



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 06:53 PM UTC

PDB ID : 4PJ0 / pdb_00004pj0
Title : Structure of T.elongatus Photosystem II, rows of dimers crystal packing
Authors : Hellmich, J.; Bommer, M.; Burkhardt, A.; Ibrahim, M.; Kern, J.; Meents, A.; Mueh, F.; Dobbek, H.; Zouni, A.
Deposited on : 2014-05-10
Resolution : 2.44 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

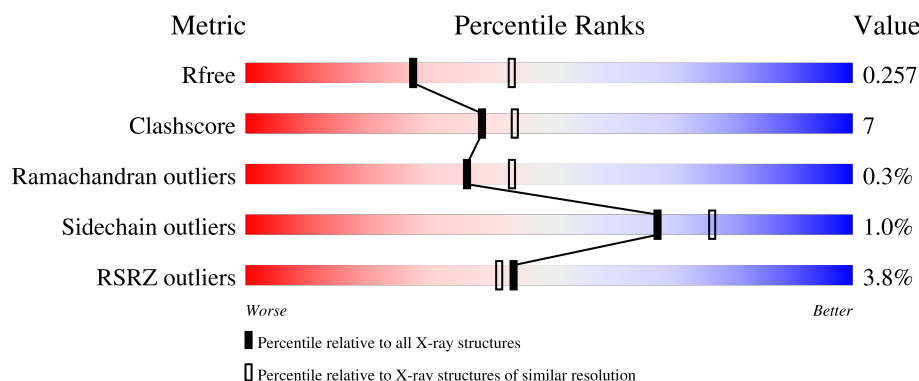
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	0% 85% 12% •
1	a	344	2% 83% 14% •
2	B	510	4% 87% 11% ••
2	b	510	3% 85% 13% ••
3	C	461	2% 82% 15% •

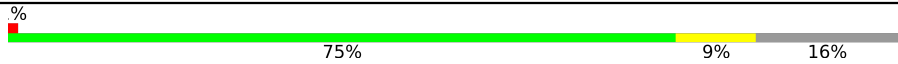
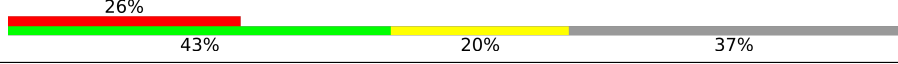
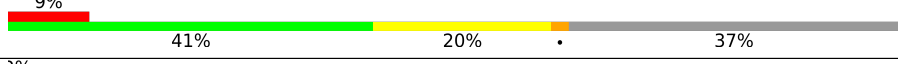
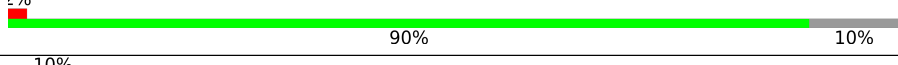
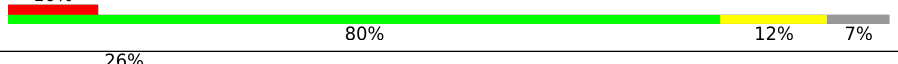
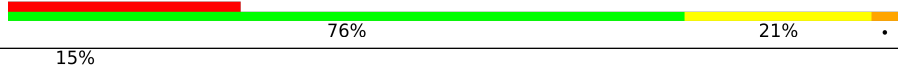
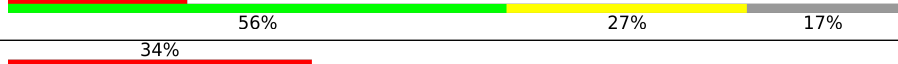
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	0	0
			3980	2611	665	691	13			
2	b	503	Total	C	N	O	S	0	0	0
			3958	2599	657	689	13			

- Molecule 3 is a protein called Photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			
3	c	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			661	431	107	123			
5	e	79	Total	C	N	O	0	0	0
			645	422	104	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	36	Total	C	N	O	0	0	0
			284	198	41	45			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			284	198	41	45			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			
12	m	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1859	1162	314	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	0	0
			249	176	35	36	2			
14	t	29	Total	C	N	O	S	0	0	0
			249	176	35	36	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	96	Total	C	N	O	0	0	0
			765	486	128	151			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	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 X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

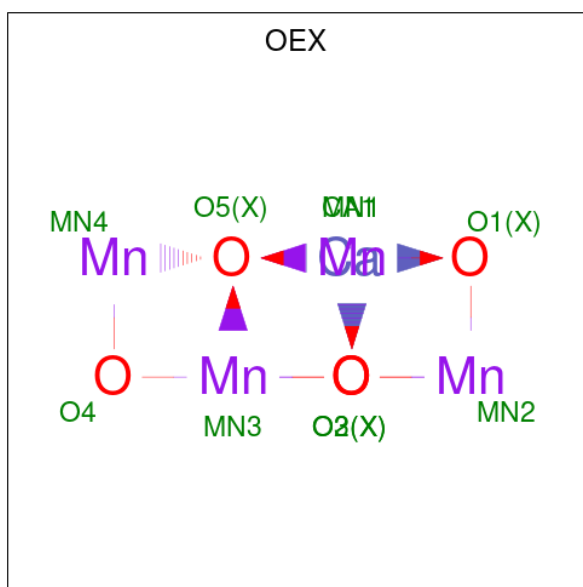
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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				
20	r	33	Total	C	N	O		0	0	0
			265	182	46	37				

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

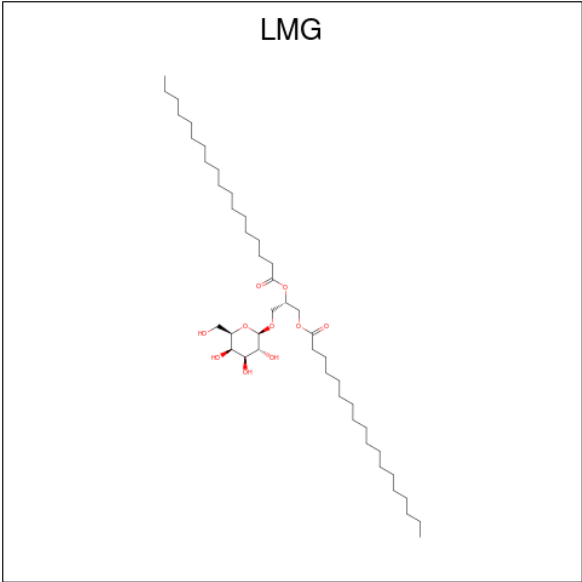


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 22 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

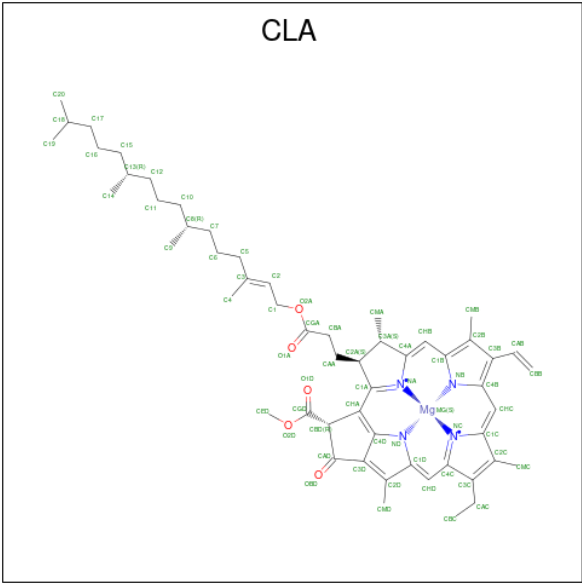


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			51	41	10		
23	A	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	D	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C	O	0	0
			51	41	10		
23	c	1	Total	C	O	0	0
			51	41	10		
23	c	1	Total	C	O	0	0
			51	41	10		
23	d	1	Total	C	O	0	0
			51	41	10		

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

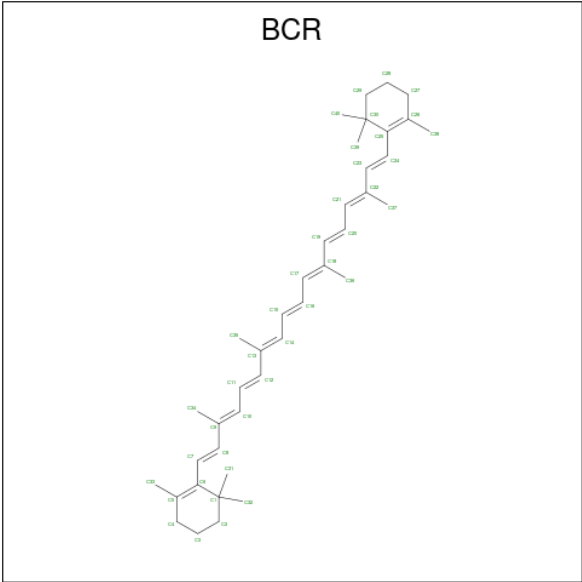
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



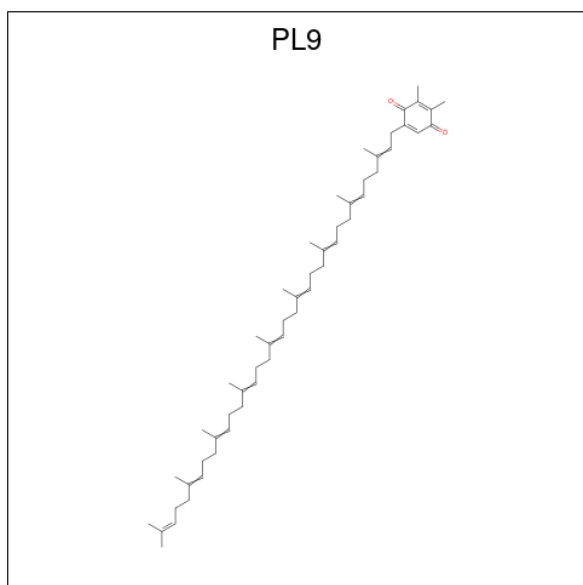
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0

- Molecule 27 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: C₅₃H₈₀O₂).



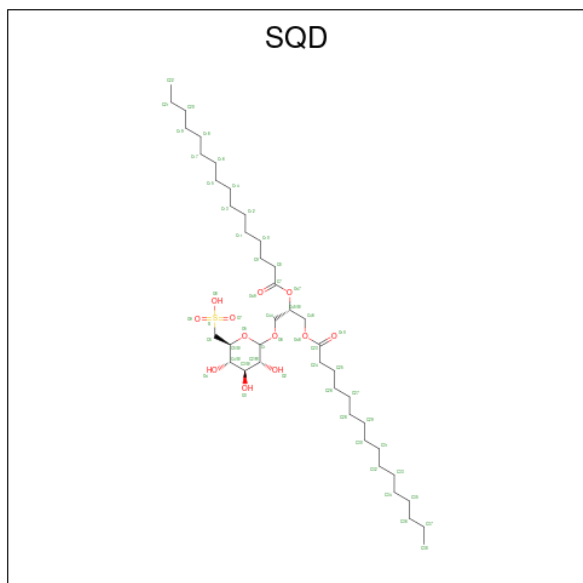
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

Continued on next page...

Continued from previous page...

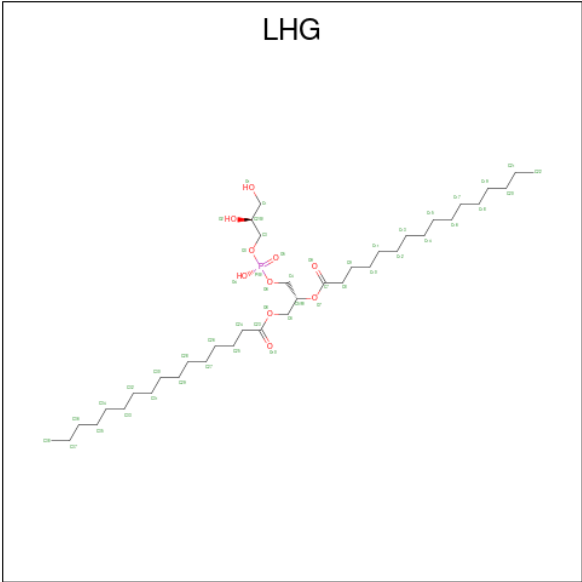
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



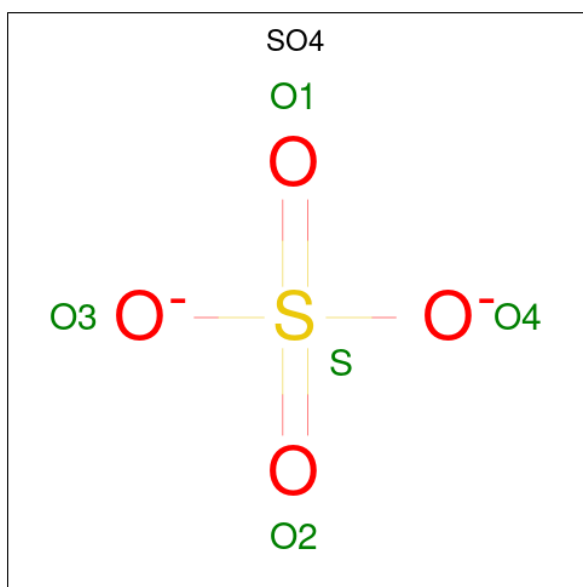
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			43	30	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



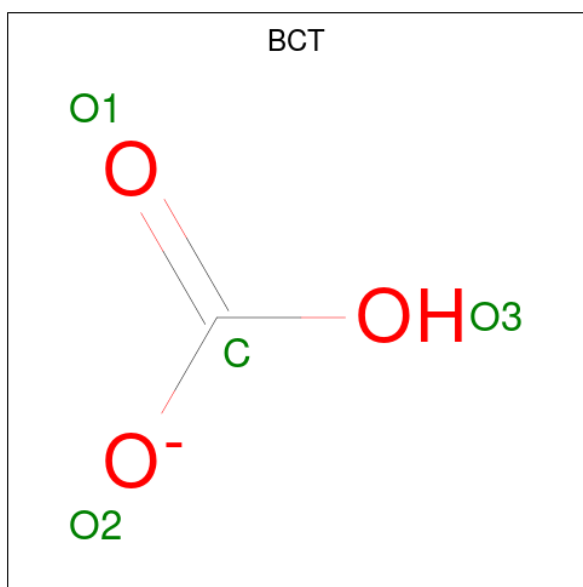
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	E	1	Total	C	O	P	0	0
			42	31	10	1		
29	L	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			42	31	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 30 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	O	S	0	0
			5	4	1		
30	O	1	Total	O	S	0	0
			5	4	1		
30	O	1	Total	O	S	0	0
			5	4	1		
30	U	1	Total	O	S	0	0
			5	4	1		
30	V	1	Total	O	S	0	0
			5	4	1		
30	a	1	Total	O	S	0	0
			5	4	1		
30	d	1	Total	O	S	0	0
			5	4	1		
30	o	1	Total	O	S	0	0
			5	4	1		
30	u	1	Total	O	S	0	0
			5	4	1		
30	u	1	Total	O	S	0	0
			5	4	1		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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

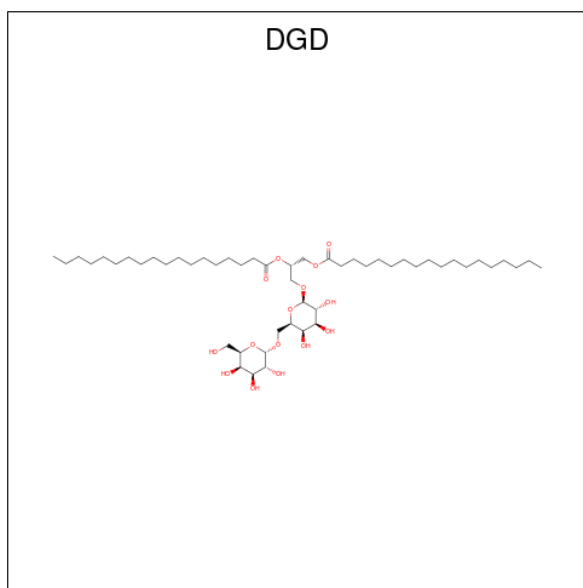
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	6	Total	C	0	0
			68	68		
32	C	1	Total	C	0	0
			15	15		
32	D	1	Total	C	0	0
			15	15		
32	I	1	Total	C	0	0
			14	14		
32	J	1	Total	C	0	0
			11	11		
32	M	2	Total	C	0	0
			26	26		
32	T	2	Total	C	0	0
			27	27		
32	X	1	Total	C	0	0
			10	10		
32	b	5	Total	C	0	0
			60	60		
32	c	1	Total	C	0	0
			15	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	d	1	Total C 15 15	0	0
32	i	1	Total C 16 16	0	0
32	j	1	Total C 15 15	0	0
32	k	1	Total C 9 9	0	0
32	m	2	Total C 25 25	0	0
32	t	1	Total C 15 15	0	0
32	x	1	Total C 16 16	0	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



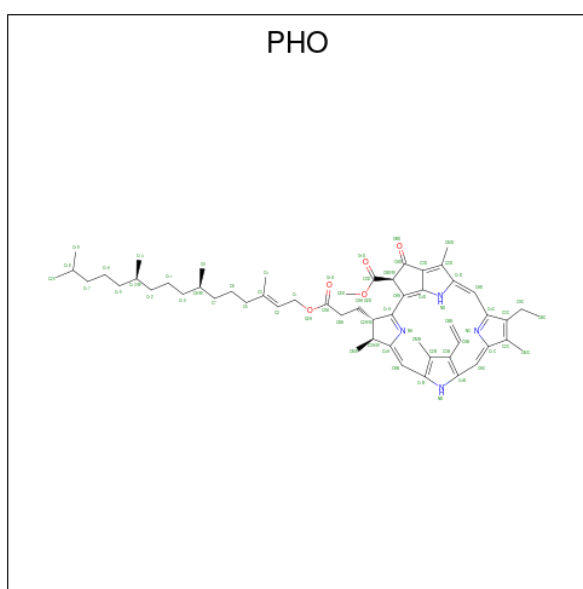
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	H	1	Total C O 62 47 15	0	0

Continued on next page...

Continued from previous page...

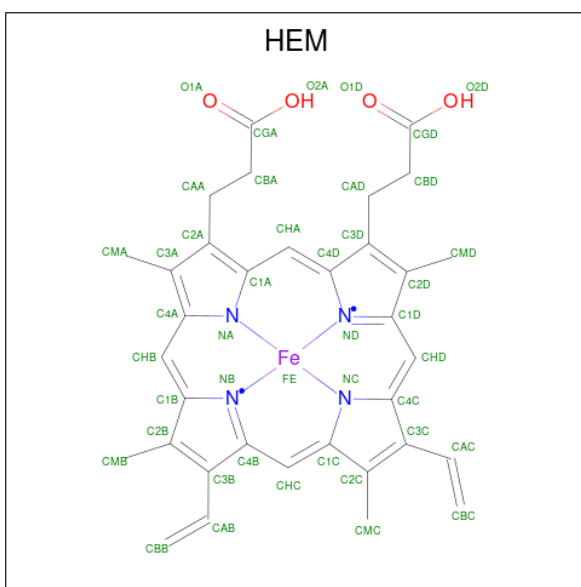
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



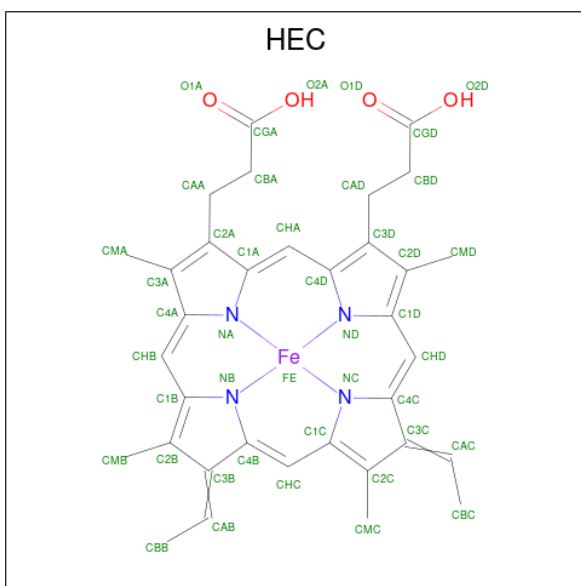
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	N	O	0	0
			64	55	4	5		
34	D	1	Total	C	N	O	0	0
			64	55	4	5		
34	a	1	Total	C	N	O	0	0
			64	55	4	5		
34	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	33	Total O 33 33	0	0
37	B	42	Total O 42 42	0	0
37	C	24	Total O 24 24	0	0
37	D	27	Total O 27 27	0	0
37	E	2	Total O 2 2	0	0
37	H	8	Total O 8 8	0	0
37	L	1	Total O 1 1	0	0
37	O	15	Total O 15 15	0	0
37	T	3	Total O 3 3	0	0
37	U	6	Total O 6 6	0	0
37	V	9	Total O 9 9	0	0
37	X	1	Total O 1 1	0	0
37	a	24	Total O 24 24	0	0
37	b	37	Total O 37 37	0	0
37	c	26	Total O 26 26	0	0
37	d	17	Total O 17 17	0	0
37	h	1	Total O 1 1	0	0
37	i	1	Total O 1 1	0	0
37	j	1	Total O 1 1	0	0
37	l	3	Total O 3 3	0	0
37	m	1	Total O 1 1	0	0

Continued on next page...

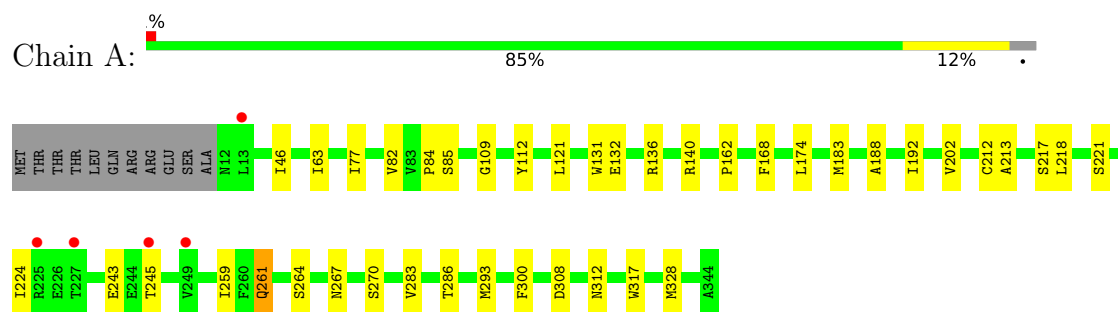
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	o	11	Total 11	O 11	0	0
37	t	1	Total 1	O 1	0	0
37	u	7	Total 7	O 7	0	0
37	v	3	Total 3	O 3	0	0

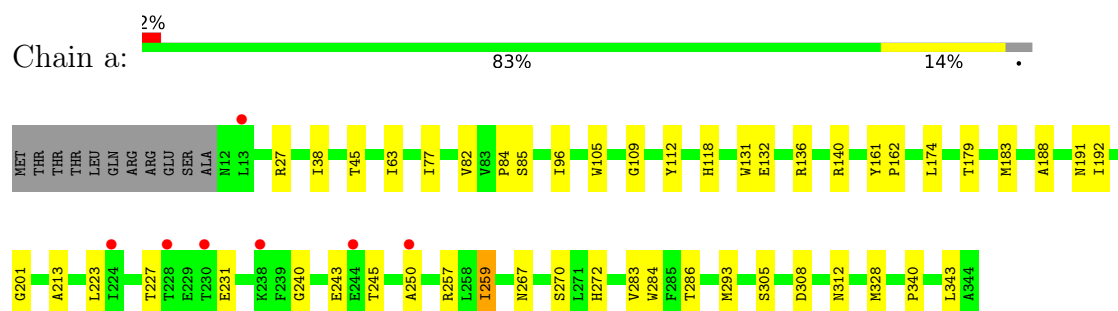
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

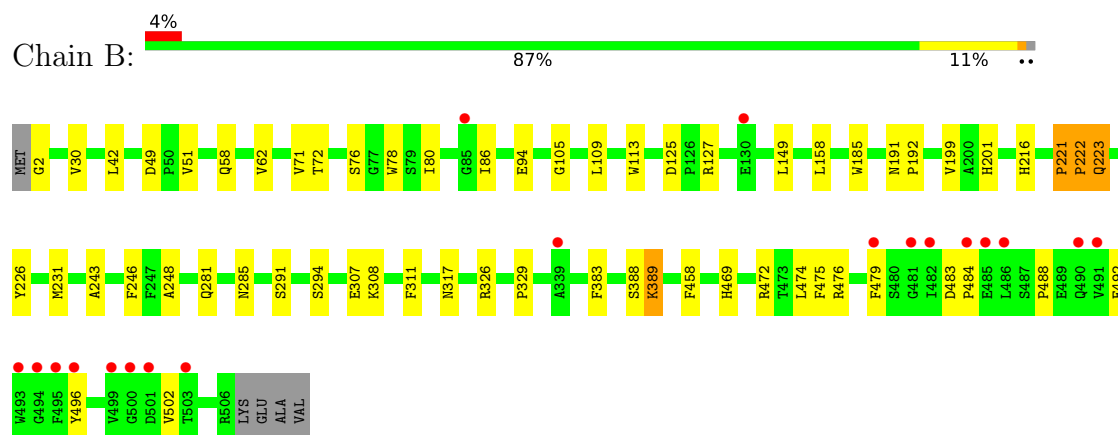
- Molecule 1: Photosystem Q(B) protein 1



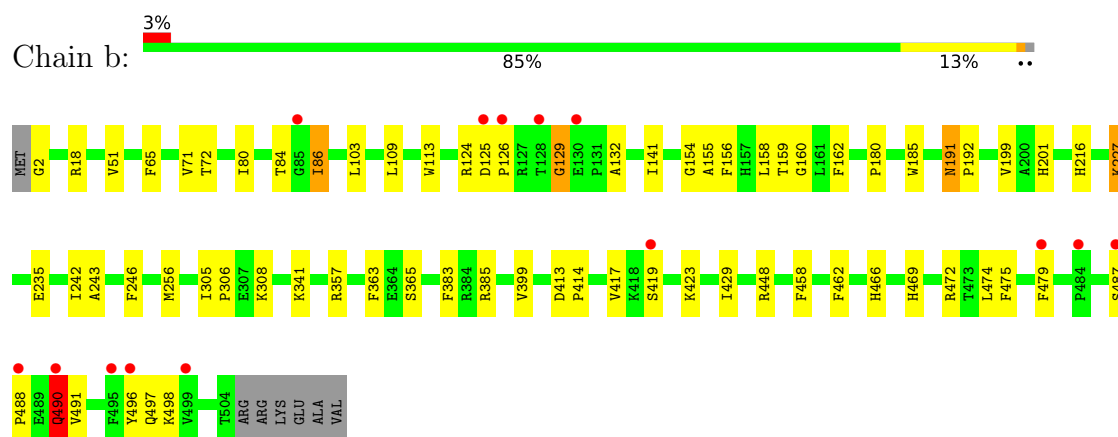
- Molecule 1: Photosystem Q(B) protein 1



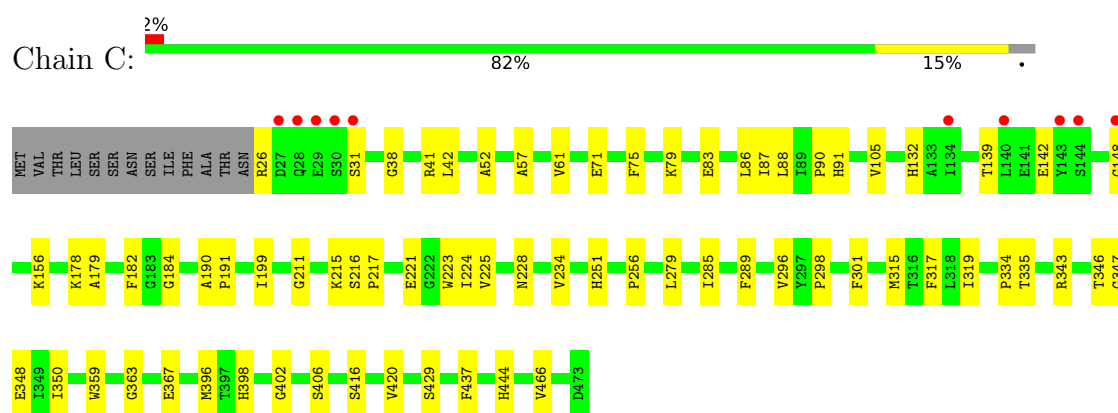
- Molecule 2: CP47 protein



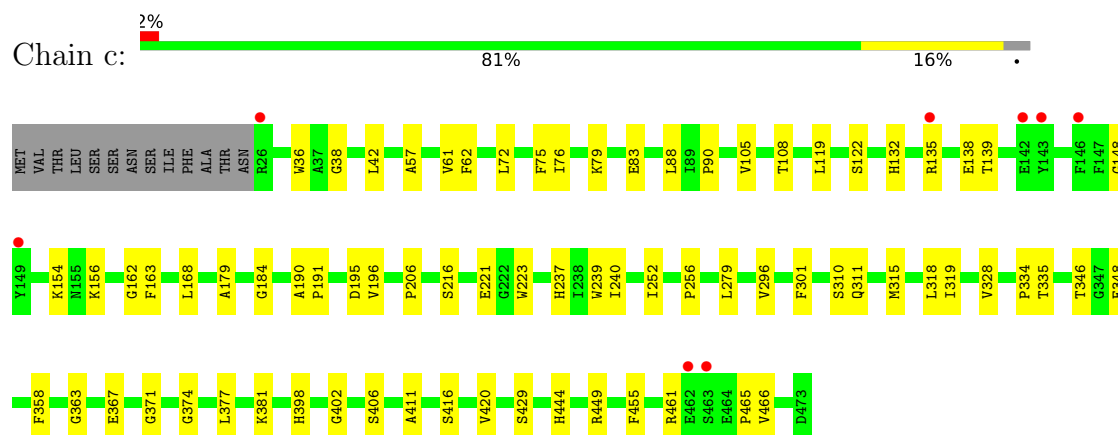
- Molecule 2: CP47 protein



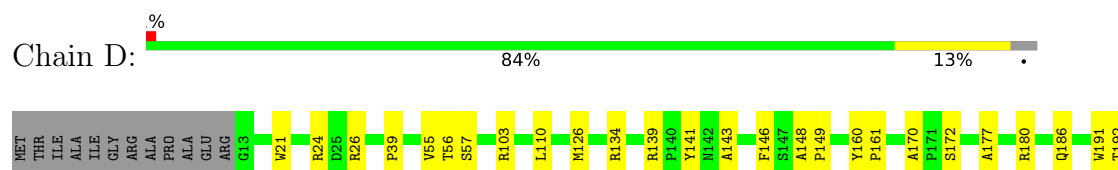
• Molecule 3: Photosystem II CP43 protein



• Molecule 3: Photosystem II CP43 protein

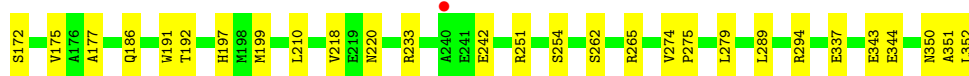
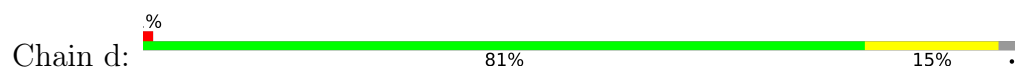


• Molecule 4: Photosystem II D2 protein

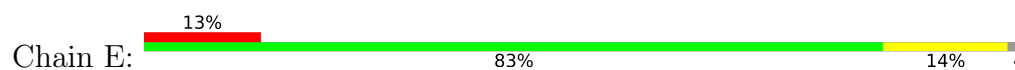




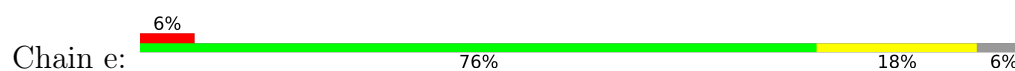
• Molecule 4: Photosystem II D2 protein



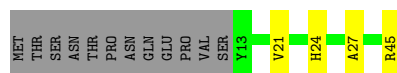
• Molecule 5: Cytochrome b559 subunit alpha



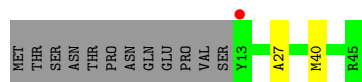
• Molecule 5: Cytochrome b559 subunit alpha



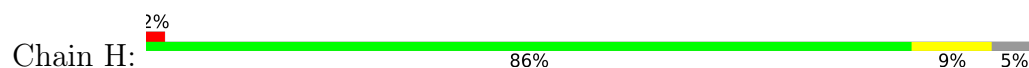
• Molecule 6: Cytochrome b559 subunit beta



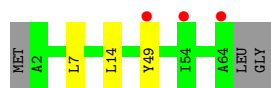
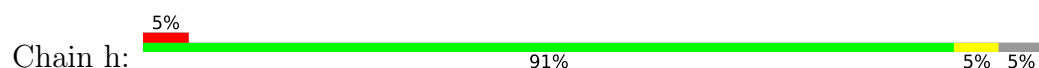
• Molecule 6: Cytochrome b559 subunit beta



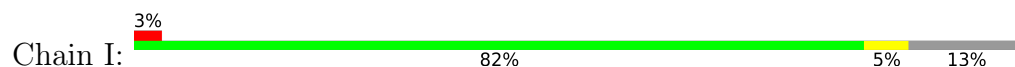
• Molecule 7: Photosystem II reaction center protein H



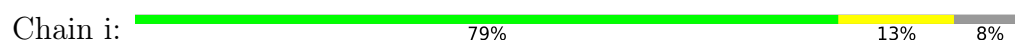
- Molecule 7: Photosystem II reaction center protein H



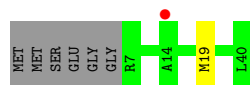
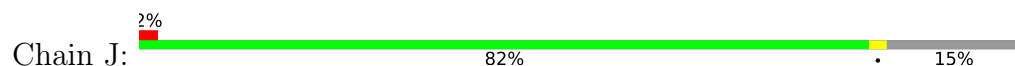
- Molecule 8: Photosystem II reaction center protein I



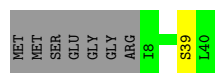
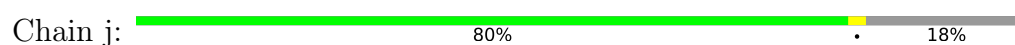
- Molecule 8: Photosystem II reaction center protein I



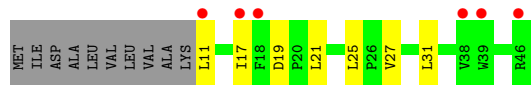
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

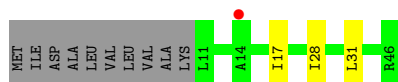


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K





- Molecule 11: Photosystem II reaction center protein L

Chain L: 86% 11% .



- Molecule 11: Photosystem II reaction center protein L

Chain L: 78% 19% .



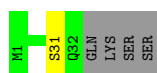
- Molecule 12: Photosystem II reaction center protein M

Chain M: 72% 17% 11%



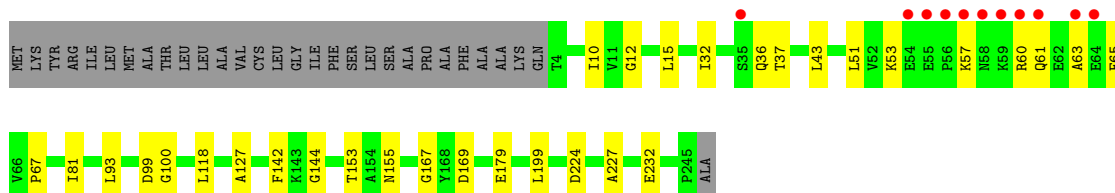
- Molecule 12: Photosystem II reaction center protein M

Chain m: 86% . 11%



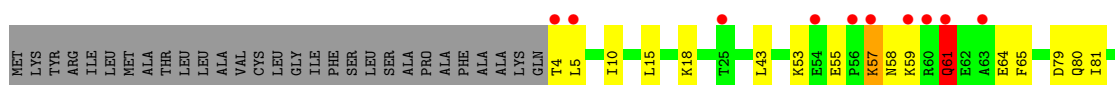
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 4% 77% 12% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 4% 75% 14% 11%

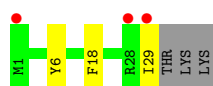
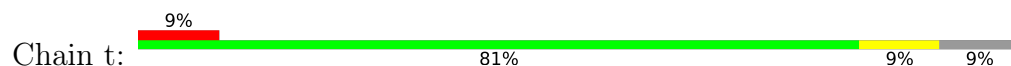




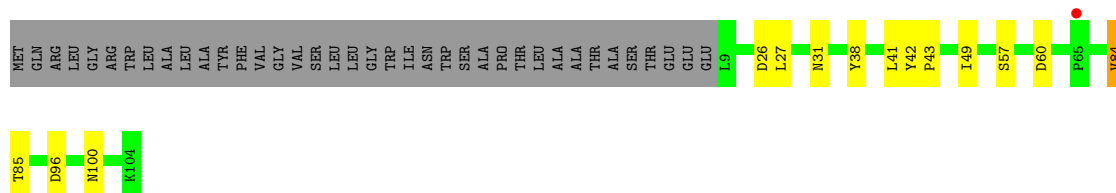
- Molecule 14: Photosystem II reaction center protein T



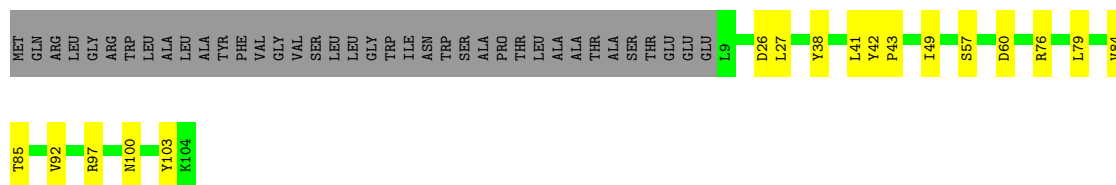
- Molecule 14: Photosystem II reaction center protein T



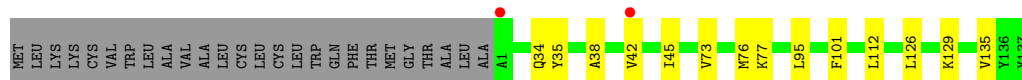
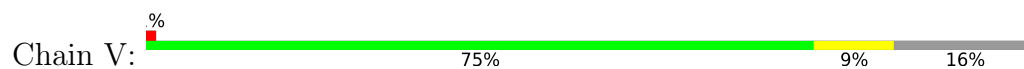
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

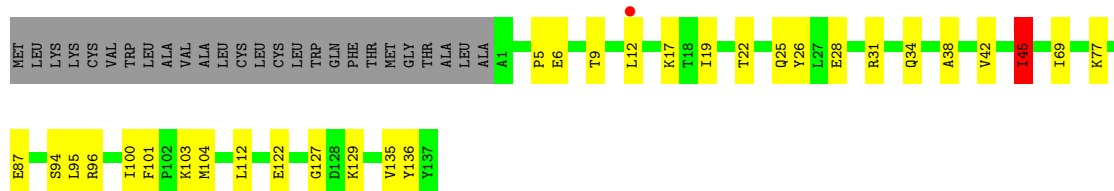


- Molecule 16: Cytochrome c-550

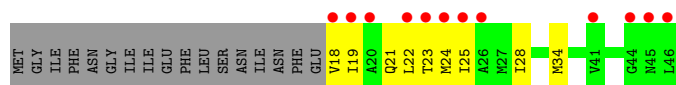
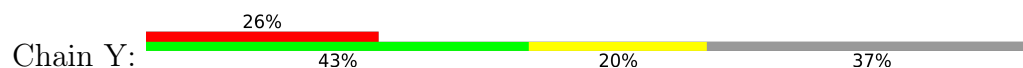


- Molecule 16: Cytochrome c-550

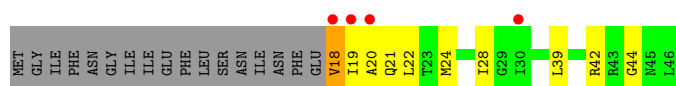
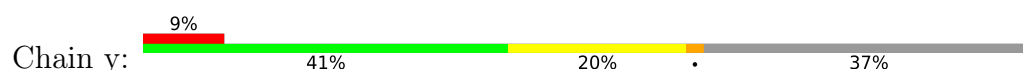




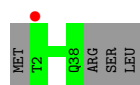
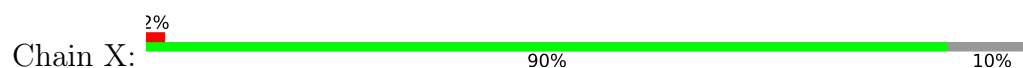
• Molecule 17: Photosystem II reaction center protein Ycf12



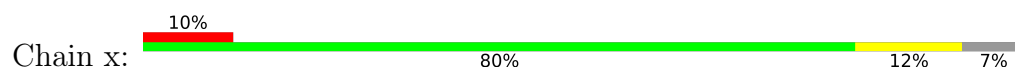
• Molecule 17: Photosystem II reaction center protein Ycf12



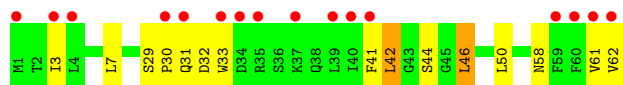
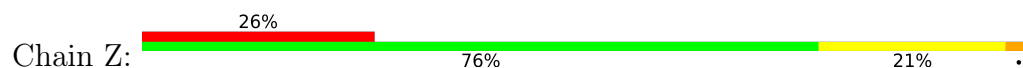
• Molecule 18: Photosystem II reaction center X protein



• Molecule 18: Photosystem II reaction center X protein

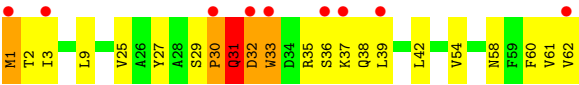


• Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z

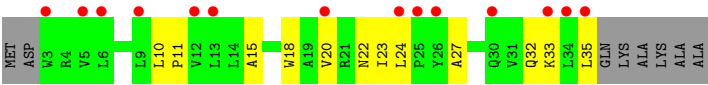




● Molecule 20: Photosystem II protein Y



● 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	116.45Å 218.89Å 302.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.44 49.12 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.12-2.44) 98.3 (49.12-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.216 , 0.256 0.218 , 0.257	Depositor DCC
R_{free} test set	14111 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	50236	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: FE, UNL, HEM, CL, CLA, SQD, LMG, BCT, PL9, HEC, OEX, DGD, PHO, SO4, LHG, BCR

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	0.29	0/2702	0.74	1/3685 (0.0%)
1	a	0.28	0/2702	0.71	0/3685
2	B	0.29	0/4120	0.74	7/5614 (0.1%)
2	b	0.28	0/4098	0.73	4/5586 (0.1%)
3	C	0.27	0/3579	0.71	0/4872
3	c	0.28	0/3579	0.73	3/4872 (0.1%)
4	D	0.27	0/2801	0.69	0/3818
4	d	0.28	0/2801	0.70	0/3818
5	E	0.28	0/680	0.76	0/929
5	e	0.29	0/664	0.72	0/907
6	F	0.33	0/278	0.77	0/379
6	f	0.32	0/278	0.77	0/379
7	H	0.28	0/511	0.69	0/697
7	h	0.27	0/511	0.69	0/697
8	I	0.29	0/273	0.71	0/370
8	i	0.33	0/293	0.81	0/395
9	J	0.27	0/255	0.73	0/346
9	j	0.26	0/244	0.73	0/332
10	K	0.43	0/294	0.97	2/405 (0.5%)
10	k	0.40	0/294	0.81	0/405
11	L	0.27	0/303	0.65	0/412
11	l	0.27	0/303	0.64	0/412
12	M	0.31	0/252	0.80	0/344
12	m	0.32	0/252	0.78	0/344
13	O	0.26	0/1890	0.67	0/2564
13	o	0.27	0/1896	0.72	2/2571 (0.1%)
14	T	0.26	0/258	0.69	0/349
14	t	0.27	0/258	0.68	0/349
15	U	0.26	0/776	0.65	0/1052
15	u	0.25	0/776	0.64	0/1052
16	V	0.29	0/1085	0.73	2/1473 (0.1%)
16	v	0.28	0/1085	0.73	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.29	0/216	0.73	0/289
17	y	0.33	0/216	0.87	0/289
18	X	0.27	0/273	0.71	0/370
18	x	0.27	0/284	0.70	0/384
19	Z	0.32	0/490	0.78	0/669
19	z	0.50	0/490	1.00	2/669 (0.3%)
20	R	0.32	0/279	0.74	0/383
20	r	0.35	0/271	0.86	1/372 (0.3%)
All	All	0.28	0/42610	0.73	24/58011 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
19	z	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	223	GLN	N-CA-C	-12.26	96.61	111.69
2	b	490	GLN	N-CA-C	-8.50	102.91	113.28
2	b	129	GLY	N-CA-C	-7.30	104.65	114.95
19	z	32	ASP	N-CA-C	7.05	120.89	111.30
10	K	19	ASP	CA-C-N	-6.65	111.52	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	PRO	Peptide
19	z	31	GLN	Peptide

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	2617	0	2514	33	0
1	a	2617	0	2514	38	0
2	B	3980	0	3841	49	0
2	b	3958	0	3815	58	0
3	C	3466	0	3389	49	0
3	c	3466	0	3389	49	0
4	D	2706	0	2608	38	0
4	d	2706	0	2608	46	0
5	E	661	0	643	9	0
5	e	645	0	628	13	0
6	F	269	0	277	5	0
6	f	269	0	277	2	0
7	H	498	0	518	5	0
7	h	498	0	518	4	0
8	I	266	0	282	2	0
8	i	286	0	308	4	0
9	J	249	0	262	0	0
9	j	238	0	249	1	0
10	K	284	0	292	4	0
10	k	284	0	292	2	0
11	L	296	0	304	3	0
11	l	296	0	304	9	0
12	M	249	0	268	6	0
12	m	249	0	268	2	0
13	O	1859	0	1833	18	0
13	o	1865	0	1838	23	0
14	T	249	0	255	8	0
14	t	249	0	255	4	0
15	U	765	0	767	8	0
15	u	765	0	767	10	0
16	V	1064	0	1073	9	0
16	v	1064	0	1073	19	0
17	Y	215	0	246	5	0
17	y	215	0	246	7	0
18	X	270	0	299	0	0
18	x	281	0	312	5	0
19	Z	479	0	516	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	479	0	516	20	0
20	R	273	0	305	7	0
20	r	265	0	301	6	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	102	0	144	1	0
23	B	102	0	144	3	0
23	C	102	0	144	4	0
23	D	51	0	72	0	0
23	a	102	0	144	2	0
23	b	102	0	144	1	0
23	c	102	0	144	5	0
23	d	51	0	72	2	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	195	0	216	7	0
25	B	1040	0	1152	34	0
25	C	845	0	936	36	0
25	D	195	0	216	10	0
25	a	260	0	288	11	0
25	b	1040	0	1152	32	0
25	c	845	0	936	41	0
25	d	130	0	144	4	0
26	A	40	0	56	3	0
26	B	120	0	168	14	0
26	C	120	0	168	8	0
26	D	40	0	56	2	0
26	H	40	0	56	2	0
26	K	40	0	56	4	0
26	T	40	0	56	6	0
26	a	40	0	56	3	0
26	b	120	0	168	6	0
26	c	80	0	112	5	0
26	d	40	0	56	4	0
26	h	40	0	56	4	0
26	k	40	0	56	3	0
26	t	40	0	56	5	0
26	z	40	0	56	10	0
27	A	55	0	80	6	0
27	D	55	0	80	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	a	55	0	80	6	0
27	d	55	0	80	4	0
28	A	54	0	78	2	0
28	F	43	0	53	2	0
28	L	108	0	156	10	0
28	a	54	0	78	5	0
28	f	43	0	53	0	0
29	A	98	0	148	13	0
29	D	49	0	74	5	0
29	E	42	0	57	0	0
29	L	49	0	74	4	0
29	a	91	0	131	6	0
29	d	98	0	148	11	0
29	l	49	0	74	3	0
30	A	5	0	0	0	0
30	O	10	0	0	0	0
30	U	5	0	0	0	0
30	V	5	0	0	0	0
30	a	5	0	0	0	0
30	d	5	0	0	0	0
30	o	5	0	0	0	0
30	u	10	0	0	0	0
31	A	4	0	0	0	0
31	a	4	0	0	0	0
32	B	68	0	0	0	0
32	C	15	0	0	0	0
32	D	15	0	0	0	0
32	I	14	0	0	0	0
32	J	11	0	0	0	0
32	M	26	0	0	0	0
32	T	27	0	0	0	0
32	X	10	0	0	0	0
32	b	60	0	0	0	0
32	c	15	0	0	0	0
32	d	15	0	0	0	0
32	i	16	0	0	0	0
32	j	15	0	0	0	0
32	k	9	0	0	0	0
32	m	25	0	0	0	0
32	t	15	0	0	0	0
32	x	16	0	0	0	0
33	C	186	0	246	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	H	62	0	82	0	0
33	c	186	0	246	3	0
33	h	62	0	82	2	0
34	D	128	0	148	6	0
34	a	64	0	74	2	0
34	d	64	0	74	1	0
35	E	43	0	30	3	0
35	e	43	0	30	5	0
36	V	43	0	30	0	0
36	v	43	0	30	0	0
37	A	33	0	0	0	0
37	B	42	0	0	1	0
37	C	24	0	0	0	0
37	D	27	0	0	0	0
37	E	2	0	0	0	0
37	H	8	0	0	0	0
37	L	1	0	0	0	0
37	O	15	0	0	0	0
37	T	3	0	0	1	0
37	U	6	0	0	0	0
37	V	9	0	0	0	0
37	X	1	0	0	0	0
37	a	24	0	0	0	0
37	b	37	0	0	1	0
37	c	26	0	0	0	0
37	d	17	0	0	0	0
37	h	1	0	0	0	0
37	i	1	0	0	0	0
37	j	1	0	0	0	0
37	l	3	0	0	0	0
37	m	1	0	0	0	0
37	o	11	0	0	0	0
37	t	1	0	0	0	0
37	u	7	0	0	0	0
37	v	3	0	0	0	0
All	All	50236	0	50766	684	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 7.

The worst 5 of 684 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)
17:y:18:VAL:HG23	17:y:19:ILE:HD12	1.61	0.83
25:B:604:CLA:H93	25:B:605:CLA:HAB	1.66	0.77
3:c:79:LYS:HG3	16:v:103:LYS:HD3	1.68	0.75
25:C:503:CLA:H172	25:C:510:CLA:HBB2	1.68	0.74
25:A:607:CLA:HAB	25:D:404:CLA:H72	1.69	0.73

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	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	36	44
1	a	331/344 (96%)	324 (98%)	6 (2%)	1 (0%)	36	44
2	B	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
2	b	501/510 (98%)	482 (96%)	18 (4%)	1 (0%)	43	53
3	C	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	43	53
3	c	446/461 (97%)	435 (98%)	9 (2%)	2 (0%)	30	36
4	D	338/352 (96%)	326 (96%)	12 (4%)	0	100	100
4	d	338/352 (96%)	323 (96%)	14 (4%)	1 (0%)	36	44
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	31/38 (82%)	31 (100%)	0	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	32/40 (80%)	32 (100%)	0	0	100	100
9	j	31/40 (78%)	31 (100%)	0	0	100	100
10	K	34/46 (74%)	31 (91%)	3 (9%)	0	100	100
10	k	34/46 (74%)	34 (100%)	0	0	100	100
11	L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	228 (95%)	11 (5%)	1 (0%)	30	36
13	o	241/272 (89%)	225 (93%)	13 (5%)	3 (1%)	10	10
14	T	27/32 (84%)	27 (100%)	0	0	100	100
14	t	27/32 (84%)	26 (96%)	1 (4%)	0	100	100
15	U	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
15	u	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
16	v	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	21
17	Y	27/46 (59%)	26 (96%)	1 (4%)	0	100	100
17	y	27/46 (59%)	24 (89%)	2 (7%)	1 (4%)	2	1
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	6
19	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	3	1
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	31/41 (76%)	29 (94%)	2 (6%)	0	100	100
All	All	5199/5700 (91%)	5010 (96%)	173 (3%)	16 (0%)	36	44

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	30	PRO
13	o	57	LYS
3	c	416	SER
13	o	58	ASN

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	270/280 (96%)	268 (99%)	2 (1%)	76	83
1	a	270/280 (96%)	269 (100%)	1 (0%)	84	89
2	B	403/407 (99%)	399 (99%)	4 (1%)	68	77
2	b	401/407 (98%)	398 (99%)	3 (1%)	76	83
3	C	350/362 (97%)	350 (100%)	0	100	100
3	c	350/362 (97%)	350 (100%)	0	100	100
4	D	275/283 (97%)	275 (100%)	0	100	100
4	d	275/283 (97%)	274 (100%)	1 (0%)	84	89
5	E	71/73 (97%)	70 (99%)	1 (1%)	59	70
5	e	70/73 (96%)	69 (99%)	1 (1%)	59	70
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	53 (100%)	0	100	100
7	h	53/55 (96%)	53 (100%)	0	100	100
8	I	30/35 (86%)	30 (100%)	0	100	100
8	i	32/35 (91%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	37
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	29/37 (78%)	27 (93%)	2 (7%)	14	18
10	k	29/37 (78%)	28 (97%)	1 (3%)	32	45
11	L	34/35 (97%)	33 (97%)	1 (3%)	37	49
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	29 (100%)	0	100	100
13	O	206/228 (90%)	203 (98%)	3 (2%)	57	69
13	o	206/228 (90%)	204 (99%)	2 (1%)	68	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	26/29 (90%)	26 (100%)	0	100	100
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	82 (99%)	1 (1%)	63	74
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	45
17	Y	22/37 (60%)	19 (86%)	3 (14%)	3	3
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	10
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	48 (92%)	4 (8%)	12	14
19	z	52/52 (100%)	47 (90%)	5 (10%)	8	8
20	R	29/33 (88%)	28 (97%)	1 (3%)	32	45
20	r	28/33 (85%)	28 (100%)	0	100	100
All	All	4318/4660 (93%)	4275 (99%)	43 (1%)	68	77

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	k	17	ILE
20	R	31	VAL
13	o	61	GLN
16	v	17	LYS
17	y	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	332	GLN
4	d	255	GLN
16	v	25	GLN
4	d	250	ASN
4	d	336	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 191 ligands modelled in this entry, 6 are monoatomic and 29 are unknown - leaving 156 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
23	LMG	A	612	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	3 (5%)
26	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.83	12 (21%)
25	CLA	b	613	-	69,73,73	1.58	7 (10%)	82,113,113	1.16	9 (10%)
30	SO4	O	301	-	4,4,4	0.23	0	6,6,6	0.08	0
23	LMG	C	519	-	51,51,55	0.95	2 (3%)	59,59,63	0.99	3 (5%)
27	PL9	D	407	-	55,55,55	0.63	2 (3%)	68,69,69	1.69	17 (25%)
30	SO4	o	301	-	4,4,4	0.23	0	6,6,6	0.09	0
30	SO4	V	202	-	4,4,4	0.23	0	6,6,6	0.14	0
26	BCR	T	101	-	41,41,41	0.69	0	56,56,56	2.06	12 (21%)
21	OEX	A	601	1,37,3	0,15,15	-	-	-	-	-
25	CLA	C	504	-	69,73,73	1.61	7 (10%)	82,113,113	1.15	8 (9%)
25	CLA	C	507	-	69,73,73	1.58	7 (10%)	82,113,113	1.16	8 (9%)
33	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	0.95	3 (3%)
25	CLA	b	601	-	69,73,73	1.60	9 (13%)	82,113,113	1.16	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	d	403	-	69,73,73	1.59	9 (13%)	82,113,113	1.13	8 (9%)
26	BCR	k	102	-	41,41,41	0.70	0	56,56,56	1.86	17 (30%)
23	LMG	B	620	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)
23	LMG	a	603	-	51,51,55	0.94	2 (3%)	59,59,63	1.09	6 (10%)
25	CLA	c	513	-	69,73,73	1.60	8 (11%)	82,113,113	1.19	9 (10%)
30	SO4	u	202	-	4,4,4	0.24	0	6,6,6	0.08	0
26	BCR	h	101	-	41,41,41	0.68	0	56,56,56	1.98	13 (23%)
23	LMG	A	603	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	3 (5%)
21	OEX	a	601	1,37,3	0,15,15	-	-	-	-	-
30	SO4	a	617	-	4,4,4	0.24	0	6,6,6	0.07	0
23	LMG	C	521	-	51,51,55	0.97	3 (5%)	59,59,63	1.11	4 (6%)
28	SQD	L	103	-	52,54,54	1.12	3 (5%)	62,65,65	1.12	4 (6%)
25	CLA	c	503	-	69,73,73	1.57	8 (11%)	82,113,113	1.20	8 (9%)
33	DGD	C	516	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	4 (5%)
34	PHO	D	401	-	58,69,69	1.36	6 (10%)	55,99,99	1.65	4 (7%)
26	BCR	B	618	-	41,41,41	0.67	0	56,56,56	1.87	11 (19%)
26	BCR	K	101	-	41,41,41	0.71	0	56,56,56	1.80	14 (25%)
29	LHG	d	407	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	2 (3%)
25	CLA	b	615	-	69,73,73	1.57	7 (10%)	82,113,113	1.20	8 (9%)
35	HEM	e	101	5,6	50,50,50	1.38	6 (12%)	67,82,82	1.02	3 (4%)
25	CLA	B	609	-	69,73,73	1.60	9 (13%)	82,113,113	1.18	10 (12%)
26	BCR	B	617	-	41,41,41	0.68	0	56,56,56	1.97	17 (30%)
25	CLA	C	505	-	69,73,73	1.59	8 (11%)	82,113,113	1.17	8 (9%)
25	CLA	b	608	-	69,73,73	1.61	8 (11%)	82,113,113	1.17	9 (10%)
23	LMG	b	620	-	51,51,55	0.94	2 (3%)	59,59,63	1.04	5 (8%)
25	CLA	C	501	-	69,73,73	1.59	8 (11%)	82,113,113	1.16	9 (10%)
25	CLA	b	616	-	69,73,73	1.59	9 (13%)	82,113,113	1.21	9 (10%)
29	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
25	CLA	b	607	37	69,73,73	1.58	8 (11%)	82,113,113	1.19	9 (10%)
23	LMG	c	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.05	4 (6%)
25	CLA	b	610	37	69,73,73	1.61	8 (11%)	82,113,113	1.20	9 (10%)
25	CLA	C	508	-	69,73,73	1.59	8 (11%)	82,113,113	1.19	8 (9%)
23	LMG	B	624	-	51,51,55	0.94	2 (3%)	59,59,63	0.98	3 (5%)
25	CLA	a	606	-	69,73,73	1.57	8 (11%)	82,113,113	1.22	9 (10%)
25	CLA	c	501	-	69,73,73	1.58	8 (11%)	82,113,113	1.18	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	F	101	-	41,43,54	1.23	3 (7%)	51,54,65	1.25	7 (13%)
27	PL9	A	610	-	55,55,55	0.64	2 (3%)	68,69,69	1.77	20 (29%)
26	BCR	b	618	-	41,41,41	0.63	0	56,56,56	1.97	17 (30%)
25	CLA	c	507	-	69,73,73	1.58	7 (10%)	82,113,113	1.16	8 (9%)
25	CLA	A	606	-	69,73,73	1.59	8 (11%)	82,113,113	1.23	8 (9%)
26	BCR	A	609	-	41,41,41	0.67	0	56,56,56	1.86	12 (21%)
25	CLA	B	611	-	69,73,73	1.59	7 (10%)	82,113,113	1.20	9 (10%)
25	CLA	b	602	-	69,73,73	1.64	9 (13%)	82,113,113	1.25	8 (9%)
23	LMG	b	624	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	3 (5%)
33	DGD	h	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.90	2 (2%)
25	CLA	a	608	-	69,73,73	1.62	9 (13%)	82,113,113	1.18	10 (12%)
26	BCR	c	521	-	41,41,41	0.64	0	56,56,56	2.07	12 (21%)
25	CLA	b	612	-	69,73,73	1.59	7 (10%)	82,113,113	1.19	9 (10%)
25	CLA	B	605	-	69,73,73	1.58	8 (11%)	82,113,113	1.20	8 (9%)
25	CLA	B	614	-	69,73,73	1.59	8 (11%)	82,113,113	1.21	9 (10%)
30	SO4	A	615	-	4,4,4	0.24	0	6,6,6	0.09	0
25	CLA	B	602	-	69,73,73	1.60	8 (11%)	82,113,113	1.23	9 (10%)
33	DGD	c	517	-	63,63,67	0.87	2 (3%)	77,77,81	0.90	3 (3%)
29	LHG	a	616	-	41,41,48	1.01	2 (4%)	44,47,54	1.11	3 (6%)
25	CLA	c	508	-	69,73,73	1.58	8 (11%)	82,113,113	1.19	9 (10%)
29	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.09	4 (7%)
25	CLA	B	615	-	69,73,73	1.56	8 (11%)	82,113,113	1.20	8 (9%)
26	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.84	14 (25%)
25	CLA	b	614	-	69,73,73	1.59	8 (11%)	82,113,113	1.22	8 (9%)
25	CLA	C	513	-	69,73,73	1.59	8 (11%)	82,113,113	1.18	9 (10%)
25	CLA	b	609	-	69,73,73	1.60	9 (13%)	82,113,113	1.16	9 (10%)
27	PL9	d	405	-	55,55,55	0.63	2 (3%)	68,69,69	1.70	19 (27%)
33	DGD	c	515	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	4 (5%)
33	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	0.89	3 (3%)
25	CLA	B	603	-	69,73,73	1.58	8 (11%)	82,113,113	1.21	9 (10%)
25	CLA	B	607	37	69,73,73	1.60	8 (11%)	82,113,113	1.19	9 (10%)
25	CLA	C	503	-	69,73,73	1.57	7 (10%)	82,113,113	1.18	9 (10%)
25	CLA	c	511	3	69,73,73	1.58	8 (11%)	82,113,113	1.13	10 (12%)
33	DGD	c	516	-	63,63,67	0.88	2 (3%)	77,77,81	0.93	4 (5%)
28	SQD	f	101	-	41,43,54	1.26	3 (7%)	51,54,65	1.28	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCT	A	616	22	3,3,3	0.58	0	2,3,3	0.23	0
26	BCR	t	102	-	41,41,41	0.67	0	56,56,56	2.07	14 (25%)
29	LHG	A	614	-	48,48,48	0.95	2 (4%)	51,54,54	1.02	2 (3%)
25	CLA	C	502	-	69,73,73	1.60	8 (11%)	82,113,113	1.17	9 (10%)
25	CLA	C	509	-	69,73,73	1.59	8 (11%)	82,113,113	1.15	9 (10%)
29	LHG	A	613	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
30	SO4	d	410	-	4,4,4	0.23	0	6,6,6	0.07	0
23	LMG	a	614	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	3 (5%)
25	CLA	c	502	-	69,73,73	1.61	8 (11%)	82,113,113	1.17	9 (10%)
25	CLA	c	510	-	69,73,73	1.58	7 (10%)	82,113,113	1.20	9 (10%)
29	LHG	L	102	-	48,48,48	0.93	2 (4%)	51,54,54	1.11	4 (7%)
27	PL9	a	612	-	55,55,55	0.65	2 (3%)	68,69,69	1.69	19 (27%)
30	SO4	O	302	-	4,4,4	0.23	0	6,6,6	0.07	0
23	LMG	D	409	-	51,51,55	0.95	2 (3%)	59,59,63	0.99	3 (5%)
29	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
25	CLA	B	604	-	69,73,73	1.57	7 (10%)	82,113,113	1.18	10 (12%)
26	BCR	D	406	-	41,41,41	0.69	0	56,56,56	2.23	15 (26%)
28	SQD	L	101	-	52,54,54	1.15	3 (5%)	62,65,65	3.07	8 (12%)
25	CLA	a	607	37	69,73,73	1.62	8 (11%)	82,113,113	1.22	9 (10%)
30	SO4	u	201	-	4,4,4	0.24	0	6,6,6	0.07	0
31	BCT	a	618	22	3,3,3	0.59	0	2,3,3	0.74	0
26	BCR	H	101	-	41,41,41	0.65	0	56,56,56	2.05	13 (23%)
25	CLA	D	403	37	69,73,73	1.61	8 (11%)	82,113,113	1.23	9 (10%)
26	BCR	C	514	-	41,41,41	0.67	0	56,56,56	1.94	14 (25%)
26	BCR	b	619	-	41,41,41	0.71	0	56,56,56	1.94	13 (23%)
25	CLA	D	404	-	69,73,73	1.60	8 (11%)	82,113,113	1.18	8 (9%)
28	SQD	a	613	-	52,54,54	1.11	3 (5%)	62,65,65	1.19	7 (11%)
34	PHO	d	402	-	58,69,69	1.32	6 (10%)	55,99,99	1.70	4 (7%)
35	HEM	E	102	5,6	50,50,50	1.38	6 (12%)	67,82,82	0.99	2 (2%)
25	CLA	C	512	-	69,73,73	1.57	8 (11%)	82,113,113	1.15	8 (9%)
34	PHO	a	609	-	58,69,69	1.34	6 (10%)	55,99,99	1.64	3 (5%)
23	LMG	d	408	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)
25	CLA	B	608	-	69,73,73	1.59	8 (11%)	82,113,113	1.16	9 (10%)
25	CLA	A	607	-	69,73,73	1.61	8 (11%)	82,113,113	1.17	9 (10%)
25	CLA	B	601	-	69,73,73	1.61	9 (13%)	82,113,113	1.16	8 (9%)
25	CLA	B	610	-	69,73,73	1.62	8 (11%)	82,113,113	1.21	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	608	-	69,73,73	1.60	8 (11%)	82,113,113	1.17	8 (9%)
25	CLA	D	405	-	69,73,73	1.59	9 (13%)	82,113,113	1.16	9 (10%)
26	BCR	z	101	-	41,41,41	0.68	0	56,56,56	1.87	10 (17%)
36	HEC	V	201	16	46,50,50	1.35	4 (8%)	58,82,82	1.67	3 (5%)
25	CLA	c	512	-	69,73,73	1.58	8 (11%)	82,113,113	1.14	8 (9%)
25	CLA	c	505	-	69,73,73	1.61	8 (11%)	82,113,113	1.17	7 (8%)
25	CLA	b	611	-	69,73,73	1.60	8 (11%)	82,113,113	1.19	9 (10%)
25	CLA	B	613	-	69,73,73	1.58	7 (10%)	82,113,113	1.18	9 (10%)
25	CLA	C	506	-	69,73,73	1.61	7 (10%)	82,113,113	1.17	9 (10%)
25	CLA	B	616	-	69,73,73	1.58	9 (13%)	82,113,113	1.28	9 (10%)
25	CLA	C	511	3	69,73,73	1.57	7 (10%)	82,113,113	1.15	10 (12%)
29	LHG	a	615	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
33	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	0.91	3 (3%)
25	CLA	b	604	-	69,73,73	1.57	7 (10%)	82,113,113	1.18	10 (12%)
25	CLA	d	401	-	69,73,73	1.61	8 (11%)	82,113,113	1.18	8 (9%)
25	CLA	c	506	-	69,73,73	1.61	9 (13%)	82,113,113	1.19	8 (9%)
34	PHO	D	402	-	58,69,69	1.31	6 (10%)	55,99,99	1.66	4 (7%)
26	BCR	d	404	-	41,41,41	0.73	0	56,56,56	2.04	13 (23%)
25	CLA	c	509	-	69,73,73	1.58	8 (11%)	82,113,113	1.16	9 (10%)
28	SQD	A	611	-	52,54,54	1.10	3 (5%)	62,65,65	1.21	6 (9%)
26	BCR	b	617	-	41,41,41	0.67	0	56,56,56	2.03	15 (26%)
26	BCR	C	522	-	41,41,41	0.64	0	56,56,56	2.08	15 (26%)
26	BCR	a	611	-	41,41,41	0.68	0	56,56,56	1.80	12 (21%)
29	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.10	3 (6%)
25	CLA	b	603	-	69,73,73	1.60	8 (11%)	82,113,113	1.18	9 (10%)
36	HEC	v	201	16	46,50,50	1.36	4 (8%)	58,82,82	1.72	3 (5%)
25	CLA	b	606	-	69,73,73	1.59	8 (11%)	82,113,113	1.17	7 (8%)
30	SO4	U	201	-	4,4,4	0.24	0	6,6,6	0.08	0
23	LMG	c	518	-	51,51,55	0.94	2 (3%)	59,59,63	0.98	3 (5%)
26	BCR	B	619	-	41,41,41	0.74	0	56,56,56	1.94	16 (28%)
25	CLA	C	510	-	69,73,73	1.60	7 (10%)	82,113,113	1.21	9 (10%)
25	CLA	a	610	-	69,73,73	1.60	8 (11%)	82,113,113	1.18	9 (10%)
25	CLA	b	605	-	69,73,73	1.59	8 (11%)	82,113,113	1.19	8 (9%)
25	CLA	B	612	-	69,73,73	1.59	8 (11%)	82,113,113	1.17	9 (10%)
25	CLA	c	504	-	69,73,73	1.59	8 (11%)	82,113,113	1.16	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	606	-	69,73,73	1.59	8 (11%)	82,113,113	1.20	9 (10%)

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
23	LMG	A	612	-	-	11/46/66/70	0/1/1/1
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	CLA	b	613	-	1/1/15/20	1/39/115/115	-
23	LMG	C	519	-	-	9/46/66/70	0/1/1/1
27	PL9	D	407	-	-	8/53/73/73	0/1/1/1
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
25	CLA	C	507	-	1/1/15/20	5/39/115/115	-
25	CLA	C	504	-	1/1/15/20	6/39/115/115	-
33	DGD	C	517	-	-	12/51/91/95	0/2/2/2
25	CLA	b	601	-	1/1/15/20	7/39/115/115	-
25	CLA	d	403	-	1/1/15/20	2/39/115/115	-
26	BCR	k	102	-	-	4/29/63/63	0/2/2/2
23	LMG	B	620	-	-	4/46/66/70	0/1/1/1
23	LMG	a	603	-	-	11/46/66/70	0/1/1/1
25	CLA	c	513	-	1/1/15/20	3/39/115/115	-
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
23	LMG	A	603	-	-	15/46/66/70	0/1/1/1
23	LMG	C	521	-	-	17/46/66/70	0/1/1/1
28	SQD	L	103	-	-	18/49/69/69	0/1/1/1
25	CLA	c	503	-	1/1/15/20	4/39/115/115	-
33	DGD	C	516	-	-	8/51/91/95	0/2/2/2
34	PHO	D	401	-	-	5/37/103/103	0/5/6/6
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
29	LHG	d	407	-	-	16/53/53/53	-
25	CLA	b	615	-	1/1/15/20	4/39/115/115	-
35	HEM	e	101	5,6	-	7/14/54/54	-
25	CLA	B	609	-	1/1/15/20	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	CLA	C	505	-	1/1/15/20	2/39/115/115	-
25	CLA	b	608	-	1/1/15/20	2/39/115/115	-
25	CLA	C	501	-	1/1/15/20	0/39/115/115	-
23	LMG	b	620	-	-	4/46/66/70	0/1/1/1
25	CLA	b	616	-	1/1/15/20	4/39/115/115	-
29	LHG	D	408	-	-	5/53/53/53	-
25	CLA	b	607	37	1/1/15/20	5/39/115/115	-
25	CLA	b	610	37	1/1/15/20	3/39/115/115	-
23	LMG	c	520	-	-	13/46/66/70	0/1/1/1
25	CLA	C	508	-	1/1/15/20	0/39/115/115	-
23	LMG	B	624	-	-	10/46/66/70	0/1/1/1
25	CLA	a	606	-	1/1/15/20	1/39/115/115	-
25	CLA	c	501	-	1/1/15/20	2/39/115/115	-
28	SQD	F	101	-	-	5/38/58/69	0/1/1/1
27	PL9	A	610	-	-	8/53/73/73	0/1/1/1
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	CLA	c	507	-	1/1/15/20	7/39/115/115	-
25	CLA	A	606	-	1/1/15/20	1/39/115/115	-
26	BCR	A	609	-	-	0/29/63/63	0/2/2/2
25	CLA	B	611	-	1/1/15/20	1/39/115/115	-
25	CLA	b	602	-	1/1/15/20	2/39/115/115	-
23	LMG	b	624	-	-	9/46/66/70	0/1/1/1
33	DGD	h	102	-	-	7/51/91/95	0/2/2/2
25	CLA	a	608	-	1/1/15/20	2/39/115/115	-
26	BCR	c	521	-	-	0/29/63/63	0/2/2/2
25	CLA	b	612	-	1/1/15/20	0/39/115/115	-
25	CLA	B	605	-	1/1/15/20	6/39/115/115	-
25	CLA	B	614	-	1/1/15/20	7/39/115/115	-
25	CLA	B	602	-	1/1/15/20	8/39/115/115	-
33	DGD	c	517	-	-	1/51/91/95	0/2/2/2
29	LHG	a	616	-	-	8/46/46/53	-
25	CLA	c	508	-	1/1/15/20	0/39/115/115	-
29	LHG	l	101	-	-	17/53/53/53	-
25	CLA	B	615	-	1/1/15/20	5/39/115/115	-
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	614	-	1/1/15/20	10/39/115/115	-
25	CLA	C	513	-	1/1/15/20	2/39/115/115	-
25	CLA	b	609	-	1/1/15/20	4/39/115/115	-
27	PL9	d	405	-	-	8/53/73/73	0/1/1/1
33	DGD	c	515	-	-	8/51/91/95	0/2/2/2
33	DGD	H	102	-	-	5/51/91/95	0/2/2/2
25	CLA	B	603	-	1/1/15/20	1/39/115/115	-
25	CLA	B	607	37	1/1/15/20	7/39/115/115	-
25	CLA	C	503	-	1/1/15/20	1/39/115/115	-
25	CLA	c	511	3	1/1/15/20	0/39/115/115	-
33	DGD	c	516	-	-	8/51/91/95	0/2/2/2
28	SQD	f	101	-	-	11/38/58/69	0/1/1/1
26	BCR	t	102	-	-	8/29/63/63	0/2/2/2
29	LHG	A	614	-	-	4/53/53/53	-
25	CLA	C	502	-	1/1/15/20	3/39/115/115	-
25	CLA	C	509	-	1/1/15/20	0/39/115/115	-
29	LHG	A	613	-	-	6/53/53/53	-
23	LMG	a	614	-	-	5/46/66/70	0/1/1/1
25	CLA	c	502	-	1/1/15/20	2/39/115/115	-
25	CLA	c	510	-	1/1/15/20	4/39/115/115	-
29	LHG	L	102	-	-	15/53/53/53	-
27	PL9	a	612	-	-	7/53/73/73	0/1/1/1
23	LMG	D	409	-	-	3/46/66/70	0/1/1/1
29	LHG	d	406	-	-	4/53/53/53	-
25	CLA	B	604	-	1/1/15/20	0/39/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
28	SQD	L	101	-	-	16/49/69/69	0/1/1/1
25	CLA	a	607	37	1/1/15/20	3/39/115/115	-
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
25	CLA	D	403	37	1/1/15/20	3/39/115/115	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	CLA	D	404	-	1/1/15/20	2/39/115/115	-
28	SQD	a	613	-	-	7/49/69/69	0/1/1/1
34	PHO	d	402	-	-	1/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	E	102	5,6	-	8/14/54/54	-
25	CLA	C	512	-	1/1/15/20	4/39/115/115	-
34	PHO	a	609	-	-	6/37/103/103	0/5/6/6
23	LMG	d	408	-	-	3/46/66/70	0/1/1/1
25	CLA	B	608	-	1/1/15/20	1/39/115/115	-
25	CLA	A	607	-	1/1/15/20	3/39/115/115	-
25	CLA	B	610	-	1/1/15/20	3/39/115/115	-
25	CLA	B	601	-	1/1/15/20	8/39/115/115	-
25	CLA	A	608	-	1/1/15/20	6/39/115/115	-
25	CLA	D	405	-	1/1/15/20	2/39/115/115	-
26	BCR	z	101	-	-	1/29/63/63	0/2/2/2
36	HEC	V	201	16	-	4/14/54/54	-
25	CLA	c	512	-	1/1/15/20	6/39/115/115	-
25	CLA	c	505	-	1/1/15/20	2/39/115/115	-
25	CLA	b	611	-	1/1/15/20	2/39/115/115	-
25	CLA	B	613	-	1/1/15/20	1/39/115/115	-
25	CLA	C	506	-	1/1/15/20	8/39/115/115	-
25	CLA	B	616	-	1/1/15/20	2/39/115/115	-
25	CLA	C	511	3	1/1/15/20	0/39/115/115	-
29	LHG	a	615	-	-	7/53/53/53	-
33	DGD	C	518	-	-	4/51/91/95	0/2/2/2
25	CLA	b	604	-	1/1/15/20	3/39/115/115	-
25	CLA	d	401	-	1/1/15/20	0/39/115/115	-
25	CLA	c	506	-	1/1/15/20	2/39/115/115	-
34	PHO	D	402	-	-	1/37/103/103	0/5/6/6
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	1/39/115/115	-
28	SQD	A	611	-	-	5/49/69/69	0/1/1/1
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
26	BCR	C	522	-	-	0/29/63/63	0/2/2/2
26	BCR	a	611	-	-	0/29/63/63	0/2/2/2
29	LHG	E	101	-	-	9/46/46/53	-
25	CLA	b	603	-	1/1/15/20	4/39/115/115	-
36	HEC	v	201	16	-	3/14/54/54	-
25	CLA	b	606	-	1/1/15/20	4/39/115/115	-
23	LMG	c	518	-	-	8/46/66/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	CLA	C	510	-	1/1/15/20	3/39/115/115	-
25	CLA	a	610	-	1/1/15/20	6/39/115/115	-
25	CLA	b	605	-	1/1/15/20	4/39/115/115	-
25	CLA	B	612	-	1/1/15/20	0/39/115/115	-
25	CLA	c	504	-	1/1/15/20	3/39/115/115	-
25	CLA	B	606	-	1/1/15/20	3/39/115/115	-

The worst 5 of 691 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	MG-NB	-6.50	1.92	2.05
25	C	506	CLA	MG-NB	-6.47	1.93	2.05
25	a	607	CLA	MG-NB	-6.47	1.93	2.05
25	A	607	CLA	MG-NB	-6.44	1.93	2.05
25	C	504	CLA	MG-NB	-6.43	1.93	2.05

The worst 5 of 1156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	101	SQD	O9-S-C6	-14.06	85.76	106.76
28	L	101	SQD	O8-S-O9	-11.51	82.59	111.40
34	a	609	PHO	C4D-CHA-CBD	-10.48	103.43	108.45
34	d	402	PHO	C4D-CHA-CBD	-10.46	103.44	108.45
34	D	401	PHO	C4D-CHA-CBD	-10.25	103.54	108.45

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	608	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND

5 of 662 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	C	521	LMG	O6-C1-O1-C7
25	A	607	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	601	CLA	C2B-C3B-CAB-CBB
25	B	601	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

130 monomers are involved in 323 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	514	BCR	4	0
25	b	613	CLA	4	0
23	C	519	LMG	1	0
27	D	407	PL9	3	0
26	T	101	BCR	6	0
25	C	504	CLA	2	0
25	C	507	CLA	2	0
33	C	517	DGD	4	0
25	b	601	CLA	3	0
25	d	403	CLA	1	0
26	k	102	BCR	3	0
23	B	620	LMG	3	0
23	a	603	LMG	1	0
25	c	513	CLA	7	0
26	h	101	BCR	4	0
23	A	603	LMG	1	0
23	C	521	LMG	3	0
28	L	103	SQD	4	0
25	c	503	CLA	5	0
33	C	516	DGD	4	0
34	D	401	PHO	1	0
26	B	618	BCR	4	0
26	K	101	BCR	4	0
29	d	407	LHG	8	0
25	b	615	CLA	3	0
35	e	101	HEM	5	0
25	B	609	CLA	3	0
26	B	617	BCR	6	0
25	C	505	CLA	5	0
25	b	608	CLA	2	0
25	C	501	CLA	4	0
25	b	616	CLA	2	0
29	D	408	LHG	5	0
25	b	607	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	520	LMG	3	0
25	b	610	CLA	1	0
25	C	508	CLA	4	0
25	a	606	CLA	2	0
25	c	501	CLA	3	0
28	F	101	SQD	2	0
27	A	610	PL9	6	0
26	b	618	BCR	1	0
25	c	507	CLA	3	0
25	A	606	CLA	3	0
26	A	609	BCR	3	0
25	B	611	CLA	3	0
25	b	602	CLA	2	0
23	b	624	LMG	1	0
33	h	102	DGD	2	0
25	a	608	CLA	1	0
26	c	521	BCR	1	0
25	b	612	CLA	2	0
25	B	605	CLA	4	0
25	B	614	CLA	3	0
25	B	602	CLA	2	0
29	a	616	LHG	2	0
25	c	508	CLA	7	0
29	l	101	LHG	3	0
25	B	615	CLA	1	0
26	C	515	BCR	2	0
25	b	614	CLA	1	0
25	C	513	CLA	5	0
25	b	609	CLA	3	0
27	d	405	PL9	4	0
25	B	603	CLA	3	0
25	B	607	CLA	2	0
25	C	503	CLA	4	0
25	c	511	CLA	2	0
33	c	516	DGD	3	0
26	t	102	BCR	5	0
29	A	614	LHG	8	0
25	C	502	CLA	1	0
25	C	509	CLA	2	0
29	A	613	LHG	5	0
23	a	614	LMG	1	0
25	c	502	CLA	2	0

Continued on next page...

Continued from previous page...

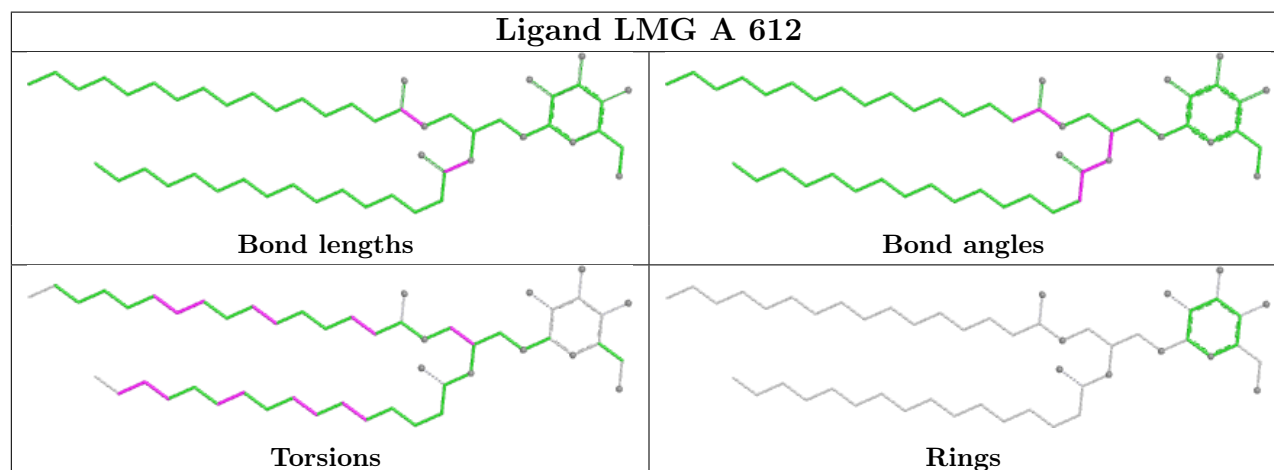
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	510	CLA	5	0
29	L	102	LHG	4	0
27	a	612	PL9	6	0
29	d	406	LHG	3	0
25	B	604	CLA	3	0
26	D	406	BCR	2	0
28	L	101	SQD	6	0
25	a	607	CLA	4	0
26	H	101	BCR	2	0
25	D	403	CLA	3	0
26	C	514	BCR	5	0
26	b	619	BCR	4	0
25	D	404	CLA	6	0
28	a	613	SQD	5	0
34	d	402	PHO	1	0
35	E	102	HEM	3	0
25	C	512	CLA	3	0
34	a	609	PHO	2	0
23	d	408	LMG	2	0
25	B	608	CLA	1	0
25	A	607	CLA	2	0
25	B	601	CLA	2	0
25	A	608	CLA	2	0
25	D	405	CLA	1	0
26	z	101	BCR	10	0
25	c	512	CLA	3	0
25	c	505	CLA	6	0
25	b	611	CLA	2	0
25	B	613	CLA	5	0
25	C	506	CLA	5	0
25	B	616	CLA	4	0
25	C	511	CLA	3	0
29	a	615	LHG	4	0
33	C	518	DGD	1	0
25	b	604	CLA	3	0
25	d	401	CLA	3	0
25	c	506	CLA	4	0
34	D	402	PHO	5	0
26	d	404	BCR	4	0
25	c	509	CLA	3	0
28	A	611	SQD	2	0
26	b	617	BCR	1	0

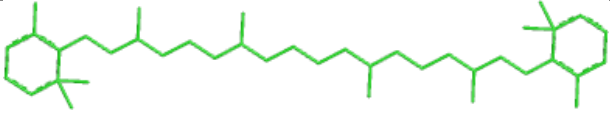
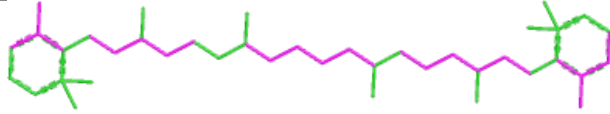
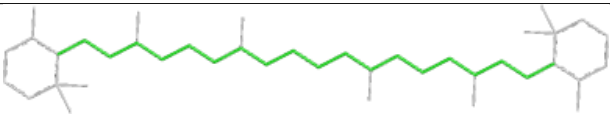
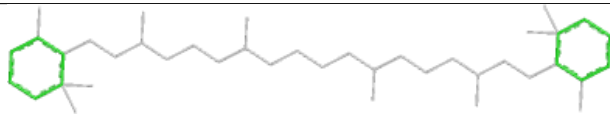
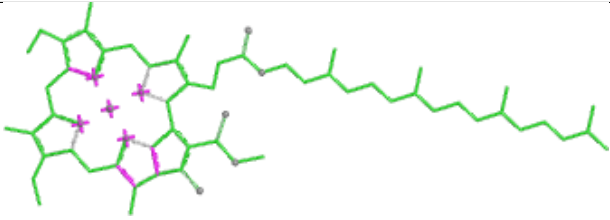
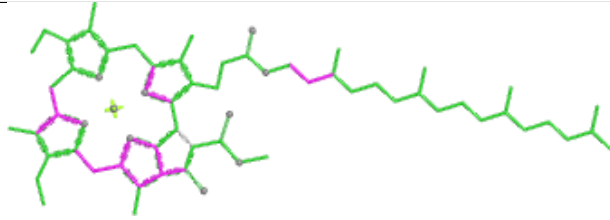
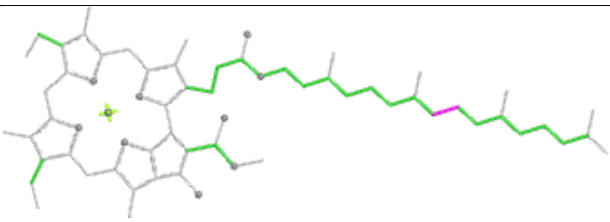
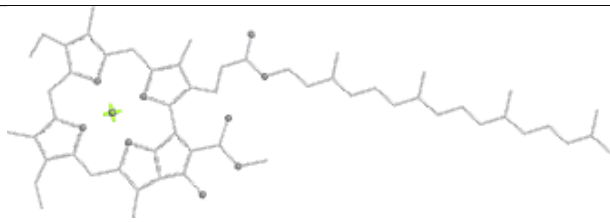
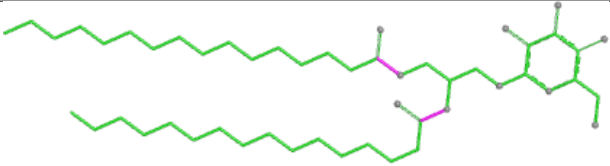
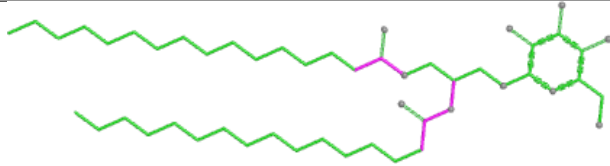
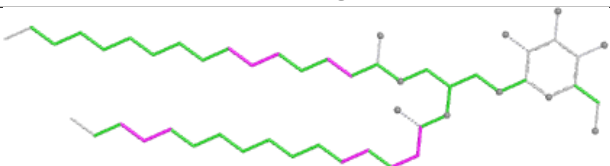
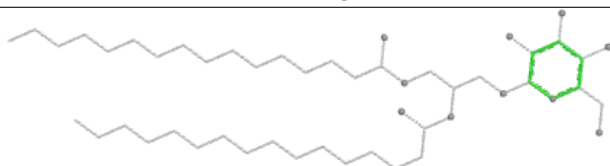
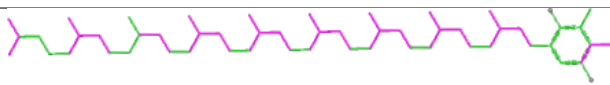
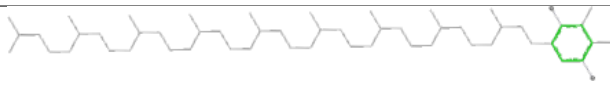
Continued on next page...

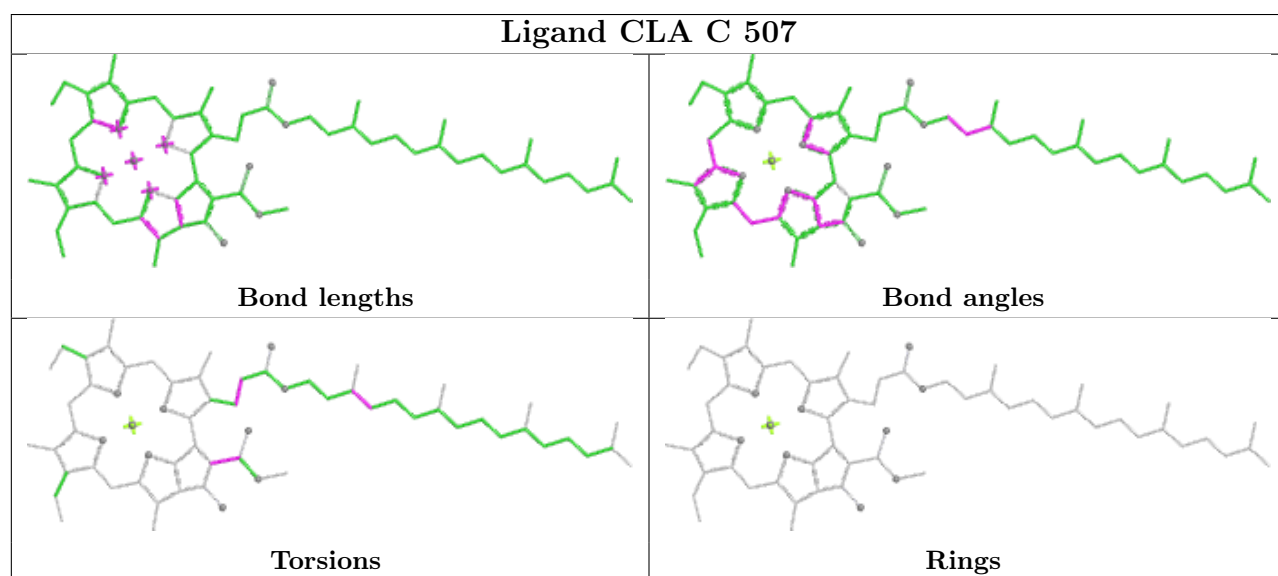
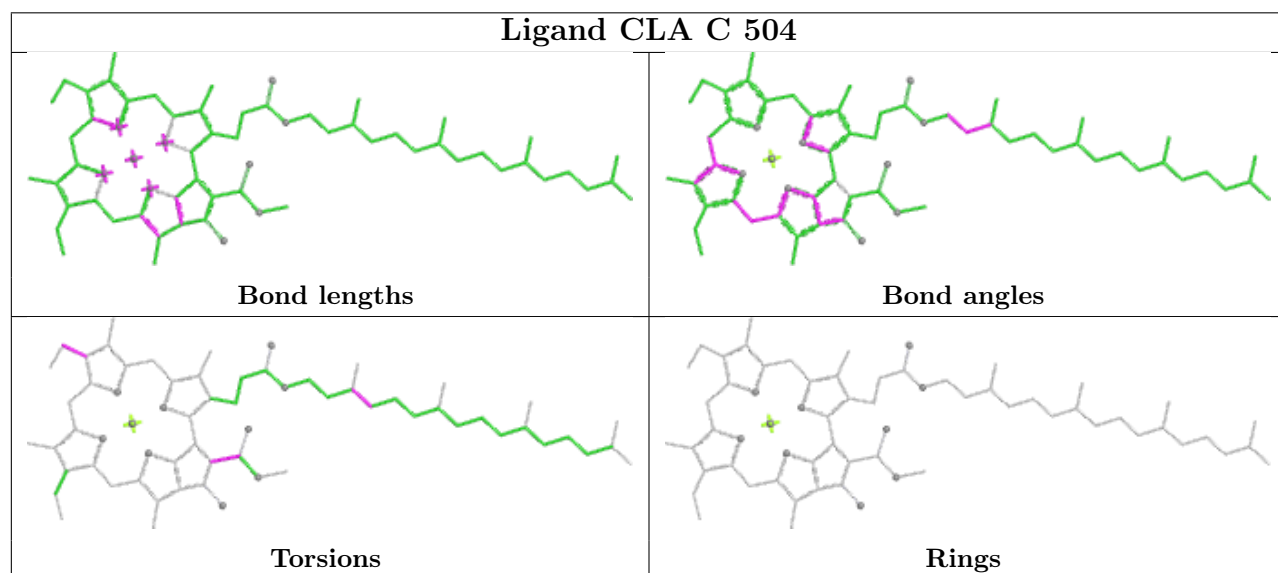
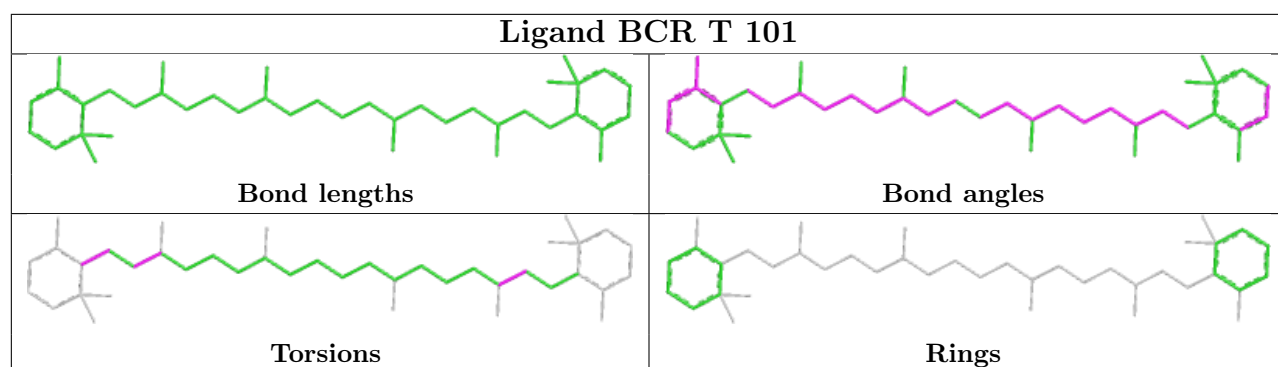
Continued from previous page...

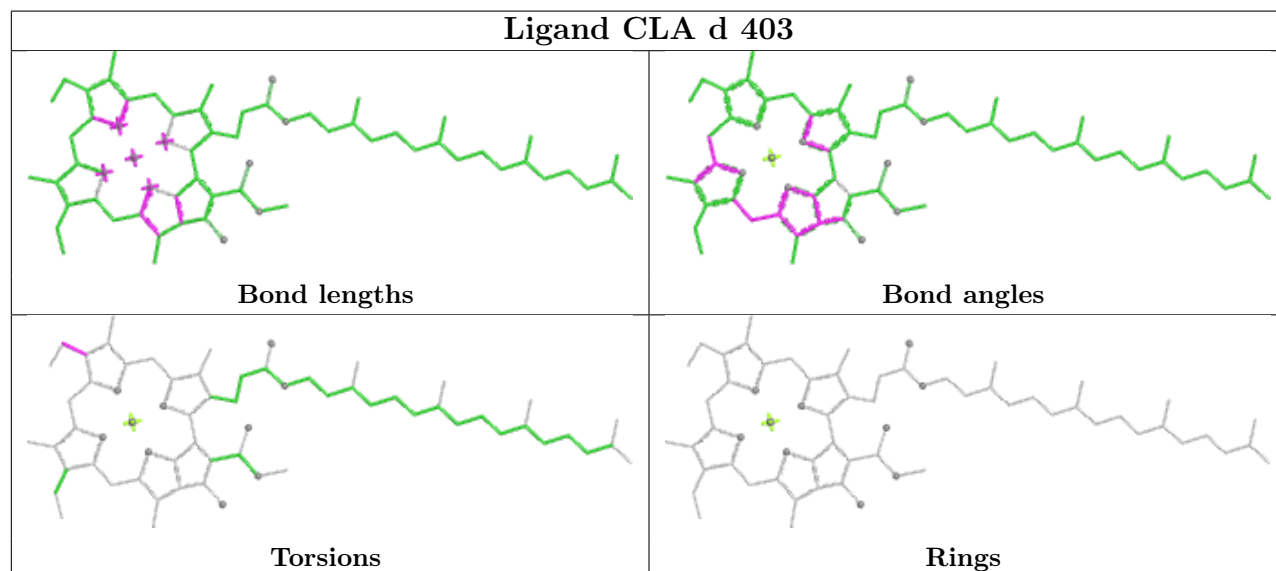
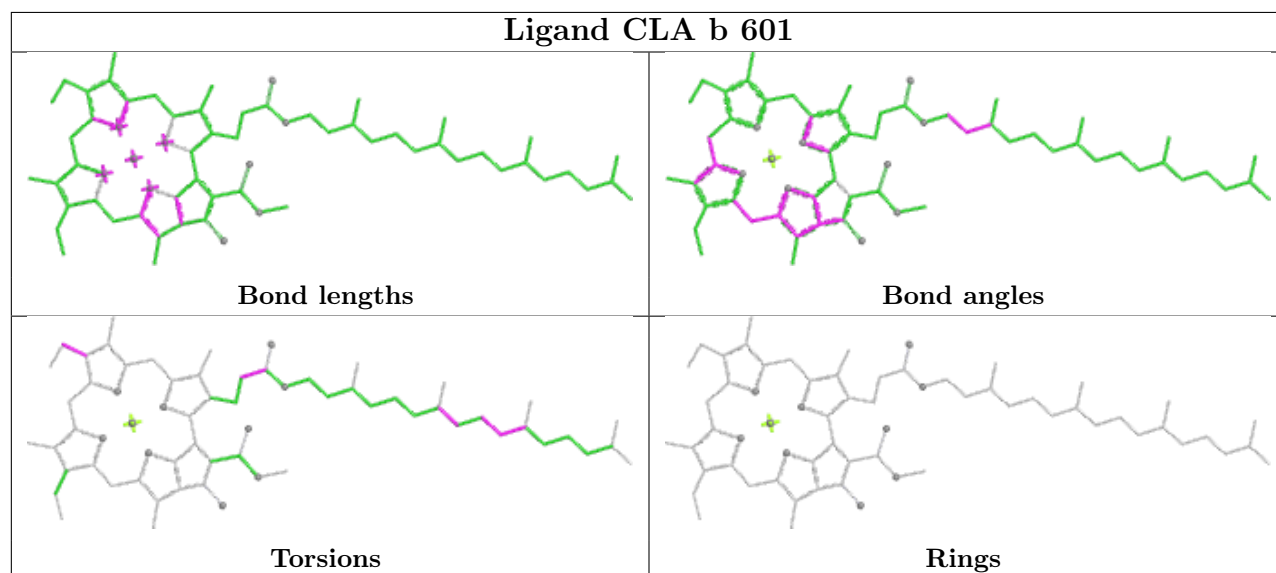
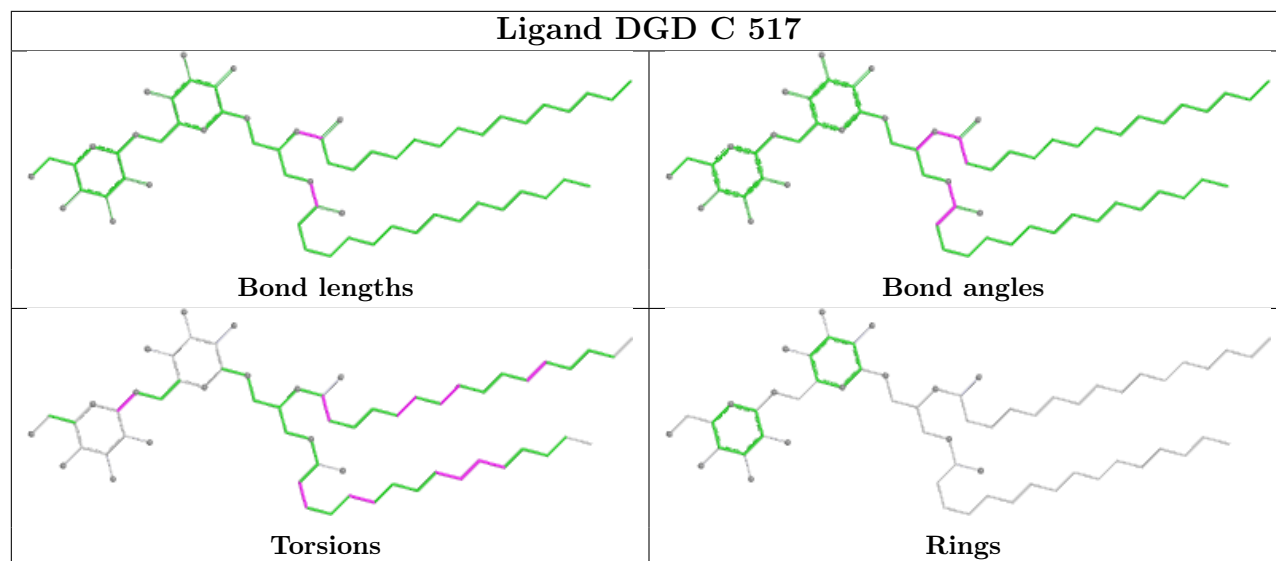
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	522	BCR	1	0
26	a	611	BCR	3	0
25	b	603	CLA	1	0
25	b	606	CLA	3	0
23	c	518	LMG	2	0
26	B	619	BCR	4	0
25	C	510	CLA	3	0
25	a	610	CLA	4	0
25	b	605	CLA	3	0
25	B	612	CLA	1	0
25	c	504	CLA	1	0
25	B	606	CLA	1	0

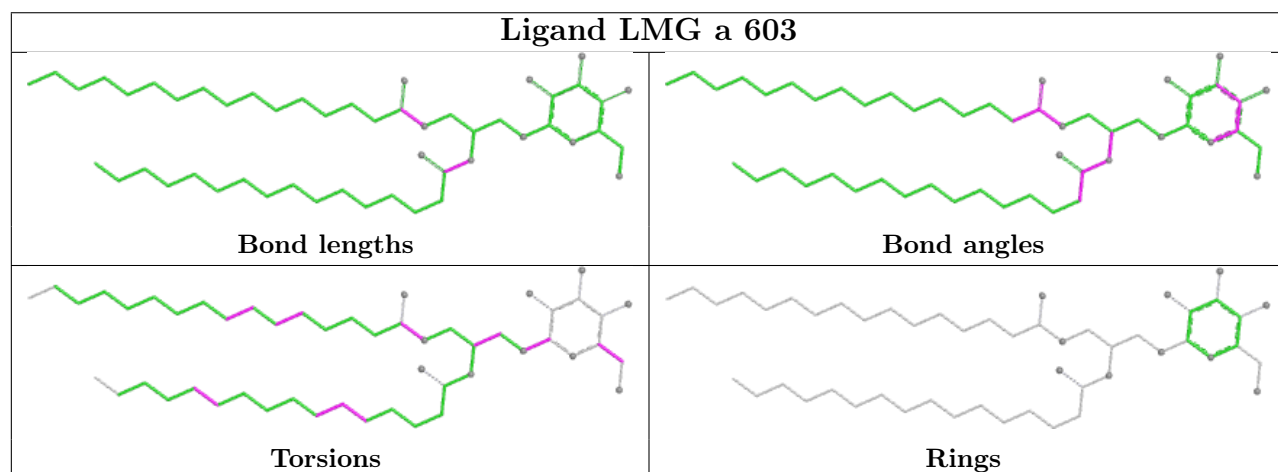
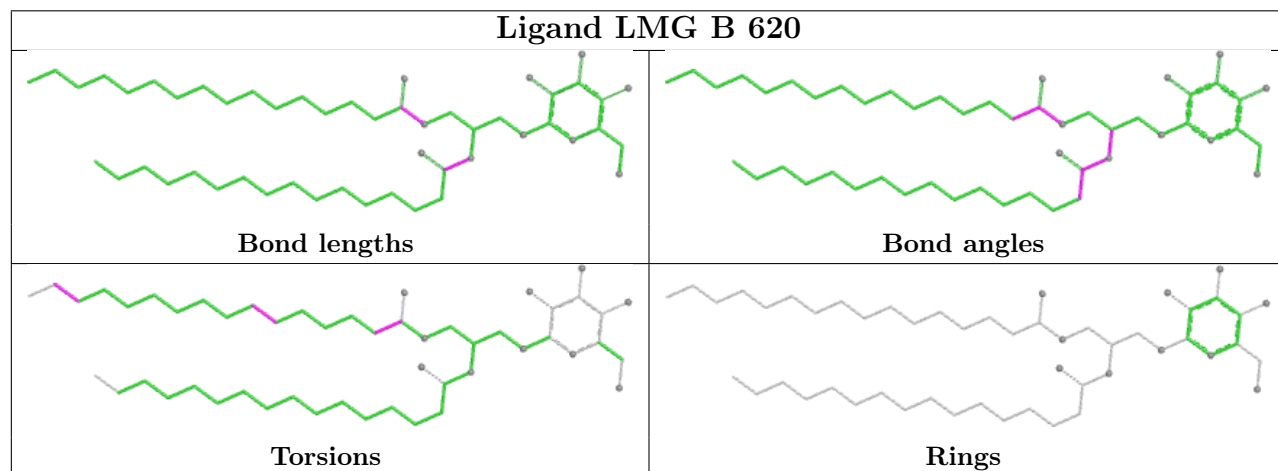
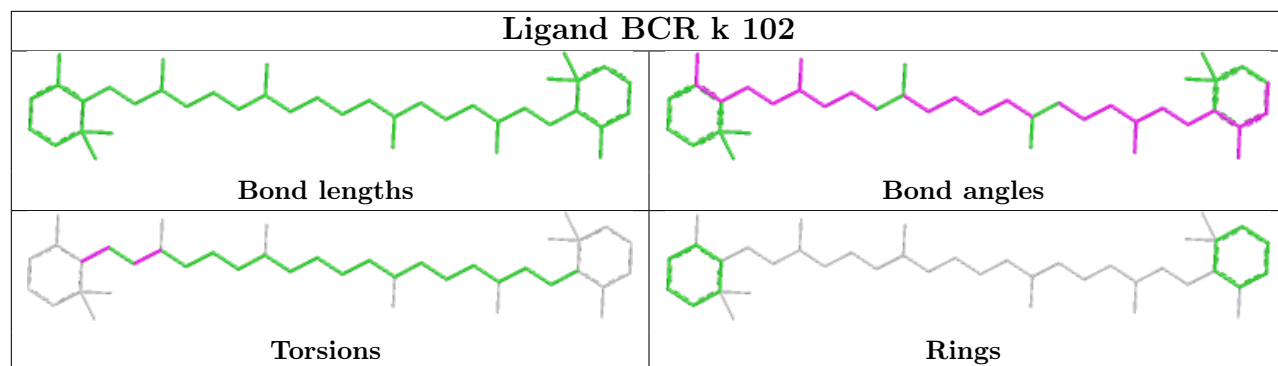
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

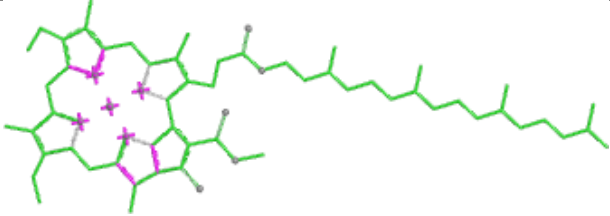
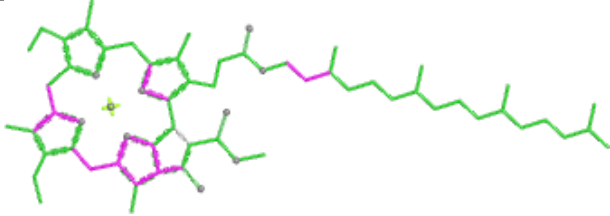
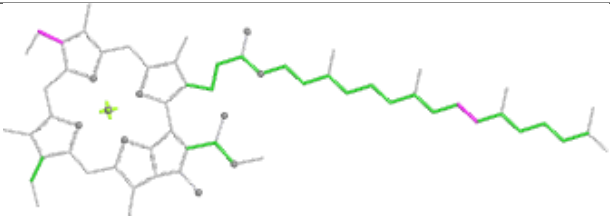
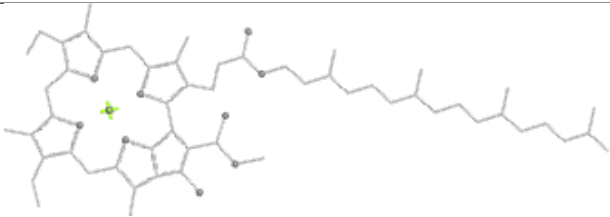
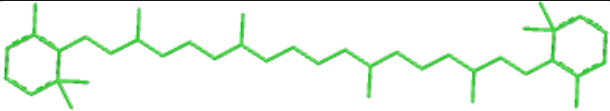
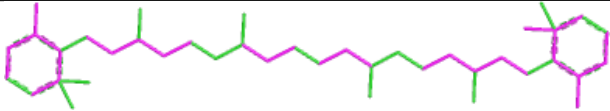
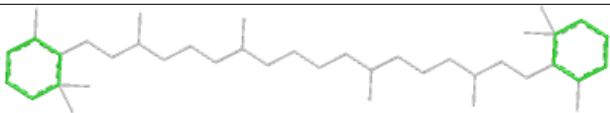
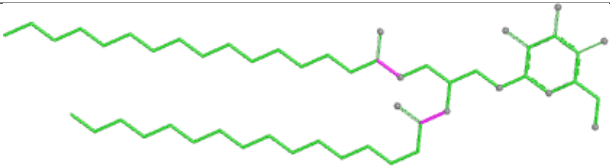
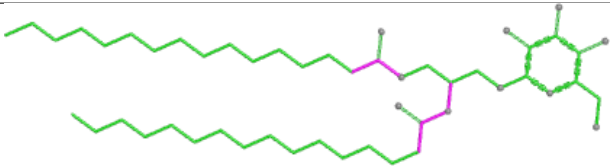
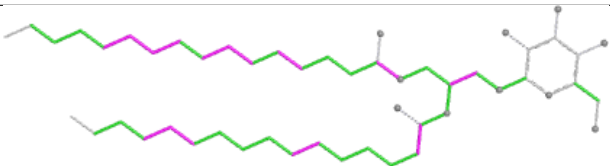
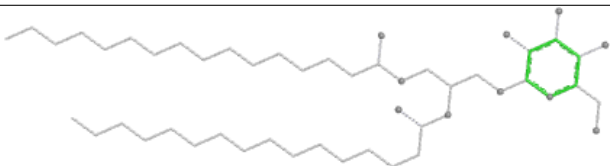


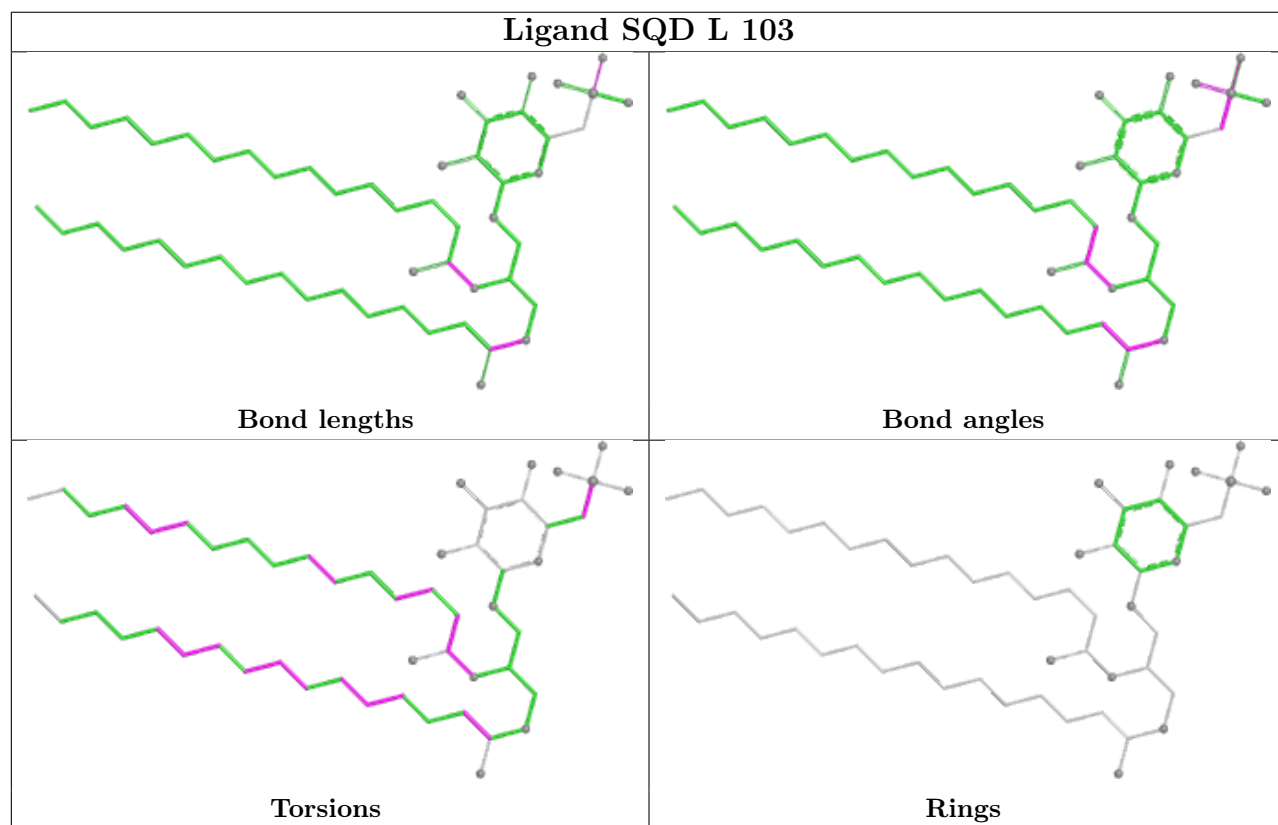
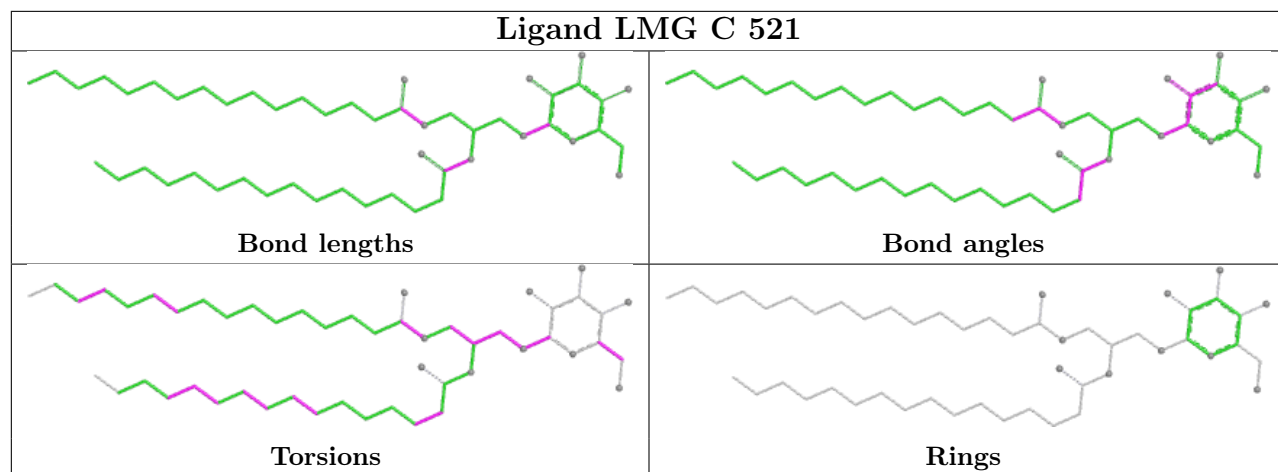
Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

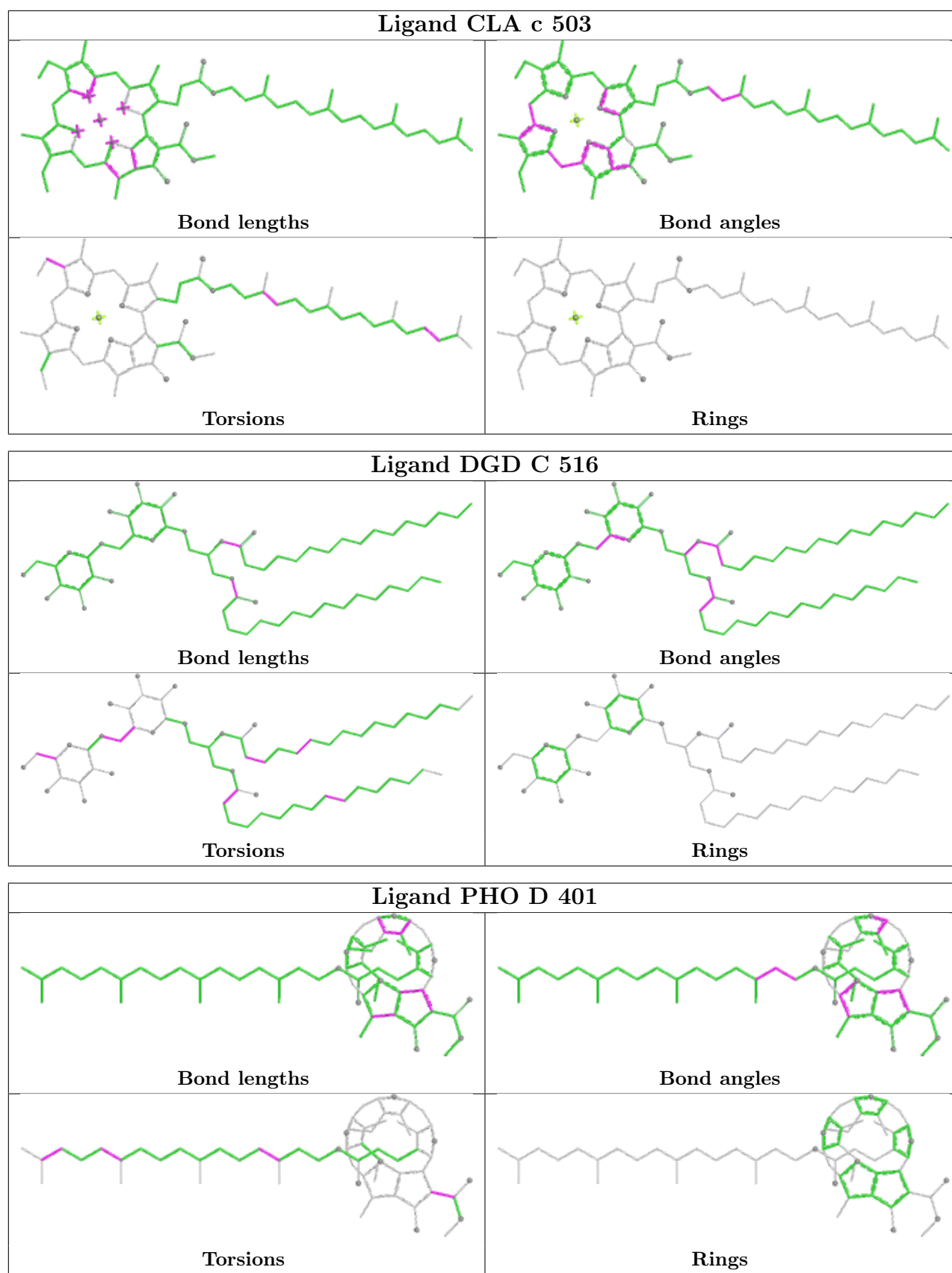


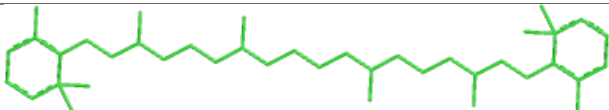
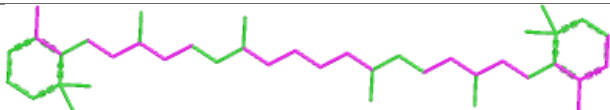
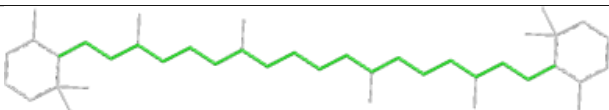
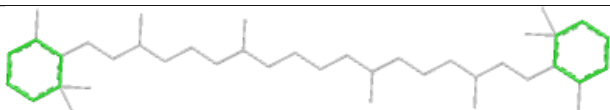


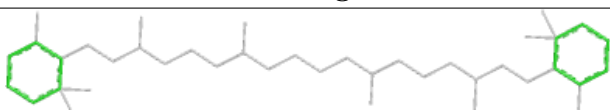


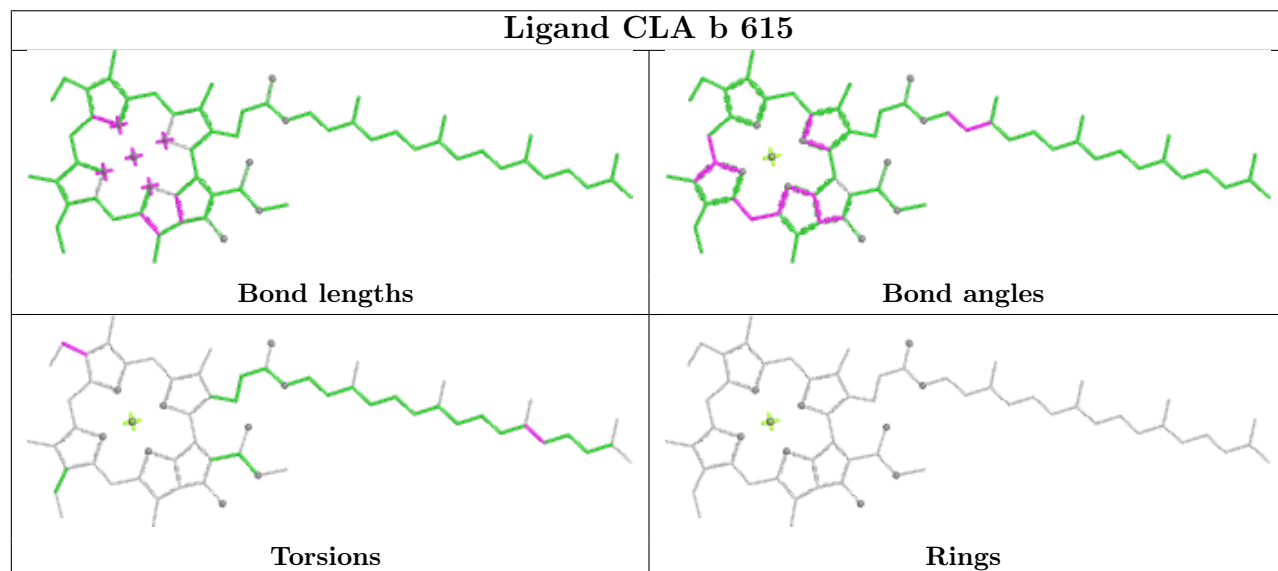
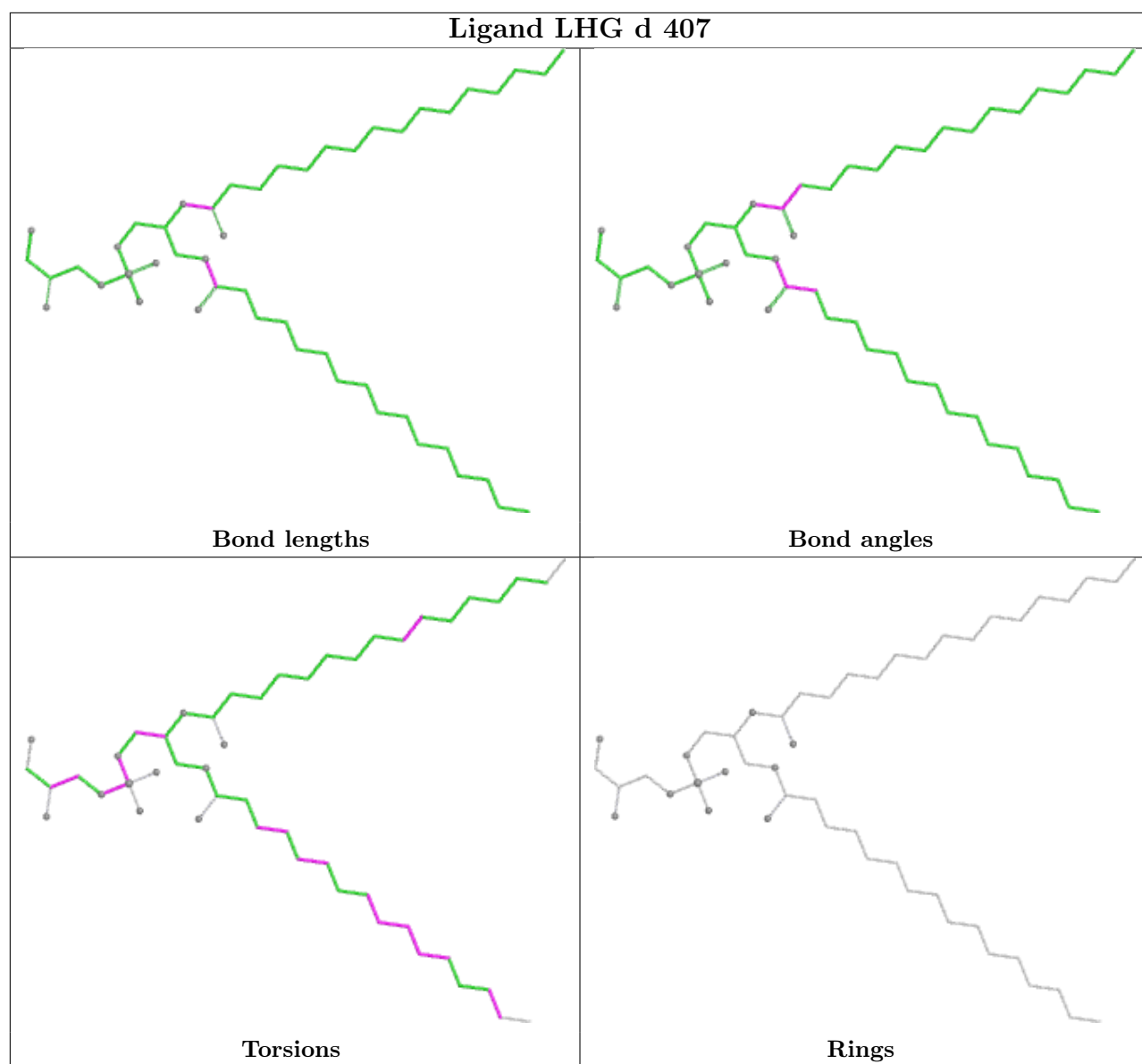
Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 603	
 Bond lengths	 Bond angles
 Torsions	 Rings



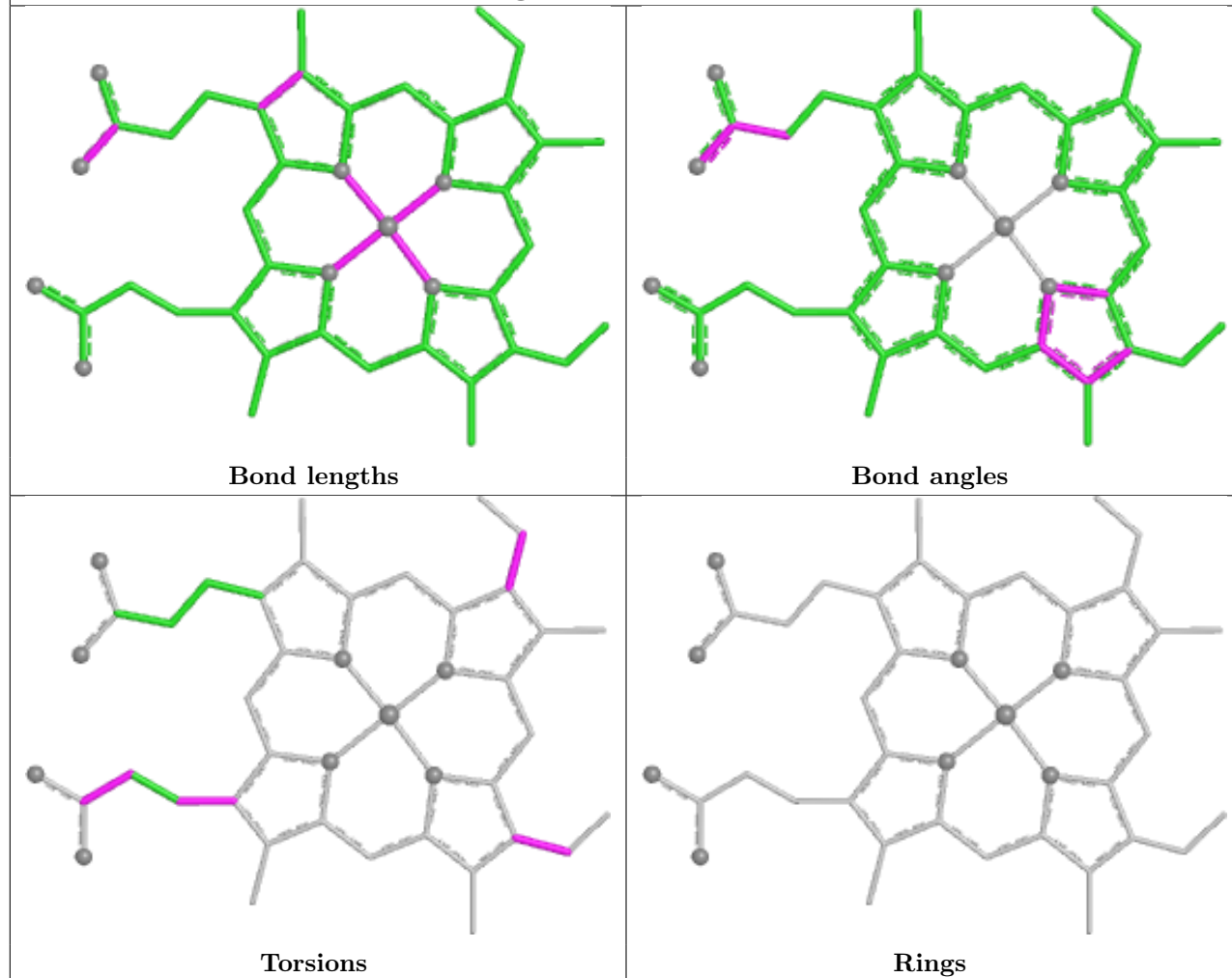


Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

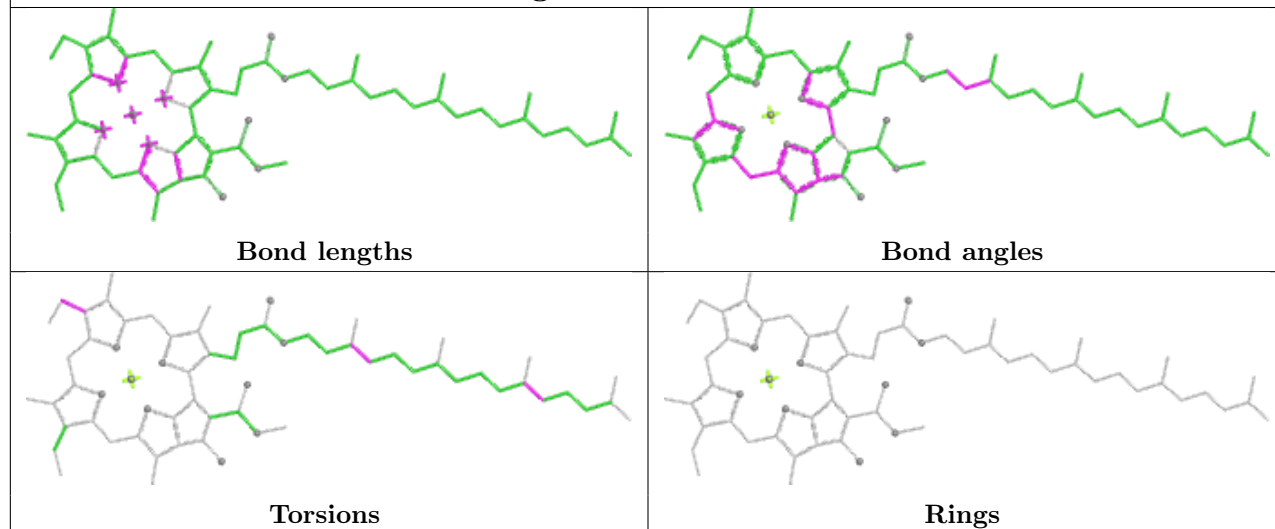
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

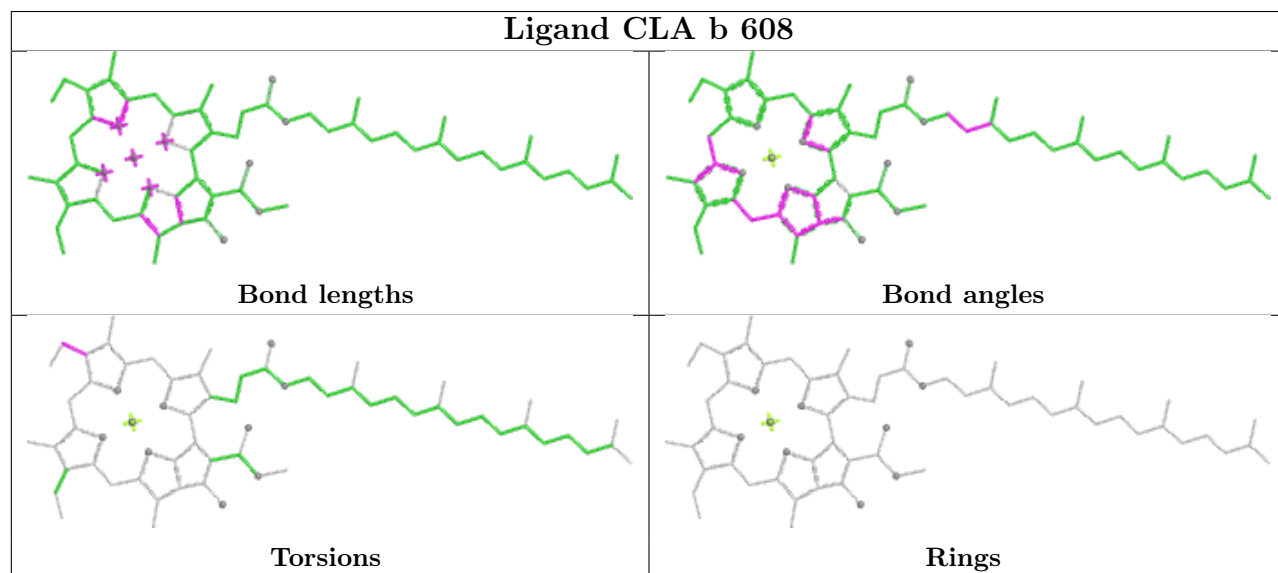
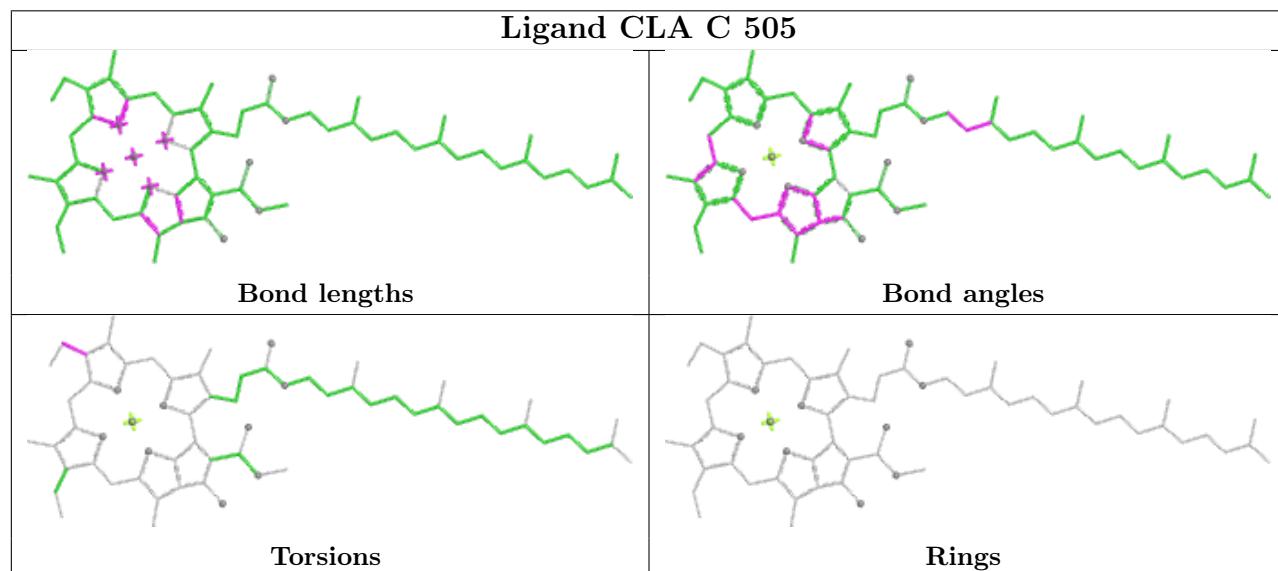
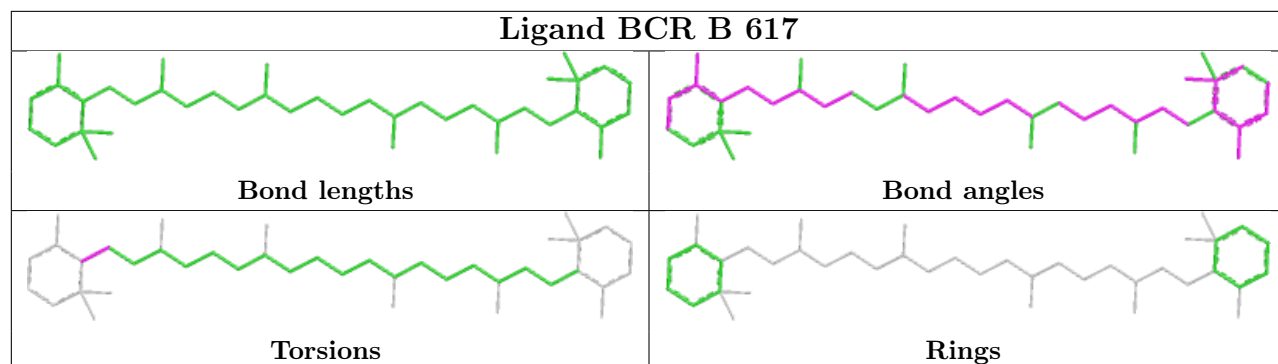


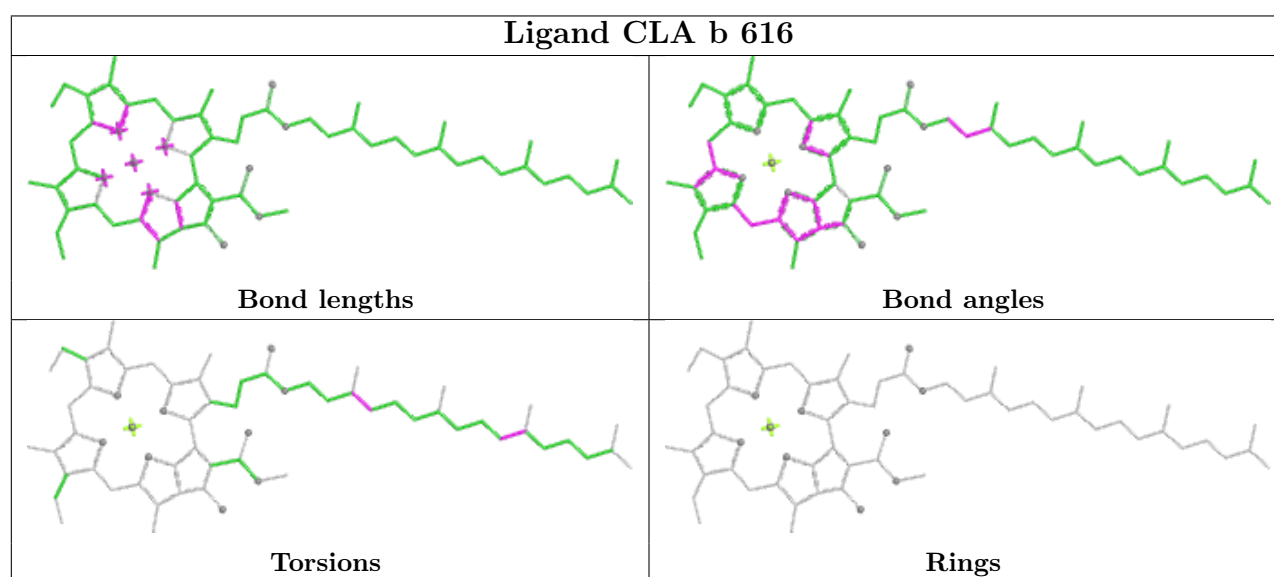
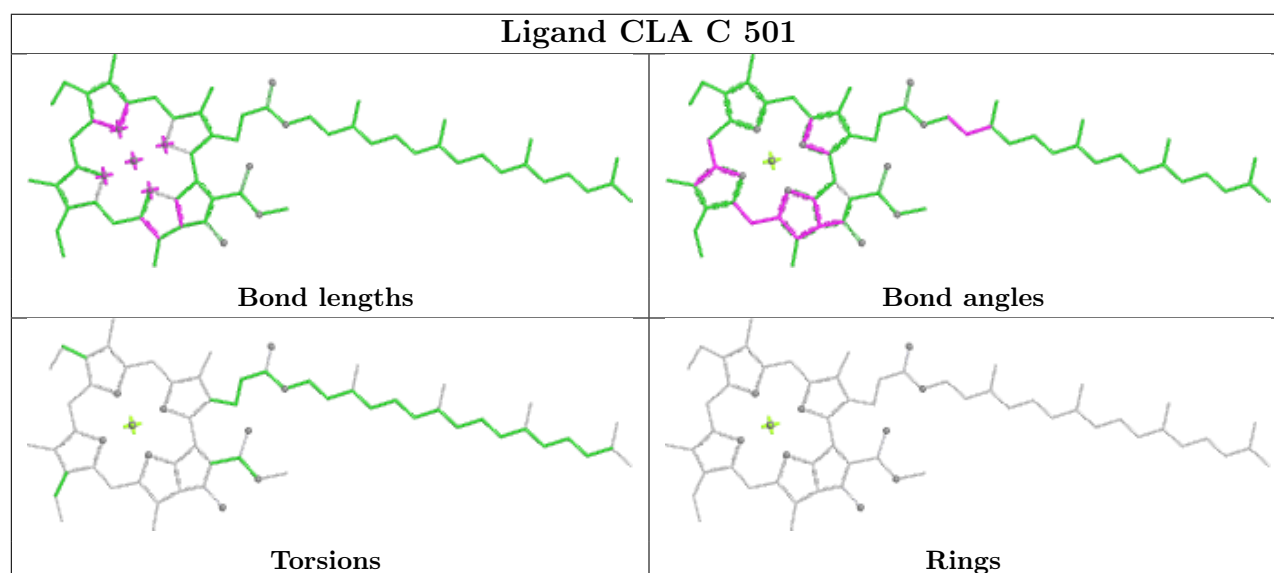
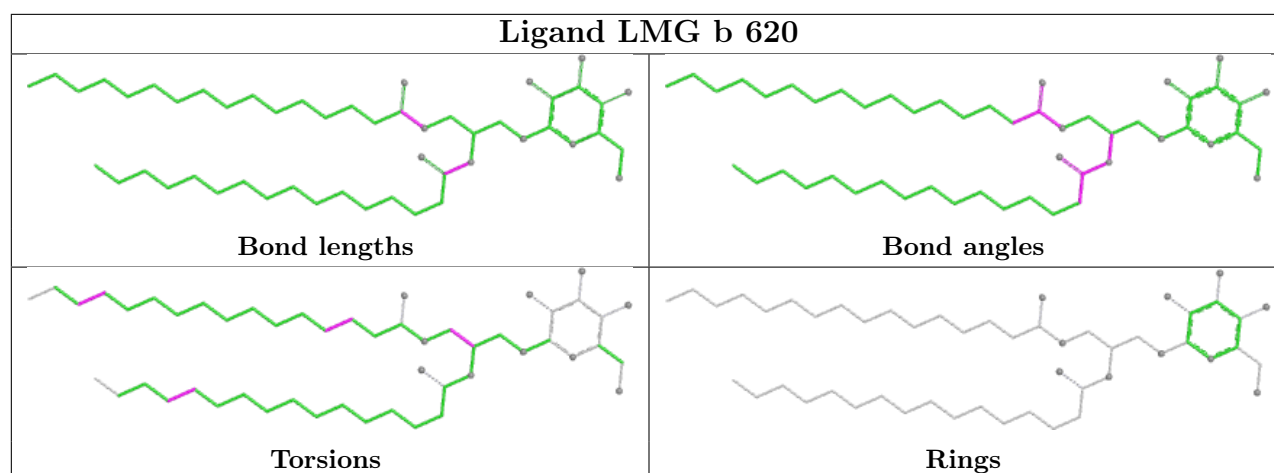
Ligand HEM e 101

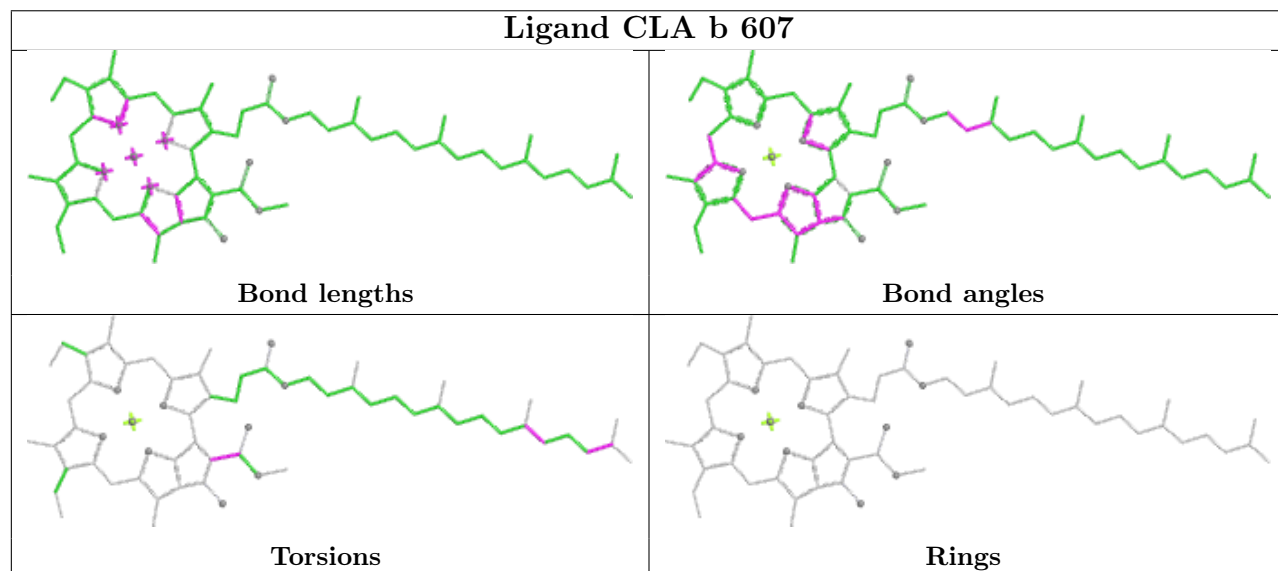
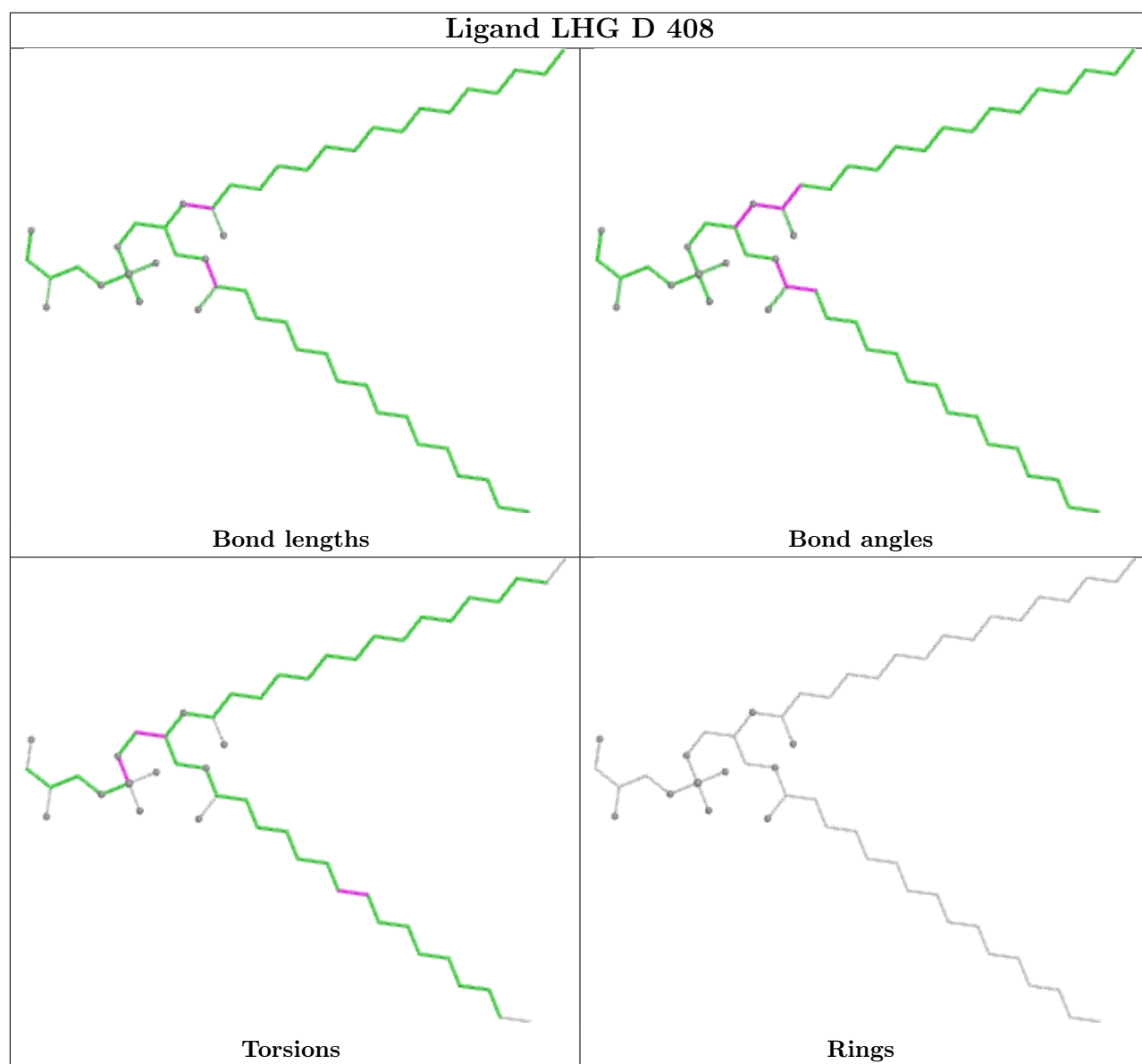


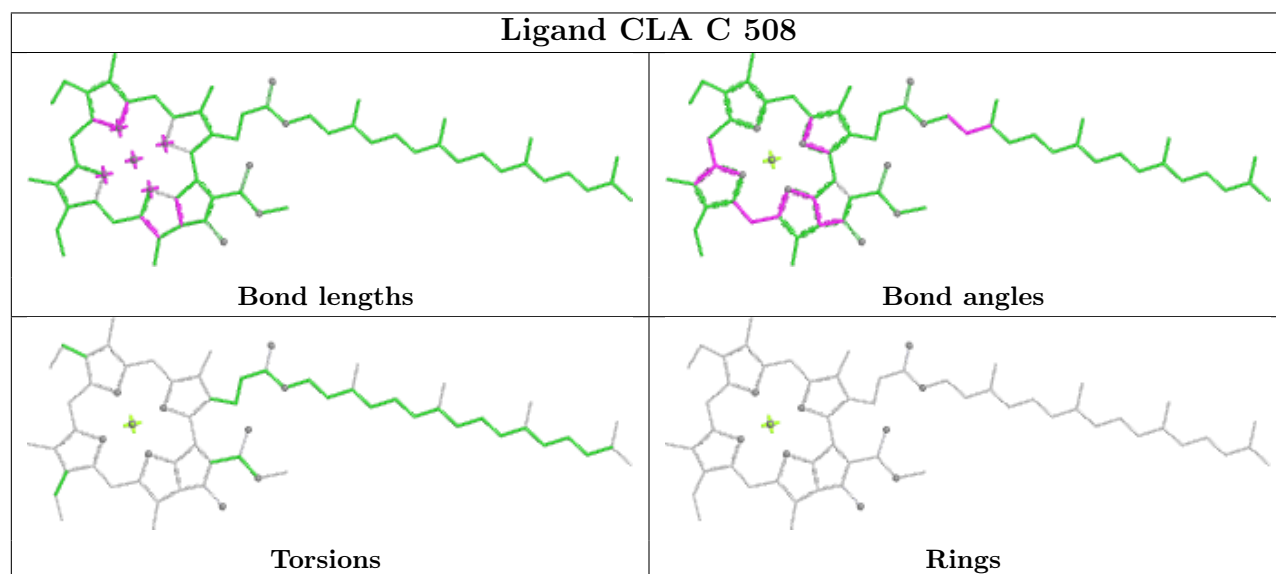
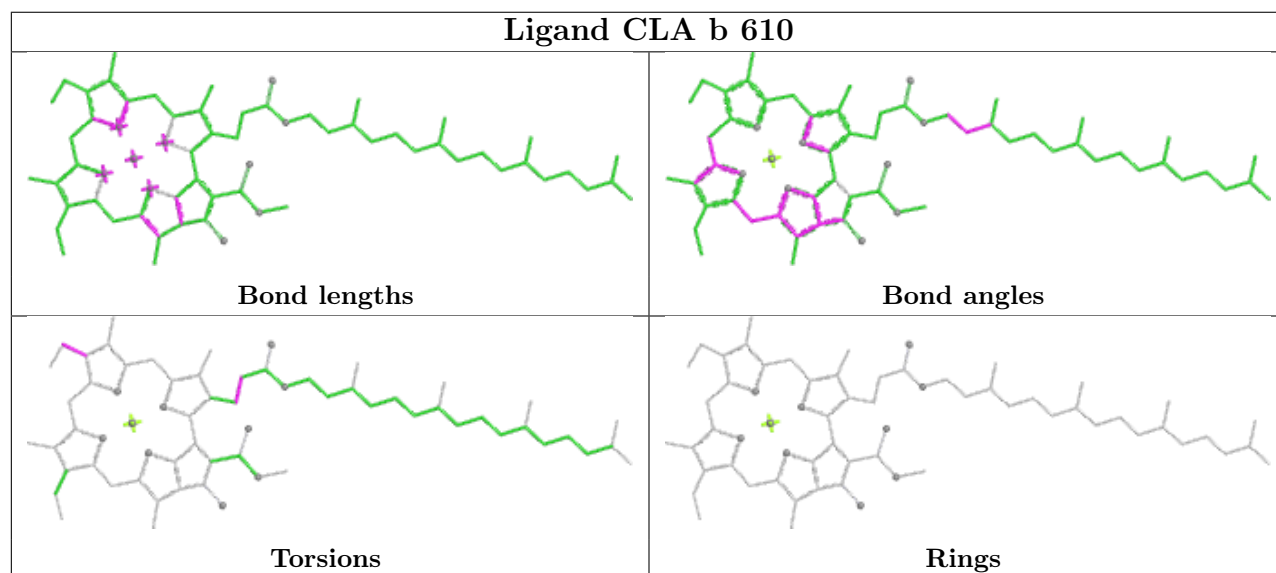
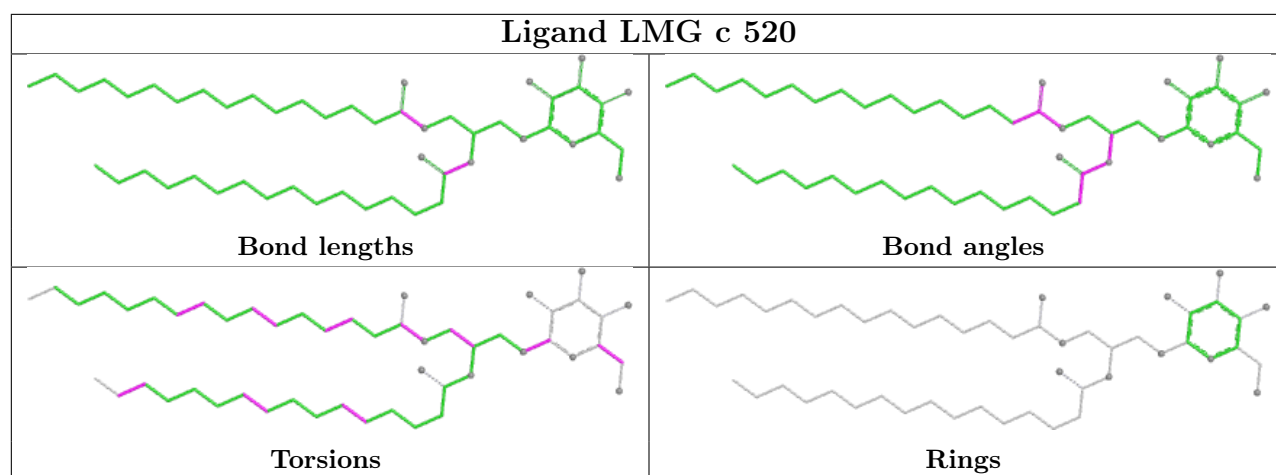
Ligand CLA B 609

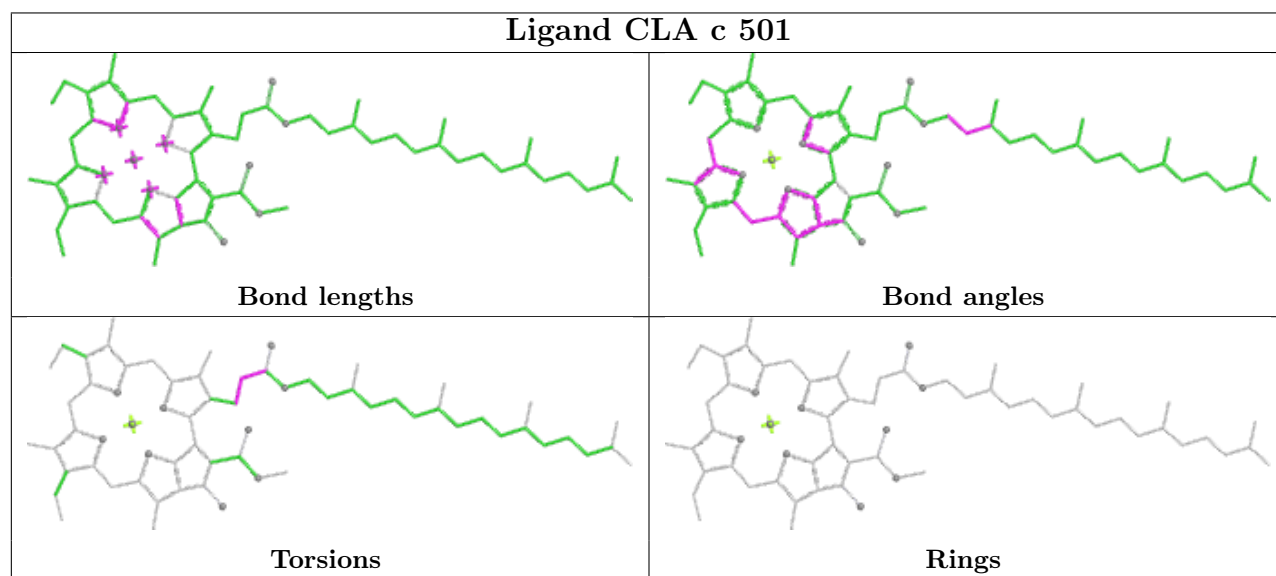
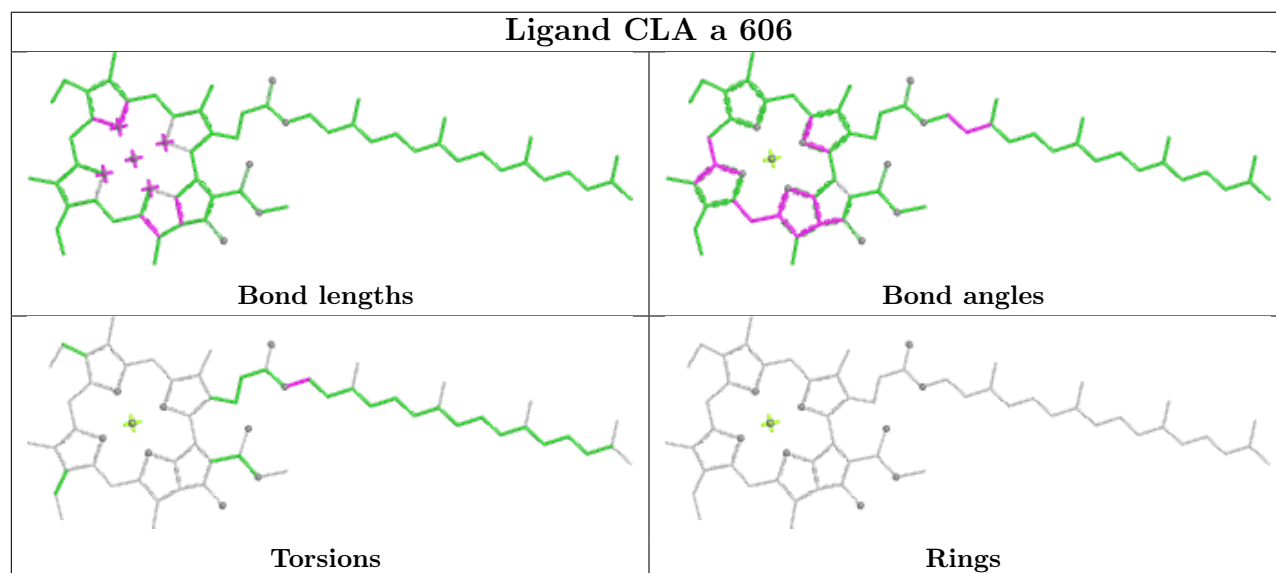
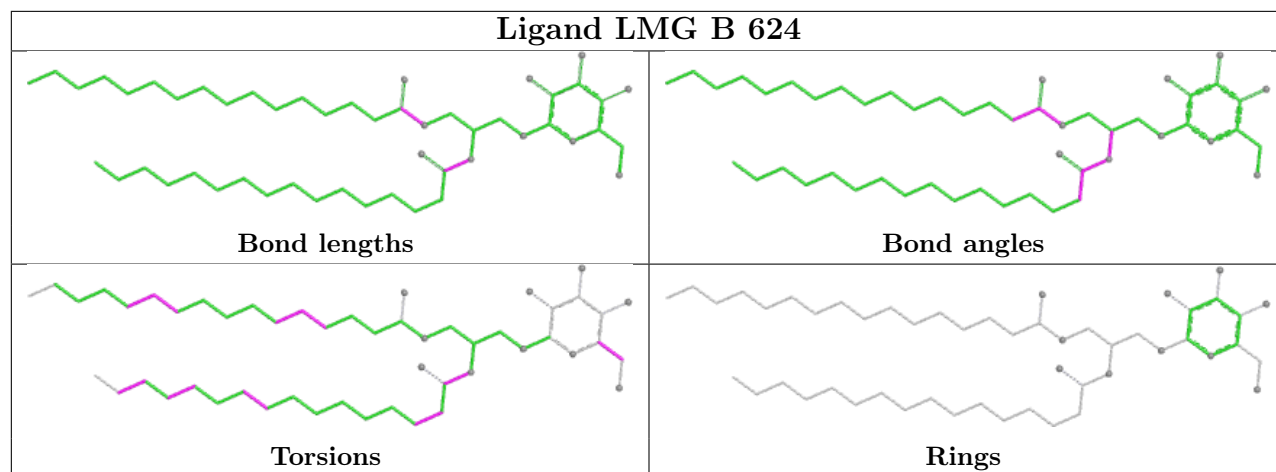


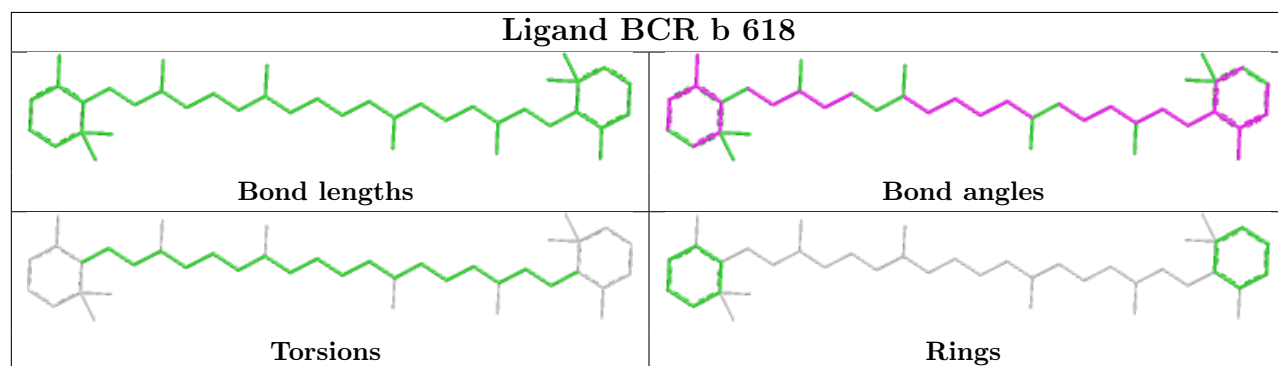
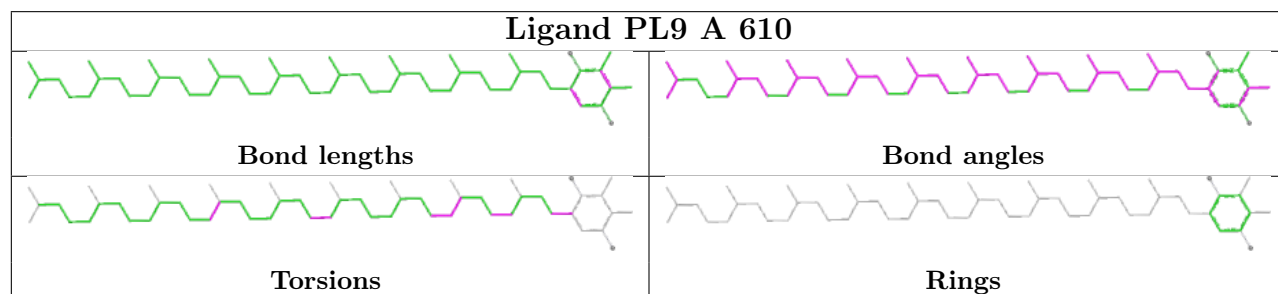
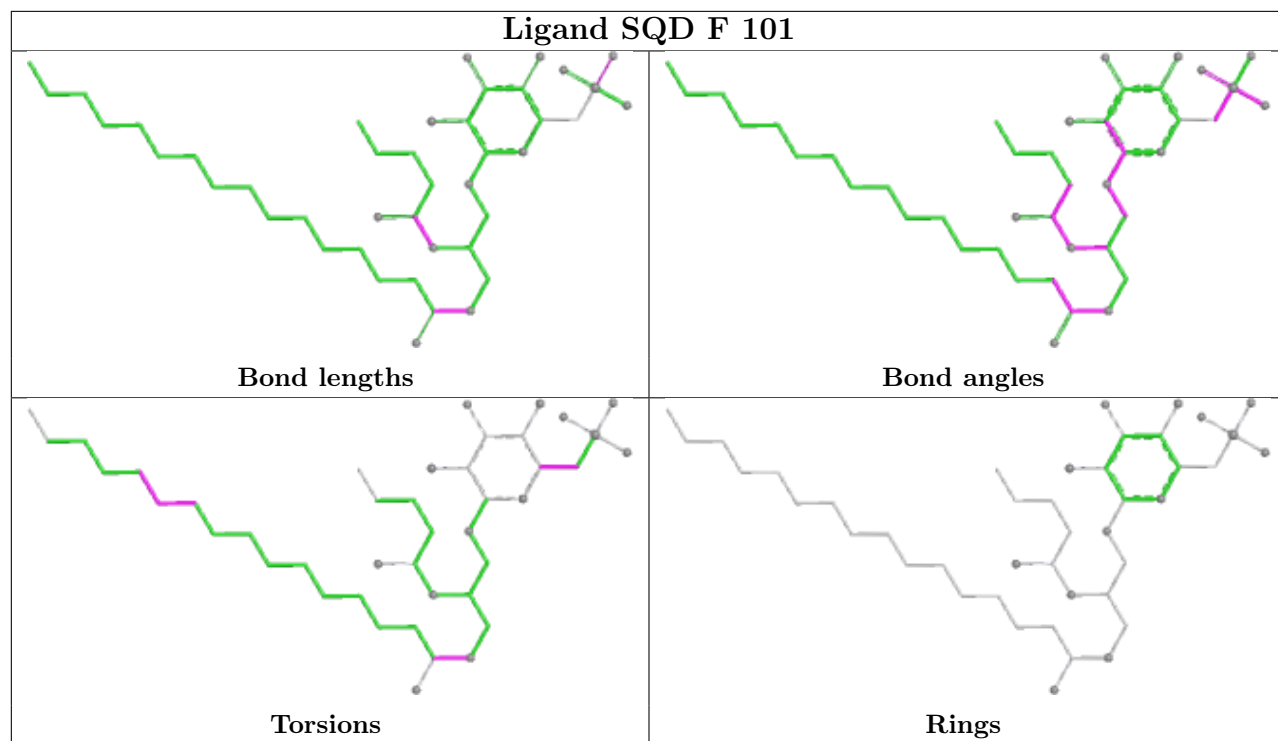


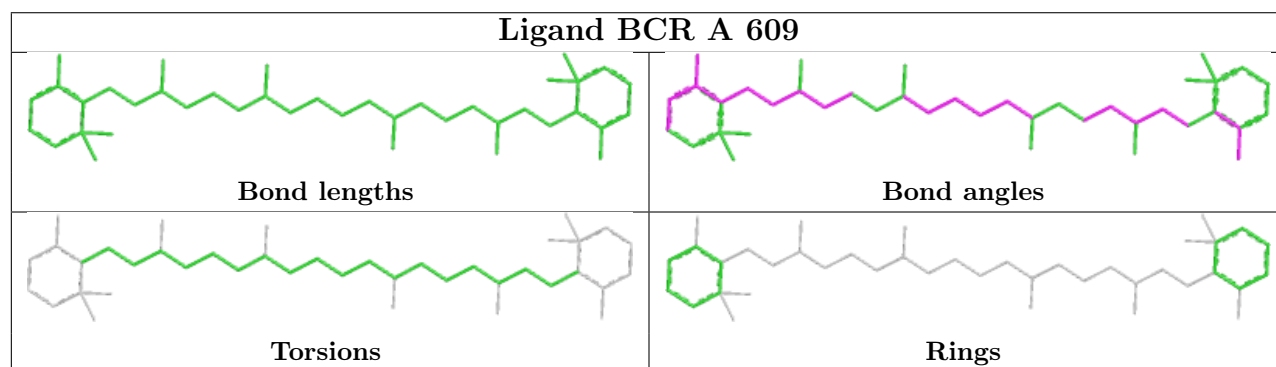
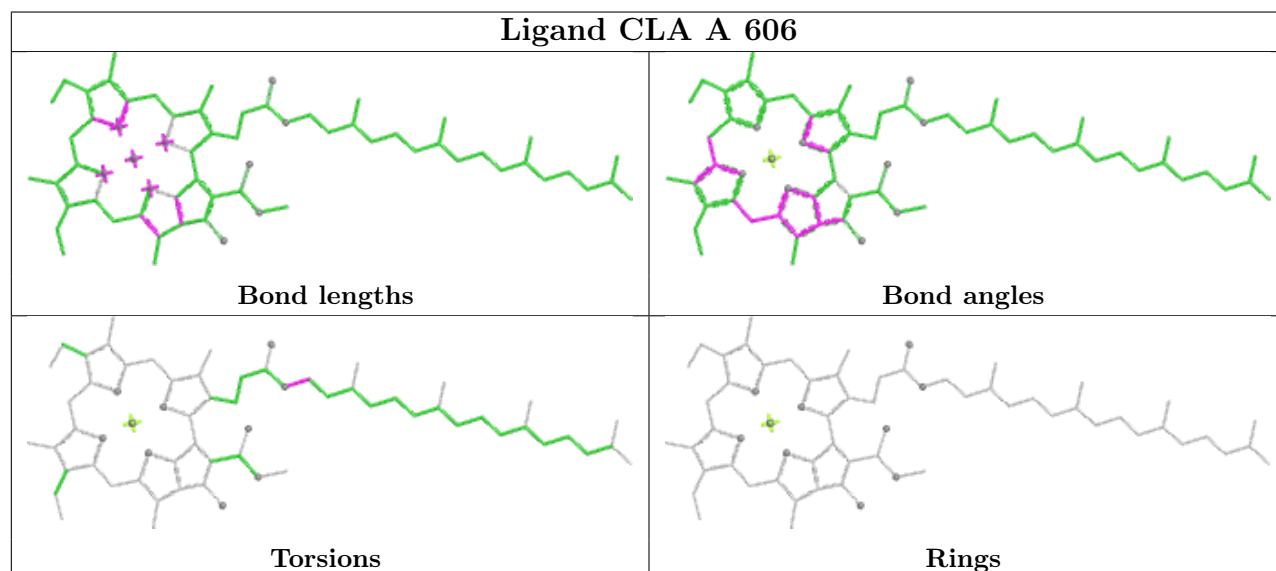
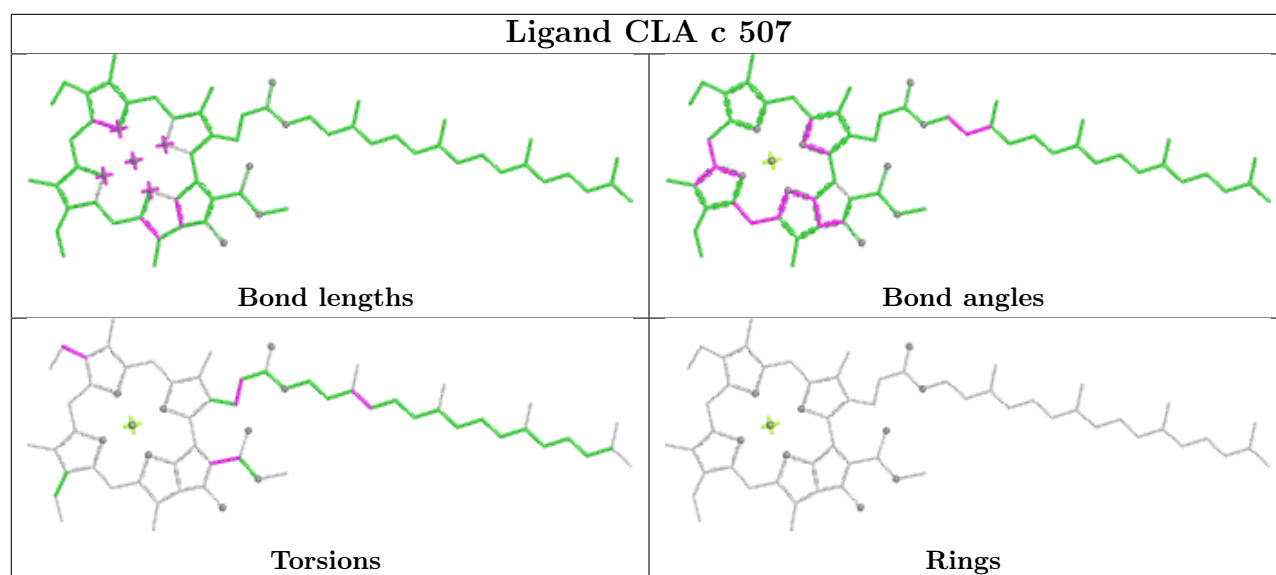


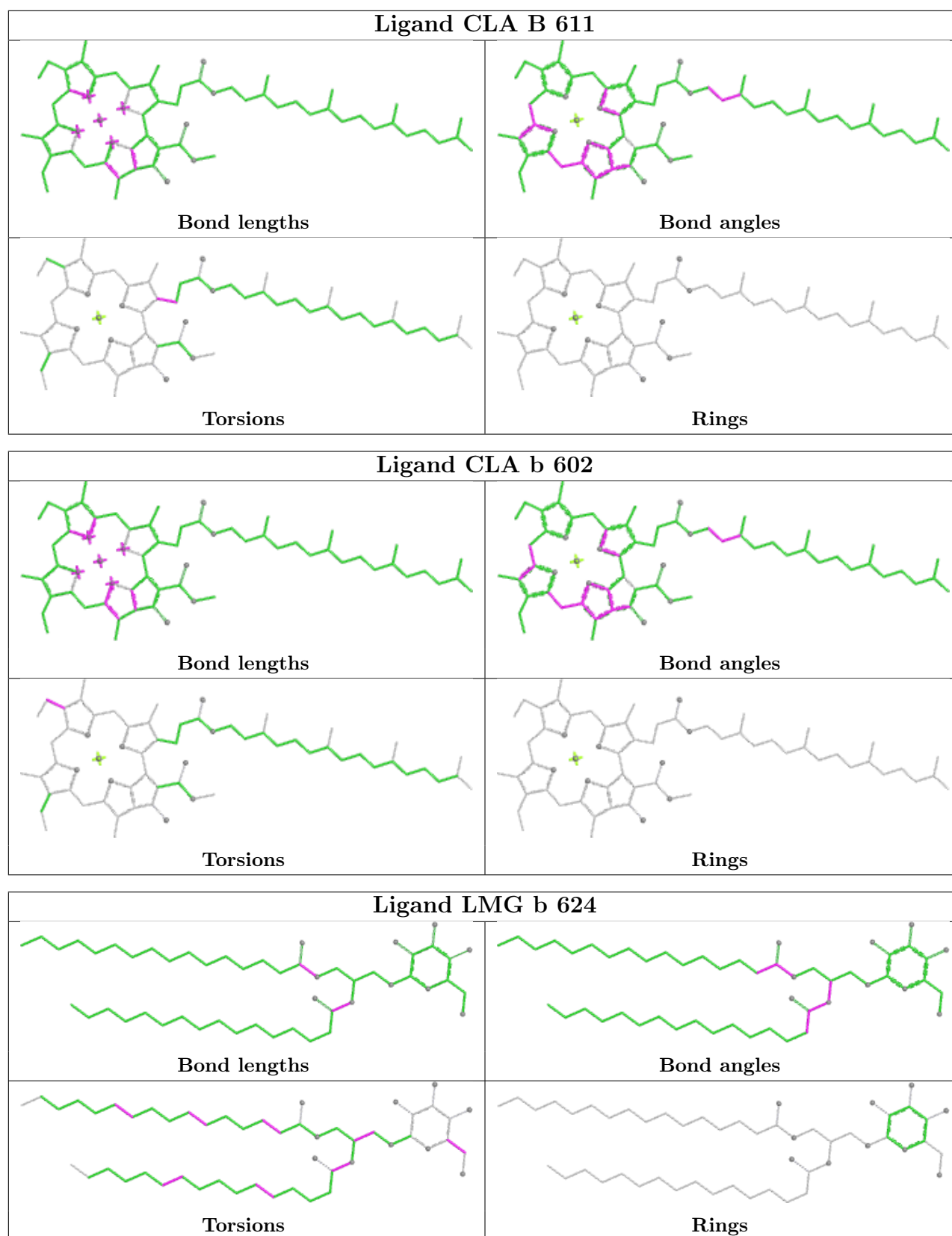


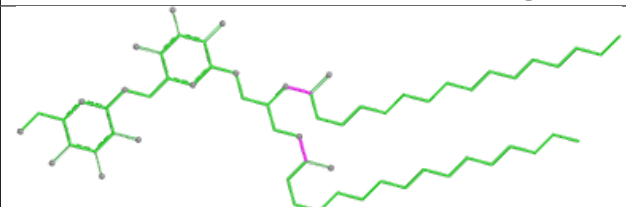
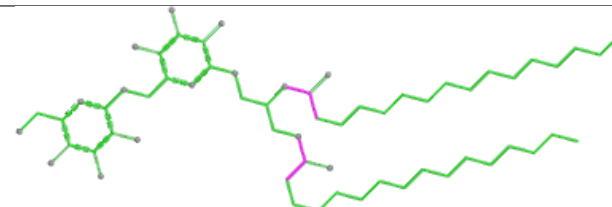
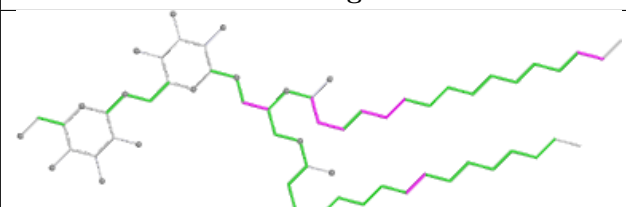
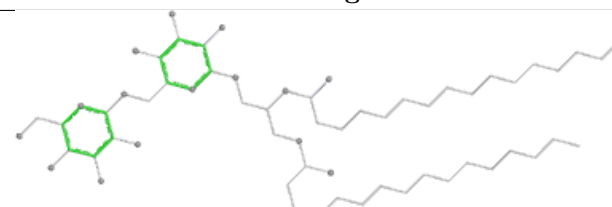


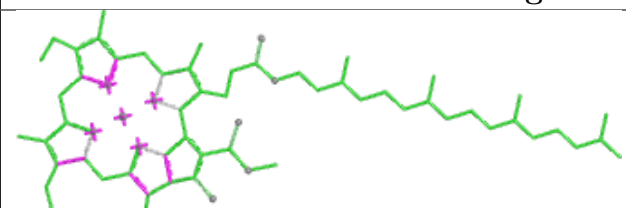
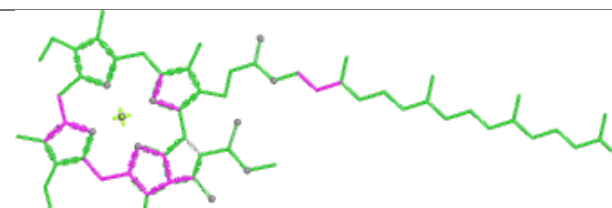
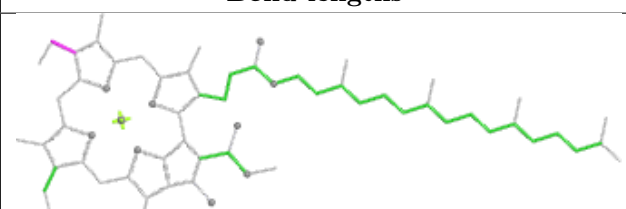
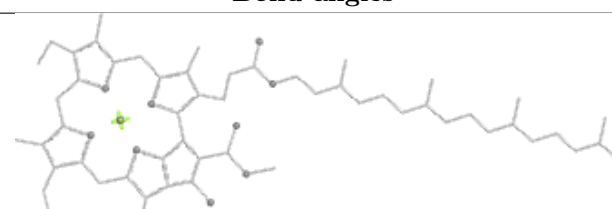


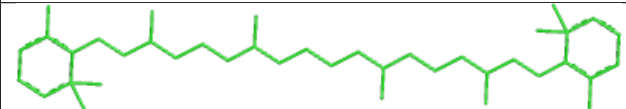
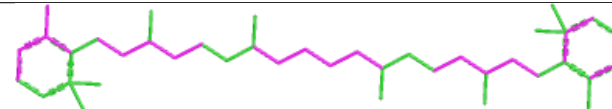
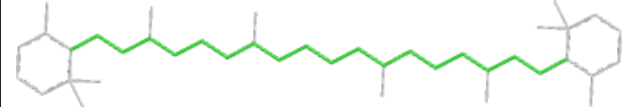
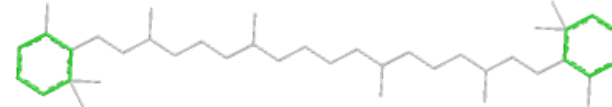


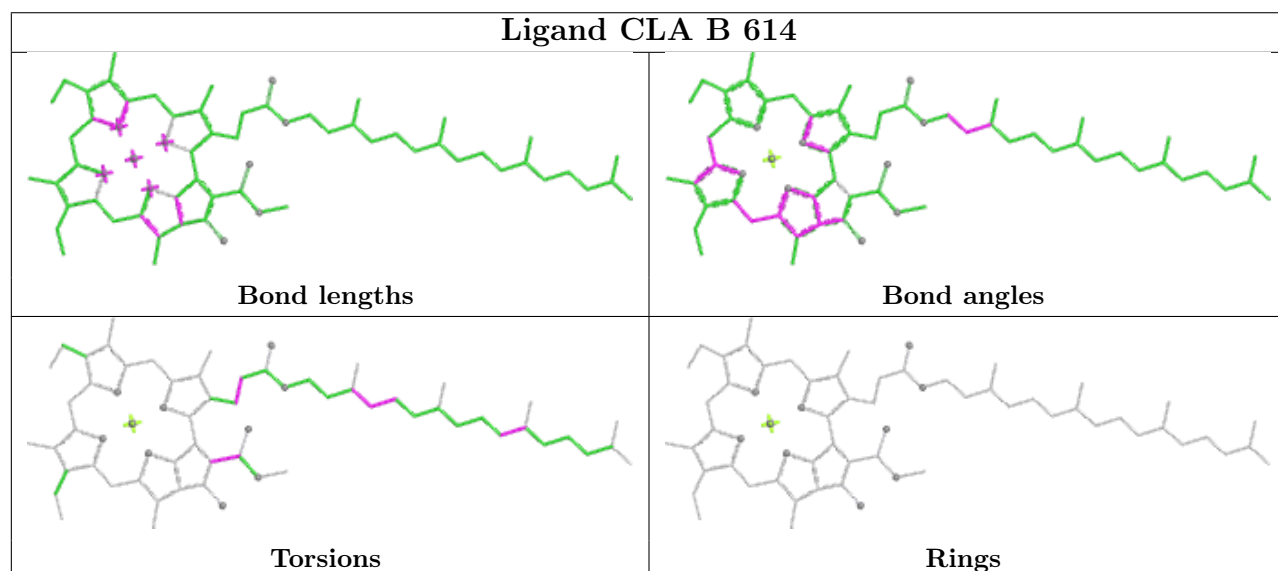
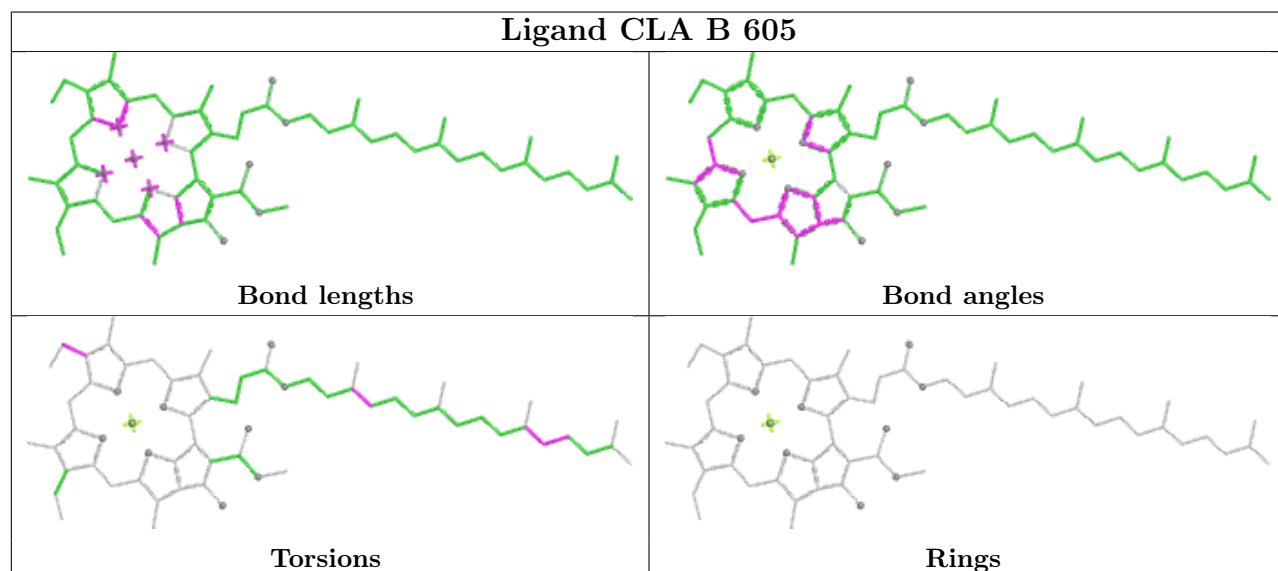
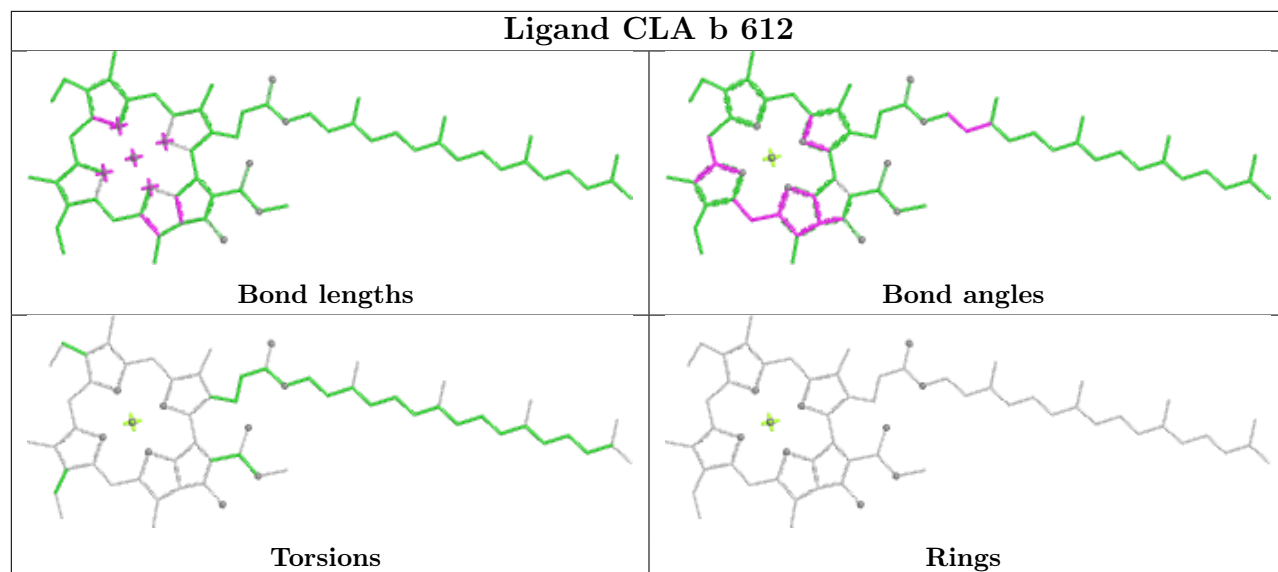


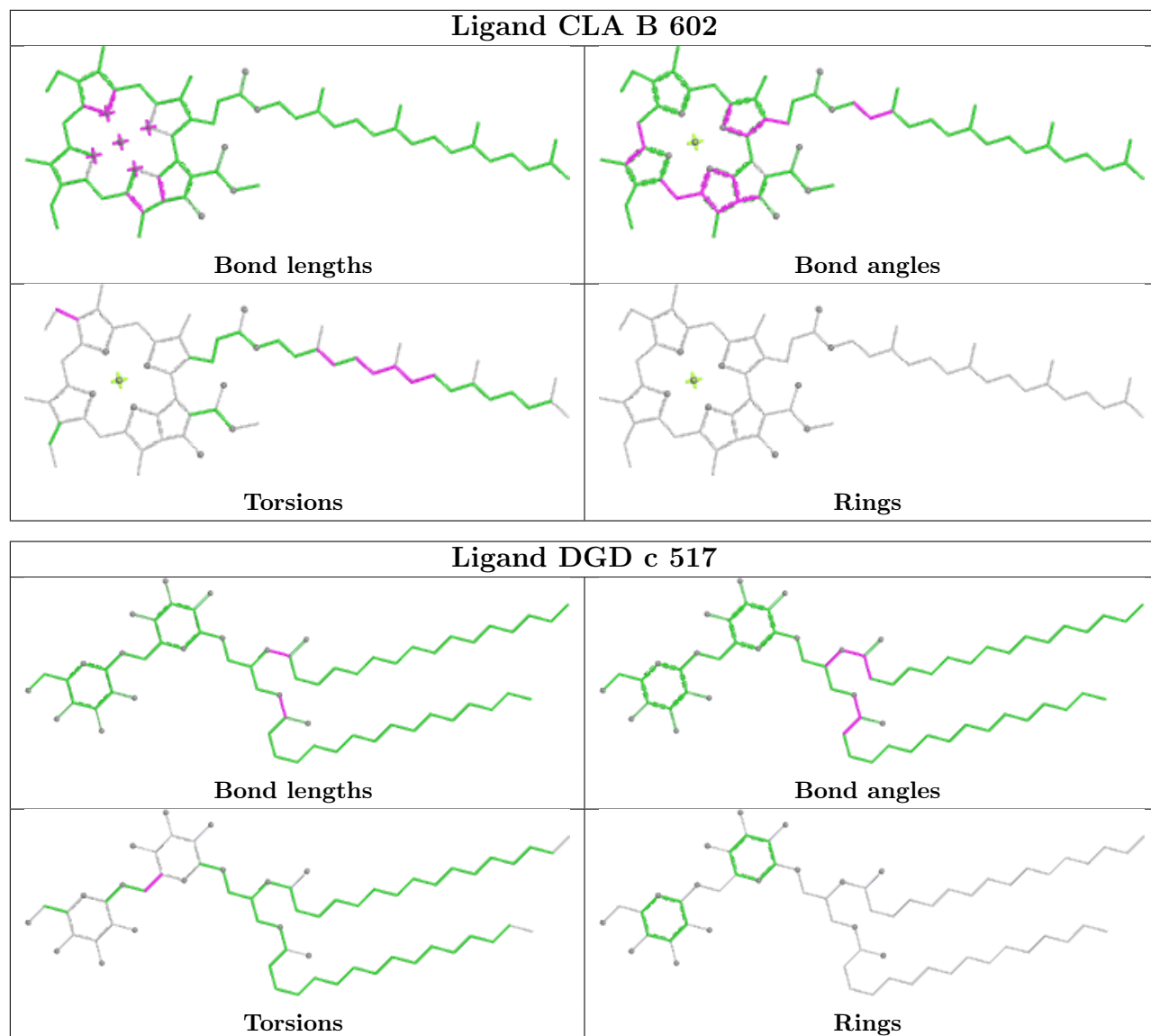


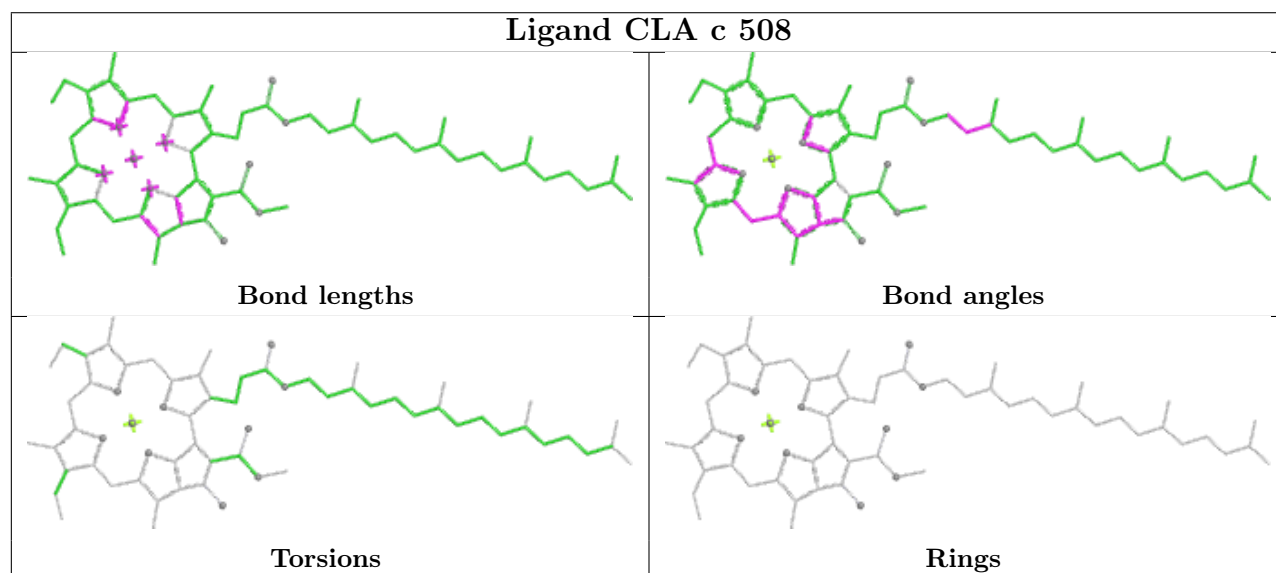
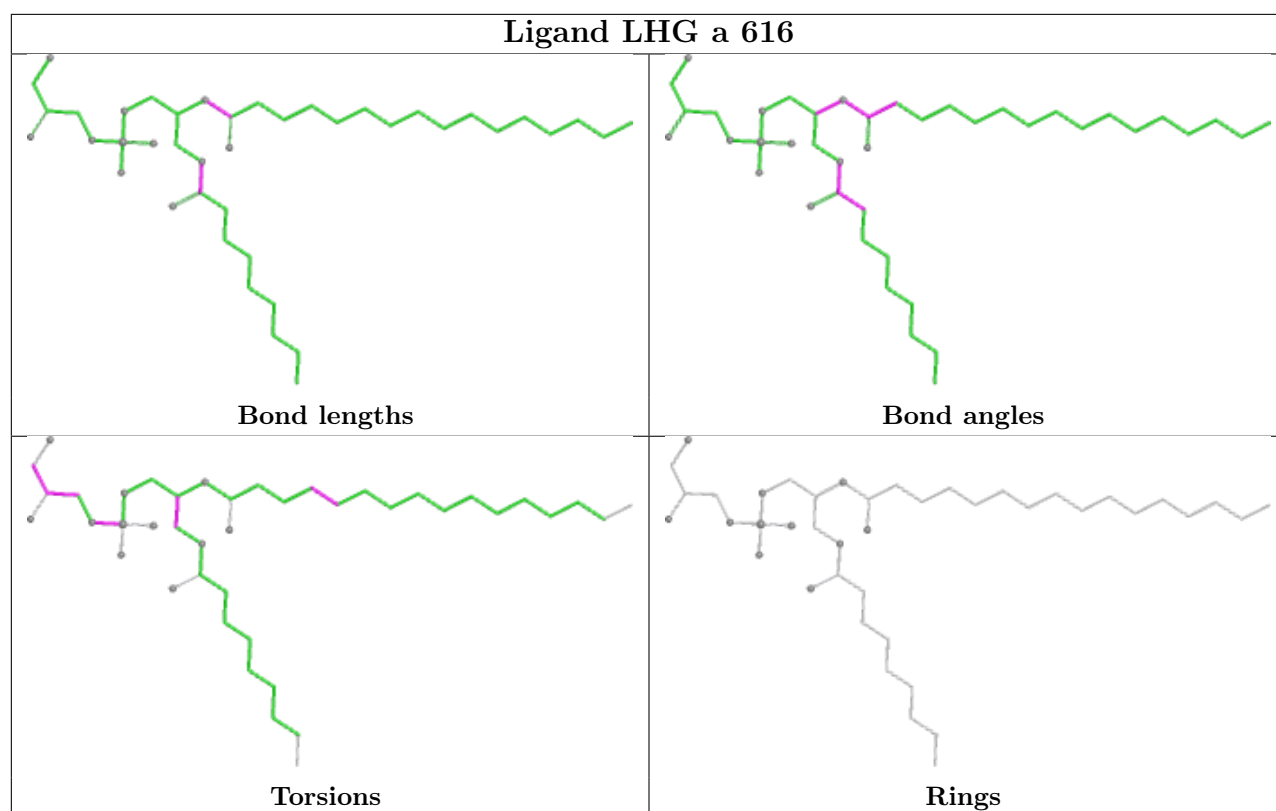
Ligand DGD h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

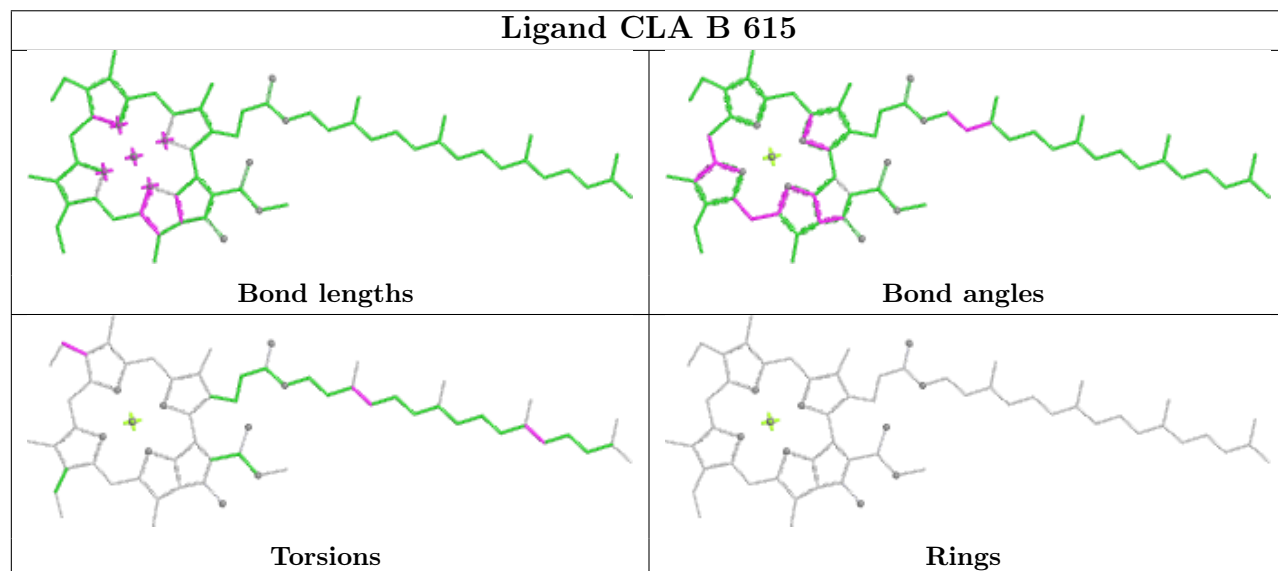
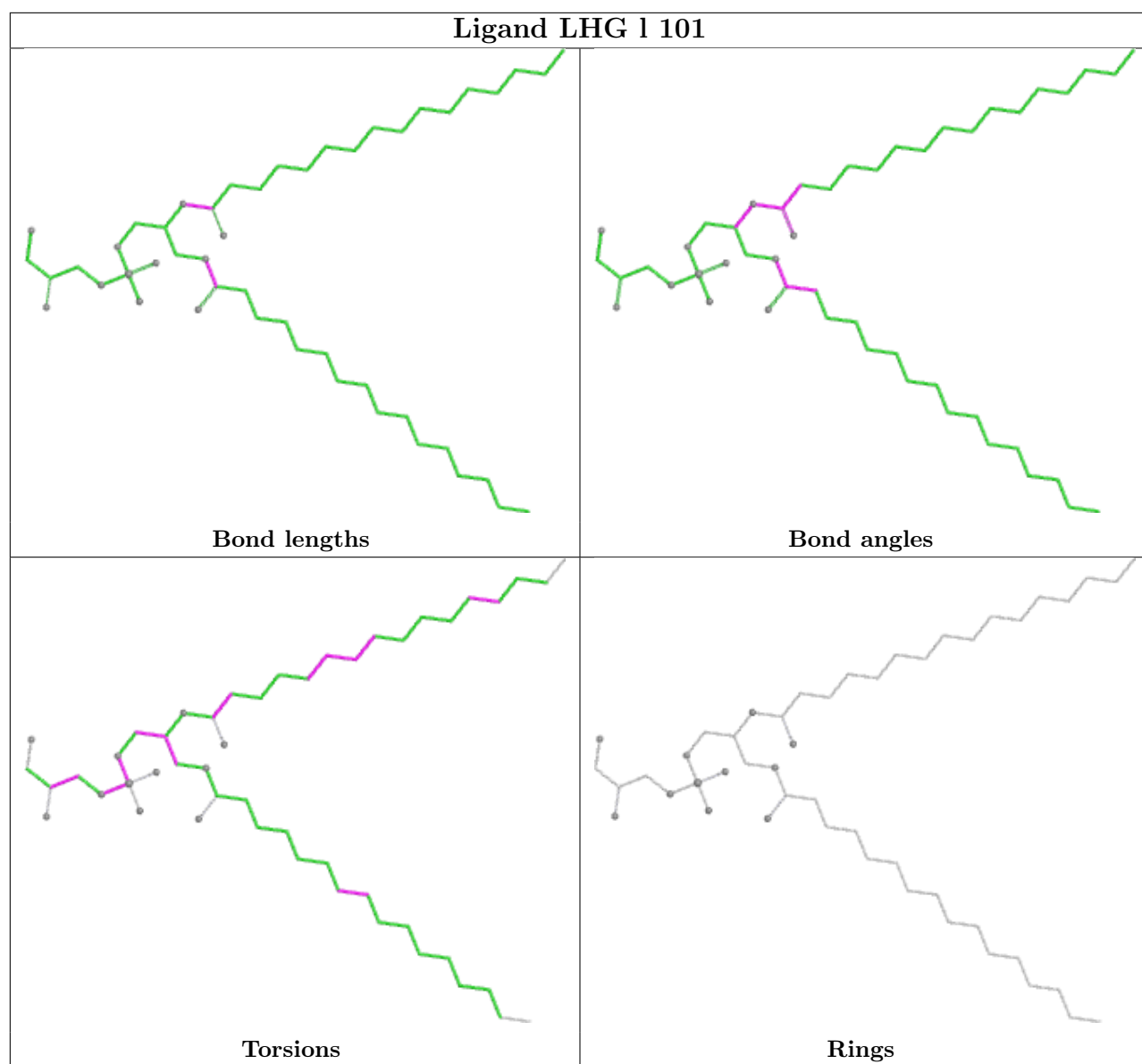
Ligand CLA a 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

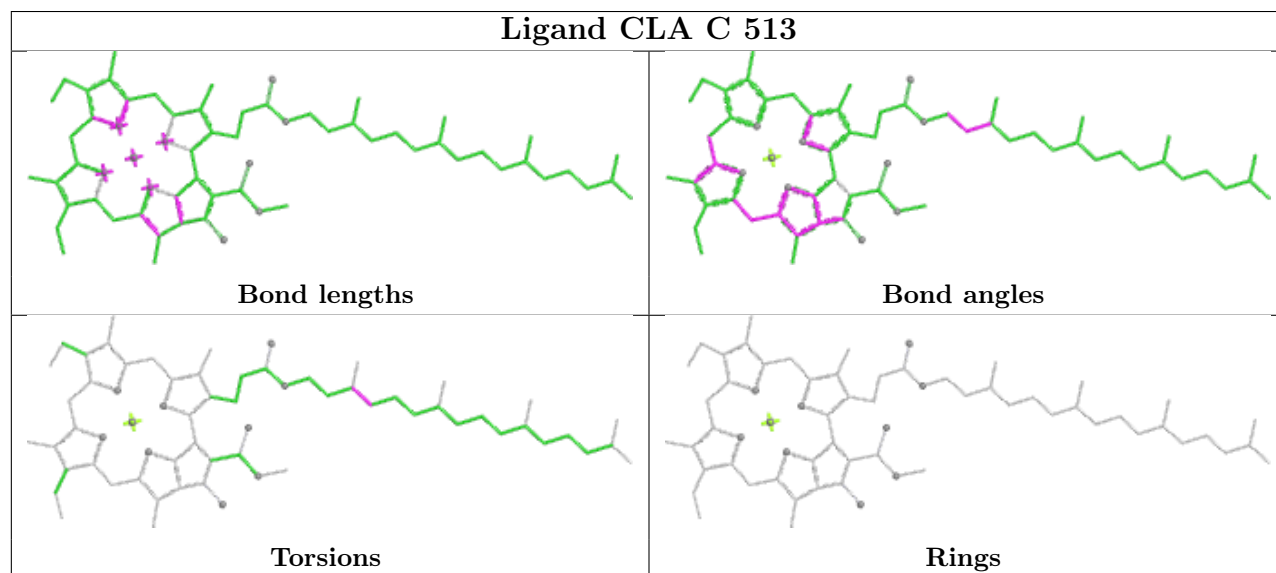
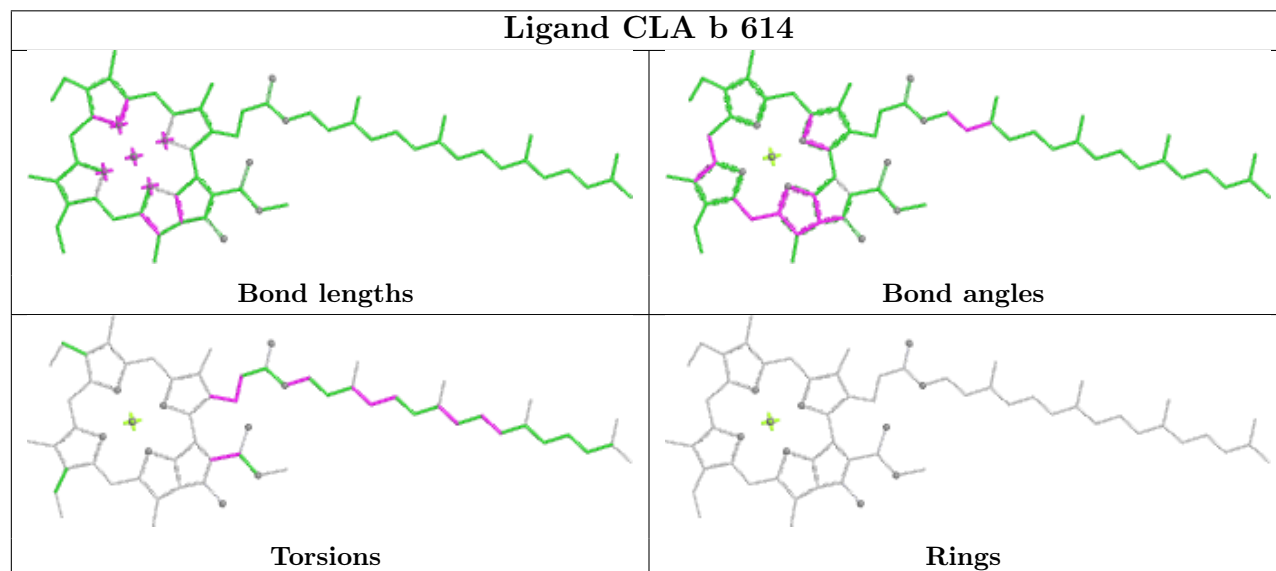
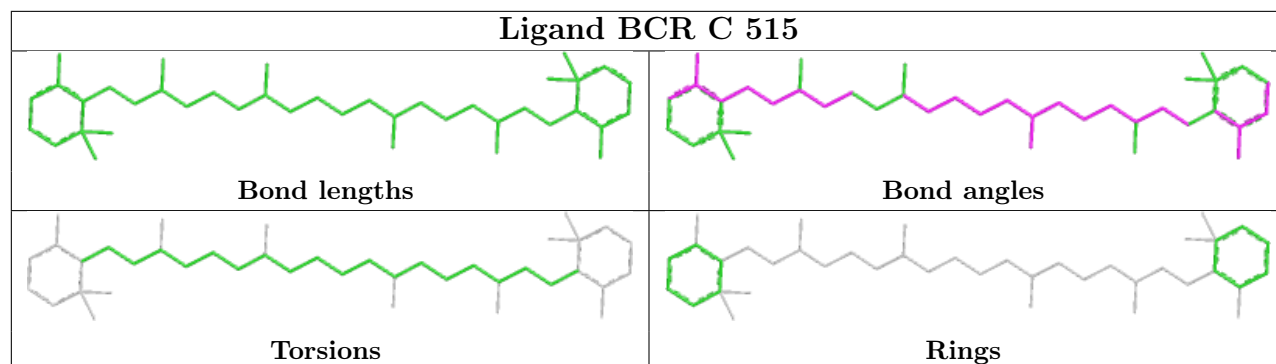
Ligand BCR c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

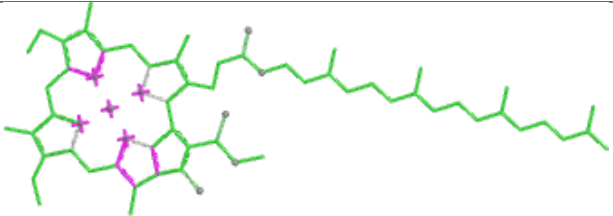
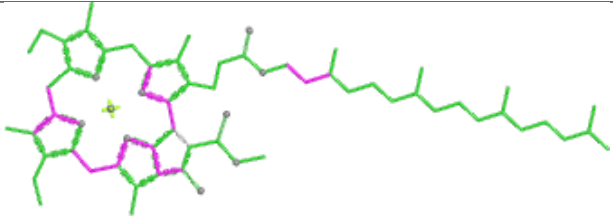
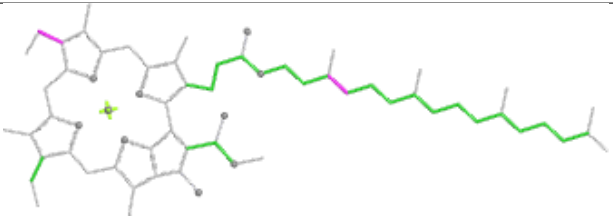
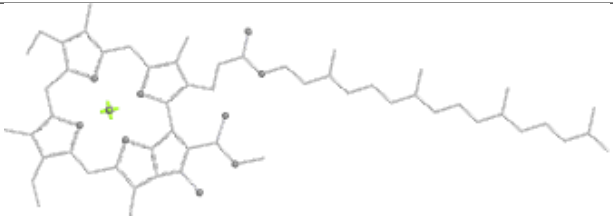
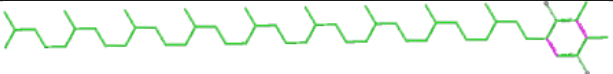
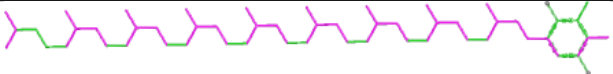
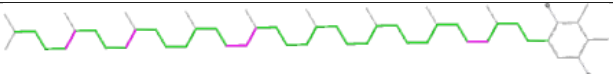
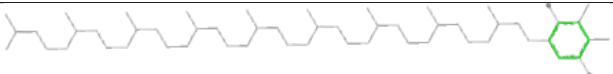
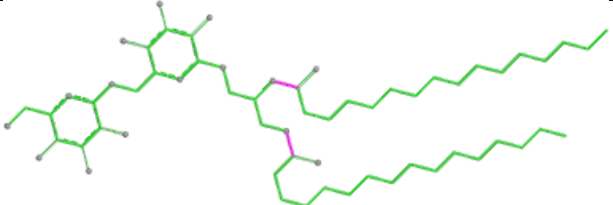
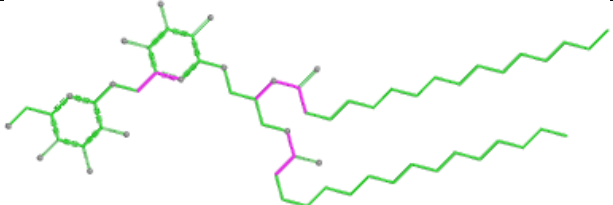
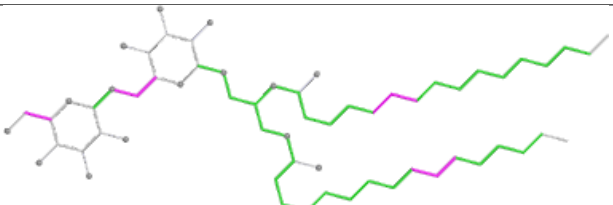
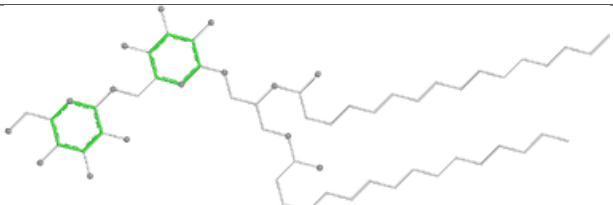


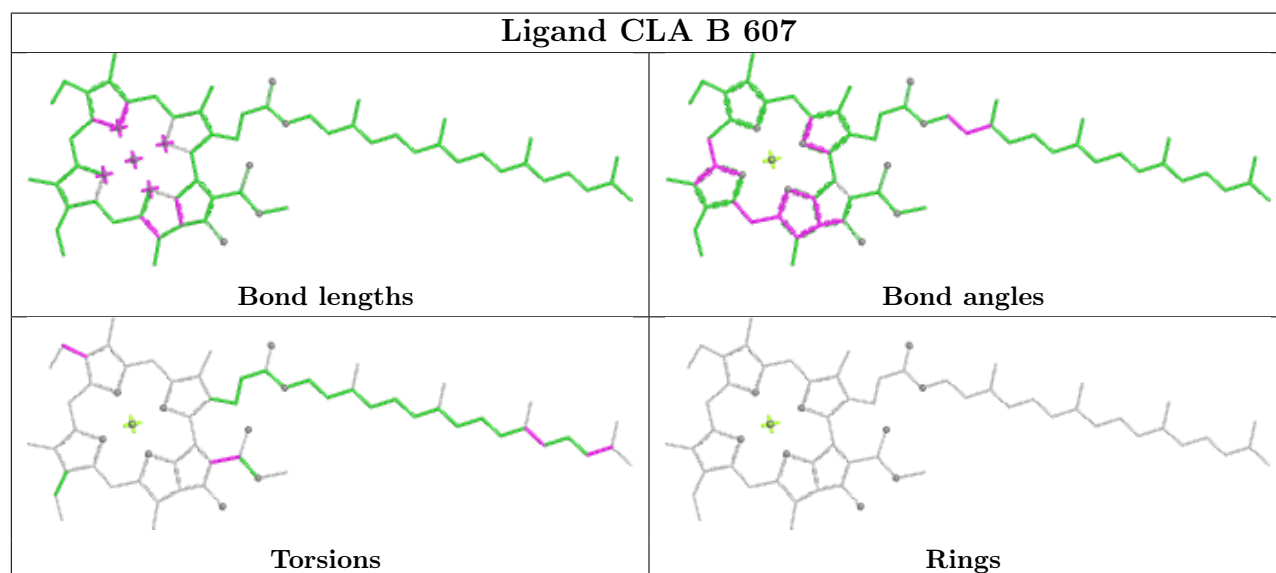
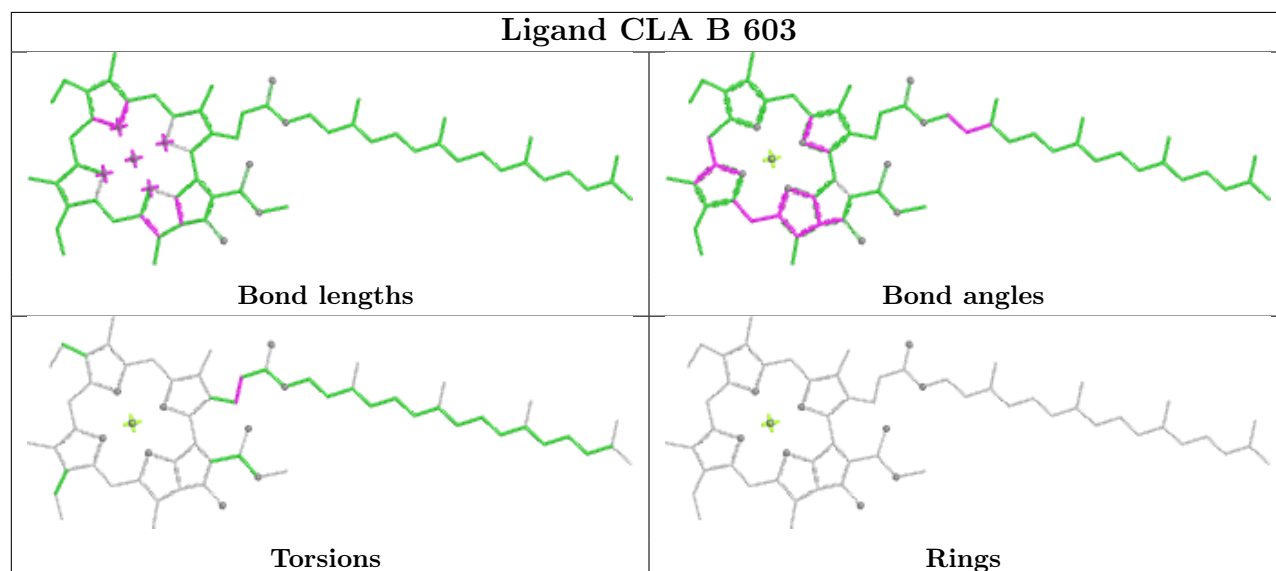
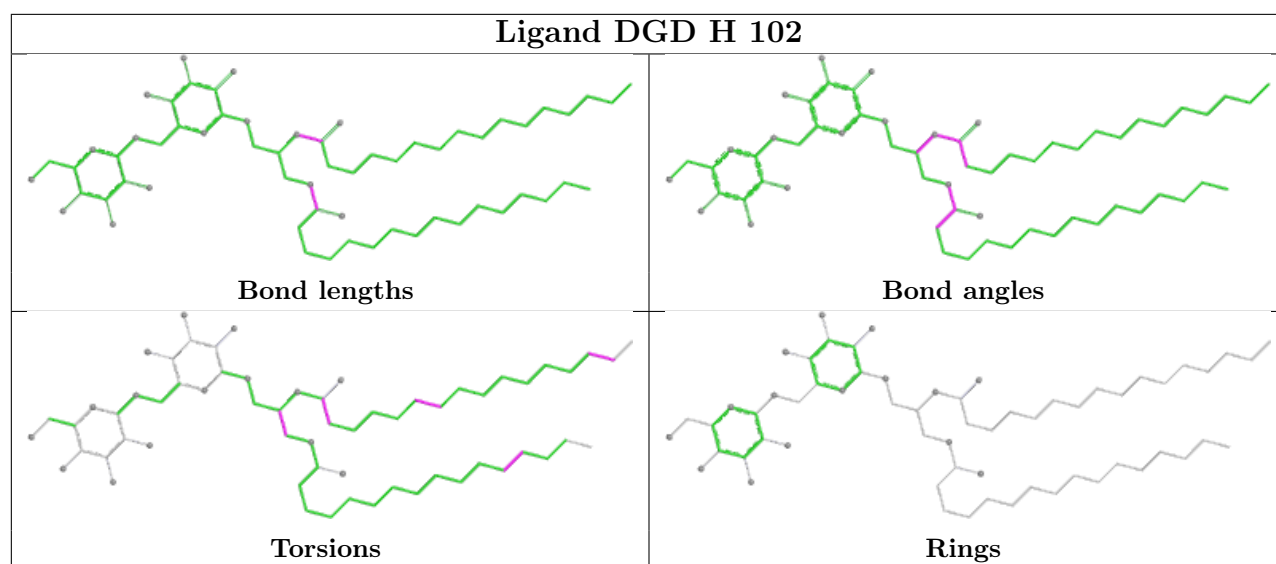


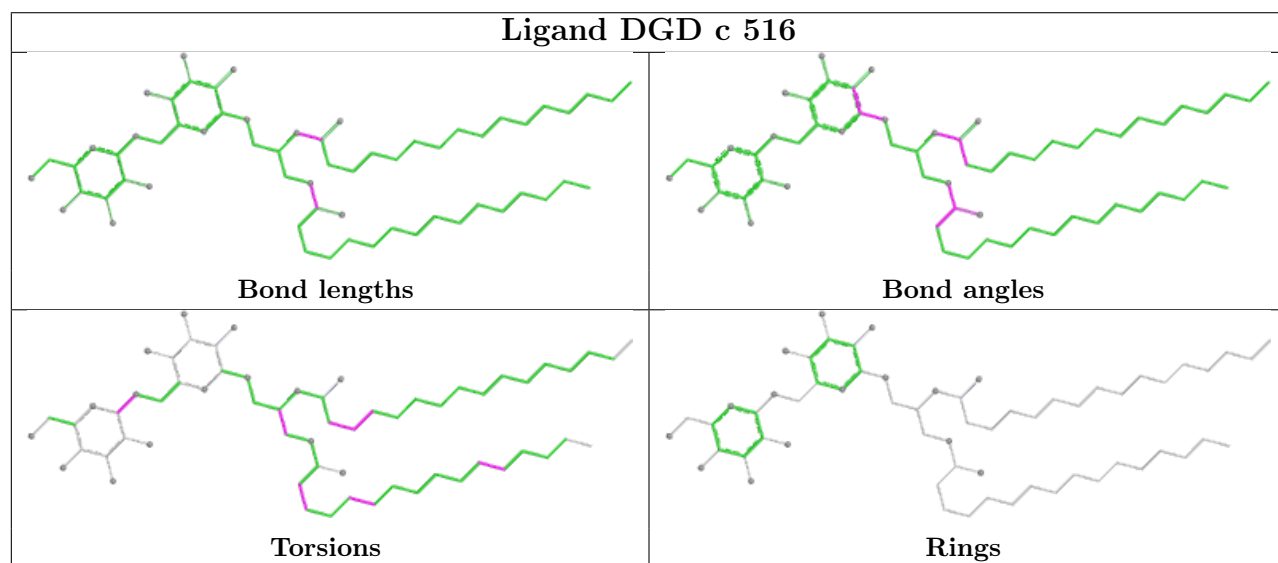
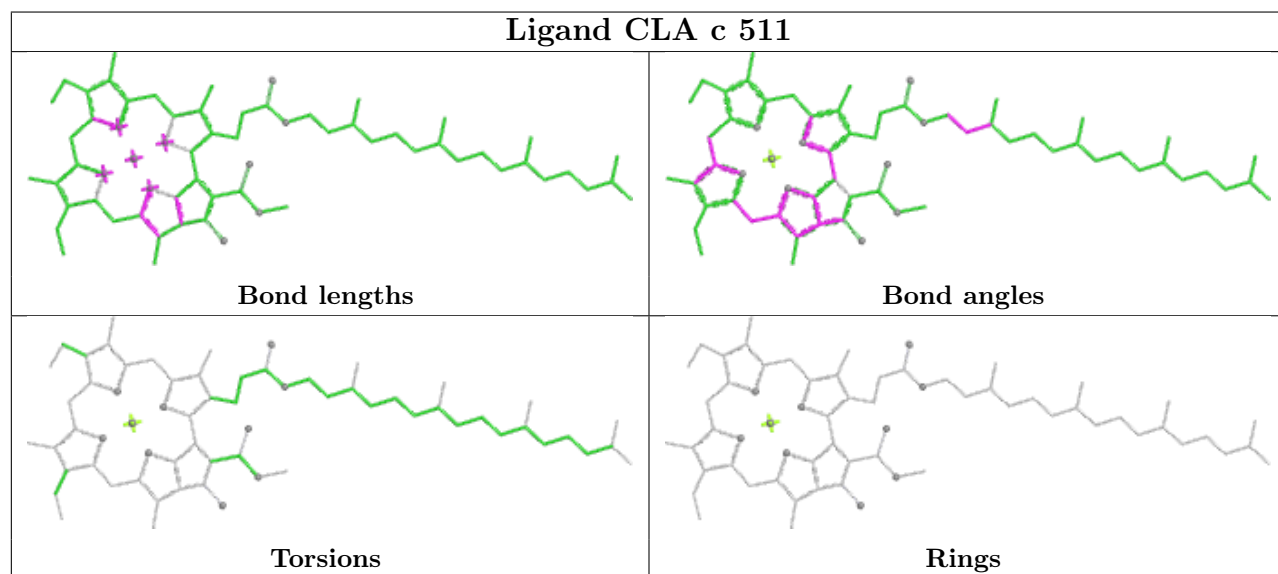
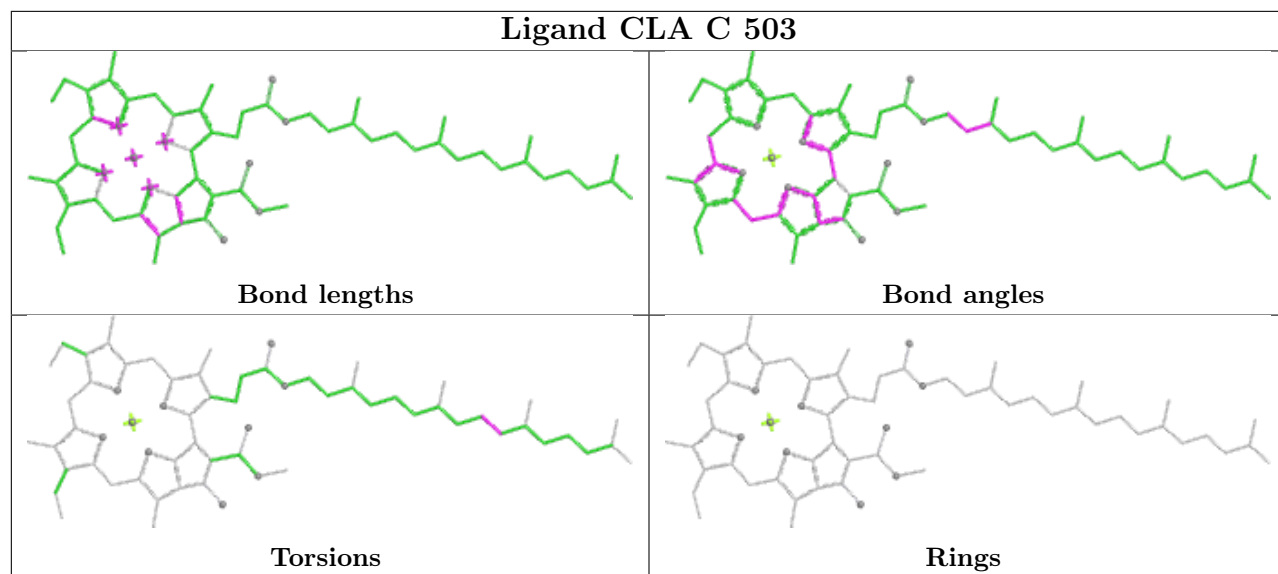


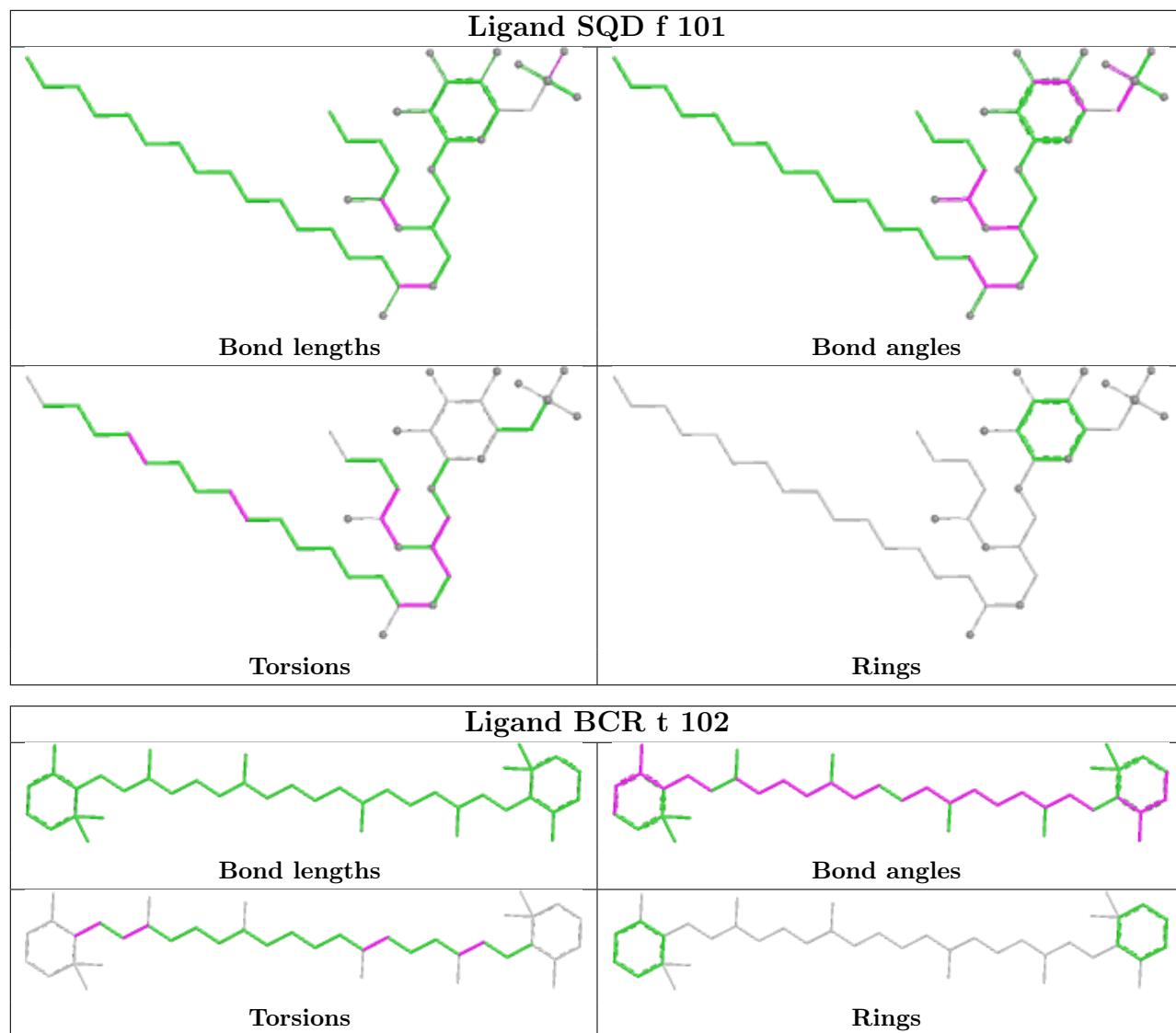


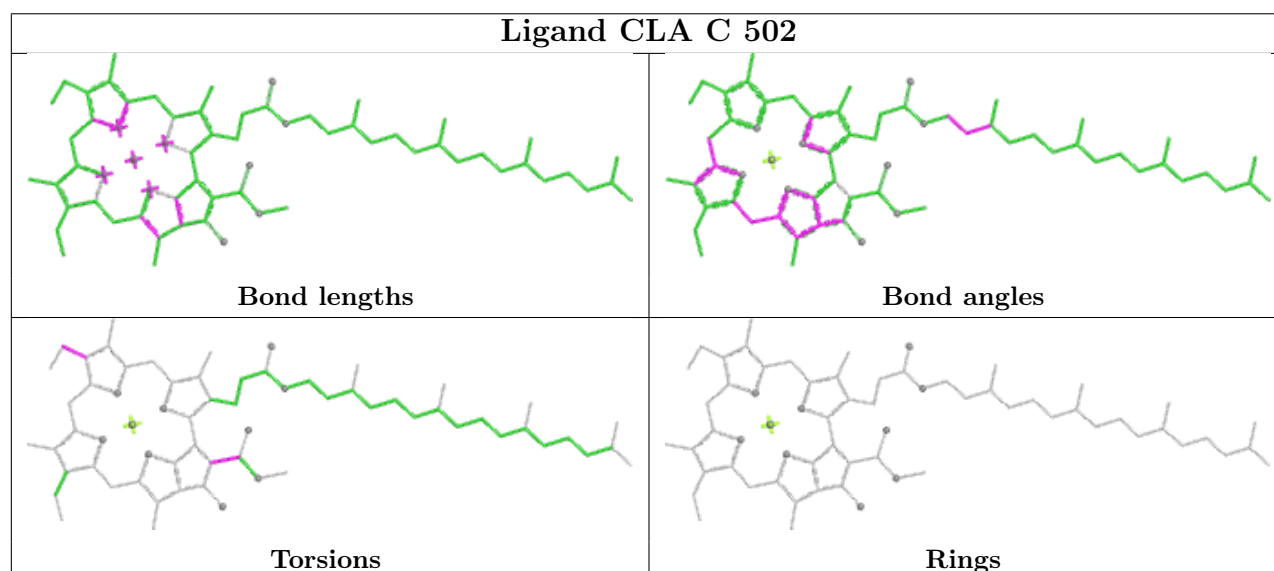
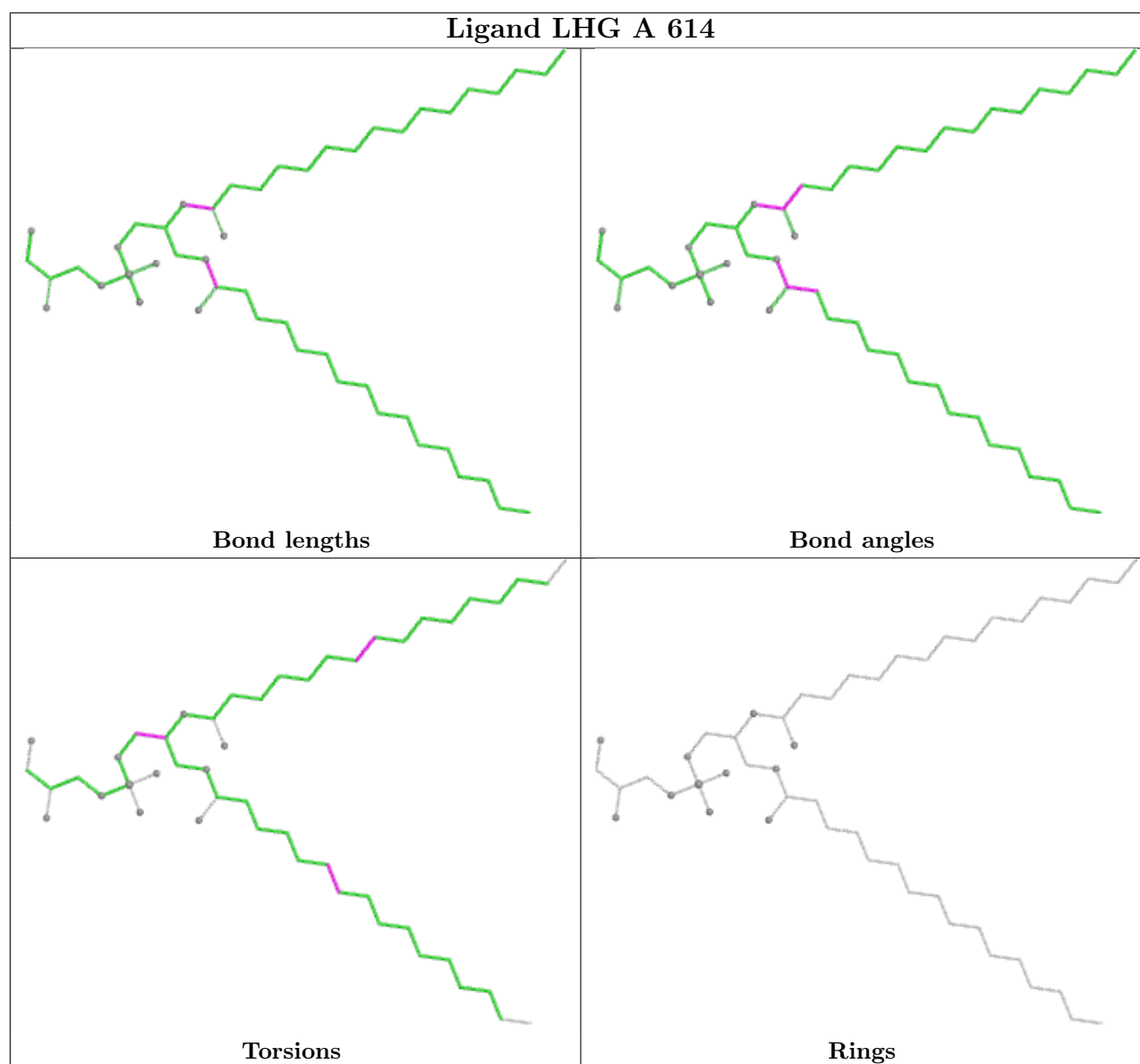


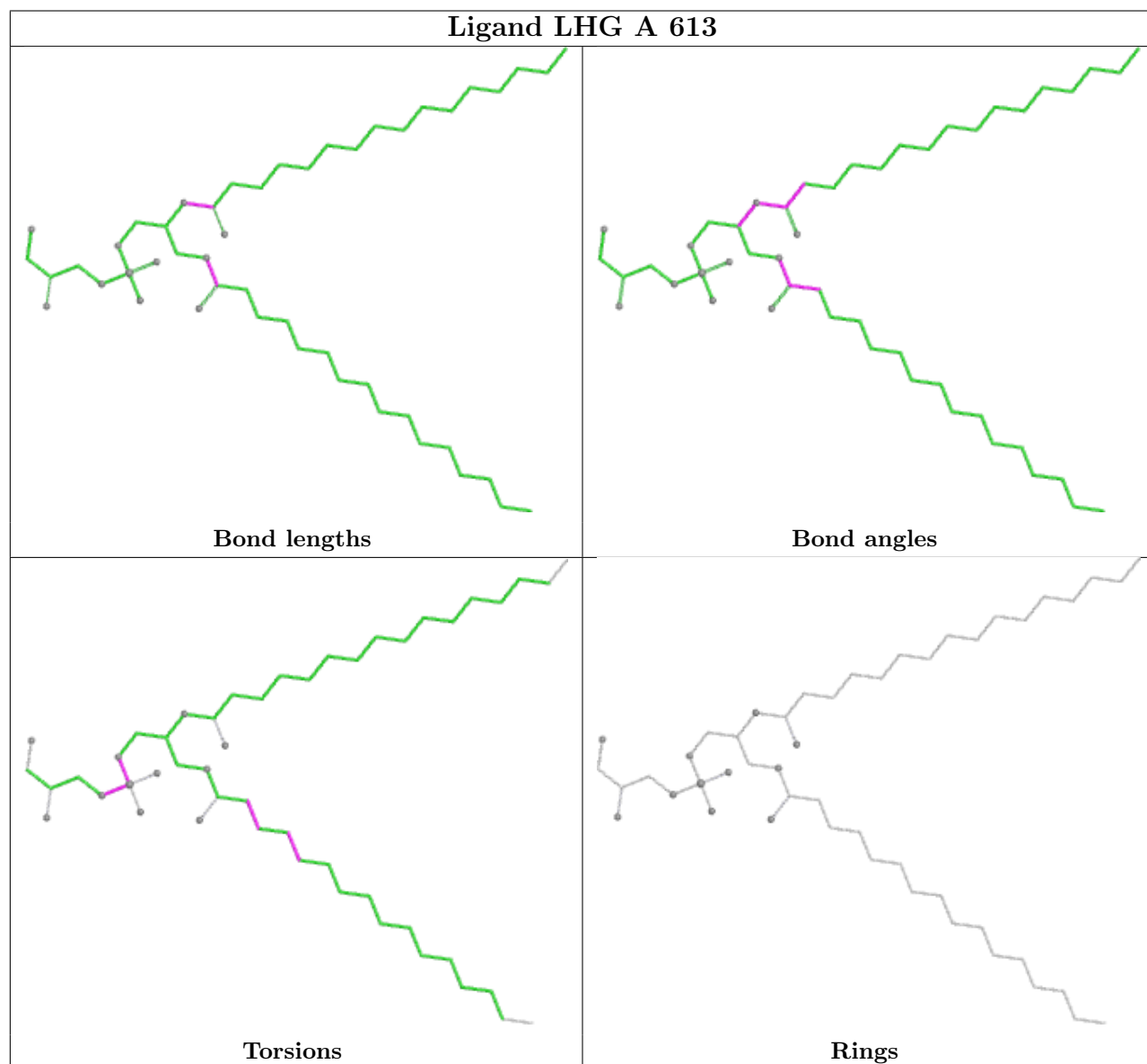
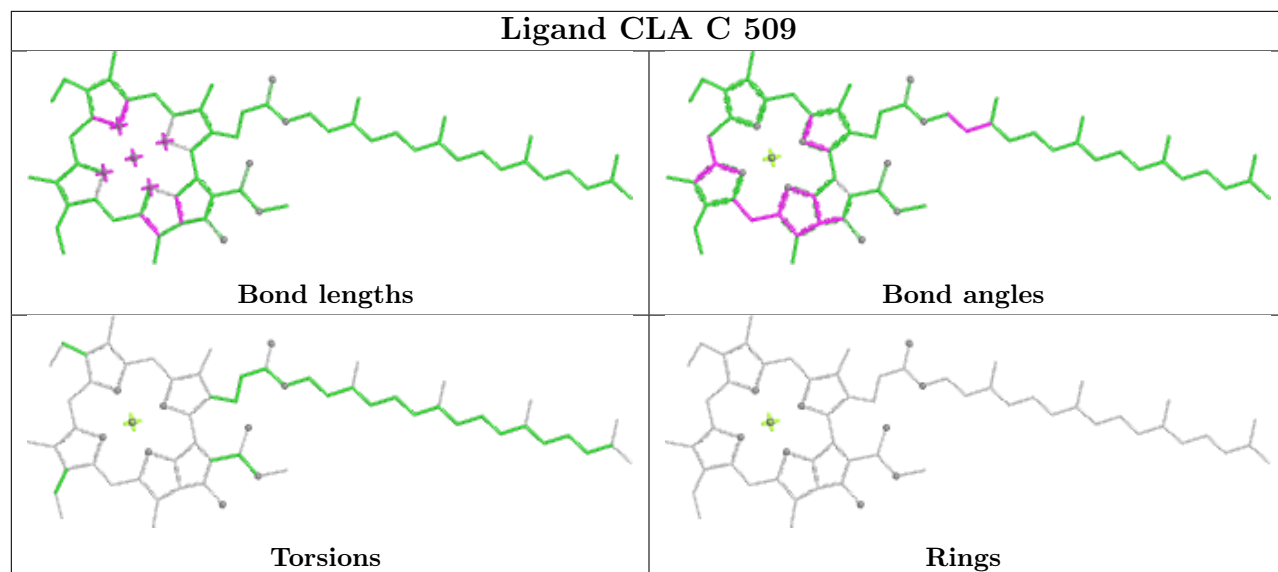
Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

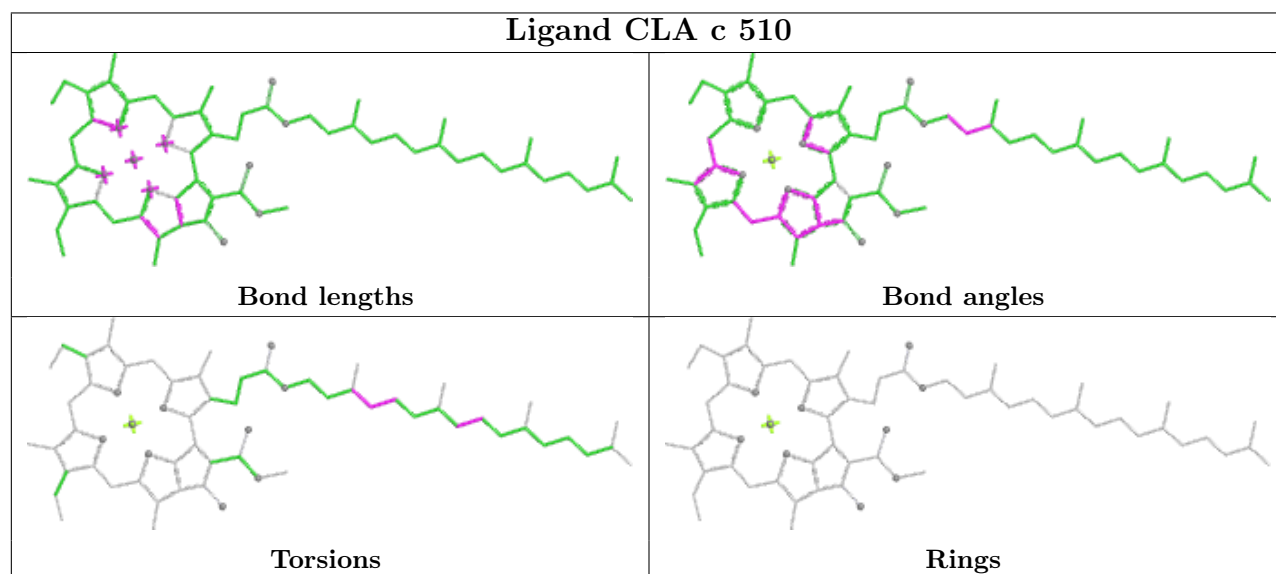
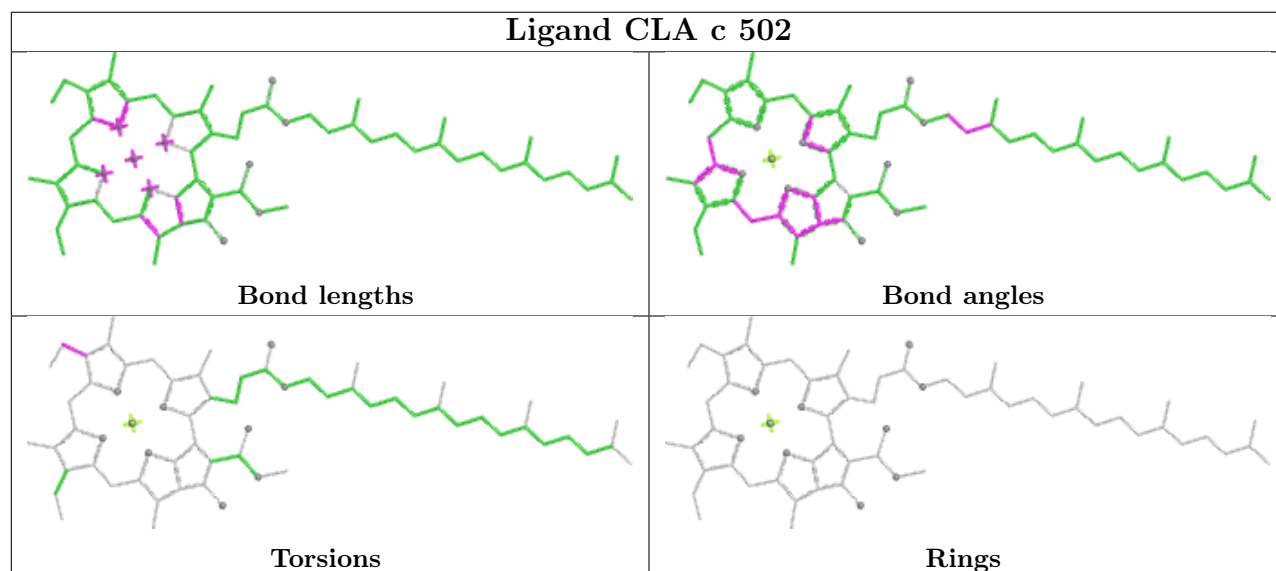
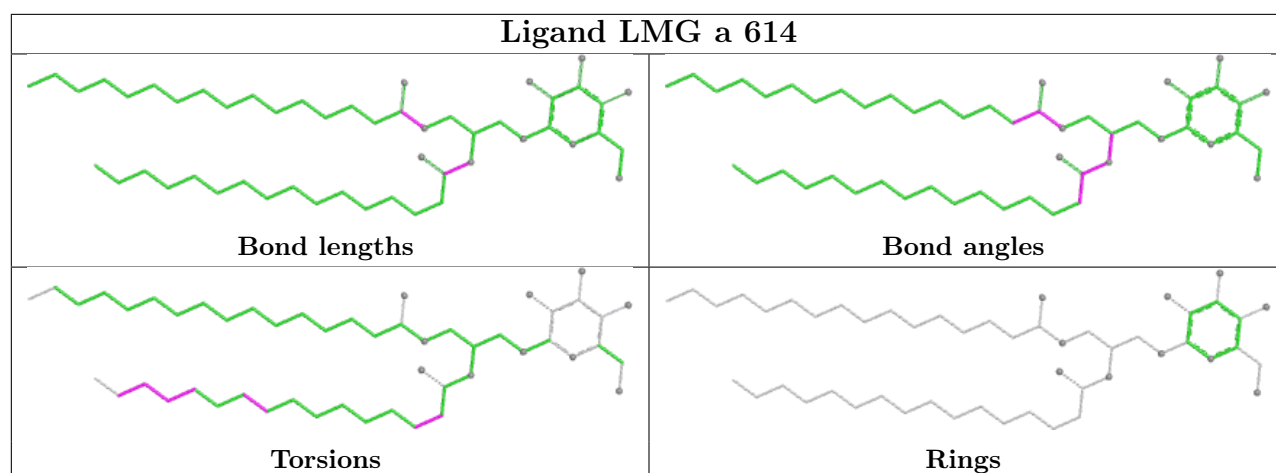


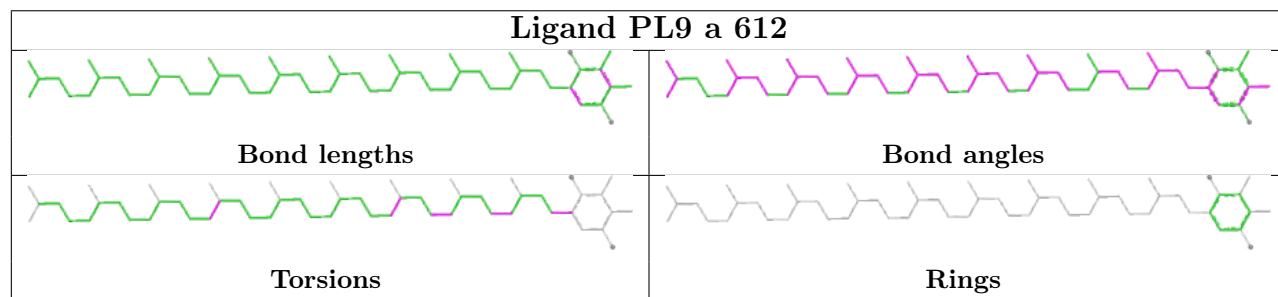
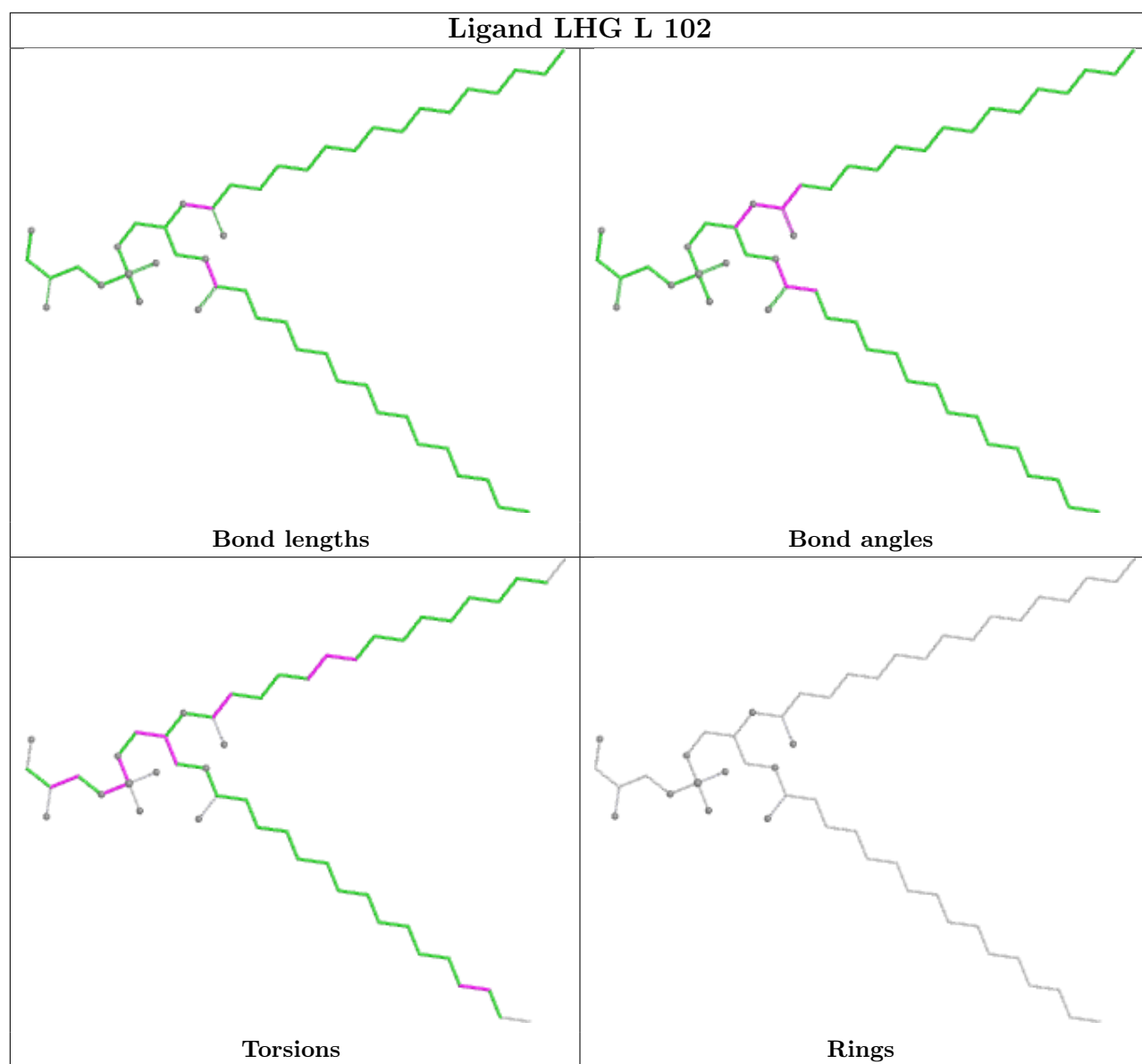


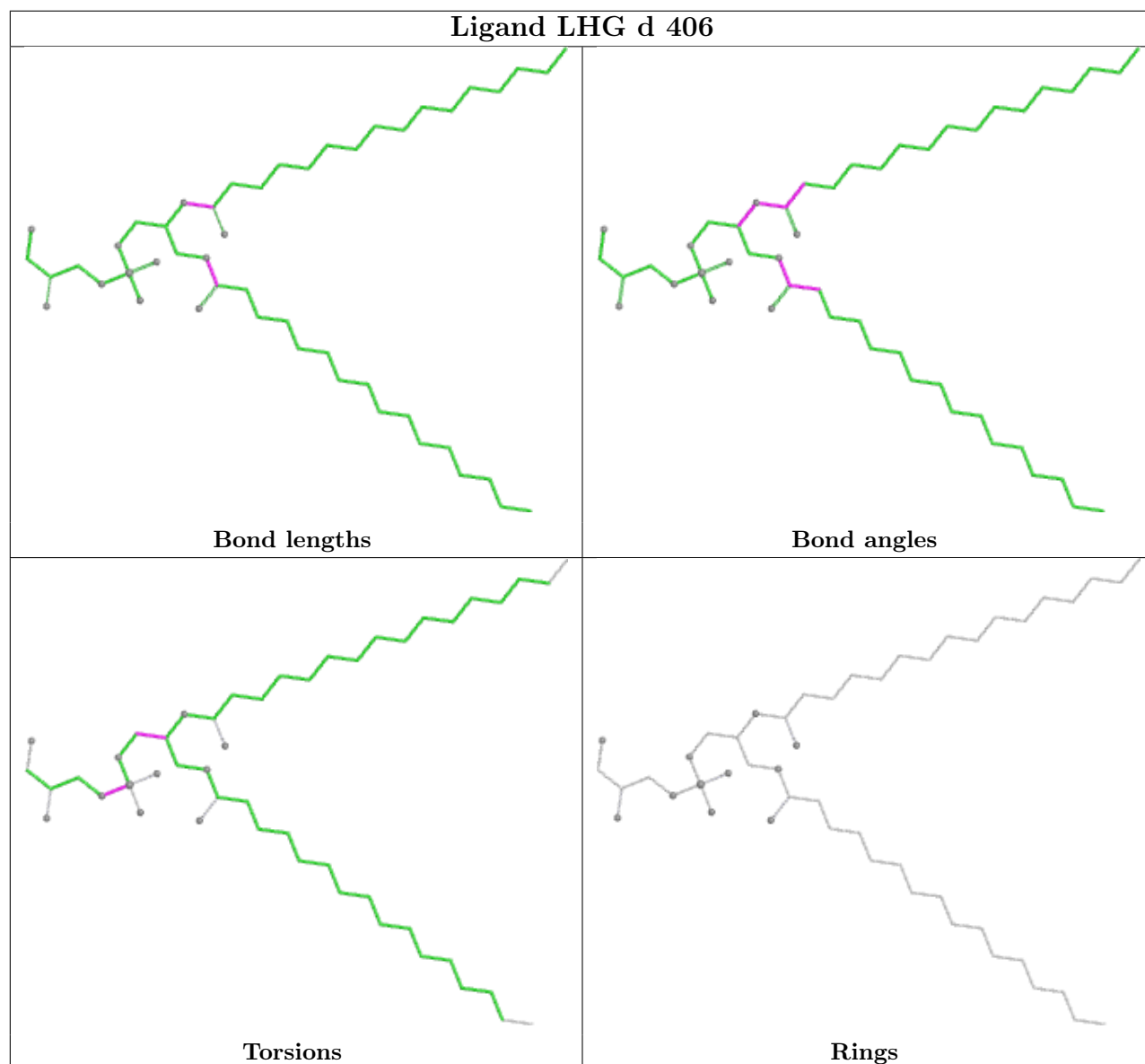
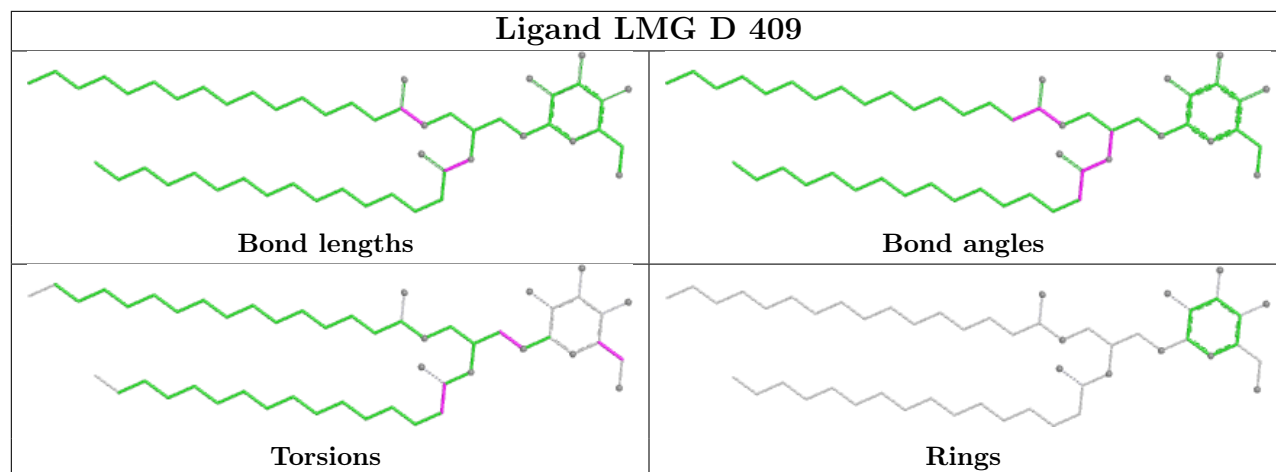


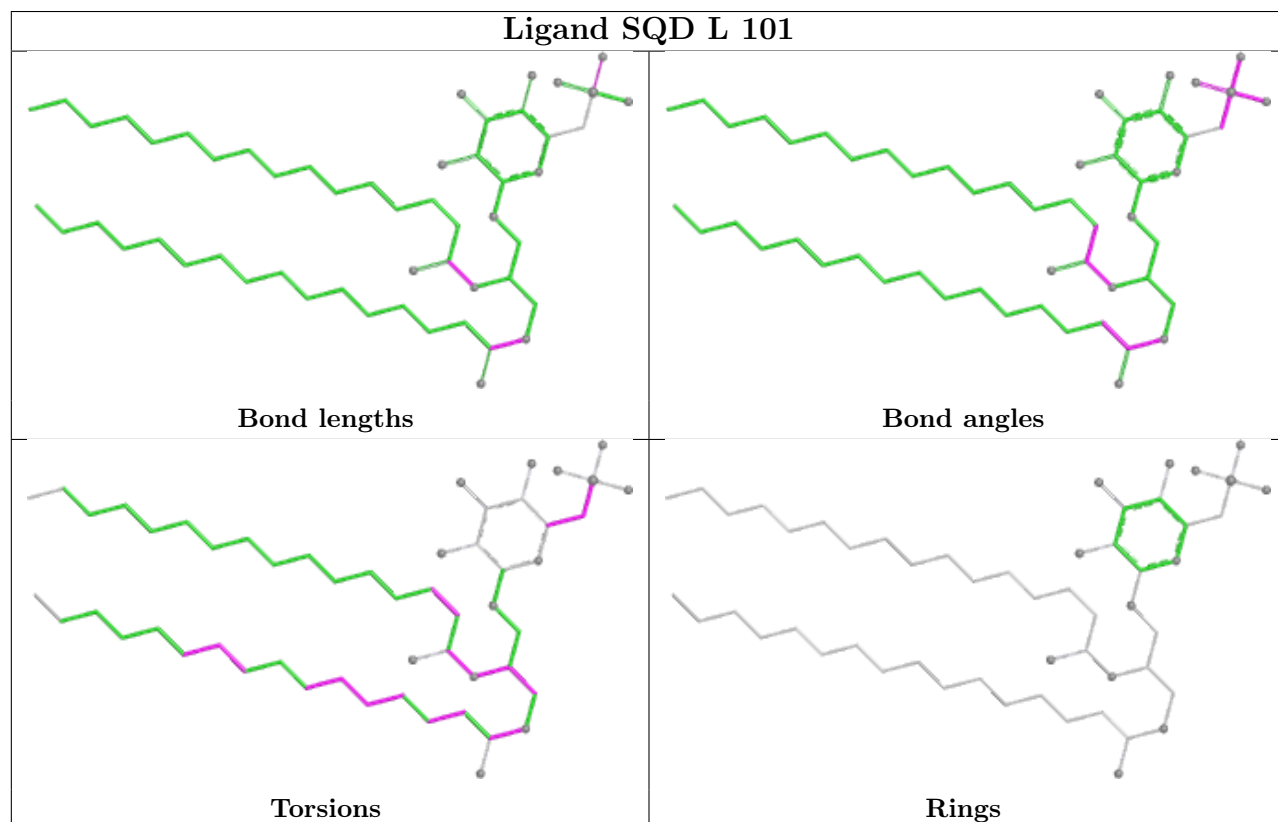
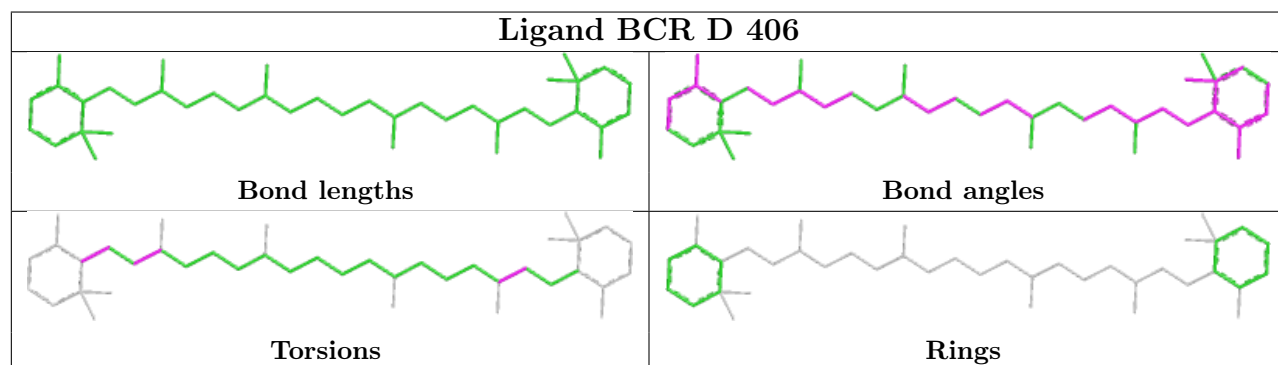
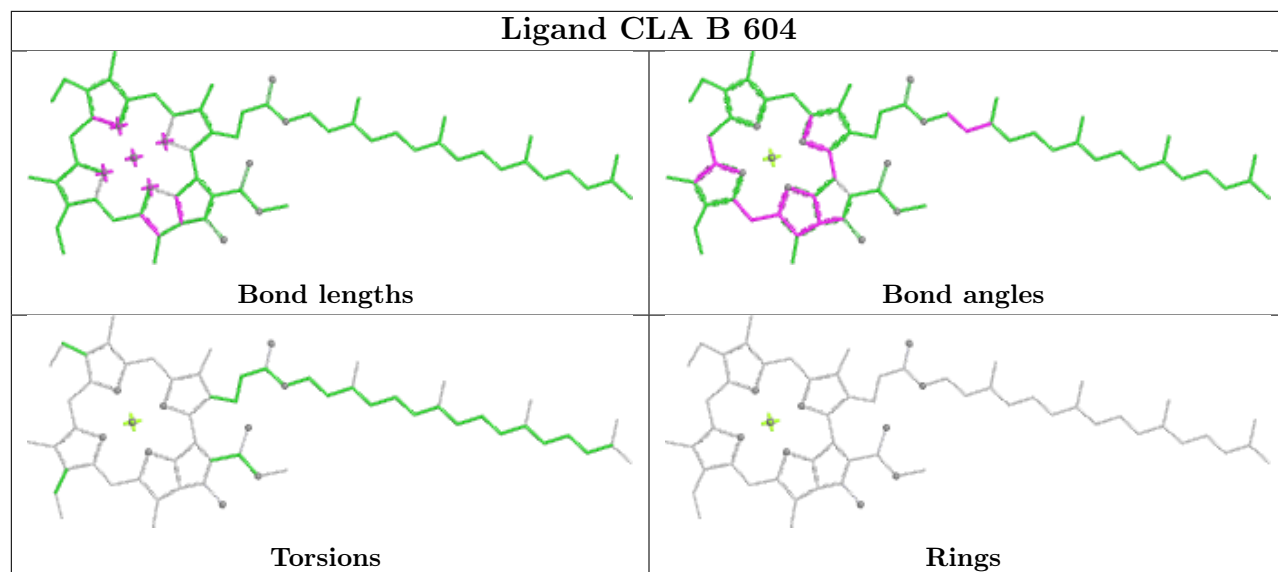


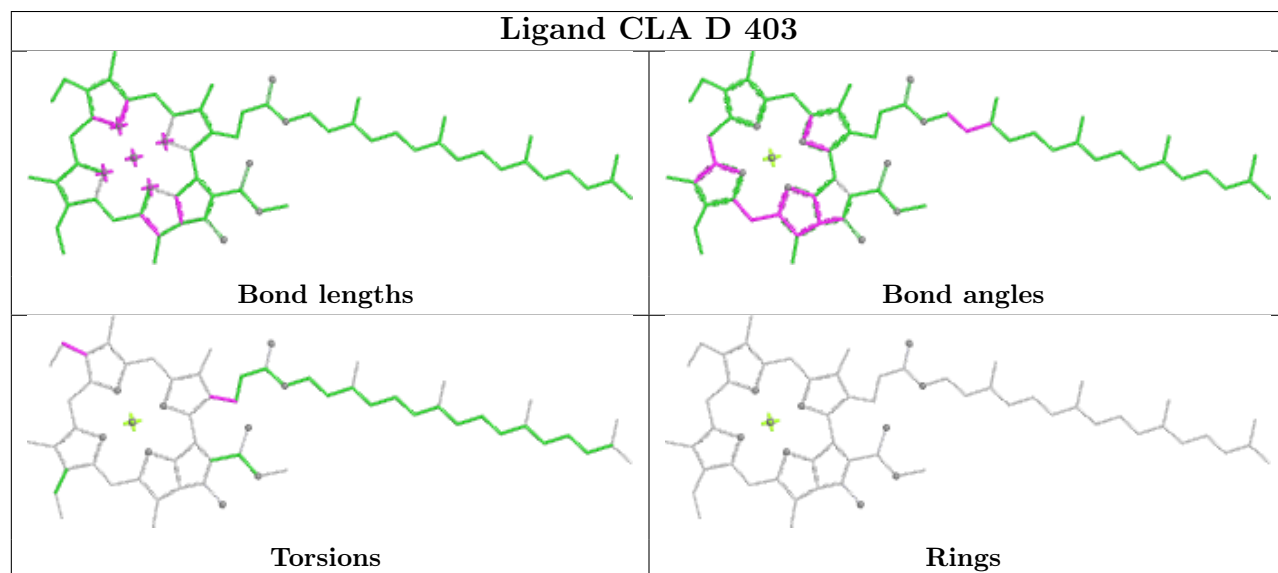
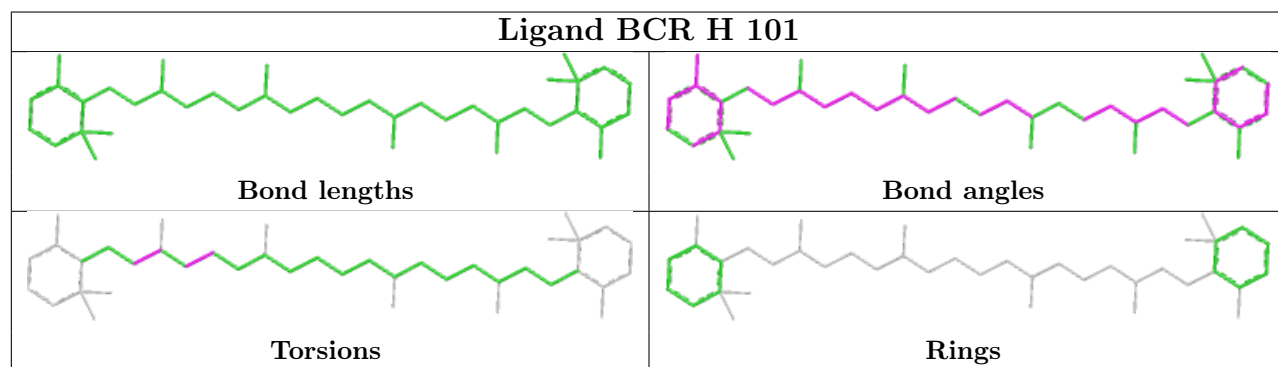
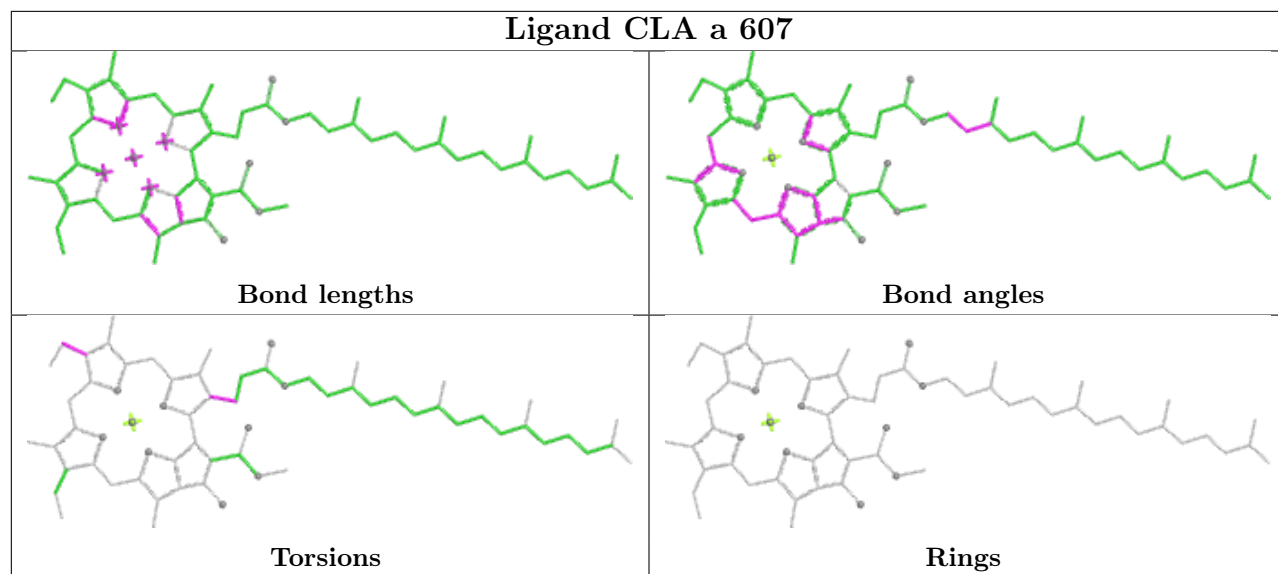


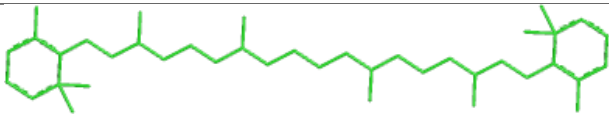
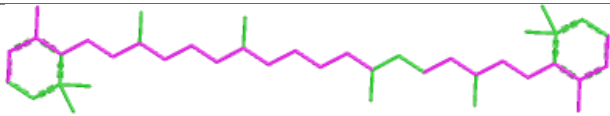
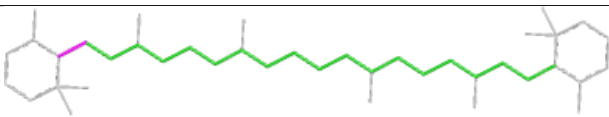
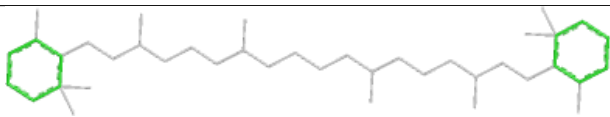


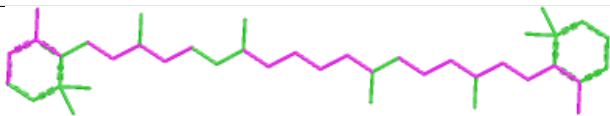
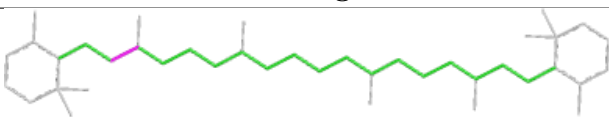
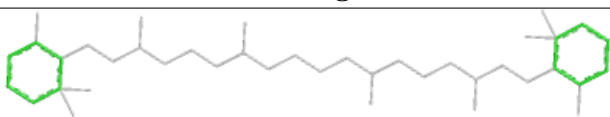


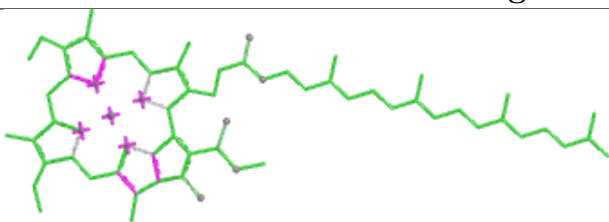
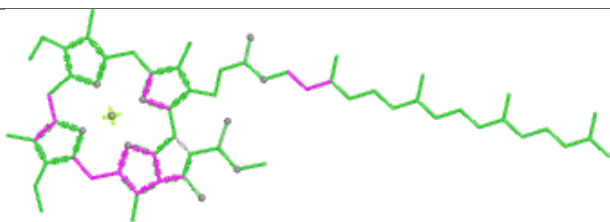
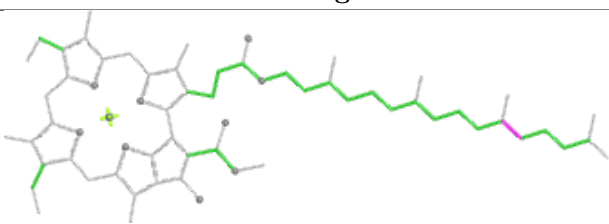
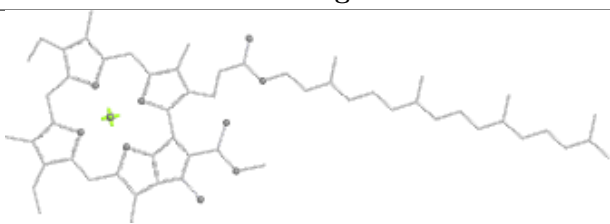


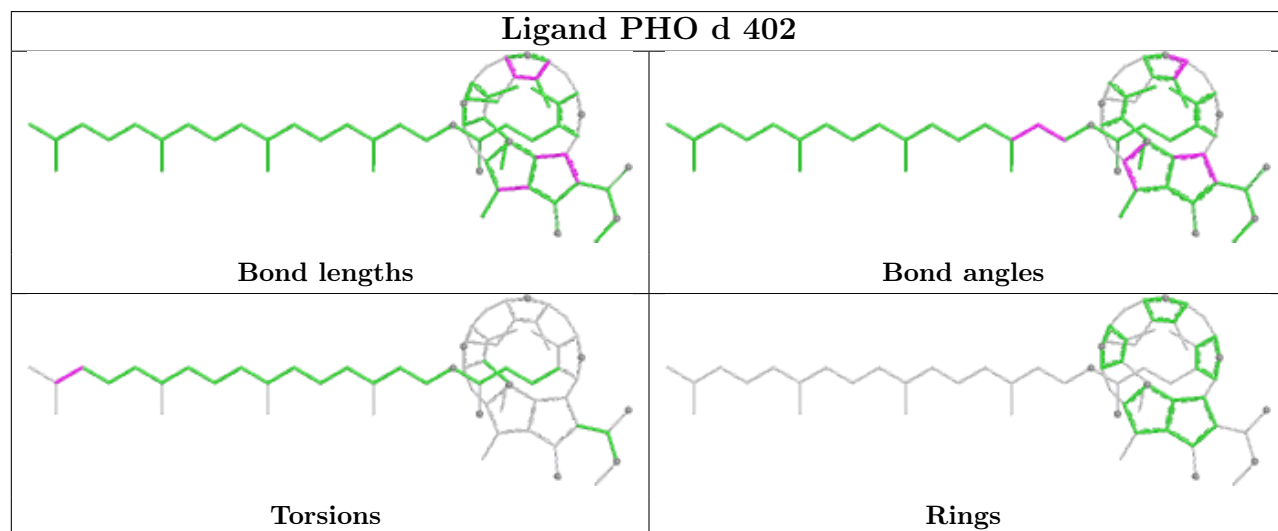
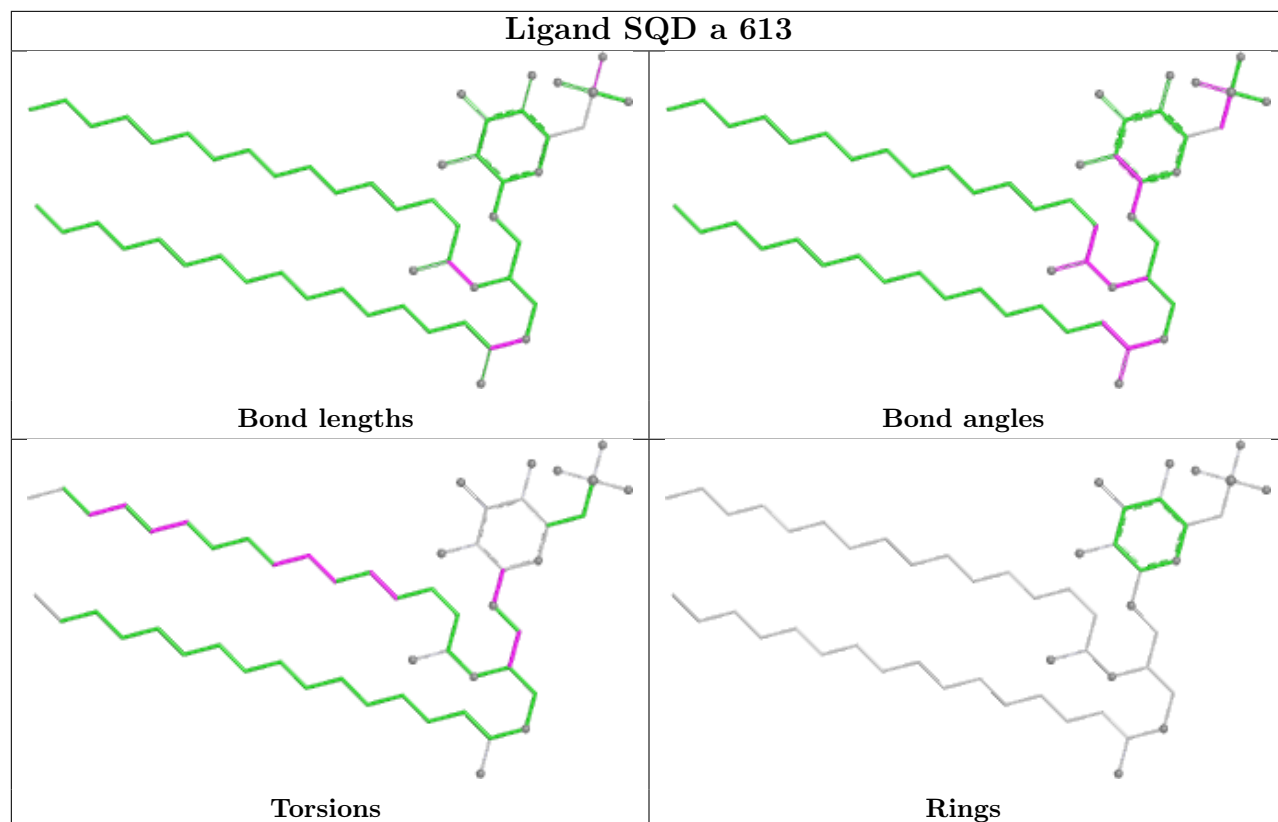


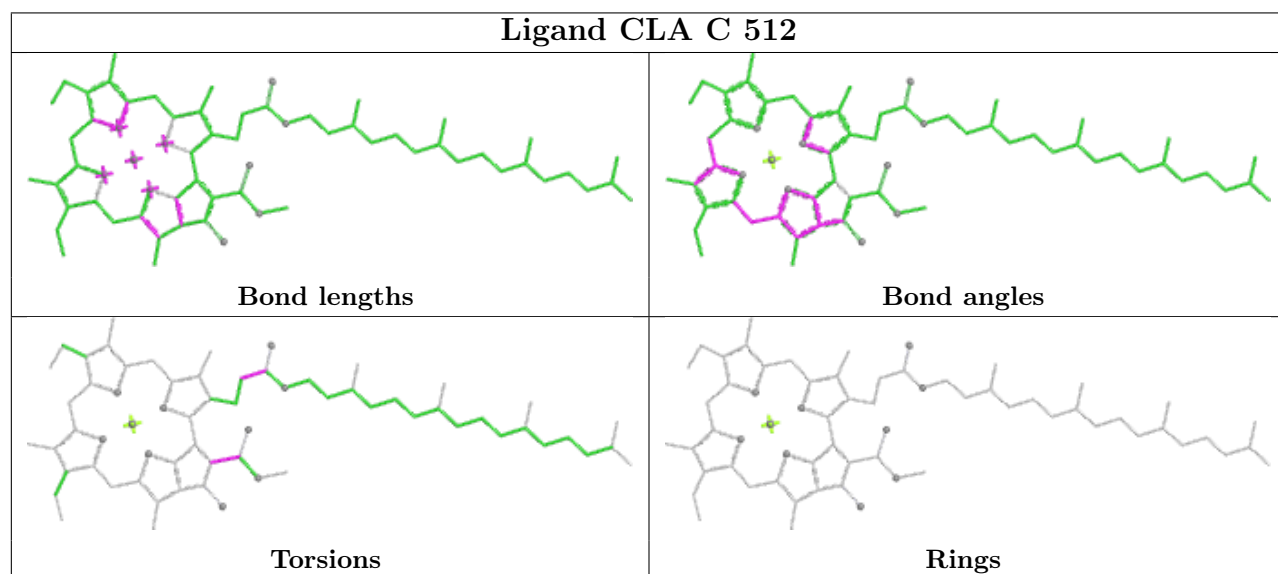
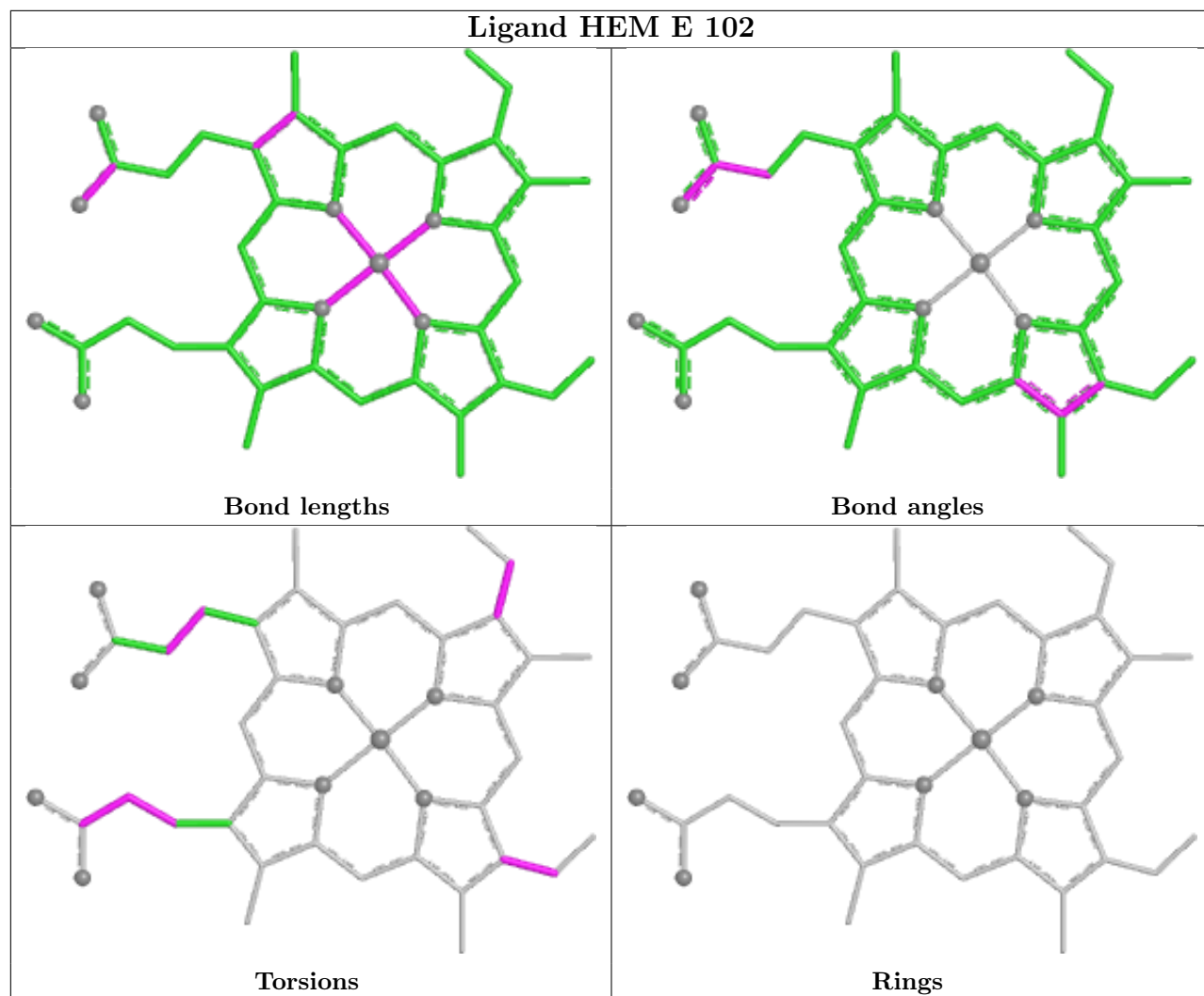


Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

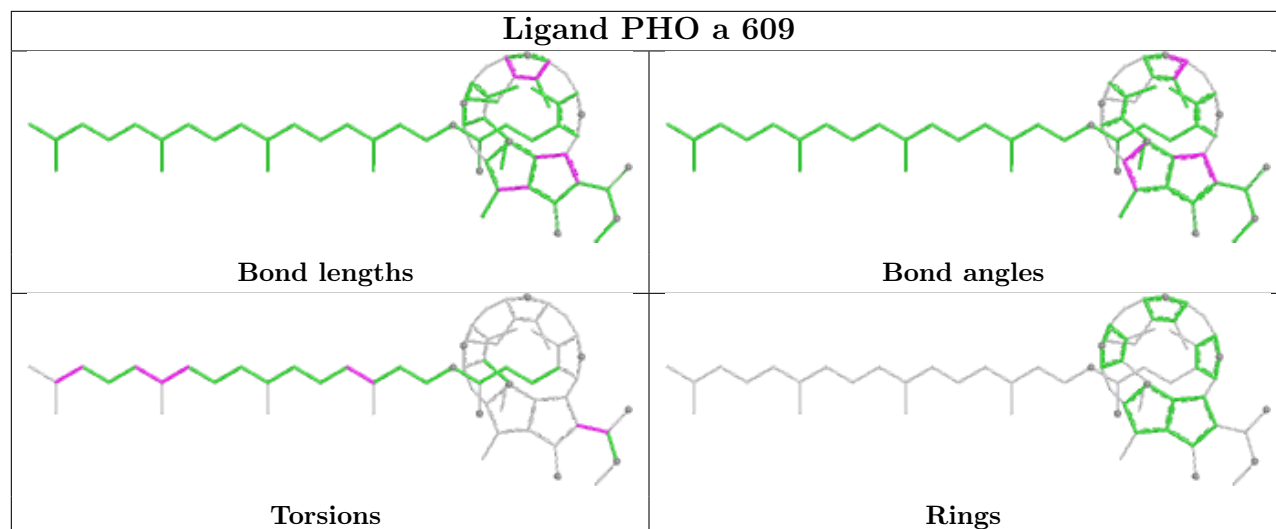
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

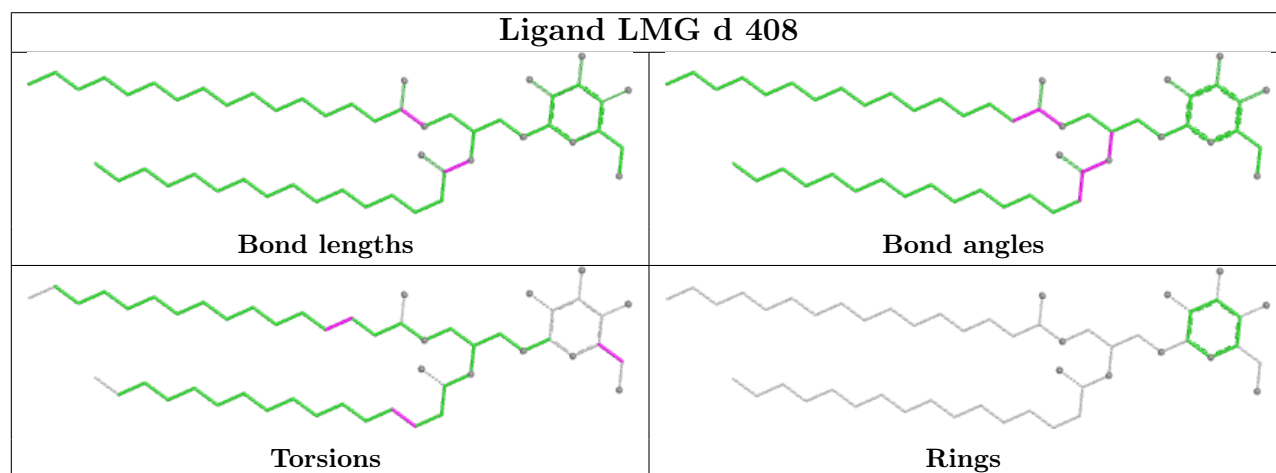




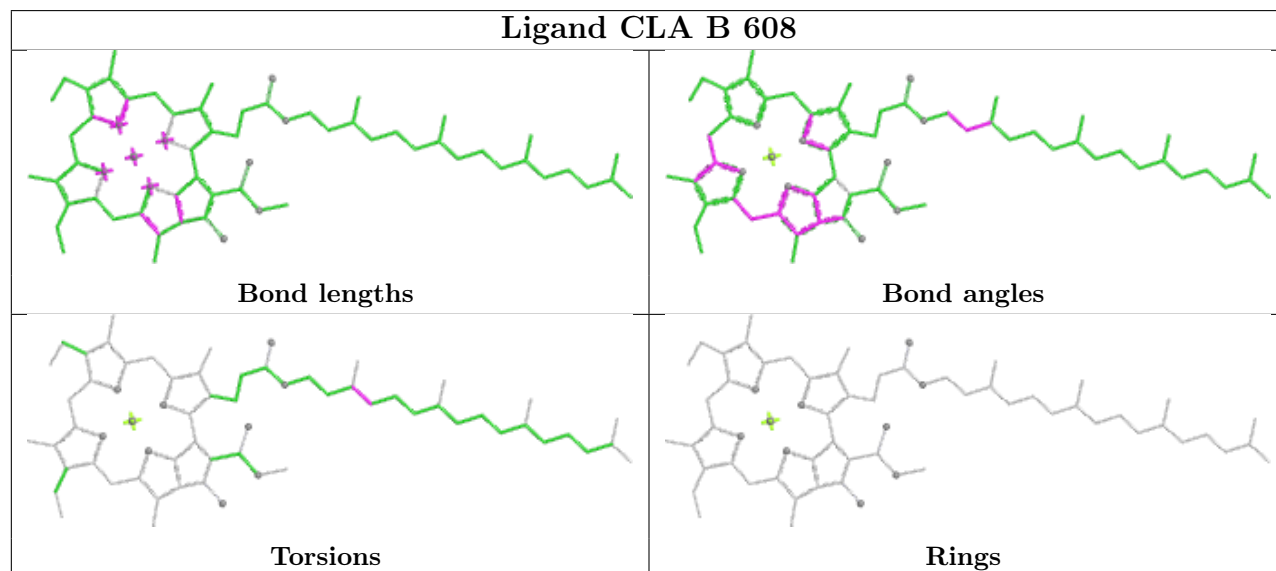
Ligand PHO a 609

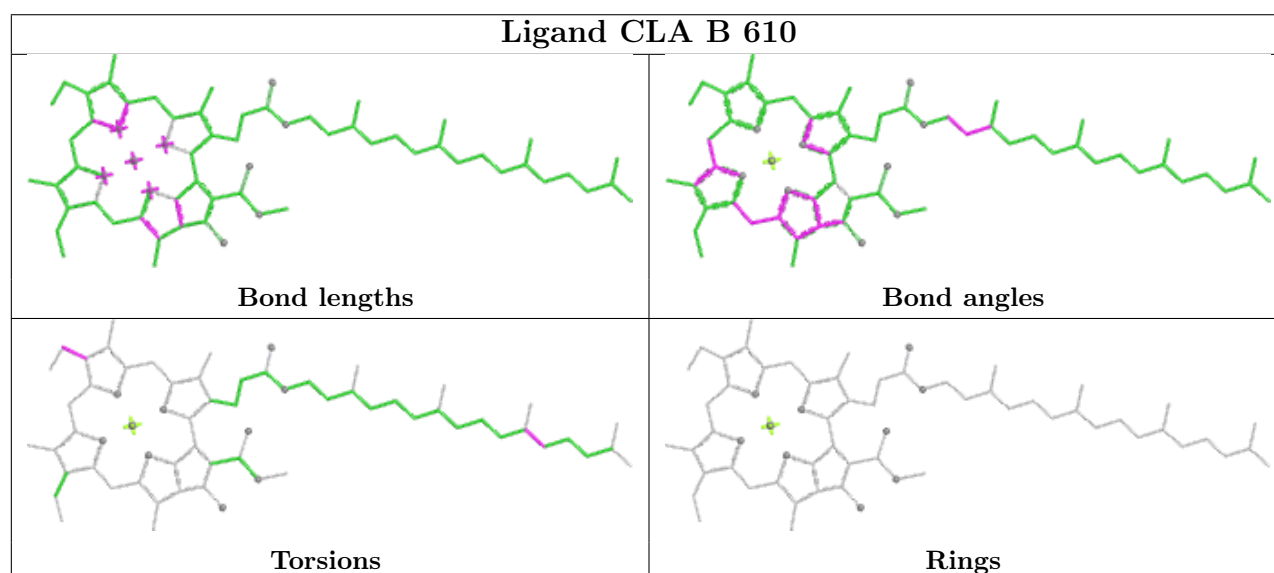
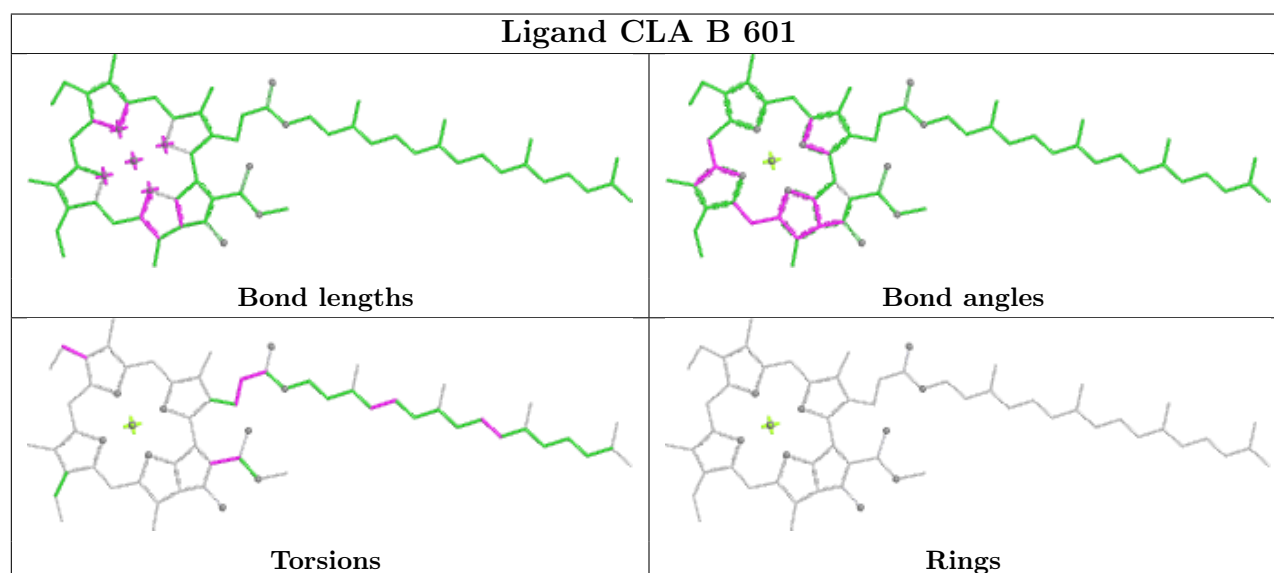
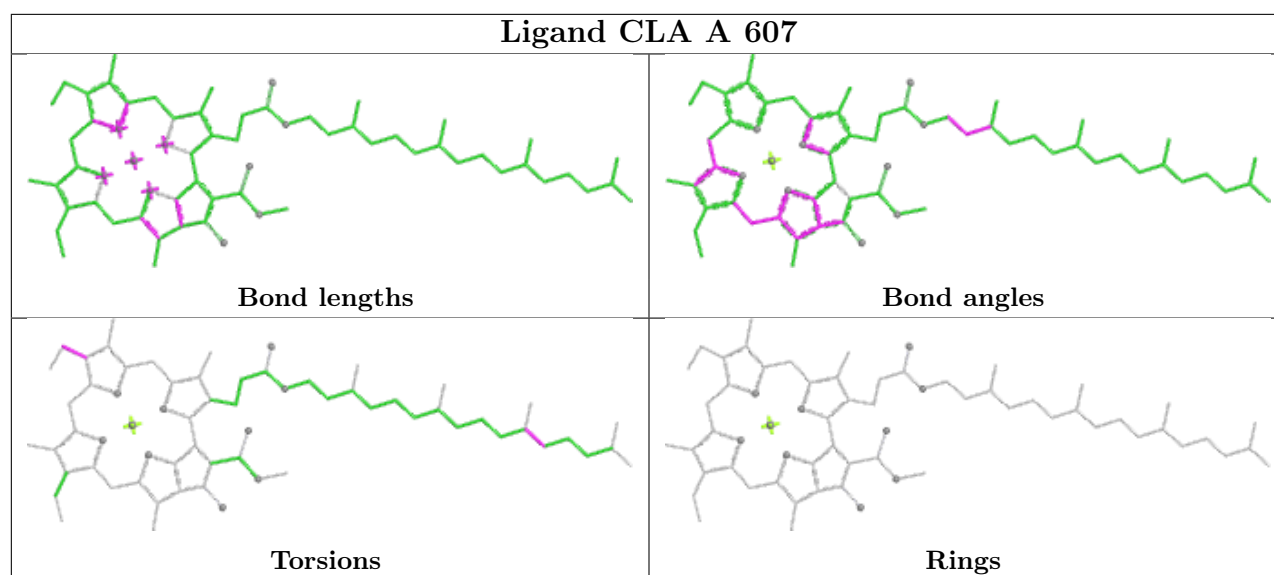


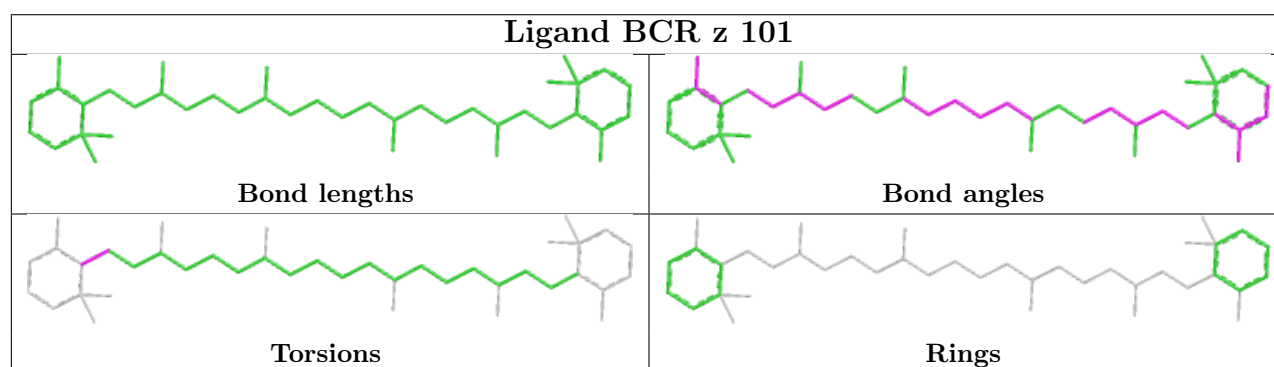
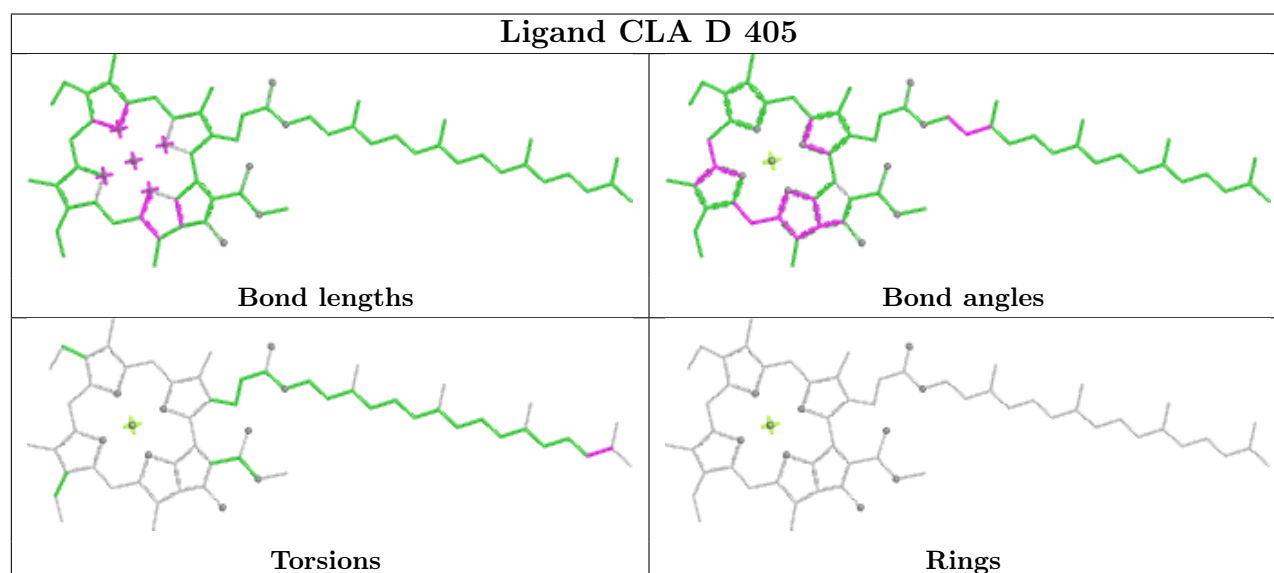
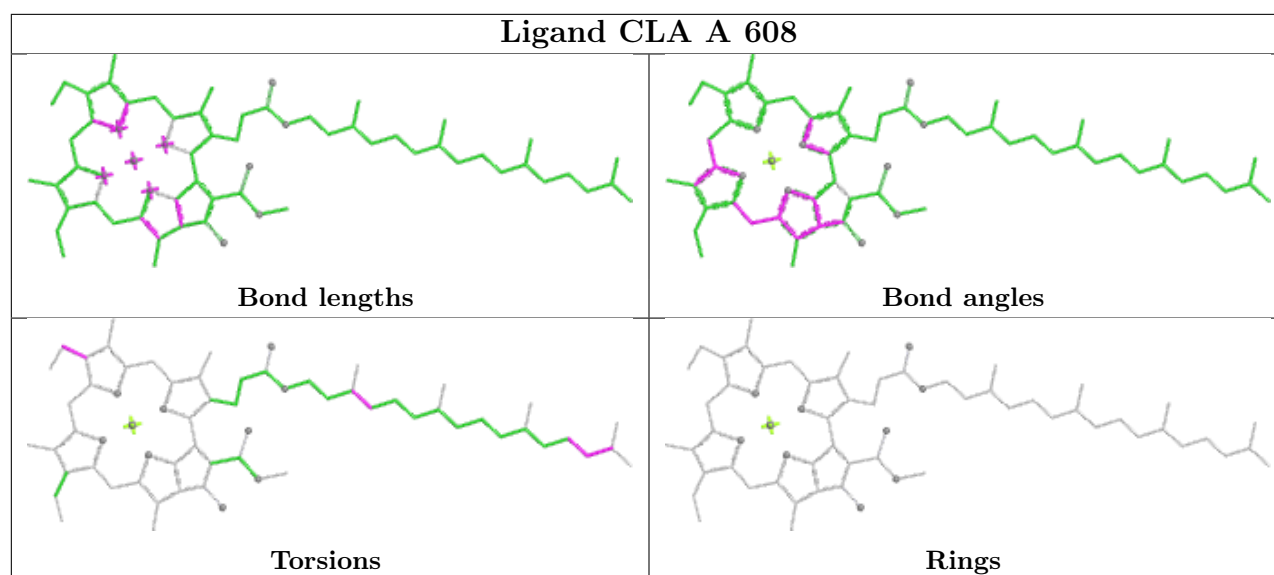
Ligand LMG d 408



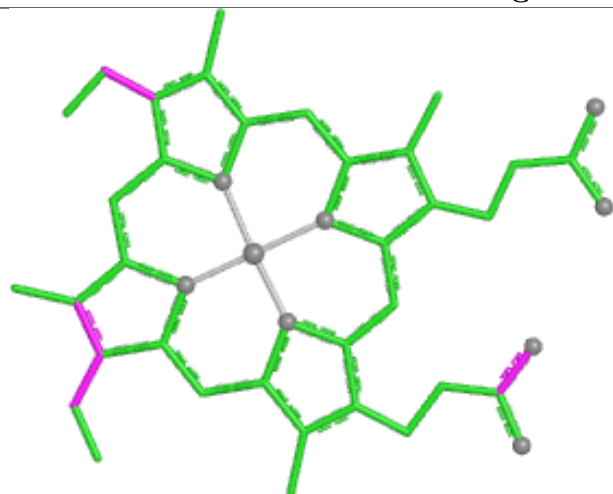
Ligand CLA B 608



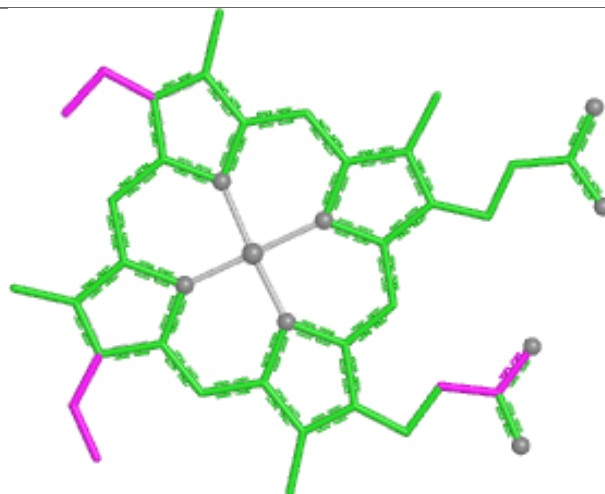




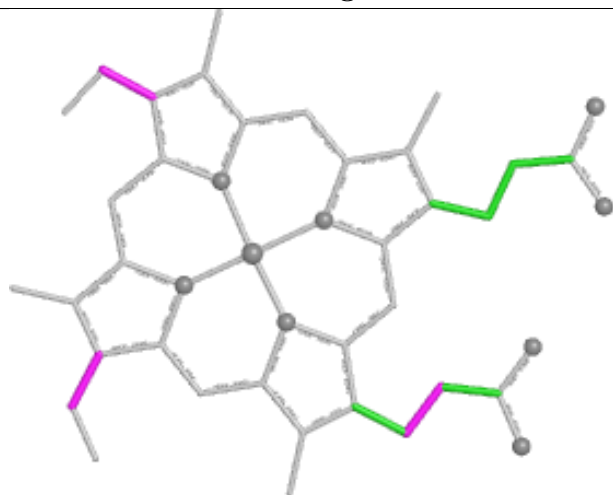
Ligand HEC V 201



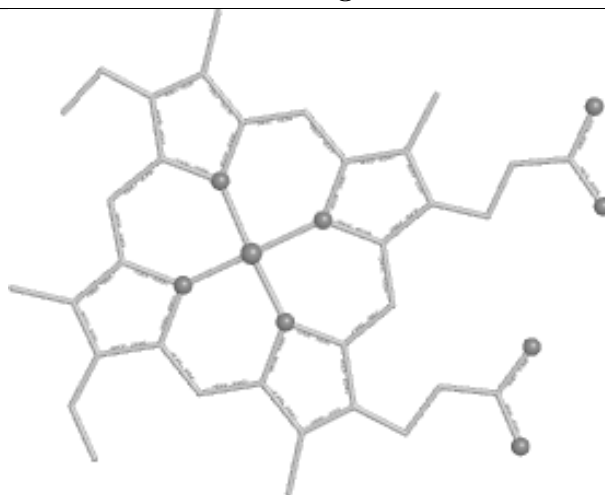
Bond lengths



Bond angles

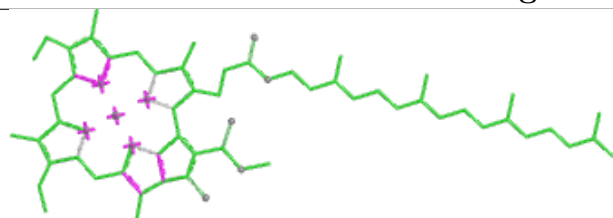


Torsions

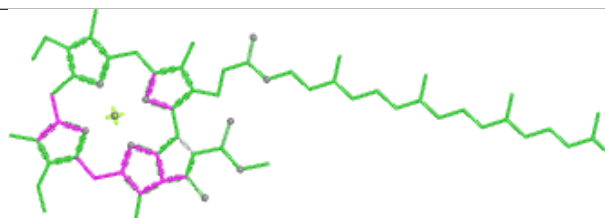


Rings

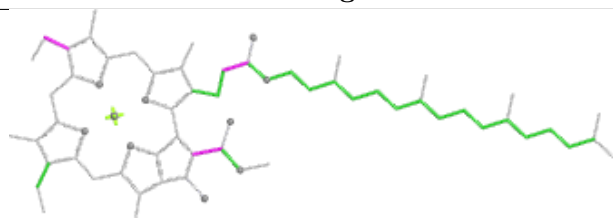
Ligand CLA c 512



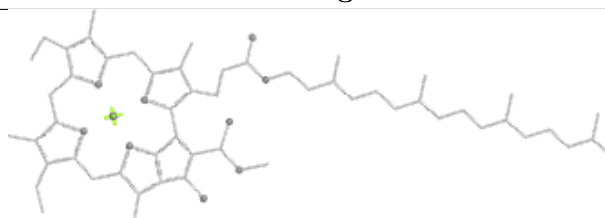
Bond lengths



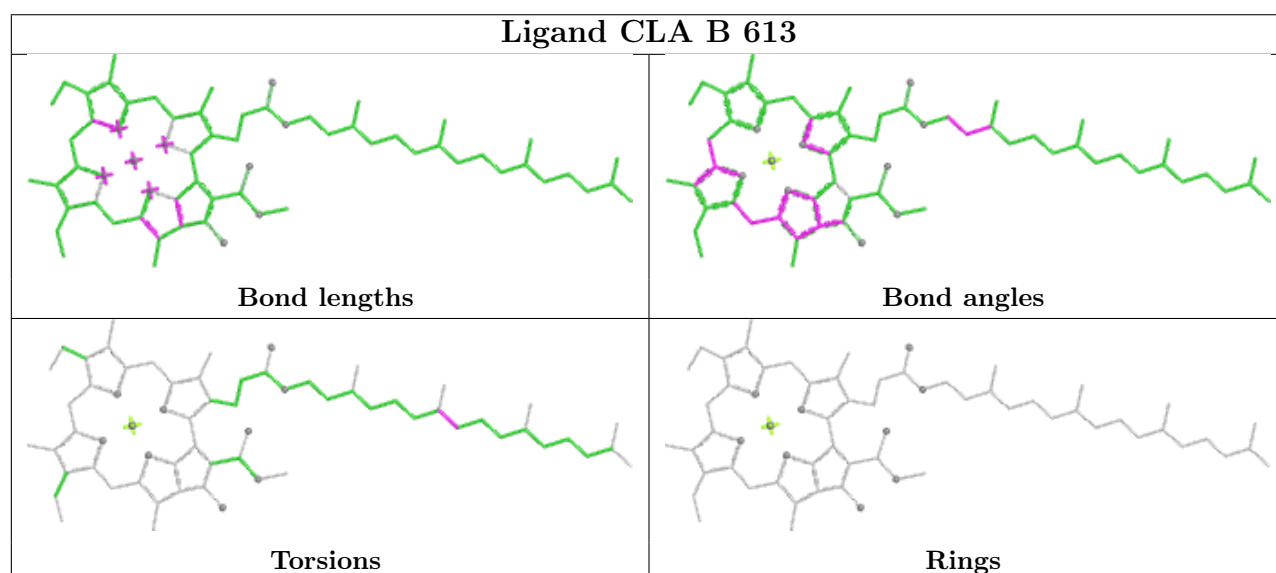
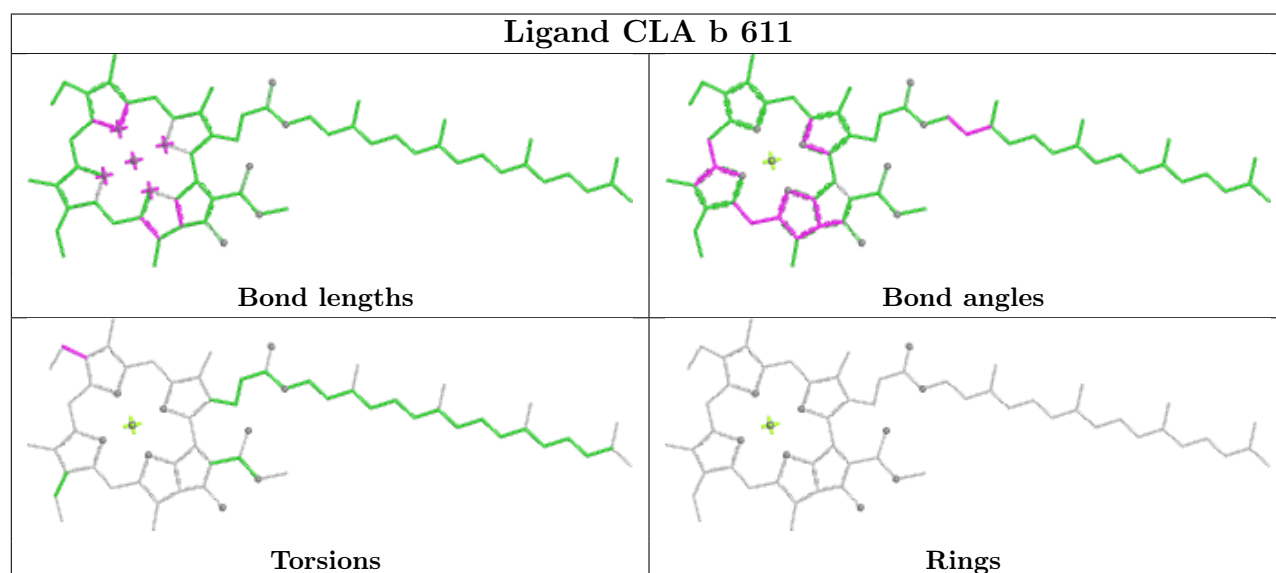
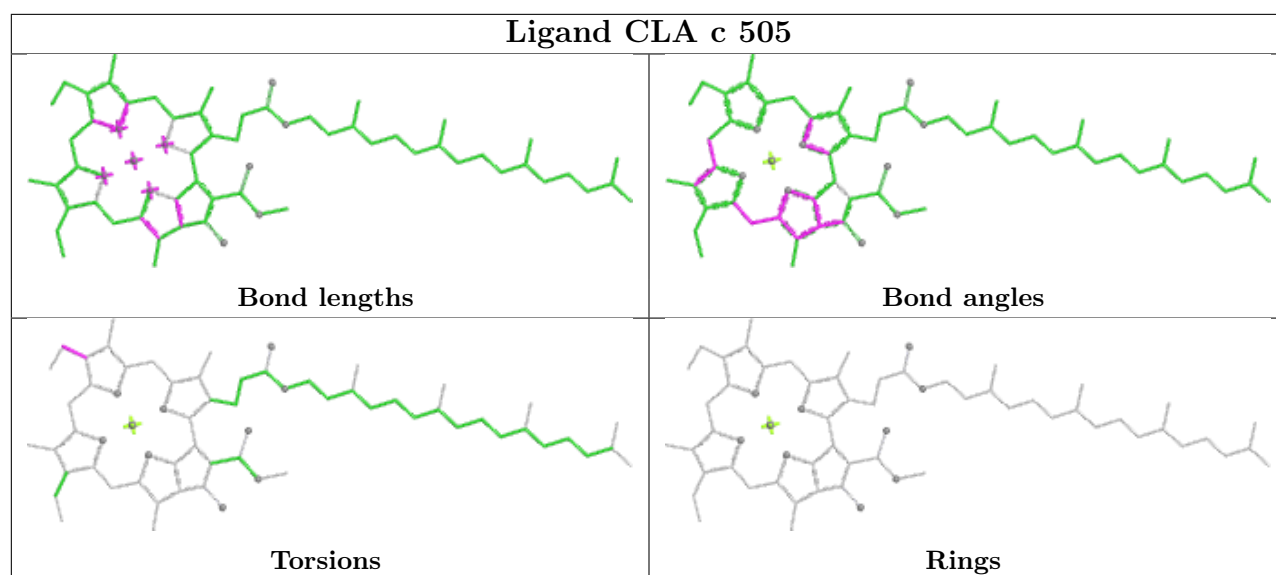
Bond angles

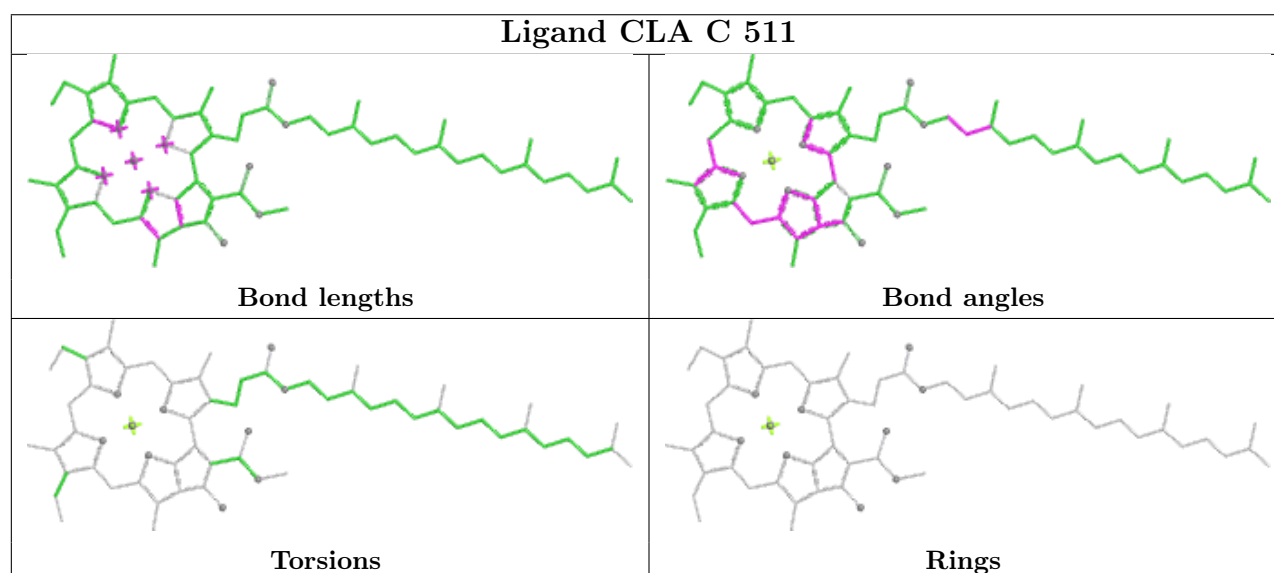
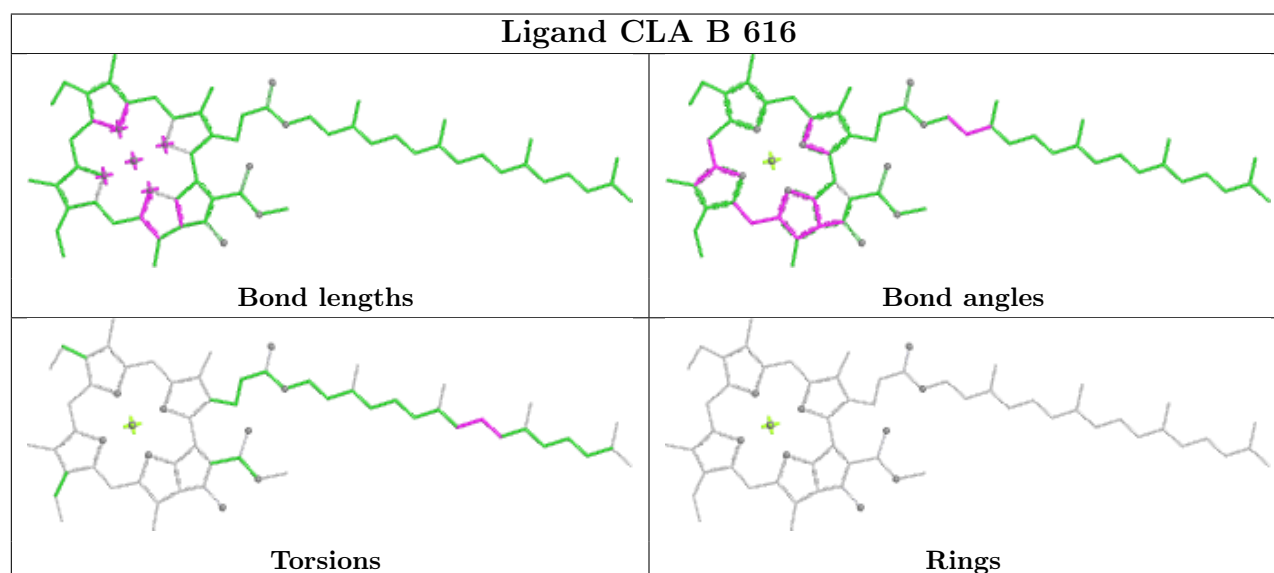
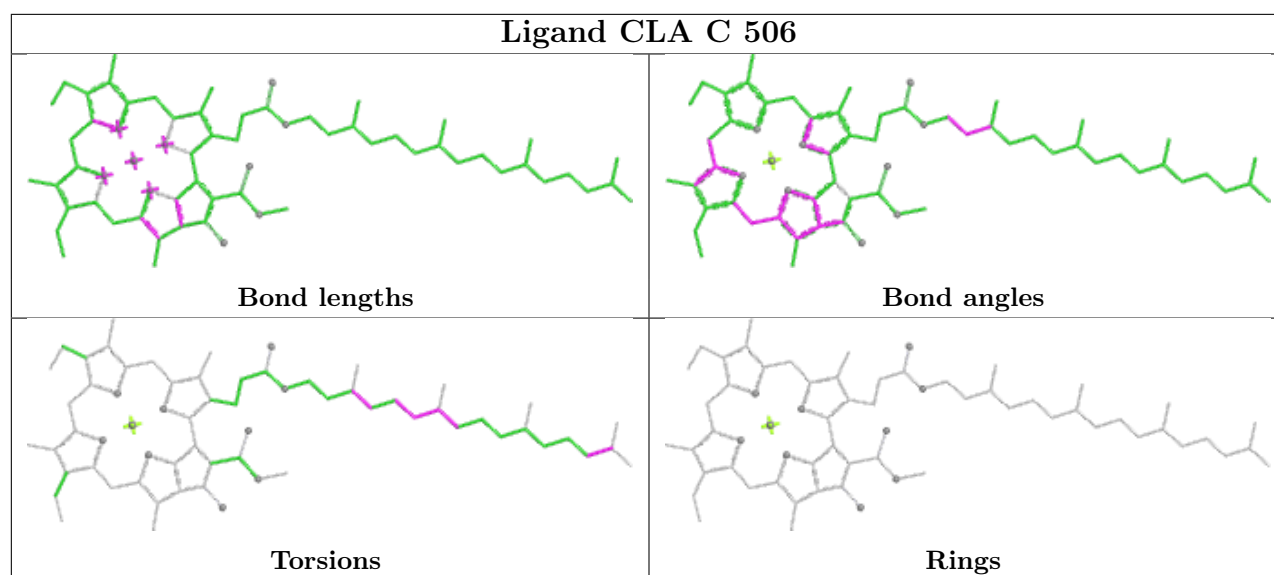


Torsions

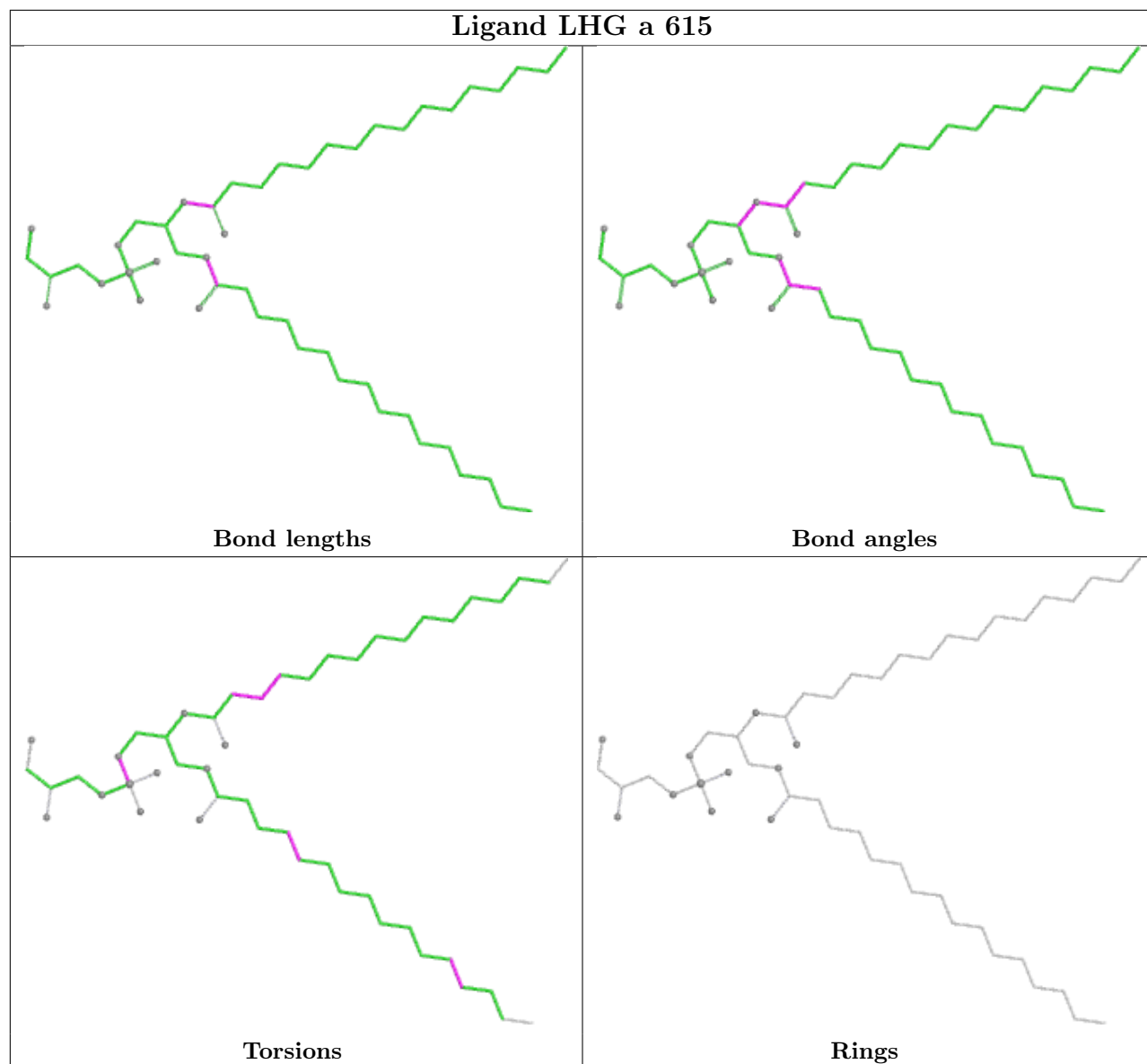


Rings

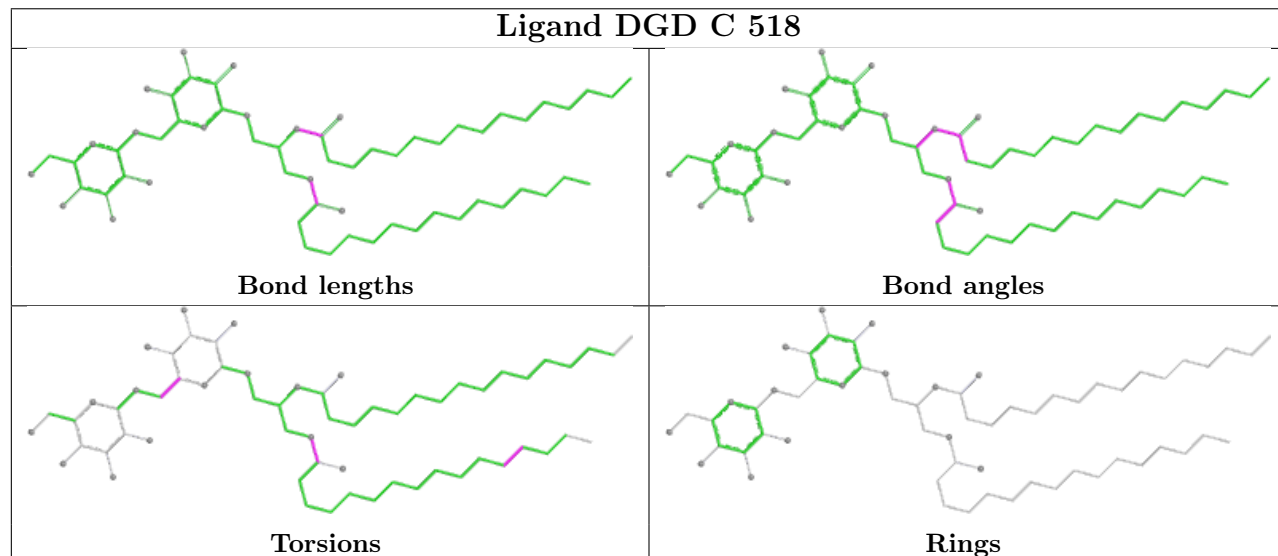


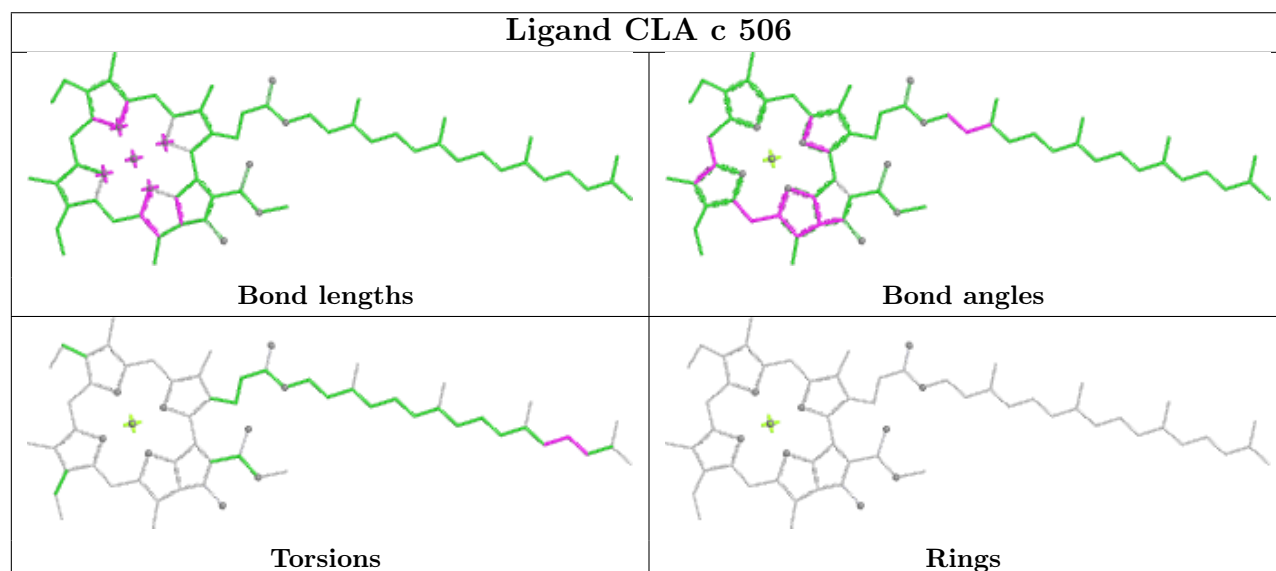
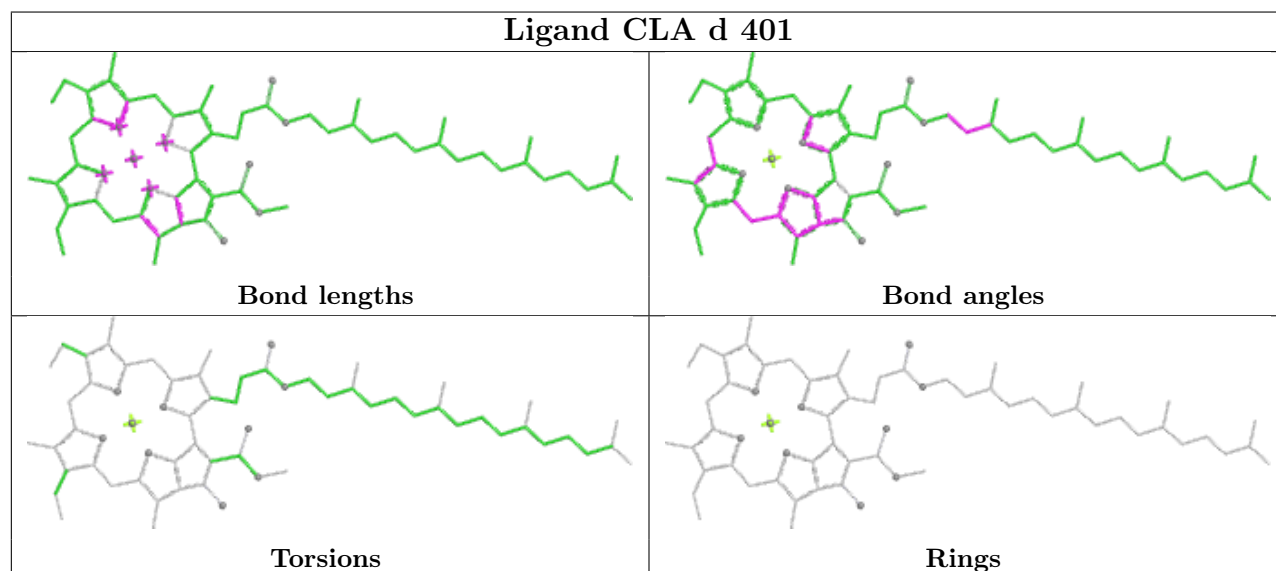
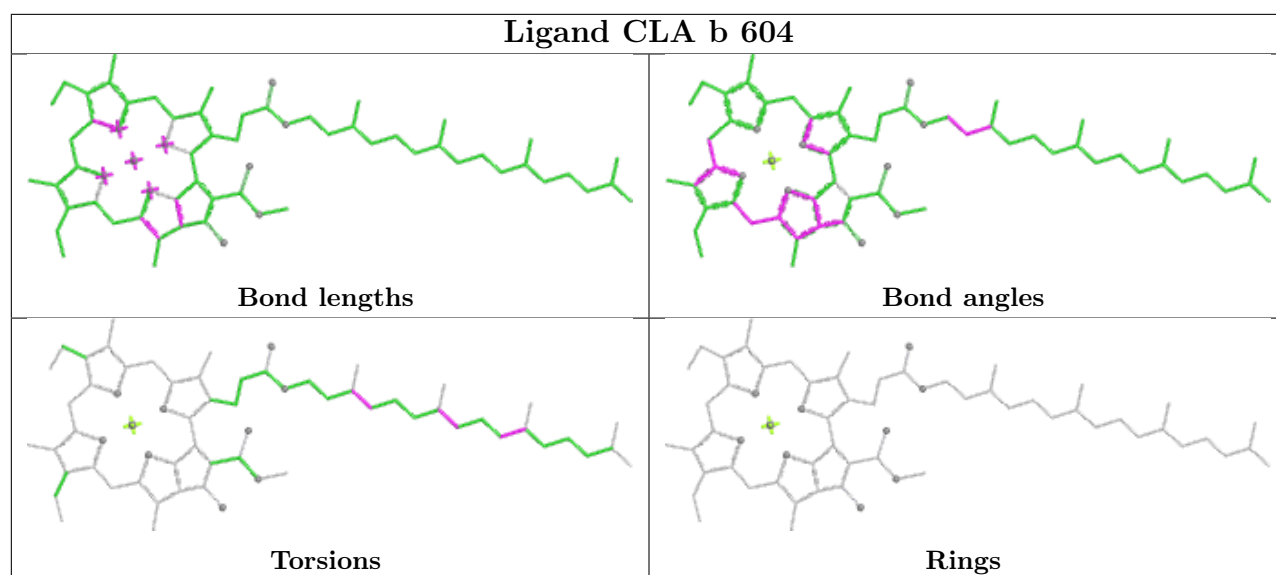


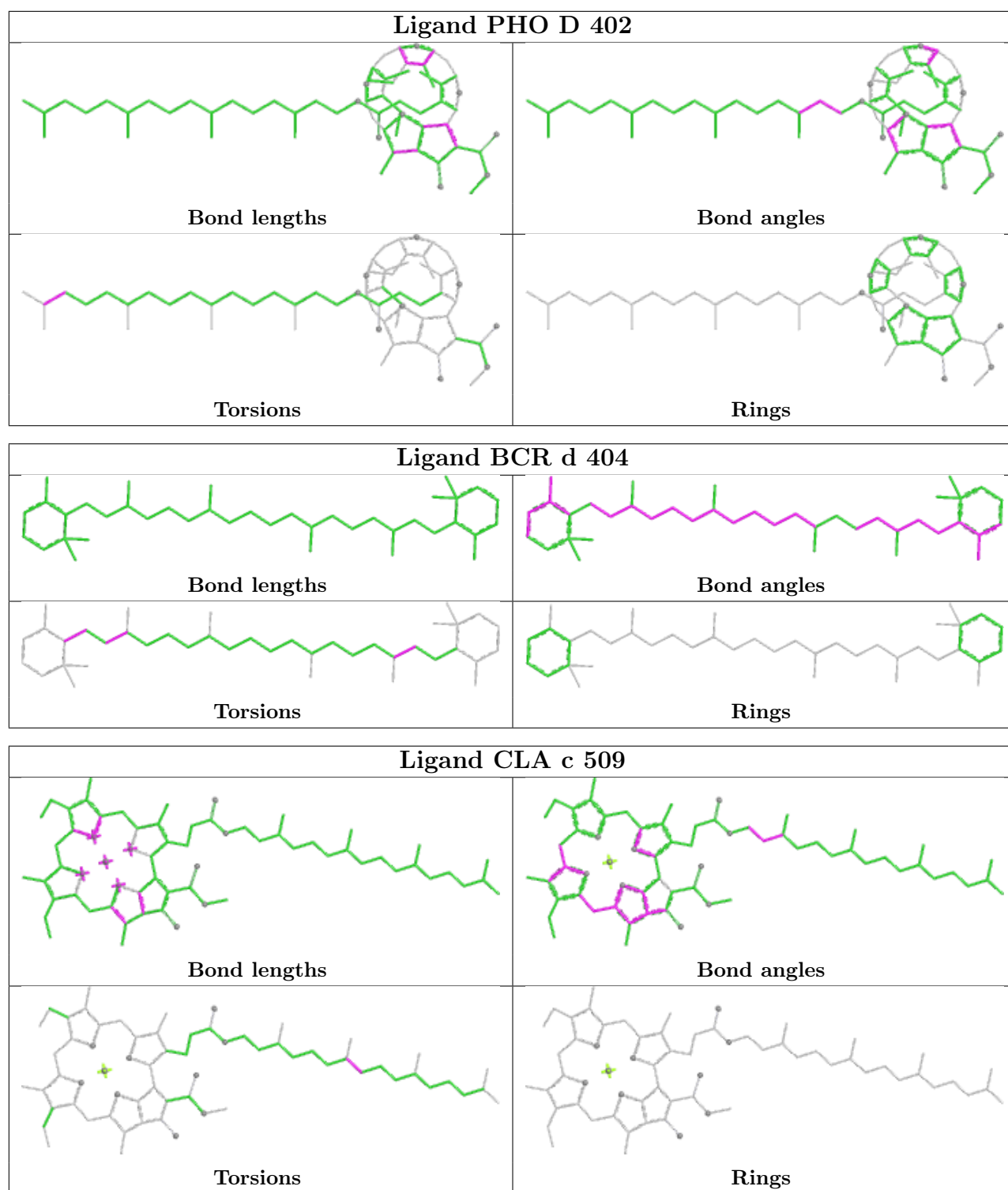
Ligand LHG a 615

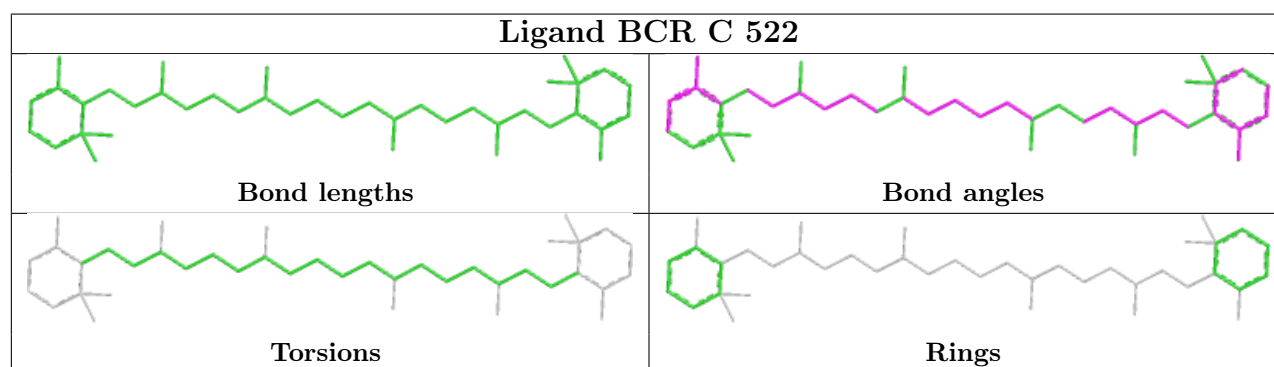
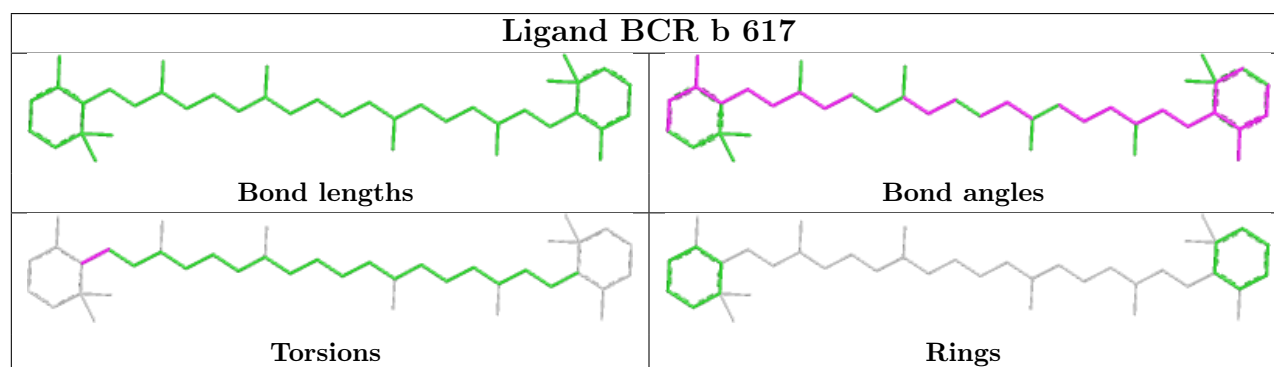
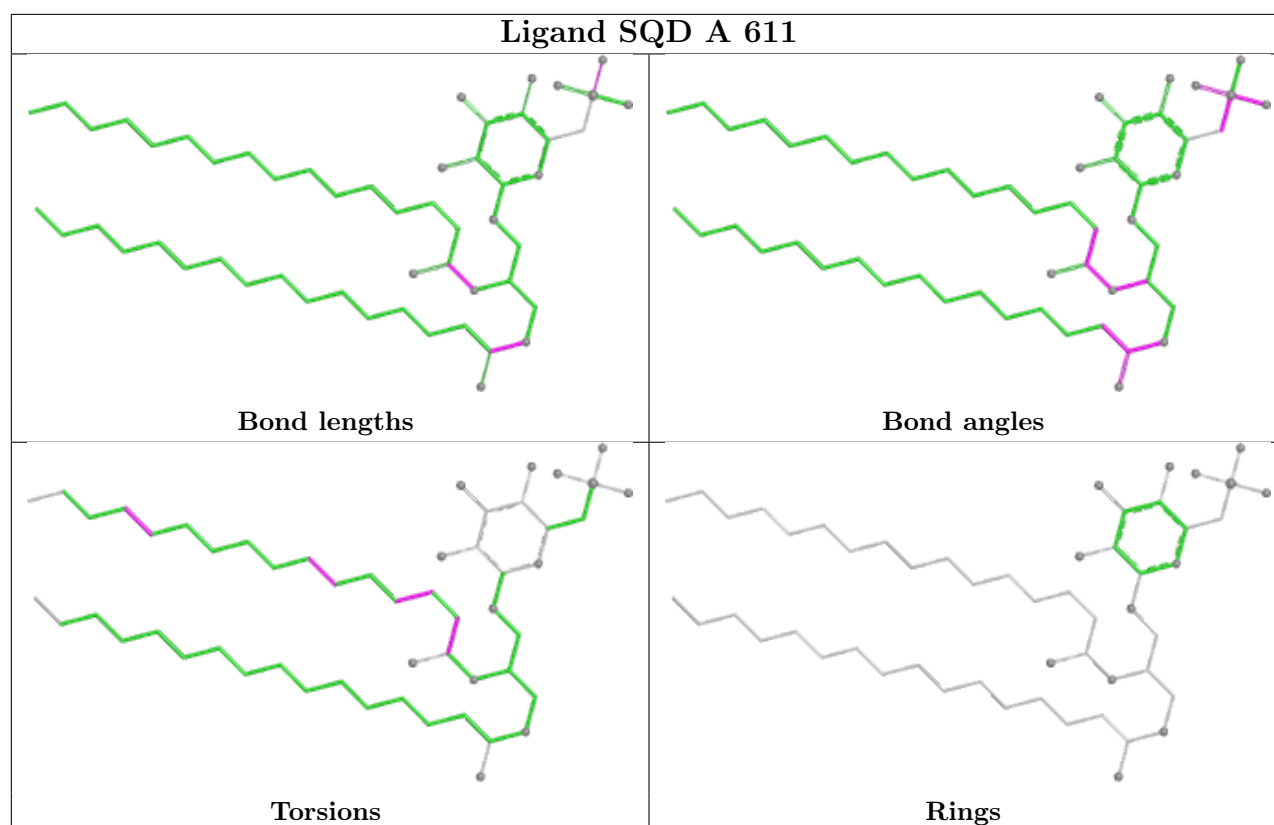


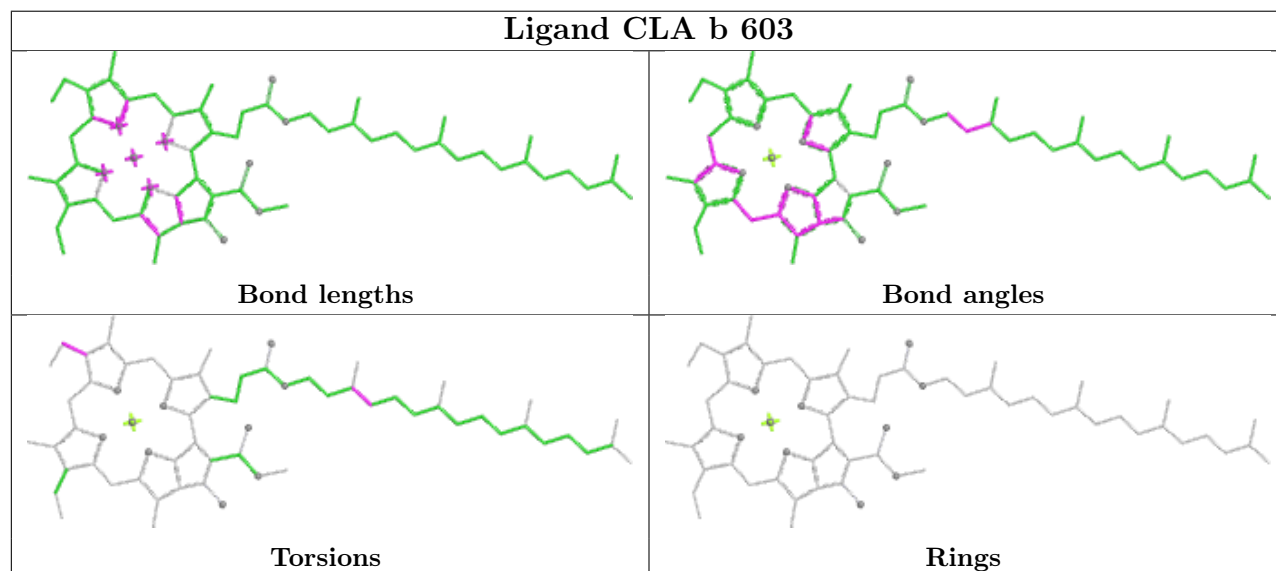
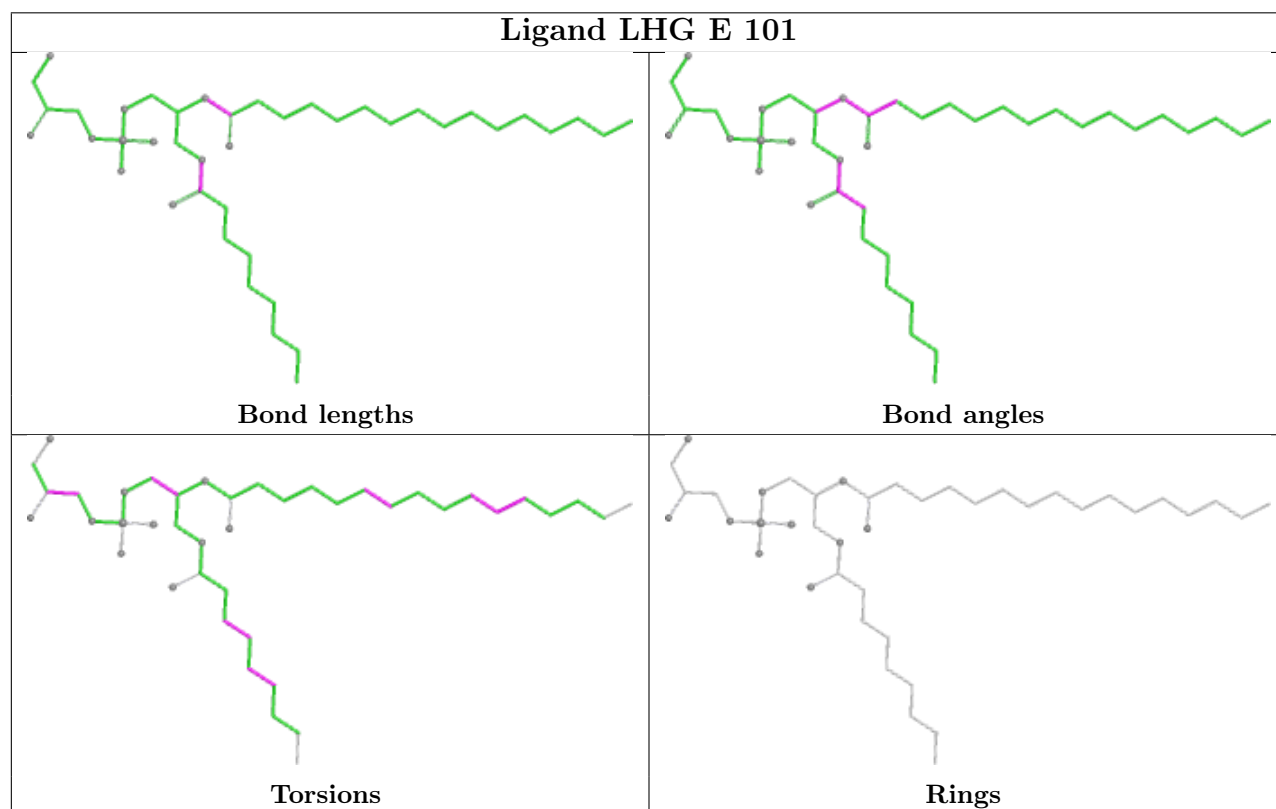
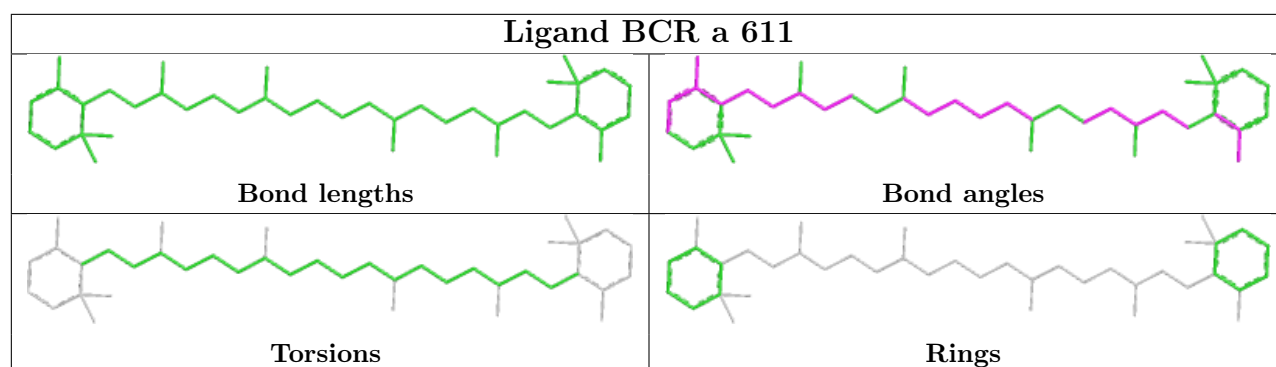
Ligand DGD C 518



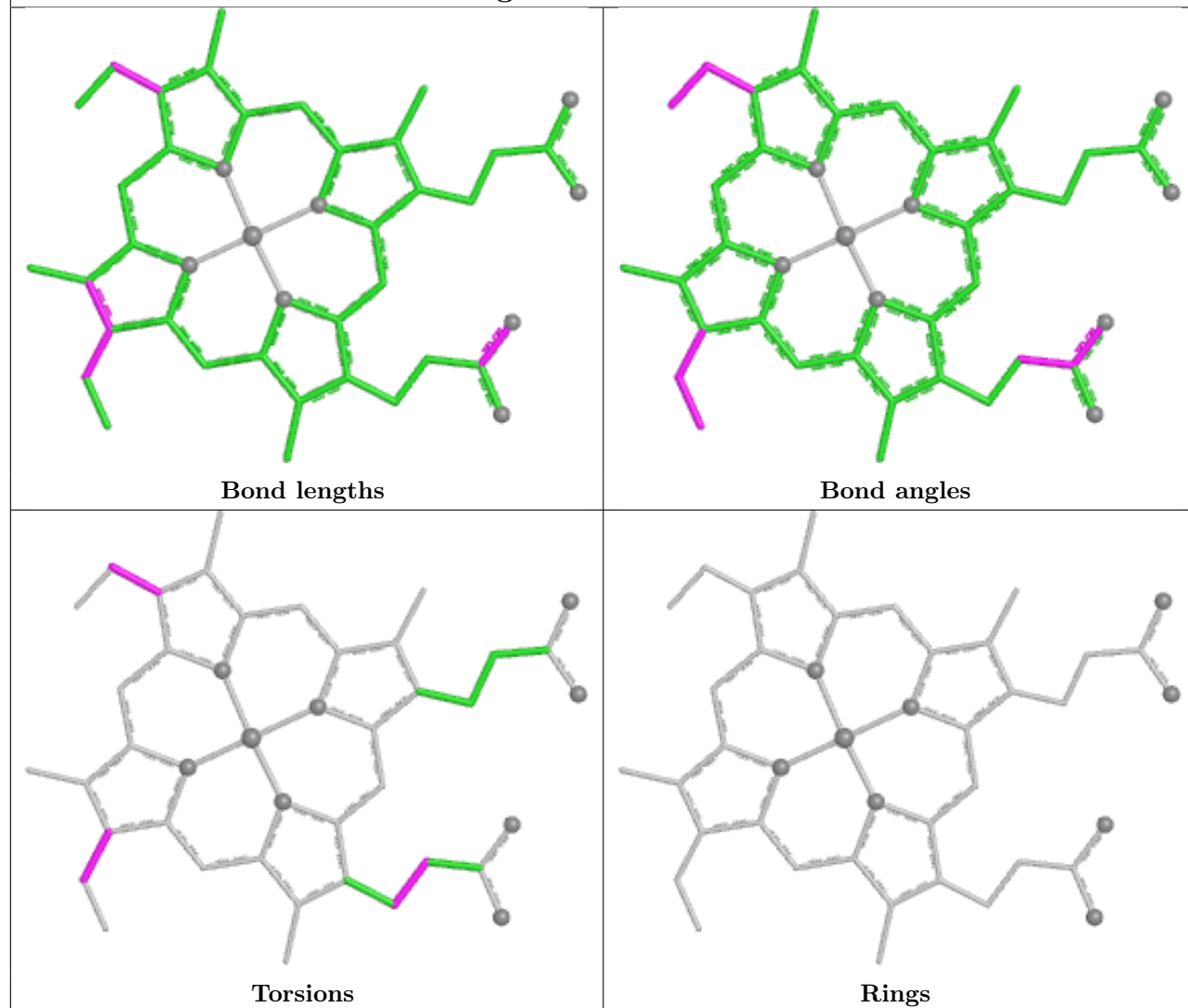




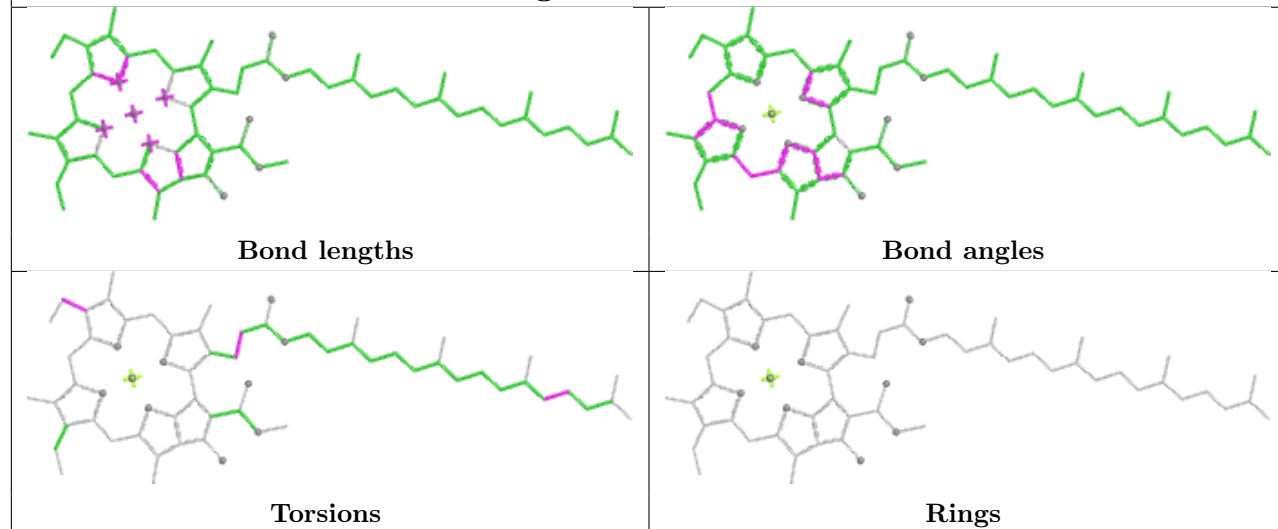


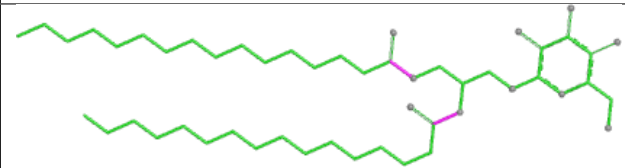
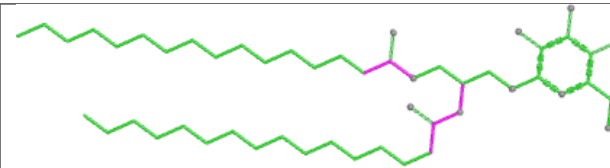
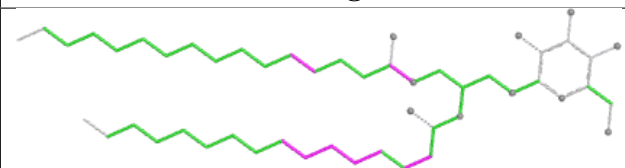
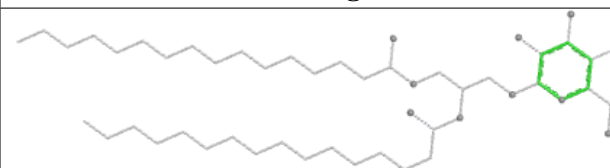


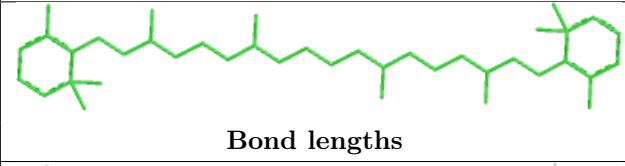
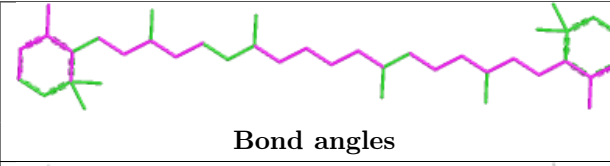
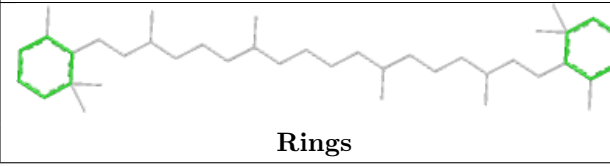
Ligand HEC v 201

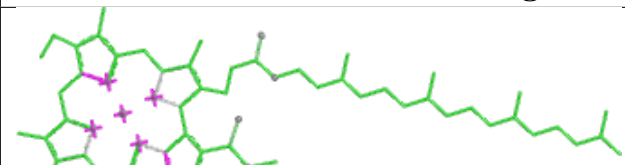
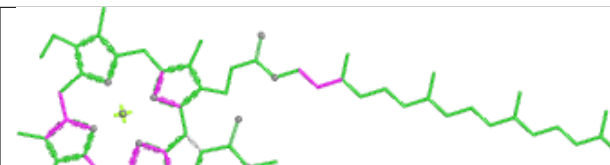
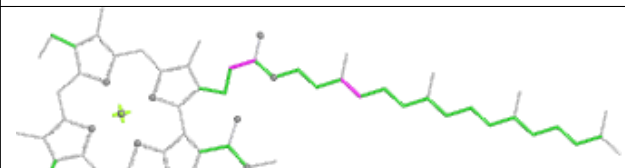
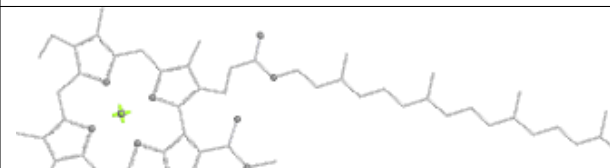


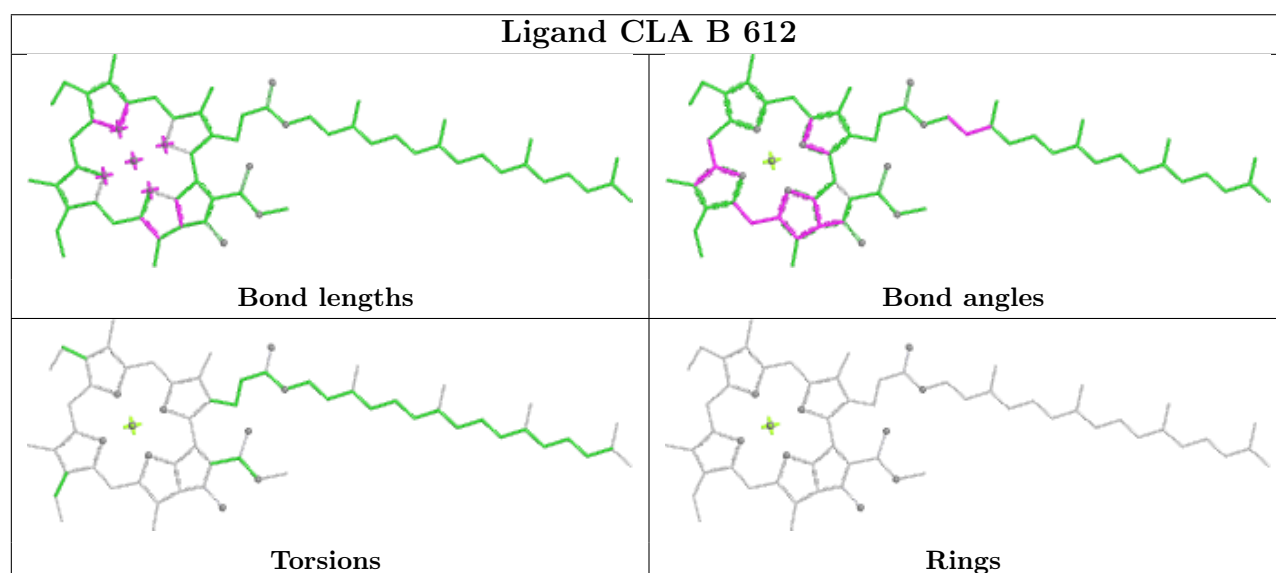
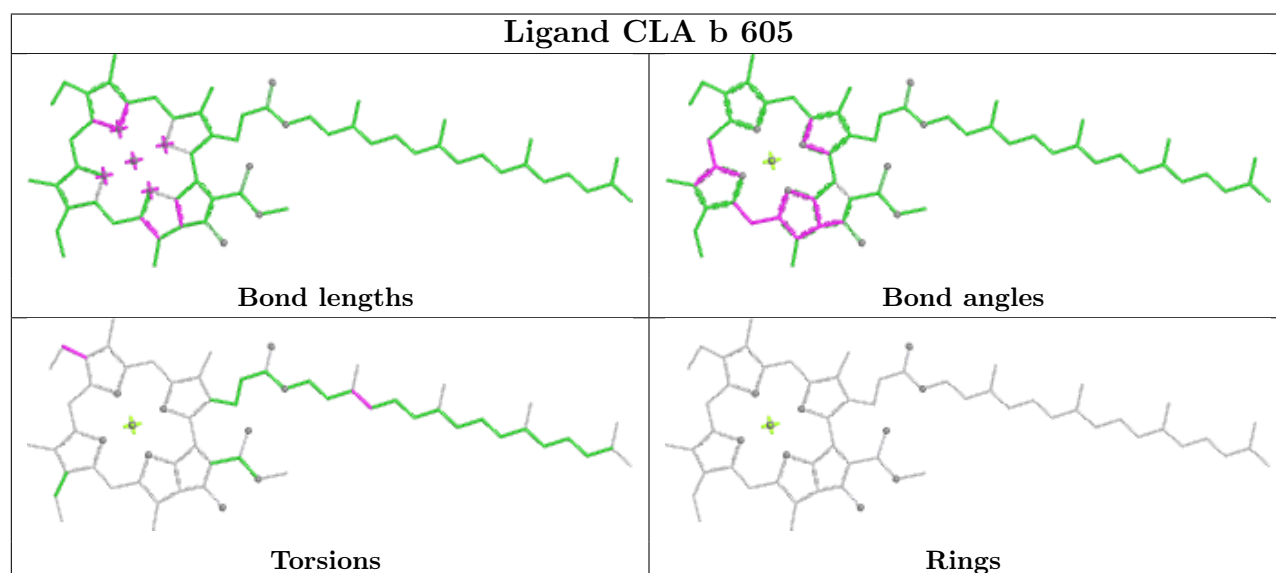
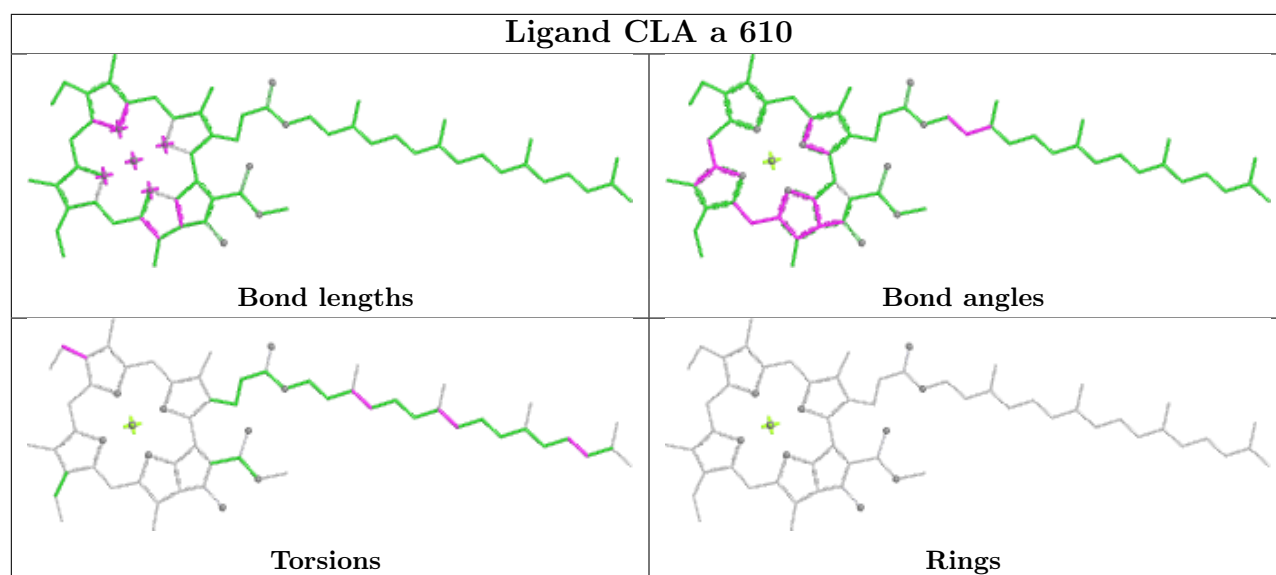
Ligand CLA b 606

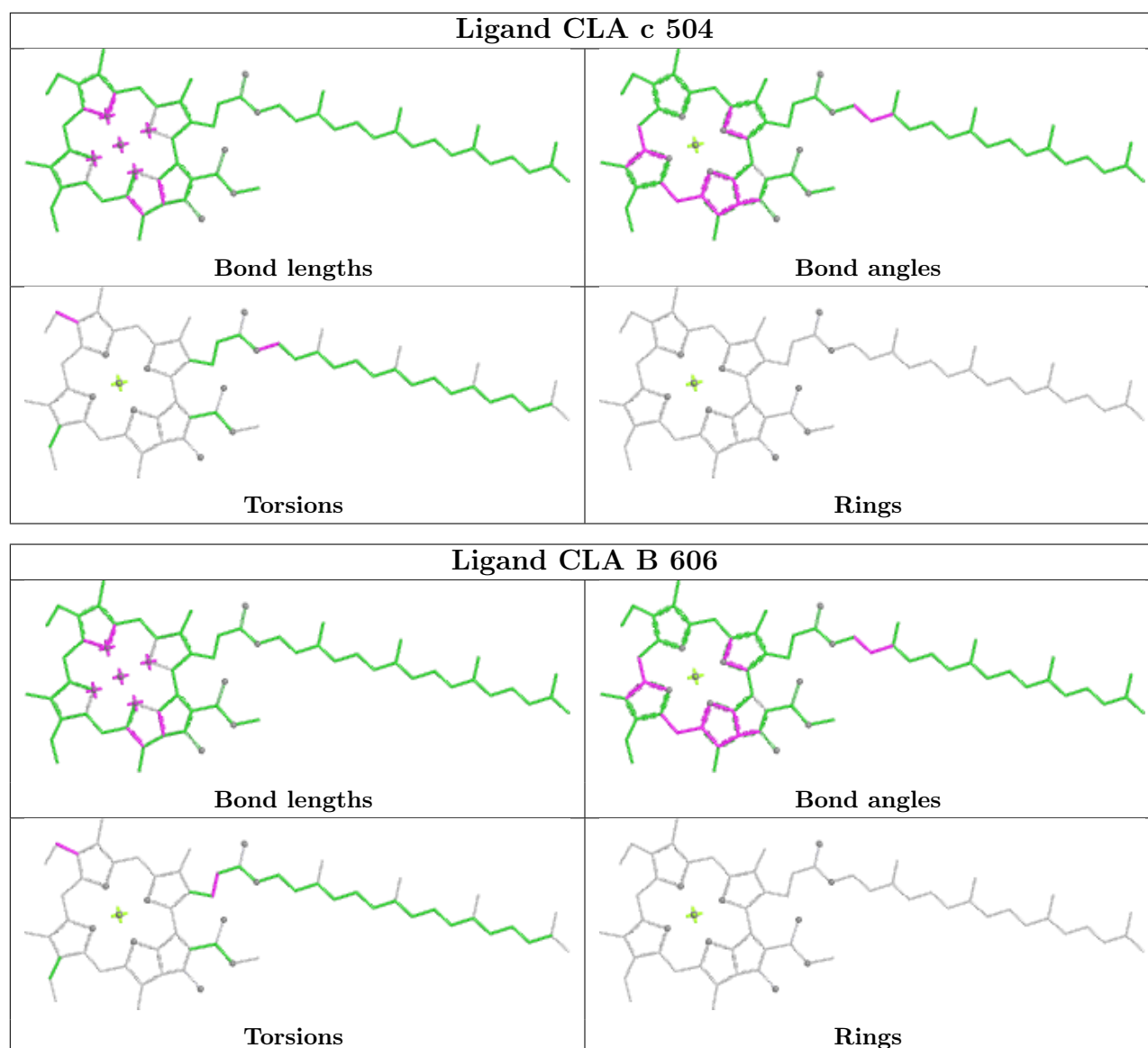


Ligand LMG c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings





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	333/344 (96%)	-0.01	5 (1%) 72 73	24, 32, 54, 72	0
1	a	333/344 (96%)	0.06	7 (2%) 63 64	24, 34, 62, 76	0
2	B	505/510 (99%)	0.07	19 (3%) 44 42	24, 35, 61, 84	0
2	b	503/510 (98%)	0.15	14 (2%) 55 54	26, 38, 67, 87	0
3	C	448/461 (97%)	0.17	10 (2%) 62 63	24, 40, 59, 77	0
3	c	448/461 (97%)	0.22	8 (1%) 67 68	29, 42, 60, 80	0
4	D	340/352 (96%)	-0.01	5 (1%) 72 73	25, 34, 52, 70	0
4	d	340/352 (96%)	0.06	2 (0%) 85 87	26, 37, 59, 74	0
5	E	82/84 (97%)	0.94	11 (13%) 7 5	39, 57, 71, 75	0
5	e	79/84 (94%)	0.95	5 (6%) 26 23	43, 58, 71, 81	0
6	F	33/45 (73%)	0.43	0 100 100	42, 49, 63, 71	0
6	f	33/45 (73%)	0.74	1 (3%) 52 52	46, 52, 73, 82	0
7	H	63/66 (95%)	0.33	1 (1%) 70 72	34, 41, 48, 60	0
7	h	63/66 (95%)	0.58	3 (4%) 35 33	39, 48, 59, 69	0
8	I	33/38 (86%)	-0.05	1 (3%) 52 52	30, 36, 44, 55	0
8	i	35/38 (92%)	0.17	0 100 100	31, 39, 56, 66	0
9	J	34/40 (85%)	0.58	1 (2%) 53 53	40, 53, 64, 78	0
9	j	33/40 (82%)	0.66	0 100 100	43, 52, 61, 65	0
10	K	36/46 (78%)	1.09	6 (16%) 4 3	52, 61, 75, 77	0
10	k	36/46 (78%)	0.83	1 (2%) 55 54	48, 60, 76, 78	0
11	L	36/37 (97%)	-0.09	0 100 100	26, 33, 53, 59	0
11	l	36/37 (97%)	-0.09	0 100 100	28, 35, 50, 62	0
12	M	32/36 (88%)	0.07	0 100 100	30, 36, 56, 58	0
12	m	32/36 (88%)	0.14	0 100 100	30, 38, 57, 63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/272 (88%)	0.33	11 (4%) 38 35	30, 44, 70, 104	0
13	o	243/272 (89%)	0.42	12 (4%) 35 32	28, 45, 72, 108	0
14	T	29/32 (90%)	0.02	2 (6%) 23 19	26, 35, 56, 62	0
14	t	29/32 (90%)	0.10	3 (10%) 12 9	31, 36, 55, 67	0
15	U	96/134 (71%)	0.35	1 (1%) 79 81	34, 43, 64, 72	0
15	u	96/134 (71%)	0.33	0 100 100	35, 45, 58, 65	0
16	V	137/163 (84%)	0.39	2 (1%) 72 73	33, 44, 56, 64	0
16	v	137/163 (84%)	0.51	1 (0%) 84 85	37, 50, 67, 82	0
17	Y	29/46 (63%)	1.87	12 (41%) 0 0	63, 76, 95, 96	0
17	y	29/46 (63%)	1.43	4 (13%) 6 5	61, 71, 90, 91	0
18	X	37/41 (90%)	0.32	1 (2%) 56 55	42, 50, 65, 79	0
18	x	38/41 (92%)	0.57	4 (10%) 11 9	41, 52, 74, 84	0
19	Z	62/62 (100%)	1.47	16 (25%) 1 1	57, 73, 104, 111	0
19	z	62/62 (100%)	1.44	9 (14%) 6 4	62, 74, 100, 107	0
20	R	34/41 (82%)	1.56	8 (23%) 2 1	61, 74, 88, 92	0
20	r	33/41 (80%)	1.70	14 (42%) 0 0	64, 73, 86, 91	0
All	All	5279/5700 (92%)	0.28	200 (3%) 44 42	24, 41, 72, 111	0

The worst 5 of 200 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	49	TYR	5.8
13	O	56	PRO	5.3
17	y	18	VAL	5.1
19	Z	33	TRP	4.9
17	Y	19	ILE	4.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
30	SO4	u	202	5/5	0.67	0.17	64,73,90,96	0
32	UNL	D	410	15/-	0.72	0.25	36,44,67,68	0
30	SO4	V	202	5/5	0.74	0.25	71,72,81,81	0
32	UNL	i	101	16/-	0.74	0.20	33,42,48,48	0
28	SQD	L	103	54/54	0.77	0.17	34,53,92,102	0
32	UNL	b	621	10/-	0.77	0.18	32,41,44,46	0
32	UNL	B	626	9/-	0.77	0.19	35,40,44,47	0
27	PL9	a	612	55/55	0.78	0.20	48,64,76,81	0
32	UNL	b	625	16/-	0.80	0.16	37,43,48,49	0
32	UNL	B	622	8/-	0.80	0.20	38,42,45,46	0
32	UNL	m	101	10/-	0.80	0.16	44,53,58,59	0
28	SQD	L	101	54/54	0.81	0.15	34,54,89,94	0
32	UNL	M	101	10/-	0.81	0.17	45,49,60,62	0
32	UNL	T	102	15/-	0.82	0.18	36,46,51,51	0
28	SQD	f	101	43/54	0.82	0.19	55,77,85,88	0
32	UNL	b	622	12/-	0.82	0.18	37,47,51,51	0
29	LHG	E	101	42/49	0.82	0.15	44,67,78,83	0
27	PL9	A	610	55/55	0.82	0.16	34,52,63,70	0
23	LMG	a	603	51/55	0.82	0.16	37,52,70,80	0
32	UNL	J	101	11/-	0.83	0.22	48,58,64,67	0
32	UNL	j	101	15/-	0.83	0.18	43,53,57,59	0
23	LMG	C	519	51/55	0.83	0.17	48,64,79,84	0
23	LMG	B	624	51/55	0.84	0.14	41,50,60,66	0
32	UNL	B	627	12/-	0.84	0.15	33,39,45,50	0
23	LMG	b	624	51/55	0.84	0.15	43,59,69,72	0
30	SO4	a	617	5/5	0.84	0.18	52,57,70,79	0
26	BCR	K	101	40/40	0.84	0.16	51,61,70,73	0
23	LMG	A	603	51/55	0.84	0.14	36,49,64,72	0
23	LMG	c	520	51/55	0.85	0.15	41,54,74,79	0
23	LMG	B	620	51/55	0.85	0.14	27,50,57,64	0
28	SQD	a	613	54/54	0.85	0.16	37,65,73,77	0
26	BCR	c	521	40/40	0.85	0.16	43,53,62,66	0
23	LMG	a	614	51/55	0.85	0.15	34,50,68,75	0
32	UNL	d	409	15/-	0.85	0.16	39,45,52,53	0
29	LHG	a	616	42/49	0.85	0.16	53,71,80,87	0
32	UNL	I	101	14/-	0.85	0.15	32,41,48,49	0
23	LMG	C	521	51/55	0.85	0.15	38,51,63,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	513	65/65	0.86	0.14	51,62,77,82	0
30	SO4	O	302	5/5	0.86	0.18	65,66,78,80	0
25	CLA	b	601	65/65	0.86	0.14	39,59,77,84	0
28	SQD	F	101	43/54	0.86	0.17	46,63,76,85	0
30	SO4	u	201	5/5	0.86	0.14	63,66,73,73	0
26	BCR	C	514	40/40	0.86	0.15	50,58,65,66	0
32	UNL	B	621	10/-	0.86	0.15	34,41,45,46	0
32	UNL	b	626	9/-	0.86	0.18	32,45,53,56	0
23	LMG	A	612	51/55	0.86	0.15	38,52,61,63	0
23	LMG	b	620	51/55	0.86	0.14	31,44,58,60	0
26	BCR	d	404	40/40	0.86	0.14	38,50,62,67	0
26	BCR	z	101	40/40	0.86	0.14	49,59,63,67	0
32	UNL	m	102	15/-	0.86	0.14	34,43,51,52	0
32	UNL	B	623	13/-	0.87	0.15	36,40,48,51	0
23	LMG	c	518	51/55	0.87	0.15	38,58,76,80	0
32	UNL	c	519	15/-	0.87	0.15	40,46,51,53	0
32	UNL	M	102	16/-	0.87	0.13	28,43,53,56	0
31	BCT	a	618	4/4	0.87	0.12	36,38,43,44	0
32	UNL	T	103	12/-	0.87	0.13	35,42,49,49	0
30	SO4	o	301	5/5	0.87	0.20	62,68,71,91	0
26	BCR	k	102	40/40	0.87	0.15	48,59,65,65	0
32	UNL	t	101	15/-	0.87	0.13	31,49,57,57	0
26	BCR	h	101	40/40	0.88	0.12	34,44,52,53	0
25	CLA	C	511	65/65	0.88	0.13	42,58,67,70	0
25	CLA	C	512	65/65	0.88	0.13	45,56,66,71	0
32	UNL	x	101	16/-	0.88	0.12	31,42,52,54	0
28	SQD	A	611	54/54	0.89	0.14	32,57,74,79	0
30	SO4	d	410	5/5	0.89	0.10	73,73,83,84	0
25	CLA	c	513	65/65	0.89	0.14	45,60,76,79	0
26	BCR	B	619	40/40	0.89	0.12	33,39,46,50	0
25	CLA	B	601	65/65	0.89	0.12	36,49,72,80	0
32	UNL	b	623	13/-	0.89	0.15	37,44,53,54	0
26	BCR	C	522	40/40	0.89	0.14	45,55,63,64	0
26	BCR	t	102	40/40	0.89	0.12	28,39,45,49	0
29	LHG	A	614	49/49	0.89	0.15	29,48,70,78	0
26	BCR	D	406	40/40	0.89	0.14	28,45,64,66	0
26	BCR	H	101	40/40	0.89	0.12	32,37,53,54	0
29	LHG	d	407	49/49	0.89	0.16	38,50,68,76	0
30	SO4	A	615	5/5	0.89	0.21	49,50,62,64	0
30	SO4	O	301	5/5	0.89	0.15	51,67,76,82	0
25	CLA	C	503	65/65	0.89	0.11	32,44,49,50	0
27	PL9	d	405	55/55	0.89	0.13	29,37,50,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	DGD	C	517	62/66	0.89	0.13	36,50,69,82	0
25	CLA	c	511	65/65	0.90	0.12	39,54,62,66	0
25	CLA	c	512	65/65	0.90	0.13	44,57,65,68	0
32	UNL	B	625	16/-	0.90	0.12	37,42,49,50	0
23	LMG	d	408	51/55	0.90	0.14	35,49,72,80	0
32	UNL	k	101	9/-	0.90	0.13	44,52,56,56	0
25	CLA	C	510	65/65	0.90	0.11	36,46,58,68	0
32	UNL	C	520	15/-	0.90	0.12	31,42,47,47	0
27	PL9	D	407	55/55	0.90	0.13	21,37,44,47	0
30	SO4	U	201	5/5	0.90	0.10	47,60,63,71	5
29	LHG	a	615	49/49	0.90	0.12	32,42,53,62	0
33	DGD	c	516	62/66	0.90	0.14	32,46,78,87	0
25	CLA	C	502	65/65	0.91	0.10	35,43,48,50	0
26	BCR	A	609	40/40	0.91	0.10	24,34,39,40	0
26	BCR	B	618	40/40	0.91	0.10	23,35,48,50	0
23	LMG	D	409	51/55	0.91	0.14	31,48,74,83	0
29	LHG	L	102	49/49	0.91	0.11	27,39,46,50	0
25	CLA	C	508	65/65	0.91	0.12	36,43,79,88	0
26	BCR	C	515	40/40	0.91	0.12	30,40,50,54	0
29	LHG	d	406	49/49	0.91	0.11	25,41,48,53	0
25	CLA	b	614	65/65	0.91	0.11	25,38,57,65	0
29	LHG	l	101	49/49	0.91	0.11	28,39,50,53	0
25	CLA	c	503	65/65	0.91	0.10	33,43,50,57	0
25	CLA	B	614	65/65	0.91	0.11	27,36,57,61	0
25	CLA	B	616	65/65	0.91	0.13	26,36,78,87	0
26	BCR	T	101	40/40	0.91	0.12	30,41,48,50	0
26	BCR	a	611	40/40	0.91	0.10	26,35,41,44	0
26	BCR	b	617	40/40	0.91	0.11	31,41,48,51	0
33	DGD	C	518	62/66	0.91	0.13	30,46,63,70	0
26	BCR	b	619	40/40	0.91	0.12	35,44,50,54	0
33	DGD	h	102	62/66	0.91	0.12	35,44,51,56	0
25	CLA	c	508	65/65	0.92	0.12	35,44,73,77	0
25	CLA	c	509	65/65	0.92	0.11	32,45,56,61	0
25	CLA	c	510	65/65	0.92	0.11	41,46,53,57	0
25	CLA	a	608	65/65	0.92	0.12	28,36,75,85	0
25	CLA	C	504	65/65	0.92	0.11	35,49,67,75	0
25	CLA	b	606	65/65	0.92	0.10	24,35,55,62	0
26	BCR	b	618	40/40	0.92	0.10	27,36,41,48	0
25	CLA	d	403	65/65	0.92	0.12	28,39,77,85	0
25	CLA	C	509	65/65	0.92	0.10	35,43,55,60	0
25	CLA	b	615	65/65	0.92	0.10	31,39,49,52	0
29	LHG	A	613	49/49	0.92	0.12	21,37,47,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	616	65/65	0.92	0.11	28,42,62,69	0
25	CLA	C	505	65/65	0.92	0.11	29,39,49,57	0
25	CLA	c	504	65/65	0.92	0.12	35,42,61,74	0
33	DGD	H	102	62/66	0.92	0.10	27,36,47,58	0
31	BCT	A	616	4/4	0.92	0.11	28,33,33,38	0
33	DGD	c	517	62/66	0.92	0.12	33,45,66,77	0
25	CLA	c	507	65/65	0.92	0.11	31,41,50,52	0
34	PHO	d	402	64/64	0.92	0.10	29,40,48,54	0
25	CLA	c	501	65/65	0.93	0.09	27,39,45,54	0
25	CLA	c	502	65/65	0.93	0.09	31,41,49,55	0
25	CLA	a	607	65/65	0.93	0.10	22,30,37,45	0
25	CLA	B	609	65/65	0.93	0.10	28,36,43,52	0
25	CLA	c	505	65/65	0.93	0.10	32,40,48,51	0
25	CLA	c	506	65/65	0.93	0.11	35,44,66,73	0
25	CLA	B	606	65/65	0.93	0.10	25,33,57,62	0
25	CLA	b	604	65/65	0.93	0.10	23,34,50,58	0
25	CLA	B	615	65/65	0.93	0.10	28,36,47,55	0
25	CLA	b	610	65/65	0.93	0.10	23,35,45,48	0
25	CLA	b	611	65/65	0.93	0.10	23,36,45,48	0
25	CLA	b	612	65/65	0.93	0.10	24,34,43,48	0
25	CLA	B	608	65/65	0.93	0.09	21,32,41,47	0
26	BCR	c	514	40/40	0.93	0.11	26,42,50,53	0
32	UNL	X	101	10/-	0.93	0.14	36,38,40,40	0
25	CLA	C	506	65/65	0.93	0.10	32,41,67,71	0
25	CLA	C	507	65/65	0.93	0.11	26,41,51,57	0
34	PHO	D	402	64/64	0.93	0.09	24,33,41,49	0
34	PHO	a	609	64/64	0.93	0.09	24,30,39,42	0
26	BCR	B	617	40/40	0.93	0.09	32,38,44,47	0
25	CLA	A	607	65/65	0.94	0.11	23,36,71,74	0
25	CLA	b	608	65/65	0.94	0.10	28,40,49,56	0
25	CLA	b	609	65/65	0.94	0.10	28,41,55,60	0
25	CLA	A	606	65/65	0.94	0.09	19,29,35,47	0
25	CLA	B	602	65/65	0.94	0.10	21,34,47,50	0
25	CLA	B	610	65/65	0.94	0.09	20,29,37,40	0
25	CLA	b	613	65/65	0.94	0.09	21,29,52,58	0
25	CLA	D	403	65/65	0.94	0.09	23,30,39,49	0
33	DGD	C	516	62/66	0.94	0.11	25,35,67,72	0
25	CLA	D	405	65/65	0.94	0.11	24,35,63,68	0
25	CLA	a	606	65/65	0.94	0.08	19,30,40,48	0
29	LHG	D	408	49/49	0.94	0.10	20,36,45,51	0
33	DGD	c	515	62/66	0.94	0.12	26,37,70,73	0
25	CLA	B	612	65/65	0.94	0.08	25,31,40,44	0

Continued on next page...

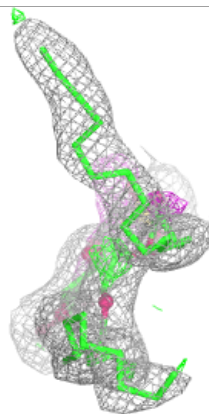
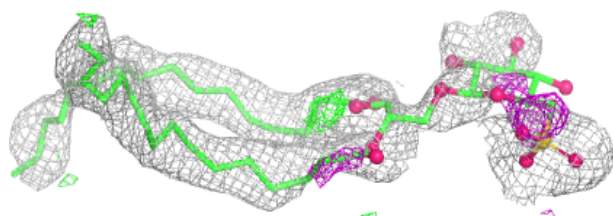
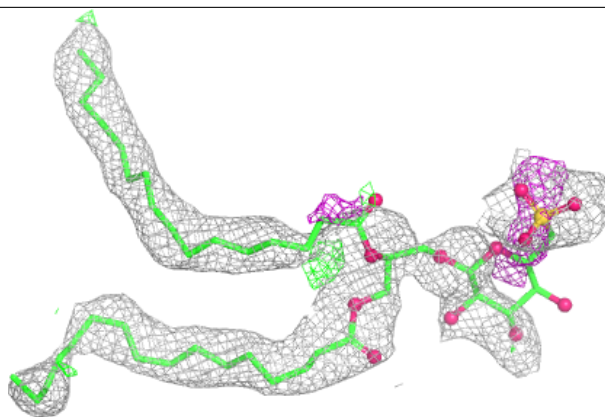
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	603	65/65	0.94	0.09	21,31,48,53	0
25	CLA	B	604	65/65	0.94	0.09	20,32,50,65	0
25	CLA	b	602	65/65	0.94	0.09	29,41,55,60	0
25	CLA	b	603	65/65	0.94	0.10	24,36,50,60	0
25	CLA	B	605	65/65	0.94	0.08	21,30,37,42	0
35	HEM	E	102	43/43	0.94	0.13	42,53,68,74	0
35	HEM	e	101	43/43	0.94	0.12	49,57,69,72	0
25	CLA	C	501	65/65	0.95	0.08	21,34,46,51	0
25	CLA	B	611	65/65	0.95	0.08	19,27,39,42	0
25	CLA	b	605	65/65	0.95	0.09	24,33,42,47	0
34	PHO	D	401	64/64	0.95	0.08	24,30,36,39	0
25	CLA	a	610	65/65	0.95	0.10	23,30,65,76	0
25	CLA	b	607	65/65	0.95	0.09	22,29,42,44	0
24	CL	a	604	1/1	0.95	0.09	40,40,40,40	0
25	CLA	d	401	65/65	0.95	0.08	20,30,45,53	0
25	CLA	B	613	65/65	0.95	0.08	21,30,50,60	0
36	HEC	v	201	43/43	0.95	0.10	29,39,47,55	0
25	CLA	D	404	65/65	0.96	0.08	18,28,40,43	0
25	CLA	B	607	65/65	0.96	0.09	19,28,53,54	0
24	CL	A	604	1/1	0.96	0.07	35,35,35,35	0
22	FE	a	602	1/1	0.96	0.06	37,37,37,37	0
36	HEC	V	201	43/43	0.96	0.10	31,38,46,48	0
25	CLA	A	608	65/65	0.96	0.10	14,27,68,74	0
21	OEX	A	601	10/10	0.98	0.06	34,40,52,57	0
24	CL	a	605	1/1	0.98	0.05	38,38,38,38	1
21	OEX	a	601	10/10	0.98	0.06	33,37,46,51	0
24	CL	A	605	1/1	0.99	0.02	26,26,26,26	0
22	FE	A	602	1/1	0.99	0.03	34,34,34,34	0

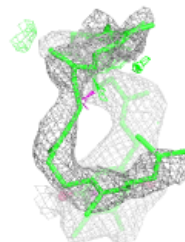
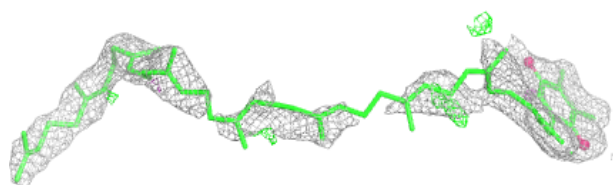
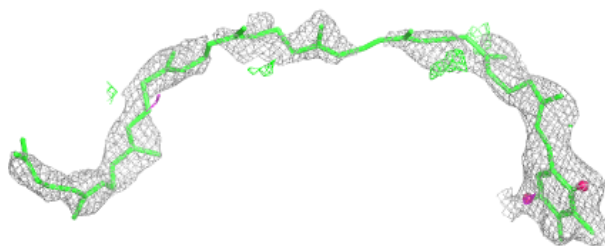
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SQD L 103:

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

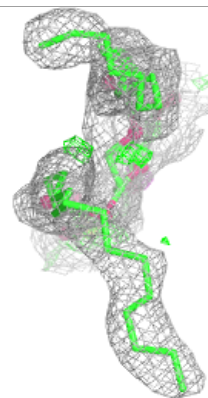
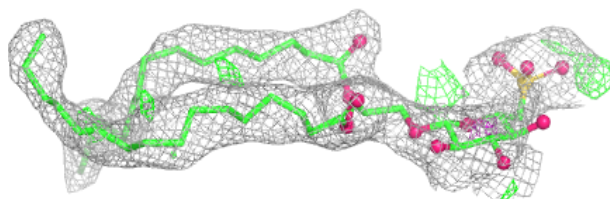
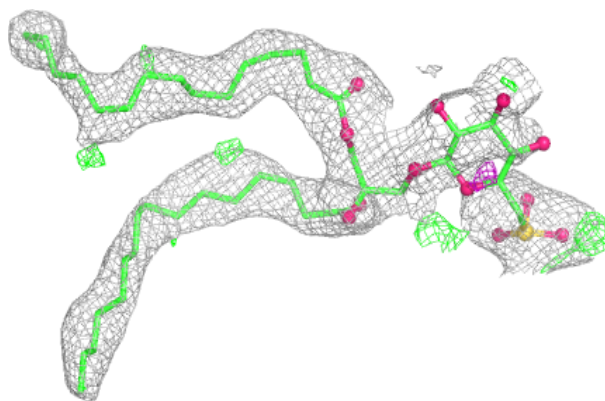
**Electron density around PL9 a 612:**

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

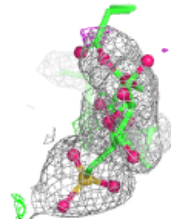
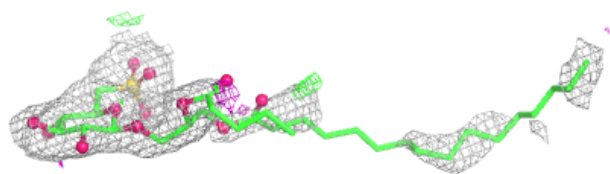
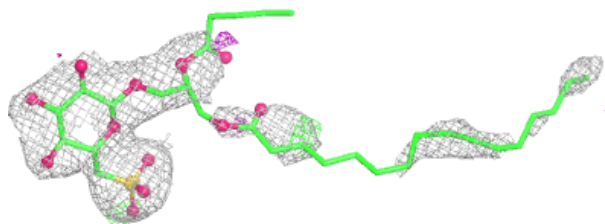


Electron density around SQD L 101:

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

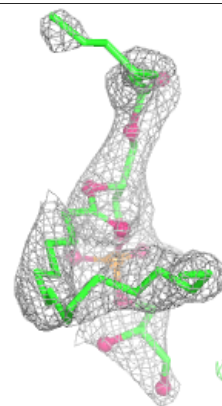
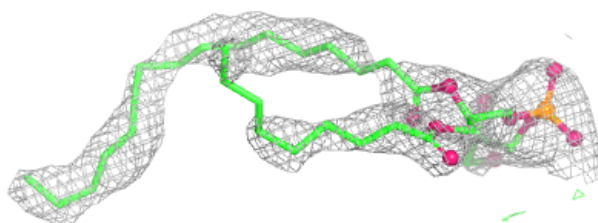
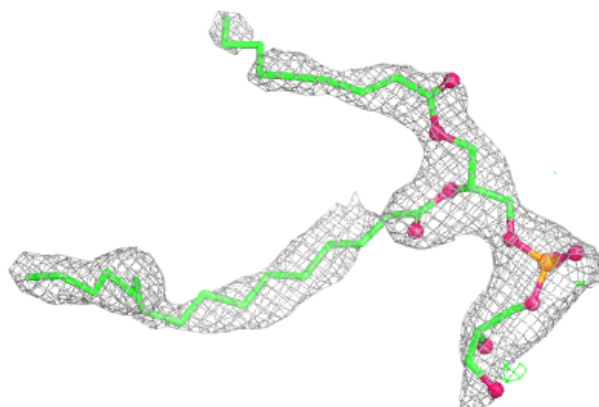
**Electron density around SQD f 101:**

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

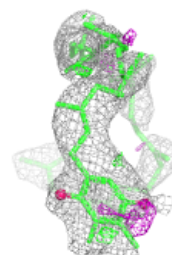
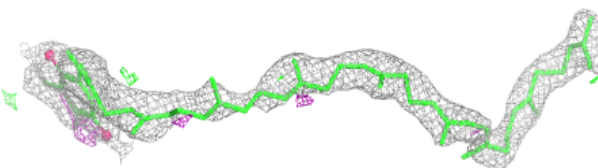
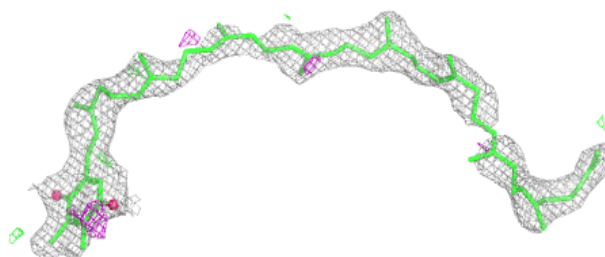


Electron density around LHG E 101:

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

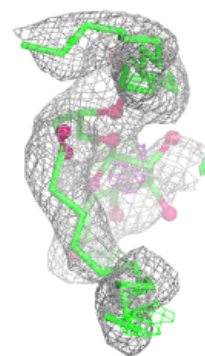
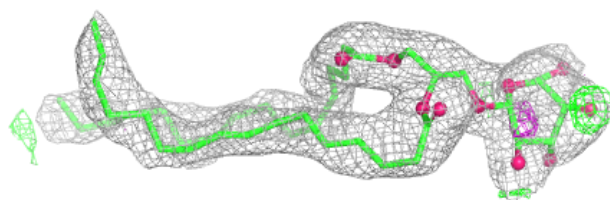
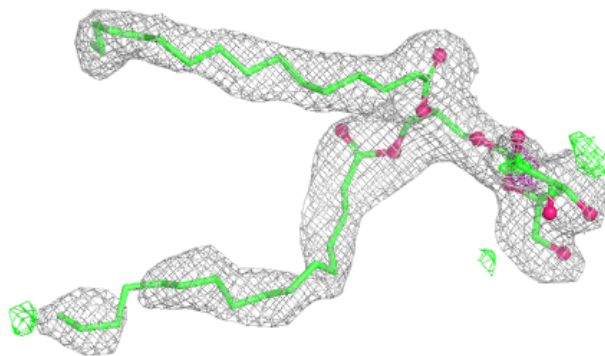
**Electron density around PL9 A 610:**

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

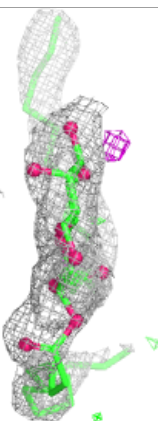
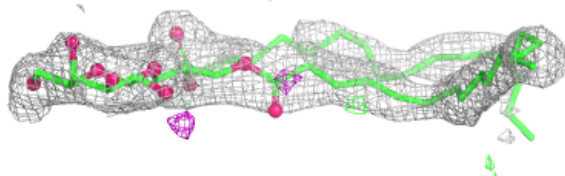
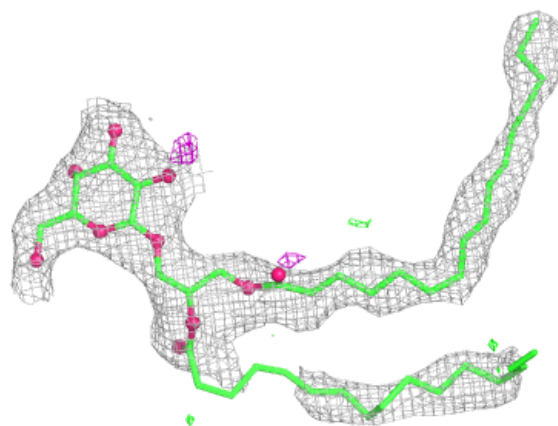


Electron density around LMG a 603:

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

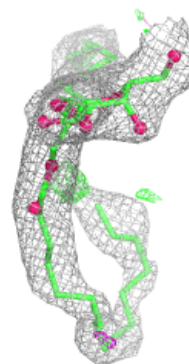
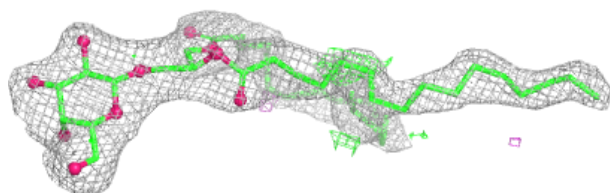
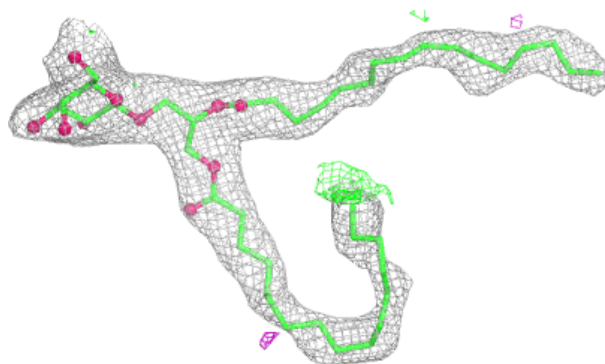
**Electron density around LMG C 519:**

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

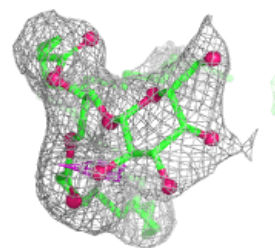
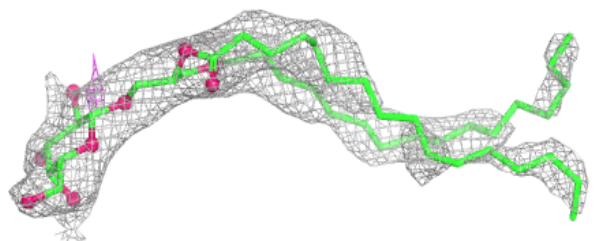
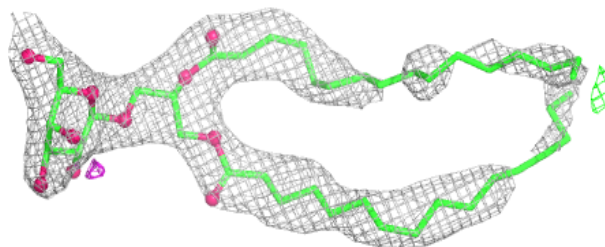


Electron density around LMG B 624:

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

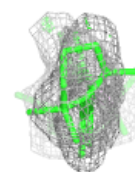
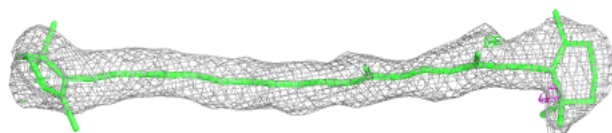
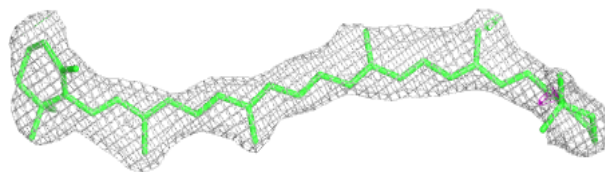
**Electron density around LMG b 624:**

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

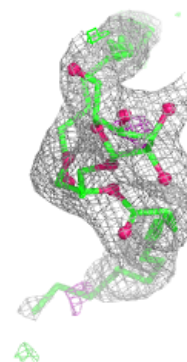
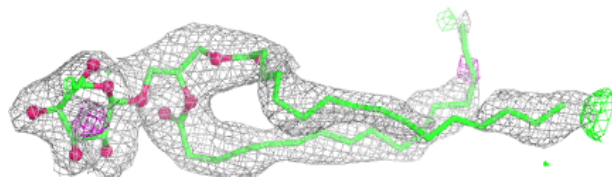
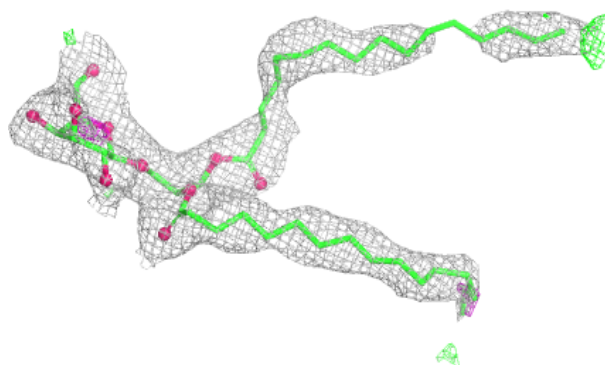


Electron density around BCR K 101:

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

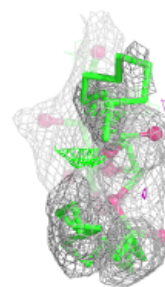
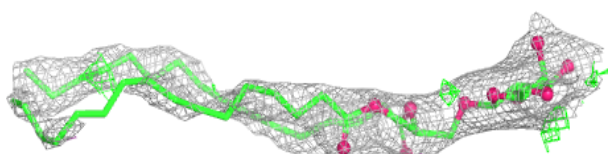
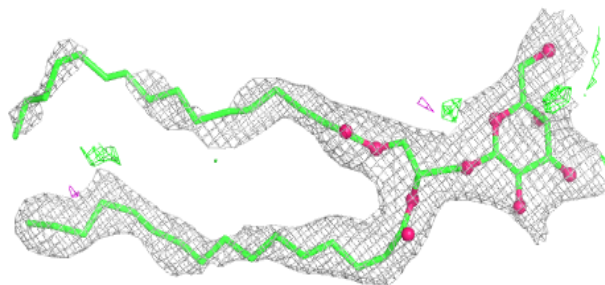
**Electron density around LMG A 603:**

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

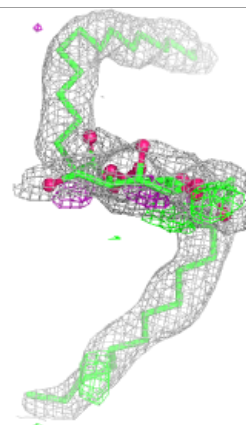
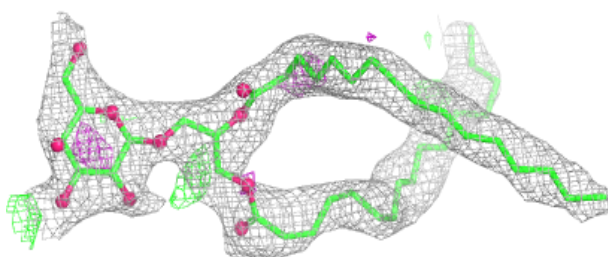
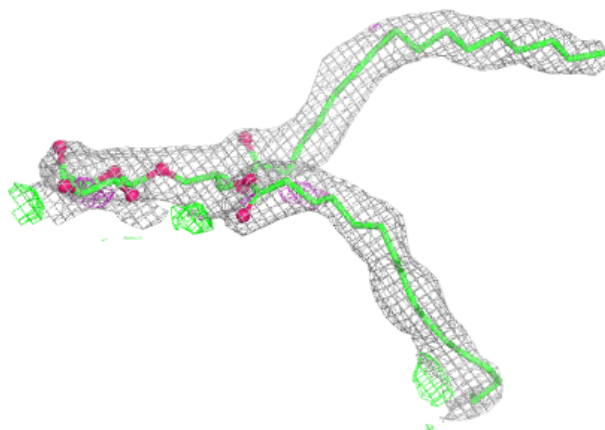


Electron density around LMG c 520:

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

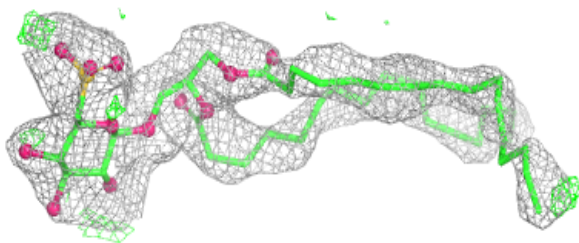
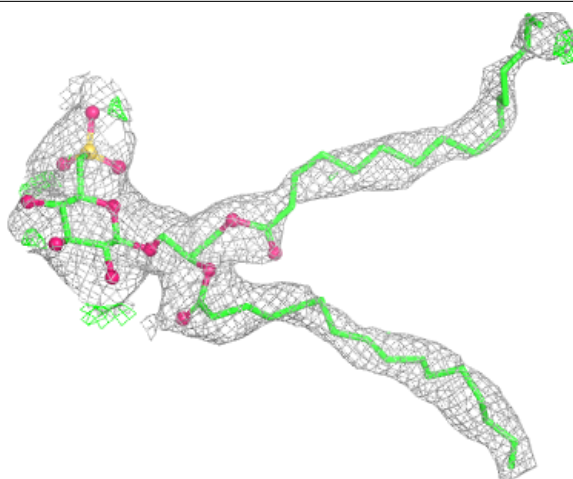
**Electron density around LMG B 620:**

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



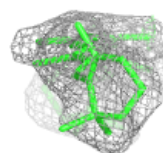
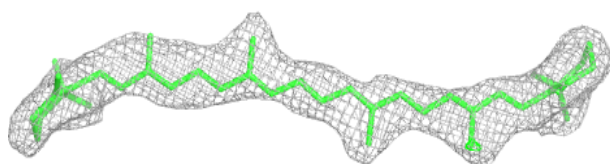
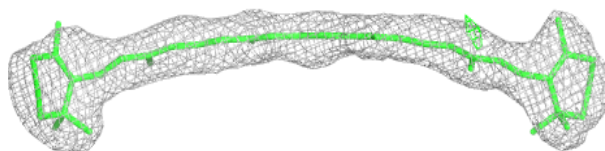
Electron density around SQD a 613:

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

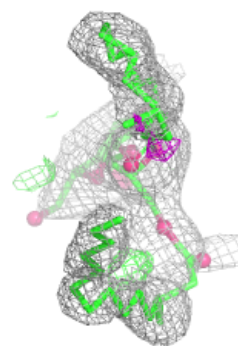
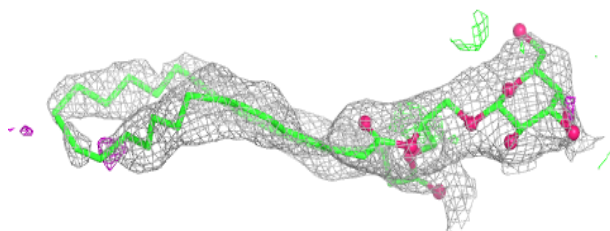
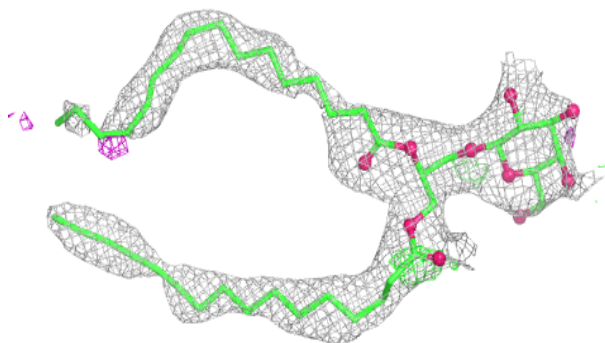


Electron density around BCR c 521:

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

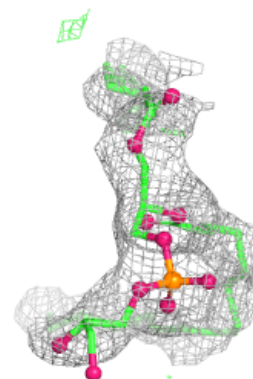
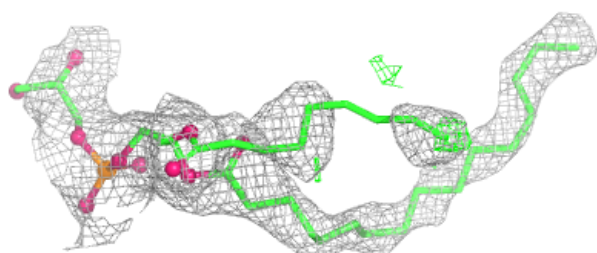
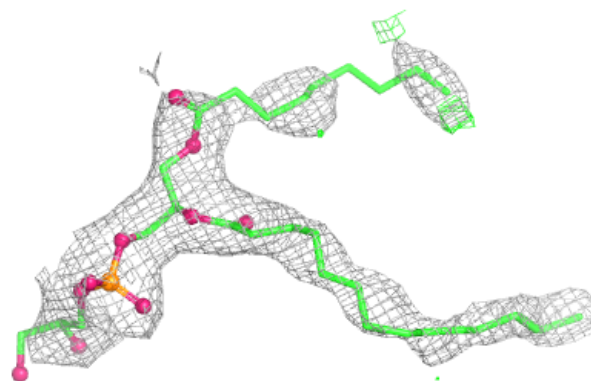
**Electron density around LMG a 614:**

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

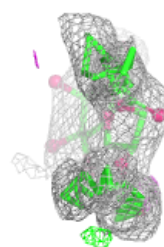
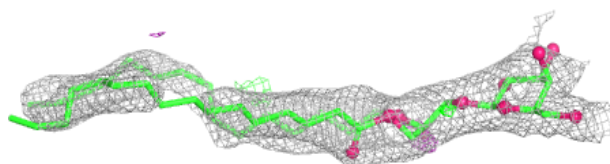
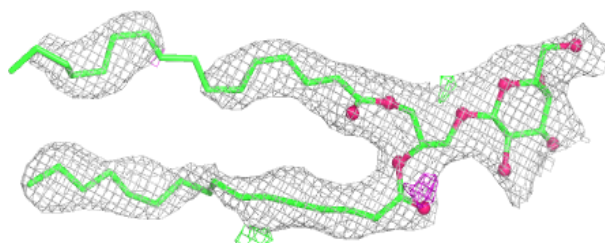


Electron density around LHG a 616:

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

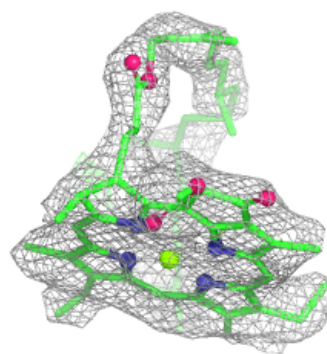
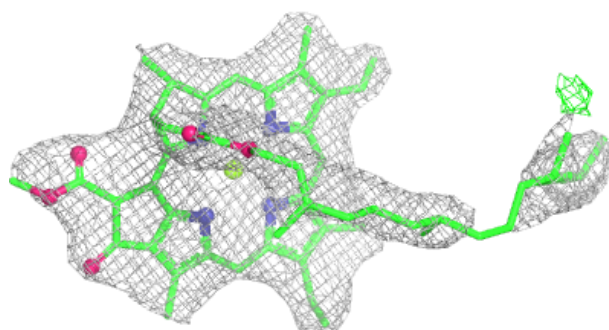
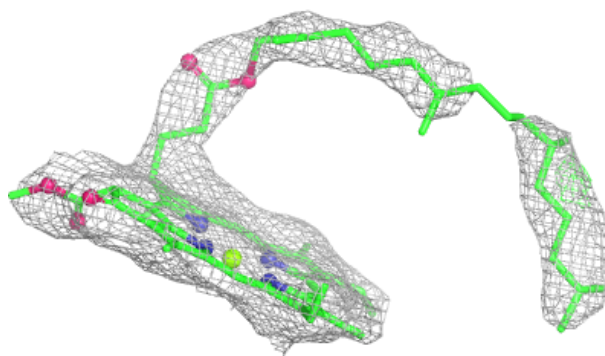
**Electron density around LMG C 521:**

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

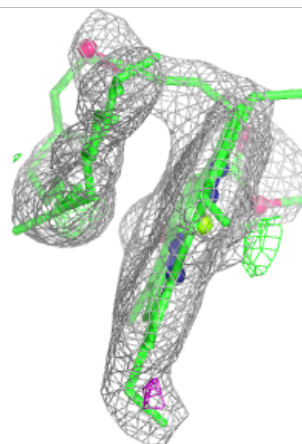
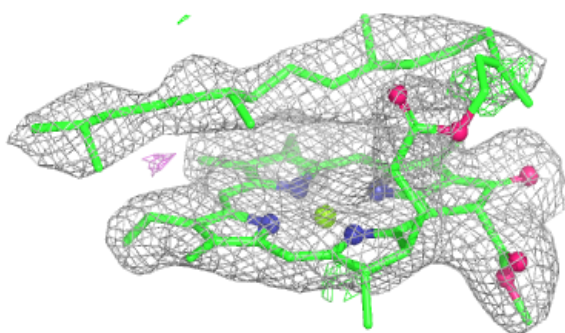
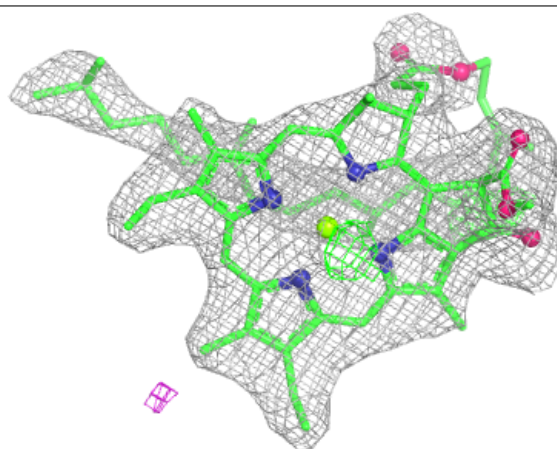


Electron density around CLA C 513:

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

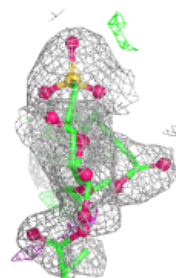
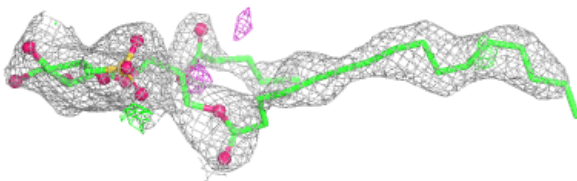
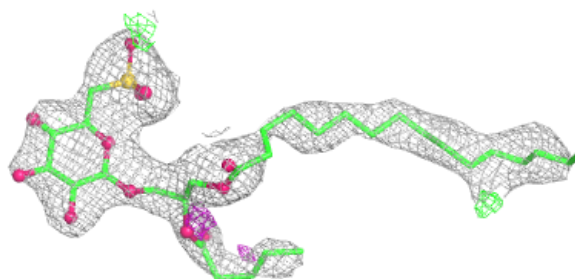
**Electron density around CLA b 601:**

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

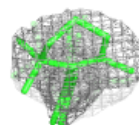
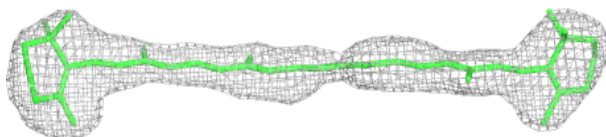
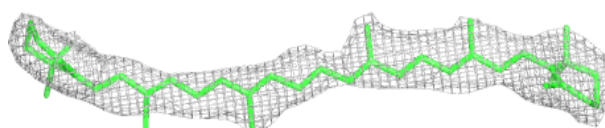


Electron density around SQD F 101:

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

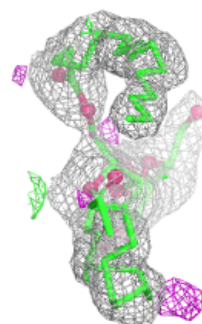
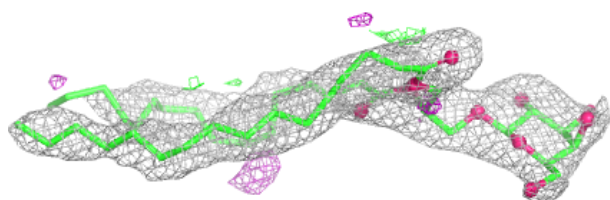
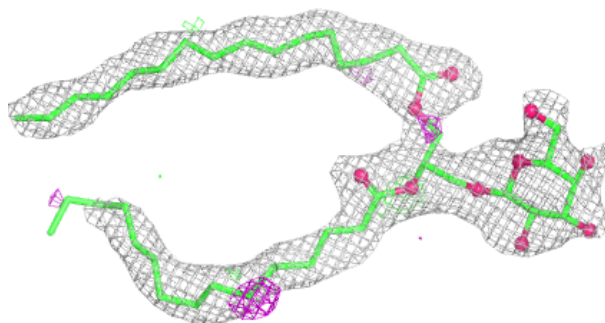
**Electron density around BCR C 514:**

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

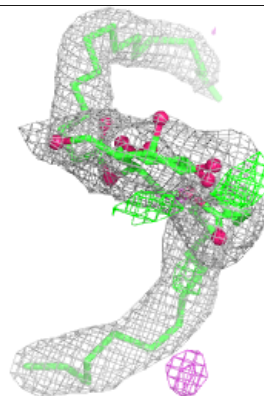
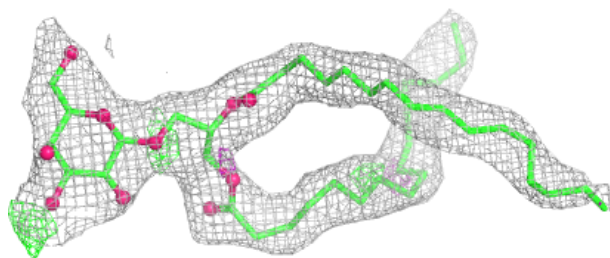
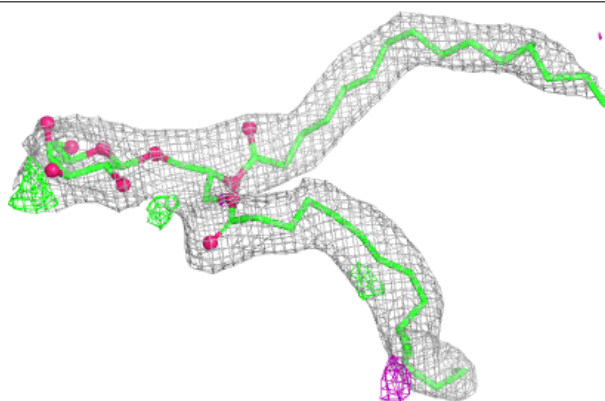


Electron density around LMG A 612:

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

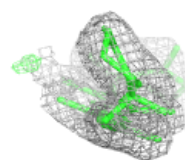
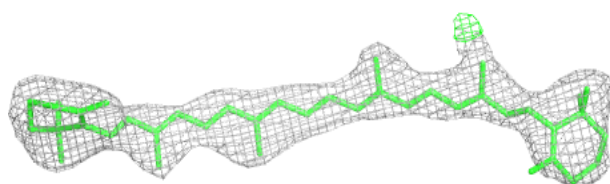
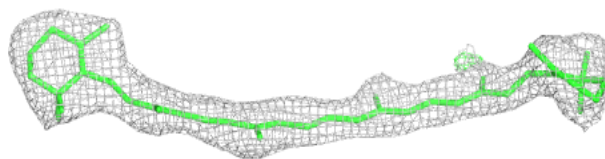
**Electron density around LMG b 620:**

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

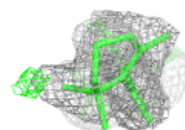
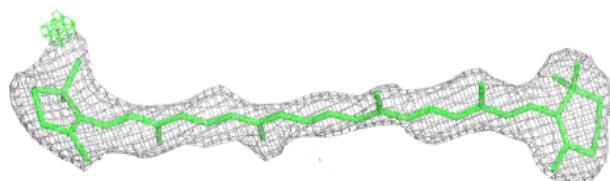
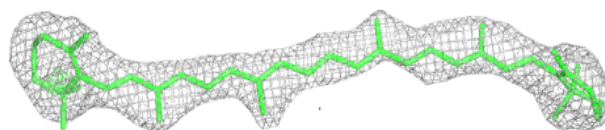


Electron density around BCR d 404:

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

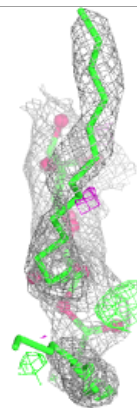
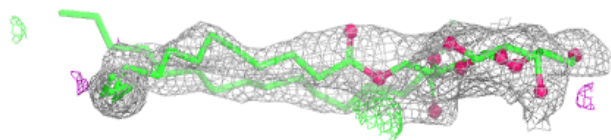
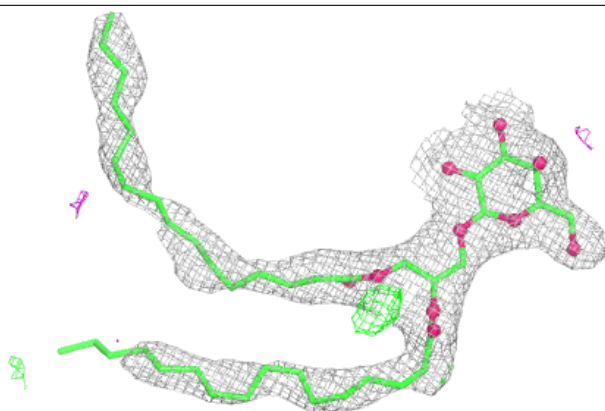
**Electron density around BCR z 101:**

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

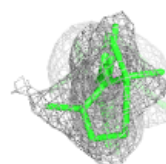
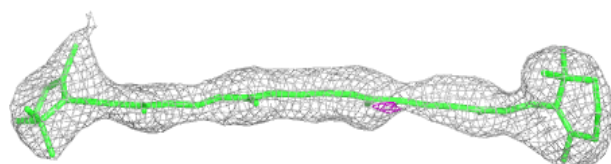


Electron density around LMG c 518:

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

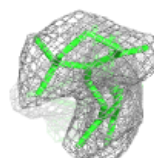
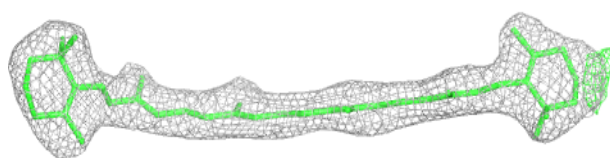
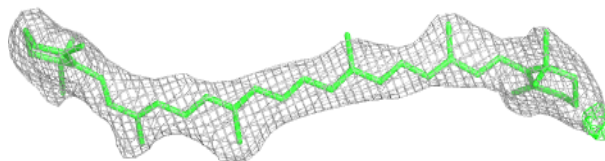
**Electron density around BCR k 102:**

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

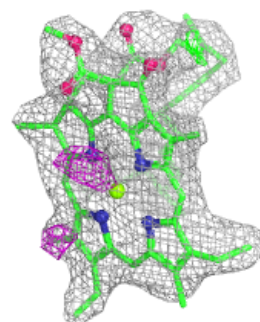
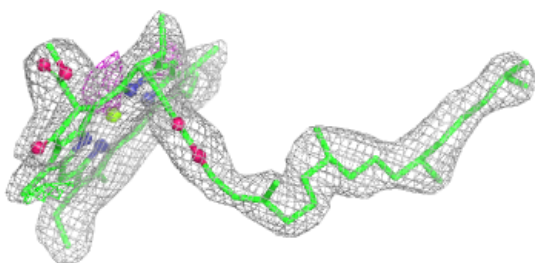
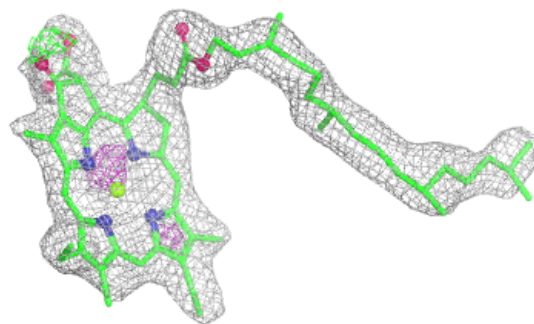


Electron density around BCR h 101:

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

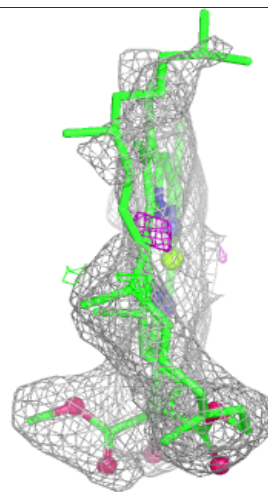
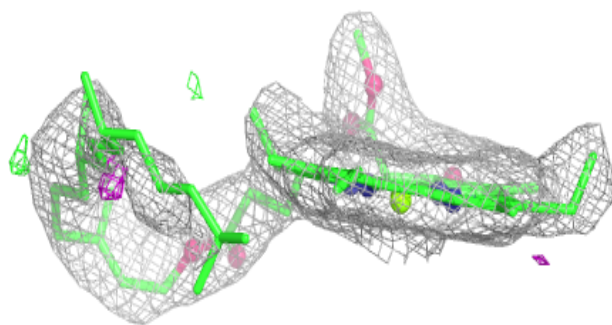
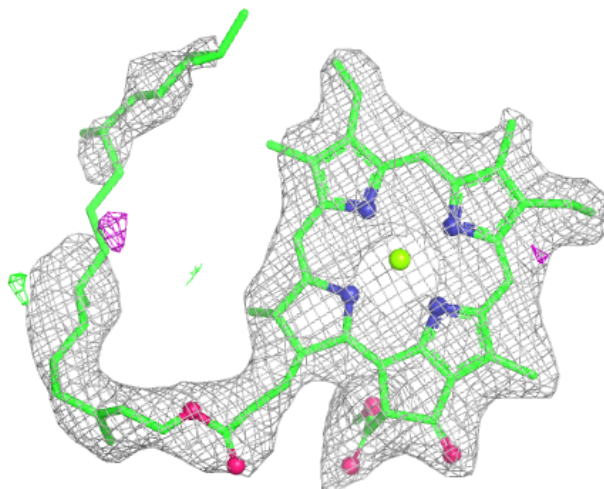
**Electron density around CLA C 511:**

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



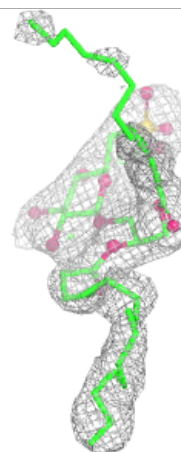
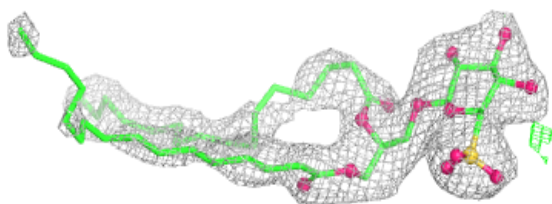
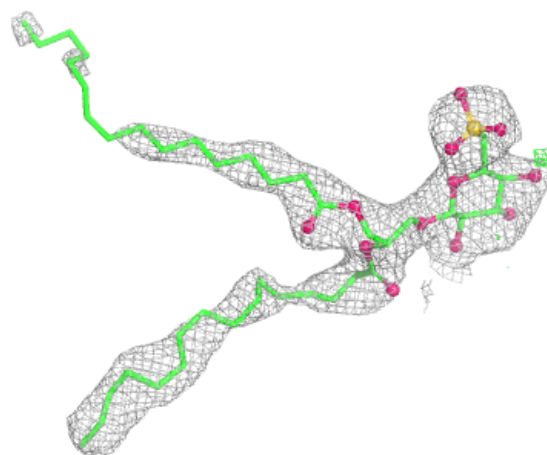
Electron density around CLA C 512:

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



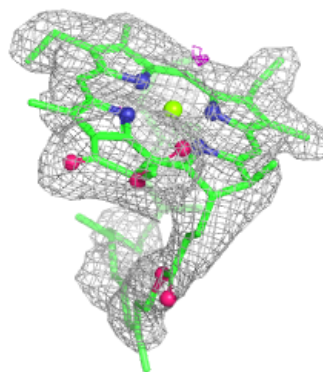
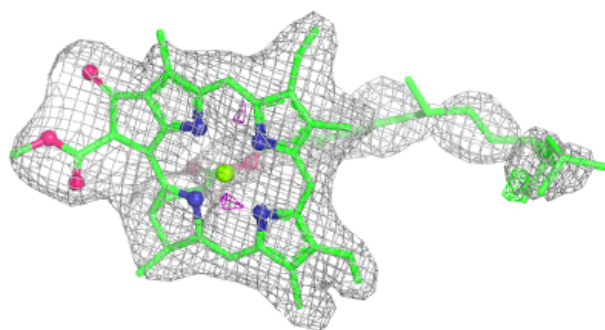
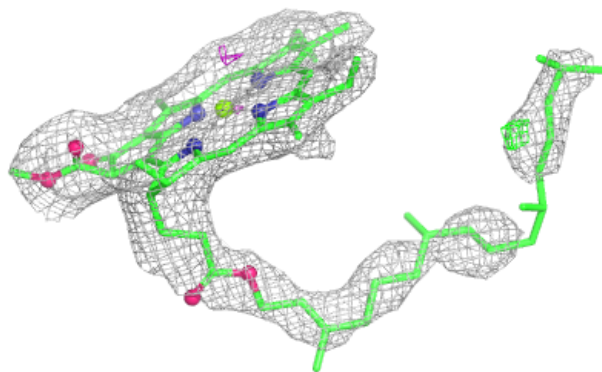
Electron density around SQD A 611:

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

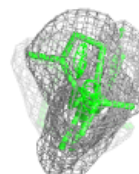
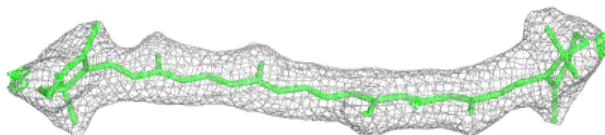
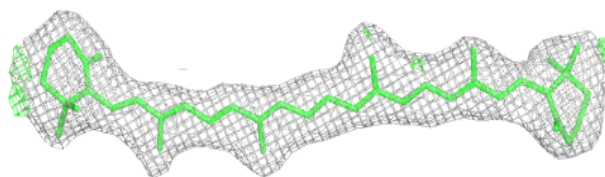


Electron density around CLA c 513:

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

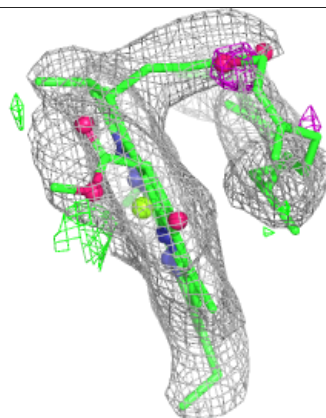
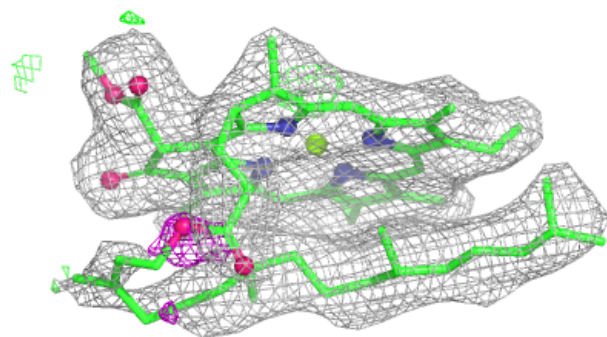
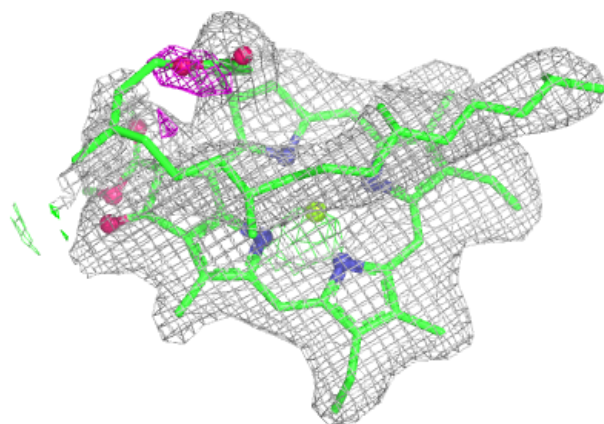
**Electron density around BCR B 619:**

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

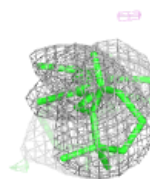
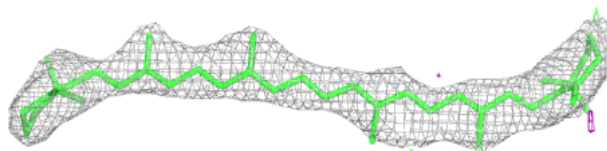
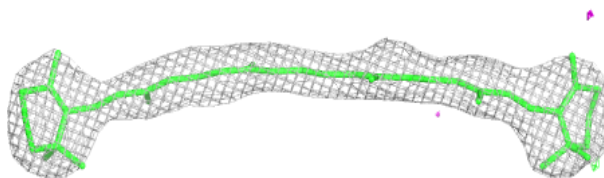


Electron density around CLA B 601:

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

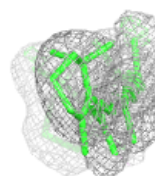
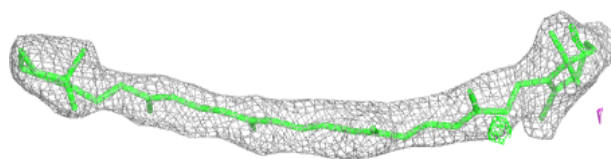
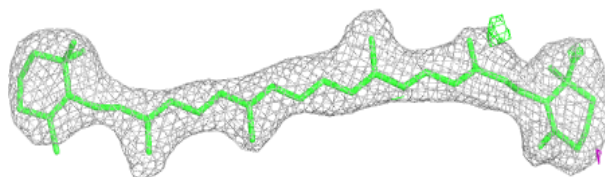
**Electron density around BCR C 522:**

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

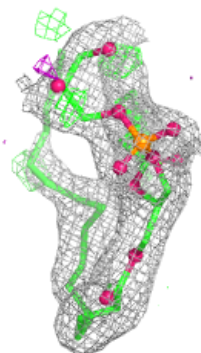
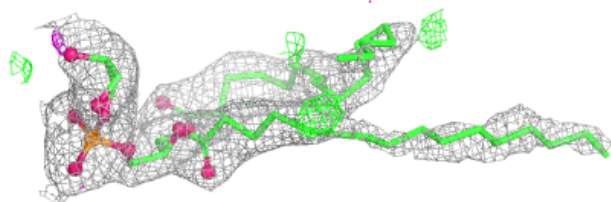
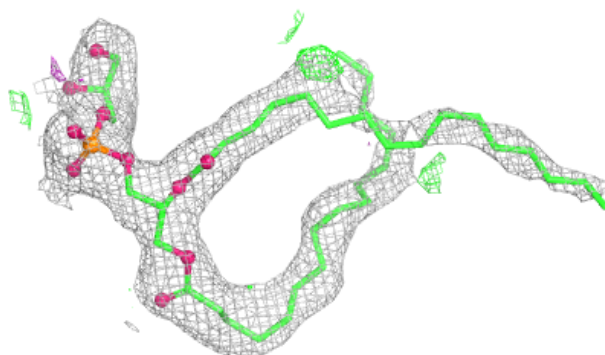


Electron density around BCR t 102:

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

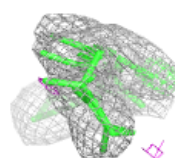
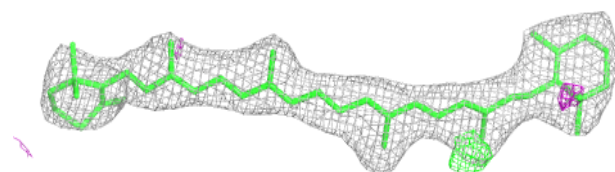
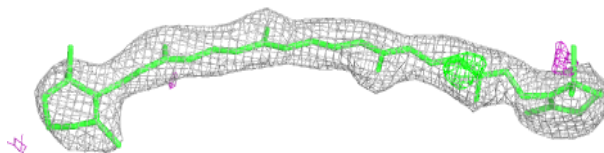
**Electron density around LHG A 614:**

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

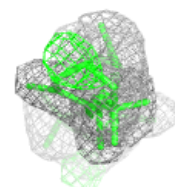
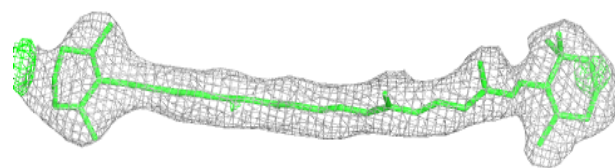
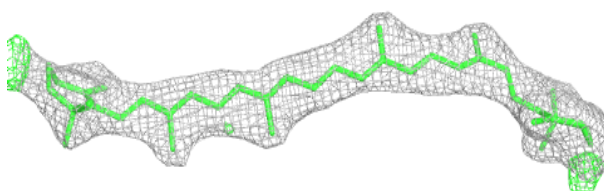


Electron density around BCR D 406:

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

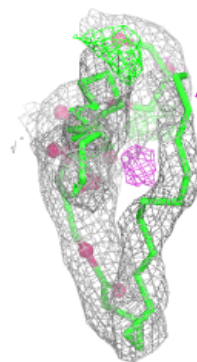
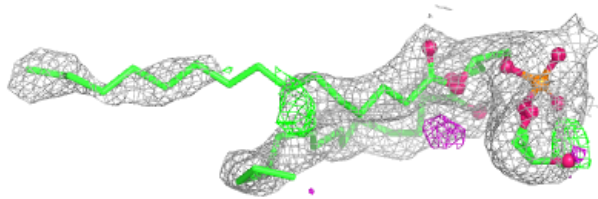
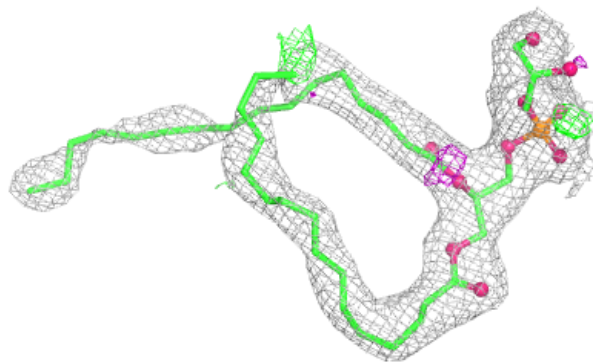
**Electron density around BCR H 101:**

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



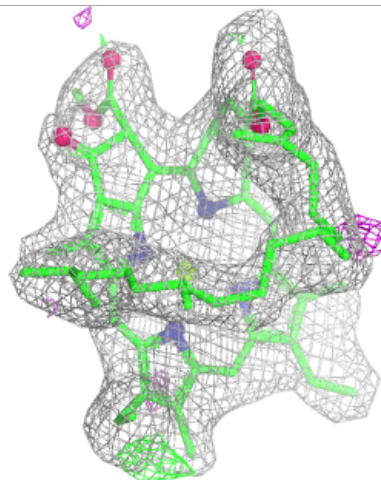
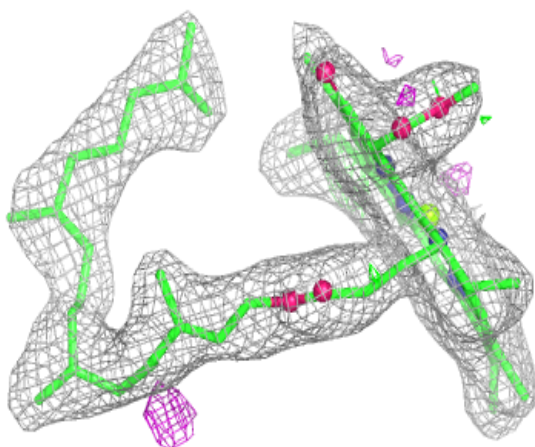
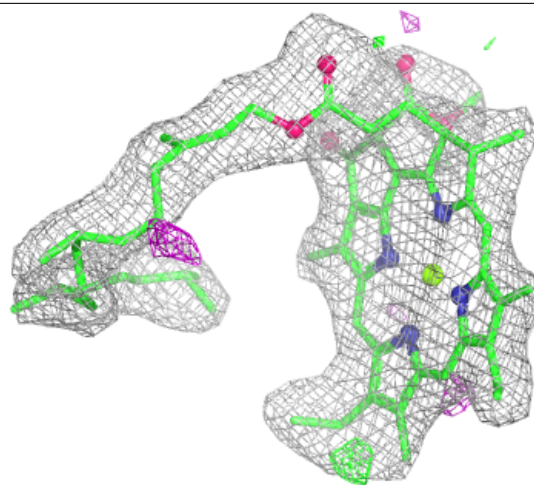
Electron density around LHG d 407:

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



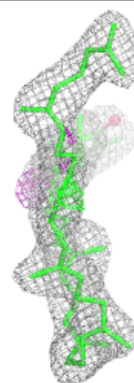
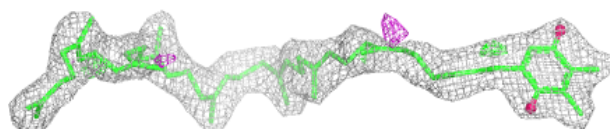
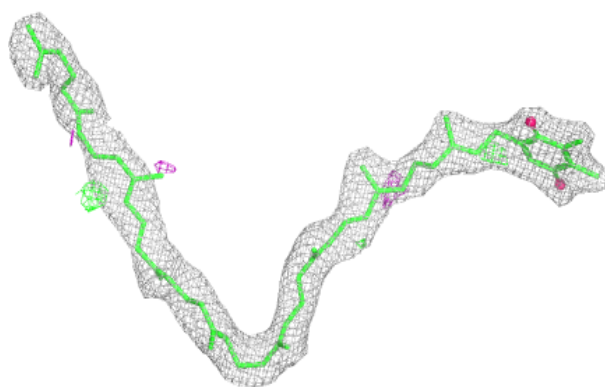
Electron density around CLA C 503:

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

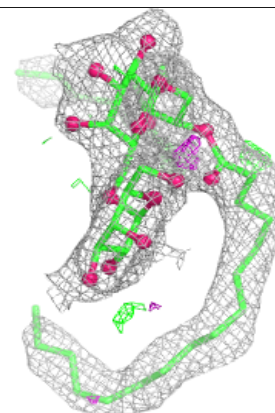
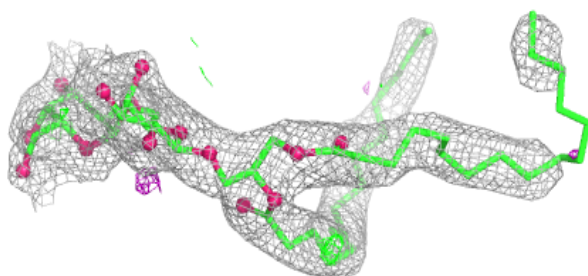
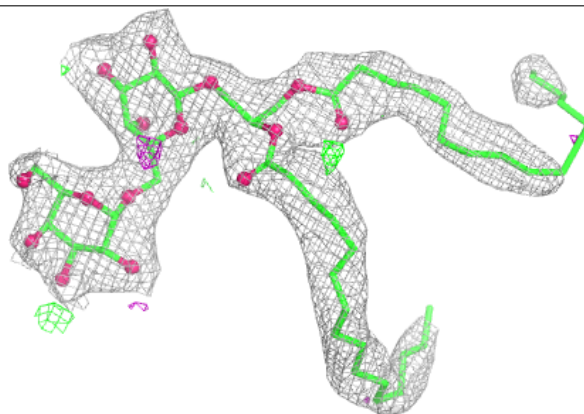


Electron density around PL9 d 405:

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

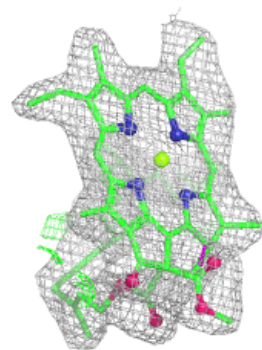
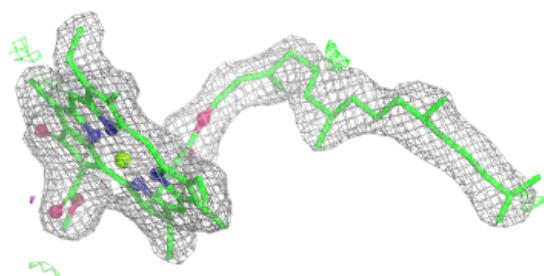
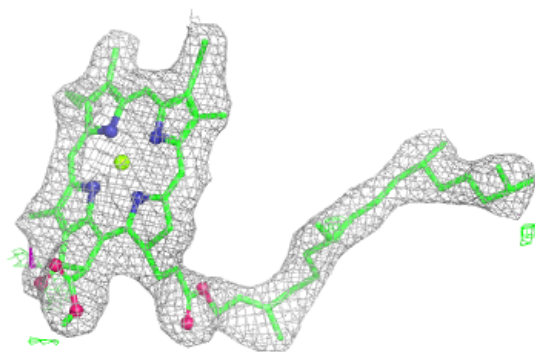
**Electron density around DGD C 517:**

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



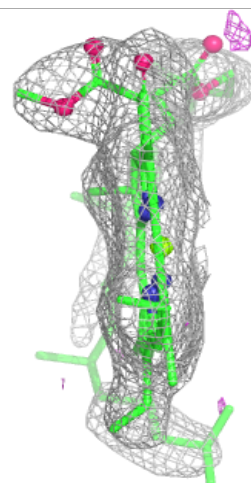
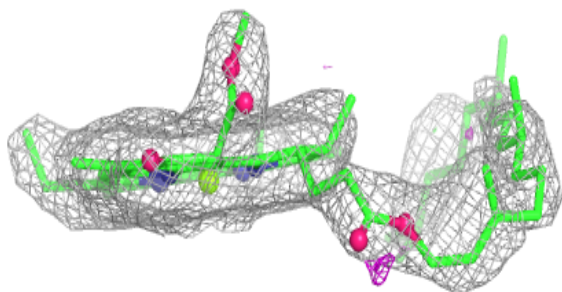
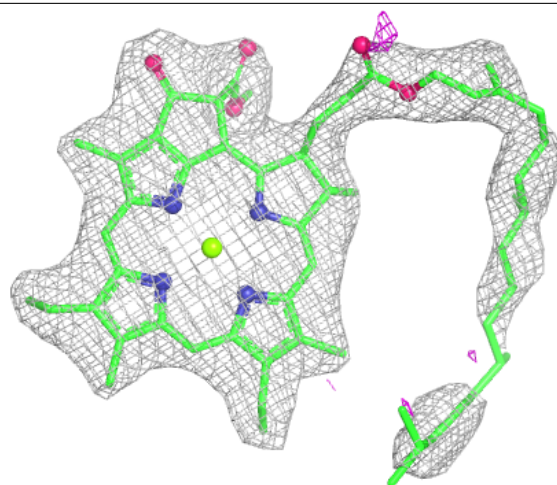
Electron density around CLA c 511:

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



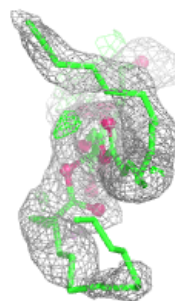
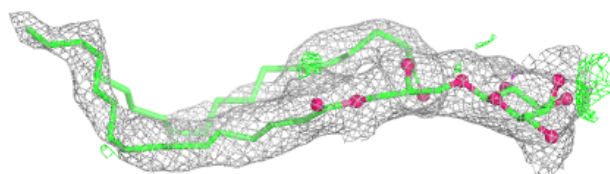
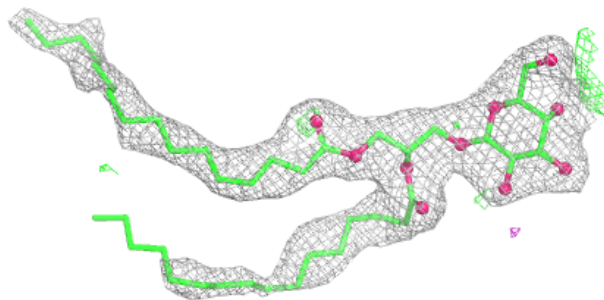
Electron density around CLA c 512:

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



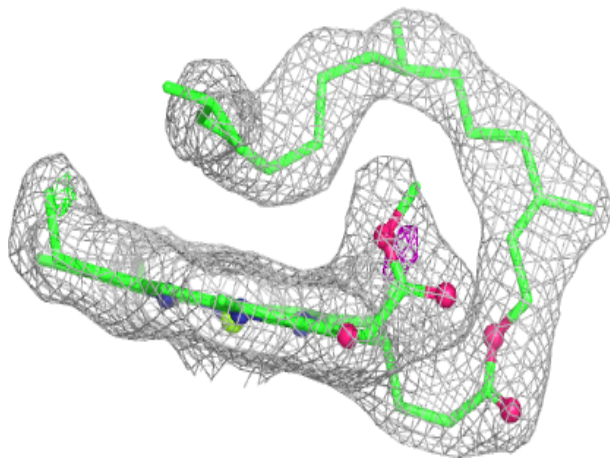
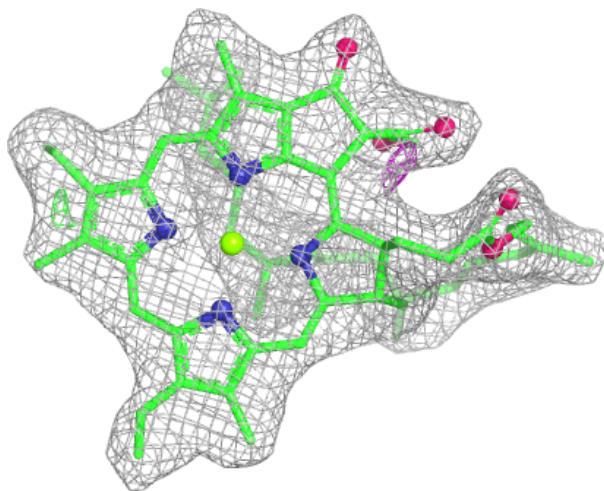
Electron density around LMG d 408:

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



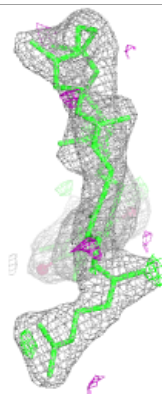
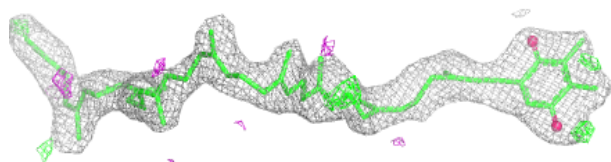
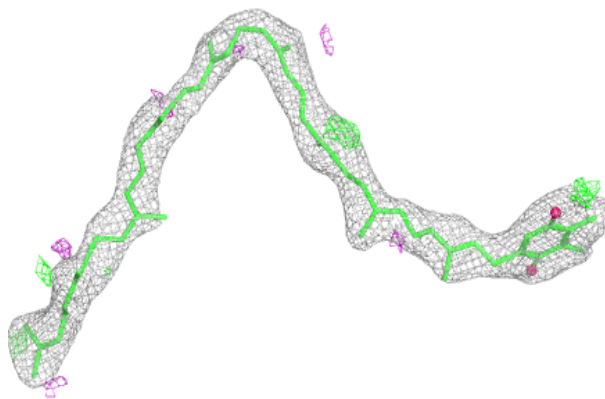
Electron density around CLA C 510:

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

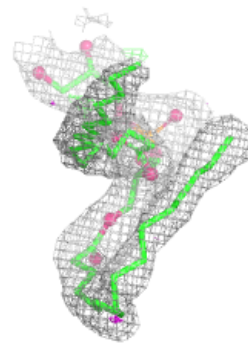
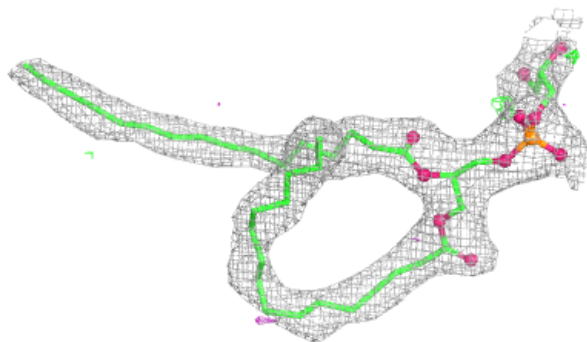


Electron density around PL9 D 407:

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

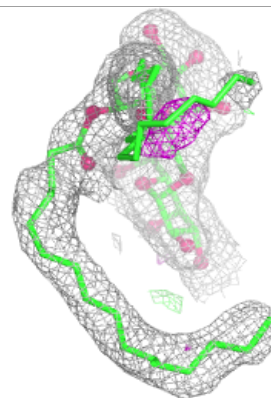
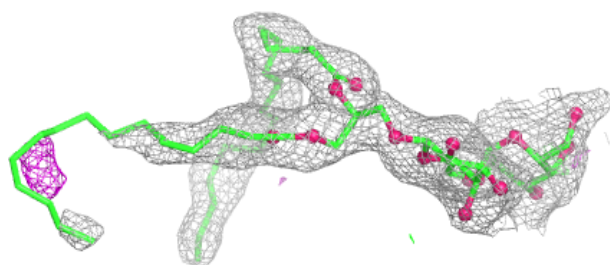
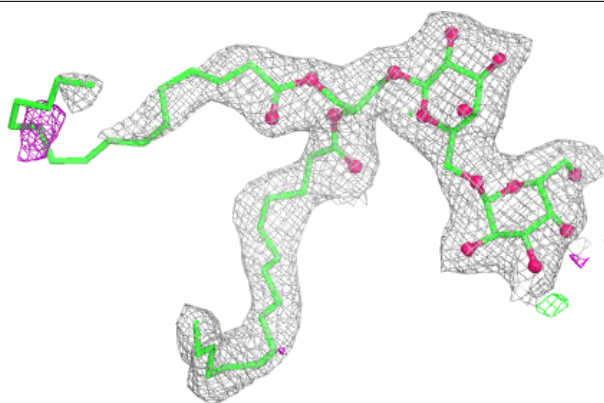
**Electron density around LHG a 615:**

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

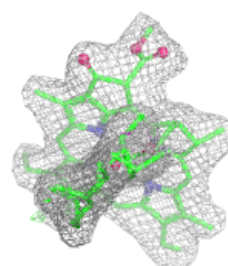
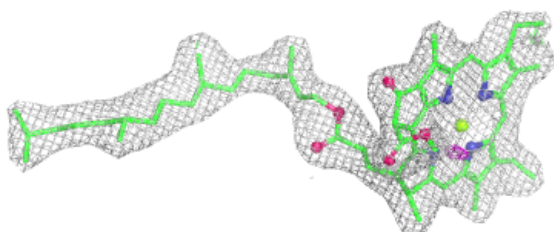
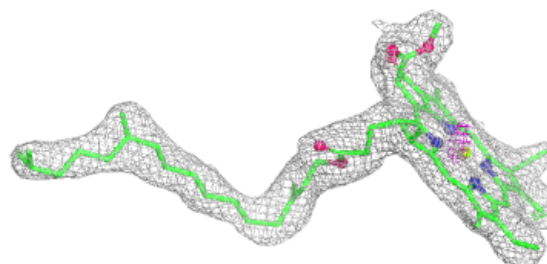


Electron density around DGD c 516:

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

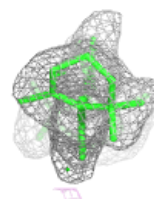
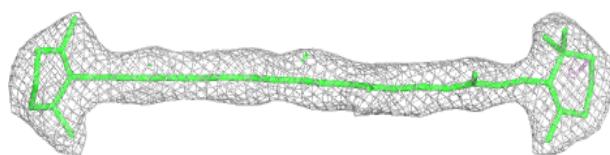
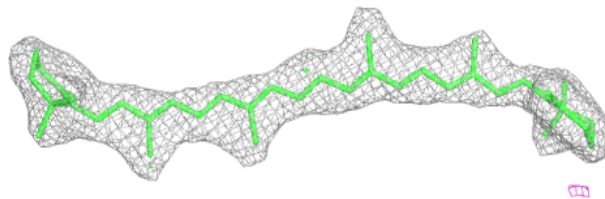
**Electron density around CLA C 502:**

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

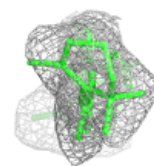
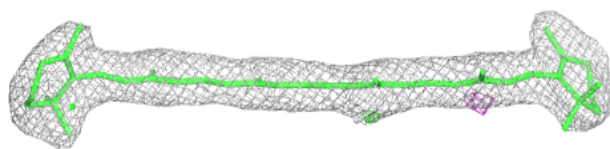
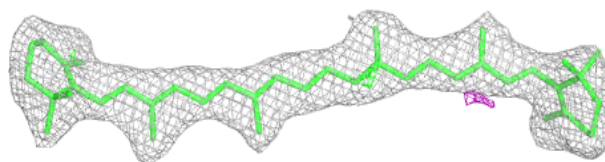


Electron density around BCR A 609:

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

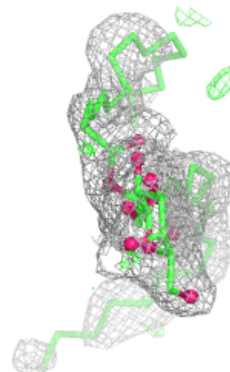
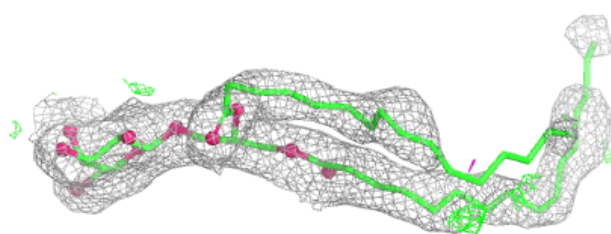
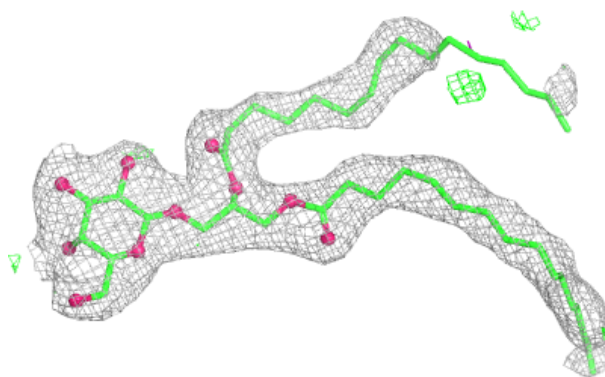
**Electron density around BCR B 618:**

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



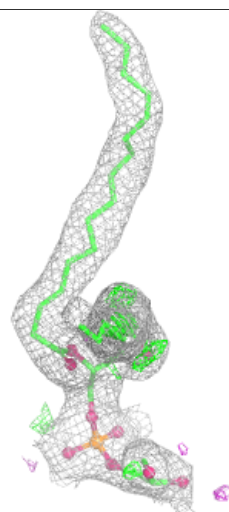
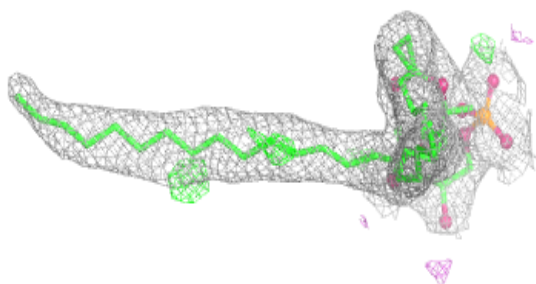
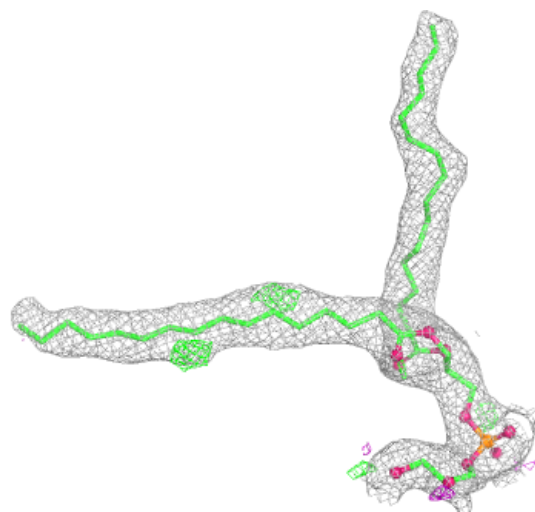
Electron density around LMG D 409:

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



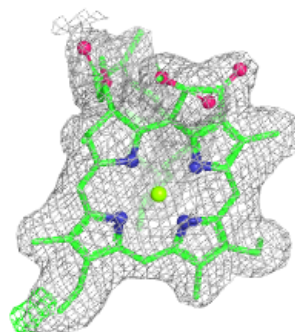
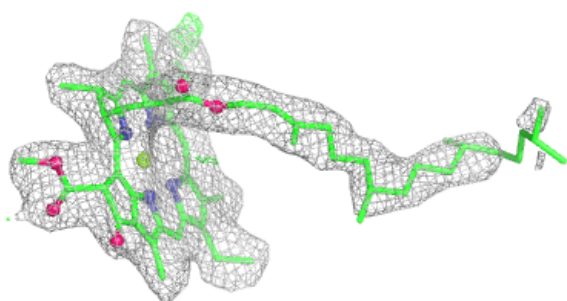
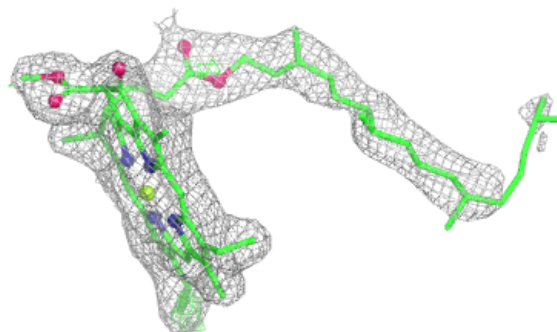
Electron density around LHG L 102:

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

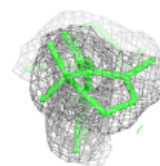
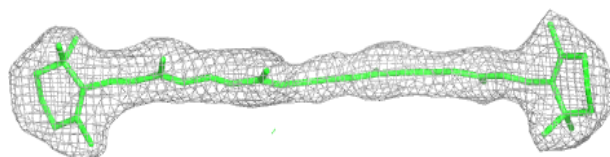
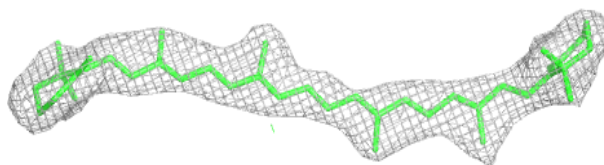


Electron density around CLA C 508:

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

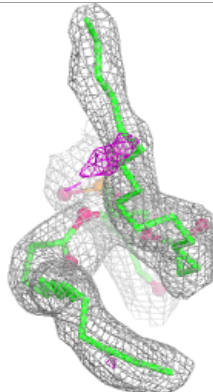
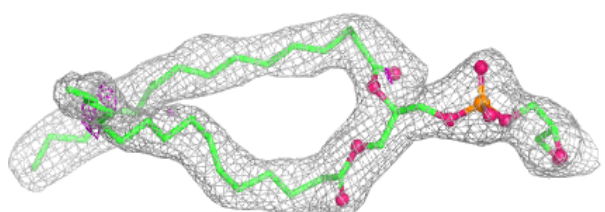
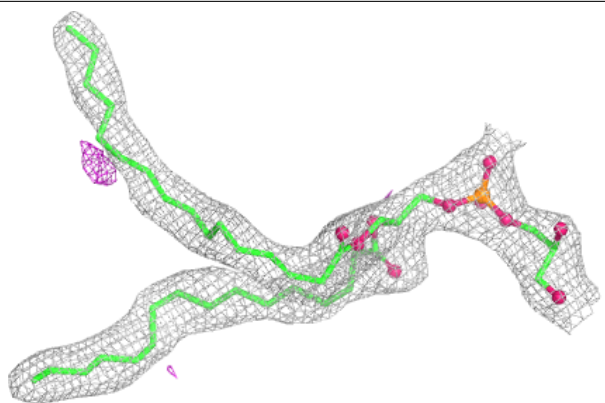
**Electron density around BCR C 515:**

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

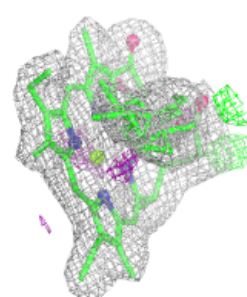
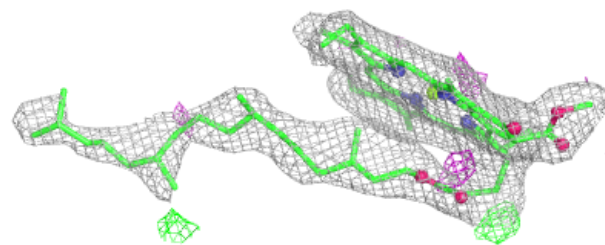
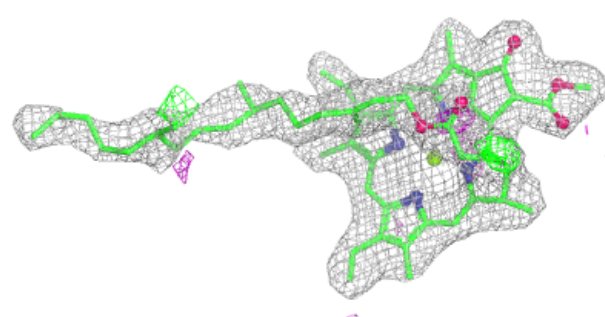


Electron density around LHG d 406:

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

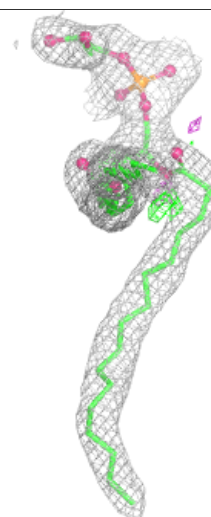
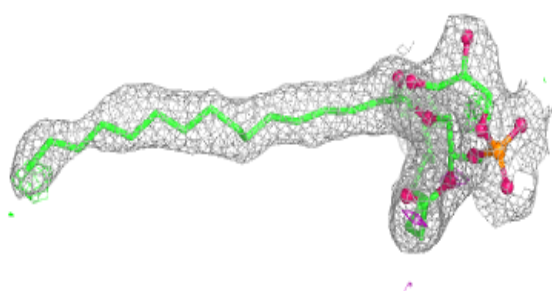
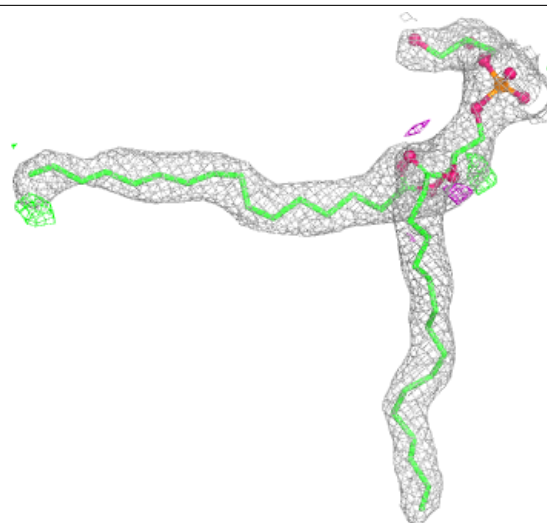
**Electron density around CLA b 614:**

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



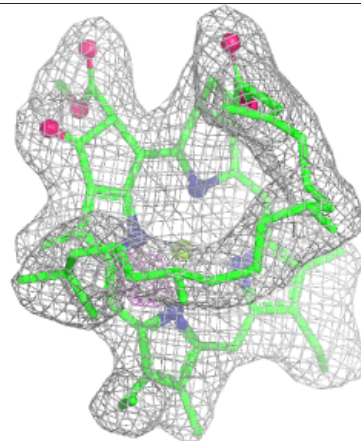
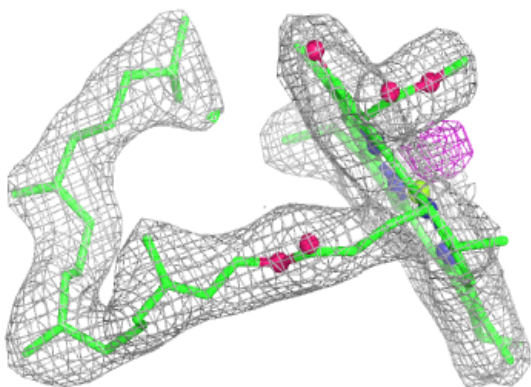
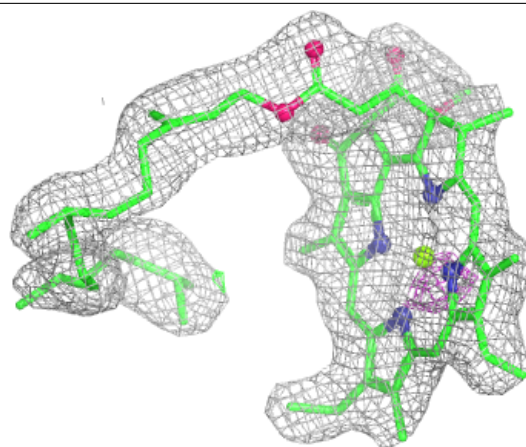
Electron density around LHG 1 101:

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

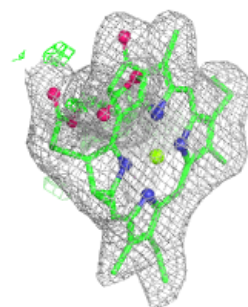
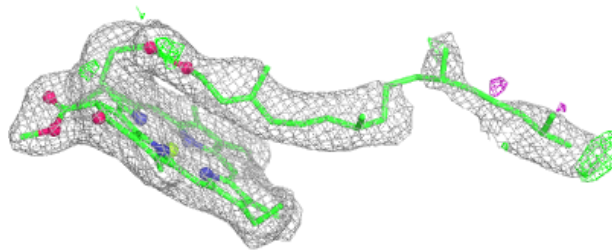
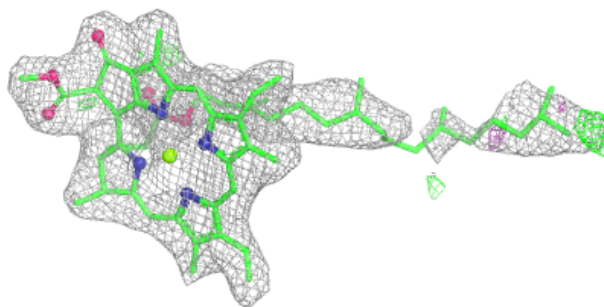


Electron density around CLA c 503:

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

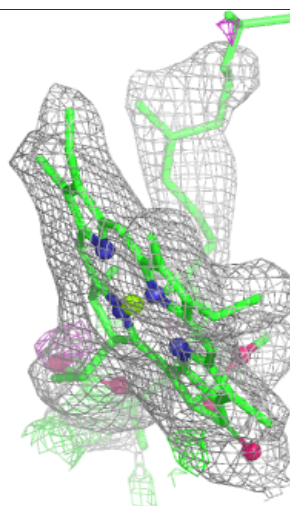
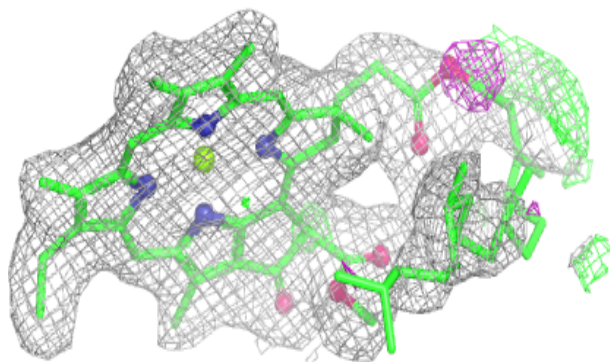
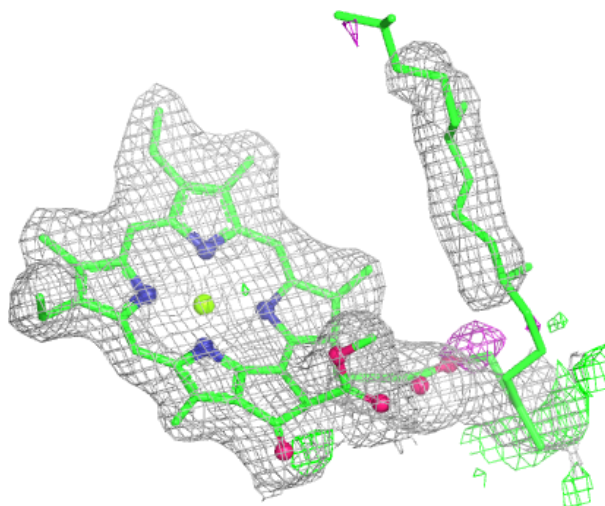
**Electron density around CLA B 614:**

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



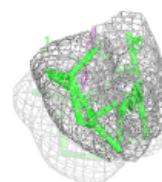
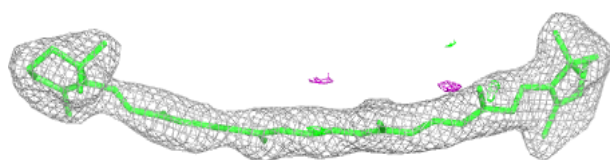
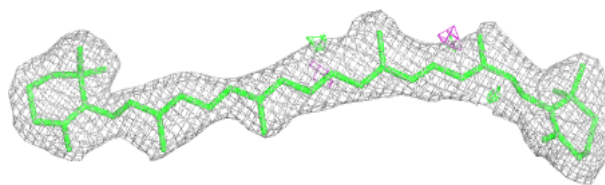
Electron density around CLA B 616:

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

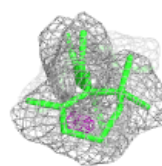
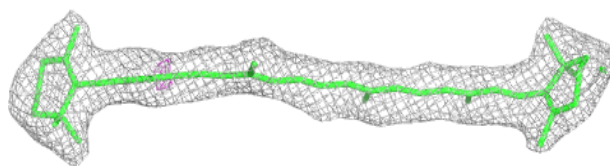
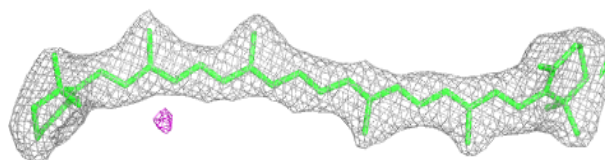


Electron density around BCR T 101:

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

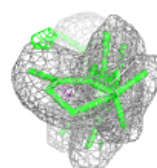
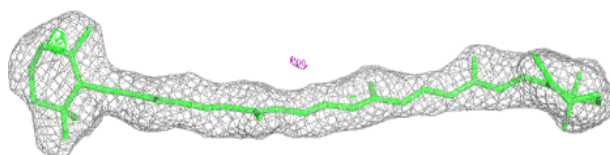
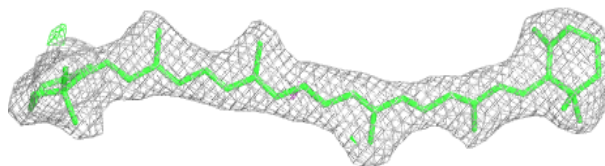
**Electron density around BCR a 611:**

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

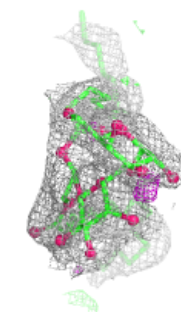
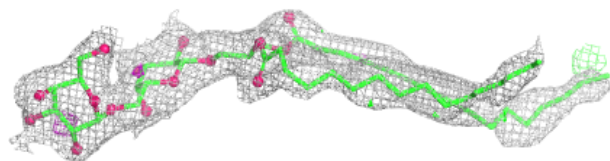
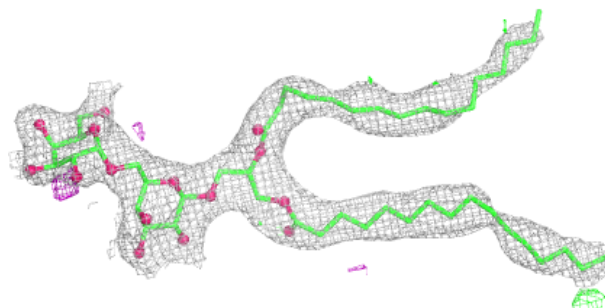


Electron density around BCR b 617:

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

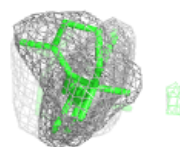
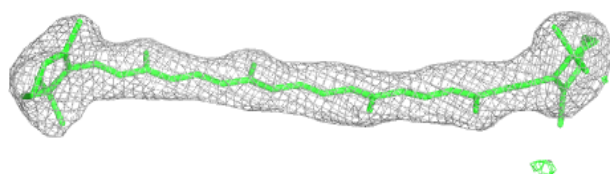
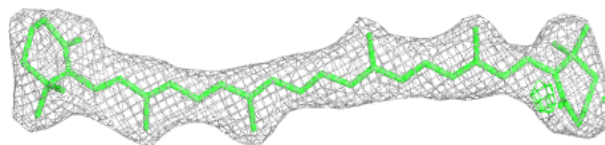
**Electron density around DGD C 518:**

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

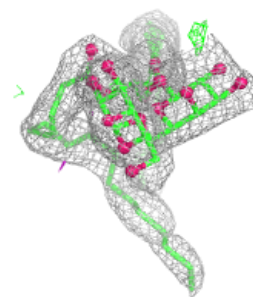
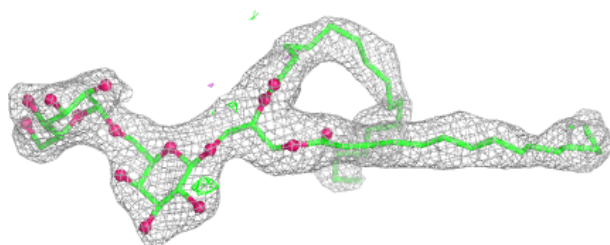
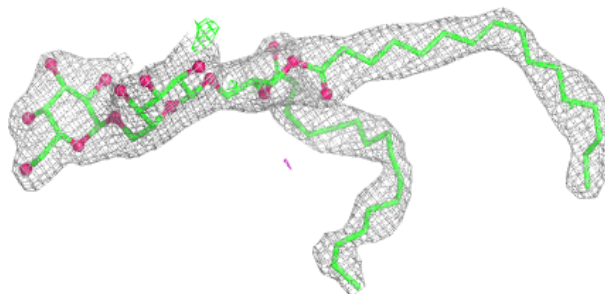


Electron density around BCR b 619:

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

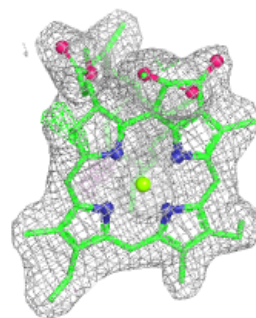
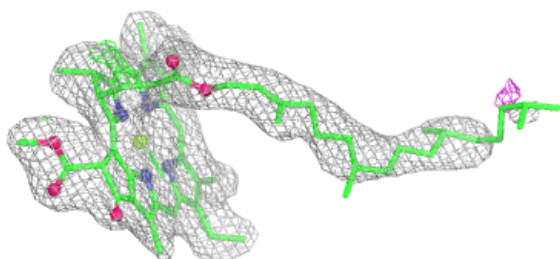
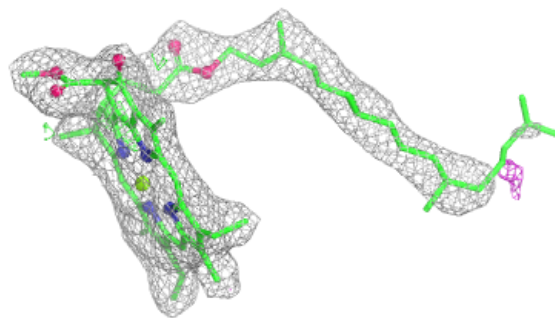
**Electron density around DGD h 102:**

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



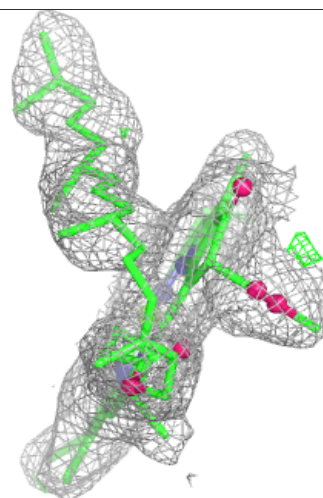
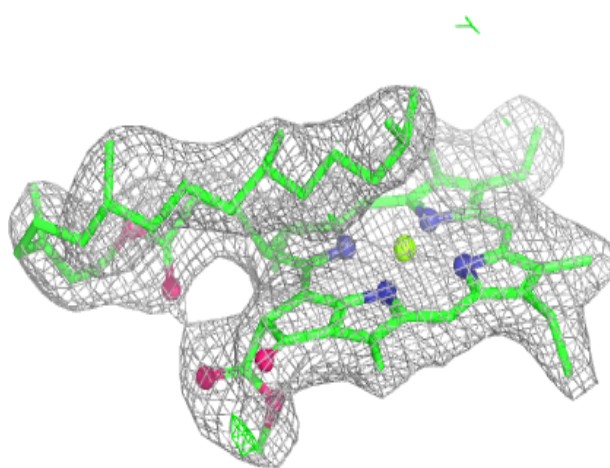
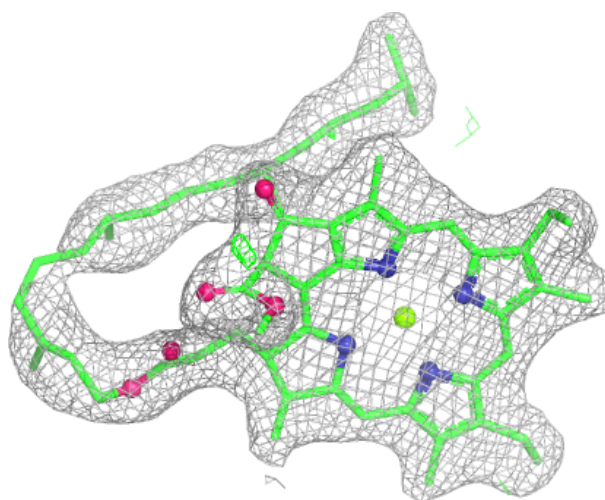
Electron density around CLA c 508:

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



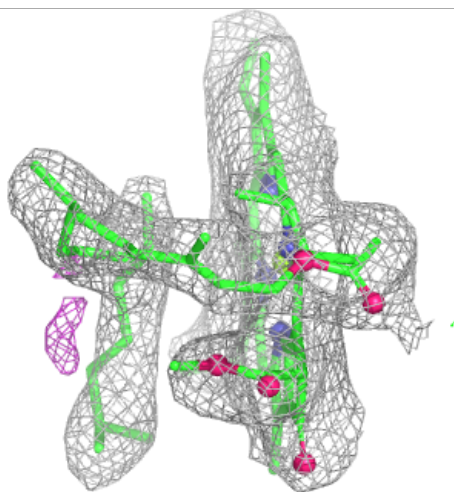
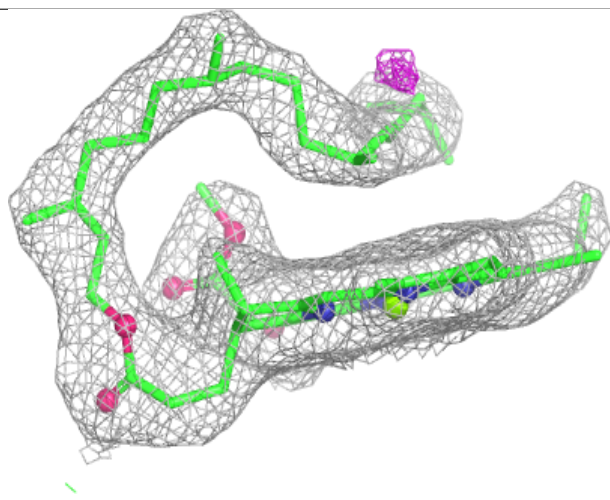
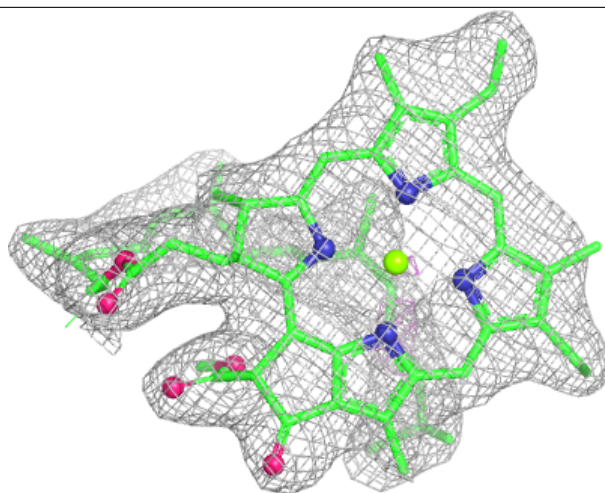
Electron density around CLA c 509:

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



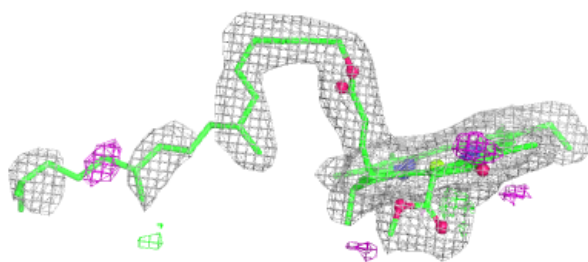
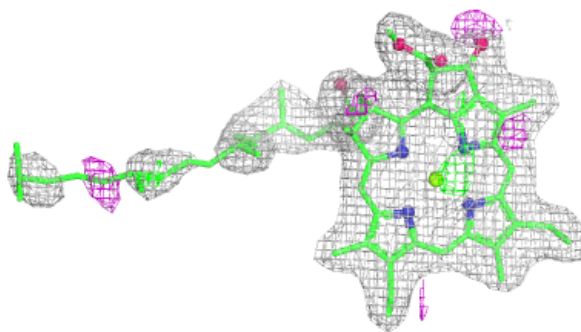
Electron density around CLA c 510:

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

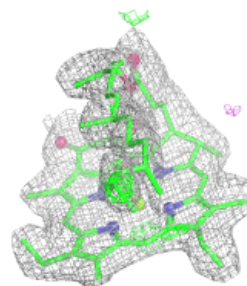
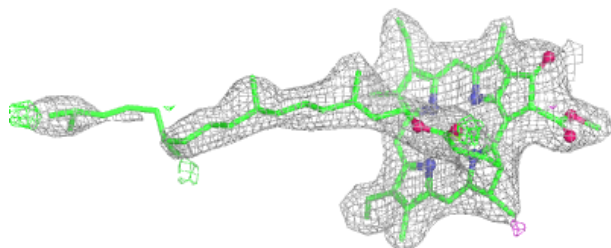
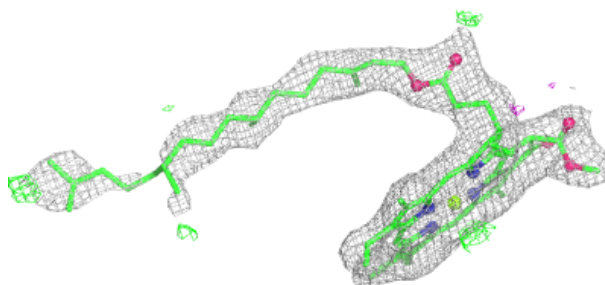


Electron density around CLA a 608:

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

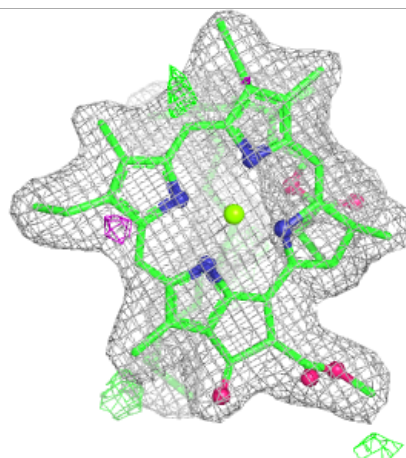
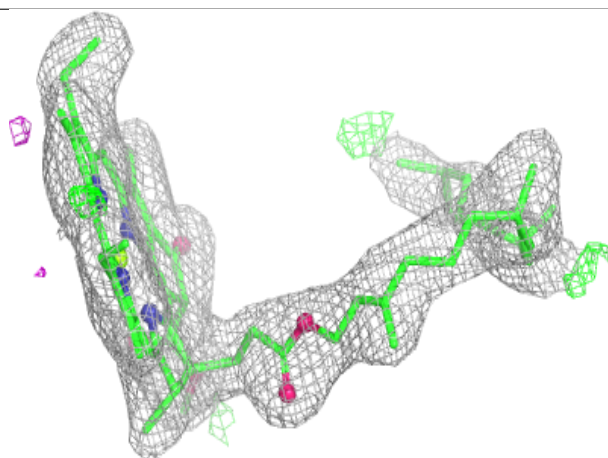
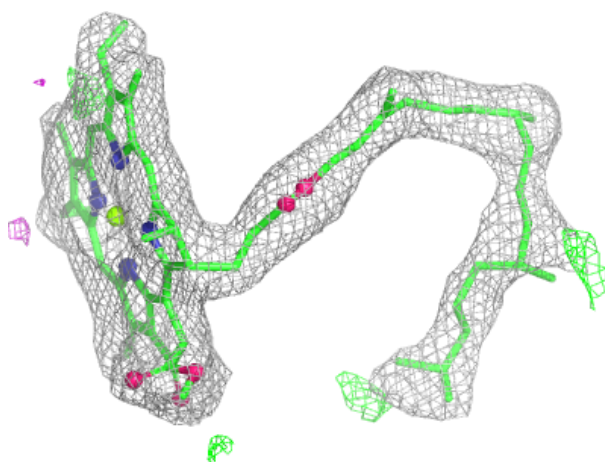
**Electron density around CLA C 504:**

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



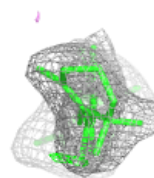
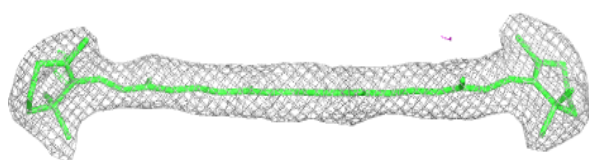
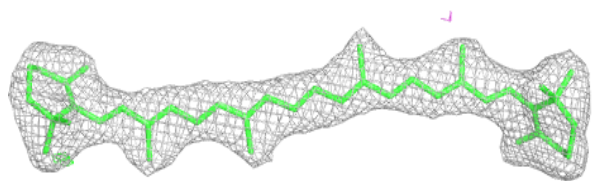
Electron density around CLA b 606:

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

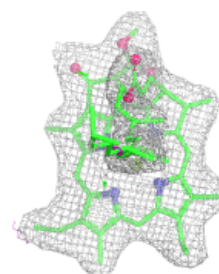
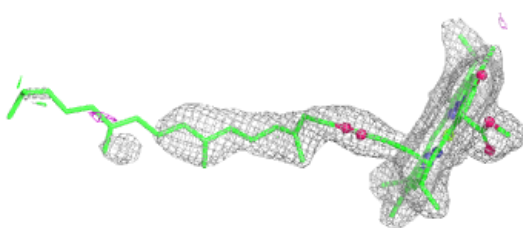
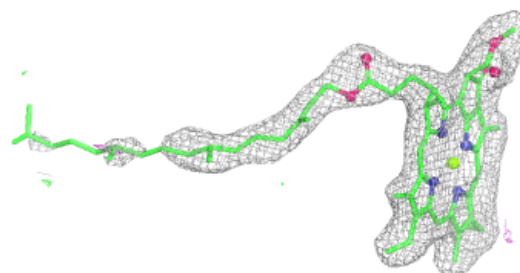


Electron density around BCR b 618:

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

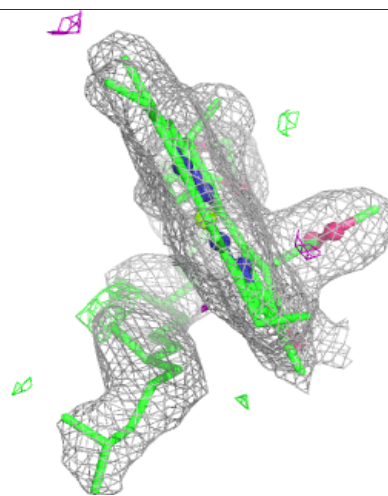
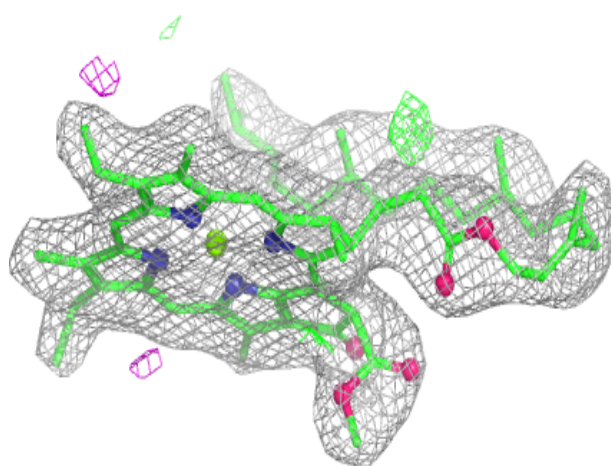
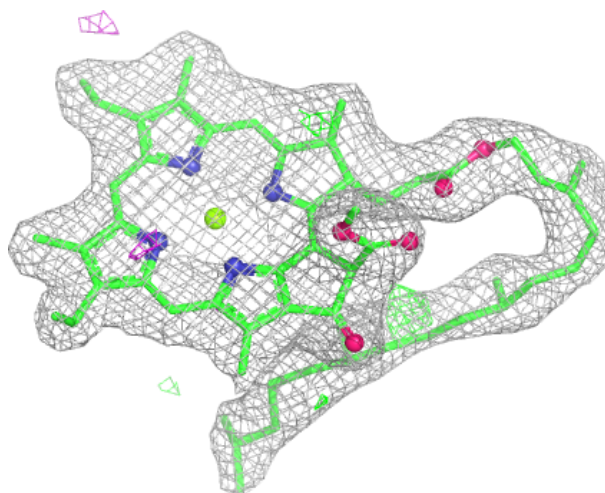
**Electron density around CLA d 403:**

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



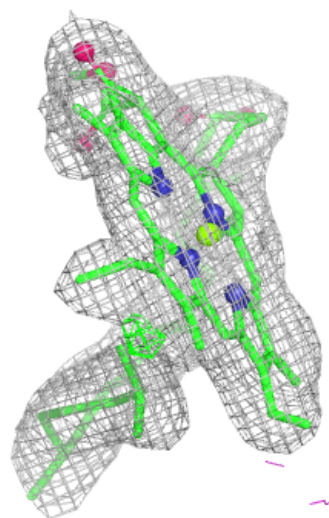
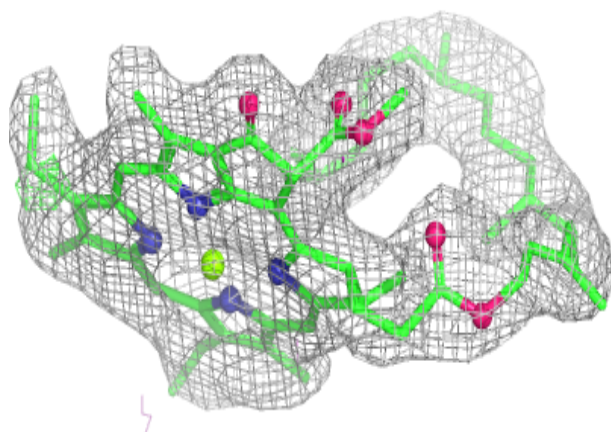
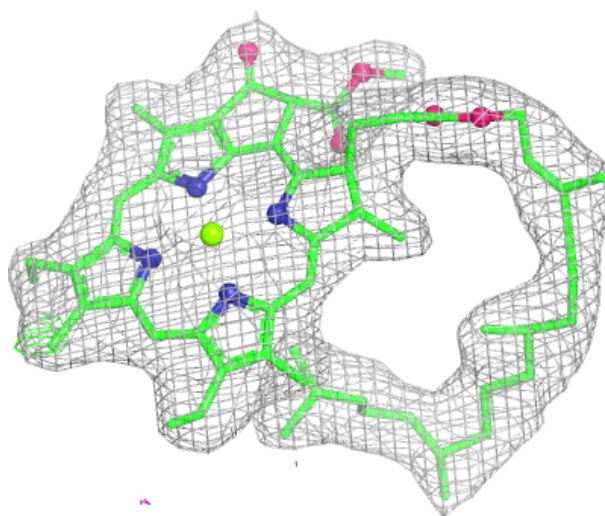
Electron density around CLA C 509:

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



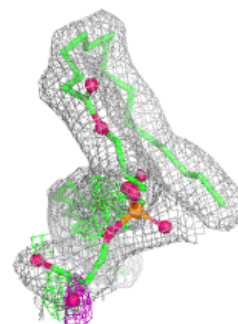
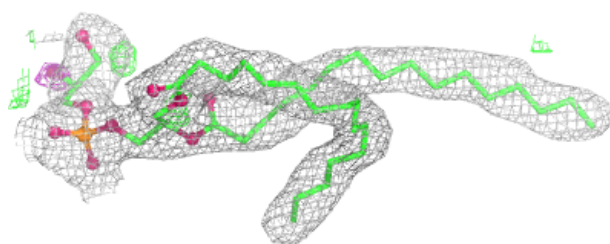
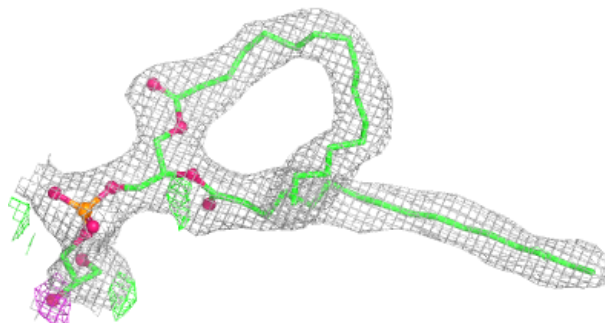
Electron density around CLA b 615:

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



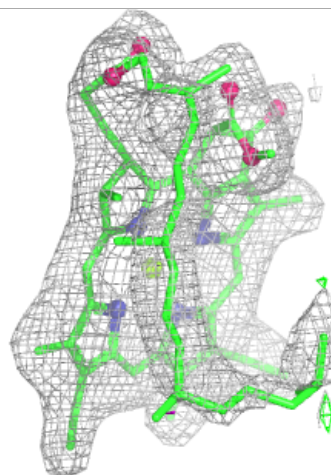
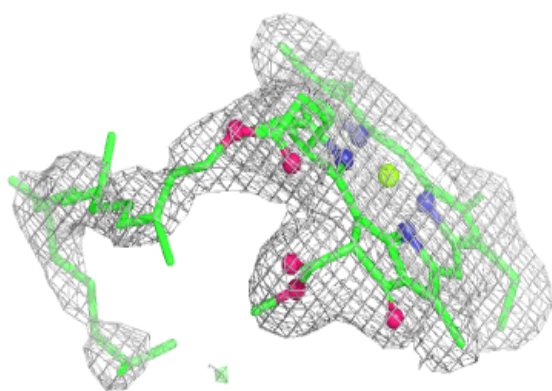
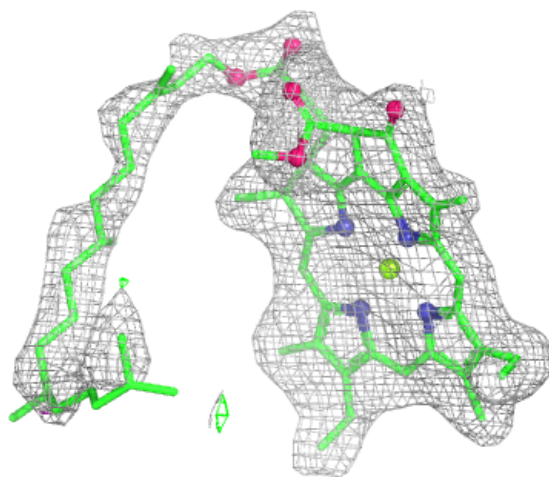
Electron density around LHG A 613:

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



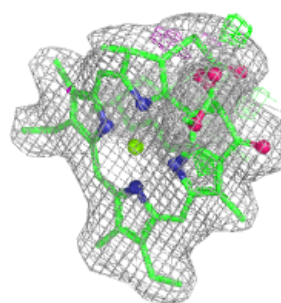
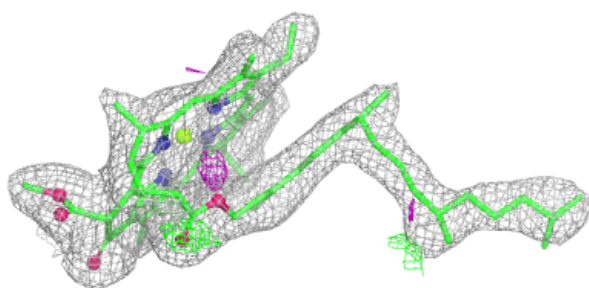
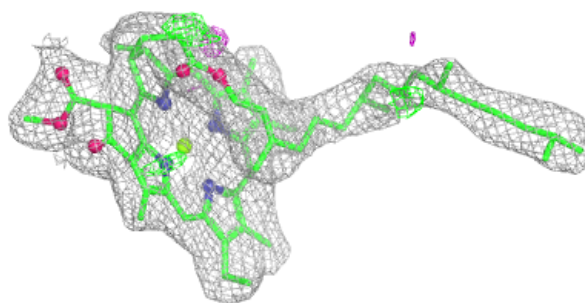
Electron density around CLA b 616:

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

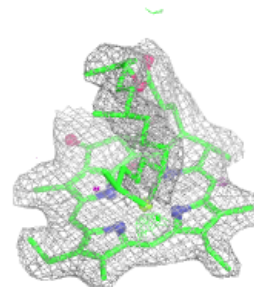
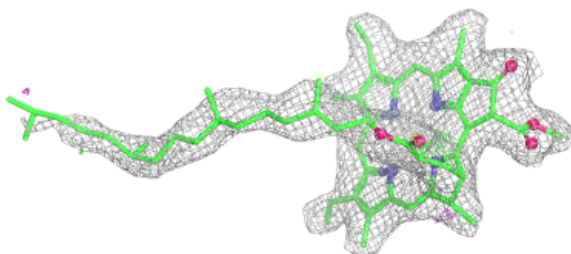
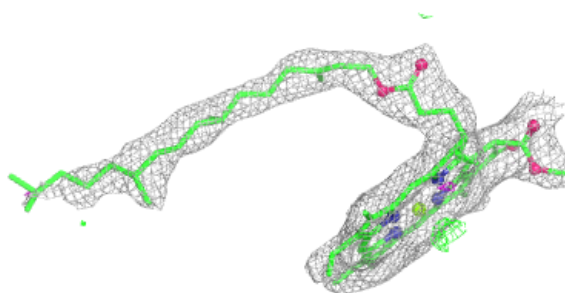


Electron density around CLA C 505:

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

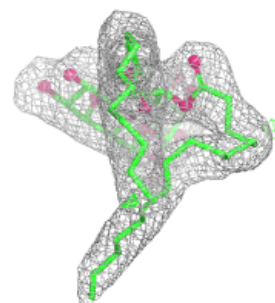
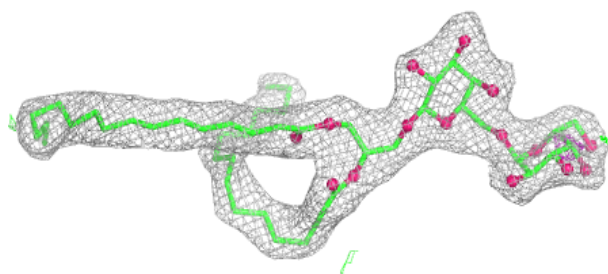
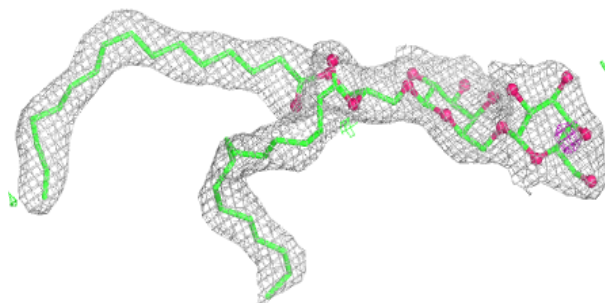
**Electron density around CLA c 504:**

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

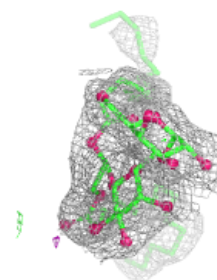
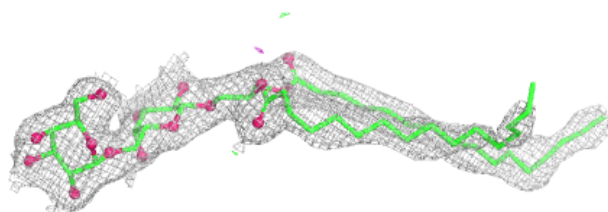
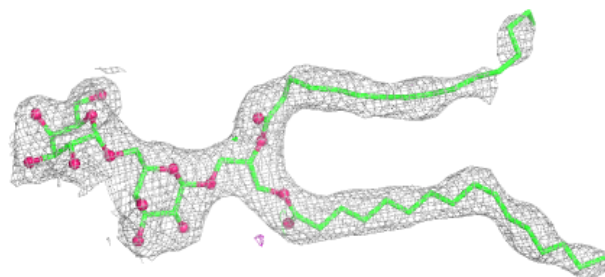


Electron density around DGD H 102:

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

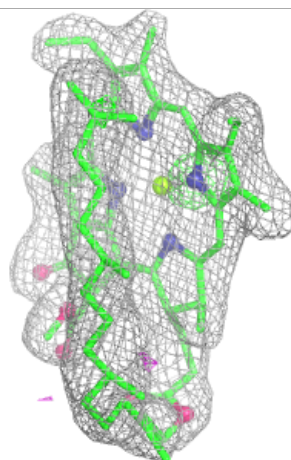
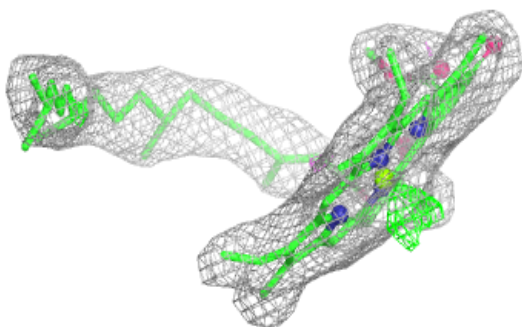
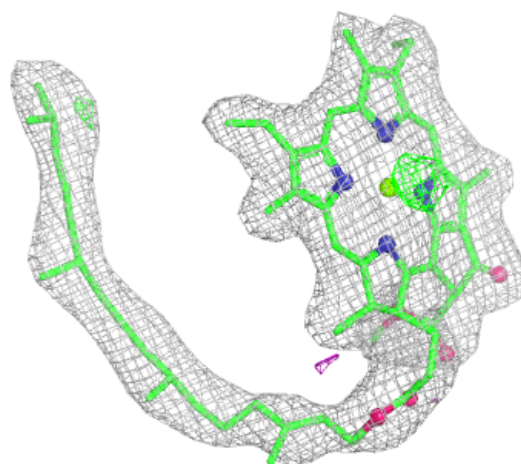
**Electron density around DGD c 517:**

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



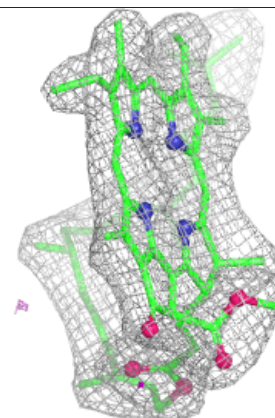
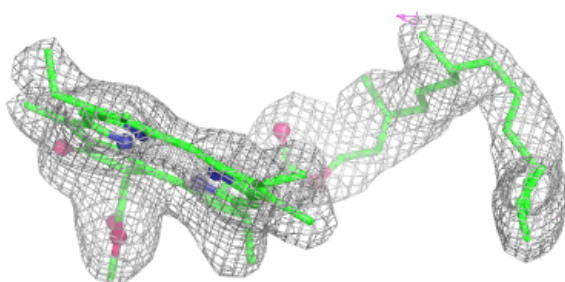
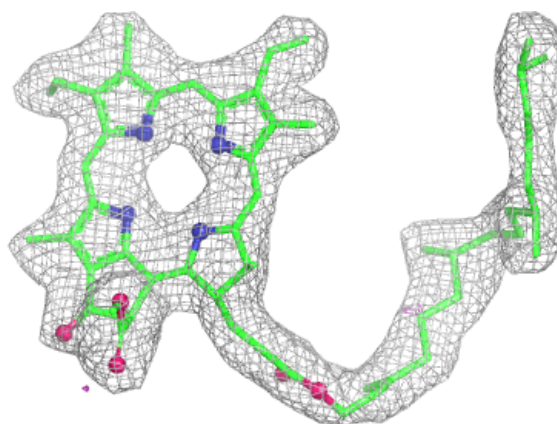
Electron density around CLA c 507:

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

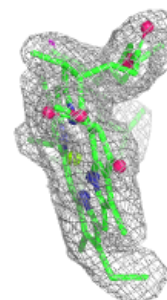
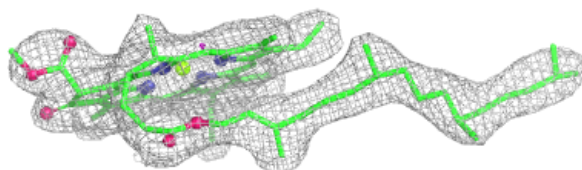
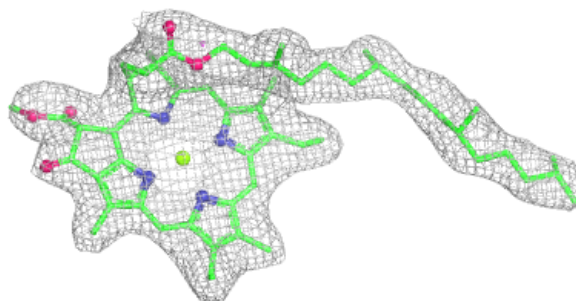


Electron density around PHO d 402:

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

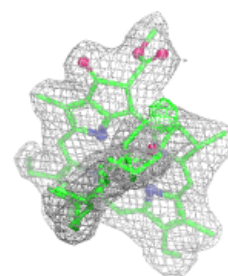
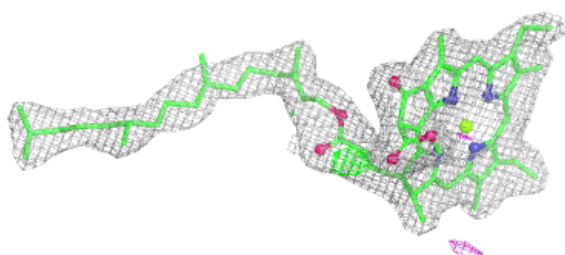
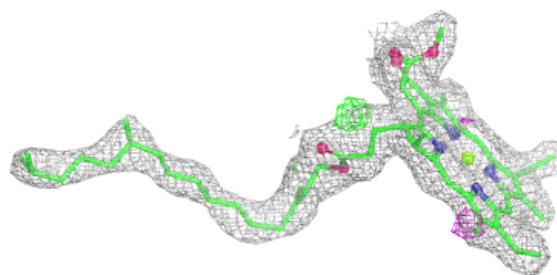
**Electron density around CLA c 501:**

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

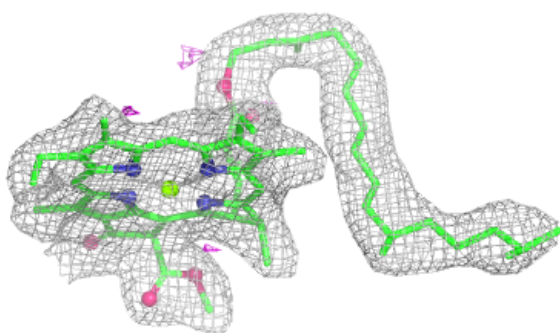
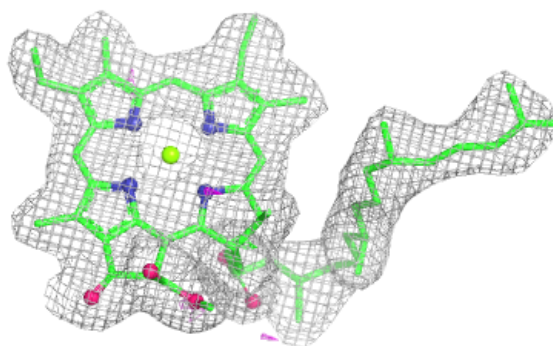


Electron density around CLA c 502:

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

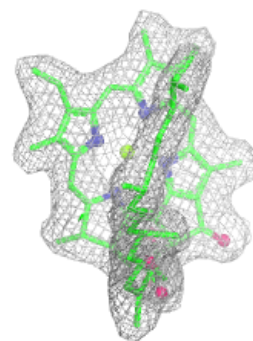
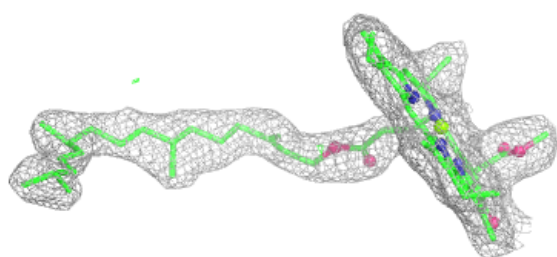
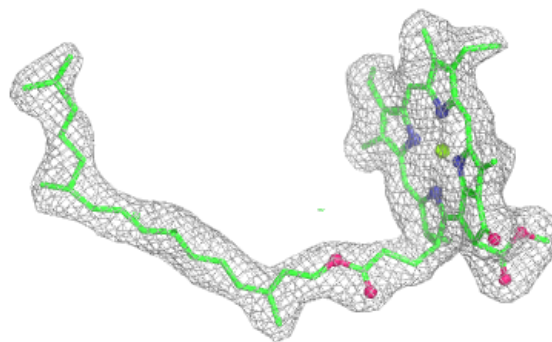
**Electron density around CLA a 607:**

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

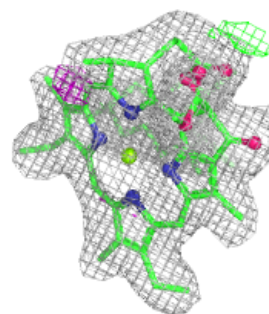
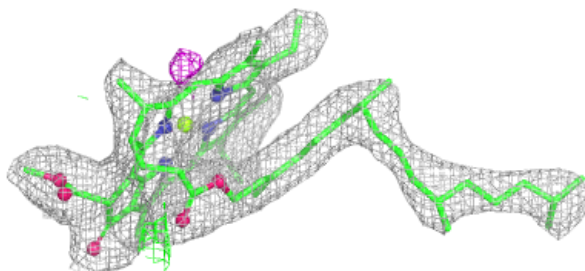
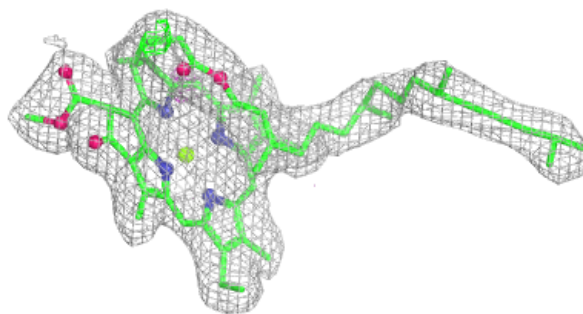


Electron density around CLA B 609:

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

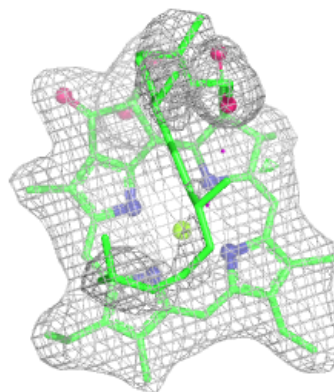
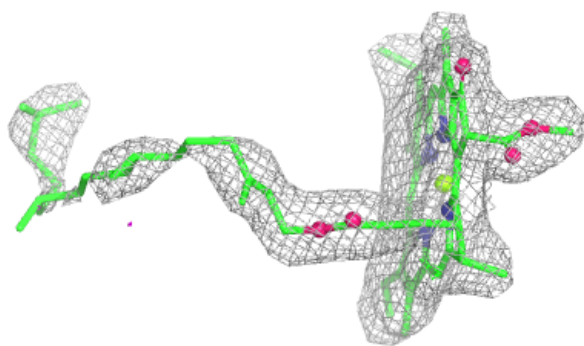
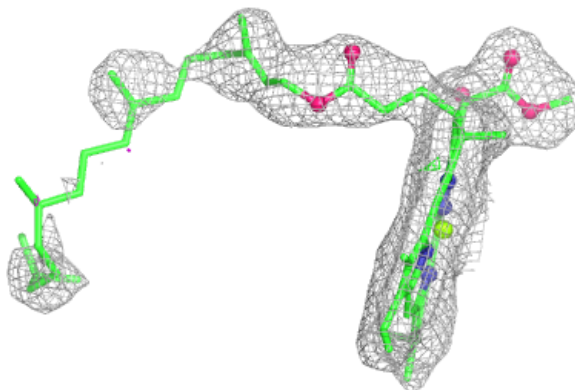
**Electron density around CLA c 505:**

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



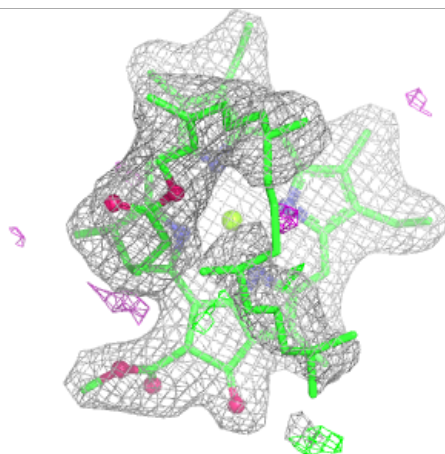
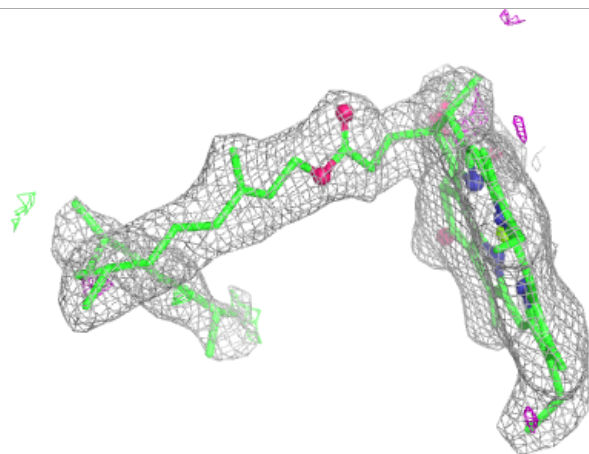
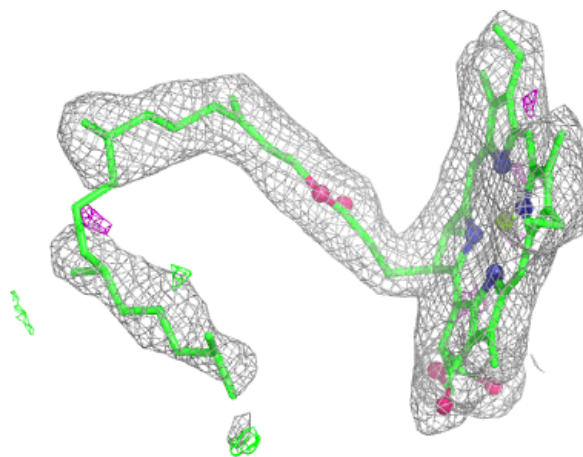
Electron density around CLA c 506:

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



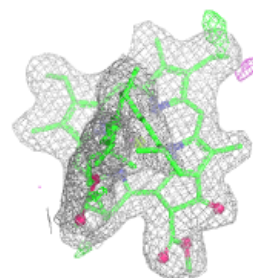
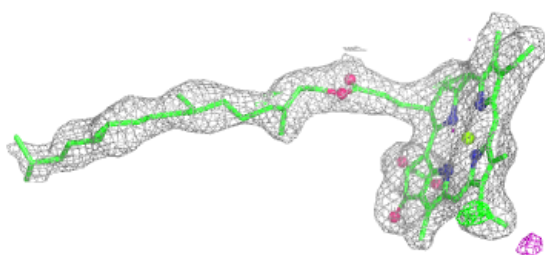
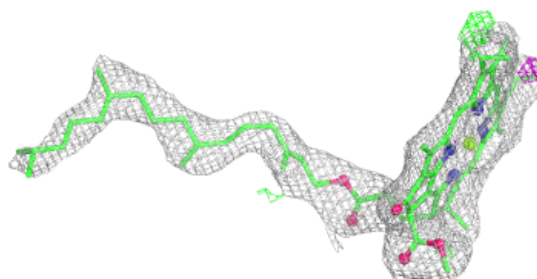
Electron density around CLA B 606:

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



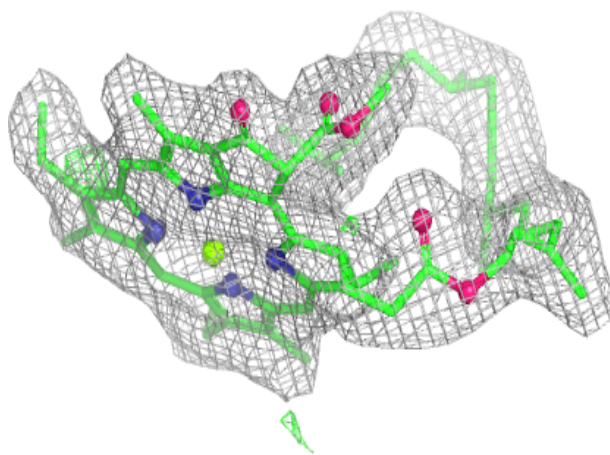
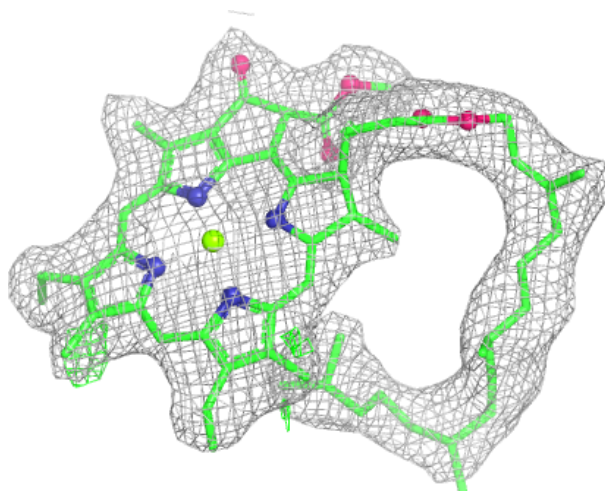
Electron density around CLA b 604:

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



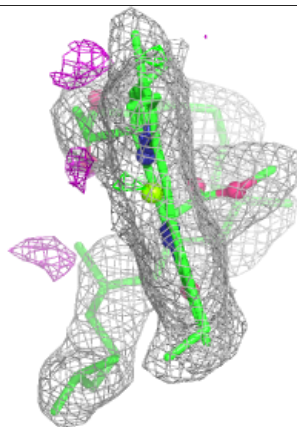
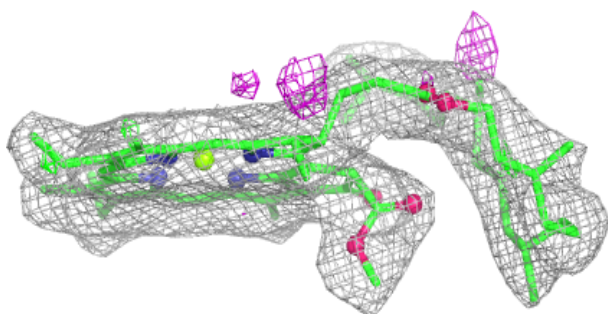
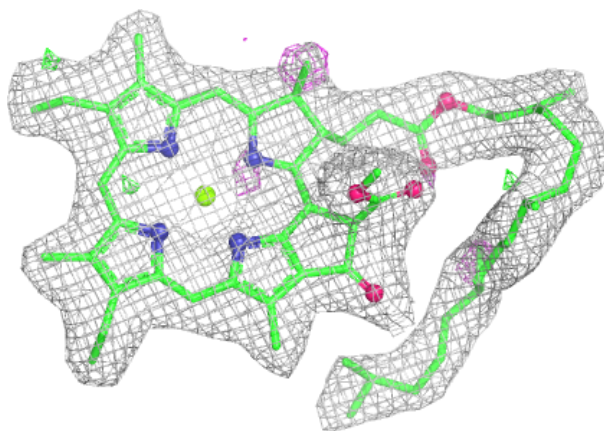
Electron density around CLA B 615:

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



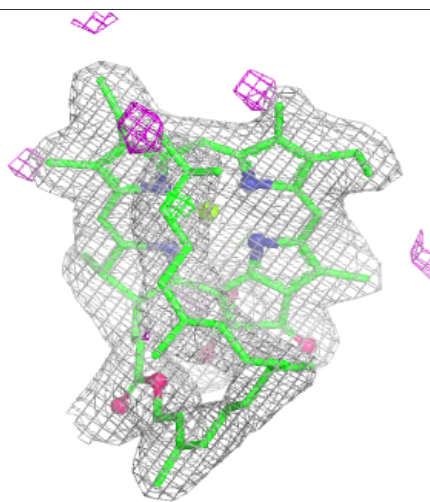
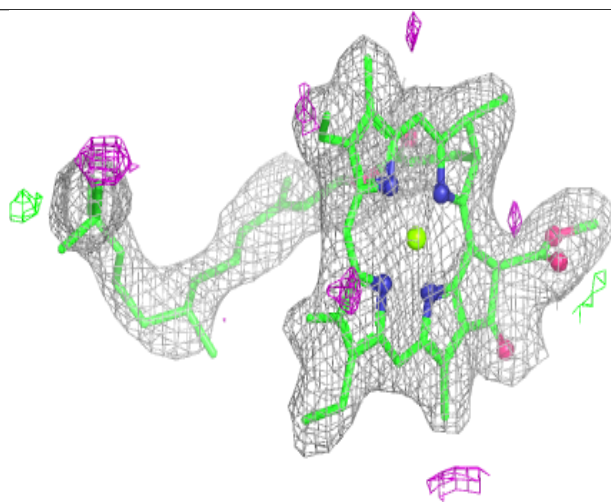
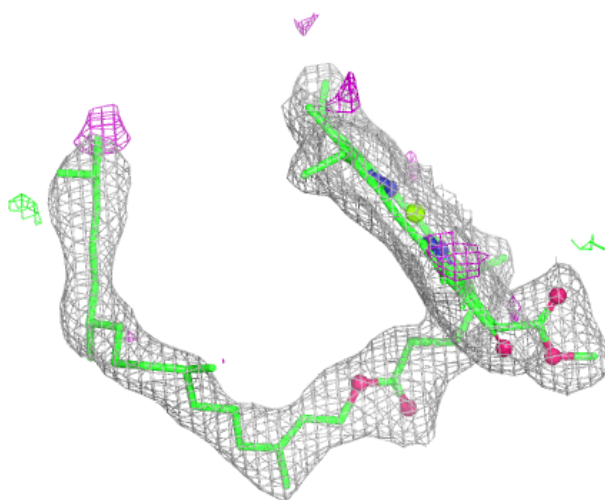
Electron density around CLA b 610:

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



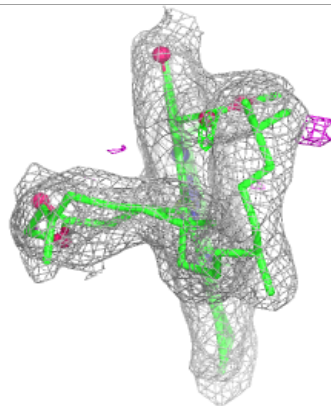
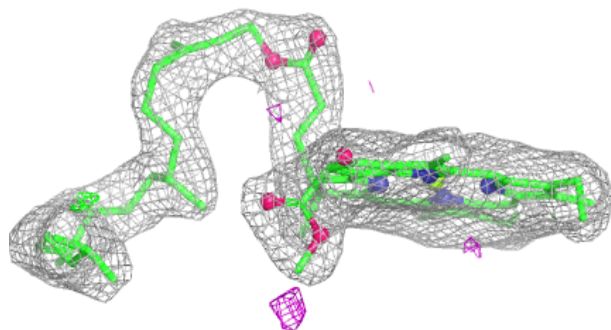
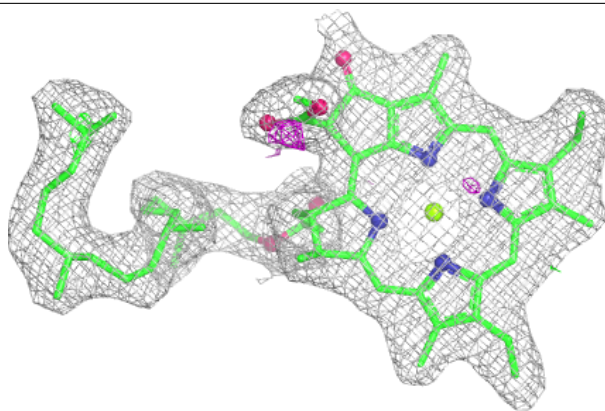
Electron density around CLA b 611:

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

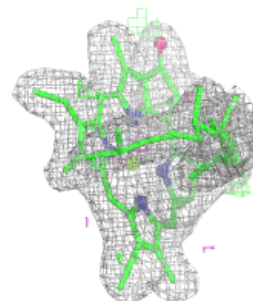
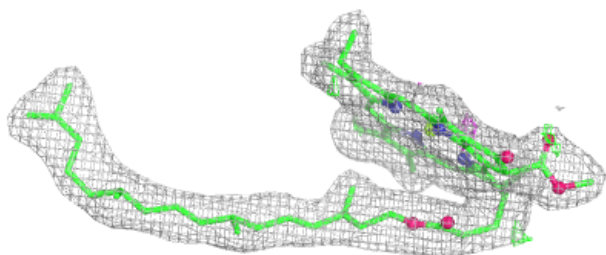
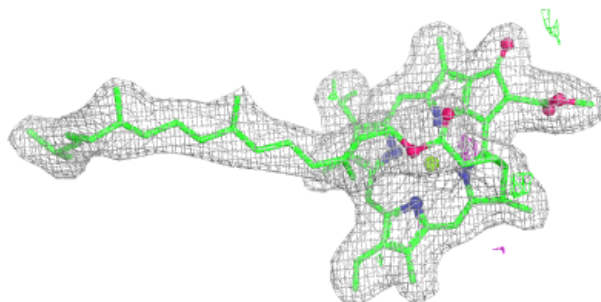


Electron density around CLA b 612:

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

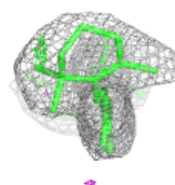
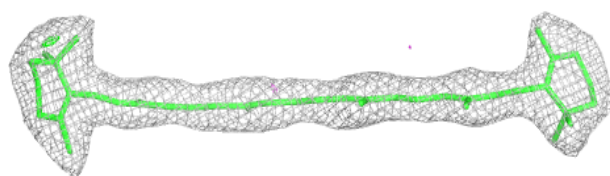
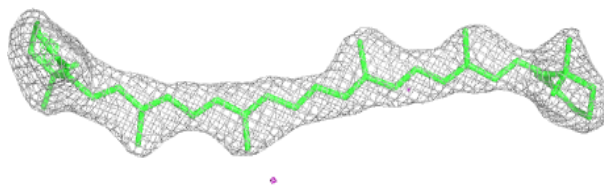
**Electron density around CLA B 608:**

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

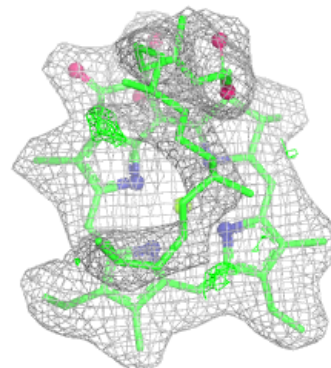
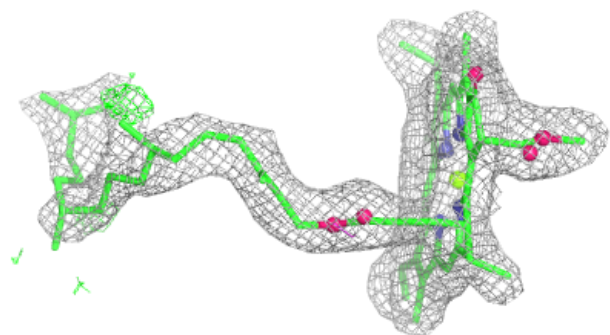
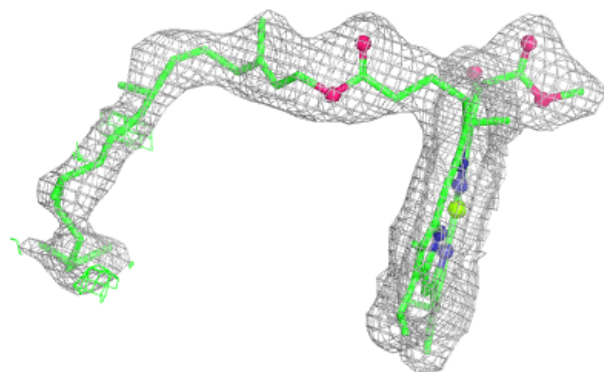


Electron density around BCR c 514:

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

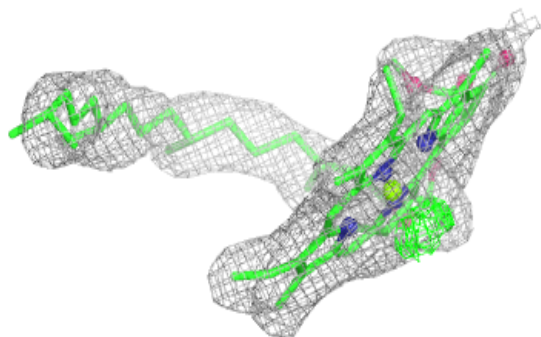
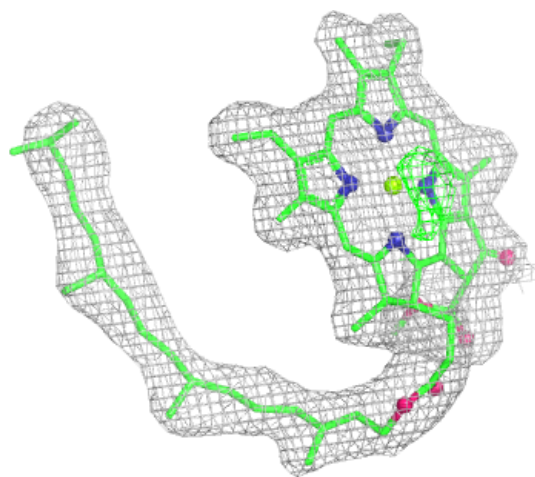
**Electron density around CLA C 506:**

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



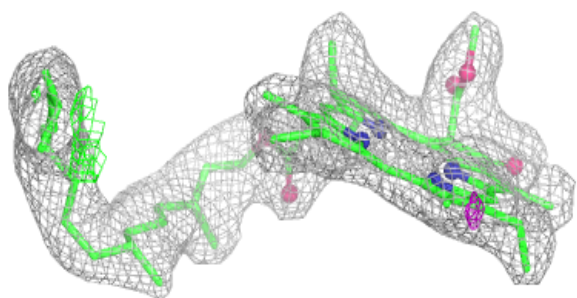
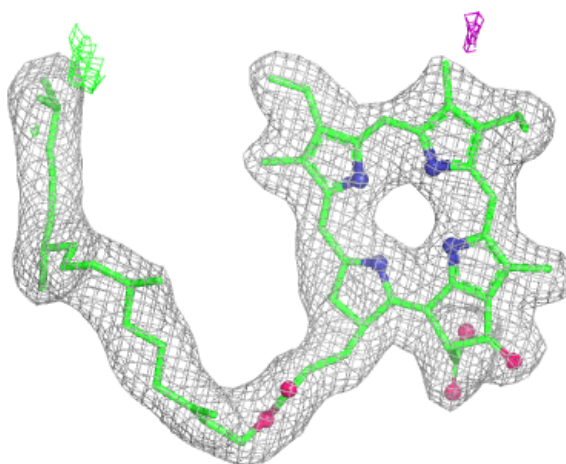
Electron density around CLA C 507:

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



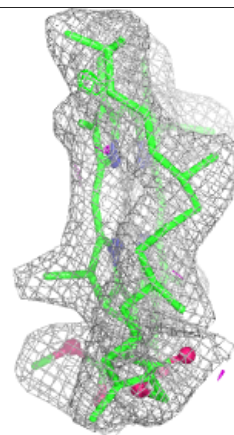
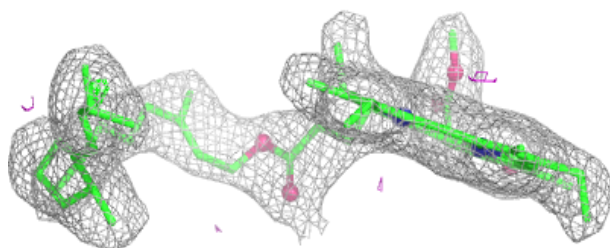
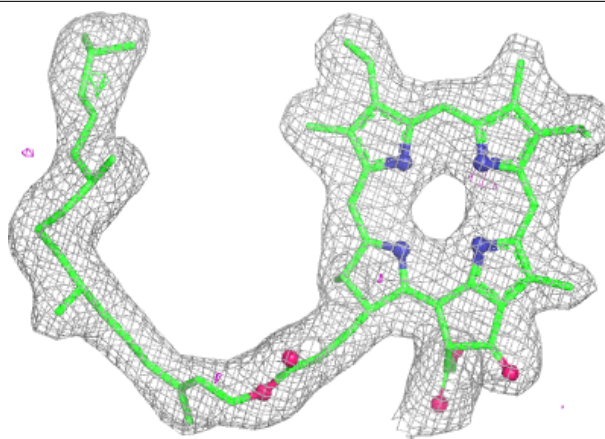
Electron density around PHO D 402:

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

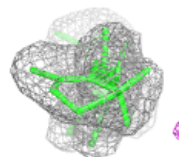
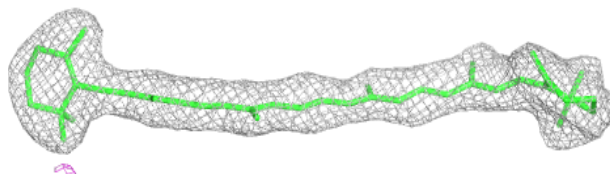
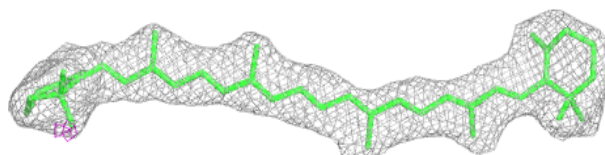


Electron density around PHO a 609:

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

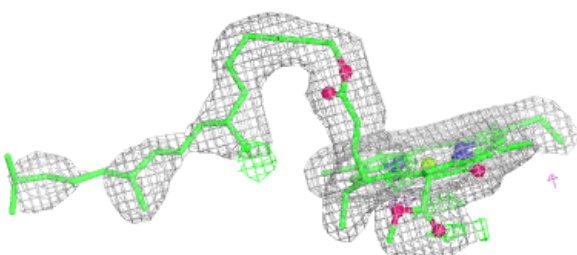
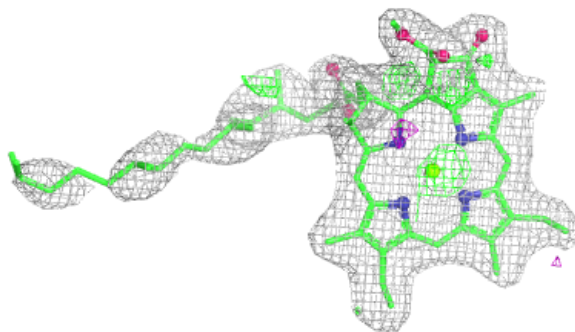
**Electron density around BCR B 617:**

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

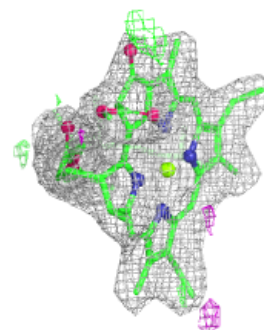
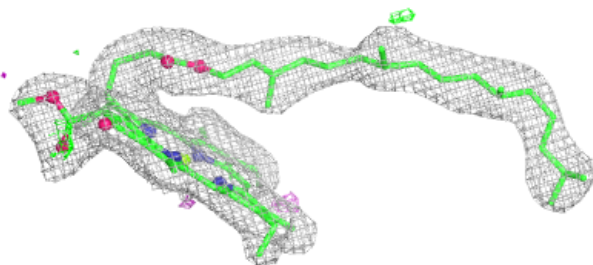
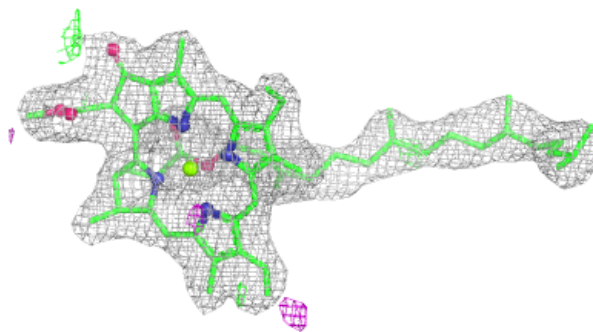


Electron density around CLA A 607:

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

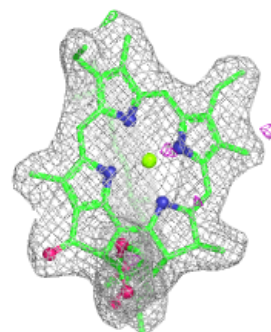
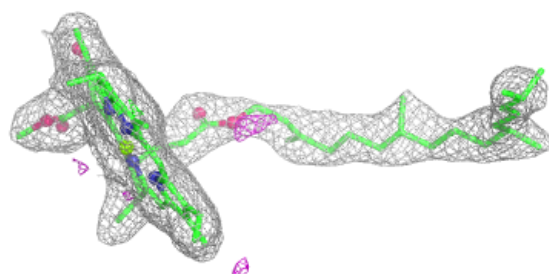
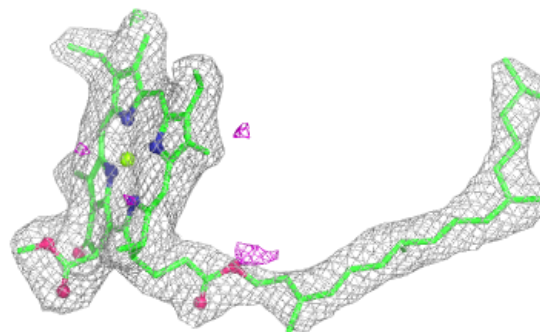
**Electron density around CLA b 608:**

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

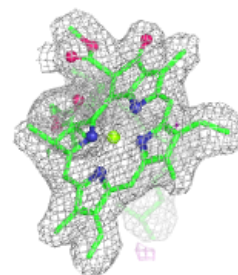
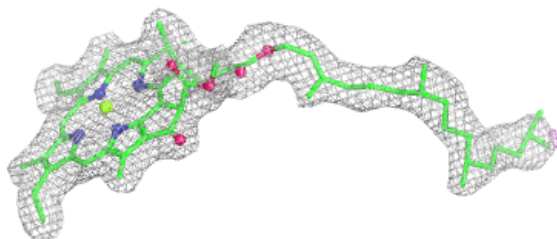
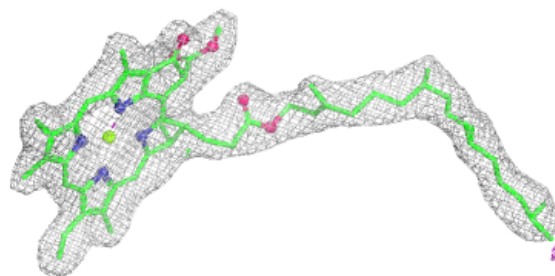


Electron density around CLA b 609:

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

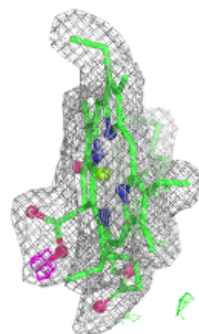
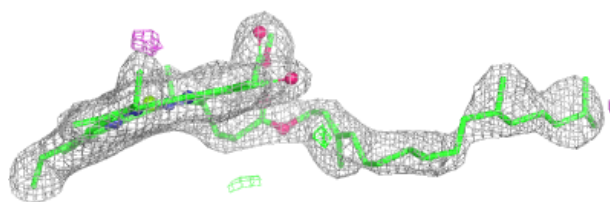
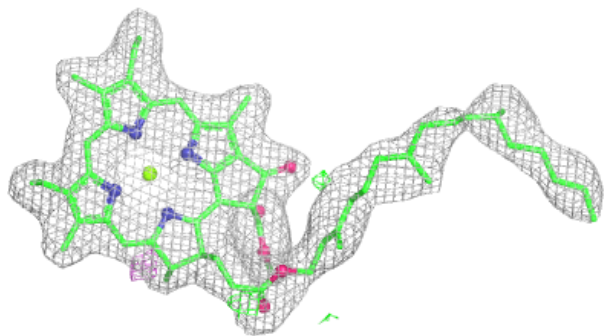
**Electron density around CLA A 606:**

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

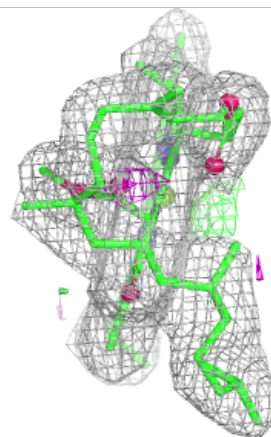
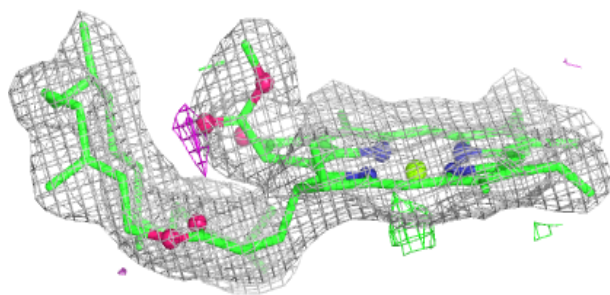
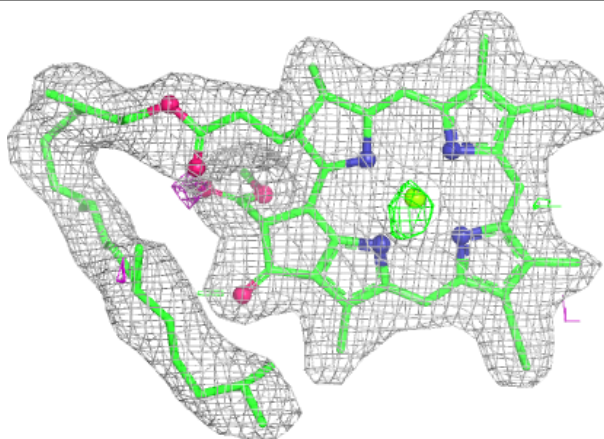


Electron density around CLA B 602:

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

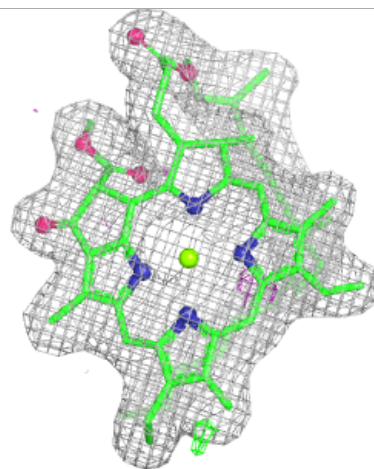
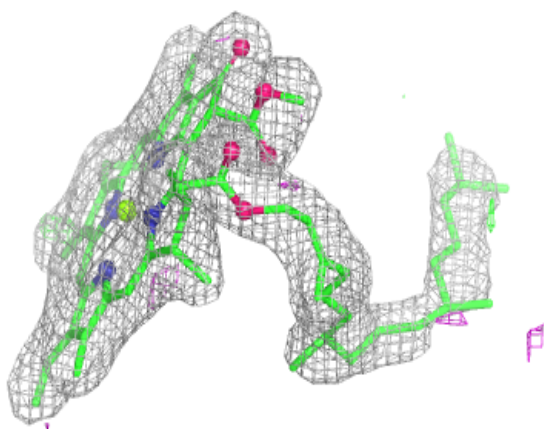
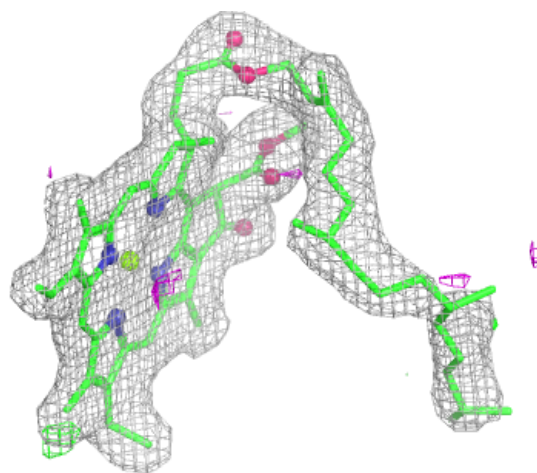
**Electron density around CLA B 610:**

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



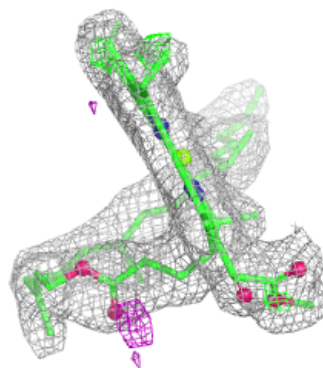
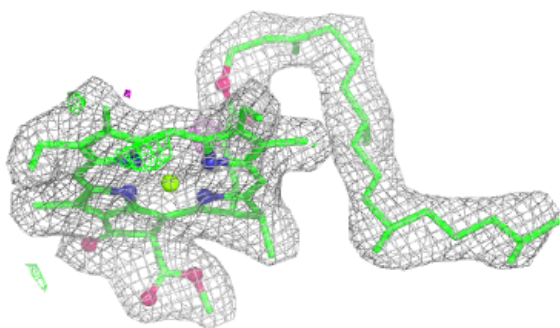
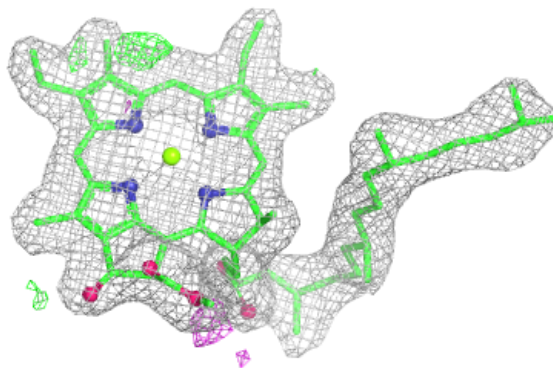
Electron density around CLA b 613:

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

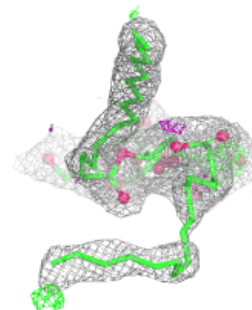
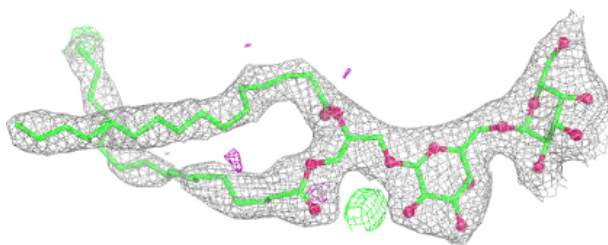
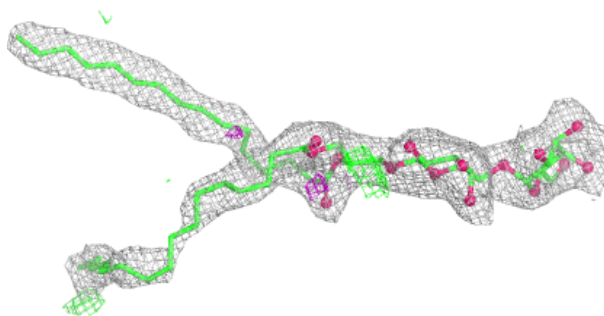


Electron density around CLA D 403:

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

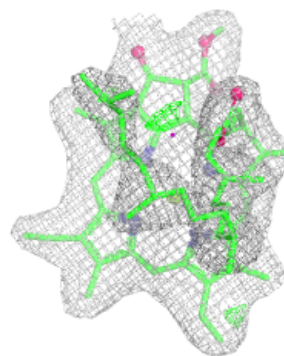
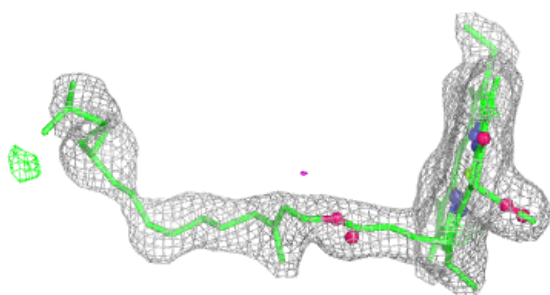
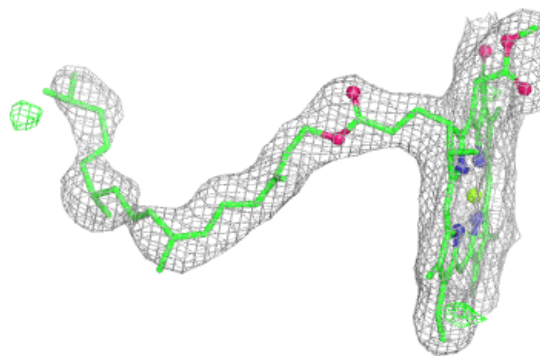
**Electron density around DGD C 516:**

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

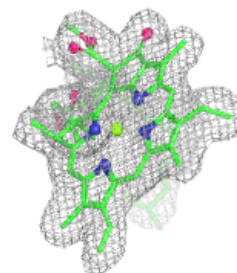
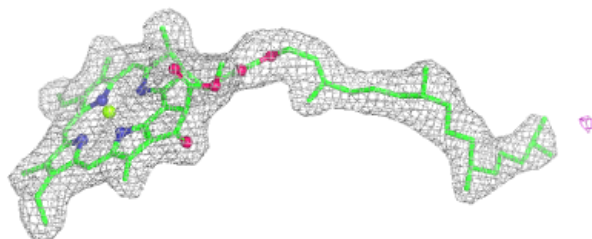
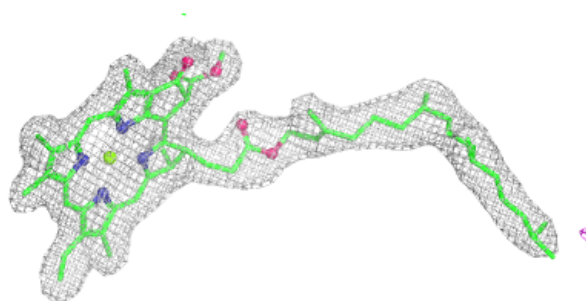


Electron density around CLA D 405:

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

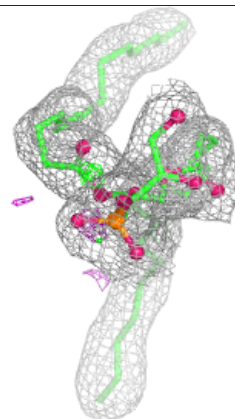
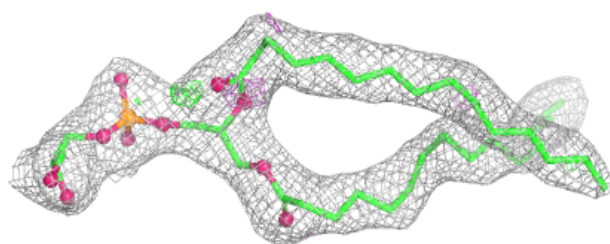
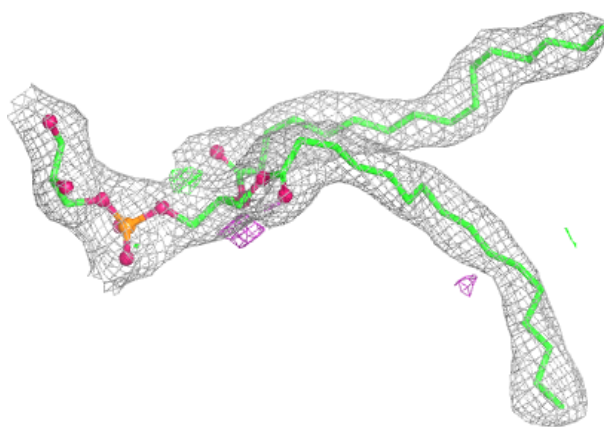
**Electron density around CLA a 606:**

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

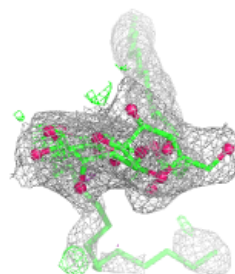
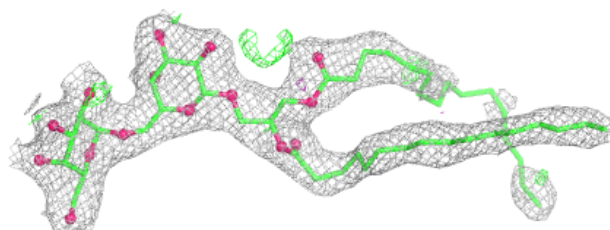
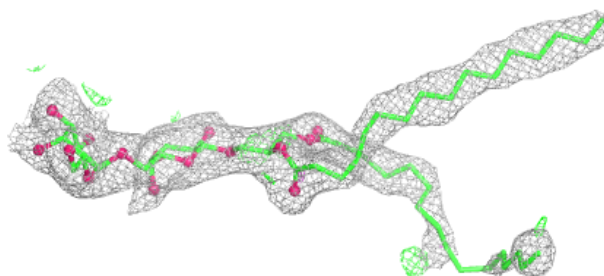


Electron density around LHG D 408:

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

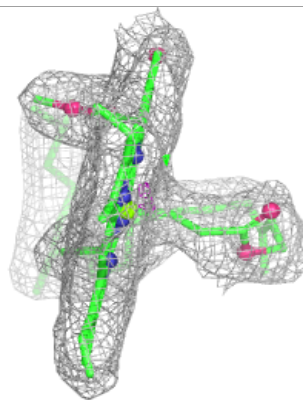
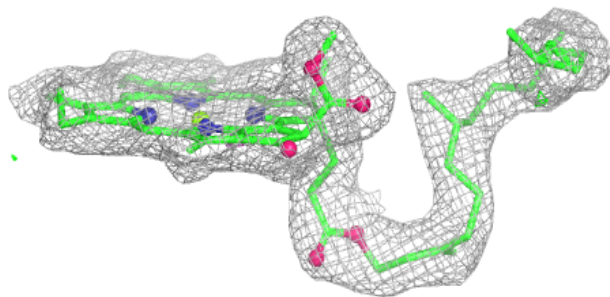
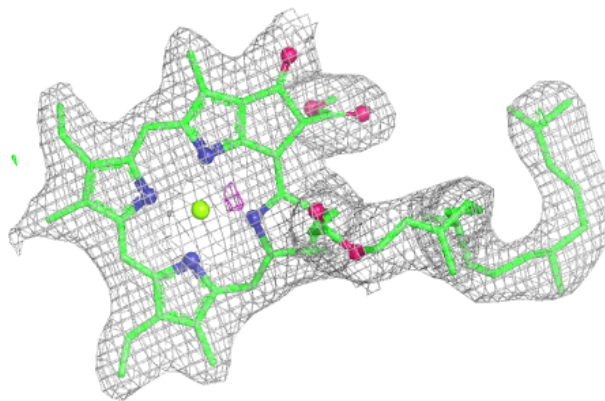
**Electron density around DGD c 515:**

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

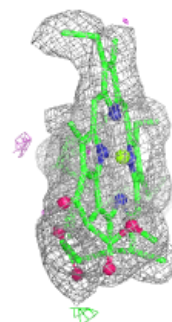
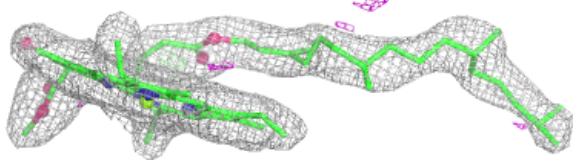
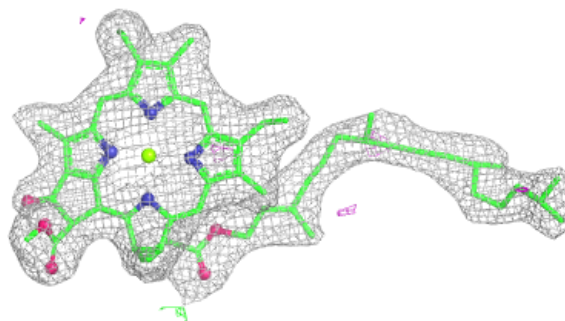


Electron density around CLA B 612:

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

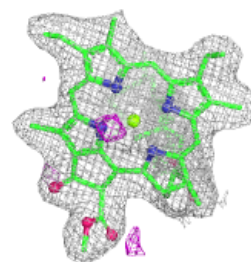
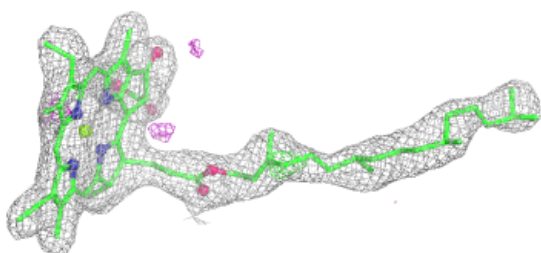
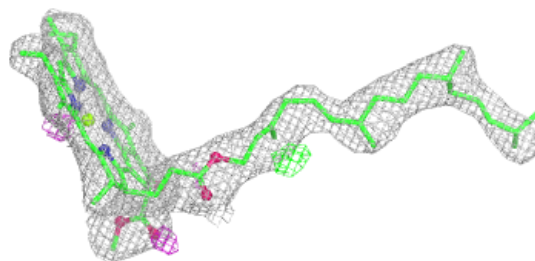
**Electron density around CLA B 603:**

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

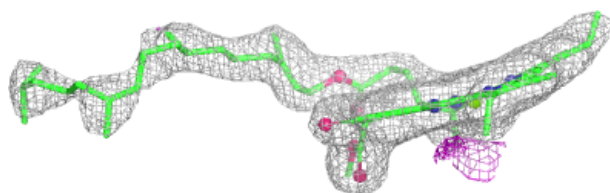
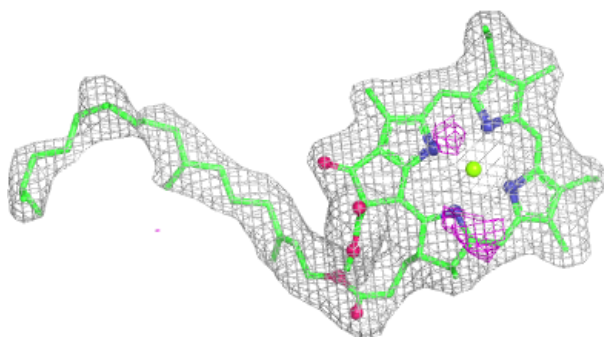


Electron density around CLA B 604:

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

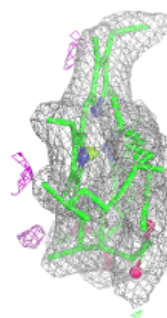
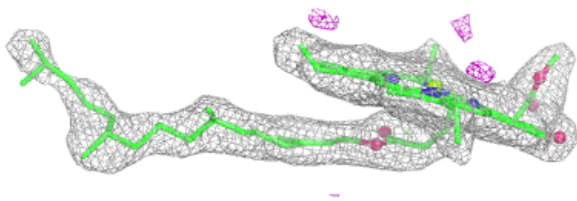
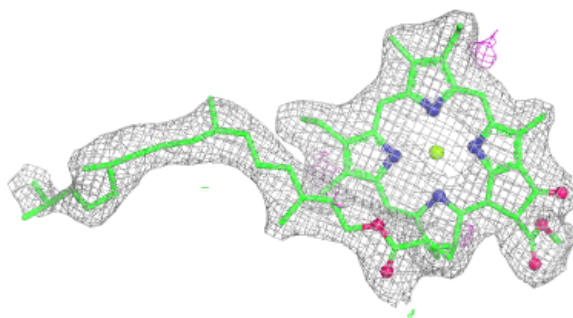
**Electron density around CLA b 602:**

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

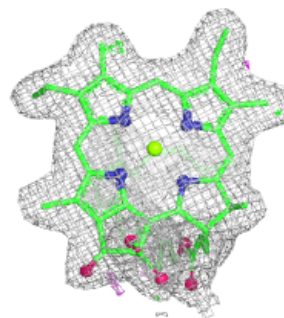
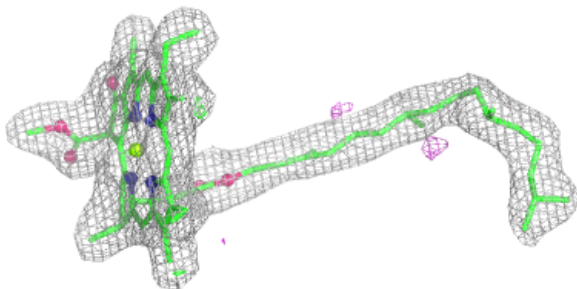
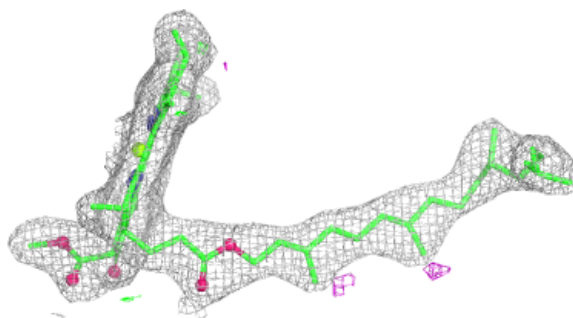


Electron density around CLA b 603:

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

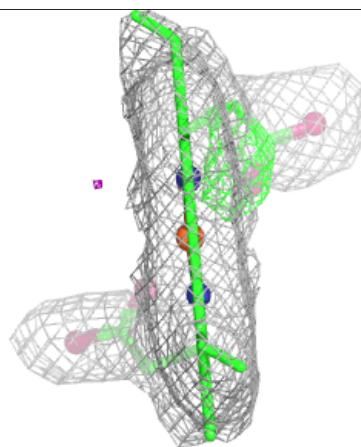
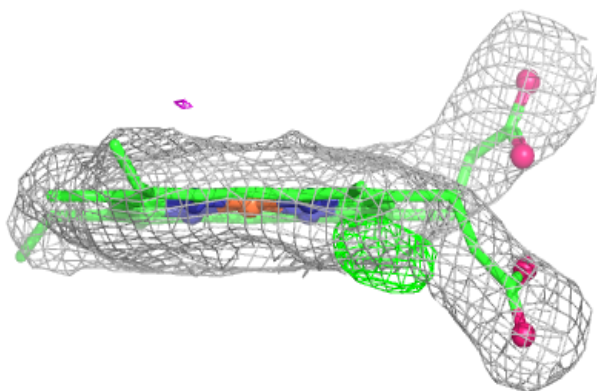
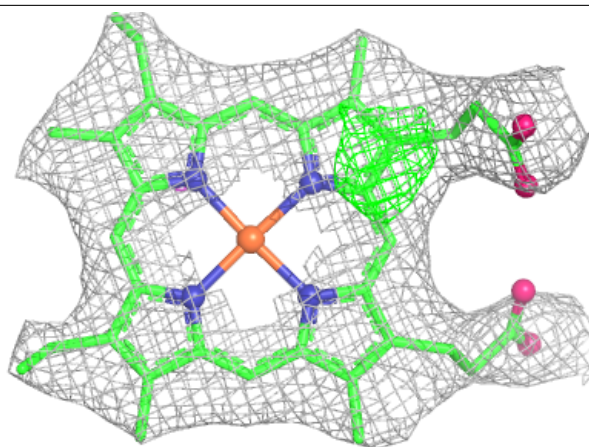
**Electron density around CLA B 605:**

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



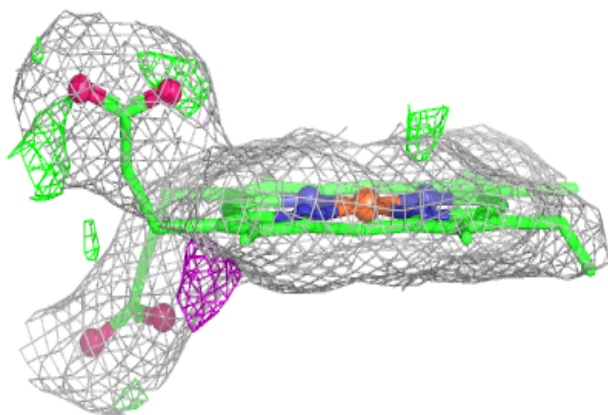
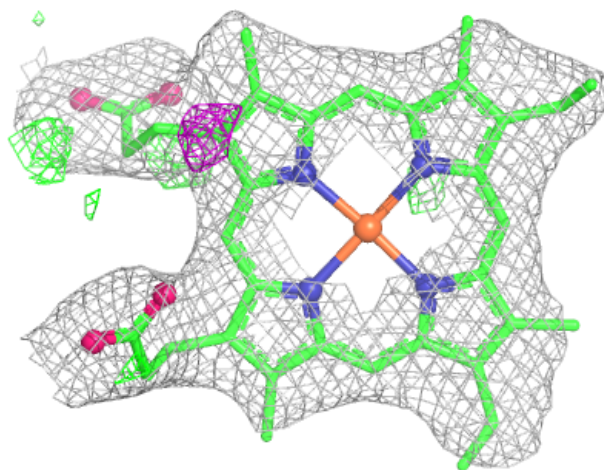
Electron density around HEM E 102:

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



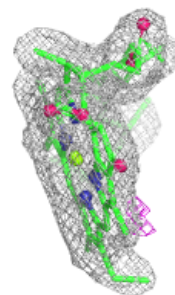
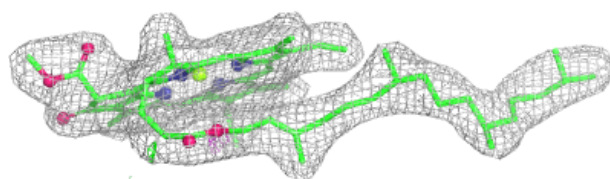
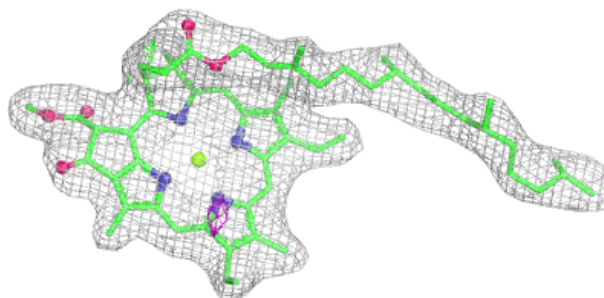
Electron density around HEM e 101:

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



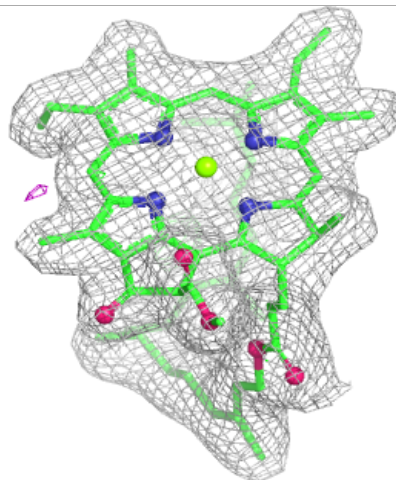
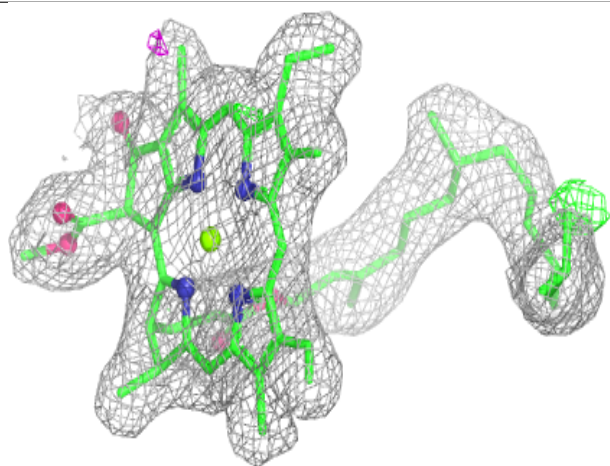
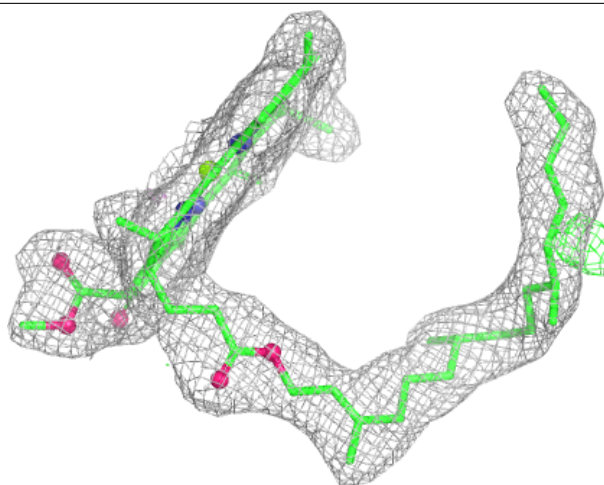
Electron density around CLA C 501:

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



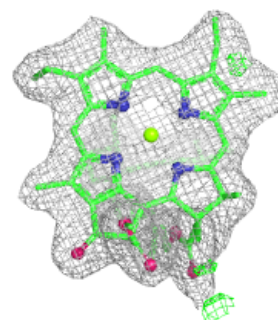
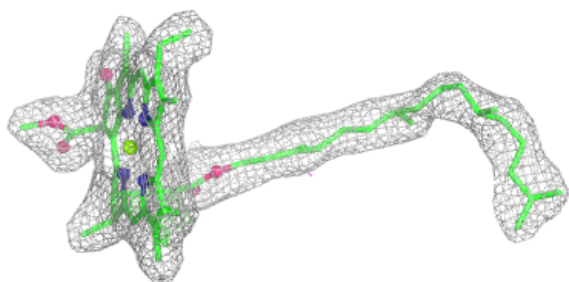
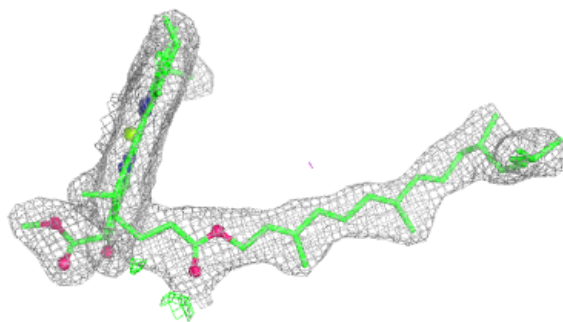
Electron density around CLA B 611:

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



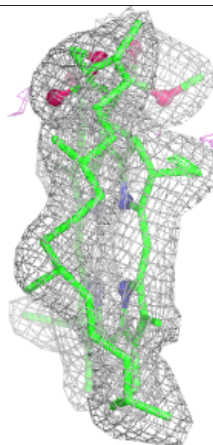
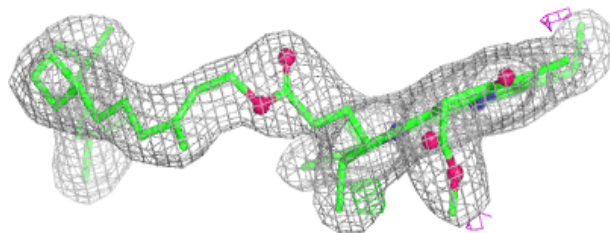
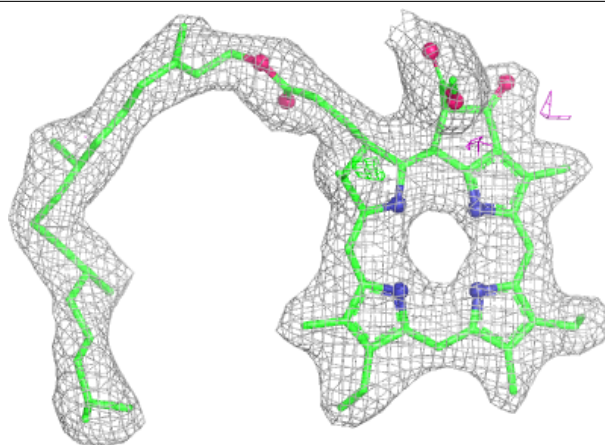
Electron density around CLA b 605:

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



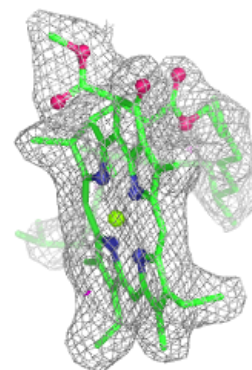
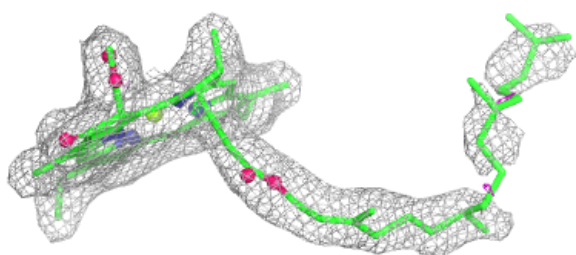
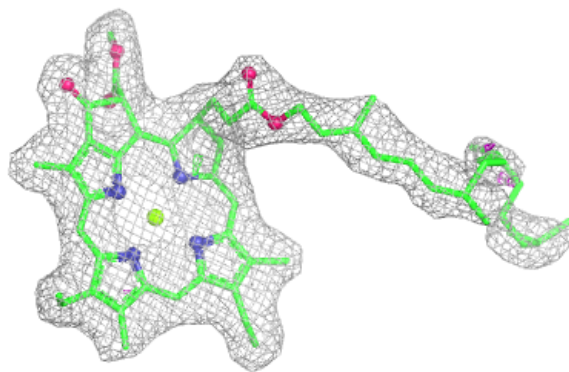
Electron density around PHO D 401:

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

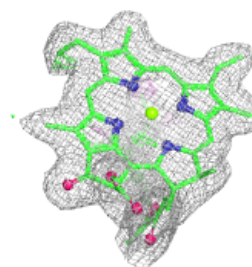
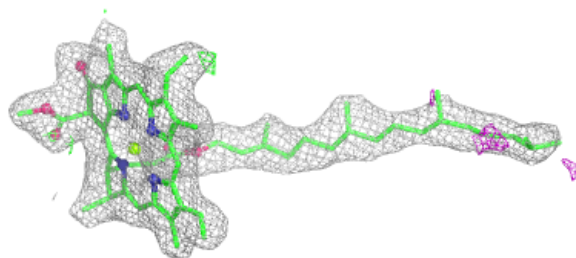
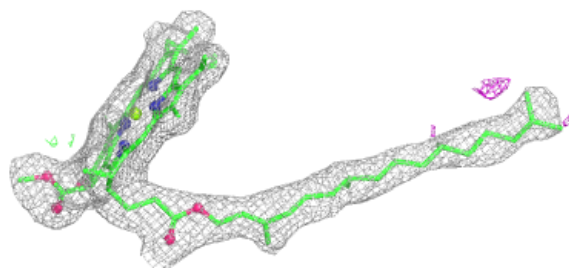


Electron density around CLA a 610:

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

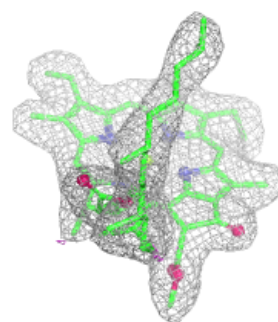
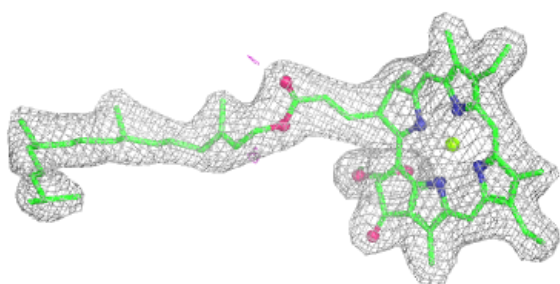
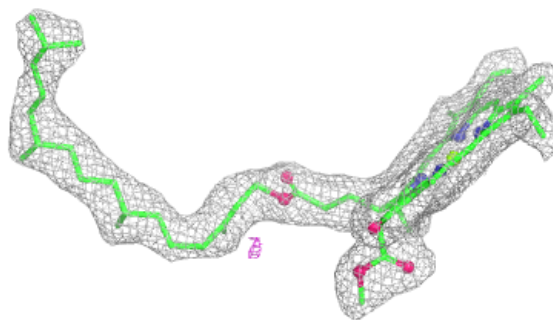
**Electron density around CLA b 607:**

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



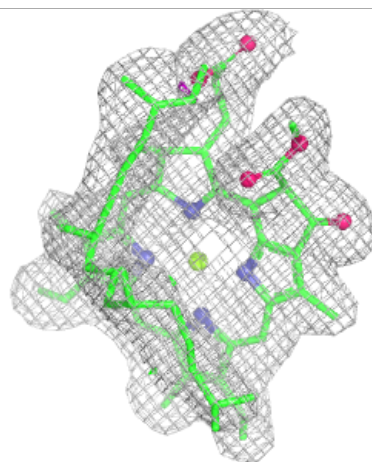
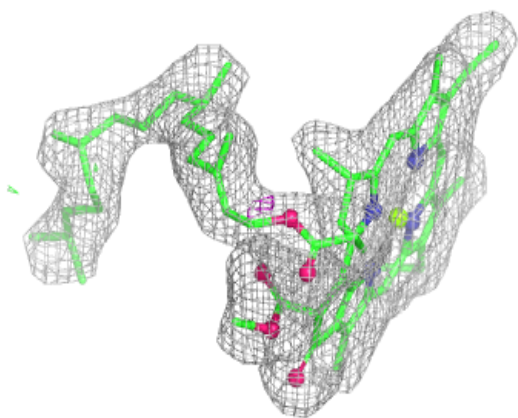
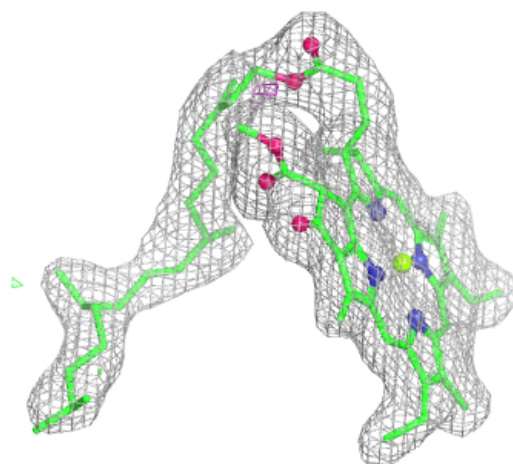
Electron density around CLA d 401:

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



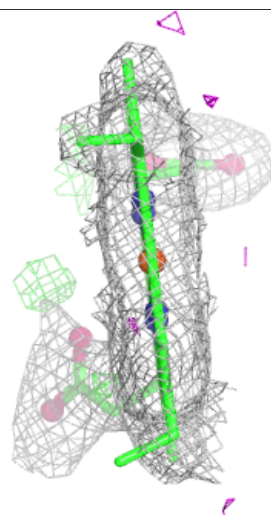
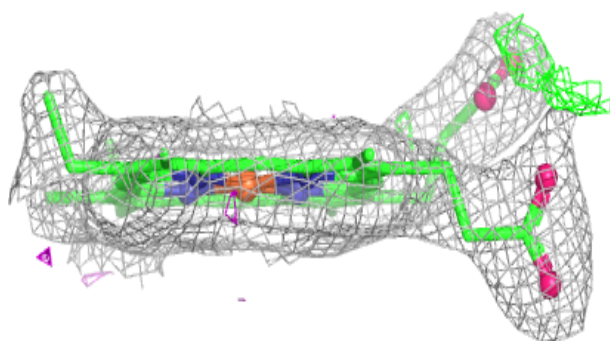
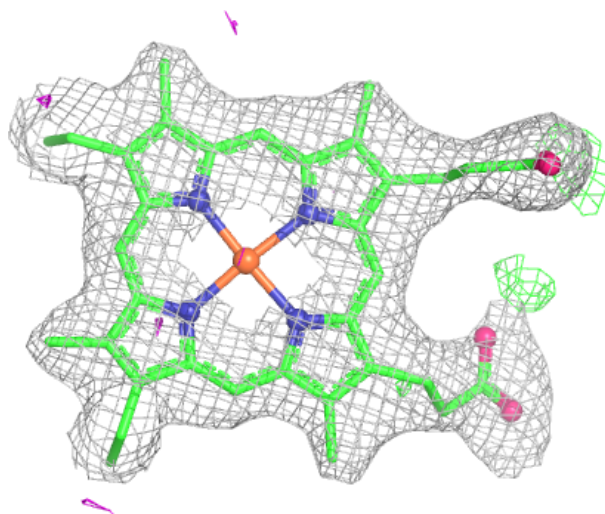
Electron density around CLA B 613:

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



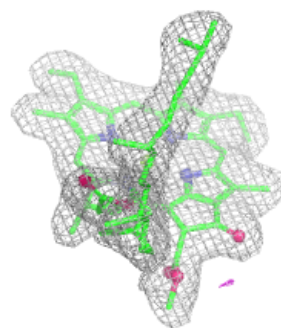
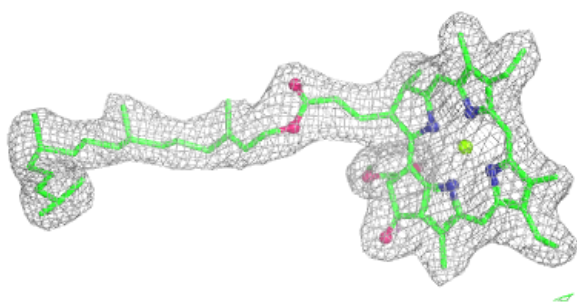
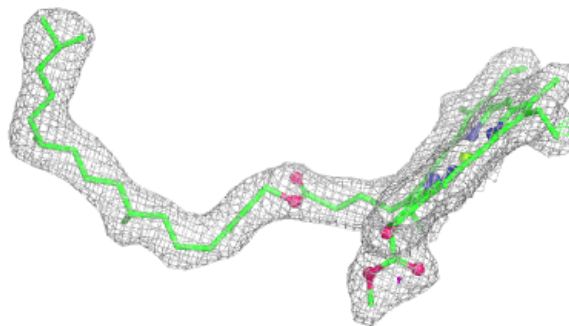
Electron density around HEC v 201:

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

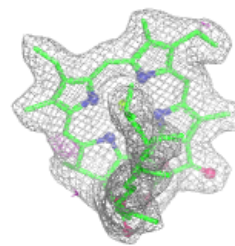
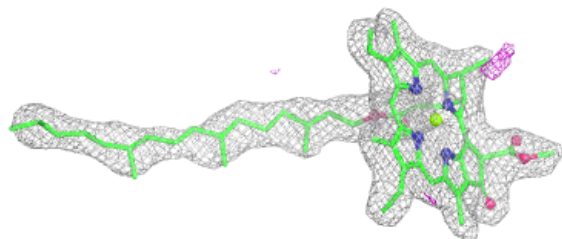
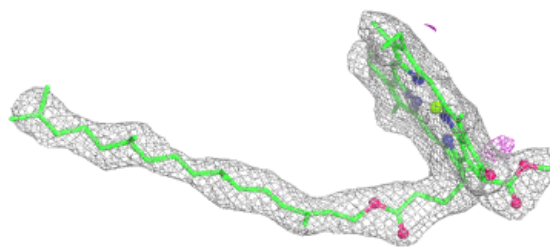


Electron density around CLA D 404:

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

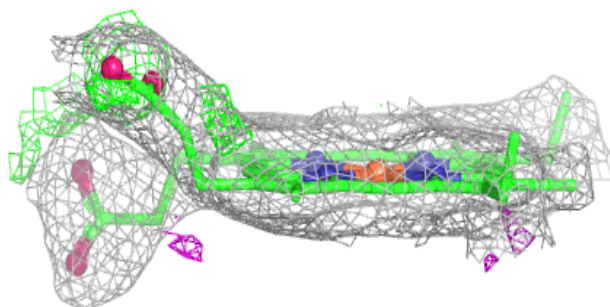
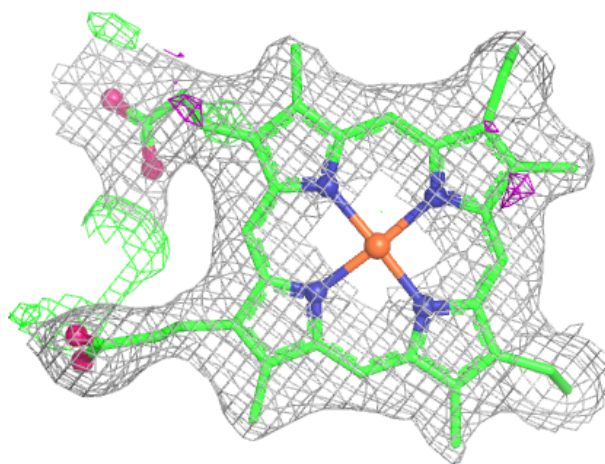
**Electron density around CLA B 607:**

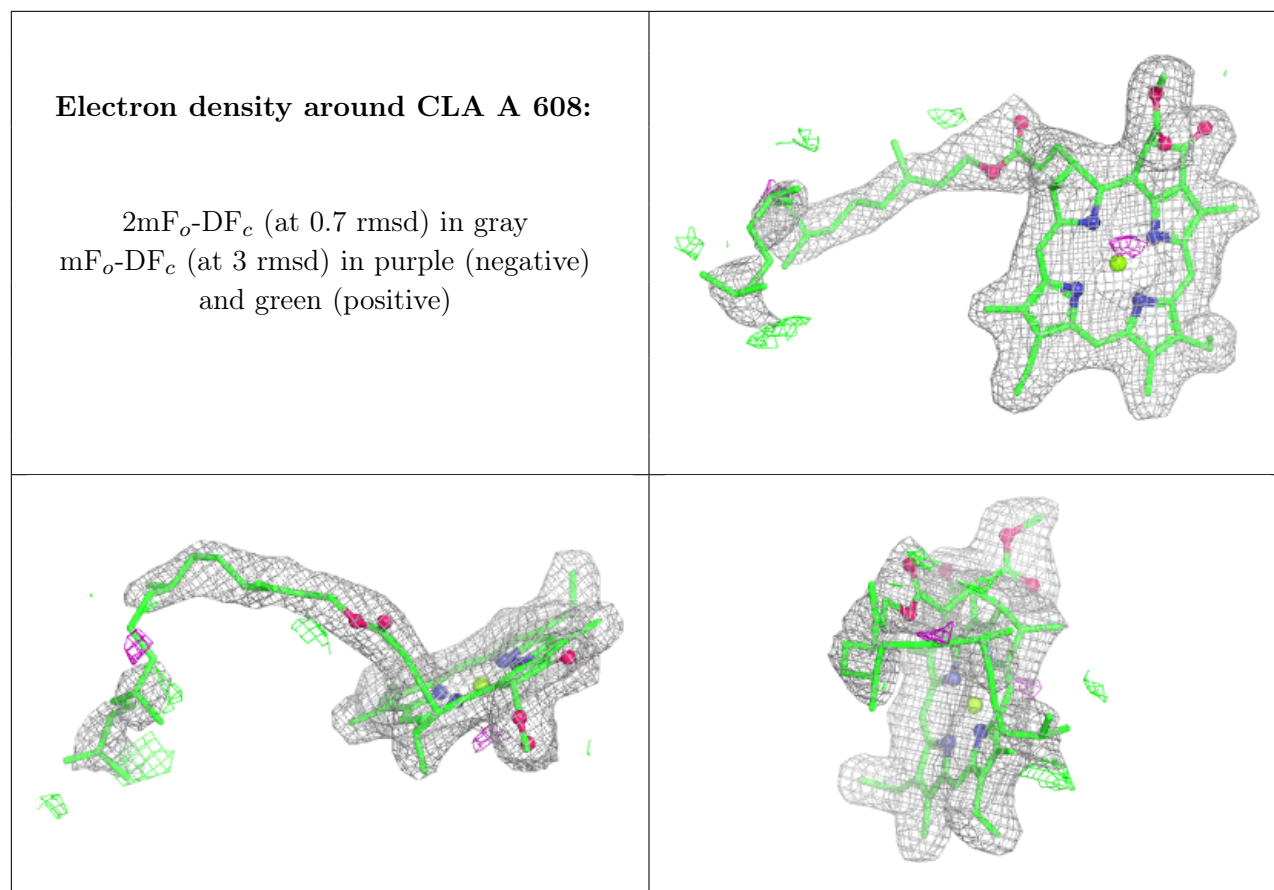
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.