



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:49 PM EDT

PDB ID : 8F4K / pdb_00008f4k
Title : RT XFEL structure of the three-flash state of Photosystem II (3F, S0-rich) at 2.16 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 : 2.16 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

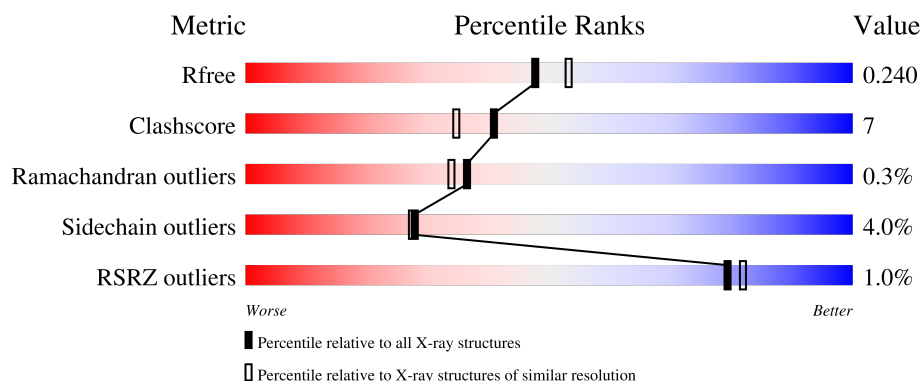
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

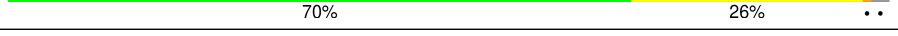
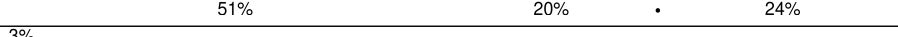
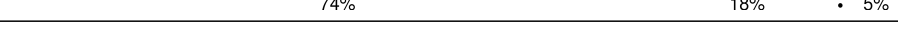
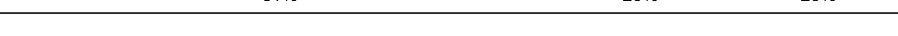
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

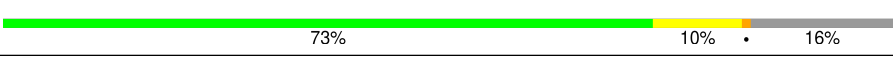
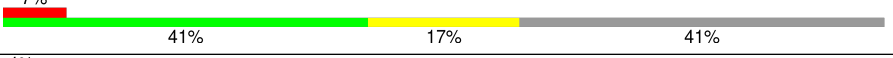
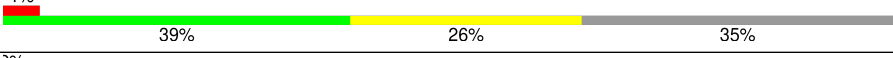
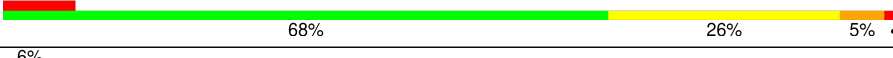
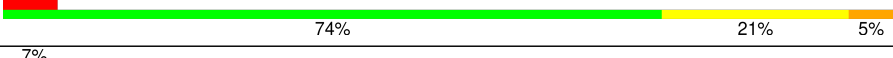
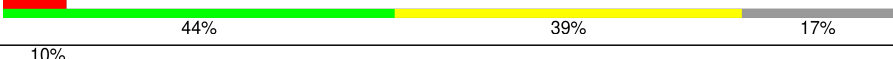
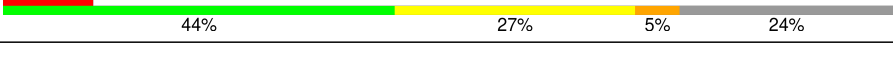
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	

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
36	HEC	V	201	X	-	-	-
36	HEC	v	201	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 53024 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
			3113	2030	513	551	19			
1	a	334	Total	C	N	O	S	0	64	0
			3110	2027	513	551	19			

- 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
			3509	2302	586	607	14			
3	c	451	Total	C	N	O	S	0	12	0
			3583	2343	602	624	14			

- 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
			2731	1809	446	464	12			
4	d	341	Total	C	N	O	S	0	3	0
			2737	1813	446	466	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- 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			
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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- 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			

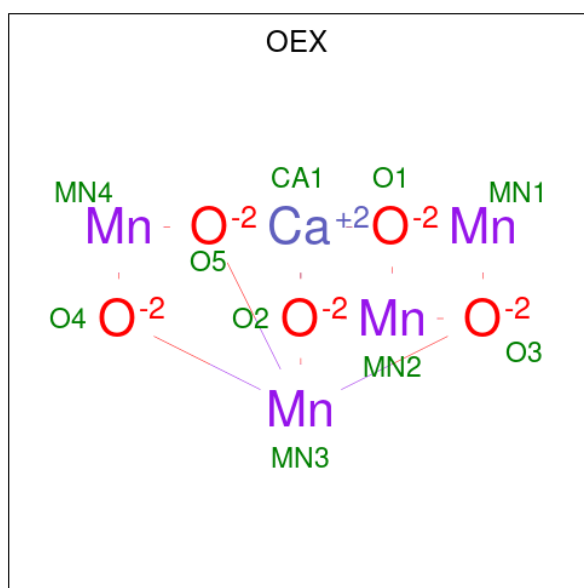
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

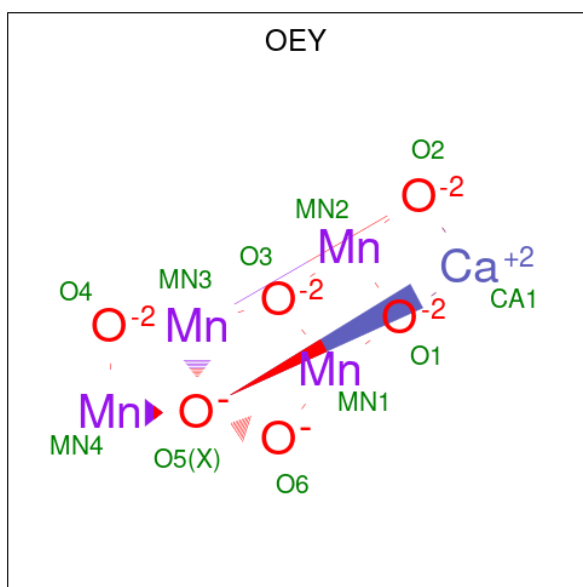
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
20	r	31	Total	C	N	O	0	0	0
			246	166	43	37			

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 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
22	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
22	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

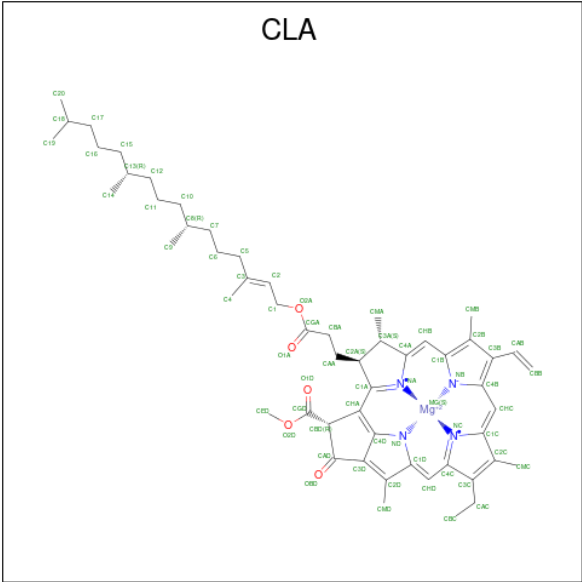
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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 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 59	C 49	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

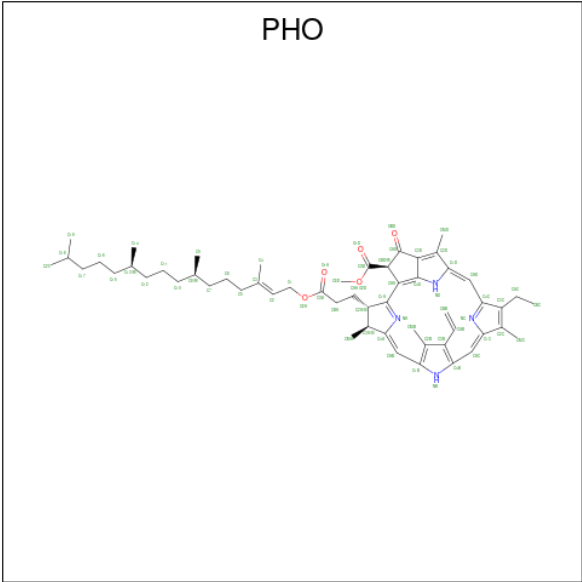
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

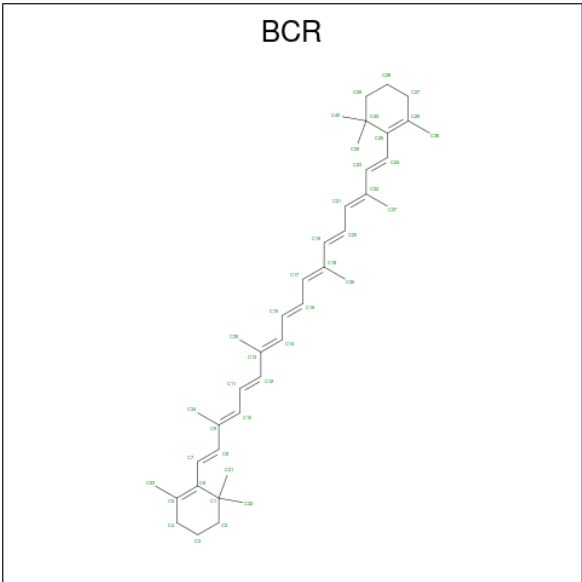
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 64	C 54	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N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

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



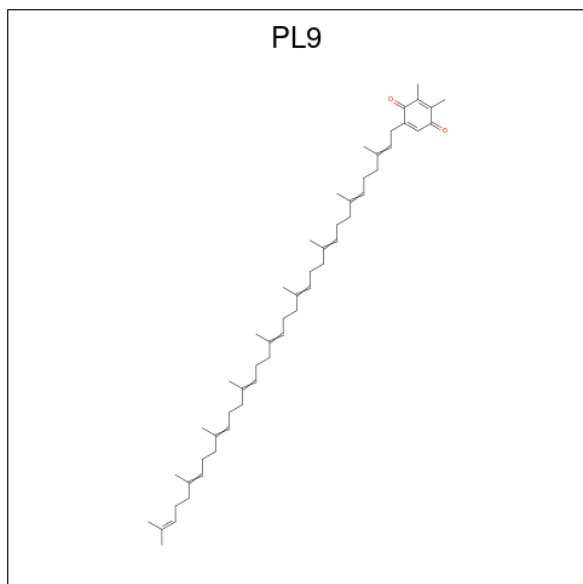
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



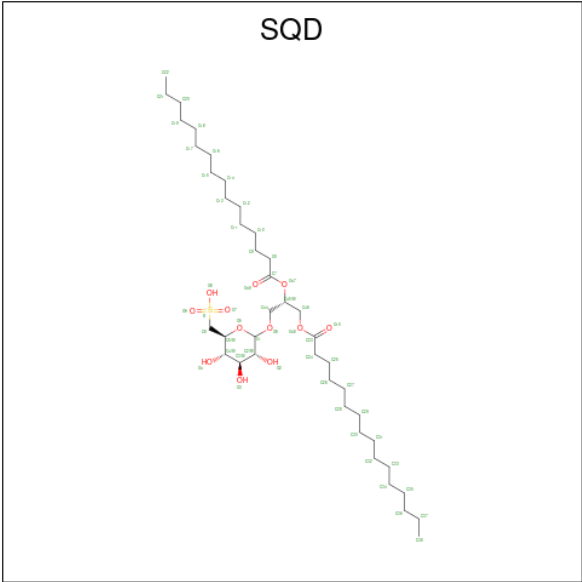
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	Z	1	Total 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
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	c	1	Total C 40 40	0	0
27	d	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	x	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: $C_{53}H_{80}O_2$).



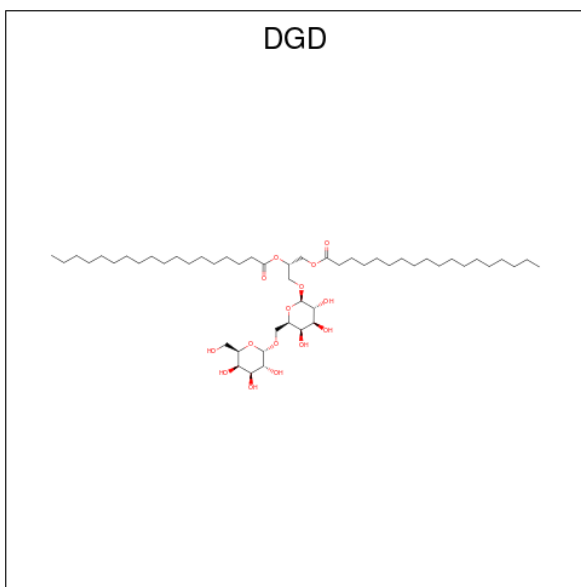
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			55	53	2		
28	D	1	Total	C	O	0	0
			55	53	2		
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



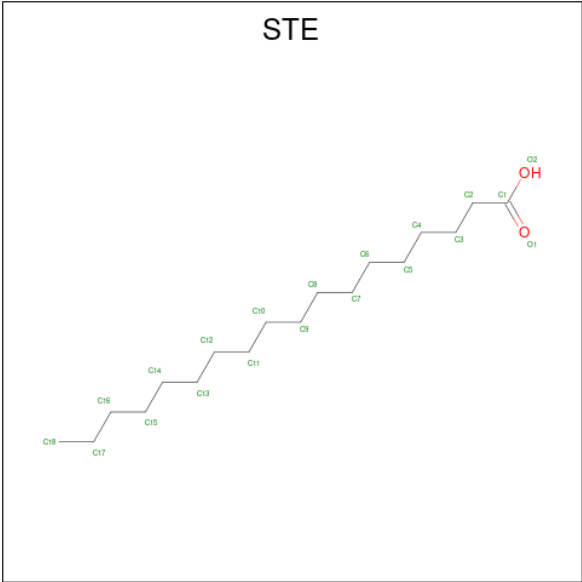
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			36	25	10	1		
29	T	1	Total	C	O		0	0
			39	35	4			
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O		0	0
			36	31	5			
29	b	1	Total	C	O	S	0	0
			49	36	12	1		
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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

- Molecule 31 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



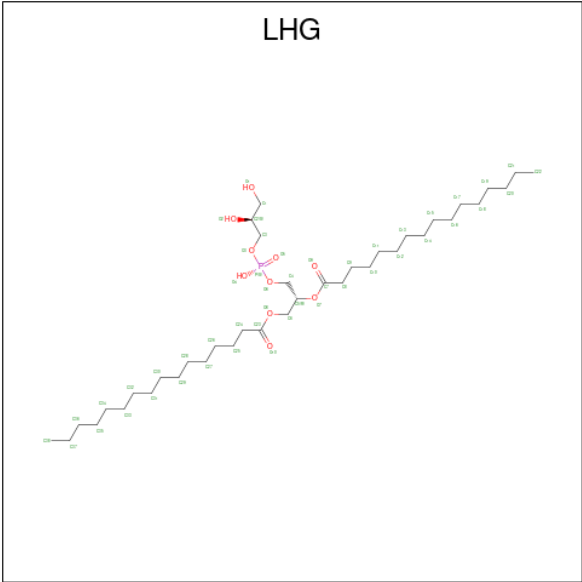
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			17	15	2		
31	B	1	Total	C	O	0	0
			12	10	2		
31	B	1	Total	C	O	0	0
			18	16	2		
31	B	1	Total	C	O	0	0
			12	10	2		
31	B	1	Total	C		0	0
			16	16			
31	C	1	Total	C	O	0	0
			12	10	2		
31	C	1	Total	C	O	0	0
			12	10	2		
31	C	1	Total	C		0	0
			16	16			
31	D	1	Total	C	O	0	0
			20	18	2		
31	E	1	Total	C	O	0	0
			12	10	2		
31	H	1	Total	C		0	0
			18	18			
31	I	1	Total	C		0	0
			15	15			
31	J	1	Total	C	O	0	0
			12	10	2		
31	M	1	Total	C	O	0	0
			15	13	2		

Continued on next page...

Continued from previous page...

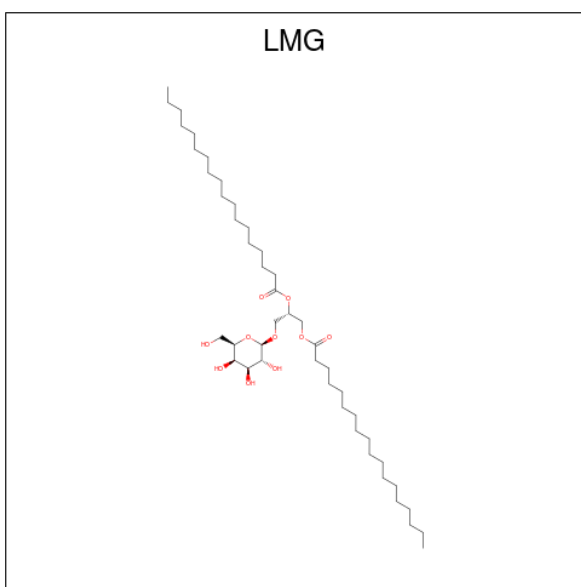
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	M	1	Total C 10 10	0	0
31	M	1	Total C 15 15	0	0
31	T	1	Total C 16 16	0	0
31	a	1	Total C O 12 10 2	0	0
31	b	1	Total C O 20 18 2	0	0
31	b	1	Total C O 16 14 2	0	0
31	b	1	Total C O 20 18 2	0	0
31	b	1	Total C 10 10	0	0
31	c	1	Total C O 20 18 2	0	0
31	c	1	Total C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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



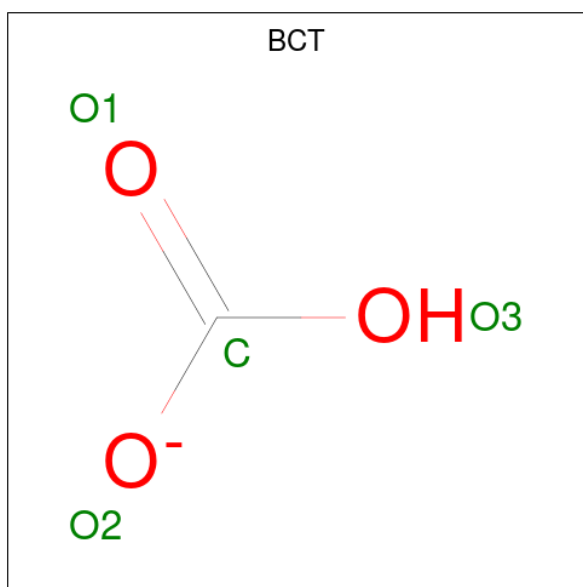
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			47	36	10	1		
32	E	1	Total	C	O	P	0	0
			49	38	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	b	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



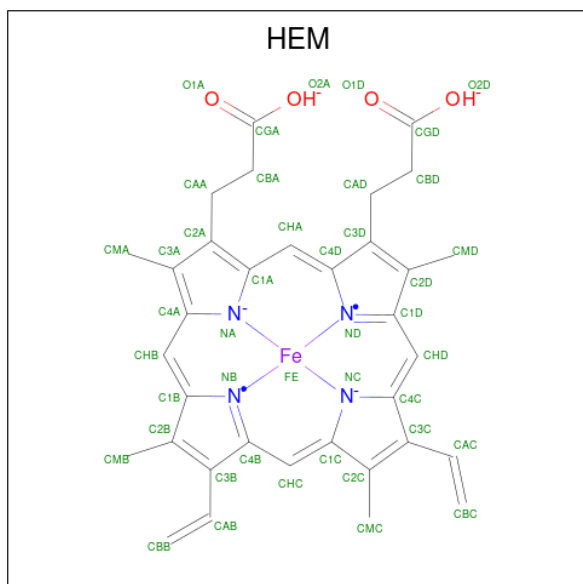
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			48	38	10		
33	C	1	Total	C	O	0	0
			48	38	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			33	27	6		
33	D	1	Total	C	O	0	0
			28	24	4		
33	M	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			55	45	10		
33	c	1	Total	C	O	0	0
			37	27	10		
33	c	1	Total	C	O	0	0
			48	38	10		
33	c	1	Total	C	O	0	0
			49	39	10		
33	d	1	Total	C	O	0	0
			23	21	2		
33	d	1	Total	C	O	0	0
			44	34	10		

- 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	a	1	Total	C	O	0	0
			4	1	3		

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



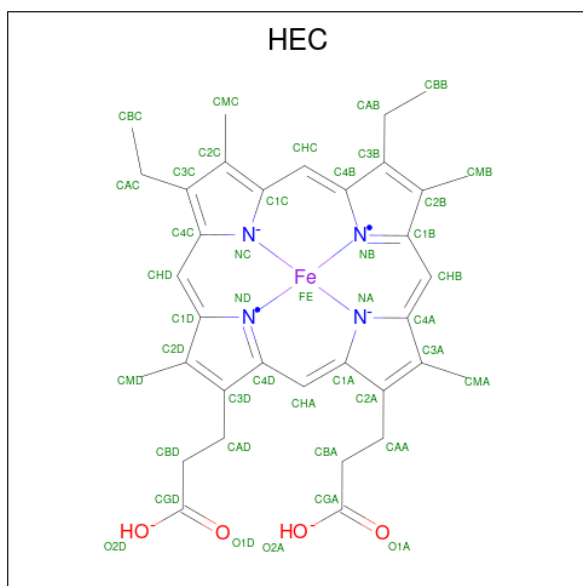
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	121	Total	O		
			125	125	0	4
37	B	161	Total	O		
			161	161	0	0
37	C	150	Total	O		
			150	150	0	0
37	D	112	Total	O		
			112	112	0	0
37	E	20	Total	O		
			20	20	0	0
37	F	7	Total	O		
			7	7	0	0

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	20	Total 20	O 20	0	0
37	J	17	Total 17	O 17	0	0
37	K	4	Total 4	O 4	0	0
37	L	8	Total 8	O 8	0	0
37	M	3	Total 3	O 3	0	0
37	O	76	Total 76	O 76	0	0
37	T	9	Total 9	O 9	0	0
37	U	32	Total 32	O 32	0	0
37	V	52	Total 52	O 52	0	0
37	X	7	Total 7	O 7	0	0
37	Z	2	Total 2	O 2	0	0
37	R	7	Total 7	O 7	0	0
37	a	102	Total 106	O 106	0	4
37	b	163	Total 163	O 163	0	0
37	c	145	Total 145	O 145	0	0
37	d	93	Total 93	O 93	0	0
37	e	18	Total 18	O 18	0	0
37	f	8	Total 8	O 8	0	0
37	h	18	Total 18	O 18	0	0
37	i	11	Total 11	O 11	0	0

Continued on next page...

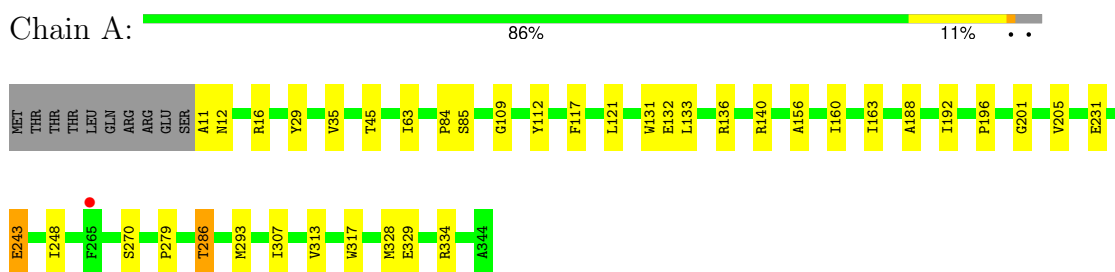
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	j	6	Total 6	O 6	0	0
37	k	4	Total 4	O 4	0	0
37	l	5	Total 5	O 5	0	0
37	m	6	Total 6	O 6	0	0
37	o	79	Total 79	O 79	0	0
37	t	9	Total 9	O 9	0	0
37	u	39	Total 39	O 39	0	0
37	v	46	Total 46	O 46	0	0
37	y	3	Total 3	O 3	0	0
37	x	2	Total 2	O 2	0	0
37	z	8	Total 8	O 8	0	0
37	r	8	Total 8	O 8	0	0

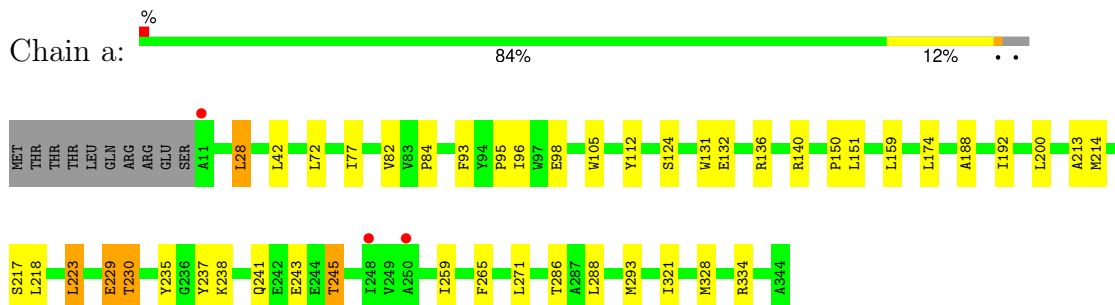
3 Residue-property plots [i](#)

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.

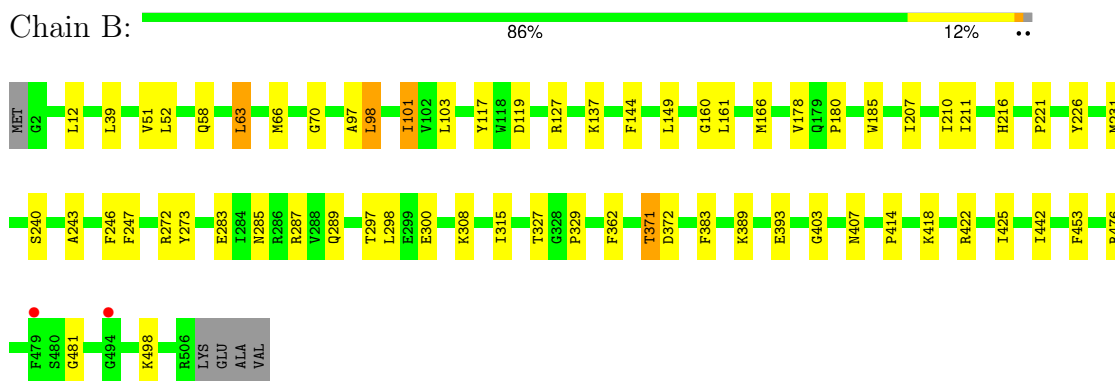
- Molecule 1: Photosystem II protein D1 1



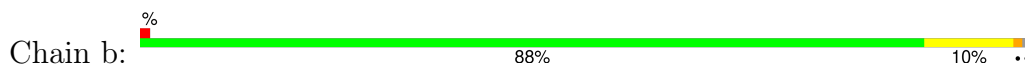
- Molecule 1: Photosystem II protein D1 1

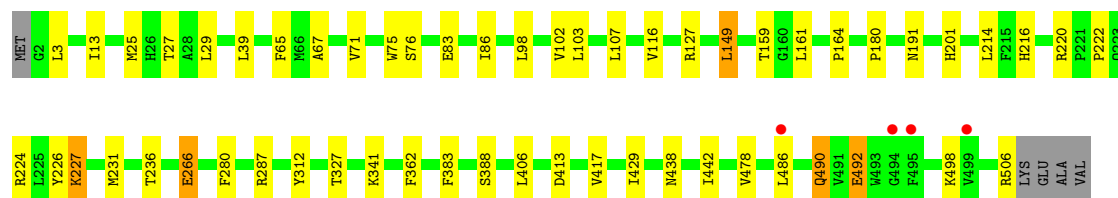


- Molecule 2: Photosystem II CP47 reaction center protein



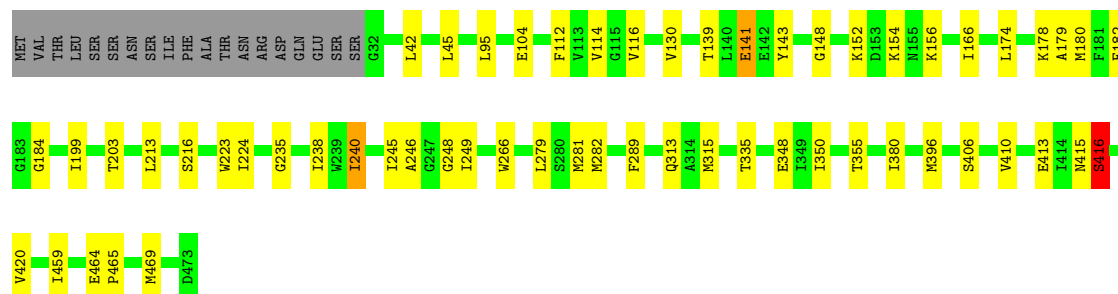
- Molecule 2: Photosystem II CP47 reaction center protein





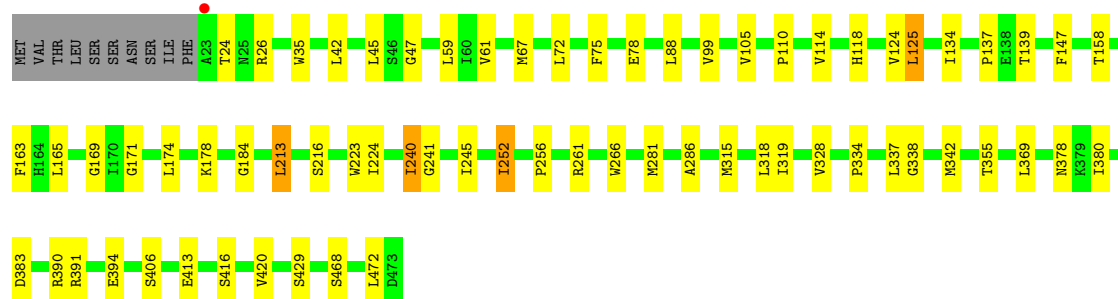
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 83% 12%



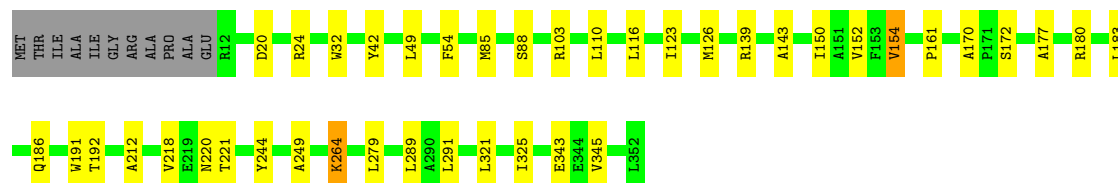
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 83% 14%



• Molecule 4: Photosystem II D2 protein

Chain D: 85% 11%



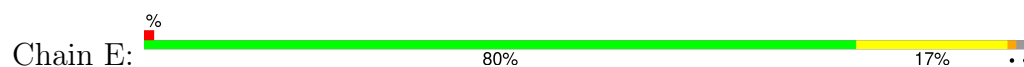
• Molecule 4: Photosystem II D2 protein

Chain d: 81% 16%





- Molecule 5: Cytochrome b559 subunit alpha



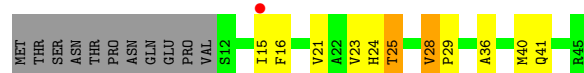
- Molecule 5: Cytochrome b559 subunit alpha



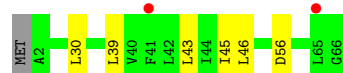
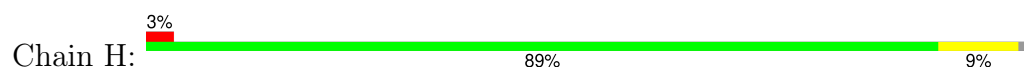
- Molecule 6: Cytochrome b559 subunit beta



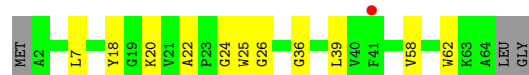
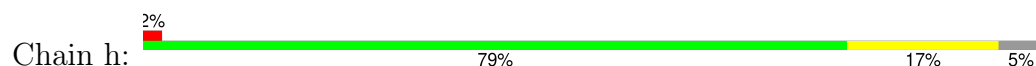
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

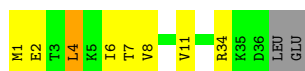


- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

Chain I:  74% 18% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  87% 8% 5%



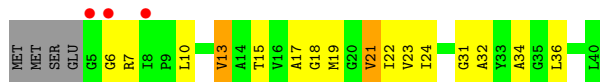
- Molecule 9: Photosystem II reaction center protein J

Chain J:  72% 18% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  8% 50% 35% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  67% 11% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  61% 20% 20%



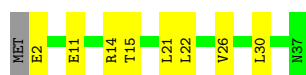
- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 



- Molecule 12: Photosystem II reaction center protein M

Chain M: 



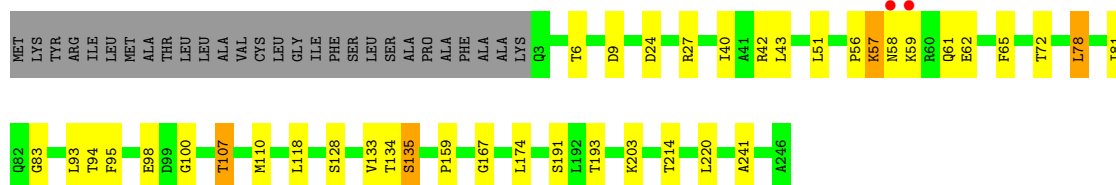
- Molecule 12: Photosystem II reaction center protein M

Chain m: 



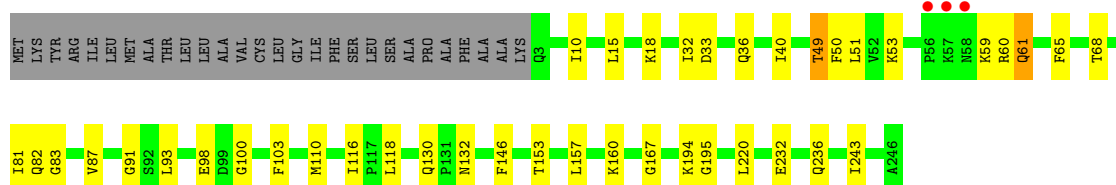
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 



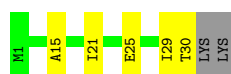
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 

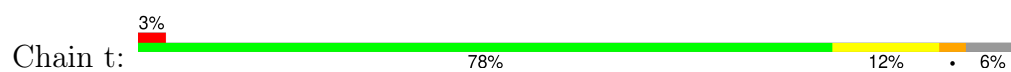


- Molecule 14: Photosystem II reaction center protein T

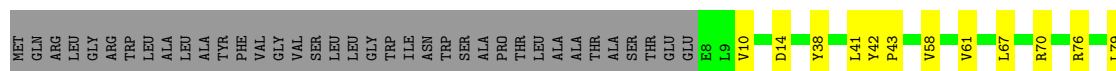
Chain T: 



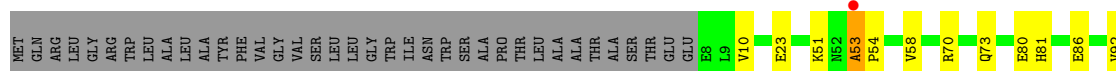
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



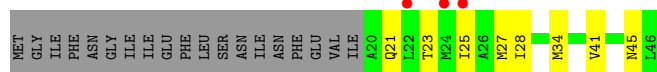
- Molecule 16: Cytochrome c-550



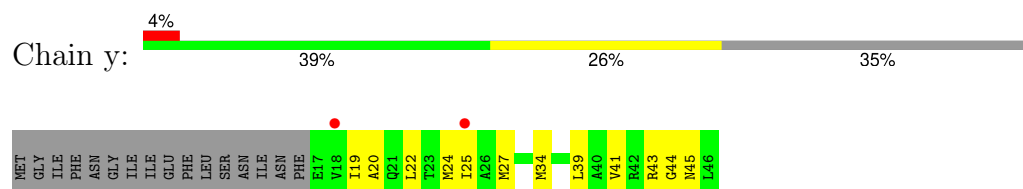
- Molecule 16: Cytochrome c-550



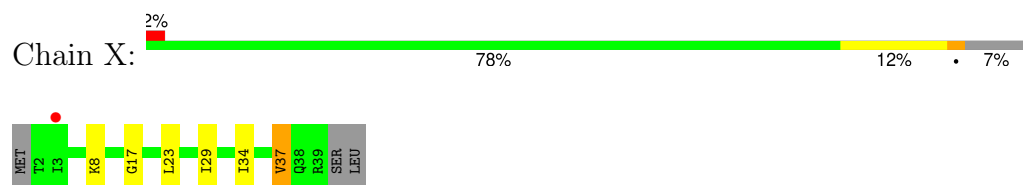
- Molecule 17: Photosystem II reaction center protein Ycf12



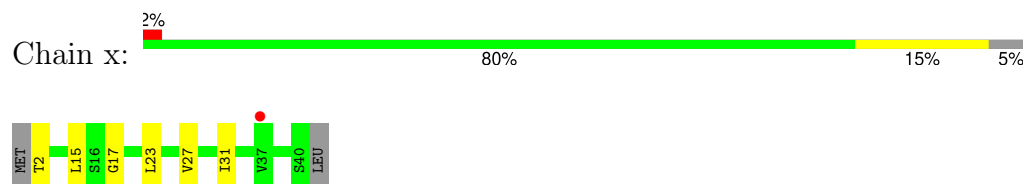
- Molecule 17: Photosystem II reaction center protein Ycf12



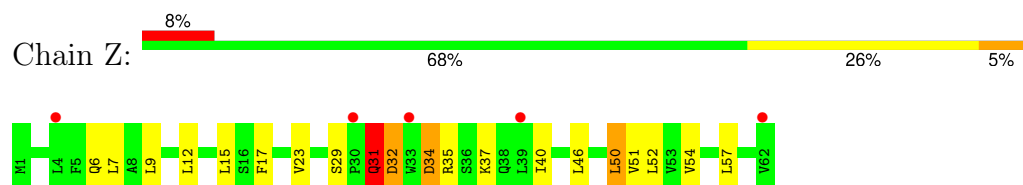
- Molecule 18: Photosystem II reaction center X protein



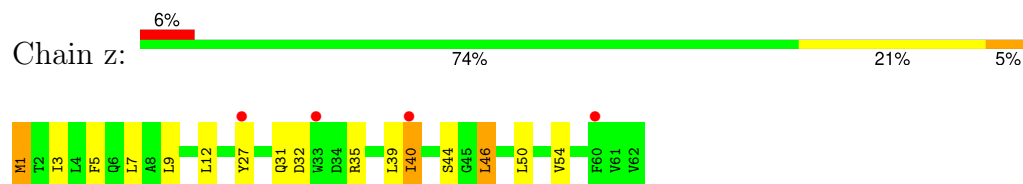
- Molecule 18: Photosystem II reaction center X protein



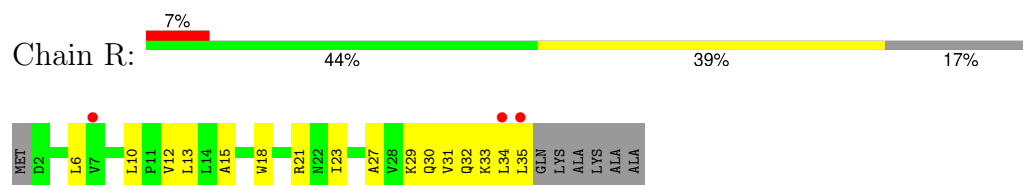
- Molecule 19: Photosystem II reaction center protein Z



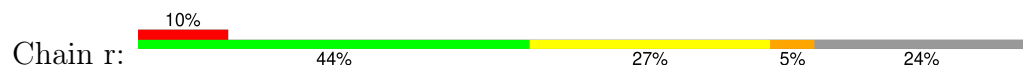
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.99Å 221.75Å 307.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.52 – 2.16 33.52 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.1 (33.52-2.16) 84.7 (33.52-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.241 0.185 , 0.240	Depositor DCC
R_{free} test set	3779 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53024	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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: CLA, BCT, DGD, HEC, FE2, OEX, PHO, OEY, BCR, CL, LHG, SQD, PL9, HEM, STE, FME, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/3212	0.49	0/4376
1	a	0.29	0/3209	0.48	0/4372
2	B	0.33	0/4155	0.50	0/5661
2	b	0.31	0/4118	0.48	0/5611
3	C	0.31	0/3625	0.47	0/4935
3	c	0.29	0/3705	0.45	0/5042
4	D	0.34	0/2825	0.51	0/3847
4	d	0.33	0/2834	0.51	0/3859
5	E	0.27	0/688	0.42	0/940
5	e	0.23	0/683	0.42	0/932
6	F	0.29	0/284	0.43	0/387
6	f	0.26	0/284	0.50	0/387
7	H	0.36	0/523	0.53	0/713
7	h	0.30	0/511	0.43	0/697
8	I	0.32	0/293	0.49	0/396
8	i	0.35	0/293	0.45	0/396
9	J	0.28	0/263	0.44	0/356
9	j	0.25	0/263	0.42	0/356
10	K	0.26	0/303	0.46	0/416
10	k	0.25	0/303	0.41	0/416
11	L	0.34	0/311	0.49	0/422
11	l	0.33	0/303	0.46	0/412
12	M	0.33	0/249	0.56	0/341
12	m	0.35	0/244	0.52	0/334
13	O	0.31	0/1904	0.52	0/2585
13	o	0.33	0/1905	0.49	0/2583
14	T	0.36	0/257	0.51	0/349
14	t	0.33	0/255	0.50	0/346
15	U	0.28	0/785	0.48	0/1064
15	u	0.31	0/785	0.50	0/1064
16	V	0.31	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.28	0/1085	0.43	0/1473
17	Y	0.22	0/197	0.37	0/264
17	y	0.21	0/219	0.35	0/294
18	X	0.26	0/284	0.43	0/384
18	x	0.23	0/289	0.36	0/391
19	Z	0.21	0/490	0.38	0/669
19	z	0.18	0/488	0.32	0/666
20	R	0.28	0/277	0.55	0/380
20	r	0.24	0/252	0.37	0/347
All	All	0.30	0/44038	0.48	0/59936

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	3113	0	2981	29	0
1	a	3110	0	2972	36	0
2	B	4005	0	3871	45	0
2	b	3978	0	3836	44	0
3	C	3509	0	3426	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	42	0
4	D	2731	0	2637	35	0
4	d	2737	0	2643	44	0
5	E	666	0	651	14	0
5	e	664	0	648	14	0
6	F	275	0	282	4	0
6	f	275	0	282	11	0
7	H	510	0	532	5	0
7	h	498	0	518	11	0
8	I	296	0	311	4	0
8	i	296	0	311	3	0
9	J	257	0	268	5	0
9	j	257	0	268	10	0
10	K	293	0	305	2	0
10	k	293	0	305	4	0
11	L	304	0	316	7	0
11	l	296	0	304	5	0
12	M	256	0	269	7	0
12	m	251	0	267	7	0
13	O	1870	0	1830	27	0
13	o	1874	0	1846	26	0
14	T	258	0	261	4	0
14	t	256	0	256	4	0
15	U	774	0	773	7	0
15	u	774	0	773	7	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	12	0
17	Y	196	0	217	3	0
17	y	218	0	241	5	0
18	X	281	0	312	4	0
18	x	286	0	314	3	0
19	Z	479	0	516	12	0
19	z	477	0	509	8	0
20	R	271	0	298	10	0
20	r	246	0	263	8	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	11	0	0	1	0
22	a	11	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	6	0
25	B	970	0	1067	41	0
25	C	839	0	922	24	0
25	D	130	0	144	5	0
25	H	65	0	72	3	0
25	a	195	0	216	10	0
25	b	970	0	1067	44	0
25	c	839	0	919	25	0
25	d	195	0	216	6	0
25	h	65	0	72	4	0
26	A	64	0	74	0	0
26	D	64	0	74	5	0
26	a	64	0	74	2	0
26	d	64	0	74	5	0
27	A	40	0	56	0	0
27	B	120	0	168	7	0
27	C	40	0	56	5	0
27	D	40	0	56	1	0
27	H	40	0	56	1	0
27	K	40	0	56	1	0
27	T	40	0	56	4	0
27	Y	40	0	56	1	0
27	Z	40	0	56	1	0
27	a	40	0	56	0	0
27	b	120	0	168	6	0
27	c	120	0	168	6	0
27	d	40	0	56	2	0
27	k	40	0	56	0	0
27	t	40	0	56	5	0
27	x	40	0	56	4	0
28	A	55	0	80	5	0
28	D	55	0	80	0	0
28	a	55	0	80	5	0
28	d	55	0	80	3	0
29	A	52	0	71	3	0
29	B	54	0	78	4	0
29	D	36	0	46	1	0
29	T	39	0	65	1	0
29	a	90	0	134	4	0
29	b	49	0	65	4	0
29	f	41	0	49	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	66	0	96	9	0
30	C	186	0	246	9	0
30	H	62	0	82	4	0
30	a	44	0	75	2	0
30	c	186	0	246	6	0
30	h	62	0	82	3	0
31	B	75	0	117	2	0
31	C	40	0	63	2	0
31	D	20	0	35	1	0
31	E	12	0	16	0	0
31	H	18	0	35	1	0
31	I	15	0	26	2	0
31	J	12	0	16	0	0
31	M	40	0	67	0	0
31	T	16	0	31	0	0
31	a	12	0	16	0	0
31	b	66	0	110	1	0
31	c	32	0	51	1	0
31	d	17	0	26	1	0
31	j	12	0	16	0	0
31	l	18	0	35	0	0
31	m	12	0	16	0	0
31	t	24	0	36	2	0
31	x	20	0	35	0	0
32	B	49	0	74	3	0
32	D	96	0	141	5	0
32	E	49	0	74	2	0
32	L	49	0	74	1	0
32	b	49	0	74	3	0
32	d	88	0	125	4	0
32	e	42	0	57	0	0
32	l	49	0	74	5	0
33	C	96	0	132	7	0
33	D	112	0	157	4	0
33	M	51	0	72	2	0
33	b	106	0	158	3	0
33	c	134	0	181	6	0
33	d	67	0	92	1	0
34	D	4	0	1	1	0
34	a	4	0	1	0	0
35	F	43	0	30	3	0
35	e	43	0	30	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	43	0	30	0	0
36	v	43	0	30	0	0
37	A	125	0	0	3	0
37	B	161	0	0	0	0
37	C	150	0	0	4	0
37	D	112	0	0	1	0
37	E	20	0	0	0	0
37	F	7	0	0	0	0
37	H	28	0	0	0	0
37	I	20	0	0	1	0
37	J	17	0	0	1	0
37	K	4	0	0	0	0
37	L	8	0	0	1	0
37	M	3	0	0	0	0
37	O	76	0	0	4	0
37	R	7	0	0	0	0
37	T	9	0	0	0	0
37	U	32	0	0	0	0
37	V	52	0	0	1	0
37	X	7	0	0	1	0
37	Z	2	0	0	0	0
37	a	106	0	0	0	0
37	b	163	0	0	2	0
37	c	145	0	0	1	0
37	d	93	0	0	0	0
37	e	18	0	0	0	0
37	f	8	0	0	0	0
37	h	18	0	0	1	0
37	i	11	0	0	0	0
37	j	6	0	0	2	0
37	k	4	0	0	0	0
37	l	5	0	0	0	0
37	m	6	0	0	0	0
37	o	79	0	0	0	0
37	r	8	0	0	1	0
37	t	9	0	0	0	0
37	u	39	0	0	1	0
37	v	46	0	0	1	0
37	x	2	0	0	0	0
37	y	3	0	0	0	0
37	z	8	0	0	0	0
All	All	53024	0	52753	681	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 681 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)
28:A:611:PL9:H361	6:F:25:THR:HG21	1.49	0.95
3:C:245:ILE:O	37:C:601:HOH:O	1.85	0.94
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.62	0.81
5:e:57:ALA:H	5:e:60:GLN:HE21	1.29	0.81
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.64	0.79

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	395/344 (115%)	391 (99%)	4 (1%)	0	100	100
1	a	395/344 (115%)	387 (98%)	7 (2%)	1 (0%)	36	34
2	B	507/510 (99%)	501 (99%)	6 (1%)	0	100	100
2	b	503/510 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	451/461 (98%)	441 (98%)	9 (2%)	1 (0%)	43	44
3	c	461/461 (100%)	448 (97%)	12 (3%)	1 (0%)	43	44
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
10	K	35/46 (76%)	33 (94%)	2 (6%)	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%)	27 (90%)	3 (10%)	0	100	100
13	O	243/272 (89%)	231 (95%)	8 (3%)	4 (2%)	7	3
13	o	242/272 (89%)	234 (97%)	7 (3%)	1 (0%)	30	26
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	13
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	22 (88%)	2 (8%)	1 (4%)	2	0
17	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	7	2
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
20	r	29/41 (71%)	29 (100%)	0	0	100	100
All	All	5386/5700 (94%)	5234 (97%)	138 (3%)	14 (0%)	36	34

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
19	Z	31	GLN
13	O	62	GLU
13	O	134	THR

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	322/280 (115%)	314 (98%)	8 (2%)	42	45
1	a	321/280 (115%)	310 (97%)	11 (3%)	32	33
2	B	407/407 (100%)	395 (97%)	12 (3%)	37	39
2	b	402/407 (99%)	388 (96%)	14 (4%)	32	32
3	C	353/362 (98%)	341 (97%)	12 (3%)	32	33
3	c	362/362 (100%)	347 (96%)	15 (4%)	27	26
4	D	277/283 (98%)	274 (99%)	3 (1%)	65	72
4	d	278/283 (98%)	271 (98%)	7 (2%)	42	45
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	40
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	9
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	31
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	8
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	56
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	56
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	2
10	K	30/37 (81%)	26 (87%)	4 (13%)	4	1
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	39
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	5
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	3
13	O	206/228 (90%)	200 (97%)	6 (3%)	37	39
13	o	207/228 (91%)	200 (97%)	7 (3%)	32	33
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	27
15	U	84/112 (75%)	82 (98%)	2 (2%)	43	47
15	u	84/112 (75%)	81 (96%)	3 (4%)	31	31
16	V	117/138 (85%)	116 (99%)	1 (1%)	70	77
16	v	117/138 (85%)	114 (97%)	3 (3%)	40	43
17	Y	19/37 (51%)	16 (84%)	3 (16%)	2	1
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	4
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	4
19	Z	52/52 (100%)	42 (81%)	10 (19%)	1	0
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
20	R	28/33 (85%)	21 (75%)	7 (25%)	0	0
20	r	25/33 (76%)	19 (76%)	6 (24%)	1	0
All	All	4450/4654 (96%)	4272 (96%)	178 (4%)	28	27

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	413[A]	GLU
12	m	13	LEU
4	d	230	SER
6	f	25	THR
13	o	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	338	GLN
18	x	33	GLN
3	c	378	ASN
20	r	30	GLN
13	o	155	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	1.02	0	8,9,11	1.02	1 (12%)
12	FME	M	1	12	8,9,10	1.05	1 (12%)	8,9,11	0.99	0
14	FME	t	1	14	8,9,10	1.13	1 (12%)	8,9,11	1.07	0
12	FME	m	1	12	8,9,10	1.01	1 (12%)	8,9,11	0.63	0
14	FME	T	1	14	8,9,10	0.99	0	8,9,11	0.82	0
8	FME	i	1	8	8,9,10	1.01	0	8,9,11	1.17	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
8	FME	I	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	4/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

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	-
8	FME	i	1	8	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.39	1.43	1.46
12	M	1	FME	CA-N	-2.20	1.43	1.46
12	m	1	FME	CA-N	-2.16	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.69	114.70	109.50
8	I	1	FME	CB-CA-N	2.07	114.29	110.52

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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
32	LHG	B	620	-	48,48,48	0.84	1 (2%)	51,54,54	1.36	7 (13%)
25	CLA	B	602	2	69,73,73	1.27	9 (13%)	82,113,113	1.29	6 (7%)
25	CLA	b	611	2	69,73,73	1.18	7 (10%)	82,113,113	1.37	12 (14%)
32	LHG	L	101	-	48,48,48	0.76	2 (4%)	51,54,54	1.19	3 (5%)
25	CLA	C	513	3	69,73,73	1.28	6 (8%)	82,113,113	1.32	7 (8%)
27	BCR	B	616	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	6 (10%)
28	PL9	A	611	-	55,55,55	0.90	2 (3%)	68,69,69	1.42	12 (17%)
29	SQD	a	613	-	52,54,54	1.55	7 (13%)	62,65,65	1.86	13 (20%)
25	CLA	B	609	37	69,73,73	1.12	6 (8%)	82,113,113	1.35	9 (10%)
27	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.25	6 (10%)
31	STE	E	102	-	11,11,19	0.76	0	11,11,19	1.17	0
25	CLA	c	508	3	68,72,73	1.39	8 (11%)	80,111,113	1.35	6 (7%)
31	STE	b	624	-	15,15,19	0.74	0	15,15,19	0.97	0
25	CLA	C	509	3	69,73,73	1.31	10 (14%)	82,113,113	1.41	9 (10%)
31	STE	d	411	-	16,16,19	0.64	0	16,16,19	1.22	1 (6%)
21	OEX	A	601[B]	1,3,37	0,14,14	-	-	-	-	-
25	CLA	b	603	2	69,73,73	1.15	8 (11%)	82,113,113	1.65	14 (17%)
27	BCR	c	516	-	41,41,41	1.05	3 (7%)	56,56,56	1.22	6 (10%)
32	LHG	d	408	-	38,38,48	0.76	1 (2%)	41,44,54	1.15	3 (7%)
22	OXY	A	602[A]	1,3,37	0,16,16	-	-	-	-	-
29	SQD	D	408	-	34,36,54	1.50	6 (17%)	42,45,65	2.44	12 (28%)
25	CLA	B	613	2	69,73,73	1.28	7 (10%)	82,113,113	1.27	7 (8%)
30	DGD	H	103	-	63,63,67	1.13	4 (6%)	77,77,81	1.36	9 (11%)
30	DGD	c	517	-	63,63,67	1.01	7 (11%)	77,77,81	1.36	8 (10%)
25	CLA	D	404	4	69,73,73	1.30	9 (13%)	82,113,113	1.30	8 (9%)
25	CLA	h	101	37	69,73,73	1.31	9 (13%)	82,113,113	1.41	7 (8%)
25	CLA	C	504	37	63,67,73	1.34	7 (11%)	74,105,113	1.32	12 (16%)
29	SQD	b	619	-	47,49,54	1.62	8 (17%)	57,60,65	1.92	14 (24%)
33	LMG	b	620	-	51,51,55	0.94	3 (5%)	59,59,63	1.54	10 (16%)
33	LMG	d	409	-	21,21,55	0.50	0	20,20,63	1.23	2 (10%)
30	DGD	C	516	-	63,63,67	1.09	8 (12%)	77,77,81	1.33	8 (10%)
25	CLA	C	502	3	69,73,73	1.46	9 (13%)	82,113,113	1.33	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	507	37	69,73,73	1.23	10 (14%)	82,113,113	1.46	8 (9%)
27	BCR	D	405	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	4 (7%)
25	CLA	c	503	3	69,73,73	1.33	9 (13%)	82,113,113	1.36	8 (9%)
25	CLA	c	505	3	69,73,73	1.29	7 (10%)	82,113,113	1.28	7 (8%)
25	CLA	c	506	3	69,73,73	1.37	9 (13%)	82,113,113	1.26	5 (6%)
25	CLA	A	607	37	69,73,73	1.16	5 (7%)	82,113,113	1.28	8 (9%)
31	STE	B	619	-	16,16,19	0.71	0	16,16,19	1.03	0
34	BCT	a	606	23	3,3,3	1.17	0	2,3,3	2.88	1 (50%)
27	BCR	d	405	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	6 (10%)
25	CLA	b	604	2	69,73,73	1.25	7 (10%)	82,113,113	1.52	10 (12%)
34	BCT	D	401	23	3,3,3	1.07	0	2,3,3	3.18	1 (50%)
27	BCR	T	101	-	41,41,41	0.99	3 (7%)	56,56,56	1.23	4 (7%)
27	BCR	t	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.36	8 (14%)
28	PL9	d	406	-	55,55,55	1.15	3 (5%)	68,69,69	1.55	13 (19%)
25	CLA	b	607	2	69,73,73	1.40	8 (11%)	82,113,113	1.38	12 (14%)
33	LMG	b	622	-	55,55,55	0.82	1 (1%)	63,63,63	1.39	8 (12%)
25	CLA	c	511	3	69,73,73	1.37	7 (10%)	82,113,113	1.43	5 (6%)
33	LMG	D	407	-	51,51,55	0.76	2 (3%)	59,59,63	1.36	7 (11%)
31	STE	B	623	-	17,17,19	0.57	0	17,17,19	1.23	1 (5%)
25	CLA	B	614	2	69,73,73	1.28	7 (10%)	82,113,113	1.28	8 (9%)
30	DGD	C	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.43	6 (7%)
33	LMG	c	522	-	48,48,55	0.88	2 (4%)	56,56,63	1.26	8 (14%)
31	STE	b	621	-	19,19,19	0.62	0	19,19,19	1.04	1 (5%)
25	CLA	B	601	2	69,73,73	1.18	8 (11%)	82,113,113	1.36	10 (12%)
30	DGD	h	102	-	63,63,67	0.96	4 (6%)	77,77,81	1.41	9 (11%)
33	LMG	M	101	-	51,51,55	0.85	0	59,59,63	1.38	7 (11%)
29	SQD	B	621	-	52,54,54	1.59	9 (17%)	62,65,65	1.76	12 (19%)
22	OXY	a	602[A]	1,3,37	0,16,16	-	-	-	-	-
27	BCR	Y	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	5 (8%)
31	STE	C	522	-	15,15,19	0.39	0	14,14,19	0.70	0
26	PHO	D	402	-	58,69,69	2.10	10 (17%)	55,99,99	1.61	8 (14%)
29	SQD	A	613	-	50,52,54	1.61	7 (14%)	60,63,65	1.89	11 (18%)
25	CLA	C	505	3	69,73,73	1.40	7 (10%)	82,113,113	1.26	8 (9%)
31	STE	B	624	-	11,11,19	0.65	0	11,11,19	1.29	1 (9%)
25	CLA	D	403	4	69,73,73	1.29	6 (8%)	82,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	606	37	69,73,73	1.20	9 (13%)	82,113,113	1.29	7 (8%)
25	CLA	b	612	2	69,73,73	1.30	8 (11%)	82,113,113	1.39	12 (14%)
27	BCR	b	616	-	41,41,41	1.05	3 (7%)	56,56,56	1.27	7 (12%)
31	STE	B	622	-	11,11,19	0.66	0	11,11,19	1.32	1 (9%)
25	CLA	a	607	1	69,73,73	1.27	9 (13%)	82,113,113	1.31	7 (8%)
25	CLA	d	403	4	69,73,73	1.22	6 (8%)	82,113,113	1.13	5 (6%)
27	BCR	K	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	7 (12%)
25	CLA	A	606	1	69,73,73	1.08	5 (7%)	82,113,113	1.18	5 (6%)
25	CLA	B	603	2	69,73,73	1.31	7 (10%)	82,113,113	1.54	8 (9%)
25	CLA	C	510	3	69,73,73	1.23	9 (13%)	82,113,113	1.31	8 (9%)
33	LMG	C	519	-	48,48,55	0.85	2 (4%)	56,56,63	1.34	8 (14%)
31	STE	c	523	-	11,11,19	0.75	0	11,11,19	1.21	1 (9%)
25	CLA	c	501	3	69,73,73	1.22	8 (11%)	82,113,113	1.45	7 (8%)
25	CLA	b	605	2	69,73,73	1.43	5 (7%)	82,113,113	1.50	8 (9%)
26	PHO	a	608	-	58,69,69	2.11	9 (15%)	55,99,99	1.38	7 (12%)
31	STE	M	102	-	14,14,19	0.64	0	14,14,19	1.13	1 (7%)
21	OEX	a	601[B]	1,3,37	0,14,14	-	-	-	-	-
30	DGD	c	519	-	63,63,67	0.88	2 (3%)	77,77,81	1.45	14 (18%)
29	SQD	T	103	-	38,38,54	1.75	5 (13%)	40,40,65	1.23	3 (7%)
25	CLA	C	501	3	69,73,73	1.41	8 (11%)	82,113,113	1.44	10 (12%)
25	CLA	A	609	1	58,62,73	1.30	6 (10%)	68,99,113	1.29	9 (13%)
33	LMG	c	524	-	49,49,55	0.86	4 (8%)	57,57,63	1.35	7 (12%)
26	PHO	A	608	-	58,69,69	1.99	8 (13%)	55,99,99	1.52	8 (14%)
33	LMG	C	515	-	48,48,55	0.93	2 (4%)	56,56,63	1.32	6 (10%)
31	STE	T	102	-	15,15,19	0.35	0	14,14,19	0.95	0
27	BCR	A	610	-	41,41,41	0.94	2 (4%)	56,56,56	1.38	6 (10%)
31	STE	C	520	-	11,11,19	0.70	0	11,11,19	1.49	1 (9%)
28	PL9	D	406	-	55,55,55	1.00	4 (7%)	68,69,69	1.51	14 (20%)
25	CLA	c	513	3	69,73,73	1.20	7 (10%)	82,113,113	1.27	7 (8%)
25	CLA	b	602	2	69,73,73	1.34	10 (14%)	82,113,113	1.46	12 (14%)
32	LHG	b	623	-	48,48,48	0.72	2 (4%)	51,54,54	1.31	7 (13%)
27	BCR	Z	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
25	CLA	b	615	2	64,68,73	1.19	7 (10%)	76,107,113	1.44	7 (9%)
25	CLA	c	509	3	69,73,73	1.16	6 (8%)	82,113,113	1.35	5 (6%)
30	DGD	A	614	-	67,67,67	1.15	8 (11%)	81,81,81	1.30	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	d	401	37	69,73,73	1.19	6 (8%)	82,113,113	1.28	8 (9%)
31	STE	t	102	-	13,13,19	0.69	0	13,13,19	1.28	2 (15%)
25	CLA	b	609	37	69,73,73	1.41	8 (11%)	82,113,113	1.39	12 (14%)
36	HEC	v	201	16	50,50,50	1.71	5 (10%)	68,82,82	1.44	7 (10%)
33	LMG	D	412	-	26,26,55	0.55	0	26,26,63	1.36	1 (3%)
25	CLA	B	611	2	69,73,73	1.16	8 (11%)	82,113,113	1.50	11 (13%)
31	STE	c	521	-	19,19,19	0.64	0	19,19,19	0.95	0
31	STE	a	616	-	11,11,19	0.85	0	11,11,19	1.01	0
25	CLA	c	504	37	64,68,73	1.18	6 (9%)	76,107,113	1.31	9 (11%)
25	CLA	c	502	3	69,73,73	1.23	8 (11%)	82,113,113	1.33	10 (12%)
31	STE	H	104	-	17,17,19	0.43	0	16,16,19	0.66	0
30	DGD	c	518	-	63,63,67	1.03	3 (4%)	77,77,81	1.39	10 (12%)
27	BCR	x	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.16	3 (5%)
25	CLA	a	609	1	69,73,73	1.24	8 (11%)	82,113,113	1.21	6 (7%)
31	STE	B	625	-	15,15,19	0.34	0	14,14,19	0.94	0
31	STE	b	625	-	19,19,19	0.59	0	19,19,19	1.11	1 (5%)
31	STE	I	101	-	14,14,19	0.43	0	13,13,19	0.65	0
32	LHG	D	409	-	48,48,48	0.70	1 (2%)	51,54,54	1.24	7 (13%)
33	LMG	d	410	-	44,44,55	0.88	2 (4%)	52,52,63	1.34	6 (11%)
35	HEM	e	101	5,6	50,50,50	1.44	9 (18%)	67,82,82	1.33	7 (10%)
25	CLA	C	512	3	69,73,73	1.43	9 (13%)	82,113,113	1.28	7 (8%)
27	BCR	b	618	-	41,41,41	0.99	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	b	613	2	69,73,73	1.23	7 (10%)	82,113,113	1.29	7 (8%)
25	CLA	B	608	2	69,73,73	1.16	6 (8%)	82,113,113	1.27	6 (7%)
31	STE	m	101	-	11,11,19	0.70	0	11,11,19	1.53	2 (18%)
32	LHG	d	407	-	48,48,48	0.62	0	51,54,54	1.21	3 (5%)
32	LHG	l	101	-	48,48,48	0.65	0	51,54,54	1.23	7 (13%)
29	SQD	f	101	-	39,41,54	1.69	8 (20%)	49,52,65	1.85	11 (22%)
31	STE	C	521	-	11,11,19	0.71	0	11,11,19	1.26	1 (9%)
25	CLA	B	606	37	69,73,73	1.25	7 (10%)	82,113,113	1.41	10 (12%)
25	CLA	B	612	2	69,73,73	1.44	5 (7%)	82,113,113	1.45	10 (12%)
27	BCR	c	514	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	6 (10%)
31	STE	D	413	-	19,19,19	0.61	0	19,19,19	1.07	0
32	LHG	e	102	-	41,41,48	0.81	1 (2%)	44,47,54	1.33	6 (13%)
25	CLA	B	607	2	69,73,73	1.29	8 (11%)	82,113,113	1.34	10 (12%)
25	CLA	B	615	2	64,68,73	1.33	9 (14%)	76,107,113	1.38	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	511	3	69,73,73	1.23	8 (11%)	82,113,113	1.28	6 (7%)
26	PHO	d	402	-	58,69,69	2.12	10 (17%)	55,99,99	1.59	9 (16%)
31	STE	l	102	-	17,17,19	0.35	0	16,16,19	0.83	0
27	BCR	b	617	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	6 (10%)
25	CLA	C	506	3	69,73,73	1.46	10 (14%)	82,113,113	1.33	7 (8%)
25	CLA	c	512	3	69,73,73	1.37	10 (14%)	82,113,113	1.31	10 (12%)
31	STE	J	101	-	11,11,19	0.71	0	11,11,19	1.19	1 (9%)
25	CLA	a	612	37	69,73,73	1.32	6 (8%)	82,113,113	1.32	9 (10%)
25	CLA	B	604	2	69,73,73	1.28	7 (10%)	82,113,113	1.25	9 (10%)
27	BCR	k	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.06	2 (3%)
31	STE	x	102	-	19,19,19	0.64	0	19,19,19	1.00	1 (5%)
35	HEM	F	101	5,6	50,50,50	1.41	7 (14%)	67,82,82	1.14	3 (4%)
31	STE	t	103	-	9,9,19	0.48	0	8,8,19	0.55	0
27	BCR	B	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.35	8 (14%)
31	STE	j	101	-	11,11,19	0.73	0	11,11,19	1.28	1 (9%)
31	STE	M	104	-	14,14,19	0.35	0	13,13,19	0.82	0
36	HEC	V	201	16	50,50,50	1.74	7 (14%)	68,82,82	1.36	8 (11%)
33	LMG	D	411	-	31,31,55	0.65	0	33,33,63	1.26	2 (6%)
30	DGD	a	615	-	43,43,67	0.84	2 (4%)	45,45,81	1.45	6 (13%)
33	LMG	c	520	-	37,37,55	0.96	1 (2%)	45,45,63	1.32	6 (13%)
27	BCR	a	610	-	41,41,41	0.97	2 (4%)	56,56,56	1.12	4 (7%)
31	STE	b	626	-	9,9,19	0.34	0	8,8,19	0.78	0
25	CLA	B	605	2	69,73,73	1.36	9 (13%)	82,113,113	1.48	8 (9%)
25	CLA	d	404	4	69,73,73	1.19	7 (10%)	82,113,113	1.21	9 (10%)
25	CLA	H	101	37	69,73,73	1.31	9 (13%)	82,113,113	1.30	8 (9%)
27	BCR	C	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	5 (8%)
25	CLA	b	608	2	69,73,73	1.26	9 (13%)	82,113,113	1.19	8 (9%)
27	BCR	H	102	-	41,41,41	0.96	1 (2%)	56,56,56	1.27	6 (10%)
29	SQD	a	614	-	35,35,54	1.77	5 (14%)	37,37,65	1.35	4 (10%)
25	CLA	b	614	2	69,73,73	1.47	11 (15%)	82,113,113	1.29	5 (6%)
25	CLA	B	610	2	69,73,73	1.27	7 (10%)	82,113,113	1.42	10 (12%)
31	STE	M	103	-	9,9,19	0.37	0	8,8,19	0.71	0
32	LHG	E	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.20	5 (9%)
25	CLA	b	601	2	69,73,73	1.17	7 (10%)	82,113,113	1.38	9 (10%)
32	LHG	D	410	-	46,46,48	0.92	2 (4%)	49,52,54	1.20	6 (12%)
27	BCR	c	515	-	41,41,41	1.08	3 (7%)	56,56,56	1.27	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DGD	C	517	-	63,63,67	1.01	6 (9%)	77,77,81	1.43	13 (16%)
25	CLA	A	612	37	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
25	CLA	c	510	3	69,73,73	1.24	10 (14%)	82,113,113	1.36	9 (10%)
25	CLA	C	503	3	69,73,73	1.31	8 (11%)	82,113,113	1.46	10 (12%)
25	CLA	c	507	37	69,73,73	1.34	9 (13%)	82,113,113	1.36	9 (10%)
28	PL9	a	611	-	55,55,55	0.69	1 (1%)	68,69,69	1.62	12 (17%)
25	CLA	C	508	3	69,73,73	1.39	10 (14%)	82,113,113	1.36	8 (9%)
25	CLA	b	610	2	69,73,73	1.19	8 (11%)	82,113,113	1.40	6 (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
32	LHG	B	620	-	-	14/53/53/53	-
25	CLA	B	602	2	-	12/39/115/115	-
25	CLA	b	611	2	-	8/39/115/115	-
32	LHG	L	101	-	-	22/53/53/53	-
25	CLA	C	513	3	-	14/39/115/115	-
27	BCR	B	616	-	-	4/29/63/63	0/2/2/2
28	PL9	A	611	-	-	29/53/73/73	0/1/1/1
29	SQD	a	613	-	-	25/49/69/69	0/1/1/1
25	CLA	B	609	37	-	5/39/115/115	-
27	BCR	B	617	-	-	5/29/63/63	0/2/2/2
31	STE	E	102	-	-	5/9/9/17	-
25	CLA	c	508	3	-	6/38/114/115	-
31	STE	b	624	-	-	11/13/13/17	-
25	CLA	C	509	3	-	14/39/115/115	-
31	STE	d	411	-	-	11/14/14/17	-
27	BCR	c	516	-	-	5/29/63/63	0/2/2/2
25	CLA	b	603	2	-	9/39/115/115	-
32	LHG	d	408	-	-	15/43/43/53	-
30	DGD	c	517	-	-	28/51/91/95	0/2/2/2
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
25	CLA	B	613	2	-	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	H	103	-	-	17/51/91/95	0/2/2/2
25	CLA	D	404	4	-	6/39/115/115	-
25	CLA	h	101	37	-	19/39/115/115	-
25	CLA	C	504	37	-	8/32/108/115	-
29	SQD	b	619	-	-	21/44/64/69	0/1/1/1
33	LMG	b	620	-	-	16/46/66/70	0/1/1/1
33	LMG	d	409	-	-	10/17/17/70	-
30	DGD	C	516	-	-	24/51/91/95	0/2/2/2
25	CLA	C	502	3	-	8/39/115/115	-
25	CLA	C	507	37	-	10/39/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
25	CLA	c	503	3	-	14/39/115/115	-
25	CLA	c	505	3	-	10/39/115/115	-
25	CLA	c	506	3	-	15/39/115/115	-
25	CLA	A	607	37	-	9/39/115/115	-
31	STE	B	619	-	-	6/14/14/17	-
27	BCR	d	405	-	-	10/29/63/63	0/2/2/2
25	CLA	b	604	2	-	9/39/115/115	-
27	BCR	T	101	-	-	11/29/63/63	0/2/2/2
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
28	PL9	d	406	-	-	8/53/73/73	0/1/1/1
25	CLA	b	607	2	-	7/39/115/115	-
33	LMG	b	622	-	-	18/50/70/70	0/1/1/1
25	CLA	c	511	3	-	9/39/115/115	-
33	LMG	D	407	-	-	16/46/66/70	0/1/1/1
31	STE	B	623	-	-	10/15/15/17	-
25	CLA	B	614	2	-	11/39/115/115	-
30	DGD	C	518	-	-	20/51/91/95	0/2/2/2
33	LMG	c	522	-	-	23/43/63/70	0/1/1/1
31	STE	b	621	-	-	10/17/17/17	-
25	CLA	B	601	2	-	11/39/115/115	-
30	DGD	h	102	-	-	17/51/91/95	0/2/2/2
33	LMG	M	101	-	-	28/46/66/70	0/1/1/1
29	SQD	B	621	-	-	30/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
31	STE	C	522	-	-	3/13/13/17	-
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
29	SQD	A	613	-	-	18/47/67/69	0/1/1/1
25	CLA	C	505	3	-	11/39/115/115	-
31	STE	B	624	-	-	4/9/9/17	-
25	CLA	D	403	4	-	10/39/115/115	-
25	CLA	b	606	37	-	18/39/115/115	-
25	CLA	b	612	2	-	11/39/115/115	-
27	BCR	b	616	-	-	4/29/63/63	0/2/2/2
31	STE	B	622	-	-	6/9/9/17	-
25	CLA	a	607	1	-	6/39/115/115	-
25	CLA	d	403	4	-	12/39/115/115	-
27	BCR	K	101	-	-	9/29/63/63	0/2/2/2
25	CLA	A	606	1	-	9/39/115/115	-
25	CLA	B	603	2	-	11/39/115/115	-
25	CLA	C	510	3	-	12/39/115/115	-
33	LMG	C	519	-	-	23/43/63/70	0/1/1/1
31	STE	c	523	-	-	3/9/9/17	-
25	CLA	c	501	3	-	3/39/115/115	-
25	CLA	b	605	2	-	7/39/115/115	-
26	PHO	a	608	-	-	5/37/103/103	0/5/6/6
31	STE	M	102	-	-	7/12/12/17	-
30	DGD	c	519	-	-	17/51/91/95	0/2/2/2
29	SQD	T	103	-	-	13/39/39/69	-
25	CLA	C	501	3	-	6/39/115/115	-
25	CLA	A	609	1	-	3/26/102/115	-
33	LMG	c	524	-	-	26/44/64/70	0/1/1/1
26	PHO	A	608	-	-	4/37/103/103	0/5/6/6
33	LMG	C	515	-	-	26/43/63/70	0/1/1/1
31	STE	T	102	-	-	8/13/13/17	-
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
31	STE	C	520	-	-	5/9/9/17	-
28	PL9	D	406	-	-	8/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	513	3	-	7/39/115/115	-
25	CLA	b	602	2	-	6/39/115/115	-
32	LHG	b	623	-	-	22/53/53/53	-
27	BCR	Z	101	-	-	11/29/63/63	0/2/2/2
25	CLA	b	615	2	-	10/33/109/115	-
25	CLA	c	509	3	-	9/39/115/115	-
30	DGD	A	614	-	-	26/55/95/95	0/2/2/2
25	CLA	d	401	37	-	12/39/115/115	-
31	STE	t	102	-	-	6/11/11/17	-
25	CLA	b	609	37	-	7/39/115/115	-
36	HEC	v	201	16	1/1/3/7	4/14/54/54	-
33	LMG	D	412	-	-	15/22/22/70	-
25	CLA	B	611	2	-	9/39/115/115	-
31	STE	c	521	-	-	12/17/17/17	-
31	STE	a	616	-	-	2/9/9/17	-
25	CLA	c	504	37	-	10/33/109/115	-
25	CLA	c	502	3	-	5/39/115/115	-
31	STE	H	104	-	-	7/15/15/17	-
30	DGD	c	518	-	-	15/51/91/95	0/2/2/2
27	BCR	x	101	-	-	8/29/63/63	0/2/2/2
25	CLA	a	609	1	-	9/39/115/115	-
31	STE	B	625	-	-	8/13/13/17	-
31	STE	b	625	-	-	11/17/17/17	-
31	STE	I	101	-	-	6/12/12/17	-
32	LHG	D	409	-	-	26/53/53/53	-
33	LMG	d	410	-	-	11/39/59/70	0/1/1/1
35	HEM	e	101	5,6	-	2/14/54/54	-
25	CLA	C	512	3	-	12/39/115/115	-
27	BCR	b	618	-	-	5/29/63/63	0/2/2/2
25	CLA	b	613	2	-	14/39/115/115	-
25	CLA	B	608	2	-	5/39/115/115	-
31	STE	m	101	-	-	3/9/9/17	-
32	LHG	d	407	-	-	19/53/53/53	-
32	LHG	l	101	-	-	19/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	f	101	-	-	16/36/56/69	0/1/1/1
31	STE	C	521	-	-	2/9/9/17	-
25	CLA	B	606	37	-	11/39/115/115	-
25	CLA	B	612	2	-	19/39/115/115	-
27	BCR	c	514	-	-	9/29/63/63	0/2/2/2
31	STE	D	413	-	-	9/17/17/17	-
32	LHG	e	102	-	-	22/46/46/53	-
25	CLA	B	607	2	-	4/39/115/115	-
25	CLA	B	615	2	-	7/33/109/115	-
25	CLA	C	511	3	-	3/39/115/115	-
26	PHO	d	402	-	-	7/37/103/103	0/5/6/6
31	STE	l	102	-	-	10/15/15/17	-
27	BCR	b	617	-	-	4/29/63/63	0/2/2/2
25	CLA	C	506	3	-	13/39/115/115	-
25	CLA	c	512	3	-	25/39/115/115	-
31	STE	J	101	-	-	6/9/9/17	-
25	CLA	a	612	37	-	14/39/115/115	-
25	CLA	B	604	2	-	12/39/115/115	-
27	BCR	k	101	-	-	7/29/63/63	0/2/2/2
31	STE	x	102	-	-	10/17/17/17	-
35	HEM	F	101	5,6	-	3/14/54/54	-
31	STE	t	103	-	-	3/7/7/17	-
27	BCR	B	618	-	-	7/29/63/63	0/2/2/2
31	STE	j	101	-	-	3/9/9/17	-
31	STE	M	104	-	-	8/12/12/17	-
36	HEC	V	201	16	1/1/3/7	4/14/54/54	-
33	LMG	D	411	-	-	15/33/33/70	-
30	DGD	a	615	-	-	24/45/45/95	-
33	LMG	c	520	-	-	22/31/51/70	0/1/1/1
27	BCR	a	610	-	-	3/29/63/63	0/2/2/2
31	STE	b	626	-	-	5/7/7/17	-
25	CLA	B	605	2	-	16/39/115/115	-
25	CLA	d	404	4	-	8/39/115/115	-
25	CLA	H	101	37	-	20/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	C	514	-	-	7/29/63/63	0/2/2/2
25	CLA	b	608	2	-	3/39/115/115	-
27	BCR	H	102	-	-	3/29/63/63	0/2/2/2
29	SQD	a	614	-	-	14/37/37/69	-
25	CLA	b	614	2	-	9/39/115/115	-
25	CLA	B	610	2	-	5/39/115/115	-
31	STE	M	103	-	-	3/7/7/17	-
32	LHG	E	101	-	-	24/53/53/53	-
25	CLA	b	601	2	-	11/39/115/115	-
32	LHG	D	410	-	-	17/51/51/53	-
27	BCR	c	515	-	-	5/29/63/63	0/2/2/2
30	DGD	C	517	-	-	23/51/91/95	0/2/2/2
25	CLA	A	612	37	-	9/39/115/115	-
25	CLA	c	510	3	-	9/39/115/115	-
25	CLA	C	503	3	-	6/39/115/115	-
25	CLA	c	507	37	-	9/39/115/115	-
28	PL9	a	611	-	-	28/53/73/73	0/1/1/1
25	CLA	C	508	3	-	6/39/115/115	-
25	CLA	b	610	2	-	5/39/115/115	-

The worst 5 of 796 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	608	PHO	C1B-C2B	10.33	1.50	1.39
26	D	402	PHO	C1B-C2B	9.19	1.49	1.39
26	d	402	PHO	C1B-C2B	9.02	1.49	1.39
26	d	402	PHO	C3B-C4B	8.75	1.50	1.41
26	D	402	PHO	C3B-C4B	8.58	1.50	1.41

The worst 5 of 1132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	C4A-NA-C1A	8.71	110.66	106.68
25	C	507	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	B	603	CLA	C4A-NA-C1A	8.04	110.35	106.68
25	b	603	CLA	C4A-NA-C1A	7.96	110.31	106.68
25	h	101	CLA	C4A-NA-C1A	7.96	110.31	106.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	V	201	HEC	NA
36	v	201	HEC	NA

5 of 1942 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C12-C13-C15-C16
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C2B-C3B-CAB-CBB
25	B	614	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

144 monomers are involved in 305 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	B	620	LHG	3	0
25	B	602	CLA	3	0
25	b	611	CLA	3	0
32	L	101	LHG	1	0
25	C	513	CLA	2	0
27	B	616	BCR	2	0
28	A	611	PL9	5	0
29	a	613	SQD	2	0
25	B	609	CLA	1	0
27	B	617	BCR	2	0
25	c	508	CLA	3	0
25	C	509	CLA	1	0
31	d	411	STE	1	0
25	b	603	CLA	5	0
27	c	516	BCR	1	0
32	d	408	LHG	1	0
22	A	602[A]	OEY	1	0
29	D	408	SQD	1	0
25	B	613	CLA	2	0
30	H	103	DGD	4	0
25	D	404	CLA	1	0
25	h	101	CLA	4	0
25	C	504	CLA	4	0
29	b	619	SQD	4	0
33	b	620	LMG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	516	DGD	1	0
25	C	502	CLA	2	0
25	C	507	CLA	1	0
27	D	405	BCR	1	0
25	c	503	CLA	3	0
25	c	505	CLA	4	0
25	c	506	CLA	2	0
25	A	607	CLA	2	0
27	d	405	BCR	2	0
25	b	604	CLA	3	0
34	D	401	BCT	1	0
27	T	101	BCR	4	0
27	t	101	BCR	5	0
28	d	406	PL9	3	0
25	b	607	CLA	2	0
25	c	511	CLA	3	0
33	D	407	LMG	2	0
25	B	614	CLA	3	0
30	C	518	DGD	5	0
33	c	522	LMG	2	0
25	B	601	CLA	4	0
30	h	102	DGD	3	0
33	M	101	LMG	2	0
29	B	621	SQD	4	0
27	Y	101	BCR	1	0
31	C	522	STE	2	0
26	D	402	PHO	5	0
29	A	613	SQD	3	0
25	C	505	CLA	3	0
31	B	624	STE	1	0
25	D	403	CLA	4	0
25	b	606	CLA	5	0
25	b	612	CLA	2	0
27	b	616	BCR	1	0
25	a	607	CLA	4	0
25	d	403	CLA	2	0
27	K	101	BCR	1	0
25	A	606	CLA	1	0
25	B	603	CLA	2	0
25	C	510	CLA	3	0
33	C	519	LMG	5	0
31	c	523	STE	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	501	CLA	3	0
25	b	605	CLA	10	0
26	a	608	PHO	2	0
30	c	519	DGD	3	0
29	T	103	SQD	1	0
25	C	501	CLA	2	0
25	A	609	CLA	2	0
33	c	524	LMG	3	0
33	C	515	LMG	2	0
25	c	513	CLA	2	0
25	b	602	CLA	1	0
32	b	623	LHG	3	0
27	Z	101	BCR	1	0
25	b	615	CLA	3	0
25	c	509	CLA	3	0
30	A	614	DGD	9	0
25	d	401	CLA	1	0
31	t	102	STE	1	0
25	b	609	CLA	4	0
33	D	412	LMG	1	0
25	B	611	CLA	4	0
25	c	504	CLA	1	0
25	c	502	CLA	1	0
31	H	104	STE	1	0
30	c	518	DGD	5	0
27	x	101	BCR	4	0
25	a	609	CLA	4	0
31	B	625	STE	1	0
31	b	625	STE	1	0
31	I	101	STE	2	0
32	D	409	LHG	2	0
33	d	410	LMG	1	0
35	e	101	HEM	5	0
25	C	512	CLA	3	0
27	b	618	BCR	2	0
25	b	613	CLA	3	0
25	B	608	CLA	5	0
32	d	407	LHG	3	0
32	l	101	LHG	5	0
29	f	101	SQD	2	0
25	B	606	CLA	4	0
25	B	612	CLA	3	0

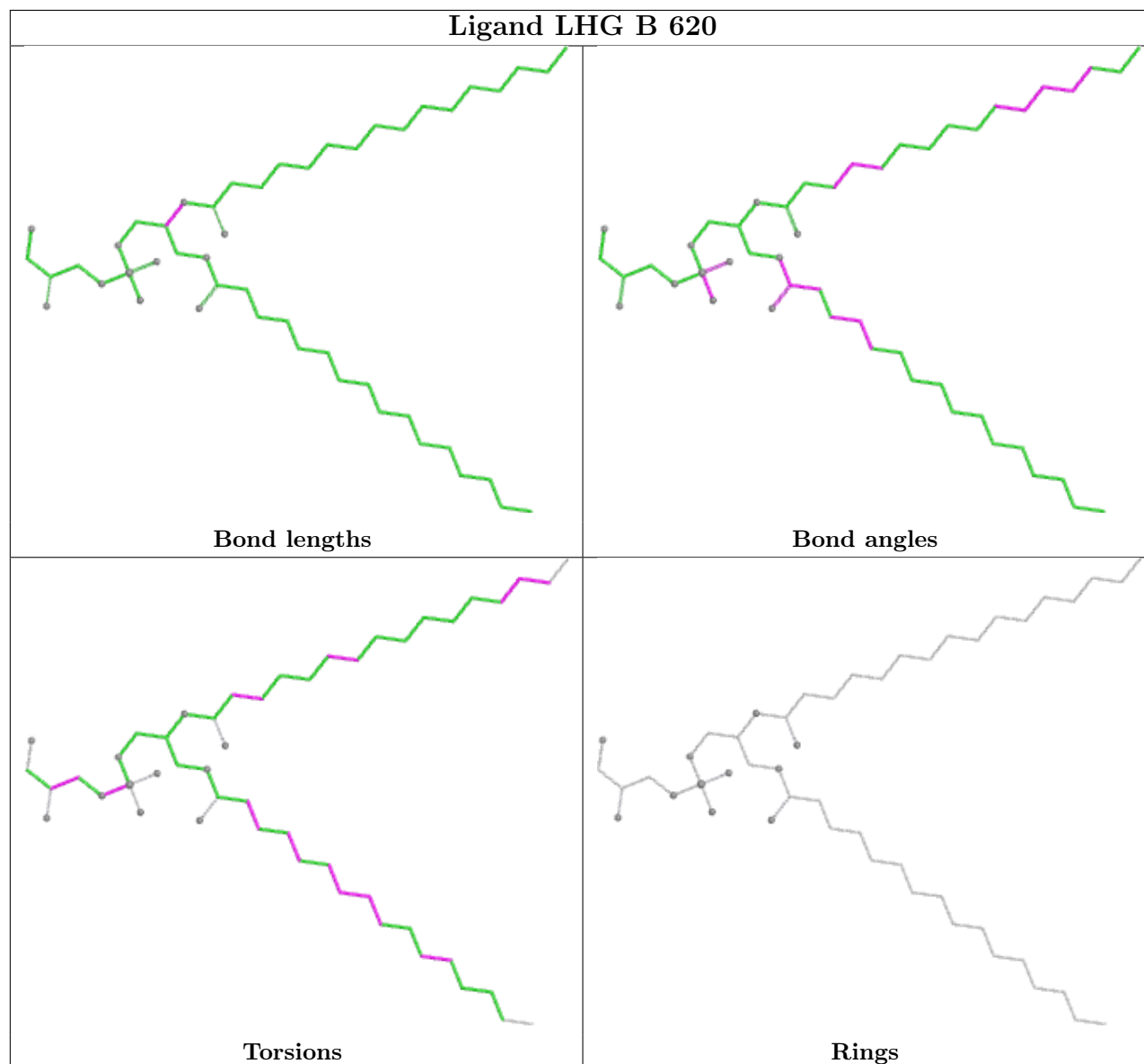
Continued on next page...

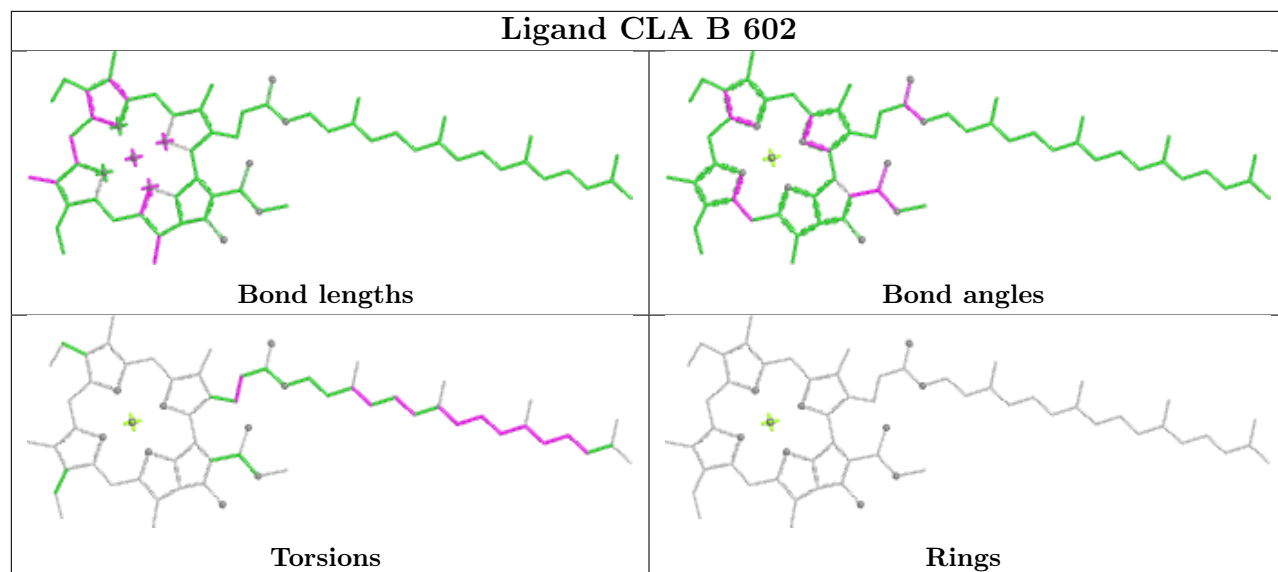
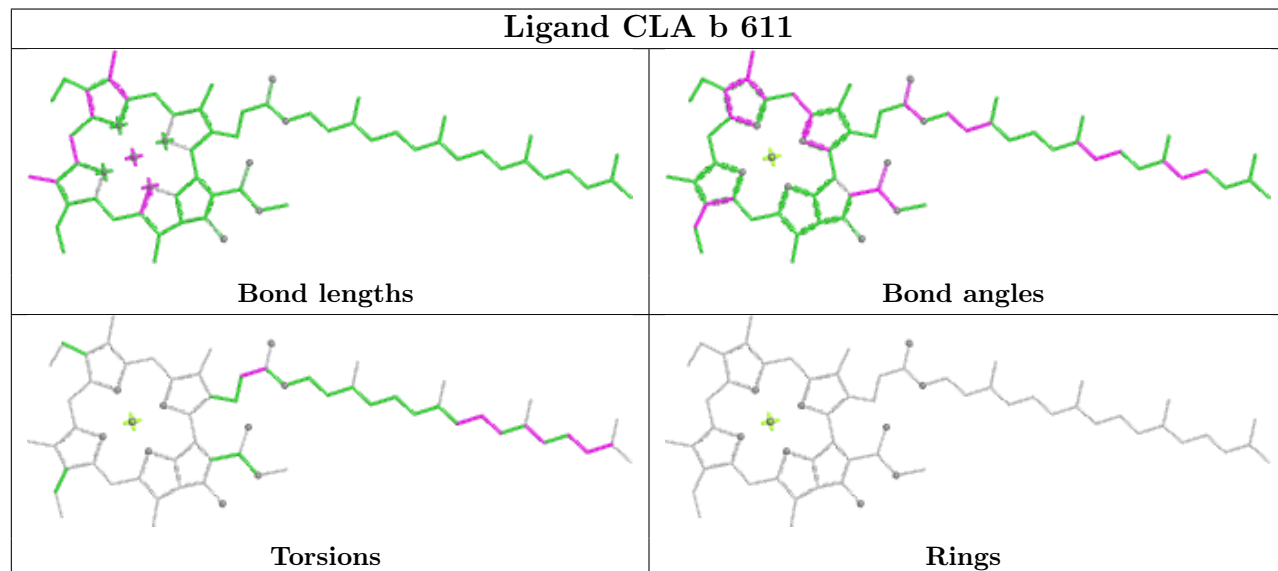
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	c	514	BCR	1	0
31	D	413	STE	1	0
25	B	607	CLA	2	0
25	B	615	CLA	2	0
25	C	511	CLA	1	0
26	d	402	PHO	5	0
27	b	617	BCR	3	0
25	C	506	CLA	1	0
25	a	612	CLA	2	0
25	B	604	CLA	5	0
35	F	101	HEM	3	0
31	t	103	STE	1	0
27	B	618	BCR	3	0
33	D	411	LMG	1	0
30	a	615	DGD	2	0
33	c	520	LMG	1	0
25	B	605	CLA	4	0
25	d	404	CLA	3	0
25	H	101	CLA	3	0
27	C	514	BCR	5	0
25	b	608	CLA	4	0
27	H	102	BCR	1	0
29	a	614	SQD	2	0
25	b	614	CLA	4	0
25	B	610	CLA	4	0
32	E	101	LHG	2	0
25	b	601	CLA	3	0
32	D	410	LHG	3	0
27	c	515	BCR	4	0
30	C	517	DGD	3	0
25	A	612	CLA	1	0
25	c	510	CLA	3	0
25	c	507	CLA	3	0
28	a	611	PL9	5	0
25	C	508	CLA	4	0

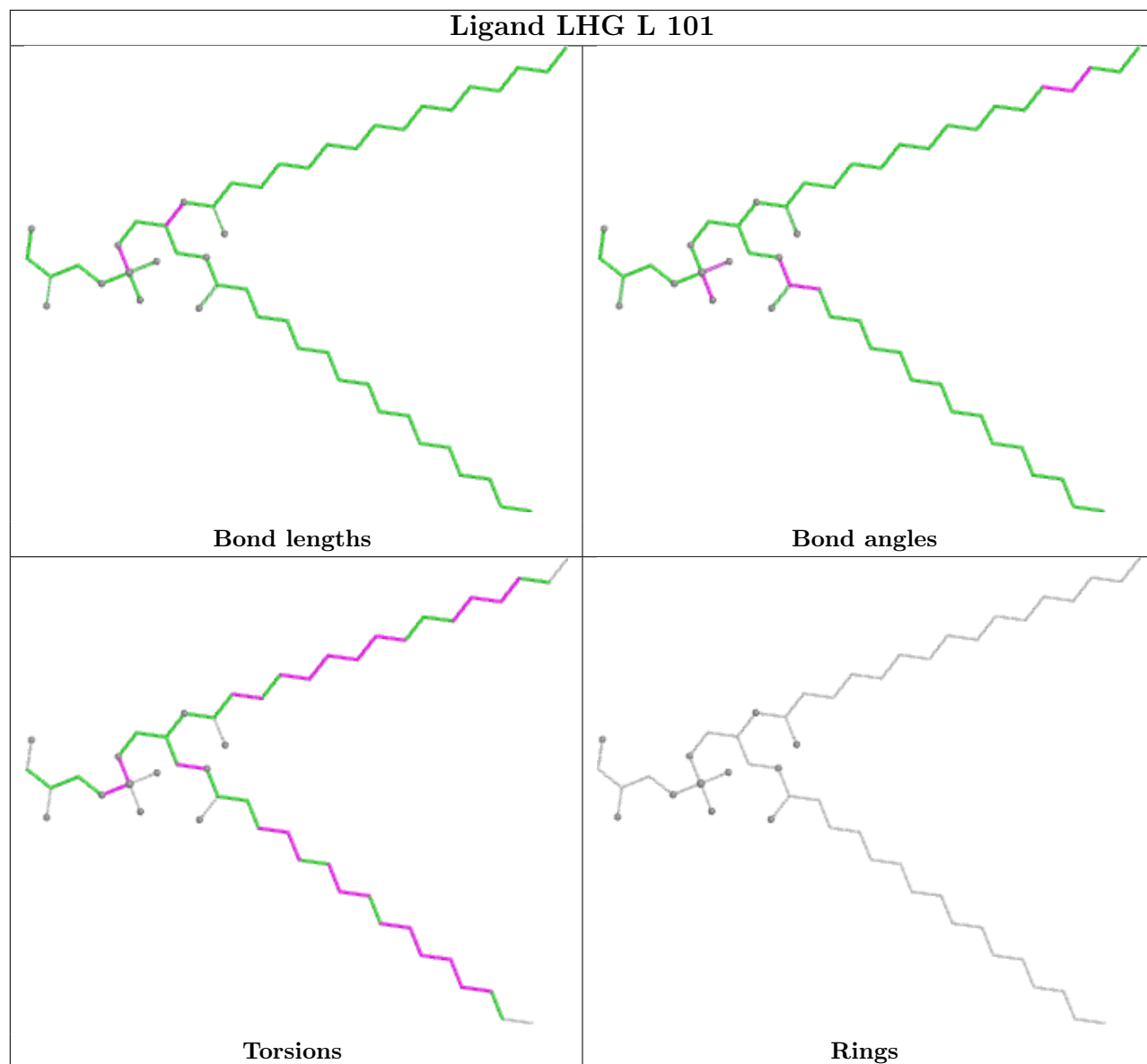
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

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

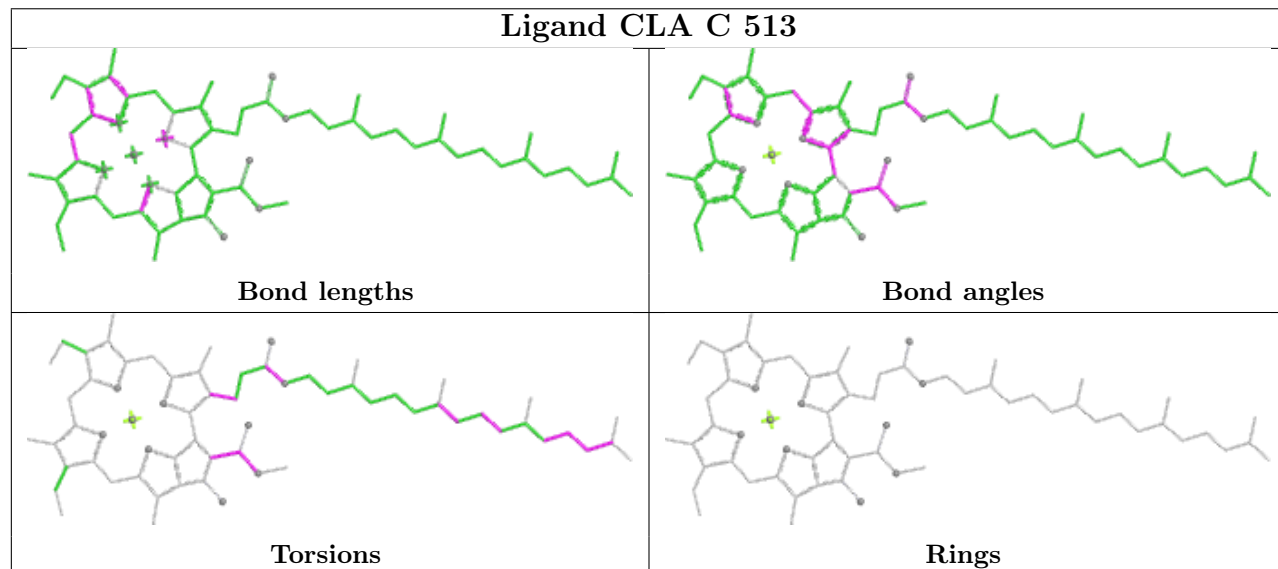


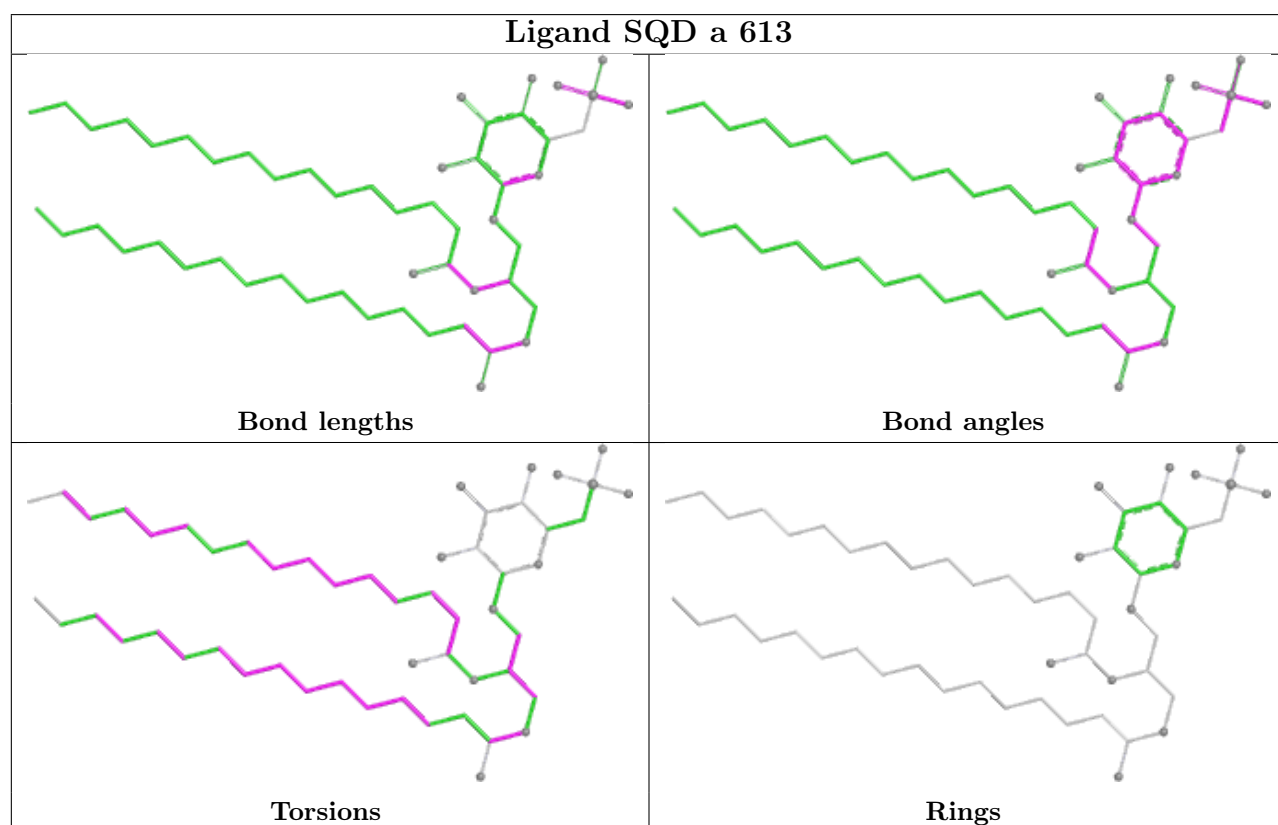
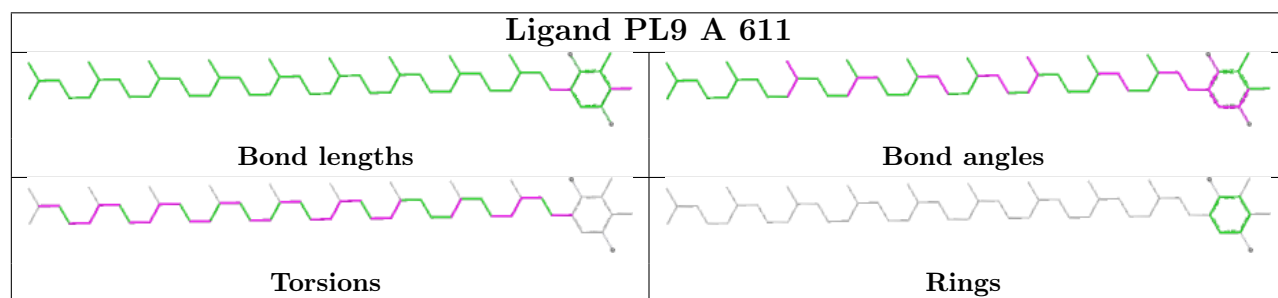
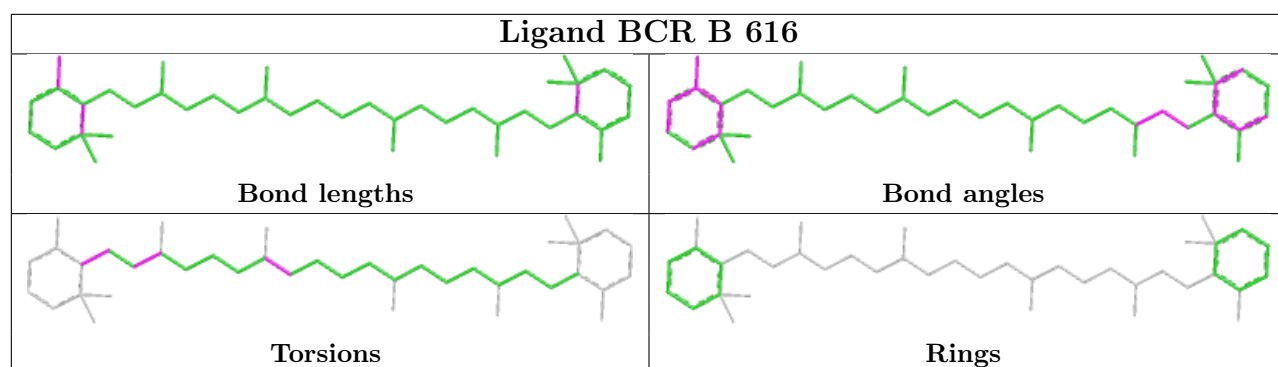
Ligand CLA B 602**Ligand CLA b 611**

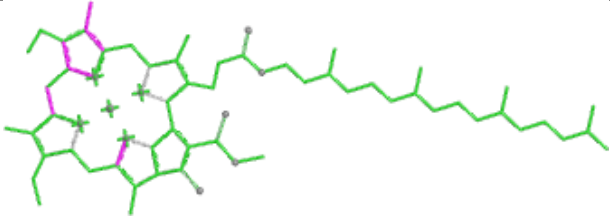
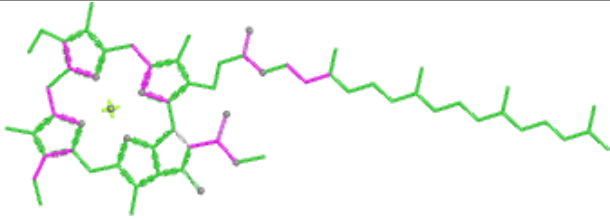
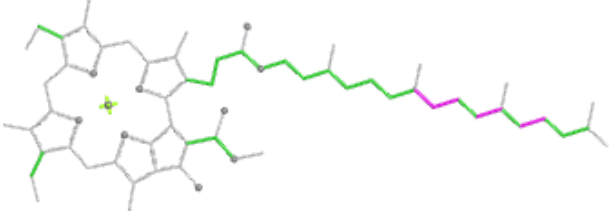
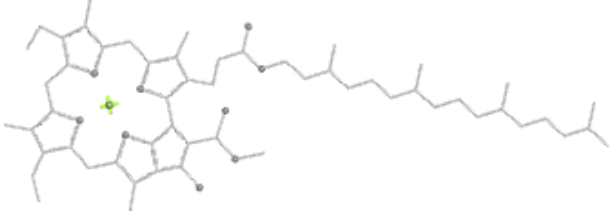
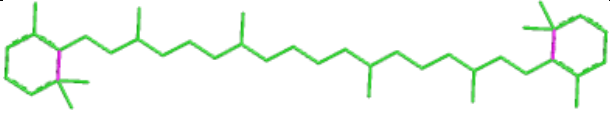
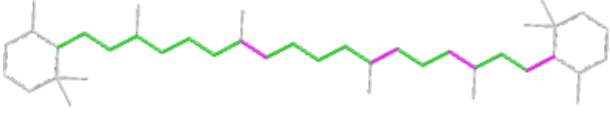
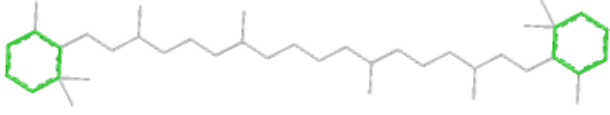
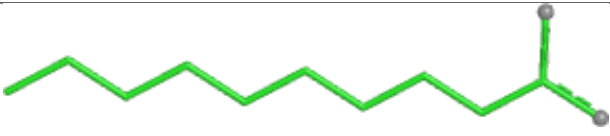
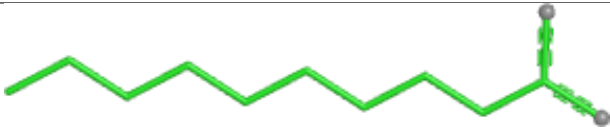
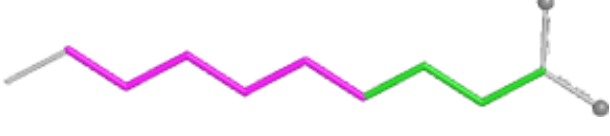
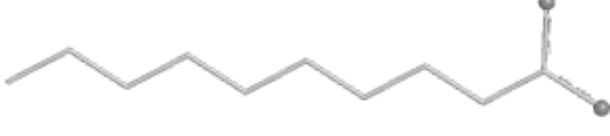
Ligand LHG L 101

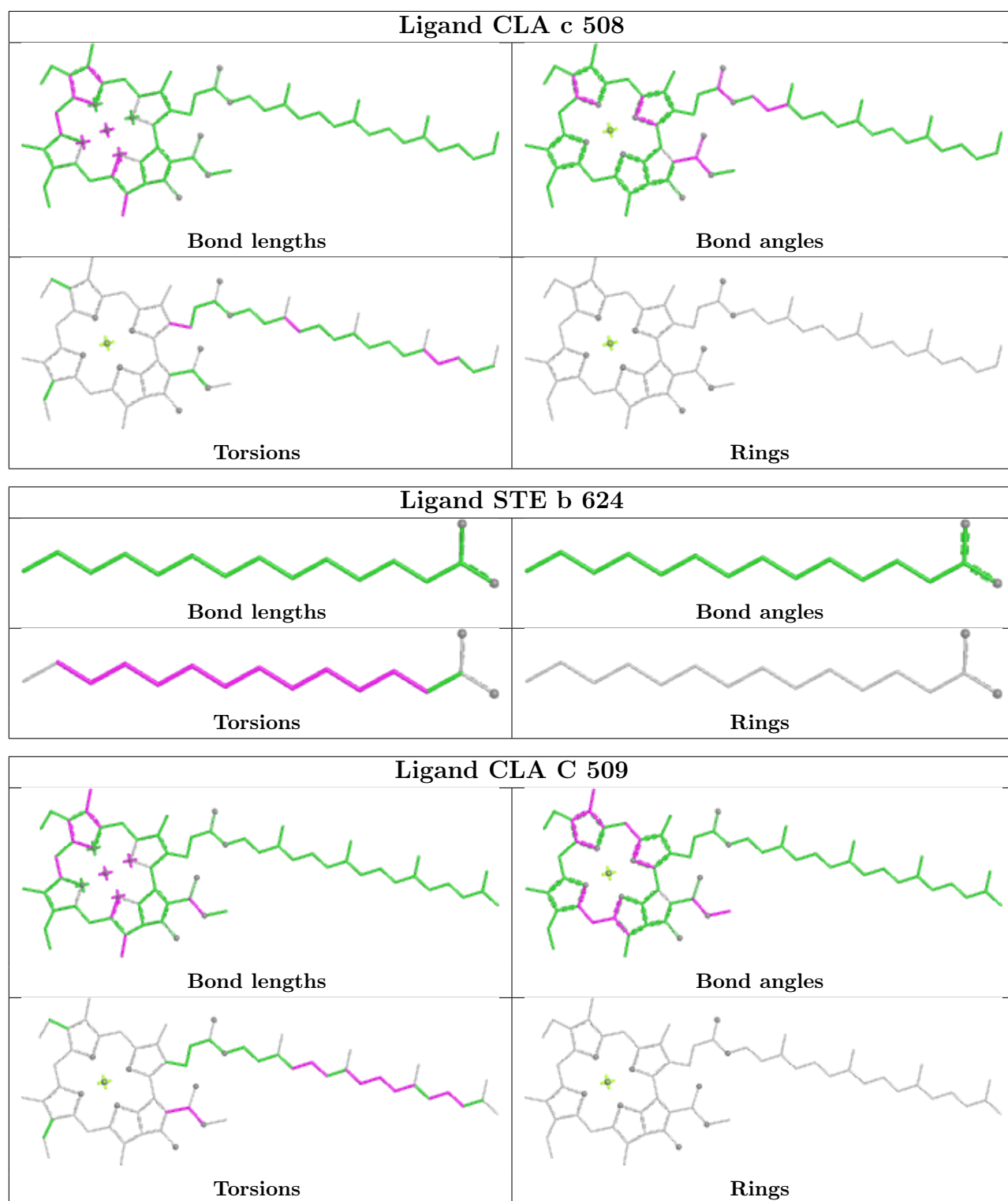


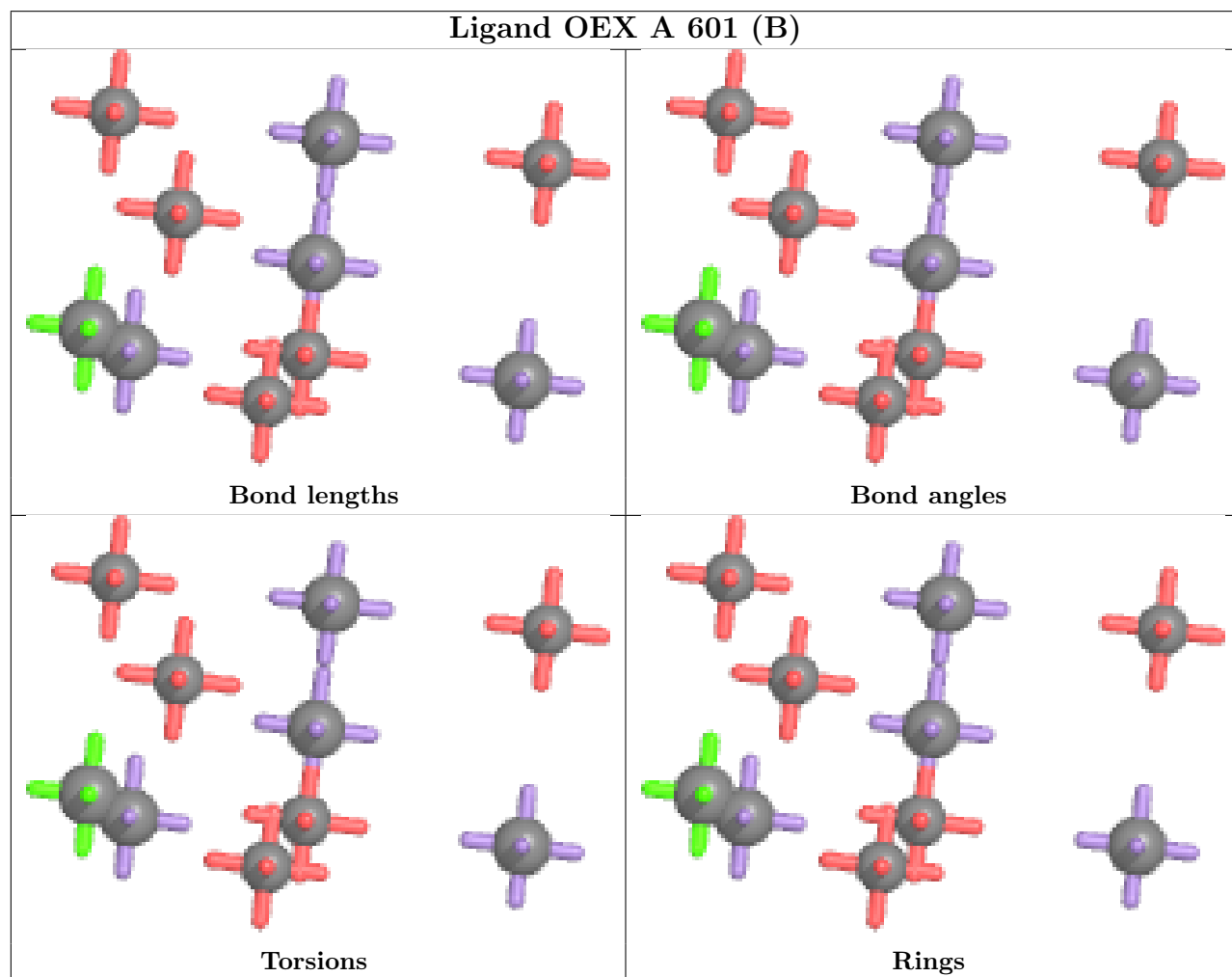
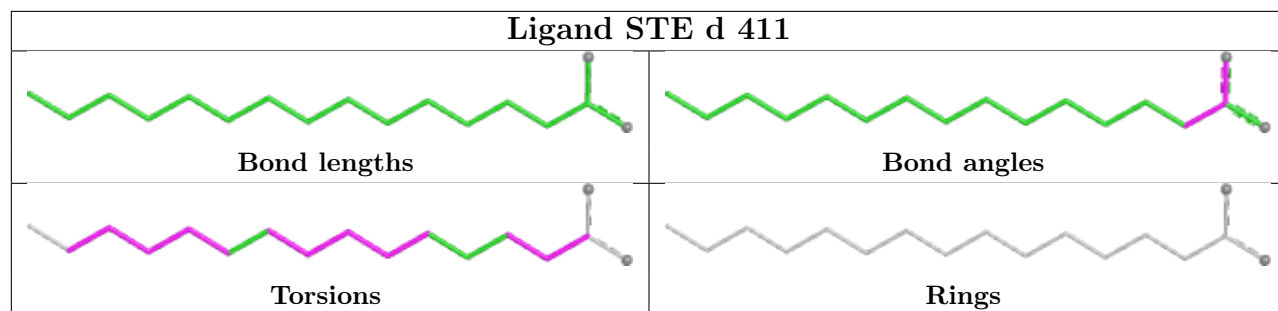
Ligand CLA C 513

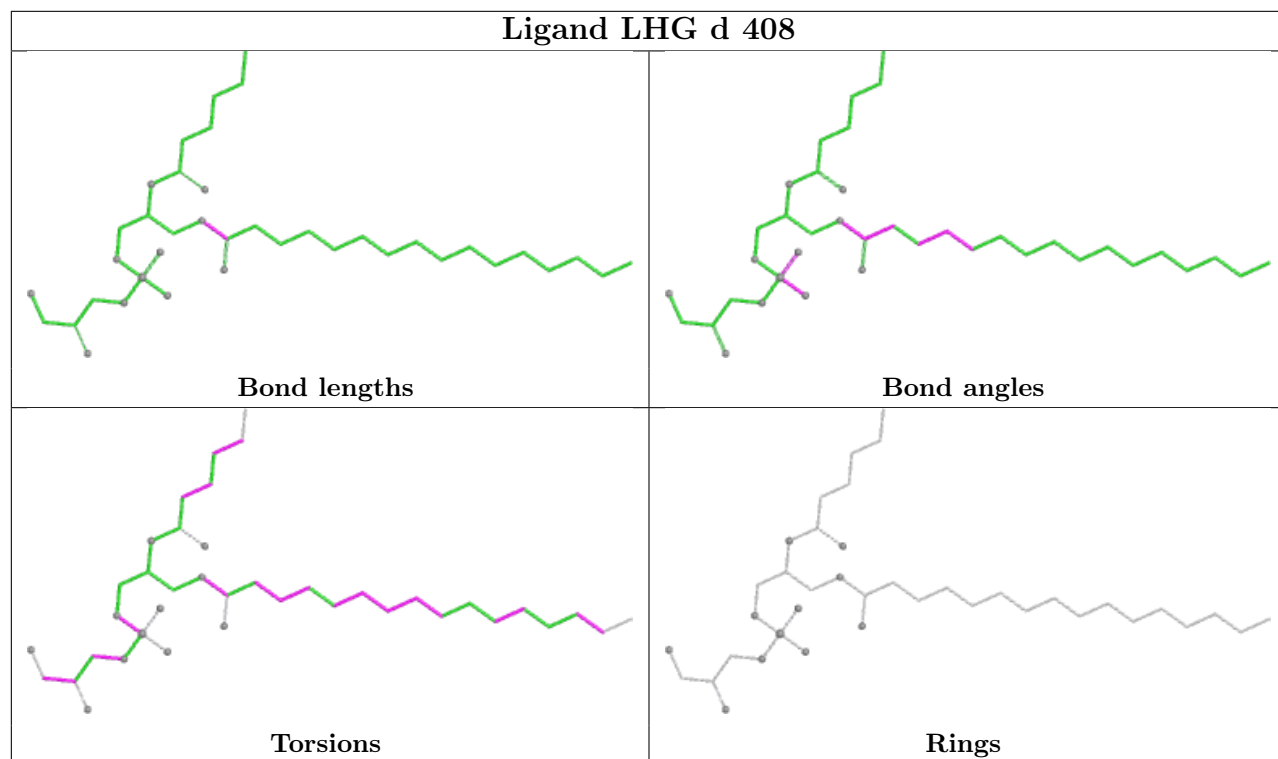
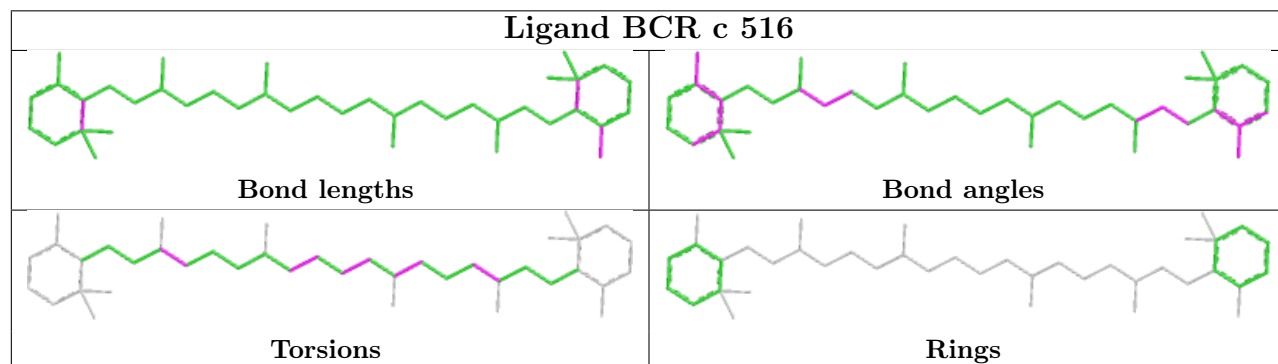
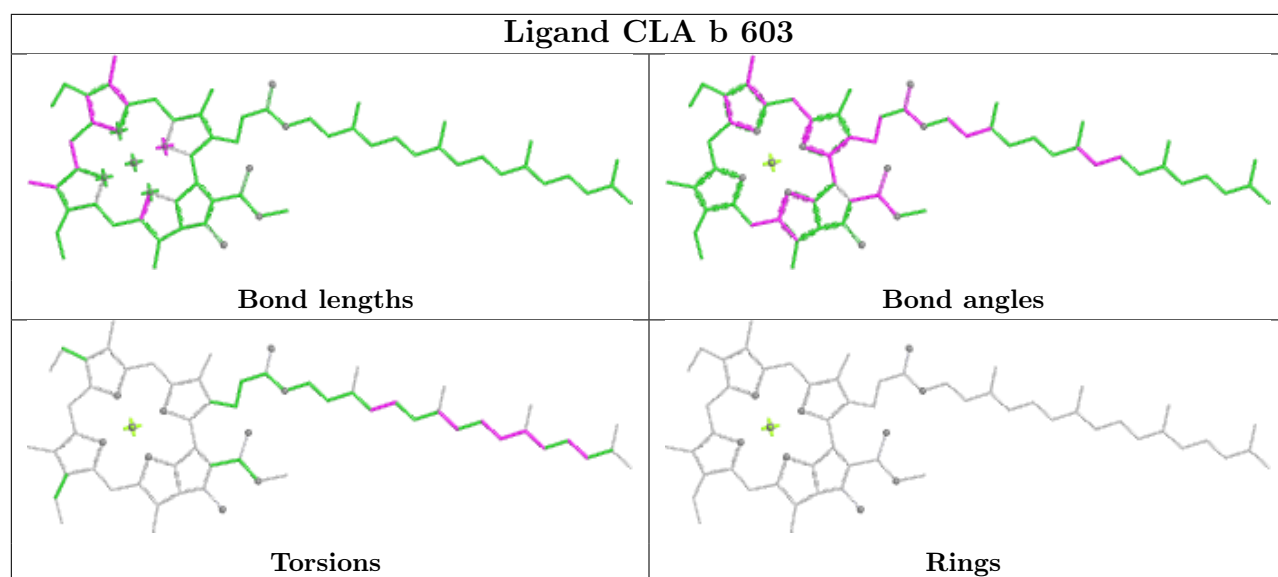


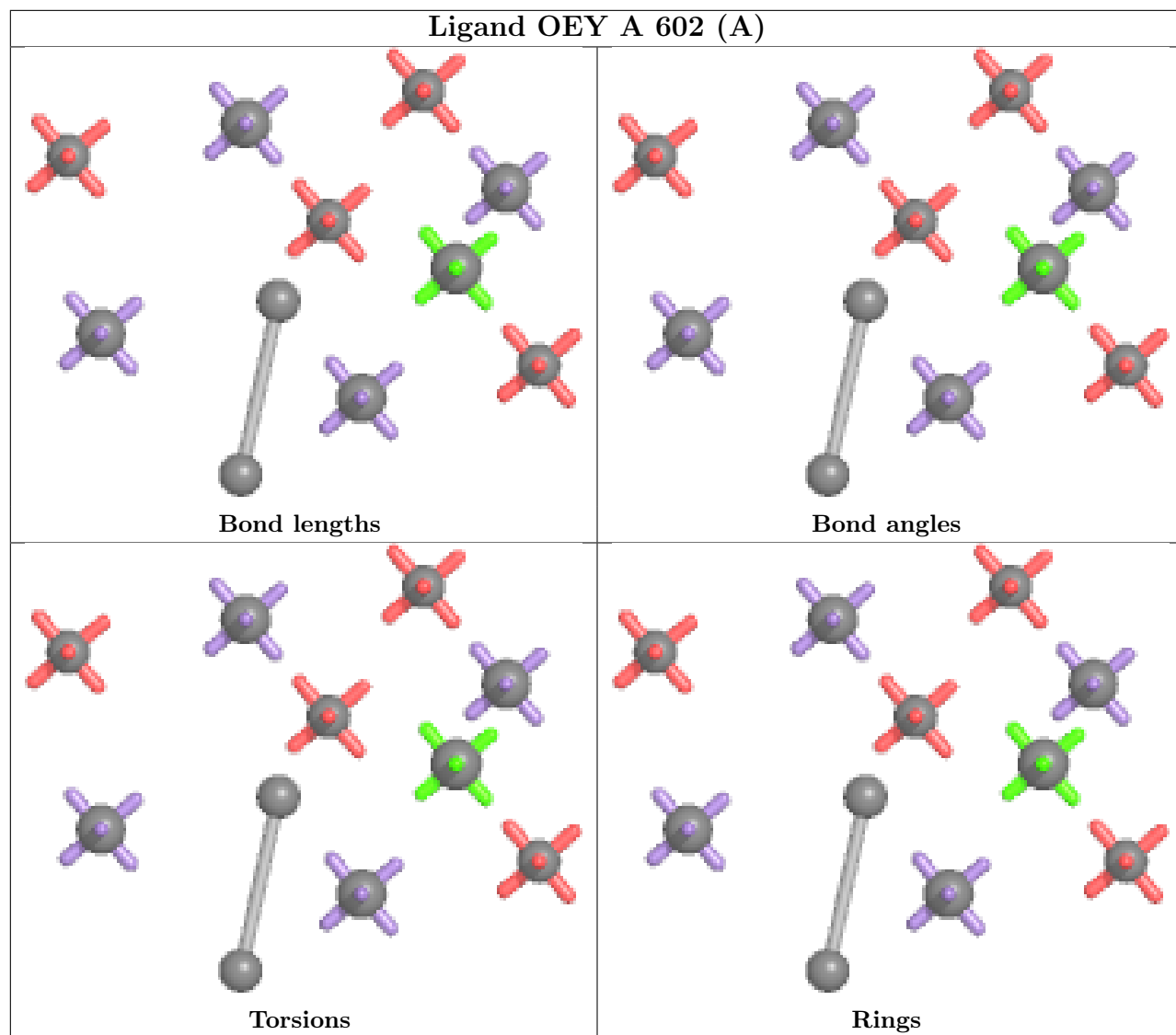


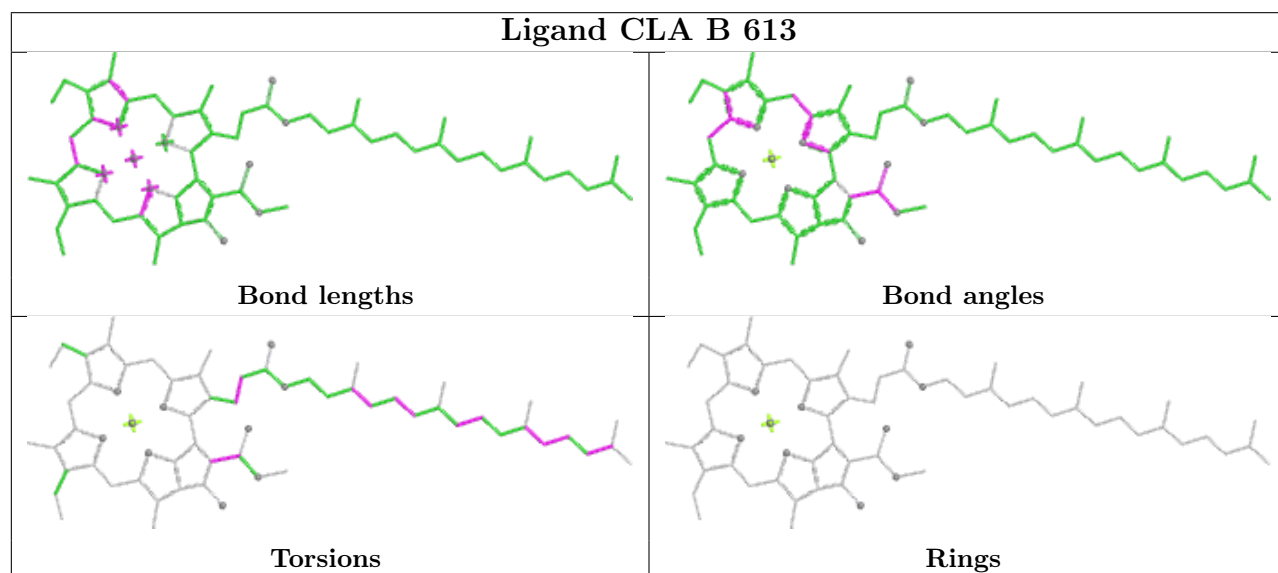
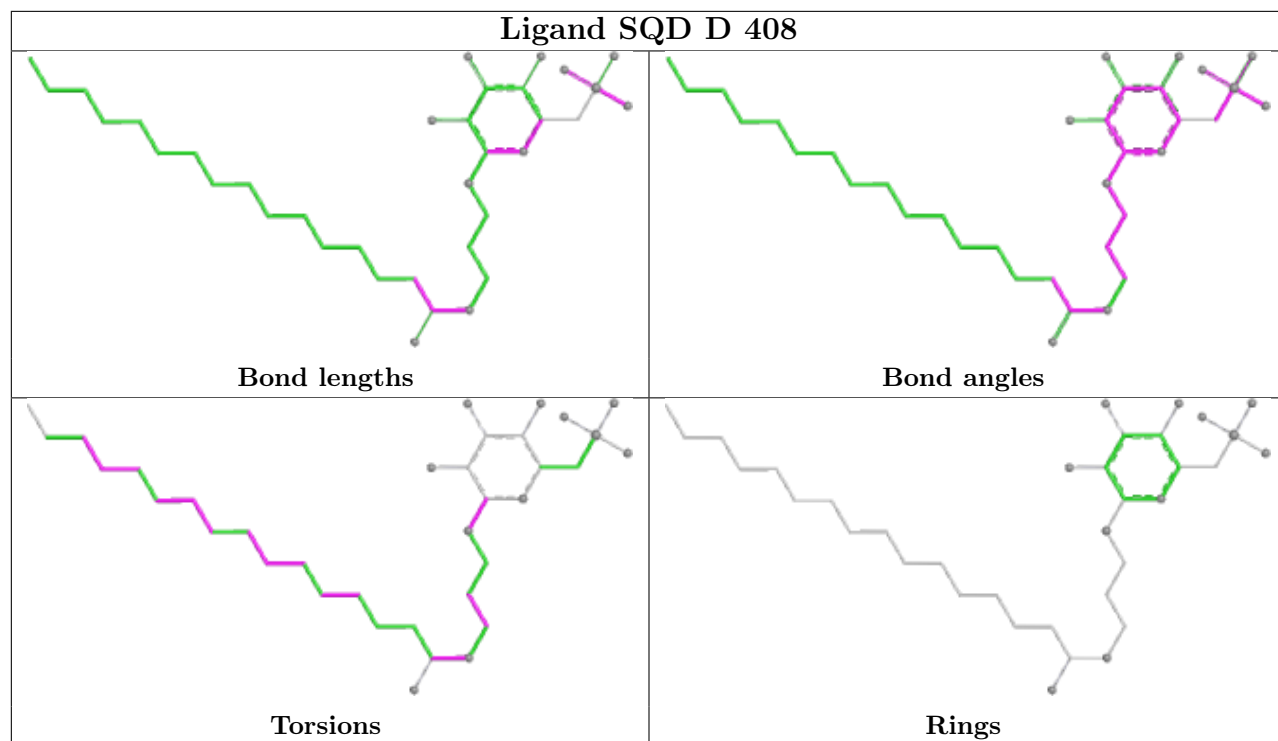
Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE E 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

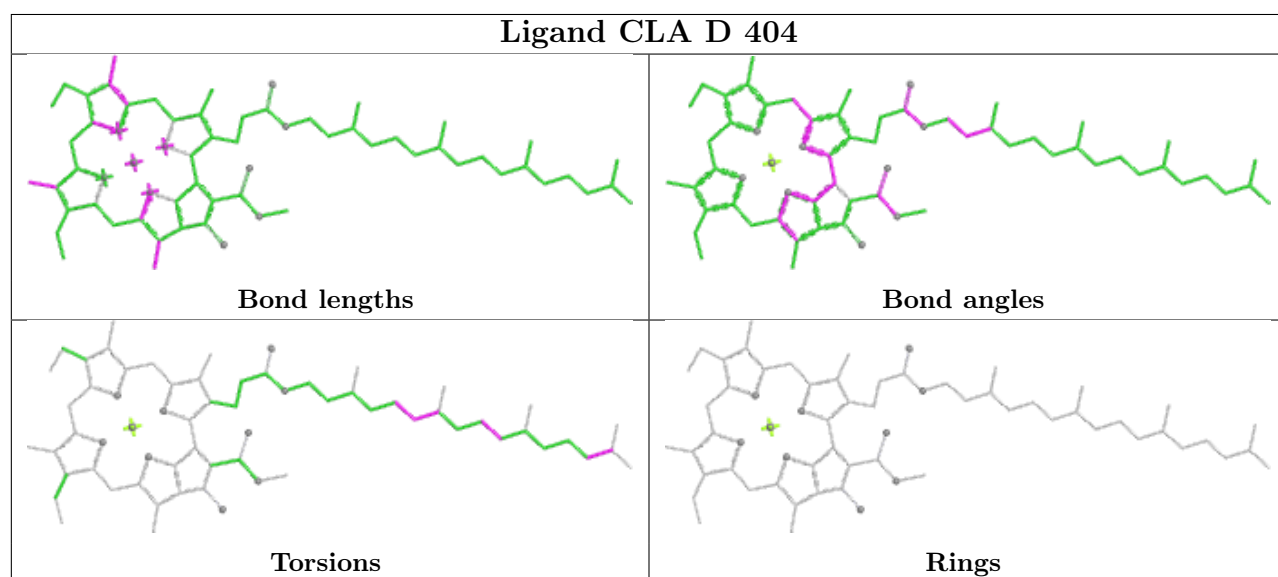
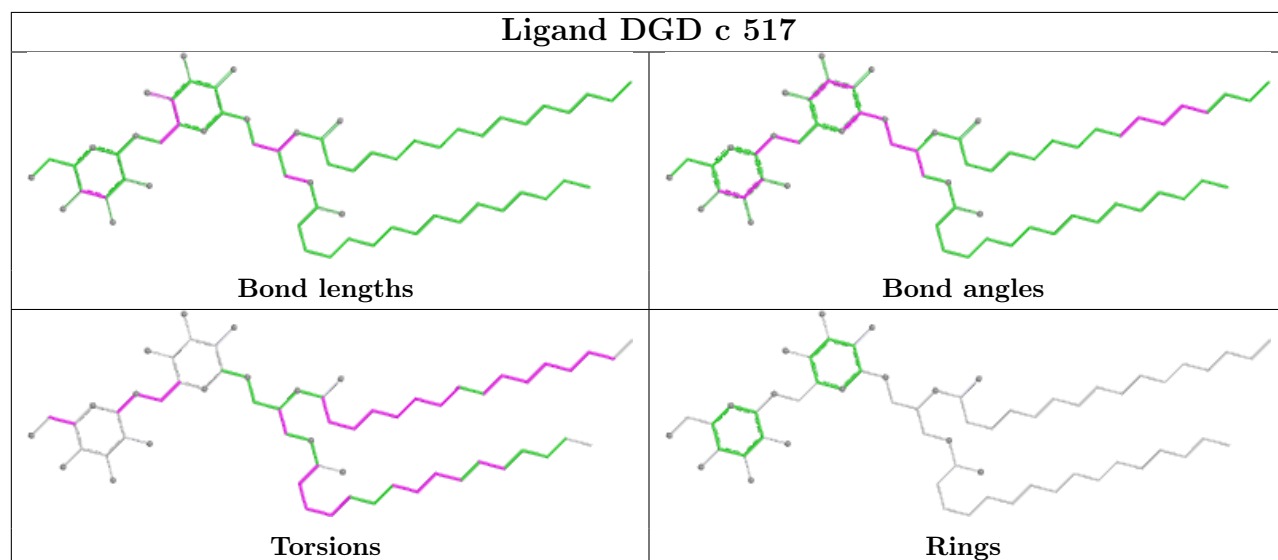
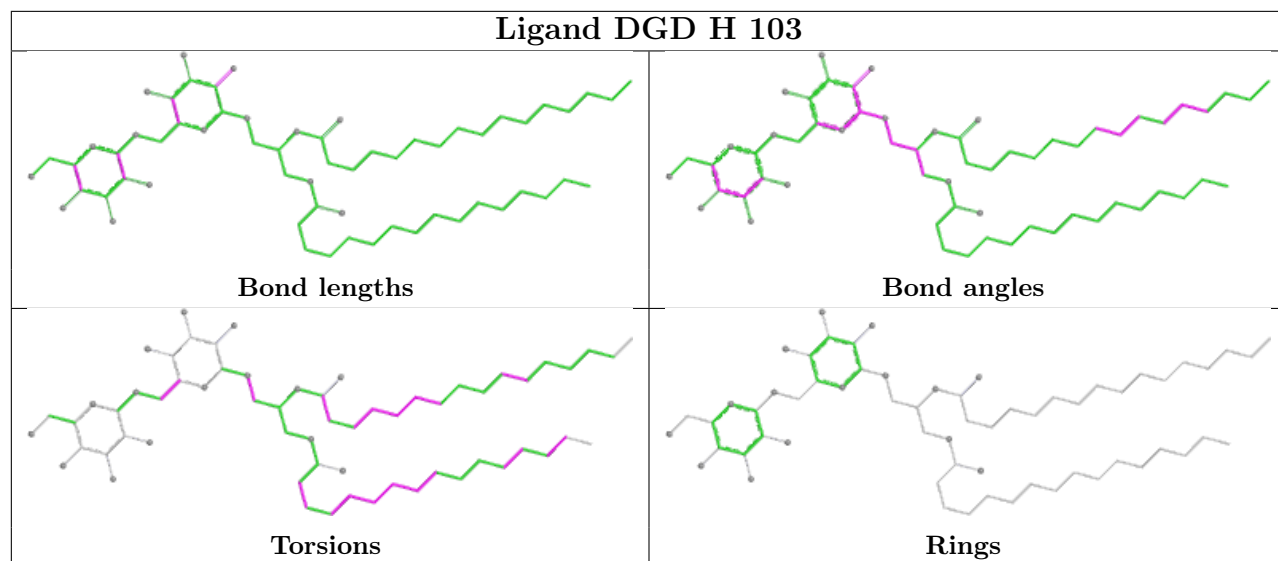


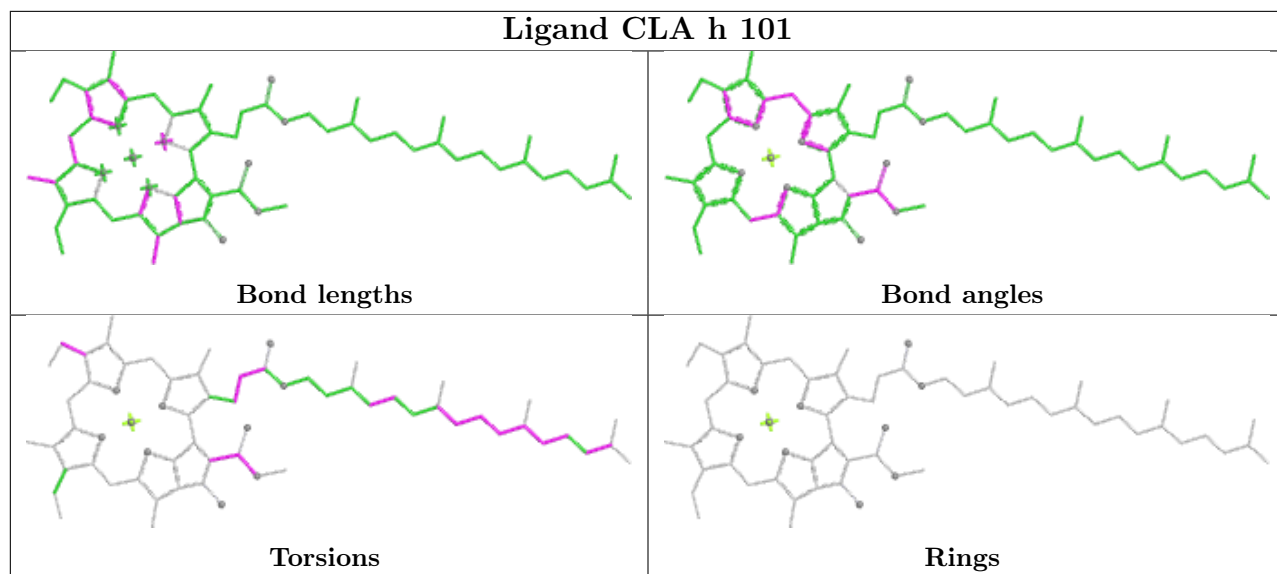
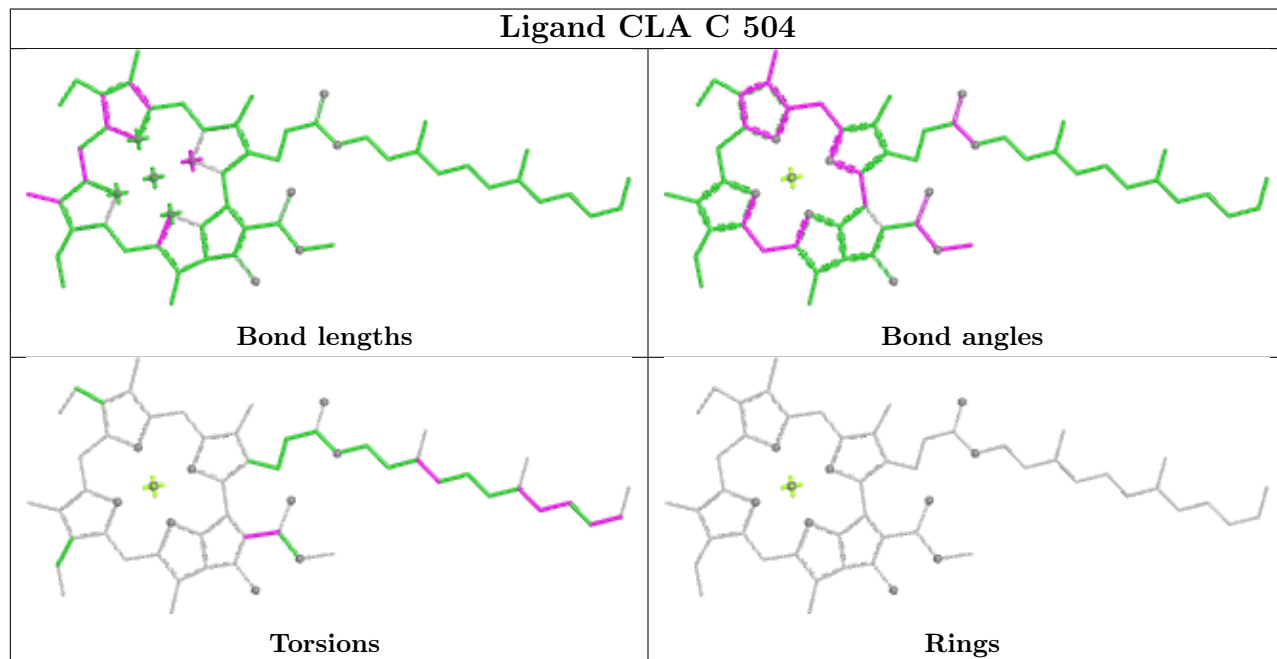


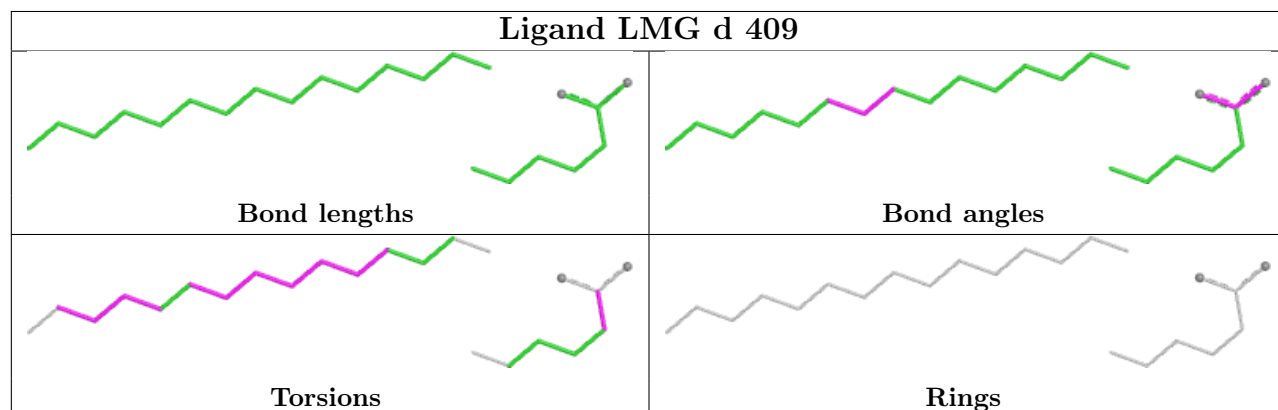
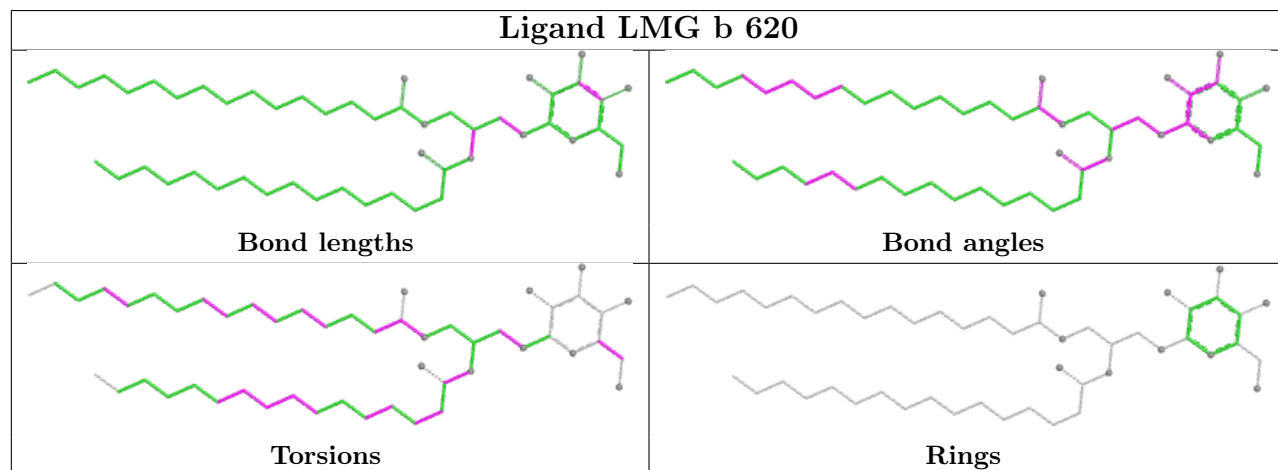
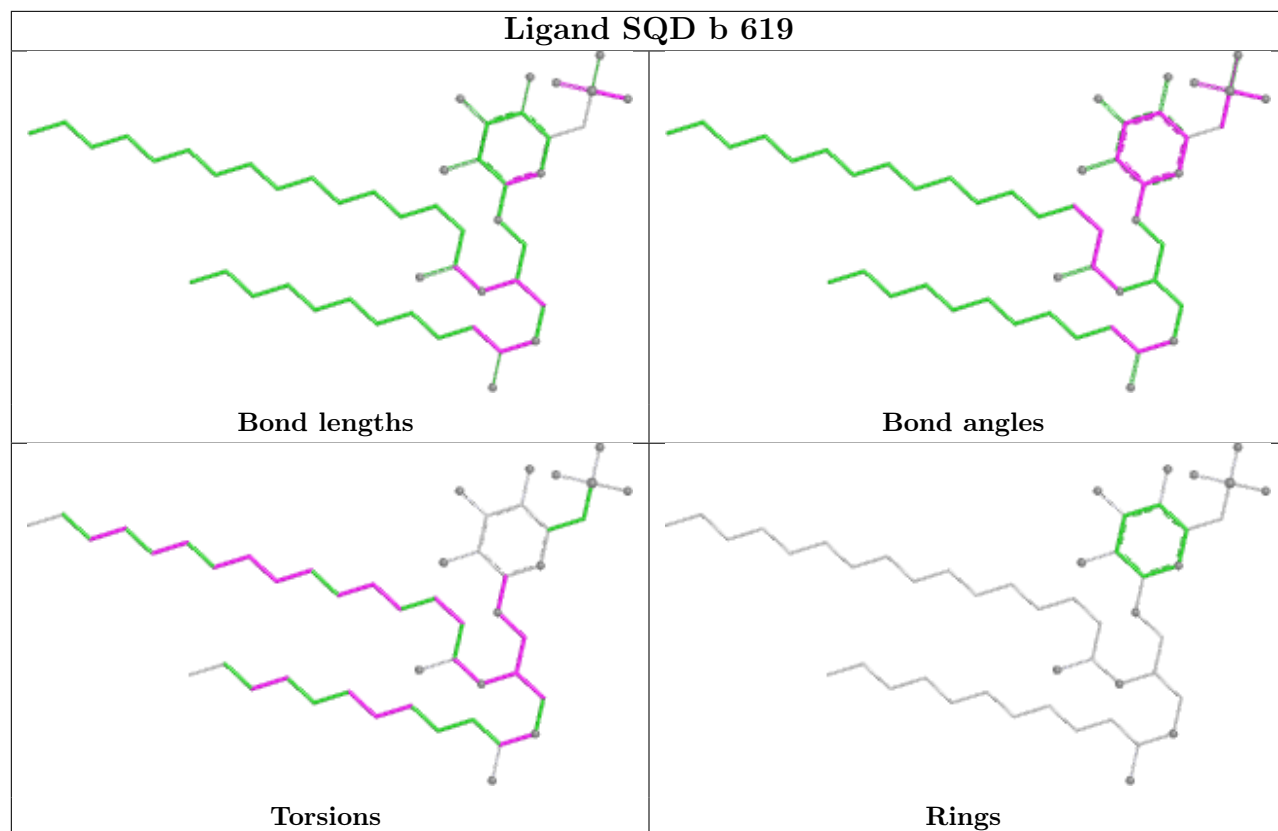


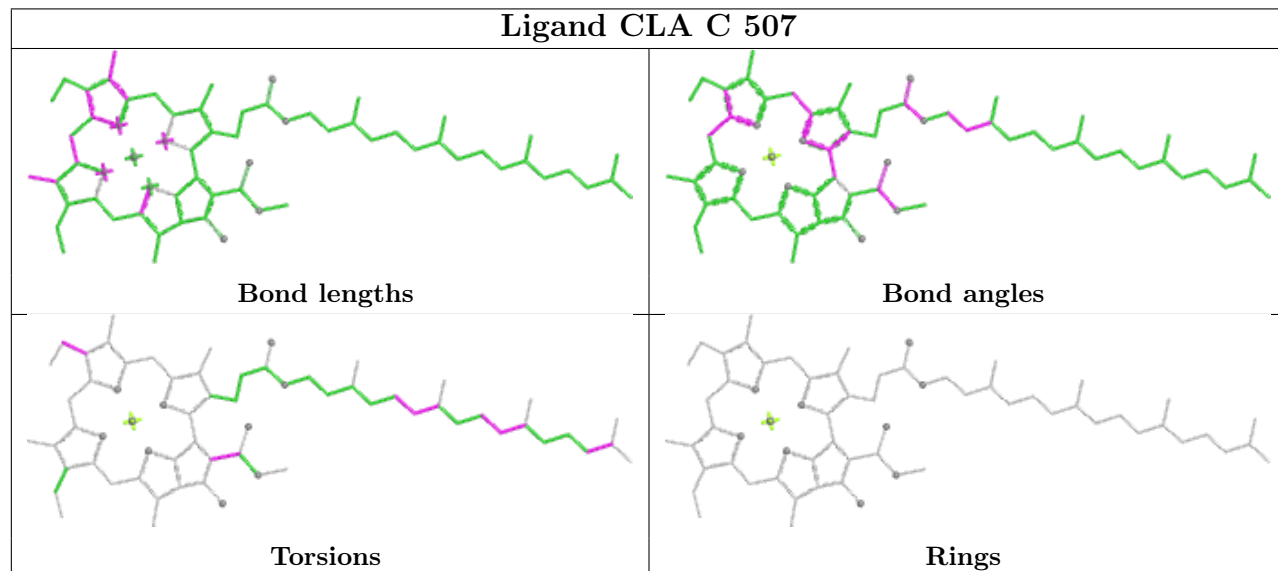
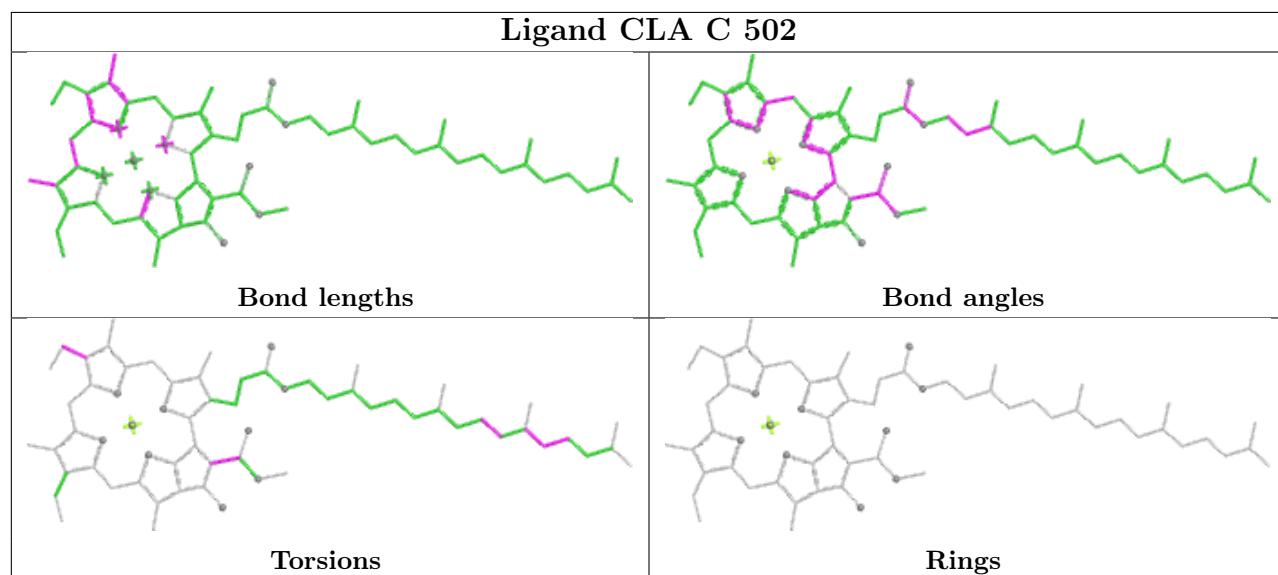
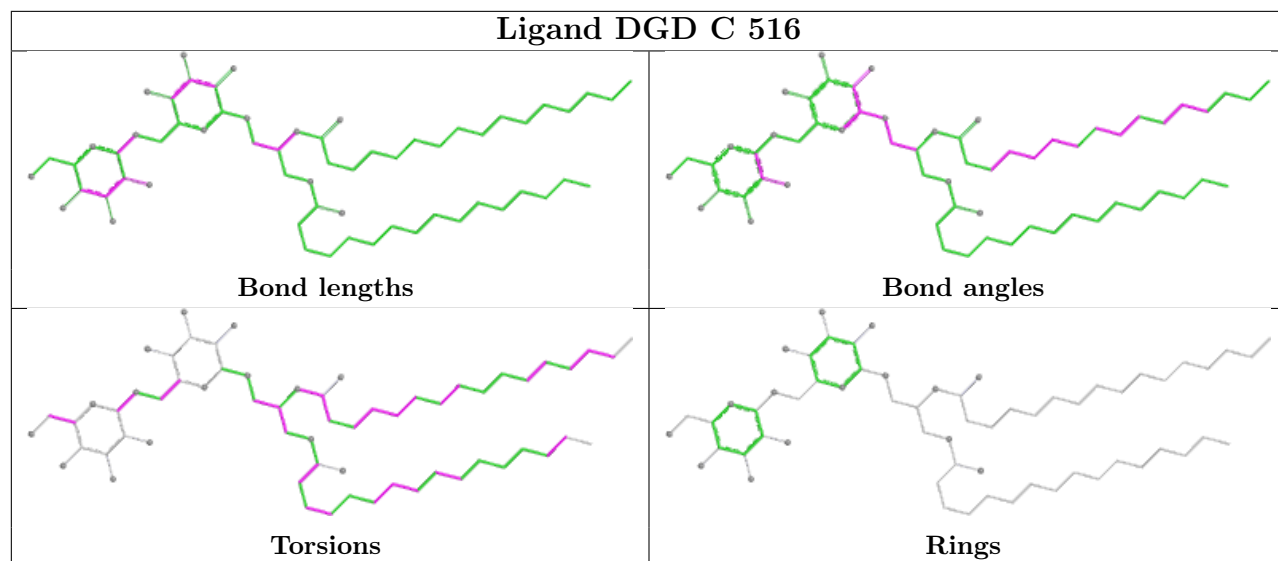


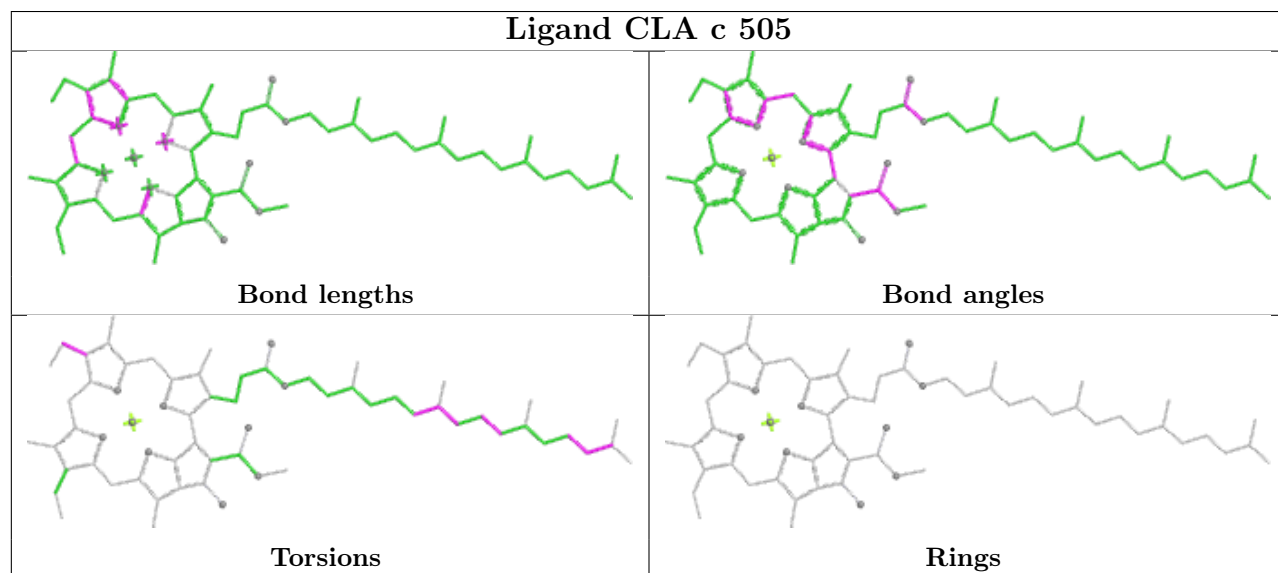
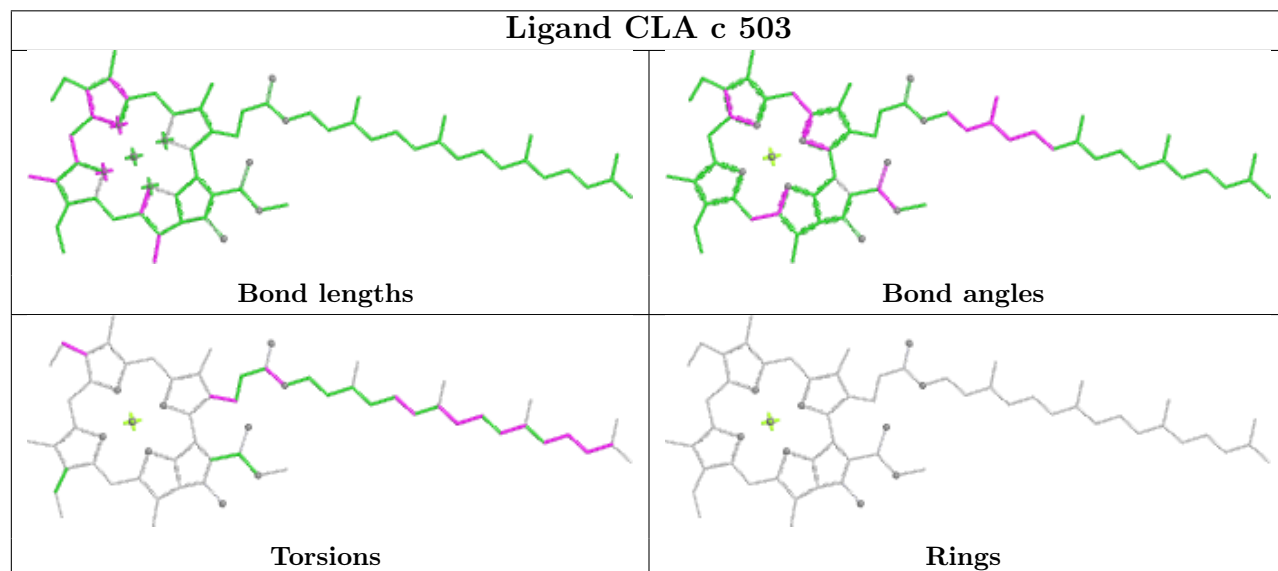
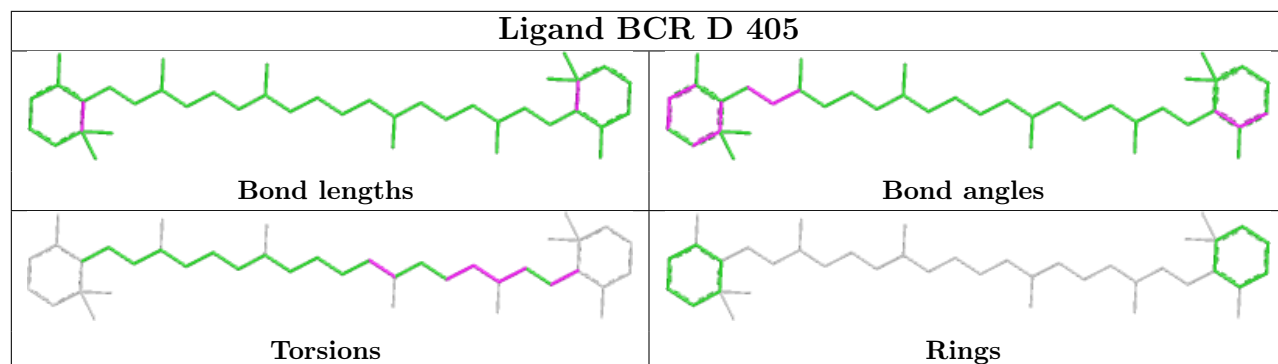




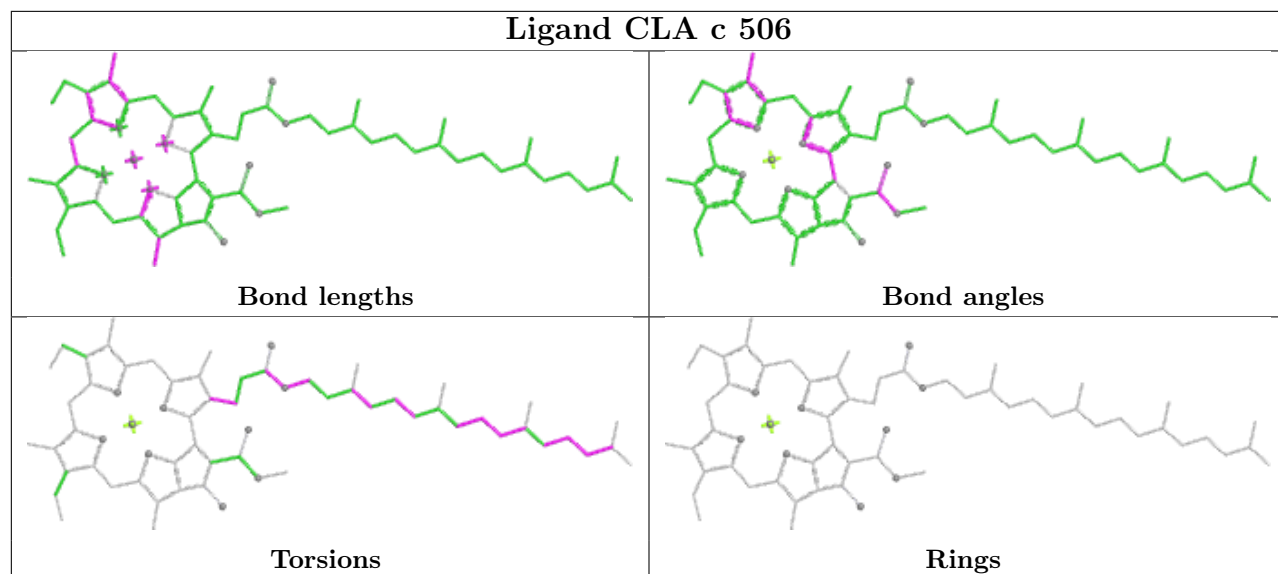
Ligand CLA h 101**Ligand CLA C 504**



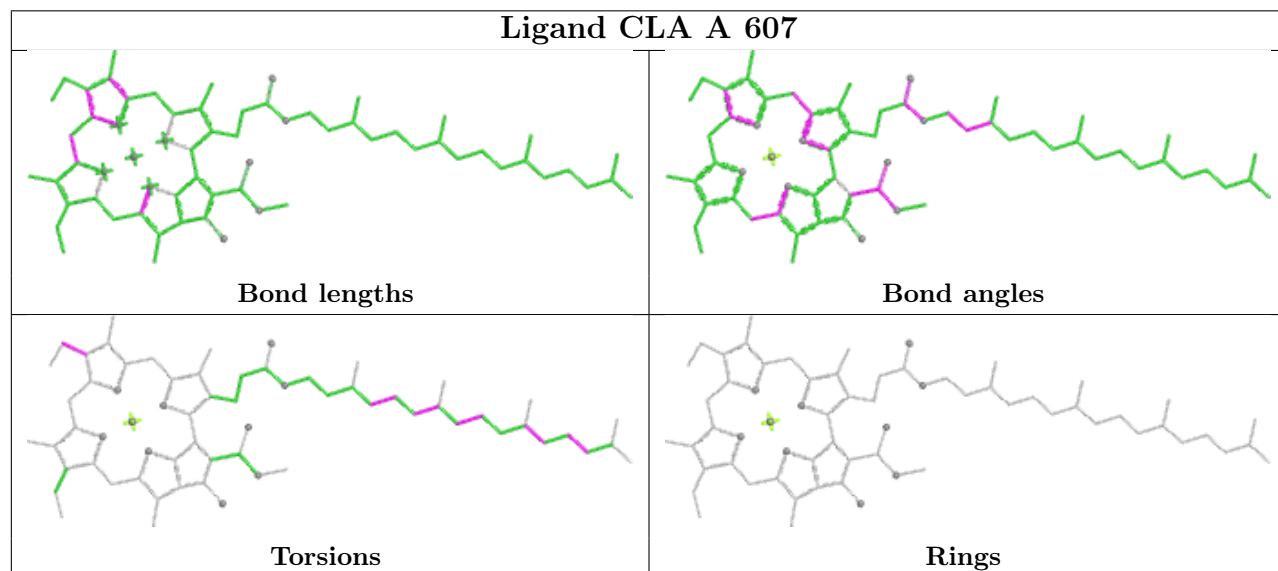




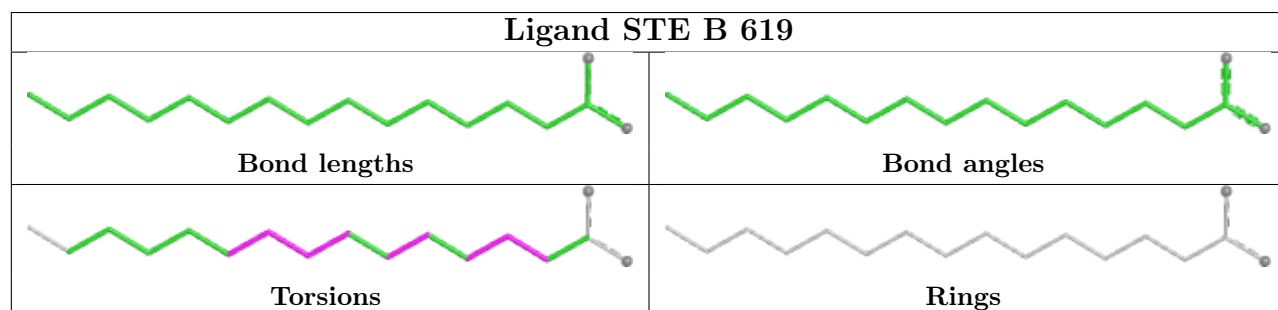
Ligand CLA c 506

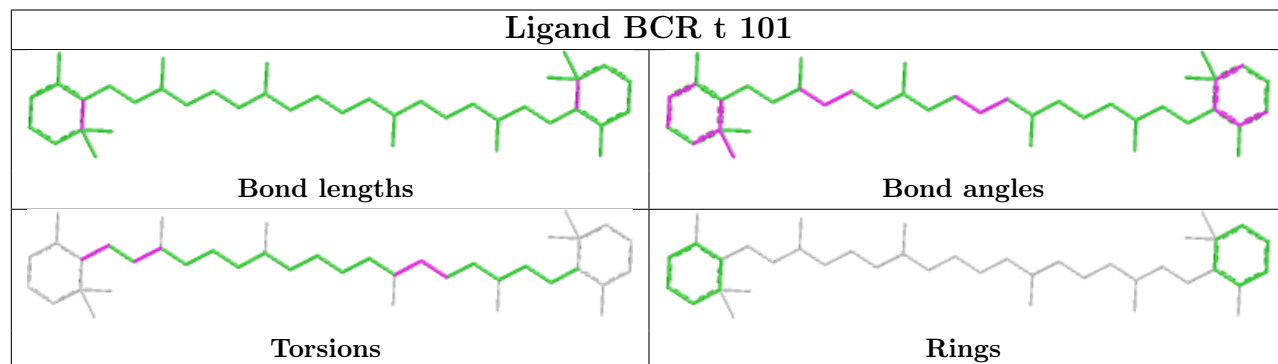
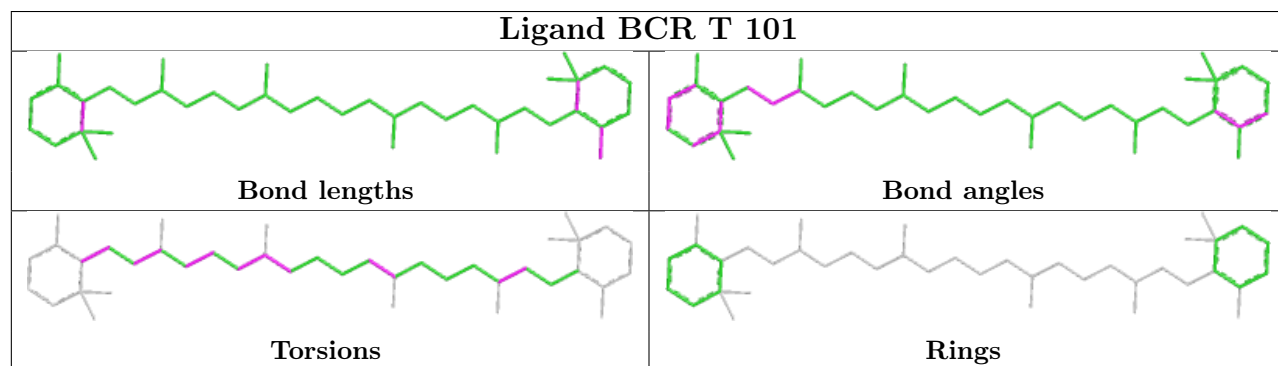
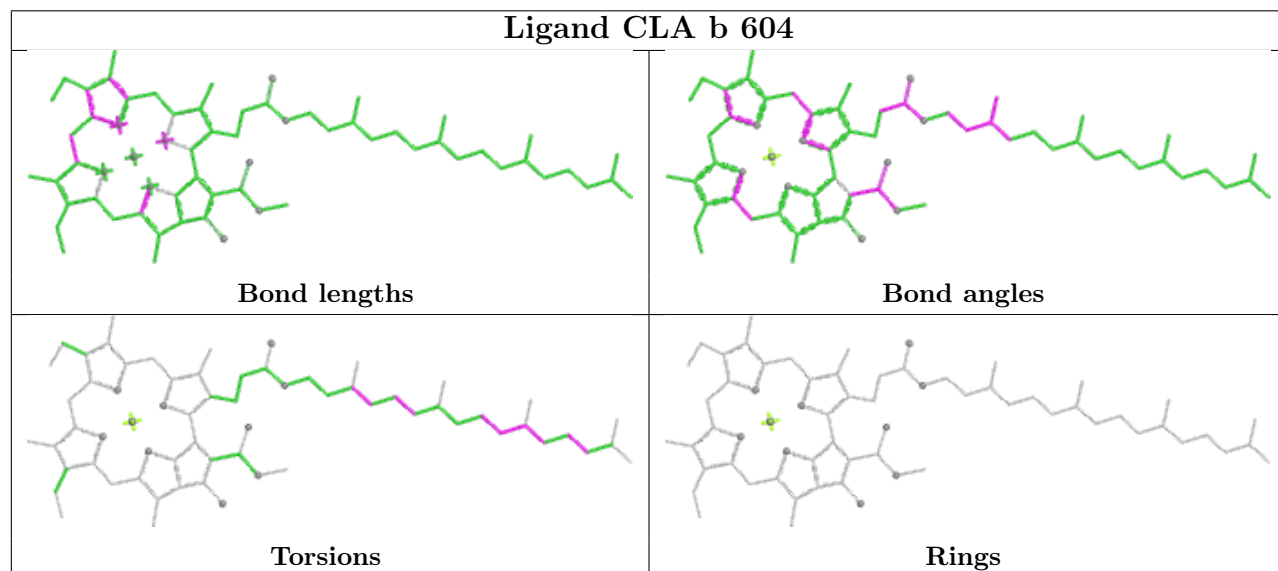
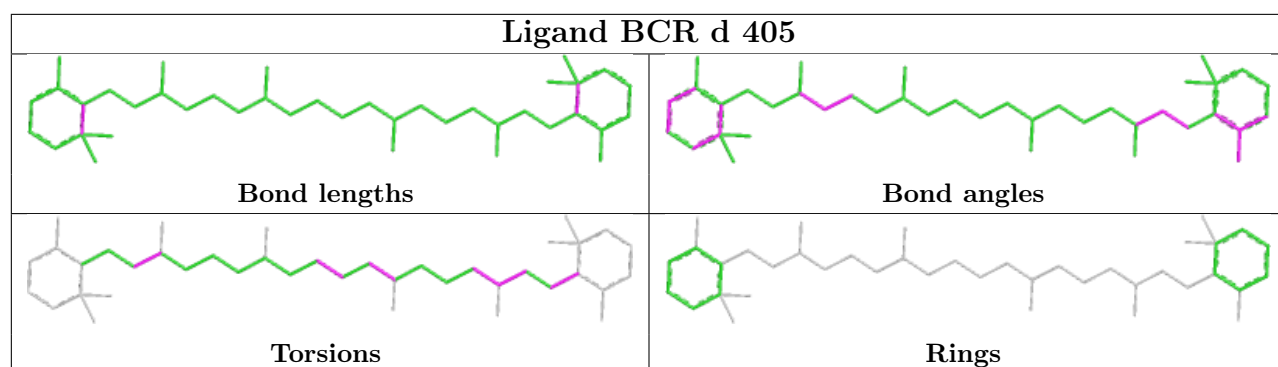


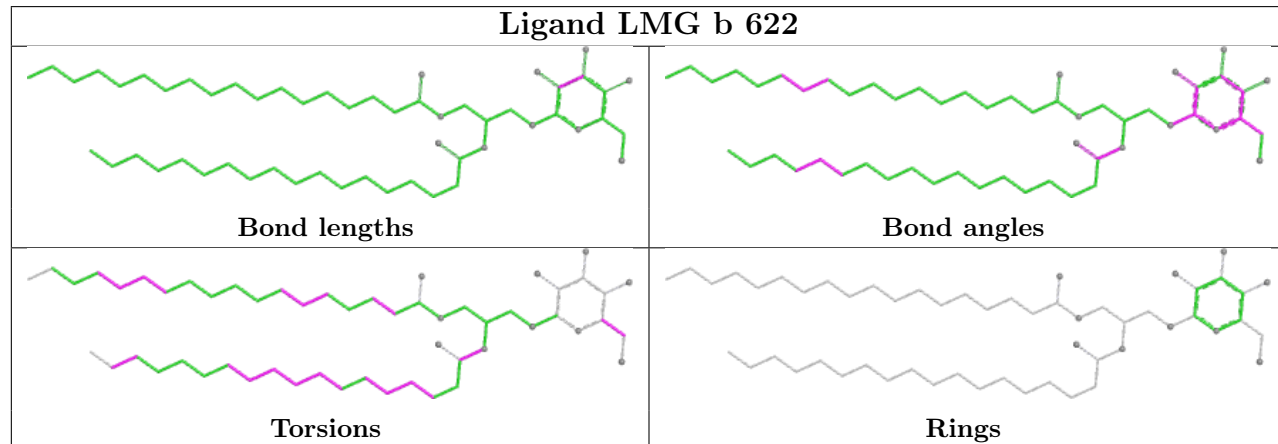
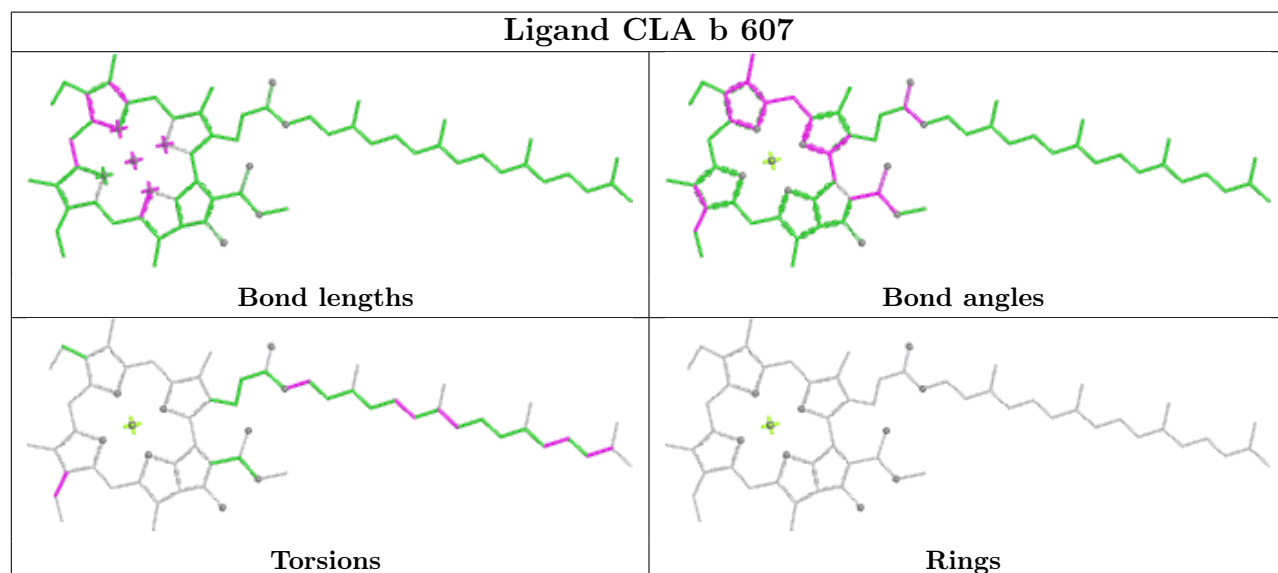
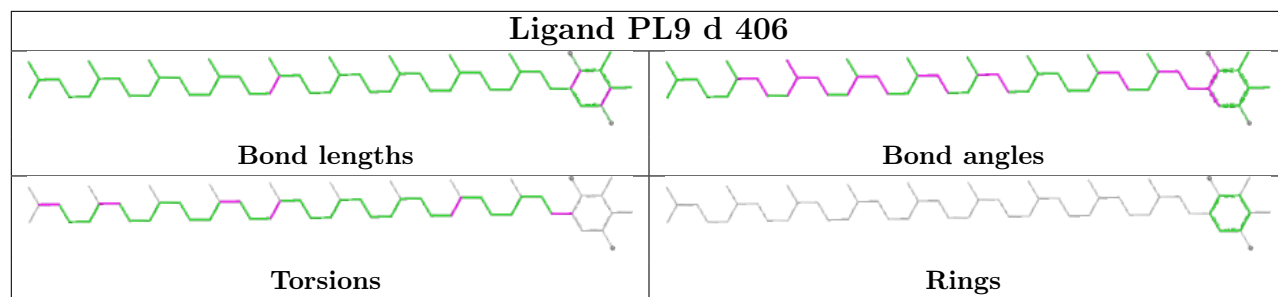
Ligand CLA A 607

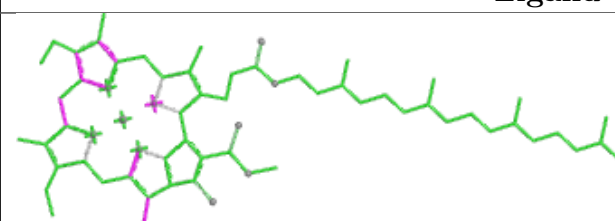
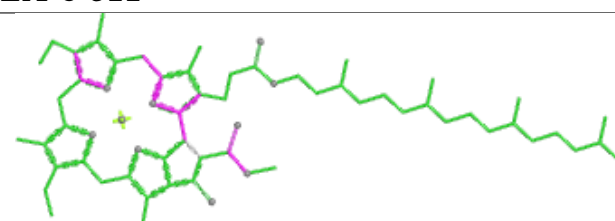
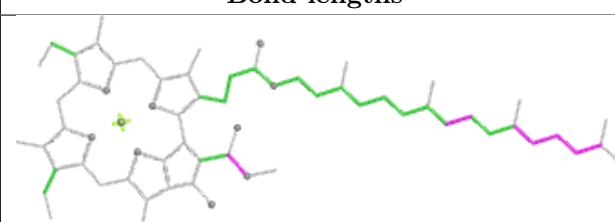
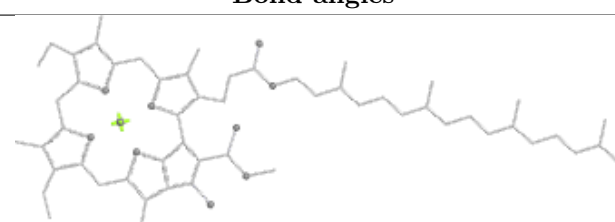


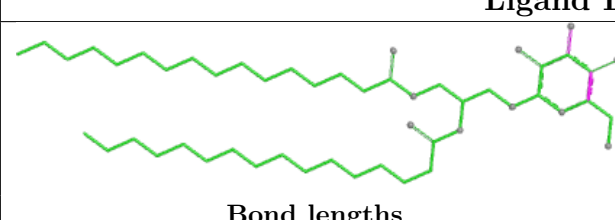
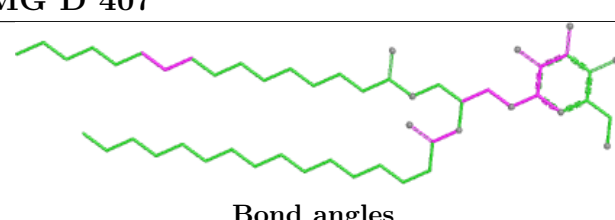
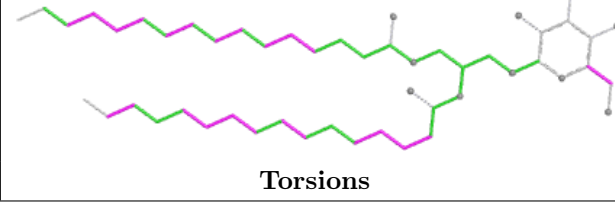
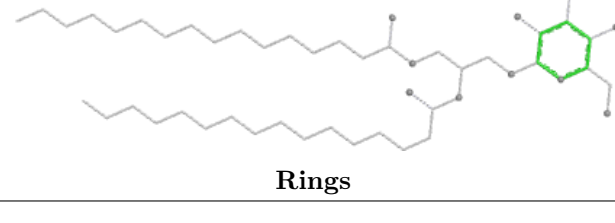
Ligand STE B 619

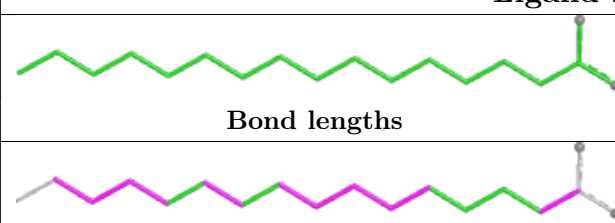
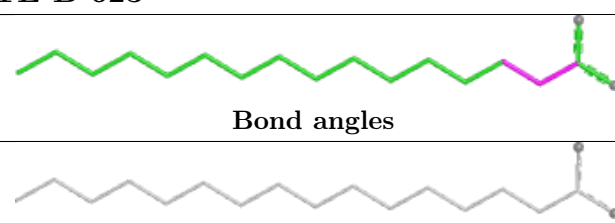


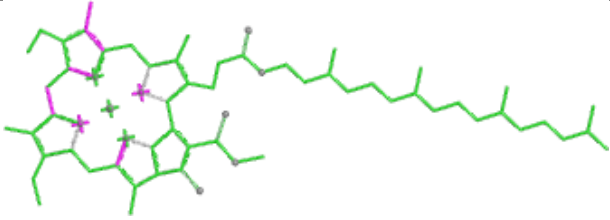
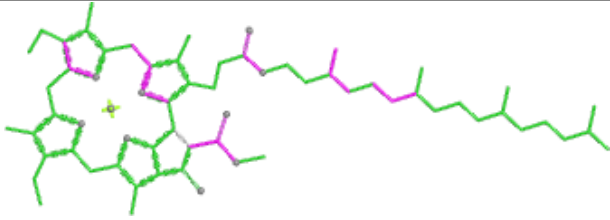
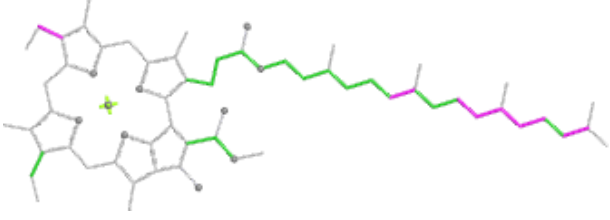
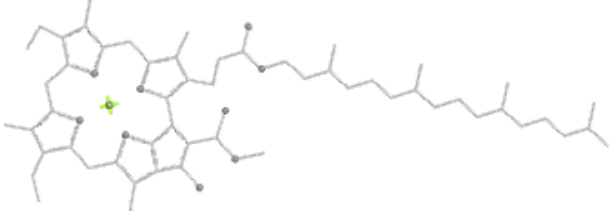
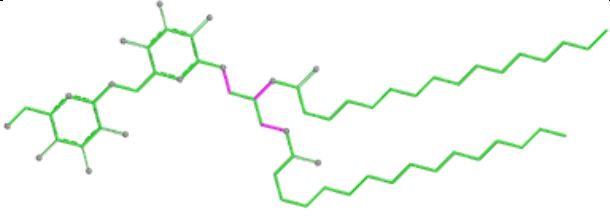
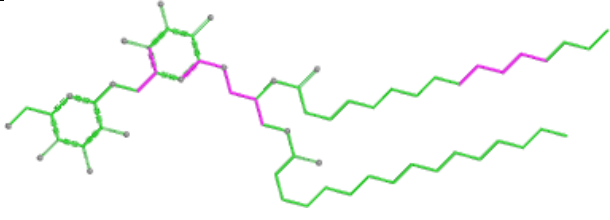
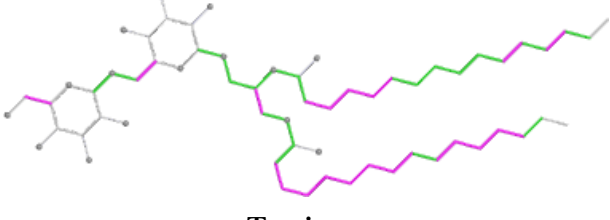
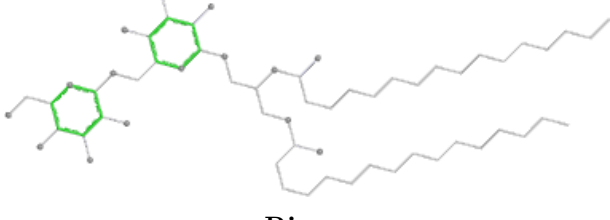
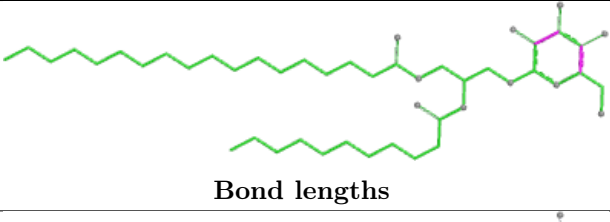
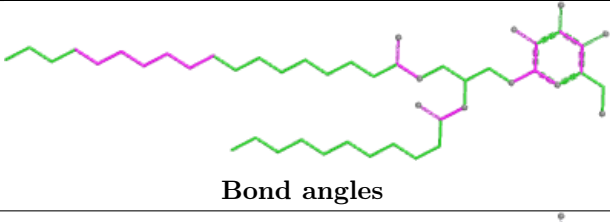
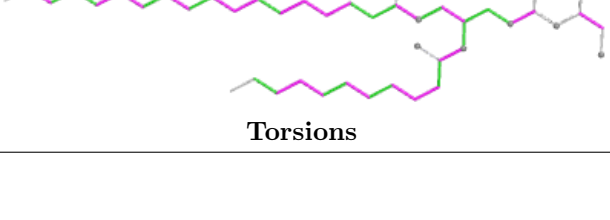


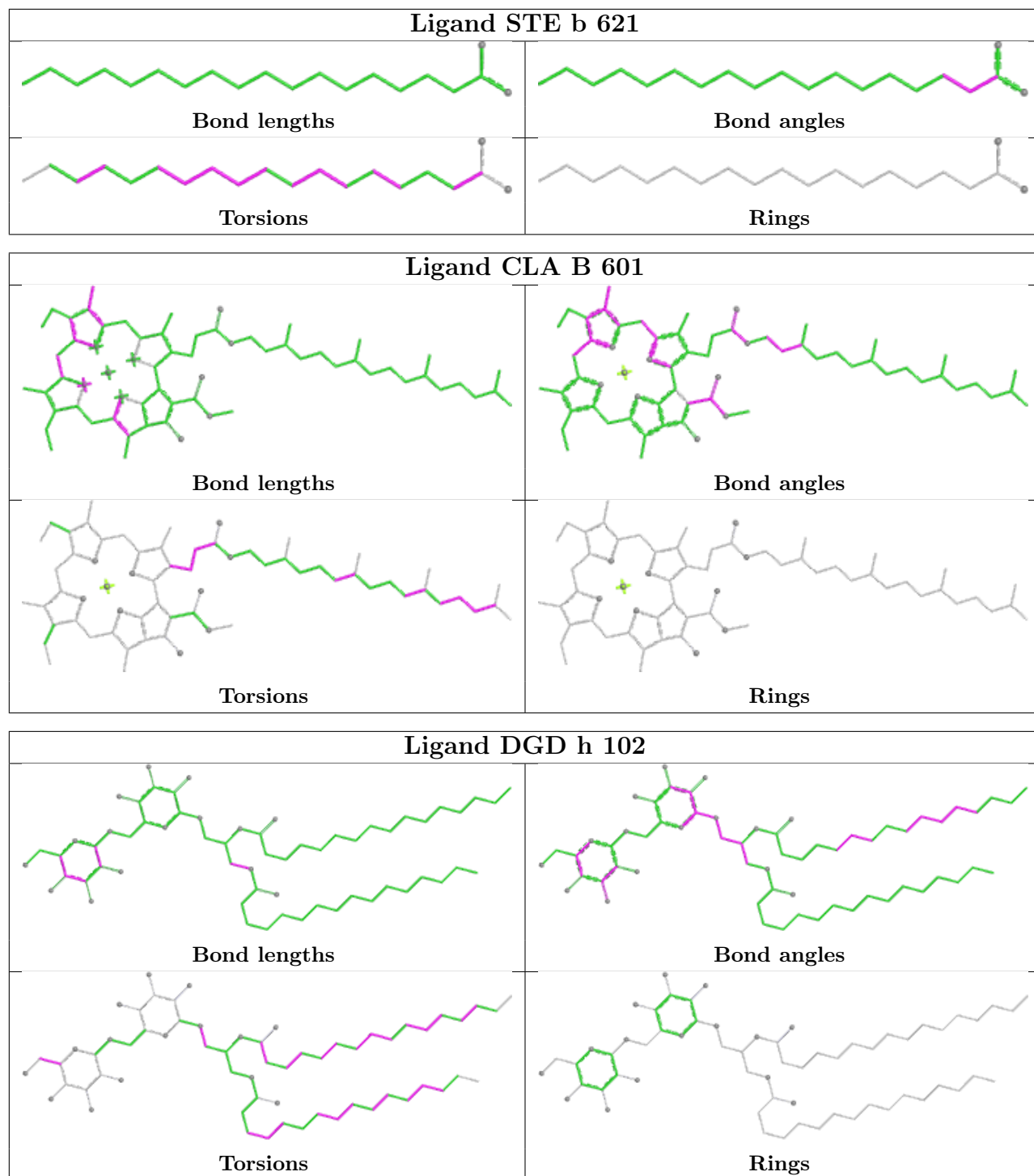


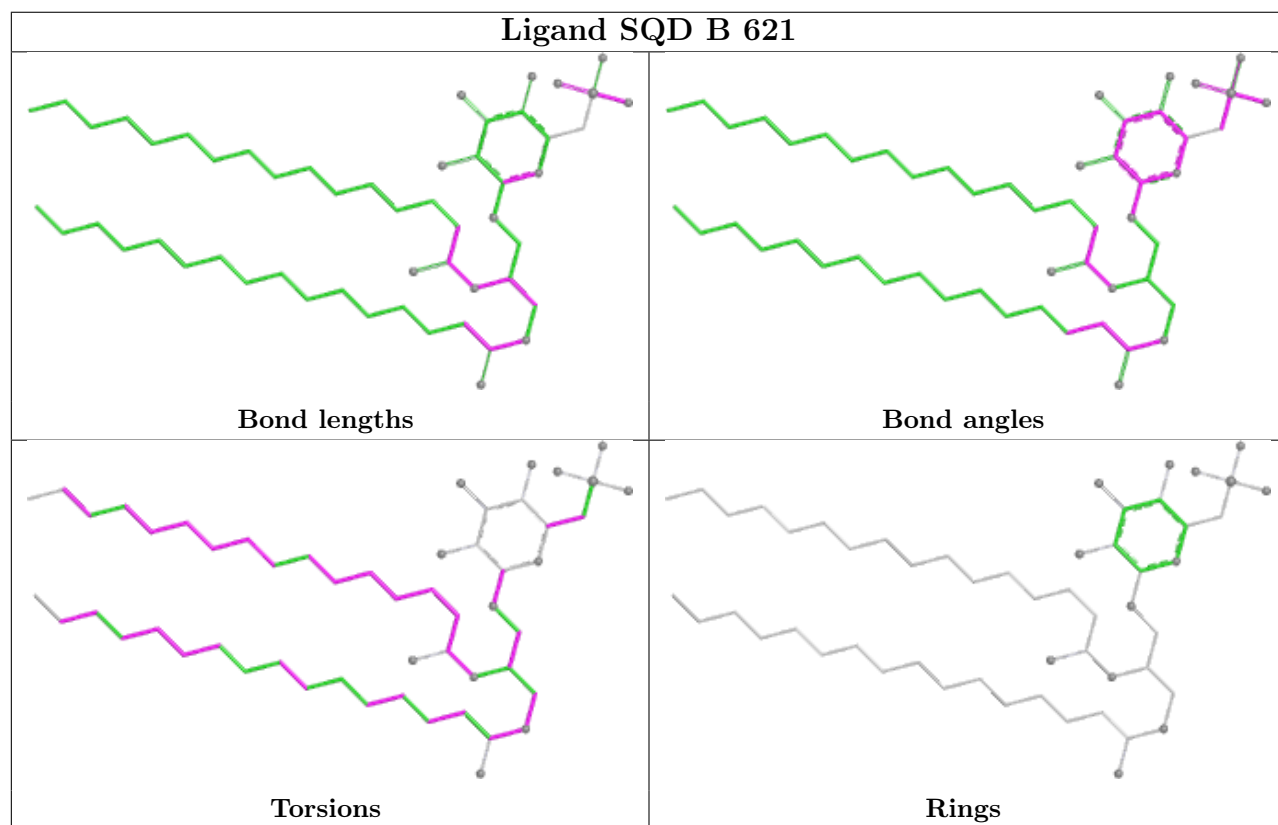
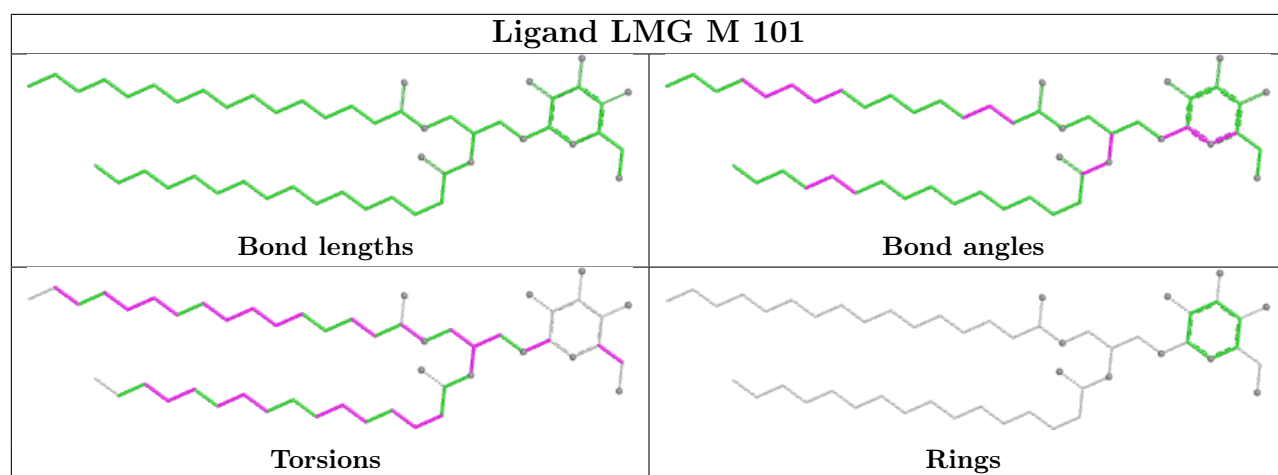
Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

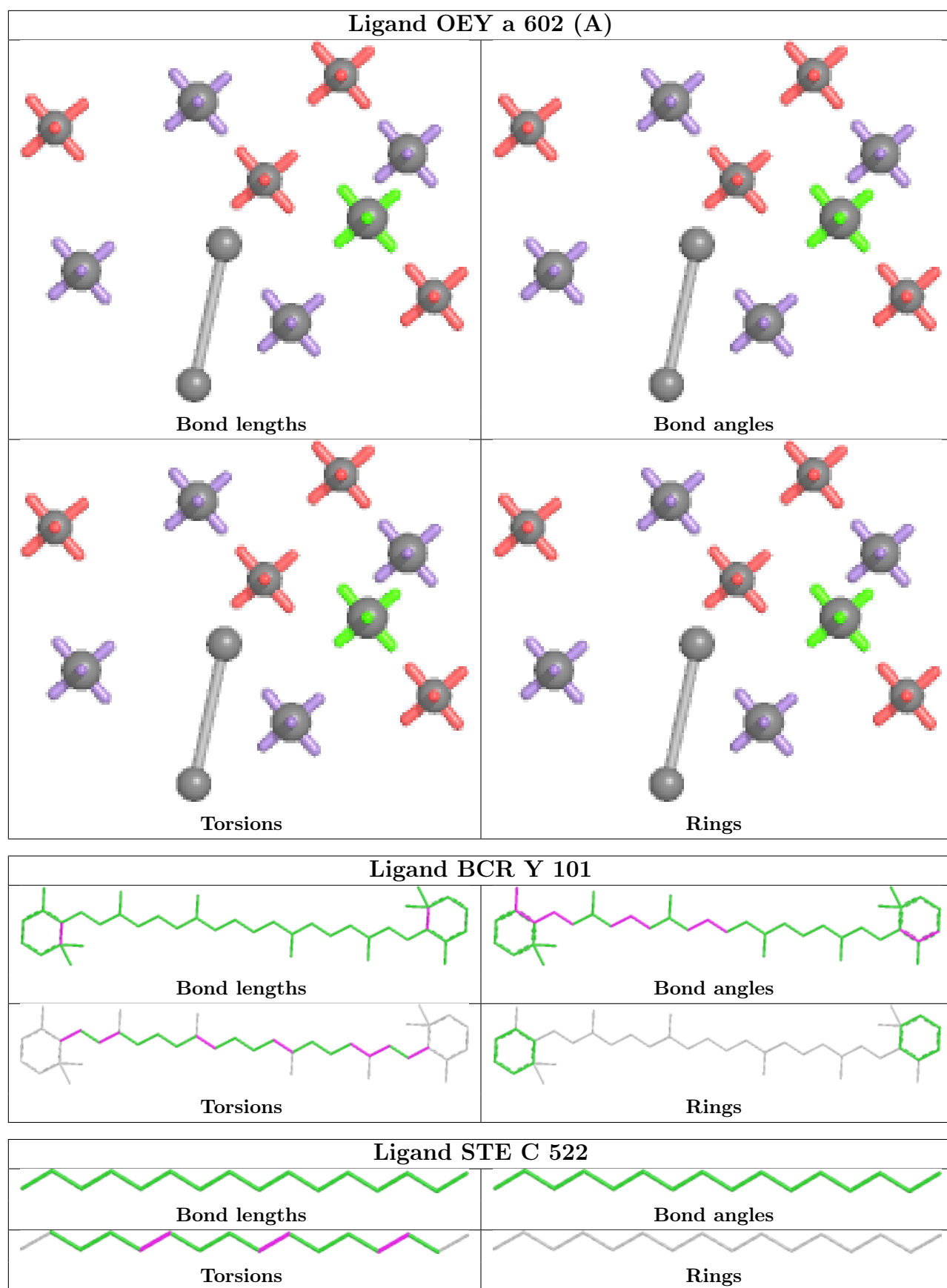
Ligand LMG D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

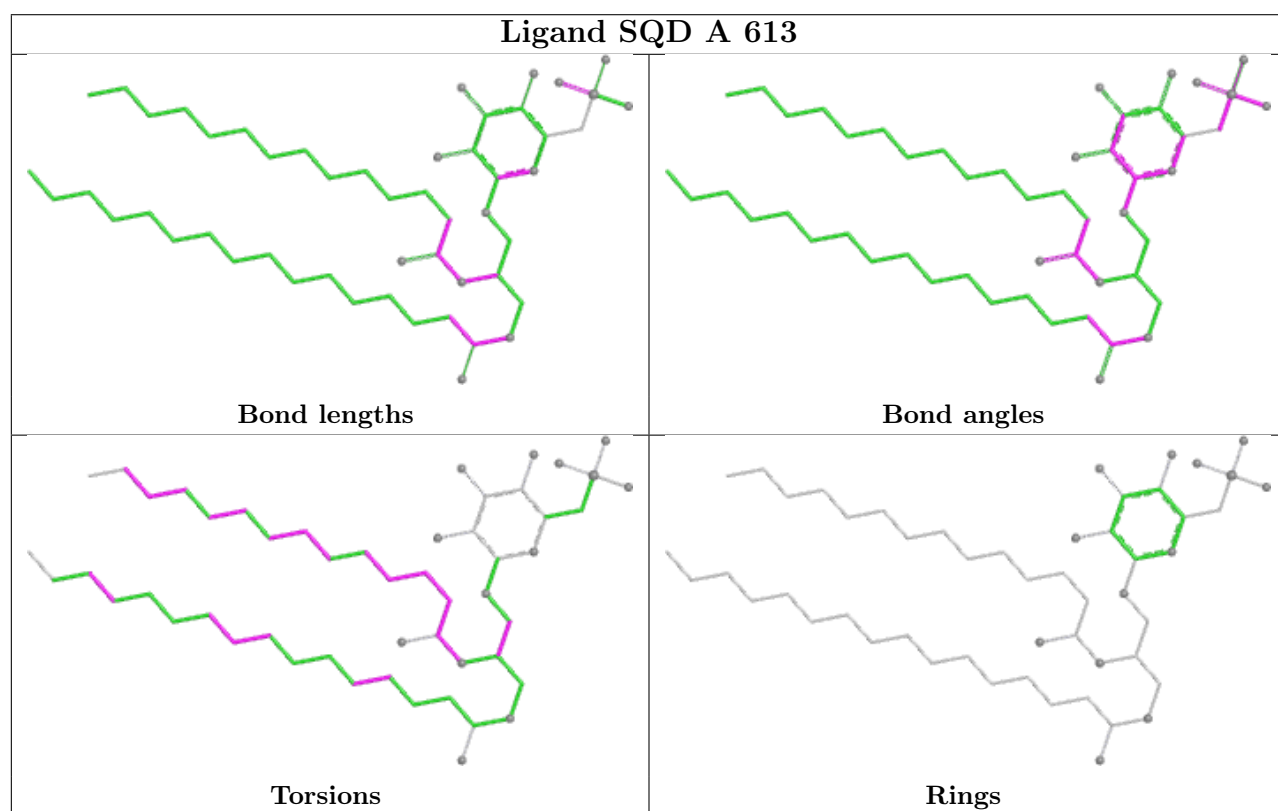
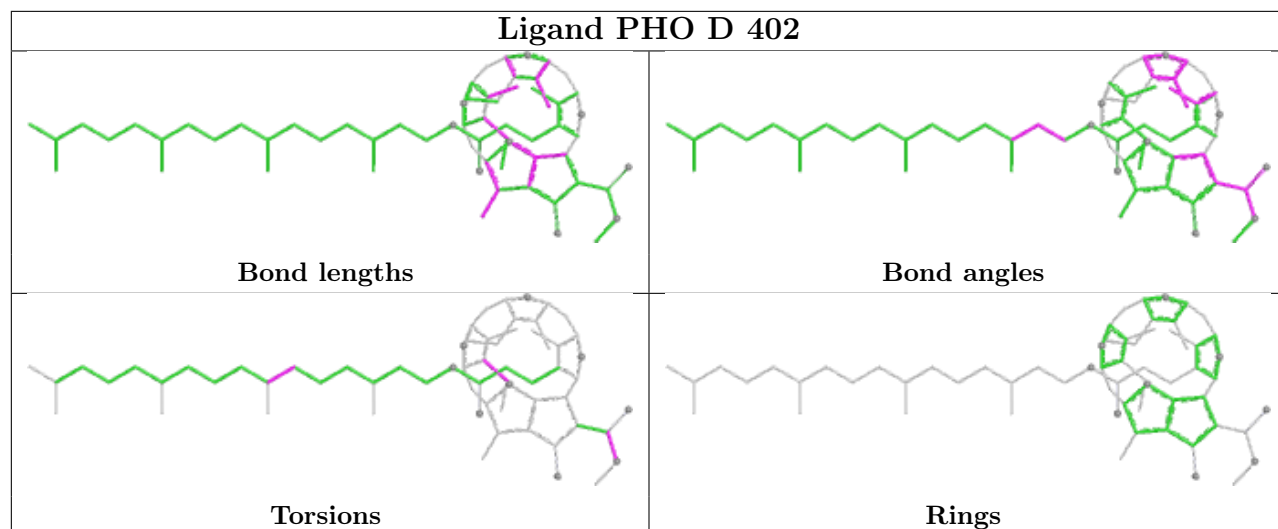
Ligand STE B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD C 518	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

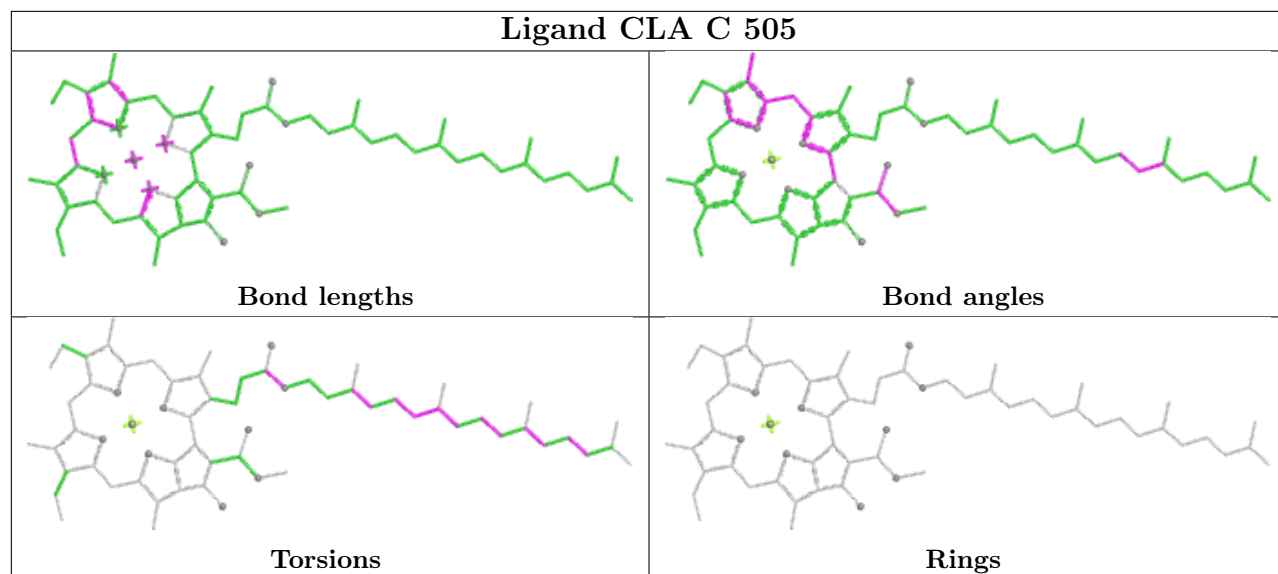




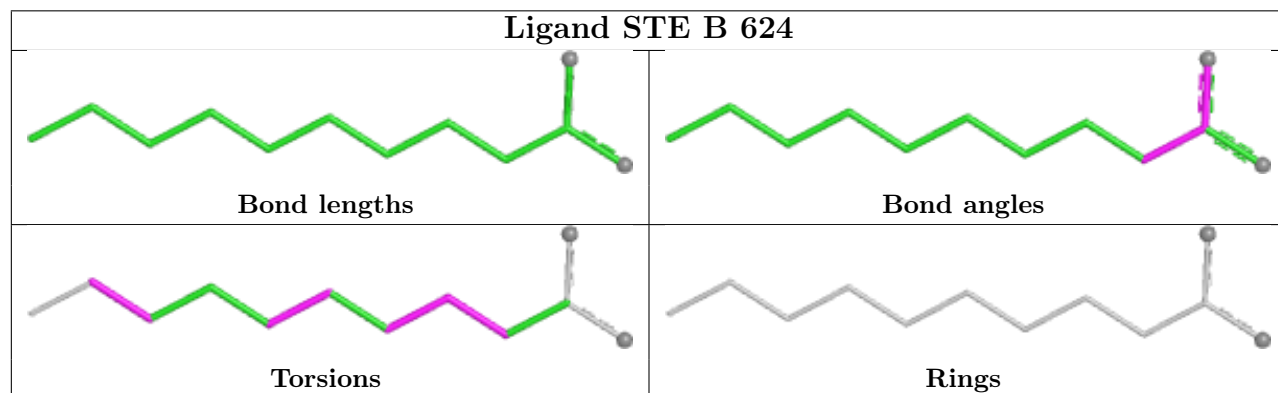




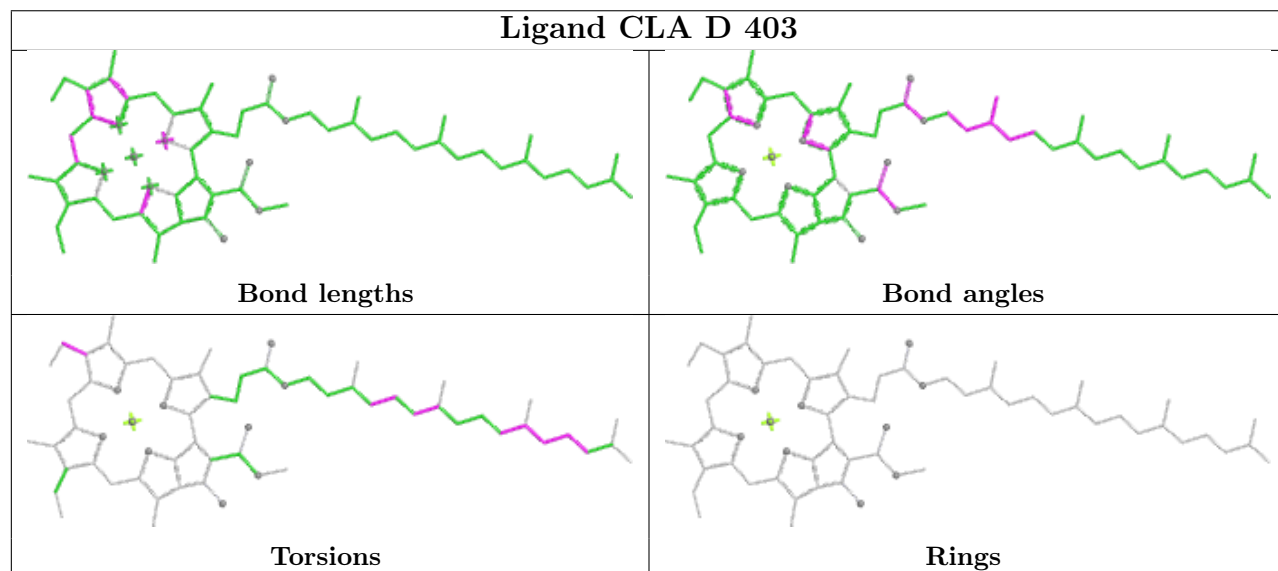
Ligand CLA C 505



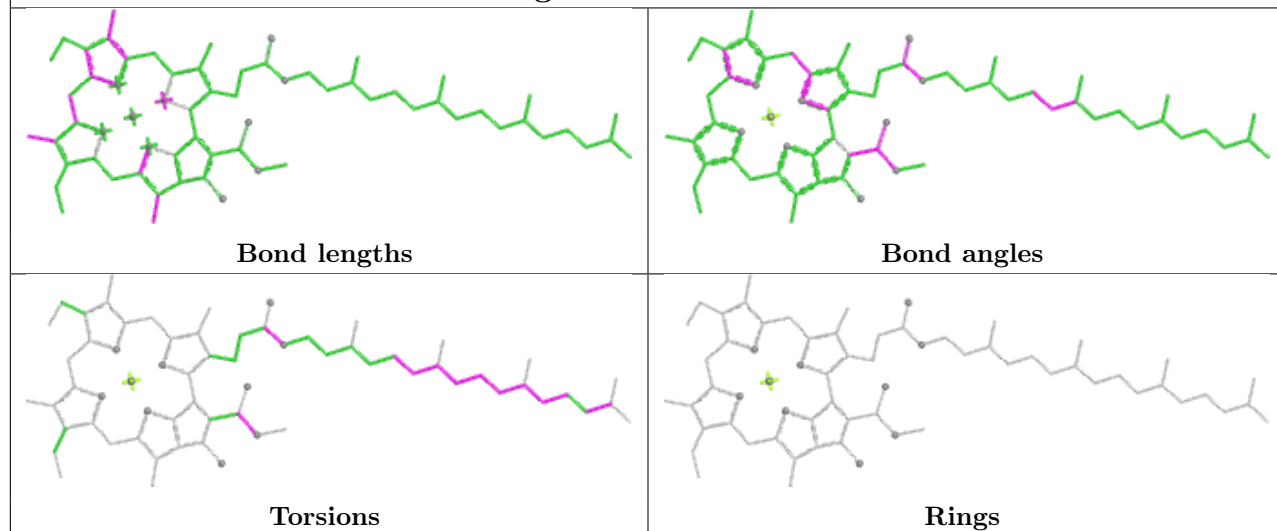
Ligand STE B 624



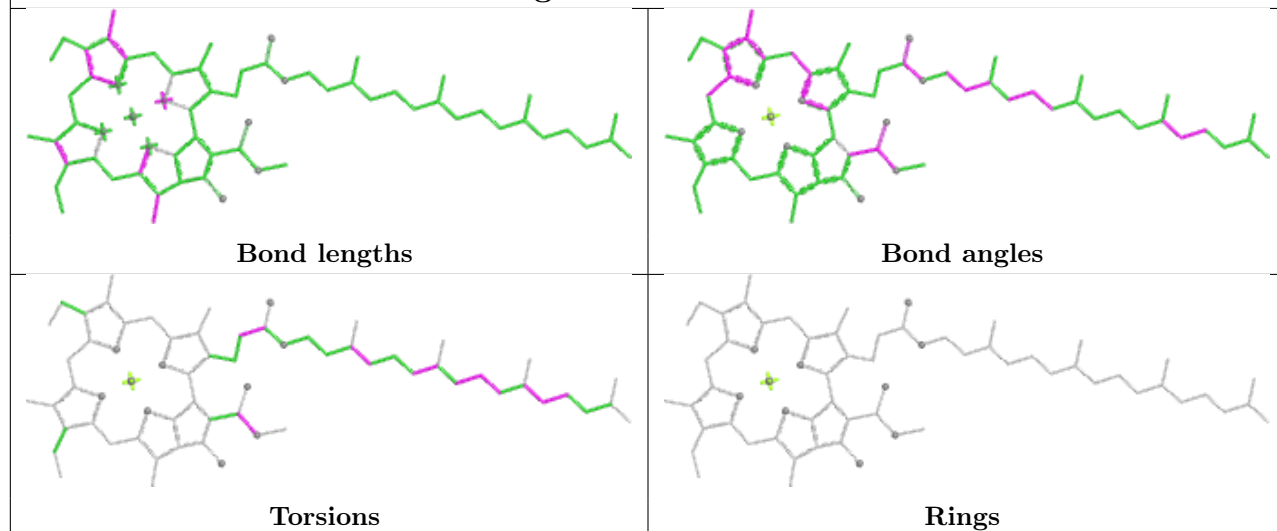
Ligand CLA D 403



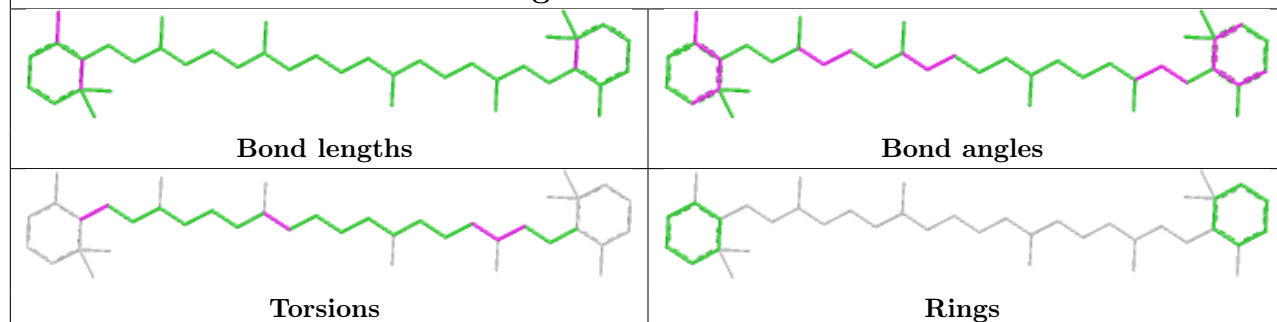
Ligand CLA b 606

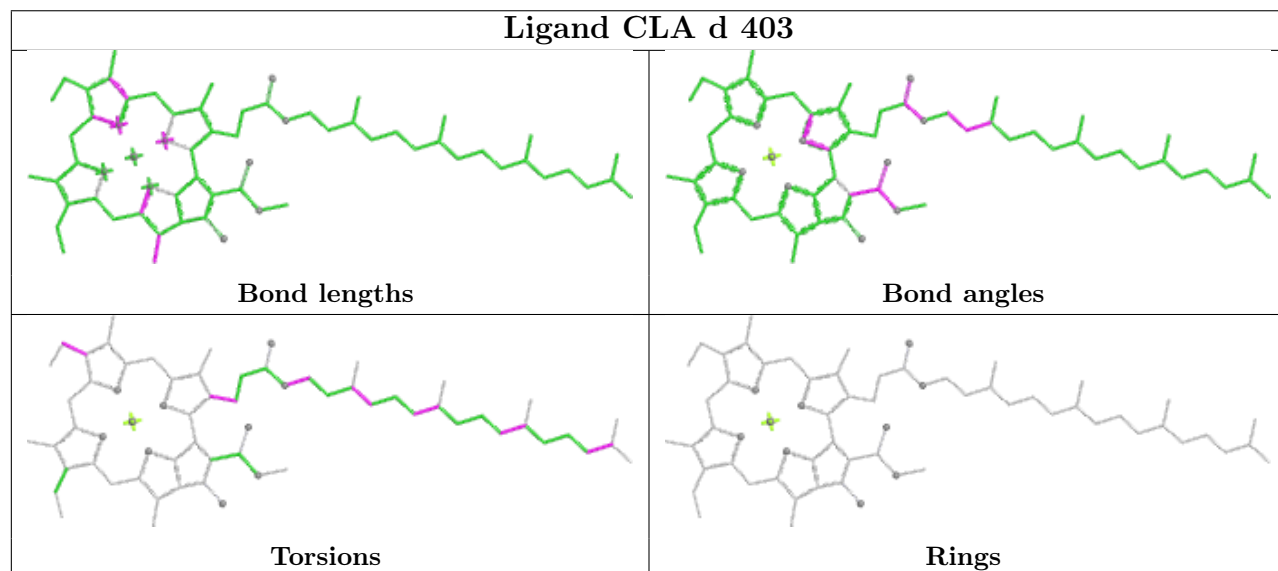
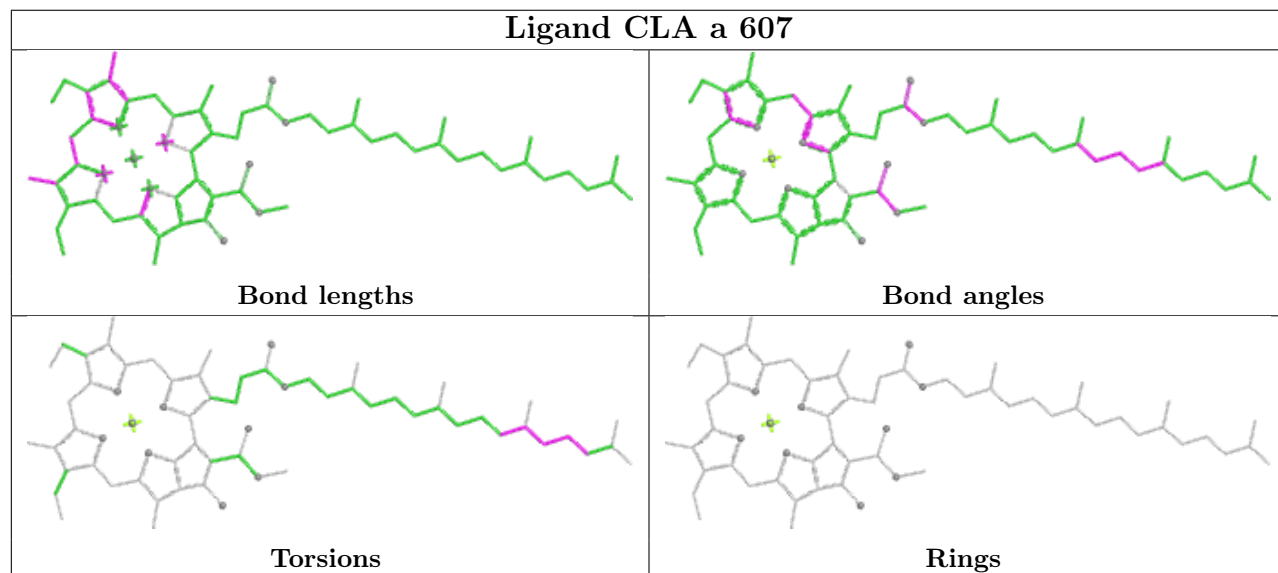
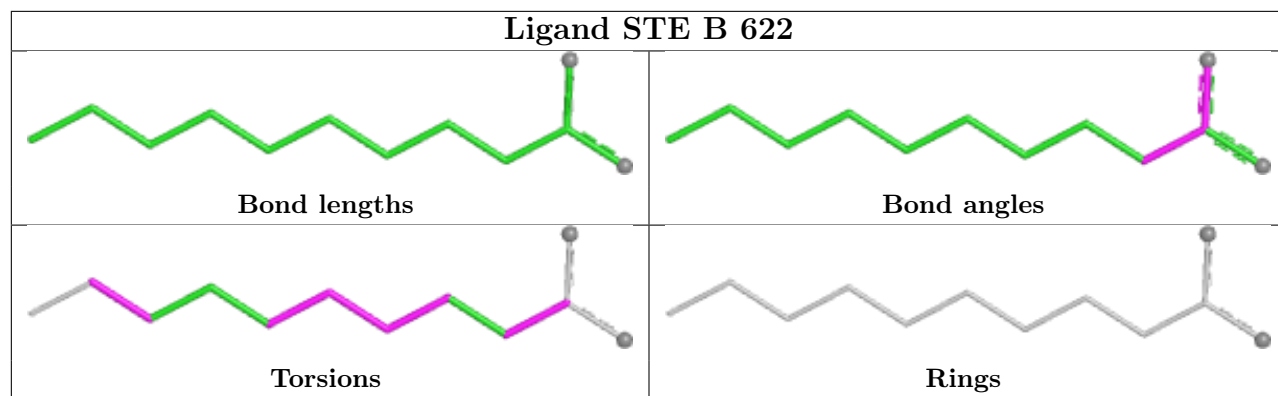


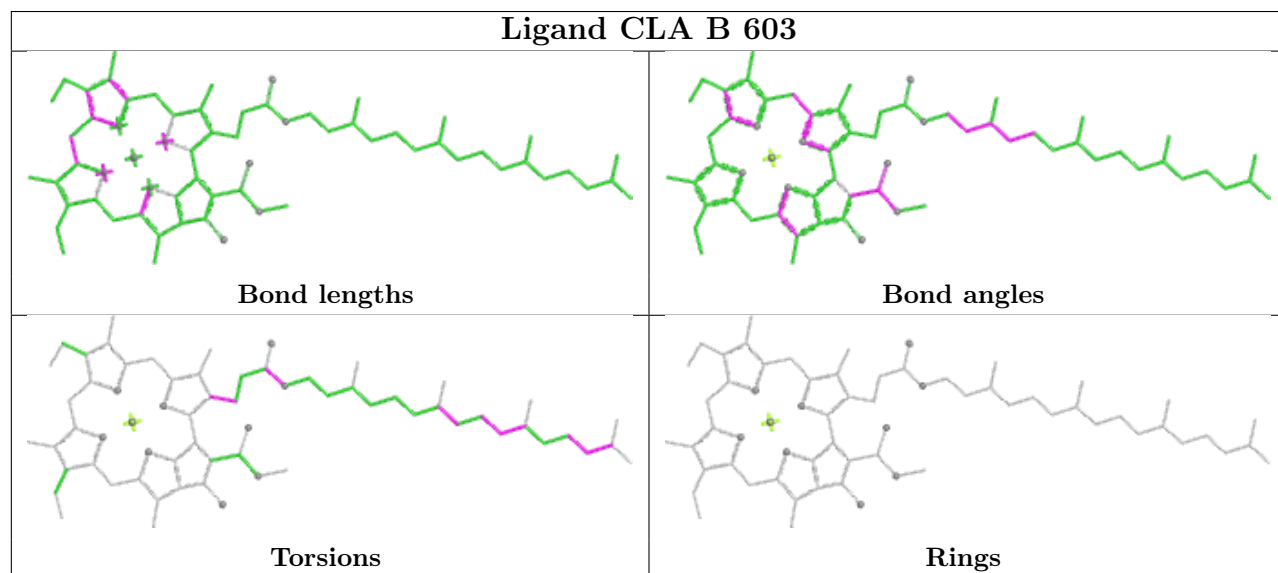
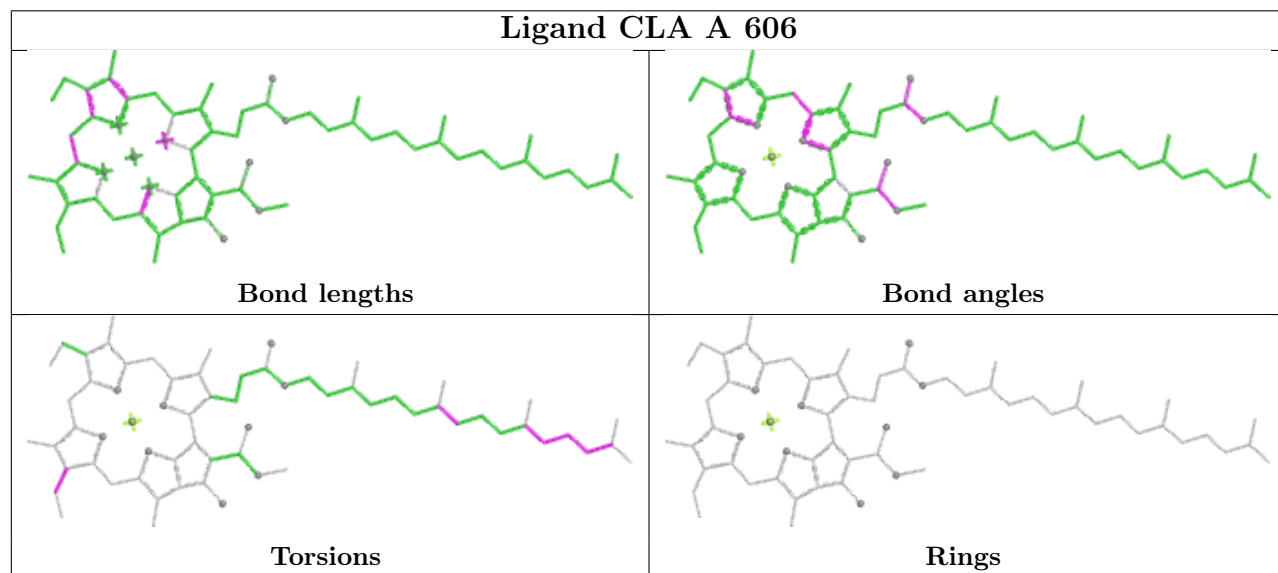
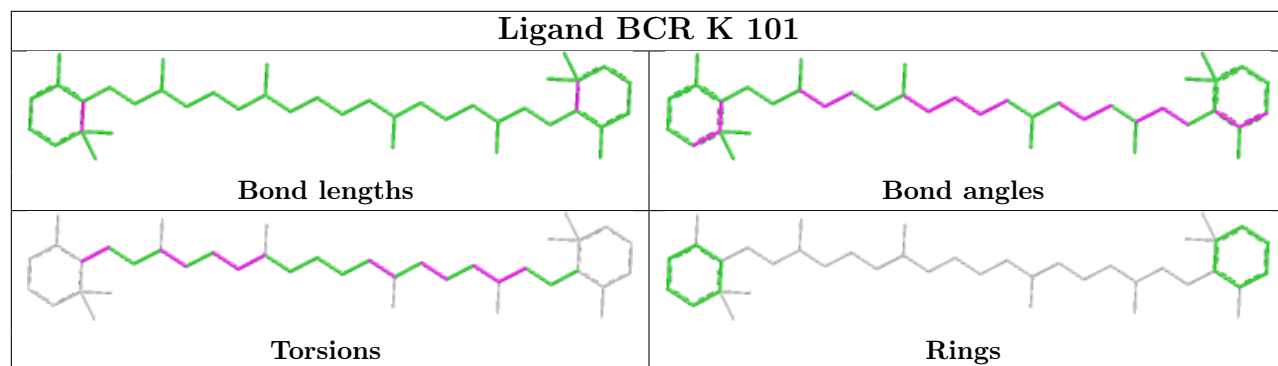
Ligand CLA b 612



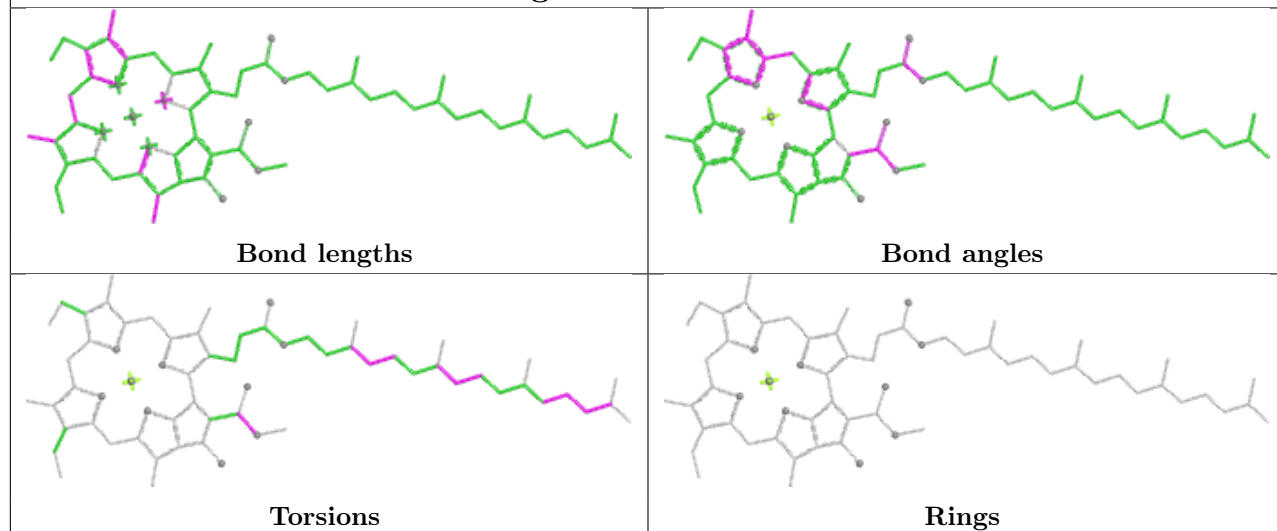
Ligand BCR b 616



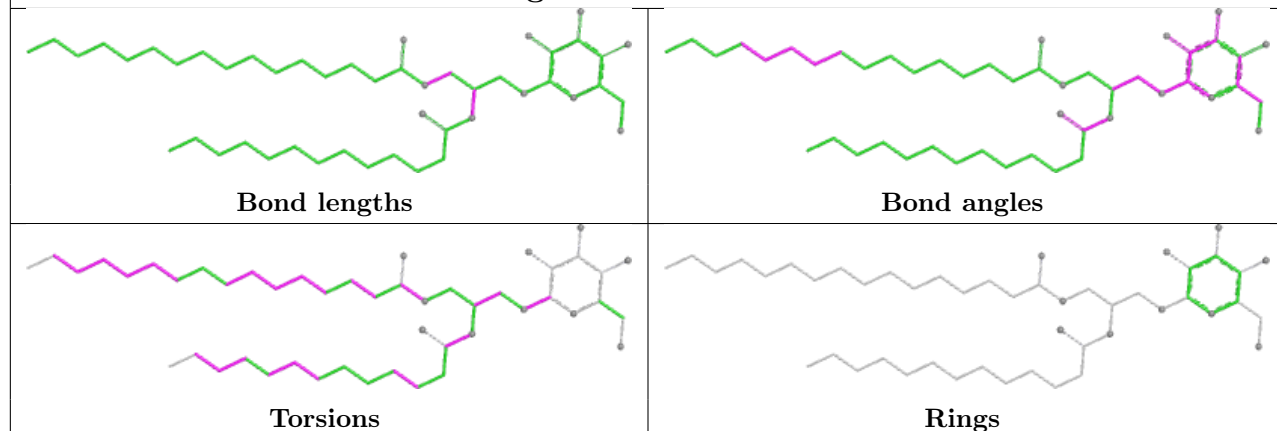




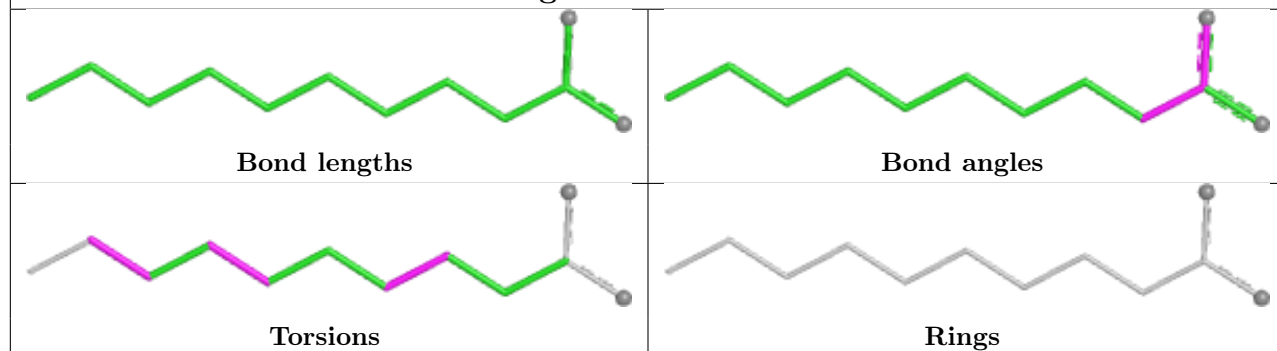
Ligand CLA C 510

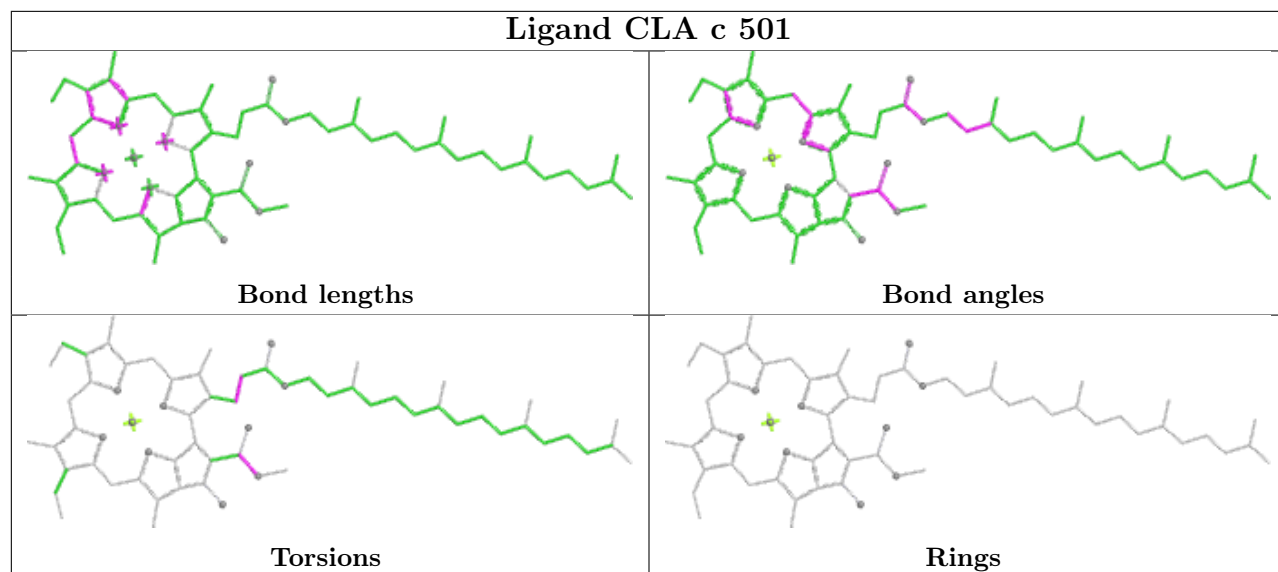
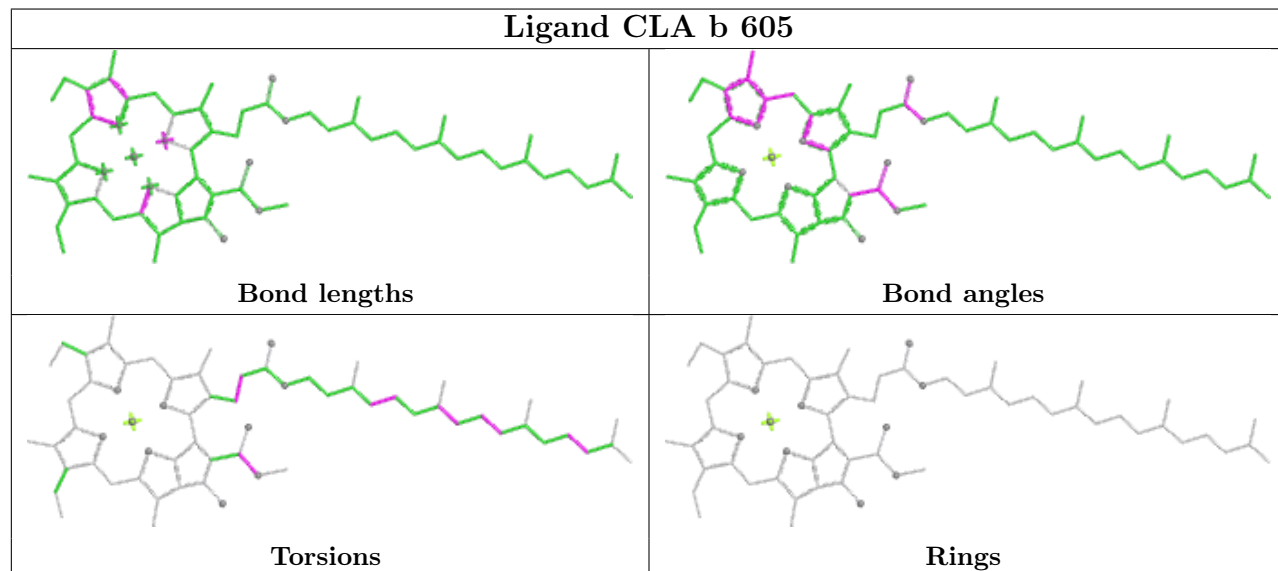
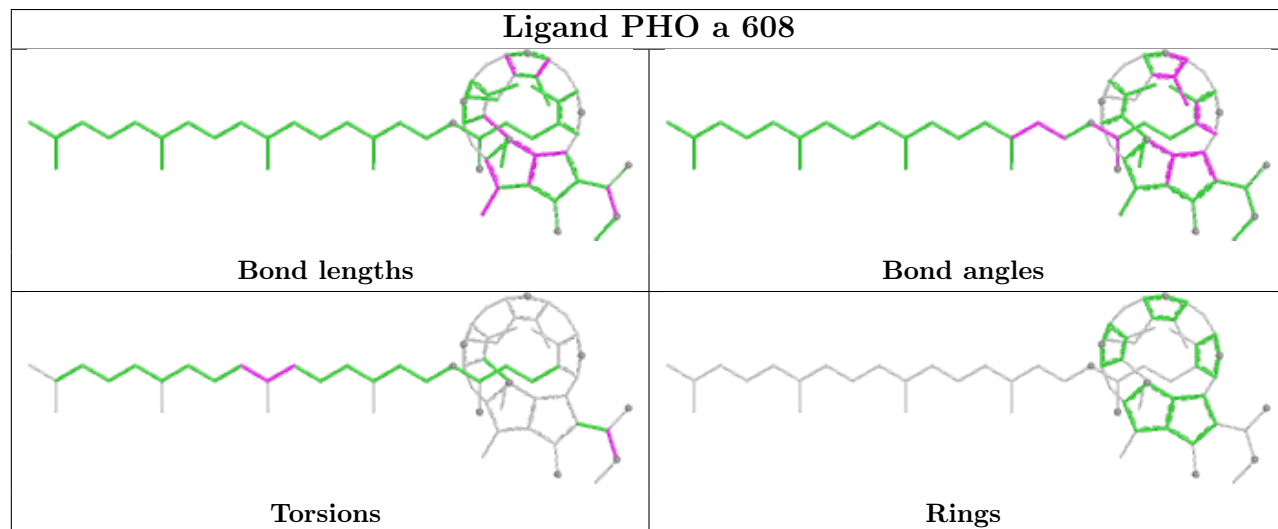


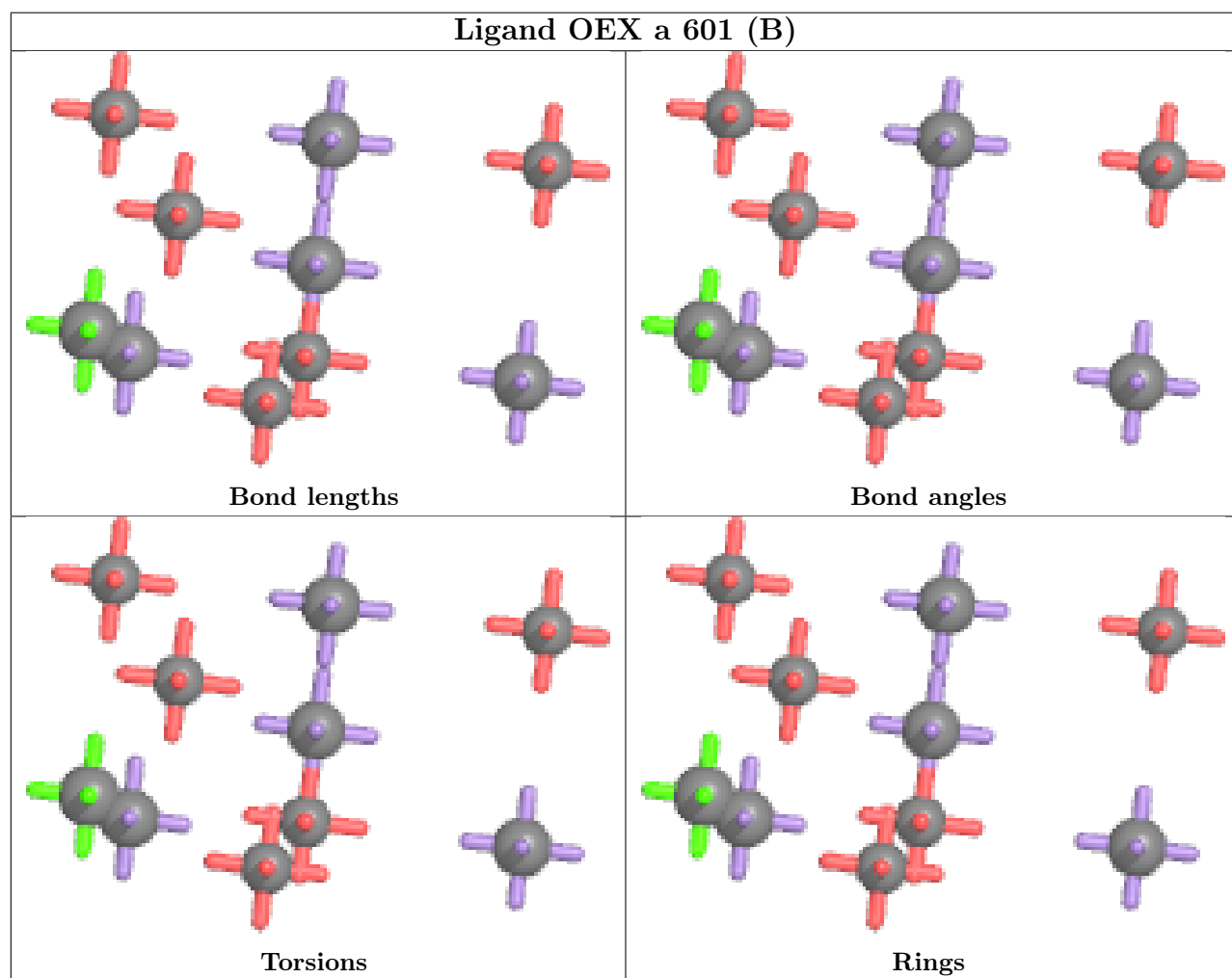
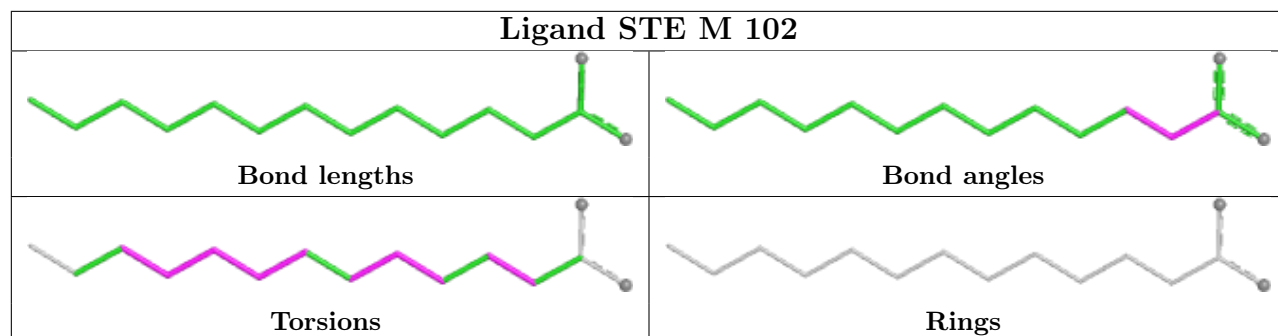
Ligand LMG C 519

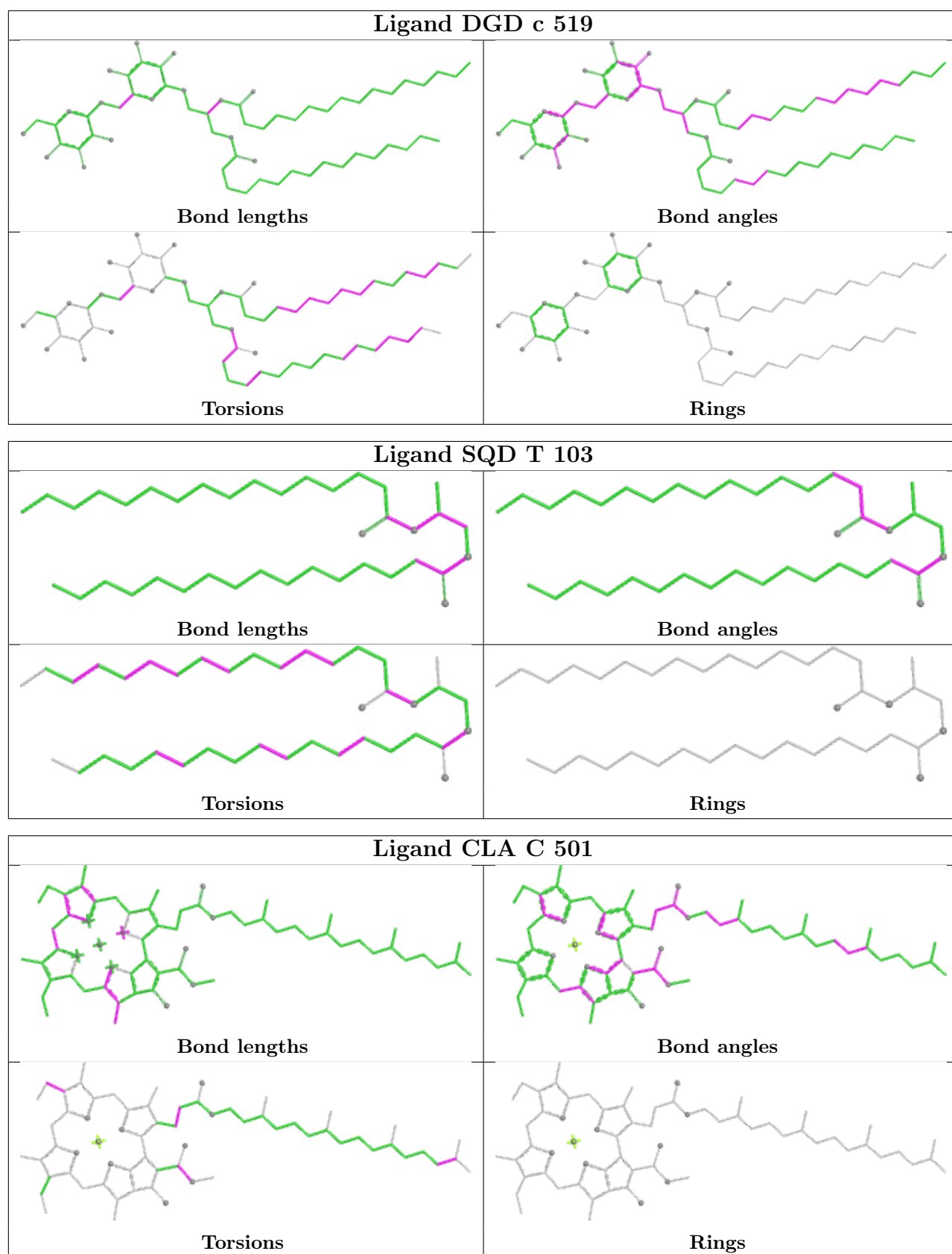


Ligand STE c 523

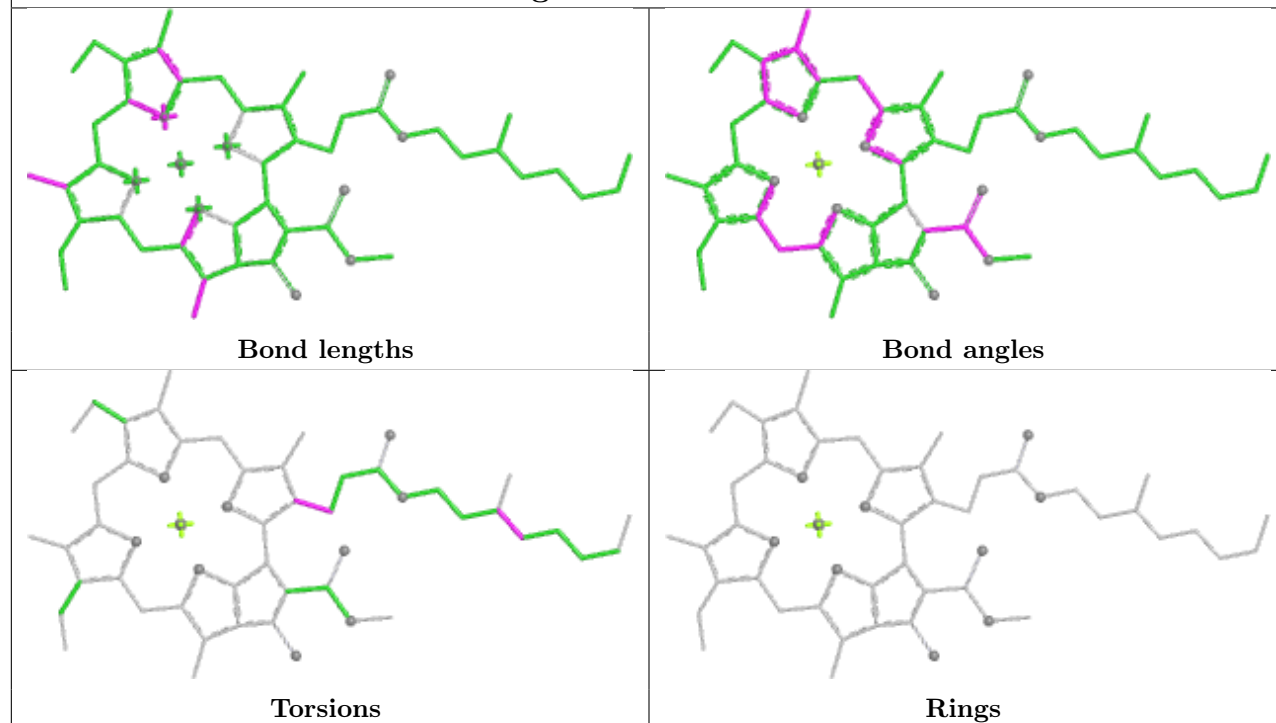


Ligand CLA c 501**Ligand CLA b 605****Ligand PHO a 608**

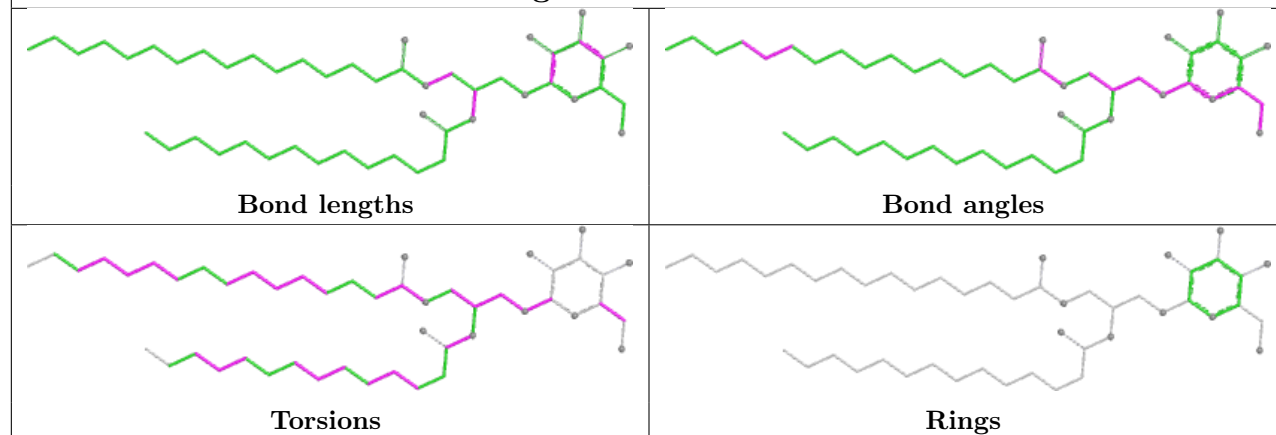




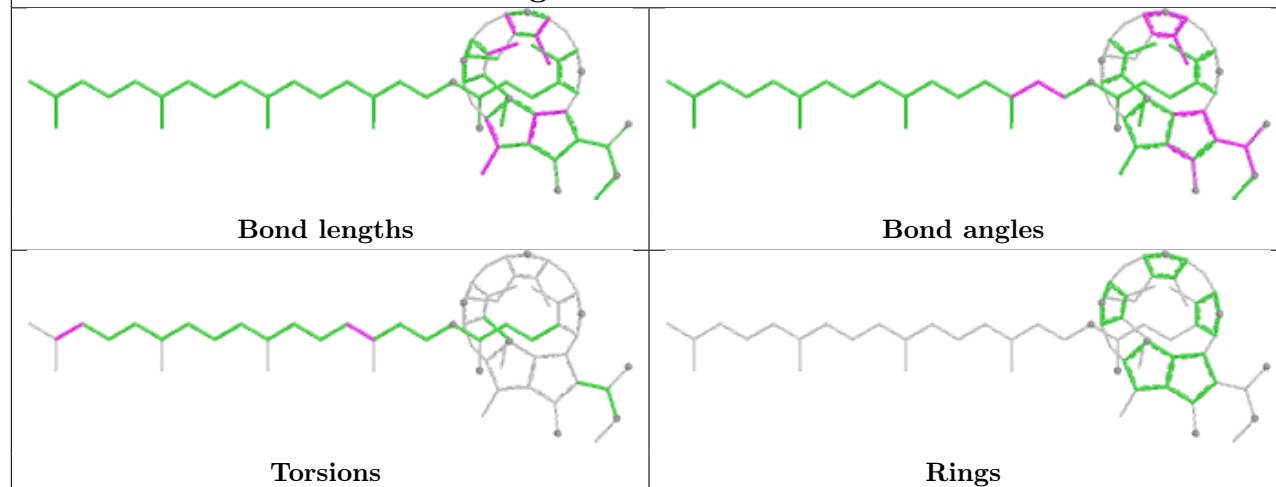
Ligand CLA A 609

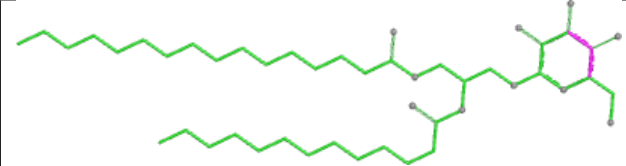
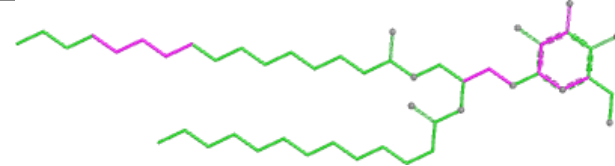
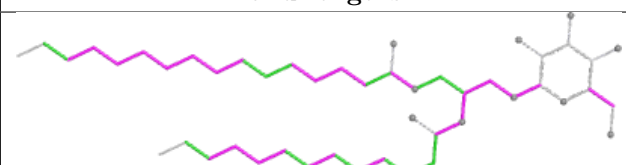
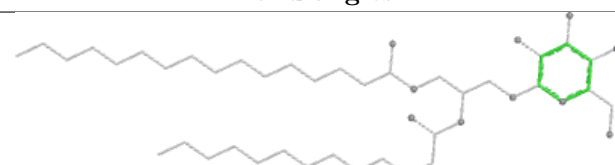


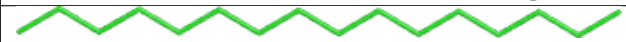
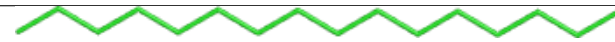
Ligand LMG c 524

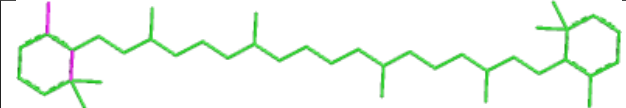
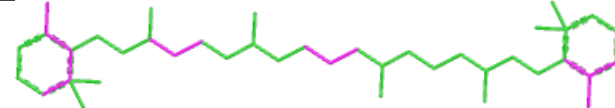
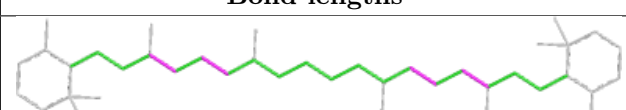
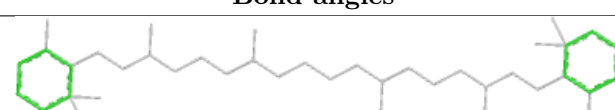


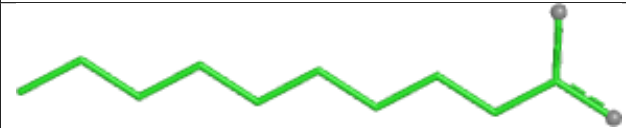
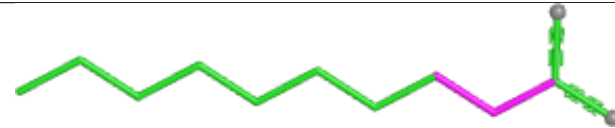
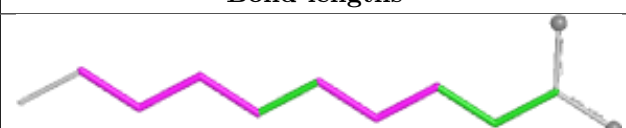
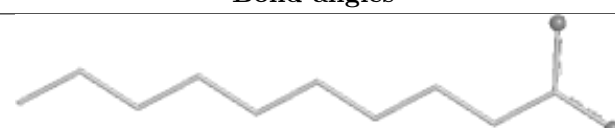
Ligand PHO A 608

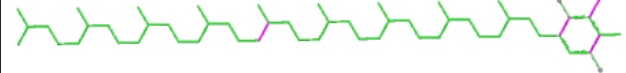
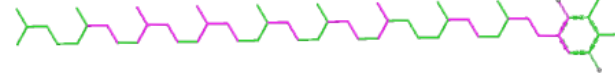
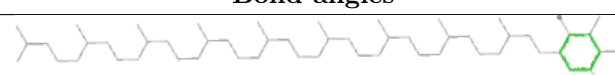


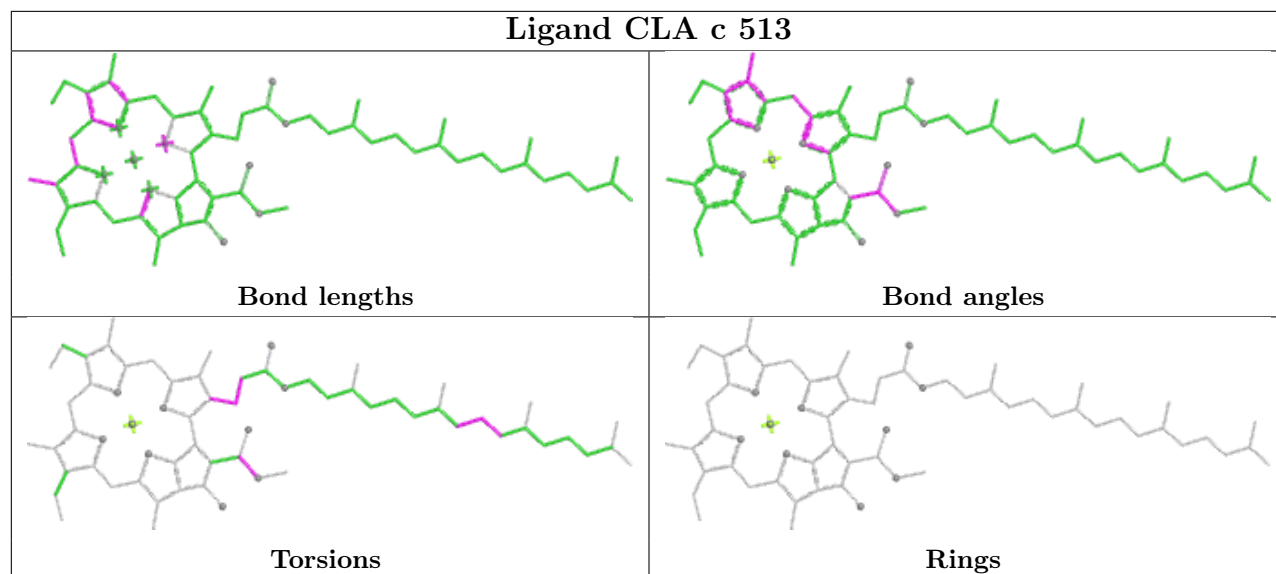
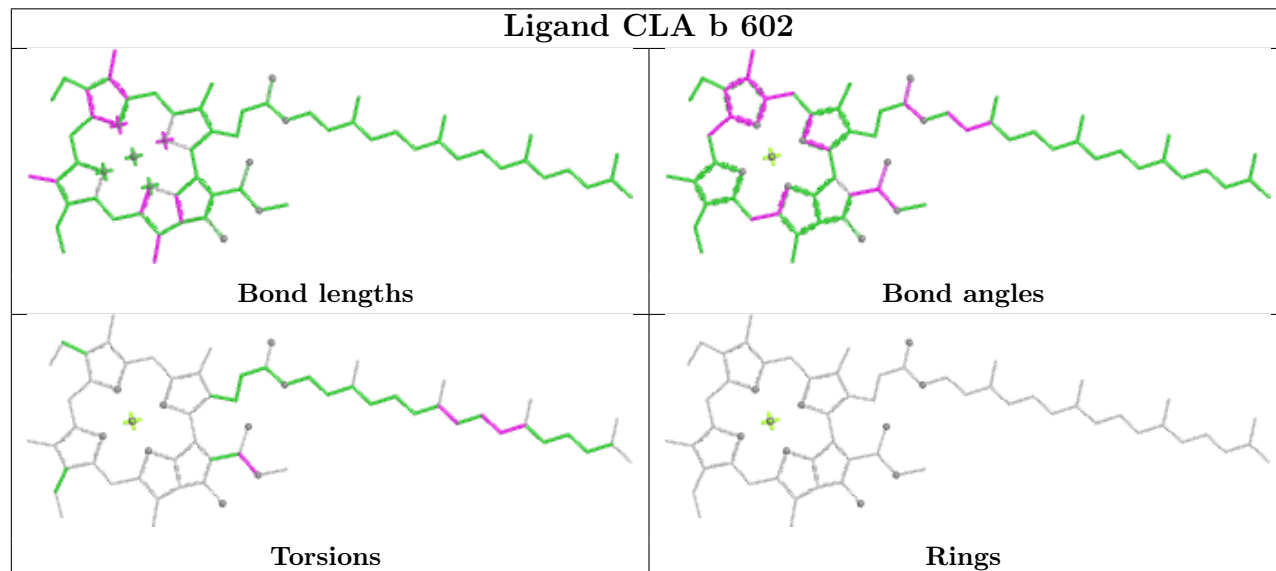
Ligand LMG C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

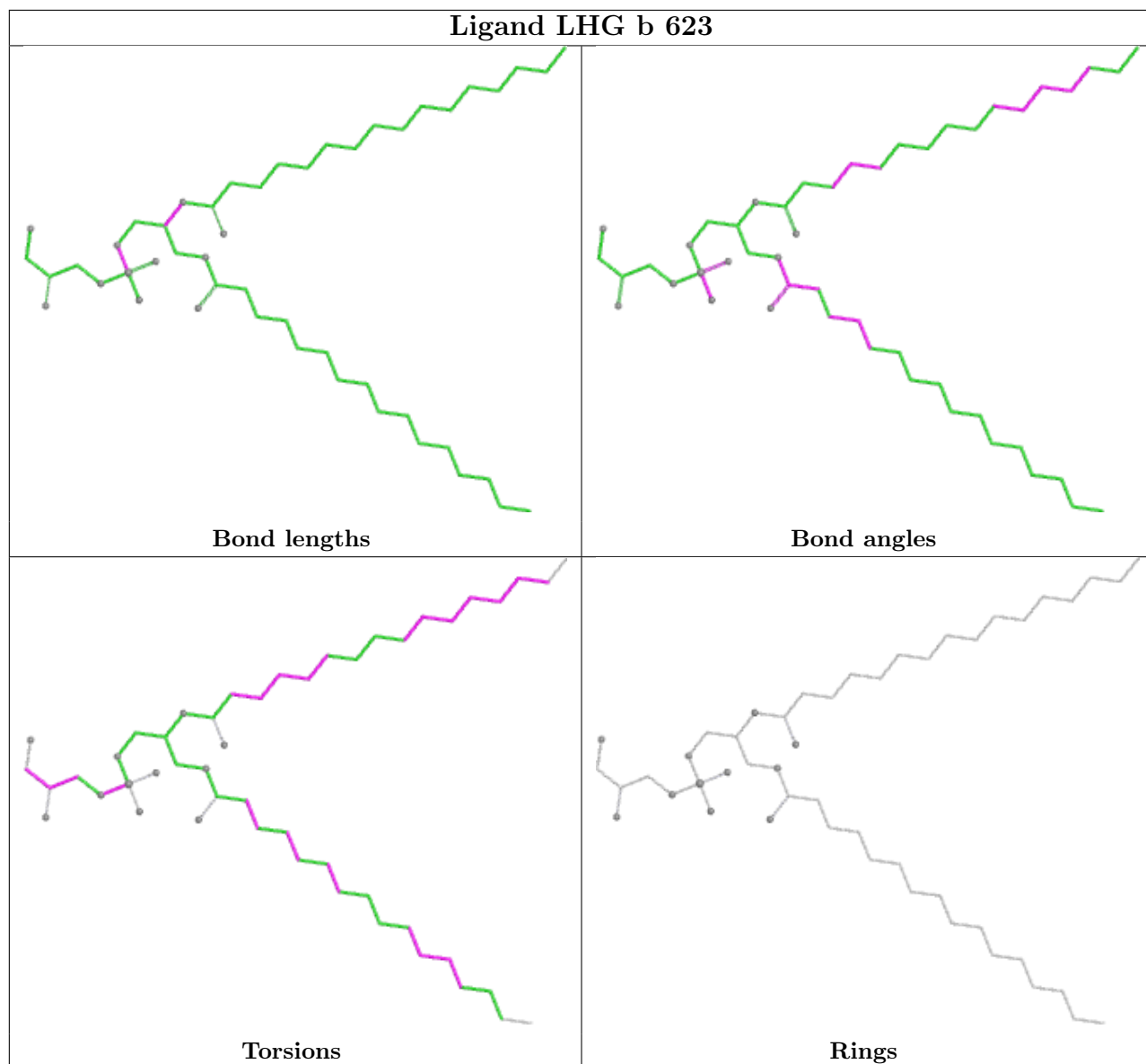
Ligand BCR A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

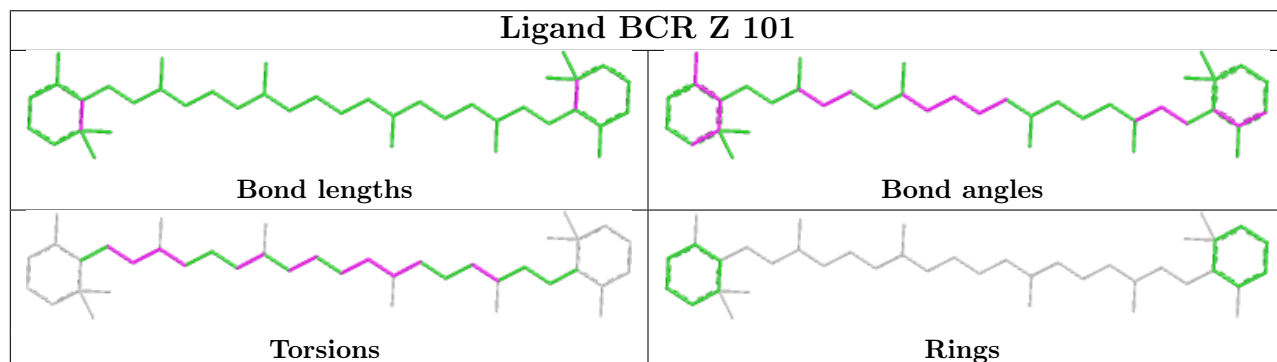
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 513**Ligand CLA b 602**

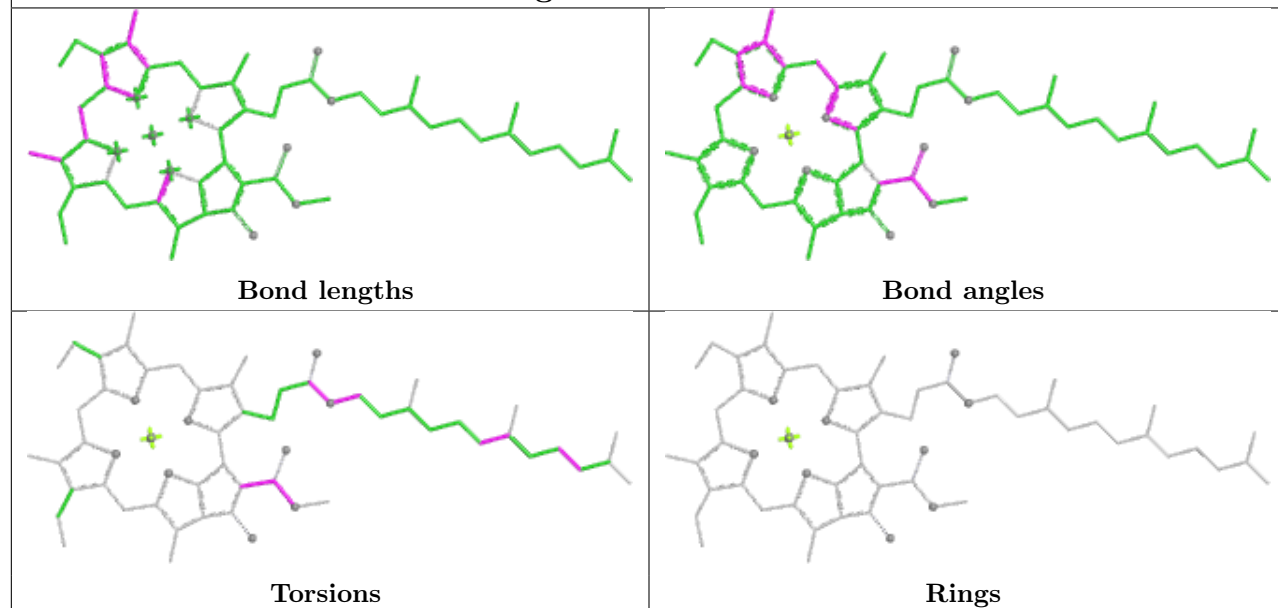
Ligand LHG b 623



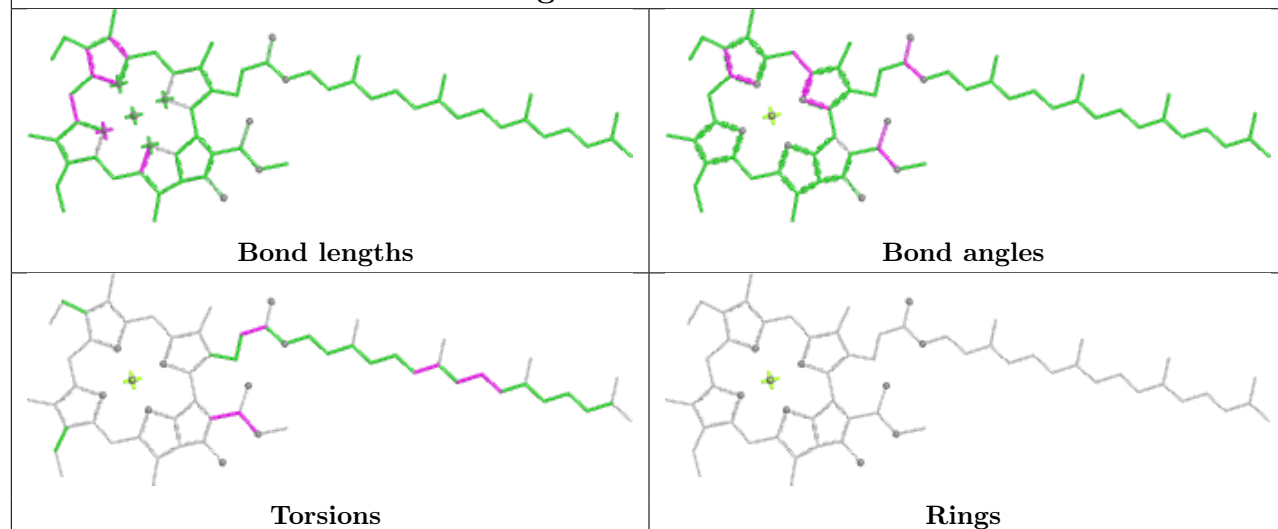
Ligand BCR Z 101



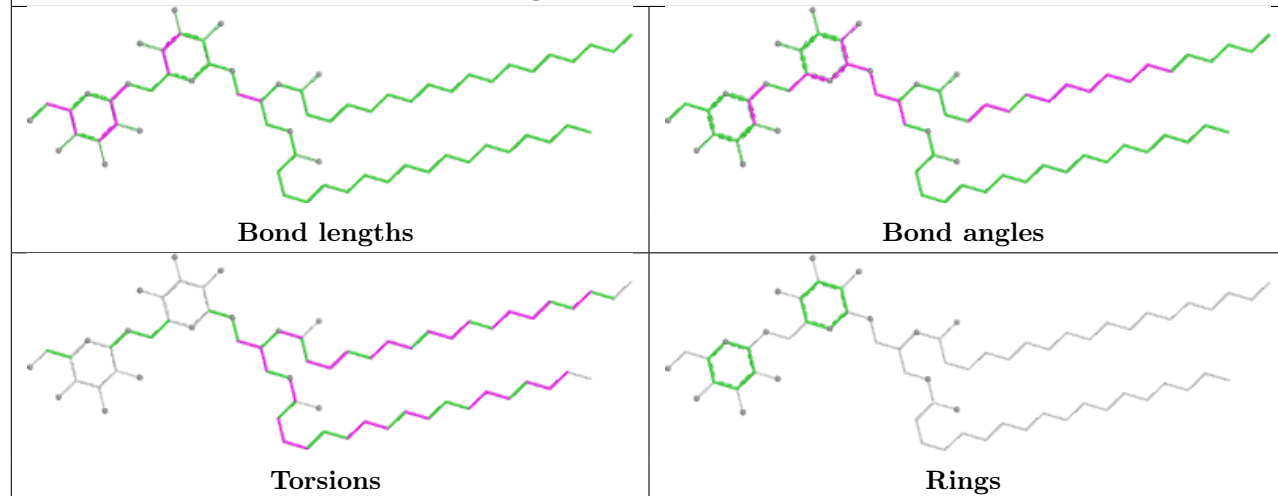
Ligand CLA b 615



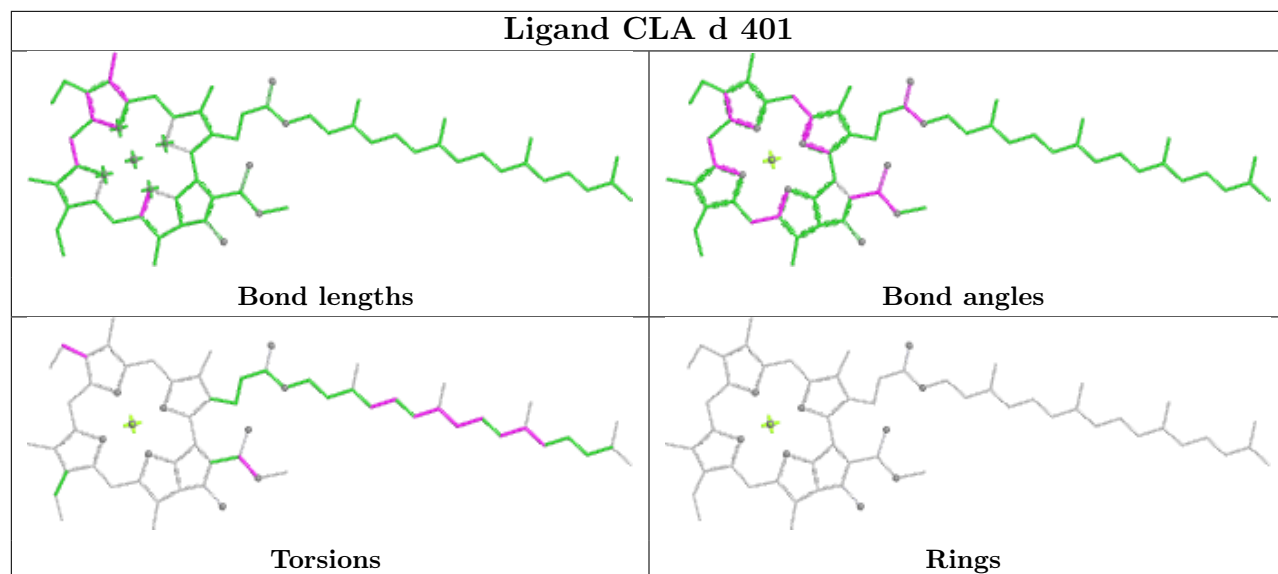
Ligand CLA c 509



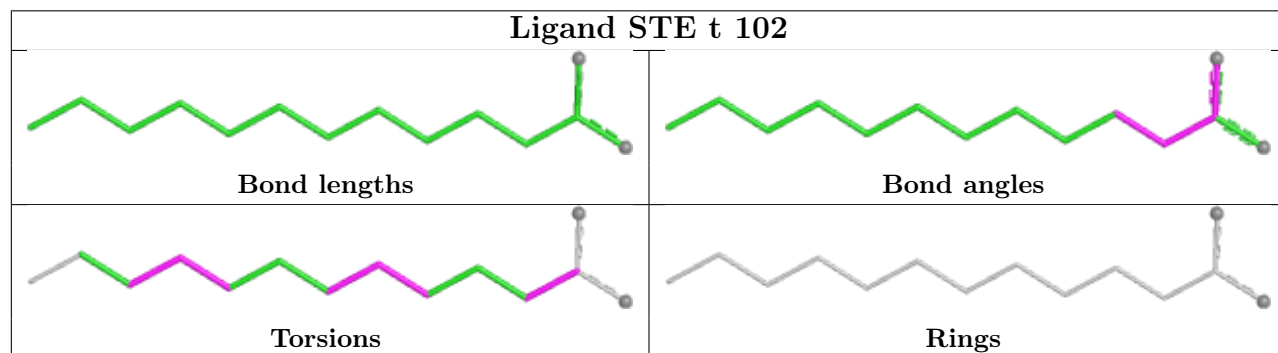
Ligand DGD A 614



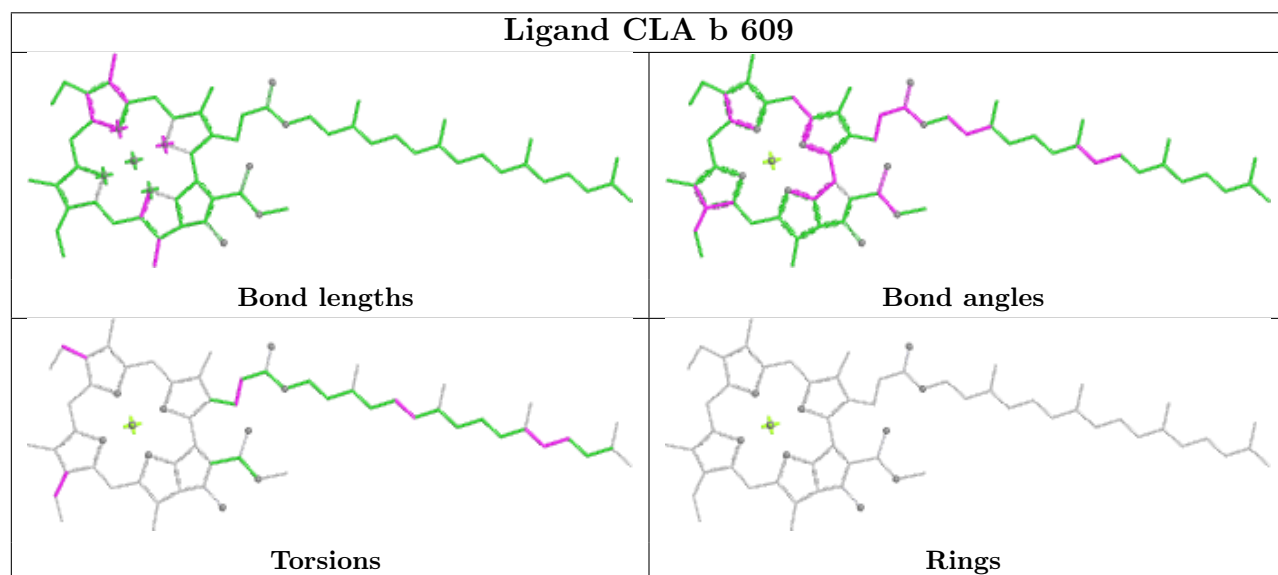
Ligand CLA d 401



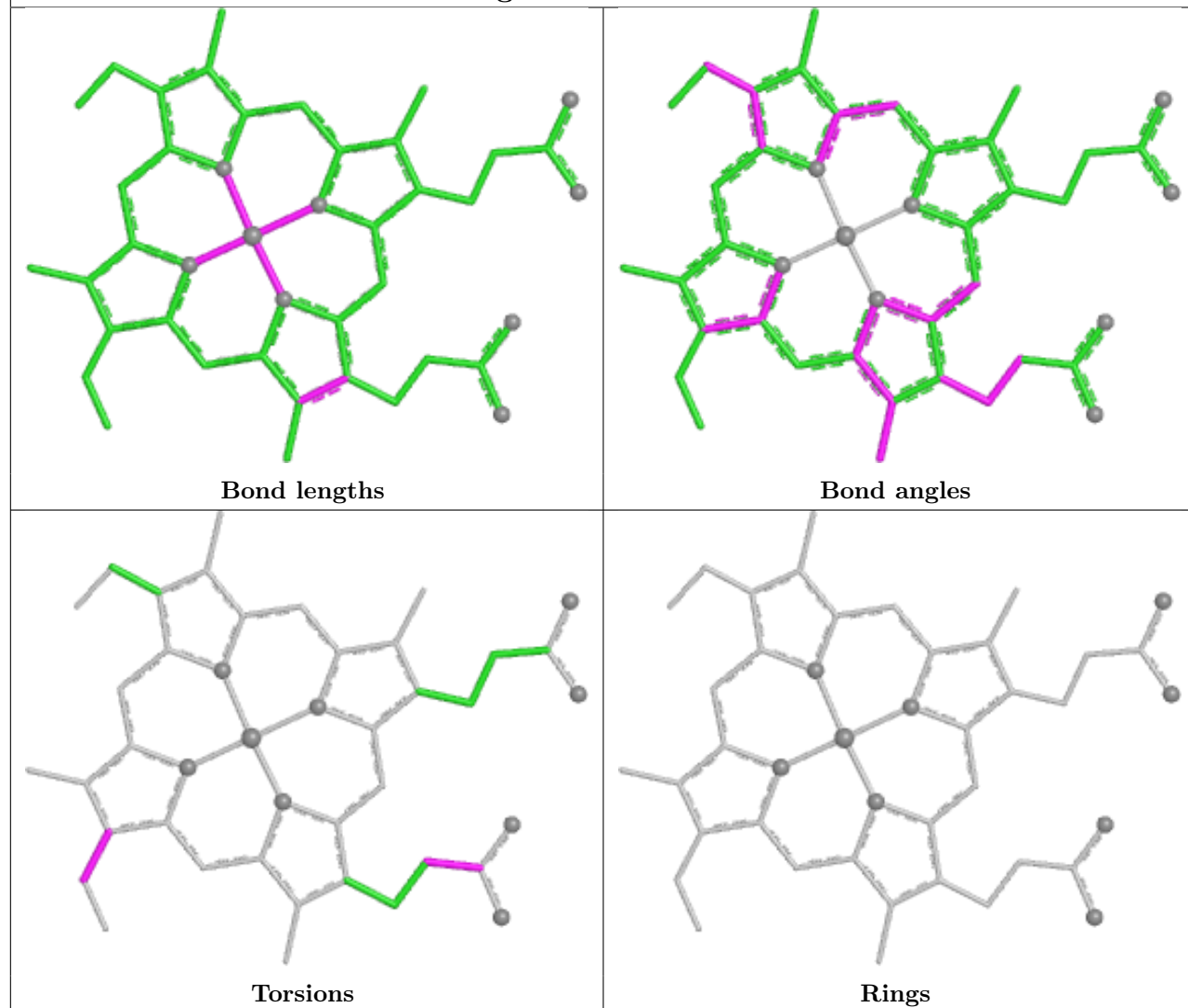
Ligand STE t 102



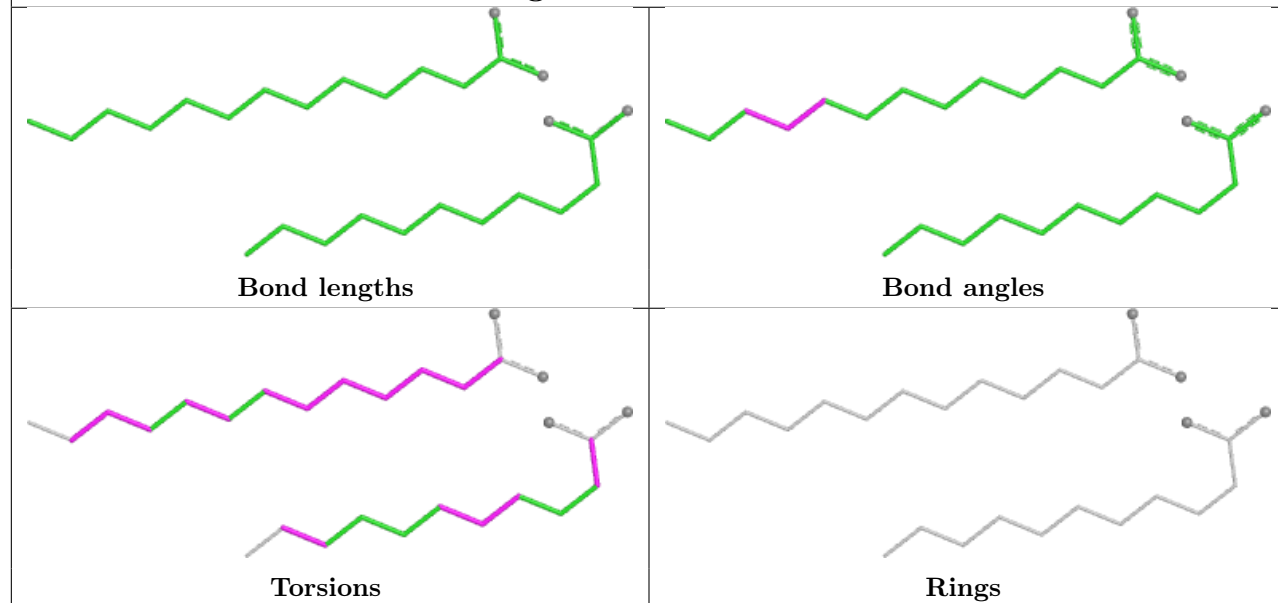
Ligand CLA b 609

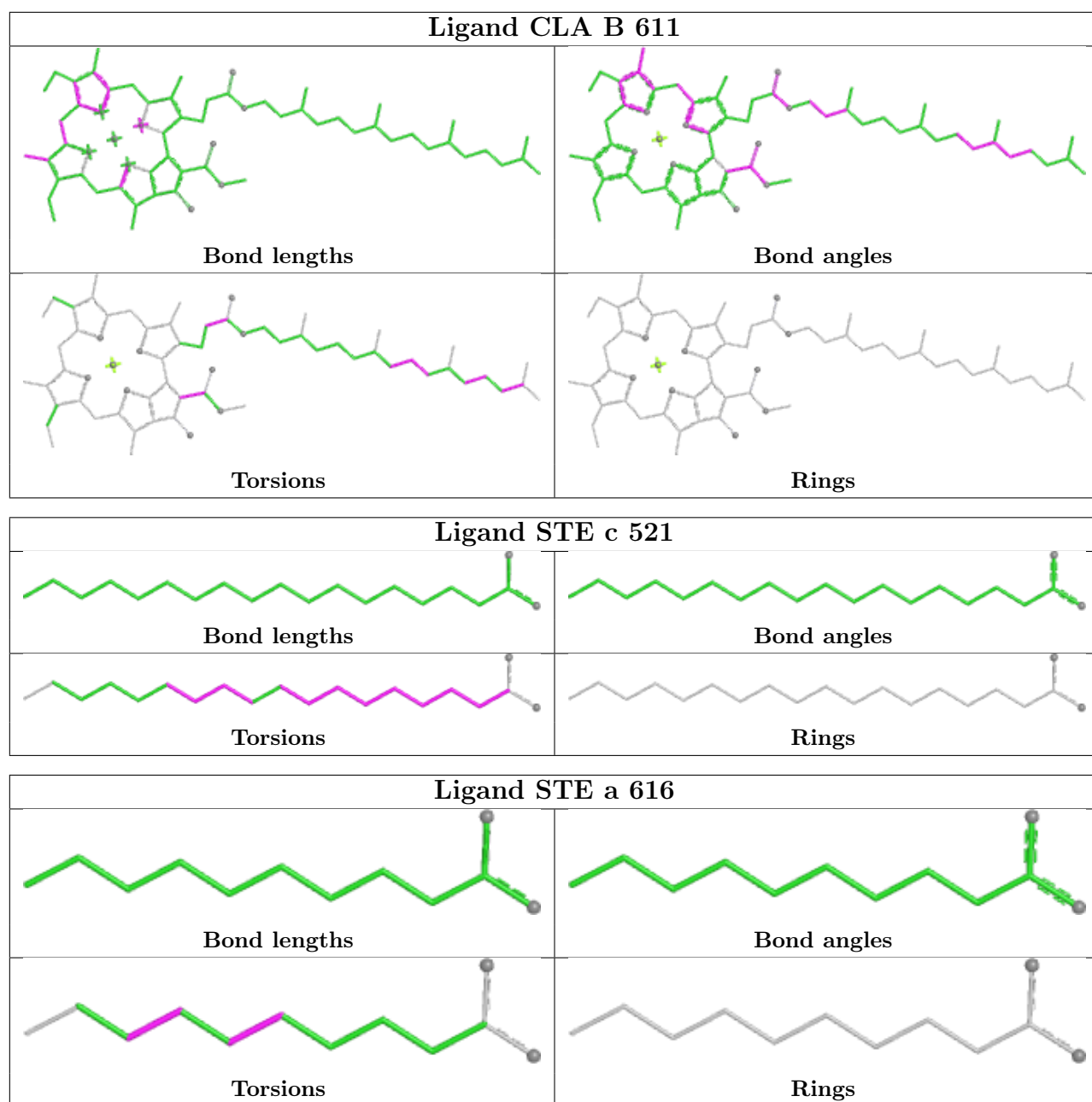


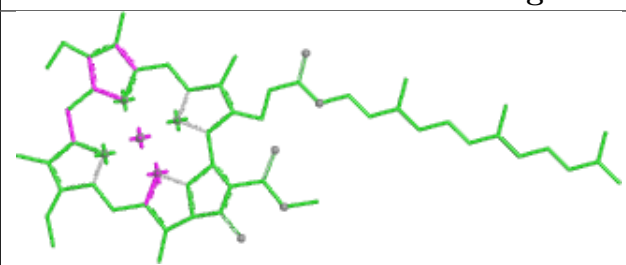
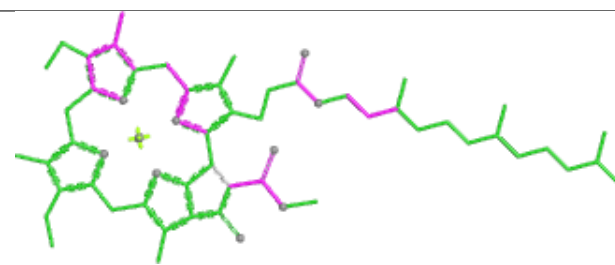
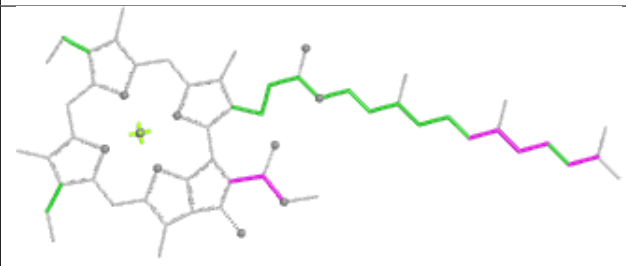
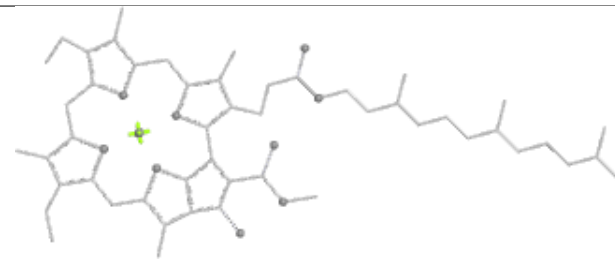
Ligand HEC v 201

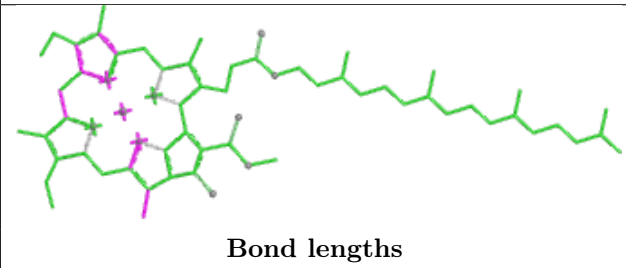
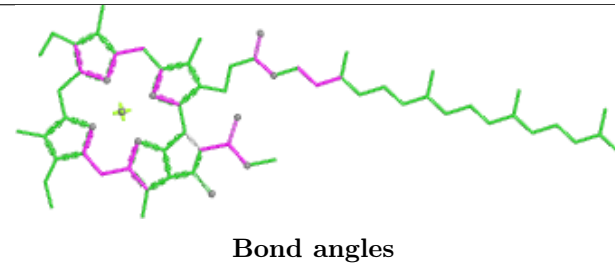
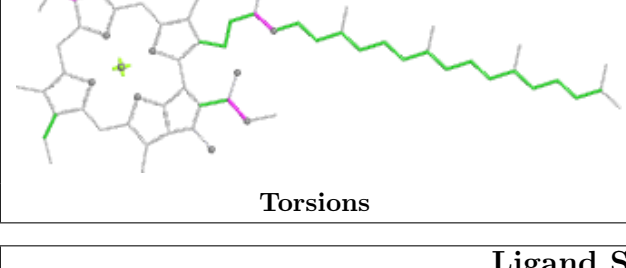
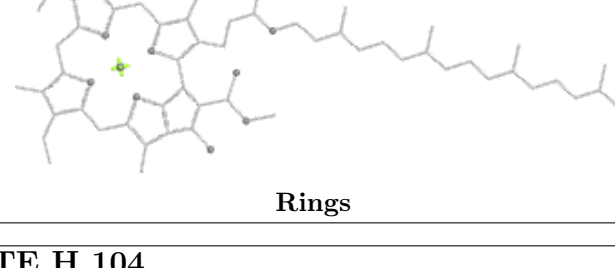


Ligand LMG D 412

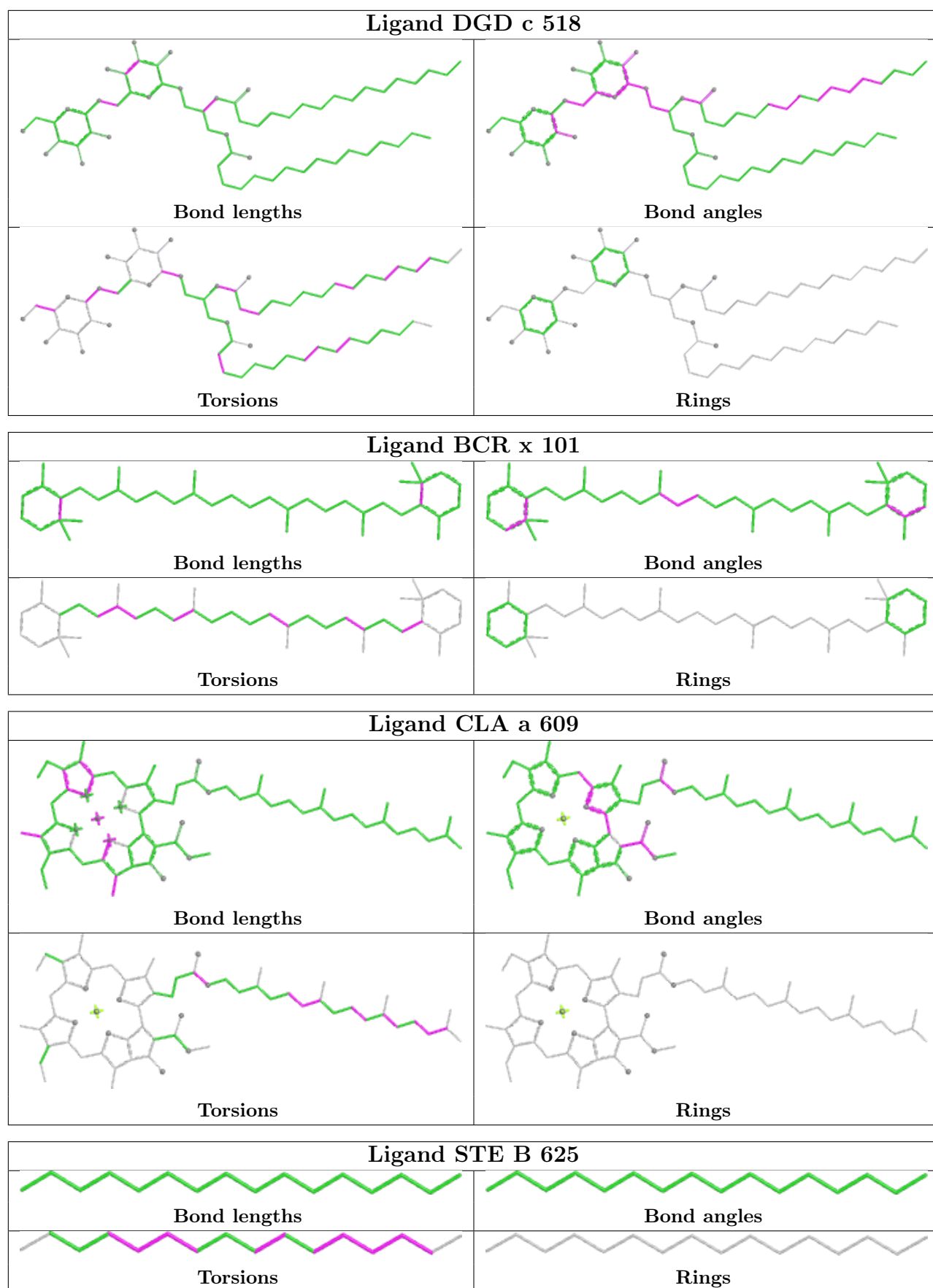


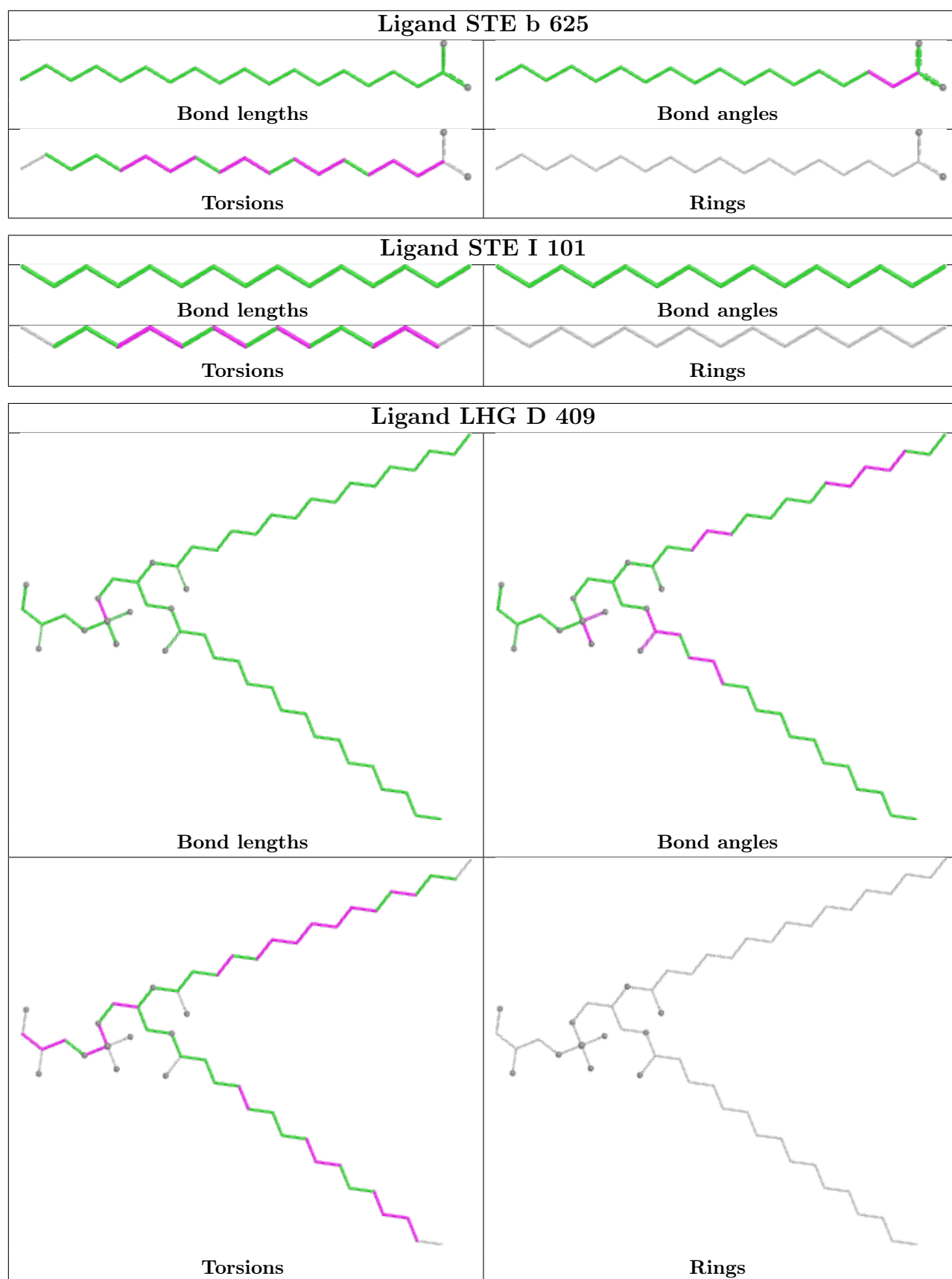


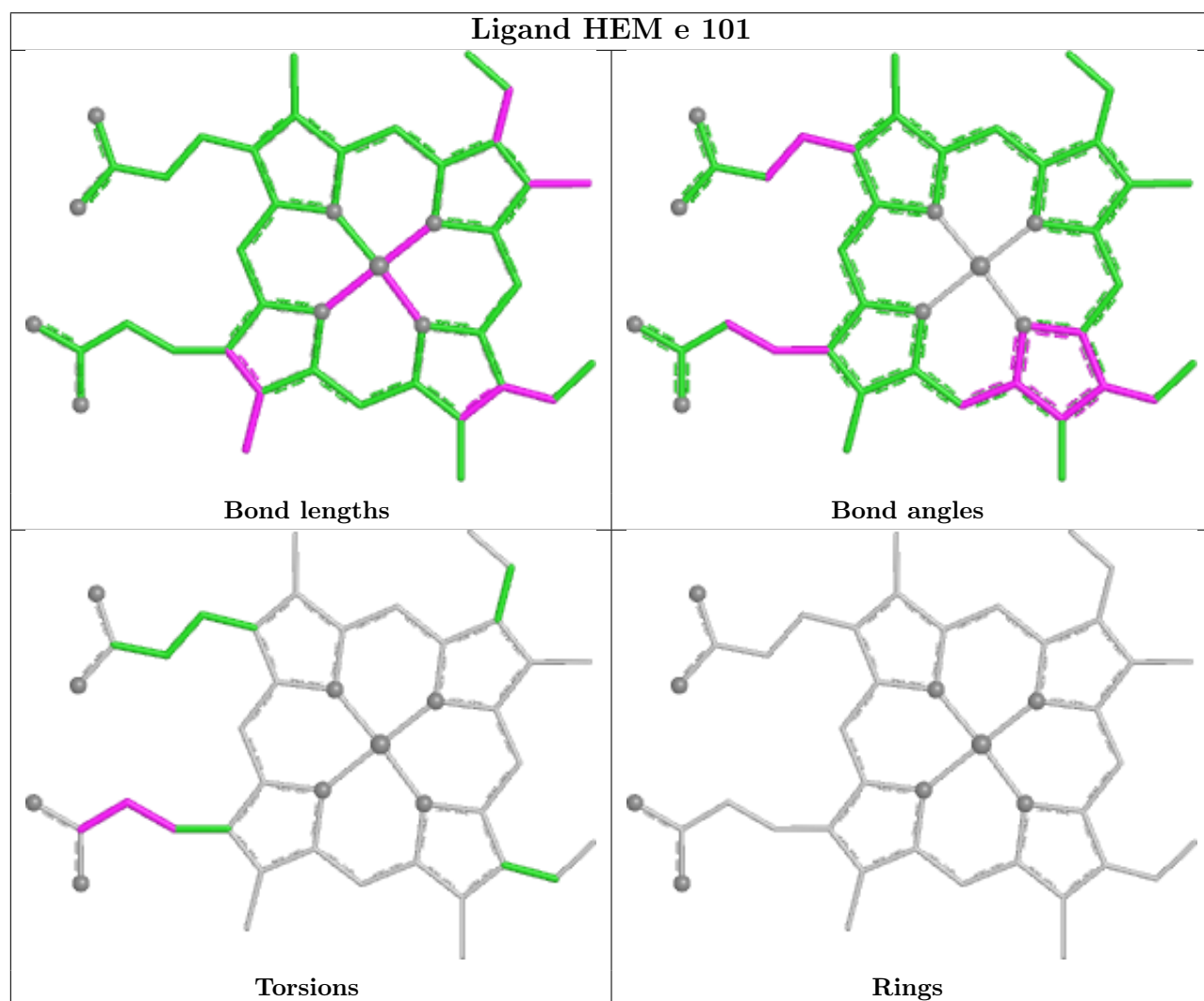
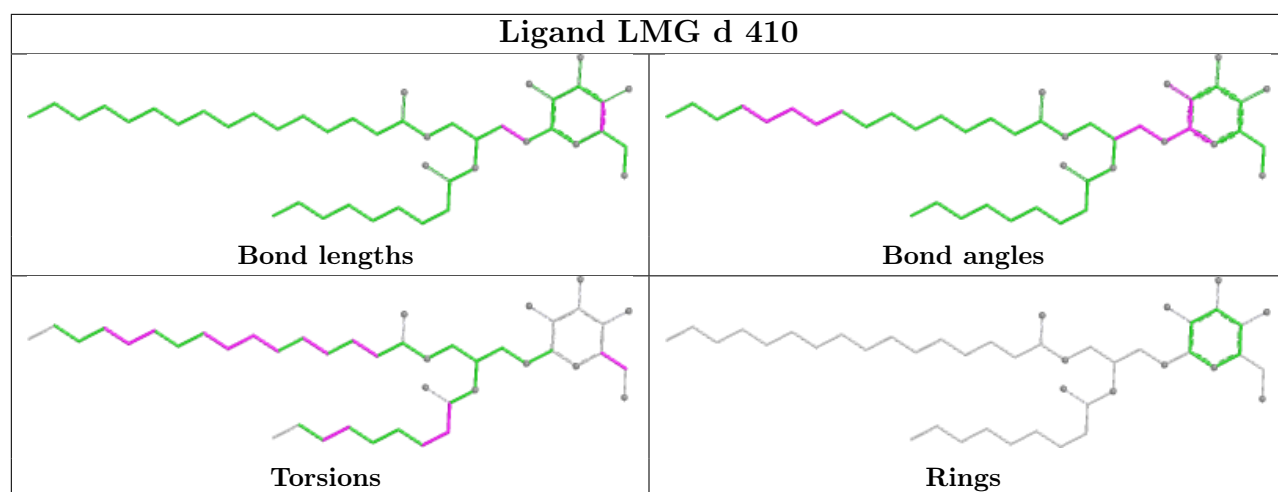
Ligand CLA c 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

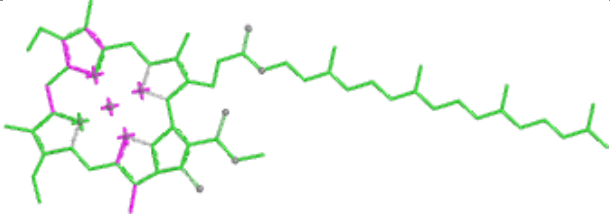
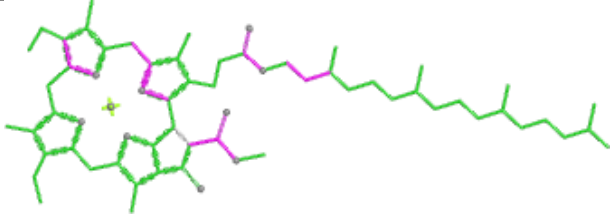
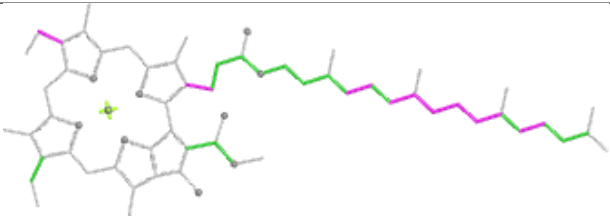
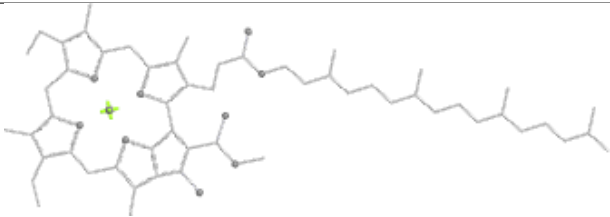
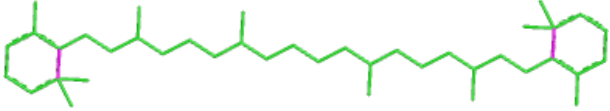
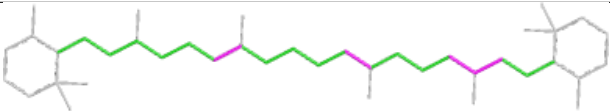
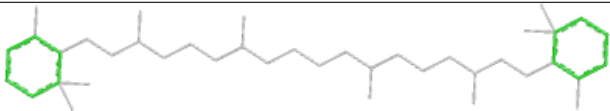
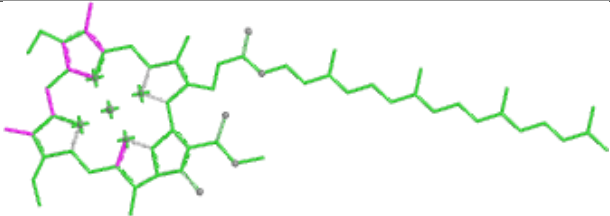
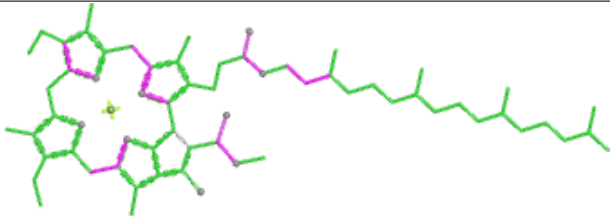
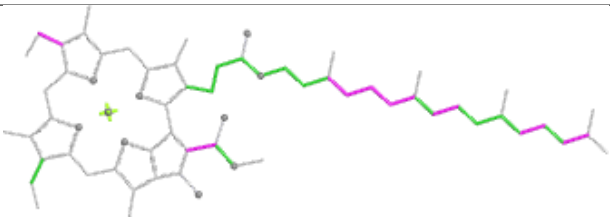
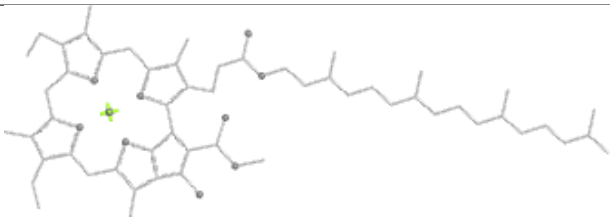
Ligand CLA c 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

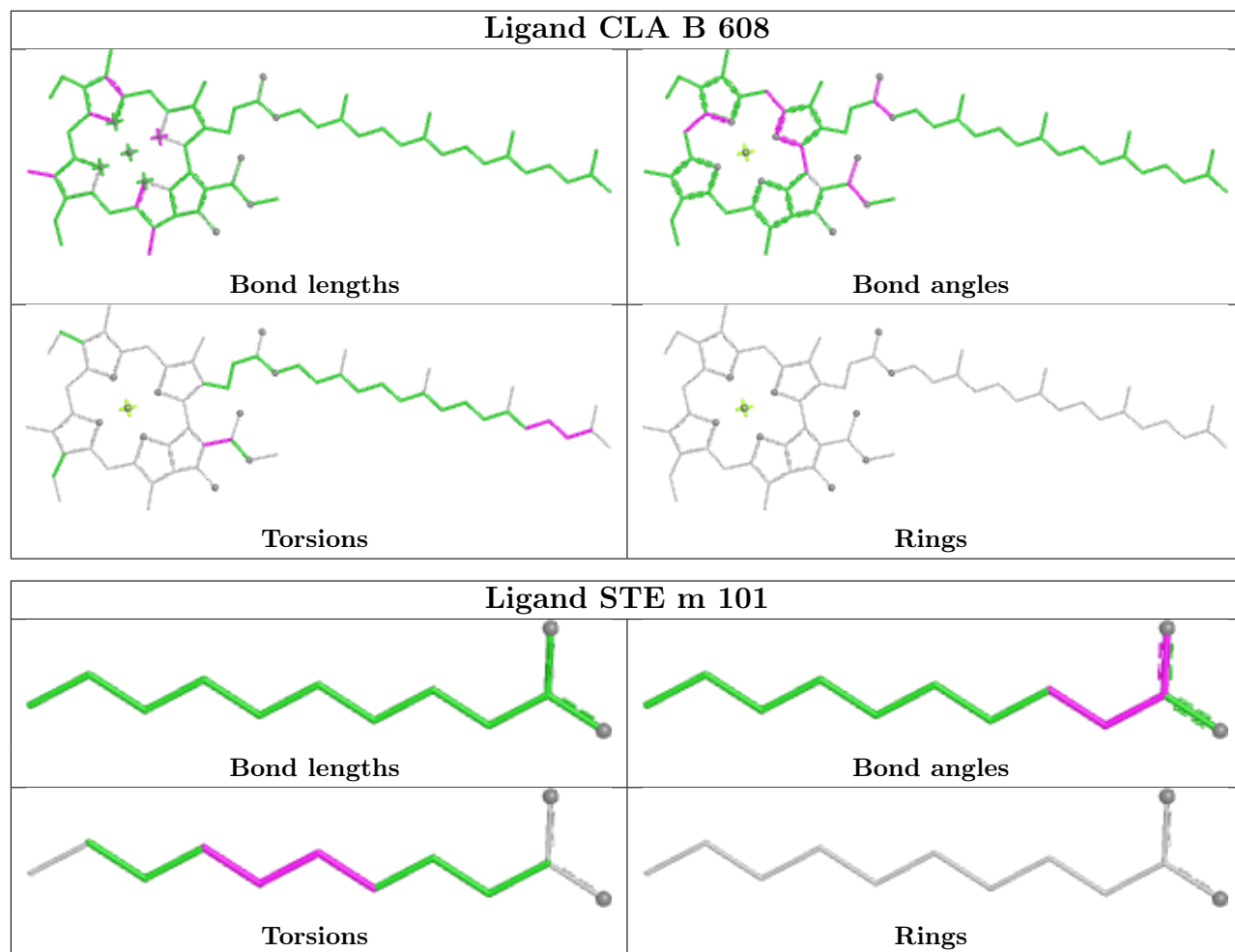
Ligand STE H 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

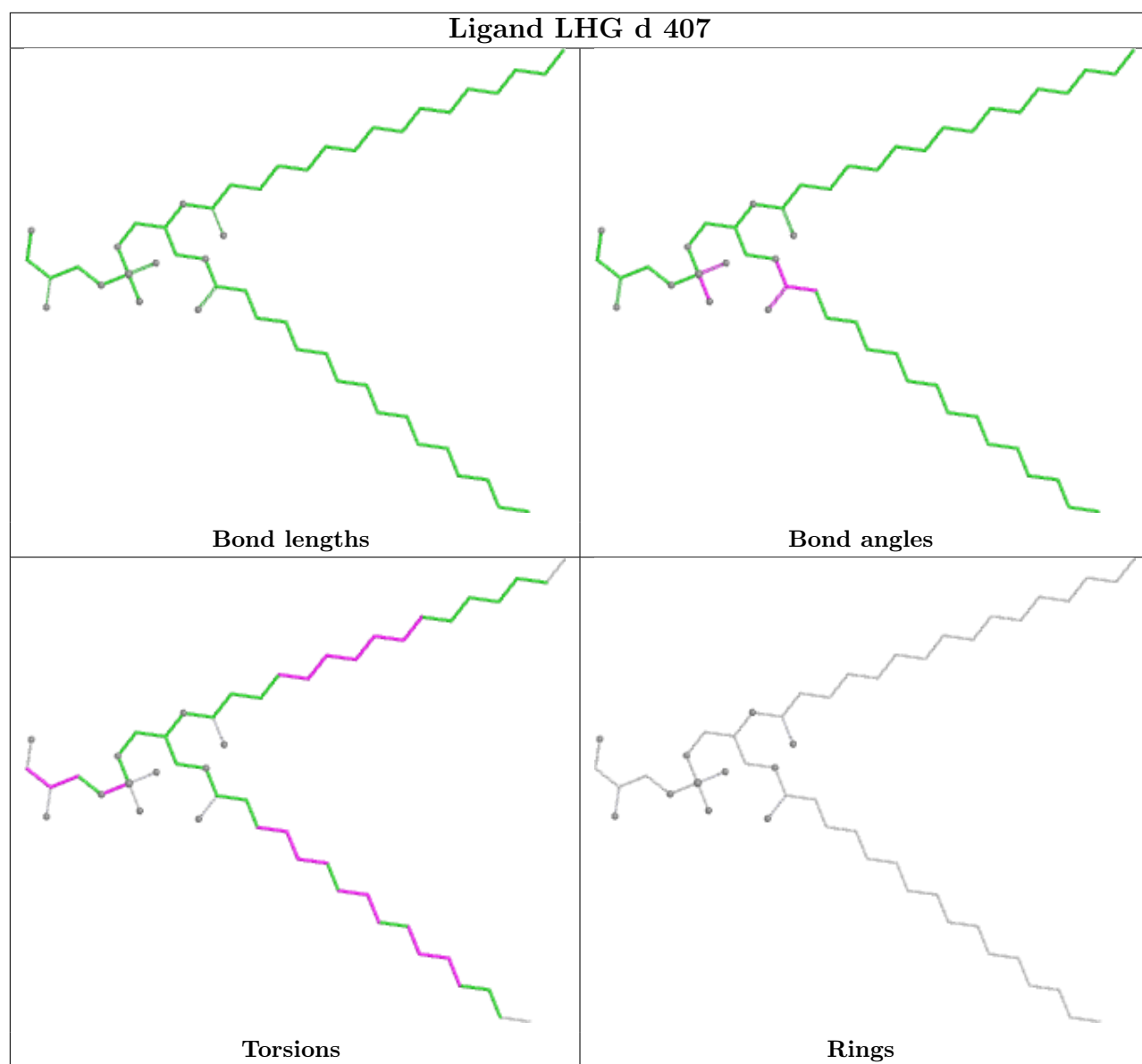


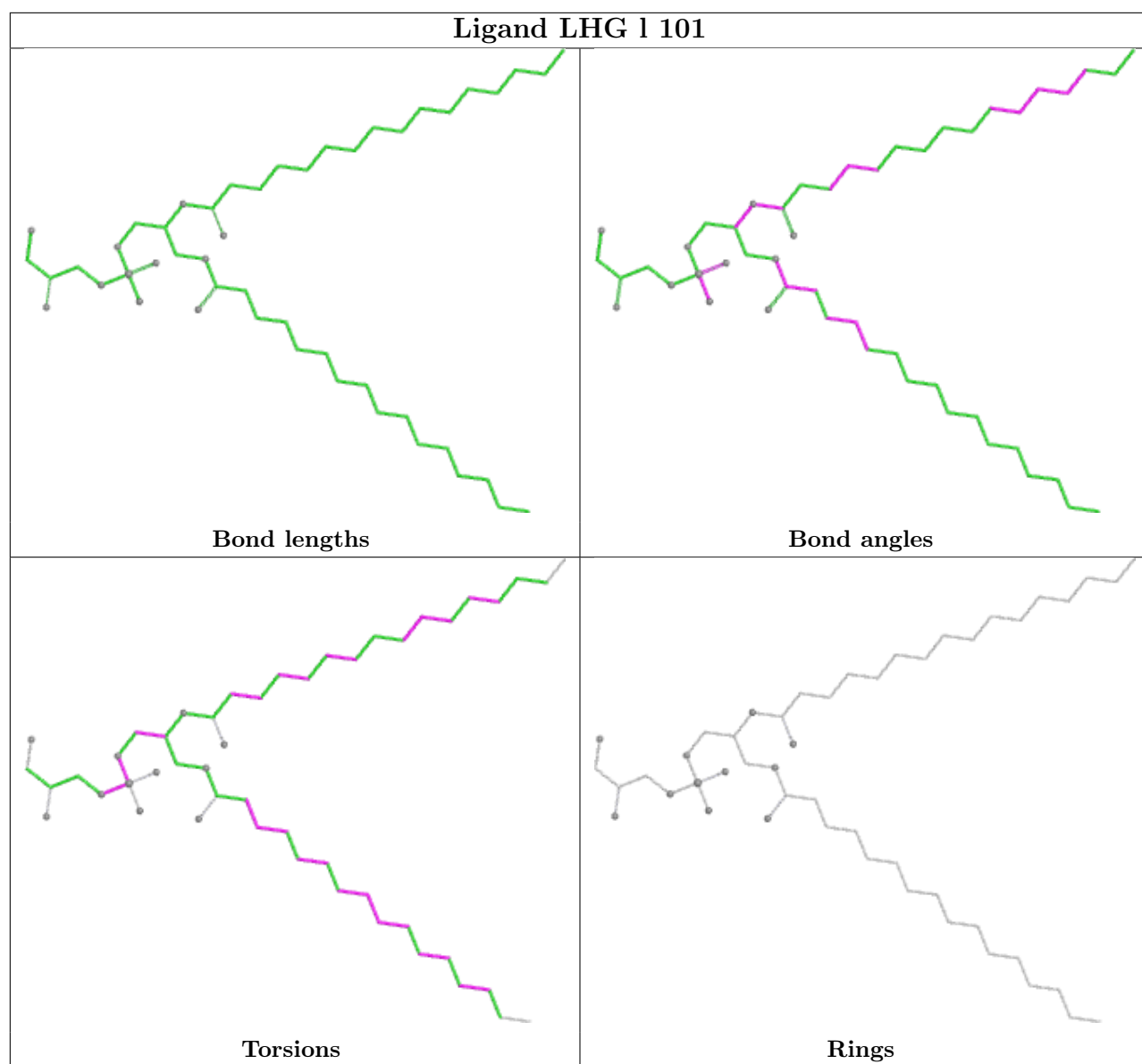


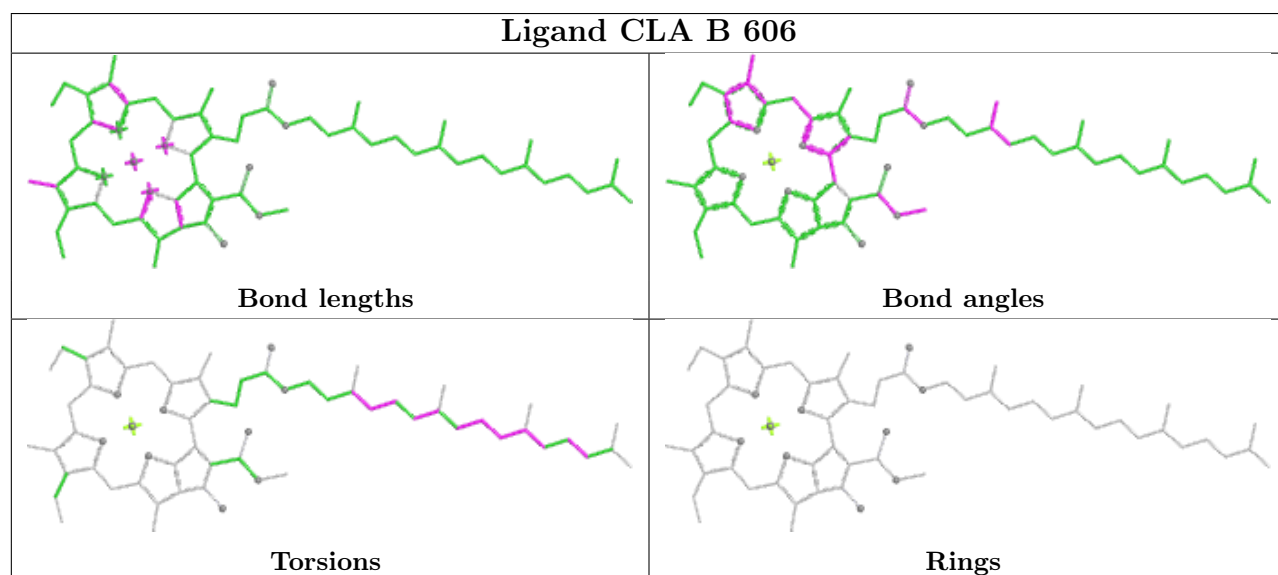
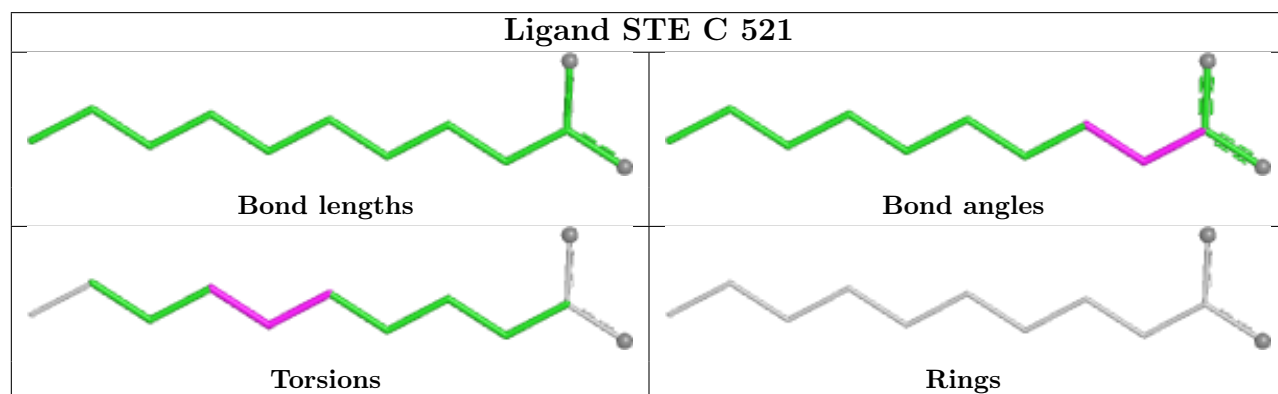
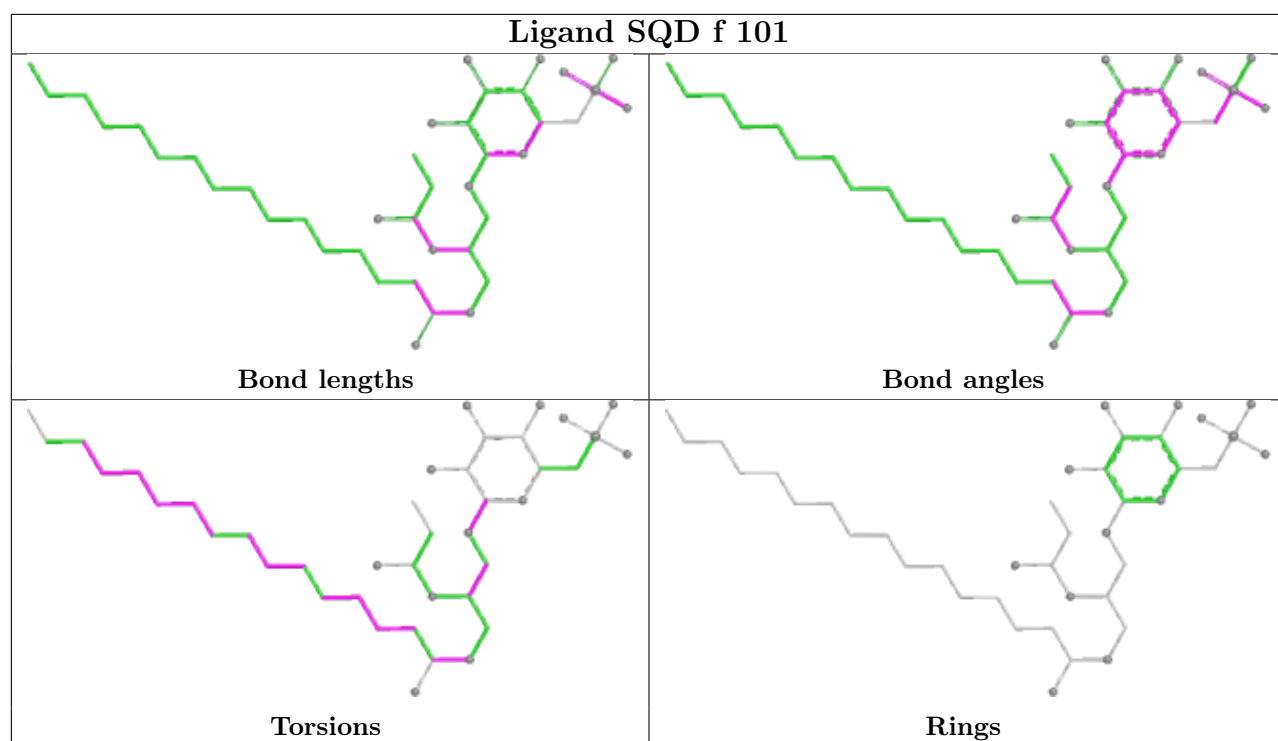


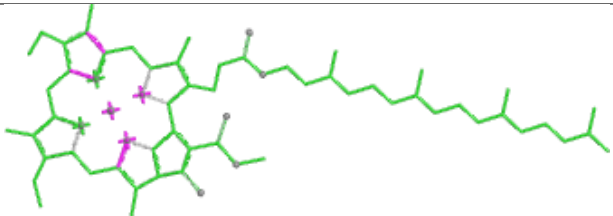
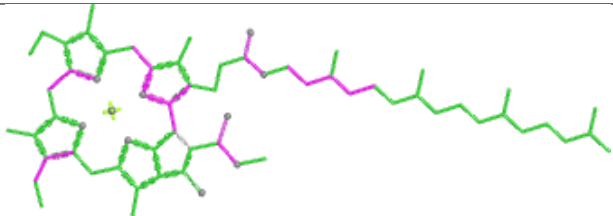
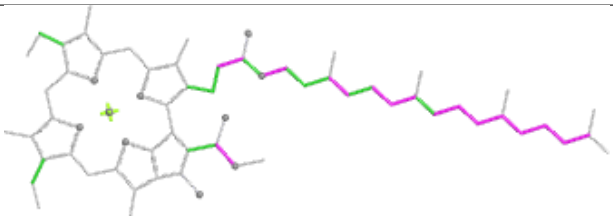
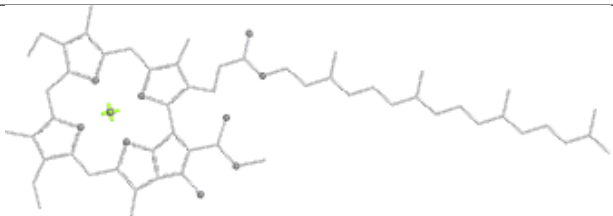
Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

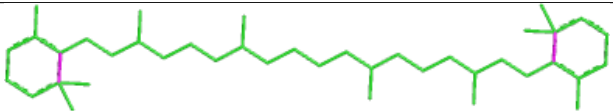
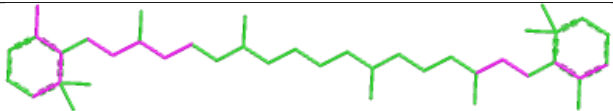
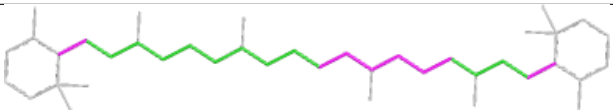
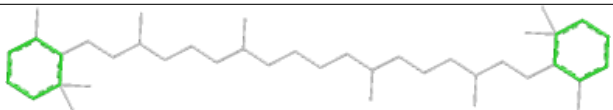


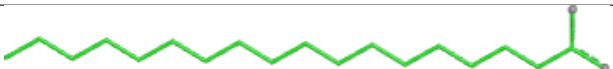
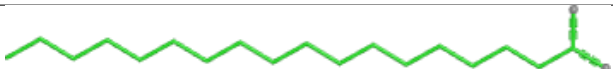
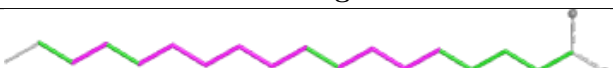
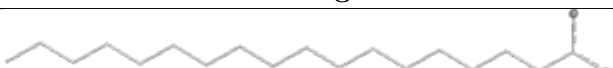




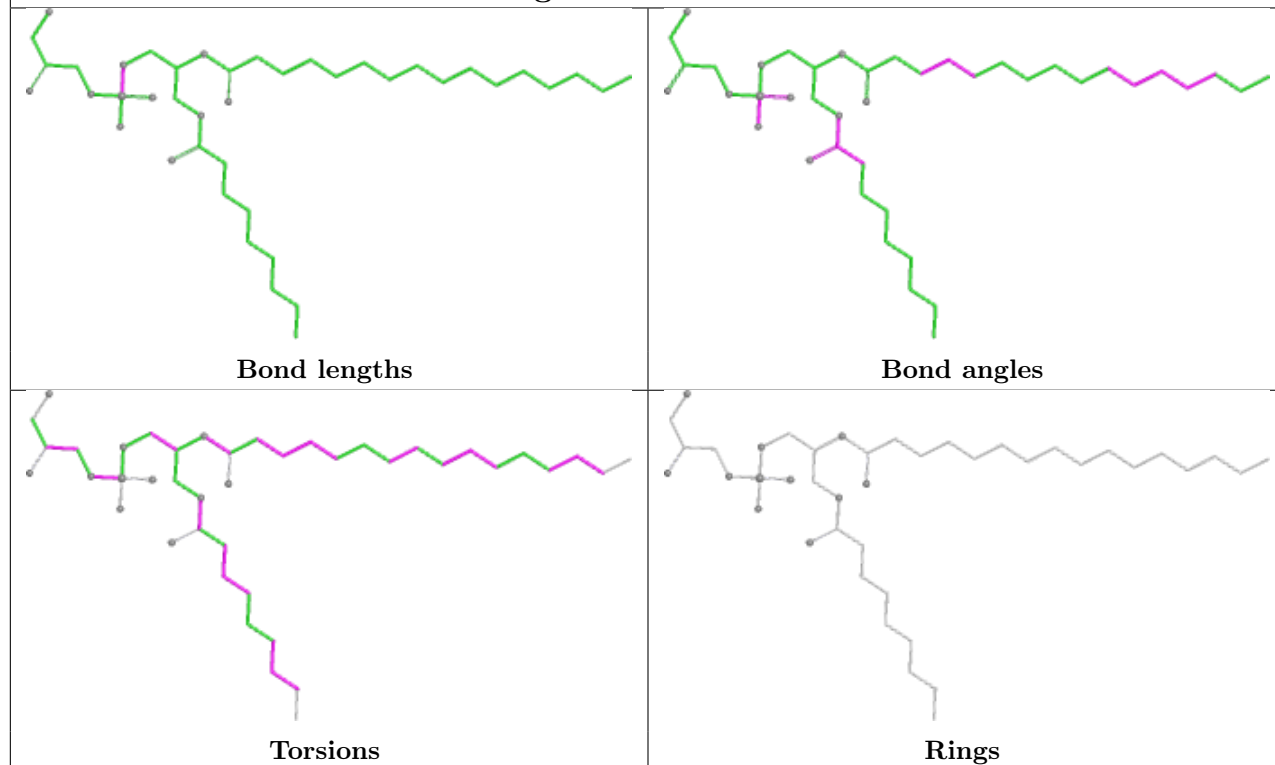


Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

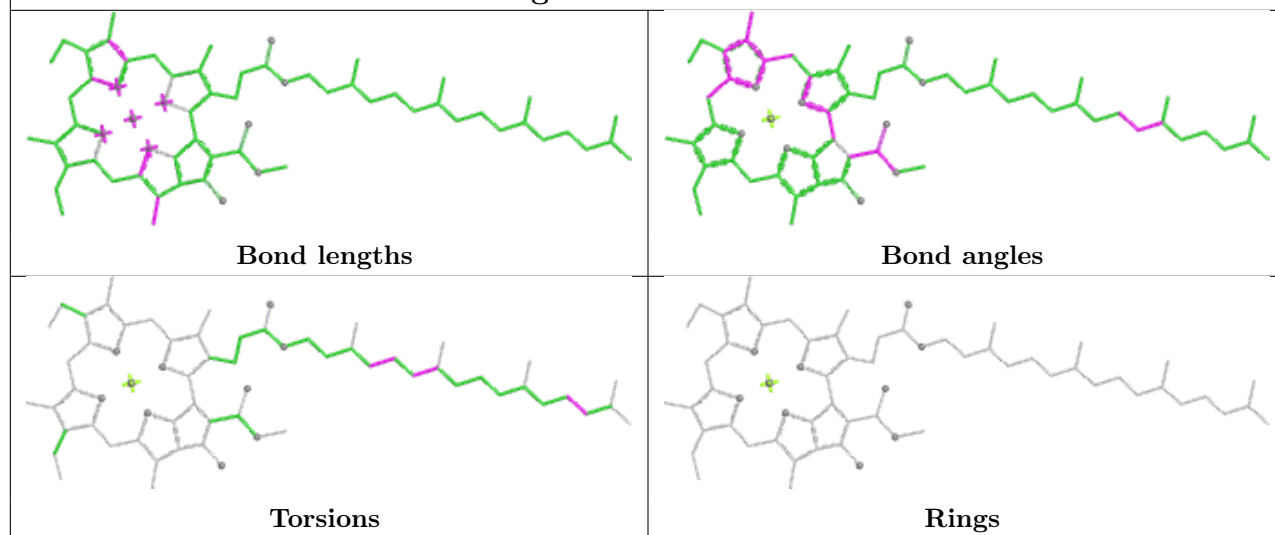
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

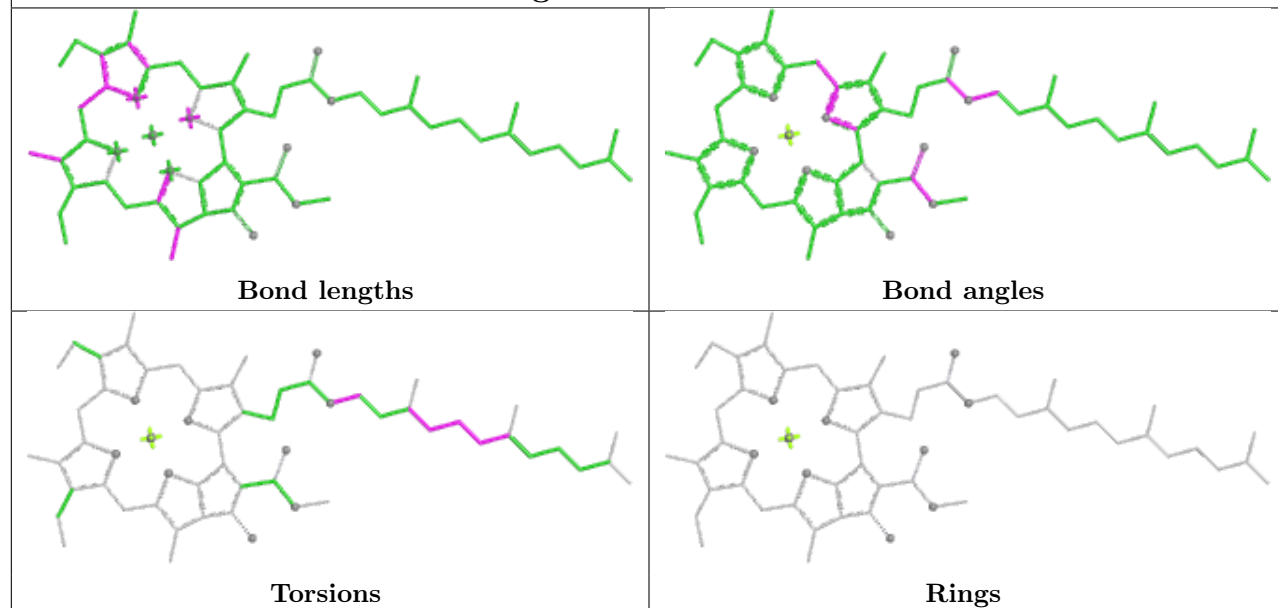
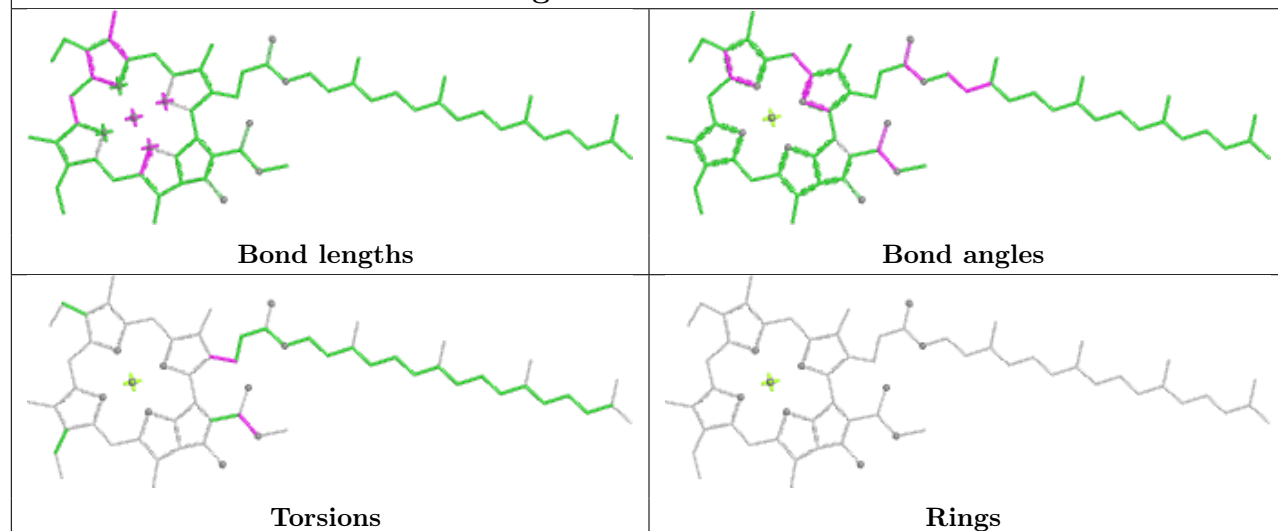
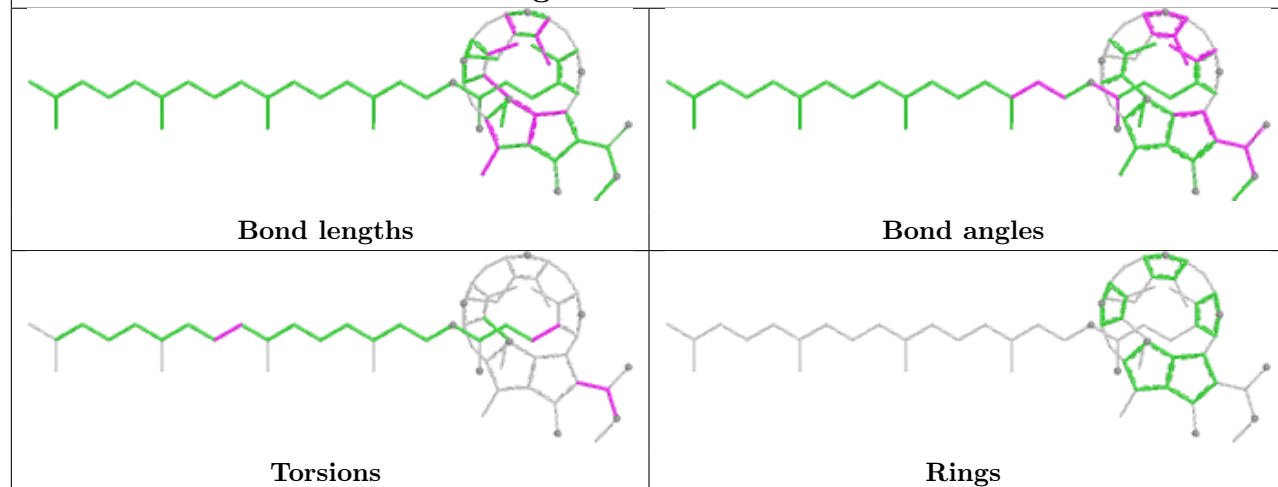
Ligand STE D 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG e 102

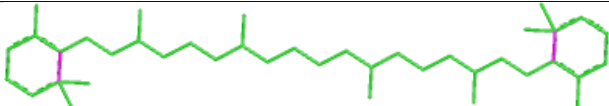
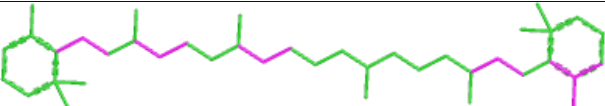
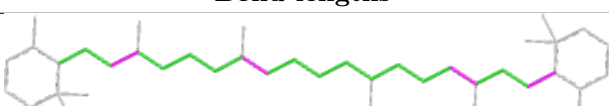
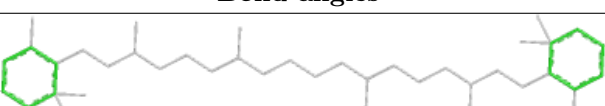


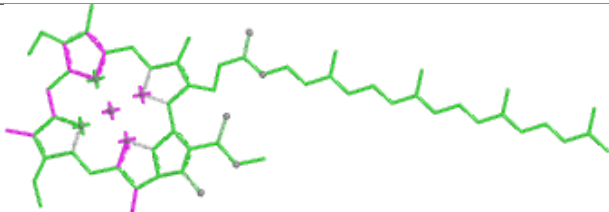
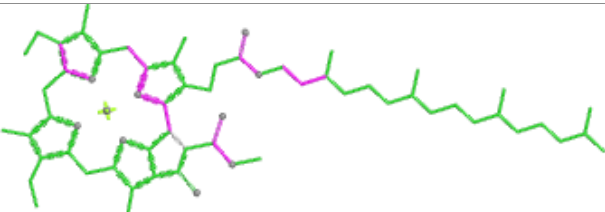
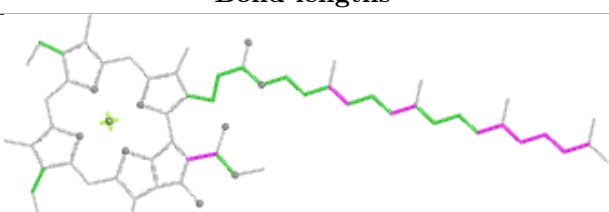
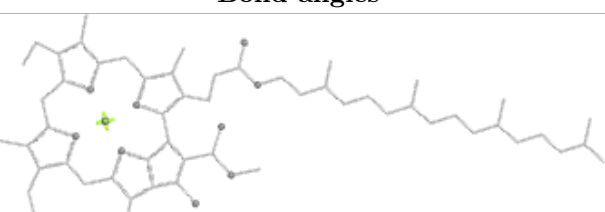
Ligand CLA B 607

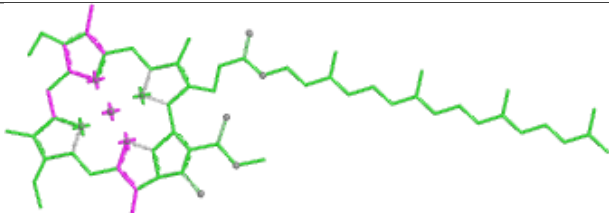
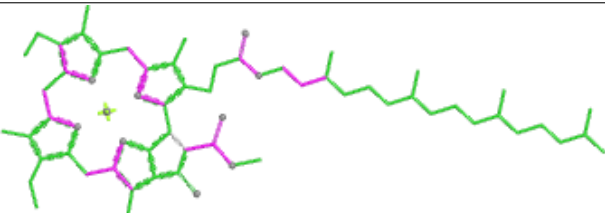
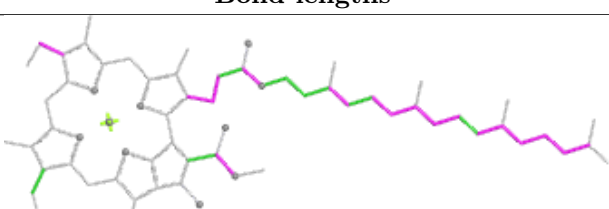
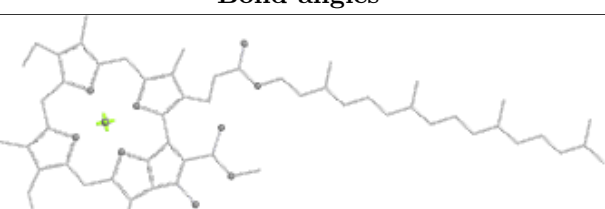


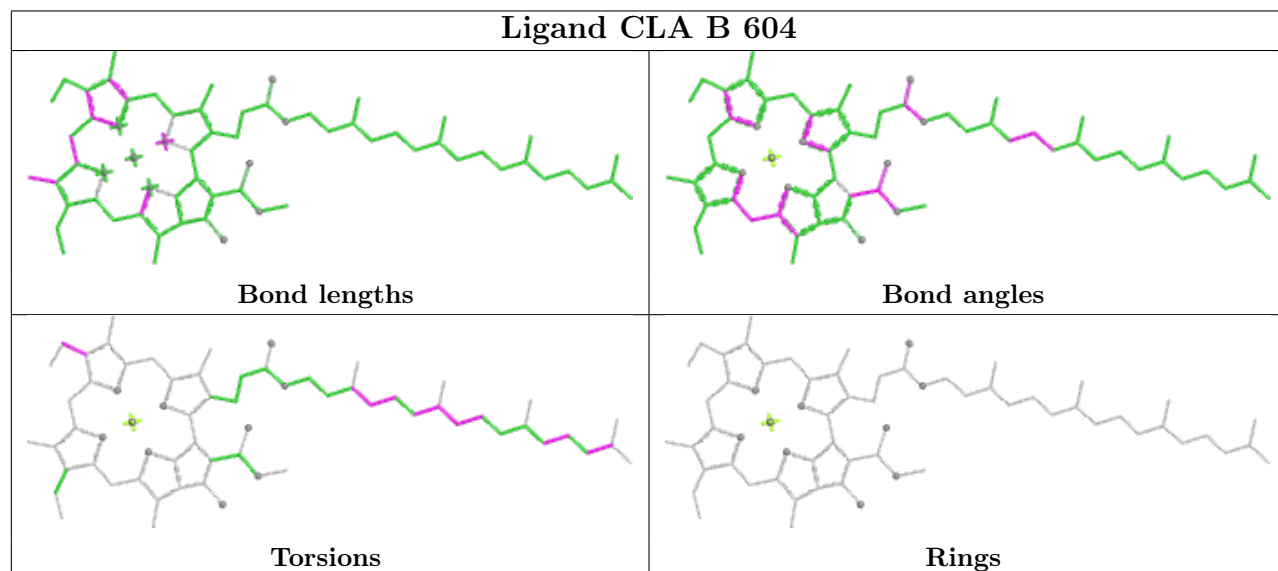
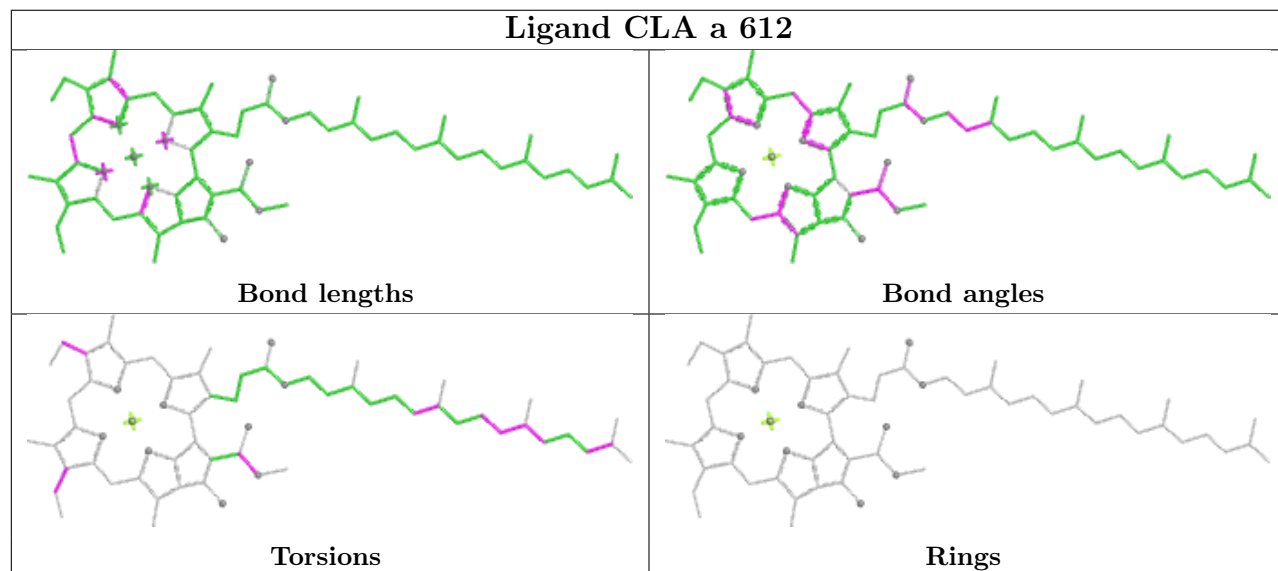
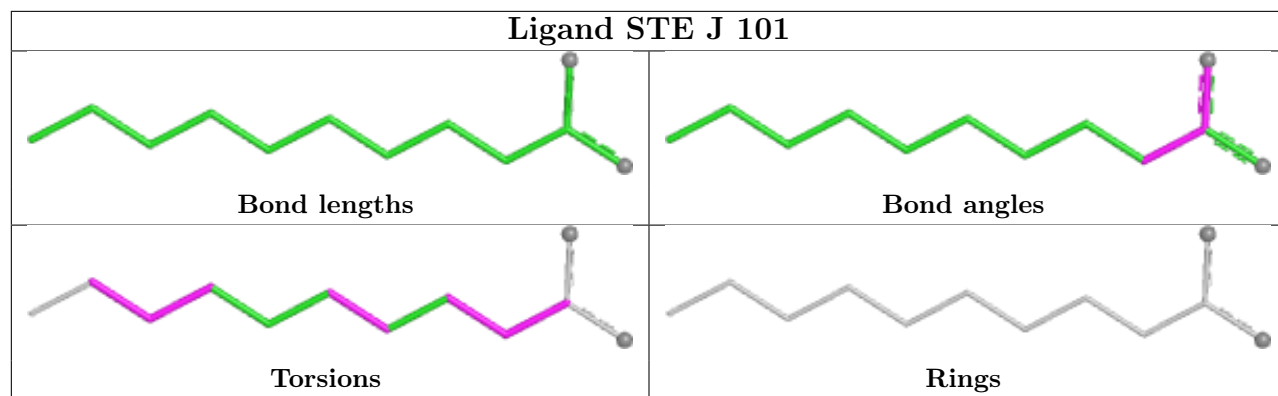
Ligand CLA B 615**Ligand CLA C 511****Ligand PHO d 402**

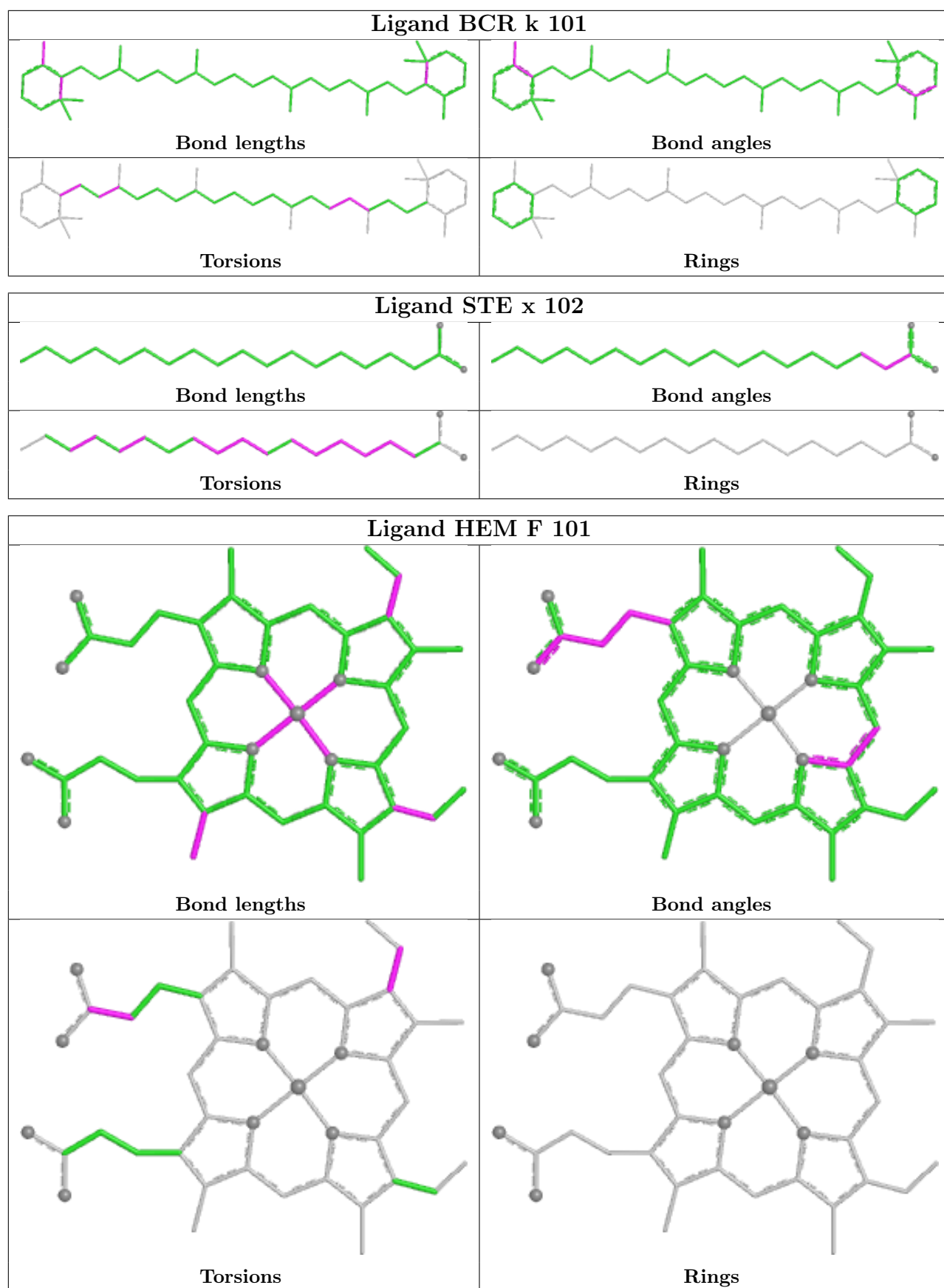
Ligand STE l 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

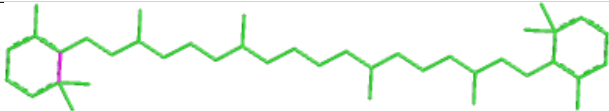
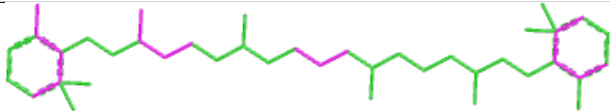
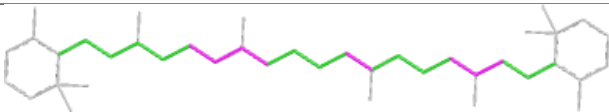
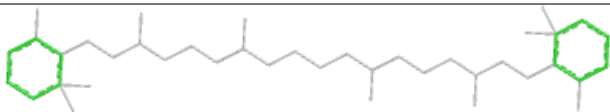
Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

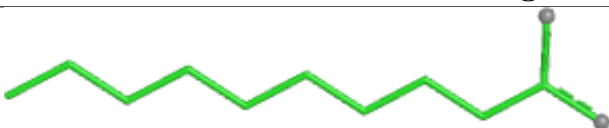
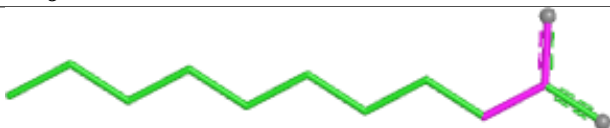
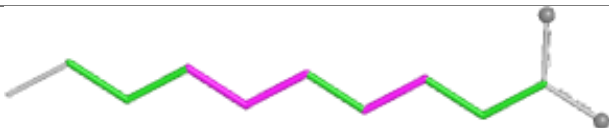
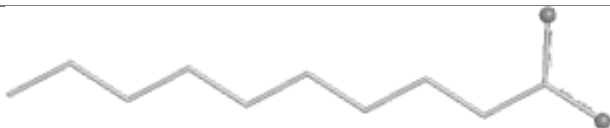
Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings





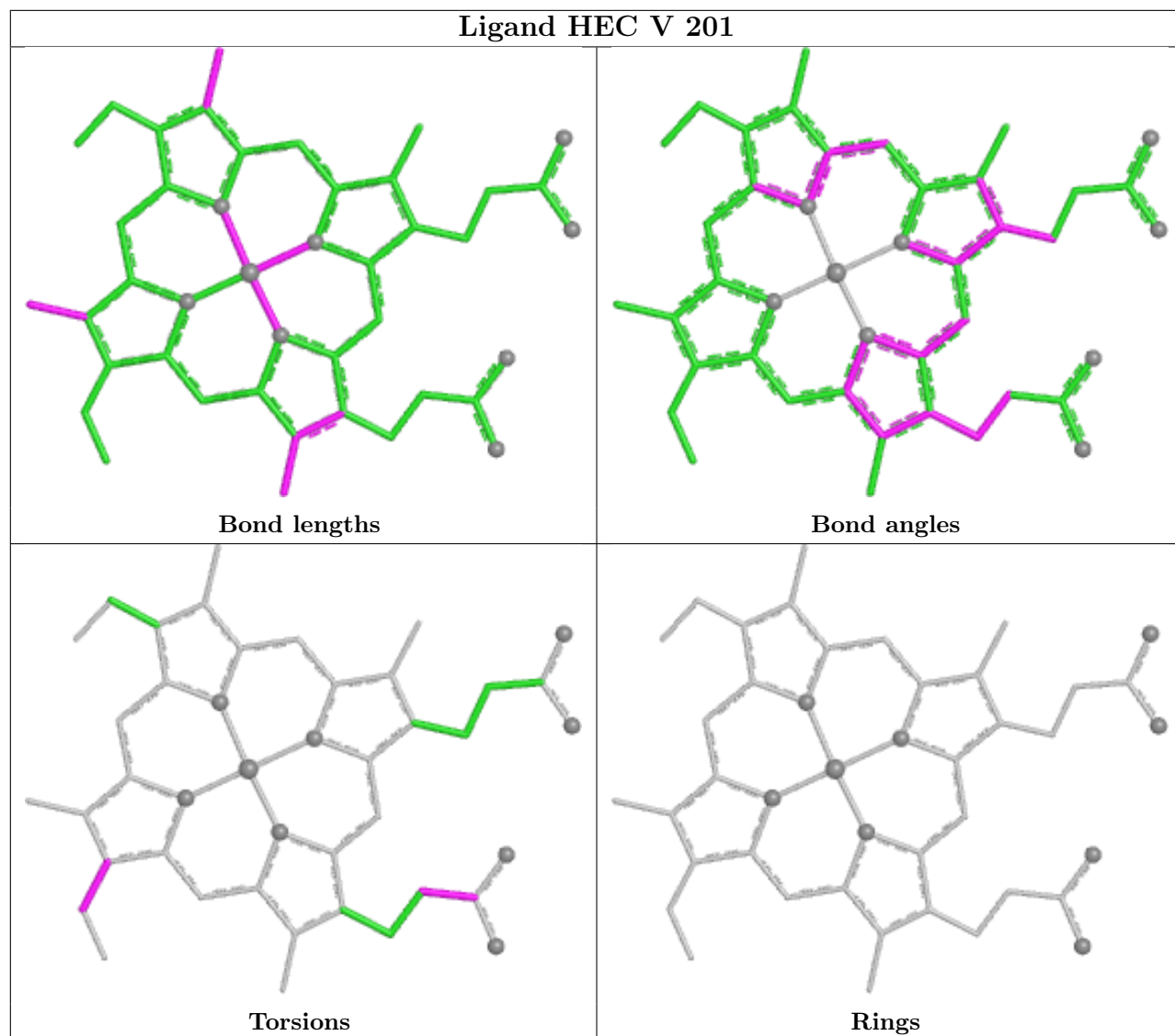
Ligand STE t 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

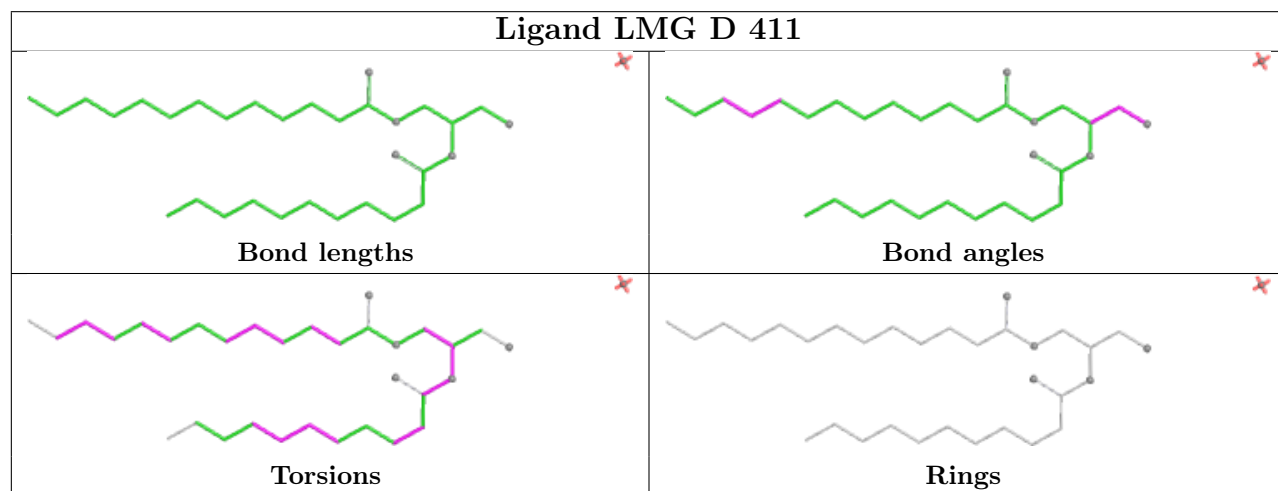
Ligand STE j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

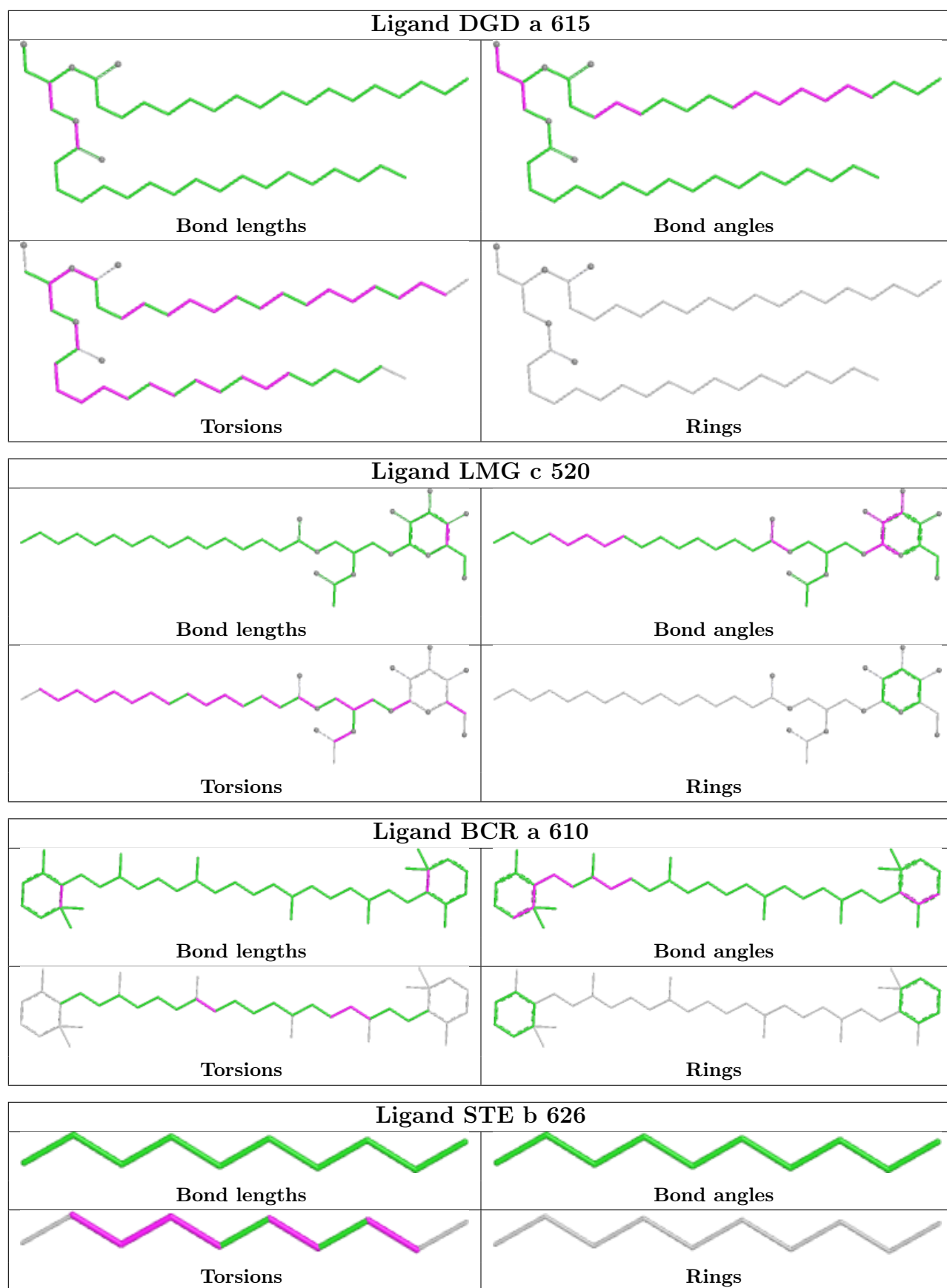
Ligand STE M 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

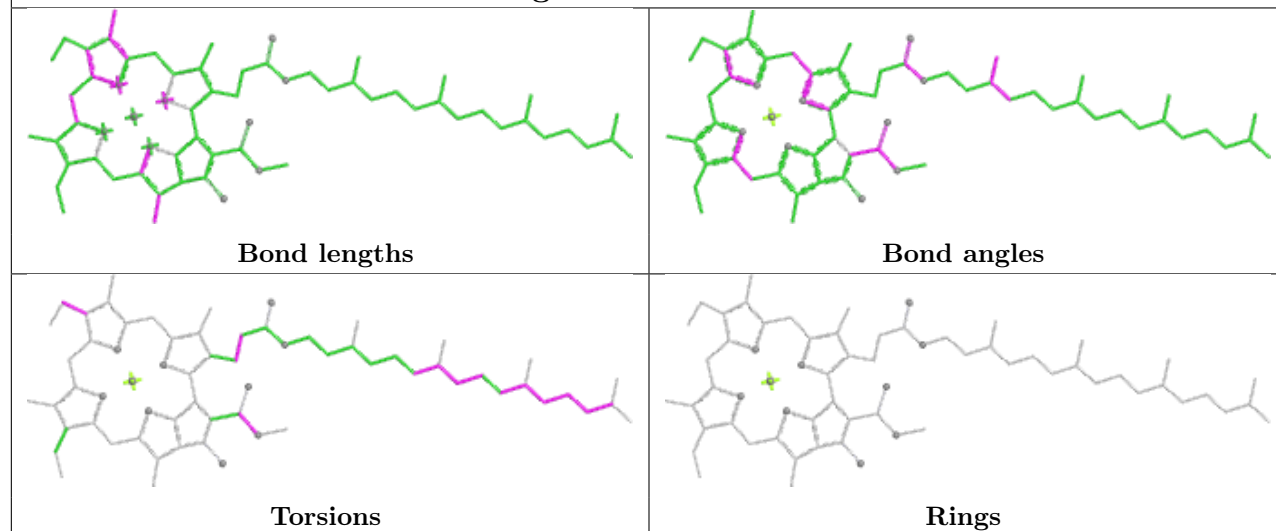
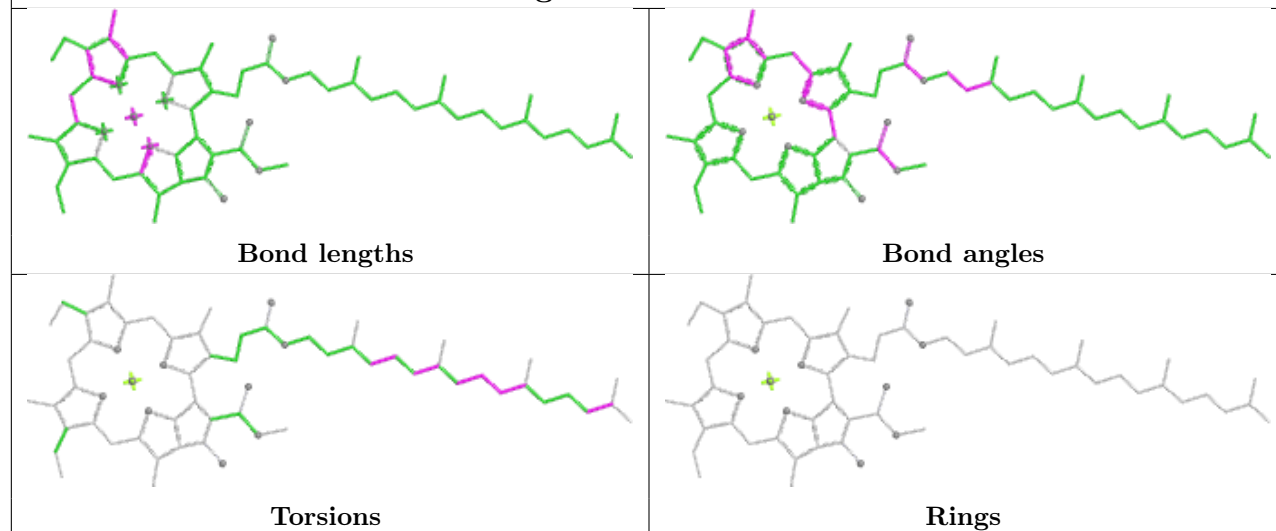
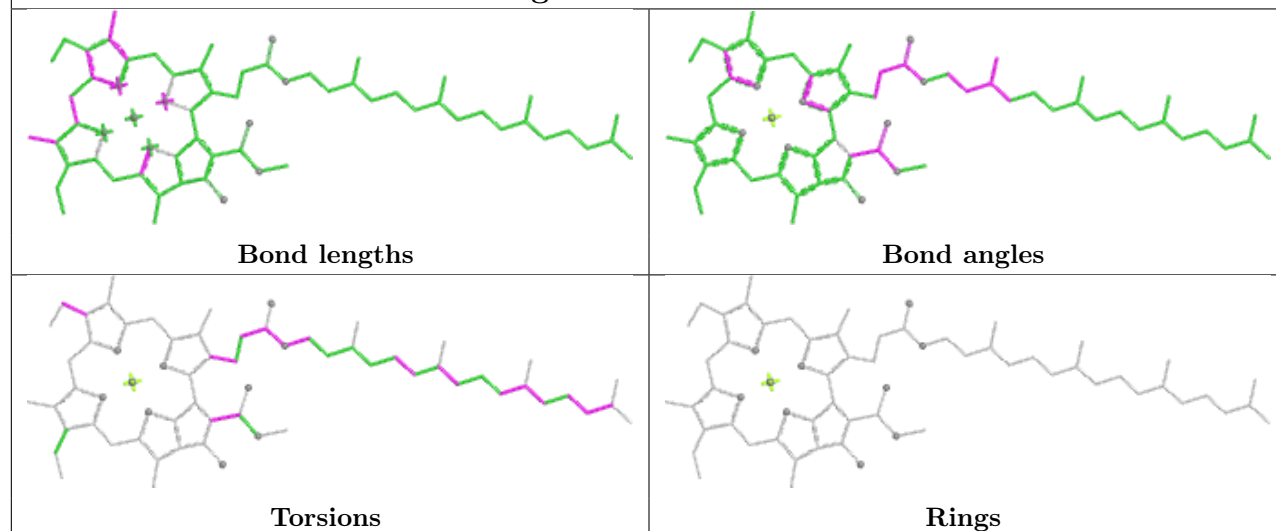
Ligand HEC V 201

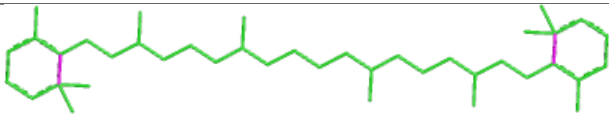
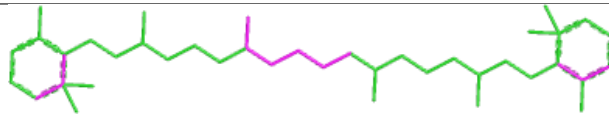
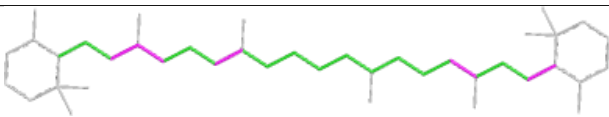
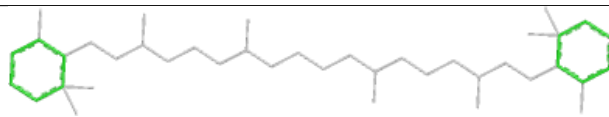


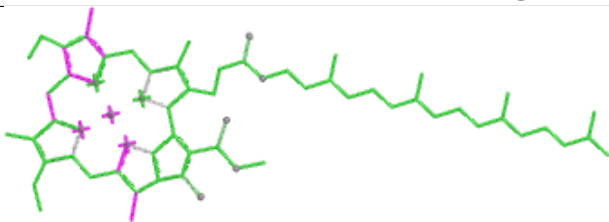
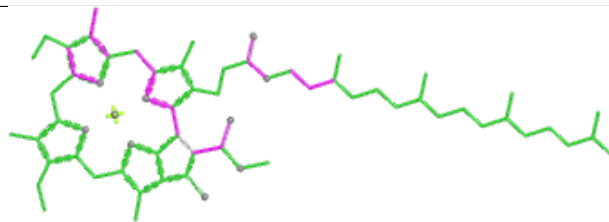
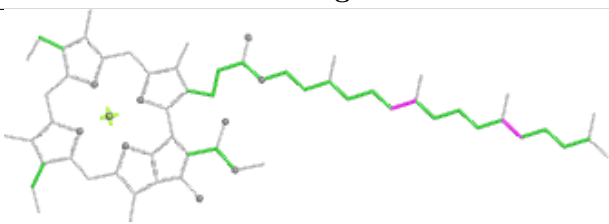
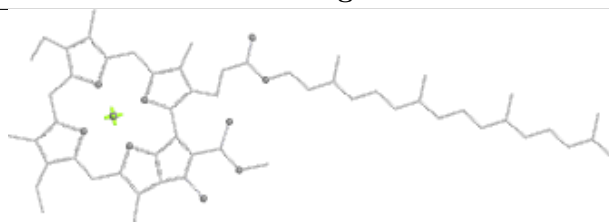
Ligand LMG D 411

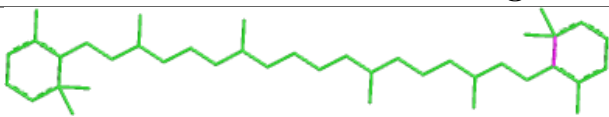
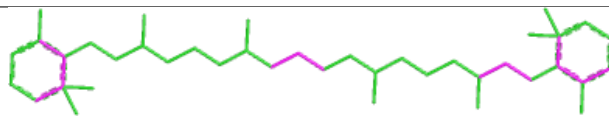
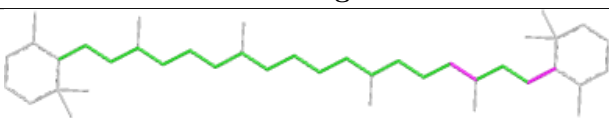
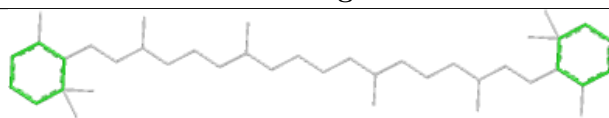


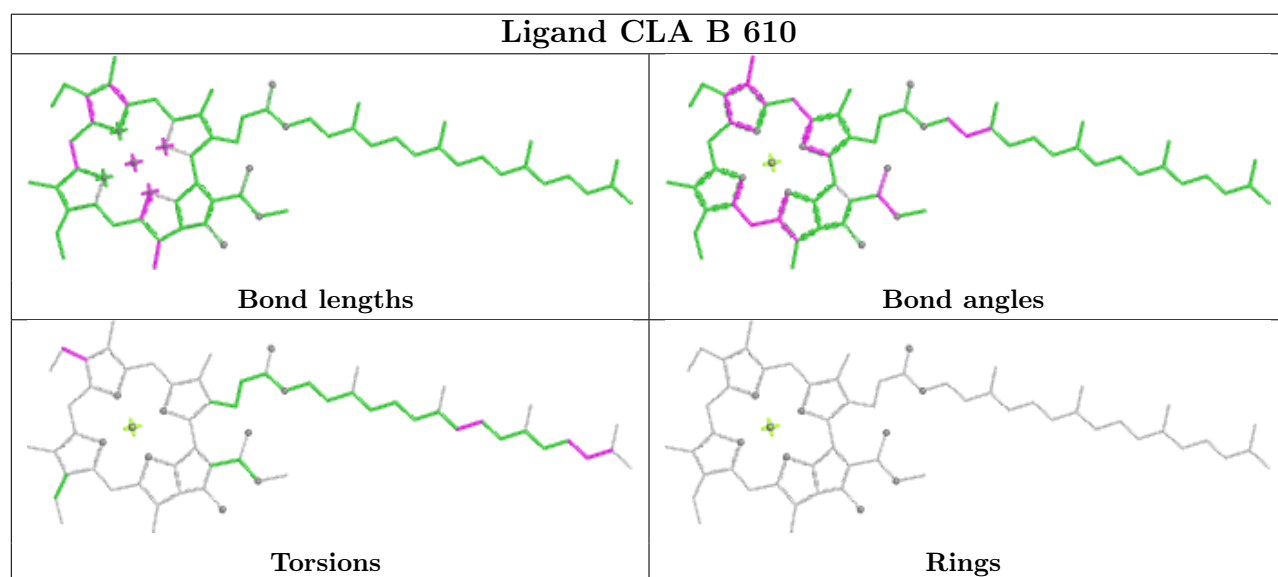
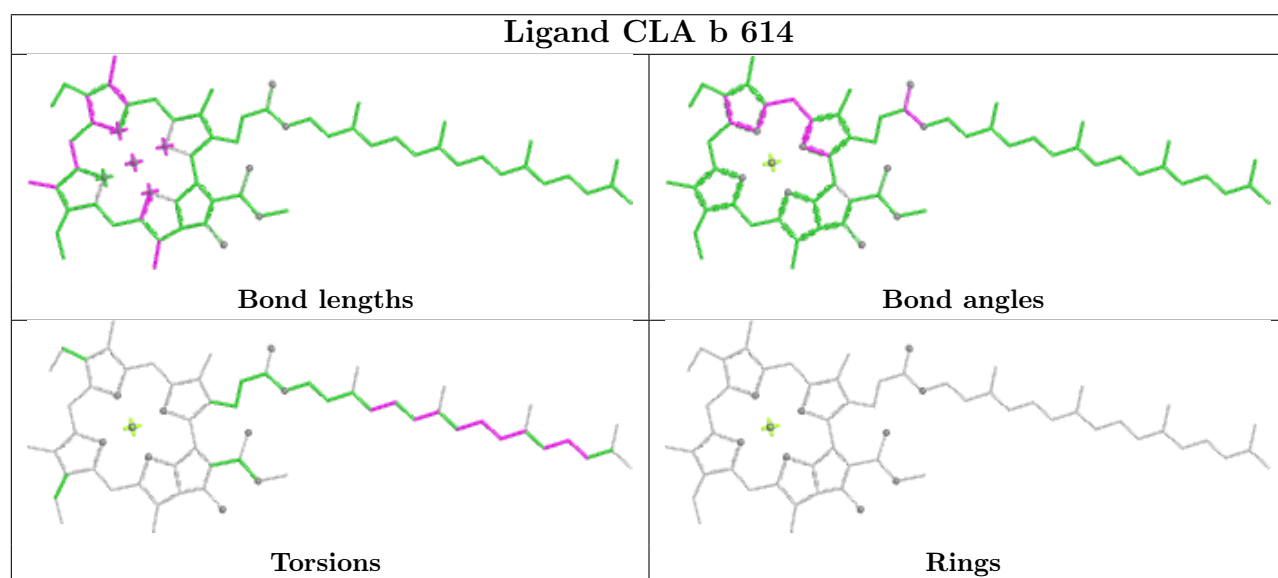
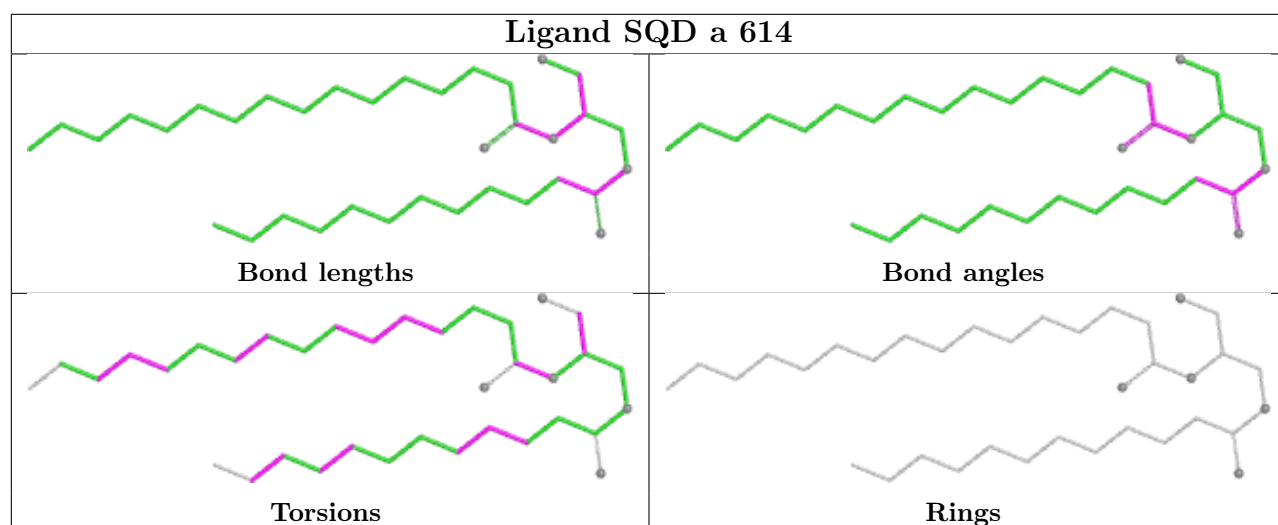


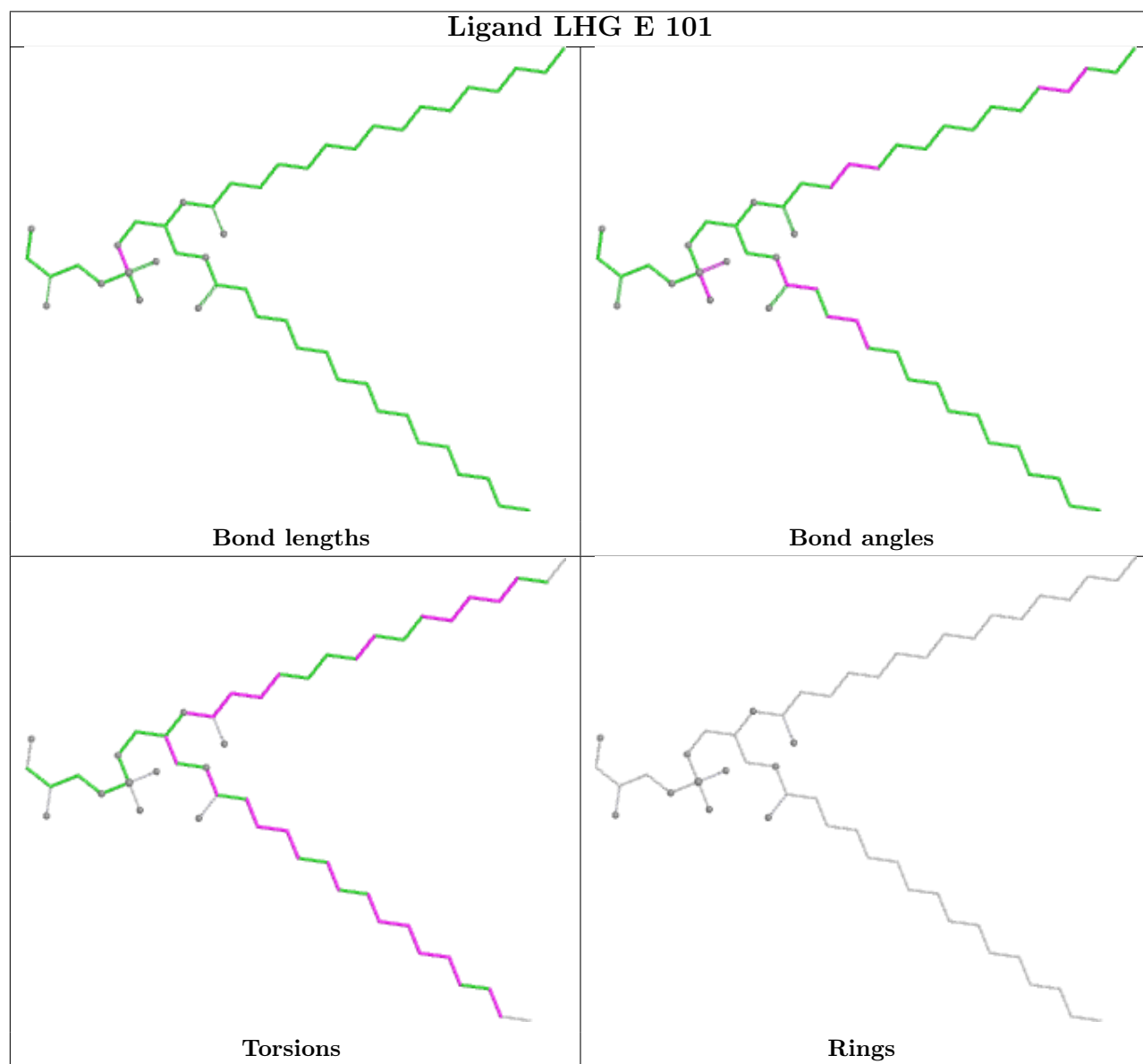
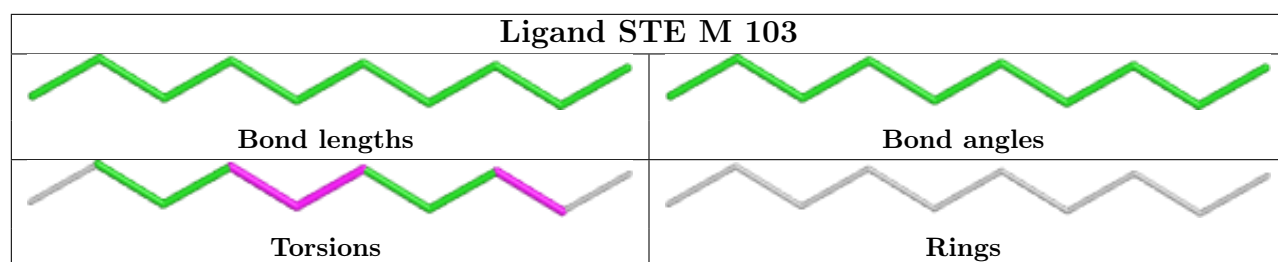
Ligand CLA B 605**Ligand CLA d 404****Ligand CLA H 101**

Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

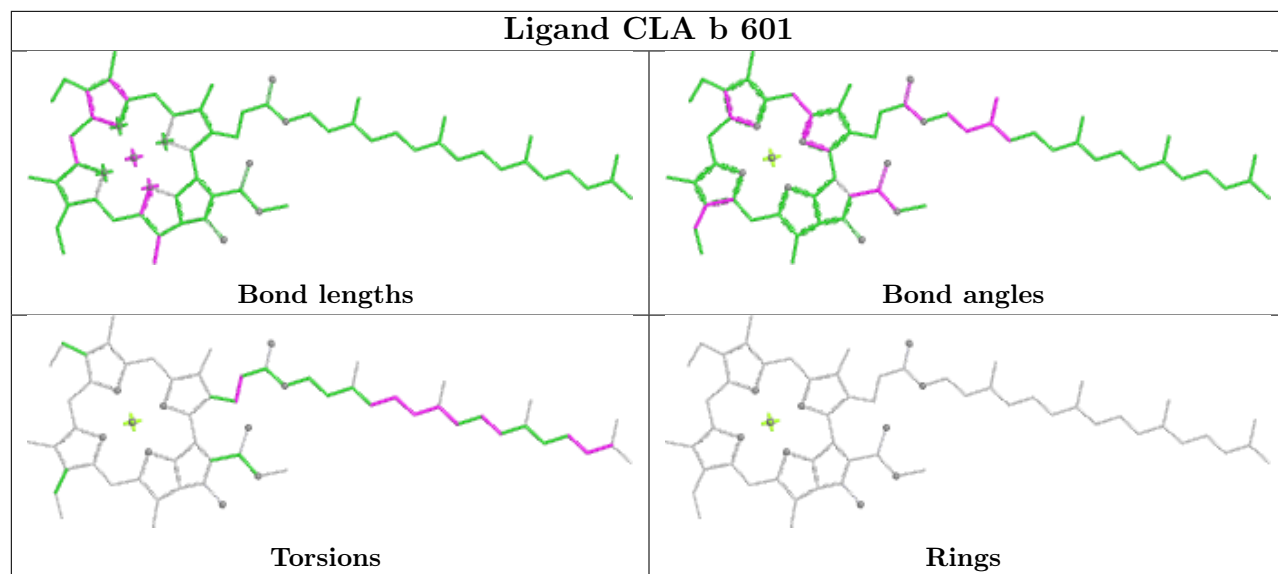
Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

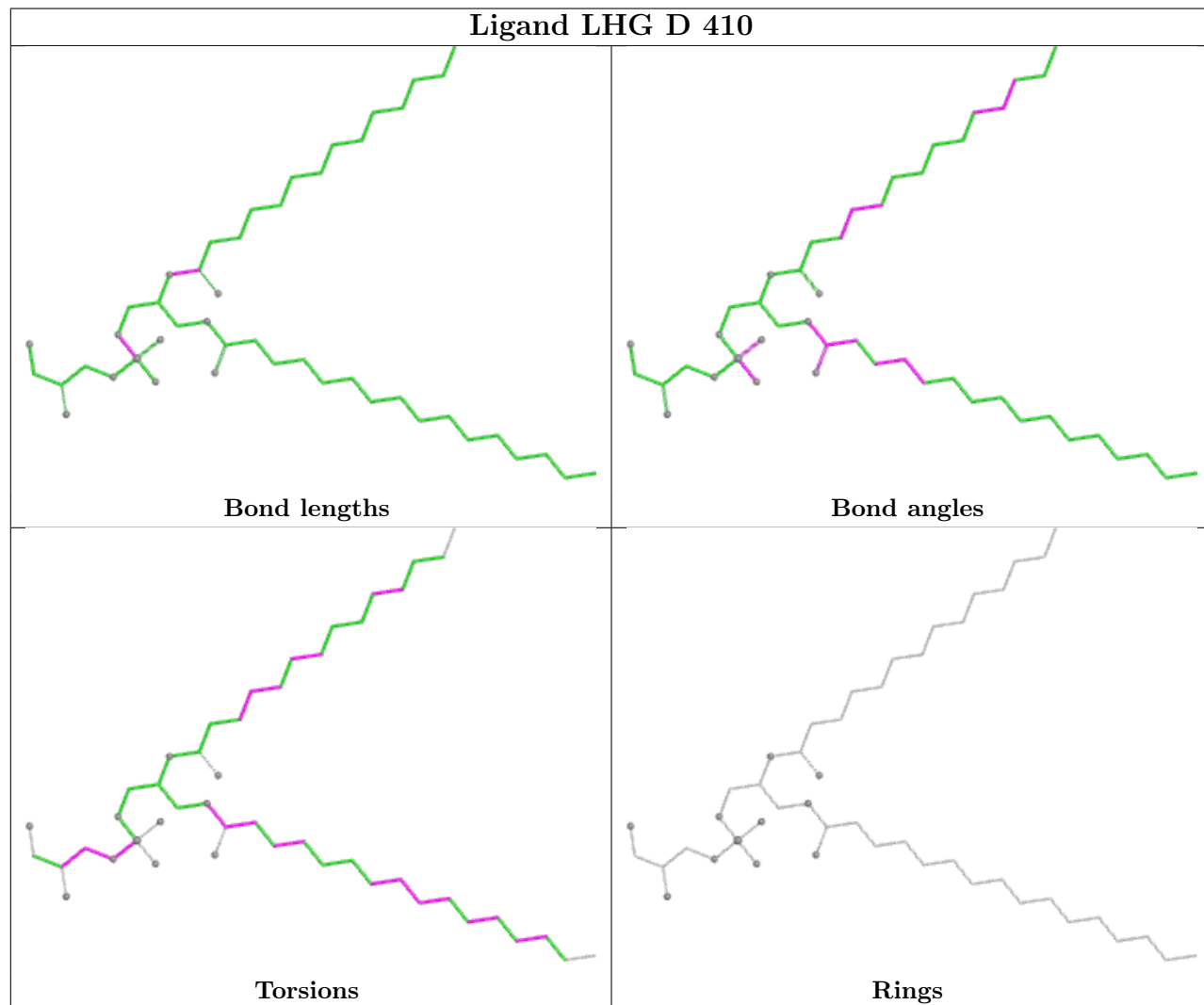


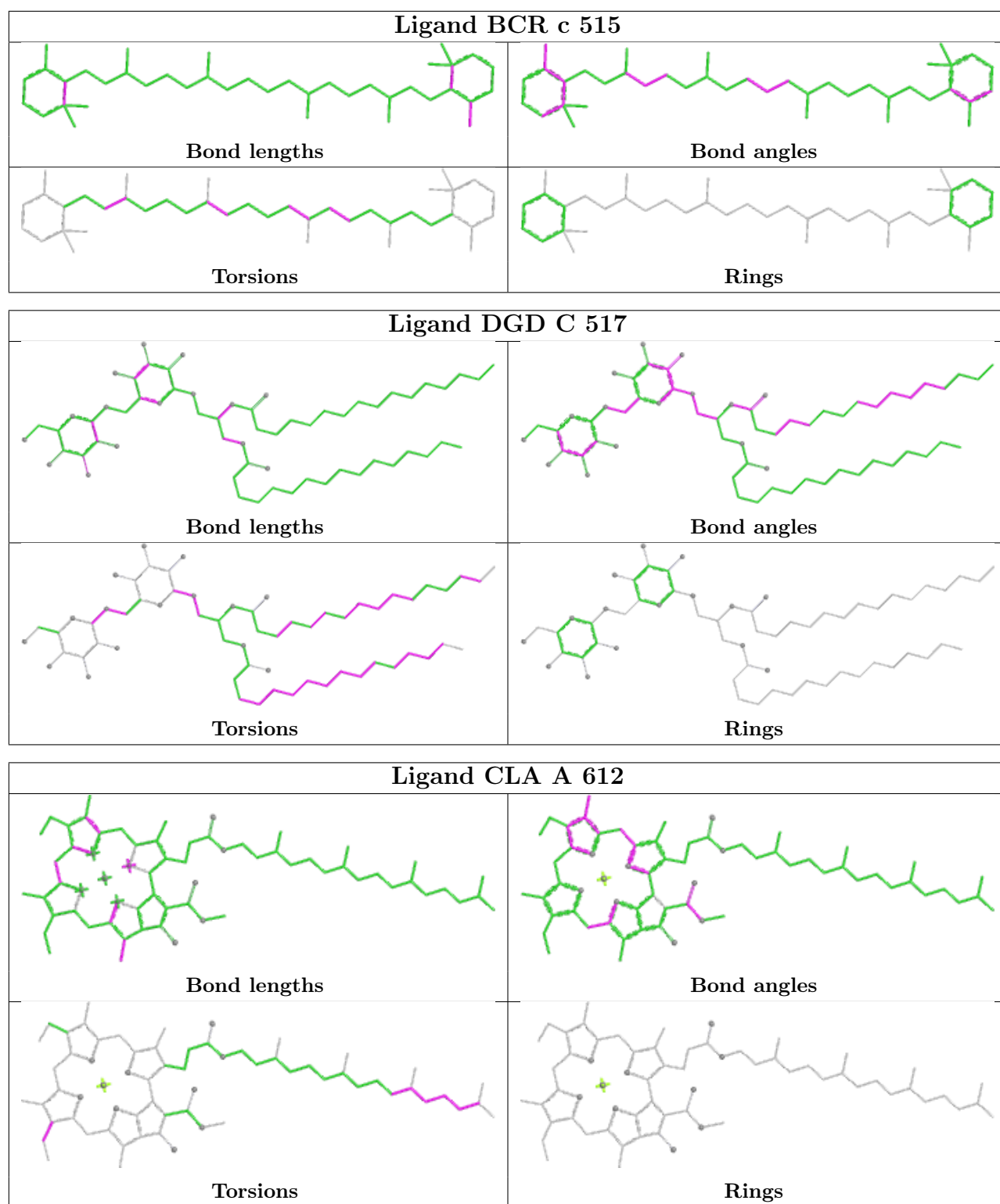


Ligand CLA b 601

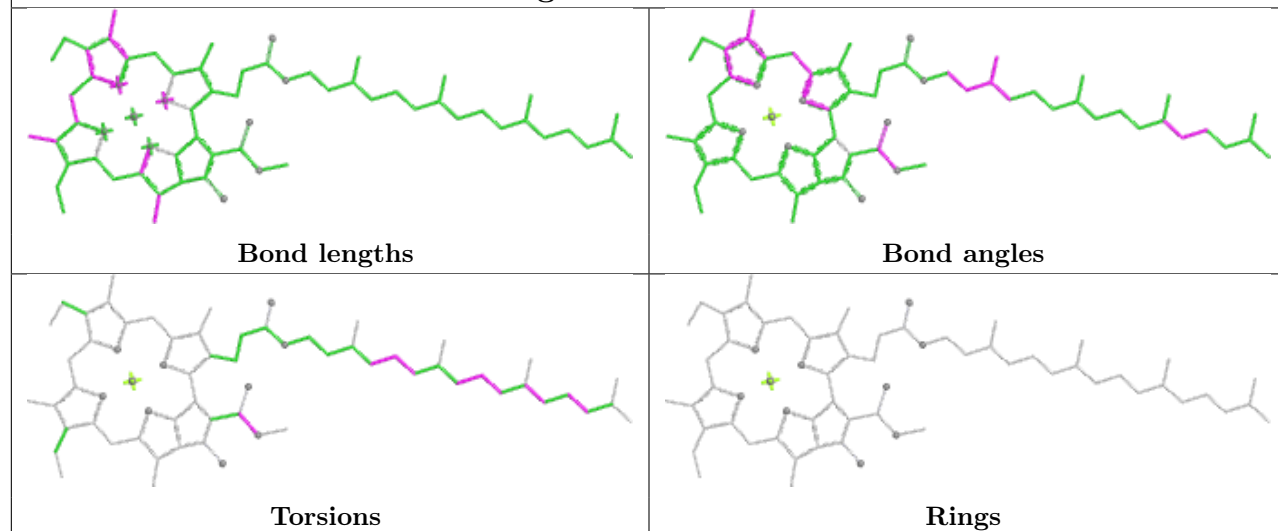


Ligand LHG D 410

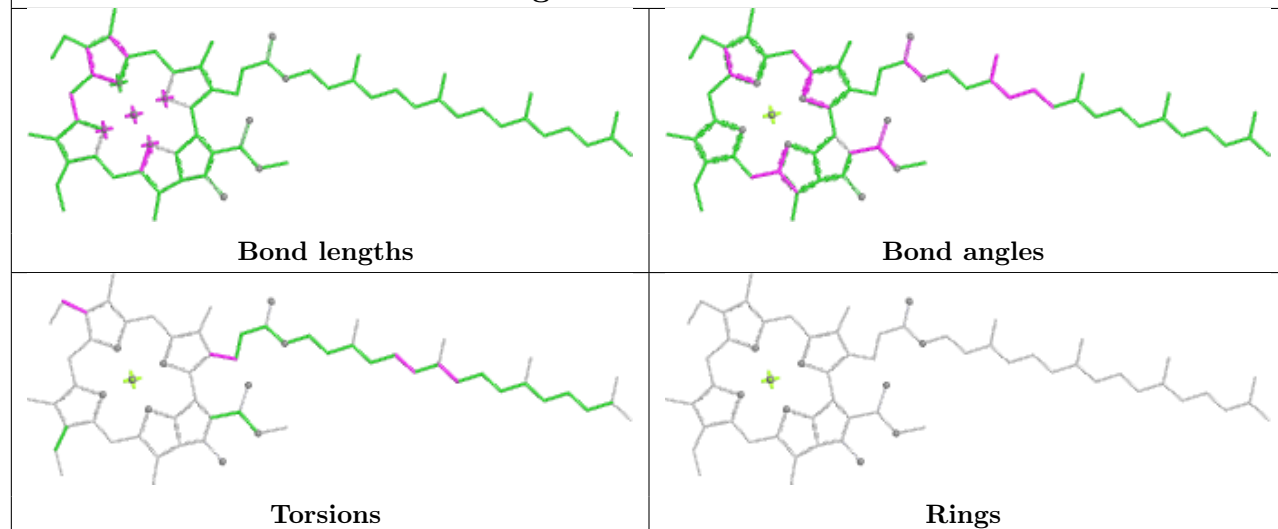




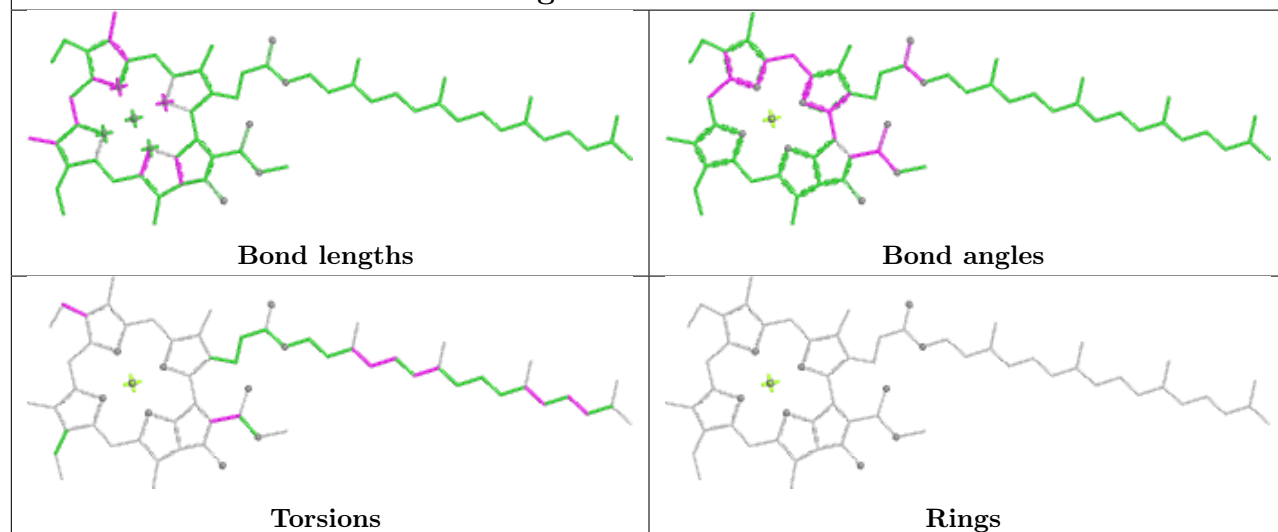
Ligand CLA c 510

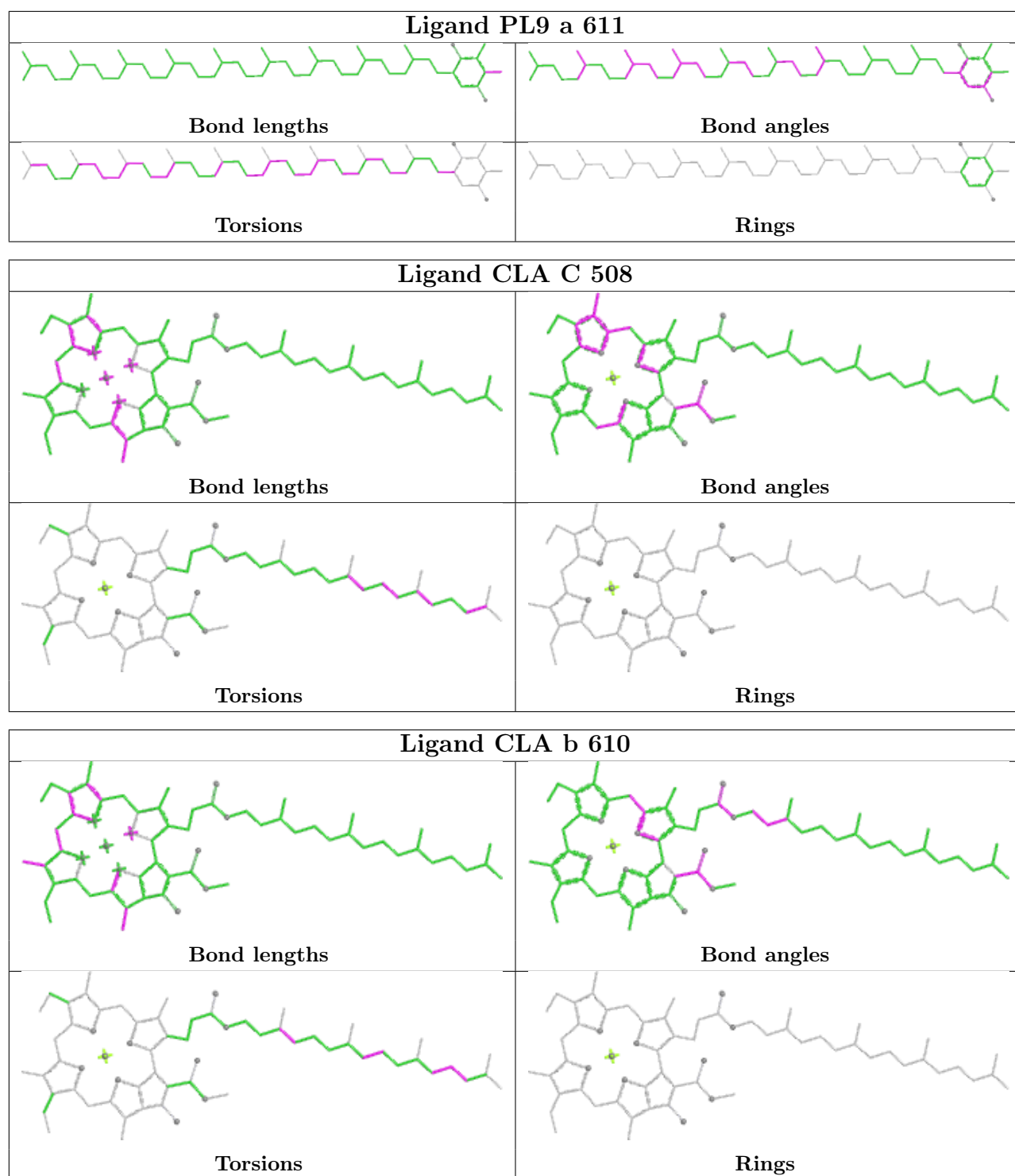


Ligand CLA C 503



Ligand CLA c 507





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.25	1 (0%) 90 91	14, 33, 54, 92	64 (19%)
1	a	334/344 (97%)	-0.17	3 (0%) 81 83	15, 35, 60, 81	64 (19%)
2	B	505/510 (99%)	-0.22	2 (0%) 88 90	21, 38, 66, 91	4 (0%)
2	b	505/510 (99%)	-0.08	4 (0%) 82 84	30, 41, 73, 115	0
3	C	442/461 (95%)	-0.14	0 100 100	16, 41, 55, 78	11 (2%)
3	c	451/461 (97%)	-0.06	1 (0%) 91 92	16, 44, 63, 104	12 (2%)
4	D	341/352 (96%)	-0.32	0 100 100	16, 35, 52, 77	2 (0%)
4	d	341/352 (96%)	-0.17	0 100 100	18, 39, 62, 82	3 (0%)
5	E	82/84 (97%)	0.32	1 (1%) 76 79	35, 55, 72, 86	1 (1%)
5	e	82/84 (97%)	0.42	2 (2%) 59 63	44, 62, 81, 90	0
6	F	34/45 (75%)	0.07	0 100 100	40, 50, 63, 89	0
6	f	34/45 (75%)	0.36	1 (2%) 53 57	47, 54, 79, 88	0
7	H	65/66 (98%)	0.02	2 (3%) 51 55	39, 44, 60, 74	0
7	h	63/66 (95%)	0.30	1 (1%) 70 74	45, 54, 64, 70	0
8	I	35/38 (92%)	-0.09	0 100 100	37, 44, 70, 89	0
8	i	35/38 (92%)	-0.06	0 100 100	34, 44, 74, 88	0
9	J	36/40 (90%)	0.31	0 100 100	42, 55, 78, 87	0
9	j	36/40 (90%)	0.35	3 (8%) 17 19	44, 57, 90, 100	0
10	K	37/46 (80%)	0.17	0 100 100	47, 56, 74, 85	0
10	k	37/46 (80%)	0.33	0 100 100	52, 59, 73, 83	0
11	L	37/37 (100%)	-0.33	0 100 100	30, 34, 65, 75	0
11	l	36/37 (97%)	-0.36	0 100 100	30, 35, 69, 92	0
12	M	32/36 (88%)	-0.37	0 100 100	32, 37, 58, 75	0
12	m	31/36 (86%)	-0.29	0 100 100	32, 38, 56, 66	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%)	-0.01	2 (0%) 82 84	31, 46, 83, 138	1 (0%)
13	o	244/272 (89%)	0.02	3 (1%) 76 79	31, 45, 85, 119	0
14	T	29/32 (90%)	-0.38	0 100 100	31, 36, 62, 74	0
14	t	29/32 (90%)	-0.20	1 (3%) 48 52	32, 36, 75, 92	0
15	U	97/134 (72%)	0.01	0 100 100	36, 48, 71, 92	0
15	u	97/134 (72%)	-0.08	1 (1%) 79 82	35, 44, 60, 89	0
16	V	137/163 (84%)	-0.14	0 100 100	35, 44, 58, 80	0
16	v	137/163 (84%)	0.09	0 100 100	37, 51, 69, 84	0
17	Y	27/46 (58%)	0.99	3 (11%) 10 11	58, 73, 96, 106	0
17	y	30/46 (65%)	0.98	2 (6%) 24 27	66, 78, 96, 104	0
18	X	38/41 (92%)	0.17	1 (2%) 57 61	43, 55, 72, 81	0
18	x	39/41 (95%)	0.38	1 (2%) 57 61	53, 63, 87, 101	0
19	Z	62/62 (100%)	0.90	5 (8%) 18 19	57, 71, 119, 132	0
19	z	62/62 (100%)	0.81	4 (6%) 25 28	64, 74, 112, 125	0
20	R	34/41 (82%)	0.99	3 (8%) 15 17	65, 72, 85, 92	0
20	r	31/41 (75%)	1.31	4 (12%) 7 8	76, 92, 110, 126	0
All	All	5302/5700 (93%)	-0.04	51 (0%) 79 82	14, 42, 76, 138	162 (3%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	4.1
13	o	58	ASN	3.8
20	R	35	LEU	3.7
19	Z	33	TRP	3.1
14	t	30	THR	3.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.90	0.09	37,41,52,69	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	0.91	0.10	40,54,65,70	0
14	FME	T	1	10/11	0.94	0.09	39,43,55,62	0
12	FME	m	1	10/11	0.94	0.10	31,45,64,68	0
8	FME	i	1	10/11	0.95	0.10	44,51,53,54	0
8	FME	I	1	10/11	0.97	0.06	42,46,52,55	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
32	LHG	e	102	42/49	0.75	0.16	61,81,102,104	0
31	STE	H	104	18/20	0.77	0.17	53,65,74,79	0
31	STE	m	101	12/20	0.78	0.19	54,58,69,70	0
31	STE	c	523	12/20	0.78	0.14	60,71,84,87	0
31	STE	I	101	15/20	0.79	0.18	45,50,65,70	0
31	STE	E	102	12/20	0.79	0.17	62,72,82,85	0
33	LMG	b	622	55/55	0.79	0.17	50,67,82,84	0
31	STE	b	625	20/20	0.80	0.14	45,51,64,70	0
31	STE	x	102	20/20	0.80	0.15	48,56,62,63	0
31	STE	t	103	10/20	0.81	0.14	42,55,59,59	0
33	LMG	D	411	33/55	0.81	0.15	40,56,72,74	0
32	LHG	E	101	49/49	0.81	0.14	51,76,99,106	0
33	LMG	d	409	23/55	0.81	0.17	51,63,69,70	0
33	LMG	c	522	48/55	0.83	0.14	43,71,91,96	0
30	DGD	a	615	44/66	0.83	0.14	37,52,71,73	0
31	STE	j	101	12/20	0.84	0.14	51,59,67,68	0
31	STE	B	623	18/20	0.84	0.13	42,48,81,84	0
31	STE	a	616	12/20	0.84	0.12	53,62,68,70	0
29	SQD	a	614	36/54	0.84	0.14	33,56,70,76	0
29	SQD	T	103	39/54	0.84	0.14	39,56,79,80	0
31	STE	b	626	10/20	0.85	0.14	46,50,57,57	0
25	CLA	h	101	65/65	0.85	0.12	55,68,83,89	0
28	PL9	A	611	55/55	0.85	0.15	40,60,74,83	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	STE	T	102	16/20	0.85	0.15	41,47,60,63	0
31	STE	B	624	12/20	0.85	0.12	46,54,64,67	0
30	DGD	A	614	66/66	0.85	0.12	51,58,67,73	0
31	STE	d	411	17/20	0.86	0.15	45,55,69,71	0
33	LMG	C	515	48/55	0.86	0.12	42,55,67,75	0
31	STE	C	520	12/20	0.86	0.12	38,42,57,61	0
31	STE	M	104	15/20	0.87	0.14	43,54,69,75	0
29	SQD	f	101	41/54	0.87	0.14	63,77,86,93	0
31	STE	B	625	16/20	0.87	0.14	43,57,63,66	0
31	STE	b	621	20/20	0.87	0.11	42,51,67,68	0
25	CLA	H	101	65/65	0.87	0.11	42,55,81,96	0
31	STE	D	413	20/20	0.87	0.13	38,51,73,83	0
33	LMG	C	519	48/55	0.87	0.13	48,67,78,86	0
31	STE	c	521	20/20	0.87	0.12	44,57,80,82	0
28	PL9	a	611	55/55	0.87	0.14	49,64,73,77	0
33	LMG	c	520	37/55	0.87	0.11	48,61,74,78	0
31	STE	B	619	17/20	0.87	0.12	42,50,66,69	0
29	SQD	b	619	49/54	0.87	0.11	42,57,78,80	0
33	LMG	b	620	51/55	0.88	0.10	36,49,65,66	0
31	STE	B	622	12/20	0.88	0.12	42,52,59,66	0
31	STE	b	624	16/20	0.88	0.13	54,59,76,79	0
31	STE	C	522	16/20	0.88	0.14	43,52,58,66	0
31	STE	J	101	12/20	0.88	0.13	54,60,72,72	0
29	SQD	D	408	36/54	0.89	0.13	53,65,78,82	0
27	BCR	c	514	40/40	0.89	0.12	49,60,68,71	0
33	LMG	D	412	28/55	0.89	0.11	36,47,59,65	0
33	LMG	c	524	49/55	0.89	0.10	40,55,72,79	0
29	SQD	B	621	54/54	0.89	0.11	39,61,82,91	0
27	BCR	Y	101	40/40	0.90	0.10	46,56,63,65	0
31	STE	M	102	15/20	0.90	0.10	46,48,61,65	0
33	LMG	M	101	51/55	0.90	0.10	32,47,63,65	0
25	CLA	c	512	65/65	0.91	0.11	44,59,83,89	0
27	BCR	H	102	40/40	0.91	0.09	36,47,56,62	0
27	BCR	d	405	40/40	0.91	0.11	39,49,81,89	0
27	BCR	k	101	40/40	0.91	0.11	51,61,71,73	0
31	STE	M	103	10/20	0.91	0.13	30,45,57,63	0
30	DGD	H	103	62/66	0.91	0.10	35,43,52,58	0
31	STE	l	102	18/20	0.91	0.12	34,45,68,72	0
31	STE	C	521	12/20	0.91	0.11	46,53,59,63	0
31	STE	t	102	14/20	0.91	0.09	38,48,52,56	0
27	BCR	x	101	40/40	0.91	0.10	43,55,66,69	0
30	DGD	h	102	62/66	0.91	0.10	37,47,54,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	SQD	a	613	54/54	0.91	0.11	46,61,75,81	0
30	DGD	C	517	62/66	0.92	0.09	37,49,86,99	0
27	BCR	B	618	40/40	0.92	0.09	35,44,52,54	0
27	BCR	C	514	40/40	0.92	0.10	35,42,52,53	0
27	BCR	D	405	40/40	0.92	0.10	33,46,70,78	0
25	CLA	c	513	65/65	0.92	0.10	41,61,87,92	0
25	CLA	C	513	65/65	0.92	0.10	47,55,82,86	0
27	BCR	Z	101	40/40	0.92	0.11	49,56,63,65	0
27	BCR	b	617	40/40	0.92	0.08	32,40,49,53	0
25	CLA	b	615	60/65	0.93	0.09	34,44,71,75	0
27	BCR	b	618	40/40	0.93	0.09	34,47,58,62	0
33	LMG	D	407	51/55	0.93	0.10	35,49,69,72	0
29	SQD	A	613	52/54	0.93	0.10	34,53,74,76	0
27	BCR	A	610	40/40	0.93	0.07	28,34,40,42	0
27	BCR	c	516	40/40	0.93	0.12	47,53,61,69	0
30	DGD	c	518	62/66	0.93	0.09	41,49,78,82	0
27	BCR	T	101	40/40	0.93	0.07	32,40,54,59	0
25	CLA	C	503	65/65	0.93	0.09	37,44,50,59	0
32	LHG	D	410	47/49	0.93	0.10	33,43,68,78	0
27	BCR	t	101	40/40	0.93	0.07	30,39,48,51	0
25	CLA	C	512	65/65	0.93	0.10	43,53,74,86	0
33	LMG	d	410	44/55	0.93	0.10	41,49,68,79	0
34	BCT	a	606	4/4	0.93	0.08	38,40,49,51	0
25	CLA	c	511	65/65	0.94	0.10	47,55,63,66	0
27	BCR	b	616	40/40	0.94	0.08	31,42,49,51	0
25	CLA	C	511	65/65	0.94	0.10	38,51,61,67	0
32	LHG	B	620	49/49	0.94	0.09	36,43,55,59	0
25	CLA	B	605	65/65	0.94	0.08	26,39,59,63	0
25	CLA	C	506	65/65	0.94	0.09	30,43,74,79	0
32	LHG	b	623	49/49	0.94	0.10	37,47,58,62	0
30	DGD	C	516	62/66	0.94	0.10	29,38,67,72	0
27	BCR	c	515	40/40	0.94	0.09	33,46,52,58	0
26	PHO	d	402	64/64	0.94	0.07	32,40,45,49	0
25	CLA	C	508	65/65	0.94	0.09	35,44,87,96	0
27	BCR	B	616	40/40	0.94	0.07	32,40,47,50	0
30	DGD	c	519	62/66	0.94	0.09	34,49,71,78	0
27	BCR	B	617	40/40	0.94	0.07	27,36,47,49	0
25	CLA	b	607	65/65	0.94	0.08	32,42,54,57	0
25	CLA	C	510	65/65	0.94	0.08	33,44,53,57	0
28	PL9	D	406	55/55	0.94	0.08	24,34,42,47	0
25	CLA	c	502	65/65	0.94	0.08	37,44,54,62	0
25	CLA	c	503	65/65	0.94	0.08	39,47,52,53	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	K	101	40/40	0.94	0.10	43,52,57,59	0
25	CLA	c	508	64/65	0.94	0.09	36,46,77,98	0
25	CLA	c	509	65/65	0.94	0.10	41,48,59,62	0
25	CLA	A	607	65/65	0.95	0.09	28,37,84,87	0
25	CLA	c	510	65/65	0.95	0.08	40,48,55,63	0
25	CLA	C	509	65/65	0.95	0.09	33,43,54,62	0
28	PL9	d	406	55/55	0.95	0.07	29,35,40,42	0
25	CLA	B	608	65/65	0.95	0.07	28,39,48,52	0
25	CLA	B	609	65/65	0.95	0.07	25,33,41,43	0
25	CLA	d	401	65/65	0.95	0.09	33,40,73,82	0
25	CLA	d	404	65/65	0.95	0.08	34,43,76,78	0
25	CLA	B	614	65/65	0.95	0.07	29,38,57,65	0
26	PHO	D	402	64/64	0.95	0.06	26,35,40,43	0
26	PHO	a	608	64/64	0.95	0.07	29,34,38,43	0
25	CLA	B	615	60/65	0.95	0.09	31,39,74,77	0
25	CLA	C	501	65/65	0.95	0.07	29,36,45,53	0
25	CLA	a	607	65/65	0.95	0.07	26,33,39,42	0
25	CLA	a	609	65/65	0.95	0.09	23,35,70,74	0
30	DGD	C	518	62/66	0.95	0.08	33,46,68,75	0
25	CLA	b	601	65/65	0.95	0.08	32,43,50,53	0
25	CLA	b	602	65/65	0.95	0.08	29,37,58,66	0
30	DGD	c	517	62/66	0.95	0.08	31,39,61,70	0
25	CLA	b	604	65/65	0.95	0.07	26,36,44,49	0
25	CLA	b	605	65/65	0.95	0.08	31,39,60,63	0
32	LHG	d	408	39/49	0.95	0.08	34,46,57,58	0
25	CLA	C	502	65/65	0.95	0.07	36,42,52,59	0
32	LHG	l	101	49/49	0.95	0.08	33,43,50,53	0
25	CLA	b	608	65/65	0.95	0.08	34,45,56,67	0
25	CLA	b	609	65/65	0.95	0.08	30,38,48,57	0
25	CLA	b	613	65/65	0.95	0.08	31,41,61,73	0
27	BCR	a	610	40/40	0.95	0.07	24,32,42,46	0
25	CLA	b	614	65/65	0.95	0.08	31,41,52,54	0
25	CLA	B	601	65/65	0.95	0.07	30,39,51,53	0
25	CLA	c	501	65/65	0.95	0.08	28,41,48,52	0
25	CLA	C	504	59/65	0.95	0.07	35,41,63,67	0
25	CLA	C	505	65/65	0.95	0.08	30,39,54,60	0
25	CLA	c	504	60/65	0.95	0.08	37,47,76,79	0
25	CLA	c	505	65/65	0.95	0.08	33,41,54,59	0
25	CLA	c	506	65/65	0.95	0.08	38,45,71,75	0
25	CLA	c	507	65/65	0.95	0.08	35,44,54,62	0
25	CLA	B	603	65/65	0.95	0.08	25,34,58,62	0
25	CLA	B	606	65/65	0.96	0.07	20,33,52,59	0

Continued on next page...

Continued from previous page...

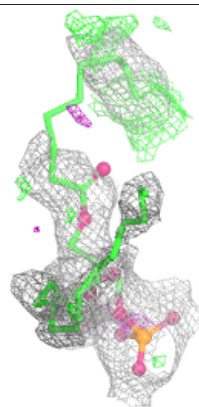
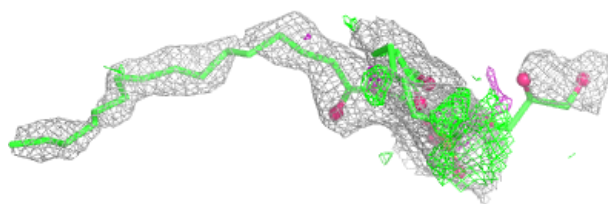
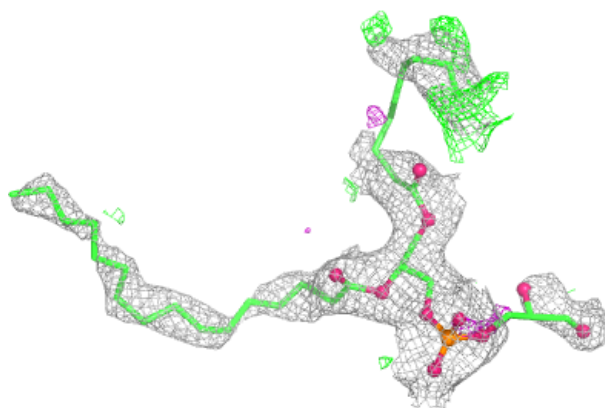
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LHG	D	409	49/49	0.96	0.07	30,38,46,48	0
25	CLA	b	610	65/65	0.96	0.07	28,37,44,50	0
25	CLA	d	403	65/65	0.96	0.07	27,35,50,61	0
32	LHG	L	101	49/49	0.96	0.07	30,39,47,58	0
25	CLA	b	611	65/65	0.96	0.07	27,36,43,49	0
32	LHG	d	407	49/49	0.96	0.08	30,41,48,53	0
25	CLA	b	612	65/65	0.96	0.07	24,34,57,65	0
26	PHO	A	608	64/64	0.96	0.06	24,30,36,40	0
25	CLA	B	607	65/65	0.96	0.06	25,35,48,52	0
25	CLA	D	403	65/65	0.96	0.06	25,31,46,50	0
25	CLA	D	404	65/65	0.96	0.07	29,39,86,94	0
25	CLA	B	602	65/65	0.96	0.07	24,34,49,56	0
25	CLA	A	612	65/65	0.96	0.06	23,30,42,47	0
25	CLA	B	610	65/65	0.96	0.06	25,33,44,48	0
25	CLA	a	612	65/65	0.96	0.06	28,33,39,43	0
25	CLA	B	611	65/65	0.96	0.07	25,33,41,44	0
25	CLA	C	507	65/65	0.96	0.07	31,40,50,55	0
25	CLA	b	603	65/65	0.96	0.08	28,34,59,72	0
25	CLA	B	612	65/65	0.96	0.07	24,33,58,64	0
25	CLA	B	613	65/65	0.96	0.08	28,36,64,70	0
25	CLA	b	606	65/65	0.96	0.07	27,35,50,60	0
25	CLA	B	604	65/65	0.96	0.07	25,32,42,46	0
34	BCT	D	401	4/4	0.96	0.06	33,38,41,42	0
25	CLA	A	606	65/65	0.96	0.06	22,29,39,46	0
35	HEM	e	101	43/43	0.96	0.09	52,59,73,80	0
35	HEM	F	101	43/43	0.97	0.09	46,52,61,71	0
25	CLA	A	609	54/65	0.97	0.06	26,32,59,61	0
24	CL	A	604	1/1	0.98	0.04	33,33,33,33	0
24	CL	a	604	1/1	0.98	0.04	34,34,34,34	0
36	HEC	V	201	43/43	0.98	0.07	32,38,45,51	0
36	HEC	v	201	43/43	0.98	0.07	36,41,47,50	0
21	OEX	a	601[B]	10/10	0.99	0.03	29,32,36,36	10
24	CL	a	605	1/1	0.99	0.10	35,35,35,35	0
22	OEY	A	602[A]	11/11	0.99	0.03	32,36,39,40	11
22	OEY	a	602[A]	11/11	0.99	0.03	35,37,40,43	11
21	OEX	A	601[B]	10/10	0.99	0.03	29,32,32,36	10
24	CL	A	605	1/1	0.99	0.04	33,33,33,33	0
23	FE2	A	603	1/1	1.00	0.01	35,35,35,35	0
23	FE2	a	603	1/1	1.00	0.02	39,39,39,39	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.

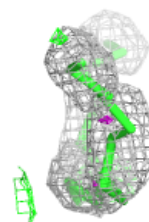
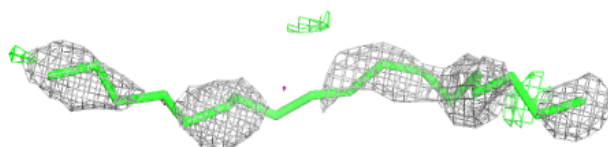
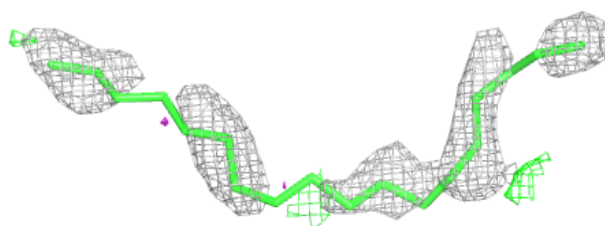
Electron density around LHG e 102:

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



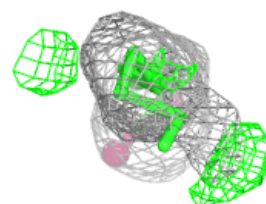
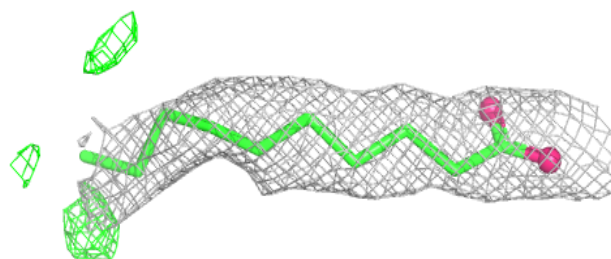
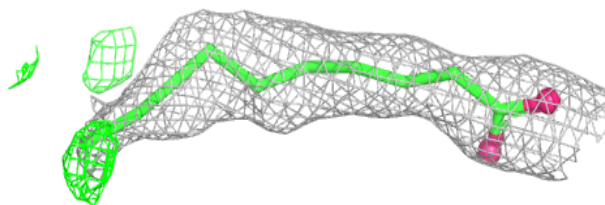
Electron density around STE H 104:

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

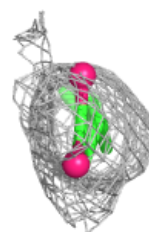
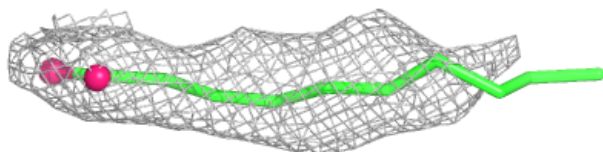
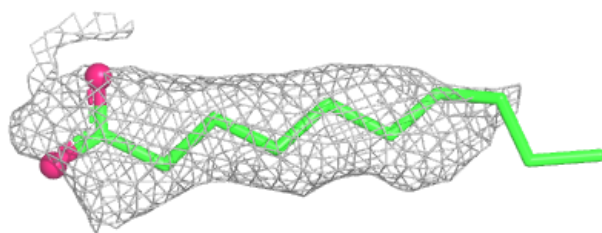


Electron density around STE m 101:

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

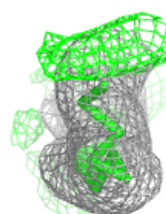
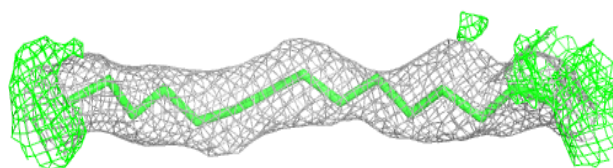
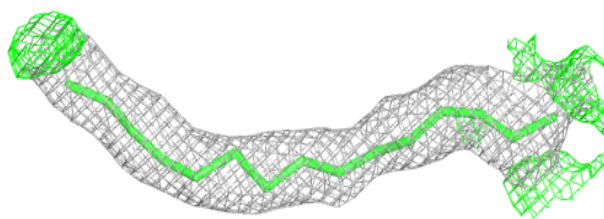
**Electron density around STE c 523:**

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

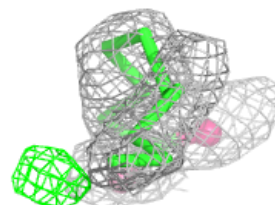
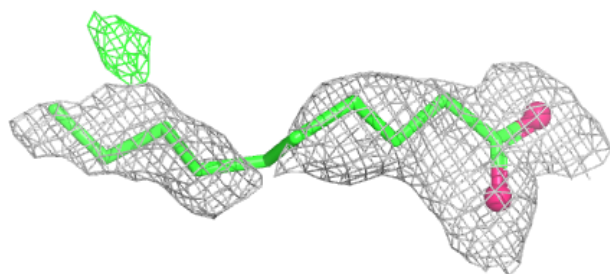
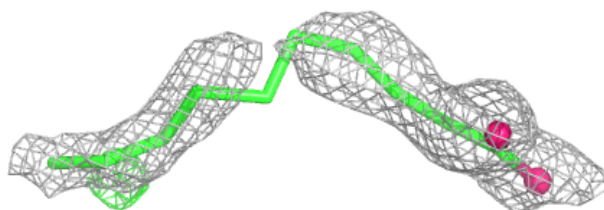


Electron density around STE I 101:

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

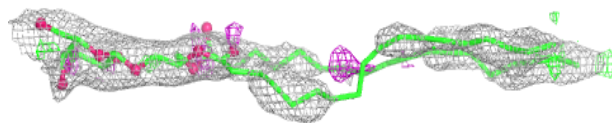
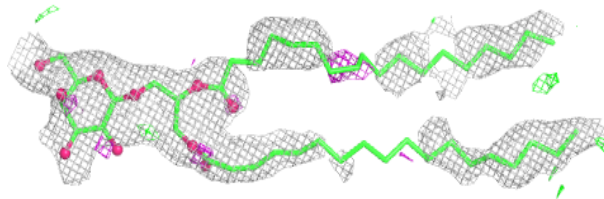
**Electron density around STE E 102:**

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

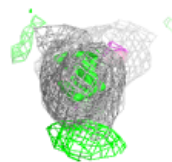
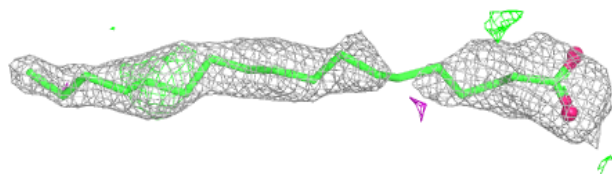
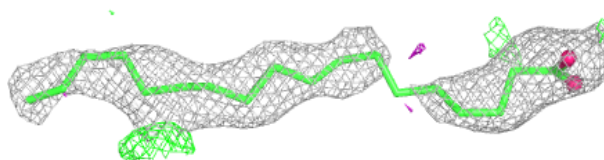


Electron density around LMG b 622:

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

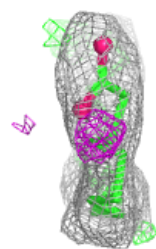
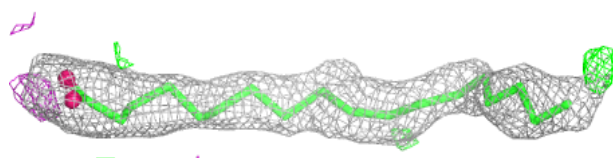
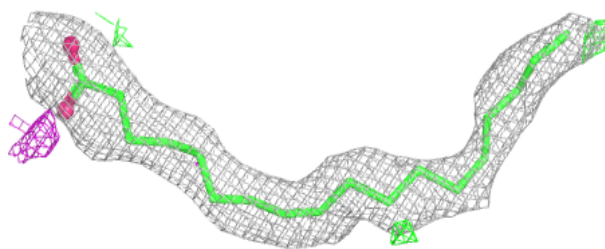
**Electron density around STE b 625:**

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

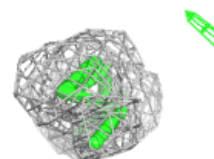
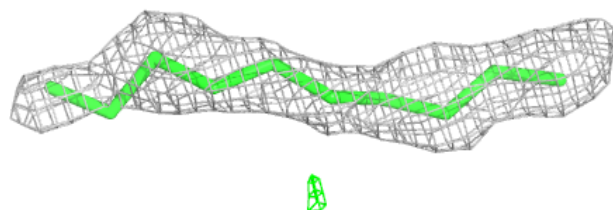
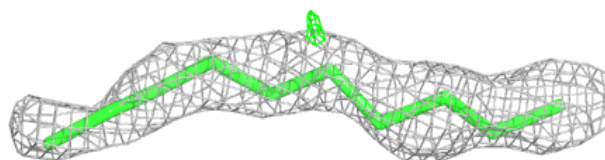


Electron density around STE x 102:

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

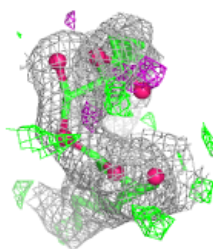
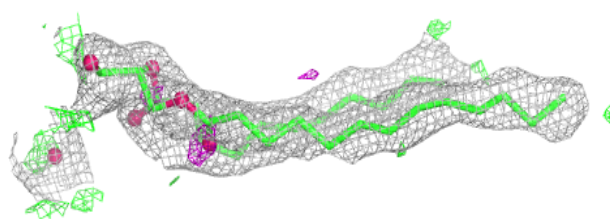
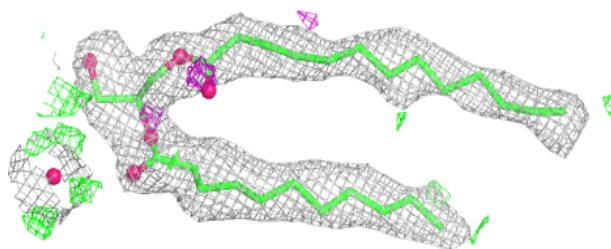
**Electron density around STE t 103:**

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



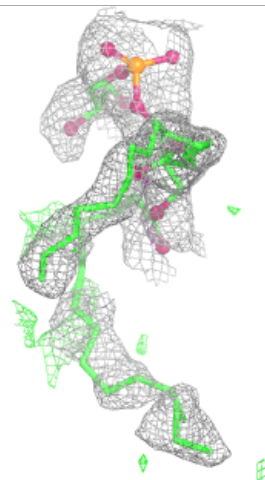
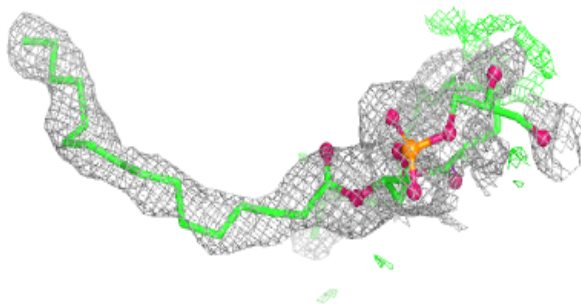
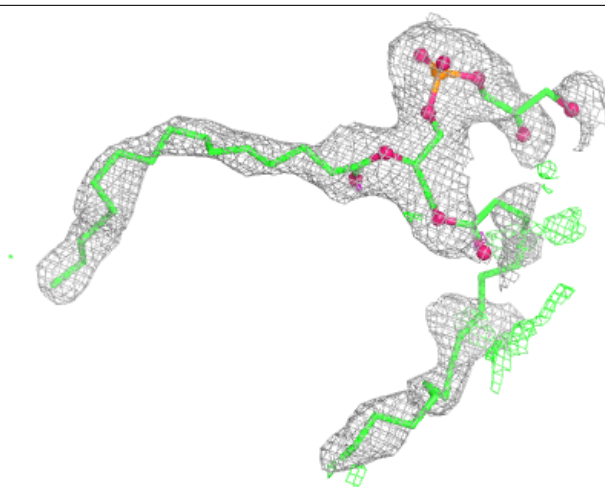
Electron density around LMG D 411:

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



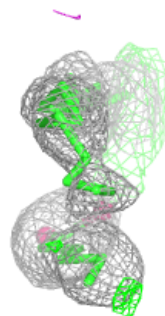
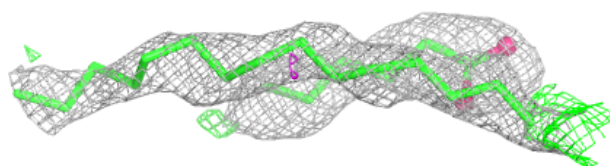
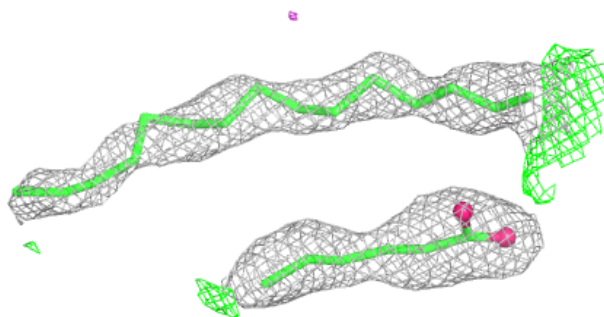
Electron density around LHG E 101:

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

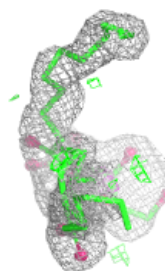
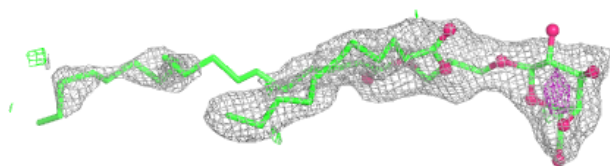
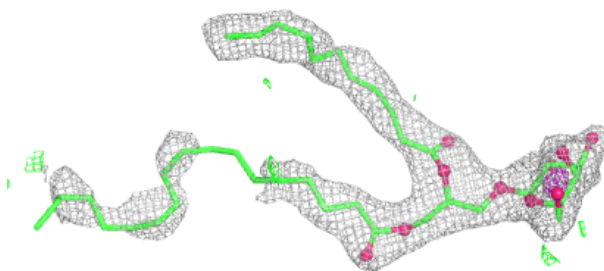


Electron density around LMG d 409:

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

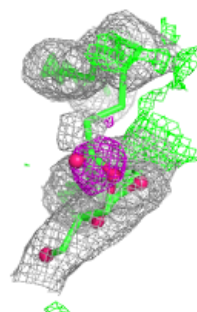
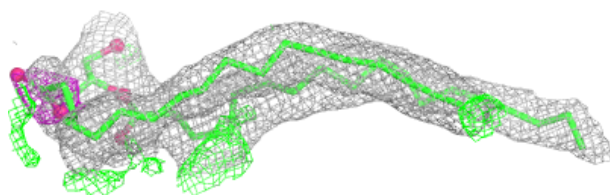
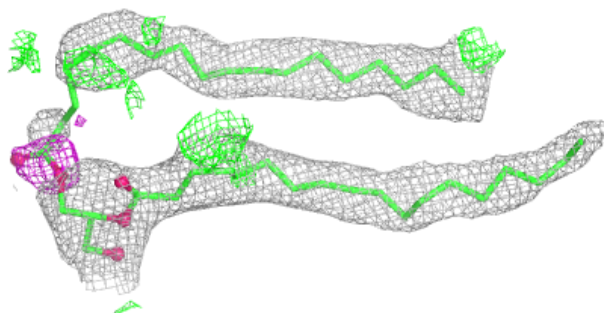
**Electron density around LMG c 522:**

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

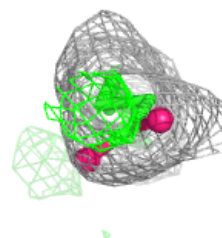
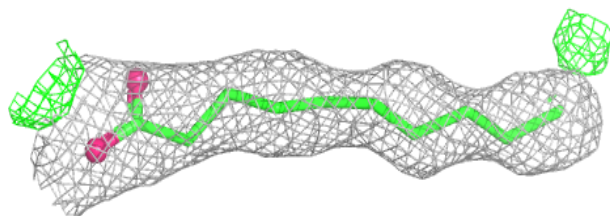
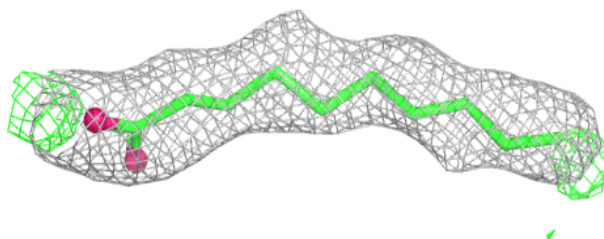


Electron density around DGD a 615:

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

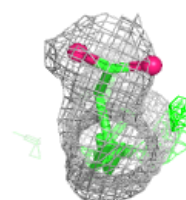
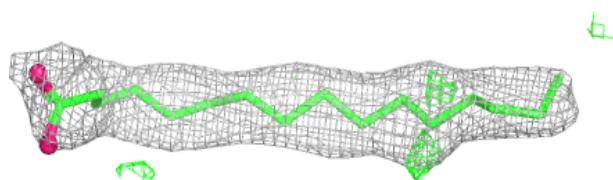
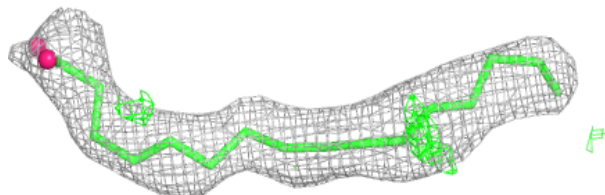
**Electron density around STE j 101:**

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

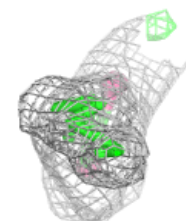
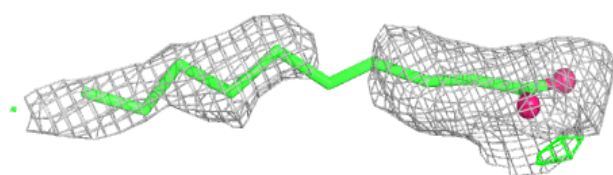
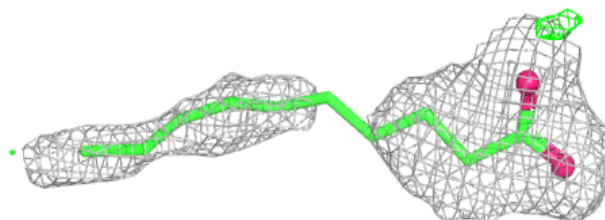


Electron density around STE B 623:

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

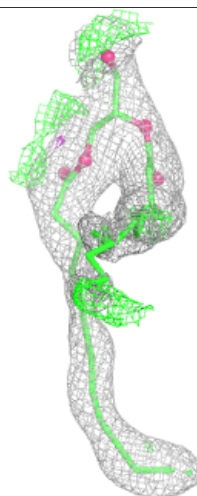
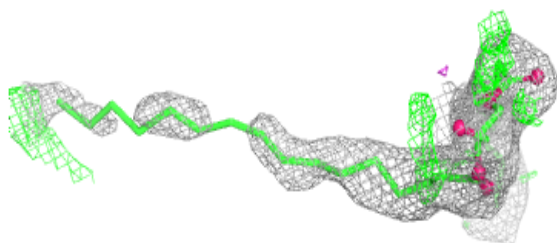
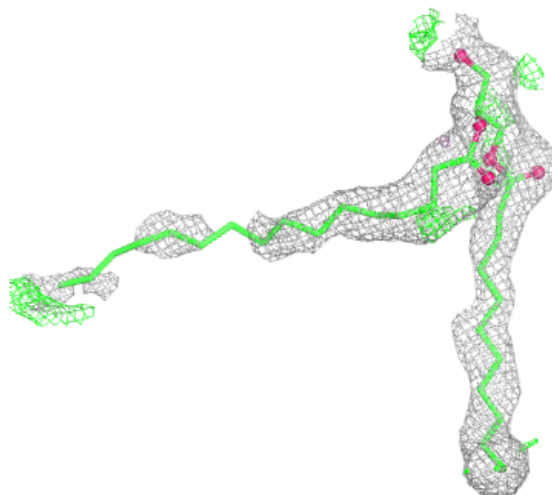
**Electron density around STE a 616:**

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



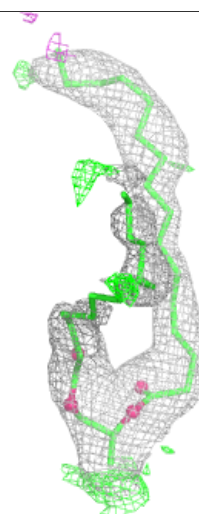
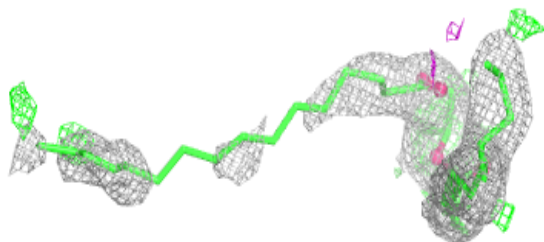
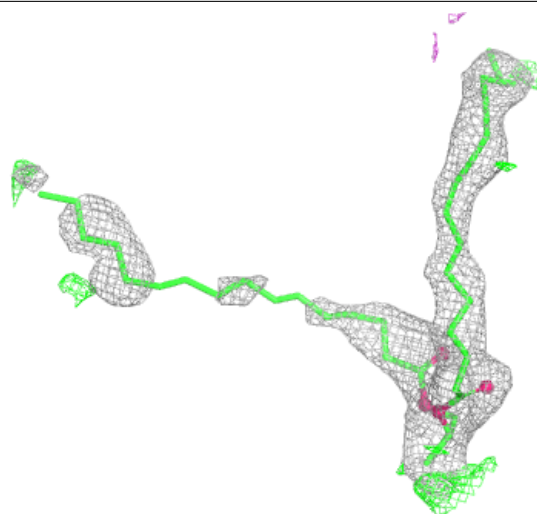
Electron density around SQD a 614:

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



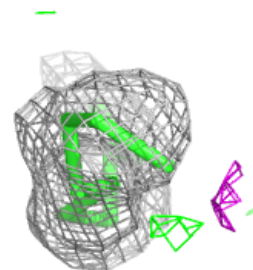
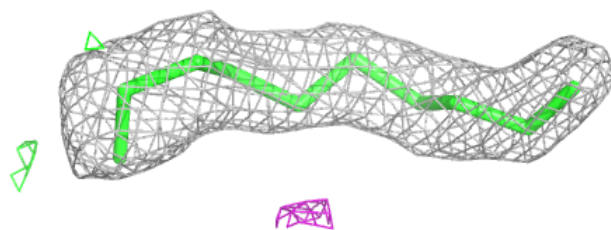
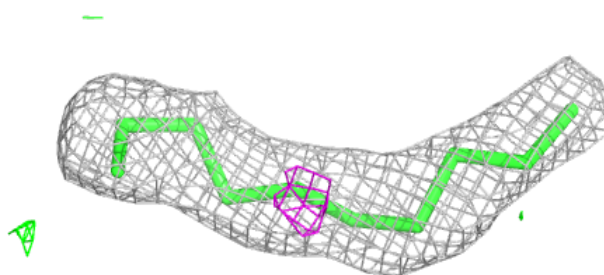
Electron density around SQD T 103:

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

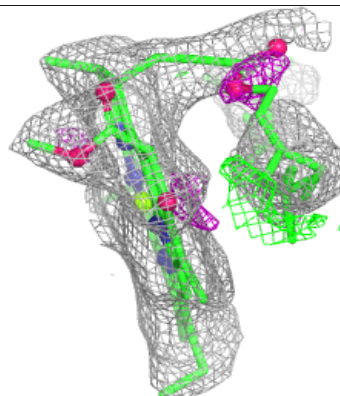
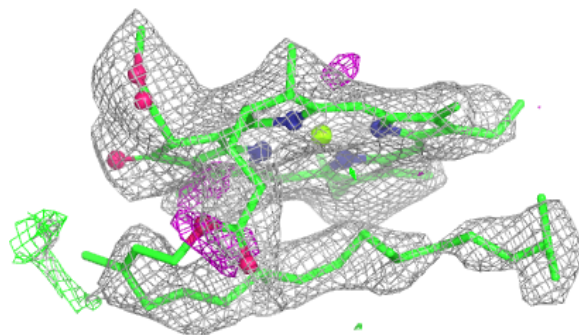
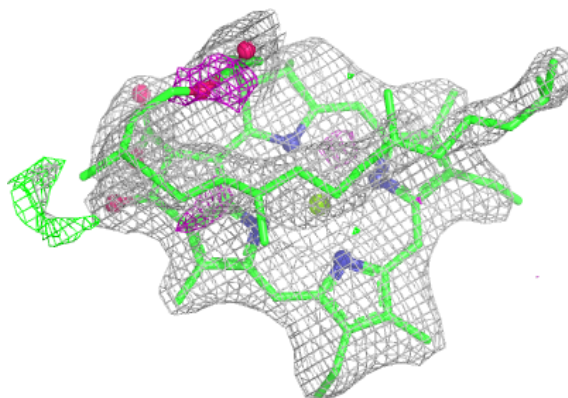


Electron density around STE b 626:

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

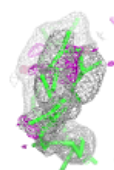
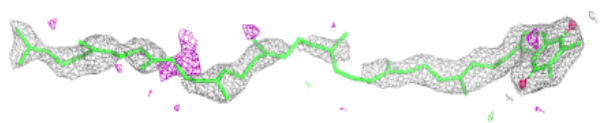
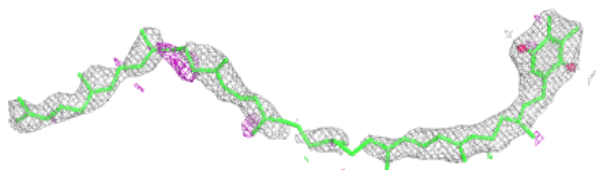
**Electron density around CLA h 101:**

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

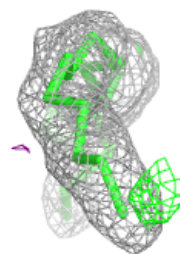
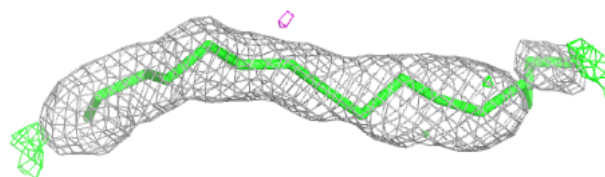
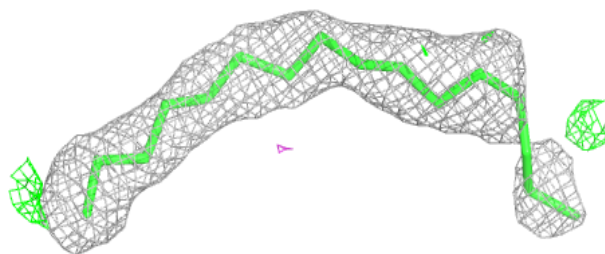


Electron density around PL9 A 611:

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

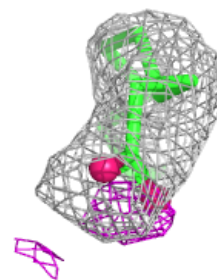
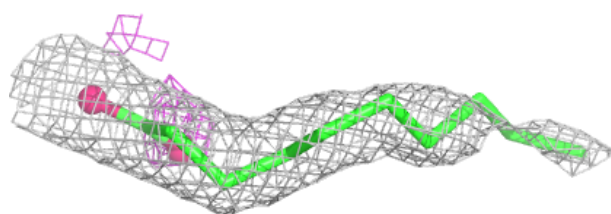
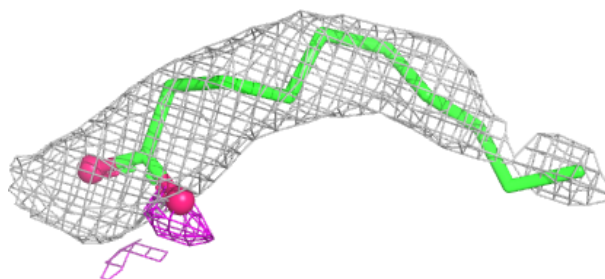
**Electron density around STE T 102:**

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

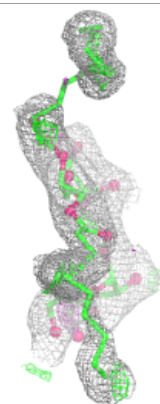
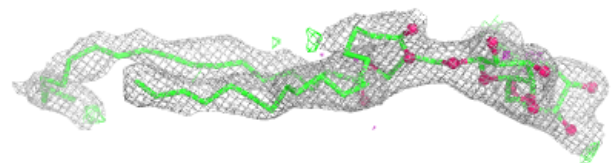
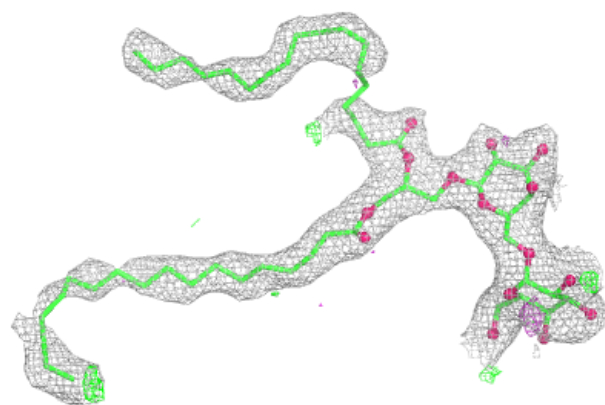


Electron density around STE B 624:

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

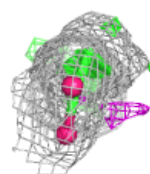
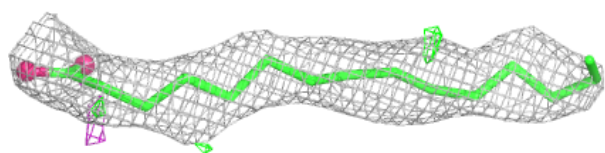
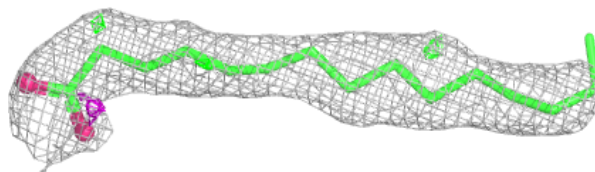
**Electron density around DGD A 614:**

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

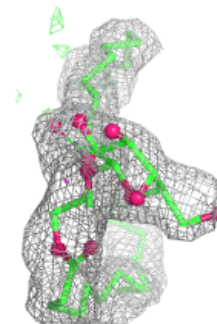
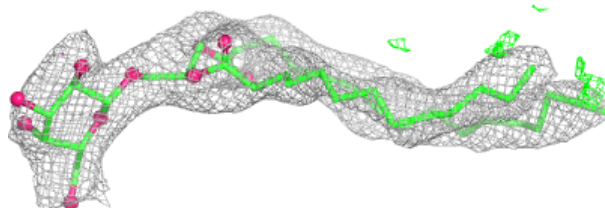
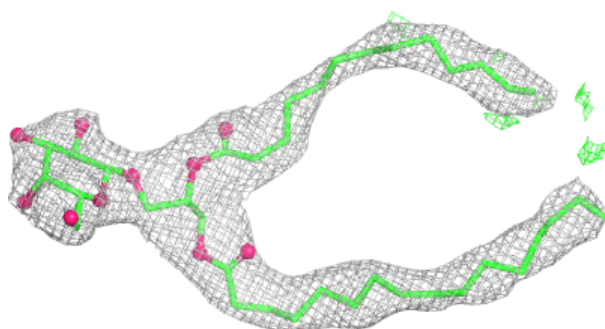


Electron density around STE d 411:

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

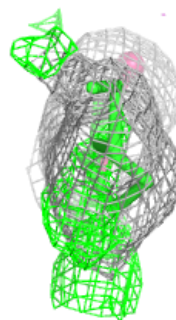
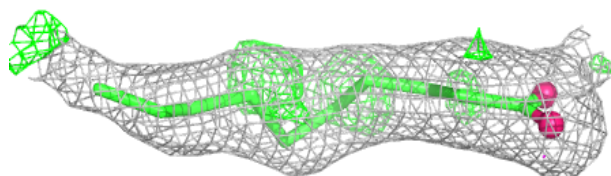
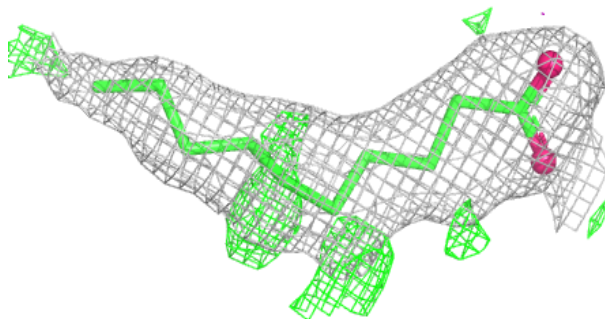
**Electron density around LMG C 515:**

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

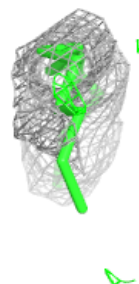
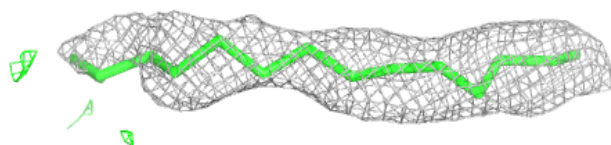
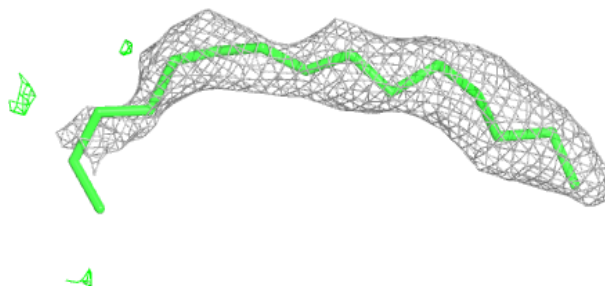


Electron density around STE C 520:

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

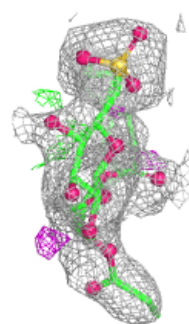
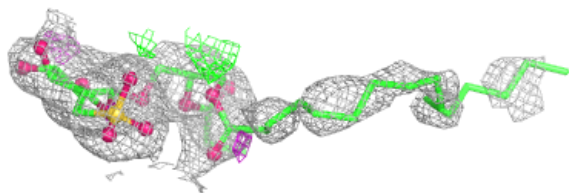
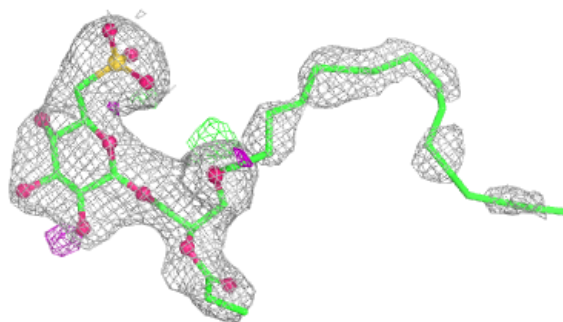
**Electron density around STE M 104:**

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

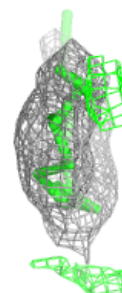
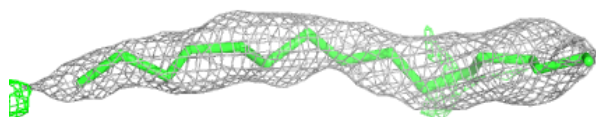
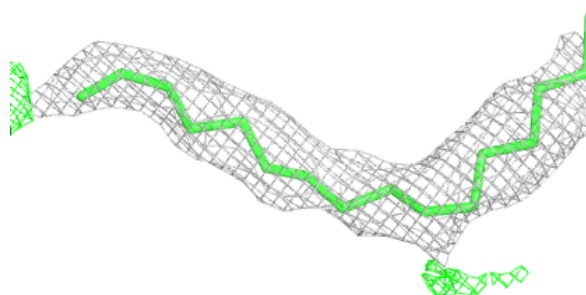


Electron density around SQD f 101:

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

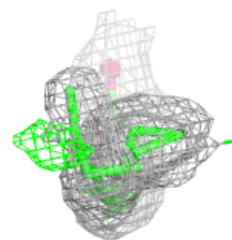
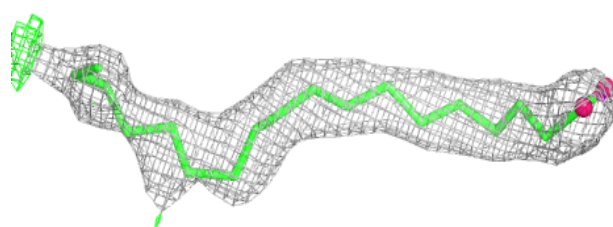
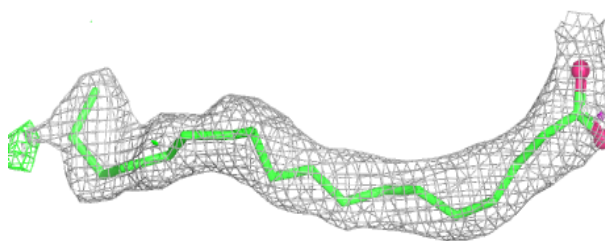
**Electron density around STE B 625:**

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

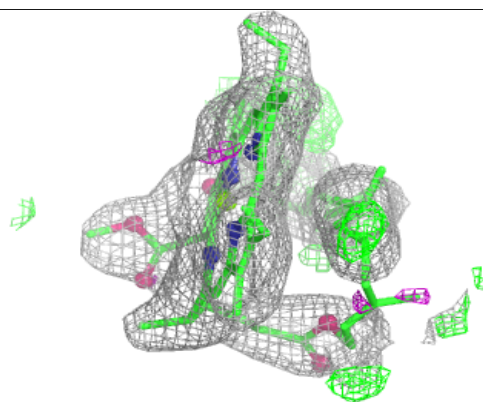
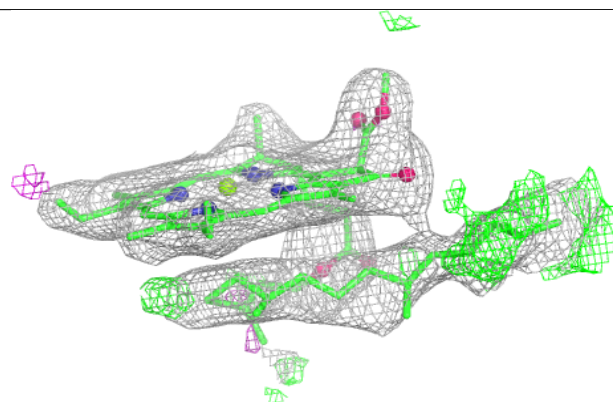
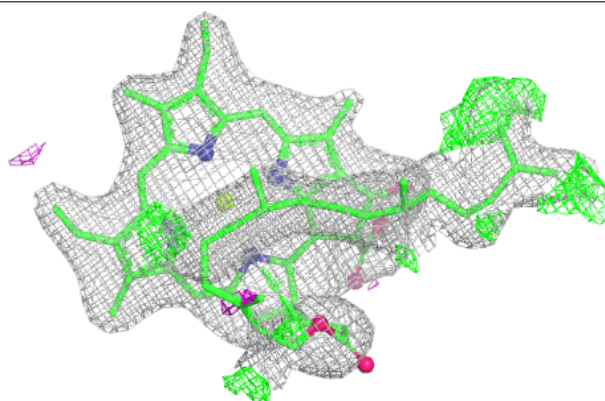


Electron density around STE b 621:

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

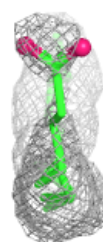
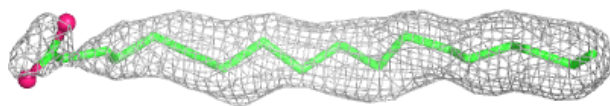
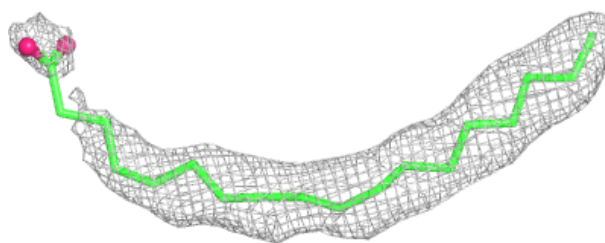
**Electron density around CLA H 101:**

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

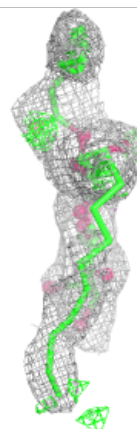
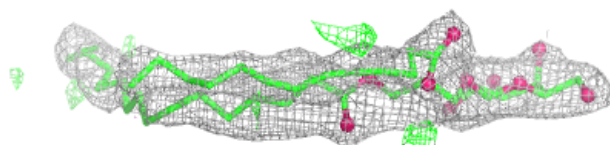
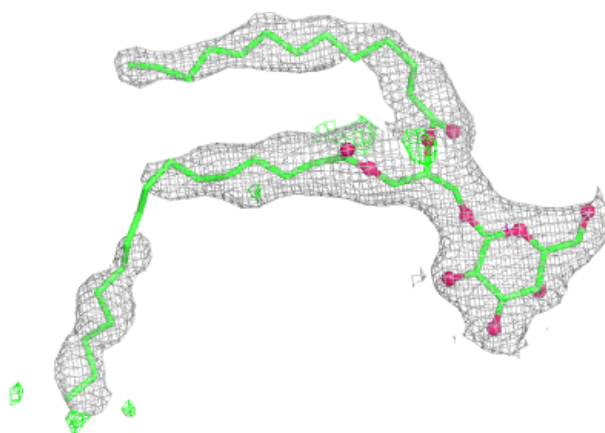


Electron density around STE D 413:

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

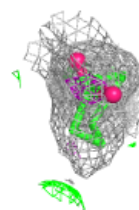
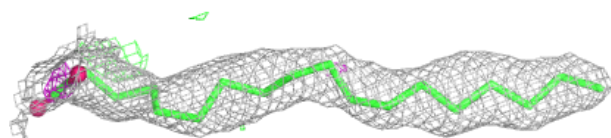
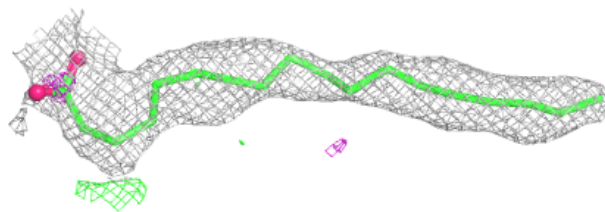
**Electron density around LMG C 519:**

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

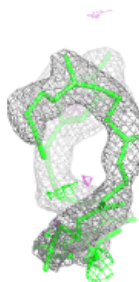
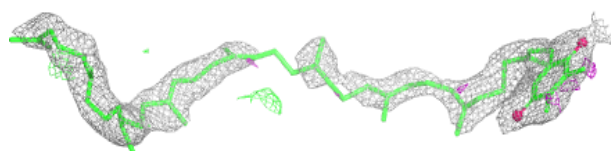
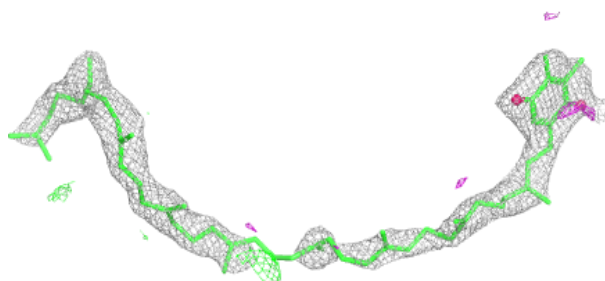


Electron density around STE c 521:

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

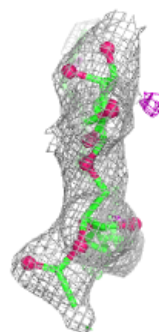
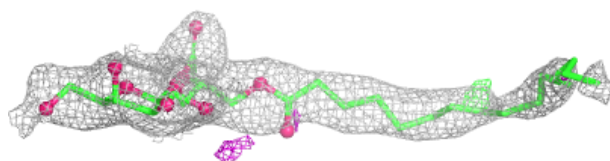
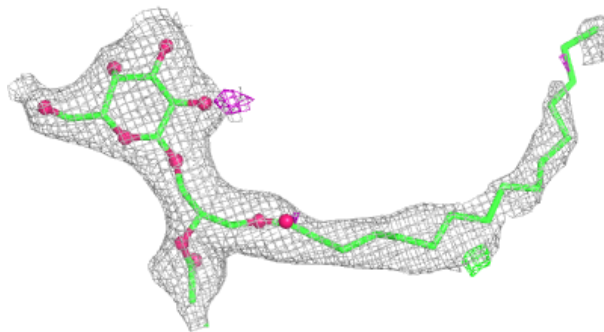
**Electron density around PL9 a 611:**

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

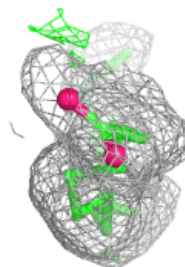
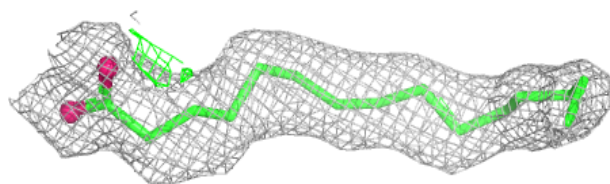
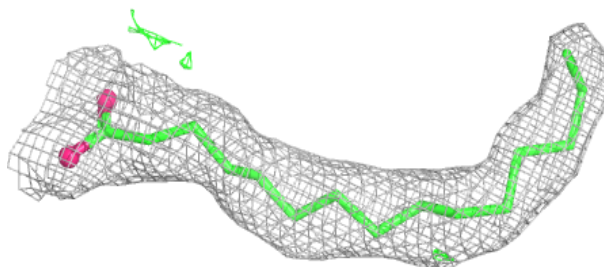


Electron density around LMG c 520:

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

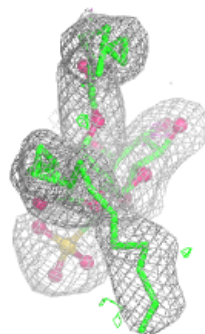
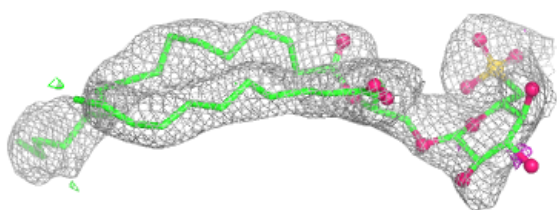
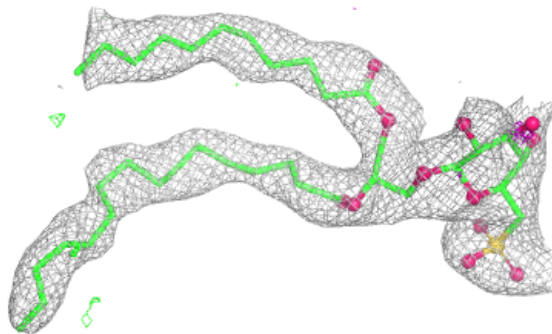
**Electron density around STE B 619:**

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

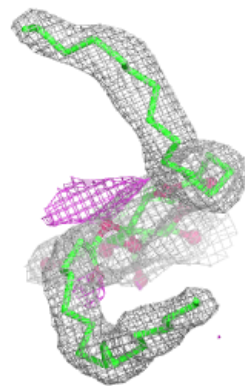
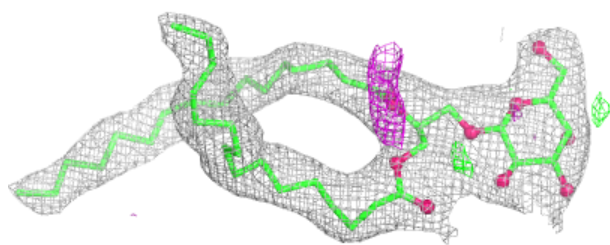
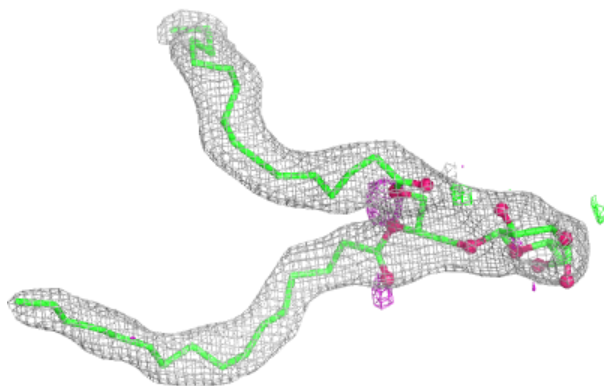


Electron density around SQD b 619:

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

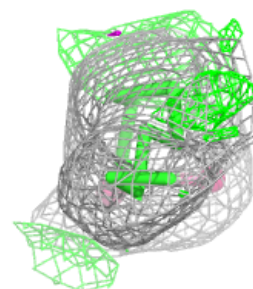
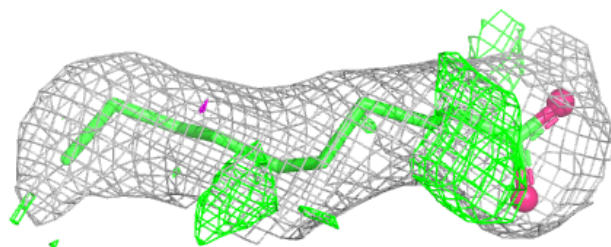
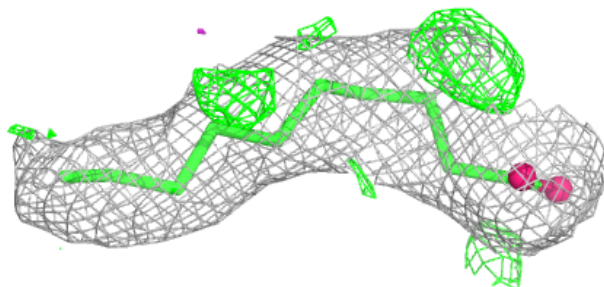
**Electron density around LMG b 620:**

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

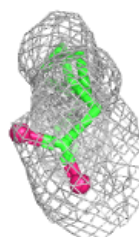
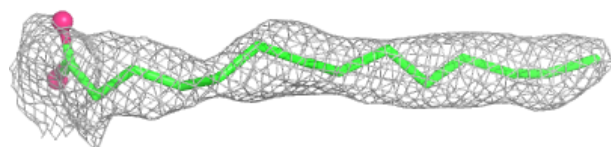
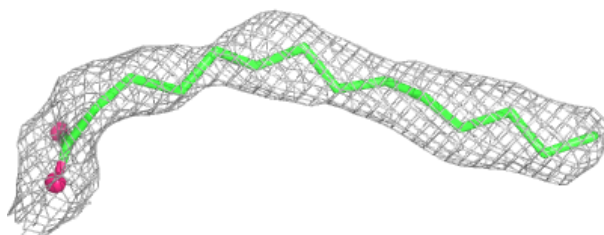


Electron density around STE B 622:

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

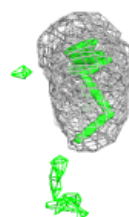
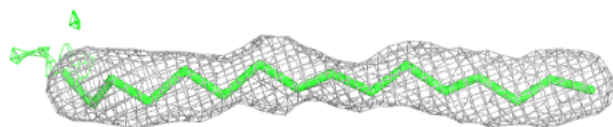
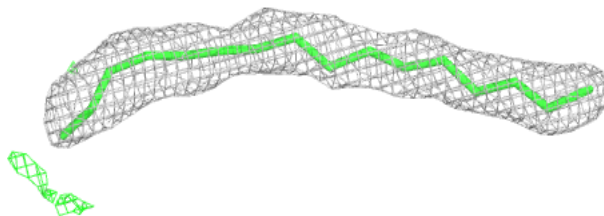
**Electron density around STE b 624:**

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

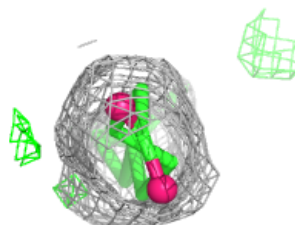
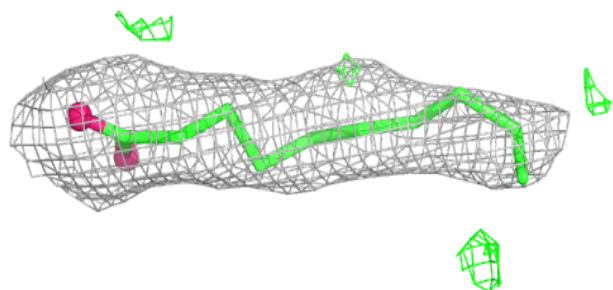
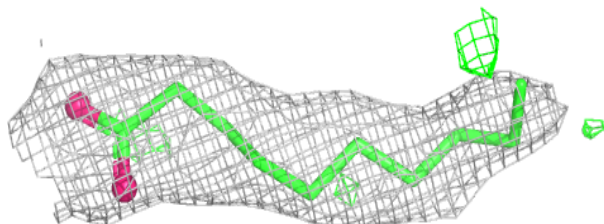


Electron density around STE C 522:

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

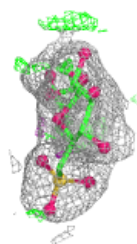
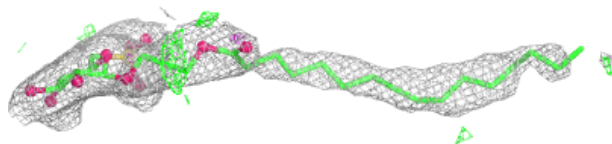
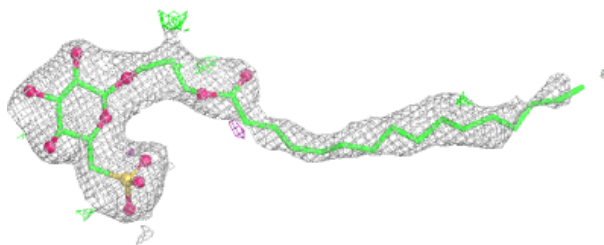
**Electron density around STE J 101:**

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

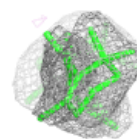
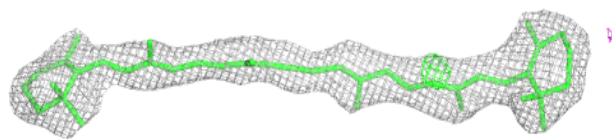
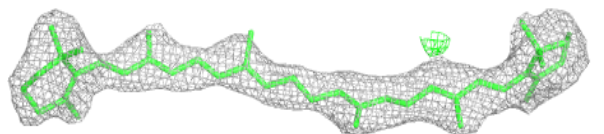


Electron density around SQD D 408:

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

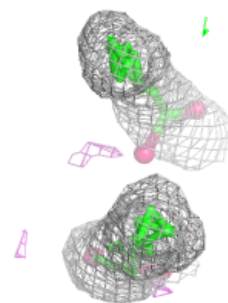
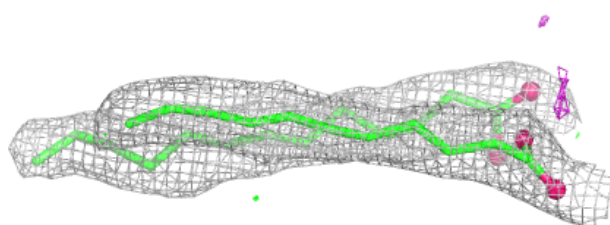
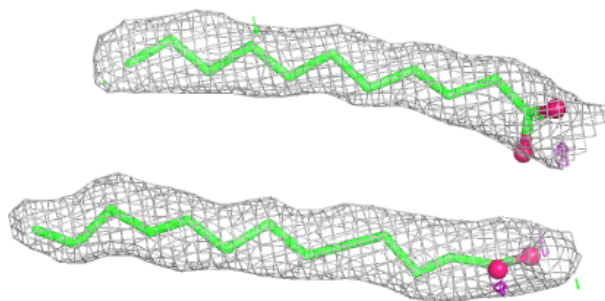
**Electron density around BCR c 514:**

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

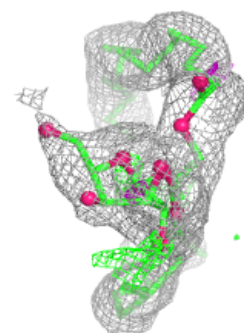
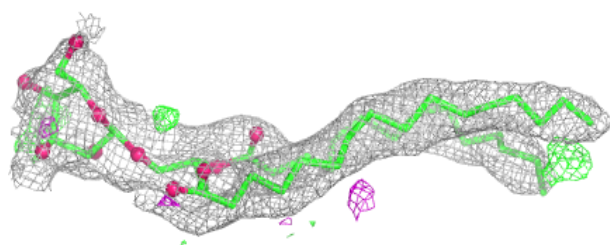
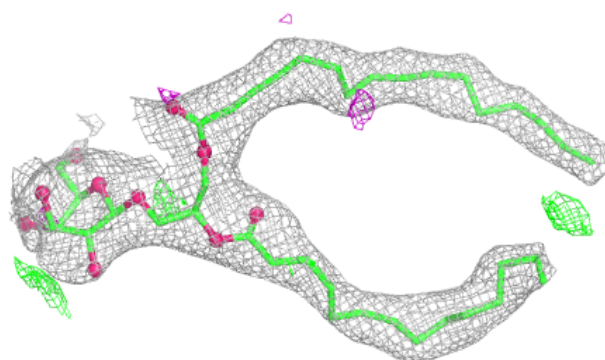


Electron density around LMG D 412:

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

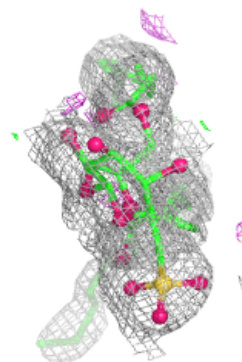
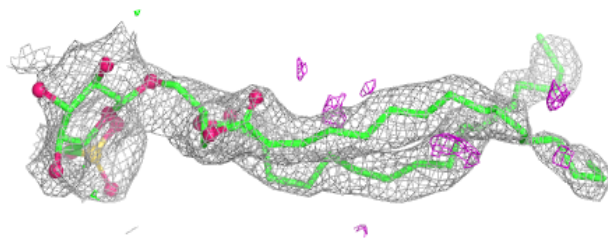
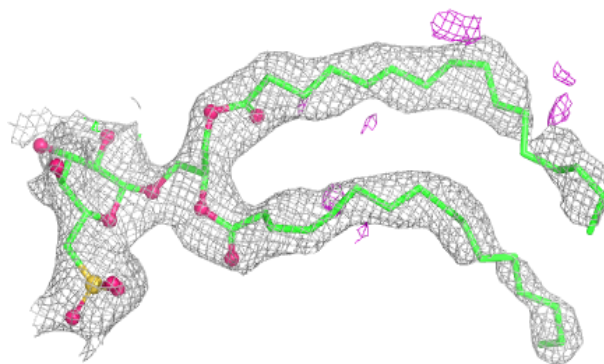
**Electron density around LMG c 524:**

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

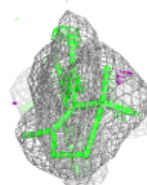
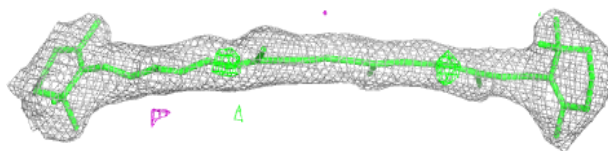
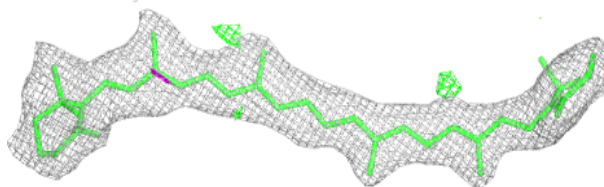


Electron density around SQD B 621:

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

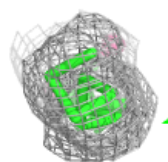
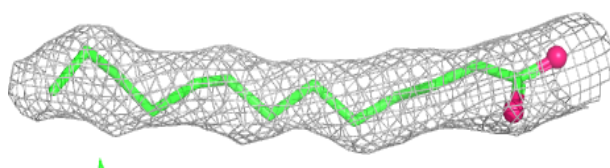
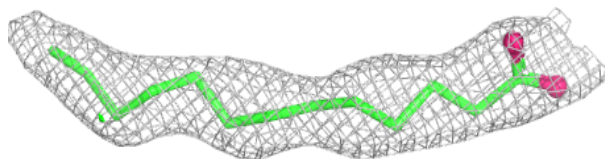
**Electron density around BCR Y 101:**

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

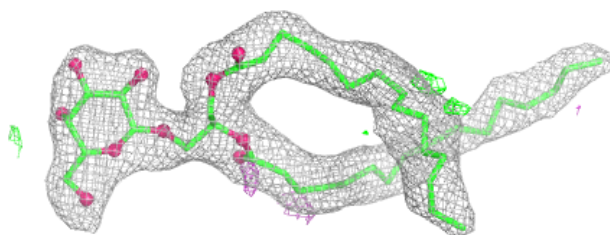
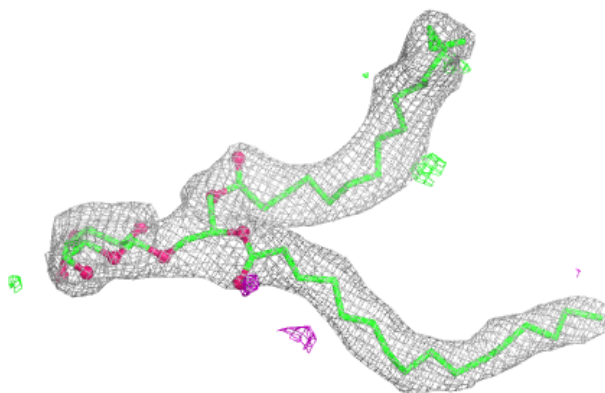


Electron density around STE M 102:

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

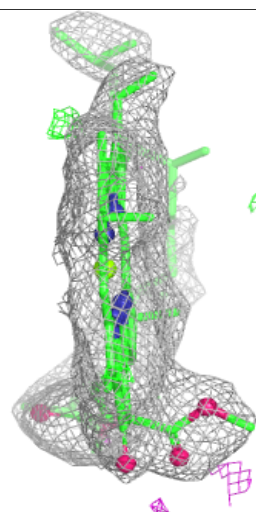
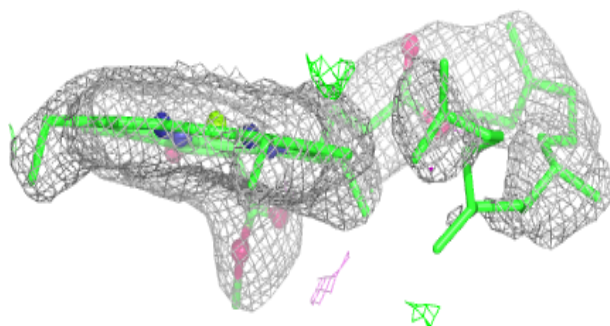
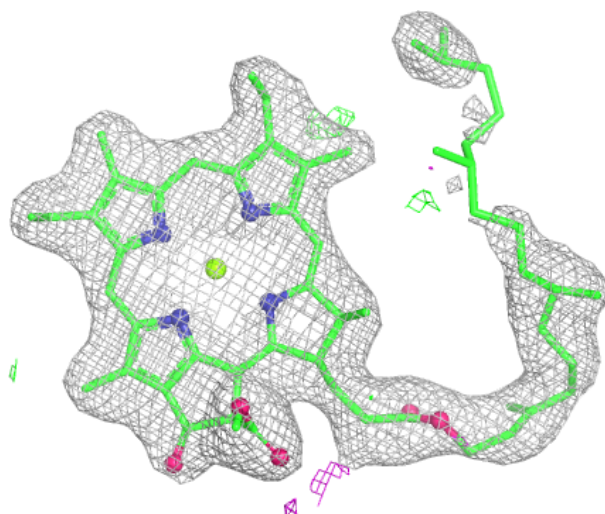
**Electron density around LMG M 101:**

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



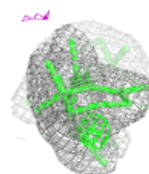
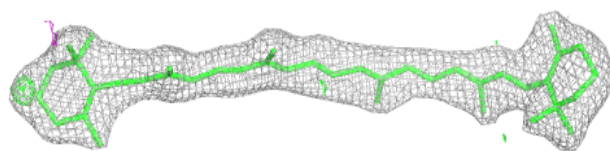
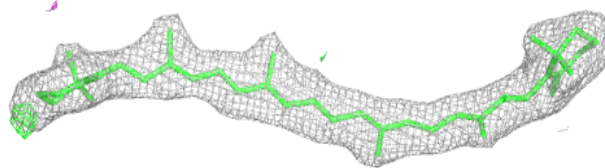
Electron density around CLA c 512:

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

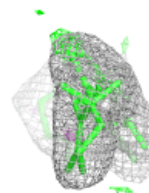
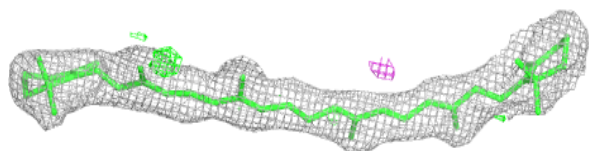
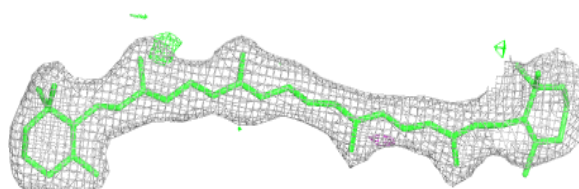


Electron density around BCR H 102:

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

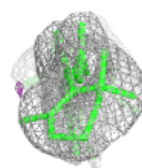
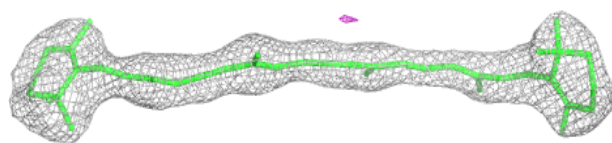
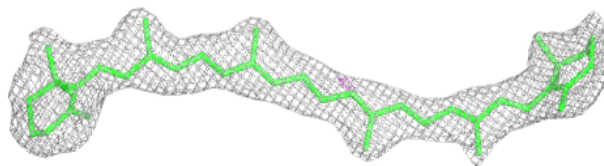
**Electron density around BCR d 405:**

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

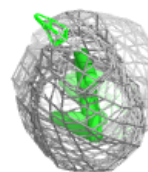
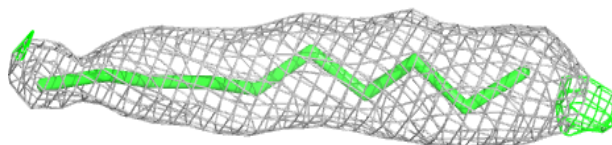
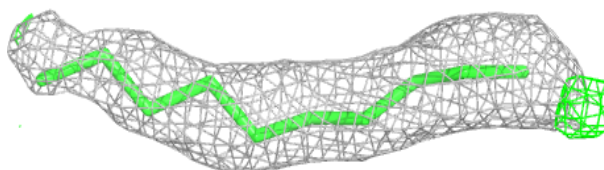


Electron density around BCR k 101:

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

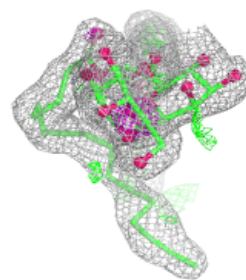
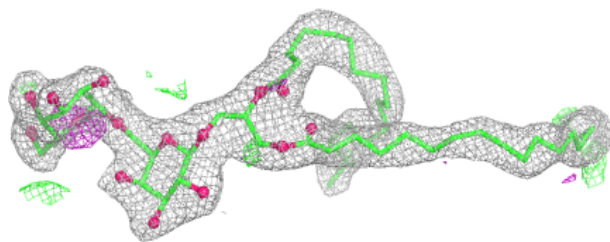
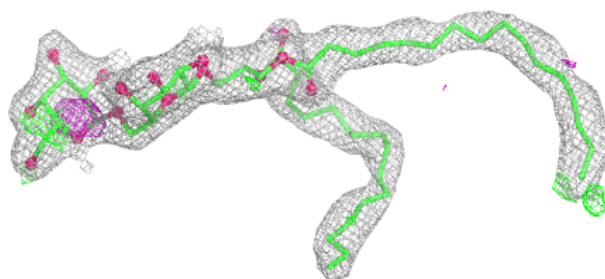
**Electron density around STE M 103:**

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

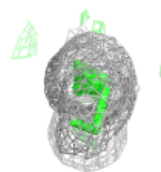
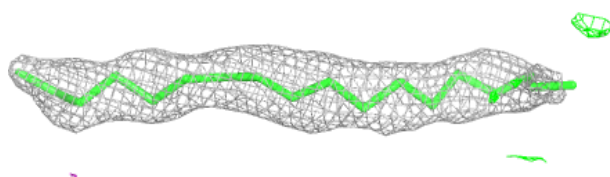
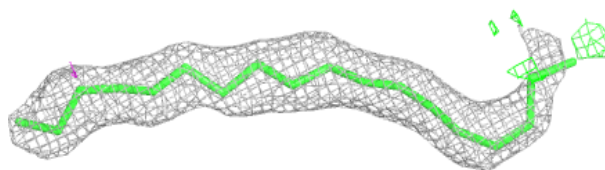


Electron density around DGD H 103:

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

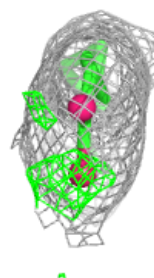
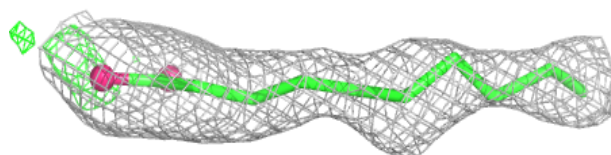
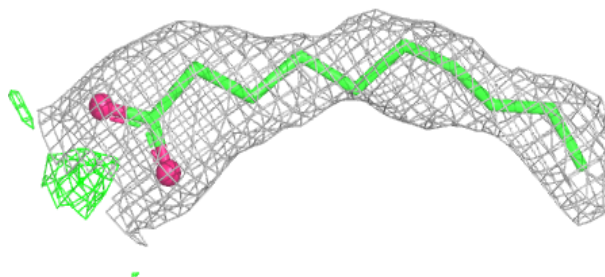
**Electron density around STE I 102:**

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

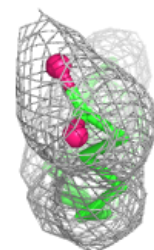
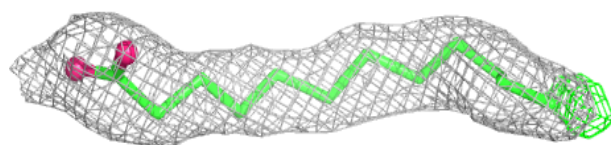
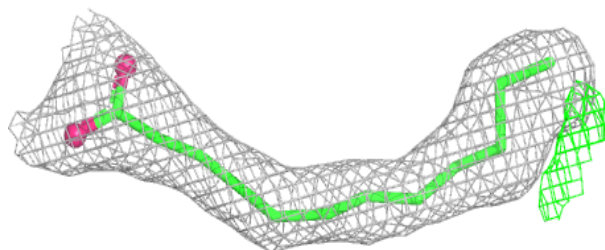


Electron density around STE C 521:

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

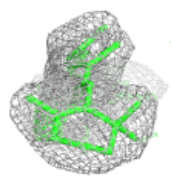
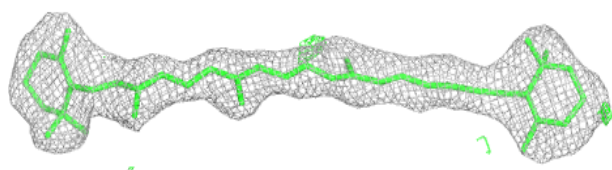
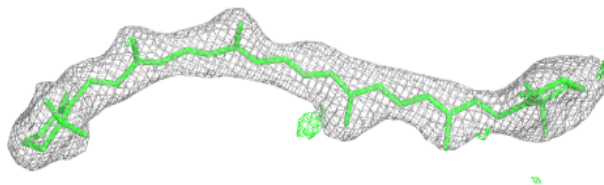
**Electron density around STE t 102:**

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

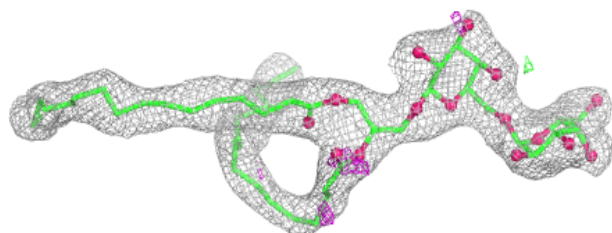
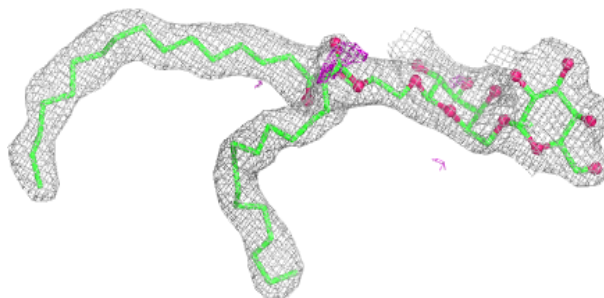


Electron density around BCR x 101:

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

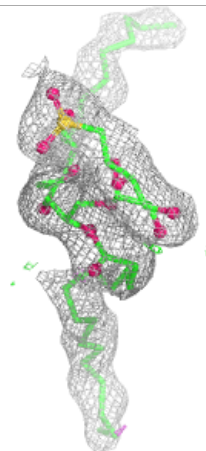
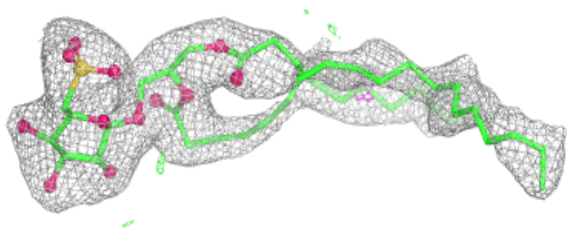
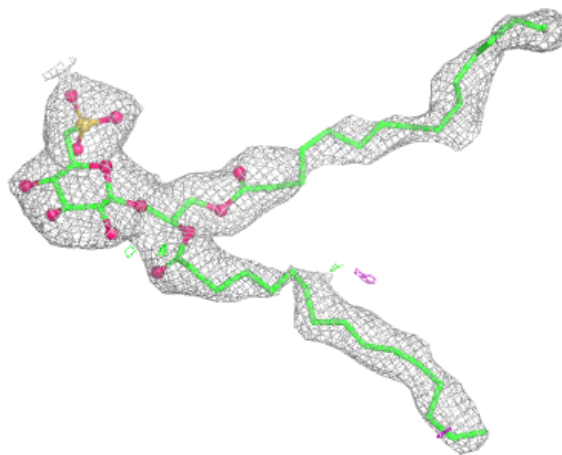
**Electron density around DGD h 102:**

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



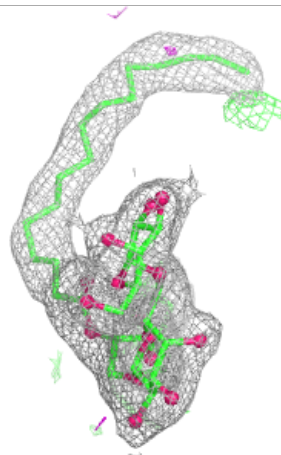
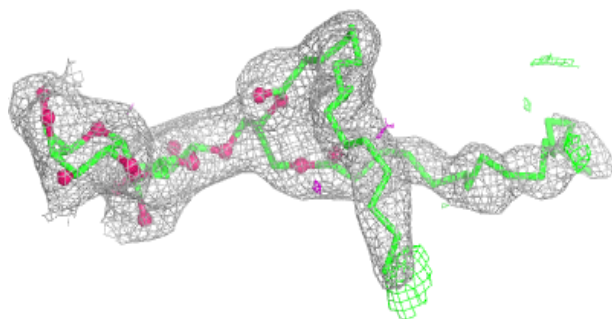
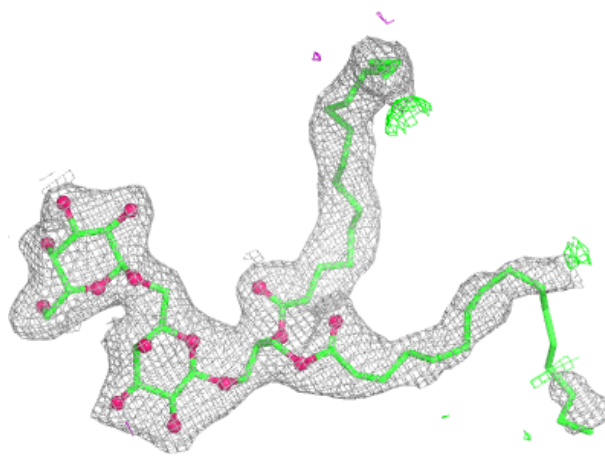
Electron density around SQD a 613:

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



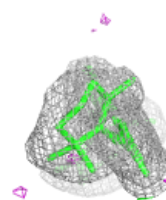
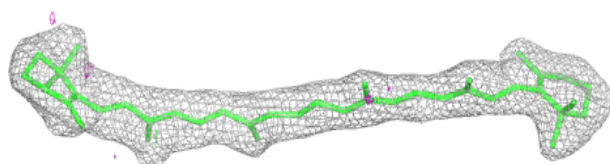
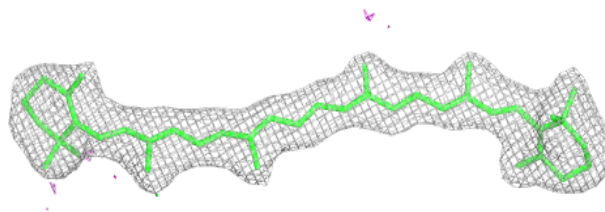
Electron density around DGD C 517:

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

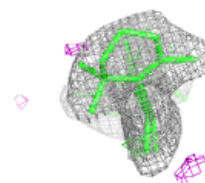
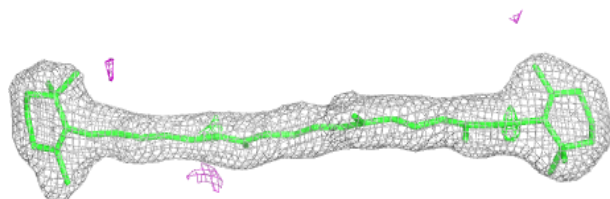
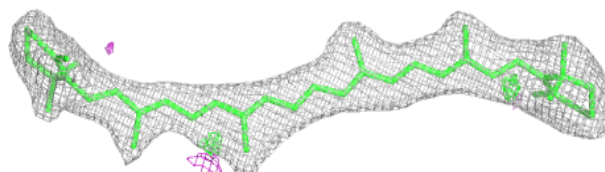


Electron density around BCR B 618:

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

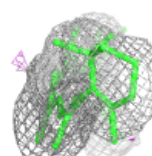
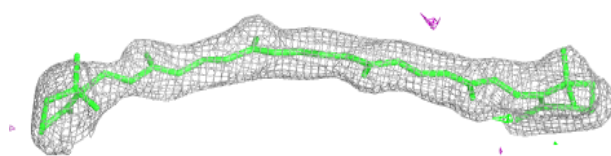
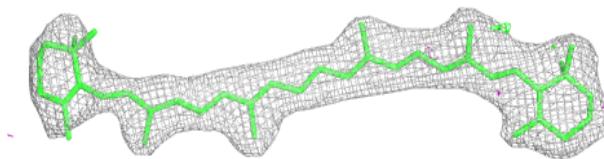
**Electron density around BCR C 514:**

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

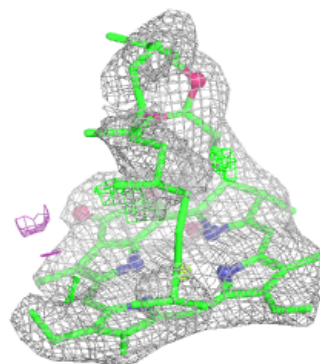
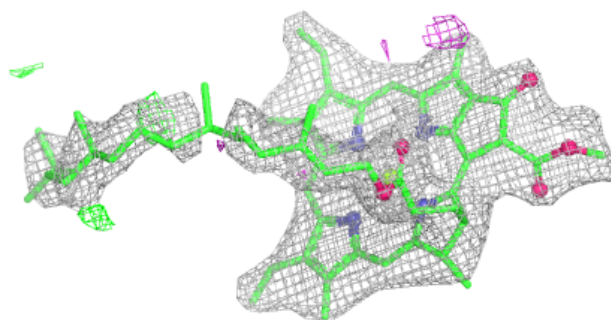
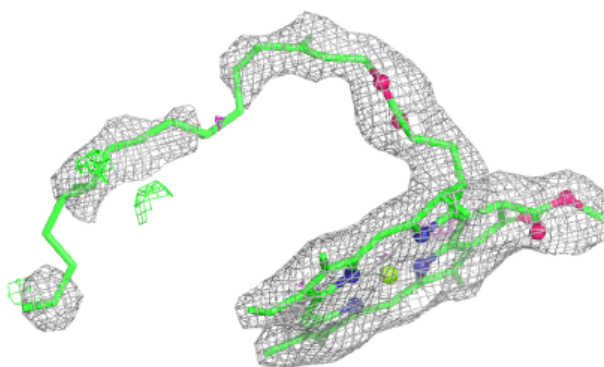


Electron density around BCR D 405:

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

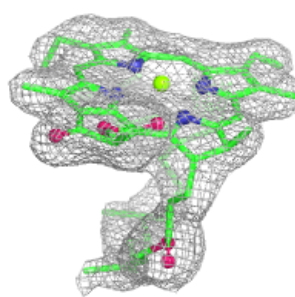
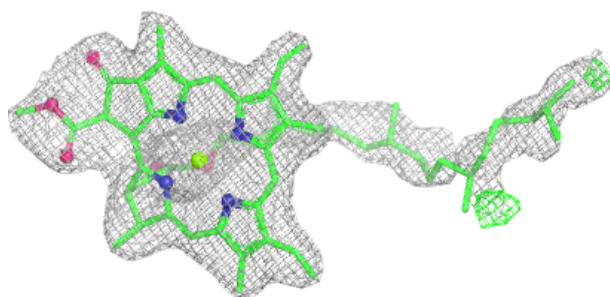
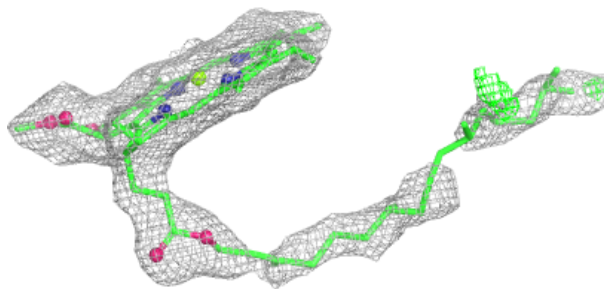
**Electron density around CLA c 513:**

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

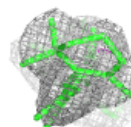
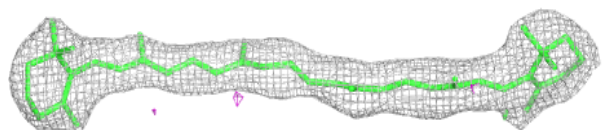
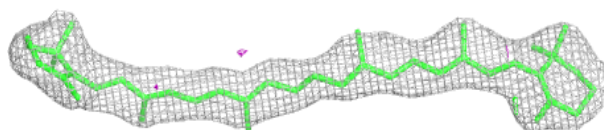


Electron density around CLA C 513:

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

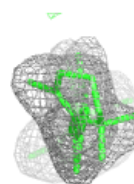
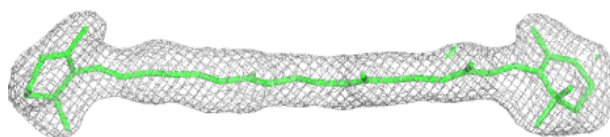
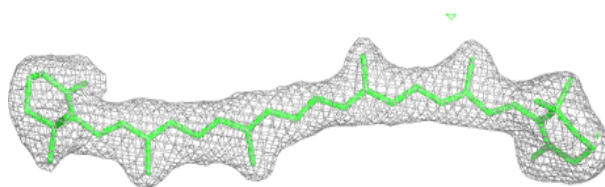
**Electron density around BCR Z 101:**

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

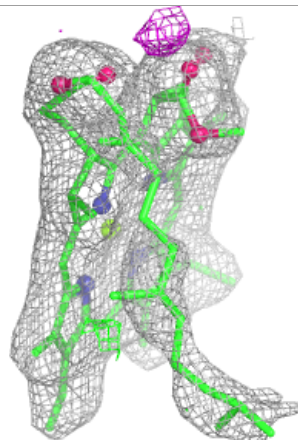
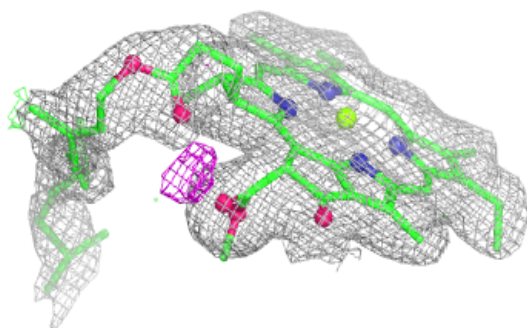
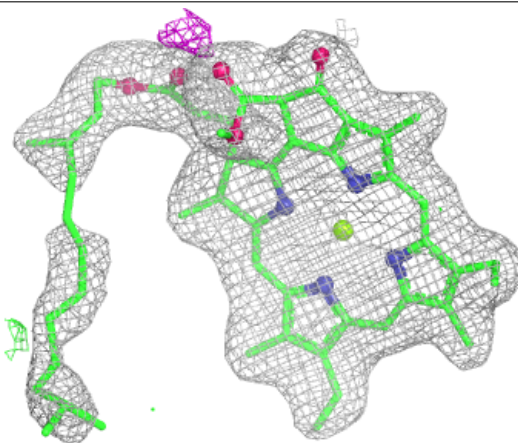


Electron density around BCR b 617:

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

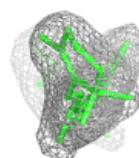
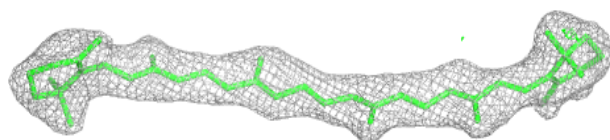
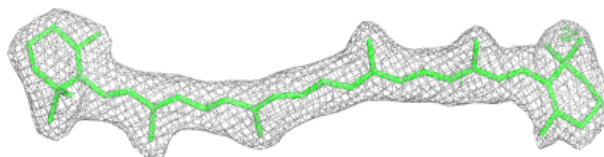
**Electron density around CLA b 615:**

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

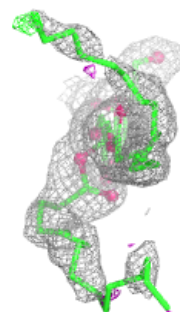
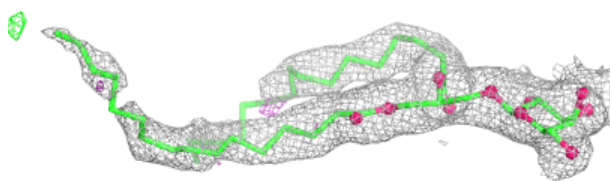
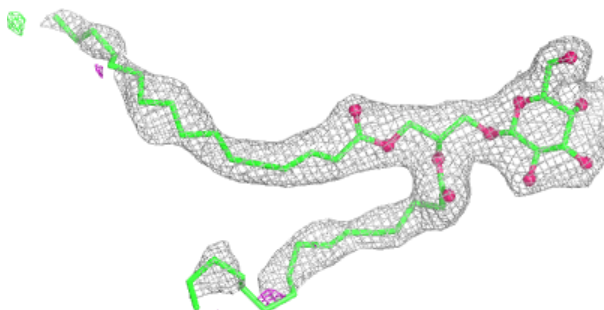


Electron density around BCR b 618:

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

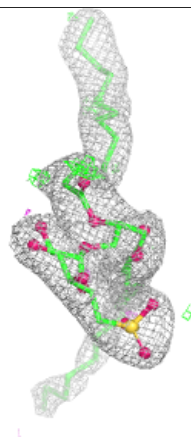
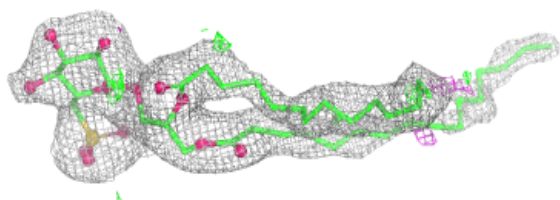
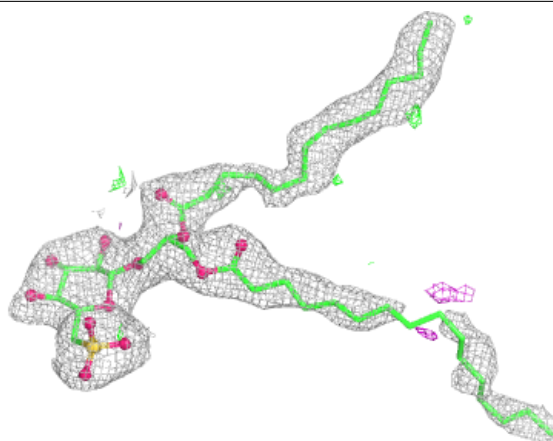
**Electron density around LMG D 407:**

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

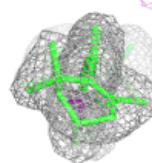
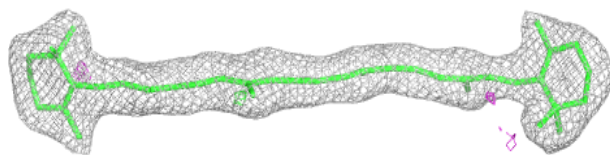
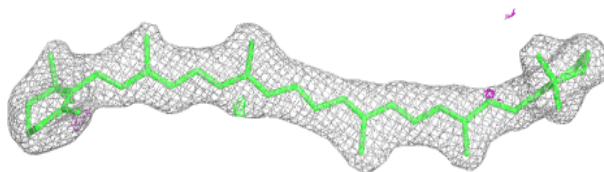


Electron density around SQD A 613:

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

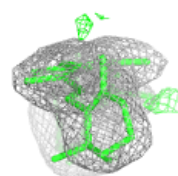
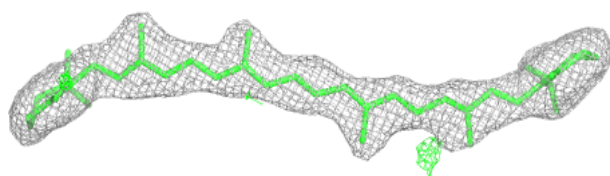
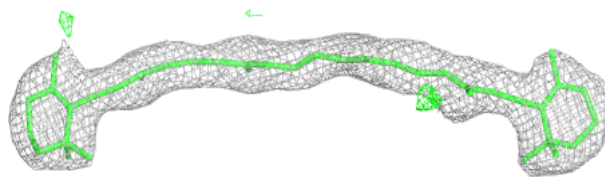
**Electron density around BCR A 610:**

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

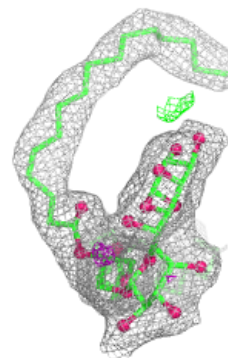
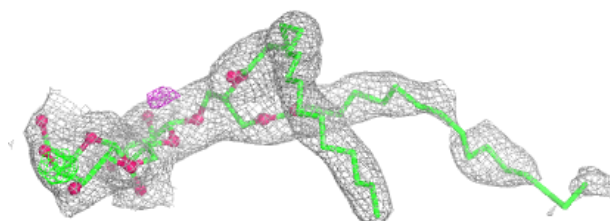


Electron density around BCR c 516:

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

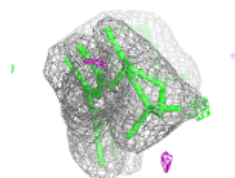
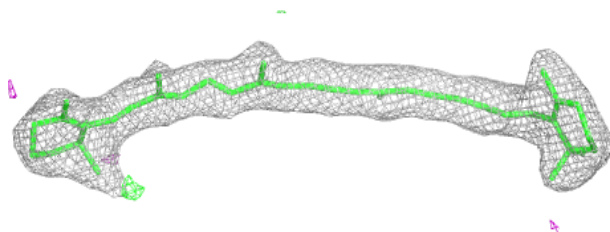
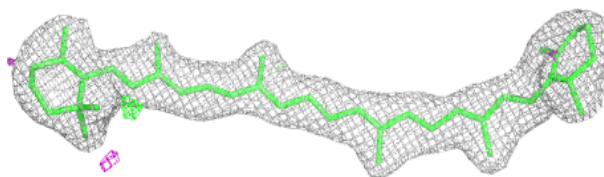
**Electron density around DGD c 518:**

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



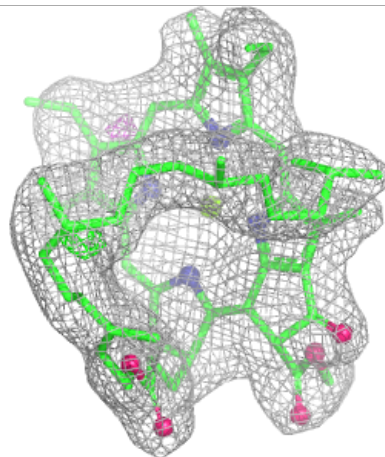
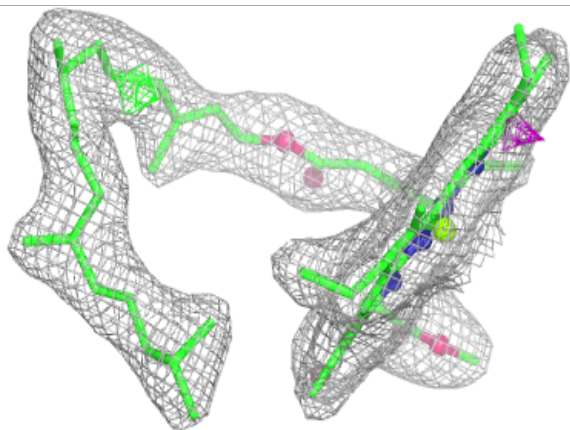
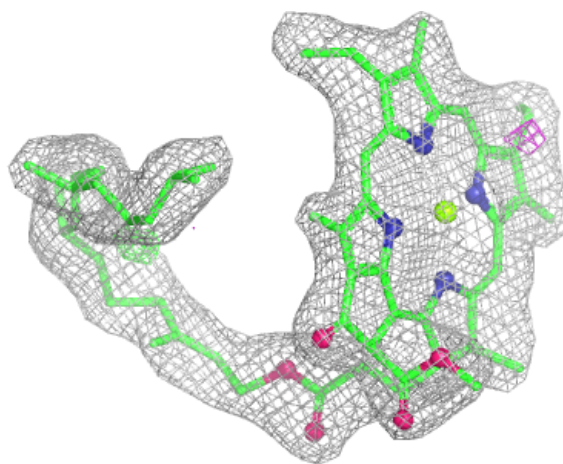
Electron density around BCR T 101:

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



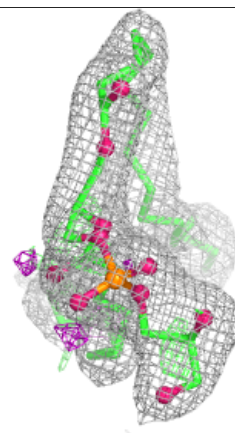
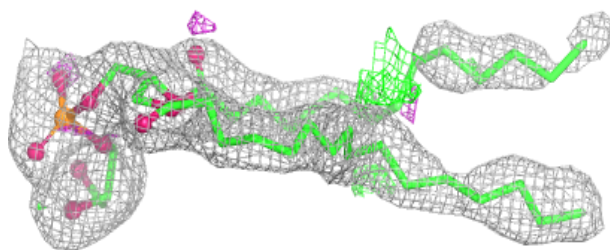
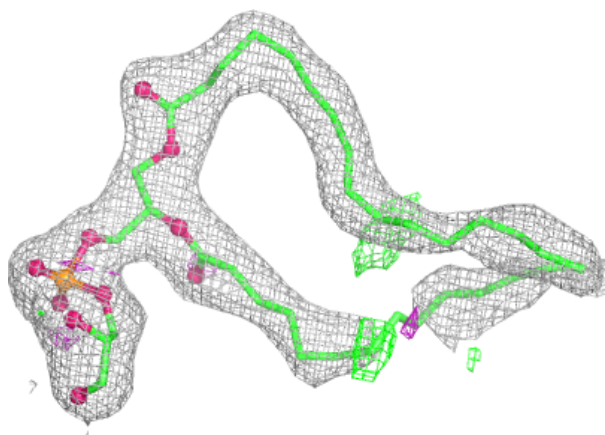
Electron density around CLA C 503:

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

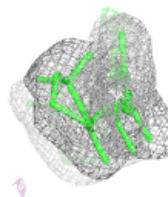
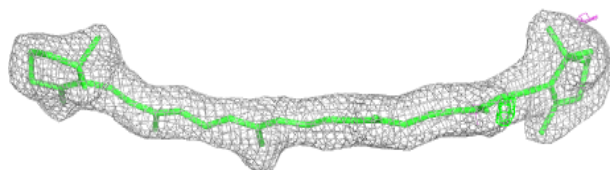
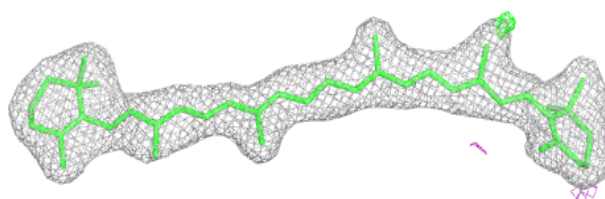


Electron density around LHG D 410:

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

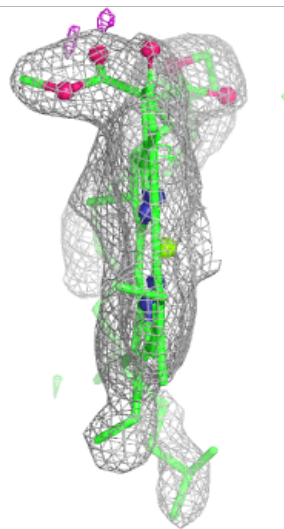
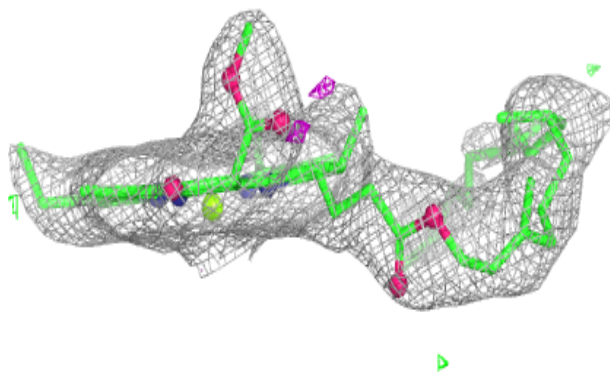
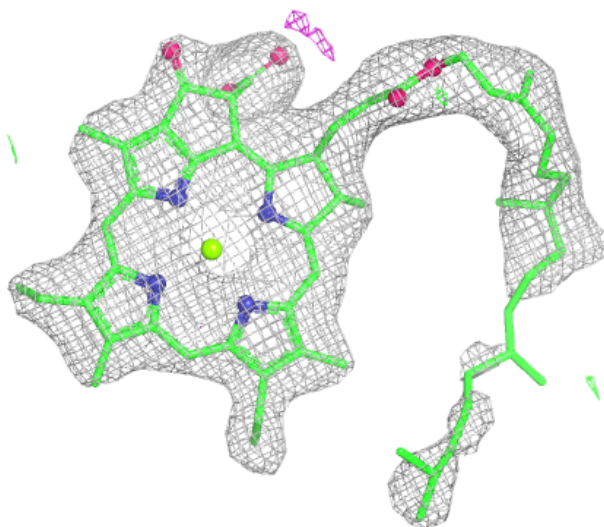
**Electron density around BCR t 101:**

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



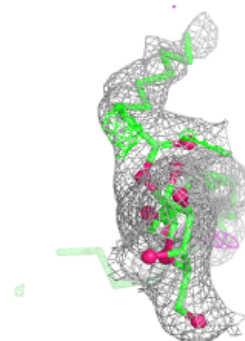
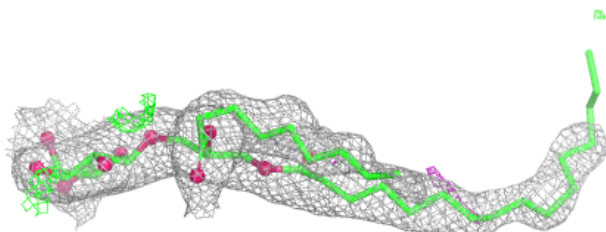
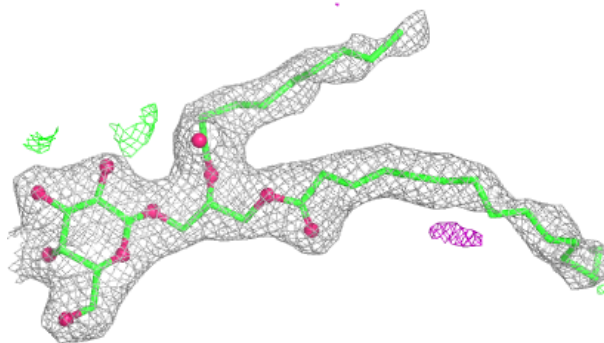
Electron density around CLA C 512:

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

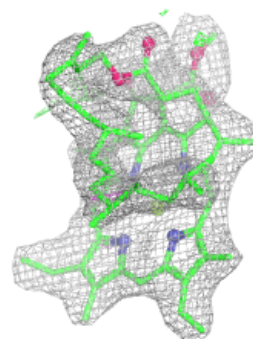
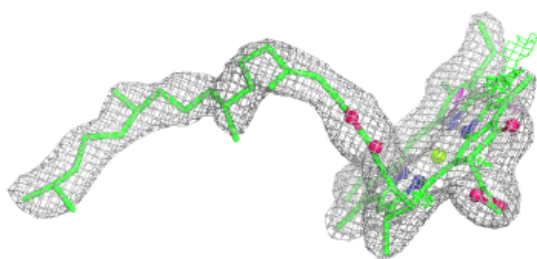
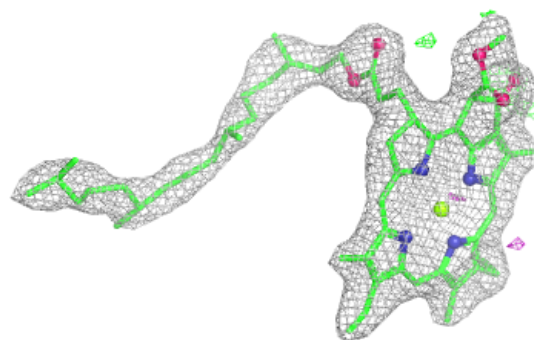


Electron density around LMG d 410:

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

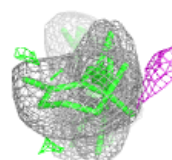
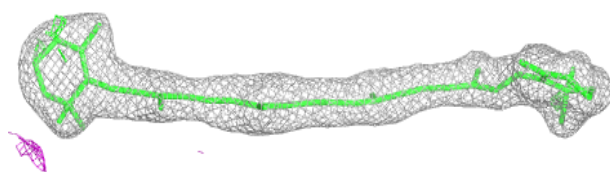
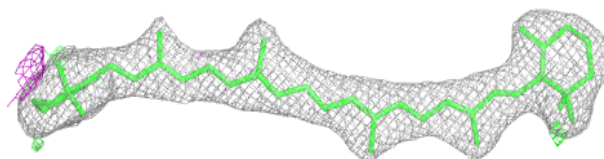
**Electron density around CLA c 511:**

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

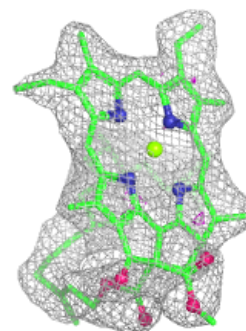
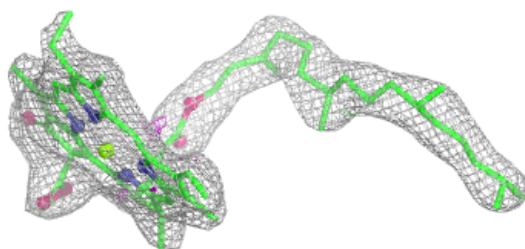
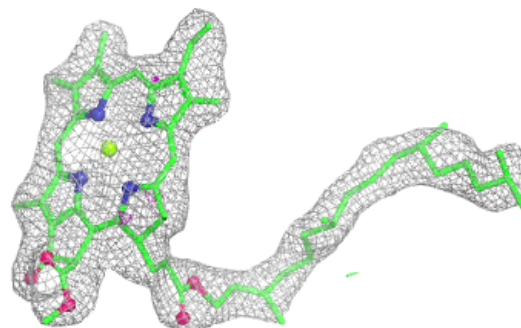


Electron density around BCR b 616:

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

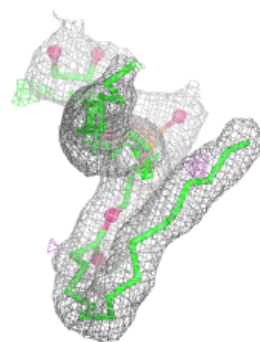
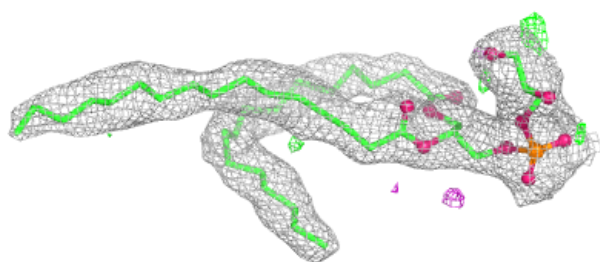
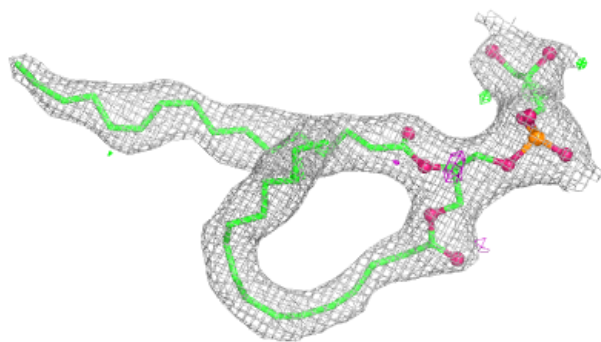
**Electron density around CLA C 511:**

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



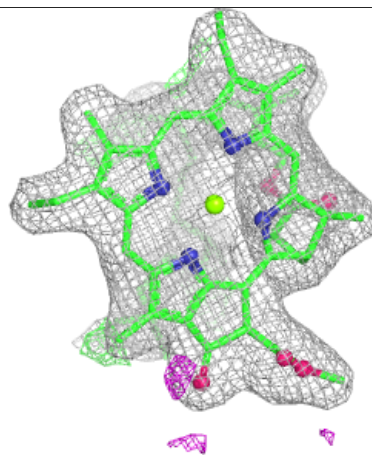
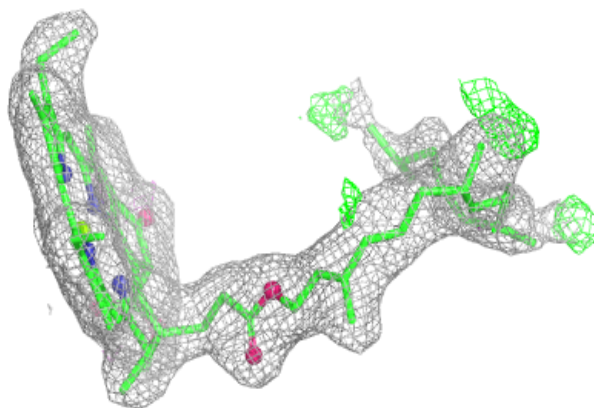
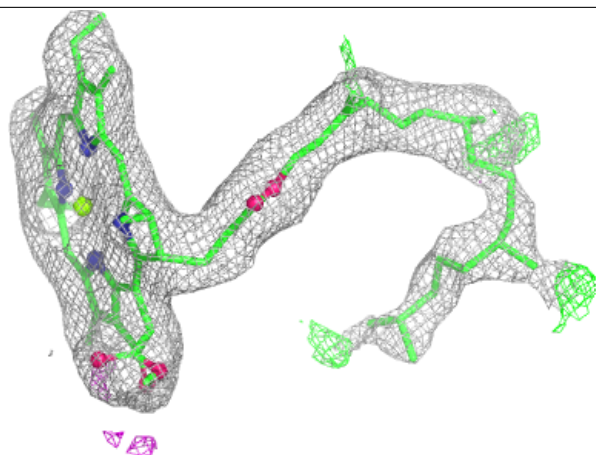
Electron density around LHG B 620:

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



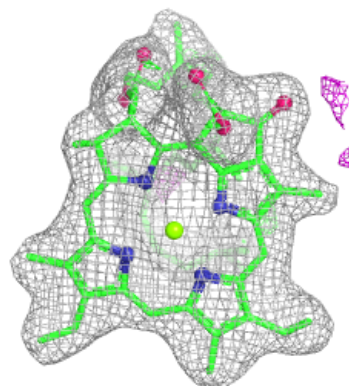
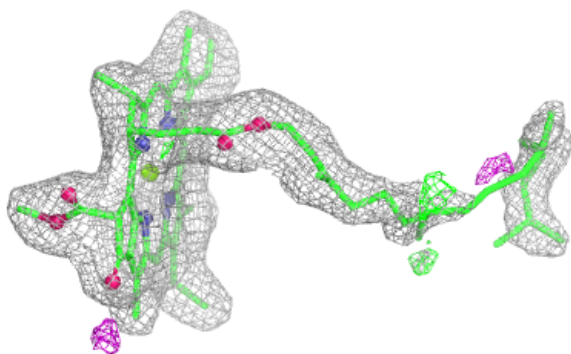
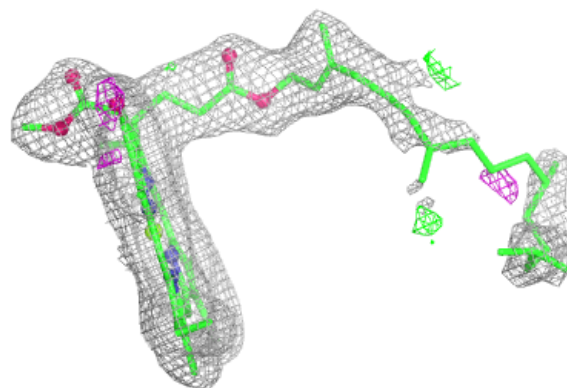
Electron density around CLA B 605:

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

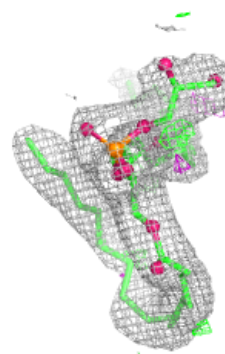
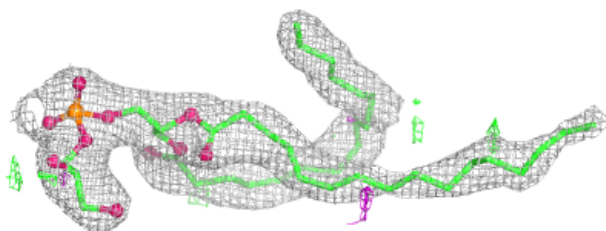
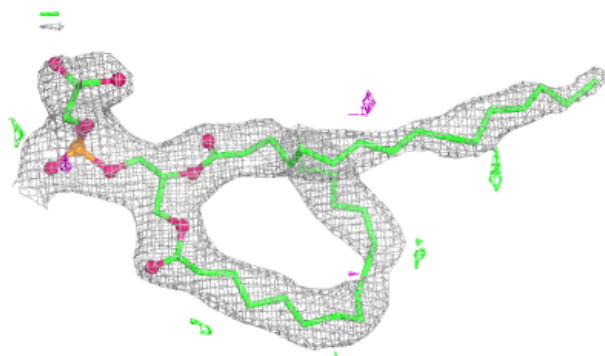


Electron density around CLA C 506:

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

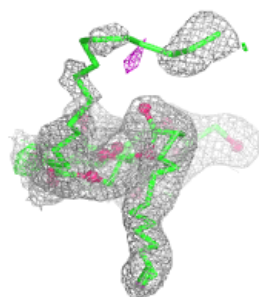
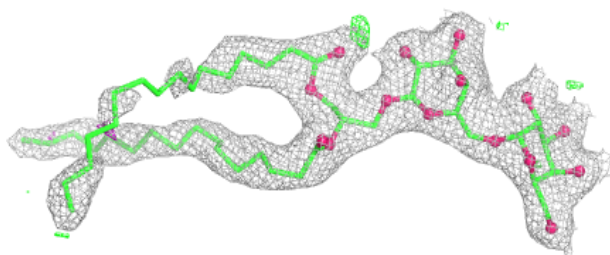
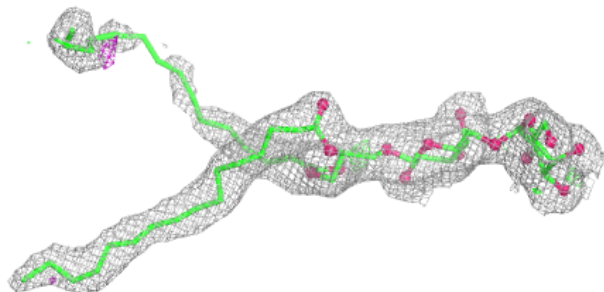
**Electron density around LHG b 623:**

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

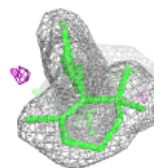
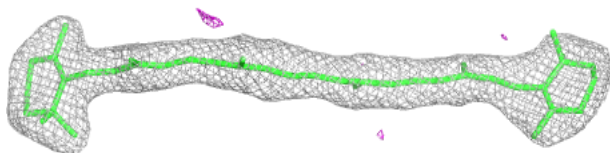
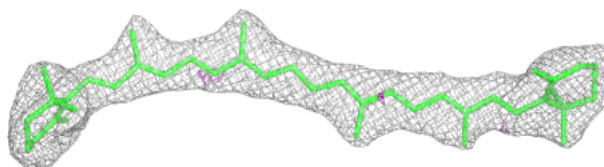


Electron density around DGD C 516:

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

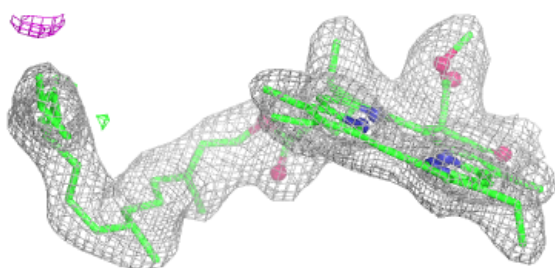
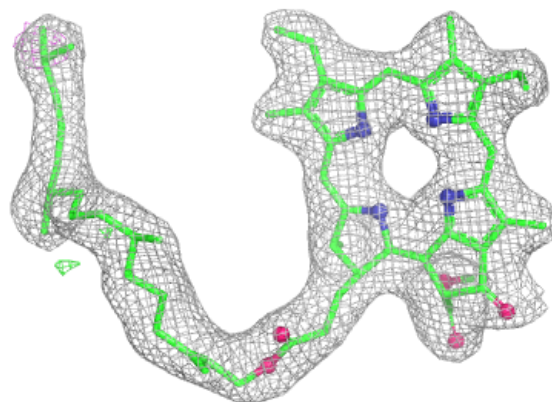
**Electron density around BCR c 515:**

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

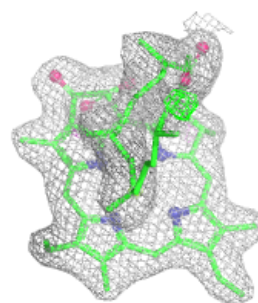
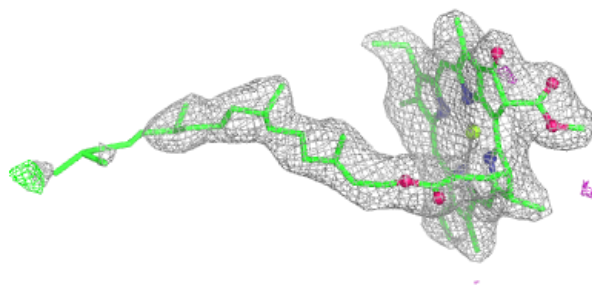
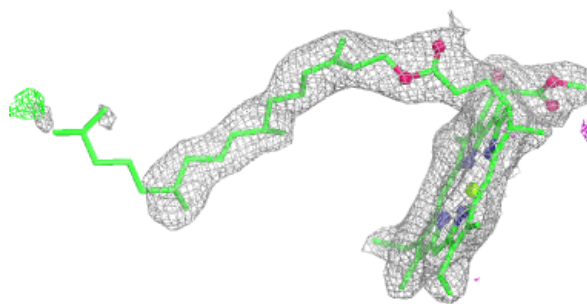


Electron density around PHO d 402:

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

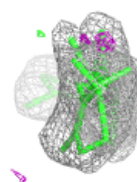
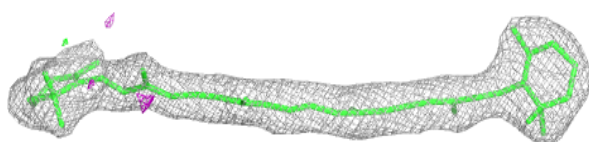
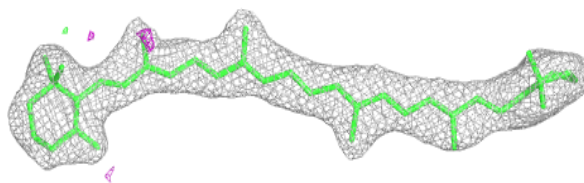
**Electron density around CLA C 508:**

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

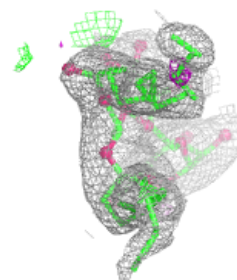
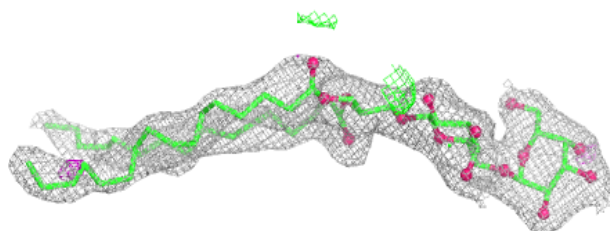
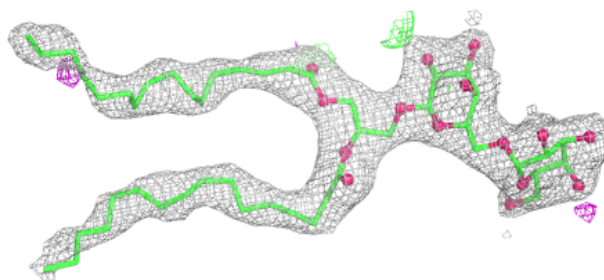


Electron density around BCR B 616:

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

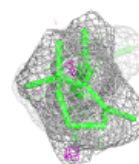
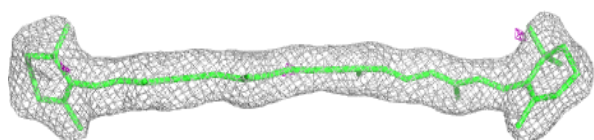
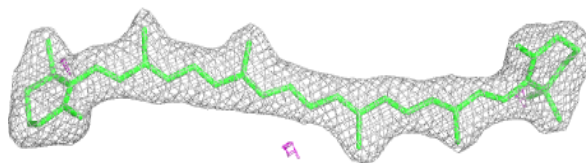
**Electron density around DGD c 519:**

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

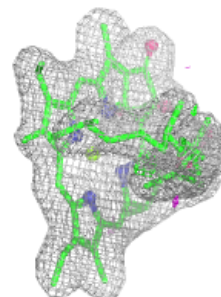
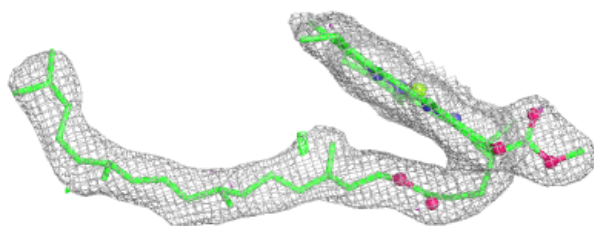
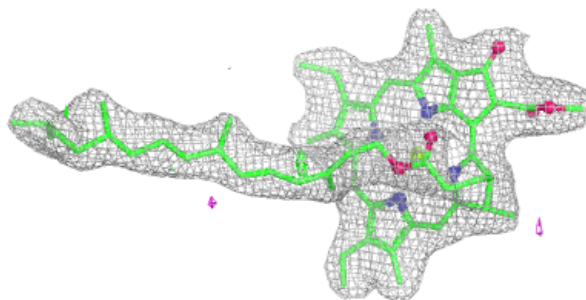


Electron density around BCR B 617:

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

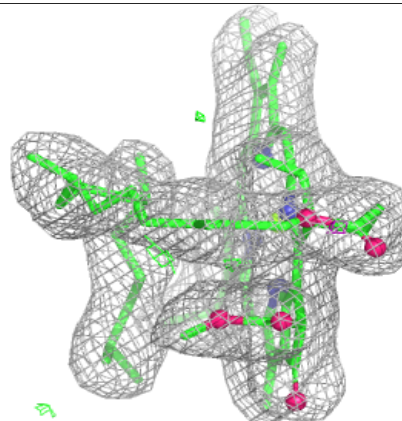
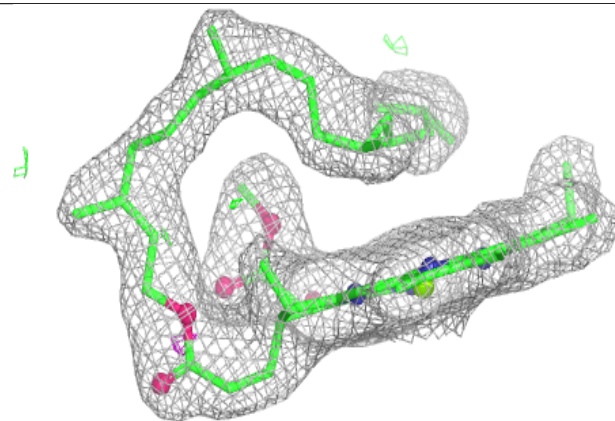
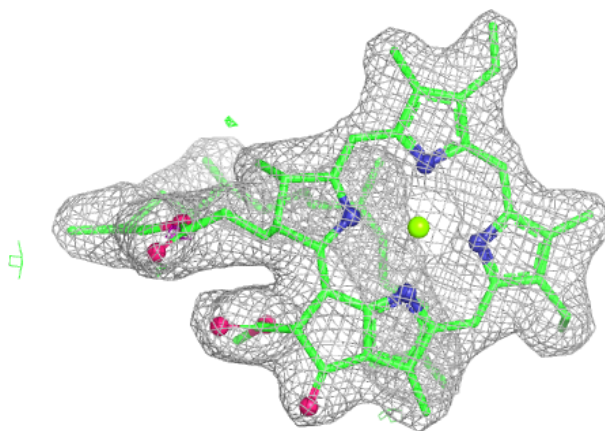
**Electron density around CLA b 607:**

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

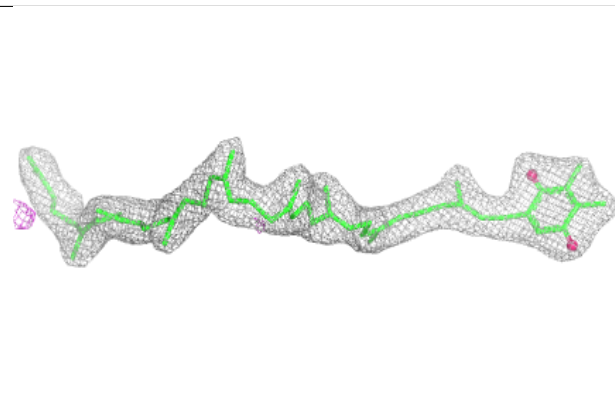
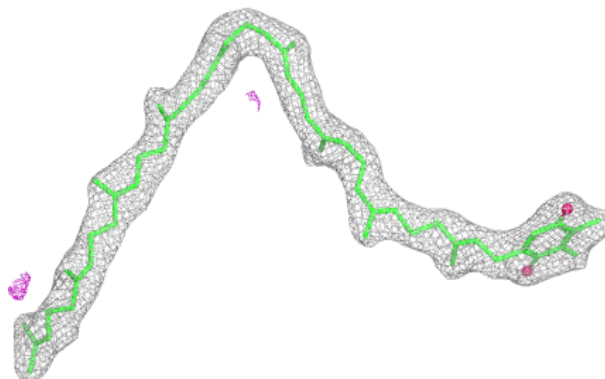


Electron density around CLA C 510:

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

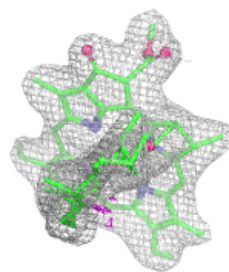
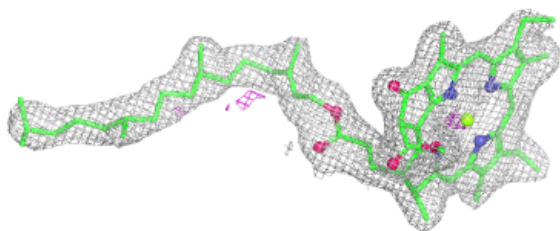
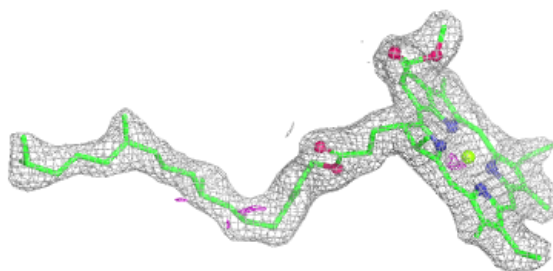
**Electron density around PL9 D 406:**

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



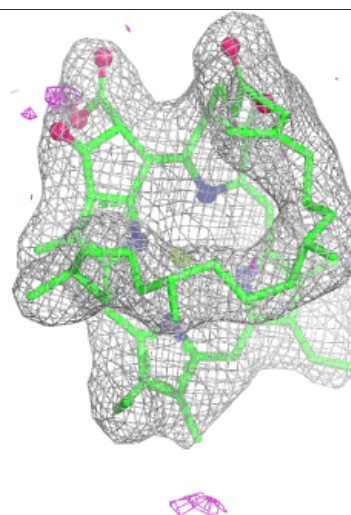
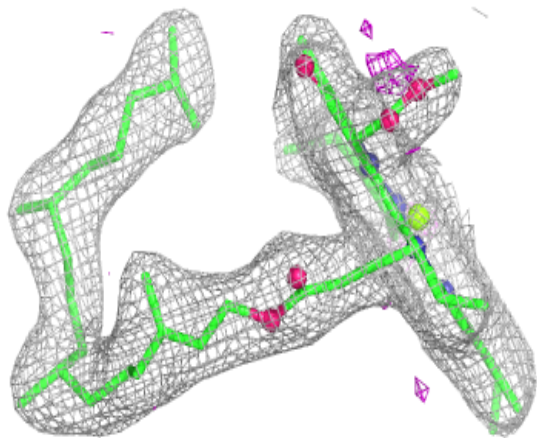
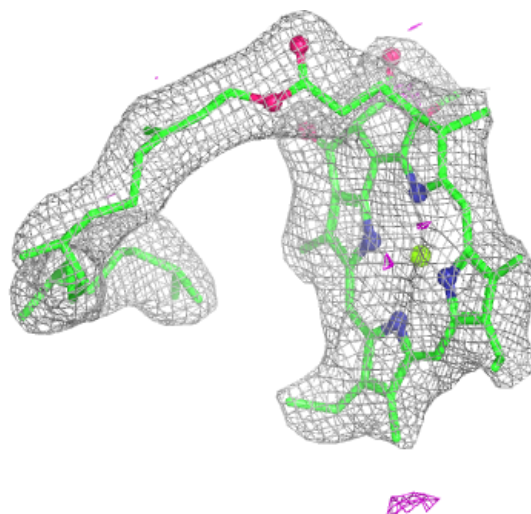
Electron density around CLA c 502:

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



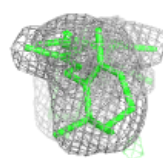
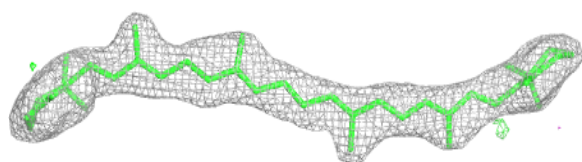
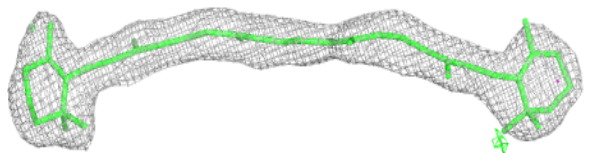
Electron density around CLA c 503:

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

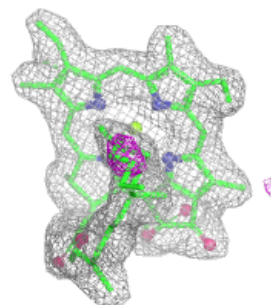
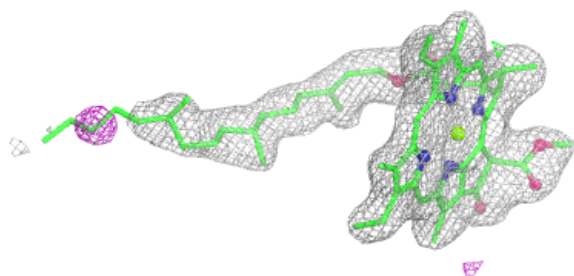
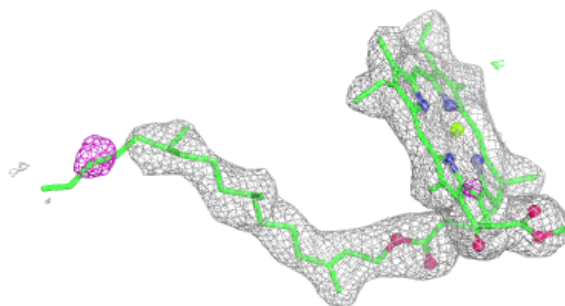


Electron density around BCR K 101:

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

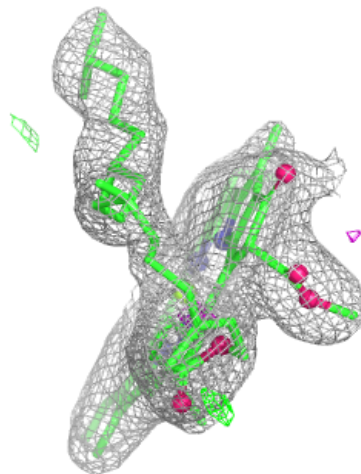
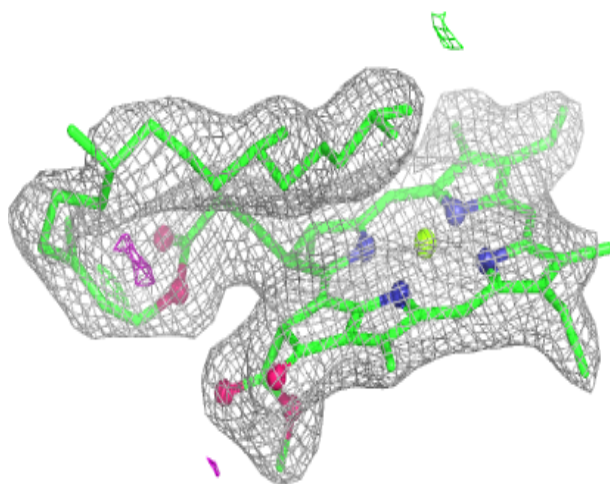
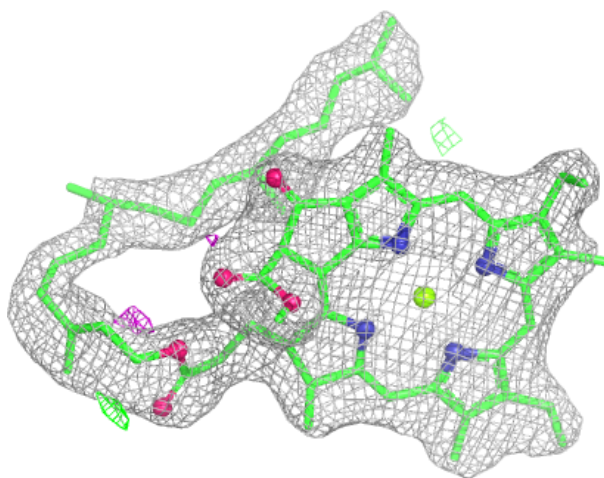
**Electron density around CLA c 508:**

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



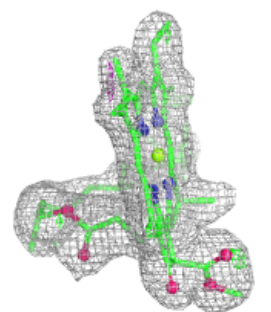
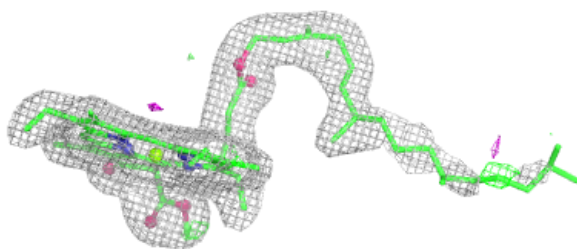
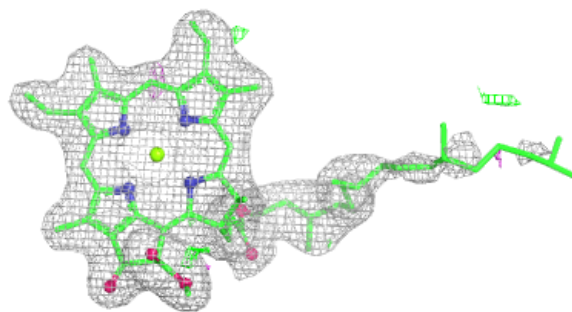
Electron density around CLA c 509:

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



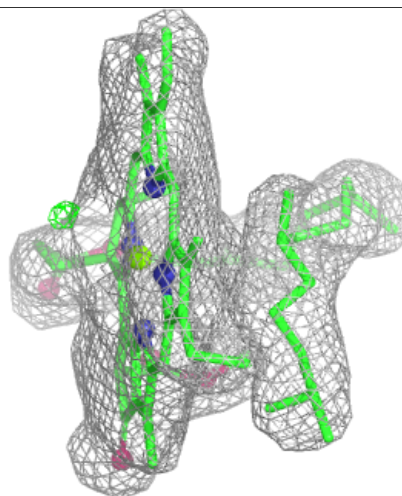
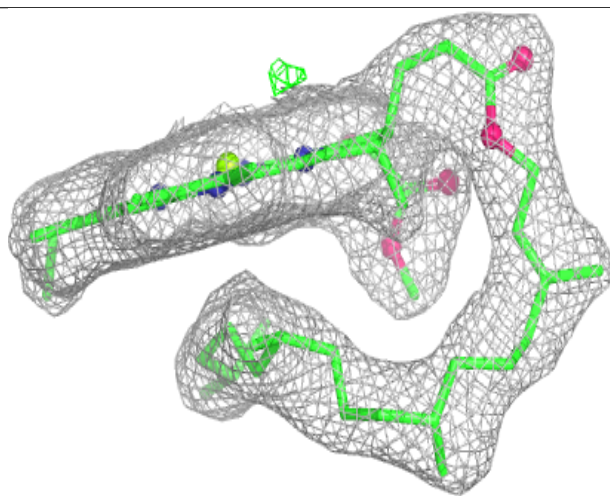
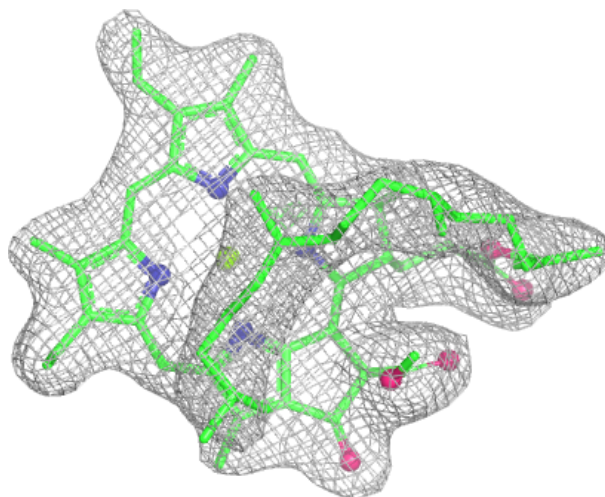
Electron density around CLA A 607:

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



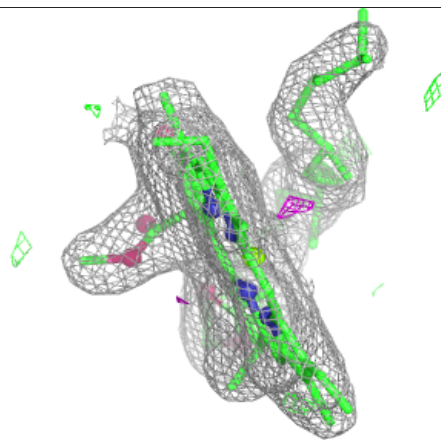
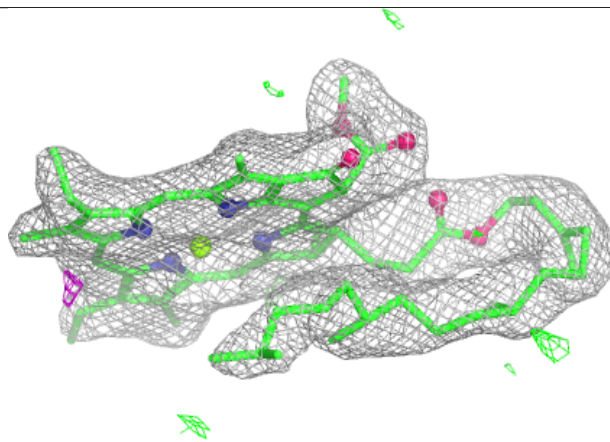
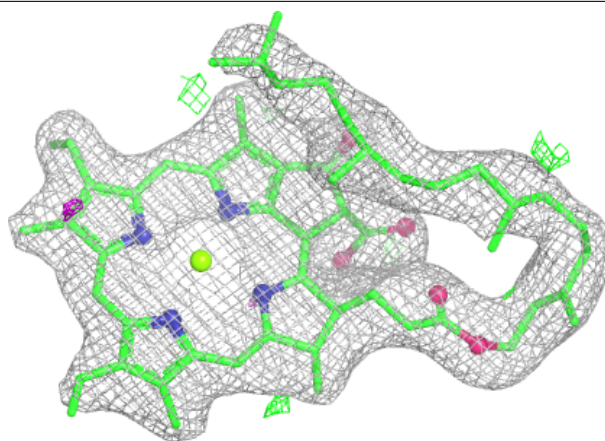
Electron density around CLA c 510:

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

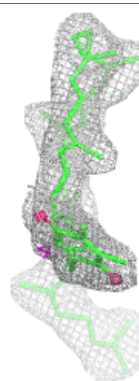
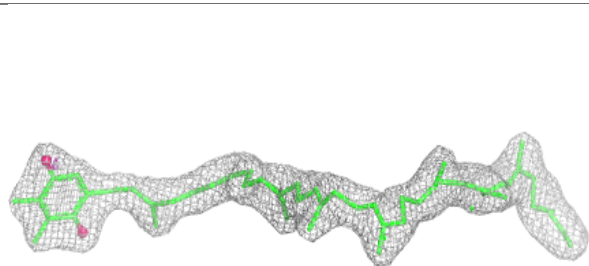
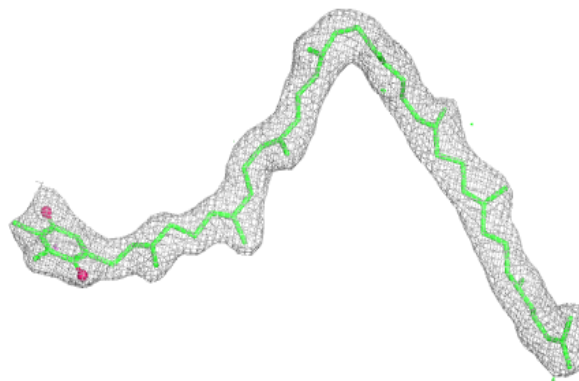


Electron density around CLA C 509:

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

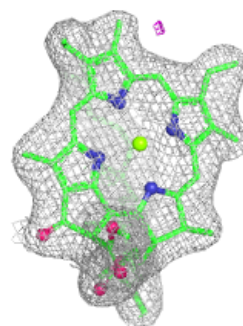
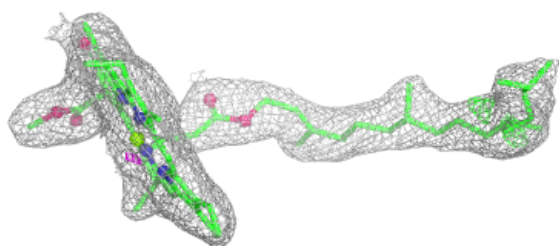
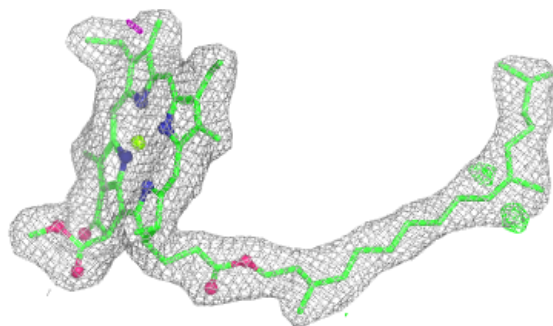
**Electron density around PL9 d 406:**

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



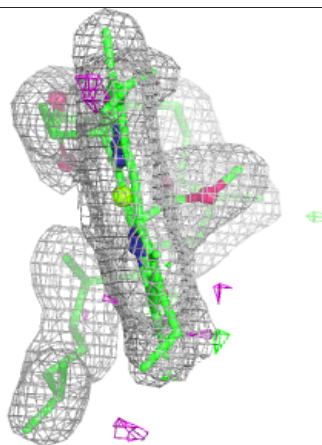
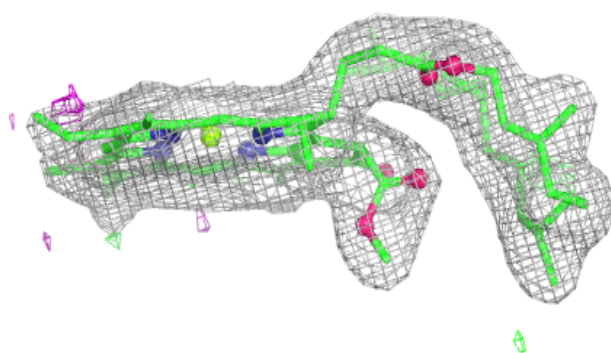
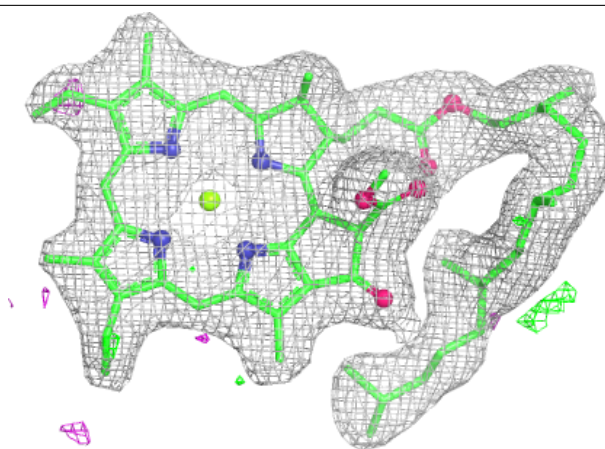
Electron density around CLA B 608:

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



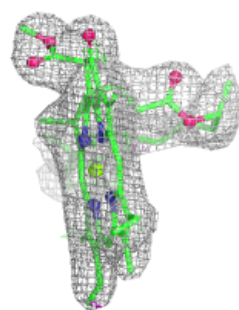
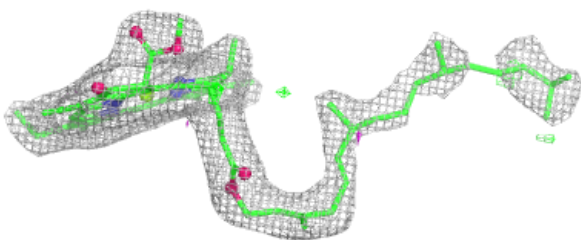
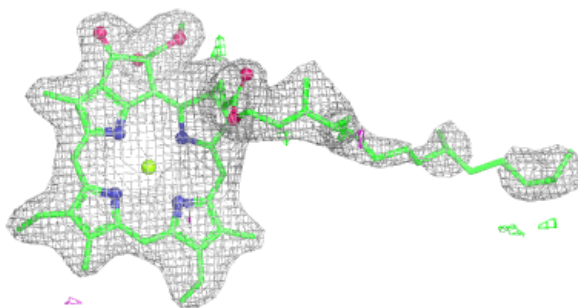
Electron density around CLA B 609:

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

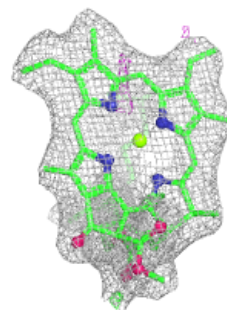
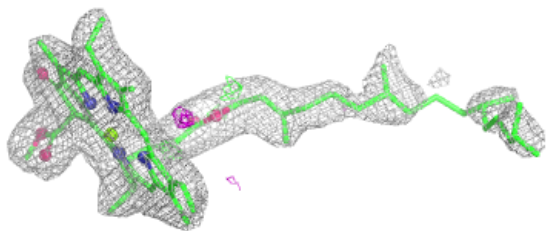
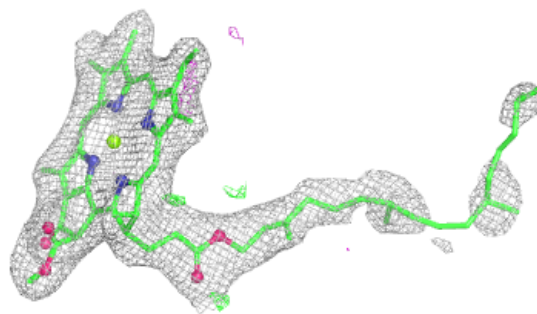


Electron density around CLA d 401:

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

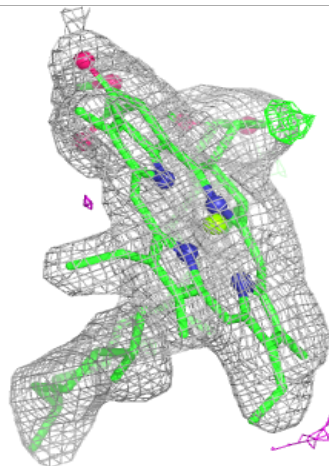
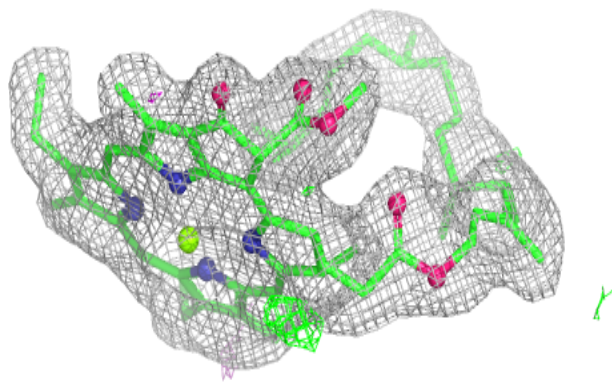
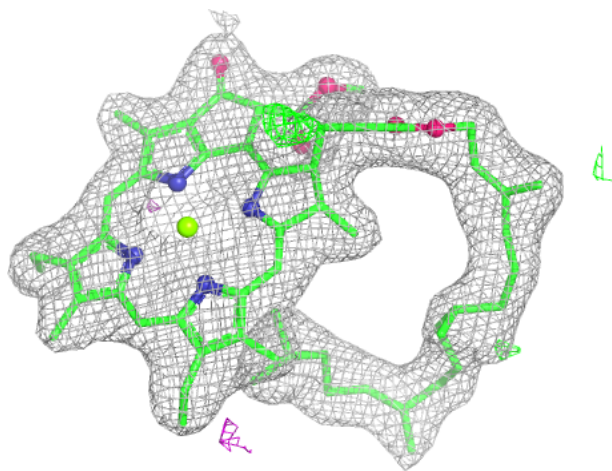
**Electron density around CLA d 404:**

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



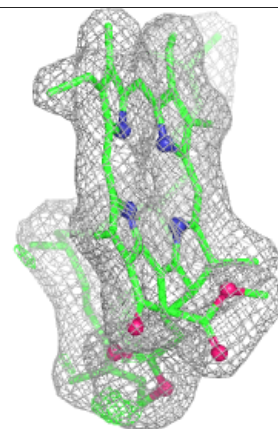
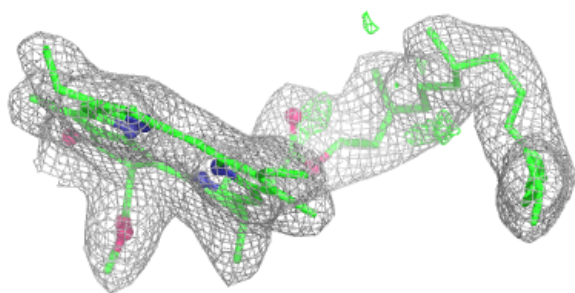
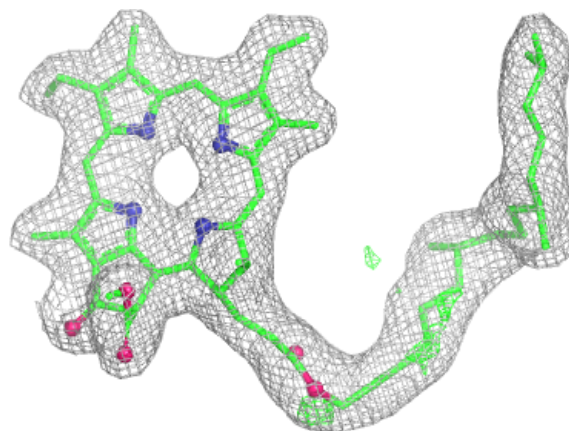
Electron density around CLA B 614:

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



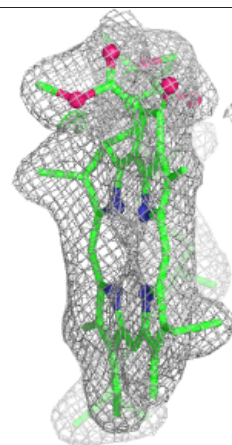
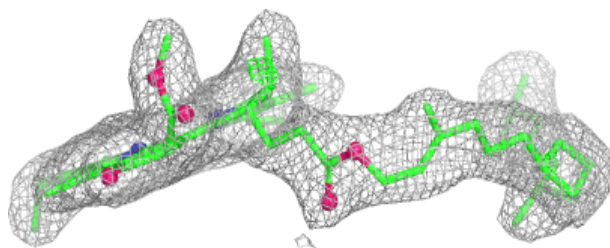
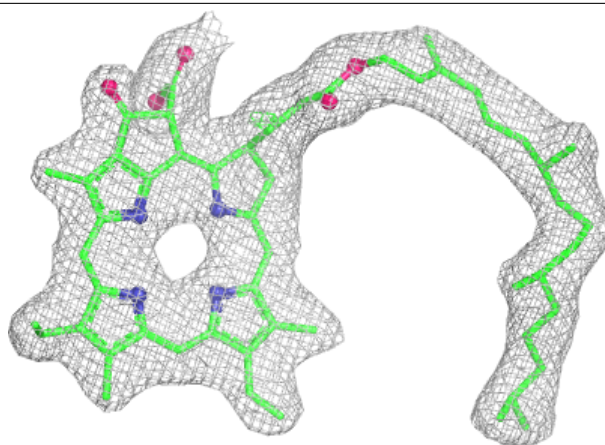
Electron density around PHO D 402:

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



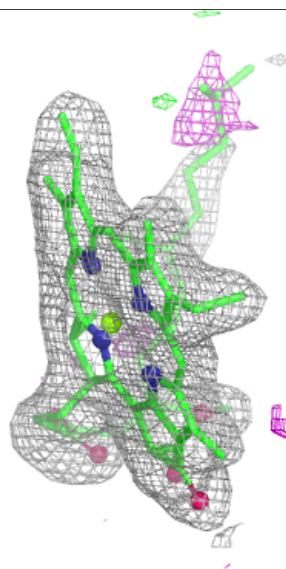
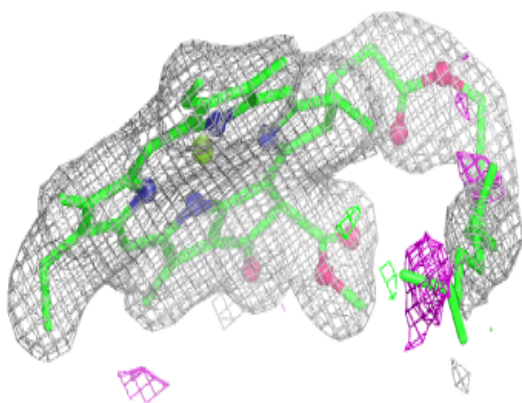
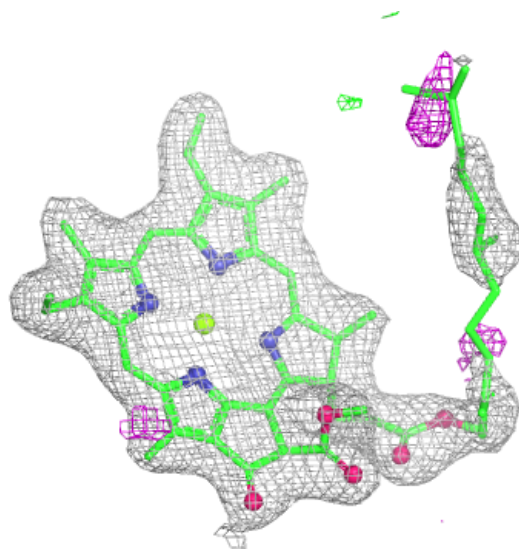
Electron density around PHO a 608:

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



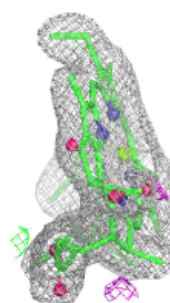
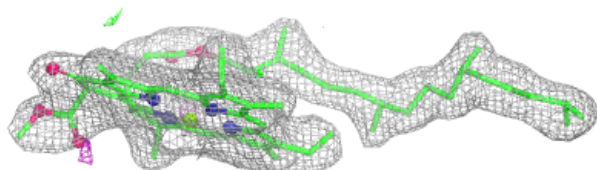
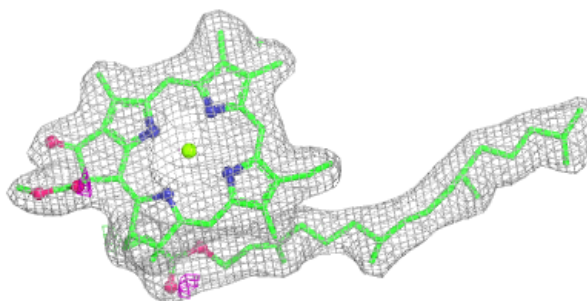
Electron density around CLA B 615:

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

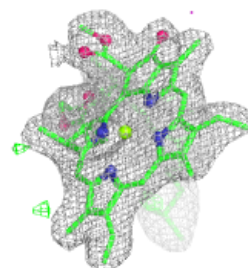
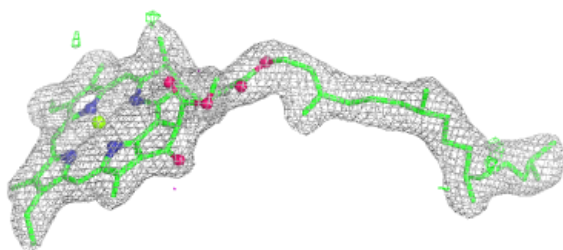
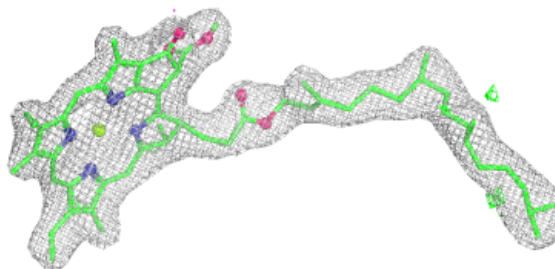


Electron density around CLA C 501:

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

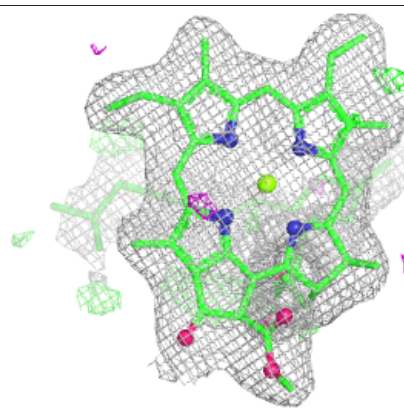
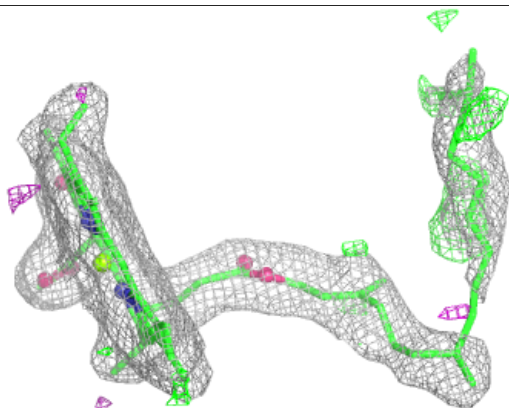
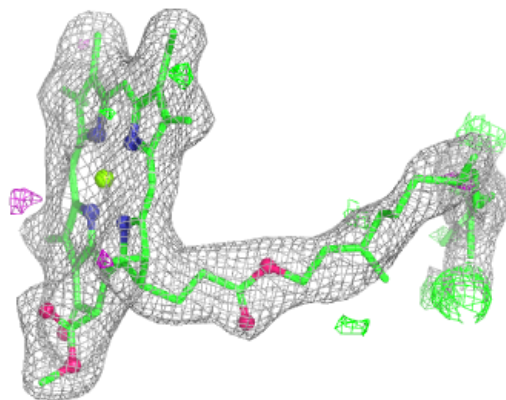
**Electron density around CLA a 607:**

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

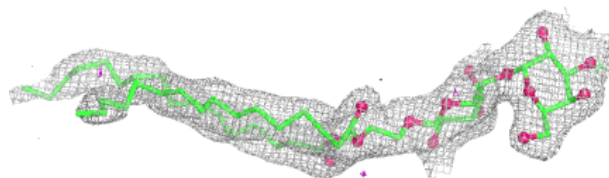
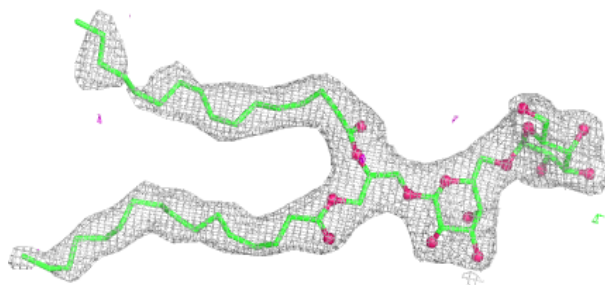


Electron density around CLA a 609:

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

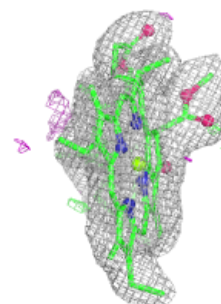
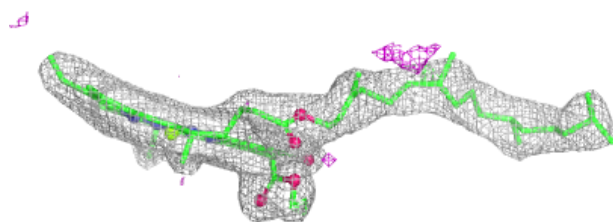
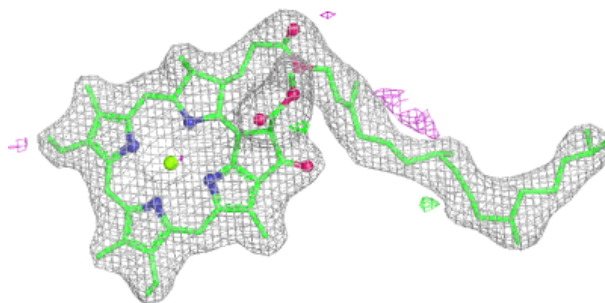
**Electron density around DGD C 518:**

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

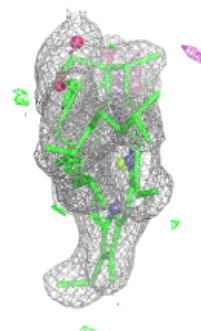
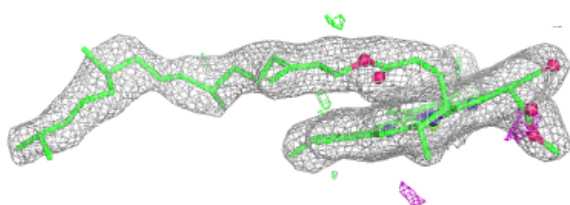
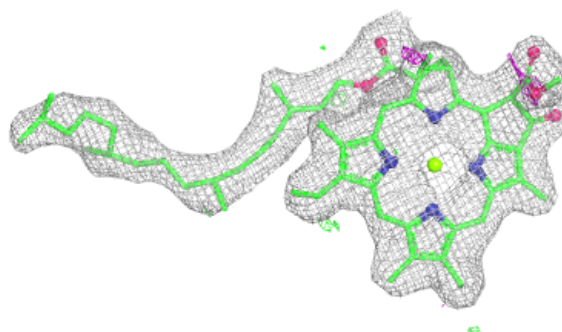


Electron density around CLA b 601:

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

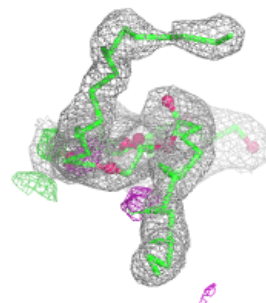
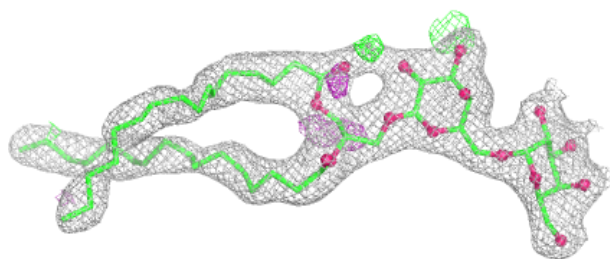
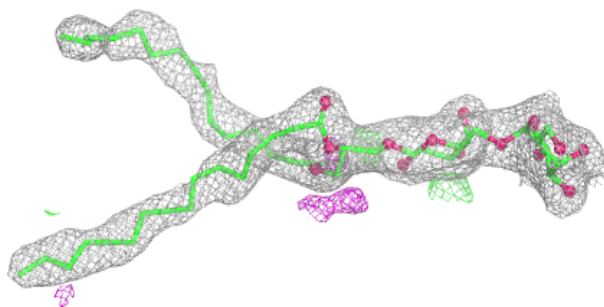
**Electron density around CLA b 602:**

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

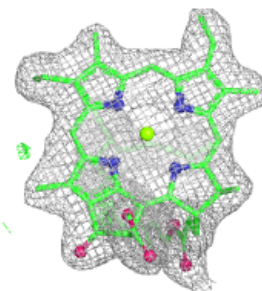
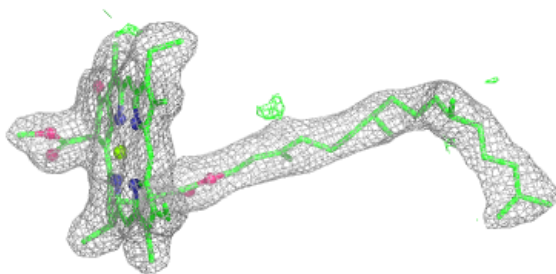
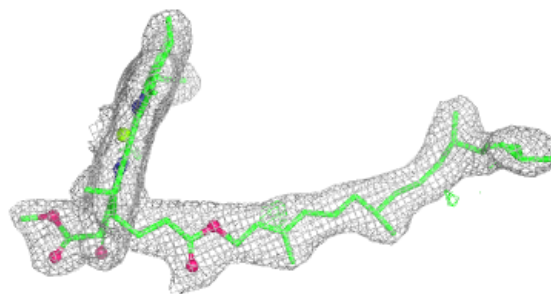


Electron density around DGD c 517:

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

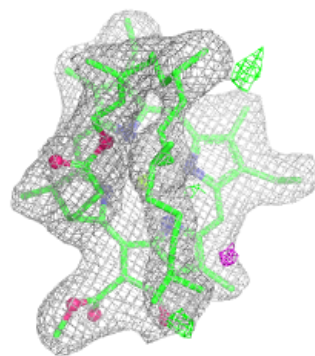
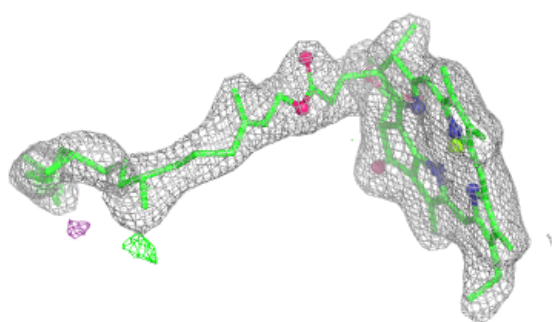
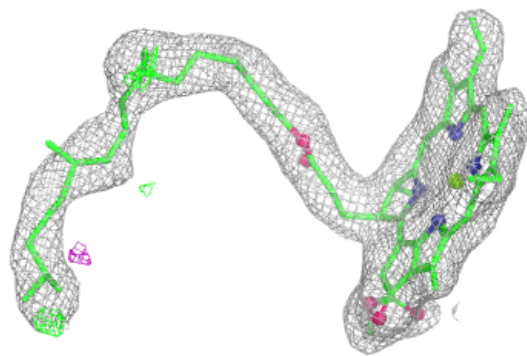
**Electron density around CLA b 604:**

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

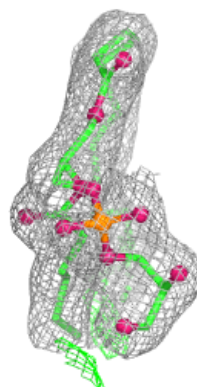
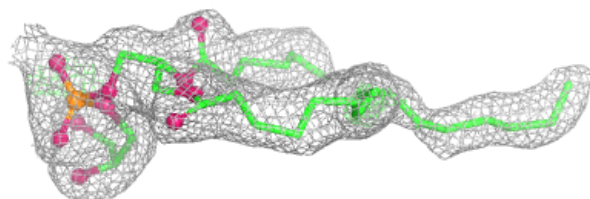
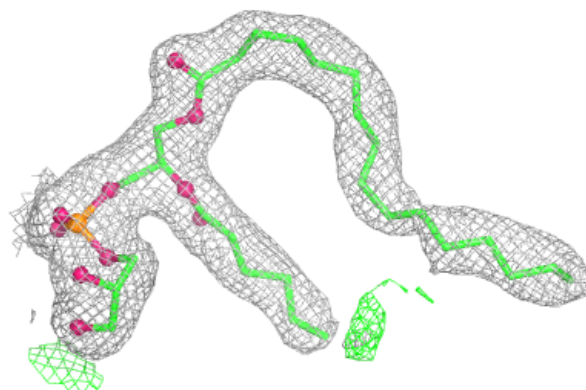


Electron density around CLA b 605:

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

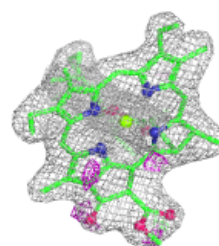
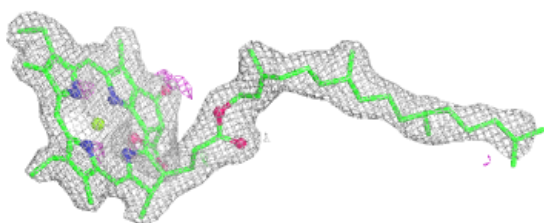
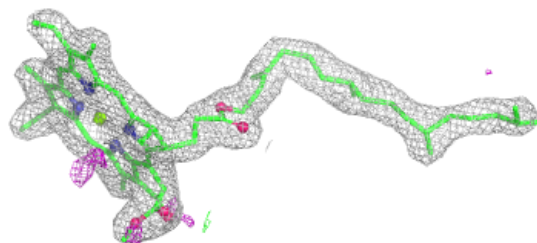
**Electron density around LHG d 408:**

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



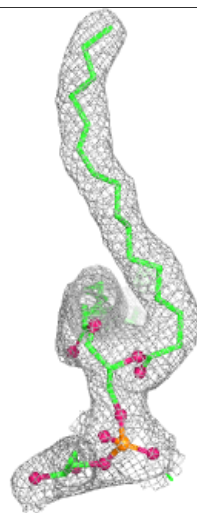
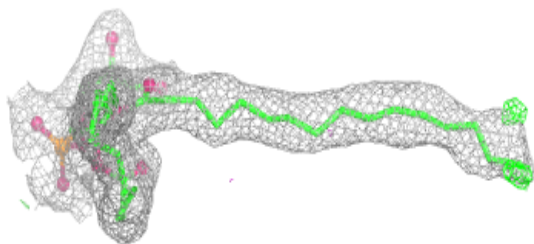
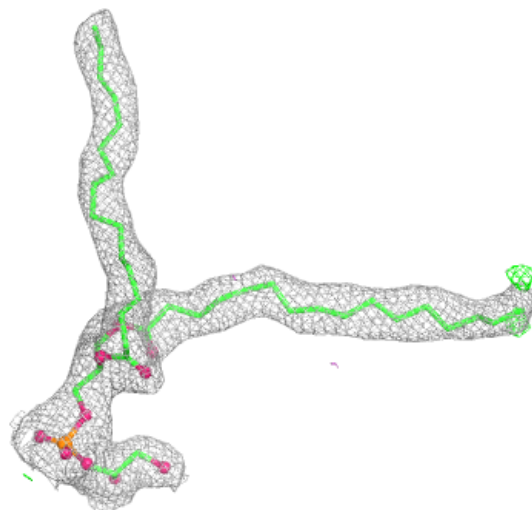
Electron density around CLA C 502:

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



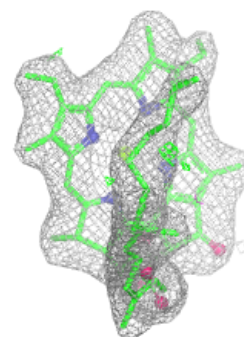
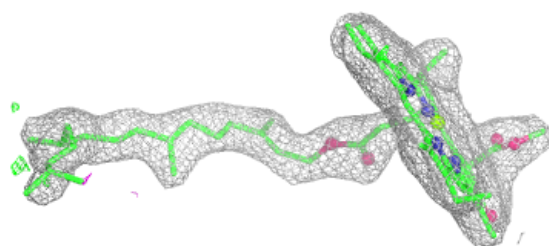
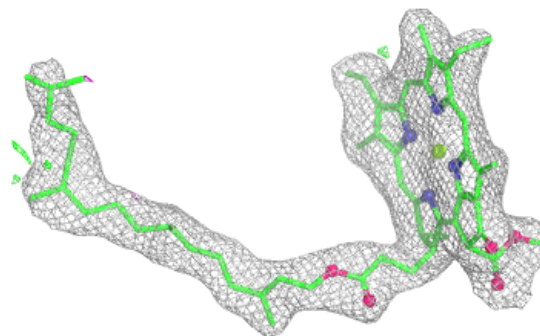
Electron density around LHG 1 101:

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

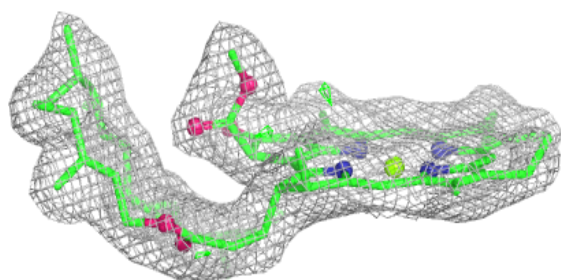
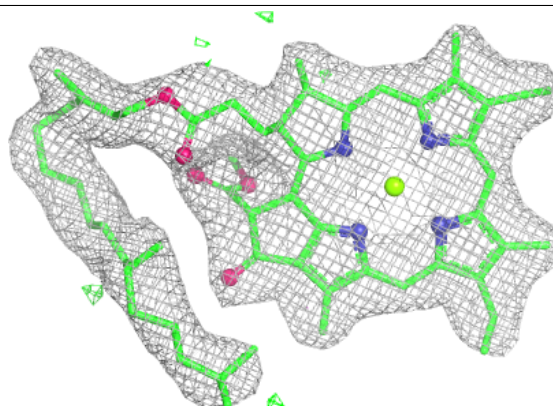


Electron density around CLA b 608:

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

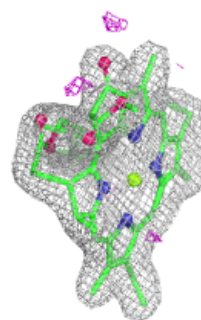
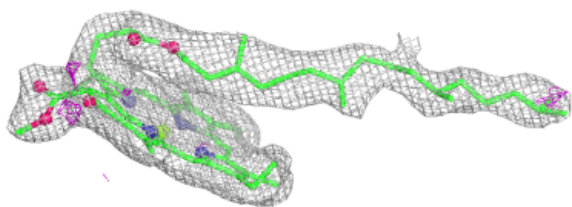
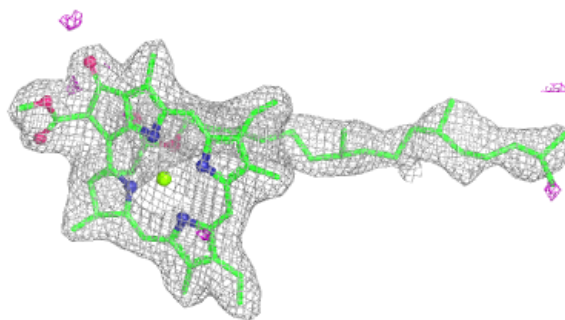
**Electron density around CLA b 609:**

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

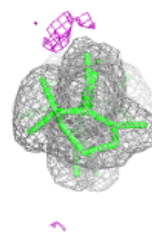
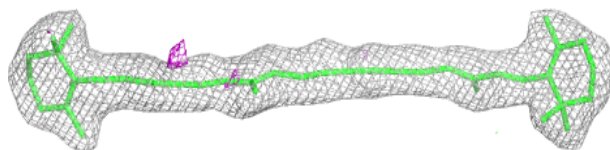
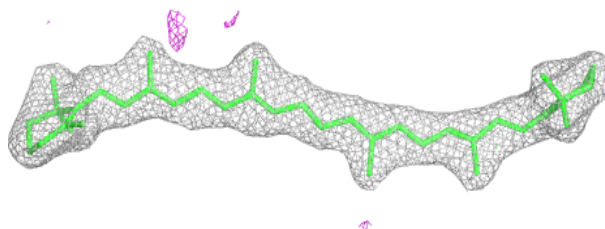


Electron density around CLA b 613:

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

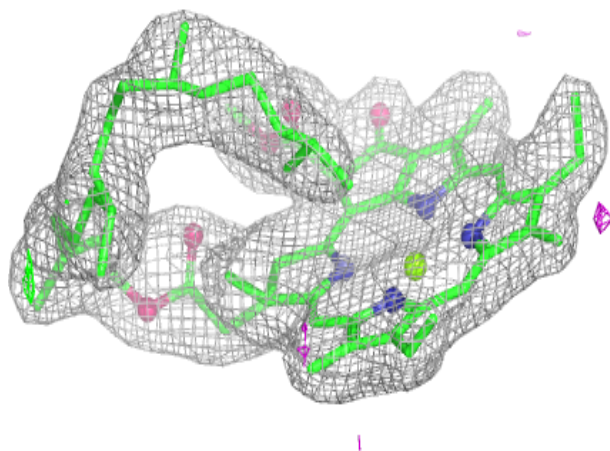
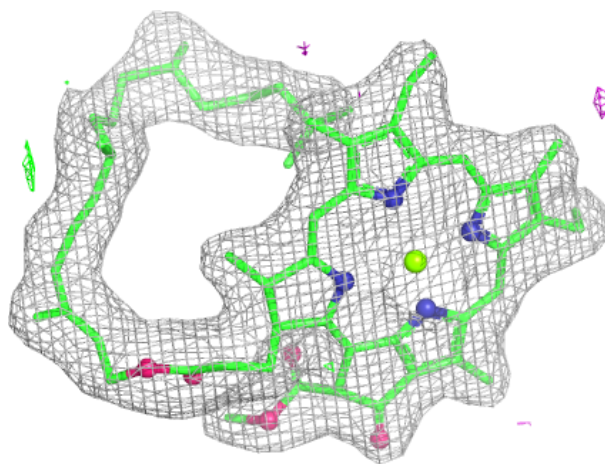
**Electron density around BCR a 610:**

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



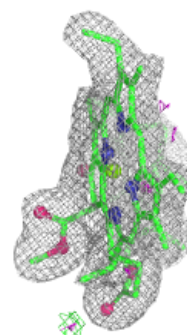
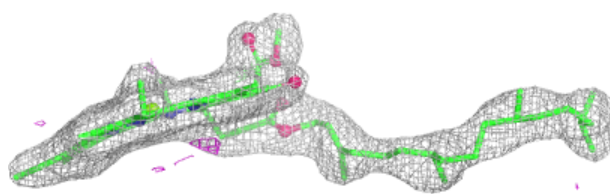
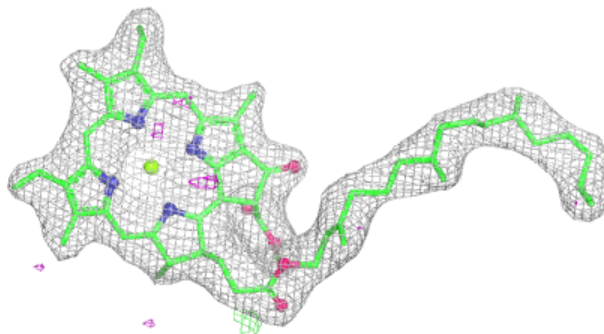
Electron density around CLA b 614:

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

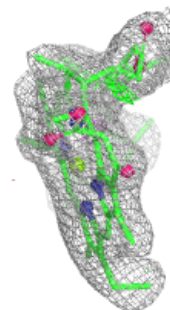
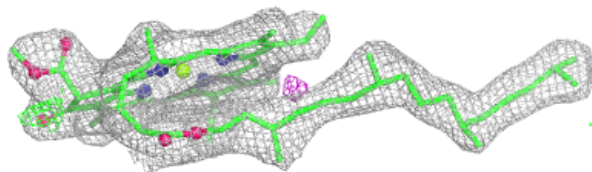
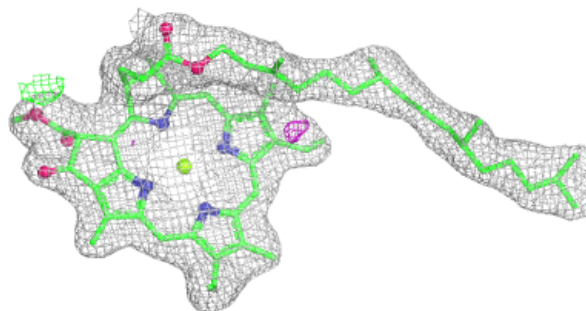


Electron density around CLA B 601:

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

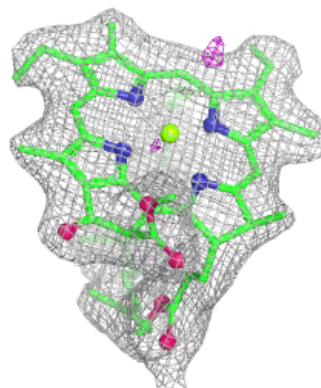
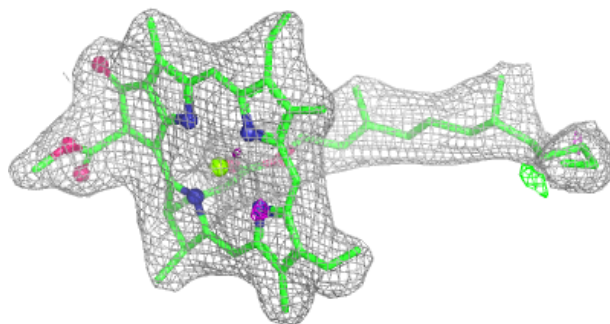
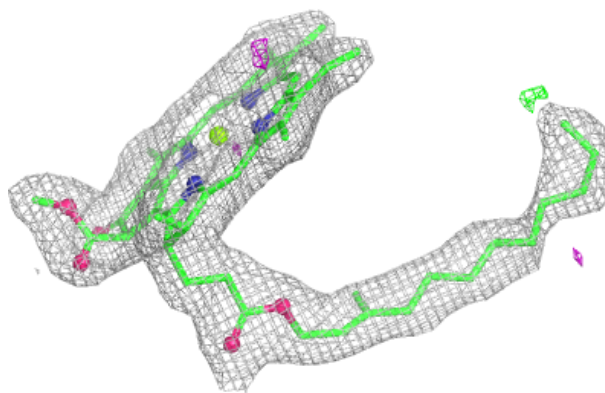
**Electron density around CLA c 501:**

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

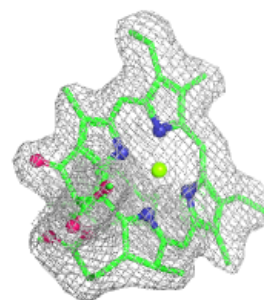
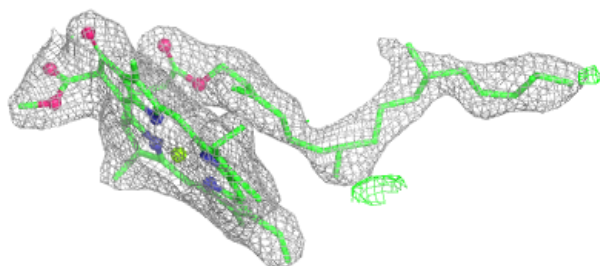
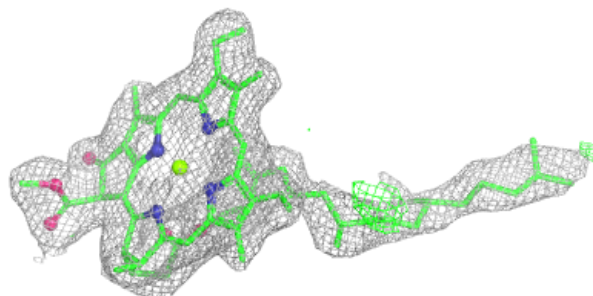


Electron density around CLA C 504:

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

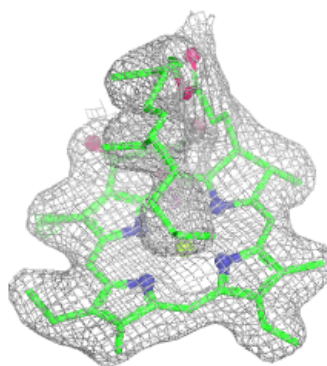
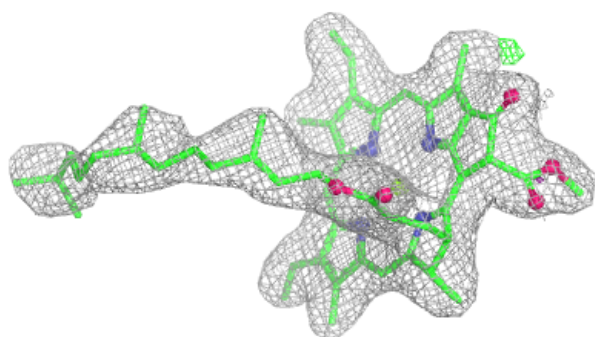
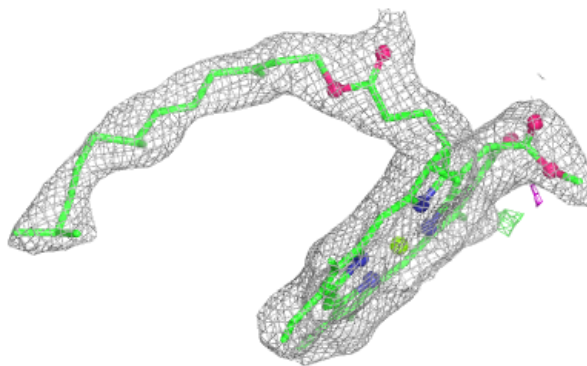
**Electron density around CLA C 505:**

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

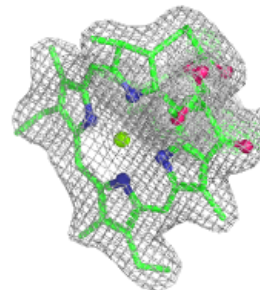
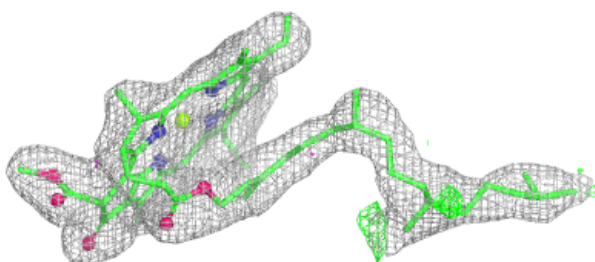
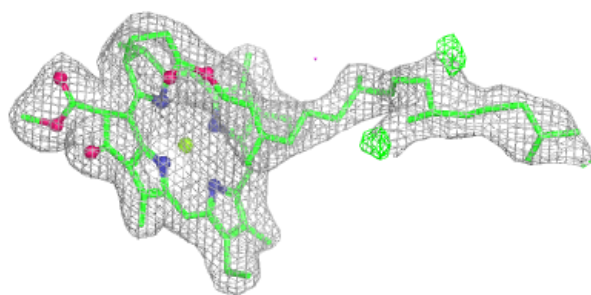


Electron density around CLA c 504:

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

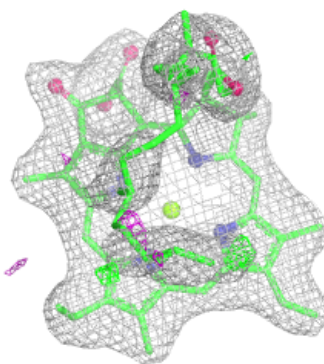
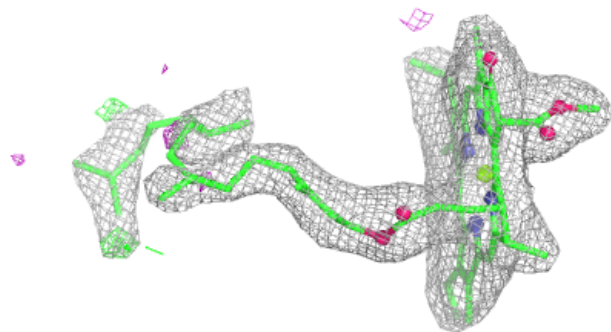
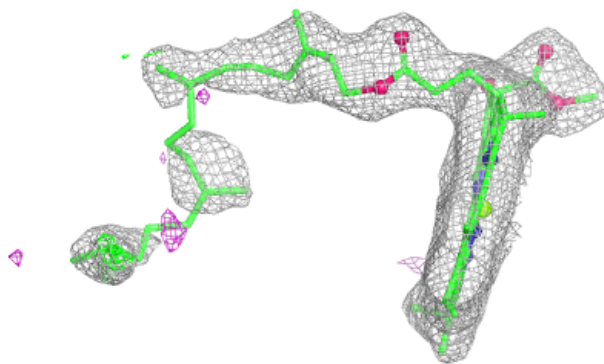
**Electron density around CLA c 505:**

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



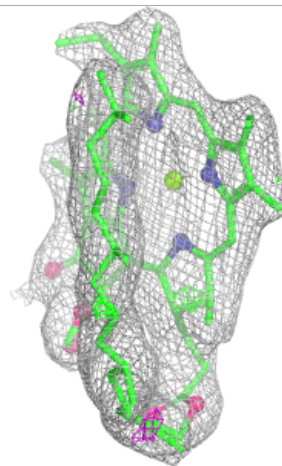
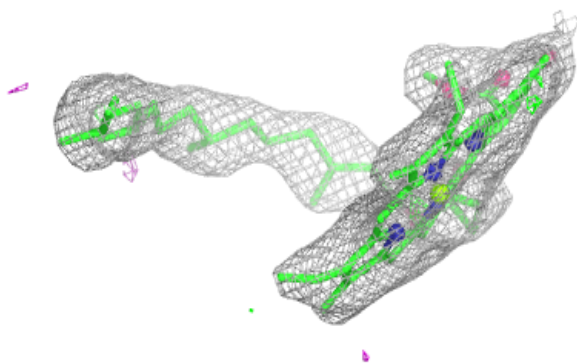
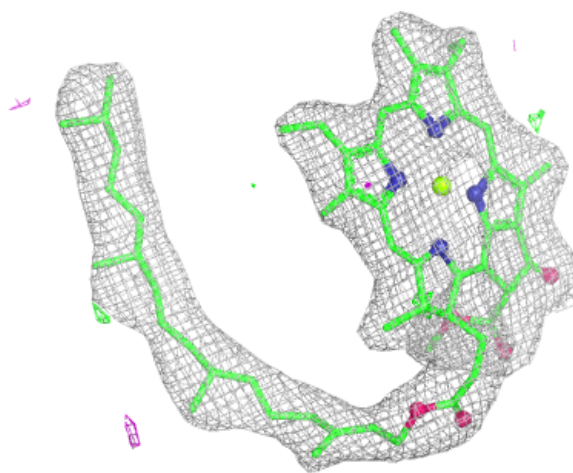
Electron density around CLA c 506:

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



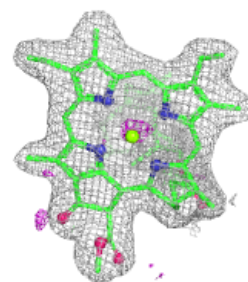
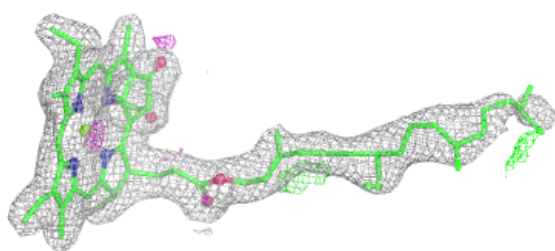
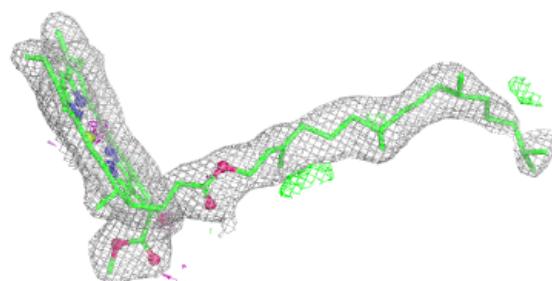
Electron density around CLA c 507:

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

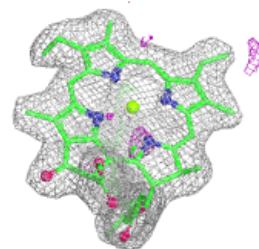
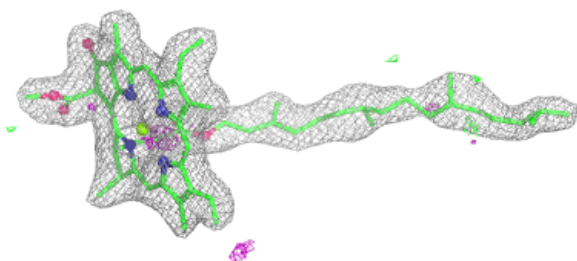
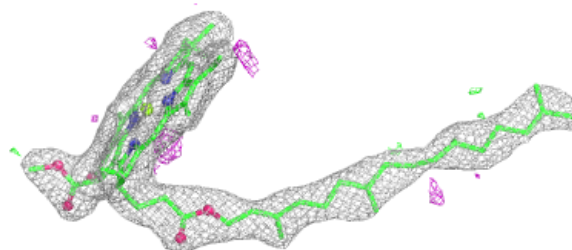


Electron density around CLA B 603:

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

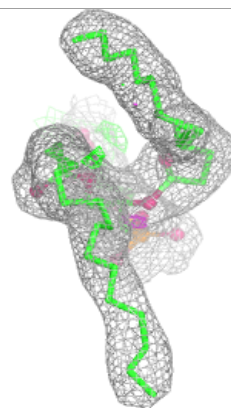
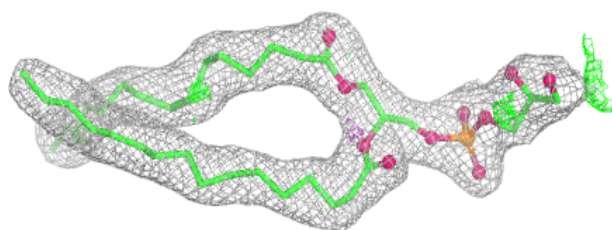
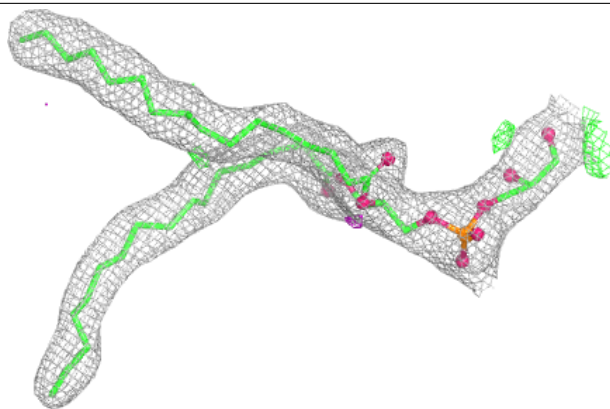
**Electron density around CLA B 606:**

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



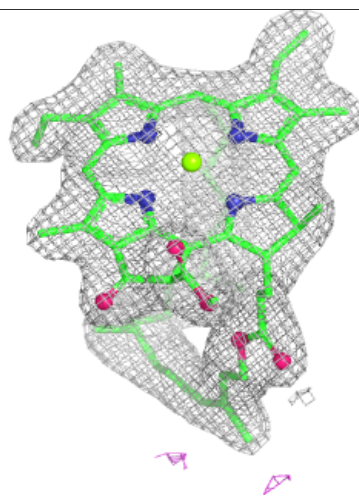
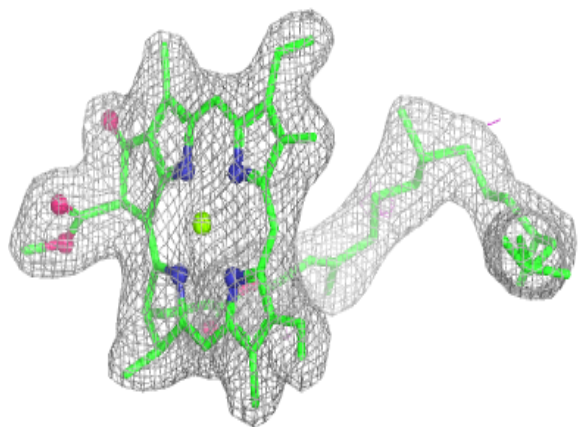
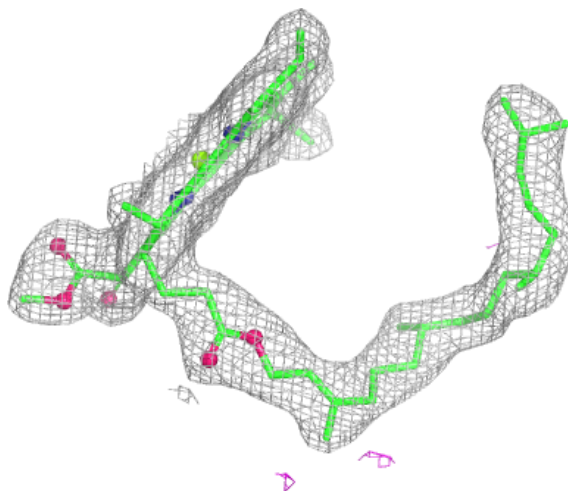
Electron density around LHG D 409:

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



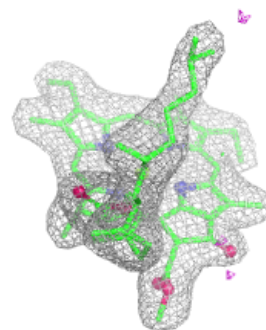
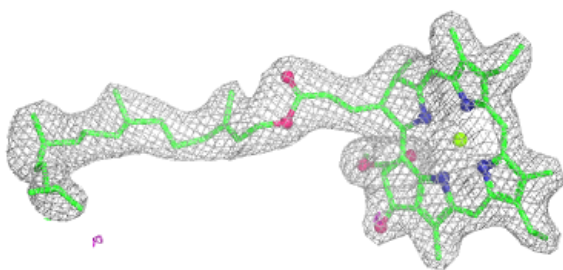
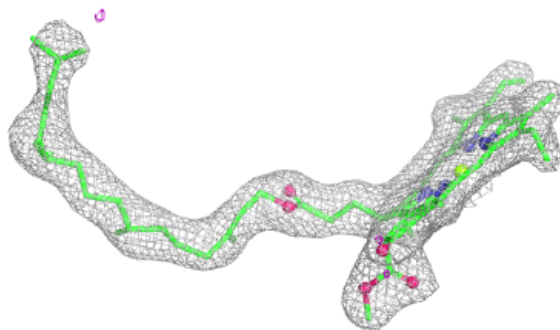
Electron density around CLA b 610:

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



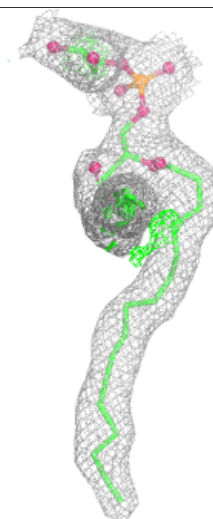
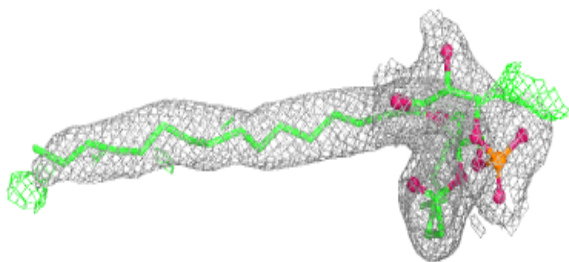
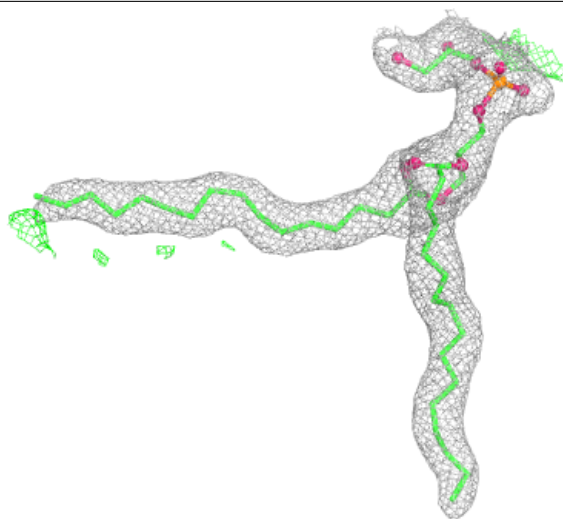
Electron density around CLA d 403:

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



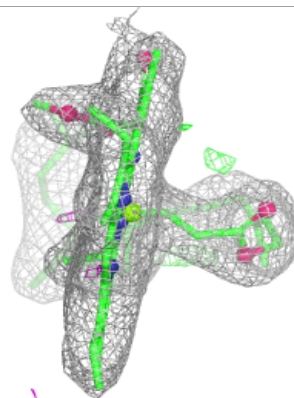
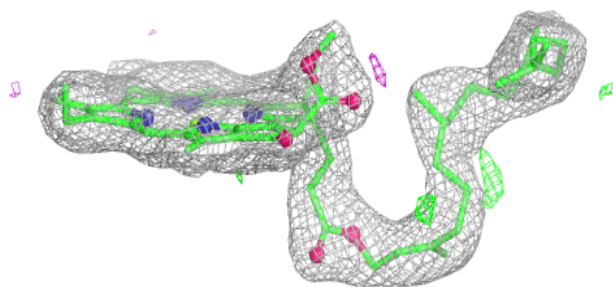
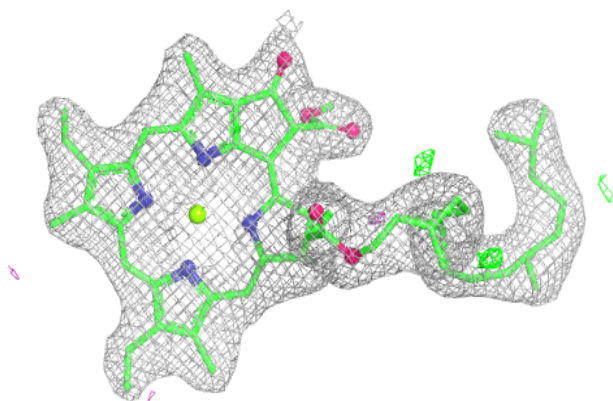
Electron density around LHG L 101:

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

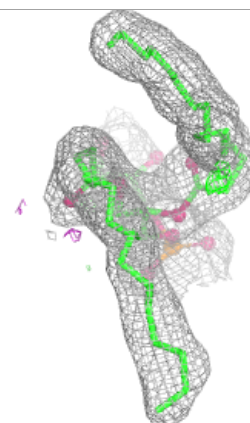
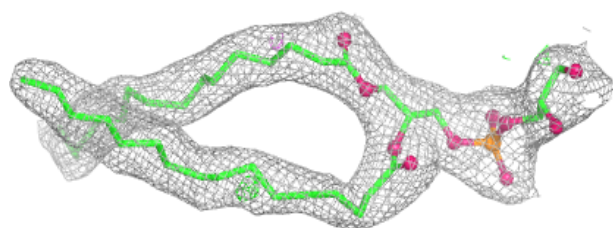
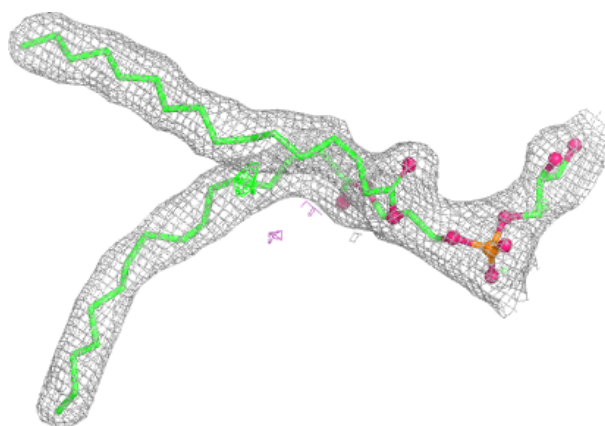


Electron density around CLA b 611:

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

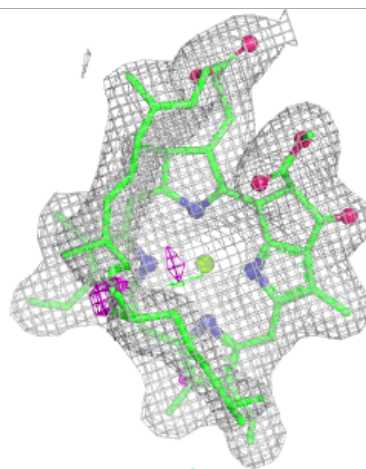
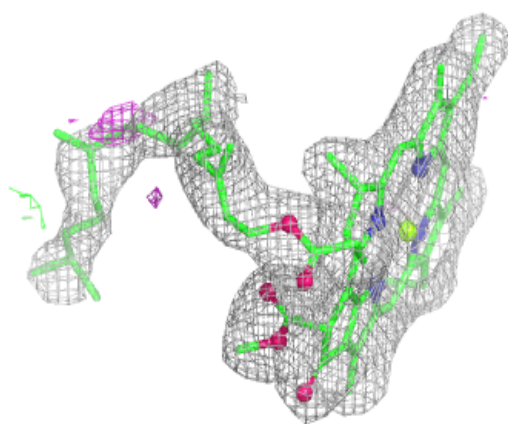
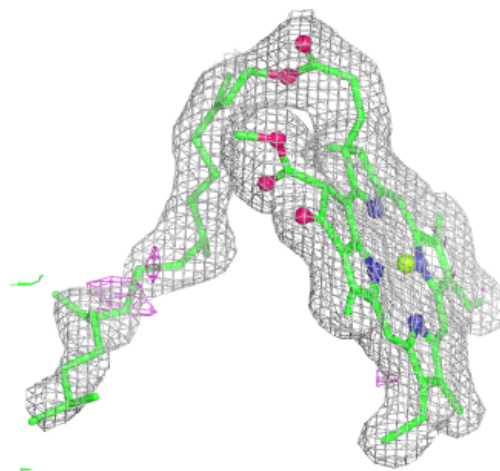
**Electron density around LHG d 407:**

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



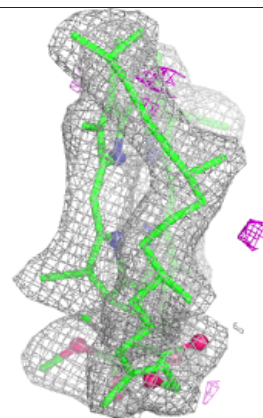
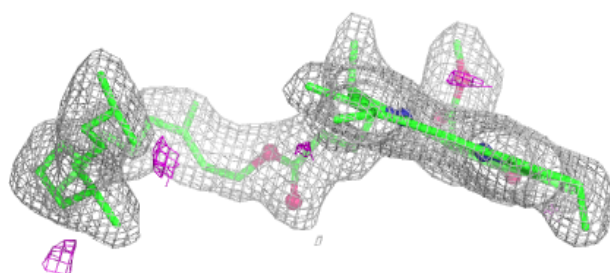
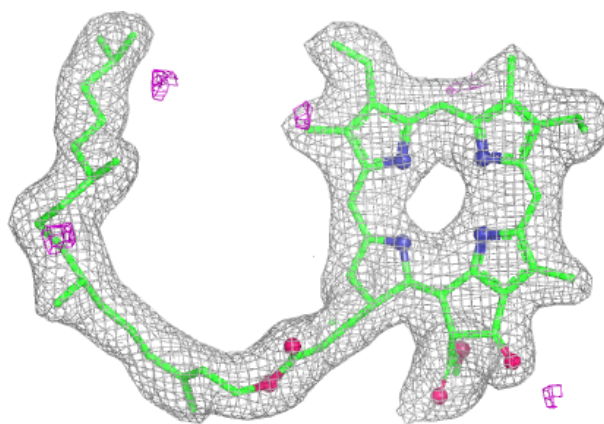
Electron density around CLA b 612:

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

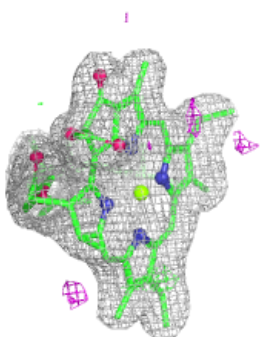
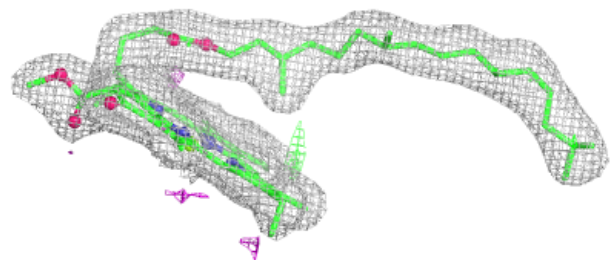
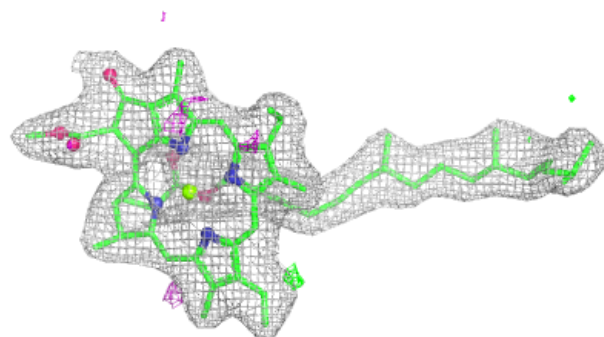


Electron density around PHO A 608:

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

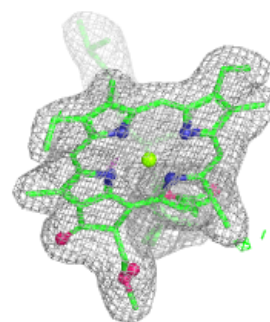
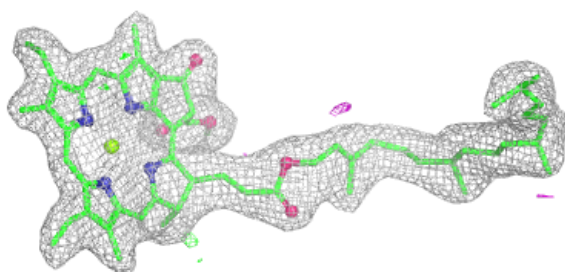
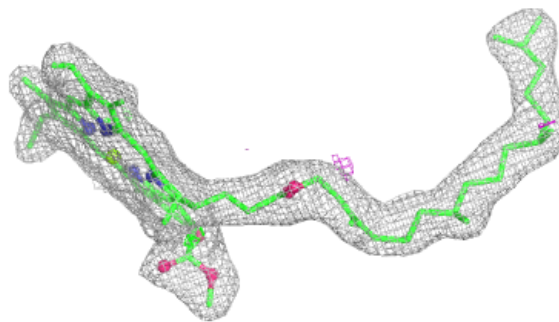
**Electron density around CLA B 607:**

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

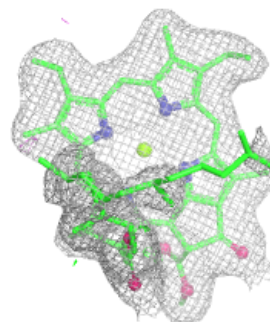
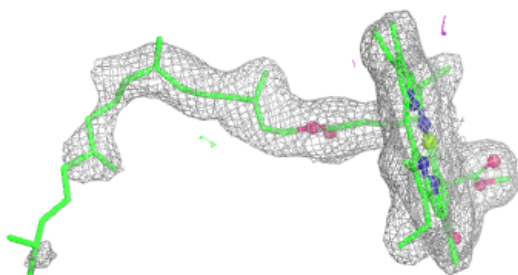
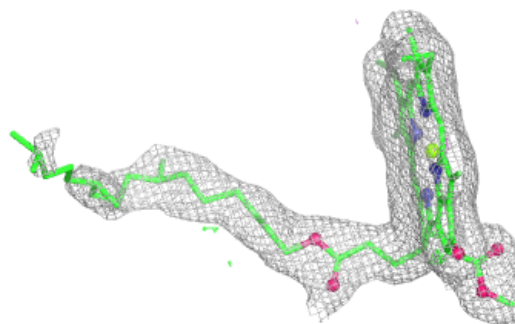


Electron density around CLA D 403:

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

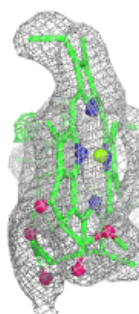
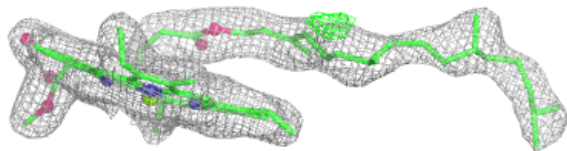
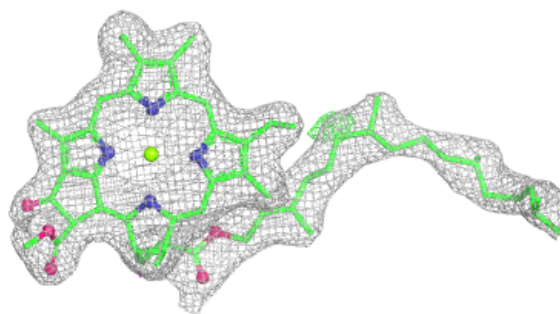
**Electron density around CLA D 404:**

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

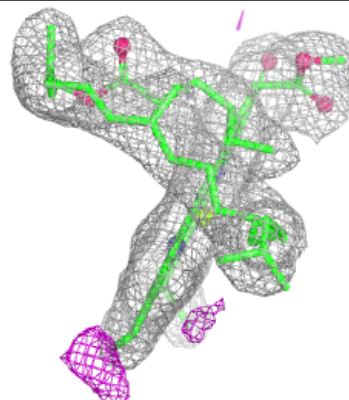
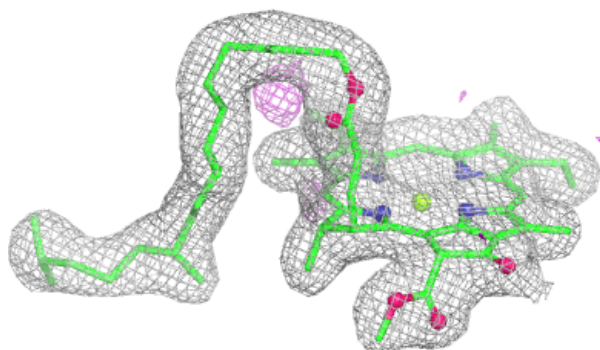
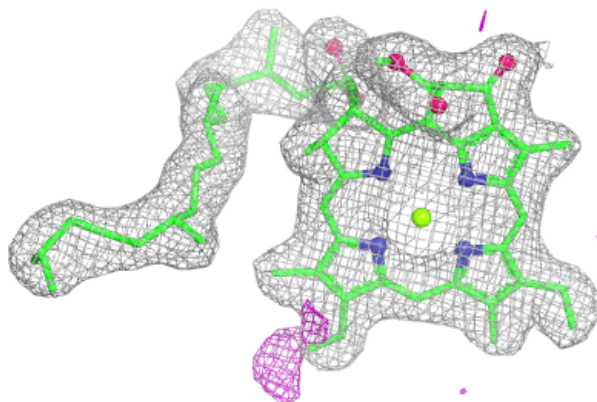


Electron density around CLA B 602:

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

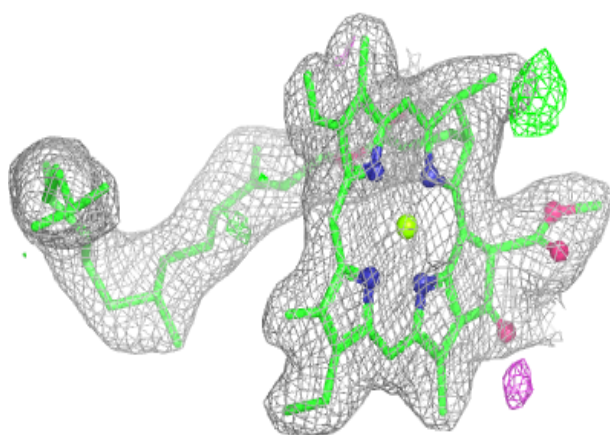
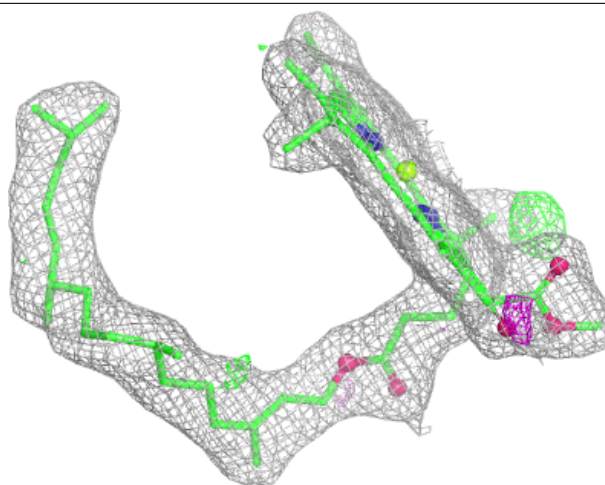
**Electron density around CLA A 612:**

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



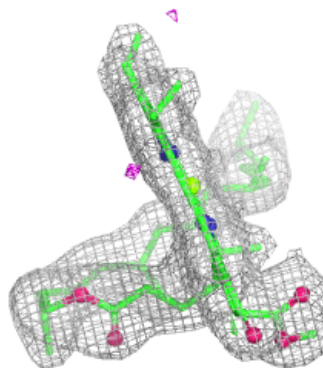
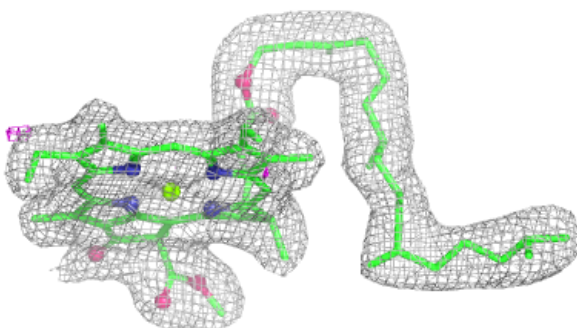
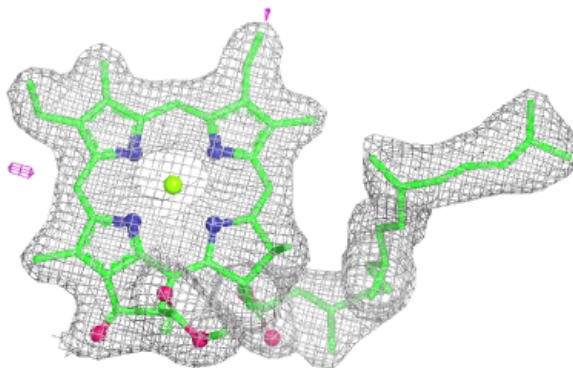
Electron density around CLA B 610:

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

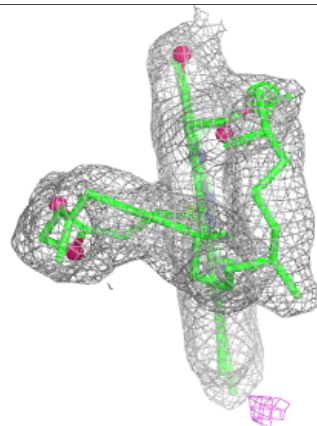
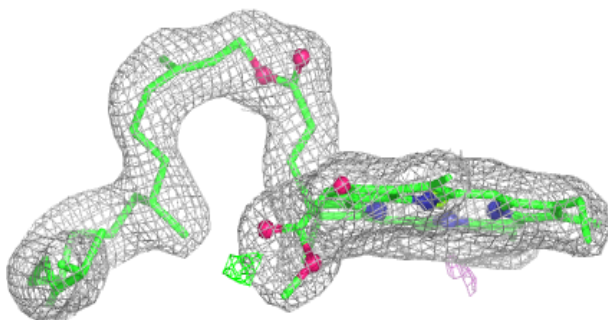
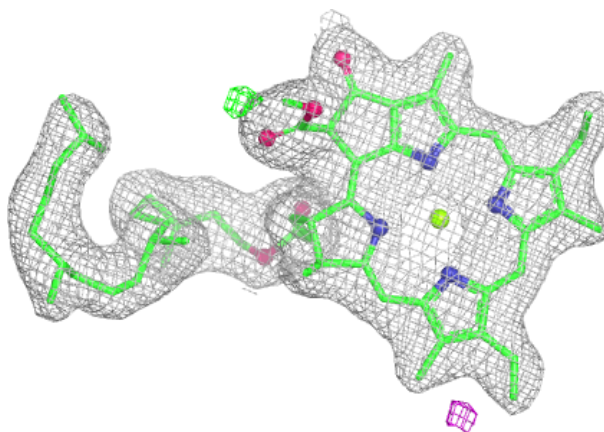


Electron density around CLA a 612:

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

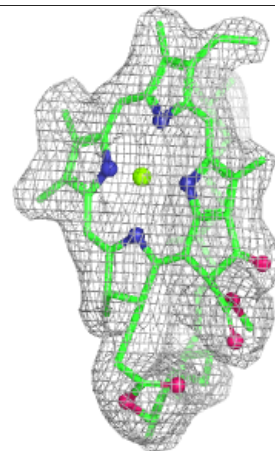
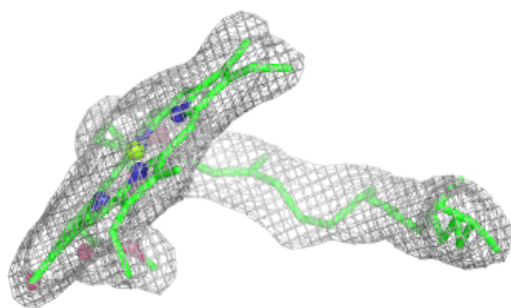
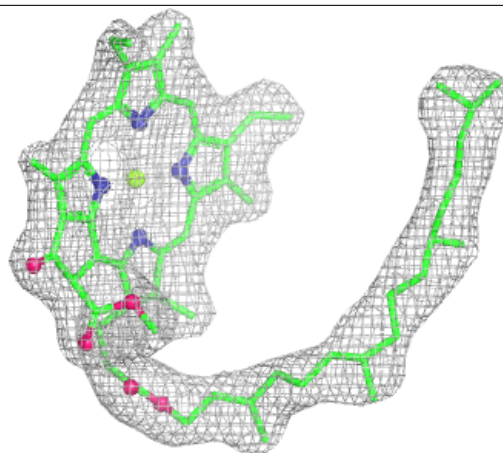
**Electron density around CLA B 611:**

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



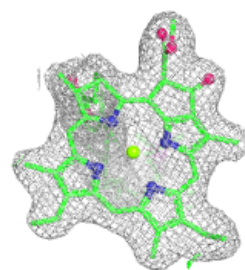
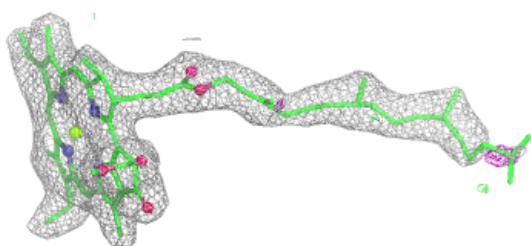
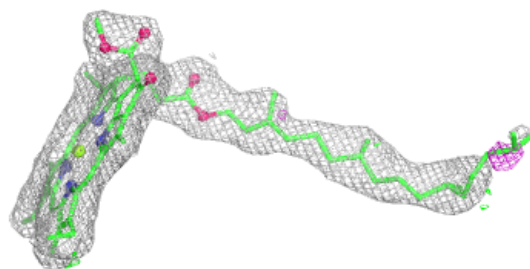
Electron density around CLA C 507:

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



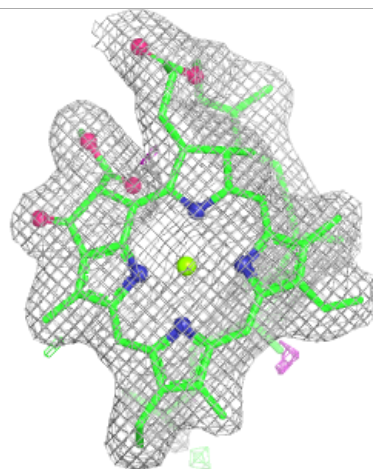
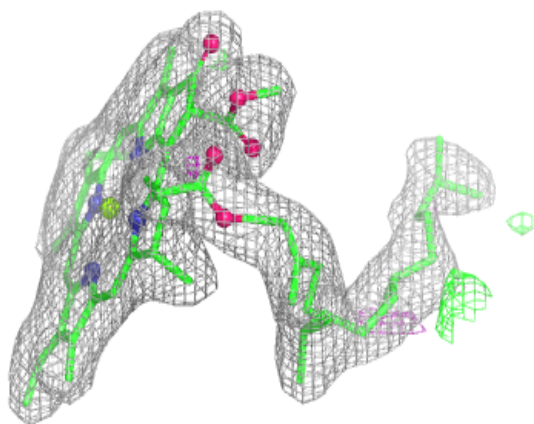
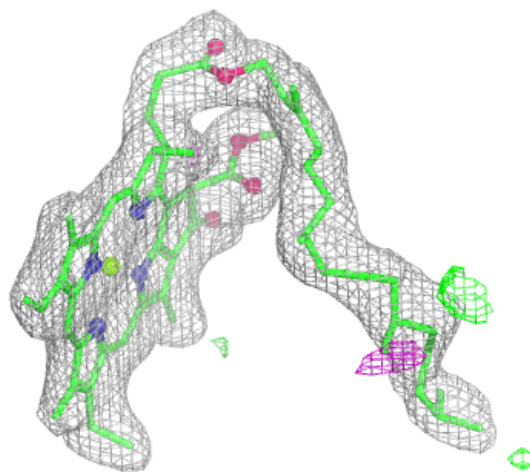
Electron density around CLA b 603:

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



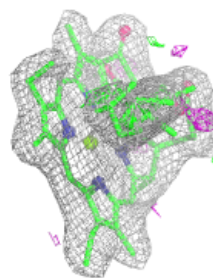
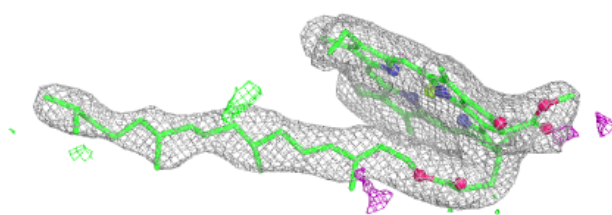
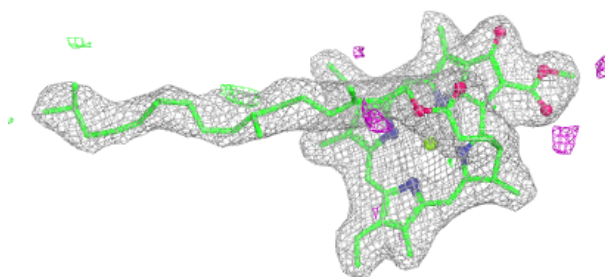
Electron density around CLA B 612:

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

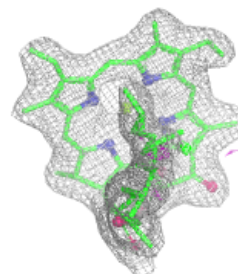
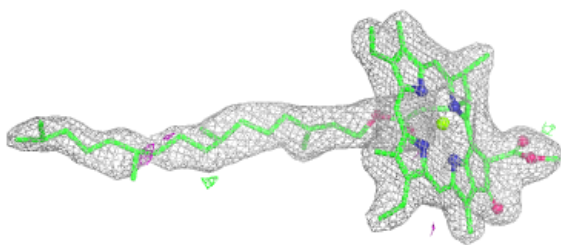
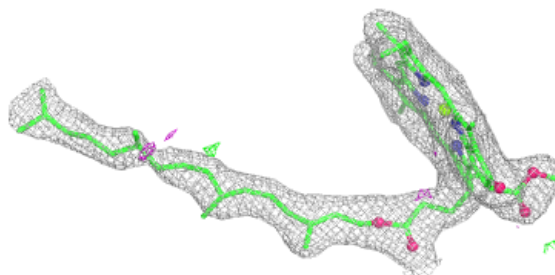


Electron density around CLA B 613:

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

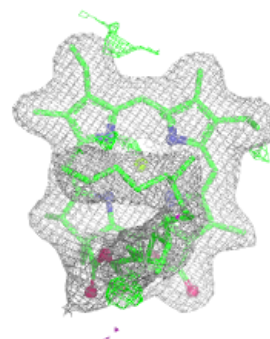
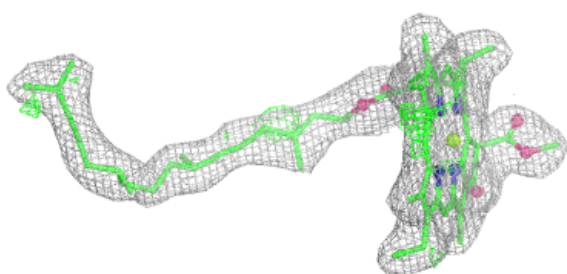
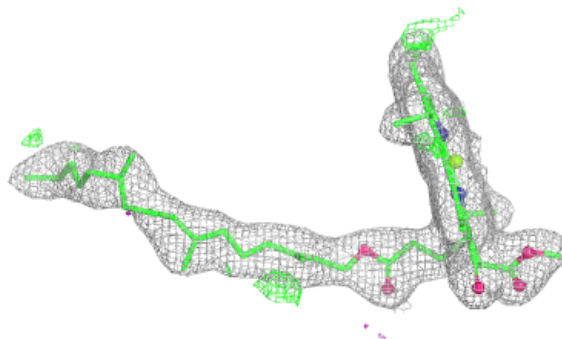
**Electron density around CLA b 606:**

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

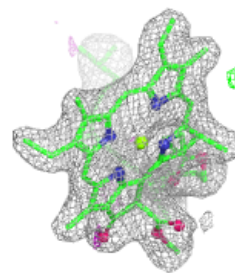
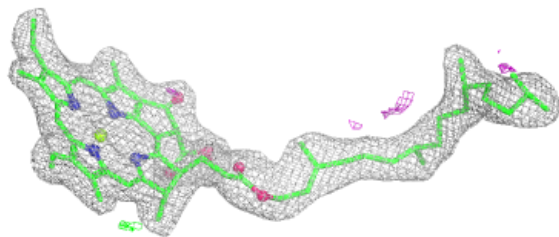
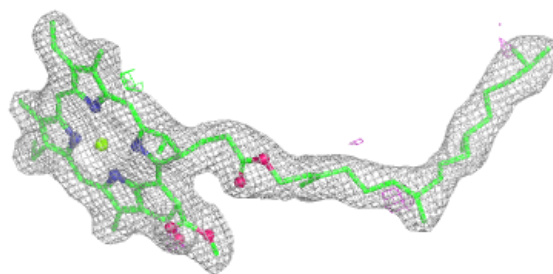


Electron density around CLA B 604:

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

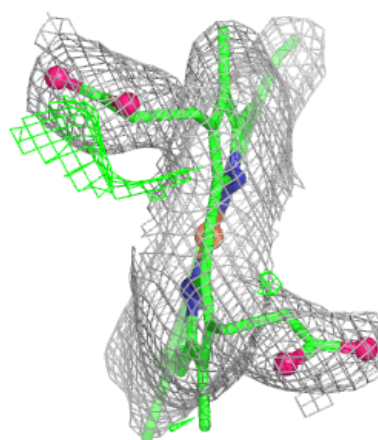
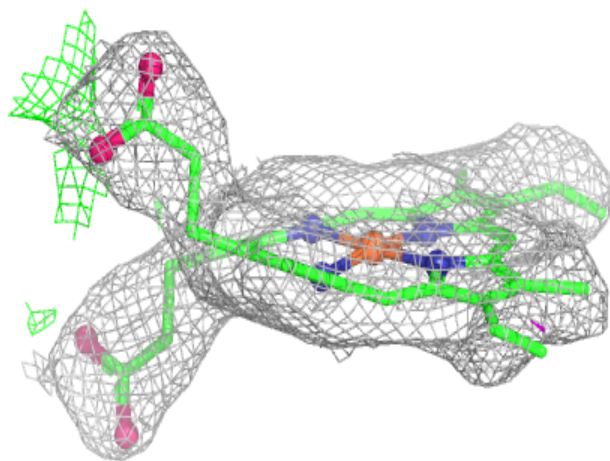
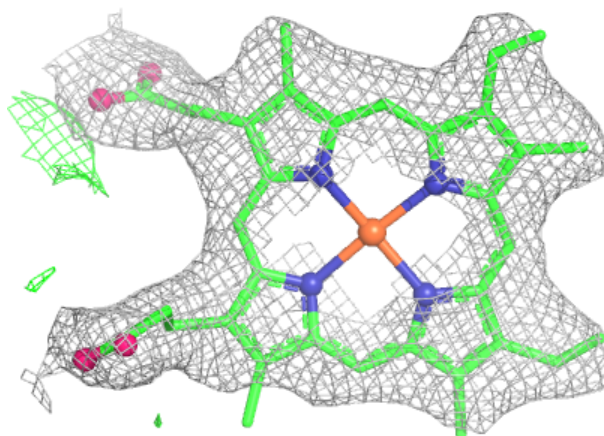
**Electron density around CLA A 606:**

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



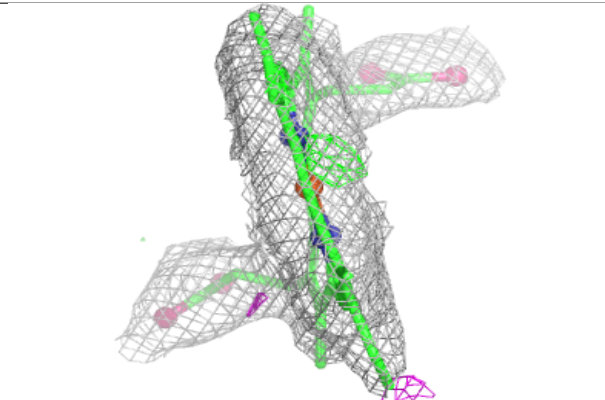
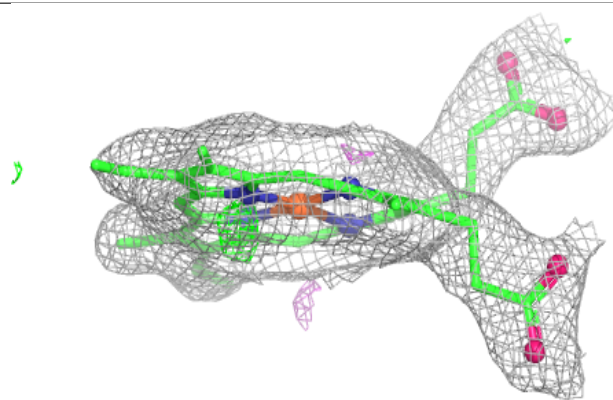
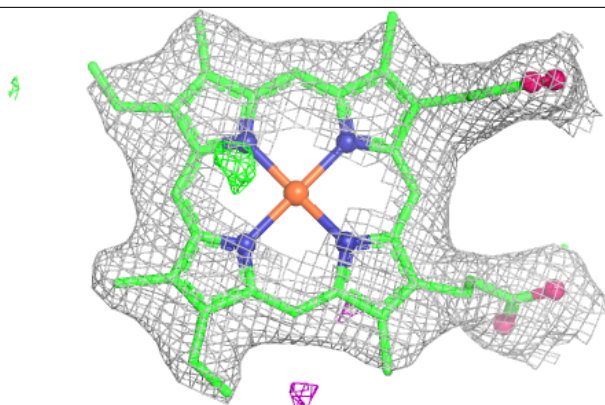
Electron density around HEM e 101:

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

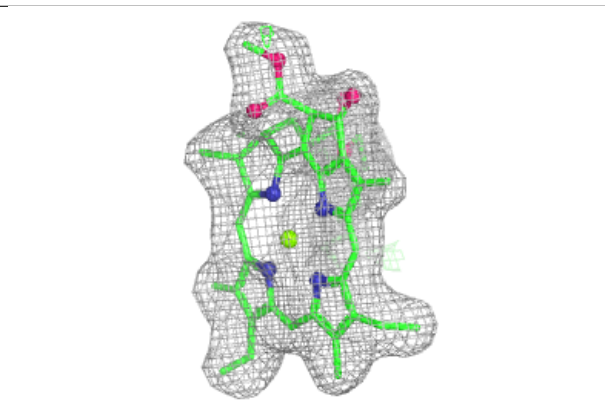
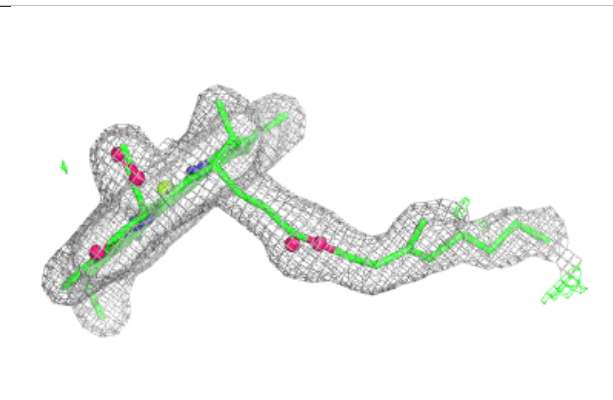
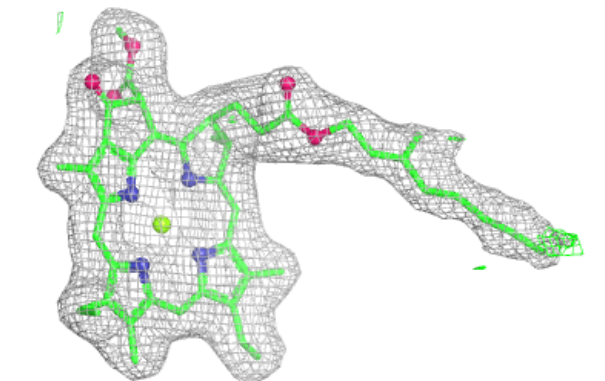


Electron density around HEM F 101:

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

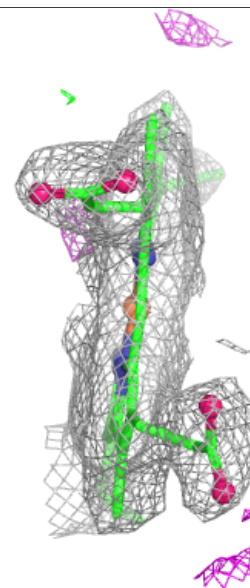
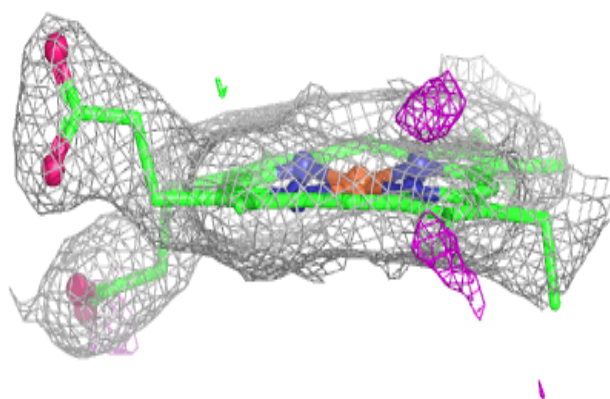
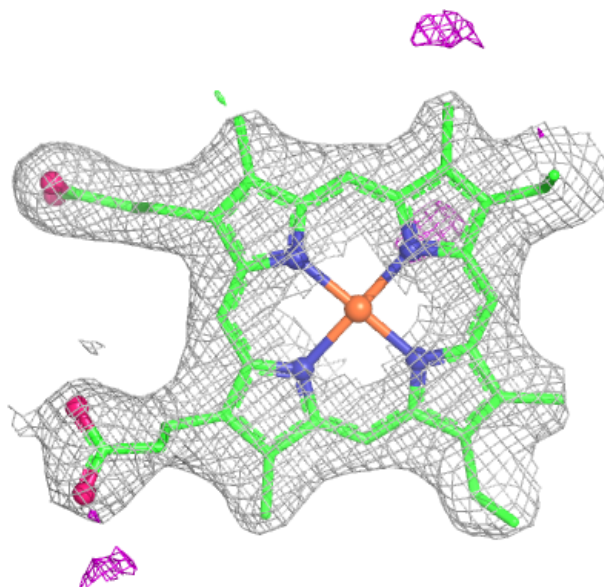
**Electron density around CLA A 609:**

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



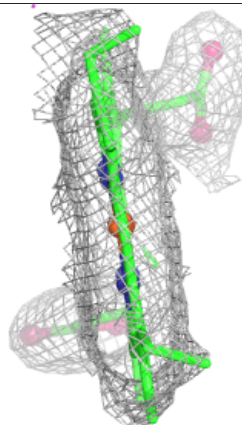
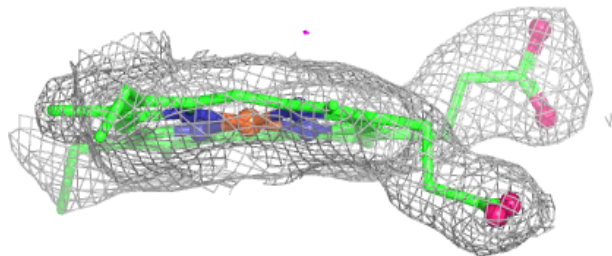
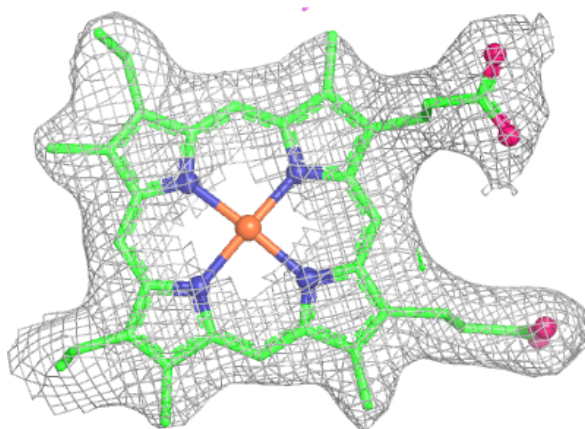
Electron density around HEC V 201:

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



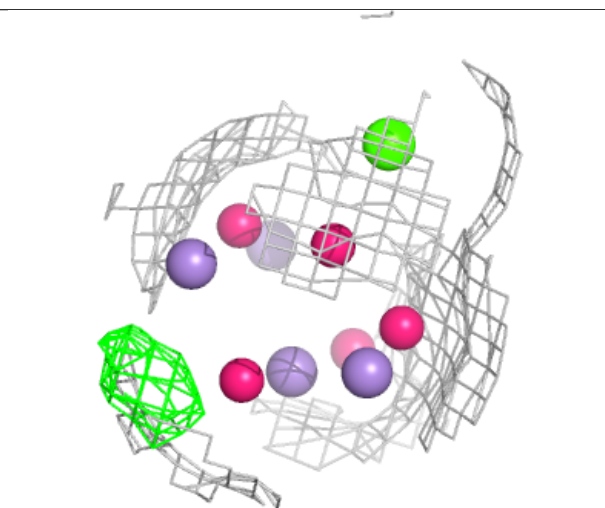
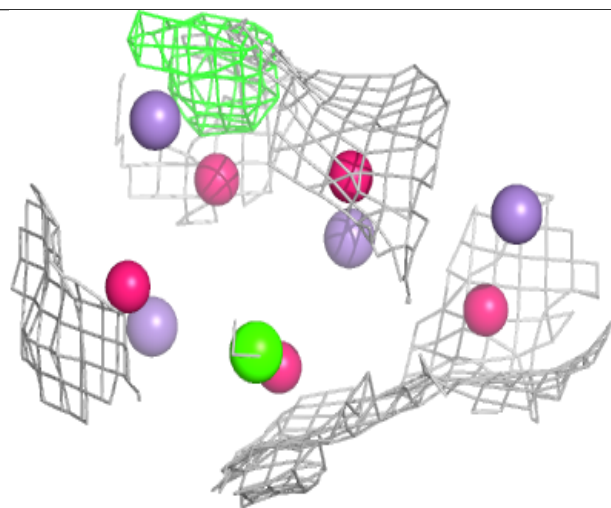
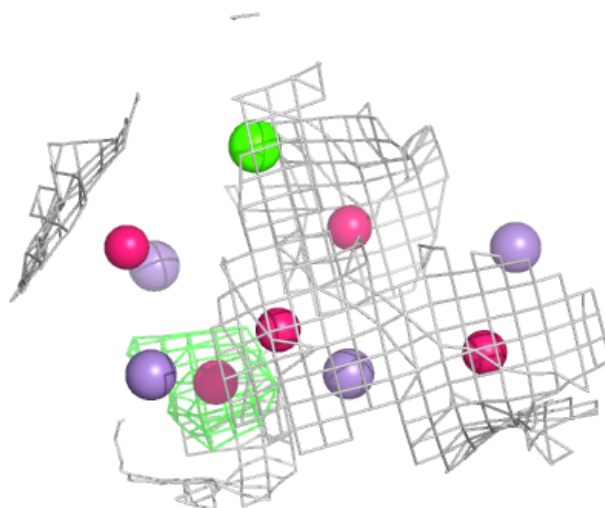
Electron density around HEC v 201:

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



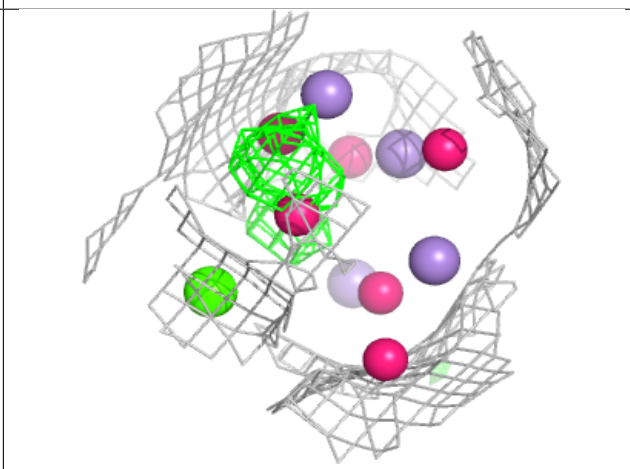
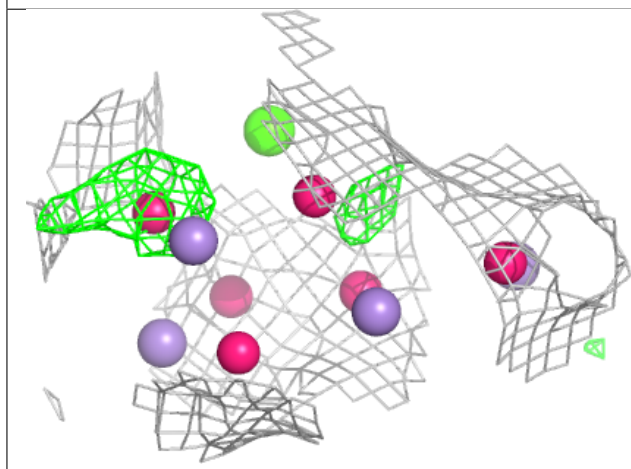
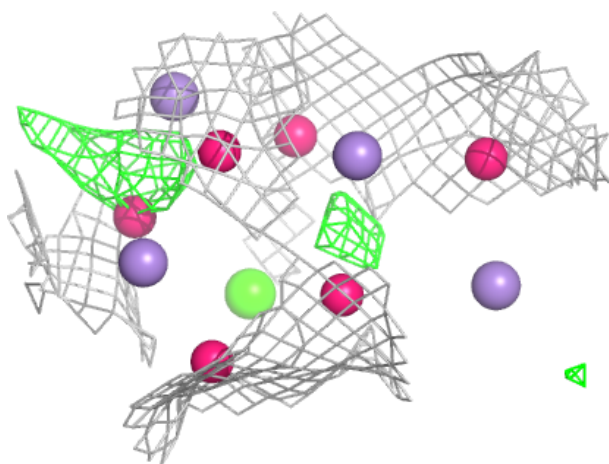
Electron density around OEX a 601 (B):

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



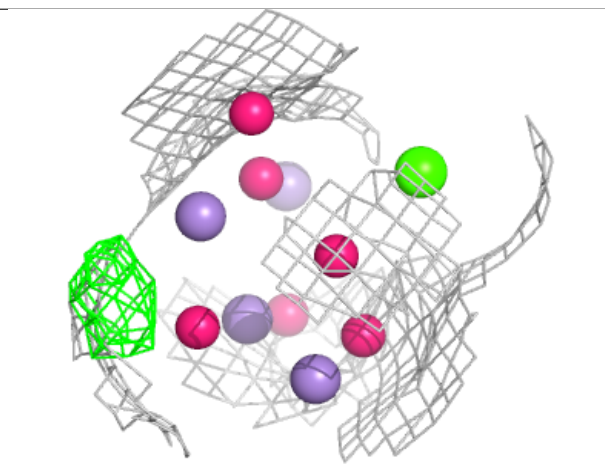
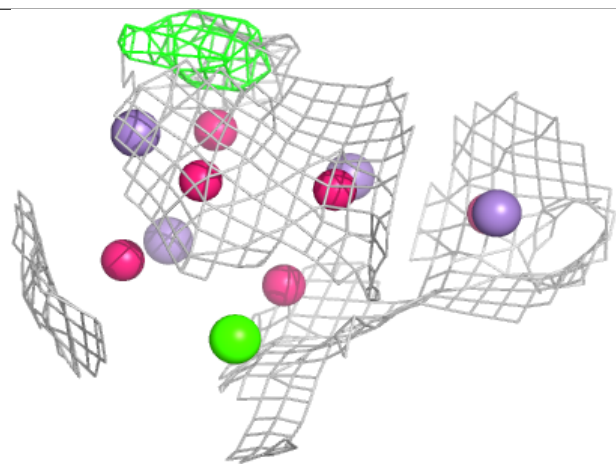
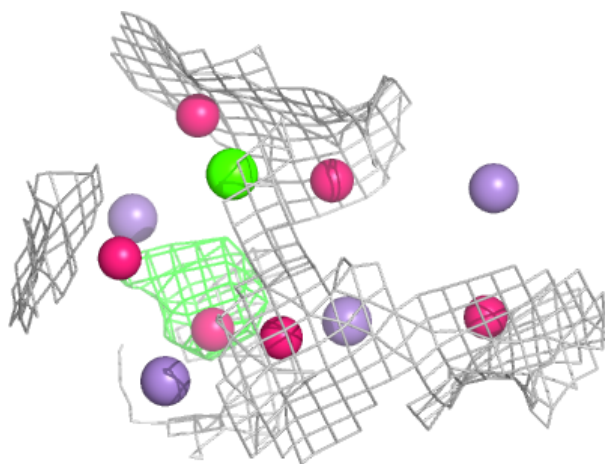
Electron density around OEY A 602 (A):

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



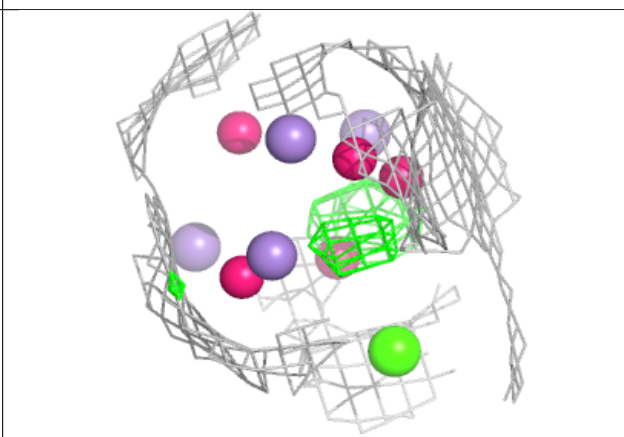
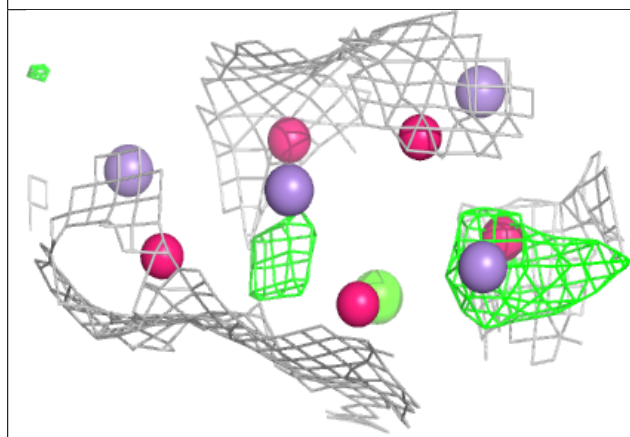
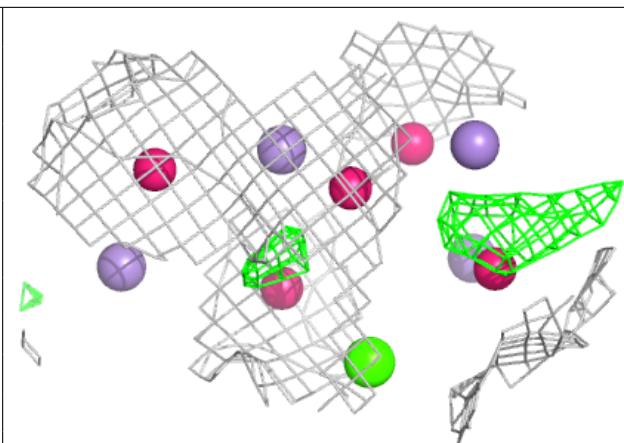
Electron density around OEY a 602 (A):

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



Electron density around OEX A 601 (B):

$2mF_o - DF_c$ (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.