



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 03:38 AM JST

PDB ID : 4UB6 / pdb_00004ub6
Title : Native structure of photosystem II (dataset-1) 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 : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

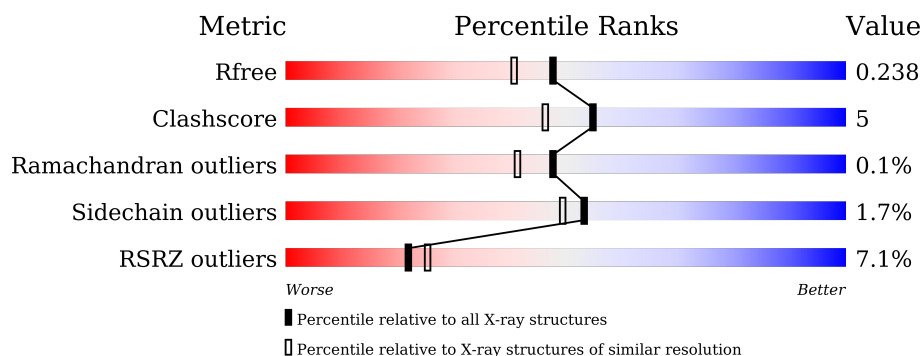
1 Overall quality at a glance

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	a	344	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
2	B	505	<div> <div>4%</div> <div>92%</div> <div>8%</div> </div>
2	b	505	<div> <div>6%</div> <div>91%</div> <div>8%</div> </div>
3	C	455	<div> <div>4%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
3	c	455	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	342	% 92% 8%
4	d	342	% 92% 8%
5	E	84	10% 88% 8% .
5	e	84	20% 80% 15% . .
6	F	44	9% 61% 14% . 23%
6	f	44	7% 50% 23% 27%
7	H	65	6% 95% 5%
7	h	65	11% 97% .
8	I	38	16% 87% 13%
8	i	38	16% 89% 8% .
9	J	39	15% 90% 8% .
9	j	39	18% 87% 10% .
10	K	37	8% 86% 14%
10	k	37	14% 81% 19%
11	L	37	8% 84% 11% 5%
11	l	37	5% 86% 14%
12	M	36	8% 75% 19% 6%
12	m	36	6% 75% 14% 6% 6%
13	O	244	7% 88% 12%
13	o	244	13% 86% 13% .
14	T	32	6% 88% 6% 6%
14	t	32	6% 88% . . 6%
15	U	104	4% 89% . 7%
15	u	104	2% 86% 7% . 7%
16	V	137	4% 97% . .

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Mol	Chain	Length	Quality of chain
16	v	137	
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
22	CL	U	201	-	-	X	-
22	CL	v	201	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54195 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
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	461	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	11	0
			4027	2643	668	703	13			
2	b	504	Total	C	N	O	S	0	12	0
			4033	2650	668	702	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

- 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	2	0
			670	439	107	124			

- 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
			280	187	43	48	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
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	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		0	0	0
			287	191	46	50				
18	x	39	Total	C	N	O		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 (CCD ID: FE2) (formula: Fe).

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

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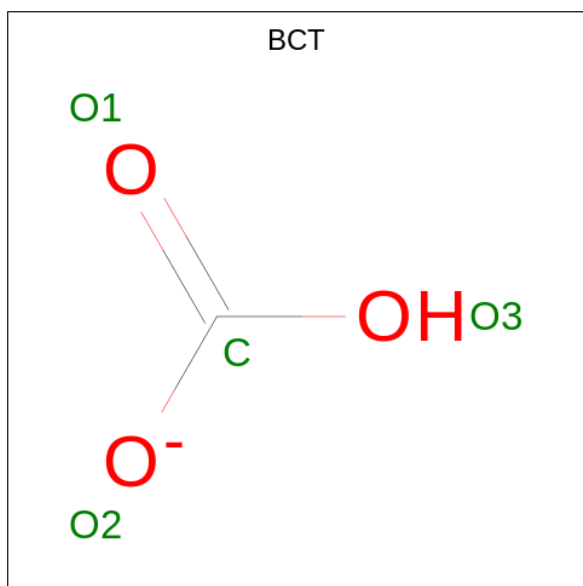
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

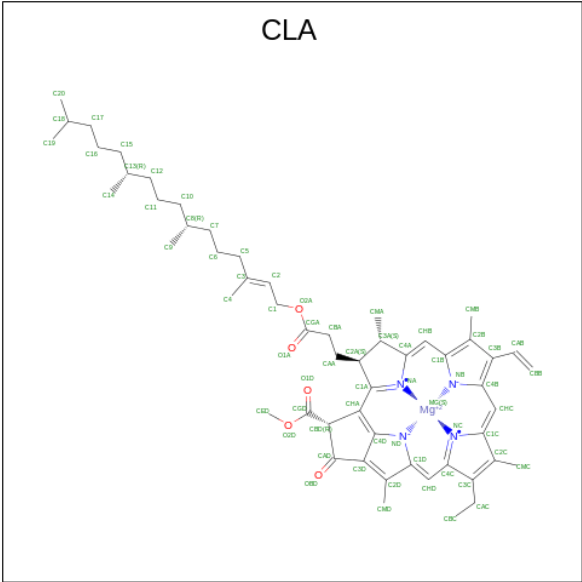
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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 (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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	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		

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

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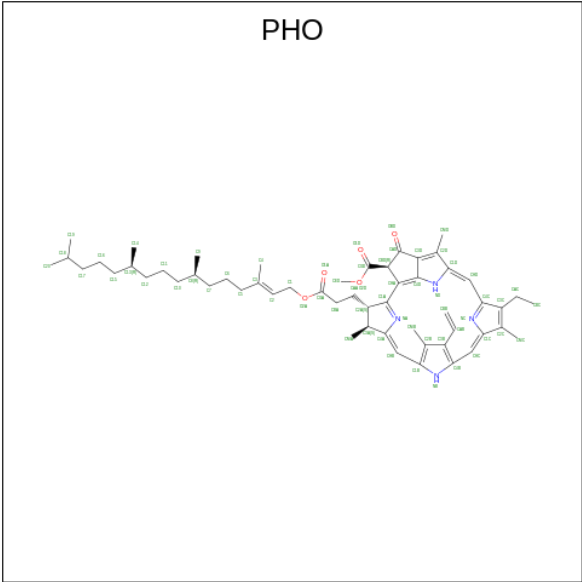
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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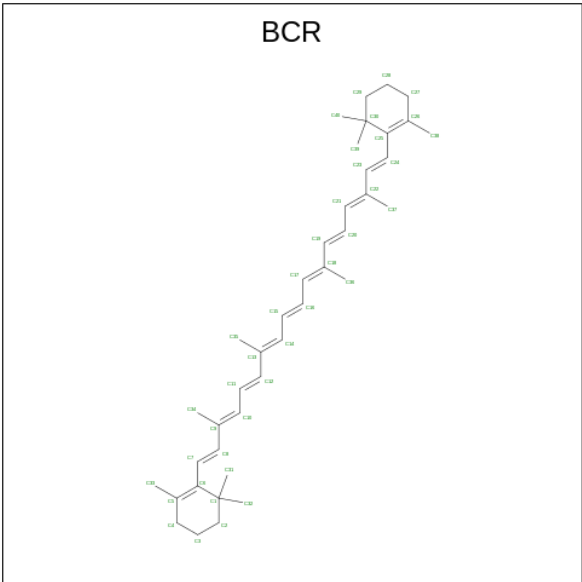
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



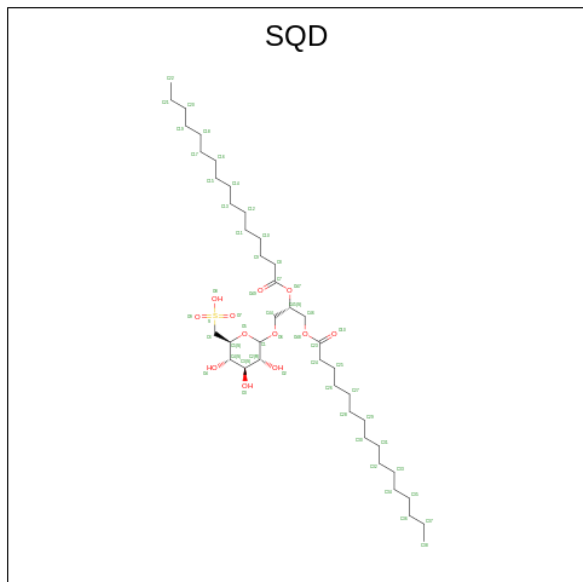
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



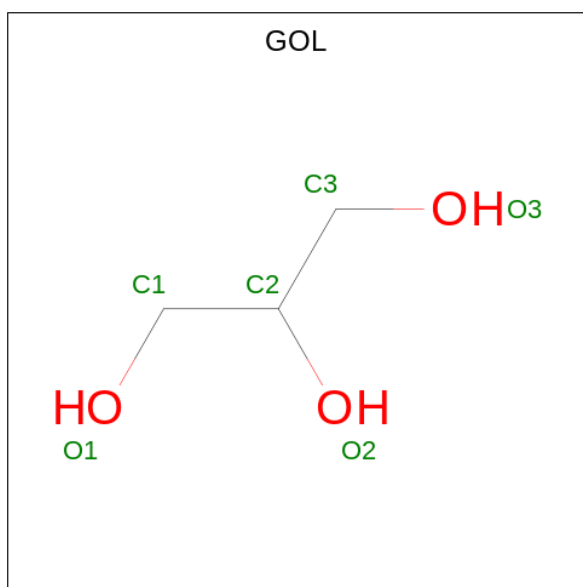
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total 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	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	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 (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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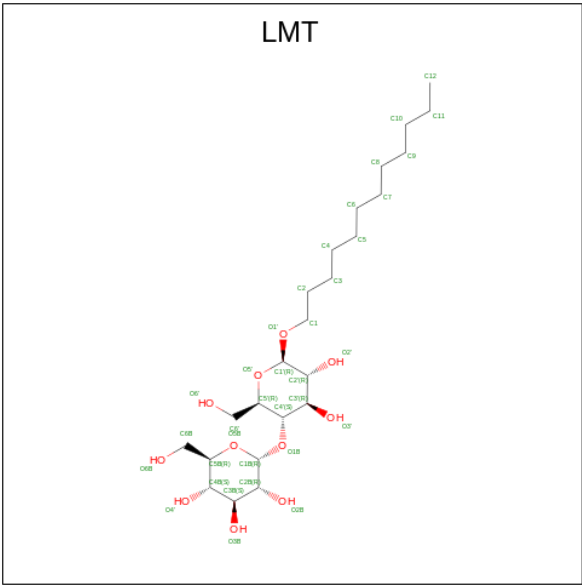
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total 6	C 3	O 3	0	0
28	T	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6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

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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 DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



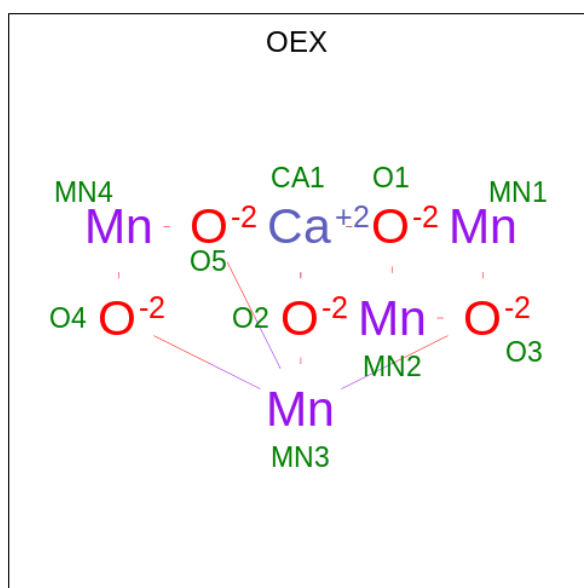
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	E	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	b	1	Total	C	O	0	0
			25	19	6		

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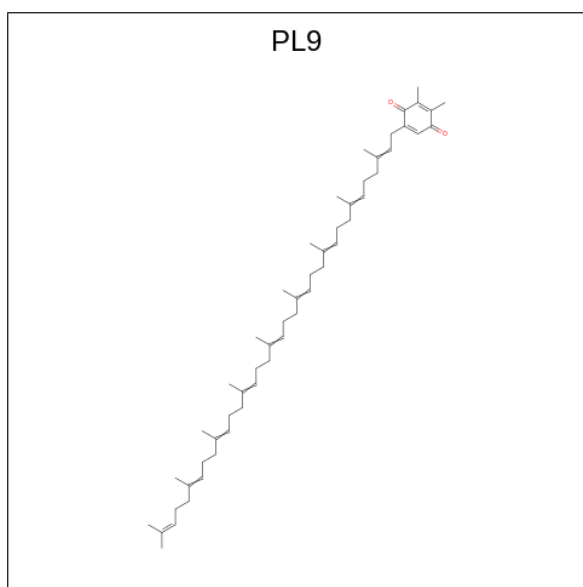
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			35	24	11		
29	f	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

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



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

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			
32	K	1	Total	C	O	0	0
			34	29	5		
32	M	1	Total	C		0	0
			10	10			
32	X	1	Total	C	O	0	0
			18	16	2		

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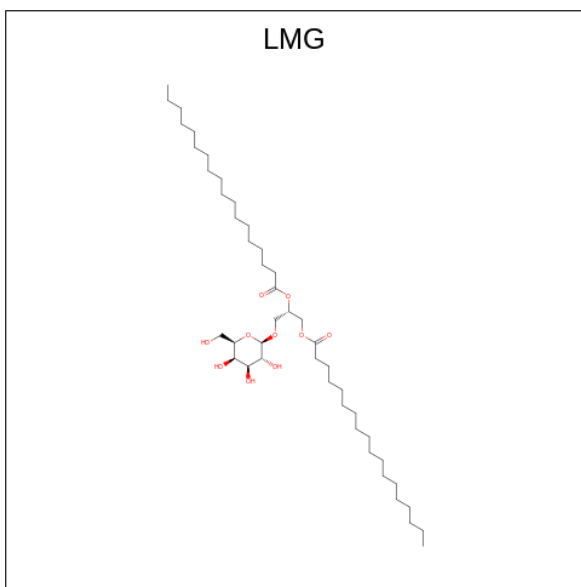
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	3	Total C O 71 63 8	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

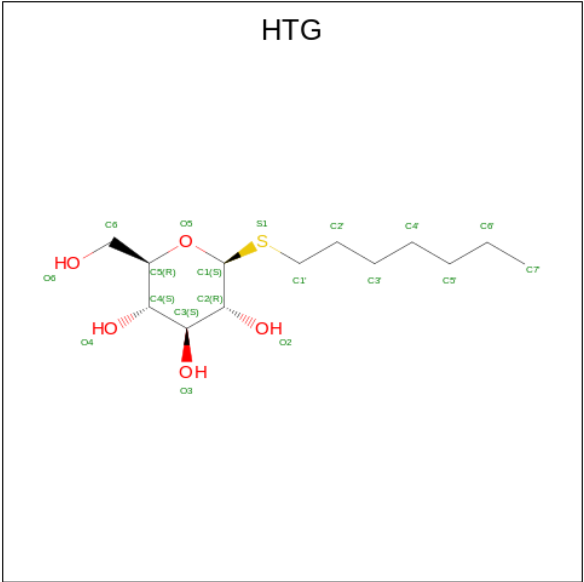
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: 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	a	1	Total	C	O	0	0
			51	41	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	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 (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



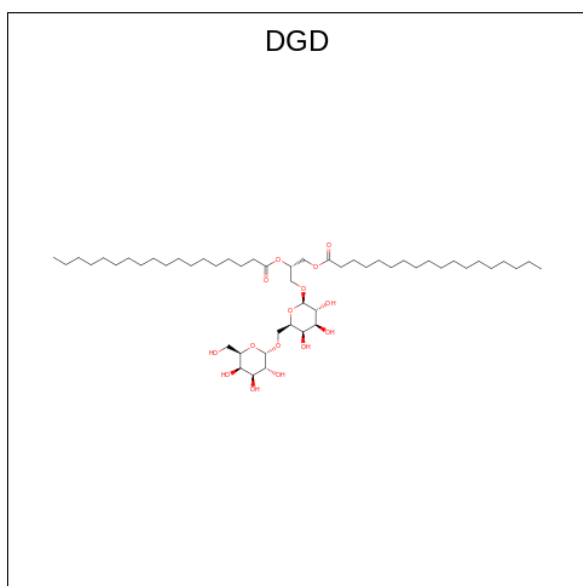
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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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) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



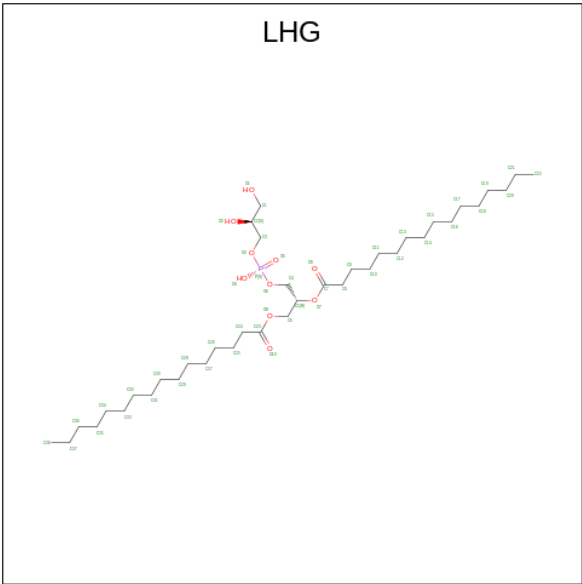
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	D	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
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 (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



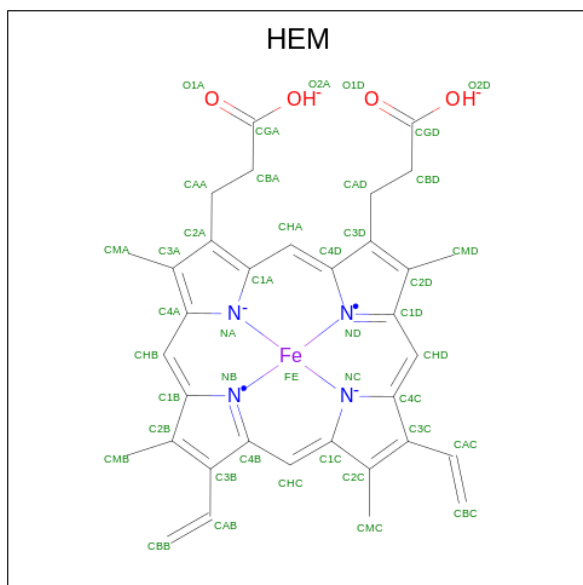
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

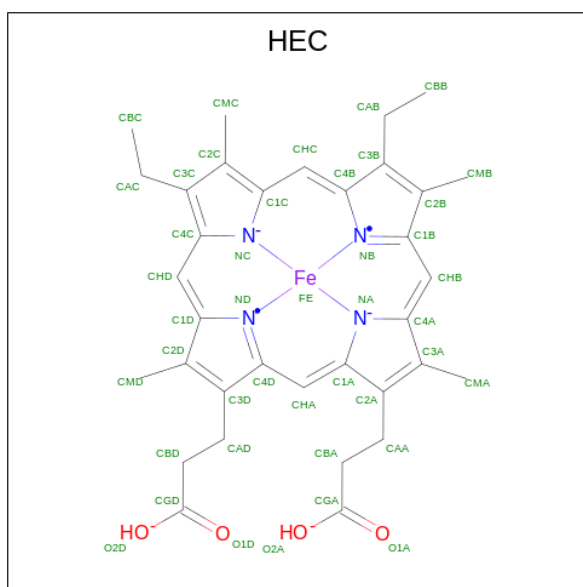


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	165	Total O 167 167	0	2
41	B	289	Total O 293 293	0	4
41	C	233	Total O 235 235	0	2
41	D	138	Total O 143 143	0	5
41	E	31	Total O 31 31	0	0
41	F	9	Total O 9 9	0	0
41	H	48	Total O 49 49	0	1
41	I	4	Total O 4 4	0	0
41	J	13	Total O 13 13	0	0
41	K	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	16	Total O 17 17	0	1
41	M	8	Total O 8 8	0	0
41	O	188	Total O 191 191	0	3
41	T	16	Total O 17 17	0	1
41	U	81	Total O 81 81	0	0
41	V	116	Total O 118 118	0	2
41	Y	4	Total O 4 4	0	0
41	X	9	Total O 9 9	0	0
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 154 154	0	1
41	b	261	Total O 264 264	0	3
41	c	197	Total O 199 199	0	2
41	d	132	Total O 137 137	0	5
41	e	17	Total O 17 17	0	0
41	f	5	Total O 5 5	0	0
41	h	41	Total O 41 41	0	0
41	i	6	Total O 6 6	0	0
41	j	7	Total O 7 7	0	0
41	k	6	Total O 6 6	0	0
41	l	10	Total O 10 10	0	0
41	m	18	Total O 18 18	0	0

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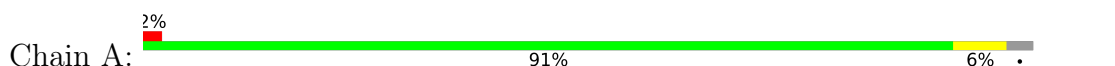
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	154	Total 155	O 155	0	1
41	t	12	Total 12	O 12	0	0
41	u	97	Total 97	O 97	0	0
41	v	89	Total 90	O 90	0	1
41	y	4	Total 4	O 4	0	0
41	x	4	Total 4	O 4	0	0

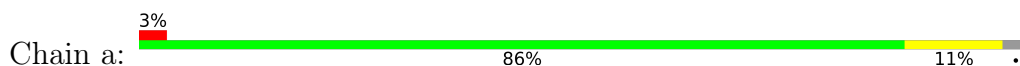
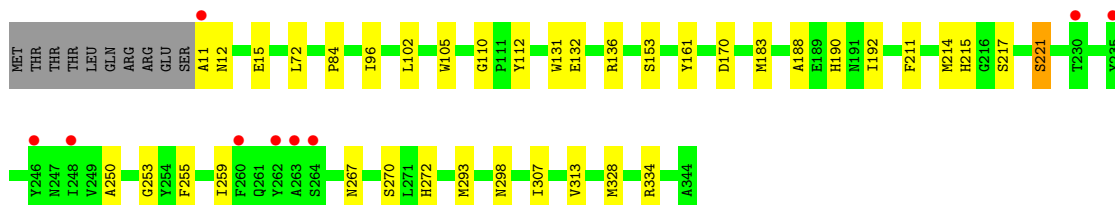
3 Residue-property plots

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.

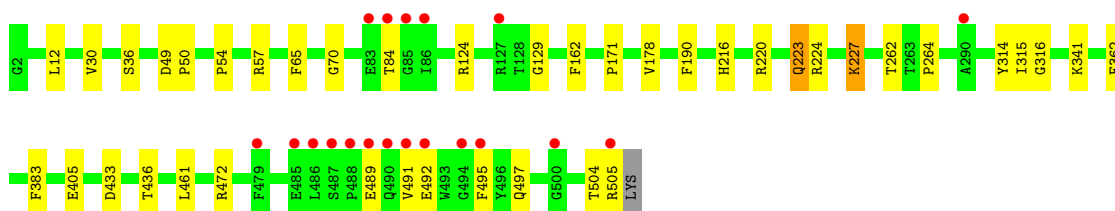
- Molecule 1: Photosystem Q(B) protein



- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

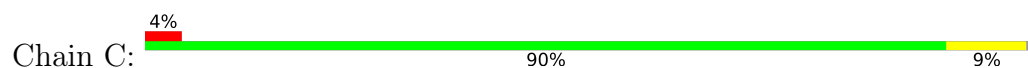
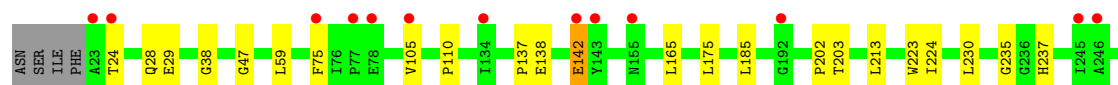


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

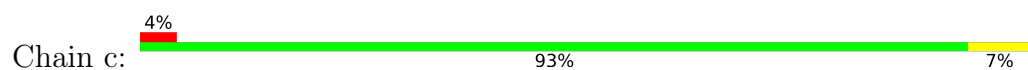
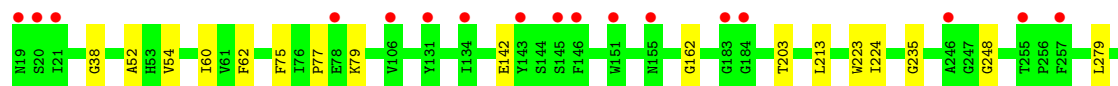




- Molecule 3: Photosystem II 44 kDa reaction center protein



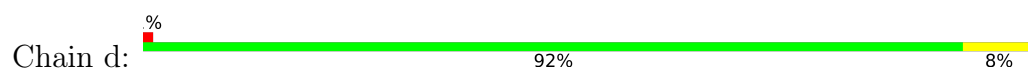
- Molecule 3: Photosystem II 44 kDa reaction center protein



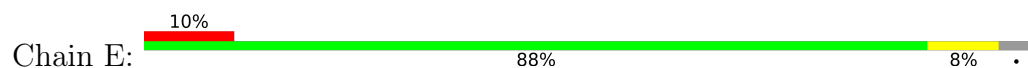
- Molecule 4: Photosystem II D2 protein



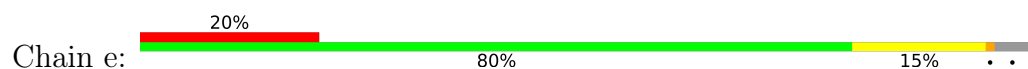
- Molecule 4: Photosystem II D2 protein

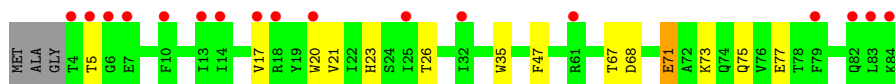


- Molecule 5: Cytochrome b559 subunit alpha

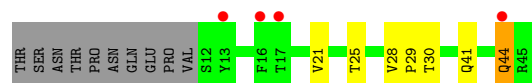


- Molecule 5: Cytochrome b559 subunit alpha

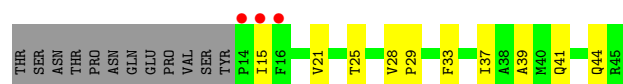




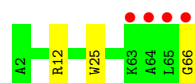
- Molecule 6: Cytochrome b559 subunit beta



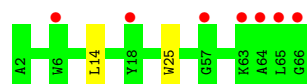
- Molecule 6: Cytochrome b559 subunit beta



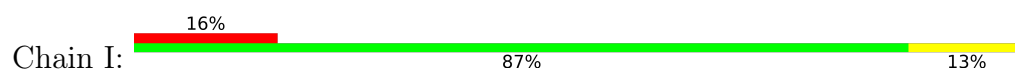
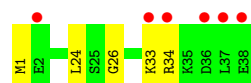
- Molecule 7: Photosystem II reaction center protein H



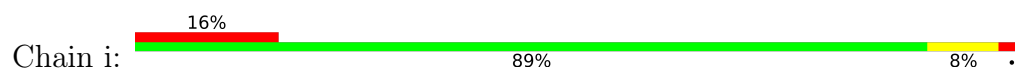
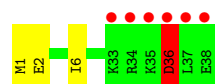
- Molecule 7: Photosystem II reaction center protein H



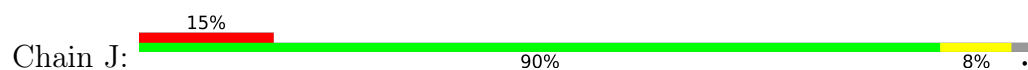
- Molecule 8: Photosystem II reaction center protein I



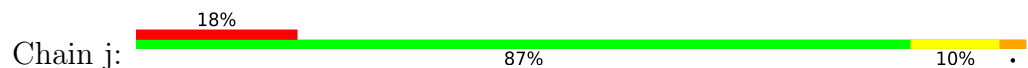
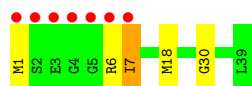
- Molecule 8: Photosystem II reaction center protein I



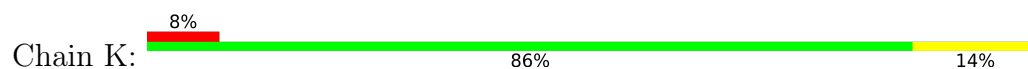
- Molecule 9: Photosystem II reaction center protein J



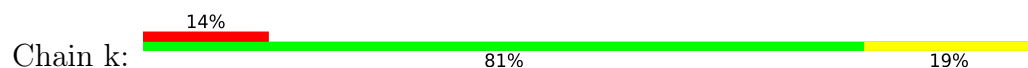
- Molecule 9: Photosystem II reaction center protein J



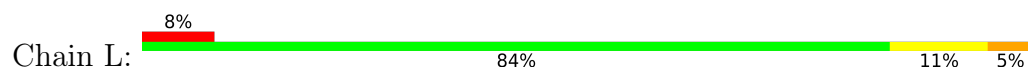
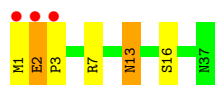
- Molecule 10: Photosystem II reaction center protein K



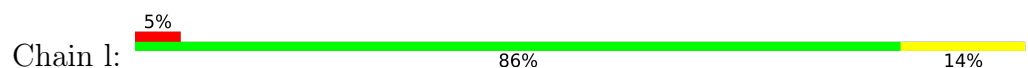
- Molecule 10: Photosystem II reaction center protein K



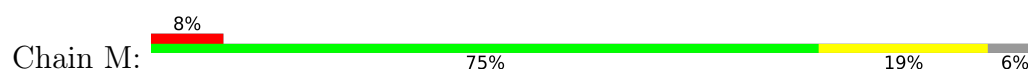
- Molecule 11: Photosystem II reaction center protein L



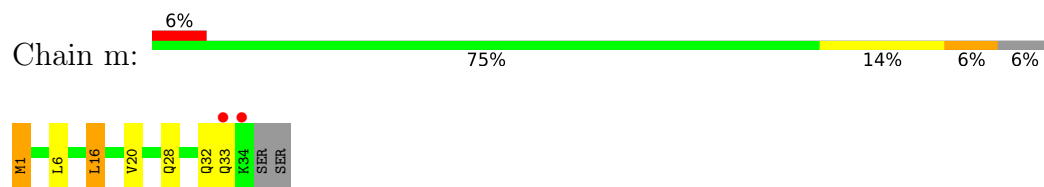
- Molecule 11: Photosystem II reaction center protein L



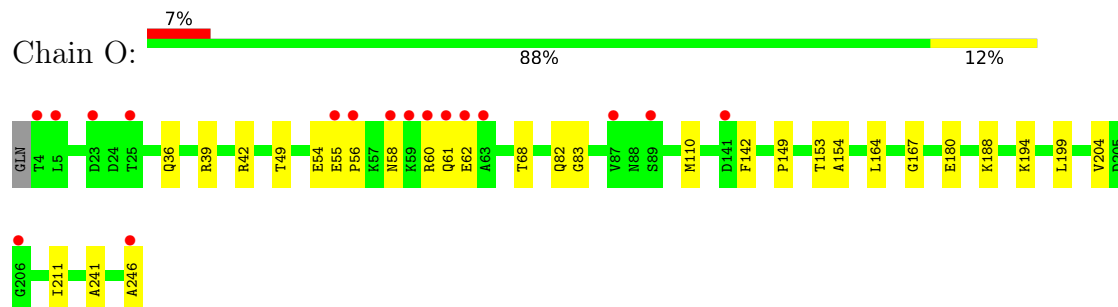
- Molecule 12: Photosystem II reaction center protein M



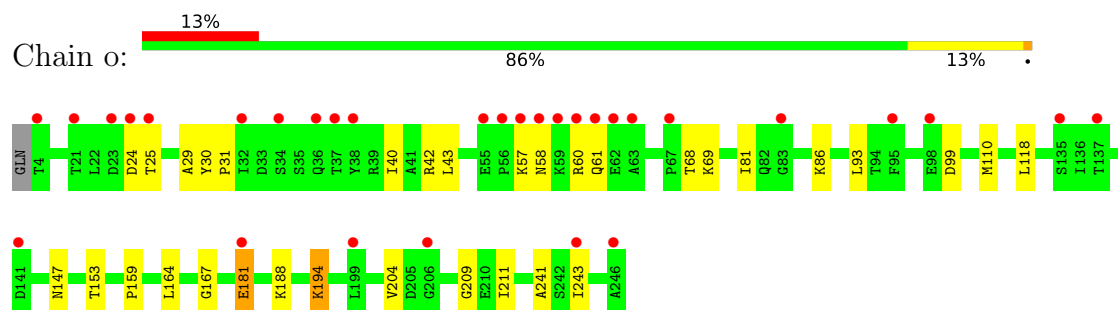
- Molecule 12: Photosystem II reaction center protein M



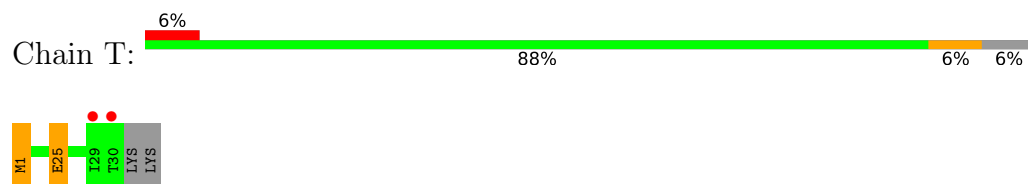
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



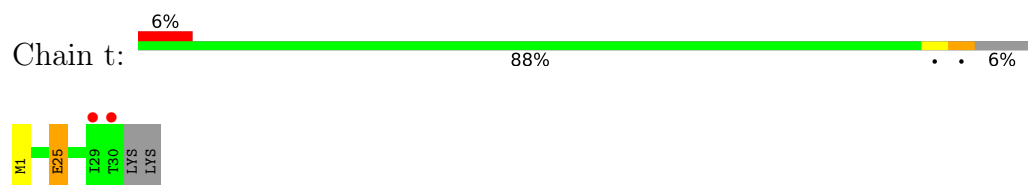
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



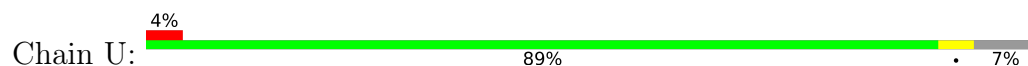
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

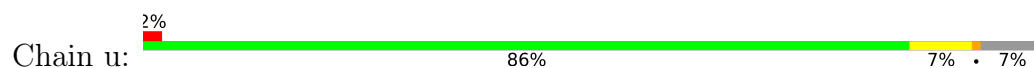
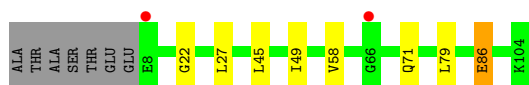


- Molecule 15: Photosystem II 12 kDa extrinsic protein





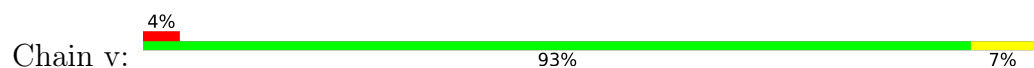
- Molecule 15: Photosystem II 12 kDa extrinsic protein



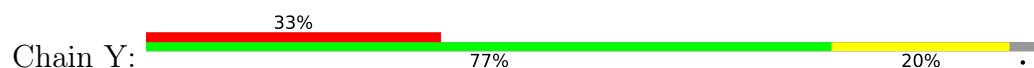
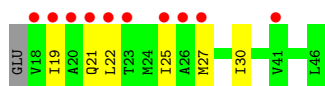
- Molecule 16: Cytochrome c-550



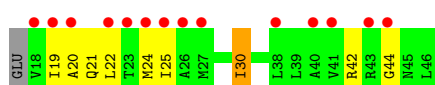
- Molecule 16: Cytochrome c-550



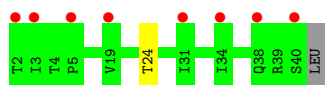
- Molecule 17: Photosystem II reaction center protein Ycf12



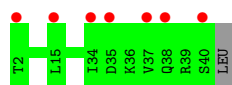
- Molecule 17: Photosystem II reaction center protein Ycf12



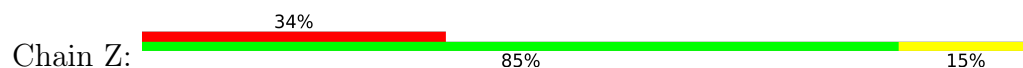
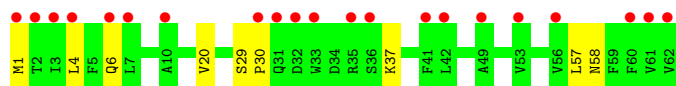
- Molecule 18: Photosystem II reaction center protein X



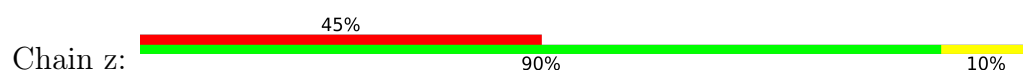
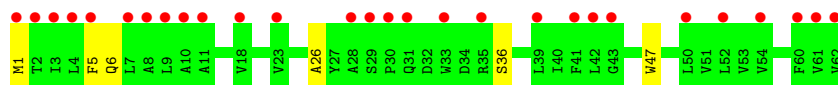
- Molecule 18: Photosystem II reaction center protein X



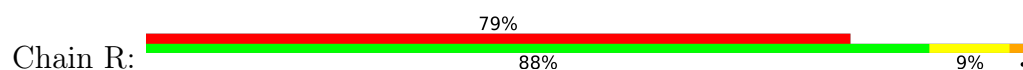
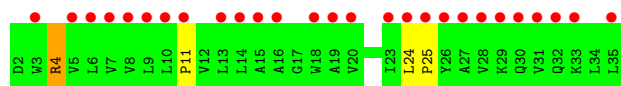
• Molecule 19: Photosystem II reaction center protein Z



• 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	123.74Å 229.99Å 288.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.29 – 1.95 62.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.29-1.95) 92.2 (62.29-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.198 , 0.238 0.198 , 0.238	Depositor DCC
R_{free} test set	29338 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	54195	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: HTG, PL9, HEM, FME, SQD, LMG, HEC, BCT, CL, UNL, LHG, PHO, OEX, LMT, CA, FE2, GOL, DGD, BCR, CLA, MG

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	0.66	0/2728	0.85	0/3719
1	a	0.65	0/2748	0.84	0/3746
2	B	0.60	0/4200	0.82	0/5721
2	b	0.57	0/4209	0.83	2/5734 (0.0%)
3	C	0.56	1/3626 (0.0%)	0.83	2/4936 (0.0%)
3	c	0.56	1/3676 (0.0%)	0.82	0/5004
4	D	0.65	0/2827	0.84	0/3852
4	d	0.63	0/2818	0.83	4/3840 (0.1%)
5	E	0.47	0/693	0.87	1/944 (0.1%)
5	e	0.45	0/695	0.78	0/948
6	F	0.52	0/284	0.79	0/387
6	f	0.56	0/265	0.85	0/360
7	H	0.51	0/535	0.84	0/728
7	h	0.47	0/524	0.78	0/713
8	I	0.43	0/311	0.85	0/419
8	i	0.48	0/311	0.79	0/419
9	J	0.53	0/278	0.81	0/376
9	j	0.51	0/286	0.86	2/386 (0.5%)
10	K	0.47	0/303	0.80	0/416
10	k	0.57	0/303	0.78	0/416
11	L	0.58	0/319	0.73	0/433
11	l	0.53	0/319	0.75	0/433
12	M	0.61	0/270	0.89	0/368
12	m	0.74	0/262	0.95	0/357
13	O	0.50	0/1958	0.82	3/2654 (0.1%)
13	o	0.48	0/1937	0.81	0/2625
14	T	0.63	0/266	0.81	0/362
14	t	0.69	0/266	0.71	0/362
15	U	0.54	0/785	0.80	0/1064
15	u	0.52	0/785	0.77	0/1064
16	V	0.56	0/1096	0.80	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.51	0/1085	0.82	1/1473 (0.1%)
17	Y	0.46	0/216	0.80	0/289
17	y	0.45	0/216	0.85	0/289
18	X	0.46	0/290	0.73	0/392
18	x	0.42	0/290	0.76	0/392
19	Z	0.43	0/490	0.76	0/669
19	z	0.45	0/490	0.85	0/669
20	R	0.38	0/279	0.73	0/383
All	All	0.57	2/43239 (0.0%)	0.82	15/58829 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	410	VAL	CA-CB	5.56	1.59	1.54
3	C	310	SER	C-O	5.41	1.30	1.24

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	v	105	ARG	N-CA-C	6.89	119.63	111.71
2	b	221	PRO	O-C-N	6.03	123.98	121.15
4	d	170	ALA	CA-C-N	-5.69	114.07	119.76
4	d	170	ALA	C-N-CA	-5.69	114.07	119.76
4	d	55	VAL	N-CA-C	5.51	116.92	108.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2634	0	2546	13	0
1	a	2645	0	2567	29	0
2	B	4027	0	3906	27	0
2	b	4033	0	3921	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3501	0	3428	26	0
3	c	3544	0	3480	22	0
4	D	2729	0	2632	22	0
4	d	2720	0	2626	21	0
5	E	668	0	658	6	0
5	e	670	0	664	11	0
6	F	275	0	282	5	0
6	f	257	0	269	5	0
7	H	519	0	545	4	0
7	h	511	0	532	5	0
8	I	314	0	328	4	0
8	i	314	0	328	2	0
9	J	272	0	279	3	0
9	j	280	0	291	4	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	309	0	327	5	0
11	l	309	0	327	5	0
12	M	274	0	299	7	0
12	m	269	0	288	8	0
13	O	1903	0	1886	16	0
13	o	1891	0	1870	18	0
14	T	264	0	267	2	0
14	t	264	0	267	1	0
15	U	774	0	773	2	0
15	u	774	0	773	5	0
16	V	1072	0	1086	3	0
16	v	1064	0	1073	6	0
17	Y	215	0	246	3	0
17	y	215	0	246	5	0
18	X	287	0	317	1	0
18	x	287	0	317	0	0
19	Z	479	0	516	5	0
19	z	479	0	516	4	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	U	1	0	0	3	0
22	a	2	0	0	0	0
22	v	1	0	0	2	0
23	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	4	0	0	0	0
24	A	260	0	288	8	0
24	B	1040	0	1152	28	0
24	C	845	0	936	29	0
24	D	130	0	144	3	0
24	a	195	0	216	5	0
24	b	1040	0	1152	23	0
24	c	845	0	936	25	0
24	d	195	0	216	5	0
25	A	128	0	148	1	0
25	a	128	0	148	1	0
26	A	40	0	56	1	0
26	B	120	0	168	7	0
26	C	80	0	112	1	0
26	D	40	0	56	2	0
26	H	40	0	56	3	0
26	K	80	0	112	4	0
26	T	40	0	56	4	0
26	a	40	0	56	3	0
26	b	120	0	168	6	0
26	c	40	0	56	2	0
26	d	40	0	56	4	0
26	h	40	0	56	2	0
26	k	80	0	112	6	0
26	t	40	0	56	7	0
26	y	40	0	56	2	0
27	A	108	0	156	7	0
27	B	54	0	78	3	0
27	F	43	0	52	3	0
27	L	54	0	78	2	0
27	a	108	0	156	4	0
27	f	43	0	53	0	0
28	A	18	0	24	1	0
28	B	42	0	56	4	0
28	C	12	0	16	2	0
28	F	6	0	7	0	0
28	O	6	0	8	0	0
28	T	12	0	16	4	0
28	V	24	0	32	0	0
28	a	18	0	24	2	0
28	b	36	0	48	4	0
28	c	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	f	6	0	6	1	0
28	o	6	0	8	0	0
28	t	6	0	8	0	0
28	v	18	0	24	2	0
29	A	35	0	46	0	0
29	B	60	0	81	2	0
29	C	35	0	46	2	0
29	E	35	0	46	1	0
29	M	35	0	46	3	0
29	a	35	0	46	2	0
29	b	50	0	70	4	0
29	c	35	0	46	1	0
29	f	35	0	46	1	0
29	m	105	0	138	7	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	55	0	80	5	0
31	D	55	0	80	1	0
31	a	55	0	80	5	0
31	d	55	0	80	1	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	K	34	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	51	0	72	2	0
34	C	153	0	216	7	0
34	J	51	0	72	3	0
34	Z	37	0	44	3	0
34	a	51	0	72	3	0
34	b	51	0	72	2	0
34	c	102	0	144	2	0
34	j	51	0	72	5	0
34	z	39	0	48	2	0
35	B	95	0	130	3	0
35	C	38	0	52	1	0
35	D	16	0	17	3	0
35	O	19	0	26	1	0
35	V	19	0	26	0	0
35	b	76	0	104	0	0
35	c	38	0	52	1	0
35	d	16	0	17	2	0
36	C	186	0	246	8	0
36	D	62	0	82	5	0
36	H	62	0	82	1	0
36	c	186	0	246	5	0
36	d	62	0	82	6	0
36	h	62	0	82	0	0
37	D	147	0	222	9	0
37	E	42	0	57	2	0
37	L	49	0	74	1	0
37	d	147	0	222	8	0
37	e	42	0	57	1	0
37	l	49	0	74	2	0
38	E	43	0	30	0	0
38	e	43	0	30	2	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	167	0	0	0	0
41	B	293	0	0	2	0
41	C	235	0	0	1	0
41	D	143	0	0	2	0
41	E	31	0	0	0	0
41	F	9	0	0	0	0
41	H	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	I	4	0	0	0	0
41	J	13	0	0	1	0
41	K	8	0	0	1	0
41	L	17	0	0	0	0
41	M	8	0	0	0	0
41	O	191	0	0	4	0
41	T	17	0	0	0	0
41	U	81	0	0	3	0
41	V	118	0	0	1	0
41	X	9	0	0	0	0
41	Y	4	0	0	0	0
41	Z	1	0	0	1	0
41	a	154	0	0	3	0
41	b	264	0	0	2	0
41	c	199	0	0	1	0
41	d	137	0	0	2	0
41	e	17	0	0	0	0
41	f	5	0	0	0	0
41	h	41	0	0	0	0
41	i	6	0	0	0	0
41	j	7	0	0	0	0
41	k	6	0	0	0	0
41	l	10	0	0	0	0
41	m	18	0	0	0	0
41	o	155	0	0	0	0
41	t	12	0	0	0	0
41	u	97	0	0	2	0
41	v	90	0	0	0	0
41	x	4	0	0	0	0
41	y	4	0	0	1	0
All	All	54195	0	52838	501	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 501 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HG2	31:A:419:PL9:H102	1.48	0.95
5:e:67:THR:H	5:e:75:GLN:HE22	1.13	0.94
12:M:16[C]:LEU:HD23	12:m:16:LEU:HD12	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.55	0.87
1:a:214:MET:HG2	31:a:417:PL9:H102	1.55	0.85

There are no symmetry-related clashes.

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%)	331 (99%)	3 (1%)	1 (0%)	36	28
1	a	338/344 (98%)	333 (98%)	4 (1%)	1 (0%)	36	28
2	B	513/505 (102%)	506 (99%)	7 (1%)	0	100	100
2	b	514/505 (102%)	506 (98%)	8 (2%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	30	21
3	c	459/455 (101%)	445 (97%)	12 (3%)	2 (0%)	30	21
4	D	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	79 (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%)	4	1
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	249/244 (102%)	240 (96%)	8 (3%)	1 (0%)	30	21
13	o	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	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%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5290/5384 (98%)	5170 (98%)	112 (2%)	8 (0%)	48	36

5 of 8 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
13	O	62	GLU

5.3.2 Protein sidechains ⓘ

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	275/279 (99%)	272 (99%)	3 (1%)	65	64
2	B	413/403 (102%)	404 (98%)	9 (2%)	45	40
2	b	414/403 (103%)	409 (99%)	5 (1%)	63	61
3	C	356/356 (100%)	349 (98%)	7 (2%)	48	43
3	c	362/356 (102%)	356 (98%)	6 (2%)	53	49
4	D	278/277 (100%)	275 (99%)	3 (1%)	65	64
4	d	277/277 (100%)	274 (99%)	3 (1%)	65	64
5	E	74/73 (101%)	73 (99%)	1 (1%)	59	56
5	e	74/73 (101%)	73 (99%)	1 (1%)	59	56
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	21
6	f	26/38 (68%)	24 (92%)	2 (8%)	12	3
7	H	55/54 (102%)	53 (96%)	2 (4%)	31	21
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	29
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	20
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	24
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	24
11	L	36/35 (103%)	33 (92%)	3 (8%)	10	3
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	30
12	M	31/32 (97%)	30 (97%)	1 (3%)	34	25
12	m	30/32 (94%)	28 (93%)	2 (7%)	15	5
13	O	214/207 (103%)	211 (99%)	3 (1%)	59	56
13	o	211/207 (102%)	204 (97%)	7 (3%)	33	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	4
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	4
15	U	84/89 (94%)	83 (99%)	1 (1%)	63	61
15	u	84/89 (94%)	83 (99%)	1 (1%)	63	61
16	V	118/117 (101%)	117 (99%)	1 (1%)	73	74
16	v	117/117 (100%)	117 (100%)	0	100	100
17	Y	22/23 (96%)	19 (86%)	3 (14%)	3	0
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	0
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	7
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	19
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	23
All	All	4395/4403 (100%)	4312 (98%)	83 (2%)	53	45

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	150	ILE
13	o	118	LEU
5	e	71	GLU
11	l	1	MET
14	t	25[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	490	GLN
13	o	155	ASN
4	d	83	ASN
19	z	6	GLN
11	l	6	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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
12	FME	m	1	12	8,9,10	0.72	0	7,9,11	1.11	1 (14%)
14	FME	T	1	14	8,9,10	0.64	0	7,9,11	1.56	1 (14%)
12	FME	M	1	12	8,9,10	0.65	0	7,9,11	1.11	0
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	2.10	4 (57%)
8	FME	i	1	8	8,9,10	0.69	0	7,9,11	1.37	1 (14%)
8	FME	I	1	8	8,9,10	0.57	0	7,9,11	1.32	2 (28%)

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
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	3.07	115.27	109.73
14	T	1	FME	C-CA-N	2.67	114.55	109.73
14	t	1	FME	O-C-CA	-2.63	117.88	124.78
14	t	1	FME	CA-N-CN	-2.56	118.89	122.82
8	I	1	FME	O-C-CA	-2.36	118.59	124.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	O1-CN-N-CA
14	T	1	FME	C-CA-CB-CG
8	I	1	FME	CA-CB-CG-SD
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	1	0
14	T	1	FME	1	0
12	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 17 are monoatomic and 18 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	512	3	69,73,73	2.05	22 (31%)	83,113,113	2.74	29 (34%)
29	LMT	m	102	-	36,36,36	0.48	0	47,47,47	0.91	1 (2%)
35	HTG	B	624	-	19,19,19	1.13	1 (5%)	23,24,24	1.39	1 (4%)
36	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	0.93	4 (5%)
29	LMT	A	417	-	36,36,36	0.50	1 (2%)	47,47,47	1.06	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	HEC	V	201	16	50,50,50	1.70	10 (20%)	68,82,82	1.79	17 (25%)
24	CLA	b	607	2	69,73,73	2.06	20 (28%)	83,113,113	2.86	32 (38%)
35	HTG	c	922	-	19,19,19	0.90	1 (5%)	23,24,24	1.34	1 (4%)
24	CLA	a	409	1	69,73,73	2.02	19 (27%)	83,113,113	2.74	35 (42%)
34	LMG	b	624	-	51,51,55	0.91	3 (5%)	59,59,63	1.05	3 (5%)
24	CLA	c	914	3	69,73,73	2.05	21 (30%)	83,113,113	2.84	30 (36%)
26	BCR	T	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.38	11 (19%)
24	CLA	A	405	1	69,73,73	2.03	19 (27%)	83,113,113	2.82	26 (31%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.07	4 (6%)
29	LMT	c	921	-	36,36,36	0.45	0	47,47,47	0.82	1 (2%)
24	CLA	b	613	2	69,73,73	2.02	19 (27%)	83,113,113	2.81	31 (37%)
24	CLA	b	617	2	69,73,73	2.01	21 (30%)	83,113,113	2.75	34 (40%)
35	HTG	C	523	-	19,19,19	0.98	2 (10%)	23,24,24	1.37	2 (8%)
29	LMT	C	522	-	36,36,36	0.48	0	47,47,47	1.27	5 (10%)
31	PL9	d	405	-	55,55,55	0.73	2 (3%)	68,69,69	1.55	14 (20%)
34	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.22	7 (11%)
35	HTG	d	412	-	16,16,19	1.11	2 (12%)	20,21,24	1.38	1 (5%)
35	HTG	b	602	-	19,19,19	1.14	2 (10%)	23,24,24	1.22	1 (4%)
34	LMG	B	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.16	3 (5%)
24	CLA	c	903	3	69,73,73	2.03	19 (27%)	83,113,113	2.78	29 (34%)
35	HTG	B	633	-	19,19,19	1.12	2 (10%)	23,24,24	1.30	1 (4%)
26	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.37	7 (12%)
24	CLA	B	602	41	69,73,73	2.05	20 (28%)	83,113,113	2.86	30 (36%)
28	GOL	f	101	33	5,5,5	0.37	0	5,5,5	0.40	0
28	GOL	C	526	-	5,5,5	0.22	0	5,5,5	0.43	0
26	BCR	b	622	-	41,41,41	1.06	1 (2%)	56,56,56	1.27	5 (8%)
28	GOL	b	629	-	5,5,5	0.34	0	5,5,5	0.15	0
34	LMG	Z	101	-	37,37,55	0.99	2 (5%)	45,45,63	1.31	6 (13%)
34	LMG	a	412	-	51,51,55	0.91	2 (3%)	59,59,63	1.15	6 (10%)
24	CLA	A	407	41	69,73,73	2.08	19 (27%)	83,113,113	2.87	33 (39%)
26	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.39	7 (12%)
25	PHO	a	420	-	58,69,69	2.82	13 (22%)	56,99,99	2.74	15 (26%)
24	CLA	C	511	3	69,73,73	2.06	20 (28%)	83,113,113	2.69	29 (34%)
28	GOL	T	101	-	5,5,5	0.41	0	5,5,5	0.31	0
24	CLA	c	906	3	69,73,73	2.01	19 (27%)	83,113,113	2.74	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	K	103	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	6 (10%)
24	CLA	A	410	1	69,73,73	2.06	18 (26%)	83,113,113	2.80	30 (36%)
28	GOL	B	631	-	5,5,5	0.42	0	5,5,5	0.47	0
29	LMT	b	601	-	25,25,36	0.46	0	30,30,47	1.35	3 (10%)
37	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.09	3 (6%)
24	CLA	b	618	2	69,73,73	2.03	20 (28%)	83,113,113	2.94	33 (39%)
35	HTG	B	625	-	19,19,19	0.83	1 (5%)	23,24,24	1.18	2 (8%)
24	CLA	B	613	2	69,73,73	2.00	20 (28%)	83,113,113	2.69	25 (30%)
24	CLA	B	617	2	69,73,73	1.99	20 (28%)	83,113,113	2.80	29 (34%)
35	HTG	b	626	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	3 (13%)
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.46	7 (14%)
26	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	4 (7%)
37	LHG	D	406	-	48,48,48	0.86	2 (4%)	51,54,54	1.09	5 (9%)
37	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.06	4 (7%)
24	CLA	B	614	2	69,73,73	2.00	19 (27%)	83,113,113	2.83	31 (37%)
24	CLA	a	407	41	69,73,73	2.07	20 (28%)	83,113,113	2.86	34 (40%)
25	PHO	A	408	-	58,69,69	2.75	11 (18%)	56,99,99	2.90	13 (23%)
24	CLA	c	908	41	69,73,73	2.01	20 (28%)	83,113,113	2.80	30 (36%)
28	GOL	V	206	-	5,5,5	0.32	0	5,5,5	0.30	0
24	CLA	C	510	3	69,73,73	2.10	20 (28%)	83,113,113	2.81	34 (40%)
28	GOL	v	203	-	5,5,5	0.28	0	5,5,5	0.61	0
35	HTG	C	524	-	19,19,19	1.03	2 (10%)	23,24,24	1.64	4 (17%)
35	HTG	b	627	-	19,19,19	1.09	2 (10%)	23,24,24	1.97	4 (17%)
27	SQD	B	621	-	53,54,54	1.05	4 (7%)	62,65,65	1.48	9 (14%)
35	HTG	V	202	-	19,19,19	1.01	2 (10%)	23,24,24	1.54	3 (13%)
24	CLA	C	513	3	69,73,73	2.00	19 (27%)	83,113,113	2.86	32 (38%)
28	GOL	B	637	-	5,5,5	0.40	0	5,5,5	0.30	0
26	BCR	B	620	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	4 (7%)
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	4 (6%)
28	GOL	B	630	-	5,5,5	0.33	0	5,5,5	0.36	0
28	GOL	c	925	-	5,5,5	0.36	0	5,5,5	0.56	0
26	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.23	5 (8%)
26	BCR	D	403	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	14 (25%)
24	CLA	B	612	2	69,73,73	2.02	20 (28%)	83,113,113	2.87	31 (37%)
24	CLA	C	514	3	69,73,73	2.02	20 (28%)	83,113,113	2.81	30 (36%)
24	CLA	D	401	4	69,73,73	1.99	19 (27%)	83,113,113	2.75	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	o	302	-	5,5,5	0.39	0	5,5,5	0.48	0
35	HTG	B	634	-	19,19,19	1.04	2 (10%)	23,24,24	1.59	3 (13%)
31	PL9	a	417	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	18 (26%)
40	HEC	v	202	16	50,50,50	1.69	7 (14%)	68,82,82	1.78	15 (22%)
36	DGD	d	406	-	63,63,67	0.93	3 (4%)	77,77,81	1.22	6 (7%)
28	GOL	T	103	-	5,5,5	0.39	0	5,5,5	0.19	0
24	CLA	B	603	2	69,73,73	2.04	20 (28%)	83,113,113	2.92	34 (40%)
35	HTG	O	303	-	19,19,19	0.95	1 (5%)	23,24,24	0.71	0
23	BCT	A	404	21	2,3,3	0.88	0	2,3,3	0.45	0
28	GOL	V	205	-	5,5,5	0.36	0	5,5,5	0.38	0
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	b	612	2	69,73,73	2.08	20 (28%)	83,113,113	2.74	29 (34%)
24	CLA	b	610	2	69,73,73	1.98	19 (27%)	83,113,113	2.91	30 (36%)
24	CLA	C	505	41	69,73,73	2.07	20 (28%)	83,113,113	2.89	28 (33%)
24	CLA	c	905	41	69,73,73	2.03	20 (28%)	83,113,113	2.83	31 (37%)
24	CLA	c	912	3	69,73,73	2.05	21 (30%)	83,113,113	2.73	29 (34%)
24	CLA	d	403	4	69,73,73	2.01	20 (28%)	83,113,113	2.82	30 (36%)
25	PHO	a	408	-	58,69,69	2.66	12 (20%)	56,99,99	2.81	13 (23%)
24	CLA	b	609	2	69,73,73	2.02	19 (27%)	83,113,113	2.92	30 (36%)
27	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.60	10 (16%)
24	CLA	b	614	41	69,73,73	2.06	20 (28%)	83,113,113	2.76	34 (40%)
26	BCR	b	623	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	9 (16%)
29	LMT	B	623	-	36,36,36	0.43	0	47,47,47	1.40	5 (10%)
24	CLA	B	616	2	69,73,73	1.98	21 (30%)	83,113,113	2.83	32 (38%)
24	CLA	B	606	2	69,73,73	2.00	20 (28%)	83,113,113	2.74	30 (36%)
35	HTG	c	923	-	19,19,19	1.14	2 (10%)	23,24,24	1.84	5 (21%)
26	BCR	c	915	-	41,41,41	1.07	1 (2%)	56,56,56	1.43	9 (16%)
24	CLA	b	620	2	69,73,73	2.02	21 (30%)	83,113,113	2.74	26 (31%)
24	CLA	C	506	3	69,73,73	2.06	20 (28%)	83,113,113	2.74	30 (36%)
27	SQD	A	412	-	53,54,54	0.99	3 (5%)	62,65,65	1.77	12 (19%)
24	CLA	c	911	3	69,73,73	2.07	20 (28%)	83,113,113	2.63	31 (37%)
35	HTG	B	626	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	2 (8%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.61	12 (21%)
24	CLA	b	619	2	69,73,73	2.01	19 (27%)	83,113,113	2.76	30 (36%)
34	LMG	C	501	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	907	3	69,73,73	2.03	20 (28%)	83,113,113	2.72	31 (37%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.00	1 (5%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.90	1 (2%)
28	GOL	b	632	-	5,5,5	0.37	0	5,5,5	0.56	0
24	CLA	b	611	41	69,73,73	2.03	20 (28%)	83,113,113	2.88	30 (36%)
24	CLA	C	504	3	69,73,73	2.02	20 (28%)	83,113,113	2.87	28 (33%)
28	GOL	b	630	-	5,5,5	0.32	0	5,5,5	0.52	0
24	CLA	b	606	2	69,73,73	2.02	21 (30%)	83,113,113	2.86	30 (36%)
24	CLA	b	615	2	69,73,73	2.00	20 (28%)	83,113,113	2.89	29 (34%)
29	LMT	B	636	-	25,25,36	0.43	0	30,30,47	0.65	0
24	CLA	D	402	4	69,73,73	2.03	19 (27%)	83,113,113	2.78	27 (32%)
29	LMT	b	625	-	25,25,36	0.52	1 (4%)	30,30,47	0.60	0
24	CLA	C	507	3	69,73,73	2.07	20 (28%)	83,113,113	2.75	33 (39%)
28	GOL	V	203	-	5,5,5	0.38	0	5,5,5	0.15	0
27	SQD	F	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.96	10 (19%)
30	OEX	a	416	1,3,41	0,14,14	-	-	-	-	-
36	DGD	c	916	-	63,63,67	0.83	2 (3%)	77,77,81	1.11	6 (7%)
24	CLA	B	608	41	69,73,73	2.02	20 (28%)	83,113,113	2.68	27 (32%)
24	CLA	c	904	3	69,73,73	2.03	20 (28%)	83,113,113	2.76	29 (34%)
28	GOL	t	102	-	5,5,5	0.40	0	5,5,5	0.23	0
28	GOL	B	628	-	5,5,5	0.27	0	5,5,5	0.42	0
30	OEX	A	418	1,3,41	0,14,14	-	-	-	-	-
28	GOL	b	631	-	5,5,5	0.33	0	5,5,5	0.46	0
27	SQD	a	402	-	53,54,54	1.06	3 (5%)	62,65,65	1.16	7 (11%)
23	BCT	a	419	21	2,3,3	0.96	0	2,3,3	0.22	0
36	DGD	c	917	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	2 (2%)
34	LMG	j	101	39	51,51,55	0.89	2 (3%)	59,59,63	0.99	4 (6%)
37	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
29	LMT	m	103	-	36,36,36	0.48	0	47,47,47	0.99	1 (2%)
28	GOL	B	629	-	5,5,5	0.41	0	5,5,5	0.56	0
28	GOL	A	415	-	5,5,5	0.42	0	5,5,5	0.27	0
24	CLA	B	611	41	69,73,73	2.09	20 (28%)	83,113,113	2.74	33 (39%)
28	GOL	b	633	-	5,5,5	0.36	0	5,5,5	0.35	0
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.31	0
26	BCR	k	101	-	41,41,41	1.10	1 (2%)	56,56,56	1.46	10 (17%)
28	GOL	a	413	-	5,5,5	0.31	0	5,5,5	0.65	0
26	BCR	a	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	5 (8%)
27	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.57	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	C	525	-	5,5,5	0.37	0	5,5,5	0.61	0
36	DGD	C	517	-	63,63,67	0.86	3 (4%)	77,77,81	1.04	4 (5%)
35	HTG	b	603	-	19,19,19	1.03	2 (10%)	23,24,24	1.47	3 (13%)
24	CLA	B	604	2	69,73,73	2.05	20 (28%)	83,113,113	2.90	29 (34%)
28	GOL	V	204	-	5,5,5	0.43	0	5,5,5	0.44	0
36	DGD	C	519	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	5 (6%)
38	HEM	E	103	6,5	50,50,50	1.50	6 (12%)	66,82,82	1.79	16 (24%)
24	CLA	c	902	3	69,73,73	1.98	19 (27%)	83,113,113	2.74	28 (33%)
28	GOL	a	415	-	5,5,5	0.40	0	5,5,5	0.46	0
34	LMG	J	101	39	51,51,55	0.88	2 (3%)	59,59,63	0.89	3 (5%)
24	CLA	B	605	2	69,73,73	1.93	19 (27%)	83,113,113	2.76	28 (33%)
24	CLA	c	913	3	69,73,73	1.99	20 (28%)	83,113,113	2.90	32 (38%)
27	SQD	f	102	-	42,43,54	1.17	3 (7%)	51,54,65	1.45	8 (15%)
24	CLA	C	502	3	69,73,73	2.01	20 (28%)	83,113,113	2.85	31 (37%)
31	PL9	D	404	-	55,55,55	0.73	2 (3%)	68,69,69	1.58	14 (20%)
34	LMG	c	919	-	51,51,55	0.97	3 (5%)	59,59,63	1.01	2 (3%)
26	BCR	A	411	-	41,41,41	1.02	1 (2%)	56,56,56	1.22	5 (8%)
29	LMT	m	104	-	36,36,36	0.51	0	47,47,47	1.01	2 (4%)
36	DGD	c	918	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	4 (5%)
26	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	7 (12%)
36	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.98	6 (7%)
28	GOL	A	413	-	5,5,5	0.25	0	5,5,5	0.52	0
24	CLA	C	503	3	69,73,73	2.06	20 (28%)	83,113,113	2.70	31 (37%)
25	PHO	A	409	-	58,69,69	2.83	15 (25%)	56,99,99	2.81	14 (25%)
28	GOL	O	302	-	5,5,5	0.32	0	5,5,5	0.44	0
27	SQD	A	416	-	53,54,54	1.03	3 (5%)	62,65,65	1.21	6 (9%)
24	CLA	B	610	2	69,73,73	1.98	18 (26%)	83,113,113	2.80	31 (37%)
24	CLA	B	615	2	69,73,73	2.04	20 (28%)	83,113,113	2.99	32 (38%)
28	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.34	0
28	GOL	B	627	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	A	406	41	69,73,73	1.99	19 (27%)	83,113,113	3.05	33 (39%)
26	BCR	t	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	7 (12%)
29	LMT	E	102	-	36,36,36	0.48	0	47,47,47	0.86	0
31	PL9	A	419	-	55,55,55	0.63	2 (3%)	68,69,69	1.83	21 (30%)
37	LHG	L	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	4 (7%)
26	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	d	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	16 (28%)
24	CLA	C	508	41	69,73,73	2.01	20 (28%)	83,113,113	2.68	28 (33%)
24	CLA	d	402	4	69,73,73	1.96	21 (30%)	83,113,113	2.91	29 (34%)
28	GOL	v	205	-	5,5,5	0.39	0	5,5,5	0.35	0
24	CLA	c	910	3	69,73,73	2.08	20 (28%)	83,113,113	2.80	30 (36%)
28	GOL	F	103	33	5,5,5	0.32	0	5,5,5	0.30	0
29	LMT	f	103	-	36,36,36	0.54	1 (2%)	47,47,47	0.93	4 (8%)
24	CLA	b	616	2	69,73,73	2.02	19 (27%)	83,113,113	2.81	30 (36%)
37	LHG	d	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	4 (7%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.29	5 (8%)
24	CLA	d	401	41	69,73,73	2.05	20 (28%)	83,113,113	2.85	31 (37%)
37	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	4 (7%)
24	CLA	C	509	3	69,73,73	2.03	20 (28%)	83,113,113	2.84	30 (36%)
26	BCR	b	621	-	41,41,41	1.12	1 (2%)	56,56,56	1.19	2 (3%)
38	HEM	e	102	6,5	50,50,50	1.57	8 (16%)	66,82,82	1.77	17 (25%)
28	GOL	v	204	-	5,5,5	0.37	0	5,5,5	0.37	0
24	CLA	b	608	2	69,73,73	2.04	20 (28%)	83,113,113	2.70	27 (32%)
24	CLA	c	909	3	69,73,73	2.03	20 (28%)	83,113,113	2.75	28 (33%)
36	DGD	D	405	-	63,63,67	0.98	3 (4%)	77,77,81	1.24	7 (9%)
24	CLA	b	605	41	69,73,73	2.07	19 (27%)	83,113,113	2.78	26 (31%)
28	GOL	B	632	-	5,5,5	0.35	0	5,5,5	0.36	0
29	LMT	a	401	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
26	BCR	B	618	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	8 (14%)
24	CLA	B	607	2	69,73,73	2.04	20 (28%)	83,113,113	2.92	32 (38%)
28	GOL	b	628	-	5,5,5	0.36	0	5,5,5	0.30	0
37	LHG	d	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
37	LHG	e	101	-	41,41,48	1.01	2 (4%)	44,47,54	0.97	2 (4%)
24	CLA	B	609	2	69,73,73	2.07	21 (30%)	83,113,113	2.78	32 (38%)
37	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	0.85	2 (3%)
28	GOL	a	414	-	5,5,5	0.39	0	5,5,5	0.43	0
24	CLA	a	406	1	69,73,73	2.04	20 (28%)	83,113,113	2.78	34 (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	512	3	-	2/39/115/115	-
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
35	HTG	B	624	-	-	1/10/30/30	0/1/1/1
36	DGD	H	102	-	-	9/51/91/95	0/2/2/2
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
40	HEC	V	201	16	1/1/3/7	4/14/54/54	-
24	CLA	b	607	2	-	8/39/115/115	-
35	HTG	c	922	-	-	4/10/30/30	0/1/1/1
24	CLA	a	409	1	-	7/39/115/115	-
34	LMG	b	624	-	-	14/46/66/70	0/1/1/1
24	CLA	c	914	3	-	12/39/115/115	-
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
24	CLA	A	405	1	-	2/39/115/115	-
34	LMG	C	521	-	-	12/46/66/70	0/1/1/1
29	LMT	c	921	-	-	4/21/61/61	0/2/2/2
24	CLA	b	613	2	-	2/39/115/115	-
24	CLA	b	617	2	-	4/39/115/115	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
29	LMT	C	522	-	-	9/21/61/61	0/2/2/2
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
34	LMG	c	920	-	-	4/46/66/70	0/1/1/1
35	HTG	d	412	-	-	0/7/27/30	0/1/1/1
35	HTG	b	602	-	-	1/10/30/30	0/1/1/1
34	LMG	B	622	-	-	12/46/66/70	0/1/1/1
24	CLA	c	903	3	-	6/39/115/115	-
35	HTG	B	633	-	-	3/10/30/30	0/1/1/1
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
28	GOL	f	101	33	-	4/4/4/4	-
28	GOL	C	526	-	-	0/4/4/4	-
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
28	GOL	b	629	-	-	0/4/4/4	-
34	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
34	LMG	a	412	-	-	10/46/66/70	0/1/1/1
24	CLA	A	407	41	-	2/39/115/115	-
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
25	PHO	a	420	-	-	2/37/103/103	0/5/6/6
24	CLA	C	511	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	c	906	3	-	6/39/115/115	-
26	BCR	K	103	-	-	2/29/63/63	0/2/2/2
24	CLA	A	410	1	-	9/39/115/115	-
28	GOL	B	631	-	-	4/4/4/4	-
29	LMT	b	601	-	-	8/17/37/61	0/1/1/2
37	LHG	E	101	-	-	21/46/46/53	-
24	CLA	b	618	2	-	17/39/115/115	-
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	B	613	2	-	4/39/115/115	-
24	CLA	B	617	2	-	9/39/115/115	-
35	HTG	b	626	-	-	1/10/30/30	0/1/1/1
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
37	LHG	D	406	-	-	6/53/53/53	-
37	LHG	D	408	-	-	11/53/53/53	-
24	CLA	B	614	2	-	9/39/115/115	-
24	CLA	a	407	41	-	6/39/115/115	-
25	PHO	A	408	-	-	5/37/103/103	0/5/6/6
24	CLA	c	908	41	-	4/39/115/115	-
28	GOL	V	206	-	-	1/4/4/4	-
24	CLA	C	510	3	-	7/39/115/115	-
28	GOL	v	203	-	-	4/4/4/4	-
35	HTG	C	524	-	-	2/10/30/30	0/1/1/1
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1
35	HTG	V	202	-	-	5/10/30/30	0/1/1/1
24	CLA	C	513	3	-	12/39/115/115	-
28	GOL	B	637	-	-	2/4/4/4	-
26	BCR	B	620	-	-	2/29/63/63	0/2/2/2
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
28	GOL	B	630	-	-	0/4/4/4	-
28	GOL	c	925	-	-	0/4/4/4	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	D	403	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	612	2	-	2/39/115/115	-
24	CLA	C	514	3	-	2/39/115/115	-
24	CLA	D	401	4	-	2/39/115/115	-
28	GOL	o	302	-	-	2/4/4/4	-
35	HTG	B	634	-	-	2/10/30/30	0/1/1/1
31	PL9	a	417	-	-	12/53/73/73	0/1/1/1
40	HEC	v	202	16	1/1/3/7	4/14/54/54	-
36	DGD	d	406	-	-	28/51/91/95	0/2/2/2
28	GOL	T	103	-	-	4/4/4/4	-
24	CLA	B	603	2	-	7/39/115/115	-
35	HTG	O	303	-	-	1/10/30/30	0/1/1/1
28	GOL	V	205	-	-	1/4/4/4	-
36	DGD	C	518	-	-	15/51/91/95	0/2/2/2
24	CLA	b	612	2	-	4/39/115/115	-
24	CLA	b	610	2	-	18/39/115/115	-
24	CLA	C	505	41	-	5/39/115/115	-
24	CLA	c	905	41	-	5/39/115/115	-
24	CLA	c	912	3	-	5/39/115/115	-
24	CLA	d	403	4	-	7/39/115/115	-
25	PHO	a	408	-	-	2/37/103/103	0/5/6/6
24	CLA	b	609	2	-	9/39/115/115	-
27	SQD	a	411	-	-	11/49/69/69	0/1/1/1
24	CLA	b	614	41	-	3/39/115/115	-
26	BCR	b	623	-	-	3/29/63/63	0/2/2/2
29	LMT	B	623	-	-	7/21/61/61	0/2/2/2
24	CLA	B	616	2	-	11/39/115/115	-
24	CLA	B	606	2	-	7/39/115/115	-
35	HTG	c	923	-	-	0/10/30/30	0/1/1/1
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
24	CLA	b	620	2	-	9/39/115/115	-
24	CLA	C	506	3	-	8/39/115/115	-
27	SQD	A	412	-	-	11/49/69/69	0/1/1/1
24	CLA	c	911	3	-	9/39/115/115	-
35	HTG	B	626	-	-	4/10/30/30	0/1/1/1
26	BCR	y	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	619	2	-	4/39/115/115	-
34	LMG	C	501	-	-	19/46/66/70	0/1/1/1
24	CLA	c	907	3	-	9/39/115/115	-
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
28	GOL	b	632	-	-	2/4/4/4	-
24	CLA	b	611	41	-	4/39/115/115	-
24	CLA	C	504	3	-	7/39/115/115	-
28	GOL	b	630	-	-	0/4/4/4	-
24	CLA	b	606	2	-	3/39/115/115	-
24	CLA	b	615	2	-	5/39/115/115	-
29	LMT	B	636	-	-	8/17/37/61	0/1/1/2
24	CLA	D	402	4	-	11/39/115/115	-
29	LMT	b	625	-	-	4/17/37/61	0/1/1/2
24	CLA	C	507	3	-	11/39/115/115	-
28	GOL	V	203	-	-	4/4/4/4	-
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
36	DGD	c	916	-	-	10/51/91/95	0/2/2/2
24	CLA	B	608	41	-	2/39/115/115	-
24	CLA	c	904	3	-	5/39/115/115	-
28	GOL	t	102	-	-	0/4/4/4	-
28	GOL	B	628	-	-	2/4/4/4	-
28	GOL	b	631	-	-	2/4/4/4	-
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
24	CLA	a	406	1	-	2/39/115/115	-
37	LHG	l	101	-	-	15/53/53/53	-
36	DGD	c	917	-	-	14/51/91/95	0/2/2/2
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1
29	LMT	m	103	-	-	3/21/61/61	0/2/2/2
28	GOL	B	629	-	-	2/4/4/4	-
28	GOL	A	415	-	-	2/4/4/4	-
24	CLA	B	611	41	-	7/39/115/115	-
28	GOL	b	633	-	-	2/4/4/4	-
28	GOL	c	924	-	-	0/4/4/4	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	a	413	-	-	0/4/4/4	-
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	-
36	DGD	C	517	-	-	15/51/91/95	0/2/2/2
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
24	CLA	B	604	2	-	6/39/115/115	-
28	GOL	V	204	-	-	2/4/4/4	-
36	DGD	C	519	-	-	8/51/91/95	0/2/2/2
38	HEM	E	103	6,5	-	4/14/54/54	-
24	CLA	c	902	3	-	5/39/115/115	-
28	GOL	a	415	-	-	2/4/4/4	-
34	LMG	J	101	39	-	13/46/66/70	0/1/1/1
24	CLA	B	605	2	-	4/39/115/115	-
24	CLA	c	913	3	-	9/39/115/115	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
24	CLA	C	502	3	-	9/39/115/115	-
31	PL9	D	404	-	-	3/53/73/73	0/1/1/1
34	LMG	c	919	-	-	16/46/66/70	0/1/1/1
26	BCR	A	411	-	-	1/29/63/63	0/2/2/2
29	LMT	m	104	-	-	7/21/61/61	0/2/2/2
36	DGD	c	918	-	-	17/51/91/95	0/2/2/2
26	BCR	K	102	-	-	6/29/63/63	0/2/2/2
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
28	GOL	A	413	-	-	2/4/4/4	-
24	CLA	C	503	3	-	6/39/115/115	-
25	PHO	A	409	-	-	0/37/103/103	0/5/6/6
28	GOL	O	302	-	-	2/4/4/4	-
27	SQD	A	416	-	-	16/49/69/69	0/1/1/1
24	CLA	B	610	2	-	3/39/115/115	-
24	CLA	B	615	2	-	18/39/115/115	-
28	GOL	A	414	-	-	2/4/4/4	-
28	GOL	B	627	-	-	1/4/4/4	-
24	CLA	A	406	41	-	4/39/115/115	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
29	LMT	E	102	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PL9	A	419	-	-	7/53/73/73	0/1/1/1
37	LHG	L	101	-	-	15/53/53/53	-
26	BCR	C	516	-	-	2/29/63/63	0/2/2/2
26	BCR	d	404	-	-	4/29/63/63	0/2/2/2
24	CLA	C	508	41	-	6/39/115/115	-
24	CLA	d	402	4	-	2/39/115/115	-
28	GOL	v	205	-	-	2/4/4/4	-
24	CLA	c	910	3	-	9/39/115/115	-
28	GOL	F	103	33	-	2/4/4/4	-
29	LMT	f	103	-	-	9/21/61/61	0/2/2/2
24	CLA	b	616	2	-	1/39/115/115	-
37	LHG	d	409	-	-	12/53/53/53	-
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
24	CLA	d	401	41	-	7/39/115/115	-
37	LHG	d	407	-	-	9/53/53/53	-
24	CLA	C	509	3	-	7/39/115/115	-
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
38	HEM	e	102	6,5	-	4/14/54/54	-
28	GOL	v	204	-	-	3/4/4/4	-
24	CLA	b	608	2	-	9/39/115/115	-
24	CLA	c	909	3	-	3/39/115/115	-
36	DGD	D	405	-	-	22/51/91/95	0/2/2/2
24	CLA	b	605	41	-	12/39/115/115	-
28	GOL	B	632	-	-	2/4/4/4	-
29	LMT	a	401	-	-	11/21/61/61	0/2/2/2
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	B	607	2	-	7/39/115/115	-
28	GOL	b	628	-	-	2/4/4/4	-
37	LHG	d	408	-	-	11/53/53/53	-
37	LHG	e	101	-	-	10/46/46/53	-
24	CLA	B	609	2	-	0/39/115/115	-
37	LHG	D	407	-	-	5/53/53/53	-
28	GOL	a	414	-	-	2/4/4/4	-
24	CLA	B	602	41	-	16/39/115/115	-

The worst 5 of 1630 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	408	PHO	C1D-C2D	9.19	1.49	1.39
25	A	409	PHO	C1B-C2B	9.14	1.49	1.39
25	a	420	PHO	C1B-C2B	9.04	1.49	1.39
25	A	408	PHO	C1B-C2B	8.77	1.49	1.39
25	a	408	PHO	C1B-C2B	8.63	1.49	1.39

The worst 5 of 2741 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	408	PHO	C2D-C1D-ND	12.74	118.32	109.53
25	A	408	PHO	C2D-C1D-ND	11.97	117.79	109.53
25	A	409	PHO	C2D-C1D-ND	11.44	117.42	109.53
25	a	420	PHO	C2D-C1D-ND	11.35	117.36	109.53
24	B	612	CLA	C1D-ND-C4D	-10.00	99.23	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	201	HEC	NA
40	v	202	HEC	NA

5 of 1295 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	410	CLA	C2-C3-C5-C6
24	A	410	CLA	C4-C3-C5-C6
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.

157 monomers are involved in 303 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	512	CLA	1	0
29	m	102	LMT	4	0
36	H	102	DGD	1	0
24	b	607	CLA	1	0
35	c	922	HTG	1	0
24	a	409	CLA	1	0
34	b	624	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	914	CLA	3	0
26	T	102	BCR	4	0
24	A	405	CLA	2	0
34	C	521	LMG	3	0
29	c	921	LMT	1	0
24	b	613	CLA	3	0
29	C	522	LMT	2	0
31	d	405	PL9	1	0
34	c	920	LMG	2	0
35	d	412	HTG	2	0
34	B	622	LMG	2	0
24	c	903	CLA	3	0
35	B	633	HTG	2	0
26	k	102	BCR	1	0
24	B	602	CLA	4	0
28	f	101	GOL	1	0
26	b	622	BCR	2	0
34	Z	101	LMG	3	0
34	a	412	LMG	3	0
26	H	101	BCR	3	0
25	a	420	PHO	1	0
24	C	511	CLA	3	0
28	T	101	GOL	1	0
24	c	906	CLA	2	0
26	K	103	BCR	3	0
24	A	410	CLA	3	0
28	B	631	GOL	1	0
29	b	601	LMT	2	0
37	E	101	LHG	2	0
24	b	618	CLA	1	0
35	B	625	HTG	1	0
24	B	613	CLA	1	0
24	B	617	CLA	5	0
34	z	101	LMG	2	0
26	C	515	BCR	1	0
37	D	406	LHG	2	0
37	D	408	LHG	7	0
24	B	614	CLA	3	0
24	c	908	CLA	2	0
24	C	510	CLA	3	0
28	v	203	GOL	2	0
35	C	524	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	621	SQD	3	0
24	C	513	CLA	3	0
28	B	637	GOL	3	0
26	B	620	BCR	2	0
34	C	520	LMG	2	0
28	c	925	GOL	2	0
26	B	619	BCR	4	0
26	D	403	BCR	2	0
24	B	612	CLA	1	0
24	C	514	CLA	4	0
24	D	401	CLA	1	0
35	B	634	HTG	1	0
31	a	417	PL9	5	0
36	d	406	DGD	6	0
28	T	103	GOL	3	0
24	B	603	CLA	2	0
35	O	303	HTG	1	0
36	C	518	DGD	2	0
24	b	612	CLA	1	0
24	b	610	CLA	1	0
24	C	505	CLA	1	0
24	c	905	CLA	1	0
24	c	912	CLA	2	0
24	d	403	CLA	1	0
24	b	609	CLA	2	0
27	a	411	SQD	3	0
26	b	623	BCR	2	0
29	B	623	LMT	1	0
24	B	616	CLA	2	0
24	B	606	CLA	1	0
26	c	915	BCR	2	0
24	b	620	CLA	2	0
24	C	506	CLA	4	0
27	A	412	SQD	5	0
24	c	911	CLA	2	0
26	y	101	BCR	2	0
24	b	619	CLA	3	0
34	C	501	LMG	2	0
24	c	907	CLA	3	0
35	D	411	HTG	3	0
29	M	101	LMT	3	0
28	b	632	GOL	2	0

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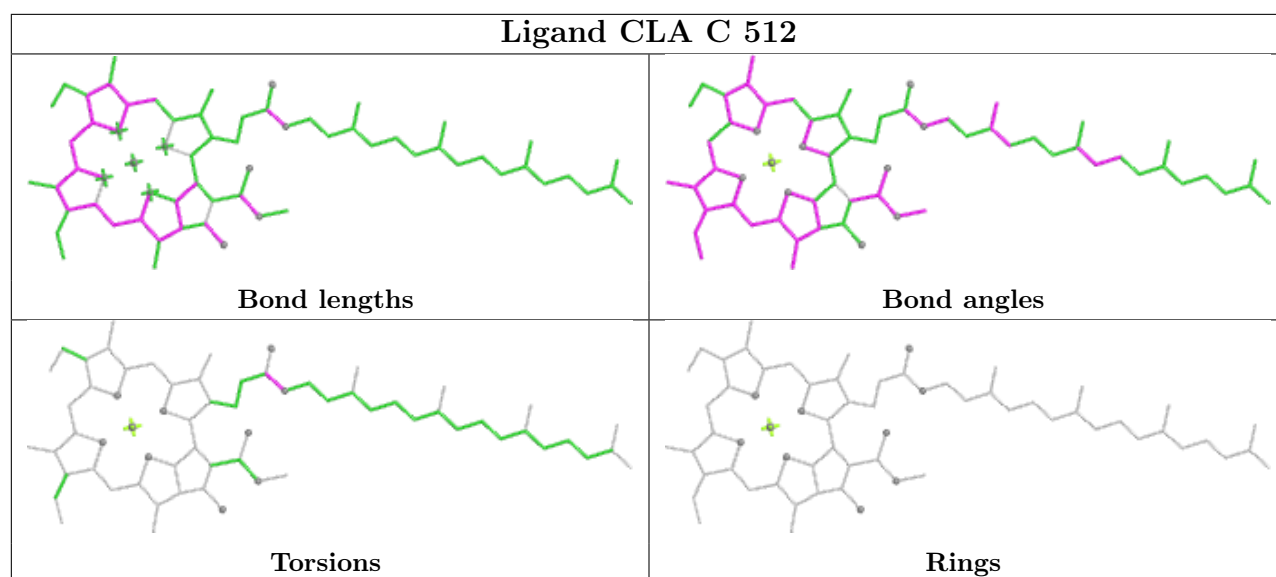
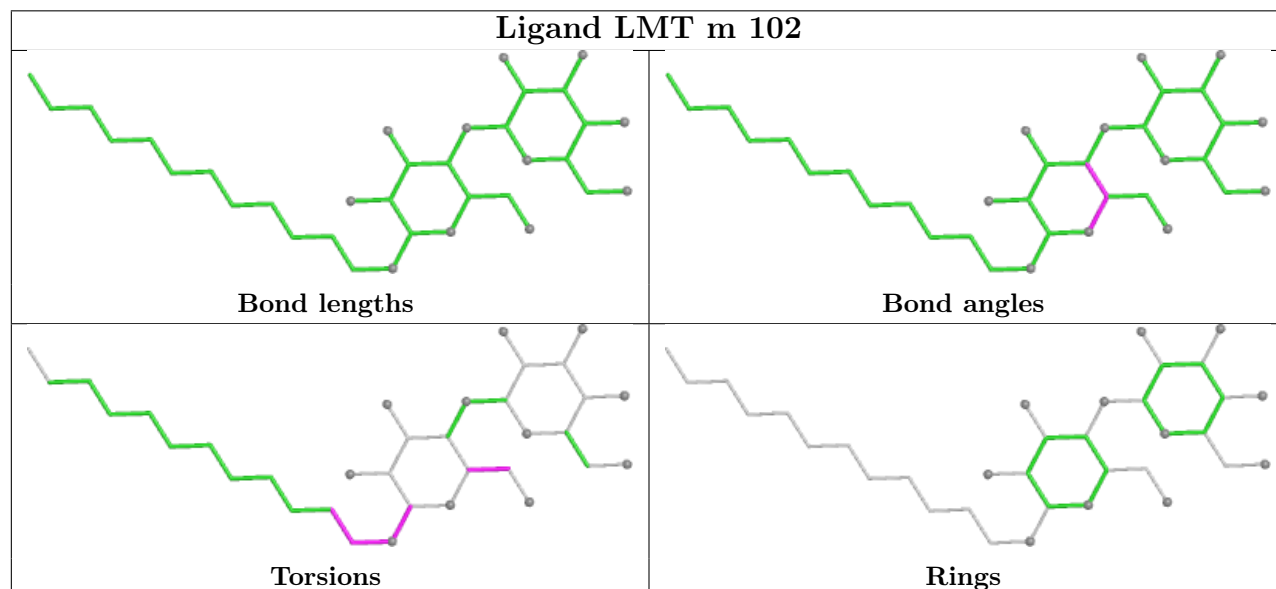
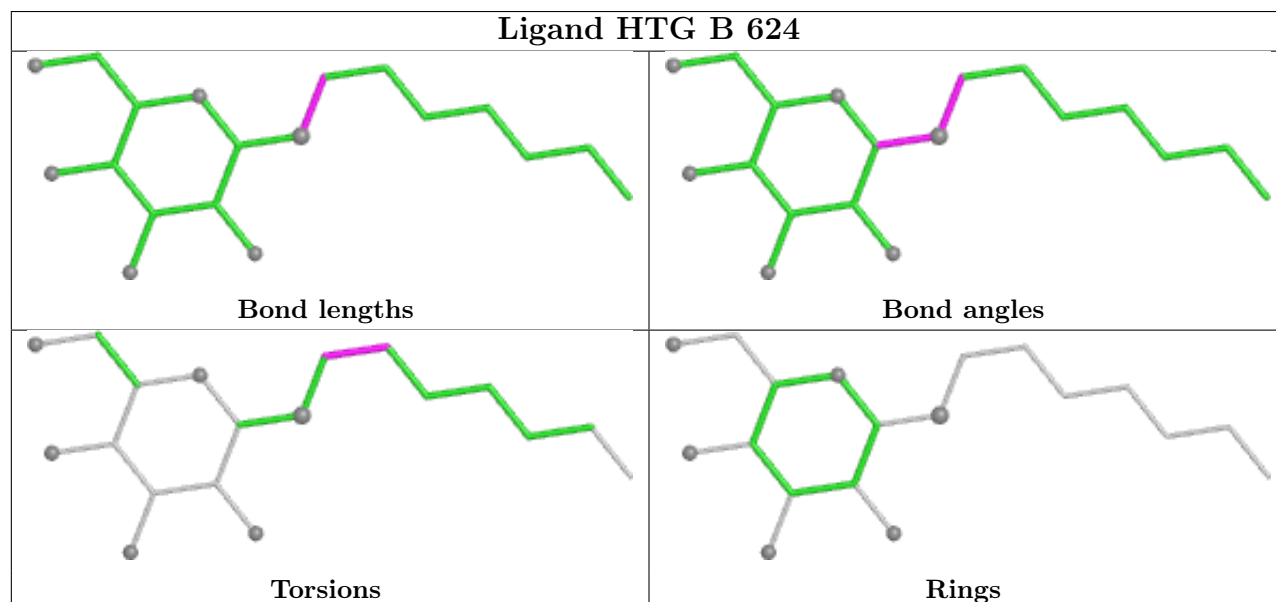
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	606	CLA	2	0
24	b	615	CLA	1	0
29	B	636	LMT	1	0
24	D	402	CLA	2	0
29	b	625	LMT	2	0
24	C	507	CLA	6	0
27	F	101	SQD	3	0
36	c	916	DGD	1	0
24	B	608	CLA	1	0
24	c	904	CLA	2	0
28	b	631	GOL	1	0
27	a	402	SQD	1	0
36	c	917	DGD	4	0
34	j	101	LMG	5	0
37	l	101	LHG	2	0
28	b	633	GOL	1	0
26	k	101	BCR	5	0
26	a	410	BCR	3	0
27	L	102	SQD	2	0
28	C	525	GOL	2	0
36	C	517	DGD	4	0
24	B	604	CLA	1	0
36	C	519	DGD	2	0
24	c	902	CLA	2	0
34	J	101	LMG	3	0
24	B	605	CLA	2	0
24	c	913	CLA	3	0
24	C	502	CLA	1	0
31	D	404	PL9	1	0
26	A	411	BCR	1	0
29	m	104	LMT	3	0
26	K	102	BCR	1	0
24	C	503	CLA	2	0
25	A	409	PHO	1	0
27	A	416	SQD	2	0
24	B	610	CLA	2	0
28	A	414	GOL	1	0
24	A	406	CLA	4	0
26	t	101	BCR	7	0
29	E	102	LMT	1	0
31	A	419	PL9	5	0
37	L	101	LHG	1	0

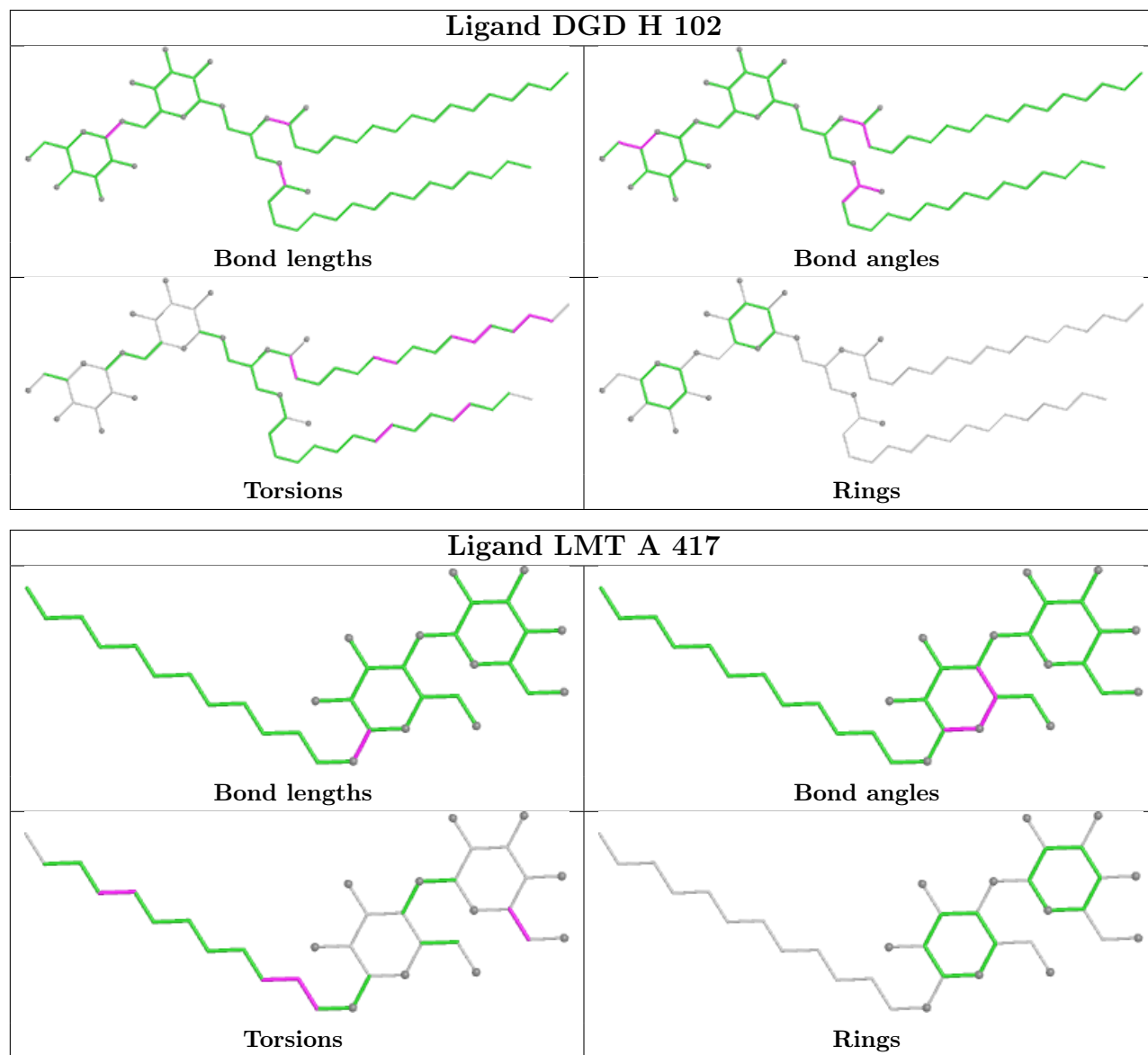
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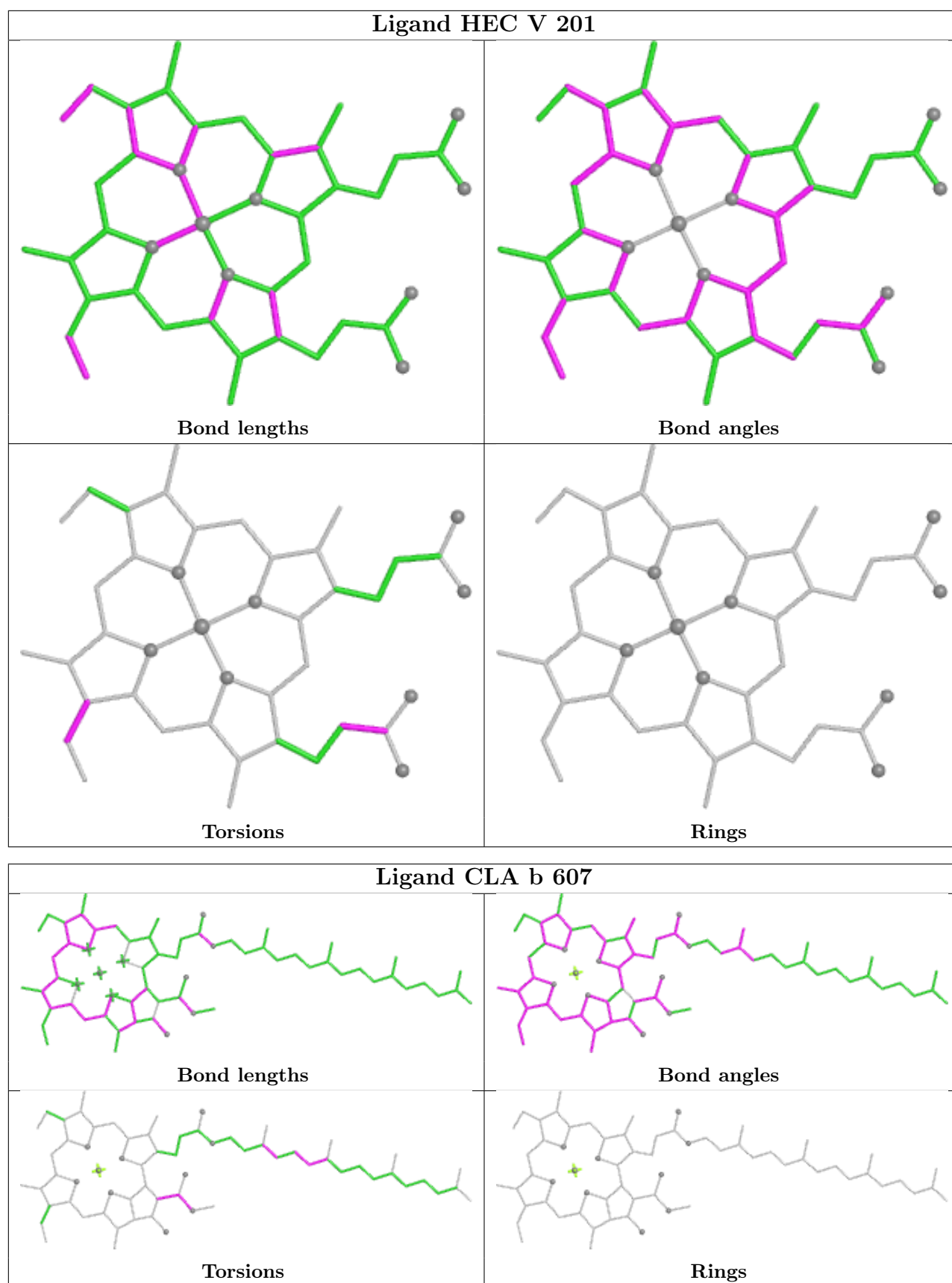
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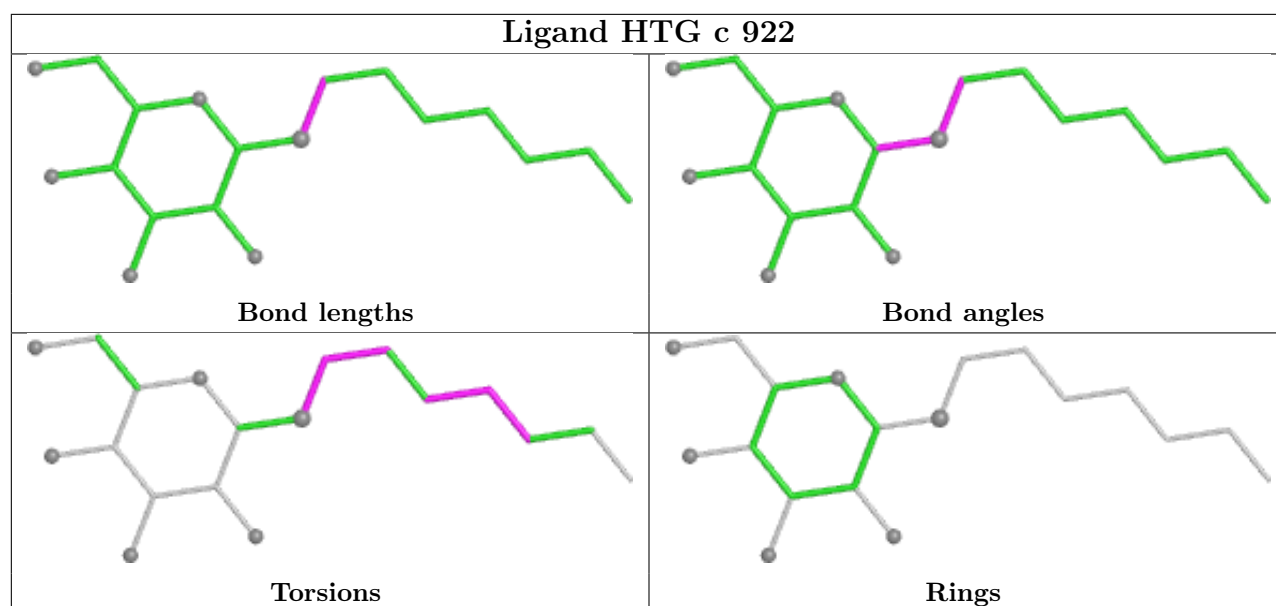
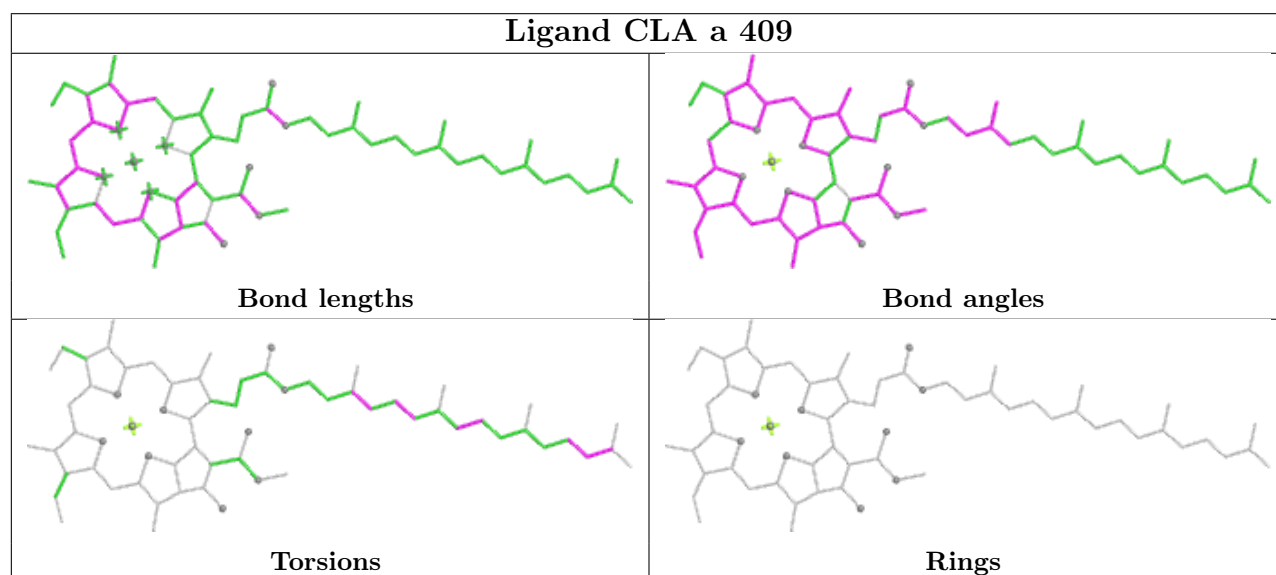
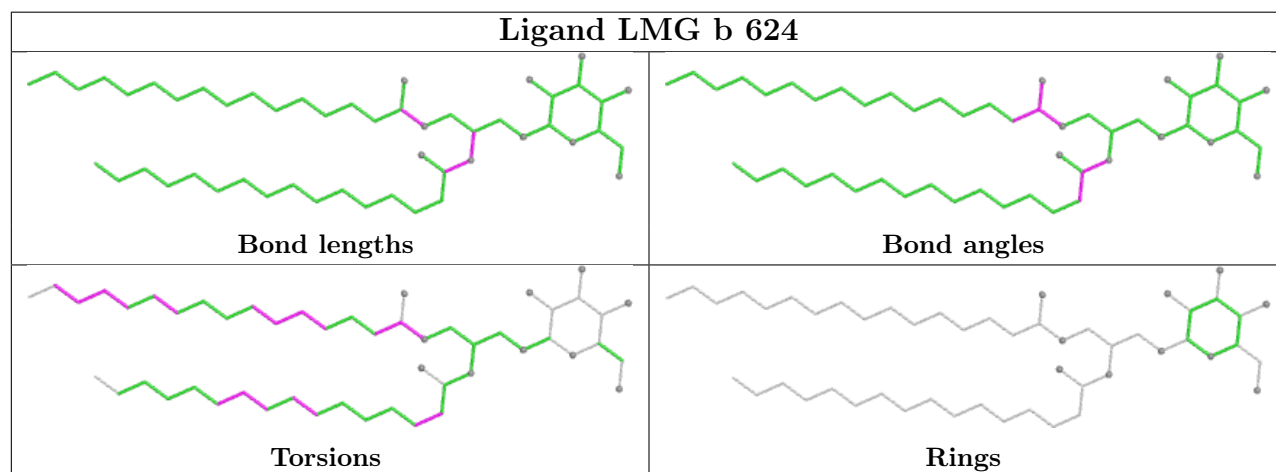
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	d	404	BCR	4	0
24	C	508	CLA	4	0
24	d	402	CLA	3	0
24	c	910	CLA	2	0
29	f	103	LMT	1	0
24	b	616	CLA	2	0
37	d	409	LHG	7	0
26	h	101	BCR	2	0
24	d	401	CLA	1	0
24	C	509	CLA	3	0
26	b	621	BCR	2	0
38	e	102	HEM	2	0
24	b	608	CLA	2	0
24	c	909	CLA	4	0
36	D	405	DGD	5	0
24	b	605	CLA	4	0
29	a	401	LMT	2	0
26	B	618	BCR	1	0
24	B	607	CLA	2	0
37	d	408	LHG	1	0
37	e	101	LHG	1	0
24	B	609	CLA	2	0
28	a	414	GOL	2	0
24	a	406	CLA	4	0

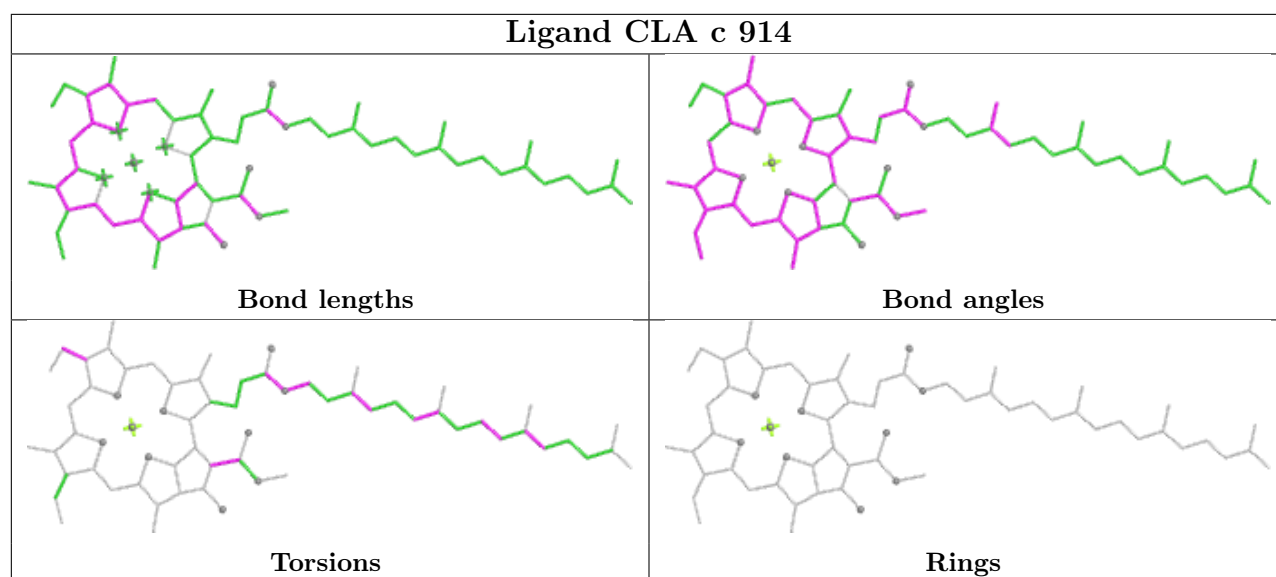
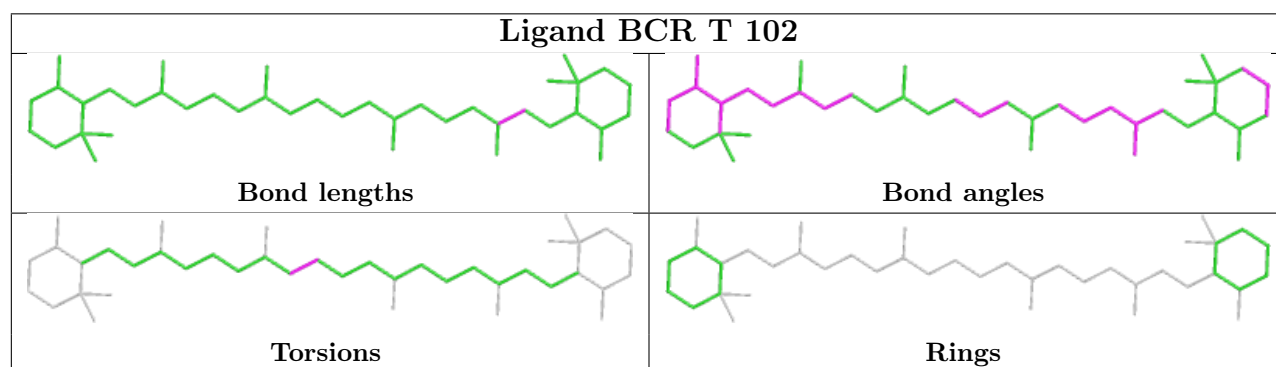
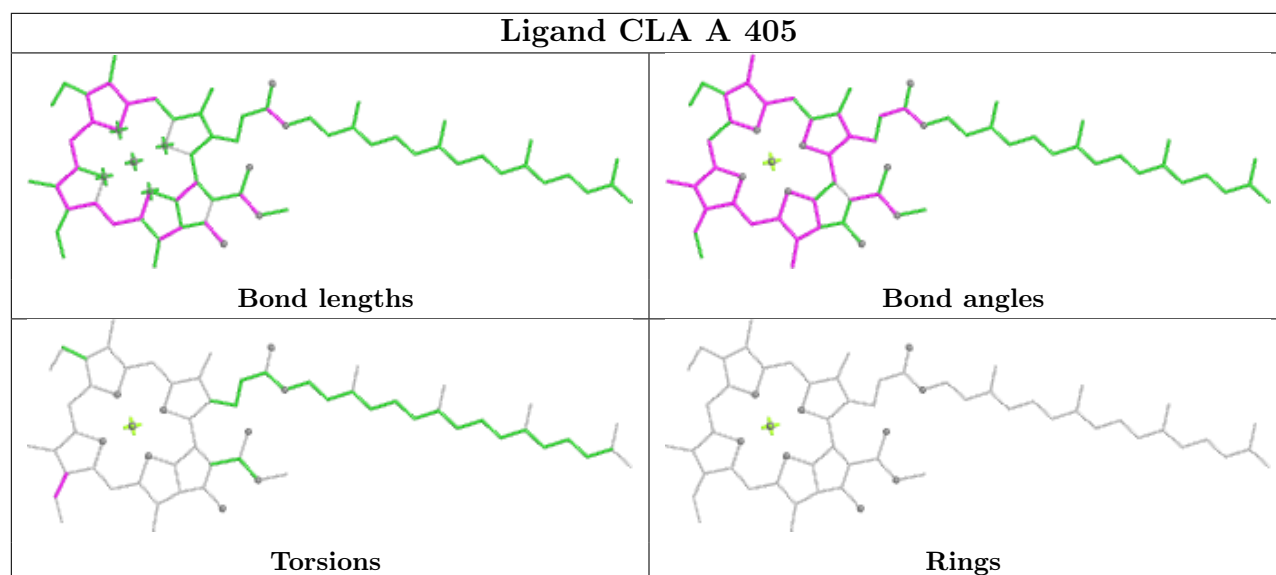
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

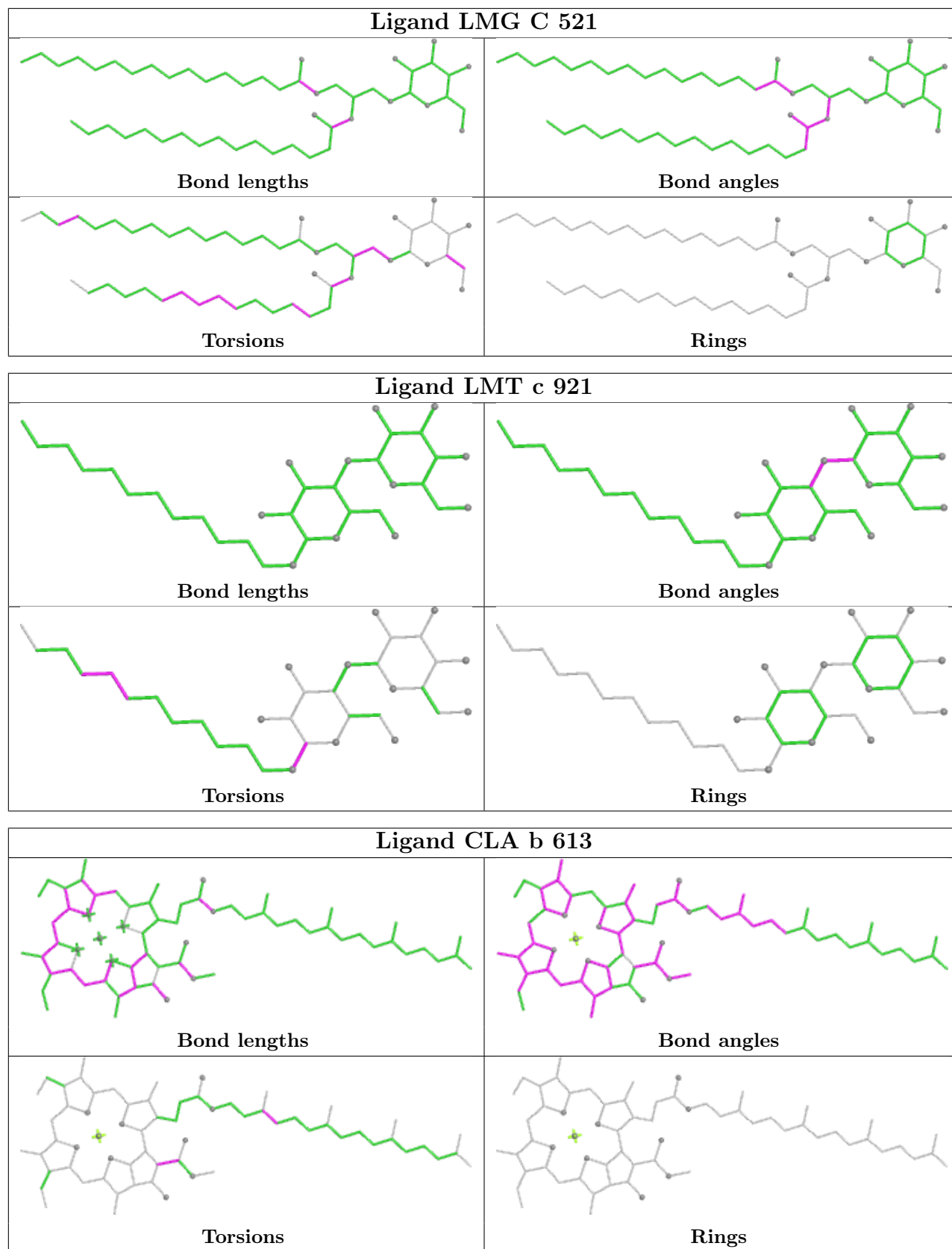


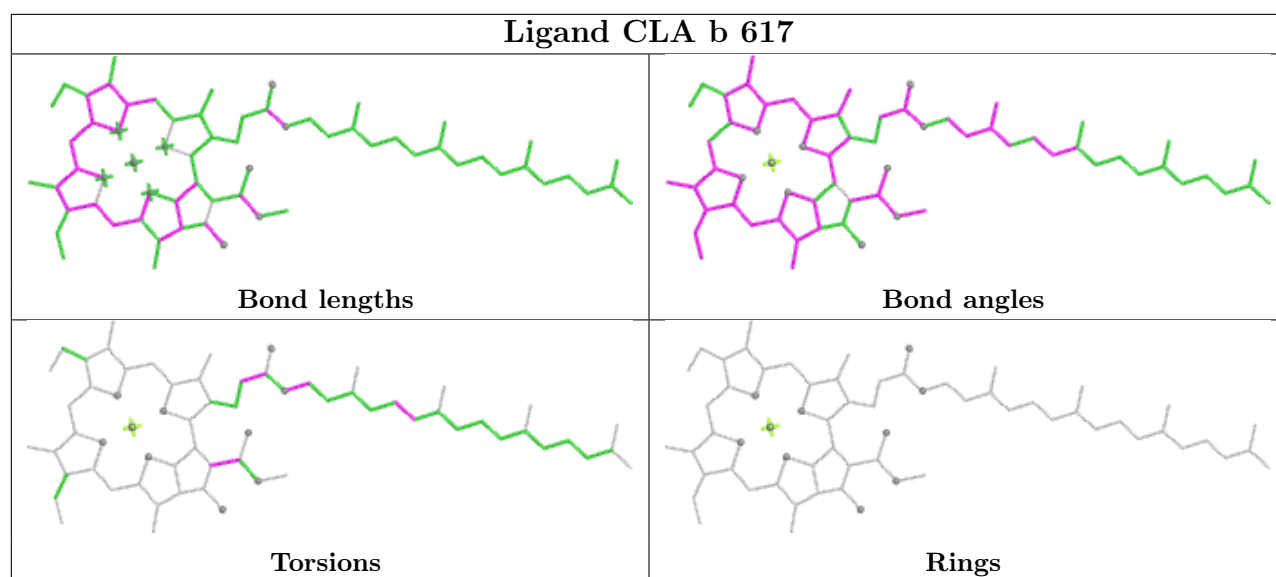
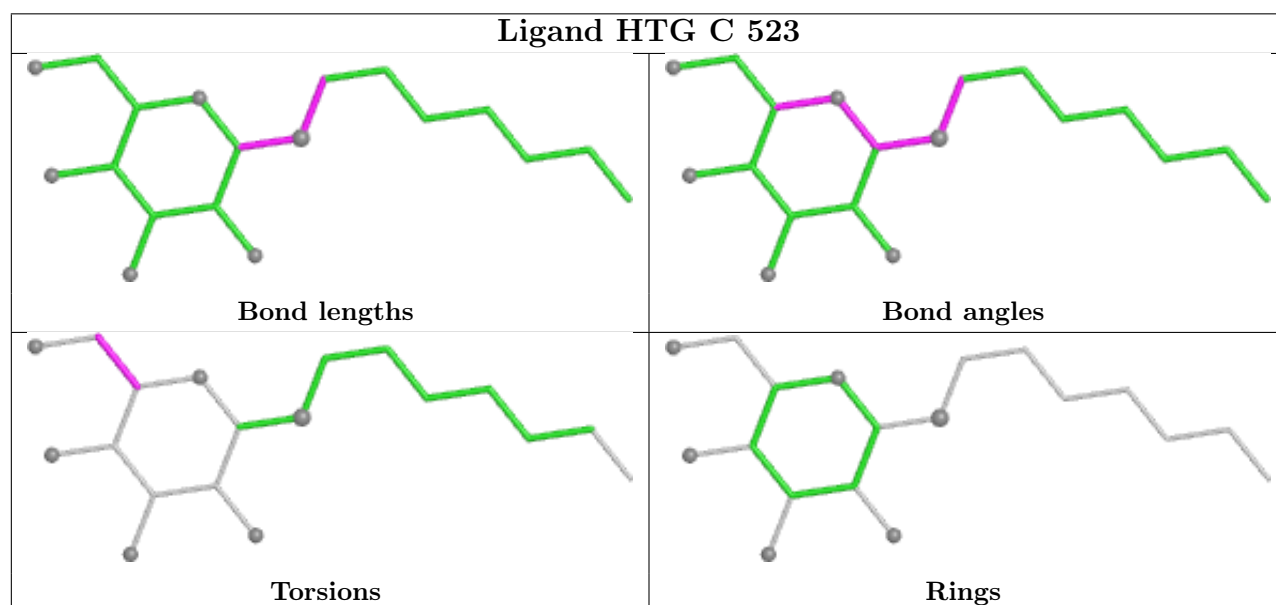
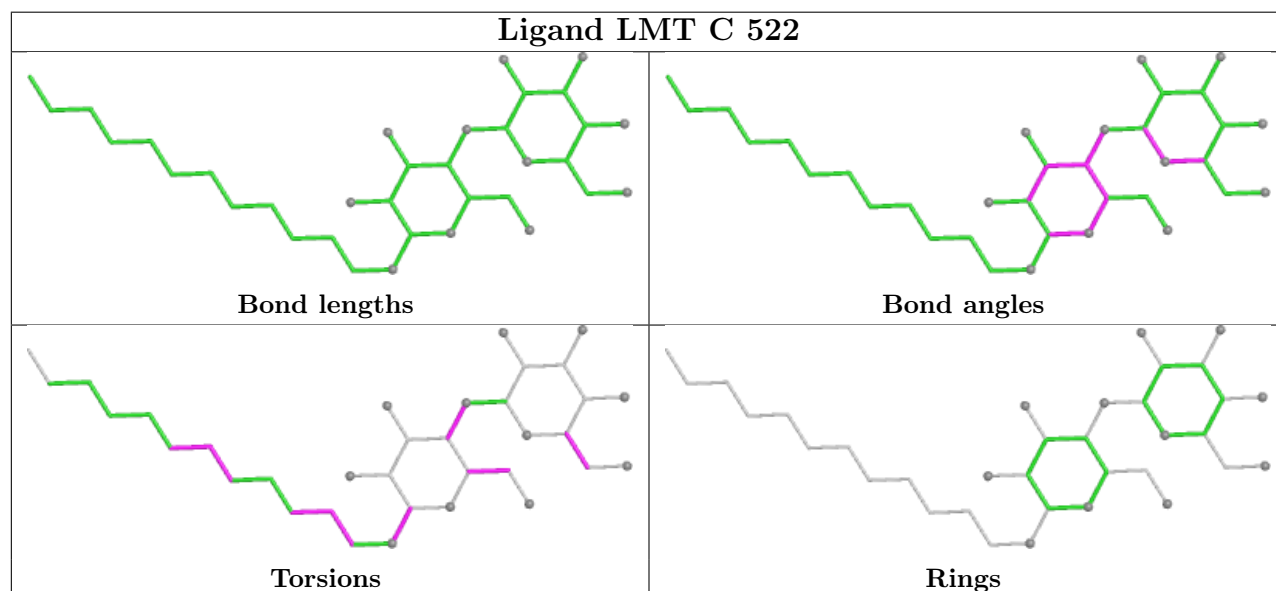


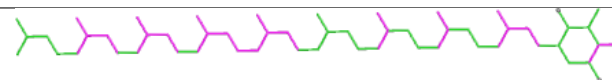
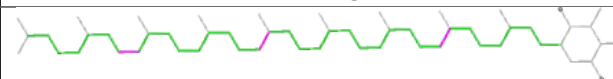
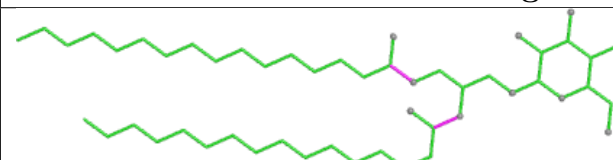
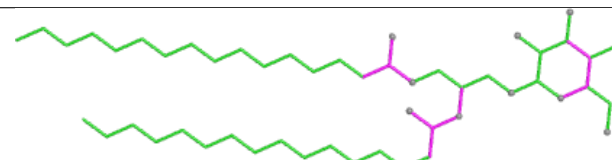
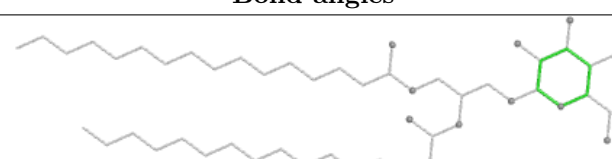
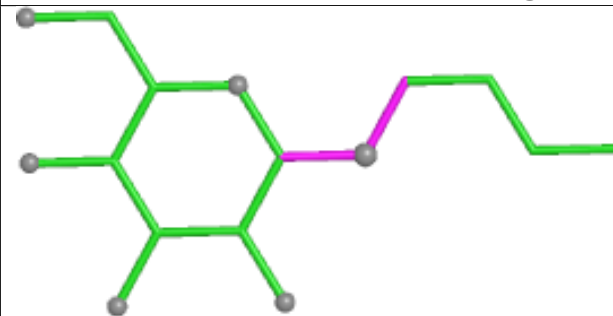
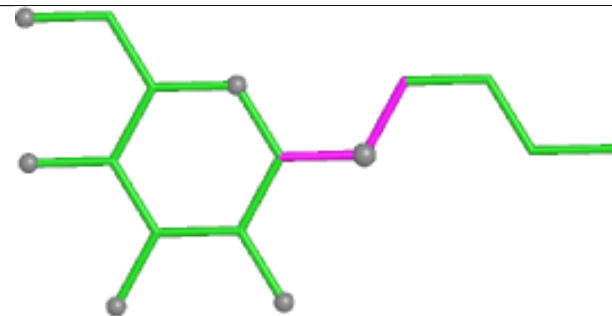
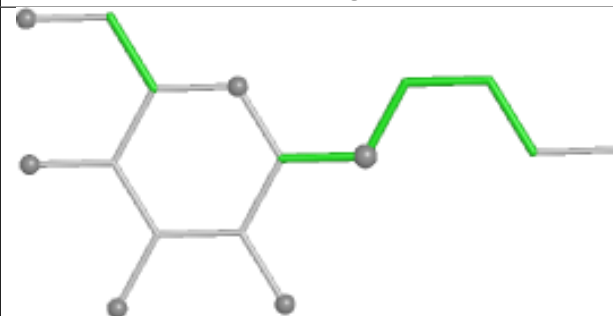
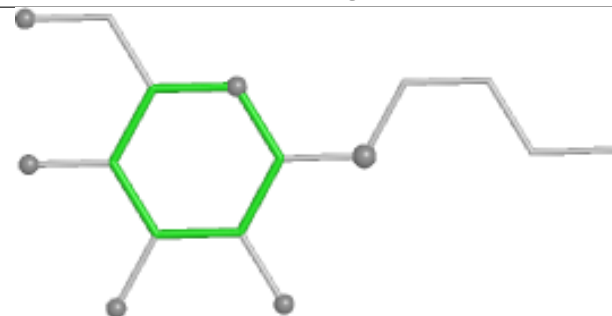


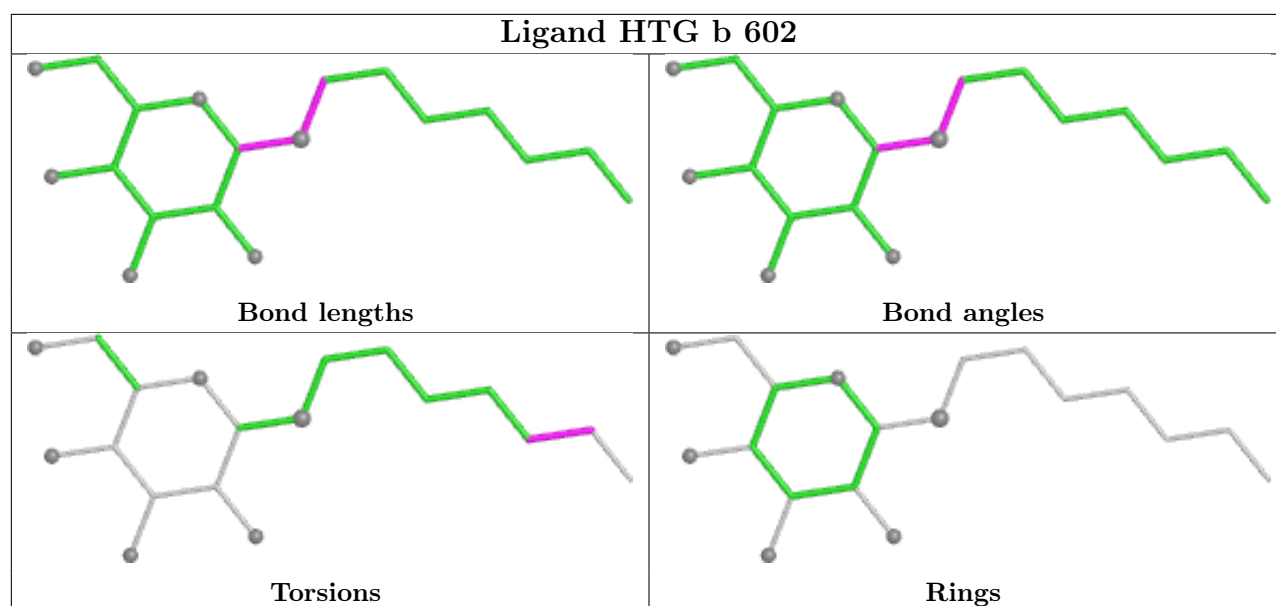
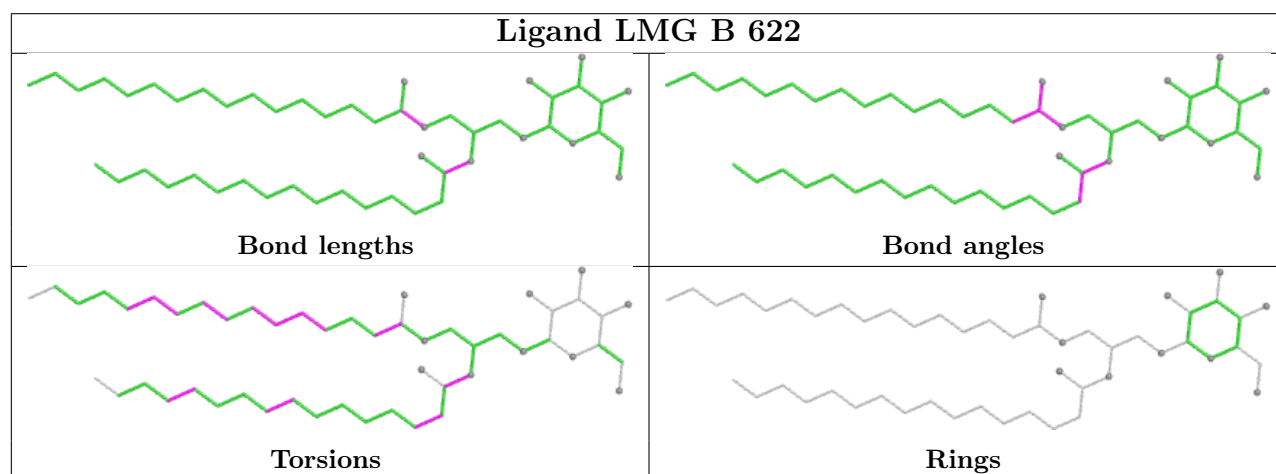
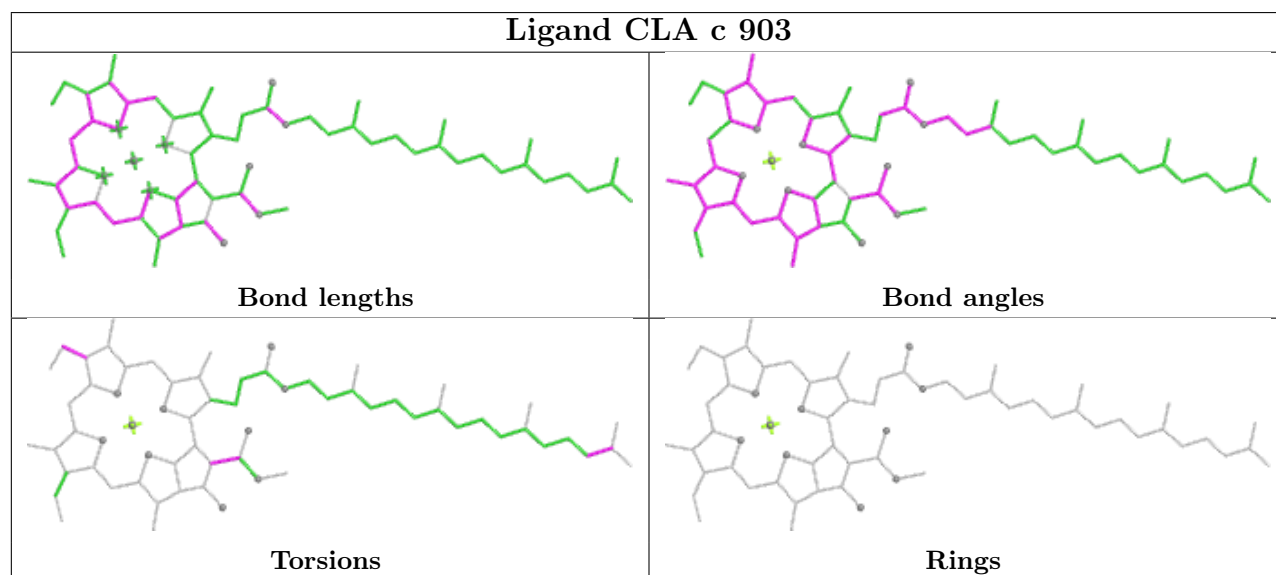


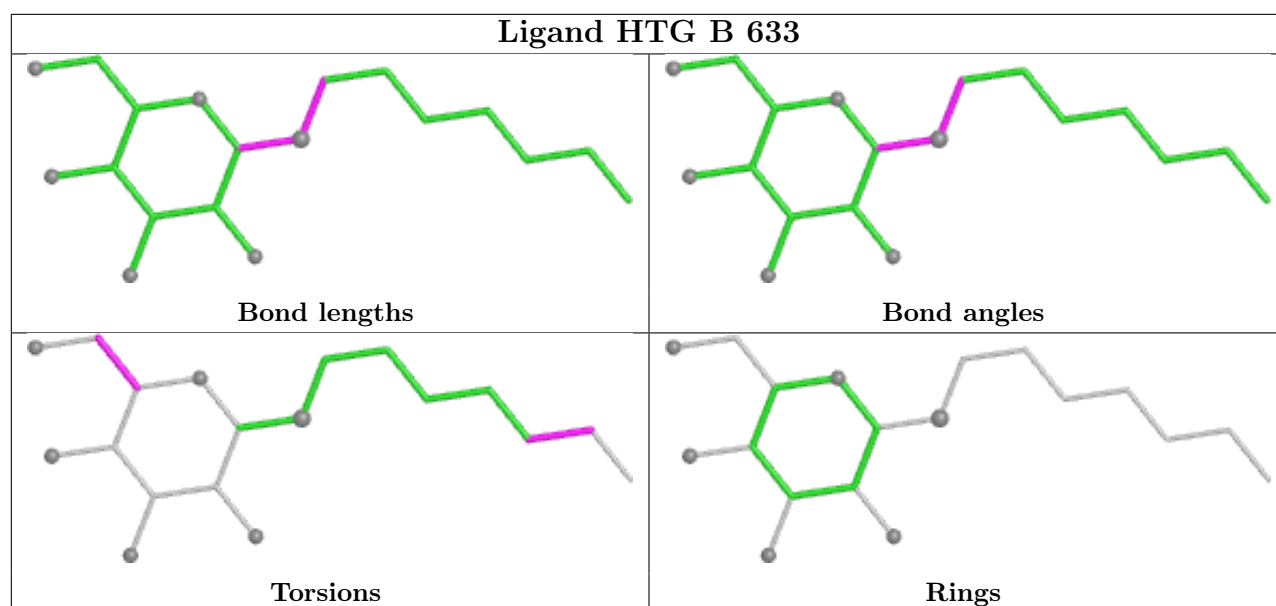
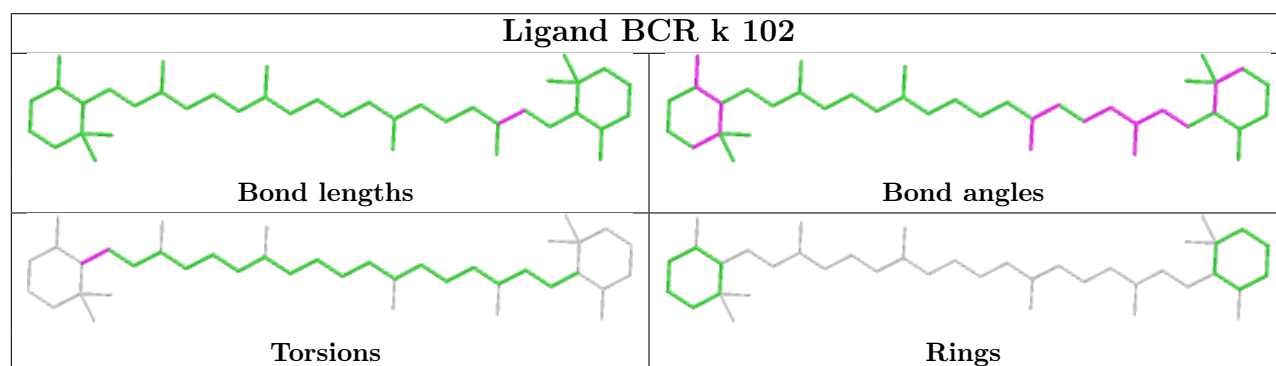
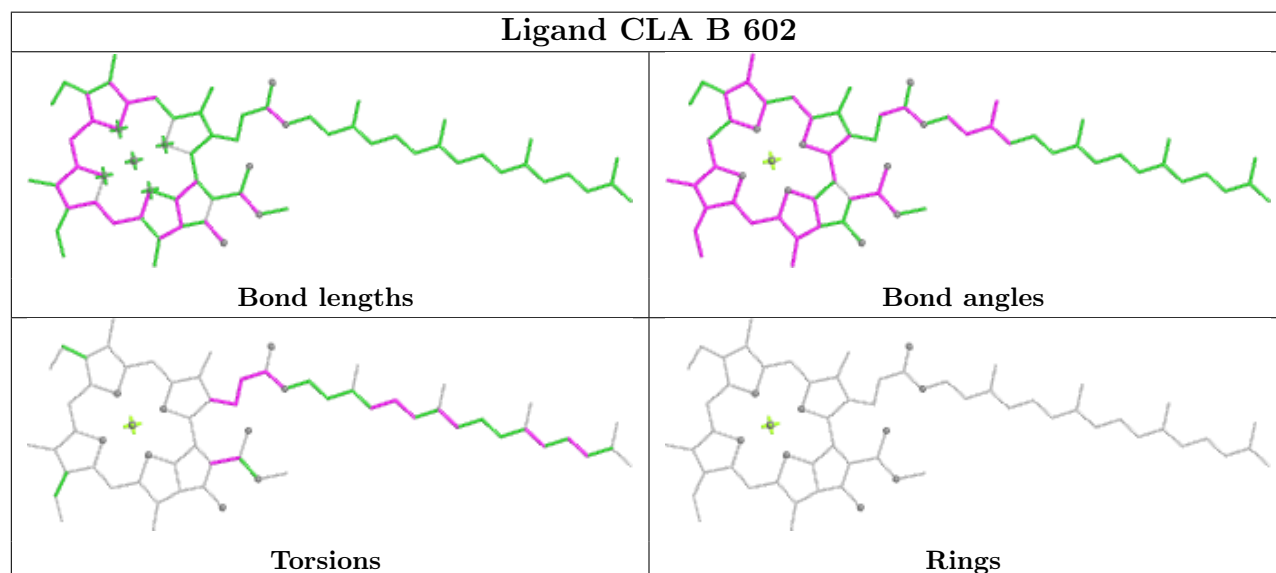


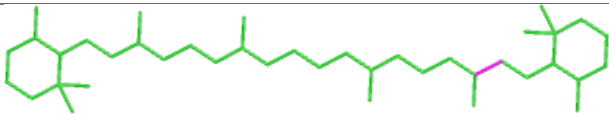
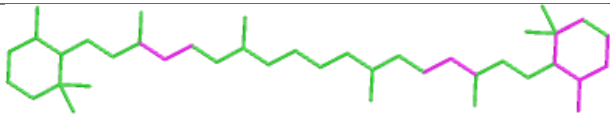
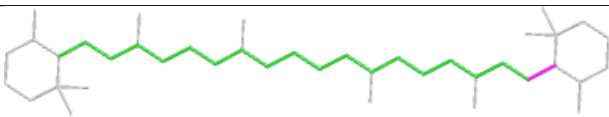
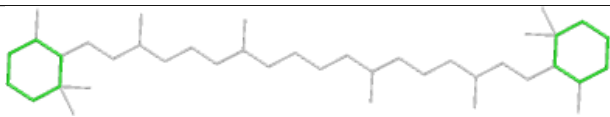


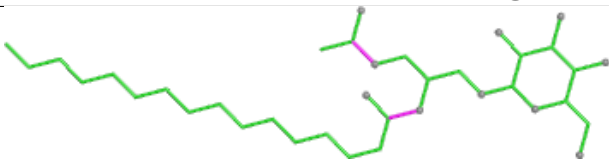
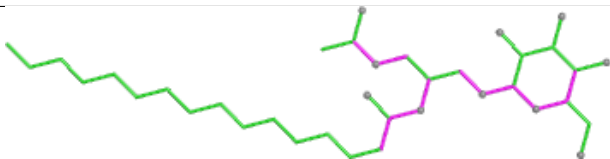
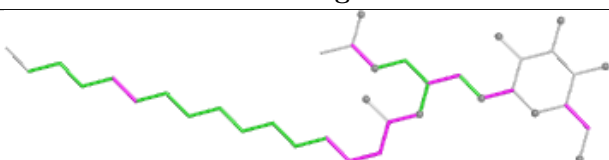
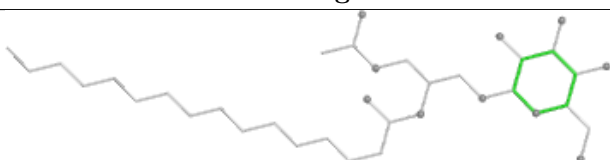


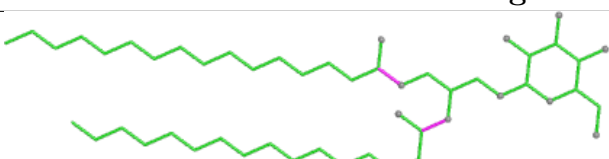
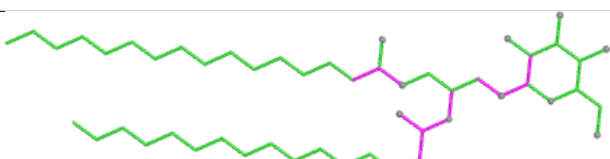
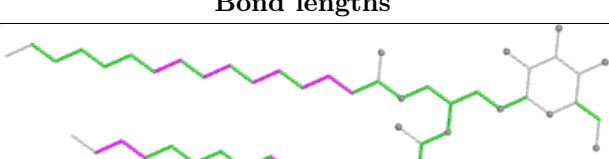
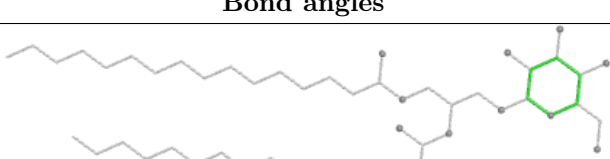
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 920	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand HTG d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

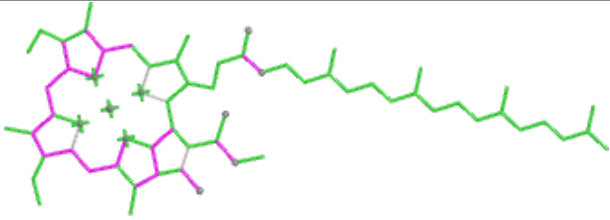
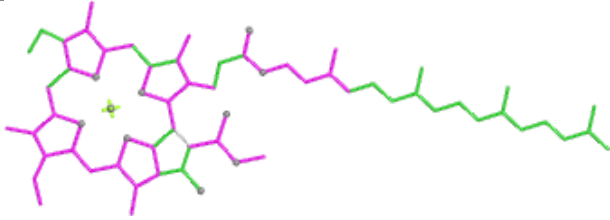
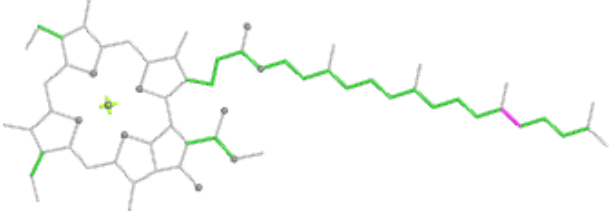
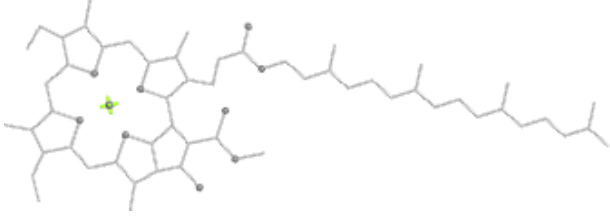
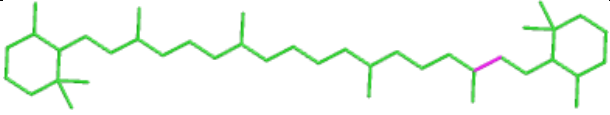
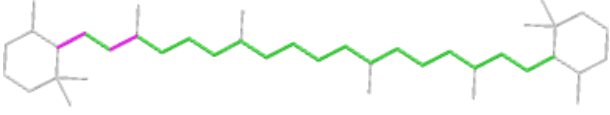
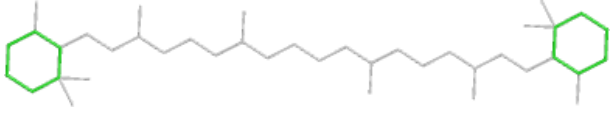
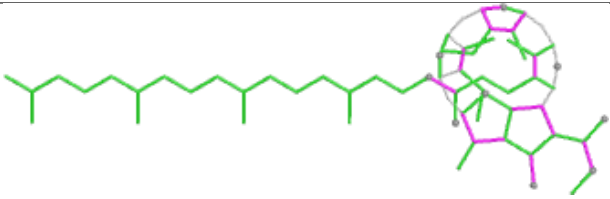
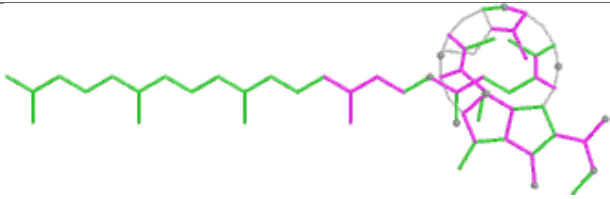
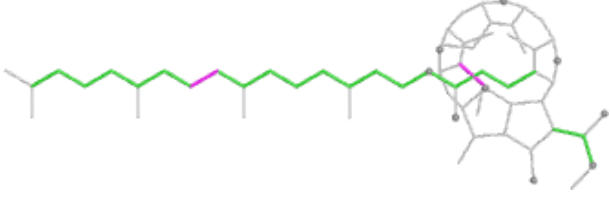
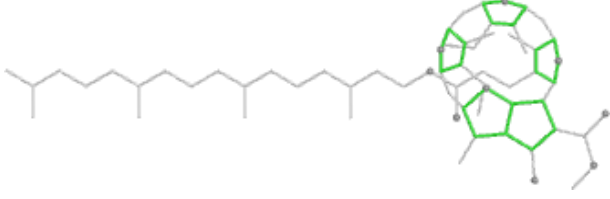


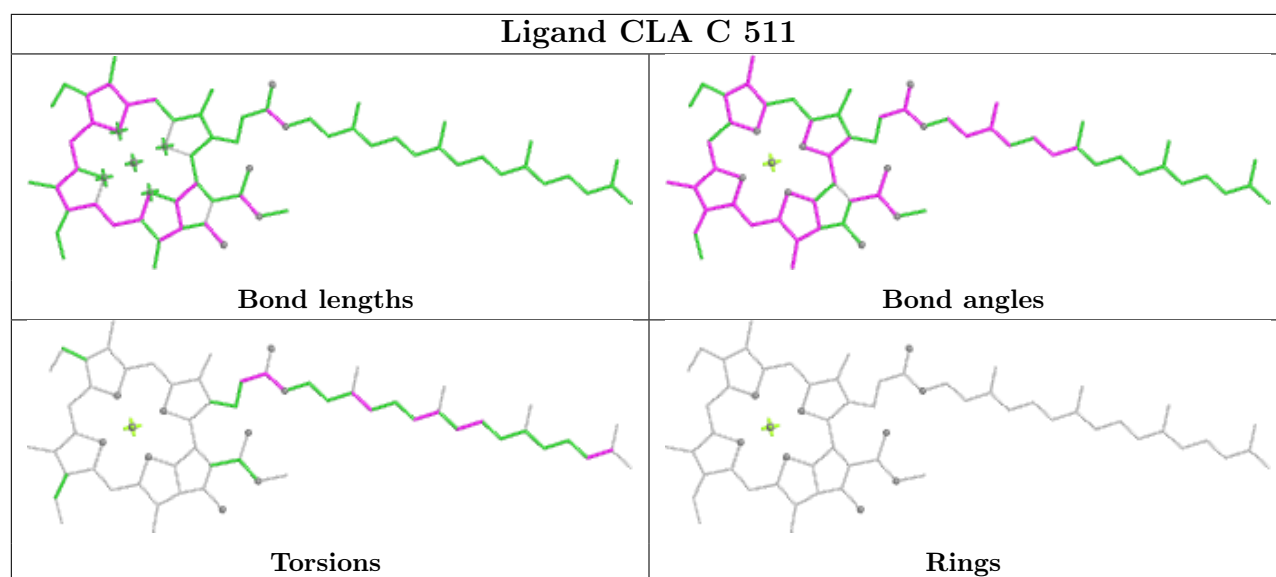
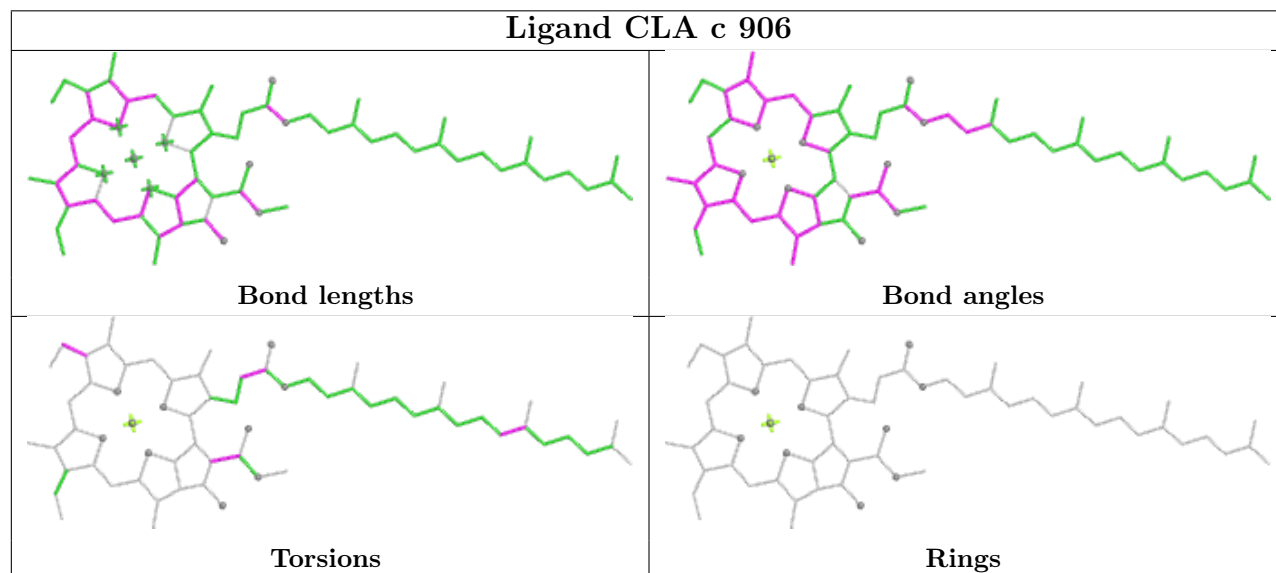
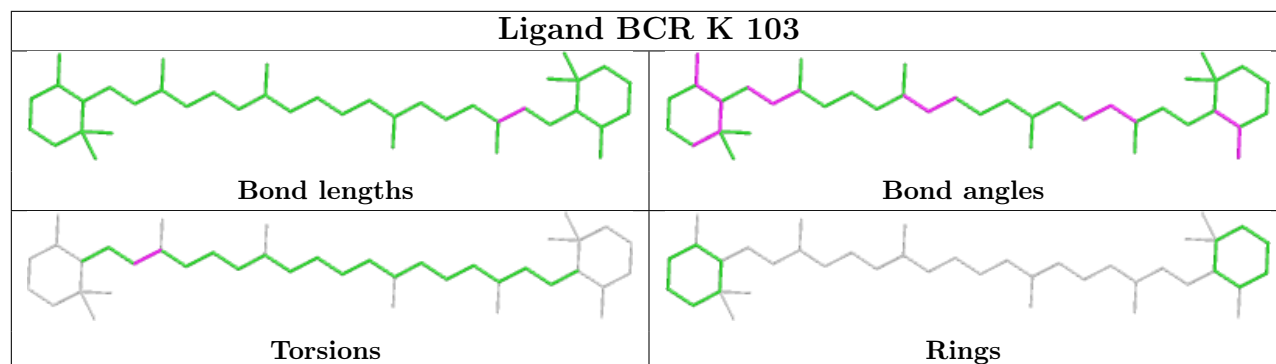


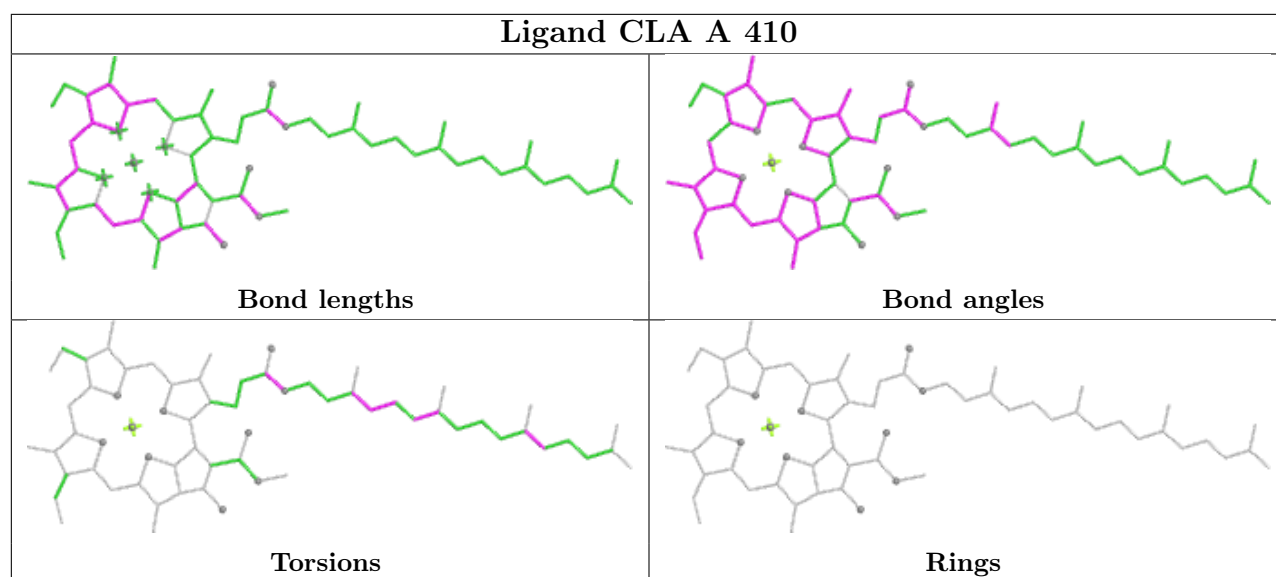
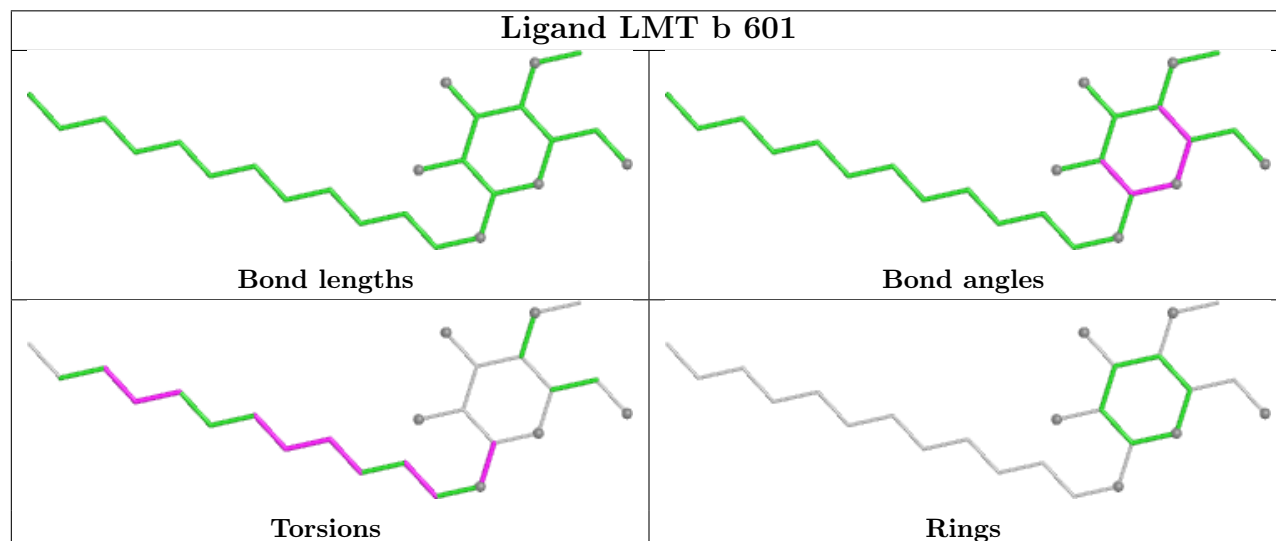
Ligand BCR b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

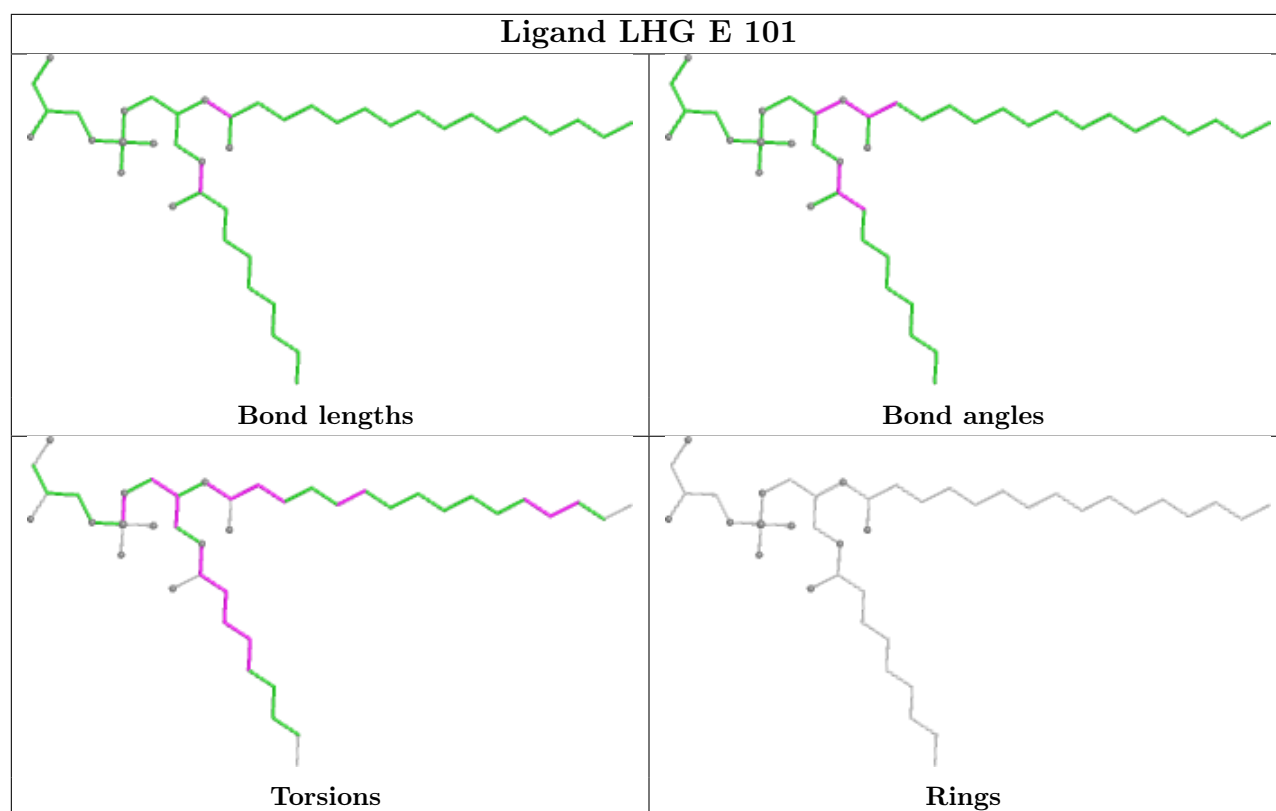
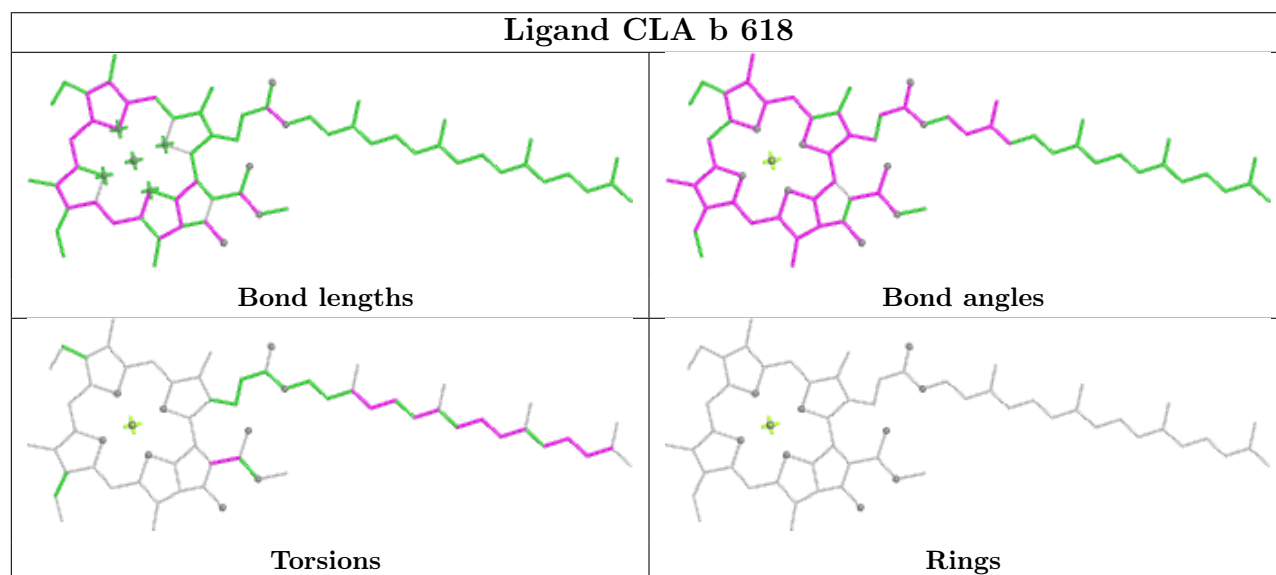
Ligand LMG Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

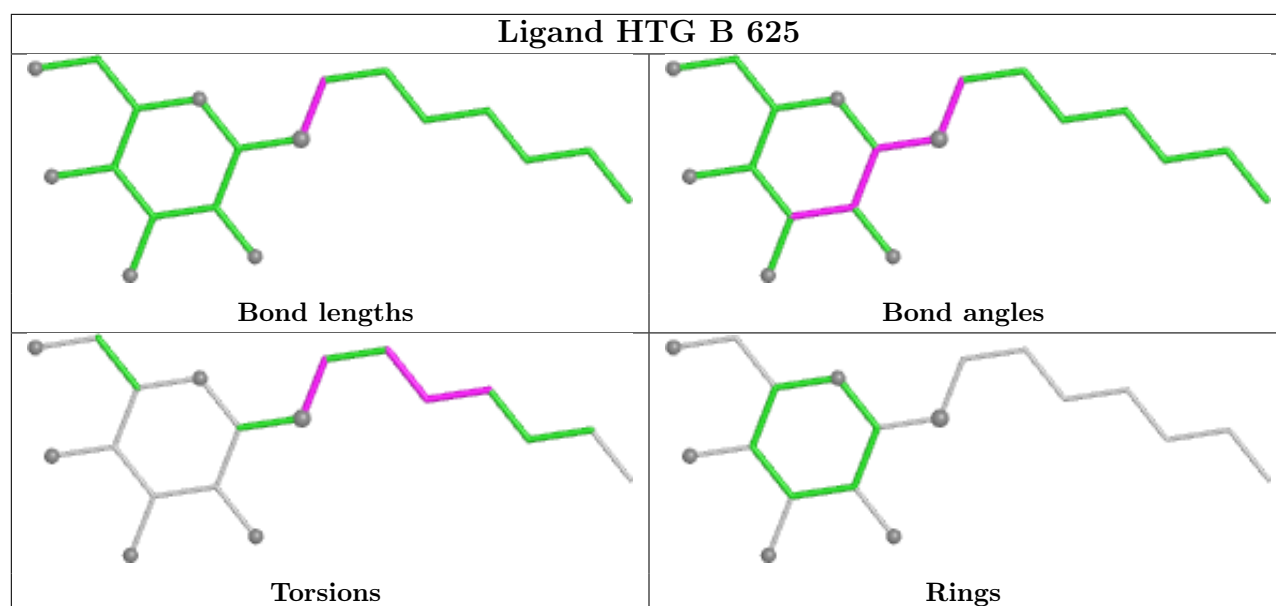
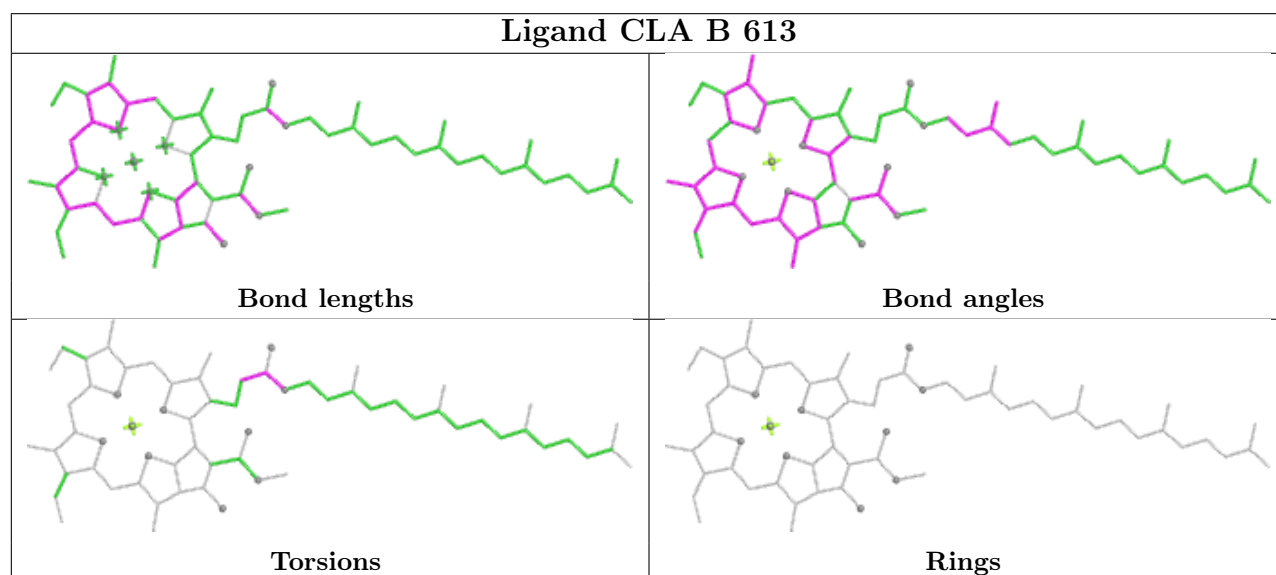
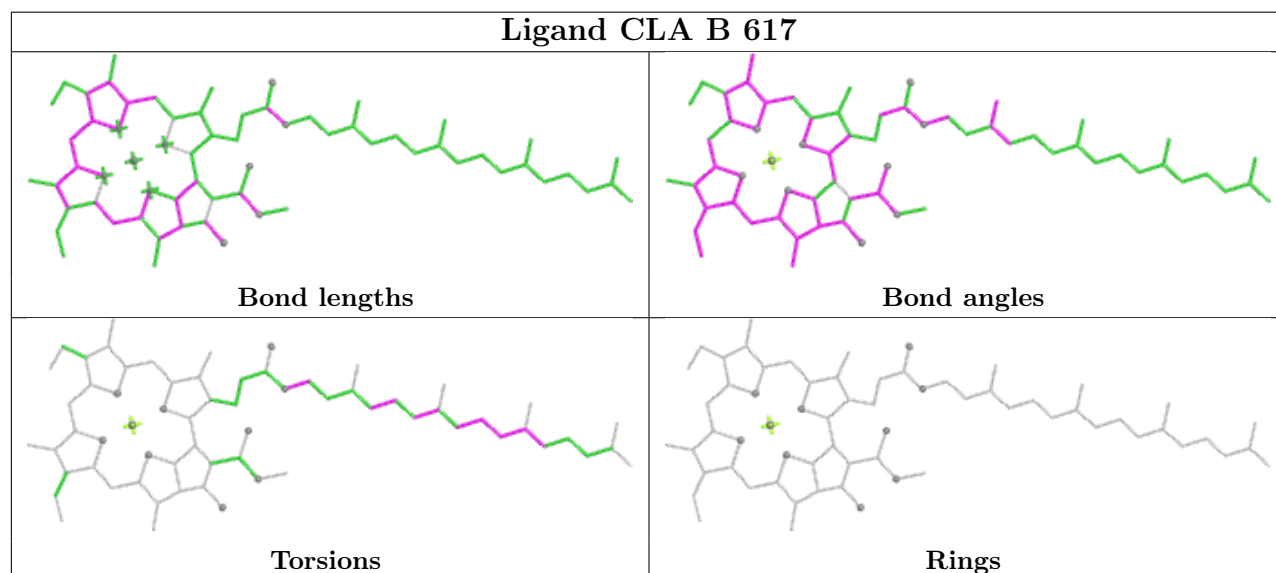
Ligand LMG a 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

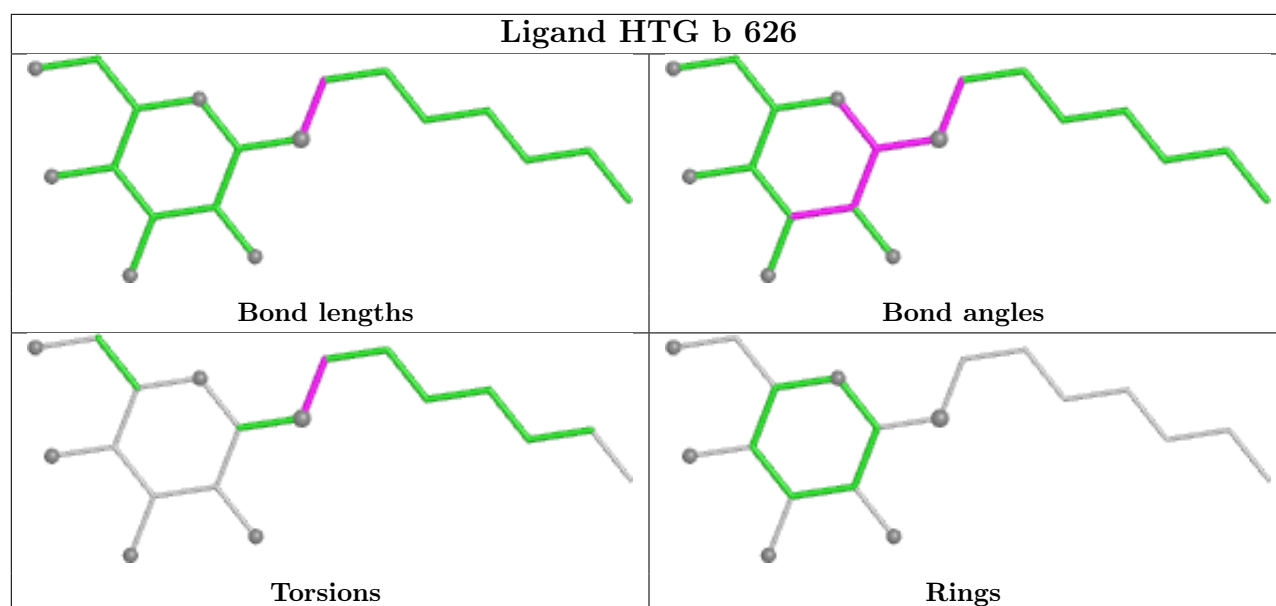
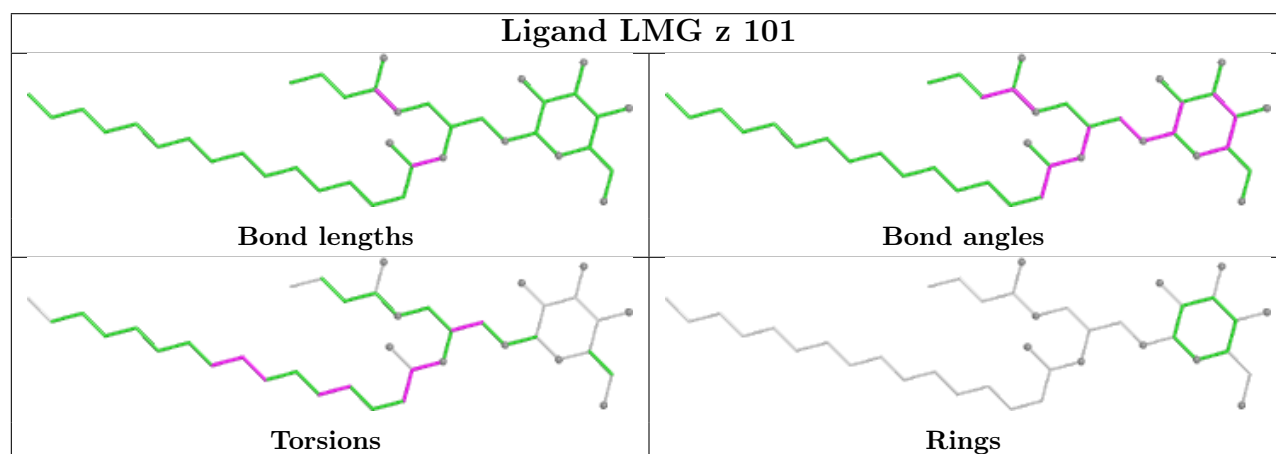
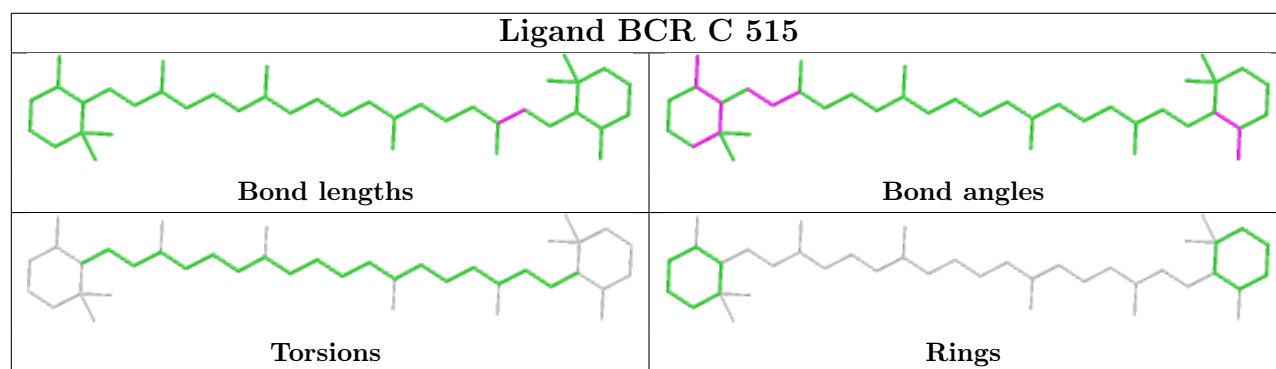
Ligand CLA A 407	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR H 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PHO a 420	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

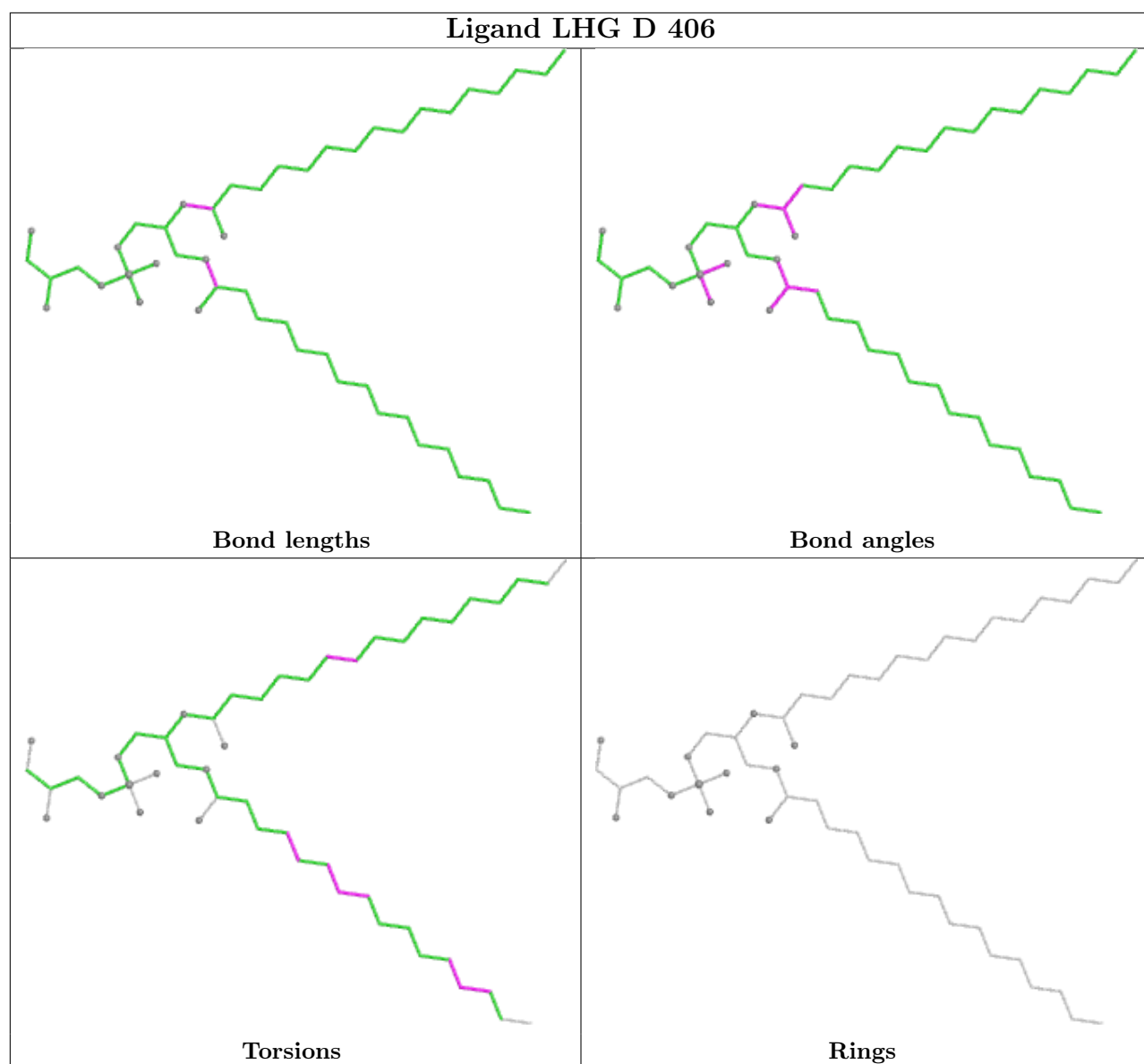


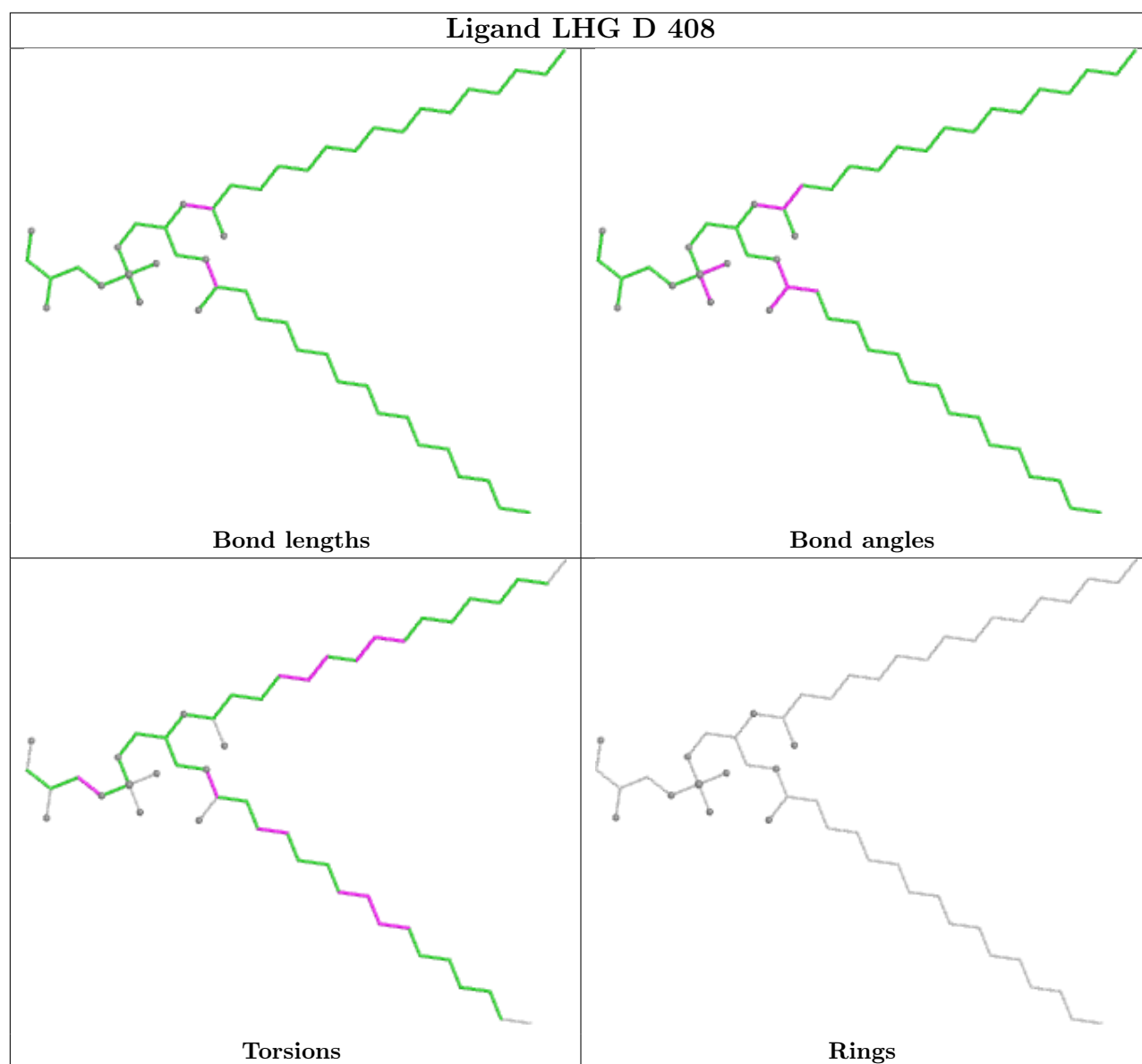
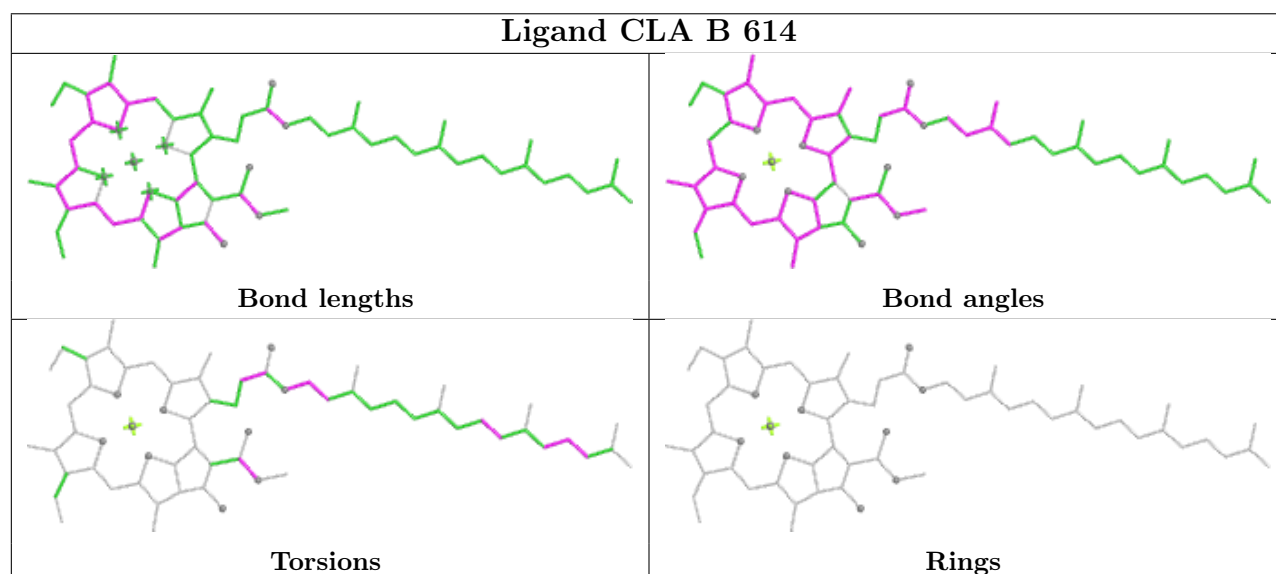




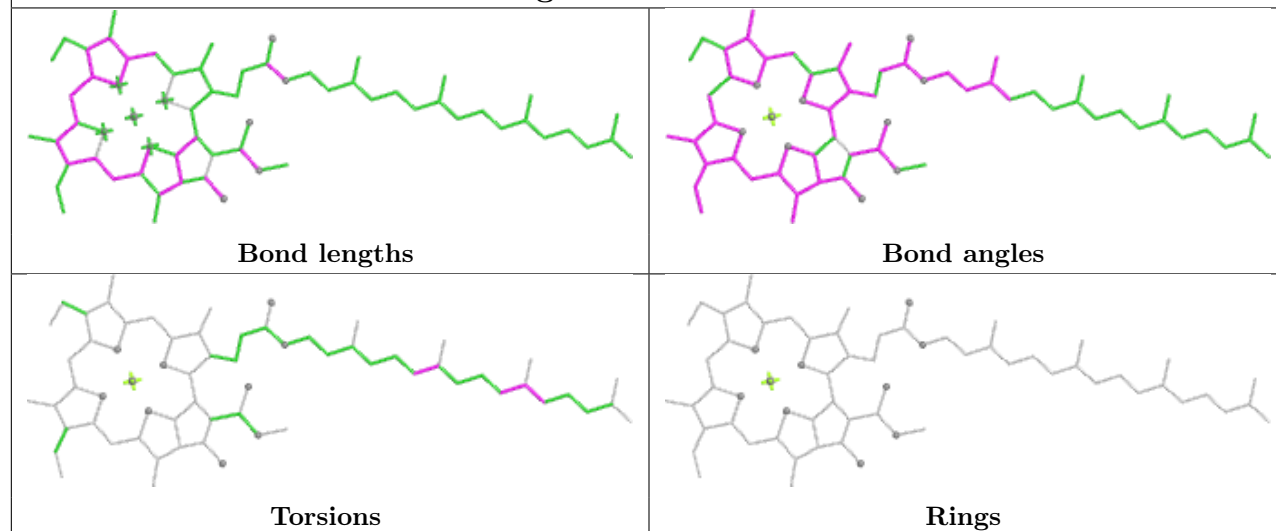




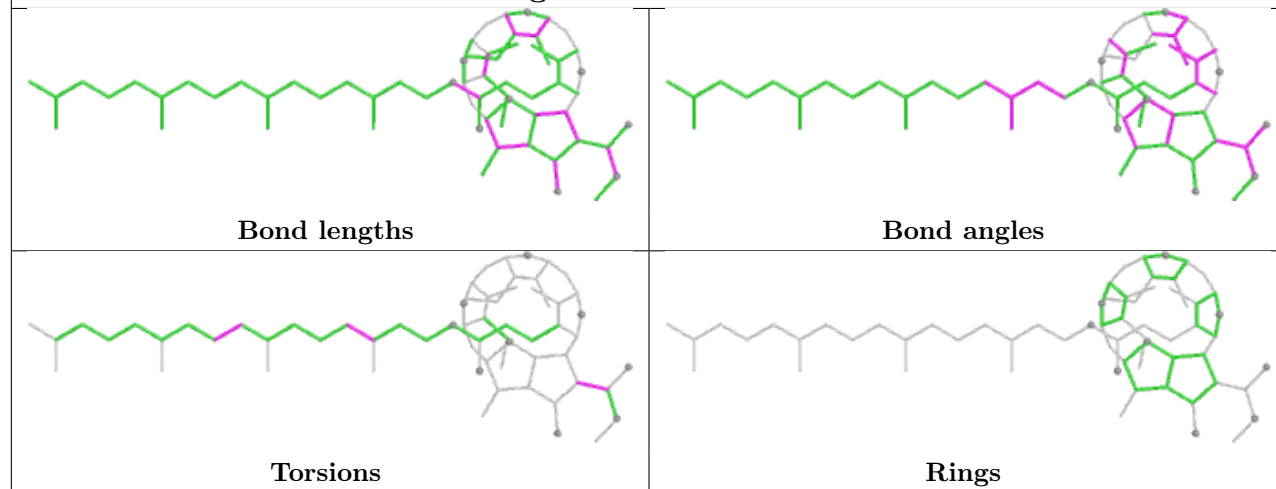




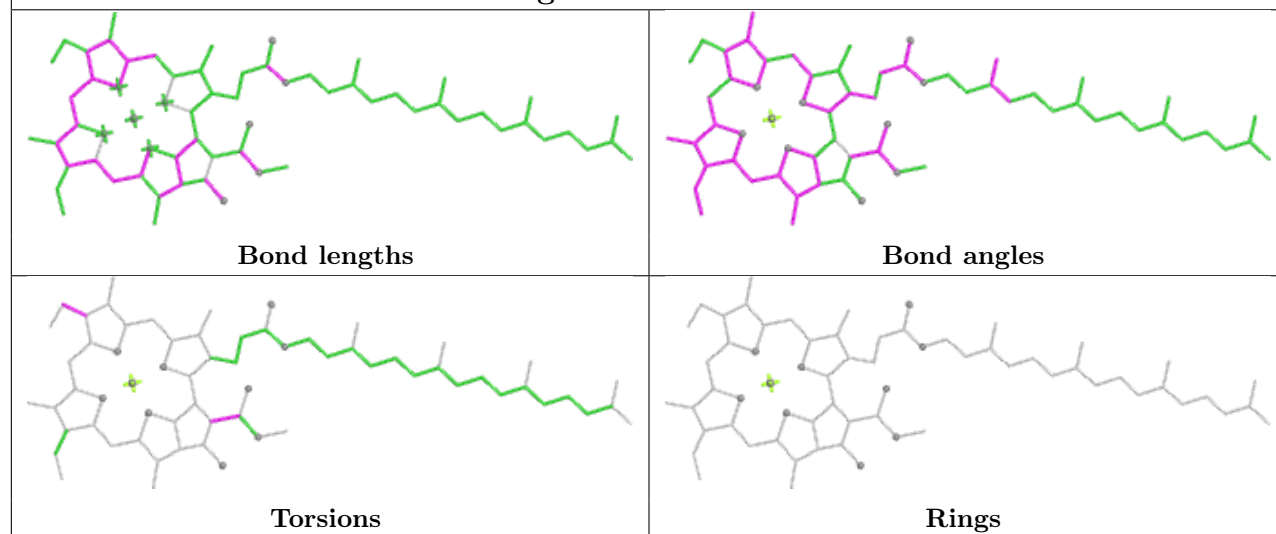
Ligand CLA a 407

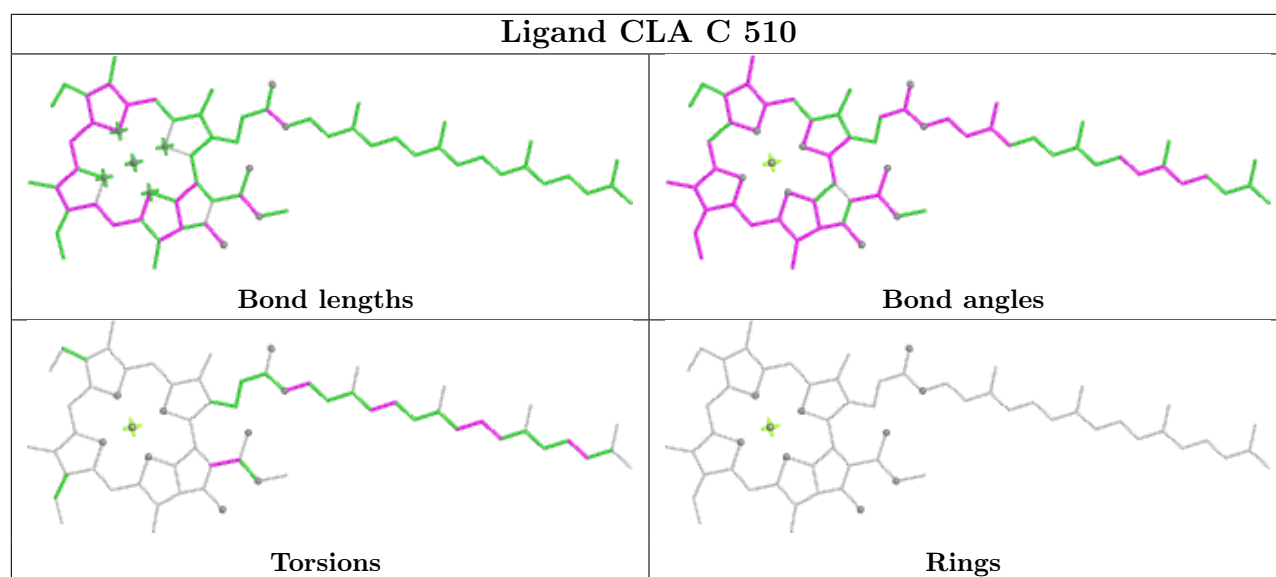
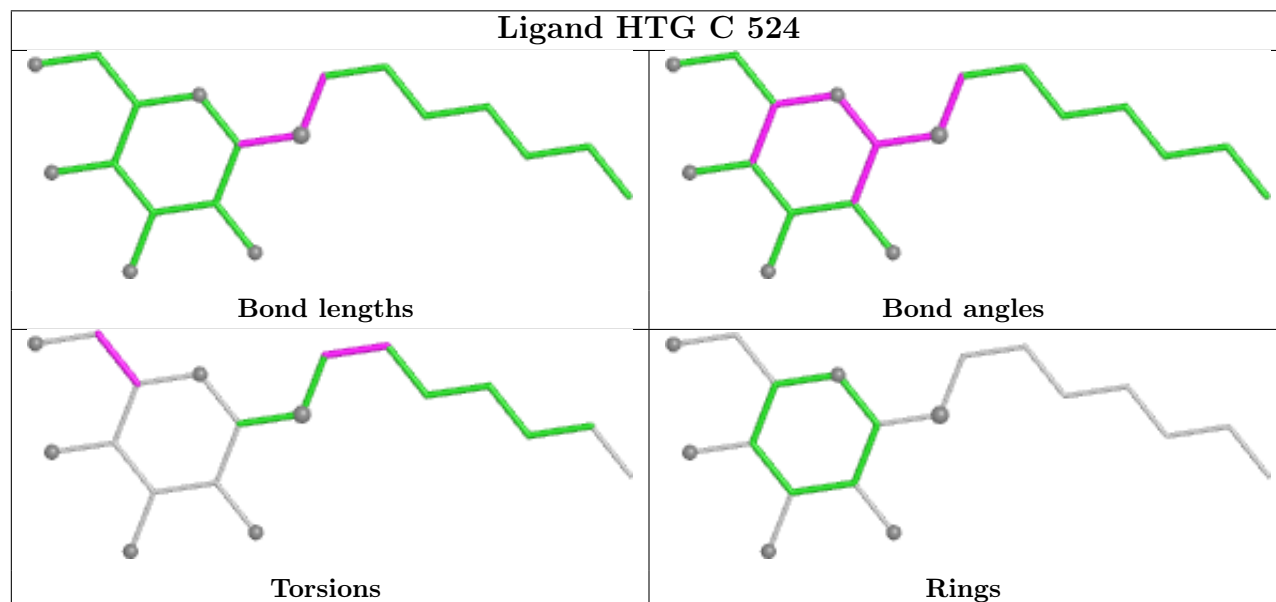
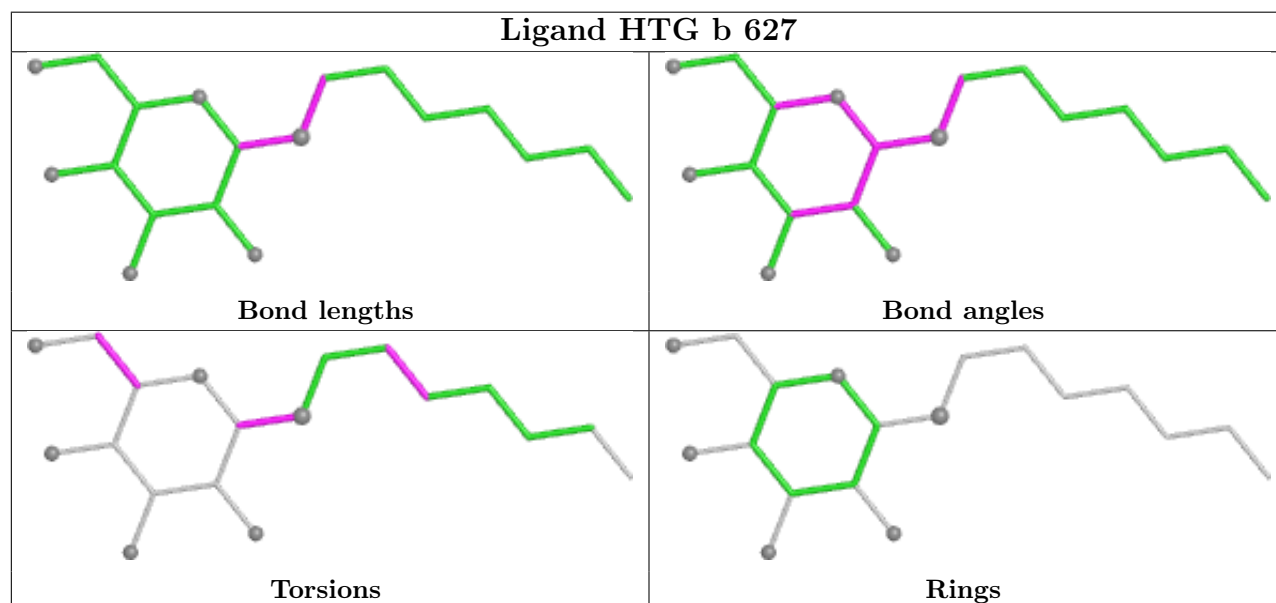


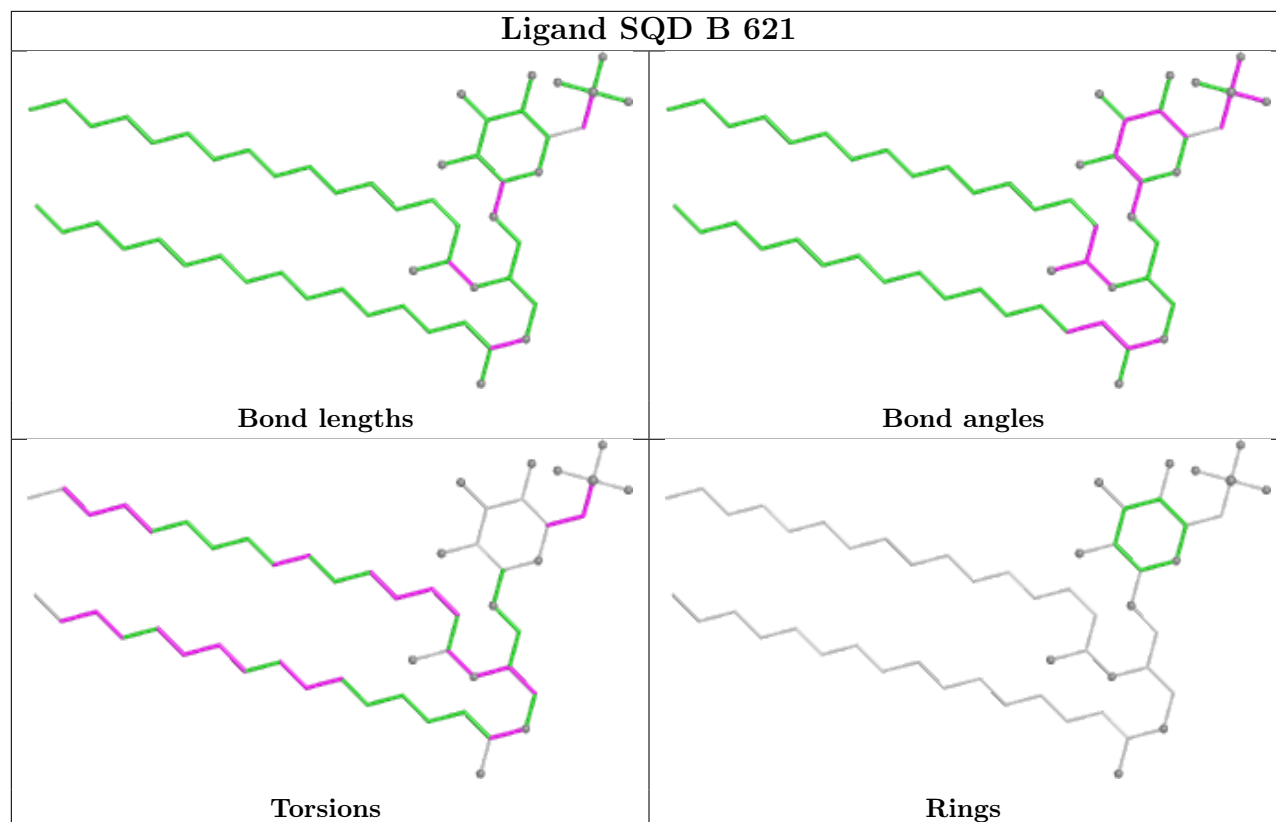
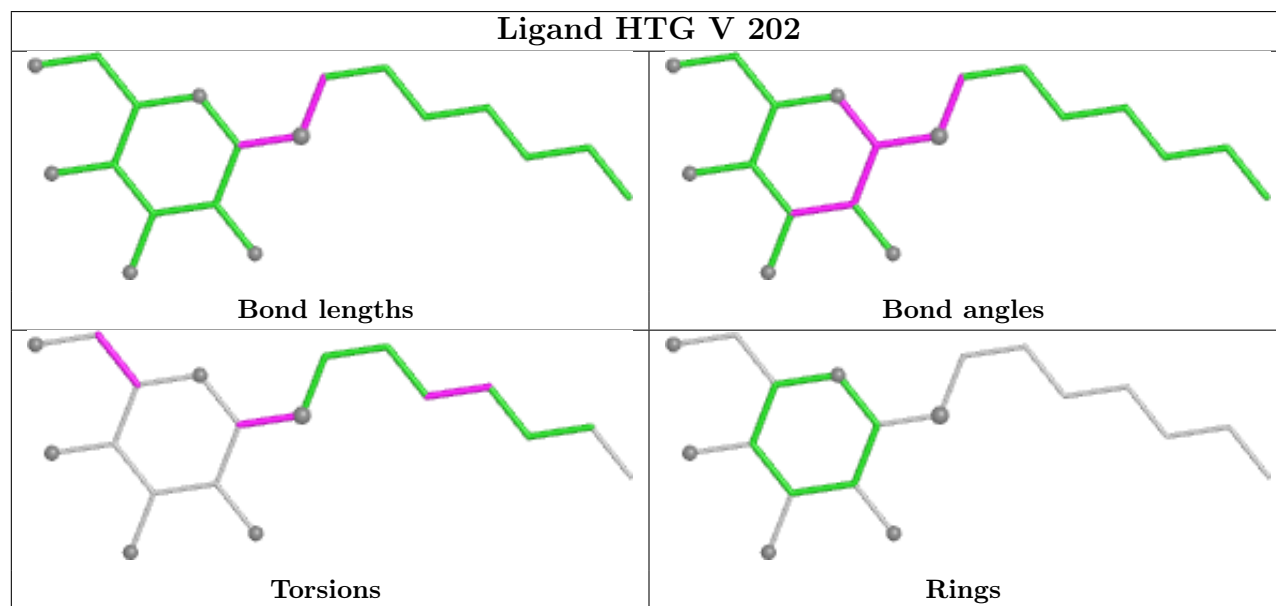
Ligand PHO A 408

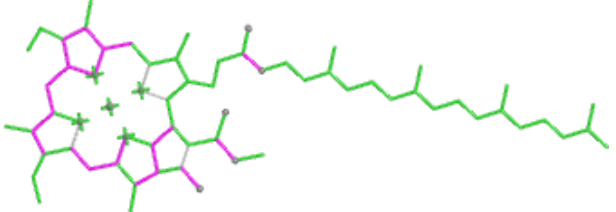
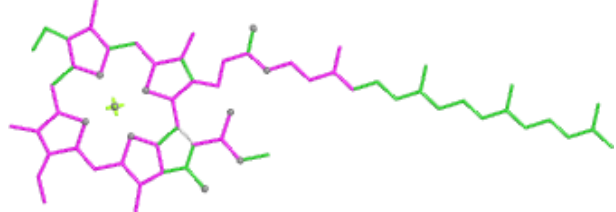
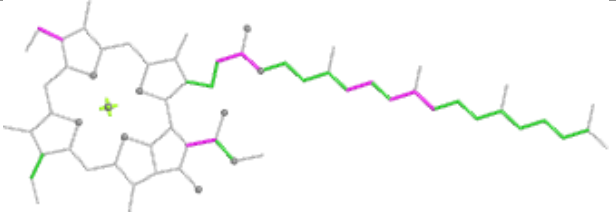
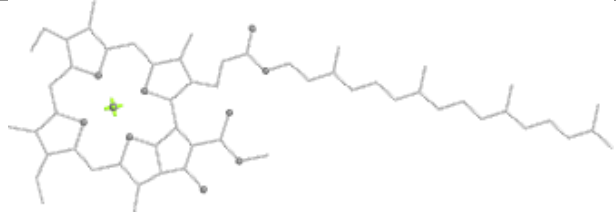
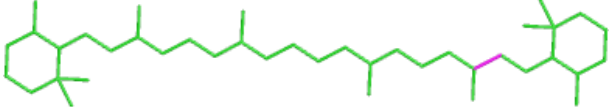
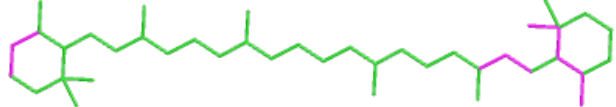
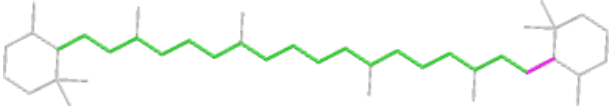
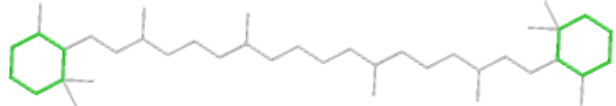
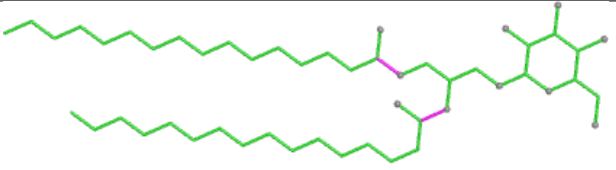
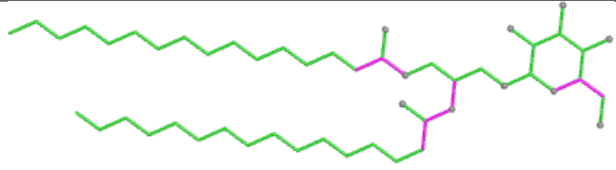
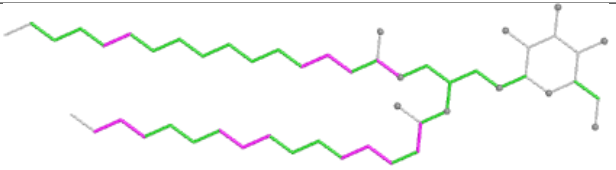
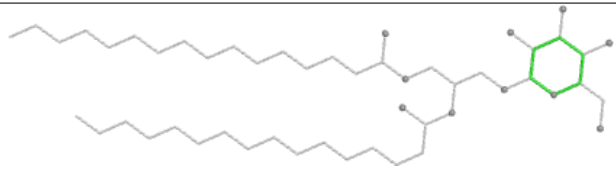


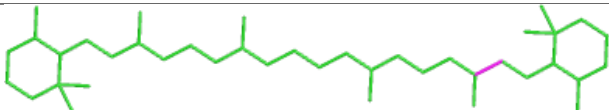
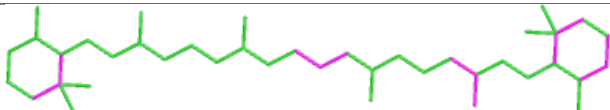
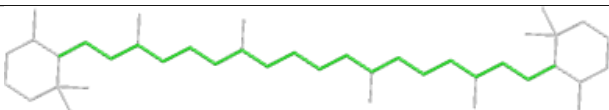
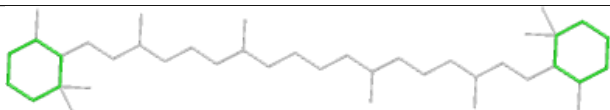
Ligand CLA c 908

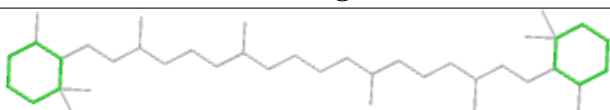


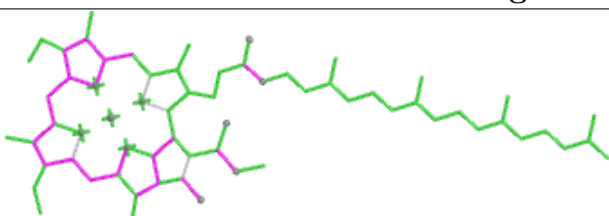
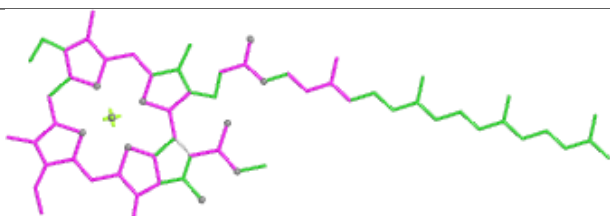
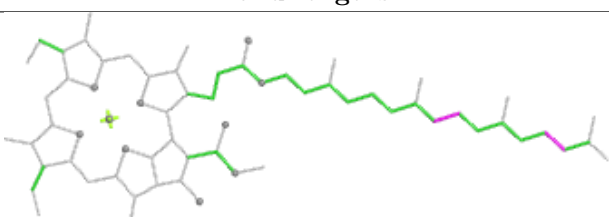
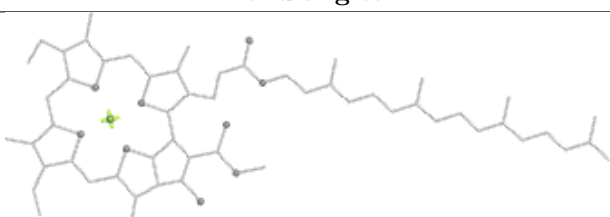


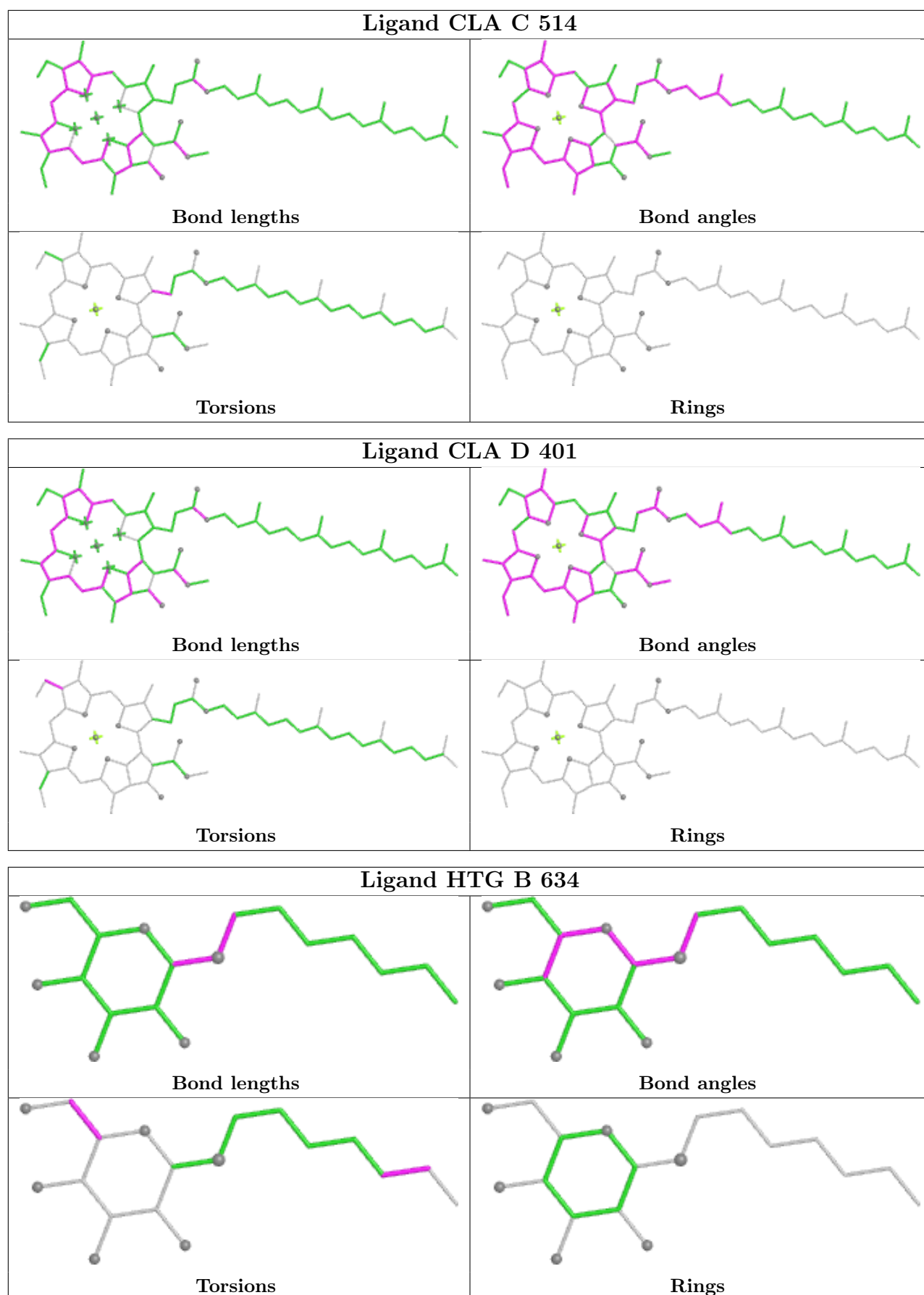


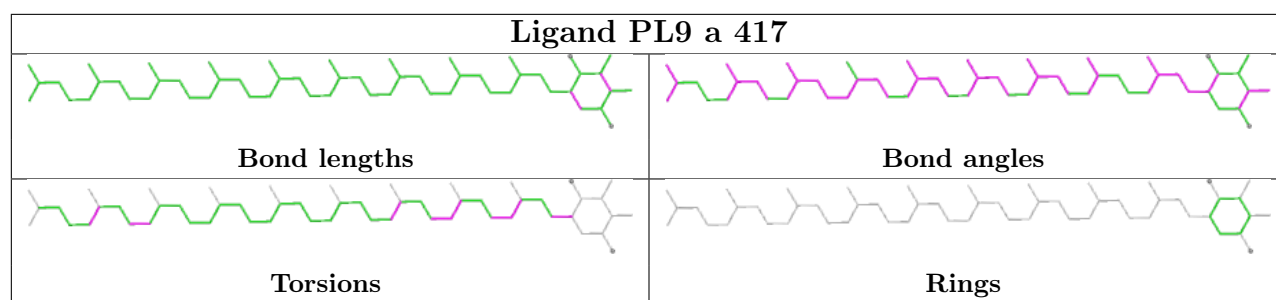
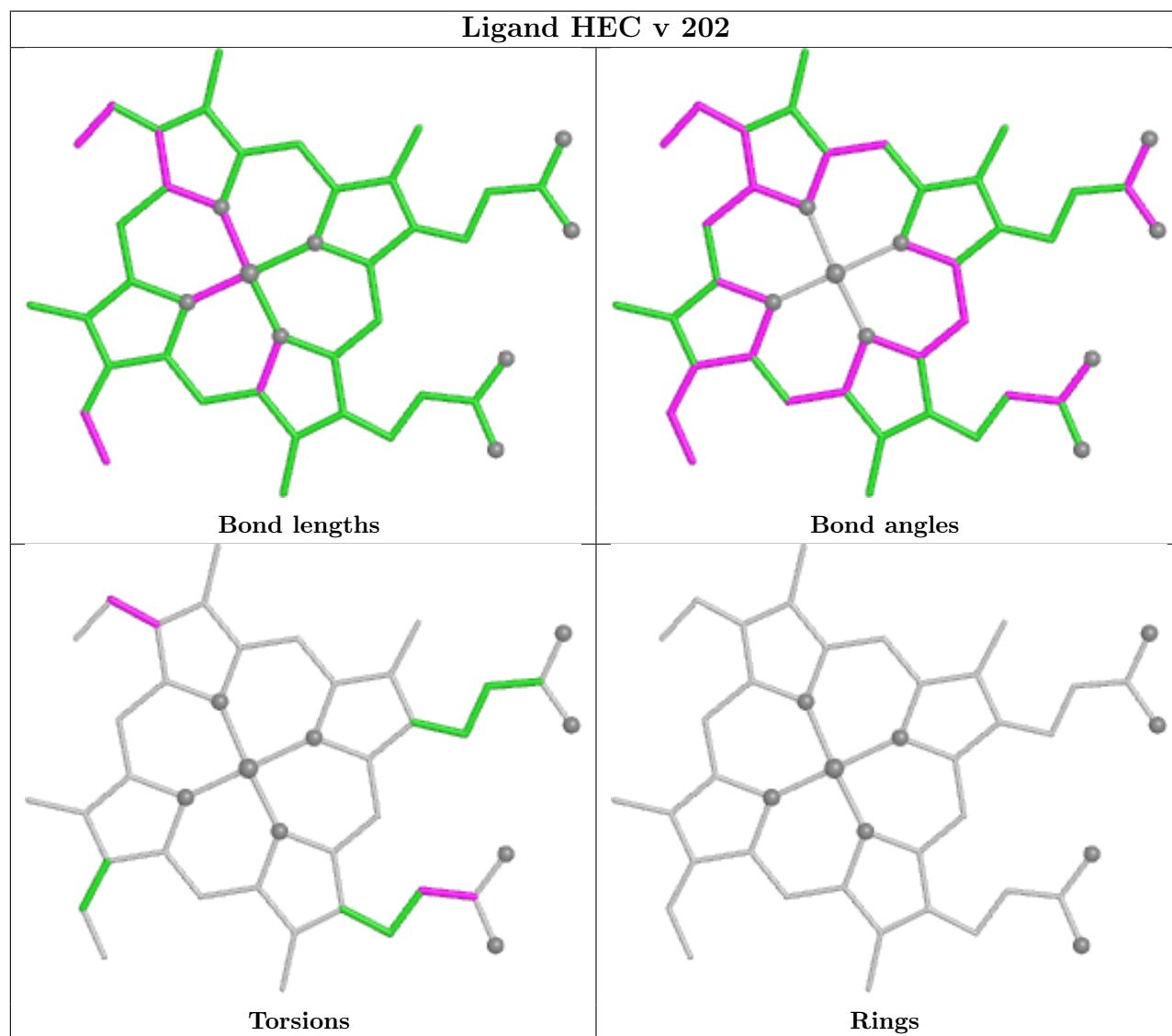
Ligand CLA C 513	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG C 520	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

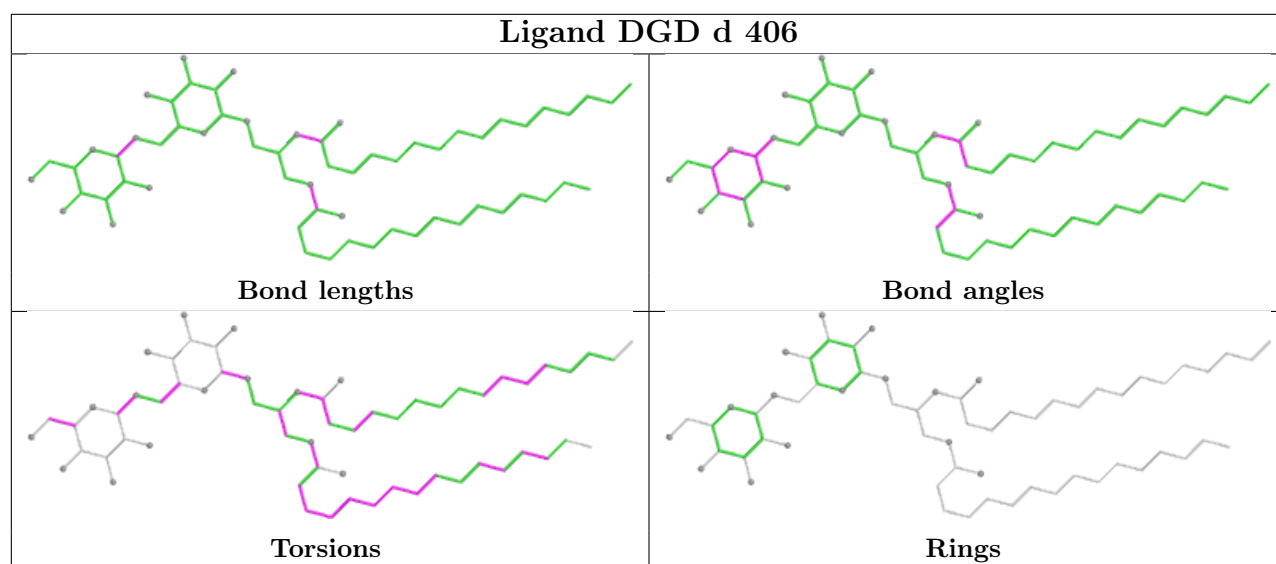
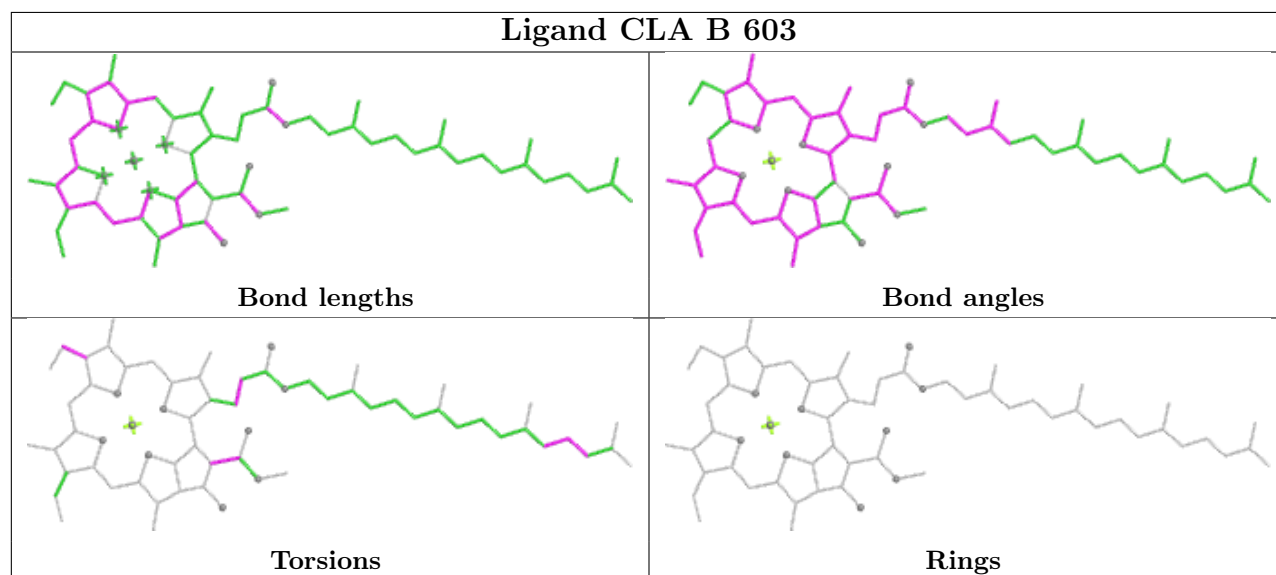
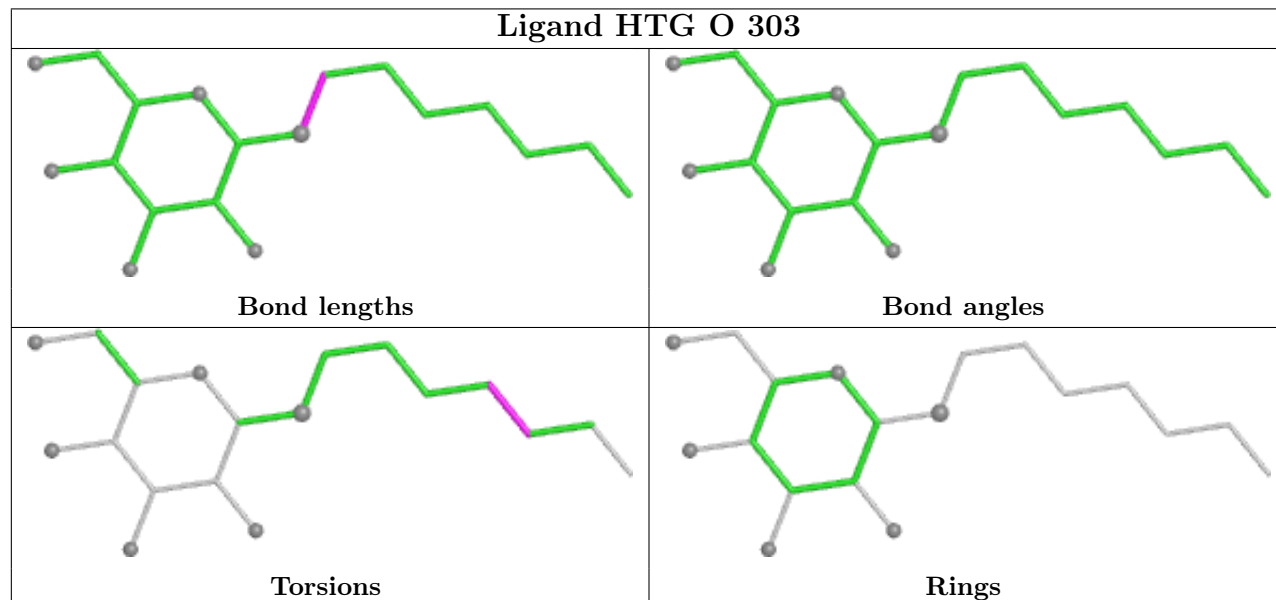
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

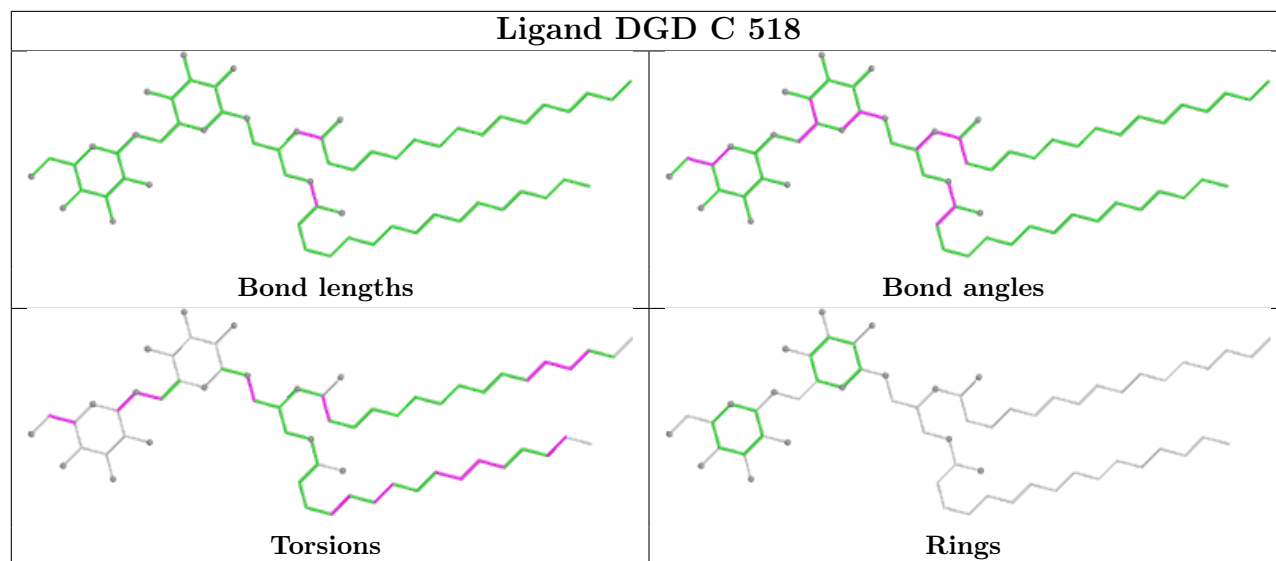
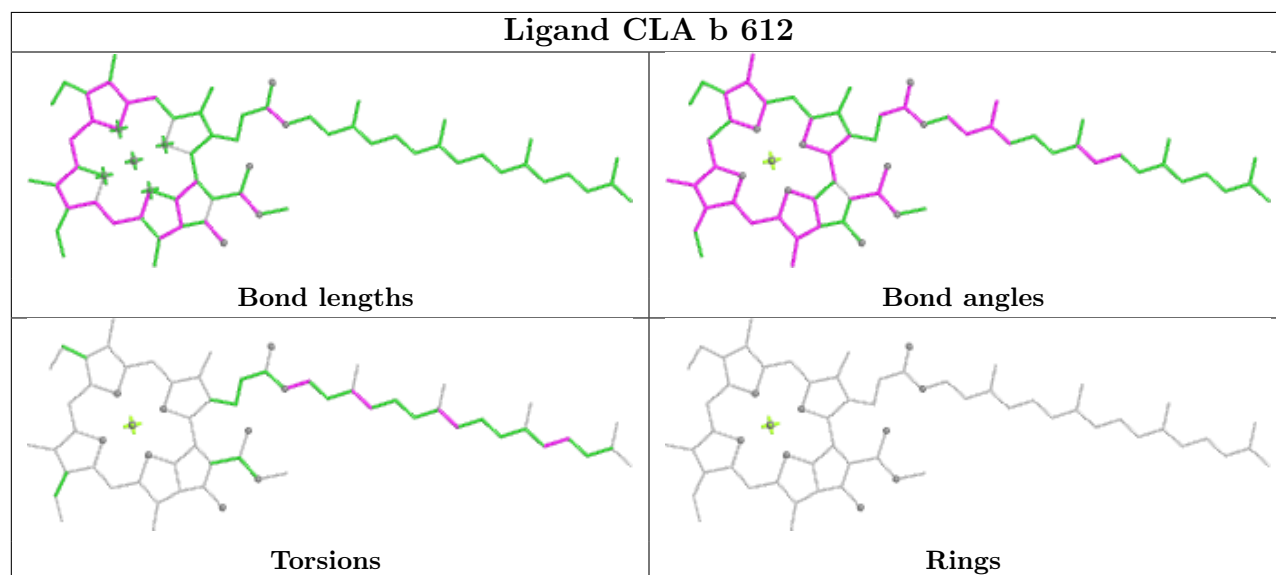
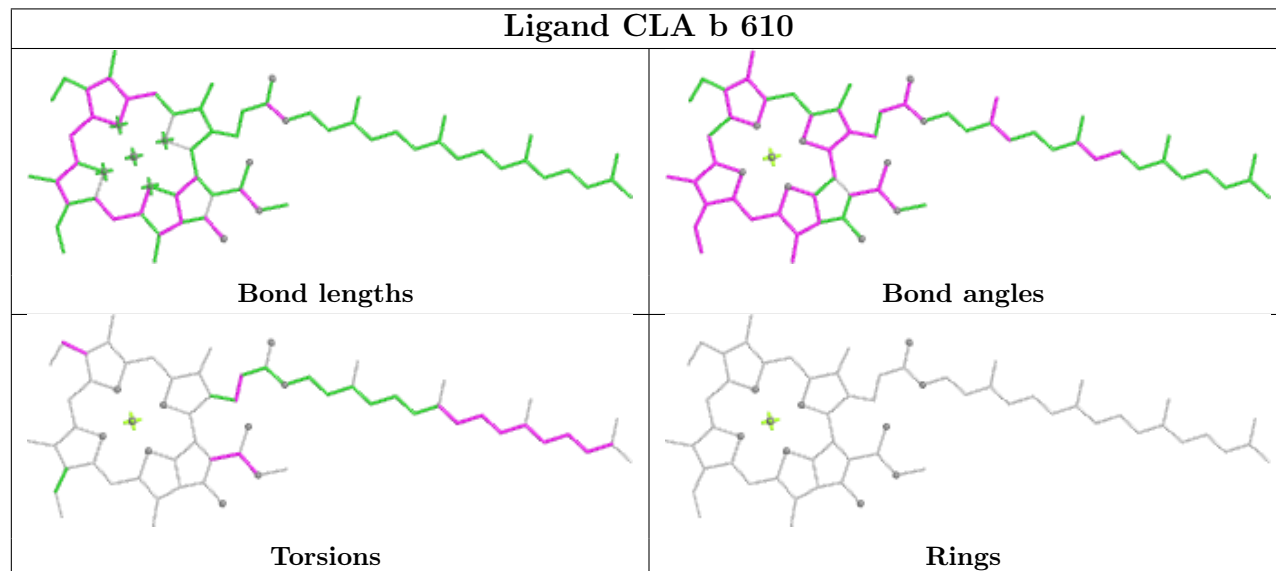
Ligand BCR D 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

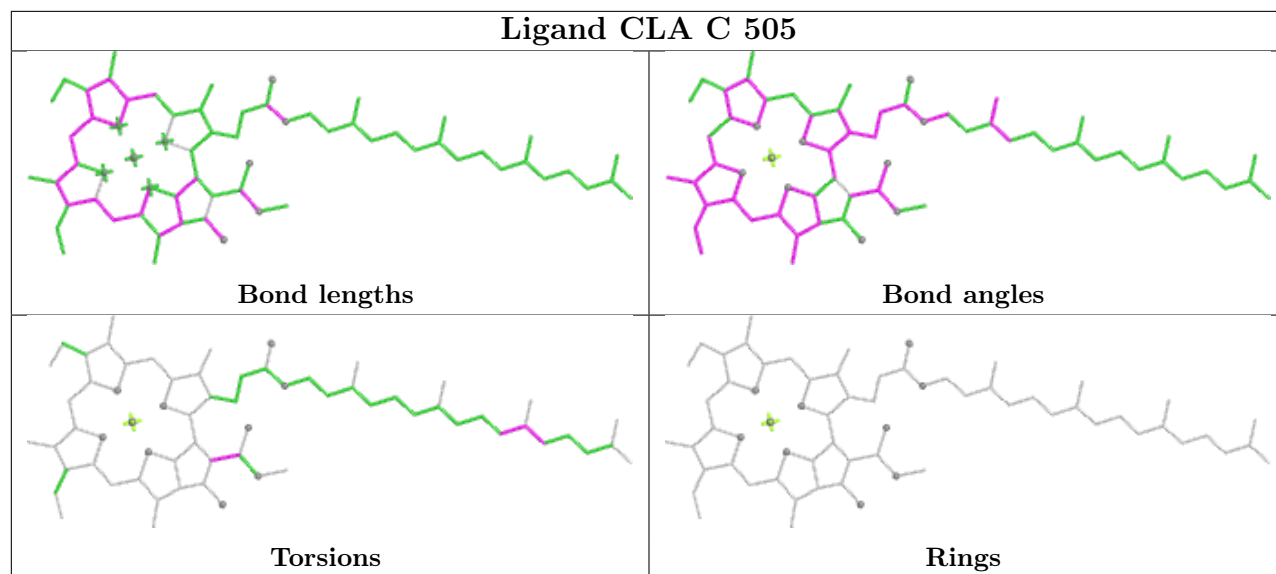
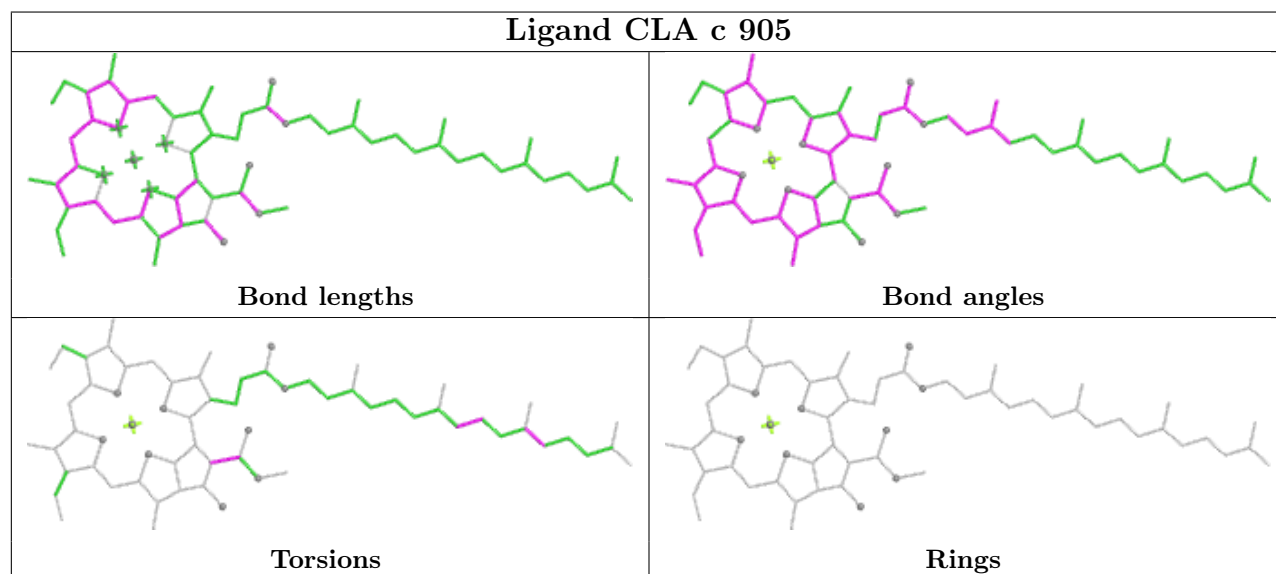
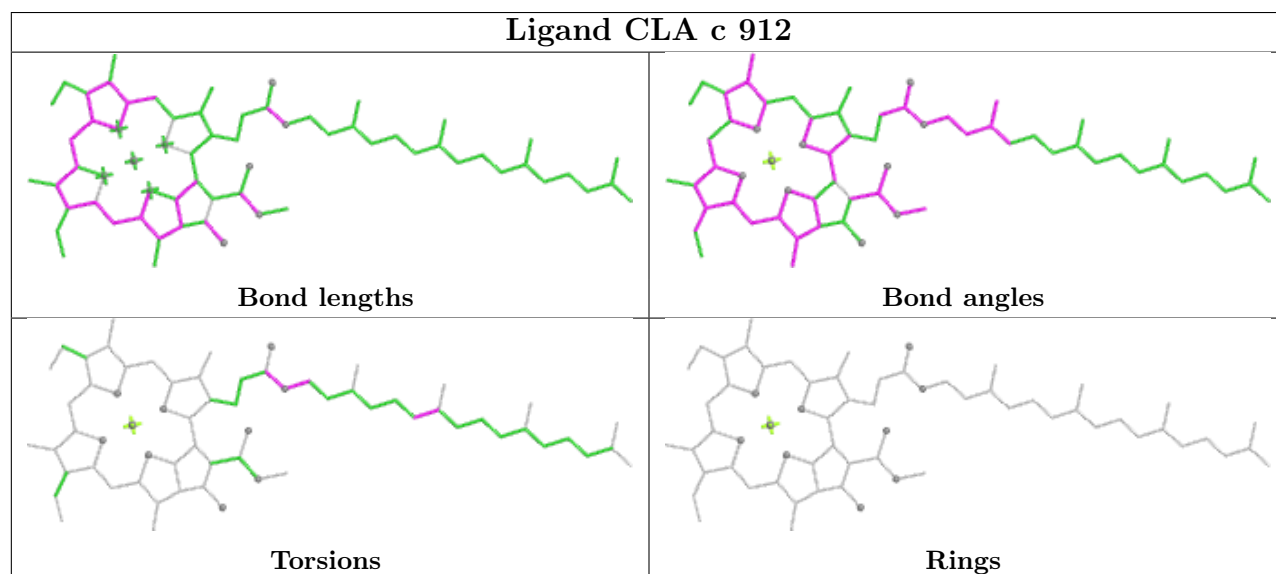
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings



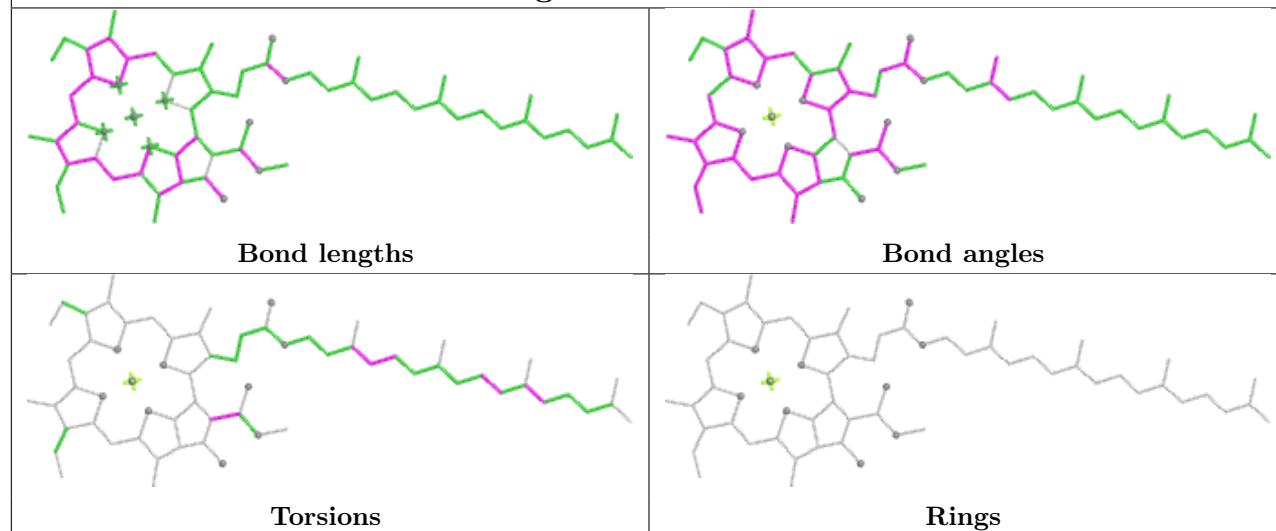




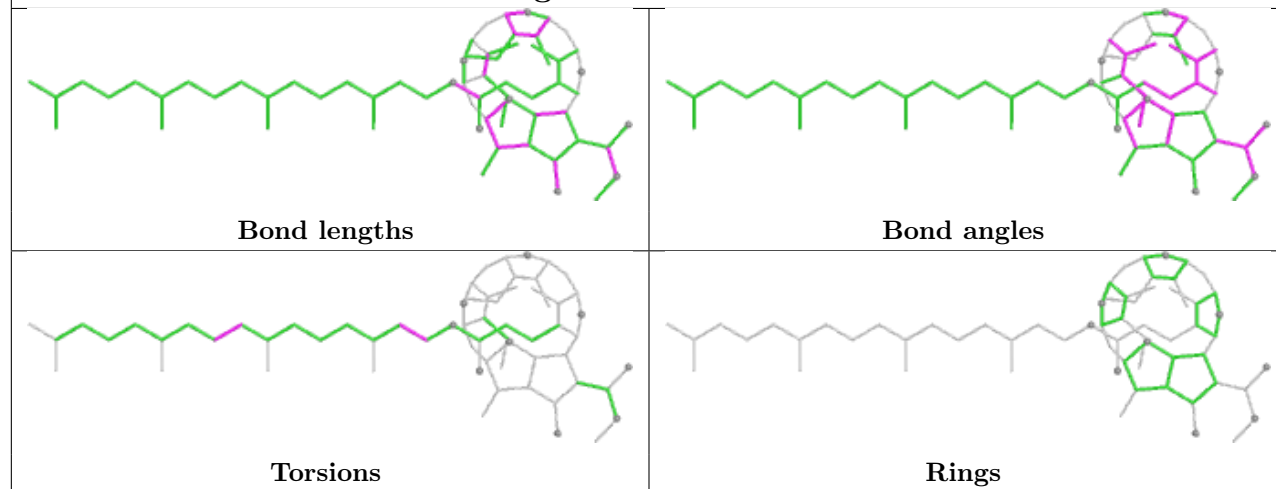




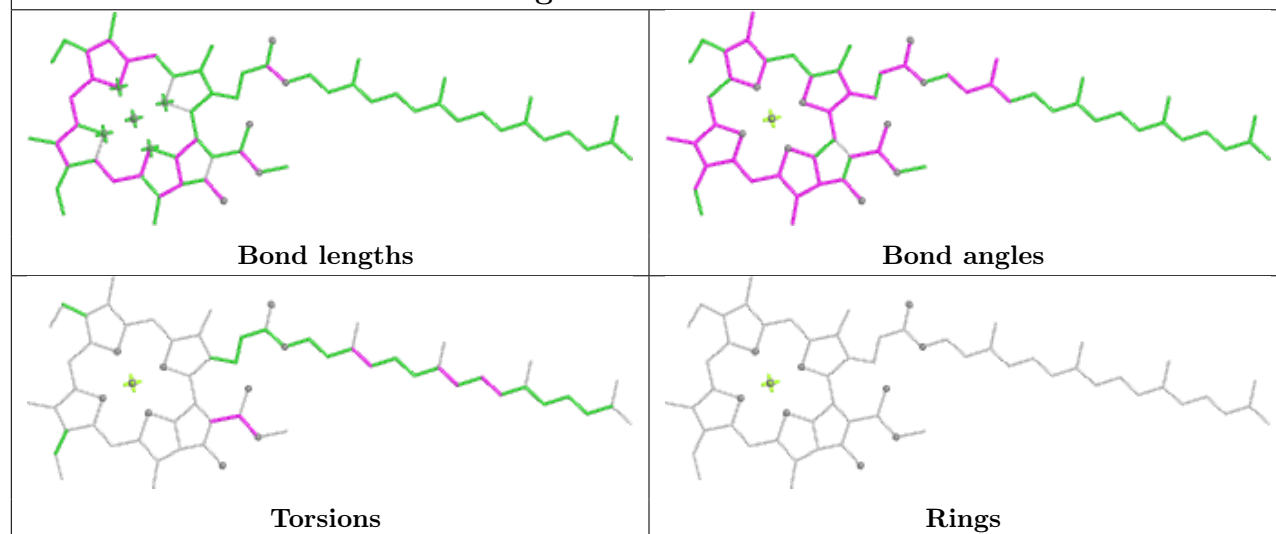
Ligand CLA d 403

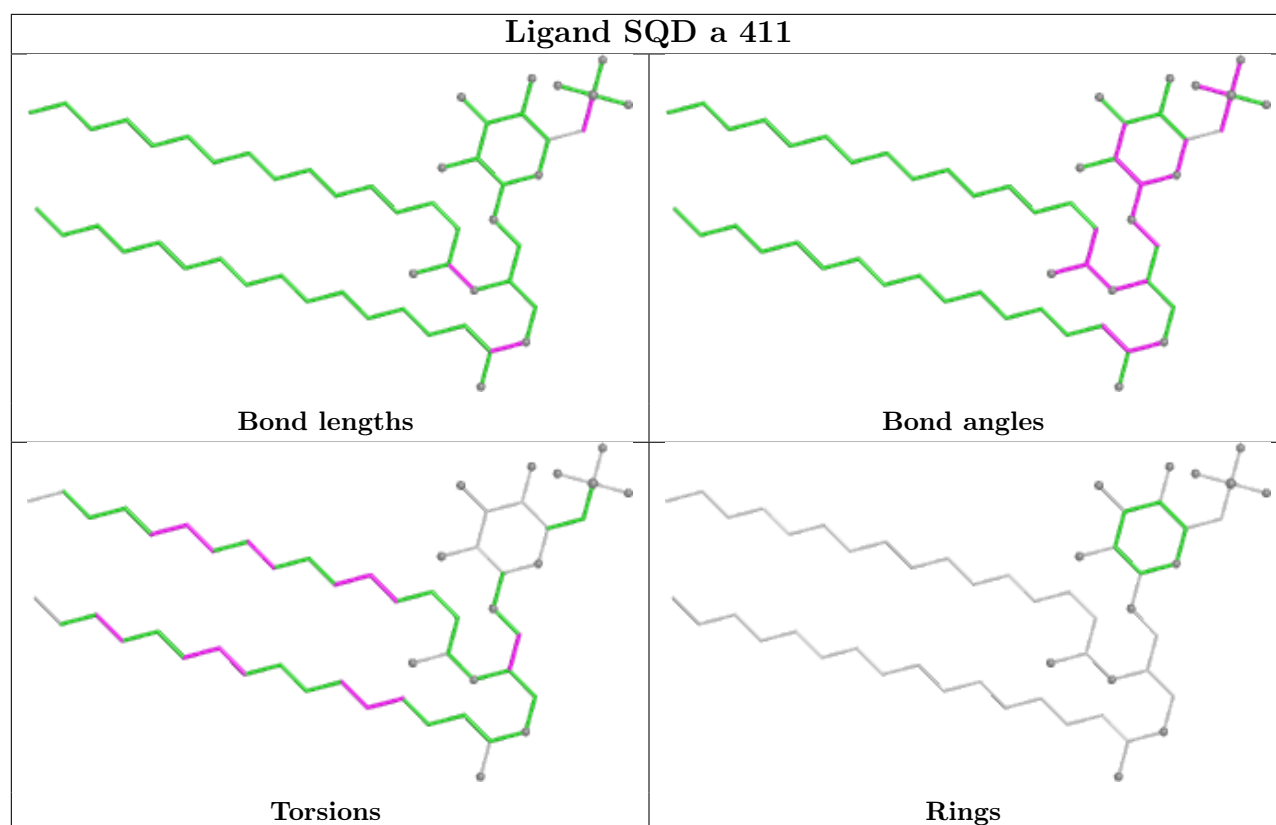
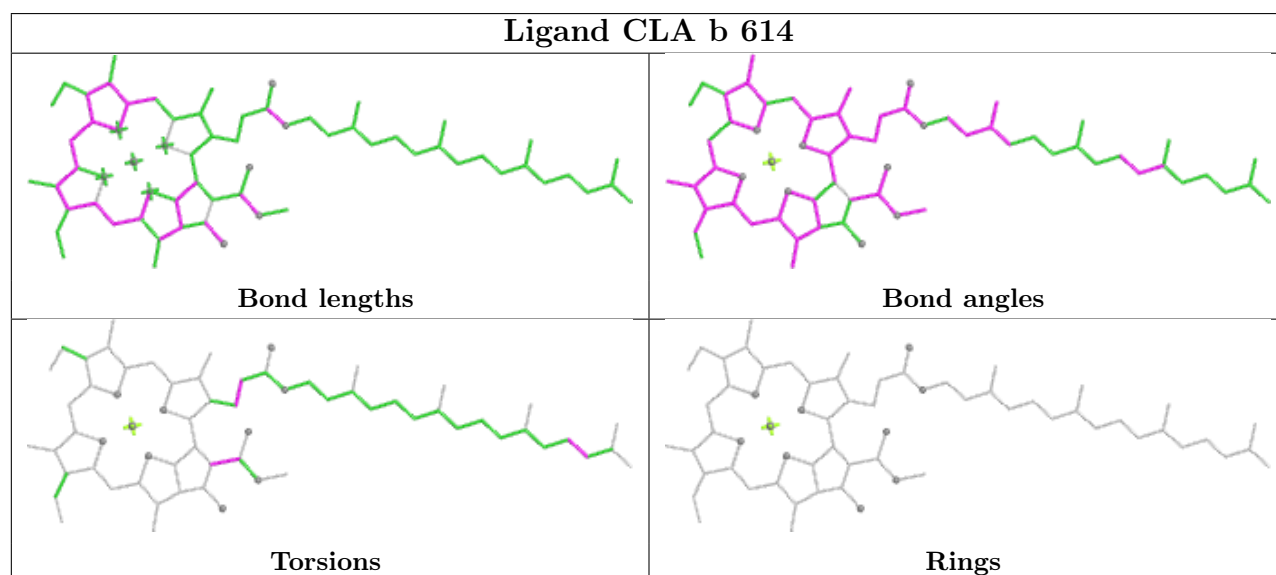
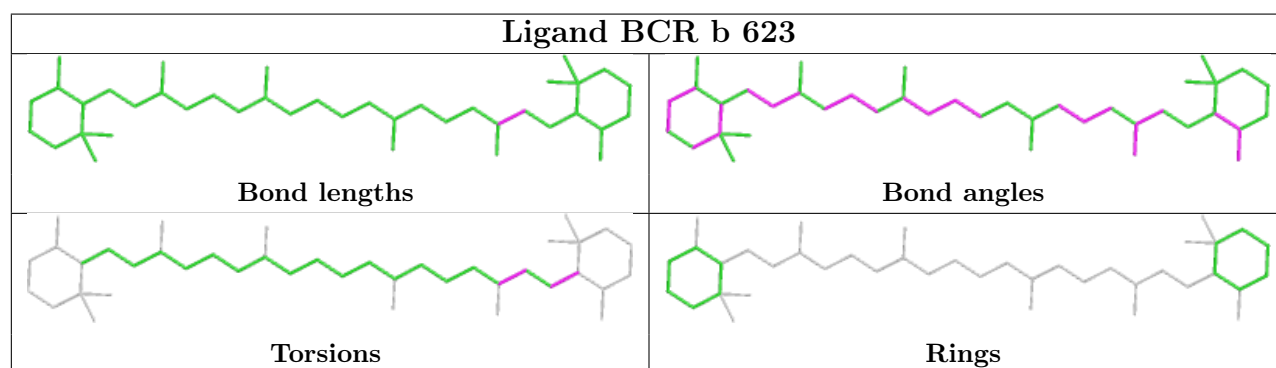


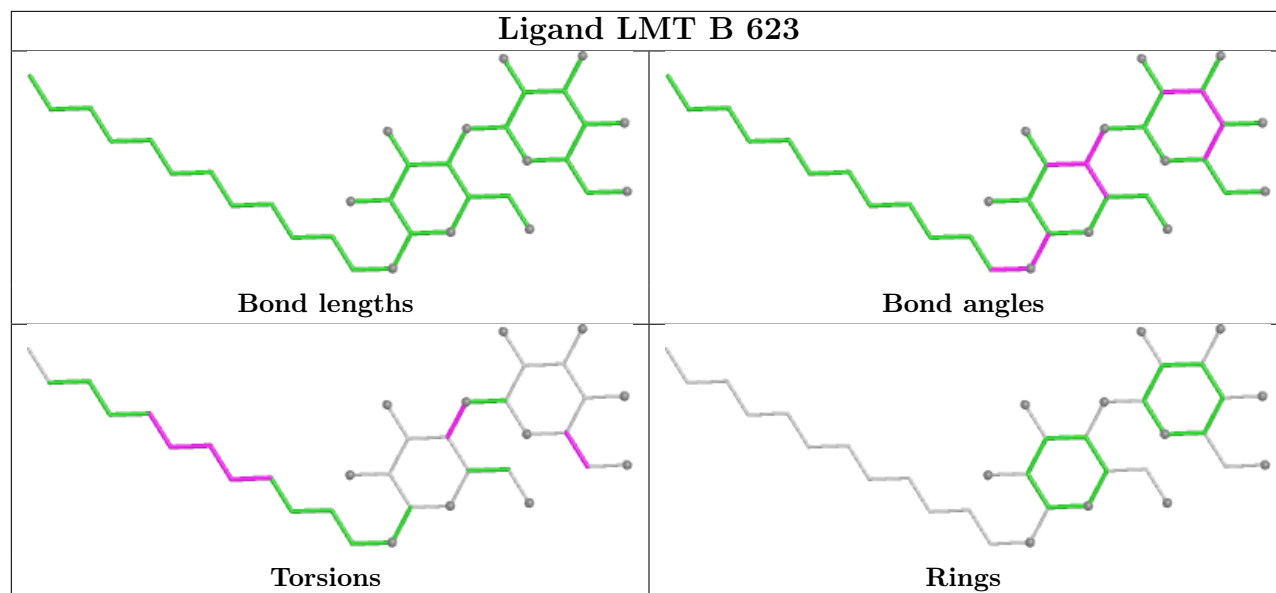
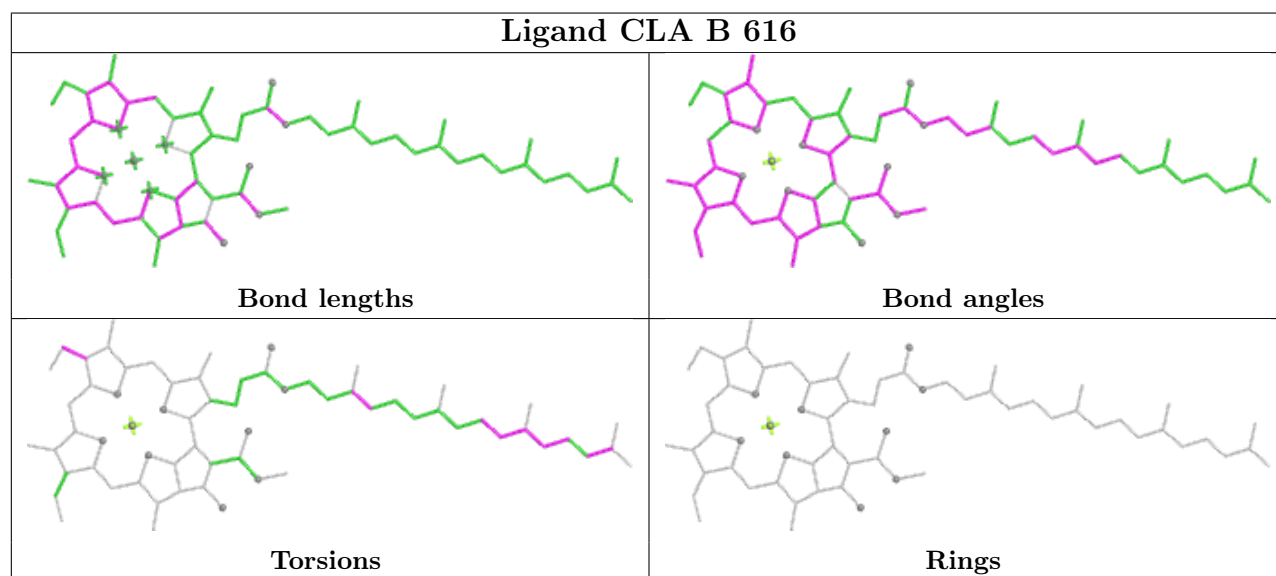
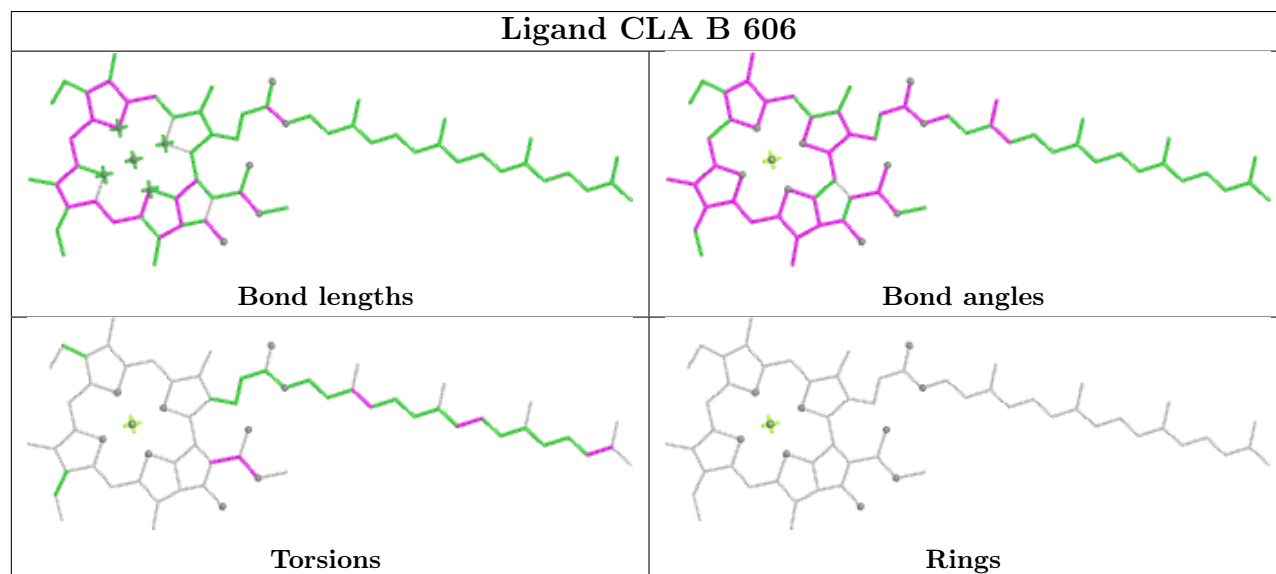
Ligand PHO a 408

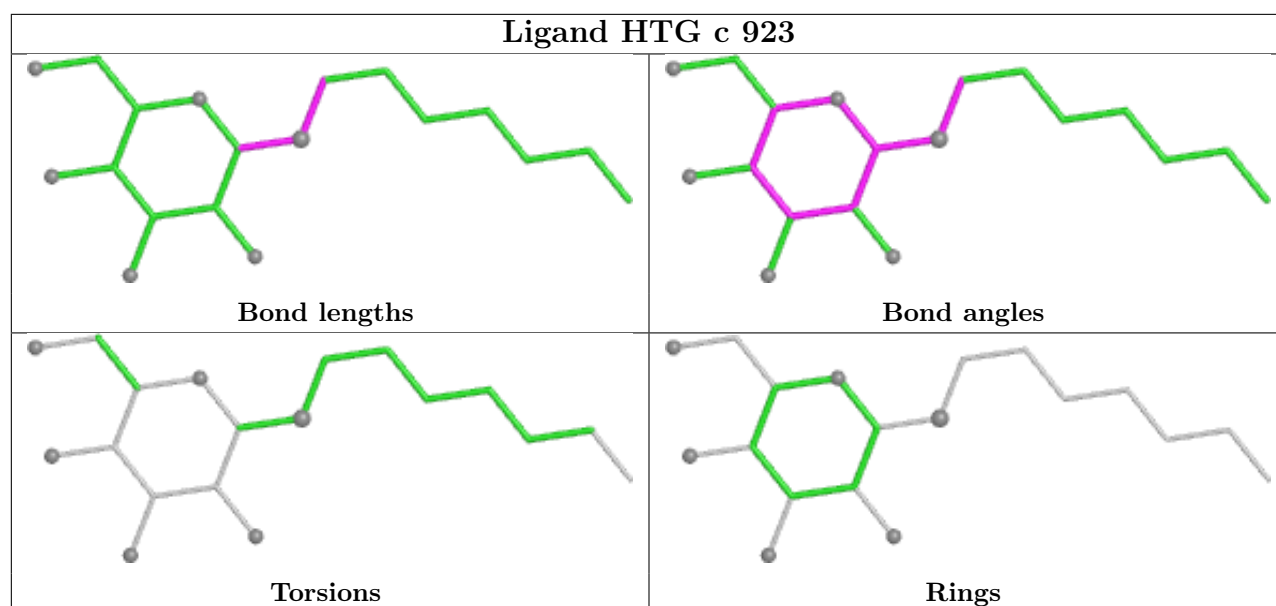
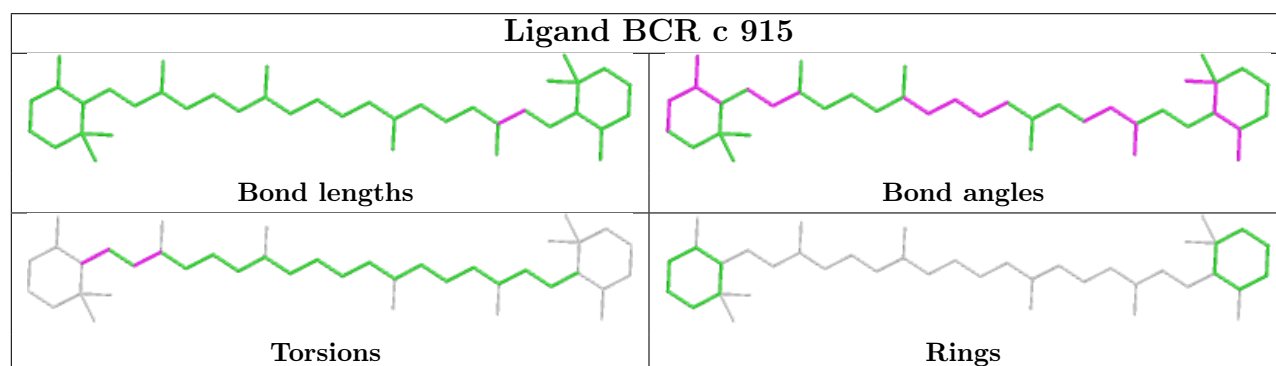
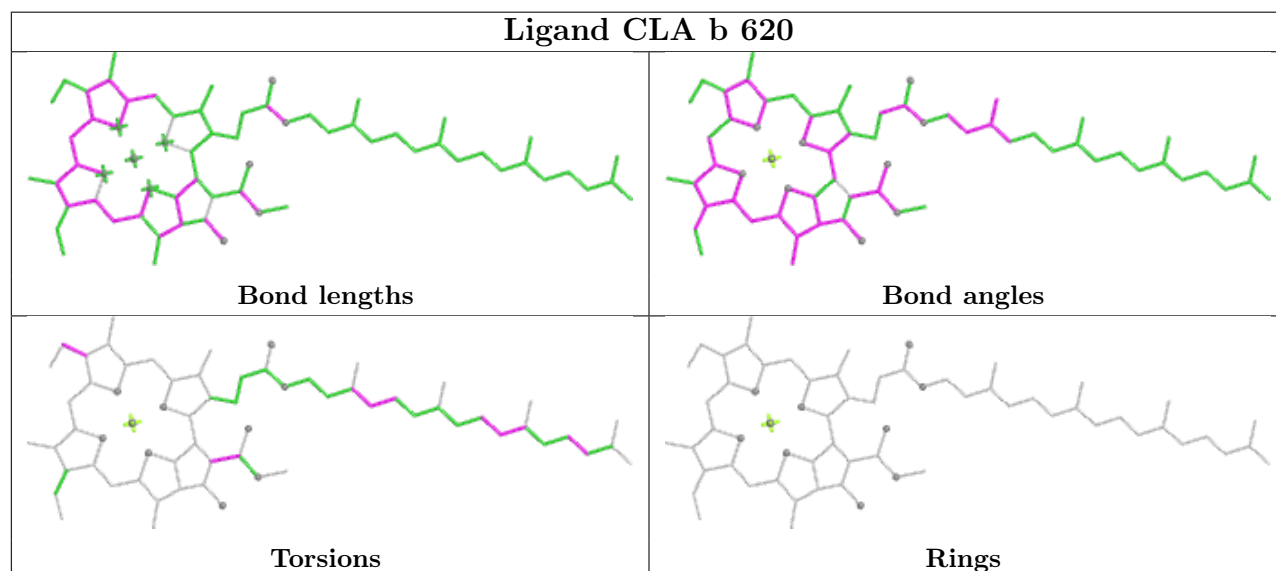


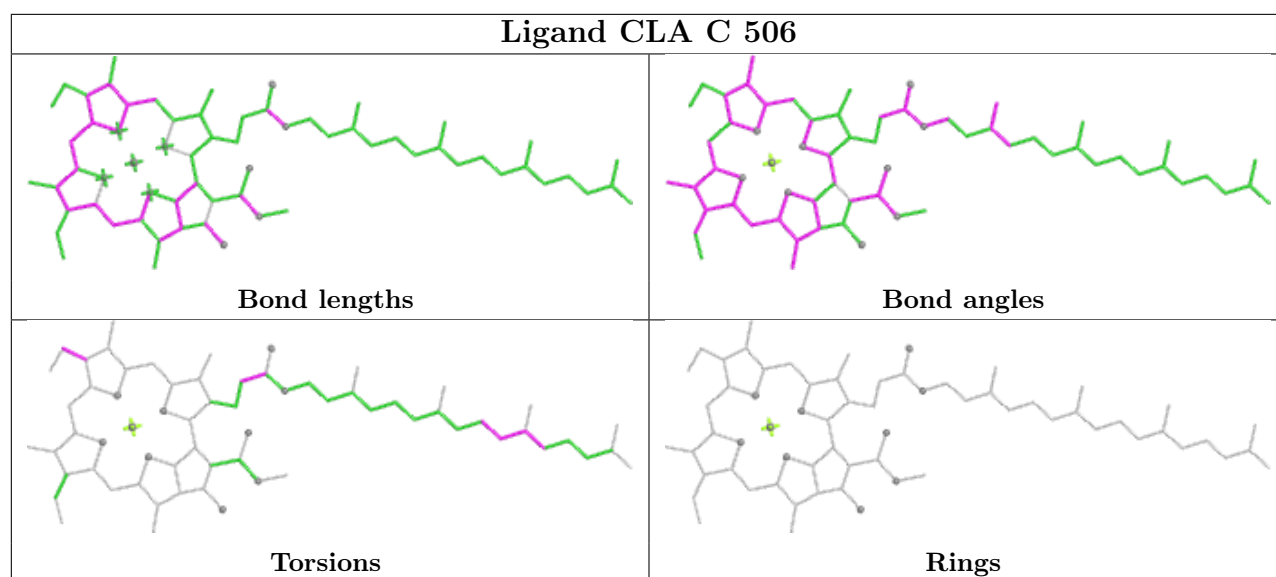
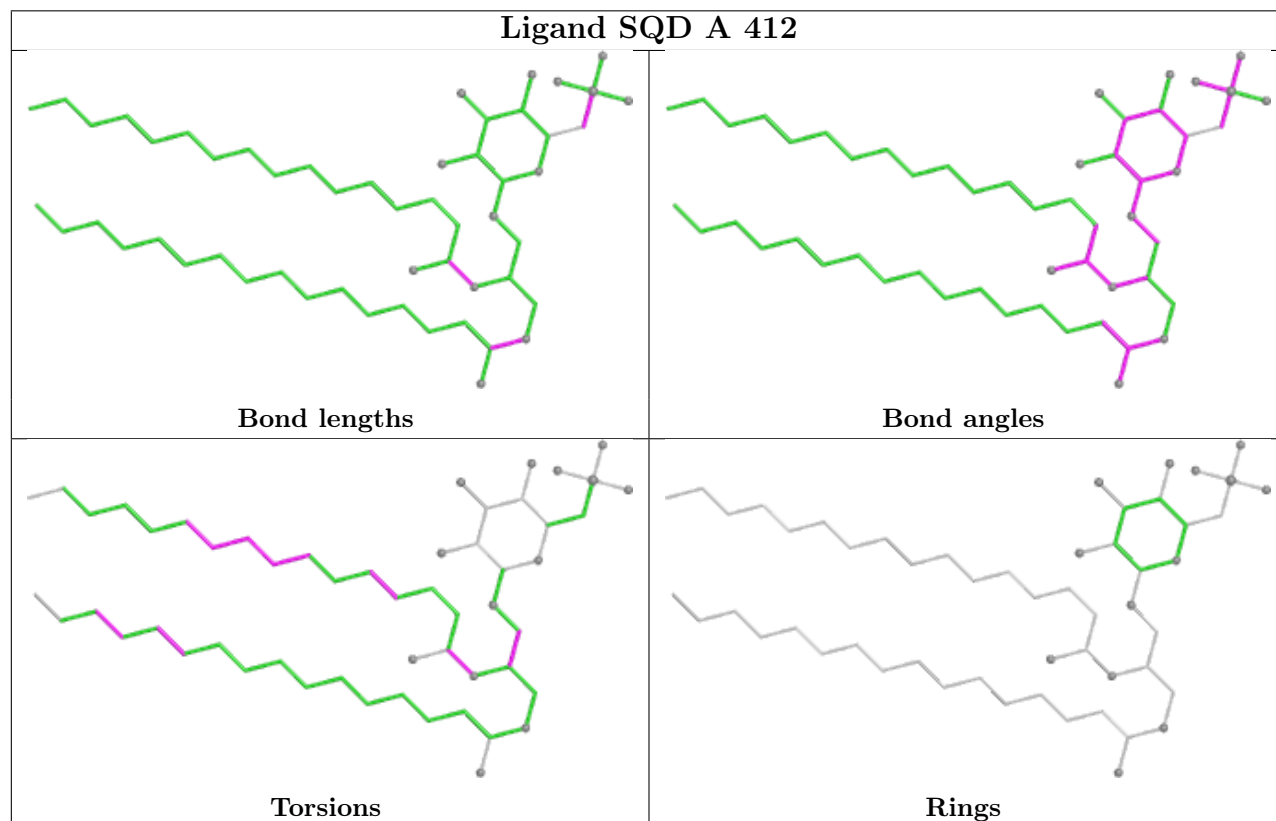
Ligand CLA b 609

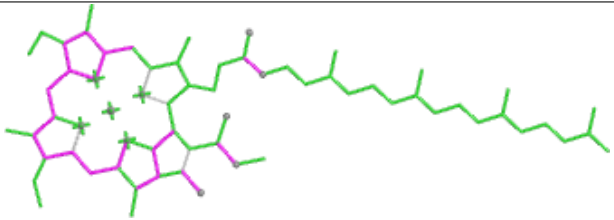
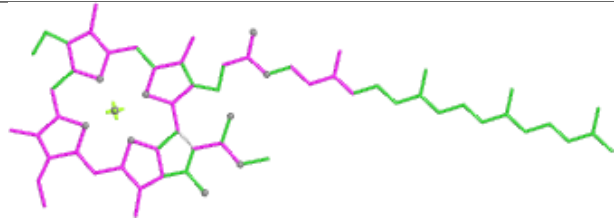
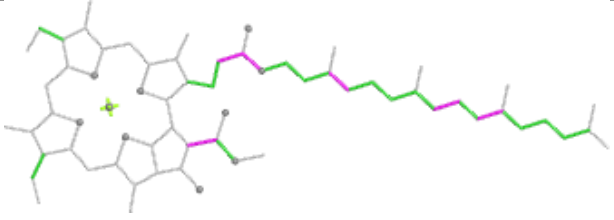
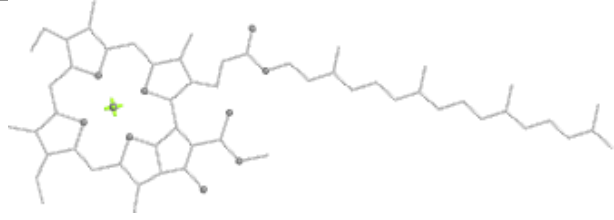


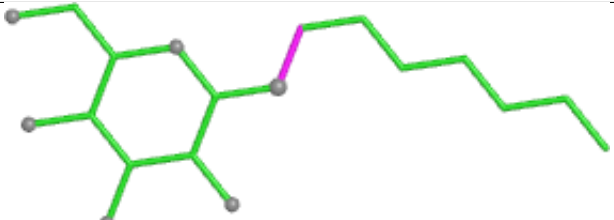
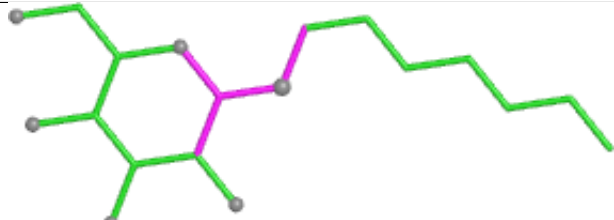
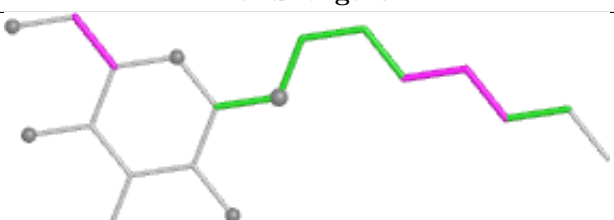
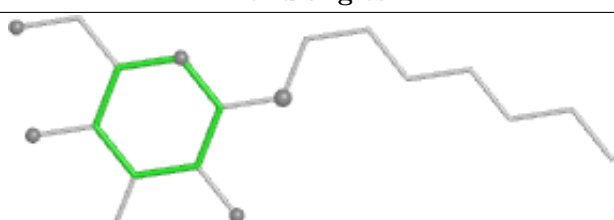


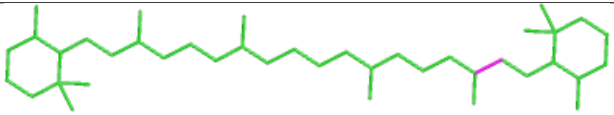
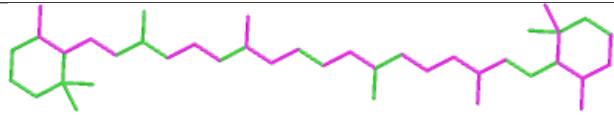
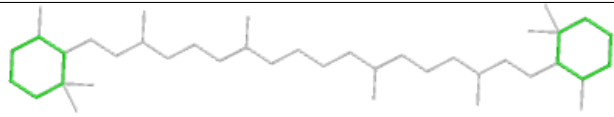


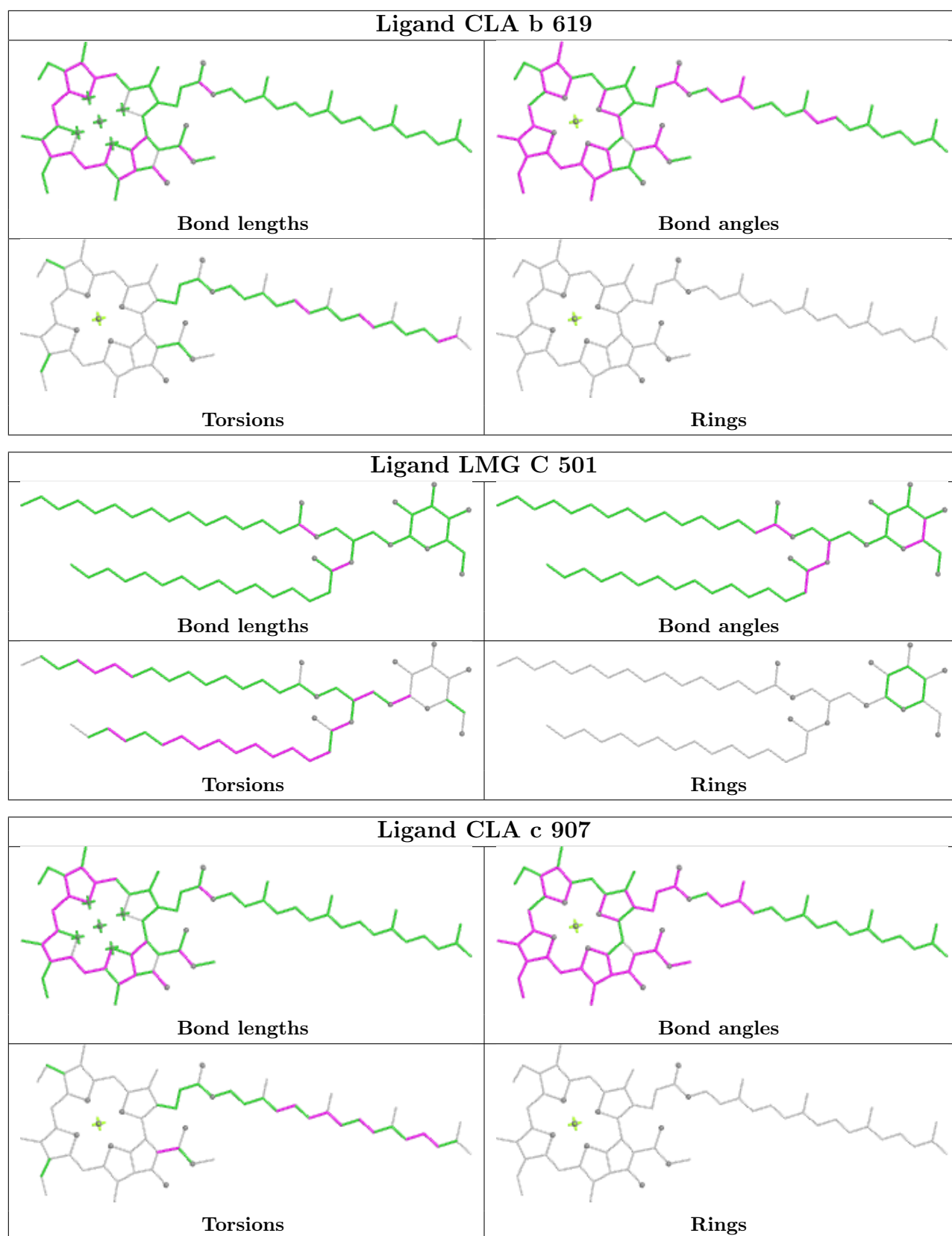


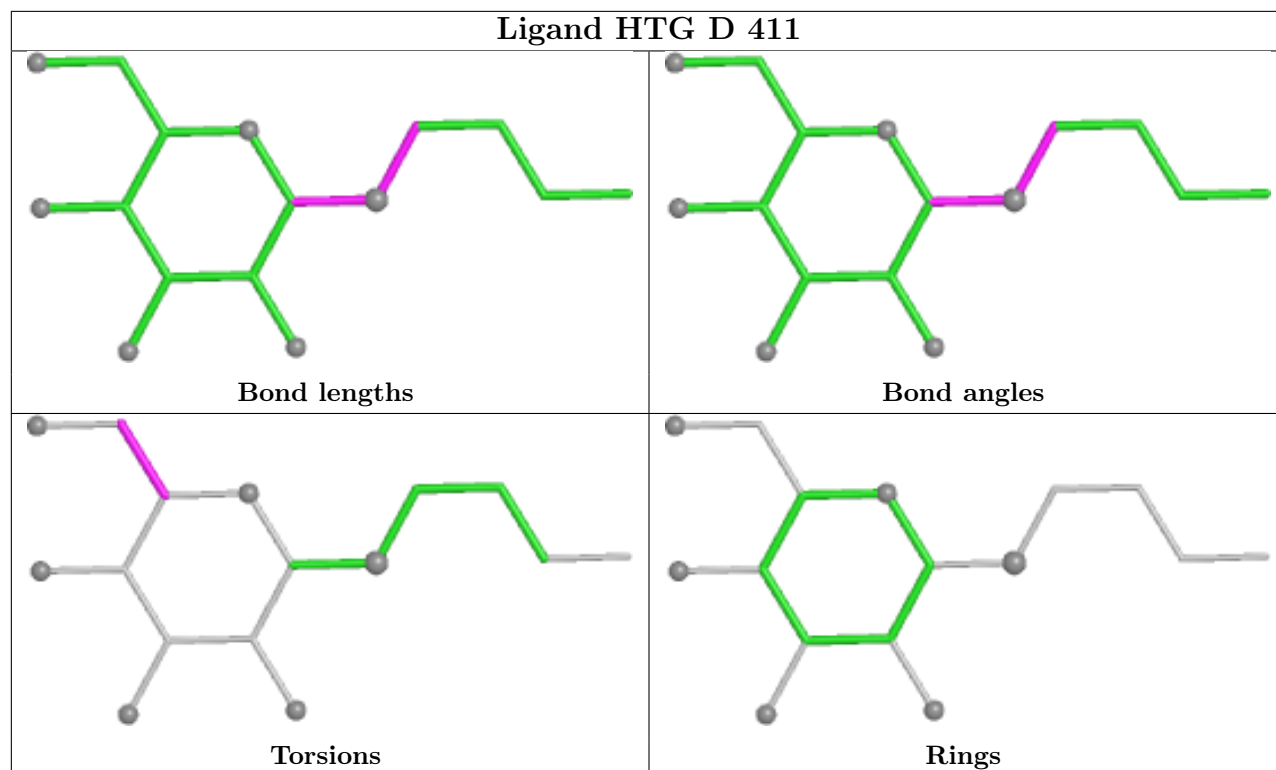
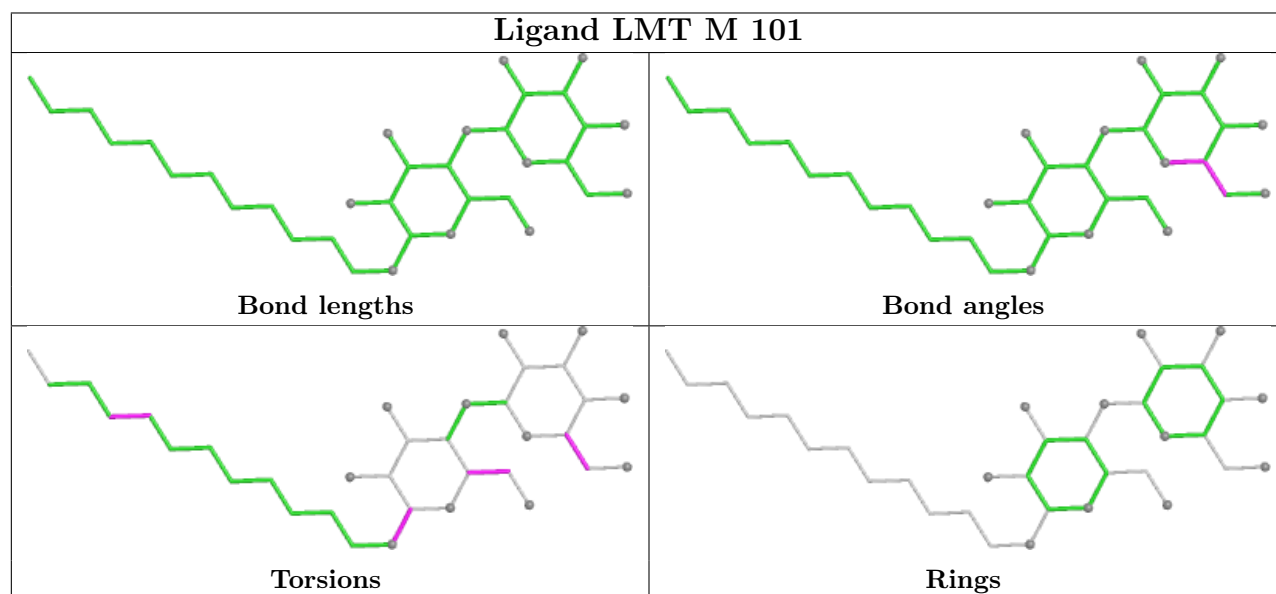


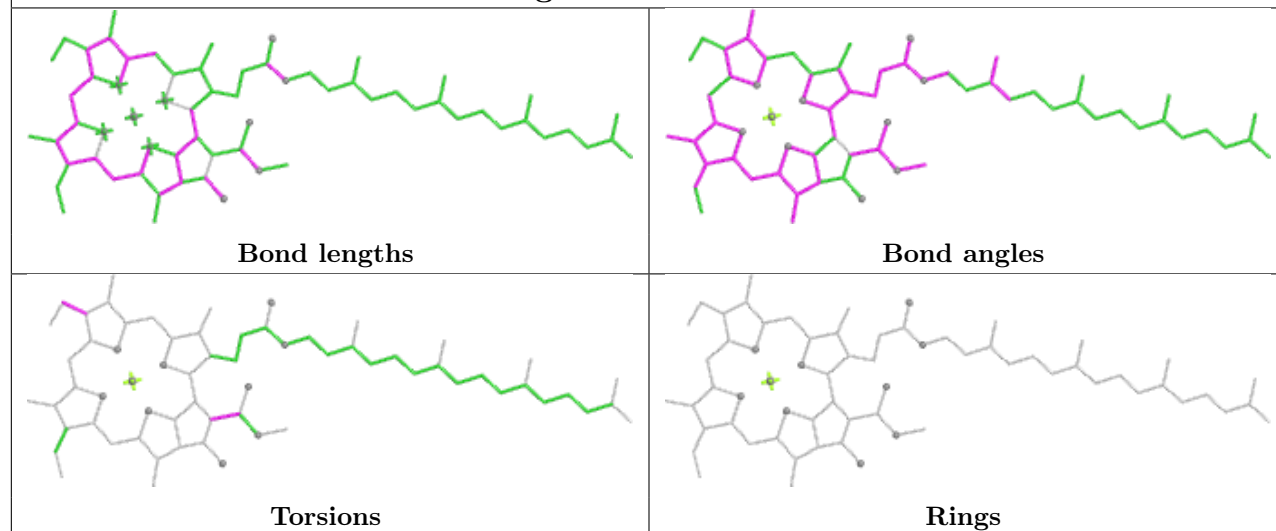
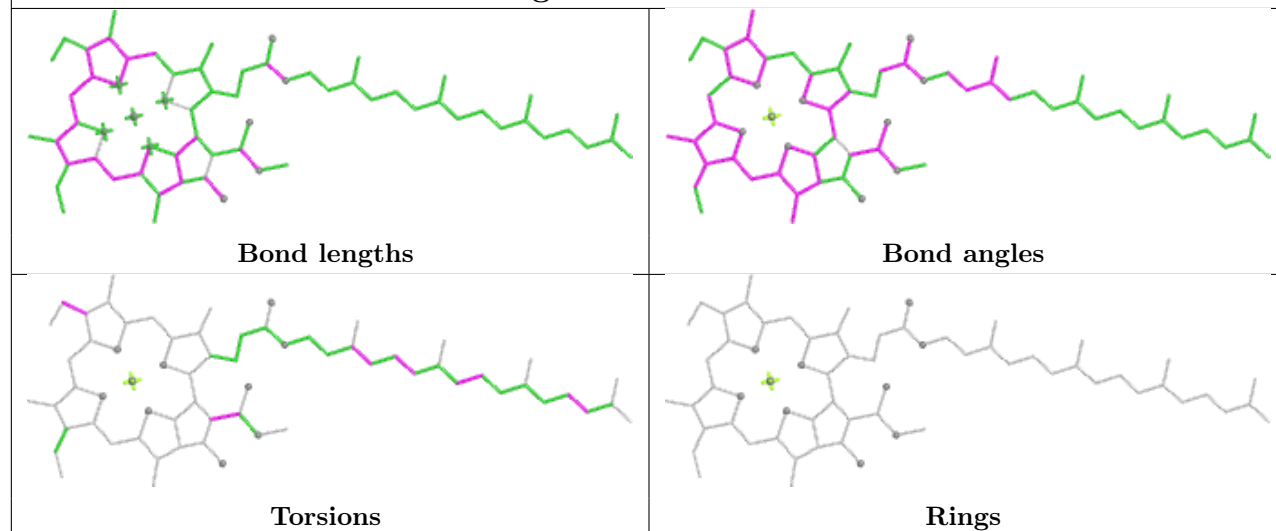
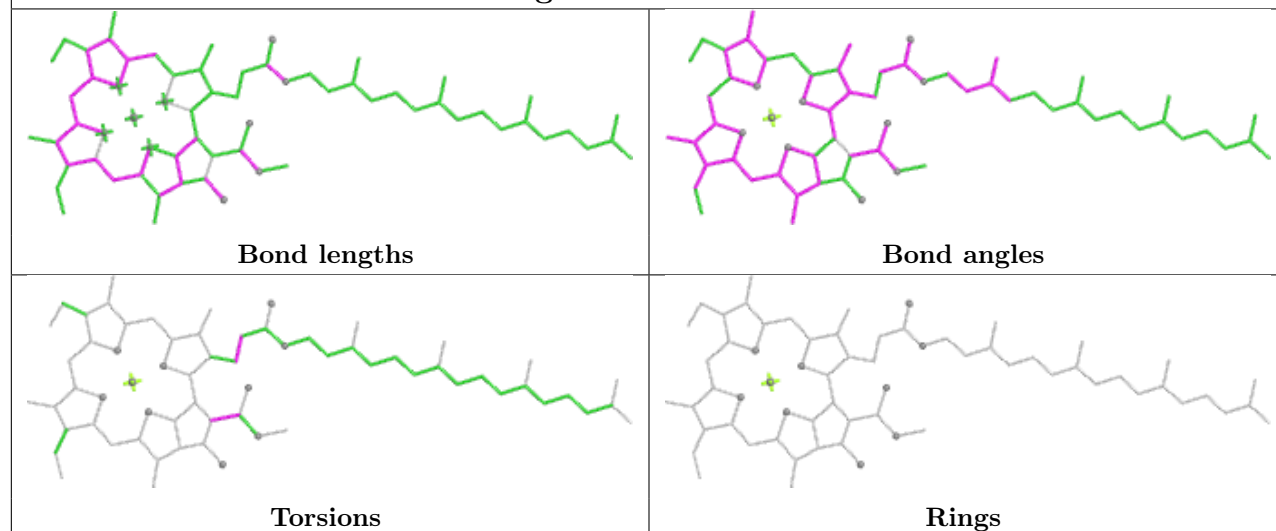
Ligand CLA c 911	
	
Bond lengths	Bond angles
	
Torsions	Rings

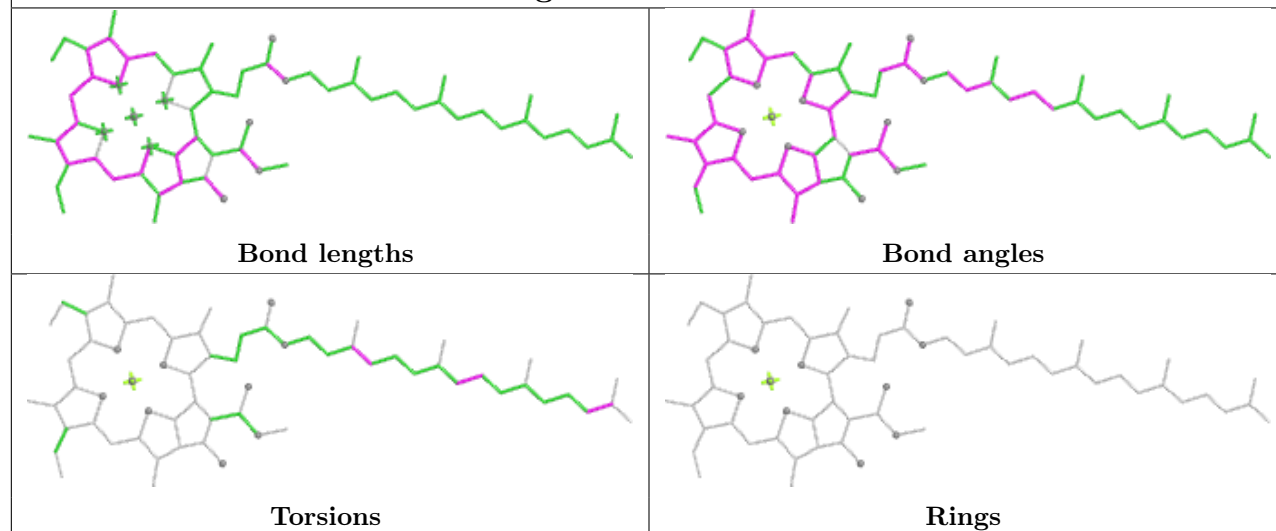
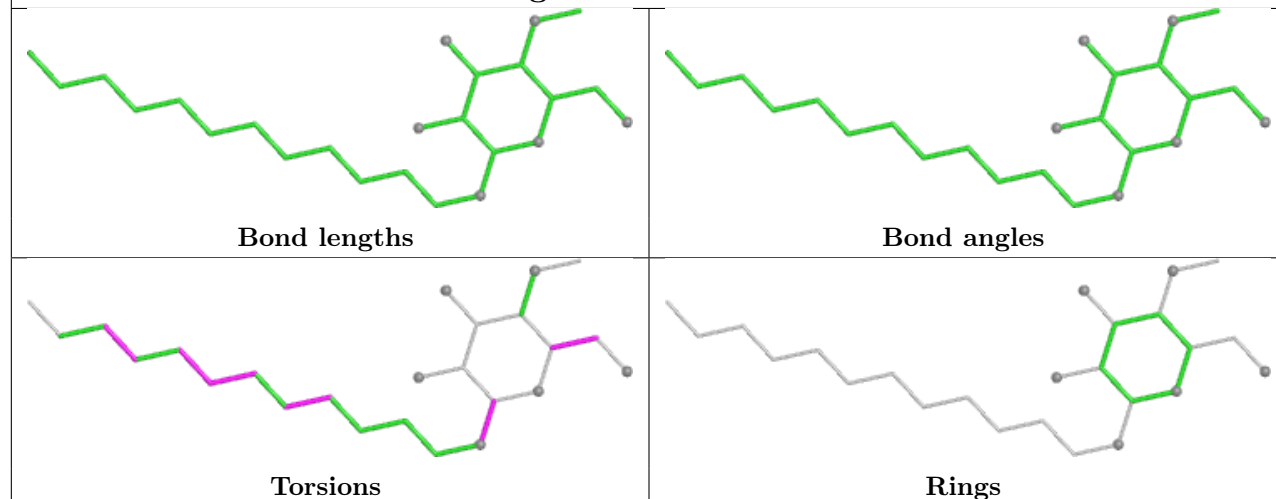
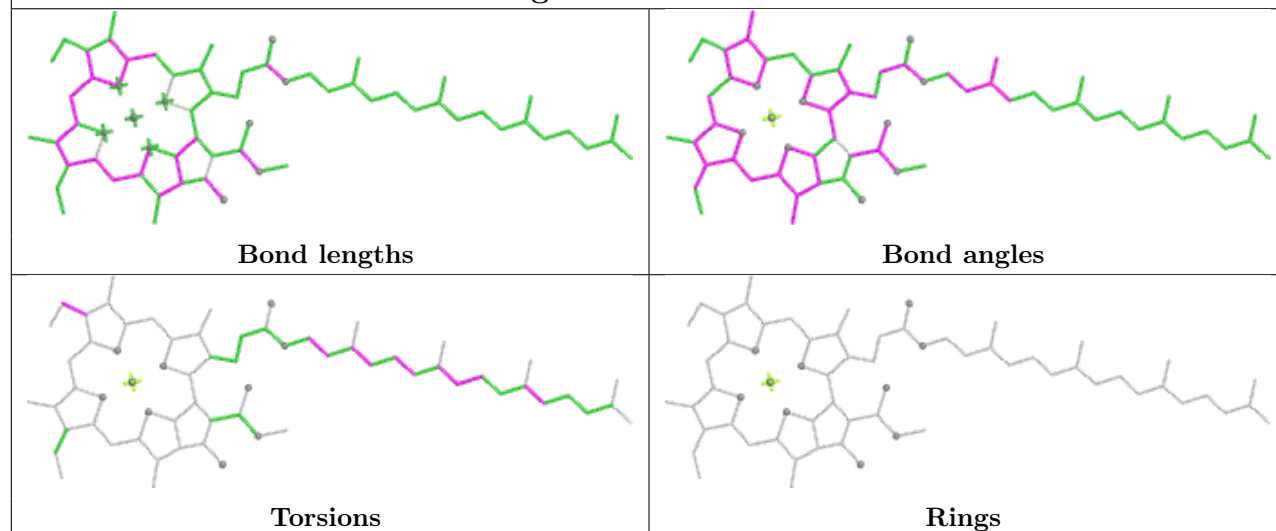
Ligand HTG B 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

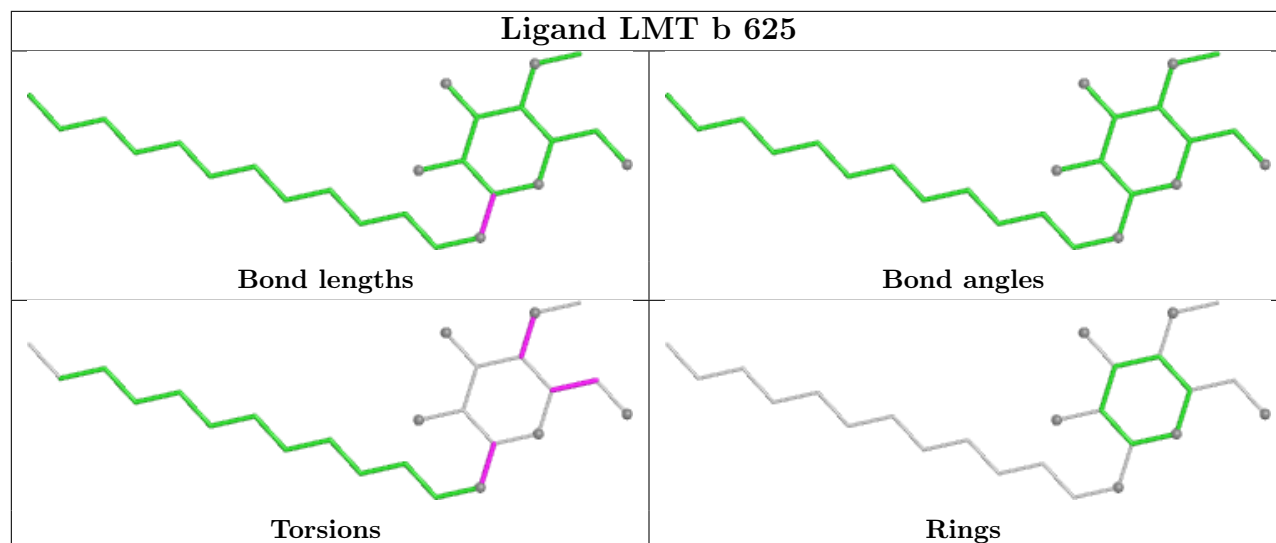
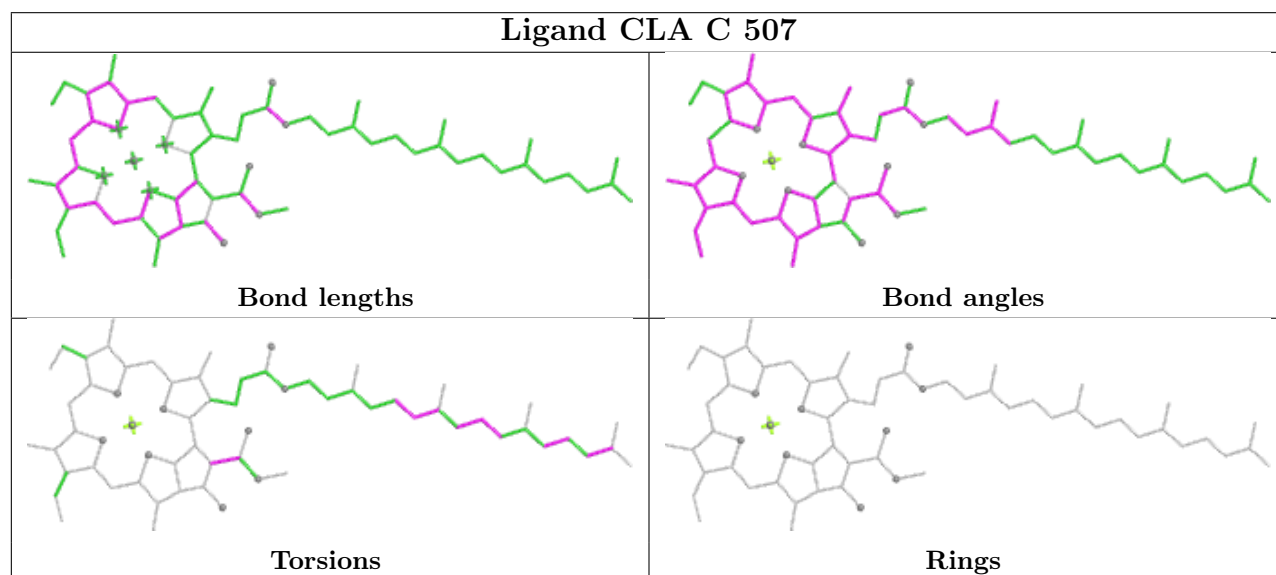
Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

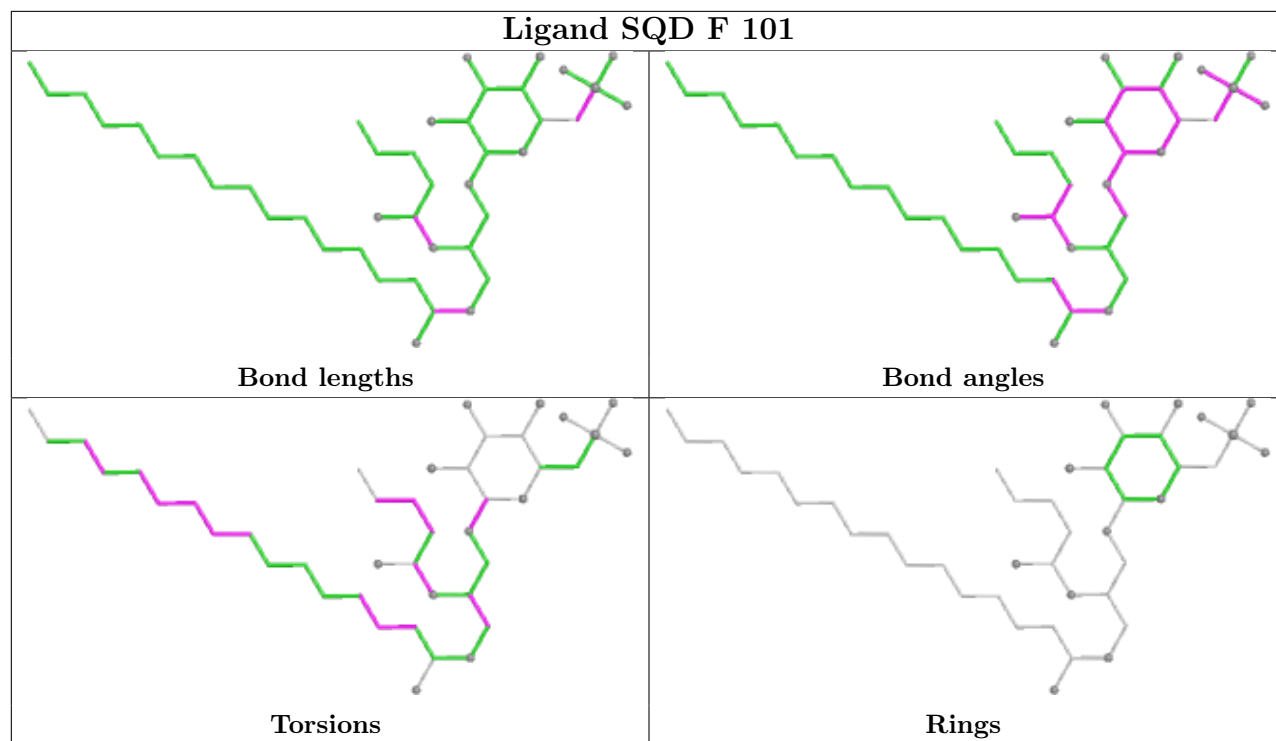
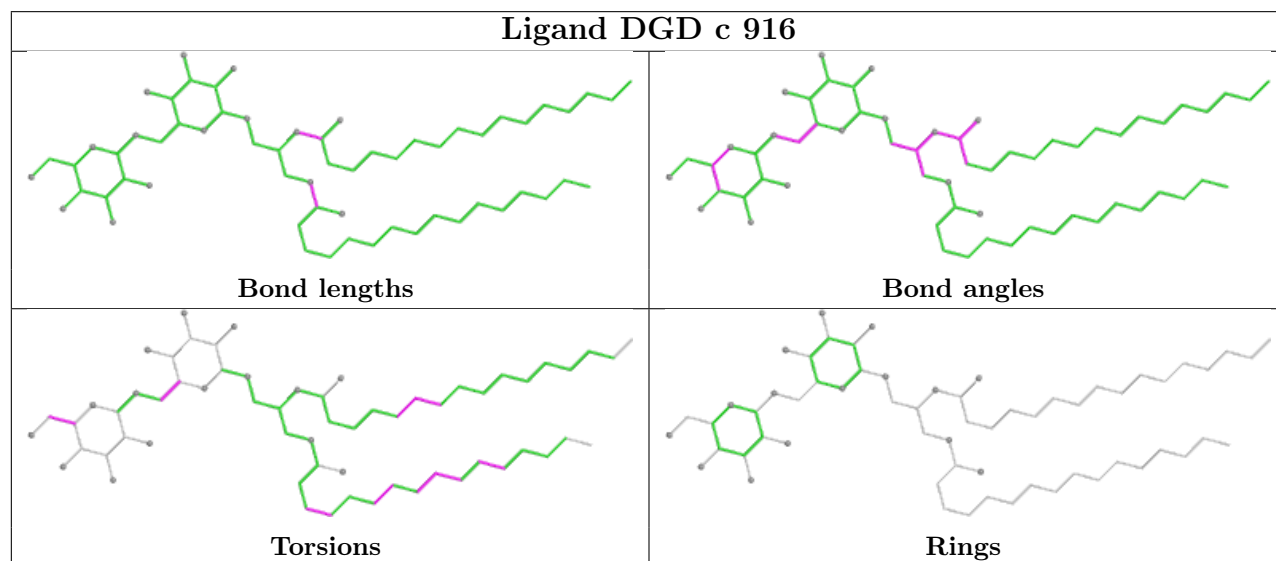


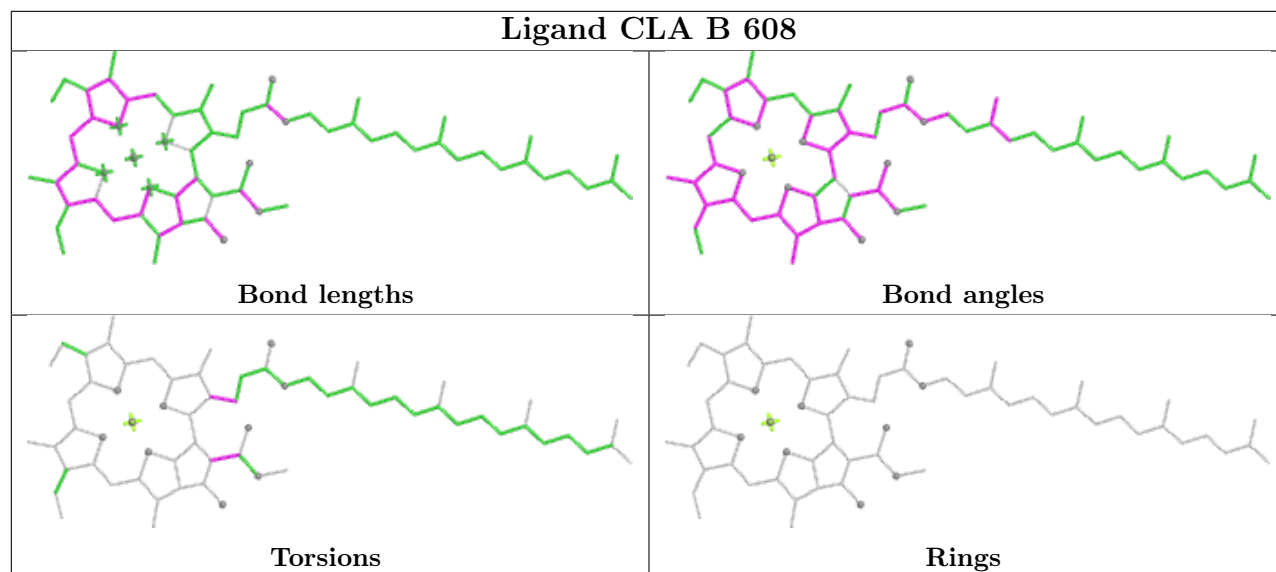
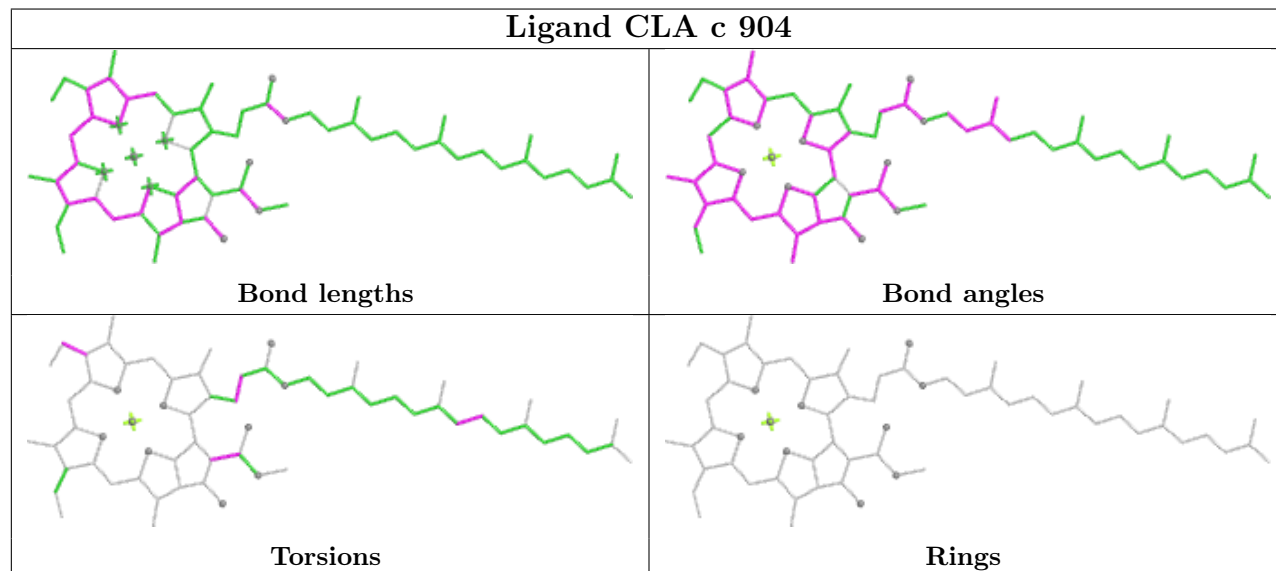


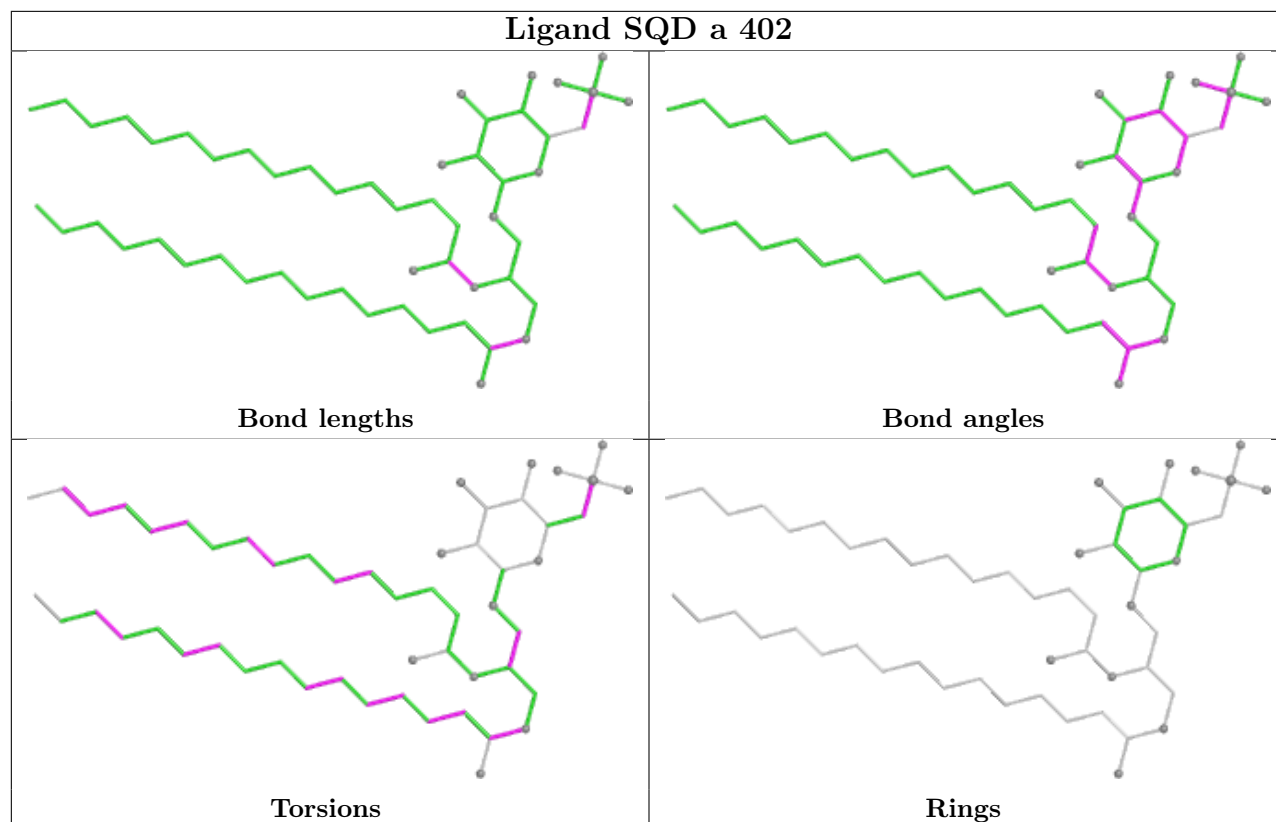
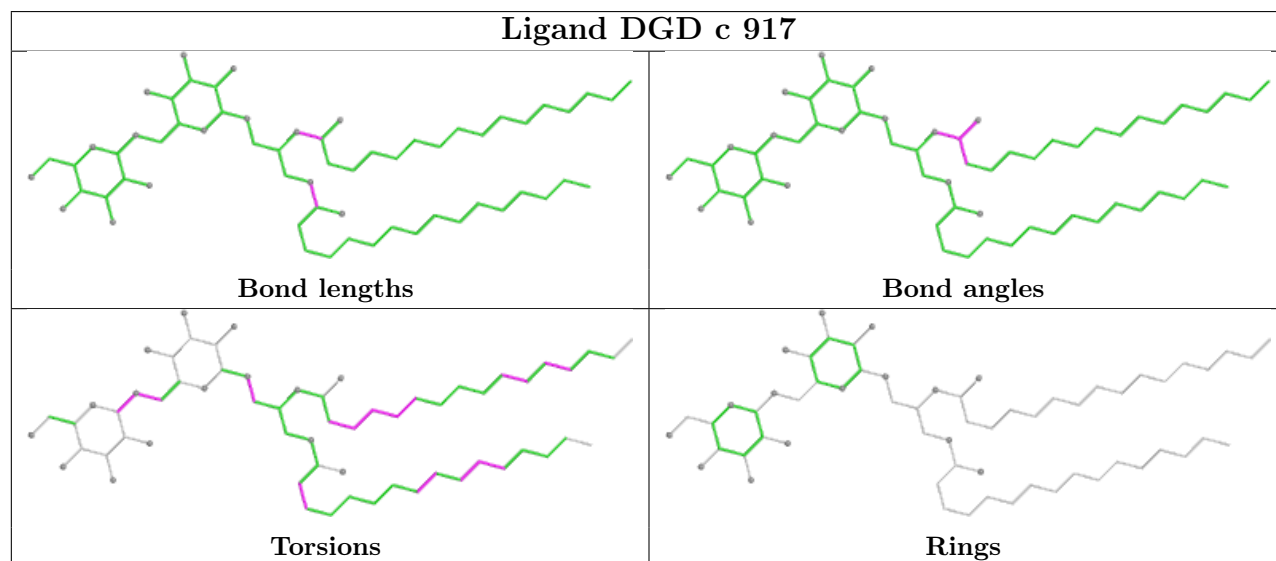
Ligand CLA b 611**Ligand CLA C 504****Ligand CLA b 606**

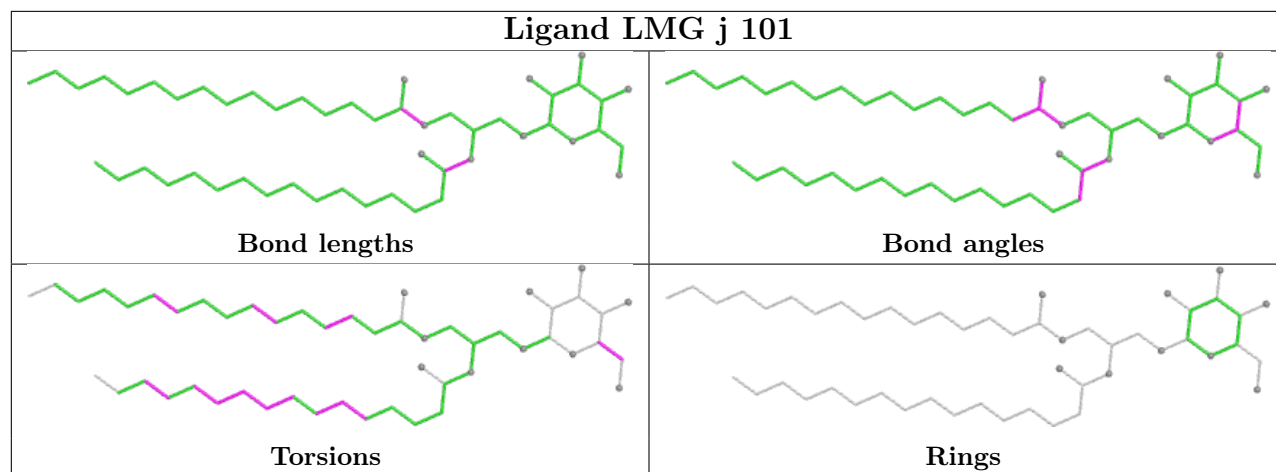
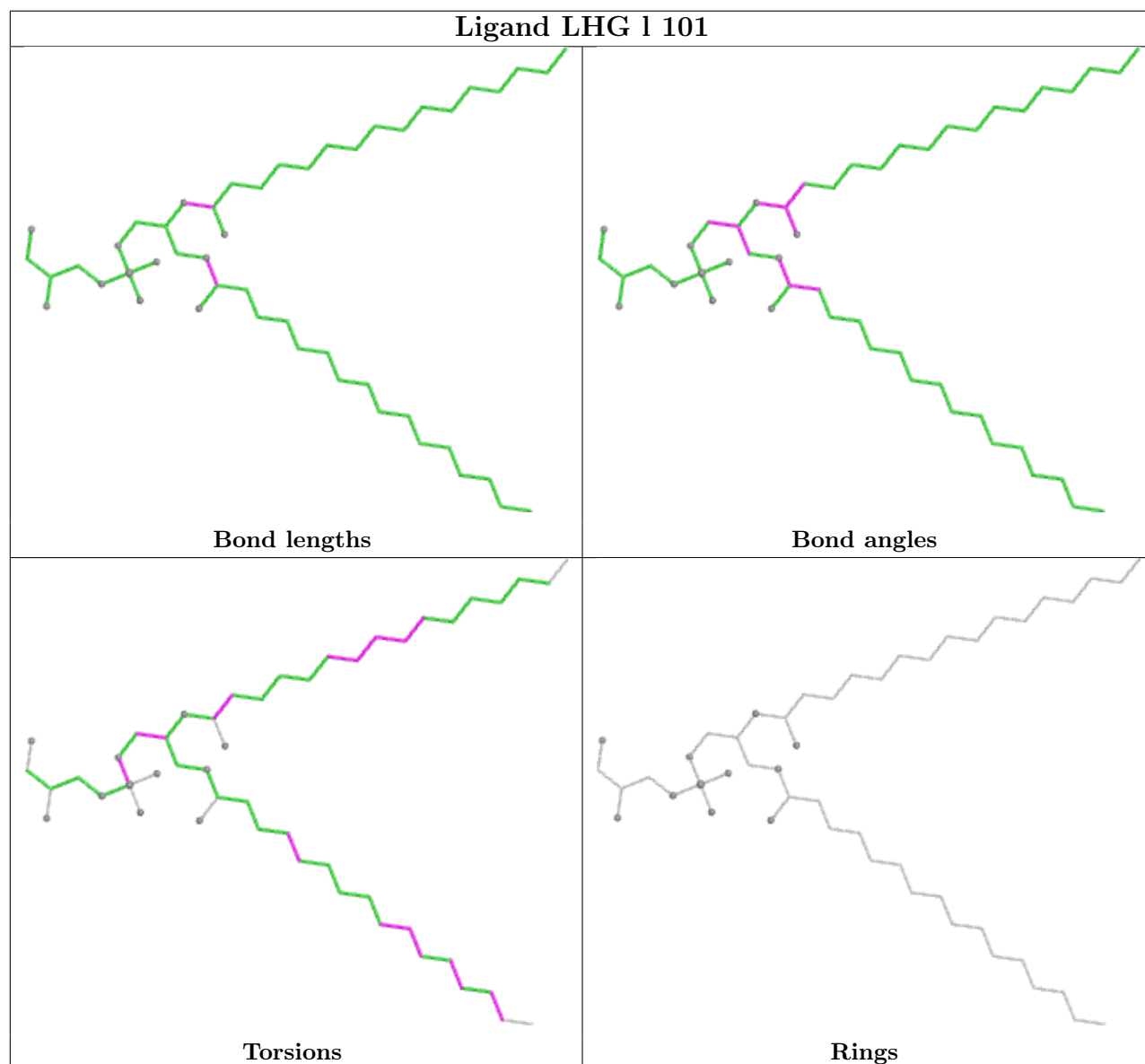
Ligand CLA b 615**Ligand LMT B 636****Ligand CLA D 402**

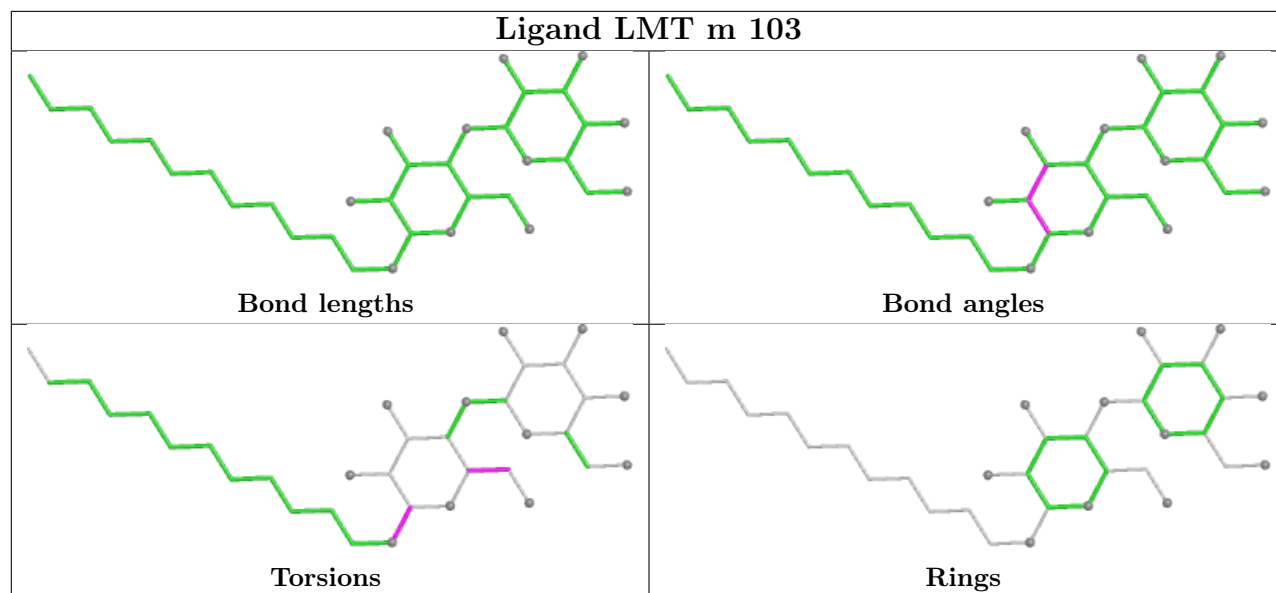
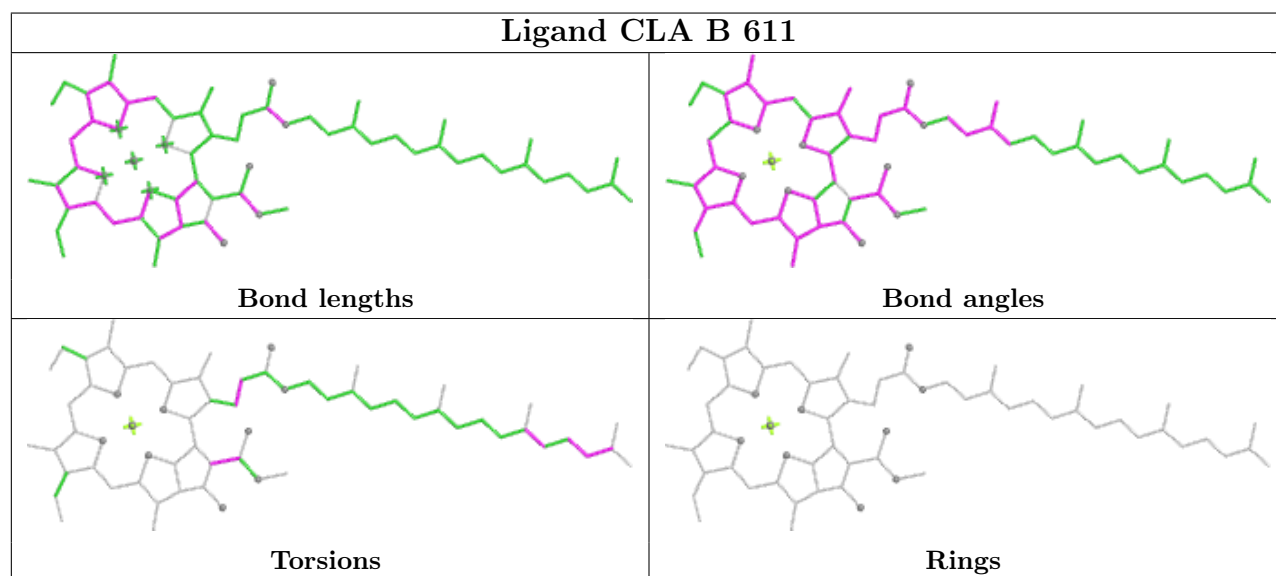
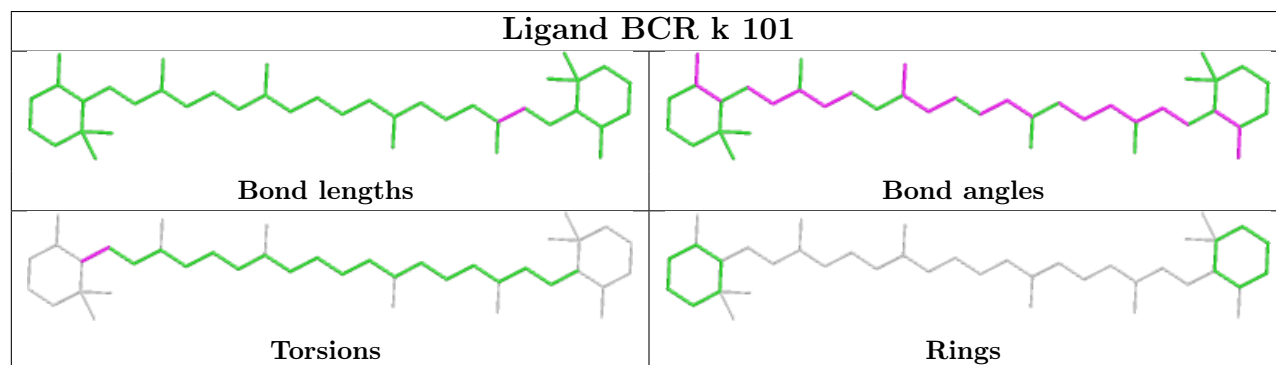


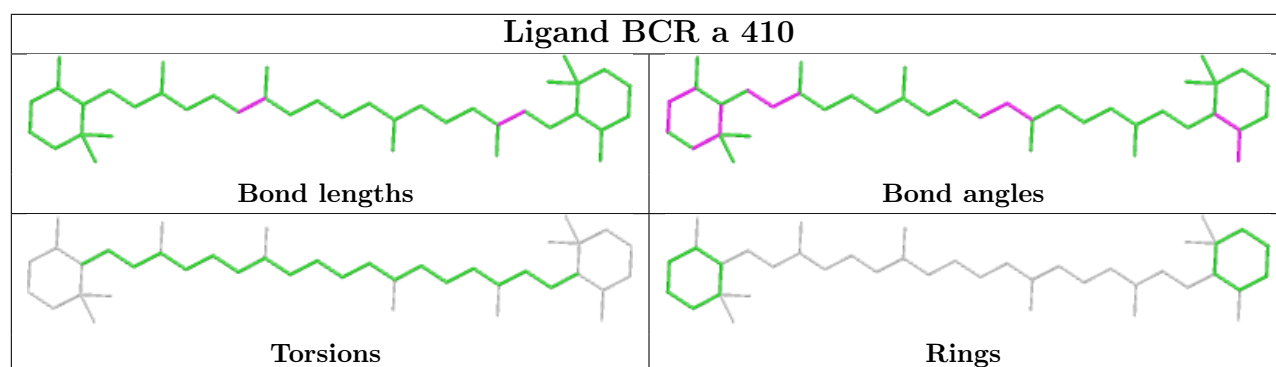
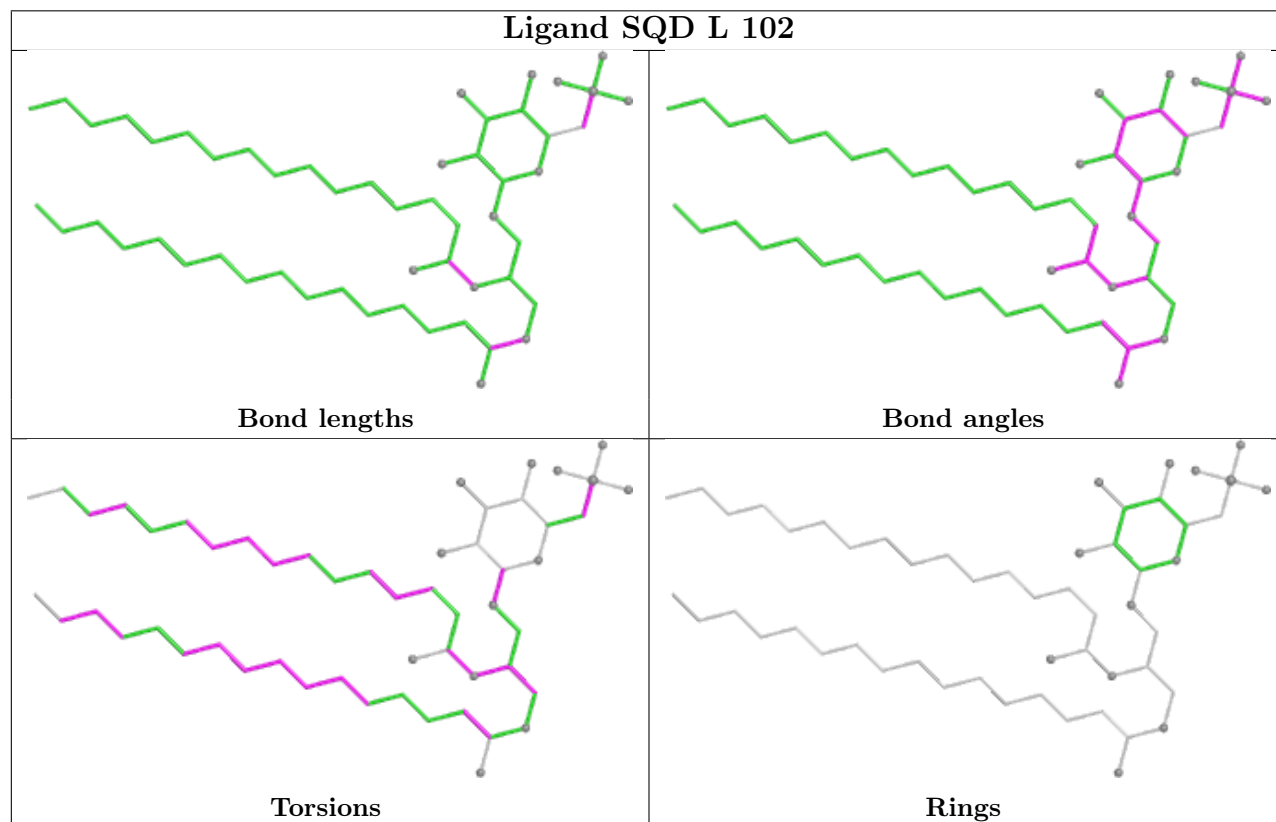
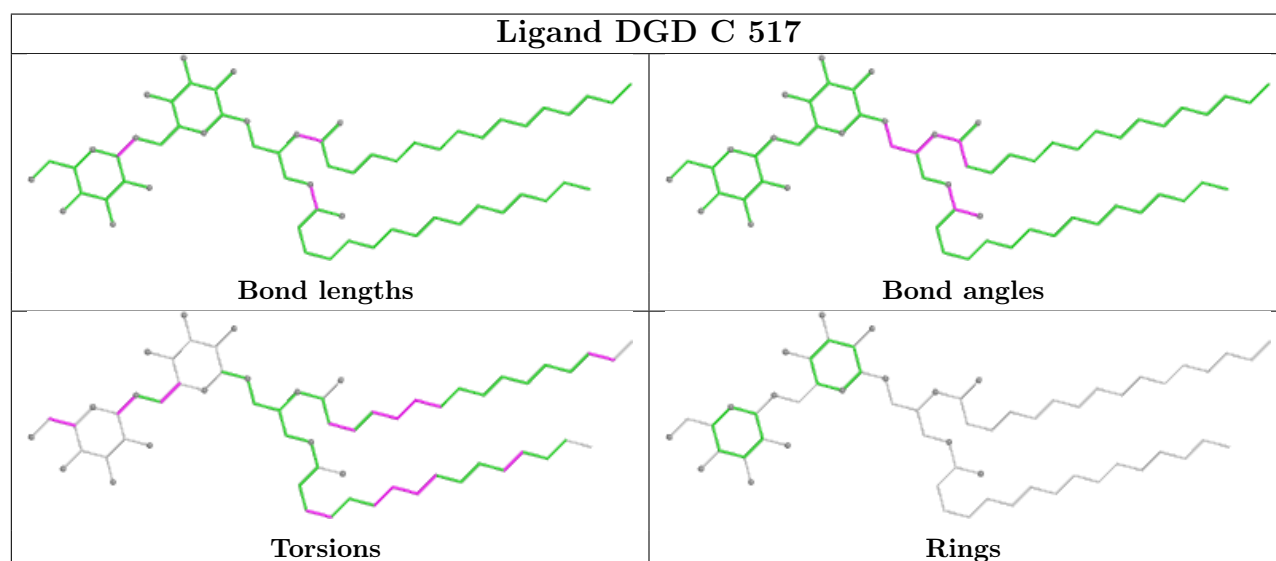


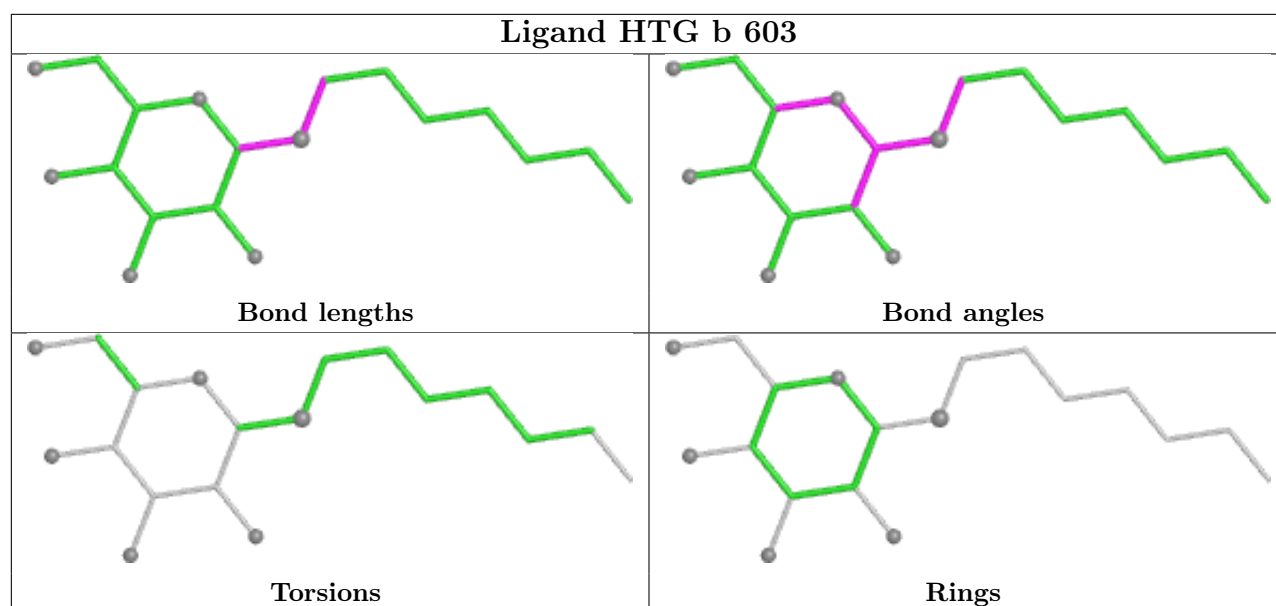
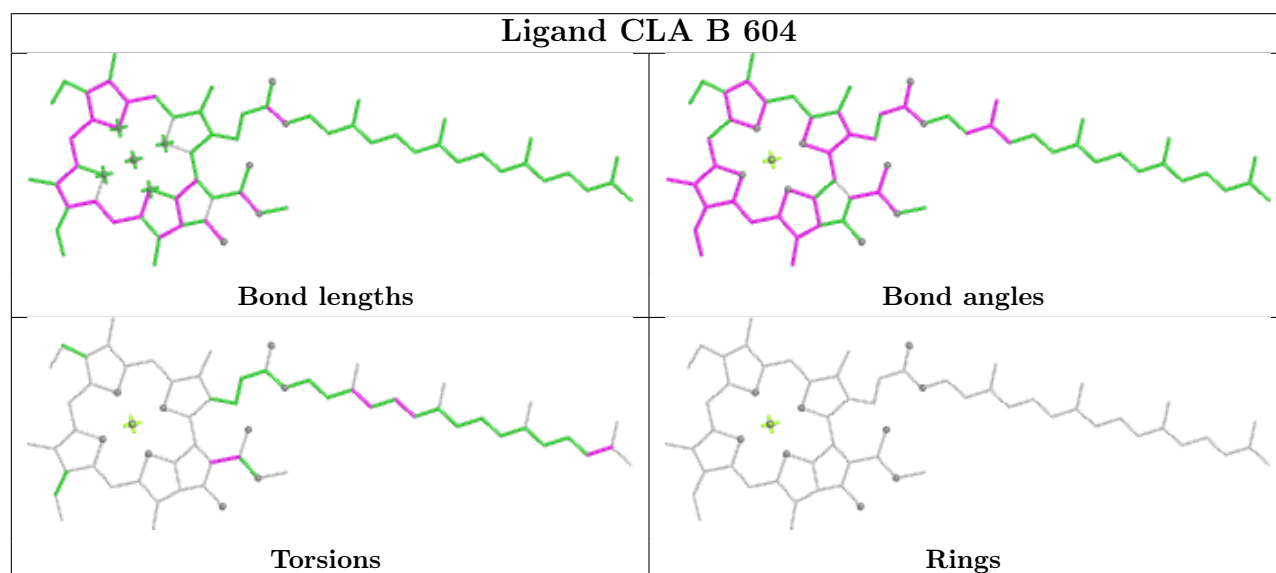
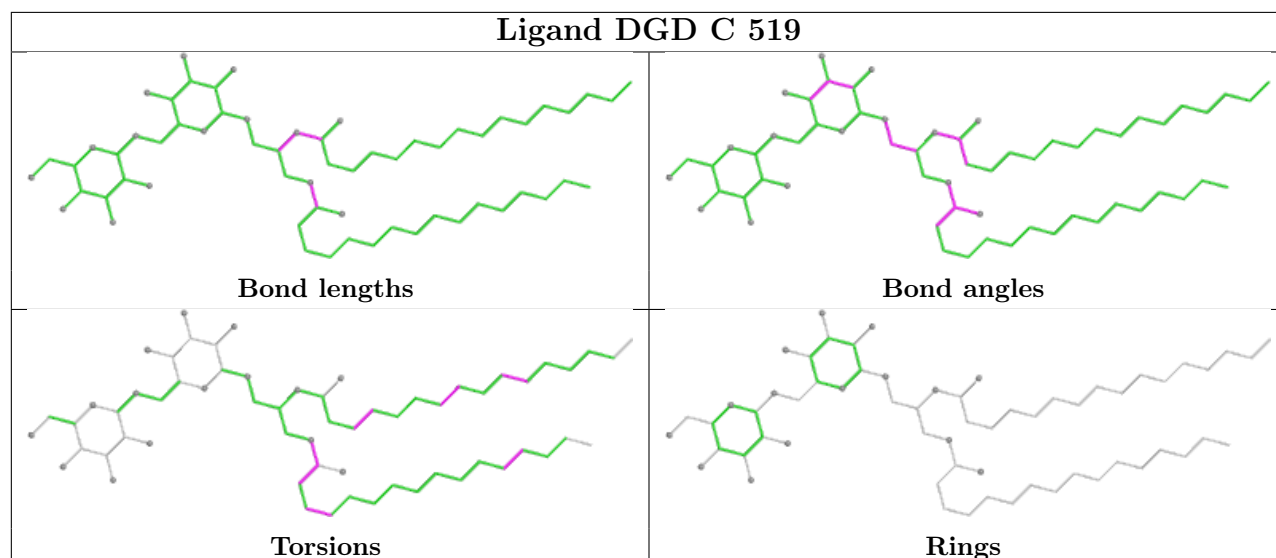
Ligand CLA B 608**Ligand CLA c 904**

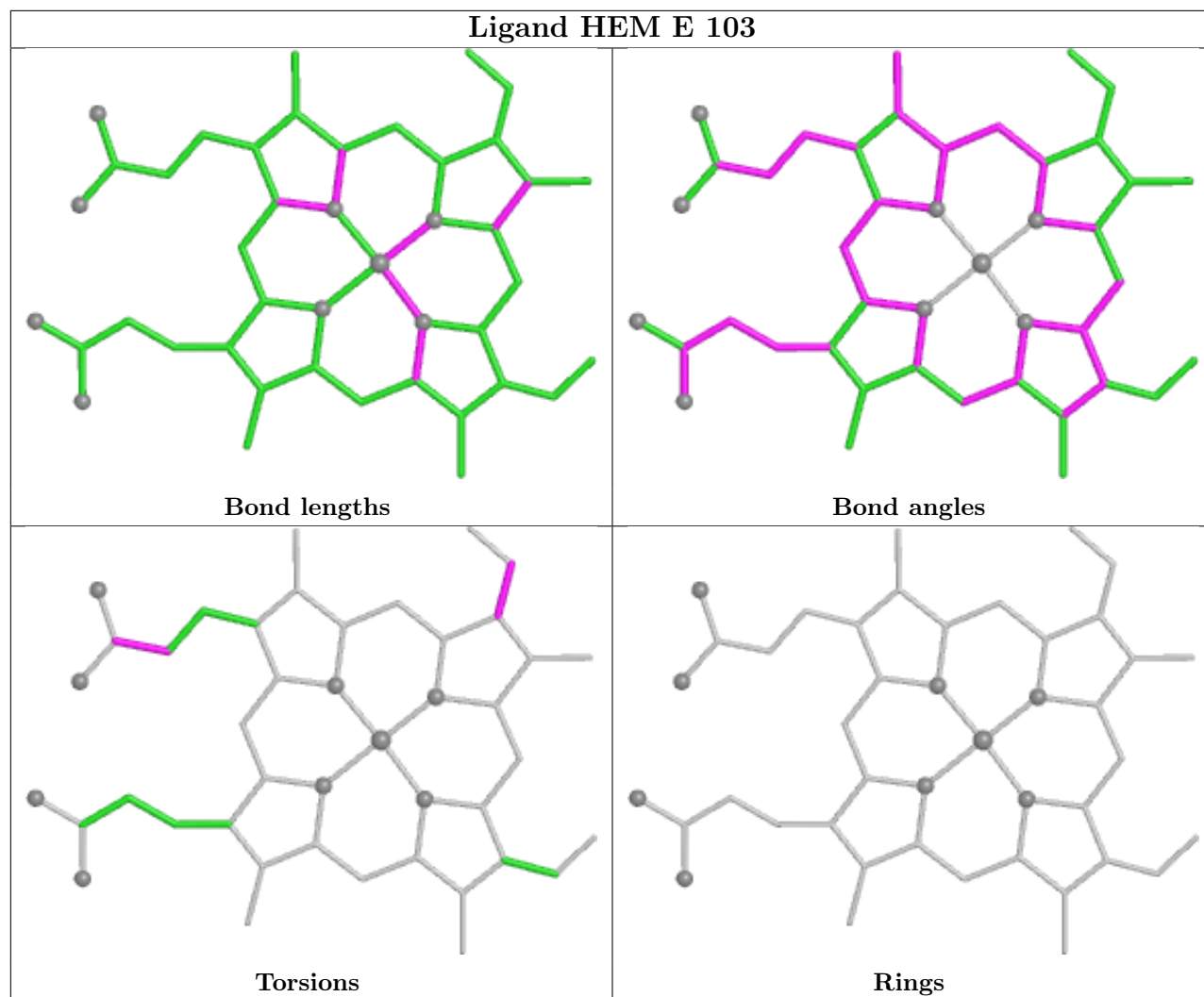
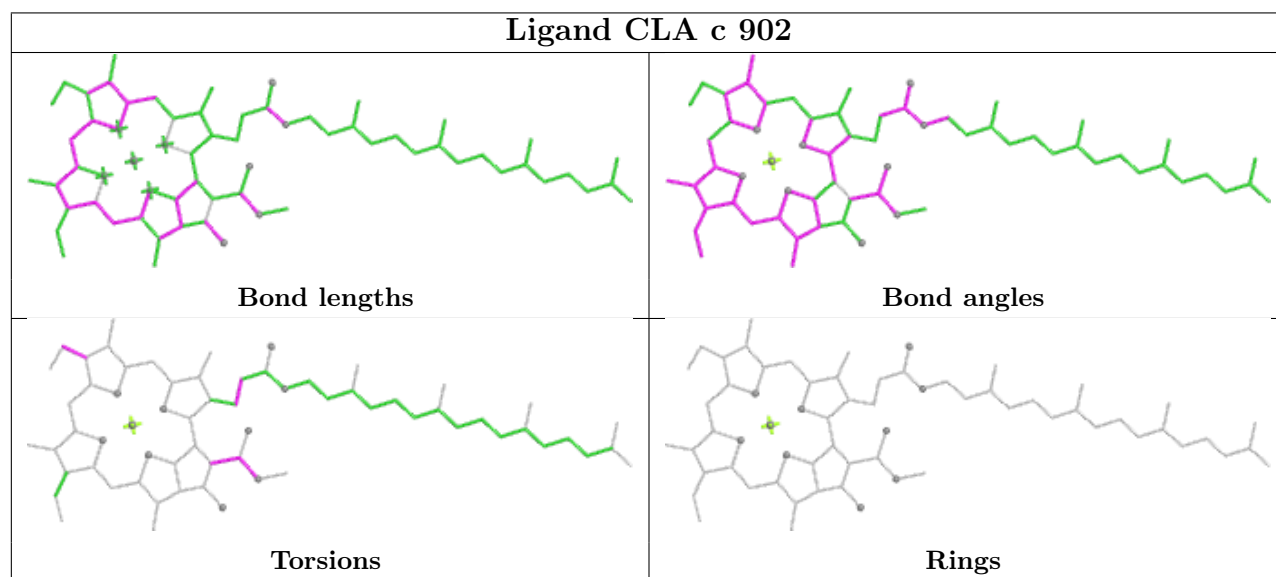


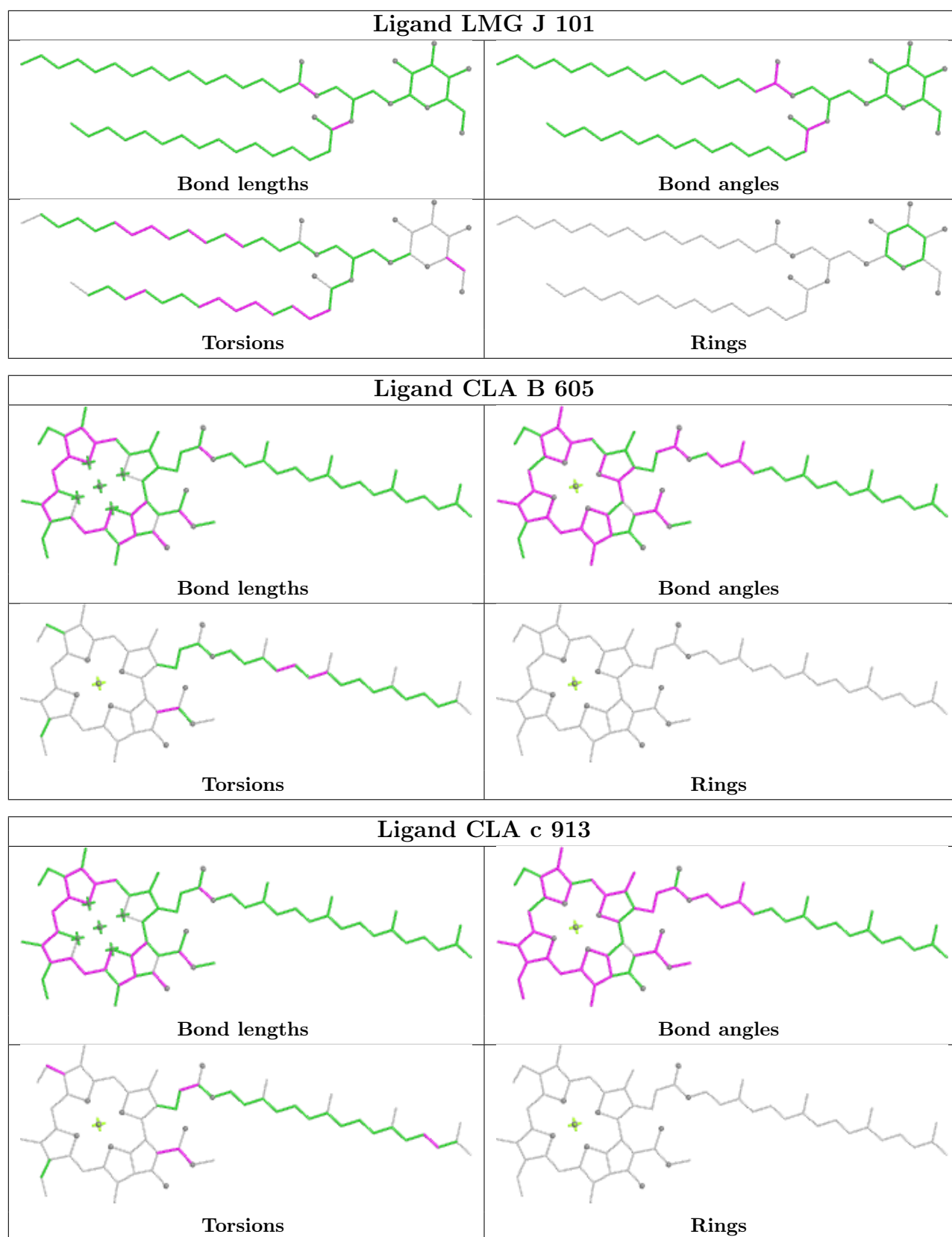


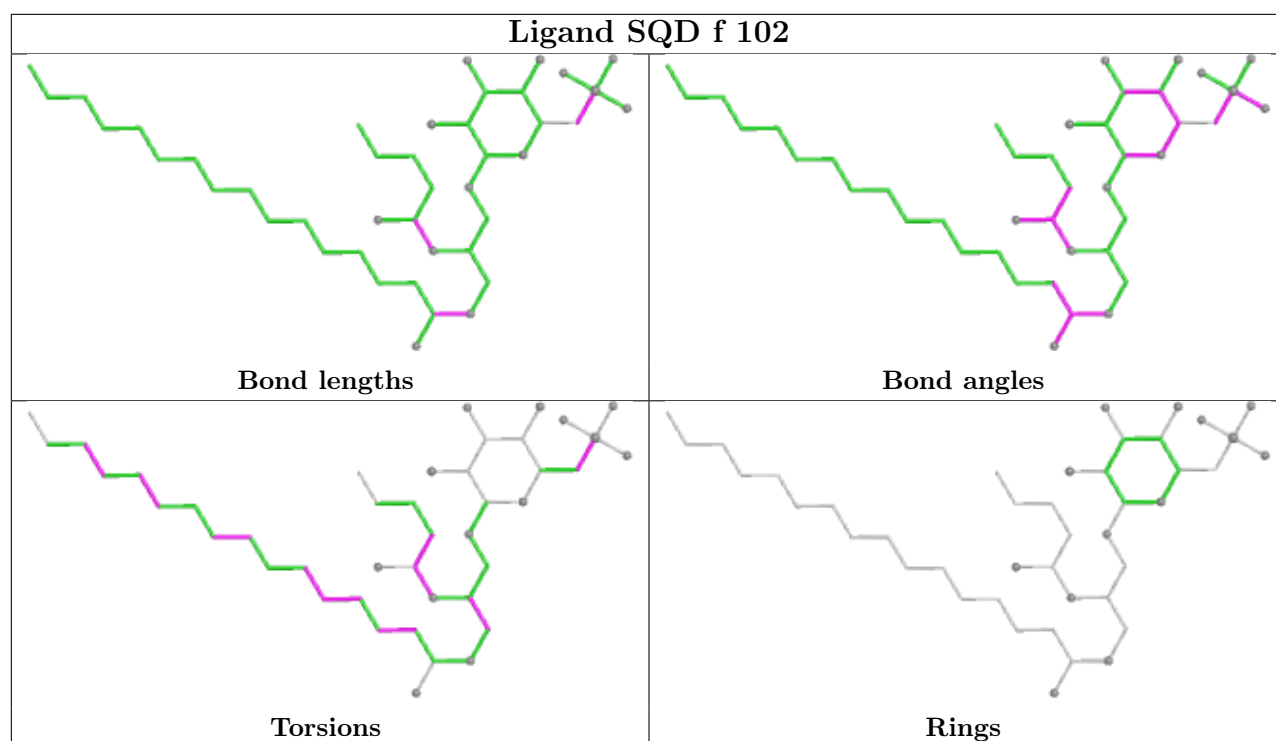
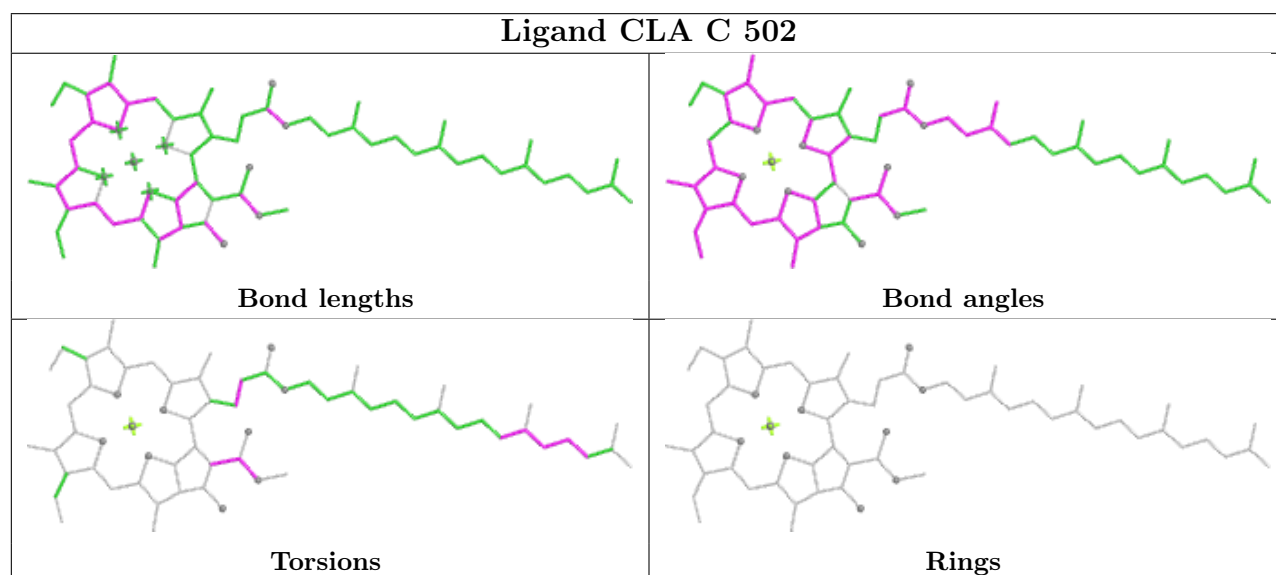
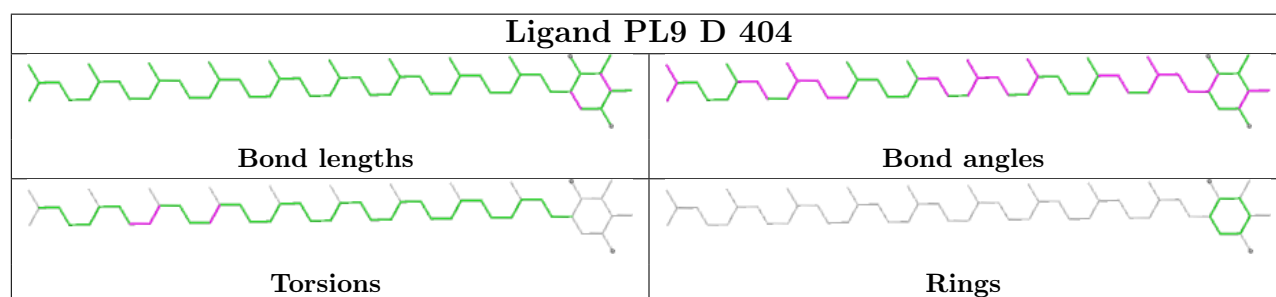


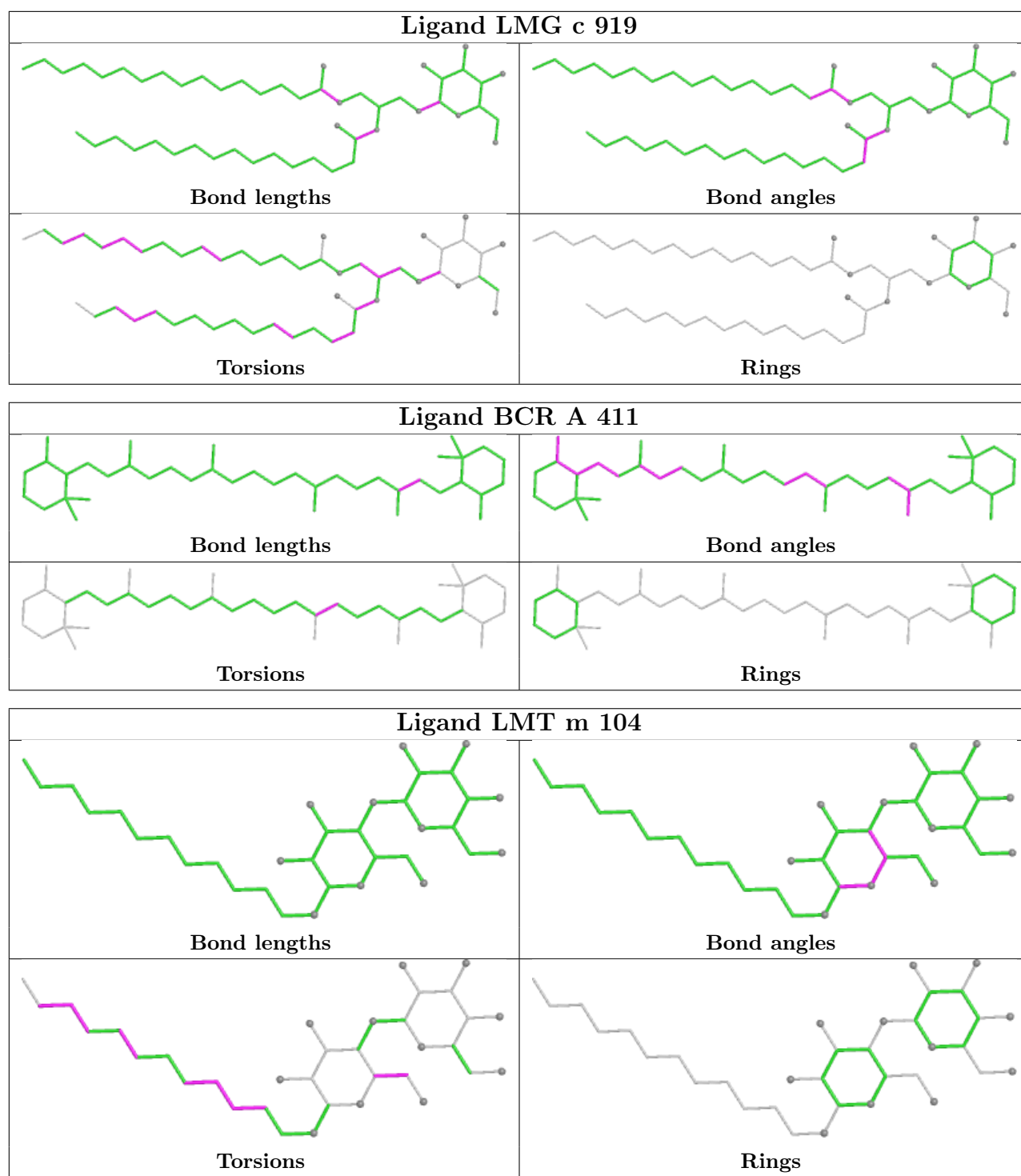


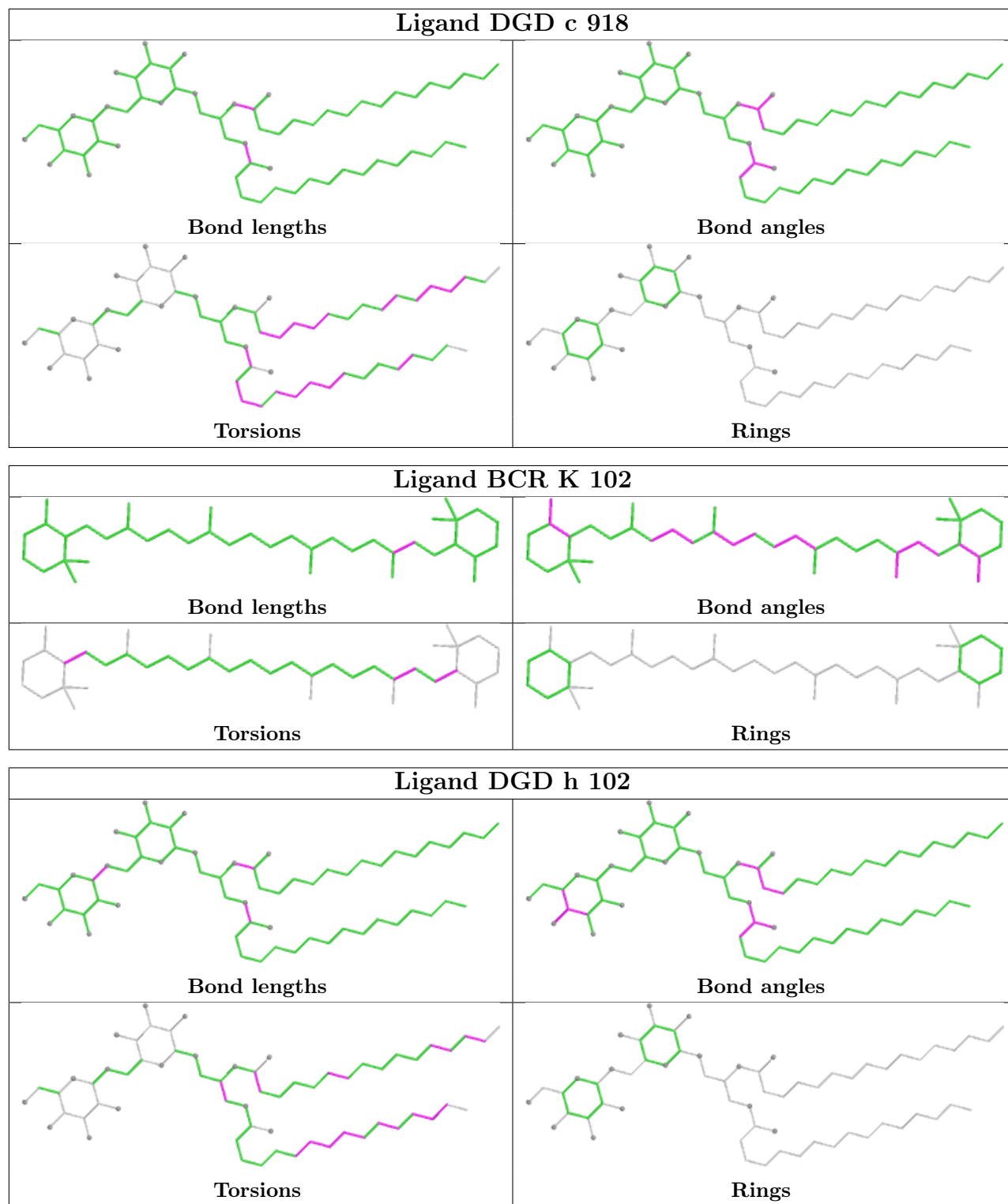


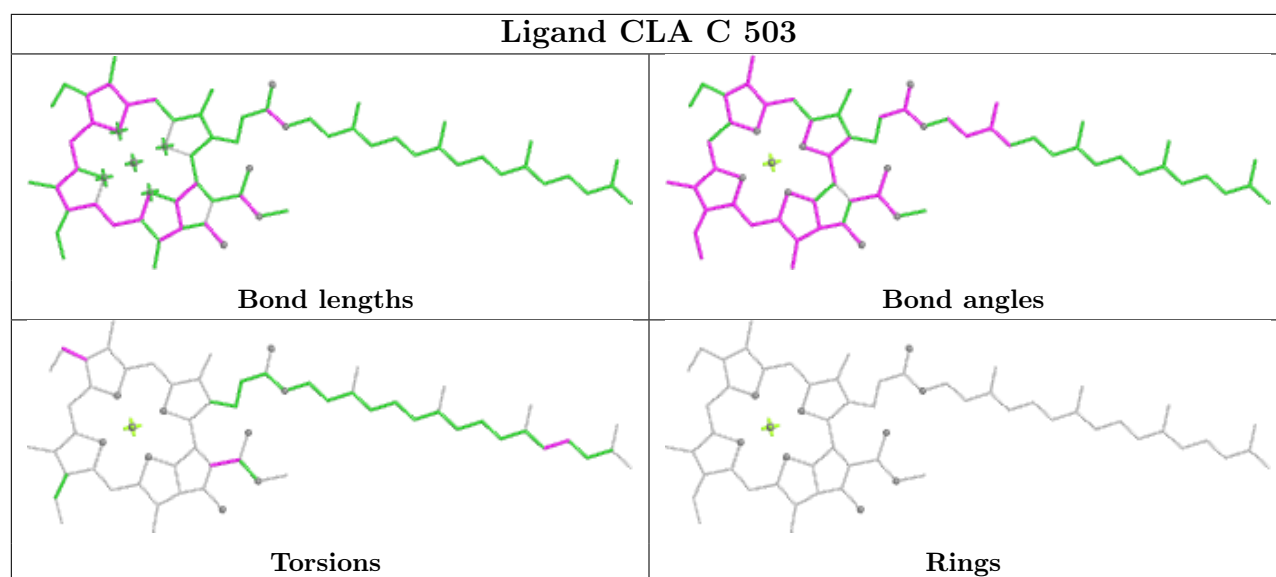
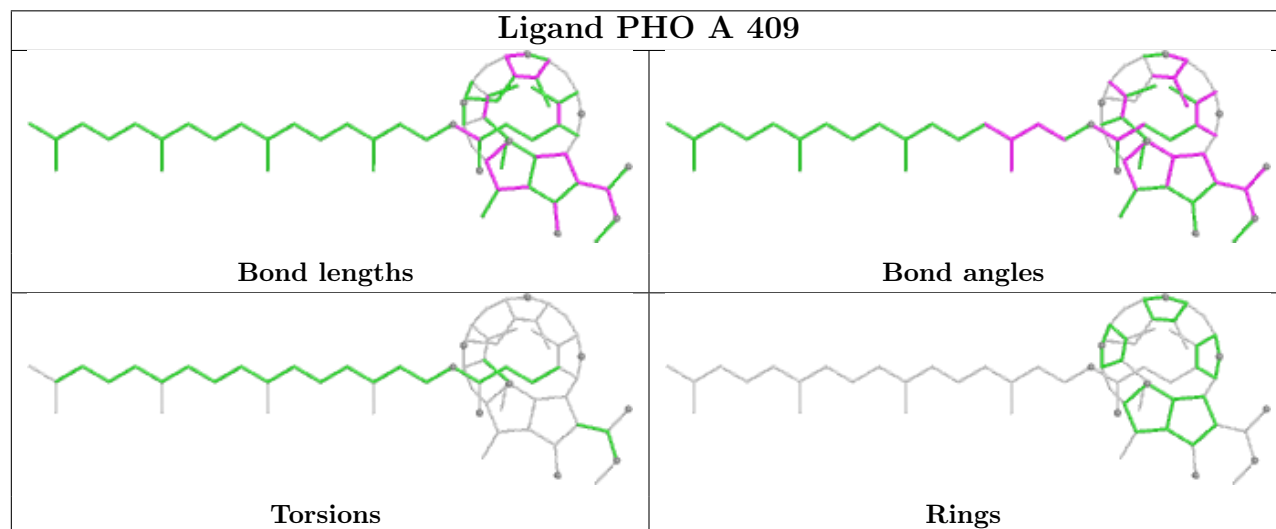


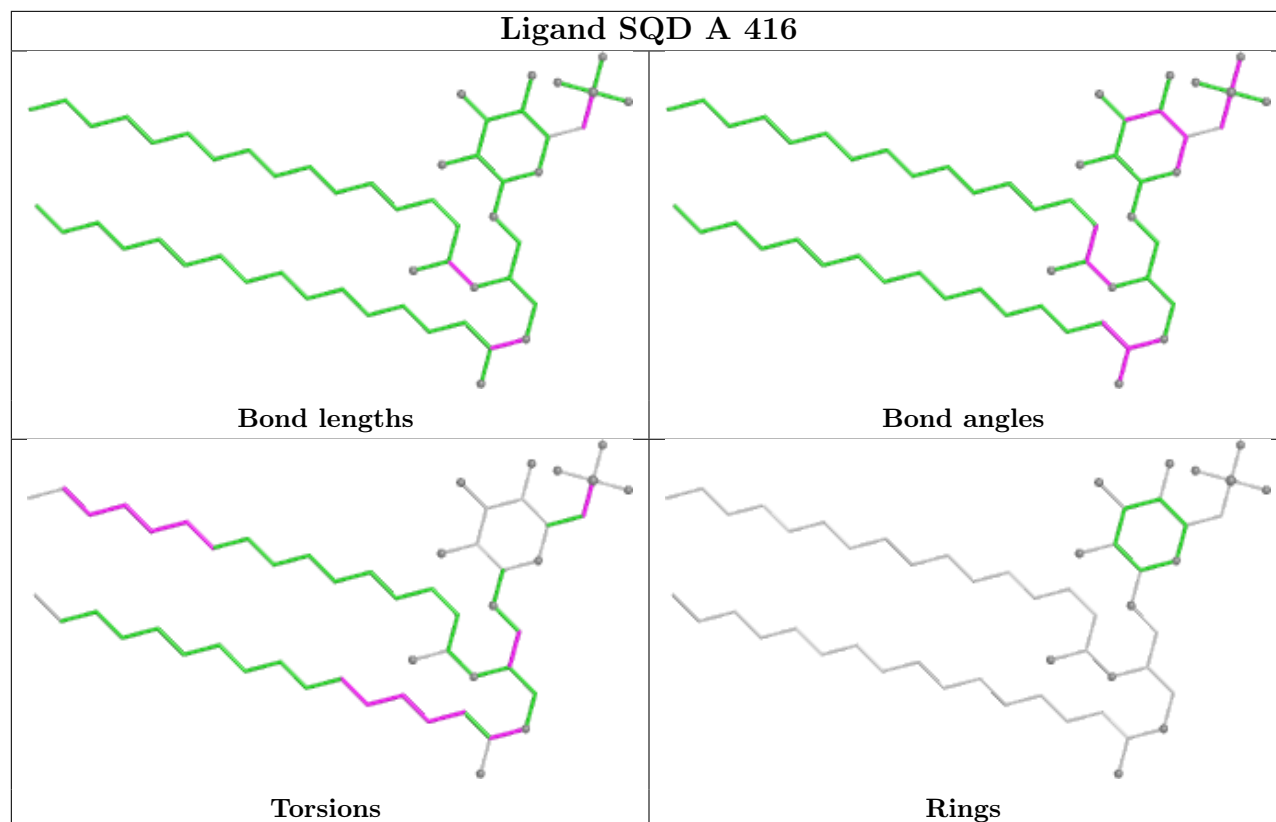
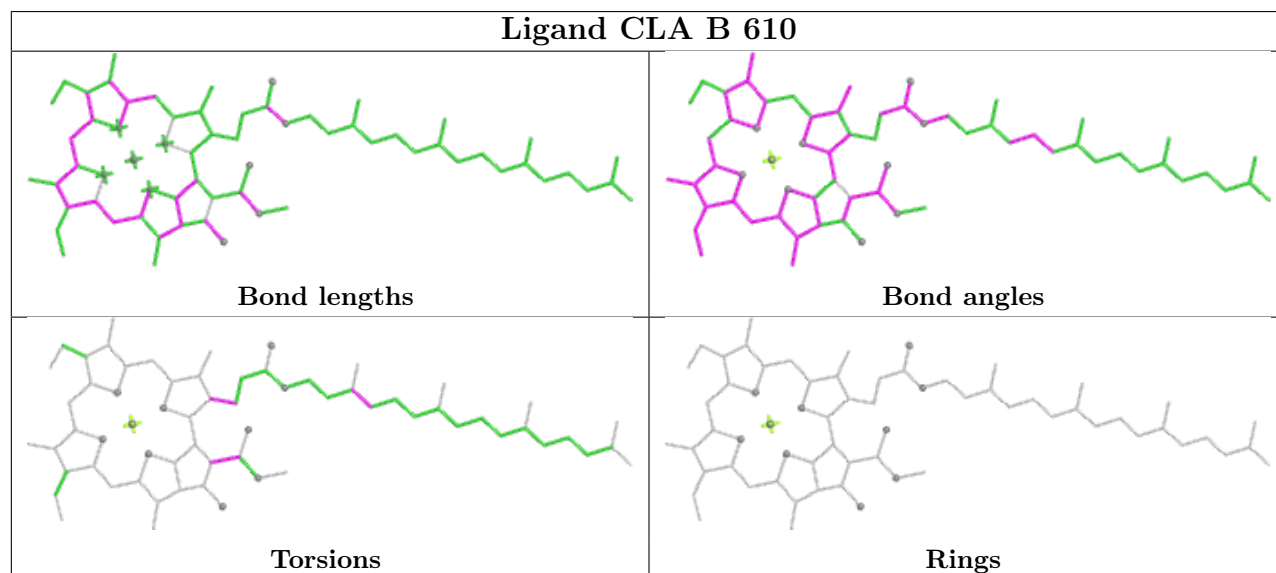


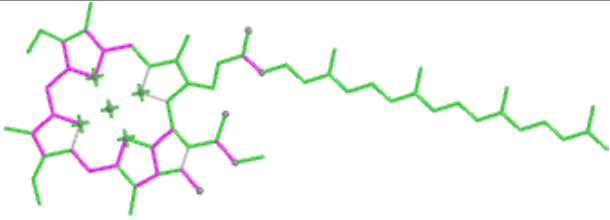
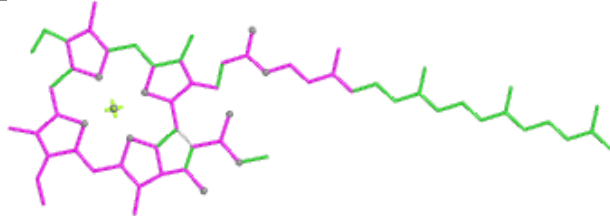
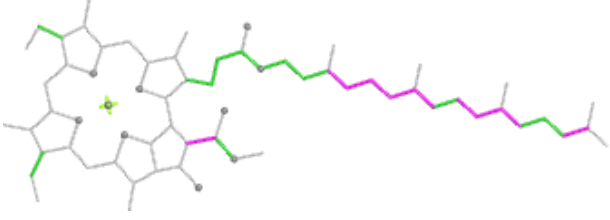
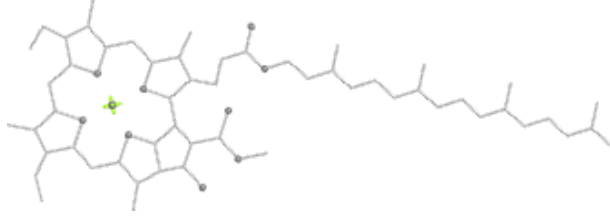
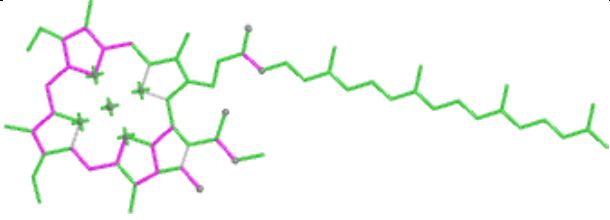
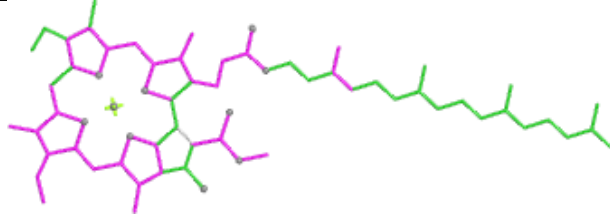
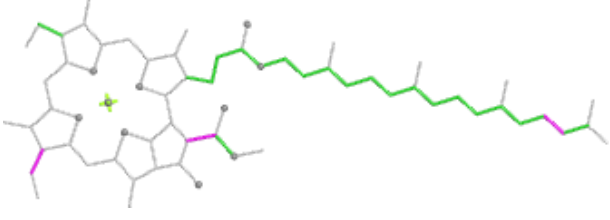
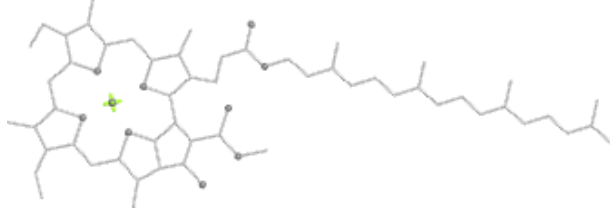
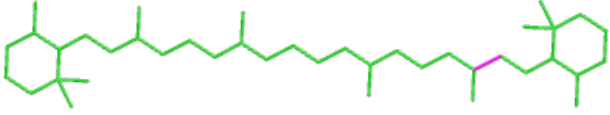
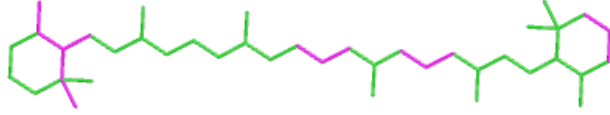
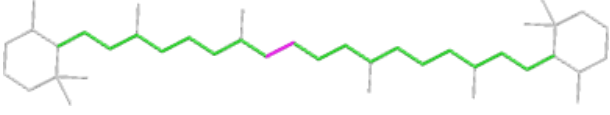
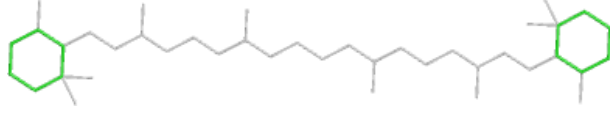


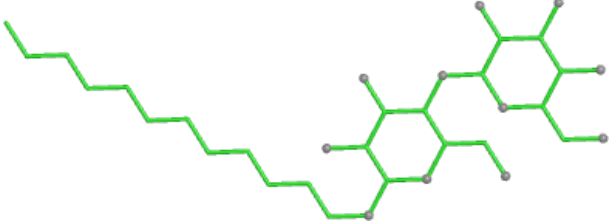
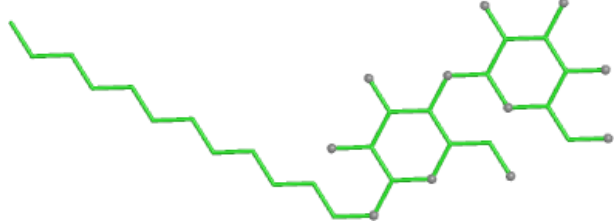
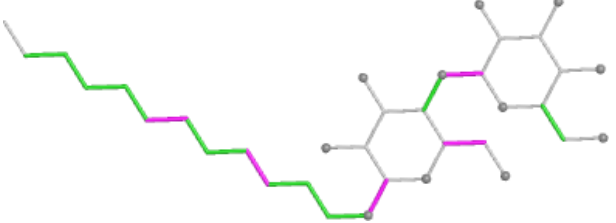
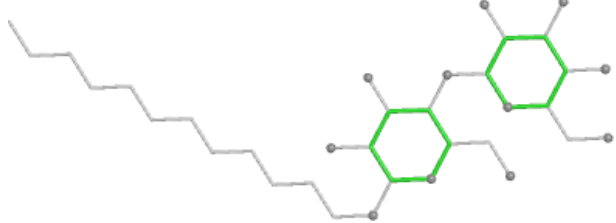
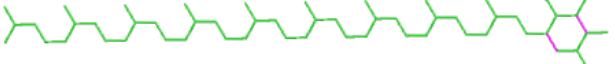
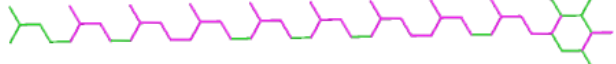
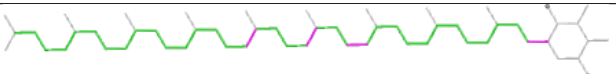
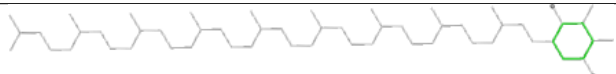


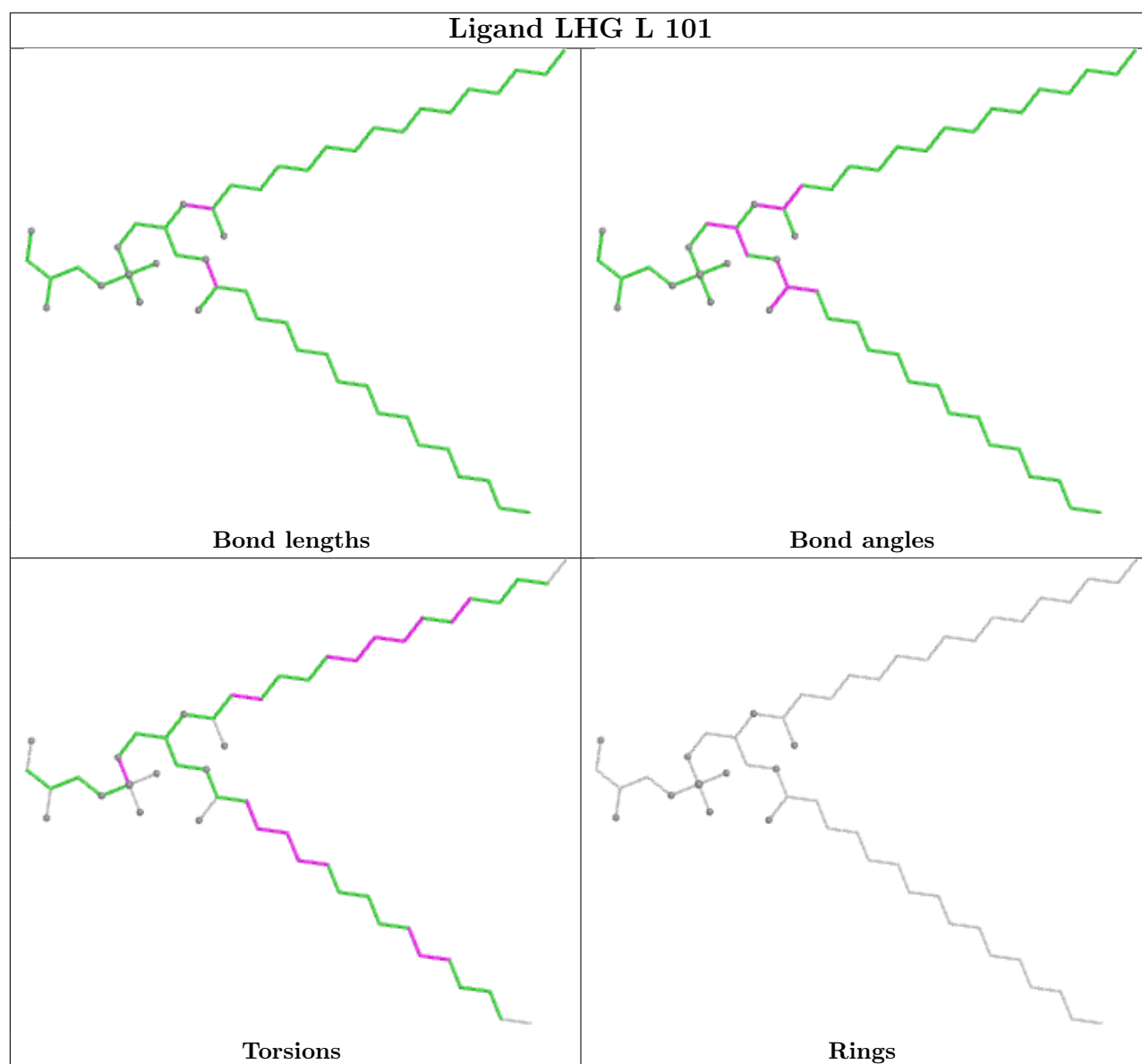
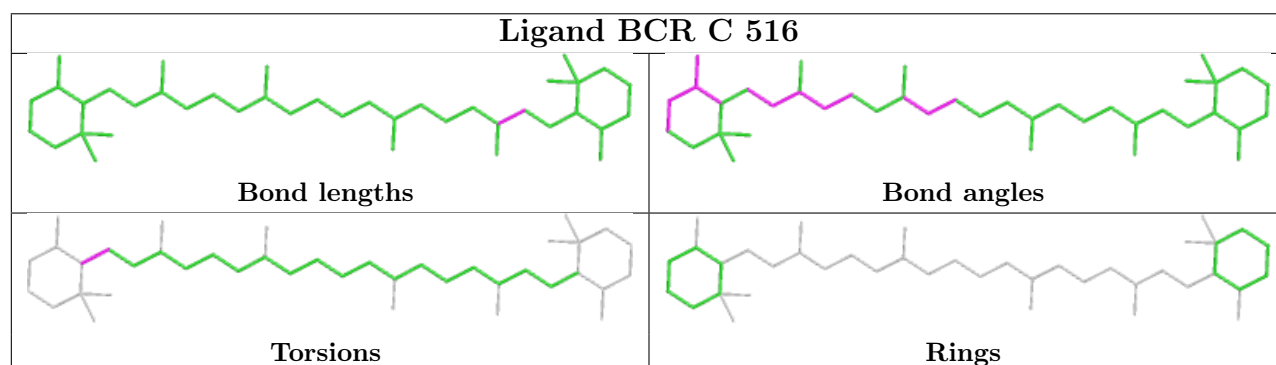


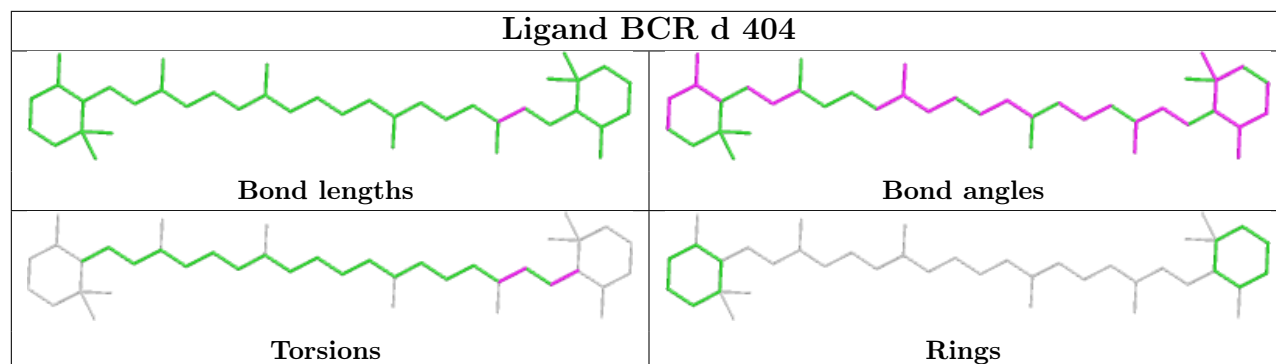
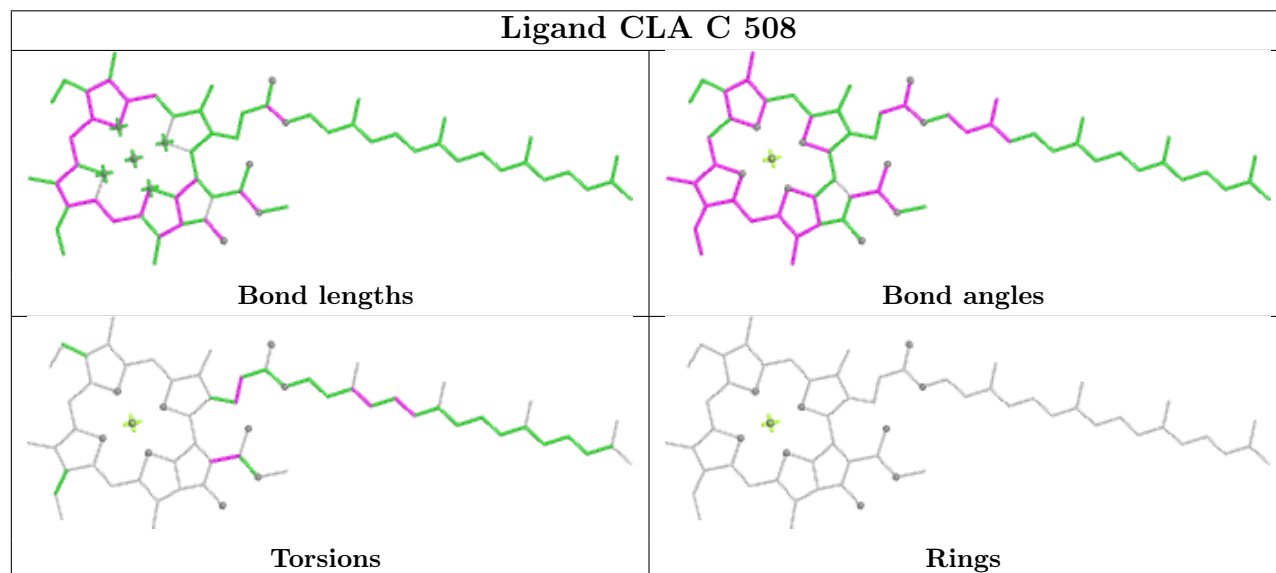
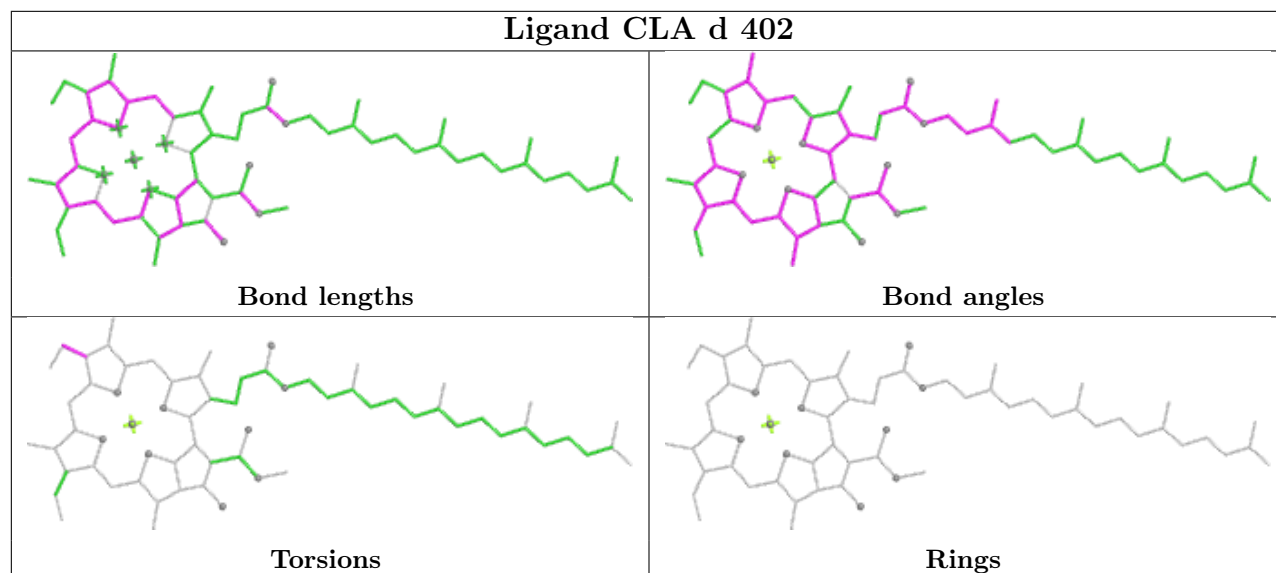




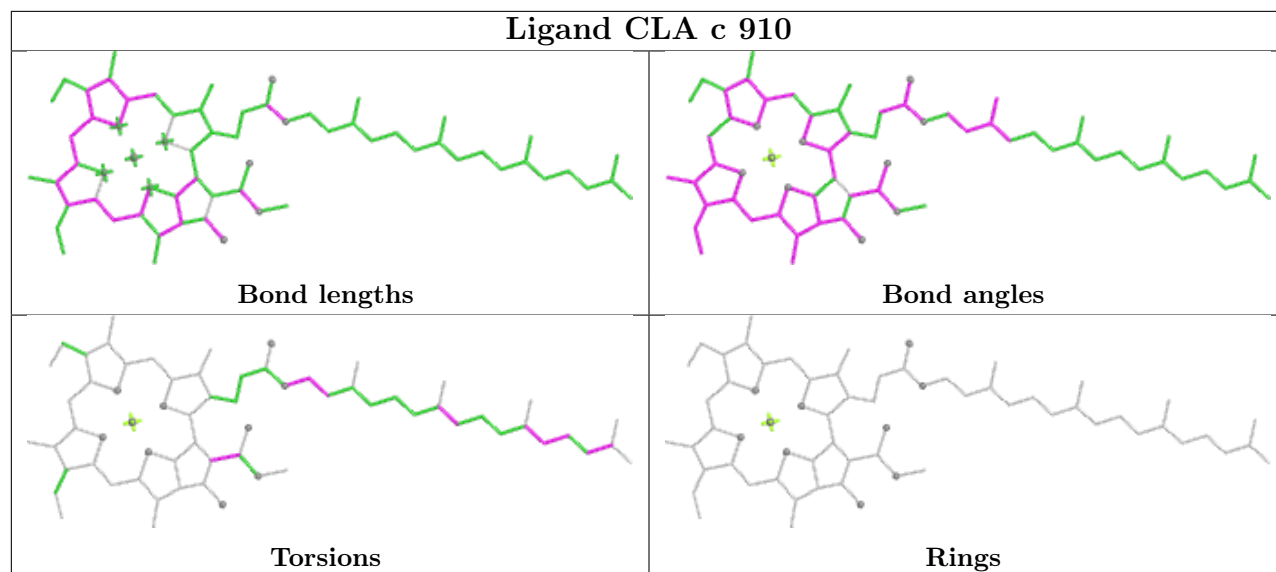
Ligand CLA B 615	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA A 406	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR t 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand LMT E 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 A 419	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

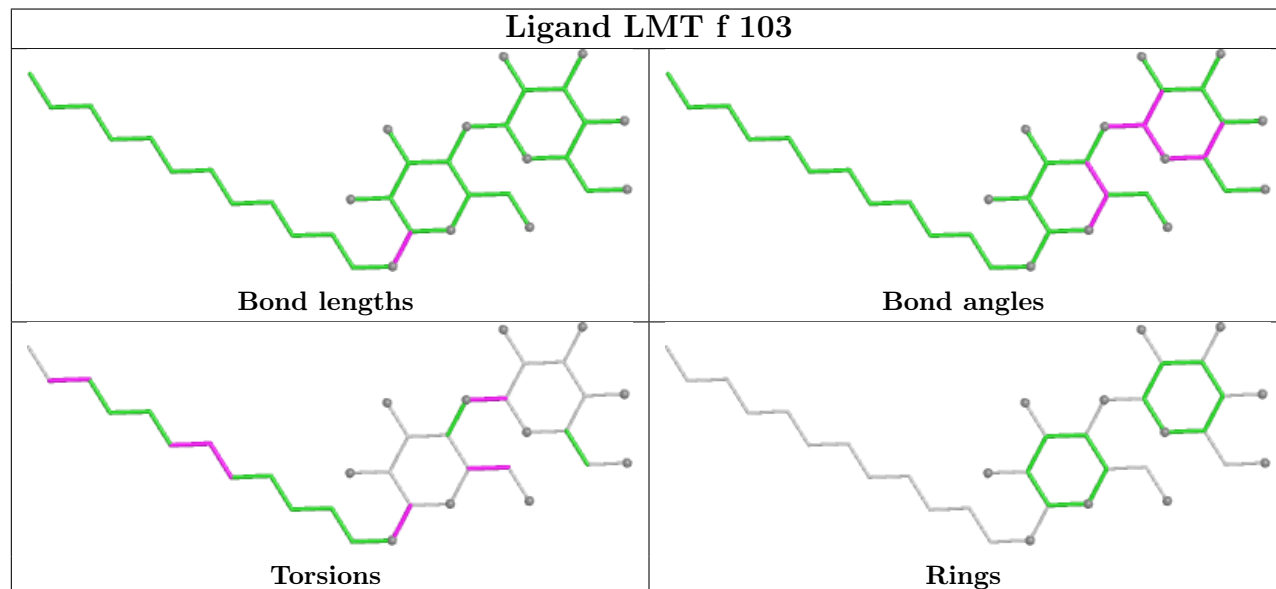


Ligand BCR d 404**Ligand CLA C 508****Ligand CLA d 402**

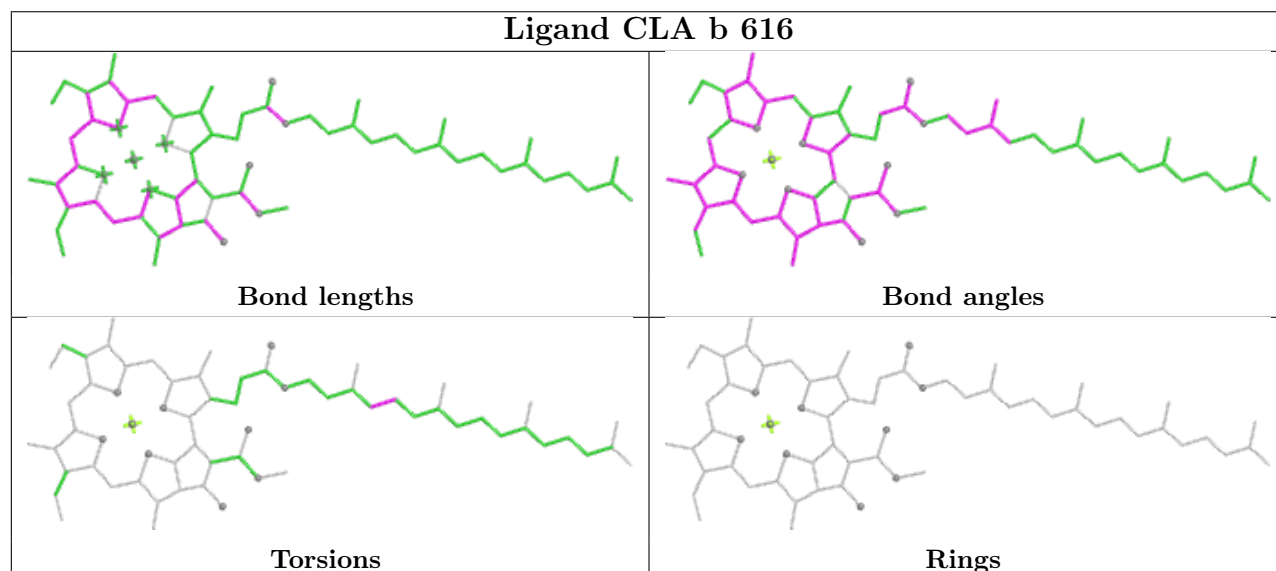
Ligand CLA c 910



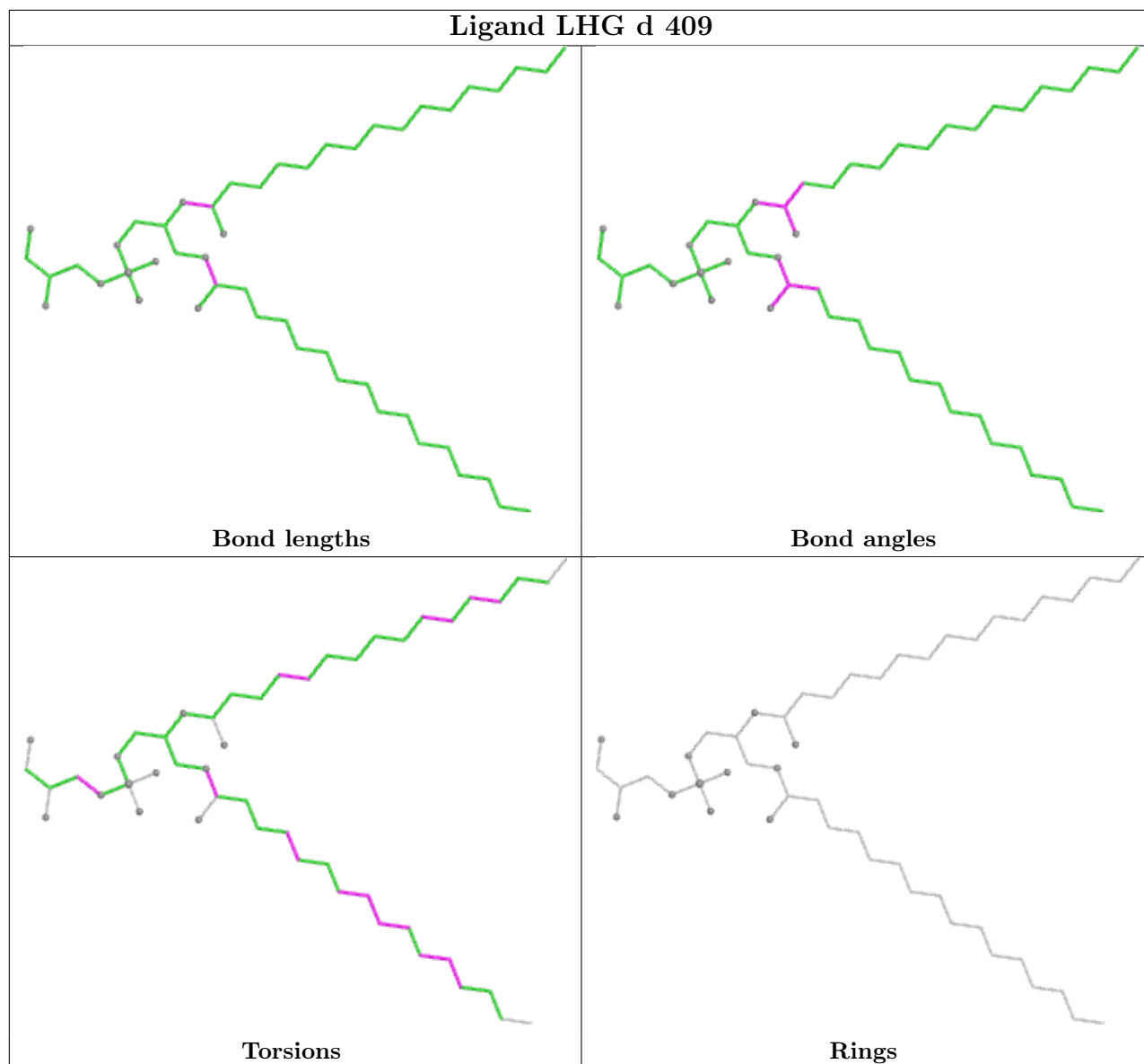
Ligand LMT f 103



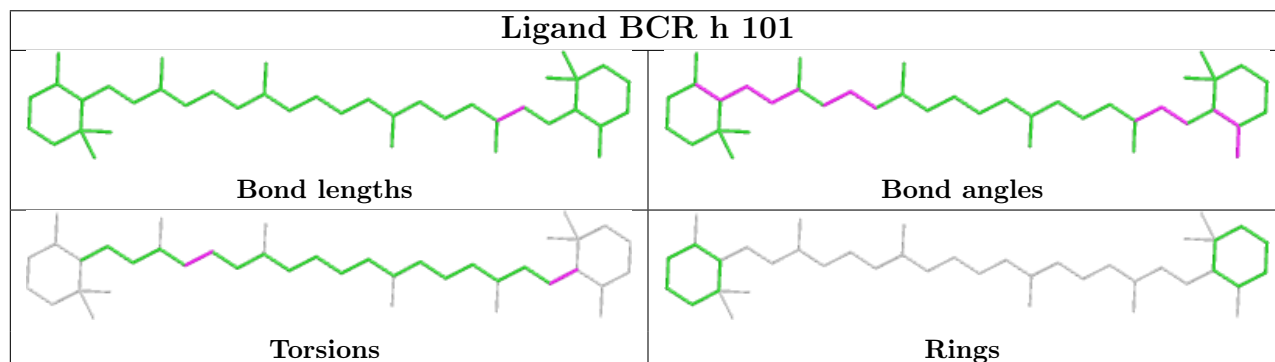
Ligand CLA b 616

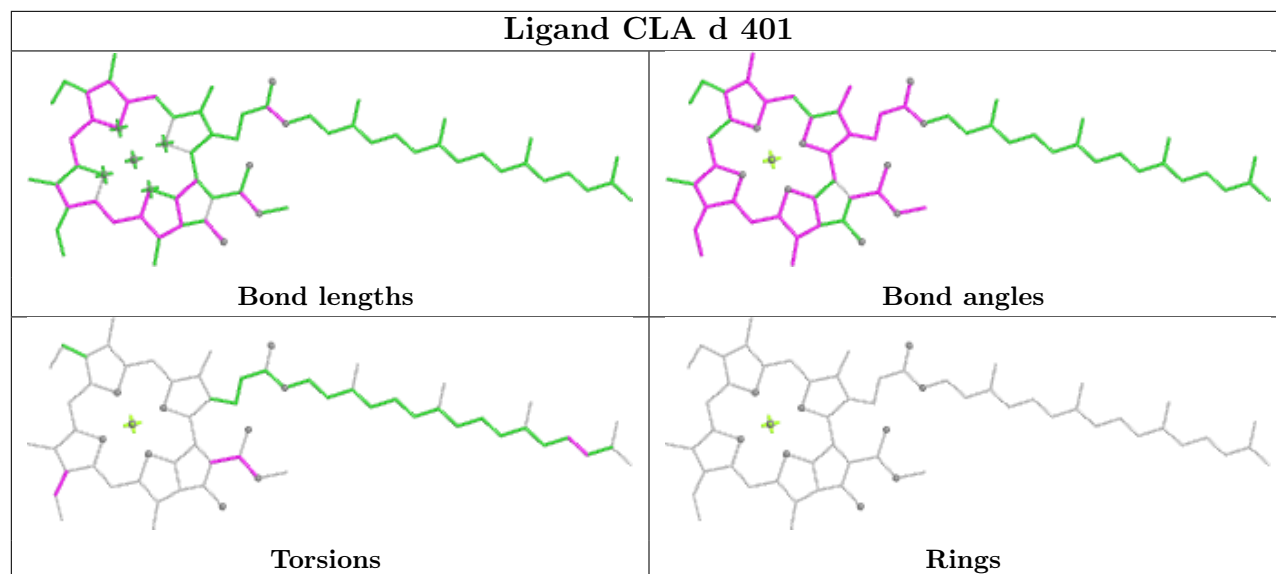
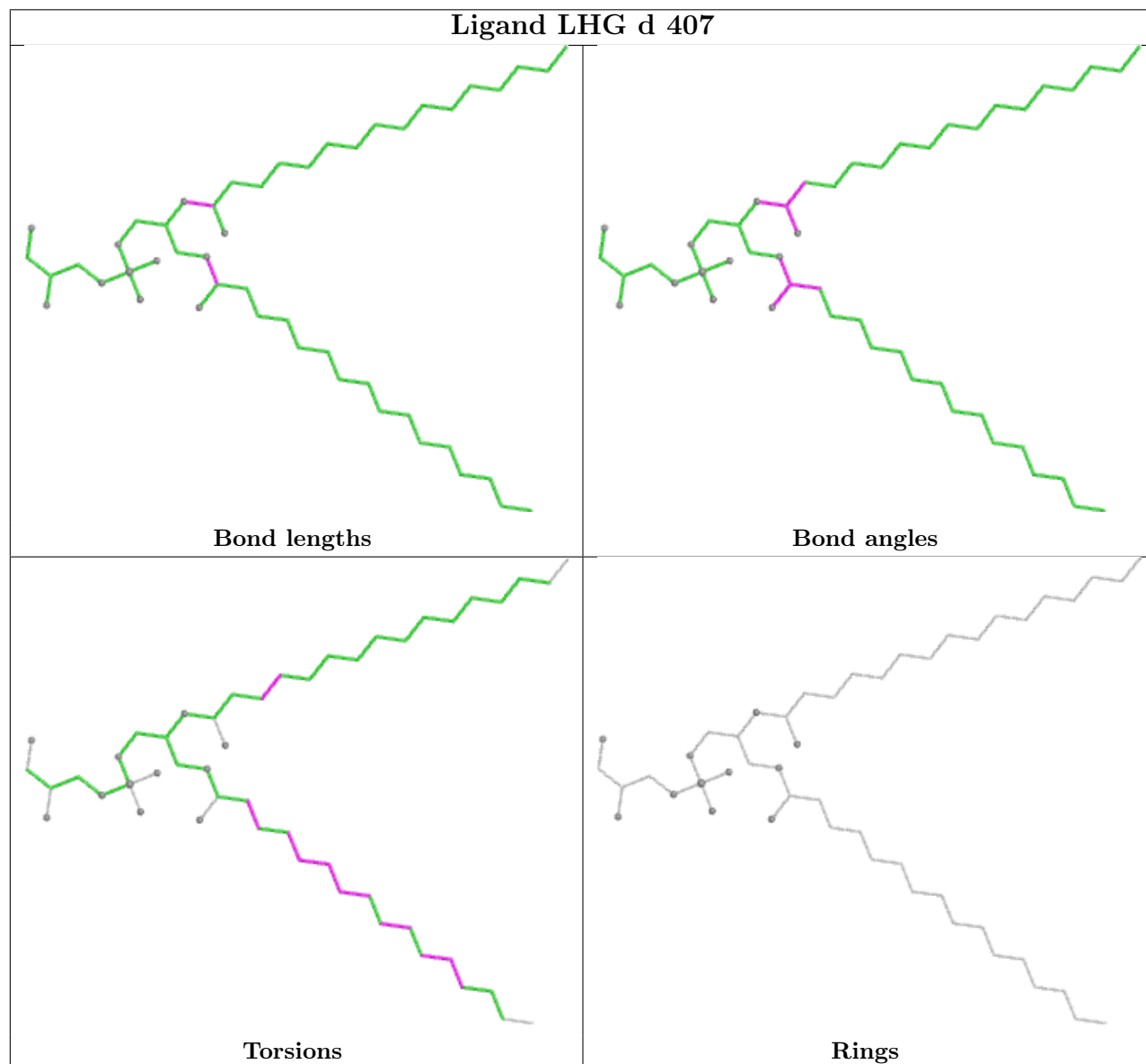


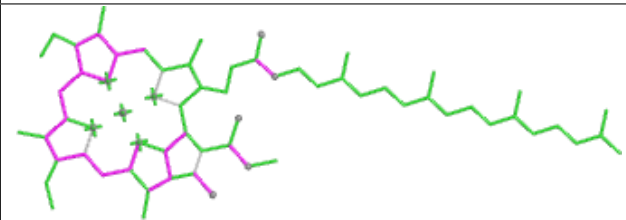
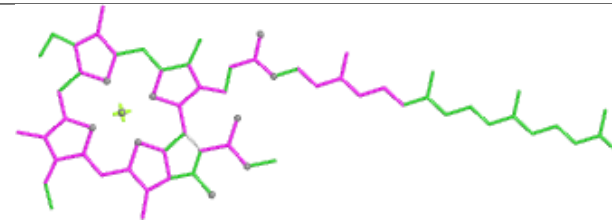
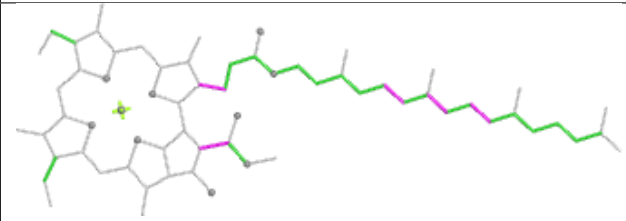
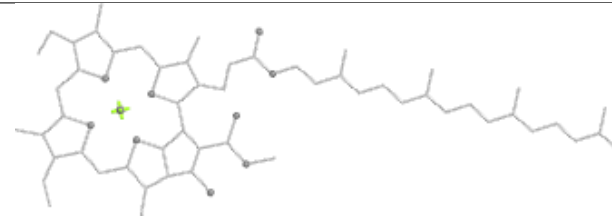
Ligand LHG d 409

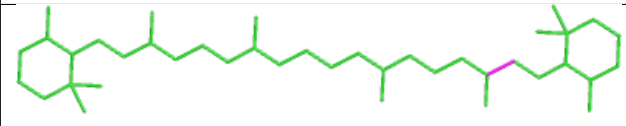
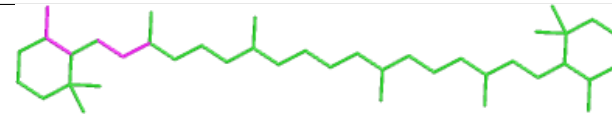
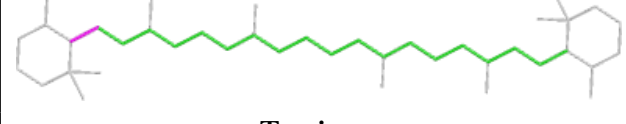
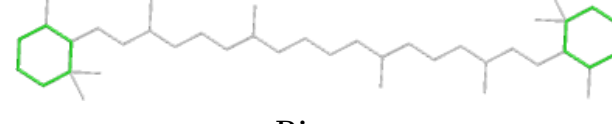


Ligand BCR h 101

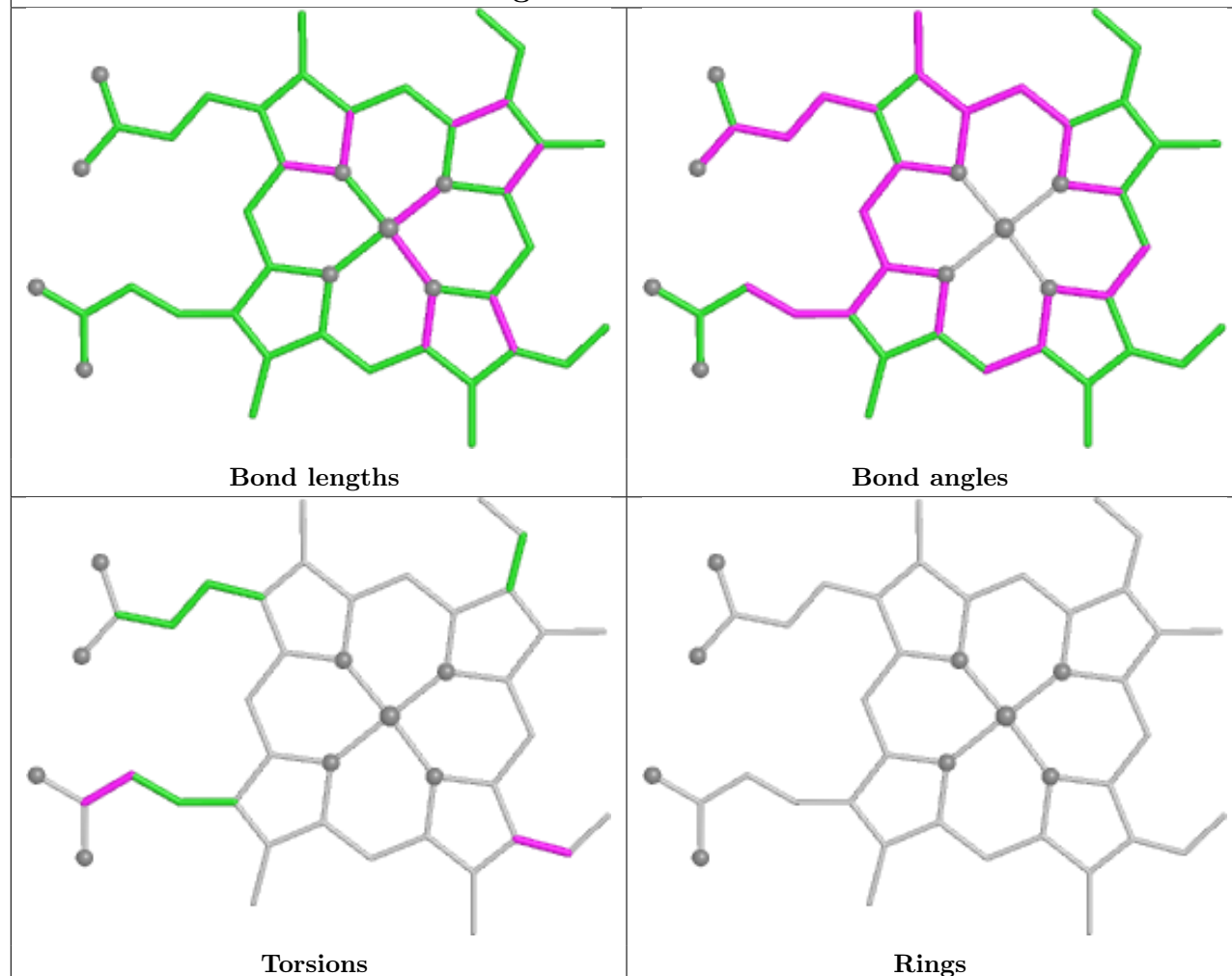




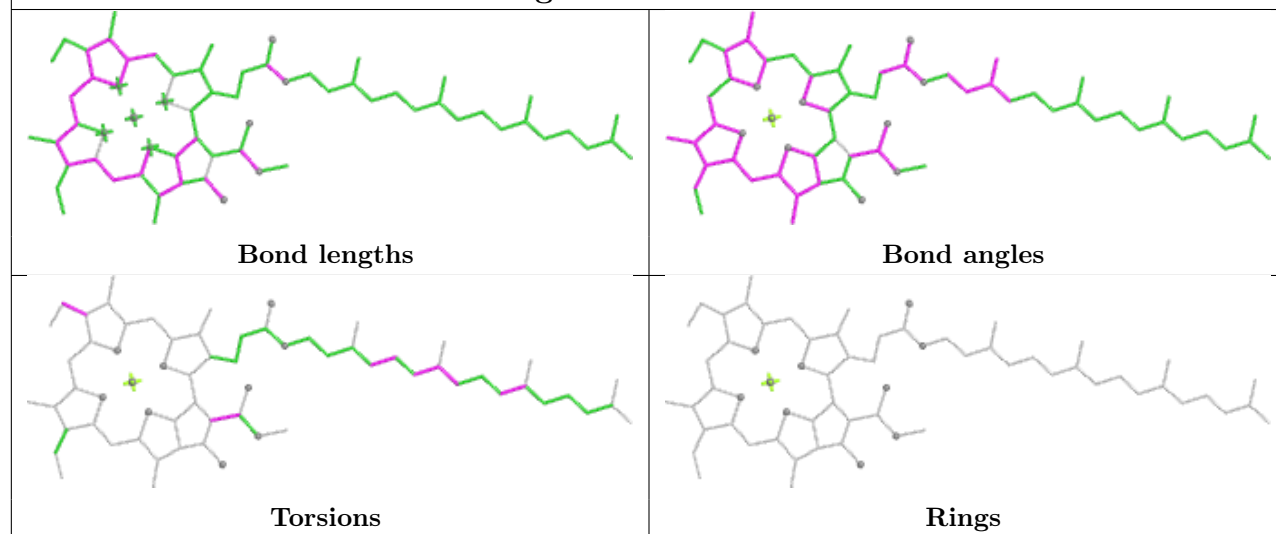
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

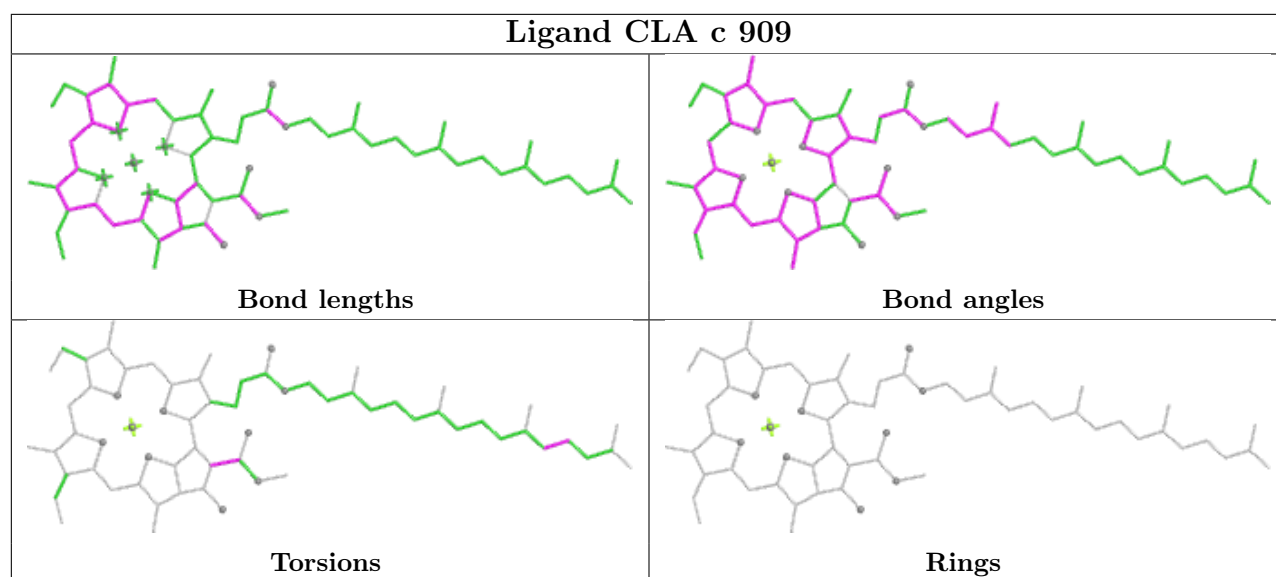
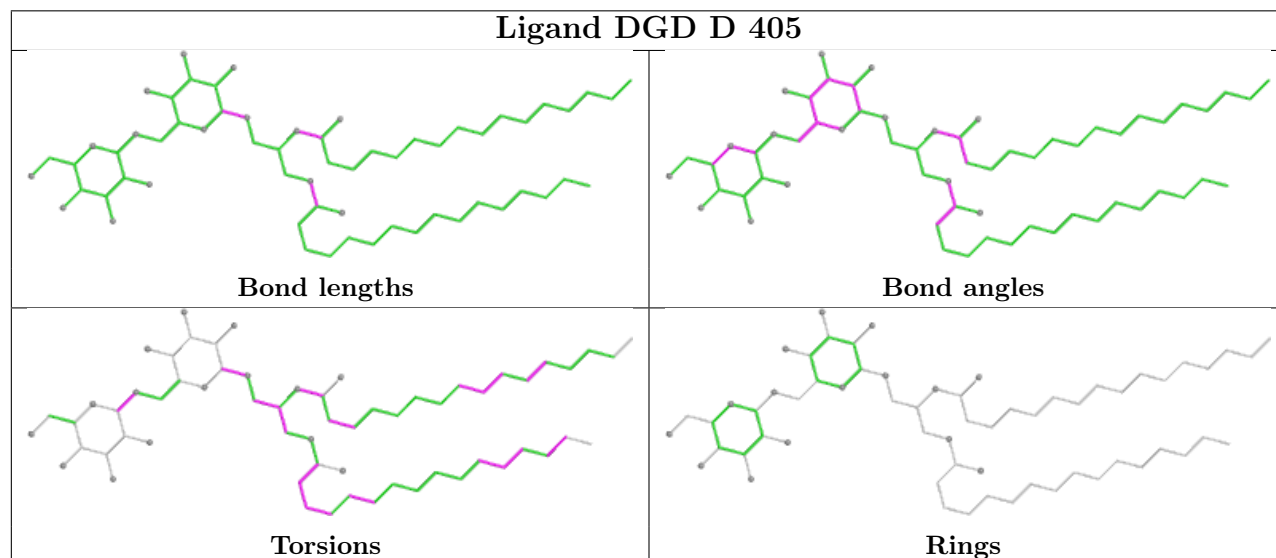
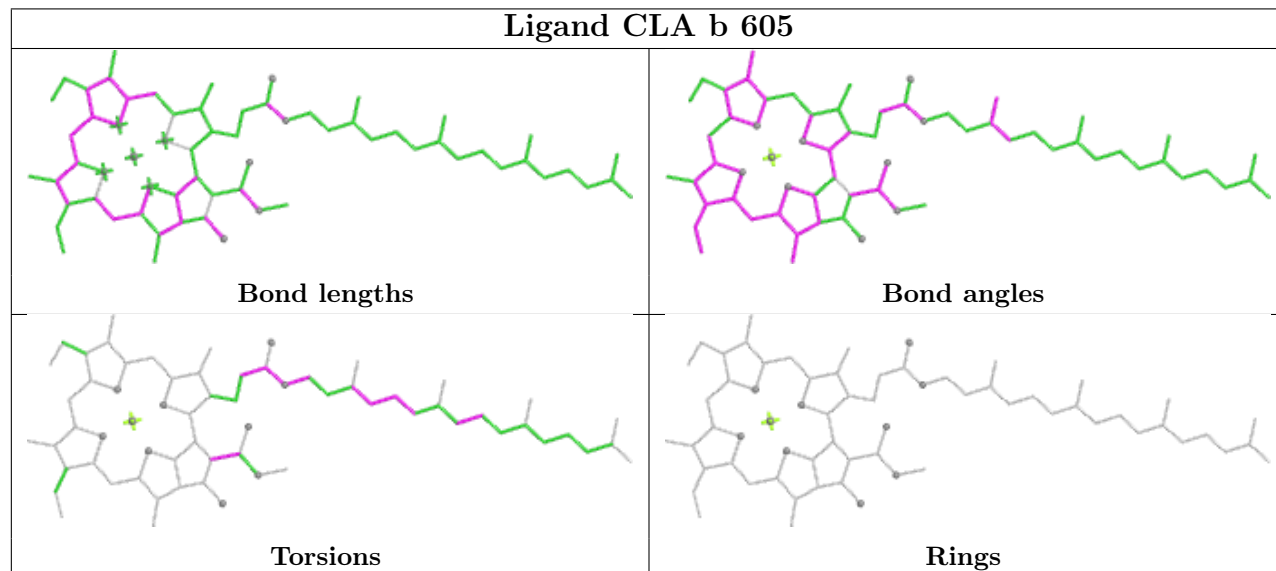
Ligand BCR b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

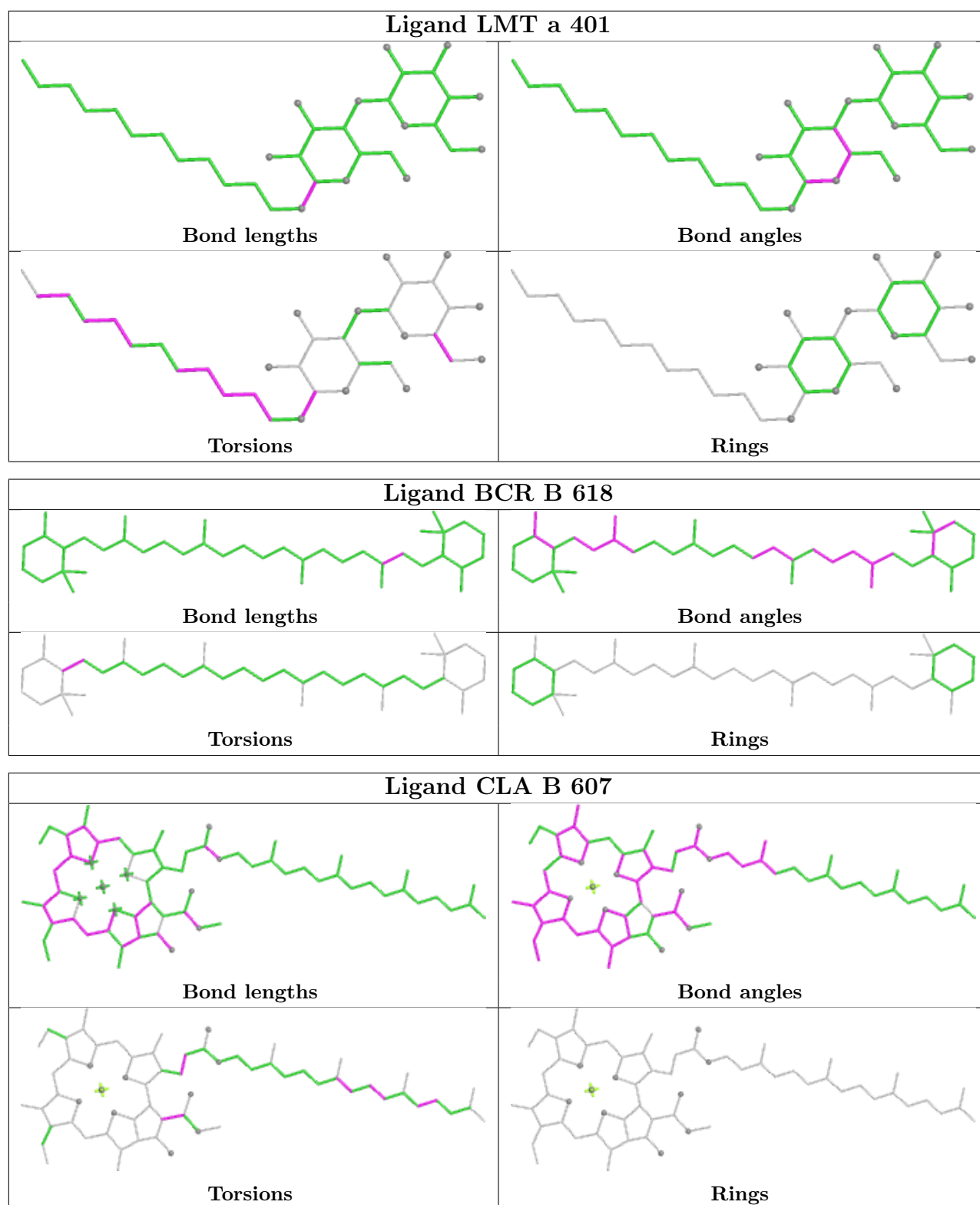
Ligand HEM e 102

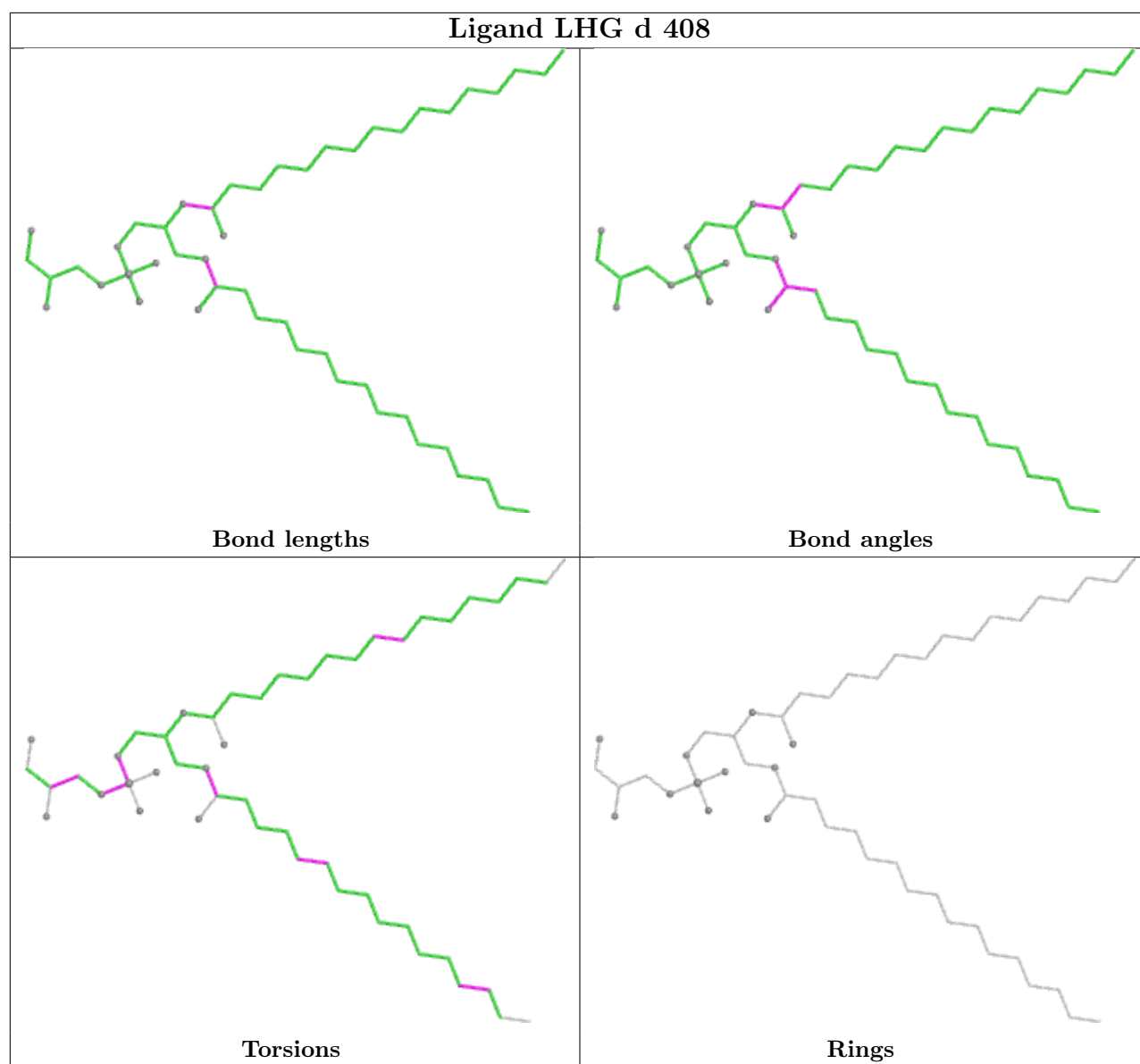


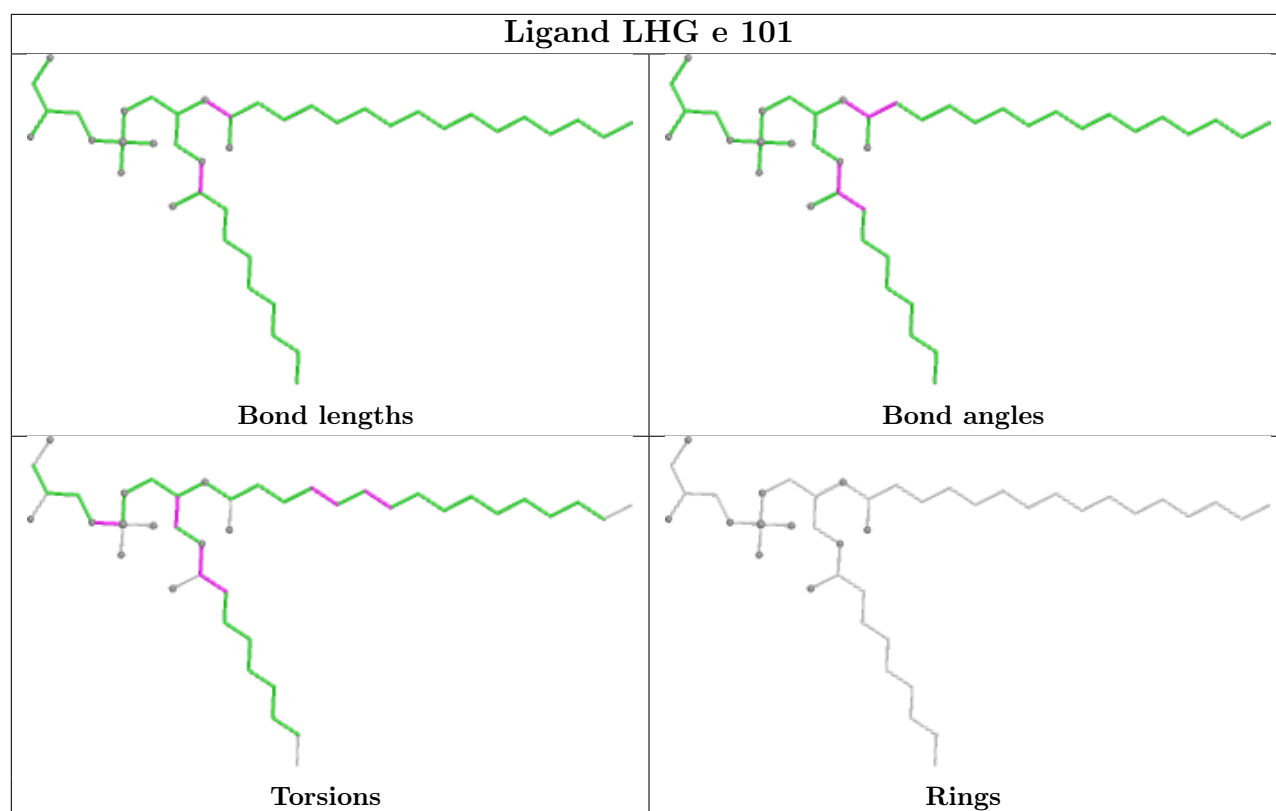
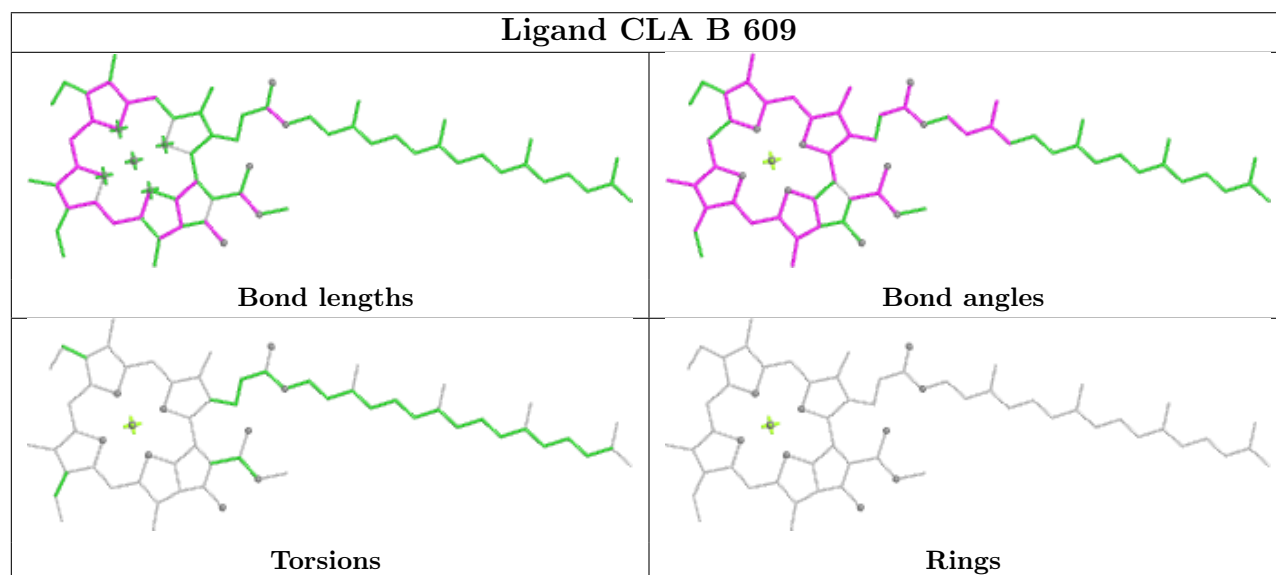
Ligand CLA b 608

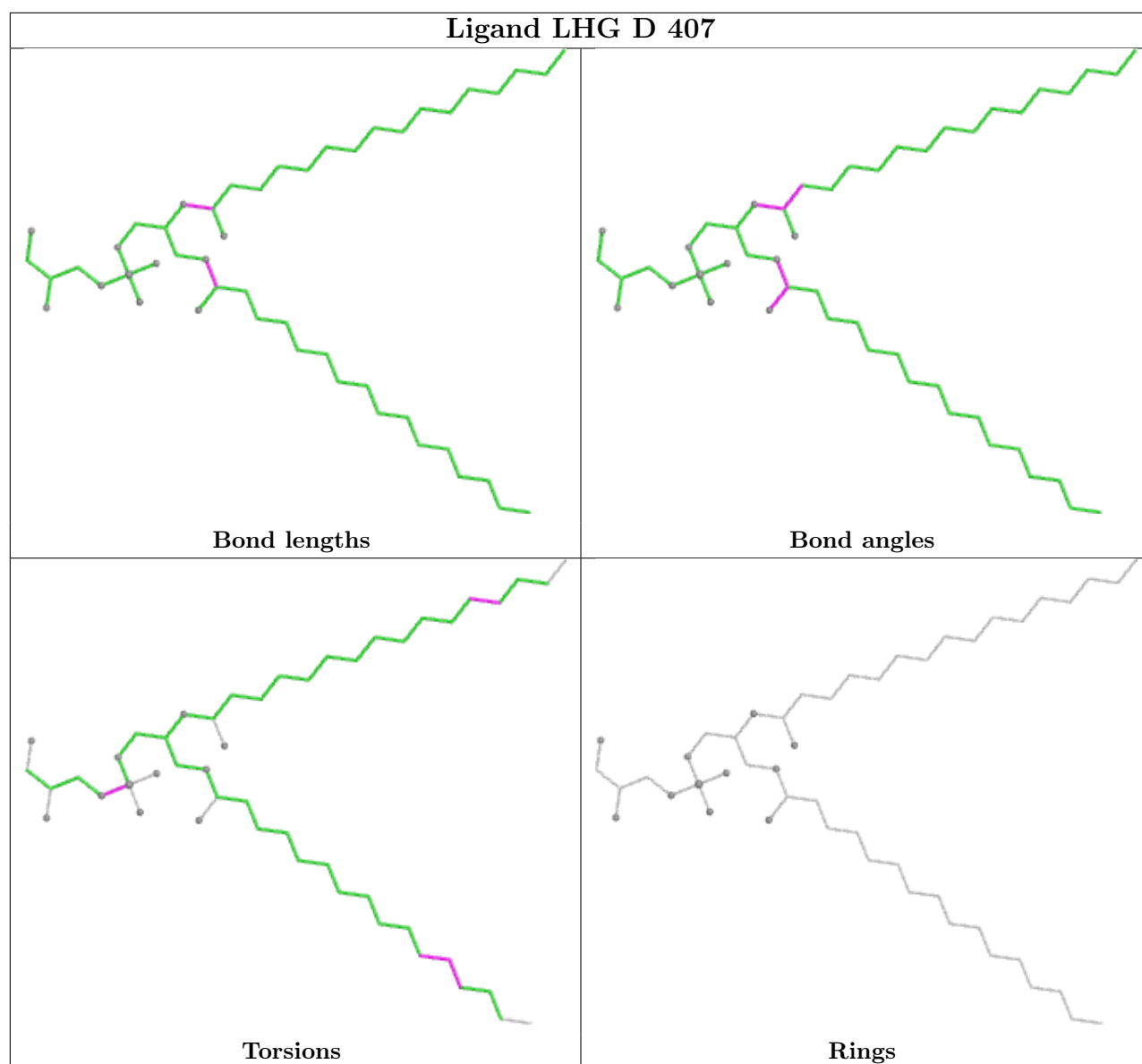
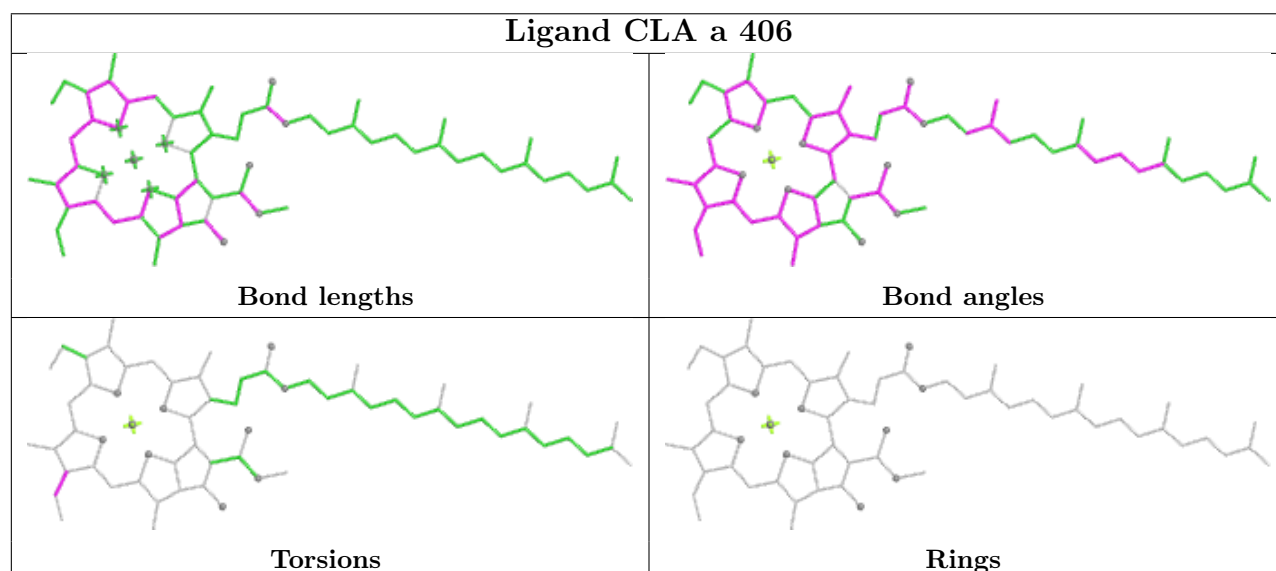












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.08	6 (1%) 67 75	13, 21, 37, 73	3 (0%)
1	a	334/344 (97%)	0.05	9 (2%) 56 62	15, 23, 47, 90	6 (1%)
2	B	504/505 (99%)	0.20	19 (3%) 44 50	14, 25, 48, 78	11 (2%)
2	b	504/505 (99%)	0.28	31 (6%) 26 31	16, 27, 58, 92	12 (2%)
3	C	451/455 (99%)	0.34	19 (4%) 40 47	17, 30, 46, 73	4 (0%)
3	c	455/455 (100%)	0.42	17 (3%) 45 52	16, 33, 49, 92	6 (1%)
4	D	342/342 (100%)	-0.09	5 (1%) 72 78	11, 22, 37, 97	1 (0%)
4	d	341/342 (99%)	-0.03	2 (0%) 85 89	12, 25, 39, 90	1 (0%)
5	E	81/84 (96%)	0.98	8 (9%) 13 14	20, 37, 66, 92	2 (2%)
5	e	81/84 (96%)	1.29	17 (20%) 2 2	23, 41, 71, 92	2 (2%)
6	F	34/44 (77%)	0.57	4 (11%) 9 10	23, 30, 50, 61	0
6	f	32/44 (72%)	0.84	3 (9%) 14 16	30, 34, 79, 84	0
7	H	65/65 (100%)	0.66	4 (6%) 26 31	18, 31, 46, 110	1 (1%)
7	h	65/65 (100%)	0.91	7 (10%) 11 12	27, 35, 52, 105	0
8	I	37/38 (97%)	1.13	6 (16%) 4 5	26, 33, 88, 108	0
8	i	37/38 (97%)	0.92	6 (16%) 4 5	27, 33, 73, 102	0
9	J	38/39 (97%)	1.07	6 (15%) 5 5	24, 35, 84, 98	0
9	j	39/39 (100%)	1.10	7 (17%) 3 3	29, 38, 84, 96	0
10	K	37/37 (100%)	0.79	3 (8%) 18 21	27, 35, 54, 65	0
10	k	37/37 (100%)	1.07	5 (13%) 7 7	30, 38, 55, 68	0
11	L	37/37 (100%)	0.04	3 (8%) 18 21	11, 19, 56, 82	1 (2%)
11	l	37/37 (100%)	0.18	2 (5%) 31 37	11, 20, 58, 83	1 (2%)
12	M	33/36 (91%)	0.27	3 (9%) 15 17	13, 21, 45, 89	1 (3%)
12	m	33/36 (91%)	0.16	2 (6%) 27 31	16, 21, 41, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.48	17 (6%) 22 26	16, 31, 66, 110	8 (3%)
13	o	243/244 (99%)	0.64	31 (12%) 7 9	15, 33, 71, 125	5 (2%)
14	T	29/32 (90%)	0.21	2 (6%) 23 26	16, 20, 43, 89	1 (3%)
14	t	29/32 (90%)	0.29	2 (6%) 23 26	16, 20, 46, 89	1 (3%)
15	U	97/104 (93%)	0.47	4 (4%) 41 48	21, 31, 54, 84	0
15	u	97/104 (93%)	0.33	2 (2%) 63 70	23, 33, 51, 84	0
16	V	137/137 (100%)	0.42	5 (3%) 46 53	16, 31, 51, 69	1 (0%)
16	v	137/137 (100%)	0.52	5 (3%) 46 53	24, 36, 57, 70	0
17	Y	29/30 (96%)	2.02	10 (34%) 1 0	35, 47, 82, 101	0
17	y	29/30 (96%)	2.00	14 (48%) 0 0	38, 50, 83, 100	0
18	X	39/40 (97%)	1.40	8 (20%) 2 2	31, 38, 75, 102	0
18	x	39/40 (97%)	1.20	7 (17%) 3 3	33, 41, 83, 102	0
19	Z	62/62 (100%)	1.84	21 (33%) 1 0	36, 47, 83, 96	0
19	z	62/62 (100%)	2.12	28 (45%) 0 0	42, 49, 82, 96	0
20	R	34/34 (100%)	3.20	27 (79%) 0 0	54, 75, 98, 106	0
All	All	5294/5384 (98%)	0.41	377 (7%) 22 25	11, 29, 61, 125	68 (1%)

The worst 5 of 377 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	10.5
7	H	65	LEU	9.2
17	Y	18	VAL	8.2
7	h	65	LEU	7.4
20	R	24	LEU	7.3

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

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
12	FME	m	1	10/11	0.92	0.15	13,32,67,68	0
14	FME	t	1	10/11	0.93	0.09	12,22,31,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	T	1	10/11	0.95	0.09	18,26,40,49	0
12	FME	M	1	10/11	0.95	0.14	23,36,70,74	0
8	FME	I	1	10/11	0.96	0.08	22,34,38,38	0
8	FME	i	1	10/11	0.97	0.08	21,31,39,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
29	LMT	f	103	35/35	0.65	0.21	43,86,107,111	0
36	DGD	D	405	62/66	0.65	0.22	48,79,113,122	0
29	LMT	E	102	35/35	0.68	0.22	43,80,109,115	0
29	LMT	C	522	35/35	0.70	0.21	52,81,102,104	0
36	DGD	d	406	62/66	0.70	0.23	38,89,122,130	0
33	CA	b	604	1/1	0.71	0.19	117,117,117,117	0
28	GOL	v	203	6/6	0.72	0.22	39,74,86,87	0
34	LMG	z	101	39/55	0.72	0.24	45,82,99,107	0
29	LMT	b	625	25/35	0.72	0.20	44,67,109,119	0
28	GOL	V	203	6/6	0.72	0.23	50,64,71,72	0
37	LHG	e	101	42/49	0.72	0.22	52,89,118,129	0
28	GOL	B	637	6/6	0.73	0.23	51,72,83,86	0
32	UNL	B	635	33/-	0.74	0.23	33,58,102,102	0
29	LMT	m	102	35/35	0.74	0.19	33,61,79,95	0
28	GOL	O	302	6/6	0.75	0.14	49,55,57,61	0
35	HTG	B	626	19/19	0.75	0.18	48,81,94,95	0
32	UNL	b	634	33/-	0.75	0.23	29,62,111,117	0
32	UNL	m	101	10/-	0.75	0.22	35,50,55,61	0
32	UNL	A	420	28/-	0.75	0.22	50,71,78,86	0
35	HTG	d	412	16/19	0.76	0.19	38,78,97,98	0
35	HTG	B	634	19/19	0.76	0.17	32,76,109,127	0
35	HTG	c	923	19/19	0.77	0.16	45,80,94,97	0
32	UNL	I	101	40/-	0.77	0.22	27,62,110,120	0
32	UNL	K	101	34/-	0.77	0.19	37,61,83,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	HTG	D	411	16/19	0.77	0.20	38,102,111,112	0
35	HTG	b	627	19/19	0.77	0.17	49,86,110,116	0
32	UNL	M	102	10/-	0.78	0.19	28,38,57,58	0
34	LMG	C	521	51/55	0.78	0.18	32,69,88,108	0
32	UNL	c	926	32/-	0.78	0.23	39,79,98,105	0
32	UNL	a	418	30/-	0.78	0.22	42,66,98,106	0
32	UNL	i	101	40/-	0.79	0.21	28,62,105,117	0
29	LMT	m	104	35/35	0.79	0.18	29,59,85,86	0
35	HTG	c	922	19/19	0.80	0.17	43,67,84,95	0
28	GOL	C	525	6/6	0.80	0.16	32,41,61,69	0
32	UNL	j	102	10/-	0.80	0.21	47,57,63,63	0
29	LMT	c	921	35/35	0.80	0.18	46,76,97,104	0
32	UNL	J	102	10/-	0.80	0.23	39,51,64,67	0
27	SQD	a	402	54/54	0.80	0.16	29,55,76,90	0
35	HTG	b	603	19/19	0.81	0.18	46,84,110,111	0
29	LMT	a	401	35/35	0.81	0.18	21,53,74,80	0
29	LMT	A	417	35/35	0.81	0.17	22,57,79,97	0
34	LMG	Z	101	37/55	0.81	0.21	30,75,96,112	0
32	UNL	d	411	36/-	0.81	0.19	32,56,104,111	0
27	SQD	L	102	54/54	0.81	0.19	24,52,86,91	0
28	GOL	v	204	6/6	0.81	0.17	54,66,71,80	0
32	UNL	D	410	40/-	0.81	0.21	24,54,93,101	0
31	PL9	a	417	55/55	0.82	0.22	41,73,92,99	0
28	GOL	B	628	6/6	0.82	0.17	33,42,54,72	0
37	LHG	E	101	42/49	0.82	0.17	22,63,78,93	0
29	LMT	B	623	35/35	0.82	0.17	26,74,96,101	0
29	LMT	B	636	25/35	0.83	0.21	24,61,106,122	0
27	SQD	A	416	54/54	0.83	0.17	26,51,78,85	0
35	HTG	C	524	19/19	0.83	0.15	41,69,99,100	0
28	GOL	b	632	6/6	0.83	0.19	38,52,59,59	0
35	HTG	V	202	19/19	0.83	0.18	40,59,77,163	0
34	LMG	c	920	51/55	0.83	0.17	33,74,88,93	0
28	GOL	T	103	6/6	0.83	0.22	52,68,70,79	0
27	SQD	f	102	43/54	0.84	0.18	41,75,103,108	0
34	LMG	a	412	51/55	0.84	0.18	33,62,84,90	0
28	GOL	a	415	6/6	0.85	0.16	48,62,65,66	0
28	GOL	B	631	6/6	0.85	0.19	30,48,62,65	0
34	LMG	C	501	51/55	0.85	0.15	34,56,76,85	0
28	GOL	c	925	6/6	0.85	0.19	34,52,63,66	0
31	PL9	A	419	55/55	0.85	0.19	28,56,91,98	0
28	GOL	t	102	6/6	0.85	0.20	22,59,67,67	0
29	LMT	M	101	35/35	0.85	0.15	23,52,69,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	T	101	6/6	0.85	0.20	54,60,61,69	0
32	UNL	d	413	18/-	0.85	0.18	30,52,81,84	0
28	GOL	A	414	6/6	0.85	0.15	30,40,43,49	0
27	SQD	B	621	54/54	0.85	0.16	26,55,94,104	0
28	GOL	A	415	6/6	0.86	0.17	36,49,64,64	0
32	UNL	D	409	17/-	0.86	0.15	30,40,63,66	0
24	CLA	c	914	65/65	0.86	0.15	35,48,81,87	0
28	GOL	V	206	6/6	0.86	0.15	47,63,66,66	0
29	LMT	m	103	35/35	0.86	0.13	19,48,62,74	0
28	GOL	a	413	6/6	0.86	0.12	30,32,37,42	0
28	GOL	B	629	6/6	0.86	0.17	28,42,50,56	0
29	LMT	b	601	25/35	0.86	0.20	18,55,104,111	0
27	SQD	F	101	43/54	0.86	0.17	34,59,81,90	0
32	UNL	d	410	17/-	0.87	0.16	34,48,82,82	0
28	GOL	F	103	6/6	0.87	0.15	60,65,71,71	0
33	CA	B	601	1/1	0.87	0.09	83,83,83,83	0
35	HTG	C	523	19/19	0.87	0.16	54,62,86,88	0
35	HTG	b	626	19/19	0.88	0.19	30,50,86,86	0
32	UNL	X	101	18/-	0.88	0.16	29,44,62,79	0
34	LMG	C	520	51/55	0.88	0.16	22,52,72,90	0
24	CLA	b	605	65/65	0.89	0.14	29,48,89,102	0
34	LMG	c	919	51/55	0.89	0.16	29,57,78,81	0
28	GOL	f	101	6/6	0.89	0.14	44,50,62,64	0
26	BCR	k	101	40/40	0.89	0.13	34,45,63,75	0
35	HTG	B	633	19/19	0.90	0.12	28,54,70,76	0
35	HTG	b	602	19/19	0.90	0.13	29,45,65,68	0
27	SQD	a	411	54/54	0.90	0.15	32,52,73,81	0
28	GOL	B	632	6/6	0.90	0.14	24,40,53,57	0
35	HTG	B	625	19/19	0.90	0.17	28,43,74,86	0
28	GOL	B	627	6/6	0.90	0.17	23,36,45,72	0
33	CA	f	104	1/1	0.91	0.09	77,77,77,77	0
34	LMG	B	622	51/55	0.91	0.11	19,32,49,71	0
24	CLA	c	913	65/65	0.91	0.11	31,40,59,65	0
24	CLA	C	507	65/65	0.91	0.12	25,40,75,77	0
26	BCR	C	515	40/40	0.91	0.11	29,38,49,53	0
26	BCR	K	103	40/40	0.91	0.09	24,30,40,43	0
28	GOL	b	628	6/6	0.91	0.10	30,35,42,53	0
34	LMG	b	624	51/55	0.91	0.11	21,36,57,81	0
28	GOL	b	631	6/6	0.91	0.12	28,41,48,51	0
26	BCR	c	915	40/40	0.91	0.10	25,34,42,45	0
26	BCR	d	404	40/40	0.91	0.11	27,36,54,60	0
28	GOL	A	413	6/6	0.91	0.10	23,30,33,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	h	101	40/40	0.91	0.10	25,35,48,52	0
24	CLA	C	513	65/65	0.91	0.11	27,40,59,71	0
24	CLA	B	602	65/65	0.91	0.13	22,40,80,101	0
26	BCR	k	102	40/40	0.92	0.10	30,37,50,61	0
26	BCR	y	101	40/40	0.92	0.11	29,37,57,63	0
28	GOL	b	629	6/6	0.92	0.12	27,36,50,54	0
28	GOL	b	630	6/6	0.92	0.11	35,39,50,53	0
27	SQD	A	412	54/54	0.92	0.13	15,45,72,85	0
26	BCR	K	102	40/40	0.92	0.09	22,30,39,47	0
28	GOL	b	633	6/6	0.92	0.14	34,60,65,65	0
34	LMG	j	101	51/55	0.92	0.13	25,35,71,81	0
24	CLA	C	514	65/65	0.92	0.11	30,42,67,73	0
24	CLA	c	902	65/65	0.92	0.10	26,32,45,52	0
28	GOL	o	302	6/6	0.92	0.11	44,50,53,58	0
26	BCR	B	620	40/40	0.92	0.09	16,26,39,49	0
24	CLA	c	907	65/65	0.92	0.13	28,37,64,72	0
26	BCR	H	101	40/40	0.92	0.10	19,32,45,59	0
24	CLA	c	912	65/65	0.93	0.10	27,36,50,54	0
26	BCR	T	102	40/40	0.93	0.08	13,26,37,42	0
24	CLA	b	610	65/65	0.93	0.11	18,31,78,87	0
24	CLA	C	512	65/65	0.93	0.09	22,30,39,45	0
24	CLA	d	403	65/65	0.93	0.11	26,31,79,93	0
34	LMG	J	101	51/55	0.93	0.12	18,32,75,81	0
25	PHO	a	420	64/64	0.93	0.08	17,24,30,33	0
24	CLA	c	904	65/65	0.93	0.09	26,33,44,47	0
26	BCR	t	101	40/40	0.93	0.09	12,26,45,48	0
24	CLA	c	905	65/65	0.93	0.09	25,32,49,68	0
31	PL9	d	405	55/55	0.93	0.08	13,19,33,44	0
26	BCR	C	516	40/40	0.93	0.09	23,32,42,43	0
28	GOL	B	630	6/6	0.93	0.10	26,32,40,42	0
36	DGD	c	916	62/66	0.93	0.11	22,31,64,82	0
36	DGD	c	917	62/66	0.93	0.11	26,35,61,87	0
26	BCR	D	403	40/40	0.93	0.10	19,30,58,70	0
36	DGD	h	102	62/66	0.93	0.10	19,31,48,60	0
24	CLA	c	906	65/65	0.93	0.10	21,28,44,56	0
37	LHG	d	407	49/49	0.93	0.11	15,31,44,53	0
37	LHG	d	409	49/49	0.93	0.14	21,32,85,88	0
24	CLA	C	504	65/65	0.93	0.08	22,28,40,45	0
37	LHG	l	101	49/49	0.93	0.10	15,27,39,56	0
22	CL	U	201	1/1	0.94	0.09	50,50,50,50	0
28	GOL	V	204	6/6	0.94	0.11	19,26,30,37	0
28	GOL	V	205	6/6	0.94	0.08	34,41,45,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	PL9	D	404	55/55	0.94	0.08	11,18,31,41	0
24	CLA	C	508	65/65	0.94	0.09	23,35,47,54	0
24	CLA	C	510	65/65	0.94	0.09	23,30,45,62	0
28	GOL	a	414	6/6	0.94	0.12	25,34,43,53	0
24	CLA	C	511	65/65	0.94	0.09	21,29,38,45	0
24	CLA	c	908	65/65	0.94	0.09	26,33,49,60	0
24	CLA	c	910	65/65	0.94	0.09	27,34,47,53	0
24	CLA	c	911	65/65	0.94	0.09	24,31,43,53	0
24	CLA	B	615	65/65	0.94	0.10	12,21,66,79	0
24	CLA	B	617	65/65	0.94	0.12	16,28,79,88	0
24	CLA	C	502	65/65	0.94	0.09	22,30,42,54	0
24	CLA	a	407	65/65	0.94	0.11	18,23,72,84	0
23	BCT	a	419	4/4	0.94	0.12	21,32,41,50	0
26	BCR	A	411	40/40	0.94	0.08	15,22,29,31	0
26	BCR	B	619	40/40	0.94	0.08	15,23,46,49	0
24	CLA	b	606	65/65	0.94	0.08	22,28,38,48	0
24	CLA	C	505	65/65	0.94	0.09	18,27,47,61	0
24	CLA	b	613	65/65	0.94	0.08	23,29,42,48	0
24	CLA	b	614	65/65	0.94	0.08	20,29,39,42	0
36	DGD	C	517	62/66	0.94	0.10	19,28,60,72	0
36	DGD	C	518	62/66	0.94	0.11	19,29,78,90	0
24	CLA	b	615	65/65	0.94	0.08	17,22,38,46	0
36	DGD	H	102	62/66	0.94	0.09	16,28,46,59	0
24	CLA	b	618	65/65	0.94	0.11	14,24,78,80	0
24	CLA	b	619	65/65	0.94	0.09	20,30,49,51	0
36	DGD	c	918	62/66	0.94	0.10	25,31,52,70	0
24	CLA	b	620	65/65	0.94	0.12	19,33,77,78	0
26	BCR	a	410	40/40	0.94	0.07	15,23,28,32	0
37	LHG	D	406	49/49	0.94	0.10	14,26,38,52	0
37	LHG	D	408	49/49	0.94	0.15	17,29,88,100	0
26	BCR	b	621	40/40	0.94	0.07	14,24,33,38	0
26	BCR	b	622	40/40	0.94	0.08	14,24,43,51	0
26	BCR	b	623	40/40	0.94	0.09	18,31,42,48	0
24	CLA	C	506	65/65	0.94	0.09	18,27,47,54	0
24	CLA	c	903	65/65	0.94	0.09	24,30,41,51	0
28	GOL	C	526	6/6	0.95	0.07	17,21,26,26	0
24	CLA	b	609	65/65	0.95	0.08	16,24,37,44	0
24	CLA	B	608	65/65	0.95	0.07	11,19,28,40	0
24	CLA	b	611	65/65	0.95	0.07	13,20,31,34	0
35	HTG	O	303	19/19	0.95	0.11	23,32,46,55	0
24	CLA	b	612	65/65	0.95	0.07	21,28,40,43	0
24	CLA	d	402	65/65	0.95	0.08	16,20,36,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	609	65/65	0.95	0.07	15,24,30,36	0
25	PHO	A	408	64/64	0.95	0.07	12,16,23,24	0
25	PHO	a	408	64/64	0.95	0.07	15,18,27,30	0
33	CA	F	102	1/1	0.95	0.08	69,69,69,69	0
24	CLA	B	610	65/65	0.95	0.08	17,24,36,45	0
24	CLA	C	509	65/65	0.95	0.09	18,25,67,82	0
26	BCR	B	618	40/40	0.95	0.07	11,23,32,35	0
24	CLA	b	616	65/65	0.95	0.07	16,23,32,44	0
36	DGD	C	519	62/66	0.95	0.09	18,29,48,55	0
24	CLA	b	617	65/65	0.95	0.08	14,22,44,52	0
24	CLA	B	611	65/65	0.95	0.07	17,25,33,50	0
24	CLA	B	613	65/65	0.95	0.07	13,20,27,33	0
24	CLA	B	614	65/65	0.95	0.08	12,20,43,55	0
22	CL	v	201	1/1	0.95	0.07	62,62,62,62	0
23	BCT	A	404	4/4	0.95	0.13	21,24,36,47	0
24	CLA	D	402	65/65	0.95	0.10	18,27,68,84	0
24	CLA	B	603	65/65	0.95	0.07	17,24,36,47	0
24	CLA	a	409	65/65	0.95	0.12	18,26,79,83	0
24	CLA	B	606	65/65	0.95	0.07	13,20,31,41	0
35	HTG	B	624	19/19	0.95	0.09	20,32,43,46	0
24	CLA	B	607	65/65	0.95	0.10	16,25,70,76	0
24	CLA	c	909	65/65	0.95	0.10	23,28,67,91	0
24	CLA	b	607	65/65	0.95	0.08	21,28,38,50	0
38	HEM	e	102	43/43	0.95	0.13	37,46,76,95	0
24	CLA	B	604	65/65	0.96	0.07	16,25,32,38	0
24	CLA	b	608	65/65	0.96	0.08	15,23,51,62	0
24	CLA	C	503	65/65	0.96	0.07	20,25,39,63	0
24	CLA	d	401	65/65	0.96	0.07	14,18,27,47	0
24	CLA	B	605	65/65	0.96	0.08	13,19,44,57	0
28	GOL	v	205	6/6	0.96	0.12	23,35,46,50	0
24	CLA	B	612	65/65	0.96	0.06	12,18,30,37	0
24	CLA	D	401	65/65	0.96	0.06	12,16,32,36	0
25	PHO	A	409	64/64	0.96	0.06	13,20,29,35	0
37	LHG	D	407	49/49	0.96	0.08	13,22,44,57	0
24	CLA	A	407	65/65	0.96	0.09	13,20,71,73	0
24	CLA	a	406	65/65	0.96	0.07	15,17,32,38	0
37	LHG	L	101	49/49	0.96	0.08	12,26,38,46	0
24	CLA	A	410	65/65	0.96	0.10	17,26,80,89	0
37	LHG	d	408	49/49	0.96	0.08	15,23,41,54	0
24	CLA	A	405	65/65	0.96	0.07	13,17,27,52	0
24	CLA	B	616	65/65	0.96	0.08	16,23,42,45	0
33	CA	O	301	1/1	0.96	0.07	53,53,53,53	0

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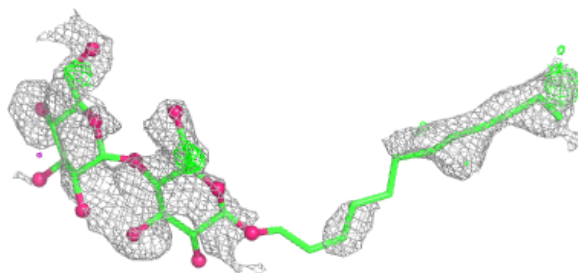
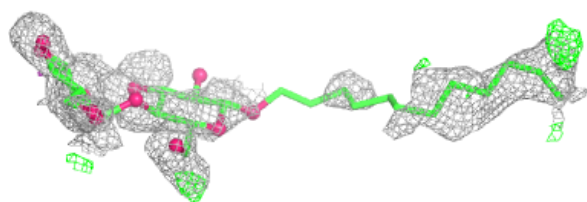
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	A	406	65/65	0.96	0.07	12,16,30,35	0
38	HEM	E	103	43/43	0.97	0.09	23,35,45,56	0
28	GOL	c	924	6/6	0.97	0.07	24,24,25,29	0
39	MG	j	103	1/1	0.97	0.09	33,33,33,33	0
40	HEC	V	201	43/43	0.97	0.08	22,25,32,39	0
40	HEC	v	202	43/43	0.97	0.08	28,31,40,46	0
33	CA	c	901	1/1	0.98	0.05	44,44,44,44	0
21	FE2	a	403	1/1	0.99	0.04	28,28,28,28	0
33	CA	o	301	1/1	0.99	0.04	54,54,54,54	0
30	OEX	A	418	10/10	0.99	0.04	15,20,24,28	0
30	OEX	a	416	10/10	0.99	0.04	18,21,24,34	0
39	MG	J	103	1/1	0.99	0.07	27,27,27,27	0
22	CL	a	404	1/1	0.99	0.04	20,20,20,20	0
22	CL	a	405	1/1	0.99	0.03	26,26,26,26	0
22	CL	A	402	1/1	0.99	0.03	18,18,18,18	0
22	CL	A	403	1/1	1.00	0.03	19,19,19,19	0
21	FE2	A	401	1/1	1.00	0.02	24,24,24,24	0

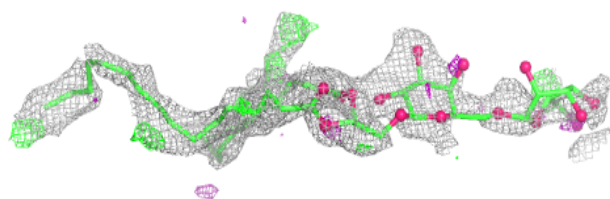
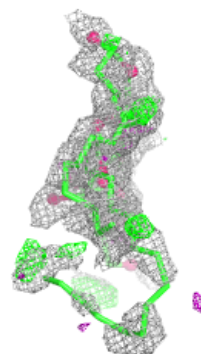
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT f 103:

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

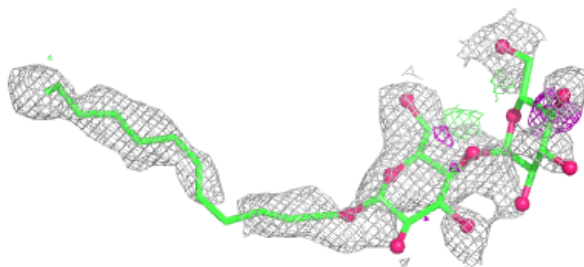
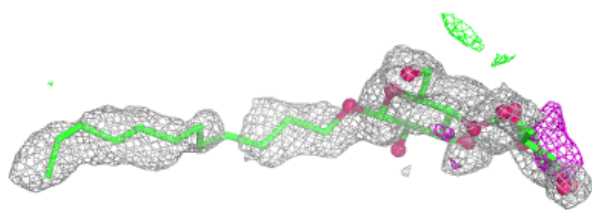
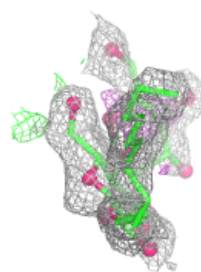
**Electron density around DGD D 405:**

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

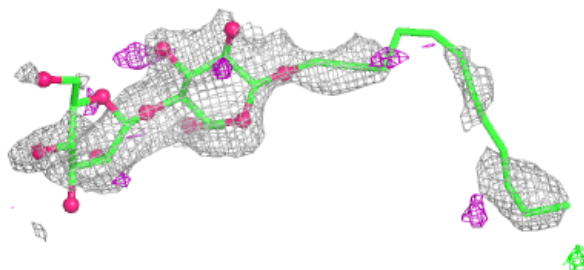
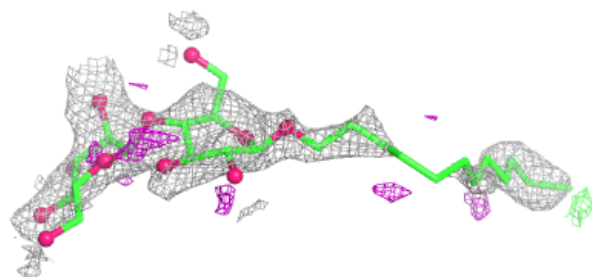
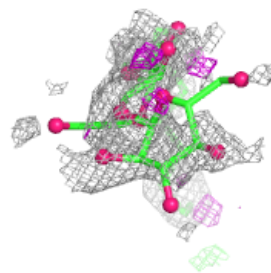


Electron density around LMT E 102:

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

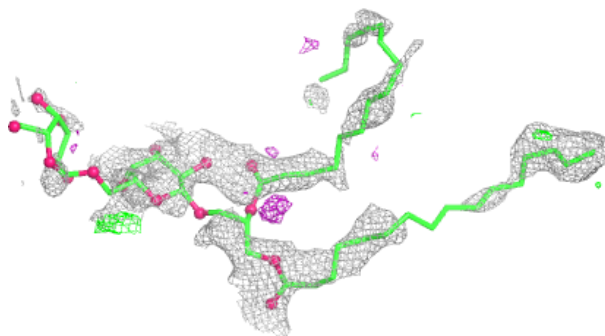
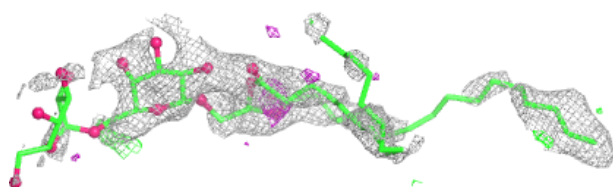
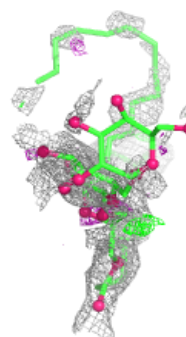
**Electron density around LMT C 522:**

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

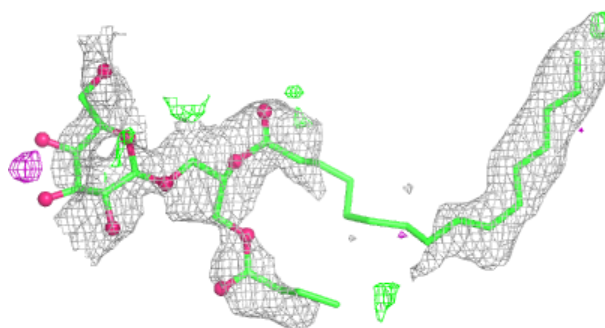
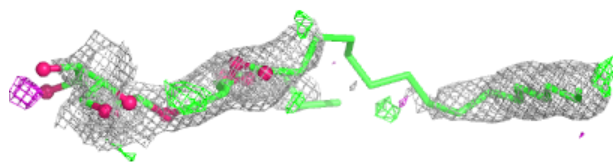
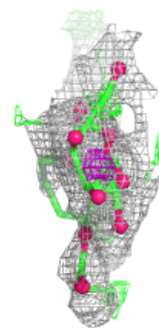


Electron density around DGD d 406:

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

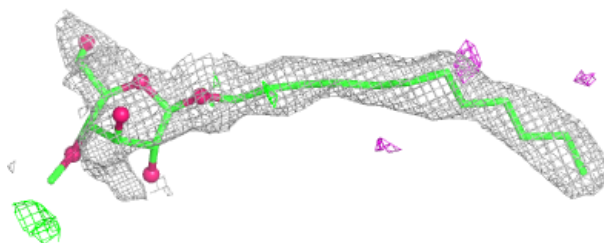
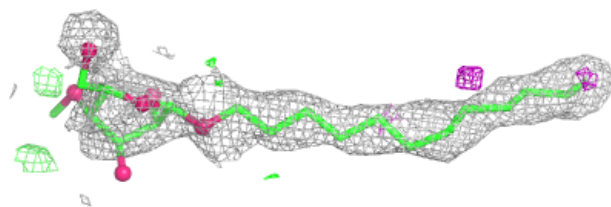
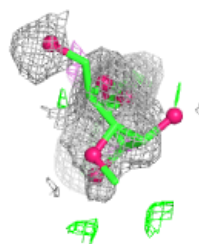
**Electron density around LMG z 101:**

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



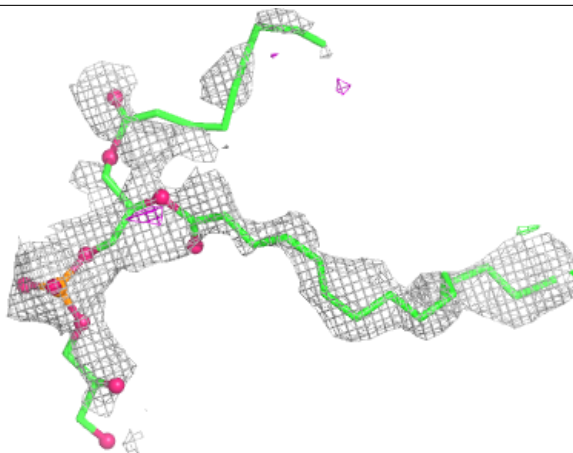
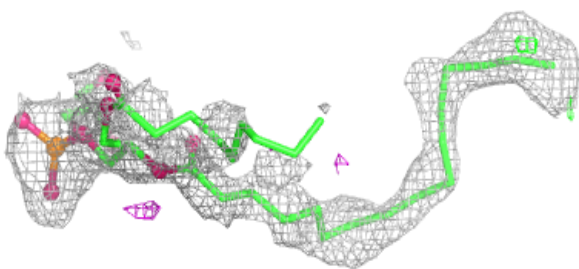
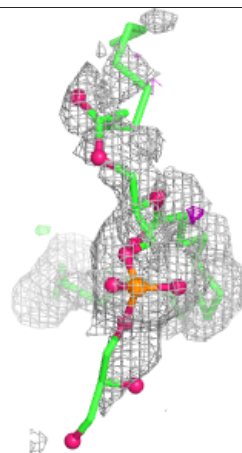
Electron density around LMT b 625:

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



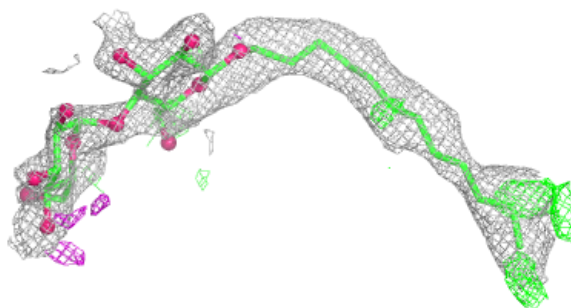
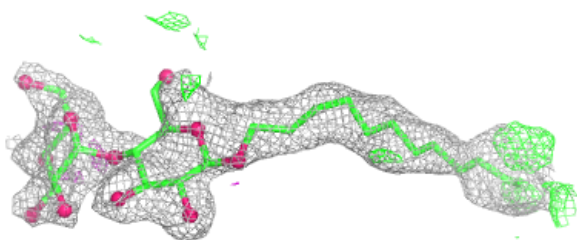
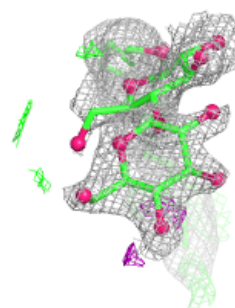
Electron density around LHG e 101:

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

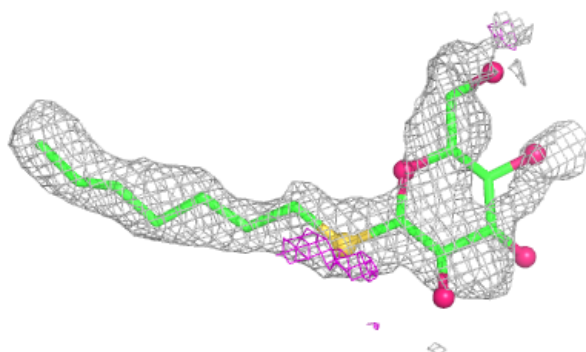
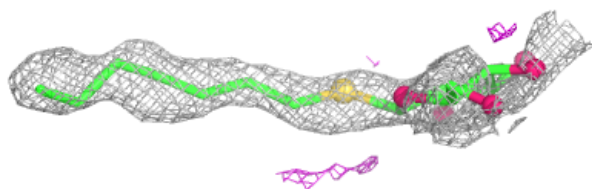
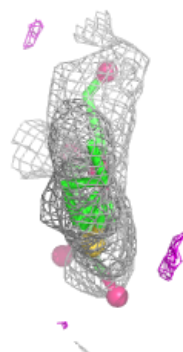


Electron density around LMT m 102:

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

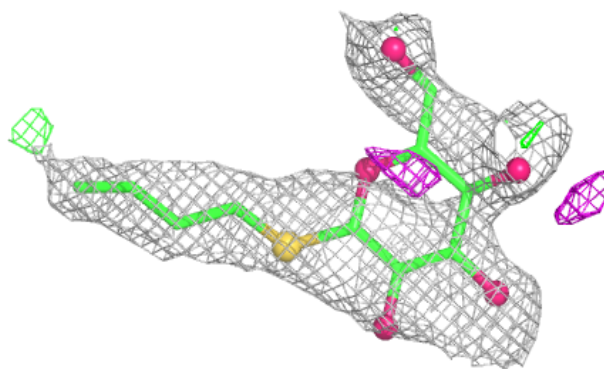
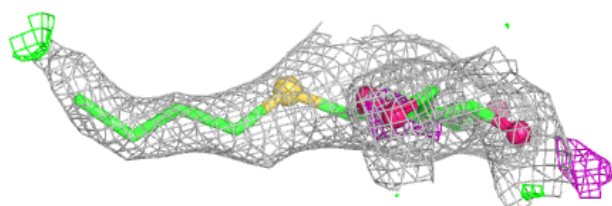
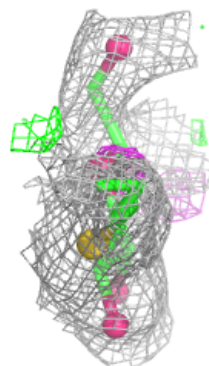
**Electron density around HTG B 626:**

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and green (positive)

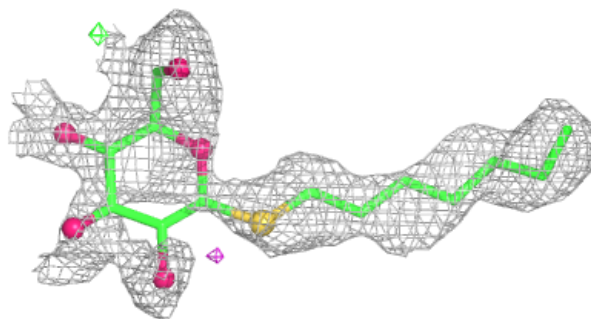
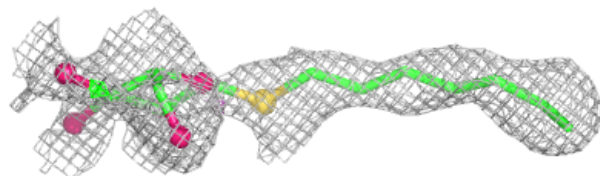
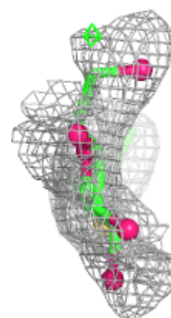


Electron density around HTG d 412:

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

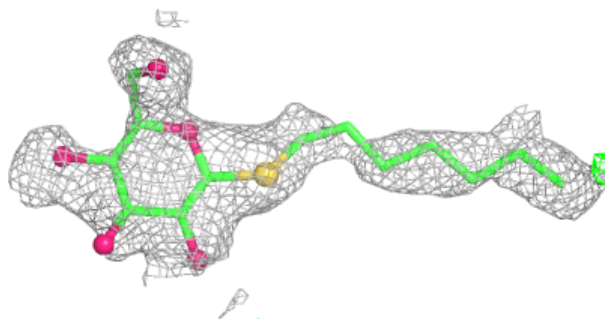
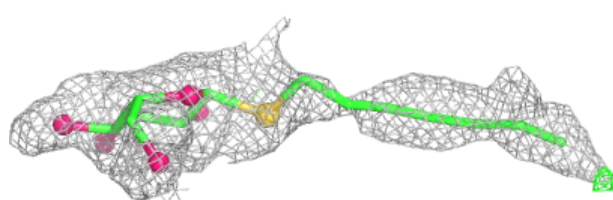
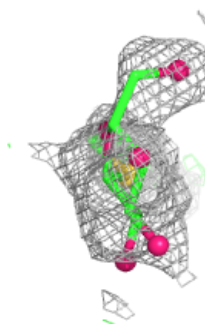
**Electron density around HTG B 634:**

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

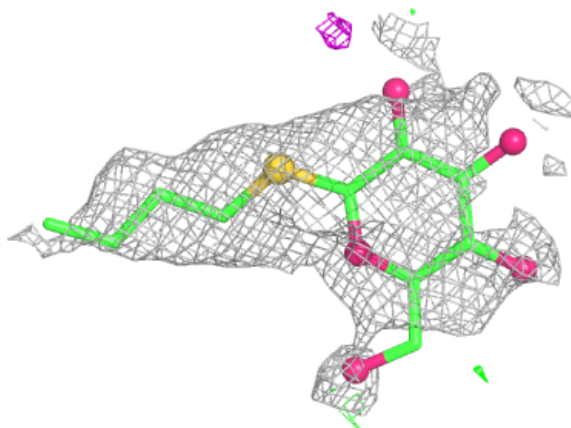
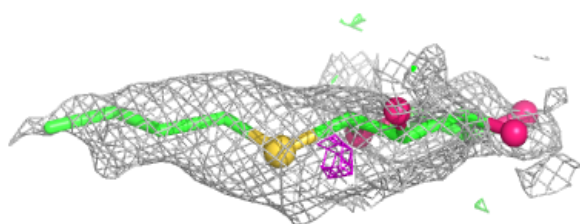
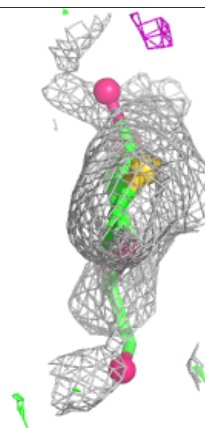


Electron density around HTG c 923:

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

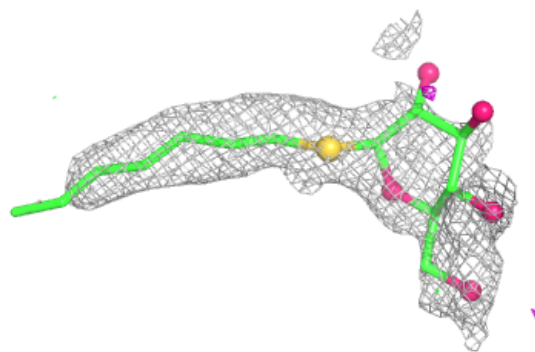
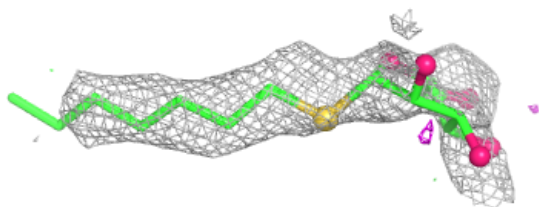
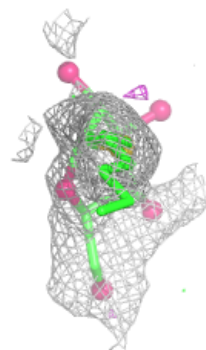
**Electron density around HTG D 411:**

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

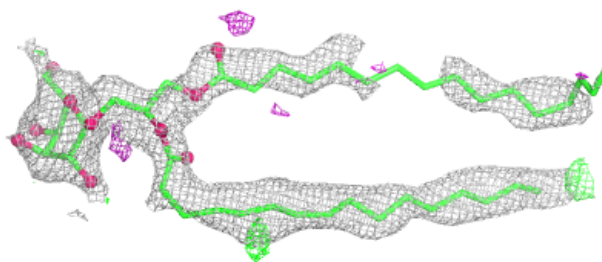
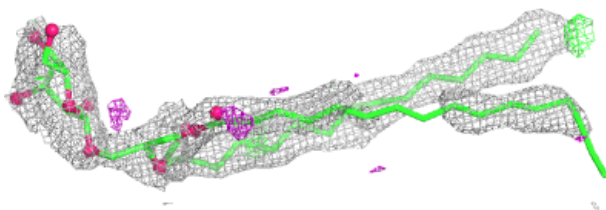
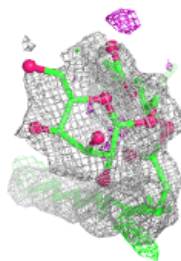


Electron density around HTG b 627:

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

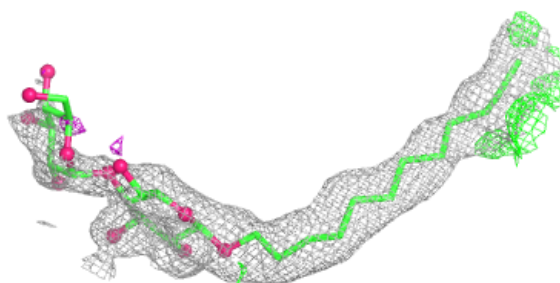
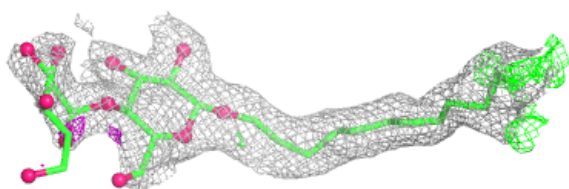
**Electron density around LMG C 521:**

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

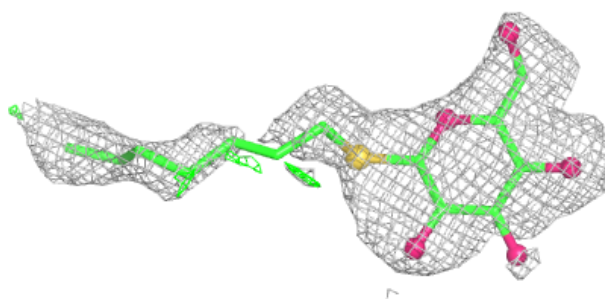
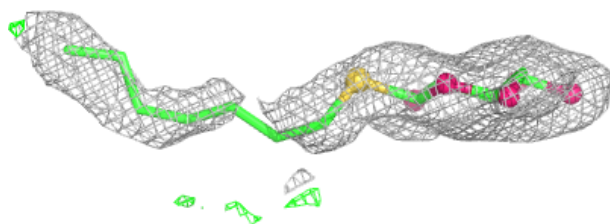
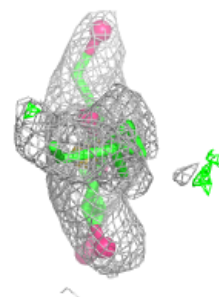


Electron density around LMT m 104:

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

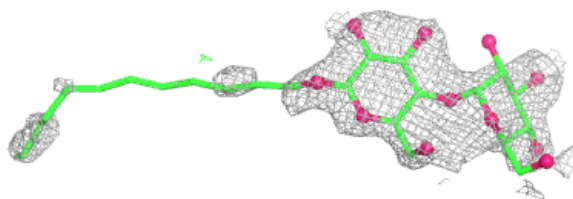
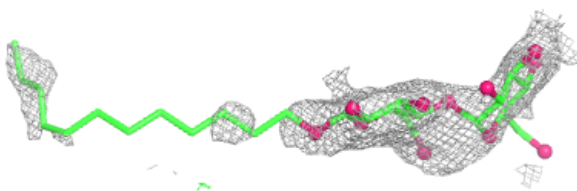
**Electron density around HTG c 922:**

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

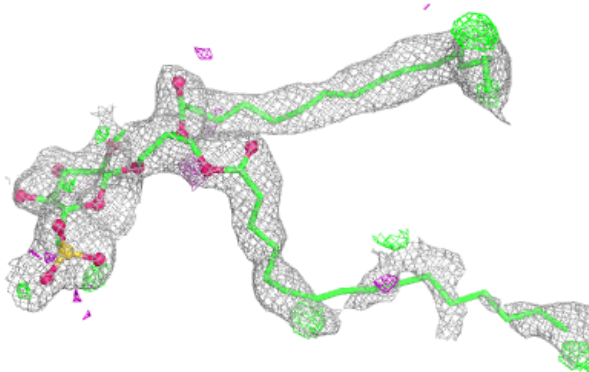
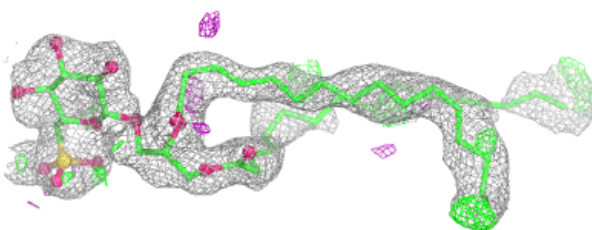
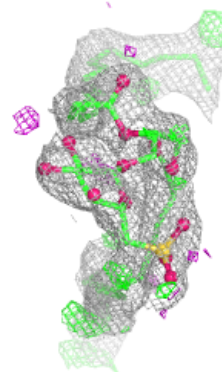


Electron density around LMT c 921:

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

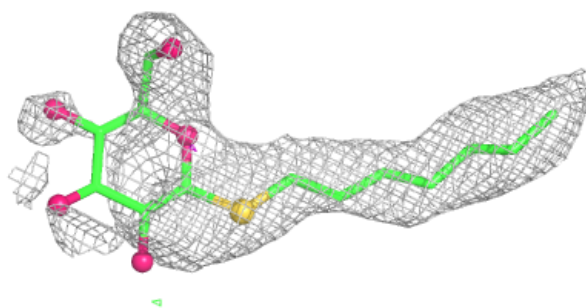
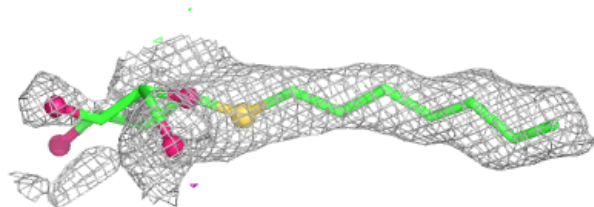
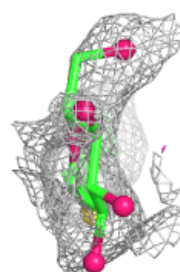
**Electron density around SQD a 402:**

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

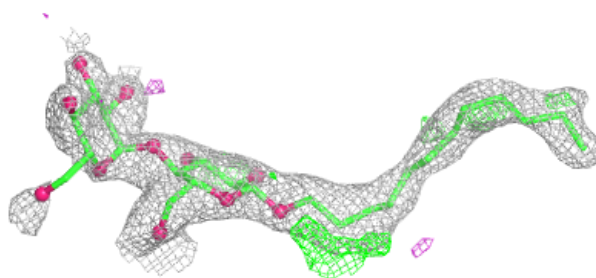
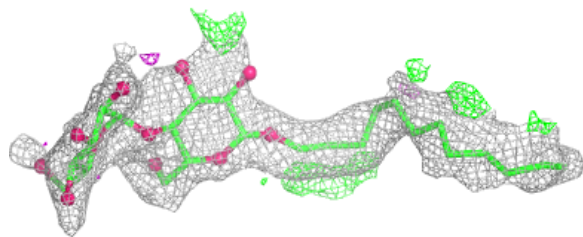
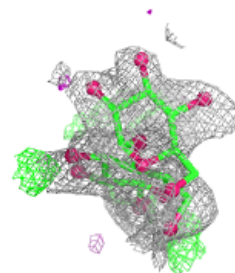


Electron density around HTG b 603:

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

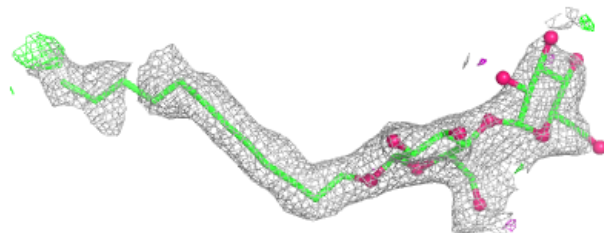
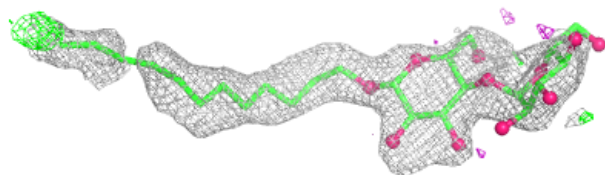
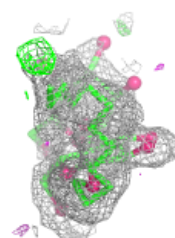
**Electron density around LMT a 401:**

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

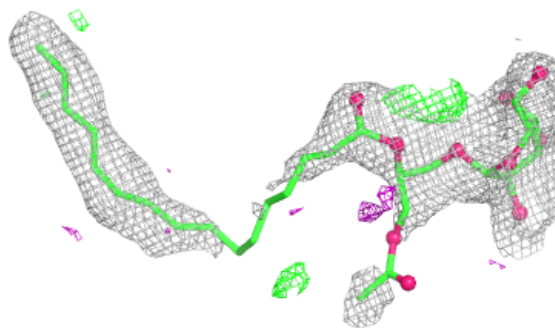
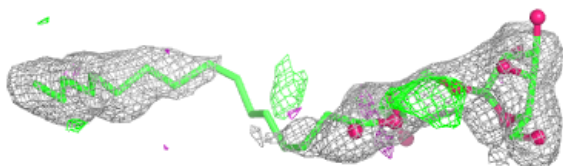
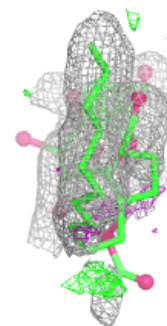


Electron density around LMT A 417:

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

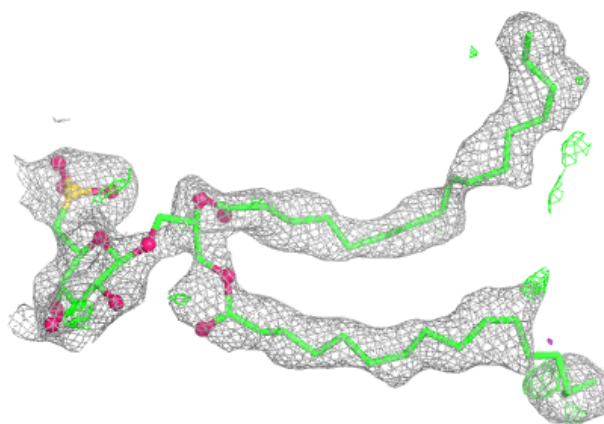
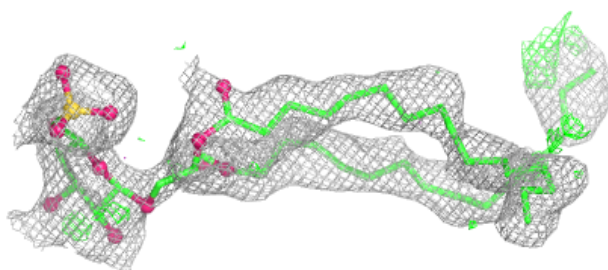
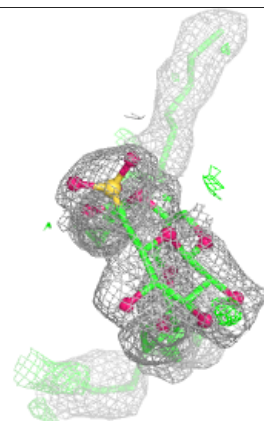
**Electron density around LMG Z 101:**

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

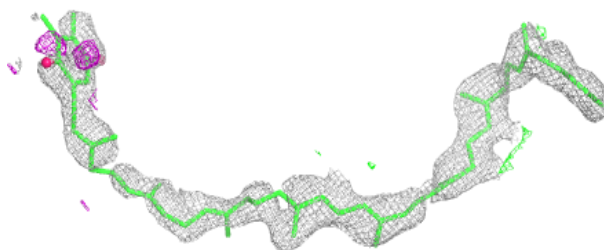
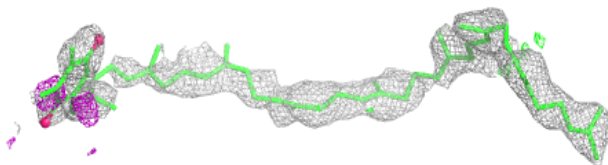
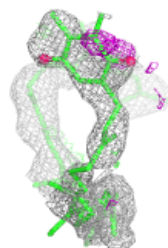


Electron density around SQD L 102:

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

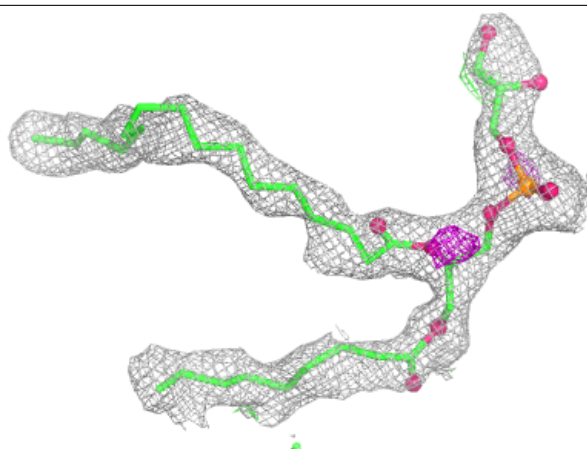
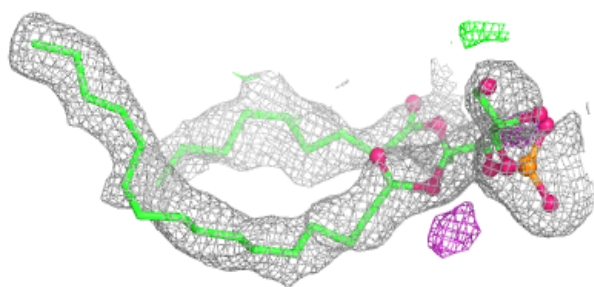
**Electron density around PL9 a 417:**

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



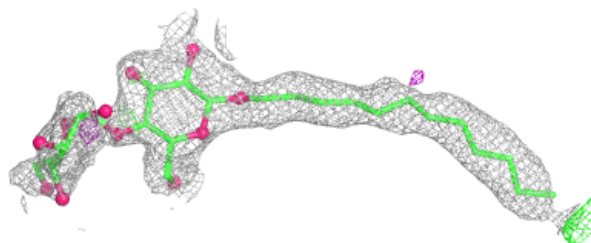
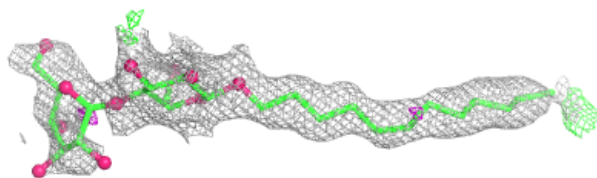
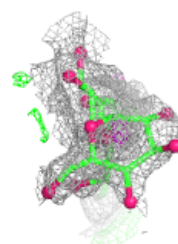
Electron density around LHG E 101:

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

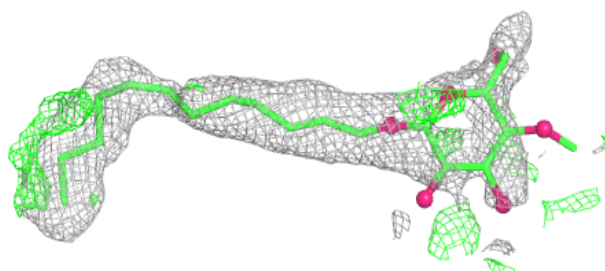
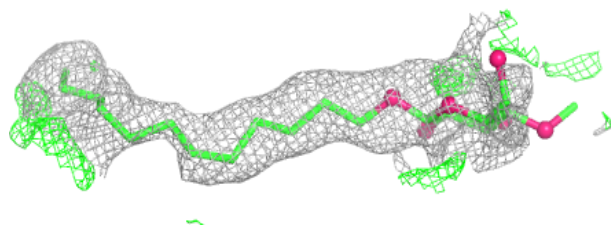
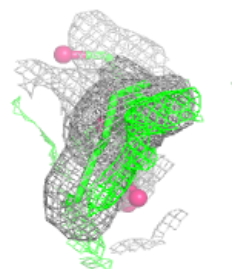


Electron density around LMT B 623:

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

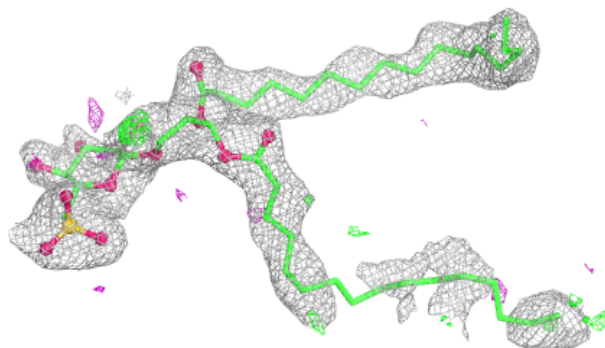
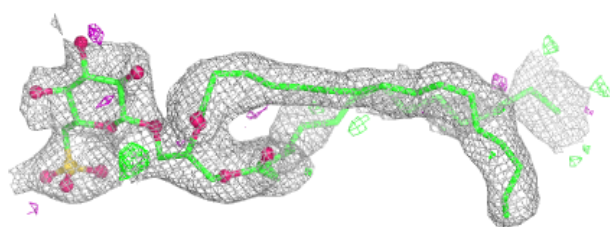
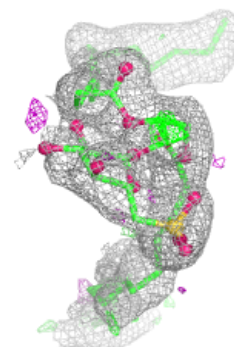
**Electron density around LMT B 636:**

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

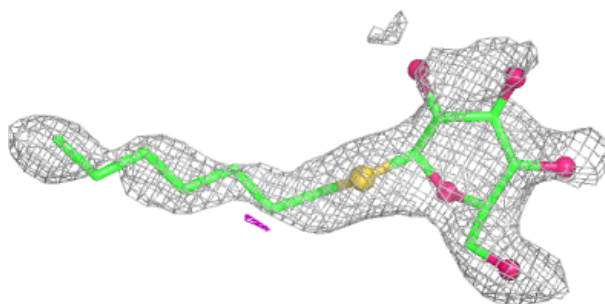
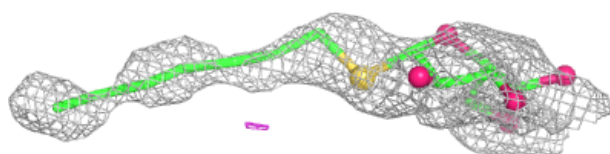
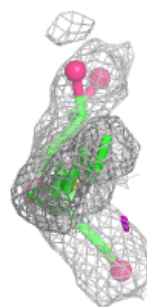


Electron density around SQD A 416:

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

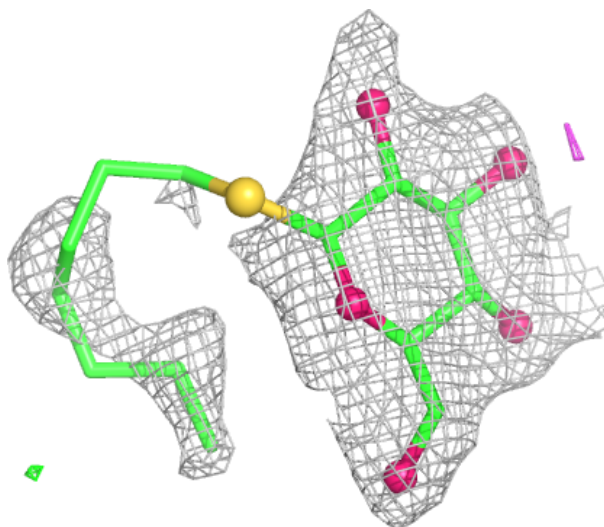
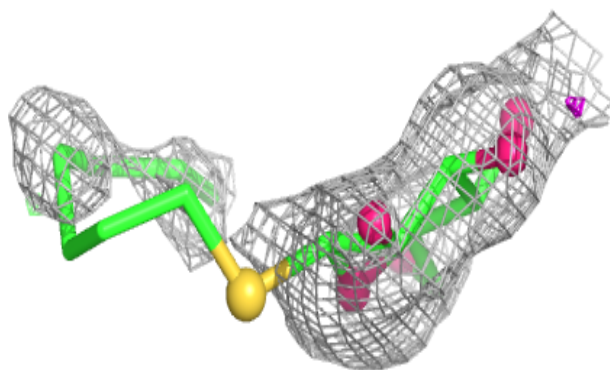
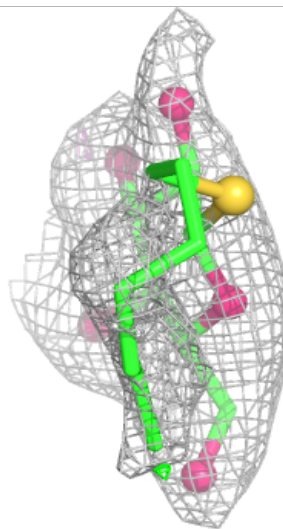
**Electron density around HTG C 524:**

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



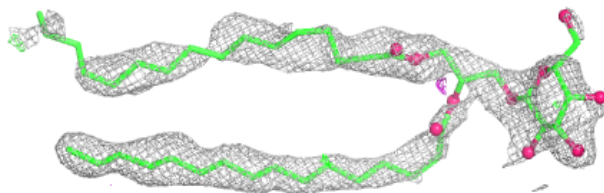
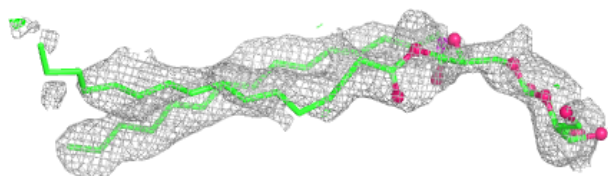
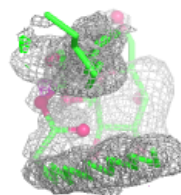
Electron density around HTG V 202:

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

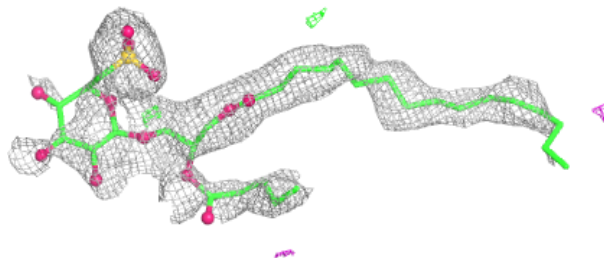
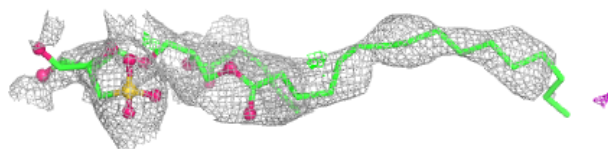
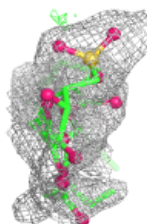


Electron density around LMG c 920:

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

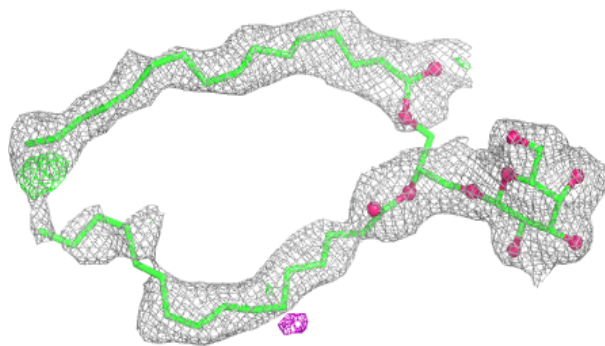
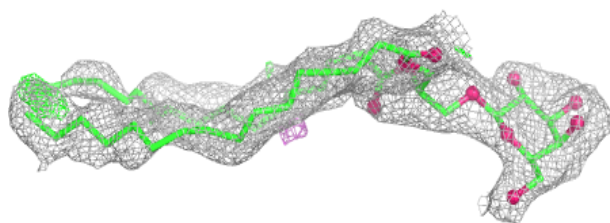
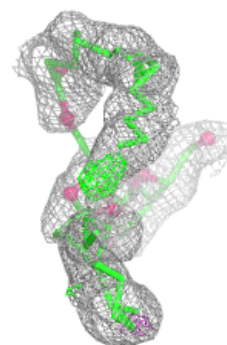
**Electron density around SQD f 102:**

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

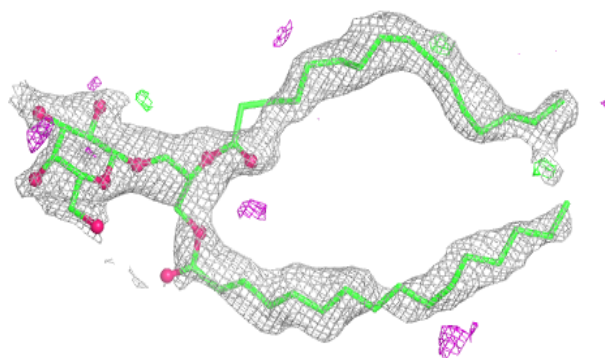
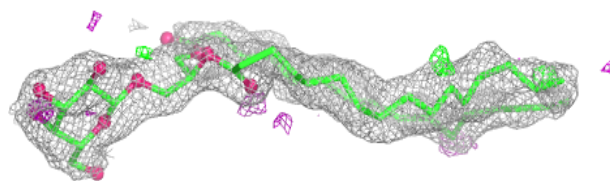
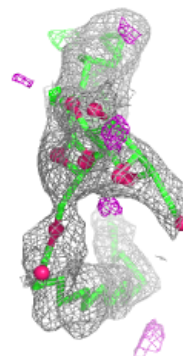


Electron density around LMG a 412:

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

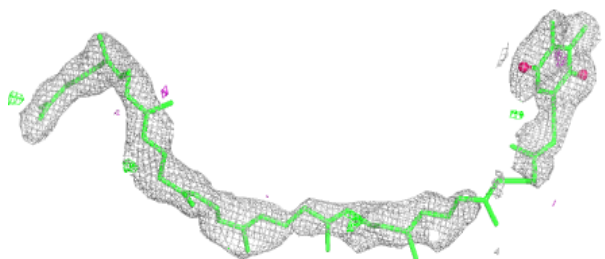
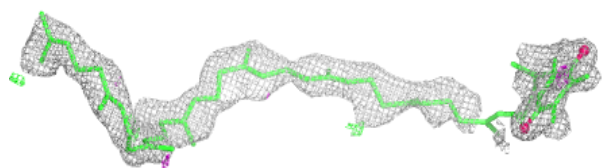
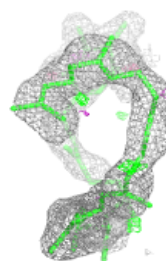
**Electron density around LMG C 501:**

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

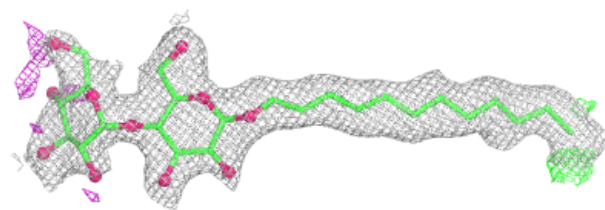
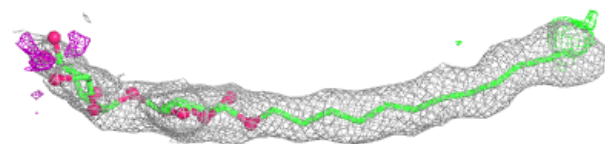
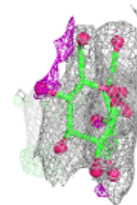


Electron density around PL9 A 419:

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

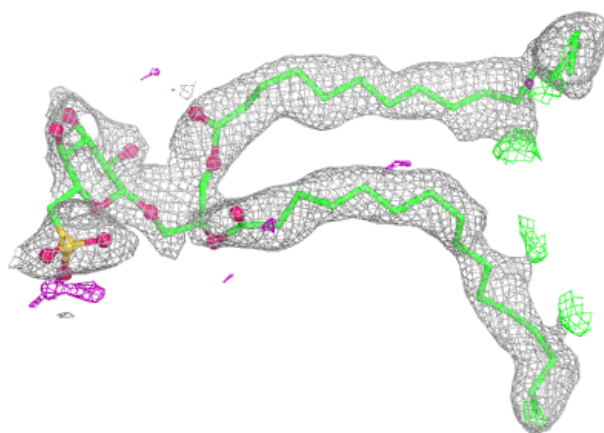
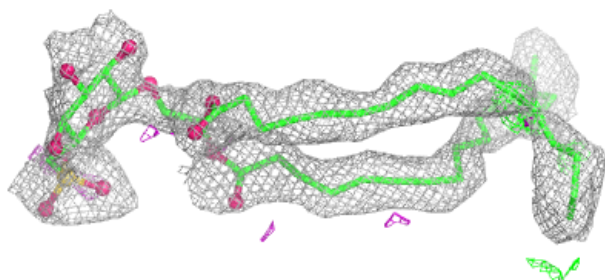
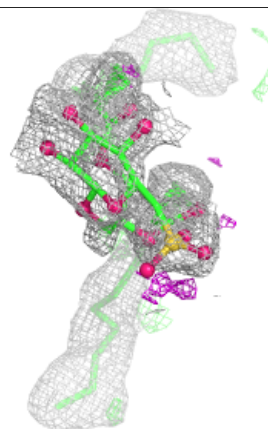
**Electron density around LMT M 101:**

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

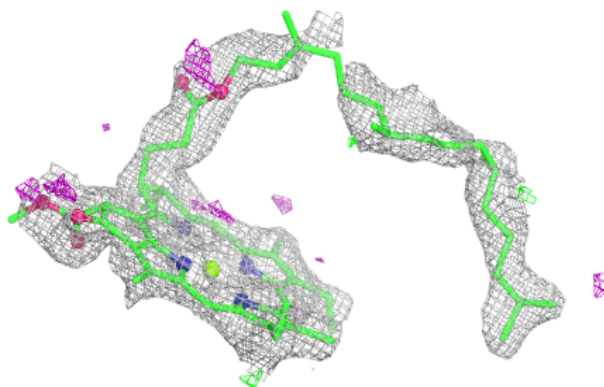
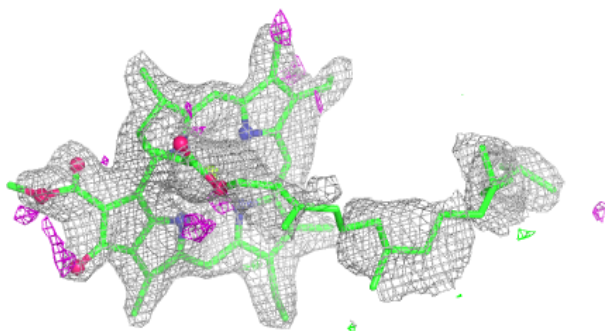
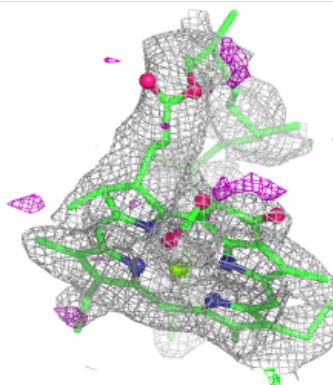


Electron density around SQD B 621:

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

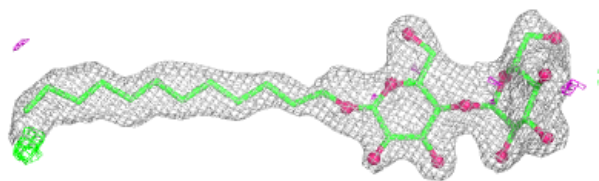
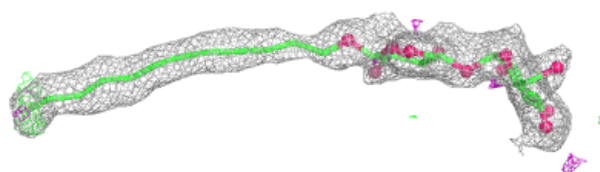
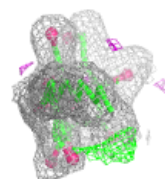
**Electron density around CLA c 914:**

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

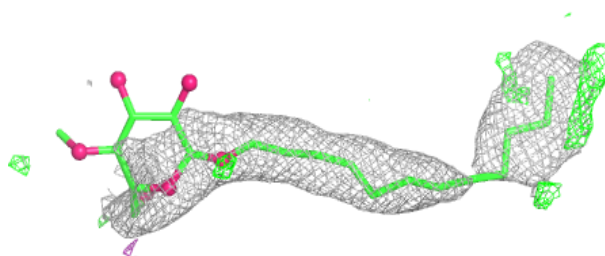
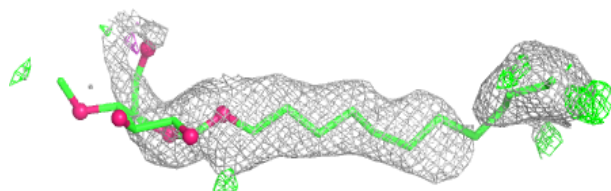
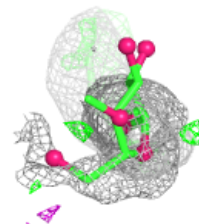


Electron density around LMT m 103:

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

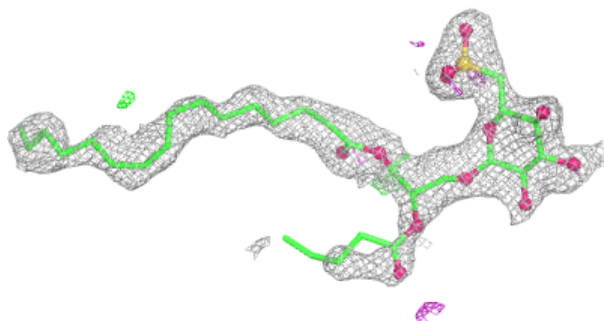
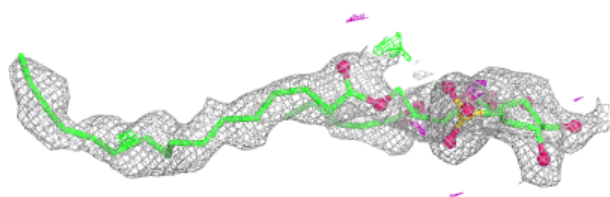
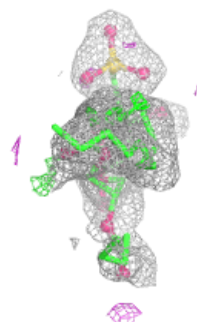
**Electron density around LMT b 601:**

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

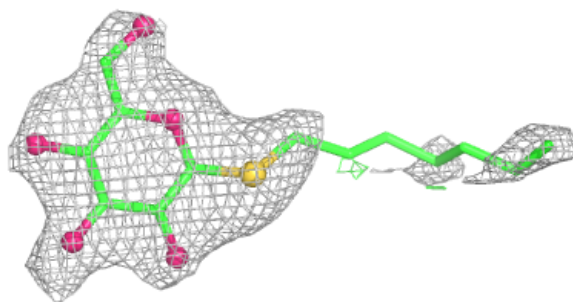
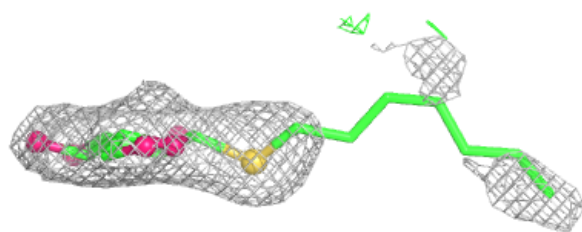
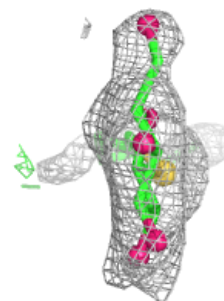


Electron density around SQD F 101:

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

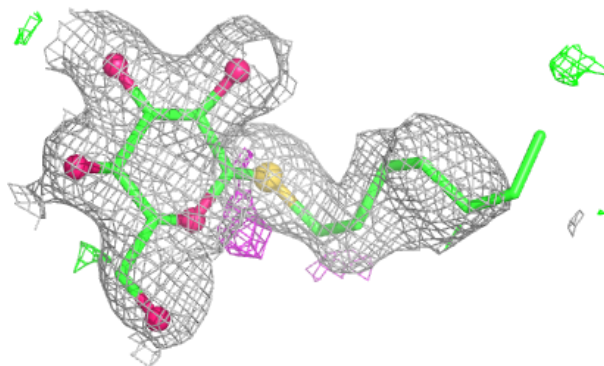
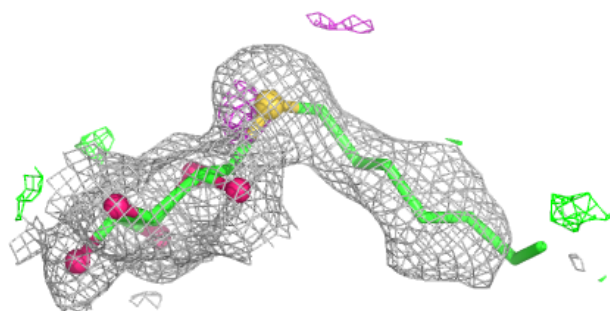
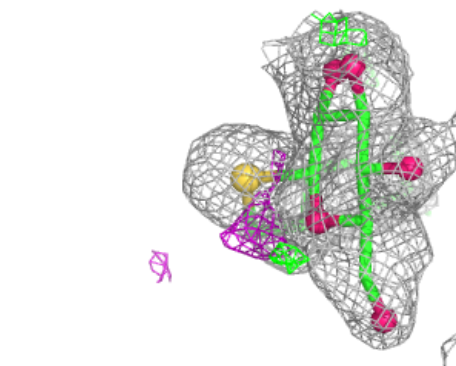
**Electron density around HTG C 523:**

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

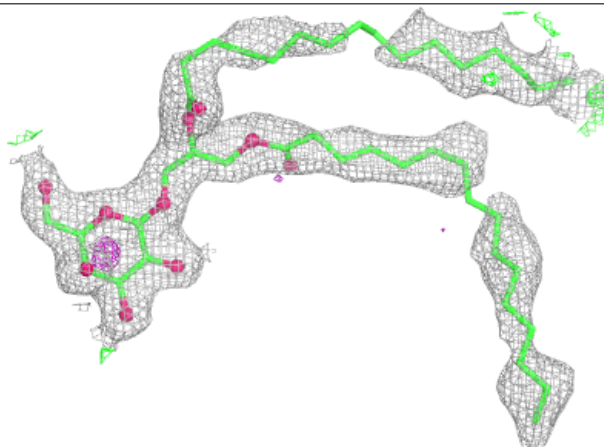
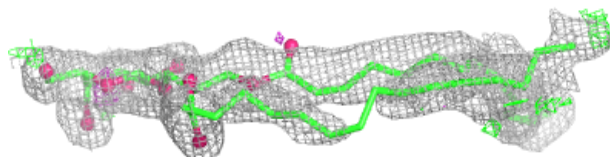
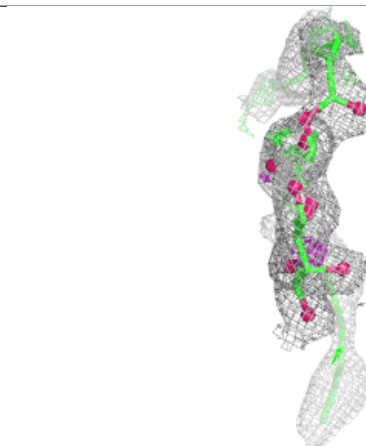


Electron density around HTG b 626:

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

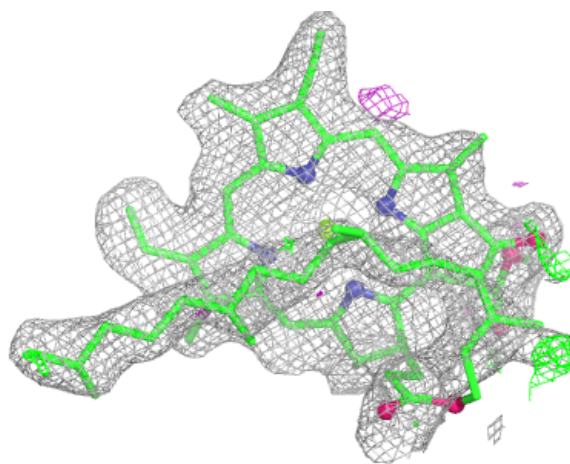
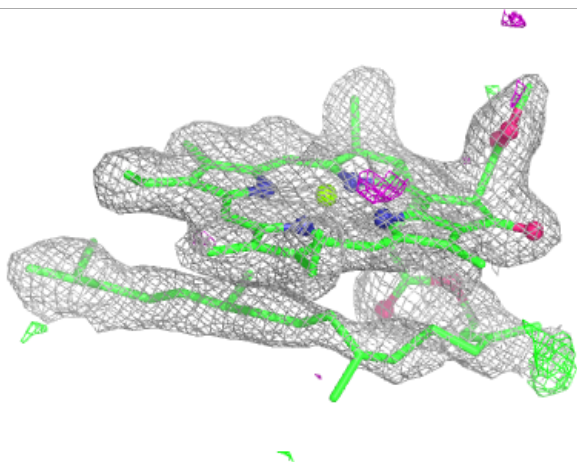
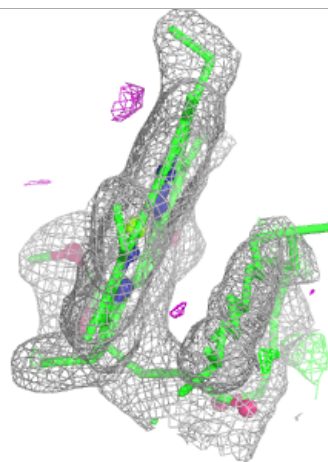
**Electron density around LMG C 520:**

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



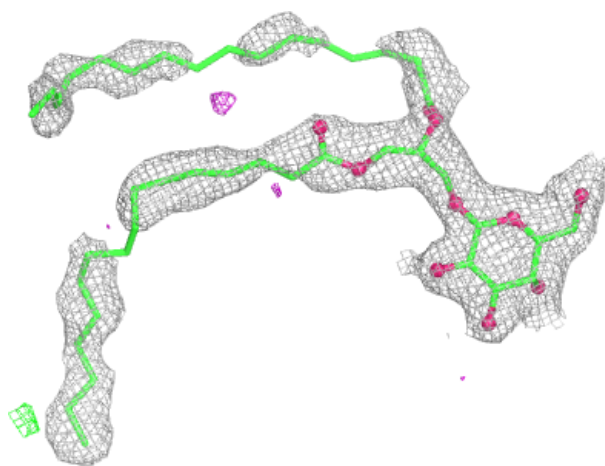
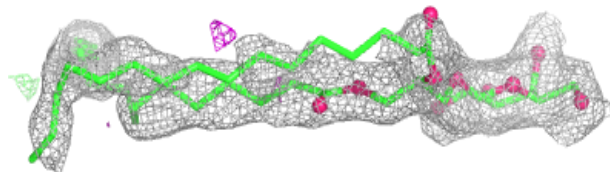
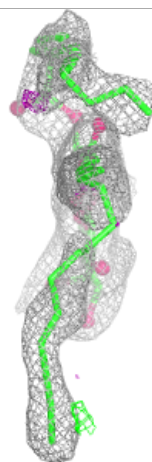
Electron density around CLA b 605:

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



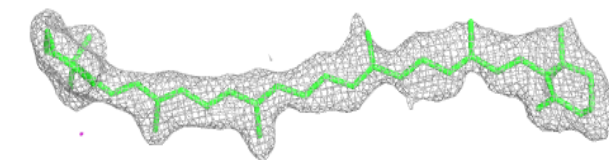
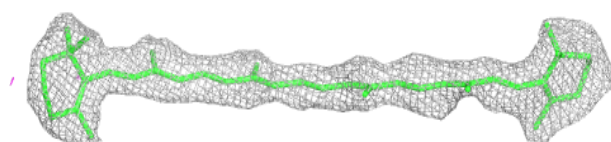
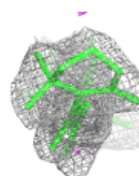
Electron density around LMG c 919:

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

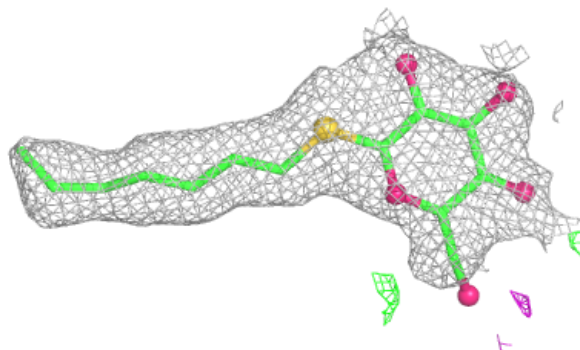
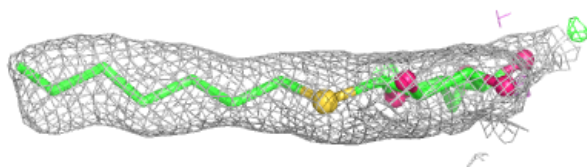
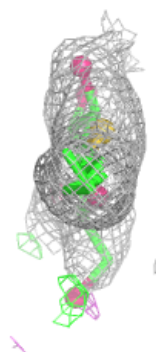


Electron density around BCR k 101:

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

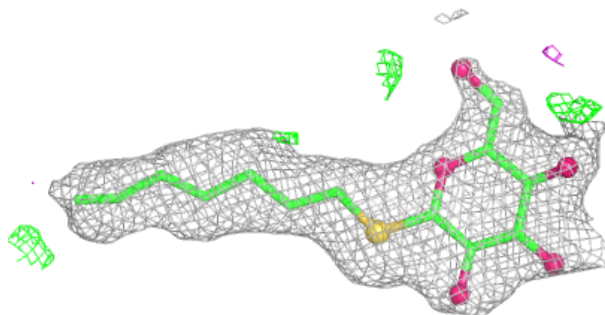
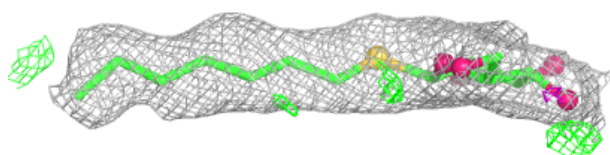
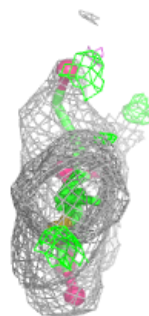
**Electron density around HTG B 633:**

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



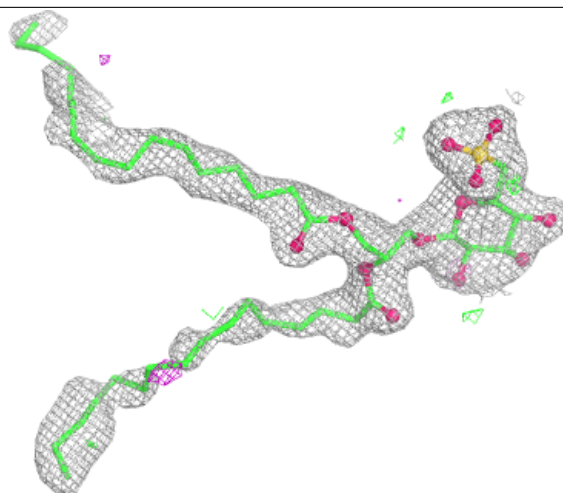
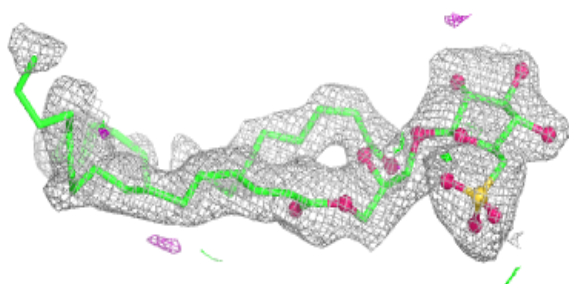
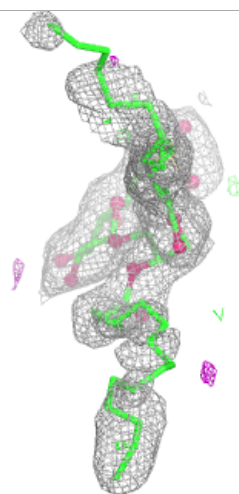
Electron density around HTG b 602:

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



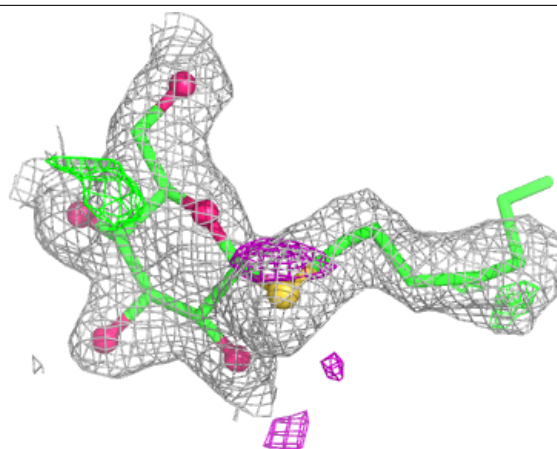
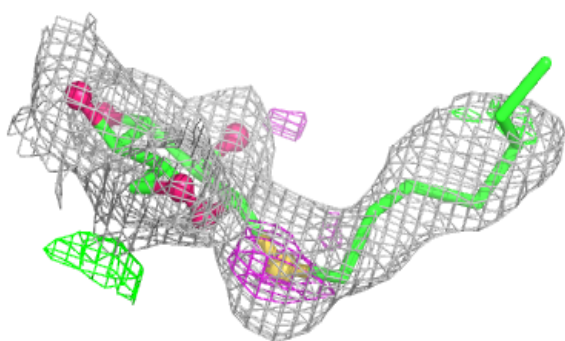
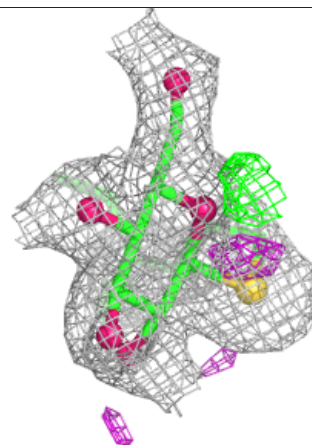
Electron density around SQD a 411:

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



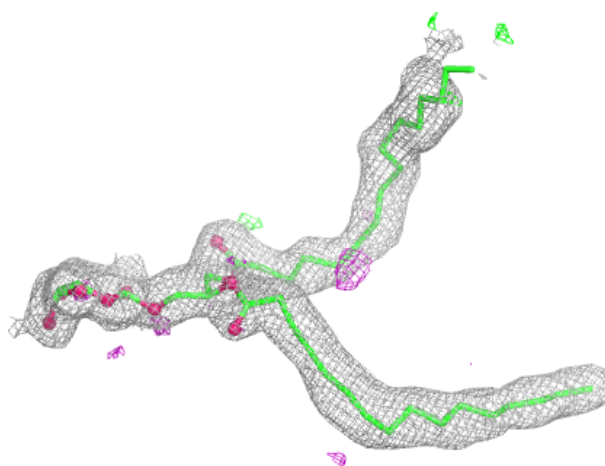
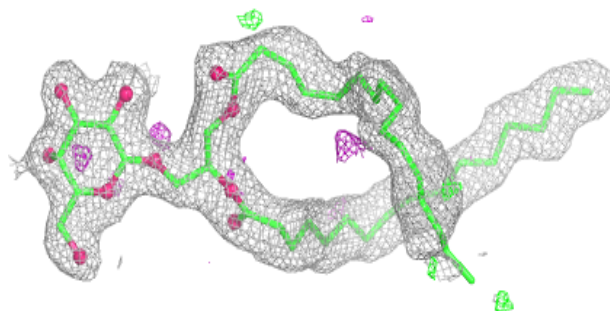
Electron density around HTG B 625:

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



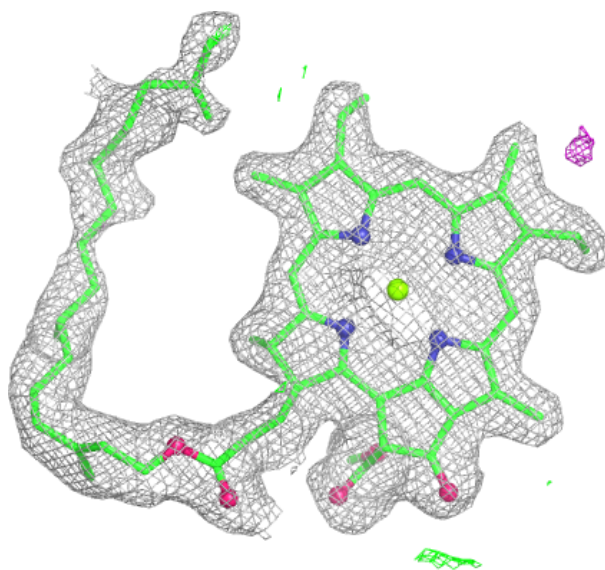
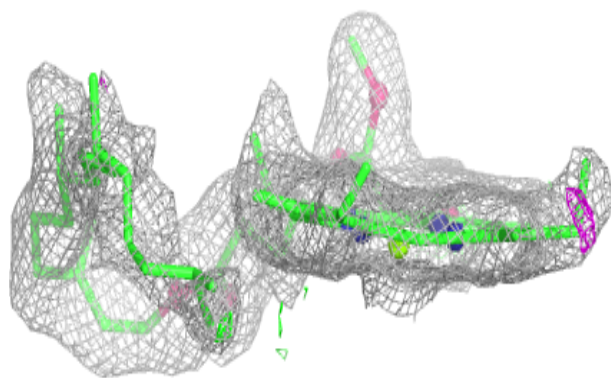
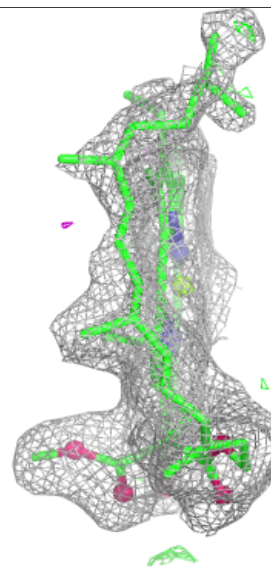
Electron density around LMG B 622:

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



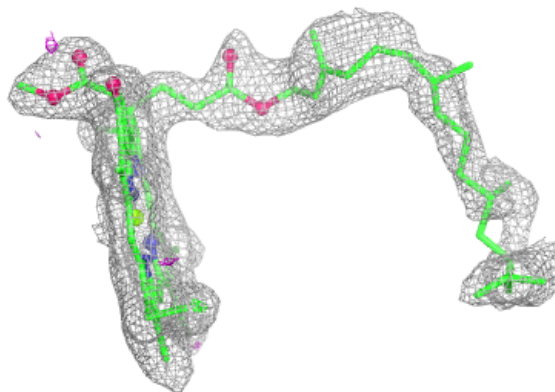
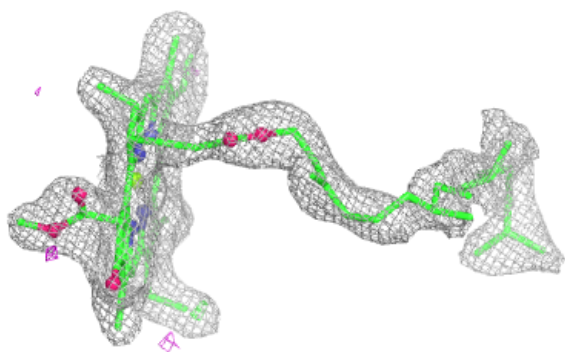
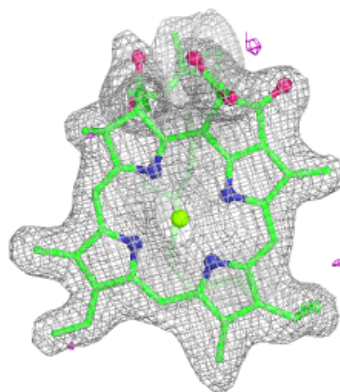
Electron density around CLA c 913:

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

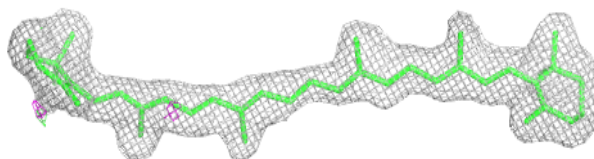
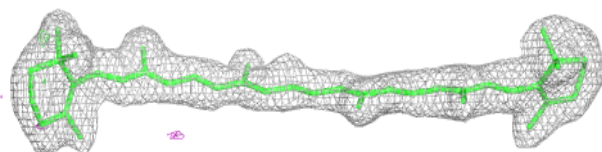
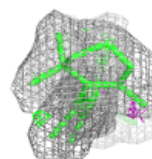


Electron density around CLA C 507:

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

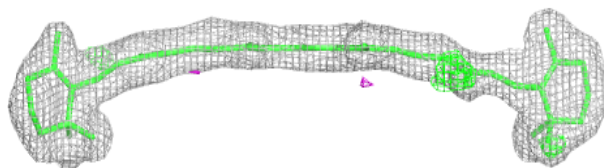
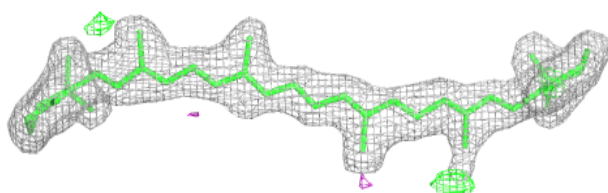
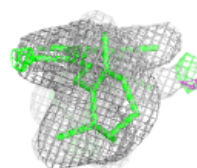
**Electron density around BCR C 515:**

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

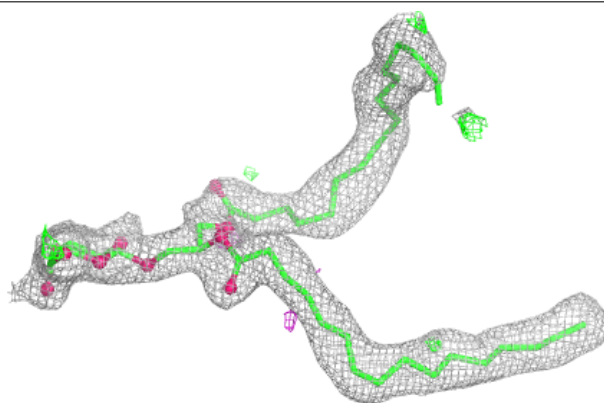
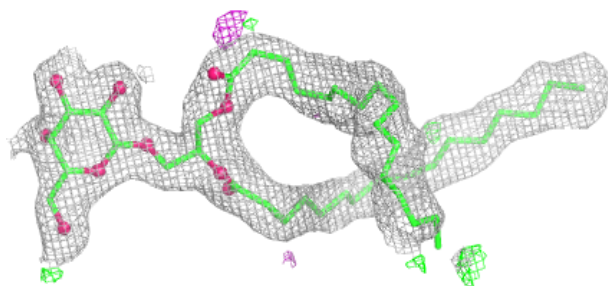
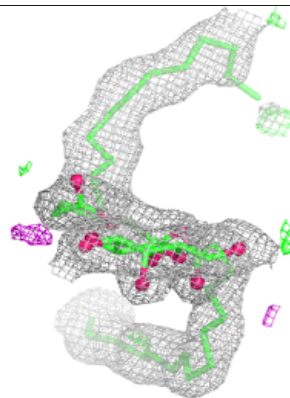


Electron density around BCR K 103:

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

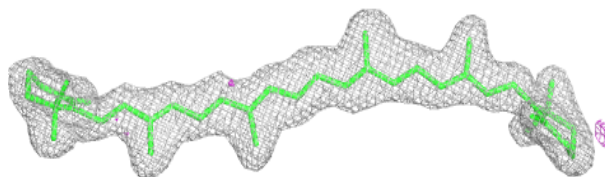
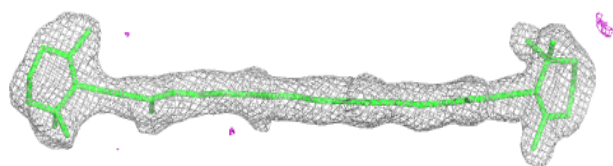
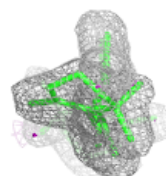
**Electron density around LMG b 624:**

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

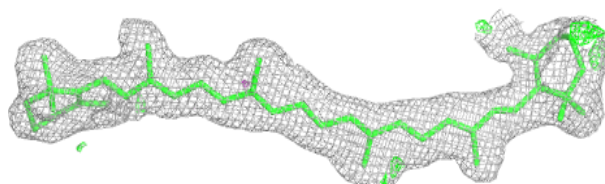
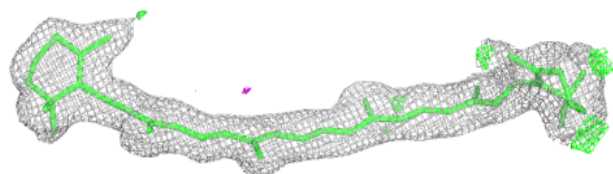
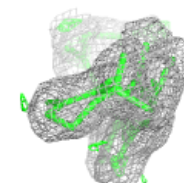


Electron density around BCR c 915:

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

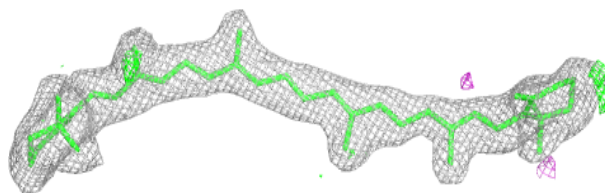
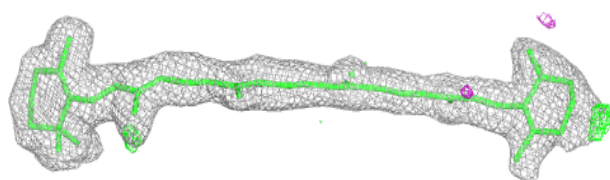
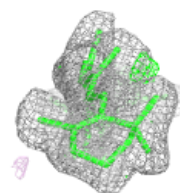
**Electron density around BCR d 404:**

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



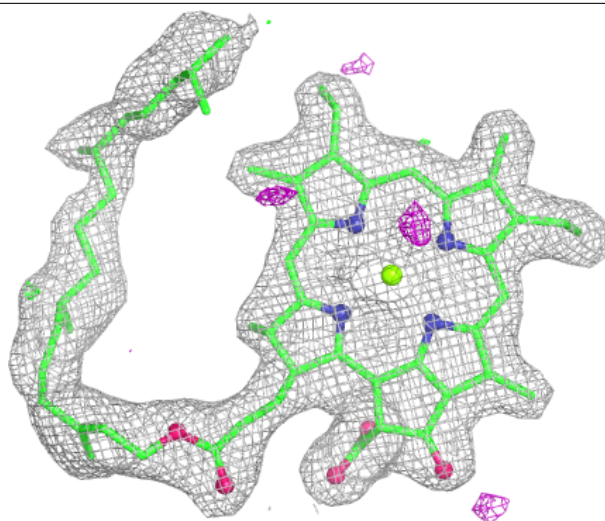
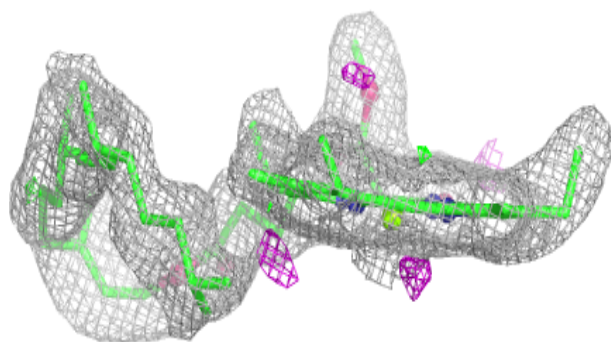
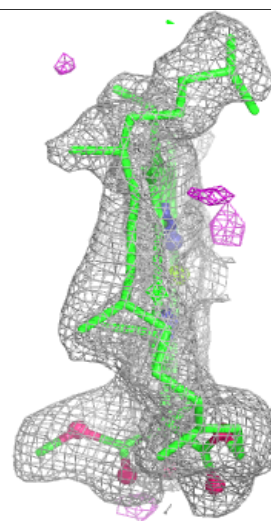
Electron density around BCR h 101:

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



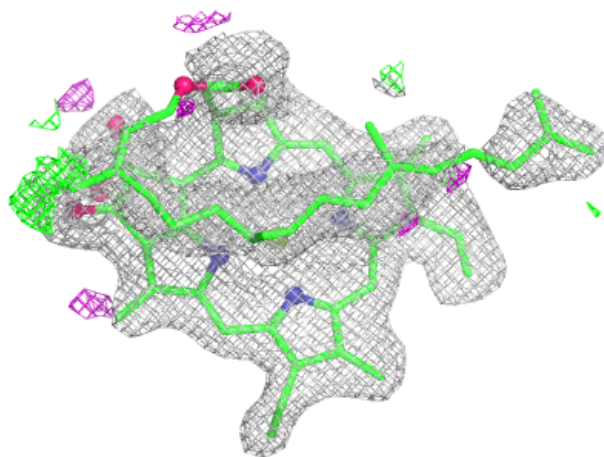
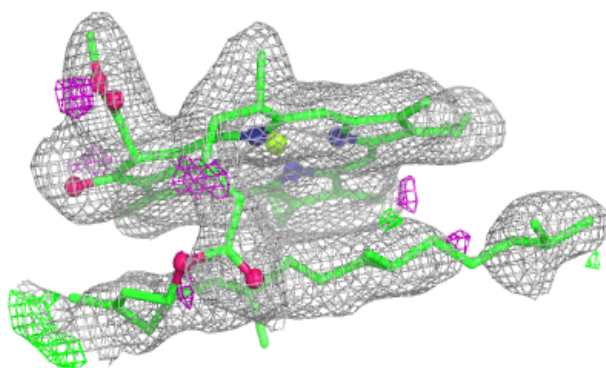
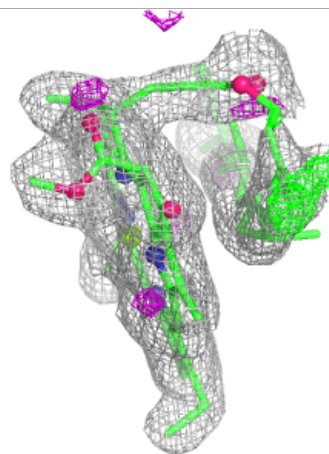
Electron density around CLA C 513:

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



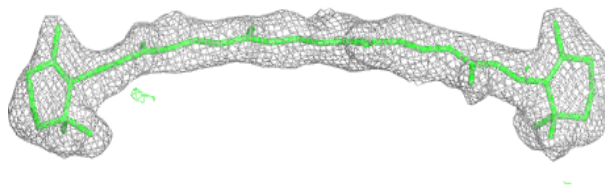
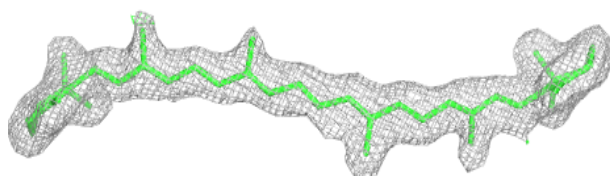
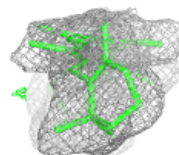
Electron density around CLA B 602:

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

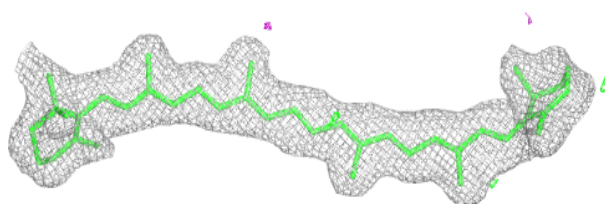
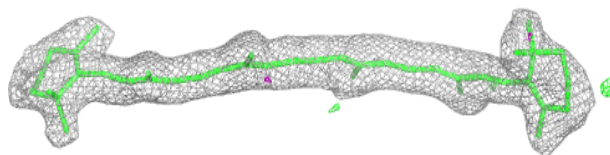
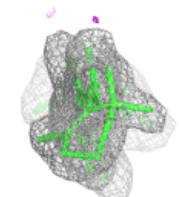


Electron density around BCR k 102:

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

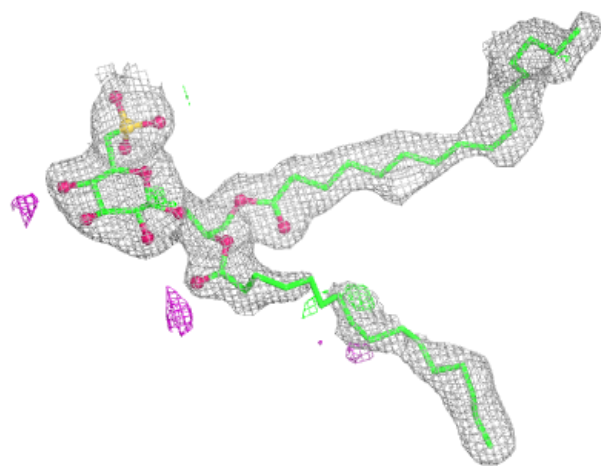
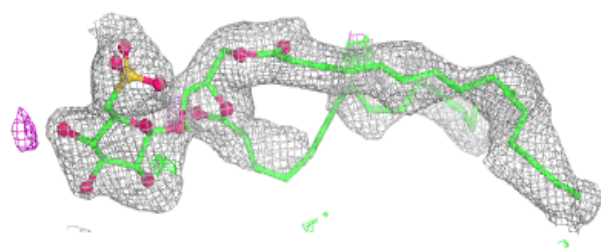
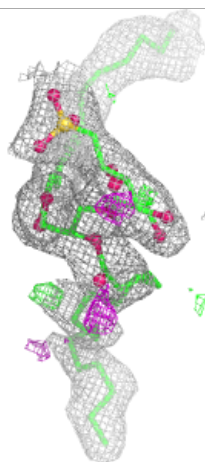
**Electron density around BCR y 101:**

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



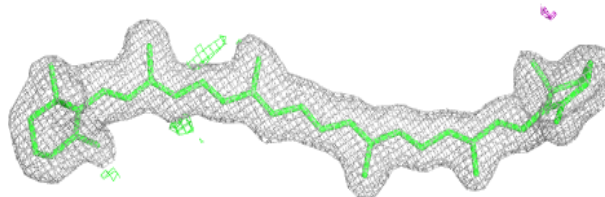
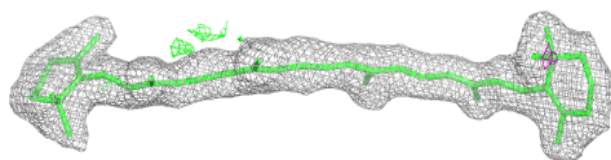
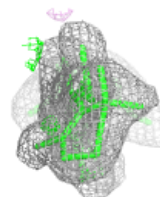
Electron density around SQD A 412:

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

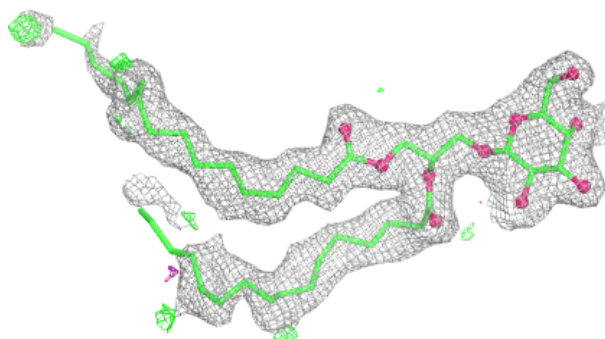
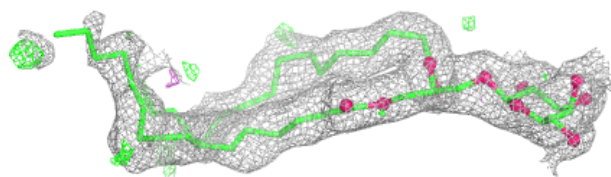
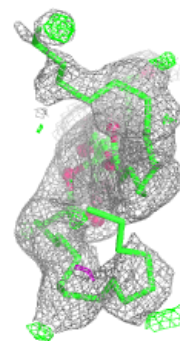


Electron density around BCR K 102:

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

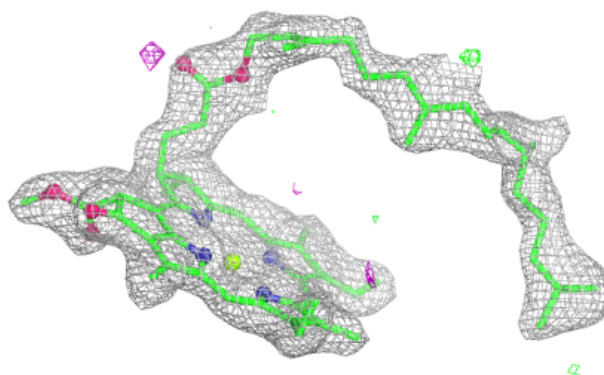
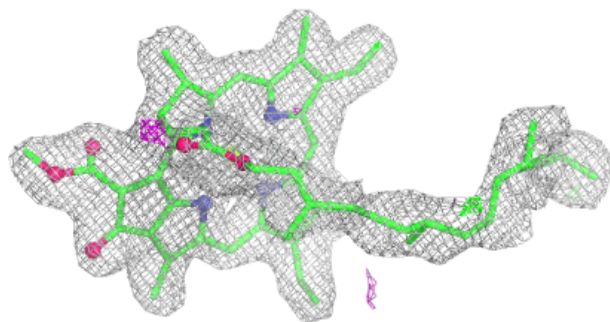
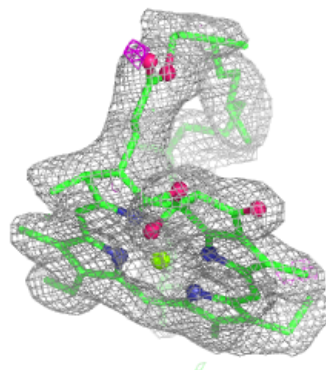
**Electron density around LMG j 101:**

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

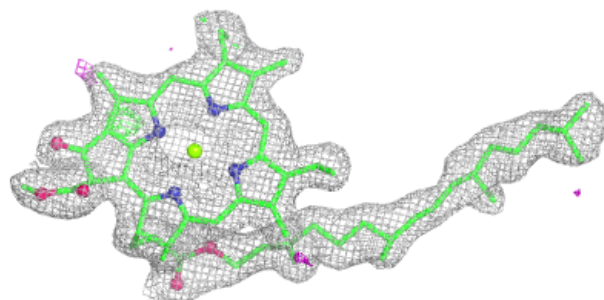
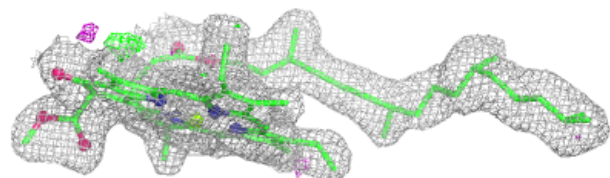
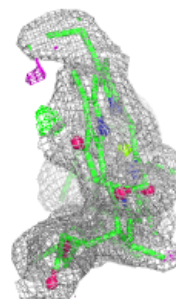


Electron density around CLA C 514:

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

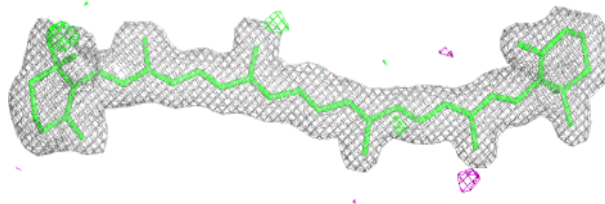
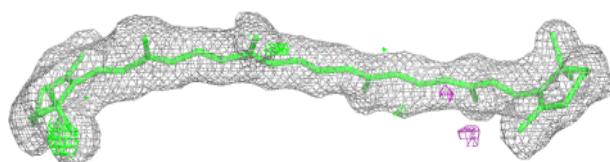
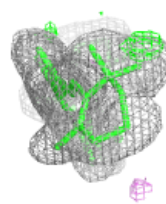
**Electron density around CLA c 902:**

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

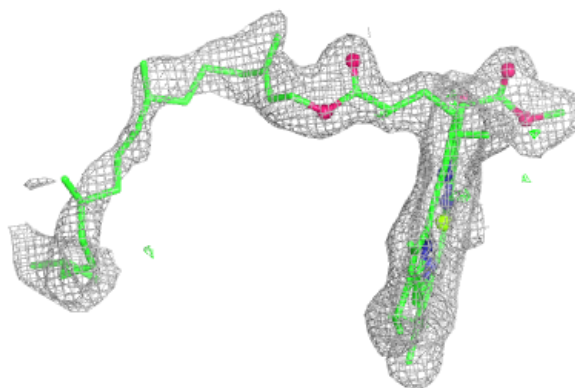
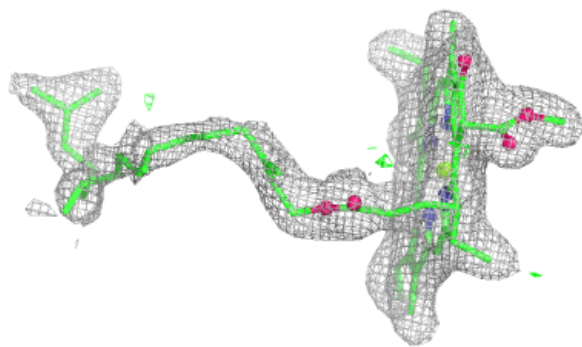
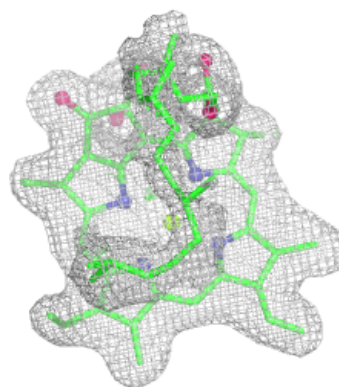


Electron density around BCR B 620:

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

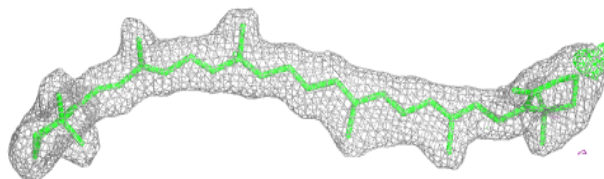
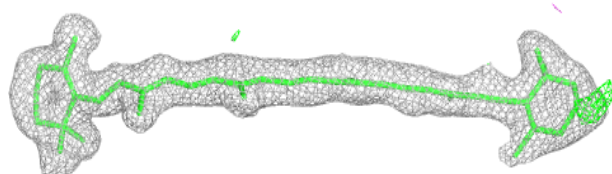
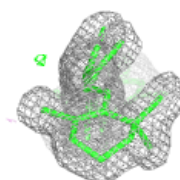
**Electron density around CLA c 907:**

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

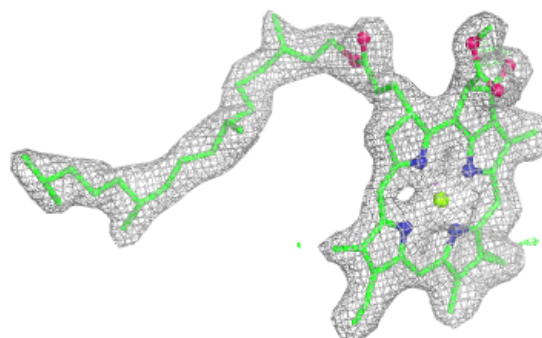
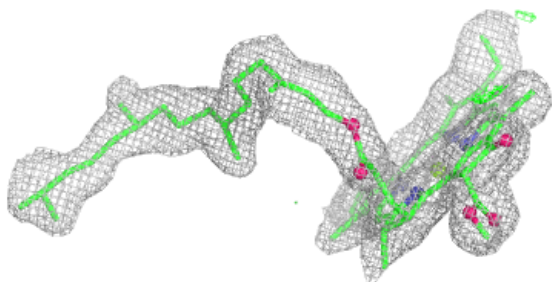
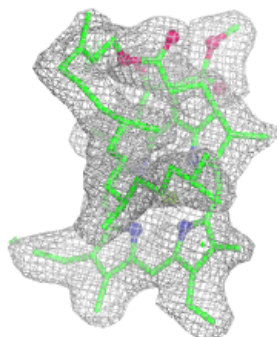


Electron density around BCR H 101:

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

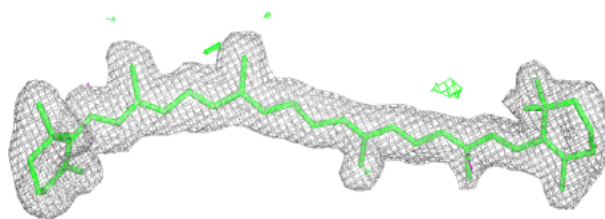
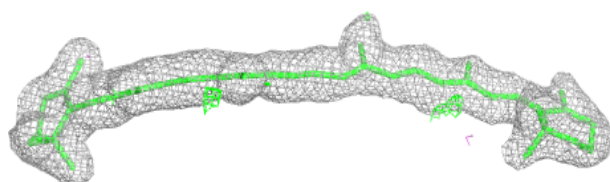
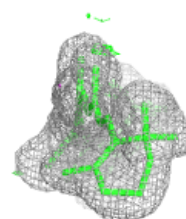
**Electron density around CLA c 912:**

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

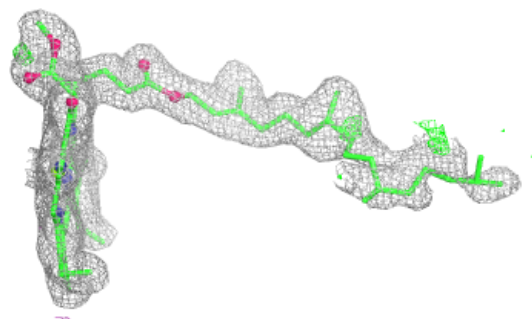
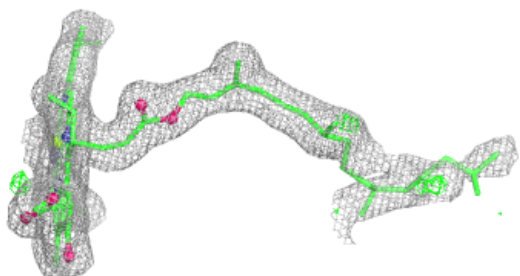
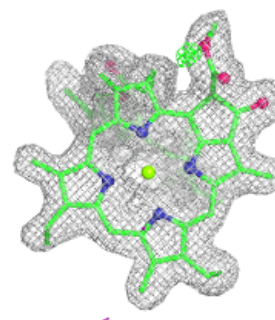


Electron density around BCR T 102:

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

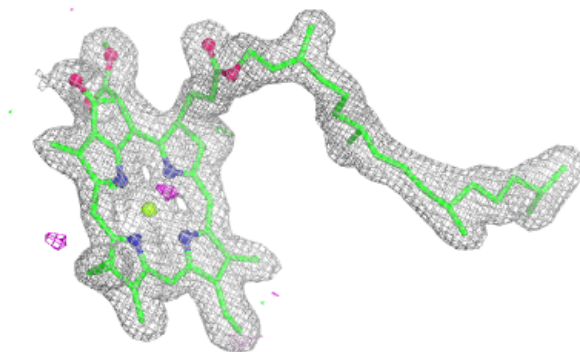
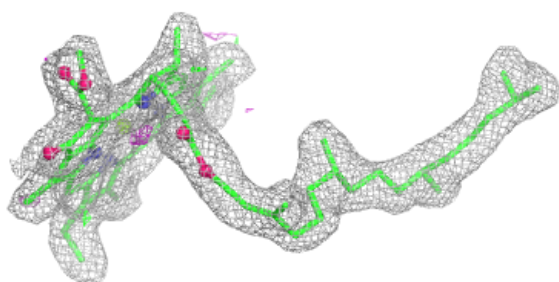
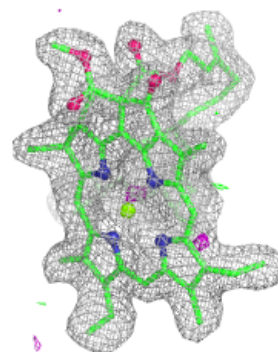
**Electron density around CLA b 610:**

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

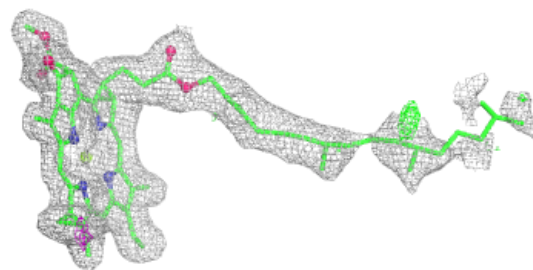
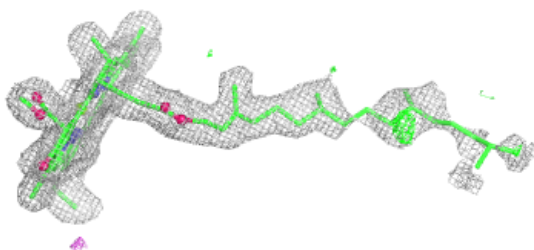
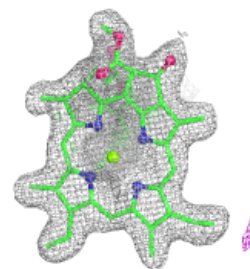


Electron density around CLA C 512:

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

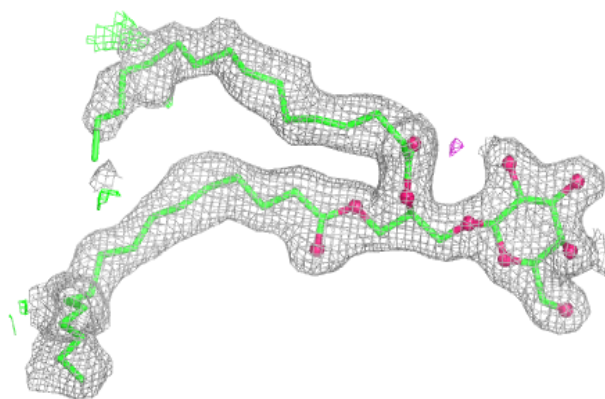
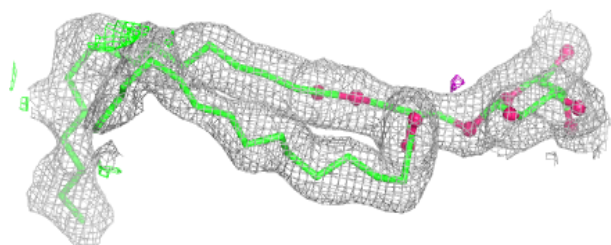
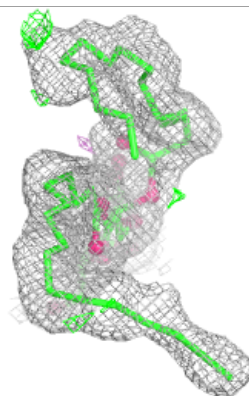
**Electron density around CLA d 403:**

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

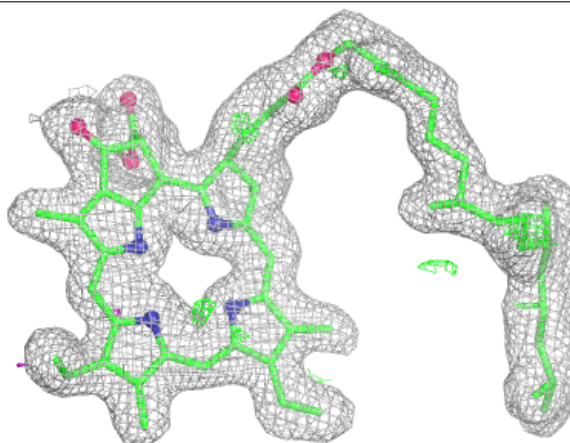
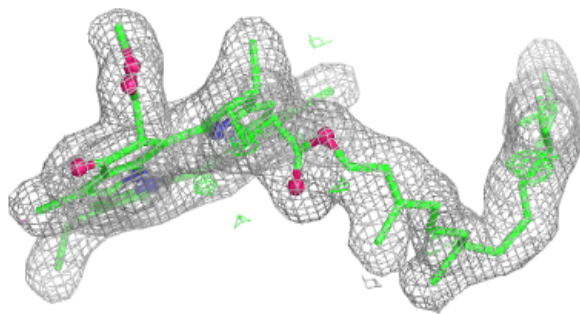
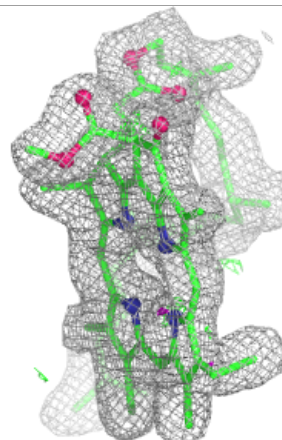


Electron density around LMG J 101:

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

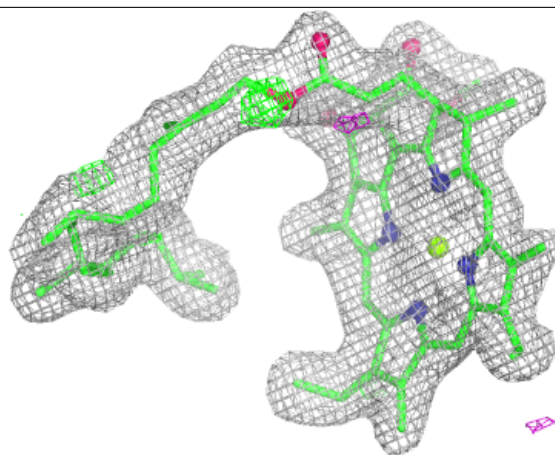
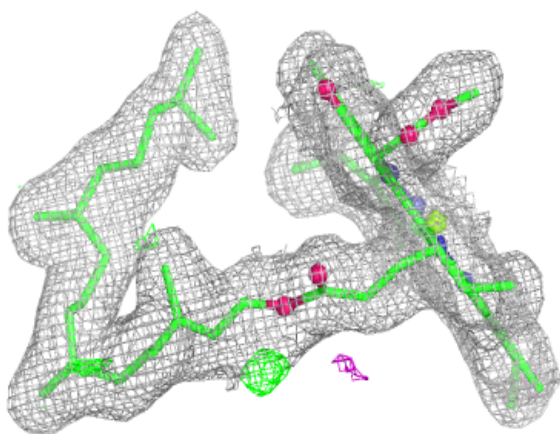
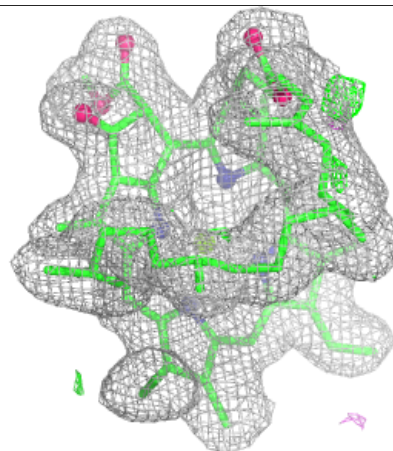
**Electron density around PHO a 420:**

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

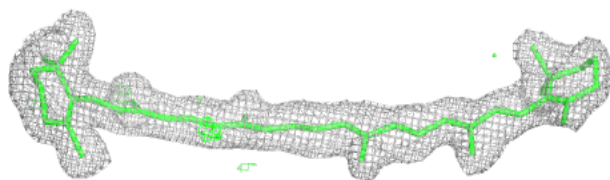
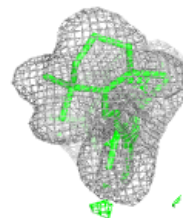


Electron density around CLA c 904:

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

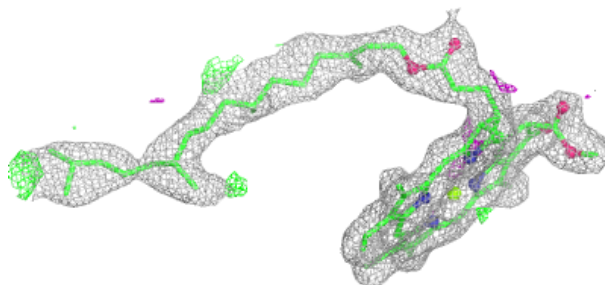
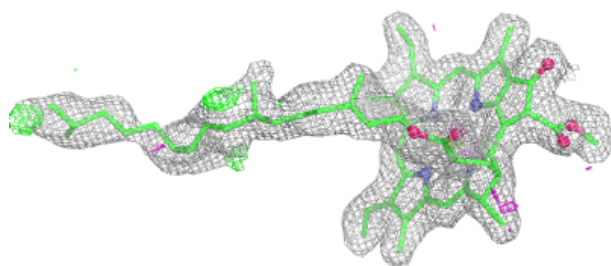
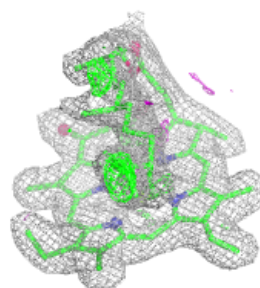
**Electron density around BCR t 101:**

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

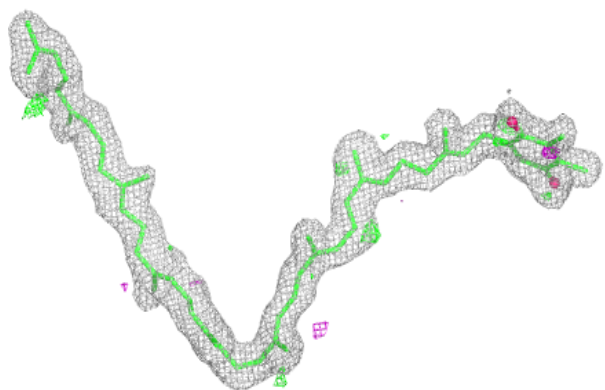
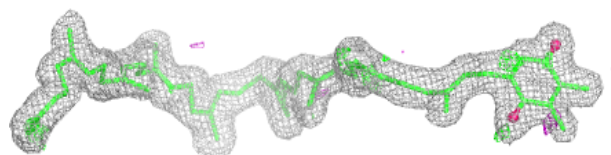
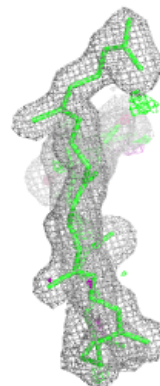


Electron density around CLA c 905:

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

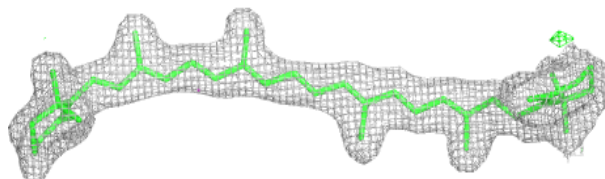
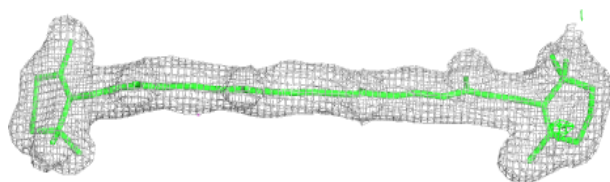
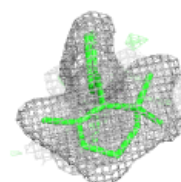
**Electron density around PL9 d 405:**

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

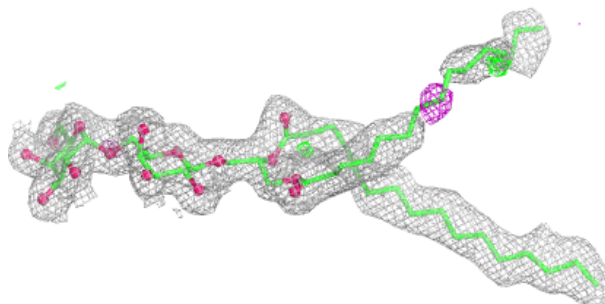
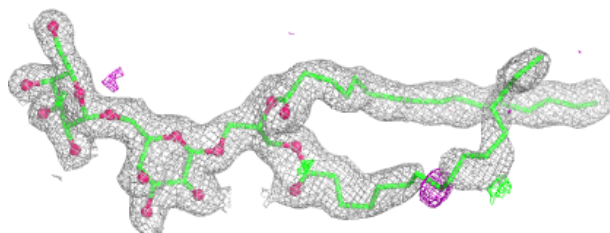
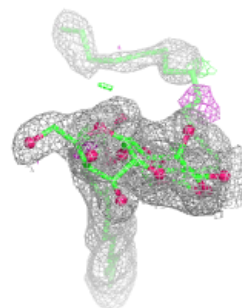


Electron density around BCR C 516:

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

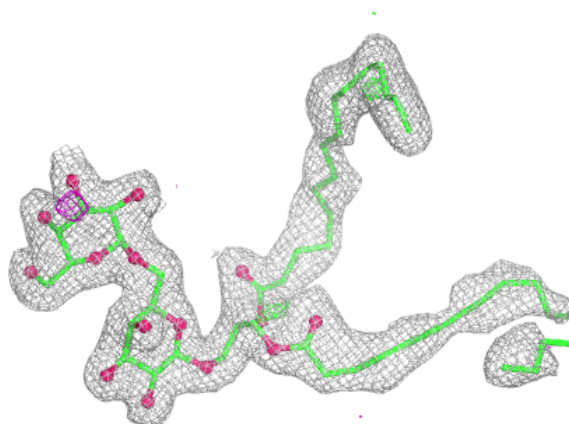
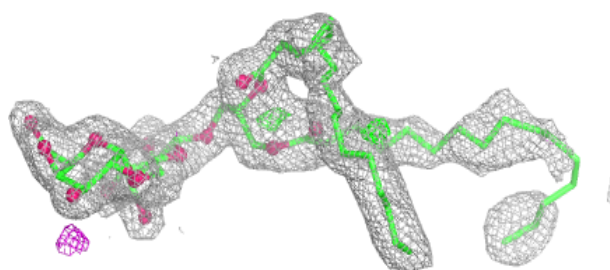
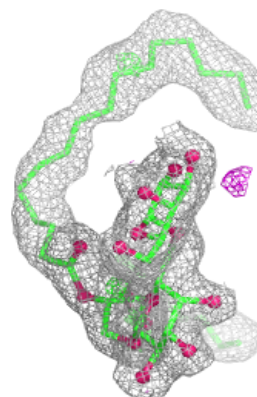
**Electron density around DGD c 916:**

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

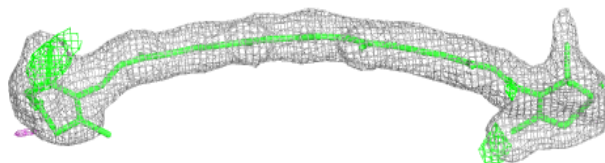
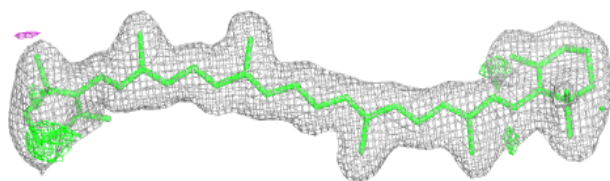
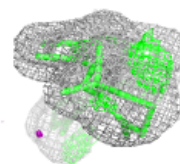


Electron density around DGD c 917:

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

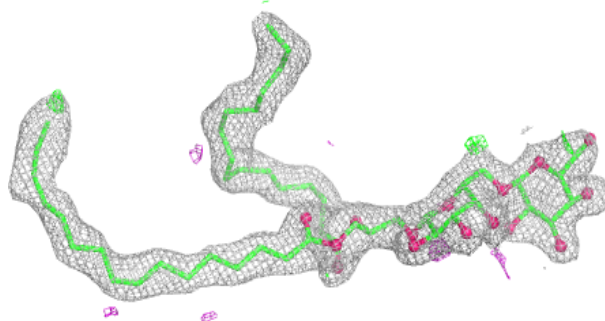
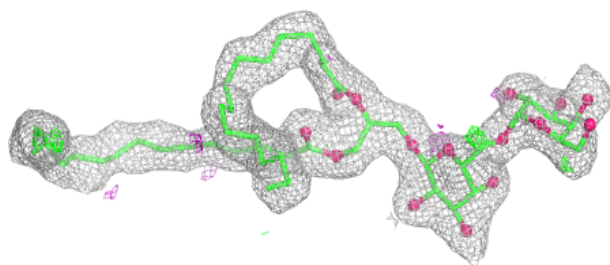
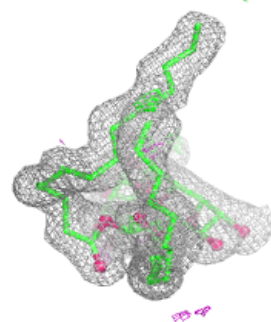
**Electron density around BCR D 403:**

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

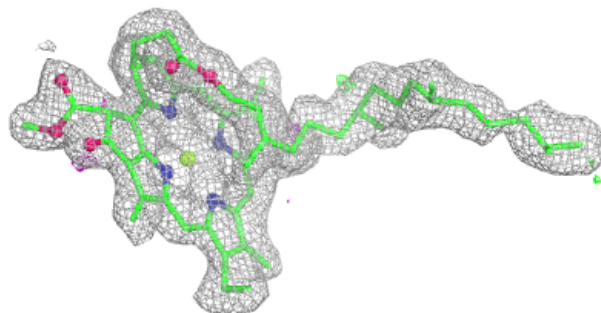
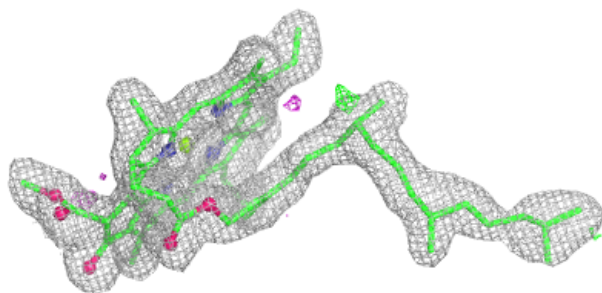
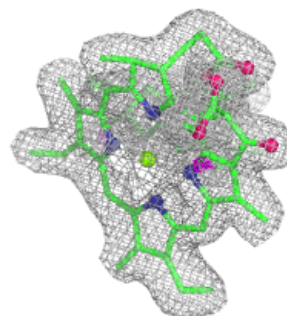


Electron density around DGD h 102:

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

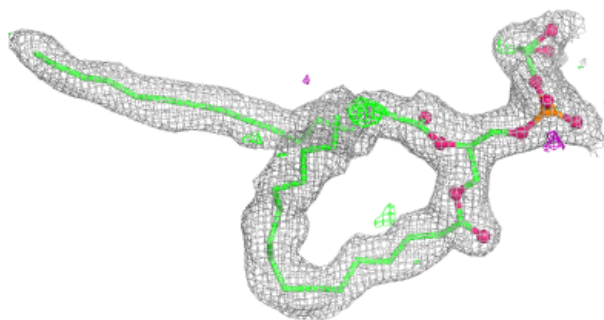
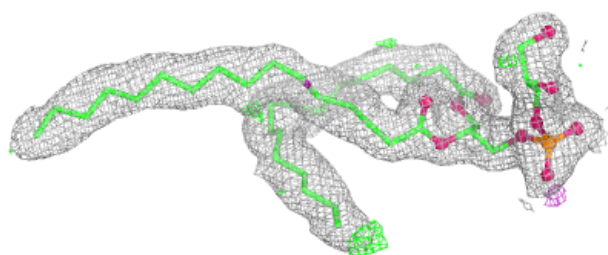
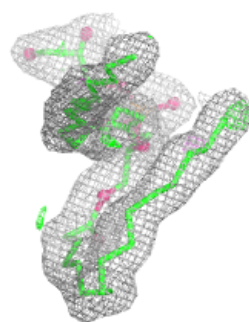
**Electron density around CLA c 906:**

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

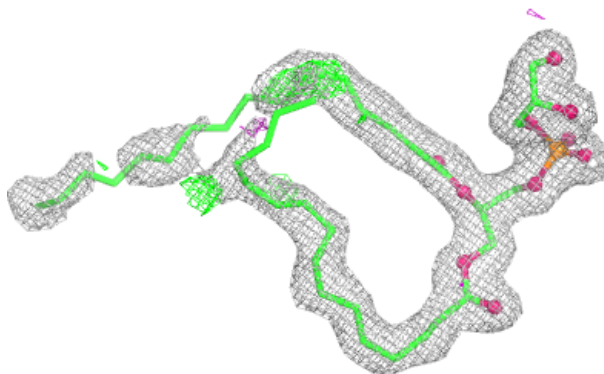
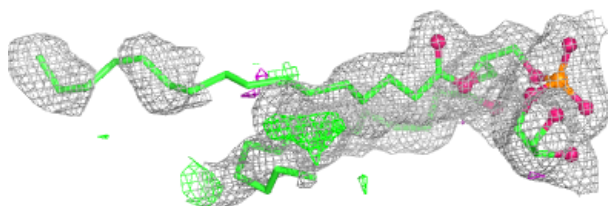


Electron density around LHG d 407:

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

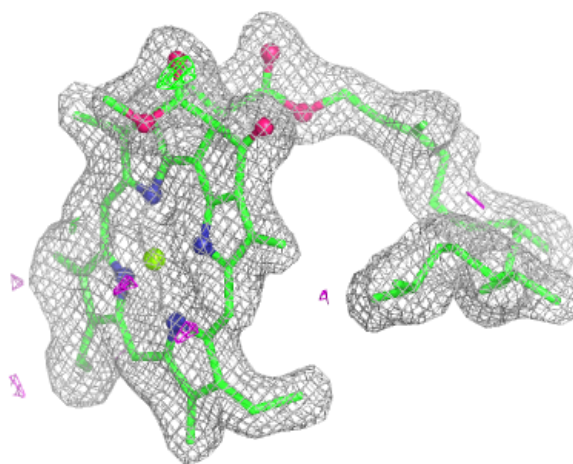
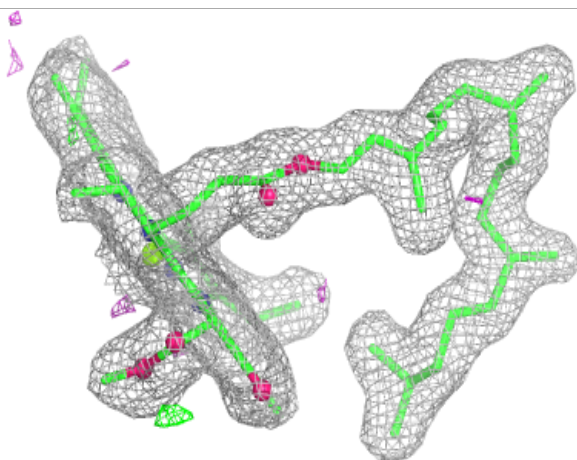
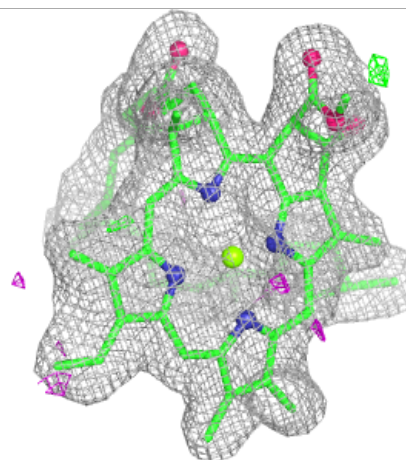
**Electron density around LHG d 409:**

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



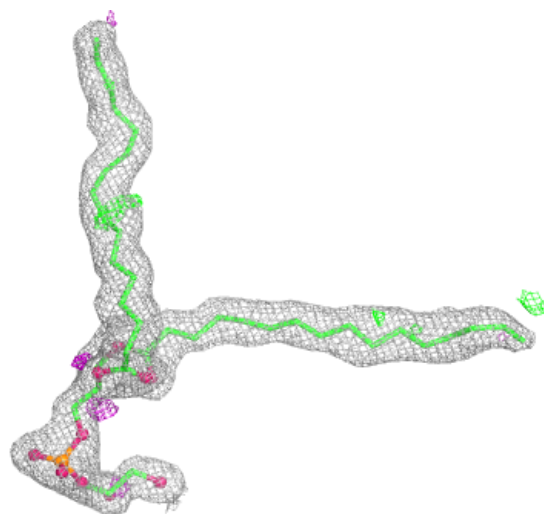
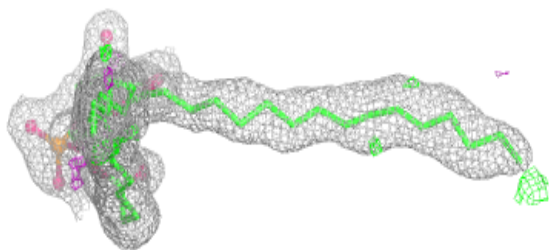
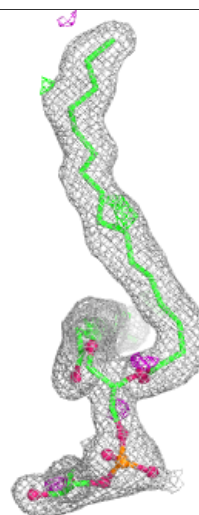
Electron density around CLA C 504:

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



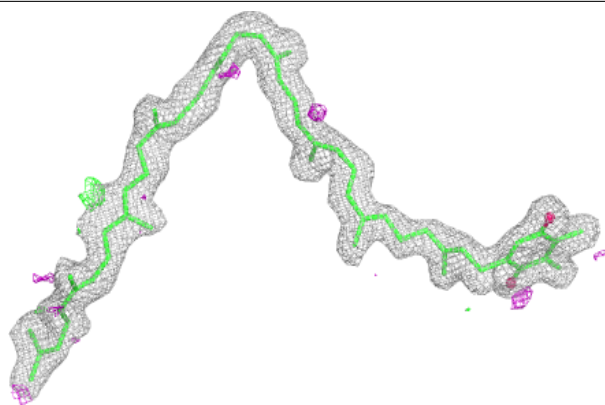
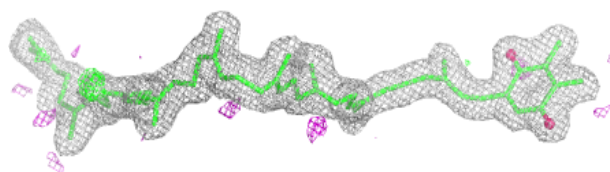
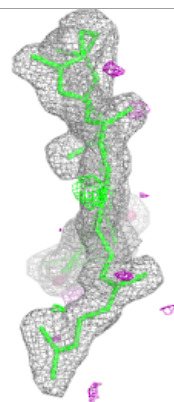
Electron density around LHG 1 101:

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



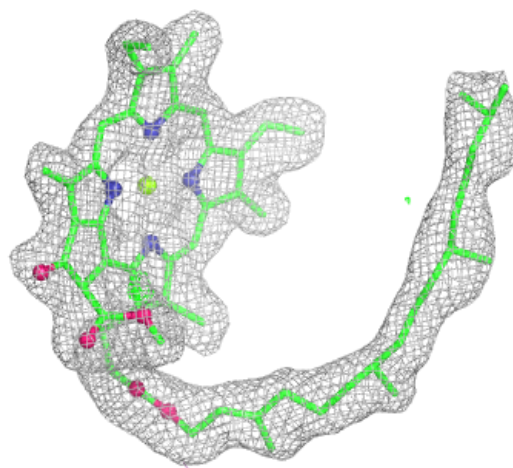
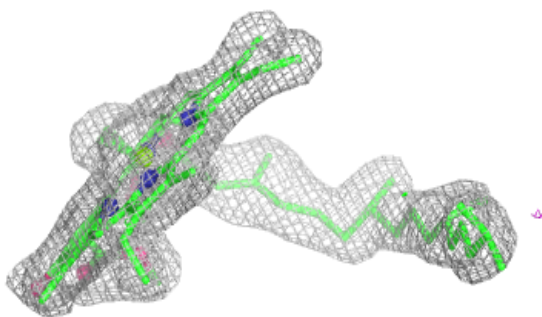
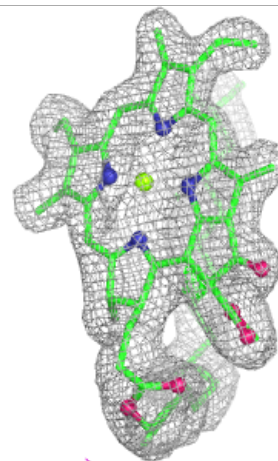
Electron density around PL9 D 404:

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



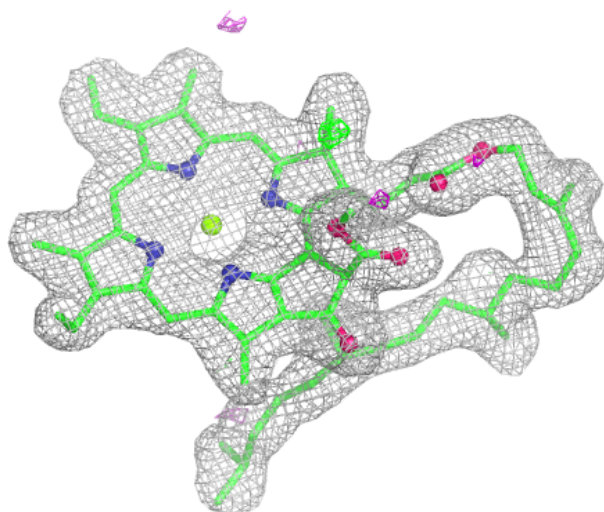
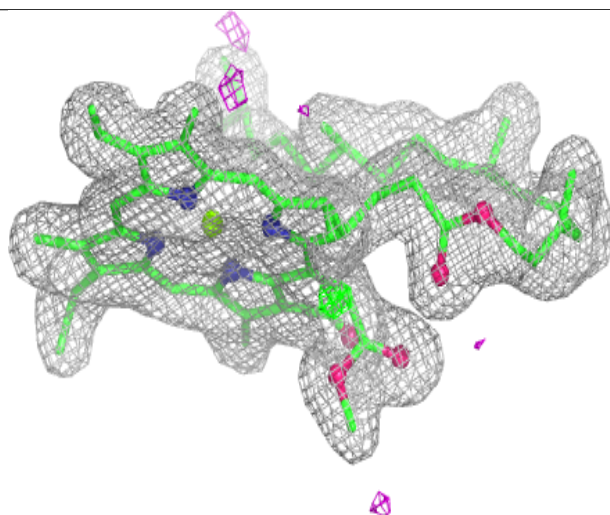
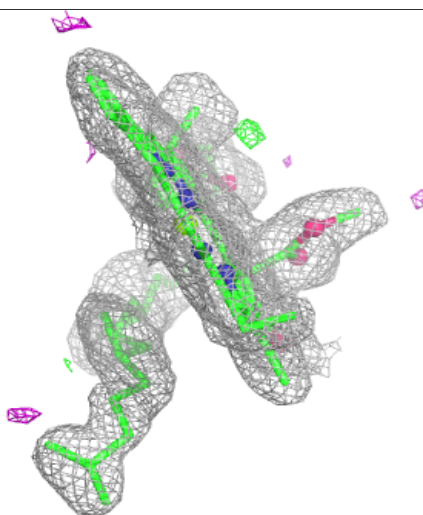
Electron density around CLA C 508:

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



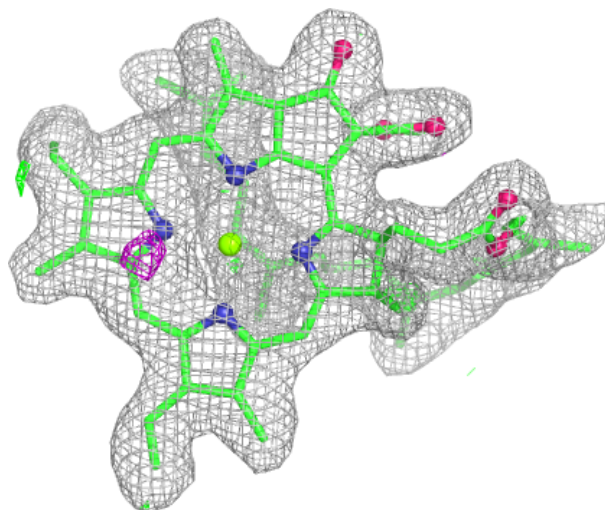
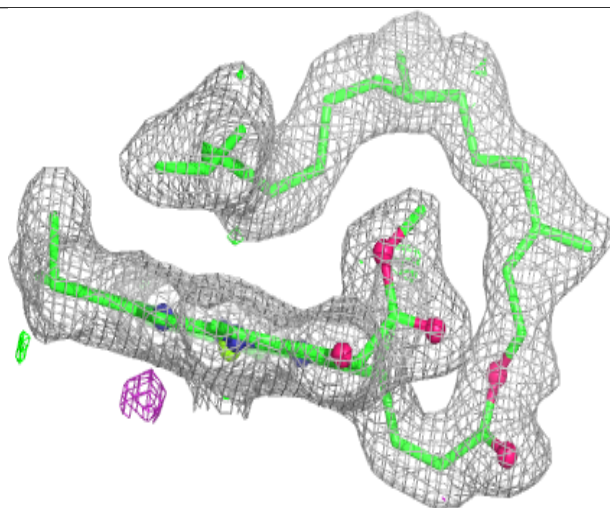
Electron density around CLA C 510:

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



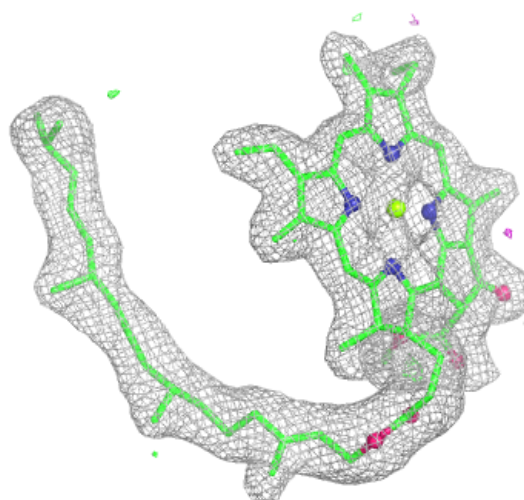
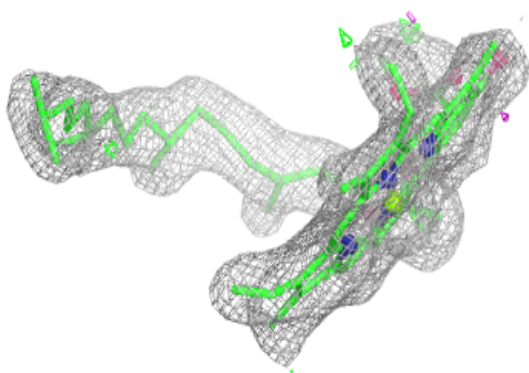
Electron density around CLA C 511:

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



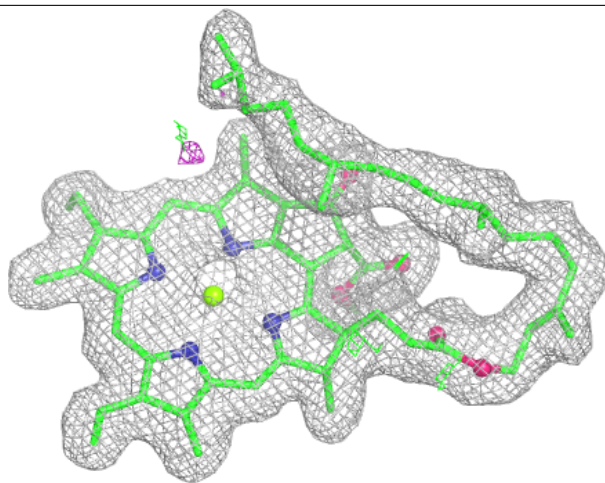
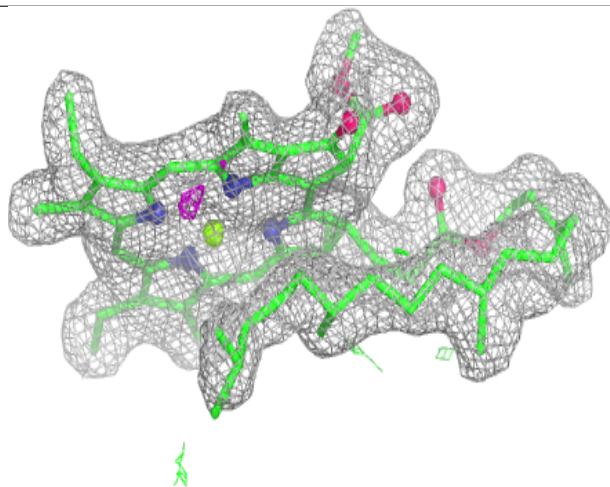
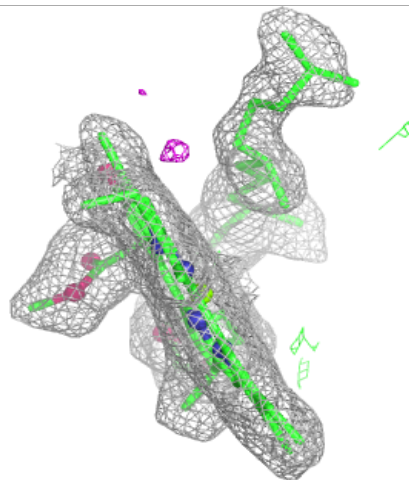
Electron density around CLA c 908:

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



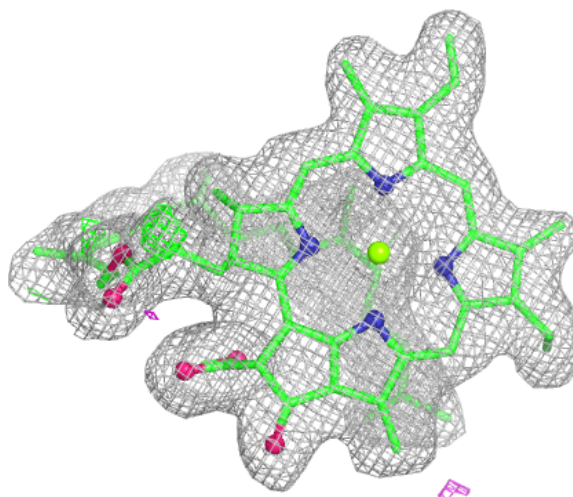
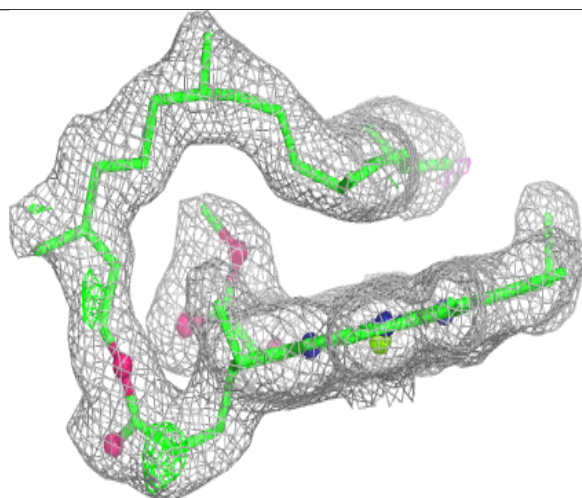
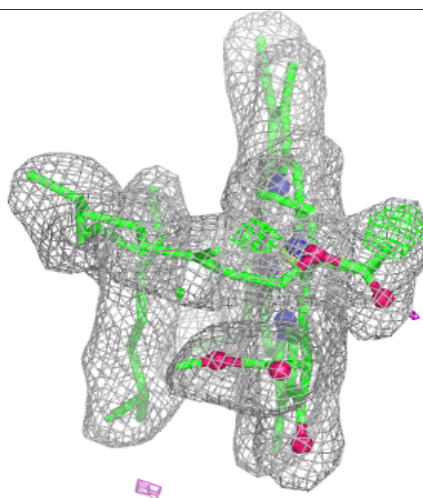
Electron density around CLA c 910:

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



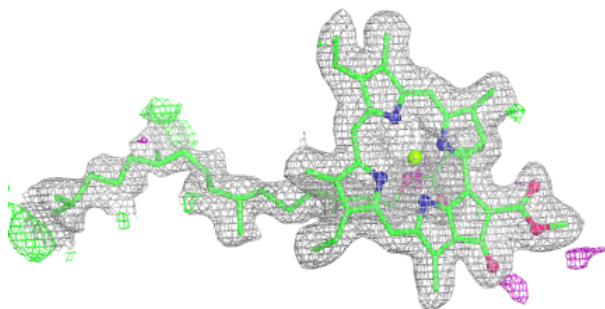
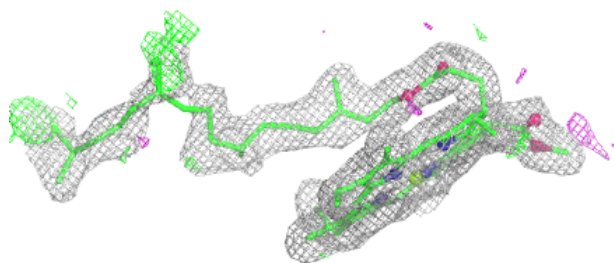
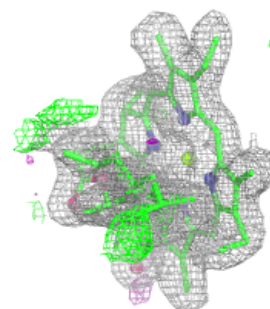
Electron density around CLA c 911:

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



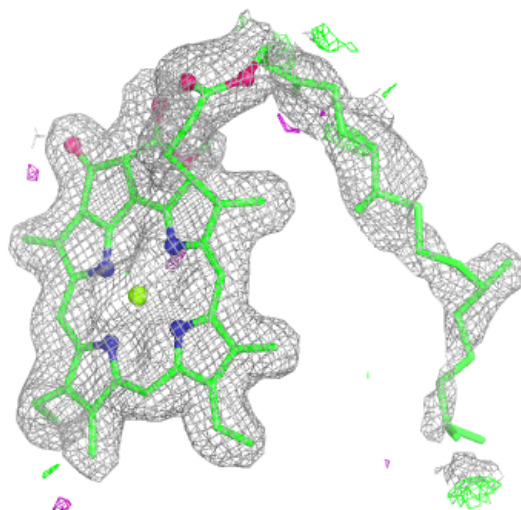
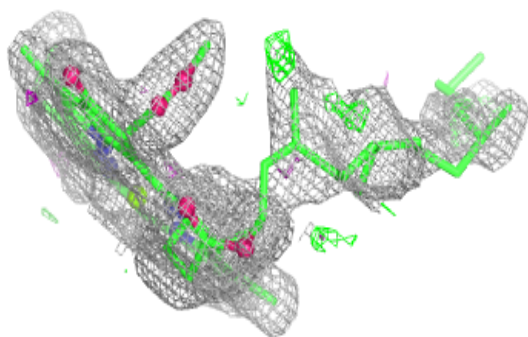
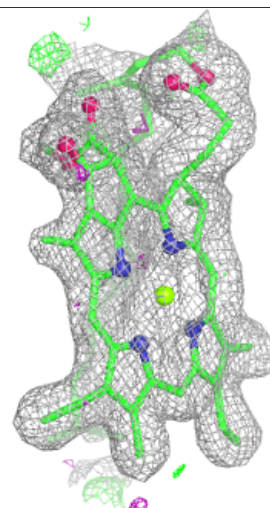
Electron density around CLA B 615:

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



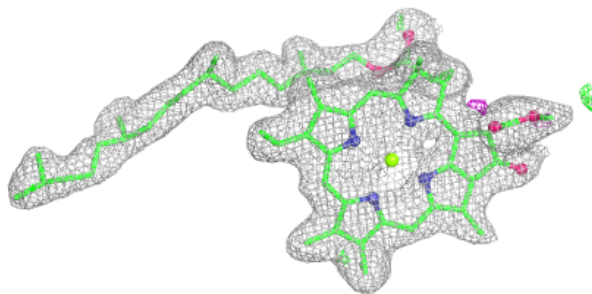
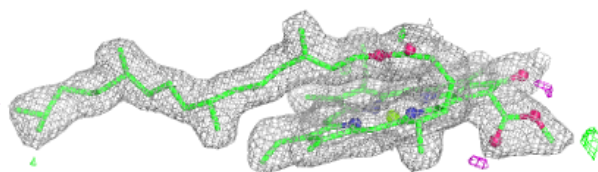
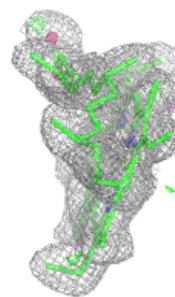
Electron density around CLA B 617:

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

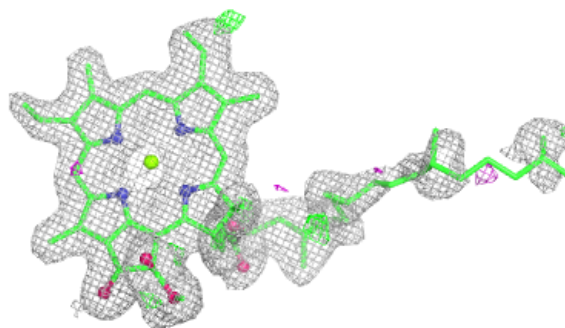
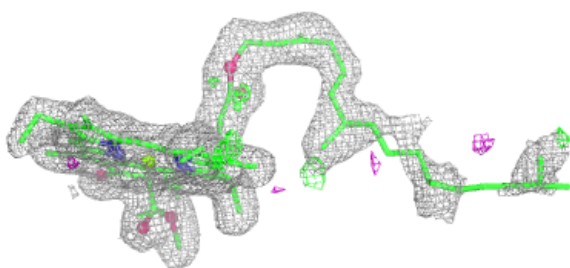
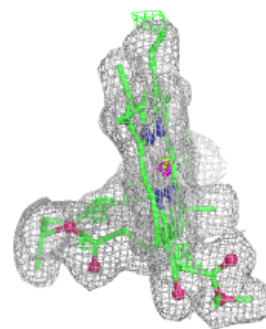


Electron density around CLA C 502:

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

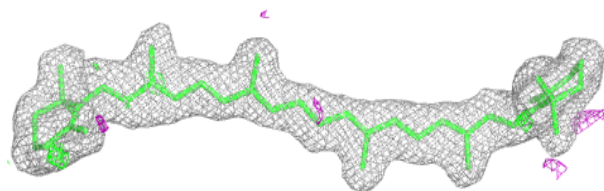
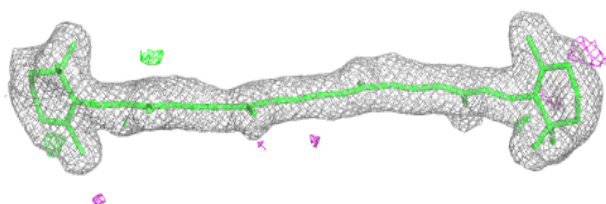
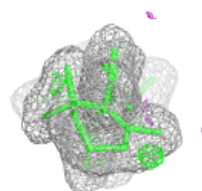
**Electron density around CLA a 407:**

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

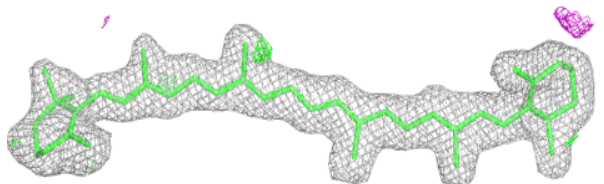
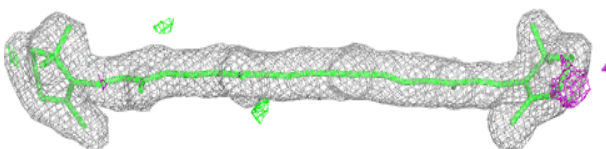
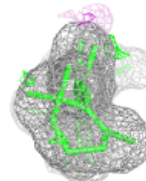


Electron density around BCR A 411:

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

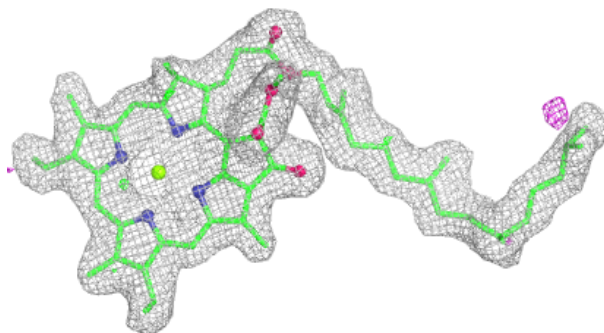
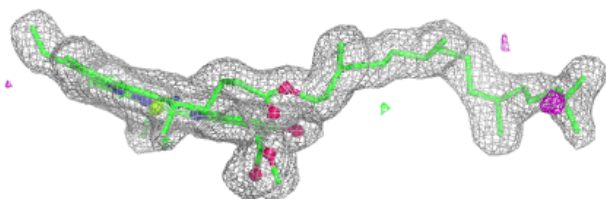
**Electron density around BCR B 619:**

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

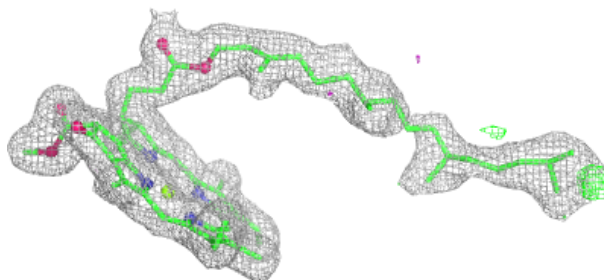
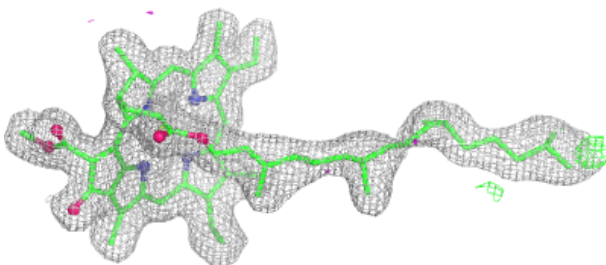
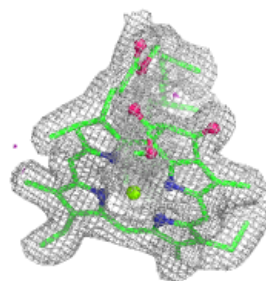


Electron density around CLA b 606:

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

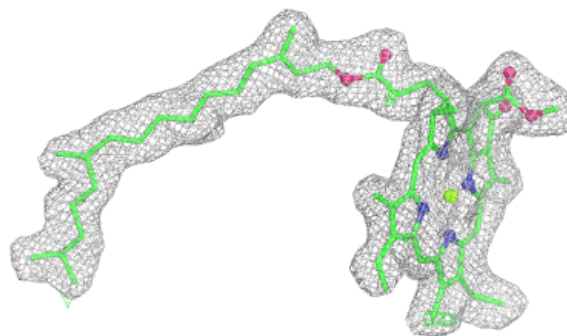
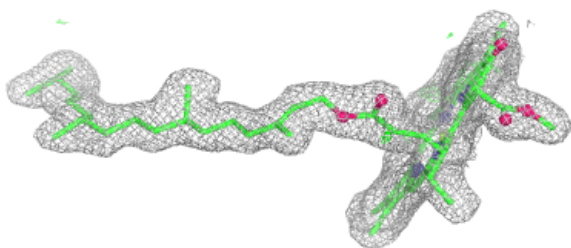
**Electron density around CLA C 505:**

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

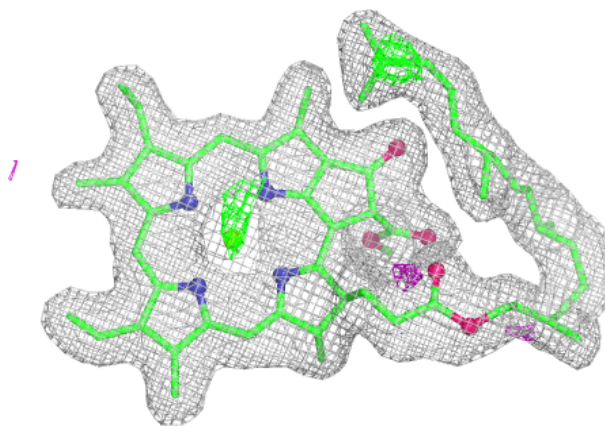
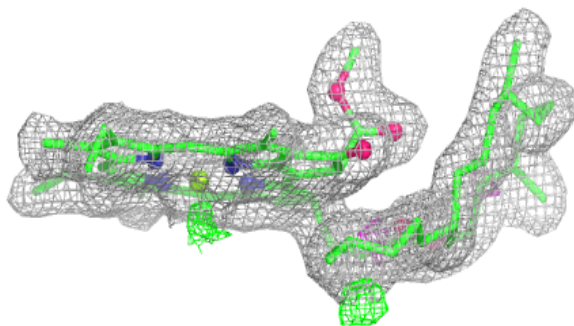
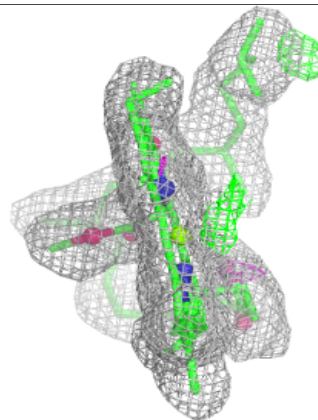


Electron density around CLA b 613:

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

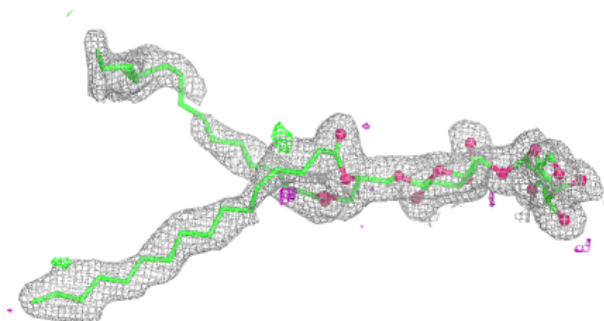
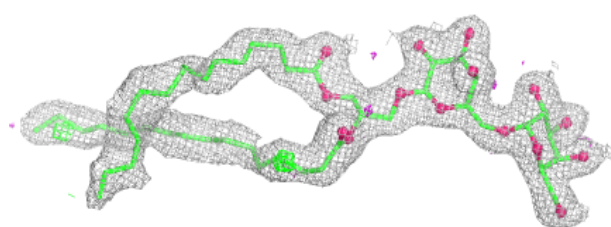
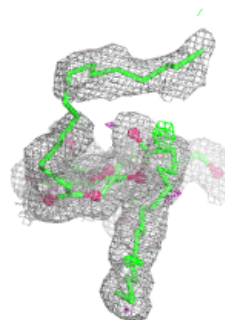
**Electron density around CLA b 614:**

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

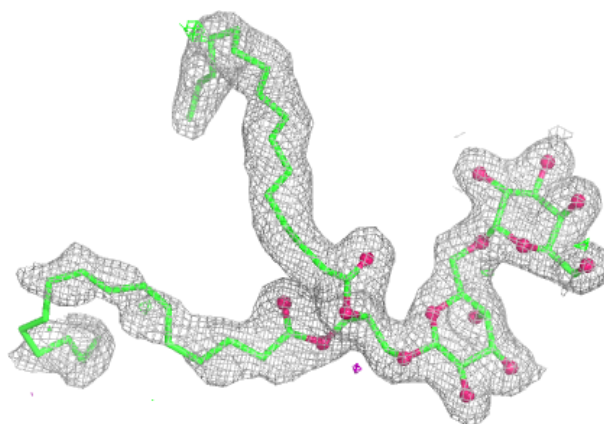
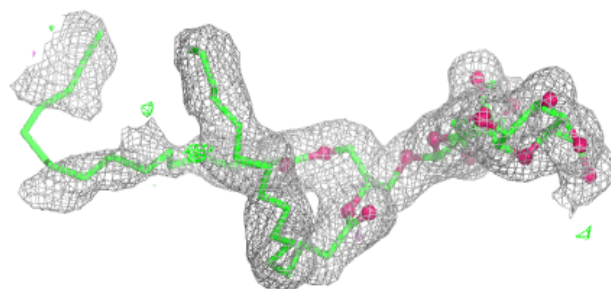
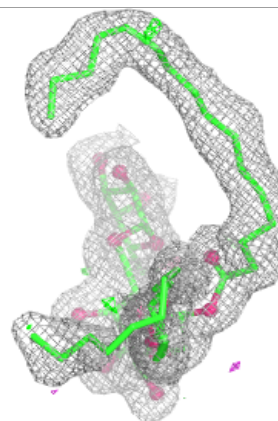


Electron density around DGD C 517:

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

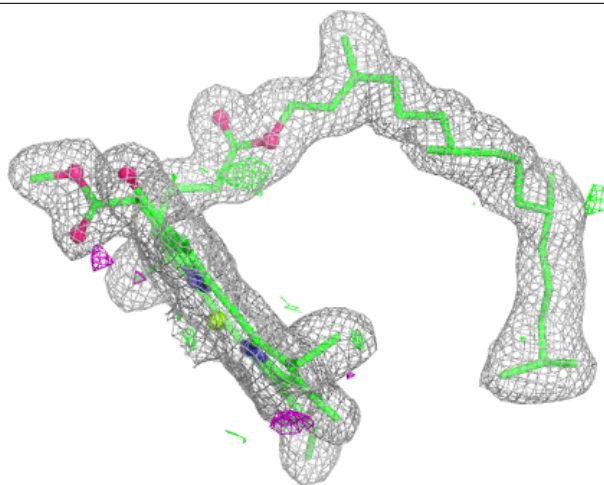
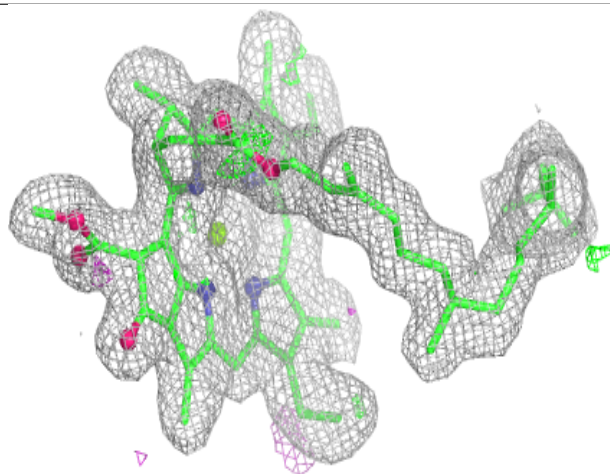
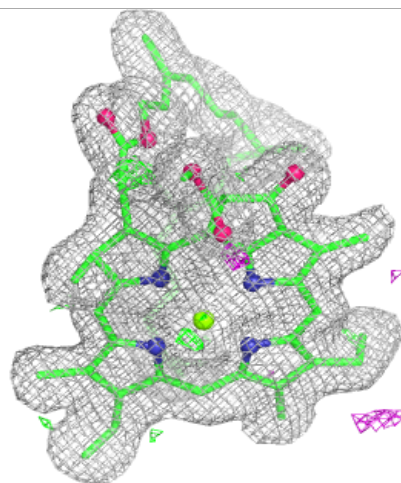
**Electron density around DGD C 518:**

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



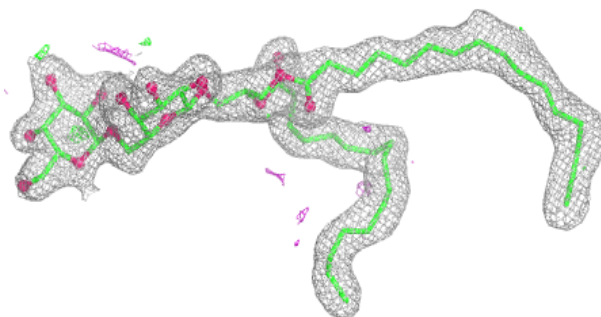
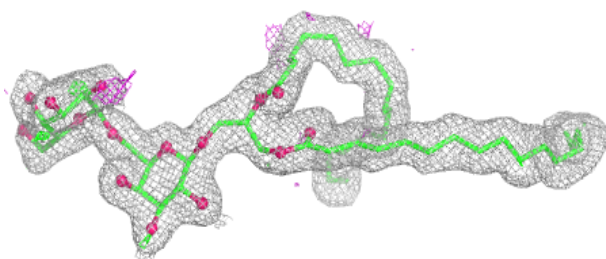
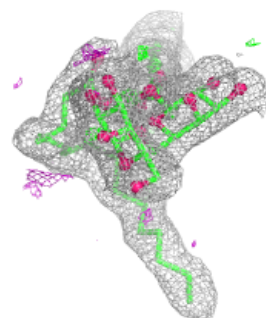
Electron density around CLA b 615:

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

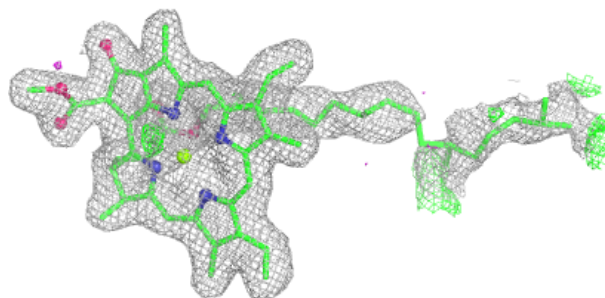
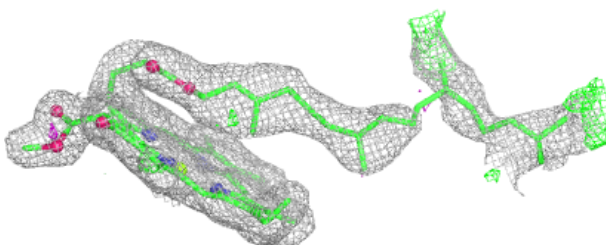
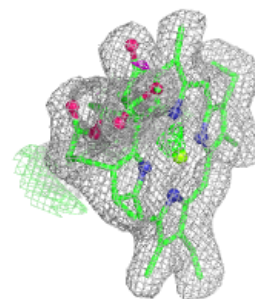


Electron density around DGD H 102:

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

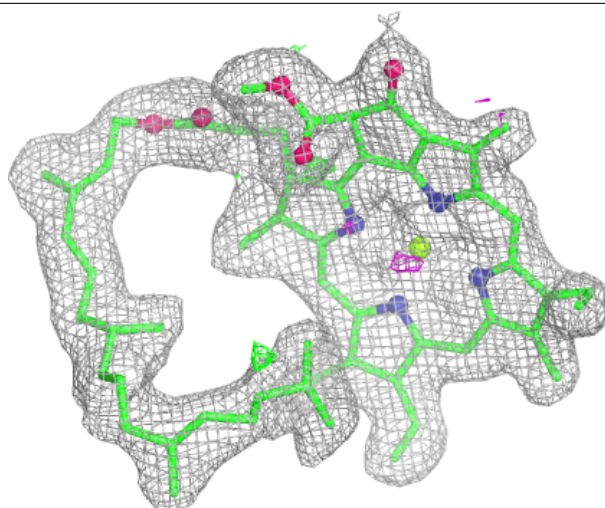
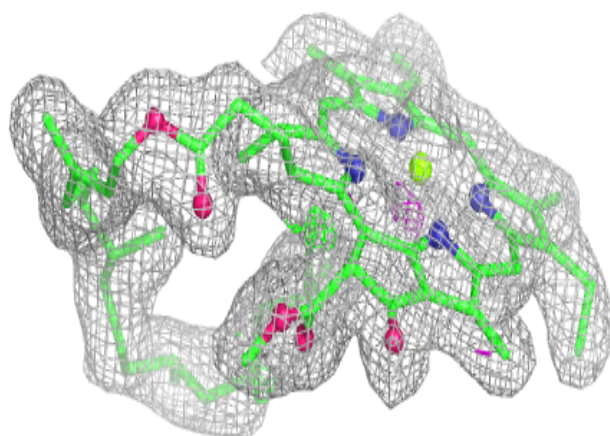
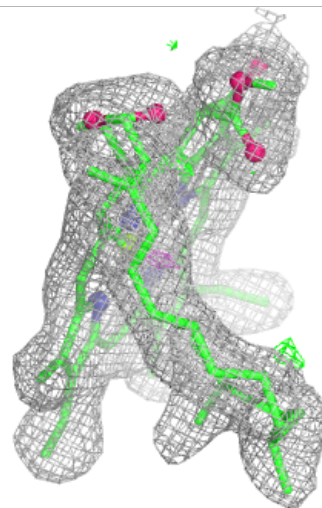
**Electron density around CLA b 618:**

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



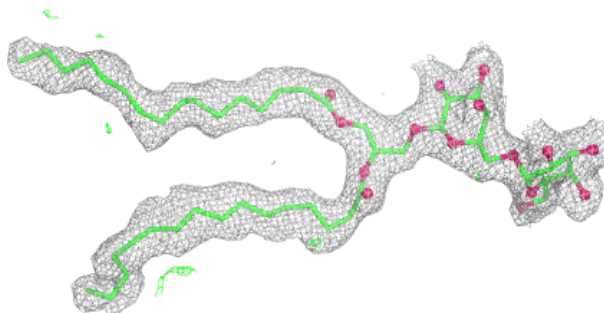
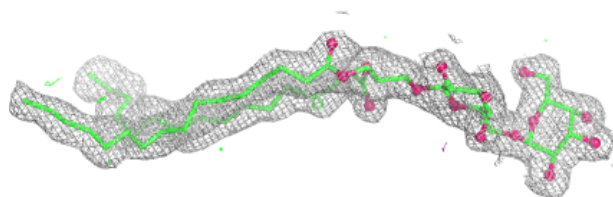
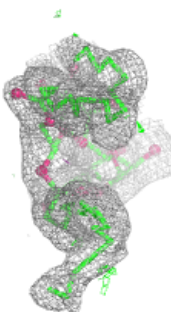
Electron density around CLA b 619:

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



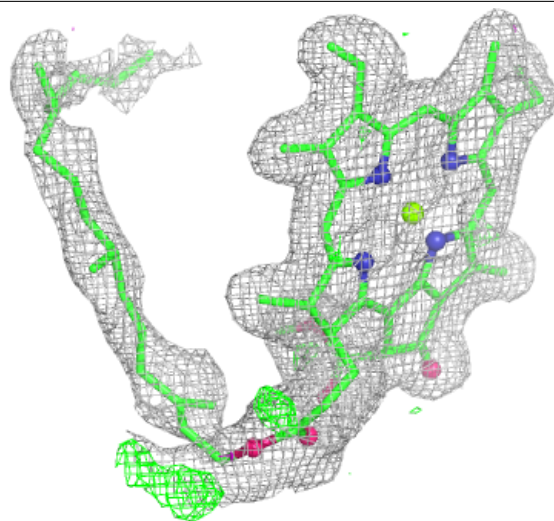
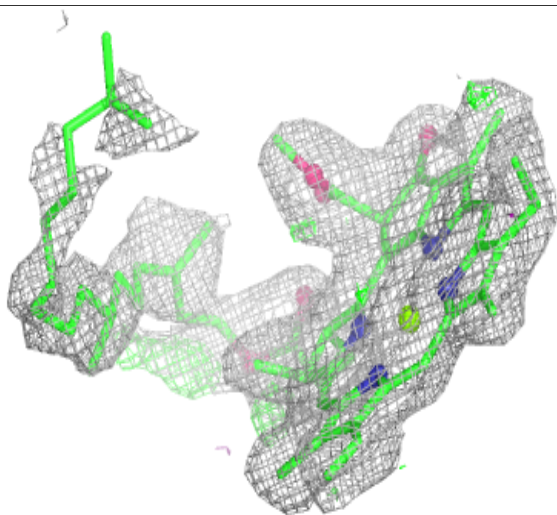
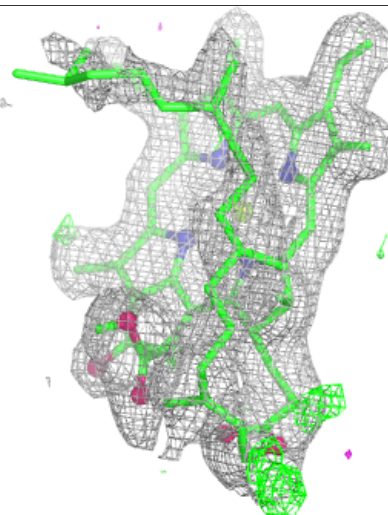
Electron density around DGD c 918:

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



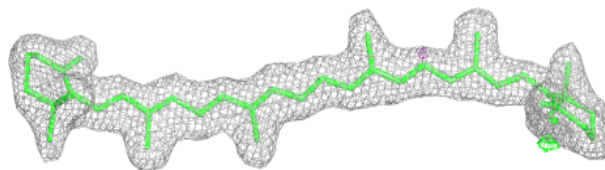
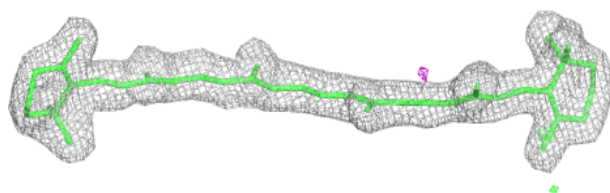
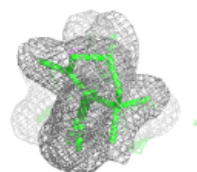
Electron density around CLA b 620:

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

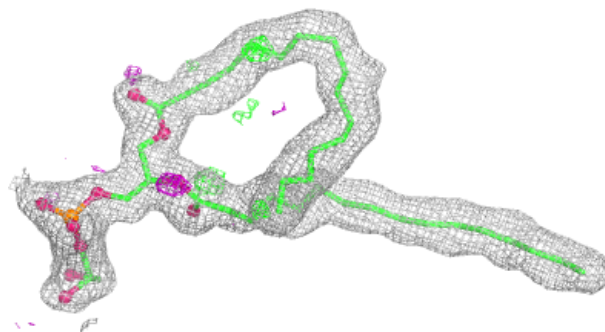
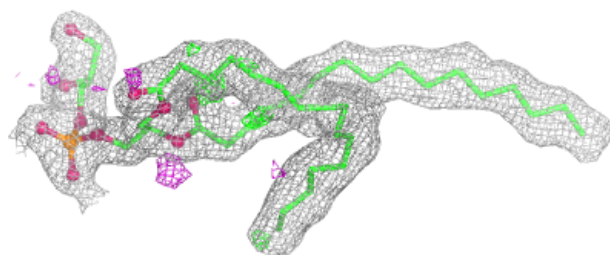


Electron density around BCR a 410:

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

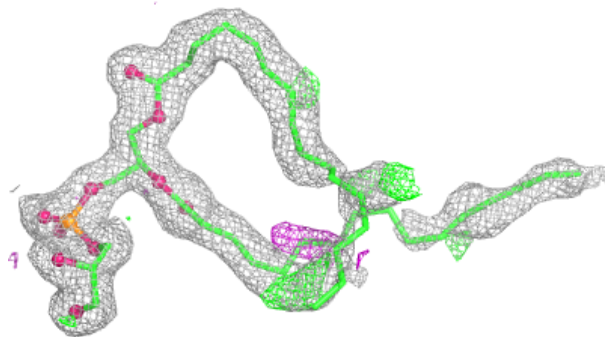
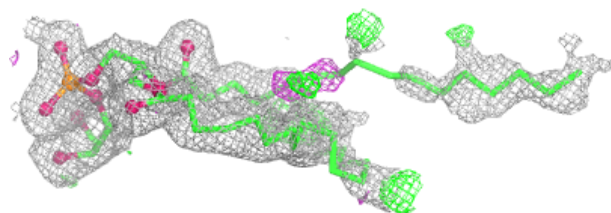
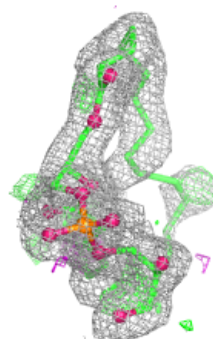
**Electron density around LHG D 406:**

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

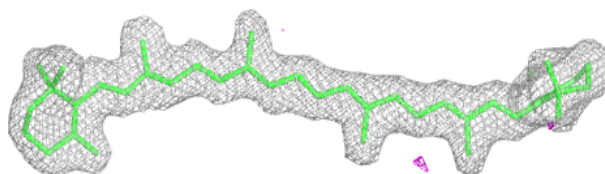
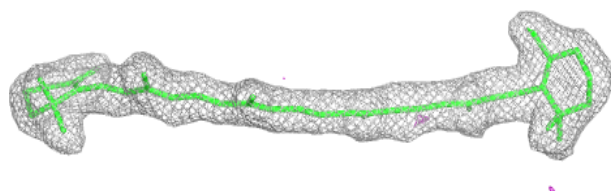
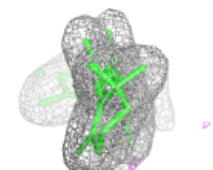


Electron density around LHG D 408:

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

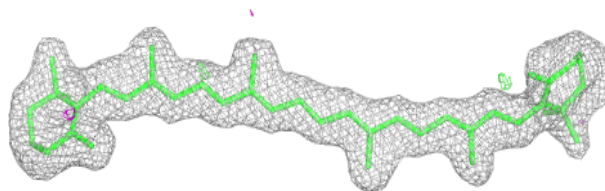
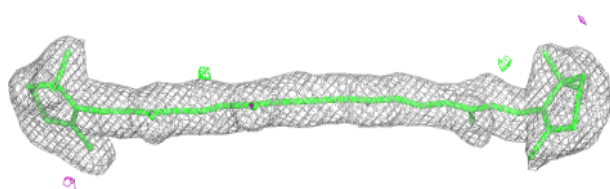
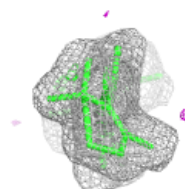
**Electron density around BCR b 621:**

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

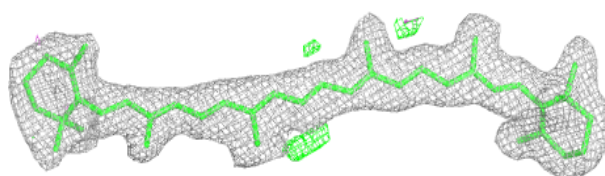
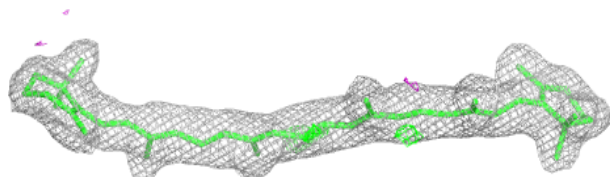
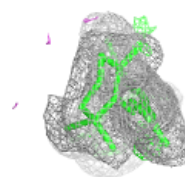


Electron density around BCR b 622:

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

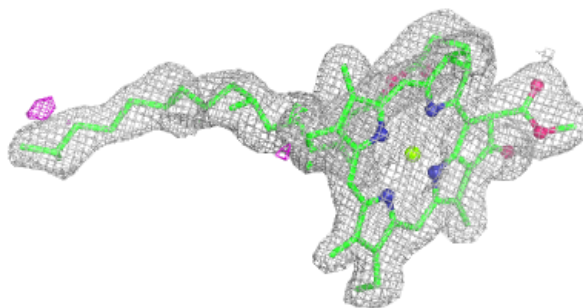
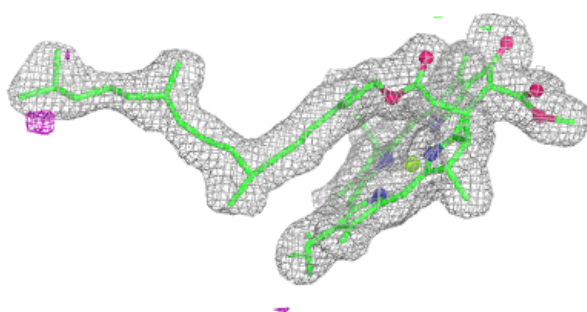
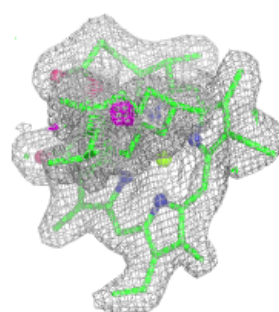
**Electron density around BCR b 623:**

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

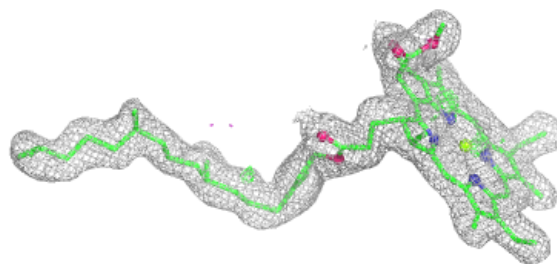
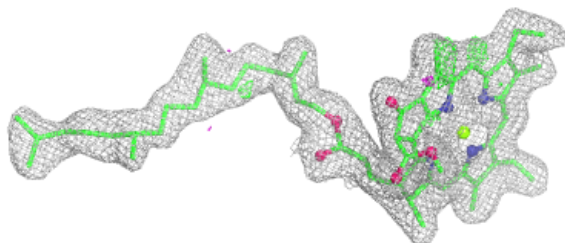
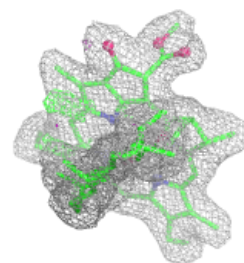


Electron density around CLA C 506:

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

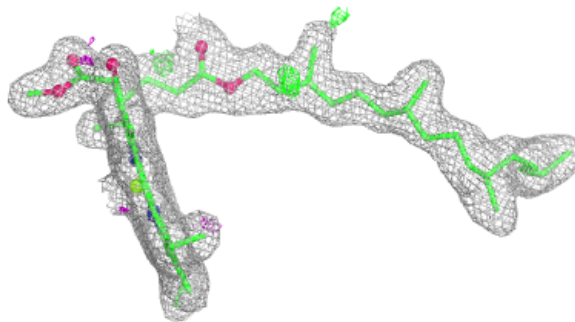
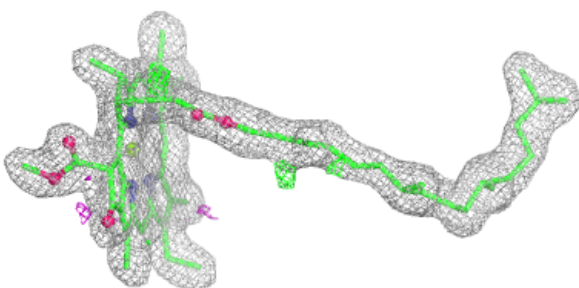
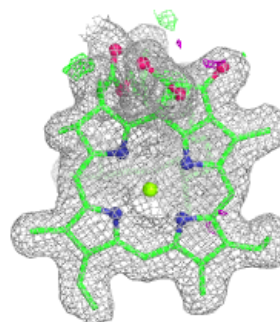
**Electron density around CLA c 903:**

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

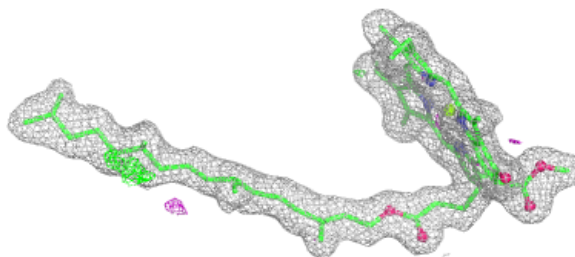
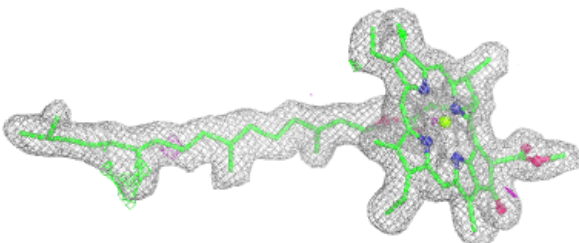
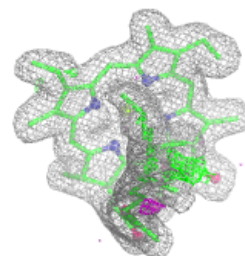


Electron density around CLA b 609:

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

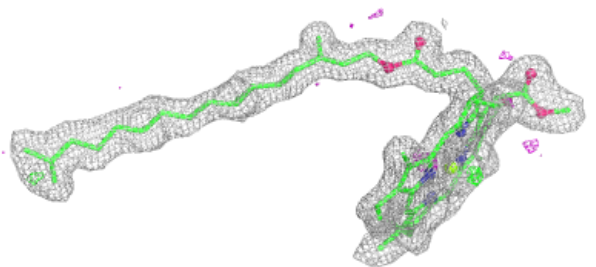
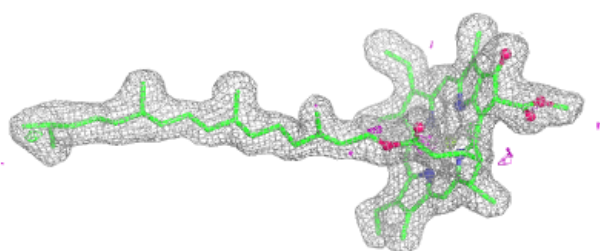
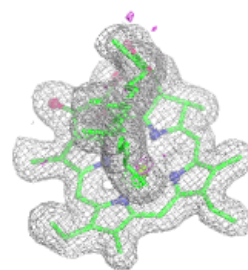
**Electron density around CLA B 608:**

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

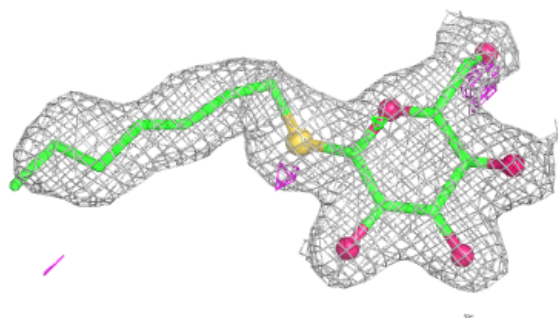
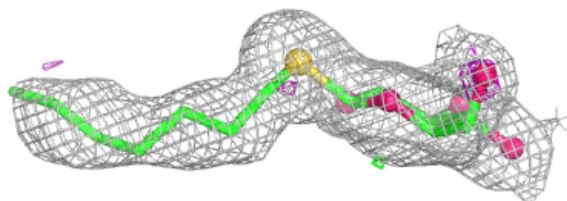
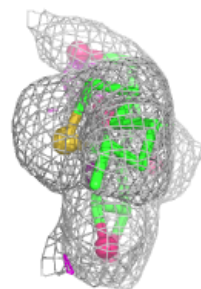


Electron density around CLA b 611:

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

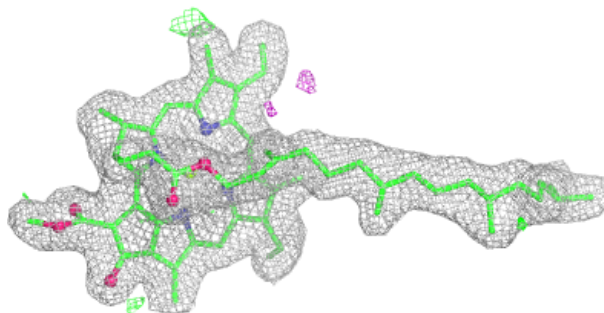
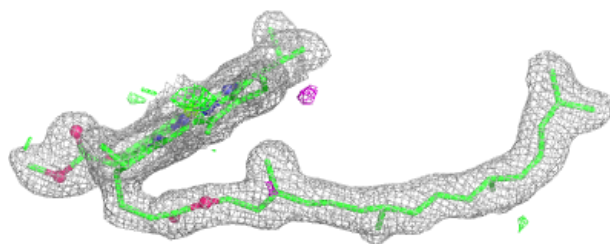
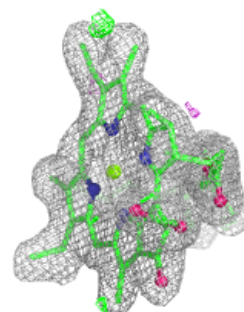
**Electron density around HTG O 303:**

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

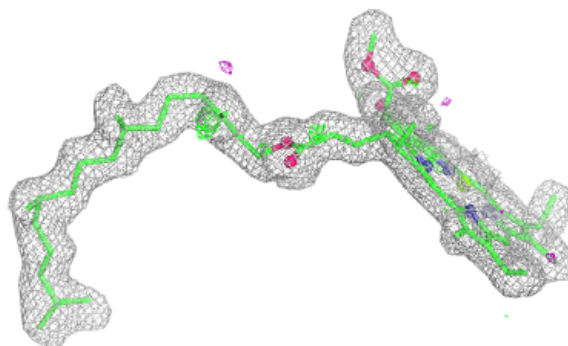
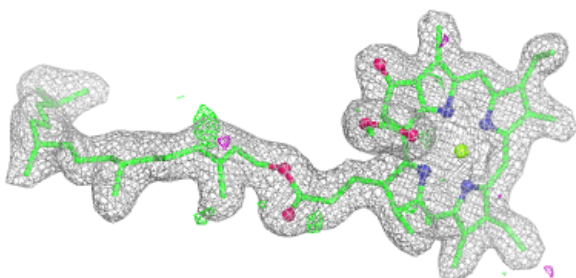
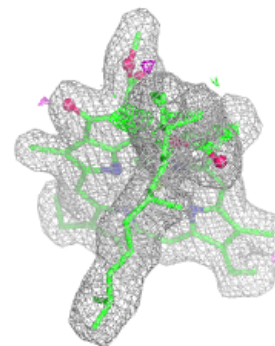


Electron density around CLA b 612:

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

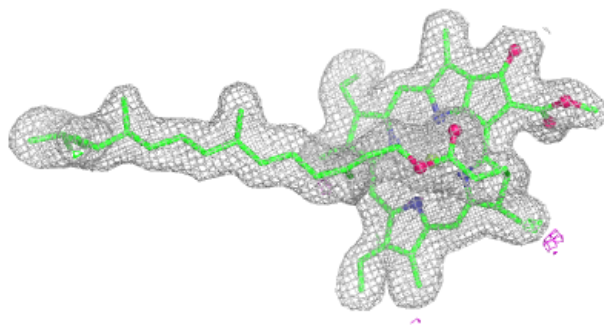
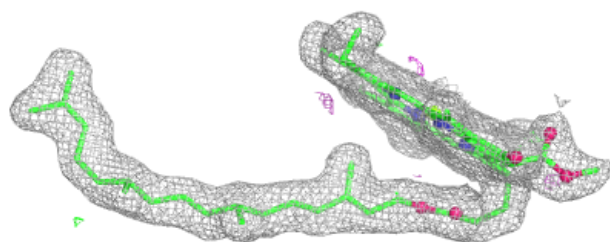
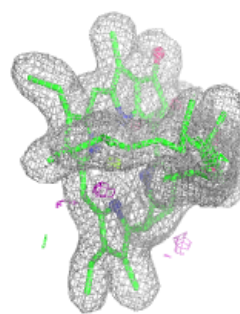
**Electron density around CLA d 402:**

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

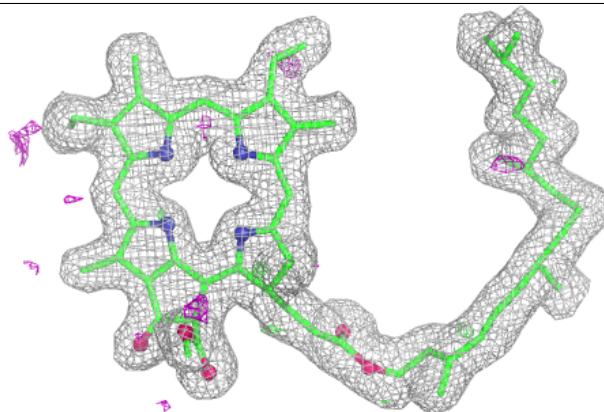
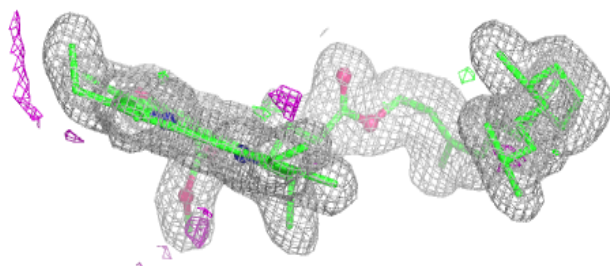


Electron density around CLA B 609:

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

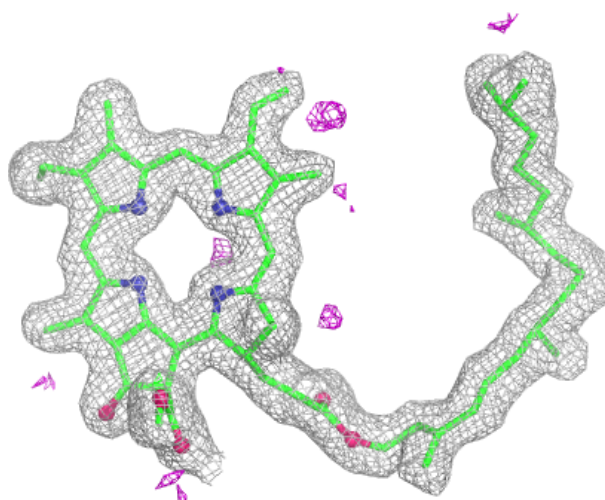
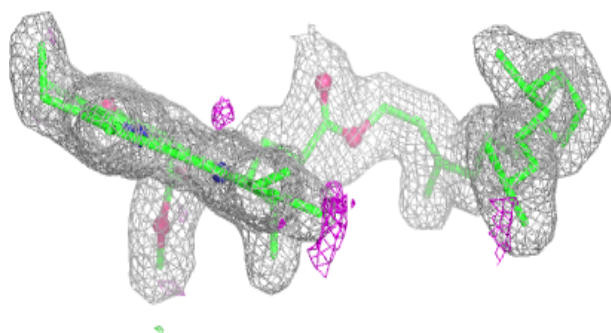
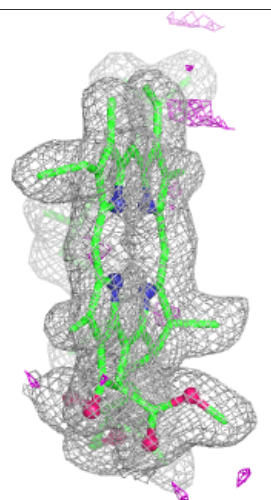
**Electron density around PHO A 408:**

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



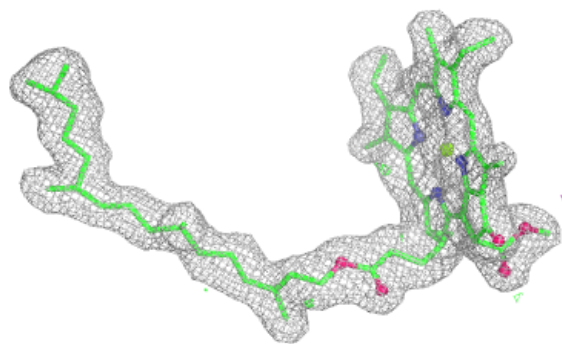
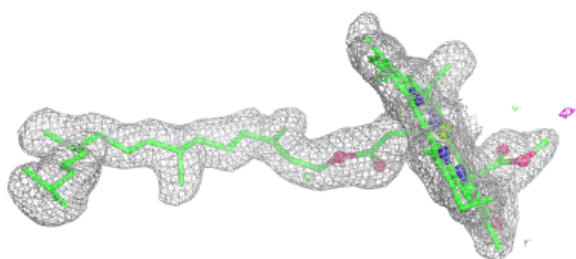
Electron density around PHO a 408:

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

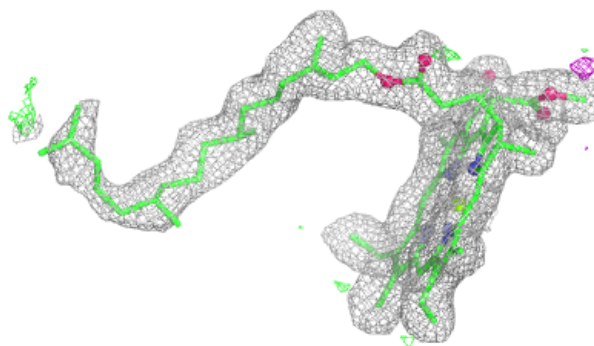
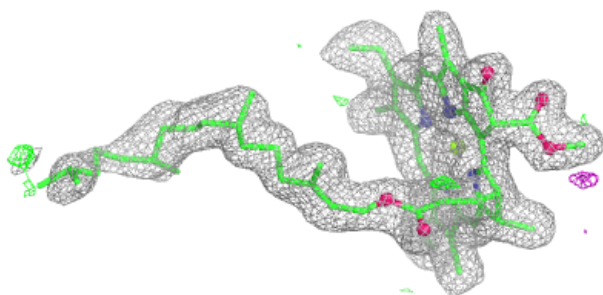
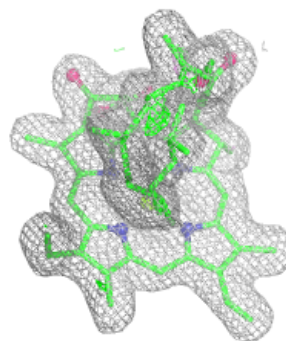


Electron density around CLA B 610:

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

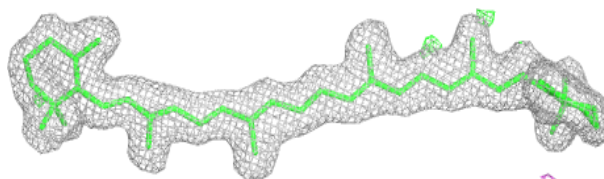
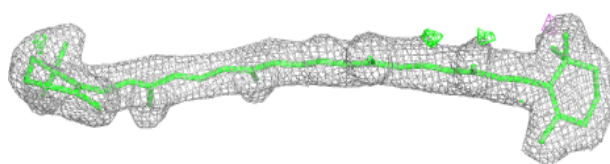
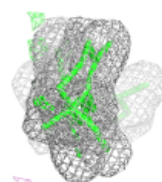
**Electron density around CLA C 509:**

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

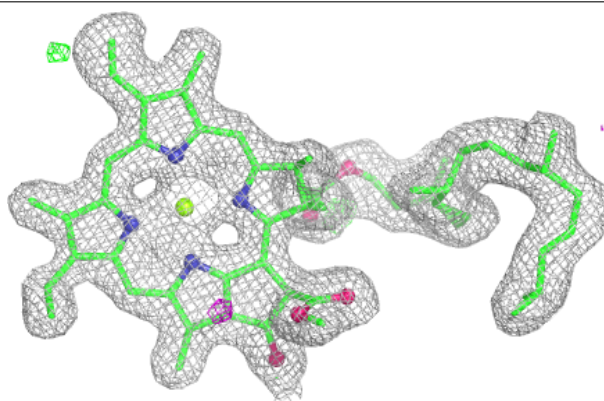
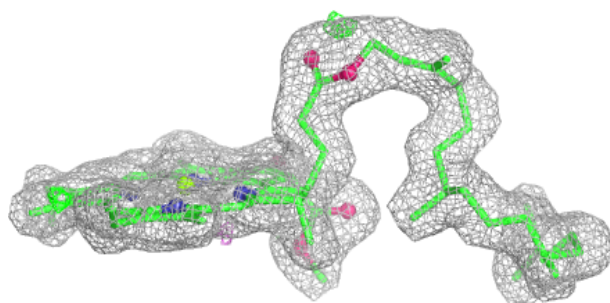
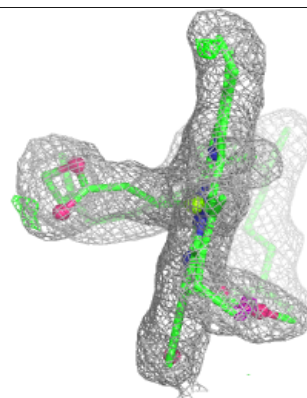


Electron density around BCR B 618:

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

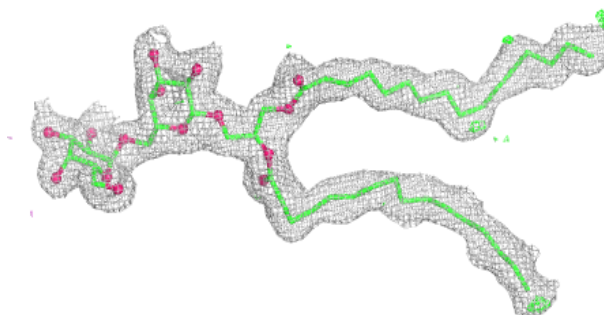
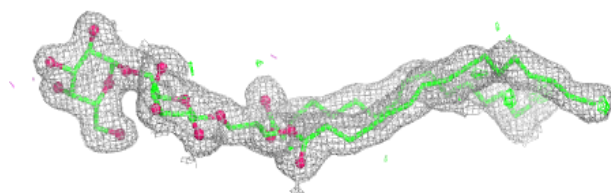
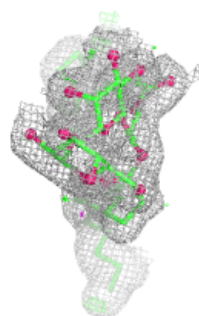
**Electron density around CLA b 616:**

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



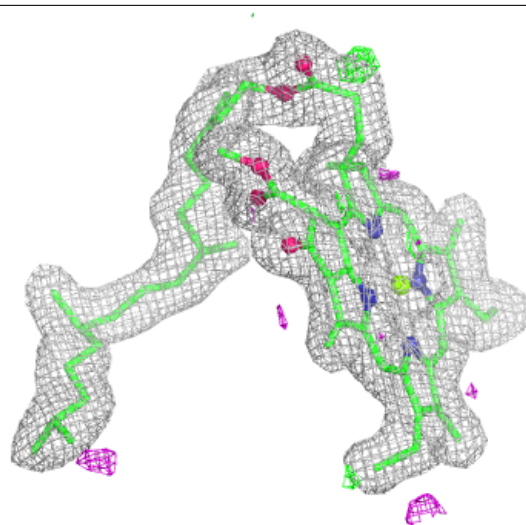
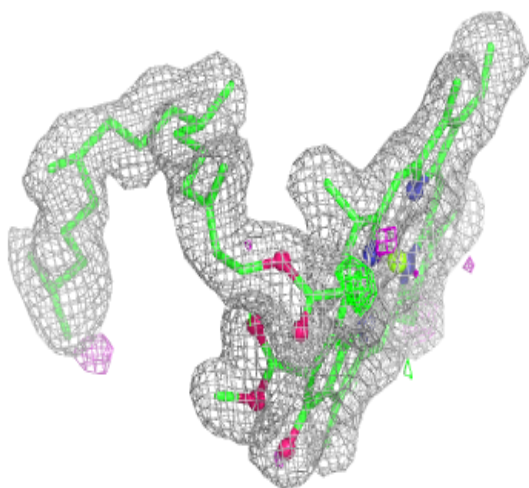
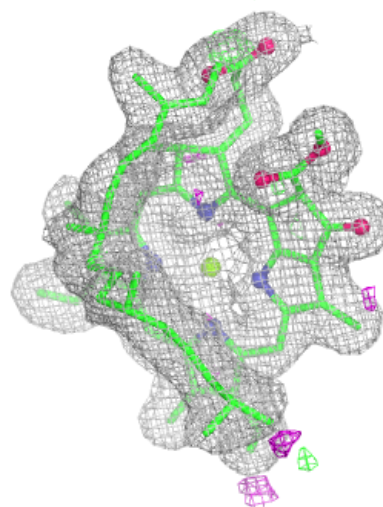
Electron density around DGD C 519:

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



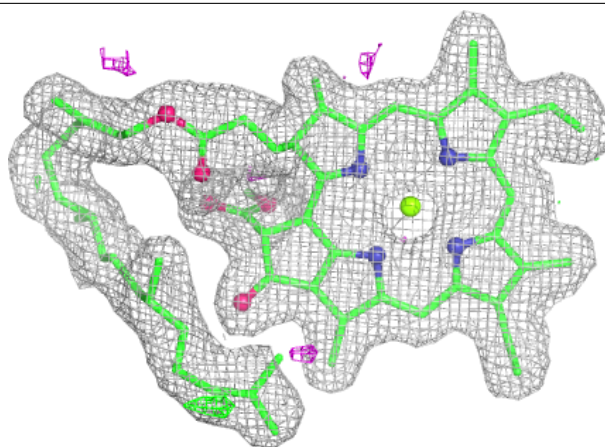
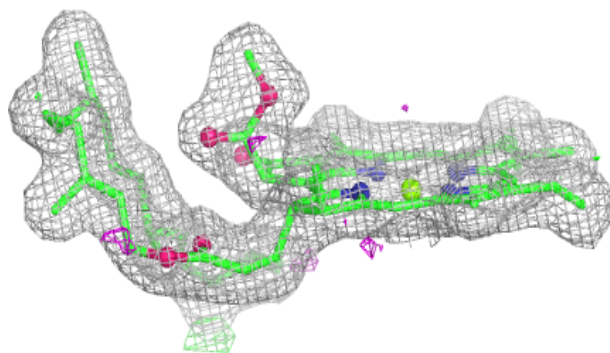
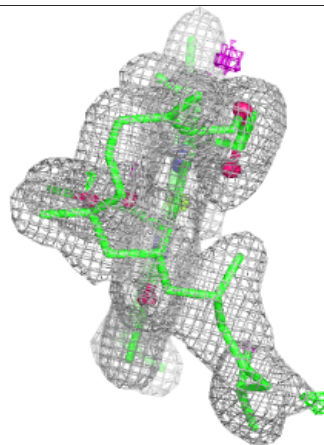
Electron density around CLA b 617:

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

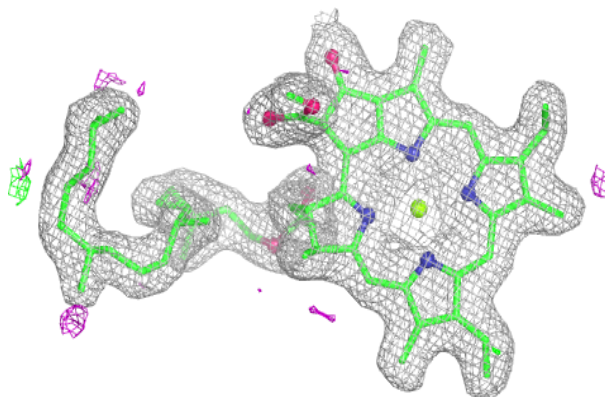
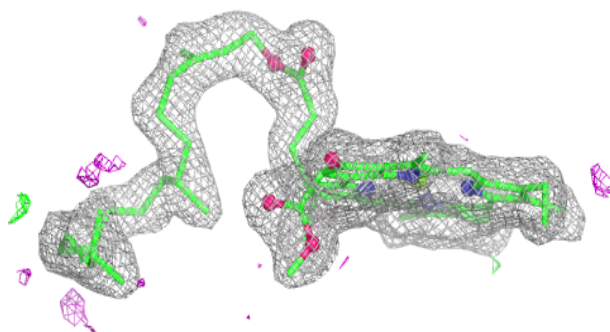


Electron density around CLA B 611:

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

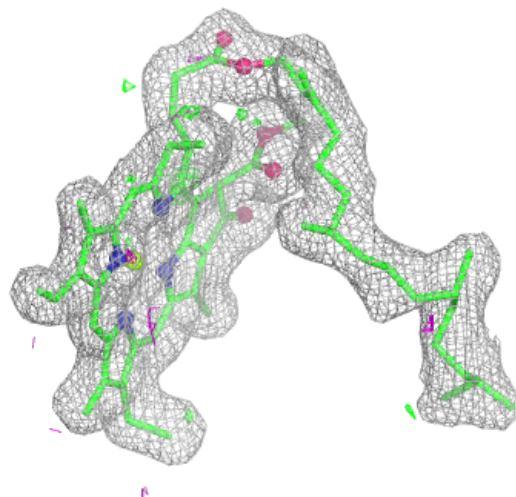
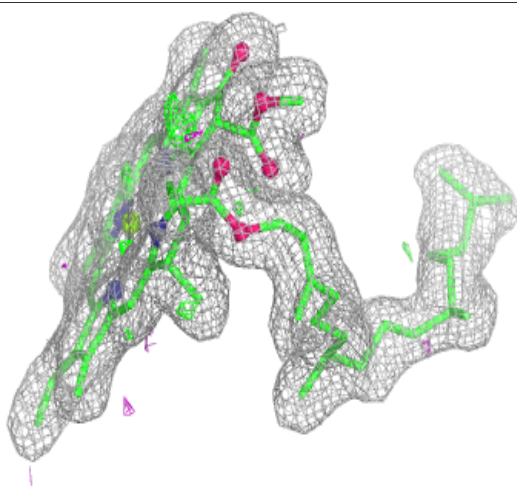
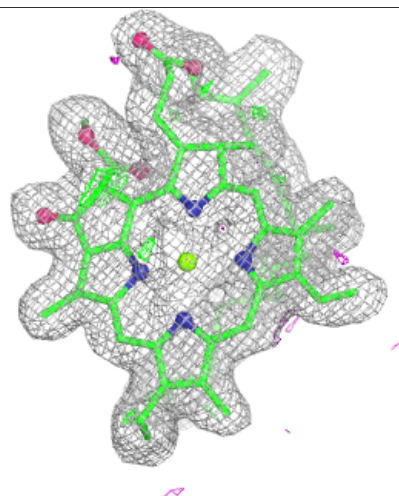
**Electron density around CLA B 613:**

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



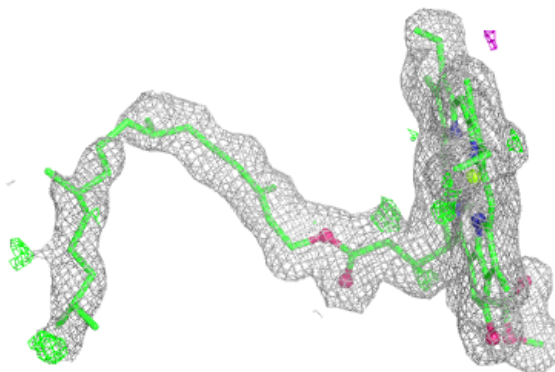
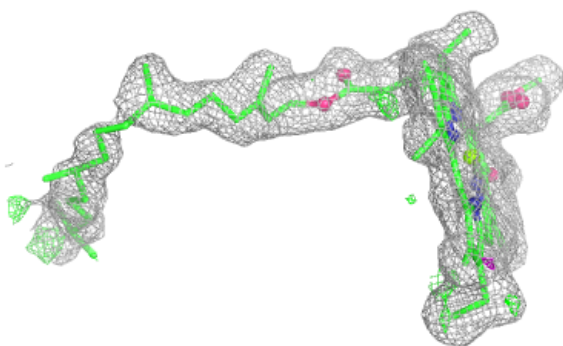
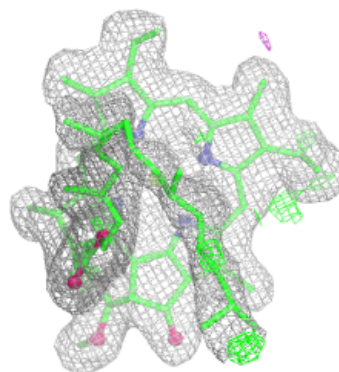
Electron density around CLA B 614:

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

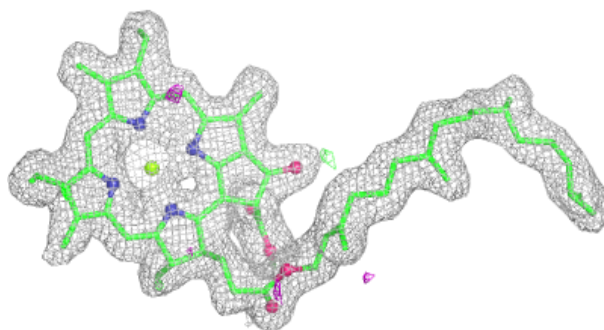
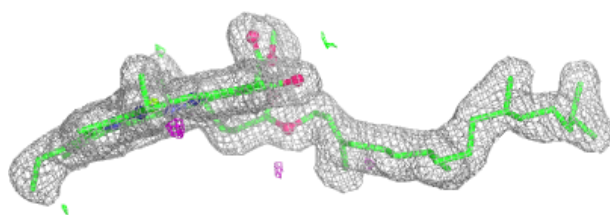
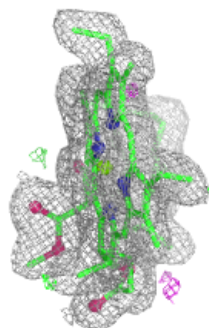


Electron density around CLA D 402:

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

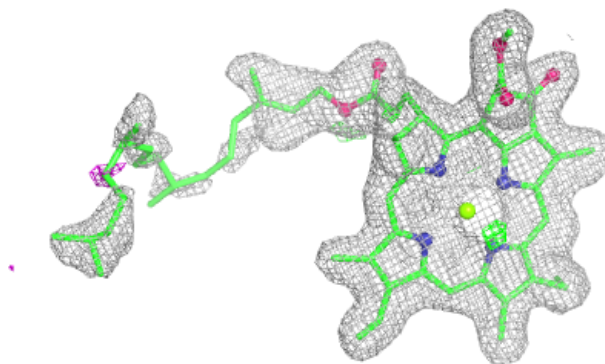
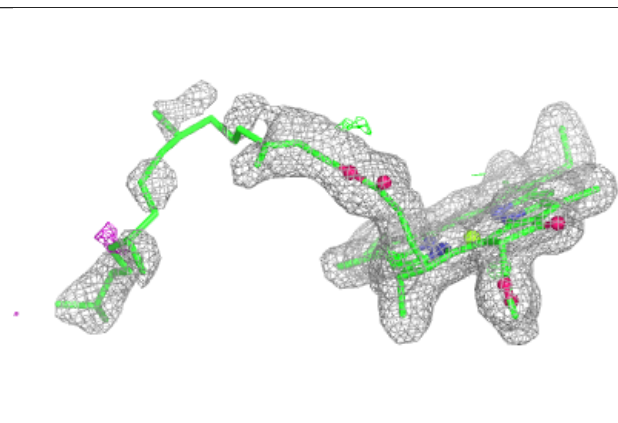
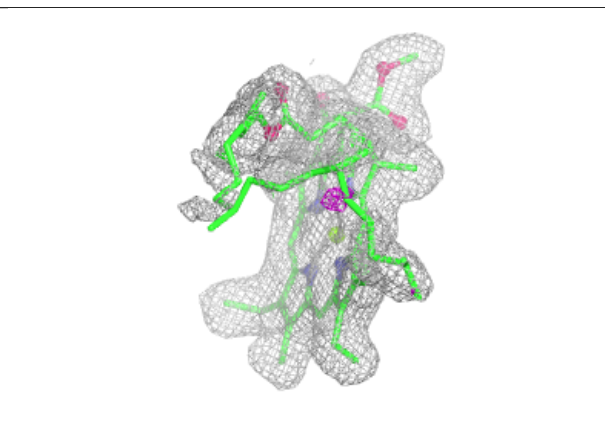
**Electron density around CLA B 603:**

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

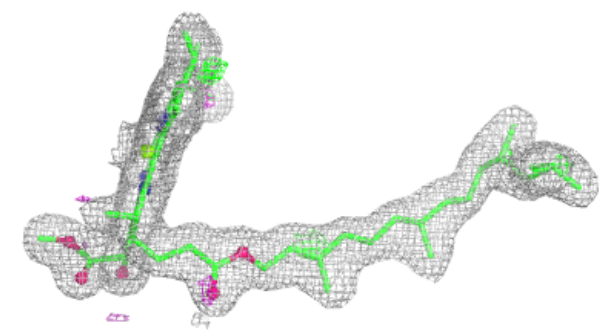
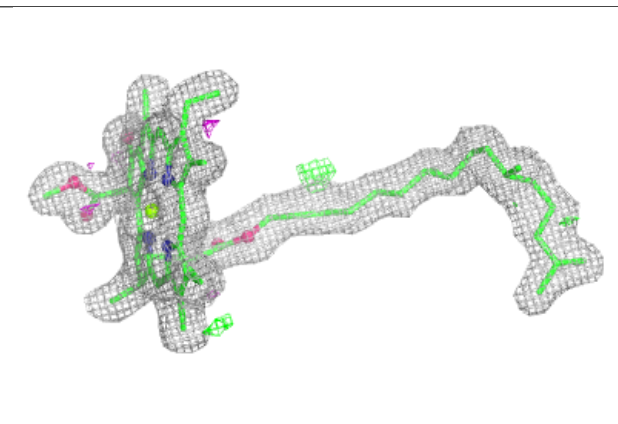
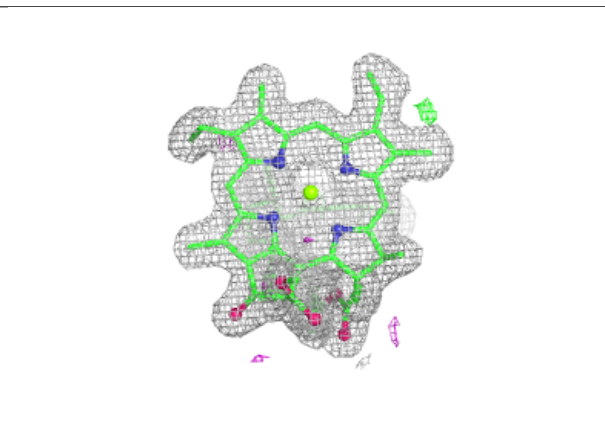


Electron density around CLA a 409:

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

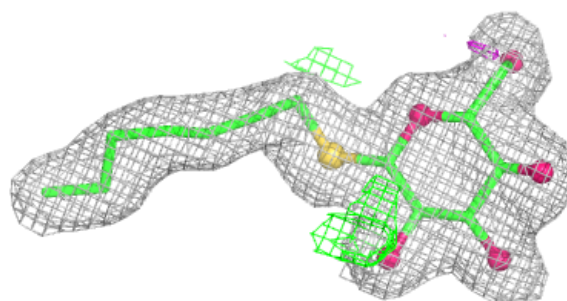
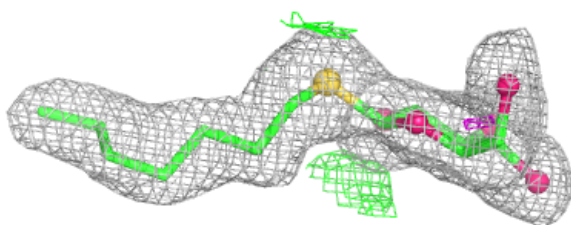
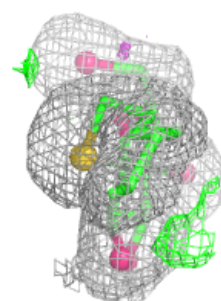
**Electron density around CLA B 606:**

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

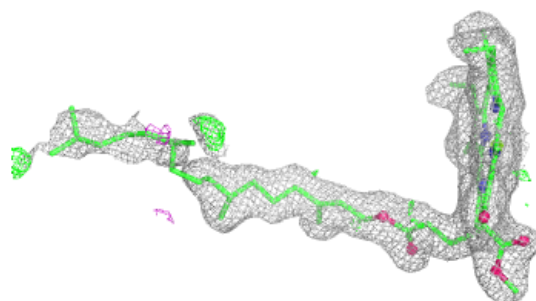
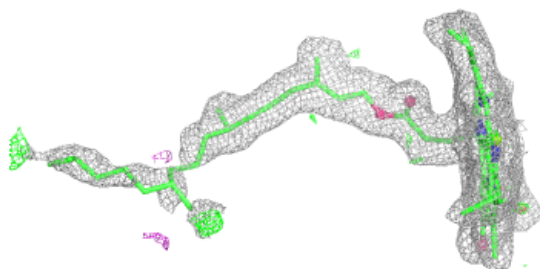
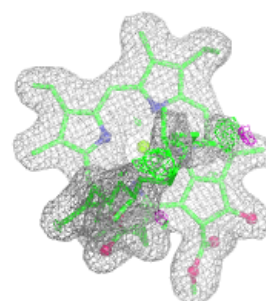


Electron density around HTG B 624:

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

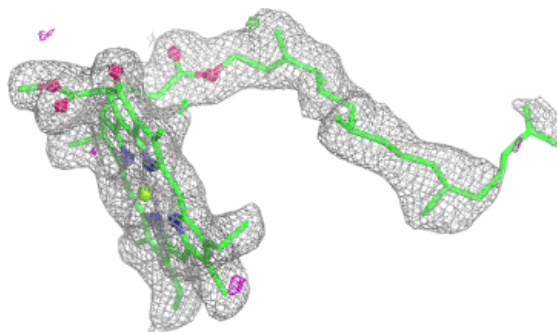
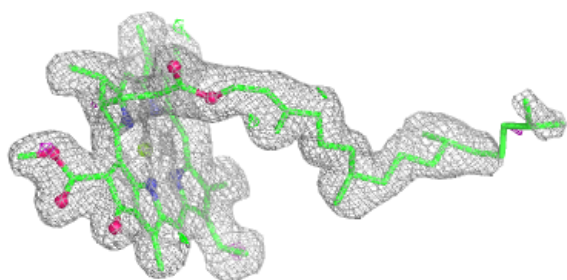
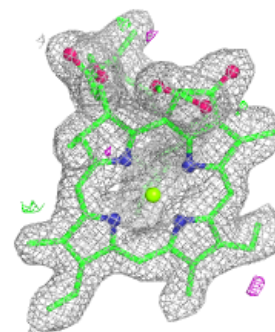
**Electron density around CLA B 607:**

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

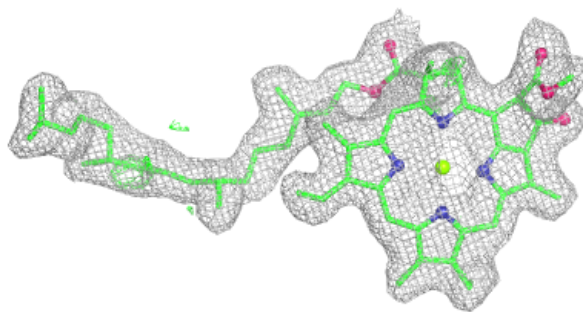
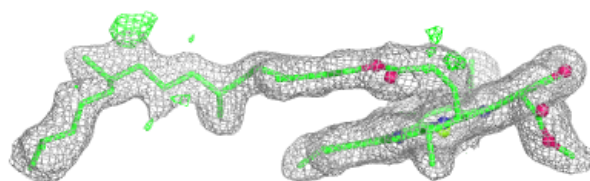
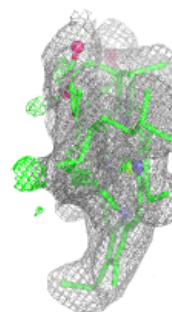


Electron density around CLA c 909:

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

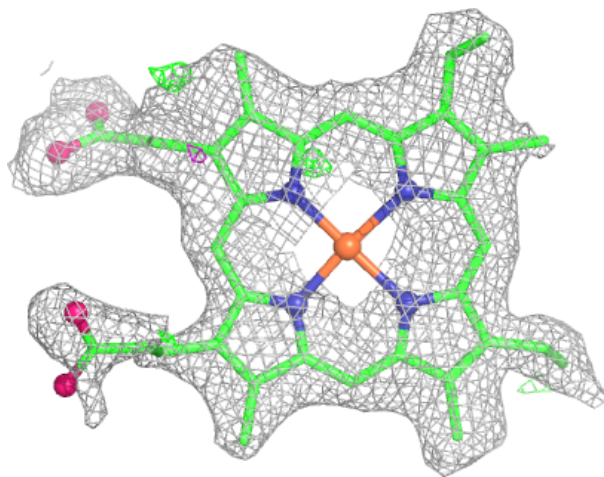
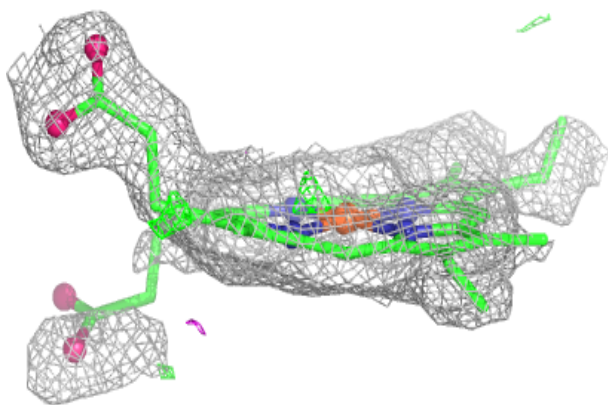
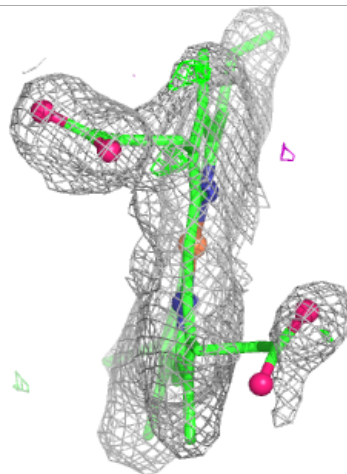
**Electron density around CLA b 607:**

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



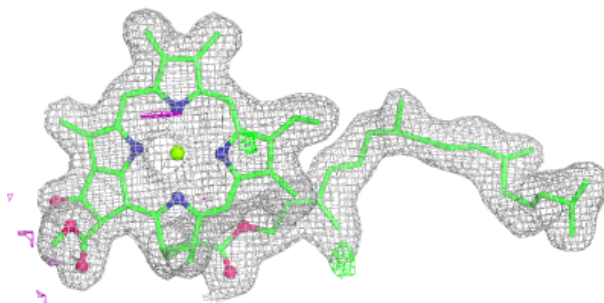
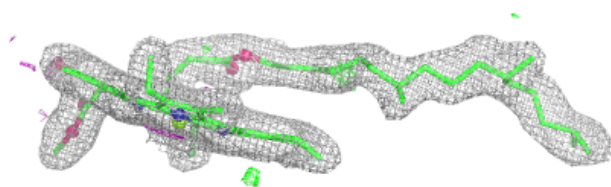
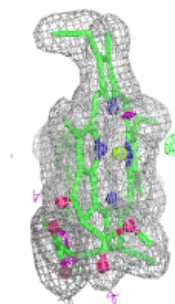
Electron density around HEM e 102:

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

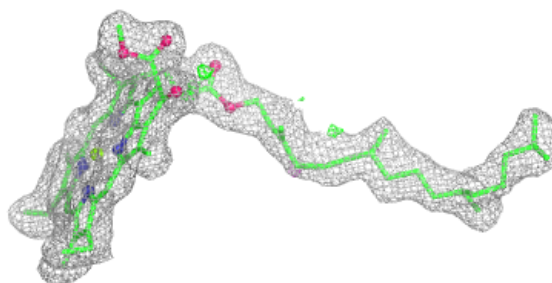
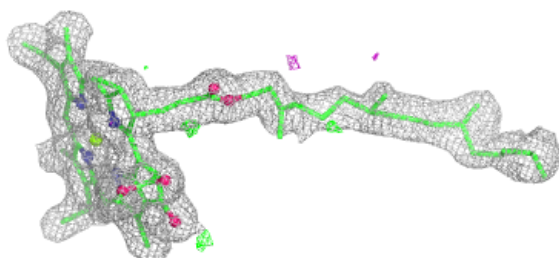
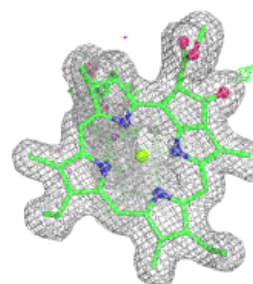


Electron density around CLA B 604:

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

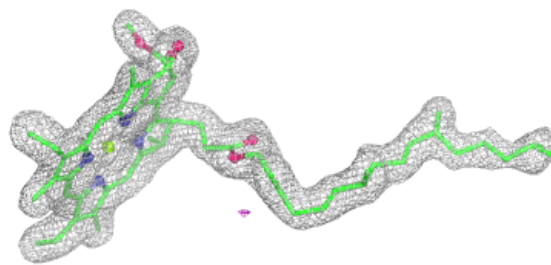
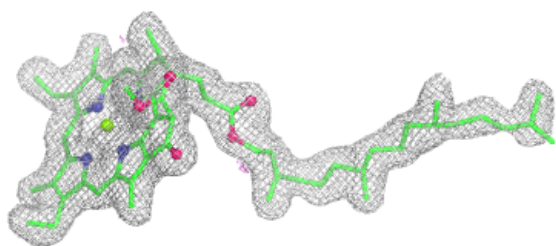
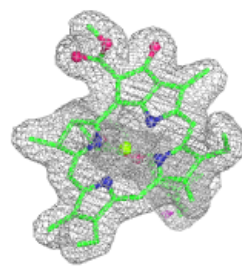
**Electron density around CLA b 608:**

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

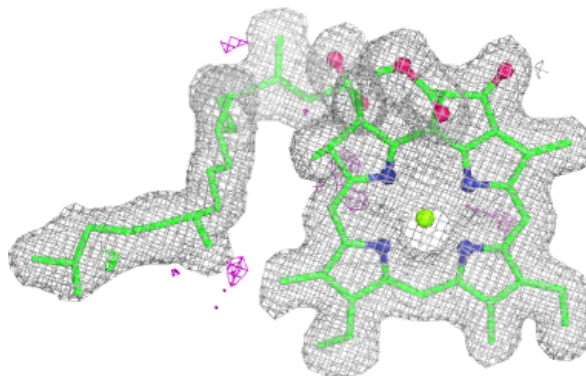
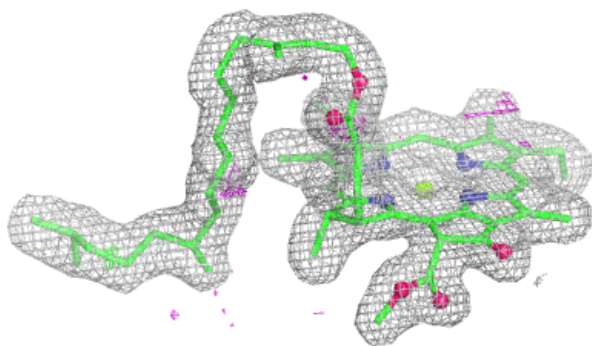
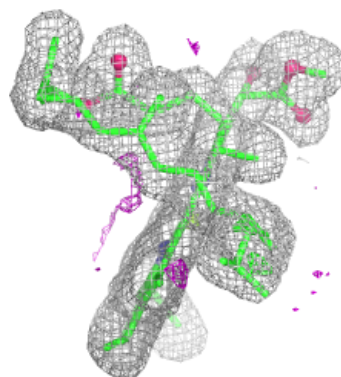


Electron density around CLA C 503:

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

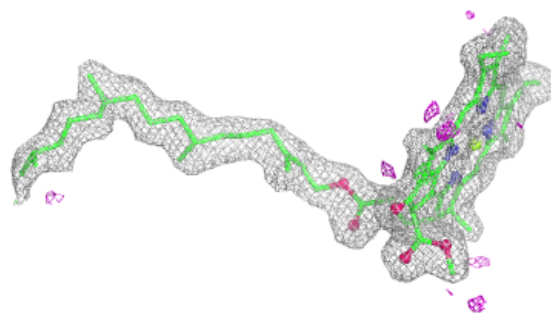
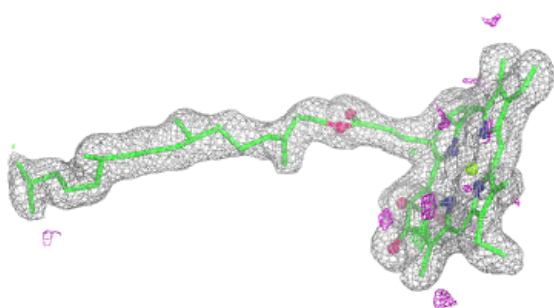
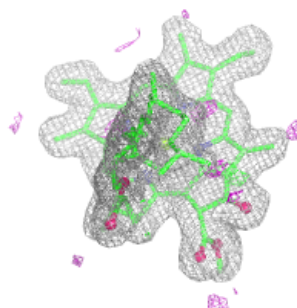
**Electron density around CLA d 401:**

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



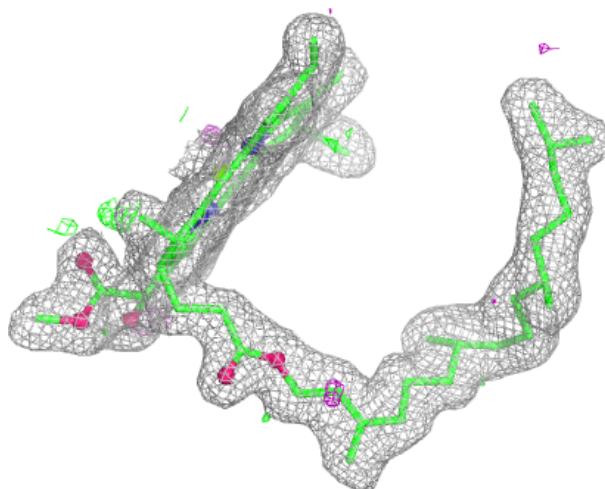
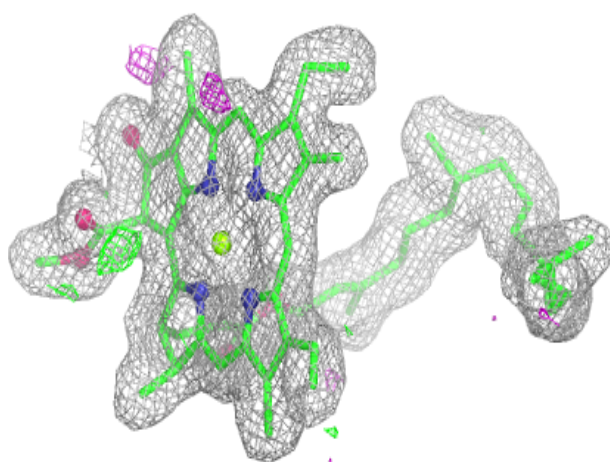
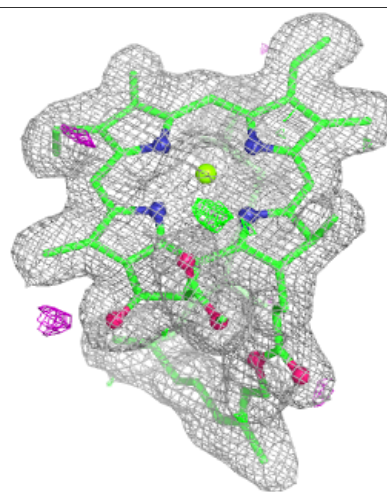
Electron density around CLA B 605:

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



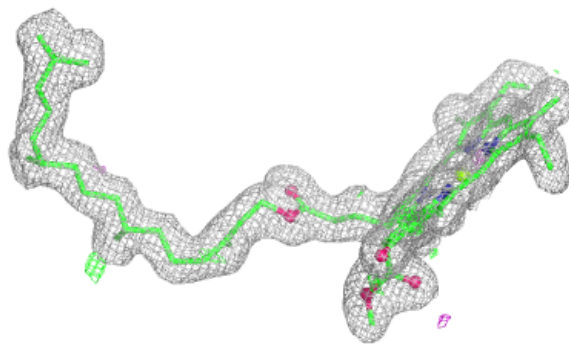
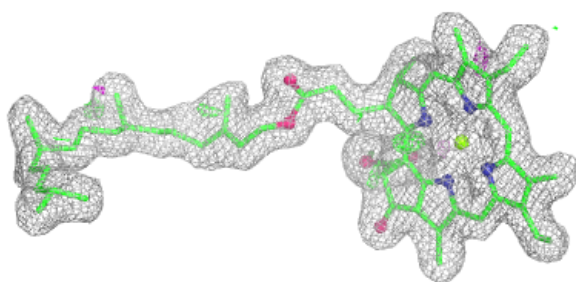
Electron density around CLA B 612:

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



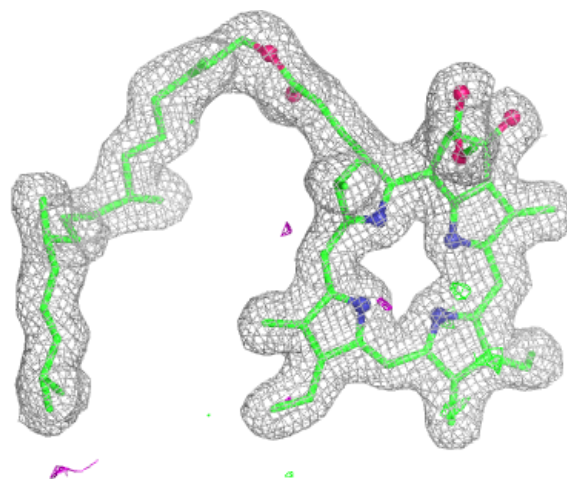
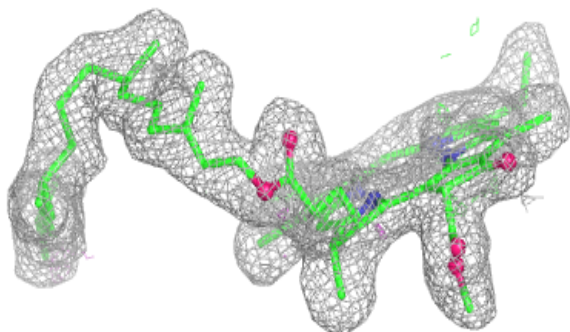
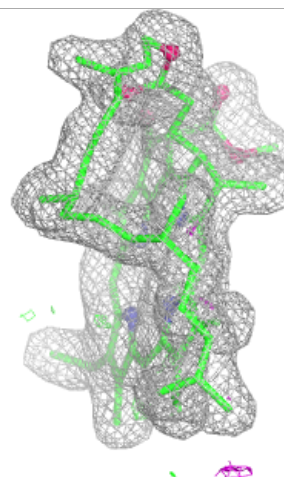
Electron density around CLA D 401:

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



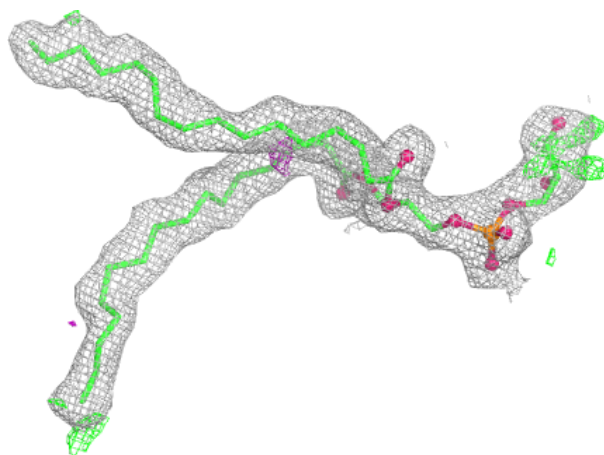
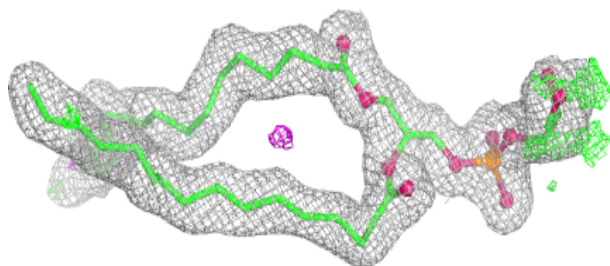
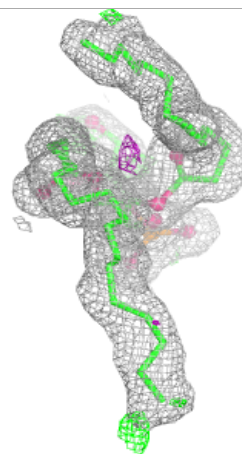
Electron density around PHO A 409:

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



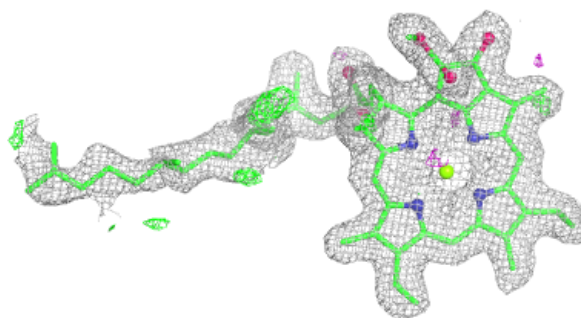
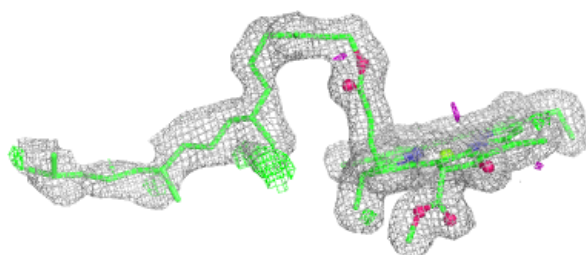
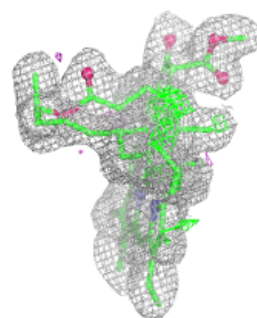
Electron density around LHG D 407:

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

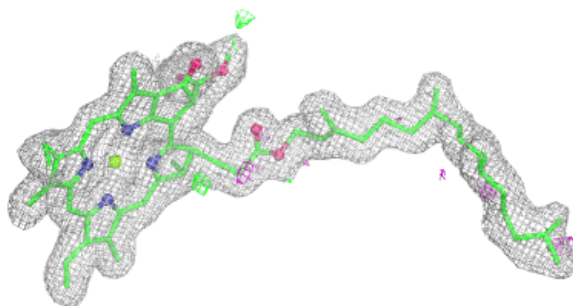
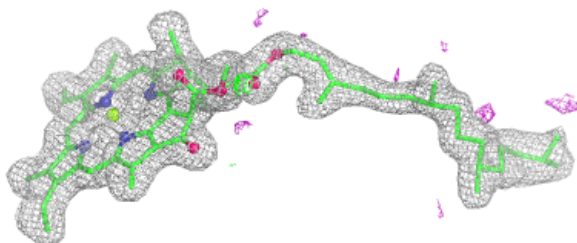
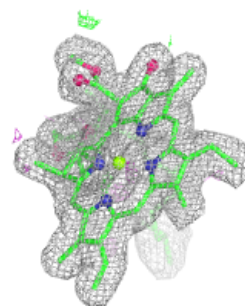


Electron density around CLA A 407:

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

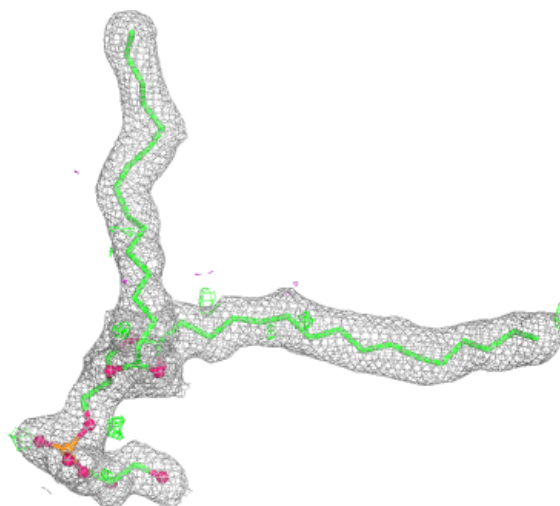
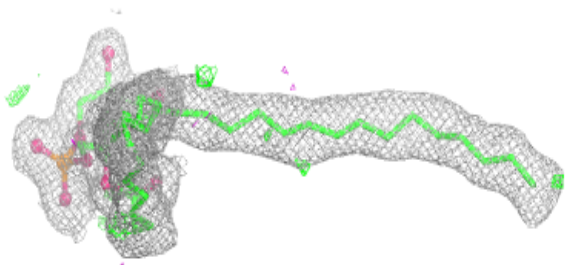
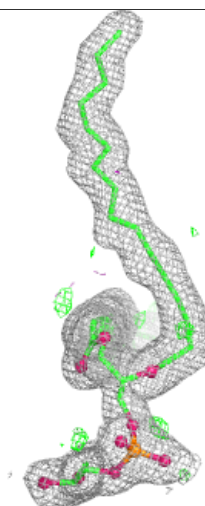
**Electron density around CLA a 406:**

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



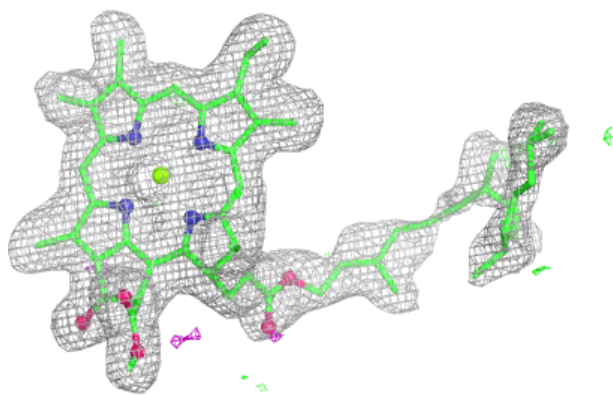
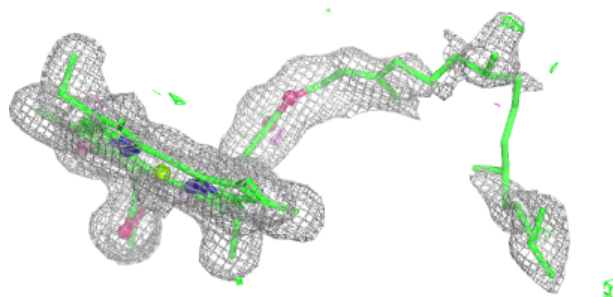
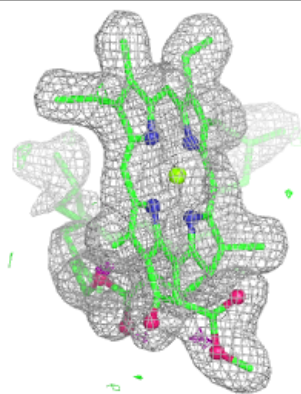
Electron density around LHG L 101:

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



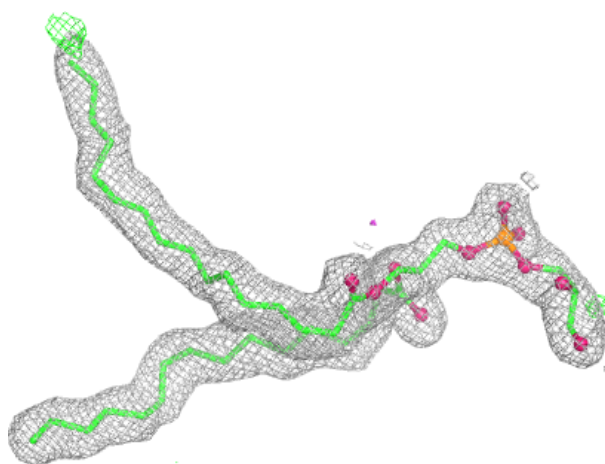
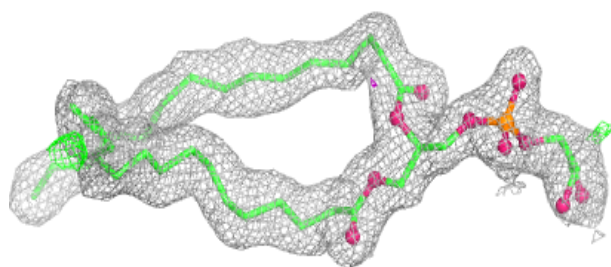
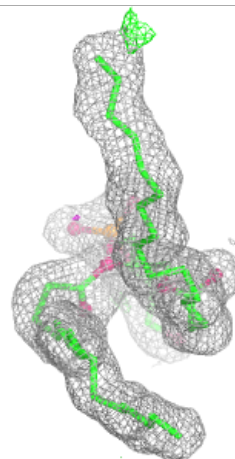
Electron density around CLA A 410:

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



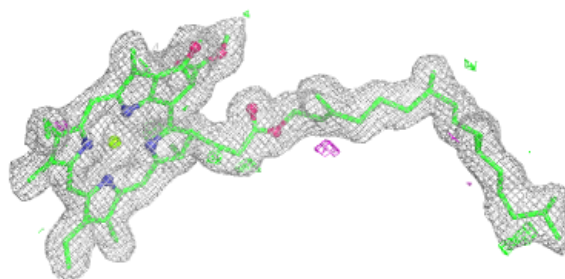
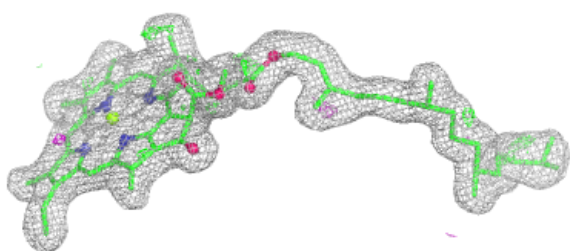
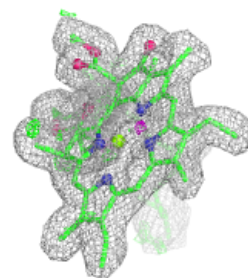
Electron density around LHG d 408:

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



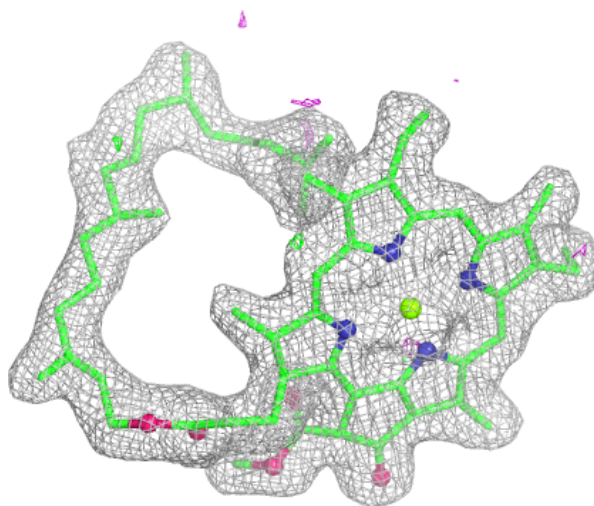
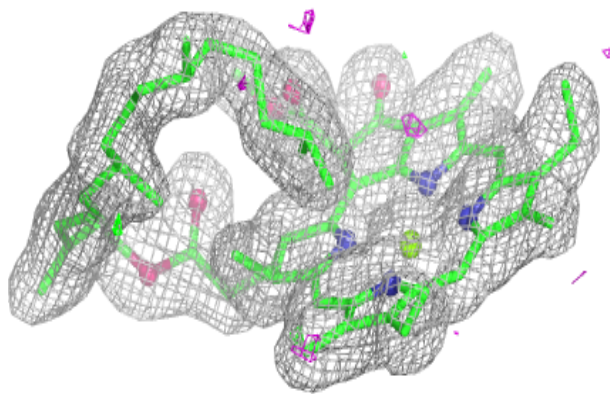
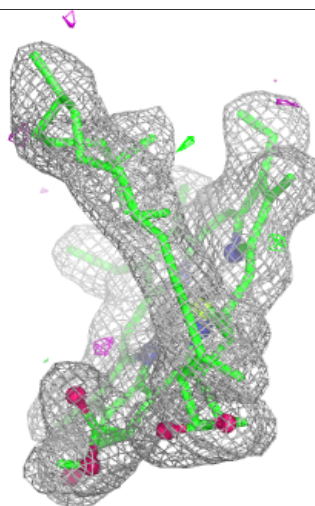
Electron density around CLA A 405:

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



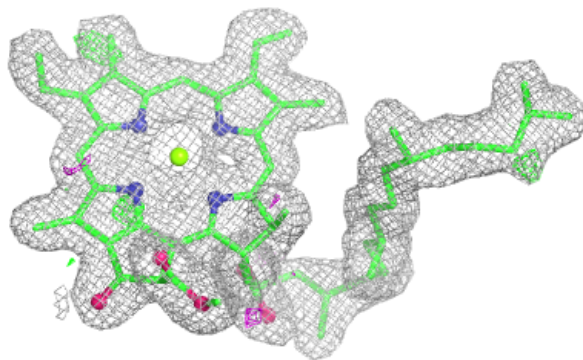
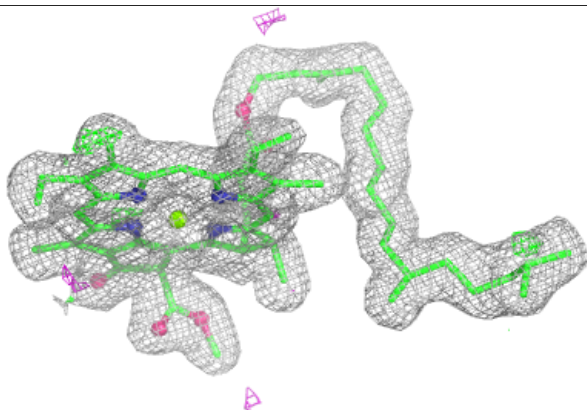
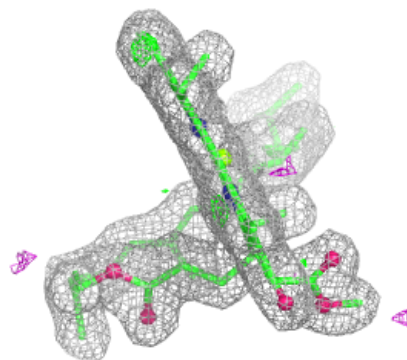
Electron density around CLA B 616:

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

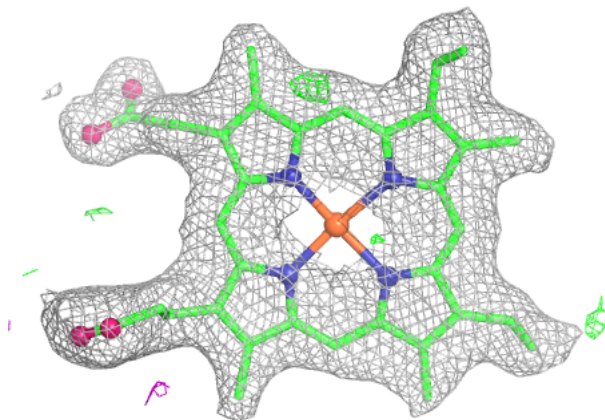
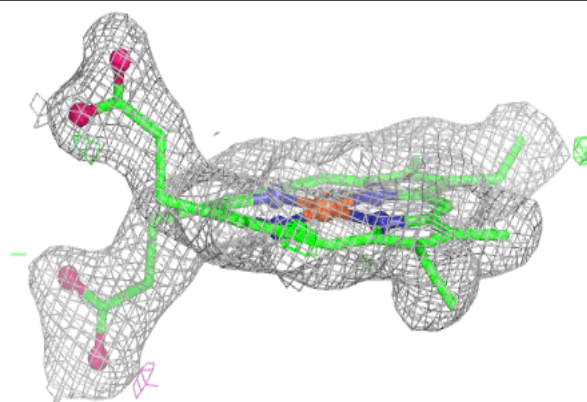


Electron density around CLA A 406:

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

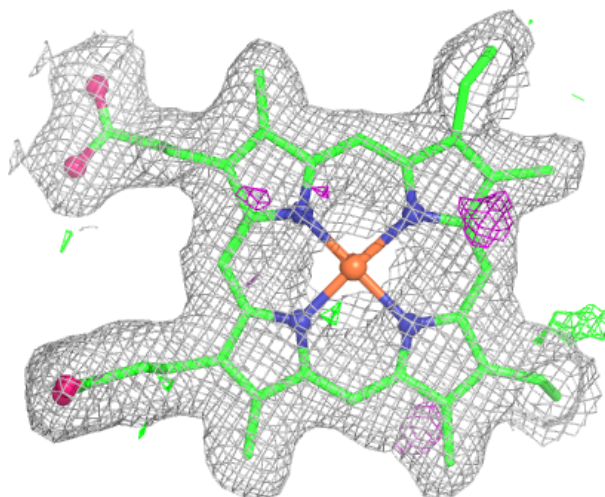
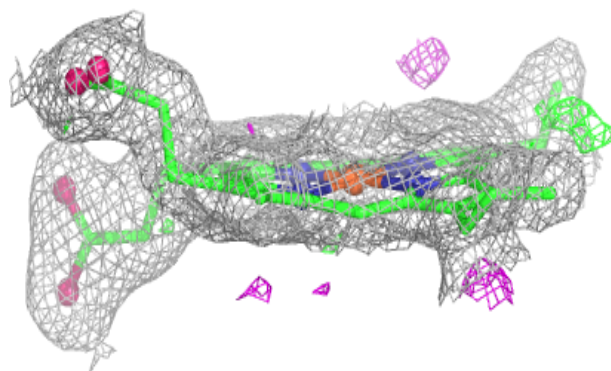
**Electron density around HEM E 103:**

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



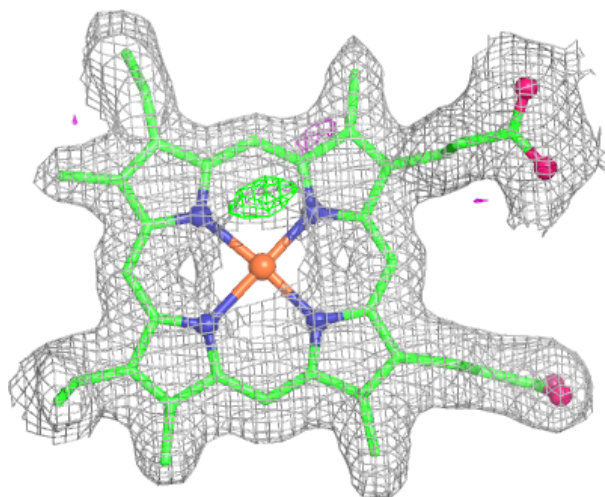
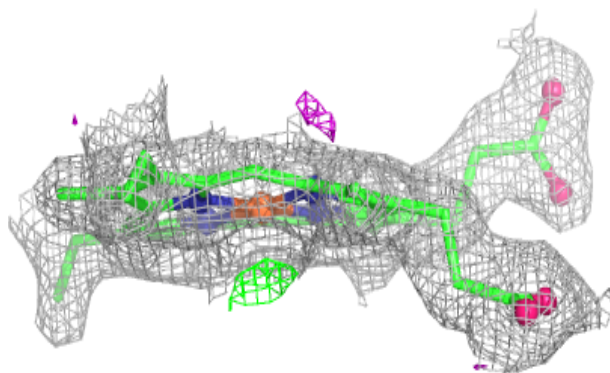
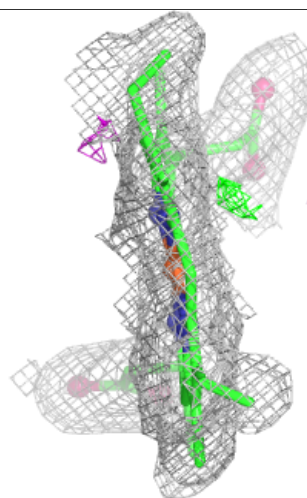
Electron density around HEC V 201:

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



Electron density around HEC v 202:

$2mF_o-DF_c$ (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.