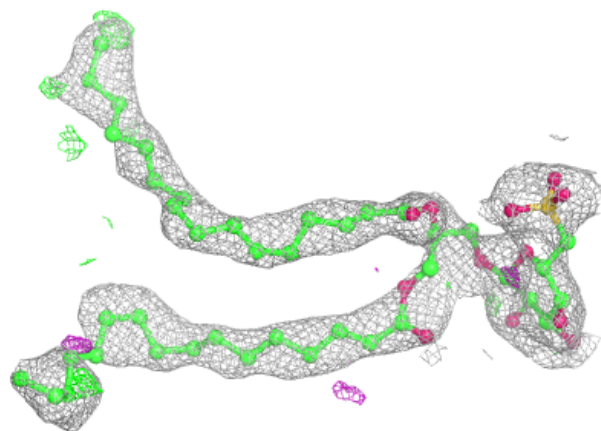
**Electron density around LMG z 101:**

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



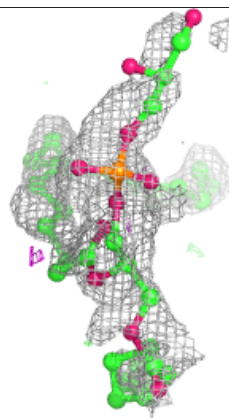
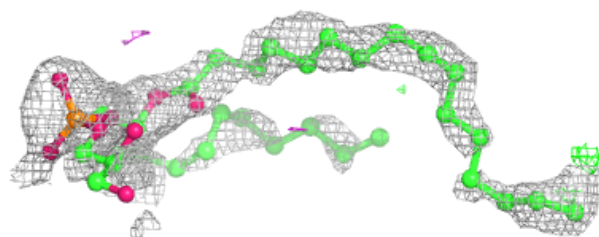
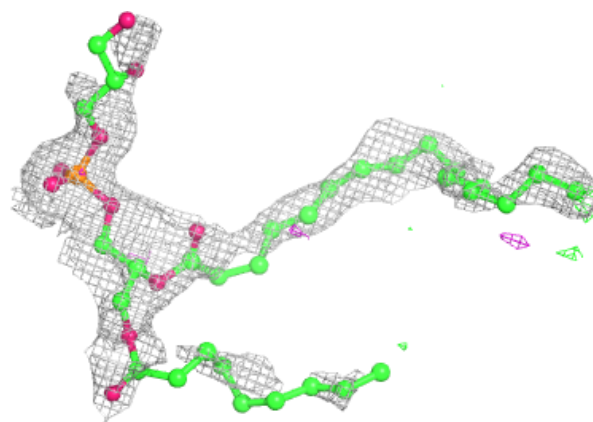
Electron density around SQD b 601:

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

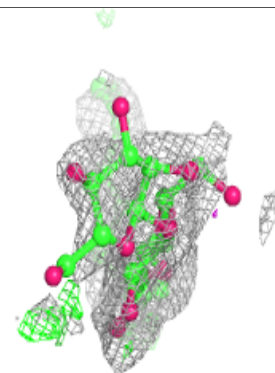
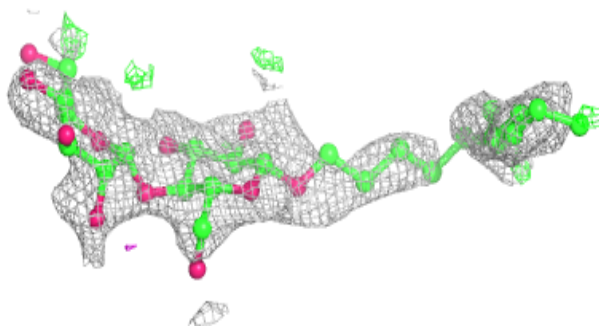
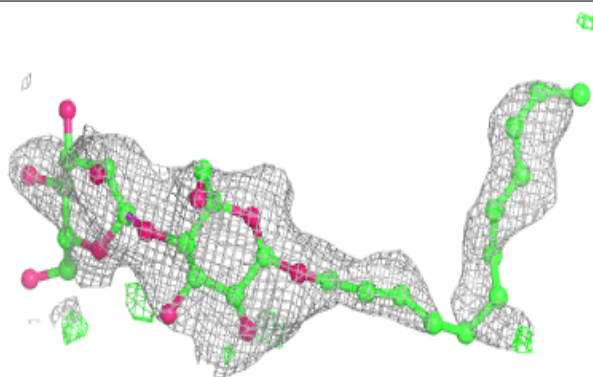


Electron density around LHG e 101:

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

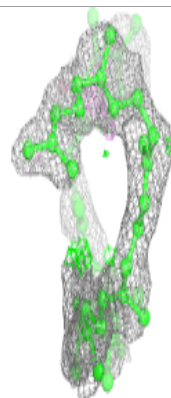
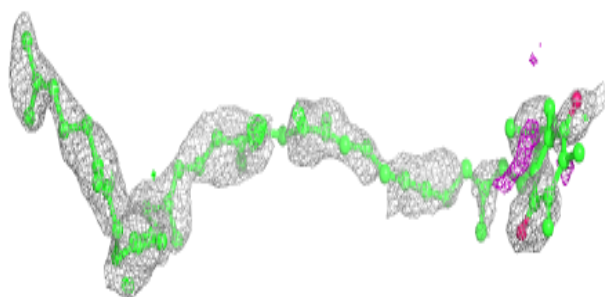
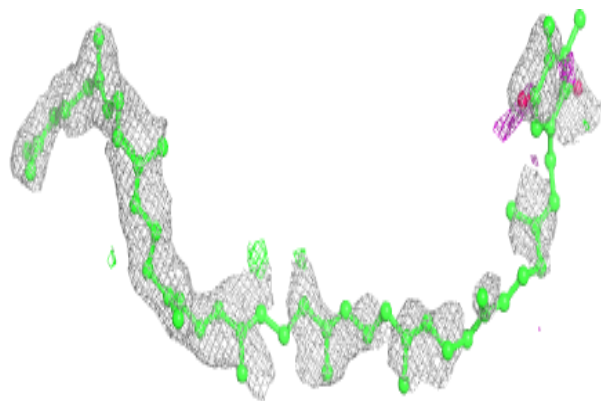
**Electron density around LMT I 102:**

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

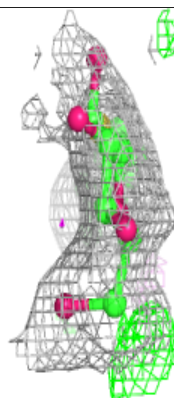
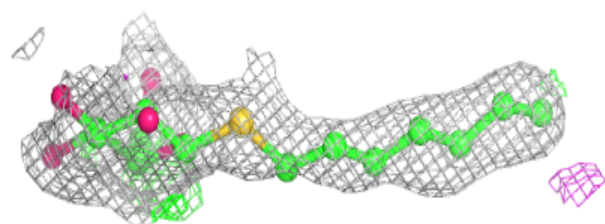
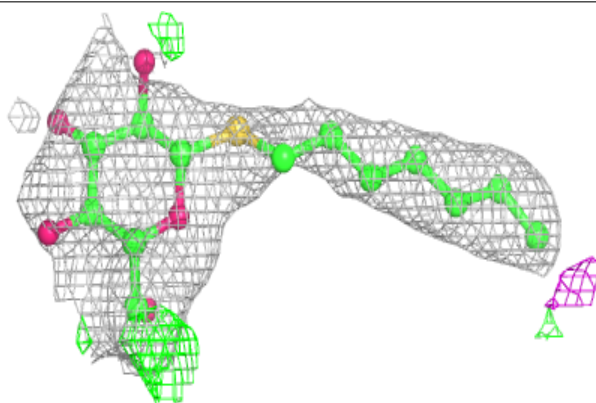


Electron density around PL9 a 416:

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

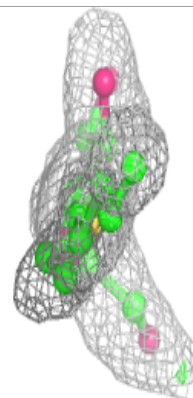
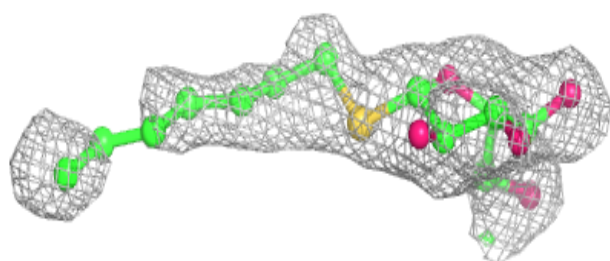
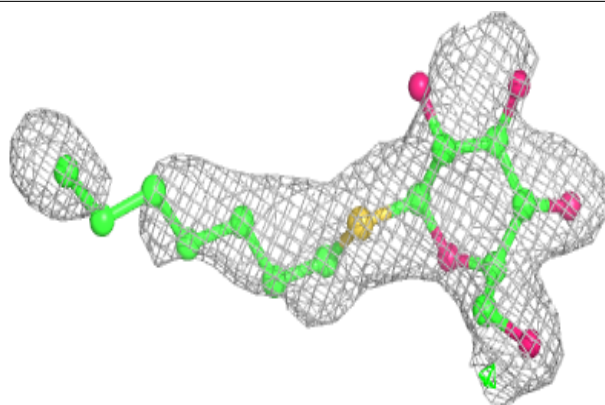
**Electron density around HTG B 631:**

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

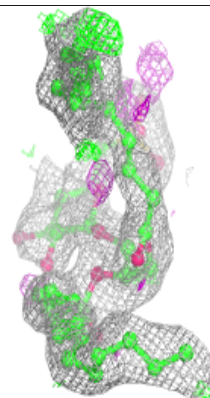
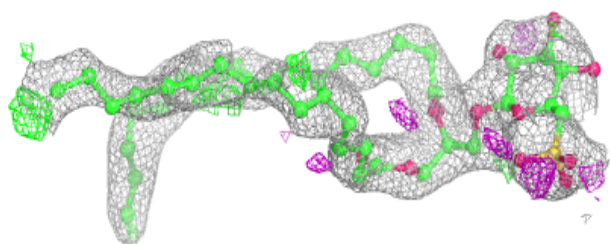
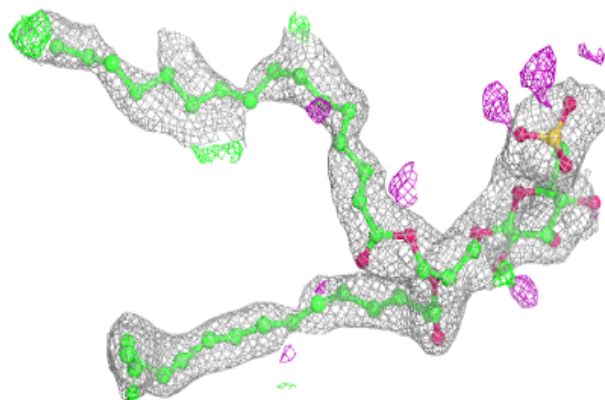


Electron density around HTG C 523:

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

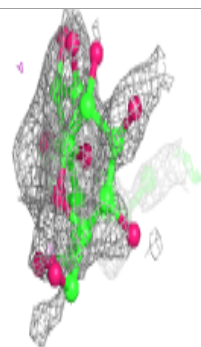
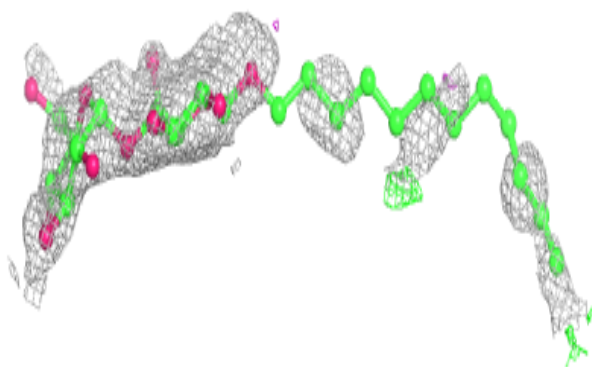
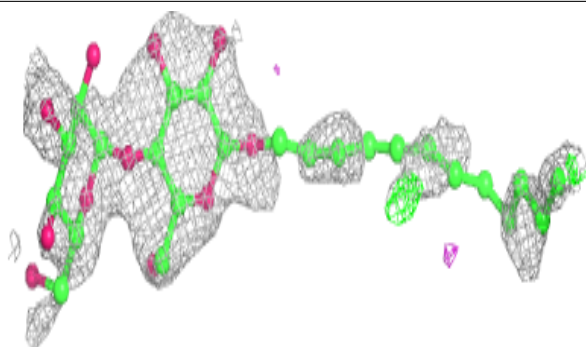
**Electron density around SQD a 402:**

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



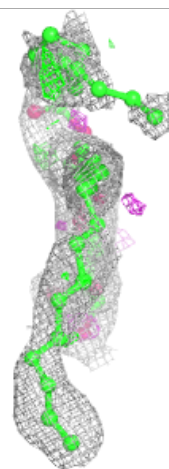
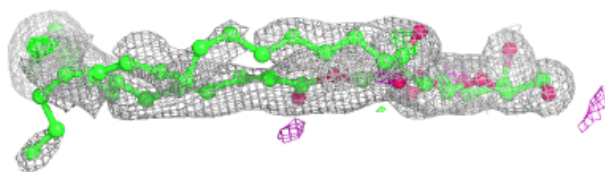
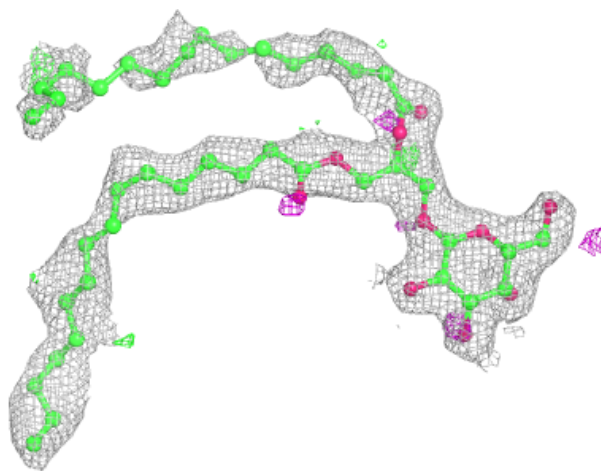
Electron density around LMT a 417:

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



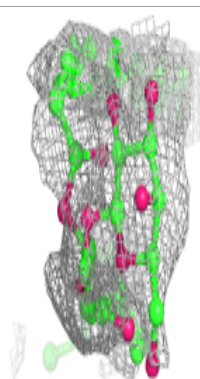
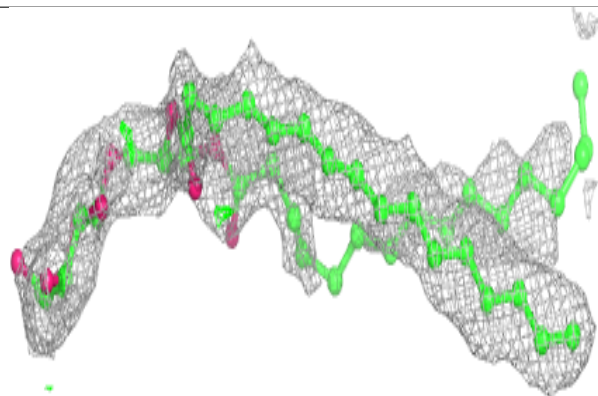
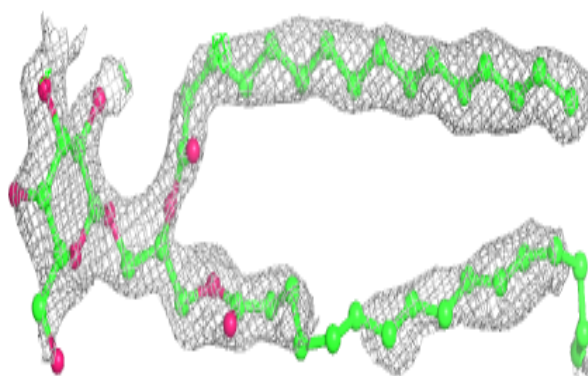
Electron density around LMG C 520:

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

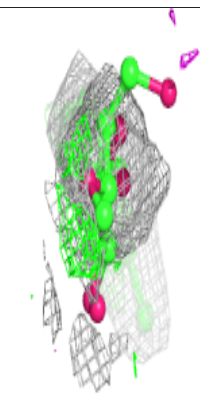
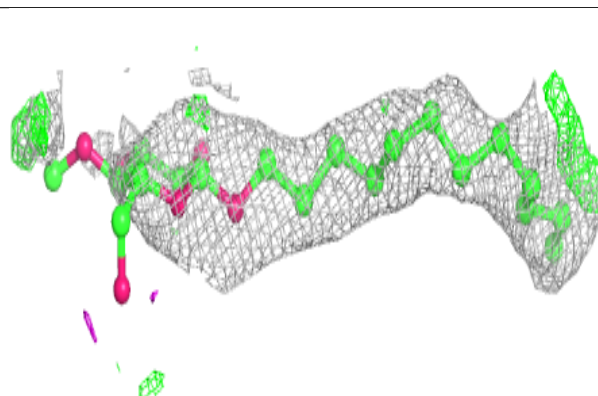
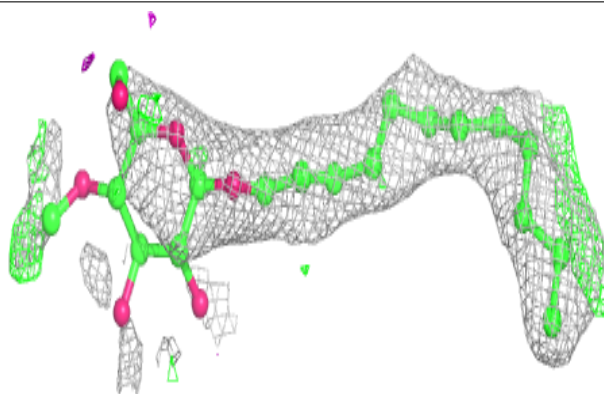


Electron density around LMG c 521:

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

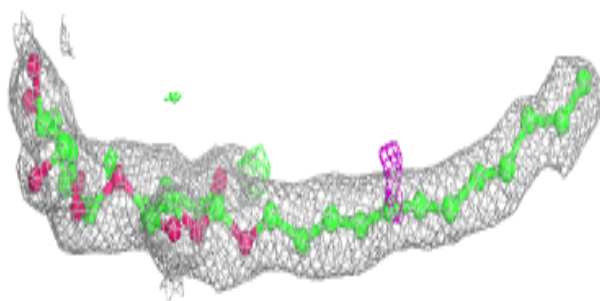
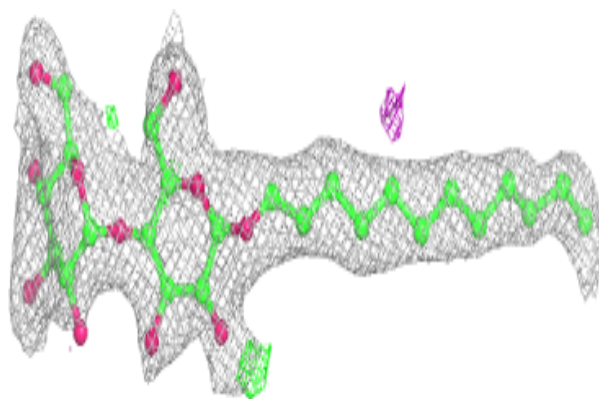
**Electron density around LMT B 634:**

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

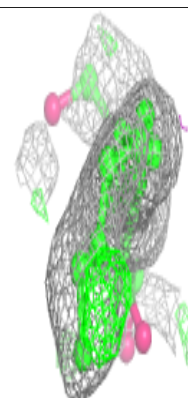
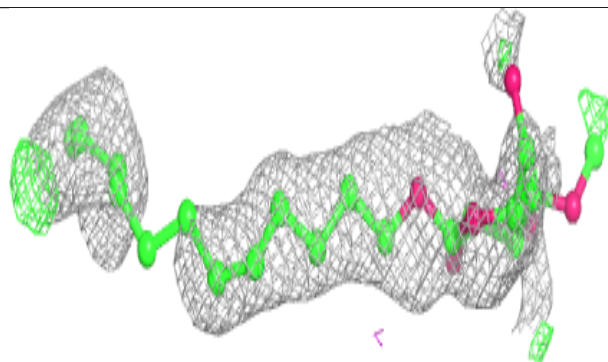
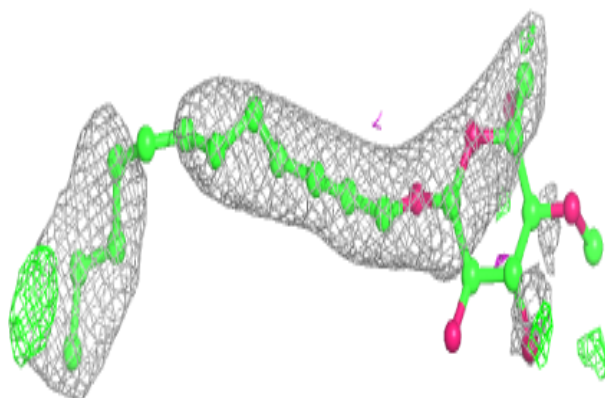


Electron density around LMT M 102:

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

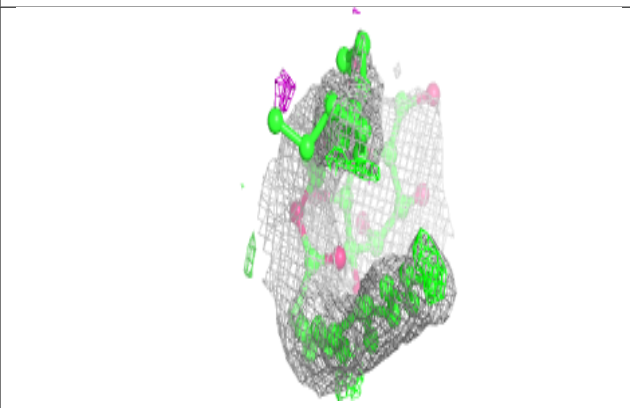
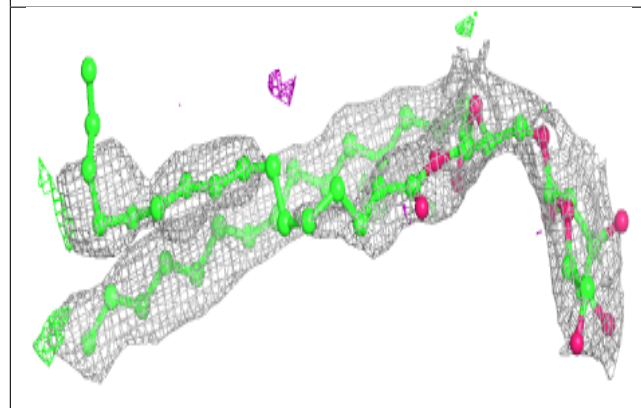
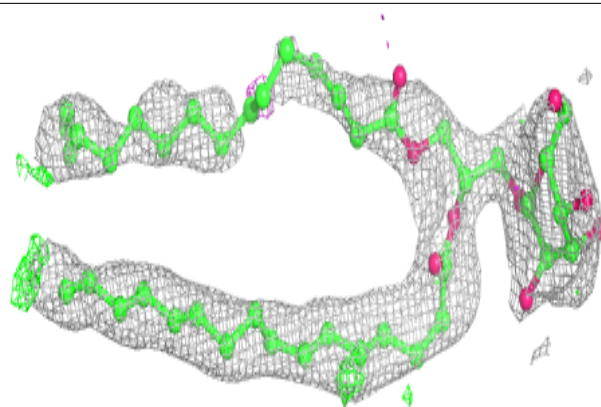
**Electron density around LMT b 602:**

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

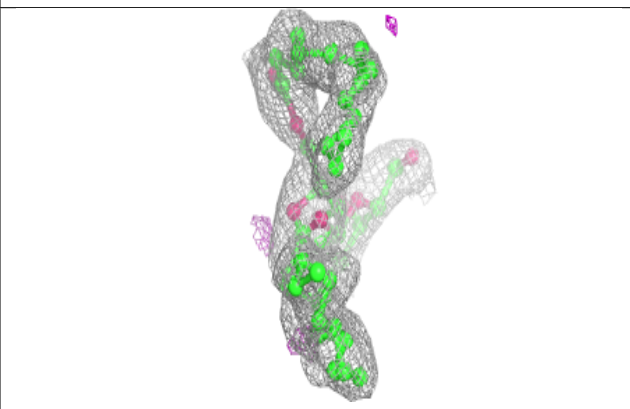
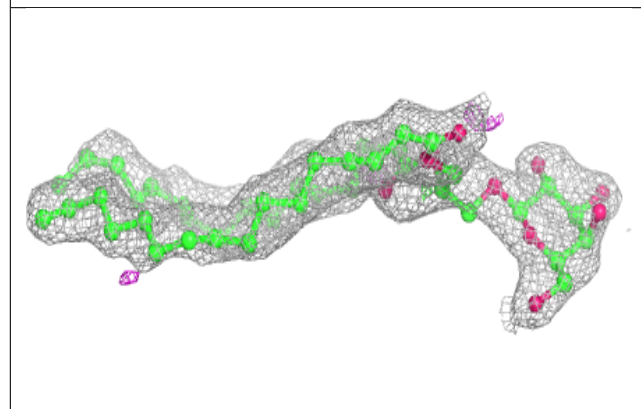
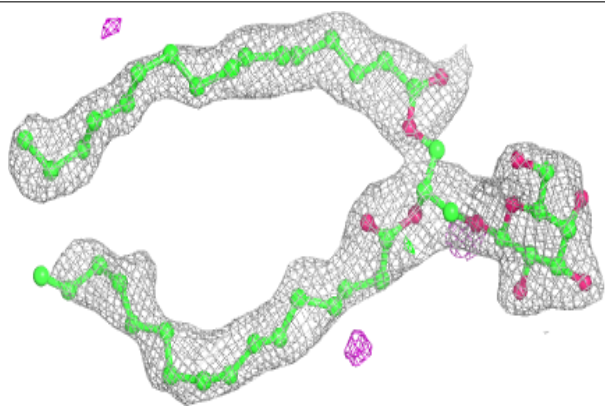


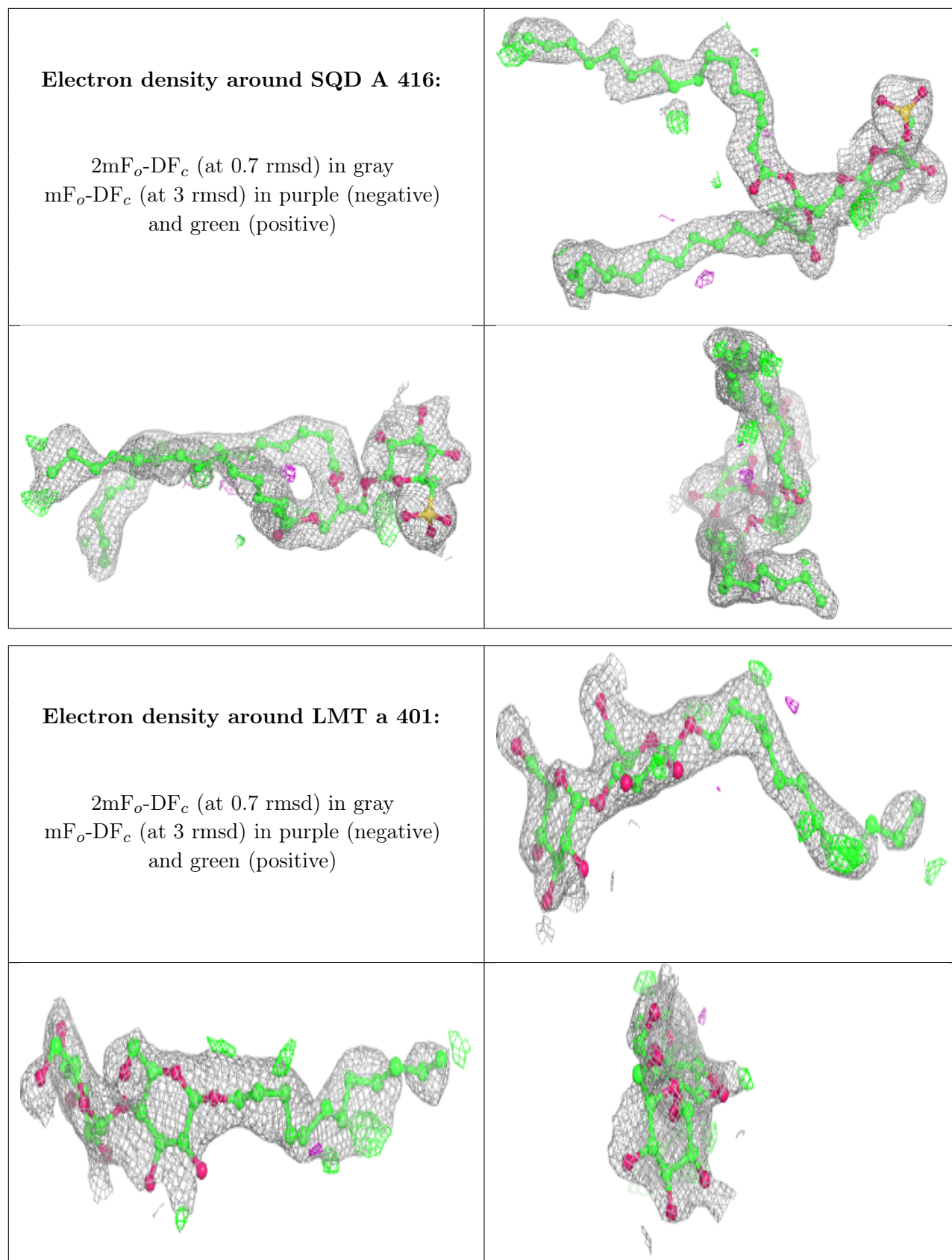
Electron density around LMG C 521:

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

**Electron density around LMG c 501:**

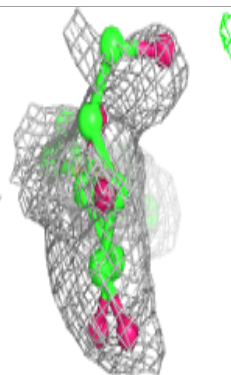
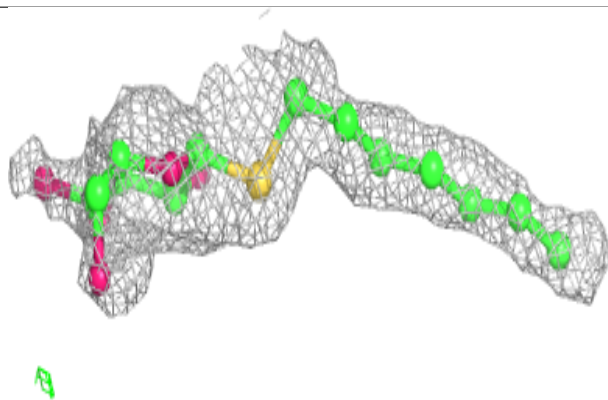
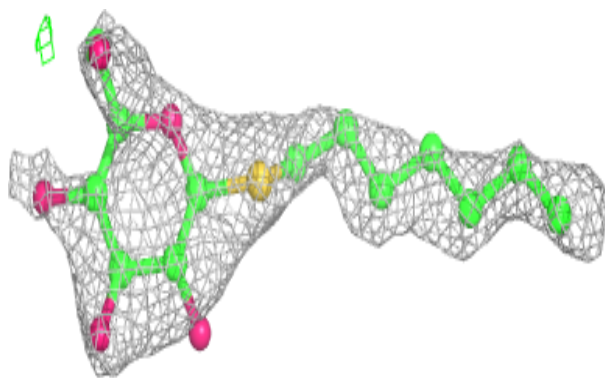
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



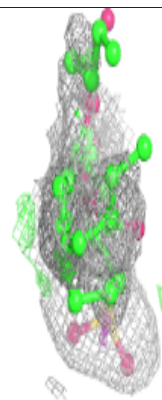
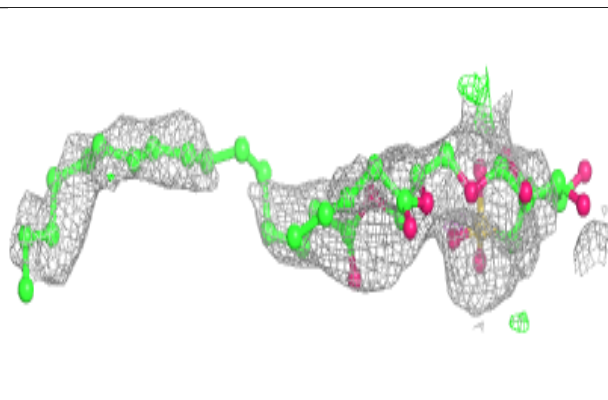
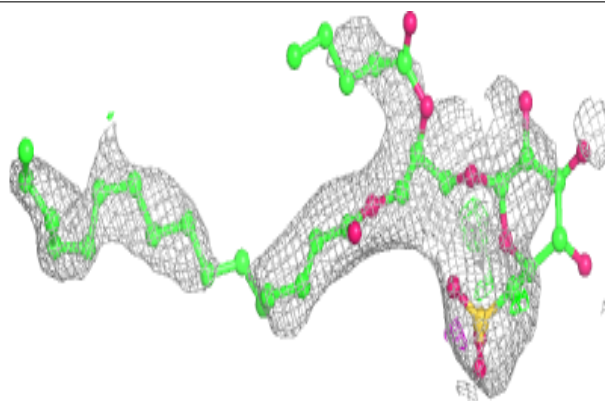


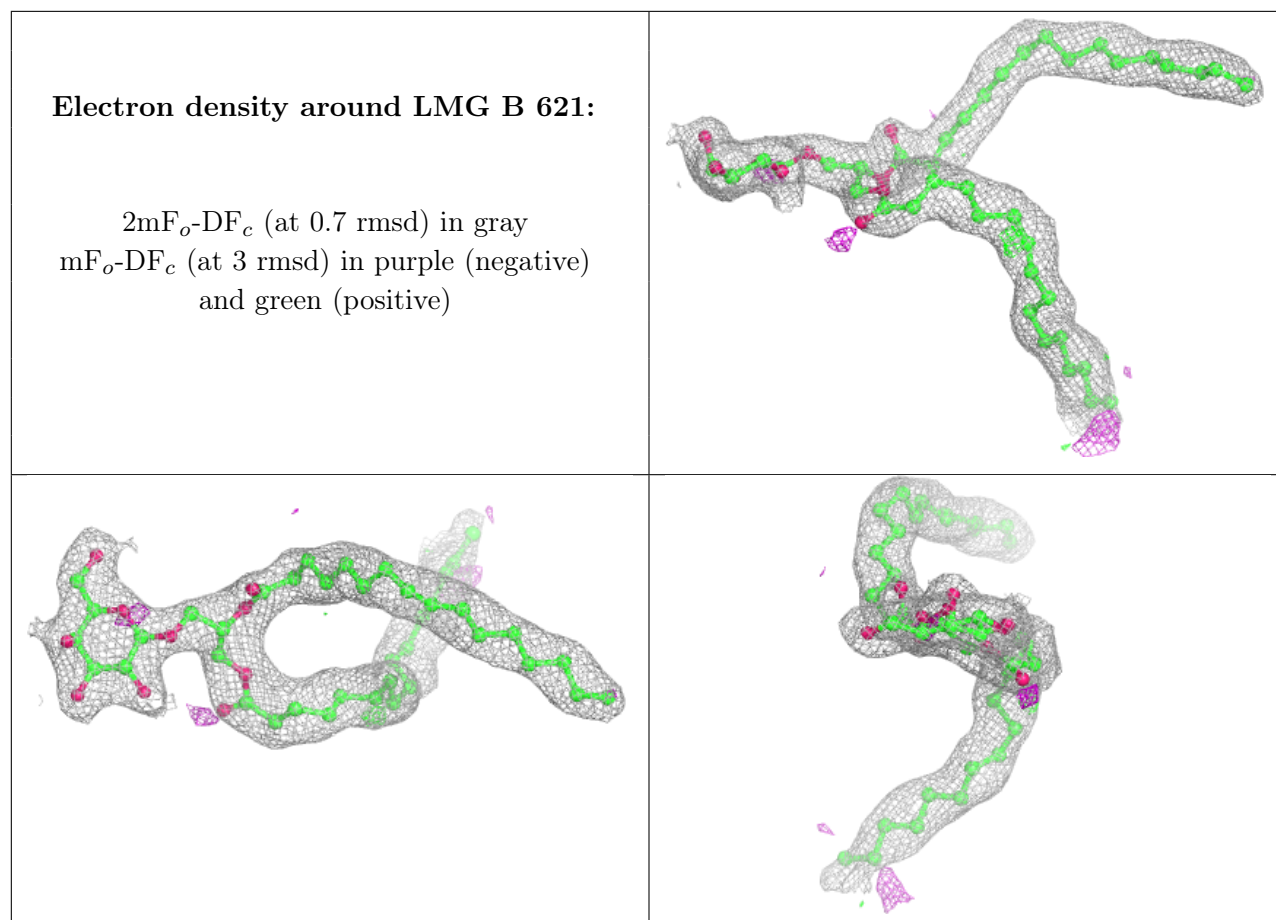
Electron density around HTG c 523:

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

**Electron density around SQD f 101:**

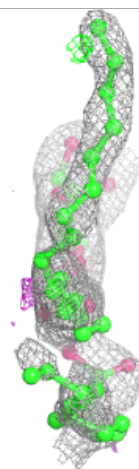
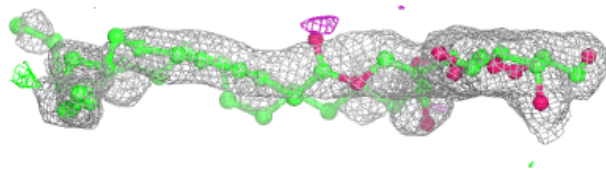
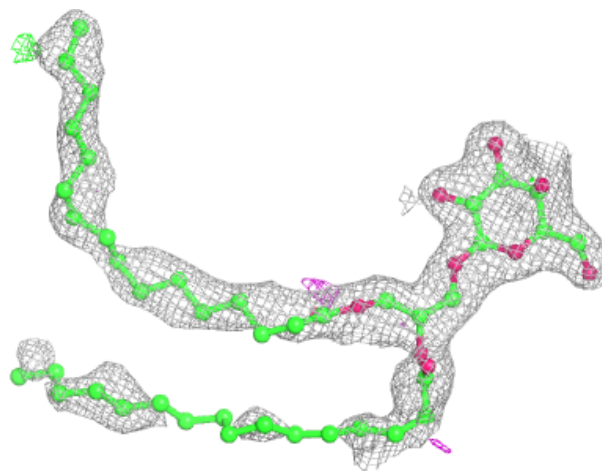
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

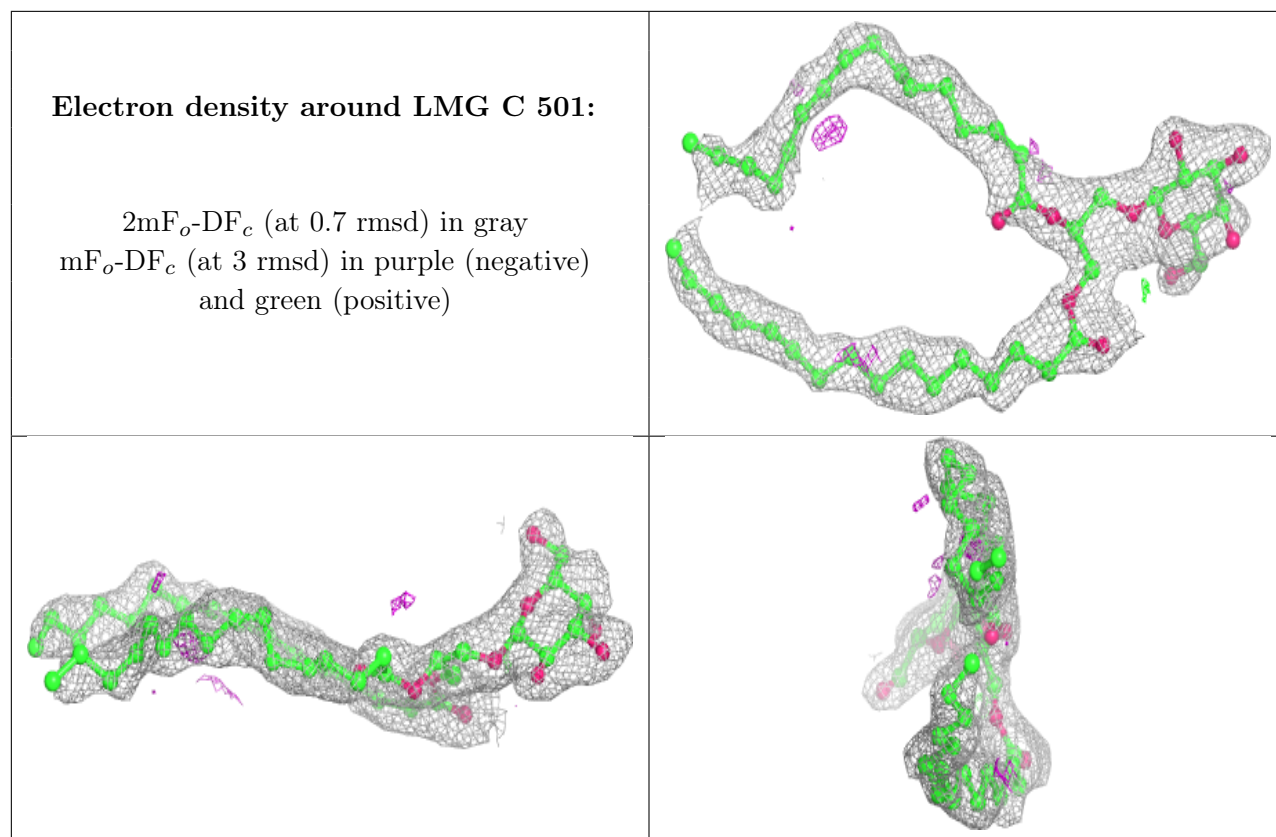




Electron density around LMG c 520:

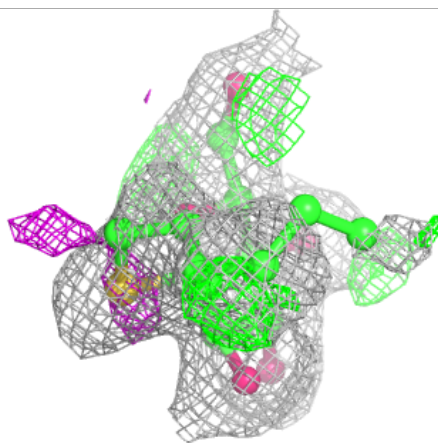
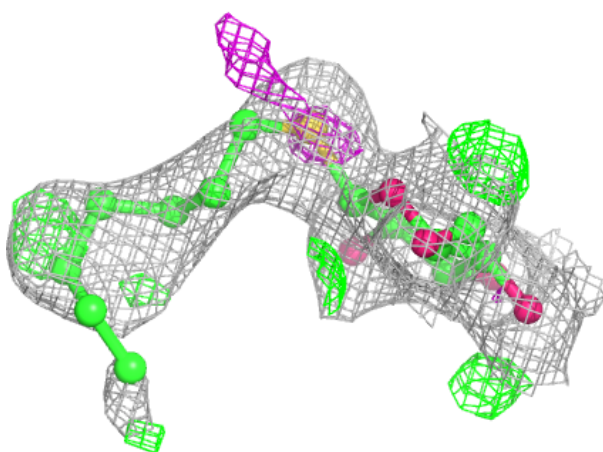
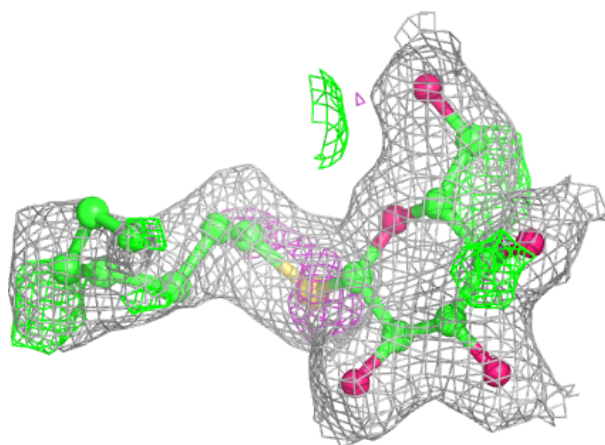
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





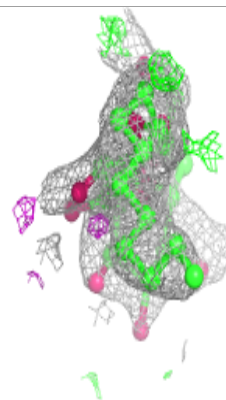
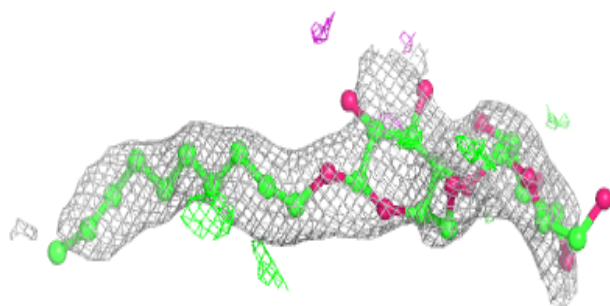
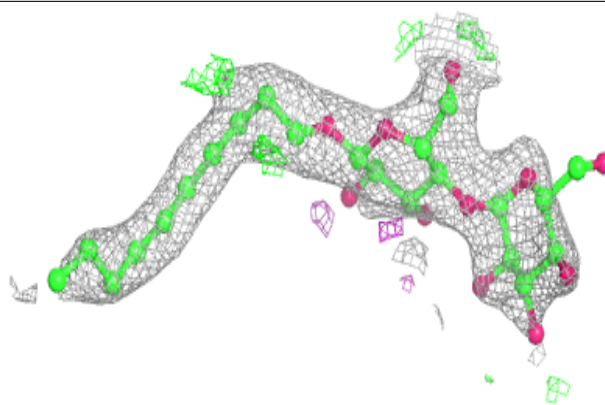
Electron density around HTG B 623:

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

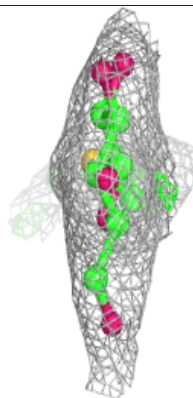
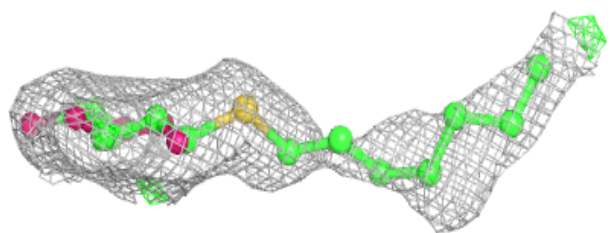
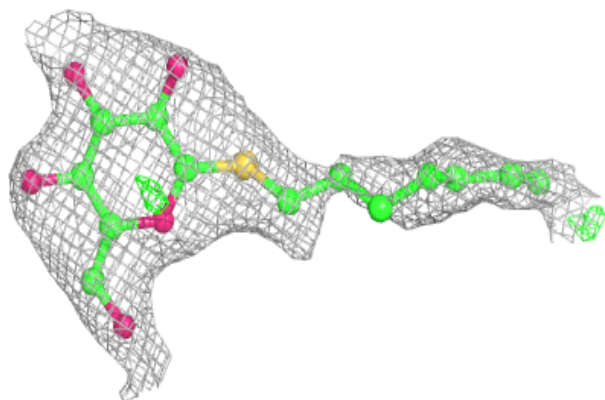


Electron density around LMT A 417:

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

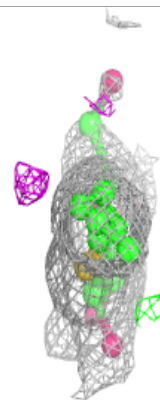
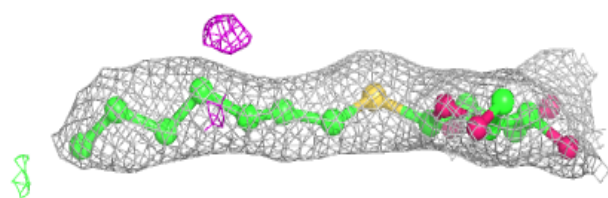
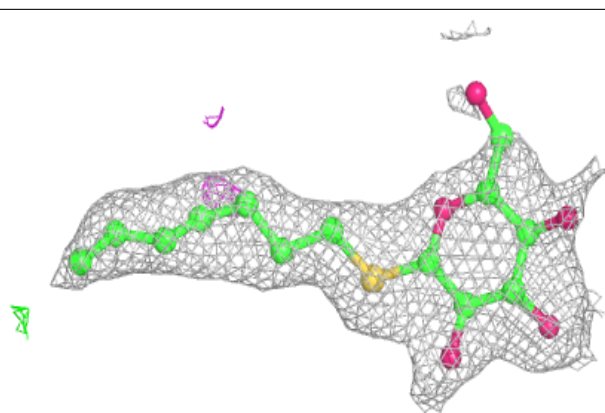
**Electron density around HTG c 522:**

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

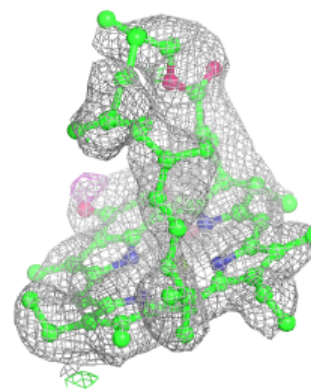
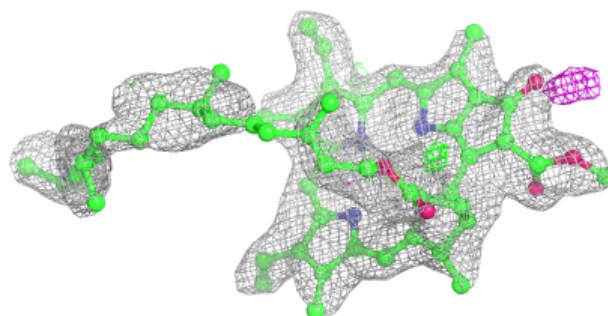
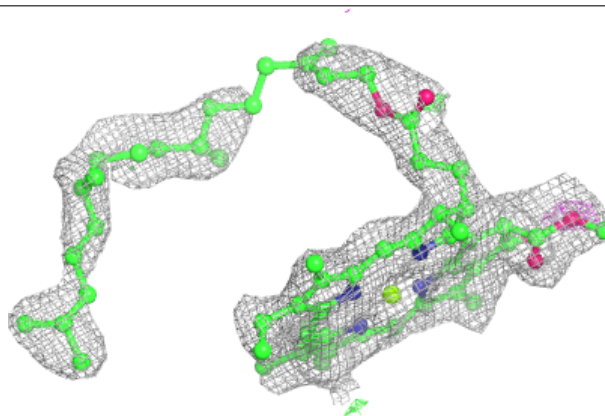


Electron density around HTG B 630:

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

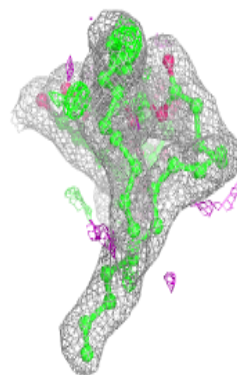
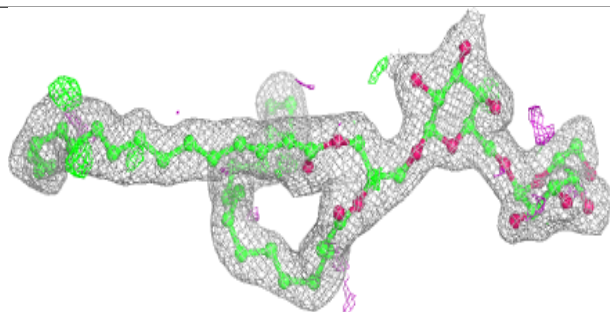
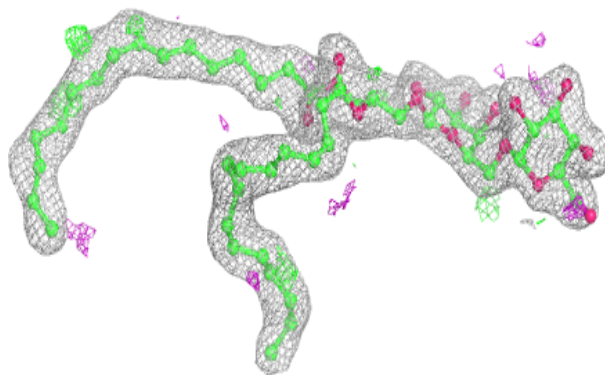
**Electron density around CLA c 515:**

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

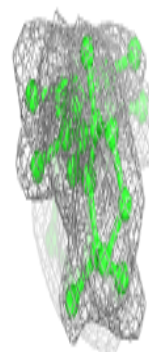
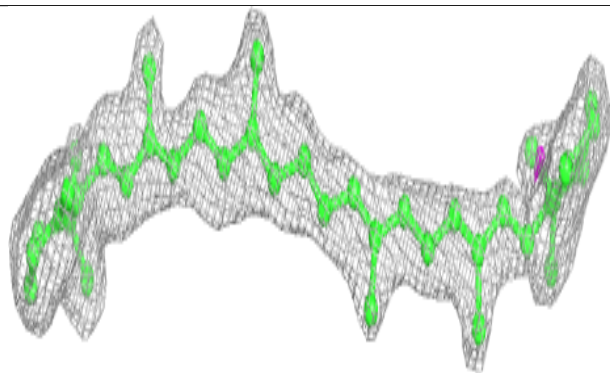
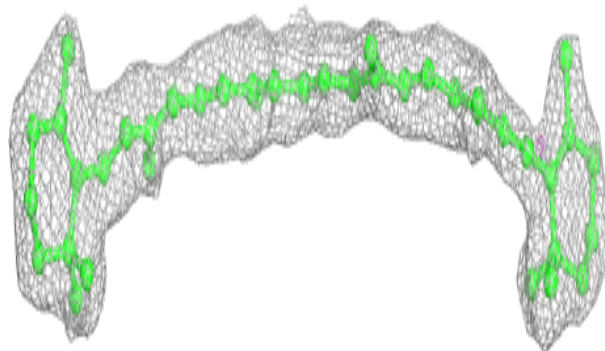


Electron density around DGD H 102:

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

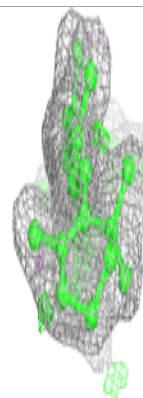
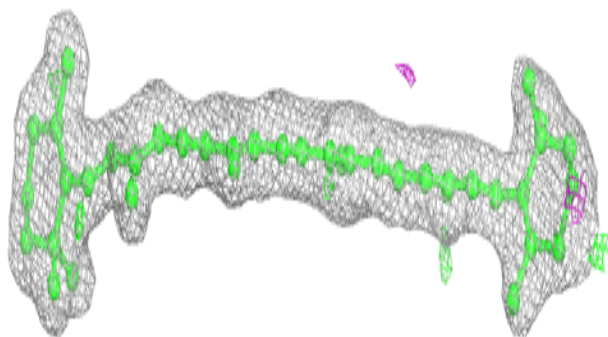
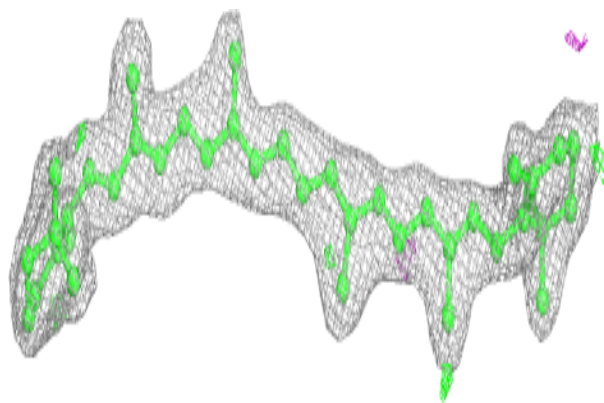
**Electron density around BCR k 103:**

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

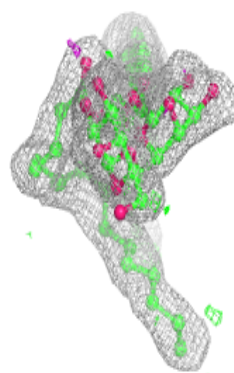
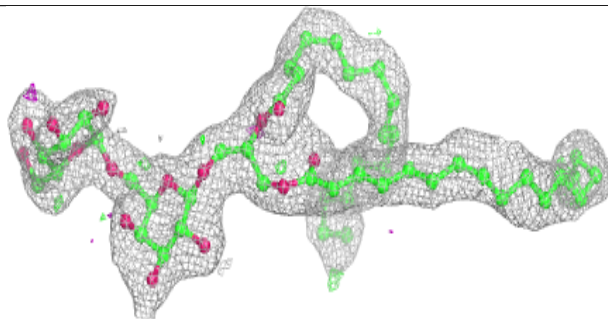
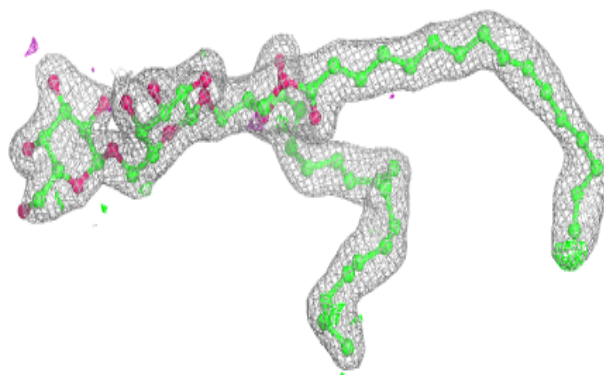


Electron density around BCR h 101:

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

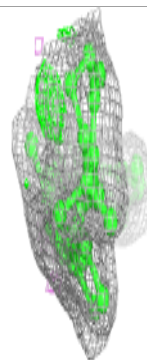
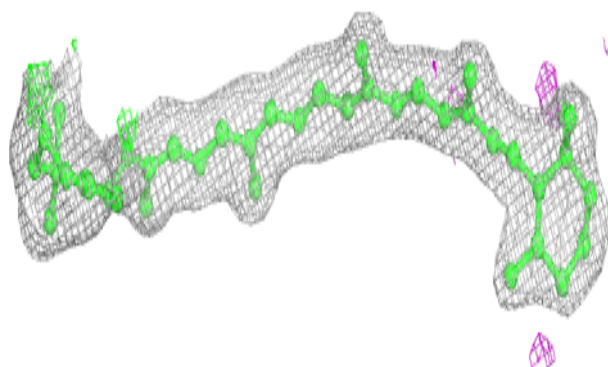
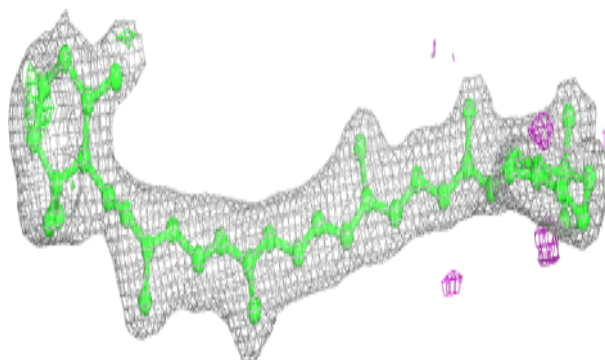
**Electron density around DGD h 102:**

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

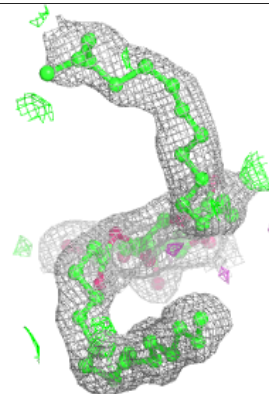
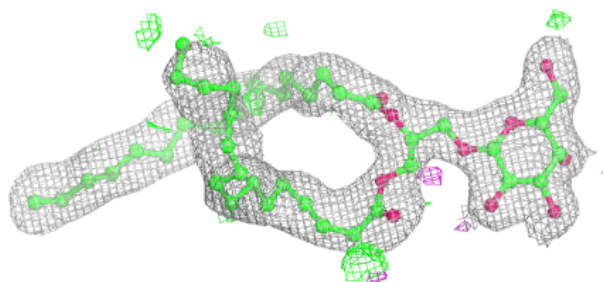
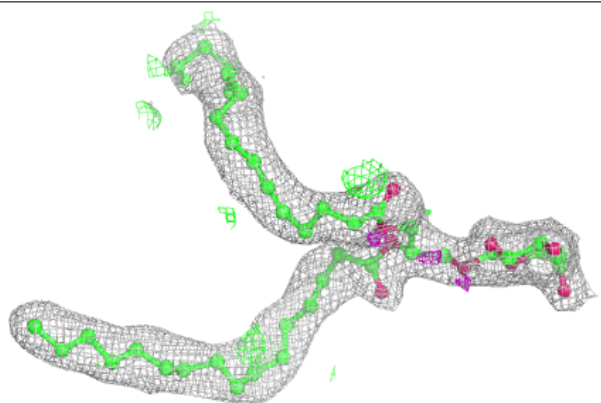


Electron density around BCR d 405:

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

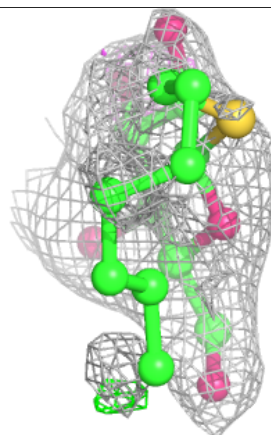
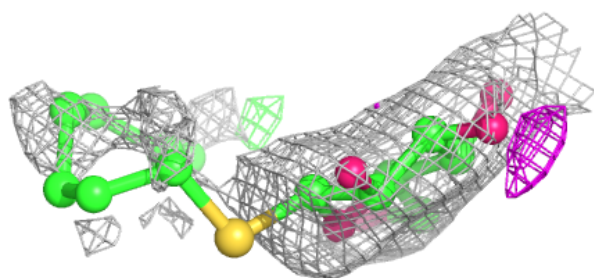
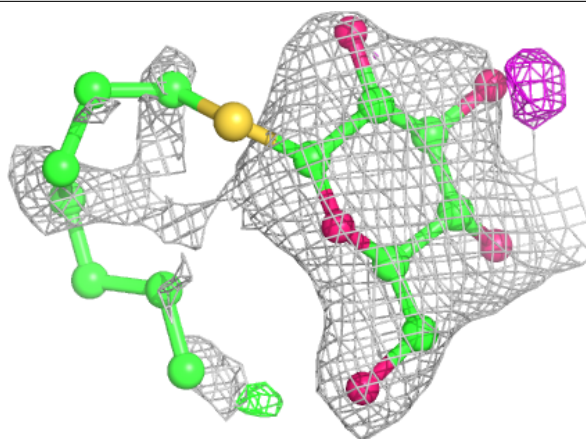
**Electron density around LMG b 625:**

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

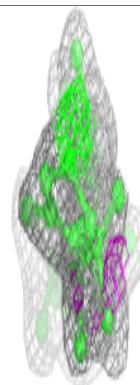
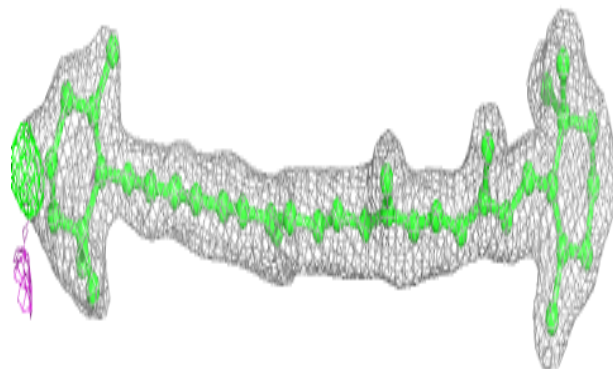
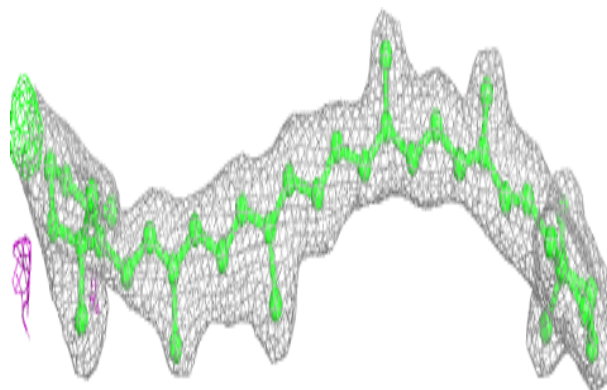


Electron density around HTG V 204:

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

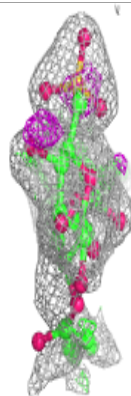
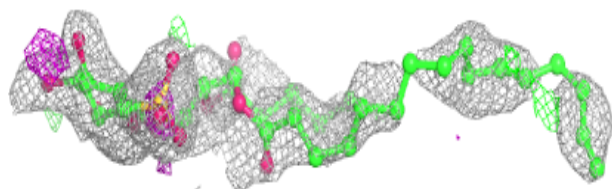
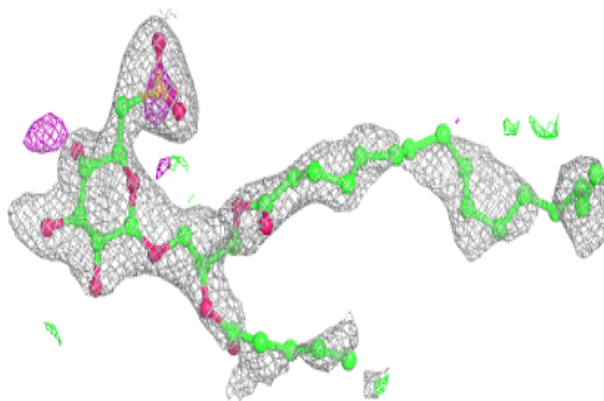
**Electron density around BCR H 101:**

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



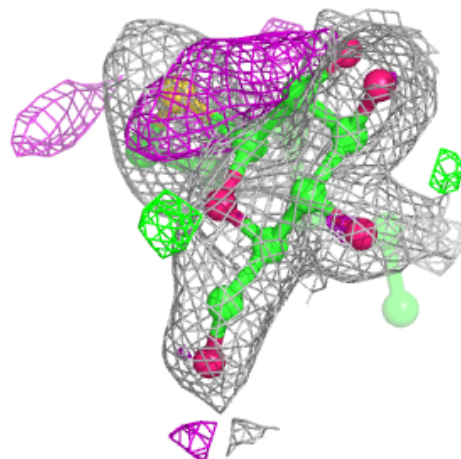
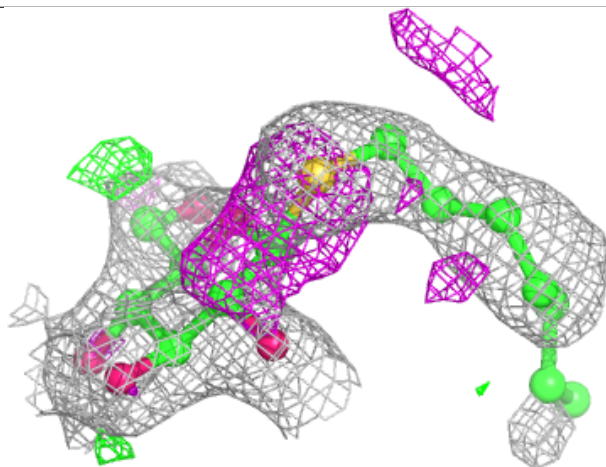
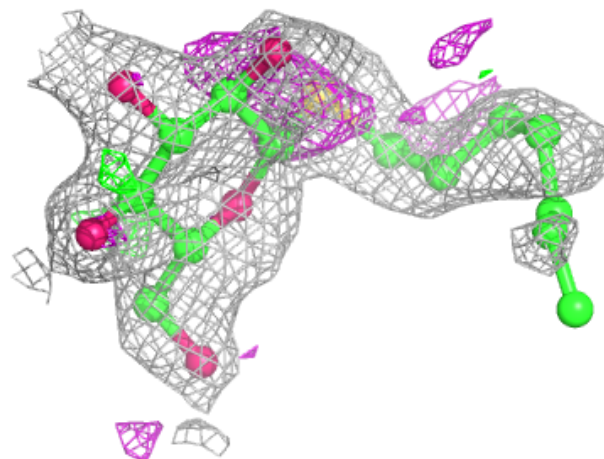
Electron density around SQD F 101:

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



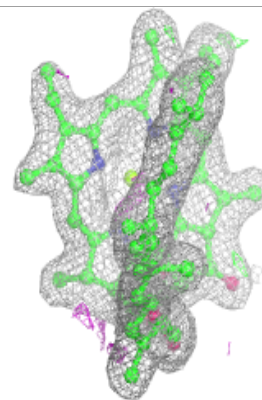
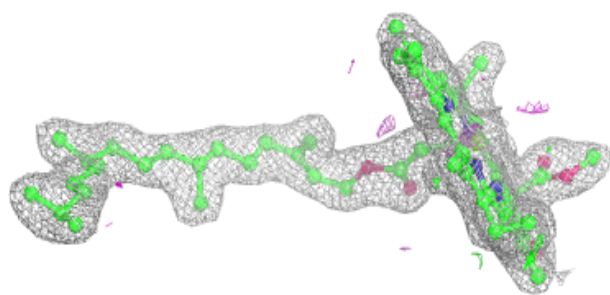
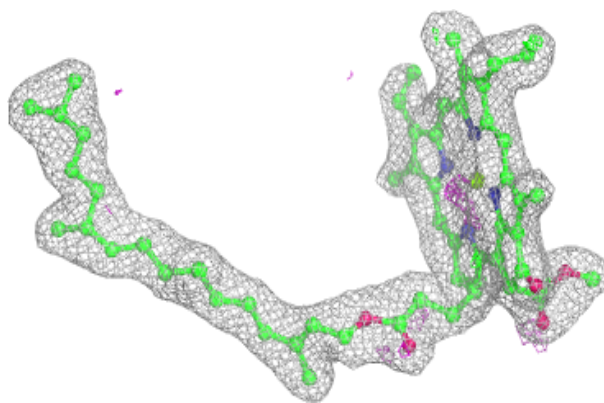
Electron density around HTG b 627:

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

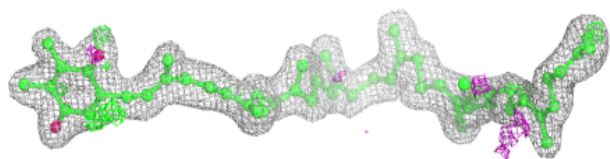
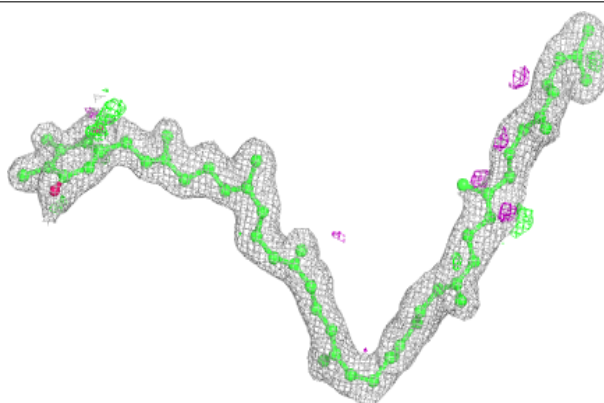


Electron density around CLA b 614:

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

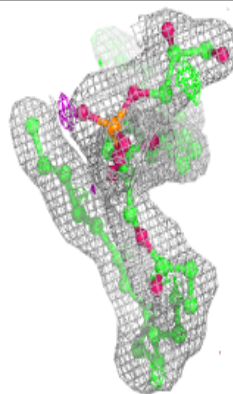
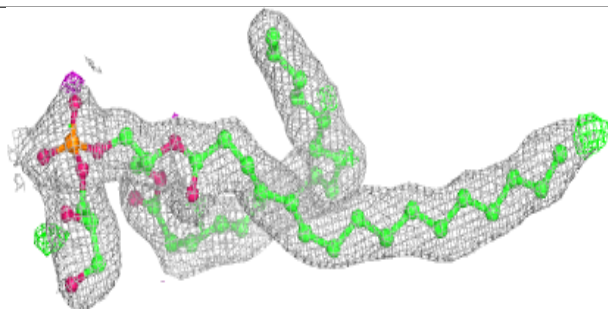
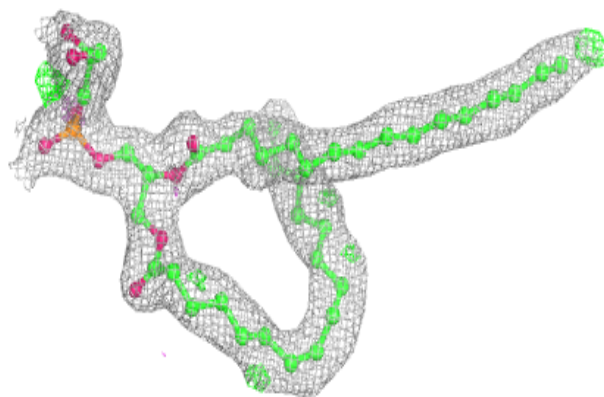
**Electron density around PL9 d 406:**

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



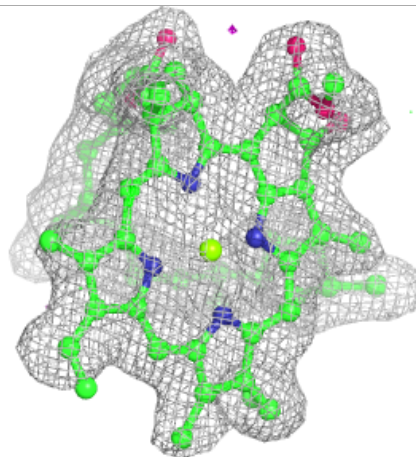
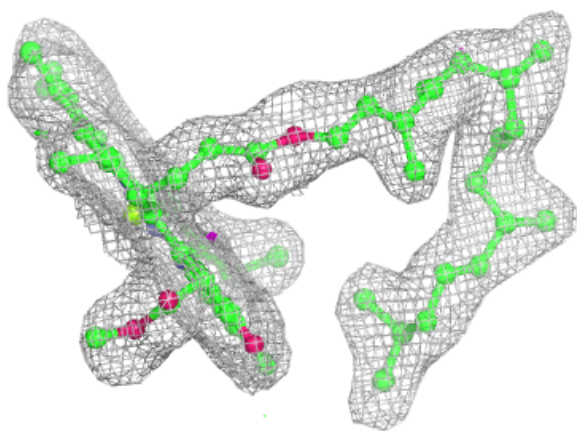
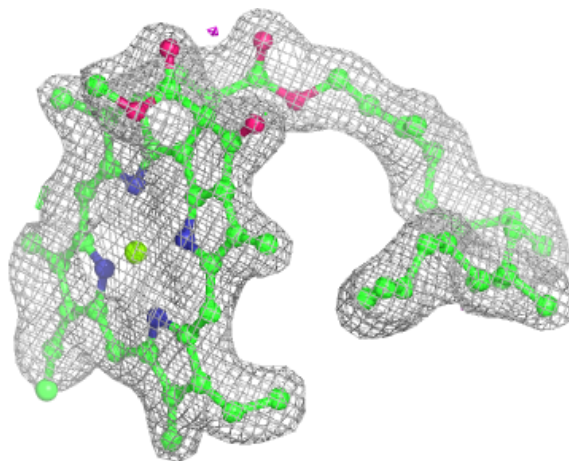
Electron density around LHG d 408:

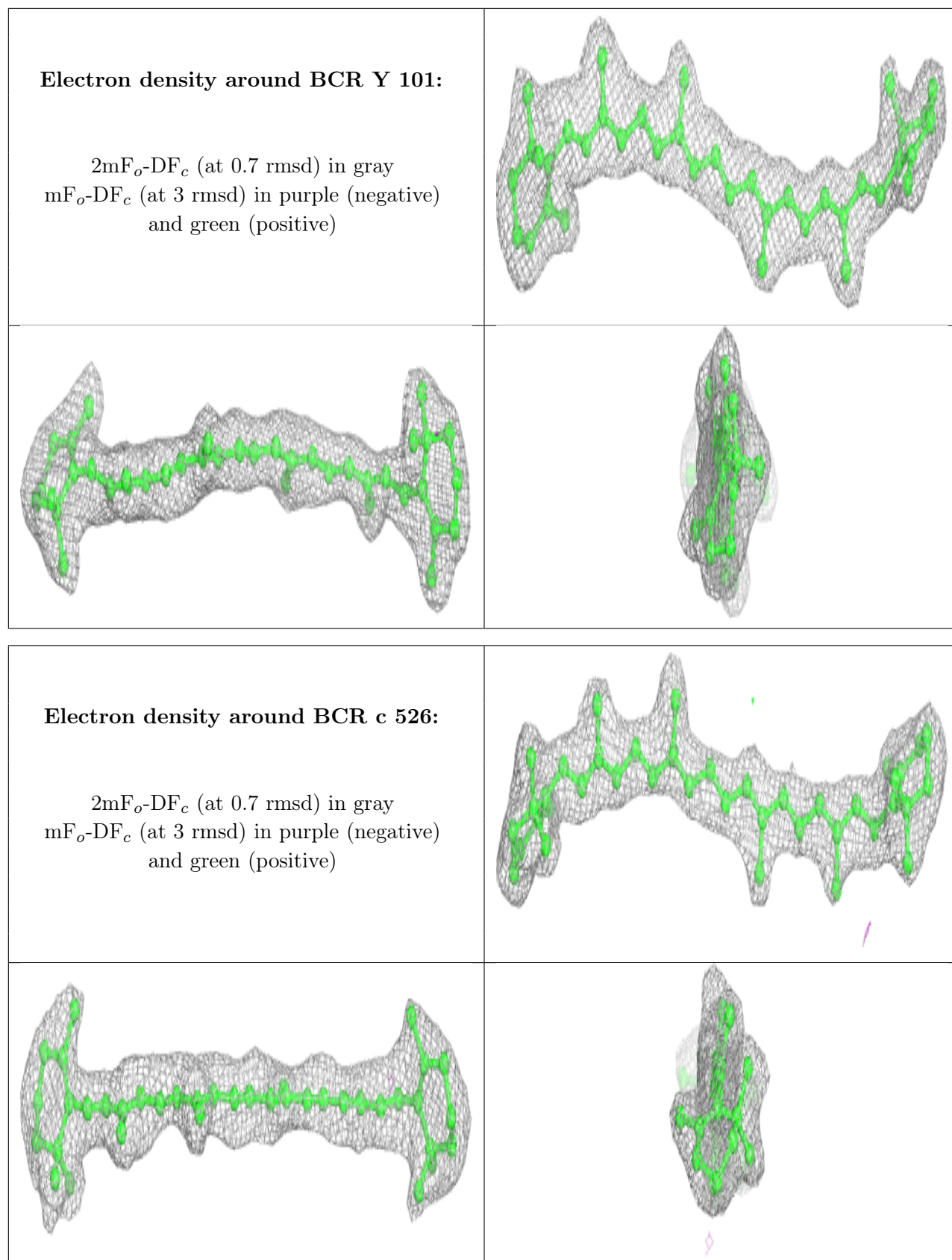
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 505:

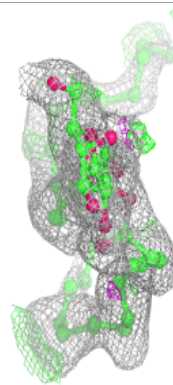
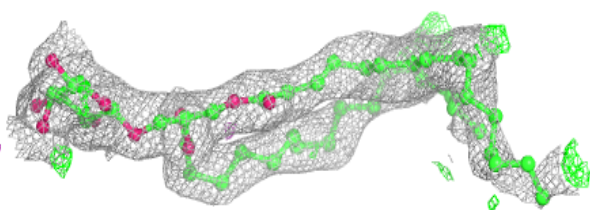
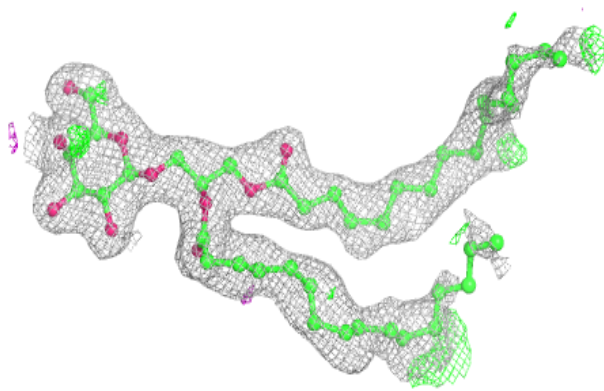
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





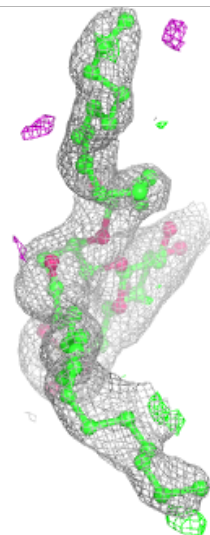
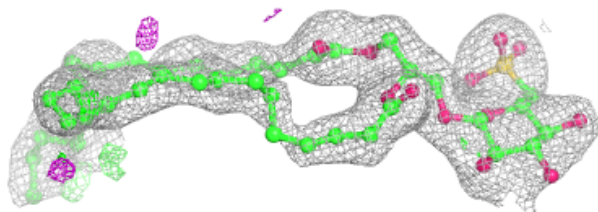
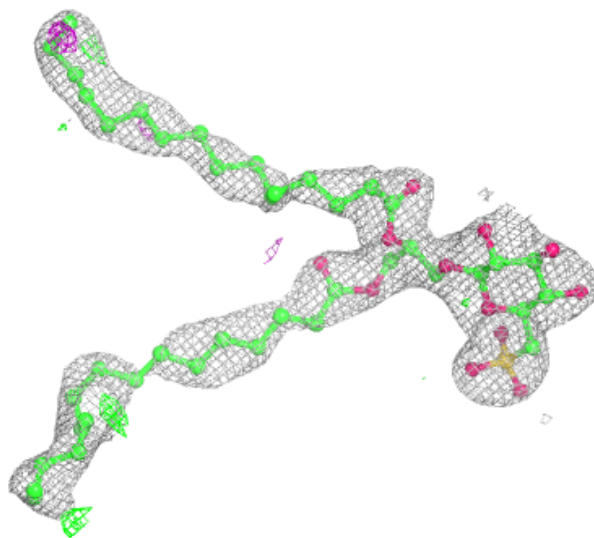
Electron density around LMG j 101:

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



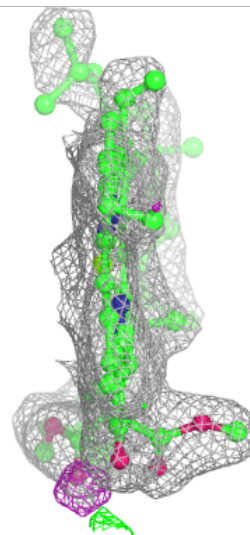
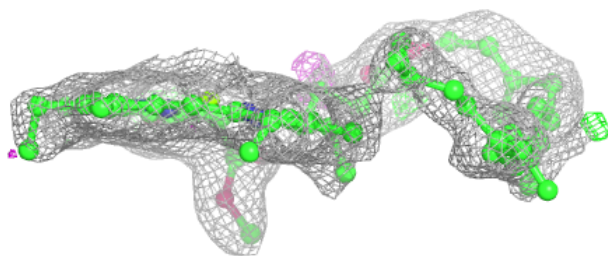
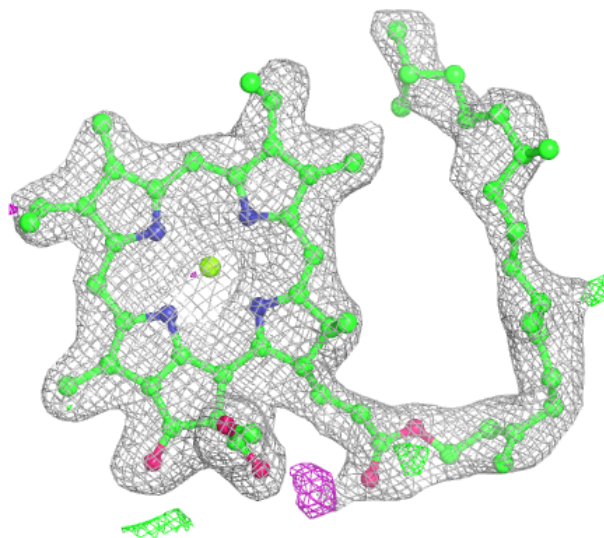
Electron density around SQD a 411:

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



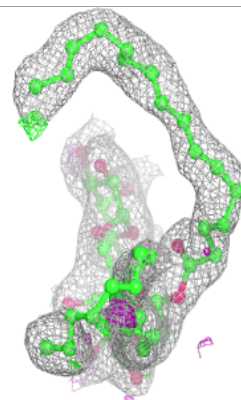
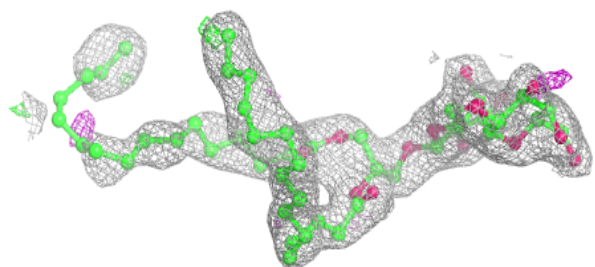
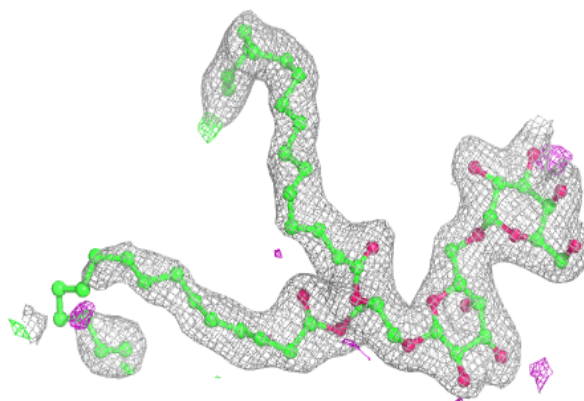
Electron density around CLA c 514:

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

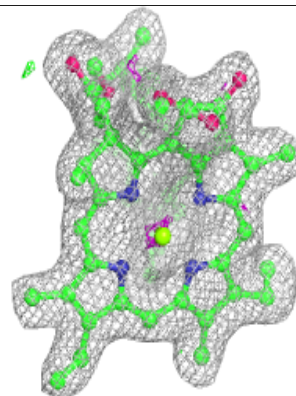
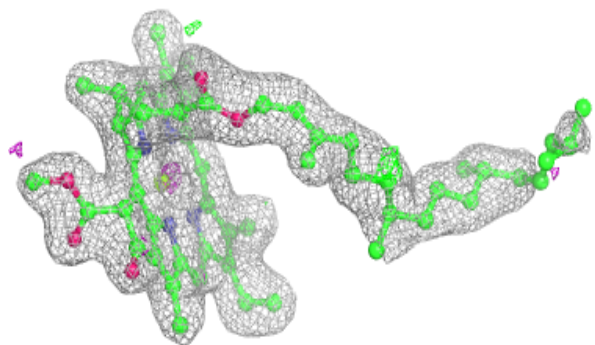
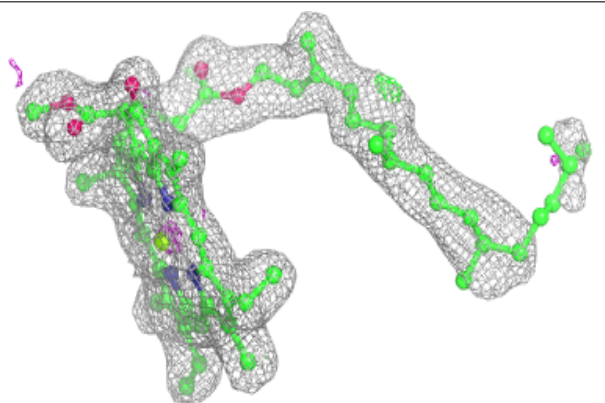


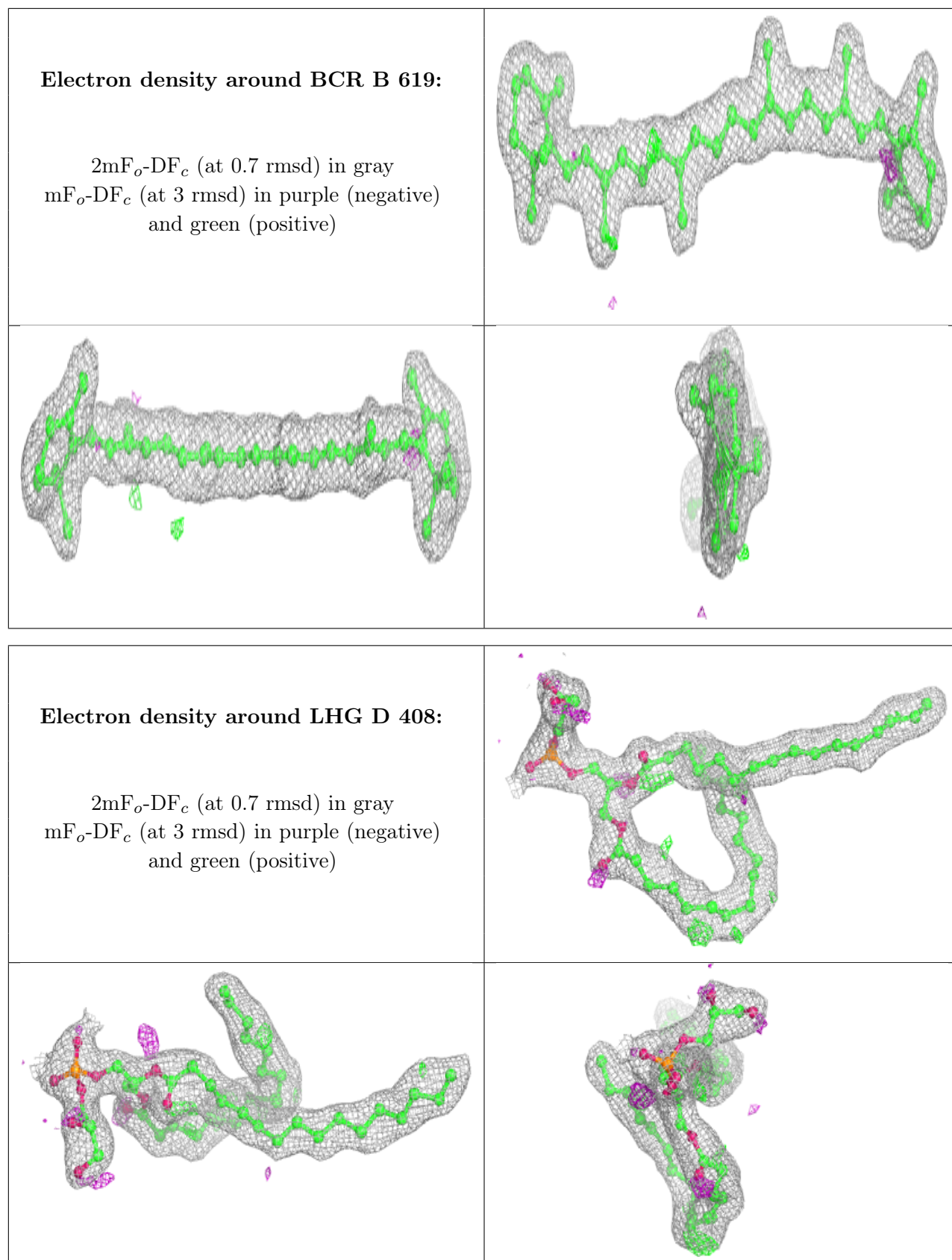
Electron density around DGD c 518:

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

**Electron density around CLA C 509:**

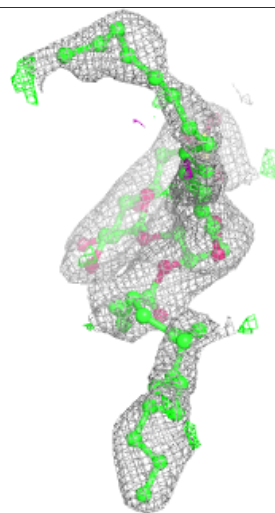
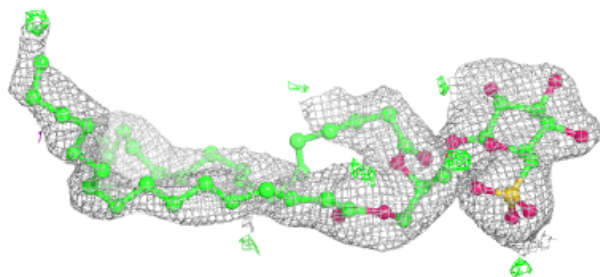
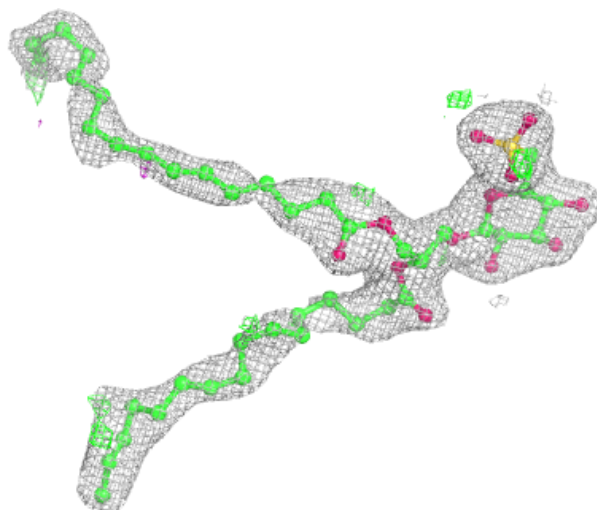
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





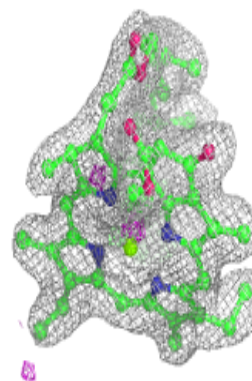
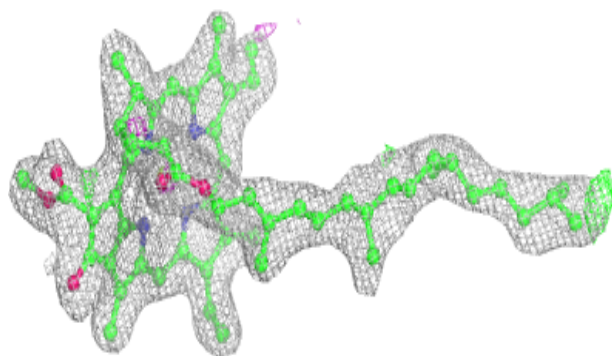
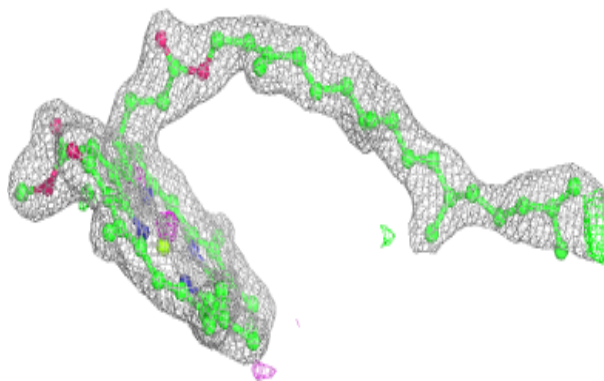
Electron density around SQD A 411:

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

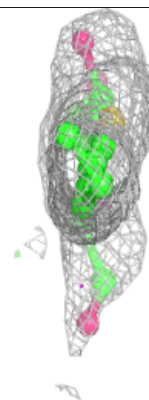
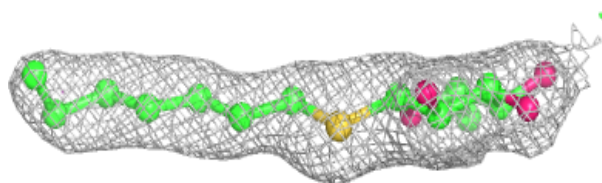
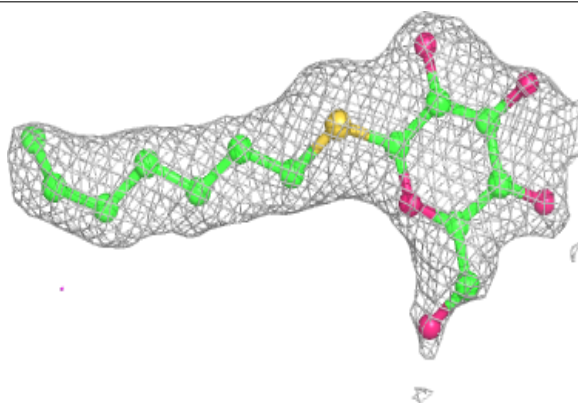


Electron density around CLA c 506:

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

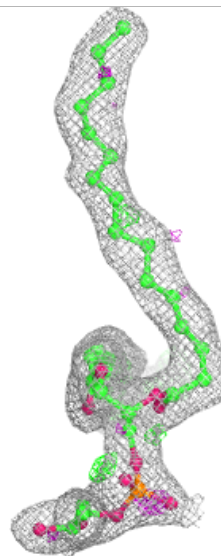
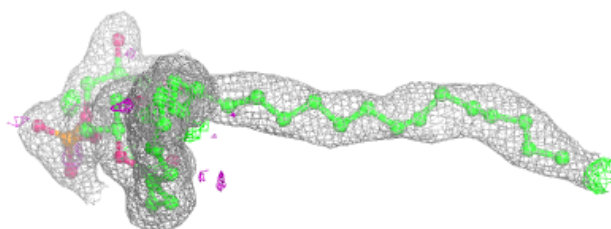
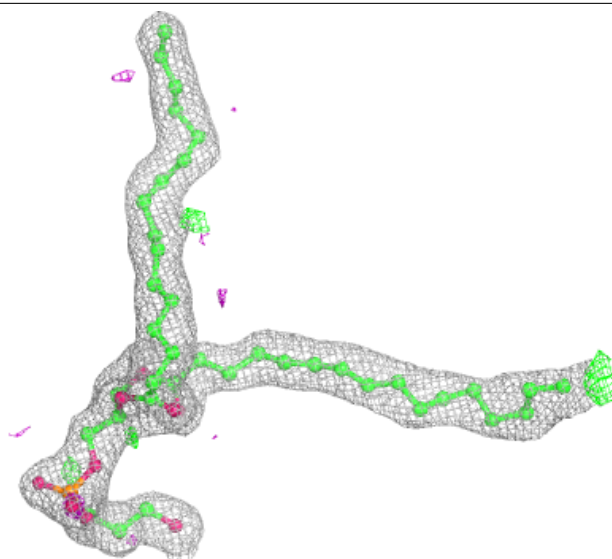
**Electron density around HTG b 603:**

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



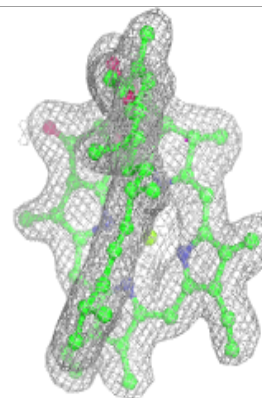
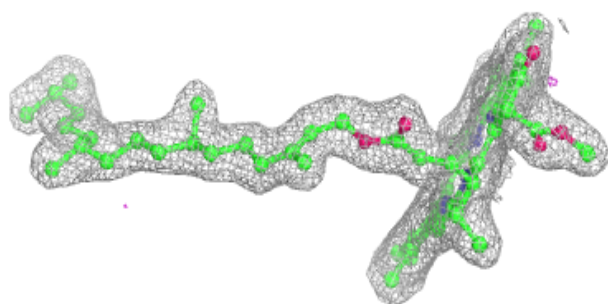
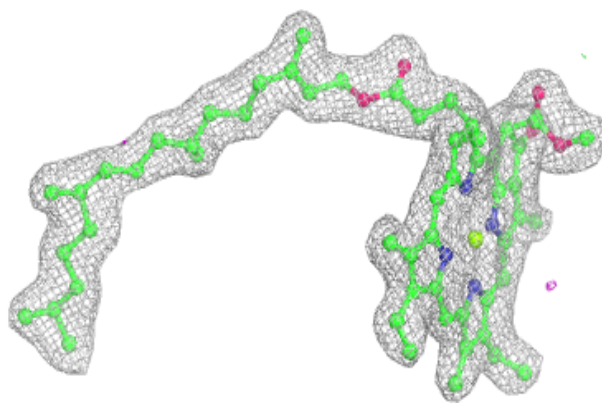
Electron density around LHG 1 102:

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

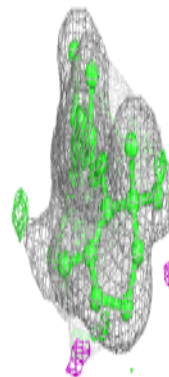
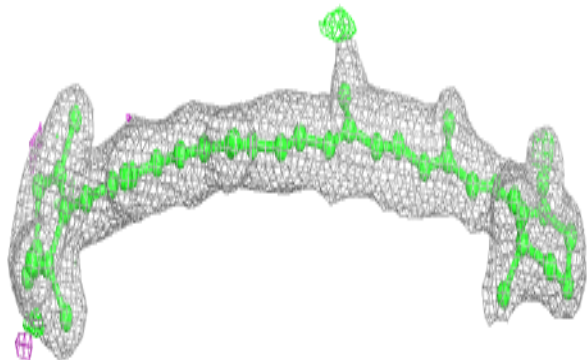
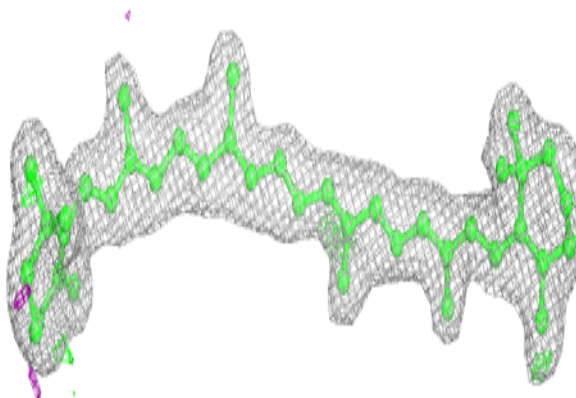


Electron density around CLA B 610:

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

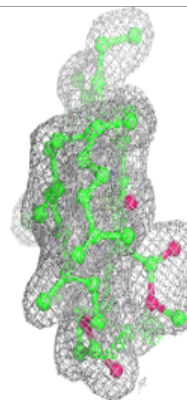
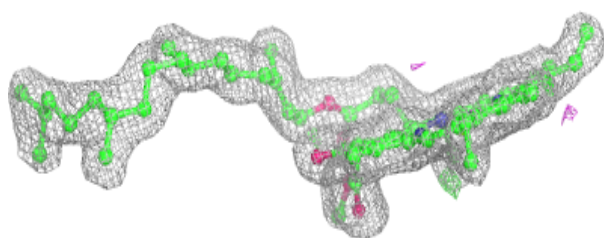
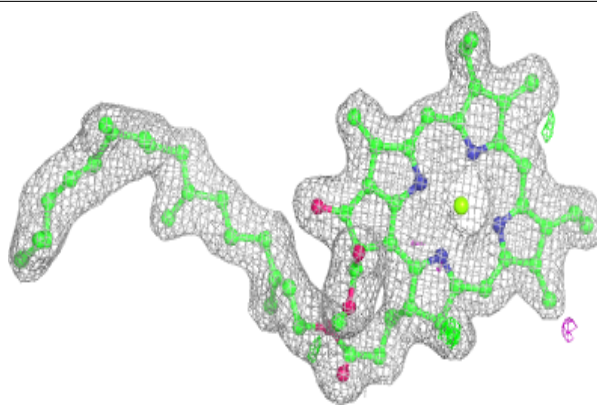
**Electron density around BCR T 102:**

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

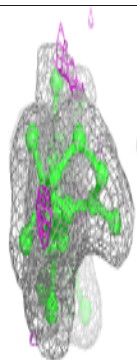
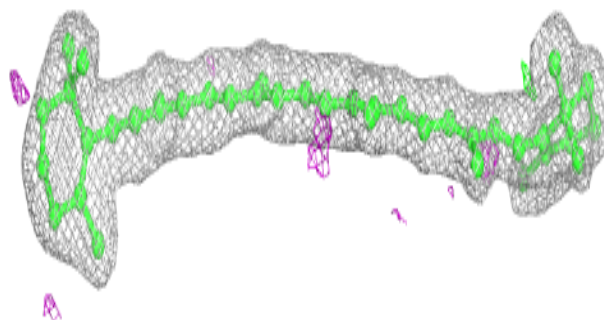
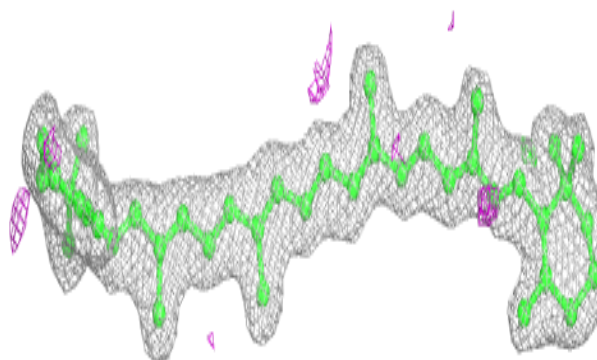


Electron density around CLA B 603:

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

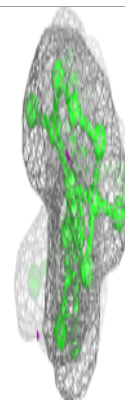
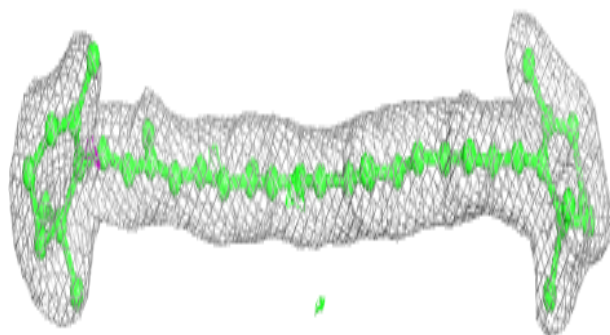
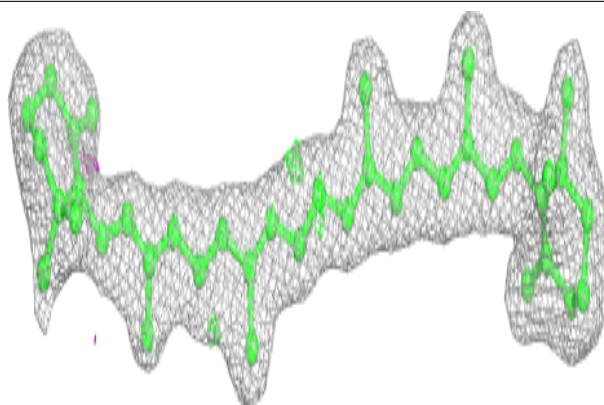
**Electron density around BCR b 622:**

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

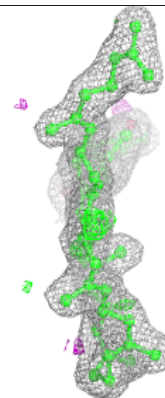
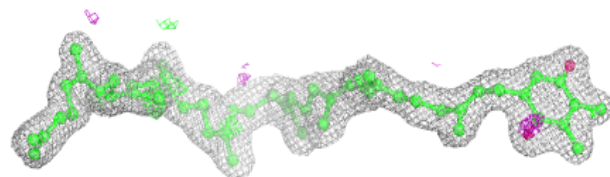
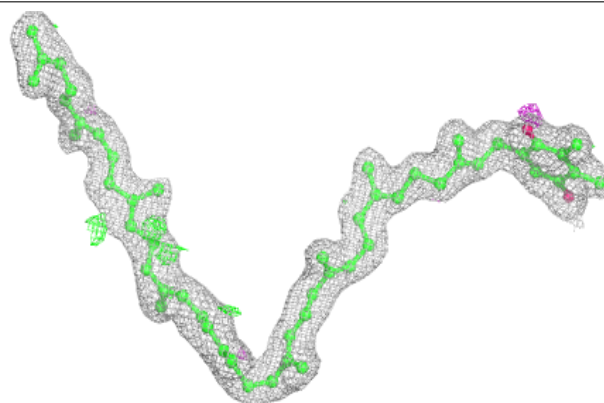


Electron density around BCR b 623:

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

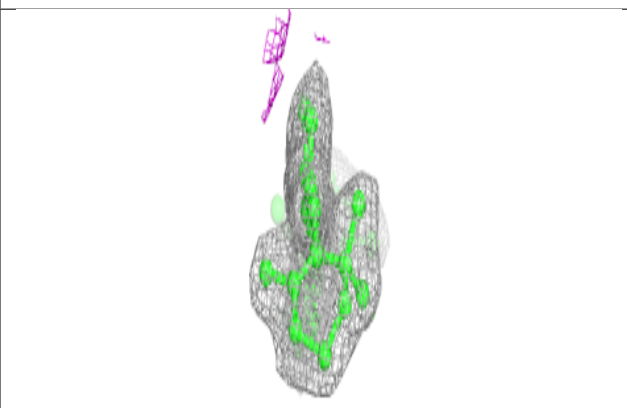
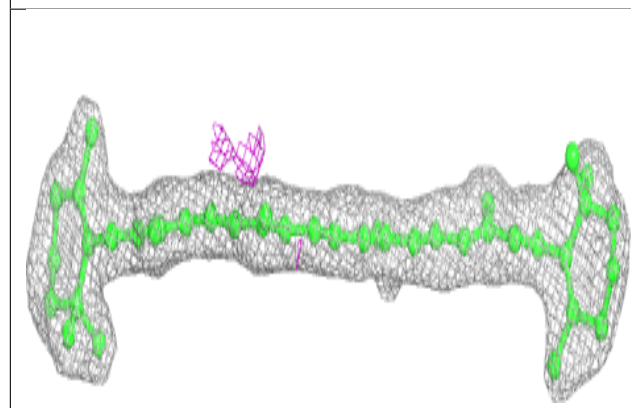
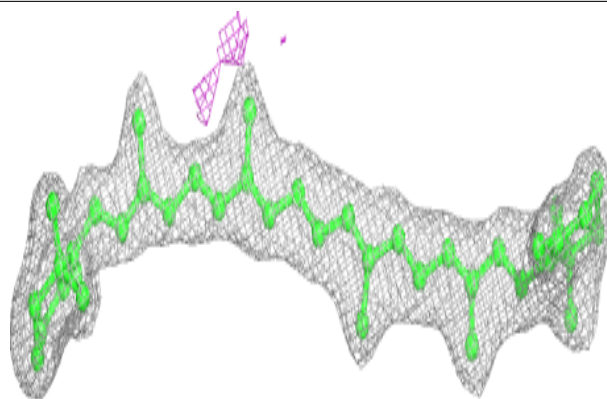
**Electron density around PL9 D 406:**

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

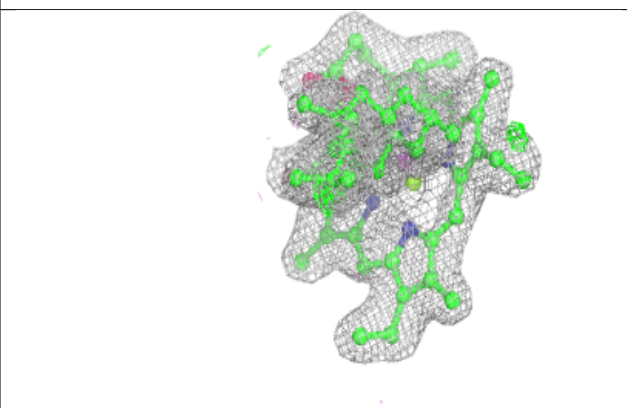
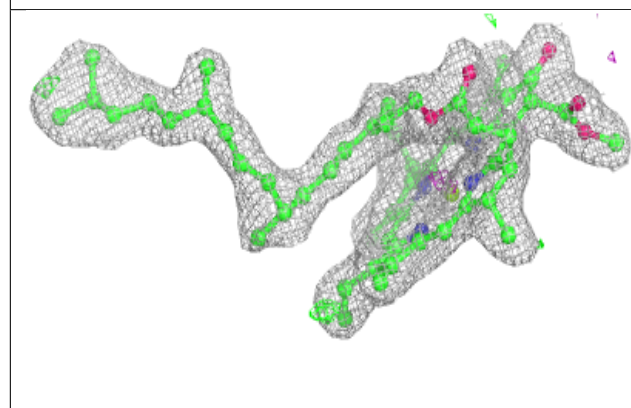
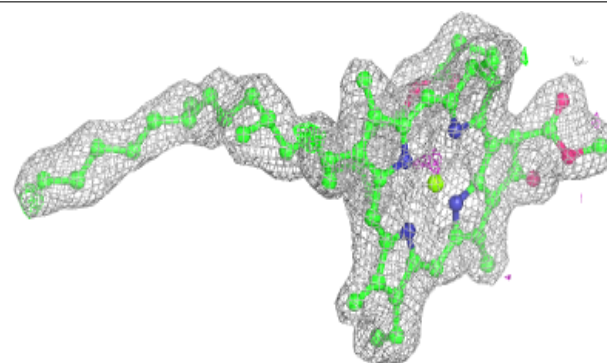


Electron density around BCR c 516:

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

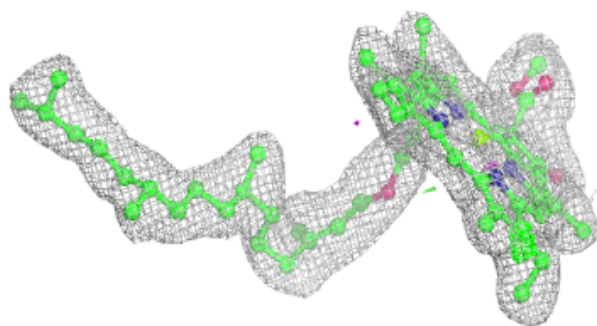
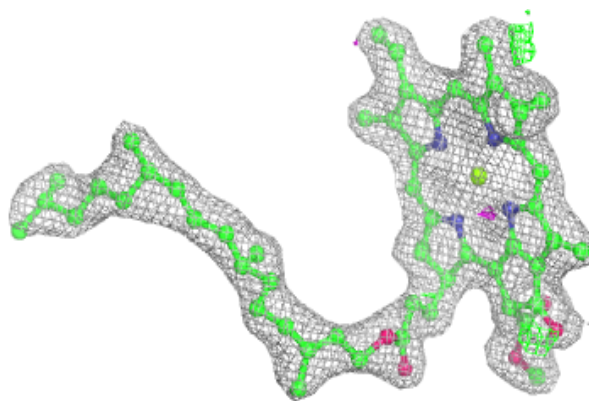
**Electron density around CLA c 507:**

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

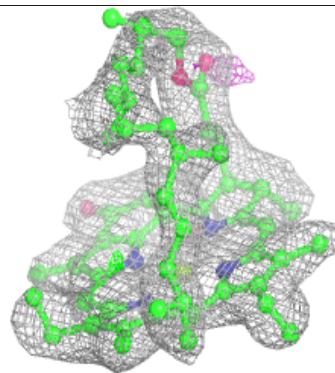
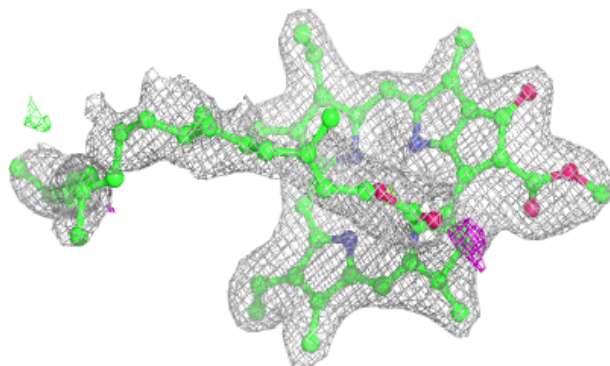
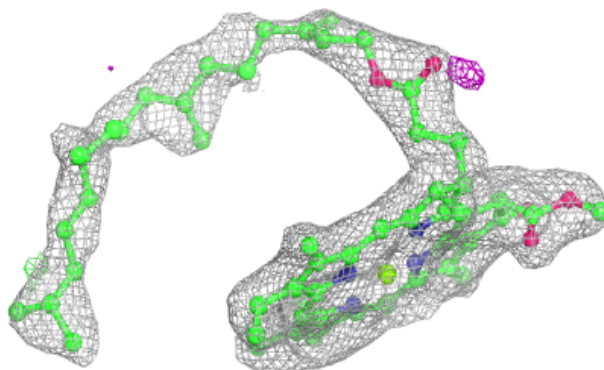


Electron density around CLA c 513:

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

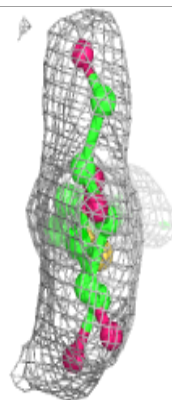
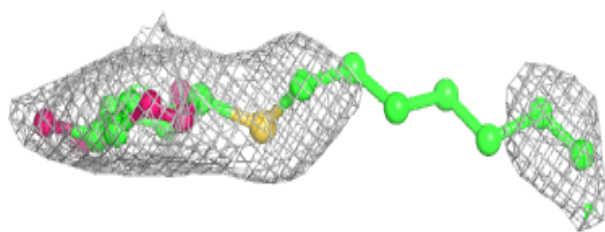
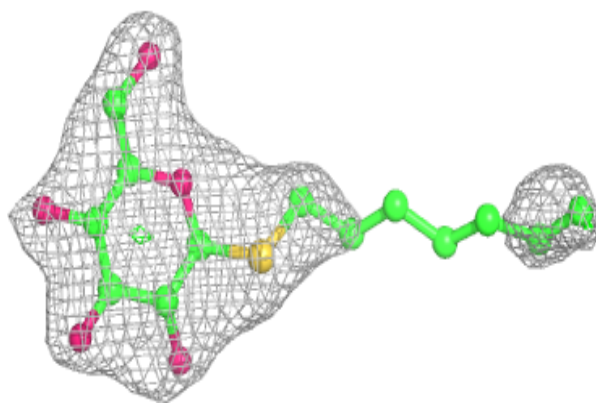
**Electron density around CLA C 514:**

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

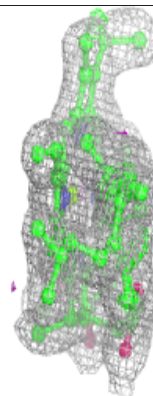
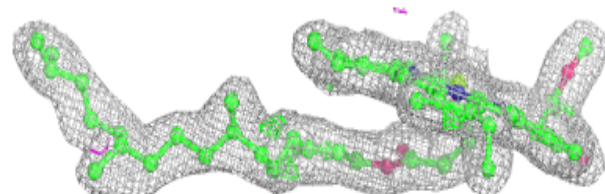
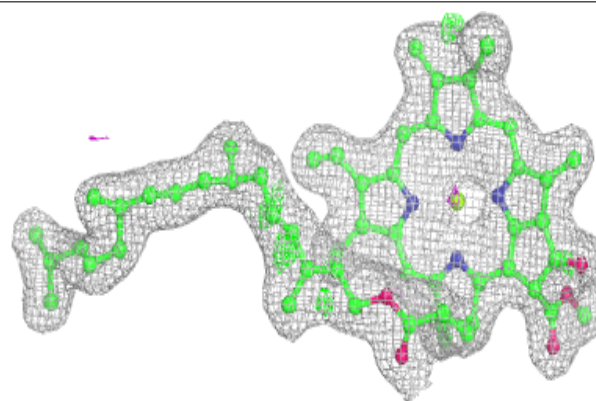


Electron density around HTG C 522:

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

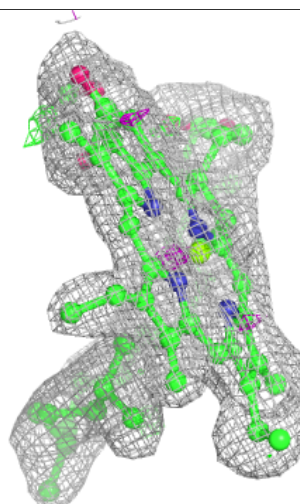
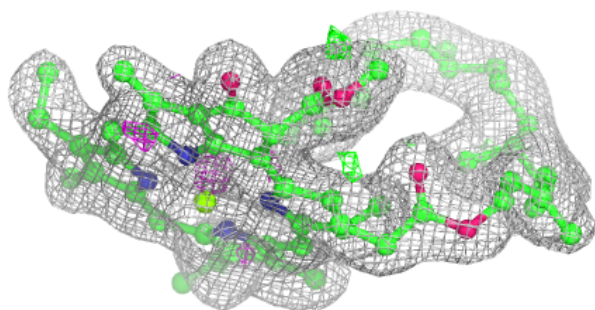
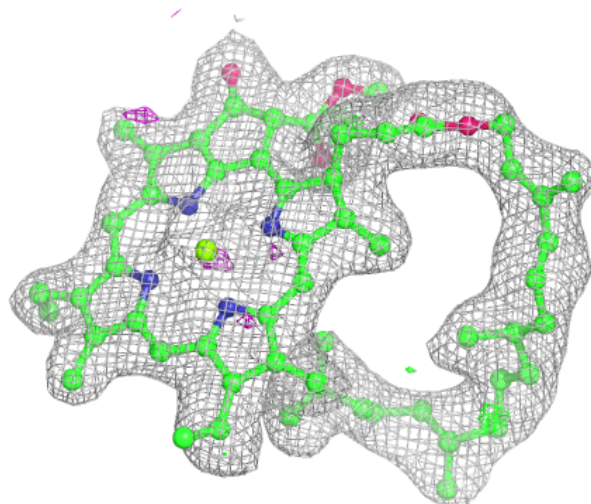
**Electron density around CLA B 604:**

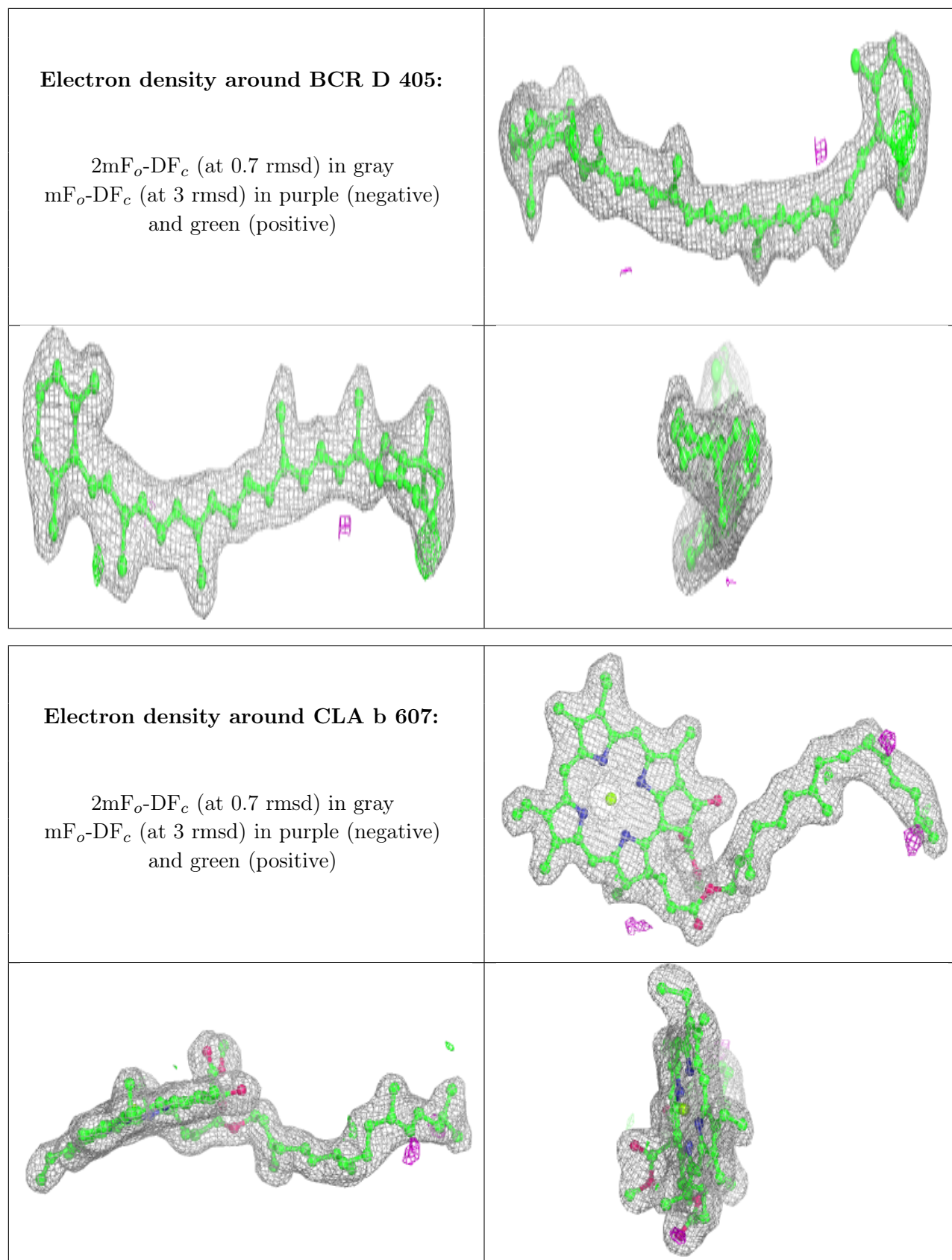
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 620:

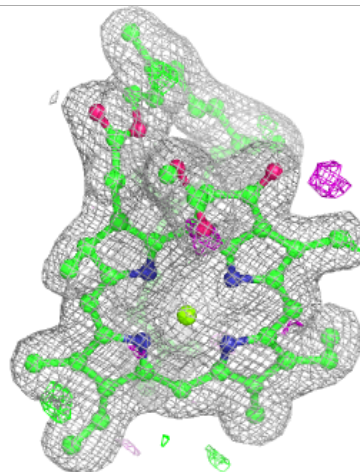
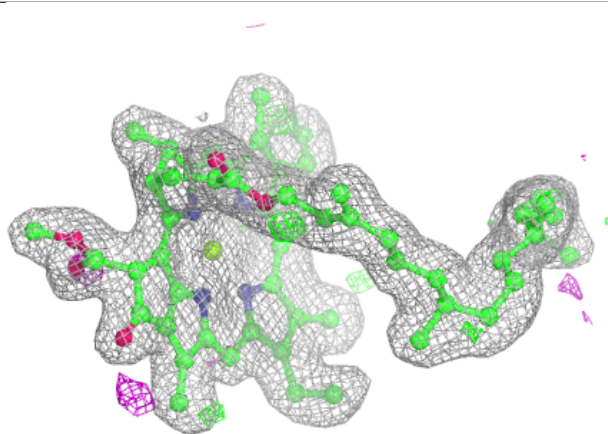
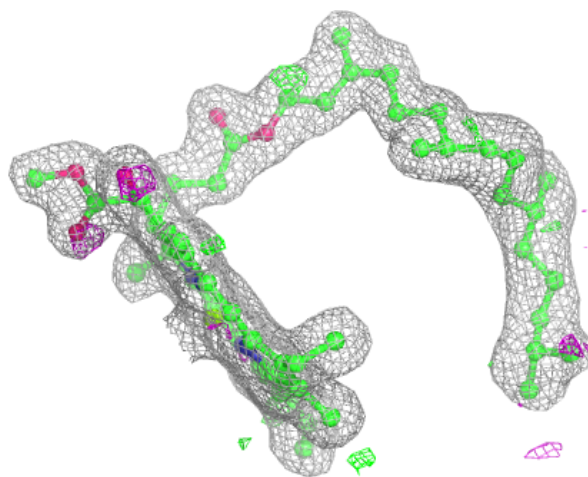
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

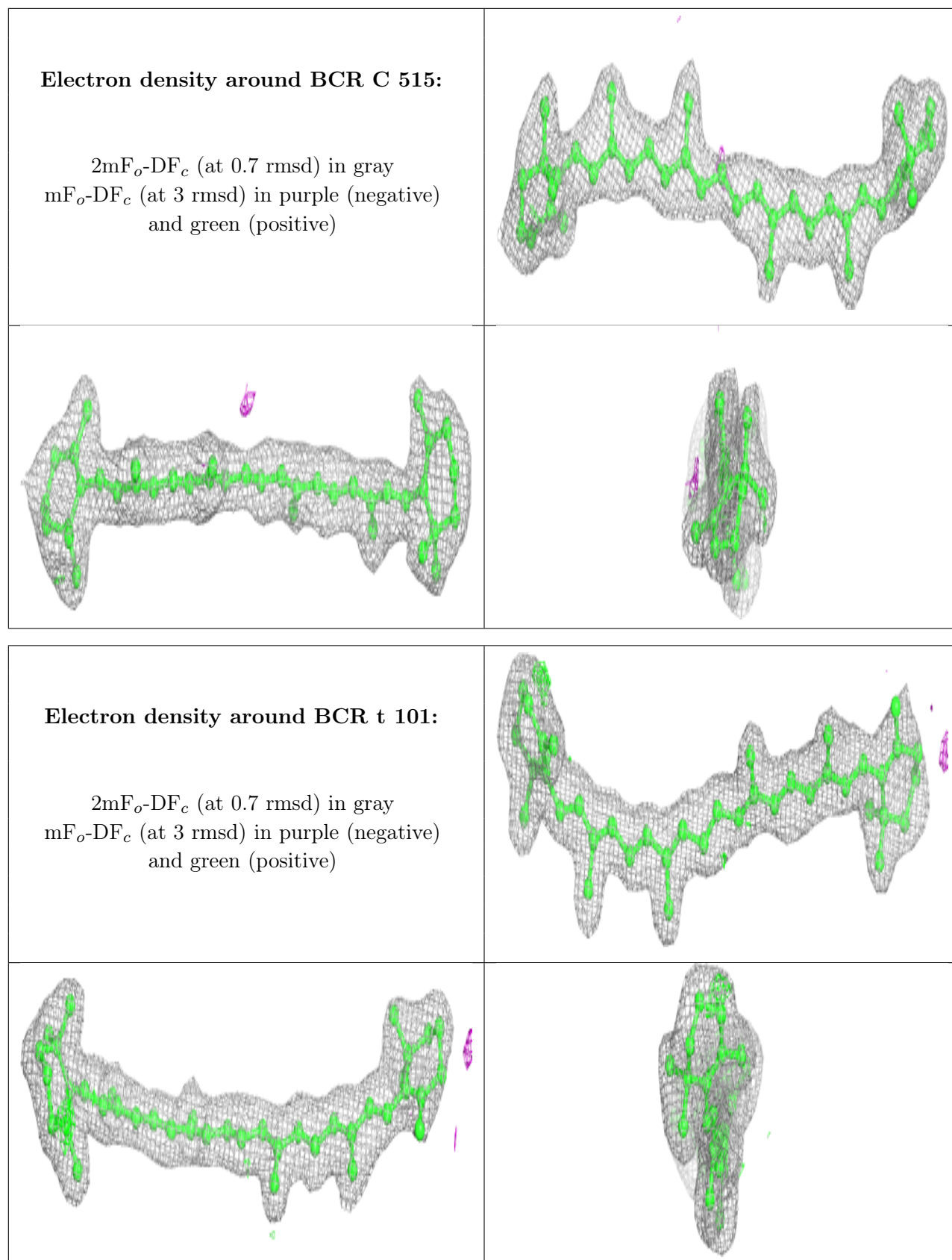




Electron density around CLA B 612:

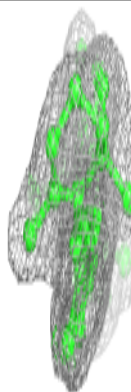
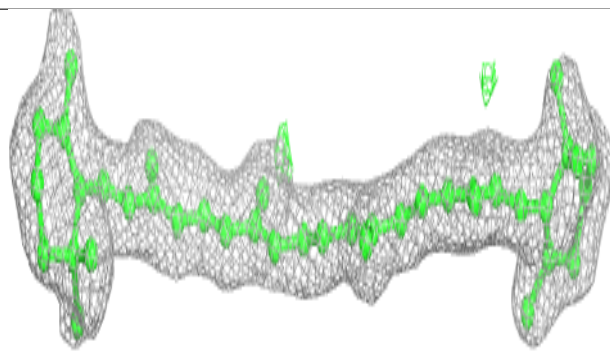
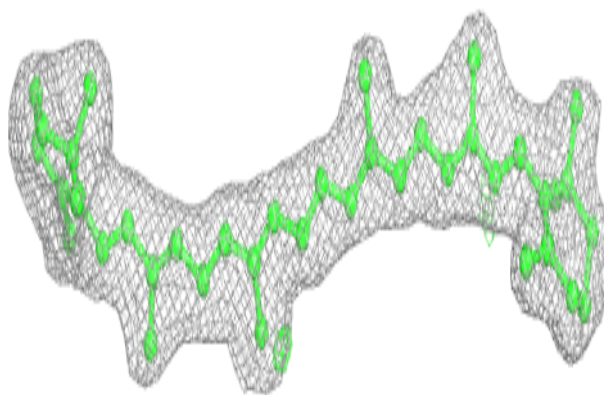
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



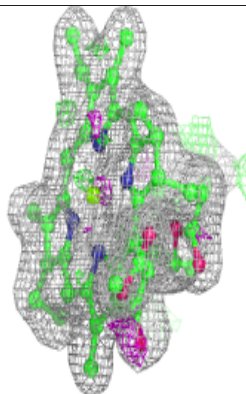
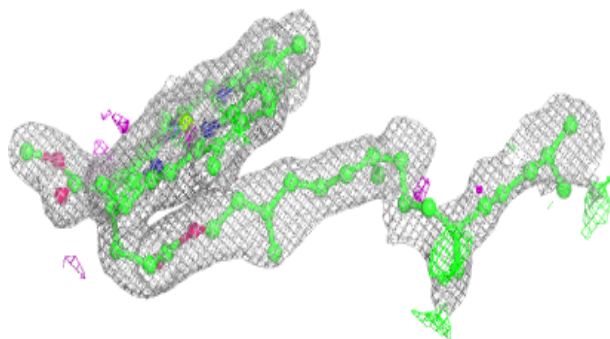
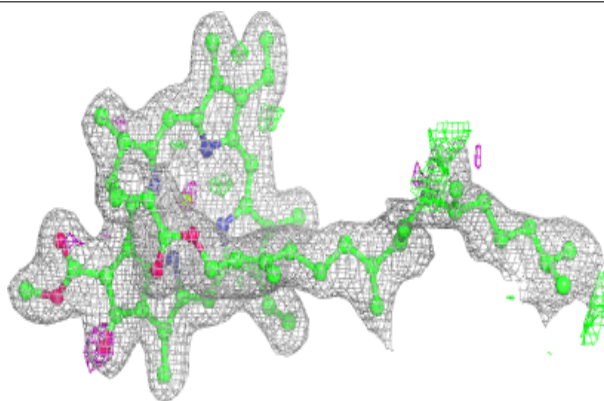


Electron density around BCR y 101:

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

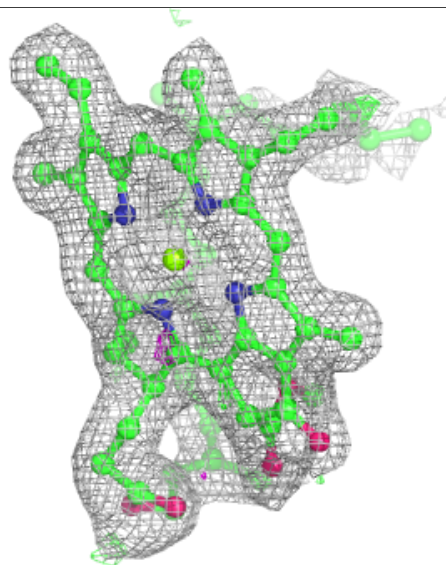
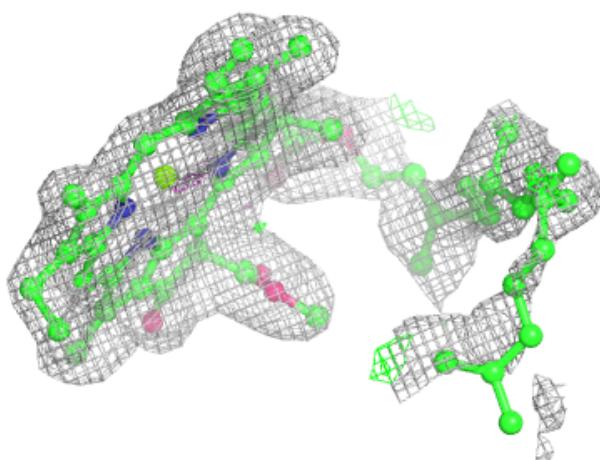
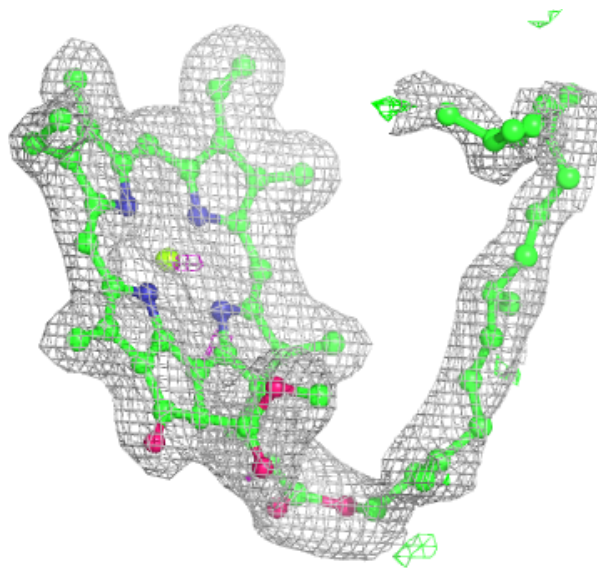
**Electron density around CLA B 615:**

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



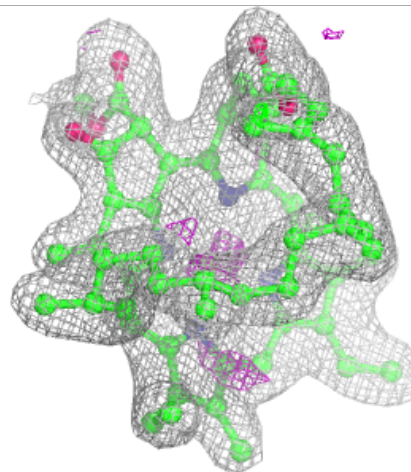
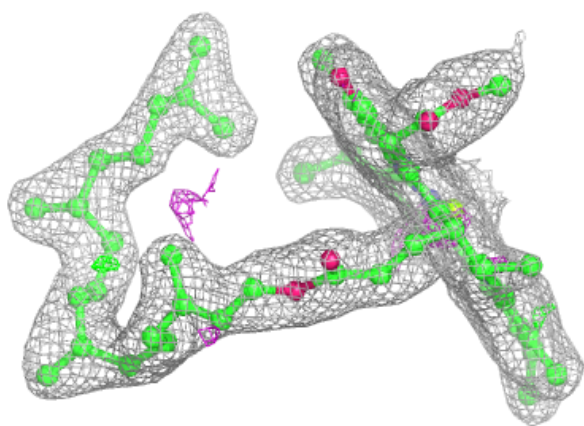
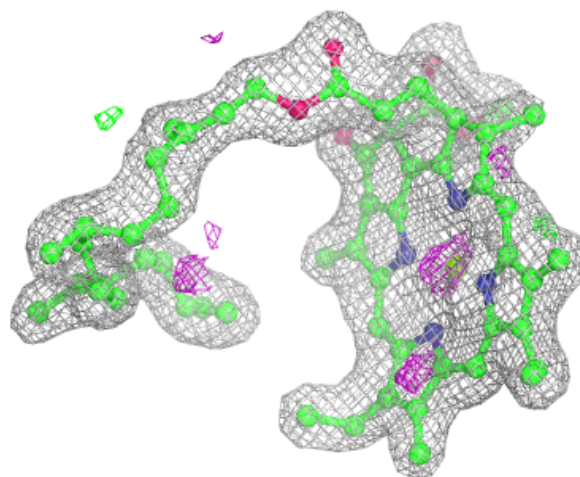
Electron density around CLA b 621:

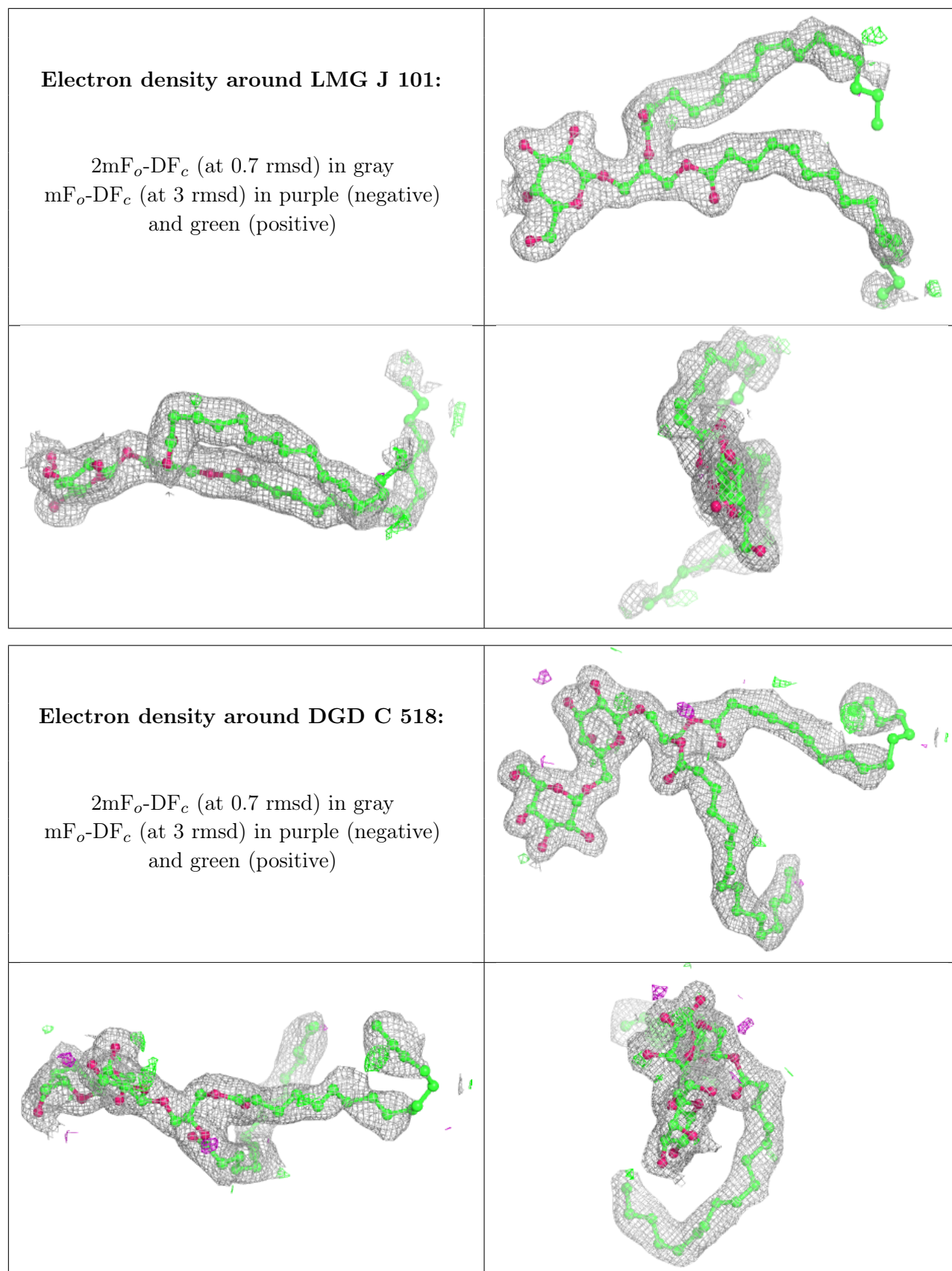
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 504:

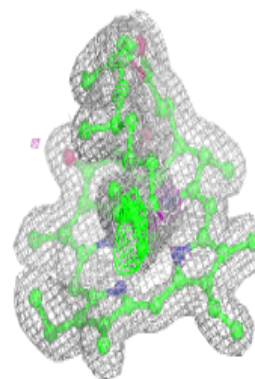
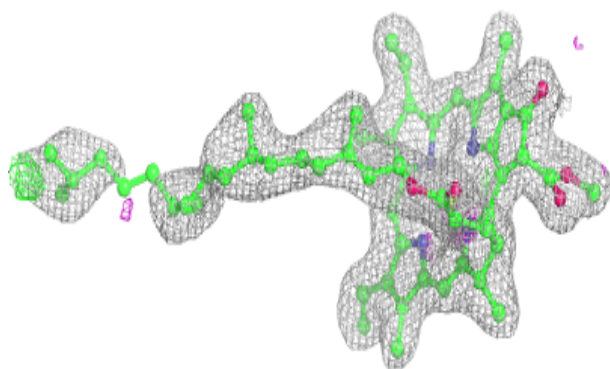
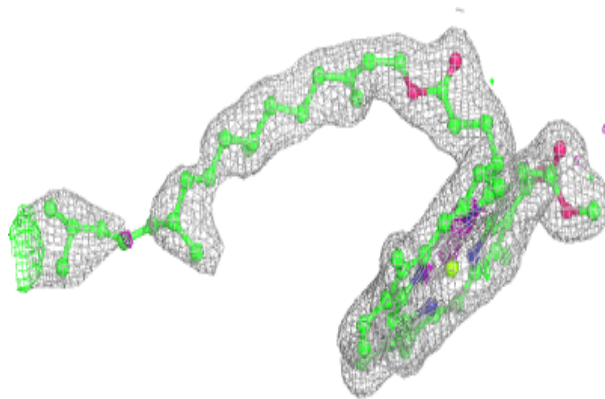
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



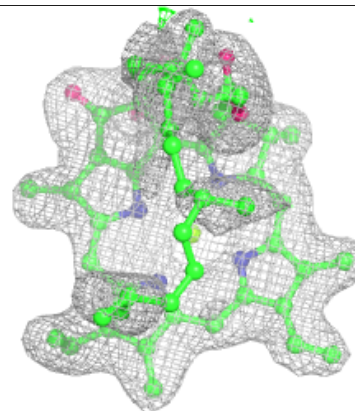
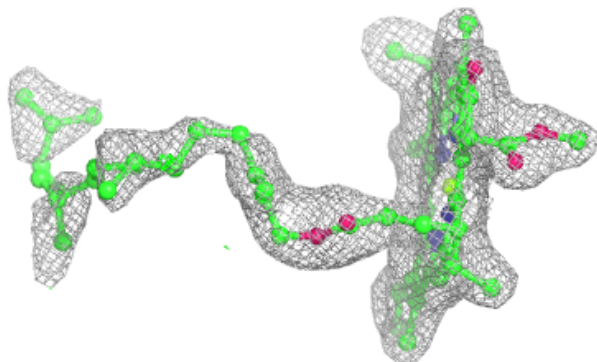
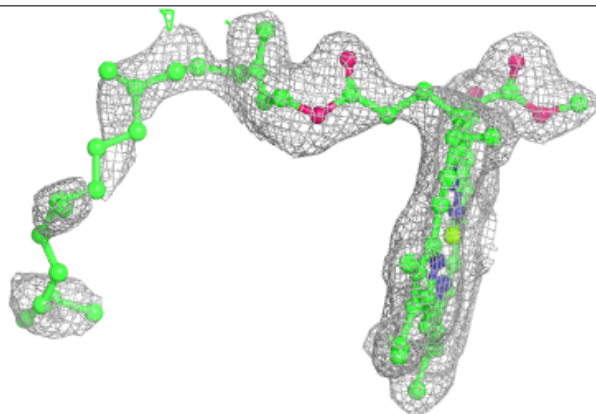


Electron density around CLA C 505:

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

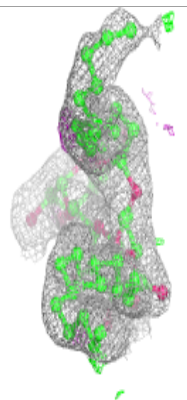
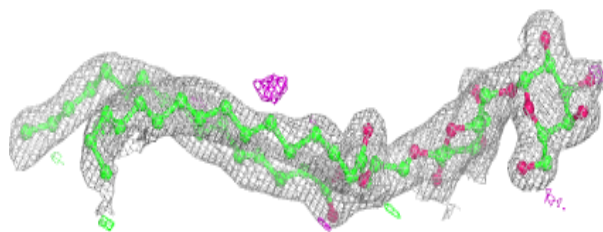
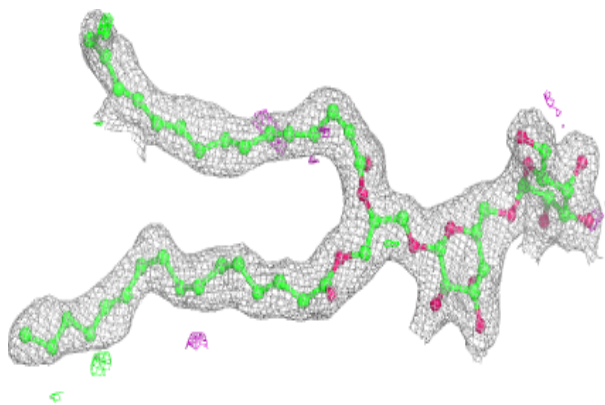
**Electron density around CLA C 507:**

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



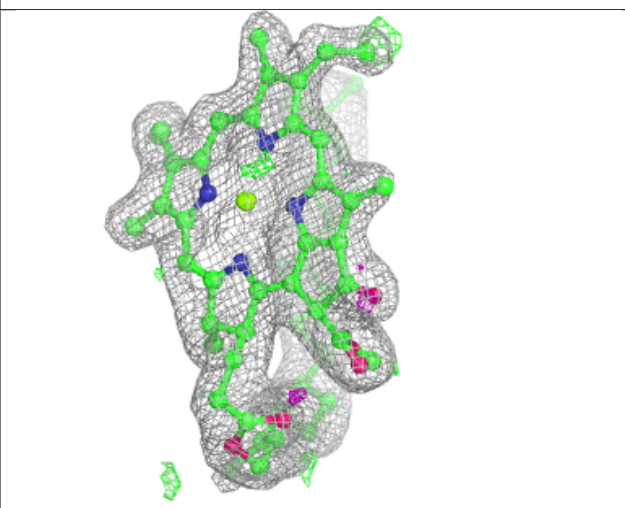
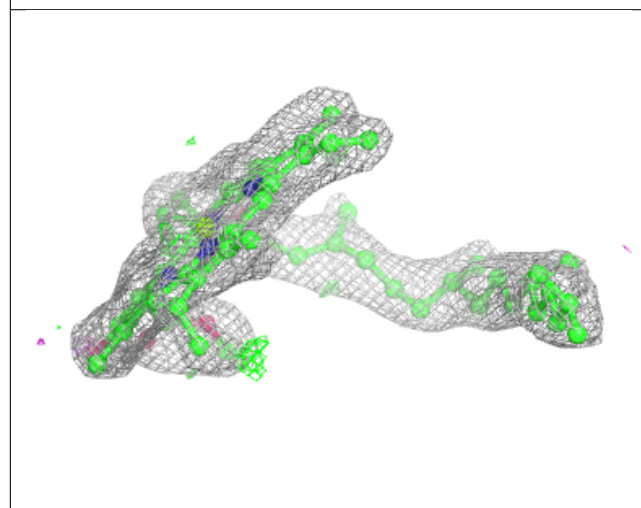
Electron density around DGD c 519:

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



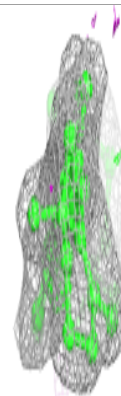
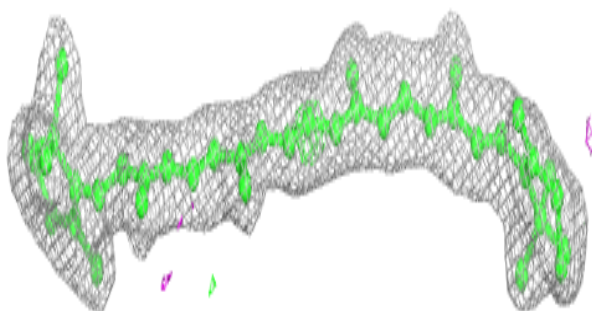
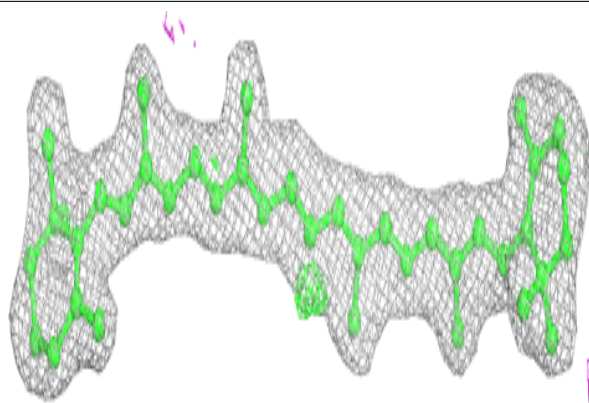
Electron density around CLA c 509:

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

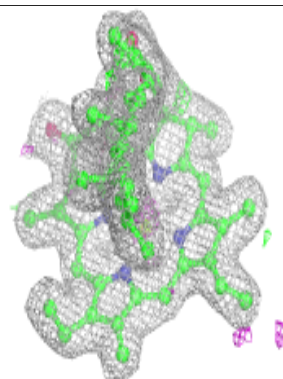
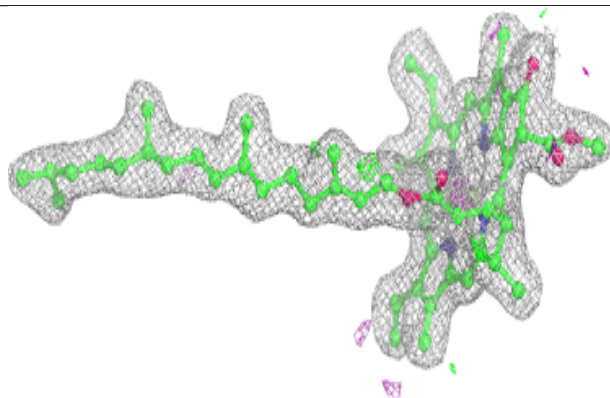
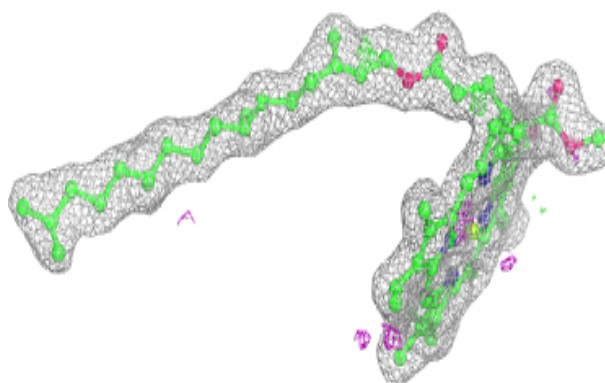


Electron density around BCR b 624:

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

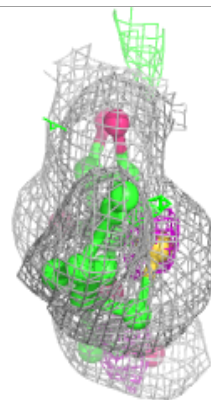
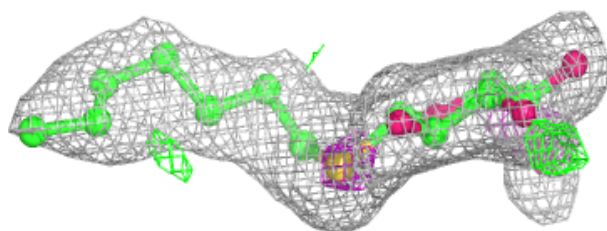
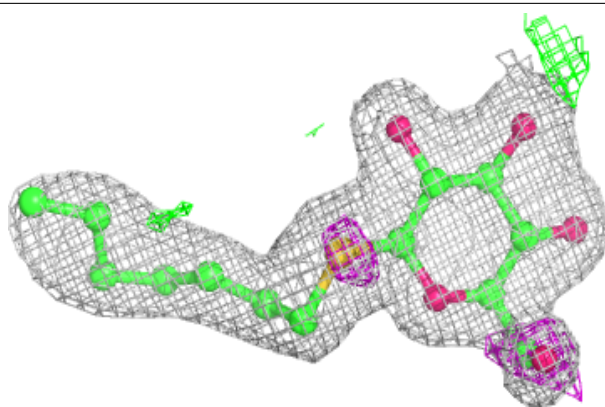
**Electron density around CLA B 608:**

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

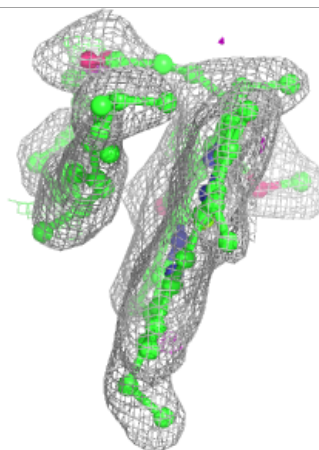
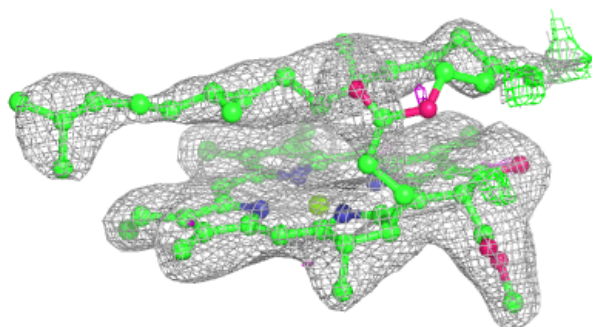
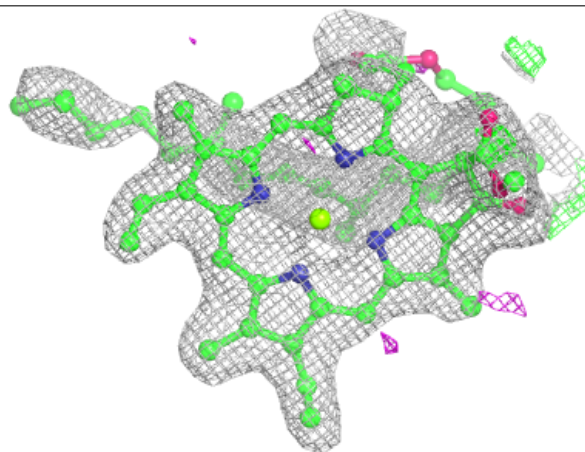


Electron density around HTG B 622:

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

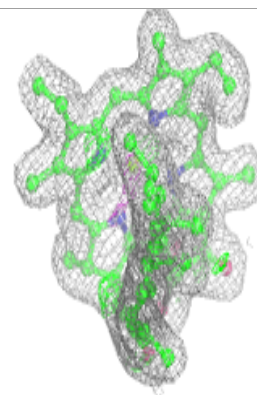
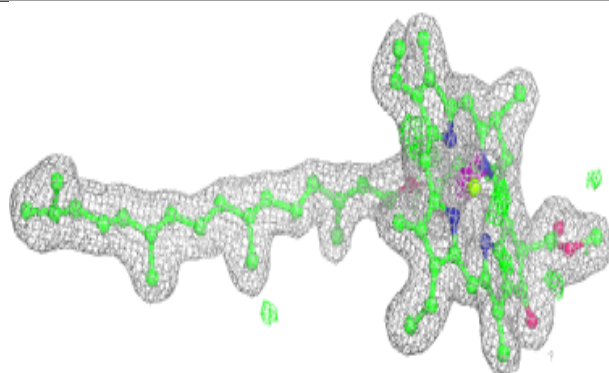
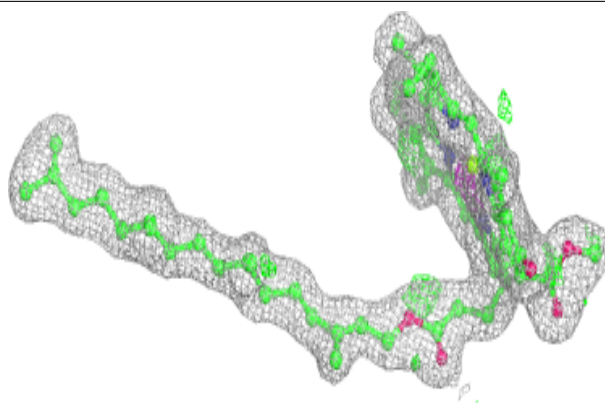
**Electron density around CLA B 602:**

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

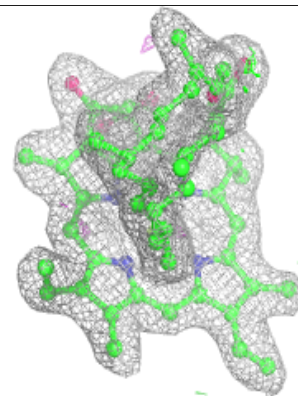
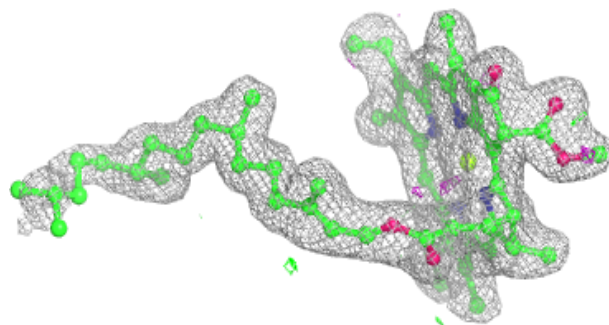
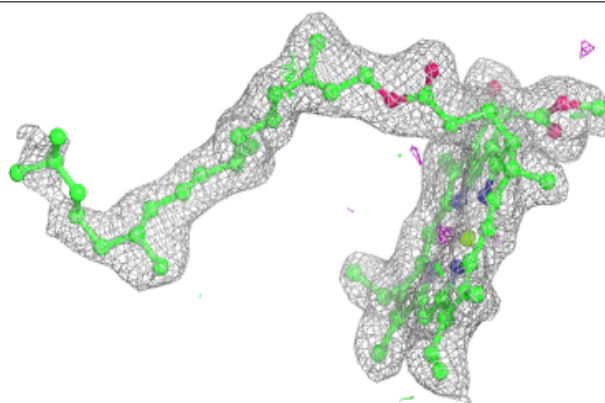


Electron density around CLA b 612:

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

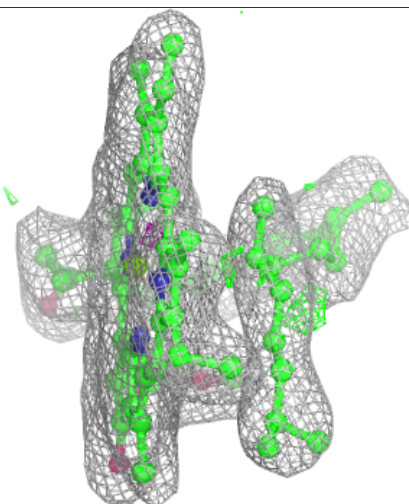
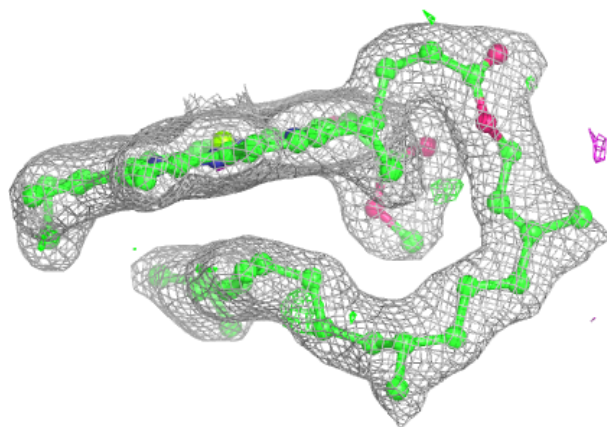
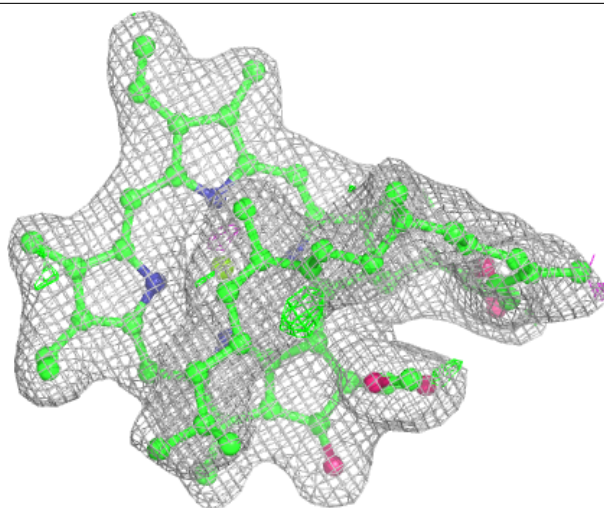
**Electron density around CLA c 510:**

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



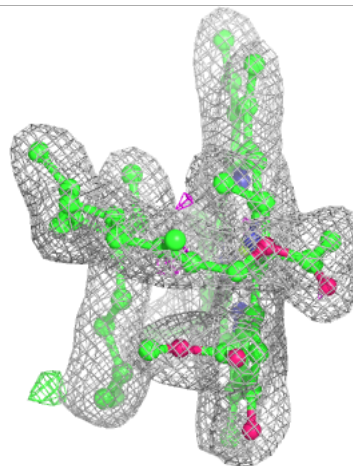
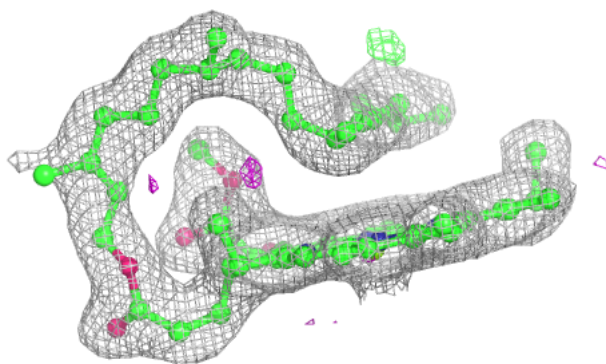
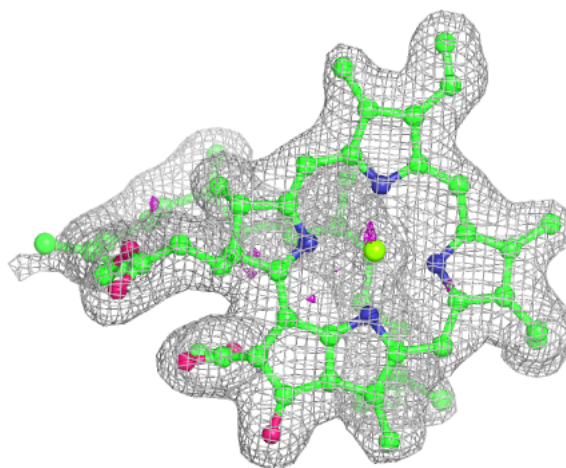
Electron density around CLA c 512:

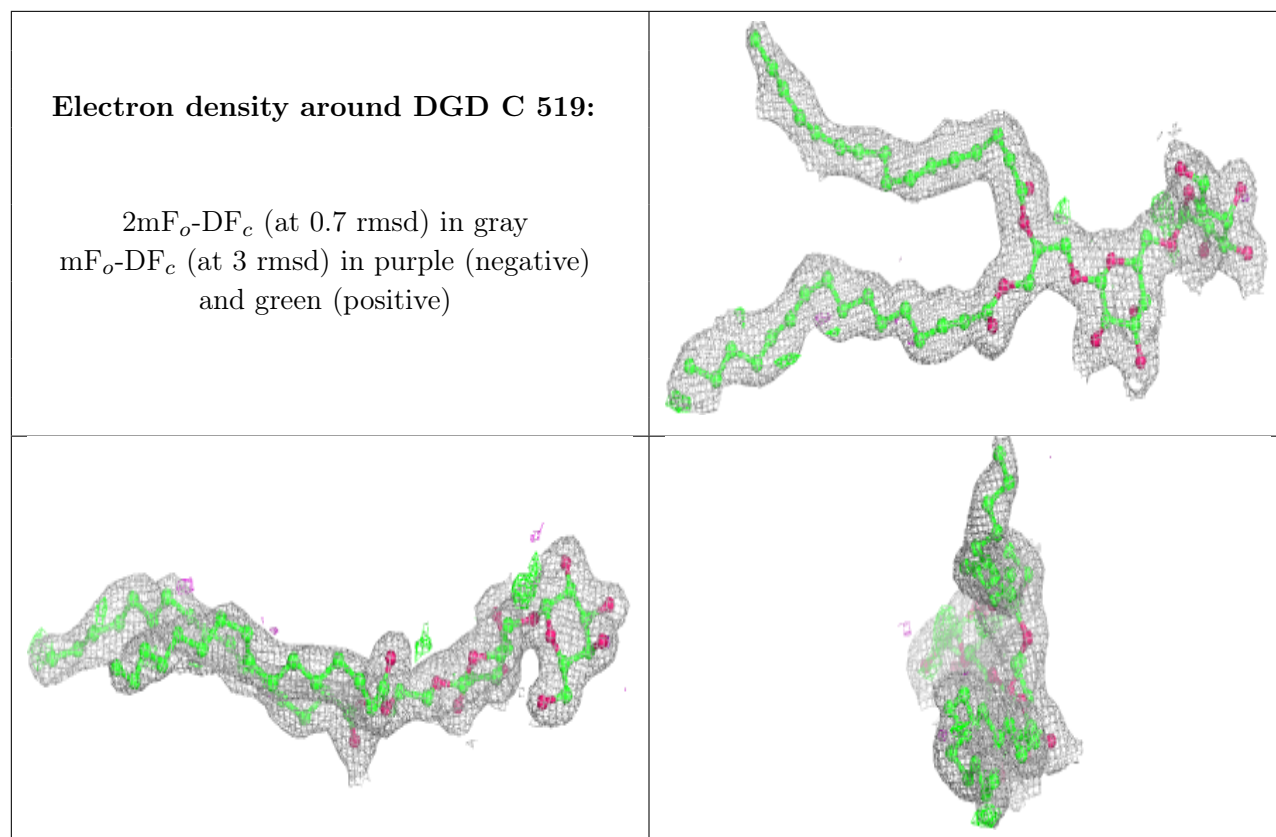
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 511:

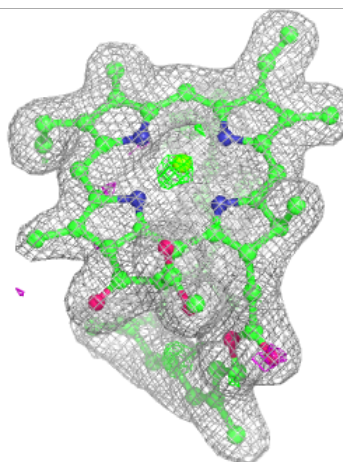
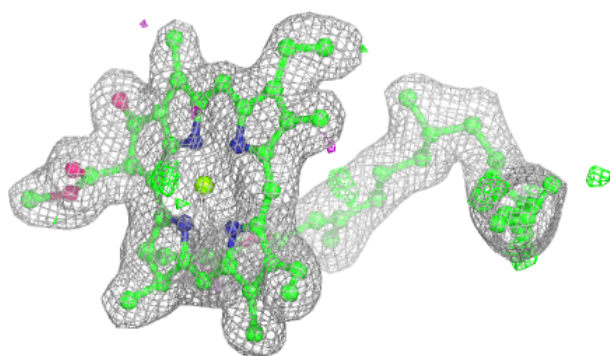
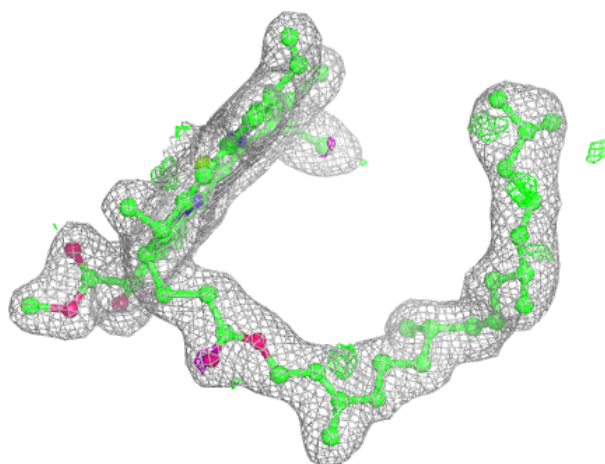
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





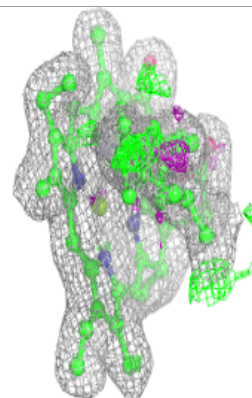
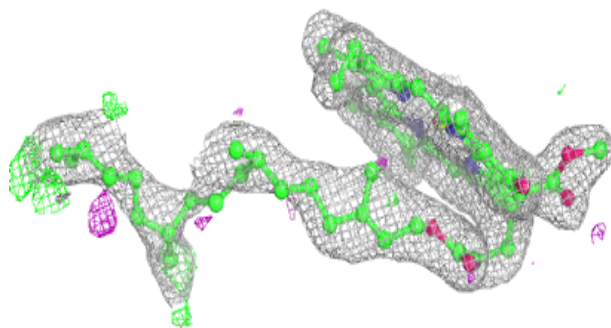
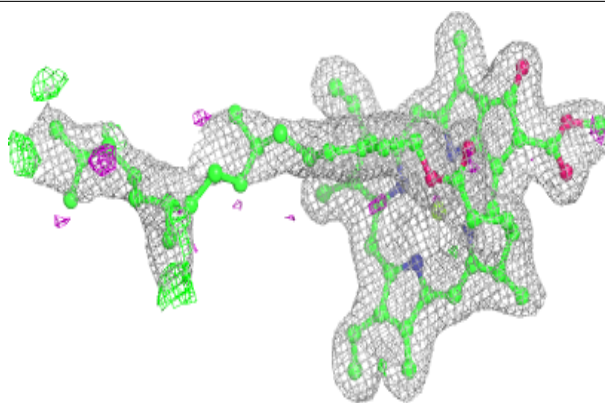
Electron density around CLA b 616:

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

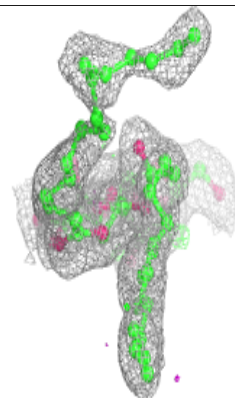
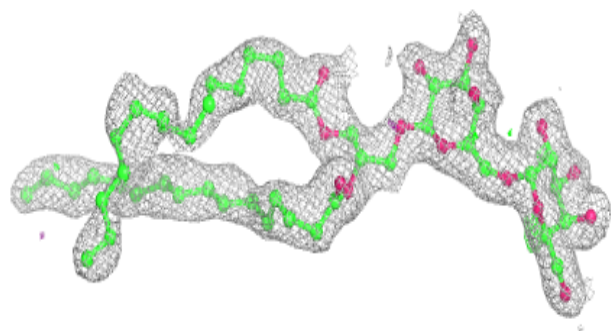
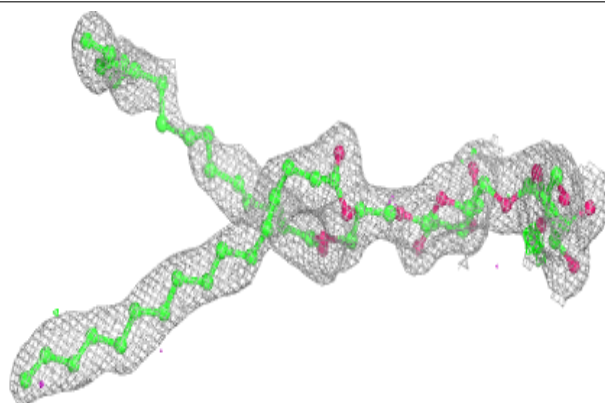


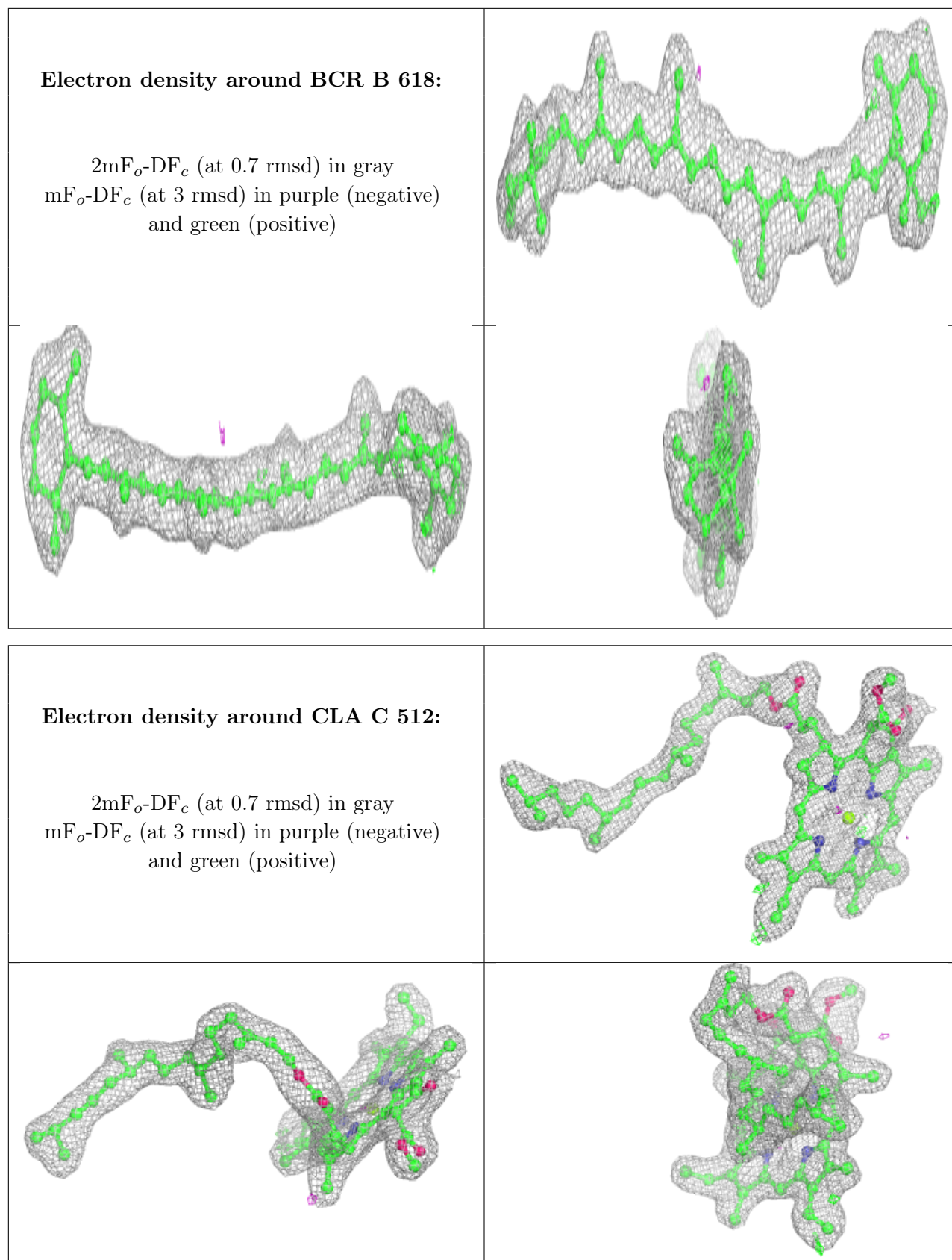
Electron density around CLA b 619:

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

**Electron density around DGD c 517:**

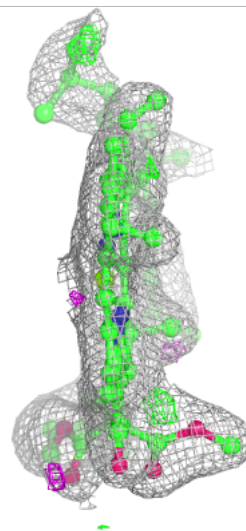
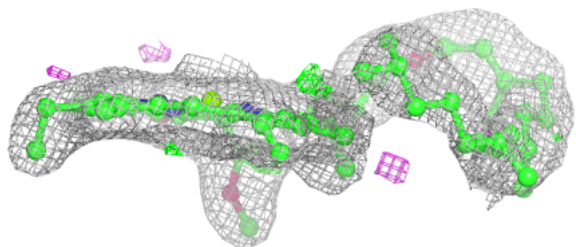
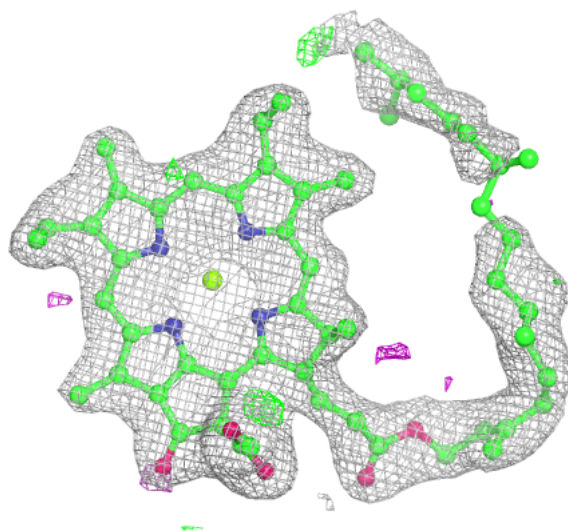
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





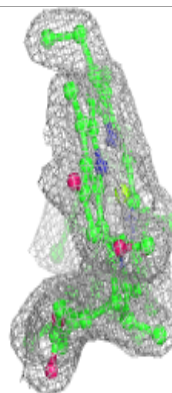
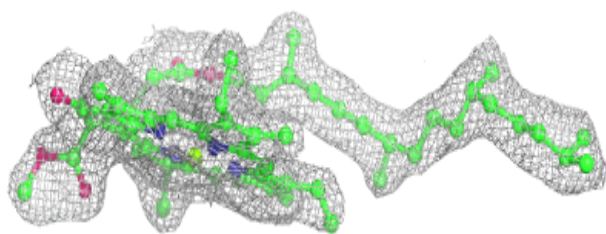
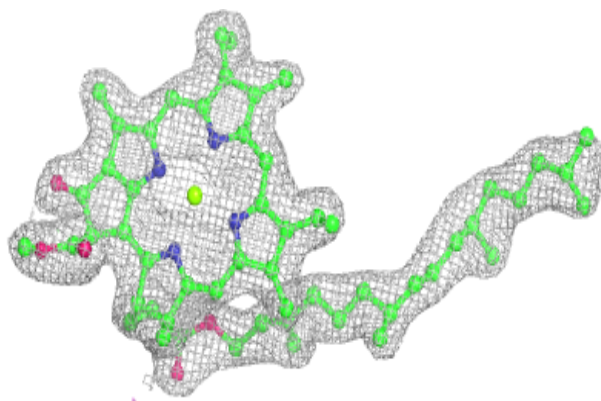
Electron density around CLA C 513:

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



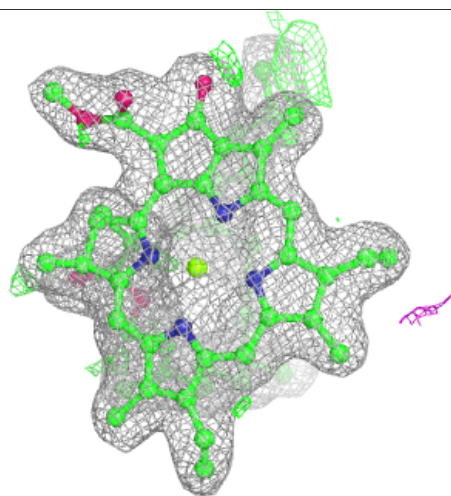
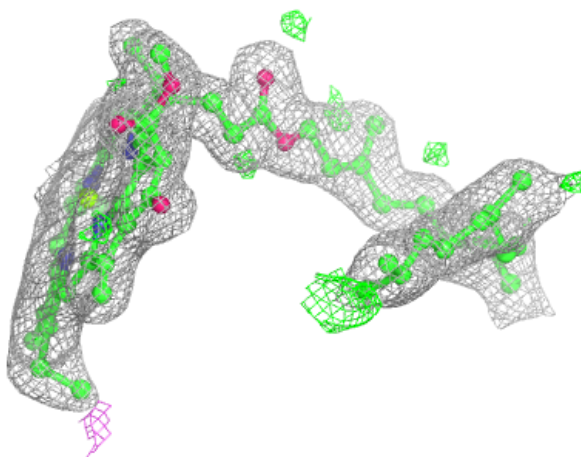
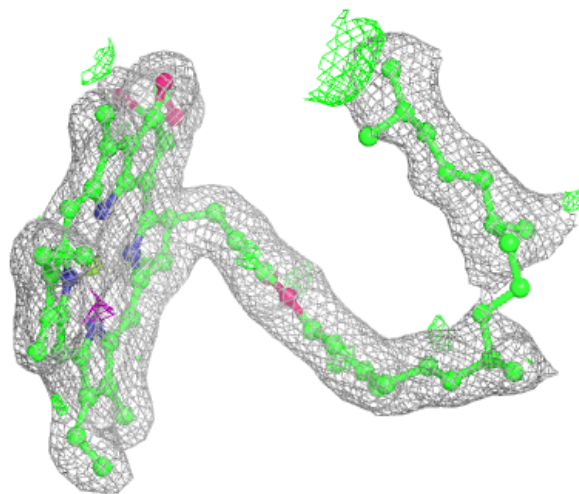
Electron density around CLA c 503:

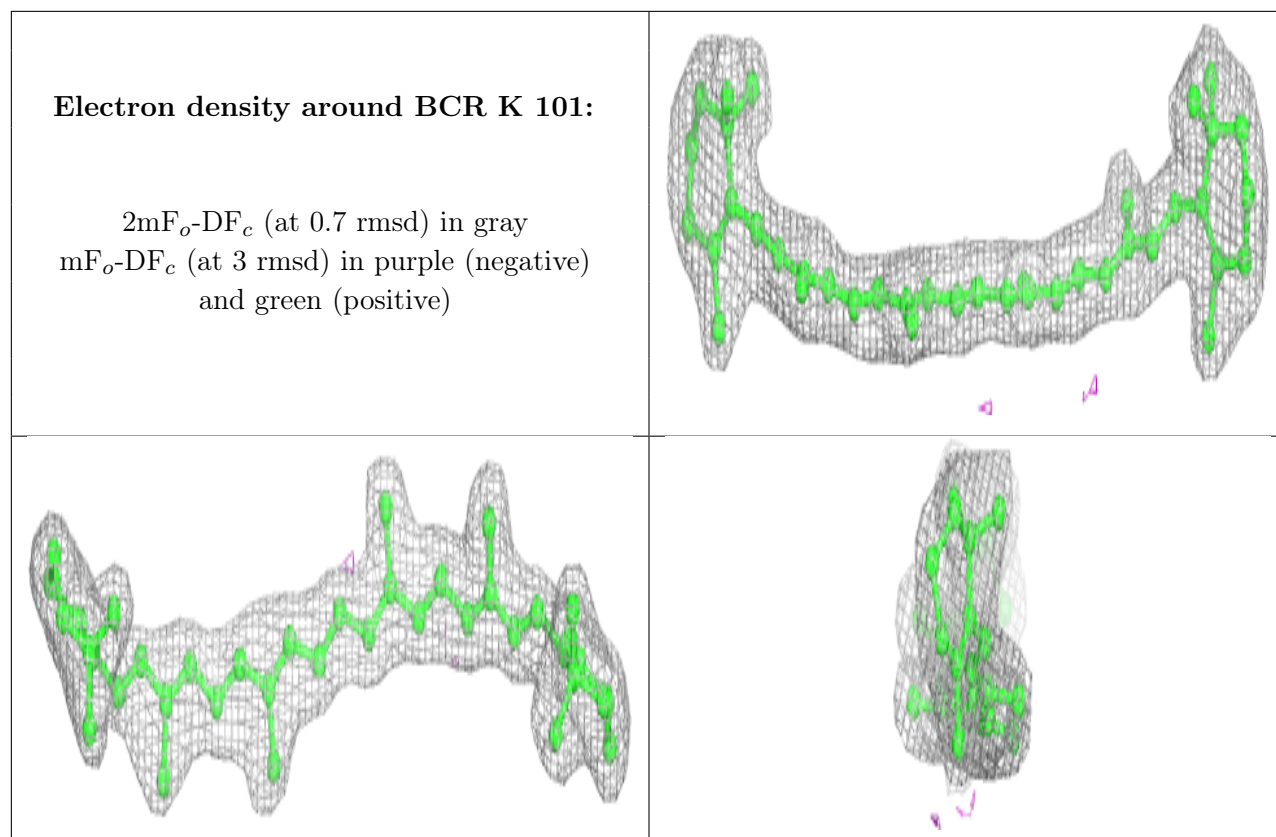
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 607:

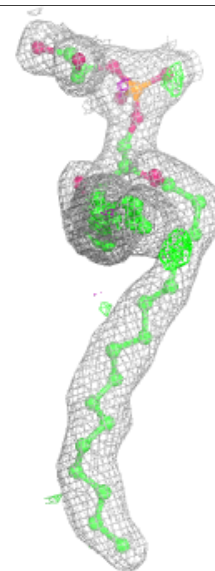
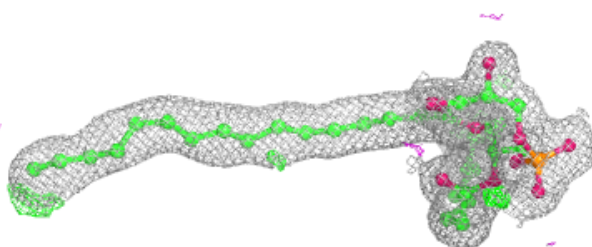
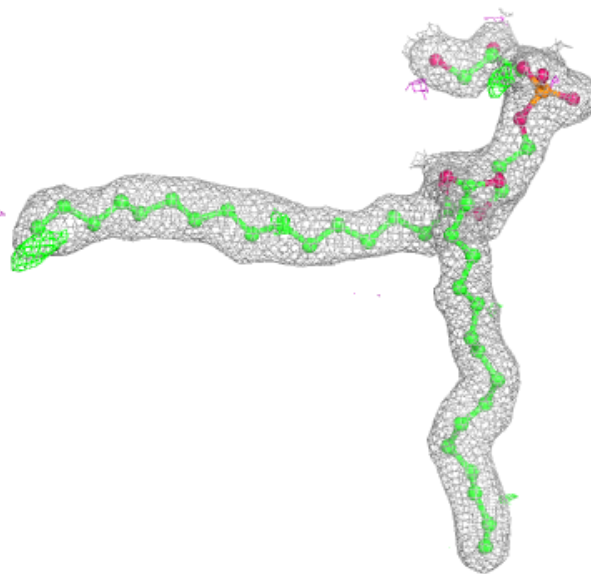
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





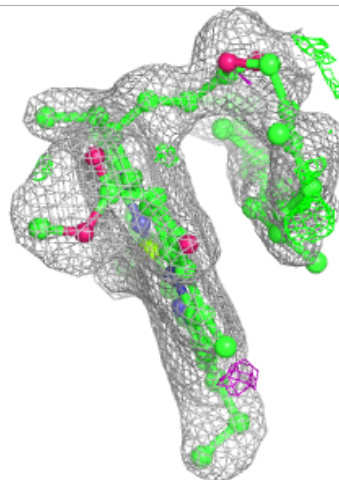
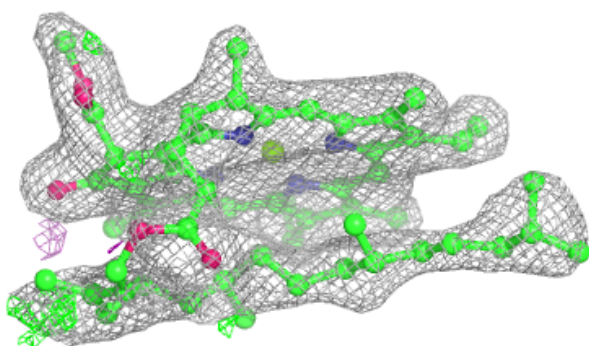
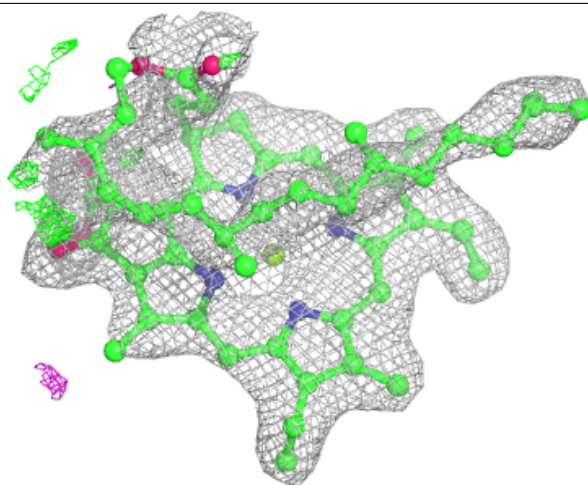
Electron density around LHG L 101:

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



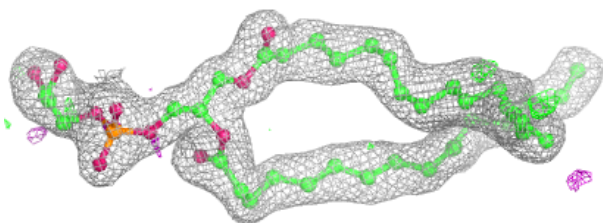
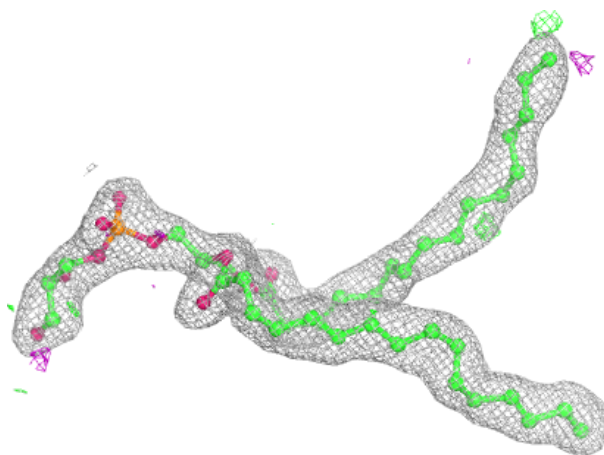
Electron density around CLA b 606:

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



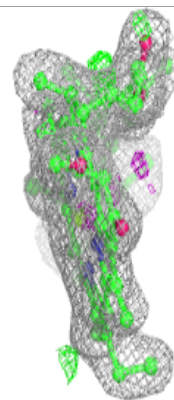
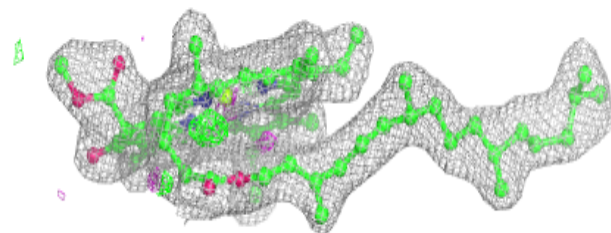
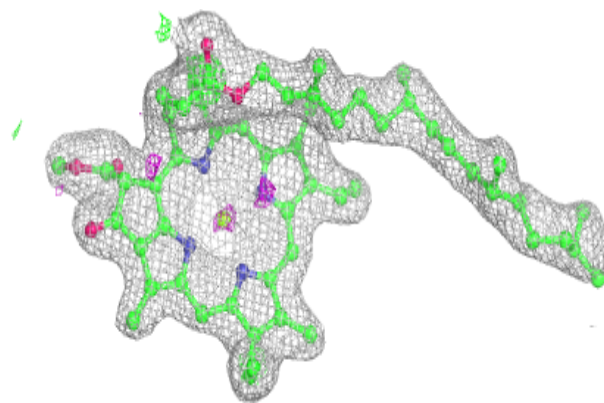
Electron density around LHG d 409:

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

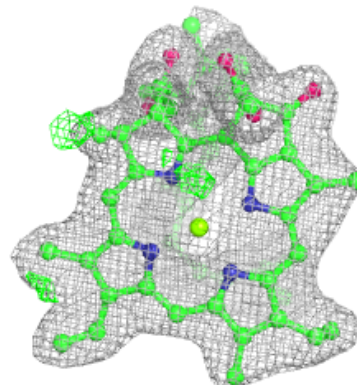
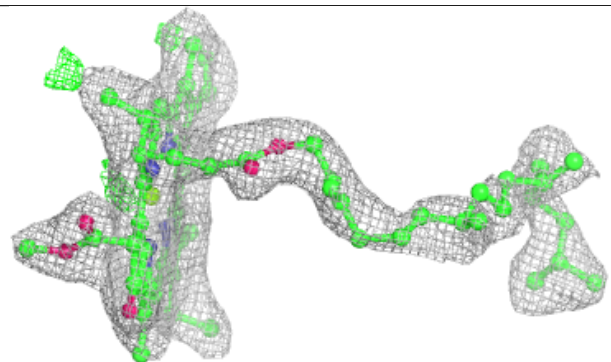
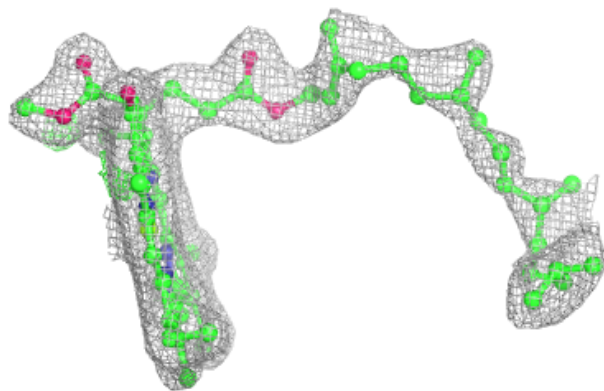


Electron density around CLA C 502:

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

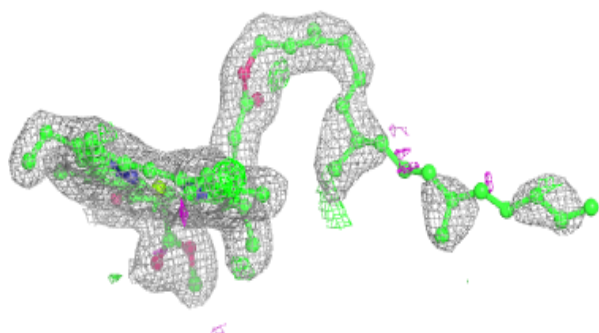
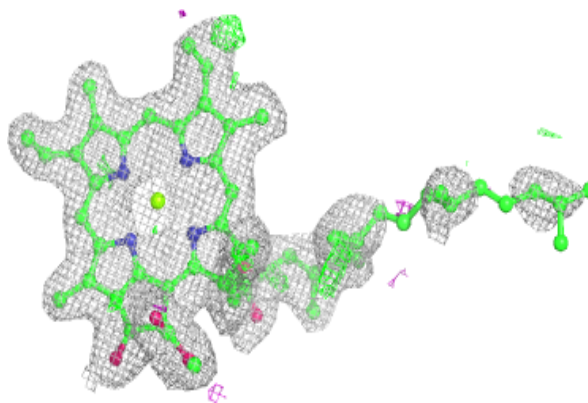
**Electron density around CLA c 508:**

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

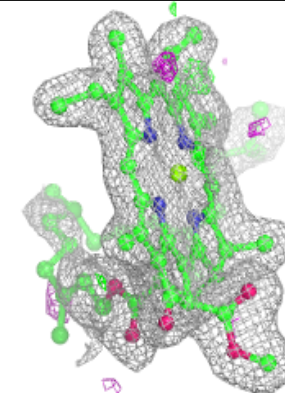
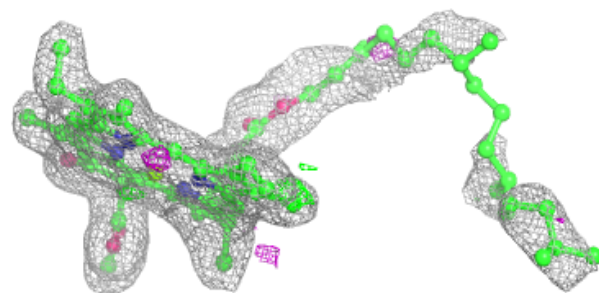
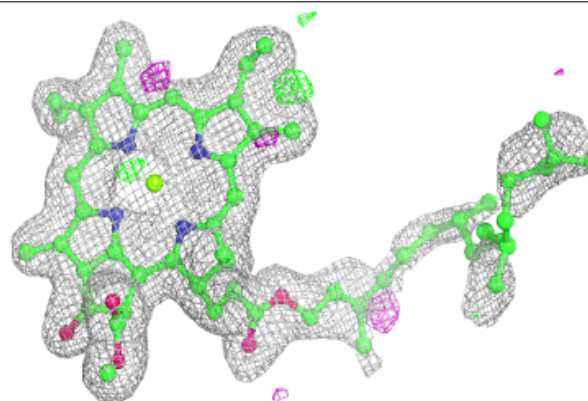


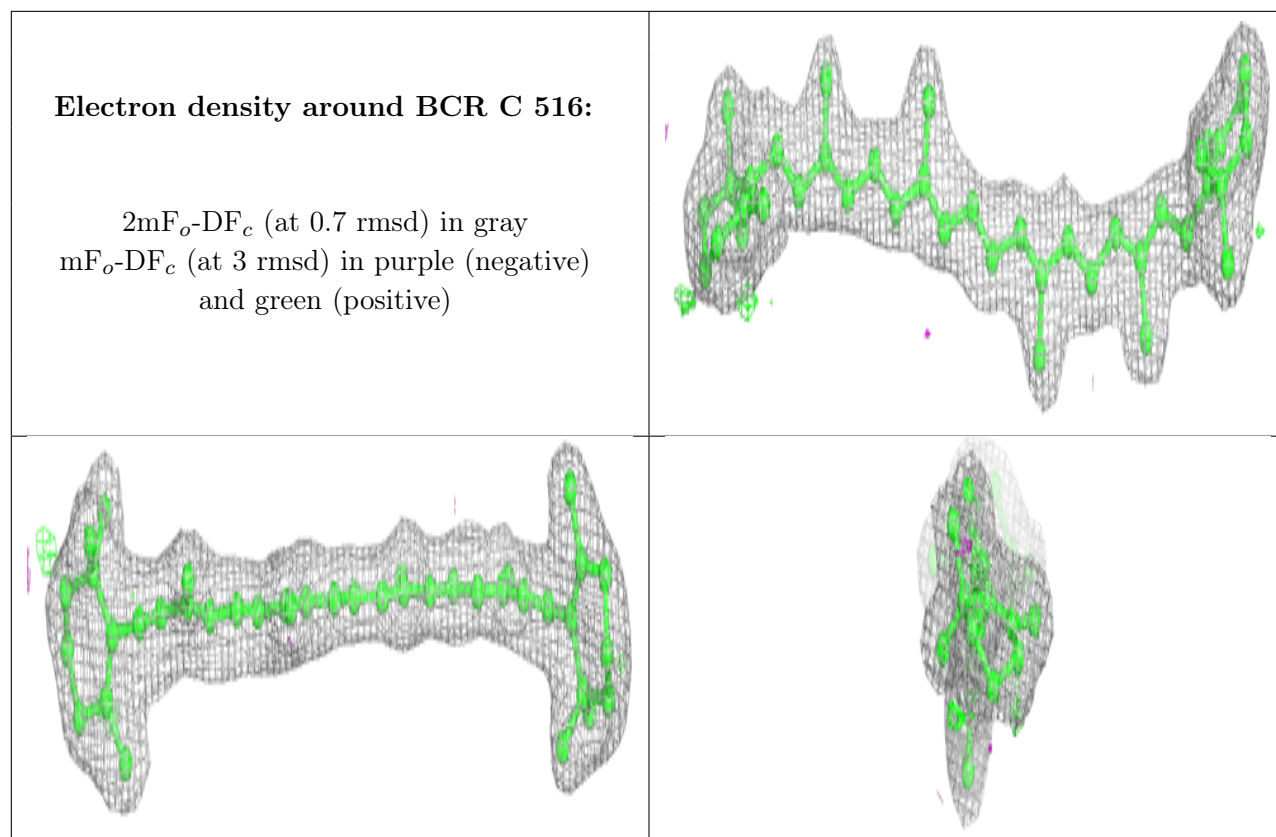
Electron density around CLA a 407:

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

**Electron density around CLA a 409:**

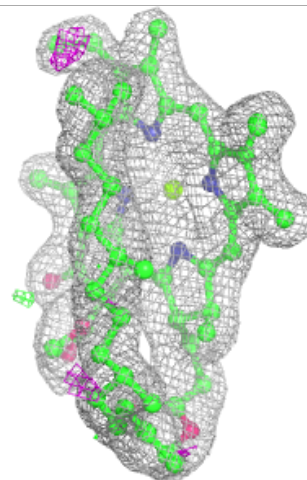
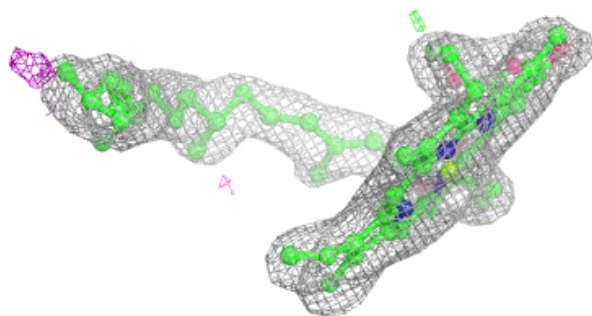
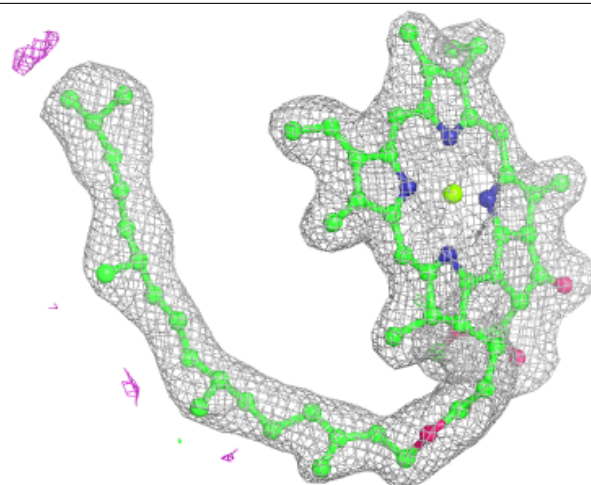
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





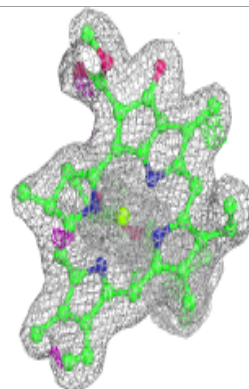
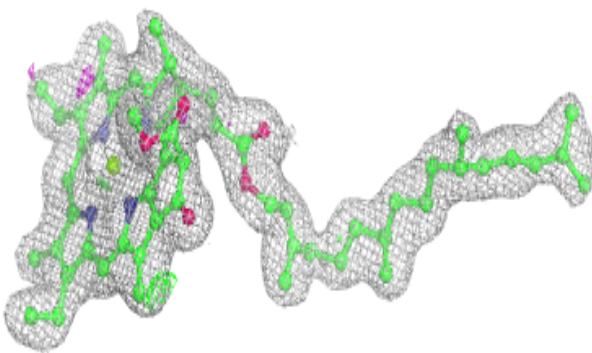
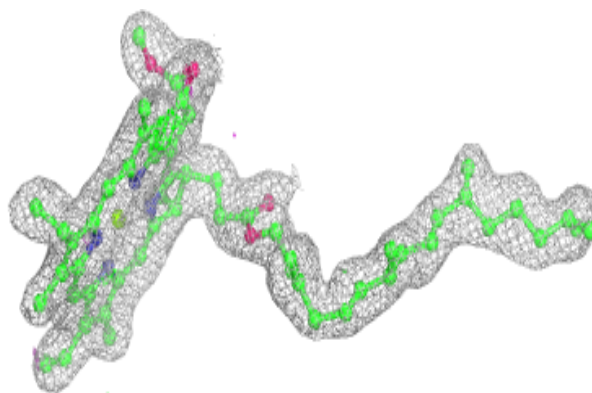
Electron density around CLA C 508:

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

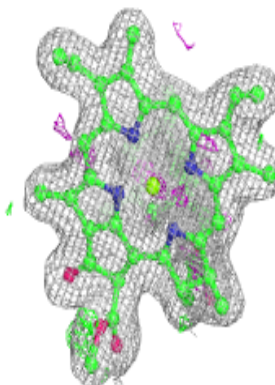
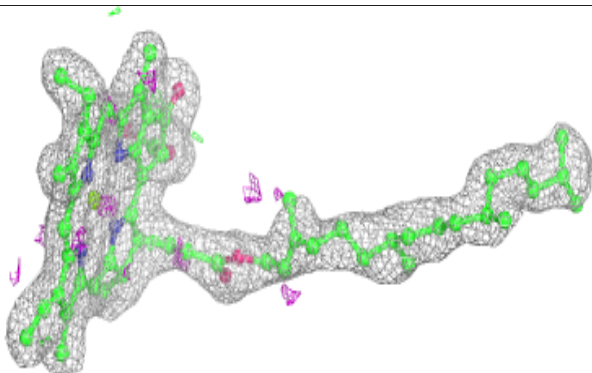
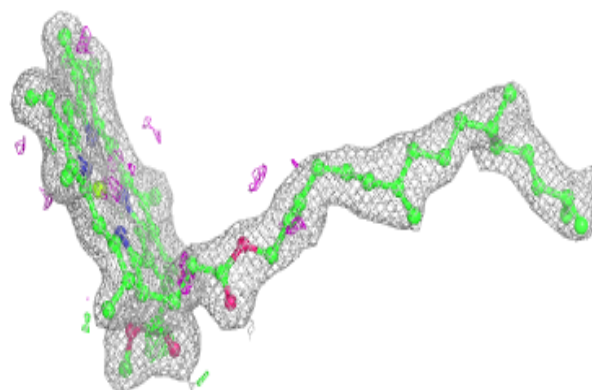


Electron density around CLA c 504:

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

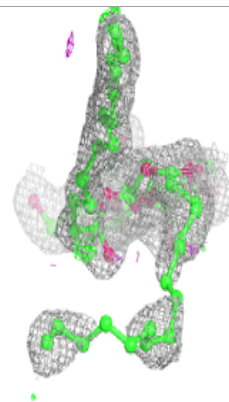
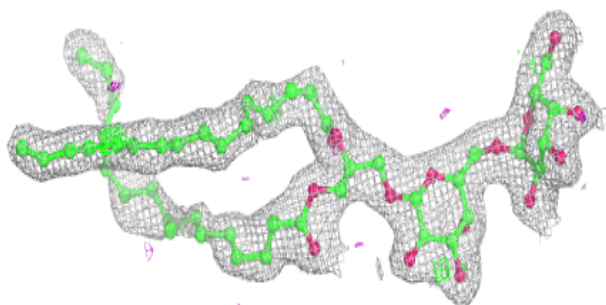
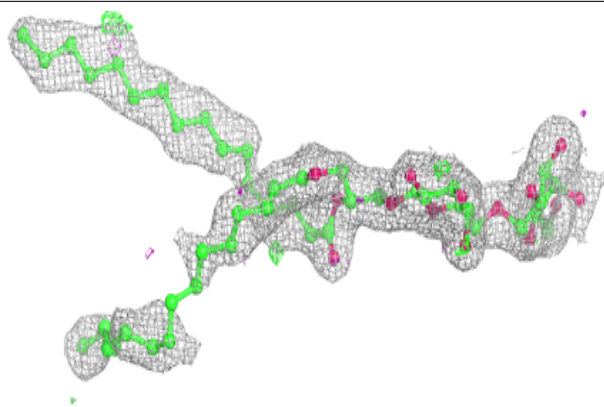
**Electron density around CLA B 605:**

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

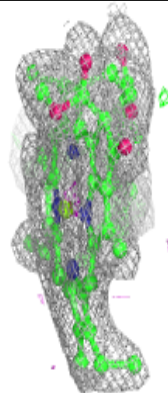
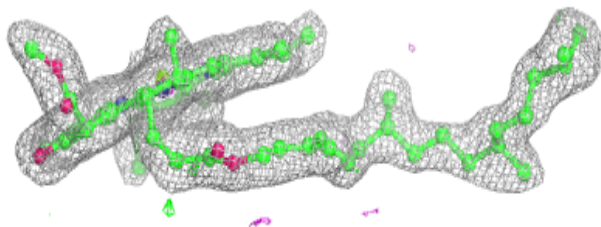
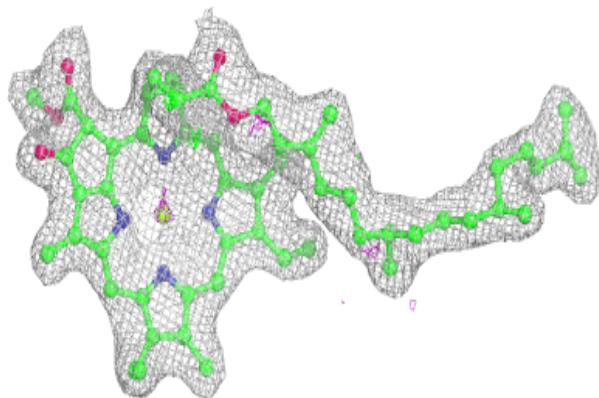


Electron density around DGD C 517:

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

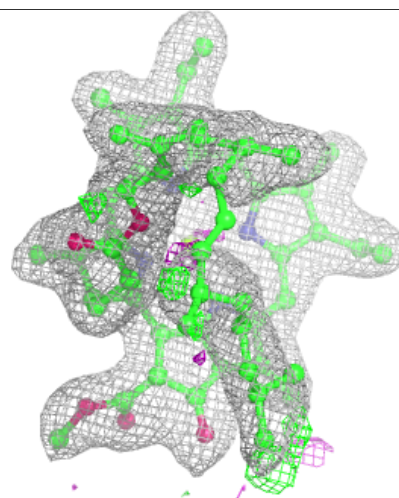
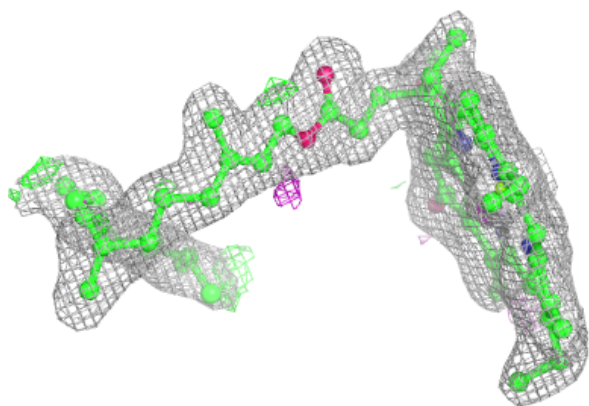
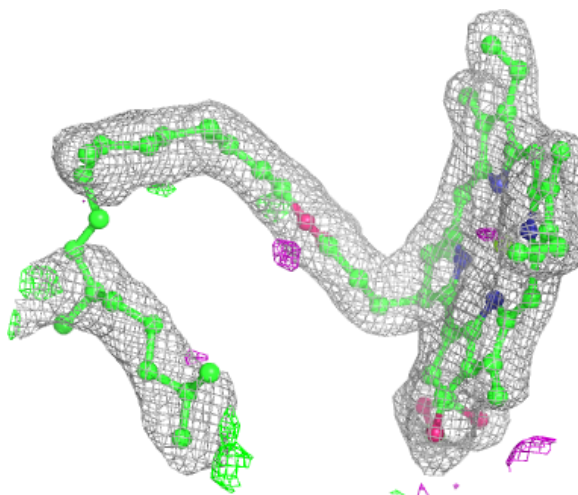
**Electron density around CLA b 608:**

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



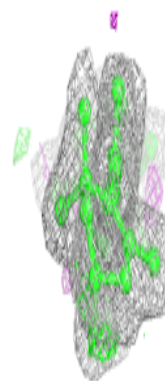
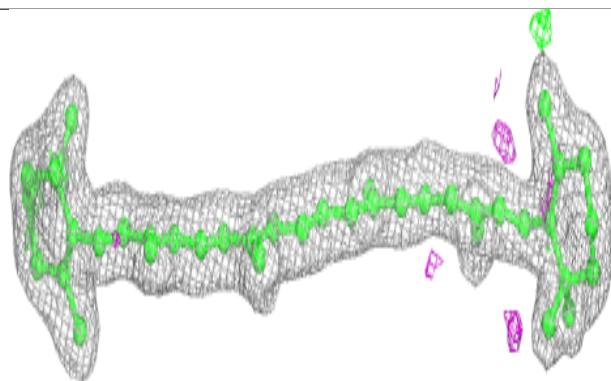
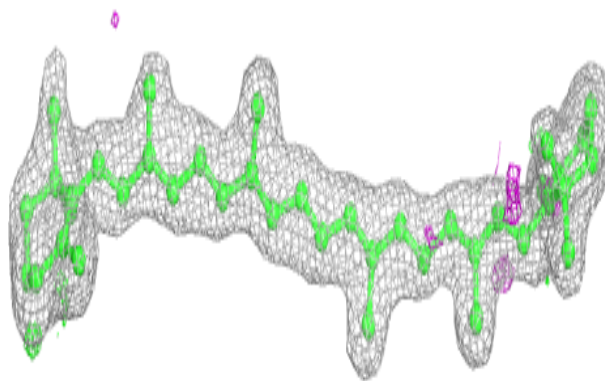
Electron density around CLA b 611:

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

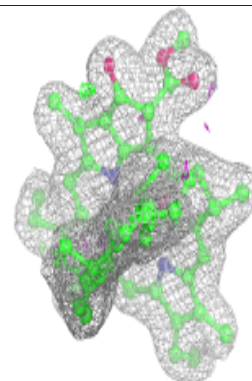
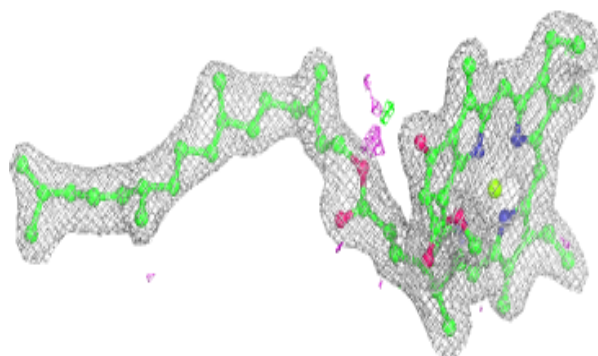
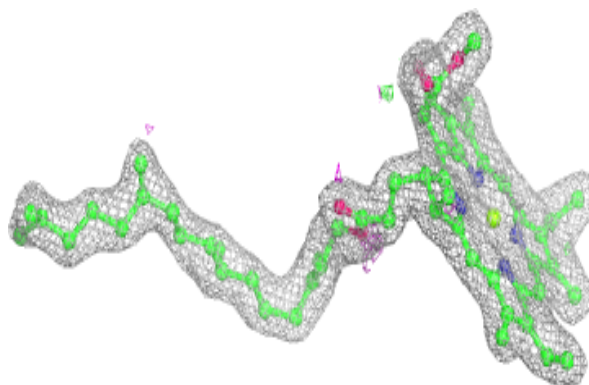


Electron density around BCR a 410:

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

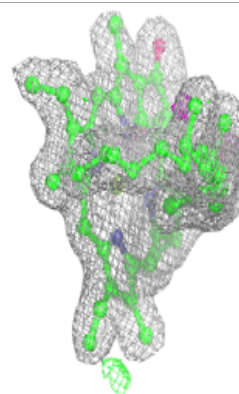
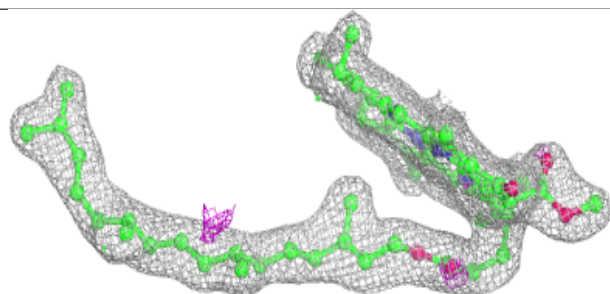
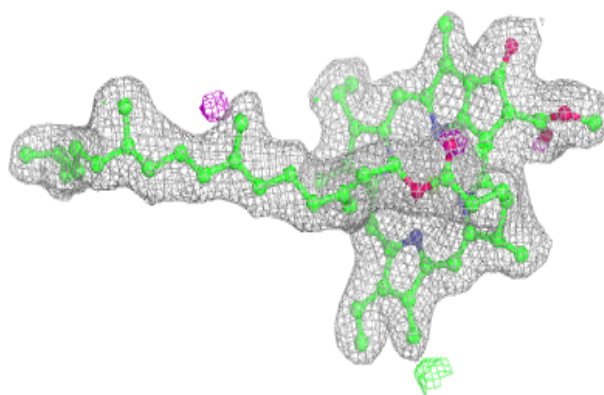
**Electron density around CLA C 503:**

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

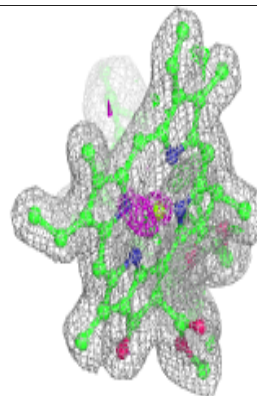
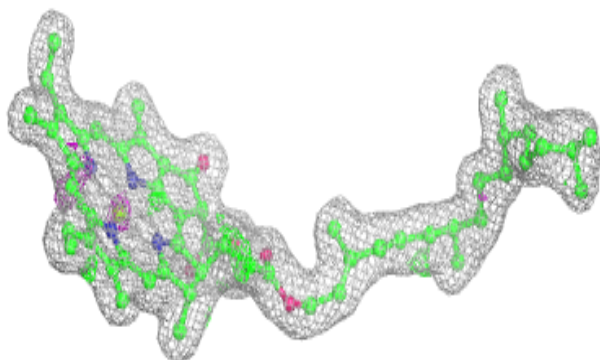
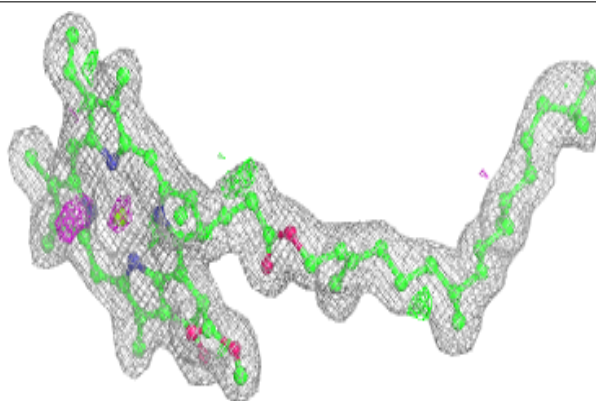


Electron density around CLA b 613:

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

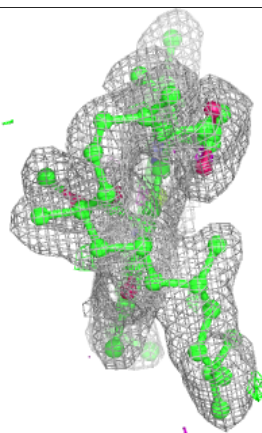
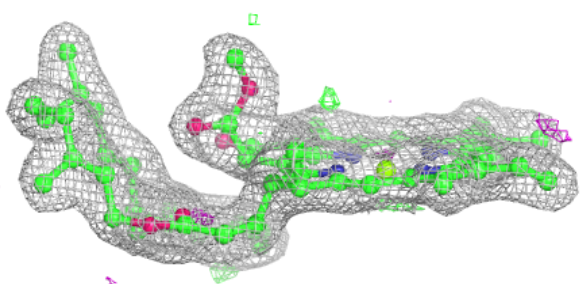
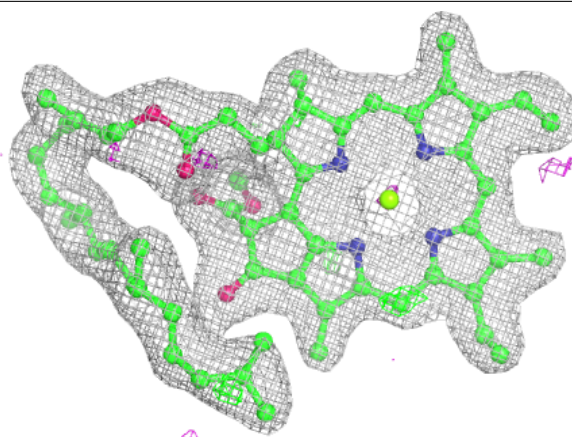
**Electron density around CLA A 405:**

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



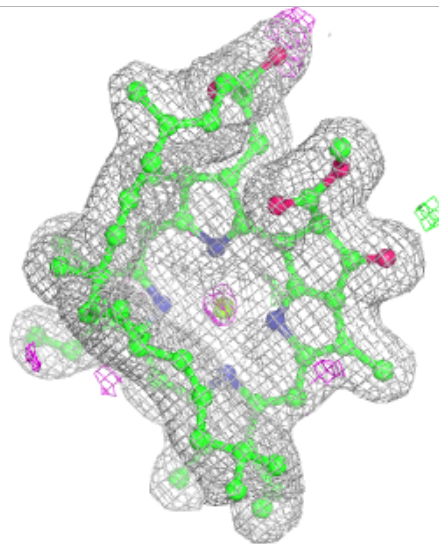
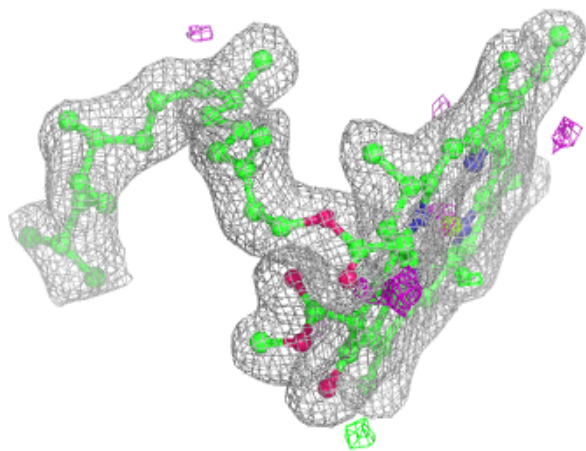
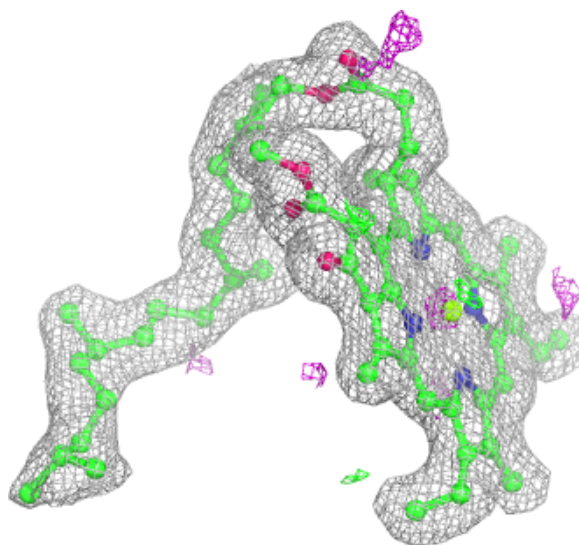
Electron density around CLA b 615:

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



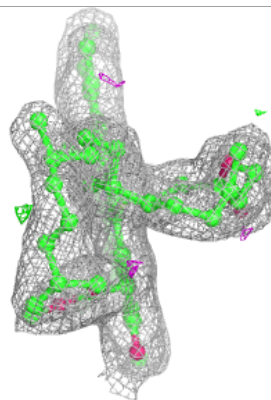
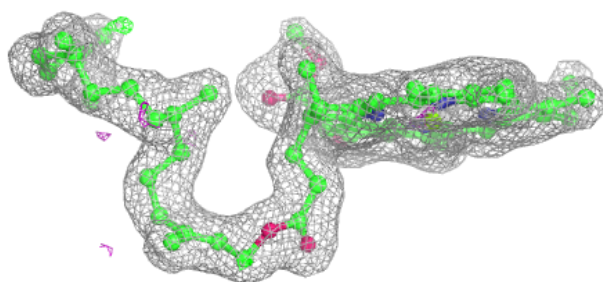
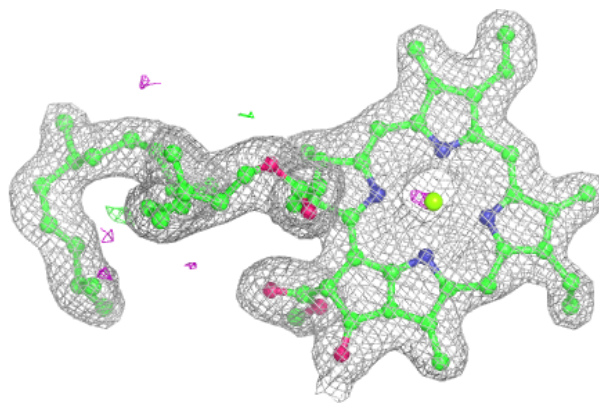
Electron density around CLA B 614:

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

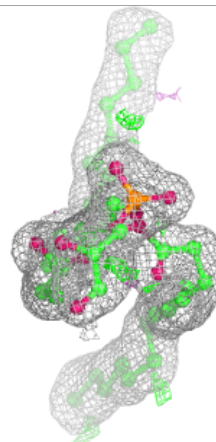
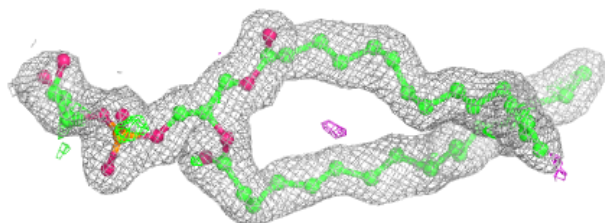
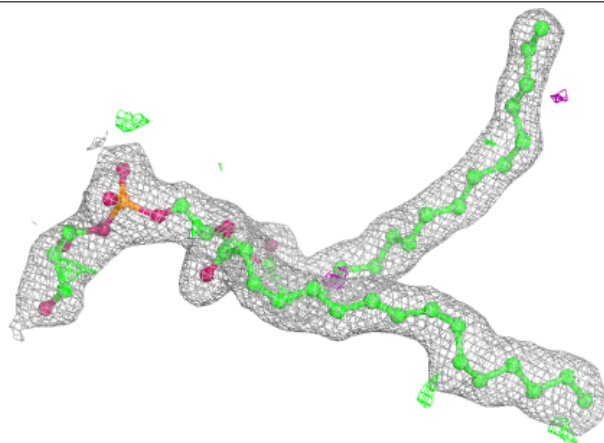


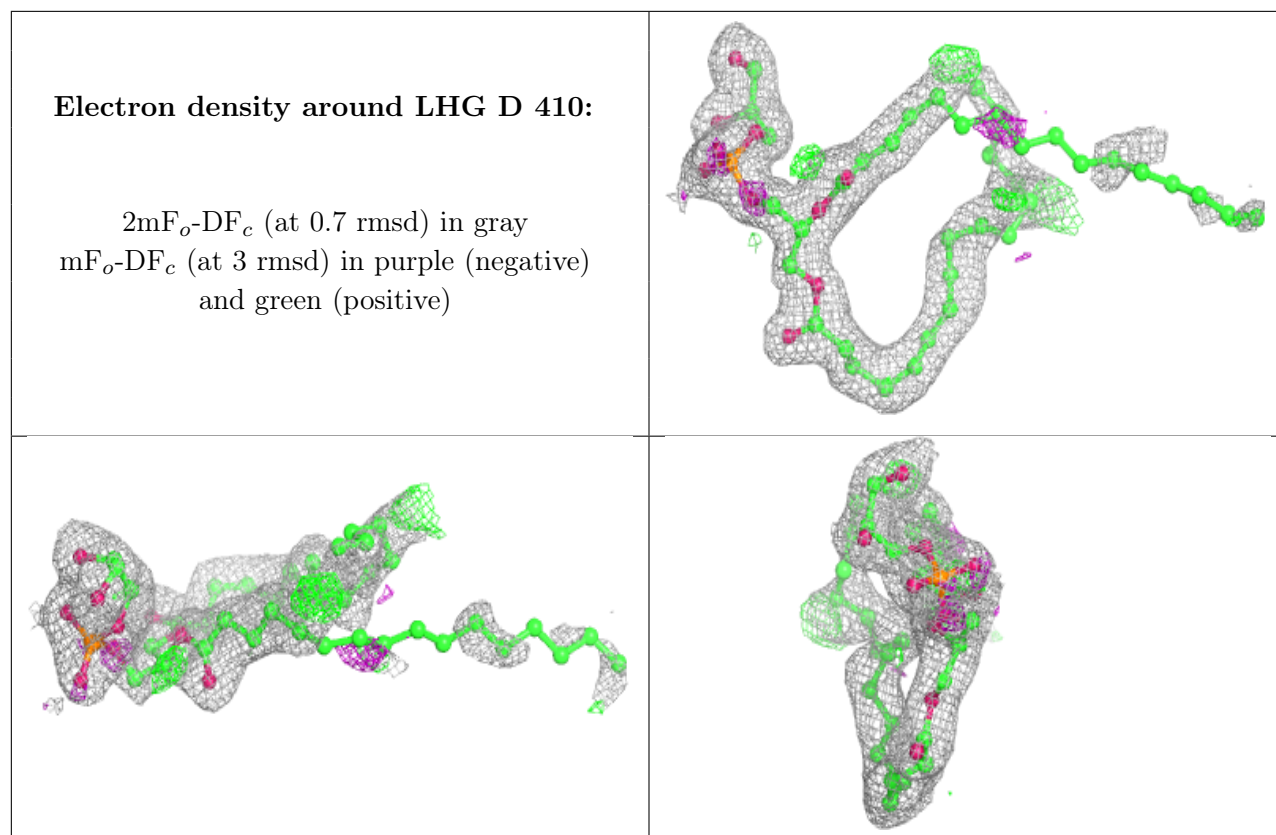
Electron density around CLA b 617:

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

**Electron density around LHG D 409:**

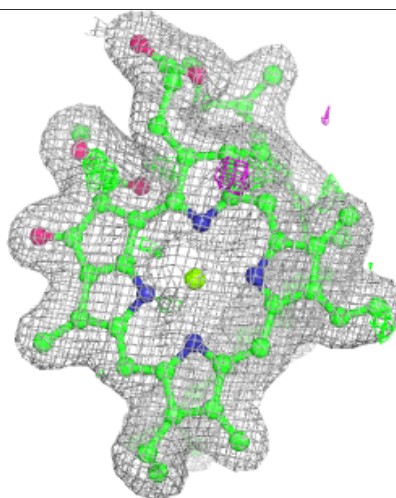
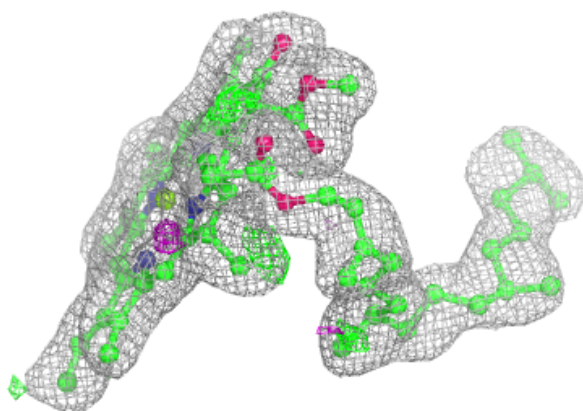
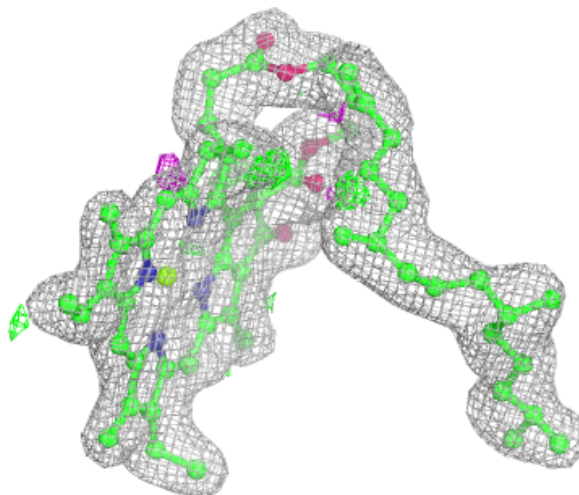
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





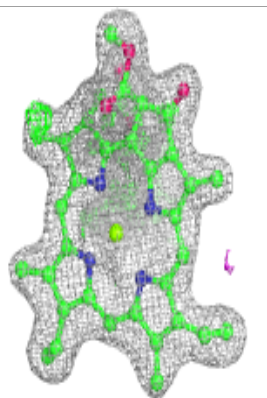
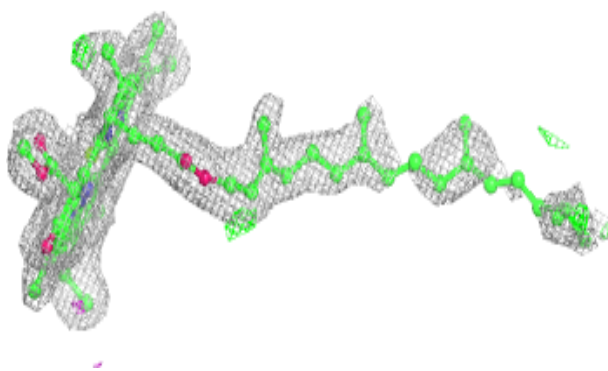
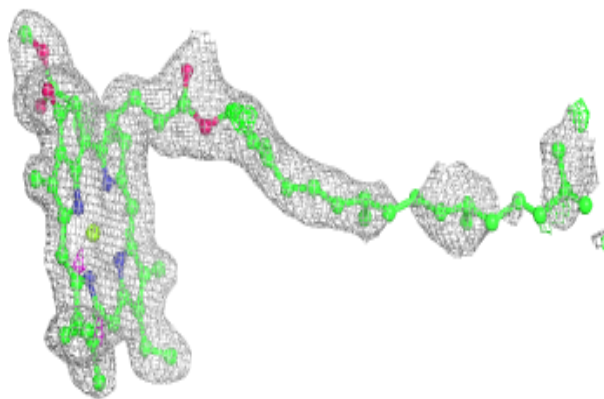
Electron density around CLA b 618:

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



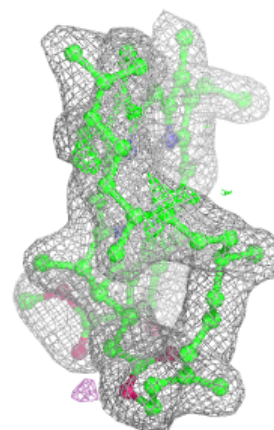
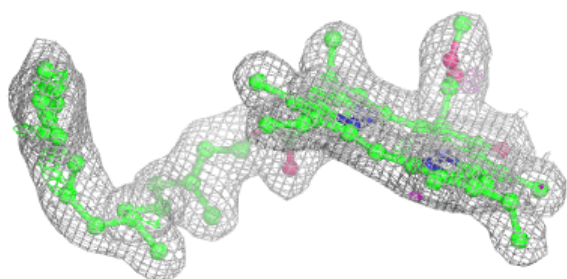
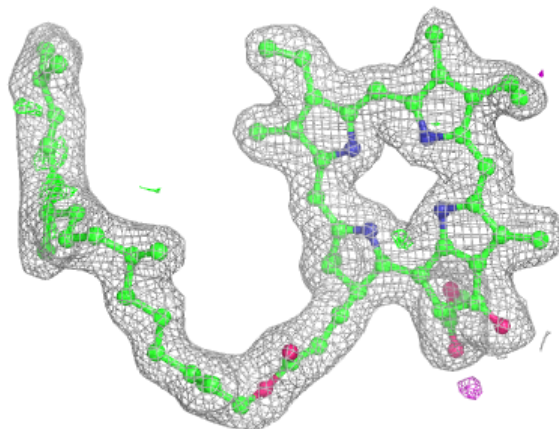
Electron density around CLA d 404:

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



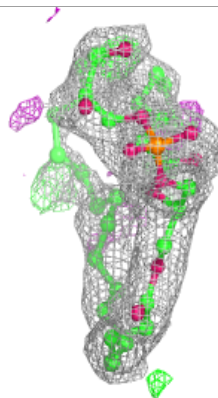
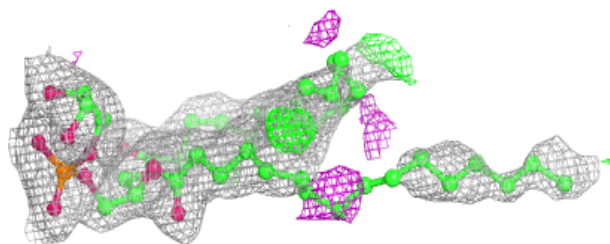
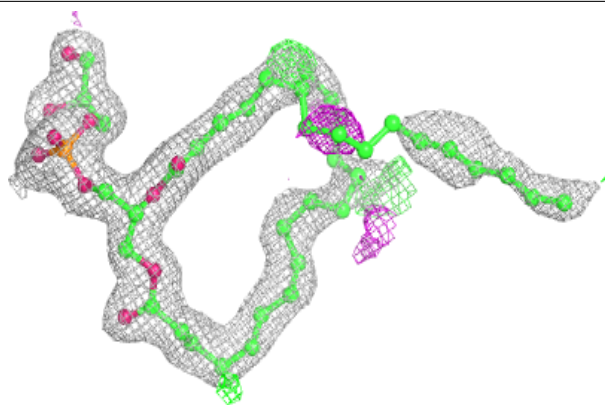
Electron density around PHO d 403:

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

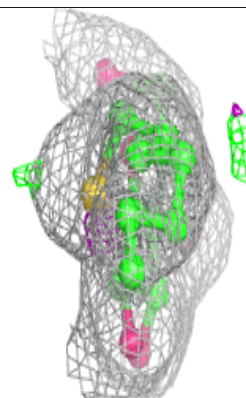
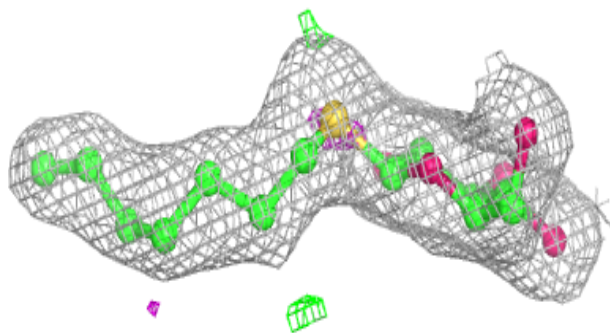
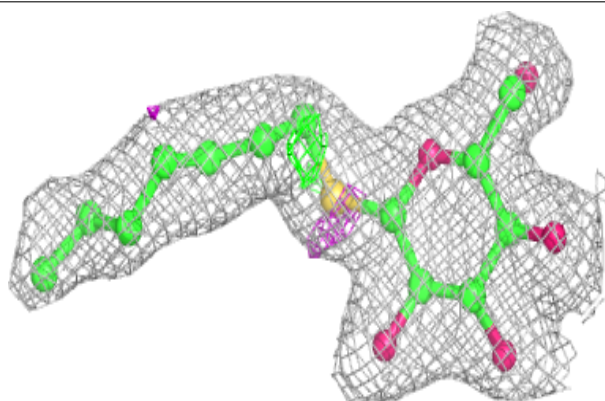


Electron density around LHG d 410:

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

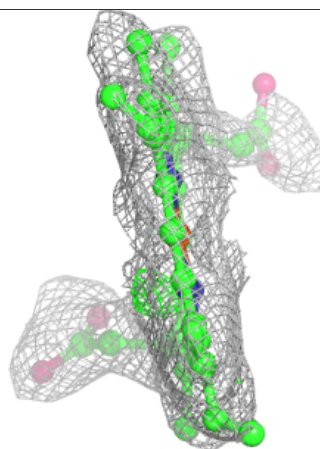
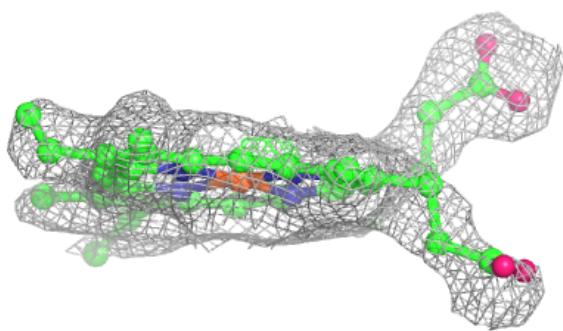
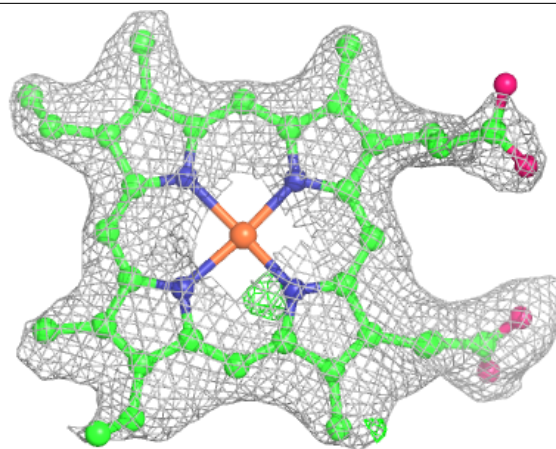
**Electron density around HTG O 303:**

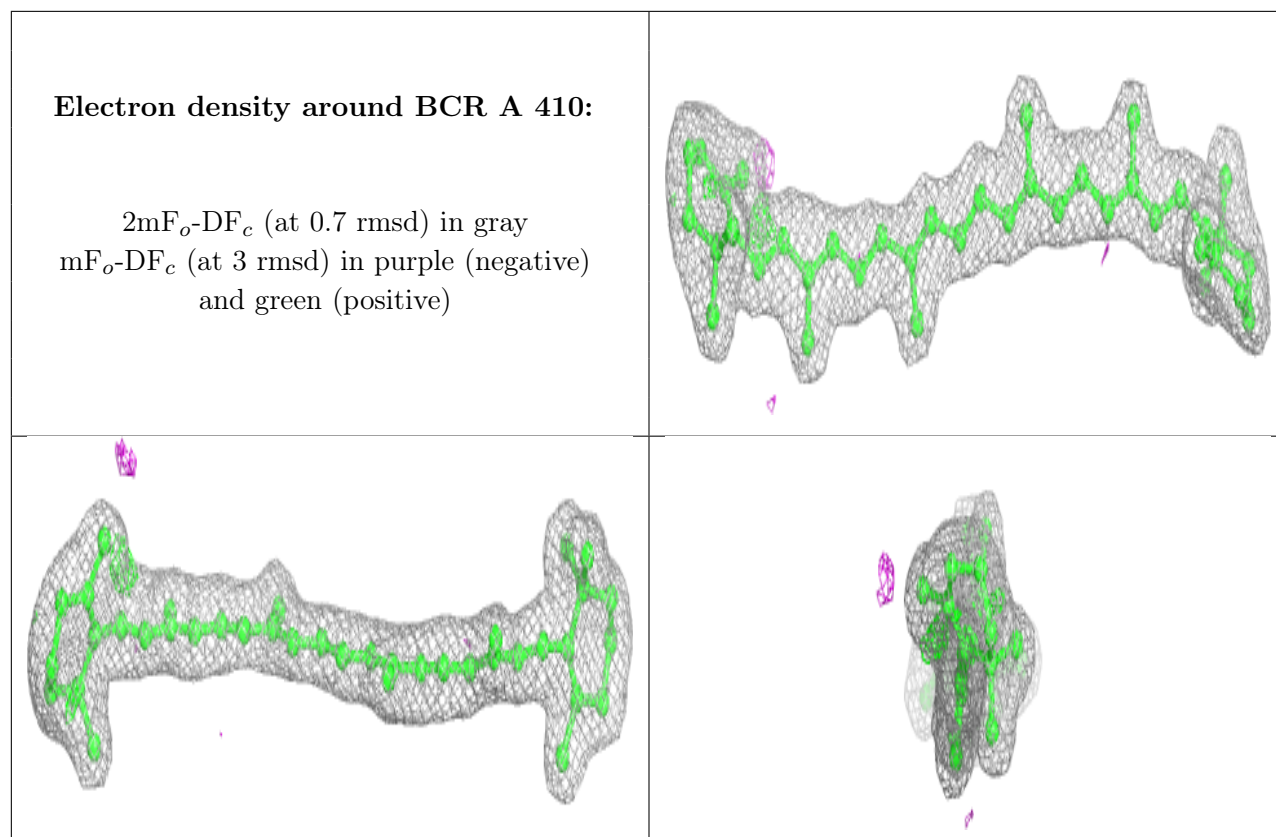
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM e 102:

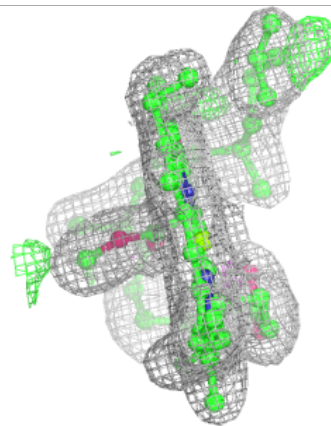
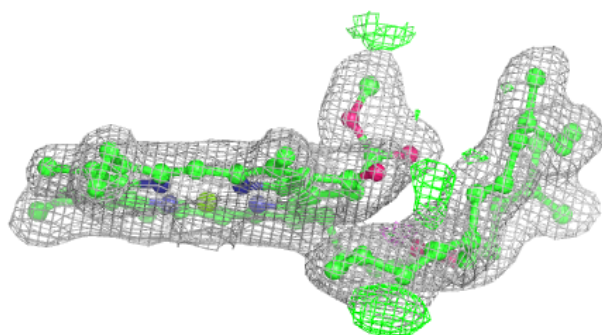
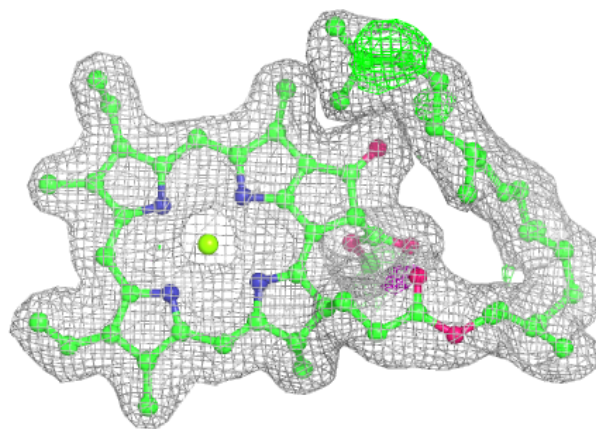
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





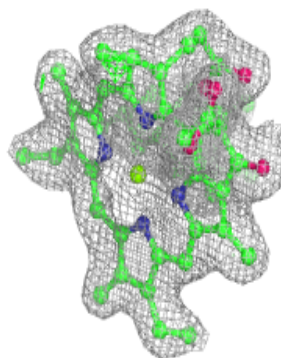
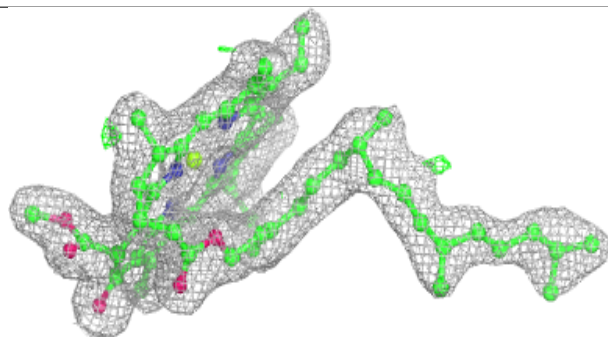
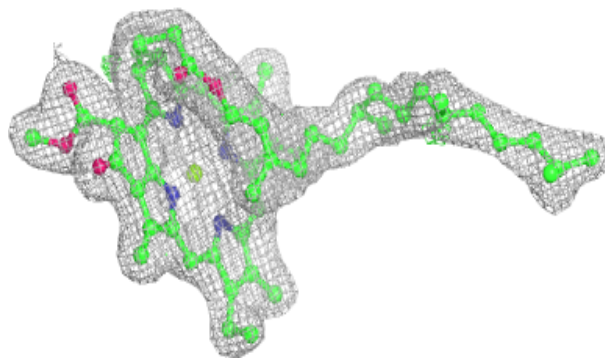
Electron density around CLA B 611:

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

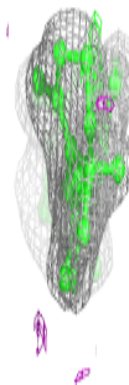
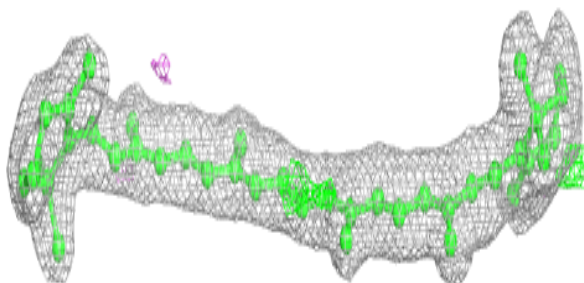
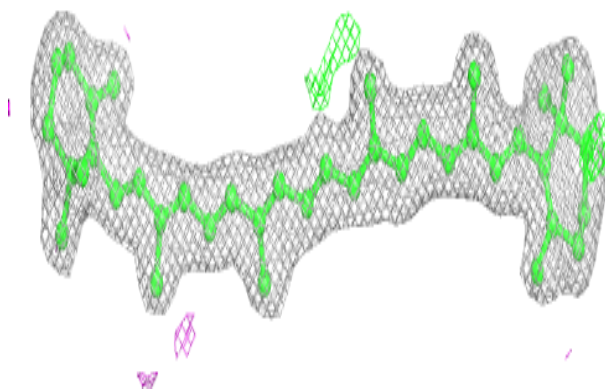


Electron density around CLA C 506:

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

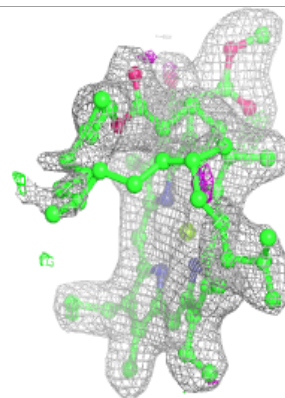
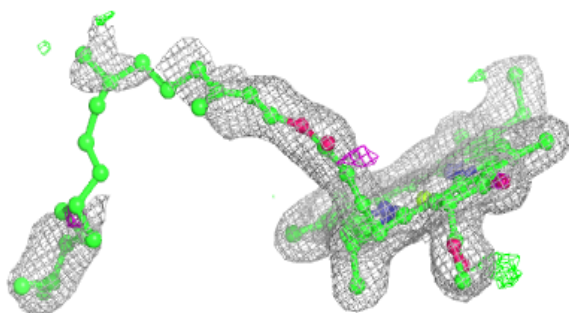
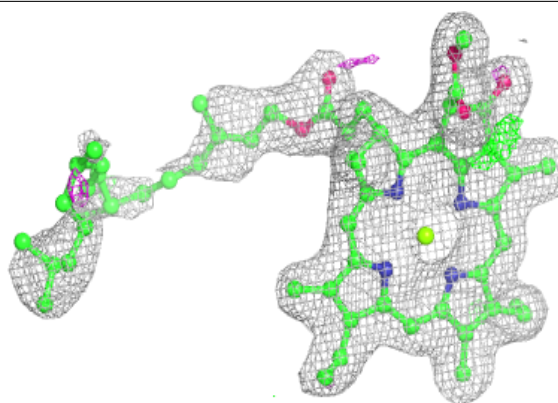
**Electron density around BCR B 620:**

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

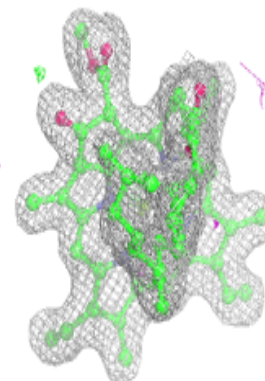
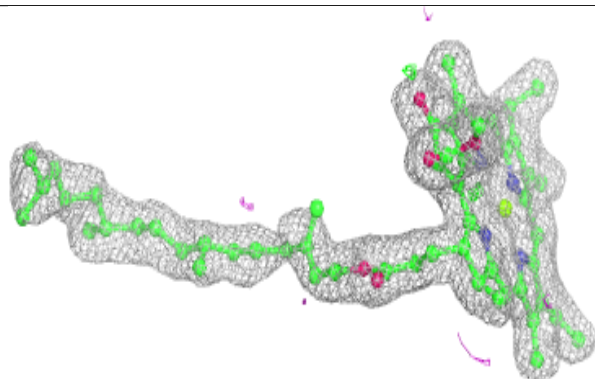
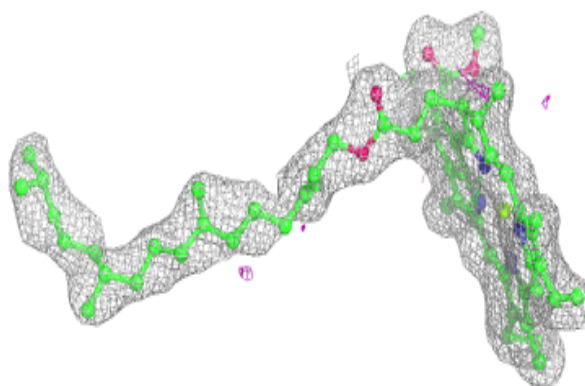


Electron density around CLA A 409:

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

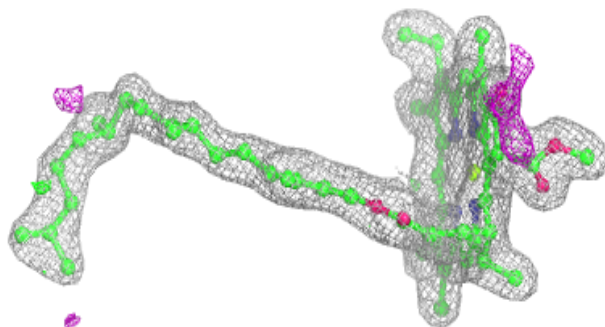
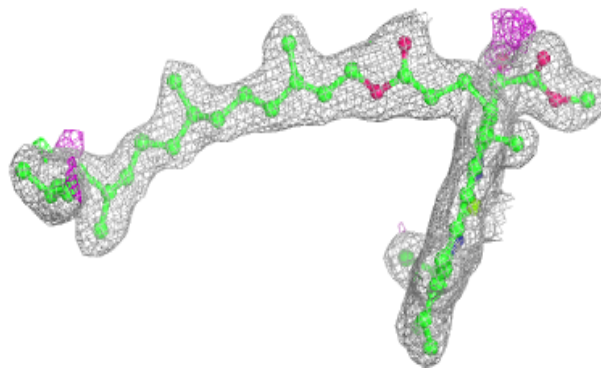
**Electron density around CLA b 609:**

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

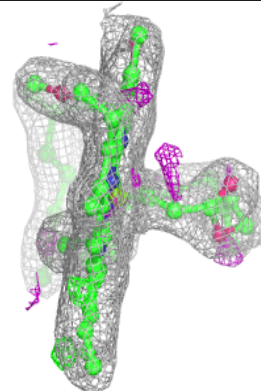
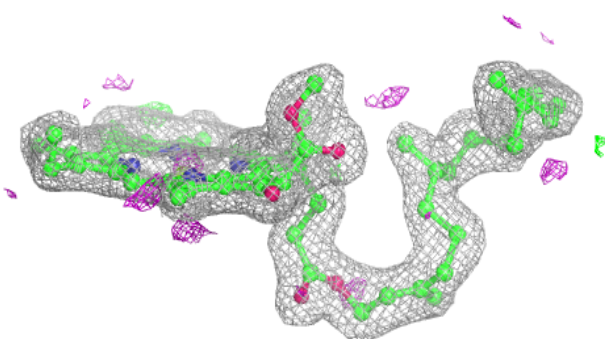
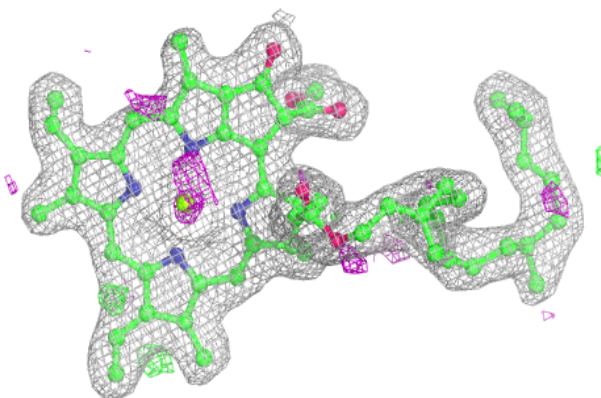


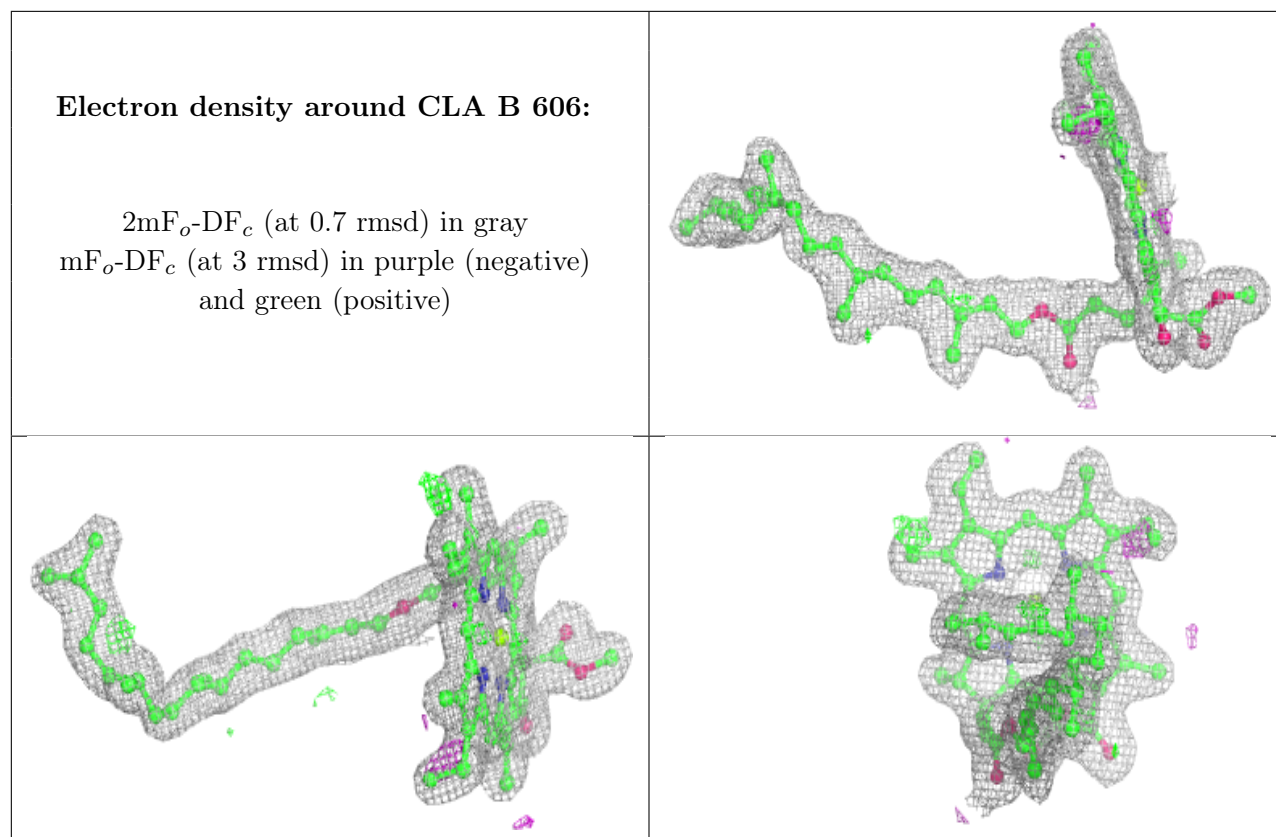
Electron density around CLA b 610:

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

**Electron density around CLA B 613:**

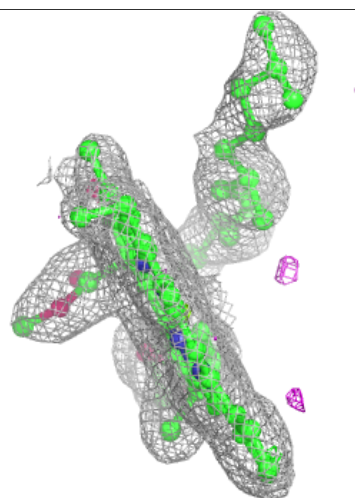
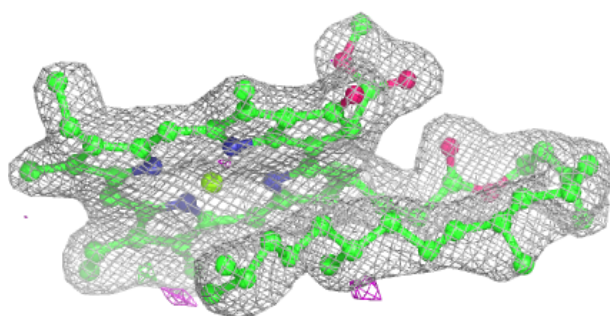
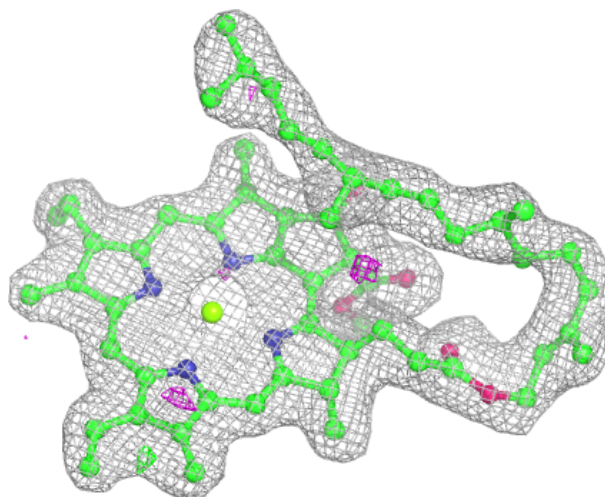
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





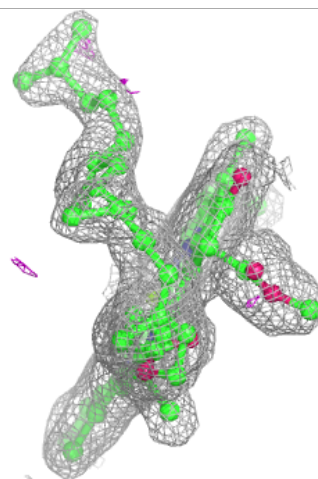
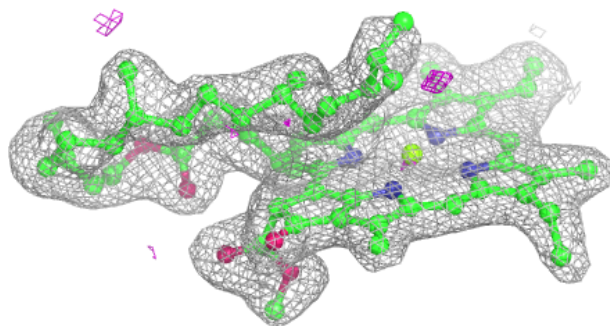
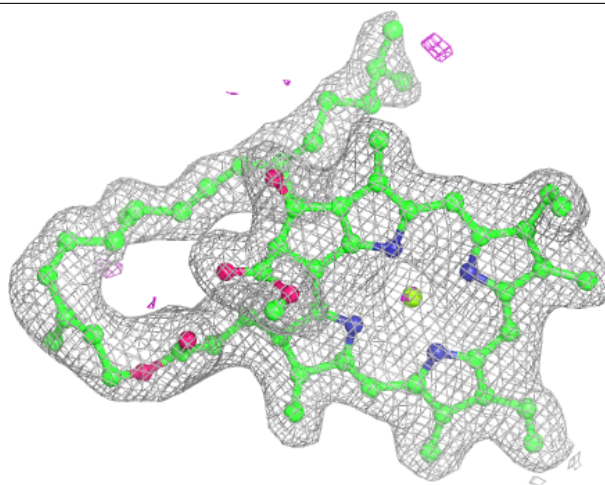
Electron density around CLA C 510:

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



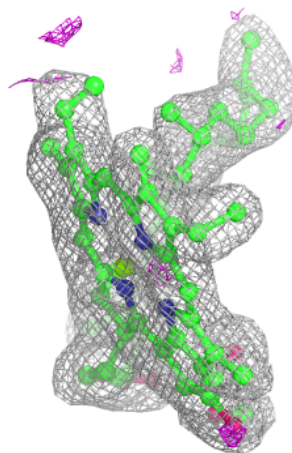
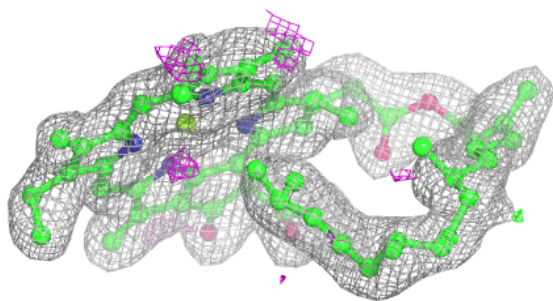
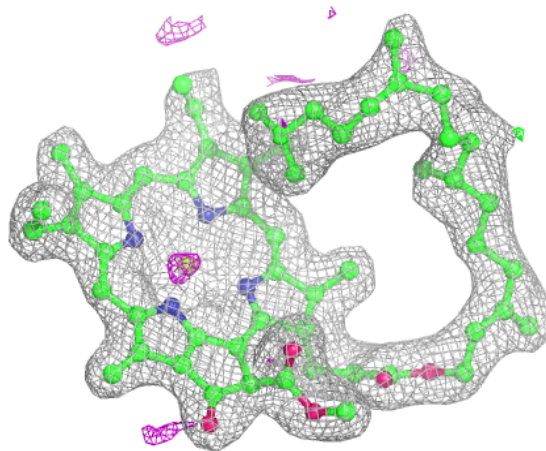
Electron density around CLA c 511:

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



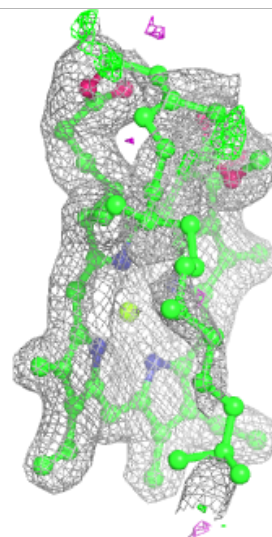
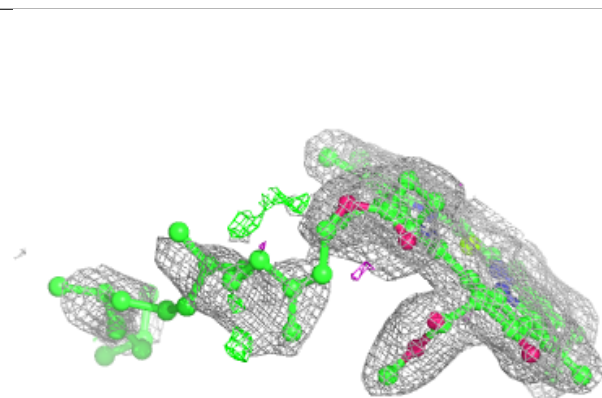
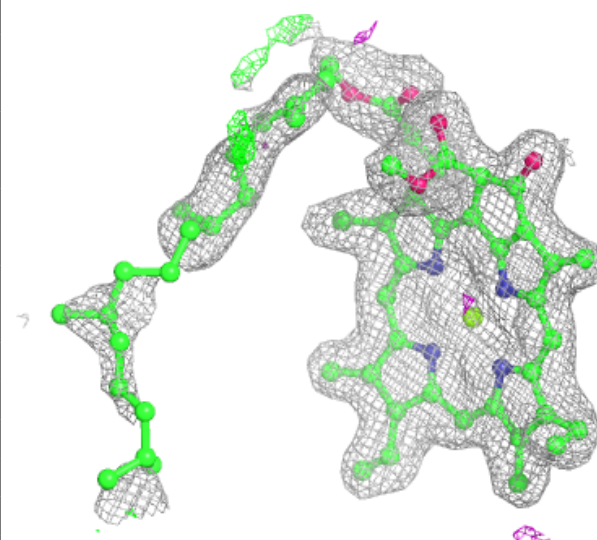
Electron density around CLA B 616:

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



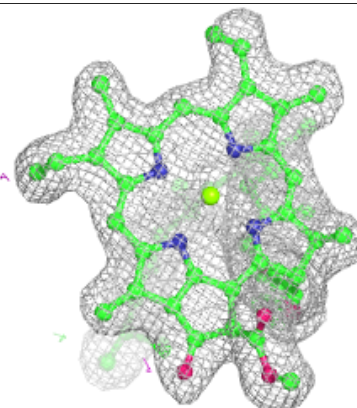
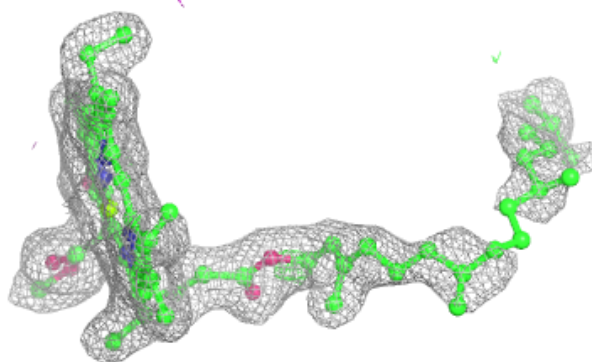
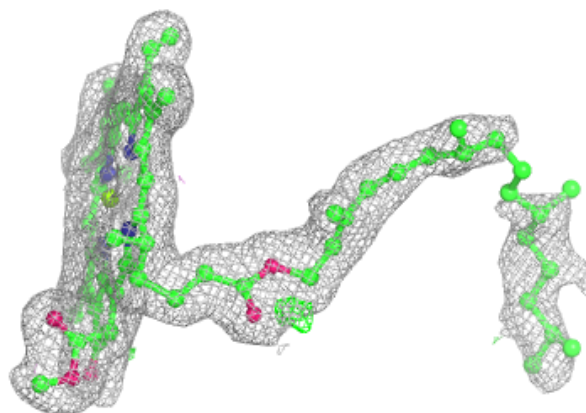
Electron density around CLA B 617:

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

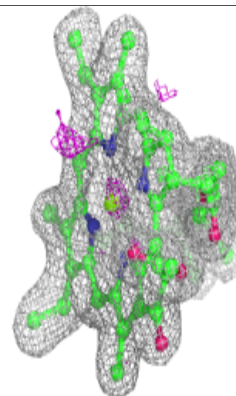
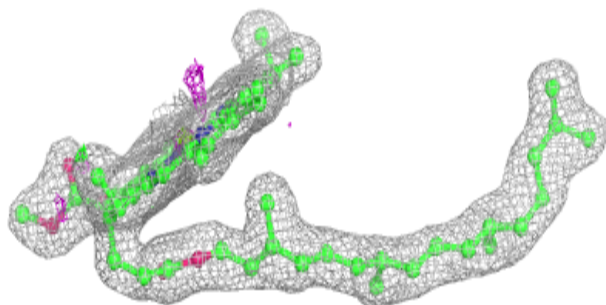
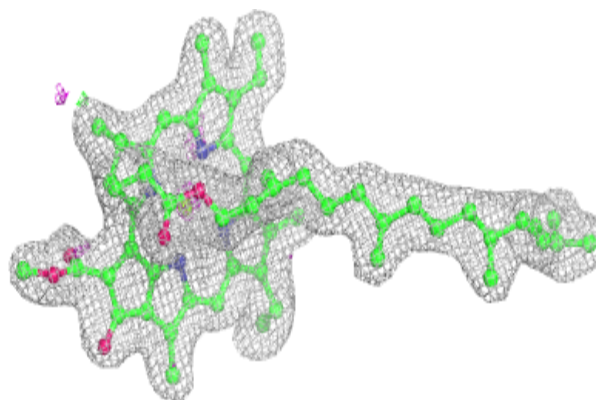


Electron density around CLA D 404:

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

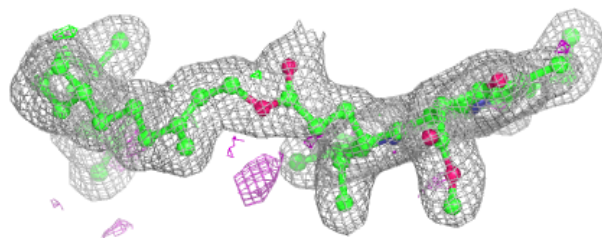
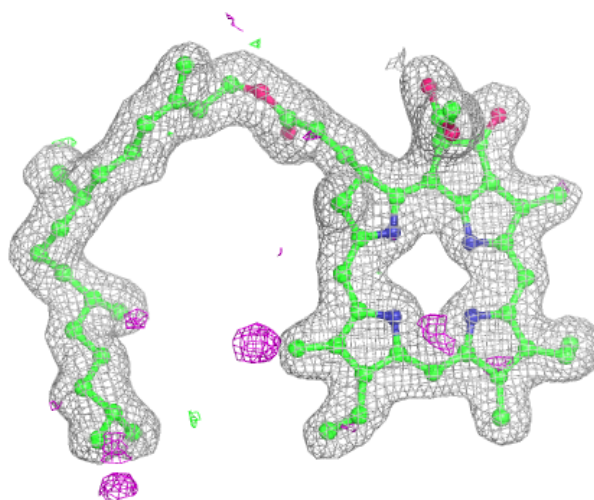
**Electron density around CLA B 609:**

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



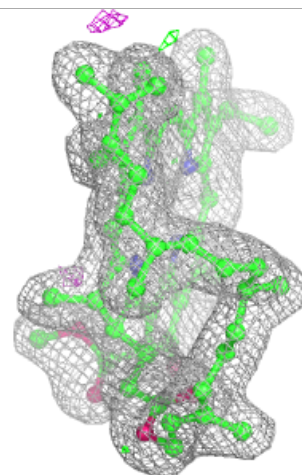
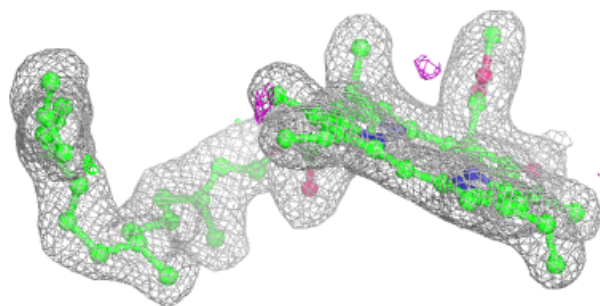
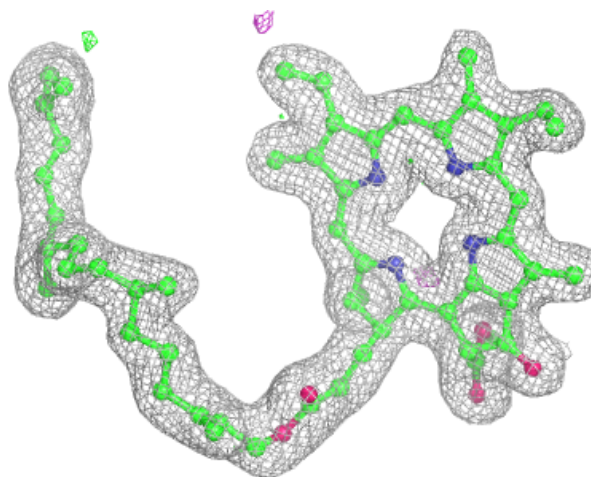
Electron density around PHO A 407:

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



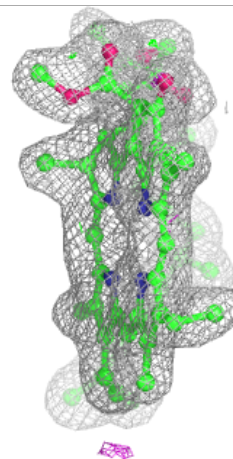
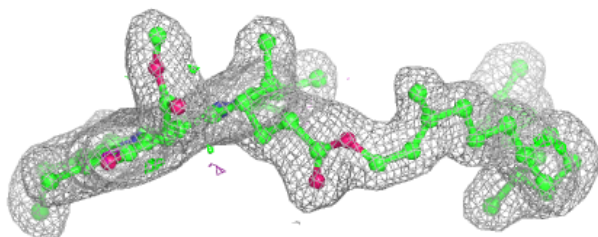
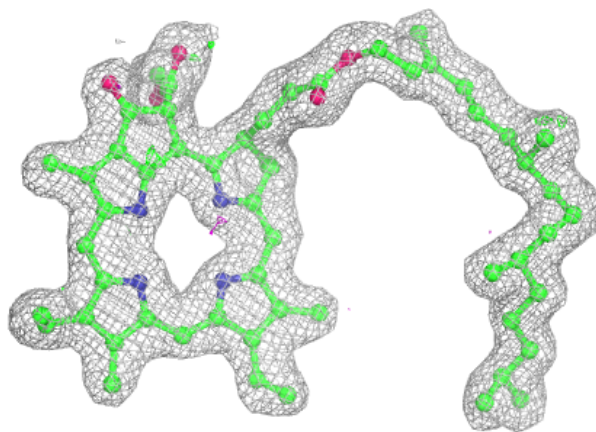
Electron density around PHO A 408:

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



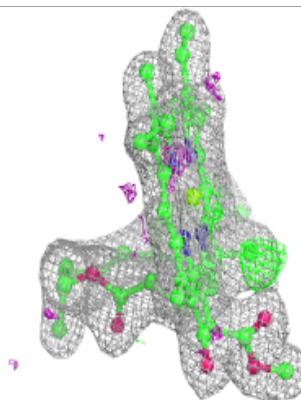
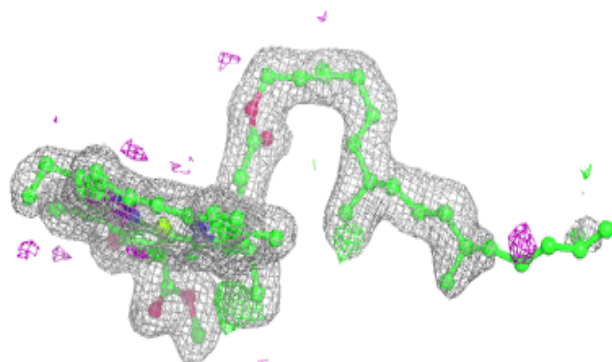
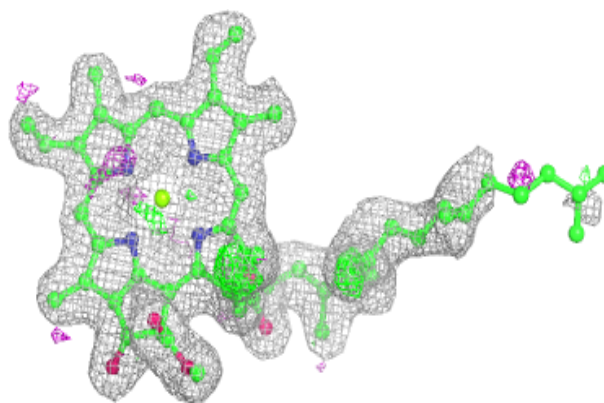
Electron density around PHO a 408:

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

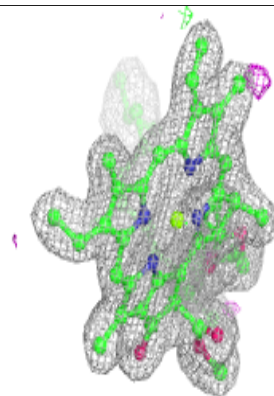
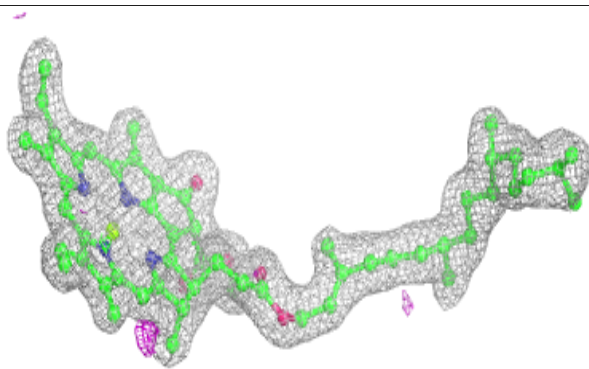
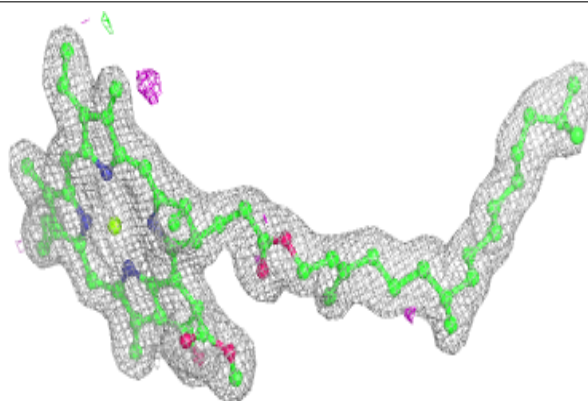


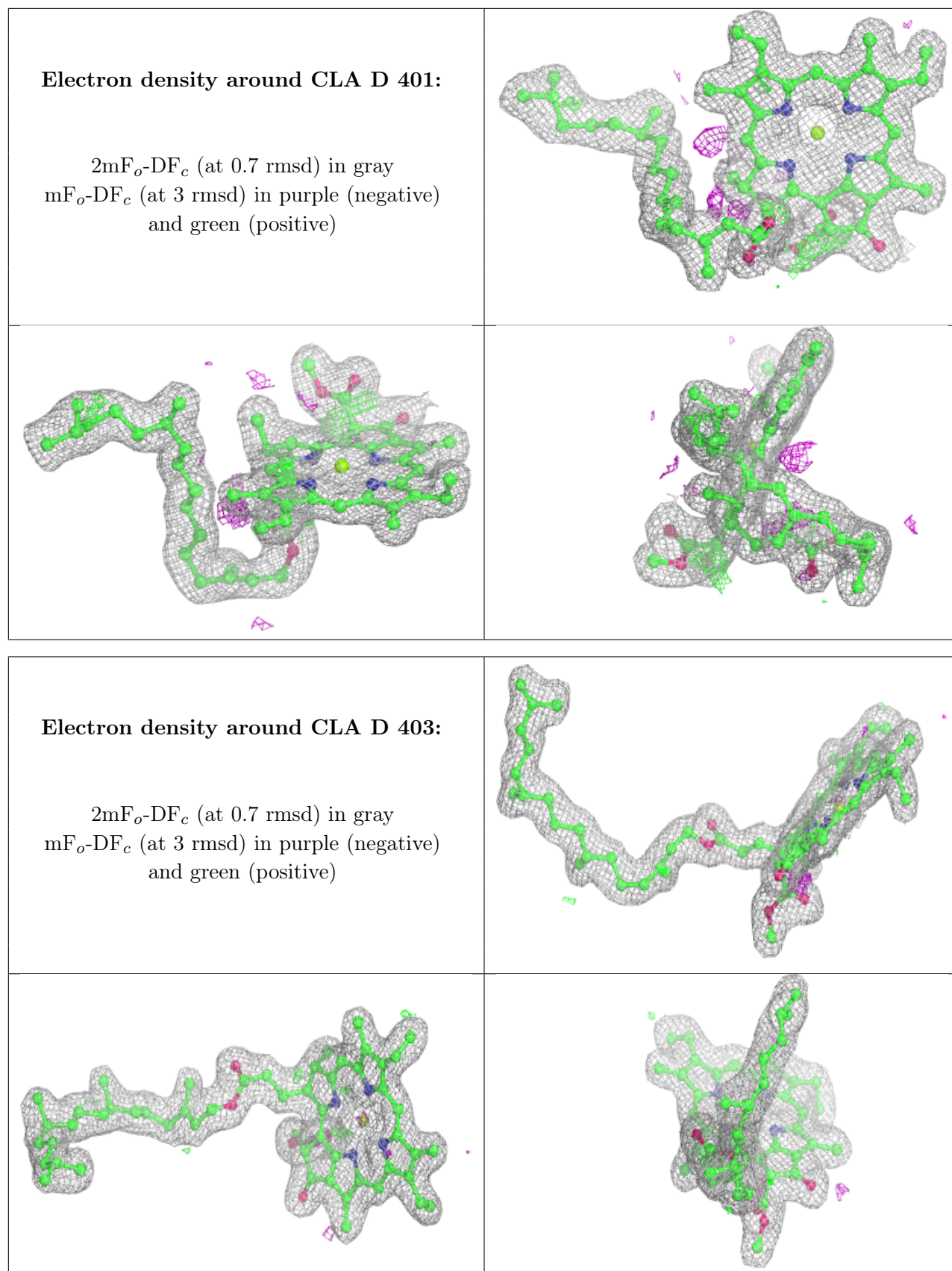
Electron density around CLA A 406:

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

**Electron density around CLA a 406:**

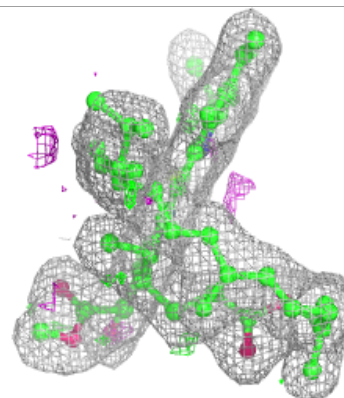
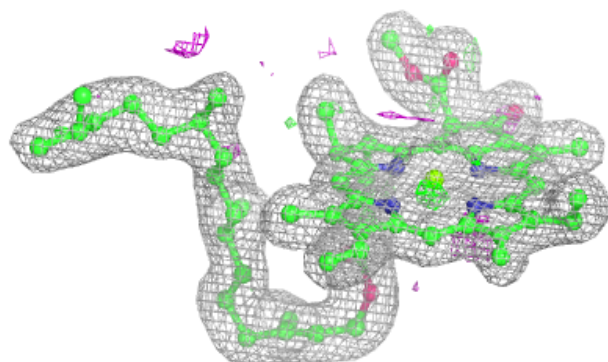
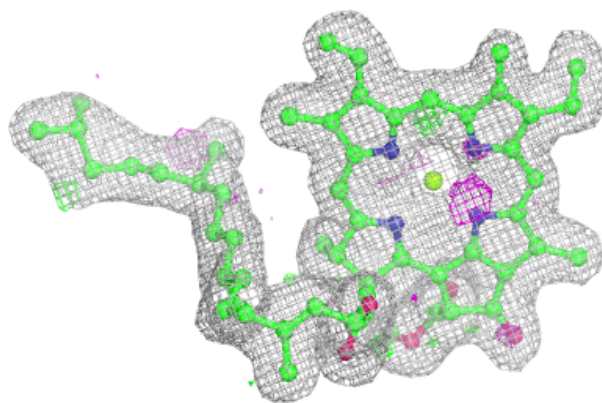
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





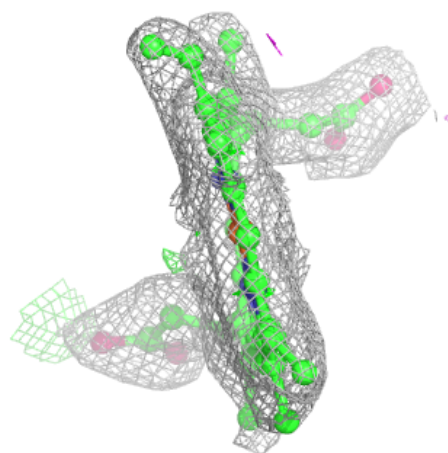
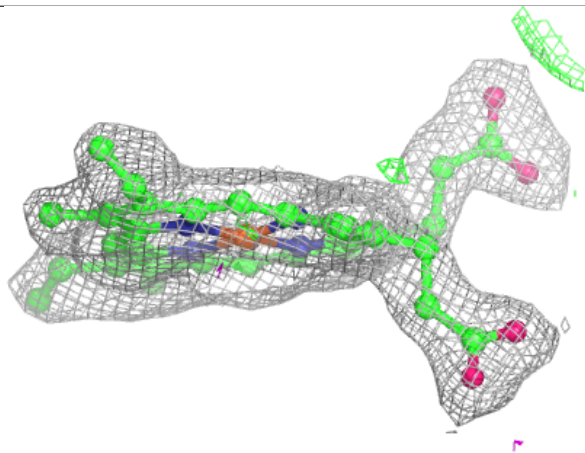
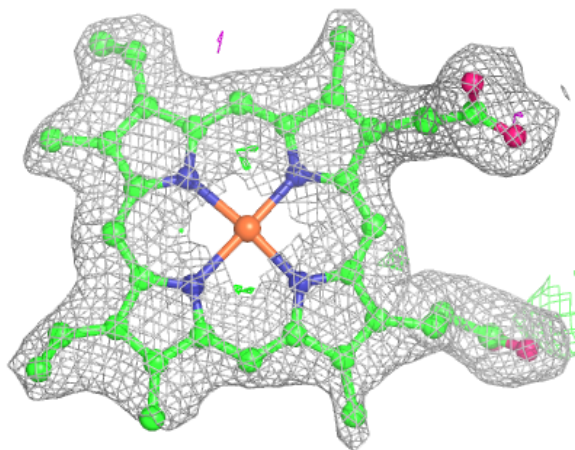
Electron density around CLA d 401:

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



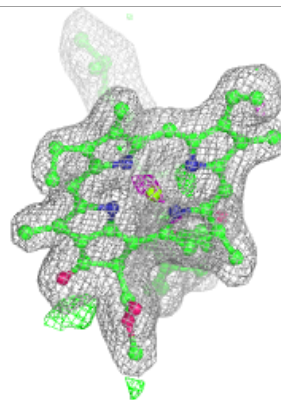
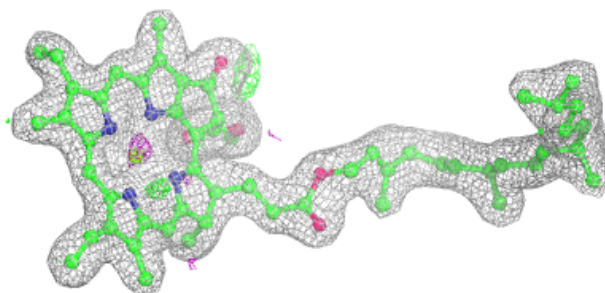
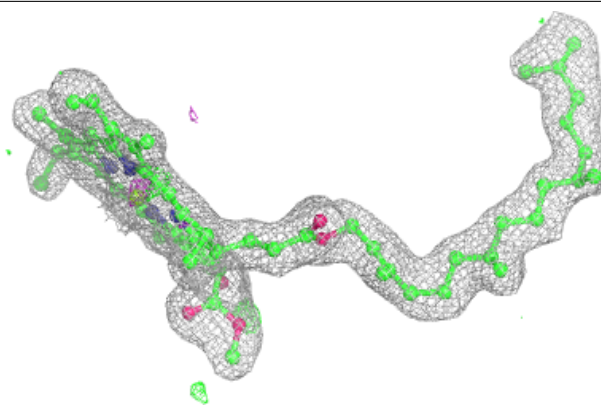
Electron density around HEM E 103:

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



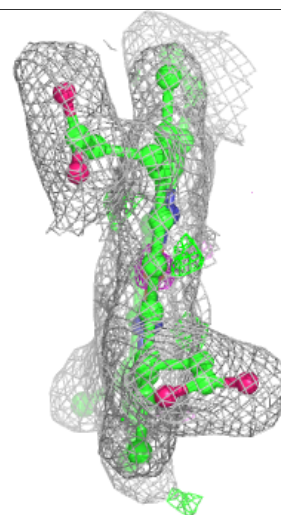
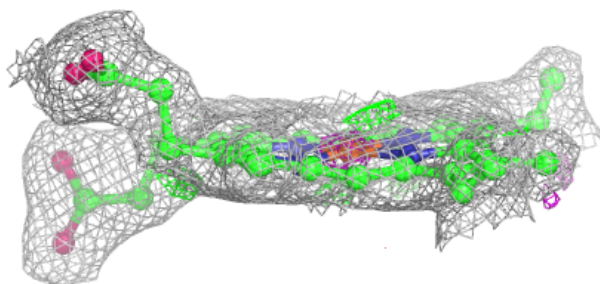
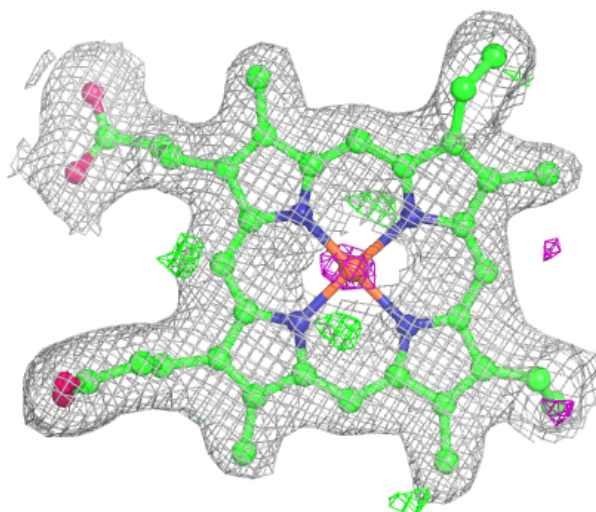
Electron density around CLA d 402:

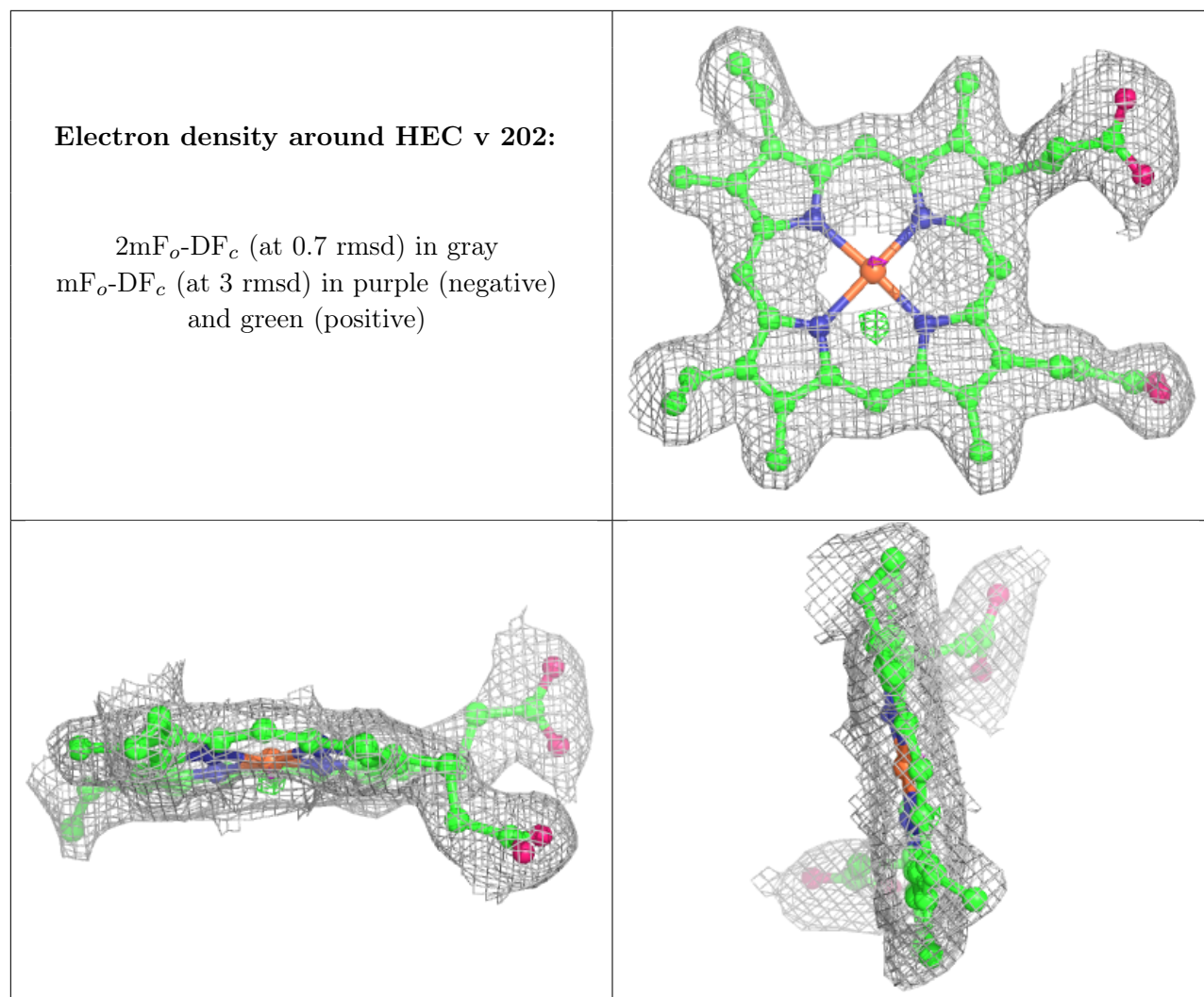
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC V 203:

$2mF_o-DF_c$ (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.