



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:44 PM UTC

PDB ID : 8F4G / pdb_00008f4g
Title : RT XFEL structure of Photosystem II 730 microseconds after the third illumination at 2.03 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.03 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

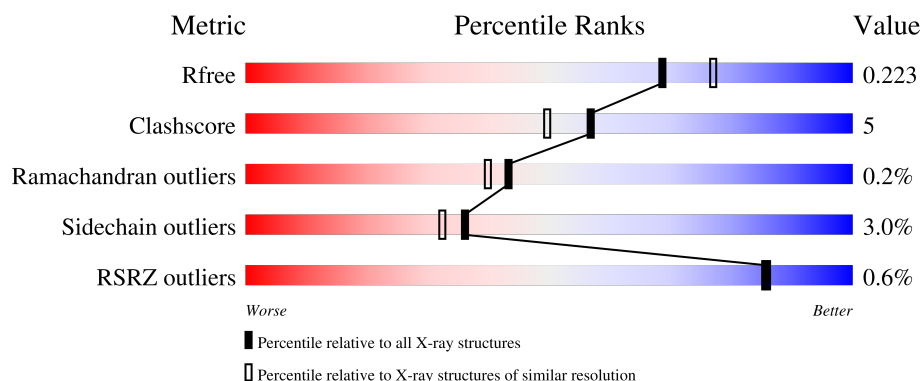
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

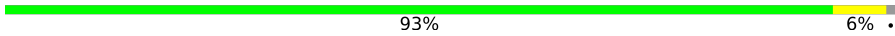
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	

Continued on next page...

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

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	a	344	 85% 10% . .
2	B	510	 93% 6% .
2	b	510	 91% 8% .
3	C	461	 89% 6% .
3	c	461	 90% 8% .
4	D	352	 89% 8% .
4	d	352	 89% 7% . .
5	E	84	 87% 10% . .
5	e	84	 79% 19% .
6	F	45	 71% . . 24%
6	f	45	 49% 22% . 24%
7	H	66	 86% 11% . .
7	h	66	 89% 6% 5%
8	I	38	 84% 11% 5%
8	i	38	 89% 5% 5%
9	J	40	 80% 10% 10%
9	j	40	 65% 22% . 10%
10	K	46	 78% . 20%
10	k	46	 67% 13% 20%
11	L	37	 86% 14%
11	l	37	 81% 14% . .
12	M	36	 72% 19% 8%
12	m	36	 75% 14% 11%
13	O	272	 81% 8% . 10%
13	o	272	 83% 6% . 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	T	32	
14	t	32	
15	U	134	
15	u	134	
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	609	X	-	-	-
25	CLA	A	612	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	609	X	-	-	-
25	CLA	B	610	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	-	-	-
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	H	101	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	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	c	501	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	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	404	X	-	-	-
25	CLA	h	101	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54517 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 II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	64	0
			3604	2343	595	643	23			
1	a	334	Total	C	N	O	S	0	64	0
			3601	2340	595	643	23			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	4	0
			4005	2631	666	695	13			
2	b	505	Total	C	N	O	S	0	0	0
			3978	2610	665	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3592	2355	601	621	15			
3	c	451	Total	C	N	O	S	0	12	0
			3666	2396	617	638	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2745	1818	448	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2751	1822	448	469	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	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	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	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
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	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	32	Total	C	N	O	S	0	0	0
			251	168	36	46	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	1	0
			1870	1168	313	385	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	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	27	Total	C	N	O	S	0	0	0
			196	128	35	30	3			
17	y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			281	188	45	48				
18	x	39	Total	C	N	O		0	0	0
			286	191	46	49				

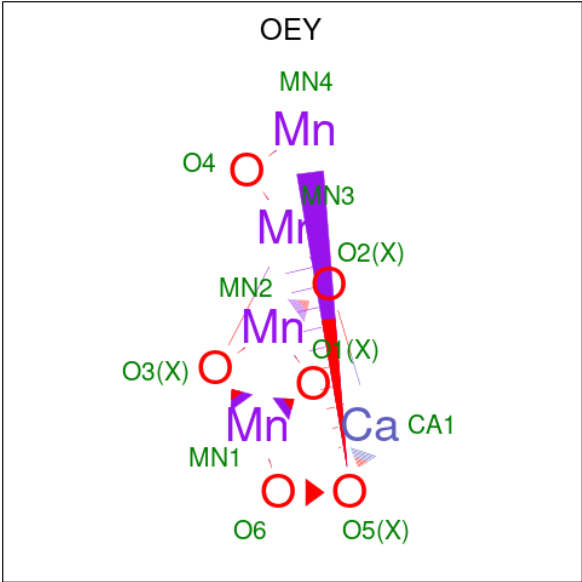
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			477	326	72	77	2			

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

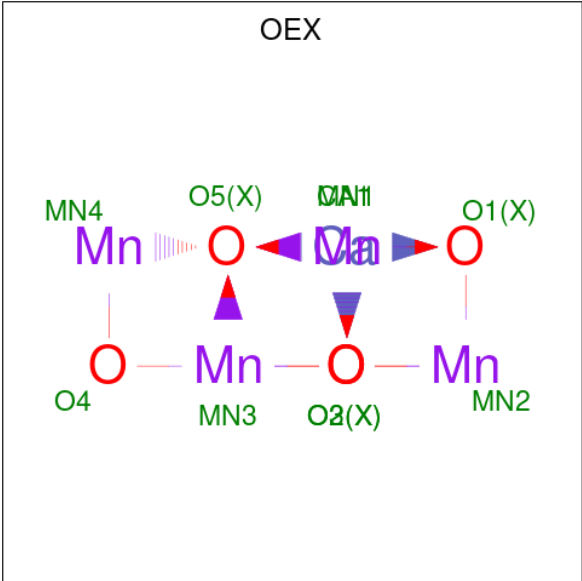
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			22	2	8	12		
21	a	1	Total	Ca	Mn	O	0	1
			22	2	8	12		

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

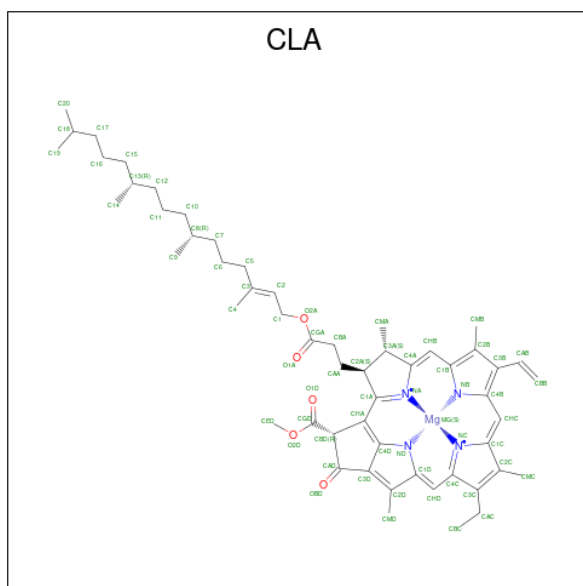
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- 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	C	Mg	N	O	0
			65	55	1	4	5	0
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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	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
25	H	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

Continued on next page...

Continued from previous page...

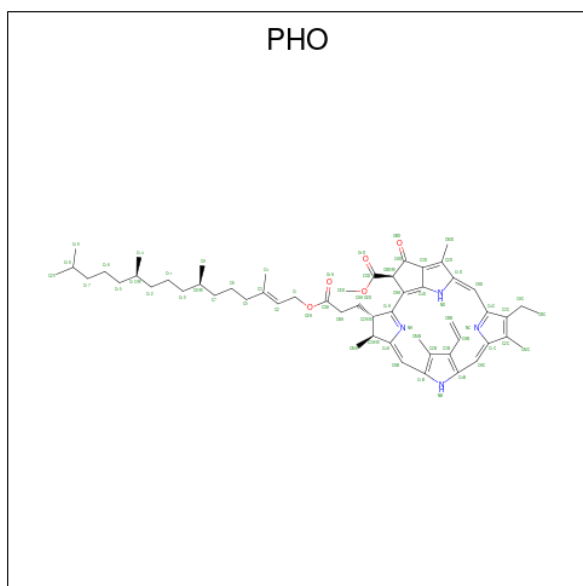
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 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 60	C 50	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 60	C 50	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 64	C 54	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...

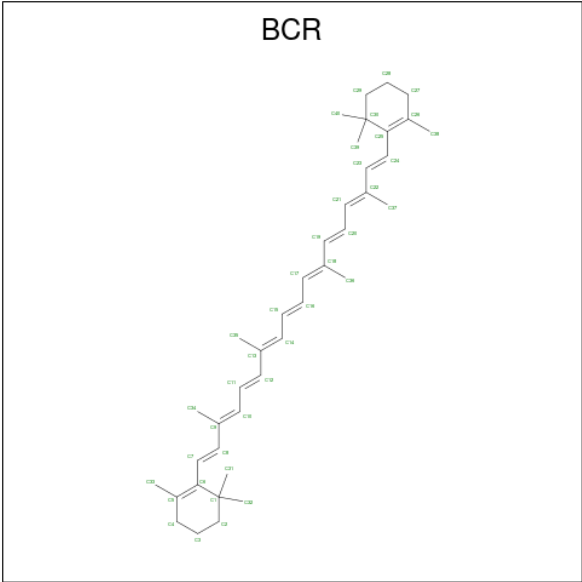
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



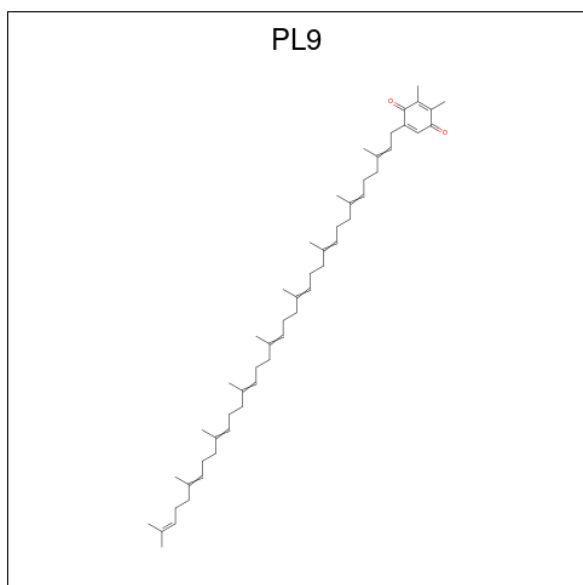
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 28 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).



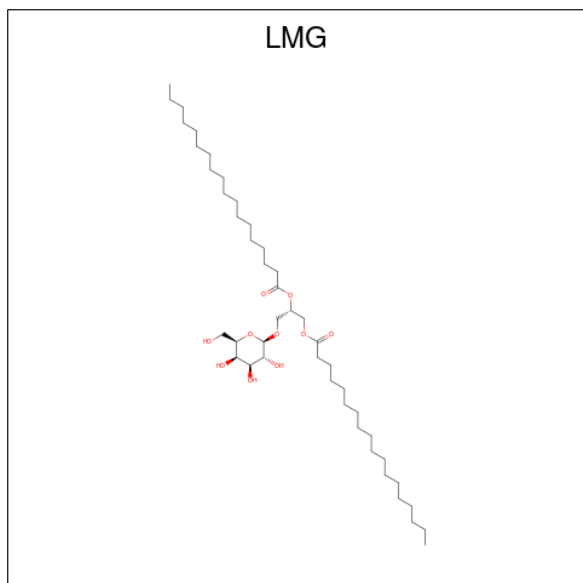
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



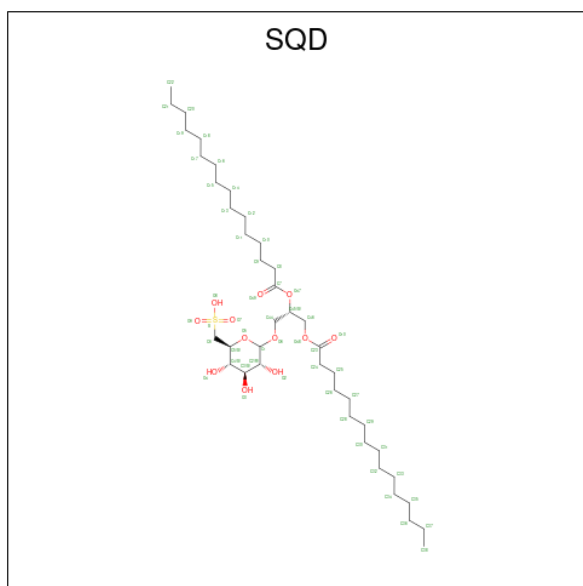
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C	O	0	0
			37	27	10		
29	c	1	Total	C	O	0	0
			48	38	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			49	39	10		
29	d	1	Total	C	O	0	0
			23	21	2		
29	d	1	Total	C	O	0	0
			44	34	10		
29	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



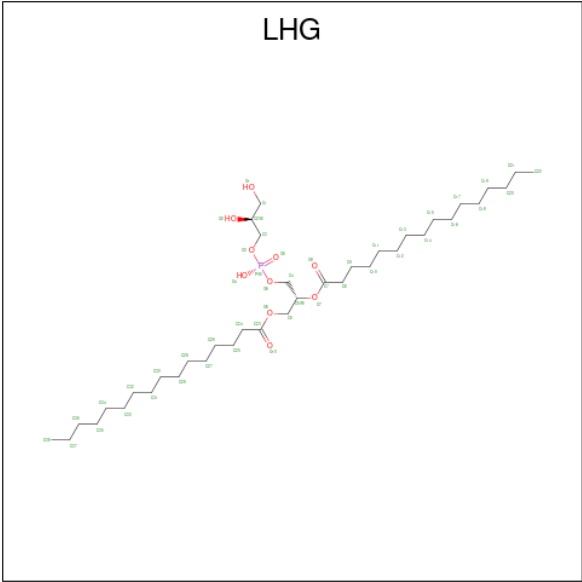
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	F	1	Total	C	O	S	0	0
			36	25	10	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36	31	5			
30	b	1	Total	C	O	S	0	0
			49	36	12	1		

Continued on next page...

Continued from previous page...

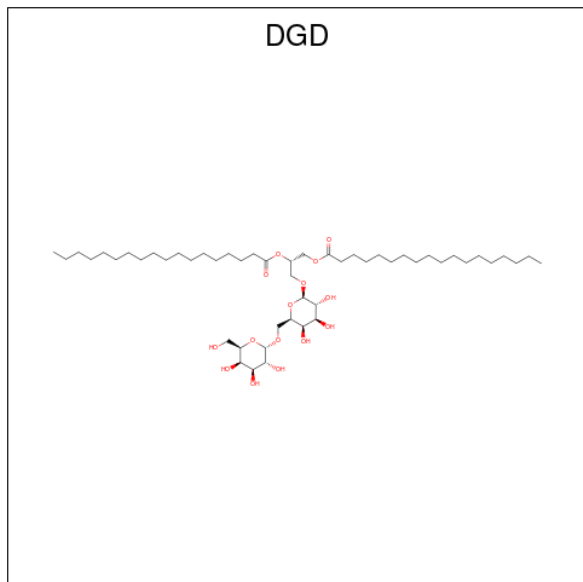
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



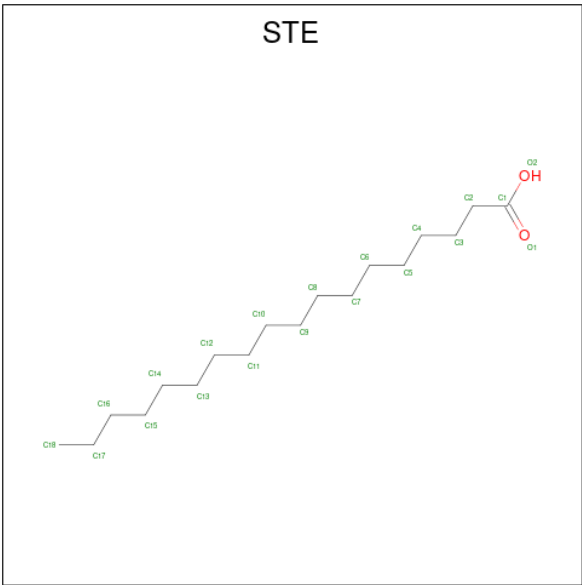
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			47	36	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	b	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			39	28	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			66	51	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		
32	H	1	Total	C	O	0	0
			62	47	15		
32	a	1	Total	C	O	0	0
			44	39	5		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	c	1	Total	C	O	0	0
			62	47	15		
32	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



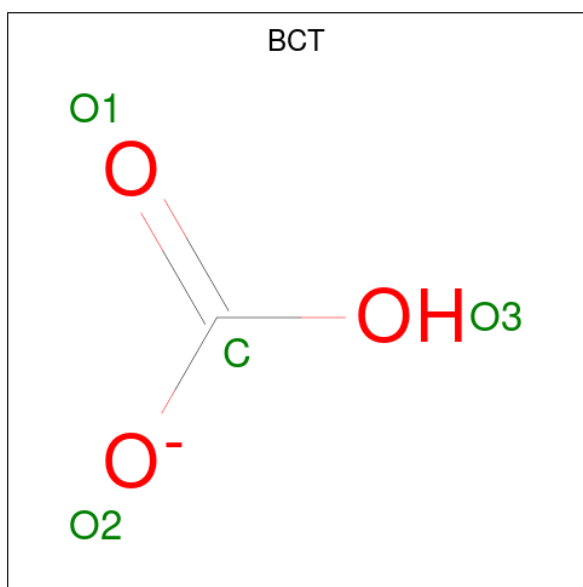
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			17	15	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C	O	0	0
			18	16	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C		0	0
			16	16			
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C		0	0
			16	16			
33	E	1	Total	C	O	0	0
			12	10	2		
33	H	1	Total	C		0	0
			18	18			
33	I	1	Total	C		0	0
			15	15			
33	J	1	Total	C	O	0	0
			12	10	2		
33	M	1	Total	C	O	0	0
			15	13	2		
33	M	1	Total	C		0	0
			10	10			

Continued on next page...

Continued from previous page...

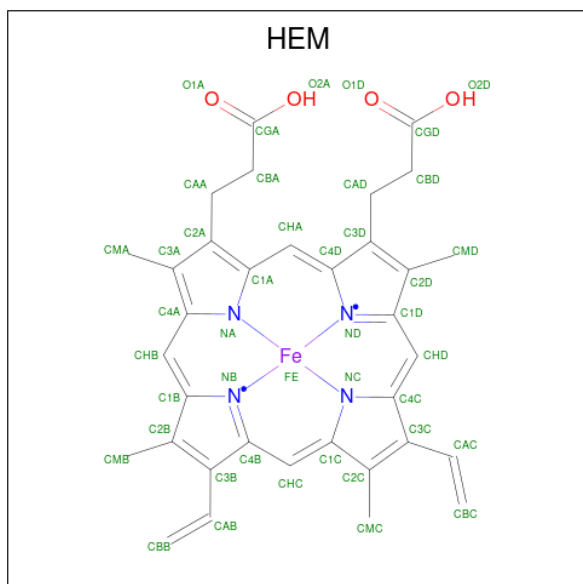
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	1	Total C O 20 18 2	0	0
33	a	1	Total C O 12 10 2	0	0
33	b	1	Total C 16 16	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 15 15	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 10 10	0	0
33	c	1	Total C O 20 18 2	0	0
33	d	1	Total C O 16 14 2	0	0
33	d	1	Total C O 17 15 2	0	0
33	j	1	Total C O 12 10 2	0	0
33	k	1	Total C O 12 10 2	0	0
33	l	1	Total C 18 18	0	0
33	m	1	Total C O 12 10 2	0	0
33	t	1	Total C O 14 12 2	0	0
33	t	1	Total C 10 10	0	0
33	x	1	Total C O 20 18 2	0	0

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	D	1	Total	C	O	0	0
			4	1	3		
34	d	1	Total	C	O	0	0
			4	1	3		

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



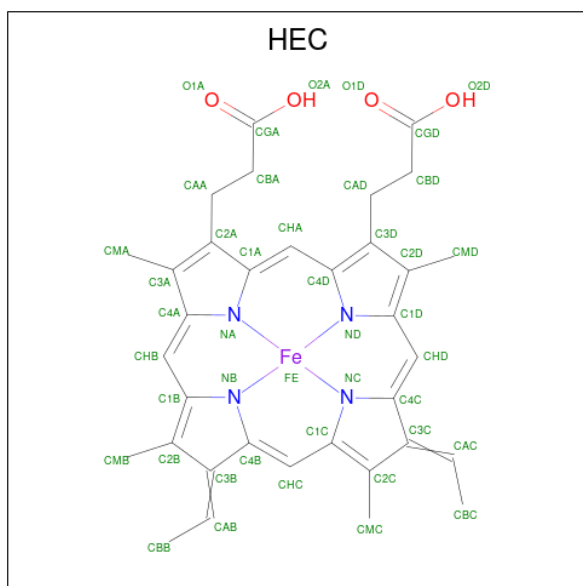
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

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

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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	142	Total	O	0	4
			150	150		
37	B	204	Total	O	0	0
			204	204		
37	C	184	Total	O	0	0
			184	184		
37	D	133	Total	O	0	0
			133	133		
37	E	21	Total	O	0	0
			21	21		
37	F	6	Total	O	0	0
			6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	28	Total 28	O 28	0	0
37	I	12	Total 12	O 12	0	0
37	J	10	Total 10	O 10	0	0
37	K	1	Total 1	O 1	0	0
37	L	10	Total 10	O 10	0	0
37	M	7	Total 7	O 7	0	0
37	O	93	Total 93	O 93	0	0
37	T	8	Total 8	O 8	0	0
37	U	43	Total 43	O 43	0	0
37	V	69	Total 69	O 69	0	0
37	Y	3	Total 3	O 3	0	0
37	X	15	Total 15	O 15	0	0
37	Z	4	Total 4	O 4	0	0
37	R	1	Total 1	O 1	0	0
37	a	115	Total 123	O 123	0	4
37	b	189	Total 189	O 189	0	0
37	c	175	Total 175	O 175	0	0
37	d	112	Total 112	O 112	0	0
37	e	18	Total 18	O 18	0	0
37	f	7	Total 7	O 7	0	0
37	h	18	Total 18	O 18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	7	Total 7	O 7	0	0
37	j	4	Total 4	O 4	0	0
37	k	7	Total 7	O 7	0	0
37	l	8	Total 8	O 8	0	0
37	m	7	Total 7	O 7	0	0
37	o	99	Total 99	O 99	0	0
37	t	11	Total 11	O 11	0	0
37	u	55	Total 55	O 55	0	0
37	v	58	Total 58	O 58	0	0
37	y	1	Total 1	O 1	0	0
37	x	10	Total 10	O 10	0	0
37	z	1	Total 1	O 1	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.

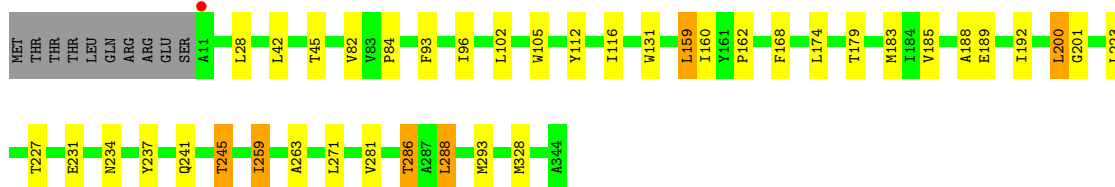
- Molecule 1: Photosystem II protein D1 1

Chain A: 



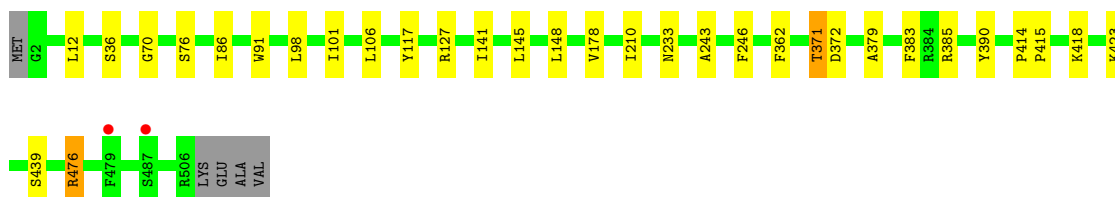
- Molecule 1: Photosystem II protein D1 1

Chain a: 



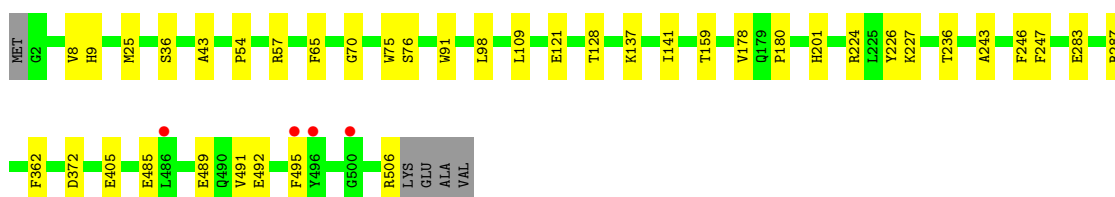
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

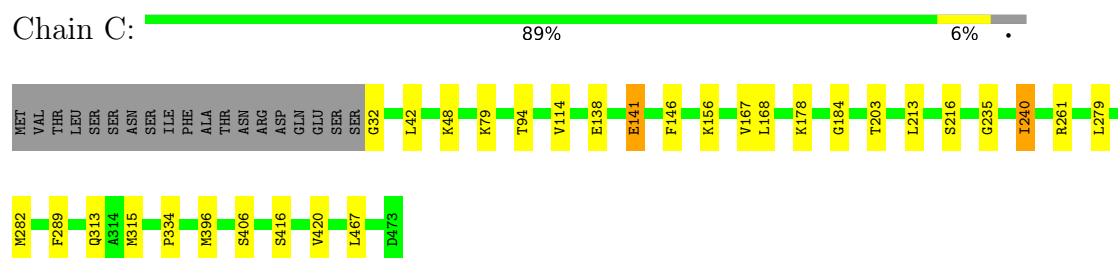


- Molecule 2: Photosystem II CP47 reaction center protein

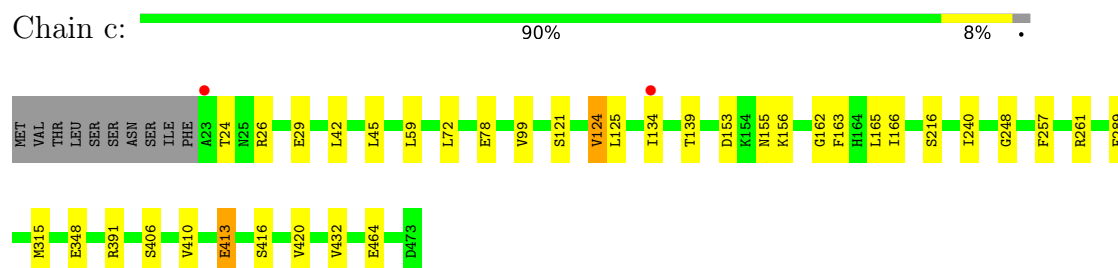
Chain b: 



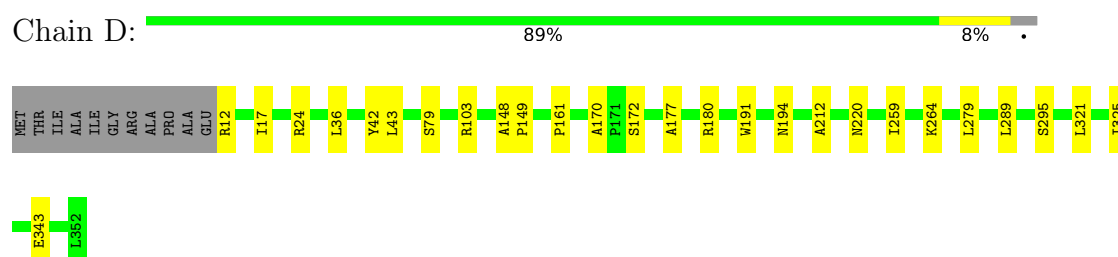
- Molecule 3: Photosystem II CP43 reaction center protein



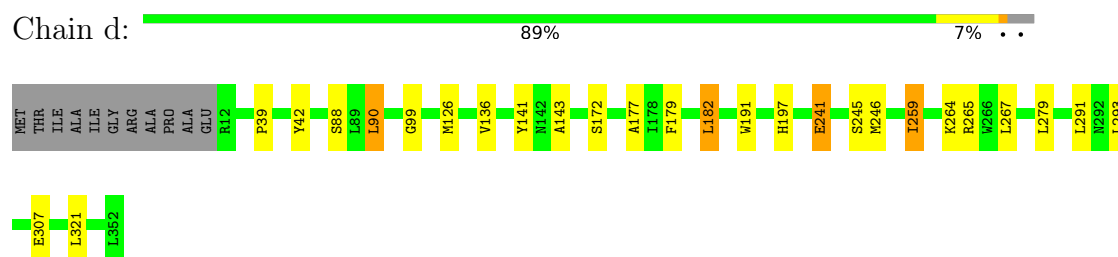
- Molecule 3: Photosystem II CP43 reaction center protein



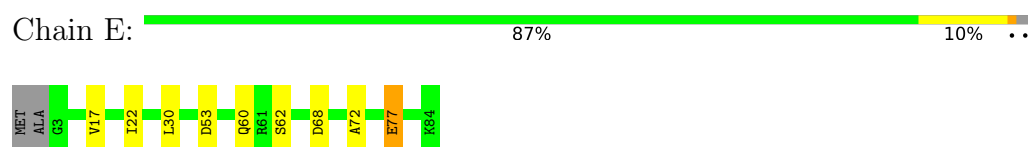
- Molecule 4: Photosystem II D2 protein



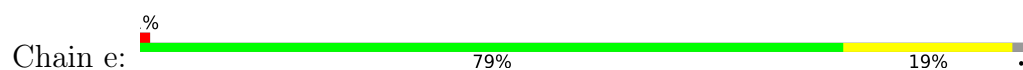
- Molecule 4: Photosystem II D2 protein



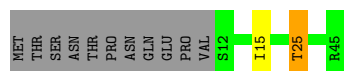
- Molecule 5: Cytochrome b559 subunit alpha



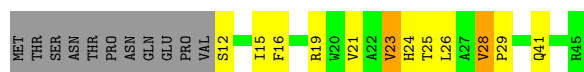
- Molecule 5: Cytochrome b559 subunit alpha



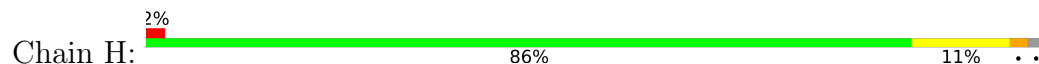
- Molecule 6: Cytochrome b559 subunit beta



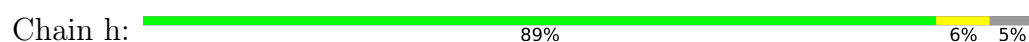
- Molecule 6: Cytochrome b559 subunit beta



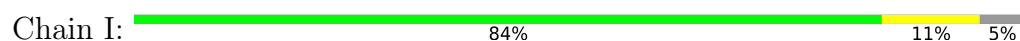
- Molecule 7: Photosystem II reaction center protein H



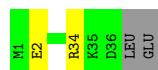
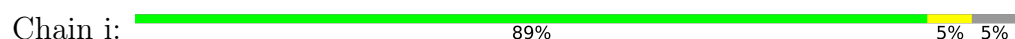
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

Chain J:  80% 10% 10%



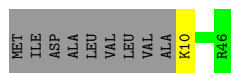
- Molecule 9: Photosystem II reaction center protein J

Chain j:  65% 22% 10%



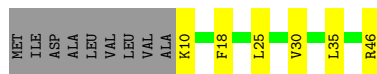
- Molecule 10: Photosystem II reaction center protein K

Chain K:  78% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  67% 13% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  81% 14% 2%



- Molecule 12: Photosystem II reaction center protein M

Chain M:  72% 19% 8%



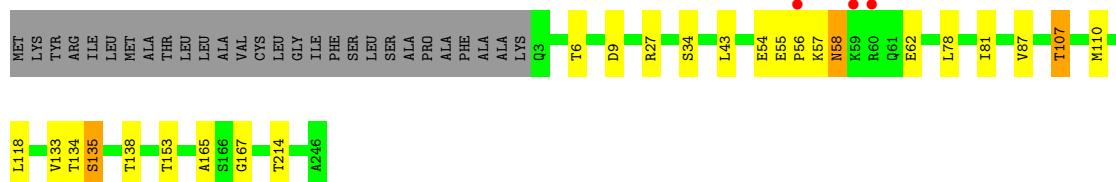
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 14% 11%



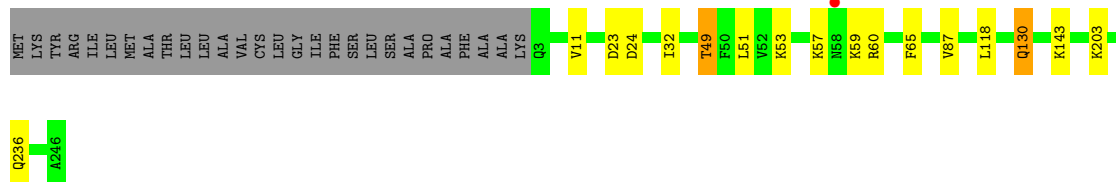
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  81% 8% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  83% 6% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 9% 6%



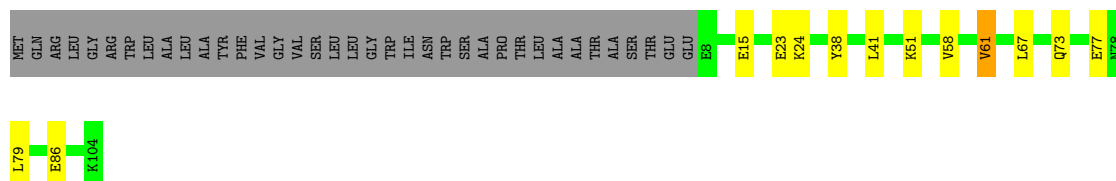
- Molecule 14: Photosystem II reaction center protein T

Chain t:  91% 6%

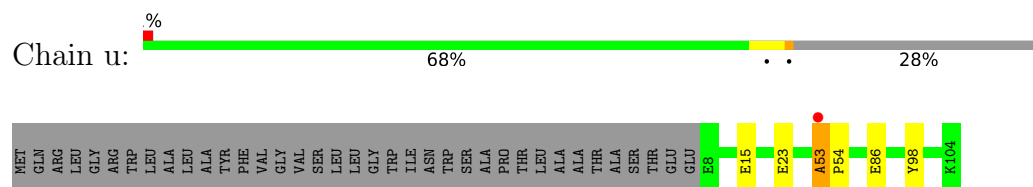


- Molecule 15: Photosystem II 12 kDa extrinsic protein

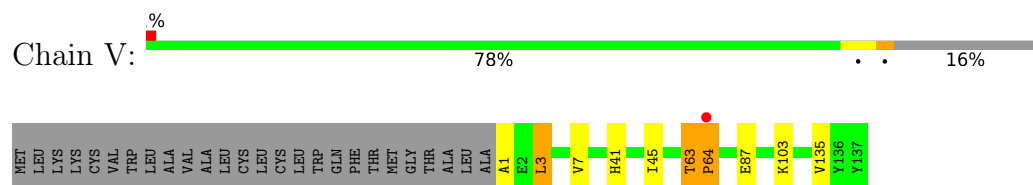
Chain U:  63% 9% 28%



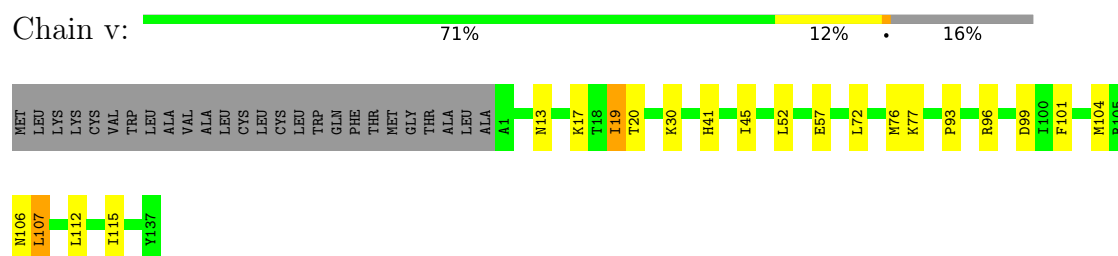
- Molecule 15: Photosystem II 12 kDa extrinsic protein



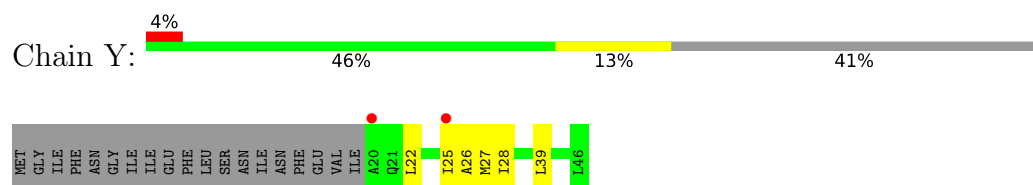
- Molecule 16: Cytochrome c-550



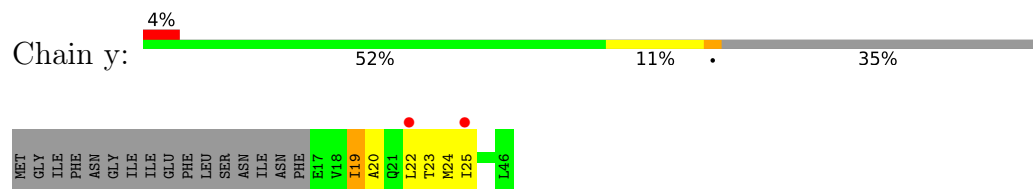
- Molecule 16: Cytochrome c-550



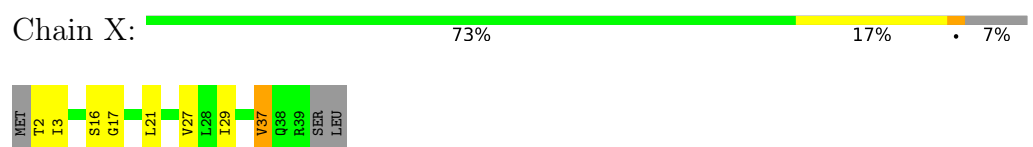
- Molecule 17: Photosystem II reaction center protein Ycf12



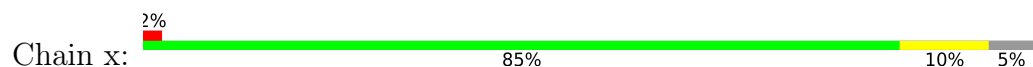
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

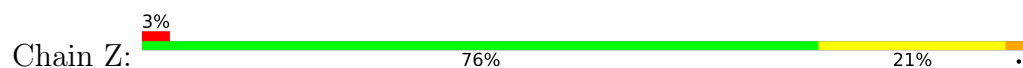


- Molecule 18: Photosystem II reaction center X protein

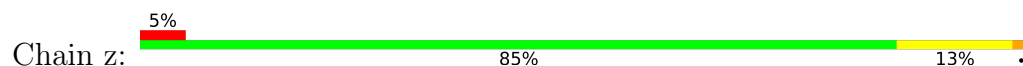




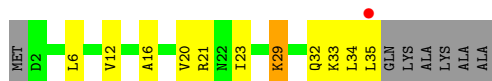
- Molecule 19: Photosystem II reaction center protein Z



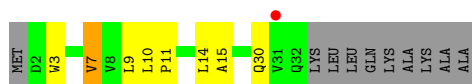
- Molecule 19: Photosystem II reaction center protein Z



- 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	117.57Å 222.91Å 310.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.03 29.87 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.87-2.03) 87.2 (29.87-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.26 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.223 0.180 , 0.223	Depositor DCC
R_{free} test set	4628 reflections (0.74%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	54517	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/3717	0.45	0/5060
1	a	0.28	0/3714	0.44	0/5056
2	B	0.32	0/4155	0.48	0/5661
2	b	0.31	0/4118	0.46	0/5611
3	C	0.30	0/3711	0.44	0/5051
3	c	0.29	0/3791	0.45	0/5158
4	D	0.35	0/2838	0.49	0/3862
4	d	0.34	0/2847	0.49	0/3874
5	E	0.25	0/688	0.41	0/940
5	e	0.23	0/683	0.41	0/932
6	F	0.25	0/284	0.42	0/387
6	f	0.24	0/284	0.48	0/387
7	H	0.30	0/523	0.45	0/713
7	h	0.27	0/511	0.47	0/697
8	I	0.28	0/293	0.46	0/396
8	i	0.31	0/293	0.46	0/396
9	J	0.25	0/263	0.40	0/356
9	j	0.23	0/263	0.38	0/356
10	K	0.24	0/303	0.41	0/416
10	k	0.22	0/303	0.38	0/416
11	L	0.33	0/311	0.45	0/422
11	l	0.35	0/303	0.45	0/412
12	M	0.32	0/249	0.50	0/341
12	m	0.33	0/244	0.51	0/334
13	O	0.29	0/1904	0.50	0/2585
13	o	0.30	0/1905	0.49	0/2583
14	T	0.31	0/257	0.48	0/349
14	t	0.29	0/255	0.46	0/346
15	U	0.28	0/785	0.45	0/1064
15	u	0.29	0/785	0.48	0/1064
16	V	0.30	0/1085	0.51	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1085	0.42	0/1473
17	Y	0.21	0/197	0.37	0/264
17	y	0.17	0/219	0.32	0/294
18	X	0.23	0/284	0.38	0/384
18	x	0.20	0/289	0.28	0/391
19	Z	0.21	0/490	0.43	0/669
19	z	0.16	0/488	0.28	0/666
20	R	0.24	0/277	0.36	0/380
20	r	0.23	0/252	0.38	0/347
All	All	0.30	0/45246	0.46	0/61566

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
16	V	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	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	3604	0	3445	17	0
1	a	3601	0	3436	35	0
2	B	4005	0	3871	19	0
2	b	3978	0	3836	26	0
3	C	3592	0	3501	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3666	0	3574	21	0
4	D	2745	0	2653	20	0
4	d	2751	0	2659	21	0
5	E	666	0	651	6	0
5	e	664	0	648	11	0
6	F	275	0	282	2	0
6	f	275	0	282	12	0
7	H	510	0	532	7	0
7	h	498	0	518	3	0
8	I	296	0	311	1	0
8	i	296	0	311	1	0
9	J	257	0	268	3	0
9	j	257	0	268	7	0
10	K	293	0	305	0	0
10	k	293	0	305	3	0
11	L	304	0	316	5	0
11	l	296	0	304	4	0
12	M	256	0	269	3	0
12	m	251	0	267	3	0
13	O	1870	0	1830	16	0
13	o	1874	0	1846	10	0
14	T	258	0	261	3	0
14	t	256	0	256	1	0
15	U	774	0	773	5	0
15	u	774	0	773	3	0
16	V	1064	0	1073	7	0
16	v	1064	0	1073	15	0
17	Y	196	0	217	5	0
17	y	218	0	241	3	0
18	X	281	0	312	6	0
18	x	286	0	314	4	0
19	Z	479	0	516	8	0
19	z	477	0	509	7	0
20	R	271	0	298	8	0
20	r	246	0	263	6	0
21	A	22	0	0	2	0
21	a	22	0	0	2	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	7	0
25	B	970	0	1067	27	0
25	C	839	0	922	18	0
25	D	130	0	144	3	0
25	H	65	0	72	1	0
25	a	260	0	288	4	0
25	b	970	0	1067	28	0
25	c	839	0	919	17	0
25	d	130	0	144	1	0
25	h	65	0	72	2	0
26	A	64	0	74	1	0
26	D	64	0	74	0	0
26	a	64	0	74	0	0
26	d	64	0	74	1	0
27	A	40	0	56	1	0
27	B	120	0	168	4	0
27	C	80	0	112	4	0
27	D	40	0	56	0	0
27	H	40	0	56	1	0
27	K	80	0	112	4	0
27	T	40	0	56	2	0
27	a	40	0	56	0	0
27	b	120	0	168	4	0
27	c	80	0	112	3	0
27	d	40	0	56	0	0
27	h	40	0	56	3	0
27	k	80	0	112	3	0
27	t	40	0	56	2	0
28	A	55	0	80	7	0
28	D	55	0	80	1	0
28	a	55	0	80	5	0
28	d	55	0	80	1	0
29	A	48	0	66	2	0
29	B	28	0	40	1	0
29	C	48	0	66	1	0
29	D	84	0	117	2	0
29	M	51	0	72	2	0
29	b	55	0	86	0	0
29	c	134	0	181	1	0
29	d	67	0	92	1	0
29	m	51	0	72	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	91	0	136	3	0
30	B	54	0	78	2	0
30	F	36	0	46	1	0
30	a	90	0	134	4	0
30	b	49	0	65	1	0
30	f	41	0	49	1	0
31	A	49	0	74	3	0
31	D	145	0	215	12	0
31	L	49	0	74	1	0
31	b	49	0	74	4	0
31	d	137	0	199	7	0
31	e	42	0	57	3	0
32	A	66	0	96	4	0
32	C	186	0	246	12	0
32	H	62	0	82	5	0
32	a	44	0	75	2	0
32	c	186	0	246	6	0
32	h	62	0	82	1	0
33	B	75	0	117	3	0
33	C	40	0	63	1	0
33	E	12	0	16	0	0
33	H	18	0	35	1	0
33	I	15	0	26	2	0
33	J	12	0	16	2	0
33	M	25	0	38	1	0
33	X	20	0	35	5	0
33	a	12	0	16	0	0
33	b	81	0	146	4	0
33	c	20	0	35	1	0
33	d	33	0	50	2	0
33	j	12	0	16	0	0
33	k	12	0	16	0	0
33	l	18	0	35	1	0
33	m	12	0	16	1	0
33	t	24	0	36	0	0
33	x	20	0	35	2	0
34	D	4	0	1	1	0
34	d	4	0	1	0	0
35	F	43	0	30	2	0
35	f	43	0	30	3	0
36	V	43	0	30	0	0
36	v	43	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A	150	0	0	3	0
37	B	204	0	0	3	0
37	C	184	0	0	3	0
37	D	133	0	0	2	0
37	E	21	0	0	0	0
37	F	6	0	0	0	0
37	H	28	0	0	0	0
37	I	12	0	0	0	0
37	J	10	0	0	0	0
37	K	1	0	0	0	0
37	L	10	0	0	0	0
37	M	7	0	0	0	0
37	O	93	0	0	2	0
37	R	1	0	0	0	0
37	T	8	0	0	1	0
37	U	43	0	0	0	0
37	V	69	0	0	1	0
37	X	15	0	0	0	0
37	Y	3	0	0	2	0
37	Z	4	0	0	0	0
37	a	123	0	0	0	0
37	b	189	0	0	3	0
37	c	175	0	0	5	0
37	d	112	0	0	1	0
37	e	18	0	0	0	0
37	f	7	0	0	1	0
37	h	18	0	0	0	0
37	i	7	0	0	1	0
37	j	4	0	0	0	0
37	k	7	0	0	0	0
37	l	8	0	0	0	0
37	m	7	0	0	0	0
37	o	99	0	0	0	0
37	t	11	0	0	0	0
37	u	55	0	0	1	0
37	v	58	0	0	1	0
37	x	10	0	0	1	0
37	y	1	0	0	0	0
37	z	1	0	0	0	0
All	All	54517	0	53863	485	0

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

The worst 5 of 485 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)
21:a:601[C]:OEY:O5	21:a:601[C]:OEY:O6	1.86	0.93
21:A:601[C]:OEY:O6	21:A:601[C]:OEY:O5	1.87	0.92
3:c:153:ASP:OD1	37:c:601:HOH:O	1.98	0.80
21:A:601[A]:OEY:O6	21:A:601[A]:OEY:O5	2.03	0.76
21:a:601[A]:OEY:O5	21:a:601[A]:OEY:O6	2.02	0.76

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	458/344 (133%)	448 (98%)	9 (2%)	1 (0%)	43	40
1	a	458/344 (133%)	448 (98%)	9 (2%)	1 (0%)	43	40
2	B	507/510 (99%)	500 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	461/461 (100%)	452 (98%)	8 (2%)	1 (0%)	43	40
3	c	471/461 (102%)	454 (96%)	16 (3%)	1 (0%)	43	40
4	D	341/352 (97%)	331 (97%)	10 (3%)	0	100	100
4	d	342/352 (97%)	332 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	56 (92%)	5 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	229 (94%)	10 (4%)	4 (2%)	7	2
13	o	242/272 (89%)	233 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	5
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	10
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5534/5700 (97%)	5386 (97%)	138 (2%)	10 (0%)	43	40

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	58	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	V	64	PRO
13	O	62	GLU
3	c	416	SER

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	374/280 (134%)	370 (99%)	4 (1%)	65	68
1	a	373/280 (133%)	363 (97%)	10 (3%)	39	37
2	B	407/407 (100%)	399 (98%)	8 (2%)	48	48
2	b	402/407 (99%)	393 (98%)	9 (2%)	45	45
3	C	361/362 (100%)	357 (99%)	4 (1%)	65	68
3	c	370/362 (102%)	357 (96%)	13 (4%)	32	27
4	D	278/283 (98%)	276 (99%)	2 (1%)	76	77
4	d	279/283 (99%)	272 (98%)	7 (2%)	42	40
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	20
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	12
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	26
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	7
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	50
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	50
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	31
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	31
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	5
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	29
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	4
12	M	28/32 (88%)	25 (89%)	3 (11%)	6	2
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	7
13	O	206/228 (90%)	200 (97%)	6 (3%)	37	34
13	o	207/228 (91%)	202 (98%)	5 (2%)	43	41
14	T	26/28 (93%)	24 (92%)	2 (8%)	12	6
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	22
15	U	84/112 (75%)	79 (94%)	5 (6%)	17	10
15	u	84/112 (75%)	82 (98%)	2 (2%)	43	41
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	53
16	v	117/138 (85%)	114 (97%)	3 (3%)	40	38
17	Y	19/37 (51%)	19 (100%)	0	100	100
17	y	22/37 (60%)	21 (96%)	1 (4%)	24	17
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	2
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	30
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	3
19	z	51/52 (98%)	48 (94%)	3 (6%)	18	10
20	R	28/33 (85%)	24 (86%)	4 (14%)	3	1
20	r	25/33 (76%)	21 (84%)	4 (16%)	2	0
All	All	4572/4654 (98%)	4438 (97%)	134 (3%)	36	34

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	60	ARG
14	t	25	GLU
20	r	7	VAL
19	Z	19	MET
19	Z	15	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
19	Z	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	409	GLN
18	x	33	GLN
2	b	338	GLN
3	c	311	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.88	0	8,9,11	1.00	0
8	FME	i	1	8	8,9,10	1.04	0	8,9,11	0.97	0
12	FME	M	1	12	8,9,10	1.01	1 (12%)	8,9,11	1.15	0
8	FME	I	1	8	8,9,10	0.93	0	8,9,11	0.97	1 (12%)
12	FME	m	1	12	8,9,10	1.00	0	8,9,11	0.59	0
14	FME	T	1	14	8,9,10	1.11	1 (12%)	8,9,11	1.21	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	2/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.20	1.43	1.46
12	M	1	FME	CA-N	-2.12	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.26	113.86	109.50
8	I	1	FME	C-CA-N	2.04	113.43	109.50

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	O-C-CA-CB
8	i	1	FME	O-C-CA-CB
12	m	1	FME	O-C-CA-CB
14	t	1	FME	O-C-CA-CB
14	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 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	$\# Z > 2$
33	STE	C	520	-	11,11,19	0.64	0	11,11,19	1.56	2 (18%)
31	LHG	D	408	-	48,48,48	0.68	1 (2%)	51,54,54	1.27	7 (13%)
33	STE	M	103	-	9,9,19	0.37	0	8,8,19	0.70	0
31	LHG	d	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.39	7 (13%)
25	CLA	a	606	-	69,73,73	1.38	9 (13%)	82,113,113	1.35	8 (9%)
25	CLA	c	504	37	64,68,73	1.24	6 (9%)	76,107,113	1.37	9 (11%)
25	CLA	C	507	37	69,73,73	1.24	7 (10%)	82,113,113	1.37	5 (6%)
33	STE	C	522	-	15,15,19	0.32	0	14,14,19	0.90	0
22	OEX	A	602[B]	1,3,37	0,15,15	-	-	-	-	-
27	BCR	H	102	-	41,41,41	0.96	1 (2%)	56,56,56	1.19	6 (10%)
25	CLA	c	508	-	68,72,73	1.34	8 (11%)	80,111,113	1.42	10 (12%)
32	DGD	c	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.42	9 (11%)
31	LHG	d	409	-	38,38,48	0.82	1 (2%)	41,44,54	1.16	3 (7%)
25	CLA	B	612	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
29	LMG	c	519	-	37,37,55	0.91	1 (2%)	45,45,63	1.34	6 (13%)
34	BCT	D	401	23	3,3,3	1.24	0	2,3,3	2.92	1 (50%)
27	BCR	k	101	-	41,41,41	1.02	3 (7%)	56,56,56	1.03	2 (3%)
32	DGD	A	617	-	67,67,67	1.06	6 (8%)	81,81,81	1.32	12 (14%)
25	CLA	b	609	37	69,73,73	1.39	7 (10%)	82,113,113	1.39	8 (9%)
27	BCR	K	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.10	2 (3%)
29	LMG	D	410	-	31,31,55	0.70	1 (3%)	33,33,63	1.21	3 (9%)
33	STE	b	624	-	14,14,19	0.32	0	13,13,19	0.90	0
29	LMG	m	101	-	51,51,55	0.73	1 (1%)	59,59,63	1.41	8 (13%)
29	LMG	D	407	-	51,51,55	0.81	2 (3%)	59,59,63	1.34	5 (8%)
25	CLA	A	607	37	69,73,73	1.14	5 (7%)	82,113,113	1.18	8 (9%)
26	PHO	d	402	-	58,69,69	2.13	8 (13%)	55,99,99	1.57	9 (16%)
25	CLA	B	615	-	64,68,73	1.48	9 (14%)	76,107,113	1.49	7 (9%)
25	CLA	b	611	-	69,73,73	1.20	9 (13%)	82,113,113	1.38	11 (13%)
25	CLA	h	101	37	69,73,73	1.26	7 (10%)	82,113,113	1.33	7 (8%)
36	HEC	v	201	16	46,50,50	1.89	5 (10%)	58,82,82	1.81	4 (6%)
27	BCR	k	102	-	41,41,41	1.01	3 (7%)	56,56,56	1.21	5 (8%)
32	DGD	h	103	-	63,63,67	0.98	5 (7%)	77,77,81	1.45	12 (15%)
25	CLA	a	607	37	69,73,73	1.17	6 (8%)	82,113,113	1.34	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	d	405	-	41,41,41	1.06	2 (4%)	56,56,56	1.12	4 (7%)
25	CLA	C	504	37	63,67,73	1.39	9 (14%)	74,105,113	1.35	10 (13%)
25	CLA	b	610	-	69,73,73	1.30	6 (8%)	82,113,113	1.29	8 (9%)
25	CLA	d	404	-	69,73,73	1.11	7 (10%)	82,113,113	1.19	8 (9%)
25	CLA	a	612	37	69,73,73	1.40	7 (10%)	82,113,113	1.32	5 (6%)
26	PHO	A	608	-	58,69,69	2.03	9 (15%)	55,99,99	1.39	6 (10%)
29	LMG	B	620	-	26,26,55	0.72	2 (7%)	26,26,63	1.24	2 (7%)
29	LMG	c	521	-	48,48,55	0.89	1 (2%)	56,56,63	1.28	6 (10%)
30	SQD	a	614	-	35,35,54	1.73	6 (17%)	37,37,65	1.37	3 (8%)
25	CLA	b	614	-	69,73,73	1.39	8 (11%)	82,113,113	1.39	5 (6%)
25	CLA	C	503	-	69,73,73	1.35	9 (13%)	82,113,113	1.46	8 (9%)
33	STE	x	101	-	19,19,19	0.53	0	19,19,19	1.27	1 (5%)
25	CLA	B	606	37	69,73,73	1.33	8 (11%)	82,113,113	1.35	6 (7%)
33	STE	c	520	-	19,19,19	0.61	0	19,19,19	0.98	0
29	LMG	M	101	-	51,51,55	0.85	2 (3%)	59,59,63	1.45	7 (11%)
25	CLA	c	501	-	69,73,73	1.18	8 (11%)	82,113,113	1.45	9 (10%)
25	CLA	B	604	-	69,73,73	1.22	7 (10%)	82,113,113	1.35	8 (9%)
25	CLA	C	505	-	69,73,73	1.20	6 (8%)	82,113,113	1.27	8 (9%)
33	STE	H	104	-	17,17,19	0.38	0	16,16,19	0.77	0
25	CLA	C	511	3	69,73,73	1.33	8 (11%)	82,113,113	1.39	4 (4%)
27	BCR	t	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.30	5 (8%)
28	PL9	D	406	-	55,55,55	1.07	4 (7%)	68,69,69	1.49	14 (20%)
34	BCT	d	401	23	3,3,3	1.20	0	2,3,3	2.88	1 (50%)
32	DGD	c	516	-	63,63,67	0.99	4 (6%)	77,77,81	1.48	13 (16%)
27	BCR	a	610	-	41,41,41	0.93	2 (4%)	56,56,56	1.15	5 (8%)
25	CLA	B	609	37	69,73,73	1.26	8 (11%)	82,113,113	1.27	10 (12%)
25	CLA	B	608	-	69,73,73	1.36	8 (11%)	82,113,113	1.42	7 (8%)
32	DGD	H	103	-	63,63,67	1.08	8 (12%)	77,77,81	1.43	12 (15%)
33	STE	d	413	-	16,16,19	0.58	0	16,16,19	1.35	2 (12%)
25	CLA	c	509	-	69,73,73	1.18	5 (7%)	82,113,113	1.39	5 (6%)
27	BCR	c	515	-	41,41,41	1.14	3 (7%)	56,56,56	1.19	6 (10%)
25	CLA	A	612	37	69,73,73	1.32	8 (11%)	82,113,113	1.28	7 (8%)
31	LHG	e	101	-	41,41,48	0.77	1 (2%)	44,47,54	1.31	6 (13%)
27	BCR	D	405	-	41,41,41	1.05	2 (4%)	56,56,56	1.17	5 (8%)
33	STE	b	620	-	15,15,19	0.37	0	14,14,19	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	502	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	5 (6%)
33	STE	B	619	-	16,16,19	0.68	0	16,16,19	1.08	0
31	LHG	A	615	-	48,48,48	0.81	3 (6%)	51,54,54	1.19	5 (9%)
25	CLA	b	604	-	69,73,73	1.30	9 (13%)	82,113,113	1.43	9 (10%)
30	SQD	a	613	-	52,54,54	1.57	7 (13%)	62,65,65	1.89	12 (19%)
35	HEM	f	101	5,6	50,50,50	1.48	9 (18%)	67,82,82	1.25	7 (10%)
21	OEY	A	601[A]	1,3,37	0,16,16	-	-	-	-	-
32	DGD	C	517	-	63,63,67	1.03	6 (9%)	77,77,81	1.33	10 (12%)
25	CLA	b	606	37	69,73,73	1.07	5 (7%)	82,113,113	1.22	9 (10%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.15	5 (8%)
27	BCR	b	618	-	41,41,41	0.97	2 (4%)	56,56,56	1.15	3 (5%)
33	STE	m	102	-	11,11,19	0.65	0	11,11,19	1.64	3 (27%)
25	CLA	C	508	-	69,73,73	1.29	7 (10%)	82,113,113	1.38	10 (12%)
25	CLA	A	606	-	69,73,73	1.23	6 (8%)	82,113,113	1.15	6 (7%)
25	CLA	c	506	-	69,73,73	1.26	8 (11%)	82,113,113	1.26	4 (4%)
33	STE	t	102	-	13,13,19	0.64	0	13,13,19	1.31	2 (15%)
25	CLA	b	613	-	69,73,73	1.24	9 (13%)	82,113,113	1.31	9 (10%)
29	LMG	C	519	-	48,48,55	0.86	2 (4%)	56,56,63	1.29	7 (12%)
25	CLA	b	612	-	69,73,73	1.33	8 (11%)	82,113,113	1.33	12 (14%)
25	CLA	c	513	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	8 (9%)
33	STE	E	101	-	11,11,19	0.74	0	11,11,19	1.17	1 (9%)
29	LMG	d	411	-	44,44,55	0.85	1 (2%)	52,52,63	1.26	6 (11%)
33	STE	b	621	-	19,19,19	0.58	0	19,19,19	1.14	1 (5%)
25	CLA	B	610	-	69,73,73	1.31	7 (10%)	82,113,113	1.32	6 (7%)
22	OEX	a	602[B]	1,3,37	0,15,15	-	-	-	-	-
32	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.35	8 (10%)
25	CLA	c	510	-	69,73,73	1.27	9 (13%)	82,113,113	1.37	9 (10%)
25	CLA	C	501	-	69,73,73	1.52	9 (13%)	82,113,113	1.49	9 (10%)
21	OEY	a	601[A]	1,3,37	0,16,16	-	-	-	-	-
25	CLA	b	602	-	69,73,73	1.30	9 (13%)	82,113,113	1.38	11 (13%)
25	CLA	b	603	-	69,73,73	1.28	7 (10%)	82,113,113	1.56	9 (10%)
33	STE	j	101	-	11,11,19	0.79	0	11,11,19	1.00	0
33	STE	B	624	-	11,11,19	0.73	0	11,11,19	1.22	1 (9%)
27	BCR	b	616	-	41,41,41	0.98	2 (4%)	56,56,56	1.30	7 (12%)
29	LMG	b	622	-	55,55,55	0.77	3 (5%)	63,63,63	1.30	7 (11%)
30	SQD	f	102	-	39,41,54	1.67	8 (20%)	49,52,65	1.80	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	503	-	69,73,73	1.23	7 (10%)	82,113,113	1.42	7 (8%)
27	BCR	b	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.08	2 (3%)
25	CLA	B	613	-	69,73,73	1.24	6 (8%)	82,113,113	1.33	10 (12%)
25	CLA	b	607	-	69,73,73	1.20	6 (8%)	82,113,113	1.32	12 (14%)
33	STE	k	103	-	11,11,19	0.73	0	11,11,19	1.20	0
25	CLA	a	609	-	69,73,73	1.15	7 (10%)	82,113,113	1.29	5 (6%)
25	CLA	D	404	-	69,73,73	1.34	8 (11%)	82,113,113	1.22	8 (9%)
25	CLA	b	605	-	69,73,73	1.28	7 (10%)	82,113,113	1.36	9 (10%)
25	CLA	c	512	-	69,73,73	1.31	9 (13%)	82,113,113	1.36	8 (9%)
31	LHG	d	408	-	48,48,48	0.63	0	51,54,54	1.20	4 (7%)
25	CLA	c	502	-	69,73,73	1.54	9 (13%)	82,113,113	1.34	9 (10%)
27	BCR	c	514	-	41,41,41	1.03	2 (4%)	56,56,56	1.20	6 (10%)
27	BCR	h	102	-	41,41,41	1.01	2 (4%)	56,56,56	1.19	4 (7%)
35	HEM	F	101	5,6	50,50,50	1.45	6 (12%)	67,82,82	1.17	3 (4%)
25	CLA	B	602	-	69,73,73	1.17	6 (8%)	82,113,113	1.39	9 (10%)
25	CLA	C	506	-	69,73,73	1.30	8 (11%)	82,113,113	1.24	6 (7%)
25	CLA	B	607	-	69,73,73	1.22	9 (13%)	82,113,113	1.28	8 (9%)
30	SQD	b	619	-	47,49,54	1.65	8 (17%)	57,60,65	1.47	7 (12%)
31	LHG	D	409	-	46,46,48	0.87	3 (6%)	49,52,54	1.21	6 (12%)
33	STE	X	101	-	19,19,19	0.55	0	19,19,19	1.19	1 (5%)
29	LMG	c	522	-	49,49,55	0.78	1 (2%)	57,57,63	1.34	6 (10%)
33	STE	a	616	-	11,11,19	0.74	0	11,11,19	1.23	2 (18%)
27	BCR	B	616	-	41,41,41	1.04	3 (7%)	56,56,56	1.23	7 (12%)
25	CLA	C	512	-	69,73,73	1.33	10 (14%)	82,113,113	1.34	9 (10%)
25	CLA	B	605	-	69,73,73	1.47	8 (11%)	82,113,113	1.48	9 (10%)
29	LMG	d	410	-	21,21,55	0.54	1 (4%)	20,20,63	1.21	2 (10%)
26	PHO	D	402	-	58,69,69	1.97	10 (17%)	55,99,99	1.41	6 (10%)
32	DGD	C	516	-	63,63,67	1.02	4 (6%)	77,77,81	1.31	11 (14%)
28	PL9	d	406	-	55,55,55	1.08	3 (5%)	68,69,69	1.58	14 (20%)
28	PL9	A	611	-	55,55,55	1.02	3 (5%)	68,69,69	1.54	12 (17%)
25	CLA	D	403	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	7 (8%)
29	LMG	A	613	-	48,48,55	0.80	0	56,56,63	1.41	9 (16%)
30	SQD	A	614	-	50,52,54	1.57	7 (14%)	60,63,65	1.93	11 (18%)
33	STE	b	626	-	9,9,19	0.36	0	8,8,19	0.72	0
27	BCR	B	618	-	41,41,41	1.05	2 (4%)	56,56,56	1.18	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	C	521	-	11,11,19	0.75	0	11,11,19	1.20	1 (9%)
33	STE	d	412	-	15,15,19	0.79	0	15,15,19	0.85	0
21	OEY	a	601[C]	1,3,37	0,16,16	-	-	-		
30	SQD	F	102	-	34,36,54	1.52	5 (14%)	42,45,65	1.79	9 (21%)
27	BCR	C	514	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	7 (12%)
28	PL9	a	611	-	55,55,55	0.69	1 (1%)	68,69,69	1.54	10 (14%)
31	LHG	D	411	-	48,48,48	0.81	1 (2%)	51,54,54	1.32	7 (13%)
25	CLA	C	510	-	69,73,73	1.26	8 (11%)	82,113,113	1.38	8 (9%)
33	STE	b	625	-	19,19,19	0.60	0	19,19,19	1.01	0
27	BCR	T	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.25	8 (14%)
25	CLA	C	509	-	69,73,73	1.29	8 (11%)	82,113,113	1.36	10 (12%)
27	BCR	A	610	-	41,41,41	0.96	2 (4%)	56,56,56	1.24	6 (10%)
33	STE	I	101	-	14,14,19	0.38	0	13,13,19	0.73	0
25	CLA	b	601	-	69,73,73	1.13	7 (10%)	82,113,113	1.36	10 (12%)
33	STE	t	103	-	9,9,19	0.34	0	8,8,19	0.81	0
25	CLA	B	611	-	69,73,73	1.16	8 (11%)	82,113,113	1.46	10 (12%)
25	CLA	c	505	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	5 (6%)
32	DGD	a	615	-	43,43,67	0.67	1 (2%)	45,45,81	1.47	6 (13%)
30	SQD	A	616	-	38,38,54	1.76	5 (13%)	40,40,65	1.12	2 (5%)
36	HEC	V	201	16	46,50,50	1.84	5 (10%)	58,82,82	1.79	4 (6%)
25	CLA	C	513	-	69,73,73	1.26	8 (11%)	82,113,113	1.37	6 (7%)
30	SQD	B	621	-	52,54,54	1.58	8 (15%)	62,65,65	1.71	12 (19%)
33	STE	l	101	-	17,17,19	0.31	0	16,16,19	0.95	0
31	LHG	L	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.19	3 (5%)
25	CLA	c	507	37	69,73,73	1.21	7 (10%)	82,113,113	1.37	6 (7%)
25	CLA	B	614	-	69,73,73	1.45	6 (8%)	82,113,113	1.38	6 (7%)
25	CLA	d	403	-	69,73,73	1.27	7 (10%)	82,113,113	1.22	7 (8%)
33	STE	B	625	-	15,15,19	0.36	0	14,14,19	0.80	0
33	STE	B	622	-	11,11,19	0.79	0	11,11,19	1.13	0
25	CLA	b	608	-	69,73,73	1.21	8 (11%)	82,113,113	1.35	11 (13%)
25	CLA	B	603	-	69,73,73	1.40	6 (8%)	82,113,113	1.58	10 (12%)
21	OEY	A	601[C]	1,3,37	0,16,16	-	-	-		
32	DGD	c	517	-	63,63,67	0.97	4 (6%)	77,77,81	1.32	10 (12%)
33	STE	B	623	-	17,17,19	0.62	0	17,17,19	1.17	0
25	CLA	H	101	37	69,73,73	1.38	9 (13%)	82,113,113	1.49	10 (12%)
25	CLA	b	615	-	64,68,73	1.09	5 (7%)	76,107,113	1.39	10 (13%)
25	CLA	A	609	-	58,62,73	1.22	5 (8%)	68,99,113	1.37	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	601	-	69,73,73	1.28	7 (10%)	82,113,113	1.31	9 (10%)
27	BCR	B	617	-	41,41,41	1.04	3 (7%)	56,56,56	1.16	4 (7%)
25	CLA	c	511	3	69,73,73	1.55	9 (13%)	82,113,113	1.38	6 (7%)
31	LHG	b	623	-	48,48,48	0.70	0	51,54,54	1.19	5 (9%)
33	STE	J	101	-	11,11,19	0.72	0	11,11,19	1.12	0
27	BCR	C	515	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	3 (5%)
26	PHO	a	608	-	58,69,69	2.11	9 (15%)	55,99,99	1.57	8 (14%)
33	STE	M	102	-	14,14,19	0.62	0	14,14,19	1.24	1 (7%)

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
33	STE	C	520	-	-	5/9/9/17	-
31	LHG	D	408	-	-	25/53/53/53	-
33	STE	M	103	-	-	2/7/7/17	-
31	LHG	d	407	-	-	18/53/53/53	-
25	CLA	a	606	-	1/1/15/20	1/39/115/115	-
25	CLA	c	504	37	1/1/14/20	9/33/109/115	-
25	CLA	C	507	37	1/1/15/20	9/39/115/115	-
33	STE	C	522	-	-	9/13/13/17	-
27	BCR	H	102	-	-	3/29/63/63	0/2/2/2
25	CLA	c	508	-	-	8/38/114/115	-
32	DGD	c	518	-	-	19/51/91/95	0/2/2/2
31	LHG	d	409	-	-	11/43/43/53	-
25	CLA	B	612	-	1/1/15/20	15/39/115/115	-
29	LMG	c	519	-	-	12/31/51/70	0/1/1/1
27	BCR	k	101	-	-	10/29/63/63	0/2/2/2
32	DGD	A	617	-	-	28/55/95/95	0/2/2/2
25	CLA	b	609	37	1/1/15/20	7/39/115/115	-
27	BCR	K	102	-	-	4/29/63/63	0/2/2/2
29	LMG	D	410	-	-	17/33/33/70	-
33	STE	b	624	-	-	10/12/12/17	-
29	LMG	m	101	-	-	22/46/66/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	D	407	-	-	16/46/66/70	0/1/1/1
25	CLA	A	607	37	1/1/15/20	12/39/115/115	-
26	PHO	d	402	-	-	5/37/103/103	0/5/6/6
25	CLA	B	615	-	1/1/14/20	12/33/109/115	-
25	CLA	b	611	-	1/1/15/20	8/39/115/115	-
25	CLA	h	101	37	1/1/15/20	18/39/115/115	-
36	HEC	v	201	16	-	6/14/54/54	-
27	BCR	k	102	-	-	0/29/63/63	0/2/2/2
32	DGD	h	103	-	-	20/51/91/95	0/2/2/2
25	CLA	a	607	37	1/1/15/20	9/39/115/115	-
27	BCR	d	405	-	-	7/29/63/63	0/2/2/2
25	CLA	C	504	37	1/1/13/20	9/32/108/115	-
25	CLA	b	610	-	1/1/15/20	6/39/115/115	-
25	CLA	d	404	-	1/1/15/20	8/39/115/115	-
25	CLA	a	612	37	1/1/15/20	2/39/115/115	-
26	PHO	A	608	-	-	1/37/103/103	0/5/6/6
29	LMG	B	620	-	-	9/22/22/70	-
29	LMG	c	521	-	-	24/43/63/70	0/1/1/1
30	SQD	a	614	-	-	22/37/37/69	-
25	CLA	b	614	-	1/1/15/20	11/39/115/115	-
25	CLA	C	503	-	1/1/15/20	6/39/115/115	-
33	STE	x	101	-	-	10/17/17/17	-
25	CLA	B	606	37	1/1/15/20	8/39/115/115	-
33	STE	c	520	-	-	8/17/17/17	-
29	LMG	M	101	-	-	14/46/66/70	0/1/1/1
25	CLA	c	501	-	1/1/15/20	4/39/115/115	-
25	CLA	B	604	-	1/1/15/20	8/39/115/115	-
25	CLA	C	505	-	1/1/15/20	12/39/115/115	-
33	STE	H	104	-	-	12/15/15/17	-
25	CLA	C	511	3	1/1/15/20	7/39/115/115	-
27	BCR	t	101	-	-	5/29/63/63	0/2/2/2
28	PL9	D	406	-	-	6/53/73/73	0/1/1/1
32	DGD	c	516	-	-	28/51/91/95	0/2/2/2
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	609	37	1/1/15/20	7/39/115/115	-
25	CLA	B	608	-	-	6/39/115/115	-
32	DGD	H	103	-	-	14/51/91/95	0/2/2/2
33	STE	d	413	-	-	9/14/14/17	-
25	CLA	c	509	-	1/1/15/20	16/39/115/115	-
27	BCR	c	515	-	-	3/29/63/63	0/2/2/2
25	CLA	A	612	37	1/1/15/20	7/39/115/115	-
31	LHG	e	101	-	-	23/46/46/53	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
33	STE	b	620	-	-	4/13/13/17	-
25	CLA	C	502	-	1/1/15/20	7/39/115/115	-
33	STE	B	619	-	-	7/14/14/17	-
31	LHG	A	615	-	-	21/53/53/53	-
25	CLA	b	604	-	1/1/15/20	7/39/115/115	-
30	SQD	a	613	-	-	21/49/69/69	0/1/1/1
35	HEM	f	101	5,6	-	5/14/54/54	-
32	DGD	C	517	-	-	16/51/91/95	0/2/2/2
25	CLA	b	606	37	1/1/15/20	15/39/115/115	-
27	BCR	K	101	-	-	6/29/63/63	0/2/2/2
27	BCR	b	618	-	-	1/29/63/63	0/2/2/2
33	STE	m	102	-	-	5/9/9/17	-
25	CLA	C	508	-	-	9/39/115/115	-
25	CLA	A	606	-	1/1/15/20	6/39/115/115	-
25	CLA	c	506	-	1/1/15/20	13/39/115/115	-
33	STE	t	102	-	-	5/11/11/17	-
25	CLA	b	613	-	1/1/15/20	16/39/115/115	-
29	LMG	C	519	-	-	18/43/63/70	0/1/1/1
25	CLA	b	612	-	1/1/15/20	10/39/115/115	-
25	CLA	c	513	-	1/1/15/20	8/39/115/115	-
33	STE	E	101	-	-	6/9/9/17	-
29	LMG	d	411	-	-	14/39/59/70	0/1/1/1
33	STE	b	621	-	-	11/17/17/17	-
25	CLA	B	610	-	1/1/15/20	6/39/115/115	-
32	DGD	C	518	-	-	16/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	510	-	1/1/15/20	14/39/115/115	-
25	CLA	C	501	-	1/1/15/20	5/39/115/115	-
25	CLA	b	602	-	1/1/15/20	10/39/115/115	-
25	CLA	b	603	-	1/1/15/20	5/39/115/115	-
33	STE	j	101	-	-	5/9/9/17	-
33	STE	B	624	-	-	1/9/9/17	-
27	BCR	b	616	-	-	5/29/63/63	0/2/2/2
29	LMG	b	622	-	-	27/50/70/70	0/1/1/1
30	SQD	f	102	-	-	12/36/56/69	0/1/1/1
25	CLA	c	503	-	1/1/15/20	7/39/115/115	-
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
25	CLA	B	613	-	1/1/15/20	10/39/115/115	-
25	CLA	b	607	-	1/1/15/20	5/39/115/115	-
33	STE	k	103	-	-	4/9/9/17	-
25	CLA	a	609	-	1/1/15/20	10/39/115/115	-
25	CLA	b	605	-	1/1/15/20	9/39/115/115	-
25	CLA	c	512	-	1/1/15/20	20/39/115/115	-
25	CLA	D	404	-	-	11/39/115/115	-
31	LHG	d	408	-	-	14/53/53/53	-
25	CLA	c	502	-	-	2/39/115/115	-
27	BCR	c	514	-	-	3/29/63/63	0/2/2/2
27	BCR	h	102	-	-	3/29/63/63	0/2/2/2
35	HEM	F	101	5,6	-	3/14/54/54	-
25	CLA	B	602	-	1/1/15/20	5/39/115/115	-
25	CLA	C	506	-	1/1/15/20	10/39/115/115	-
25	CLA	B	607	-	1/1/15/20	5/39/115/115	-
30	SQD	b	619	-	-	18/44/64/69	0/1/1/1
31	LHG	D	409	-	-	17/51/51/53	-
33	STE	X	101	-	-	12/17/17/17	-
29	LMG	c	522	-	-	23/44/64/70	0/1/1/1
33	STE	a	616	-	-	3/9/9/17	-
27	BCR	B	616	-	-	3/29/63/63	0/2/2/2
25	CLA	C	512	-	1/1/15/20	13/39/115/115	-
25	CLA	B	605	-	1/1/15/20	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	d	410	-	-	10/17/17/70	-
26	PHO	D	402	-	-	1/37/103/103	0/5/6/6
32	DGD	C	516	-	-	18/51/91/95	0/2/2/2
28	PL9	d	406	-	-	14/53/73/73	0/1/1/1
28	PL9	A	611	-	-	24/53/73/73	0/1/1/1
25	CLA	D	403	-	-	9/39/115/115	-
29	LMG	A	613	-	-	21/43/63/70	0/1/1/1
30	SQD	A	614	-	-	18/47/67/69	0/1/1/1
33	STE	b	626	-	-	4/7/7/17	-
27	BCR	B	618	-	-	2/29/63/63	0/2/2/2
33	STE	C	521	-	-	6/9/9/17	-
33	STE	d	412	-	-	6/13/13/17	-
30	SQD	F	102	-	-	14/28/48/69	0/1/1/1
27	BCR	C	514	-	-	3/29/63/63	0/2/2/2
28	PL9	a	611	-	-	24/53/73/73	0/1/1/1
31	LHG	D	411	-	-	18/53/53/53	-
25	CLA	C	510	-	1/1/15/20	7/39/115/115	-
33	STE	b	625	-	-	10/17/17/17	-
27	BCR	T	101	-	-	7/29/63/63	0/2/2/2
25	CLA	C	509	-	1/1/15/20	13/39/115/115	-
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
33	STE	I	101	-	-	6/12/12/17	-
25	CLA	b	601	-	-	8/39/115/115	-
33	STE	t	103	-	-	3/7/7/17	-
25	CLA	B	611	-	1/1/15/20	7/39/115/115	-
25	CLA	c	505	-	1/1/15/20	8/39/115/115	-
32	DGD	a	615	-	-	22/45/45/95	-
30	SQD	A	616	-	-	15/39/39/69	-
36	HEC	V	201	16	-	6/14/54/54	-
25	CLA	C	513	-	1/1/15/20	9/39/115/115	-
30	SQD	B	621	-	-	21/49/69/69	0/1/1/1
33	STE	l	101	-	-	8/15/15/17	-
31	LHG	L	101	-	-	19/53/53/53	-
25	CLA	c	507	37	1/1/15/20	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	614	-	1/1/15/20	14/39/115/115	-
25	CLA	d	403	-	-	6/39/115/115	-
33	STE	B	625	-	-	6/13/13/17	-
33	STE	B	622	-	-	7/9/9/17	-
25	CLA	b	608	-	1/1/15/20	7/39/115/115	-
25	CLA	B	603	-	1/1/15/20	8/39/115/115	-
32	DGD	c	517	-	-	15/51/91/95	0/2/2/2
33	STE	B	623	-	-	7/15/15/17	-
25	CLA	H	101	37	1/1/15/20	18/39/115/115	-
25	CLA	b	615	-	1/1/14/20	7/33/109/115	-
25	CLA	A	609	-	1/1/12/20	3/26/102/115	-
25	CLA	B	601	-	1/1/15/20	7/39/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	CLA	c	511	3	1/1/15/20	9/39/115/115	-
31	LHG	b	623	-	-	12/53/53/53	-
33	STE	J	101	-	-	4/9/9/17	-
27	BCR	C	515	-	-	2/29/63/63	0/2/2/2
26	PHO	a	608	-	-	2/37/103/103	0/5/6/6
33	STE	M	102	-	-	5/12/12/17	-

The worst 5 of 770 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	608	PHO	C1B-C2B	9.86	1.50	1.39
26	d	402	PHO	C1B-C2B	9.42	1.49	1.39
26	d	402	PHO	C3B-C4B	9.05	1.50	1.41
26	A	608	PHO	C1B-C2B	8.83	1.49	1.39
26	D	402	PHO	C1B-C2B	8.24	1.48	1.39

The worst 5 of 1082 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	603	CLA	C4A-NA-C1A	9.62	111.07	106.68
25	B	615	CLA	C4A-NA-C1A	9.03	110.80	106.68
36	V	201	HEC	CBB-CAB-C3B	-8.89	109.66	127.43
25	C	511	CLA	C4A-NA-C1A	8.70	110.65	106.68
25	b	603	CLA	C4A-NA-C1A	8.54	110.58	106.68

5 of 62 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	609	CLA	ND
25	A	612	CLA	ND
25	B	601	CLA	ND

5 of 1743 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

149 monomers are involved in 250 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	408	LHG	2	0
31	d	407	LHG	5	0
25	a	606	CLA	1	0
25	c	504	CLA	1	0
25	C	507	CLA	1	0
33	C	522	STE	1	0
27	H	102	BCR	1	0
32	c	518	DGD	4	0
31	d	409	LHG	1	0
25	B	612	CLA	5	0
34	D	401	BCT	1	0
27	k	101	BCR	1	0
32	A	617	DGD	4	0
25	b	609	CLA	1	0
27	K	102	BCR	2	0
33	b	624	STE	1	0
29	m	101	LMG	5	0
29	D	407	LMG	2	0
25	A	607	CLA	1	0
26	d	402	PHO	1	0
25	B	615	CLA	1	0
25	h	101	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	v	201	HEC	2	0
27	k	102	BCR	3	0
32	h	103	DGD	1	0
25	C	504	CLA	2	0
25	b	610	CLA	1	0
25	d	404	CLA	1	0
25	a	612	CLA	1	0
26	A	608	PHO	1	0
29	B	620	LMG	1	0
29	c	521	LMG	1	0
30	a	614	SQD	1	0
25	b	614	CLA	5	0
25	C	503	CLA	1	0
33	x	101	STE	2	0
25	B	606	CLA	3	0
33	c	520	STE	1	0
29	M	101	LMG	2	0
25	c	501	CLA	3	0
25	B	604	CLA	4	0
33	H	104	STE	1	0
25	C	511	CLA	2	0
27	t	101	BCR	2	0
28	D	406	PL9	1	0
32	c	516	DGD	2	0
25	B	609	CLA	2	0
25	B	608	CLA	1	0
32	H	103	DGD	5	0
33	d	413	STE	1	0
25	c	509	CLA	2	0
27	c	515	BCR	1	0
25	A	612	CLA	3	0
31	e	101	LHG	3	0
25	C	502	CLA	1	0
33	B	619	STE	1	0
31	A	615	LHG	3	0
25	b	604	CLA	1	0
30	a	613	SQD	3	0
35	f	101	HEM	3	0
21	A	601[A]	OEY	1	0
32	C	517	DGD	6	0
25	b	606	CLA	5	0
27	K	101	BCR	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	618	BCR	1	0
33	m	102	STE	1	0
25	C	508	CLA	2	0
25	A	606	CLA	4	0
25	c	506	CLA	1	0
25	b	613	CLA	3	0
29	C	519	LMG	1	0
25	b	612	CLA	4	0
25	c	513	CLA	1	0
33	b	621	STE	1	0
25	B	610	CLA	2	0
32	C	518	DGD	5	0
25	C	501	CLA	1	0
21	a	601[A]	OEY	1	0
25	b	602	CLA	2	0
25	b	603	CLA	1	0
27	b	616	BCR	1	0
30	f	102	SQD	1	0
25	c	503	CLA	3	0
27	b	617	BCR	2	0
25	B	613	CLA	3	0
25	b	607	CLA	1	0
25	a	609	CLA	2	0
25	D	404	CLA	3	0
25	b	605	CLA	2	0
25	c	512	CLA	4	0
31	d	408	LHG	1	0
25	c	502	CLA	1	0
27	c	514	BCR	2	0
27	h	102	BCR	3	0
35	F	101	HEM	2	0
25	B	602	CLA	1	0
25	C	506	CLA	3	0
25	B	607	CLA	1	0
30	b	619	SQD	1	0
31	D	409	LHG	2	0
33	X	101	STE	5	0
27	B	616	BCR	1	0
25	C	512	CLA	6	0
25	B	605	CLA	1	0
29	d	410	LMG	1	0
32	C	516	DGD	1	0

Continued on next page...

Continued from previous page...

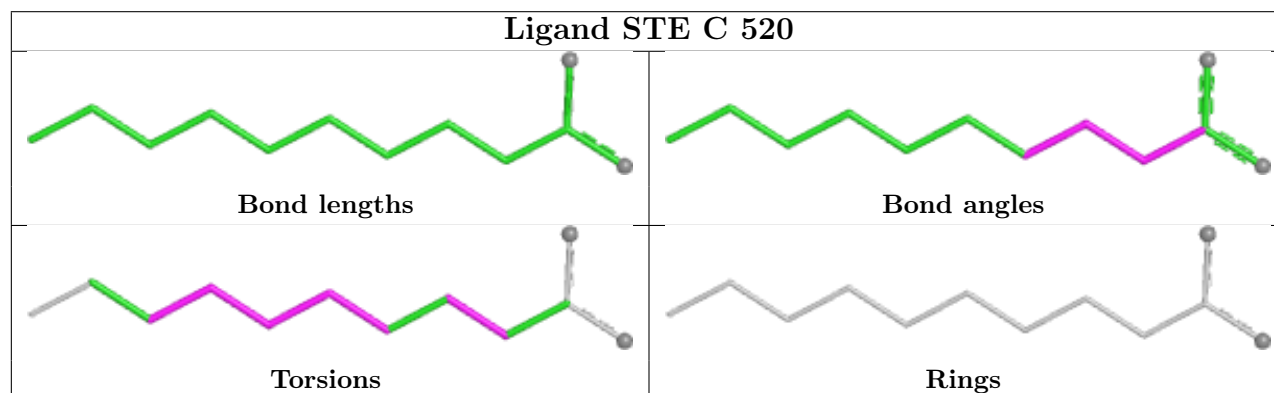
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	406	PL9	1	0
28	A	611	PL9	7	0
29	A	613	LMG	2	0
30	A	614	SQD	1	0
27	B	618	BCR	1	0
33	d	412	STE	2	0
21	a	601[C]	OEY	1	0
30	F	102	SQD	1	0
27	C	514	BCR	2	0
28	a	611	PL9	5	0
31	D	411	LHG	8	0
25	C	510	CLA	1	0
33	b	625	STE	2	0
27	T	101	BCR	2	0
25	C	509	CLA	1	0
27	A	610	BCR	1	0
33	I	101	STE	2	0
25	b	601	CLA	5	0
25	B	611	CLA	2	0
25	c	505	CLA	1	0
32	a	615	DGD	2	0
30	A	616	SQD	2	0
25	C	513	CLA	1	0
30	B	621	SQD	2	0
33	l	101	STE	1	0
31	L	101	LHG	1	0
25	c	507	CLA	2	0
25	B	614	CLA	2	0
33	B	622	STE	1	0
25	B	603	CLA	2	0
21	A	601[C]	OEY	1	0
32	c	517	DGD	2	0
33	B	623	STE	1	0
25	H	101	CLA	1	0
25	b	615	CLA	3	0
25	A	609	CLA	1	0
25	B	601	CLA	3	0
27	B	617	BCR	2	0
25	c	511	CLA	3	0
31	b	623	LHG	4	0
33	J	101	STE	2	0
27	C	515	BCR	2	0

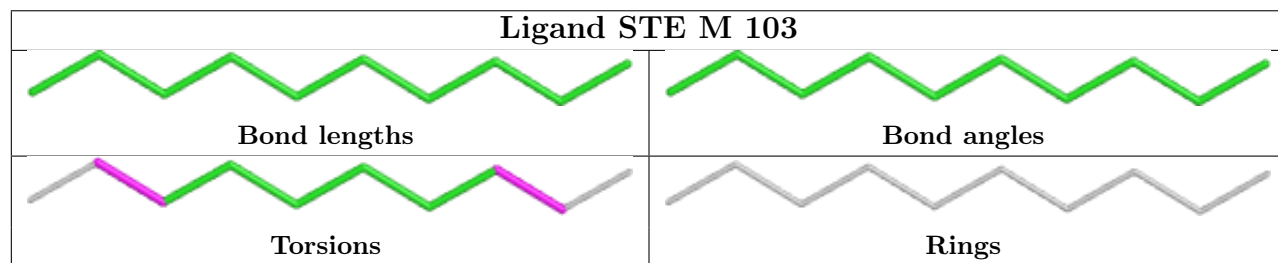
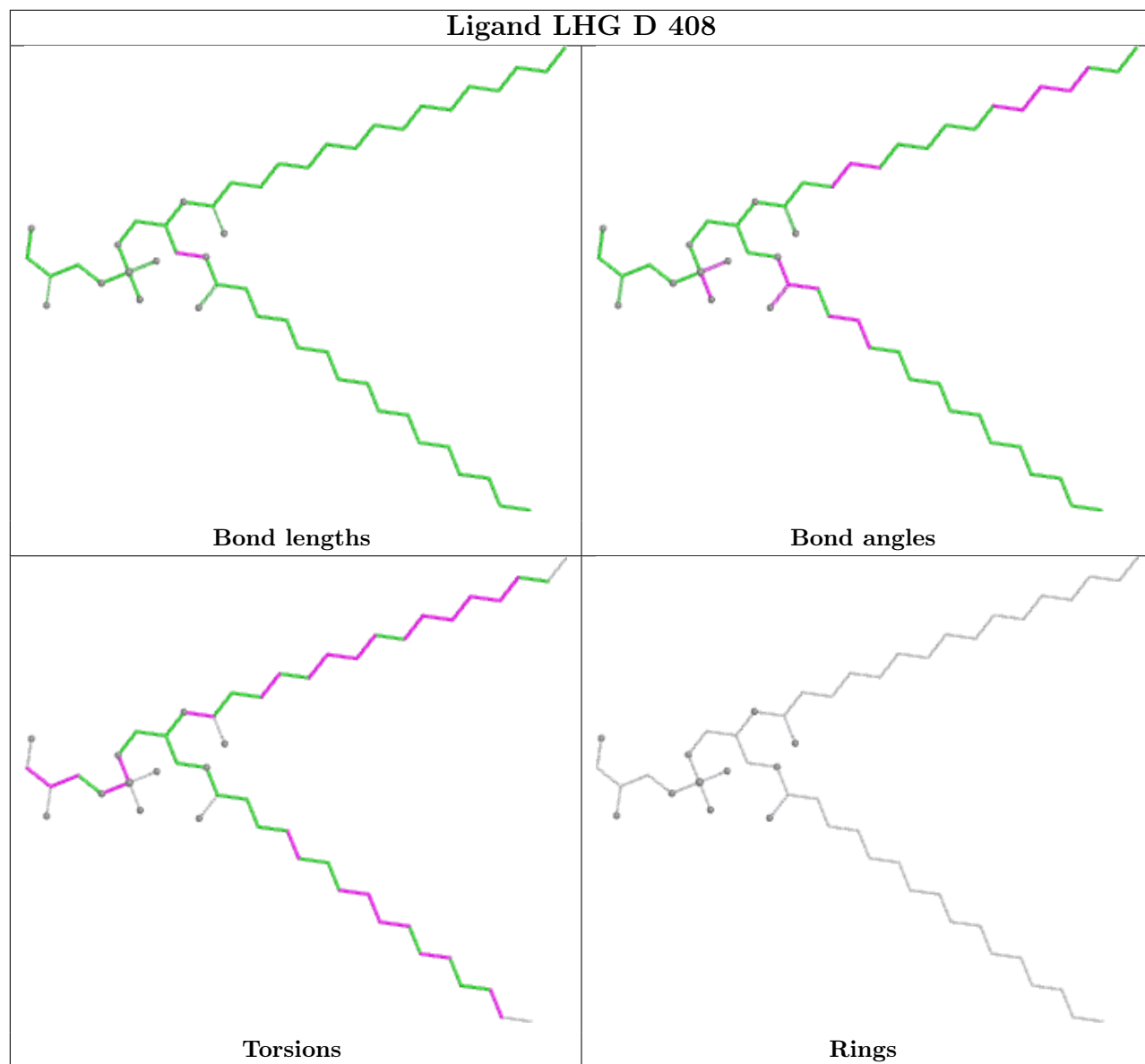
Continued on next page...

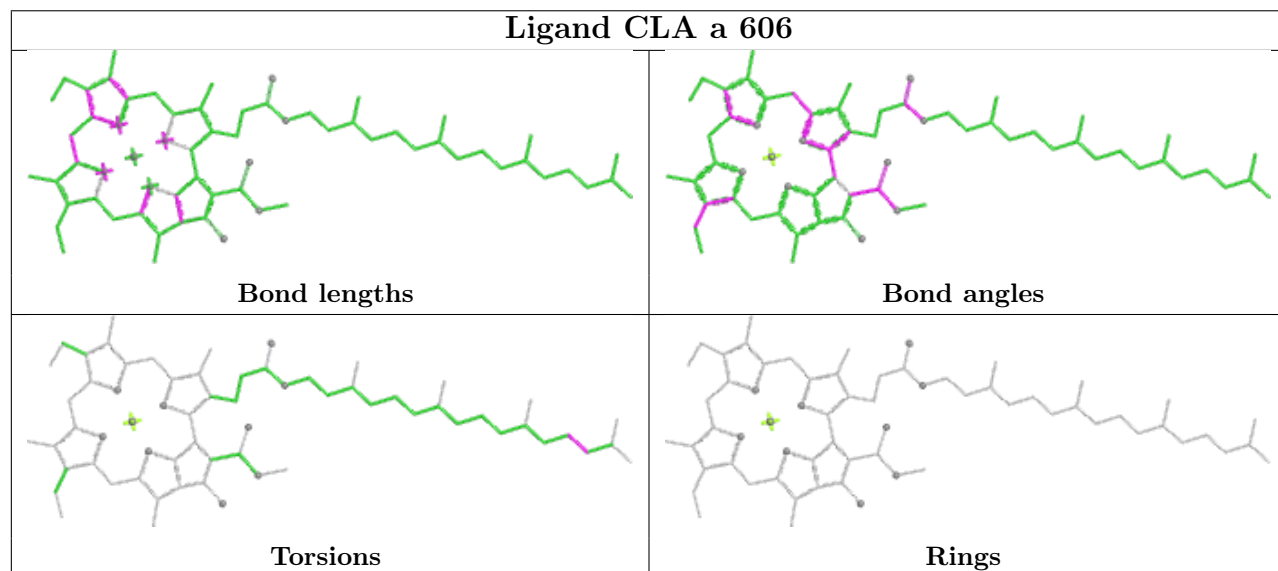
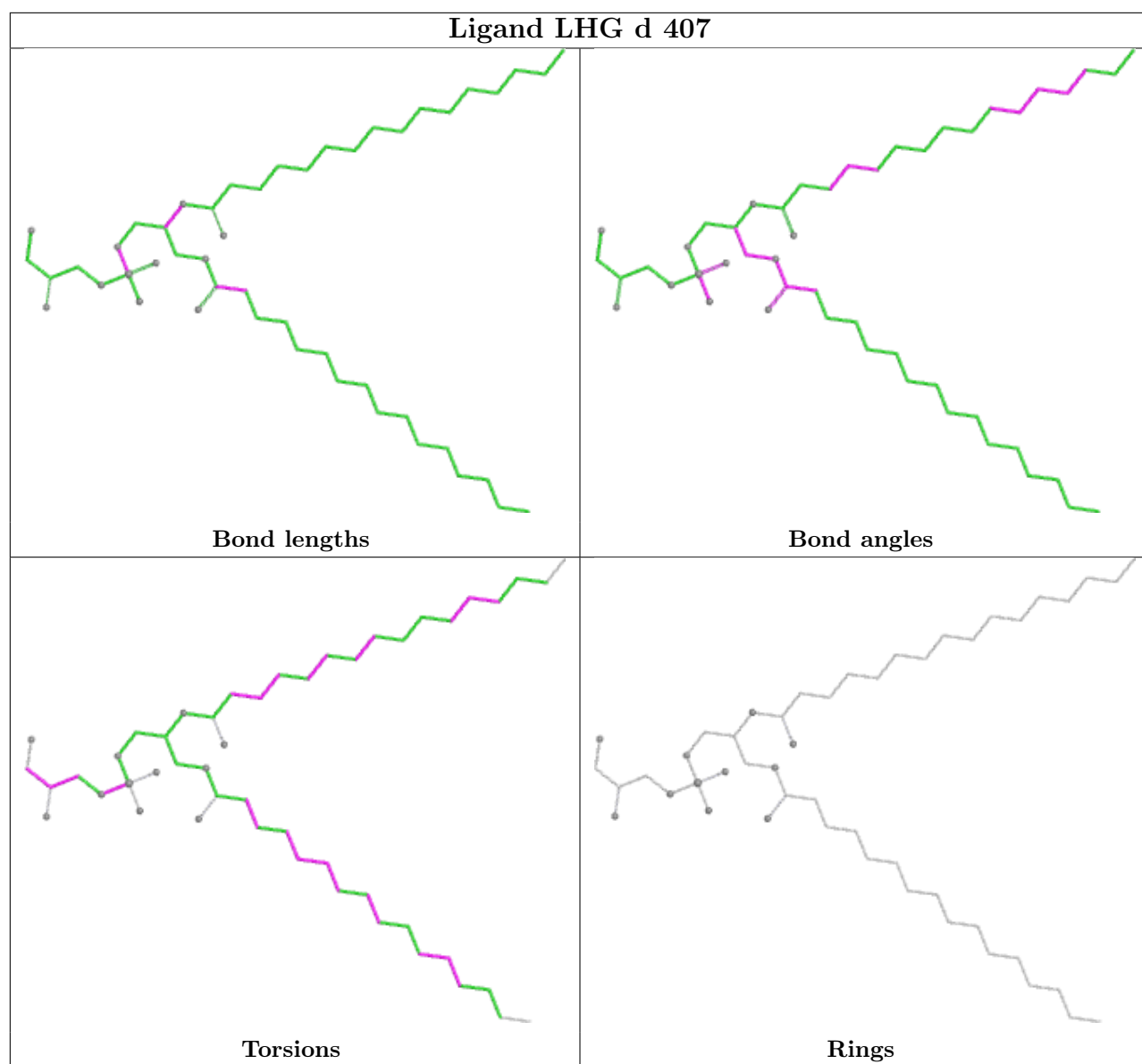
Continued from previous page...

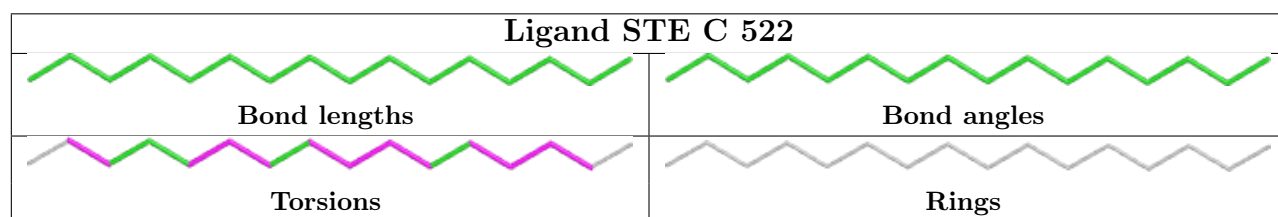
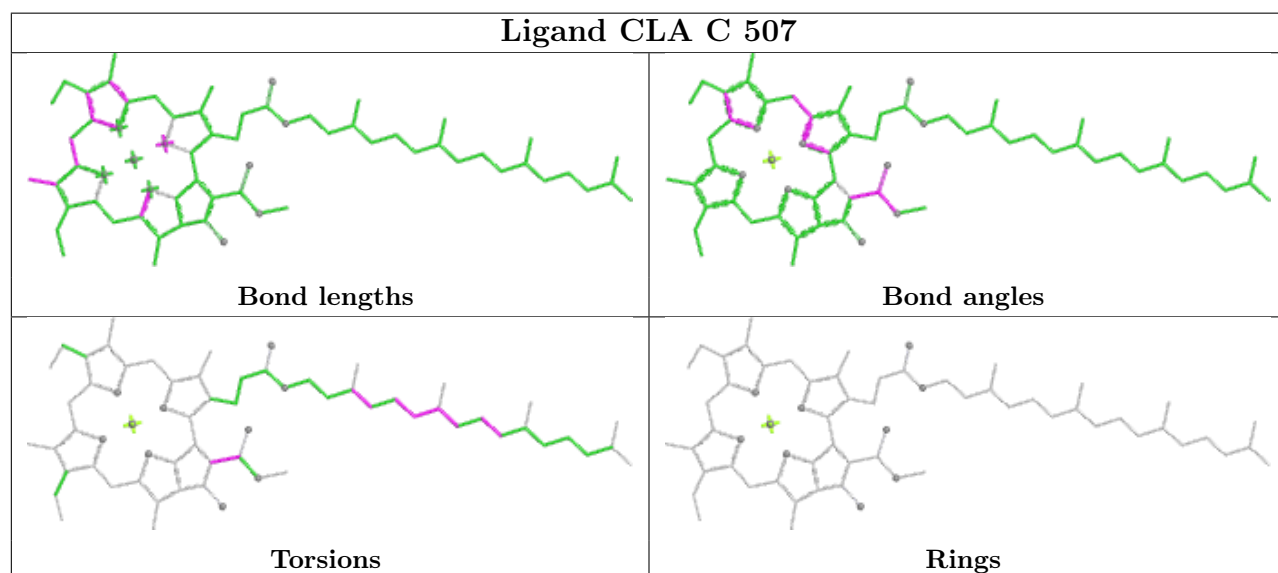
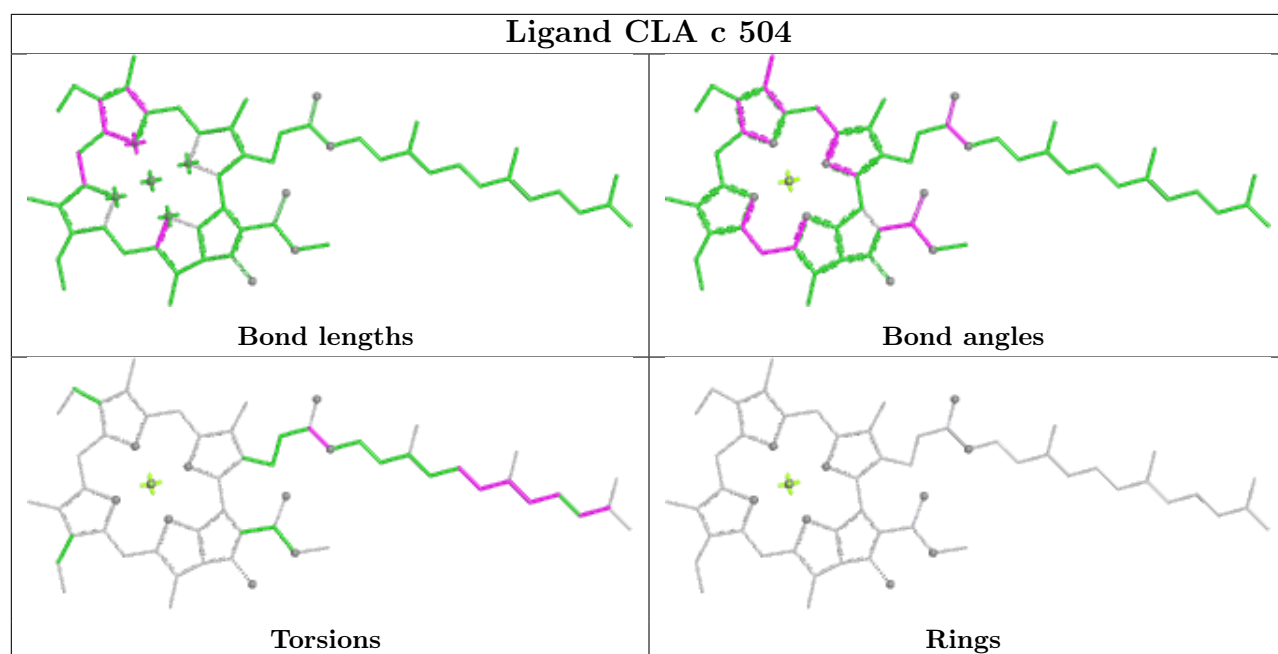
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	M	102	STE	1	0

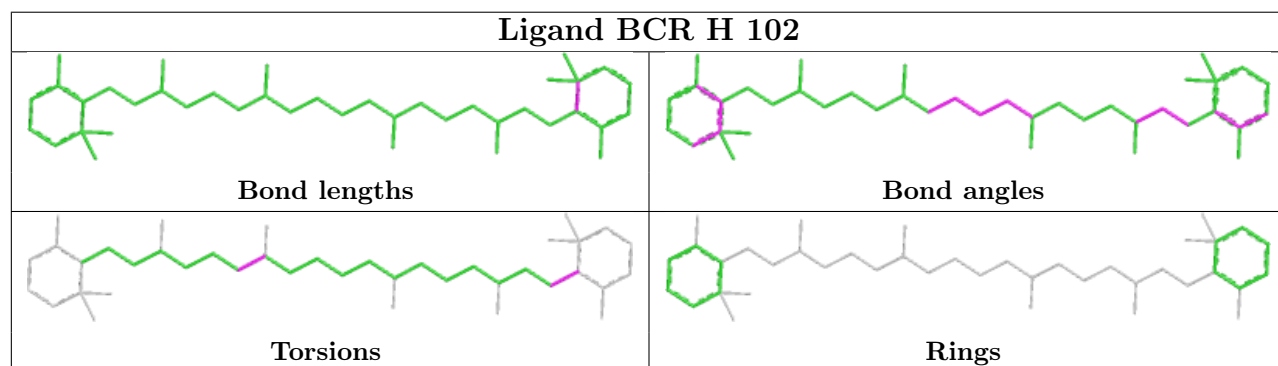
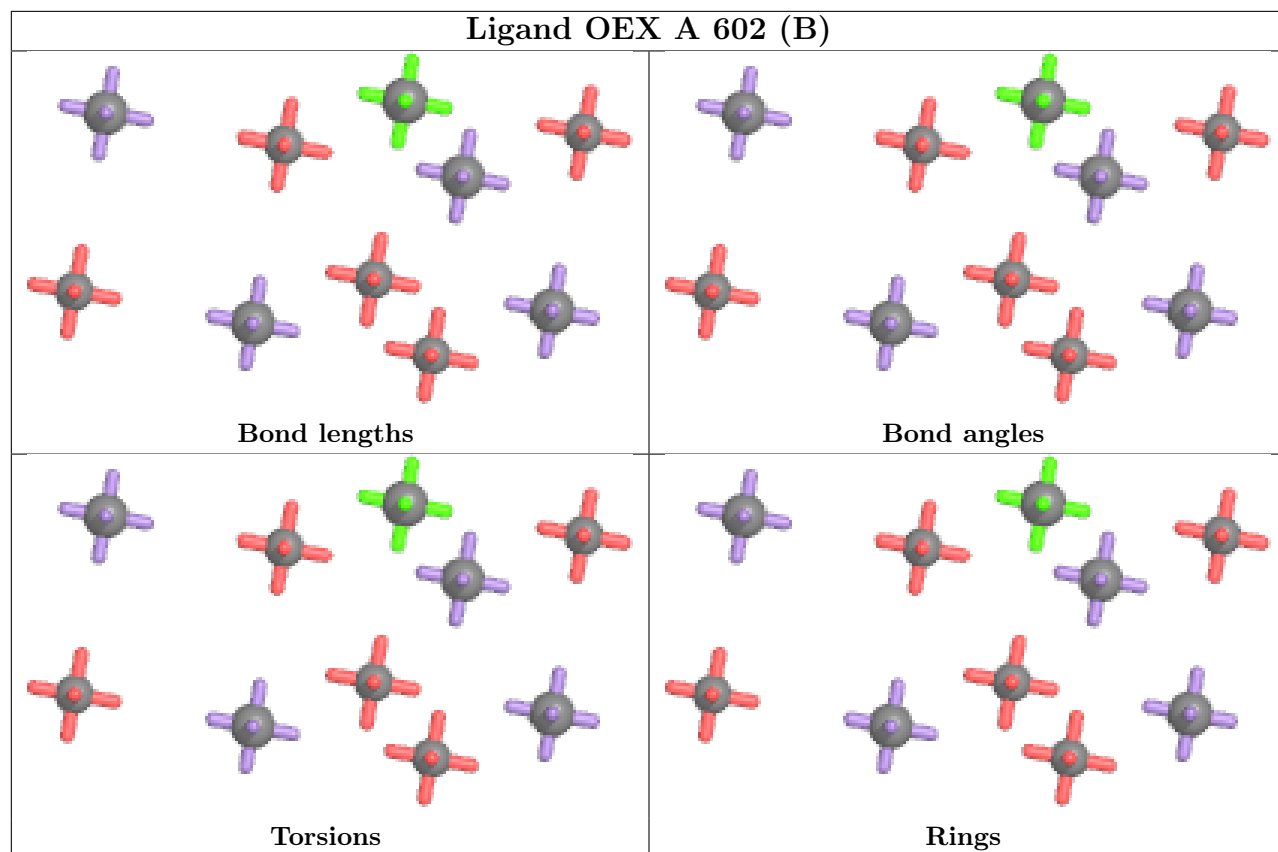
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

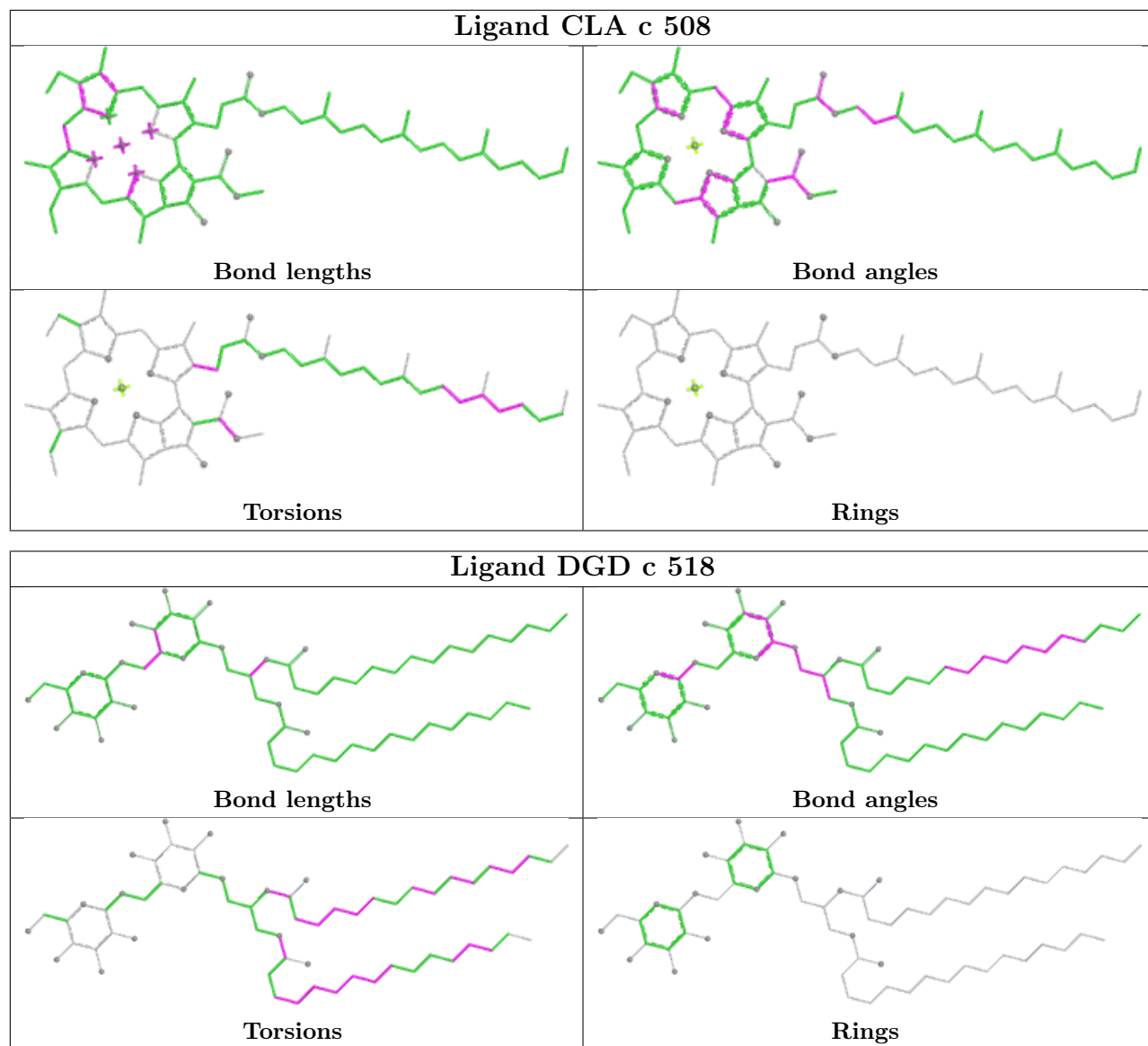


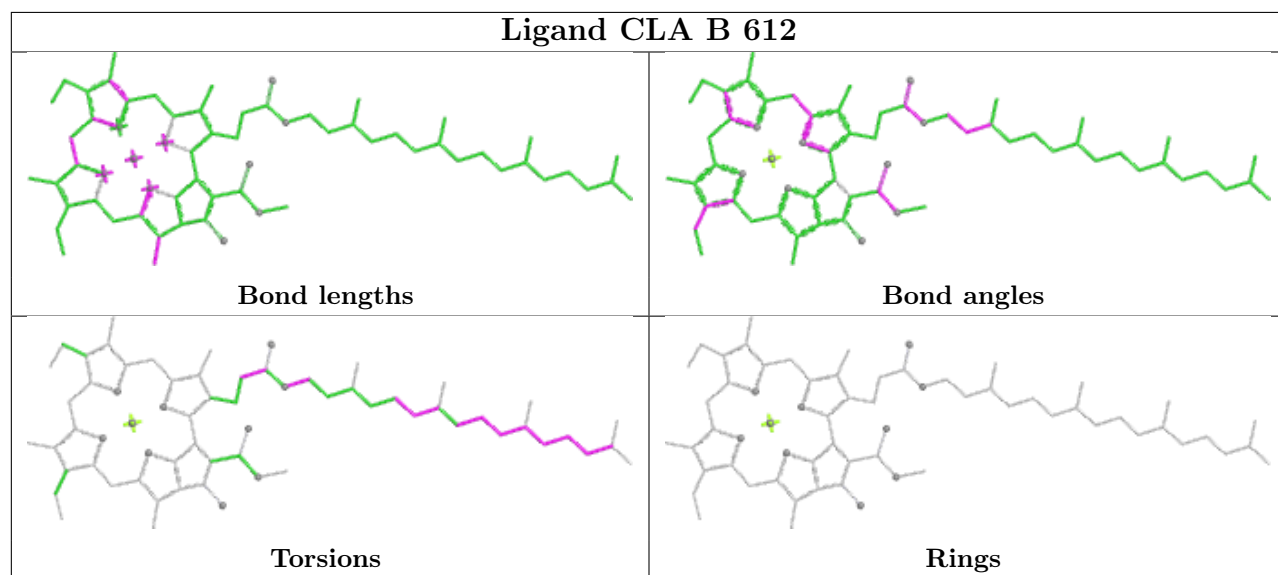
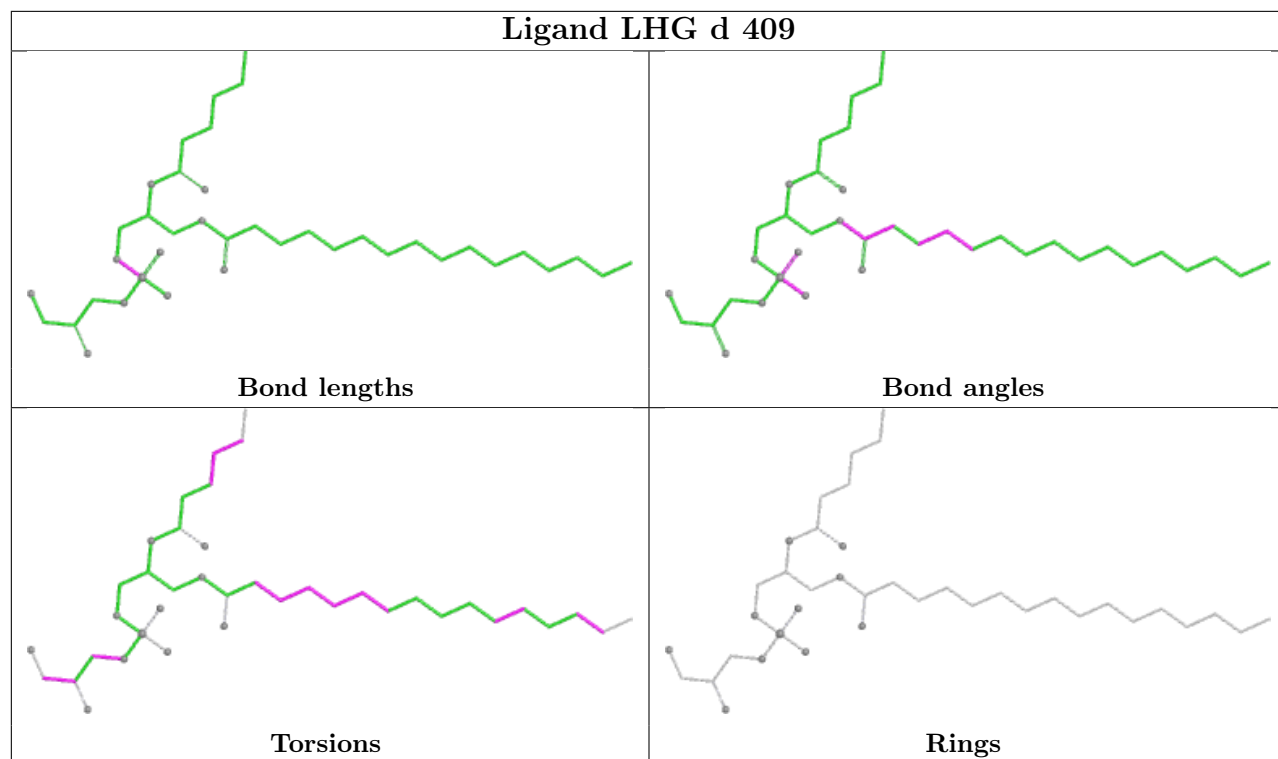


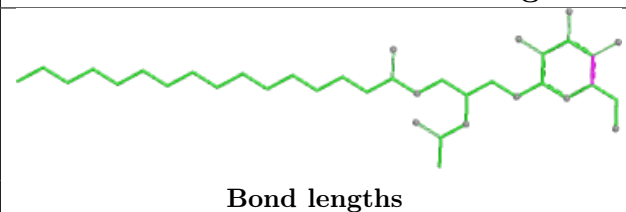
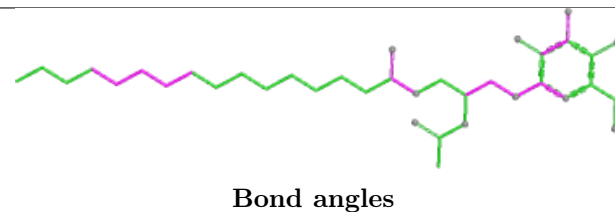
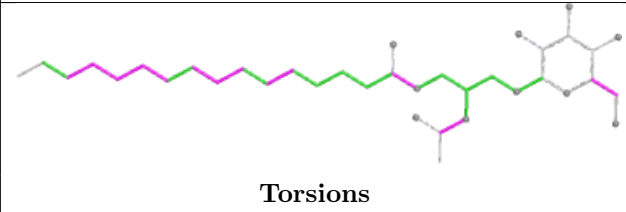
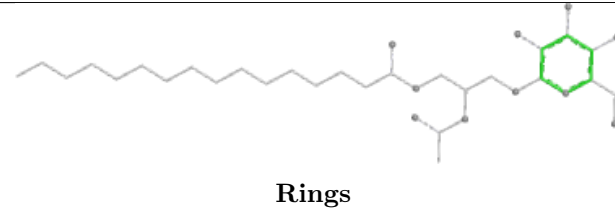


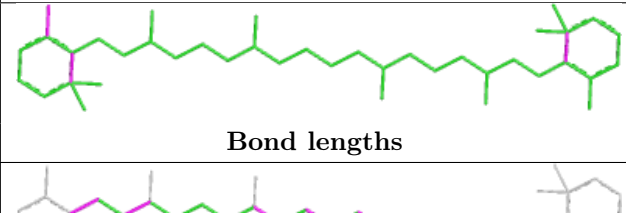
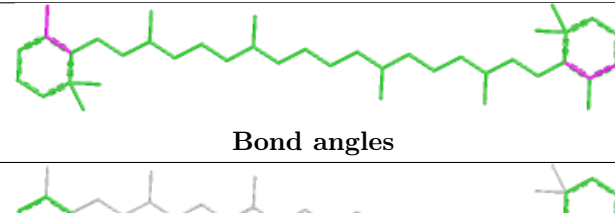
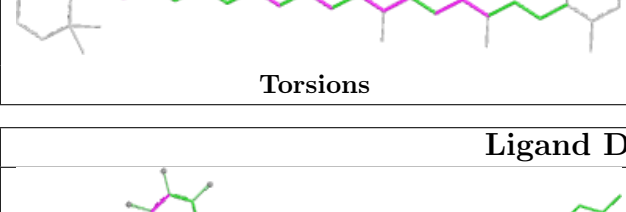


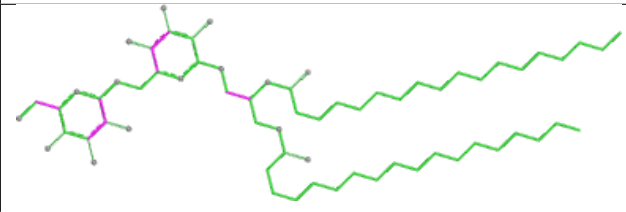
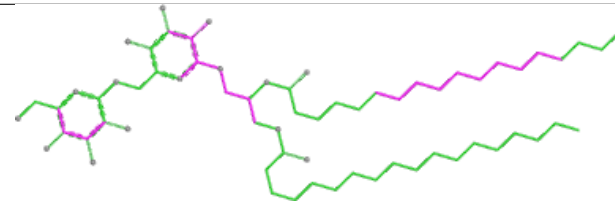
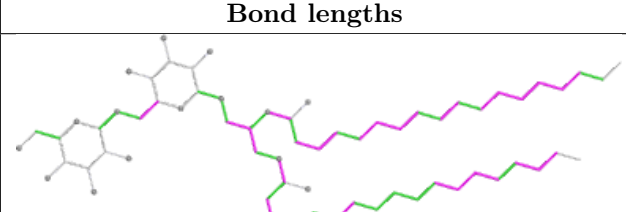
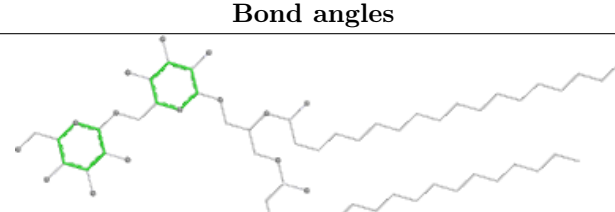


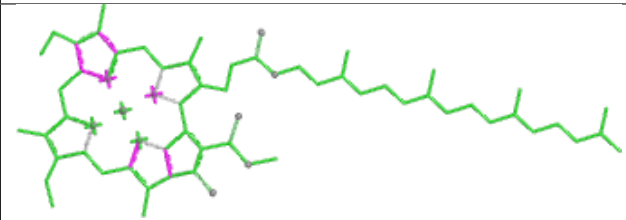
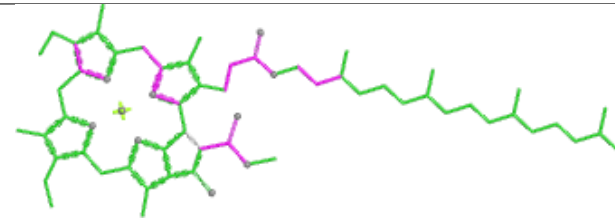
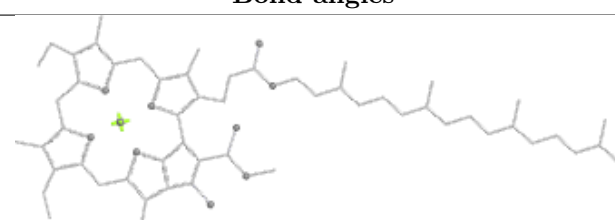


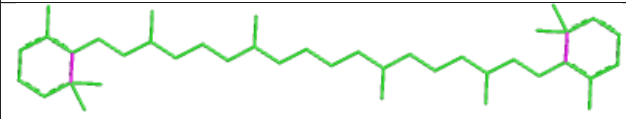
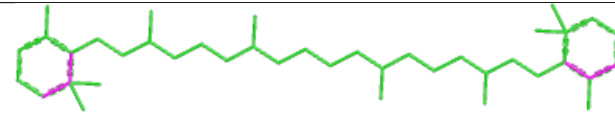
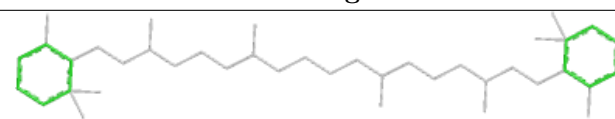


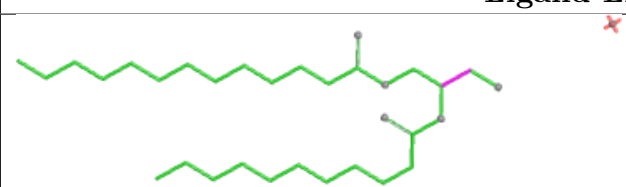
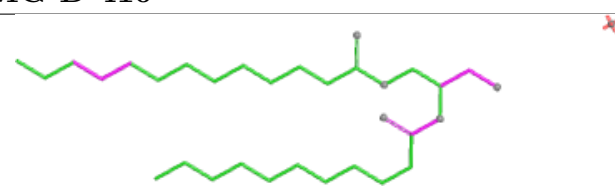
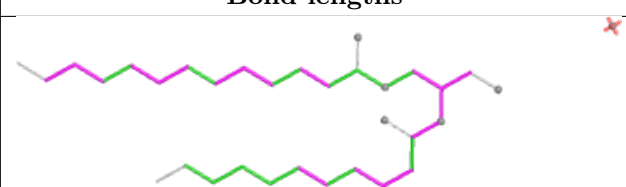
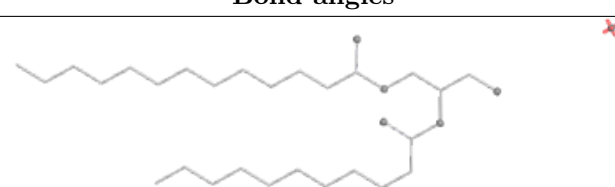
Ligand LMG c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

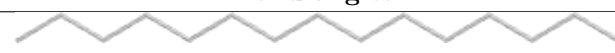
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

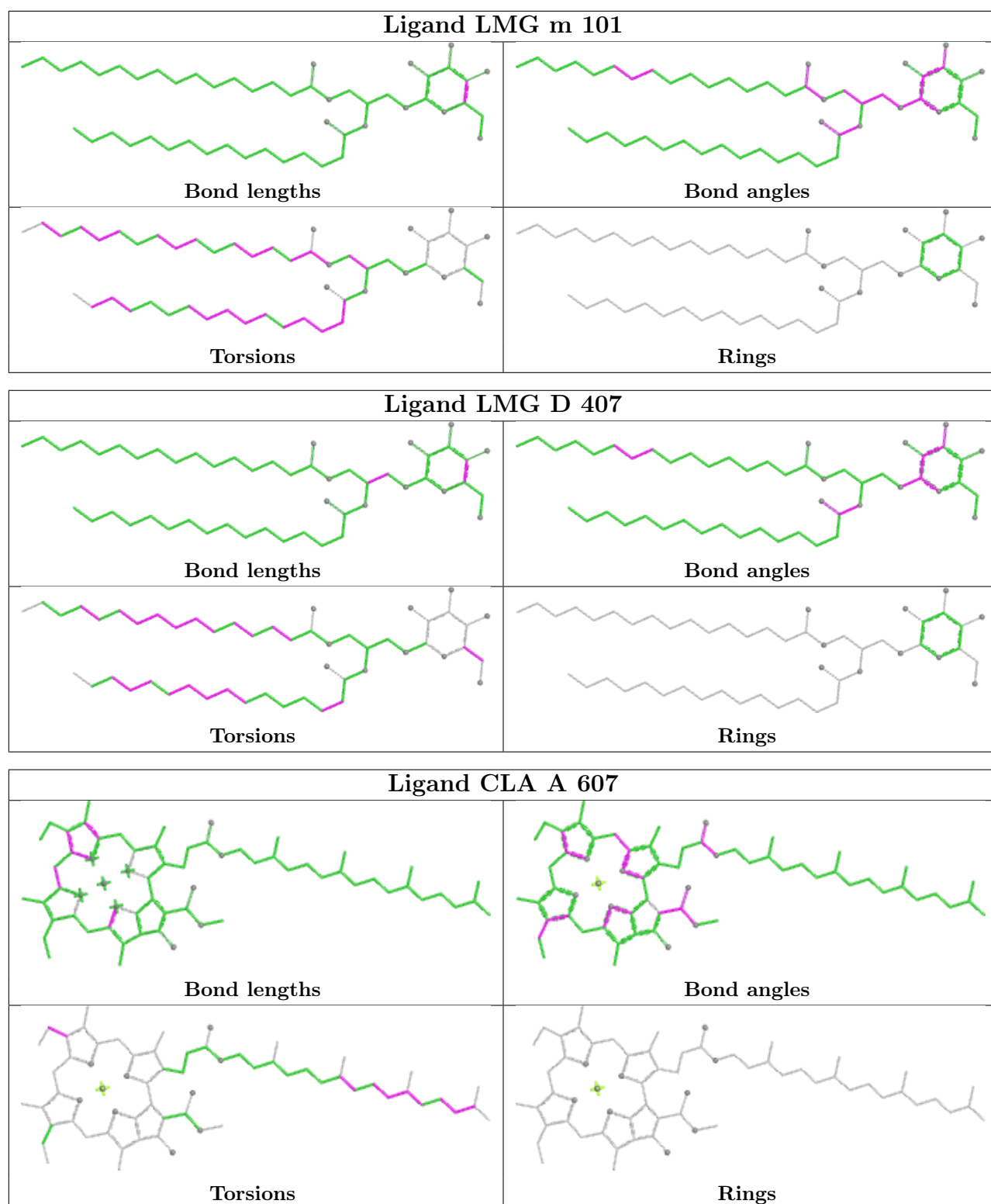
Ligand DGD A 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

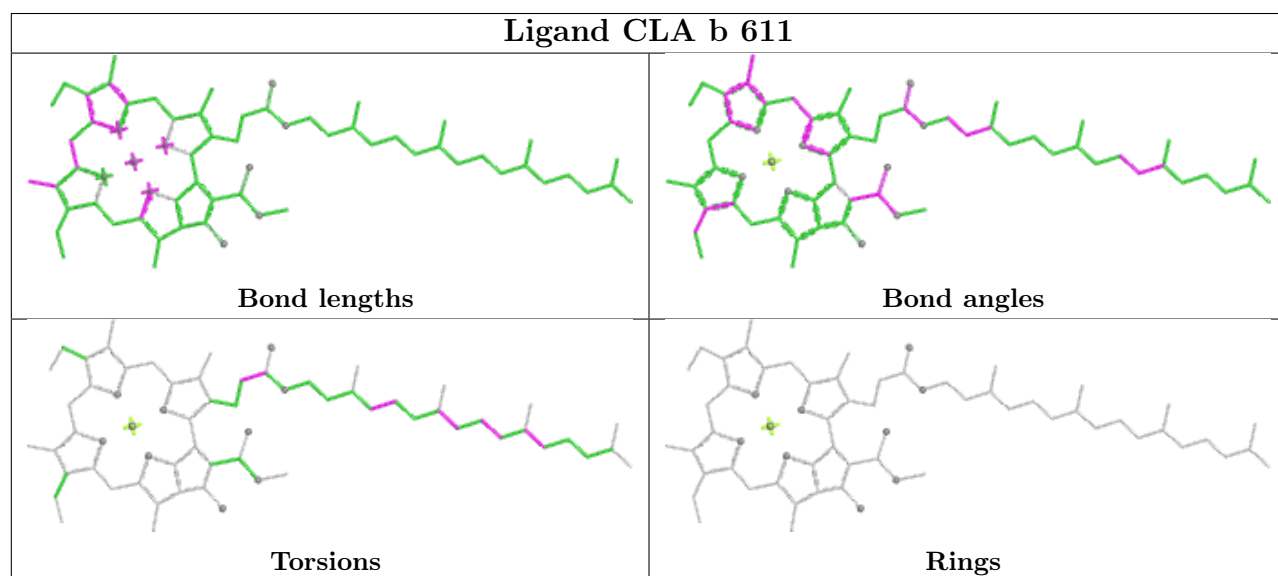
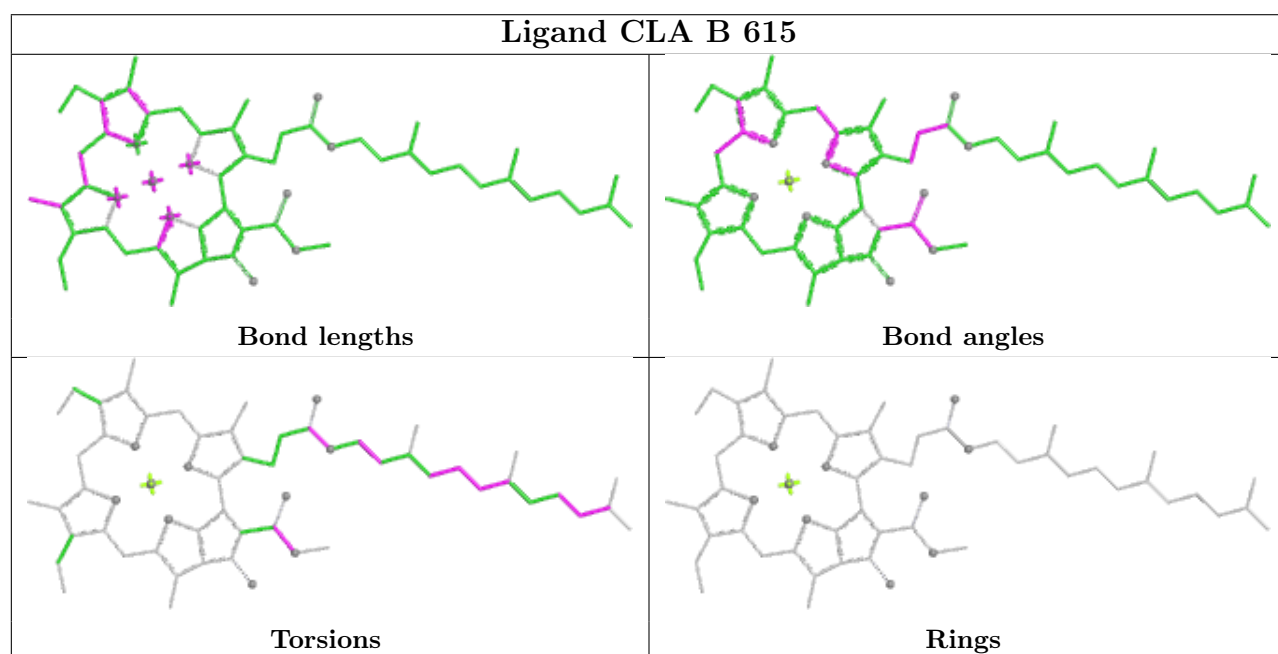
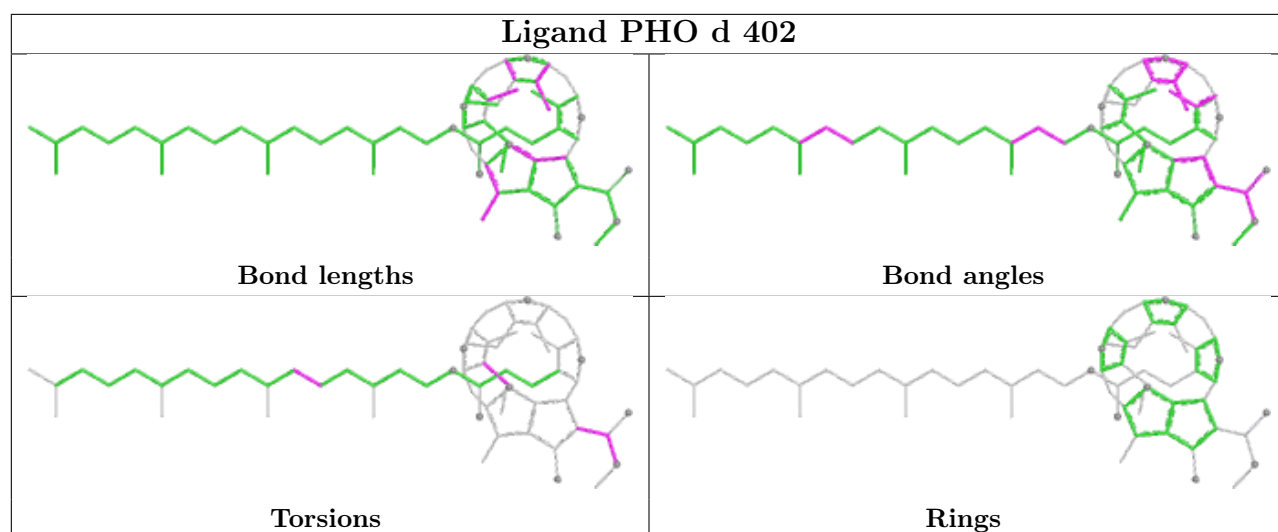
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

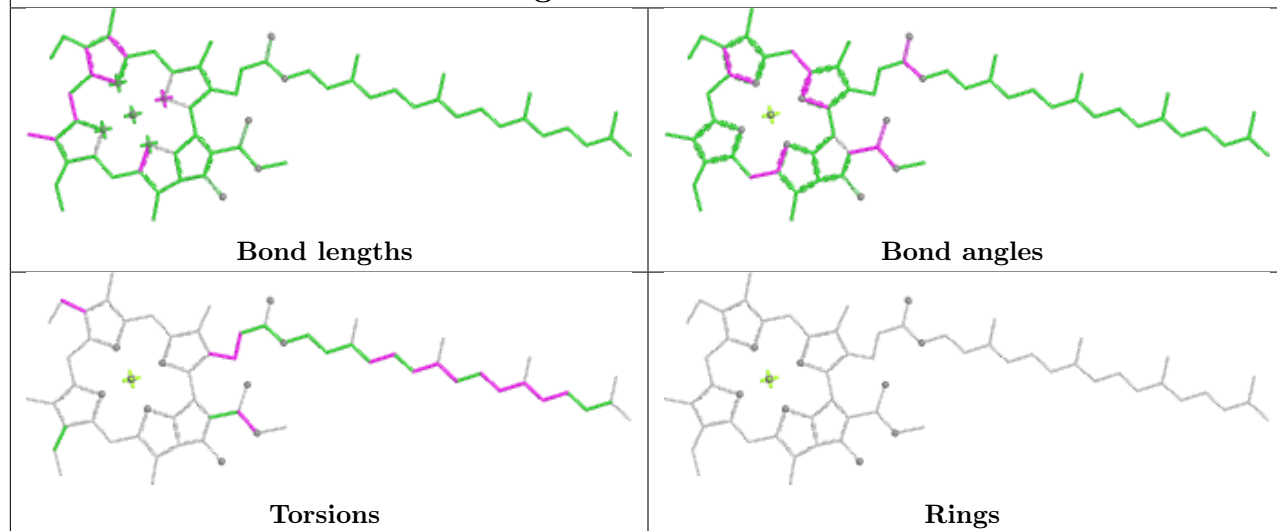
Ligand LMG D 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

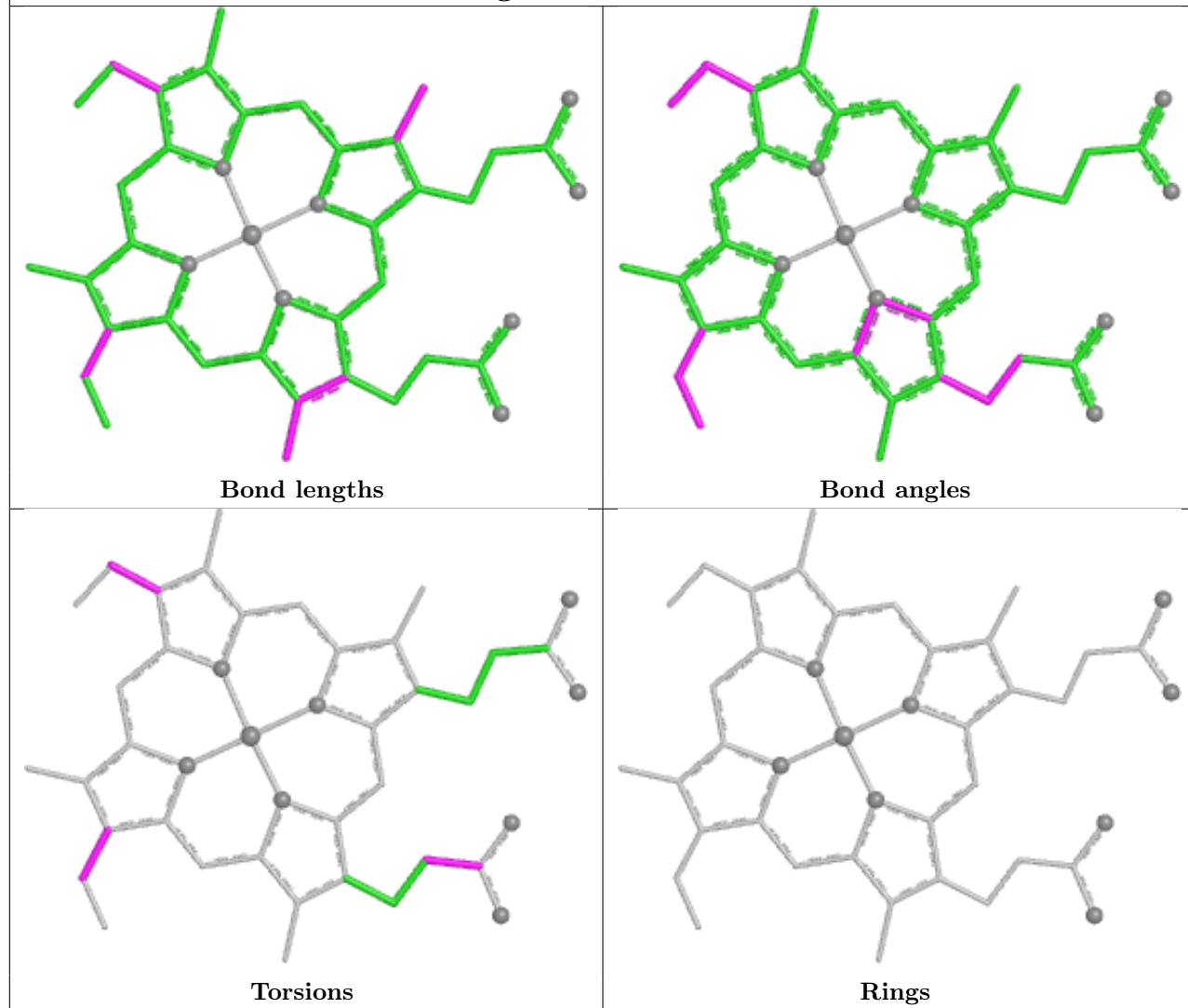


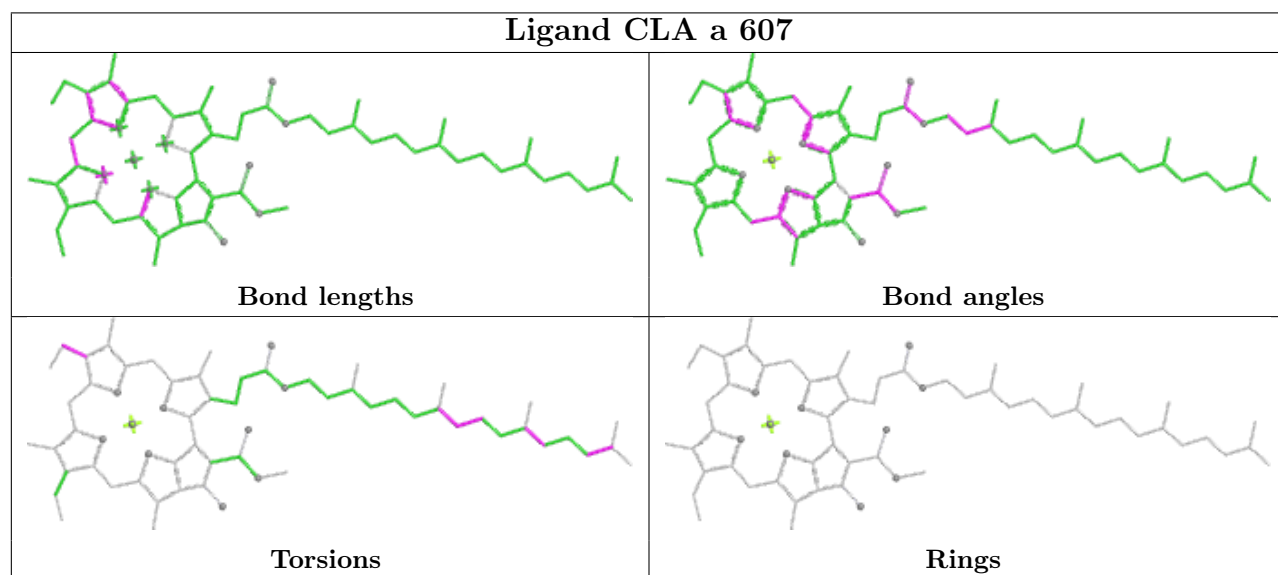
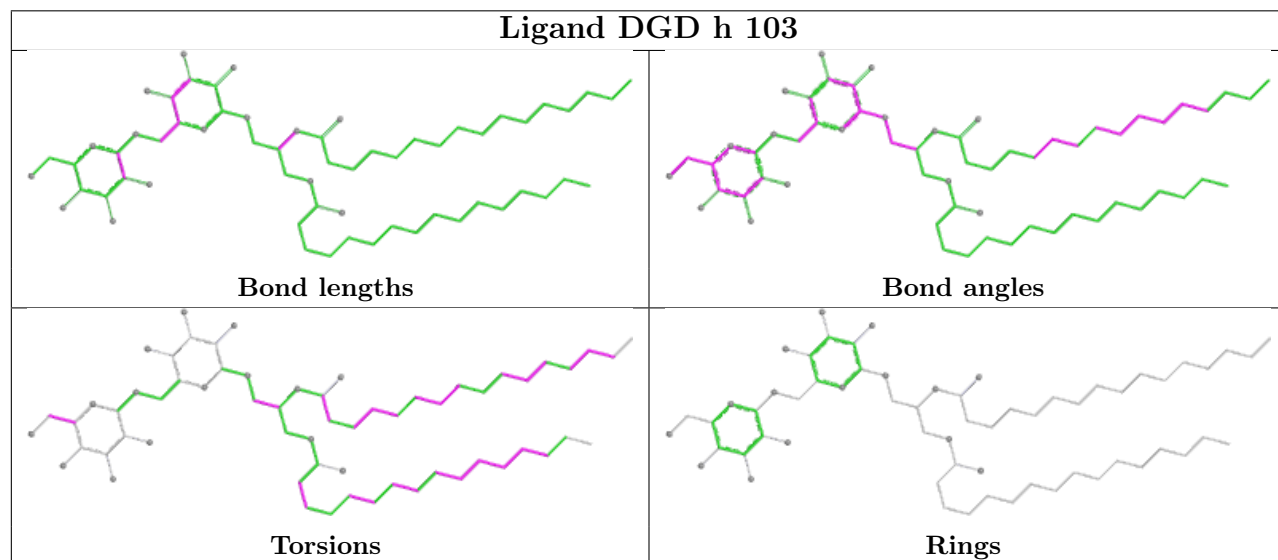
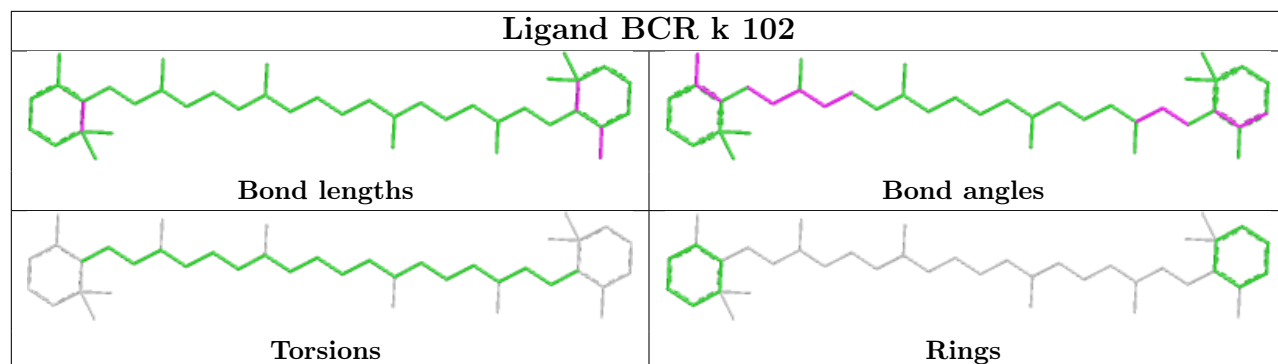


Ligand CLA h 101

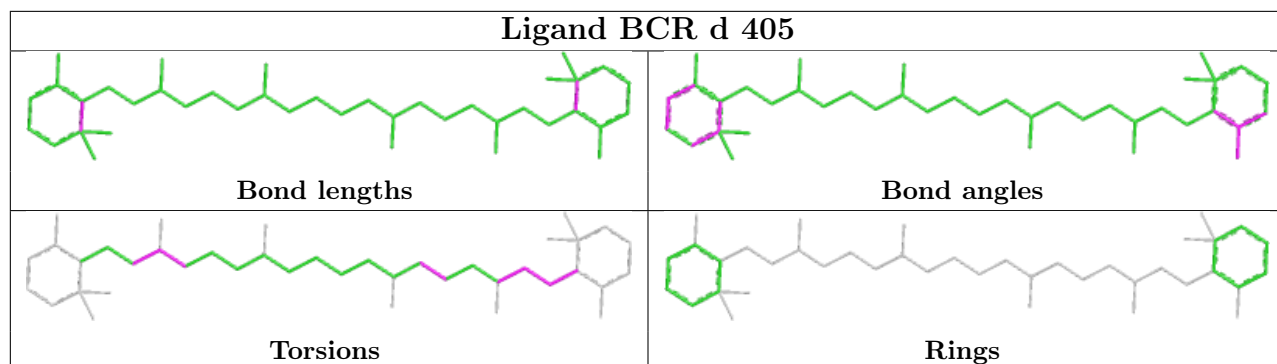


Ligand HEC v 201

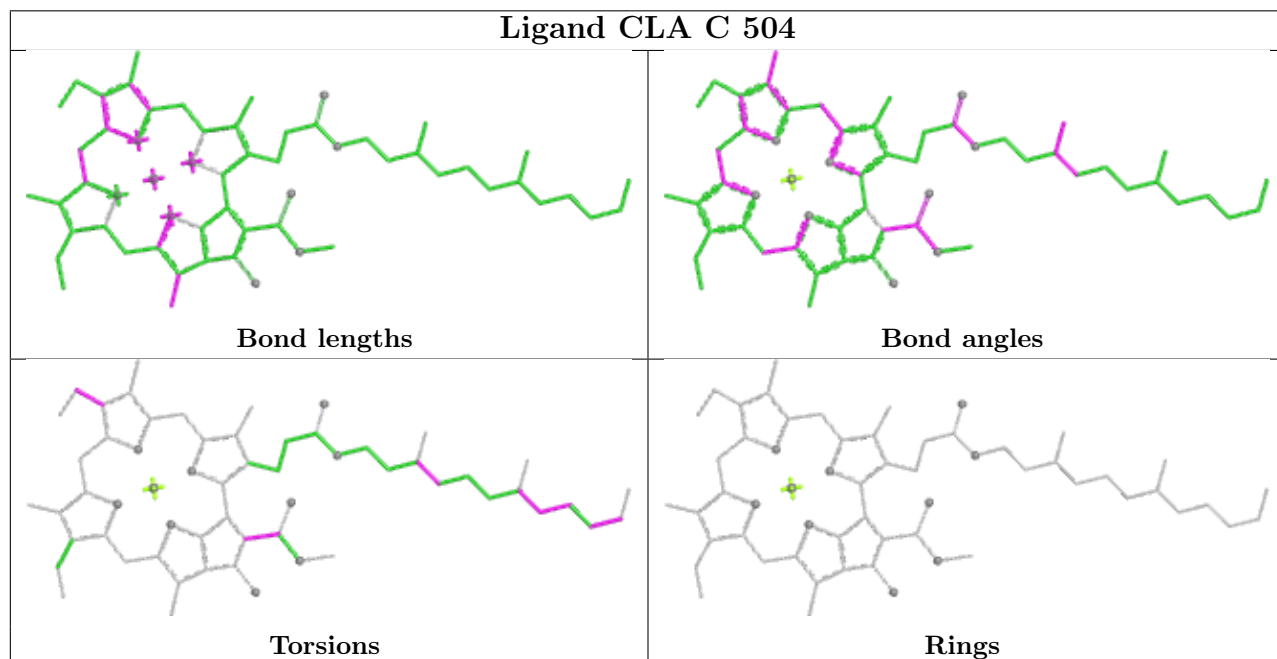




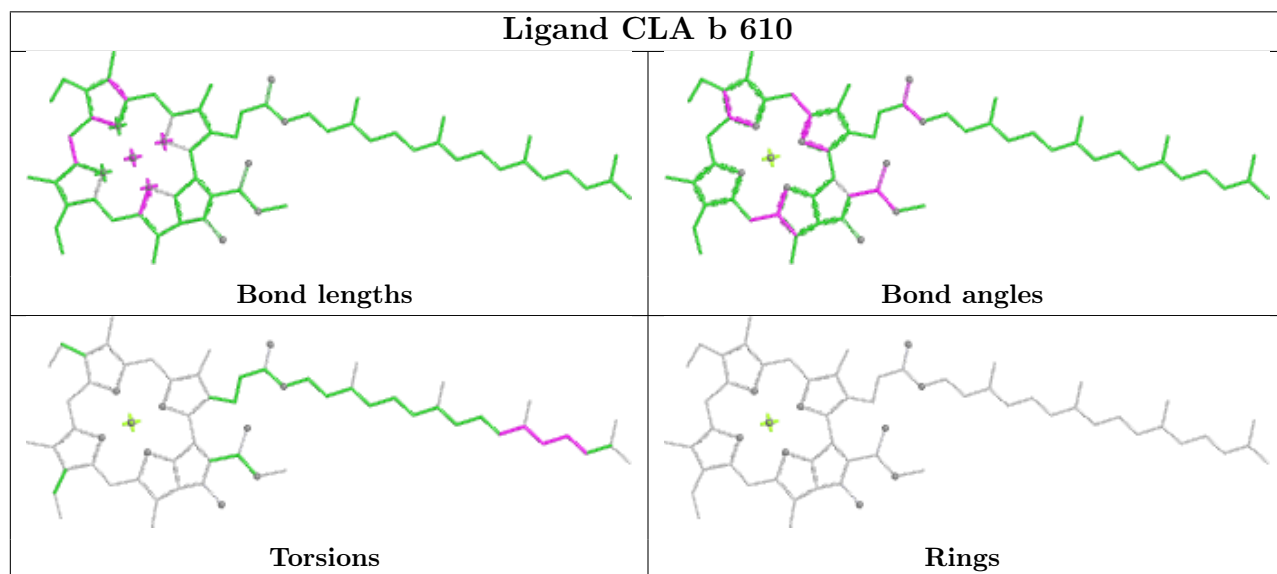
Ligand BCR d 405

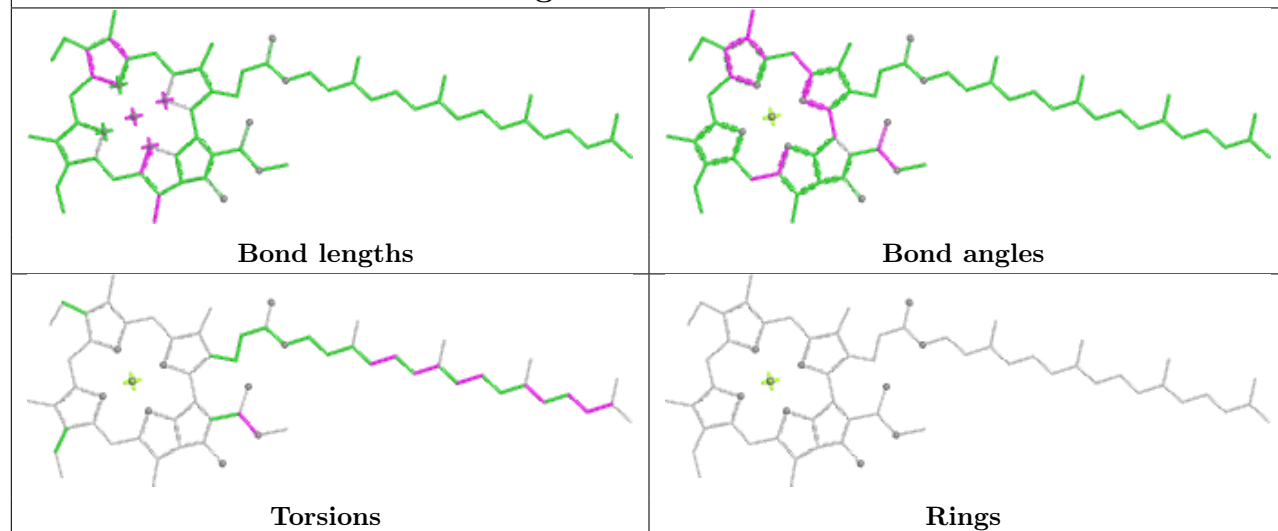
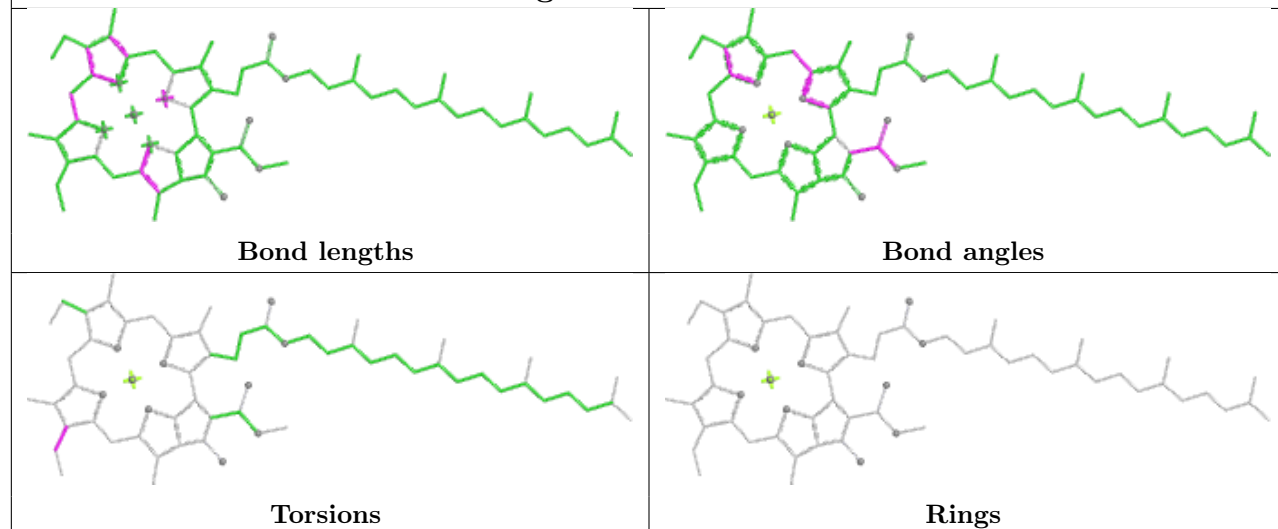
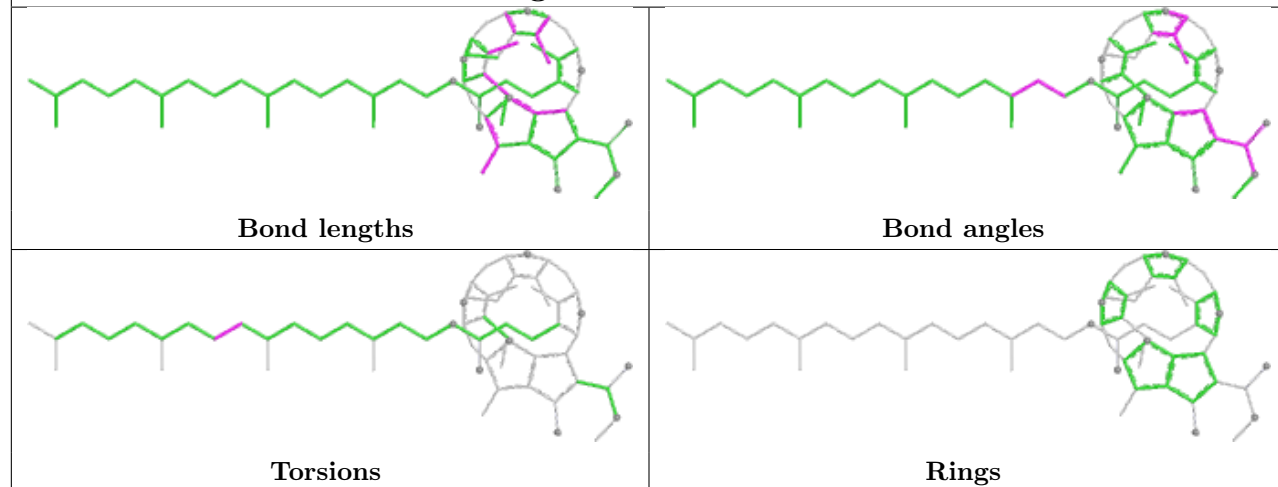


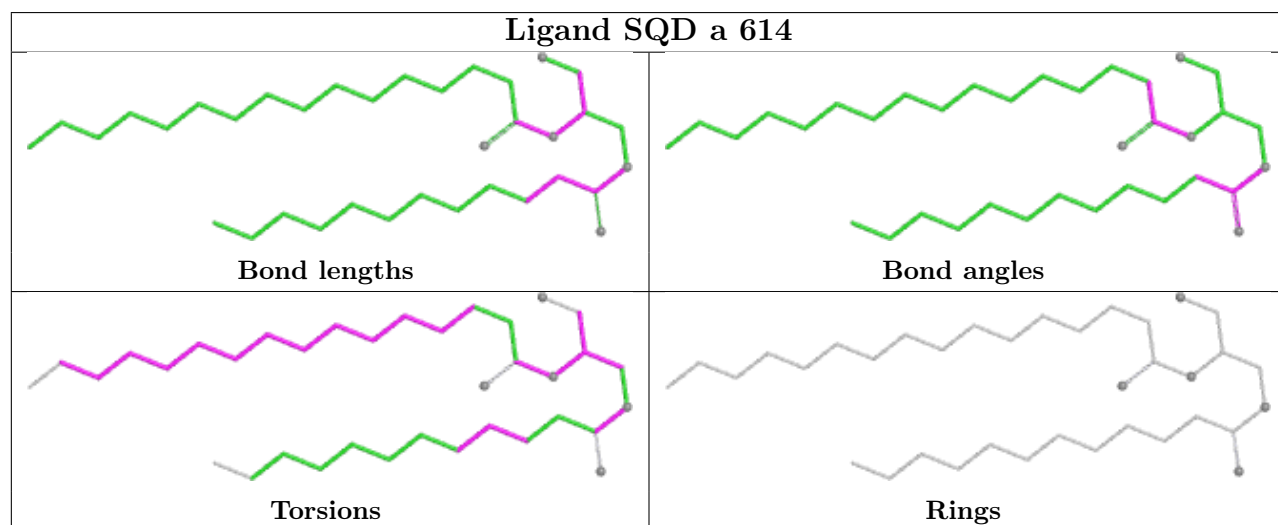
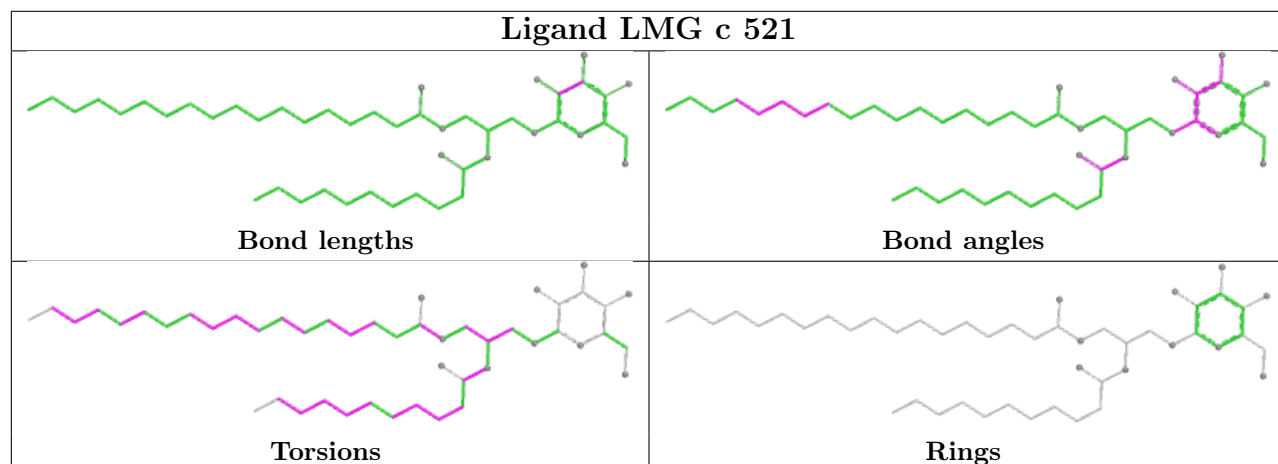
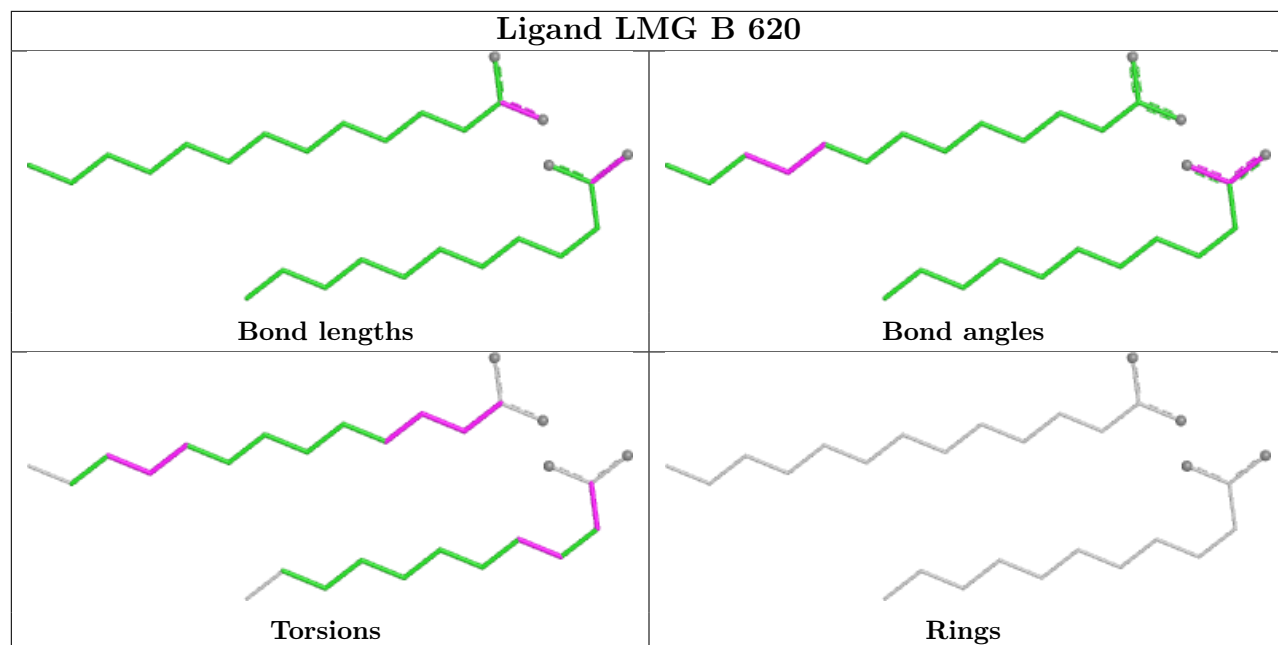
Ligand CLA C 504

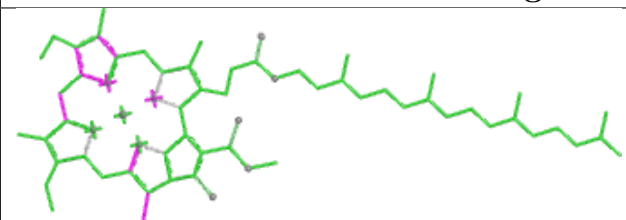
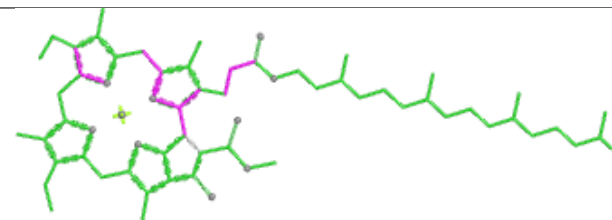
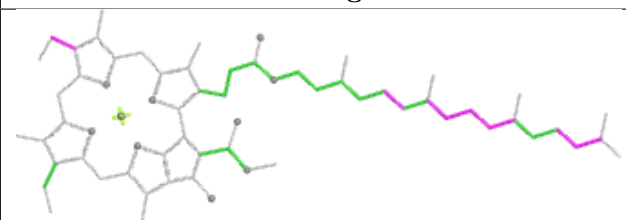
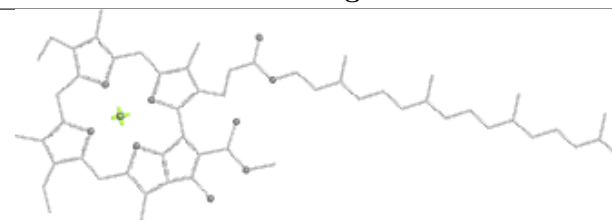


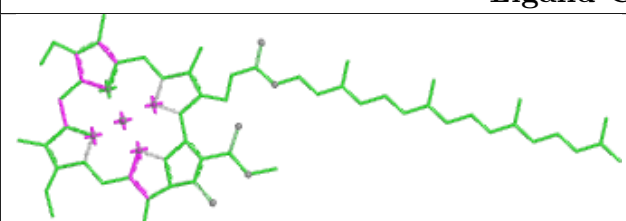
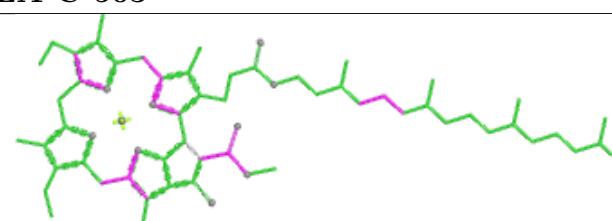
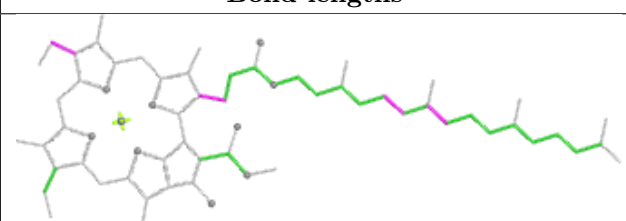
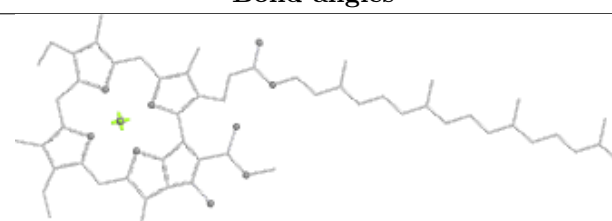
Ligand CLA b 610

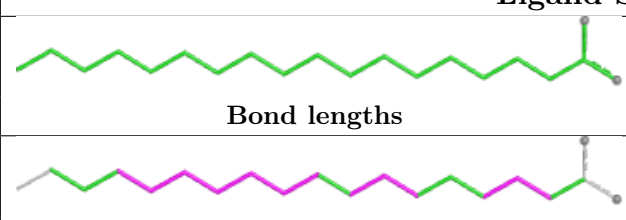
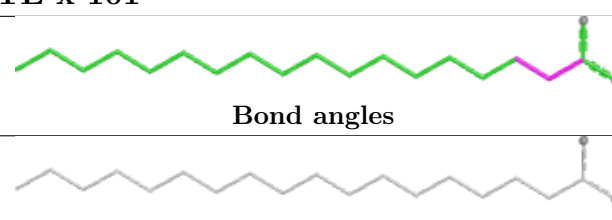
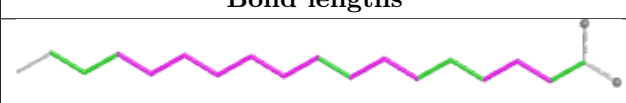
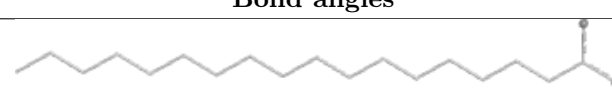


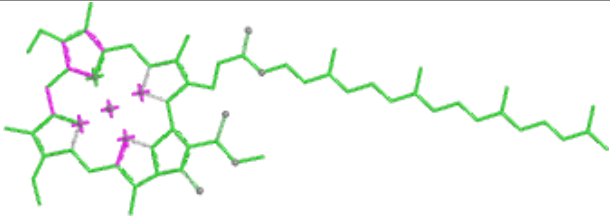
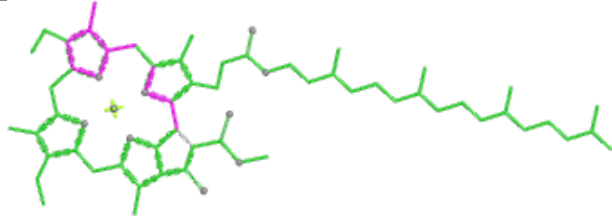
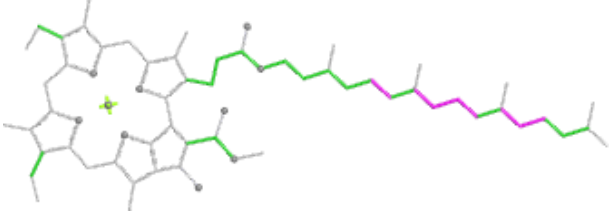
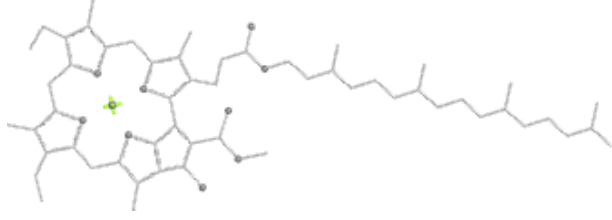
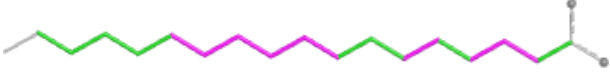
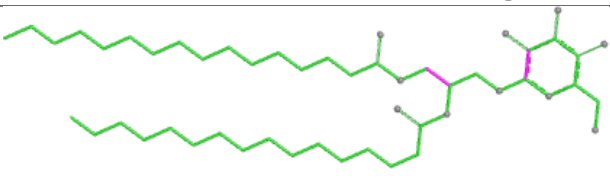
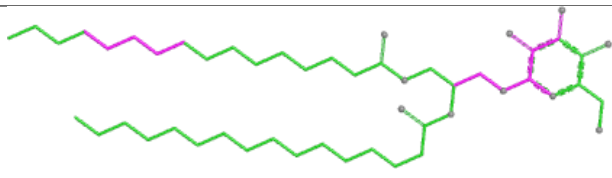
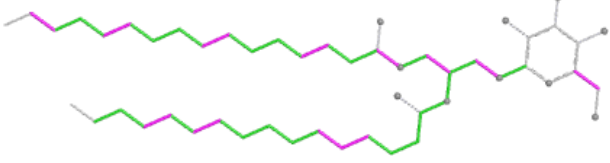
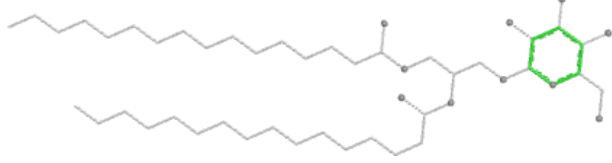
Ligand CLA d 404**Ligand CLA a 612****Ligand PHO A 608**



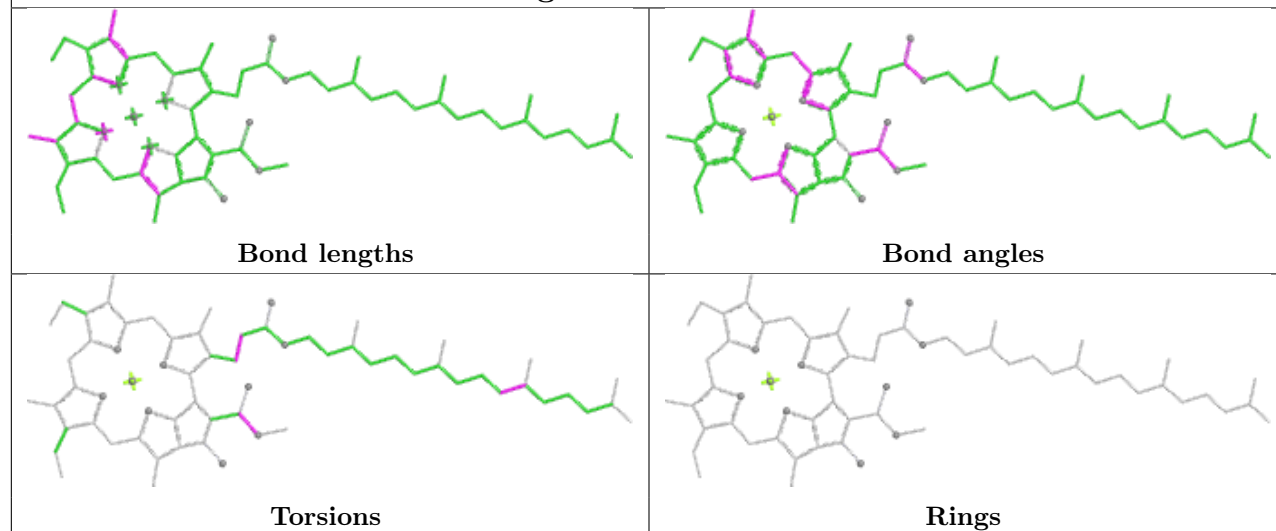
Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

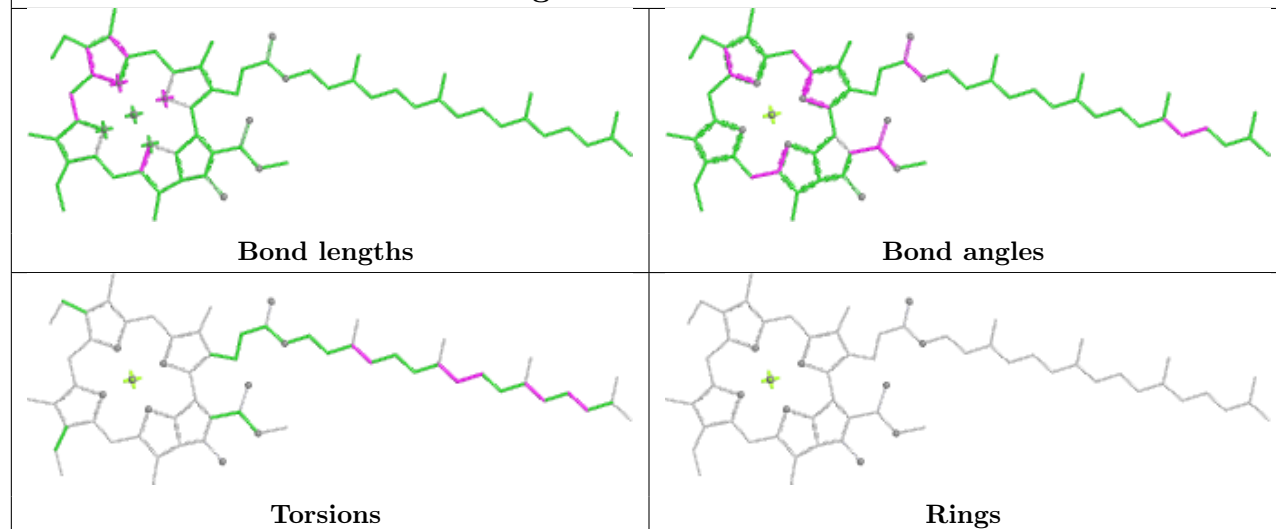
Ligand STE x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE c 520	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

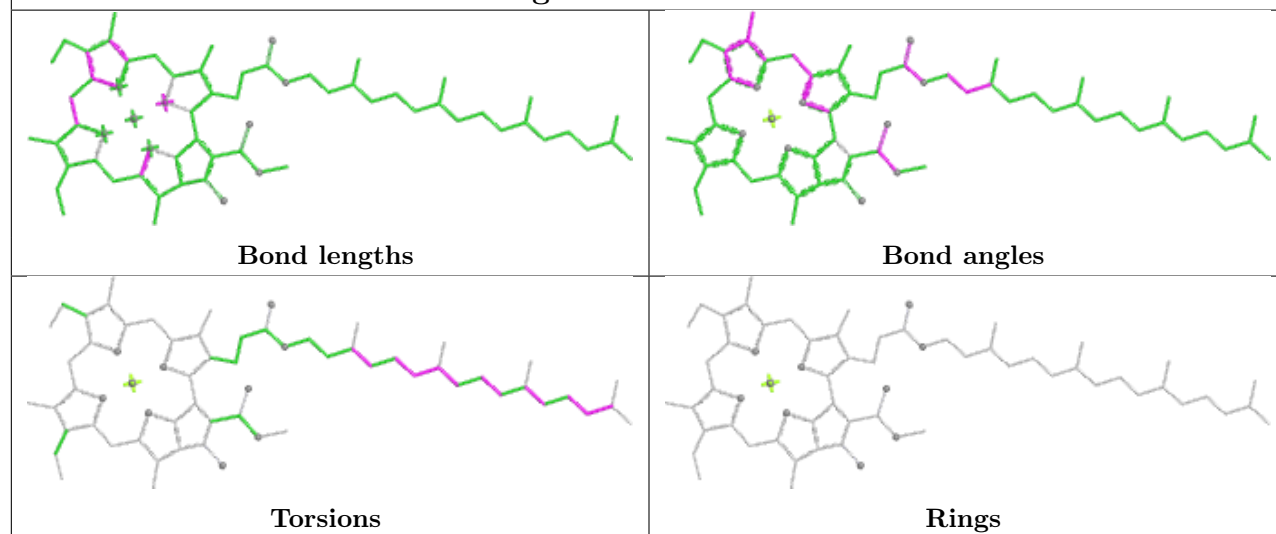
Ligand CLA c 501

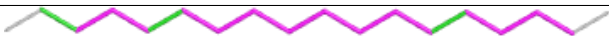


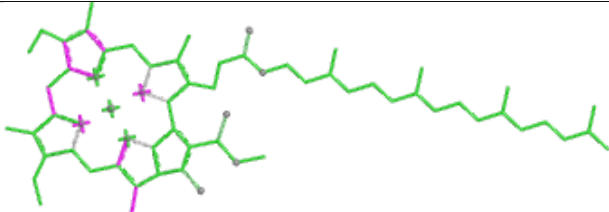
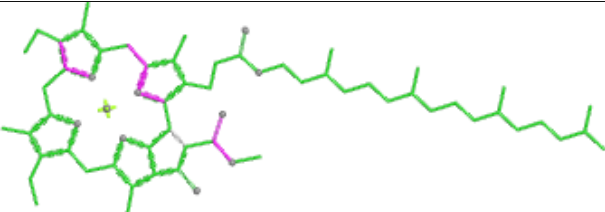
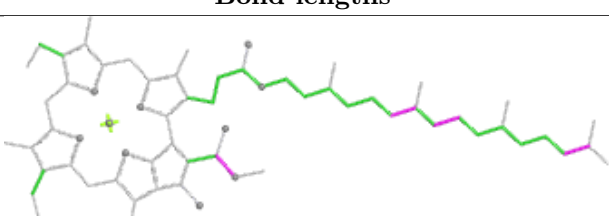
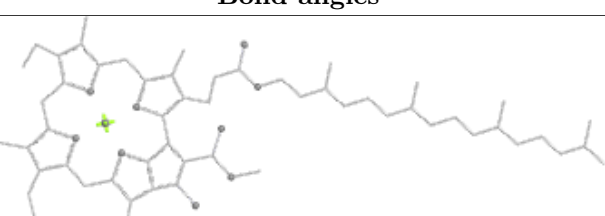
Ligand CLA B 604

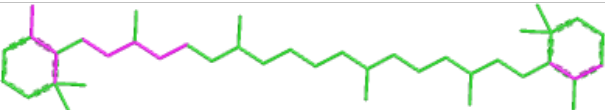
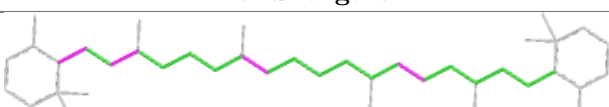
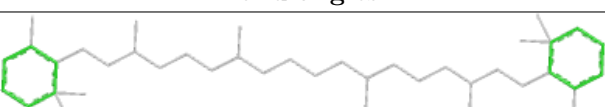


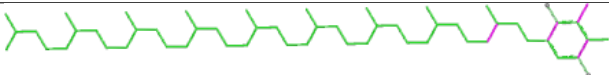
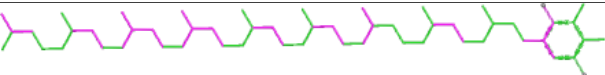
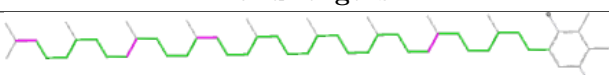
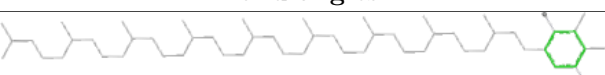
Ligand CLA C 505

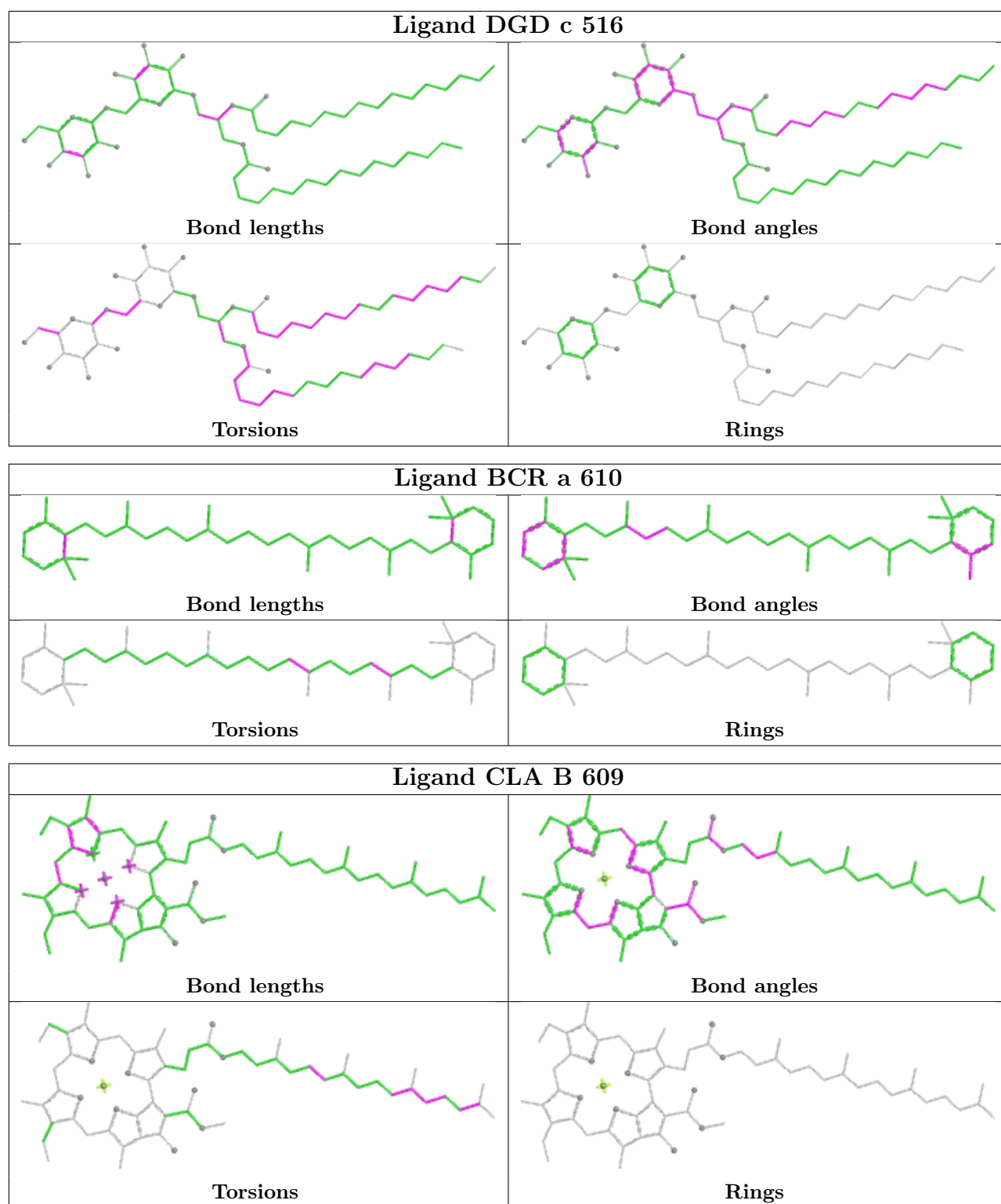


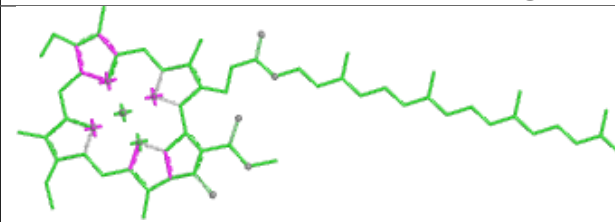
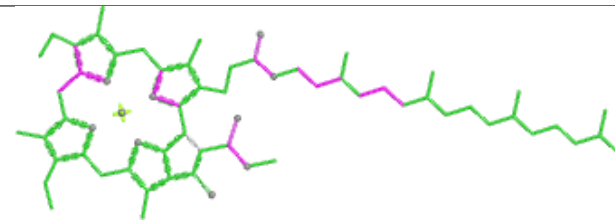
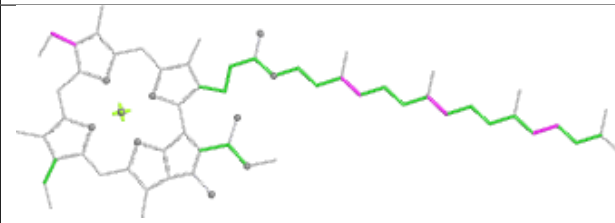
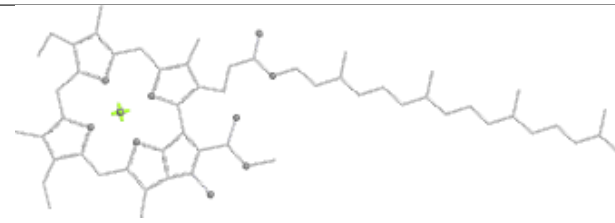
Ligand STE H 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

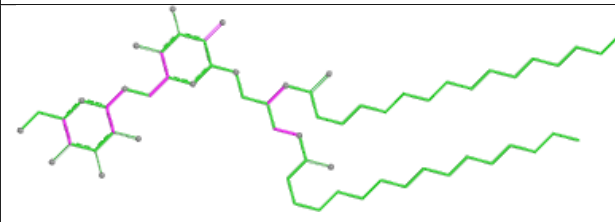
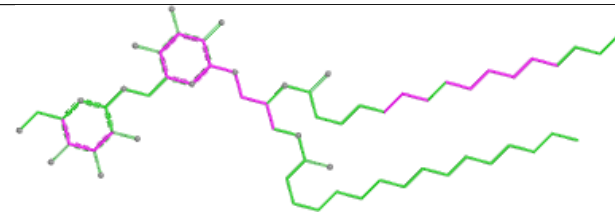
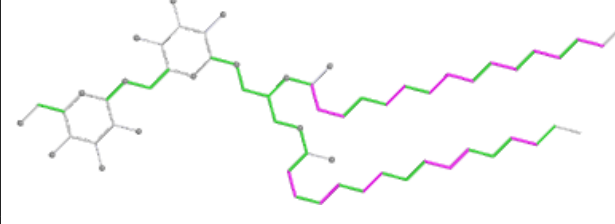
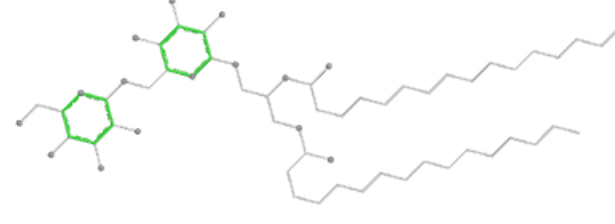
Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

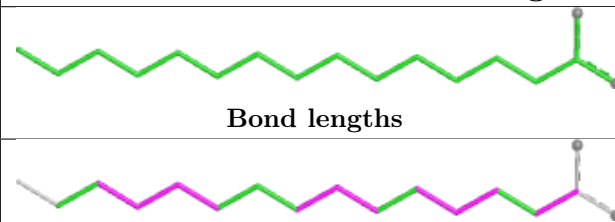
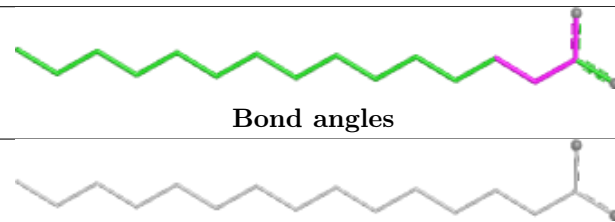
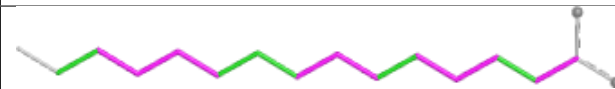
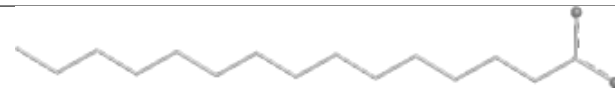
Ligand BCR t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

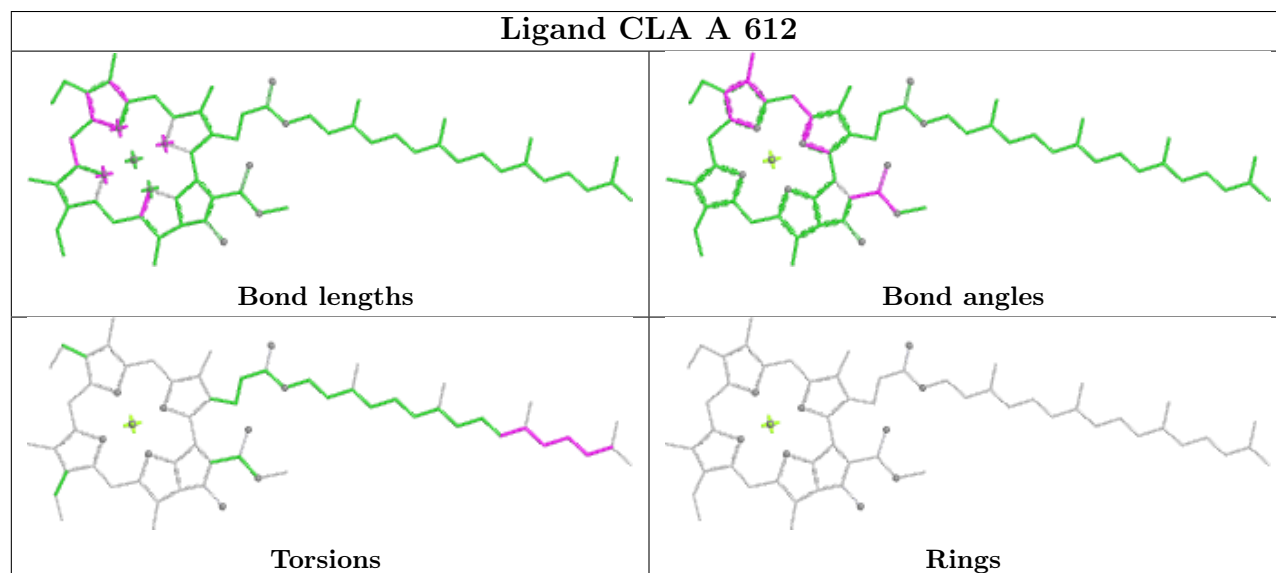
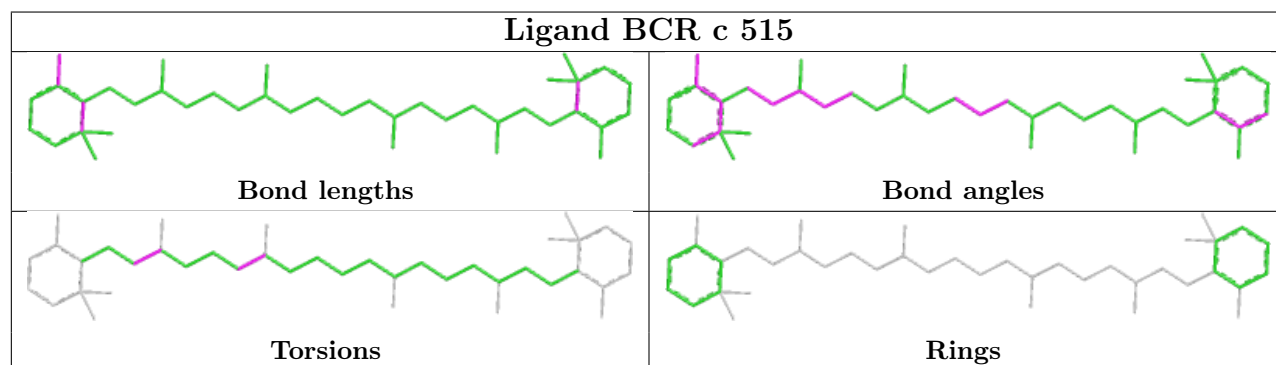
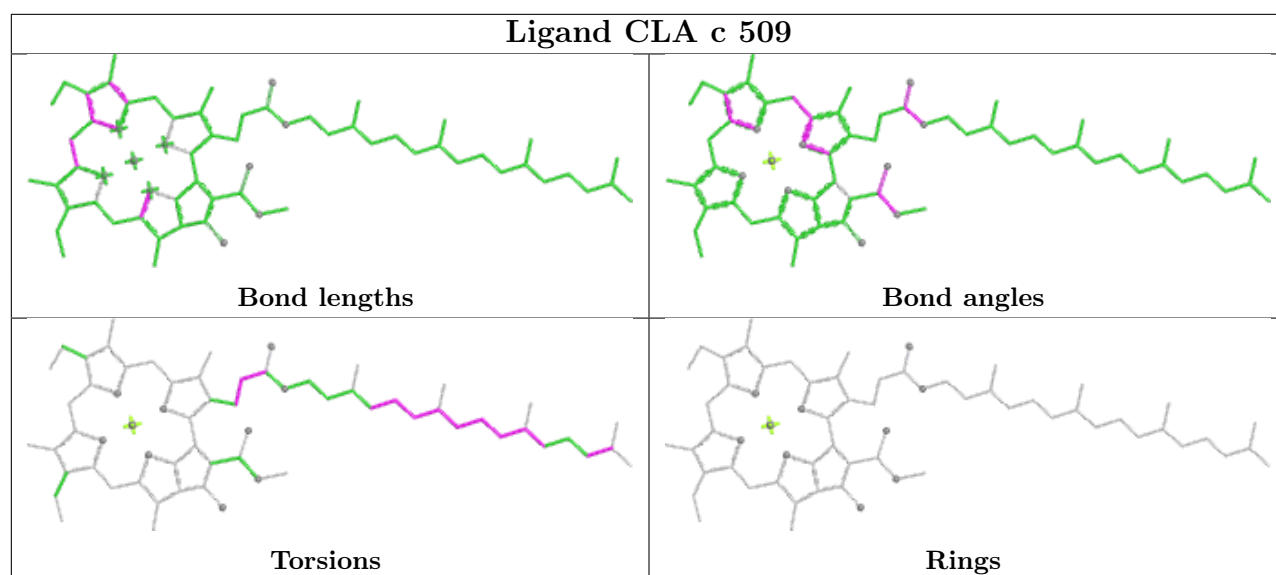
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

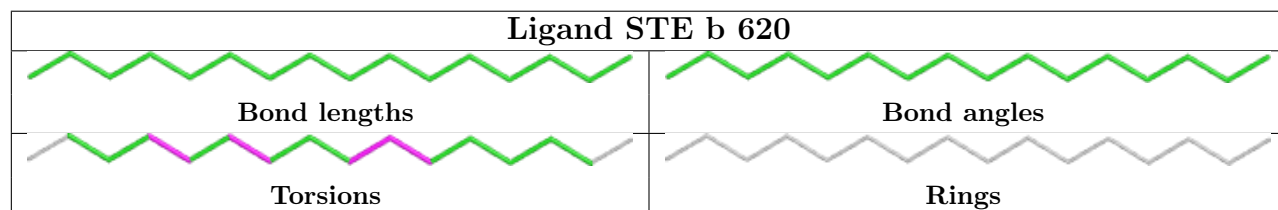
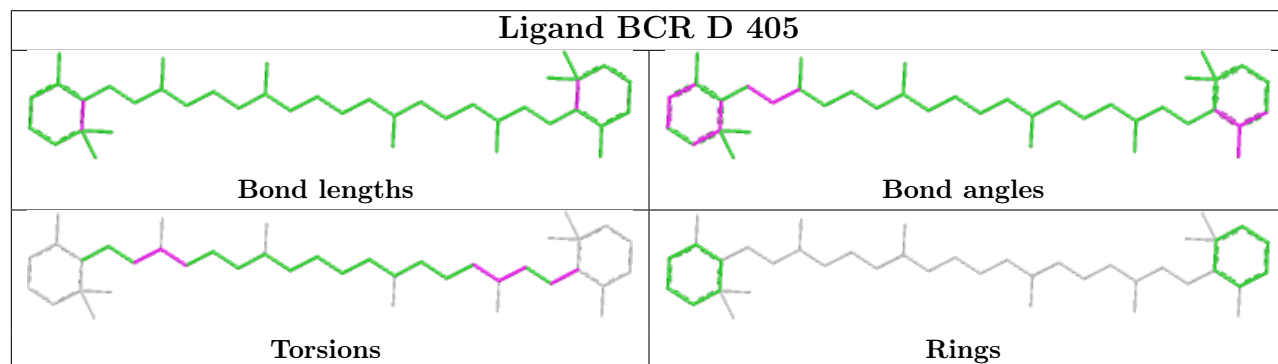
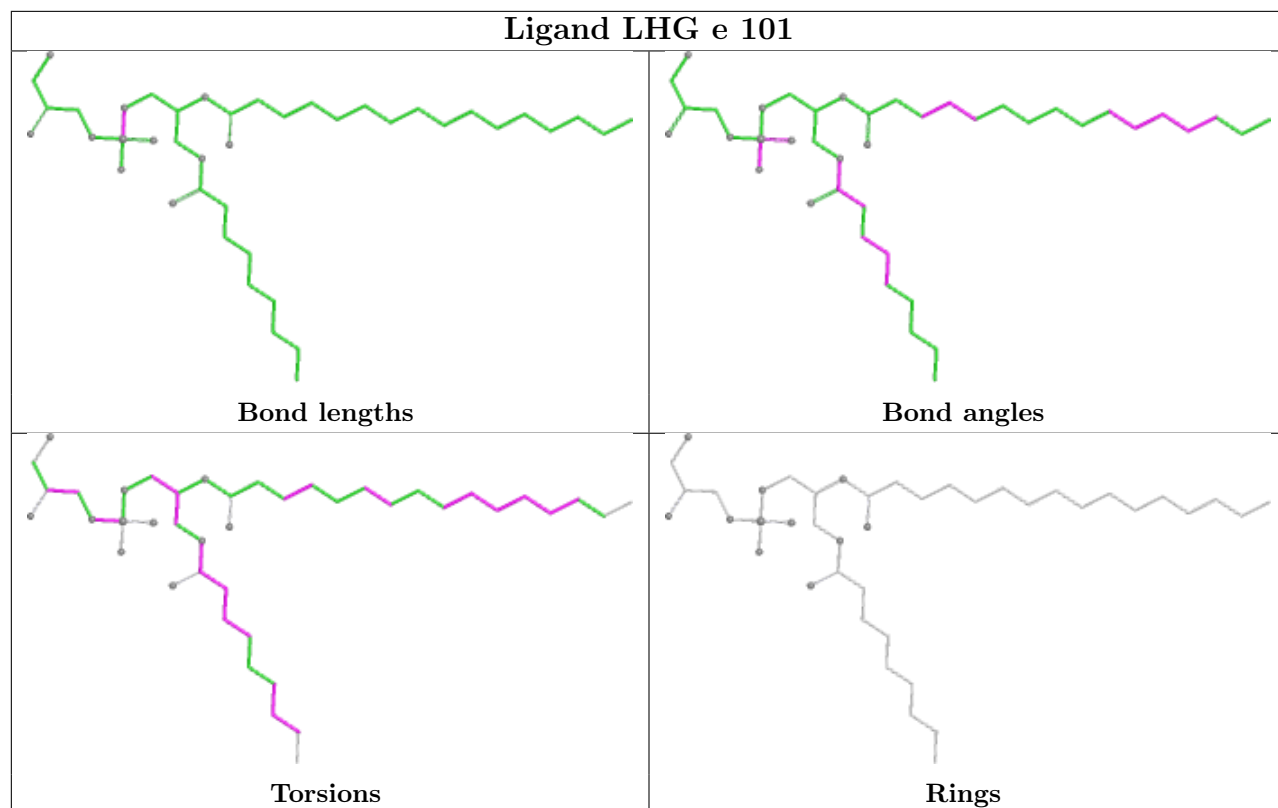


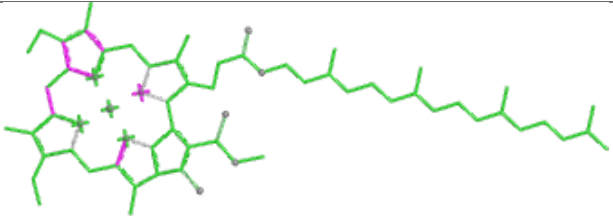
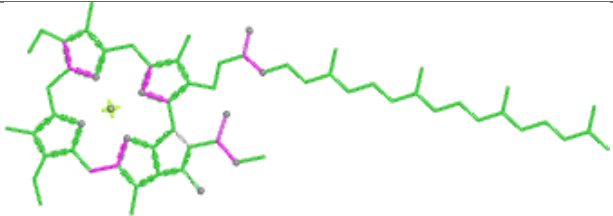
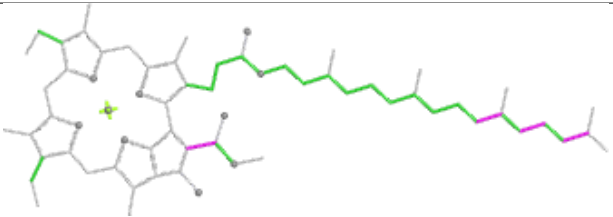
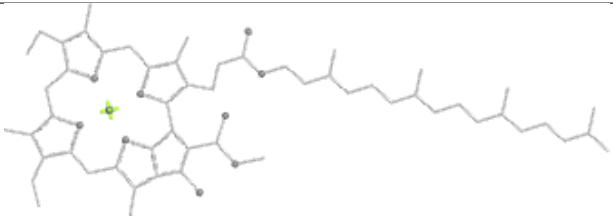
Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

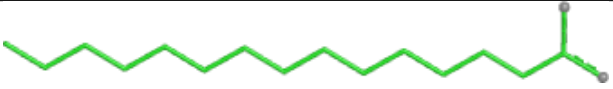
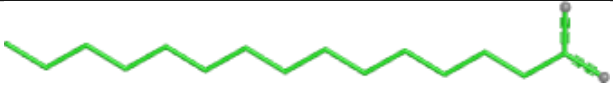
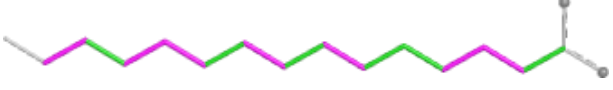
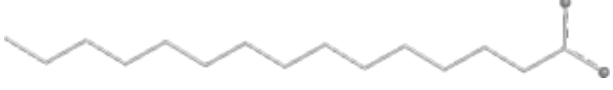
Ligand DGD H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

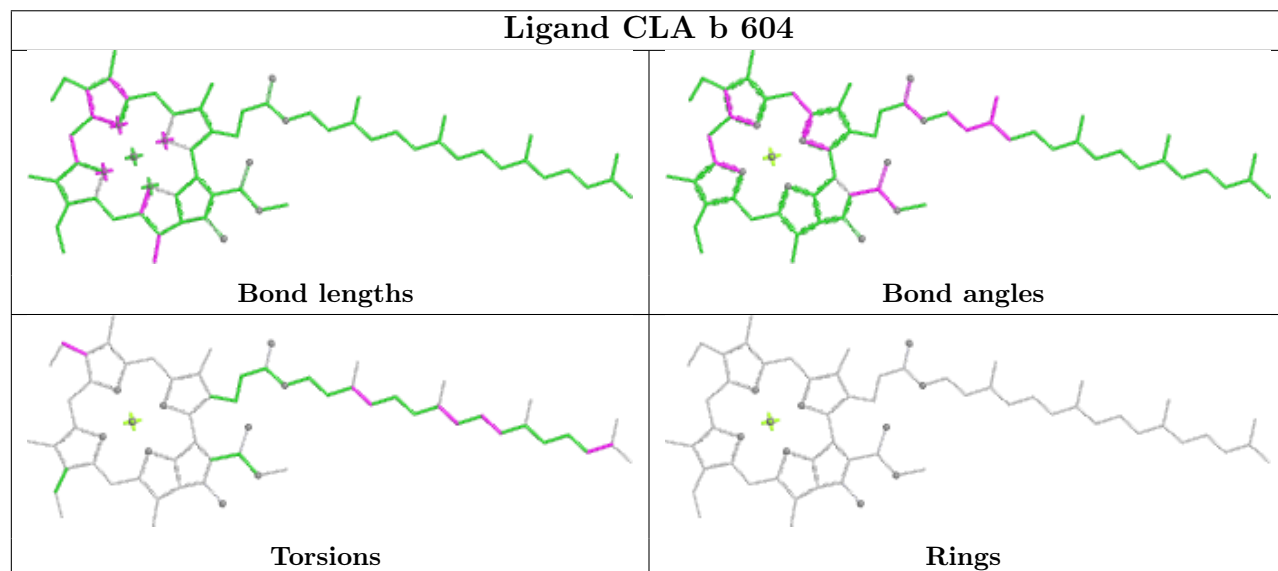
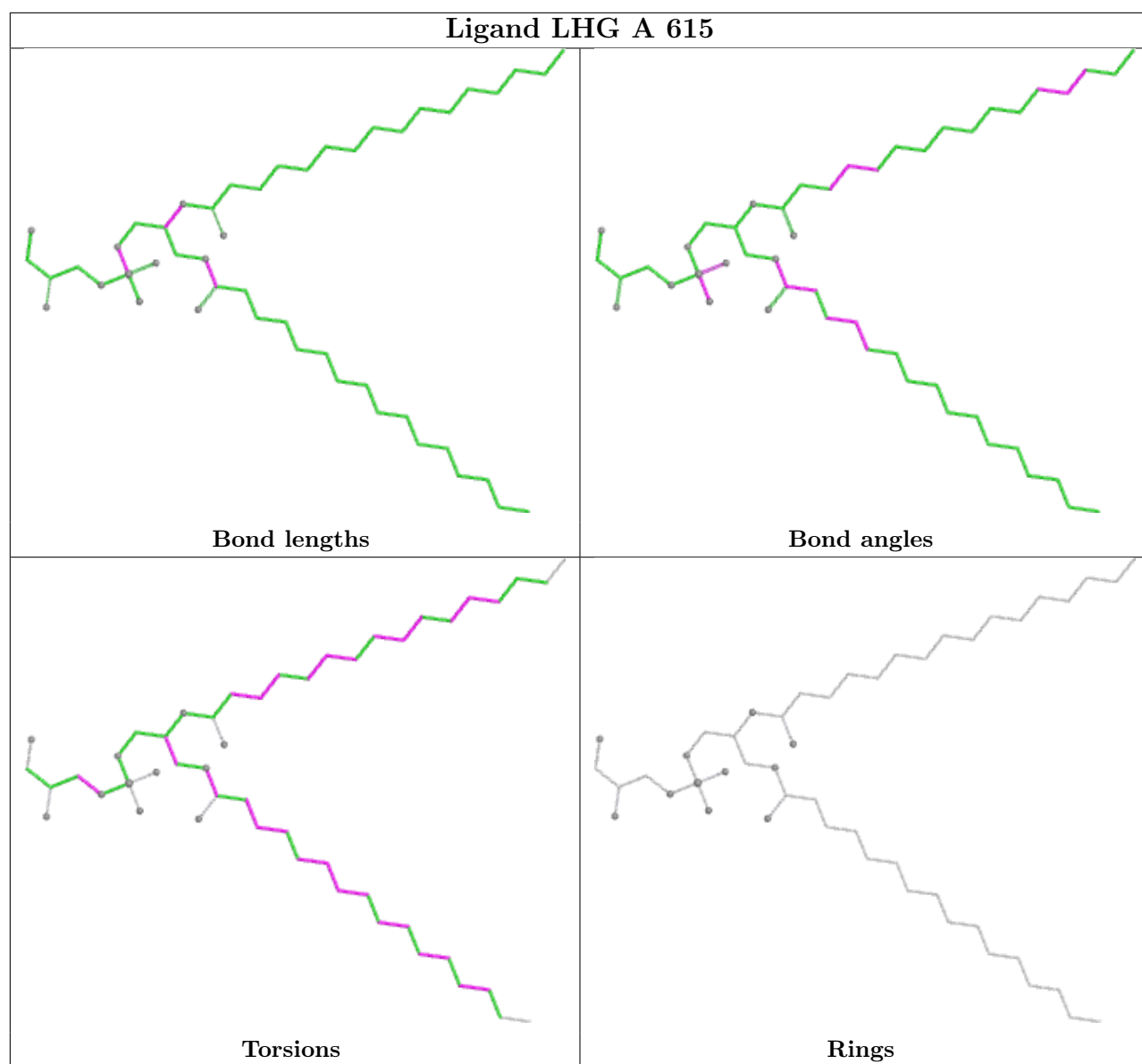
Ligand STE d 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

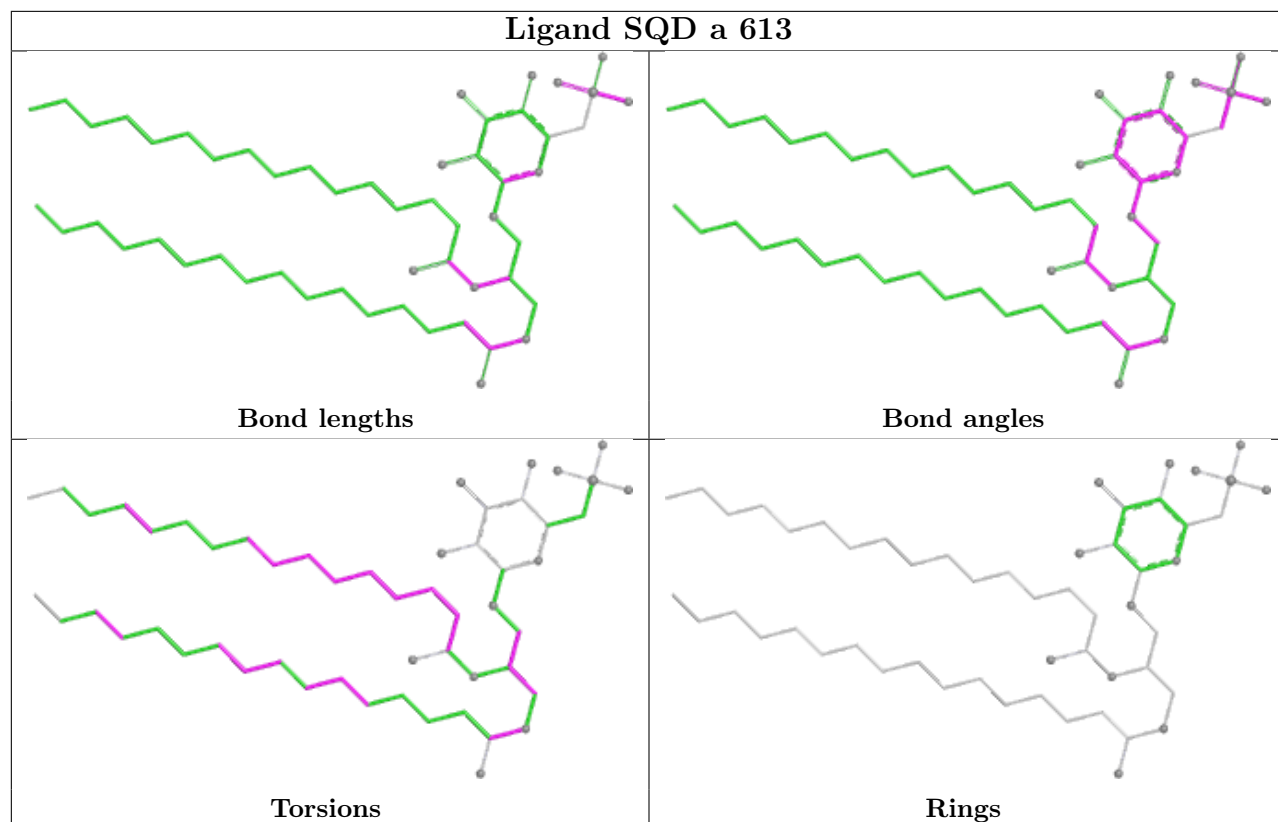




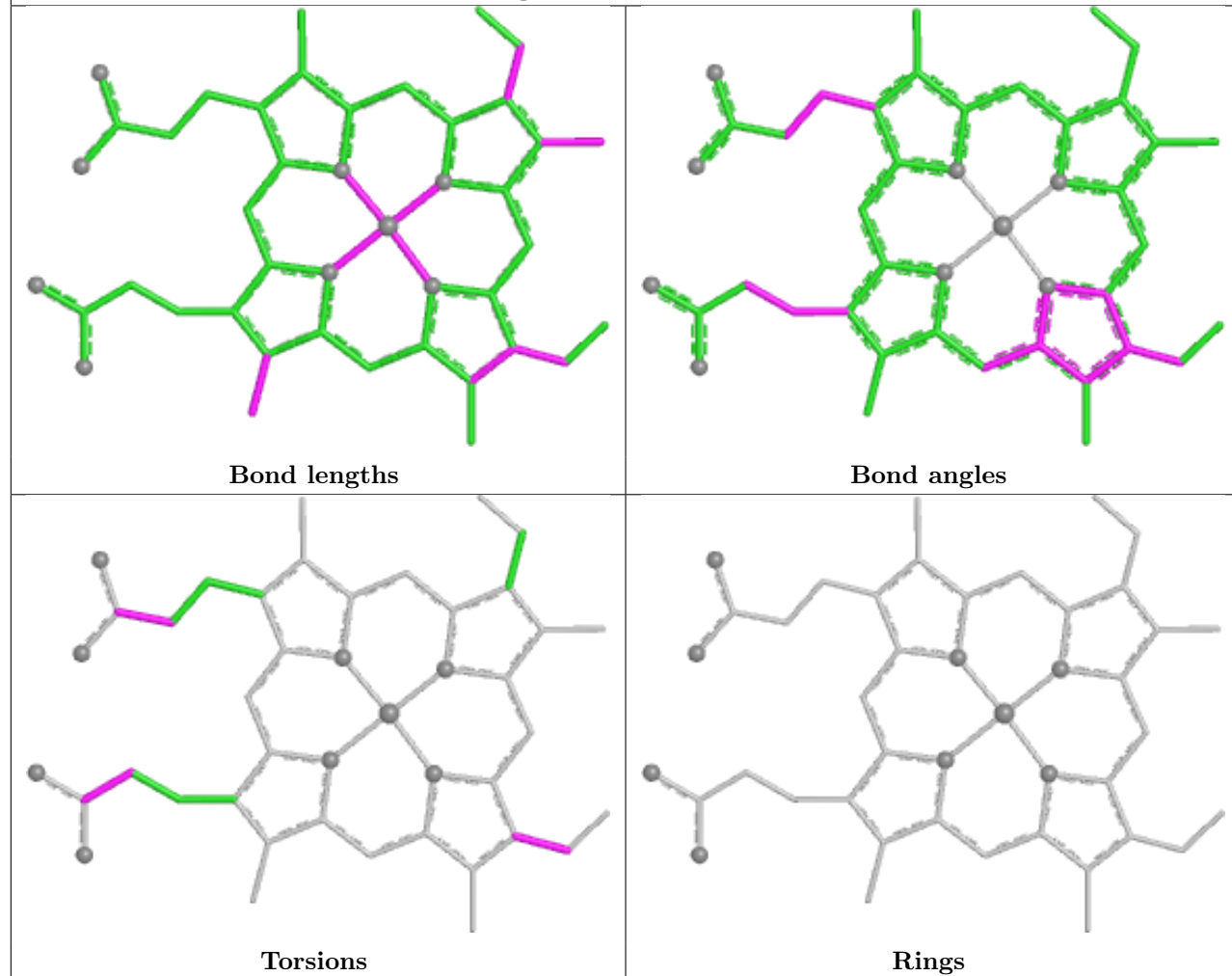
Ligand CLA C 502			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand STE B 619			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

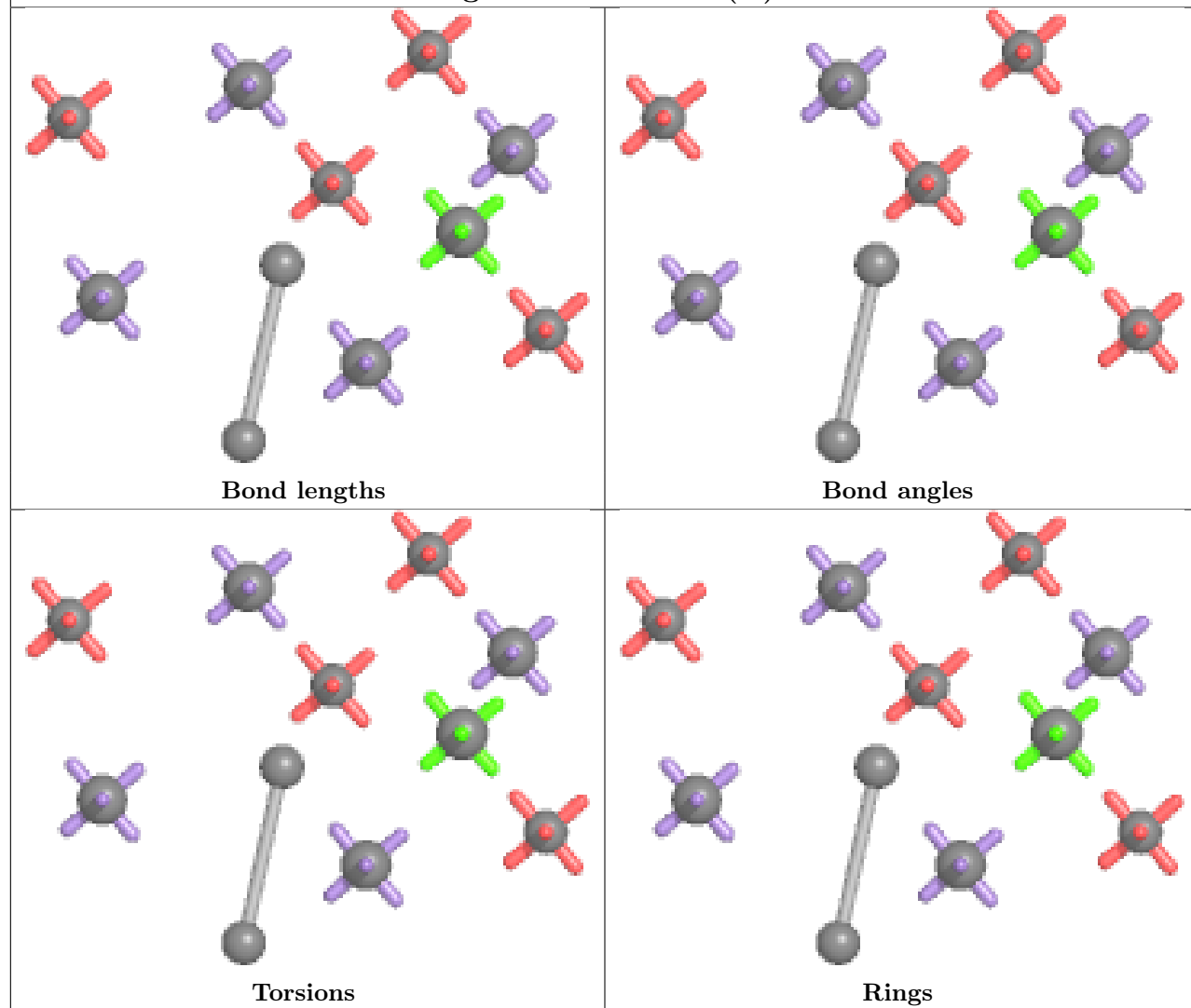




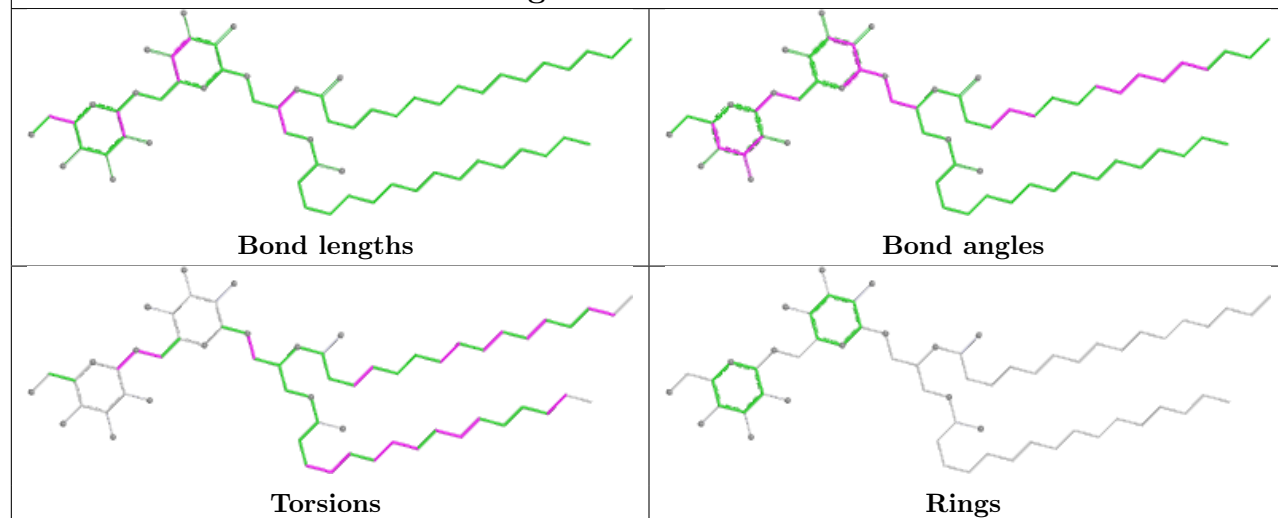
Ligand HEM f 101

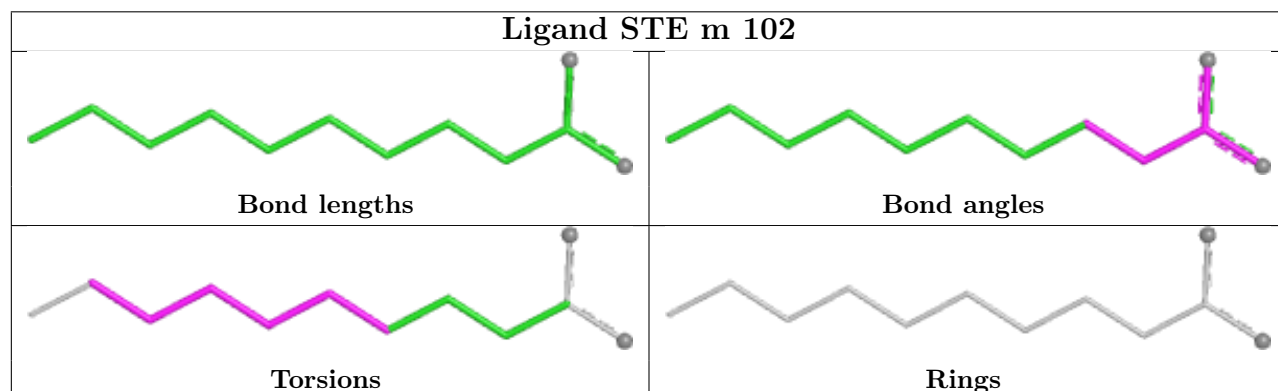
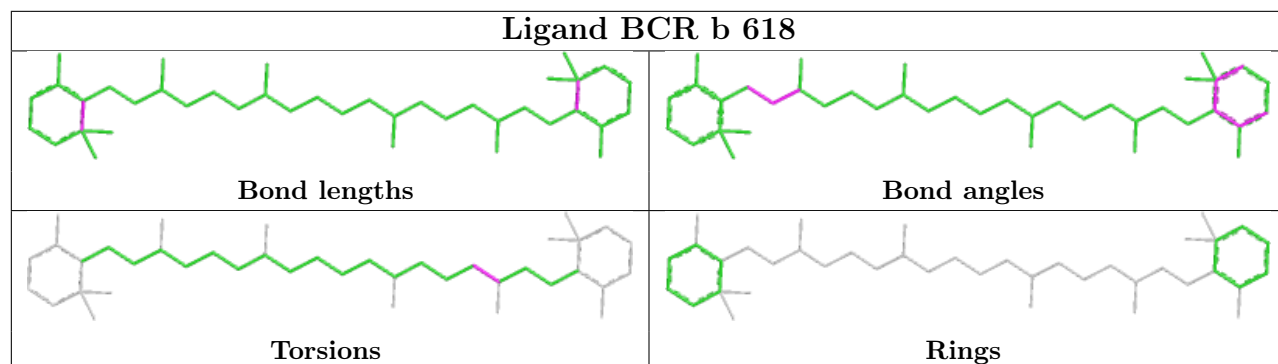
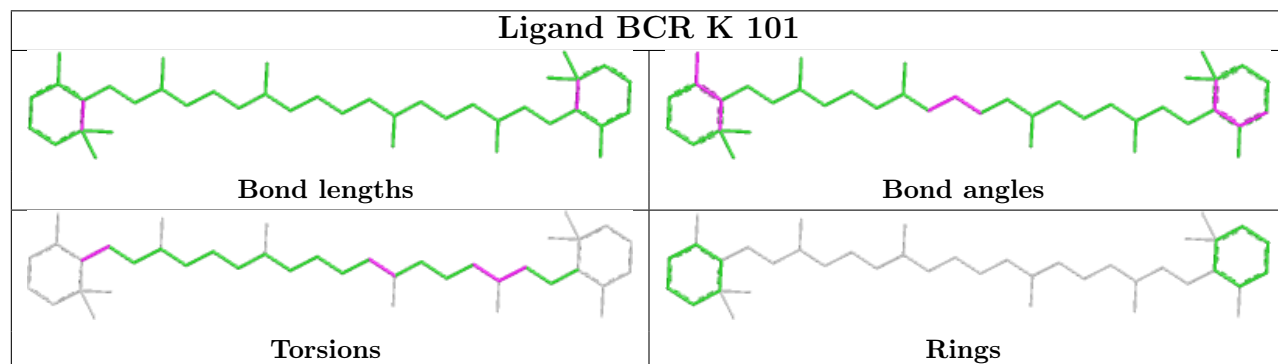
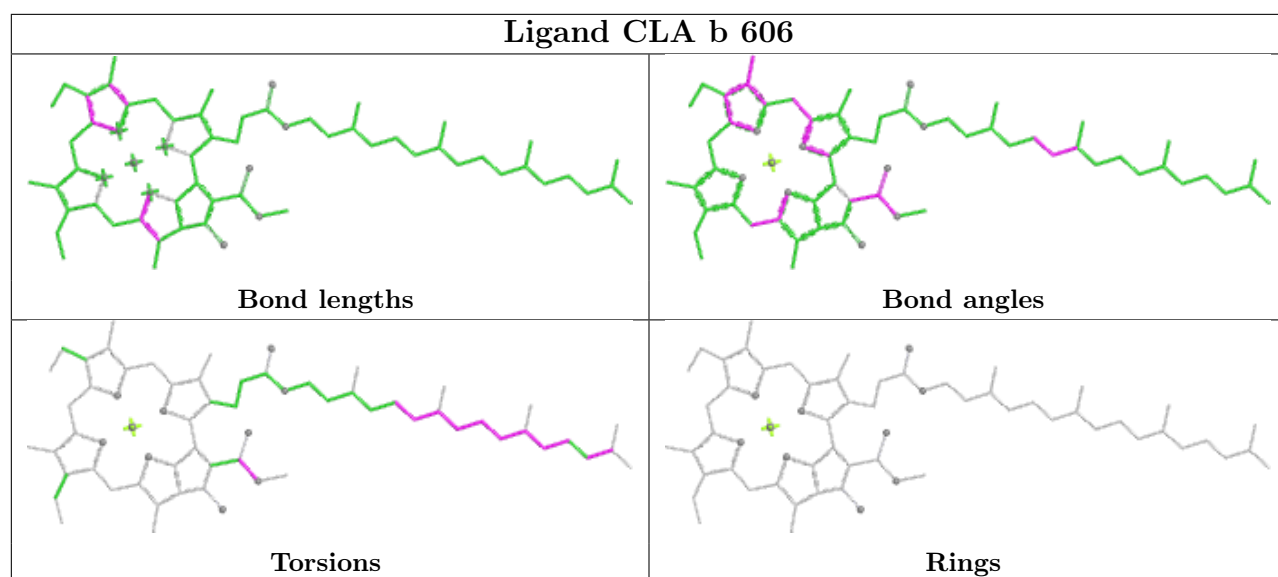


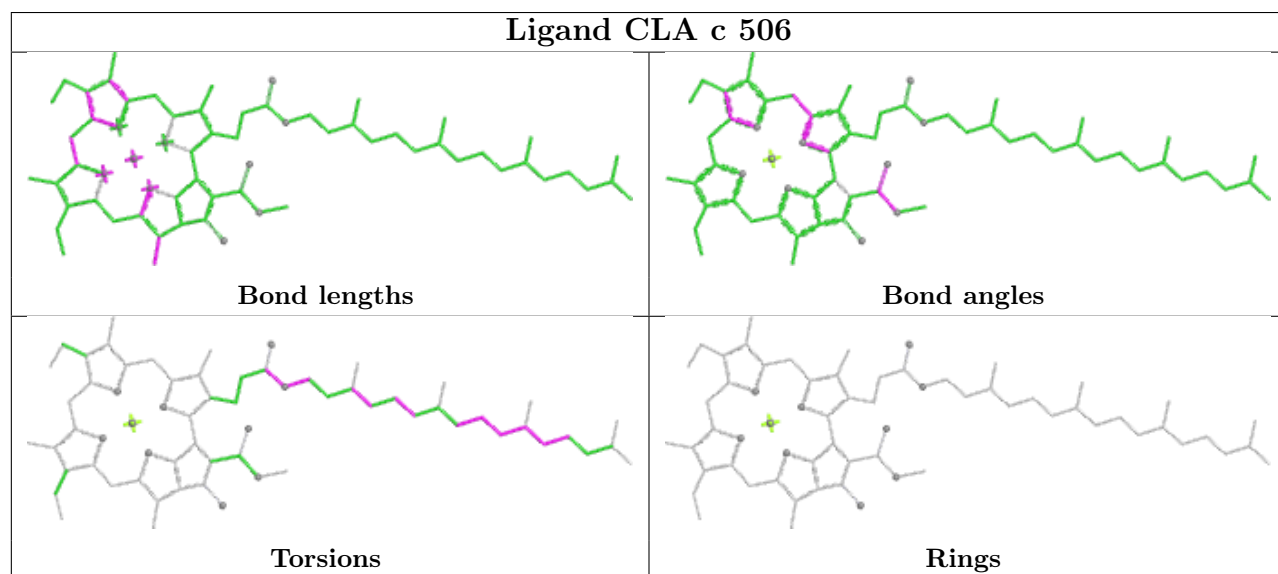
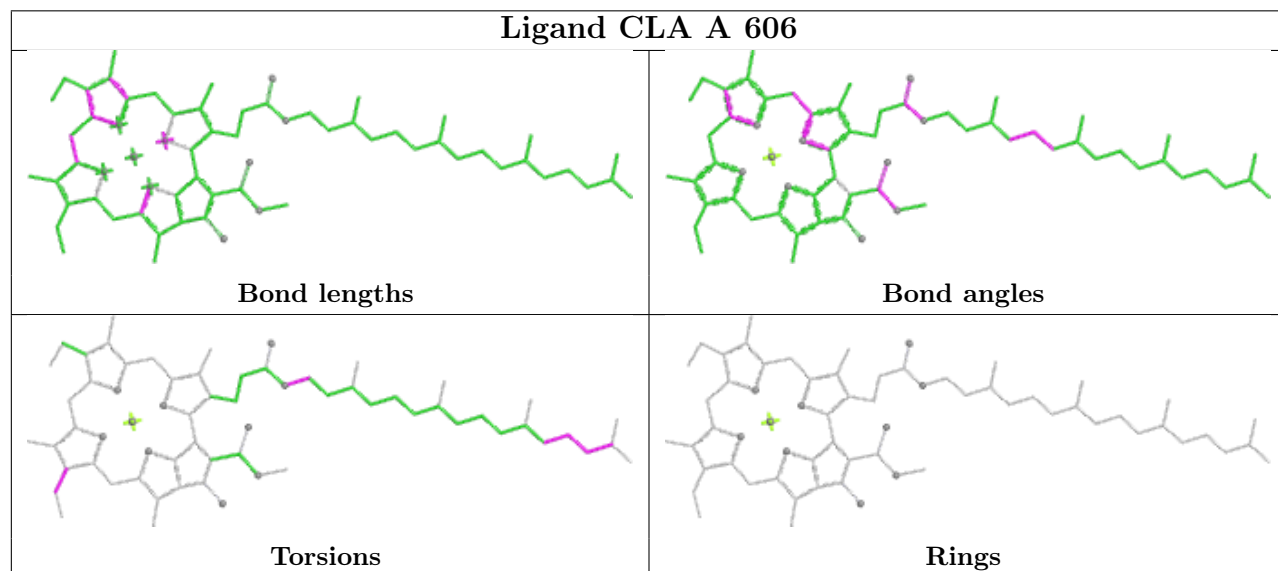
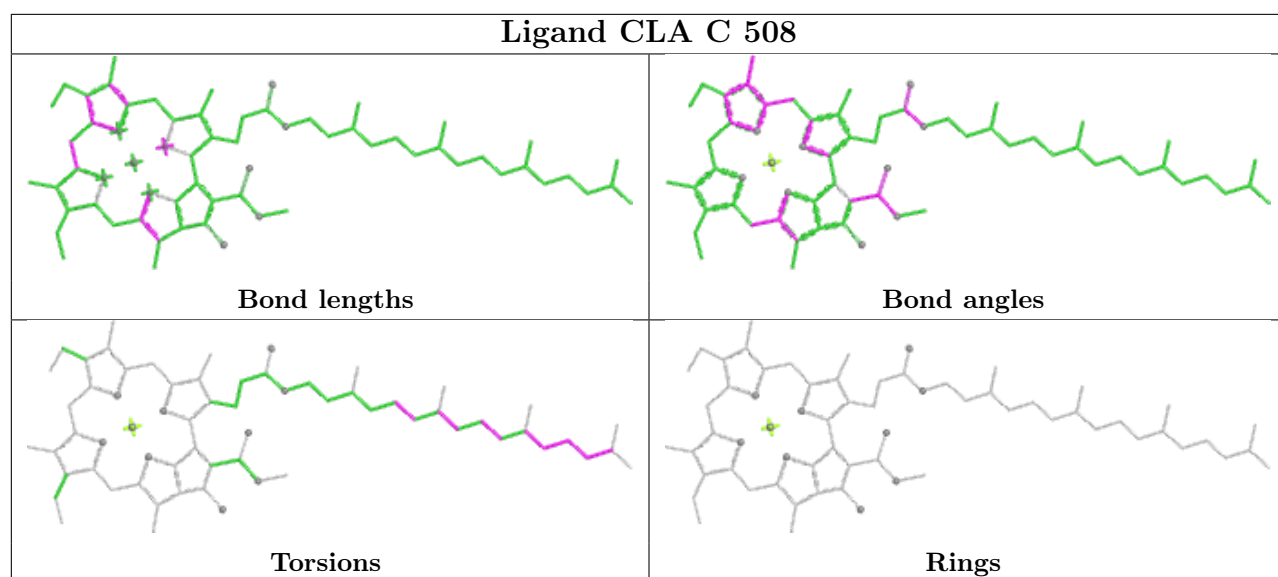
Ligand OEY A 601 (A)

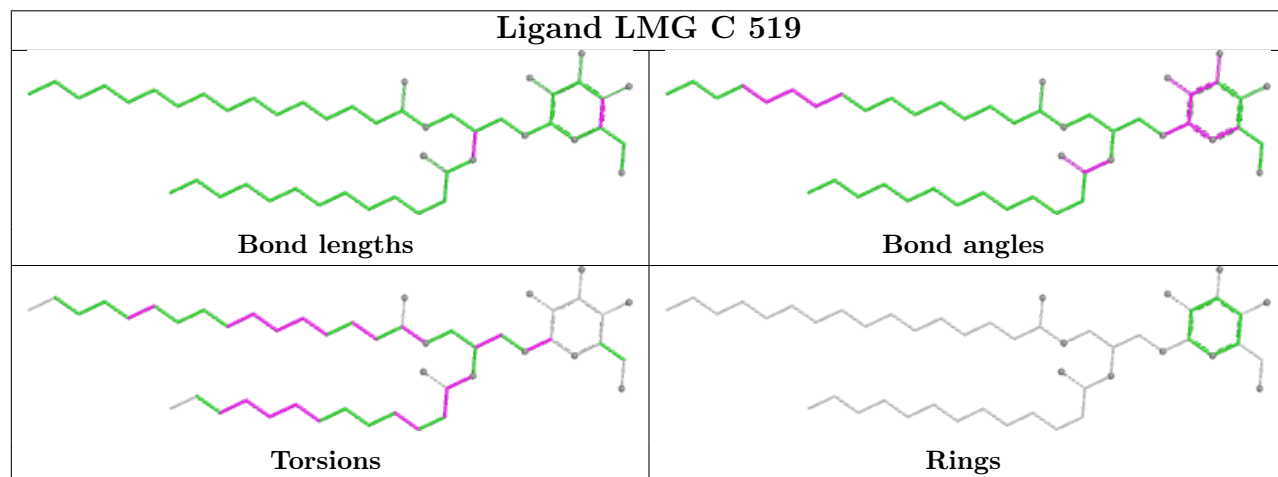
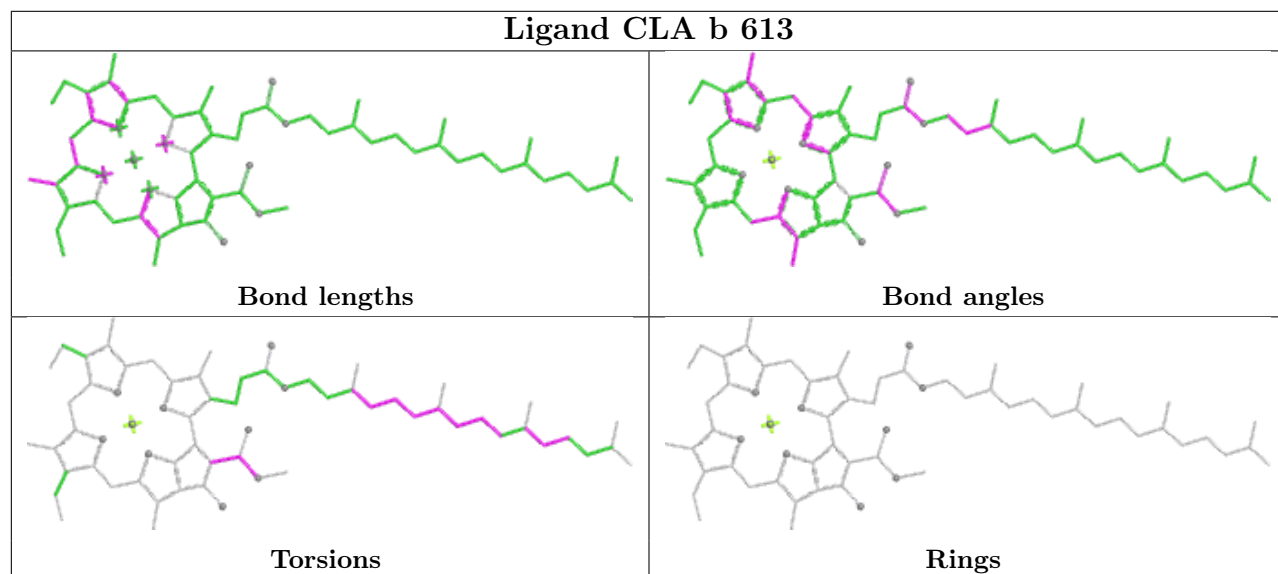
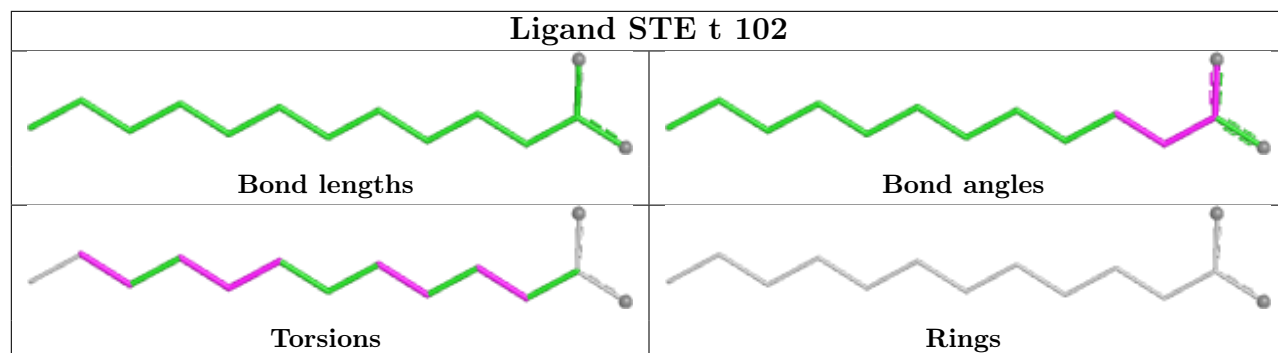


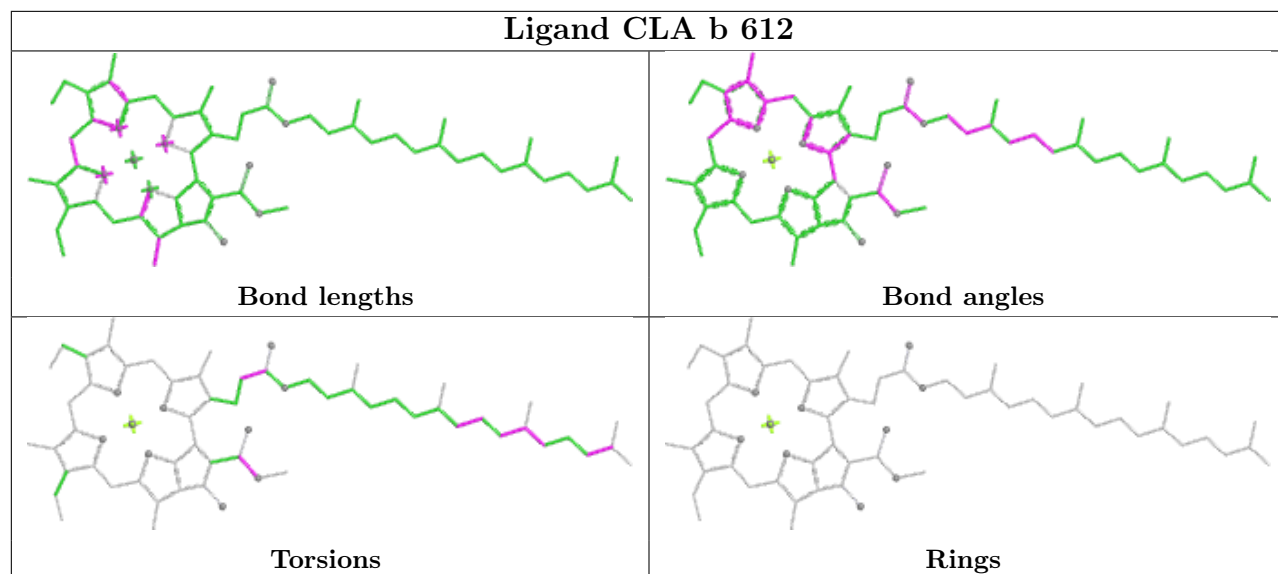
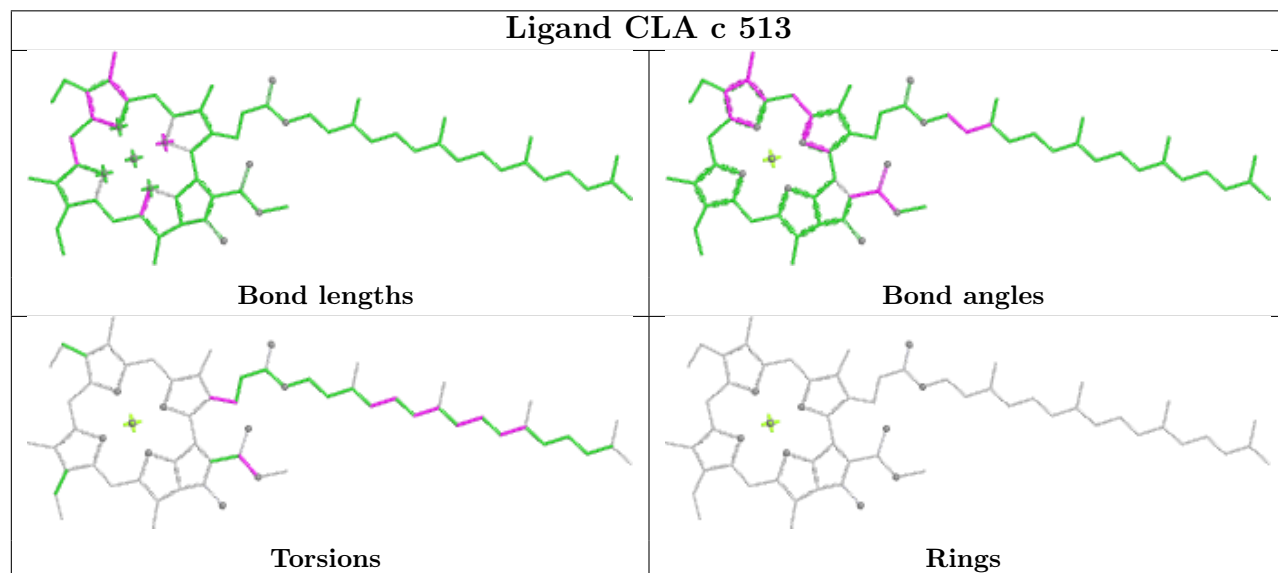
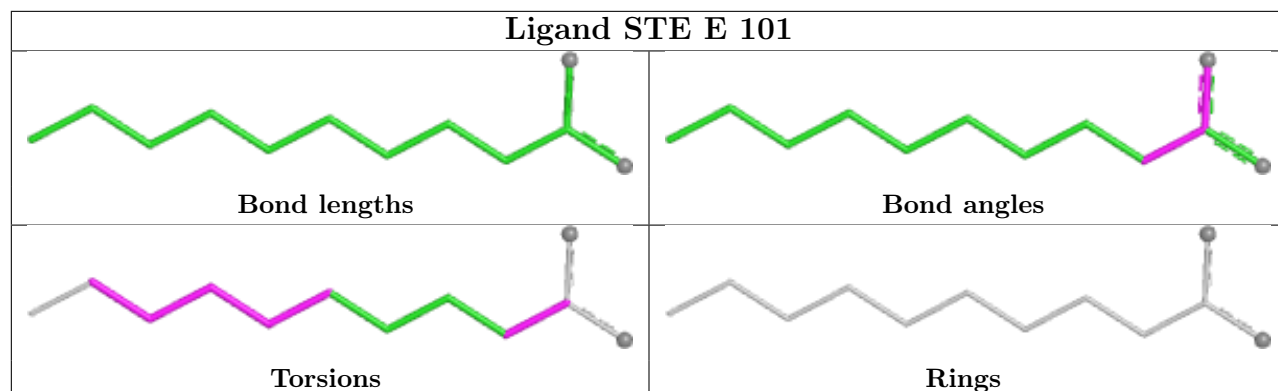
Ligand DGD C 517

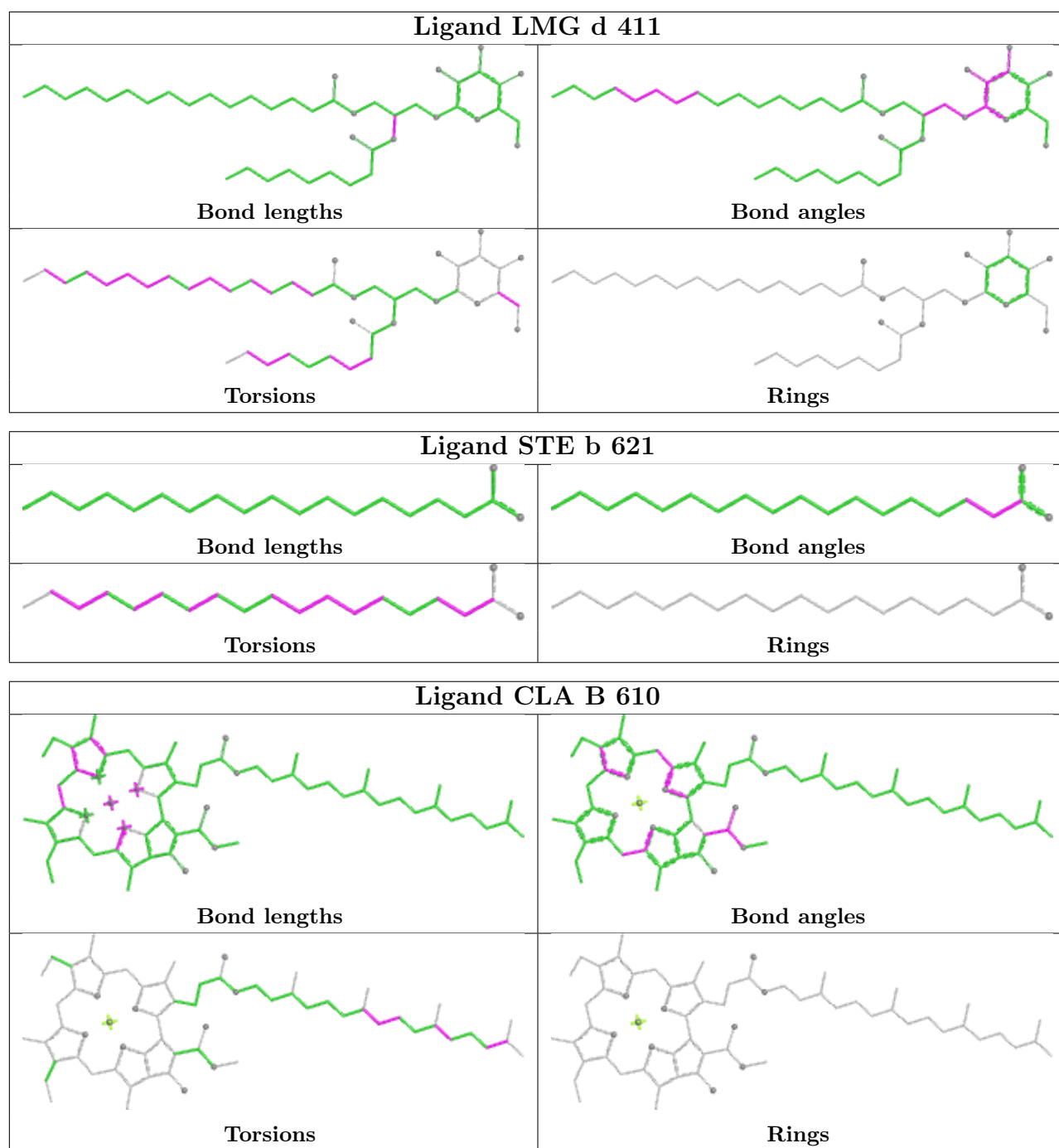




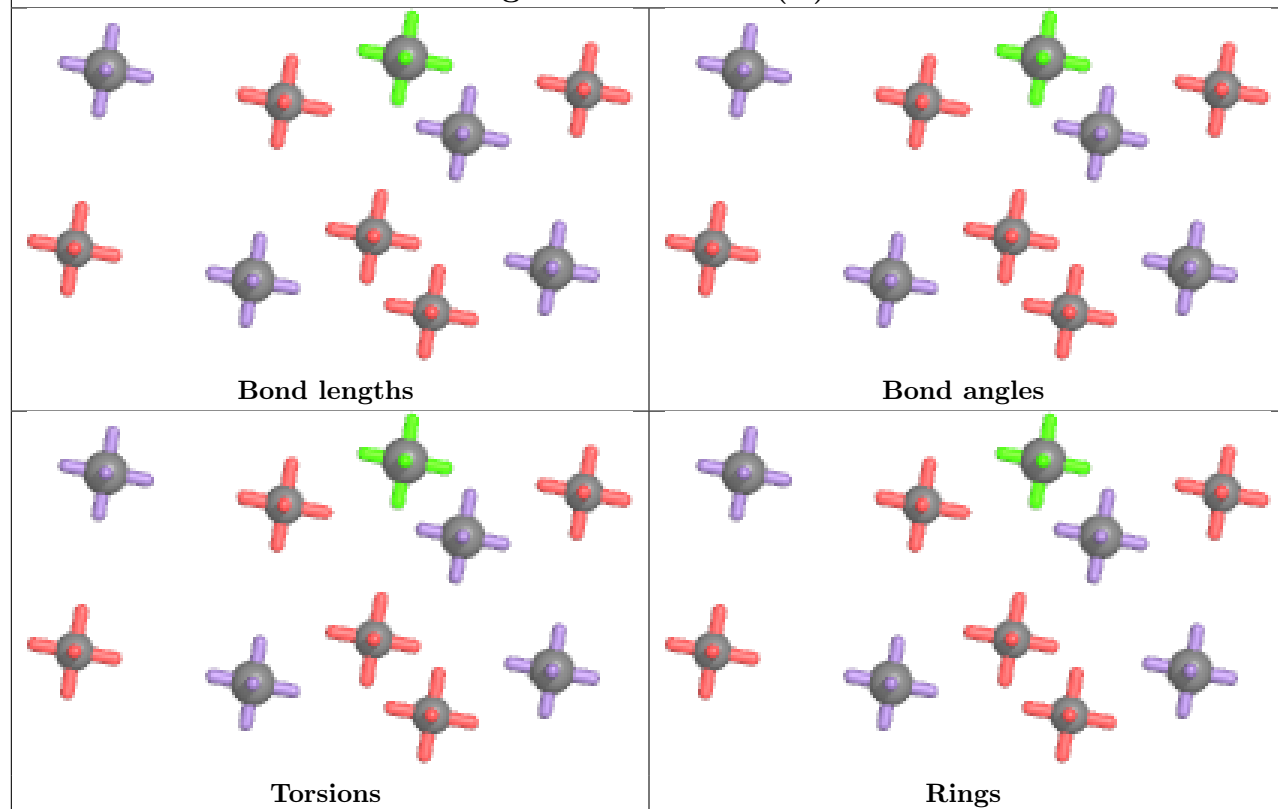




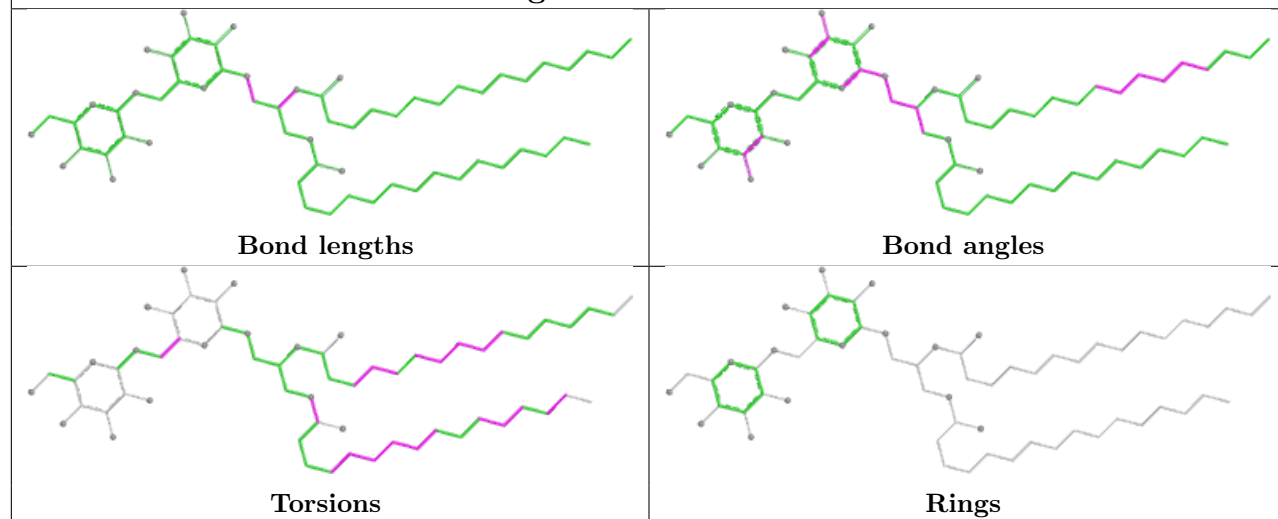
Ligand CLA b 612**Ligand CLA c 513****Ligand STE E 101**

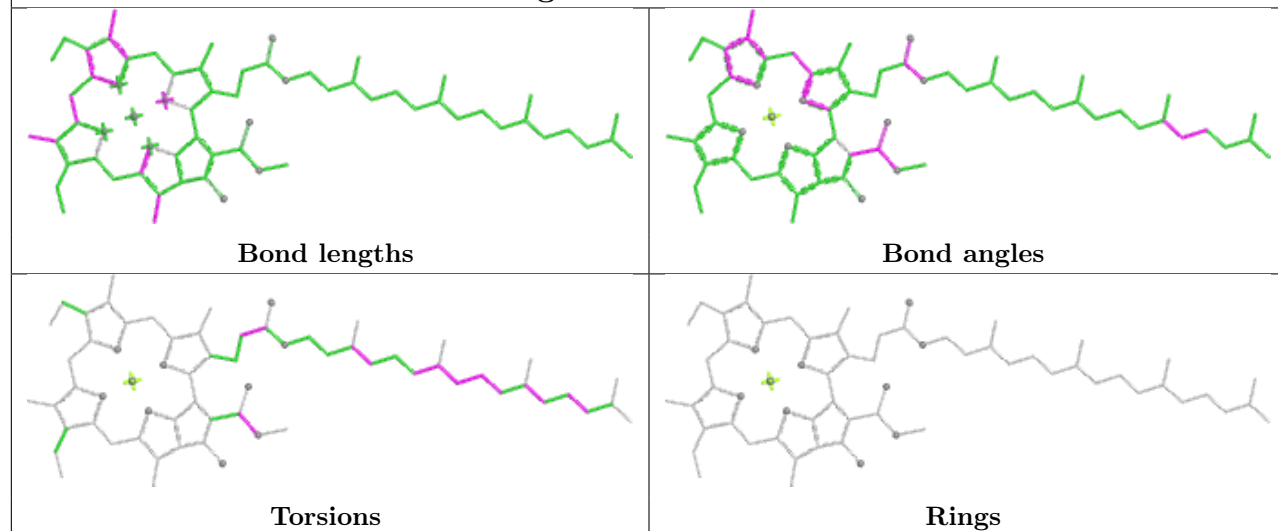
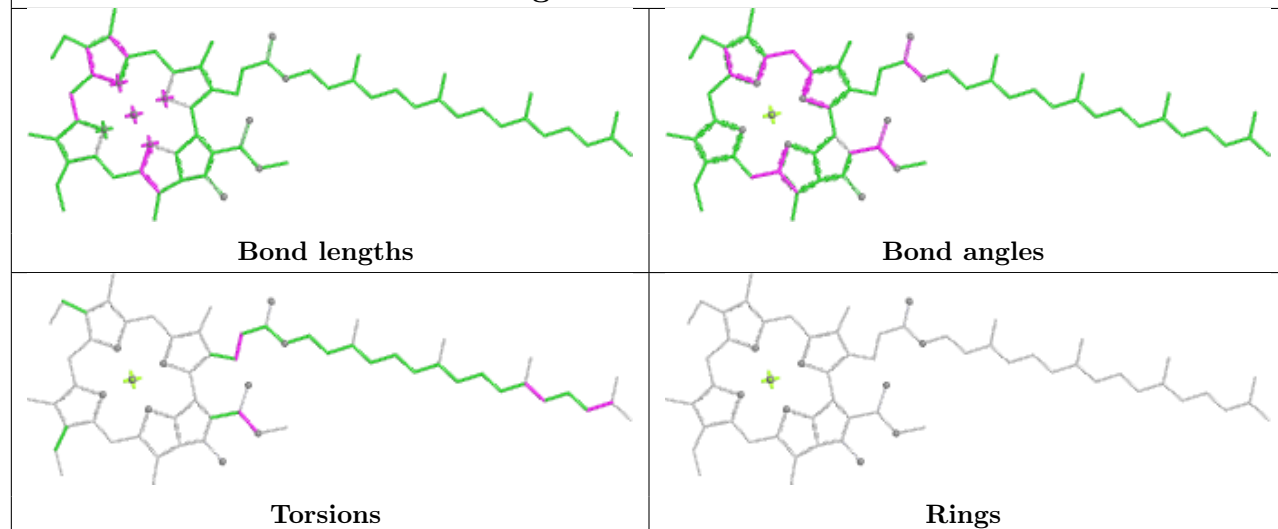


Ligand OEX a 602 (B)

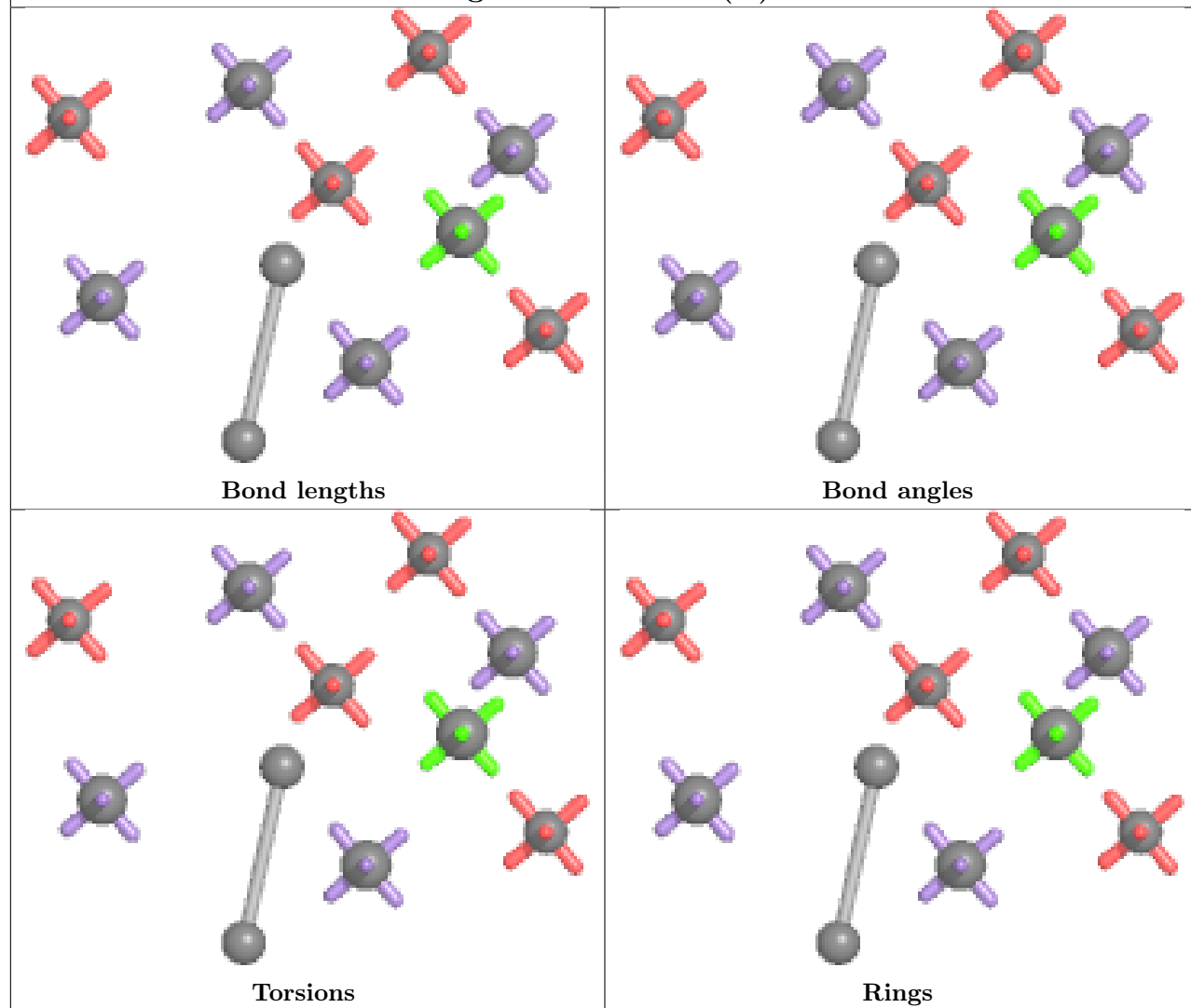


Ligand DGD C 518

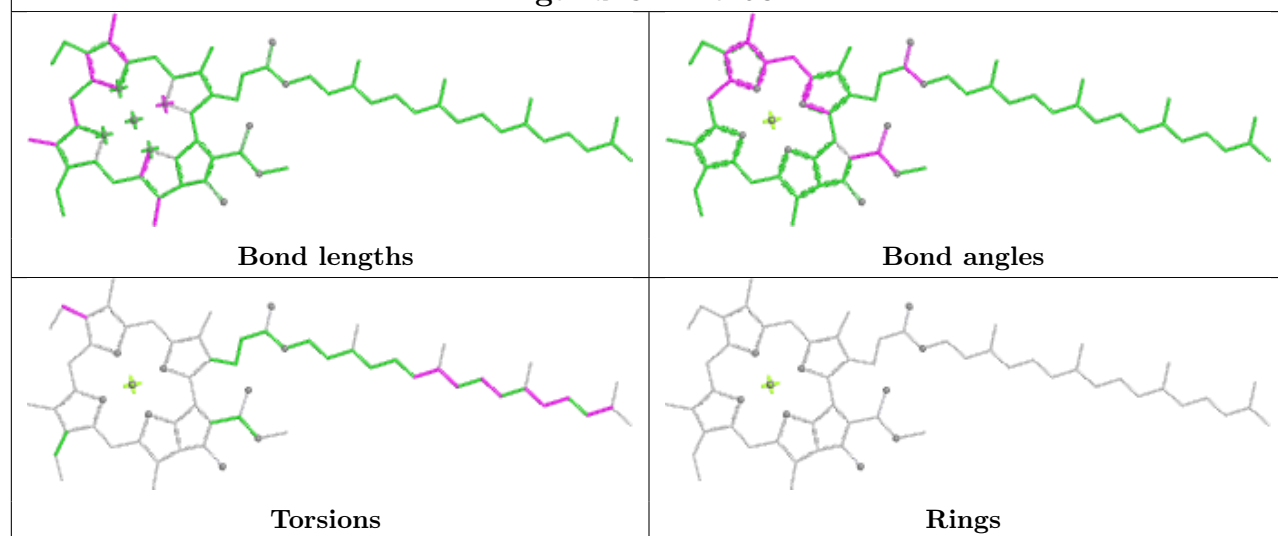


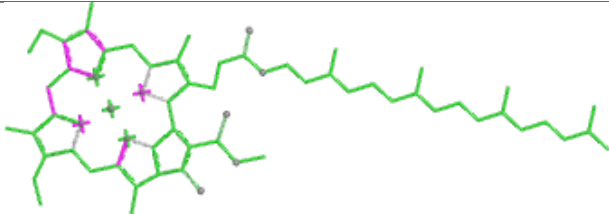
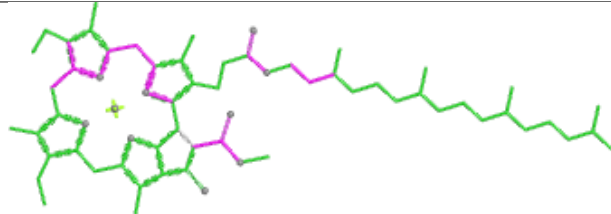
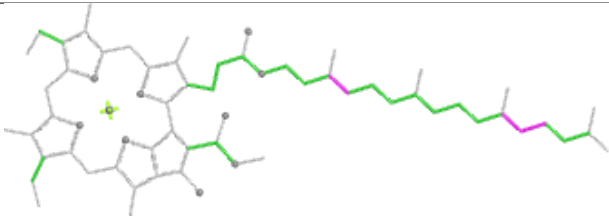
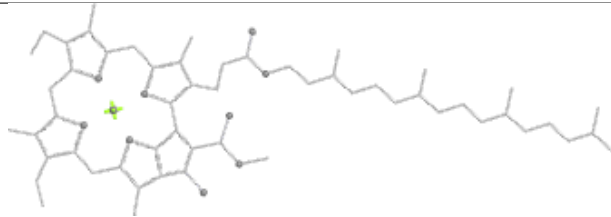
Ligand CLA c 510**Ligand CLA C 501**

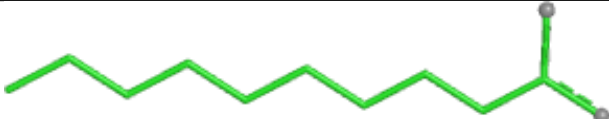
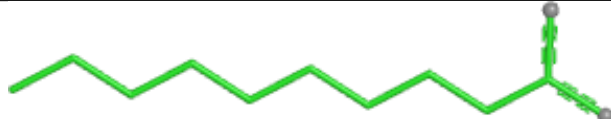
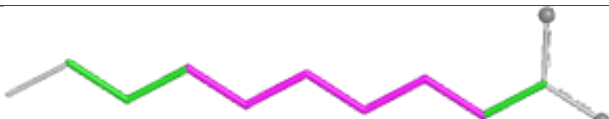
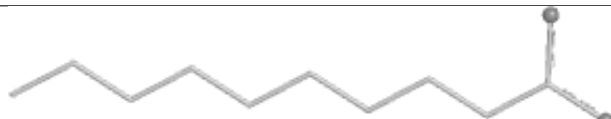
Ligand OEY a 601 (A)

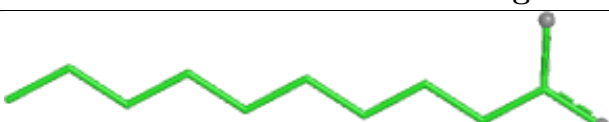
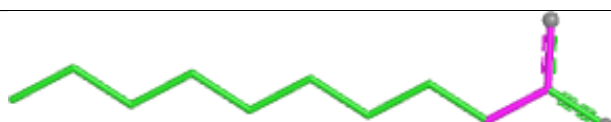
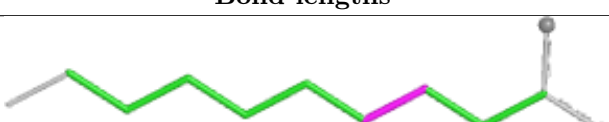
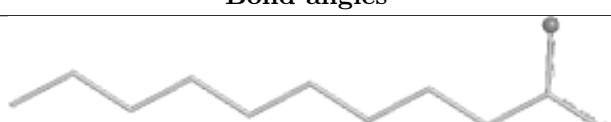


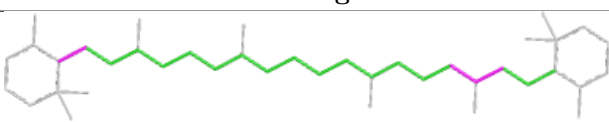
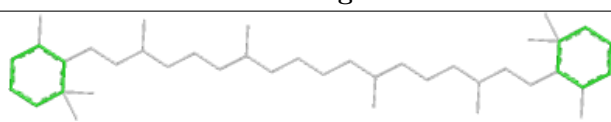
Ligand CLA b 602

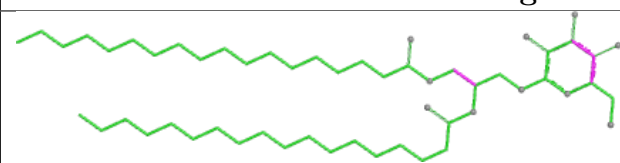
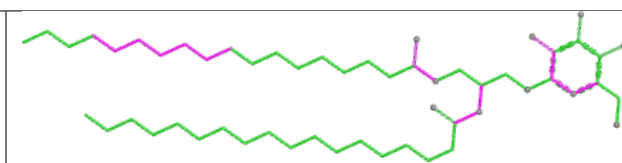
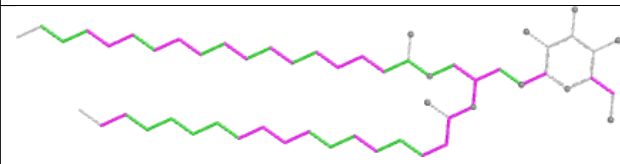
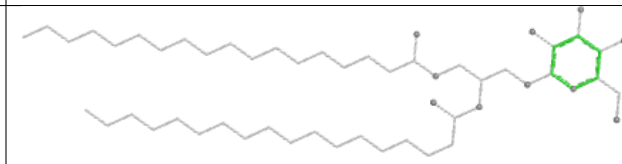


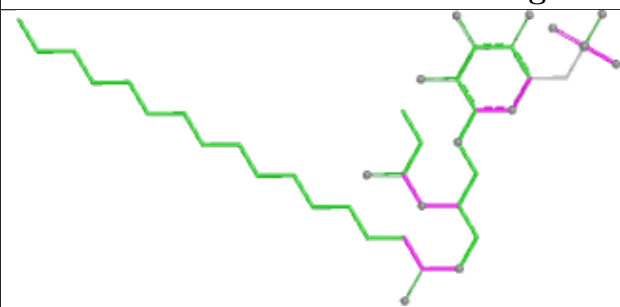
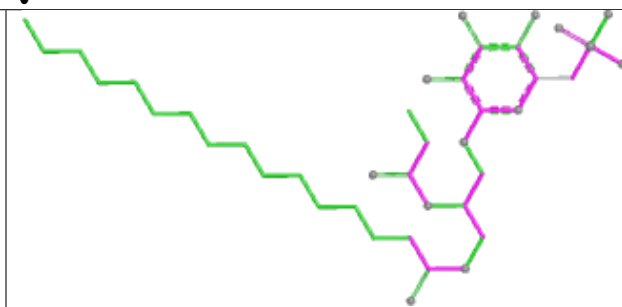
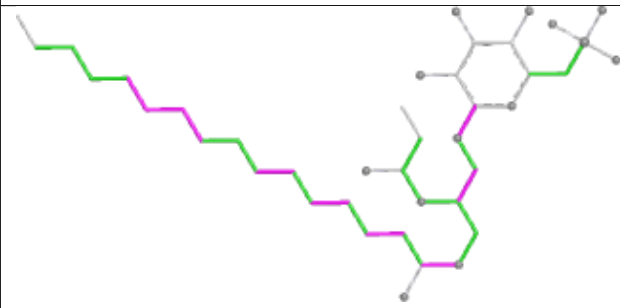
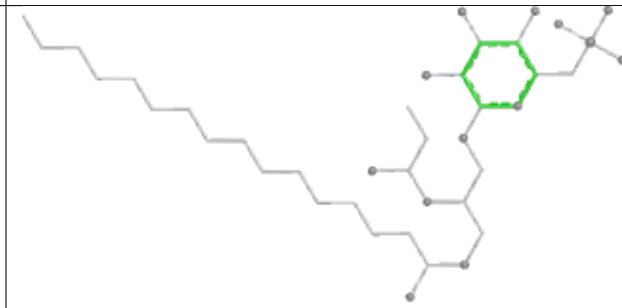
Ligand CLA b 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

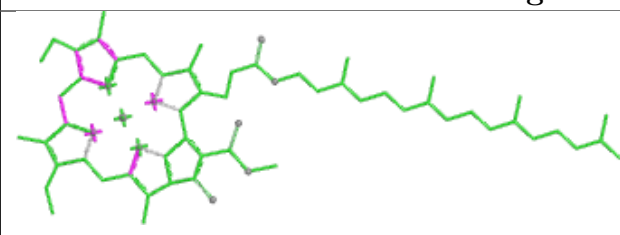
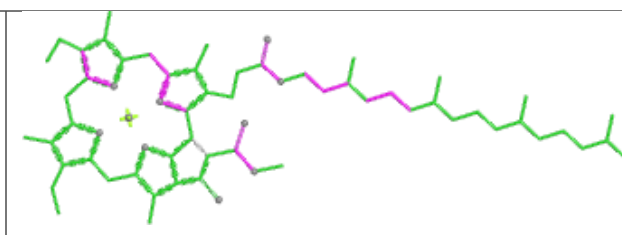
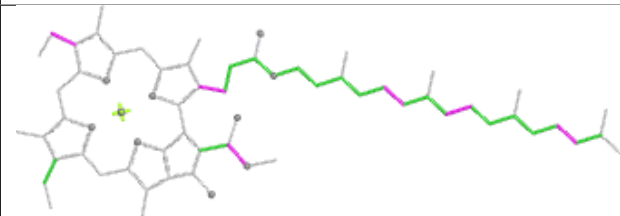
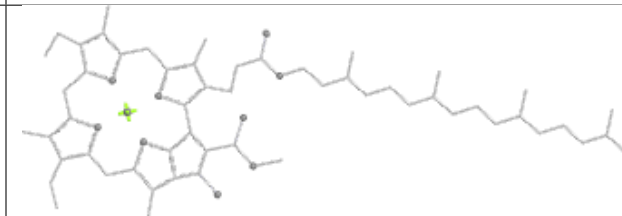
Ligand STE j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

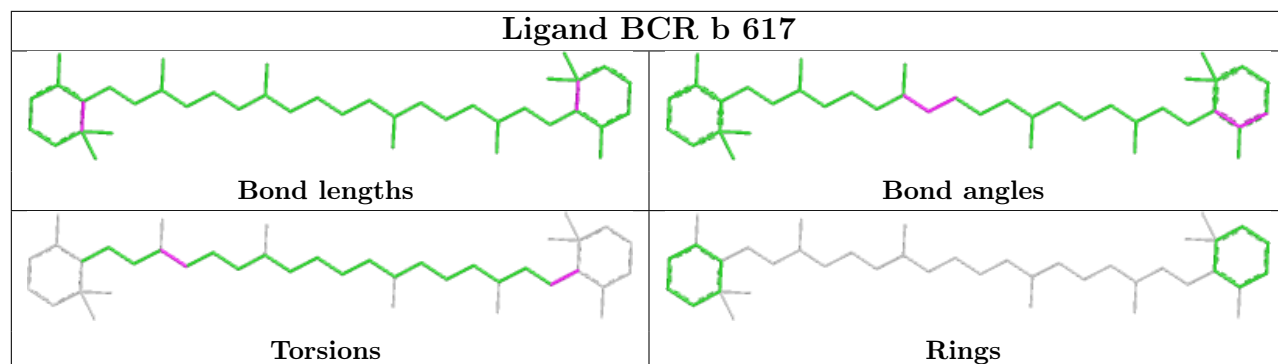
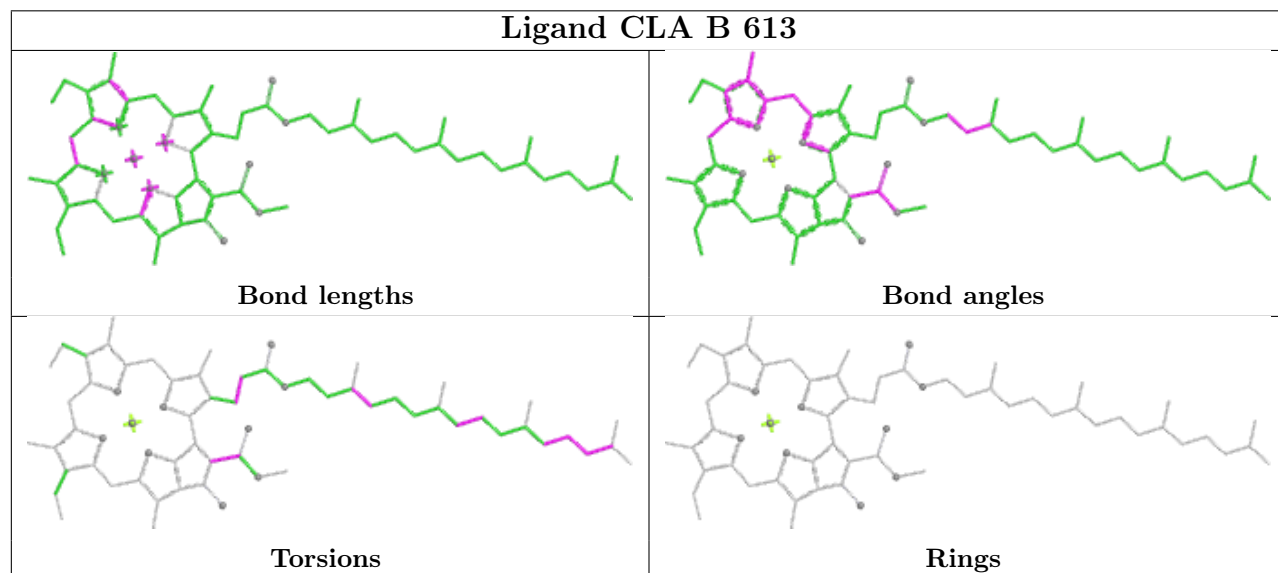
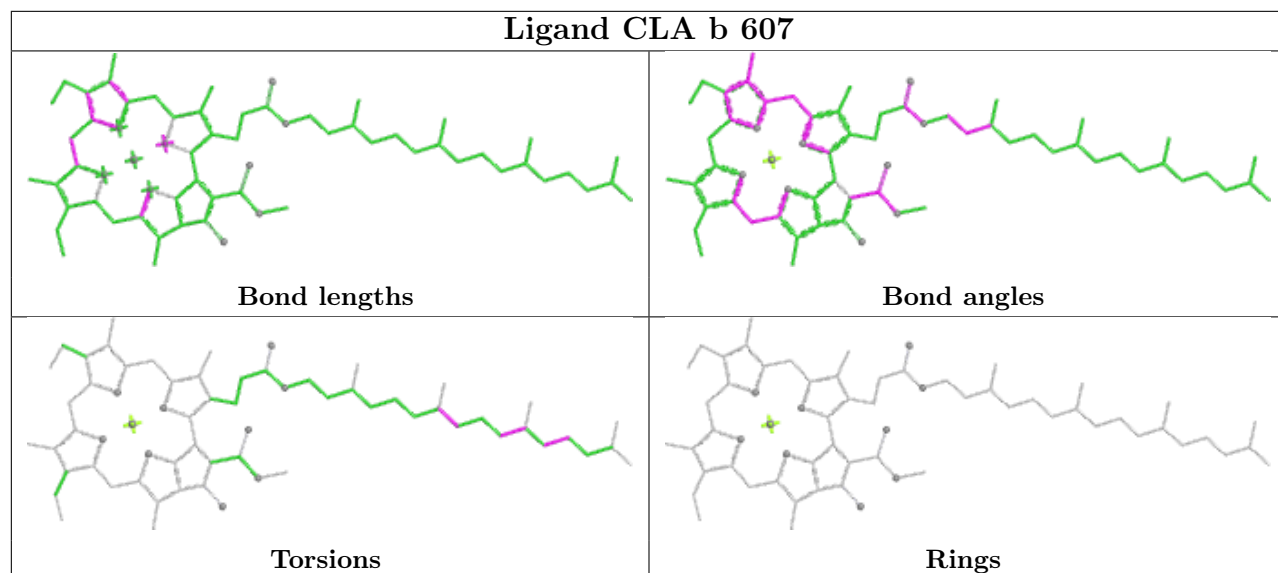
Ligand STE B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

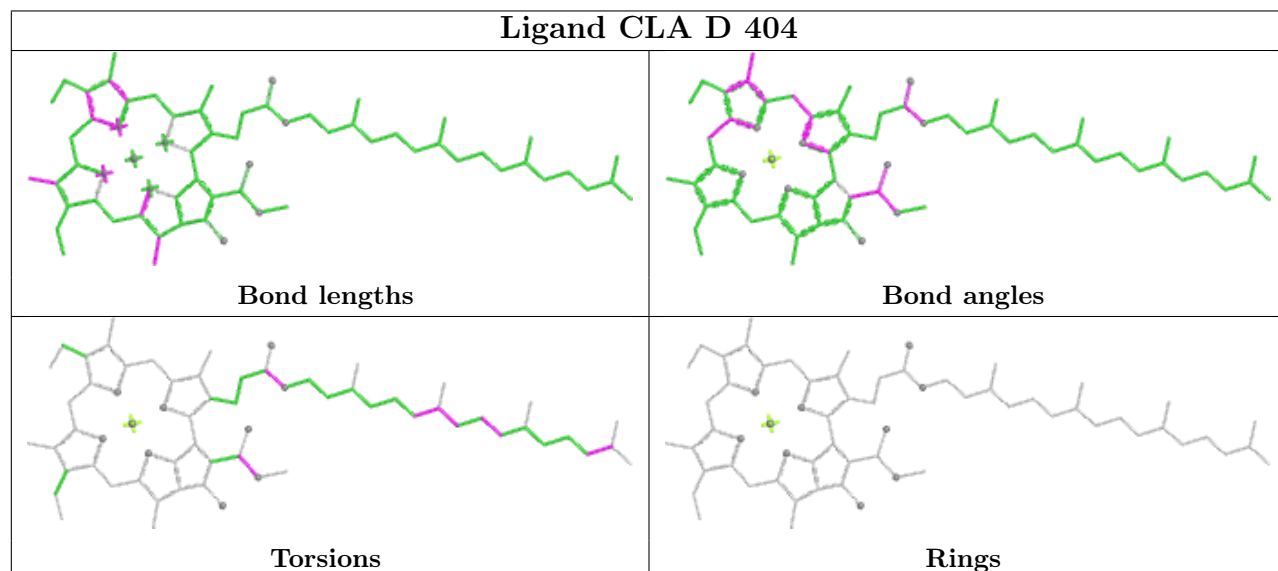
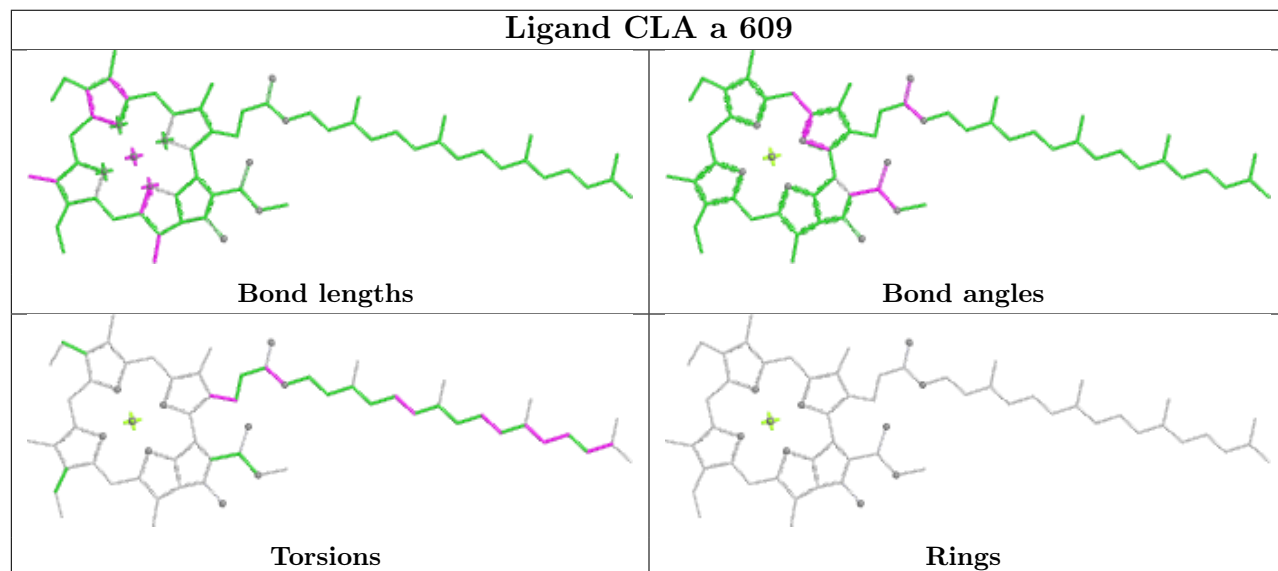
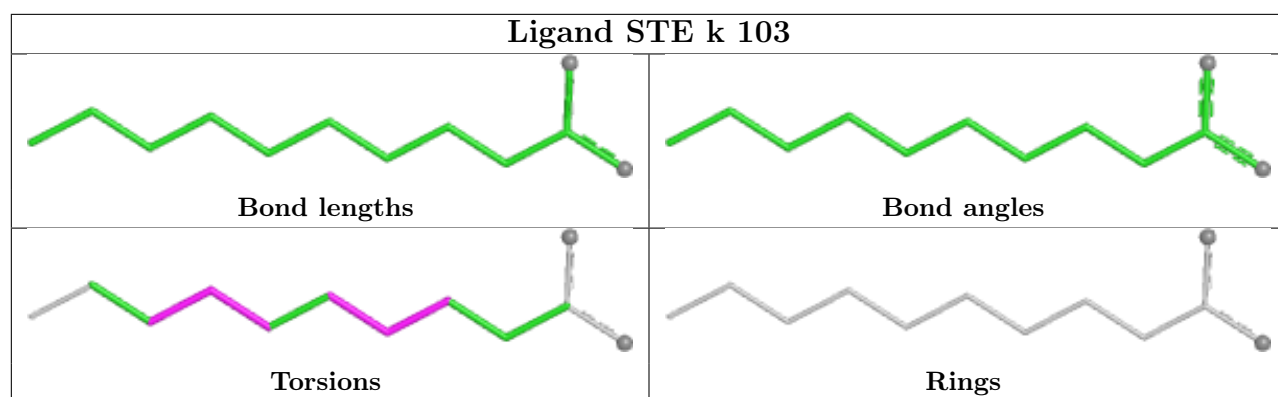
Ligand BCR b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

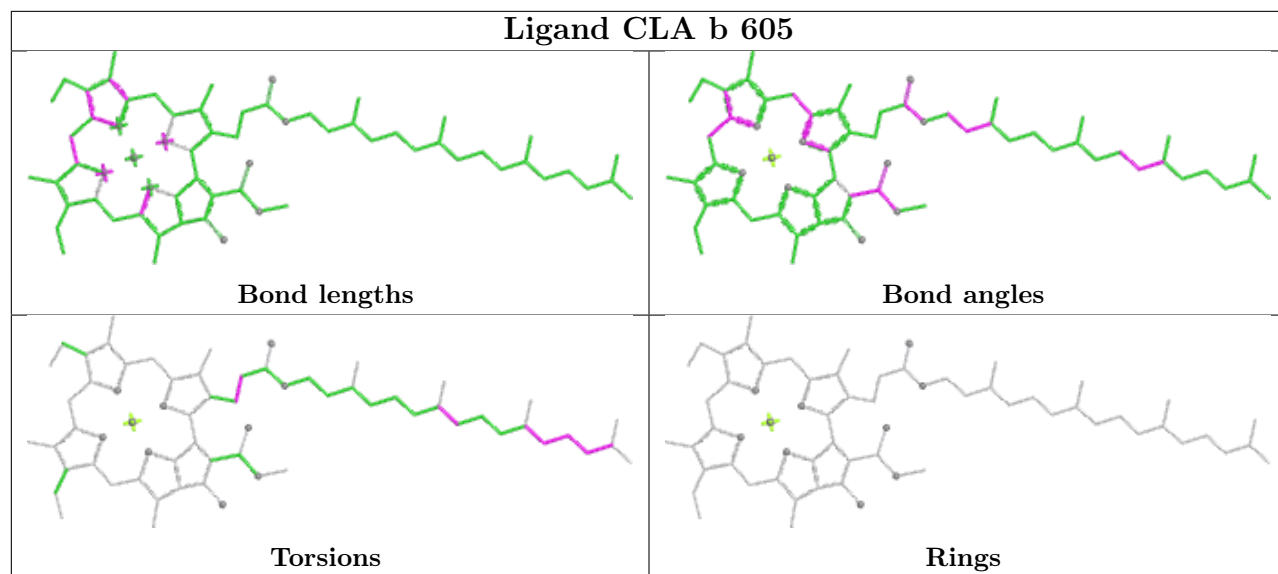
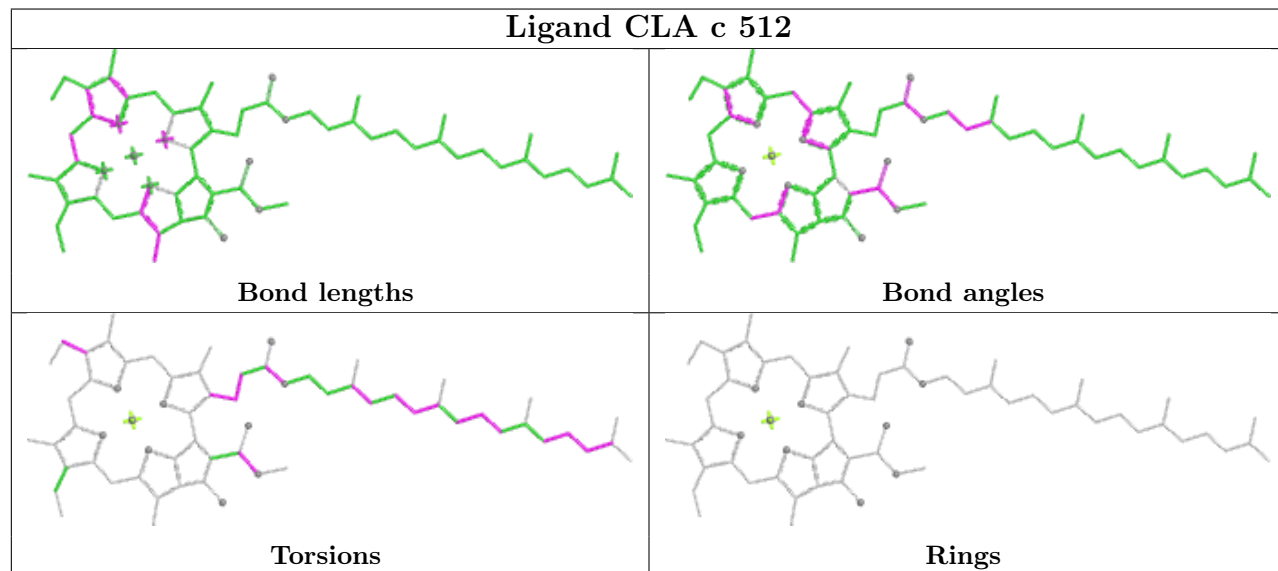
Ligand LMG b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

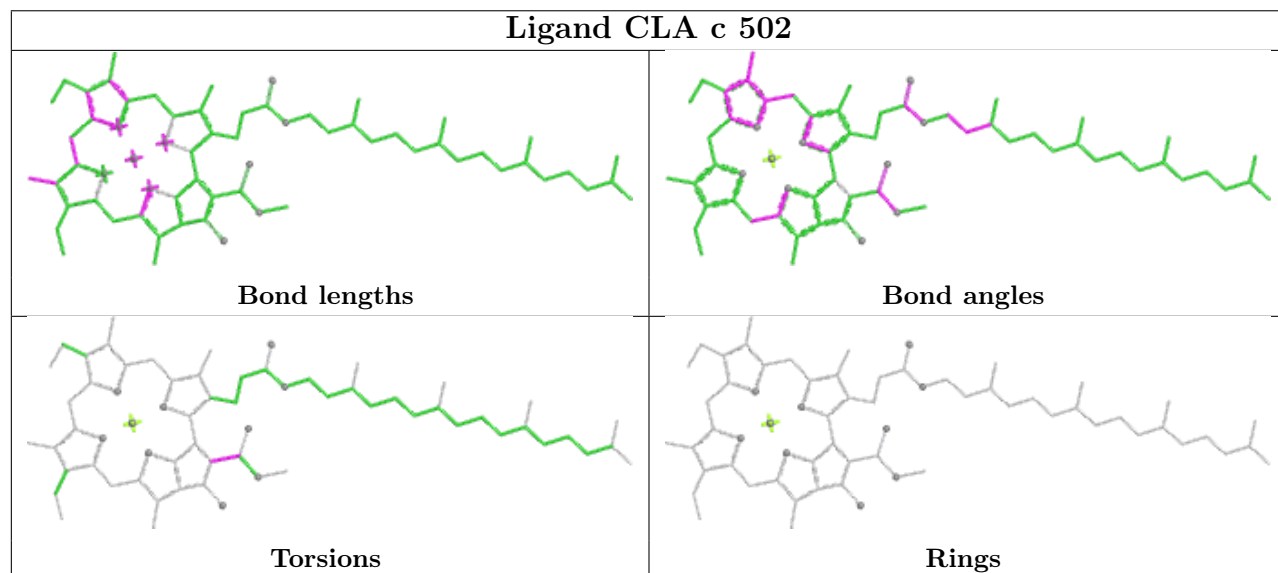
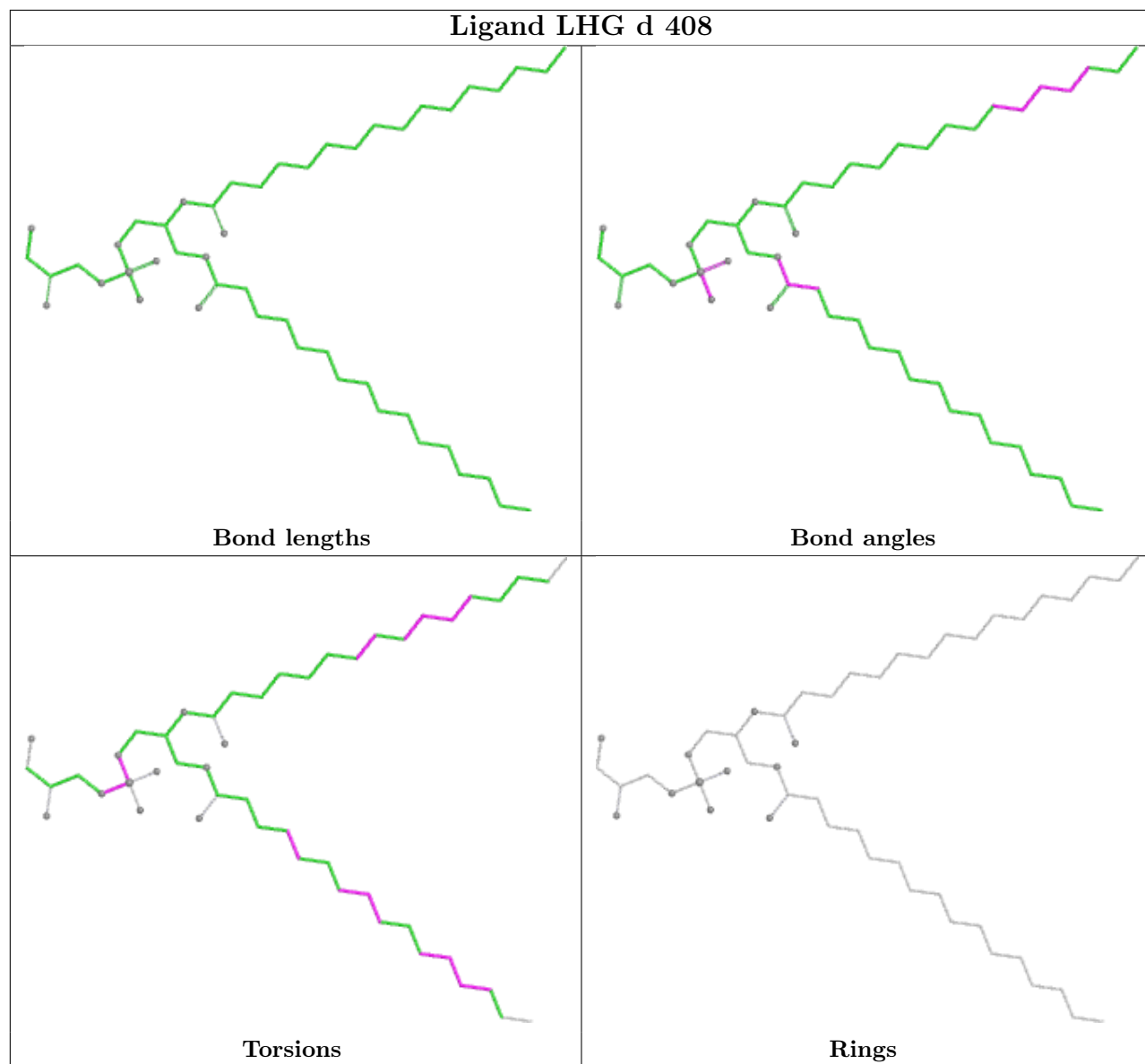
Ligand SQD f 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

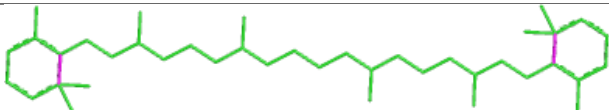
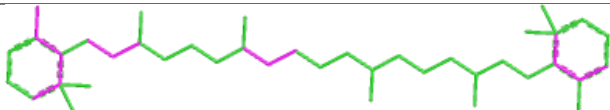
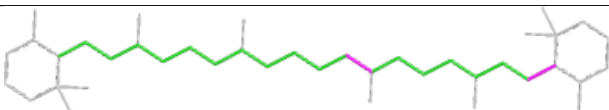
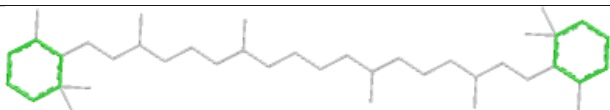
Ligand CLA c 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

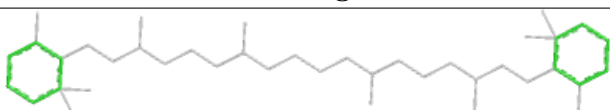
Ligand BCR b 617**Ligand CLA B 613****Ligand CLA b 607**

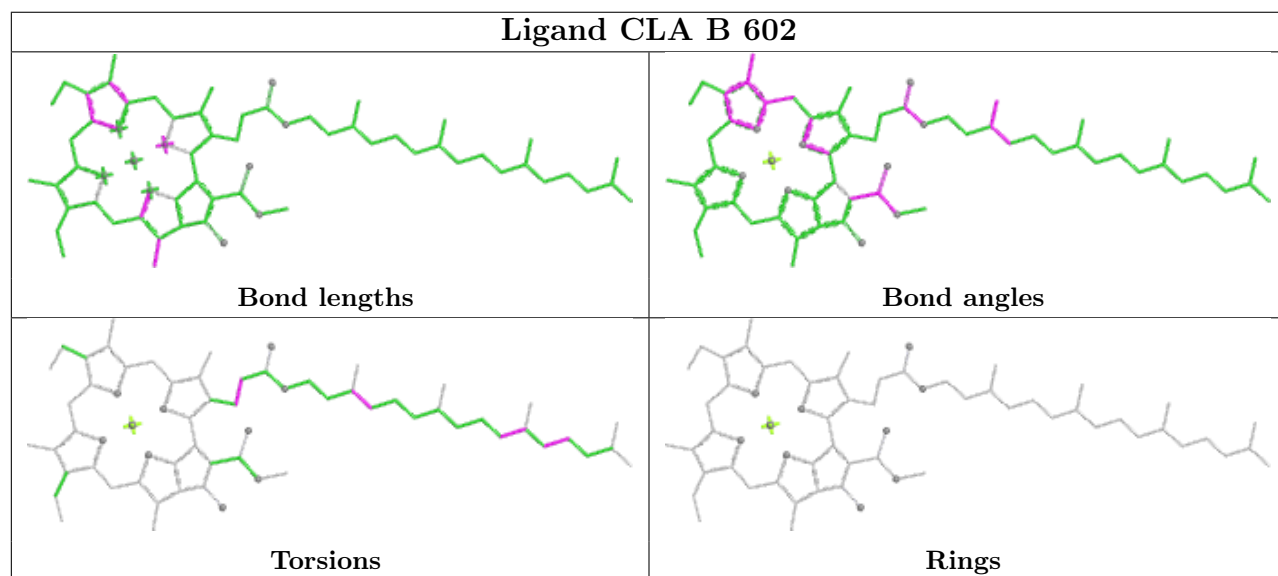
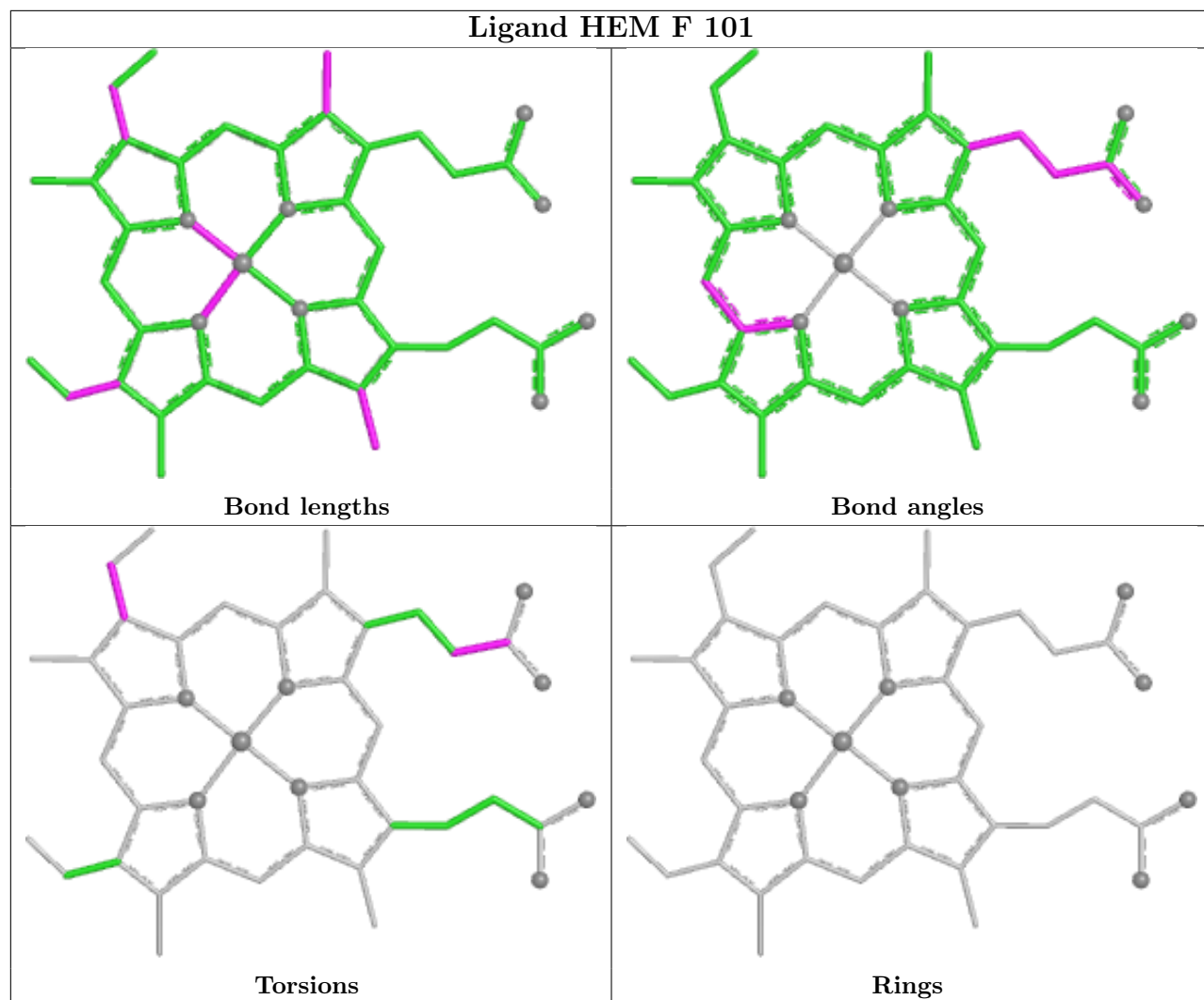


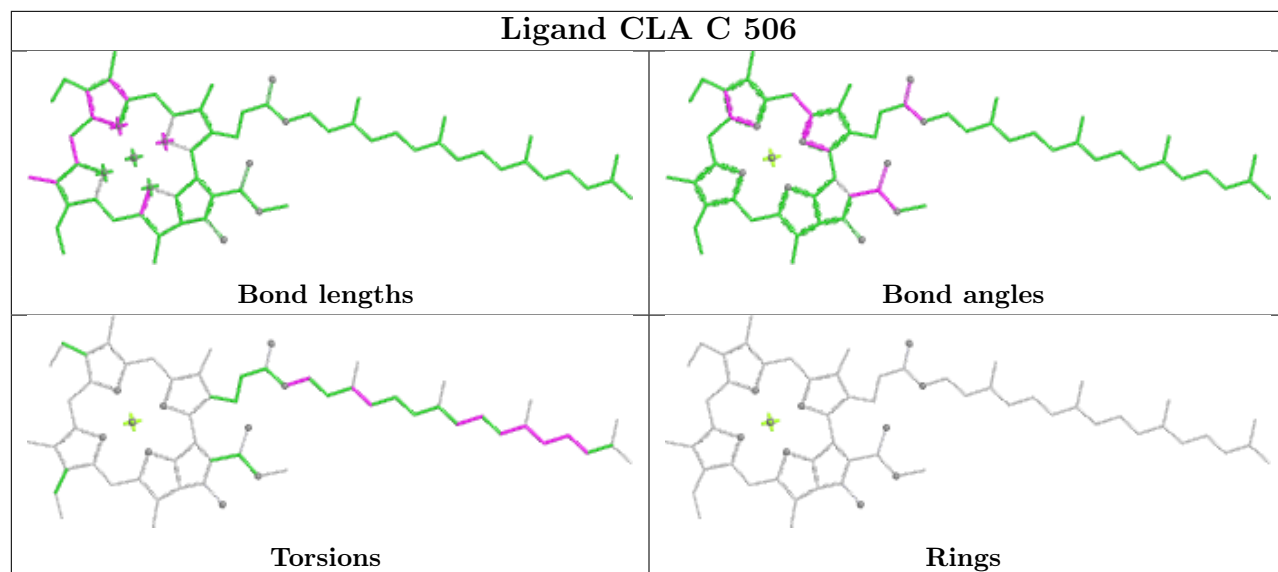
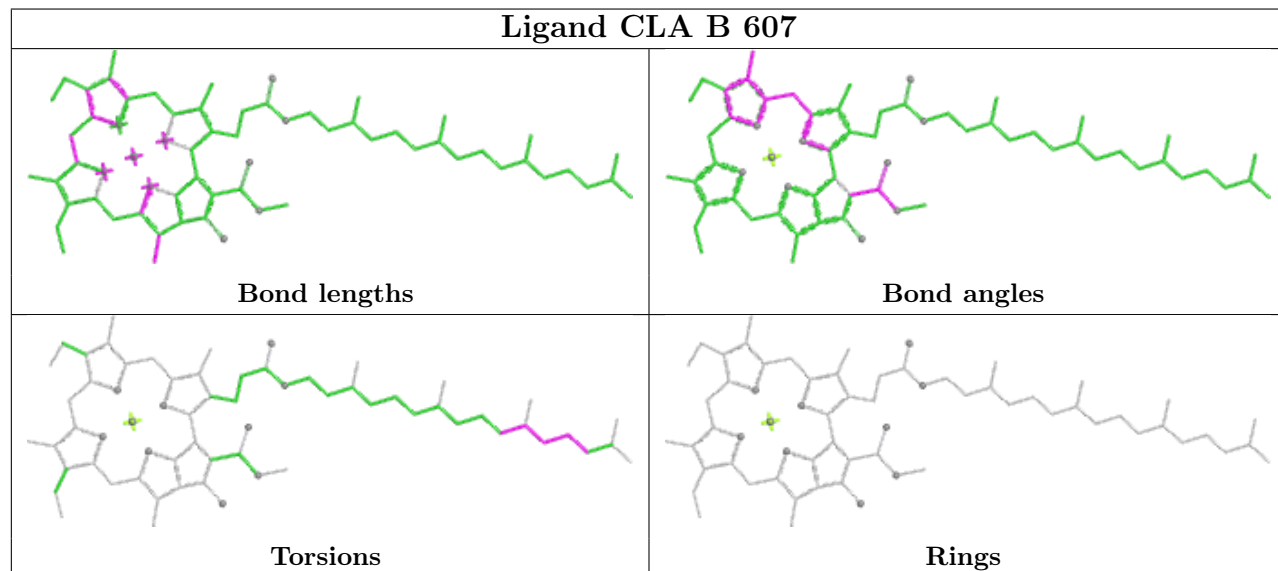
Ligand CLA b 605**Ligand CLA c 512**

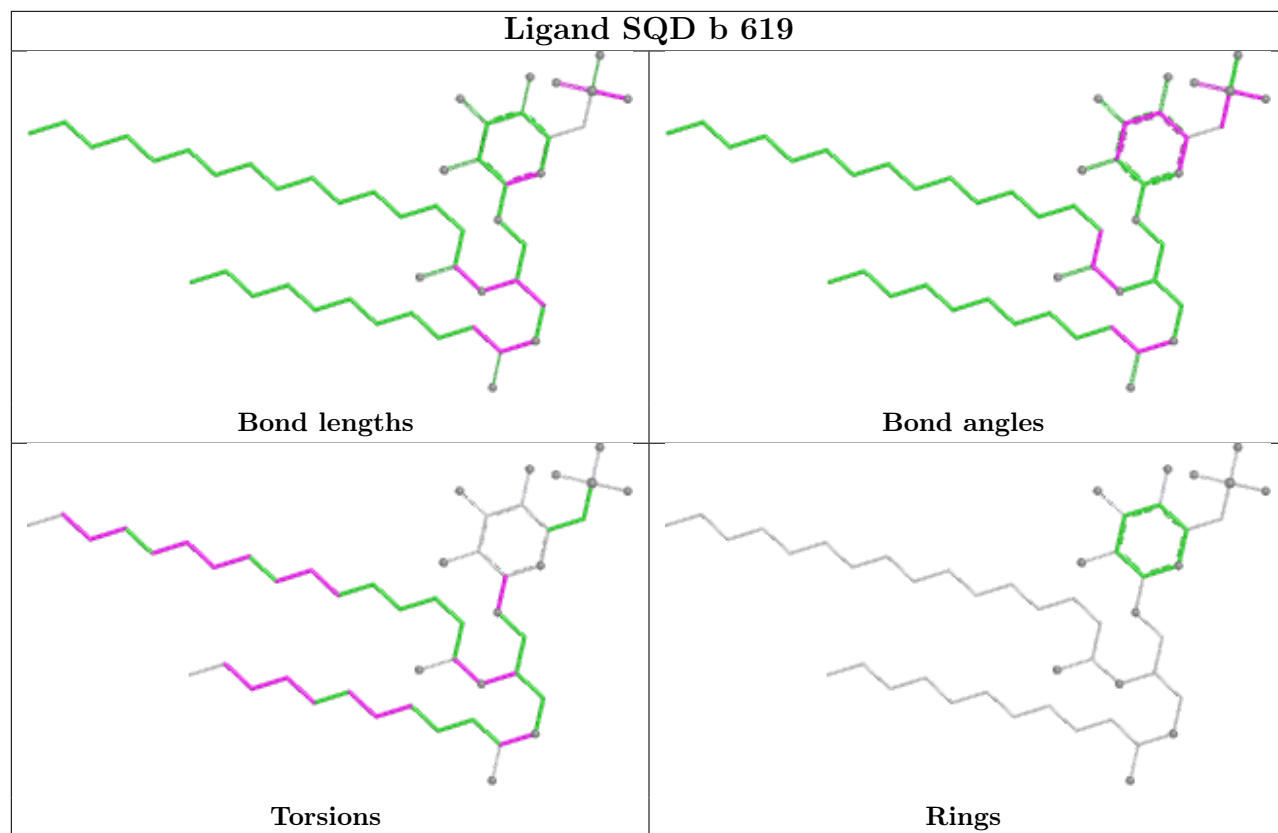


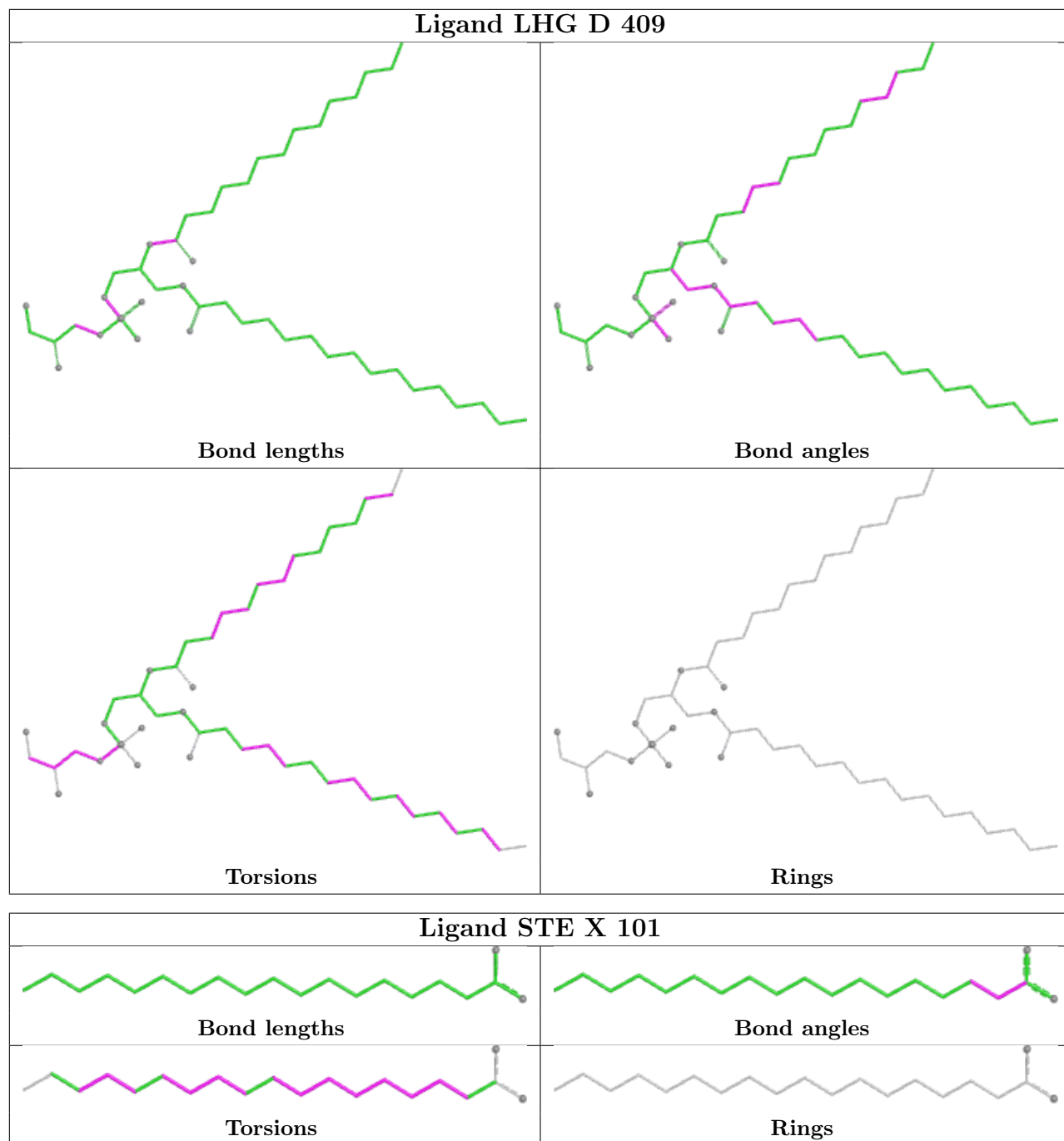
Ligand BCR c 514	
	Bond lengths
	Bond angles
	Torsions
	Rings

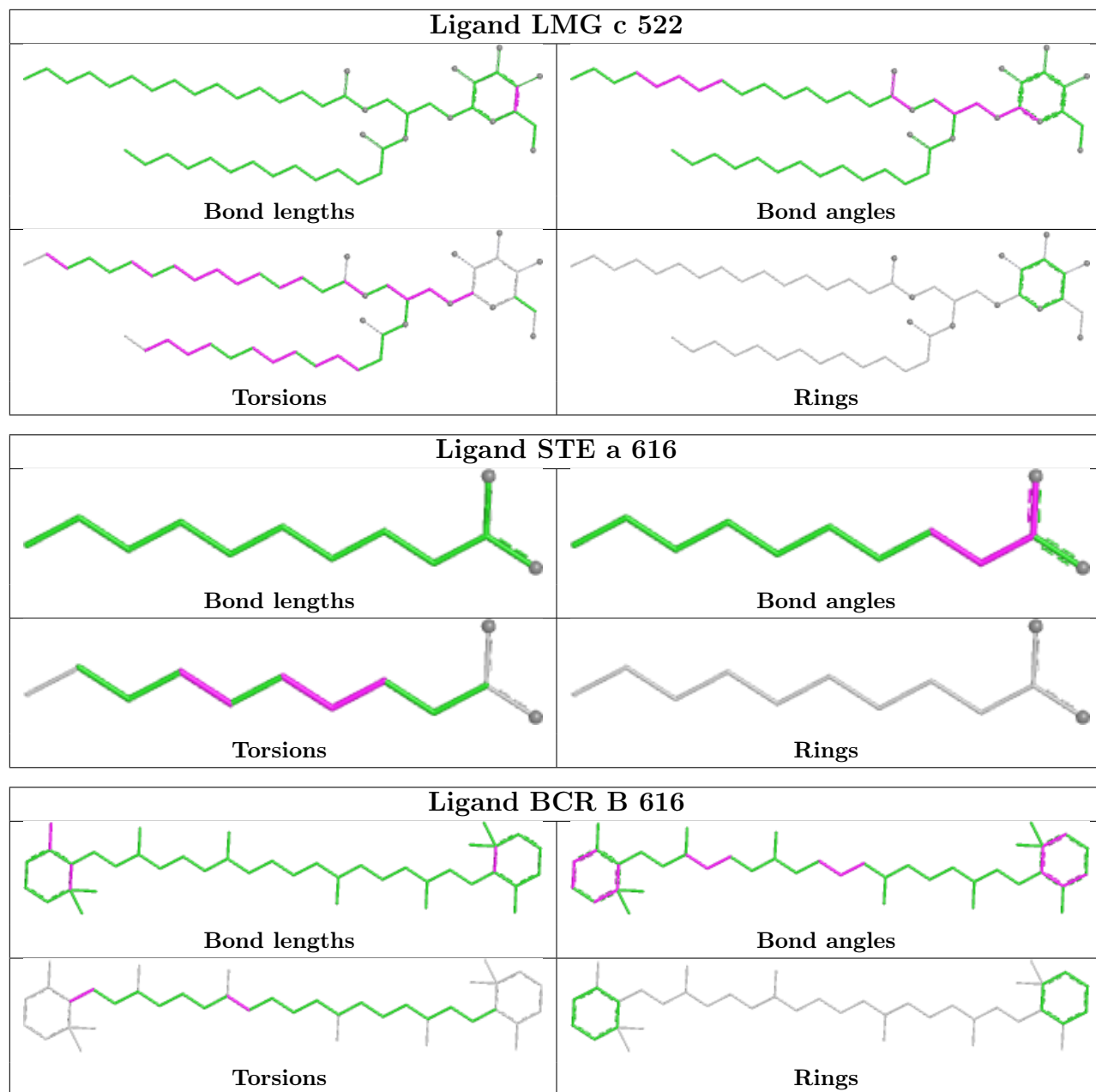
Ligand BCR h 102	
	Bond lengths
	Bond angles
	Torsions
	Rings

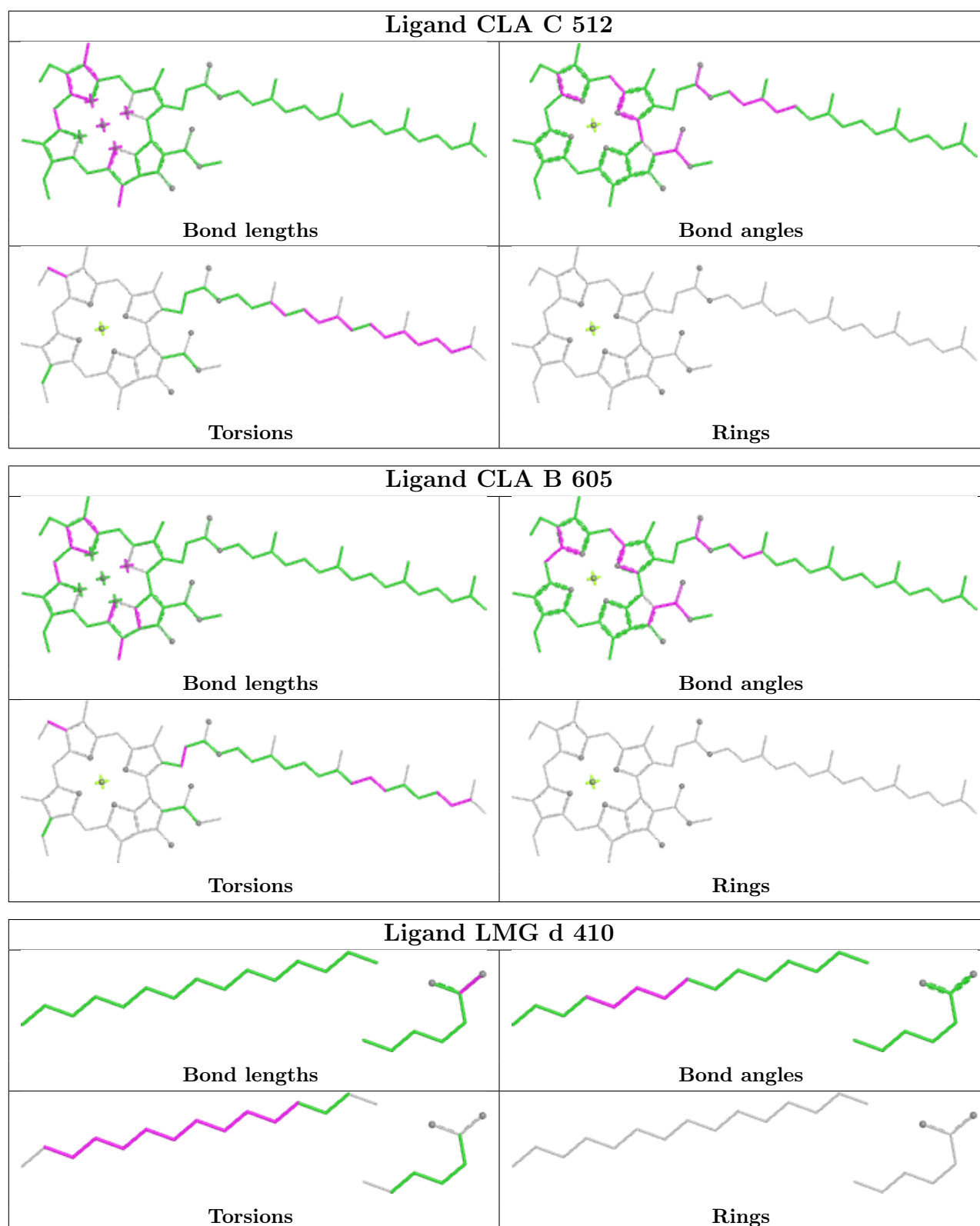


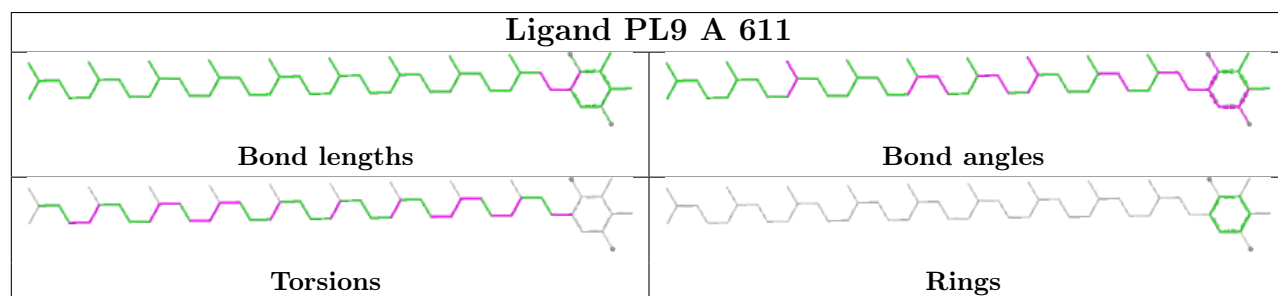
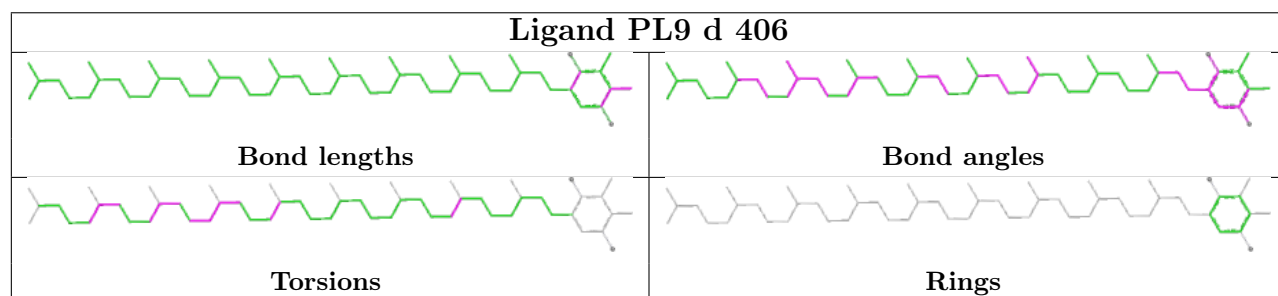
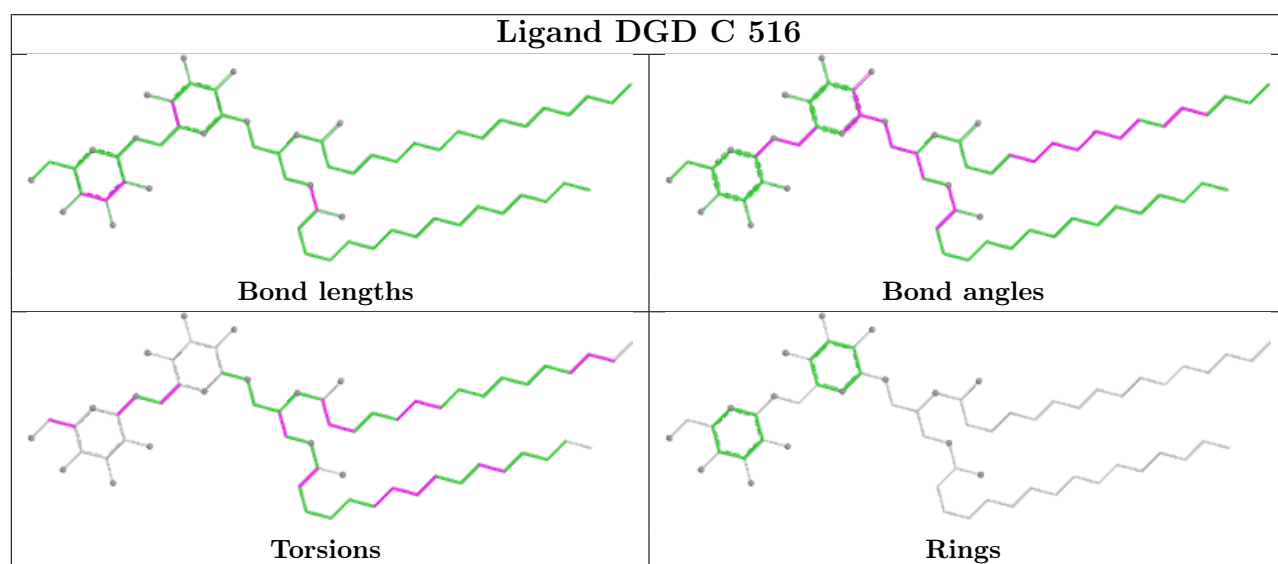
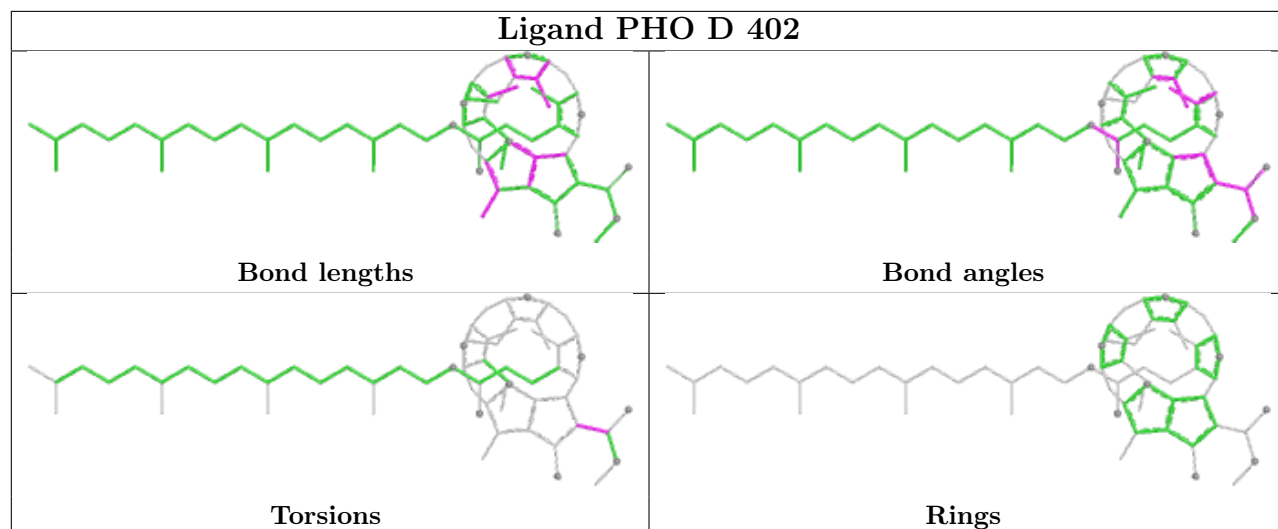
Ligand CLA C 506**Ligand CLA B 607**

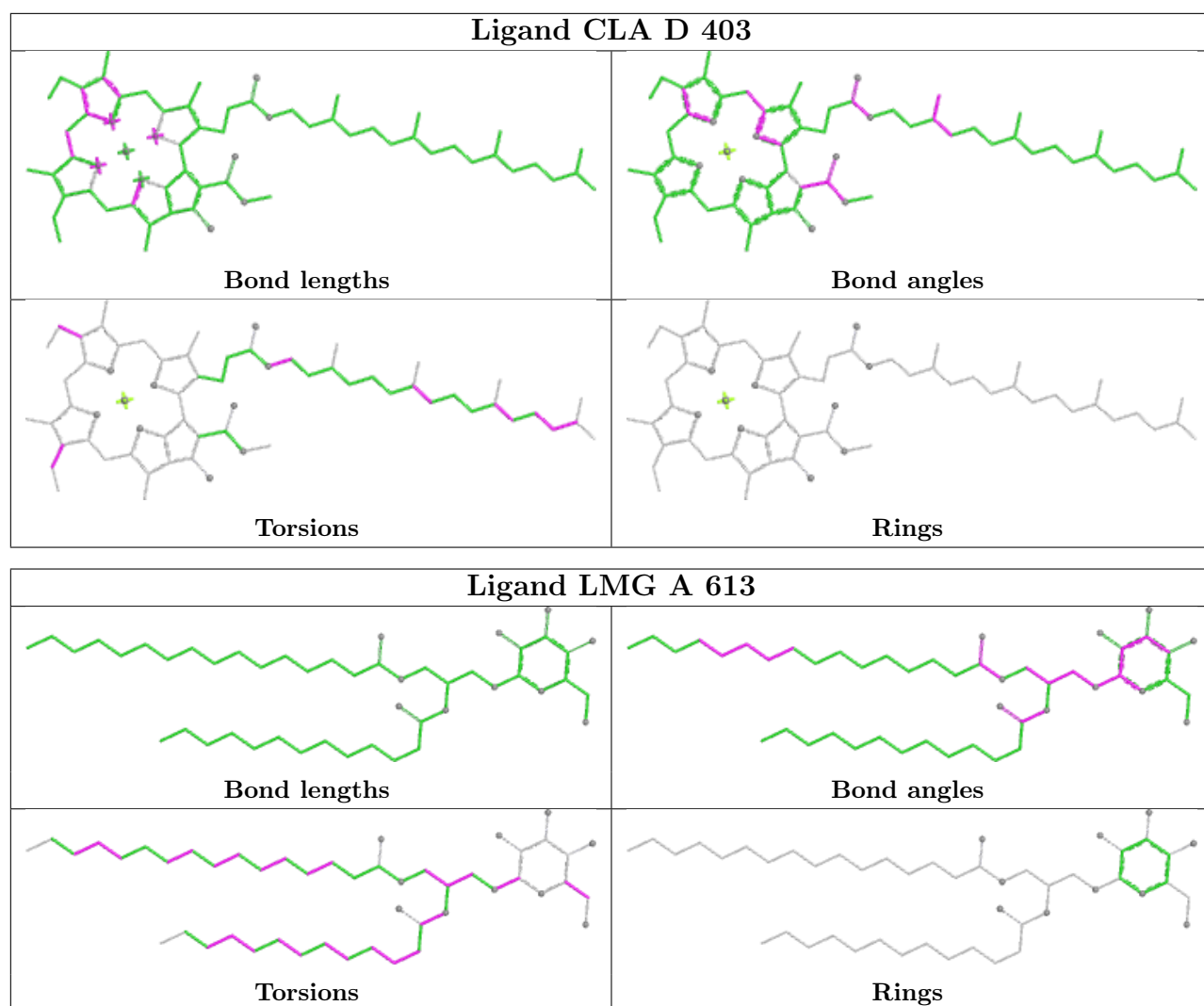


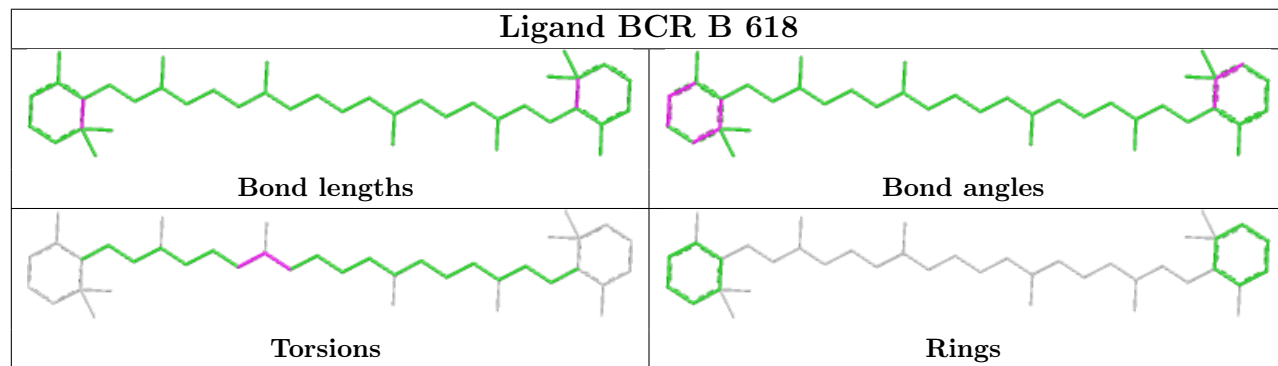
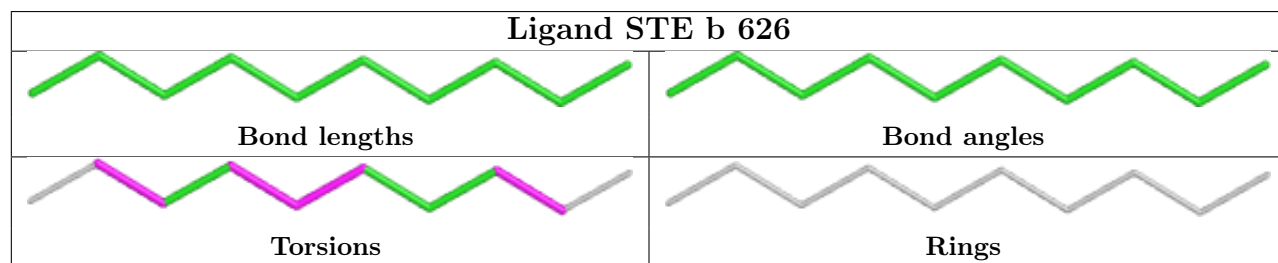
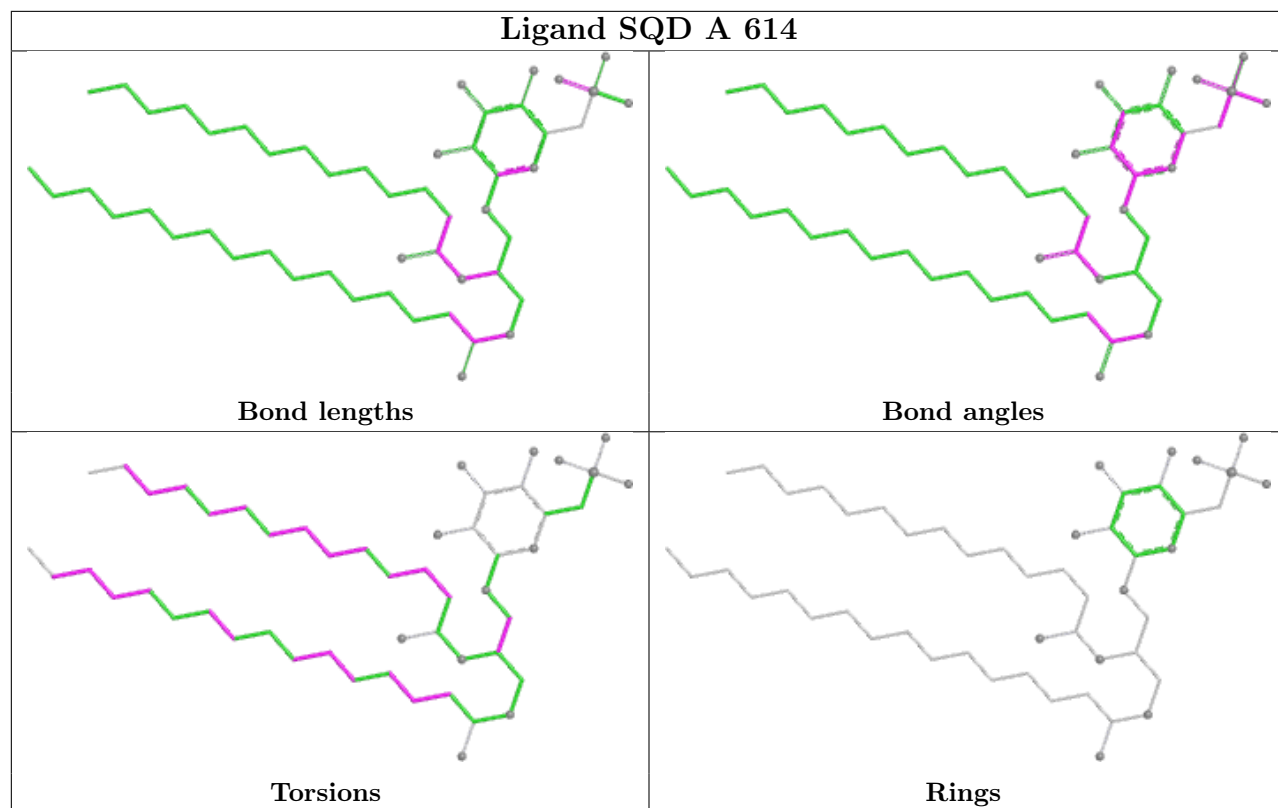


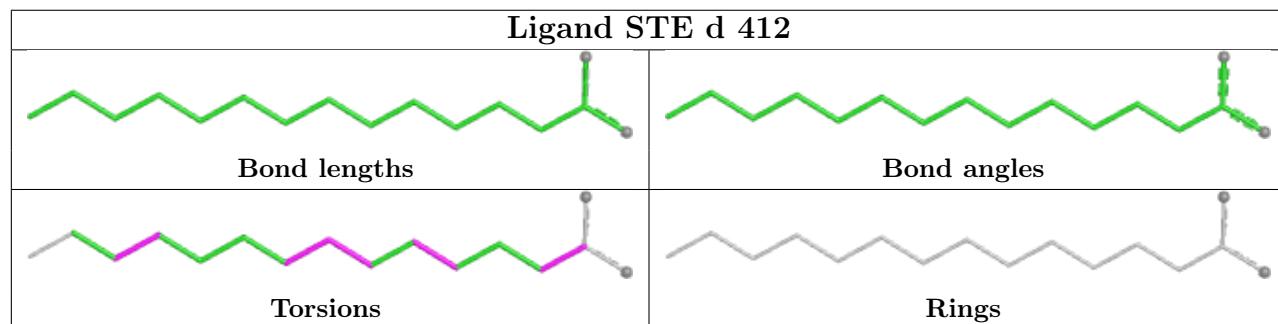
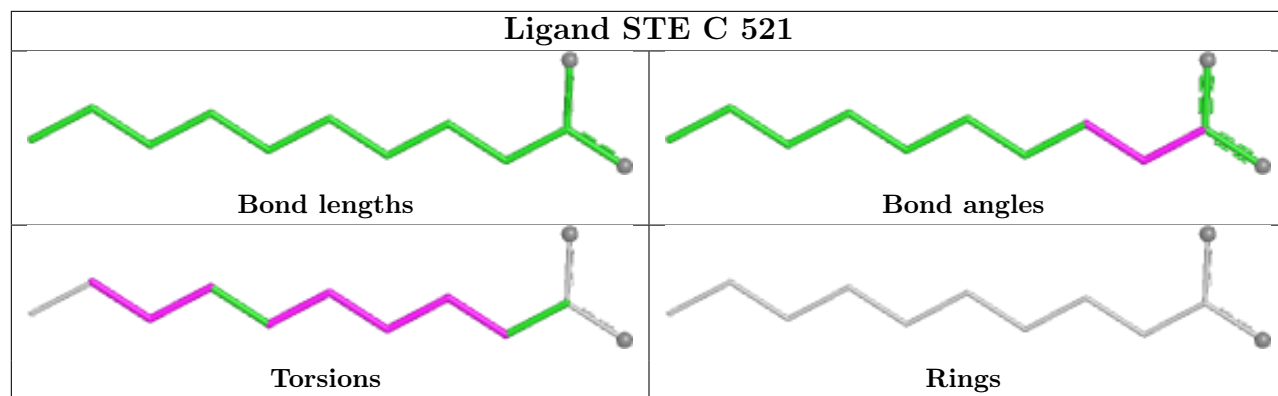




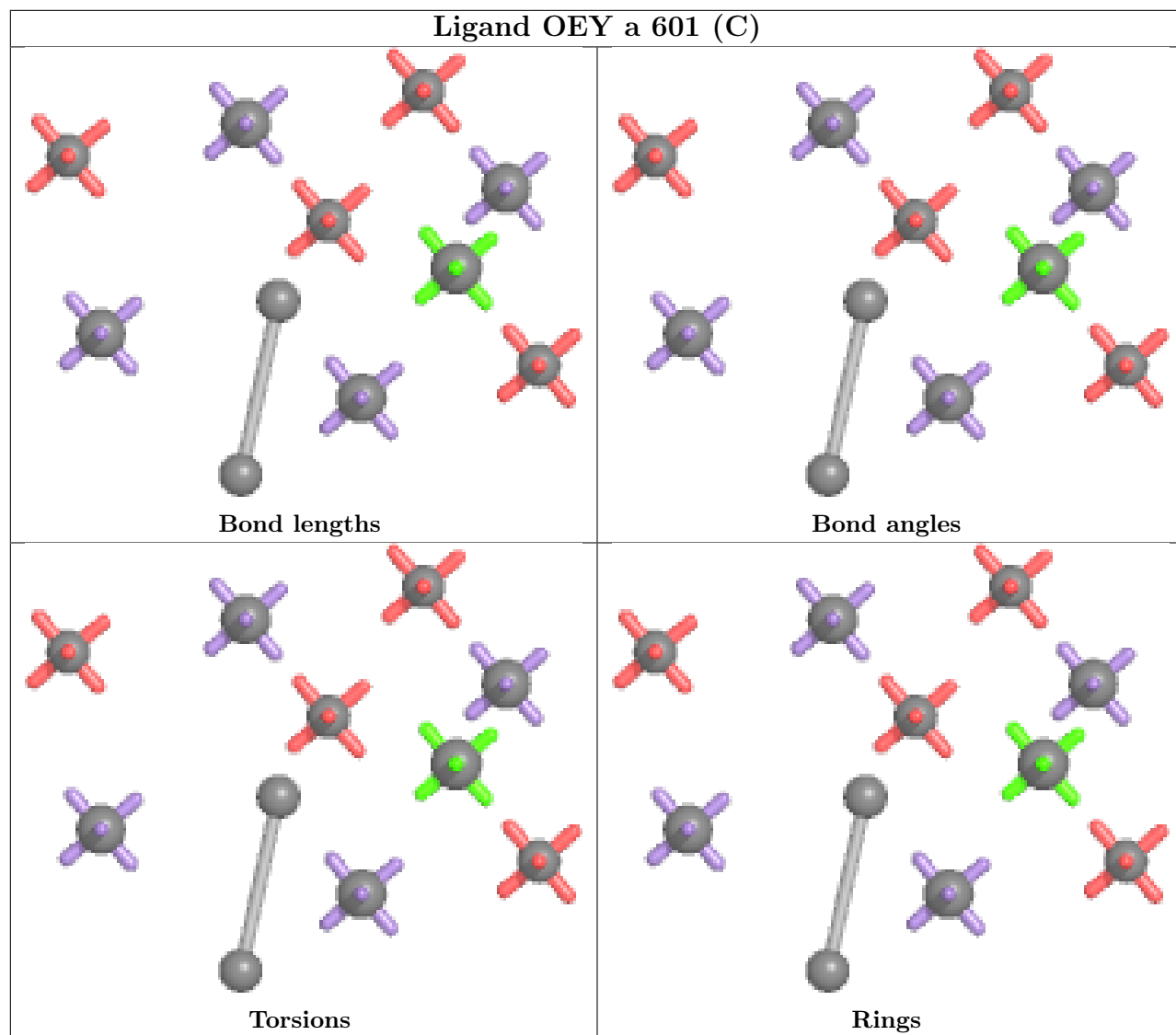


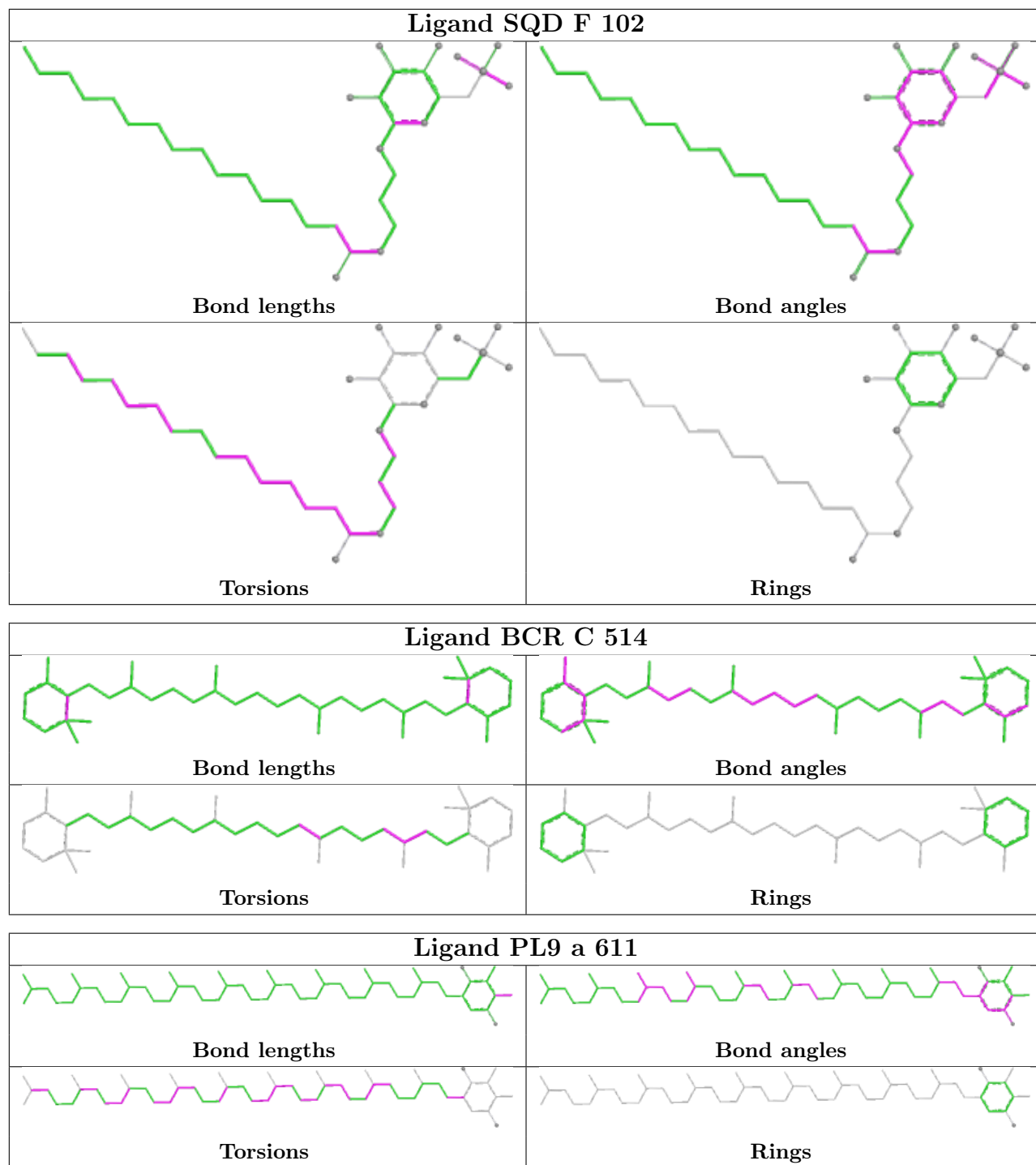


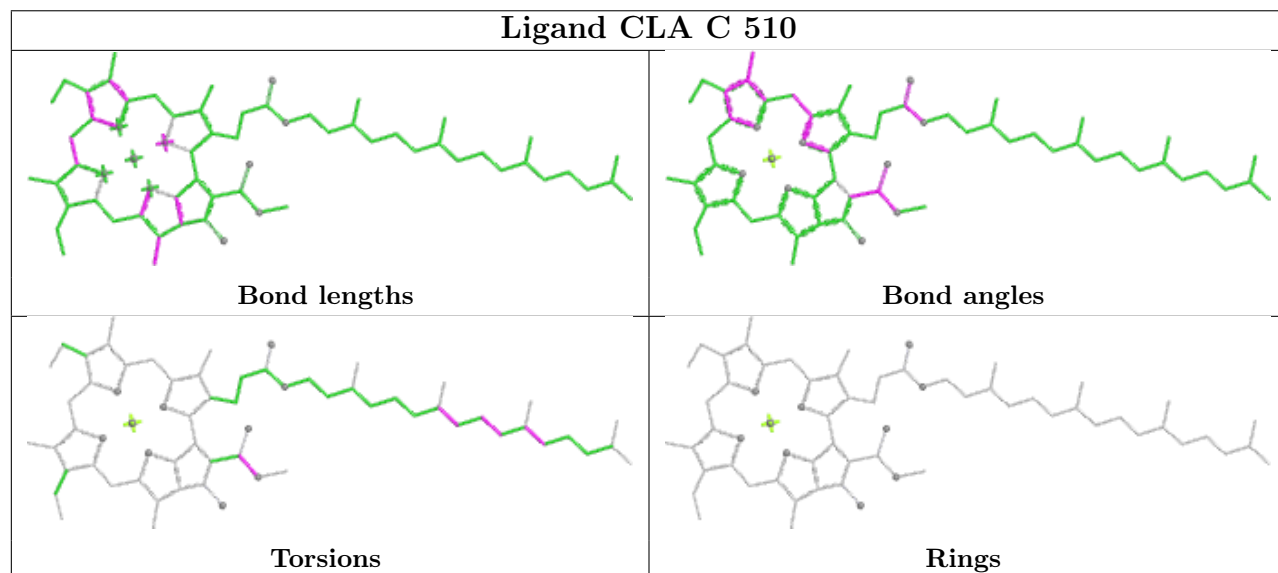
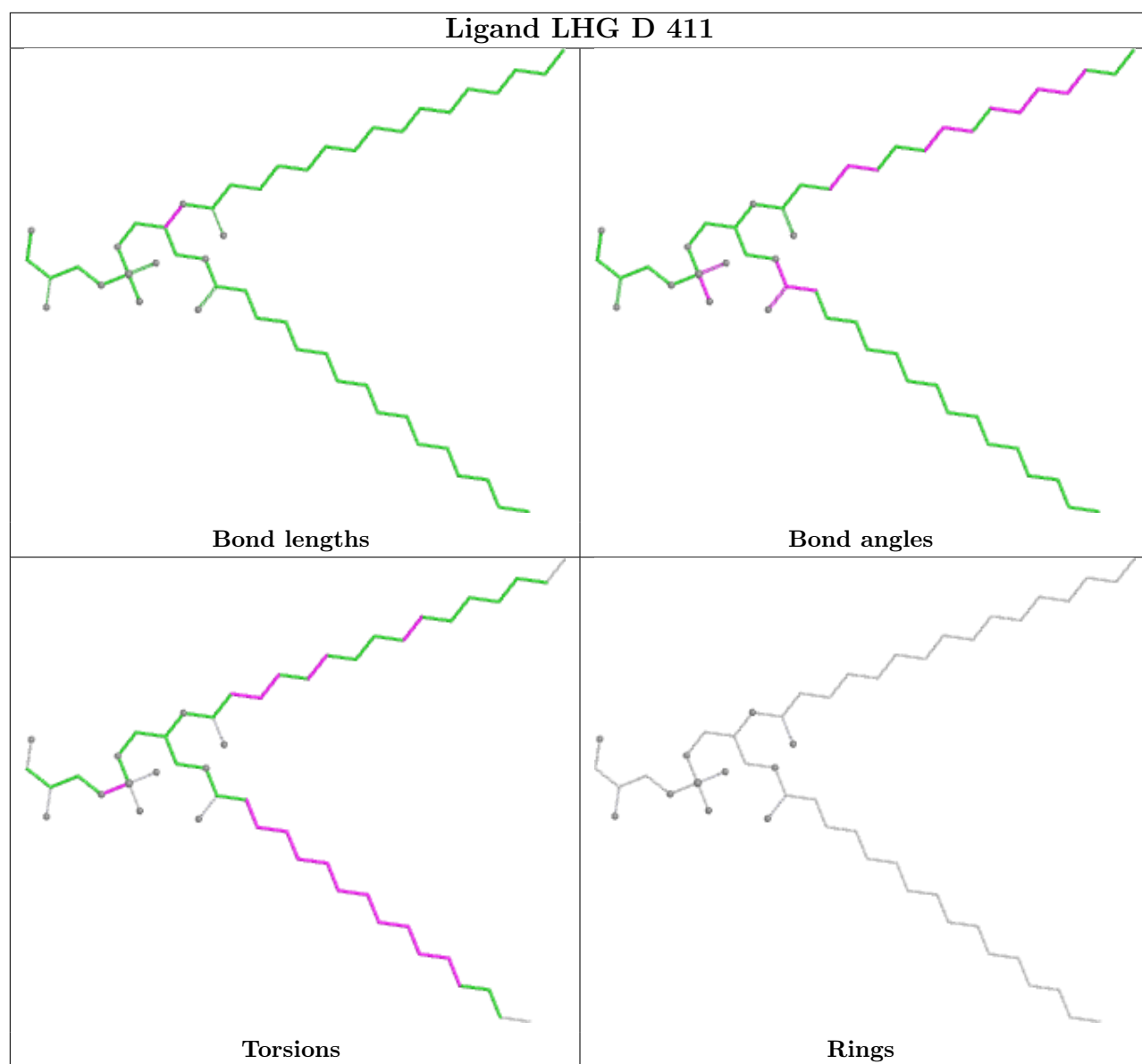


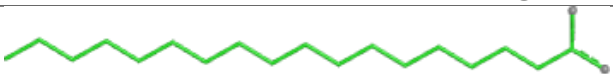
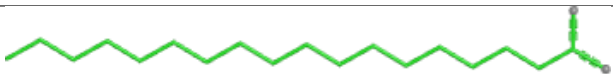
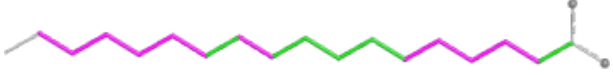


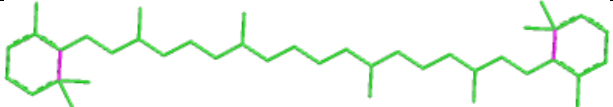
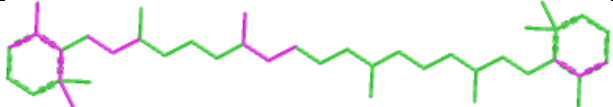
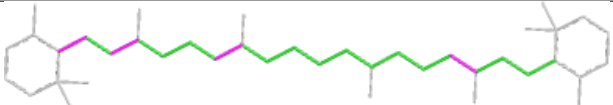
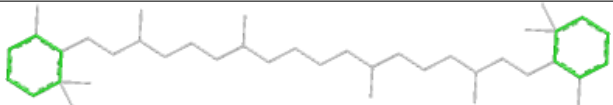
Ligand OEY a 601 (C)

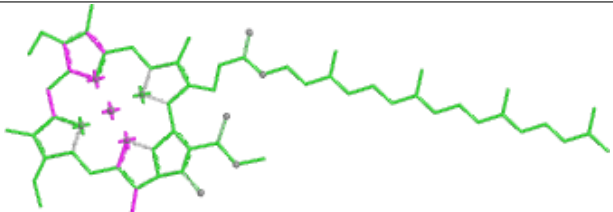
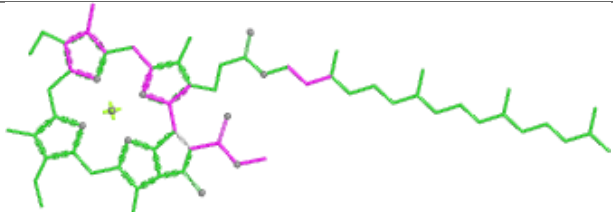
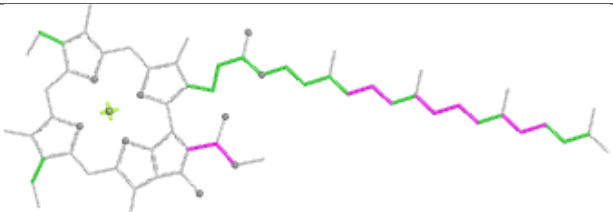
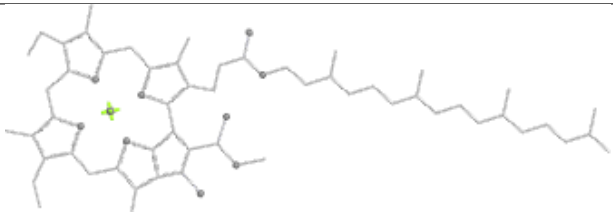


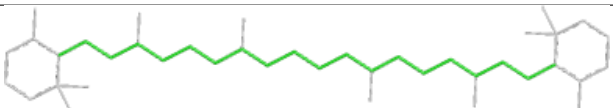
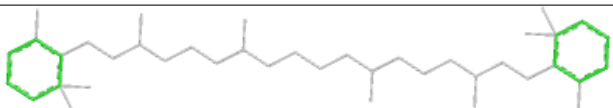


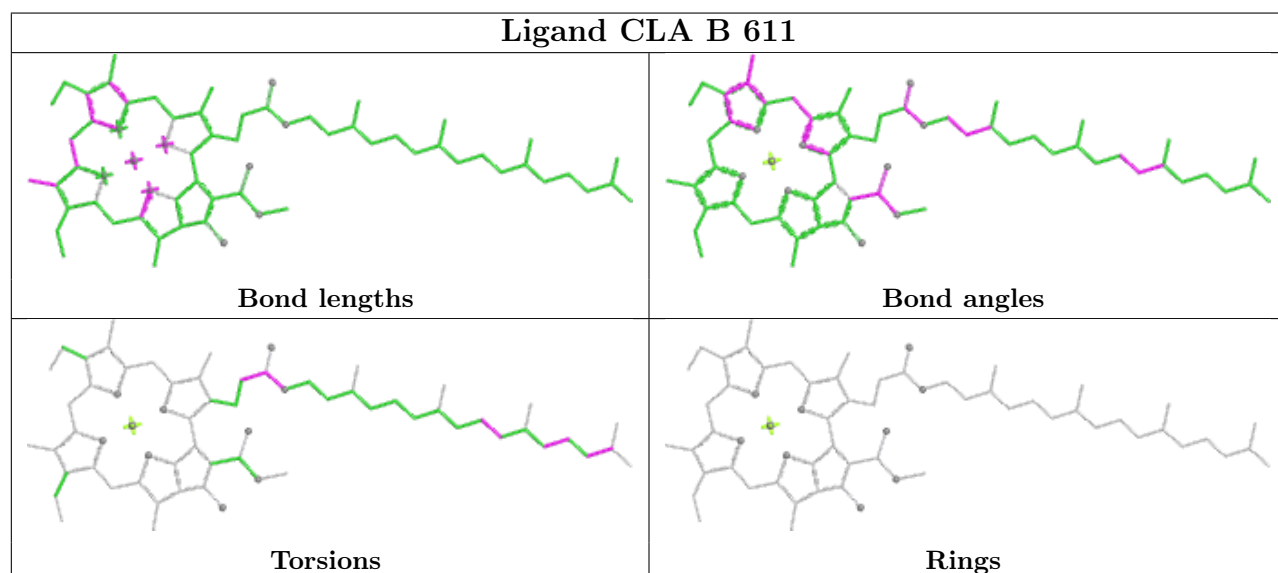
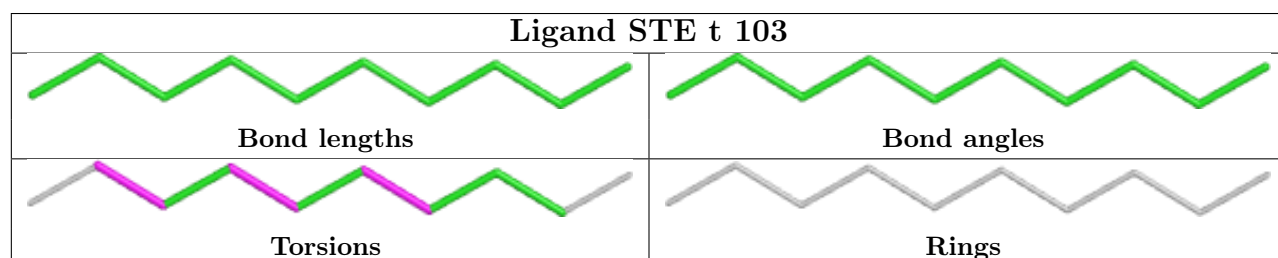
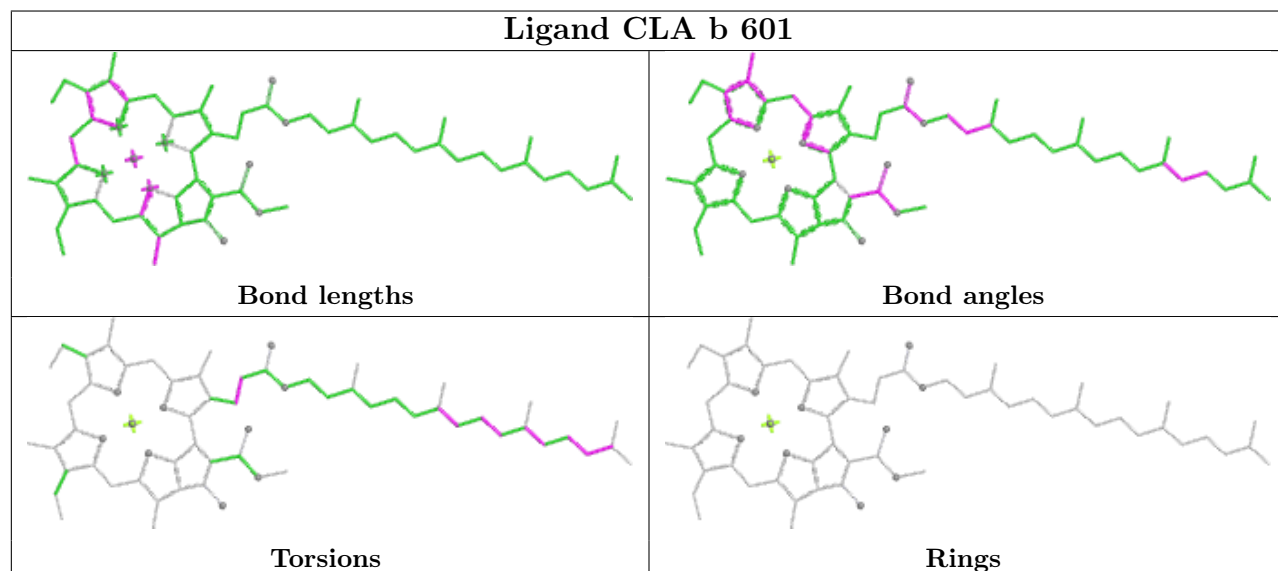
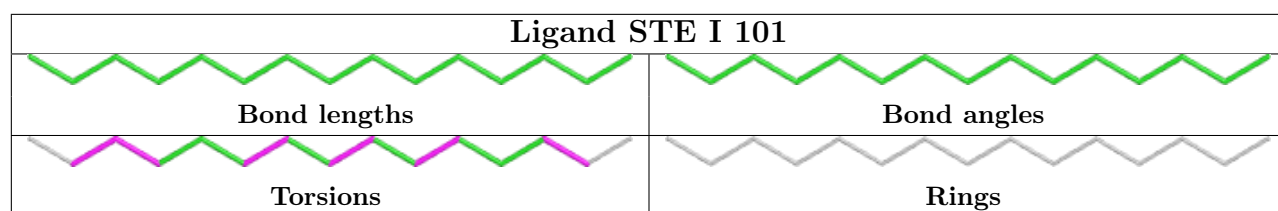


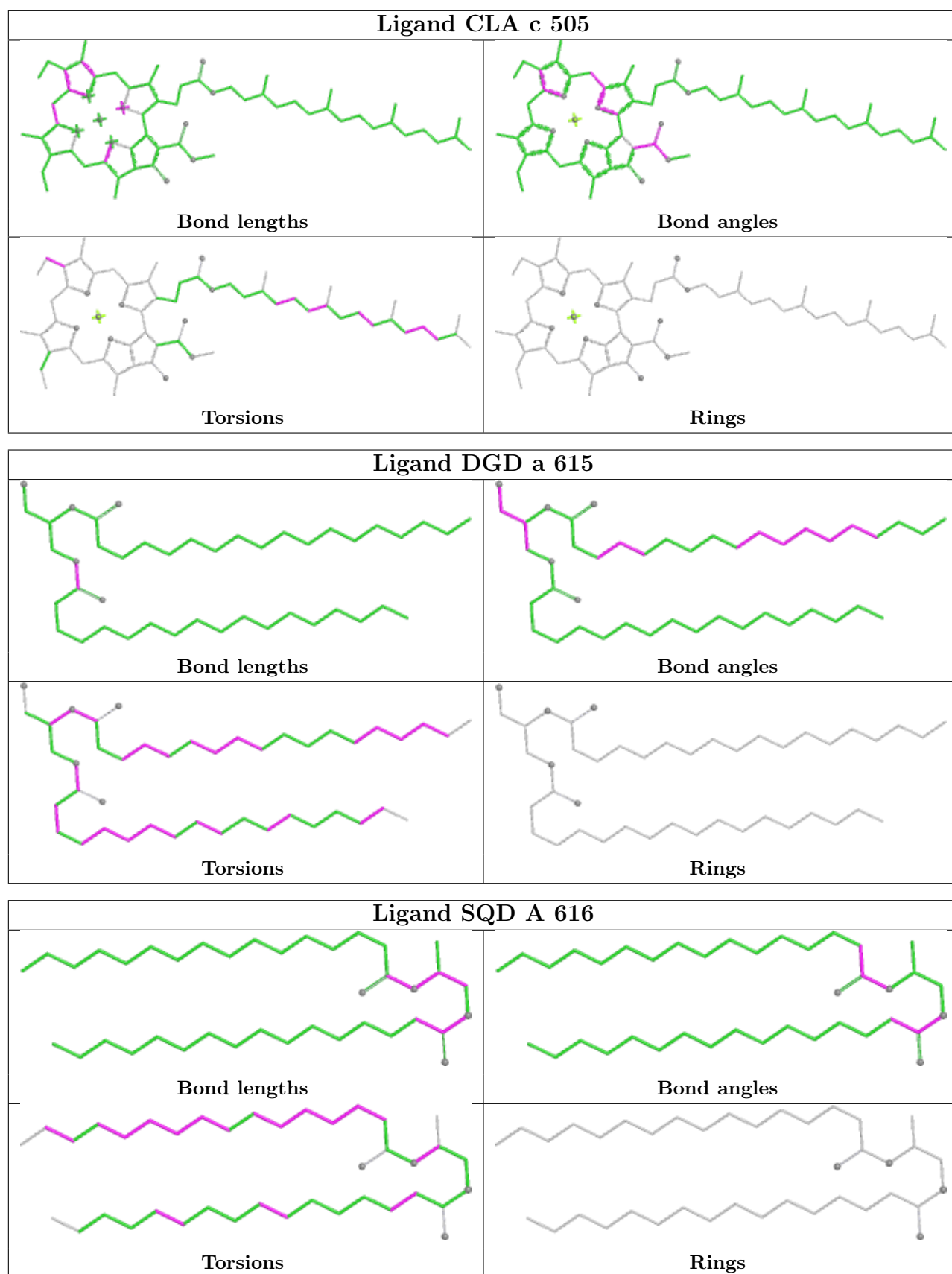
Ligand STE b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

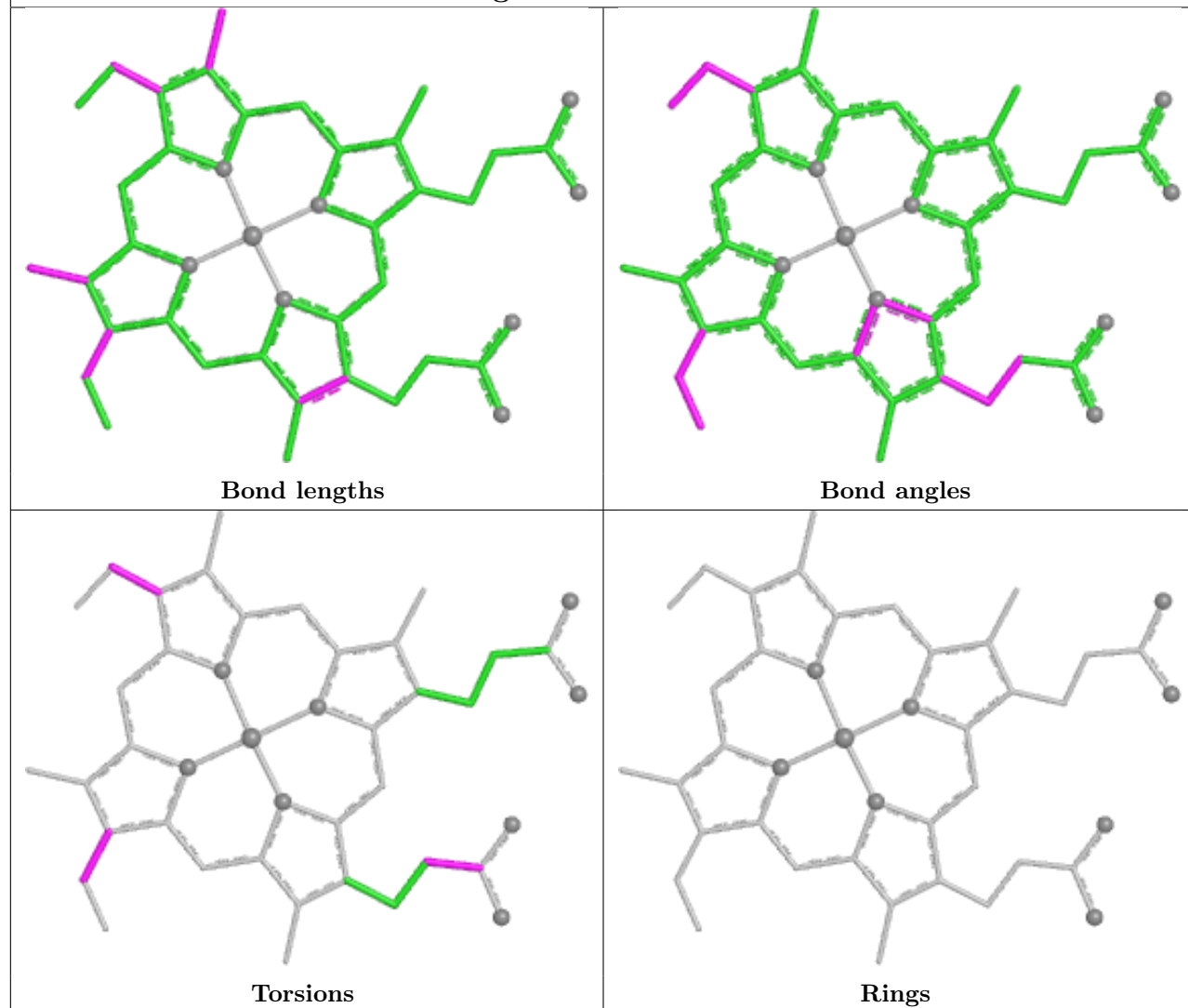
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

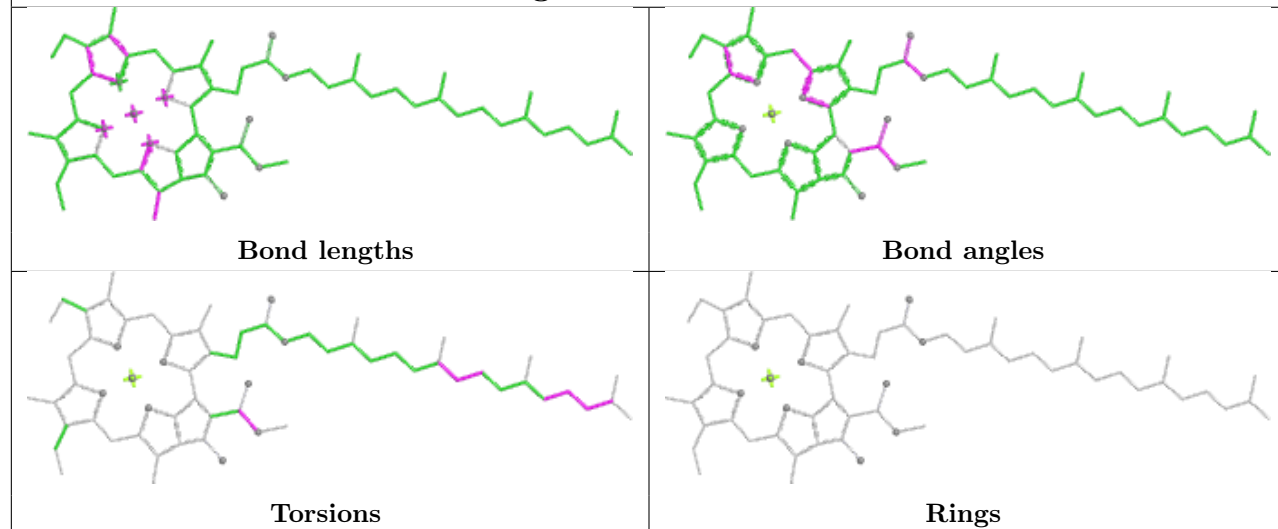


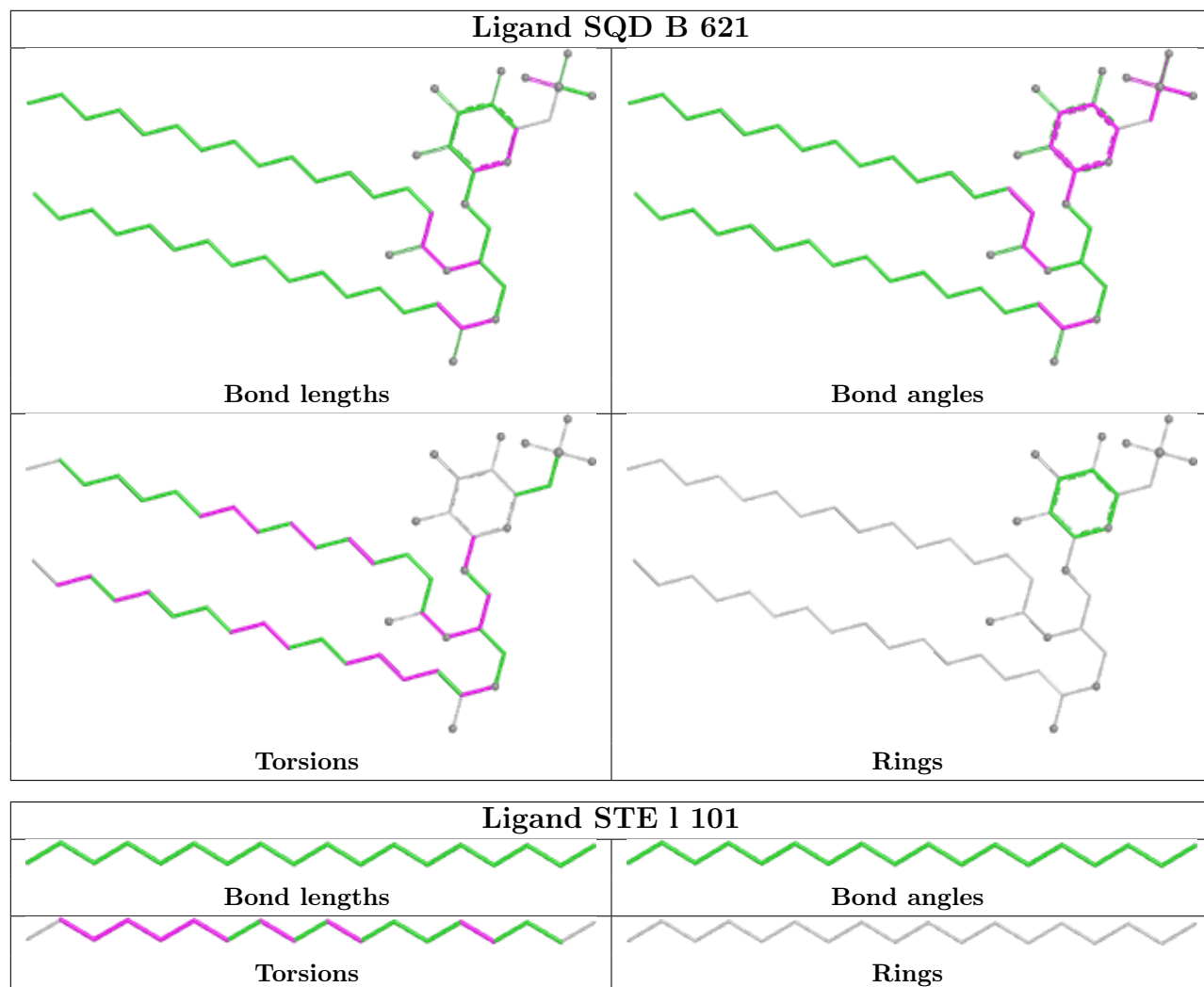


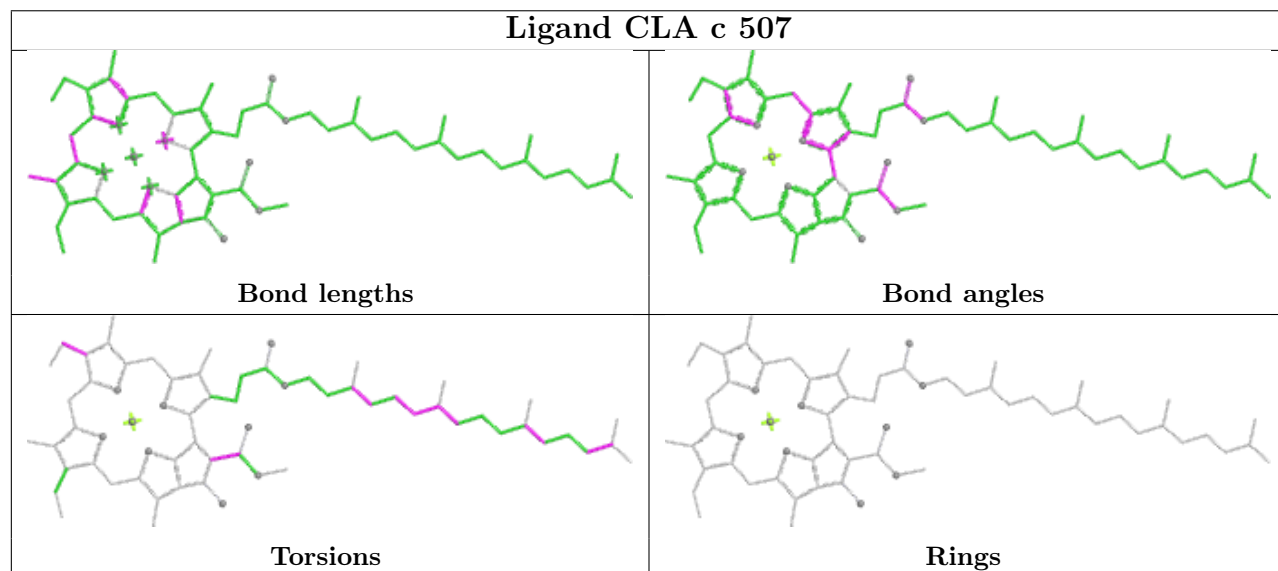
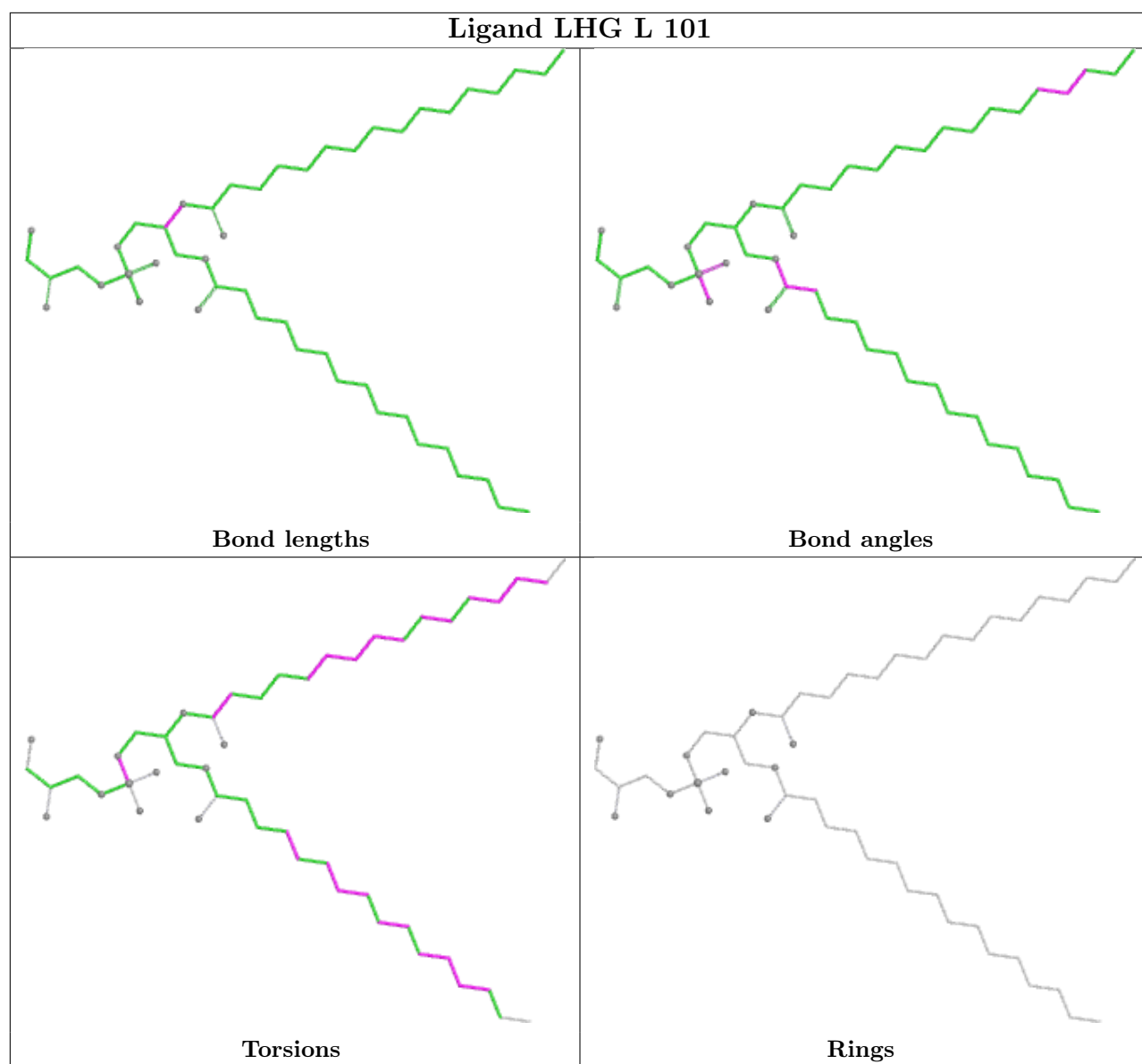
Ligand HEC V 201



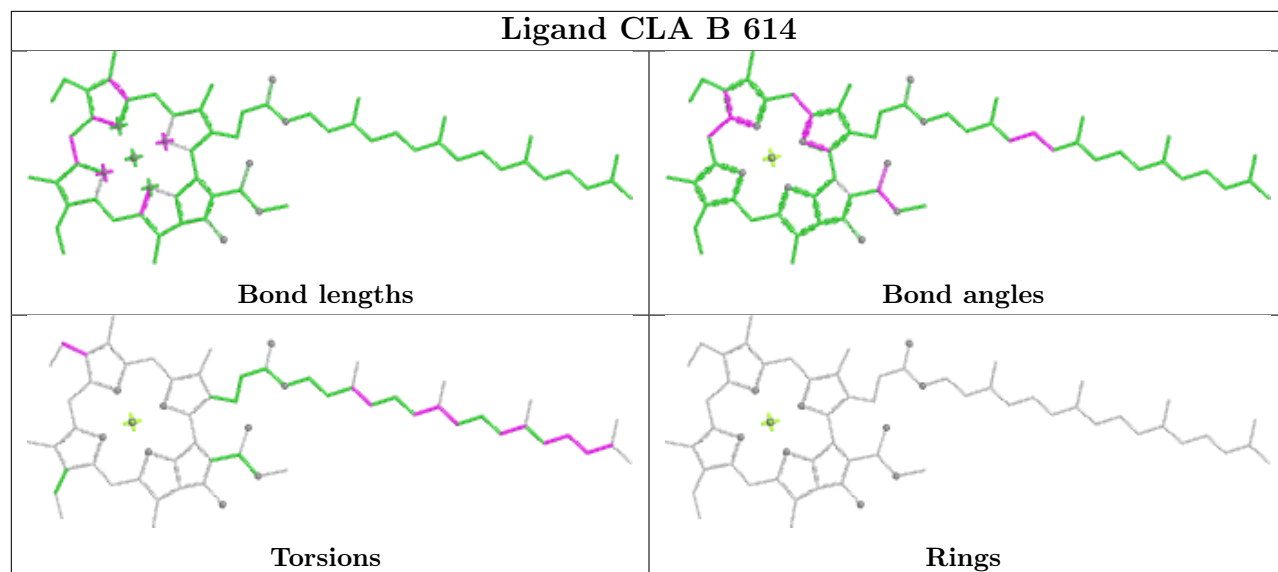
Ligand CLA C 513



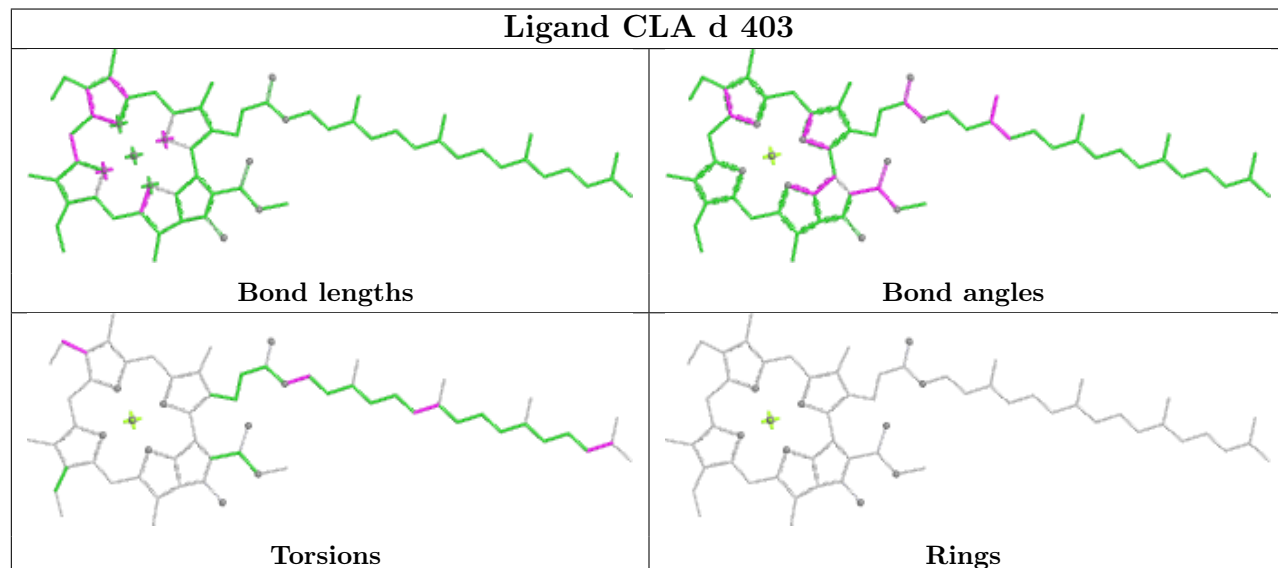




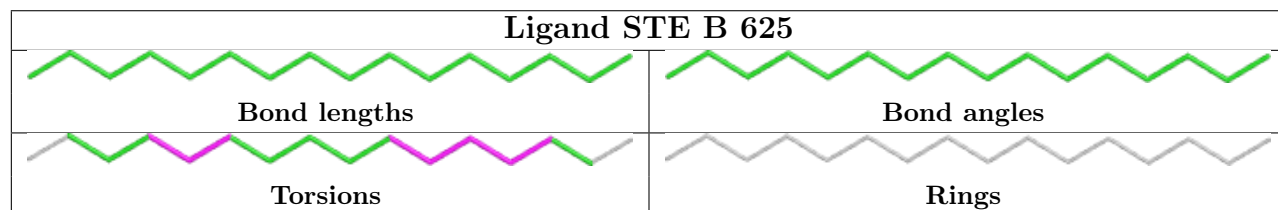
Ligand CLA B 614



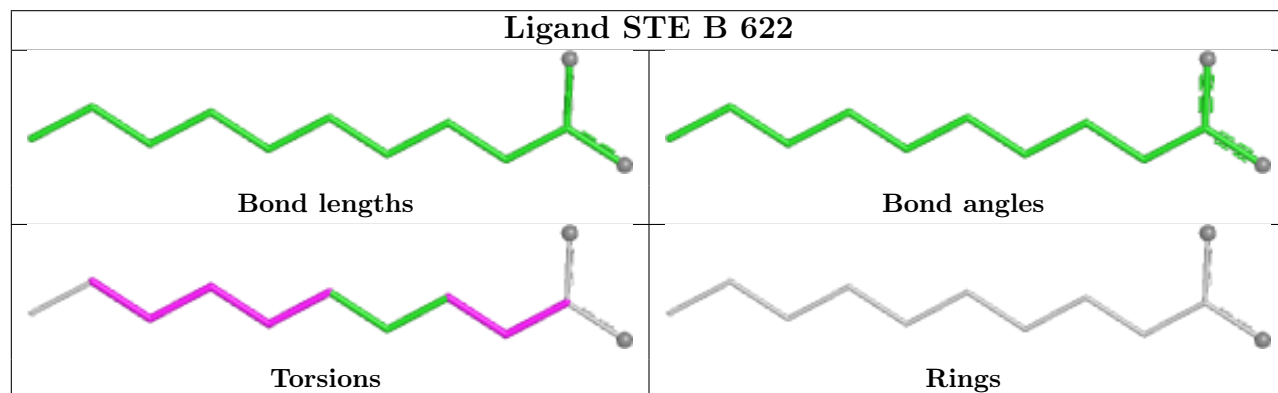
Ligand CLA d 403

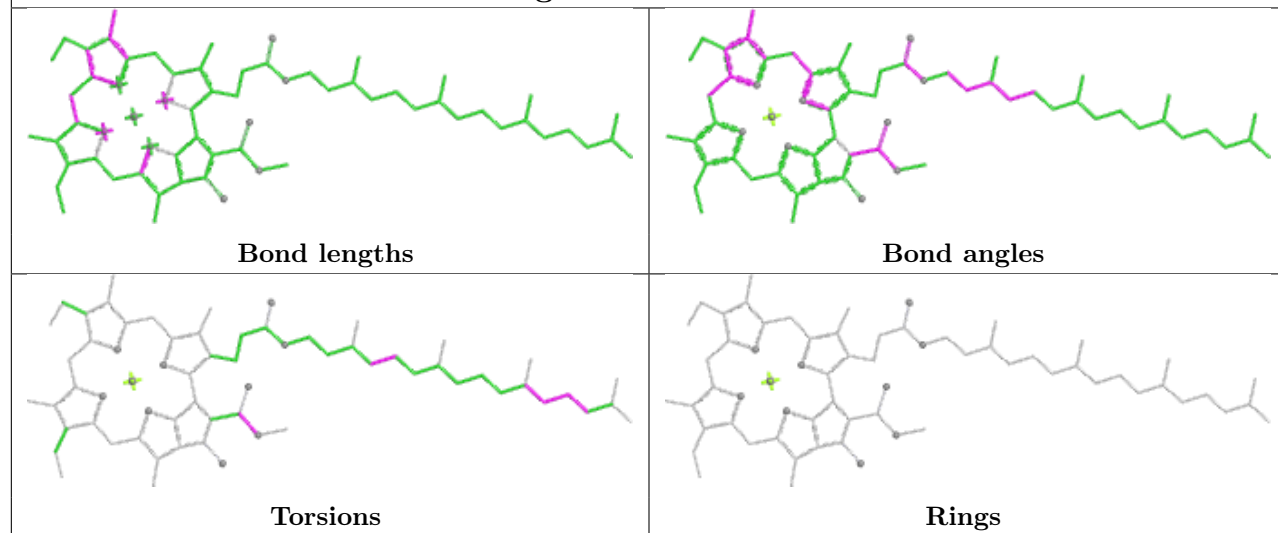
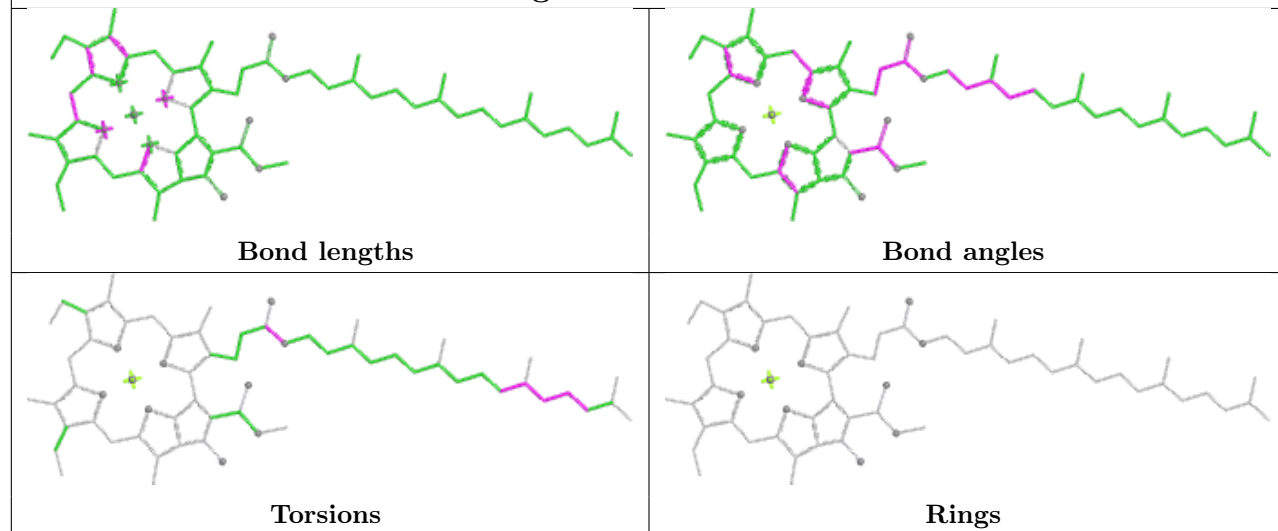


Ligand STE B 625

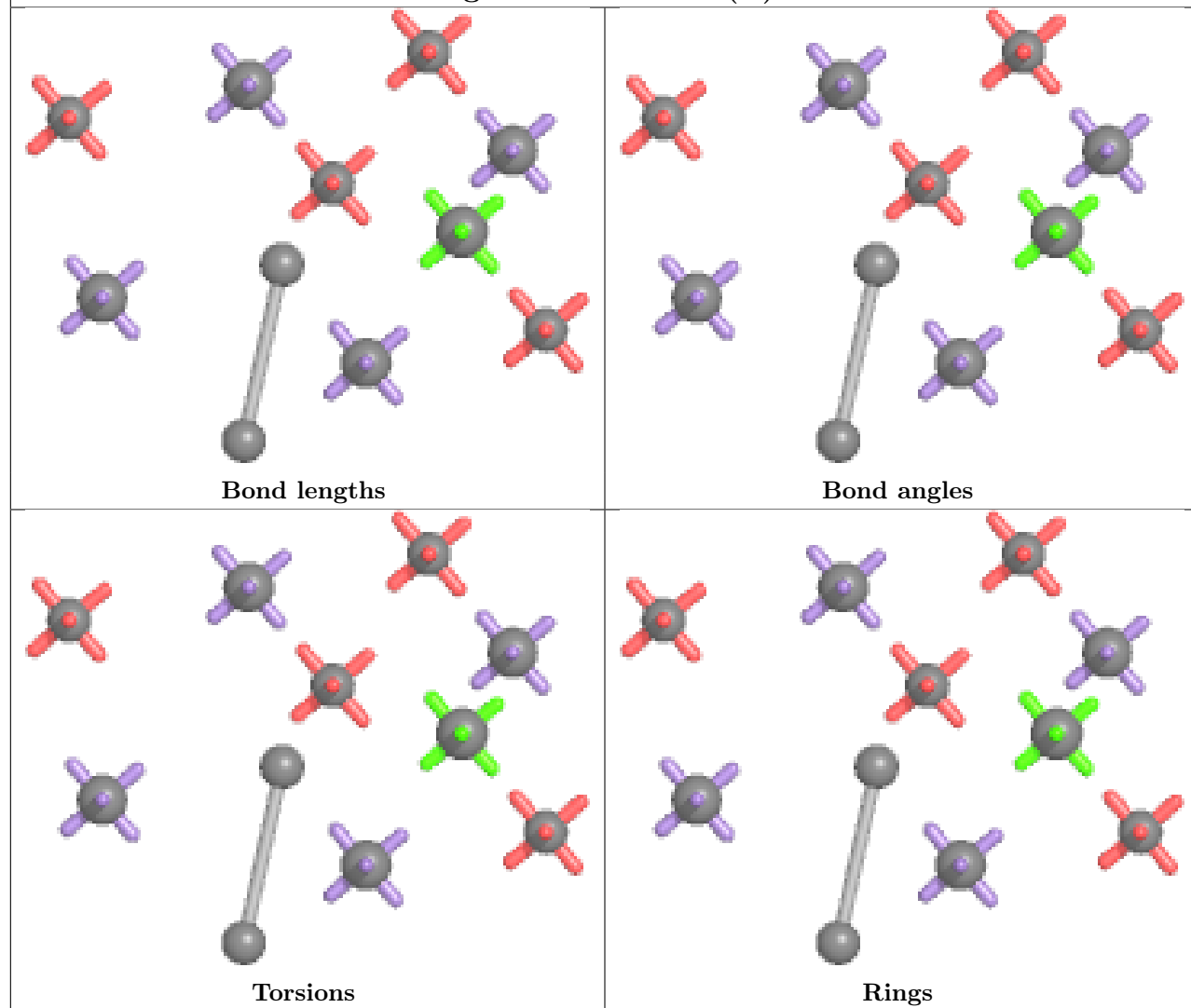


Ligand STE B 622

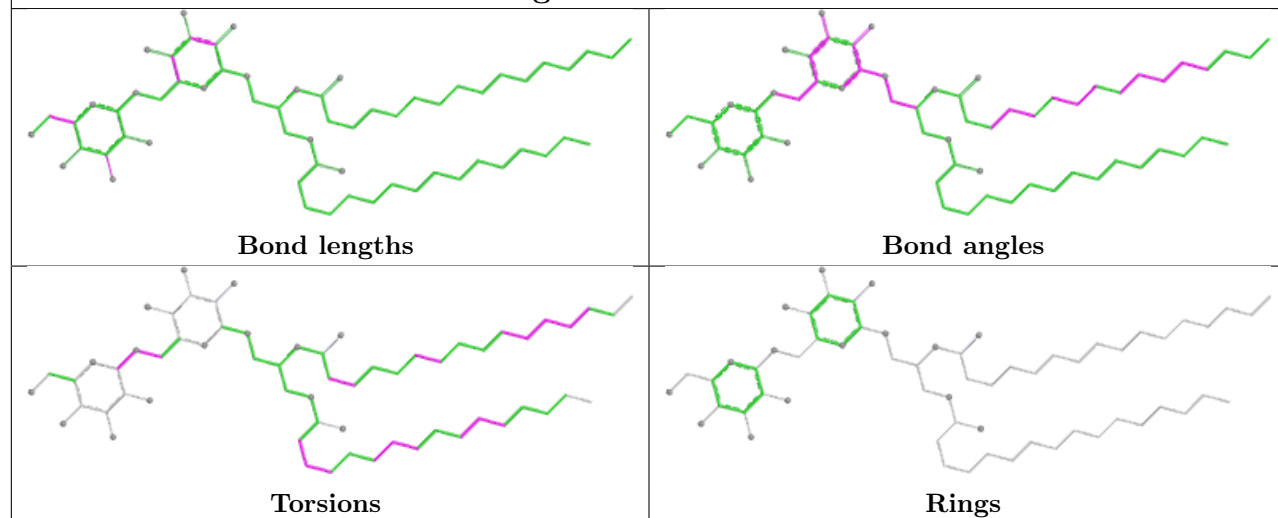


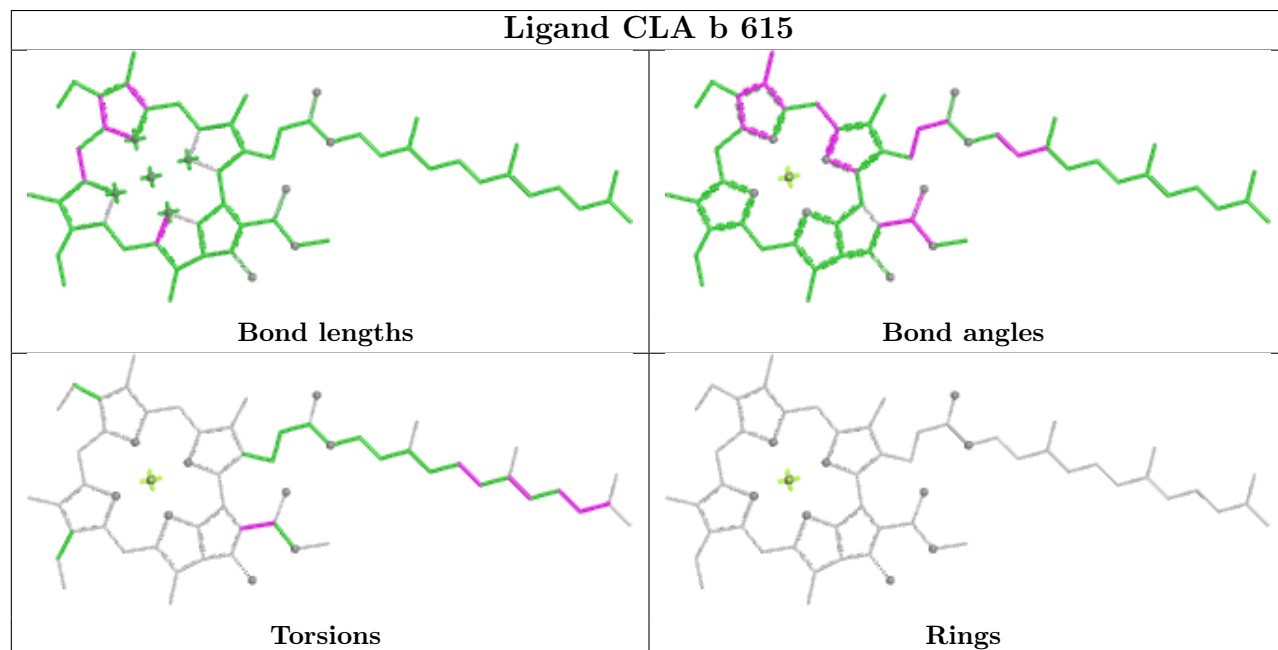
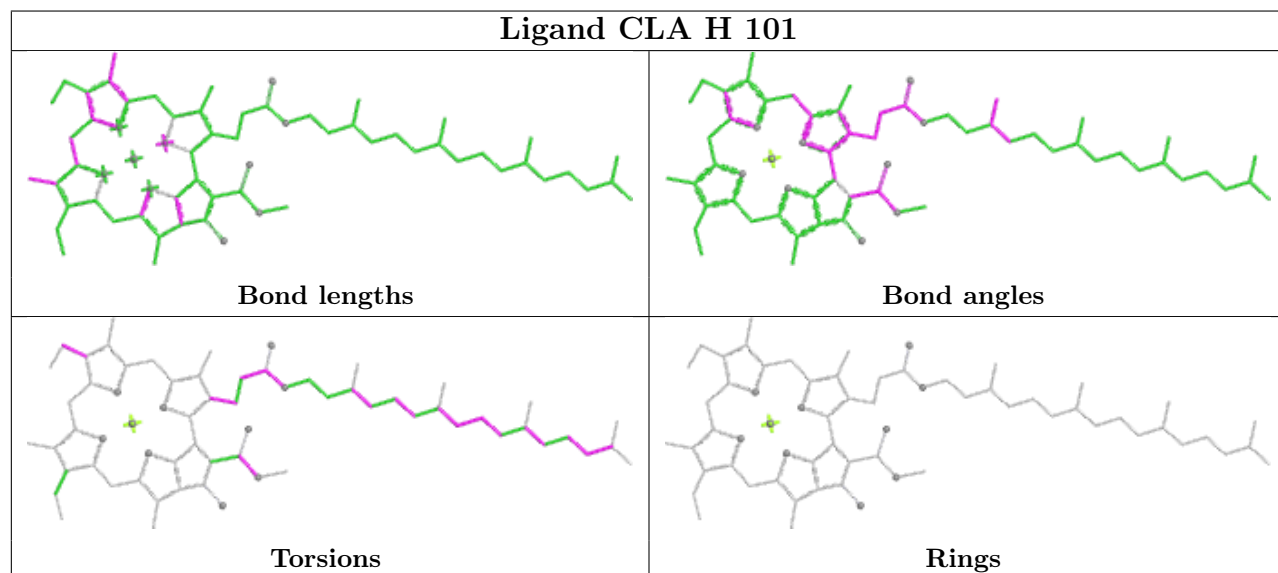
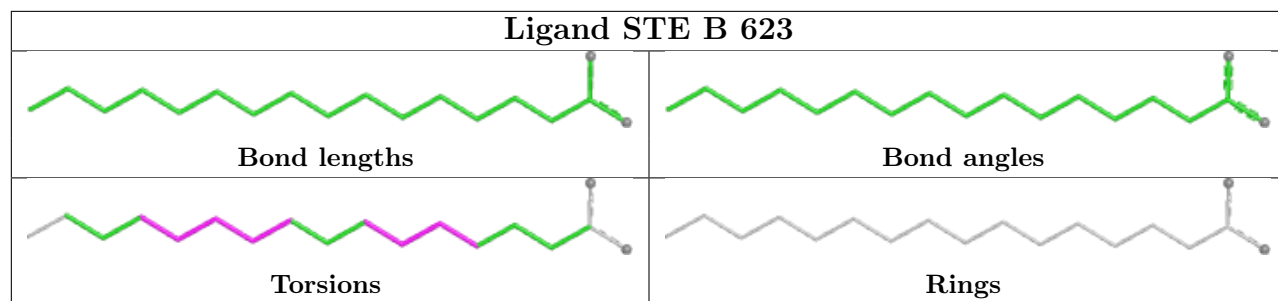
Ligand CLA b 608**Ligand CLA B 603**

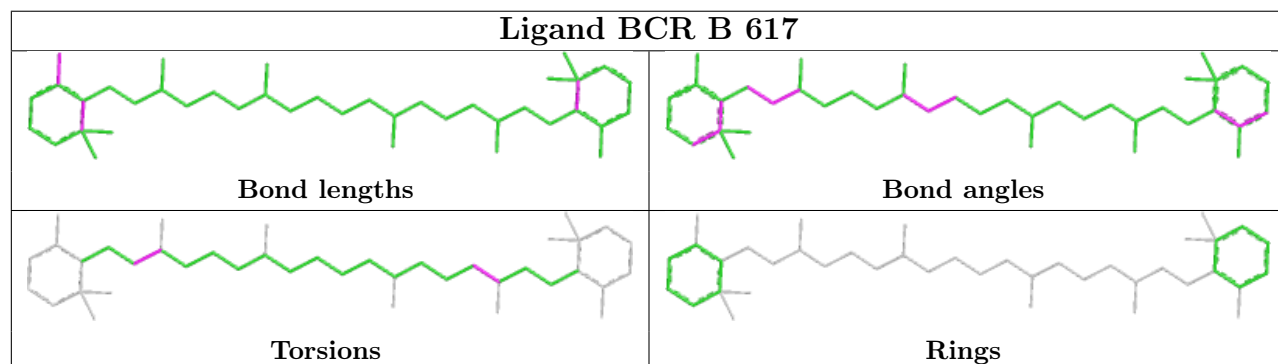
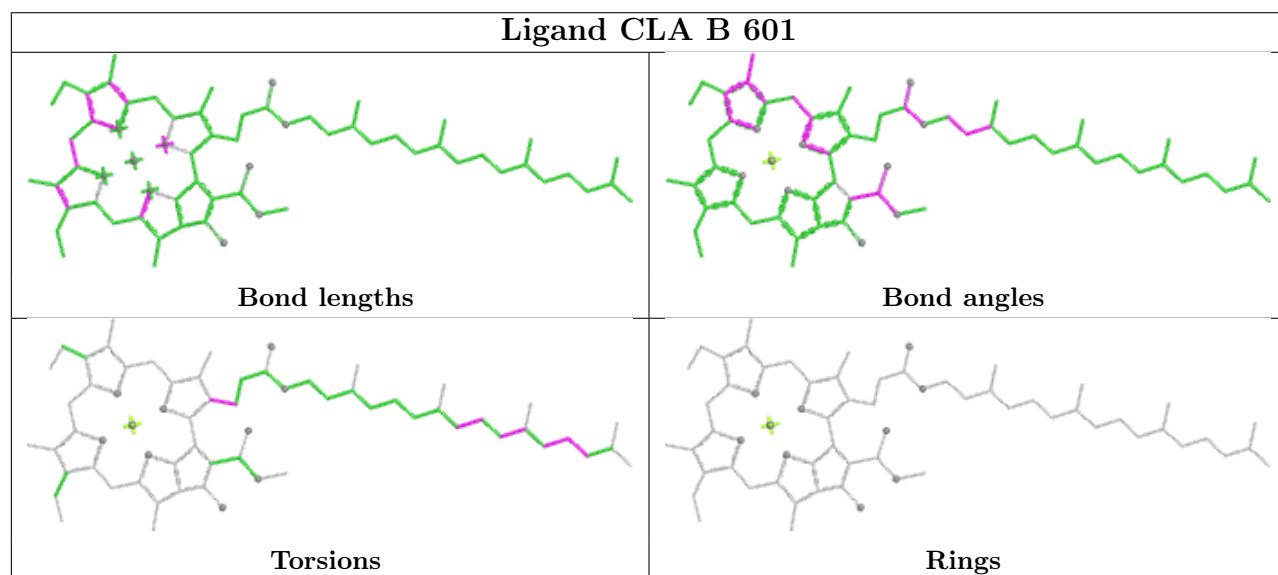
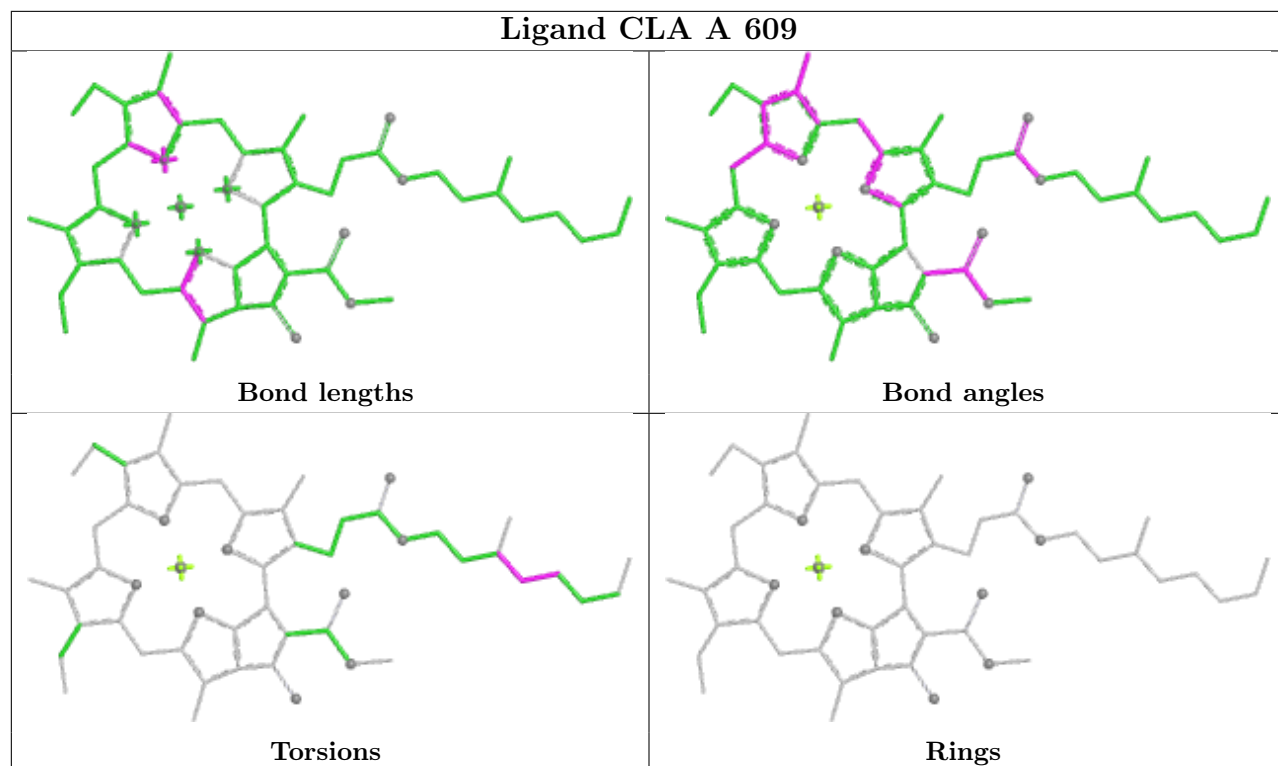
Ligand OEY A 601 (C)



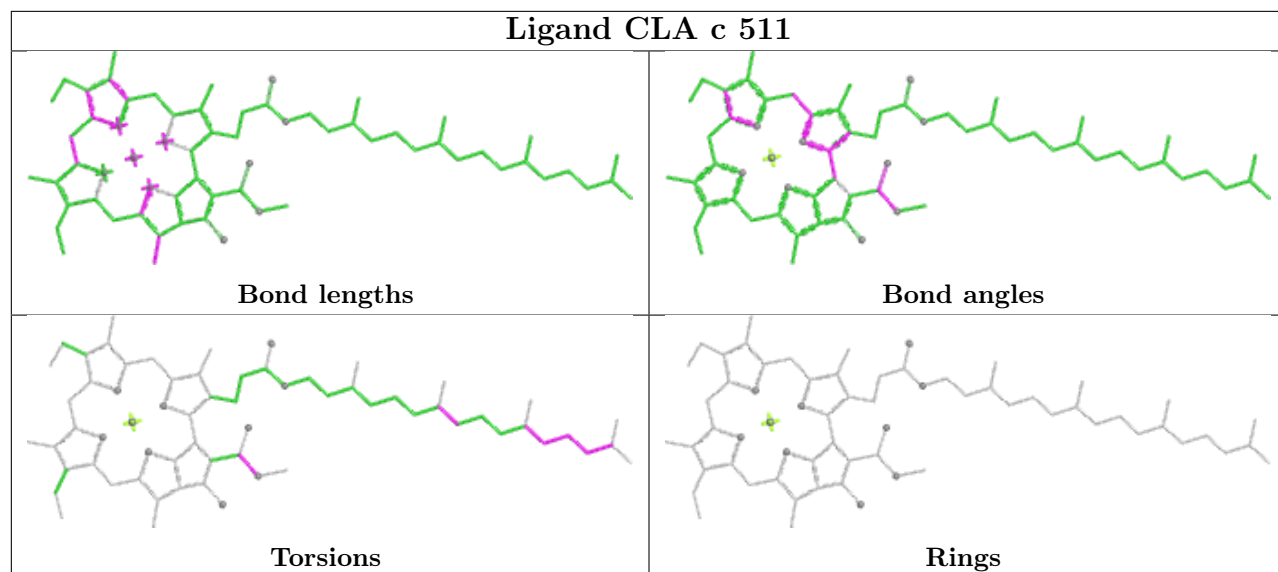
Ligand DGD c 517



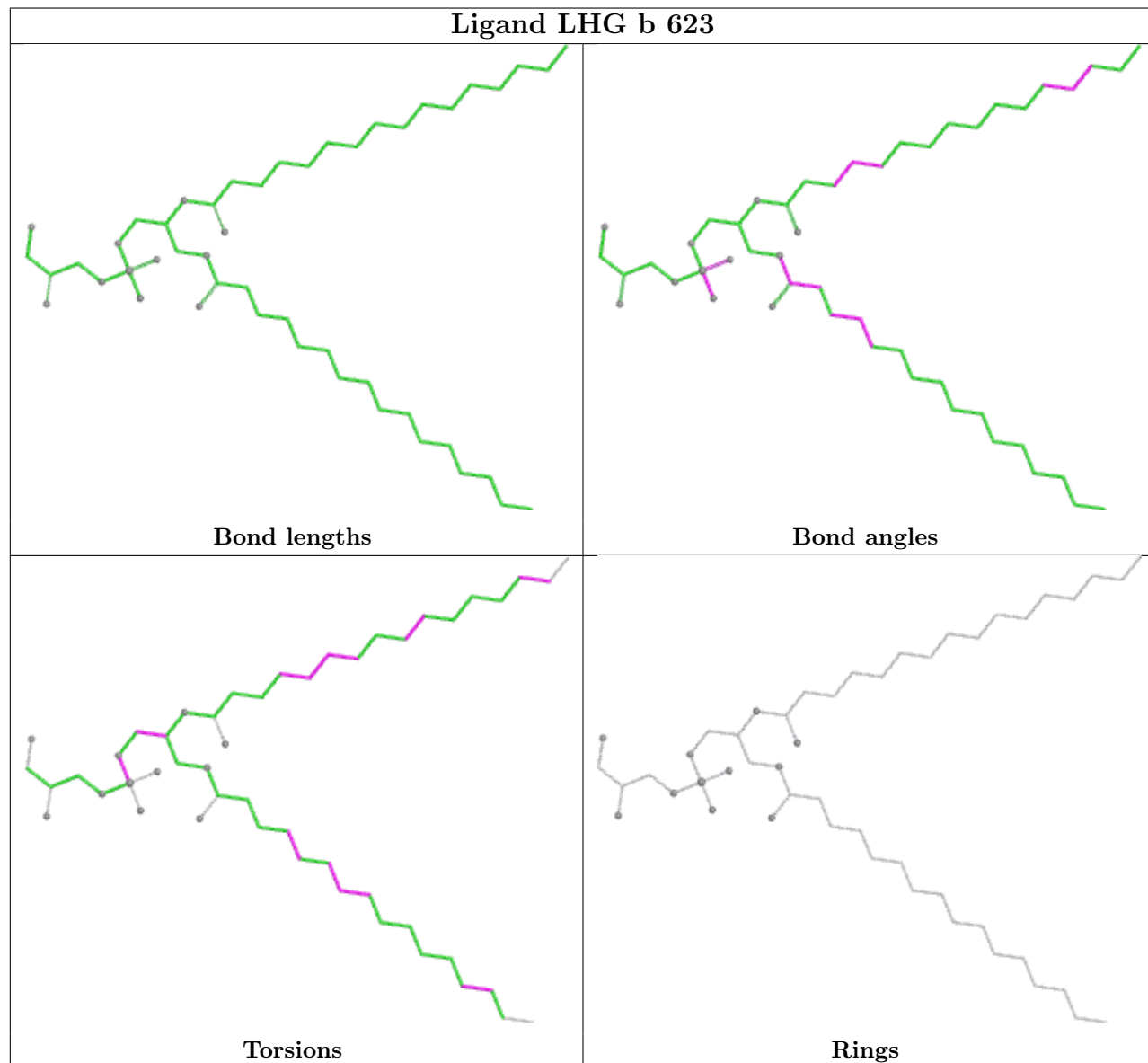


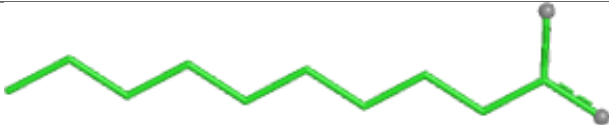
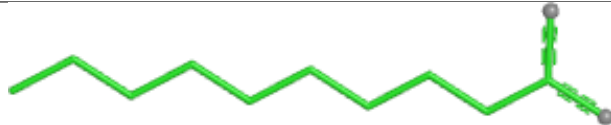
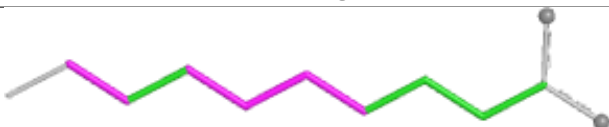
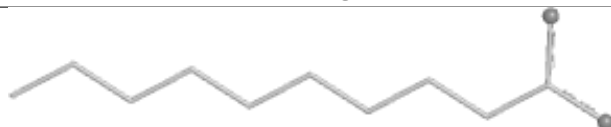


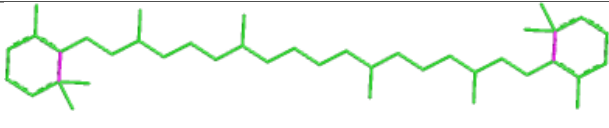
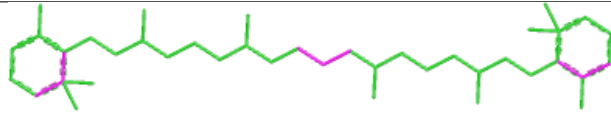
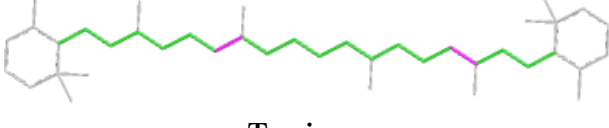
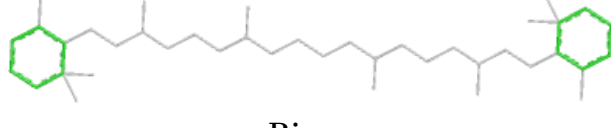
Ligand CLA c 511

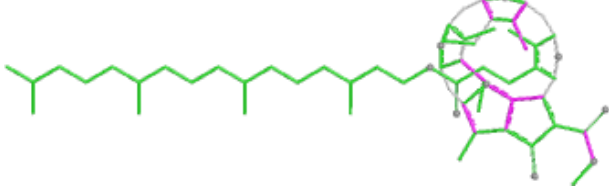
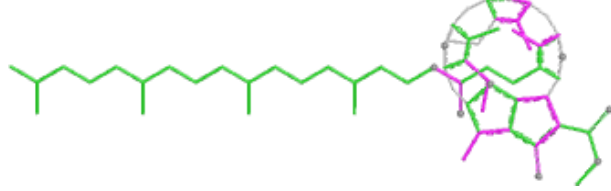
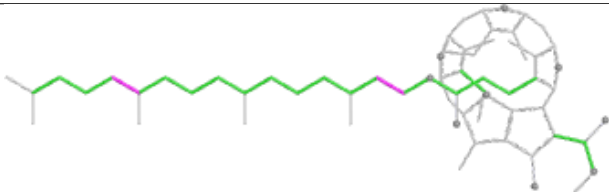
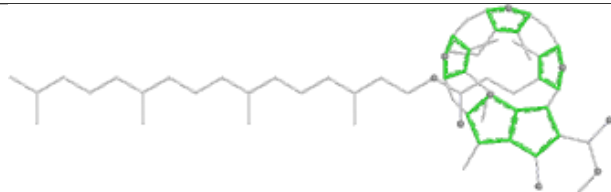


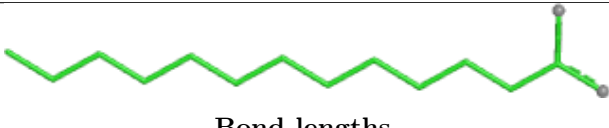
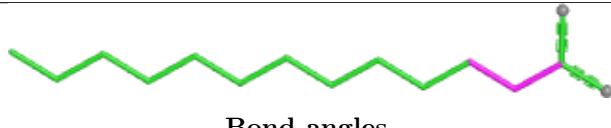
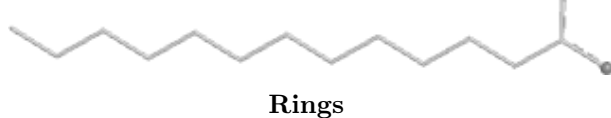
Ligand LHG b 623



Ligand STE J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO a 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE M 102	
	
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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.51	1 (0%) 90 90	8, 28, 48, 77	64 (19%)
1	a	334/344 (97%)	-0.43	1 (0%) 90 90	8, 30, 55, 76	64 (19%)
2	B	505/510 (99%)	-0.42	2 (0%) 88 89	18, 32, 60, 83	4 (0%)
2	b	505/510 (99%)	-0.31	4 (0%) 82 83	23, 35, 67, 104	0
3	C	442/461 (95%)	-0.38	0 100 100	9, 35, 51, 71	11 (2%)
3	c	451/461 (97%)	-0.25	2 (0%) 88 89	9, 39, 60, 91	12 (2%)
4	D	341/352 (96%)	-0.56	0 100 100	10, 30, 48, 74	2 (0%)
4	d	341/352 (96%)	-0.42	0 100 100	10, 33, 55, 78	3 (0%)
5	E	82/84 (97%)	0.18	0 100 100	31, 48, 66, 78	1 (1%)
5	e	82/84 (97%)	0.41	1 (1%) 76 76	39, 56, 73, 84	0
6	F	34/45 (75%)	-0.08	0 100 100	37, 44, 57, 78	0
6	f	34/45 (75%)	0.16	0 100 100	40, 49, 73, 88	0
7	H	65/66 (98%)	-0.11	1 (1%) 72 72	34, 41, 55, 67	0
7	h	63/66 (95%)	0.12	0 100 100	40, 51, 60, 62	0
8	I	35/38 (92%)	-0.19	0 100 100	32, 39, 61, 78	0
8	i	35/38 (92%)	-0.25	0 100 100	29, 38, 69, 84	0
9	J	36/40 (90%)	0.10	0 100 100	35, 49, 77, 86	0
9	j	36/40 (90%)	0.26	0 100 100	41, 54, 87, 93	0
10	K	37/46 (80%)	0.06	0 100 100	42, 50, 65, 72	0
10	k	37/46 (80%)	0.21	0 100 100	48, 55, 72, 80	0
11	L	37/37 (100%)	-0.50	0 100 100	24, 29, 58, 64	0
11	l	36/37 (97%)	-0.51	0 100 100	26, 30, 62, 73	0
12	M	32/36 (88%)	-0.49	0 100 100	28, 32, 53, 66	0
12	m	31/36 (86%)	-0.44	0 100 100	29, 32, 48, 63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.23	3 (1%) 76 76	24, 40, 74, 124	1 (0%)
13	o	244/272 (89%)	-0.23	1 (0%) 88 89	25, 39, 73, 109	0
14	T	29/32 (90%)	-0.54	0 100 100	27, 31, 55, 70	0
14	t	29/32 (90%)	-0.51	0 100 100	27, 31, 66, 82	0
15	U	97/134 (72%)	-0.23	0 100 100	32, 41, 65, 83	0
15	u	97/134 (72%)	-0.24	1 (1%) 79 80	32, 39, 55, 80	0
16	V	137/163 (84%)	-0.36	1 (0%) 84 84	29, 39, 54, 70	0
16	v	137/163 (84%)	-0.05	0 100 100	33, 47, 67, 83	0
17	Y	27/46 (58%)	0.91	2 (7%) 20 19	50, 67, 94, 100	0
17	y	30/46 (65%)	0.71	2 (6%) 24 23	61, 74, 94, 99	0
18	X	38/41 (92%)	-0.00	0 100 100	40, 50, 68, 75	0
18	x	39/41 (95%)	0.23	1 (2%) 57 57	50, 59, 81, 92	0
19	Z	62/62 (100%)	0.59	2 (3%) 50 49	53, 67, 100, 114	0
19	z	62/62 (100%)	0.69	3 (4%) 35 35	60, 72, 105, 111	0
20	R	34/41 (82%)	0.63	1 (2%) 53 53	56, 64, 74, 79	0
20	r	31/41 (75%)	1.02	1 (3%) 50 49	64, 77, 93, 97	0
All	All	5302/5700 (93%)	-0.26	30 (0%) 85 86	8, 37, 70, 124	162 (3%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	3.5
20	R	35	LEU	3.1
1	A	13	LEU	3.1
17	Y	25	ILE	2.9
2	b	495	PHE	2.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.90	0.10	29,35,51,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	M	1	10/11	0.93	0.10	38,44,61,66	0
14	FME	T	1	10/11	0.94	0.10	33,37,56,65	0
8	FME	i	1	10/11	0.96	0.07	35,47,49,49	0
8	FME	I	1	10/11	0.96	0.08	36,45,50,52	0
12	FME	m	1	10/11	0.97	0.07	31,44,62,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LHG	A	615	49/49	0.73	0.16	51,71,91,96	0
33	STE	H	104	18/20	0.74	0.17	56,64,68,70	0
29	LMG	d	410	23/55	0.75	0.20	45,65,73,75	0
29	LMG	b	622	55/55	0.76	0.17	49,63,72,77	0
28	PL9	A	611	55/55	0.78	0.15	43,60,70,73	0
33	STE	b	625	20/20	0.78	0.14	46,55,63,71	0
29	LMG	c	521	48/55	0.79	0.14	53,68,79,83	0
33	STE	d	412	16/20	0.79	0.17	51,58,80,82	0
32	DGD	a	615	44/66	0.81	0.13	36,49,61,69	0
25	CLA	h	101	65/65	0.81	0.12	47,62,78,88	0
28	PL9	a	611	55/55	0.81	0.14	42,61,73,74	0
31	LHG	e	101	42/49	0.81	0.13	57,76,89,100	0
33	STE	a	616	12/20	0.82	0.12	52,58,69,73	0
33	STE	k	103	12/20	0.82	0.13	59,71,78,80	0
29	LMG	A	613	48/55	0.83	0.11	38,52,65,68	0
33	STE	B	625	16/20	0.83	0.14	41,51,62,64	0
32	DGD	A	617	66/66	0.83	0.12	49,58,64,67	0
33	STE	J	101	12/20	0.83	0.13	49,56,60,63	0
33	STE	m	102	12/20	0.83	0.17	49,57,62,65	0
33	STE	b	624	15/20	0.84	0.14	44,48,58,59	0
33	STE	B	623	18/20	0.84	0.14	43,53,74,75	0
33	STE	b	626	10/20	0.84	0.14	45,51,59,61	0
29	LMG	D	410	33/55	0.84	0.13	31,53,76,77	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	STE	C	521	12/20	0.84	0.12	45,52,57,59	0
33	STE	b	621	20/20	0.84	0.12	40,51,61,68	0
33	STE	B	624	12/20	0.85	0.12	49,54,68,72	0
29	LMG	c	519	37/55	0.85	0.12	48,63,75,76	0
29	LMG	B	620	28/55	0.85	0.13	40,48,58,70	0
33	STE	E	101	12/20	0.85	0.12	57,62,76,78	0
29	LMG	C	519	48/55	0.85	0.13	43,63,75,78	0
30	SQD	A	616	39/54	0.85	0.12	42,52,70,72	0
30	SQD	a	614	36/54	0.85	0.12	36,55,67,70	0
33	STE	x	101	20/20	0.85	0.12	41,51,60,61	0
33	STE	B	622	12/20	0.86	0.12	45,50,58,62	0
33	STE	B	619	17/20	0.86	0.11	35,48,63,64	0
33	STE	C	520	12/20	0.86	0.14	40,44,52,55	0
33	STE	c	520	20/20	0.86	0.12	47,53,76,77	0
30	SQD	b	619	49/54	0.87	0.11	40,53,77,85	0
30	SQD	f	102	41/54	0.87	0.13	61,73,84,90	0
29	LMG	c	522	49/55	0.87	0.10	39,51,74,79	0
29	LMG	m	101	51/55	0.87	0.10	34,47,59,65	0
33	STE	X	101	20/20	0.87	0.11	40,49,63,69	0
33	STE	b	620	16/20	0.88	0.12	39,44,53,54	0
33	STE	I	101	15/20	0.88	0.13	43,49,56,57	0
33	STE	d	413	17/20	0.88	0.12	46,50,60,62	0
33	STE	j	101	12/20	0.88	0.11	50,55,58,58	0
29	LMG	M	101	51/55	0.88	0.10	31,46,60,64	0
25	CLA	H	101	65/65	0.88	0.10	36,51,74,82	0
33	STE	t	102	14/20	0.88	0.10	35,42,51,54	0
33	STE	t	103	10/20	0.88	0.11	43,55,61,62	0
27	BCR	k	101	40/40	0.88	0.11	48,57,64,65	0
33	STE	C	522	16/20	0.89	0.10	42,46,50,51	0
32	DGD	h	103	62/66	0.89	0.11	38,48,56,60	0
30	SQD	B	621	54/54	0.89	0.10	33,55,73,75	0
32	DGD	H	103	62/66	0.90	0.10	35,44,51,57	0
27	BCR	K	101	40/40	0.90	0.10	44,48,57,61	0
32	DGD	c	517	62/66	0.90	0.10	37,47,73,75	0
27	BCR	c	514	40/40	0.90	0.10	49,55,61,62	0
27	BCR	C	514	40/40	0.91	0.10	44,51,58,60	0
33	STE	M	103	10/20	0.91	0.12	44,47,53,56	0
30	SQD	F	102	36/54	0.91	0.12	45,64,68,70	0
30	SQD	a	613	54/54	0.91	0.10	37,55,72,75	0
27	BCR	d	405	40/40	0.91	0.09	38,46,77,84	0
27	BCR	h	102	40/40	0.91	0.10	40,50,61,63	0
27	BCR	D	405	40/40	0.91	0.09	34,41,69,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	BCR	H	102	40/40	0.91	0.09	33,45,51,56	0
25	CLA	C	513	65/65	0.91	0.10	45,54,76,81	0
34	BCT	d	401	4/4	0.91	0.11	34,37,41,47	0
25	CLA	c	512	65/65	0.92	0.10	43,55,73,79	0
27	BCR	B	618	40/40	0.92	0.08	27,37,49,51	0
32	DGD	C	517	62/66	0.92	0.09	36,45,80,87	0
27	BCR	k	102	40/40	0.92	0.10	43,51,59,64	0
33	STE	l	101	18/20	0.92	0.11	35,43,59,61	0
27	BCR	b	616	40/40	0.93	0.08	27,38,45,46	0
27	BCR	b	617	40/40	0.93	0.07	27,35,44,47	0
30	SQD	A	614	52/54	0.93	0.09	32,49,67,71	0
27	BCR	b	618	40/40	0.93	0.08	31,40,56,58	0
25	CLA	c	513	65/65	0.93	0.09	47,60,81,87	0
29	LMG	D	407	51/55	0.93	0.10	29,48,68,74	0
33	STE	M	102	15/20	0.93	0.09	34,40,52,63	0
27	BCR	C	515	40/40	0.93	0.08	28,38,46,52	0
25	CLA	c	503	65/65	0.93	0.08	33,41,49,54	0
27	BCR	B	617	40/40	0.93	0.07	26,34,44,50	0
25	CLA	C	503	65/65	0.93	0.08	34,39,45,51	0
27	BCR	t	101	40/40	0.93	0.07	29,35,45,46	0
27	BCR	T	101	40/40	0.93	0.07	29,35,45,49	0
25	CLA	C	508	65/65	0.94	0.09	29,36,84,88	0
28	PL9	D	406	55/55	0.94	0.07	23,29,36,38	0
31	LHG	D	409	47/49	0.94	0.10	30,38,65,73	0
31	LHG	d	407	49/49	0.94	0.09	31,44,60,64	0
27	BCR	A	610	40/40	0.94	0.06	25,31,35,37	0
25	CLA	C	510	65/65	0.94	0.08	30,38,49,52	0
32	DGD	C	516	62/66	0.94	0.09	24,34,63,68	0
25	CLA	c	504	60/65	0.94	0.07	31,43,64,68	0
25	CLA	c	508	64/65	0.94	0.09	33,41,71,84	0
25	CLA	c	509	65/65	0.94	0.09	36,42,54,56	0
25	CLA	c	511	65/65	0.94	0.10	36,50,61,66	0
32	DGD	c	518	62/66	0.94	0.08	31,45,64,69	0
25	CLA	C	512	65/65	0.94	0.09	38,46,68,74	0
25	CLA	B	605	65/65	0.94	0.08	24,32,57,61	0
27	BCR	K	102	40/40	0.94	0.09	39,47,56,60	0
25	CLA	c	505	65/65	0.95	0.07	30,37,51,56	0
25	CLA	c	506	65/65	0.95	0.08	33,41,72,76	0
25	CLA	C	502	65/65	0.95	0.07	27,35,45,50	0
31	LHG	D	411	49/49	0.95	0.08	30,39,57,64	0
31	LHG	b	623	49/49	0.95	0.08	31,40,46,50	0
25	CLA	C	504	59/65	0.95	0.07	32,39,66,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LHG	d	409	39/49	0.95	0.08	32,41,54,59	0
25	CLA	c	510	65/65	0.95	0.07	31,43,52,56	0
25	CLA	a	606	65/65	0.95	0.06	21,27,38,49	0
25	CLA	b	608	65/65	0.95	0.07	32,40,57,63	0
25	CLA	b	611	65/65	0.95	0.07	25,31,40,46	0
32	DGD	C	518	62/66	0.95	0.07	29,41,66,72	0
25	CLA	d	404	65/65	0.95	0.08	28,40,75,79	0
27	BCR	c	515	40/40	0.95	0.08	33,42,48,54	0
32	DGD	c	516	62/66	0.95	0.08	25,35,59,68	0
25	CLA	b	613	65/65	0.95	0.08	25,33,59,69	0
29	LMG	d	411	44/55	0.95	0.08	35,45,66,71	0
26	PHO	d	402	64/64	0.95	0.06	29,35,40,44	0
25	CLA	b	614	65/65	0.95	0.07	25,36,48,51	0
27	BCR	B	616	40/40	0.95	0.07	28,36,42,46	0
25	CLA	b	615	60/65	0.95	0.08	29,38,75,78	0
25	CLA	c	502	65/65	0.95	0.07	30,37,49,54	0
25	CLA	C	511	65/65	0.95	0.08	36,45,54,56	0
25	CLA	C	506	65/65	0.95	0.09	27,40,71,75	0
28	PL9	d	406	55/55	0.95	0.07	23,30,36,38	0
25	CLA	C	505	65/65	0.96	0.07	26,34,53,60	0
25	CLA	B	606	65/65	0.96	0.07	17,27,50,54	0
25	CLA	C	507	65/65	0.96	0.07	26,34,46,49	0
27	BCR	a	610	40/40	0.96	0.06	22,29,41,43	0
25	CLA	B	608	65/65	0.96	0.06	23,34,47,52	0
25	CLA	C	509	65/65	0.96	0.08	29,36,53,58	0
25	CLA	B	609	65/65	0.96	0.06	21,29,35,37	0
25	CLA	c	507	65/65	0.96	0.07	29,38,48,54	0
25	CLA	B	610	65/65	0.96	0.06	23,28,40,44	0
25	CLA	B	611	65/65	0.96	0.06	21,29,38,41	0
25	CLA	B	613	65/65	0.96	0.07	23,30,61,68	0
25	CLA	B	614	65/65	0.96	0.07	24,33,51,60	0
25	CLA	B	615	60/65	0.96	0.07	26,34,65,70	0
25	CLA	a	607	65/65	0.96	0.08	27,34,78,86	0
25	CLA	d	403	65/65	0.96	0.07	23,29,48,56	0
31	LHG	d	408	49/49	0.96	0.08	28,37,44,50	0
25	CLA	a	609	65/65	0.96	0.08	21,28,63,67	0
25	CLA	a	612	65/65	0.96	0.06	22,27,35,42	0
26	PHO	A	608	64/64	0.96	0.05	24,30,36,38	0
26	PHO	D	402	64/64	0.96	0.05	20,26,32,36	0
26	PHO	a	608	64/64	0.96	0.05	23,28,34,36	0
25	CLA	b	601	65/65	0.96	0.07	31,36,52,57	0
25	CLA	b	605	65/65	0.96	0.07	27,35,60,64	0

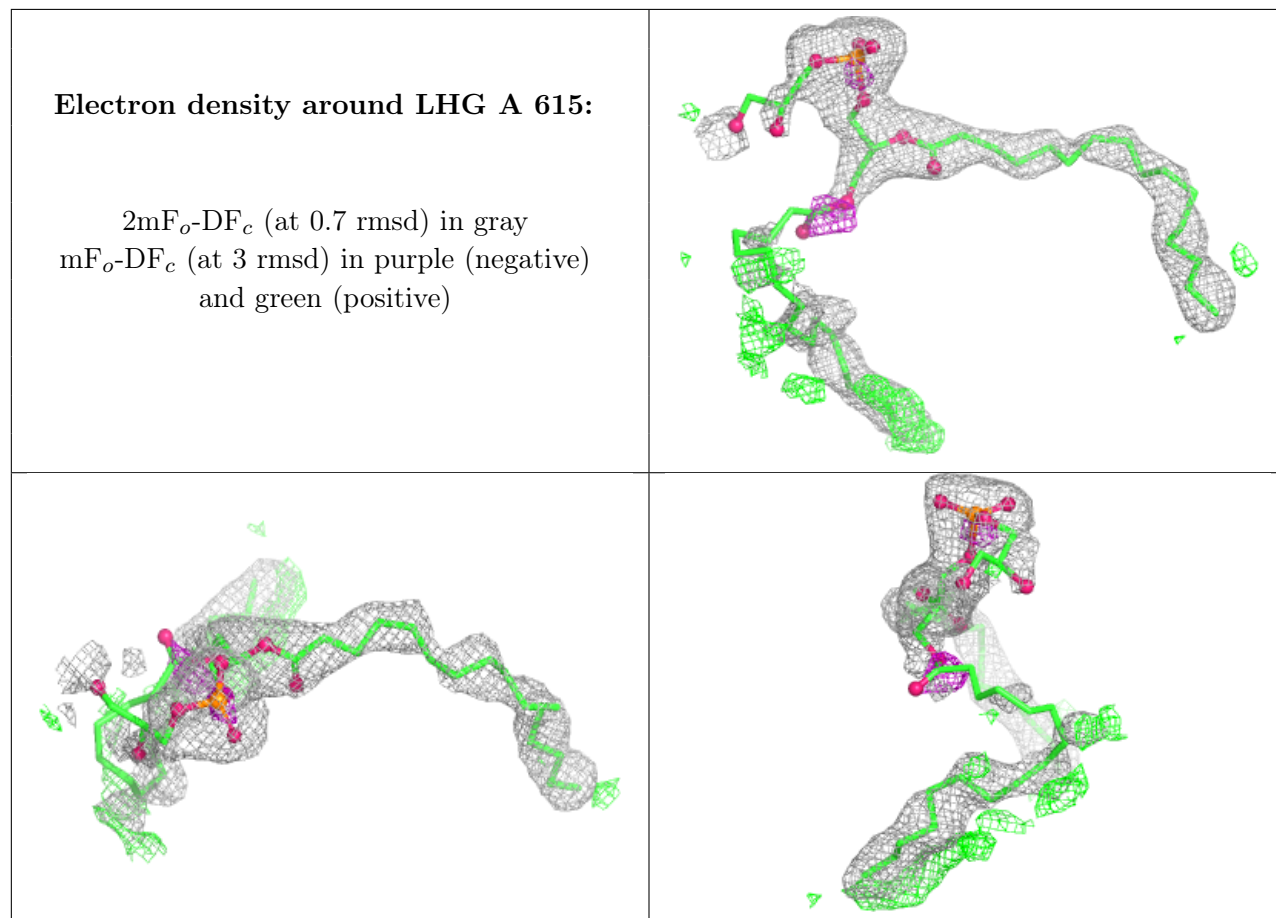
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	607	65/65	0.96	0.07	32,37,52,54	0
25	CLA	C	501	65/65	0.96	0.06	25,32,44,46	0
25	CLA	b	609	65/65	0.96	0.07	26,33,40,45	0
25	CLA	B	601	65/65	0.96	0.06	26,32,48,54	0
25	CLA	b	612	65/65	0.96	0.07	22,28,55,66	0
25	CLA	B	603	65/65	0.96	0.07	24,28,58,65	0
25	CLA	A	607	65/65	0.96	0.07	21,30,74,81	0
31	LHG	L	101	49/49	0.97	0.07	27,36,47,52	0
25	CLA	c	501	65/65	0.97	0.06	30,35,45,49	0
25	CLA	b	603	65/65	0.97	0.07	23,29,61,72	0
25	CLA	b	604	65/65	0.97	0.06	23,32,41,43	0
25	CLA	D	403	65/65	0.97	0.06	19,26,44,51	0
25	CLA	b	606	65/65	0.97	0.06	22,31,51,57	0
25	CLA	D	404	65/65	0.97	0.07	29,33,83,88	0
25	CLA	B	602	65/65	0.97	0.06	22,28,50,53	0
25	CLA	B	612	65/65	0.97	0.06	20,27,55,62	0
25	CLA	b	610	65/65	0.97	0.05	24,31,44,51	0
25	CLA	B	607	65/65	0.97	0.06	23,30,47,52	0
25	CLA	A	612	65/65	0.97	0.06	18,25,38,47	0
25	CLA	B	604	65/65	0.97	0.06	22,27,38,41	0
31	LHG	D	408	49/49	0.97	0.06	25,34,44,50	0
25	CLA	A	606	65/65	0.97	0.06	18,25,38,41	0
25	CLA	b	602	65/65	0.97	0.07	25,31,52,63	0
35	HEM	F	101	43/43	0.97	0.08	39,45,54,59	0
35	HEM	f	101	43/43	0.97	0.09	51,55,67,76	0
25	CLA	A	609	54/65	0.98	0.05	20,27,54,60	0
24	CL	A	604	1/1	0.98	0.05	27,27,27,27	0
34	BCT	D	401	4/4	0.98	0.06	33,34,35,38	0
36	HEC	V	201	43/43	0.98	0.06	24,30,37,41	0
36	HEC	v	201	43/43	0.98	0.06	28,36,41,45	0
24	CL	a	604	1/1	0.99	0.04	29,29,29,29	0
24	CL	a	605	1/1	0.99	0.07	30,30,30,30	0
21	OEY	A	601[C]	11/11	0.99	0.03	24,26,30,31	11
21	OEY	a	601[A]	11/11	0.99	0.03	27,31,33,34	11
21	OEY	a	601[C]	11/11	0.99	0.03	24,27,32,32	11
22	OEX	A	602[B]	10/10	0.99	0.03	25,29,32,32	10
22	OEX	a	602[B]	10/10	0.99	0.03	25,29,31,32	10
23	FE2	a	603	1/1	0.99	0.03	32,32,32,32	0
21	OEY	A	601[A]	11/11	0.99	0.03	28,31,33,34	11
23	FE2	A	603	1/1	1.00	0.01	30,30,30,30	0
24	CL	A	605	1/1	1.00	0.06	28,28,28,28	0

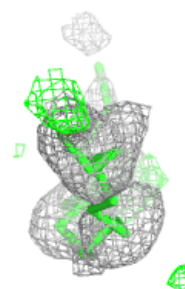
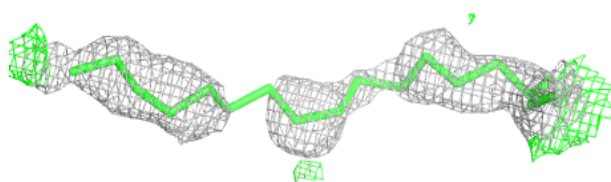
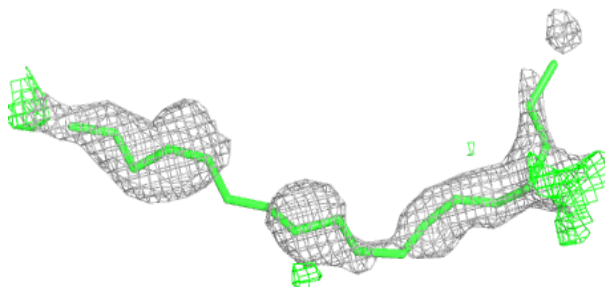
The following is a graphical depiction of the model fit to experimental electron density of all

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.

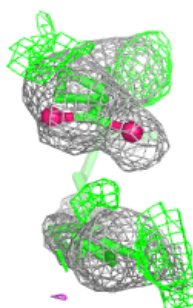
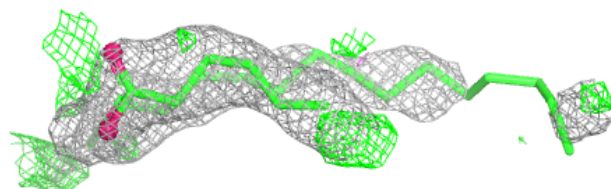
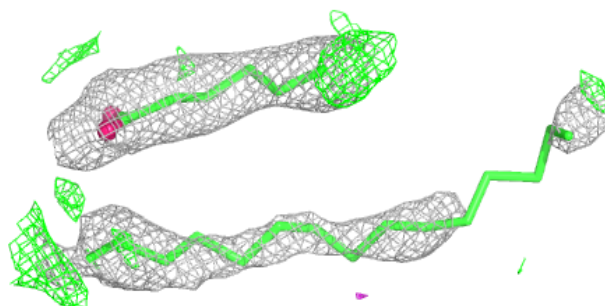


Electron density around STE H 104:

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

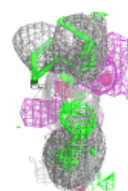
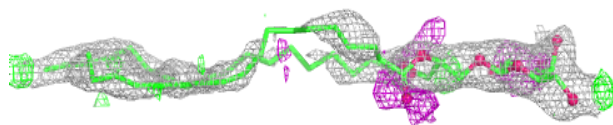
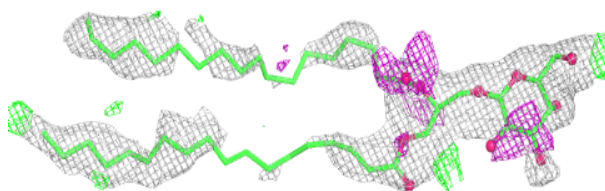
**Electron density around LMG d 410:**

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

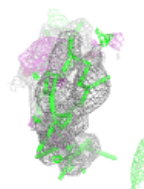
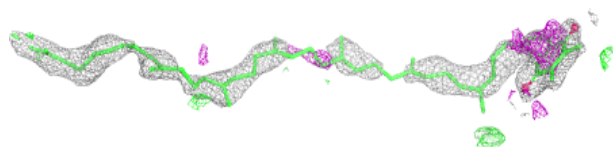
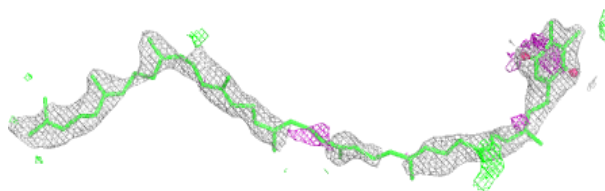


Electron density around LMG b 622:

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

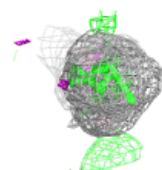
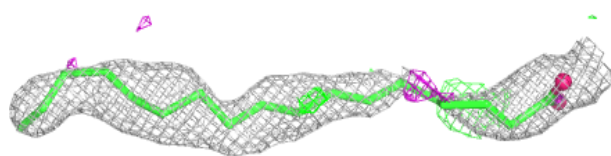
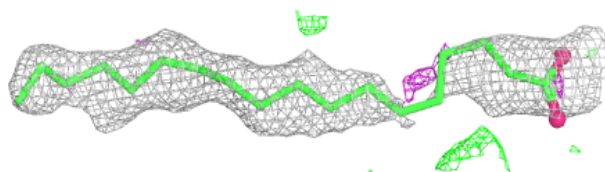
**Electron density around PL9 A 611:**

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

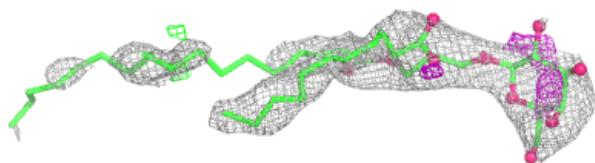
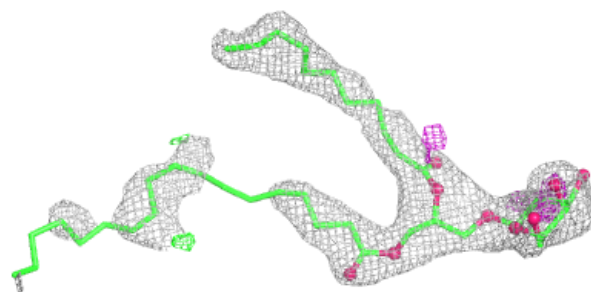


Electron density around STE b 625:

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

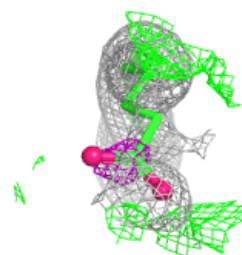
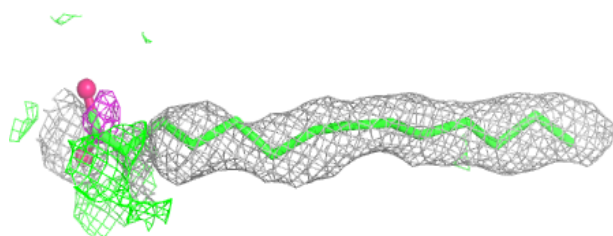
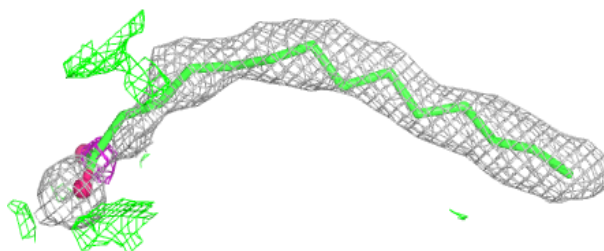
**Electron density around LMG c 521:**

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

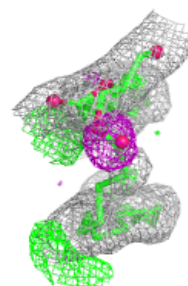
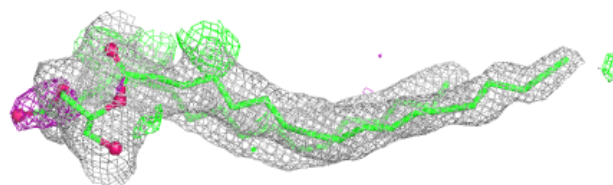
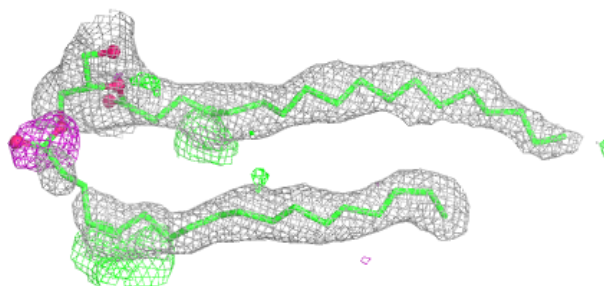


Electron density around STE d 412:

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

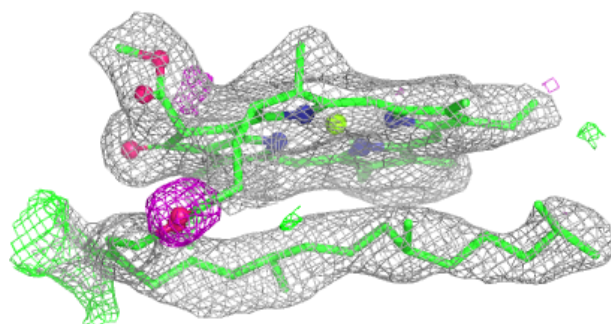
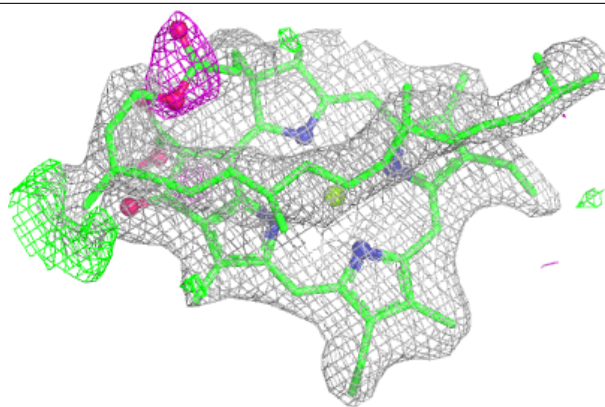
**Electron density around DGD a 615:**

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

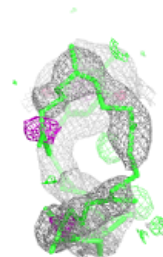
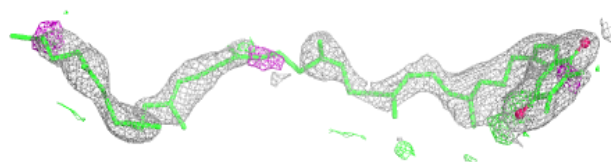
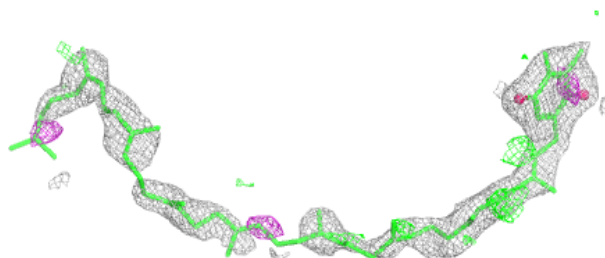


Electron density around CLA h 101:

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

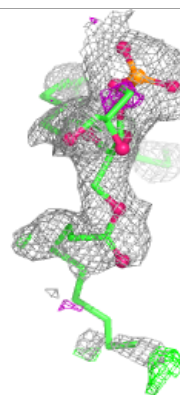
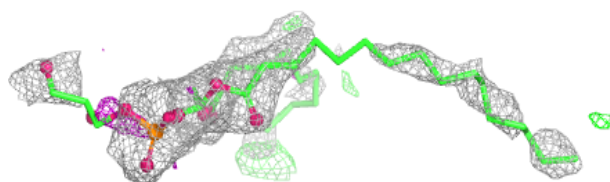
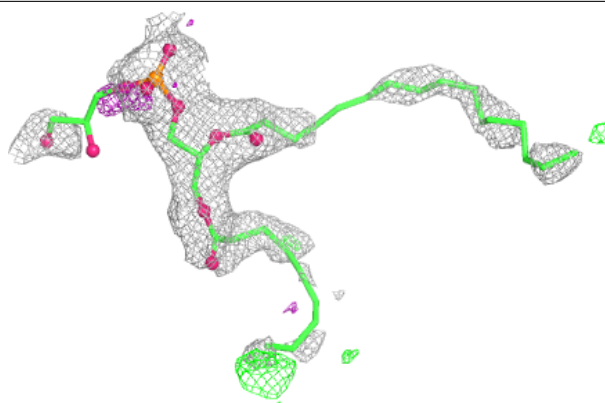
**Electron density around PL9 a 611:**

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

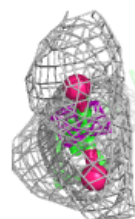
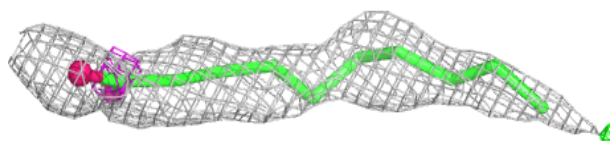
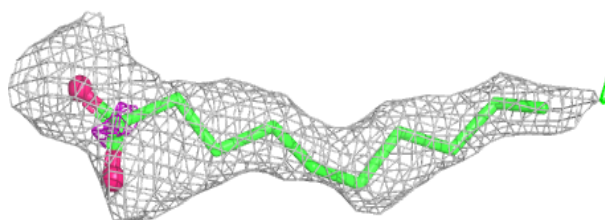


Electron density around LHG e 101:

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

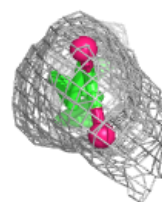
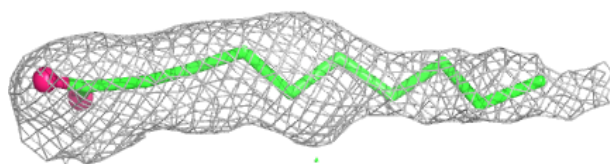
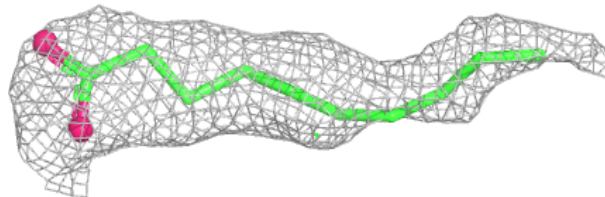
**Electron density around STE a 616:**

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

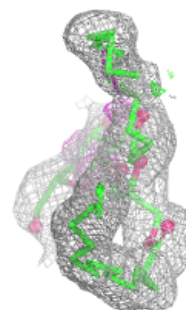
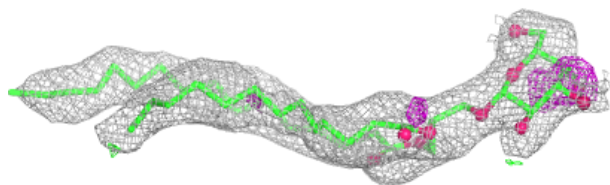
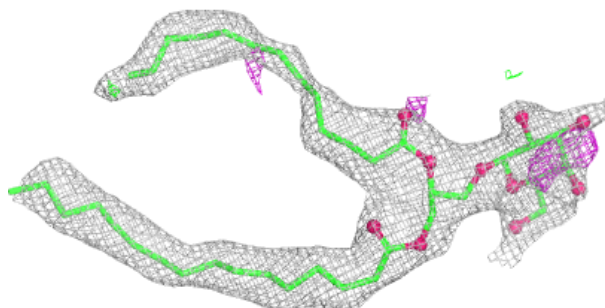


Electron density around STE k 103:

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

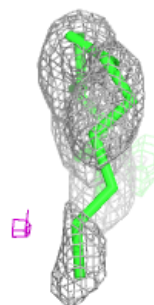
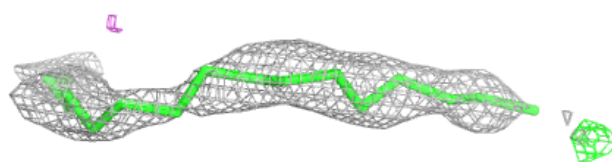
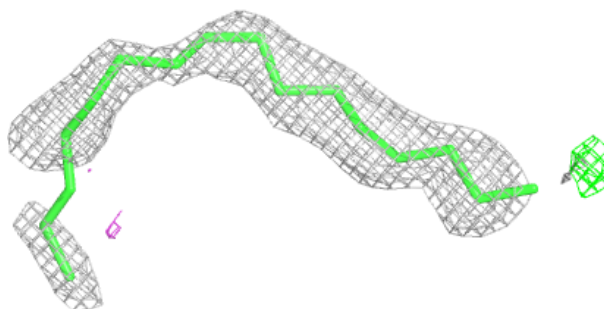
**Electron density around LMG A 613:**

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

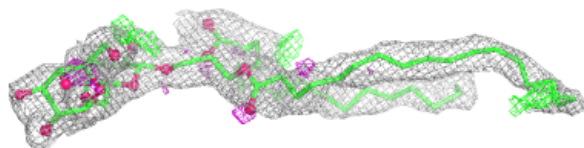
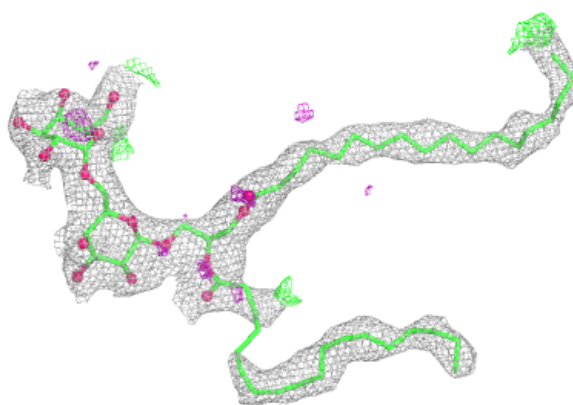


Electron density around STE B 625:

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

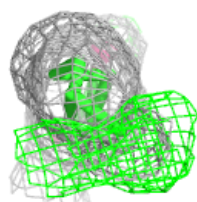
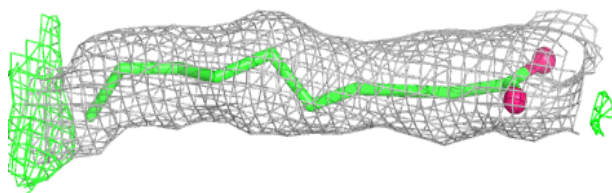
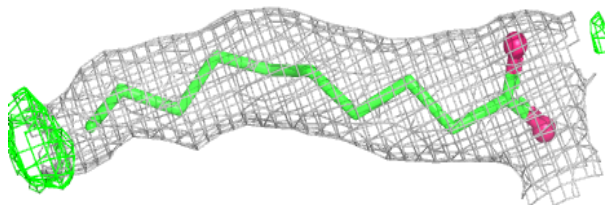
**Electron density around DGD A 617:**

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

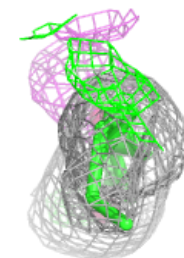
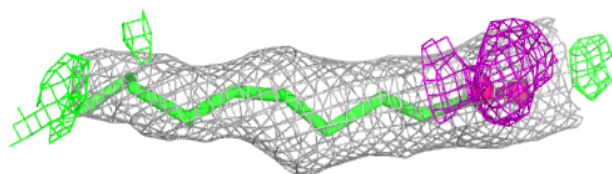
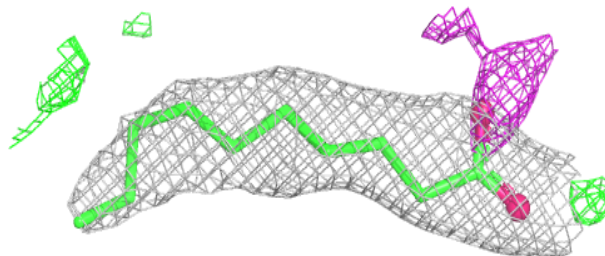


Electron density around STE J 101:

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

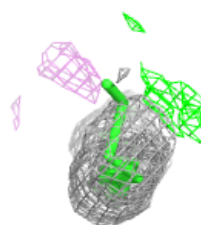
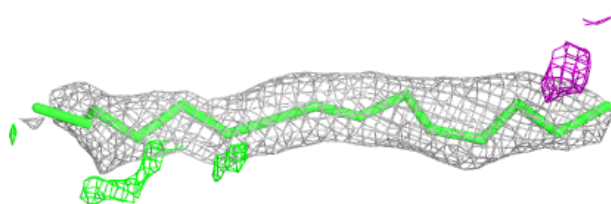
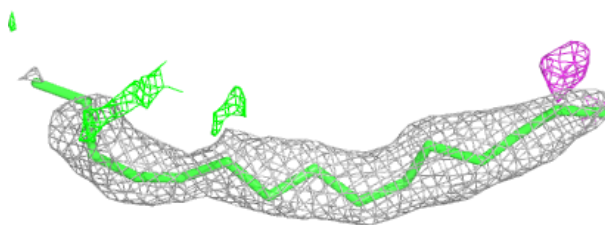
**Electron density around STE m 102:**

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

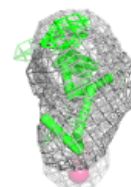
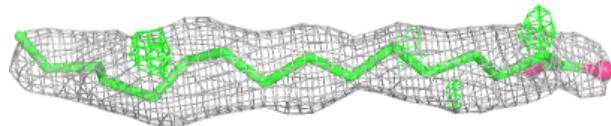
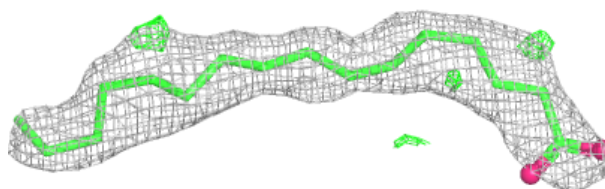


Electron density around STE b 624:

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

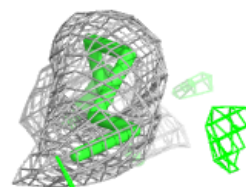
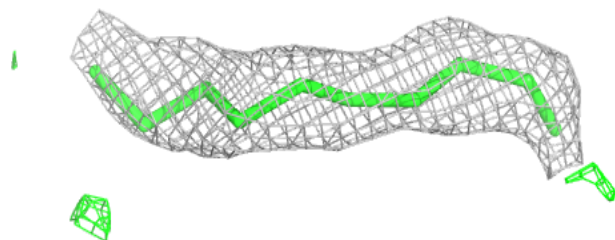
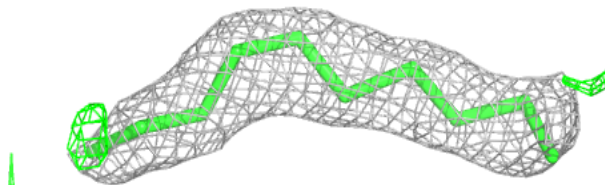
**Electron density around STE B 623:**

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

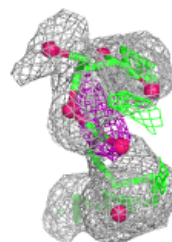
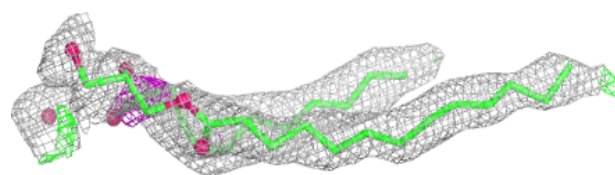
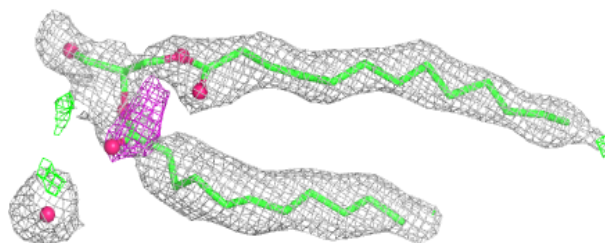


Electron density around STE b 626:

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

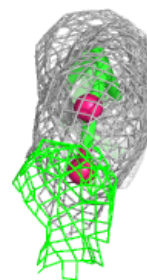
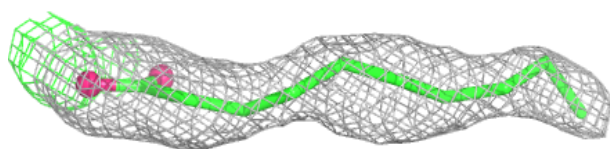
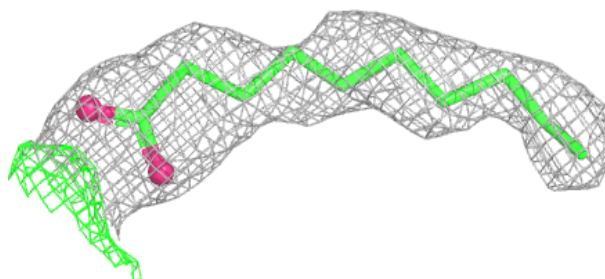
**Electron density around LMG D 410:**

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

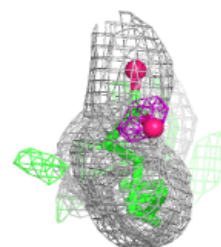
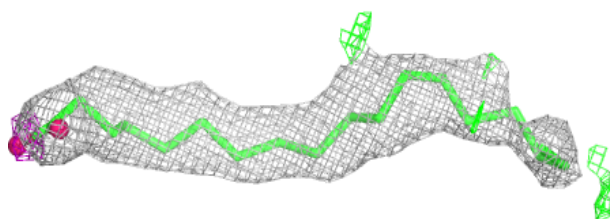
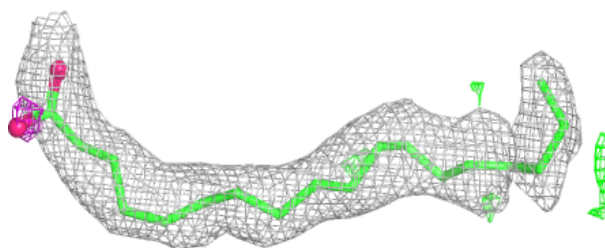


Electron density around STE C 521:

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

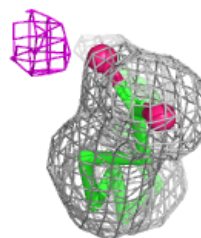
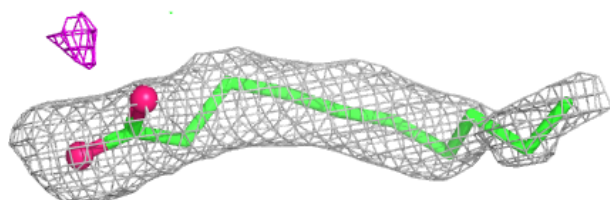
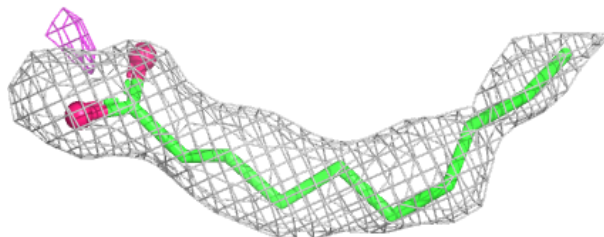
**Electron density around STE b 621:**

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

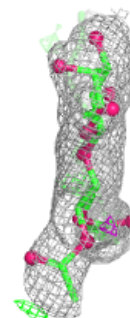
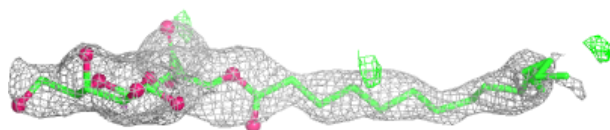
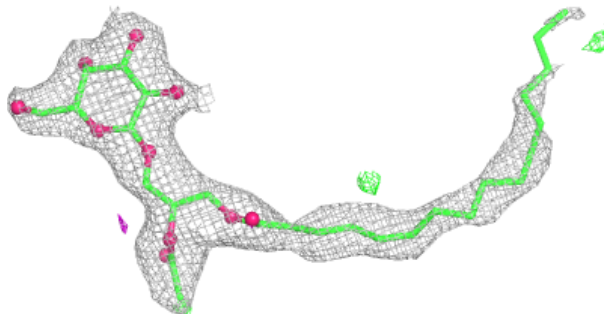


Electron density around STE B 624:

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

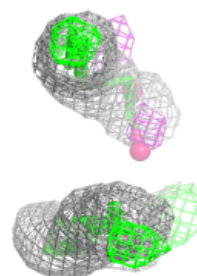
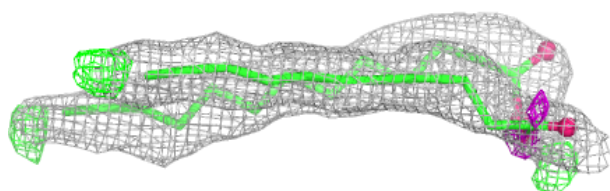
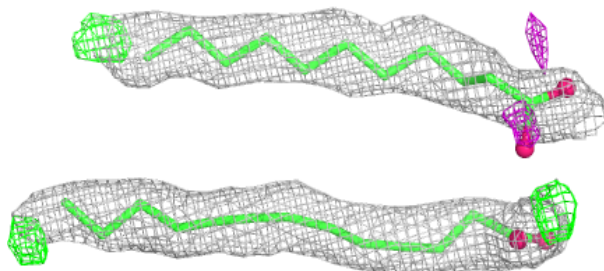
**Electron density around LMG c 519:**

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

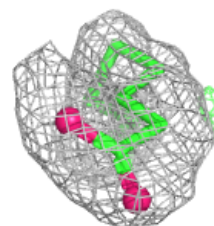
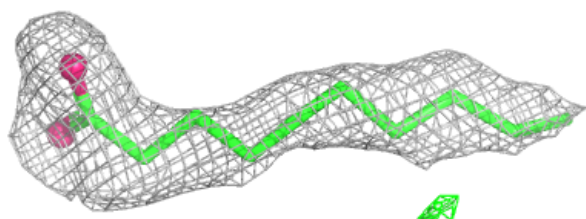
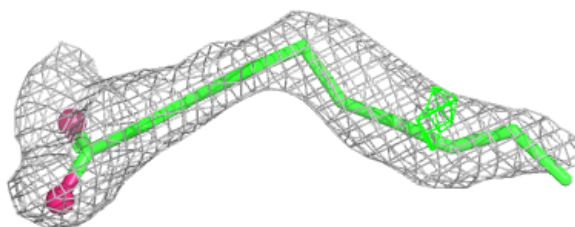


Electron density around LMG B 620:

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

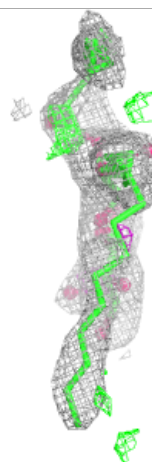
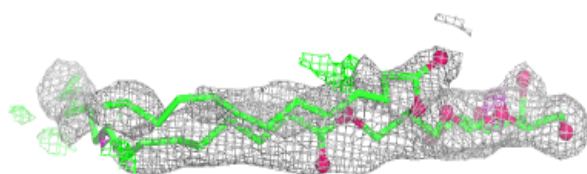
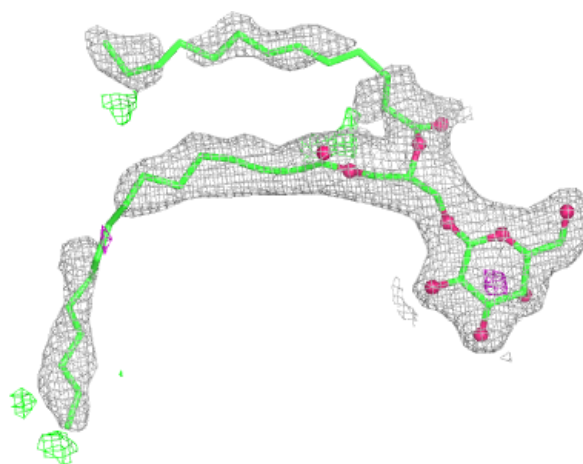
**Electron density around STE E 101:**

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



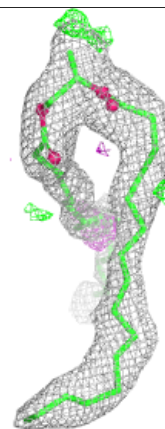
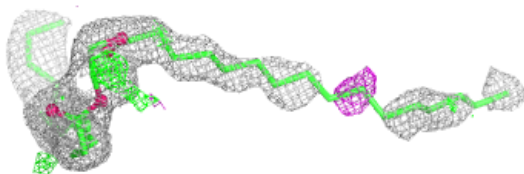
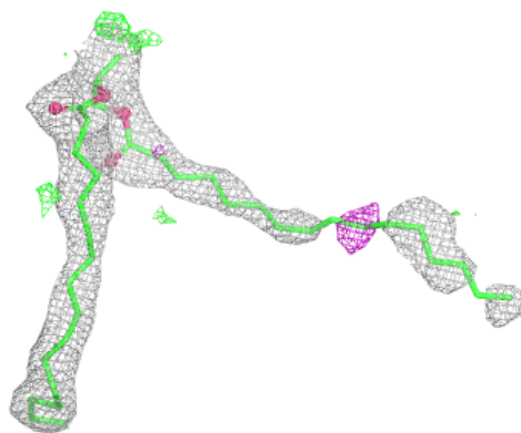
Electron density around LMG C 519:

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



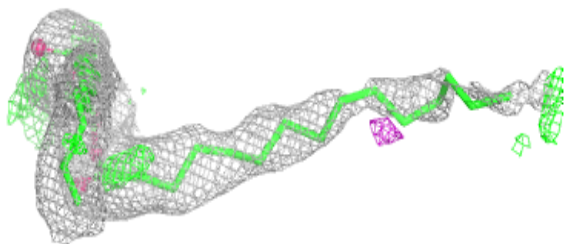
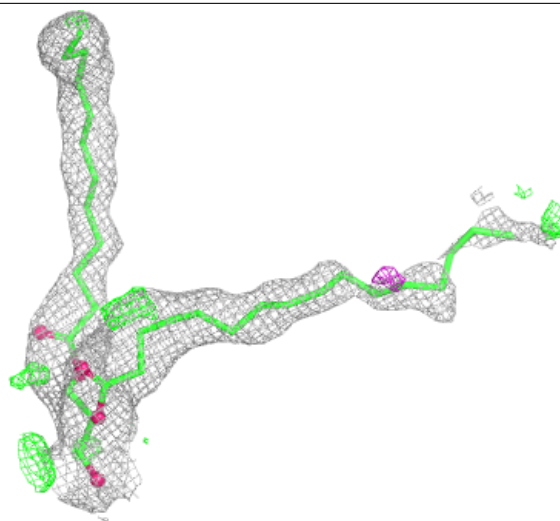
Electron density around SQD A 616:

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



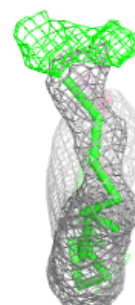
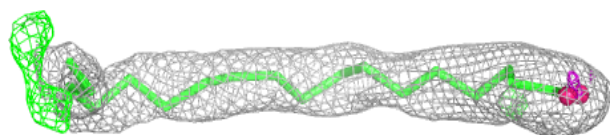
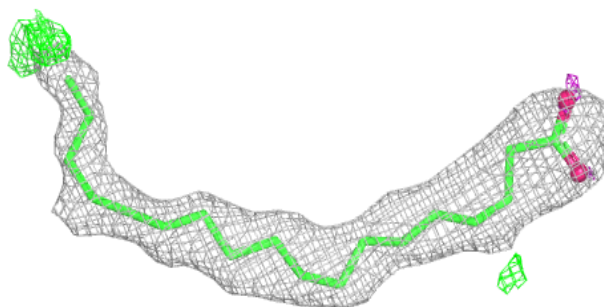
Electron density around SQD a 614:

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

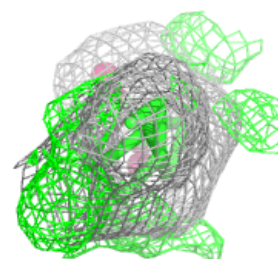
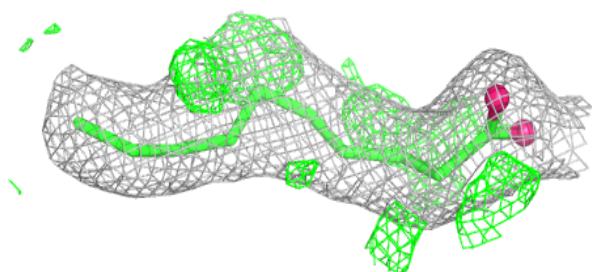
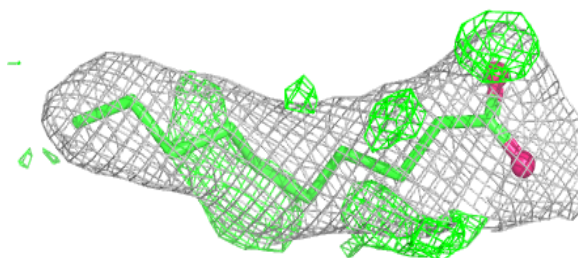


Electron density around STE x 101:

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

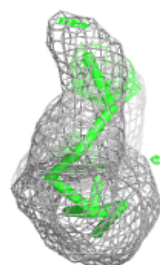
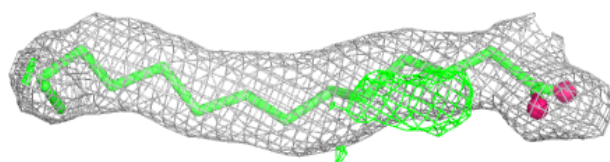
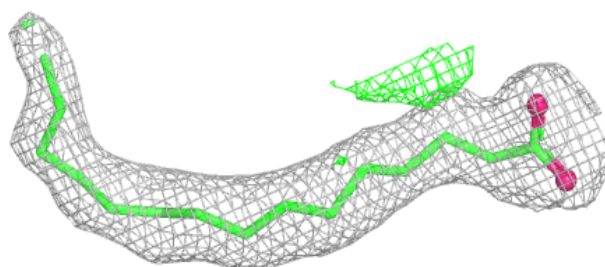
**Electron density around STE B 622:**

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

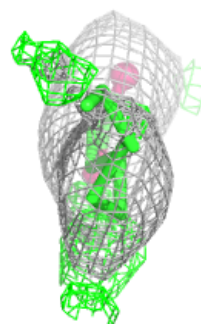
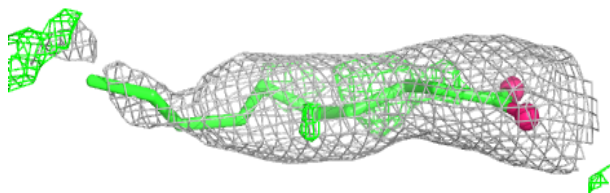
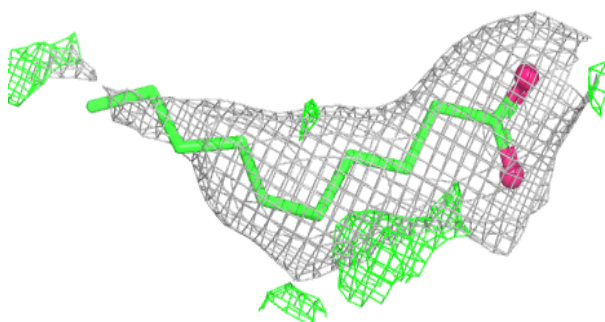


Electron density around STE B 619:

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

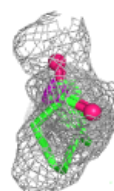
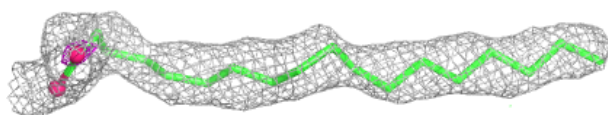
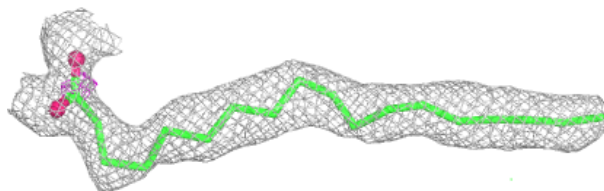
**Electron density around STE C 520:**

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

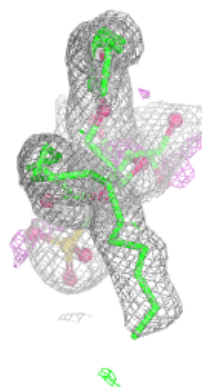
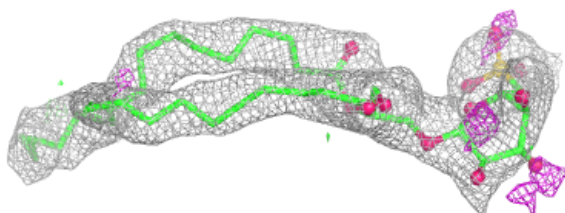
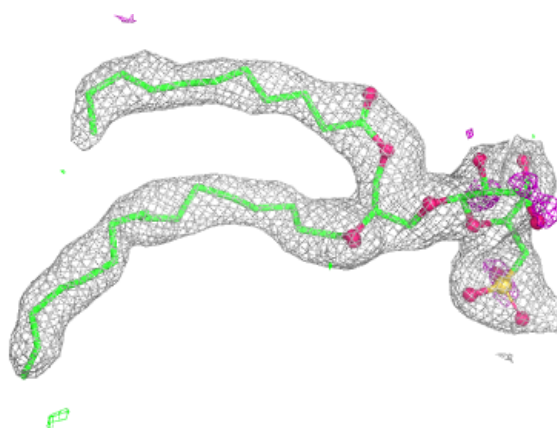


Electron density around STE c 520:

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

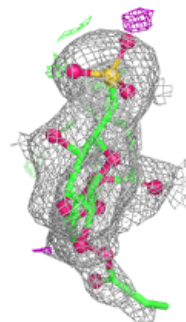
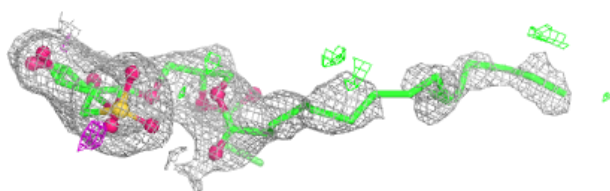
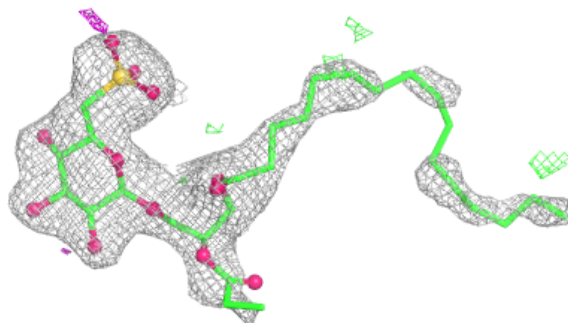
**Electron density around SQD b 619:**

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

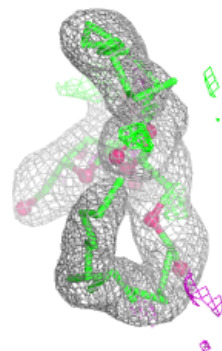
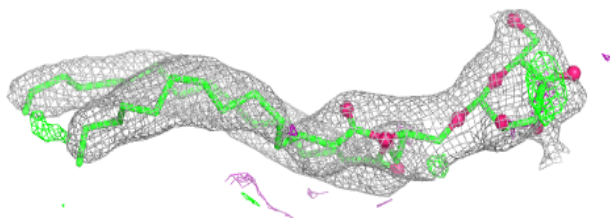
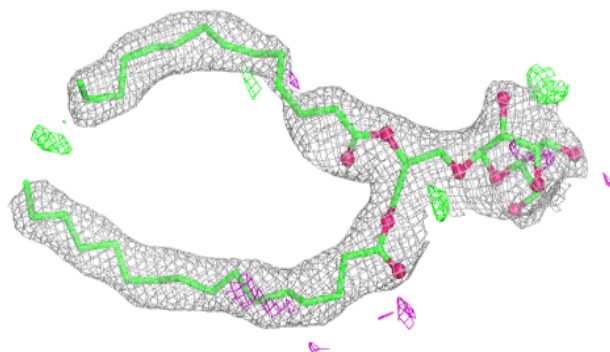


Electron density around SQD f 102:

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

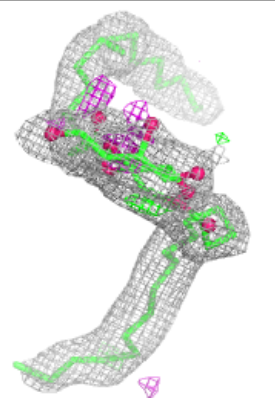
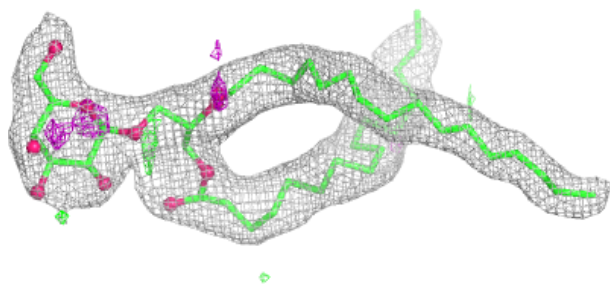
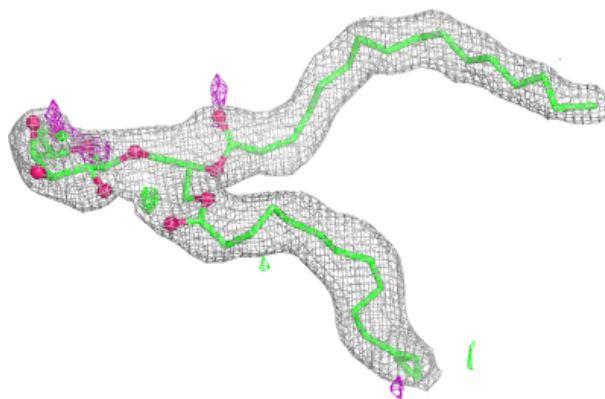
**Electron density around LMG c 522:**

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

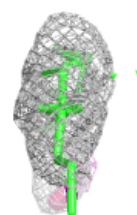
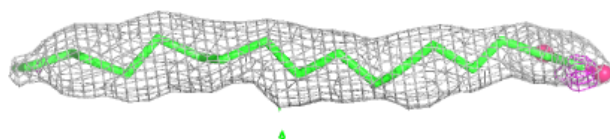
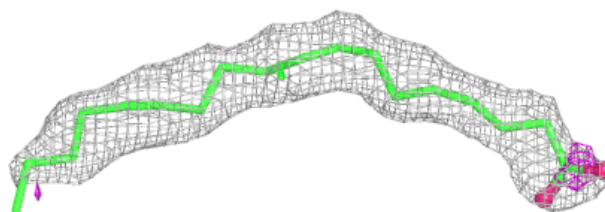


Electron density around LMG m 101:

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

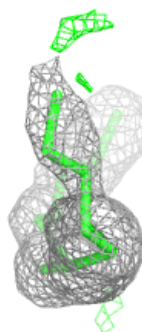
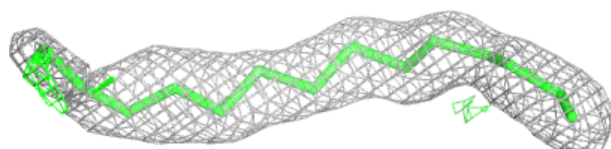
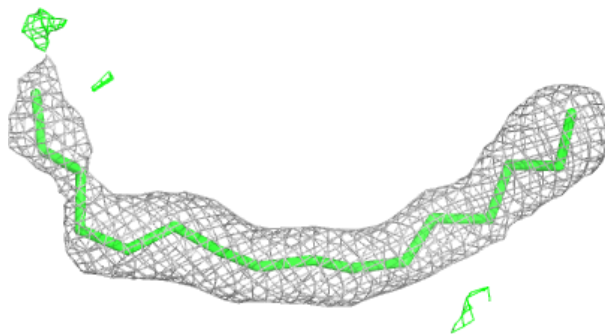
**Electron density around STE X 101:**

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

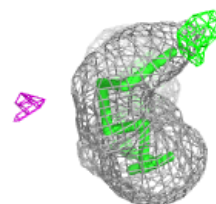
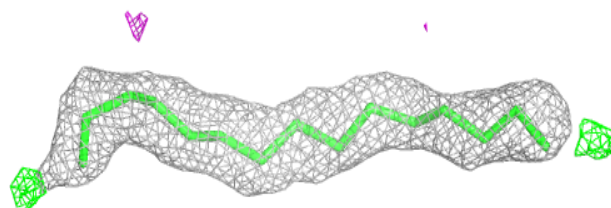
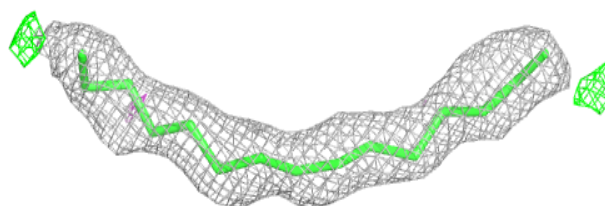


Electron density around STE b 620:

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

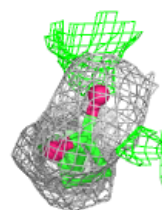
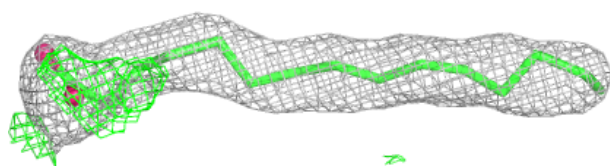
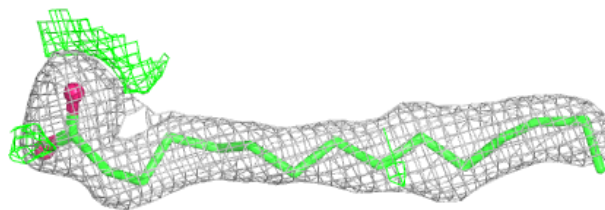
**Electron density around STE I 101:**

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

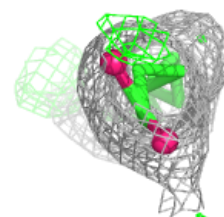
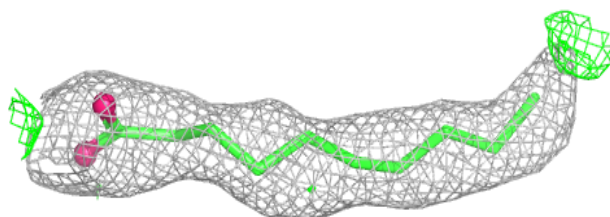
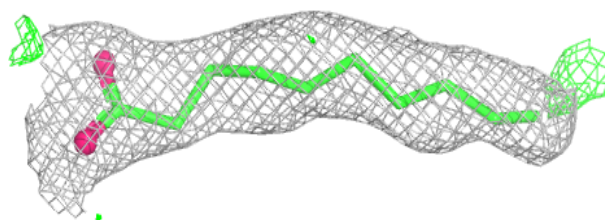


Electron density around STE d 413:

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

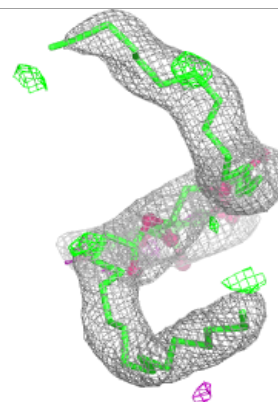
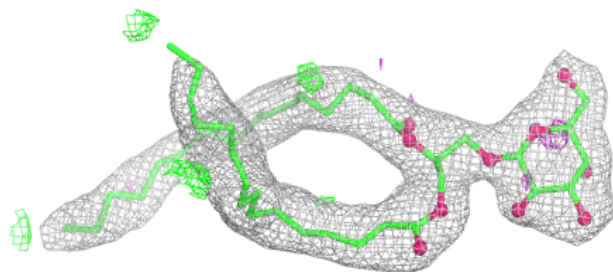
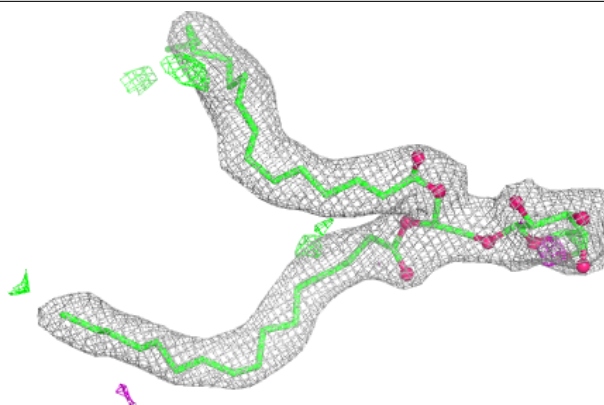
**Electron density around STE j 101:**

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

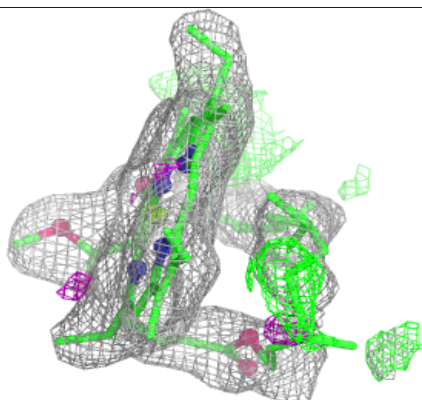
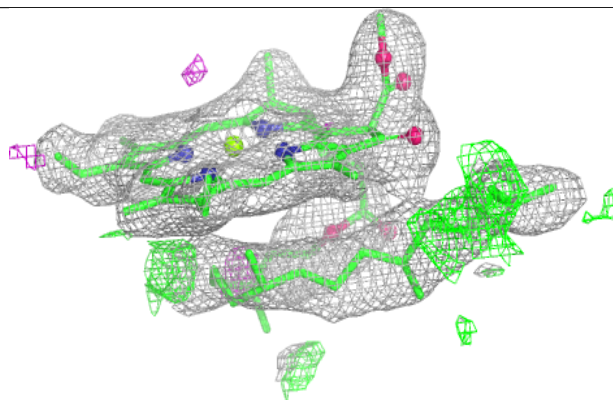
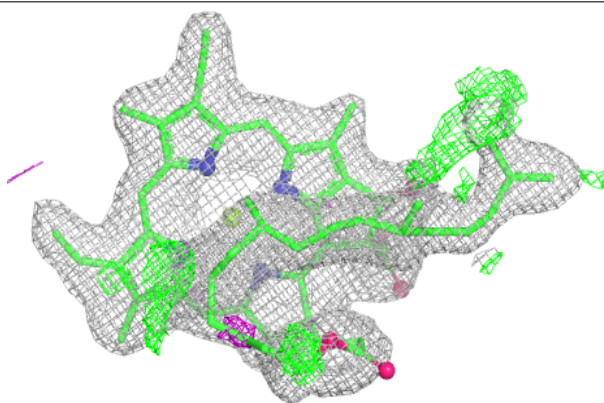


Electron density around LMG M 101:

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

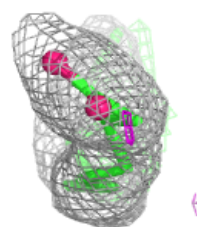
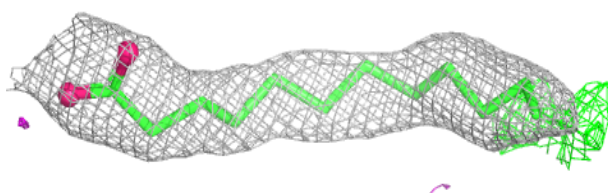
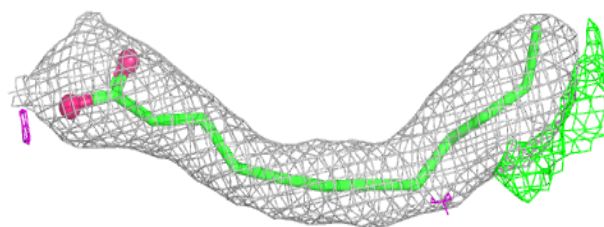
**Electron density around CLA H 101:**

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

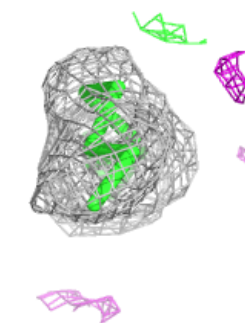
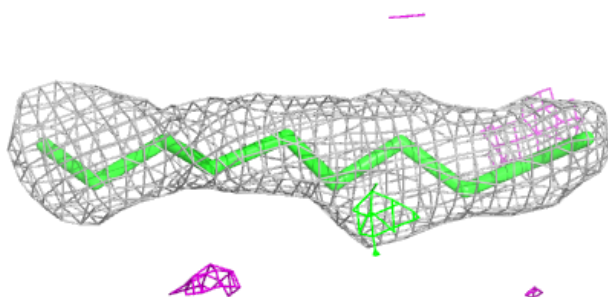


Electron density around STE t 102:

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

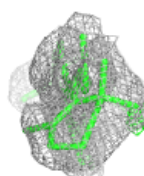
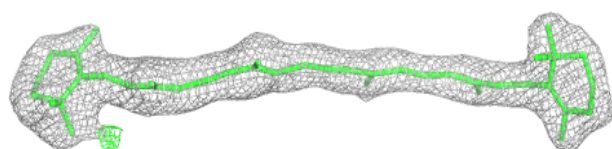
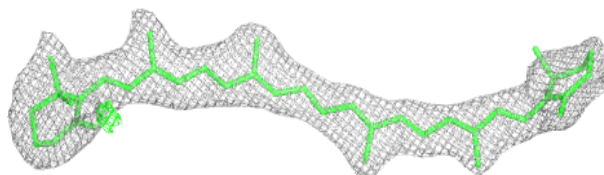
**Electron density around STE t 103:**

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

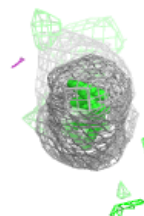
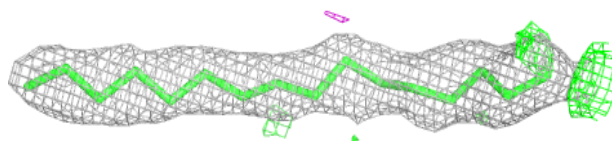
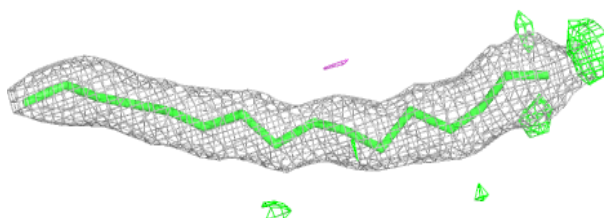


Electron density around BCR k 101:

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

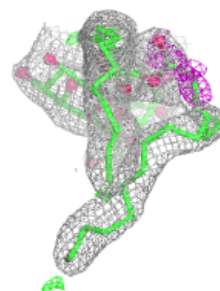
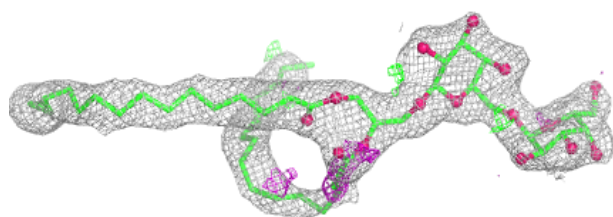
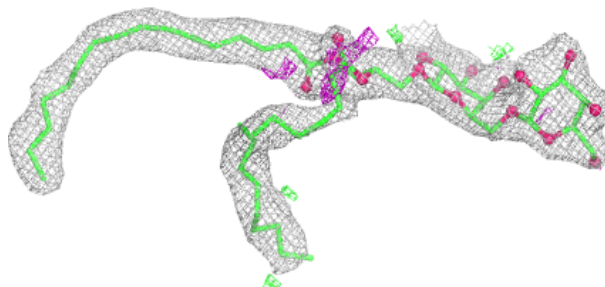
**Electron density around STE C 522:**

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

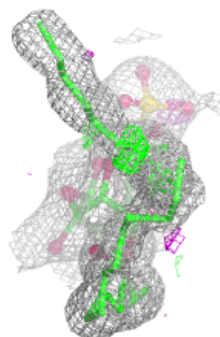
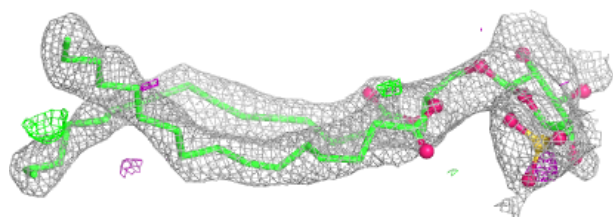
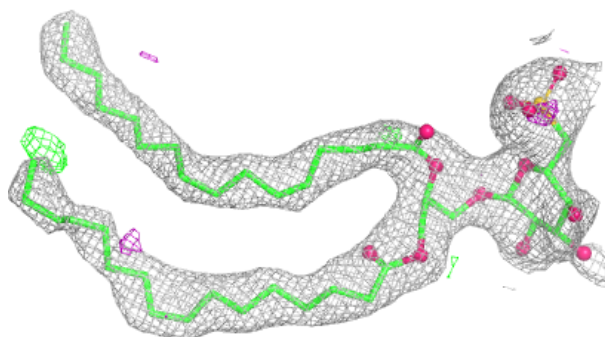


Electron density around DGD h 103:

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

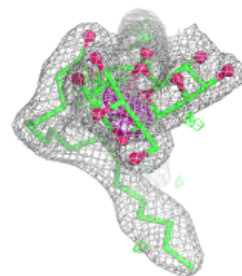
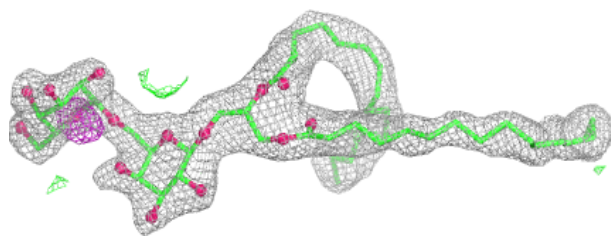
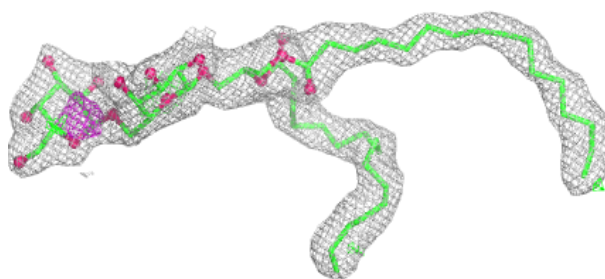
**Electron density around SQD B 621:**

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

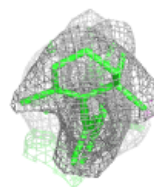
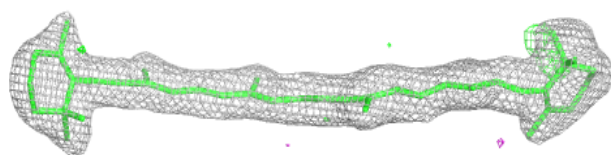
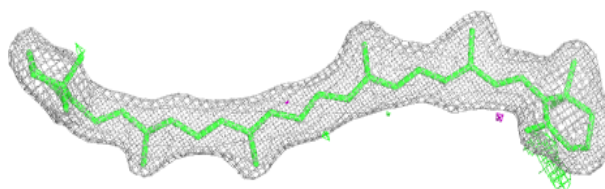


Electron density around DGD H 103:

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

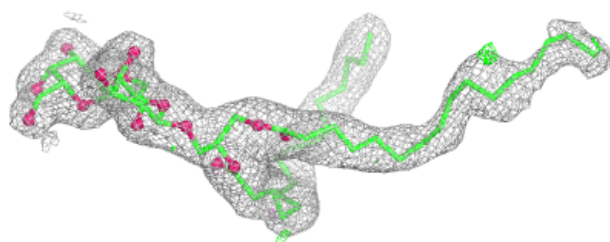
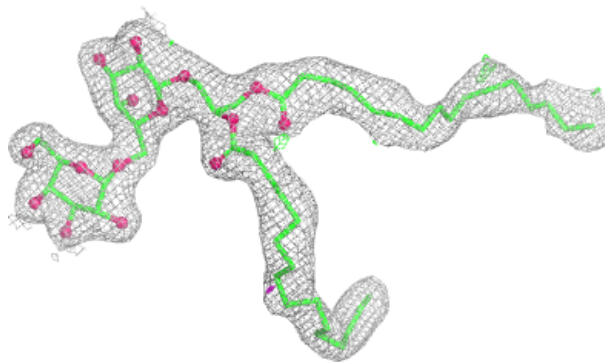
**Electron density around BCR K 101:**

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

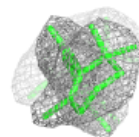
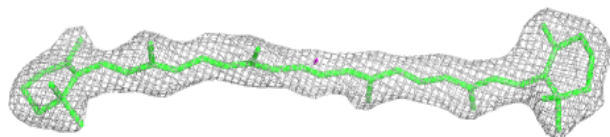
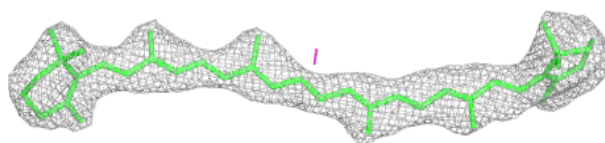


Electron density around DGD c 517:

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

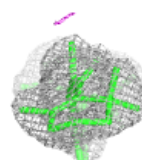
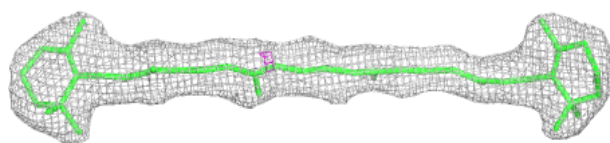
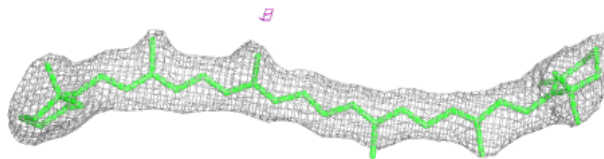
**Electron density around BCR c 514:**

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

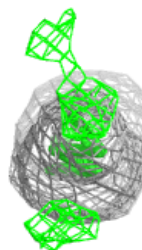
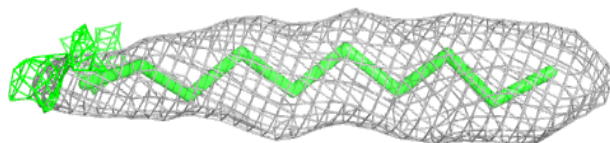
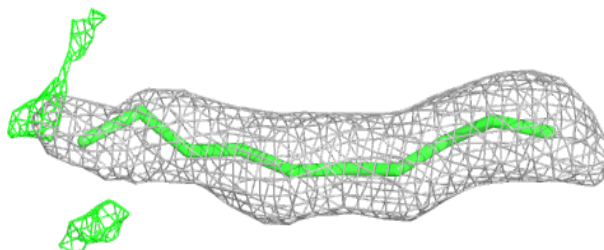


Electron density around BCR C 514:

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

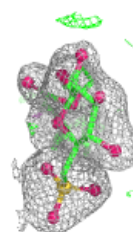
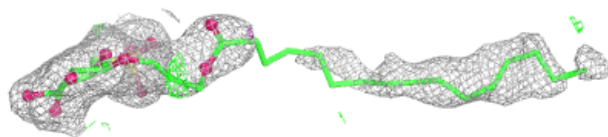
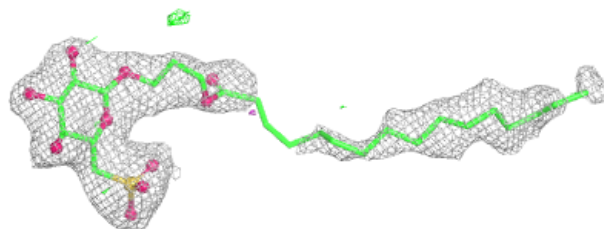
**Electron density around STE M 103:**

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



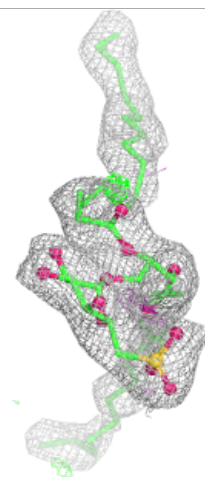
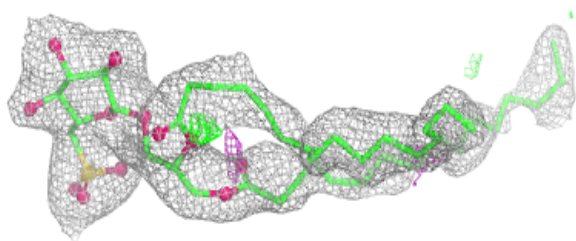
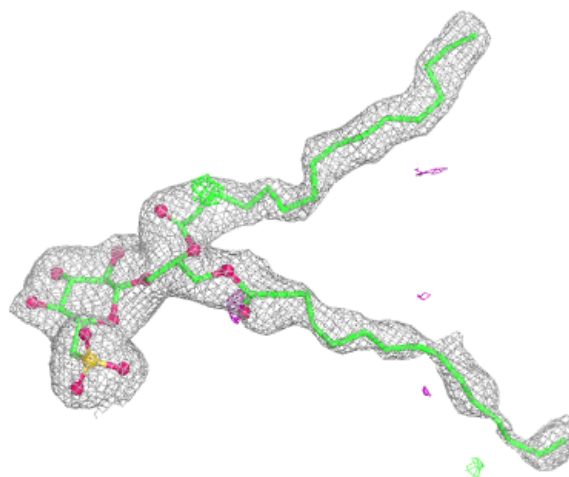
Electron density around SQD F 102:

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



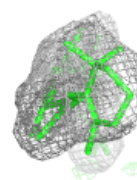
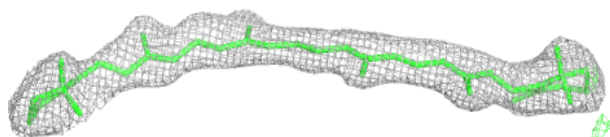
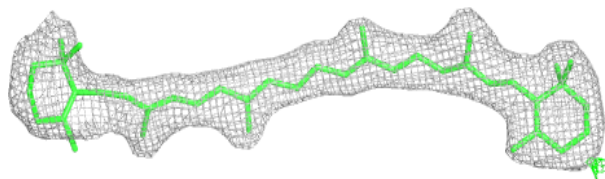
Electron density around SQD a 613:

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

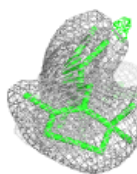
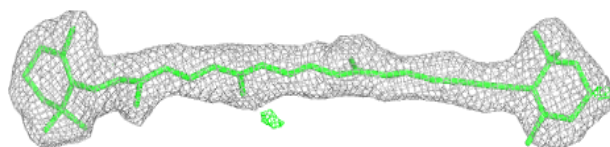
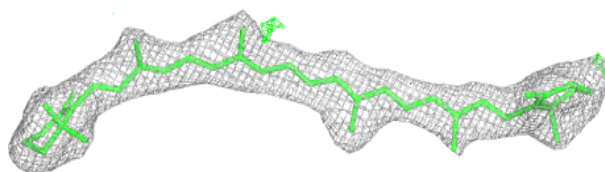


Electron density around BCR d 405:

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

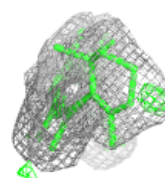
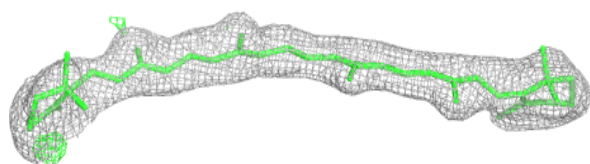
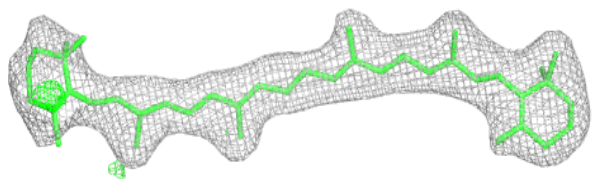
**Electron density around BCR h 102:**

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

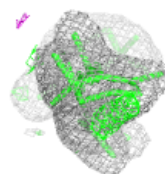
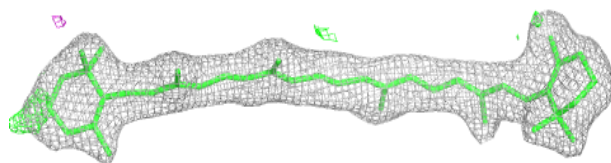
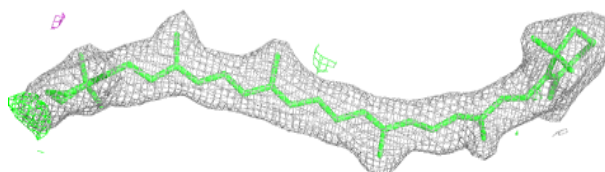


Electron density around BCR D 405:

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

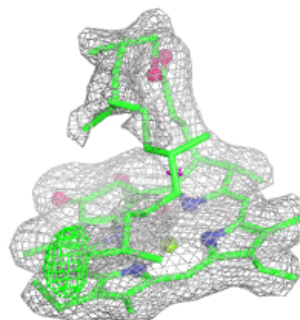
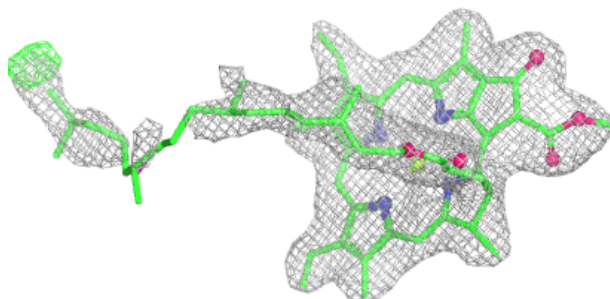
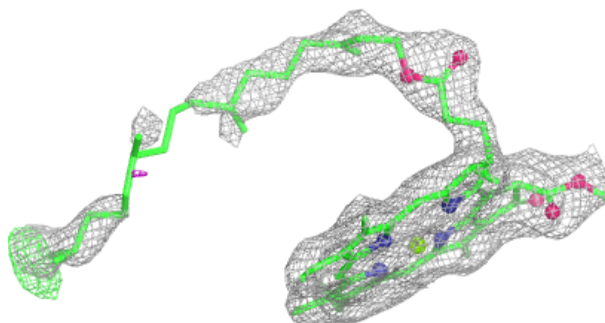
**Electron density around BCR H 102:**

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



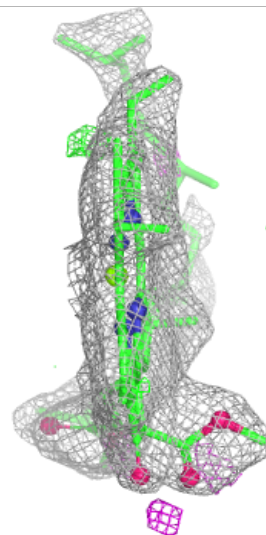
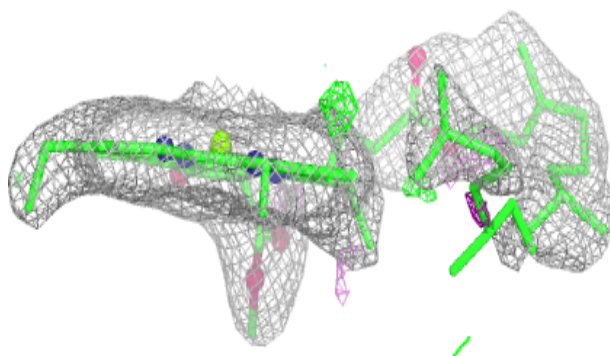
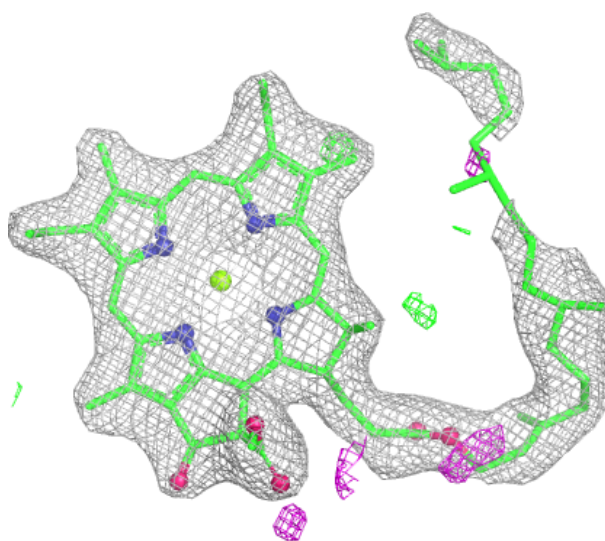
Electron density around CLA C 513:

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



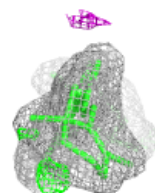
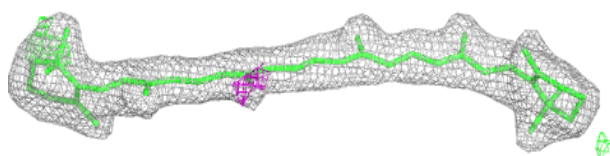
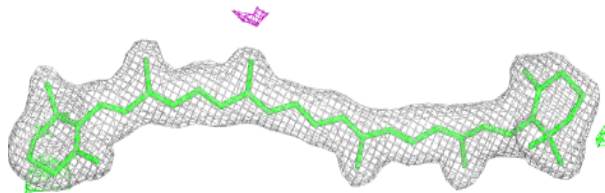
Electron density around CLA c 512:

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

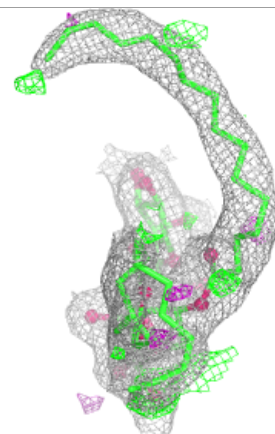
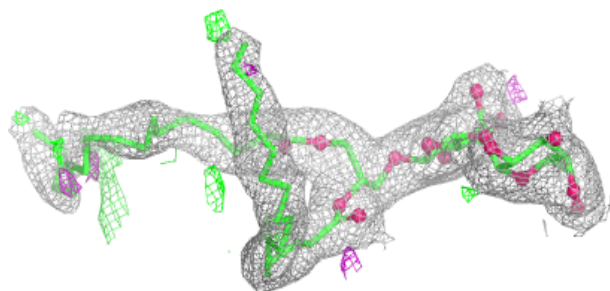
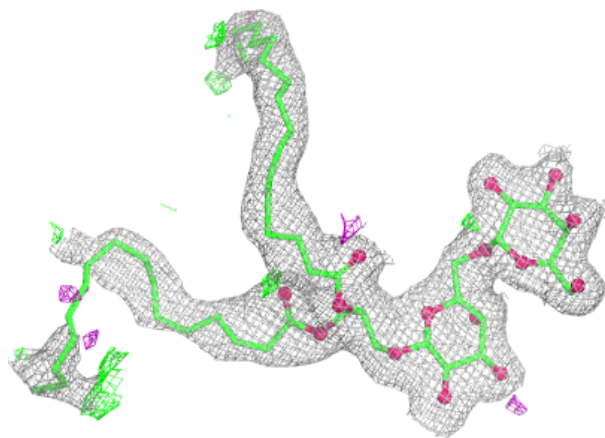


Electron density around BCR B 618:

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

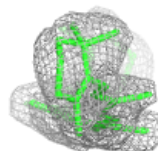
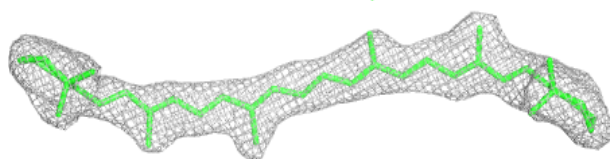
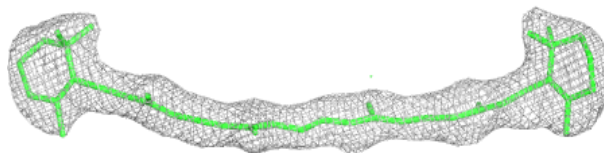
**Electron density around DGD C 517:**

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

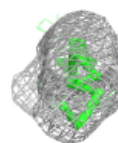
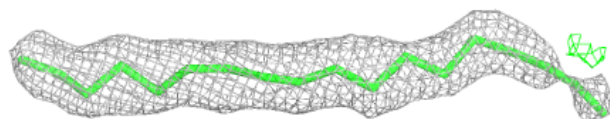
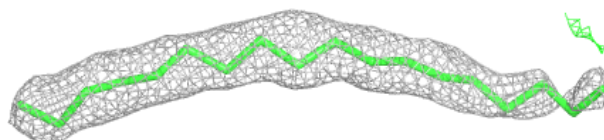


Electron density around BCR k 102:

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

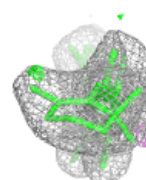
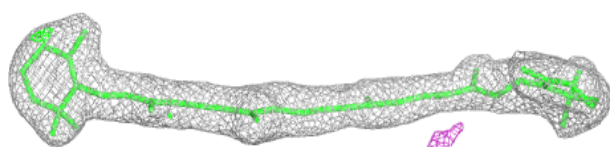
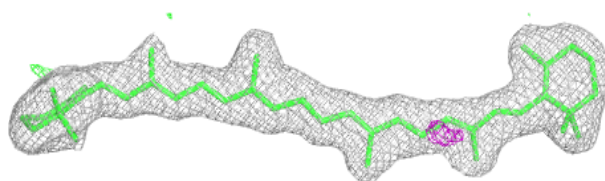
**Electron density around STE l 101:**

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

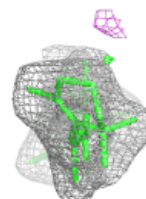
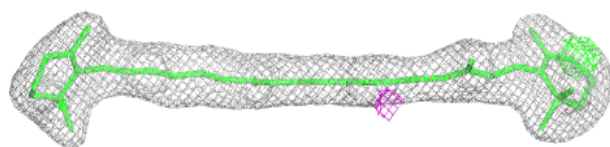
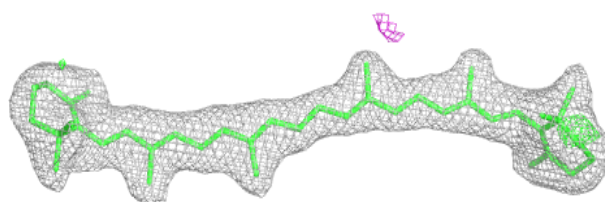


Electron density around BCR b 616:

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

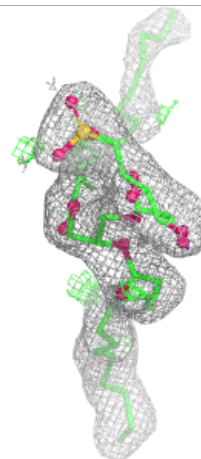
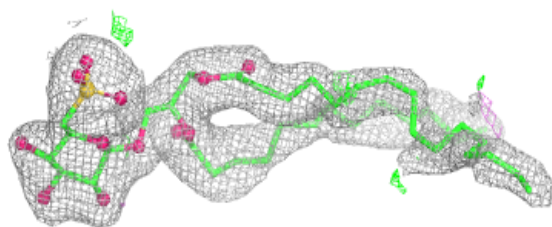
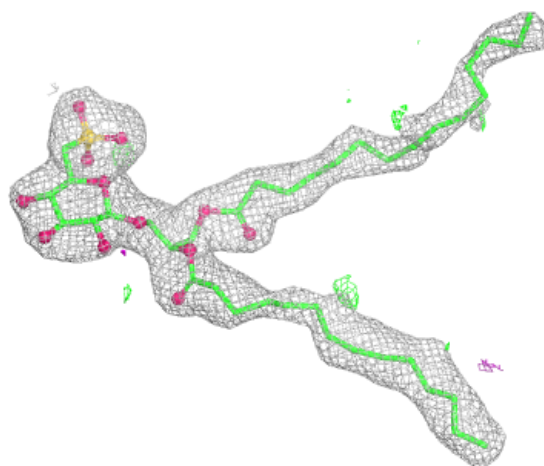
**Electron density around BCR b 617:**

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



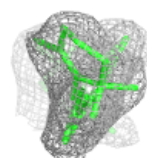
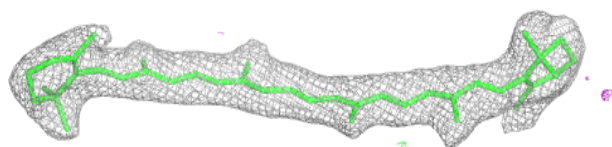
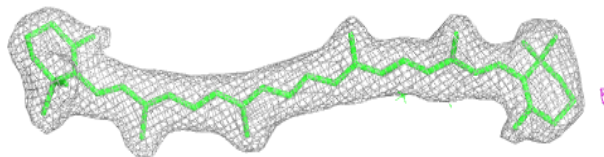
Electron density around SQD A 614:

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

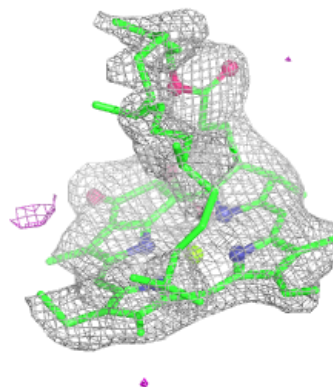
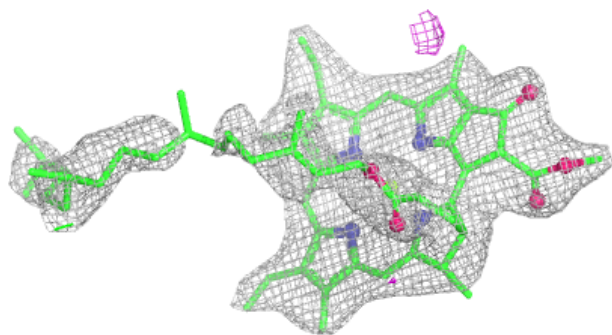
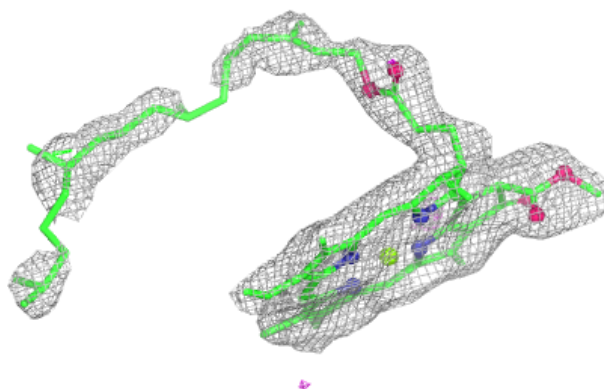


Electron density around BCR b 618:

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

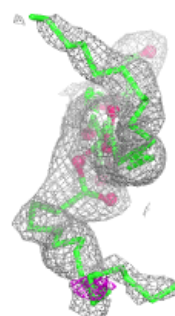
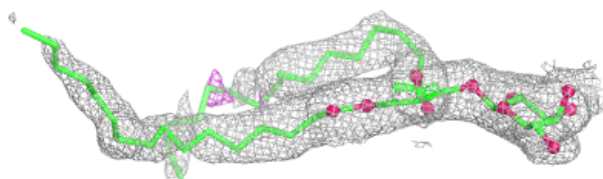
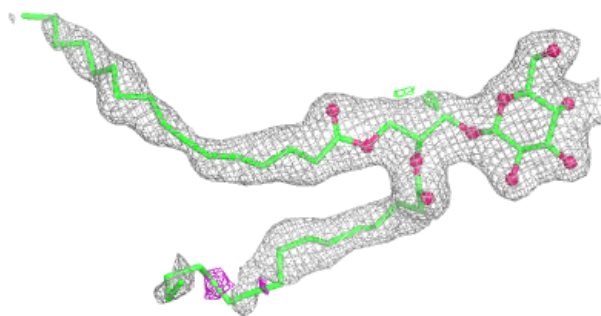
**Electron density around CLA c 513:**

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

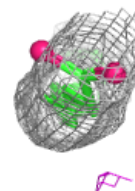
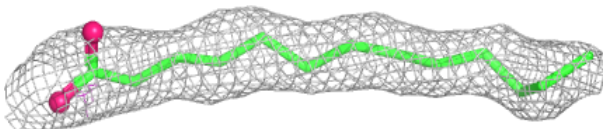
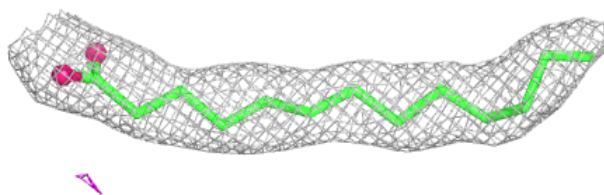


Electron density around LMG D 407:

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

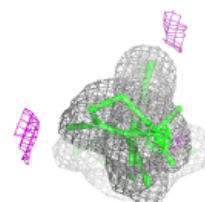
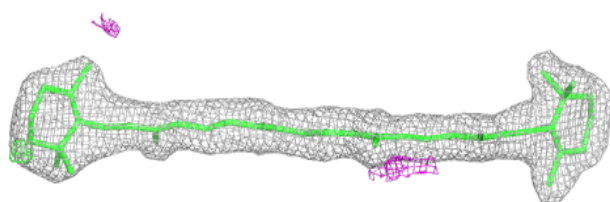
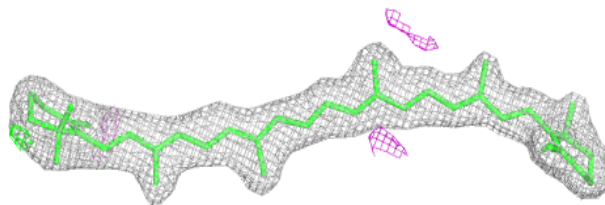
**Electron density around STE M 102:**

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

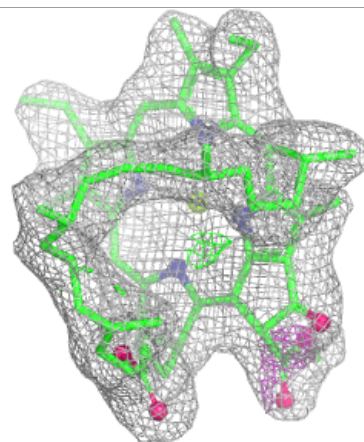
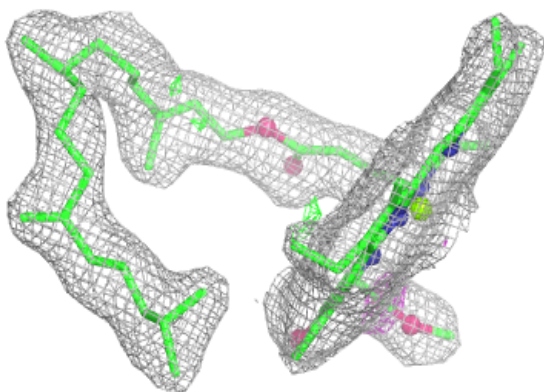
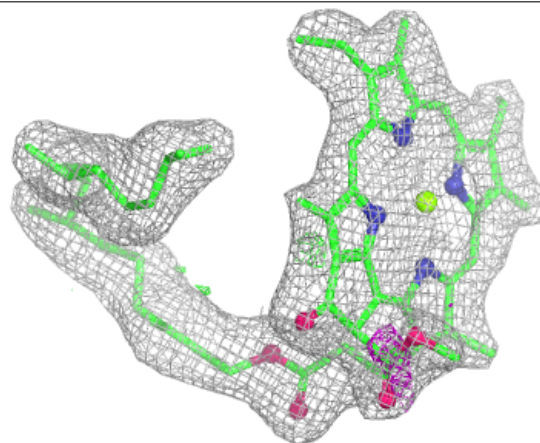


Electron density around BCR C 515:

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

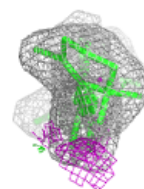
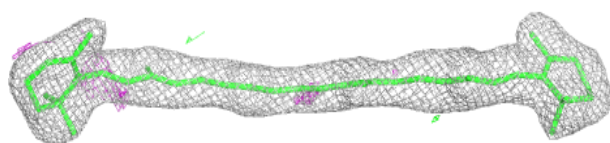
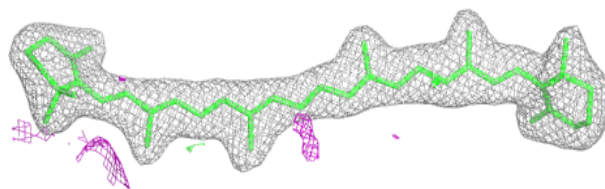
**Electron density around CLA c 503:**

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



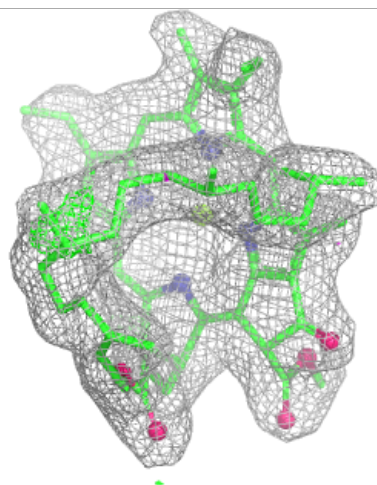
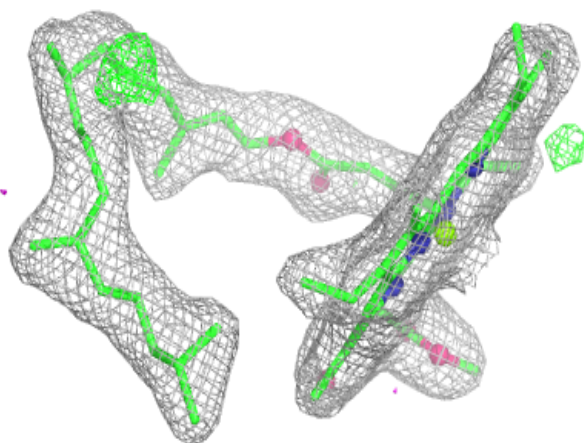
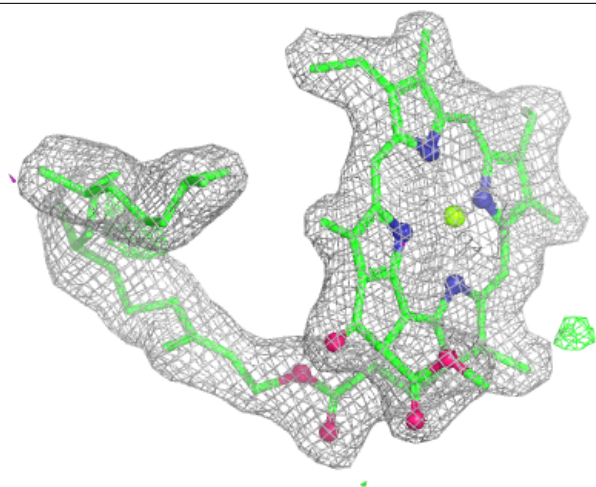
Electron density around BCR B 617:

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



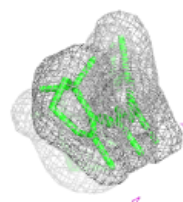
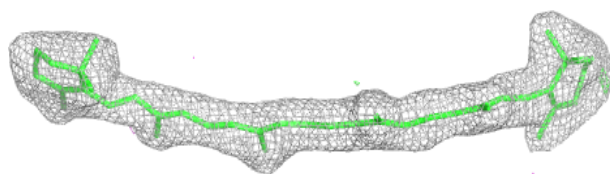
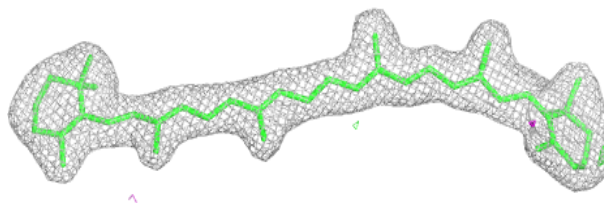
Electron density around CLA C 503:

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

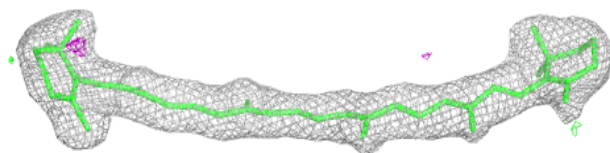
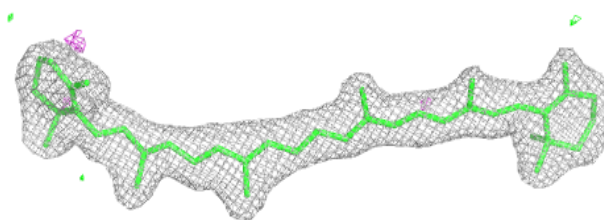


Electron density around BCR t 101:

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

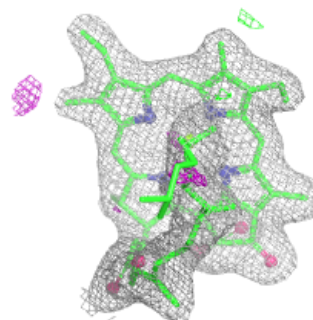
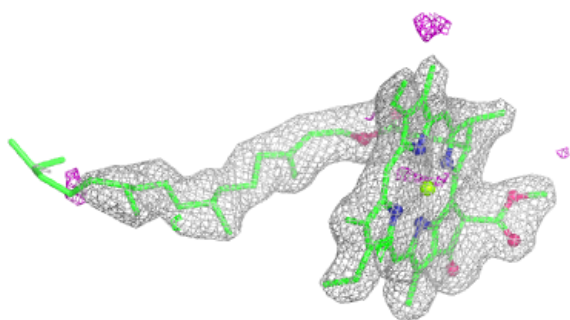
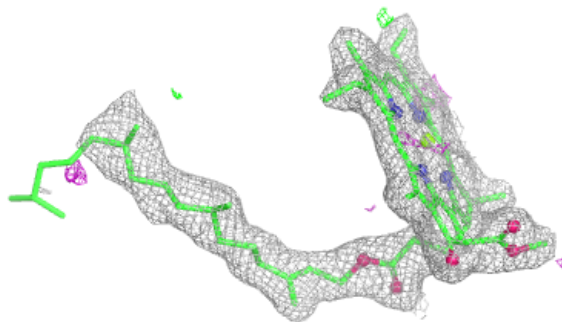
**Electron density around BCR T 101:**

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

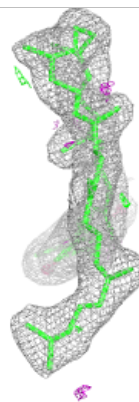
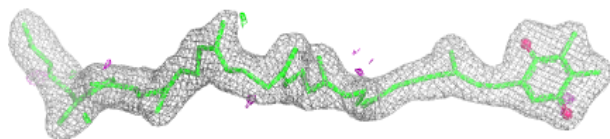
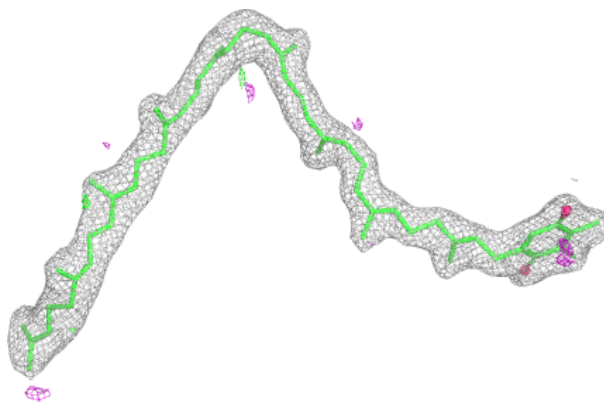


Electron density around CLA C 508:

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

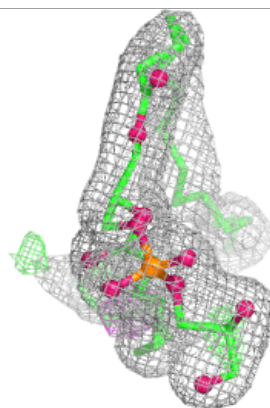
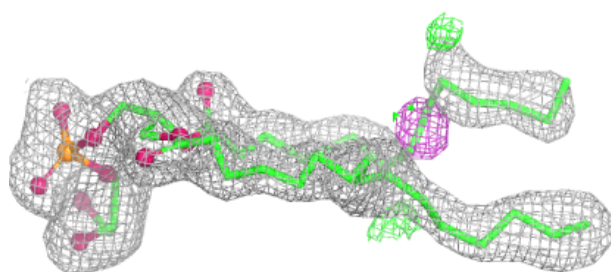
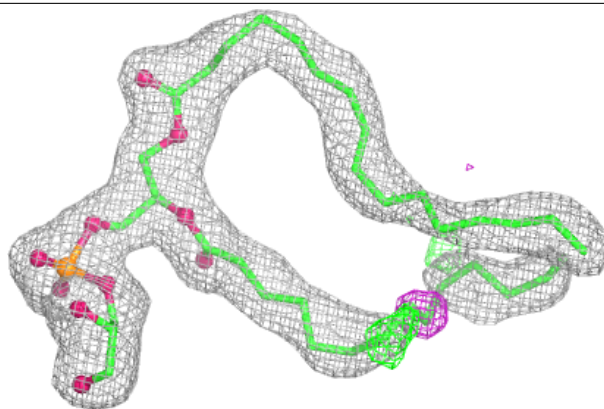
**Electron density around PL9 D 406:**

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

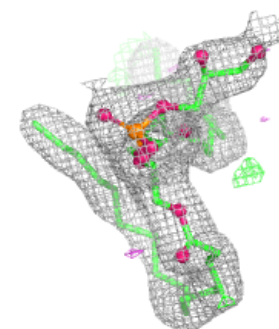
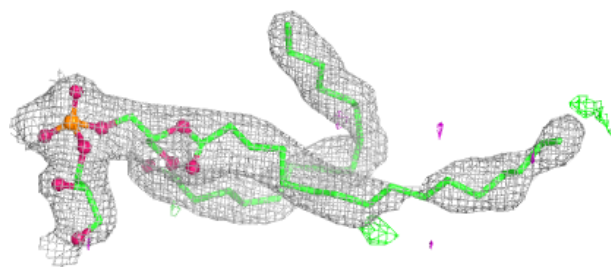
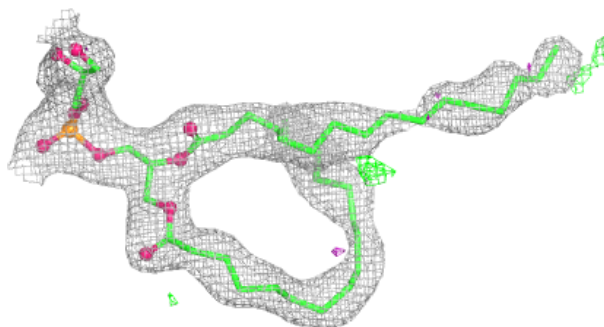


Electron density around LHG D 409:

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

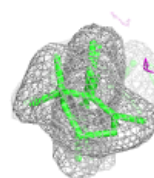
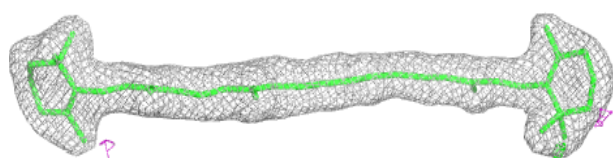
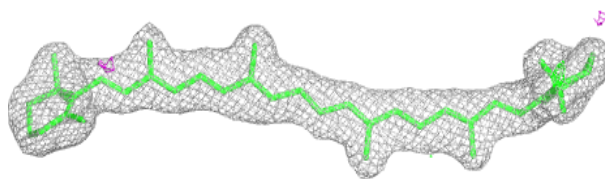
**Electron density around LHG d 407:**

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

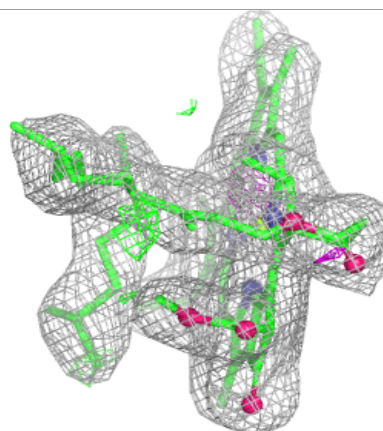
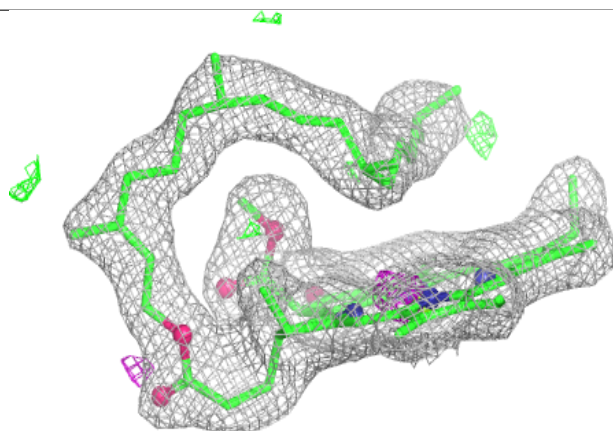
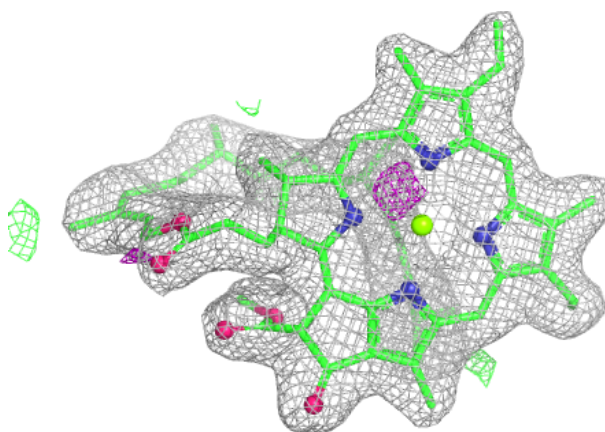


Electron density around BCR A 610:

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

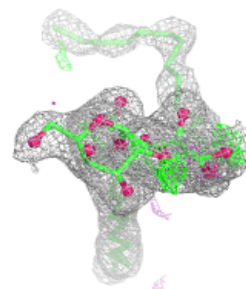
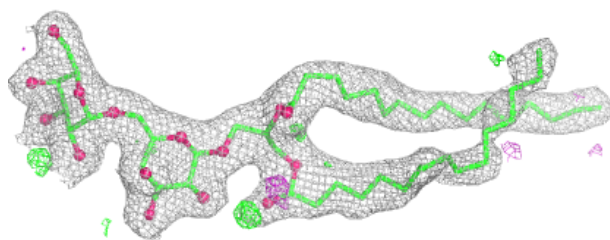
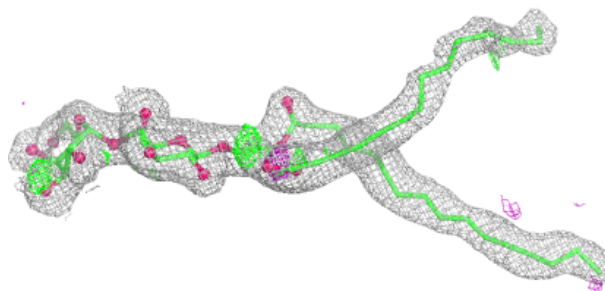
**Electron density around CLA C 510:**

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

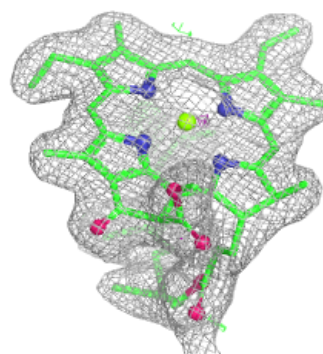
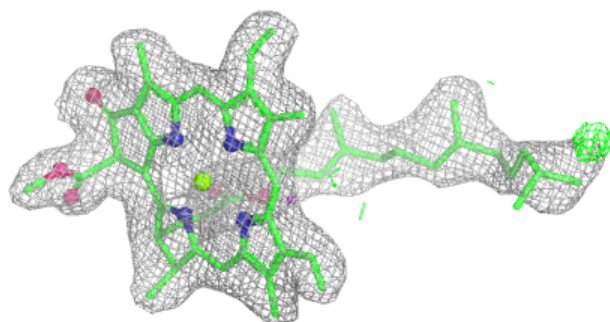
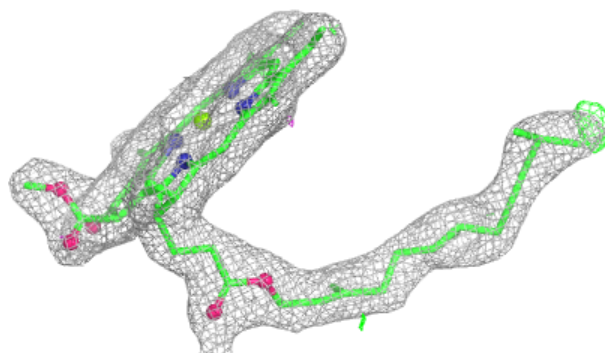


Electron density around DGD C 516:

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

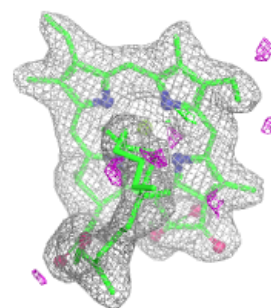
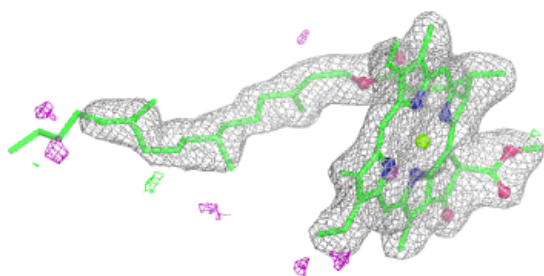
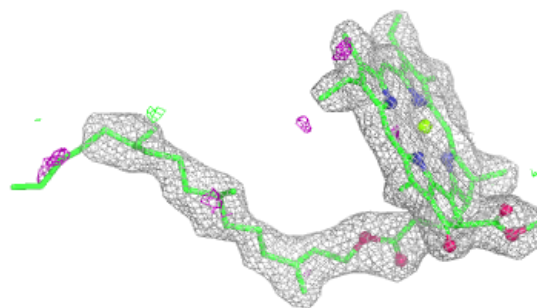
**Electron density around CLA c 504:**

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



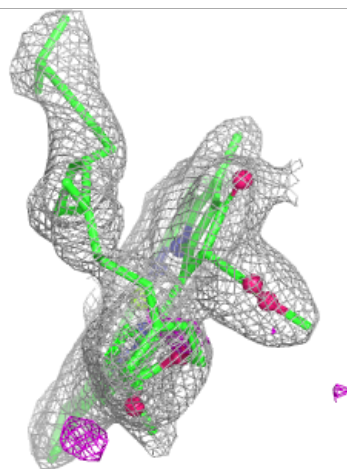
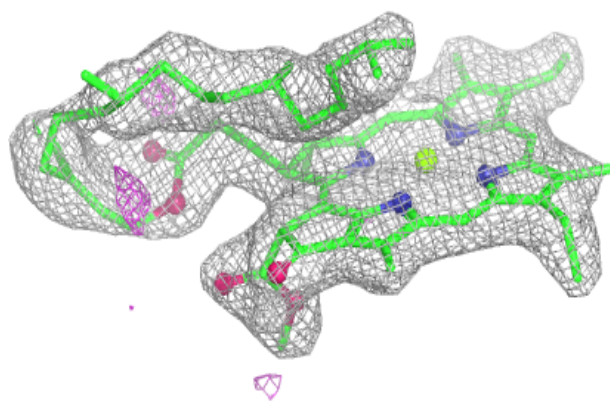
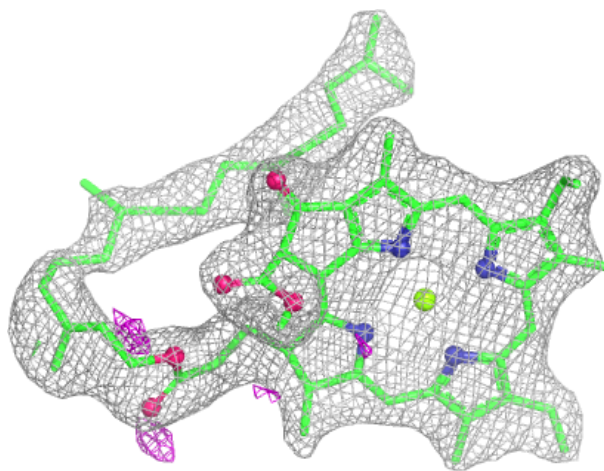
Electron density around CLA c 508:

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



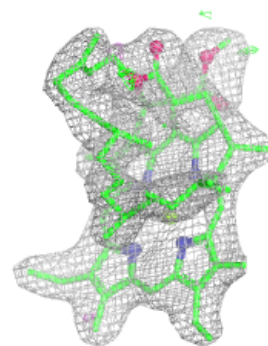
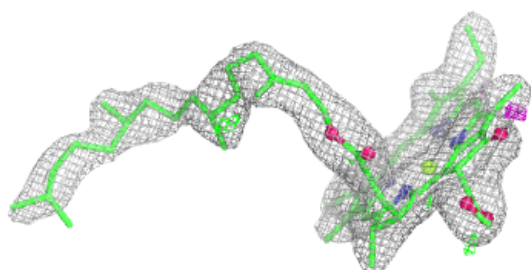
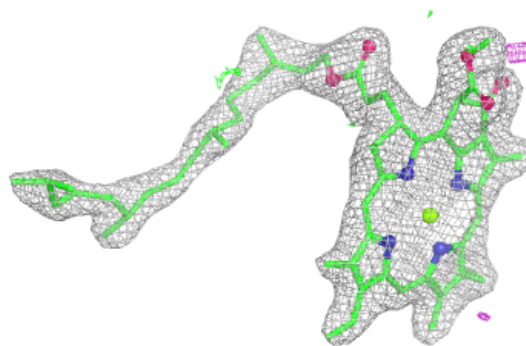
Electron density around CLA c 509:

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

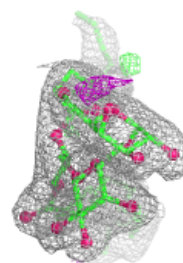
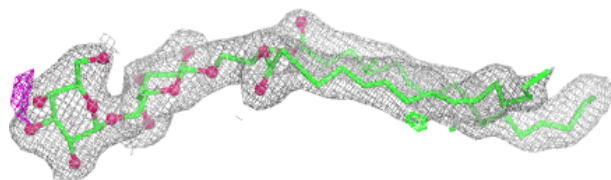
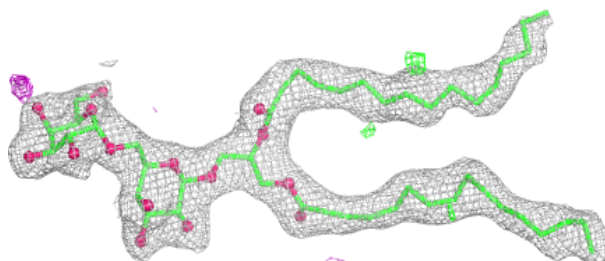


Electron density around CLA c 511:

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

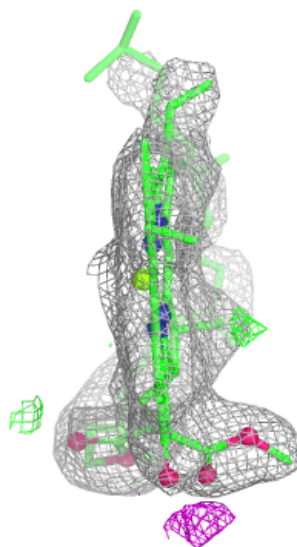
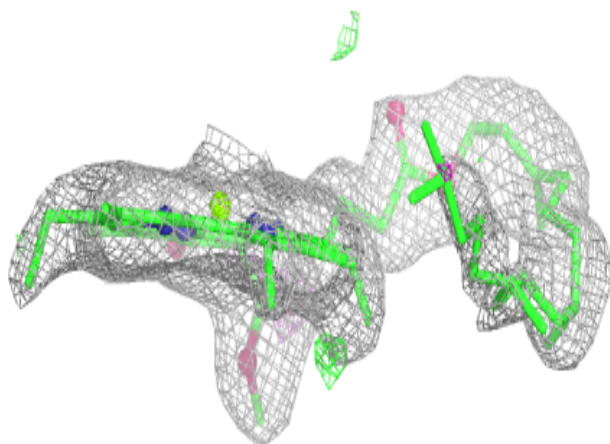
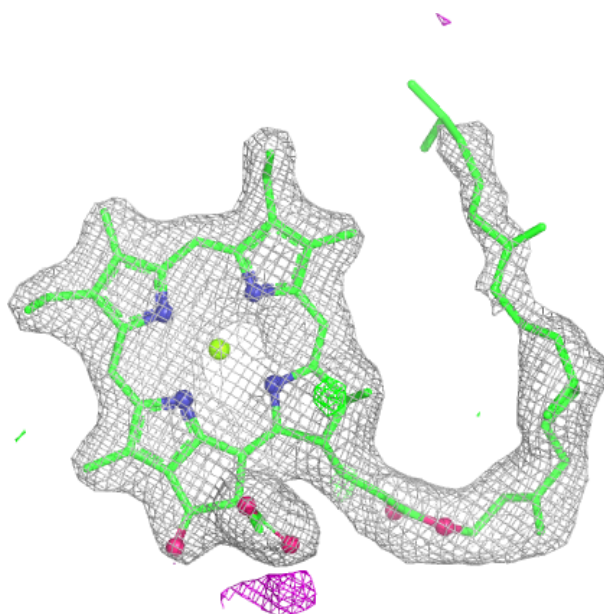
**Electron density around DGD c 518:**

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



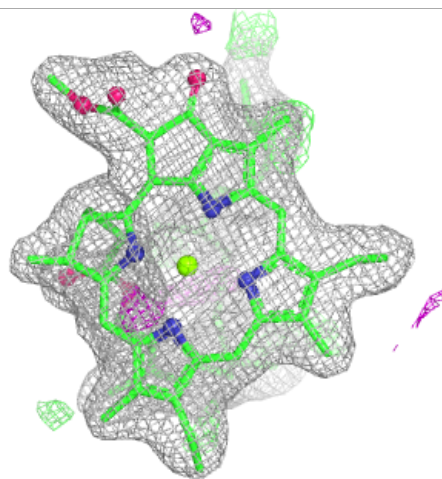
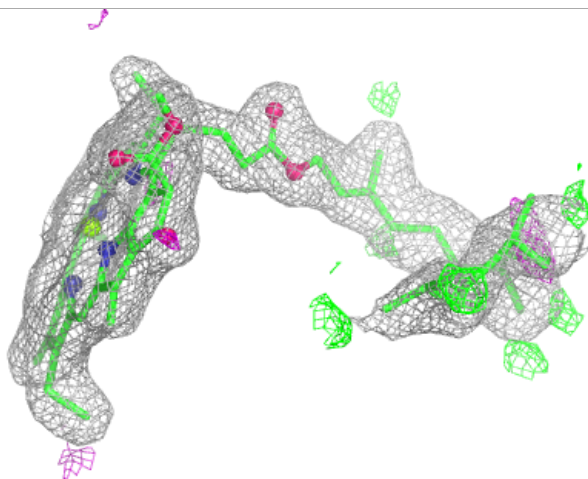
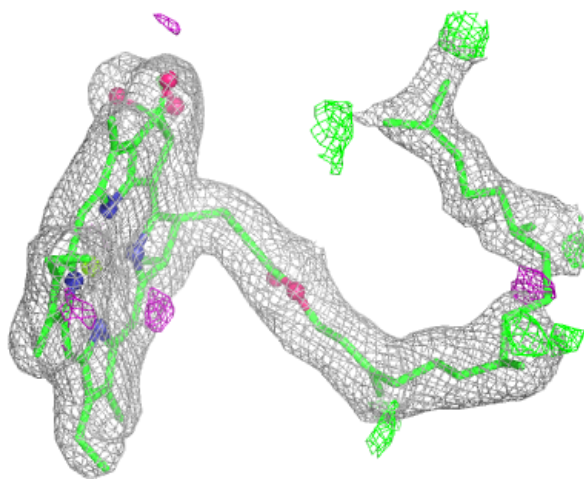
Electron density around CLA C 512:

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



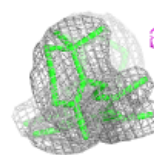
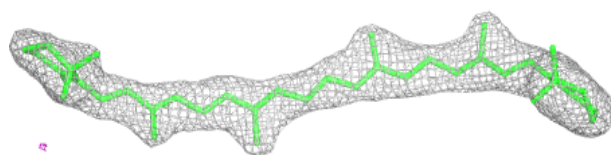
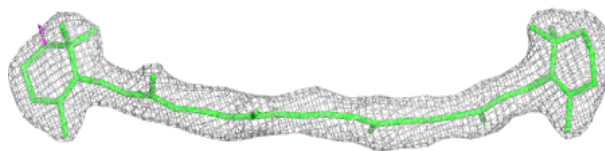
Electron density around CLA B 605:

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

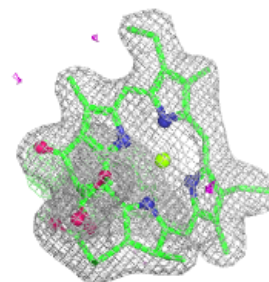
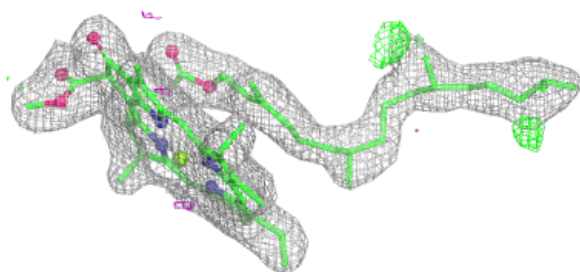
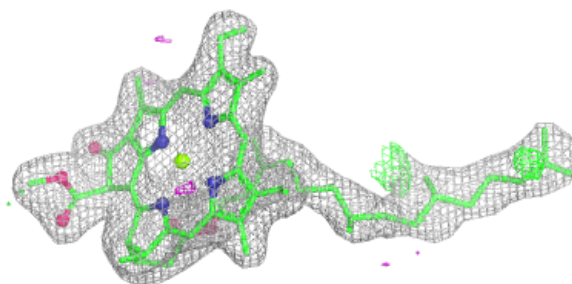


Electron density around BCR K 102:

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

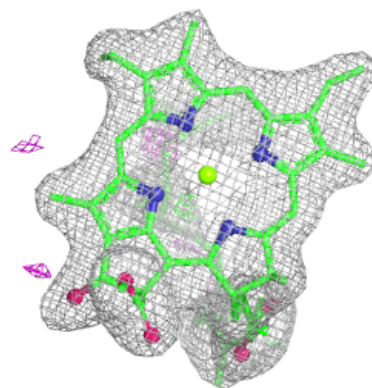
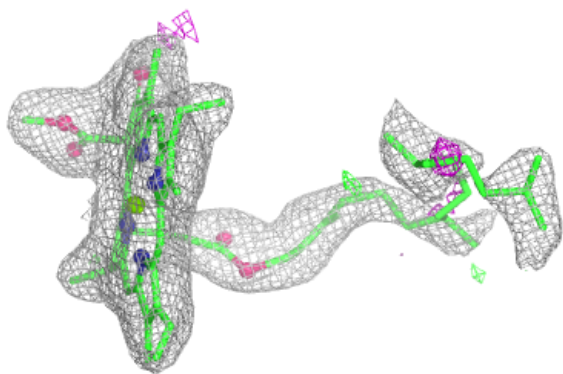
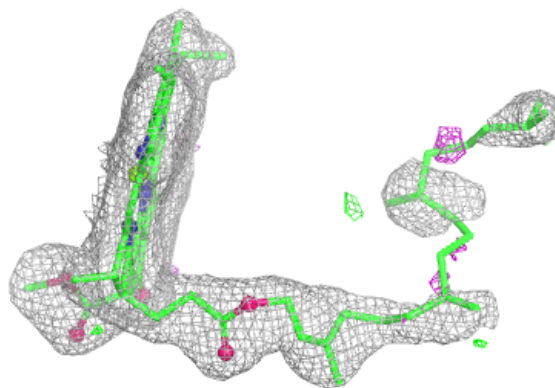
**Electron density around CLA c 505:**

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

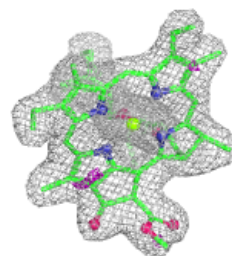
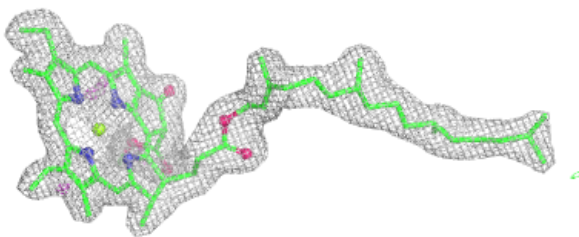
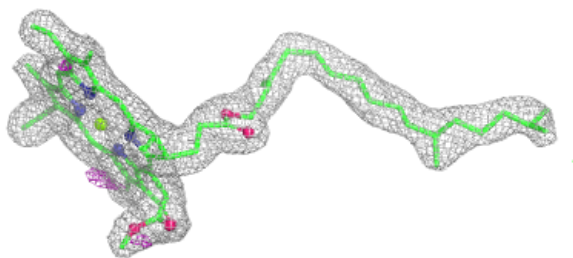


Electron density around CLA c 506:

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

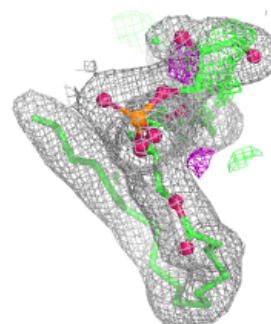
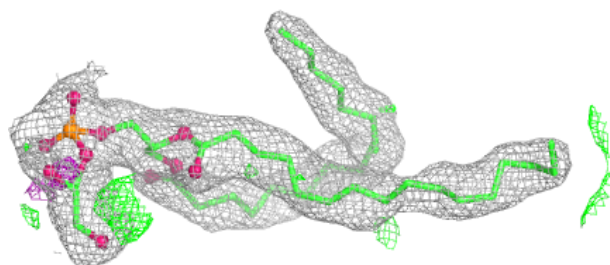
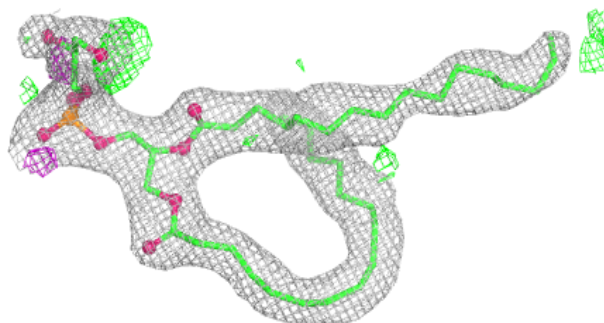
**Electron density around CLA C 502:**

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



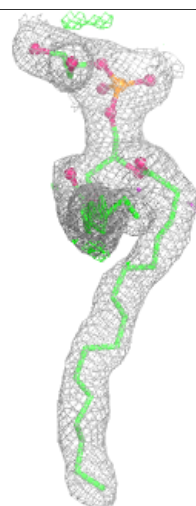
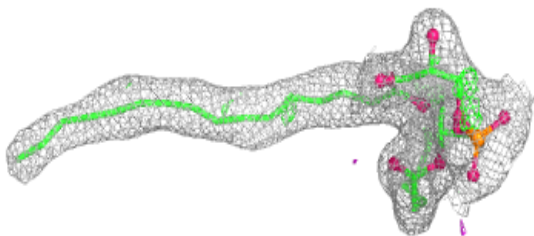
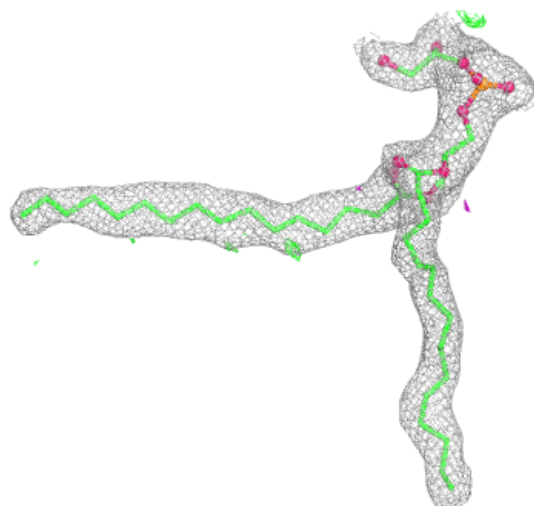
Electron density around LHG D 411:

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



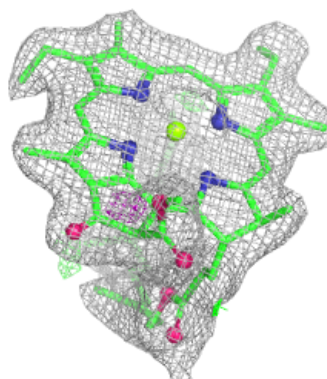
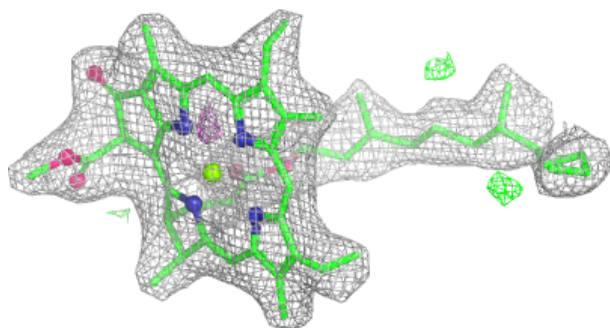
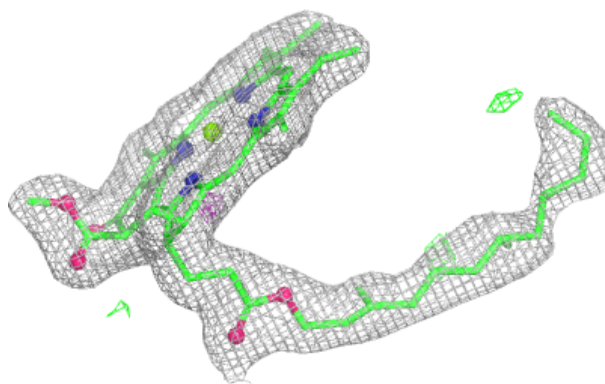
Electron density around LHG b 623:

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

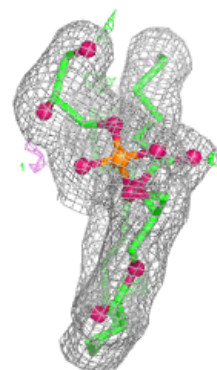
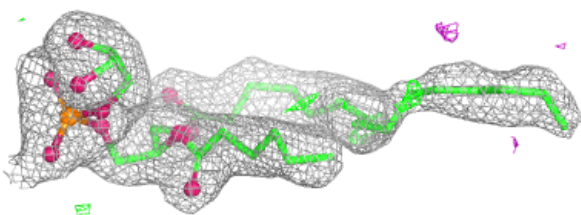
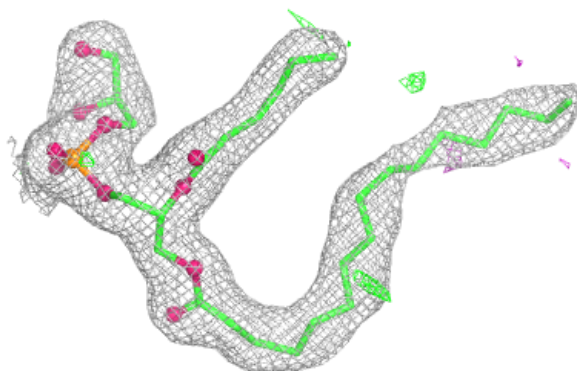


Electron density around CLA C 504:

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

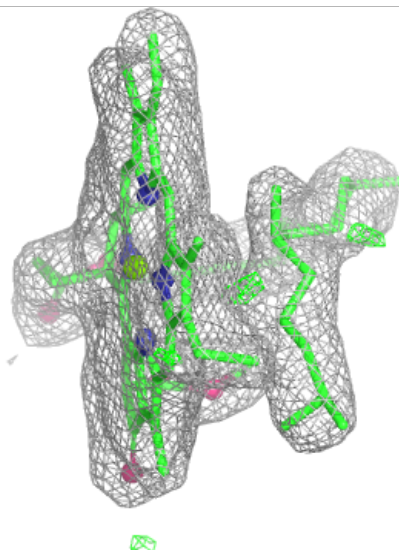
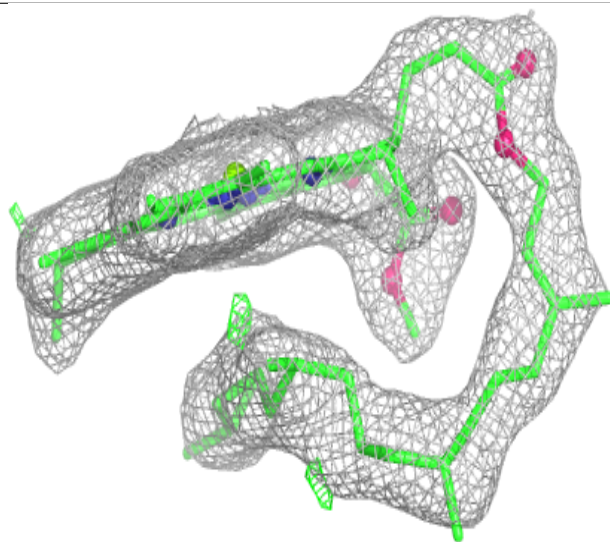
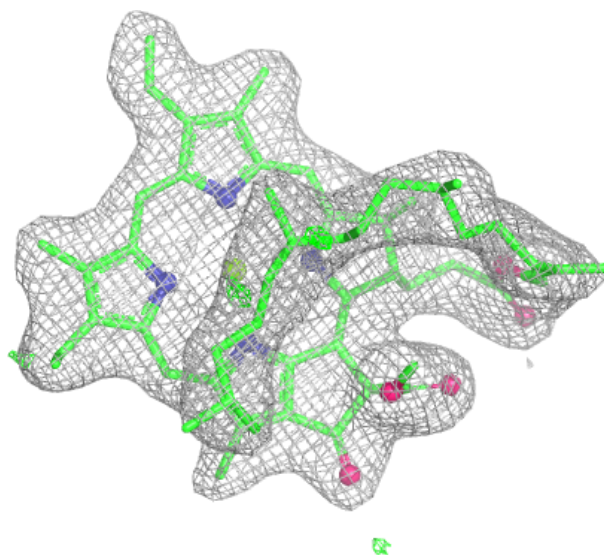
**Electron density around LHG d 409:**

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



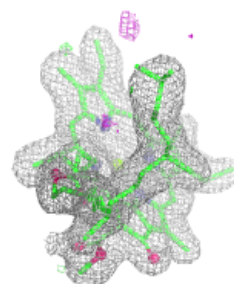
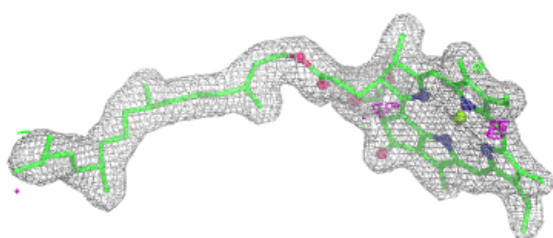
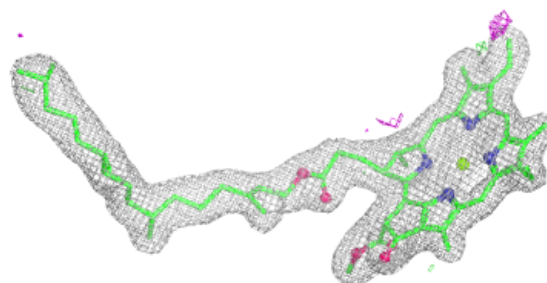
Electron density around CLA c 510:

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

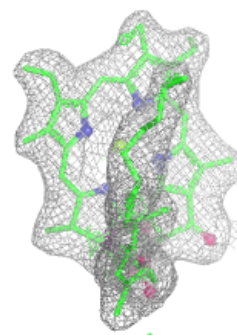
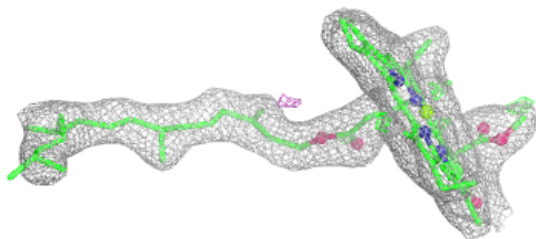
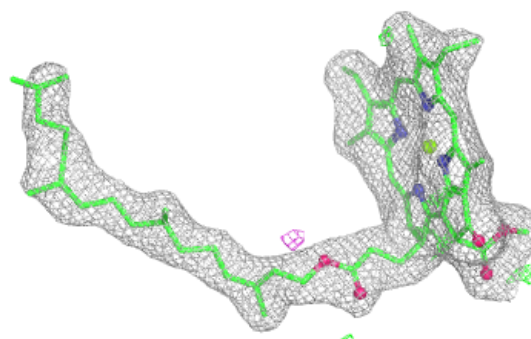


Electron density around CLA a 606:

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

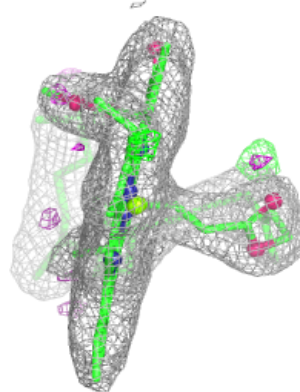
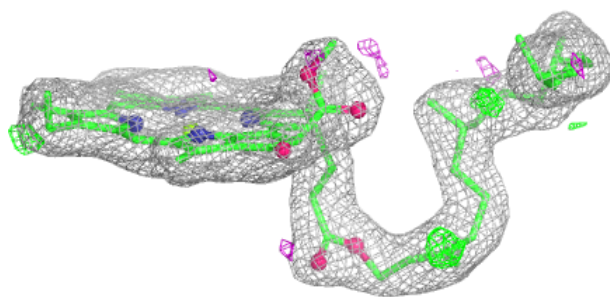
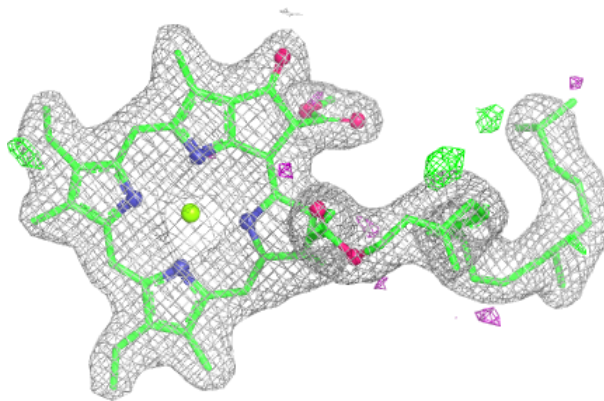
**Electron density around CLA b 608:**

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

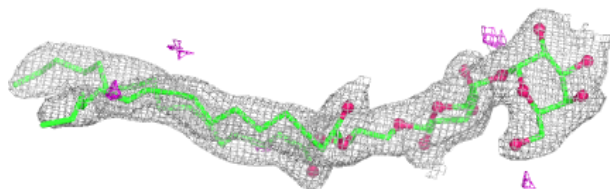
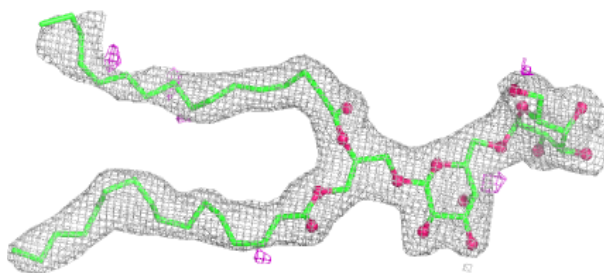


Electron density around CLA b 611:

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

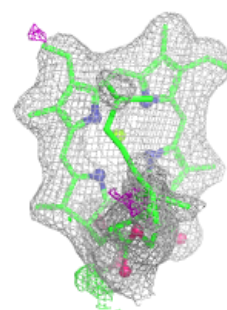
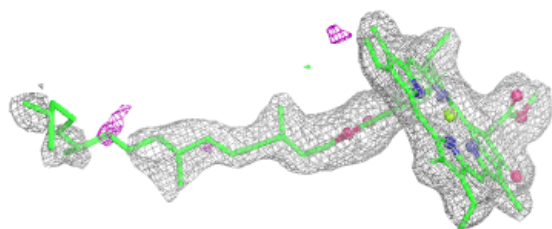
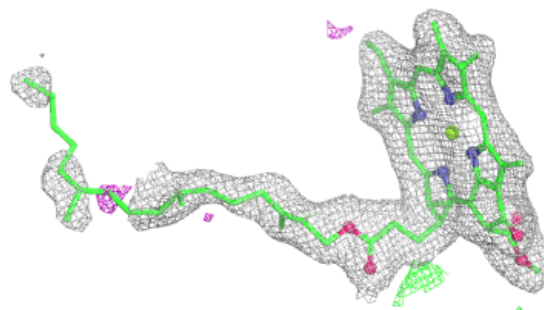
**Electron density around DGD C 518:**

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

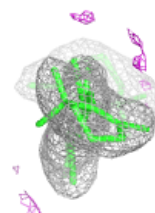
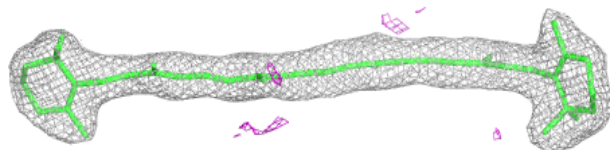
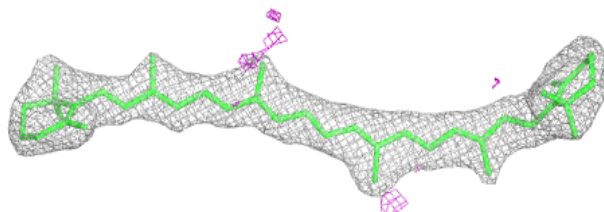


Electron density around CLA d 404:

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

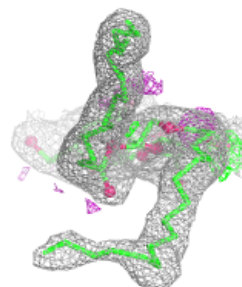
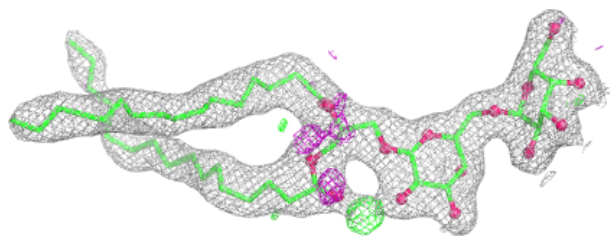
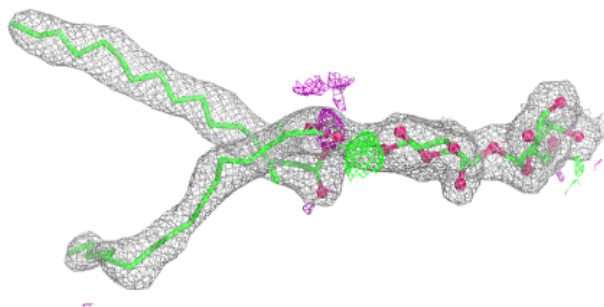
**Electron density around BCR c 515:**

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

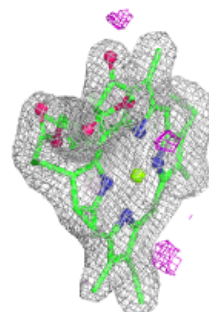
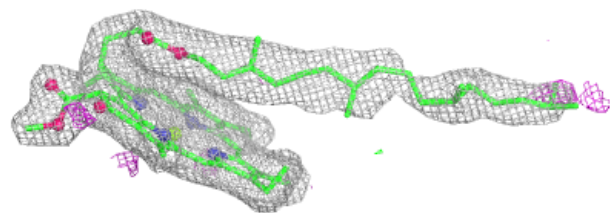
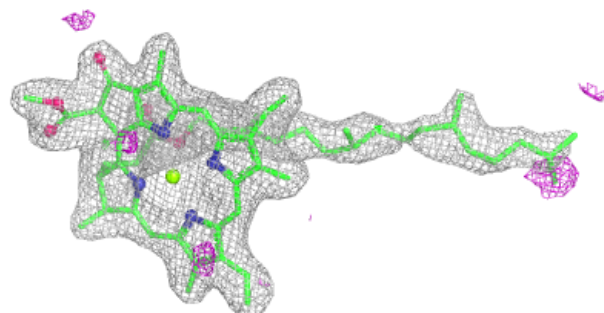


Electron density around DGD c 516:

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

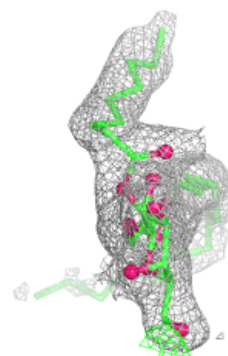
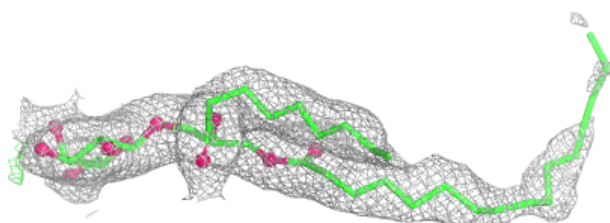
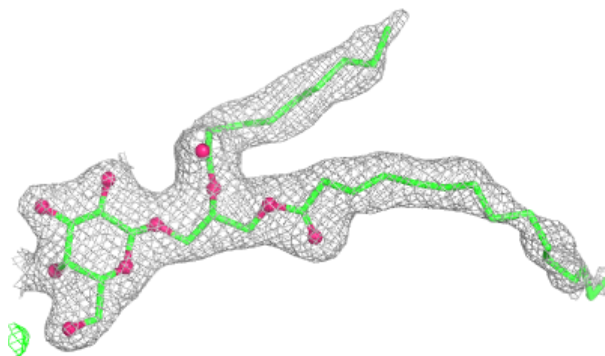
**Electron density around CLA b 613:**

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

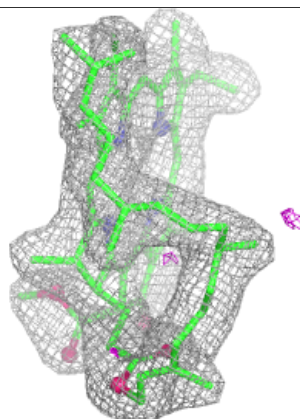
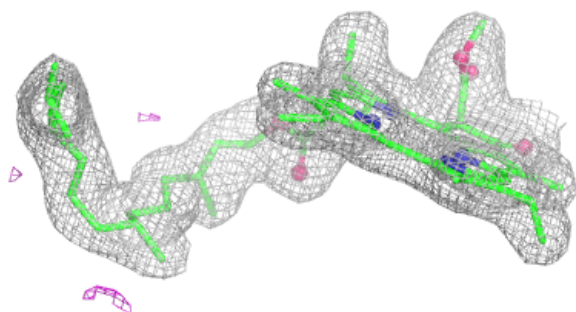
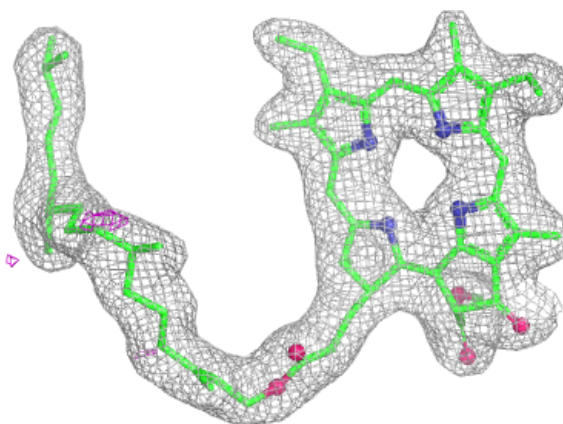


Electron density around LMG d 411:

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

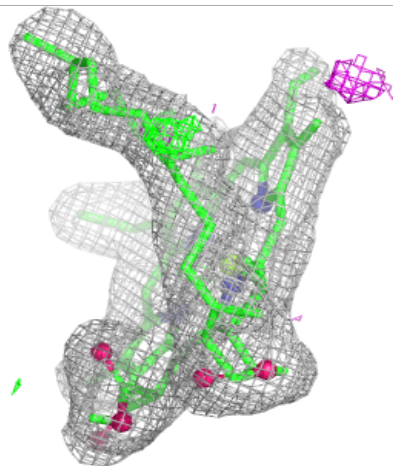
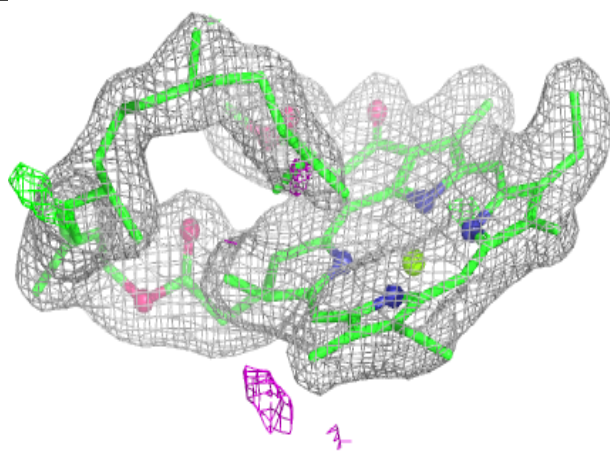
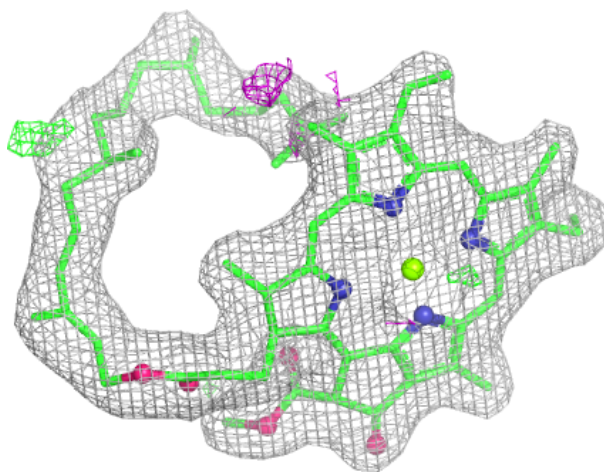
**Electron density around PHO d 402:**

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



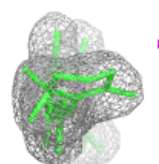
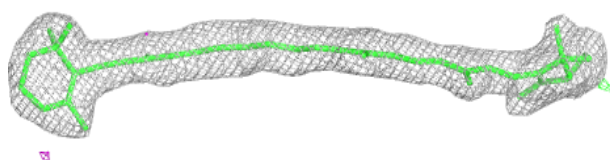
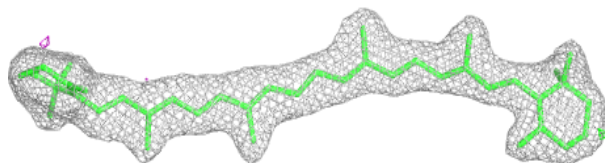
Electron density around CLA b 614:

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



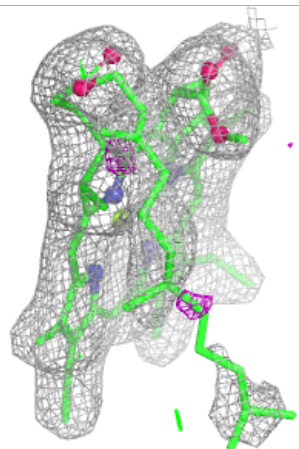
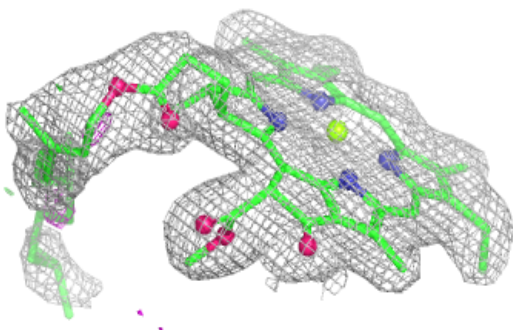
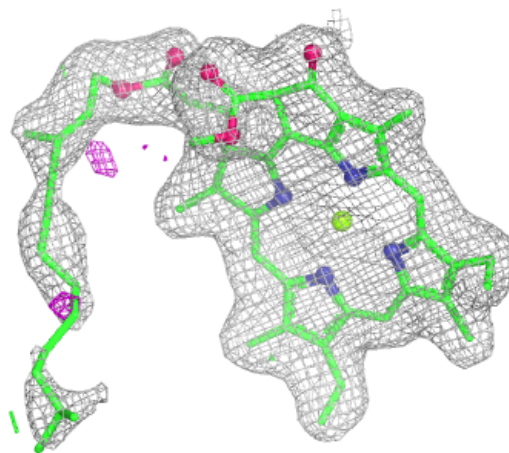
Electron density around BCR B 616:

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



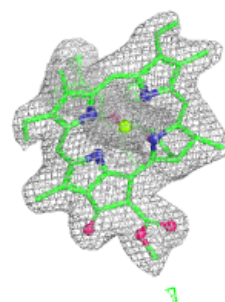
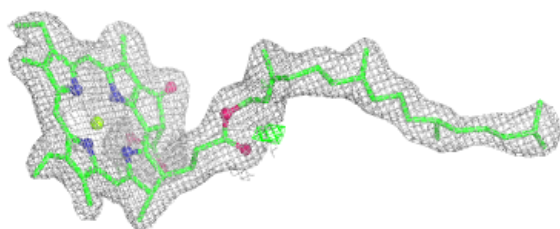
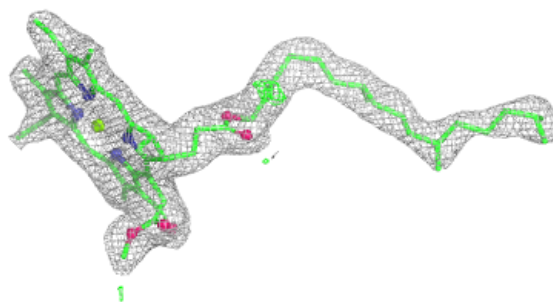
Electron density around CLA b 615:

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

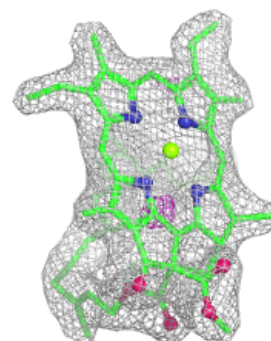
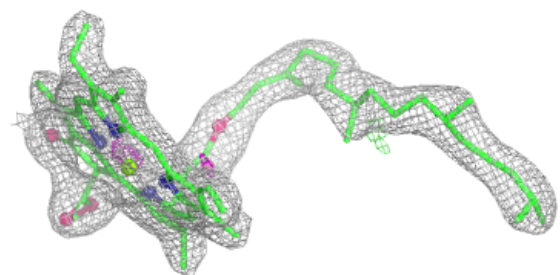
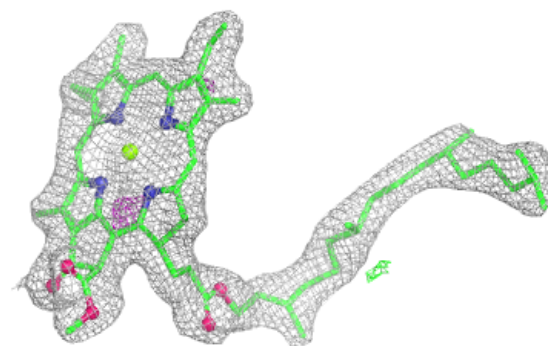


Electron density around CLA c 502:

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

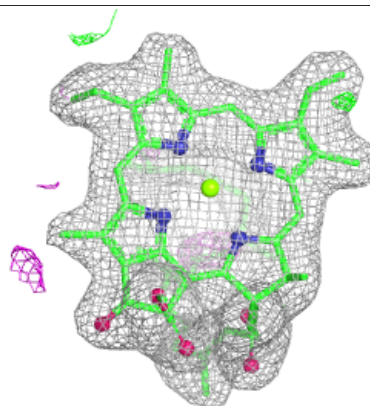
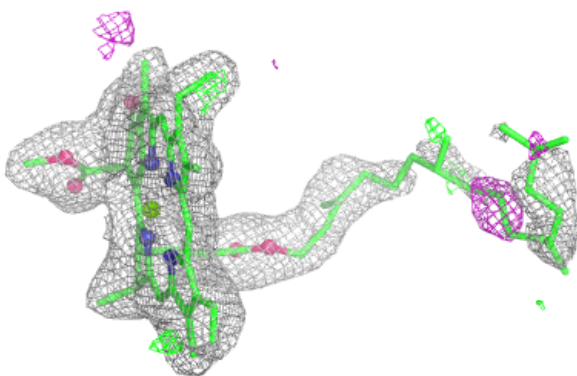
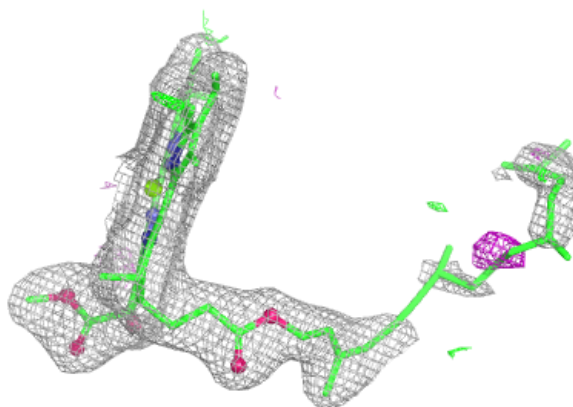
**Electron density around CLA C 511:**

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

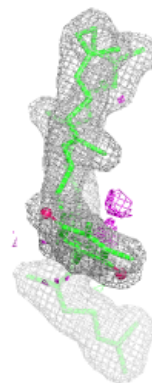
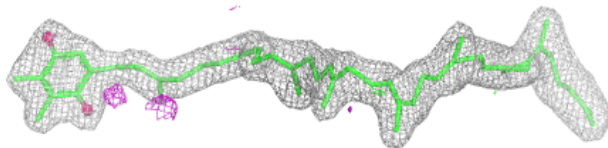
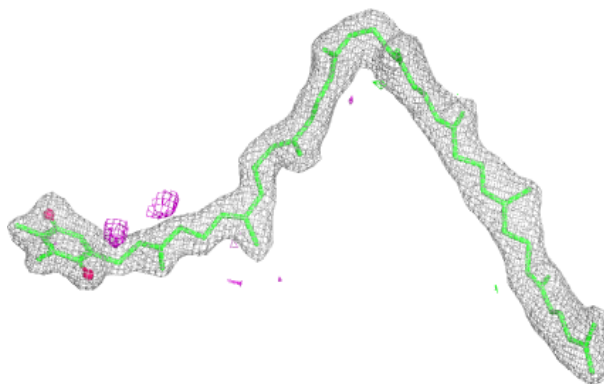


Electron density around CLA C 506:

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

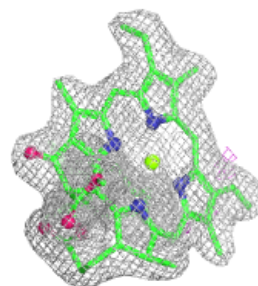
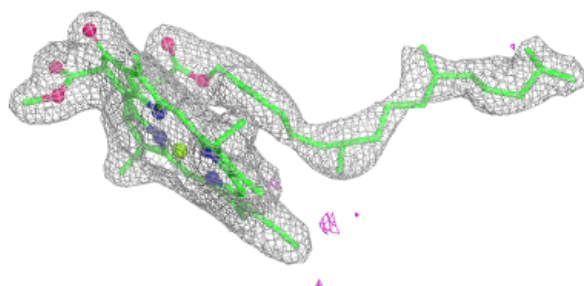
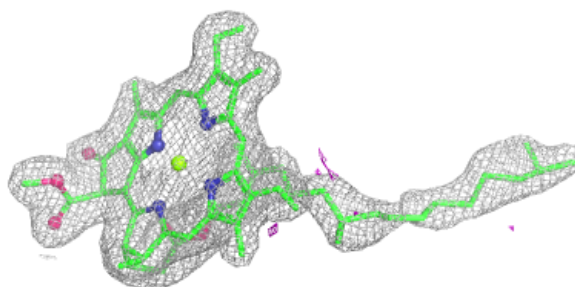
**Electron density around PL9 d 406:**

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

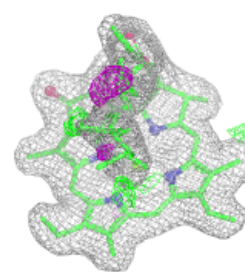
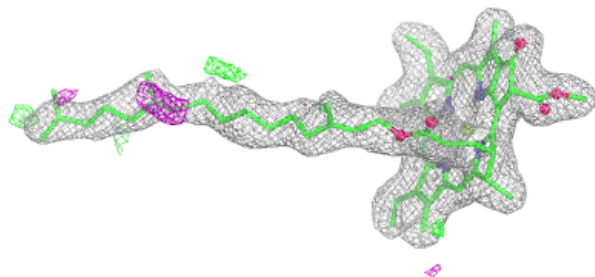
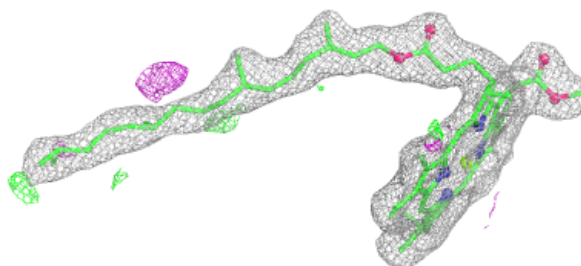


Electron density around CLA C 505:

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

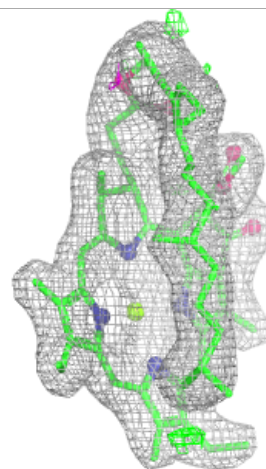
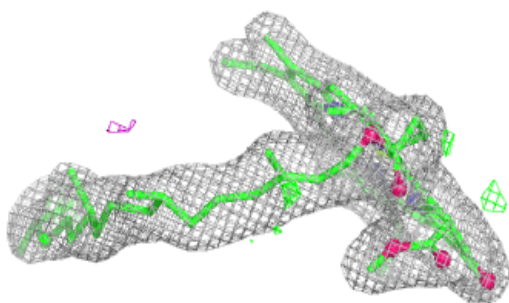
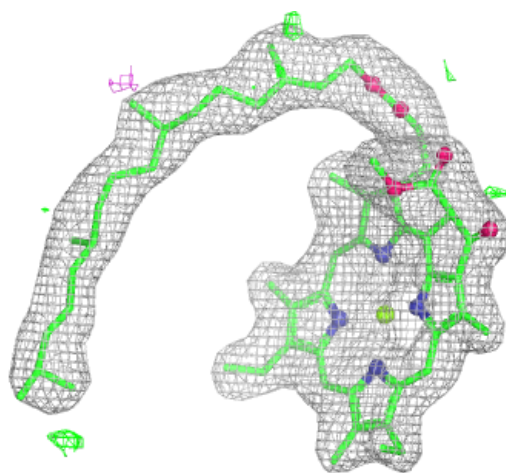
**Electron density around CLA B 606:**

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



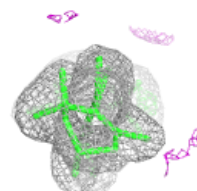
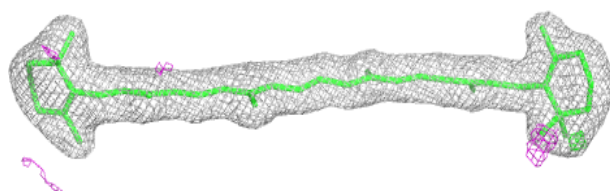
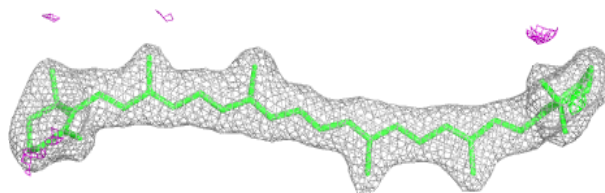
Electron density around CLA C 507:

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

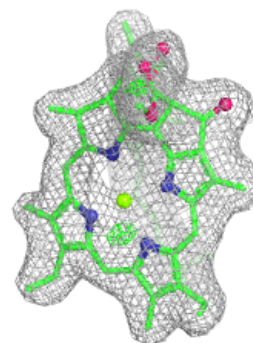
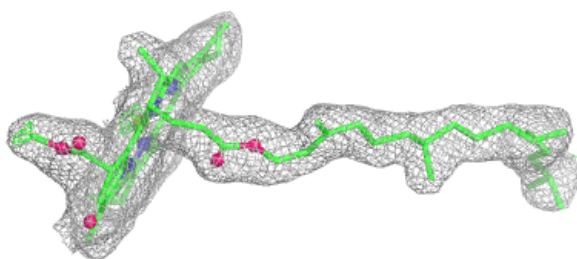
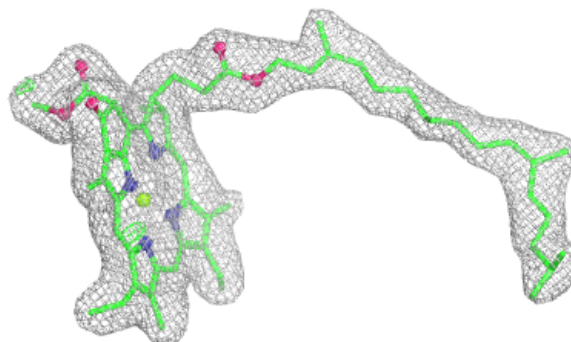


Electron density around BCR a 610:

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

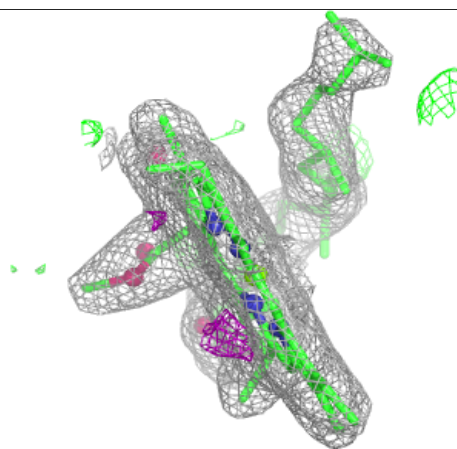
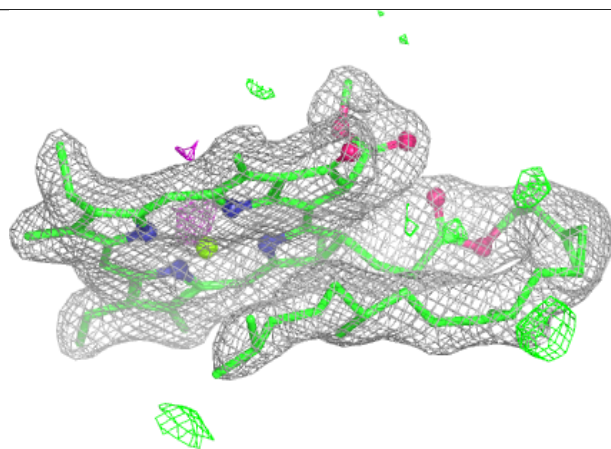
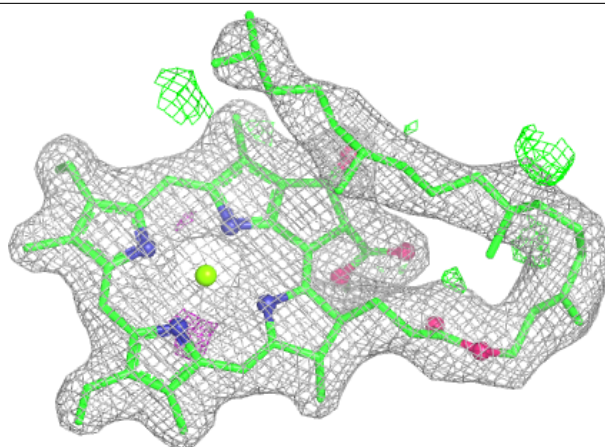
**Electron density around CLA B 608:**

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



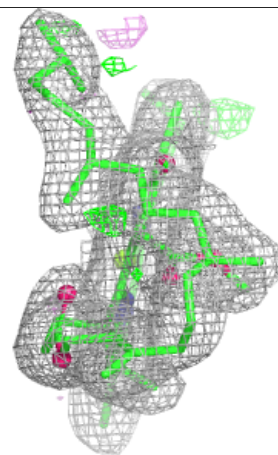
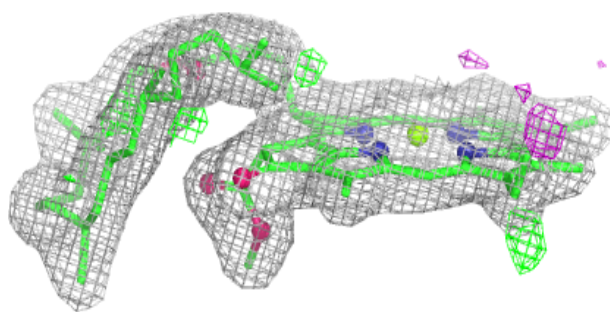
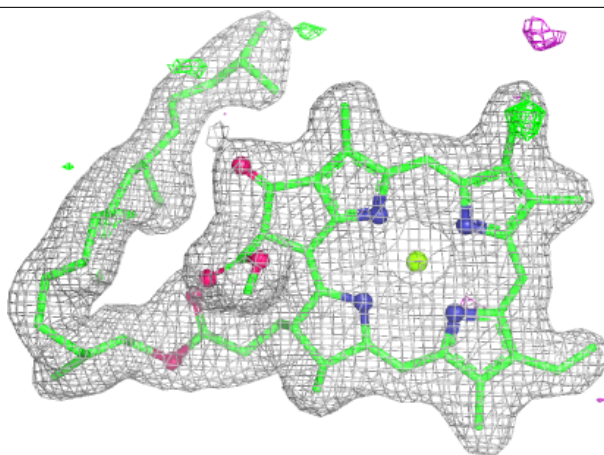
Electron density around CLA C 509:

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



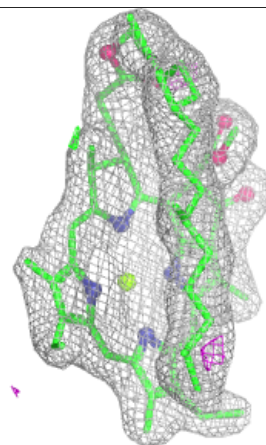
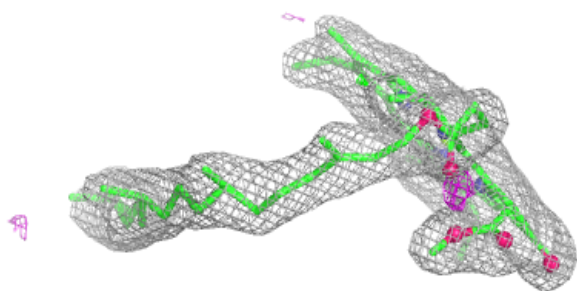
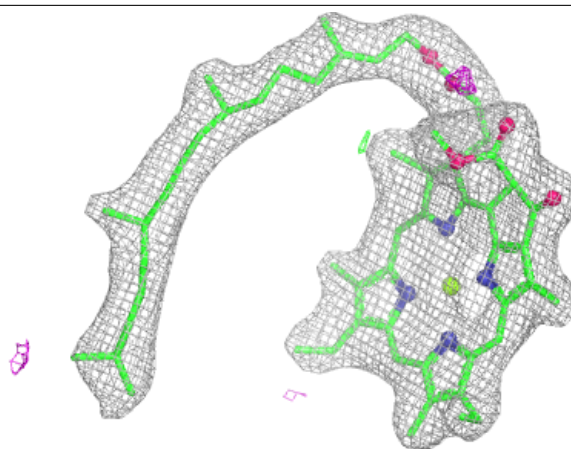
Electron density around CLA B 609:

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



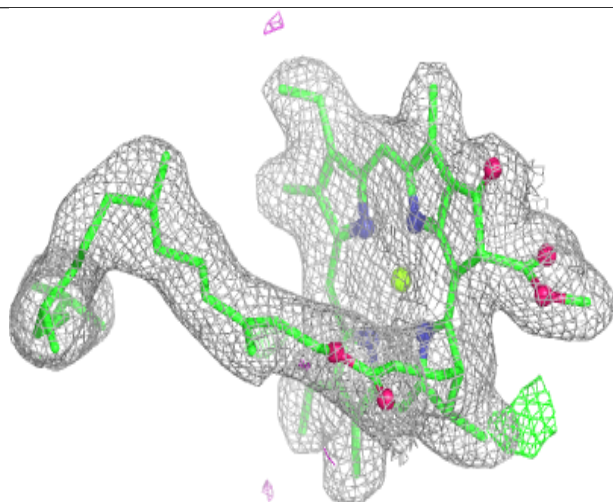
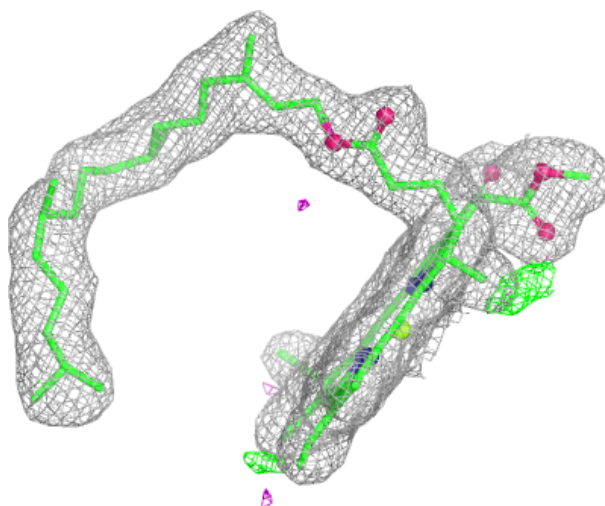
Electron density around CLA c 507:

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



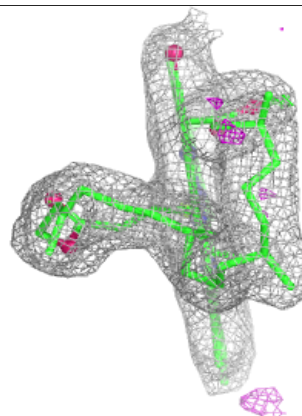
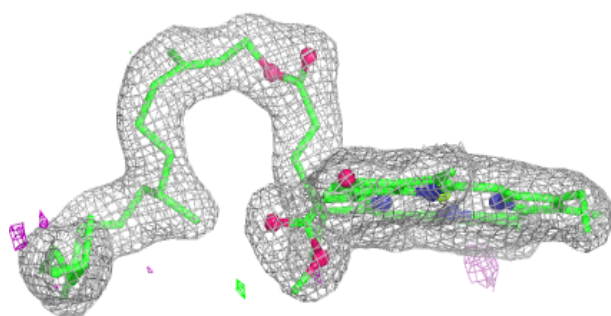
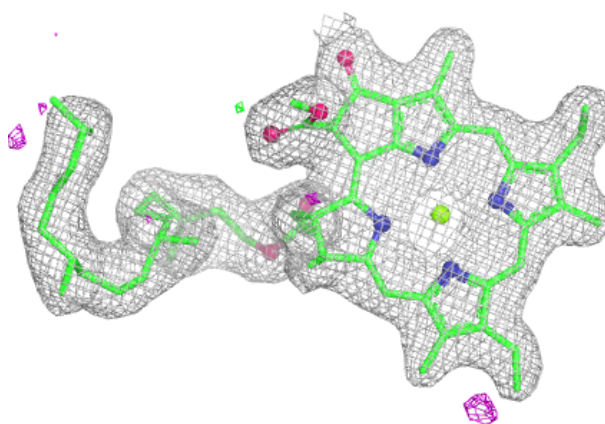
Electron density around CLA B 610:

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

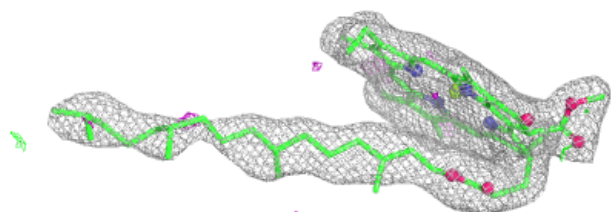
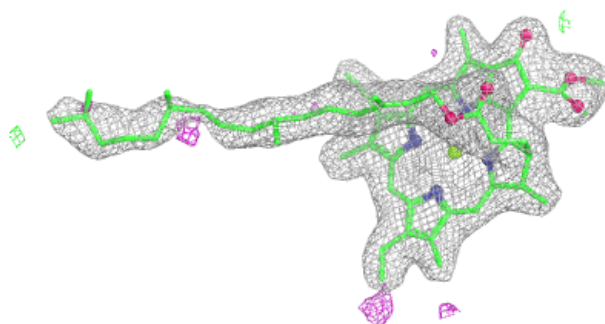


Electron density around CLA B 611:

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

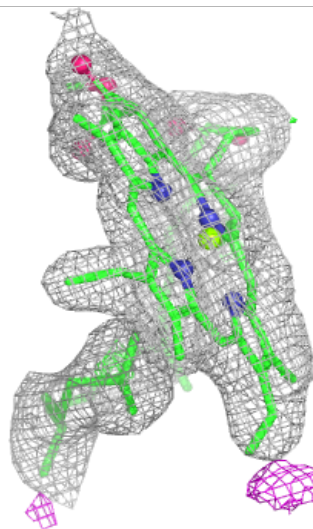
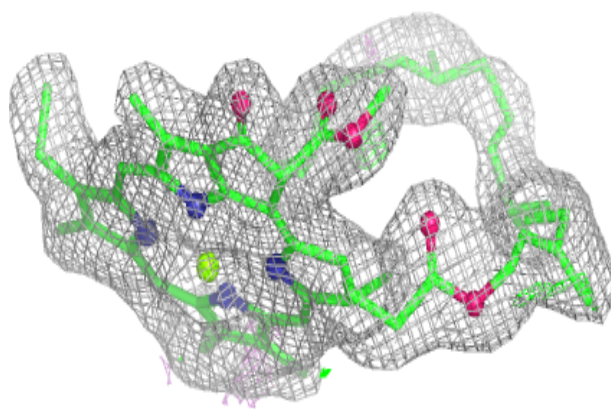
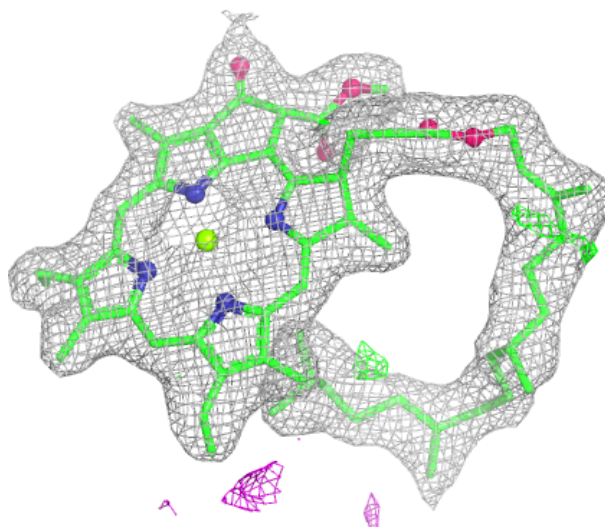
**Electron density around CLA B 613:**

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



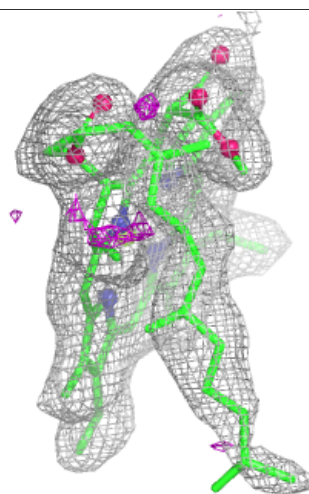
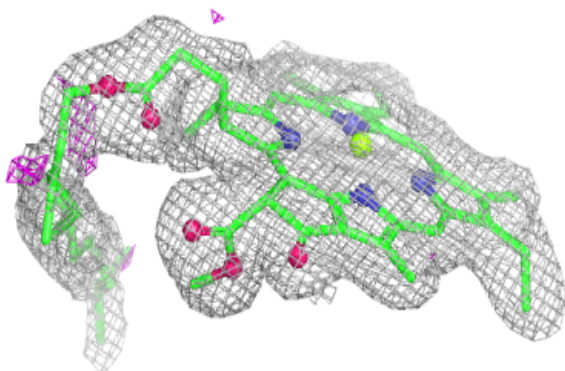
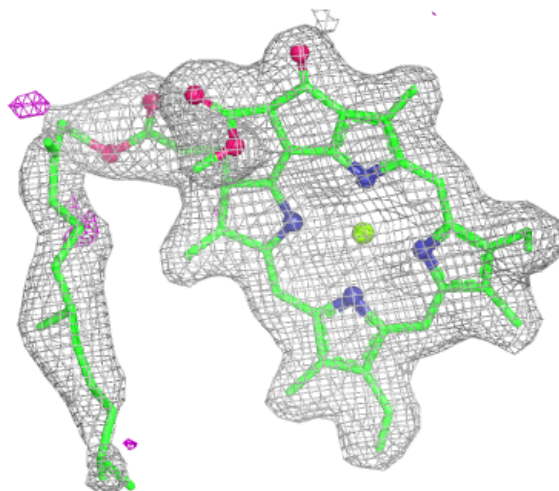
Electron density around CLA B 614:

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



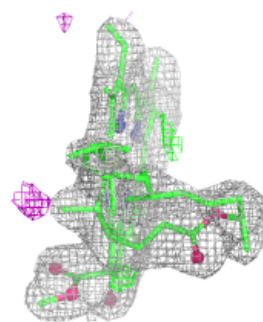
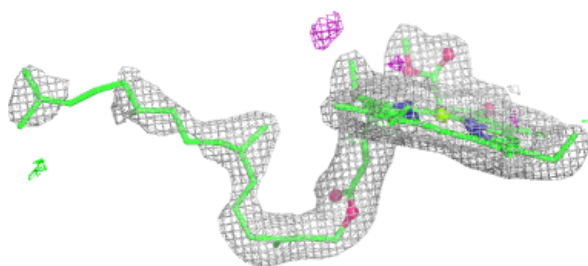
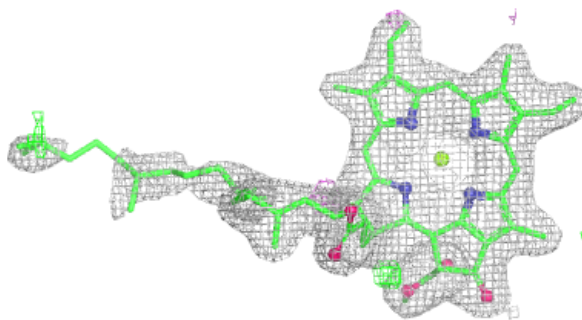
Electron density around CLA B 615:

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

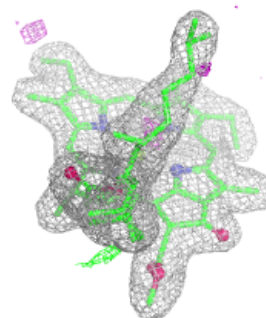
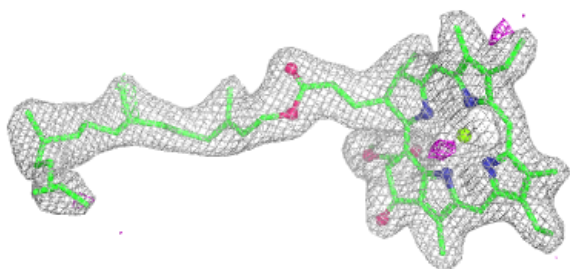
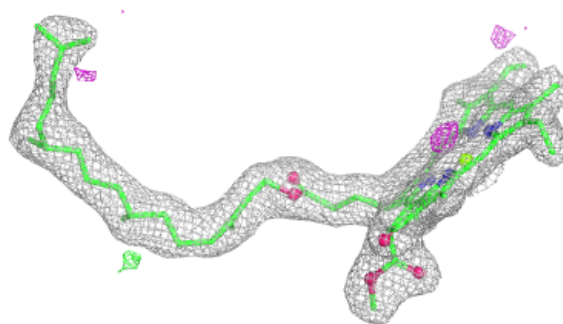


Electron density around CLA a 607:

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

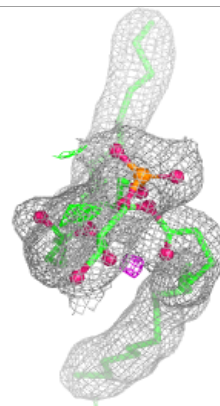
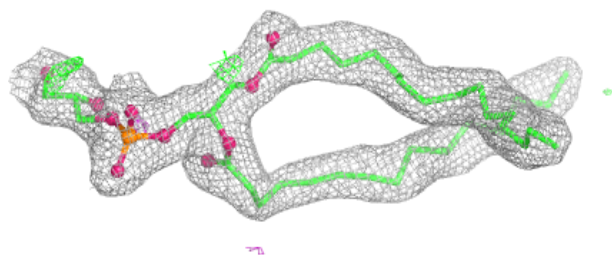
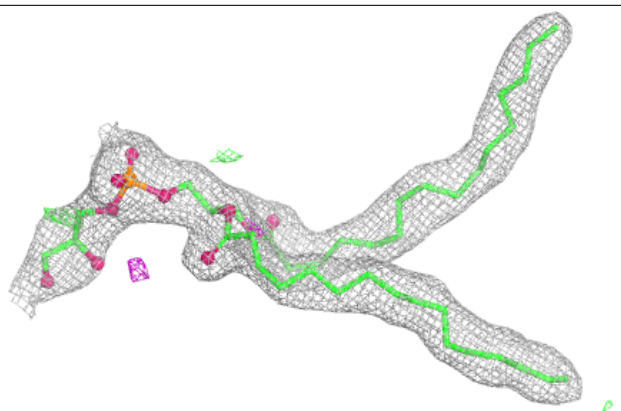
**Electron density around CLA d 403:**

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

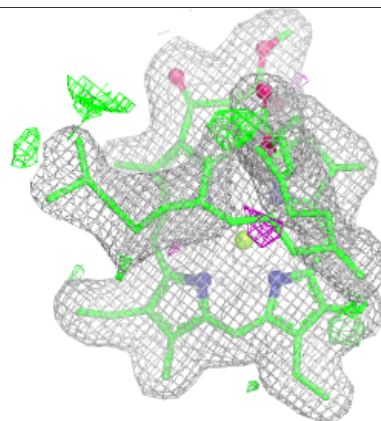
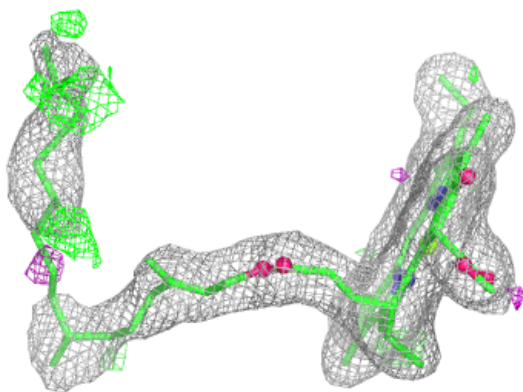
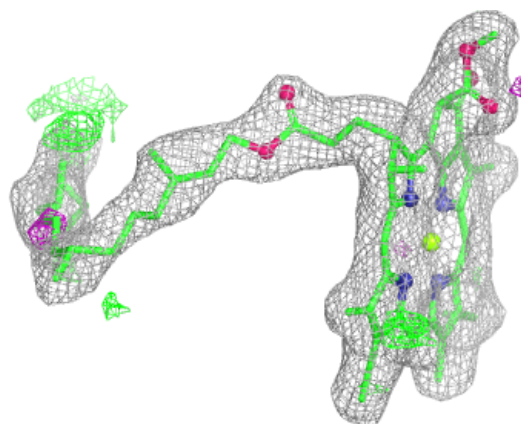


Electron density around LHG d 408:

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

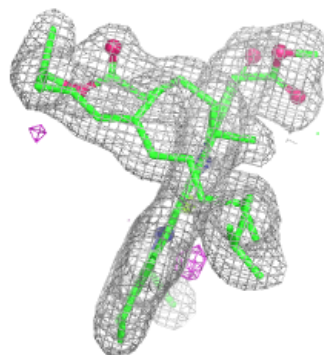
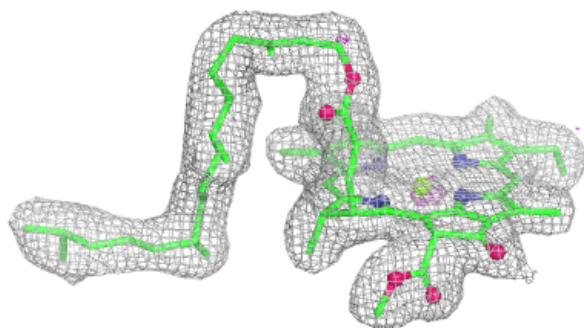
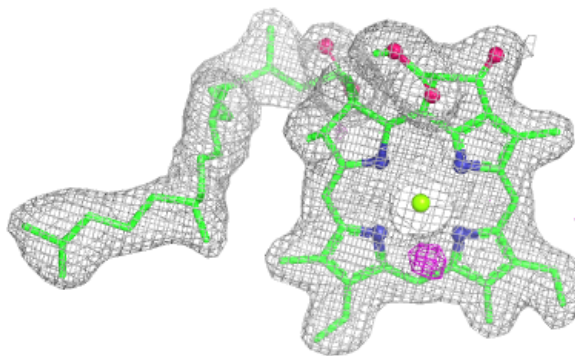
**Electron density around CLA a 609:**

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

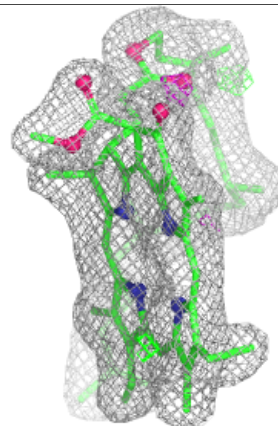
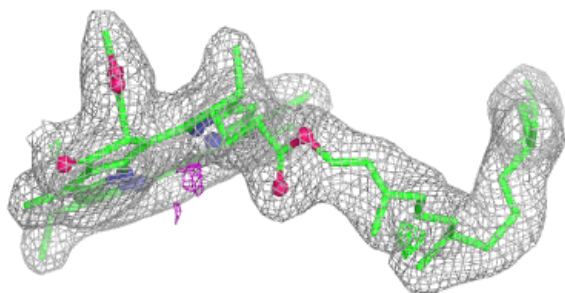
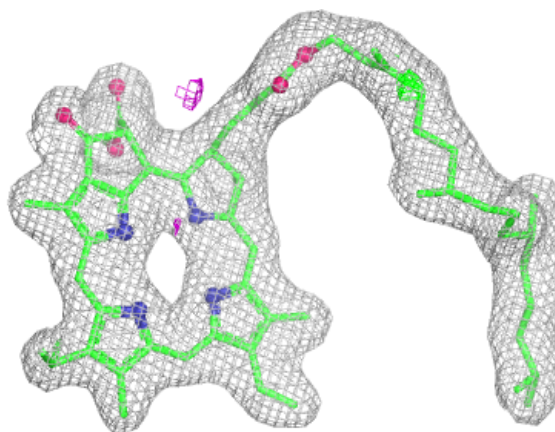


Electron density around CLA a 612:

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

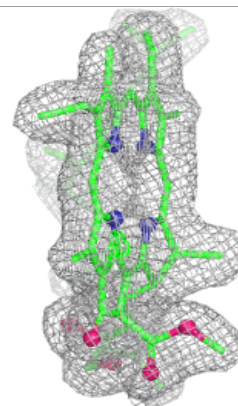
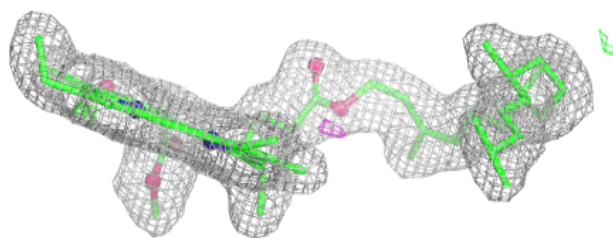
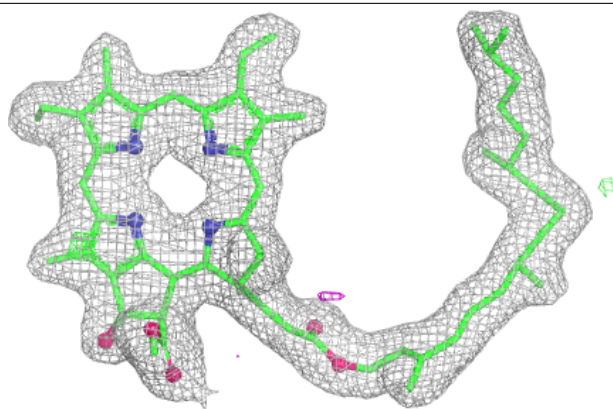
**Electron density around PHO A 608:**

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

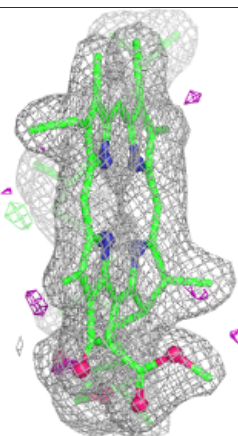
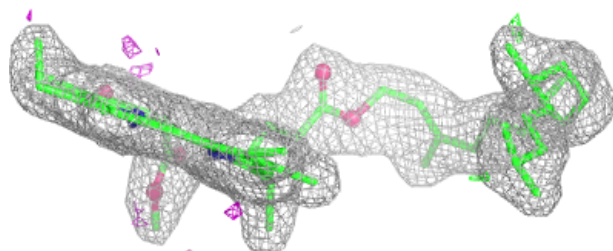
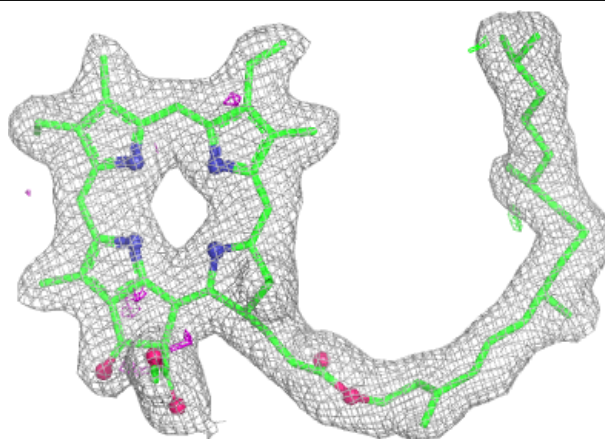


Electron density around PHO D 402:

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

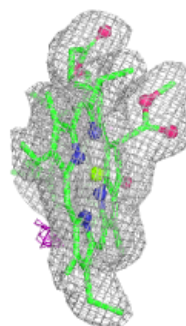
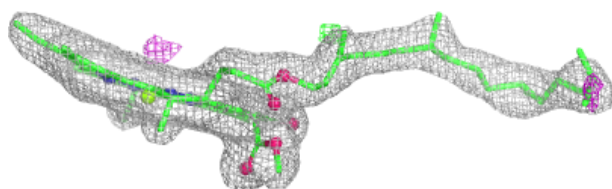
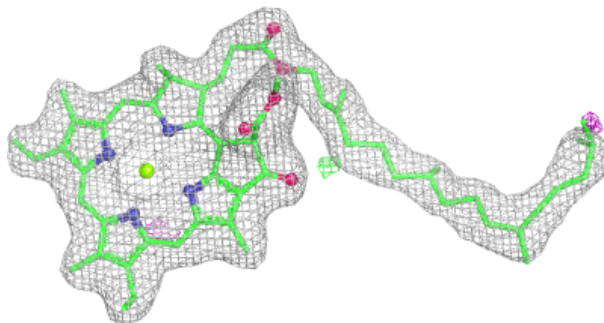
**Electron density around PHO a 608:**

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

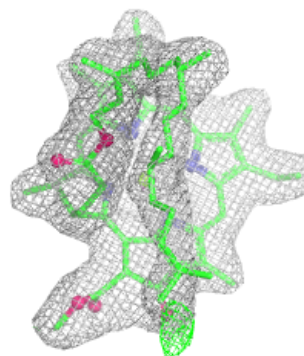
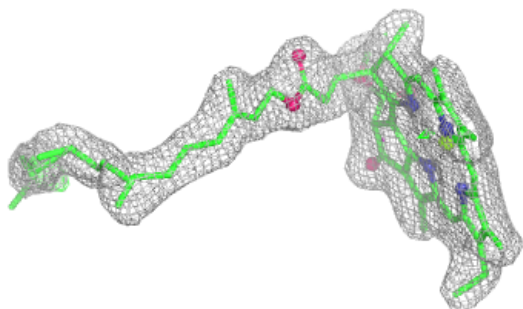
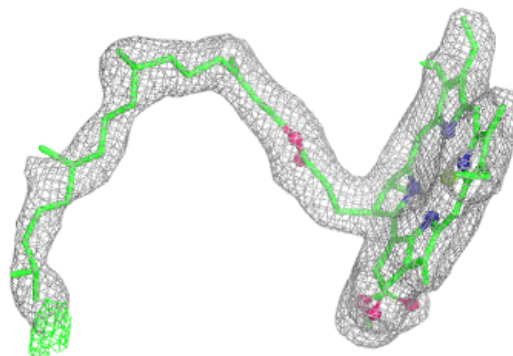


Electron density around CLA b 601:

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

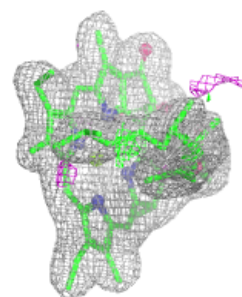
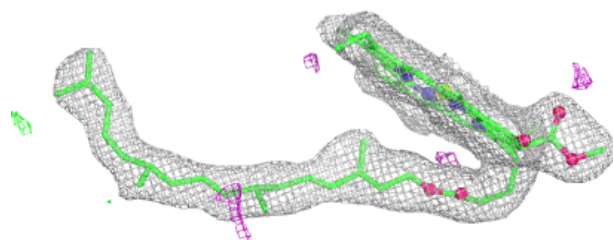
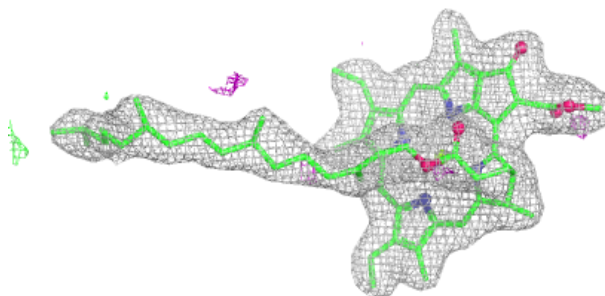
**Electron density around CLA b 605:**

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

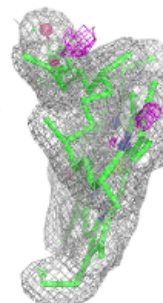
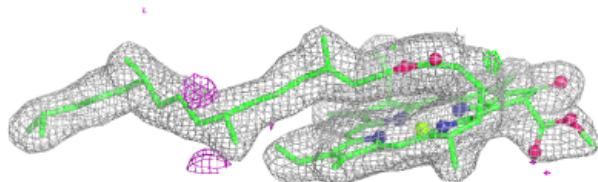
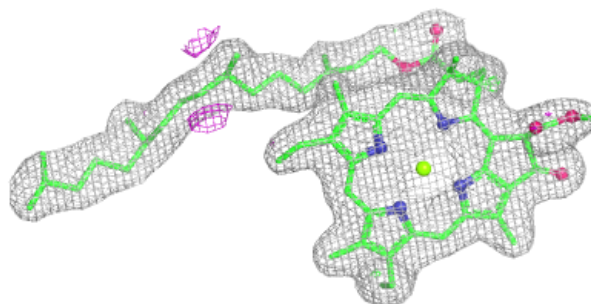


Electron density around CLA b 607:

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

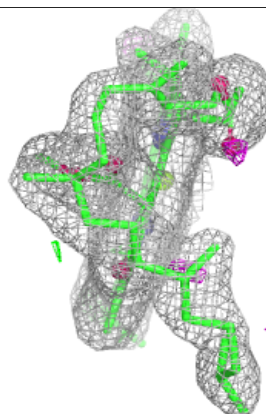
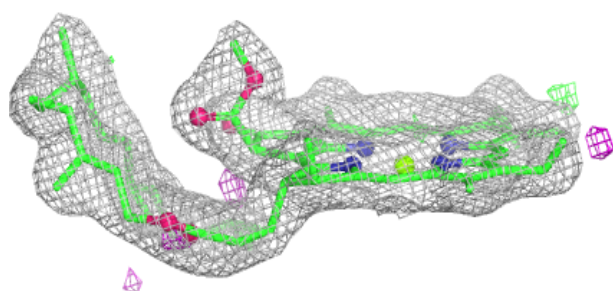
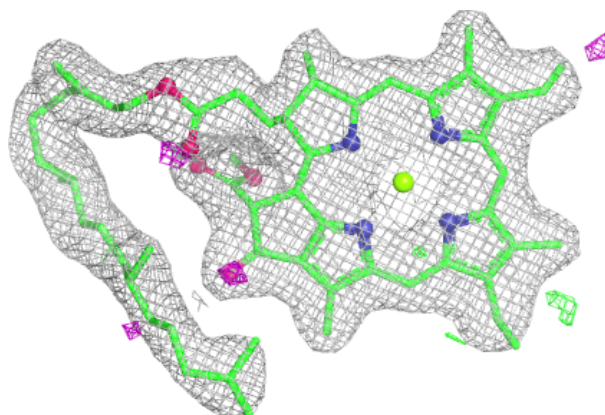
**Electron density around CLA C 501:**

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

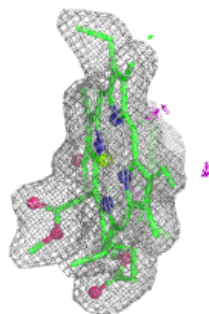
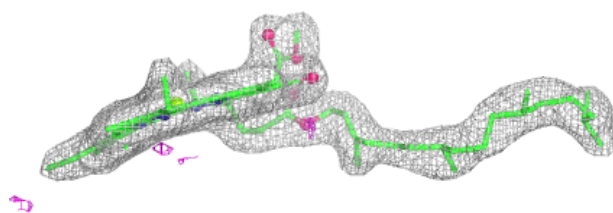
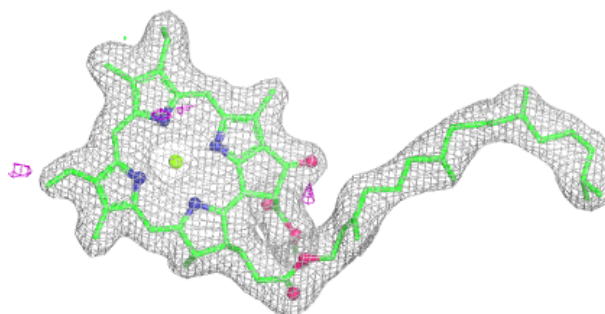


Electron density around CLA b 609:

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

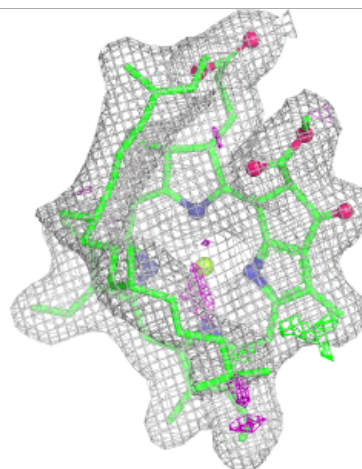
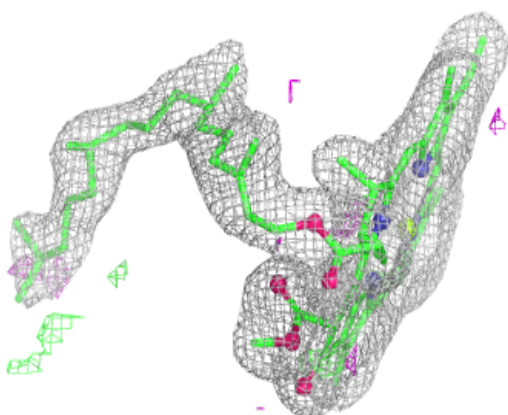
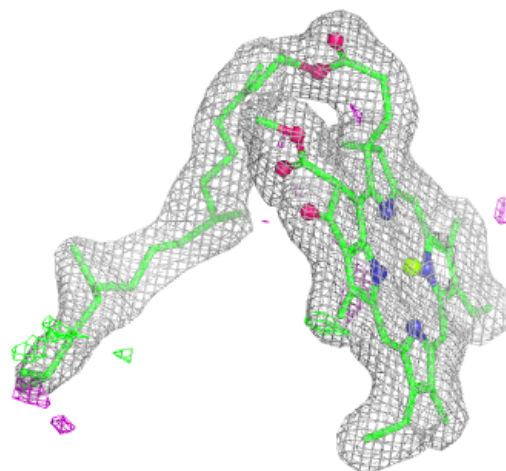
**Electron density around CLA B 601:**

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



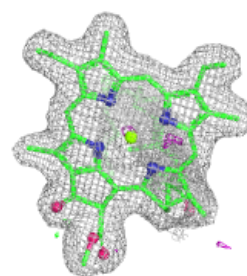
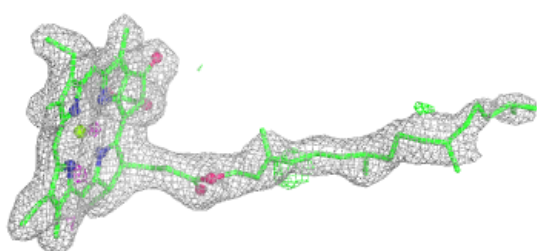
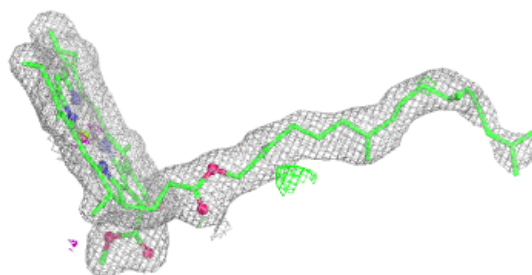
Electron density around CLA b 612:

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

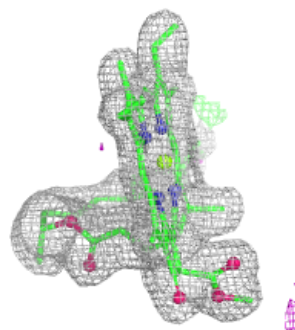
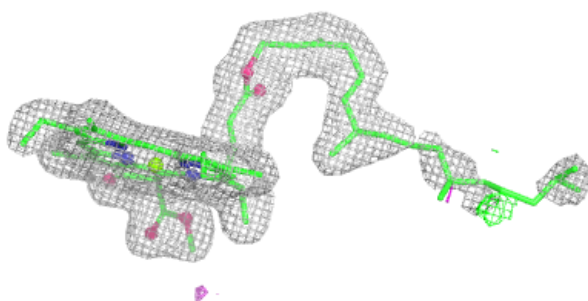
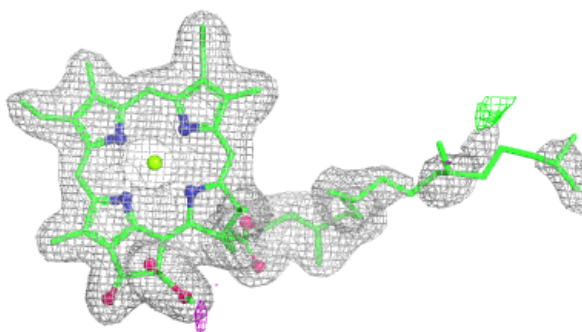


Electron density around CLA B 603:

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

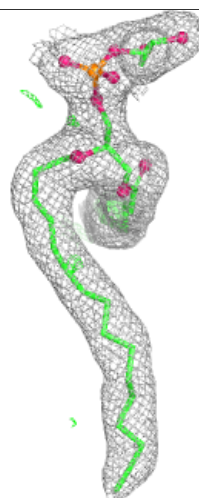
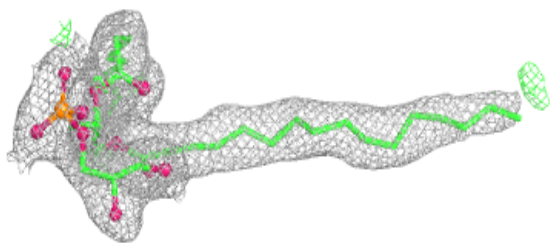
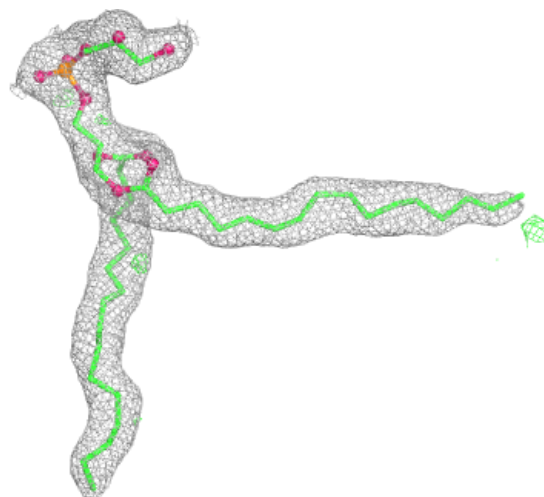
**Electron density around CLA A 607:**

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



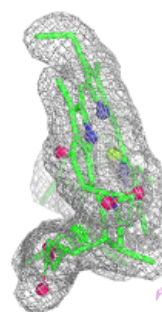
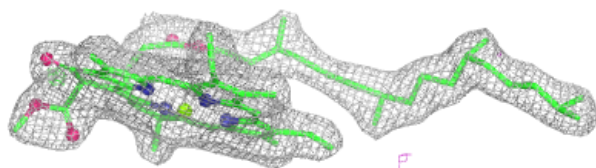
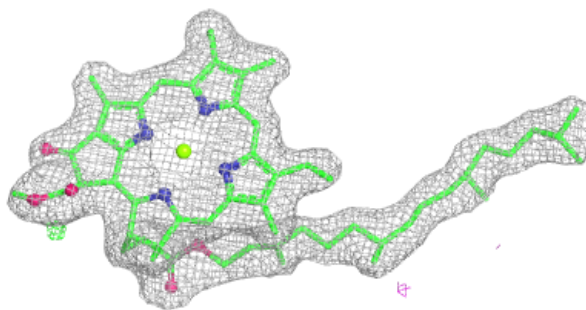
Electron density around LHG L 101:

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

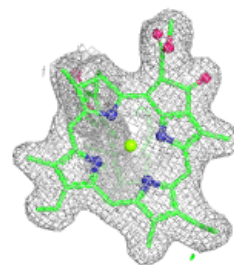
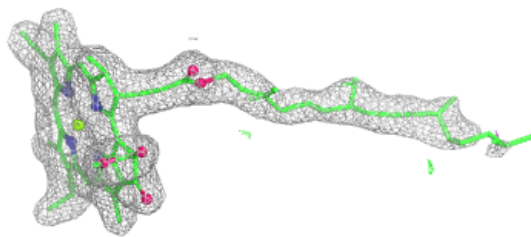
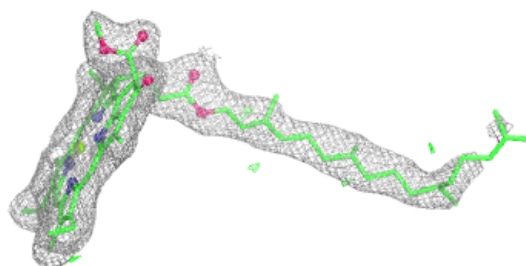


Electron density around CLA c 501:

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

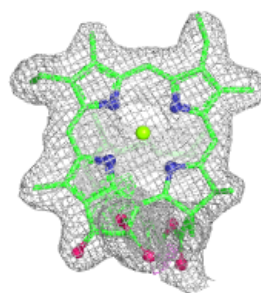
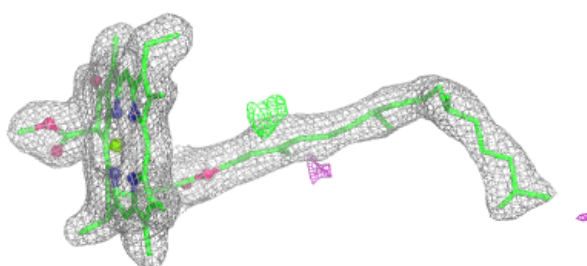
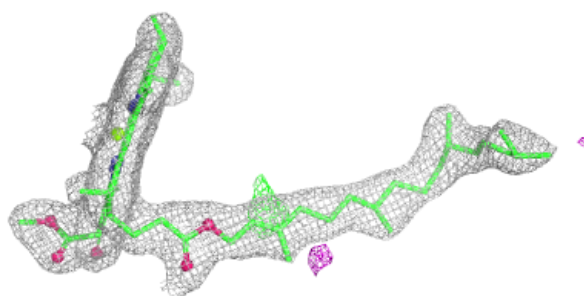
**Electron density around CLA b 603:**

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

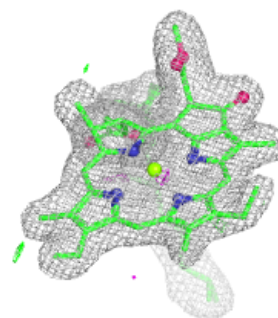
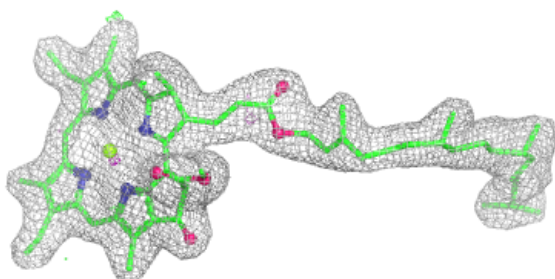
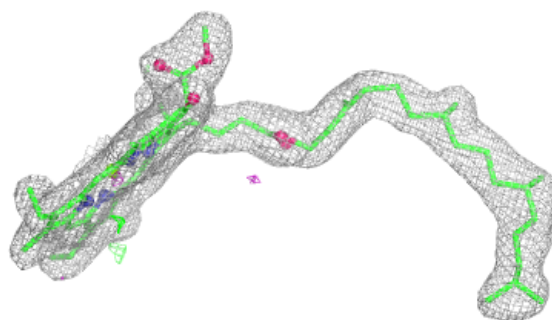


Electron density around CLA b 604:

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

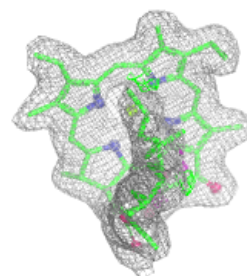
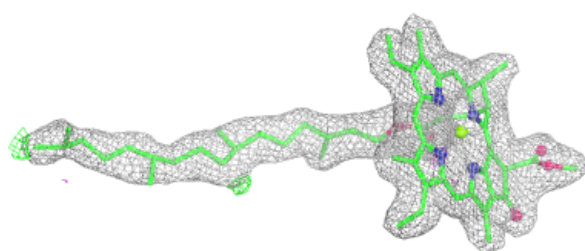
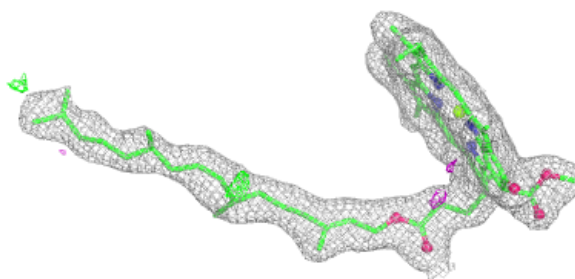
**Electron density around CLA D 403:**

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

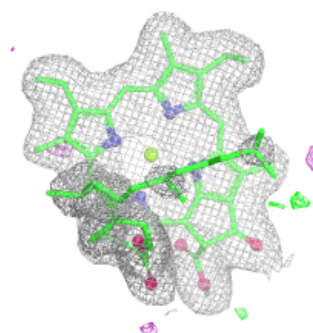
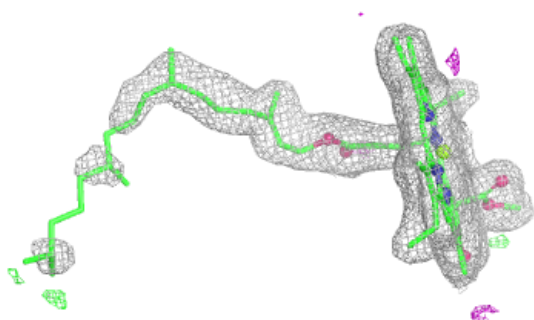
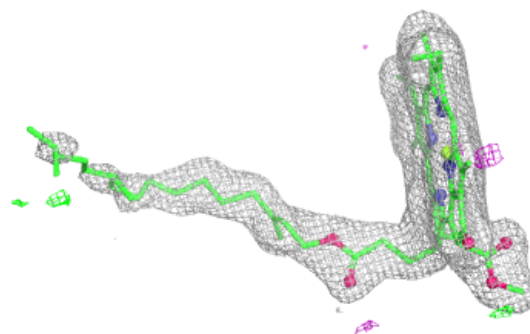


Electron density around CLA b 606:

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

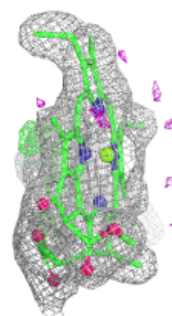
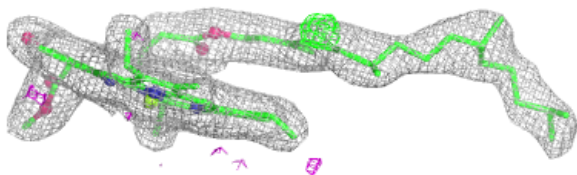
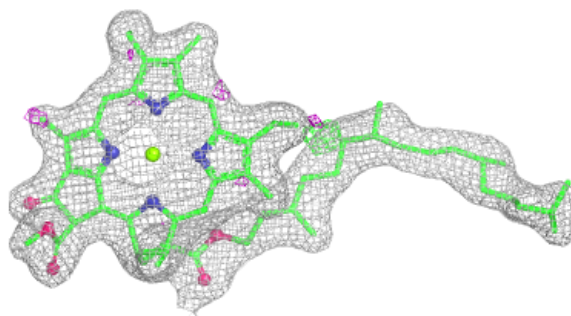
**Electron density around CLA D 404:**

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



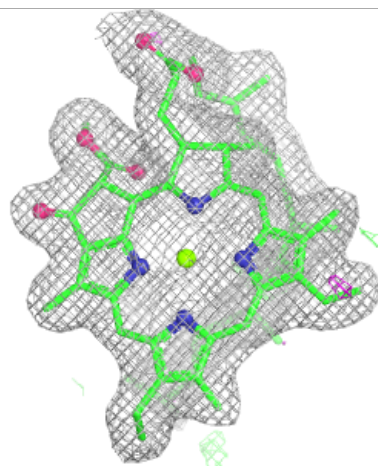
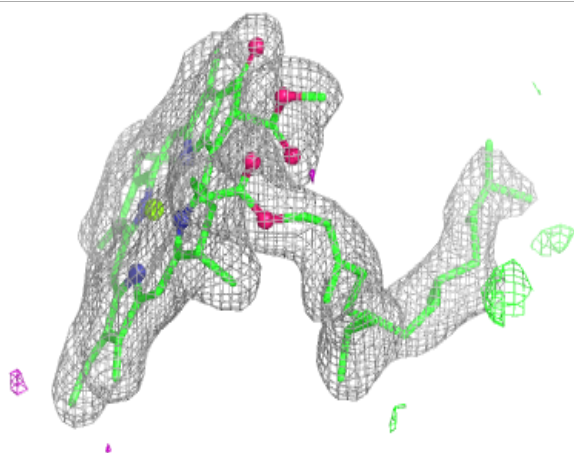
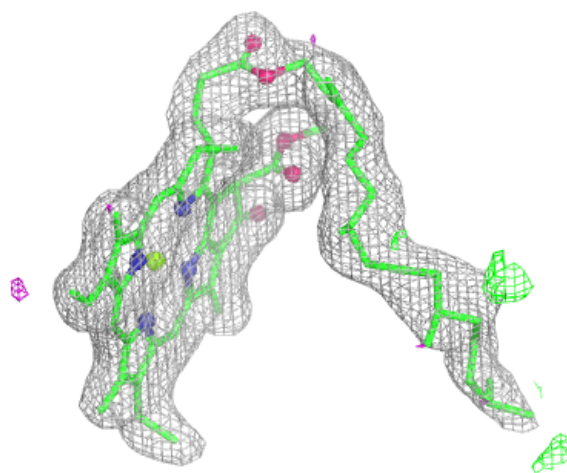
Electron density around CLA B 602:

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



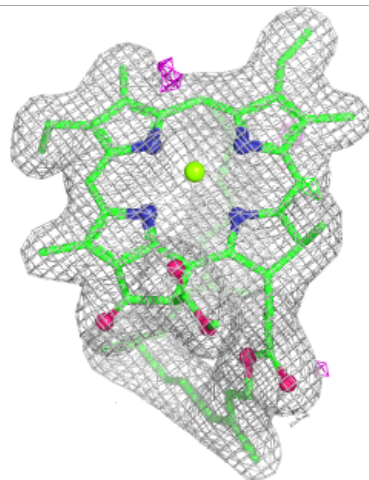
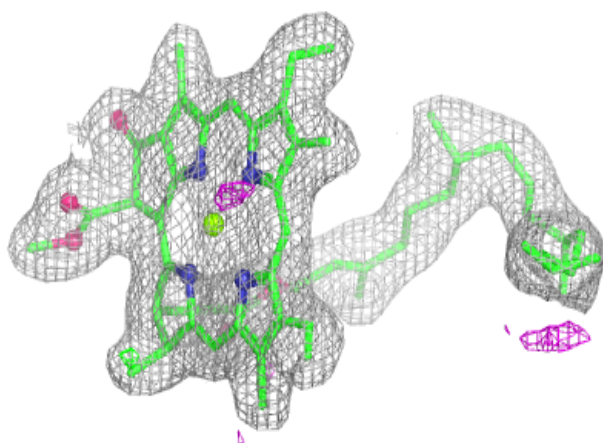
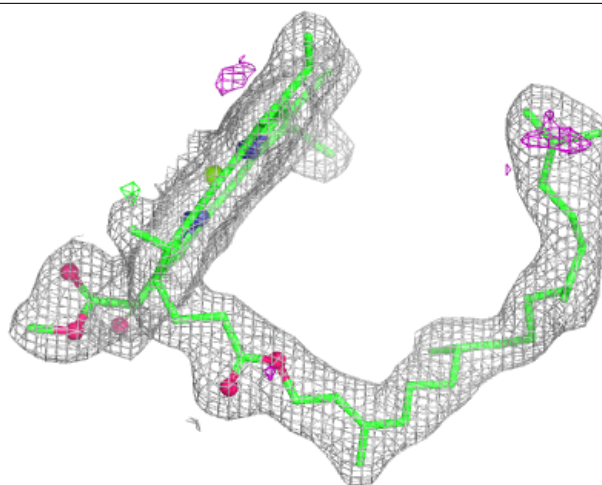
Electron density around CLA B 612:

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



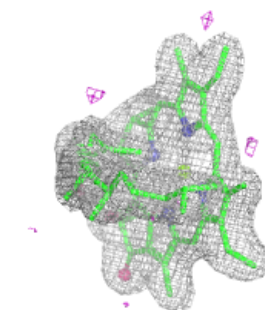
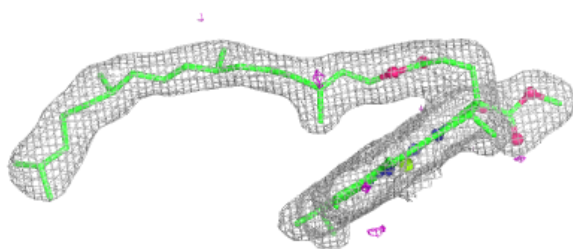
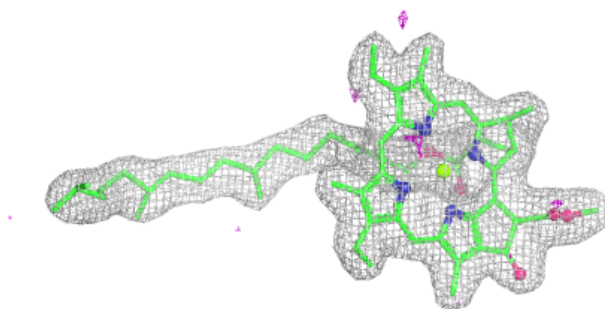
Electron density around CLA b 610:

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

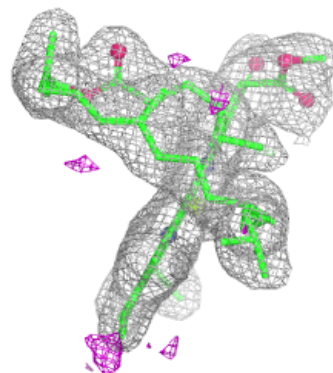
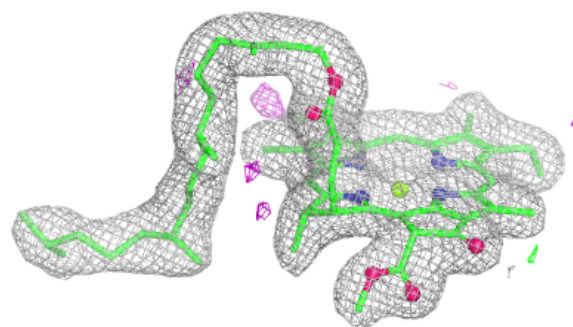
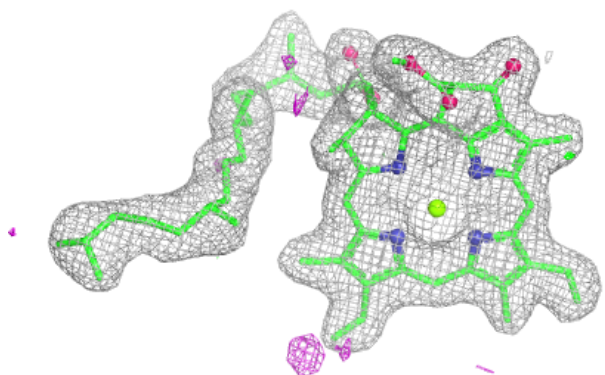


Electron density around CLA B 607:

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

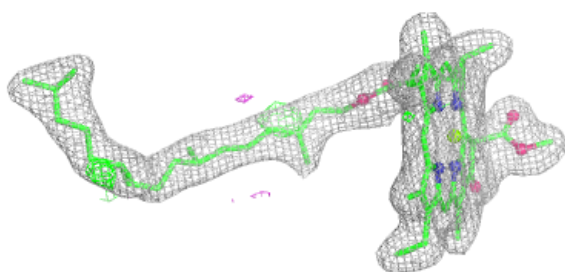
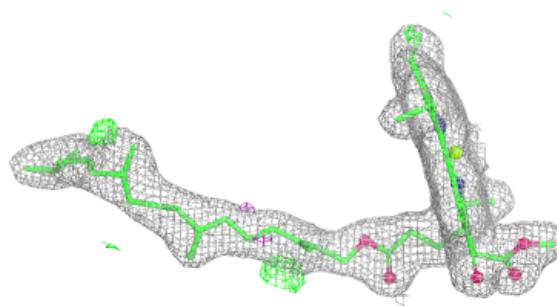
**Electron density around CLA A 612:**

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



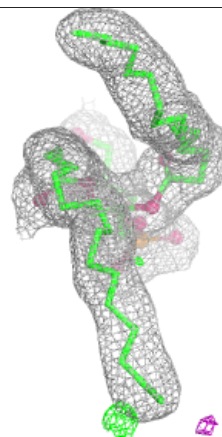
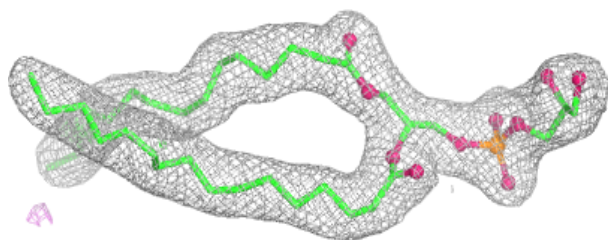
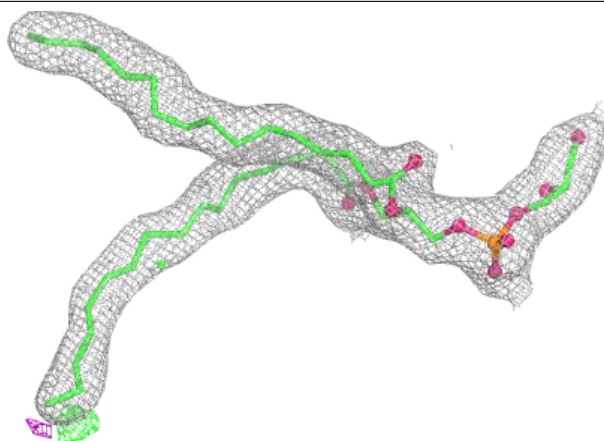
Electron density around CLA B 604:

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



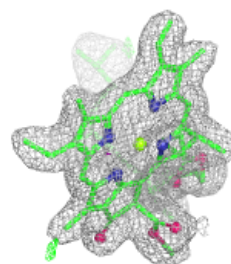
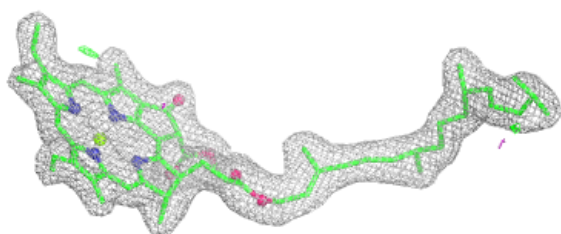
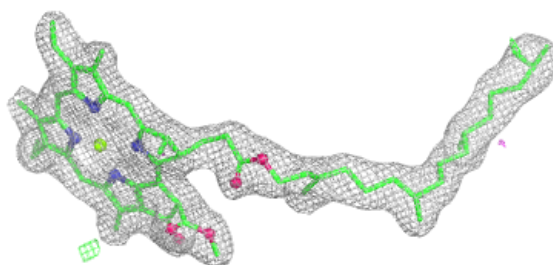
Electron density around LHG D 408:

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

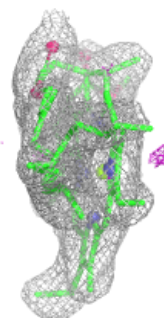
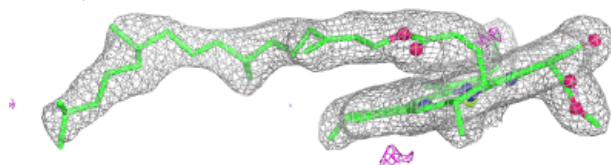
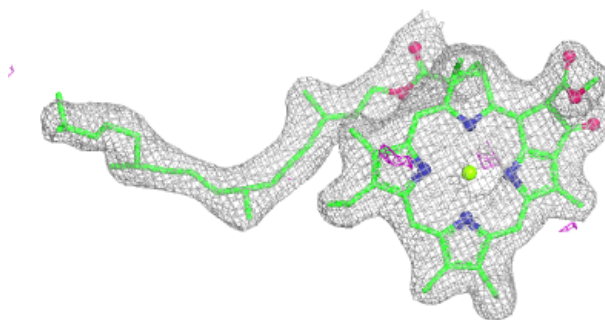


Electron density around CLA A 606:

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

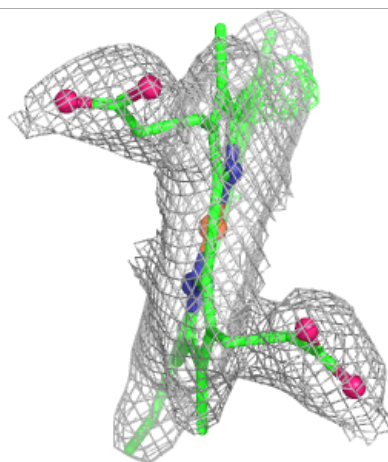
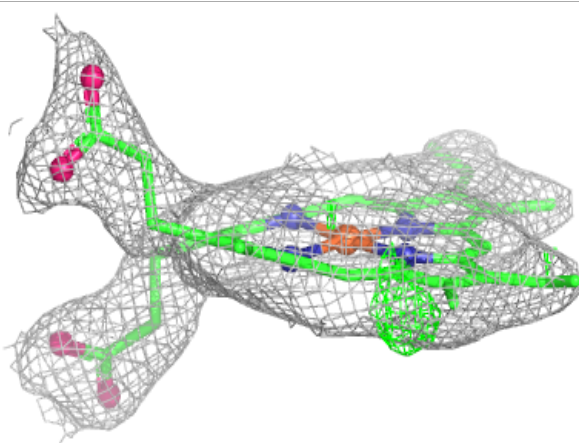
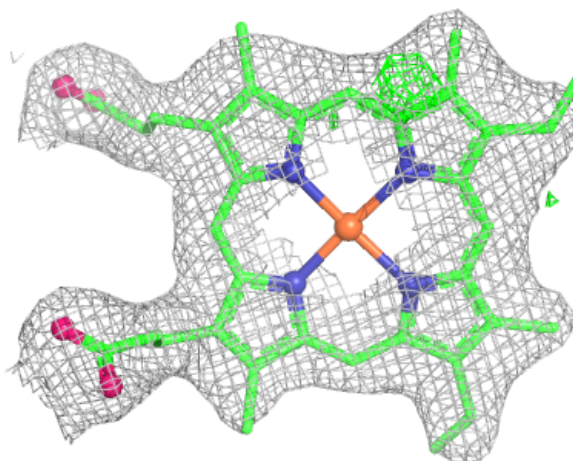
**Electron density around CLA b 602:**

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



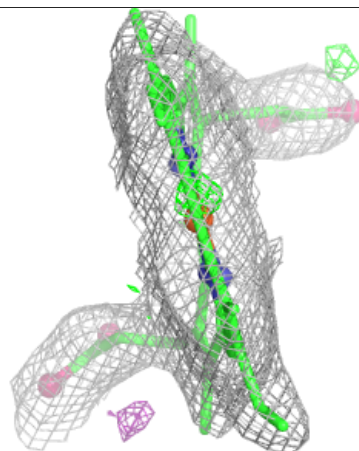
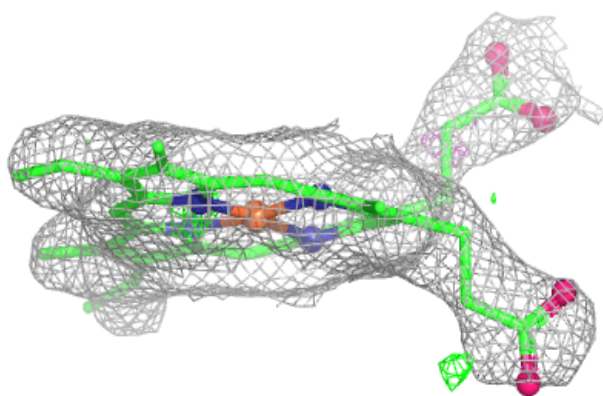
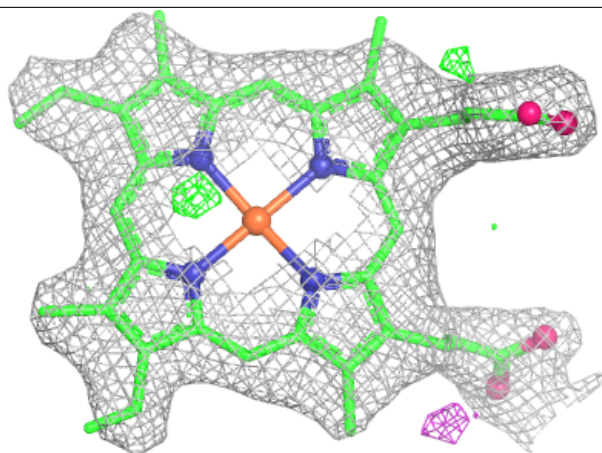
Electron density around HEM F 101:

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



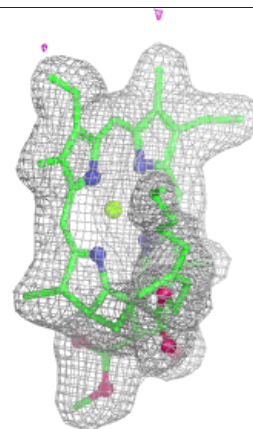
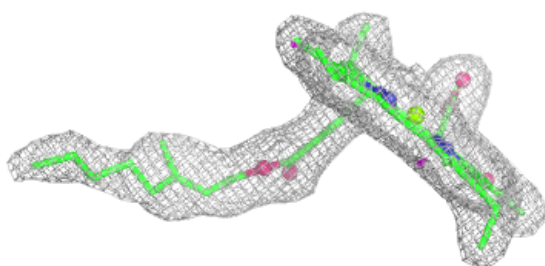
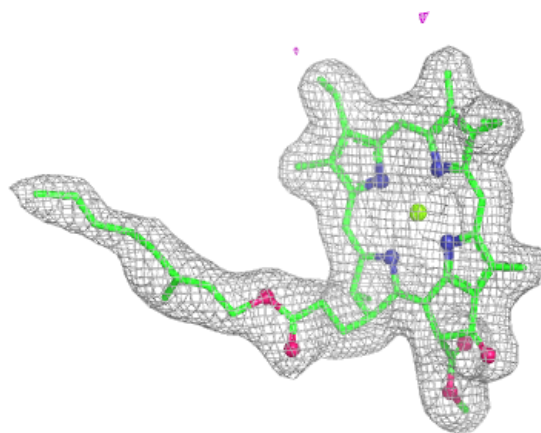
Electron density around HEM f 101:

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



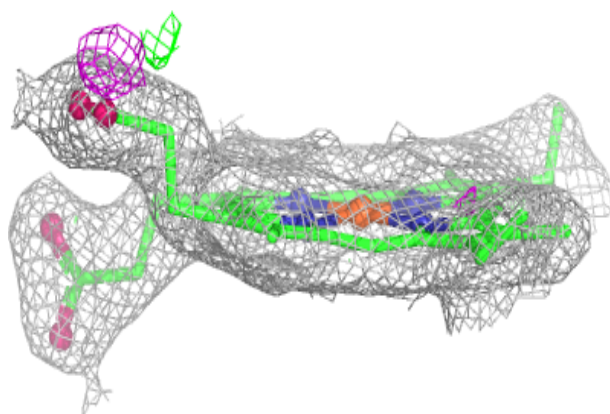
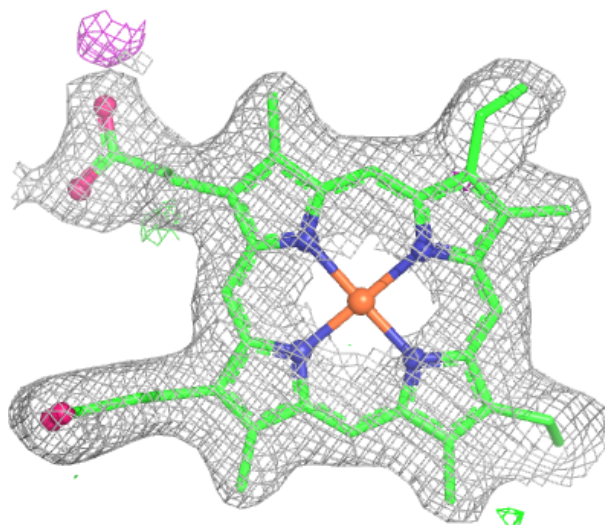
Electron density around CLA A 609:

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



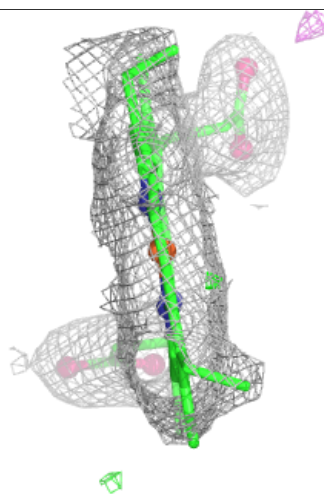
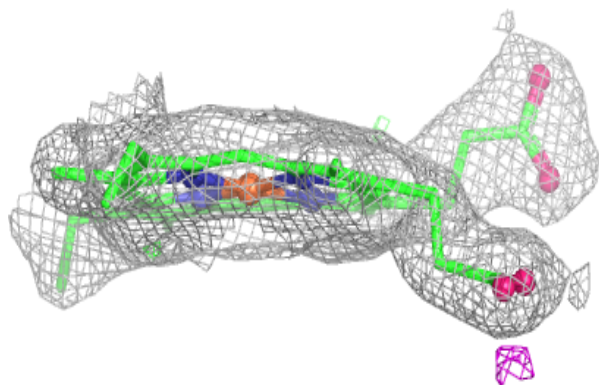
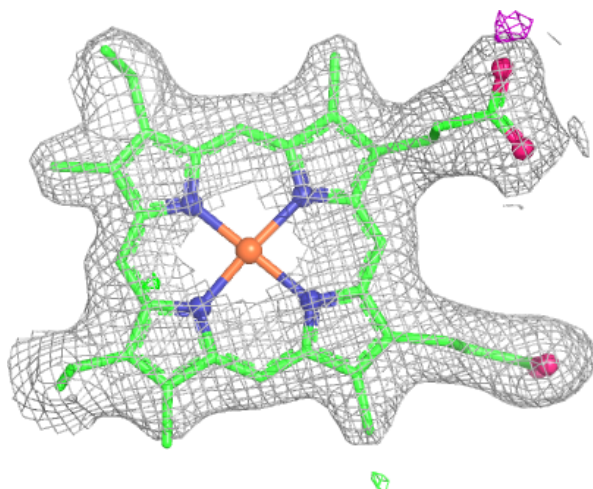
Electron density around HEC V 201:

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



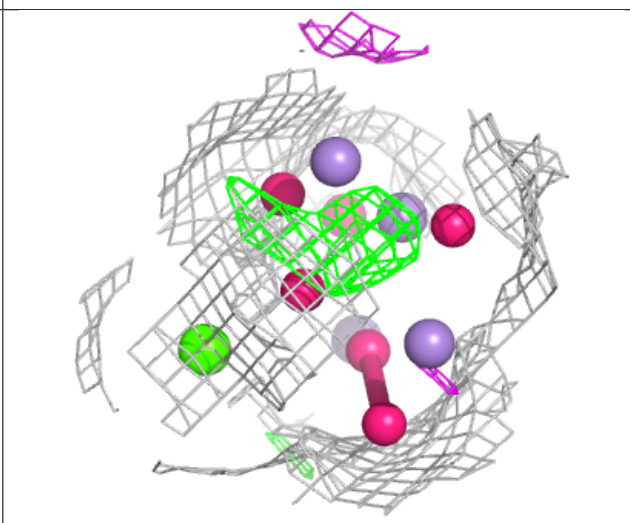
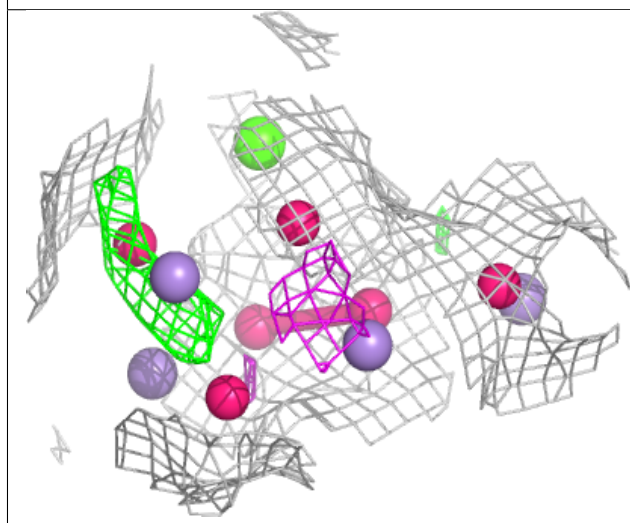
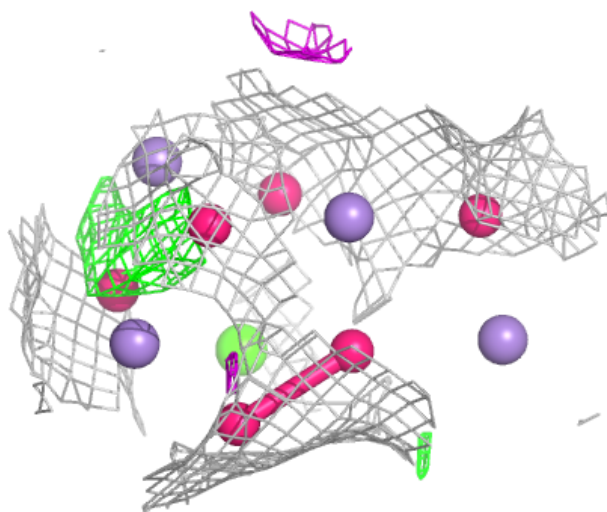
Electron density around HEC v 201:

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



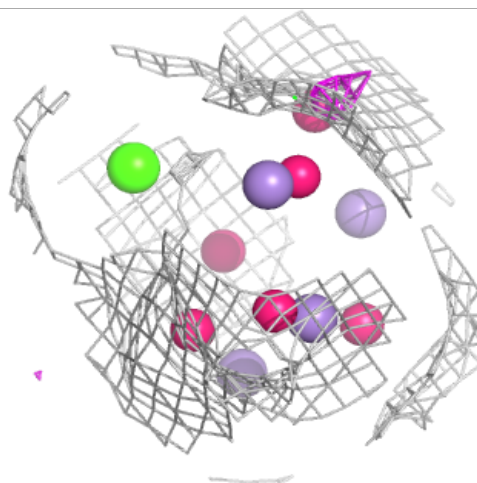
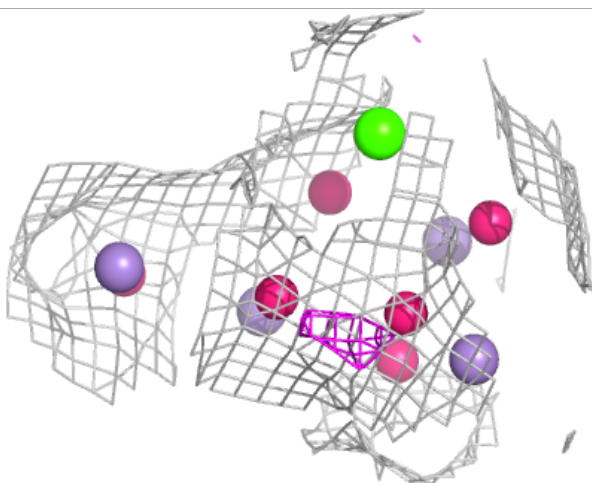
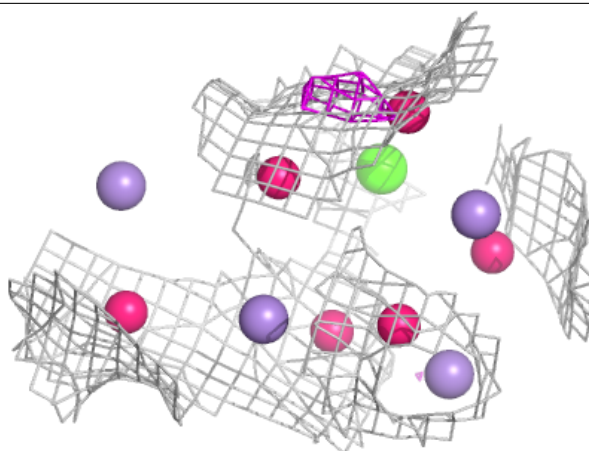
Electron density around OEY A 601 (C):

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



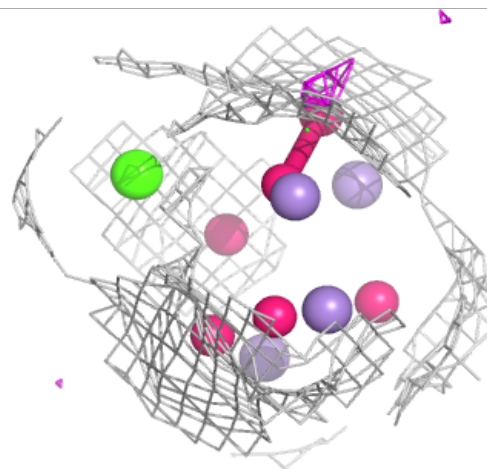
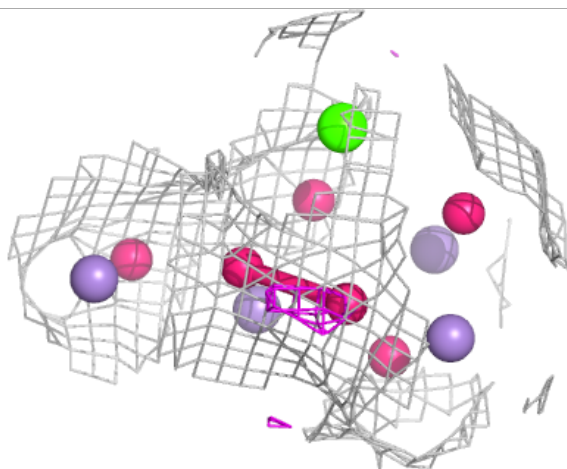
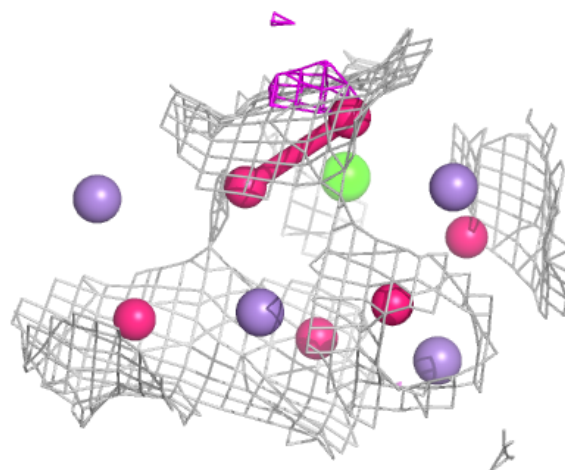
Electron density around OEY a 601 (A):

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



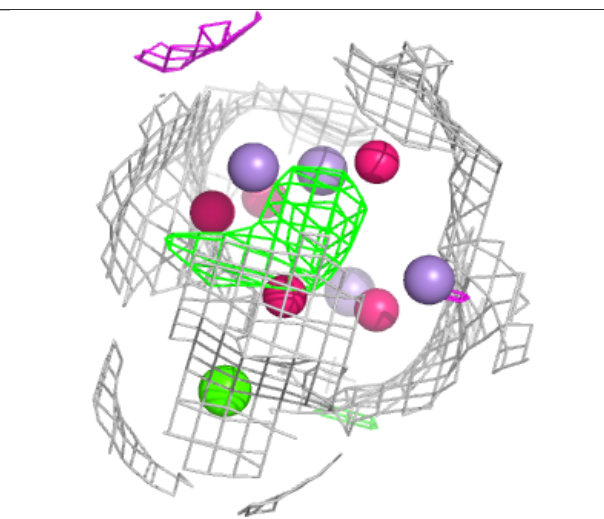
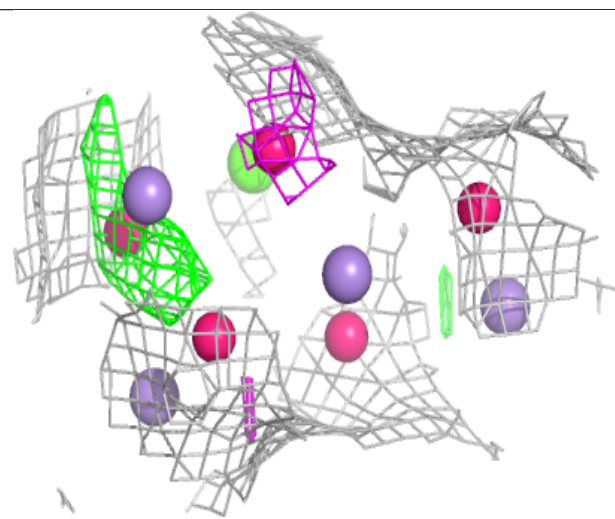
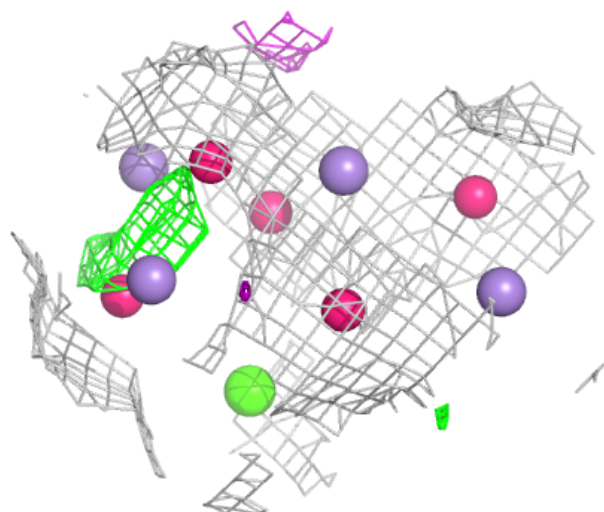
Electron density around OEY a 601 (C):

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



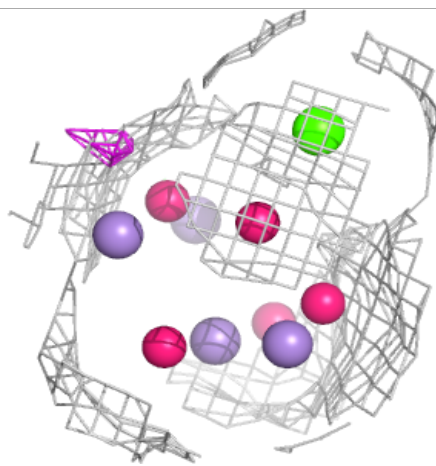
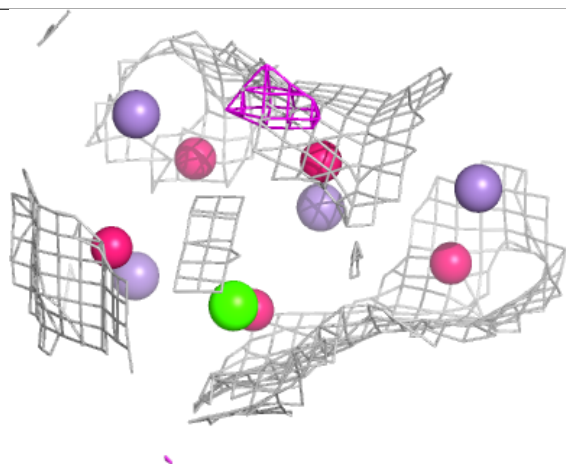
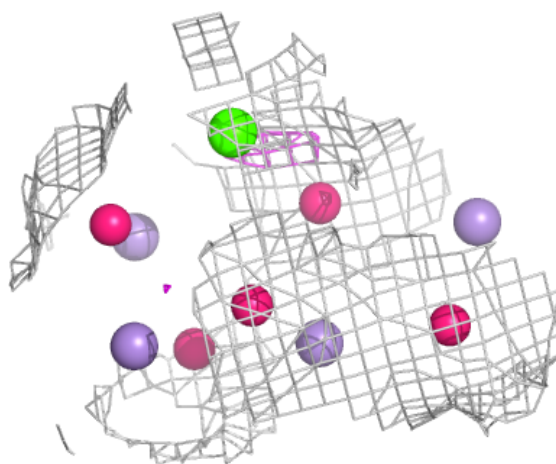
Electron density around OEX A 602 (B):

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



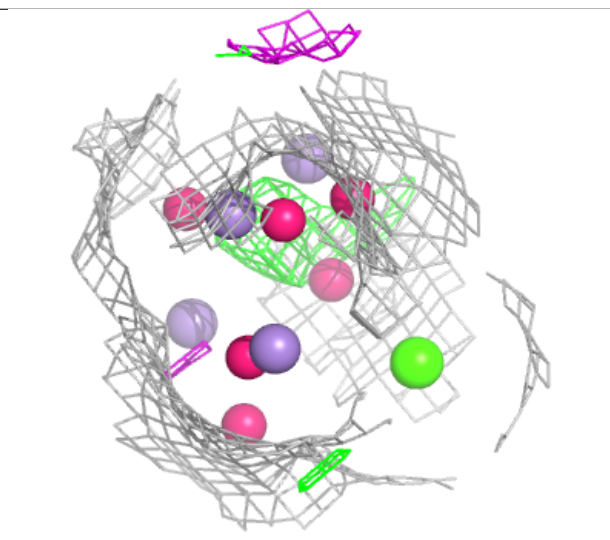
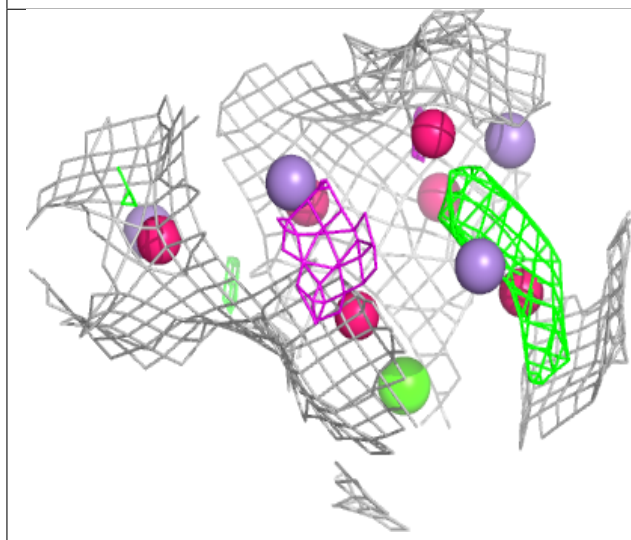
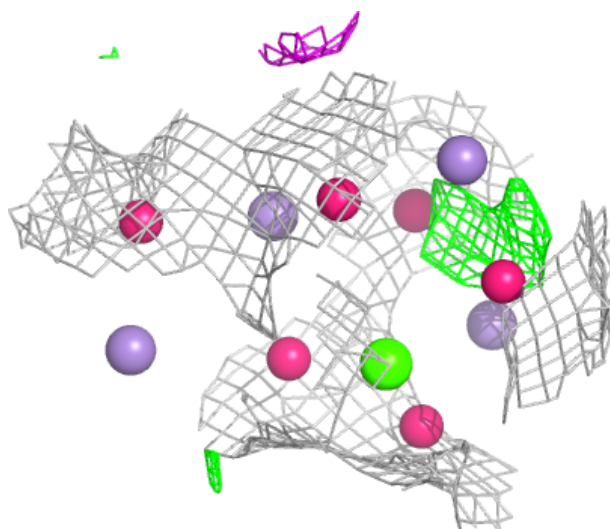
Electron density around OEX a 602 (B):

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



Electron density around OEY A 601 (A):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.