



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 08:47 AM EDT

PDB ID : 8F4J / pdb_00008f4j
Title : RT XFEL structure of Photosystem II 4000 microseconds after the third illumination at 2.00 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 : 2.00 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

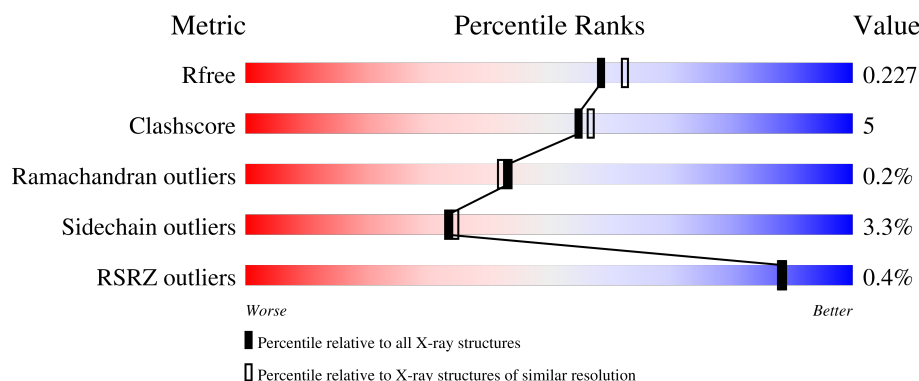
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	

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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

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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	

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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 54524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2745	1818	448	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2751	1822	448	469	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	1	0
			666	436	107	123			
5	e	82	Total	C	N	O	0	0	0
			664	434	108	122			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	36	Total	C	N	O		0	0	0
			296	197	47	52				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	32	Total	C	N	O	S	0	0	0
			251	168	36	46	1			

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

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

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

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

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

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

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

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

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

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

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

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

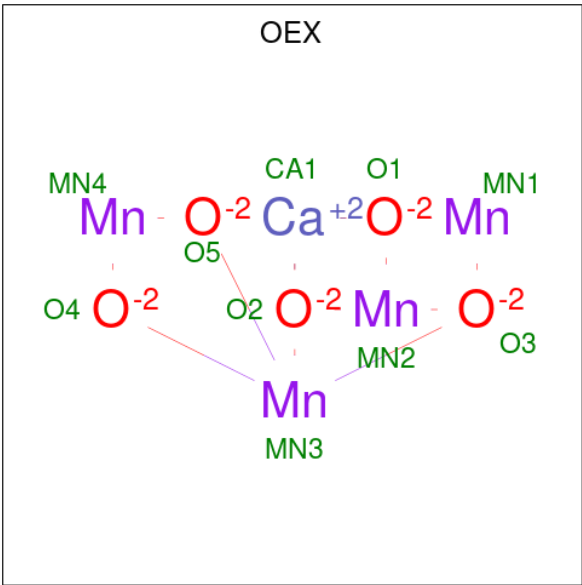
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

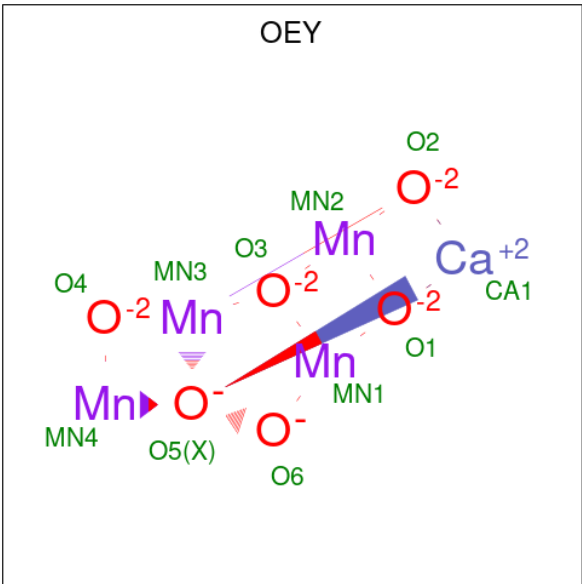
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O	S	0	0	0
			246	166	43	37				

- 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
			20	2	8	10		
21	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- 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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

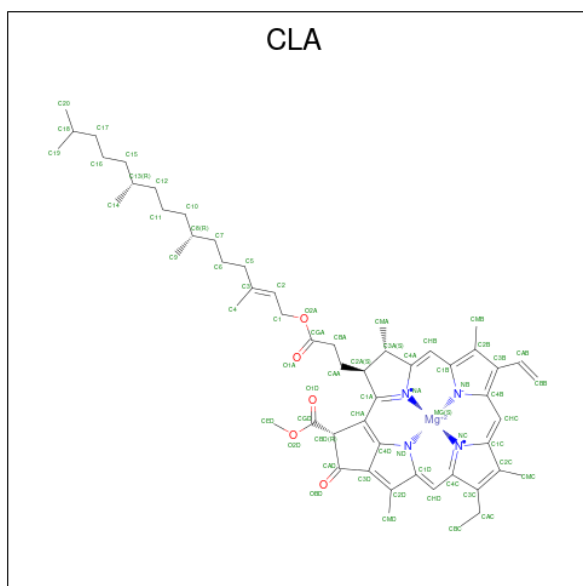
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	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
			65	55	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		

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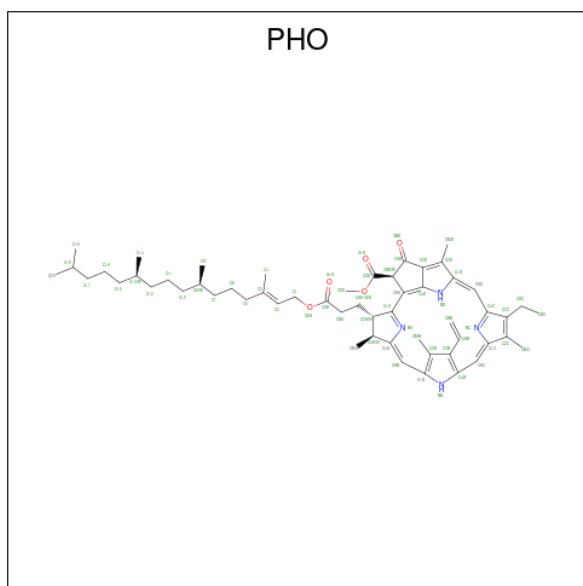
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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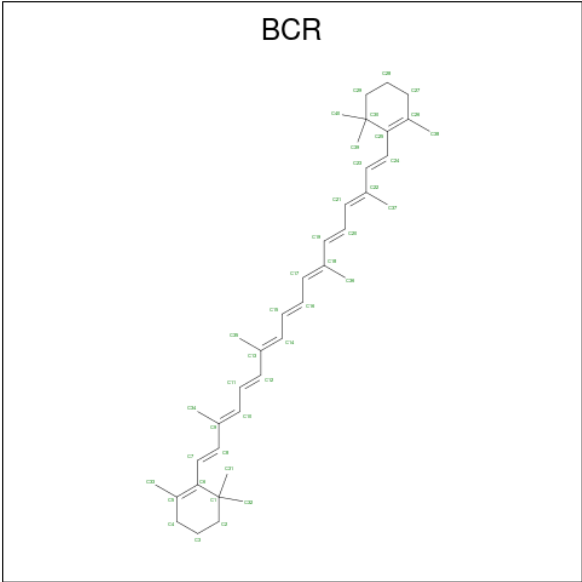
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



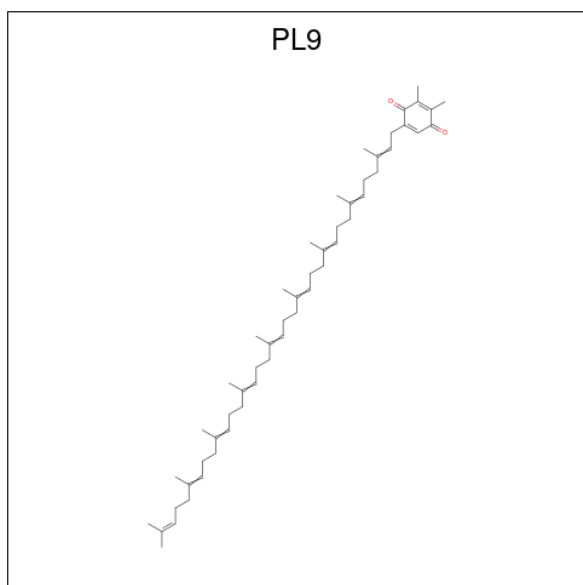
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



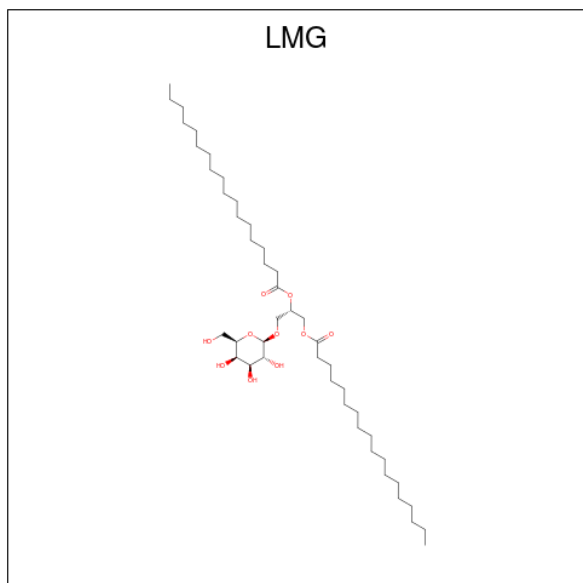
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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

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



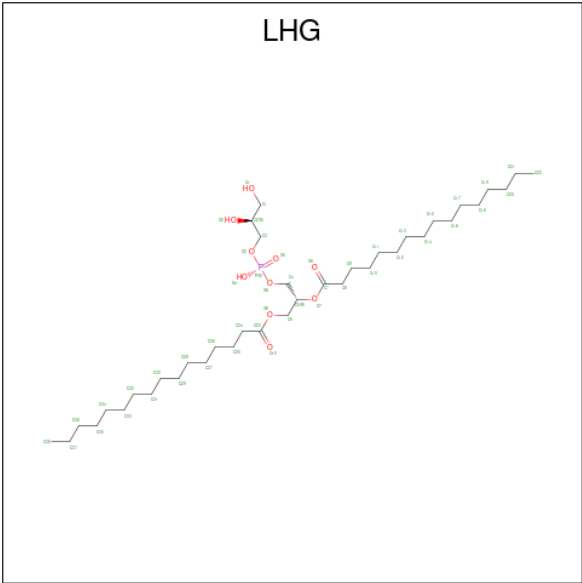
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C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

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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



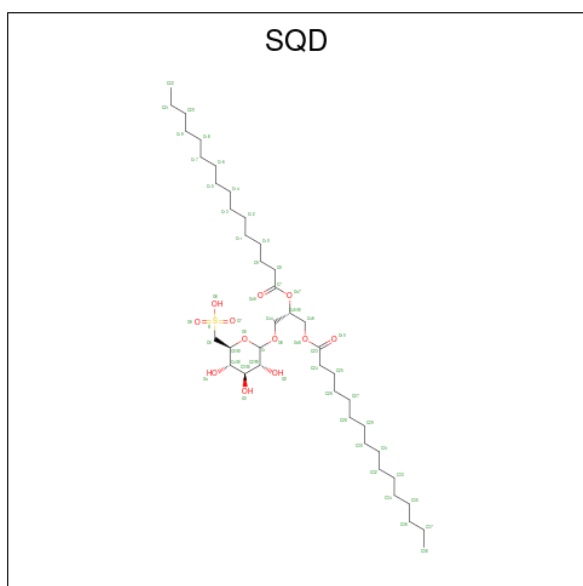
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			47	36	10	1		
30	B	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	E	1	Total	C	O	P	0	0
			49	38	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		

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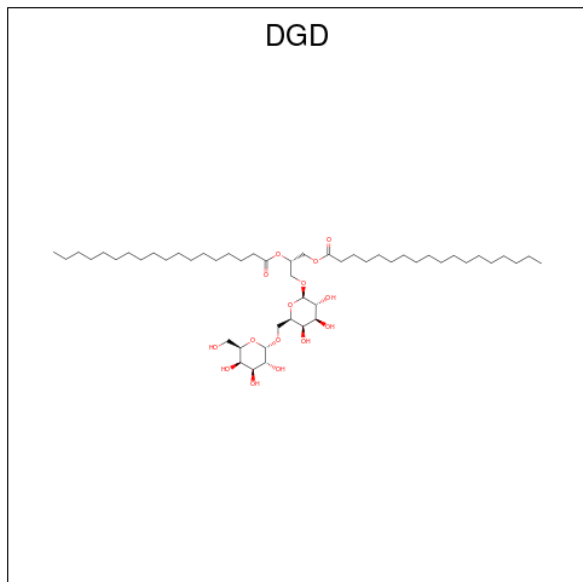
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	d	1	Total	C	O	P	0	0
			39	28	10	1		
30	e	1	Total	C	O	P	0	0
			42	31	10	1		
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



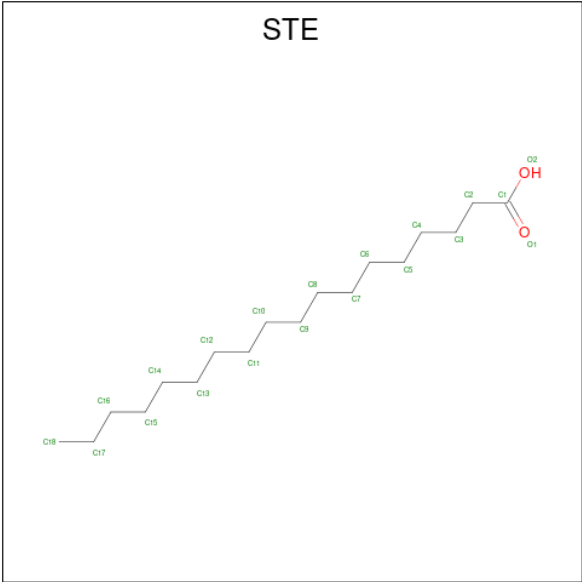
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	S	0	0
			52	39	12	1		
31	A	1	Total	C	O		0	0
			39	35	4			
31	B	1	Total	C	O	S	0	0
			54	41	12	1		
31	F	1	Total	C	O	S	0	0
			36	25	10	1		
31	a	1	Total	C	O	S	0	0
			54	41	12	1		
31	a	1	Total	C	O		0	0
			36	31	5			
31	b	1	Total	C	O	S	0	0
			49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

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



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

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



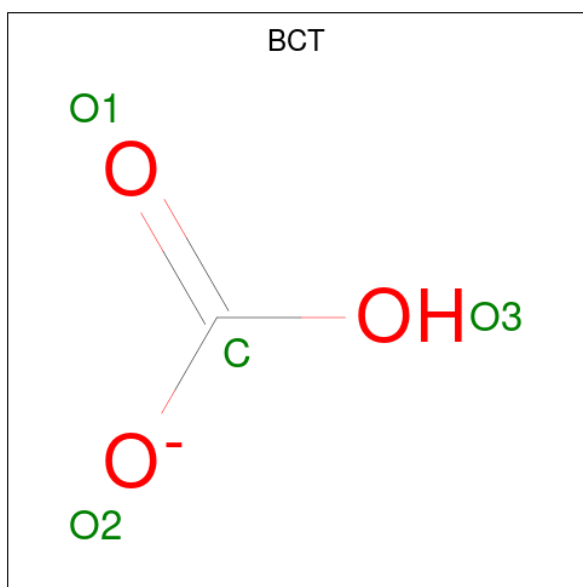
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			17	15	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C	O	0	0
			12	10	2		
33	B	1	Total	C		0	0
			16	16			
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C	O	0	0
			12	10	2		
33	C	1	Total	C		0	0
			16	16			
33	E	1	Total	C	O	0	0
		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

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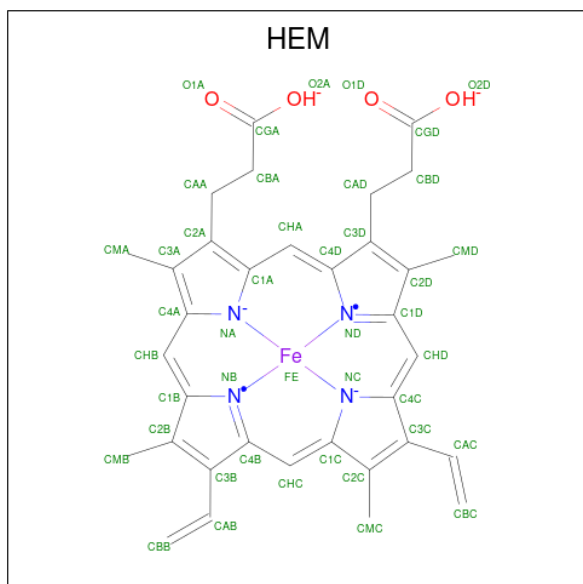
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	a	1	Total C O 12 10 2	0	0
33	b	1	Total C 16 16	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C O 16 14 2	0	0
33	b	1	Total C 15 15	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 10 10	0	0
33	c	1	Total C O 20 18 2	0	0
33	d	1	Total C O 17 15 2	0	0
33	j	1	Total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

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



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

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



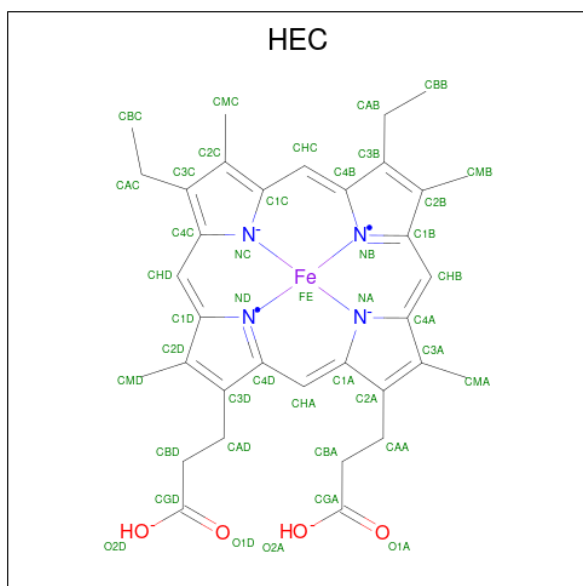
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	150	Total	O		
			158	158	0	4
37	B	214	Total	O		
			214	214	0	0
37	C	196	Total	O		
			196	196	0	0
37	D	115	Total	O		
			115	115	0	0
37	E	33	Total	O		
			33	33	0	0
37	F	6	Total	O		
			6	6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	27	Total 27	O 27	0	0
37	I	20	Total 20	O 20	0	0
37	J	13	Total 13	O 13	0	0
37	K	5	Total 5	O 5	0	0
37	L	10	Total 10	O 10	0	0
37	M	7	Total 7	O 7	0	0
37	O	89	Total 89	O 89	0	0
37	T	9	Total 9	O 9	0	0
37	U	40	Total 40	O 40	0	0
37	V	61	Total 61	O 61	0	0
37	X	12	Total 12	O 12	0	0
37	Z	6	Total 6	O 6	0	0
37	a	123	Total 131	O 131	0	4
37	b	199	Total 199	O 199	0	0
37	c	150	Total 150	O 150	0	0
37	d	109	Total 109	O 109	0	0
37	e	17	Total 17	O 17	0	0
37	f	3	Total 3	O 3	0	0
37	h	17	Total 17	O 17	0	0
37	i	17	Total 17	O 17	0	0
37	j	14	Total 14	O 14	0	0

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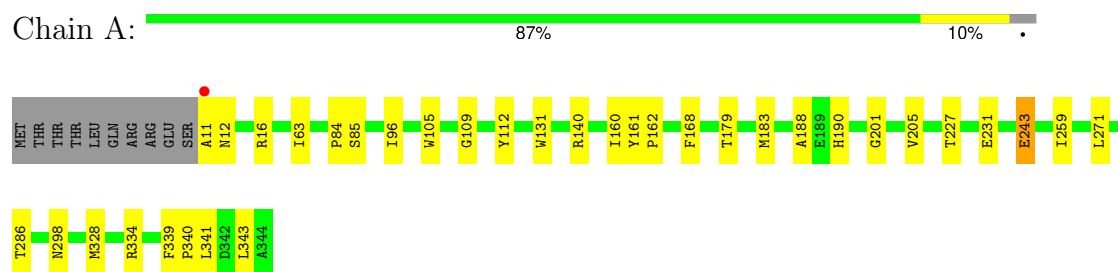
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	k	7	Total 7	O 7	0	0
37	l	7	Total 7	O 7	0	0
37	m	9	Total 9	O 9	0	0
37	o	85	Total 85	O 85	0	0
37	t	14	Total 14	O 14	0	0
37	u	48	Total 48	O 48	0	0
37	v	56	Total 56	O 56	0	0
37	x	10	Total 10	O 10	0	0
37	z	5	Total 5	O 5	0	0
37	r	2	Total 2	O 2	0	0

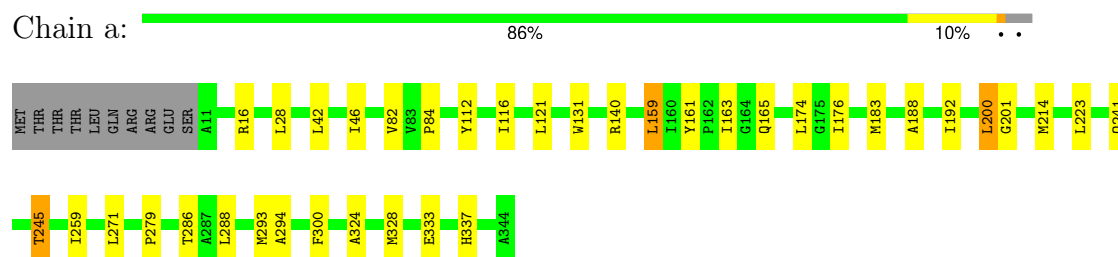
3 Residue-property plots

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

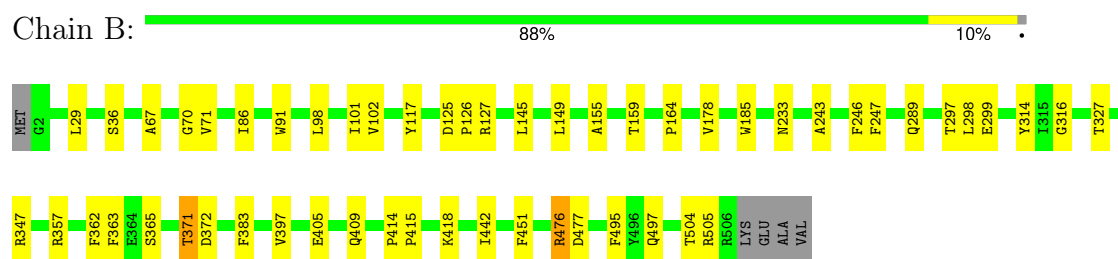
• Molecule 1: Photosystem II protein D1 1



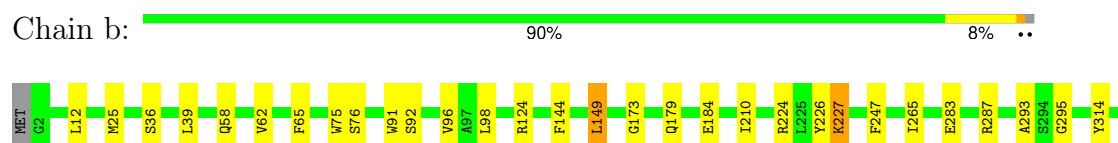
• Molecule 1: Photosystem II protein D1 1

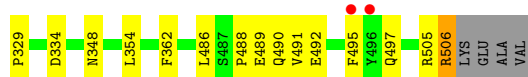


• Molecule 2: Photosystem II CP47 reaction center protein



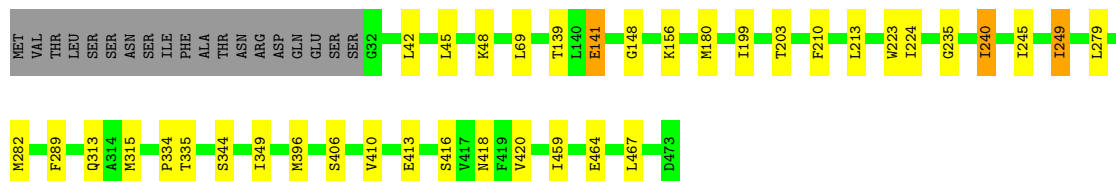
• Molecule 2: Photosystem II CP47 reaction center protein





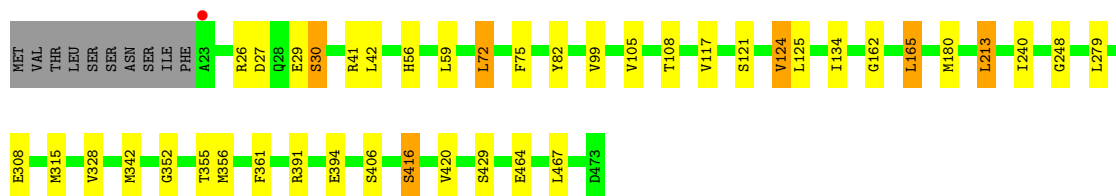
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 8% ..



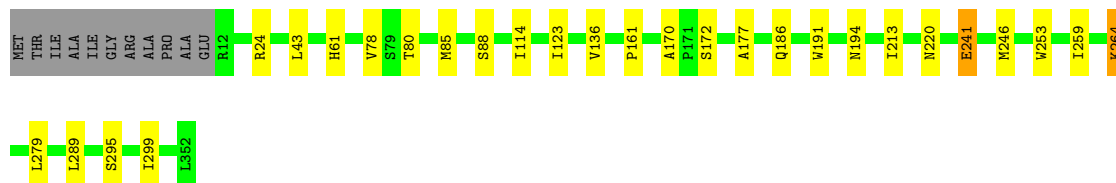
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 8% ..



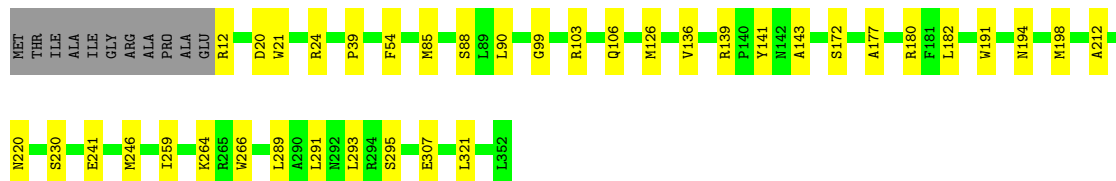
- Molecule 4: Photosystem II D2 protein

Chain D: 89% 7% ..



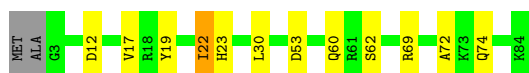
- Molecule 4: Photosystem II D2 protein

Chain d: 86% 11% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 83% 13% ..



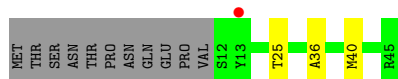
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 70% 27%



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 2% 69% 7% 24%



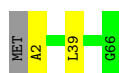
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 60% 11% 24%



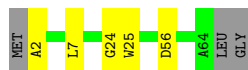
- Molecule 7: Photosystem II reaction center protein H

Chain H: 95% 5% 2%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 88% 8% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain I: 84% 11% 5%

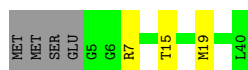
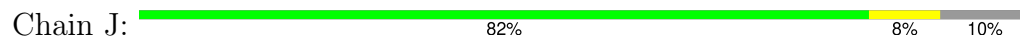


- Molecule 8: Photosystem II reaction center protein I

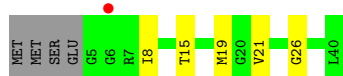
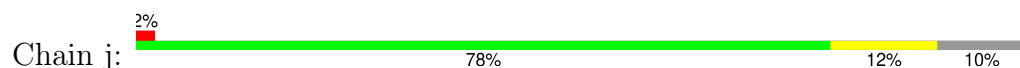
Chain i: 79% 16% 5%



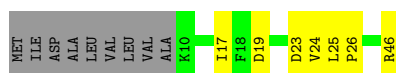
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



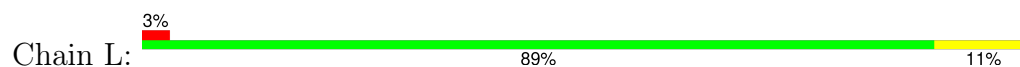
- Molecule 10: Photosystem II reaction center protein K



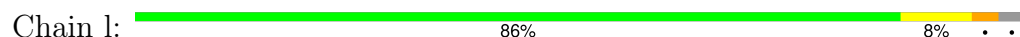
- Molecule 10: Photosystem II reaction center protein K



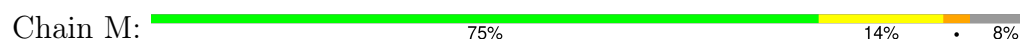
- Molecule 11: Photosystem II reaction center protein L

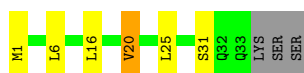


- Molecule 11: Photosystem II reaction center protein L



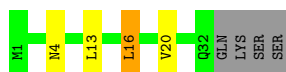
- Molecule 12: Photosystem II reaction center protein M





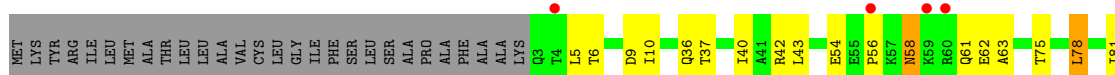
- Molecule 12: Photosystem II reaction center protein M

Chain m: 78% 8% 11%



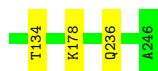
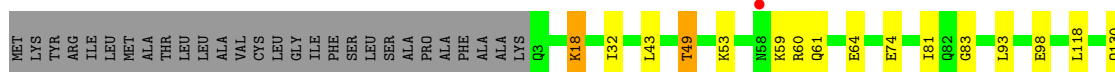
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 77% 12% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 83% 6% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 84% 9% 6%



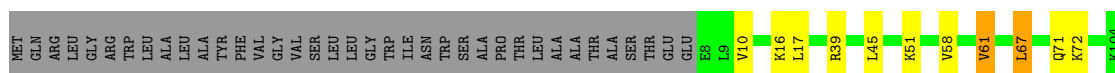
- Molecule 14: Photosystem II reaction center protein T

Chain t: 84% 9% 6%

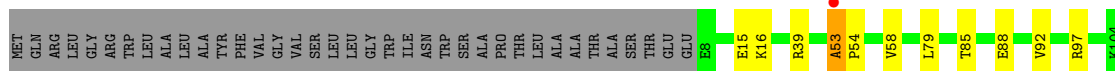


- Molecule 15: Photosystem II 12 kDa extrinsic protein

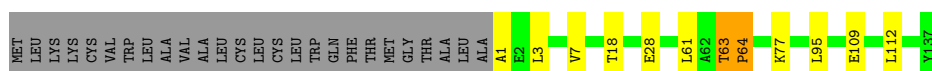
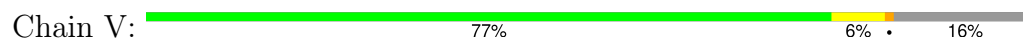
Chain U: 64% 7% 28%



- Molecule 15: Photosystem II 12 kDa extrinsic protein



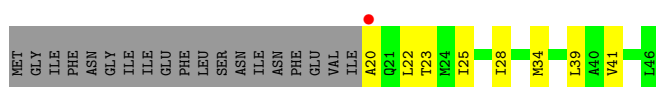
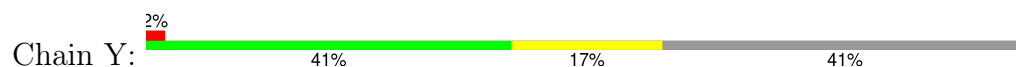
- Molecule 16: Cytochrome c-550



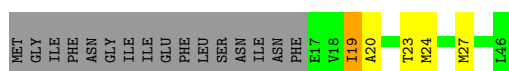
- Molecule 16: Cytochrome c-550



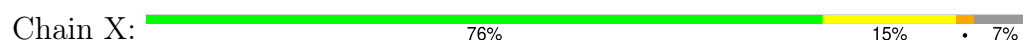
- Molecule 17: Photosystem II reaction center protein Ycf12



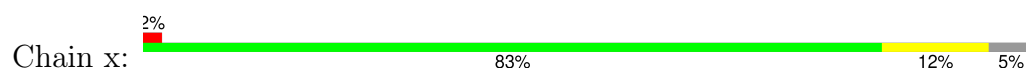
- Molecule 17: Photosystem II reaction center protein Ycf12



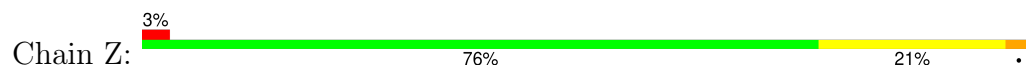
- Molecule 18: Photosystem II reaction center X protein



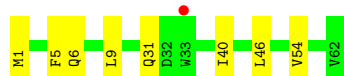
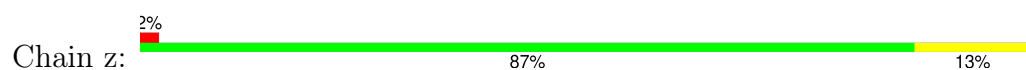
- Molecule 18: Photosystem II reaction center X protein



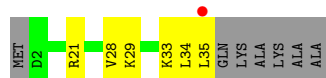
• Molecule 19: Photosystem II reaction center protein Z



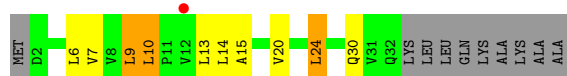
• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.34Å 222.83Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.74 – 2.00 19.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.74-2.00) 84.4 (19.74-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.226 0.182 , 0.227	Depositor DCC
R_{free} test set	4807 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	54524	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: OEY, FE2, HEC, STE, DGD, CL, LMG, LHG, CLA, BCR, SQD, HEM, OEX, PHO, FME, BCT, PL9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/3717	0.44	0/5060
1	a	0.26	0/3714	0.43	0/5056
2	B	0.32	0/4155	0.49	0/5661
2	b	0.32	0/4118	0.48	0/5611
3	C	0.31	0/3711	0.46	0/5051
3	c	0.29	0/3791	0.45	0/5158
4	D	0.34	0/2838	0.50	0/3862
4	d	0.33	0/2847	0.48	0/3874
5	E	0.26	0/688	0.45	0/940
5	e	0.24	0/683	0.45	0/932
6	F	0.30	0/284	0.47	0/387
6	f	0.25	0/284	0.52	0/387
7	H	0.32	0/523	0.50	0/713
7	h	0.28	0/511	0.45	0/697
8	I	0.30	0/293	0.46	0/396
8	i	0.32	0/293	0.43	0/396
9	J	0.26	0/263	0.41	0/356
9	j	0.23	0/263	0.43	0/356
10	K	0.27	0/303	0.42	0/416
10	k	0.27	0/303	0.43	0/416
11	L	0.34	0/311	0.45	0/422
11	l	0.33	0/303	0.46	0/412
12	M	0.31	0/249	0.49	0/341
12	m	0.31	0/244	0.51	0/334
13	O	0.32	0/1904	0.51	0/2585
13	o	0.31	0/1905	0.49	0/2583
14	T	0.32	0/257	0.54	0/349
14	t	0.33	0/255	0.45	0/346
15	U	0.27	0/785	0.47	0/1064
15	u	0.31	0/785	0.50	0/1064
16	V	0.29	0/1085	0.50	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1085	0.43	0/1473
17	Y	0.24	0/197	0.38	0/264
17	y	0.20	0/219	0.37	0/294
18	X	0.24	0/284	0.39	0/384
18	x	0.22	0/289	0.31	0/391
19	Z	0.21	0/490	0.46	0/669
19	z	0.18	0/488	0.31	0/666
20	R	0.27	0/277	0.43	0/380
20	r	0.23	0/252	0.39	0/347
All	All	0.30	0/45246	0.46	0/61566

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	V	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3604	0	3445	26	0
1	a	3601	0	3436	26	0
2	B	4005	0	3871	37	0
2	b	3978	0	3836	33	0
3	C	3592	0	3501	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3666	0	3574	25	0
4	D	2745	0	2653	19	0
4	d	2751	0	2659	29	0
5	E	666	0	651	9	0
5	e	664	0	648	17	0
6	F	275	0	282	2	0
6	f	275	0	282	6	0
7	H	510	0	532	2	0
7	h	498	0	518	3	0
8	I	296	0	311	2	0
8	i	296	0	311	3	0
9	J	257	0	268	2	0
9	j	257	0	268	4	0
10	K	293	0	305	3	0
10	k	293	0	305	7	0
11	L	304	0	316	4	0
11	l	296	0	304	1	0
12	M	256	0	269	5	0
12	m	251	0	267	4	0
13	O	1870	0	1830	22	0
13	o	1874	0	1846	9	0
14	T	258	0	261	2	0
14	t	256	0	256	1	0
15	U	774	0	773	5	0
15	u	774	0	773	7	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	20	0
17	Y	196	0	217	4	0
17	y	218	0	241	3	0
18	X	281	0	312	4	0
18	x	286	0	314	4	0
19	Z	479	0	516	7	0
19	z	477	0	509	4	0
20	R	271	0	298	0	0
20	r	246	0	263	6	0
21	A	20	0	0	0	0
21	a	20	0	0	0	0
22	A	11	0	0	1	0
22	a	11	0	0	1	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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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	1035	0	1139	29	0
25	C	839	0	922	15	0
25	D	130	0	144	2	0
25	a	260	0	288	11	0
25	b	970	0	1067	27	0
25	c	839	0	919	24	0
25	d	130	0	144	1	0
25	h	65	0	72	1	0
26	A	64	0	74	0	0
26	D	64	0	74	1	0
26	a	64	0	74	1	0
26	d	64	0	74	1	0
27	A	40	0	56	2	0
27	B	120	0	168	7	0
27	C	40	0	56	4	0
27	D	40	0	56	1	0
27	H	40	0	56	2	0
27	K	120	0	168	4	0
27	T	40	0	56	3	0
27	a	40	0	56	1	0
27	b	120	0	168	4	0
27	c	80	0	112	5	0
27	d	40	0	56	0	0
27	h	40	0	56	2	0
27	k	80	0	112	1	0
27	t	40	0	56	3	0
28	A	55	0	80	4	0
28	D	55	0	80	2	0
28	a	55	0	80	2	0
28	d	55	0	80	1	0
29	A	48	0	66	1	0
29	B	28	0	40	0	0
29	C	48	0	66	1	0
29	D	84	0	117	4	0
29	M	51	0	72	2	0
29	b	55	0	86	0	0
29	c	134	0	181	4	0
29	d	67	0	92	0	0
29	m	51	0	72	2	0
30	A	47	0	67	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	49	0	74	1	0
30	D	49	0	74	1	0
30	E	49	0	74	2	0
30	L	49	0	74	3	0
30	a	49	0	74	2	0
30	d	88	0	125	5	0
30	e	42	0	57	2	0
30	l	49	0	74	1	0
31	A	91	0	136	6	0
31	B	54	0	78	2	0
31	F	36	0	46	1	0
31	a	90	0	134	1	0
31	b	49	0	65	2	0
31	f	41	0	49	1	0
32	A	66	0	96	4	0
32	C	186	0	246	6	0
32	H	62	0	82	2	0
32	a	44	0	75	0	0
32	c	186	0	246	5	0
32	h	62	0	82	2	0
33	B	57	0	89	2	0
33	C	40	0	63	1	0
33	E	12	0	16	0	0
33	H	18	0	35	2	0
33	I	15	0	26	1	0
33	J	12	0	16	0	0
33	M	25	0	38	0	0
33	X	20	0	35	2	0
33	a	12	0	16	0	0
33	b	97	0	170	7	0
33	c	20	0	35	1	0
33	d	17	0	26	0	0
33	j	12	0	16	1	0
33	k	12	0	16	0	0
33	l	18	0	35	3	0
33	m	12	0	16	1	0
33	t	42	0	64	0	0
33	x	20	0	35	2	0
34	D	4	0	1	0	0
34	a	4	0	1	0	0
35	F	43	0	30	3	0
35	e	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	43	0	30	0	0
36	v	43	0	30	1	0
37	A	158	0	0	2	0
37	B	214	0	0	1	0
37	C	196	0	0	0	0
37	D	115	0	0	0	0
37	E	33	0	0	0	0
37	F	6	0	0	0	0
37	H	27	0	0	1	0
37	I	20	0	0	0	0
37	J	13	0	0	0	0
37	K	5	0	0	2	0
37	L	10	0	0	1	0
37	M	7	0	0	0	0
37	O	89	0	0	1	0
37	T	9	0	0	0	0
37	U	40	0	0	1	0
37	V	61	0	0	3	0
37	X	12	0	0	0	0
37	Z	6	0	0	0	0
37	a	131	0	0	1	0
37	b	199	0	0	3	0
37	c	150	0	0	1	0
37	d	109	0	0	0	0
37	e	17	0	0	0	0
37	f	3	0	0	0	0
37	h	17	0	0	0	0
37	i	17	0	0	0	0
37	j	14	0	0	0	0
37	k	7	0	0	0	0
37	l	7	0	0	0	0
37	m	9	0	0	1	0
37	o	85	0	0	0	0
37	r	2	0	0	0	0
37	t	14	0	0	0	0
37	u	48	0	0	0	0
37	v	56	0	0	1	0
37	x	10	0	0	0	0
37	z	5	0	0	0	0
All	All	54524	0	53863	507	0

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

The worst 5 of 507 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)
6:f:16:PHE:H	20:r:30:GLN:HE22	1.16	0.92
28:A:611:PL9:H361	6:F:25:THR:HG21	1.55	0.88
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.54	0.86
22:a:602[A]:OEY:O6	22:a:602[A]:OEY:O5	1.97	0.81
2:B:91:TRP:HE1	33:B:620:STE:H32	1.46	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/344 (133%)	445 (97%)	12 (3%)	1 (0%)	43	42
1	a	458/344 (133%)	440 (96%)	17 (4%)	1 (0%)	43	42
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	461/461 (100%)	449 (97%)	11 (2%)	1 (0%)	43	42
3	c	471/461 (102%)	457 (97%)	13 (3%)	1 (0%)	43	42
4	D	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
4	d	342/352 (97%)	332 (97%)	10 (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
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	9 (4%)	3 (1%)	10	6
13	o	242/272 (89%)	235 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	14
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	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%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100
20	R	32/41 (78%)	31 (97%)	0	1 (3%)	3	1
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5534/5700 (97%)	5383 (97%)	141 (2%)	10 (0%)	43	42

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO

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Mol	Chain	Res	Type
13	O	62	GLU
3	c	416	SER
15	u	53	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/280 (134%)	371 (99%)	3 (1%)	73	80
1	a	373/280 (133%)	362 (97%)	11 (3%)	37	40
2	B	407/407 (100%)	397 (98%)	10 (2%)	42	45
2	b	402/407 (99%)	396 (98%)	6 (2%)	57	64
3	C	361/362 (100%)	355 (98%)	6 (2%)	53	60
3	c	370/362 (102%)	356 (96%)	14 (4%)	29	29
4	D	278/283 (98%)	273 (98%)	5 (2%)	51	58
4	d	279/283 (99%)	273 (98%)	6 (2%)	45	50
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	25
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	41
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	10
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	29
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	13
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	25
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	10
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	200 (97%)	6 (3%)	37	40
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	28
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%)	79 (94%)	5 (6%)	17	14
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	70
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	60
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	33
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	6
18	X	31/34 (91%)	27 (87%)	4 (13%)	4	2
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	35
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
19	z	51/52 (98%)	47 (92%)	4 (8%)	11	8
20	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
20	r	25/33 (76%)	19 (76%)	6 (24%)	1	0
All	All	4572/4654 (98%)	4426 (97%)	146 (3%)	33	35

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	l	21	LEU
20	r	10	LEU
13	o	18	LYS
16	v	52	LEU
18	X	3	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	60	GLN

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Mol	Chain	Res	Type
12	m	5	GLN
18	x	33	GLN
13	O	231	HIS
13	O	219	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	T	1	14	8,9,10	1.07	0	8,9,11	0.99	1 (12%)
14	FME	t	1	14	8,9,10	1.13	1 (12%)	8,9,11	1.10	0
12	FME	m	1	12	8,9,10	0.95	0	8,9,11	0.84	0
8	FME	i	1	8	8,9,10	1.04	0	8,9,11	0.90	0
12	FME	M	1	12	8,9,10	1.05	1 (12%)	8,9,11	0.88	0
8	FME	I	1	8	8,9,10	0.95	0	8,9,11	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	1/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.20	1.43	1.46
14	t	1	FME	CA-N	-2.17	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.14	113.63	109.50

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	i	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
12	M	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	STE	X	101	-	19,19,19	0.56	0	19,19,19	1.18	1 (5%)
25	CLA	c	511	3	69,73,73	1.58	8 (11%)	82,113,113	1.46	6 (7%)
29	LMG	c	521	-	48,48,55	0.95	3 (6%)	56,56,63	1.29	7 (12%)
25	CLA	B	605	2	69,73,73	1.29	8 (11%)	82,113,113	1.37	8 (9%)
25	CLA	a	610	1	69,73,73	1.31	6 (8%)	82,113,113	1.31	7 (8%)
25	CLA	c	506	3	69,73,73	1.32	10 (14%)	82,113,113	1.21	6 (7%)
25	CLA	B	615	2	69,73,73	1.29	9 (13%)	82,113,113	1.26	6 (7%)
21	OEX	A	601[C]	37,3,1	0,14,14	-	-	-	-	-
25	CLA	C	502	3	69,73,73	1.23	9 (13%)	82,113,113	1.19	6 (7%)
29	LMG	D	407	-	51,51,55	0.75	1 (1%)	59,59,63	1.34	7 (11%)
33	STE	M	102	-	14,14,19	0.63	0	14,14,19	1.43	2 (14%)
27	BCR	B	617	-	41,41,41	1.04	3 (7%)	56,56,56	1.21	6 (10%)
33	STE	b	625	-	19,19,19	0.59	0	19,19,19	1.07	1 (5%)
31	SQD	B	623	-	52,54,54	1.56	8 (15%)	62,65,65	1.73	11 (17%)
25	CLA	B	612	2	69,73,73	1.16	6 (8%)	82,113,113	1.33	11 (13%)
33	STE	b	620	-	15,15,19	0.39	0	14,14,19	0.83	0
25	CLA	b	603	2	69,73,73	1.36	8 (11%)	82,113,113	1.44	10 (12%)
25	CLA	b	604	2	69,73,73	1.18	8 (11%)	82,113,113	1.59	11 (13%)
33	STE	H	103	-	17,17,19	0.42	0	16,16,19	0.68	0
32	DGD	C	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.35	8 (10%)
31	SQD	A	615	-	50,52,54	1.56	6 (12%)	60,63,65	1.86	10 (16%)
27	BCR	B	619	-	41,41,41	1.02	2 (4%)	56,56,56	1.28	5 (8%)
32	DGD	c	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.37	8 (10%)
36	HEC	v	201	16	50,50,50	1.68	6 (12%)	68,82,82	1.32	8 (11%)
27	BCR	C	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	6 (10%)
34	BCT	a	606	23	3,3,3	1.07	0	2,3,3	3.15	1 (50%)
36	HEC	V	201	16	50,50,50	1.67	7 (14%)	68,82,82	1.30	6 (8%)
25	CLA	b	613	2	69,73,73	1.38	9 (13%)	82,113,113	1.22	6 (7%)
35	HEM	e	101	6,5	50,50,50	1.58	7 (14%)	67,82,82	1.22	4 (5%)
30	LHG	B	622	-	48,48,48	0.74	1 (2%)	51,54,54	1.37	7 (13%)
25	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.51	11 (13%)
25	CLA	B	602	2	69,73,73	1.29	7 (10%)	82,113,113	1.34	12 (14%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	h	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.27	5 (8%)
27	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.07	3 (5%)
25	CLA	b	609	37	69,73,73	1.25	6 (8%)	82,113,113	1.28	6 (7%)
29	LMG	B	621	-	26,26,55	0.60	1 (3%)	26,26,63	1.35	2 (7%)
27	BCR	b	616	-	41,41,41	0.96	3 (7%)	56,56,56	1.23	4 (7%)
29	LMG	d	408	-	21,21,55	0.57	0	20,20,63	1.20	3 (15%)
33	STE	b	626	-	9,9,19	0.39	0	8,8,19	0.60	0
29	LMG	M	101	-	51,51,55	0.87	3 (5%)	59,59,63	1.44	10 (16%)
25	CLA	B	616	2	64,68,73	1.48	9 (14%)	76,107,113	1.36	8 (10%)
29	LMG	c	522	-	49,49,55	0.96	4 (8%)	57,57,63	1.29	4 (7%)
25	CLA	b	601	2	69,73,73	1.15	8 (11%)	82,113,113	1.41	8 (9%)
33	STE	B	620	-	16,16,19	0.70	0	16,16,19	1.06	0
25	CLA	B	606	2	69,73,73	1.38	8 (11%)	82,113,113	1.48	6 (7%)
33	STE	J	101	-	11,11,19	0.79	0	11,11,19	1.19	1 (9%)
25	CLA	C	512	3	69,73,73	1.52	10 (14%)	82,113,113	1.37	9 (10%)
25	CLA	A	612	37	69,73,73	1.21	8 (11%)	82,113,113	1.31	6 (7%)
33	STE	E	102	-	11,11,19	0.74	0	11,11,19	1.14	1 (9%)
27	BCR	b	618	-	41,41,41	0.95	2 (4%)	56,56,56	1.12	4 (7%)
21	OEX	A	601[B]	37,3,1	0,14,14	-	-	-	-	-
25	CLA	C	501	3	69,73,73	1.56	10 (14%)	82,113,113	1.43	8 (9%)
25	CLA	B	609	2	69,73,73	1.24	6 (8%)	82,113,113	1.33	9 (10%)
25	CLA	A	607	37	69,73,73	1.14	6 (8%)	82,113,113	1.35	10 (12%)
30	LHG	d	406	-	48,48,48	0.71	2 (4%)	51,54,54	1.21	5 (9%)
33	STE	C	519	-	11,11,19	0.65	0	11,11,19	1.53	1 (9%)
21	OEX	a	601[C]	37,3,1	0,14,14	-	-	-	-	-
27	BCR	d	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.18	4 (7%)
35	HEM	F	101	6,5	50,50,50	1.48	10 (20%)	67,82,82	1.22	4 (5%)
25	CLA	c	508	3	68,72,73	1.33	8 (11%)	80,111,113	1.36	8 (10%)
25	CLA	C	504	37	63,67,73	1.30	8 (12%)	74,105,113	1.27	8 (10%)
32	DGD	A	617	-	67,67,67	1.11	6 (8%)	81,81,81	1.31	8 (9%)
25	CLA	b	615	2	64,68,73	1.18	5 (7%)	76,107,113	1.37	10 (13%)
25	CLA	c	503	3	69,73,73	1.37	9 (13%)	82,113,113	1.43	6 (7%)
25	CLA	b	614	2	69,73,73	1.27	9 (13%)	82,113,113	1.31	4 (4%)
30	LHG	a	614	-	48,48,48	0.76	3 (6%)	51,54,54	1.31	7 (13%)
33	STE	b	623	-	15,15,19	0.68	0	15,15,19	1.04	0
26	PHO	a	609	-	58,69,69	2.15	9 (15%)	55,99,99	1.44	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	602	2	69,73,73	1.20	8 (11%)	82,113,113	1.29	9 (10%)
25	CLA	A	609	1	58,62,73	1.22	7 (12%)	68,99,113	1.42	8 (11%)
25	CLA	C	505	3	69,73,73	1.24	7 (10%)	82,113,113	1.30	7 (8%)
33	STE	k	103	-	11,11,19	0.75	0	11,11,19	1.09	0
33	STE	x	101	-	19,19,19	0.71	0	19,19,19	0.97	1 (5%)
33	STE	c	520	-	19,19,19	0.60	0	19,19,19	1.03	0
25	CLA	a	608	37	69,73,73	1.21	6 (8%)	82,113,113	1.35	8 (9%)
33	STE	B	625	-	11,11,19	0.68	0	11,11,19	1.31	2 (18%)
25	CLA	b	611	2	69,73,73	1.28	9 (13%)	82,113,113	1.34	9 (10%)
25	CLA	B	604	2	69,73,73	1.35	7 (10%)	82,113,113	1.53	7 (8%)
27	BCR	B	618	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
29	LMG	d	409	-	44,44,55	0.94	3 (6%)	52,52,63	1.30	6 (11%)
25	CLA	c	513	3	69,73,73	1.29	7 (10%)	82,113,113	1.28	10 (12%)
26	PHO	d	401	-	58,69,69	2.14	8 (13%)	55,99,99	1.57	10 (18%)
31	SQD	F	102	-	34,36,54	1.51	6 (17%)	42,45,65	1.95	10 (23%)
33	STE	t	103	-	9,9,19	0.35	0	8,8,19	0.80	0
25	CLA	C	511	3	69,73,73	1.37	8 (11%)	82,113,113	1.46	5 (6%)
25	CLA	h	101	37	69,73,73	1.37	9 (13%)	82,113,113	1.41	7 (8%)
25	CLA	b	608	2	69,73,73	1.29	8 (11%)	82,113,113	1.27	7 (8%)
25	CLA	B	607	37	69,73,73	1.26	6 (8%)	82,113,113	1.32	6 (7%)
25	CLA	c	501	3	69,73,73	1.22	9 (13%)	82,113,113	1.39	7 (8%)
22	OEY	A	602[A]	37,3,1	0,16,16	-	-	-	-	-
30	LHG	d	407	-	38,38,48	0.76	1 (2%)	41,44,54	1.11	2 (4%)
33	STE	a	618	-	11,11,19	0.79	0	11,11,19	1.20	2 (18%)
32	DGD	c	517	-	63,63,67	0.95	2 (3%)	77,77,81	1.41	9 (11%)
25	CLA	c	512	3	69,73,73	1.27	10 (14%)	82,113,113	1.34	7 (8%)
25	CLA	C	506	3	69,73,73	1.19	6 (8%)	82,113,113	1.22	9 (10%)
30	LHG	A	614	-	46,46,48	0.84	3 (6%)	49,52,54	1.20	6 (12%)
31	SQD	b	619	-	47,49,54	1.63	9 (19%)	57,60,65	1.73	10 (17%)
33	STE	d	410	-	16,16,19	0.61	0	16,16,19	1.30	1 (6%)
30	LHG	L	101	-	48,48,48	0.75	1 (2%)	51,54,54	1.16	2 (3%)
27	BCR	k	102	-	41,41,41	1.02	3 (7%)	56,56,56	1.15	4 (7%)
25	CLA	a	613	37	69,73,73	1.37	6 (8%)	82,113,113	1.44	7 (8%)
27	BCR	t	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.39	10 (17%)
27	BCR	c	514	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	A	610	-	41,41,41	0.97	1 (2%)	56,56,56	1.13	4 (7%)
29	LMG	A	613	-	48,48,55	0.88	2 (4%)	56,56,63	1.29	4 (7%)
29	LMG	c	519	-	37,37,55	1.01	2 (5%)	45,45,63	1.36	6 (13%)
32	DGD	c	516	-	63,63,67	0.90	4 (6%)	77,77,81	1.38	11 (14%)
33	STE	B	624	-	11,11,19	0.75	0	11,11,19	1.24	0
26	PHO	A	608	-	58,69,69	1.95	10 (17%)	55,99,99	1.44	6 (10%)
25	CLA	B	611	2	69,73,73	1.23	6 (8%)	82,113,113	1.36	6 (7%)
25	CLA	c	510	3	69,73,73	1.34	8 (11%)	82,113,113	1.35	8 (9%)
25	CLA	c	505	3	69,73,73	1.12	7 (10%)	82,113,113	1.30	6 (7%)
25	CLA	b	606	37	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
33	STE	b	621	-	19,19,19	0.65	0	19,19,19	0.95	0
33	STE	t	102	-	13,13,19	0.65	0	13,13,19	1.33	2 (15%)
27	BCR	a	611	-	41,41,41	0.96	2 (4%)	56,56,56	1.24	5 (8%)
30	LHG	D	408	-	48,48,48	0.74	2 (4%)	51,54,54	1.30	6 (11%)
25	CLA	B	601	37	69,73,73	1.40	11 (15%)	82,113,113	1.35	11 (13%)
30	LHG	E	101	-	48,48,48	0.79	2 (4%)	51,54,54	1.25	6 (11%)
31	SQD	f	101	-	39,41,54	1.68	8 (20%)	49,52,65	1.64	10 (20%)
30	LHG	e	102	-	41,41,48	0.80	1 (2%)	44,47,54	1.30	5 (11%)
28	PL9	d	405	-	55,55,55	1.05	3 (5%)	68,69,69	1.62	14 (20%)
33	STE	B	626	-	15,15,19	0.36	0	14,14,19	0.90	0
25	CLA	B	608	2	69,73,73	1.17	8 (11%)	82,113,113	1.37	10 (12%)
32	DGD	a	617	-	43,43,67	0.79	3 (6%)	45,45,81	1.41	7 (15%)
25	CLA	B	610	37	69,73,73	1.24	10 (14%)	82,113,113	1.25	9 (10%)
33	STE	I	101	-	14,14,19	0.32	0	13,13,19	0.82	0
33	STE	j	101	-	11,11,19	0.78	0	11,11,19	1.29	2 (18%)
27	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.30	5 (8%)
25	CLA	d	402	4	69,73,73	1.18	7 (10%)	82,113,113	1.26	7 (8%)
27	BCR	K	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.12	5 (8%)
25	CLA	b	612	2	69,73,73	1.22	8 (11%)	82,113,113	1.41	9 (10%)
33	STE	C	521	-	15,15,19	0.38	0	14,14,19	0.79	0
32	DGD	h	103	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	12 (15%)
25	CLA	D	403	4	69,73,73	1.29	9 (13%)	82,113,113	1.32	7 (8%)
33	STE	C	520	-	11,11,19	0.71	0	11,11,19	1.19	1 (9%)
22	OEY	a	602[A]	37,3,1	0,16,16	-	-	-	-	-
25	CLA	b	607	2	69,73,73	1.24	7 (10%)	82,113,113	1.41	10 (12%)
25	CLA	c	507	37	69,73,73	1.34	10 (14%)	82,113,113	1.42	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	SQD	a	615	-	52,54,54	1.59	7 (13%)	62,65,65	1.88	10 (16%)
31	SQD	A	616	-	38,38,54	1.78	5 (13%)	40,40,65	1.19	2 (5%)
32	DGD	C	516	-	63,63,67	1.06	5 (7%)	77,77,81	1.33	7 (9%)
25	CLA	c	504	37	64,68,73	1.16	4 (6%)	76,107,113	1.36	10 (13%)
25	CLA	C	510	3	69,73,73	1.21	7 (10%)	82,113,113	1.34	8 (9%)
25	CLA	d	403	4	69,73,73	1.24	7 (10%)	82,113,113	1.27	9 (10%)
27	BCR	T	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.31	6 (10%)
29	LMG	b	622	-	55,55,55	0.80	1 (1%)	63,63,63	1.37	12 (19%)
30	LHG	l	101	-	48,48,48	0.58	0	51,54,54	1.23	5 (9%)
34	BCT	D	401	23	3,3,3	1.07	0	2,3,3	3.28	1 (50%)
25	CLA	a	607	1	69,73,73	1.43	10 (14%)	82,113,113	1.34	6 (7%)
27	BCR	K	103	-	41,41,41	1.11	2 (4%)	56,56,56	1.13	2 (3%)
26	PHO	D	402	-	58,69,69	2.11	10 (17%)	55,99,99	1.53	7 (12%)
33	STE	m	102	-	11,11,19	0.70	0	11,11,19	1.44	2 (18%)
25	CLA	c	509	3	69,73,73	1.26	9 (13%)	82,113,113	1.42	5 (6%)
33	STE	t	104	-	17,17,19	0.65	0	17,17,19	1.10	1 (5%)
25	CLA	B	613	2	69,73,73	1.29	7 (10%)	82,113,113	1.46	11 (13%)
25	CLA	b	605	2	69,73,73	1.35	5 (7%)	82,113,113	1.48	9 (10%)
25	CLA	D	404	4	69,73,73	1.54	10 (14%)	82,113,113	1.19	8 (9%)
32	DGD	C	515	-	63,63,67	1.05	5 (7%)	77,77,81	1.36	11 (14%)
27	BCR	H	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.20	6 (10%)
25	CLA	A	606	1	69,73,73	1.32	9 (13%)	82,113,113	1.21	7 (8%)
21	OEX	a	601[B]	37,3,1	0,14,14	-	-	-	-	-
27	BCR	D	405	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	5 (8%)
29	LMG	m	101	-	51,51,55	0.91	3 (5%)	59,59,63	1.48	7 (11%)
33	STE	b	624	-	14,14,19	0.32	0	13,13,19	0.89	0
25	CLA	C	503	3	69,73,73	1.44	9 (13%)	82,113,113	1.56	9 (10%)
25	CLA	C	507	37	69,73,73	1.31	8 (11%)	82,113,113	1.39	11 (13%)
28	PL9	A	611	-	55,55,55	0.78	1 (1%)	68,69,69	1.47	13 (19%)
25	CLA	B	603	2	69,73,73	1.23	8 (11%)	82,113,113	1.22	6 (7%)
25	CLA	C	513	3	69,73,73	1.24	8 (11%)	82,113,113	1.40	7 (8%)
33	STE	l	102	-	17,17,19	0.34	0	16,16,19	0.89	0
25	CLA	C	509	3	69,73,73	1.27	11 (15%)	82,113,113	1.30	8 (9%)
27	BCR	b	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.09	4 (7%)
32	DGD	H	102	-	63,63,67	1.21	8 (12%)	77,77,81	1.33	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PL9	D	406	-	55,55,55	0.96	2 (3%)	68,69,69	1.72	12 (17%)
25	CLA	c	502	3	69,73,73	1.25	9 (13%)	82,113,113	1.27	7 (8%)
25	CLA	b	610	2	69,73,73	1.33	7 (10%)	82,113,113	1.33	10 (12%)
29	LMG	C	518	-	48,48,55	0.74	0	56,56,63	1.31	7 (12%)
29	LMG	D	409	-	31,31,55	0.84	2 (6%)	33,33,63	1.28	3 (9%)
28	PL9	a	612	-	55,55,55	0.78	2 (3%)	68,69,69	1.58	11 (16%)
33	STE	M	103	-	9,9,19	0.35	0	8,8,19	0.79	0
31	SQD	a	616	-	35,35,54	1.68	5 (14%)	37,37,65	1.43	6 (16%)
25	CLA	B	614	2	69,73,73	1.38	8 (11%)	82,113,113	1.50	9 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	X	101	-	-	8/17/17/17	-
25	CLA	c	511	3	-	9/39/115/115	-
29	LMG	c	521	-	-	23/43/63/70	0/1/1/1
25	CLA	B	605	2	-	12/39/115/115	-
25	CLA	a	610	1	-	8/39/115/115	-
25	CLA	c	506	3	-	13/39/115/115	-
25	CLA	B	615	2	-	16/39/115/115	-
25	CLA	C	502	3	-	9/39/115/115	-
29	LMG	D	407	-	-	19/46/66/70	0/1/1/1
33	STE	M	102	-	-	6/12/12/17	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
33	STE	b	625	-	-	7/17/17/17	-
31	SQD	B	623	-	-	20/49/69/69	0/1/1/1
25	CLA	B	612	2	-	7/39/115/115	-
33	STE	b	620	-	-	8/13/13/17	-
25	CLA	b	603	2	-	7/39/115/115	-
25	CLA	b	604	2	-	7/39/115/115	-
33	STE	H	103	-	-	11/15/15/17	-
32	DGD	C	517	-	-	17/51/91/95	0/2/2/2
31	SQD	A	615	-	-	14/47/67/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	B	619	-	-	4/29/63/63	0/2/2/2
36	HEC	v	201	16	1/1/3/7	4/14/54/54	-
32	DGD	c	518	-	-	19/51/91/95	0/2/2/2
27	BCR	C	514	-	-	1/29/63/63	0/2/2/2
36	HEC	V	201	16	1/1/3/7	6/14/54/54	-
25	CLA	b	613	2	-	18/39/115/115	-
35	HEM	e	101	6,5	-	3/14/54/54	-
30	LHG	B	622	-	-	16/53/53/53	-
25	CLA	C	508	3	-	7/39/115/115	-
25	CLA	B	602	2	-	7/39/115/115	-
27	BCR	K	101	-	-	11/29/63/63	0/2/2/2
27	BCR	h	102	-	-	3/29/63/63	0/2/2/2
27	BCR	k	101	-	-	8/29/63/63	0/2/2/2
25	CLA	b	609	37	-	3/39/115/115	-
29	LMG	B	621	-	-	6/22/22/70	-
27	BCR	b	616	-	-	5/29/63/63	0/2/2/2
29	LMG	d	408	-	-	11/17/17/70	-
33	STE	b	626	-	-	5/7/7/17	-
29	LMG	M	101	-	-	22/46/66/70	0/1/1/1
25	CLA	B	616	2	-	12/33/109/115	-
29	LMG	c	522	-	-	24/44/64/70	0/1/1/1
25	CLA	b	601	2	-	8/39/115/115	-
33	STE	B	620	-	-	5/14/14/17	-
25	CLA	B	606	2	-	11/39/115/115	-
33	STE	J	101	-	-	3/9/9/17	-
25	CLA	C	512	3	-	14/39/115/115	-
25	CLA	A	612	37	-	4/39/115/115	-
33	STE	E	102	-	-	6/9/9/17	-
27	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	CLA	C	501	3	-	4/39/115/115	-
25	CLA	B	609	2	-	1/39/115/115	-
25	CLA	A	607	37	-	10/39/115/115	-
30	LHG	d	406	-	-	21/53/53/53	-
33	STE	C	519	-	-	5/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	d	404	-	-	4/29/63/63	0/2/2/2
35	HEM	F	101	6,5	-	3/14/54/54	-
25	CLA	c	508	3	-	10/38/114/115	-
25	CLA	C	504	37	-	6/32/108/115	-
32	DGD	A	617	-	-	28/55/95/95	0/2/2/2
25	CLA	b	615	2	-	7/33/109/115	-
25	CLA	c	503	3	-	7/39/115/115	-
25	CLA	b	614	2	-	10/39/115/115	-
30	LHG	a	614	-	-	21/53/53/53	-
33	STE	b	623	-	-	6/13/13/17	-
26	PHO	a	609	-	-	6/37/103/103	0/5/6/6
25	CLA	b	602	2	-	9/39/115/115	-
25	CLA	A	609	1	-	2/26/102/115	-
25	CLA	C	505	3	-	8/39/115/115	-
33	STE	k	103	-	-	6/9/9/17	-
33	STE	x	101	-	-	11/17/17/17	-
33	STE	c	520	-	-	13/17/17/17	-
25	CLA	a	608	37	-	12/39/115/115	-
33	STE	B	625	-	-	5/9/9/17	-
25	CLA	b	611	2	-	5/39/115/115	-
25	CLA	B	604	2	-	10/39/115/115	-
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2
29	LMG	d	409	-	-	11/39/59/70	0/1/1/1
25	CLA	c	513	3	-	11/39/115/115	-
26	PHO	d	401	-	-	7/37/103/103	0/5/6/6
31	SQD	F	102	-	-	7/28/48/69	0/1/1/1
33	STE	t	103	-	-	4/7/7/17	-
25	CLA	C	511	3	-	3/39/115/115	-
25	CLA	h	101	37	-	14/39/115/115	-
25	CLA	b	608	2	-	9/39/115/115	-
25	CLA	B	607	37	-	6/39/115/115	-
25	CLA	c	501	3	-	5/39/115/115	-
30	LHG	d	407	-	-	11/43/43/53	-
33	STE	a	618	-	-	5/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	DGD	c	517	-	-	19/51/91/95	0/2/2/2
25	CLA	c	512	3	-	20/39/115/115	-
25	CLA	C	506	3	-	9/39/115/115	-
30	LHG	A	614	-	-	17/51/51/53	-
31	SQD	b	619	-	-	23/44/64/69	0/1/1/1
33	STE	d	410	-	-	10/14/14/17	-
30	LHG	L	101	-	-	21/53/53/53	-
27	BCR	k	102	-	-	3/29/63/63	0/2/2/2
25	CLA	a	613	37	-	3/39/115/115	-
27	BCR	t	101	-	-	1/29/63/63	0/2/2/2
27	BCR	c	514	-	-	8/29/63/63	0/2/2/2
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
29	LMG	A	613	-	-	22/43/63/70	0/1/1/1
29	LMG	c	519	-	-	13/31/51/70	0/1/1/1
32	DGD	c	516	-	-	19/51/91/95	0/2/2/2
33	STE	B	624	-	-	8/9/9/17	-
26	PHO	A	608	-	-	2/37/103/103	0/5/6/6
25	CLA	B	611	2	-	5/39/115/115	-
25	CLA	c	510	3	-	14/39/115/115	-
25	CLA	c	505	3	-	14/39/115/115	-
25	CLA	b	606	37	-	12/39/115/115	-
33	STE	b	621	-	-	10/17/17/17	-
33	STE	t	102	-	-	4/11/11/17	-
27	BCR	a	611	-	-	1/29/63/63	0/2/2/2
30	LHG	D	408	-	-	17/53/53/53	-
25	CLA	B	601	37	-	15/39/115/115	-
30	LHG	E	101	-	-	27/53/53/53	-
31	SQD	f	101	-	-	14/36/56/69	0/1/1/1
30	LHG	e	102	-	-	24/46/46/53	-
28	PL9	d	405	-	-	6/53/73/73	0/1/1/1
33	STE	B	626	-	-	2/13/13/17	-
25	CLA	B	608	2	-	4/39/115/115	-
32	DGD	a	617	-	-	21/45/45/95	-
25	CLA	B	610	37	-	6/39/115/115	-
33	STE	I	101	-	-	5/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	j	101	-	-	4/9/9/17	-
27	BCR	c	515	-	-	3/29/63/63	0/2/2/2
25	CLA	d	402	4	-	6/39/115/115	-
27	BCR	K	102	-	-	6/29/63/63	0/2/2/2
25	CLA	b	612	2	-	4/39/115/115	-
33	STE	C	521	-	-	8/13/13/17	-
32	DGD	h	103	-	-	19/51/91/95	0/2/2/2
25	CLA	D	403	4	-	4/39/115/115	-
33	STE	C	520	-	-	3/9/9/17	-
25	CLA	b	607	2	-	5/39/115/115	-
25	CLA	c	507	37	-	9/39/115/115	-
31	SQD	a	615	-	-	22/49/69/69	0/1/1/1
31	SQD	A	616	-	-	20/39/39/69	-
32	DGD	C	516	-	-	17/51/91/95	0/2/2/2
25	CLA	c	504	37	-	8/33/109/115	-
25	CLA	C	510	3	-	14/39/115/115	-
25	CLA	d	403	4	-	9/39/115/115	-
27	BCR	T	101	-	-	4/29/63/63	0/2/2/2
29	LMG	b	622	-	-	33/50/70/70	0/1/1/1
30	LHG	l	101	-	-	21/53/53/53	-
25	CLA	a	607	1	-	2/39/115/115	-
27	BCR	K	103	-	-	5/29/63/63	0/2/2/2
26	PHO	D	402	-	-	0/37/103/103	0/5/6/6
33	STE	m	102	-	-	5/9/9/17	-
25	CLA	c	509	3	-	11/39/115/115	-
33	STE	t	104	-	-	7/15/15/17	-
25	CLA	B	613	2	-	9/39/115/115	-
25	CLA	b	605	2	-	6/39/115/115	-
25	CLA	D	404	4	-	9/39/115/115	-
32	DGD	C	515	-	-	19/51/91/95	0/2/2/2
27	BCR	H	101	-	-	5/29/63/63	0/2/2/2
25	CLA	A	606	1	-	2/39/115/115	-
27	BCR	D	405	-	-	3/29/63/63	0/2/2/2
29	LMG	m	101	-	-	20/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	b	624	-	-	9/12/12/17	-
25	CLA	C	503	3	-	4/39/115/115	-
25	CLA	C	507	37	-	5/39/115/115	-
28	PL9	A	611	-	-	24/53/73/73	0/1/1/1
25	CLA	B	603	2	-	9/39/115/115	-
25	CLA	C	513	3	-	6/39/115/115	-
33	STE	l	102	-	-	8/15/15/17	-
25	CLA	C	509	3	-	14/39/115/115	-
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
32	DGD	H	102	-	-	16/51/91/95	0/2/2/2
28	PL9	D	406	-	-	13/53/73/73	0/1/1/1
25	CLA	c	502	3	-	3/39/115/115	-
25	CLA	b	610	2	-	6/39/115/115	-
29	LMG	C	518	-	-	17/43/63/70	0/1/1/1
29	LMG	D	409	-	-	20/33/33/70	-
28	PL9	a	612	-	-	15/53/73/73	0/1/1/1
33	STE	M	103	-	-	3/7/7/17	-
31	SQD	a	616	-	-	17/37/37/69	-
25	CLA	B	614	2	-	8/39/115/115	-

The worst 5 of 810 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	609	PHO	C1B-C2B	9.67	1.50	1.39
26	d	401	PHO	C1B-C2B	9.37	1.49	1.39
26	d	401	PHO	C3B-C4B	9.05	1.50	1.41
26	D	402	PHO	C3B-C4B	8.87	1.50	1.41
26	a	609	PHO	C3B-C4B	8.63	1.50	1.41

The worst 5 of 1080 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C4A-NA-C1A	9.04	110.80	106.68
25	C	511	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	c	511	CLA	C4A-NA-C1A	8.52	110.57	106.68
25	b	605	CLA	C4A-NA-C1A	8.36	110.49	106.68
25	C	508	CLA	C4A-NA-C1A	8.18	110.41	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 1722 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	607	CLA	C14-C13-C15-C16
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

133 monomers are involved in 233 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	101	STE	2	0
25	c	511	CLA	3	0
29	c	521	LMG	3	0
25	a	610	CLA	4	0
25	B	615	CLA	1	0
25	C	502	CLA	1	0
29	D	407	LMG	2	0
27	B	617	BCR	1	0
33	b	625	STE	2	0
31	B	623	SQD	2	0
25	B	612	CLA	1	0
25	b	603	CLA	3	0
25	b	604	CLA	3	0
33	H	103	STE	2	0
32	C	517	DGD	2	0
31	A	615	SQD	2	0
27	B	619	BCR	4	0
32	c	518	DGD	3	0
36	v	201	HEC	1	0
27	C	514	BCR	4	0
25	b	613	CLA	3	0
35	e	101	HEM	2	0
30	B	622	LHG	1	0
25	C	508	CLA	3	0
25	B	602	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	K	101	BCR	1	0
27	h	102	BCR	2	0
25	b	609	CLA	2	0
27	b	616	BCR	2	0
29	M	101	LMG	2	0
25	B	616	CLA	2	0
25	b	601	CLA	4	0
33	B	620	STE	1	0
25	B	606	CLA	5	0
25	C	512	CLA	2	0
25	A	612	CLA	4	0
25	B	609	CLA	1	0
25	A	607	CLA	1	0
30	d	406	LHG	4	0
33	C	519	STE	1	0
35	F	101	HEM	3	0
25	c	508	CLA	2	0
25	C	504	CLA	3	0
32	A	617	DGD	4	0
25	b	615	CLA	3	0
25	c	503	CLA	4	0
25	b	614	CLA	2	0
30	a	614	LHG	2	0
33	b	623	STE	1	0
26	a	609	PHO	1	0
25	b	602	CLA	2	0
25	C	505	CLA	4	0
33	x	101	STE	2	0
33	c	520	STE	1	0
33	B	625	STE	1	0
25	b	611	CLA	2	0
25	B	604	CLA	4	0
27	B	618	BCR	2	0
25	c	513	CLA	5	0
26	d	401	PHO	1	0
31	F	102	SQD	1	0
25	C	511	CLA	1	0
25	h	101	CLA	1	0
25	b	608	CLA	2	0
25	B	607	CLA	2	0
25	c	501	CLA	3	0
22	A	602[A]	OEY	1	0

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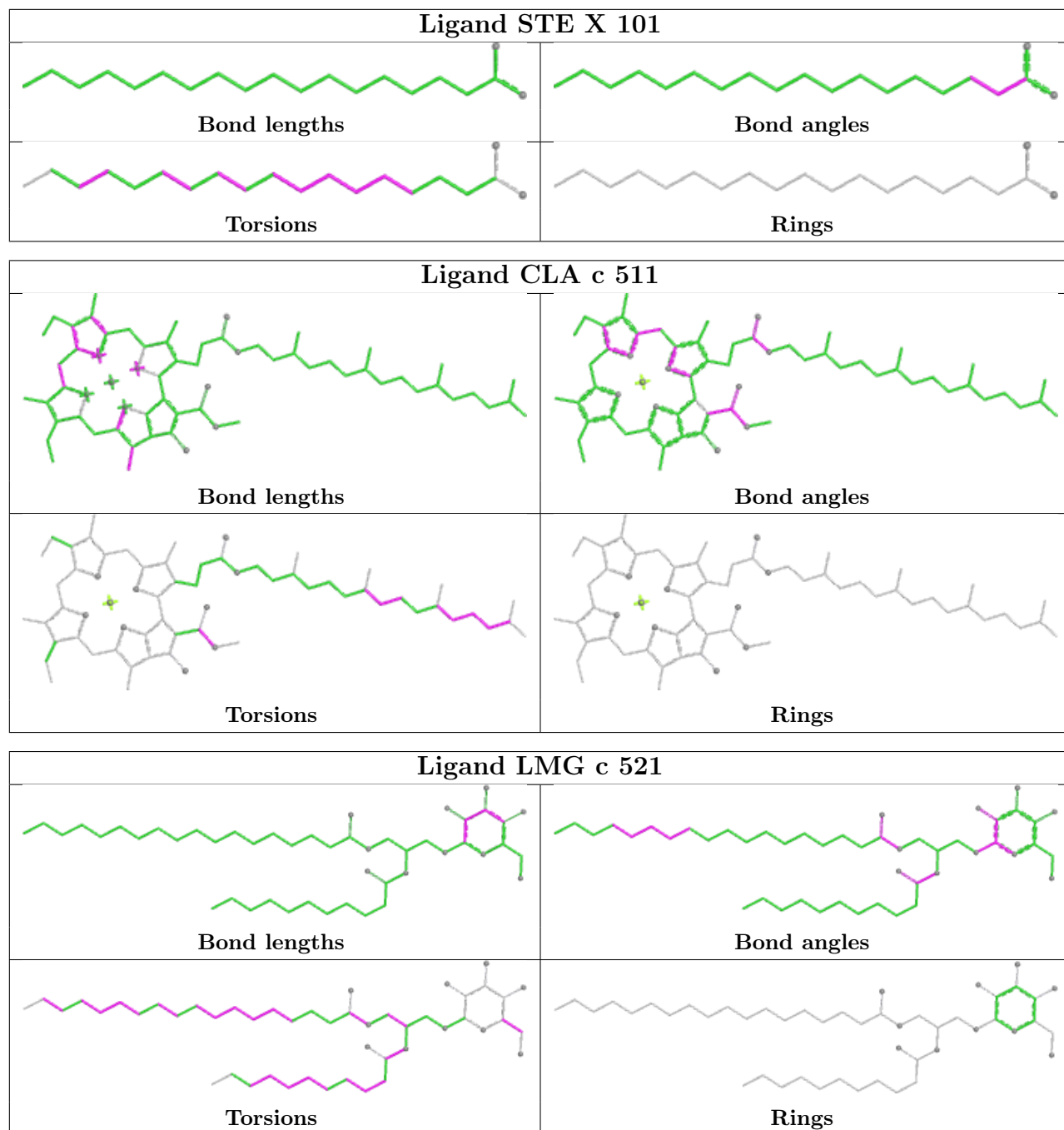
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	d	407	LHG	1	0
32	c	517	DGD	3	0
25	c	512	CLA	2	0
25	C	506	CLA	1	0
30	A	614	LHG	3	0
31	b	619	SQD	2	0
30	L	101	LHG	3	0
27	k	102	BCR	1	0
25	a	613	CLA	4	0
27	t	101	BCR	3	0
27	c	514	BCR	2	0
27	A	610	BCR	2	0
29	A	613	LMG	1	0
29	c	519	LMG	1	0
25	B	611	CLA	2	0
25	c	510	CLA	4	0
25	c	505	CLA	3	0
33	b	621	STE	4	0
27	a	611	BCR	1	0
30	D	408	LHG	1	0
25	B	601	CLA	4	0
30	E	101	LHG	2	0
31	f	101	SQD	1	0
30	e	102	LHG	2	0
28	d	405	PL9	1	0
33	I	101	STE	1	0
33	j	101	STE	1	0
27	c	515	BCR	3	0
27	K	102	BCR	2	0
25	b	612	CLA	2	0
32	h	103	DGD	2	0
25	D	403	CLA	1	0
22	a	602[A]	OEY	1	0
25	b	607	CLA	3	0
25	c	507	CLA	3	0
31	a	615	SQD	1	0
31	A	616	SQD	4	0
32	C	516	DGD	3	0
25	c	504	CLA	1	0
25	d	403	CLA	1	0
27	T	101	BCR	3	0
30	l	101	LHG	1	0

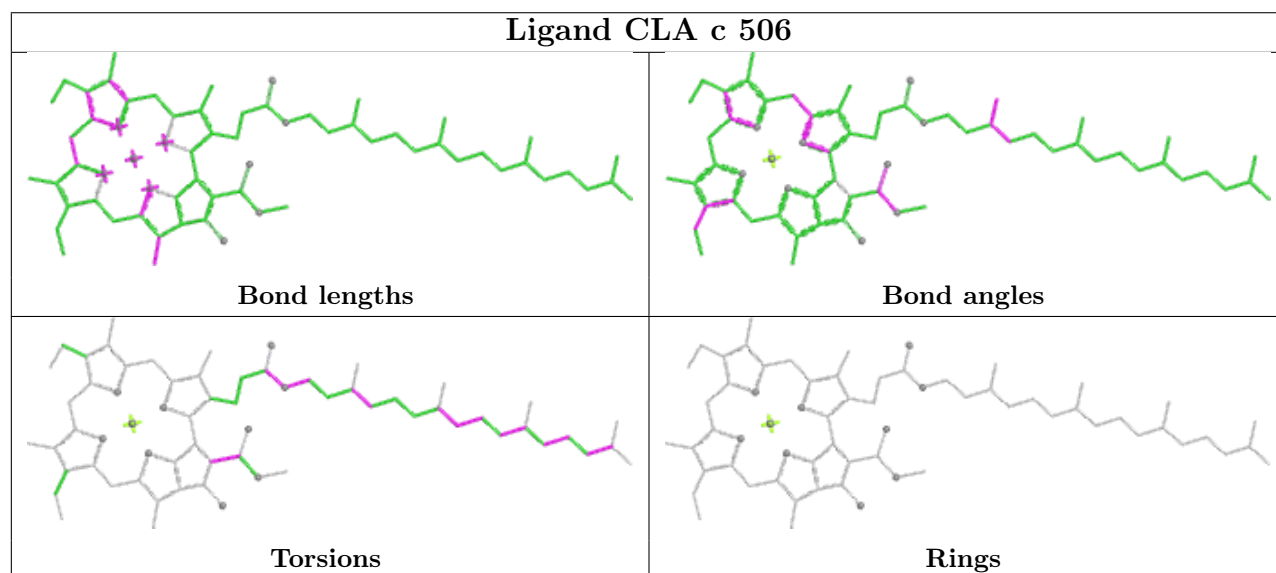
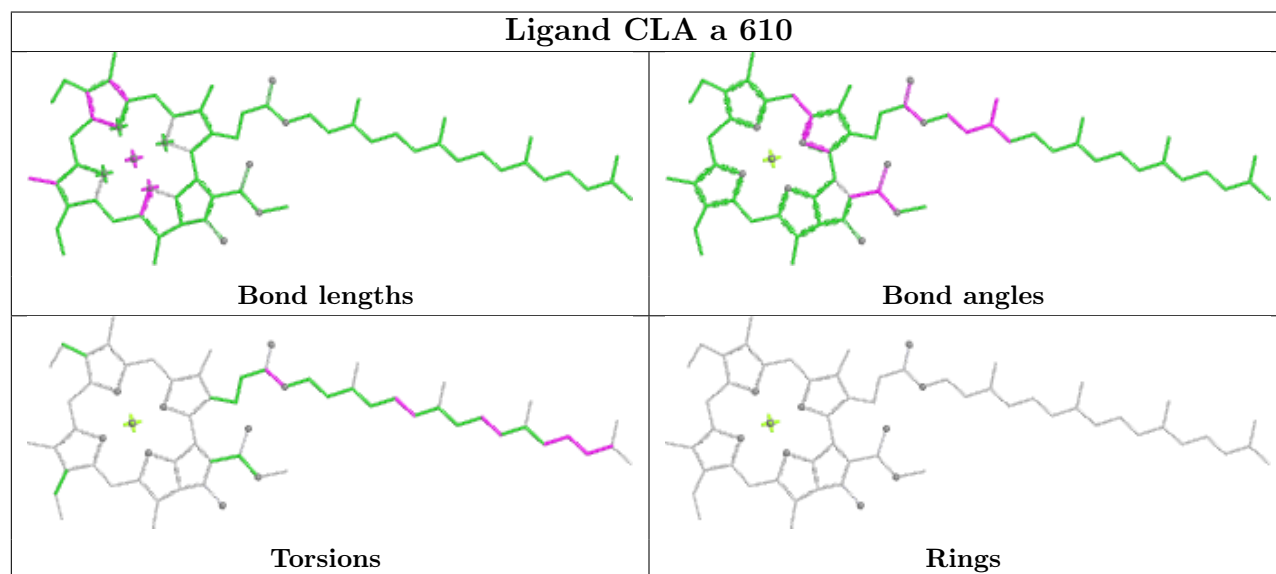
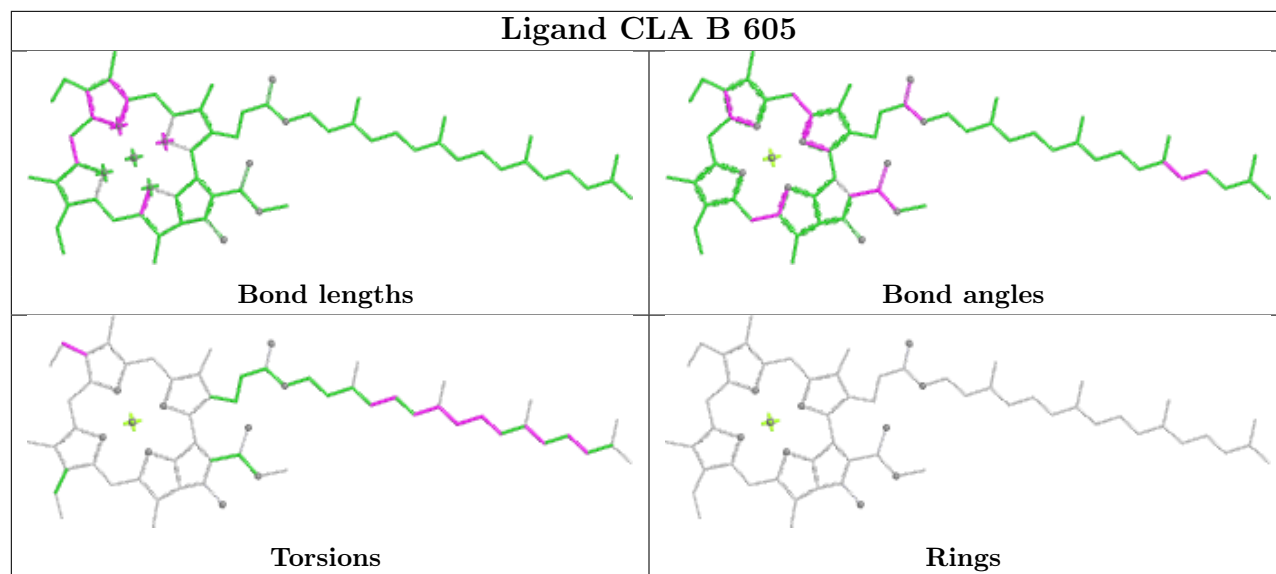
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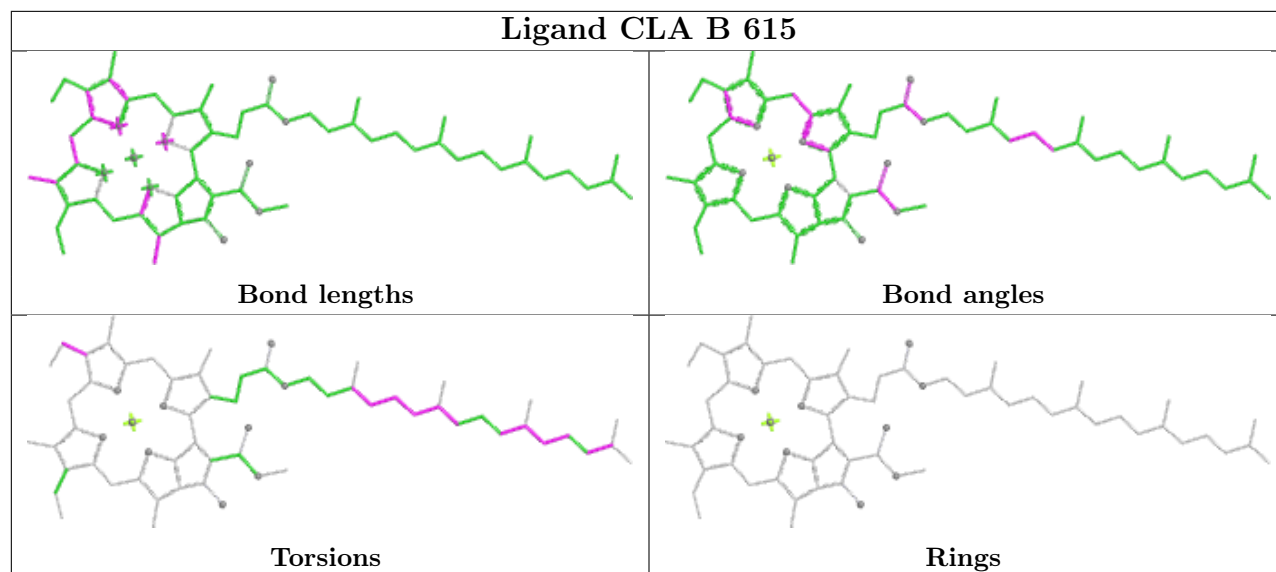
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	607	CLA	4	0
27	K	103	BCR	1	0
26	D	402	PHO	1	0
33	m	102	STE	1	0
25	B	613	CLA	1	0
25	b	605	CLA	2	0
25	D	404	CLA	1	0
32	C	515	DGD	1	0
27	H	101	BCR	2	0
25	A	606	CLA	3	0
27	D	405	BCR	1	0
29	m	101	LMG	2	0
25	C	507	CLA	1	0
28	A	611	PL9	4	0
25	B	603	CLA	1	0
33	l	102	STE	3	0
25	C	509	CLA	1	0
27	b	617	BCR	2	0
32	H	102	DGD	2	0
28	D	406	PL9	2	0
29	C	518	LMG	1	0
29	D	409	LMG	2	0
28	a	612	PL9	2	0
25	B	614	CLA	3	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.

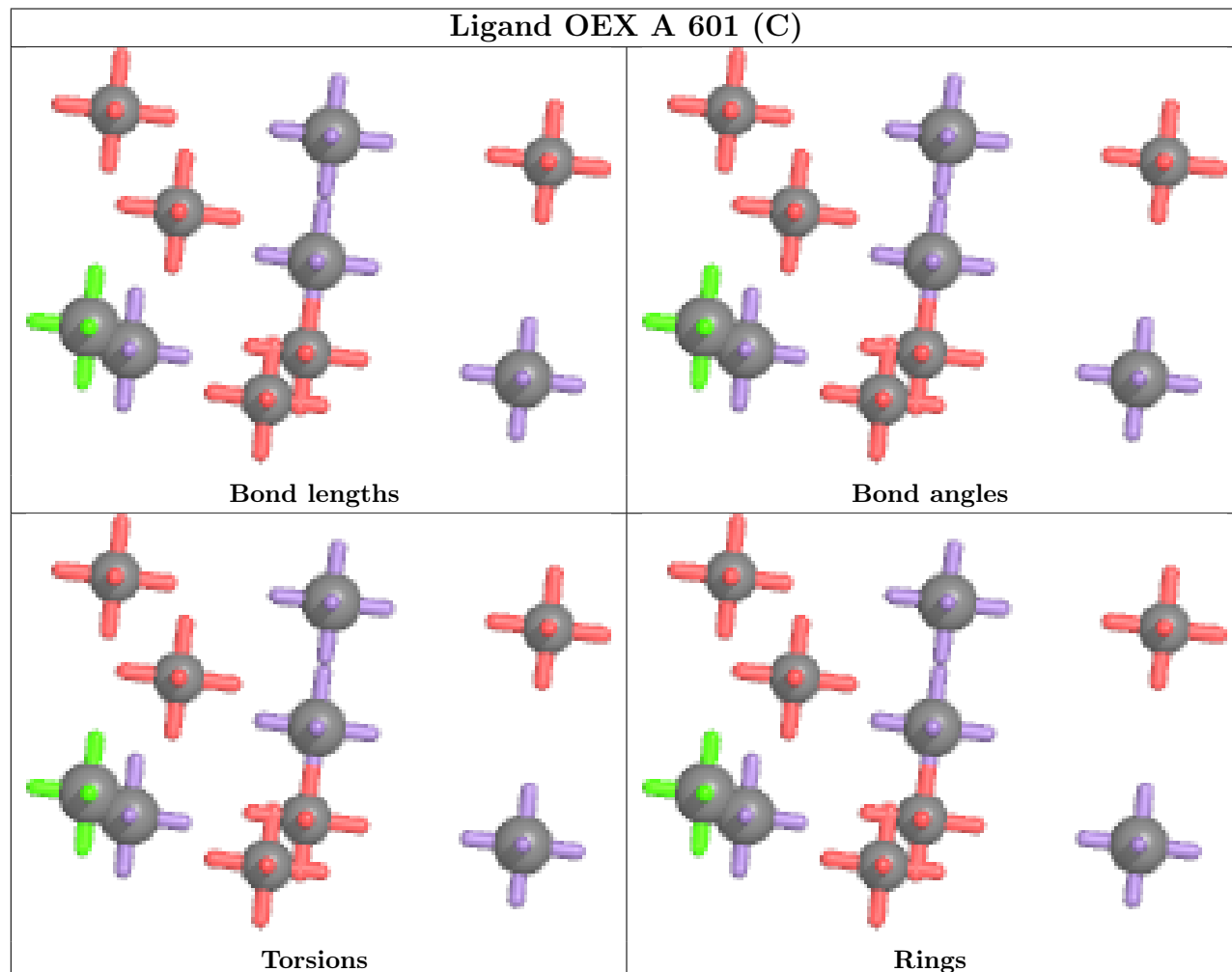


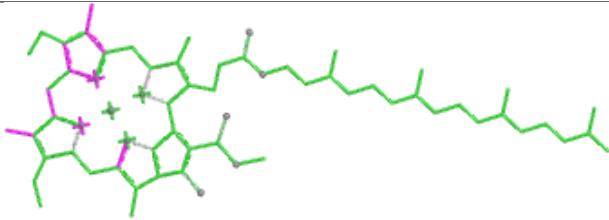
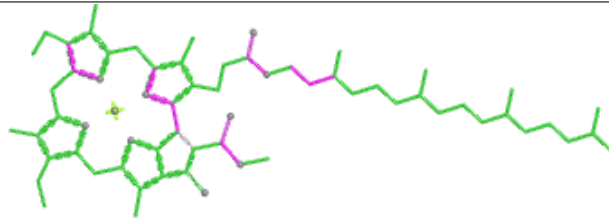
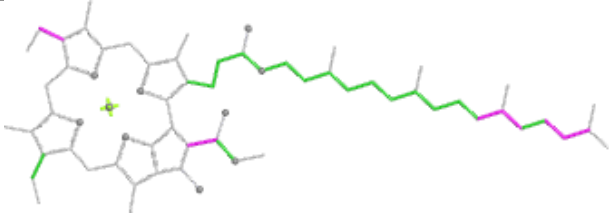
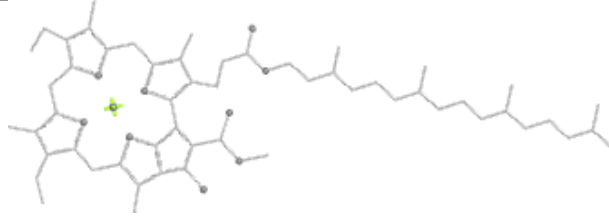


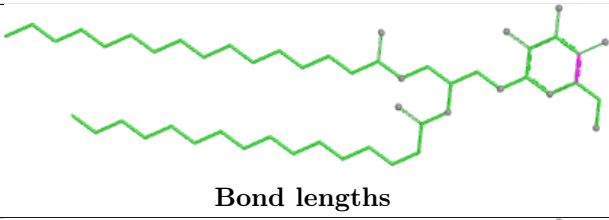
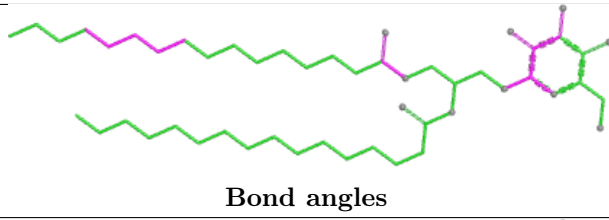
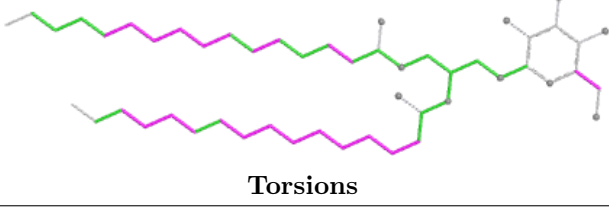
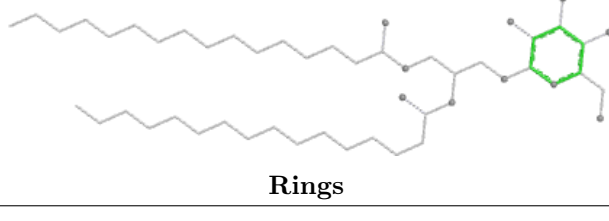
Ligand CLA B 615

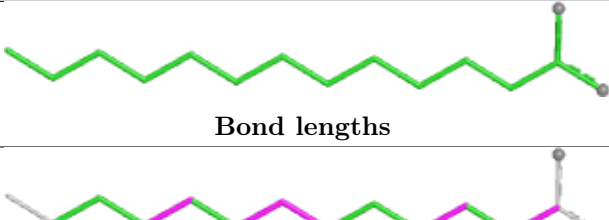
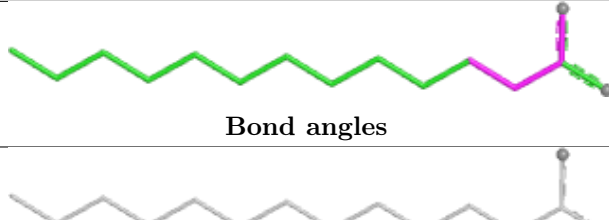
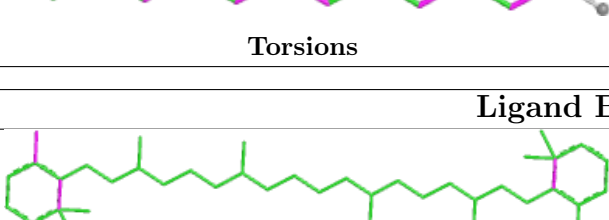


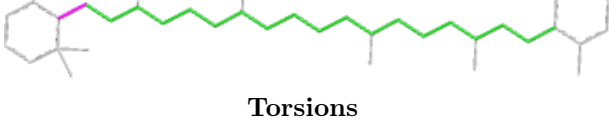
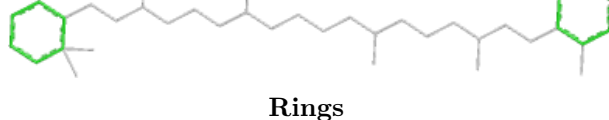
Ligand OEX A 601 (C)

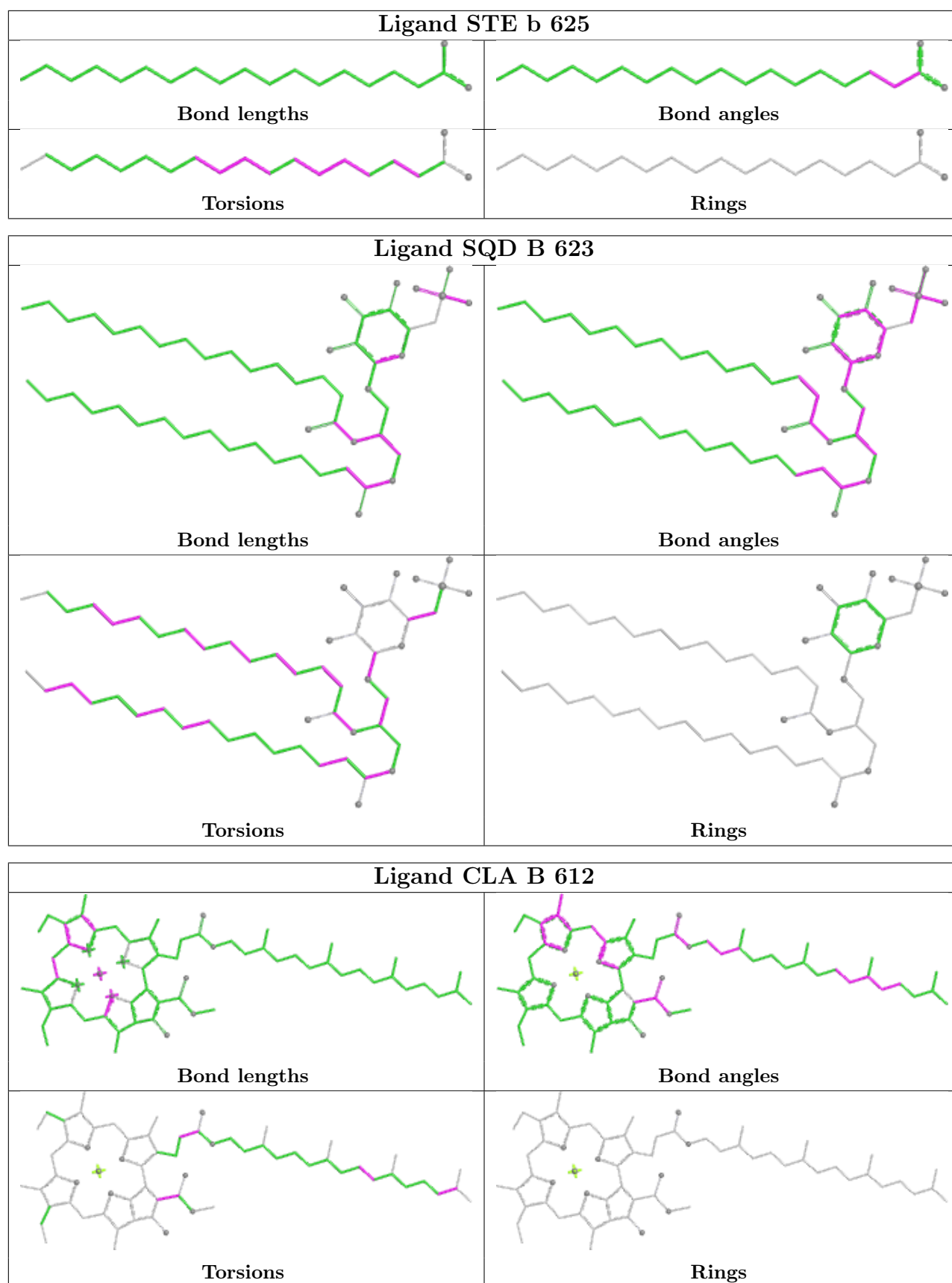


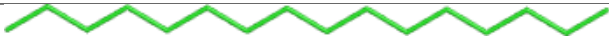
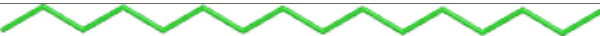
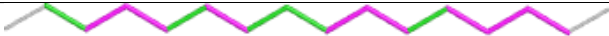
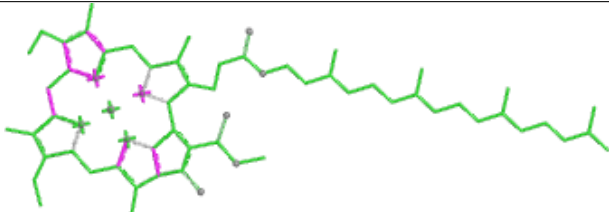
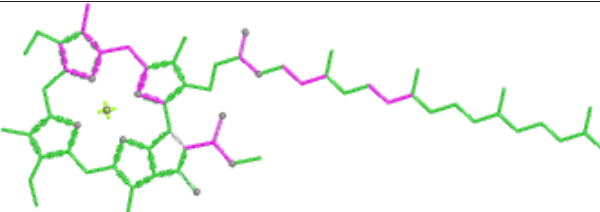
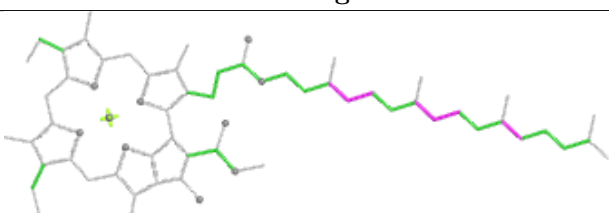
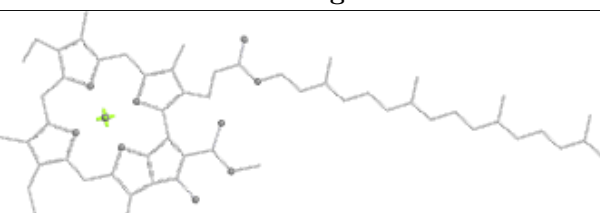
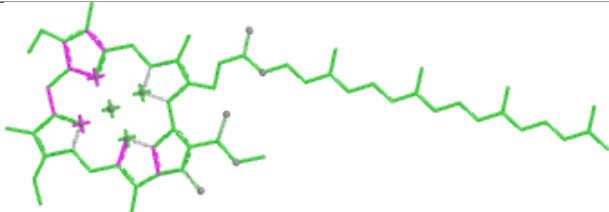
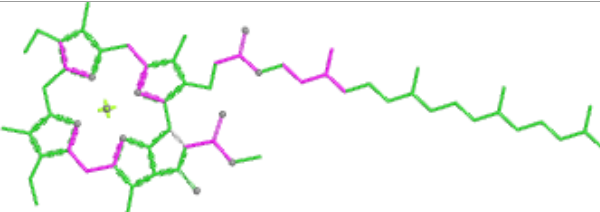
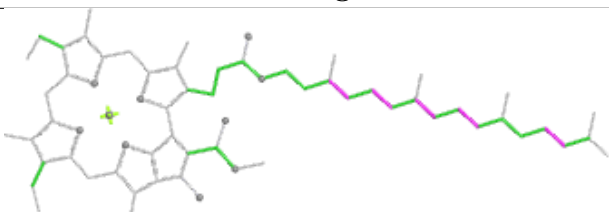
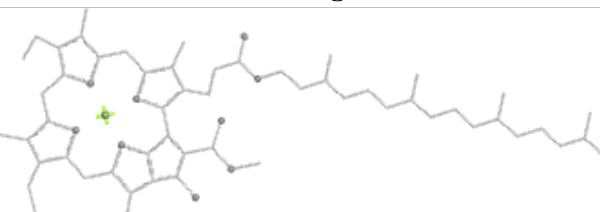
Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

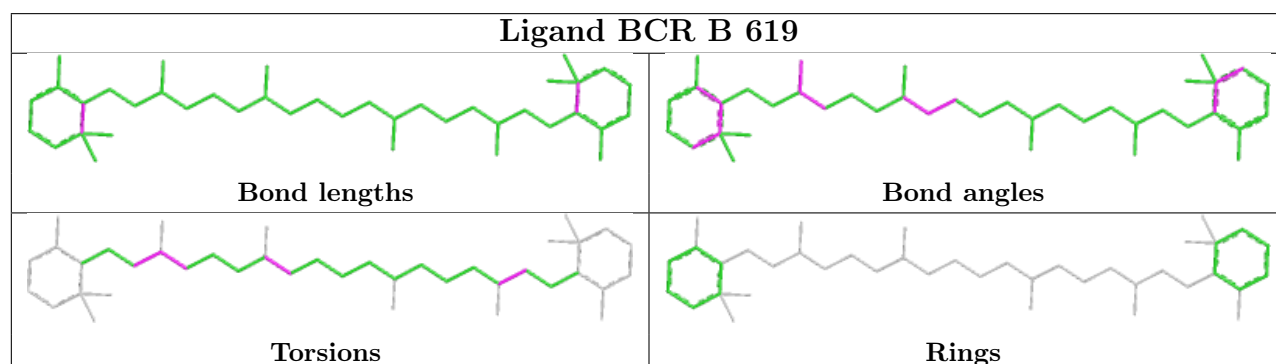
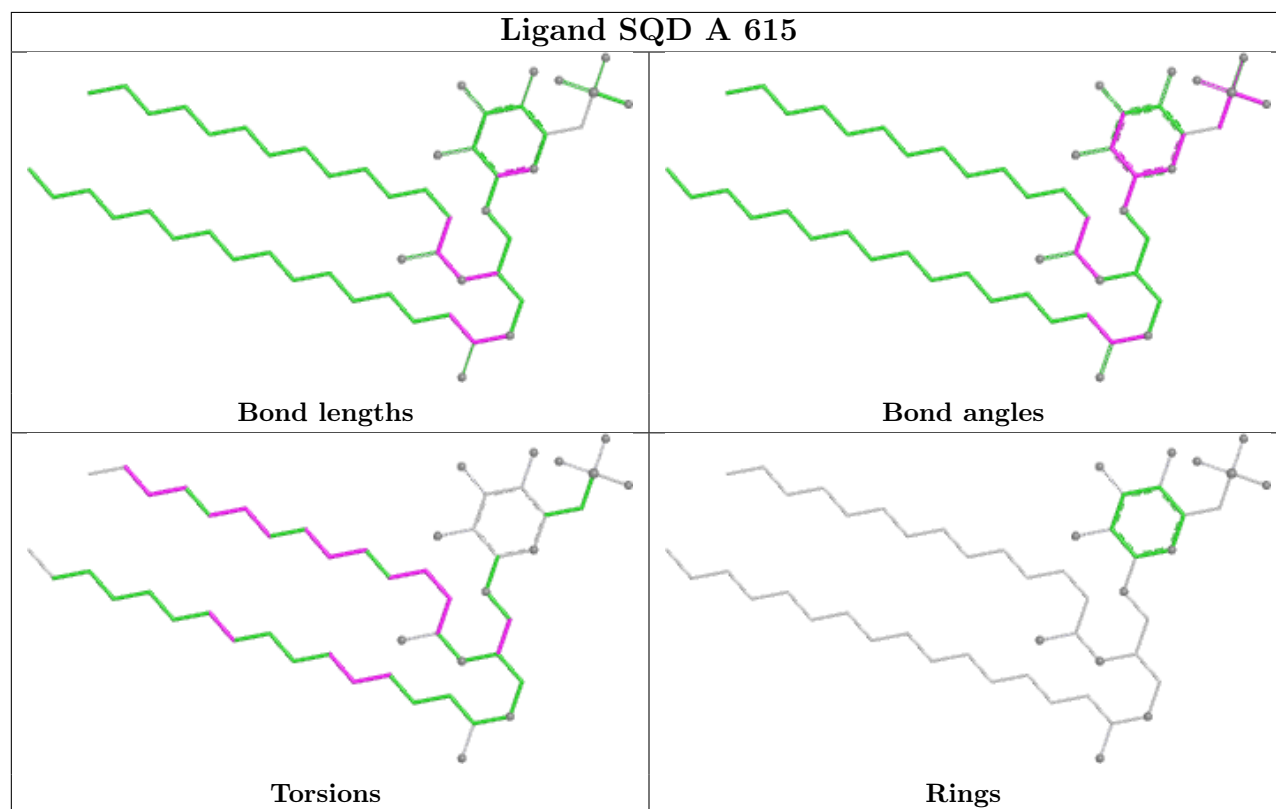
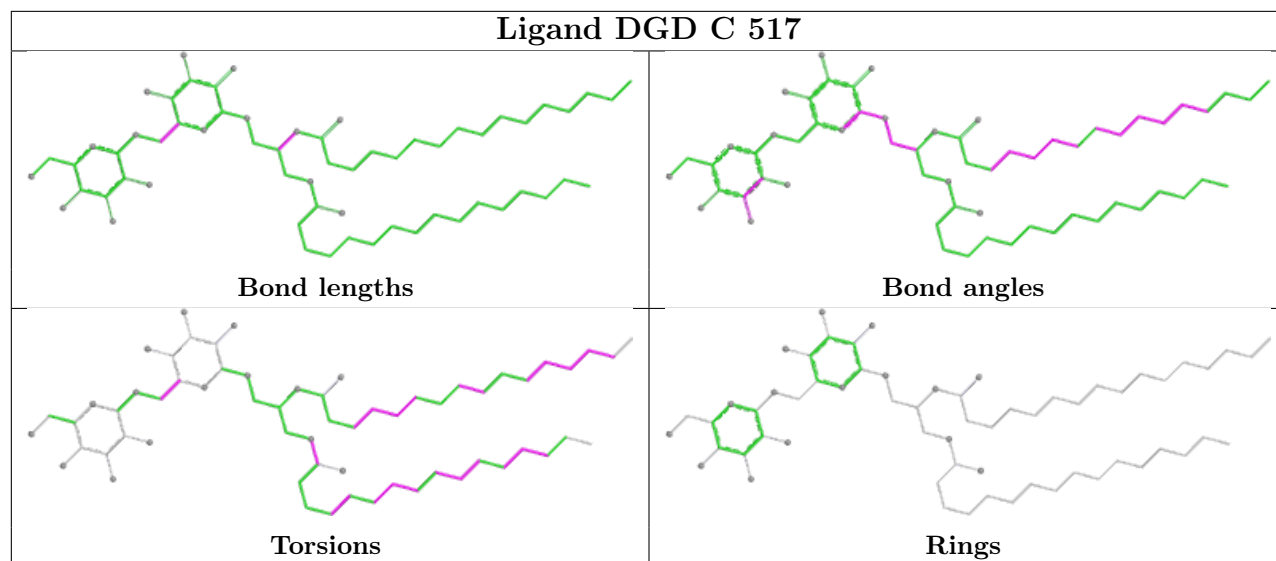
Ligand LMG D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

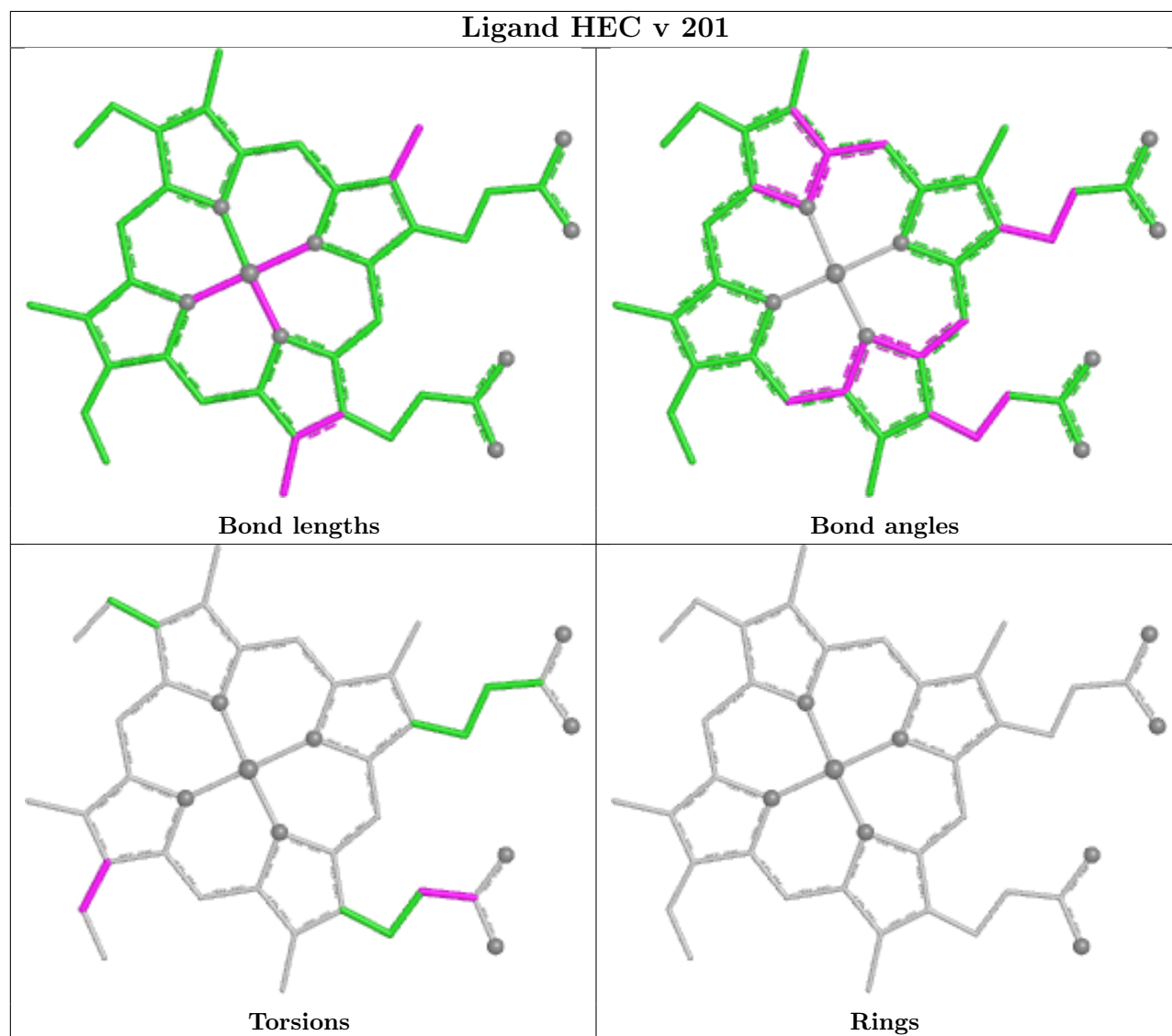
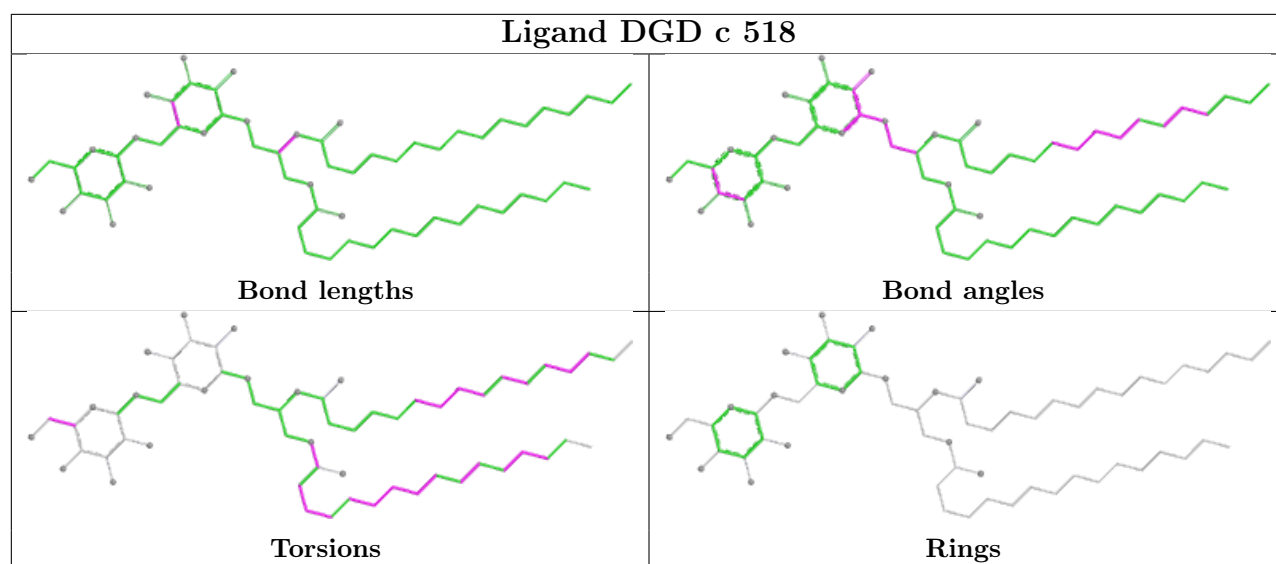
Ligand STE M 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

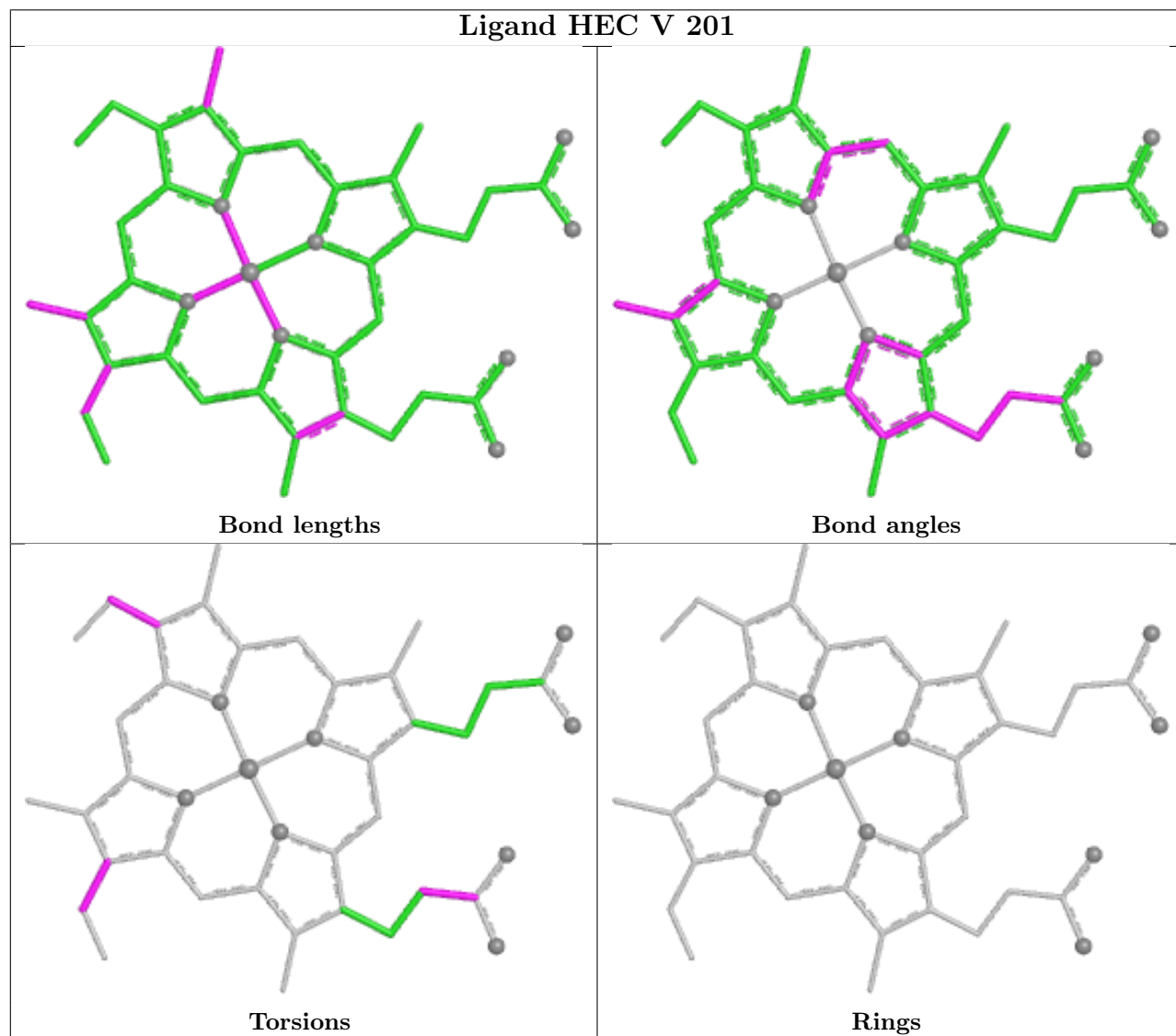
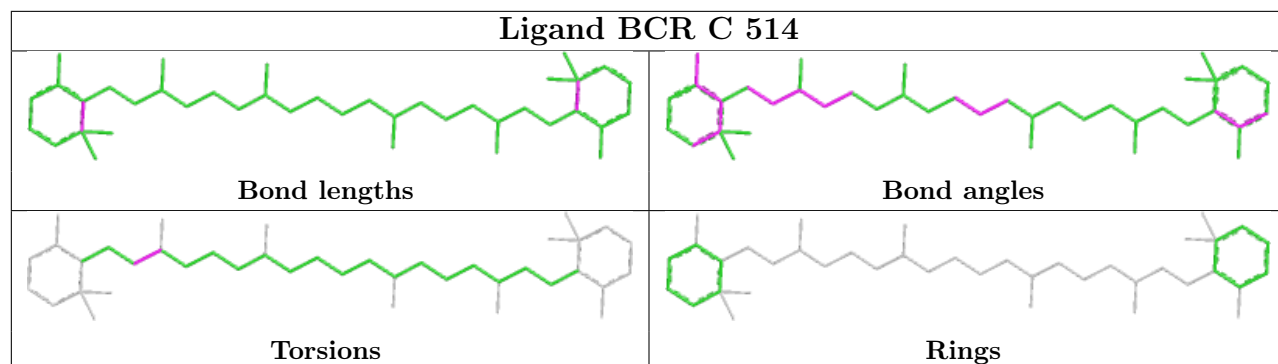
Ligand BCR B 617	
	
Bond lengths	Bond angles
Torsions	Rings



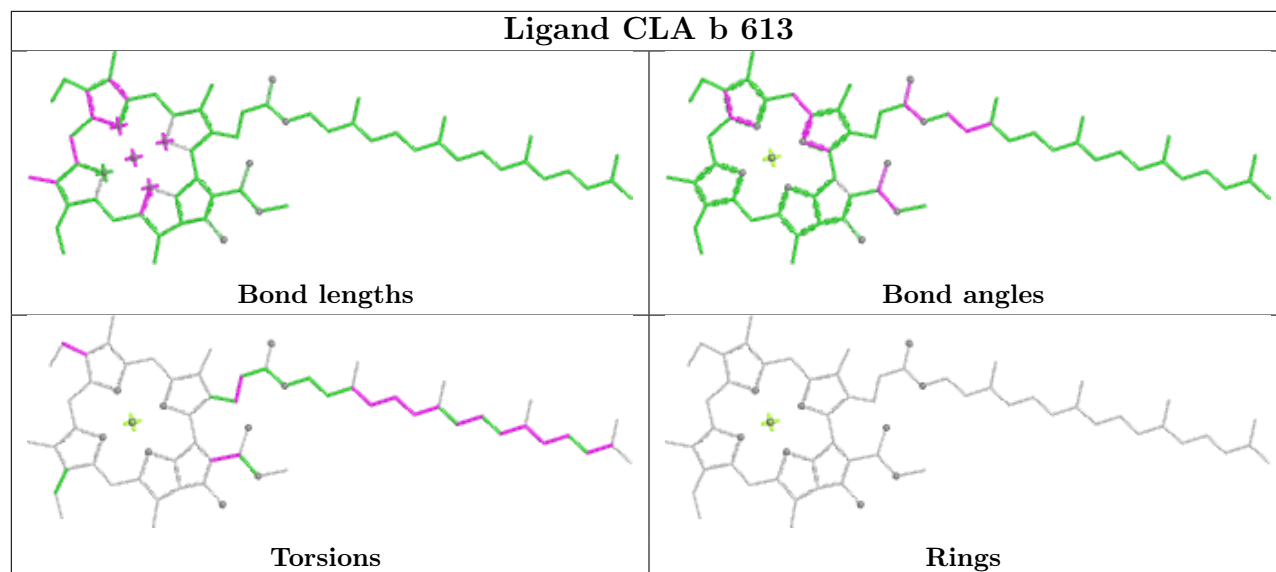
Ligand STE b 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings



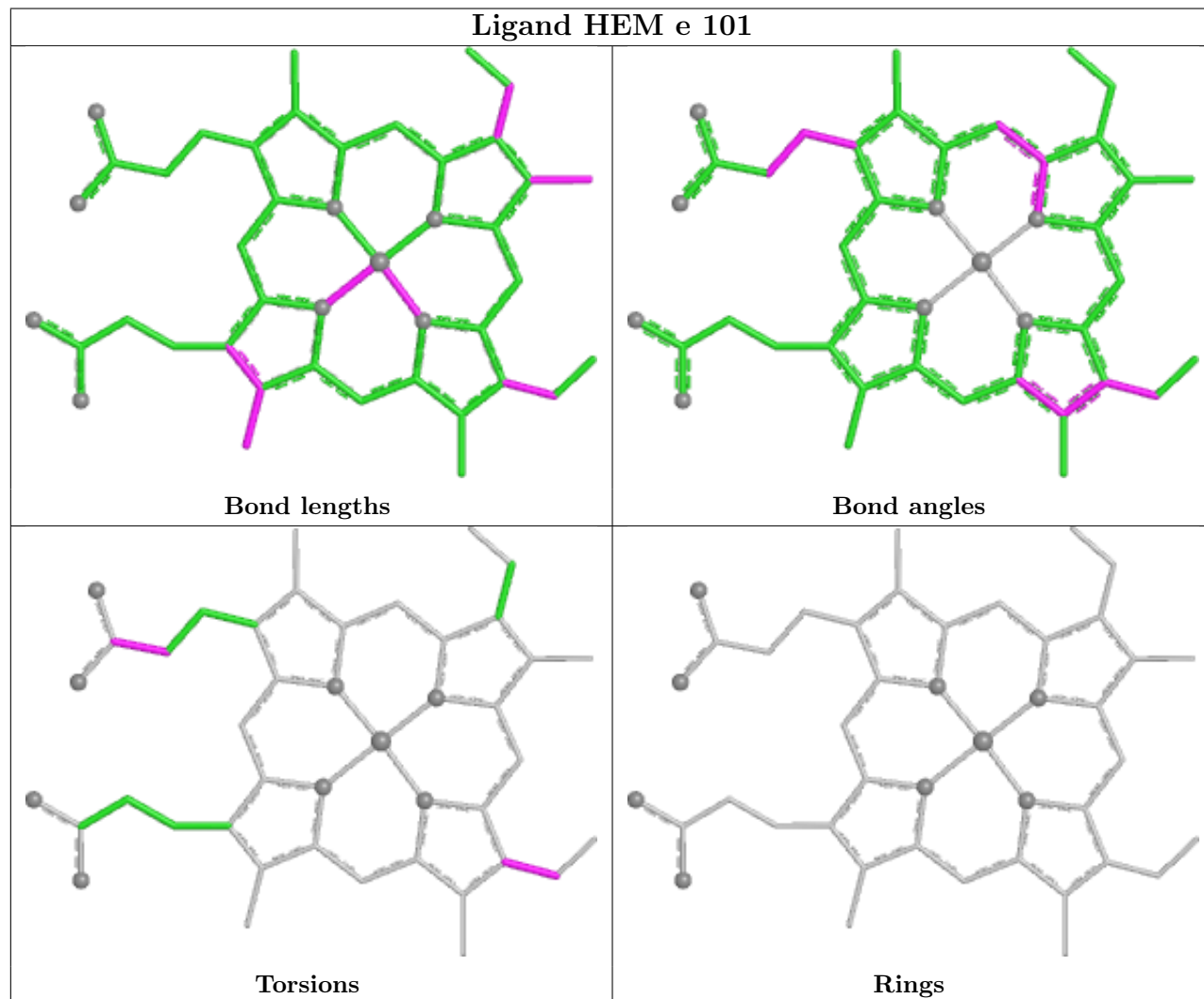


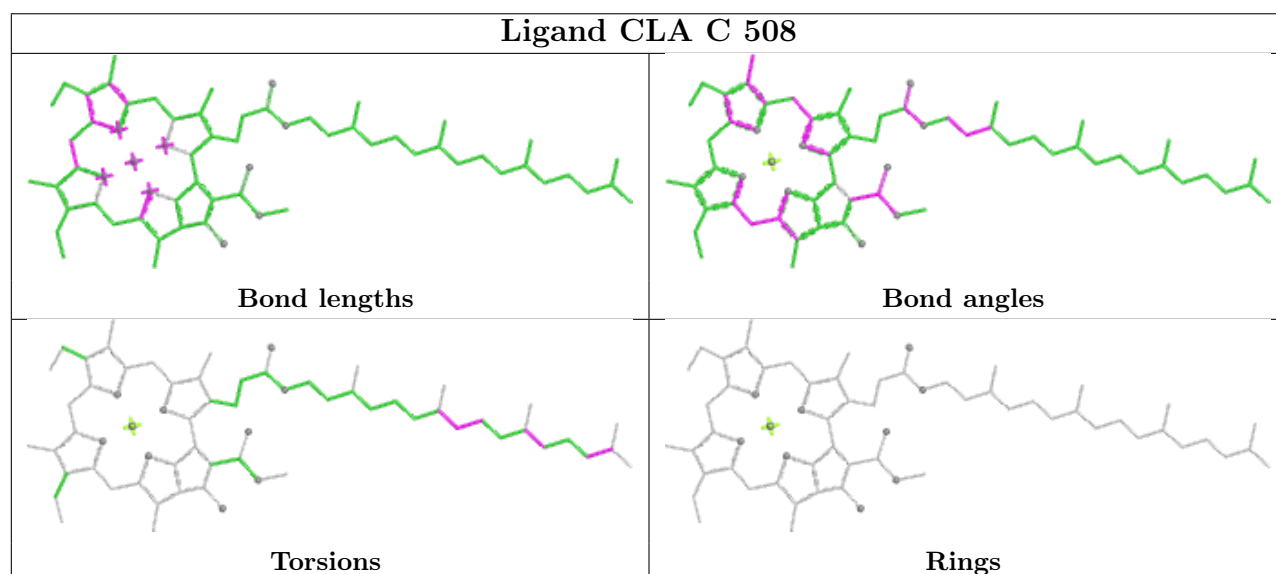
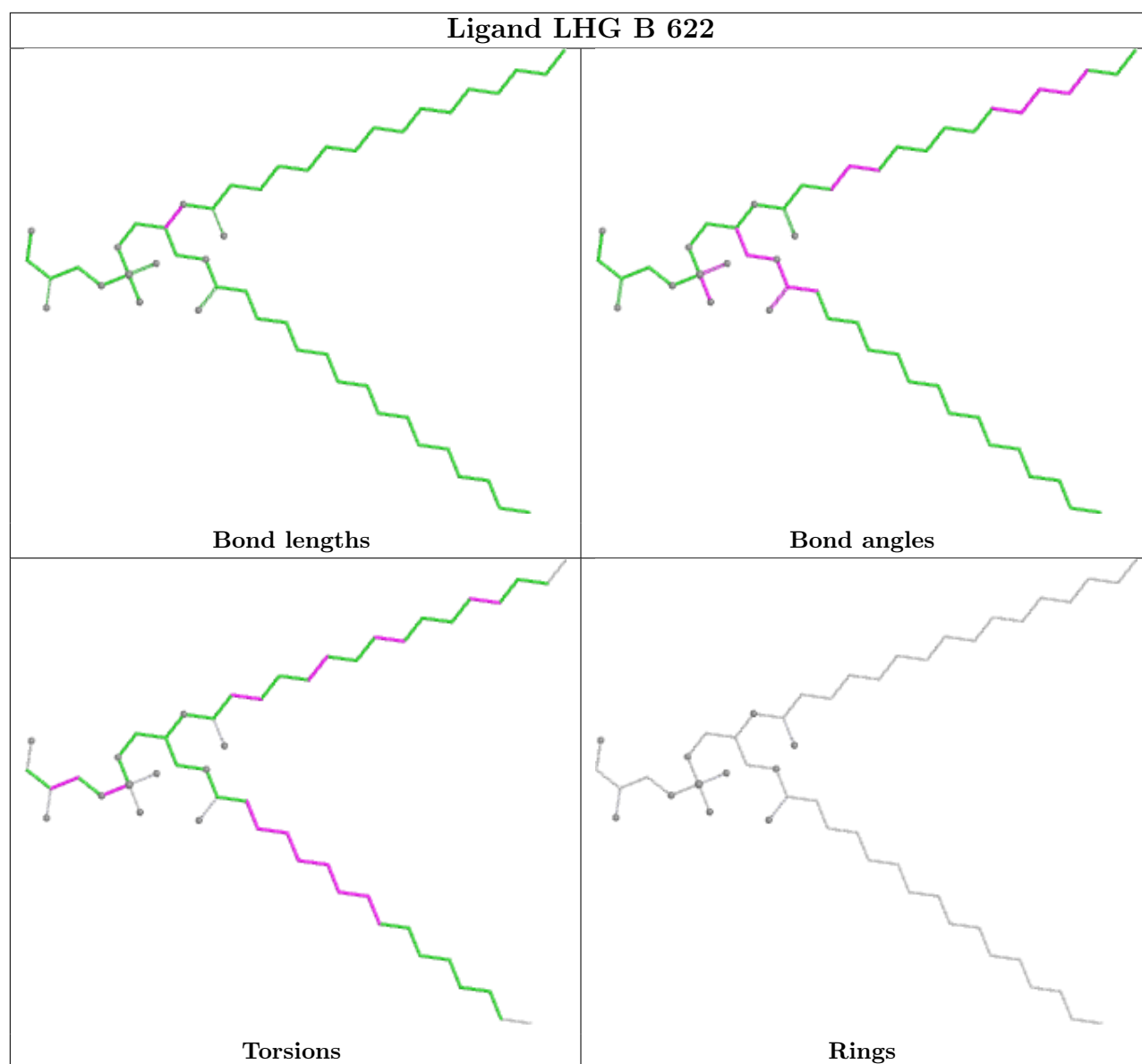


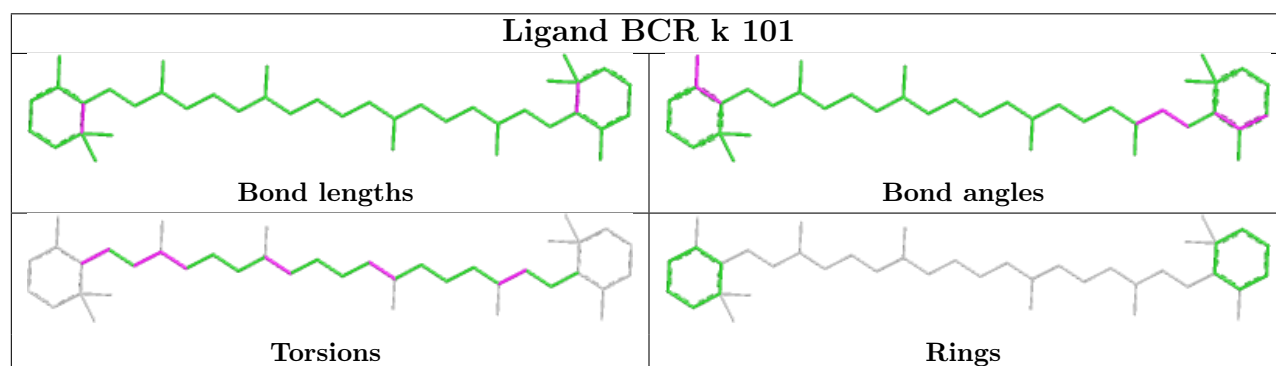
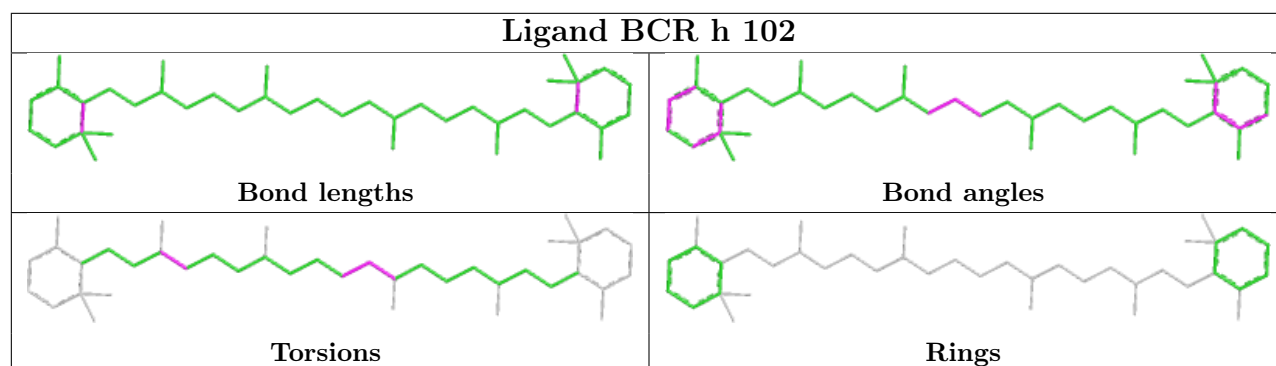
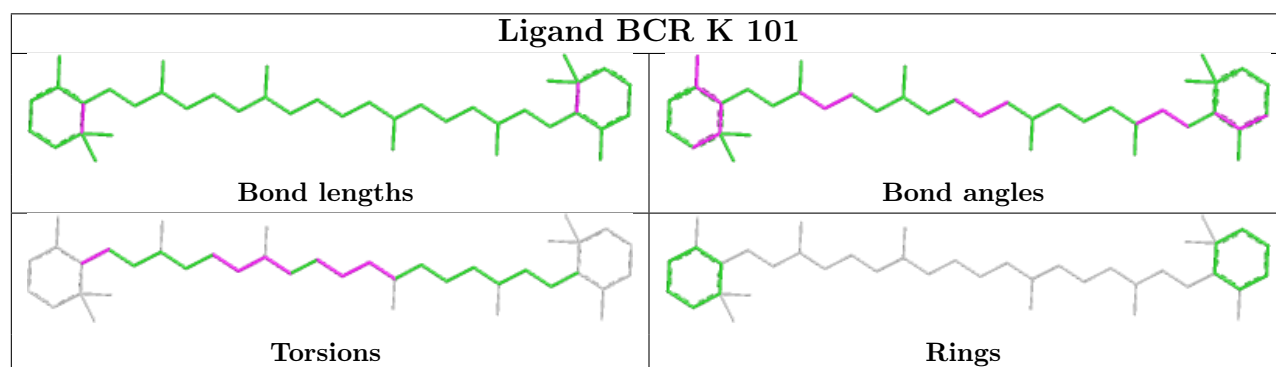
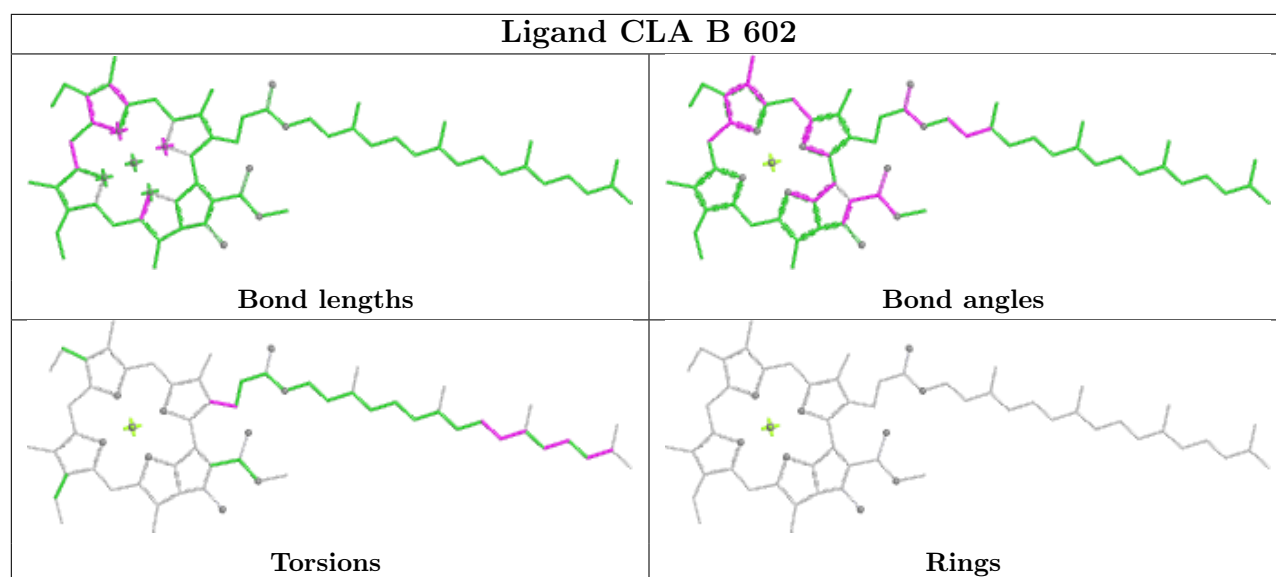
Ligand CLA b 613



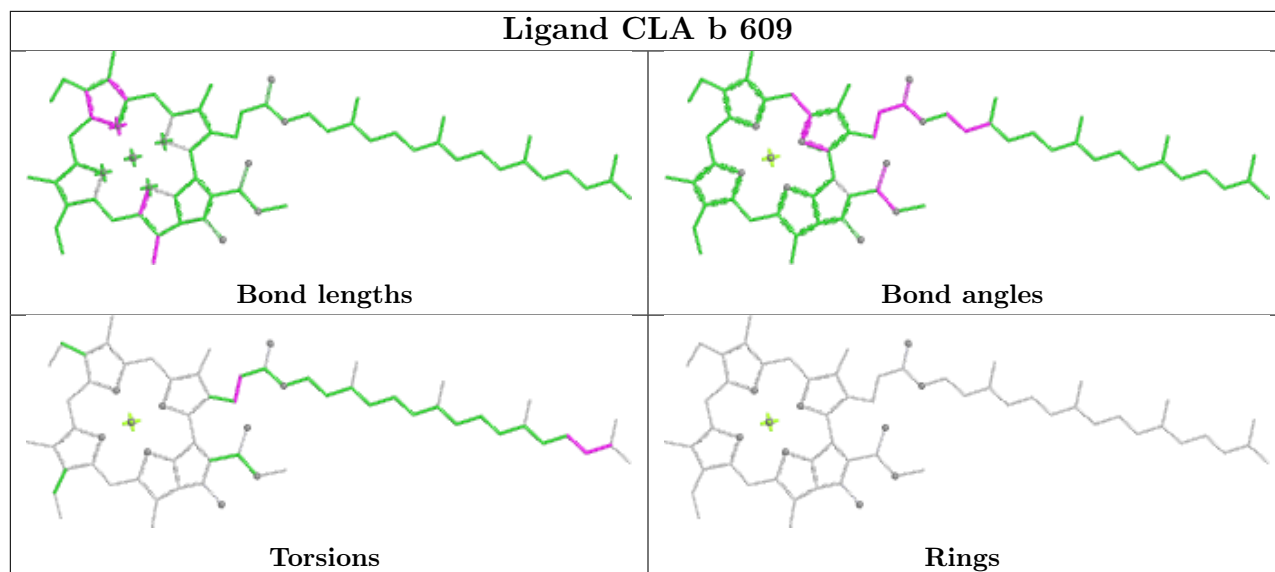
Ligand HEM e 101



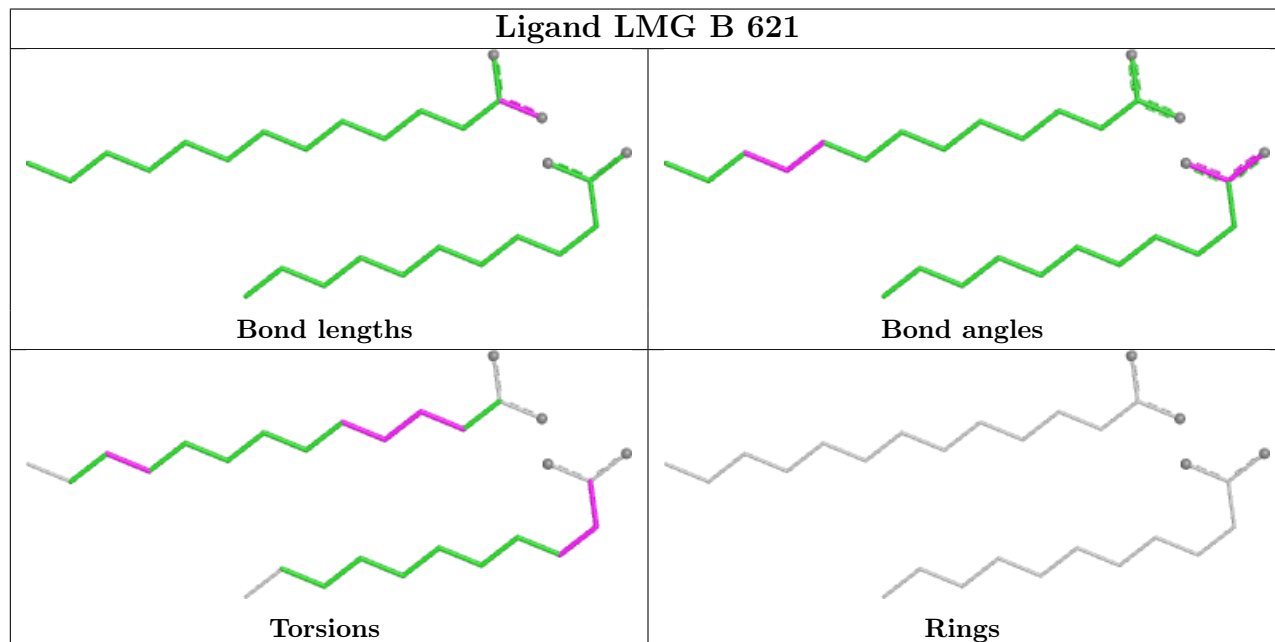




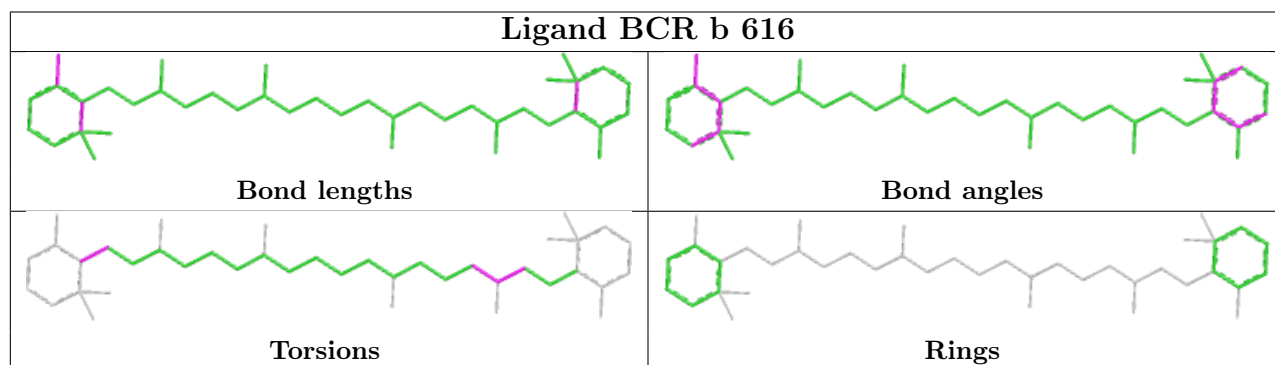
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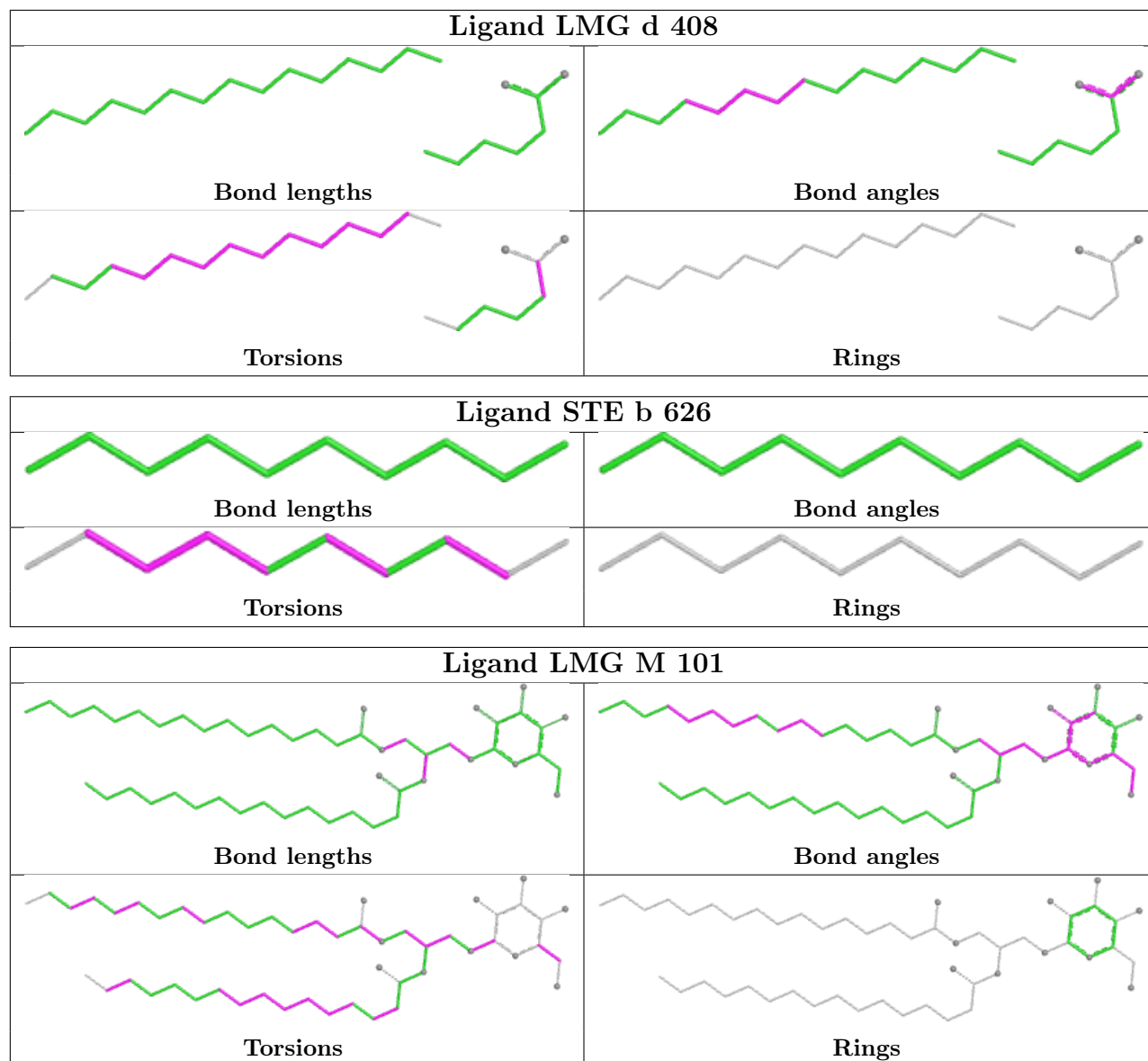


Ligand LMG B 621

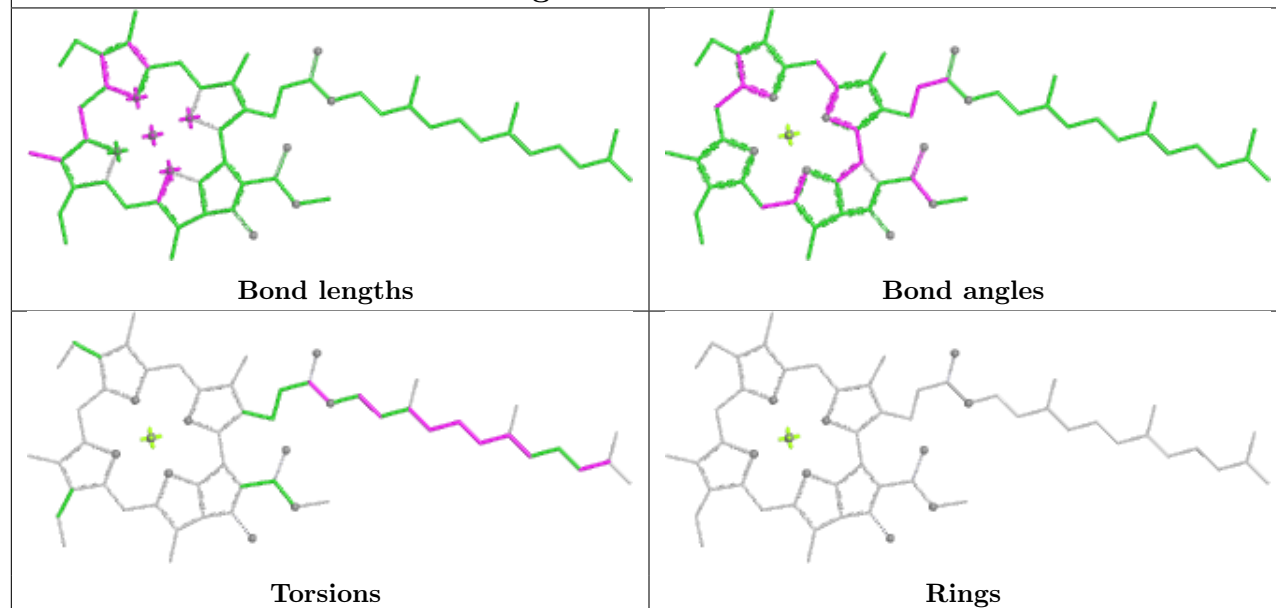


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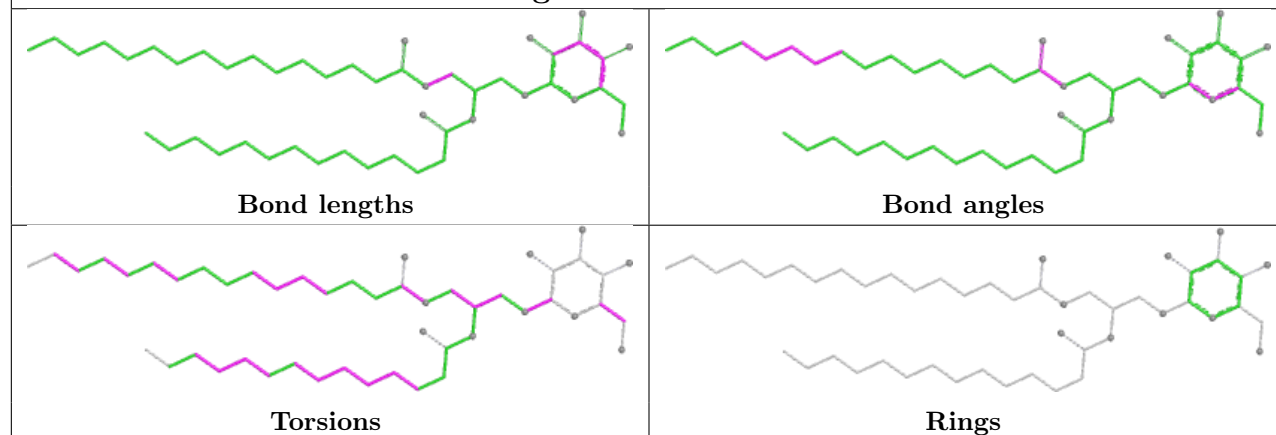




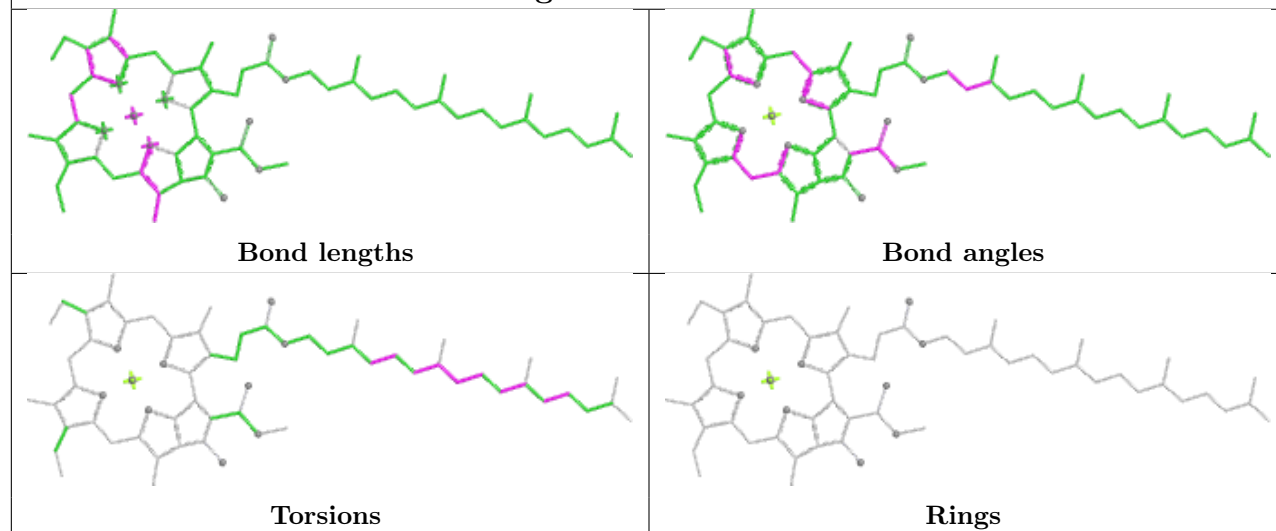
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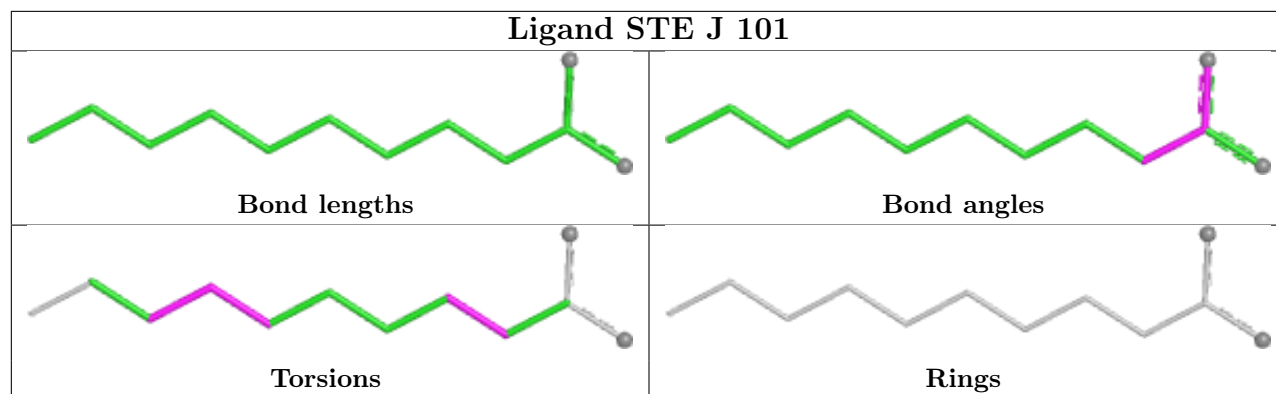
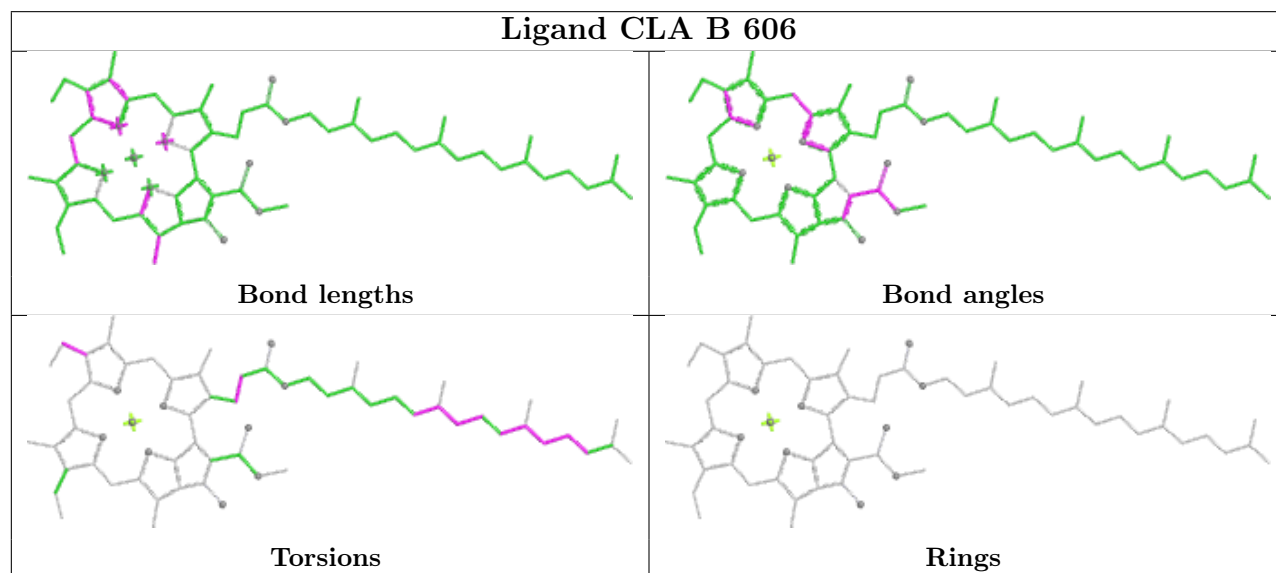
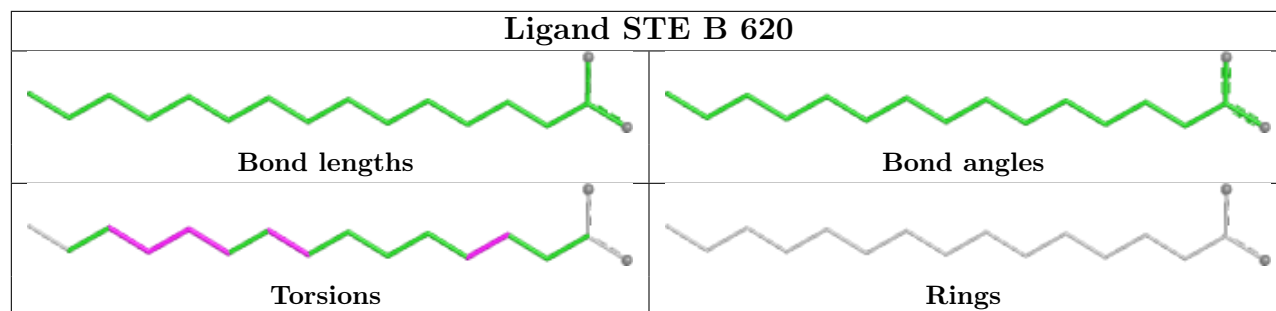


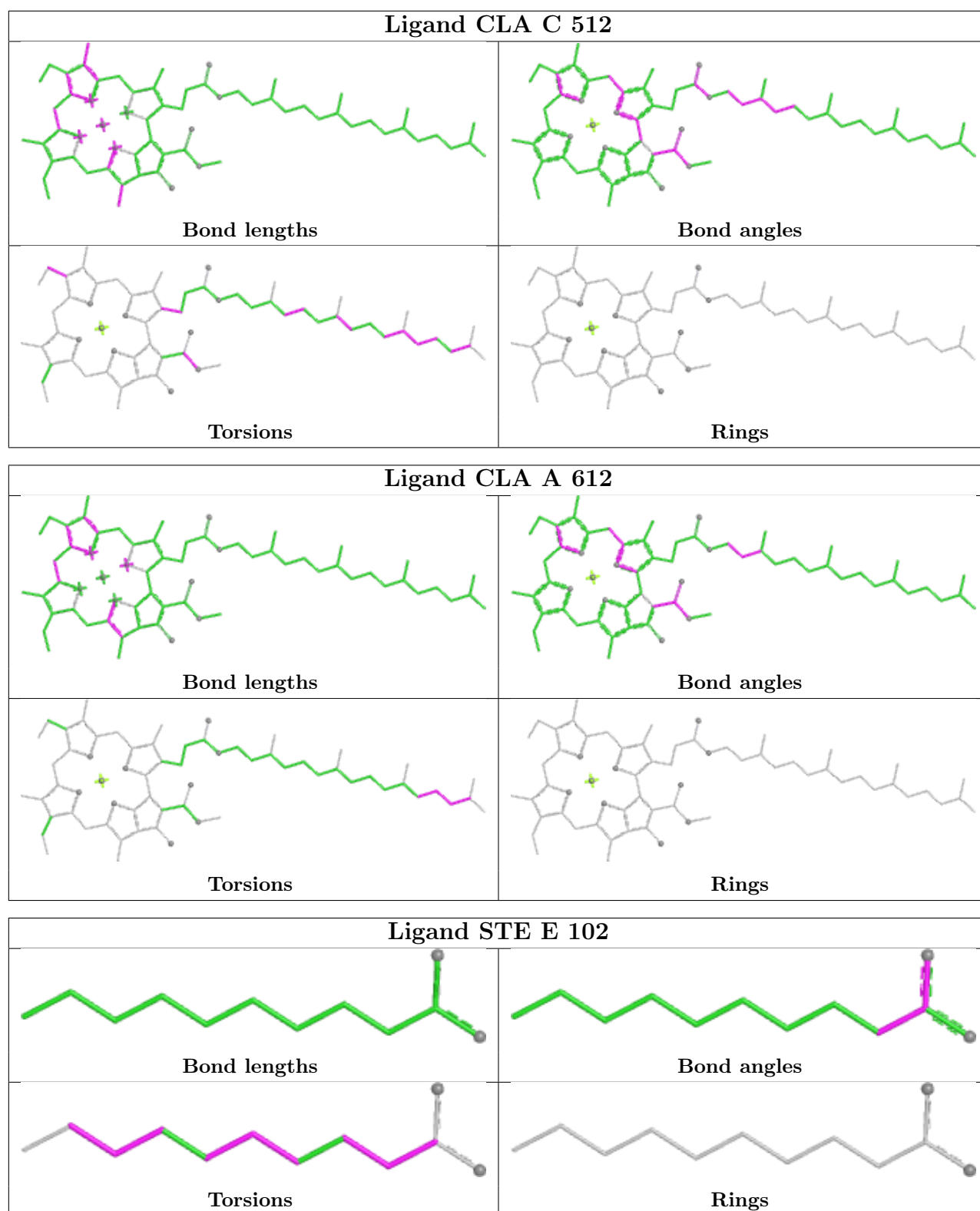
Ligand LMG c 522

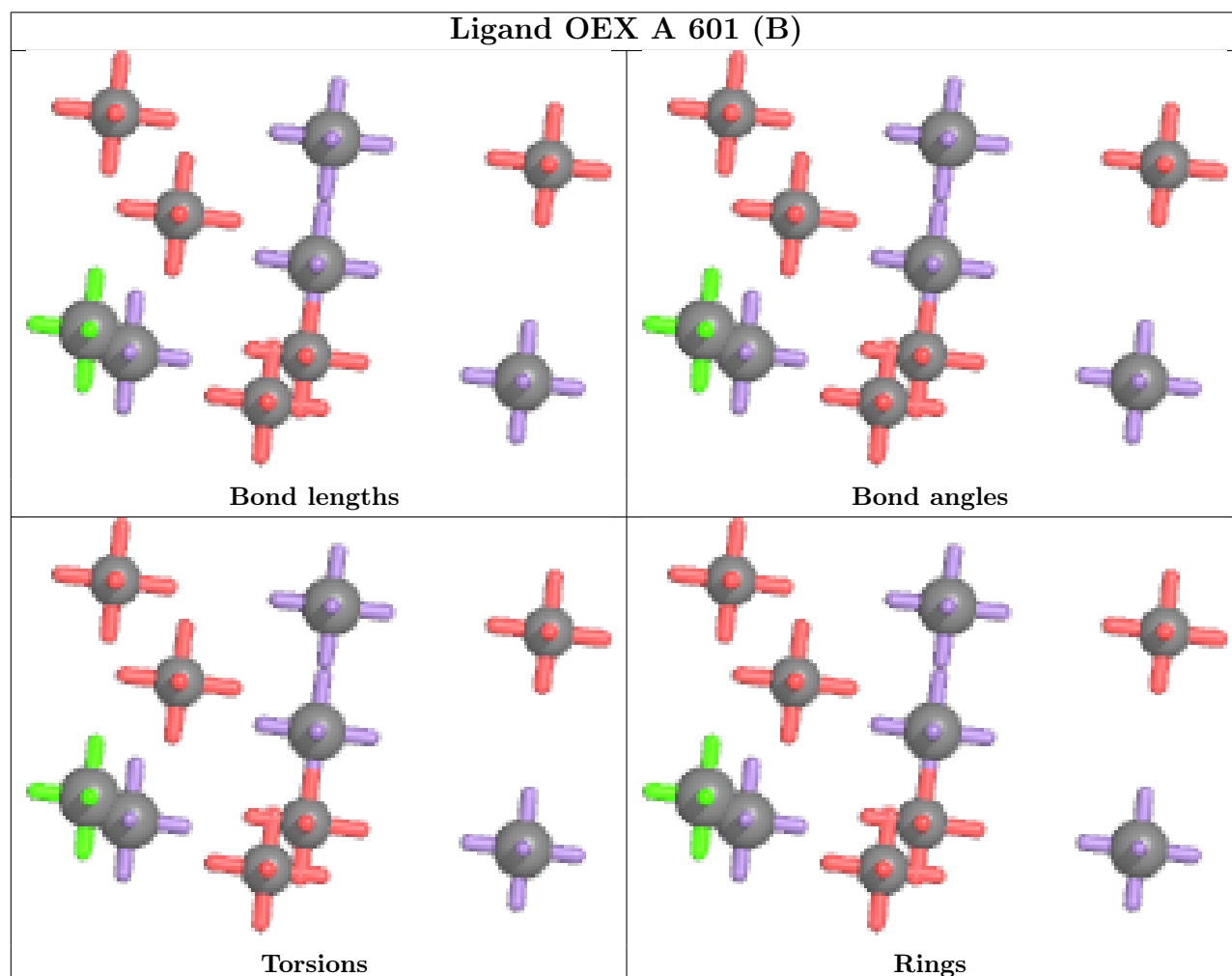
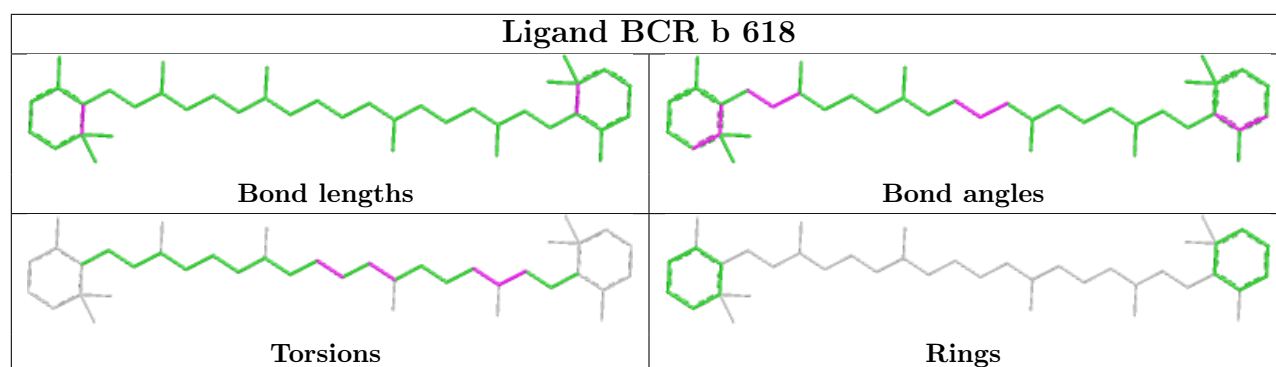


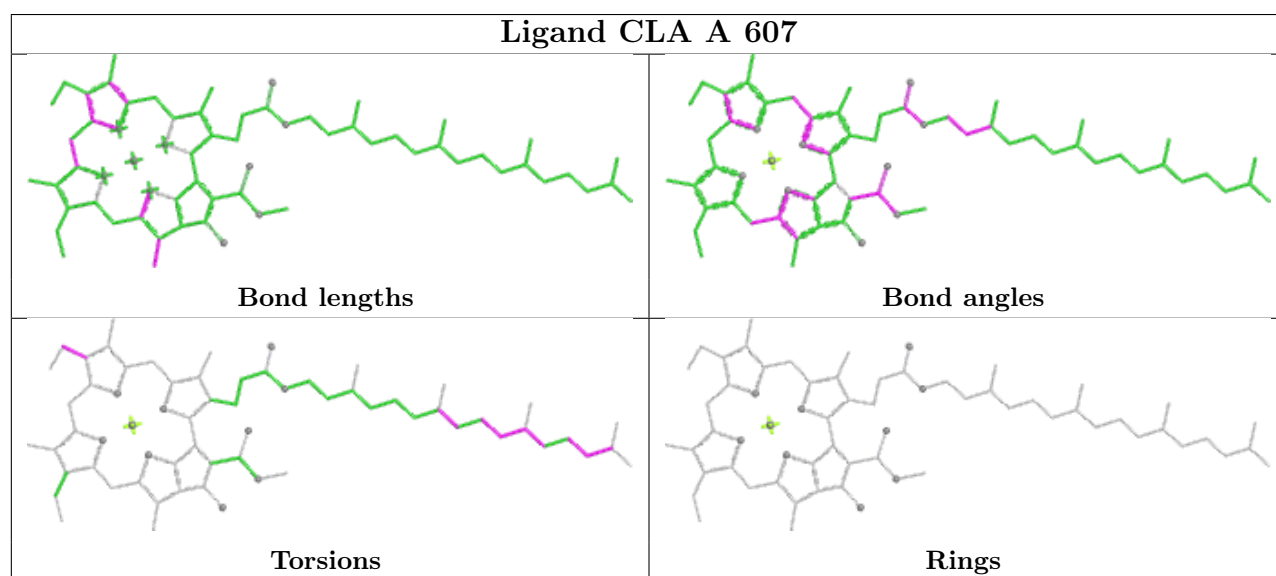
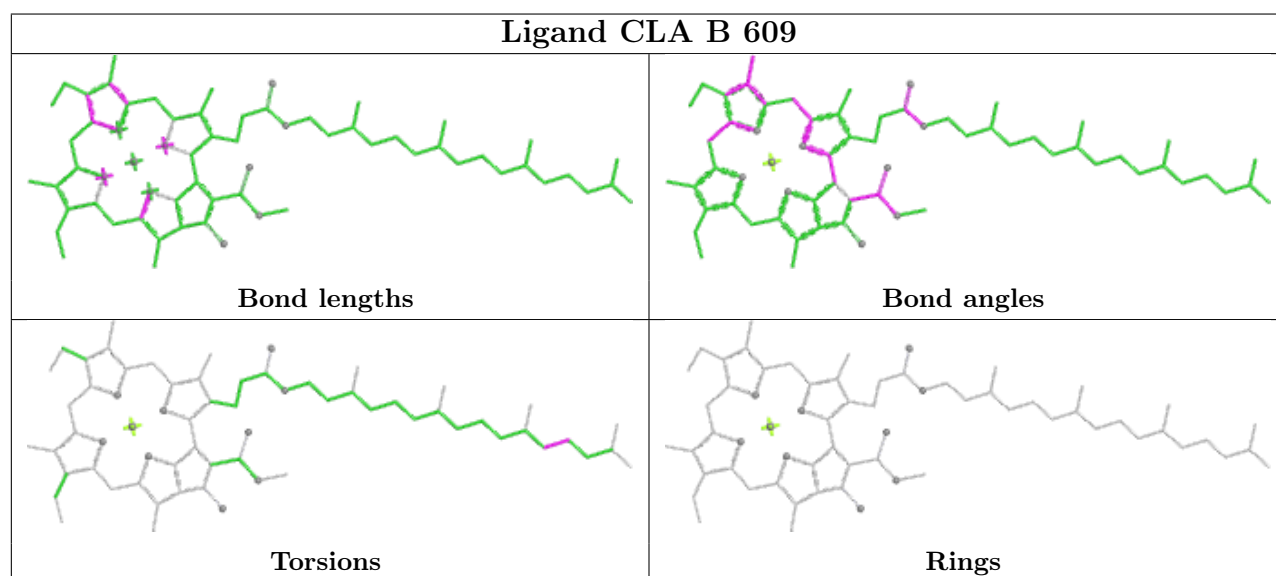
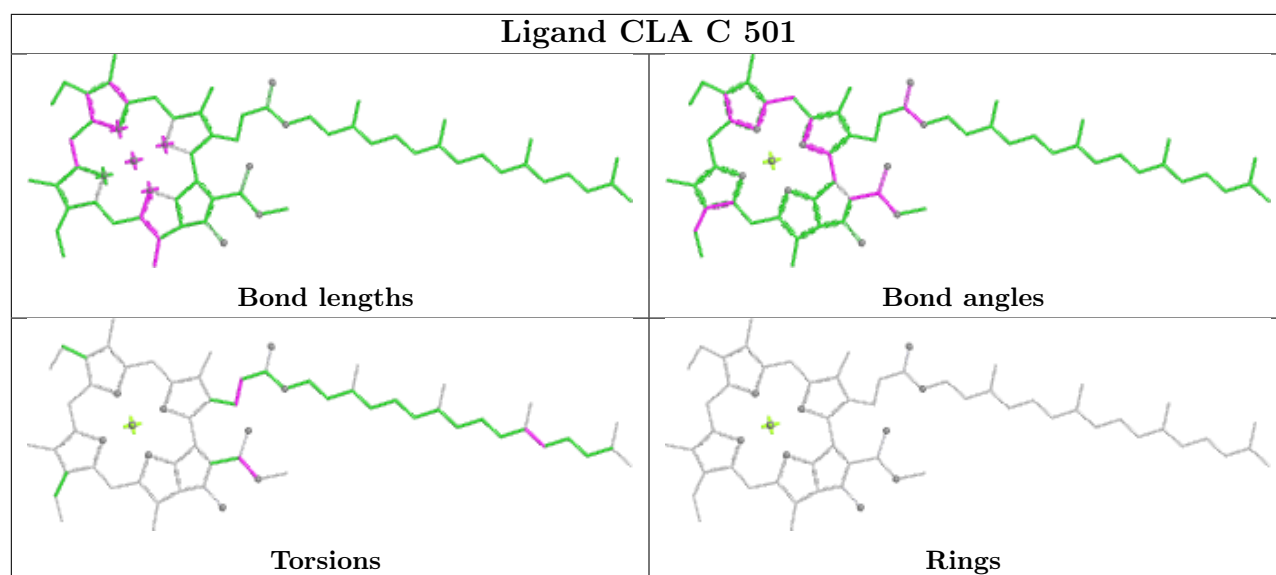
Ligand CLA b 601



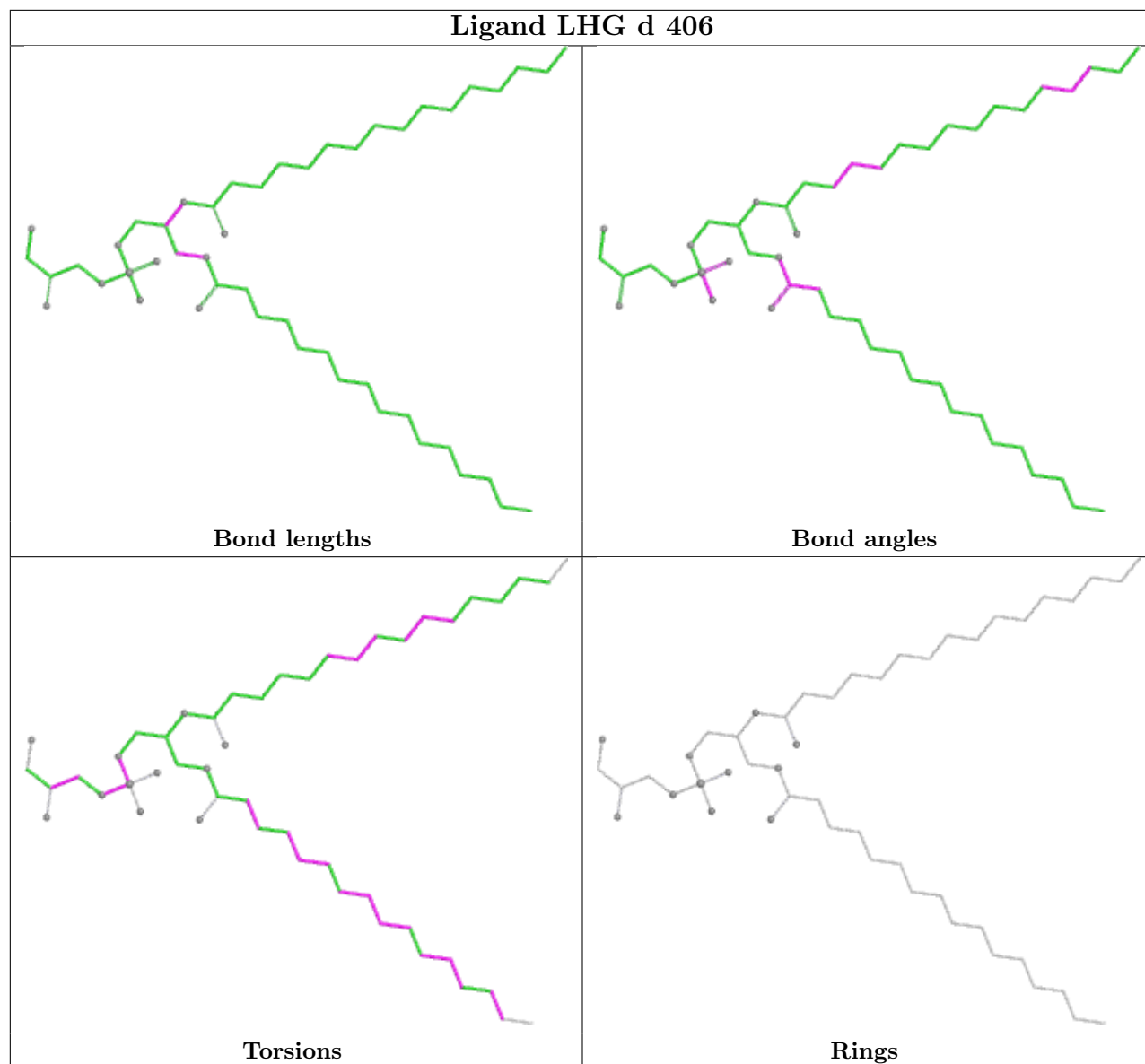




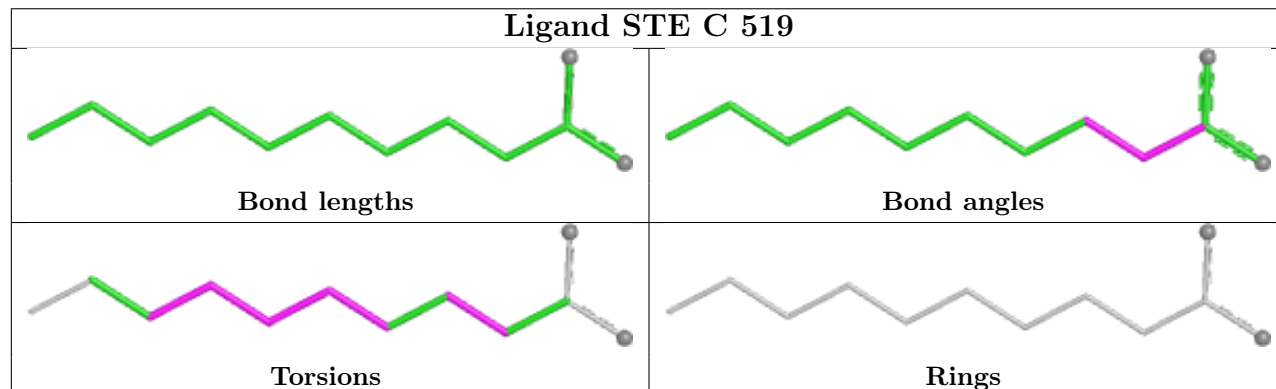




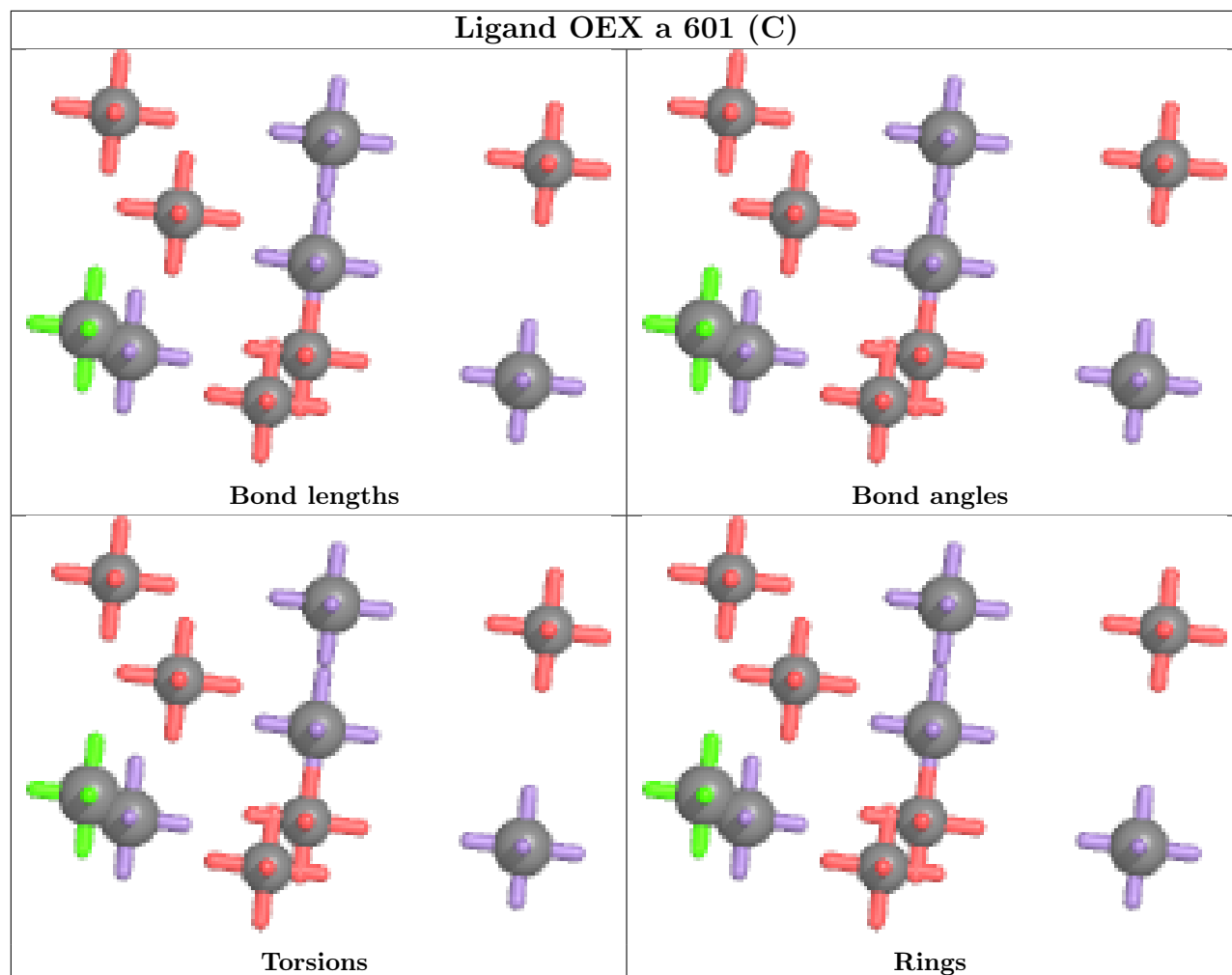
Ligand LHG d 406



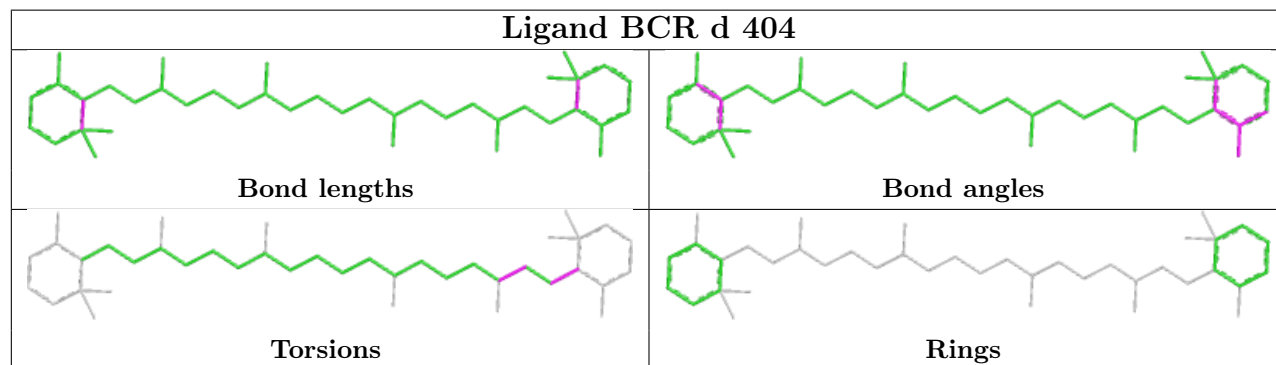
Ligand STE C 519

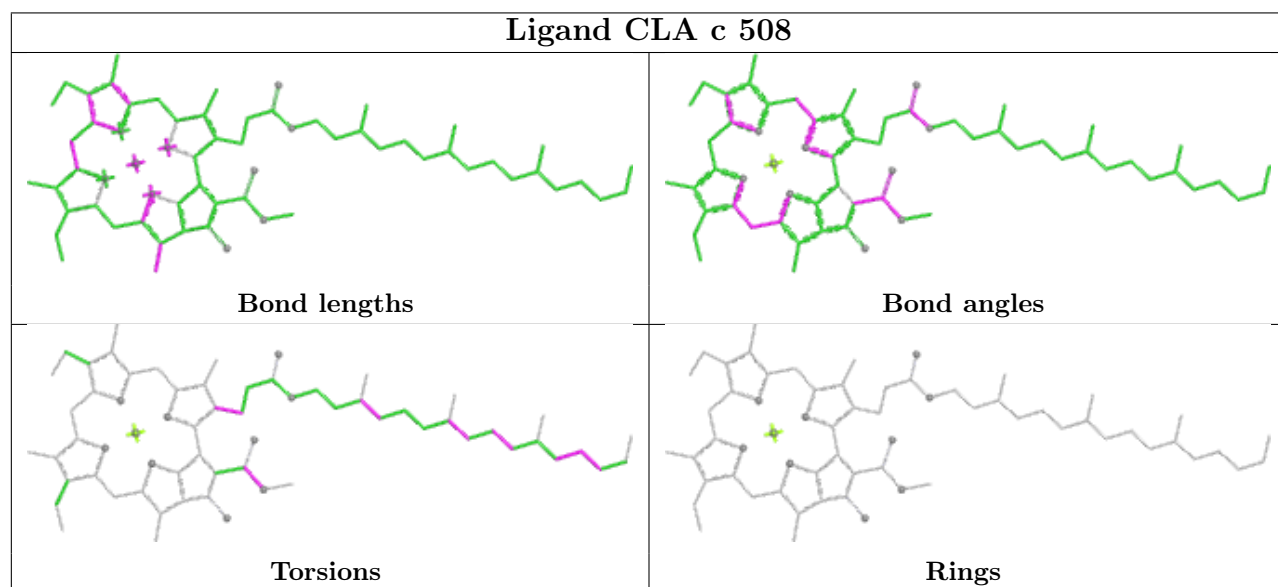
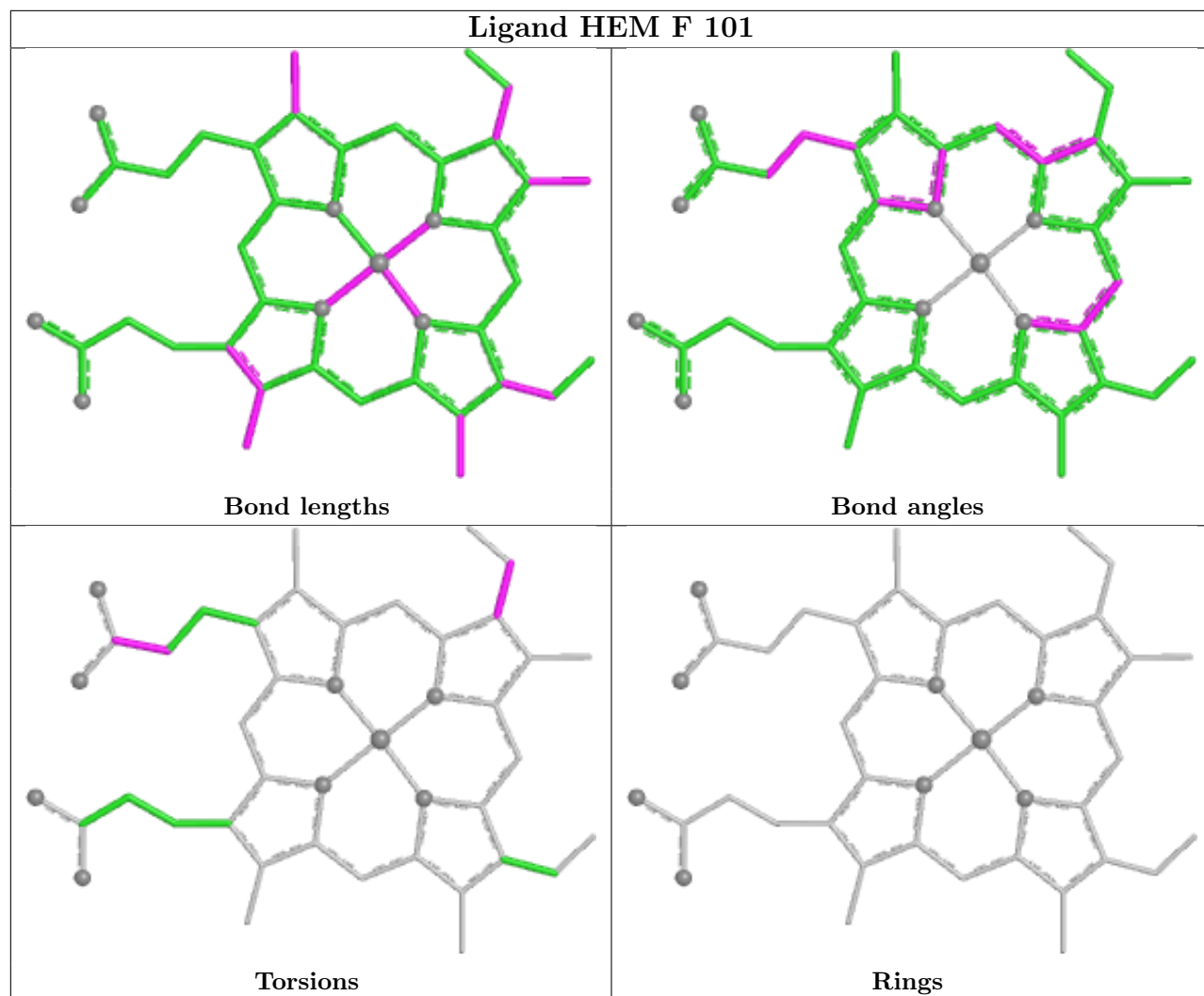


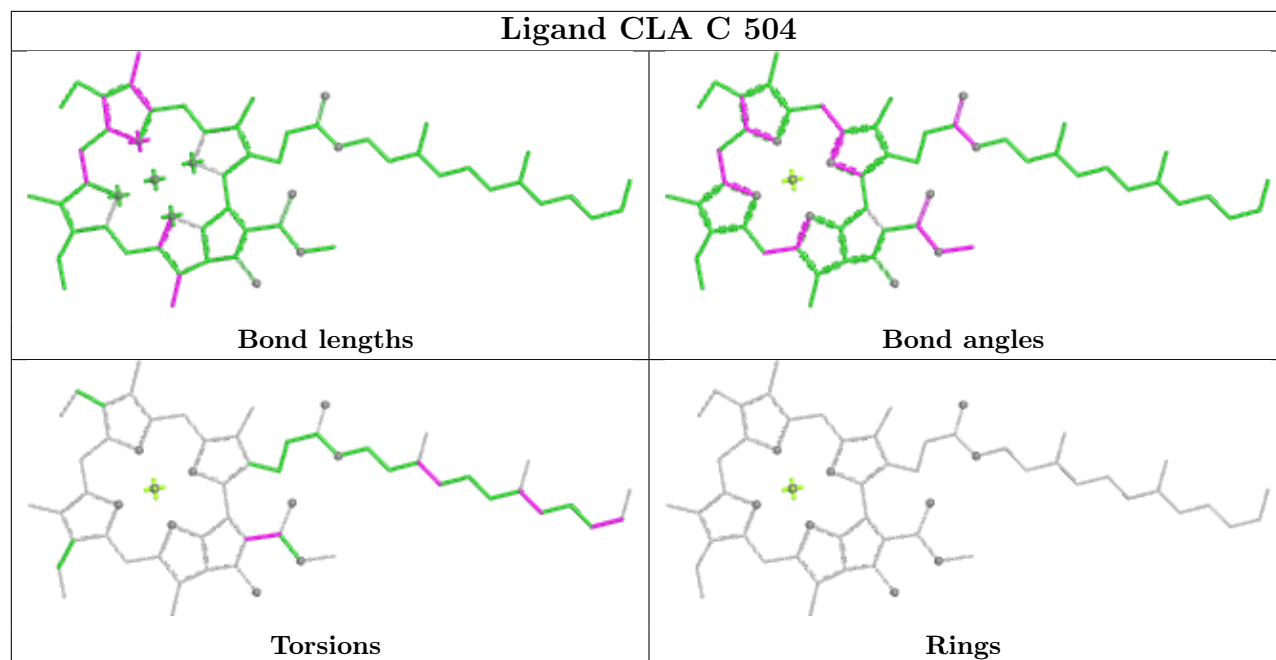
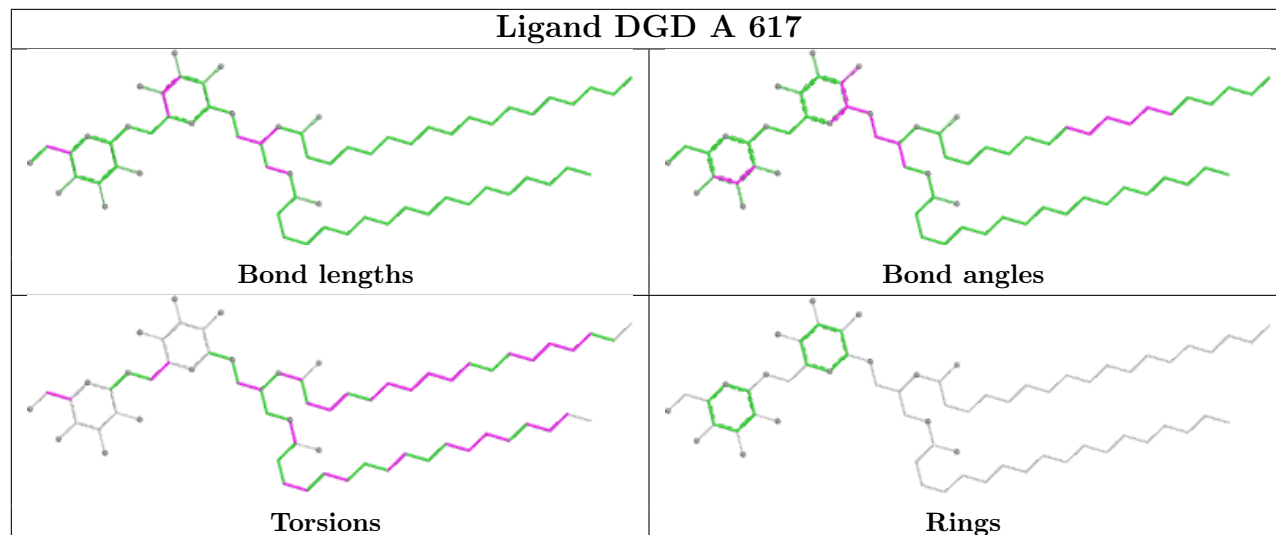
Ligand OEX a 601 (C)

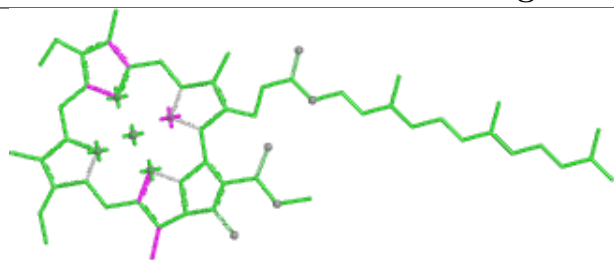
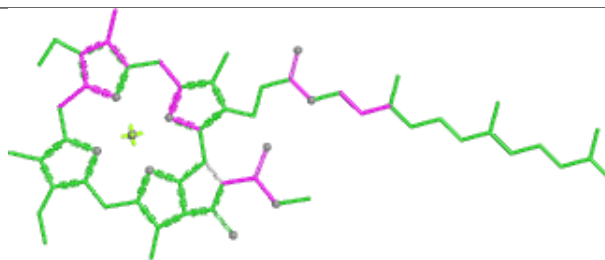
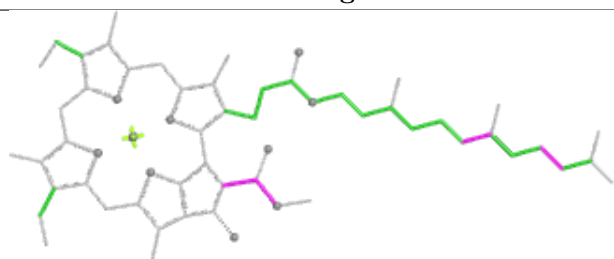
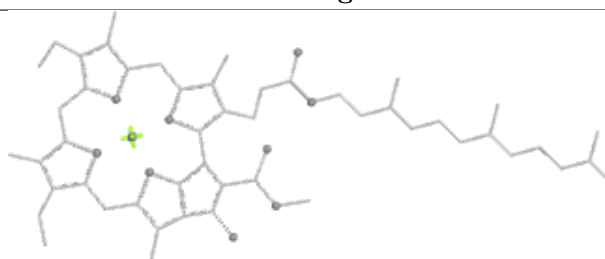
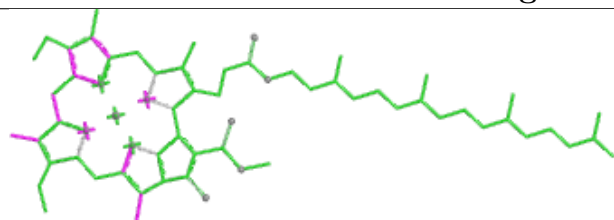
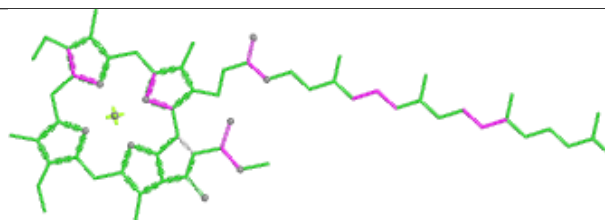
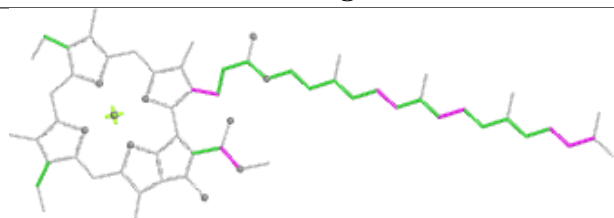
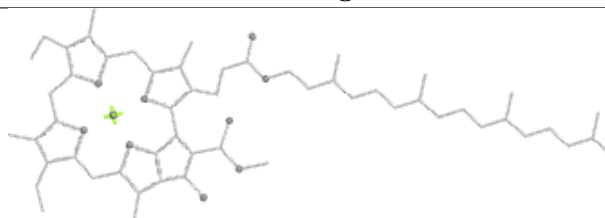


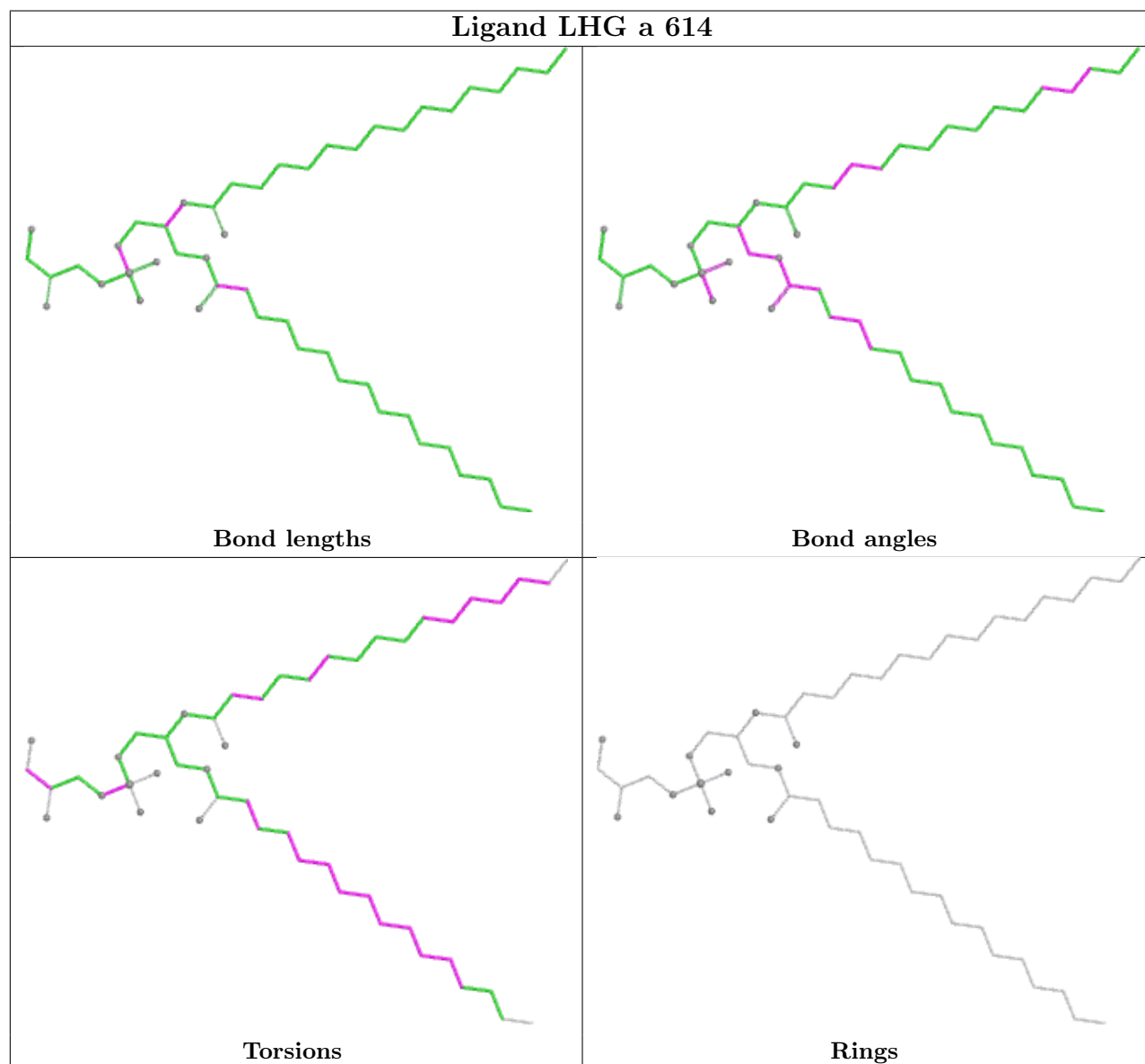
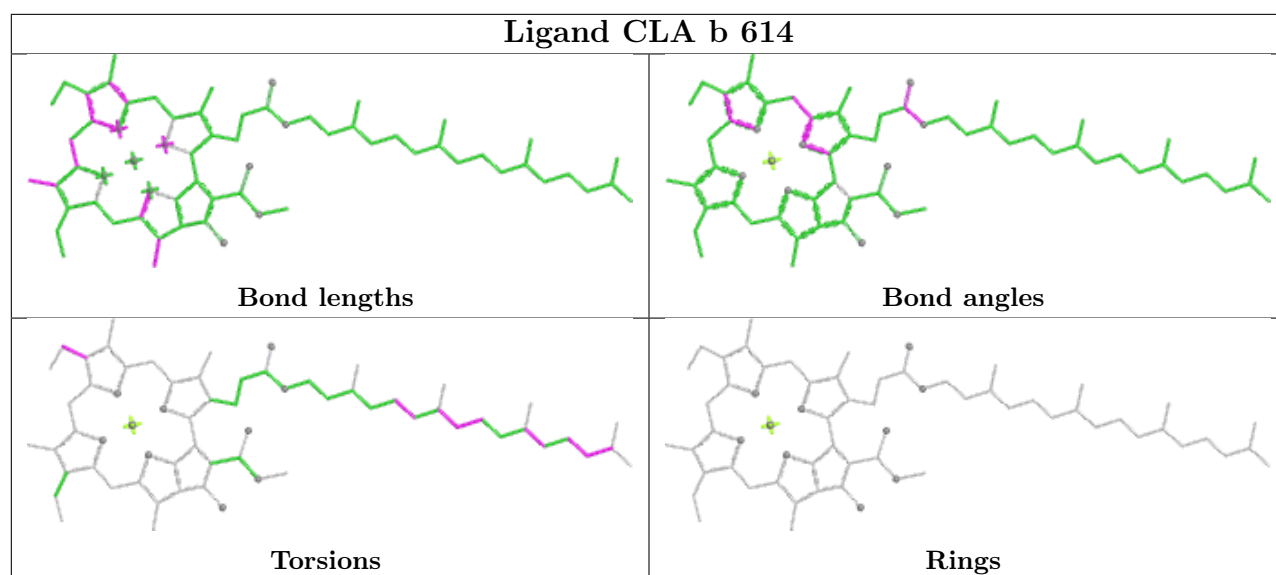
Ligand BCR d 404

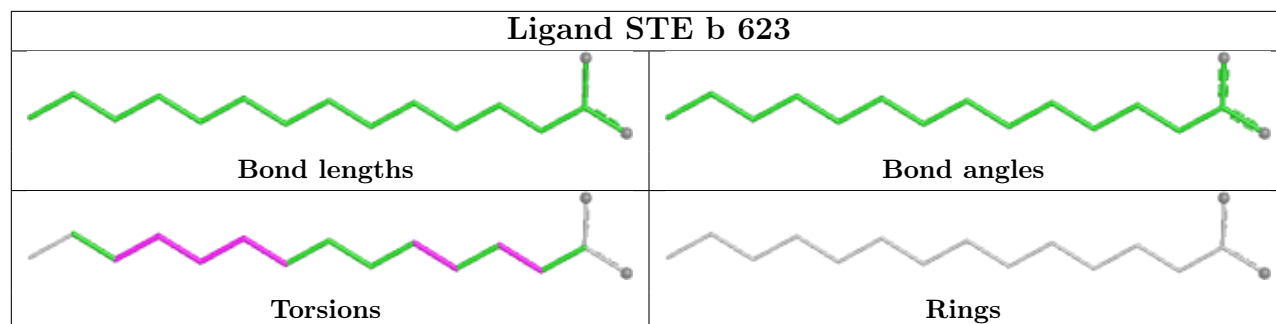
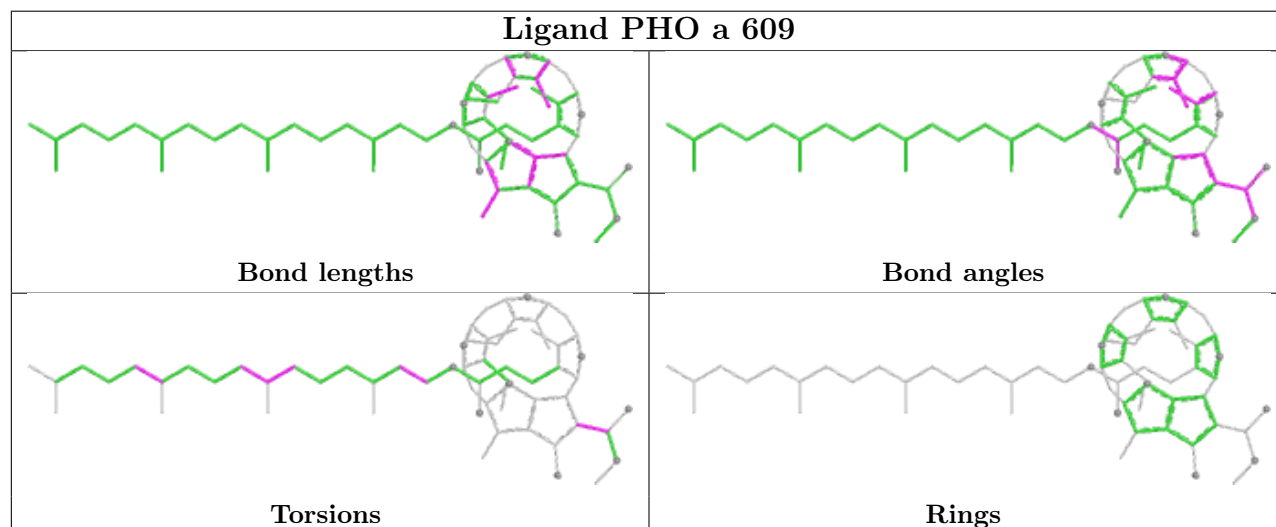
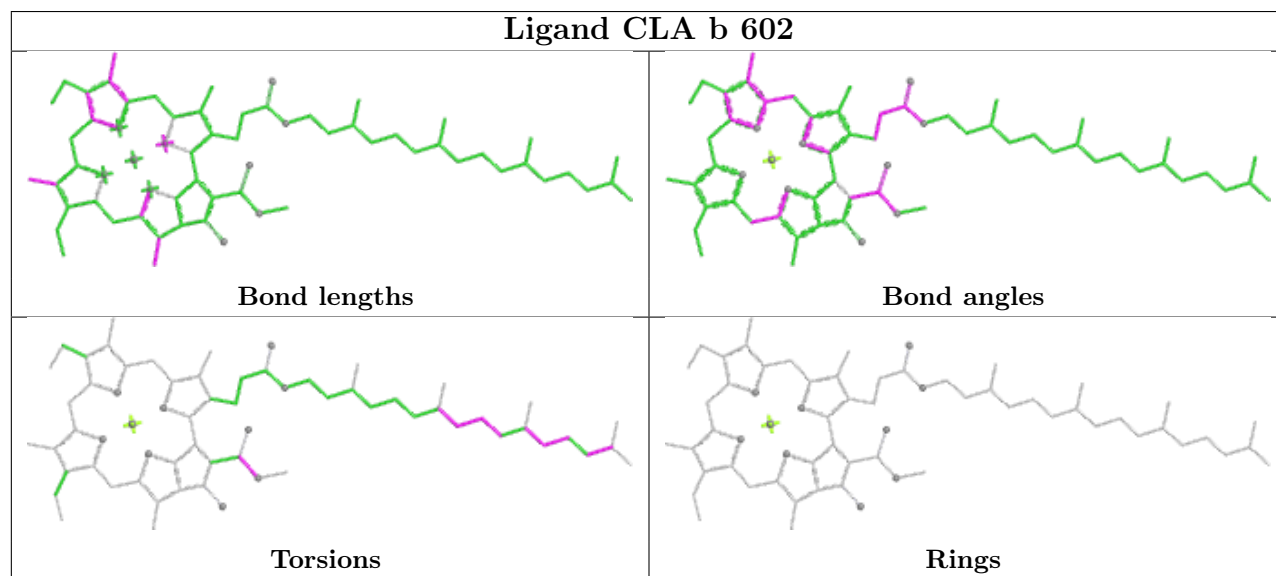


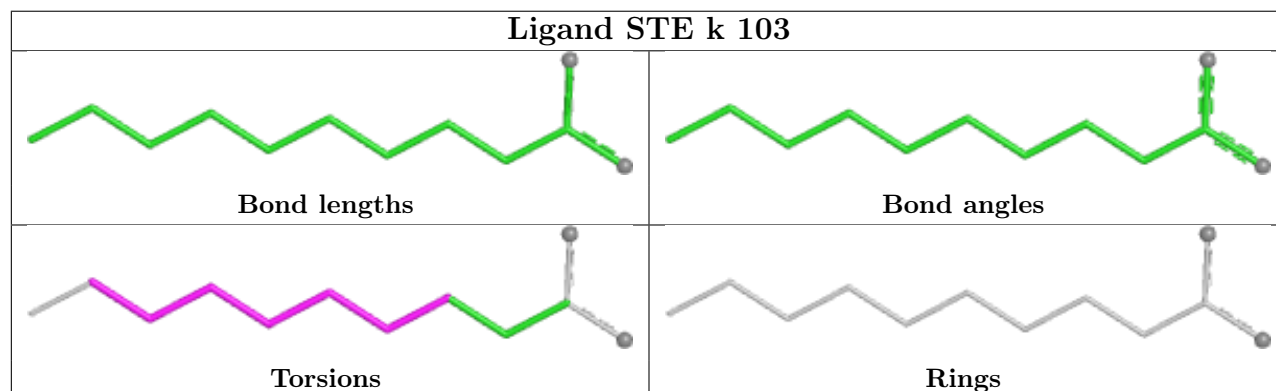
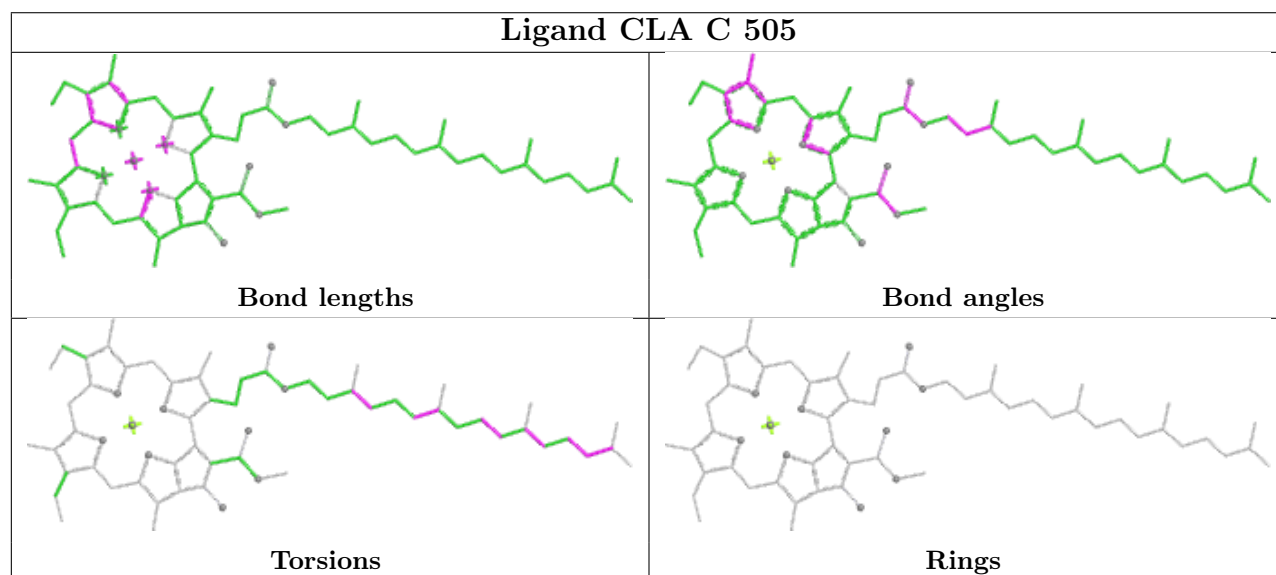
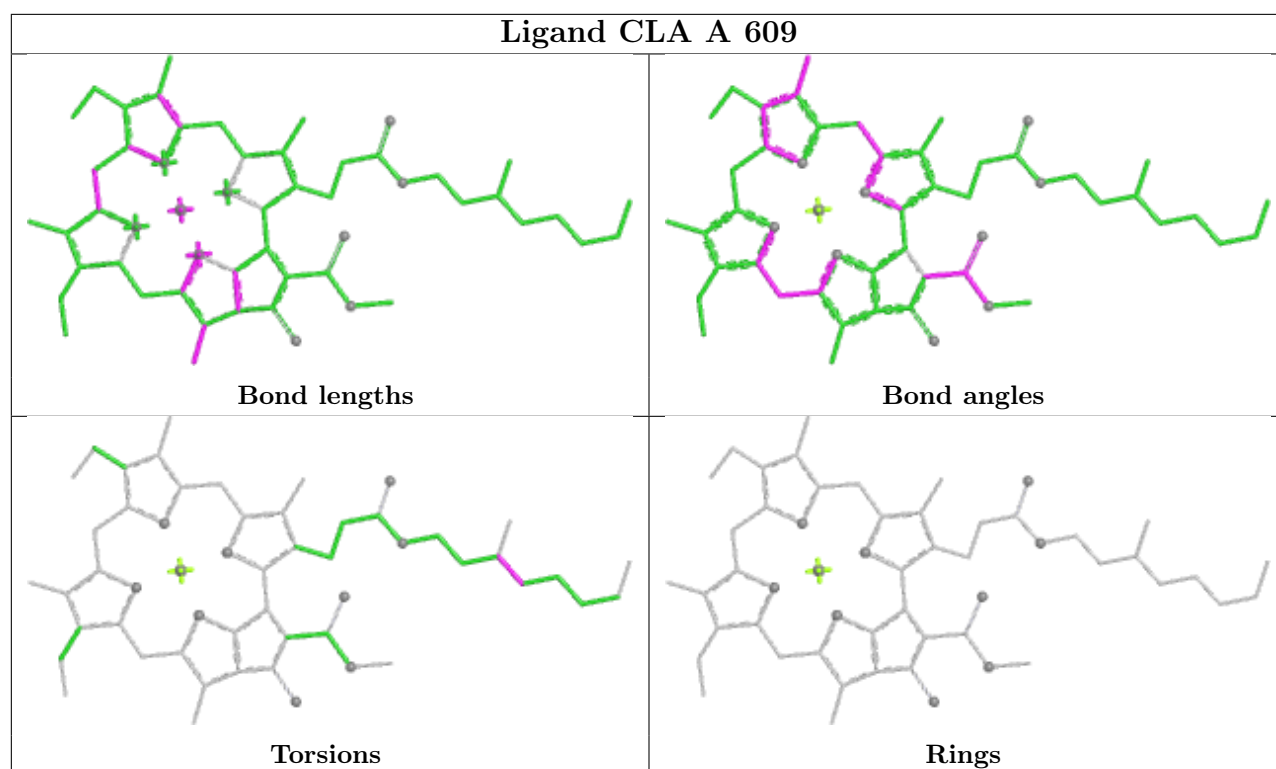


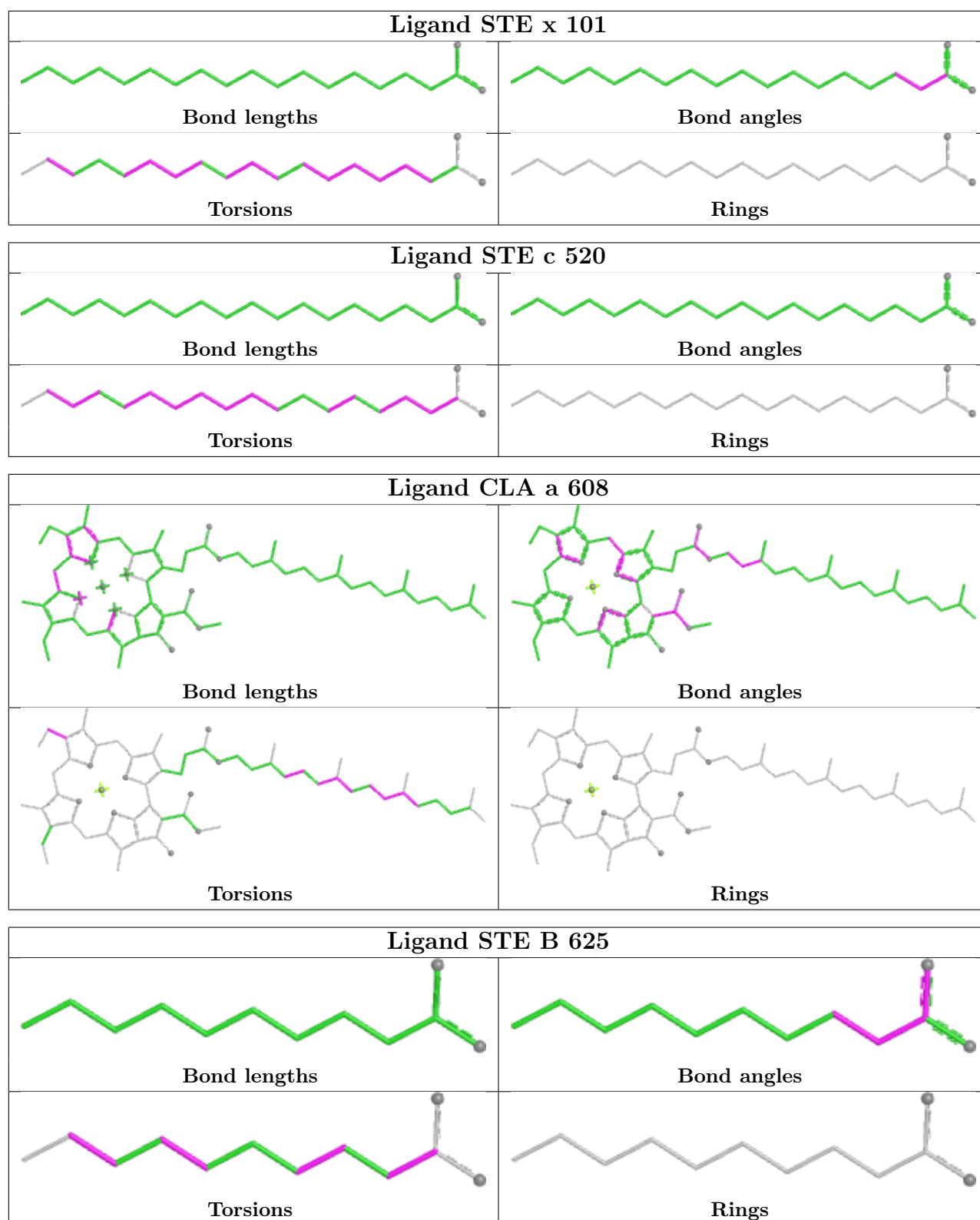
Ligand CLA C 504**Ligand DGD A 617**

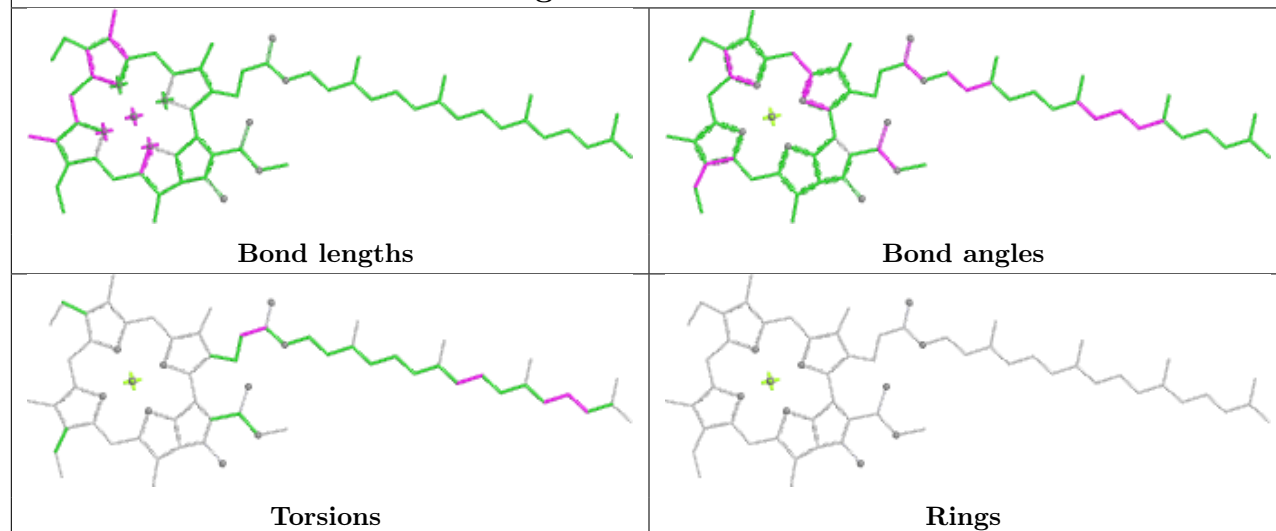
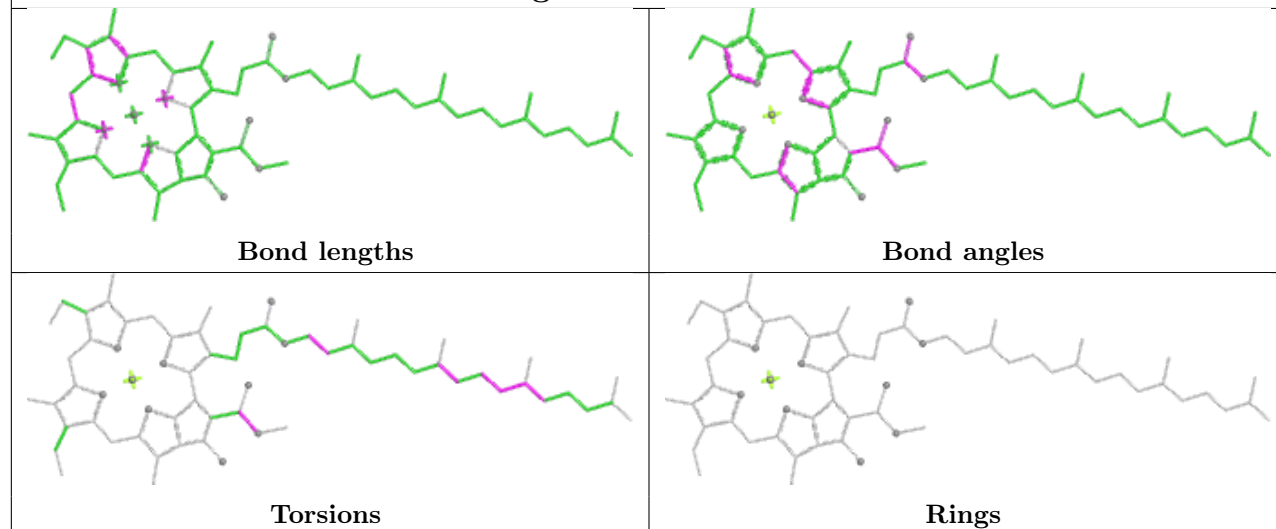
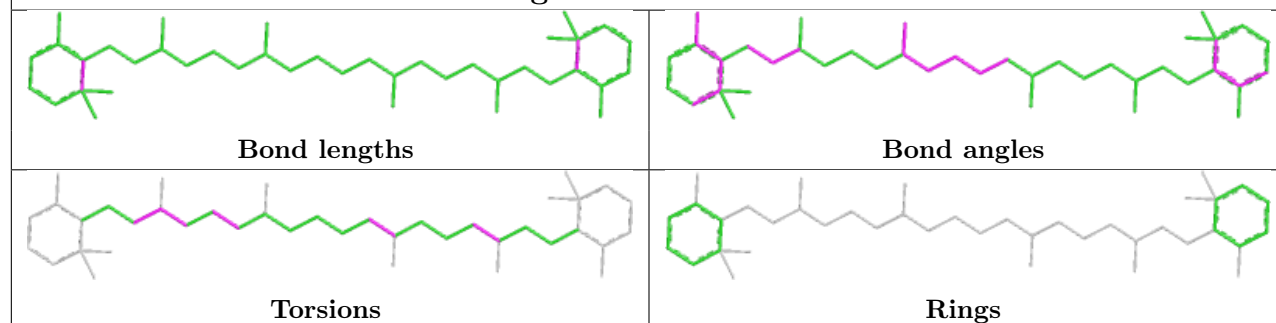
Ligand CLA b 615**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA c 503****Bond lengths****Bond angles****Torsions****Rings**

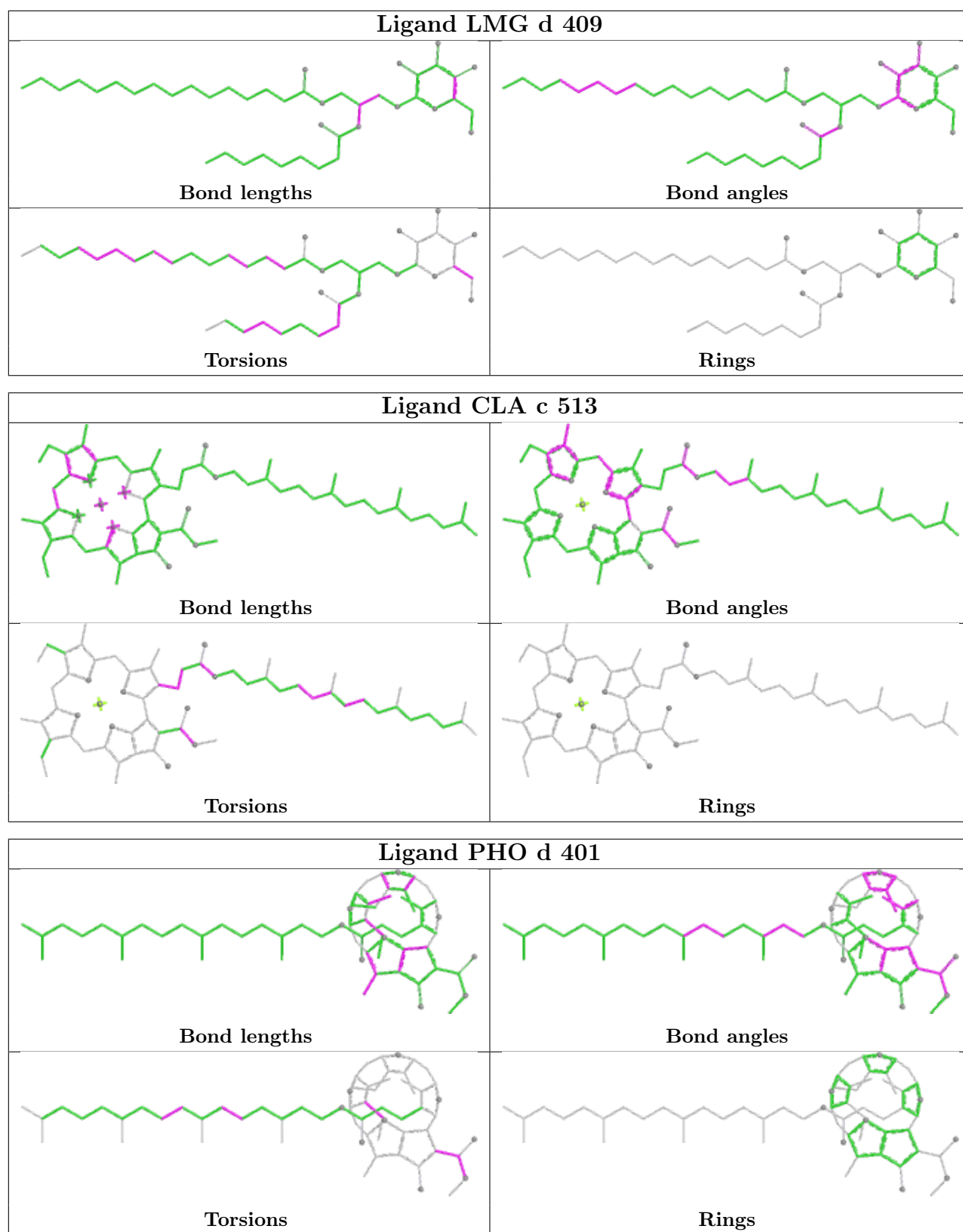


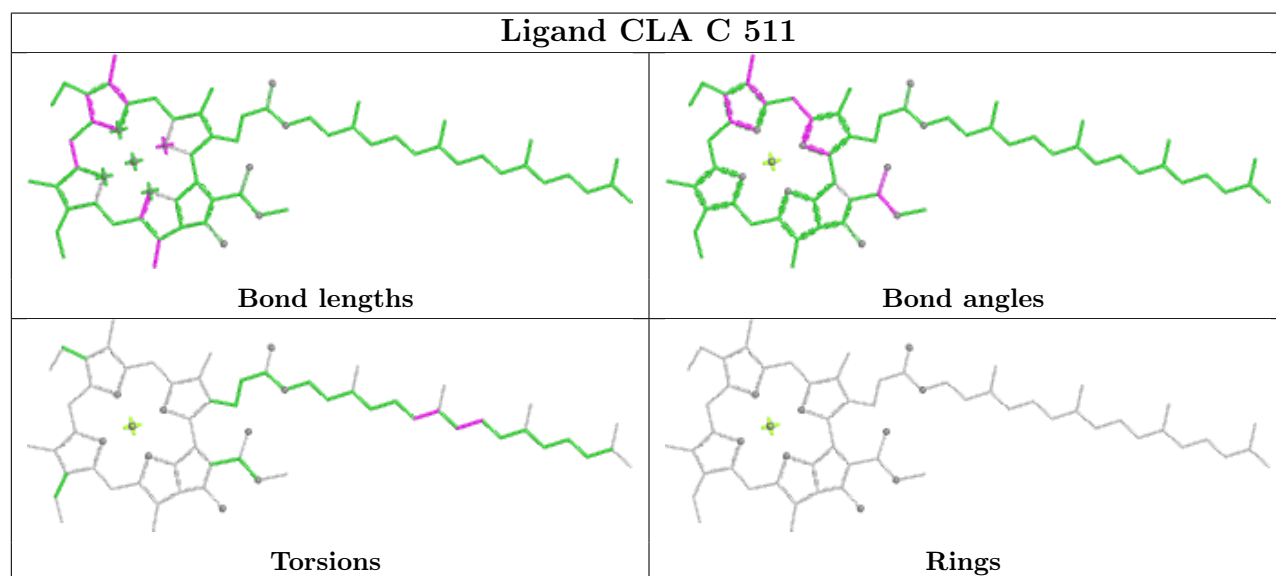
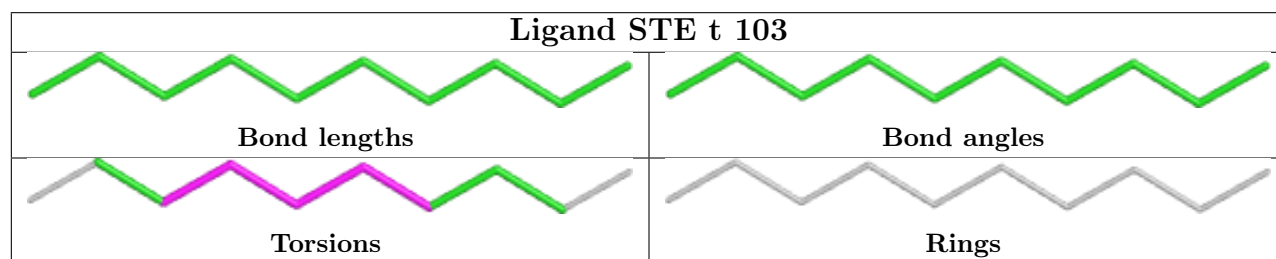
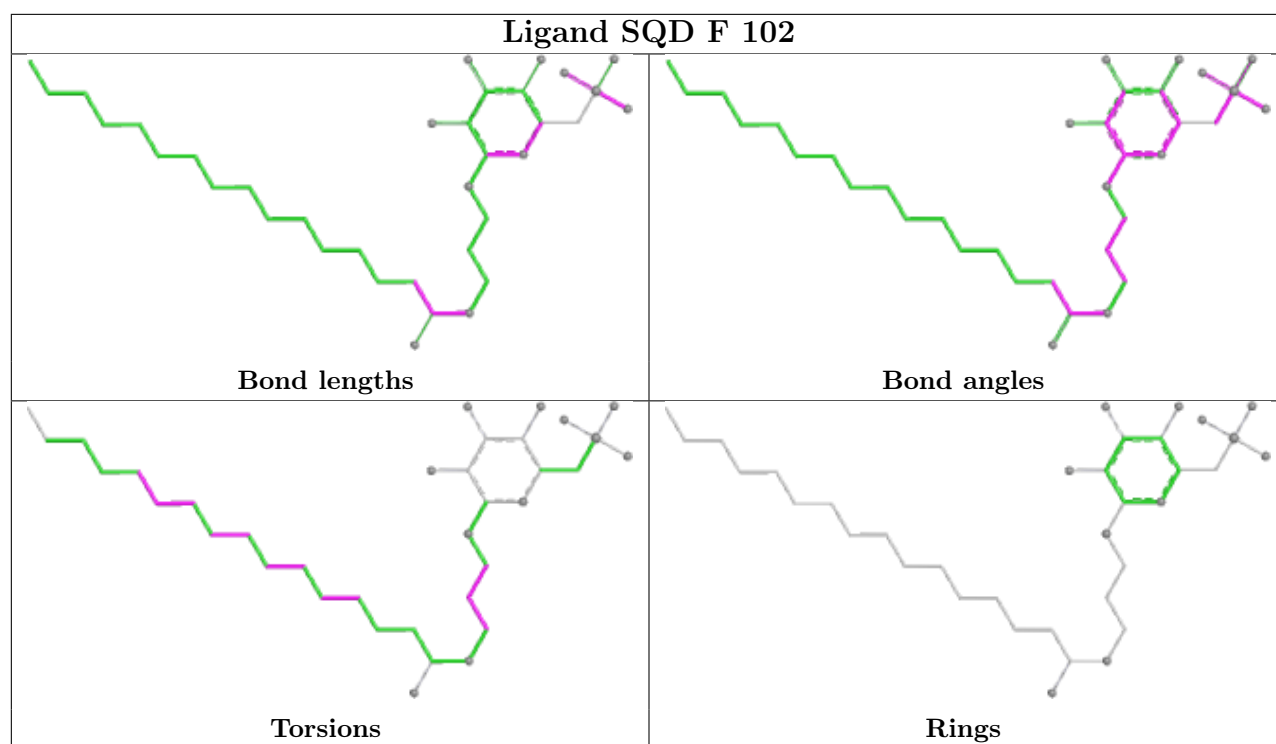
Ligand STE b 623**Ligand PHO a 609****Ligand CLA b 602**

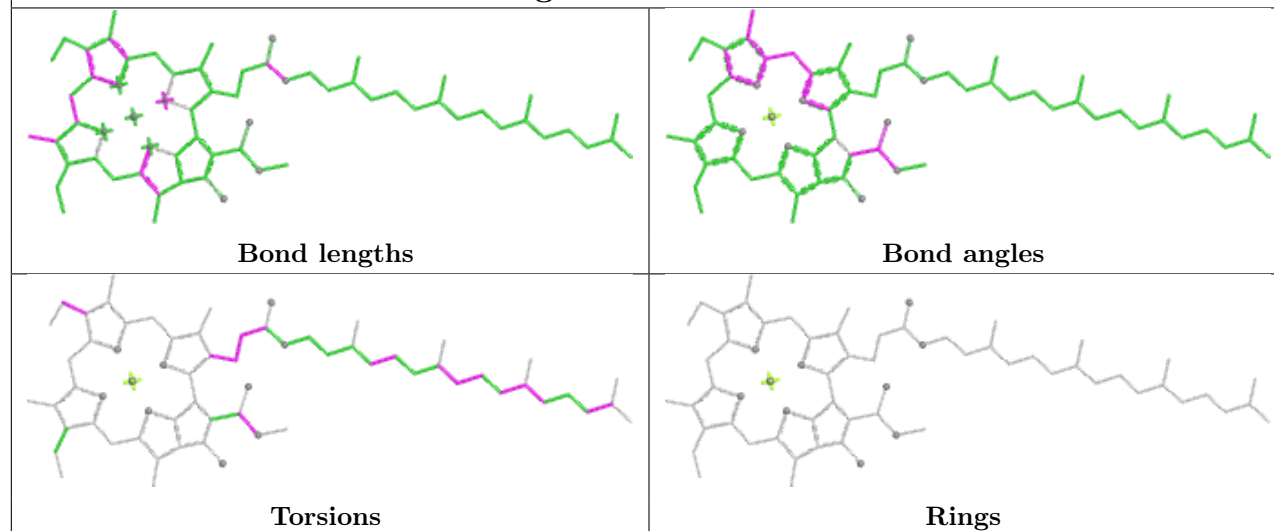
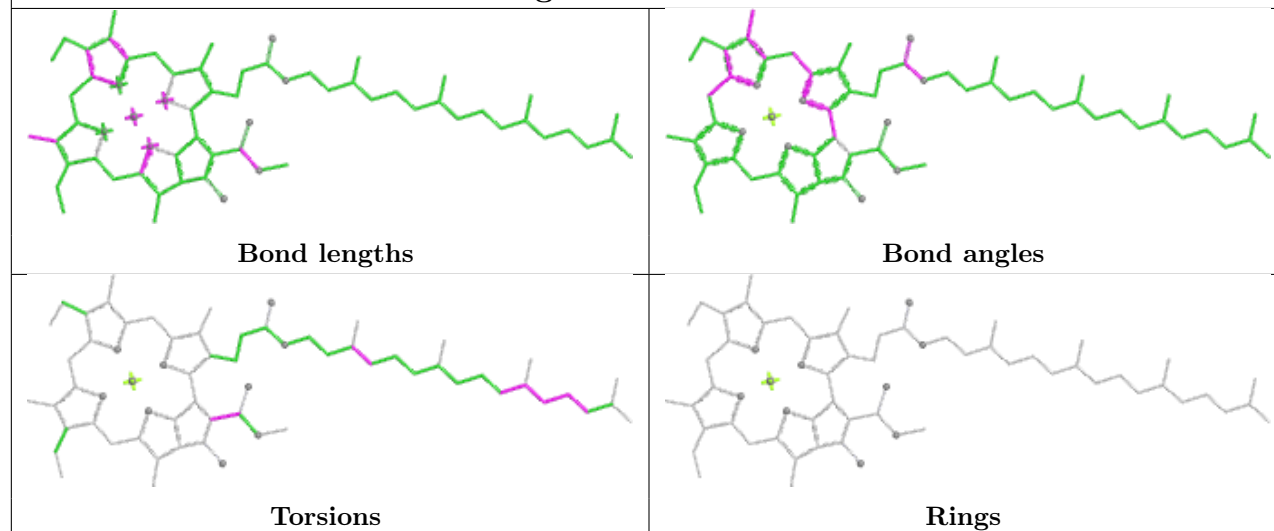
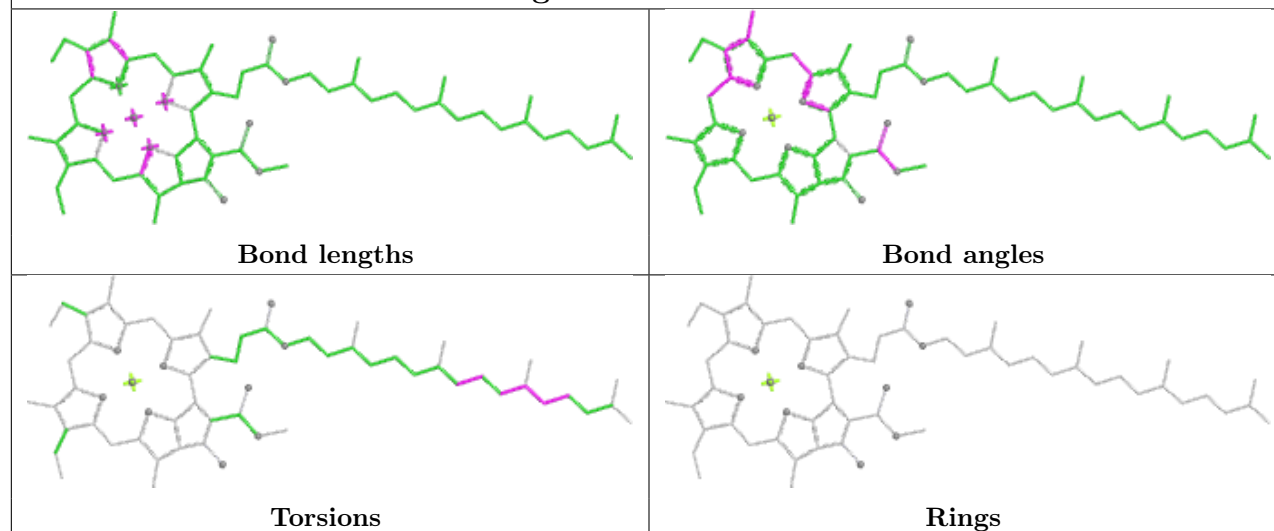


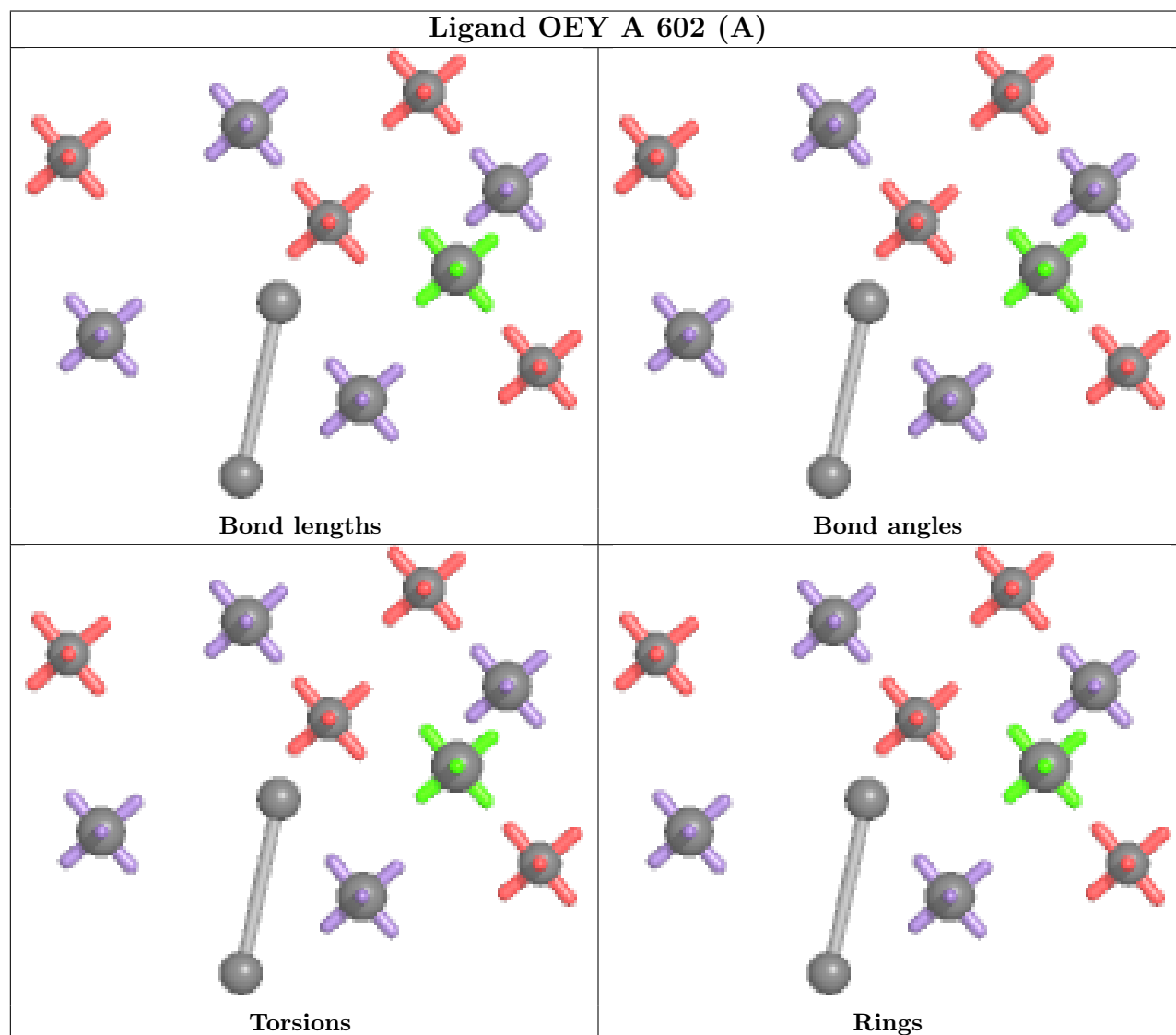
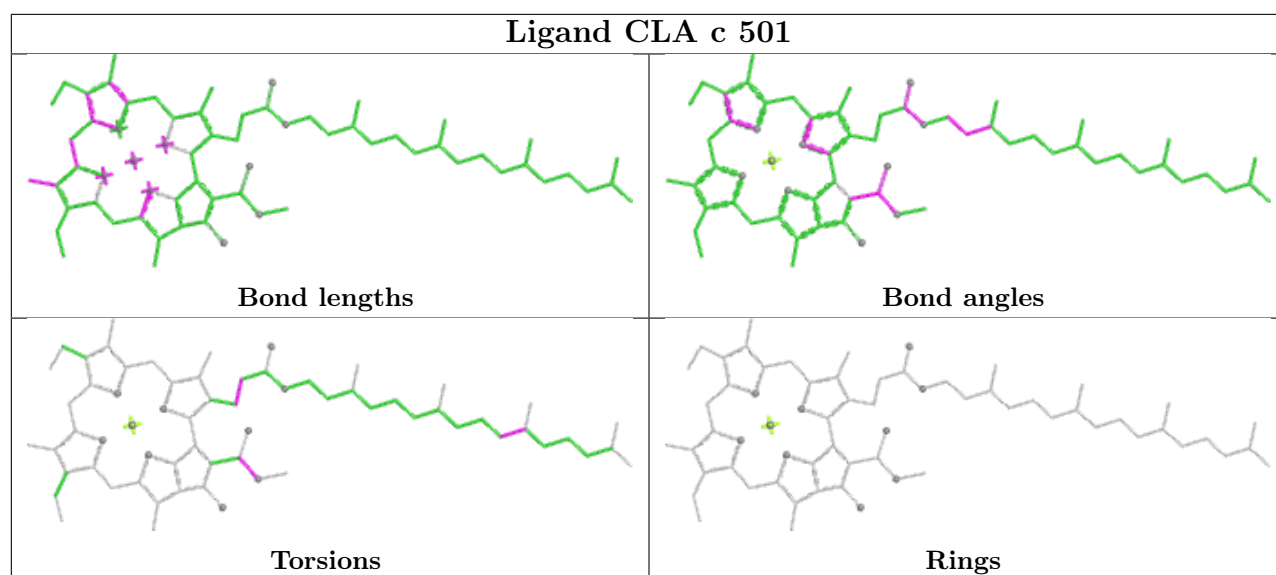


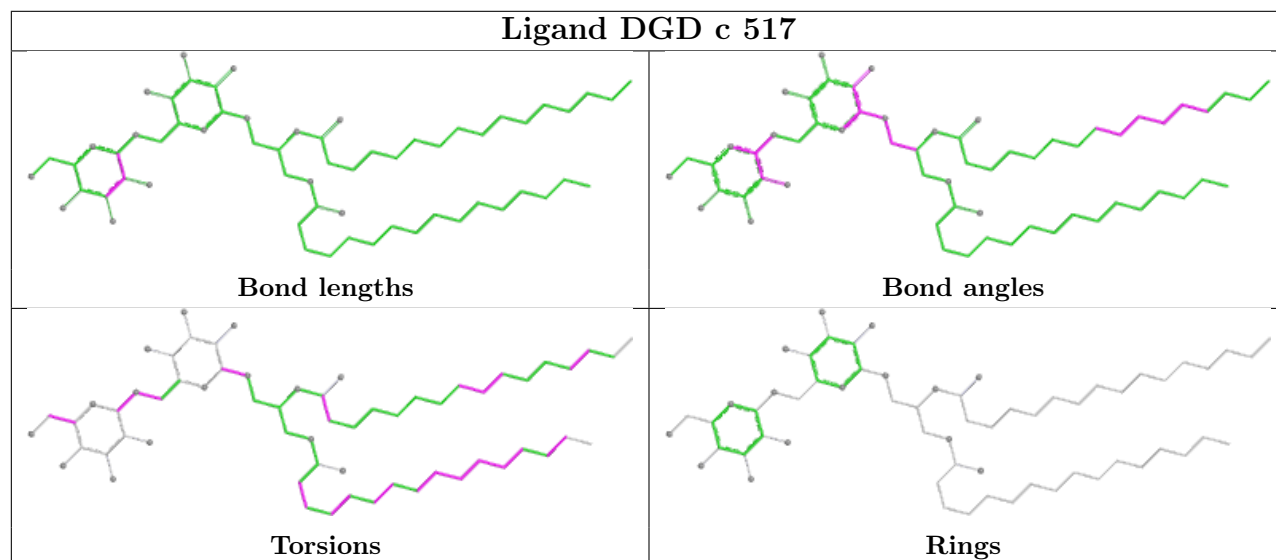
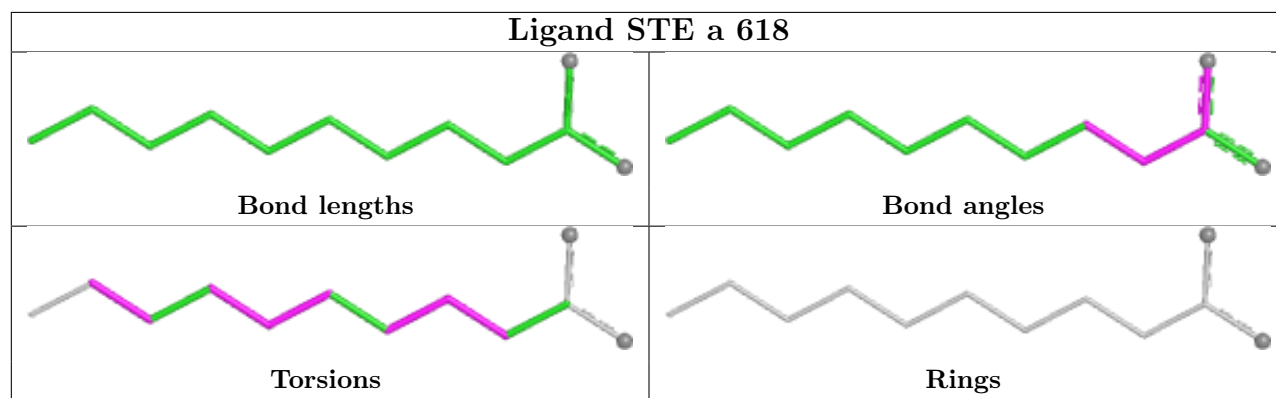
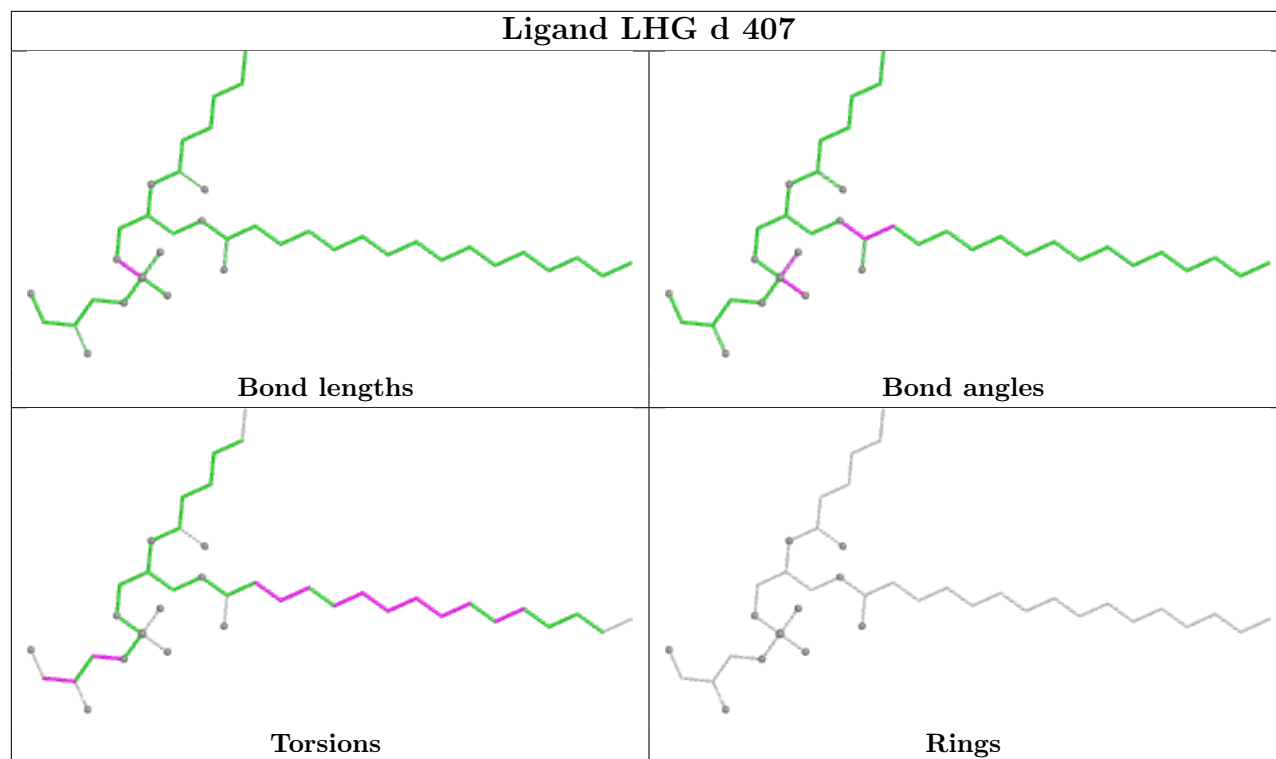
Ligand CLA b 611**Ligand CLA B 604****Ligand BCR B 618**

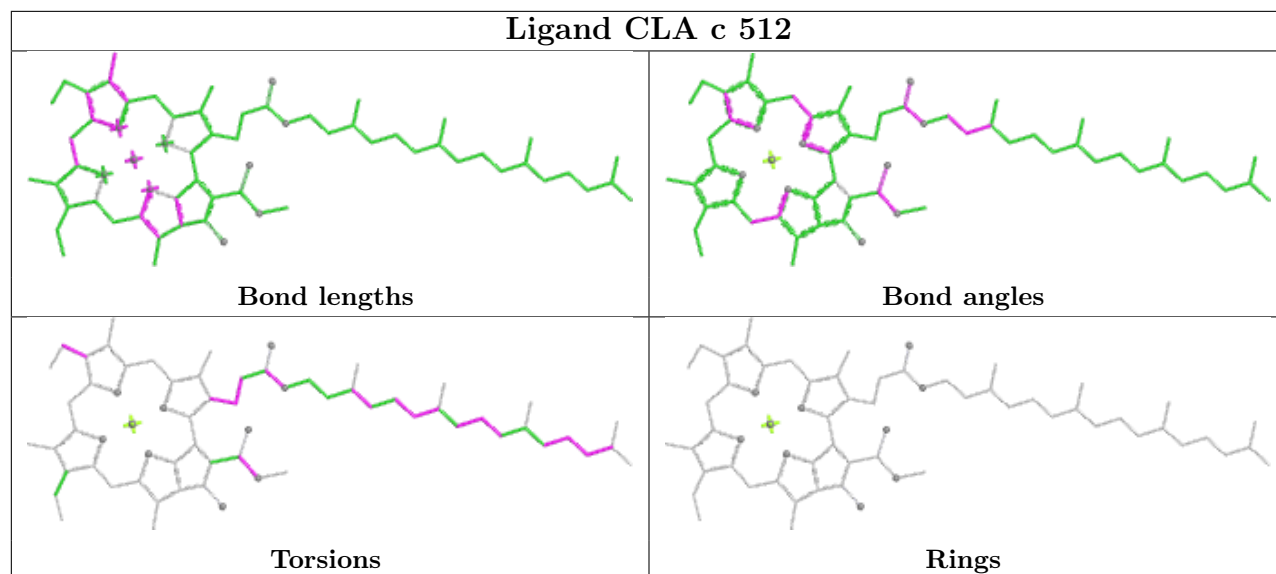
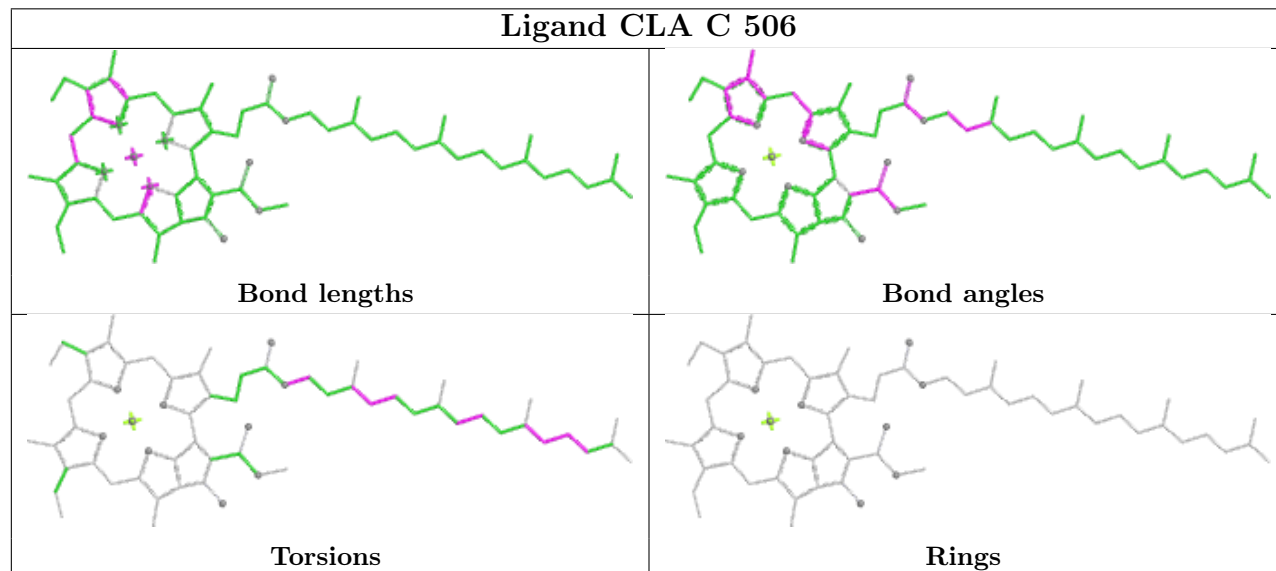


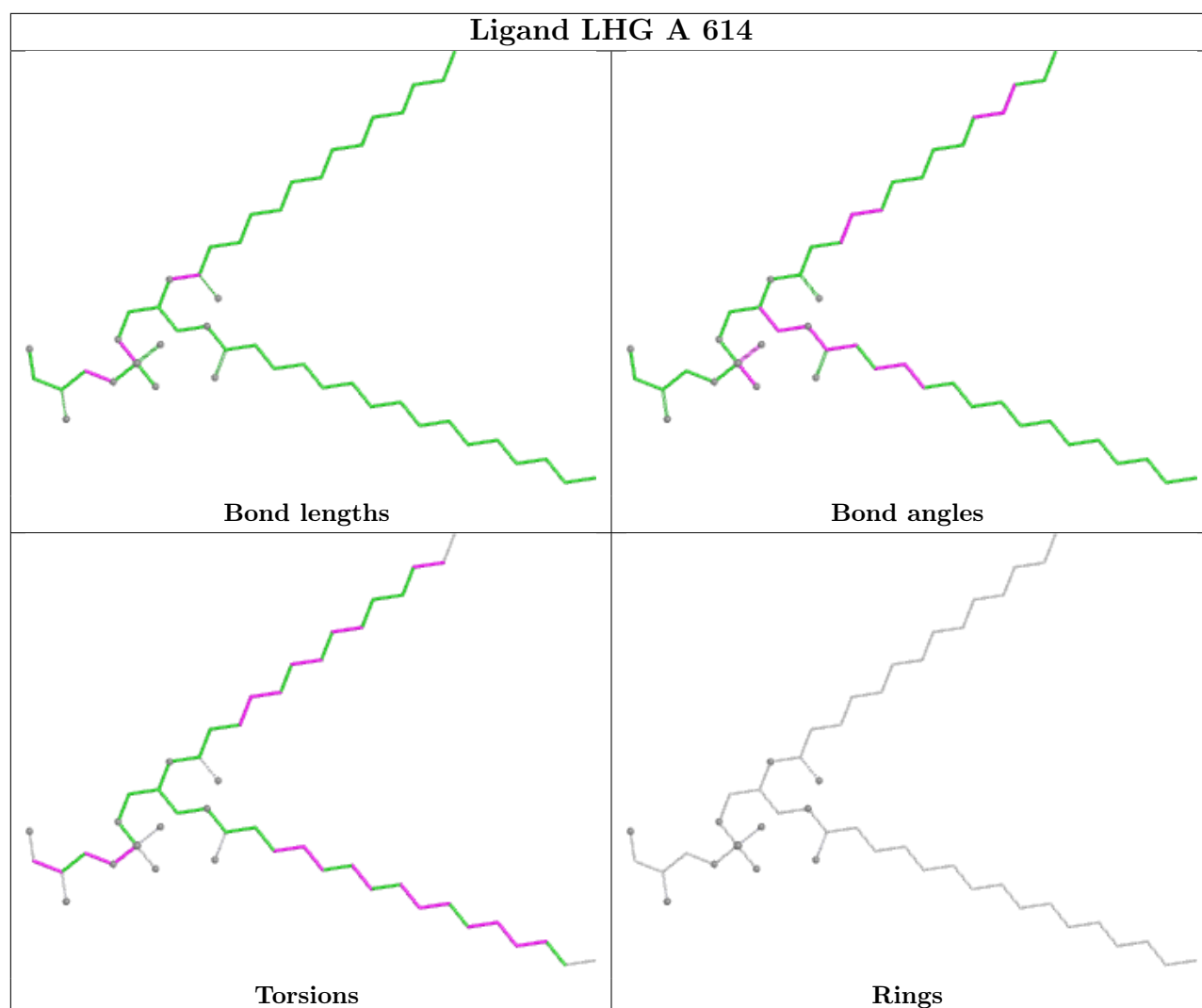


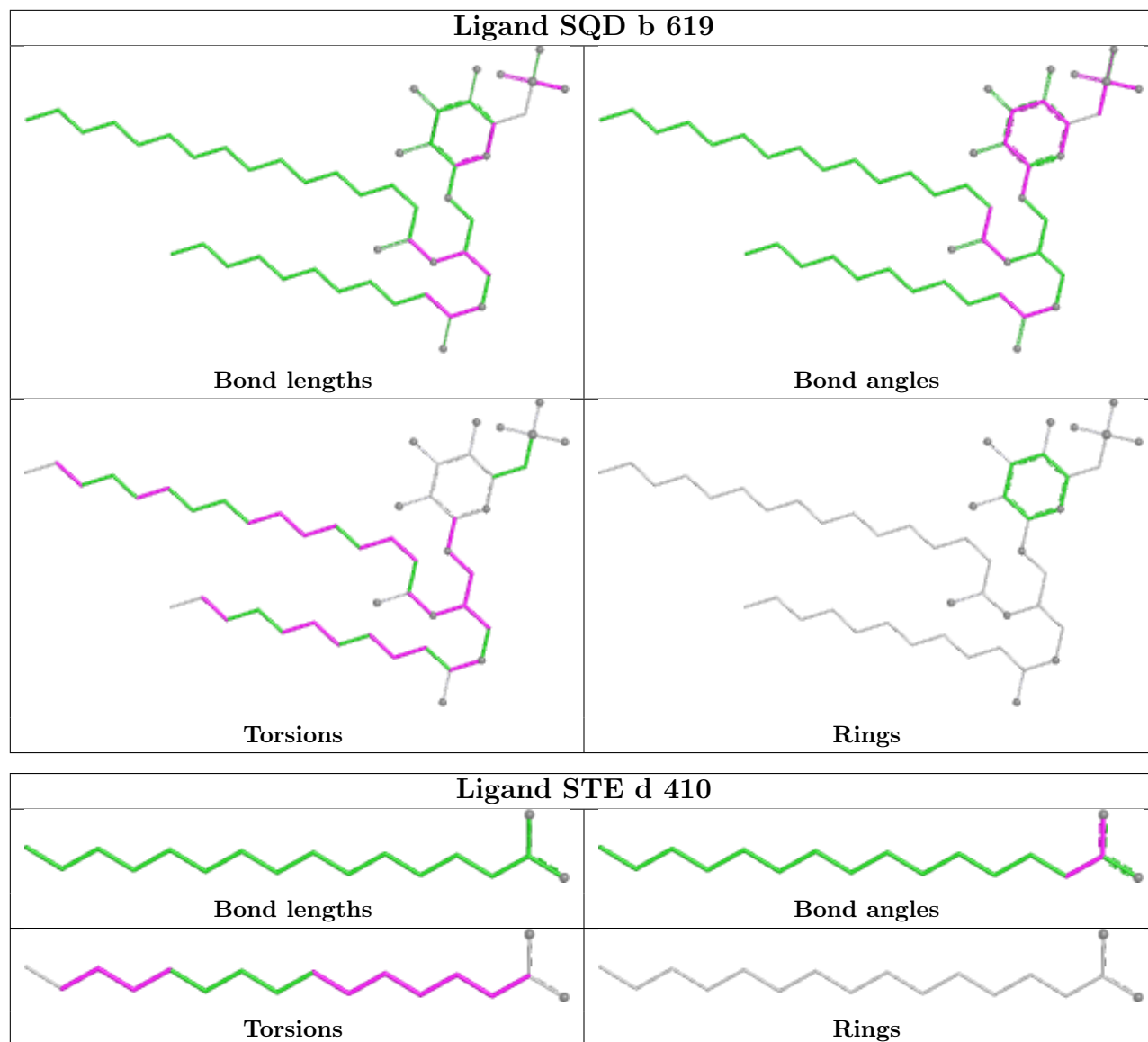
Ligand CLA h 101**Ligand CLA b 608****Ligand CLA B 607**

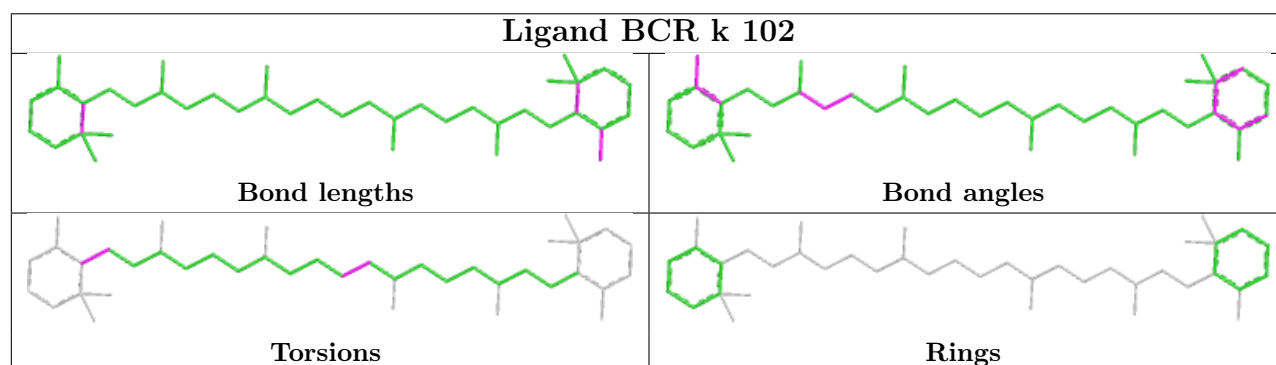
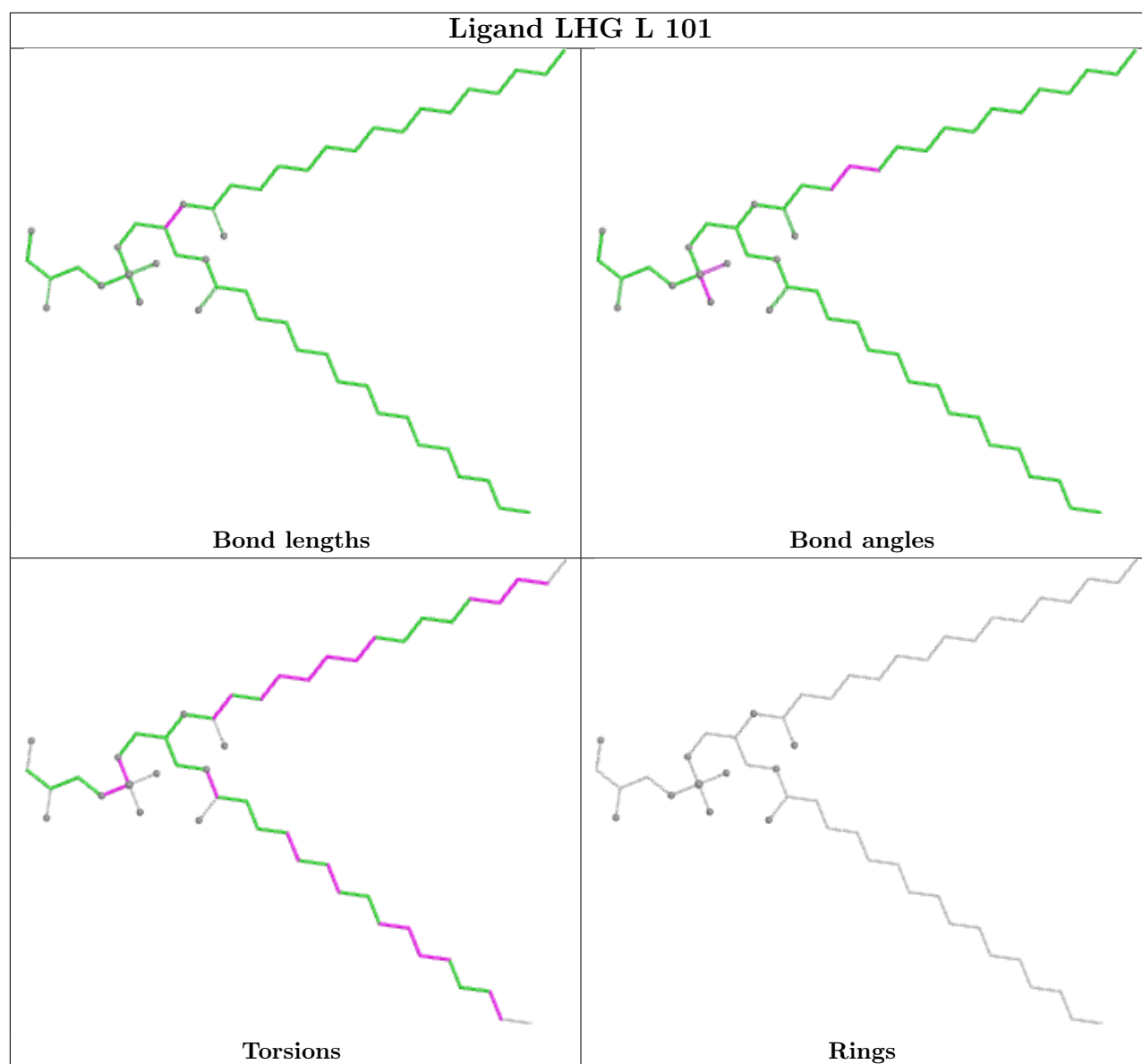


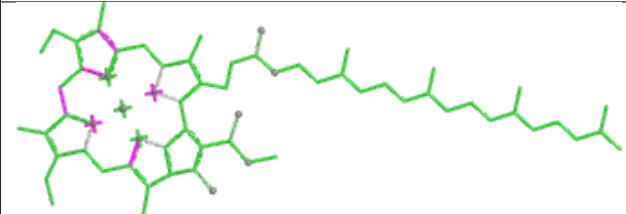
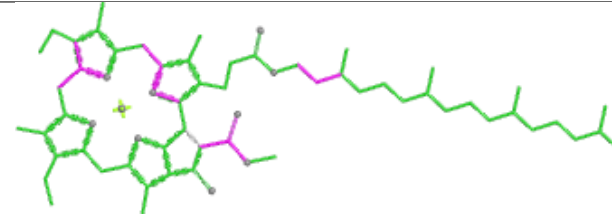
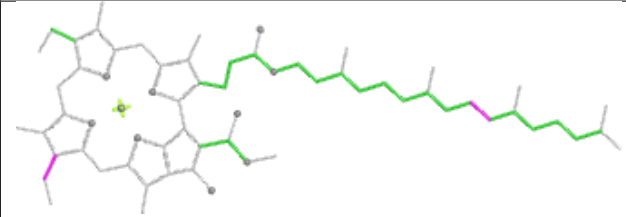
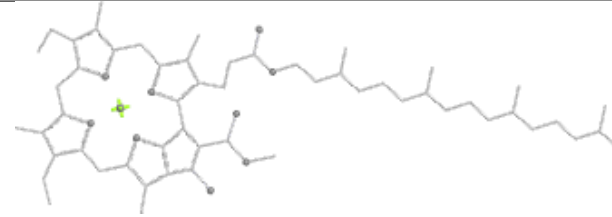


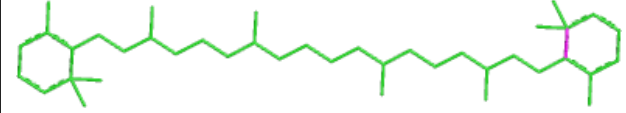
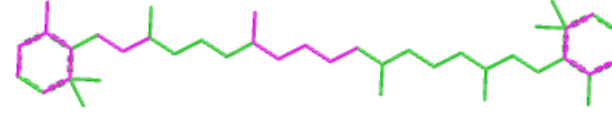
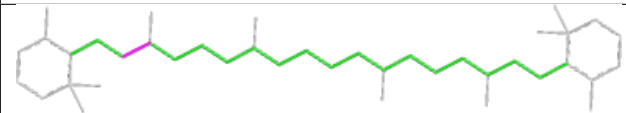
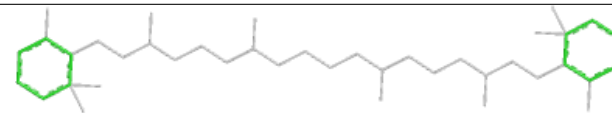
Ligand CLA c 512**Ligand CLA C 506**

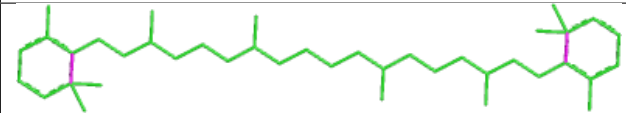
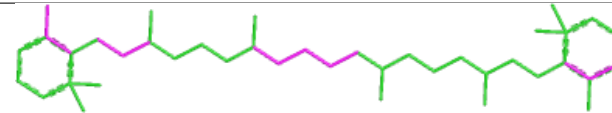
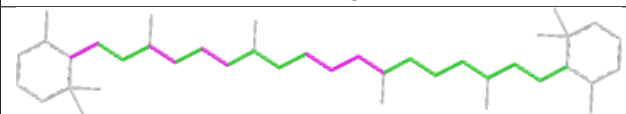
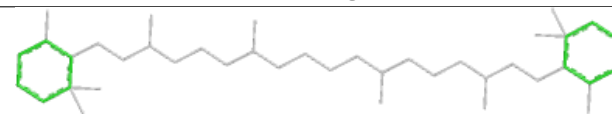


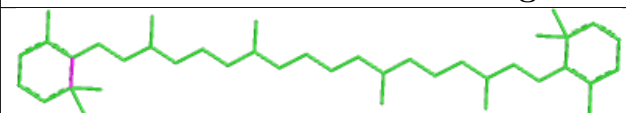
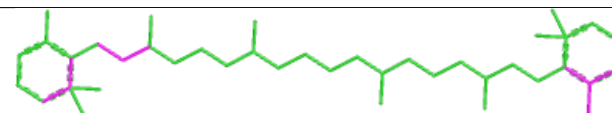
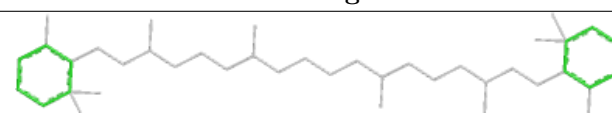


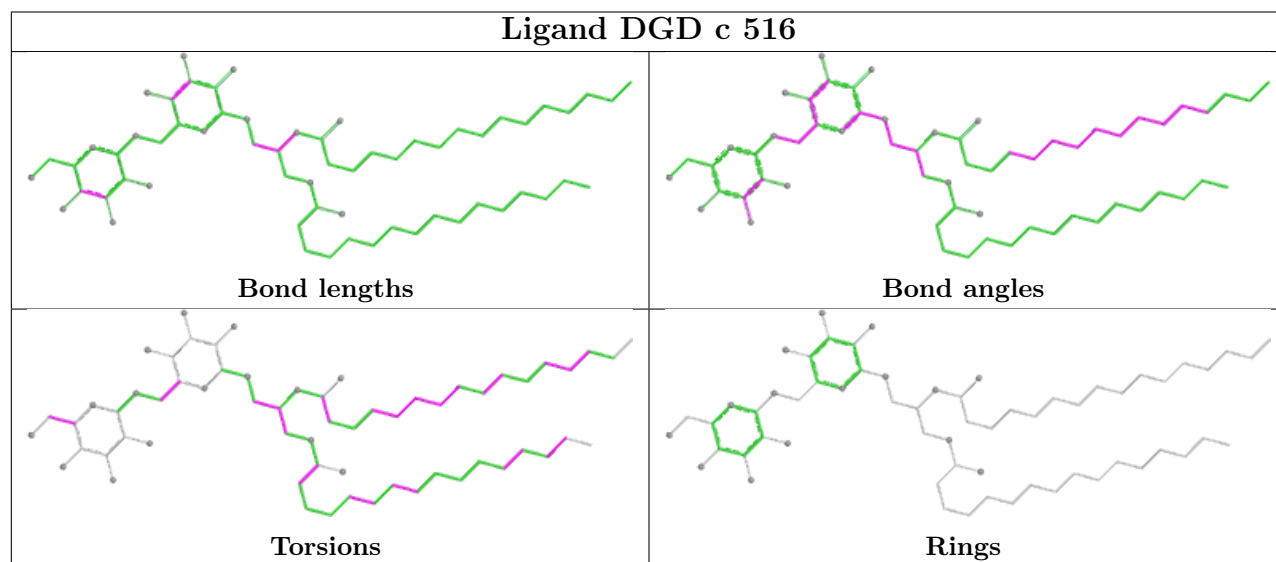
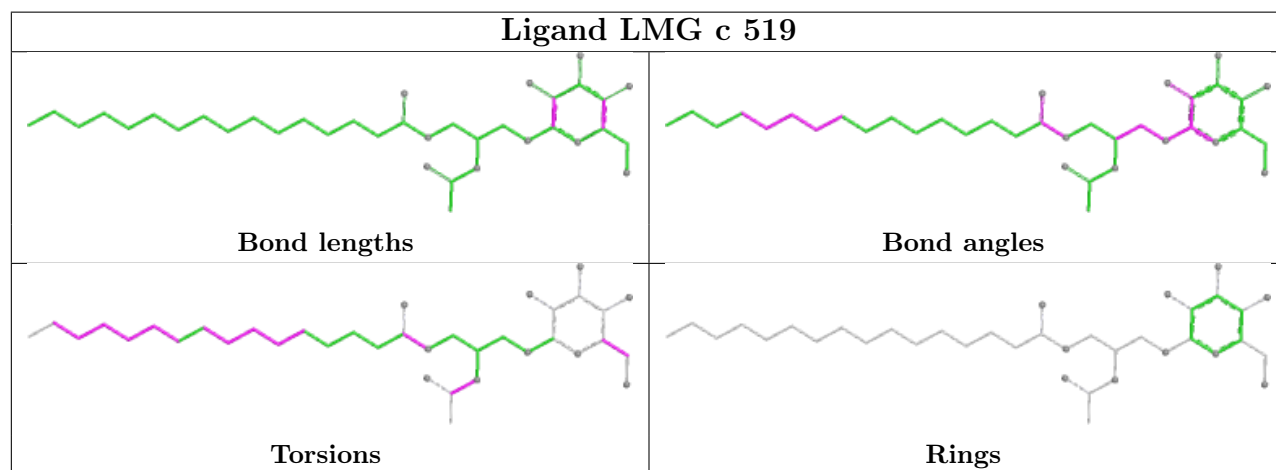
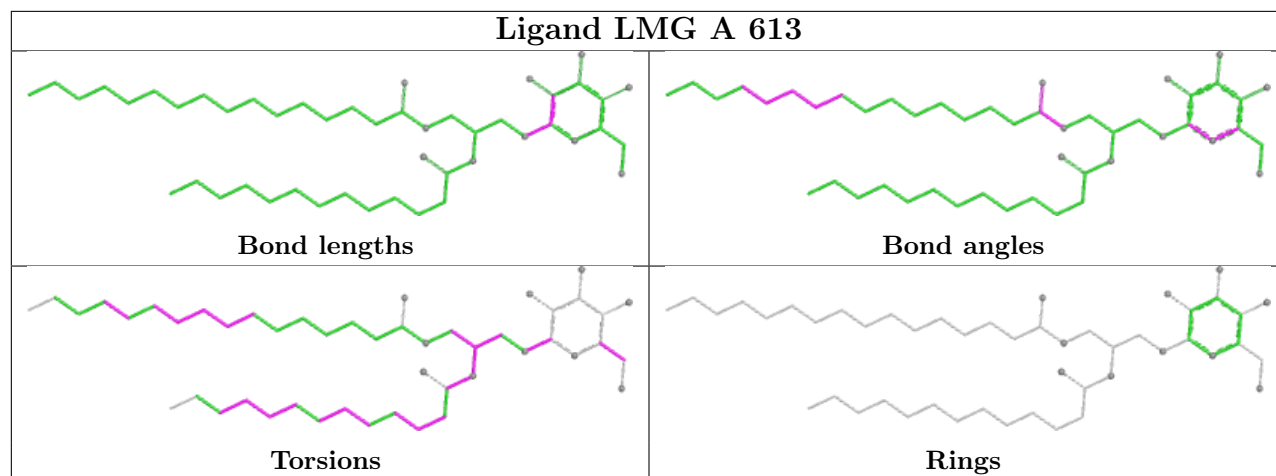


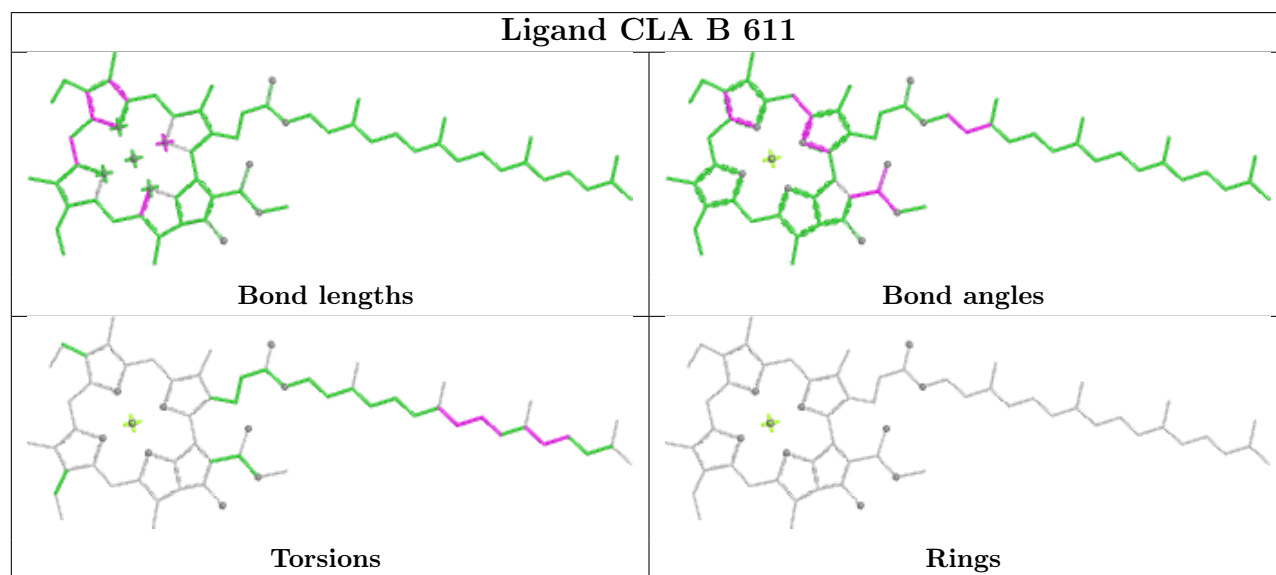
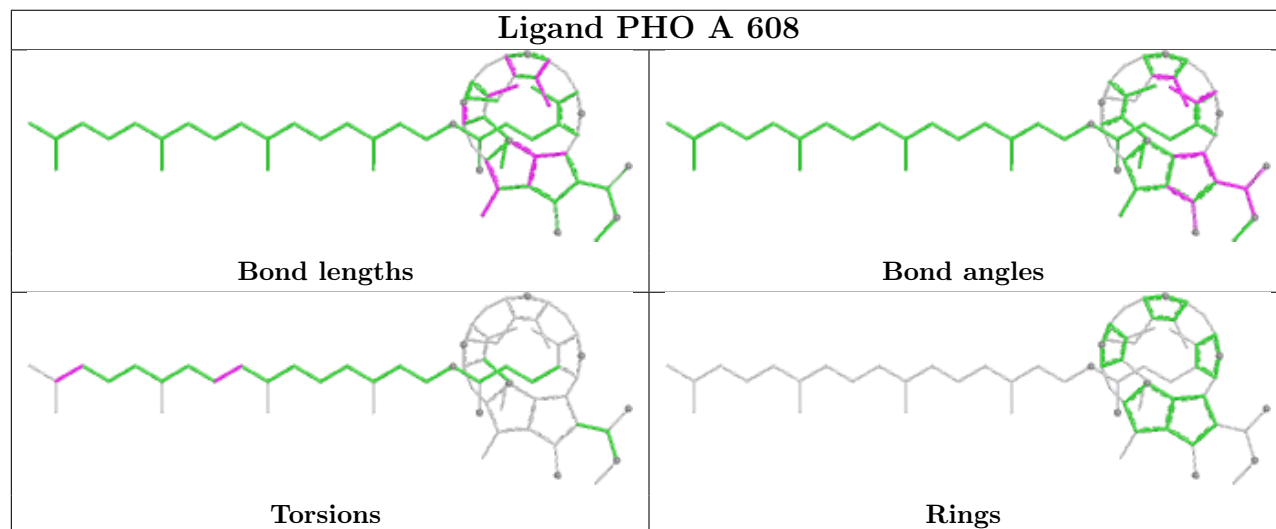
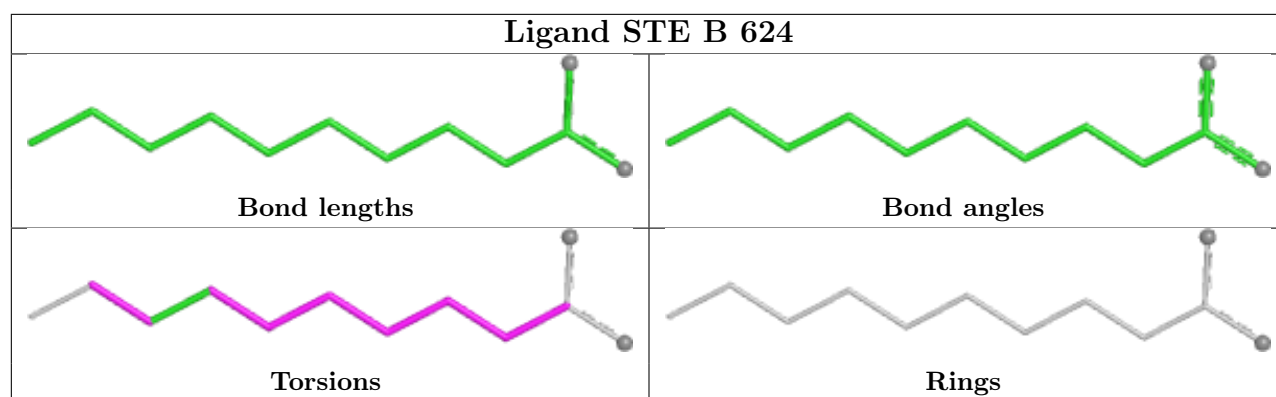
Ligand CLA a 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

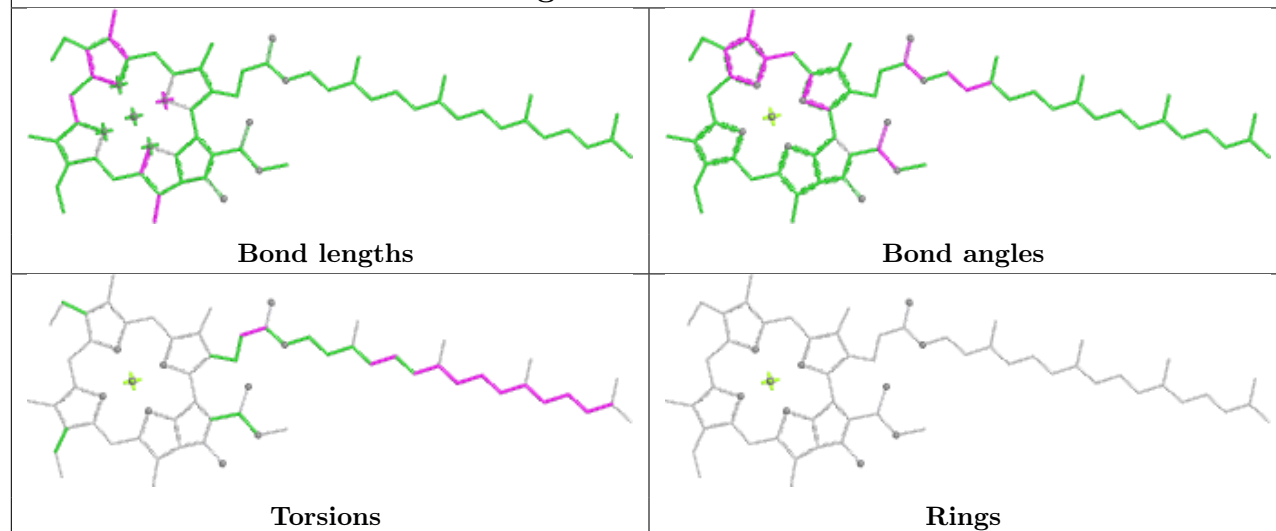
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

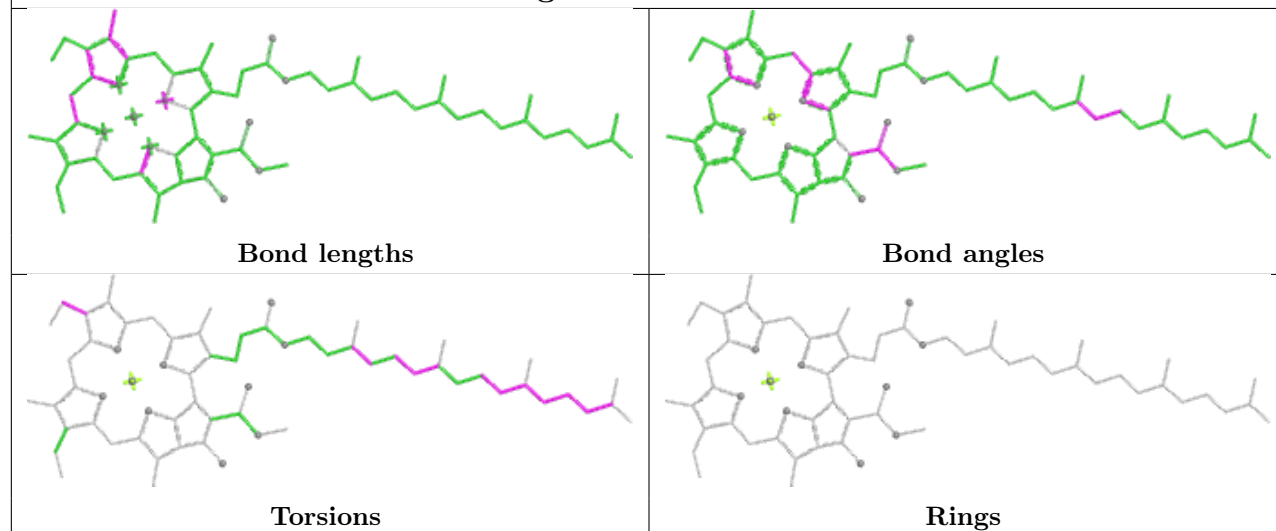




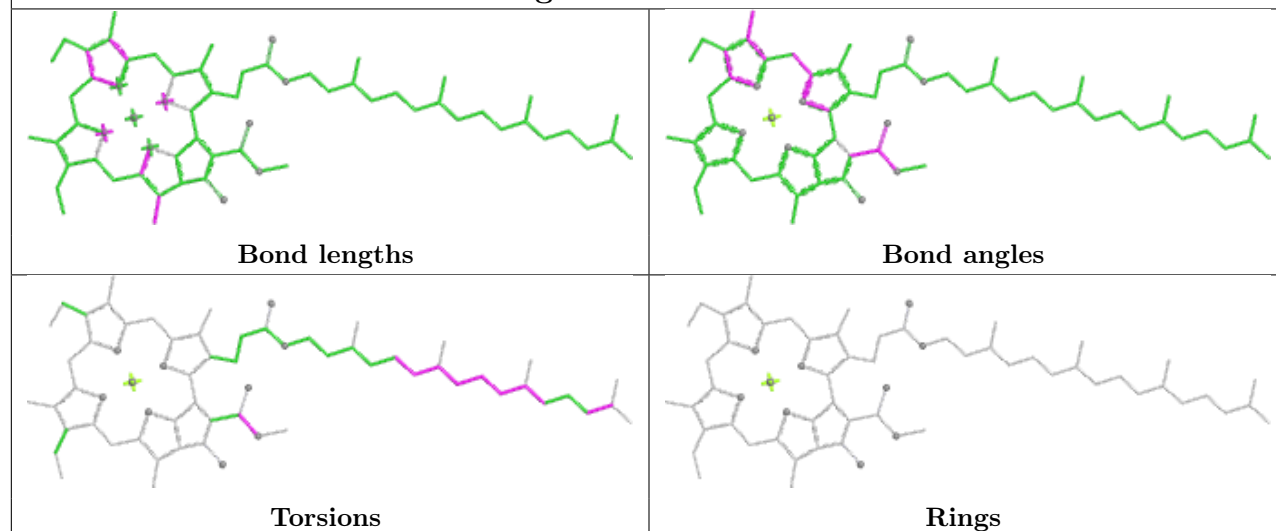
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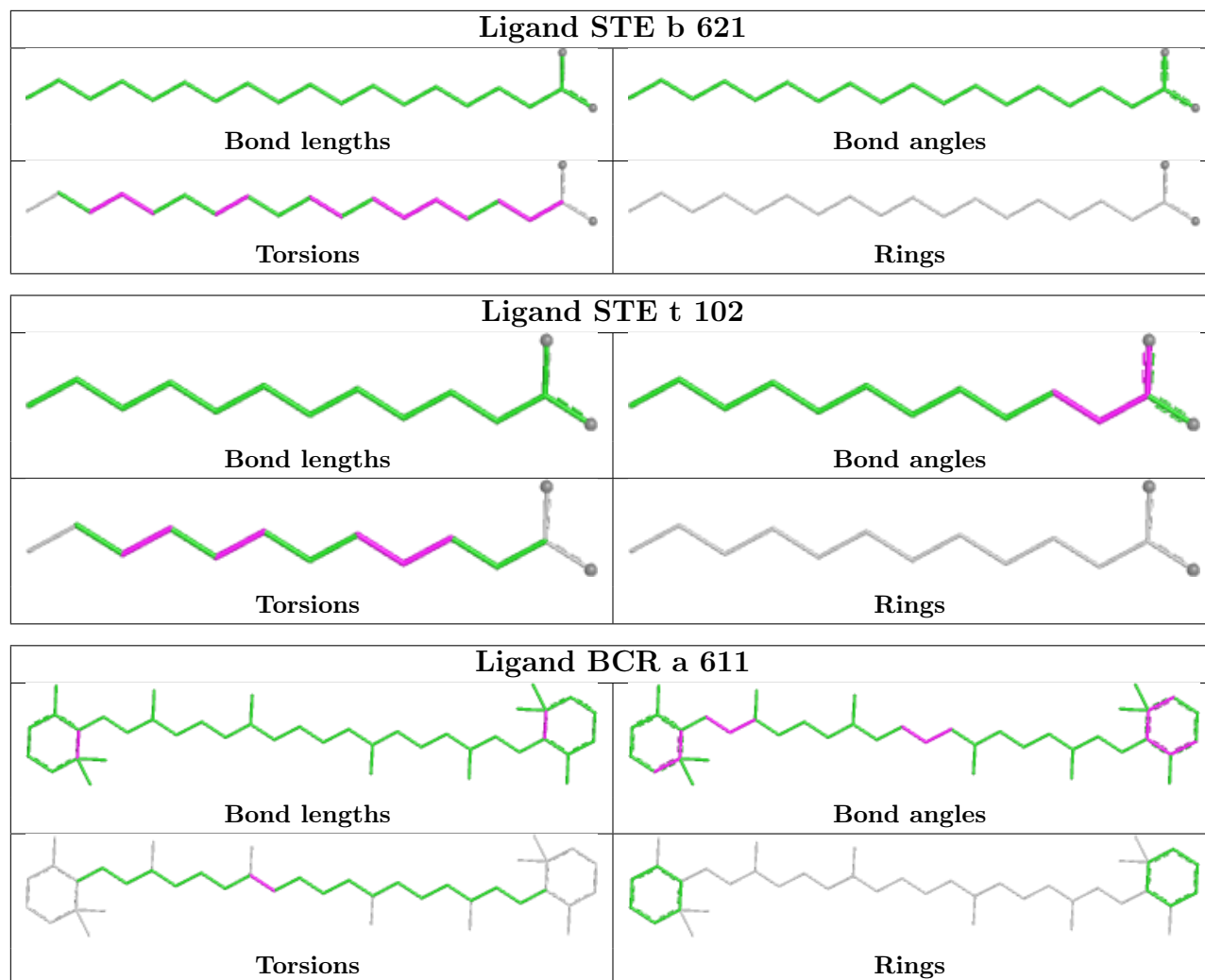


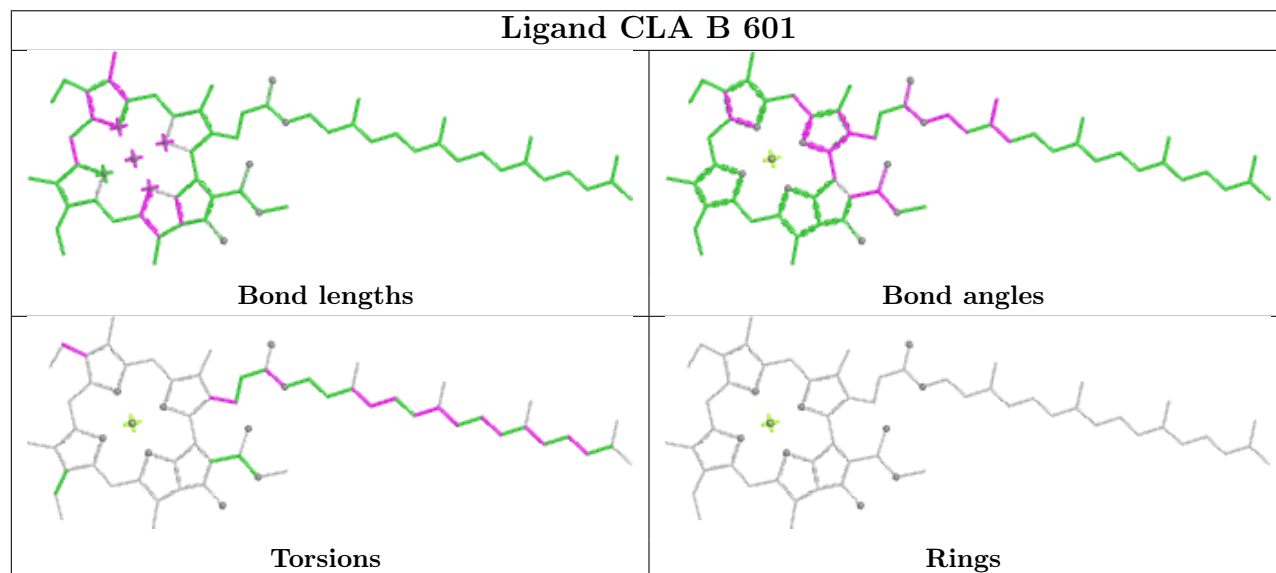
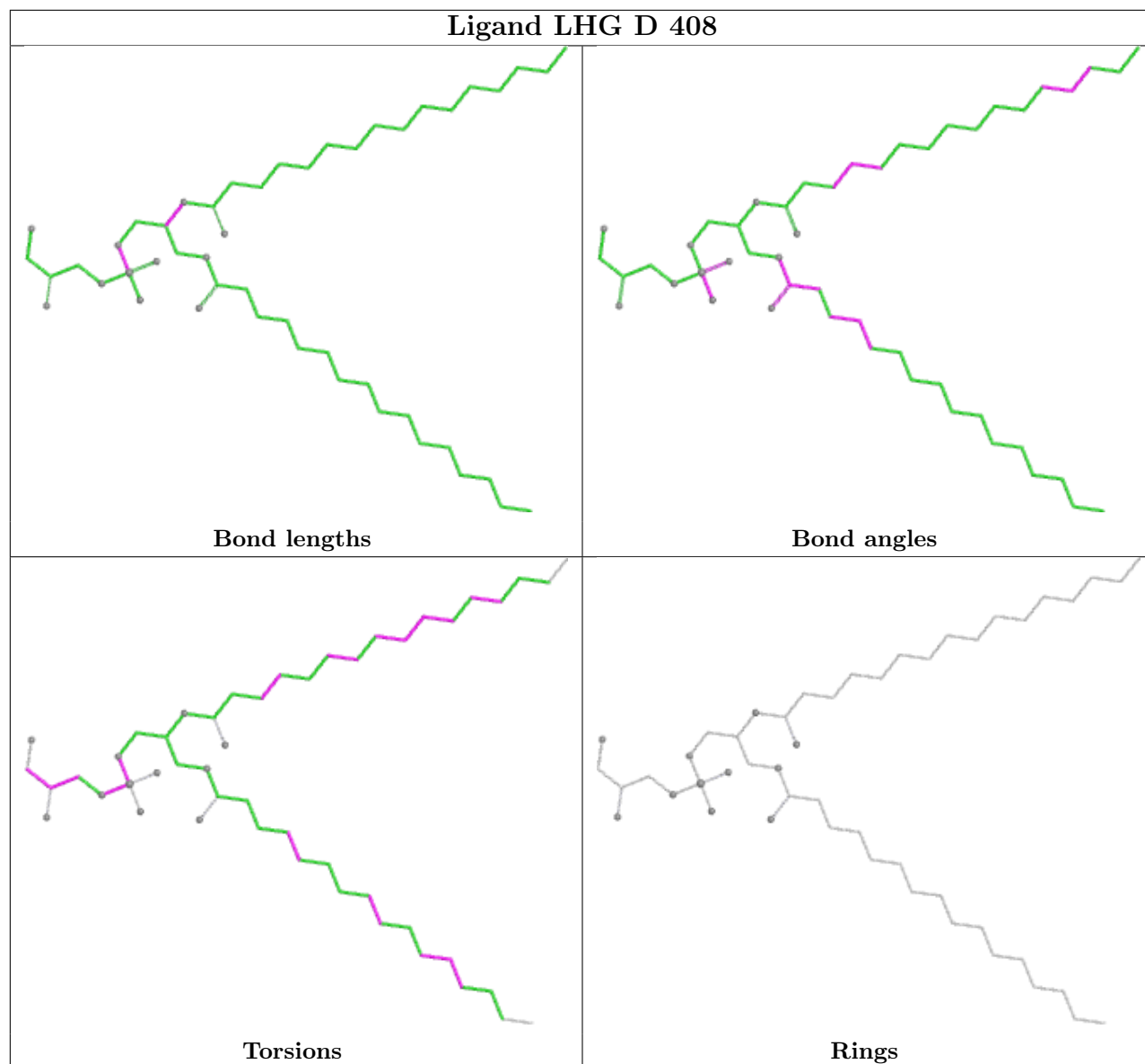
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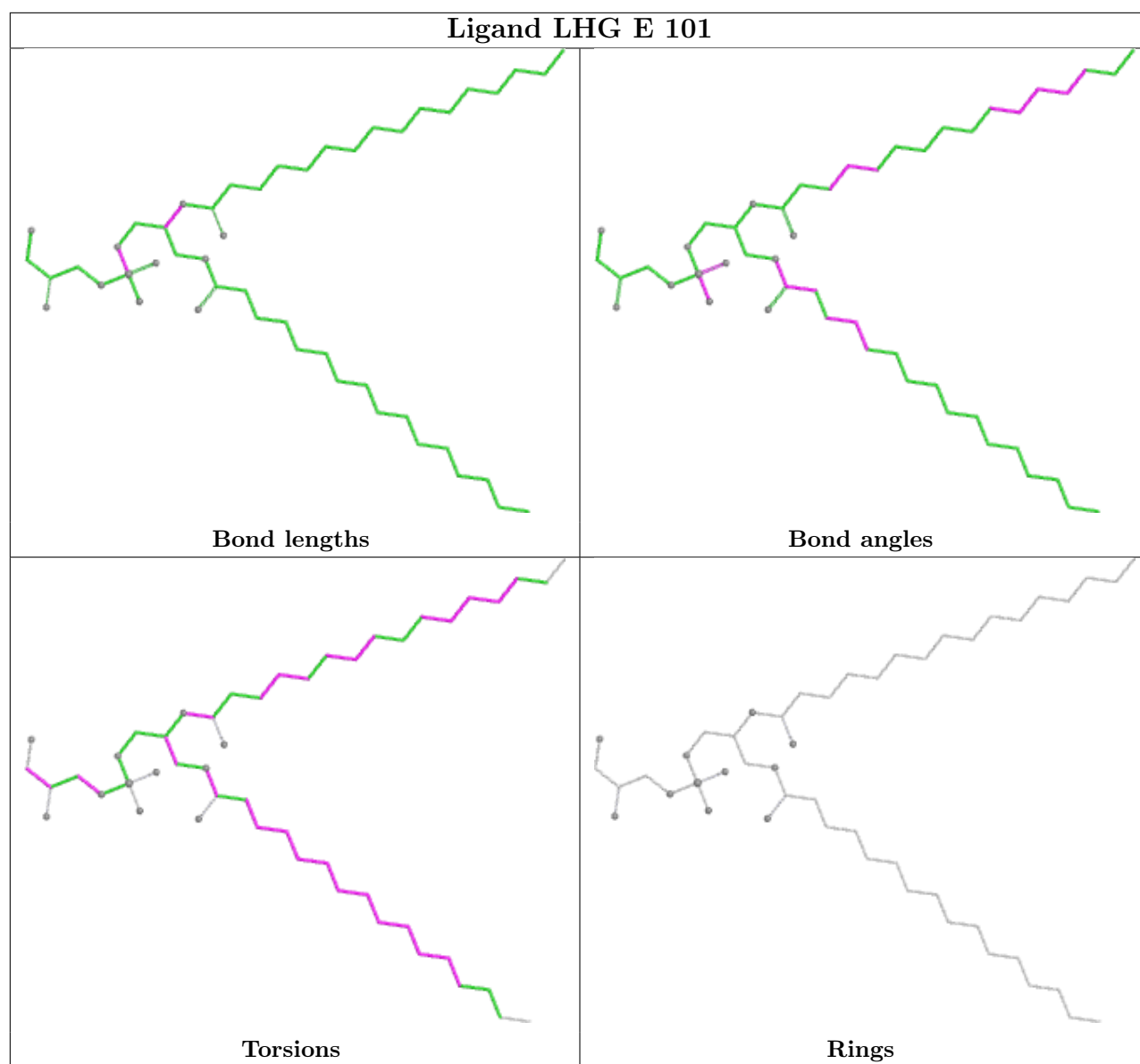


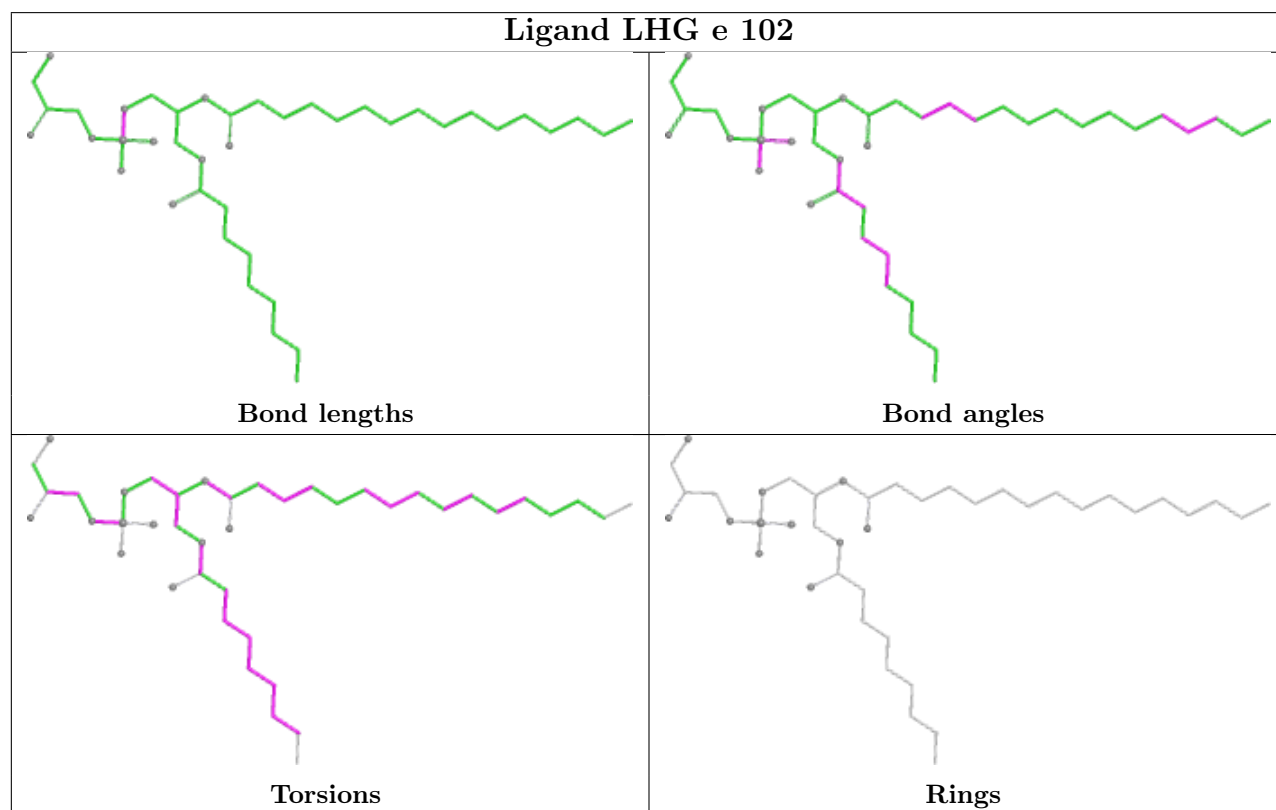
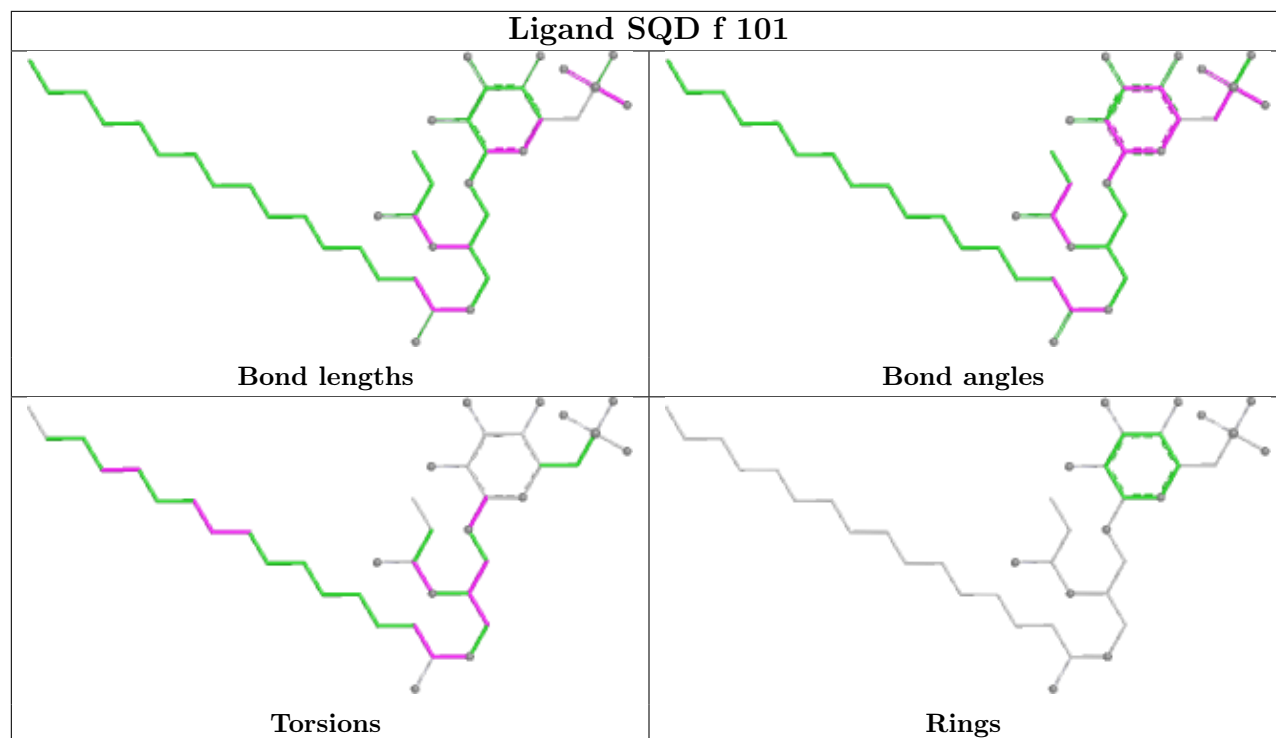
Ligand CLA b 606

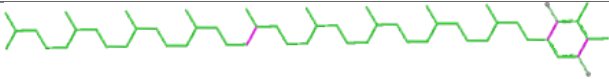
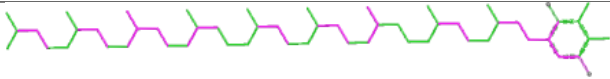
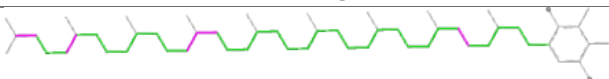
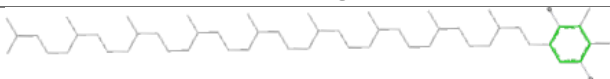


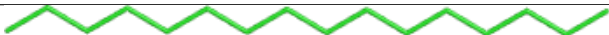
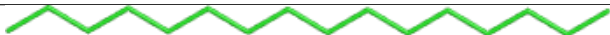


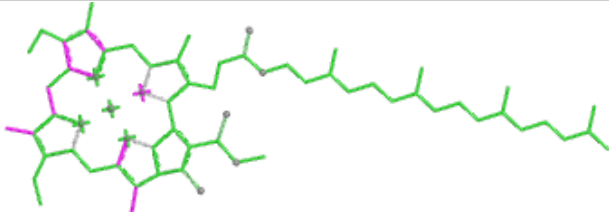
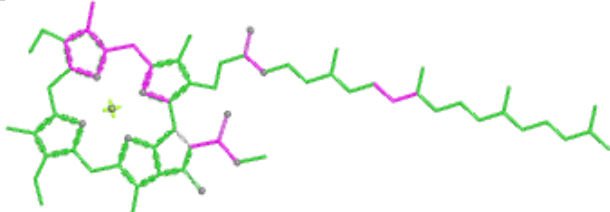
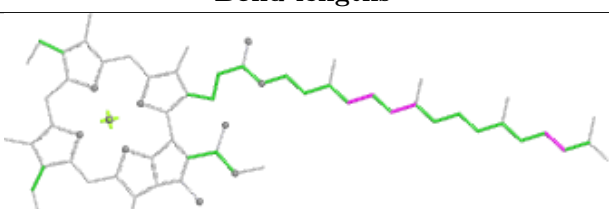
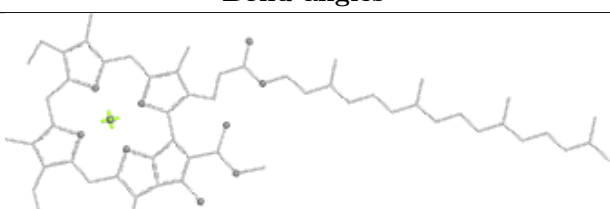


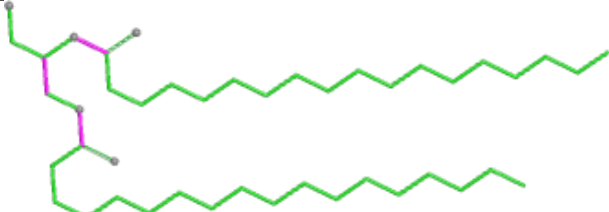
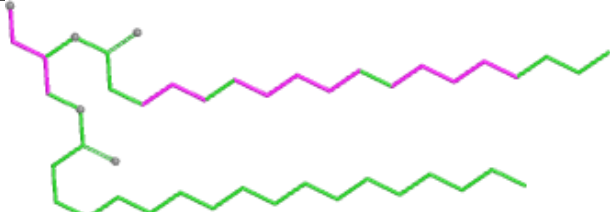
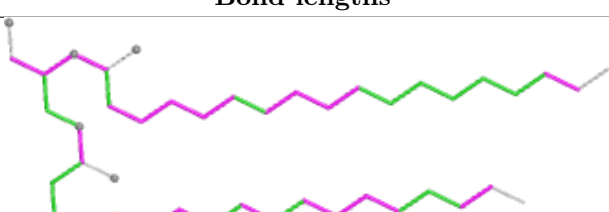
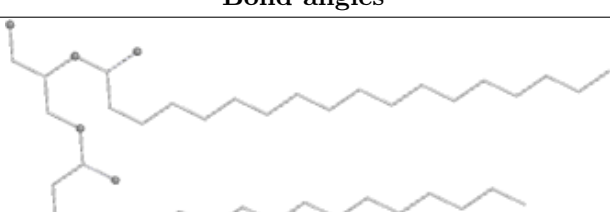


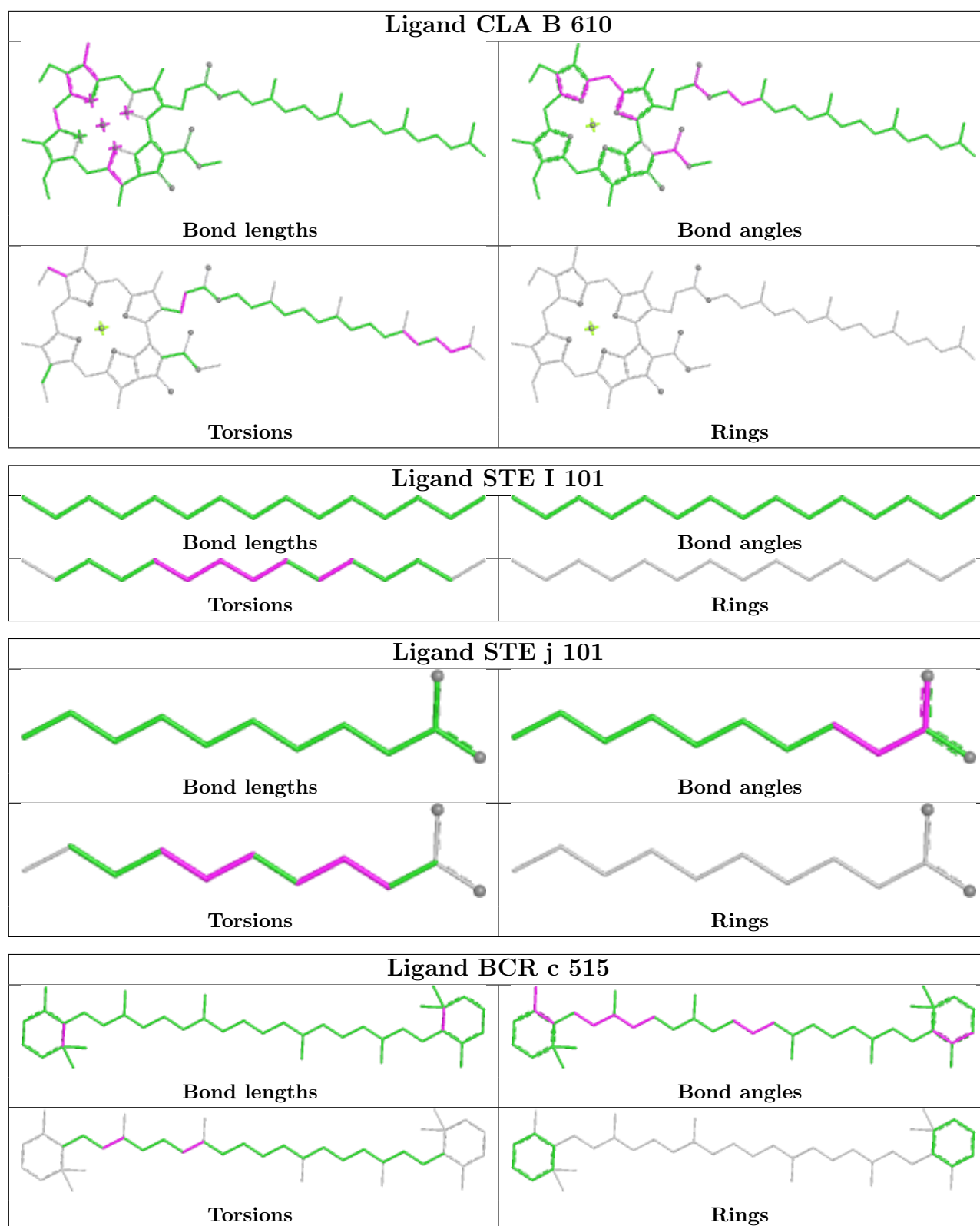


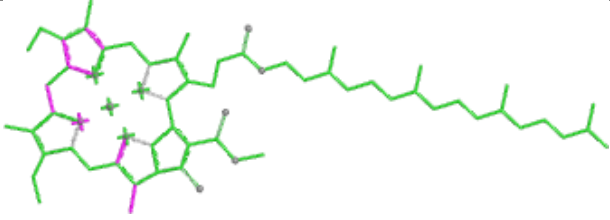
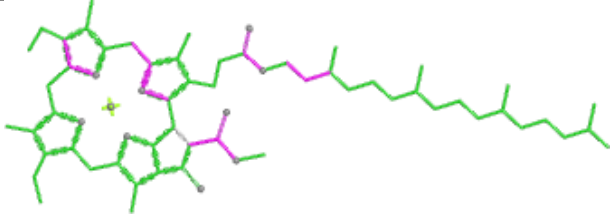
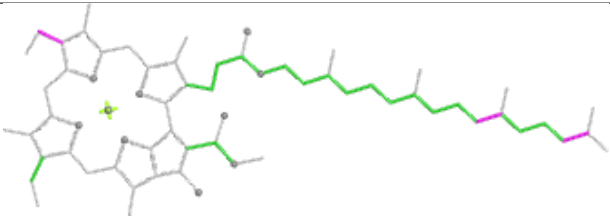
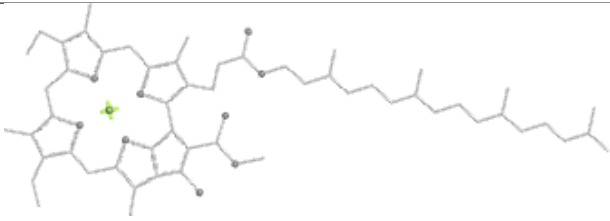
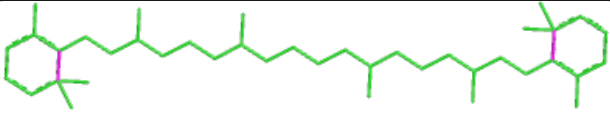
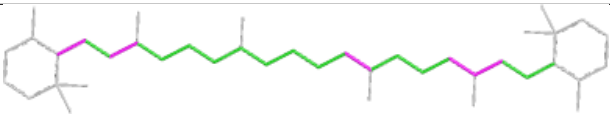
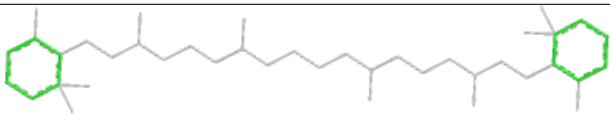
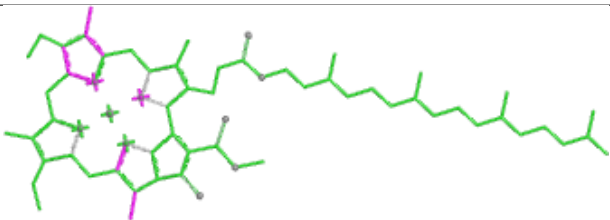
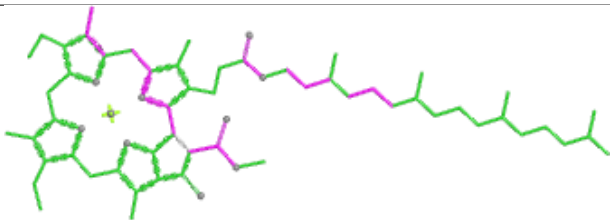
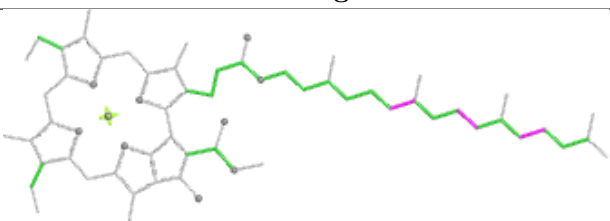
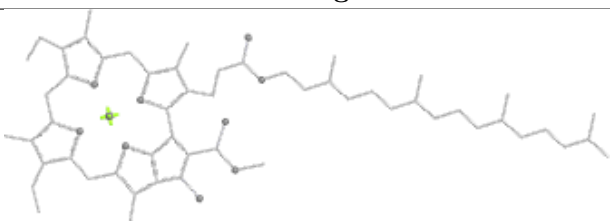
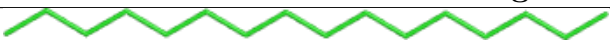
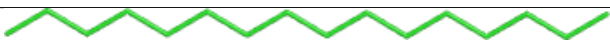
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

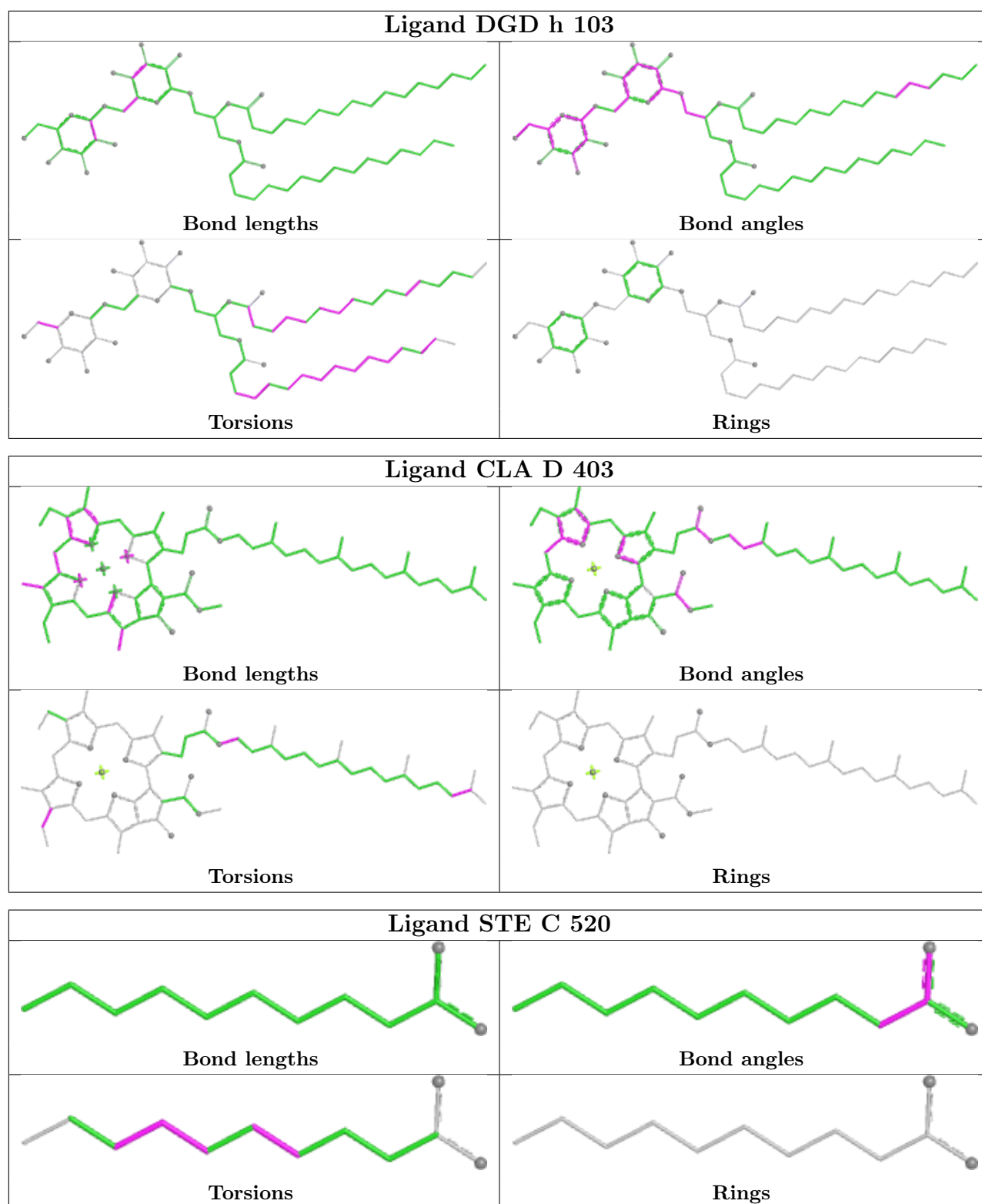
Ligand STE B 626	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

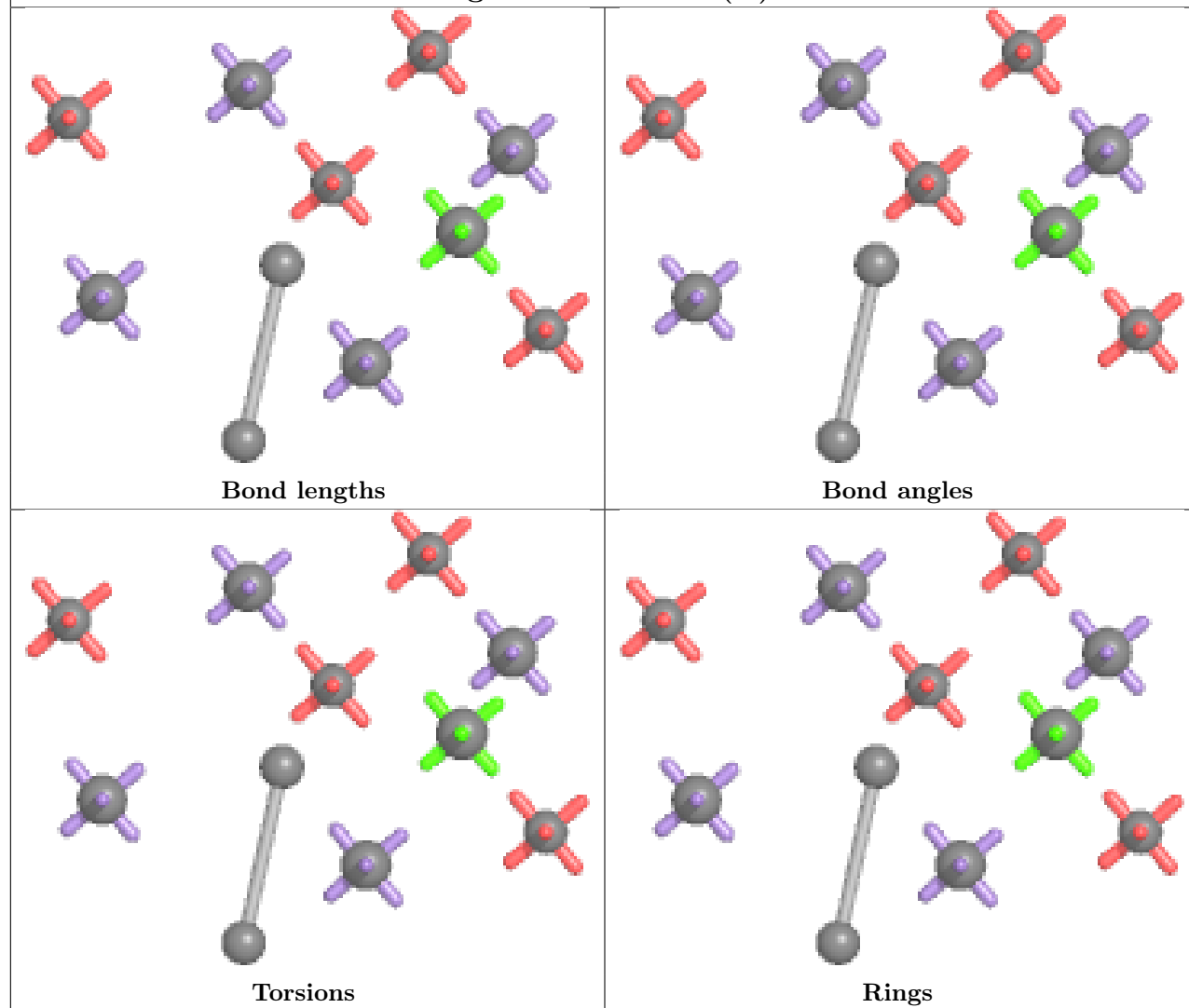
Ligand DGD a 617	
 Bond lengths	 Bond angles
 Torsions	 Rings



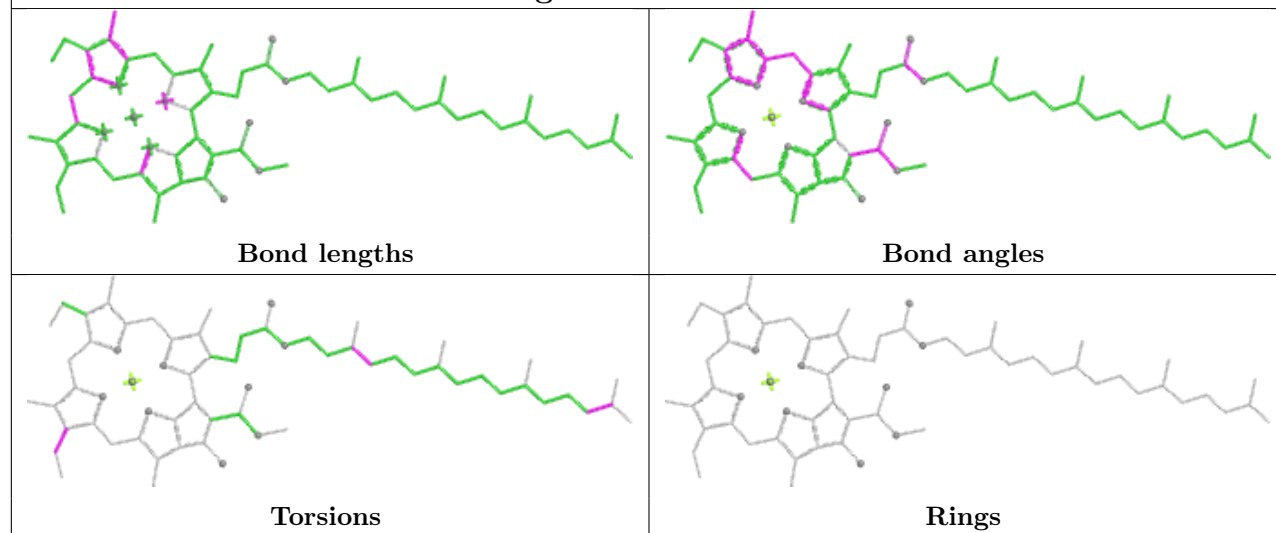
Ligand CLA d 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 612	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

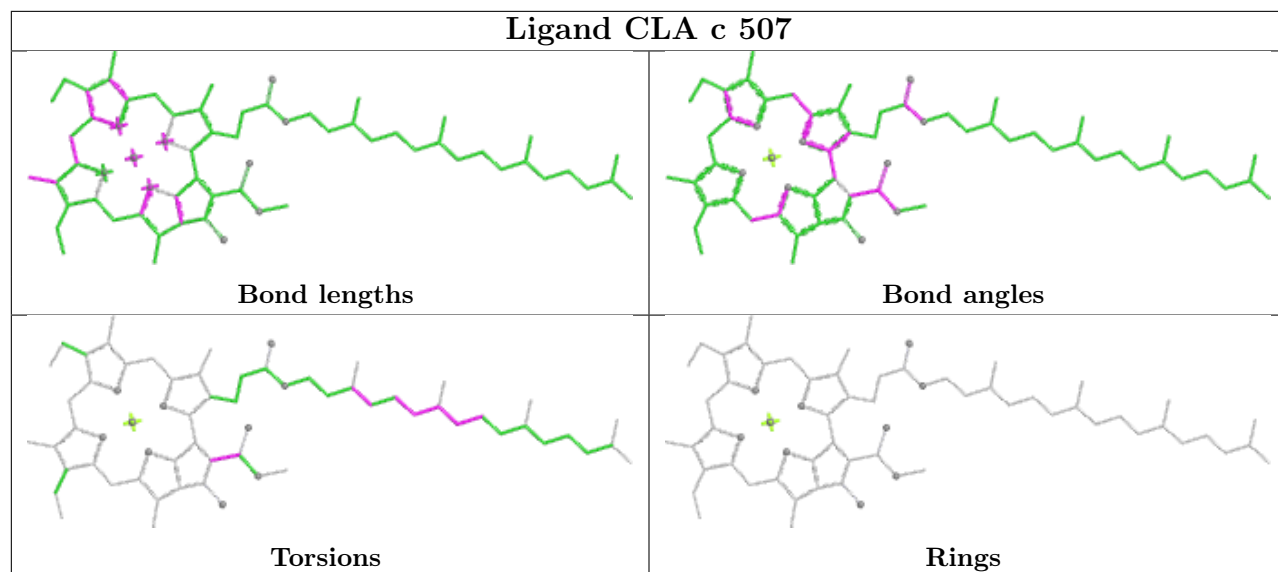
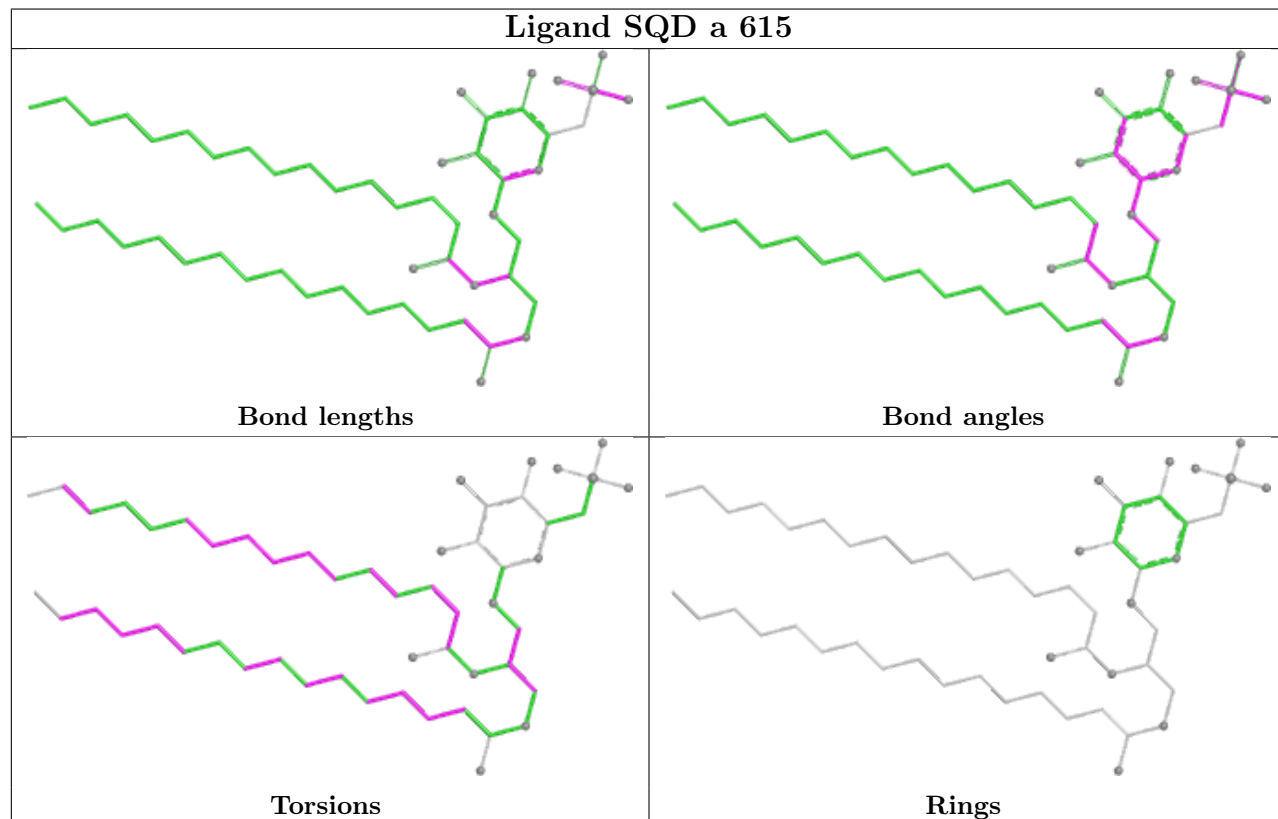


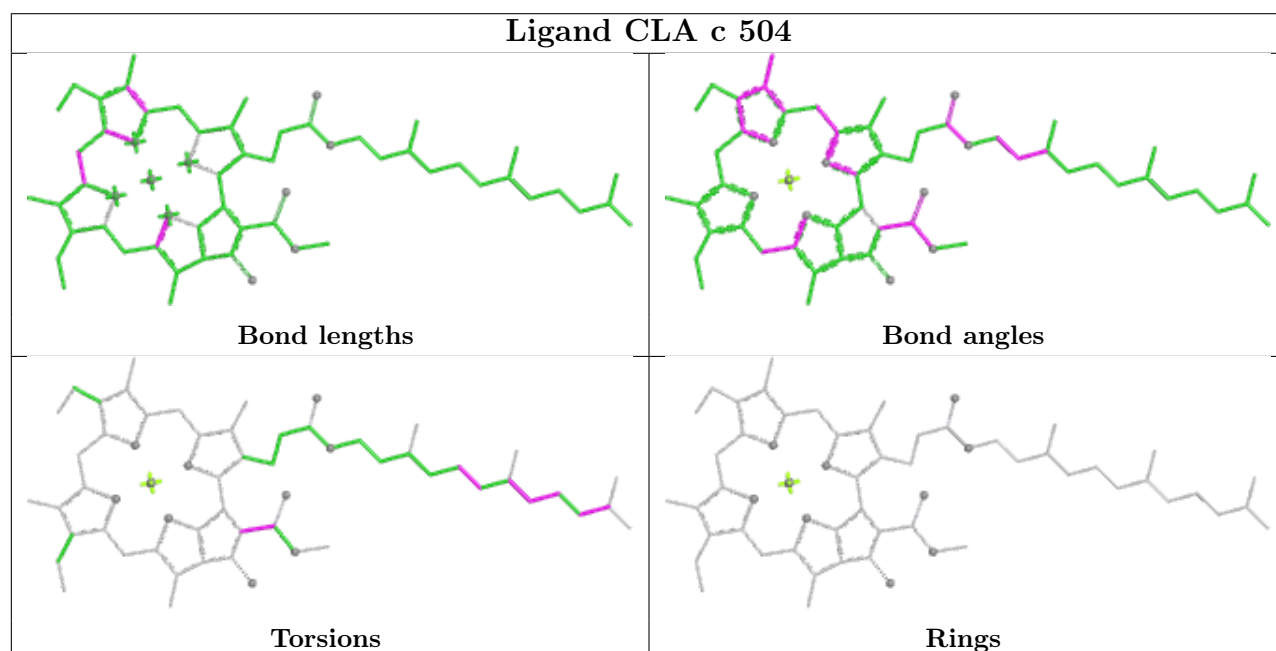
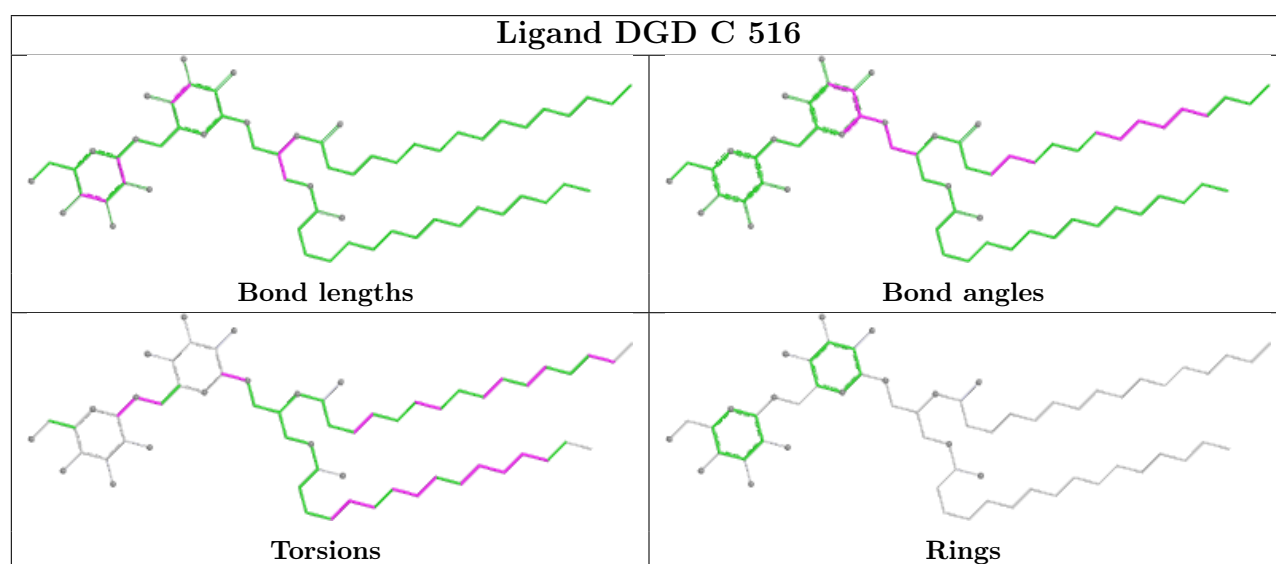
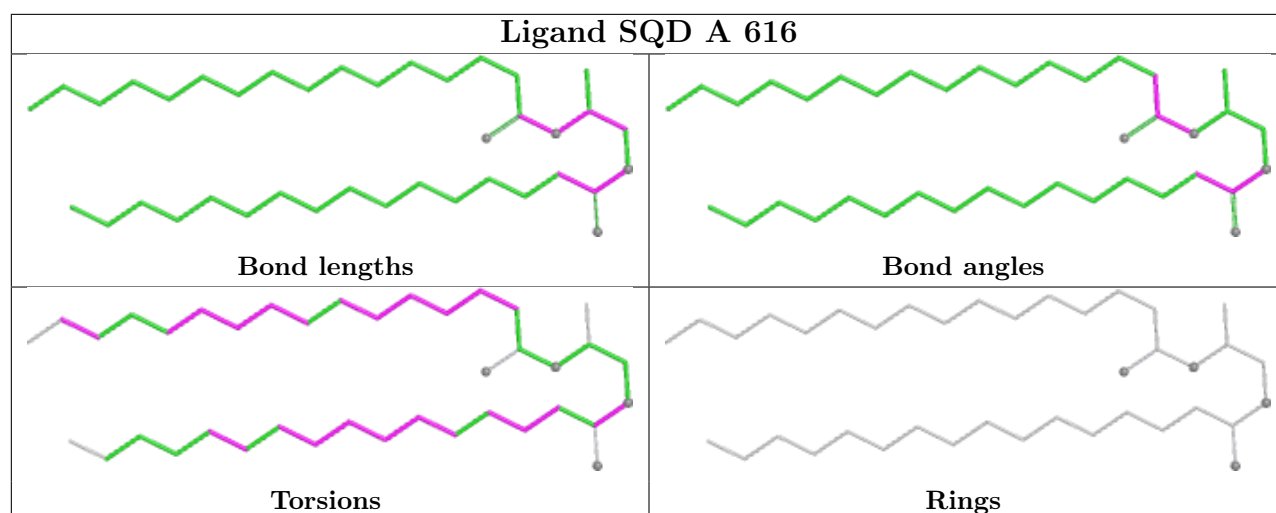
Ligand OEY a 602 (A)

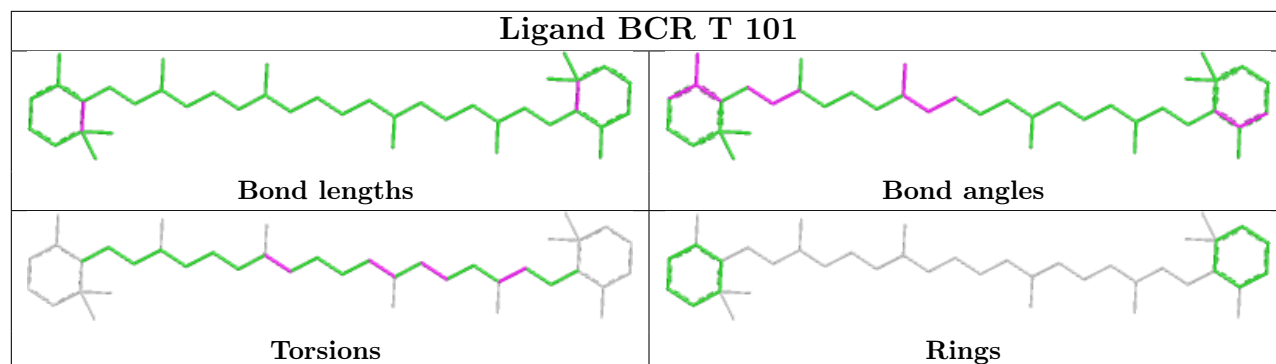
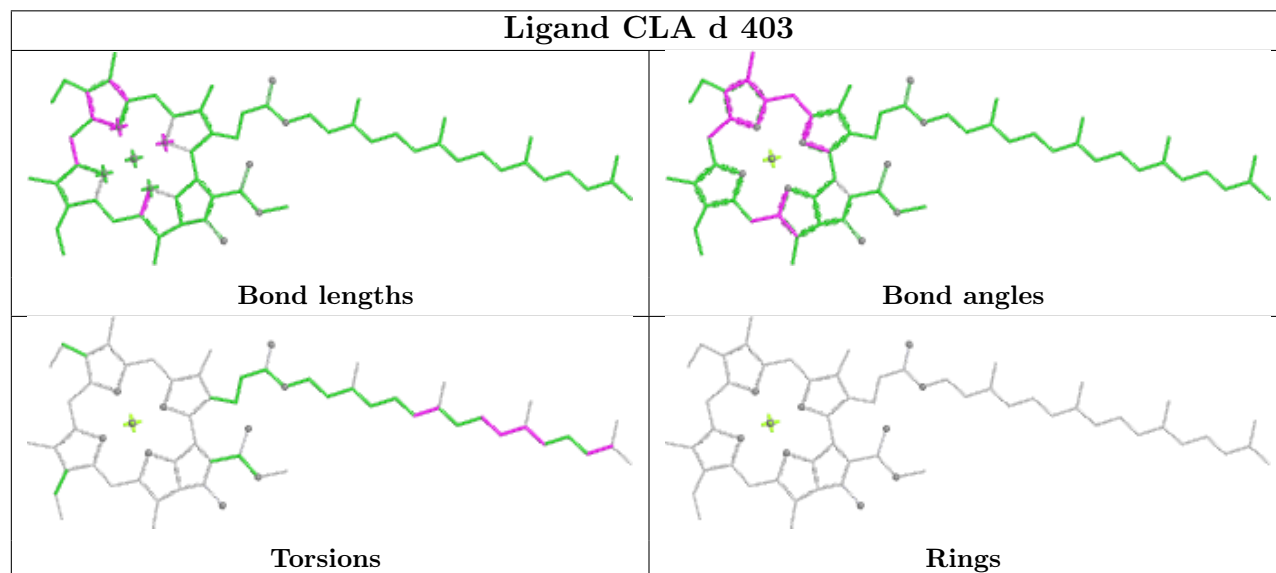
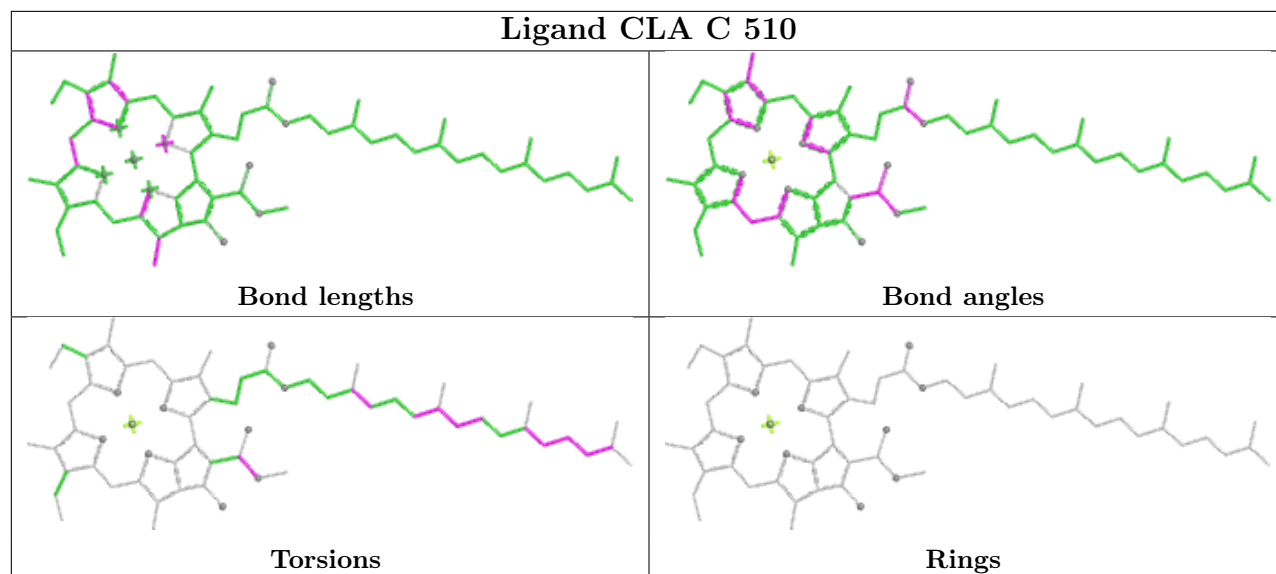


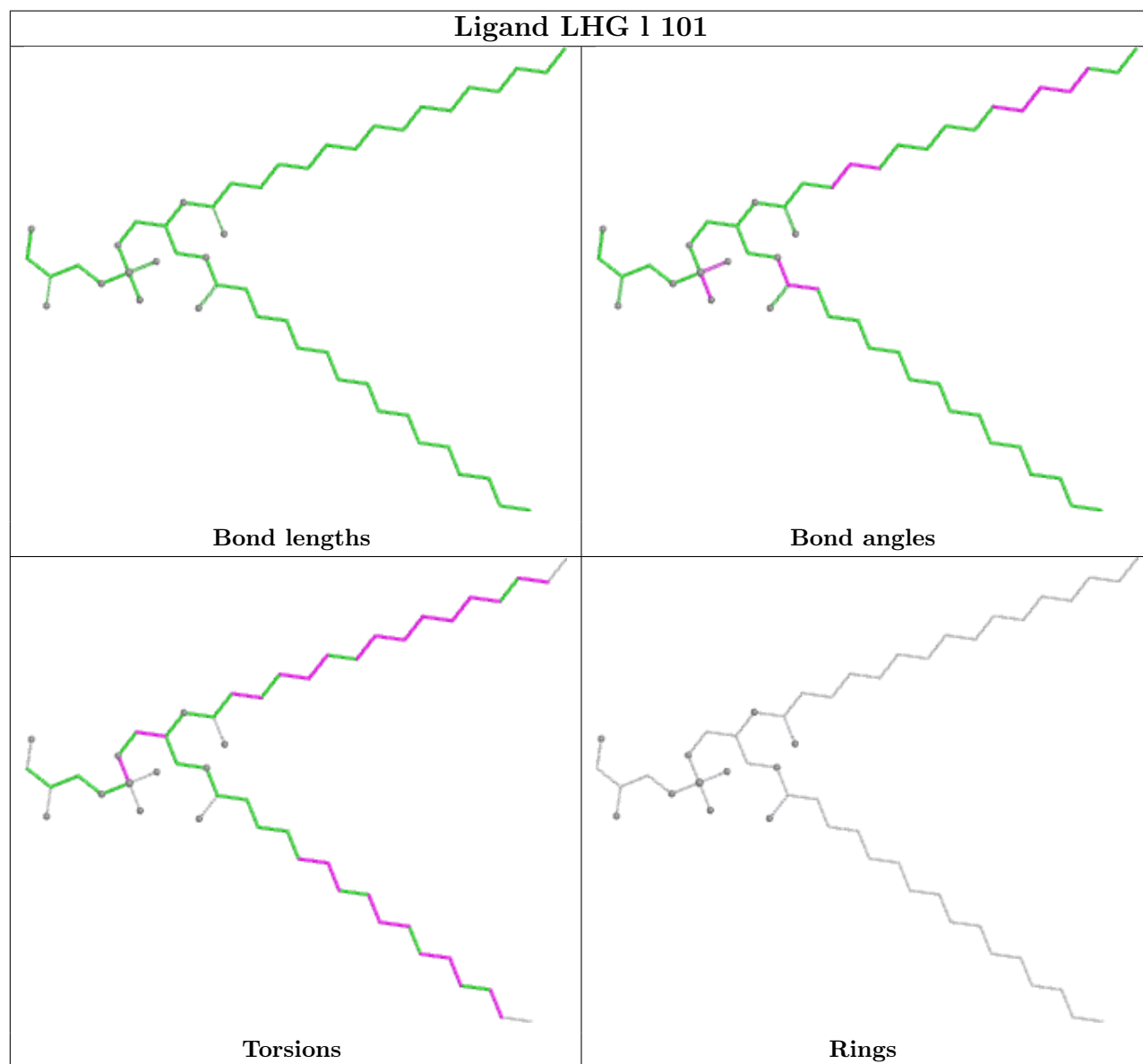
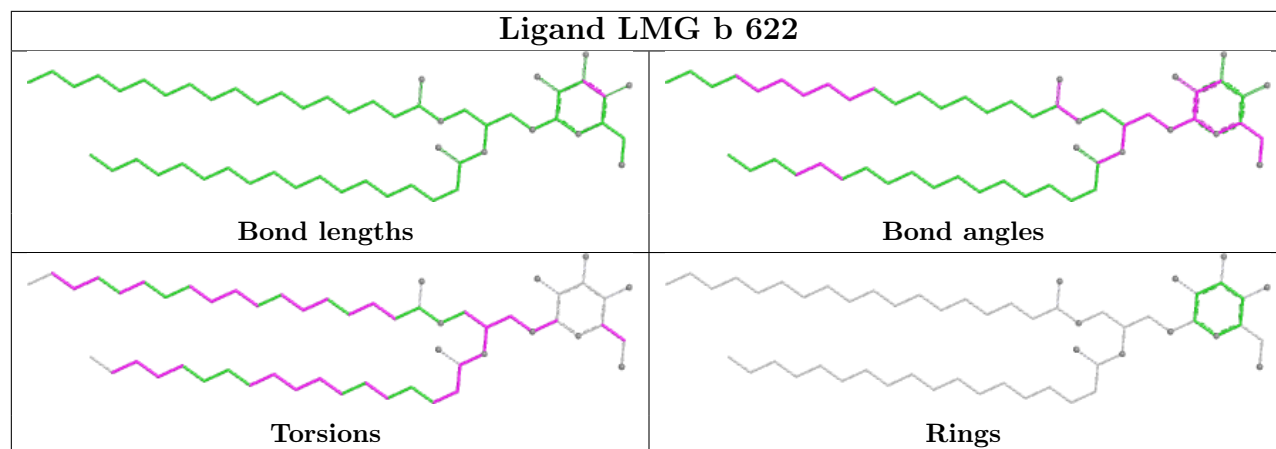
Ligand CLA b 607

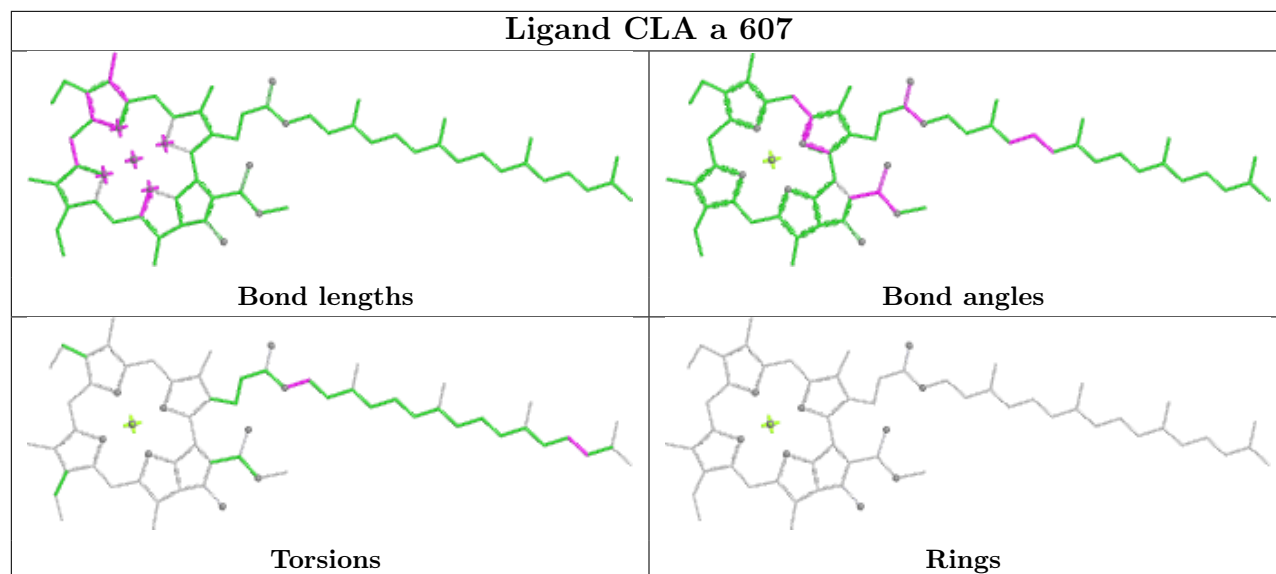
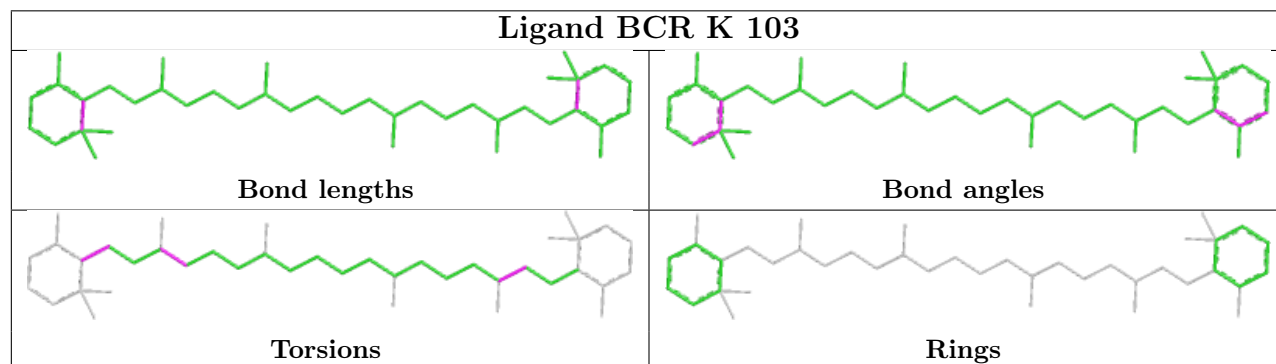
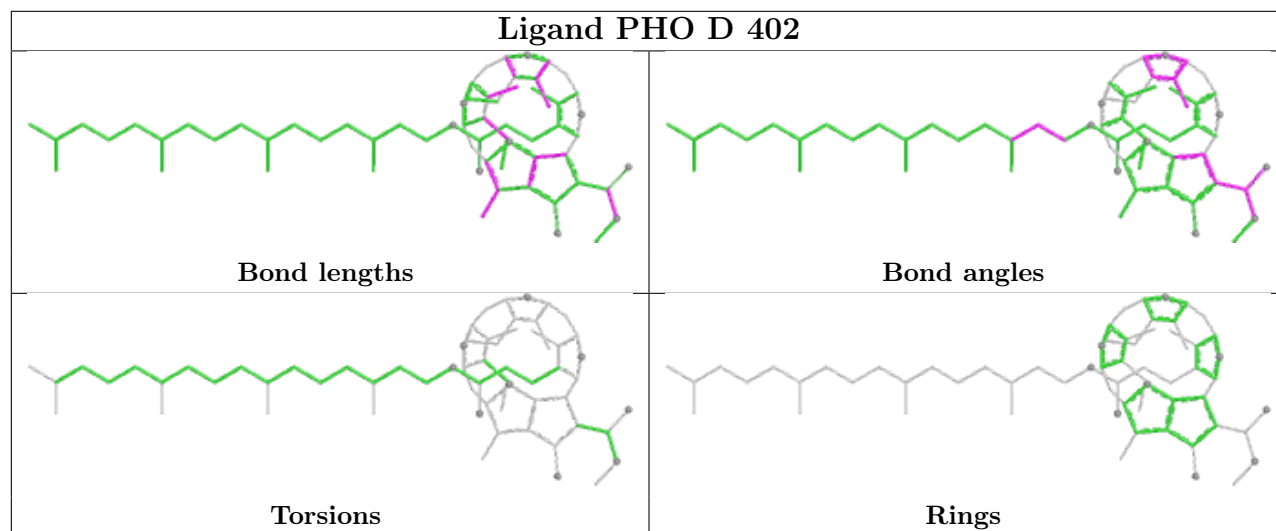


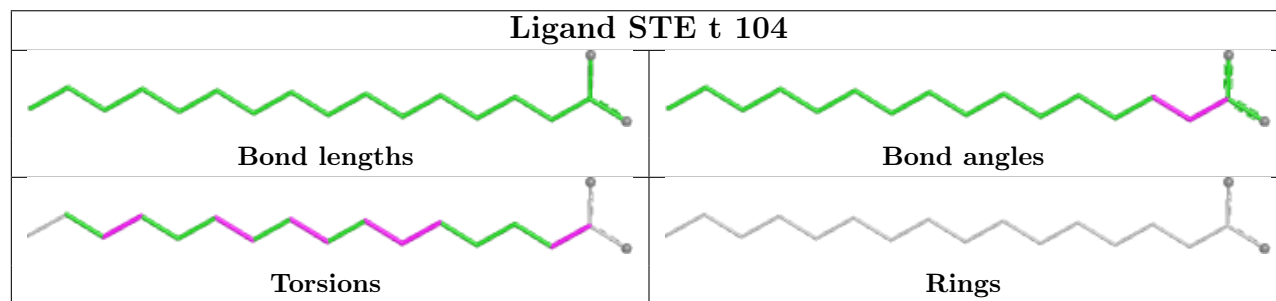
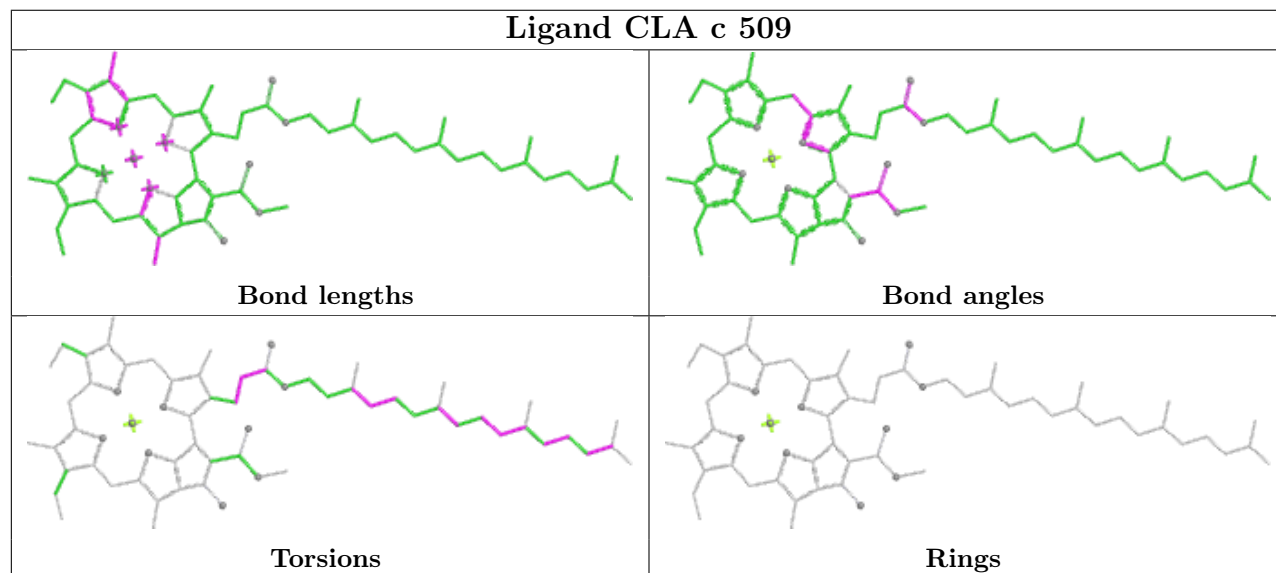
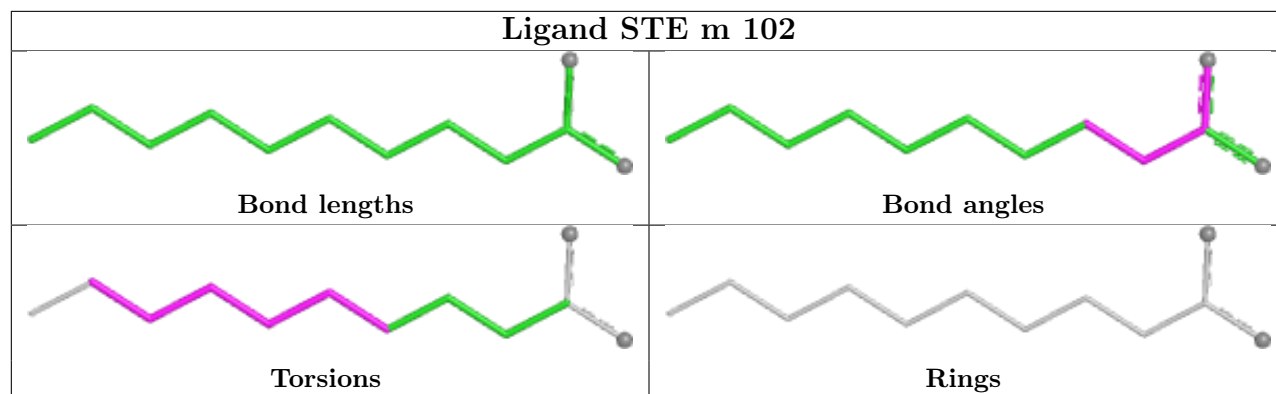
Ligand CLA c 507**Ligand SQD a 615**

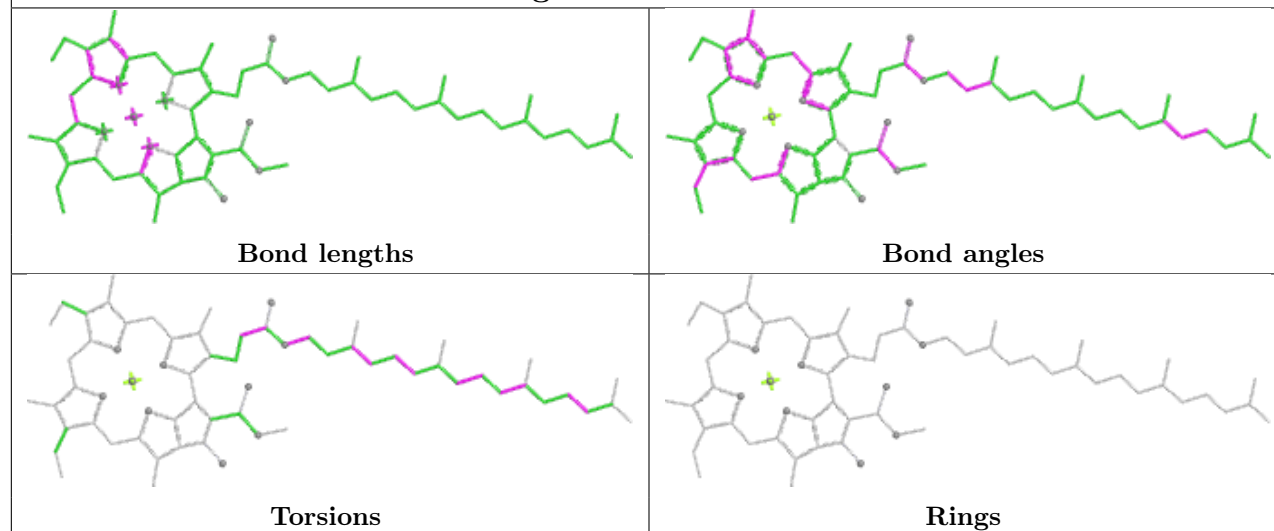
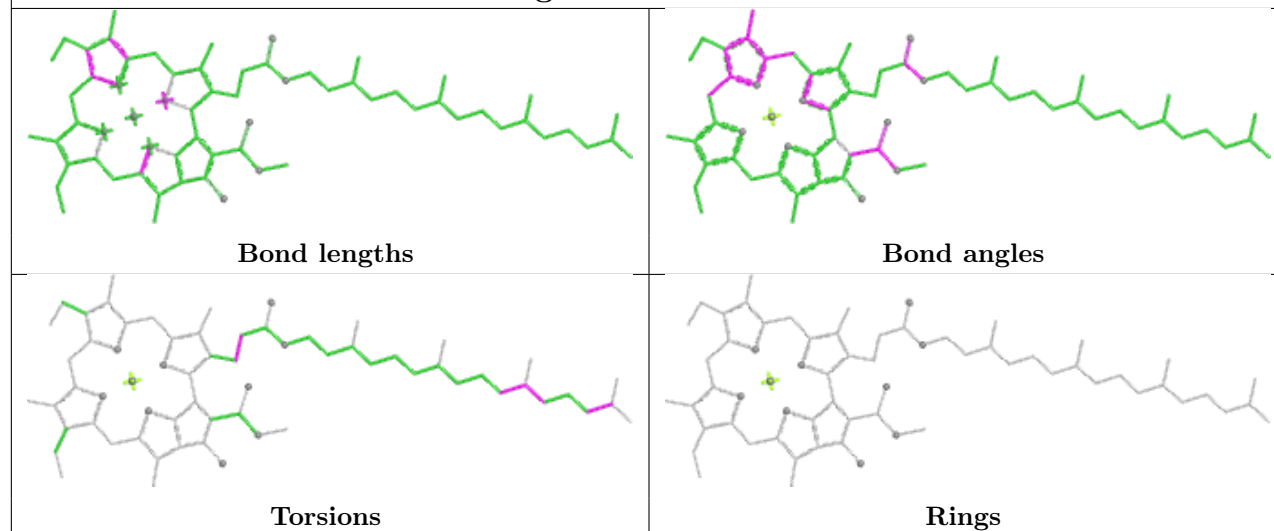
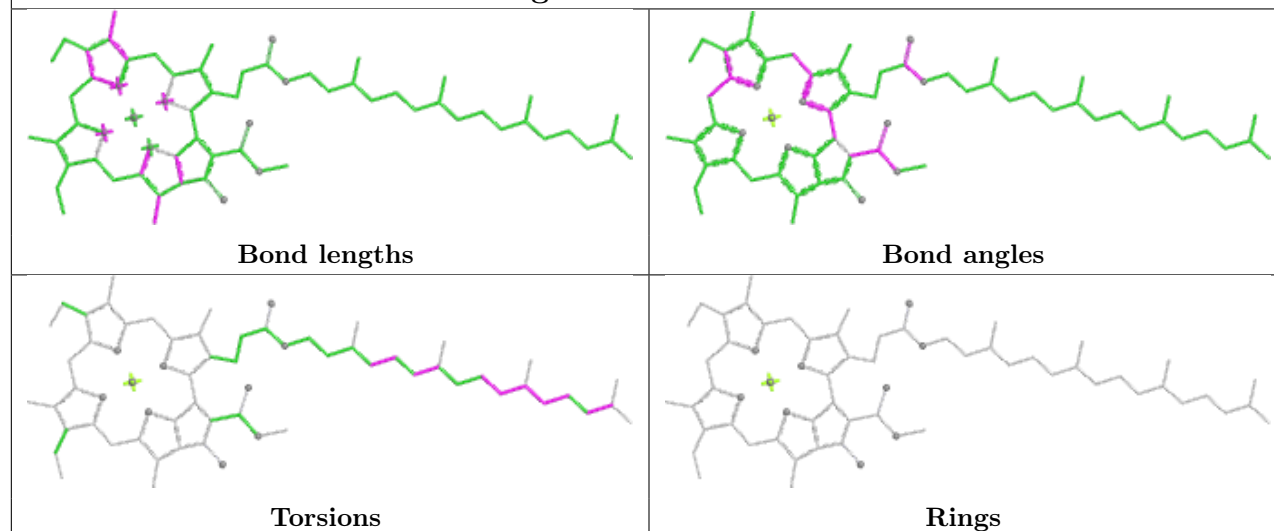


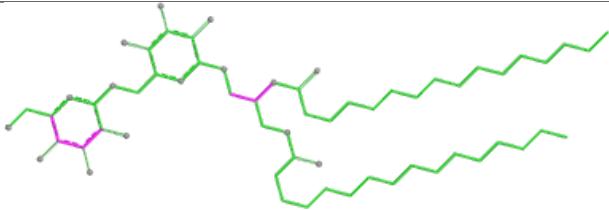
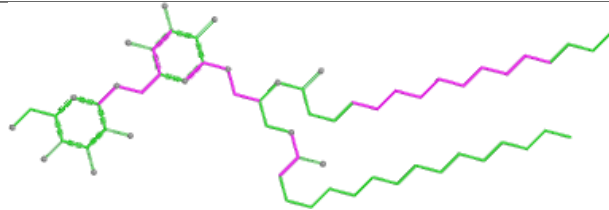
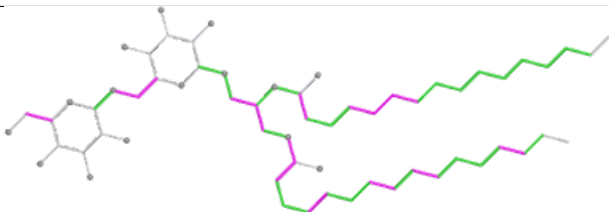
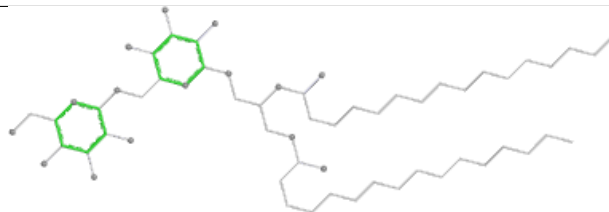


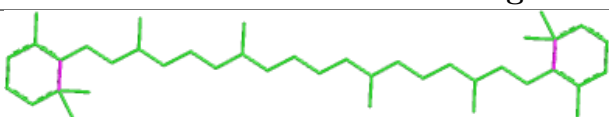
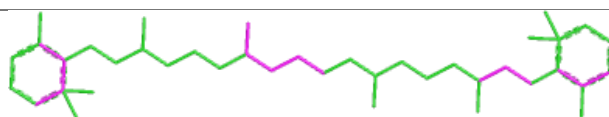
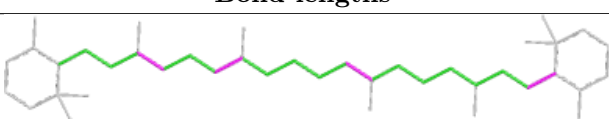
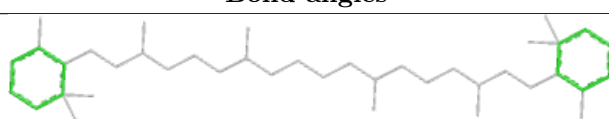


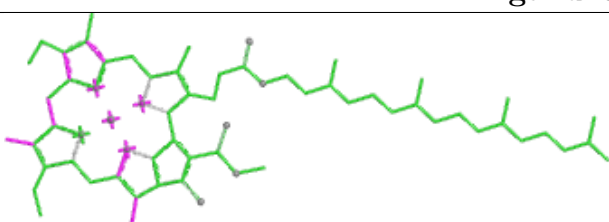
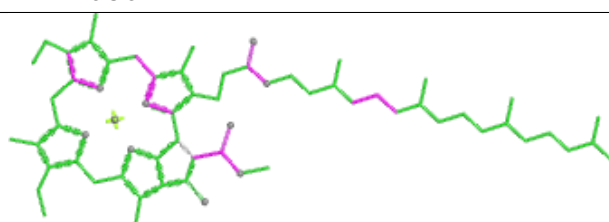
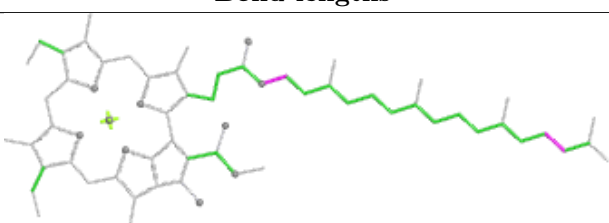
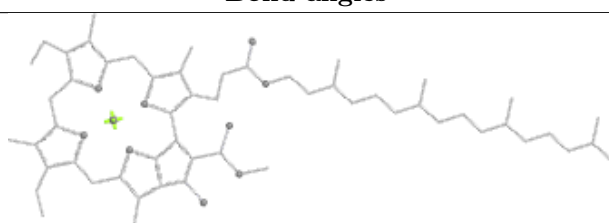
Ligand CLA a 607**Ligand BCR K 103****Ligand PHO D 402**



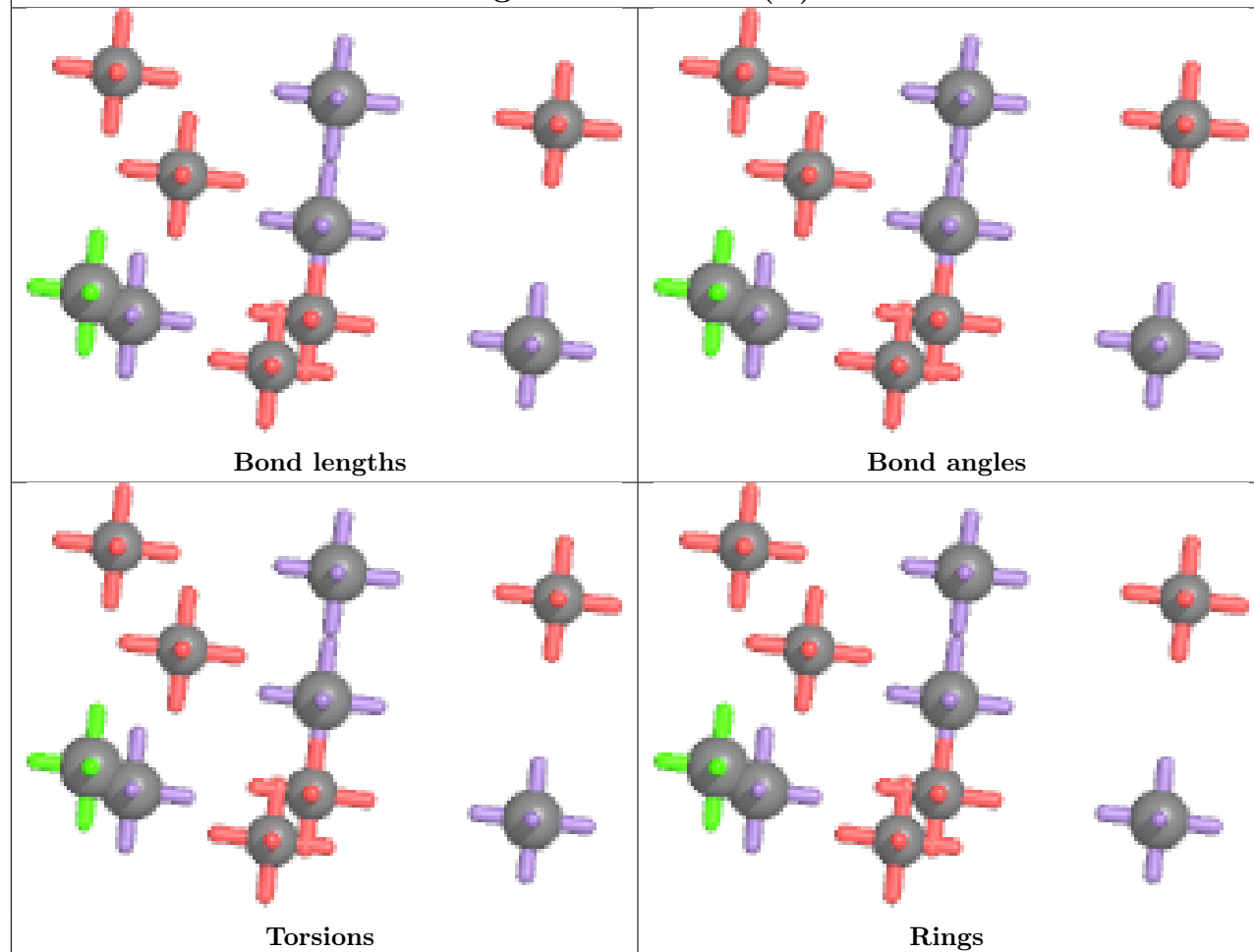
Ligand CLA B 613**Ligand CLA b 605****Ligand CLA D 404**

Ligand DGD C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

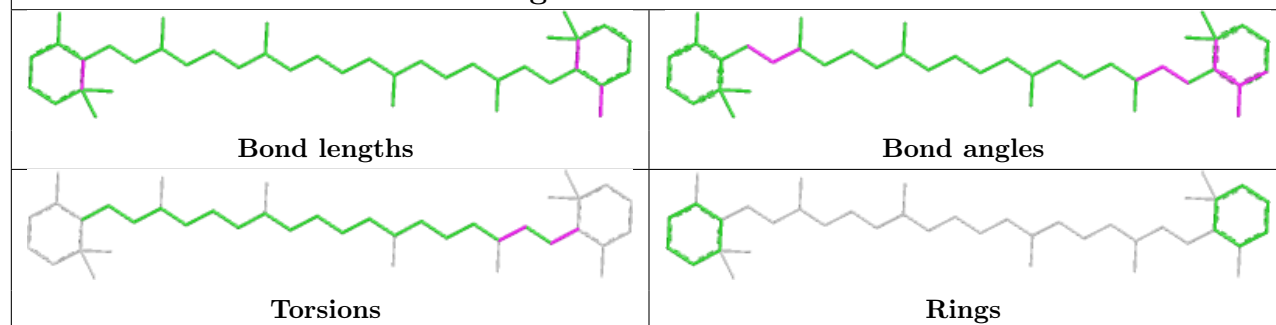
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

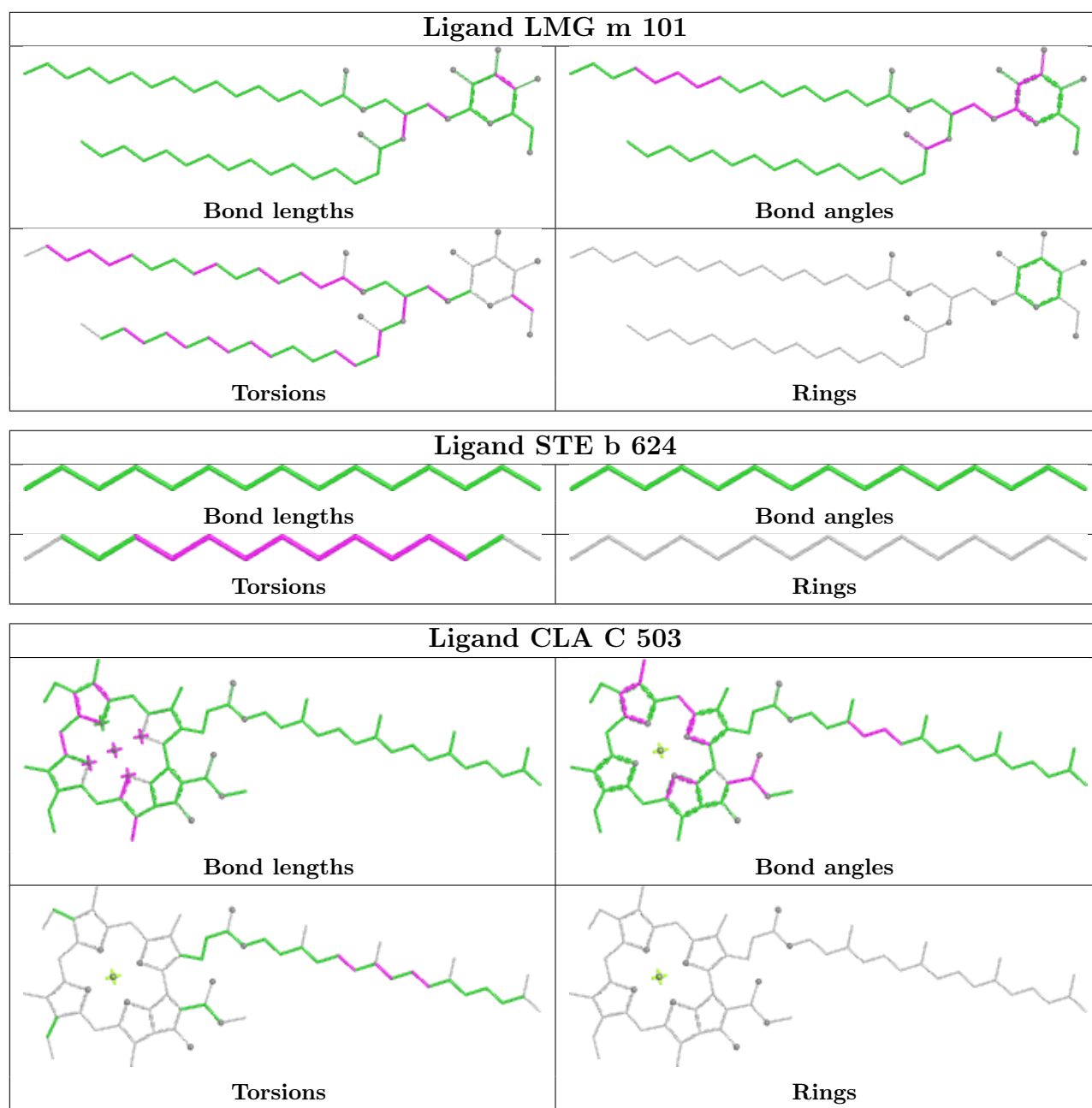
Ligand CLA A 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

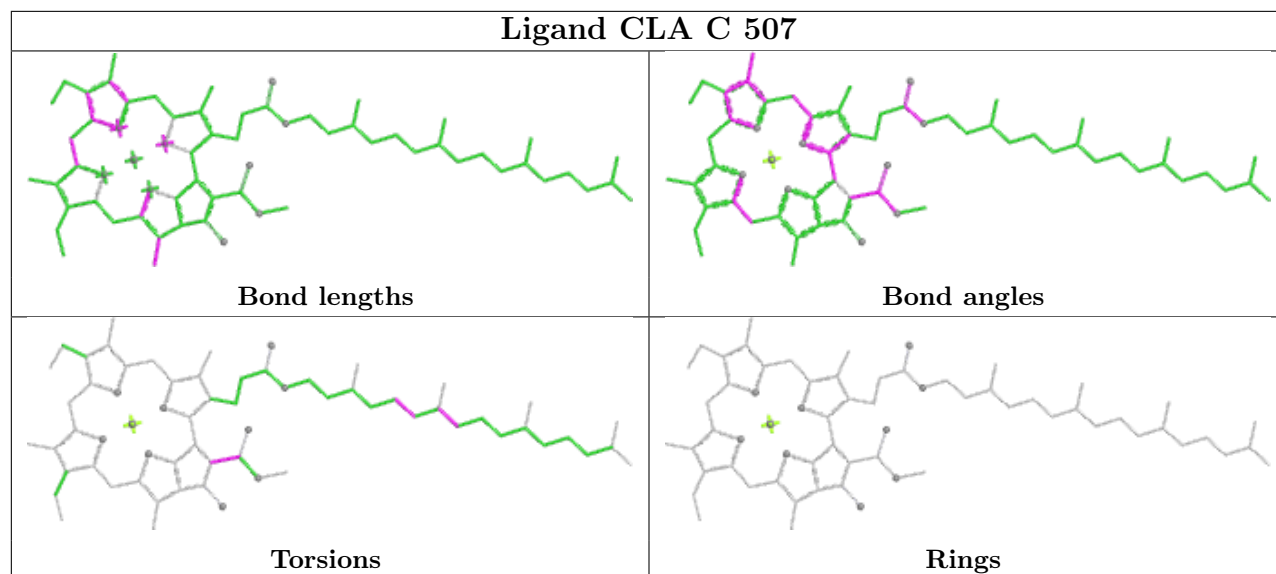
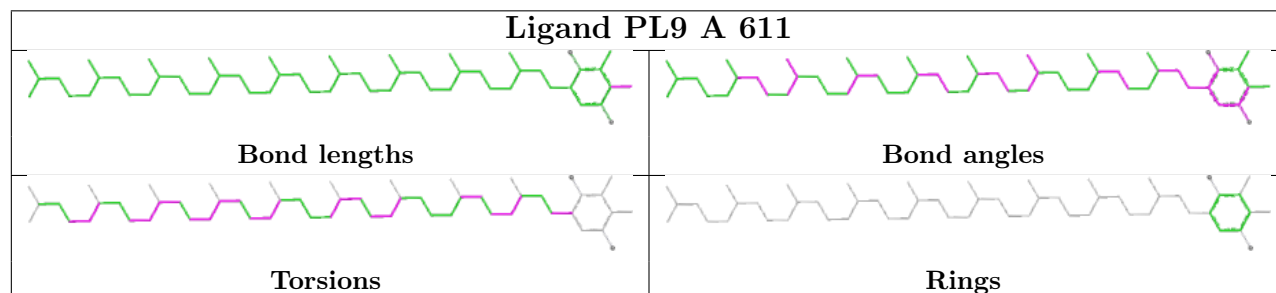
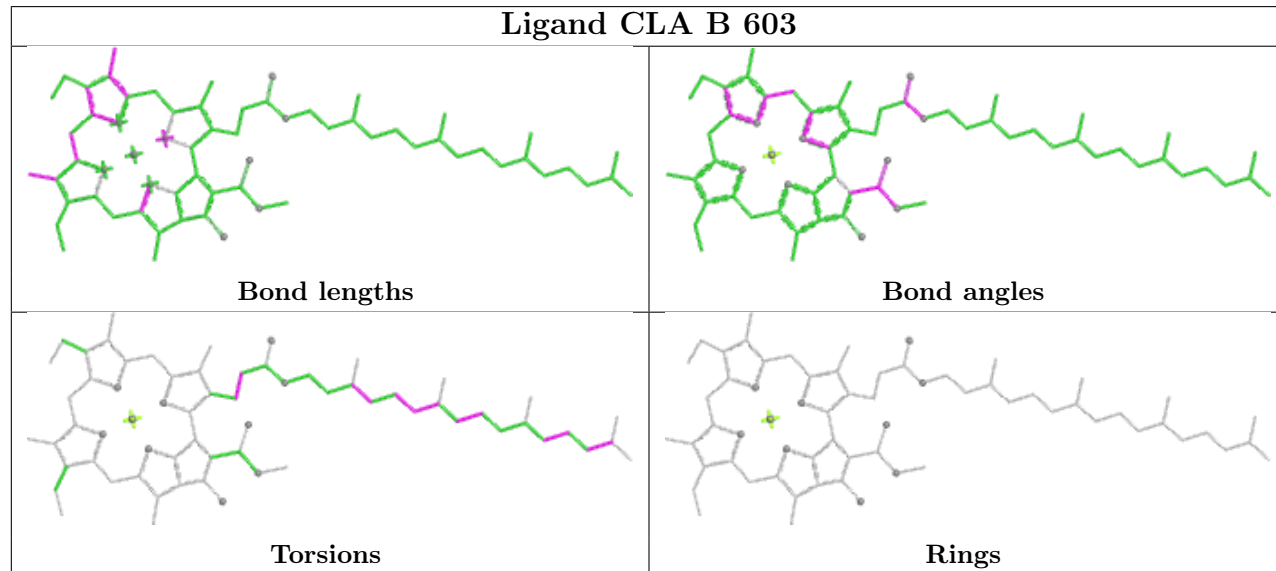
Ligand OEX a 601 (B)

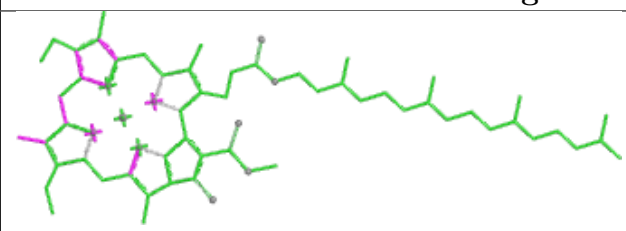
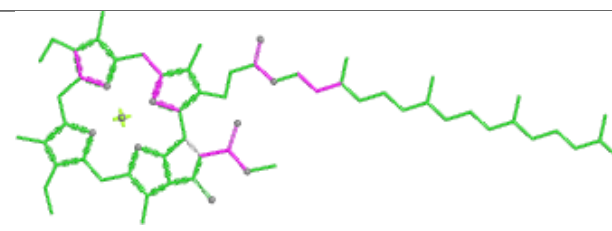
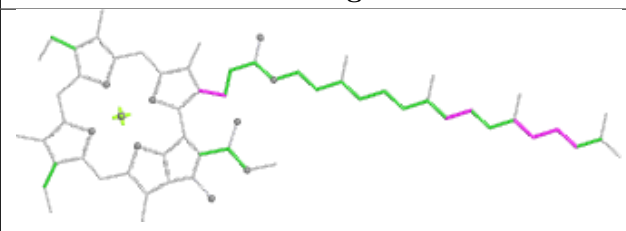
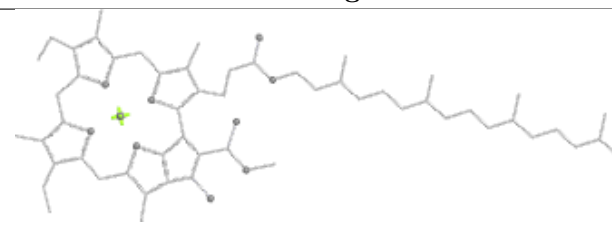


Ligand BCR D 405

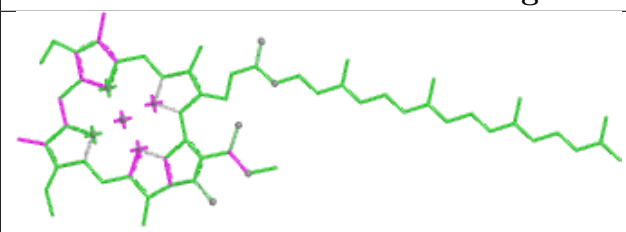
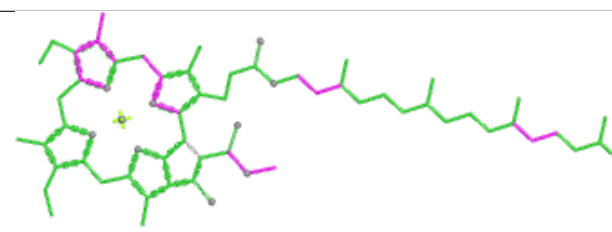
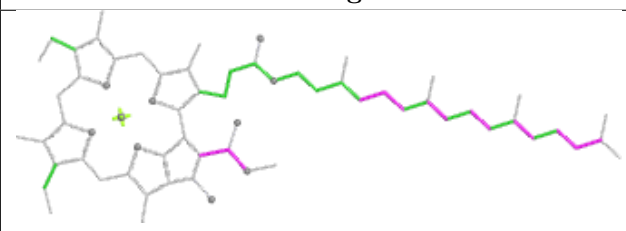
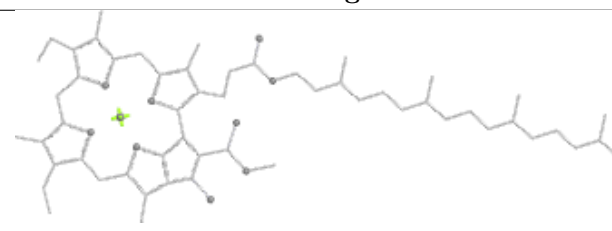


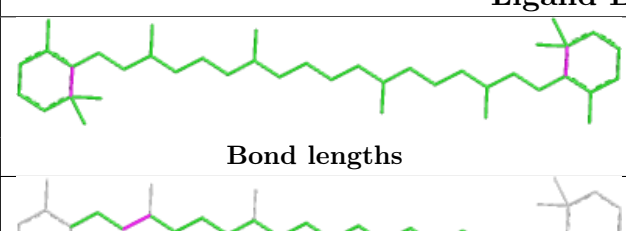
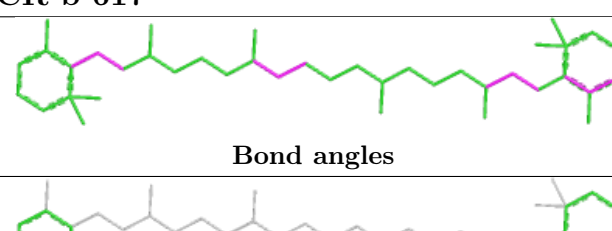


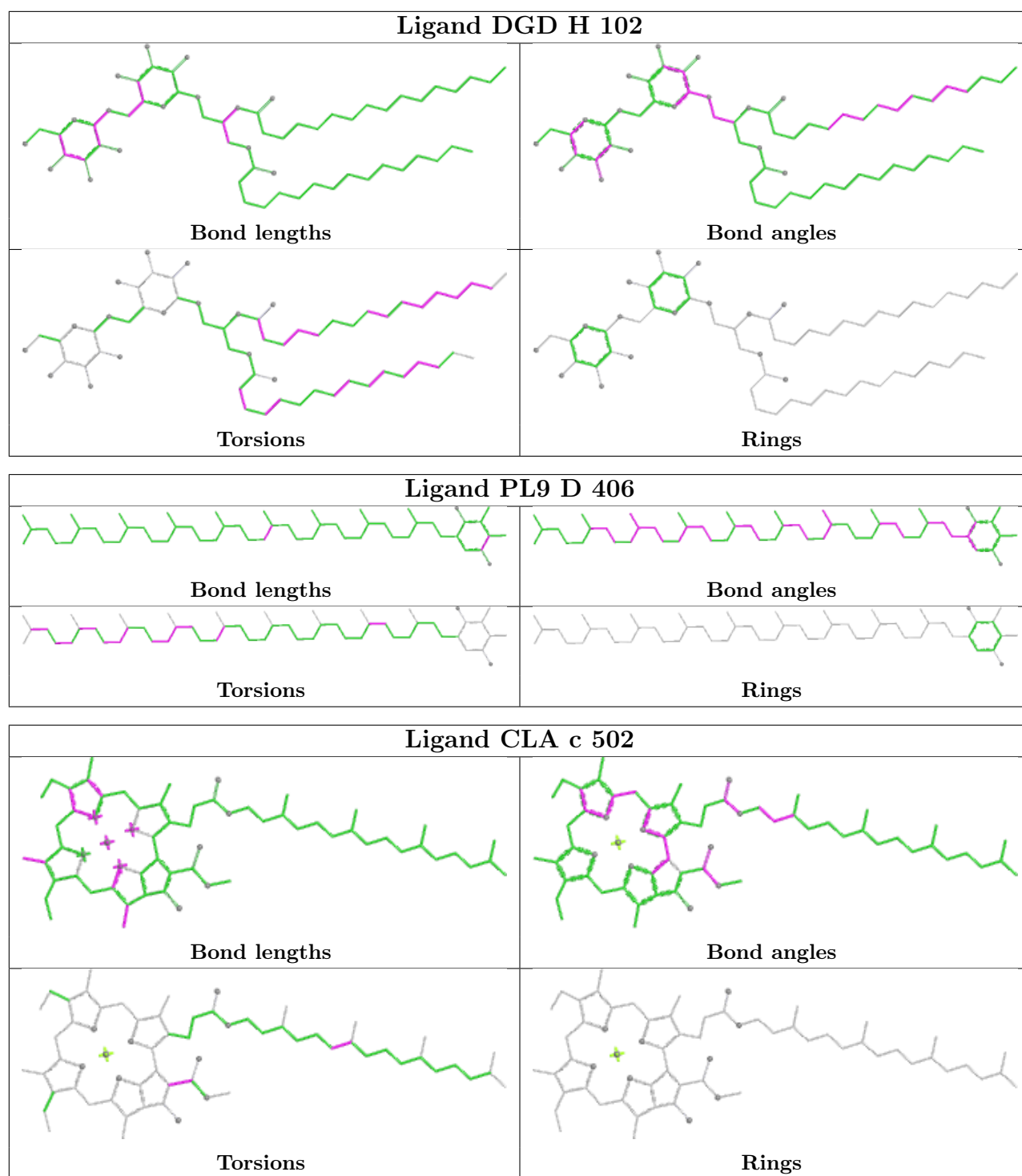
Ligand CLA C 507**Ligand PL9 A 611****Ligand CLA B 603**

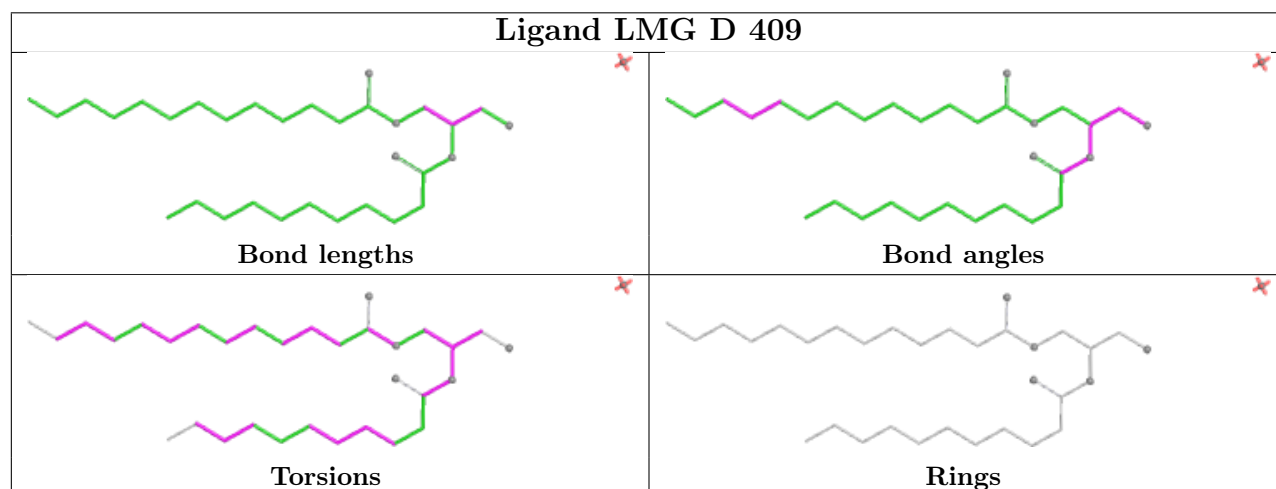
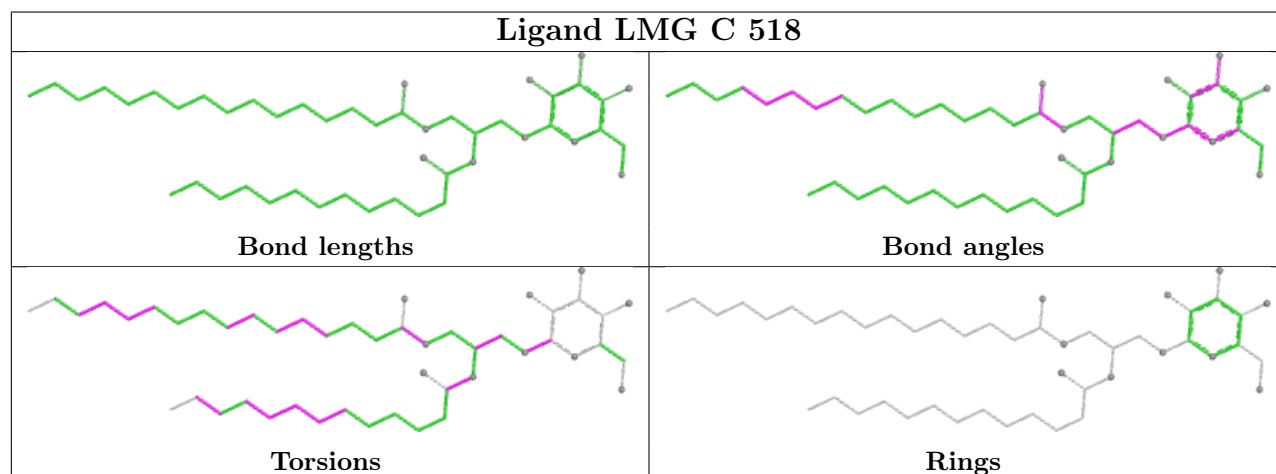
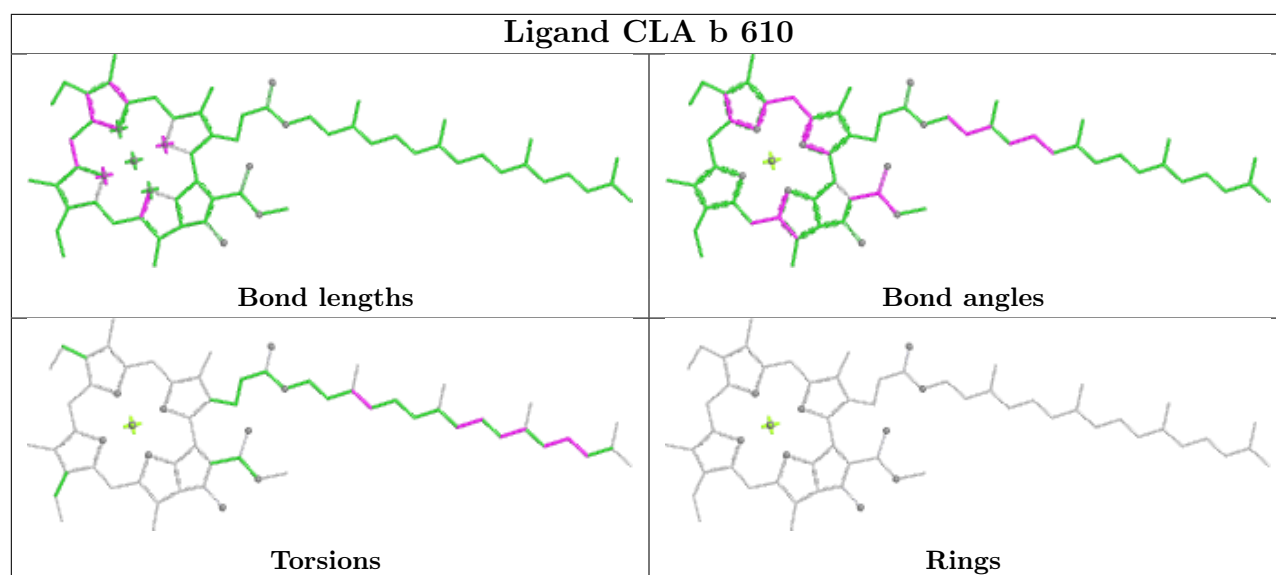
Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

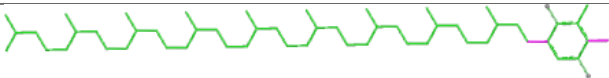
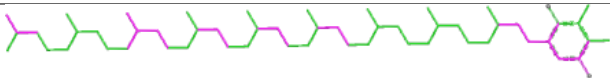
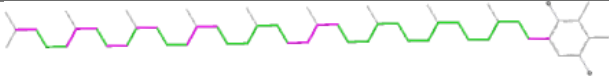
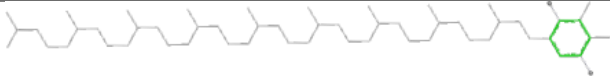
Ligand STE l 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

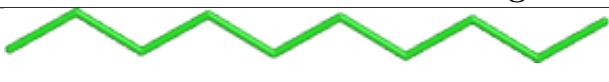
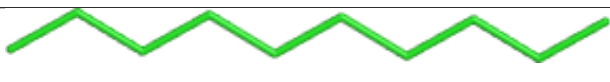
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

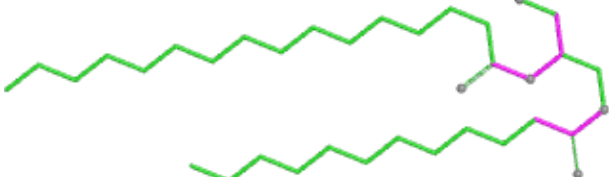
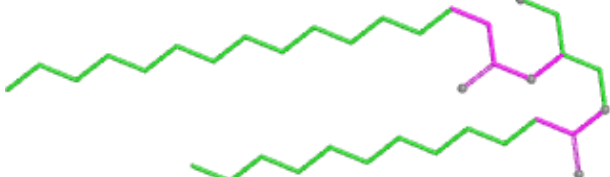
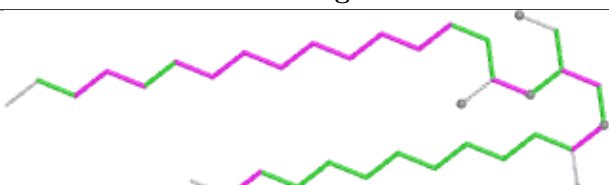
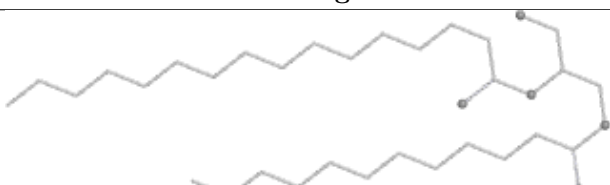
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

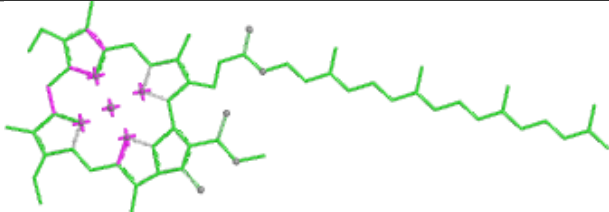
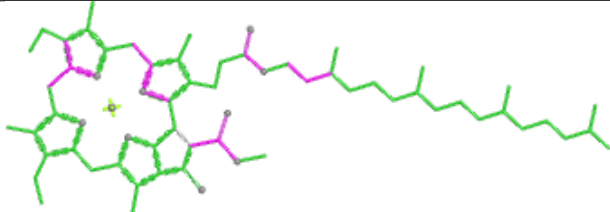
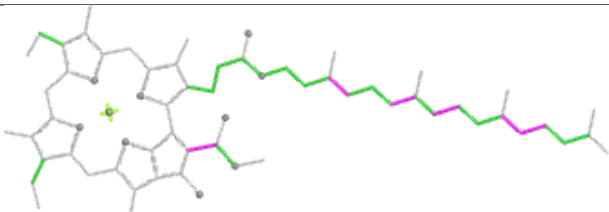
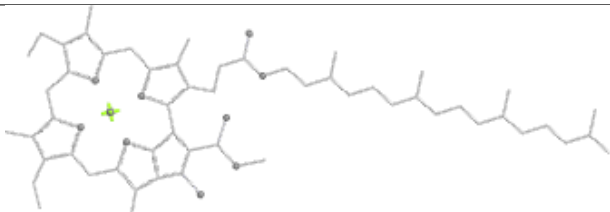




Ligand PL9 a 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE M 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD a 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.70	1 (0%) 90 89	8, 28, 47, 76	64 (19%)
1	a	334/344 (97%)	-0.58	0 100 100	8, 30, 56, 76	64 (19%)
2	B	505/510 (99%)	-0.59	0 100 100	17, 32, 60, 90	4 (0%)
2	b	505/510 (99%)	-0.48	2 (0%) 88 88	25, 35, 68, 105	0
3	C	442/461 (95%)	-0.59	0 100 100	9, 35, 50, 70	11 (2%)
3	c	451/461 (97%)	-0.45	1 (0%) 91 90	9, 39, 57, 91	12 (2%)
4	D	341/352 (96%)	-0.73	0 100 100	10, 29, 45, 78	2 (0%)
4	d	341/352 (96%)	-0.60	0 100 100	10, 33, 56, 82	3 (0%)
5	E	82/84 (97%)	-0.02	0 100 100	31, 48, 67, 83	1 (1%)
5	e	82/84 (97%)	0.11	0 100 100	37, 56, 76, 82	0
6	F	34/45 (75%)	-0.30	1 (2%) 53 52	35, 41, 58, 88	0
6	f	34/45 (75%)	-0.14	0 100 100	39, 48, 74, 88	0
7	H	65/66 (98%)	-0.35	0 100 100	32, 40, 54, 68	0
7	h	63/66 (95%)	-0.12	0 100 100	39, 49, 60, 63	0
8	I	35/38 (92%)	-0.43	0 100 100	32, 38, 62, 81	0
8	i	35/38 (92%)	-0.45	0 100 100	31, 39, 67, 81	0
9	J	36/40 (90%)	-0.25	0 100 100	33, 46, 71, 84	0
9	j	36/40 (90%)	-0.08	1 (2%) 55 54	38, 52, 83, 93	0
10	K	37/46 (80%)	-0.26	0 100 100	40, 47, 62, 70	0
10	k	37/46 (80%)	-0.06	0 100 100	46, 51, 66, 78	0
11	L	37/37 (100%)	-0.61	1 (2%) 56 55	24, 28, 60, 64	0
11	l	36/37 (97%)	-0.63	0 100 100	26, 31, 63, 87	0
12	M	32/36 (88%)	-0.54	0 100 100	27, 33, 57, 70	0
12	m	31/36 (86%)	-0.59	0 100 100	28, 32, 50, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.33	4 (1%) 70 70	25, 41, 77, 126	1 (0%)
13	o	244/272 (89%)	-0.35	1 (0%) 88 88	26, 39, 78, 115	0
14	T	29/32 (90%)	-0.74	0 100 100	26, 30, 54, 67	0
14	t	29/32 (90%)	-0.57	0 100 100	26, 31, 67, 81	0
15	U	97/134 (72%)	-0.43	0 100 100	30, 41, 66, 89	0
15	u	97/134 (72%)	-0.46	1 (1%) 79 79	31, 39, 55, 85	0
16	V	137/163 (84%)	-0.50	0 100 100	29, 38, 55, 71	0
16	v	137/163 (84%)	-0.35	0 100 100	33, 44, 63, 75	0
17	Y	27/46 (58%)	0.46	1 (3%) 45 44	49, 66, 76, 85	0
17	y	30/46 (65%)	0.23	0 100 100	56, 68, 77, 93	0
18	X	38/41 (92%)	-0.13	0 100 100	39, 48, 65, 74	0
18	x	39/41 (95%)	0.21	1 (2%) 57 56	47, 60, 80, 92	0
19	Z	62/62 (100%)	0.54	2 (3%) 50 49	52, 63, 101, 111	0
19	z	62/62 (100%)	0.26	1 (1%) 70 70	55, 64, 100, 109	0
20	R	34/41 (82%)	0.48	1 (2%) 53 52	57, 66, 78, 84	0
20	r	31/41 (75%)	0.92	1 (3%) 50 49	68, 80, 97, 101	0
All	All	5302/5700 (93%)	-0.44	20 (0%) 88 88	8, 37, 69, 126	162 (3%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	3.6
18	x	37	VAL	3.5
13	O	59	LYS	3.2
20	R	35	LEU	3.1
13	o	58	ASN	3.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.93	0.09	35,47,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	34,39,49,63	0
14	FME	t	1	10/11	0.94	0.07	30,38,53,58	0
8	FME	I	1	10/11	0.96	0.07	39,44,52,53	0
12	FME	m	1	10/11	0.97	0.06	32,46,60,66	0
8	FME	i	1	10/11	0.97	0.07	37,46,50,53	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
33	STE	H	103	18/20	0.72	0.13	56,69,71,71	0
33	STE	k	103	12/20	0.75	0.13	55,65,72,77	0
29	LMG	b	622	55/55	0.76	0.14	51,63,76,78	0
30	LHG	e	102	42/49	0.77	0.12	60,76,86,97	0
33	STE	B	625	12/20	0.77	0.13	51,56,71,74	0
29	LMG	c	521	48/55	0.77	0.13	48,66,83,91	0
33	STE	a	618	12/20	0.77	0.11	49,63,71,74	0
30	LHG	E	101	49/49	0.77	0.12	43,73,89,90	0
33	STE	E	102	12/20	0.79	0.11	58,68,81,81	0
29	LMG	d	408	23/55	0.79	0.12	48,61,69,73	0
28	PL9	A	611	55/55	0.80	0.12	39,56,70,72	0
29	LMG	D	409	33/55	0.80	0.10	32,50,67,78	0
32	DGD	a	617	44/66	0.81	0.12	36,49,71,74	0
28	PL9	a	612	55/55	0.81	0.12	41,61,74,80	0
33	STE	B	626	16/20	0.81	0.12	47,54,60,64	0
33	STE	b	623	16/20	0.81	0.10	52,57,74,79	0
33	STE	C	520	12/20	0.81	0.11	45,52,59,59	0
33	STE	B	620	17/20	0.82	0.11	32,46,61,64	0
32	DGD	A	617	66/66	0.82	0.10	47,56,65,72	0
33	STE	b	625	20/20	0.82	0.10	46,55,62,63	0
33	STE	J	101	12/20	0.82	0.11	45,52,59,63	0
33	STE	t	104	18/20	0.82	0.12	45,52,78,78	0
31	SQD	a	616	36/54	0.83	0.10	37,52,65,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	STE	t	103	10/20	0.83	0.11	46,50,56,60	0
33	STE	b	621	20/20	0.83	0.12	38,50,67,71	0
33	STE	X	101	20/20	0.84	0.12	35,44,63,75	0
29	LMG	A	613	48/55	0.84	0.10	36,54,67,76	0
33	STE	m	102	12/20	0.84	0.12	46,56,66,66	0
33	STE	t	102	14/20	0.84	0.10	41,45,59,59	0
31	SQD	A	616	39/54	0.84	0.10	41,51,73,74	0
25	CLA	h	101	65/65	0.84	0.10	46,62,82,86	0
33	STE	c	520	20/20	0.85	0.10	40,51,78,80	0
29	LMG	c	519	37/55	0.85	0.09	43,57,66,68	0
29	LMG	c	522	49/55	0.85	0.10	37,50,75,84	0
33	STE	b	624	15/20	0.85	0.11	45,51,65,66	0
33	STE	C	519	12/20	0.85	0.12	38,43,55,55	0
33	STE	b	626	10/20	0.85	0.10	43,51,58,60	0
33	STE	b	620	16/20	0.86	0.11	34,46,57,58	0
29	LMG	B	621	28/55	0.86	0.09	35,47,57,65	0
33	STE	I	101	15/20	0.86	0.11	40,50,60,63	0
31	SQD	B	623	54/54	0.86	0.10	36,59,78,86	0
29	LMG	m	101	51/55	0.86	0.09	34,48,59,63	0
31	SQD	f	101	41/54	0.86	0.11	57,75,85,87	0
33	STE	x	101	20/20	0.86	0.12	41,50,59,62	0
31	SQD	b	619	49/54	0.87	0.10	40,55,78,82	0
33	STE	j	101	12/20	0.87	0.10	47,53,56,56	0
29	LMG	C	518	48/55	0.88	0.09	39,58,70,76	0
27	BCR	k	101	40/40	0.88	0.10	44,52,60,62	0
33	STE	B	624	12/20	0.88	0.10	41,48,59,60	0
33	STE	l	102	18/20	0.89	0.10	37,44,64,64	0
33	STE	d	410	17/20	0.89	0.09	43,48,62,62	0
33	STE	C	521	16/20	0.90	0.09	34,43,57,57	0
33	STE	M	103	10/20	0.90	0.09	41,45,51,57	0
31	SQD	F	102	36/54	0.90	0.10	44,61,69,70	0
27	BCR	d	404	40/40	0.90	0.08	38,47,72,79	0
27	BCR	K	102	40/40	0.90	0.09	37,45,55,58	0
27	BCR	h	102	40/40	0.91	0.08	37,49,62,64	0
25	CLA	B	601	65/65	0.91	0.09	31,52,75,81	0
32	DGD	H	102	62/66	0.91	0.08	32,41,48,52	0
31	SQD	a	615	54/54	0.91	0.09	37,54,68,70	0
32	DGD	h	103	62/66	0.91	0.08	38,43,53,57	0
29	LMG	M	101	51/55	0.91	0.08	33,47,59,63	0
27	BCR	D	405	40/40	0.91	0.08	28,38,67,71	0
29	LMG	D	407	51/55	0.92	0.09	31,44,68,69	0
27	BCR	c	514	40/40	0.92	0.08	44,50,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	513	65/65	0.92	0.08	38,50,72,76	0
31	SQD	A	615	52/54	0.92	0.09	34,48,69,73	0
27	BCR	b	618	40/40	0.92	0.07	31,43,56,59	0
27	BCR	B	618	40/40	0.93	0.06	26,34,40,43	0
30	LHG	a	614	49/49	0.93	0.08	30,46,60,63	0
33	STE	M	102	15/20	0.93	0.07	38,44,55,64	0
25	CLA	c	512	65/65	0.93	0.08	44,52,73,80	0
27	BCR	H	101	40/40	0.93	0.07	31,41,51,53	0
27	BCR	K	101	40/40	0.93	0.07	38,47,54,56	0
32	DGD	C	516	62/66	0.93	0.07	32,42,80,88	0
25	CLA	B	606	65/65	0.93	0.07	22,32,58,64	0
27	BCR	A	610	40/40	0.93	0.06	24,31,41,42	0
32	DGD	c	517	62/66	0.93	0.07	34,44,72,76	0
32	DGD	c	518	62/66	0.93	0.08	30,42,65,70	0
27	BCR	b	616	40/40	0.94	0.06	27,37,42,45	0
27	BCR	b	617	40/40	0.94	0.06	26,34,43,46	0
25	CLA	c	506	65/65	0.94	0.07	33,41,71,75	0
27	BCR	B	617	40/40	0.94	0.06	25,33,42,43	0
27	BCR	c	515	40/40	0.94	0.06	29,42,50,53	0
25	CLA	c	508	64/65	0.94	0.07	32,38,69,88	0
27	BCR	B	619	40/40	0.94	0.06	28,38,50,53	0
25	CLA	c	511	65/65	0.94	0.08	40,47,57,62	0
27	BCR	k	102	40/40	0.94	0.08	38,47,55,58	0
32	DGD	C	515	62/66	0.94	0.07	25,33,65,72	0
25	CLA	C	506	65/65	0.94	0.07	27,37,69,71	0
25	CLA	c	513	65/65	0.94	0.08	41,55,78,82	0
25	CLA	b	605	65/65	0.94	0.07	28,36,59,62	0
32	DGD	c	516	62/66	0.94	0.07	25,35,58,68	0
27	BCR	T	101	40/40	0.94	0.06	29,35,43,46	0
30	LHG	l	101	49/49	0.94	0.07	30,39,48,54	0
34	BCT	a	606	4/4	0.94	0.08	30,36,40,46	0
29	LMG	d	409	44/55	0.95	0.07	37,44,66,73	0
27	BCR	a	611	40/40	0.95	0.05	23,31,42,44	0
30	LHG	A	614	47/49	0.95	0.08	27,38,64,73	0
30	LHG	B	622	49/49	0.95	0.07	29,39,54,57	0
25	CLA	c	504	60/65	0.95	0.06	29,37,64,68	0
25	CLA	B	609	65/65	0.95	0.06	26,34,50,54	0
25	CLA	B	616	60/65	0.95	0.07	24,32,66,70	0
25	CLA	c	509	65/65	0.95	0.07	32,39,53,57	0
25	CLA	c	510	65/65	0.95	0.06	29,41,50,54	0
25	CLA	C	503	65/65	0.95	0.06	30,36,41,46	0
25	CLA	B	602	65/65	0.95	0.06	26,32,48,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	508	65/65	0.95	0.06	29,34,74,85	0
25	CLA	d	403	65/65	0.95	0.08	30,39,72,76	0
27	BCR	t	101	40/40	0.95	0.05	25,32,45,47	0
25	CLA	C	510	65/65	0.95	0.06	29,36,47,53	0
26	PHO	d	401	64/64	0.95	0.06	23,34,40,44	0
28	PL9	d	405	55/55	0.95	0.06	22,31,38,39	0
25	CLA	C	511	65/65	0.95	0.07	27,42,51,56	0
25	CLA	C	512	65/65	0.95	0.07	34,44,75,80	0
32	DGD	C	517	62/66	0.95	0.07	25,39,64,71	0
25	CLA	B	604	65/65	0.95	0.07	22,28,57,61	0
25	CLA	a	608	65/65	0.95	0.07	26,35,73,78	0
27	BCR	C	514	40/40	0.95	0.07	29,36,46,48	0
25	CLA	A	607	65/65	0.95	0.07	24,29,76,83	0
25	CLA	b	608	65/65	0.95	0.07	30,39,55,68	0
25	CLA	b	613	65/65	0.95	0.06	27,35,63,67	0
25	CLA	b	615	60/65	0.95	0.07	30,39,77,82	0
27	BCR	K	103	40/40	0.95	0.07	32,43,51,57	0
34	BCT	D	401	4/4	0.95	0.08	35,36,39,40	0
25	CLA	c	503	65/65	0.95	0.06	31,39,45,49	0
30	LHG	d	407	39/49	0.96	0.07	31,40,56,62	0
25	CLA	b	601	65/65	0.96	0.06	30,37,51,53	0
25	CLA	B	611	65/65	0.96	0.05	21,28,40,42	0
25	CLA	d	402	65/65	0.96	0.06	23,29,49,60	0
25	CLA	b	607	65/65	0.96	0.06	29,36,52,56	0
25	CLA	C	507	65/65	0.96	0.06	26,33,46,51	0
26	PHO	D	402	64/64	0.96	0.05	20,29,34,37	0
28	PL9	D	406	55/55	0.96	0.05	21,28,36,40	0
26	PHO	a	609	64/64	0.96	0.05	21,28,33,38	0
25	CLA	b	609	65/65	0.96	0.06	28,34,41,48	0
25	CLA	b	610	65/65	0.96	0.06	22,31,46,52	0
25	CLA	b	611	65/65	0.96	0.06	21,30,42,45	0
25	CLA	b	612	65/65	0.96	0.06	20,28,59,63	0
25	CLA	B	614	65/65	0.96	0.06	22,32,62,69	0
25	CLA	b	614	65/65	0.96	0.06	28,36,51,59	0
25	CLA	C	509	65/65	0.96	0.07	27,35,49,53	0
25	CLA	c	501	65/65	0.96	0.06	28,35,43,49	0
25	CLA	c	502	65/65	0.96	0.06	26,34,51,56	0
25	CLA	B	607	65/65	0.96	0.06	19,26,51,53	0
25	CLA	C	502	65/65	0.96	0.06	27,32,44,50	0
25	CLA	c	505	65/65	0.96	0.06	27,36,54,57	0
25	CLA	B	610	65/65	0.96	0.06	22,30,36,40	0
25	CLA	c	507	65/65	0.96	0.06	28,37,49,52	0

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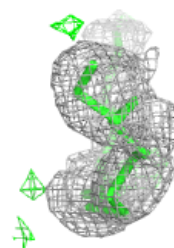
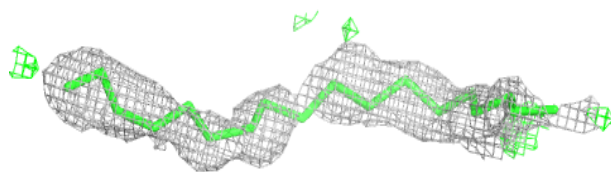
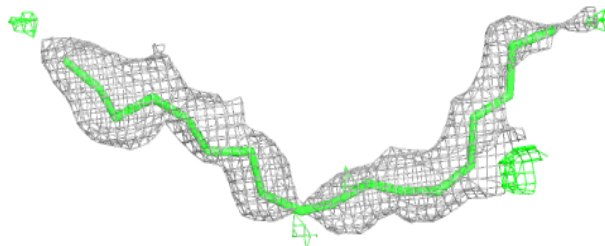
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	C	504	59/65	0.96	0.06	29,35,63,69	0
25	CLA	a	607	65/65	0.96	0.06	22,27,37,44	0
25	CLA	C	505	65/65	0.96	0.06	25,33,55,61	0
25	CLA	a	610	65/65	0.96	0.08	22,28,65,69	0
25	CLA	B	605	65/65	0.97	0.05	22,28,38,40	0
30	LHG	D	408	49/49	0.97	0.06	27,34,44,48	0
25	CLA	A	612	65/65	0.97	0.04	17,25,39,45	0
30	LHG	L	101	49/49	0.97	0.06	29,36,47,53	0
25	CLA	D	403	65/65	0.97	0.05	20,25,45,51	0
30	LHG	d	406	49/49	0.97	0.06	29,36,42,51	0
25	CLA	D	404	65/65	0.97	0.07	25,32,81,91	0
25	CLA	B	612	65/65	0.97	0.05	21,28,38,41	0
25	CLA	B	613	65/65	0.97	0.06	21,27,54,65	0
25	CLA	B	603	65/65	0.97	0.05	22,27,51,59	0
26	PHO	A	608	64/64	0.97	0.05	18,25,32,36	0
25	CLA	a	613	65/65	0.97	0.05	19,27,38,43	0
25	CLA	B	615	65/65	0.97	0.05	25,32,49,54	0
25	CLA	b	602	65/65	0.97	0.06	24,31,52,61	0
25	CLA	b	603	65/65	0.97	0.06	22,31,64,72	0
25	CLA	b	604	65/65	0.97	0.05	22,30,40,44	0
25	CLA	B	608	65/65	0.97	0.05	25,30,46,51	0
25	CLA	b	606	65/65	0.97	0.06	23,30,55,59	0
25	CLA	C	501	65/65	0.97	0.05	26,30,40,44	0
25	CLA	A	606	65/65	0.97	0.05	18,24,35,45	0
35	HEM	e	101	43/43	0.97	0.09	46,55,66,78	0
35	HEM	F	101	43/43	0.98	0.08	38,43,51,63	0
25	CLA	A	609	54/65	0.98	0.05	20,26,54,60	0
23	FE2	A	603	1/1	0.99	0.02	30,30,30,30	0
24	CL	A	604	1/1	0.99	0.03	28,28,28,28	0
24	CL	a	604	1/1	0.99	0.08	27,27,27,27	0
24	CL	a	605	1/1	0.99	0.06	29,29,29,29	0
21	OEX	A	601[B]	10/10	0.99	0.03	25,29,33,33	10
21	OEX	A	601[C]	10/10	0.99	0.03	22,25,28,28	10
21	OEX	a	601[B]	10/10	0.99	0.02	26,29,32,32	10
21	OEX	a	601[C]	10/10	0.99	0.02	21,23,25,25	10
22	OXY	A	602[A]	11/11	0.99	0.03	26,29,32,32	11
22	OXY	a	602[A]	11/11	0.99	0.03	28,30,34,34	11
36	HEC	V	201	43/43	0.99	0.05	23,30,38,42	0
36	HEC	v	201	43/43	0.99	0.05	28,33,37,43	0
23	FE2	a	603	1/1	1.00	0.01	34,34,34,34	0
24	CL	A	605	1/1	1.00	0.04	29,29,29,29	0

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

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

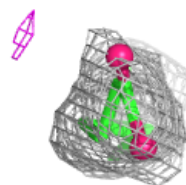
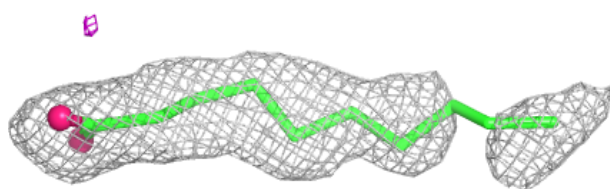
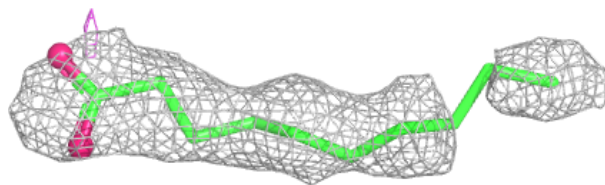
Electron density around STE H 103:

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

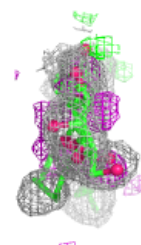
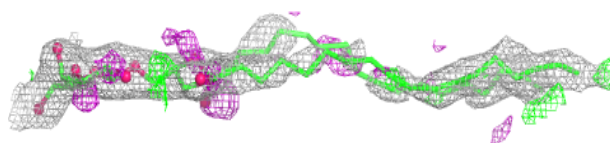
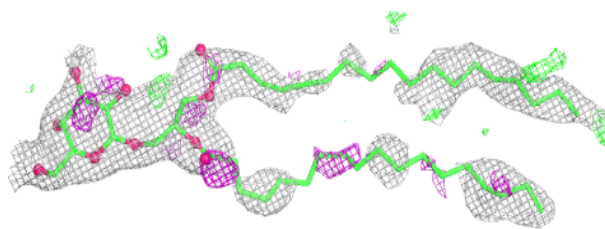


Electron density around STE k 103:

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

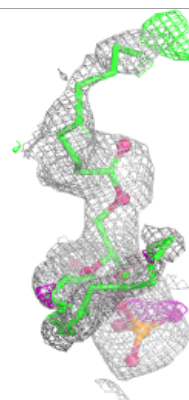
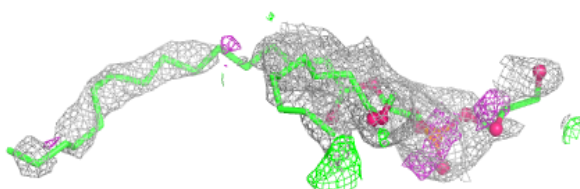
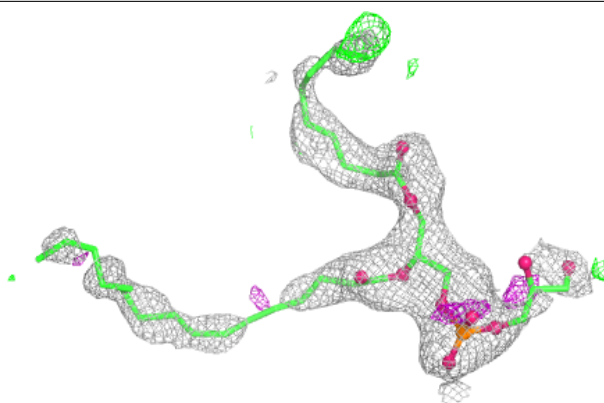
**Electron density around LMG b 622:**

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

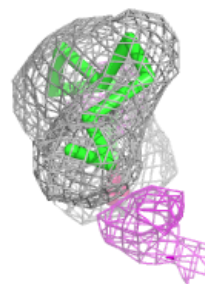
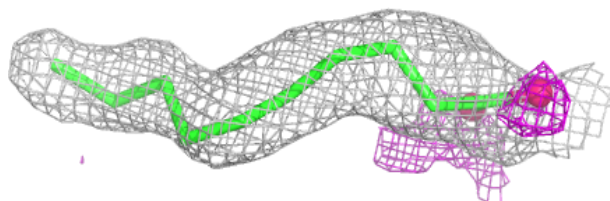
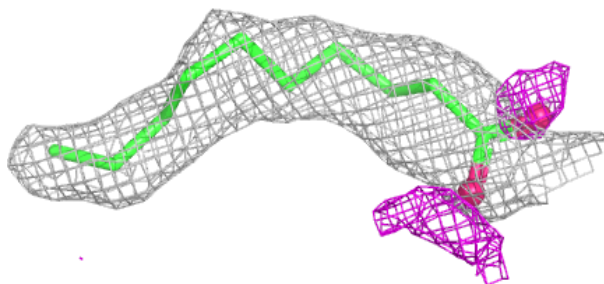


Electron density around LHG e 102:

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

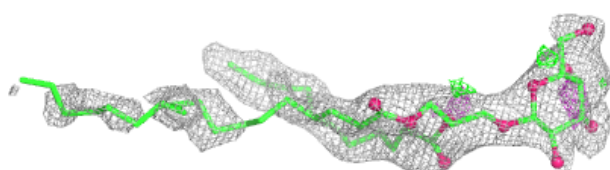
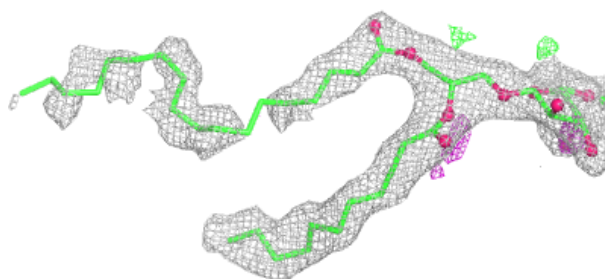
**Electron density around STE B 625:**

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

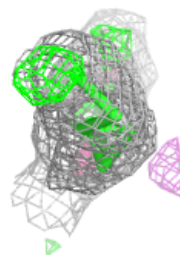
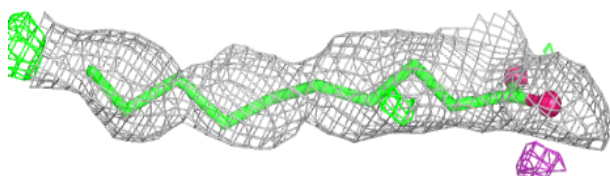
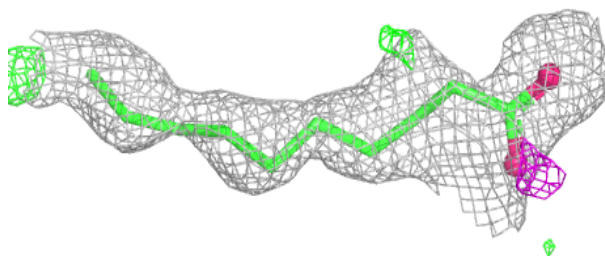


Electron density around LMG c 521:

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

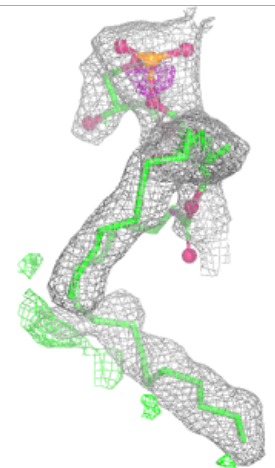
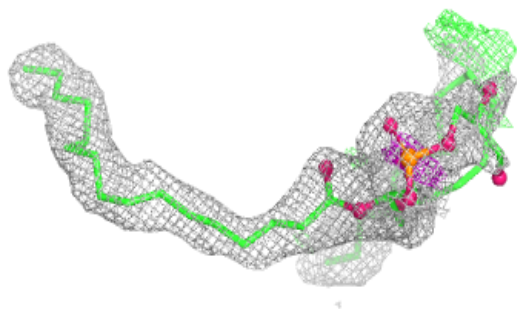
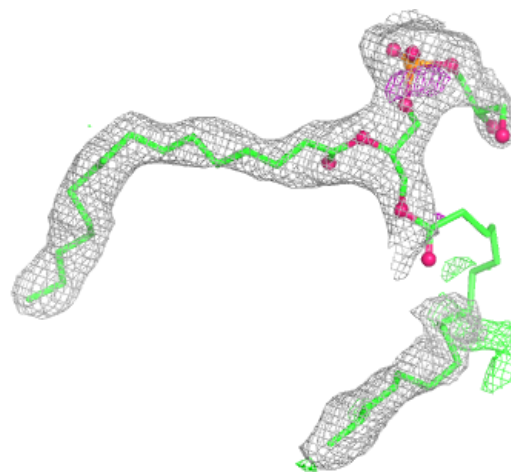
**Electron density around STE a 618:**

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



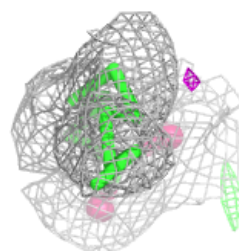
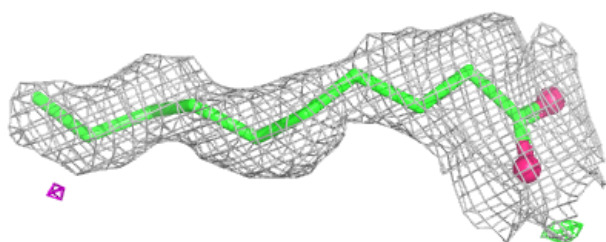
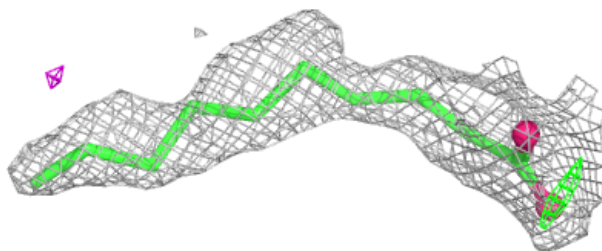
Electron density around LHG E 101:

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and green (positive)

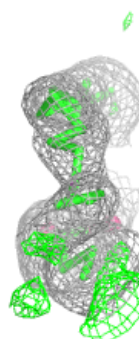
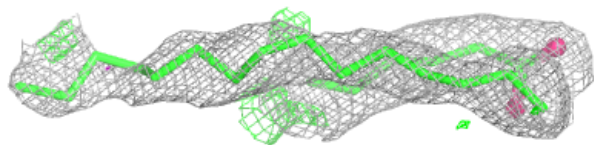
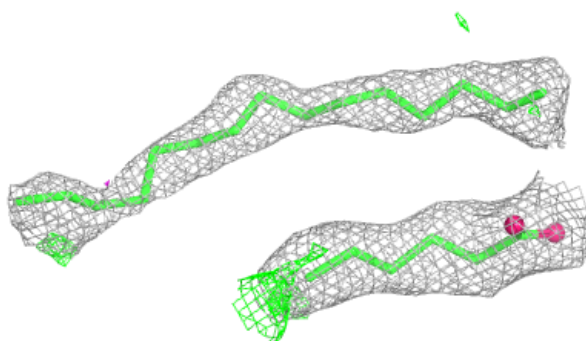


Electron density around STE E 102:

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and green (positive)

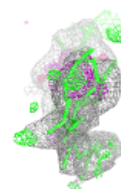
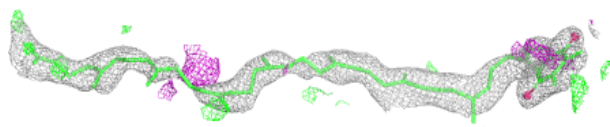
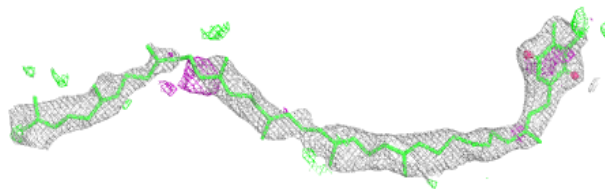
**Electron density around LMG d 408:**

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

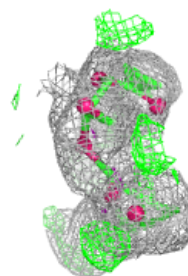
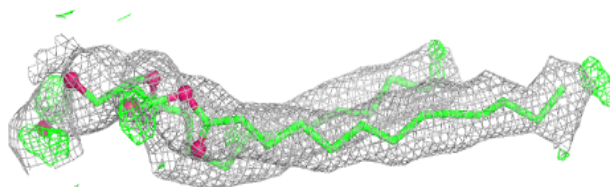
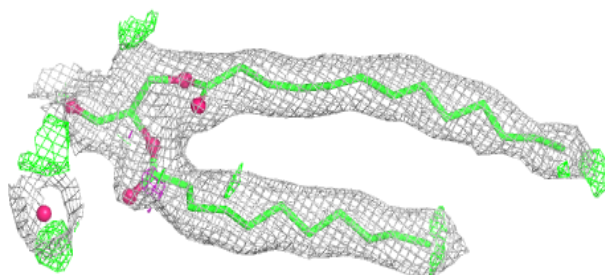


Electron density around PL9 A 611:

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

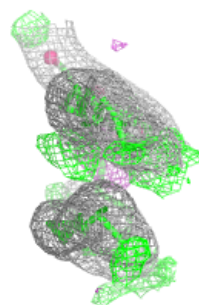
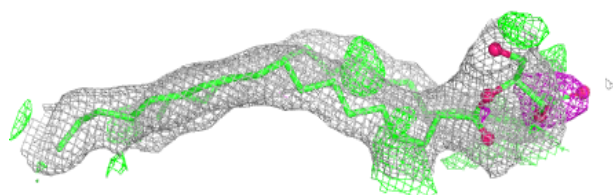
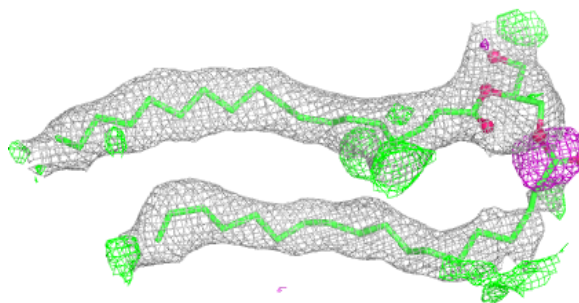
**Electron density around LMG D 409:**

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

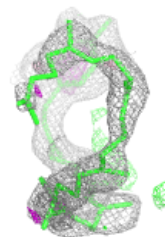
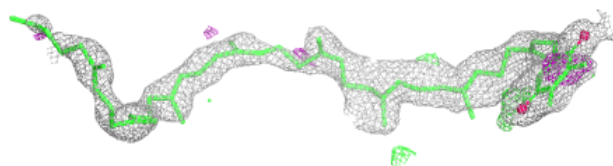
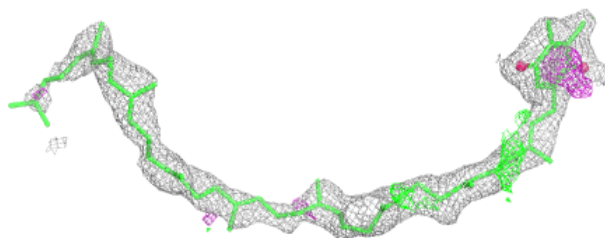


Electron density around DGD a 617:

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

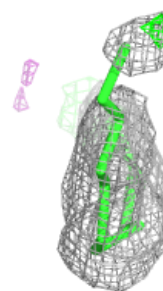
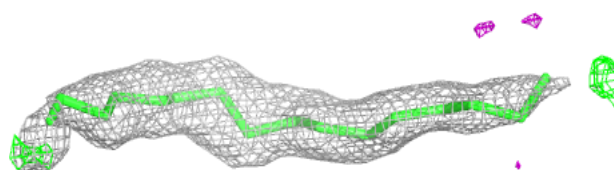
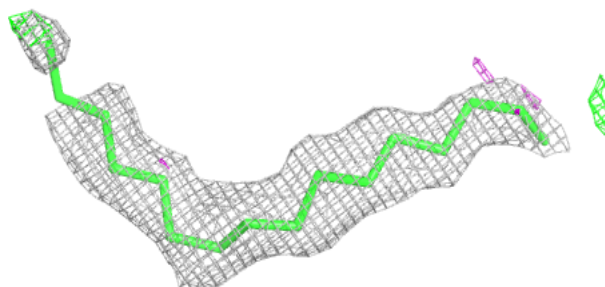
**Electron density around PL9 a 612:**

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

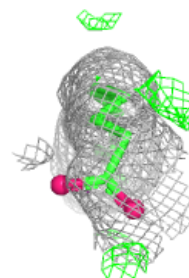
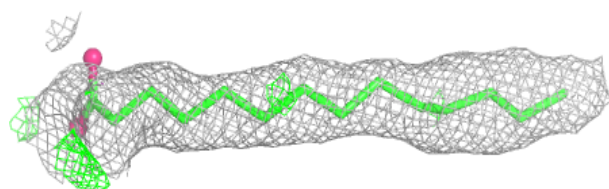
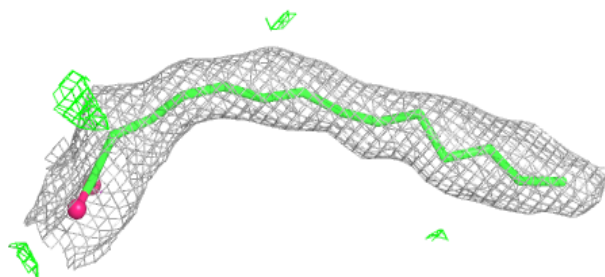


Electron density around STE B 626:

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

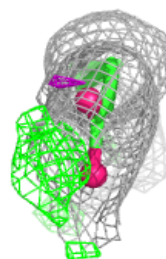
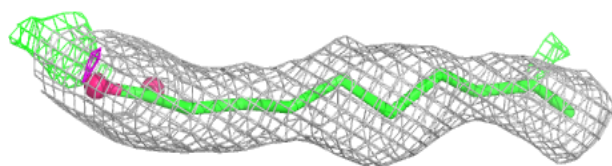
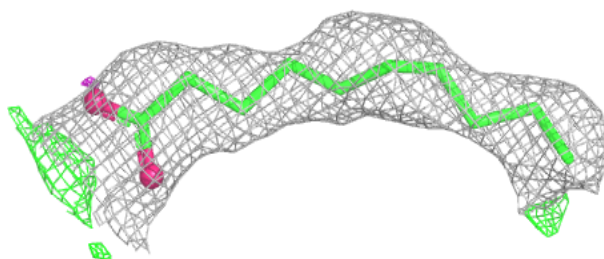
**Electron density around STE b 623:**

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

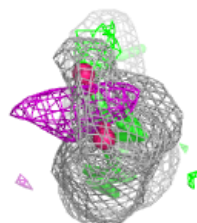
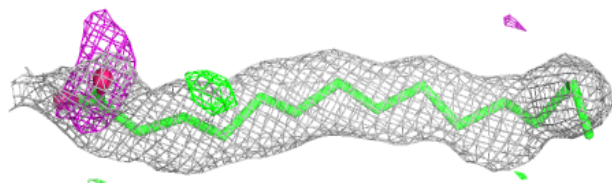
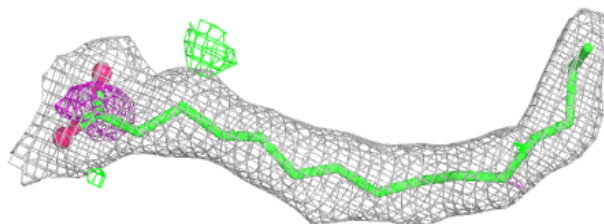


Electron density around STE C 520:

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

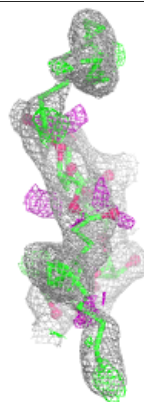
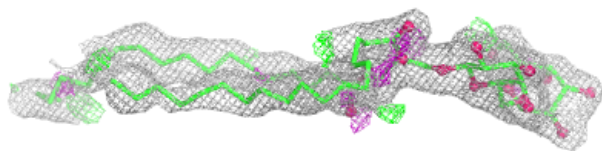
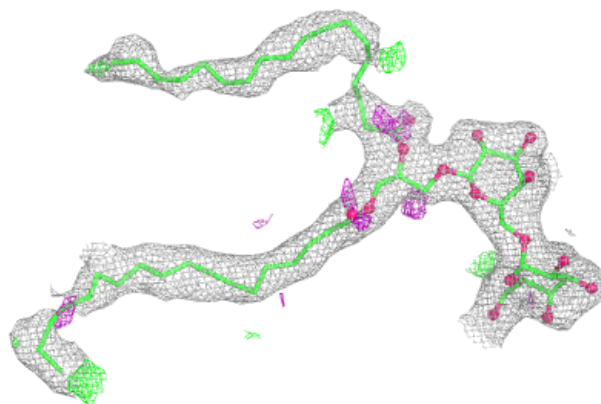
**Electron density around STE B 620:**

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

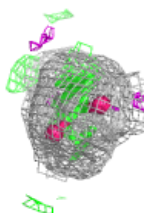
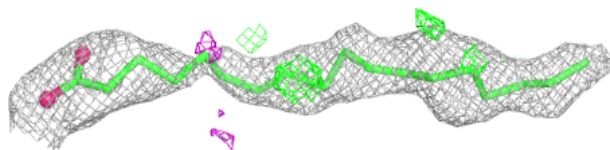
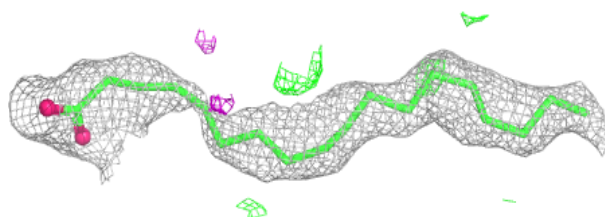


Electron density around DGD A 617:

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

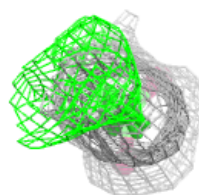
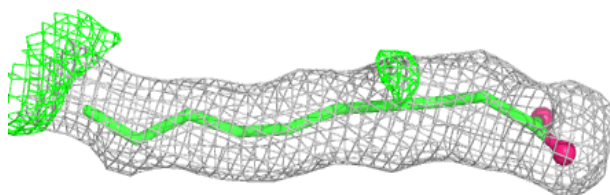
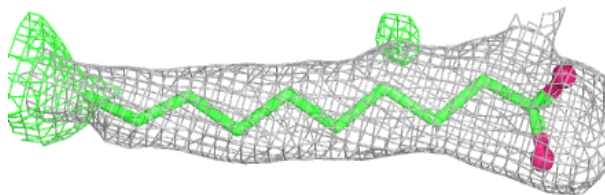
**Electron density around STE b 625:**

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

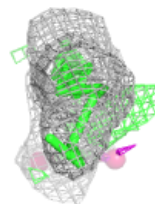
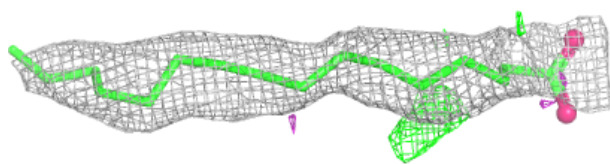
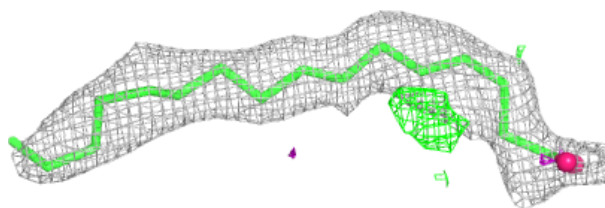


Electron density around STE J 101:

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

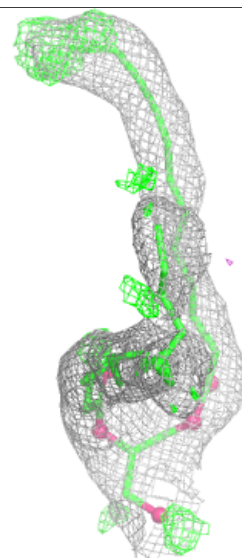
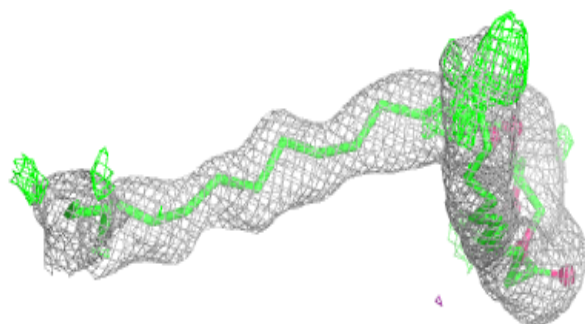
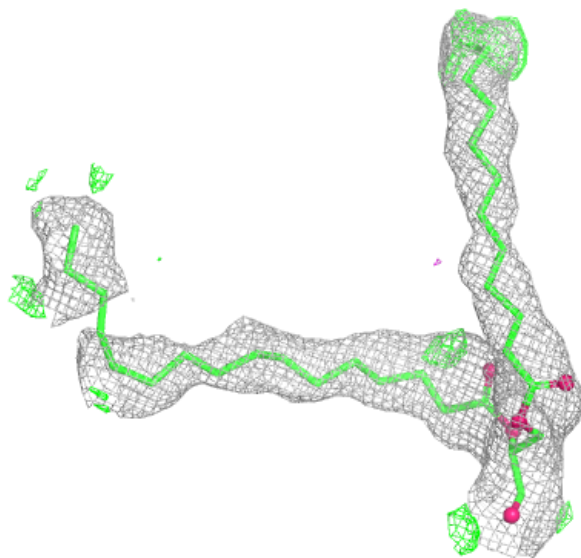
**Electron density around STE t 104:**

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



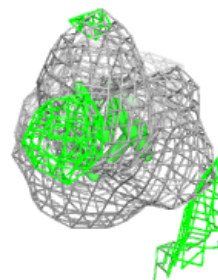
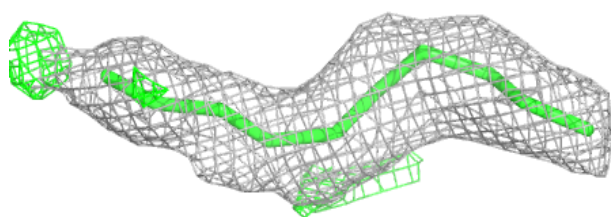
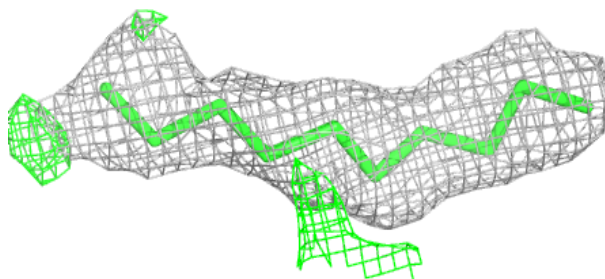
Electron density around SQD a 616:

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

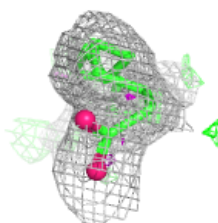
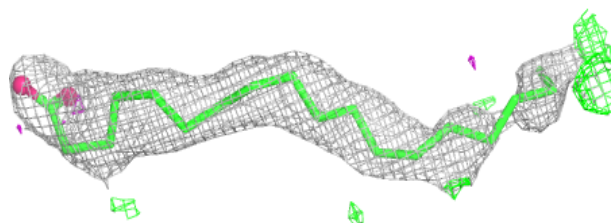
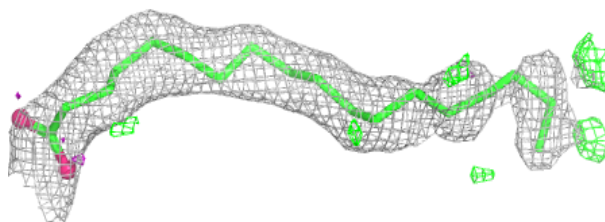


Electron density around STE t 103:

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

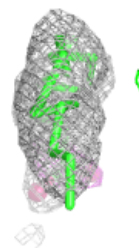
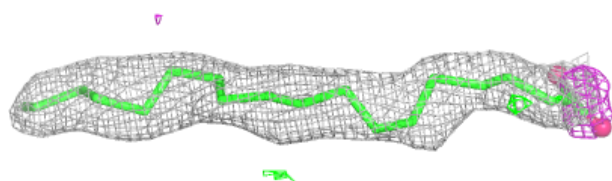
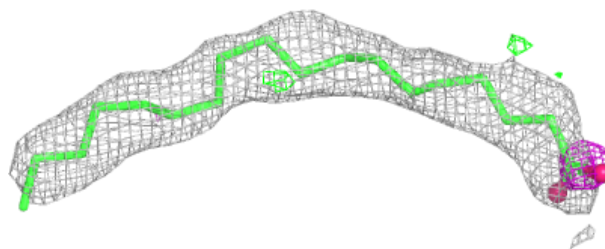
**Electron density around STE b 621:**

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

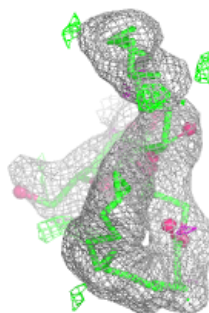
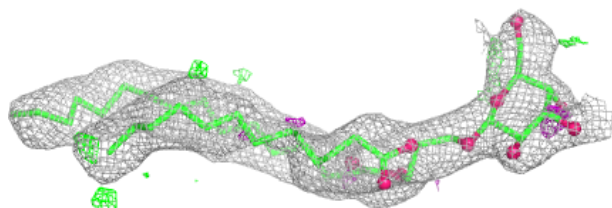
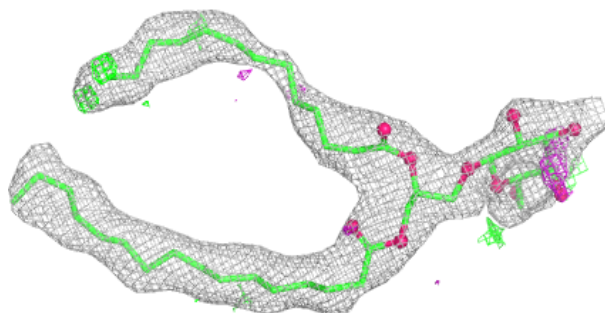


Electron density around STE X 101:

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

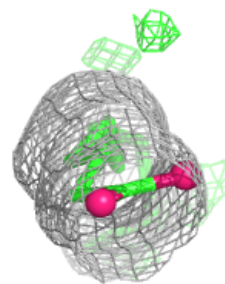
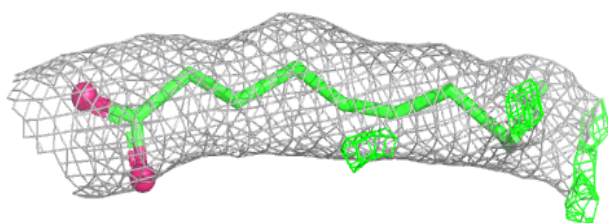
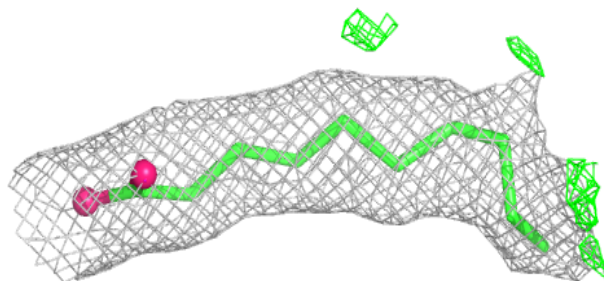
**Electron density around LMG A 613:**

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

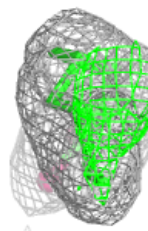
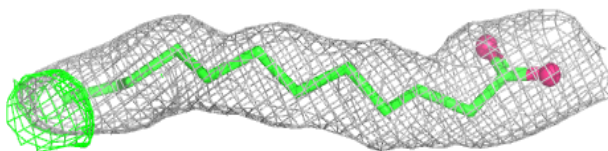
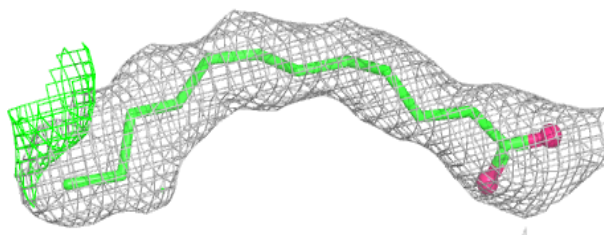


Electron density around STE m 102:

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

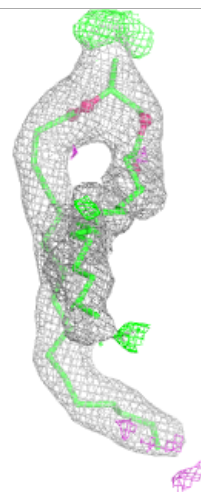
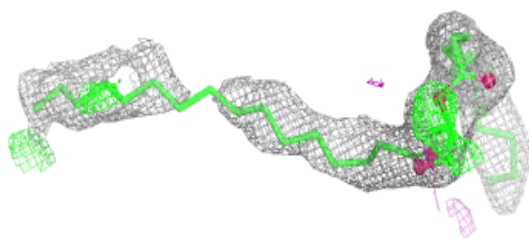
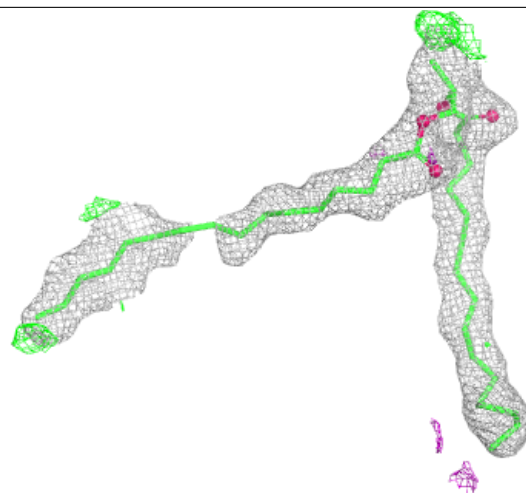
**Electron density around STE t 102:**

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



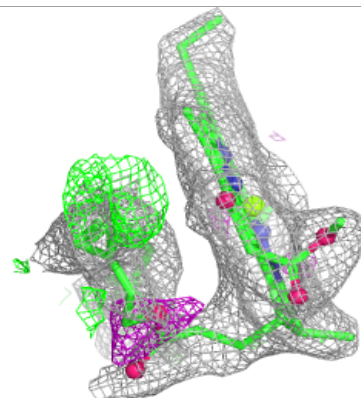
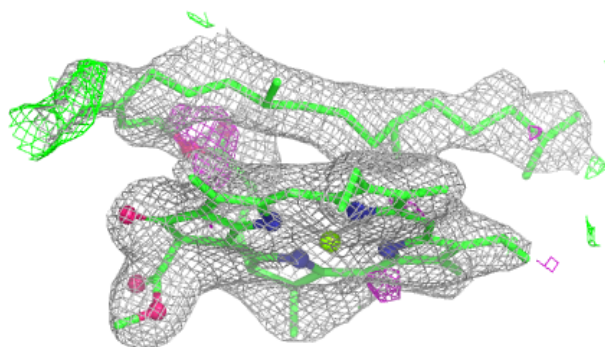
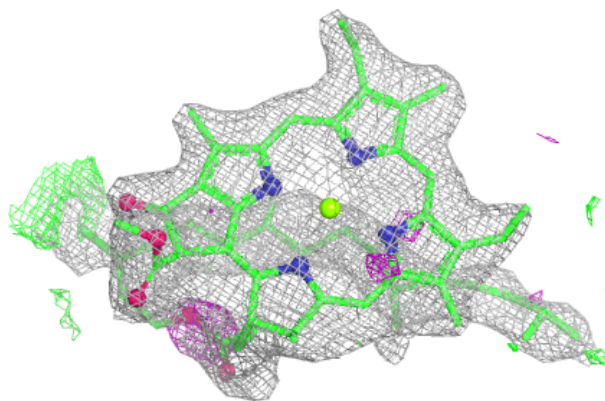
Electron density around SQD A 616:

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

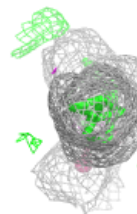
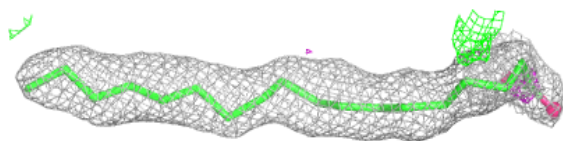
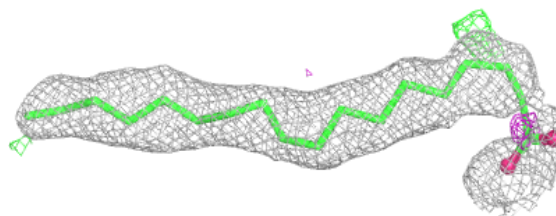


Electron density around CLA h 101:

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

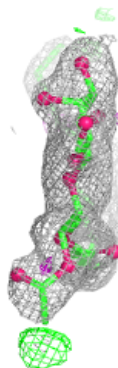
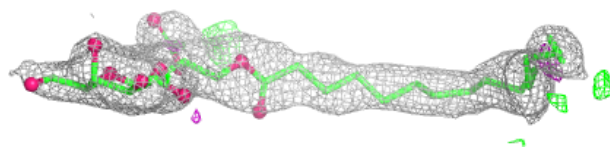
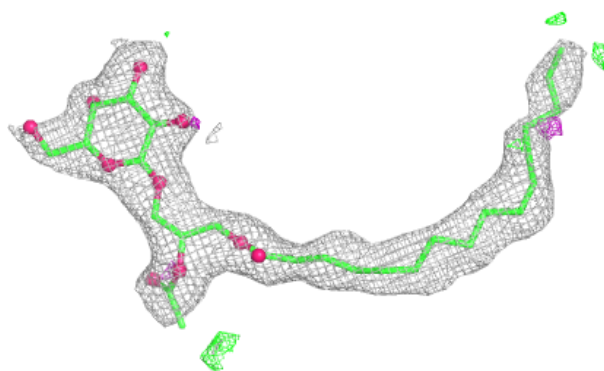
**Electron density around STE c 520:**

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

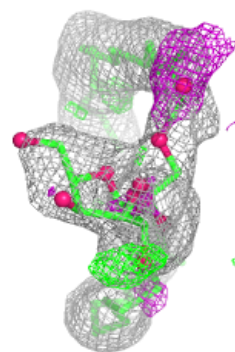
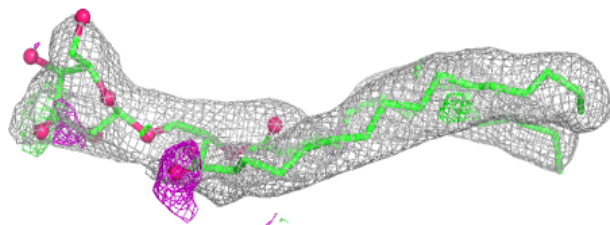
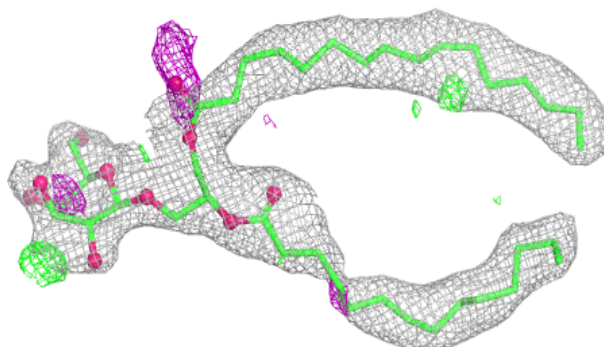


Electron density around LMG c 519:

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

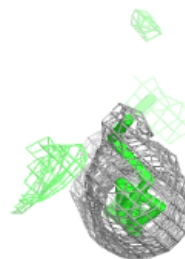
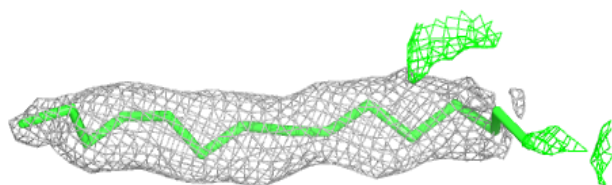
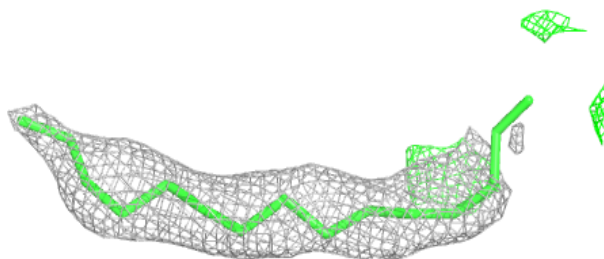
**Electron density around LMG c 522:**

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

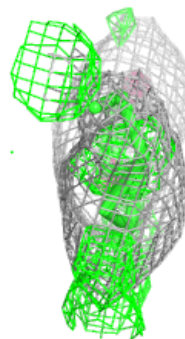
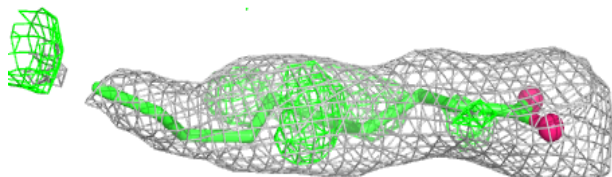
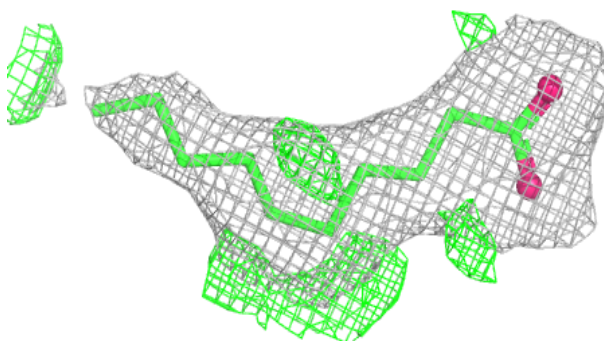


Electron density around STE b 624:

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

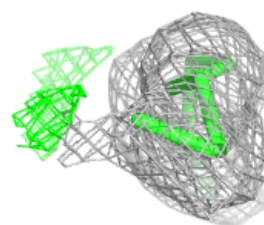
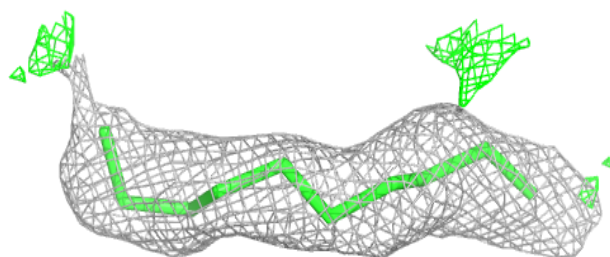
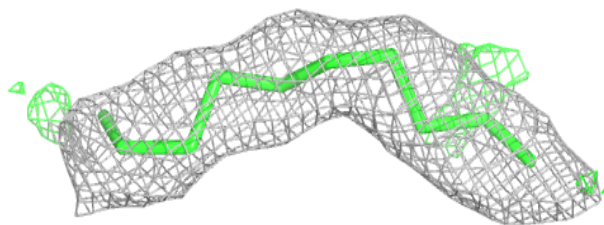
**Electron density around STE C 519:**

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

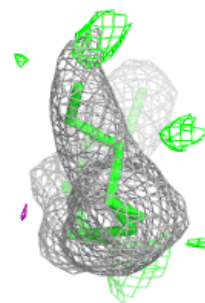
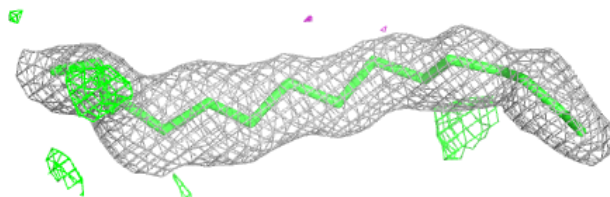
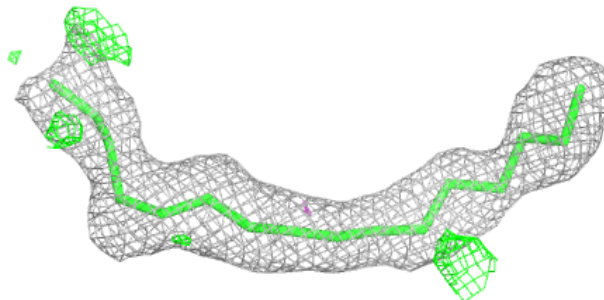


Electron density around STE b 626:

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

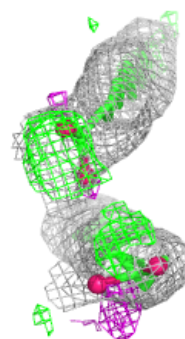
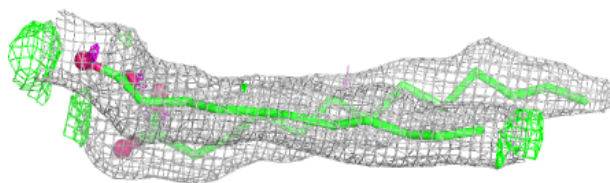
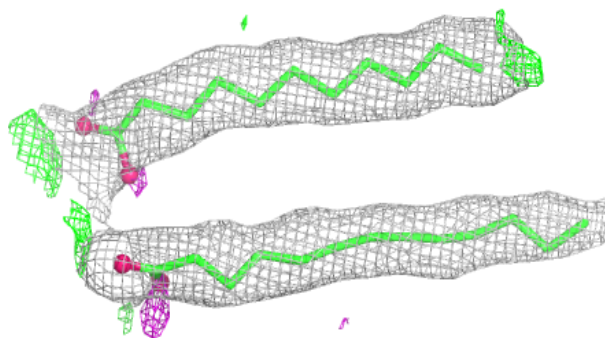
**Electron density around STE b 620:**

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

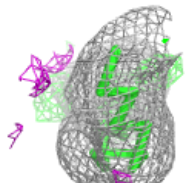
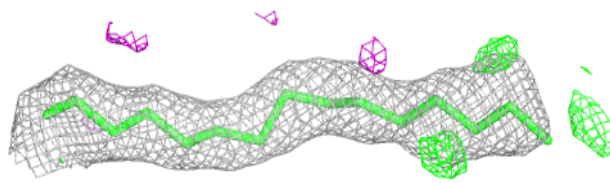
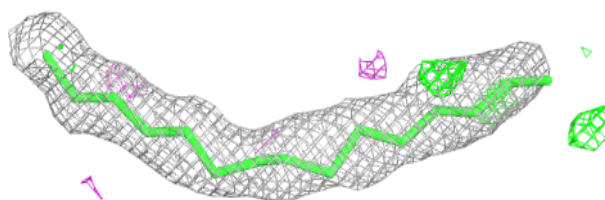


Electron density around LMG B 621:

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

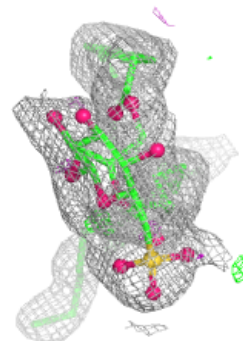
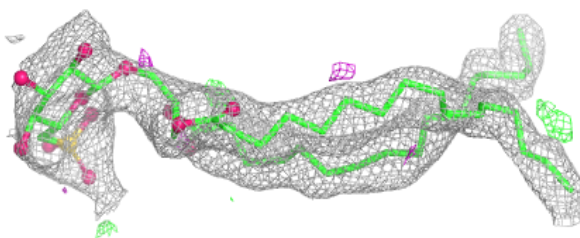
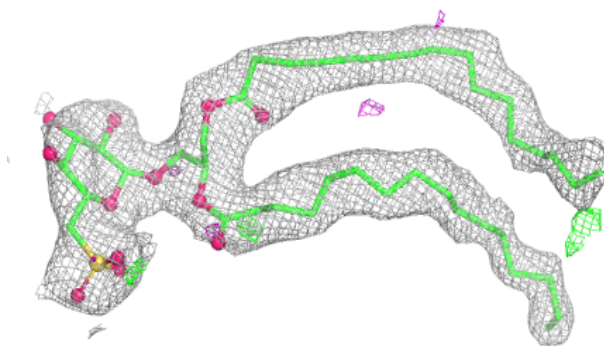
**Electron density around STE I 101:**

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

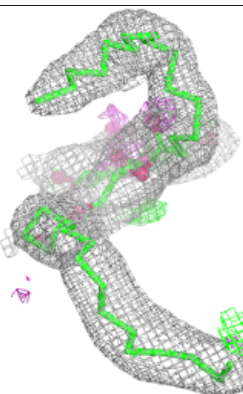
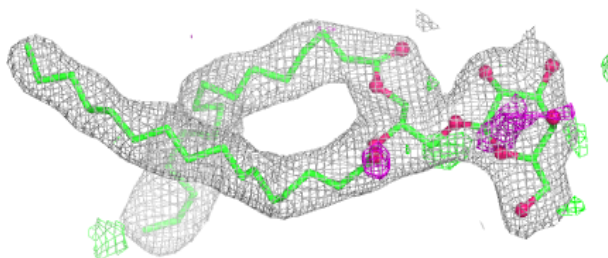
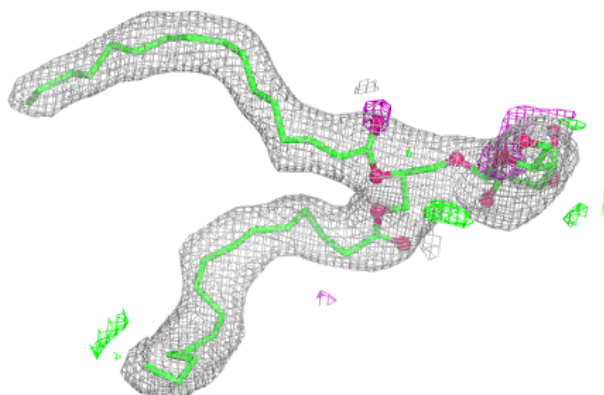


Electron density around SQD B 623:

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

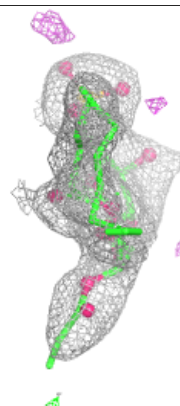
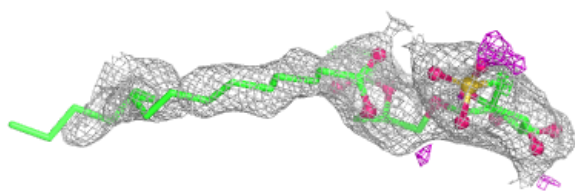
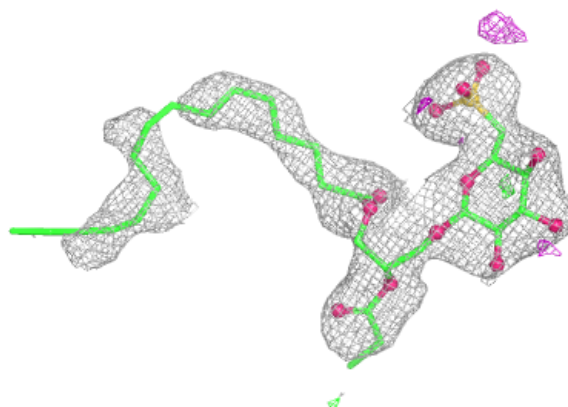
**Electron density around LMG m 101:**

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

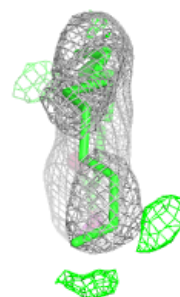
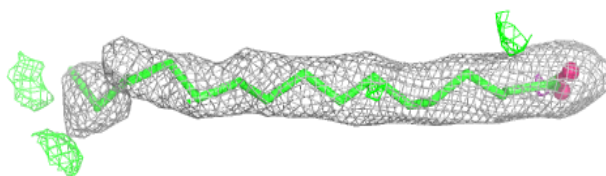
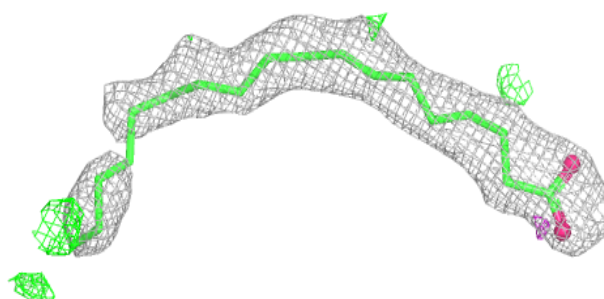


Electron density around SQD f 101:

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

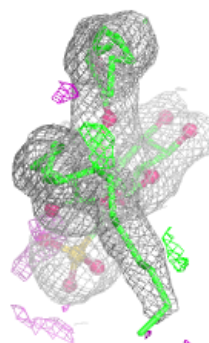
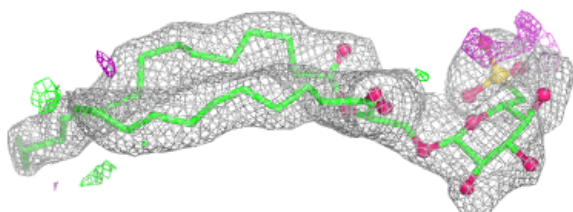
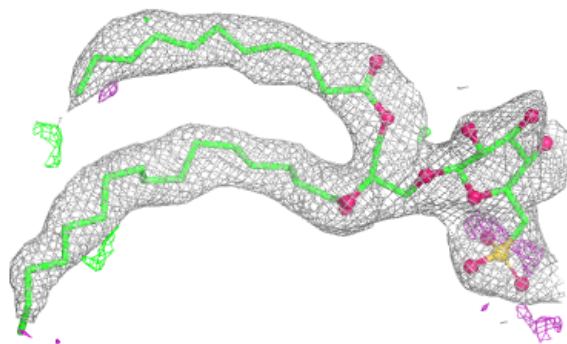
**Electron density around STE x 101:**

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

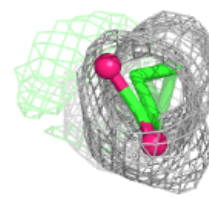
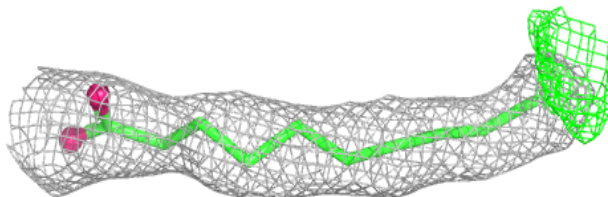
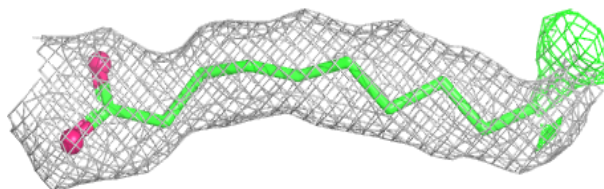


Electron density around SQD b 619:

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

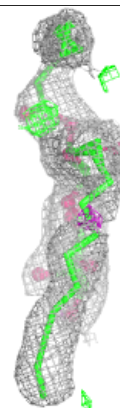
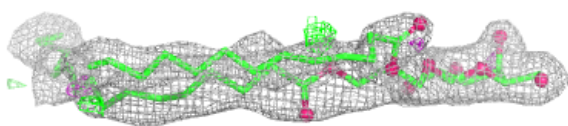
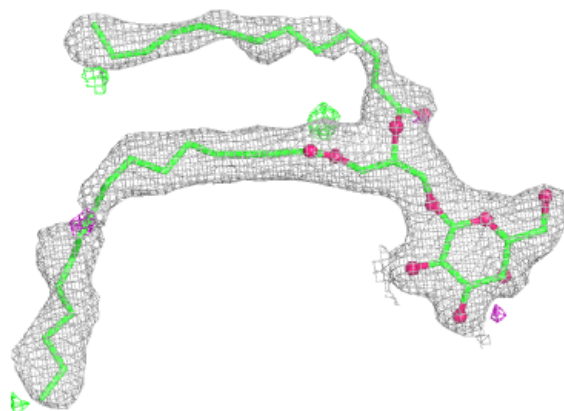
**Electron density around STE j 101:**

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

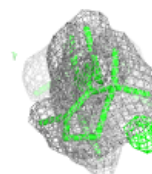
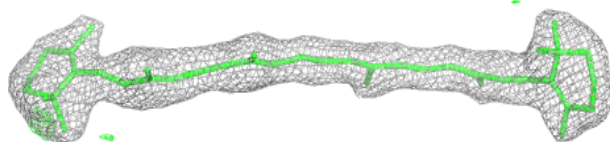
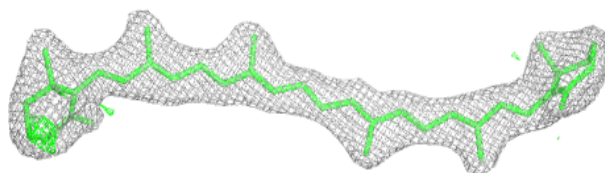


Electron density around LMG C 518:

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

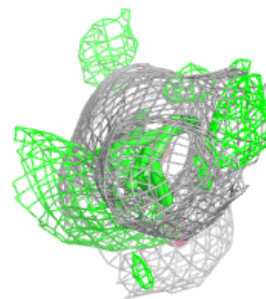
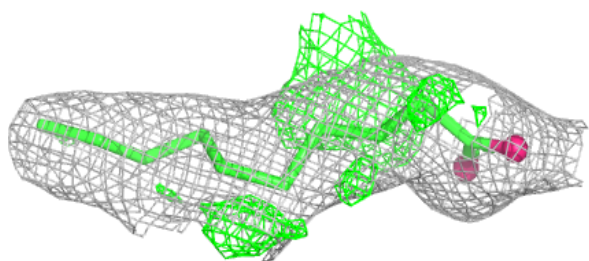
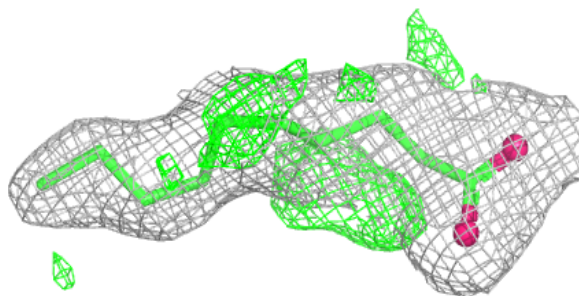
**Electron density around BCR k 101:**

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

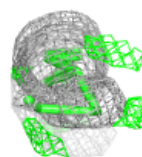
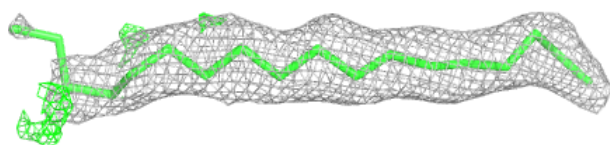
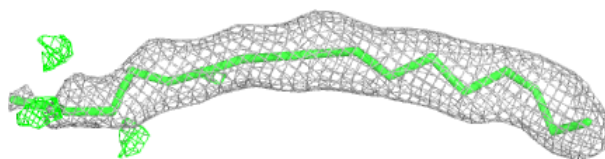


Electron density around STE B 624:

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

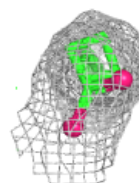
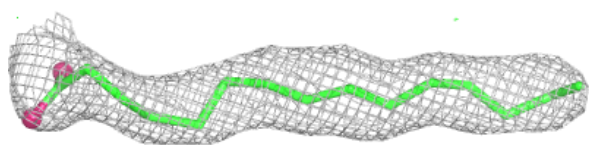
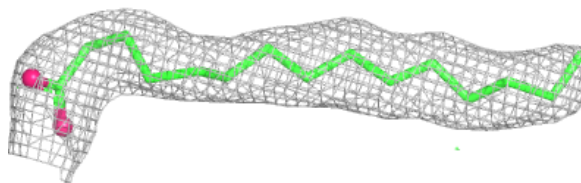
**Electron density around STE I 102:**

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

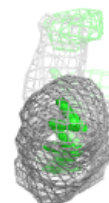
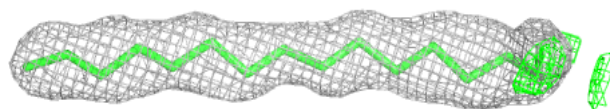
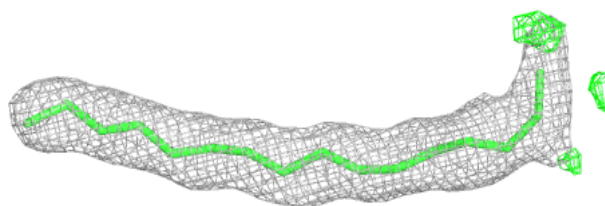


Electron density around STE d 410:

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

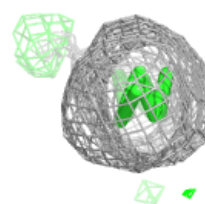
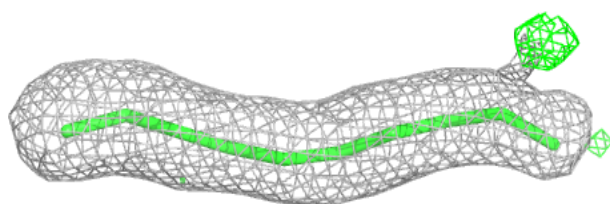
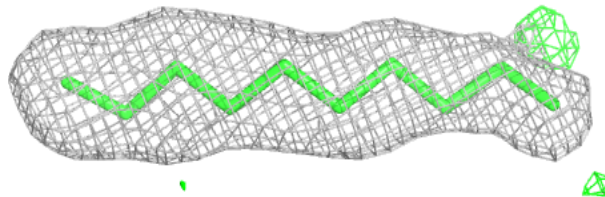
**Electron density around STE C 521:**

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

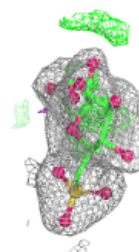
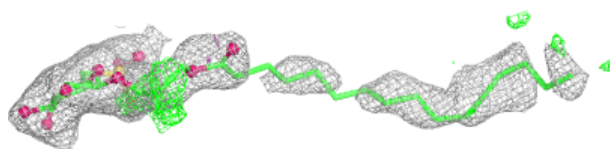
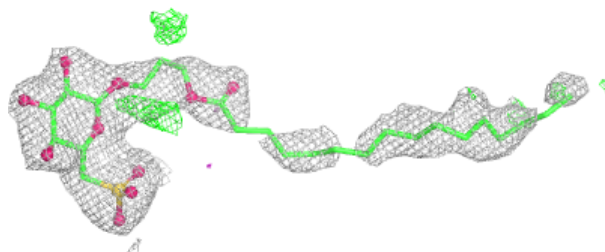


Electron density around STE M 103:

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

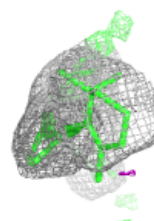
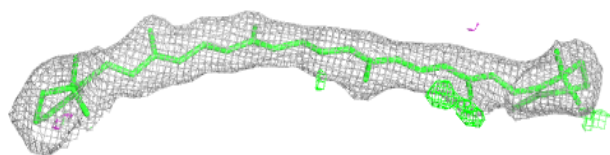
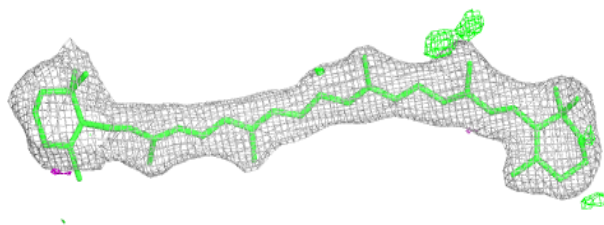
**Electron density around SQD F 102:**

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

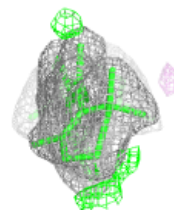
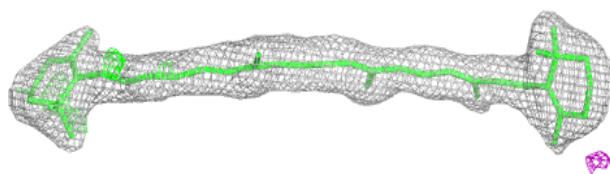
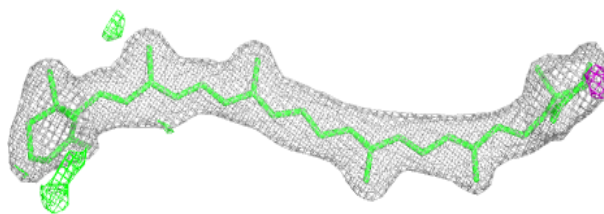


Electron density around BCR d 404:

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

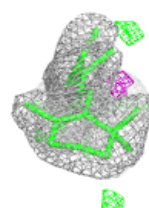
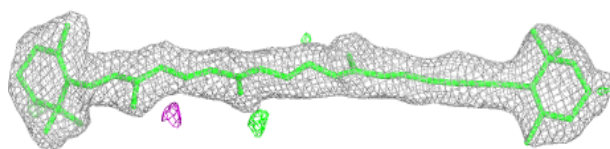
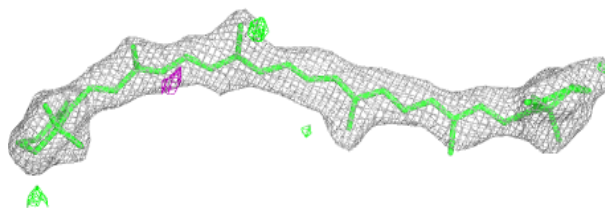
**Electron density around BCR K 102:**

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



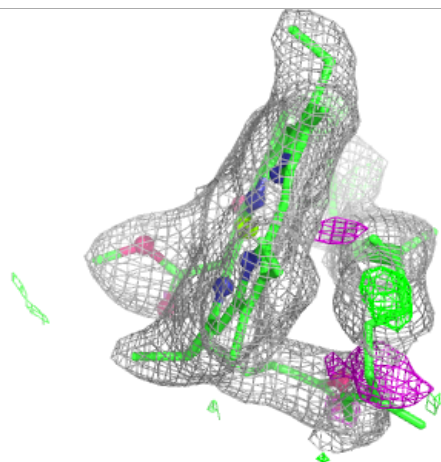
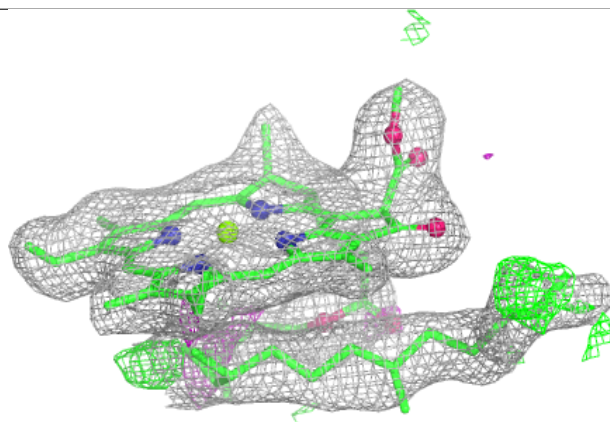
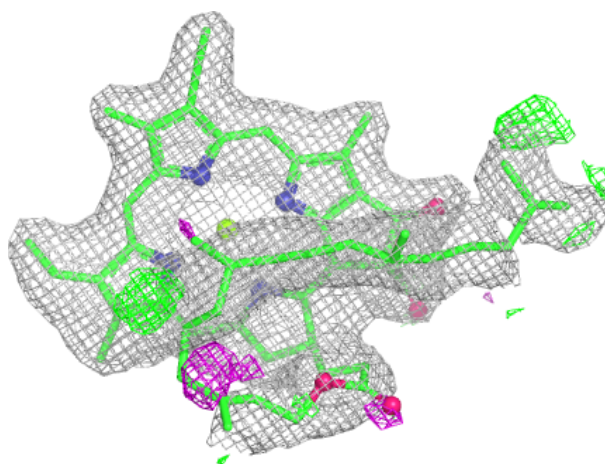
Electron density around BCR h 102:

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



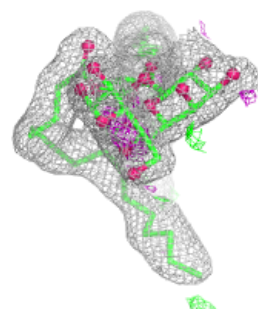
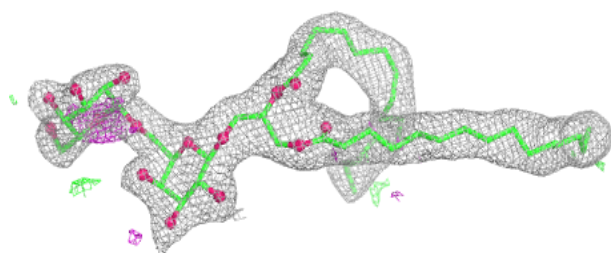
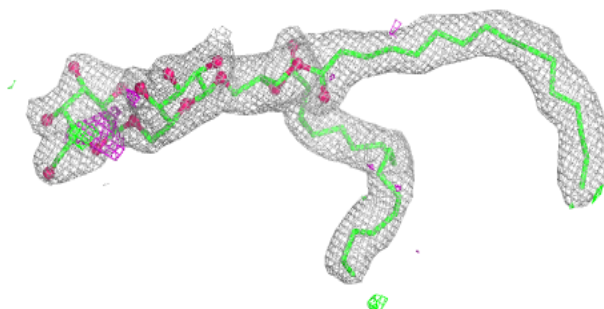
Electron density around CLA B 601:

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

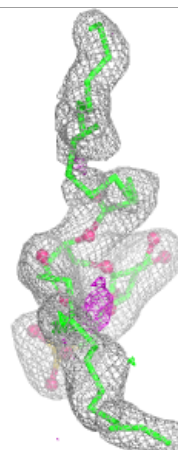
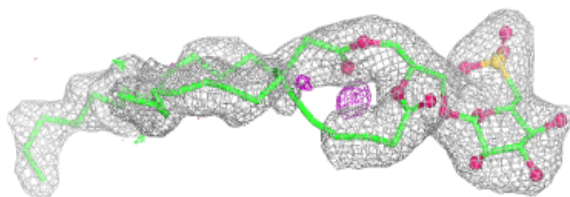
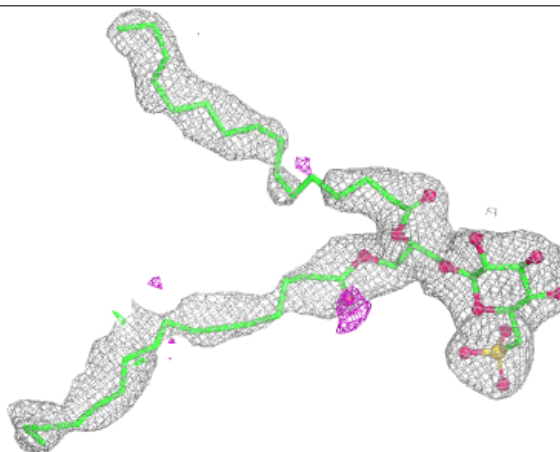


Electron density around DGD H 102:

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

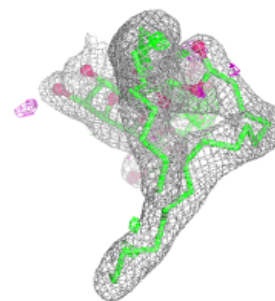
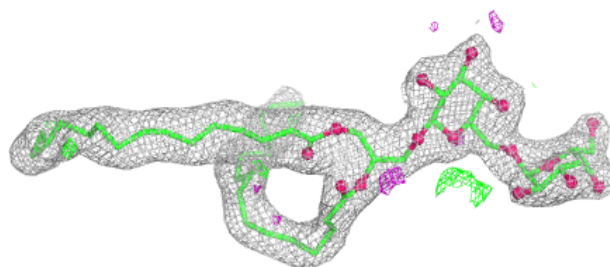
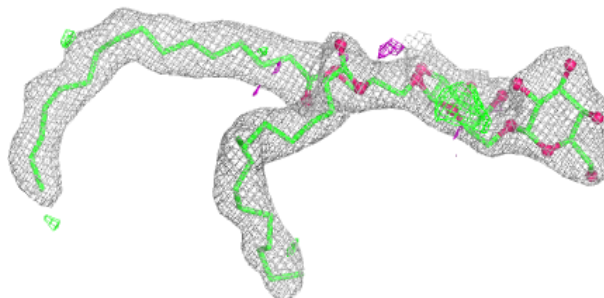
**Electron density around SQD a 615:**

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

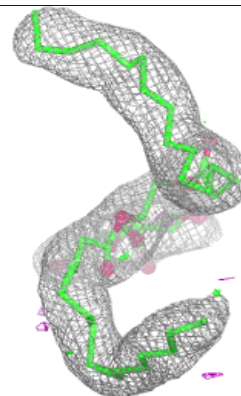
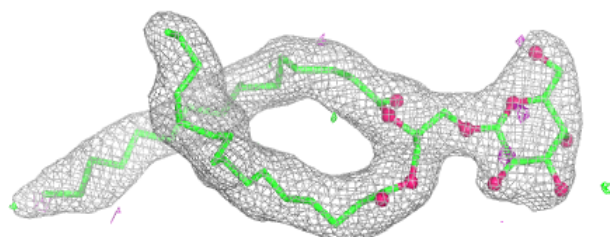
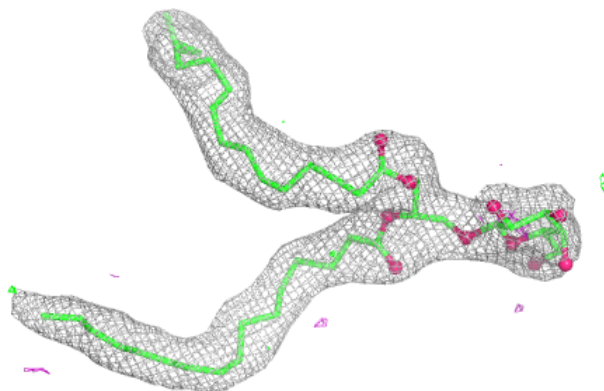


Electron density around DGD h 103:

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

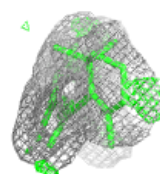
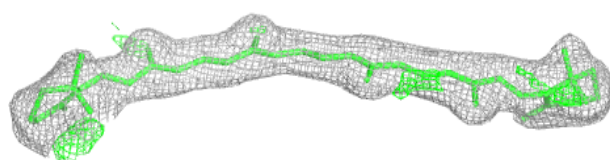
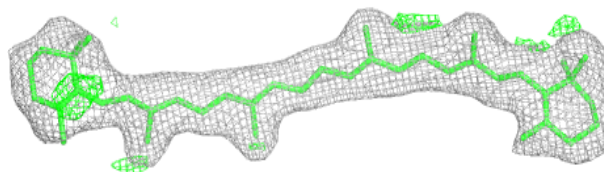
**Electron density around LMG M 101:**

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

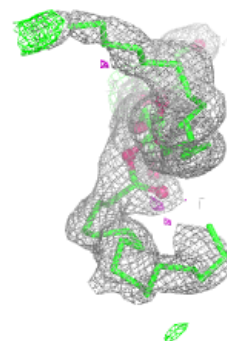
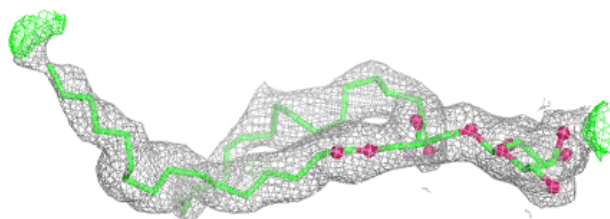
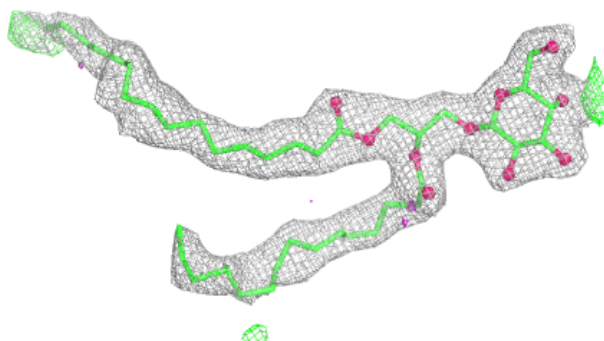


Electron density around BCR D 405:

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

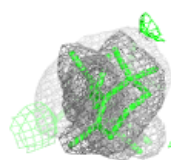
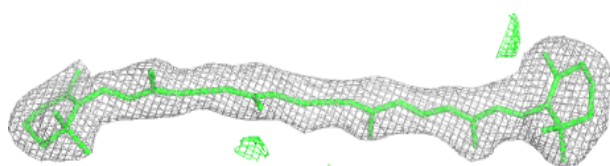
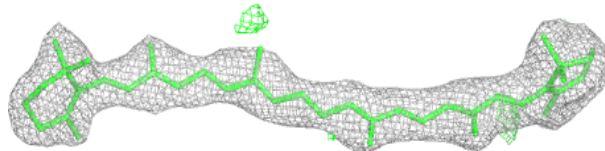
**Electron density around LMG D 407:**

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

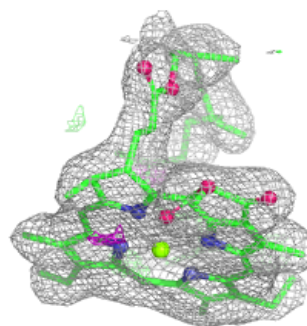
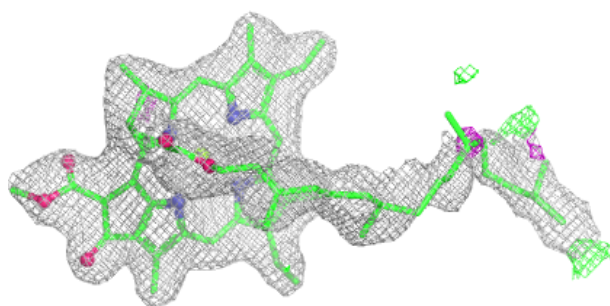
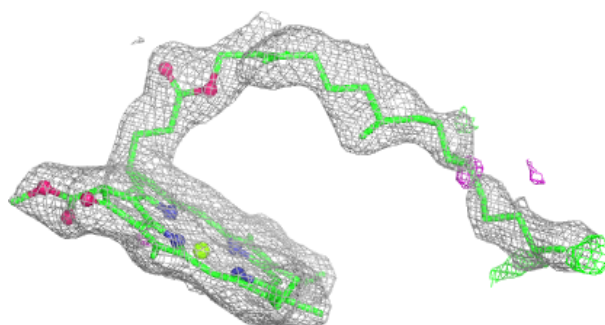


Electron density around BCR c 514:

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

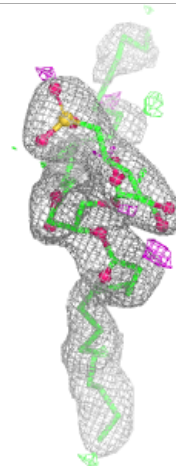
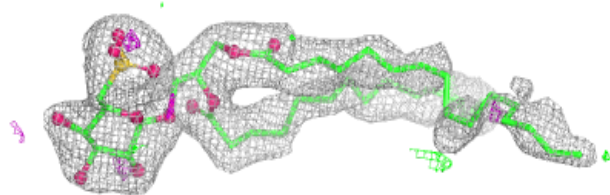
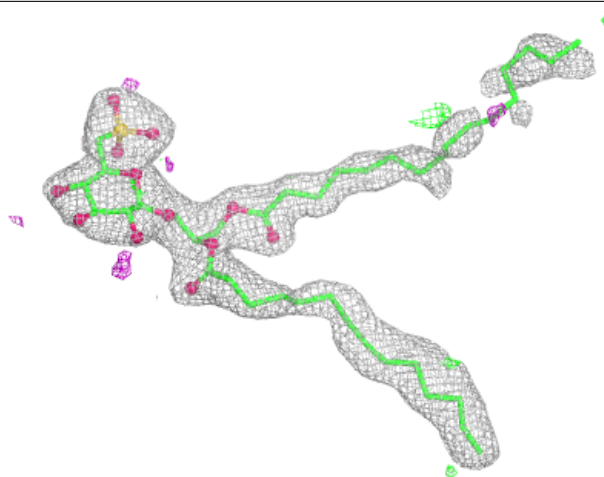
**Electron density around CLA C 513:**

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



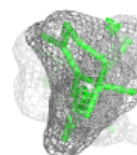
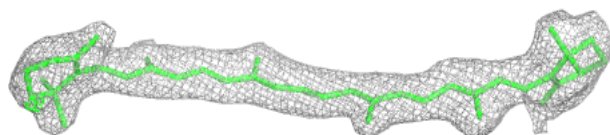
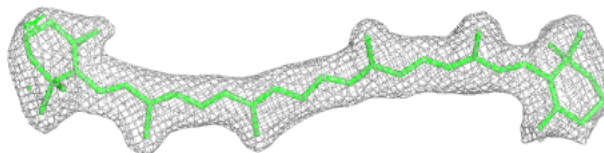
Electron density around SQD A 615:

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

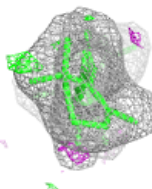
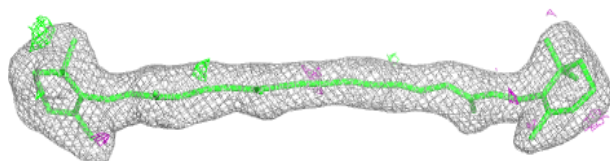
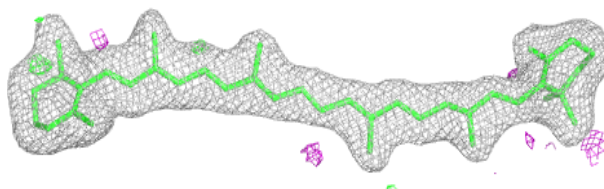


Electron density around BCR b 618:

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

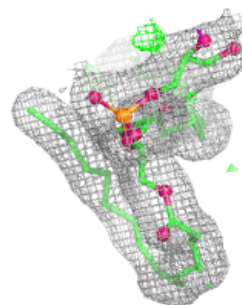
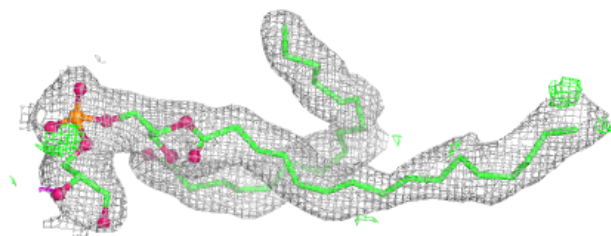
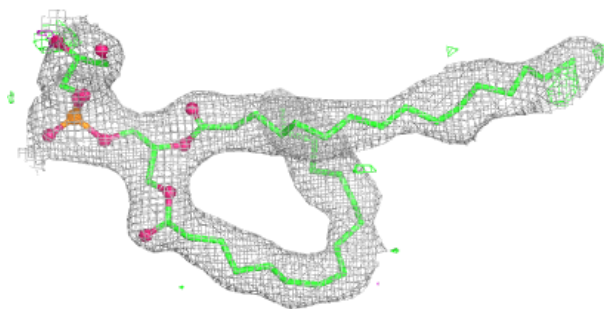
**Electron density around BCR B 618:**

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

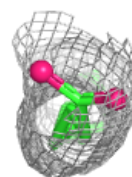
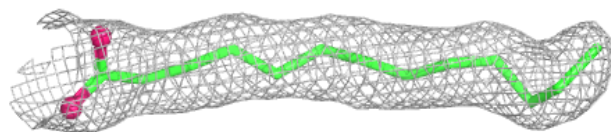
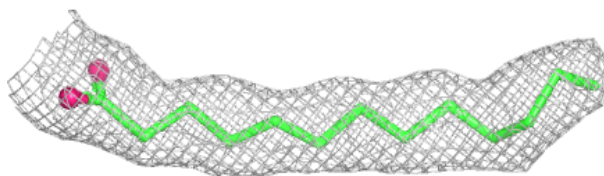


Electron density around LHG a 614:

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

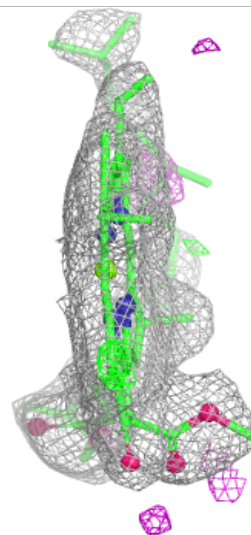
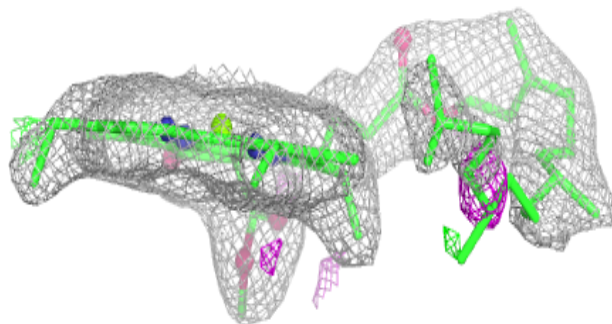
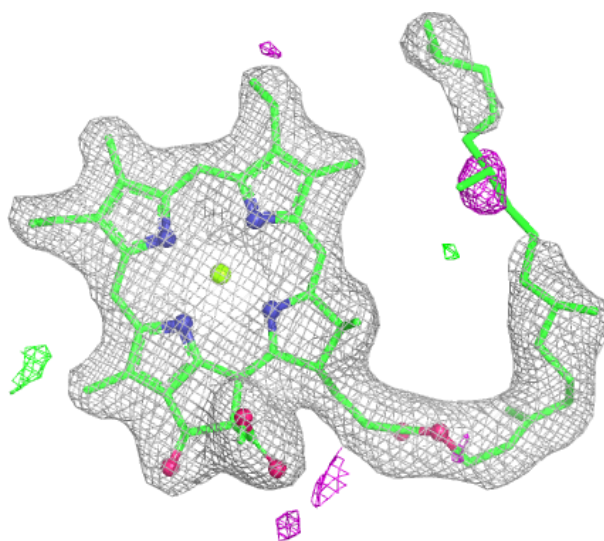
**Electron density around STE M 102:**

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



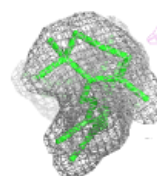
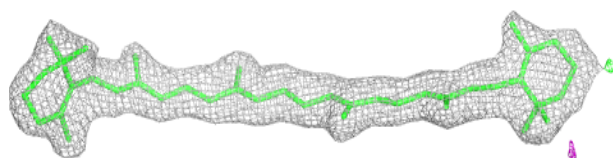
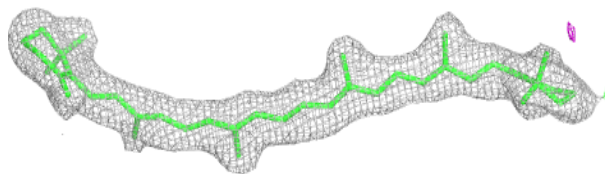
Electron density around CLA c 512:

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

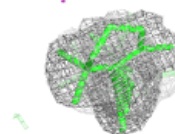
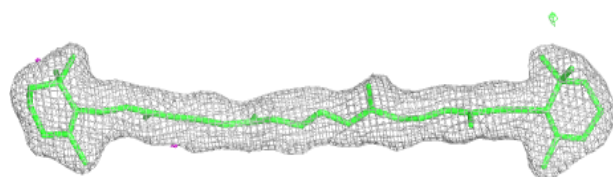
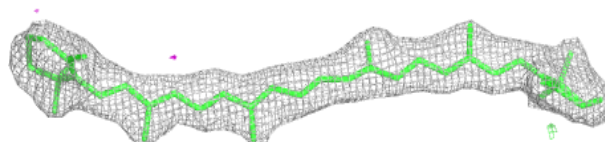


Electron density around BCR H 101:

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

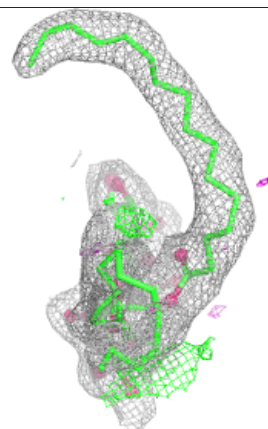
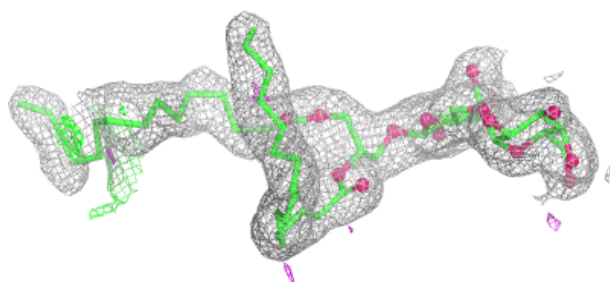
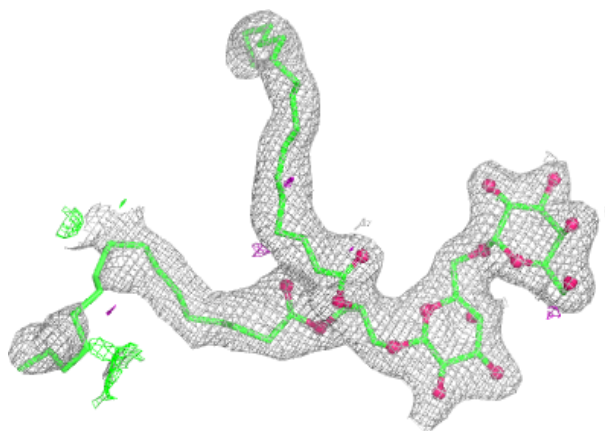
**Electron density around BCR K 101:**

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



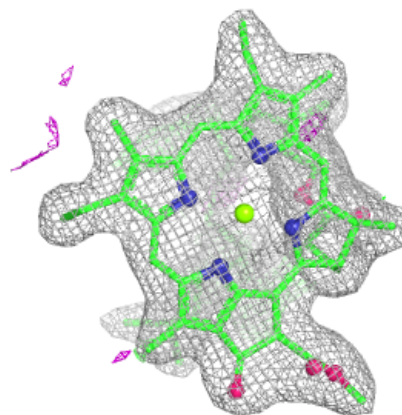
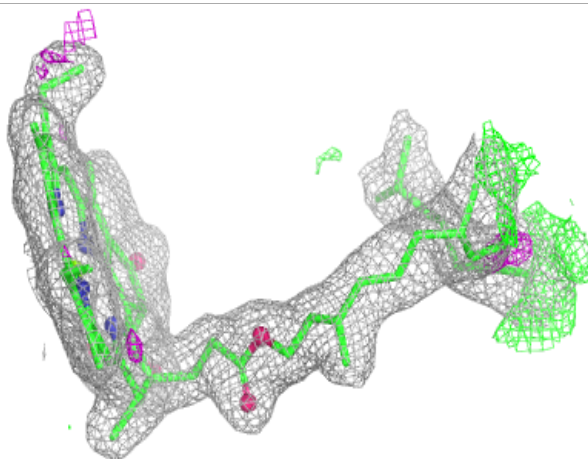
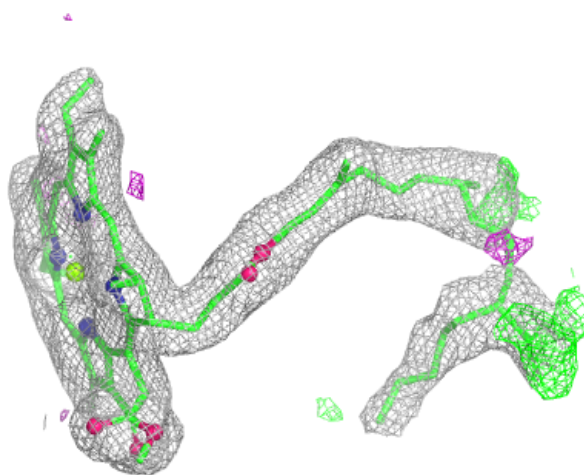
Electron density around DGD C 516:

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



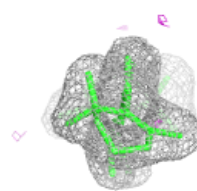
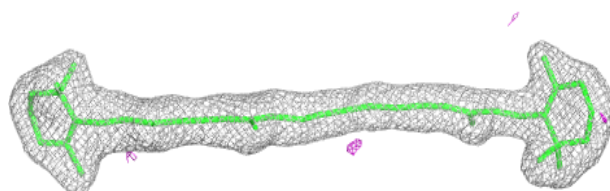
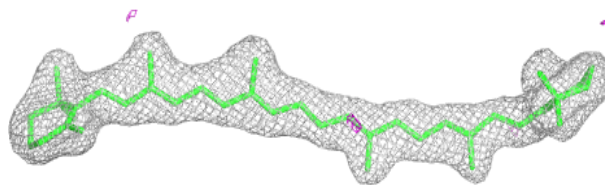
Electron density around CLA B 606:

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

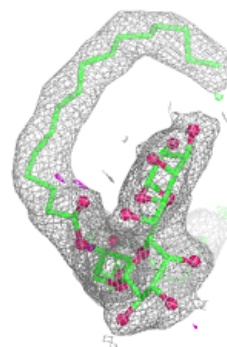
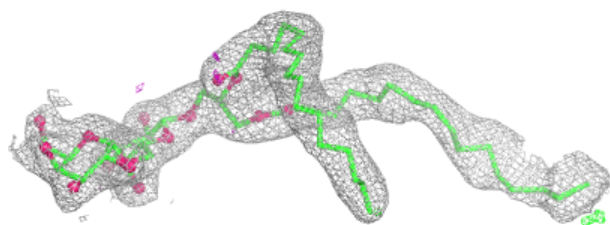
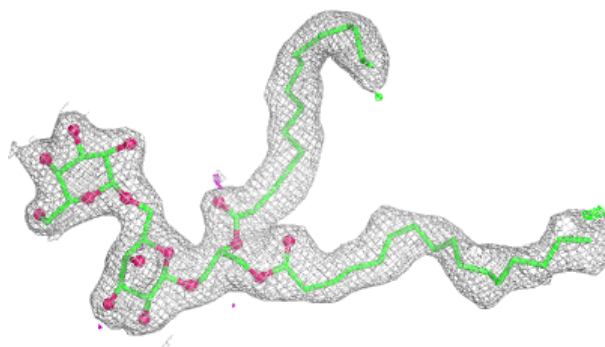


Electron density around BCR A 610:

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

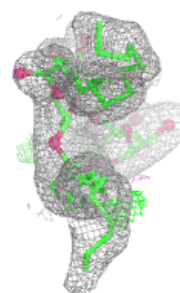
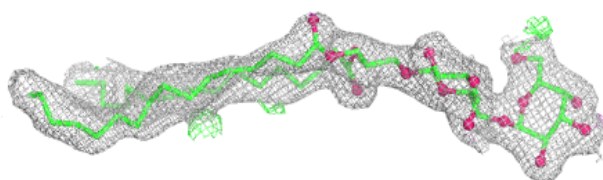
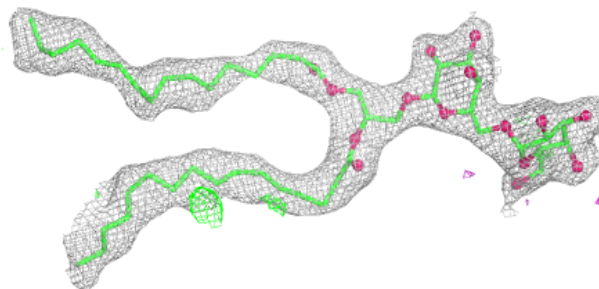
**Electron density around DGD c 517:**

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

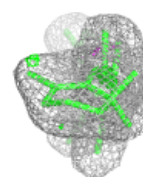
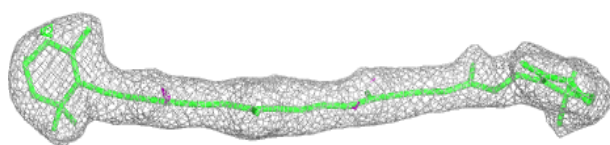
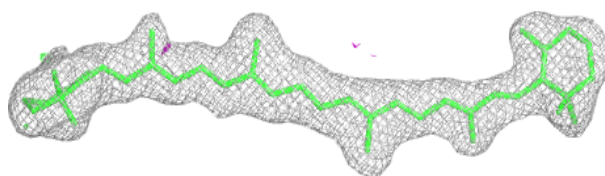


Electron density around DGD c 518:

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

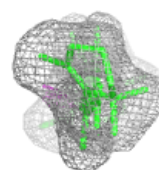
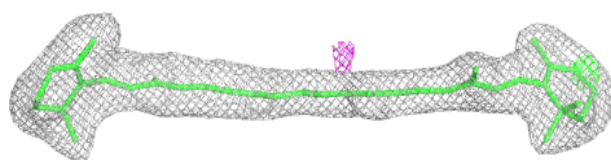
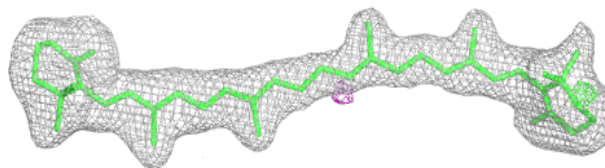
**Electron density around BCR b 616:**

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

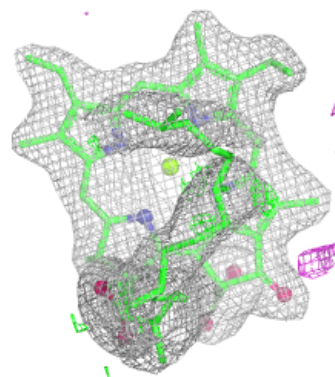
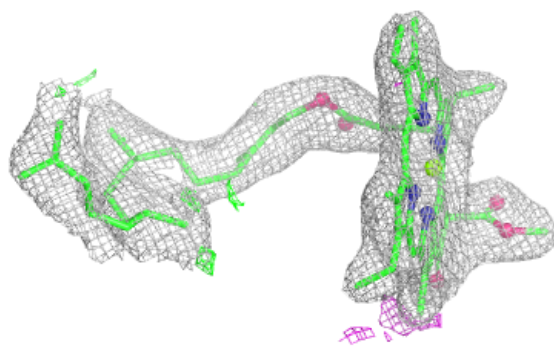
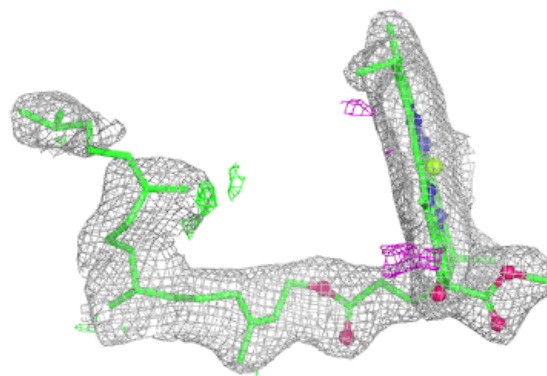


Electron density around BCR b 617:

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

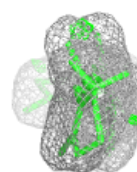
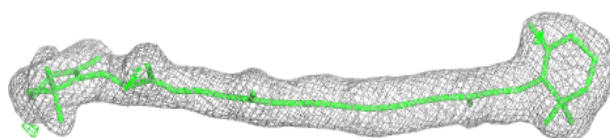
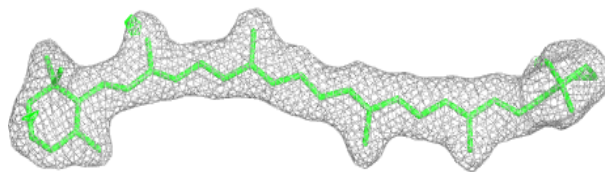
**Electron density around CLA c 506:**

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

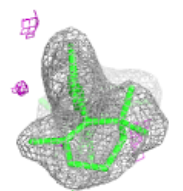
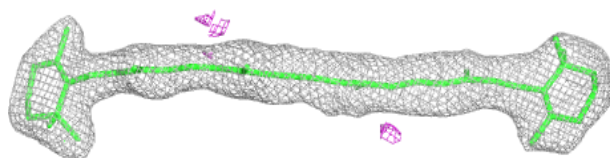
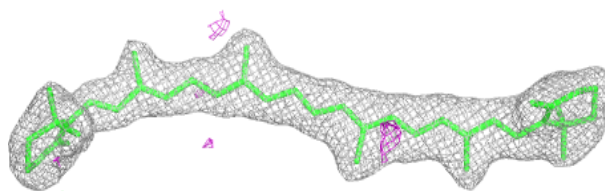


Electron density around BCR B 617:

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

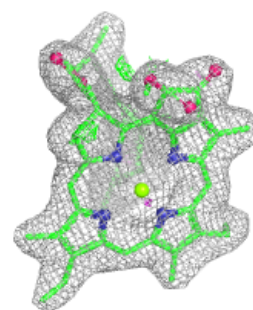
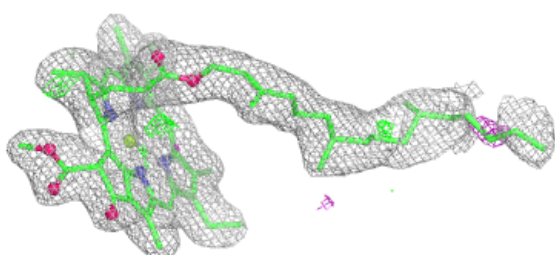
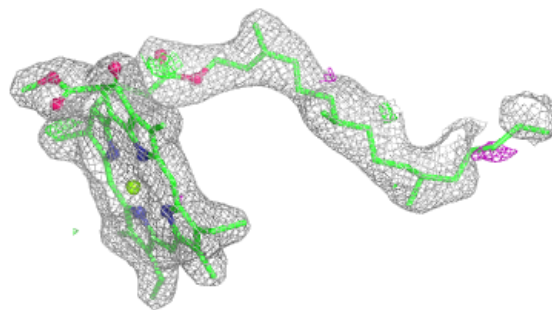
**Electron density around BCR c 515:**

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

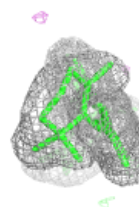
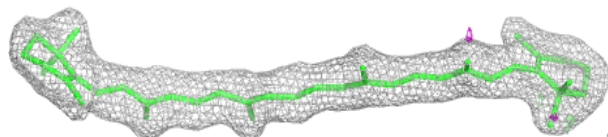
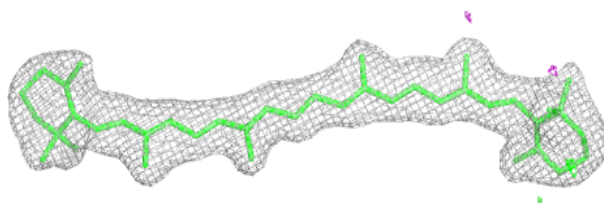


Electron density around CLA c 508:

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

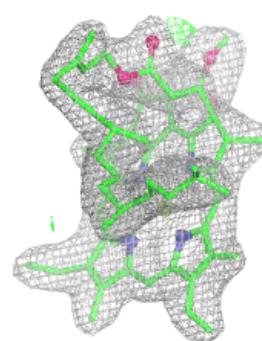
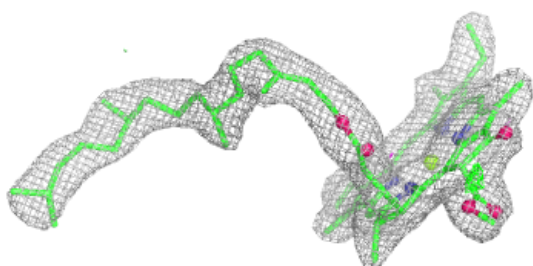
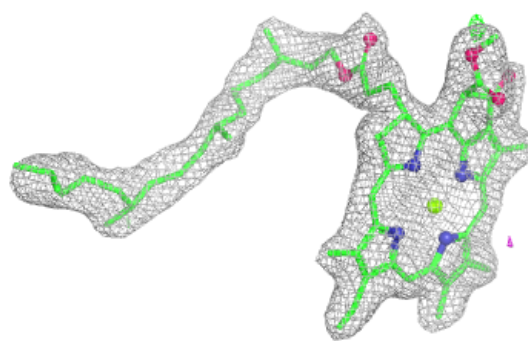
**Electron density around BCR B 619:**

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

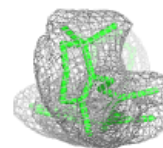
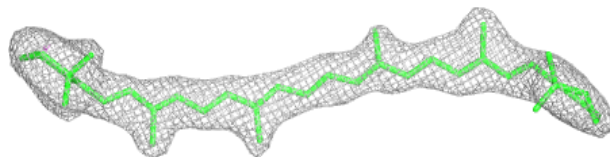
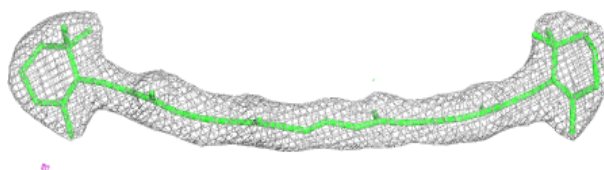


Electron density around CLA c 511:

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

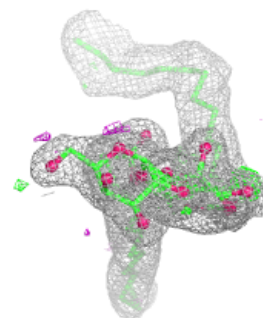
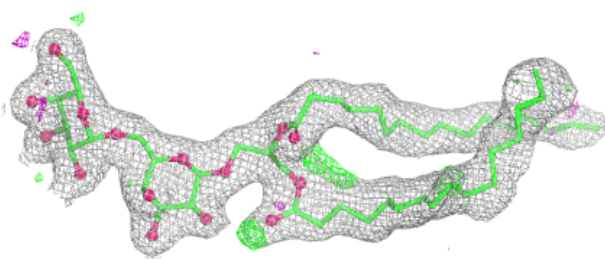
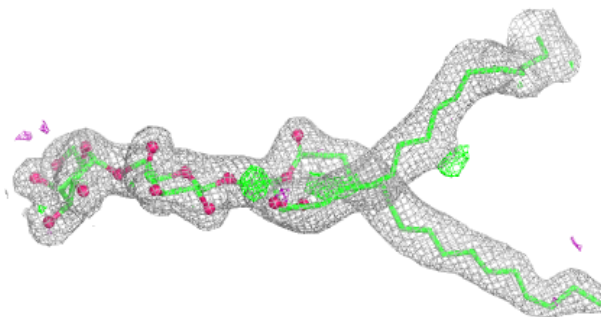
**Electron density around BCR k 102:**

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

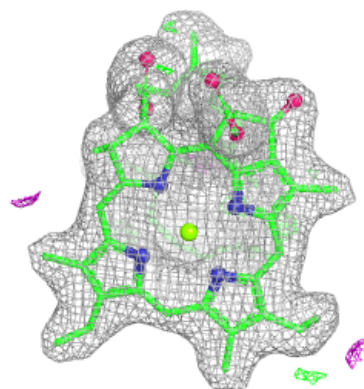
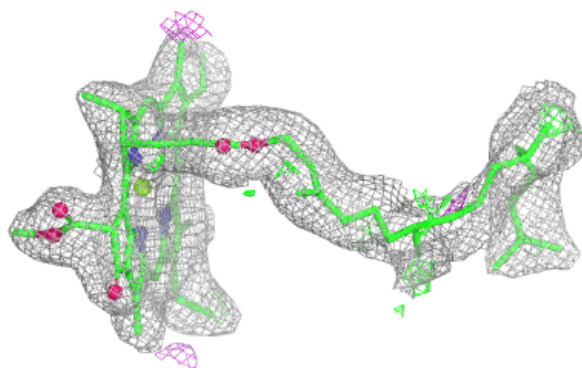
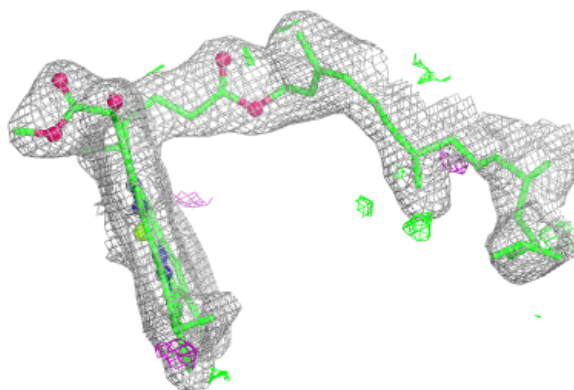


Electron density around DGD C 515:

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

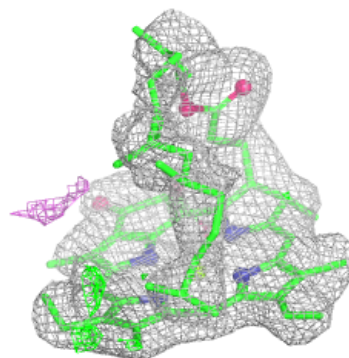
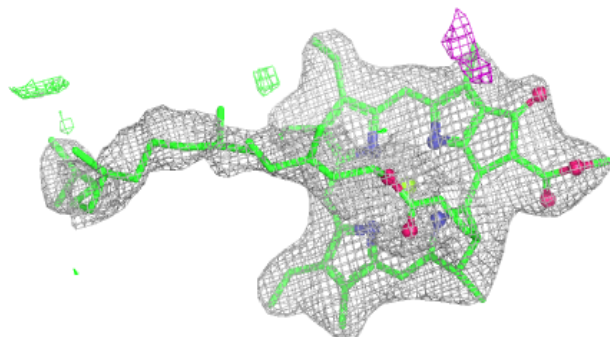
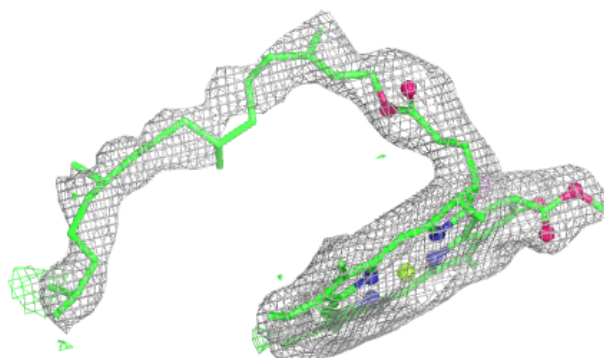
**Electron density around CLA C 506:**

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

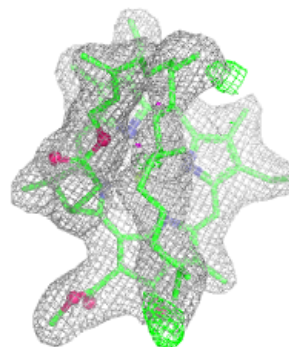
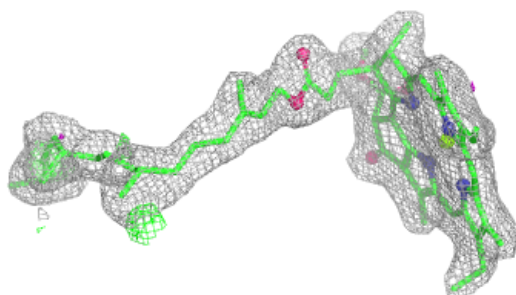
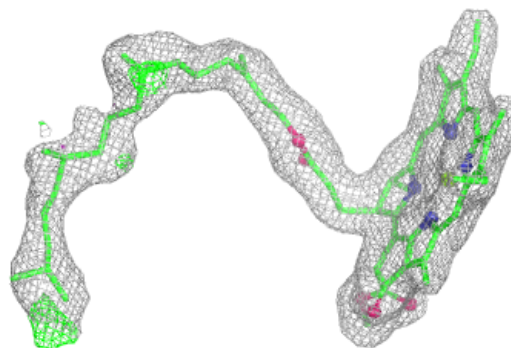


Electron density around CLA c 513:

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

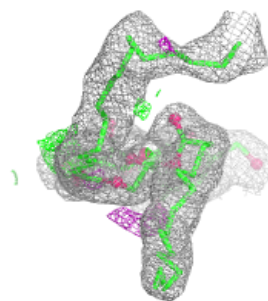
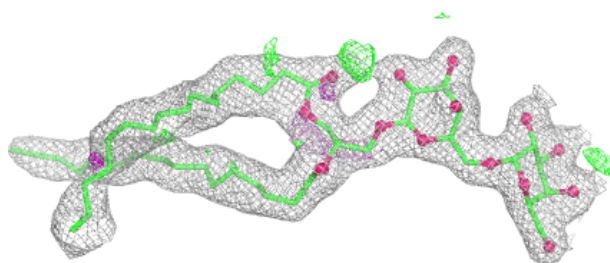
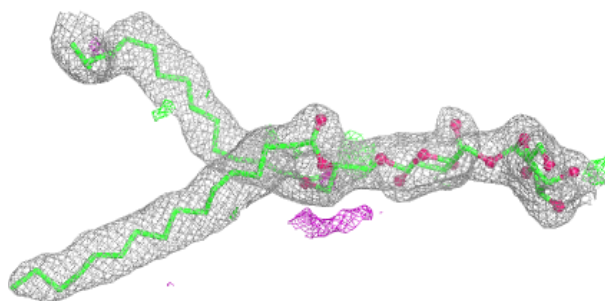
**Electron density around CLA b 605:**

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

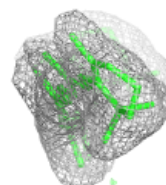
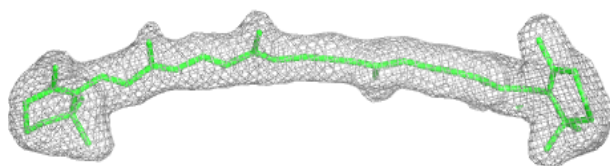
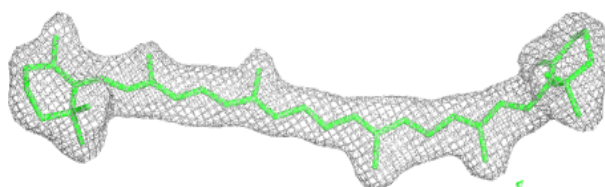


Electron density around DGD c 516:

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

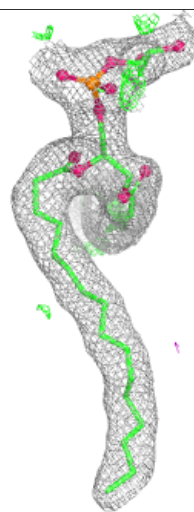
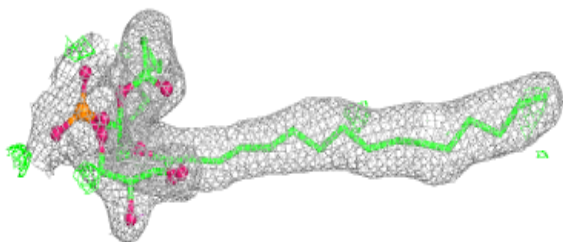
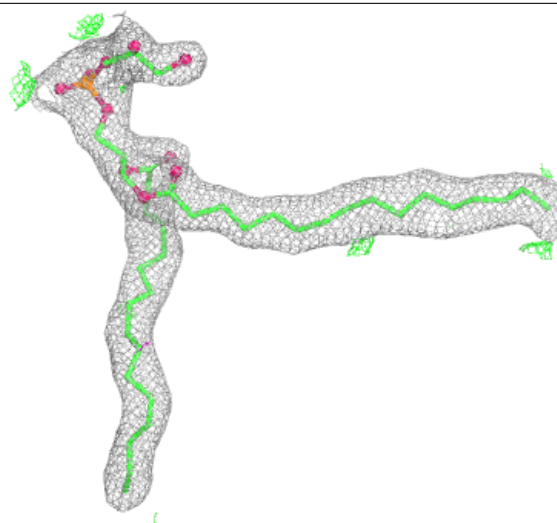
**Electron density around BCR T 101:**

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



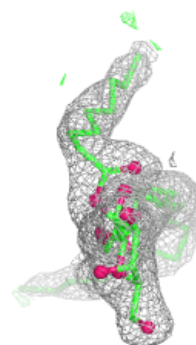
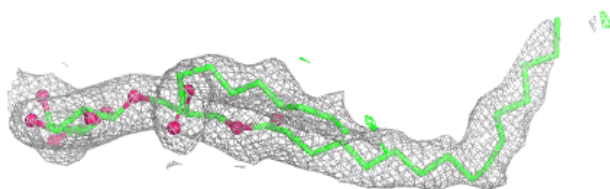
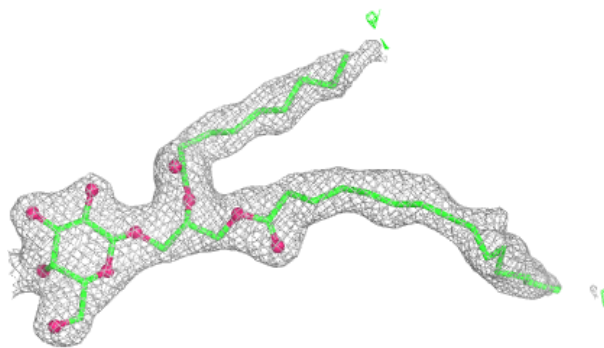
Electron density around LHG 1 101:

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

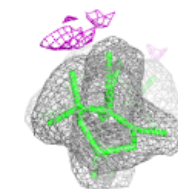
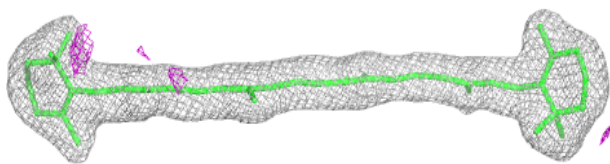
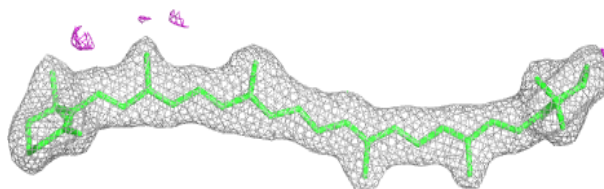


Electron density around LMG d 409:

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

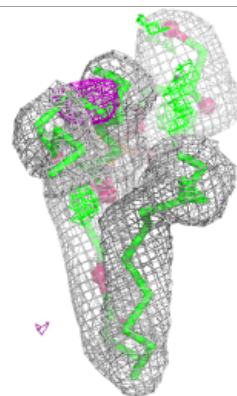
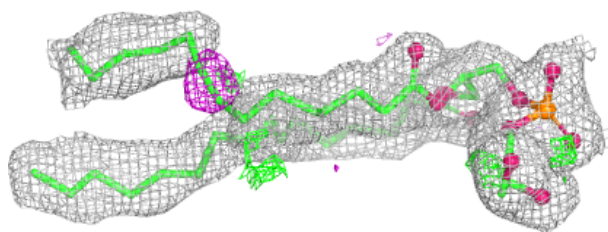
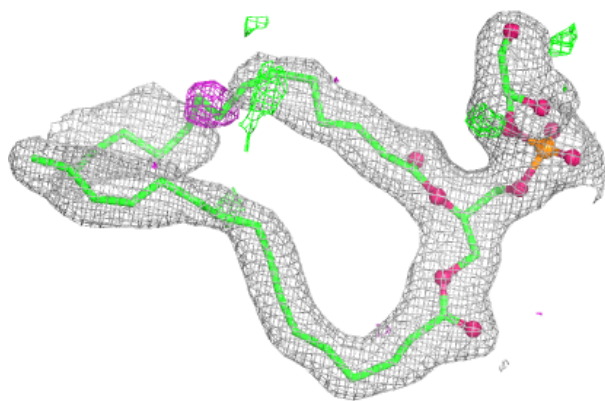
**Electron density around BCR a 611:**

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

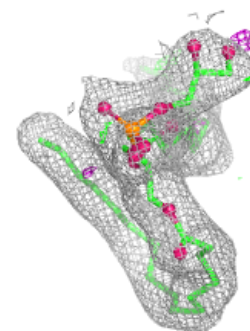
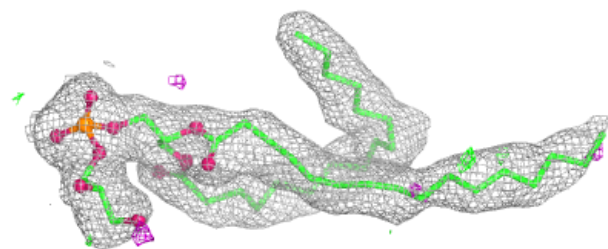
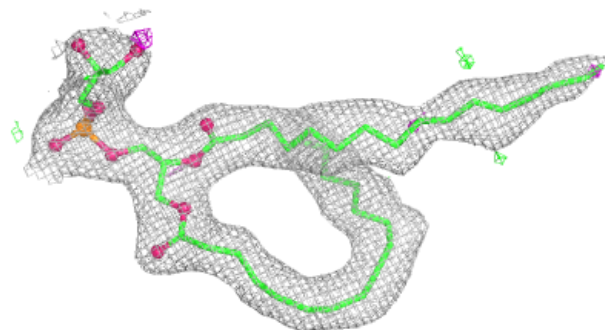


Electron density around LHG A 614:

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

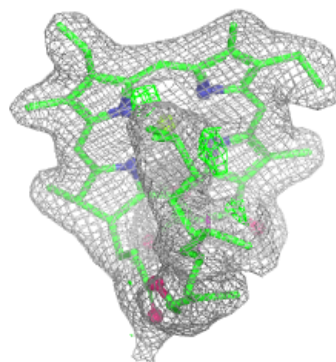
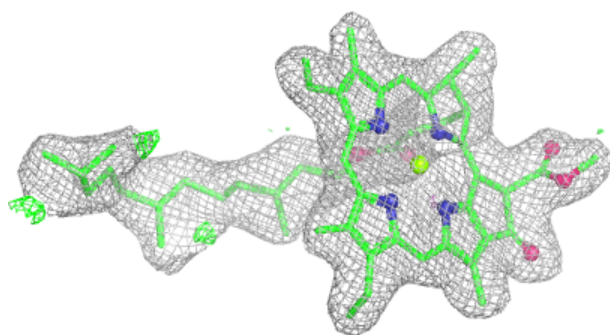
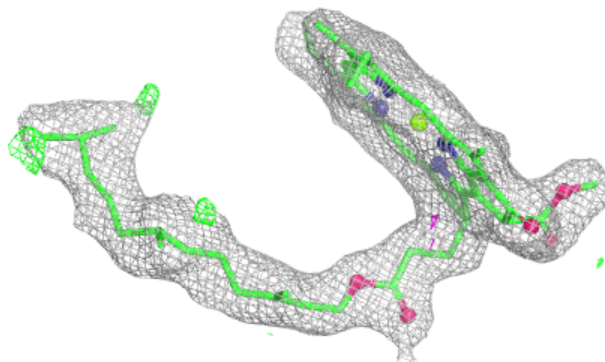
**Electron density around LHG B 622:**

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

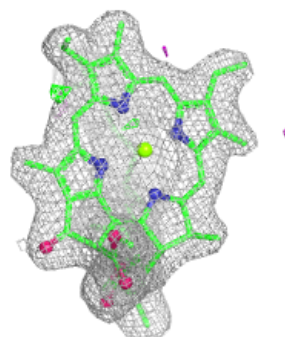
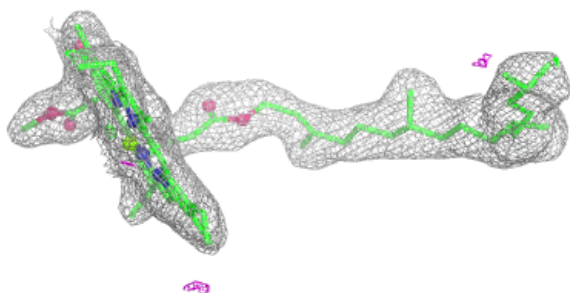
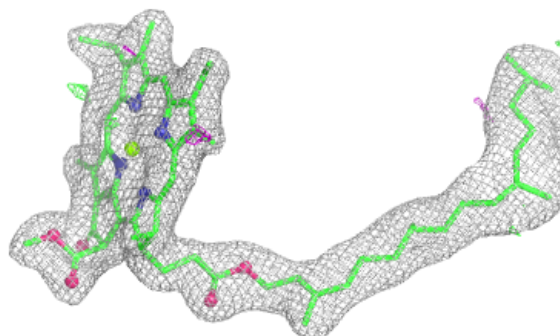


Electron density around CLA c 504:

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

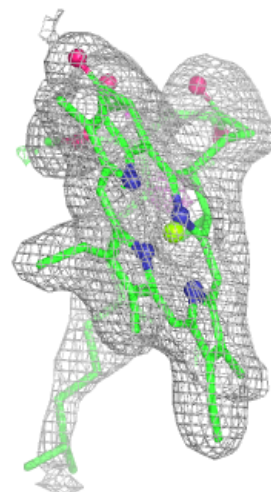
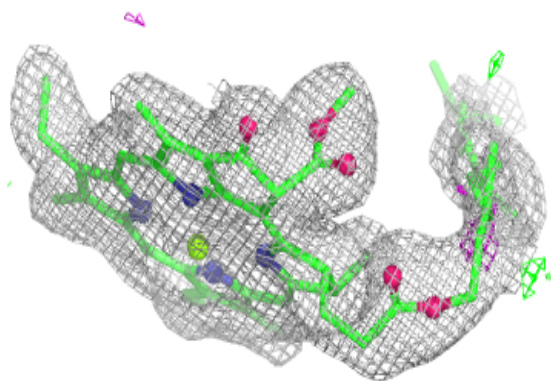
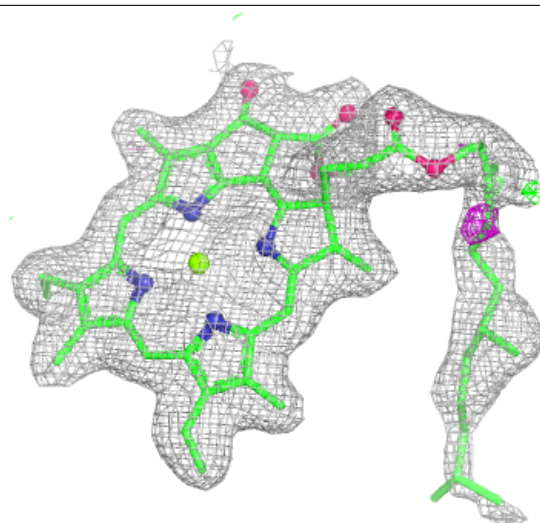
**Electron density around CLA B 609:**

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



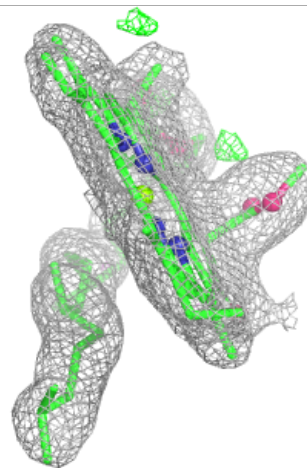
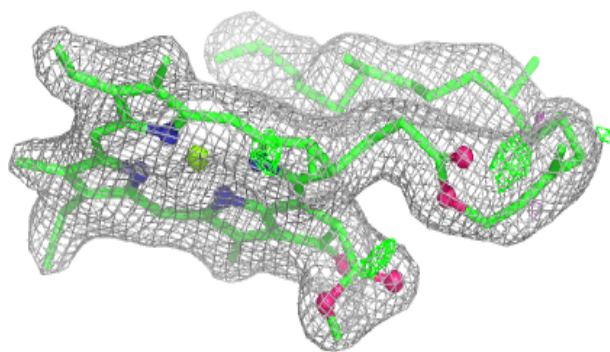
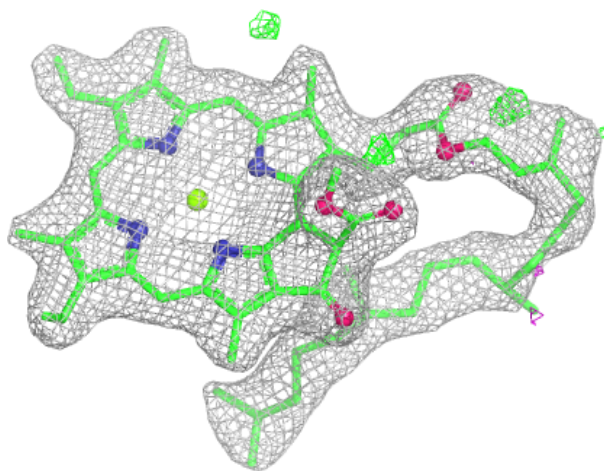
Electron density around CLA B 616:

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



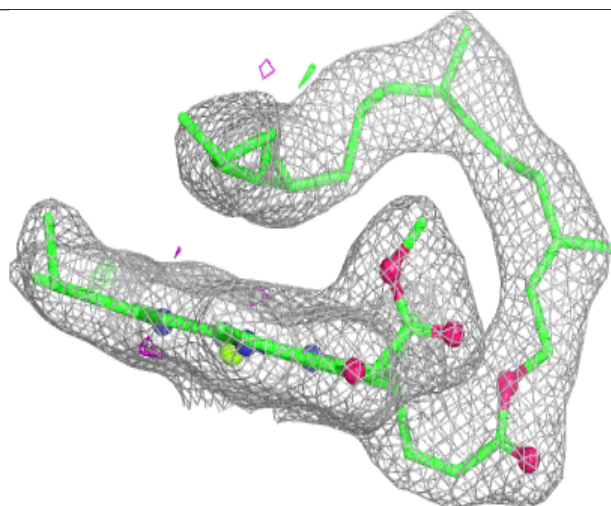
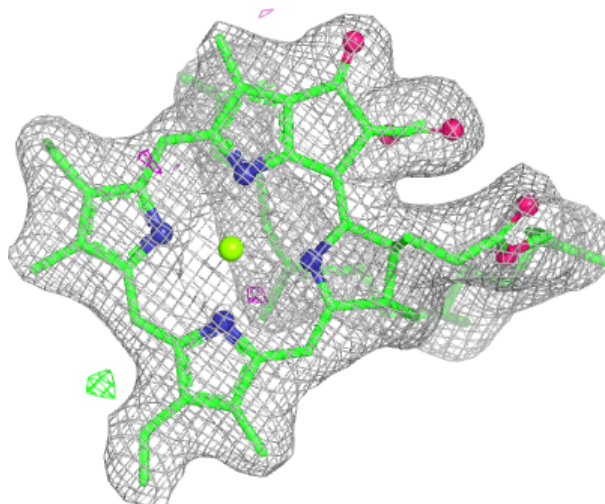
Electron density around CLA c 509:

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



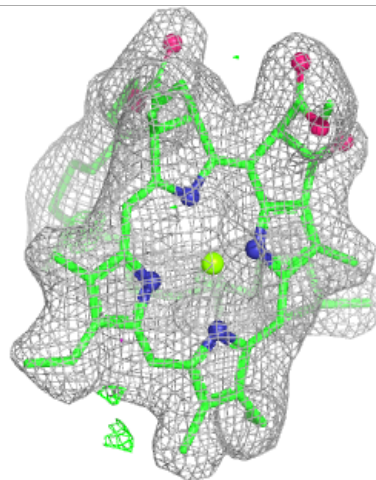
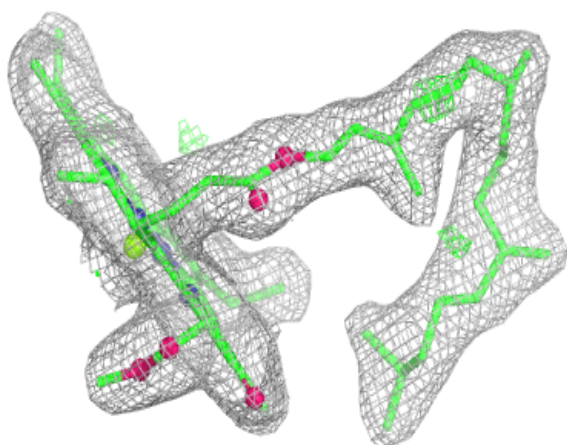
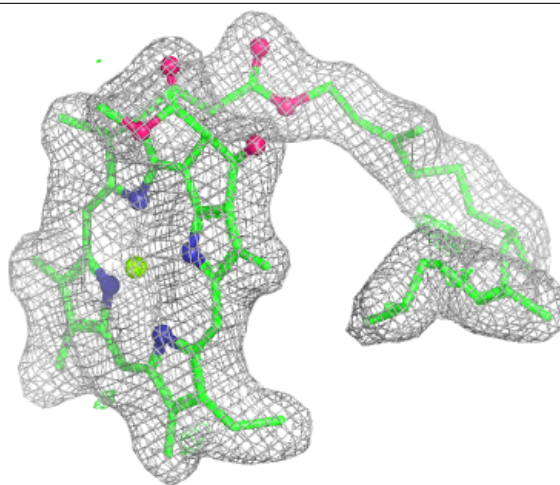
Electron density around CLA c 510:

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



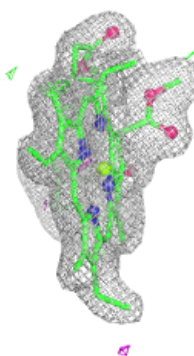
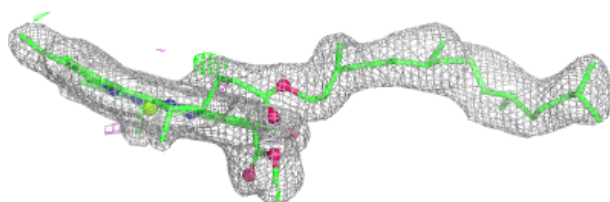
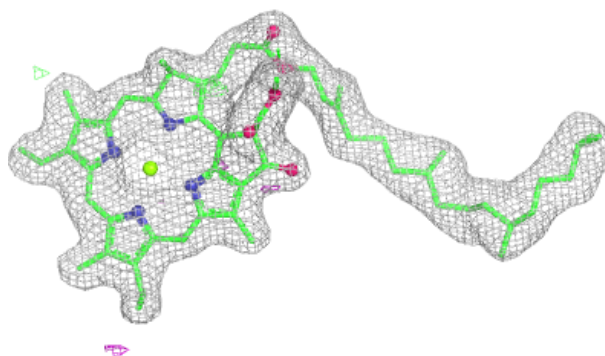
Electron density around CLA C 503:

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

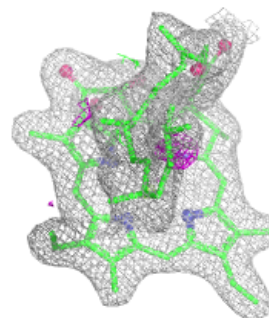
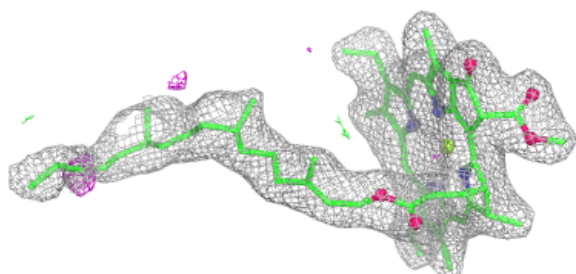
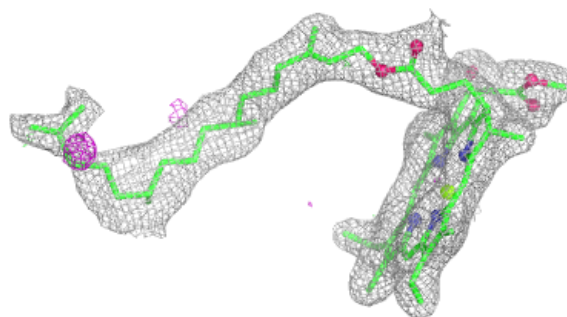


Electron density around CLA B 602:

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

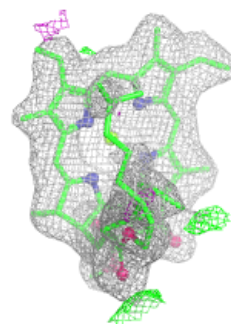
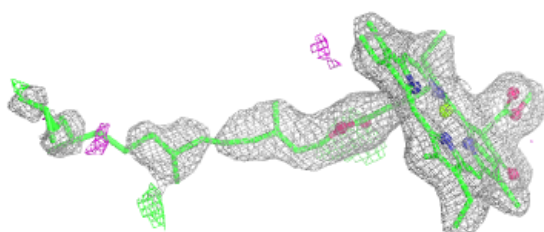
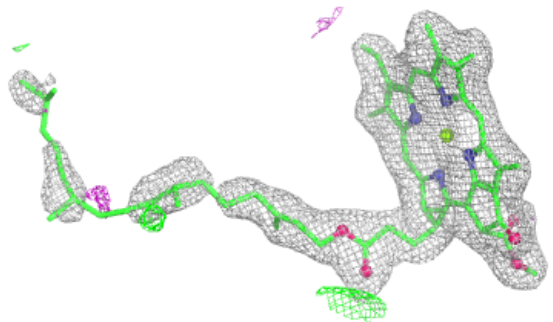
**Electron density around CLA C 508:**

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

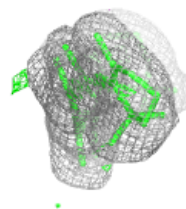
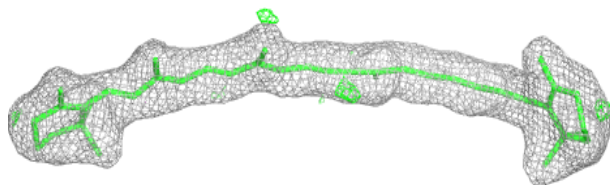
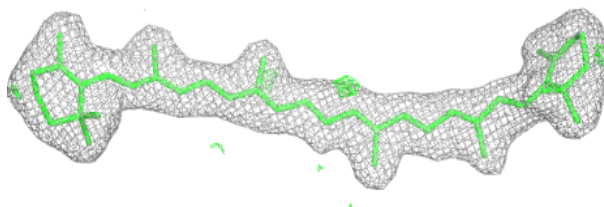


Electron density around CLA d 403:

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

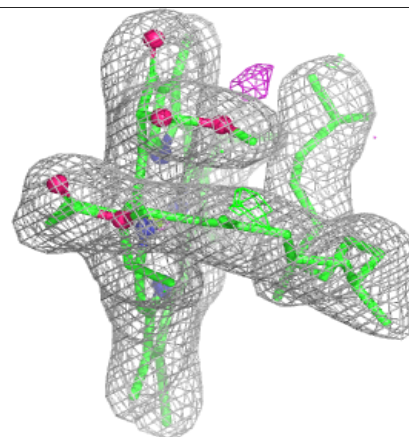
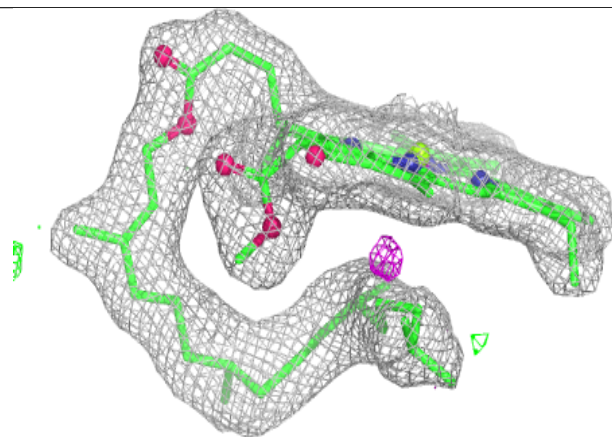
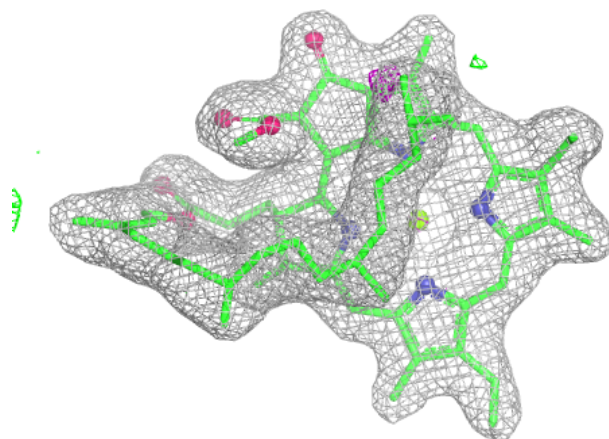
**Electron density around BCR t 101:**

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



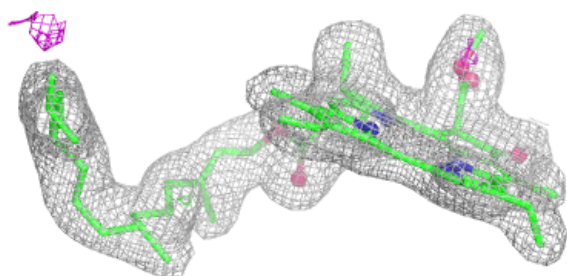
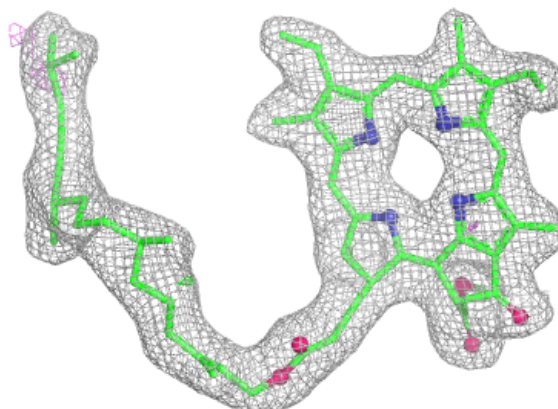
Electron density around CLA C 510:

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

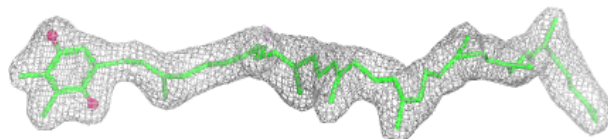
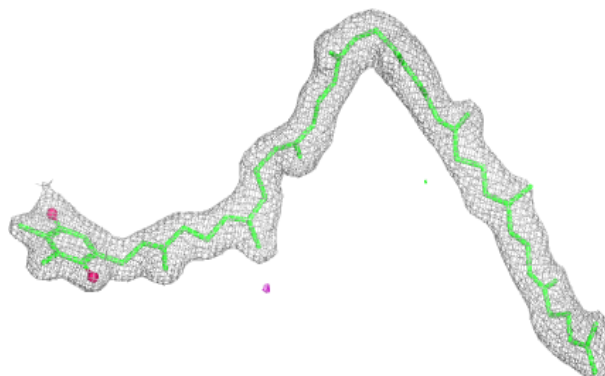


Electron density around PHO d 401:

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

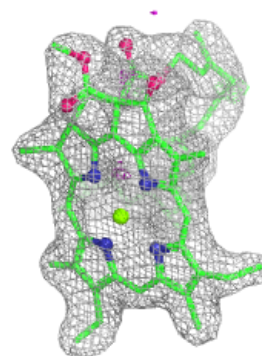
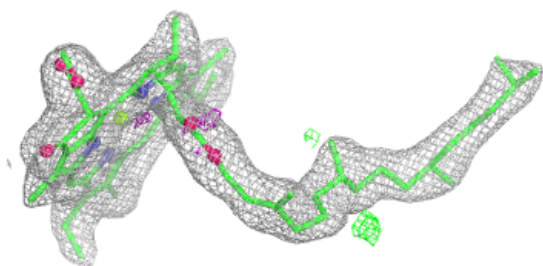
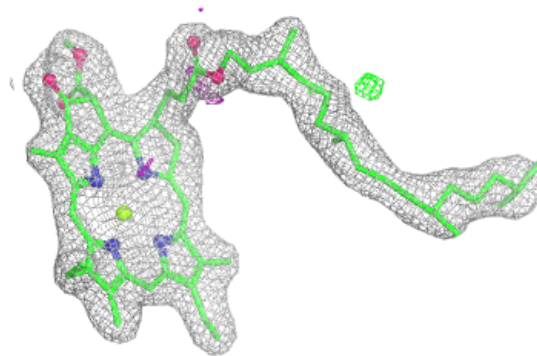
**Electron density around PL9 d 405:**

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



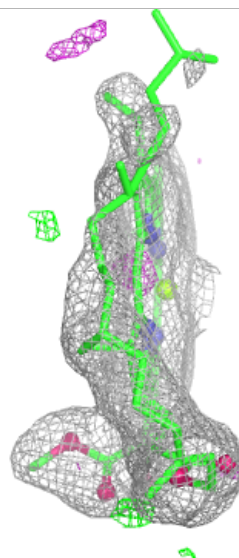
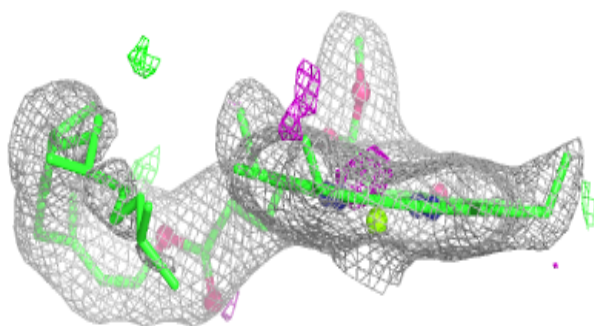
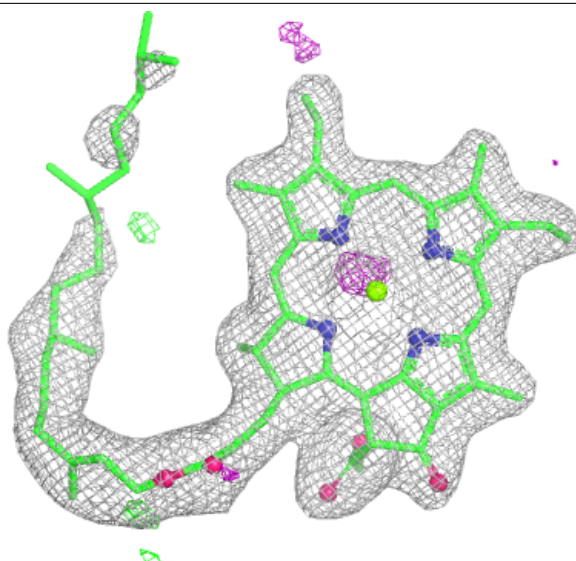
Electron density around CLA C 511:

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



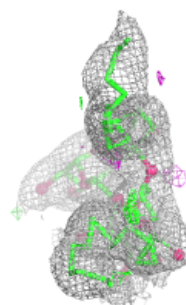
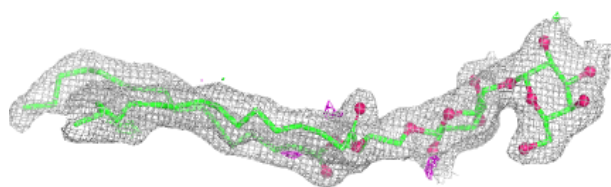
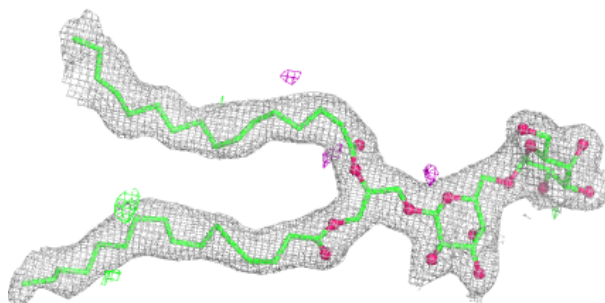
Electron density around CLA C 512:

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

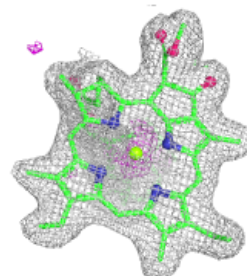
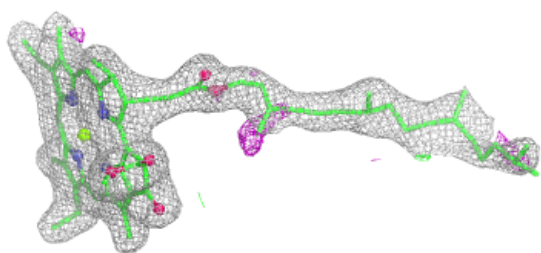
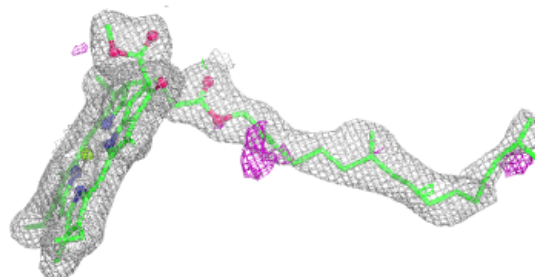


Electron density around DGD C 517:

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

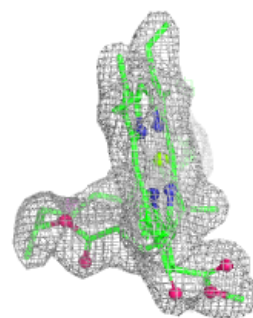
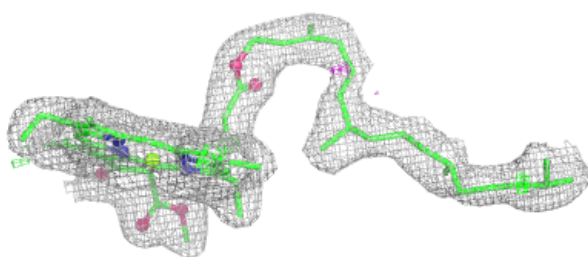
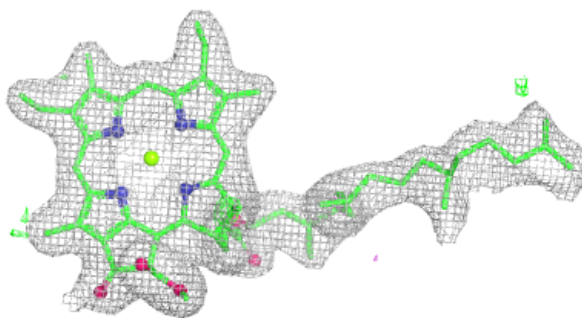
**Electron density around CLA B 604:**

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

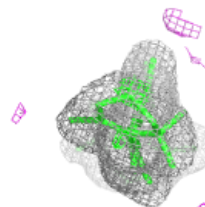
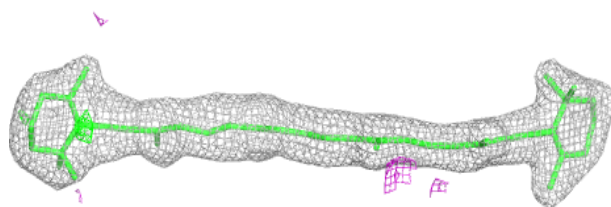
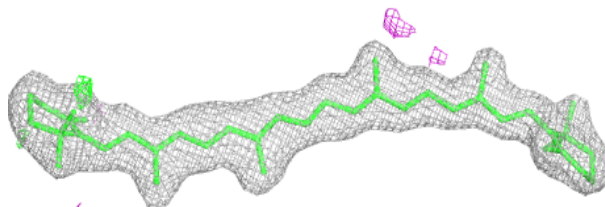


Electron density around CLA a 608:

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

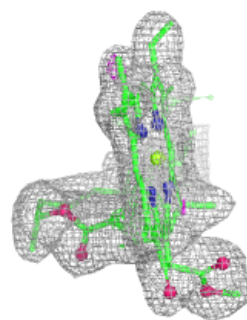
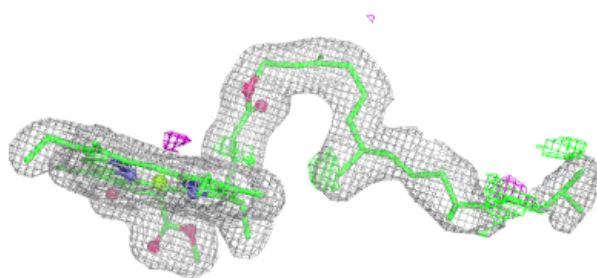
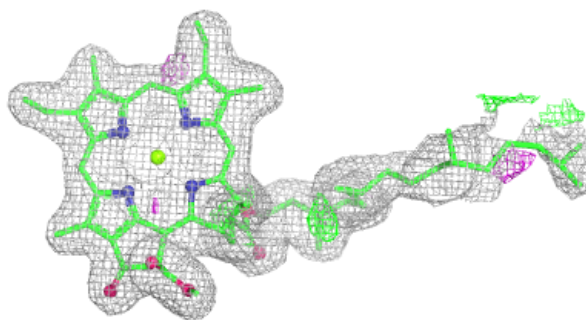
**Electron density around BCR C 514:**

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

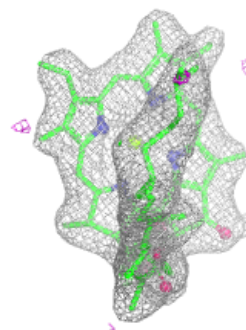
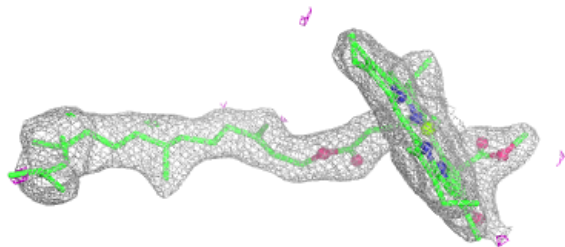
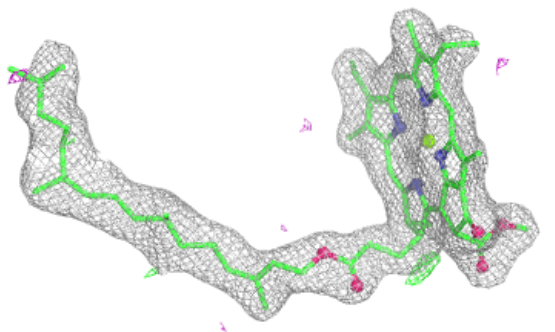


Electron density around CLA A 607:

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

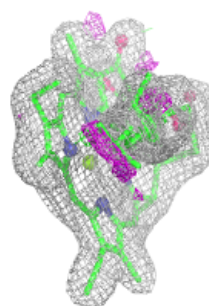
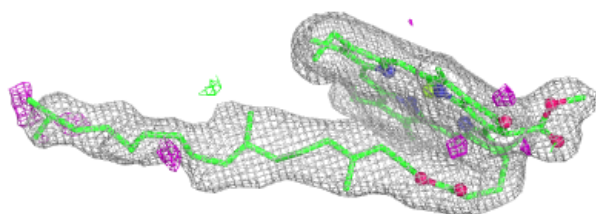
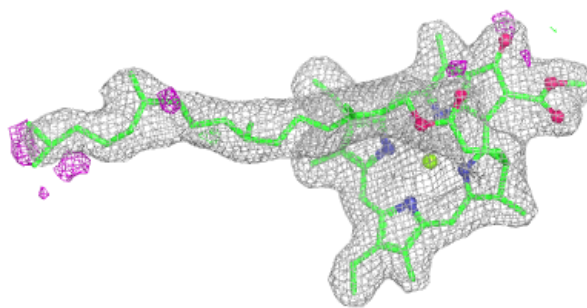
**Electron density around CLA b 608:**

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



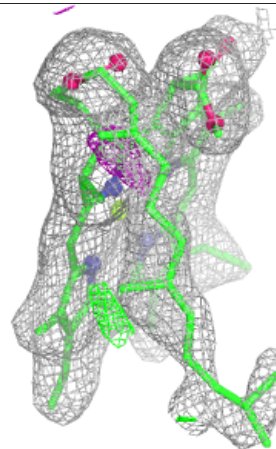
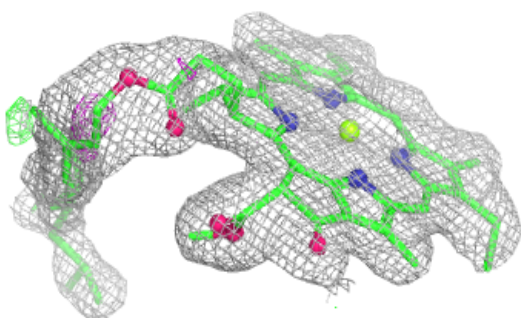
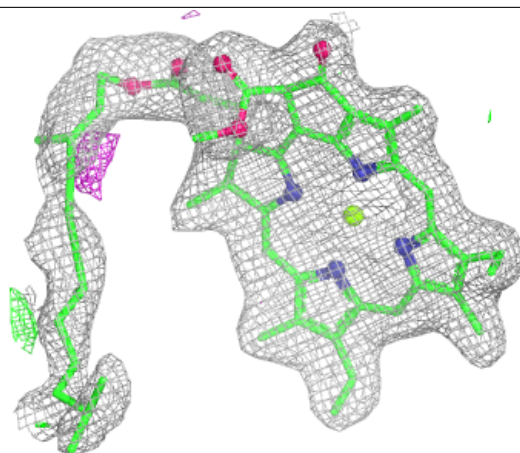
Electron density around CLA b 613:

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

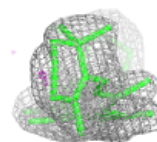
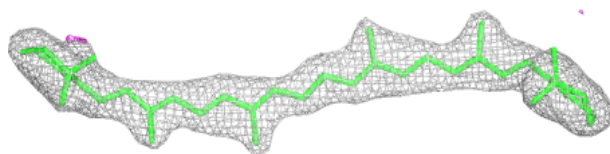
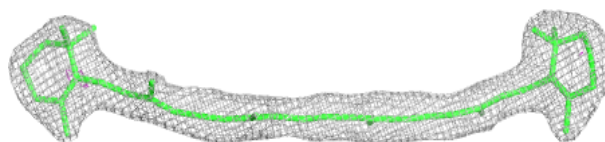


Electron density around CLA b 615:

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

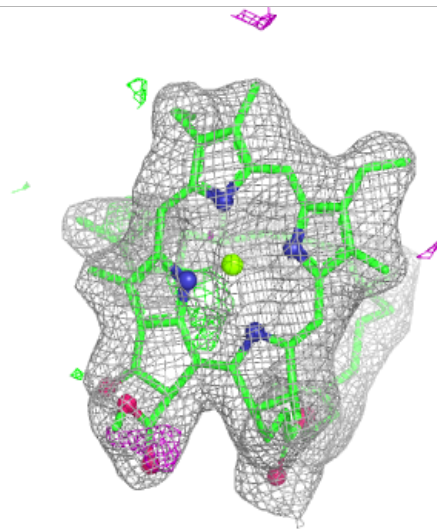
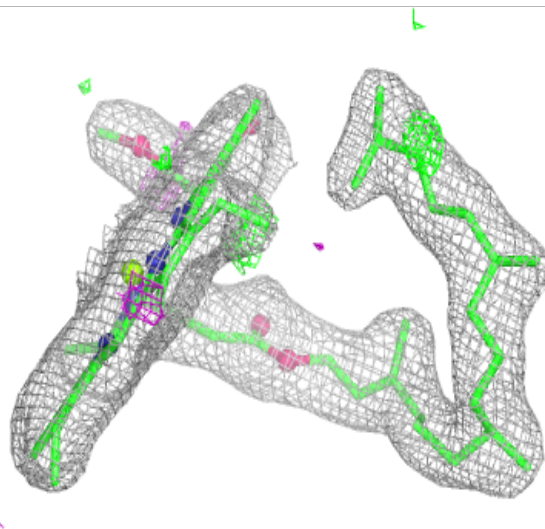
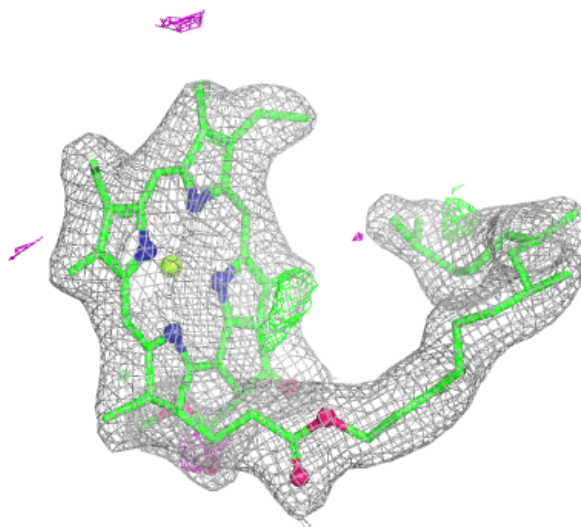
**Electron density around BCR K 103:**

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



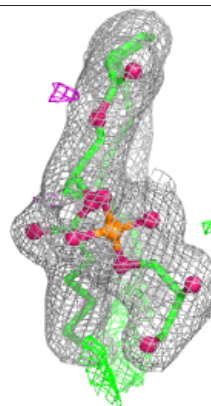
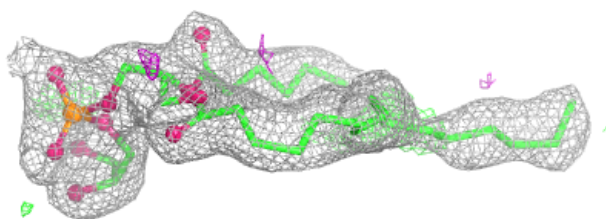
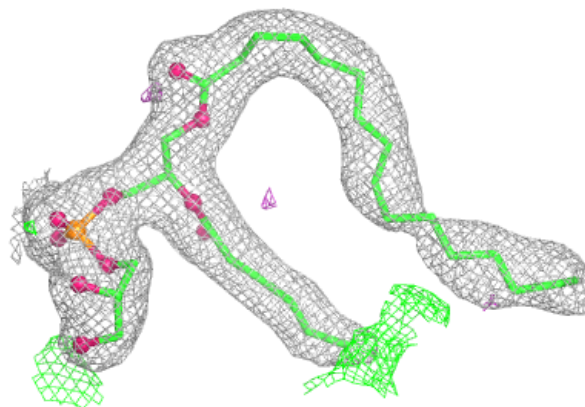
Electron density around CLA c 503:

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

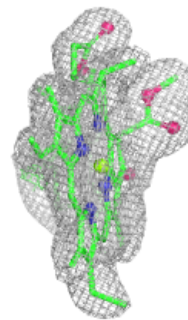
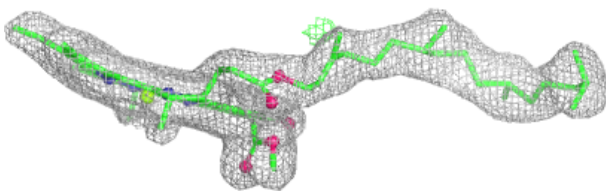
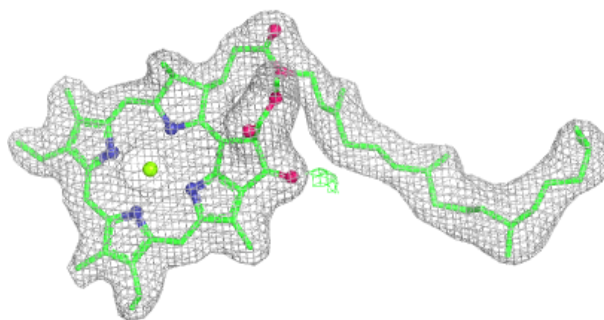


Electron density around LHG d 407:

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

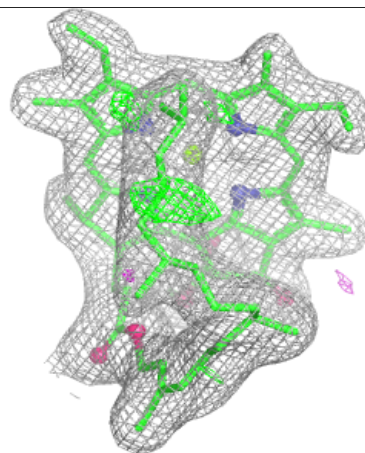
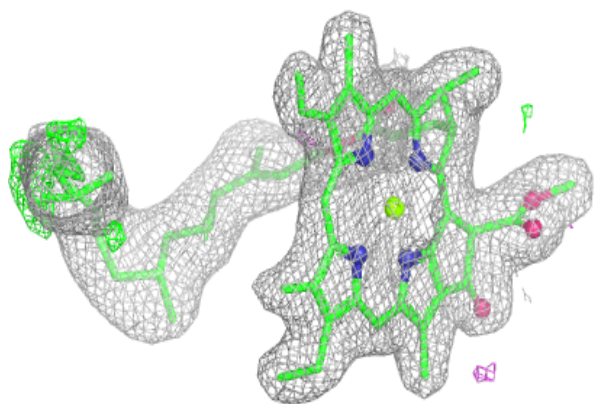
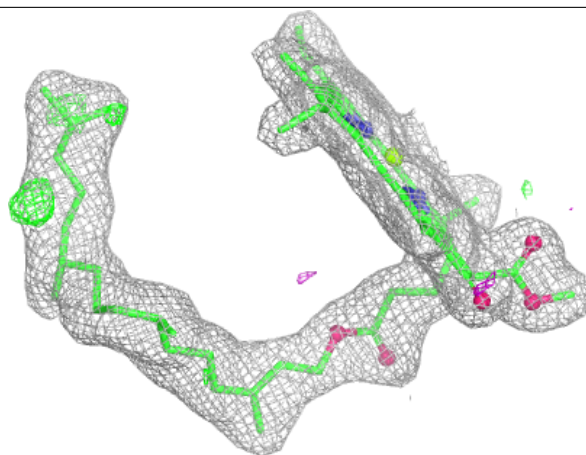
**Electron density around CLA b 601:**

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



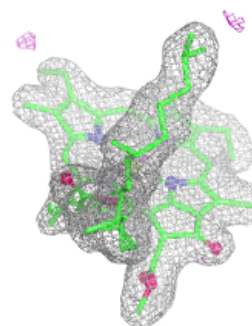
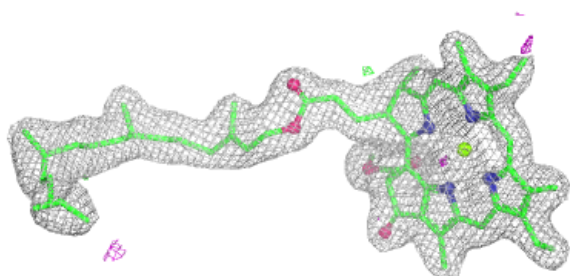
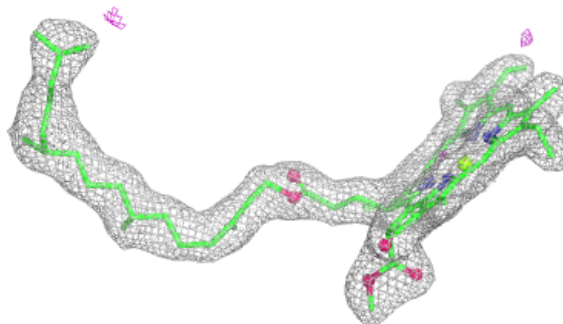
Electron density around CLA B 611:

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

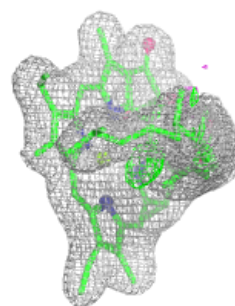
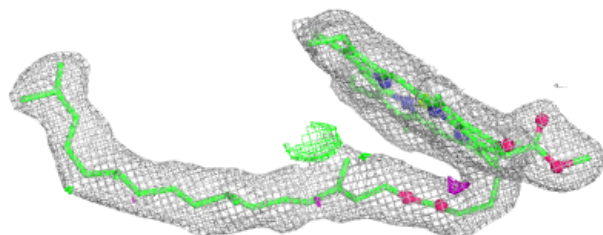
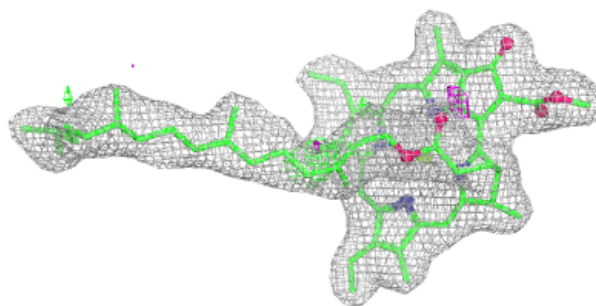


Electron density around CLA d 402:

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

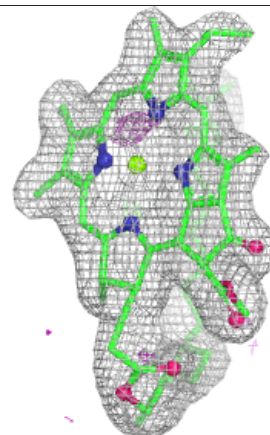
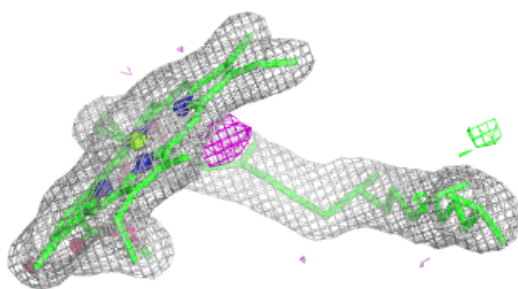
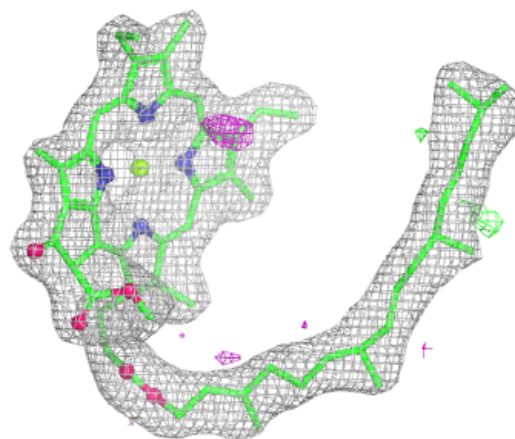
**Electron density around CLA b 607:**

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



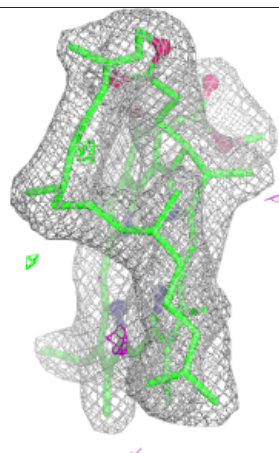
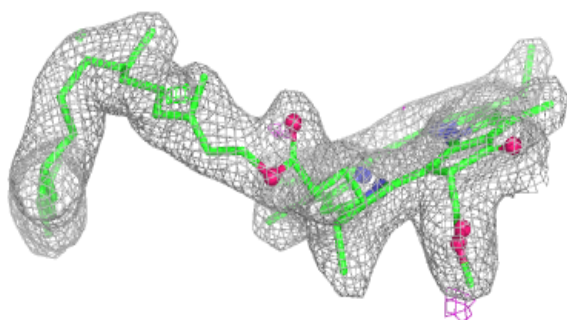
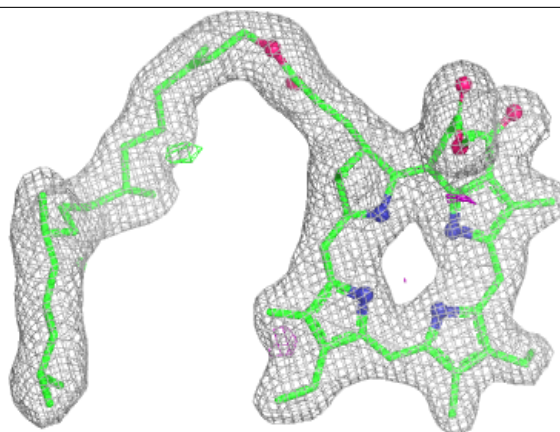
Electron density around CLA C 507:

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

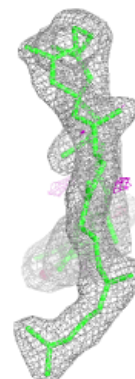
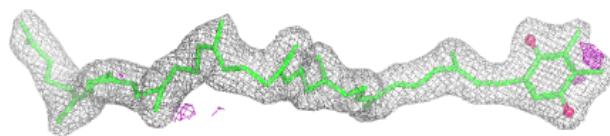
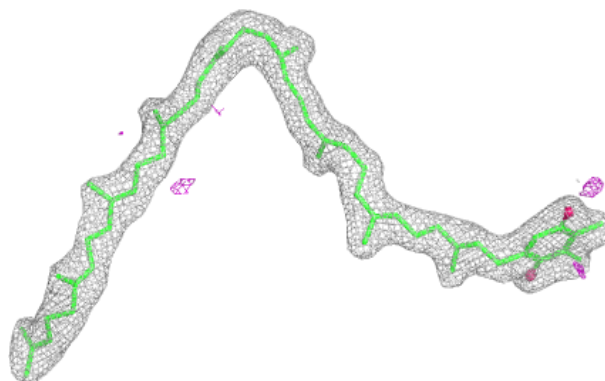


Electron density around PHO D 402:

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

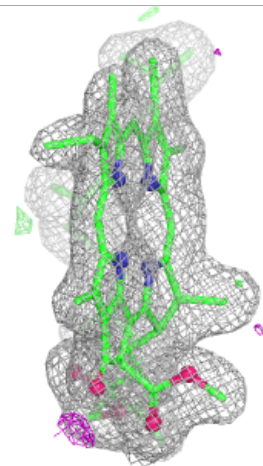
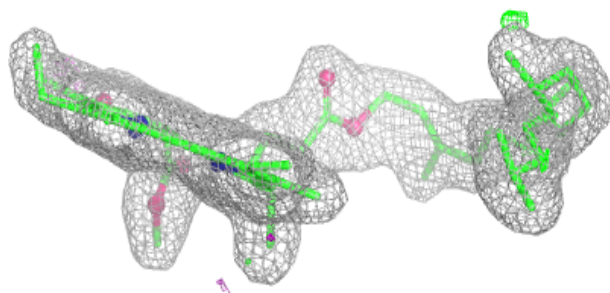
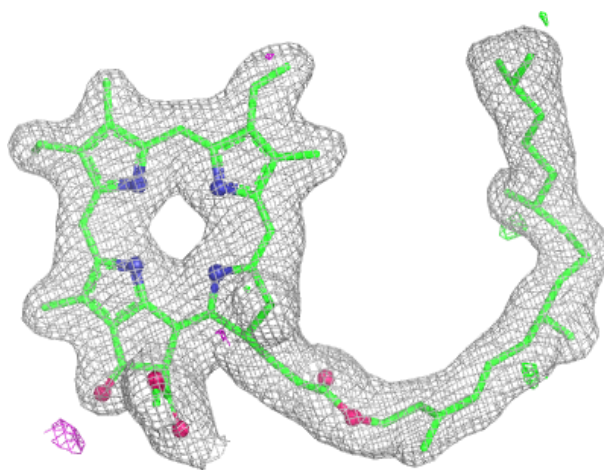
**Electron density around PL9 D 406:**

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



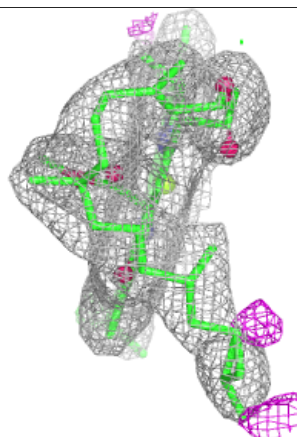
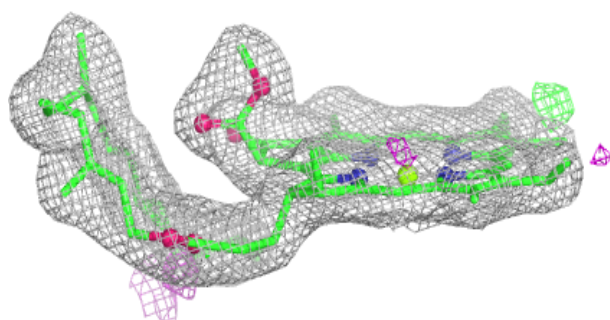
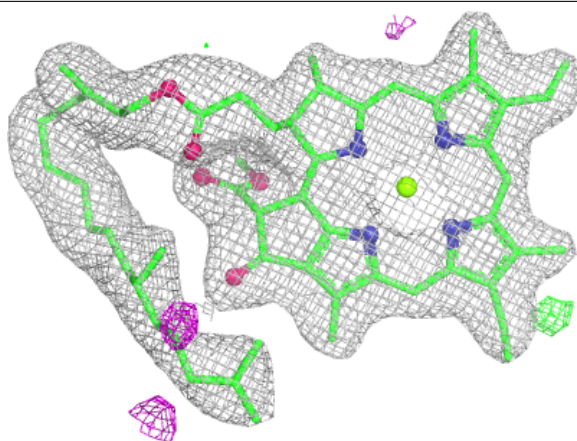
Electron density around PHO a 609:

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



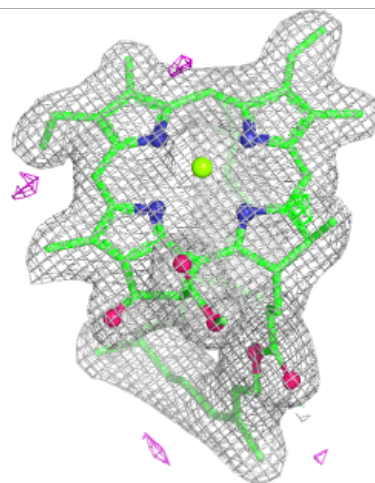
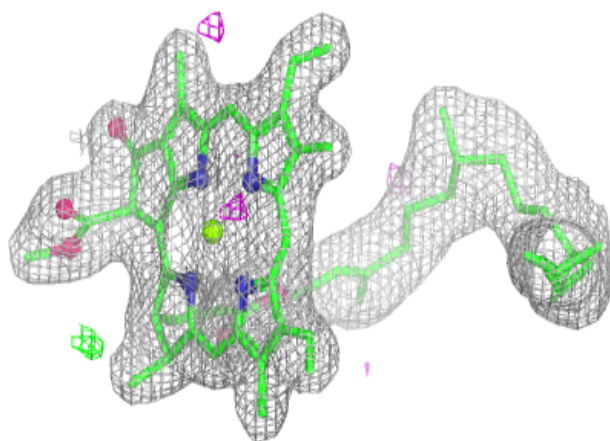
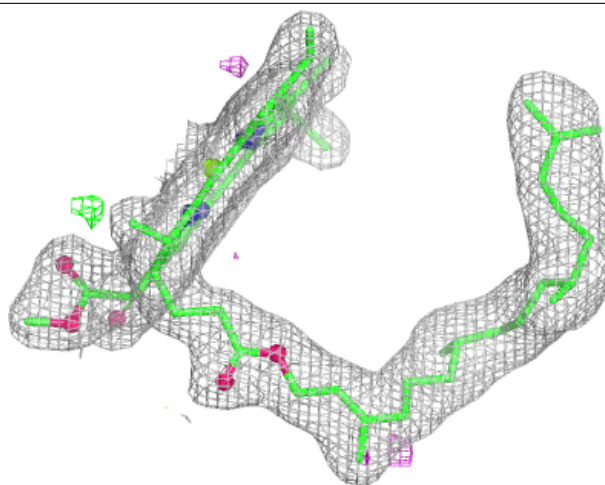
Electron density around CLA b 609:

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



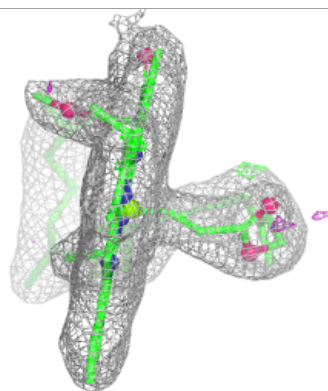
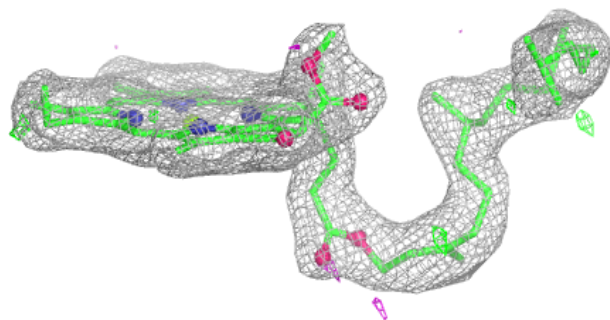
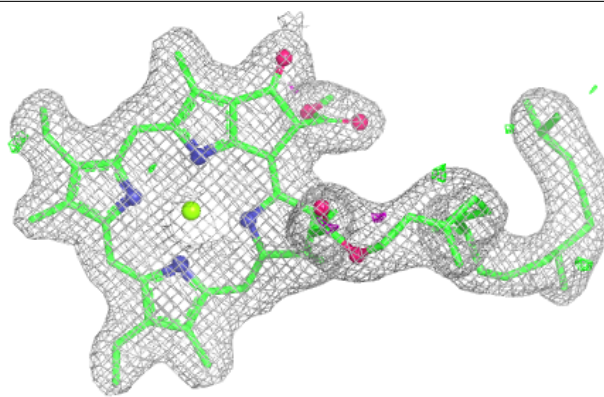
Electron density around CLA b 610:

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



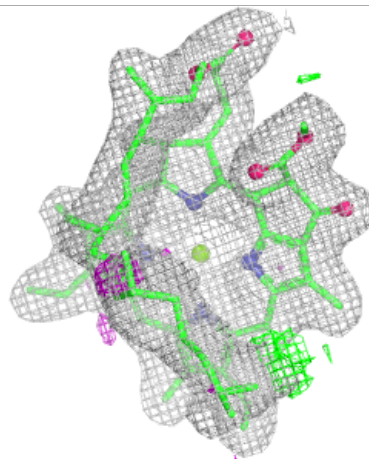
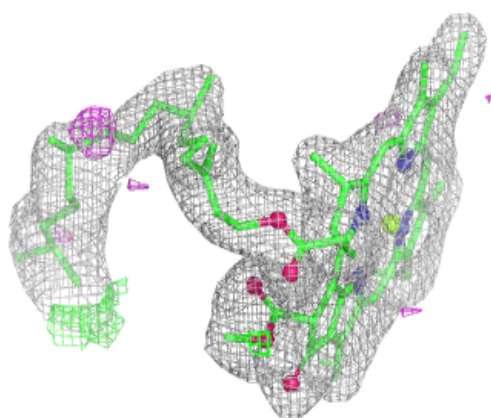
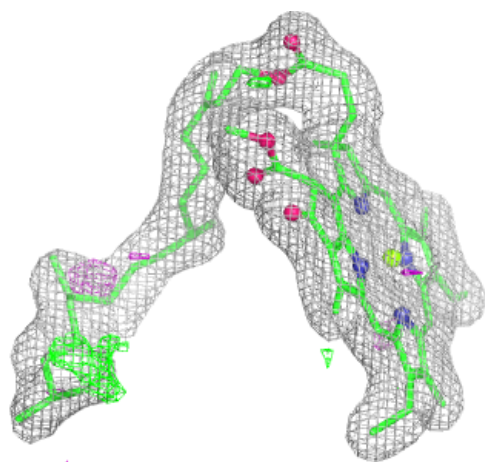
Electron density around CLA b 611:

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



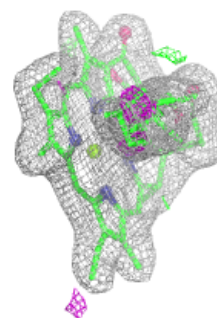
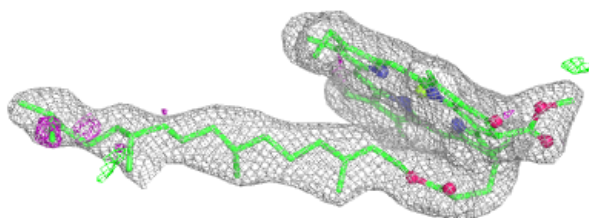
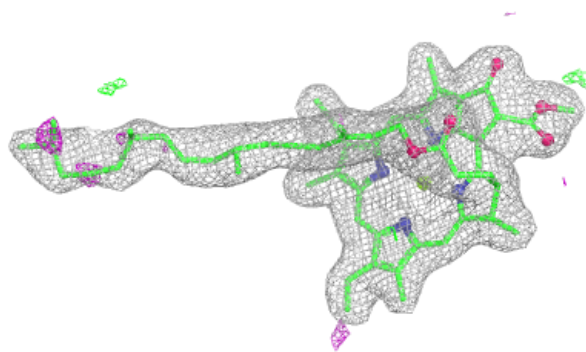
Electron density around CLA b 612:

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



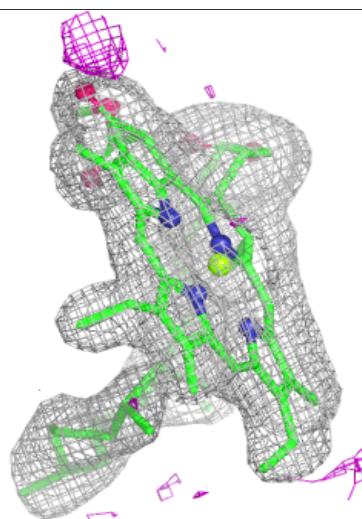
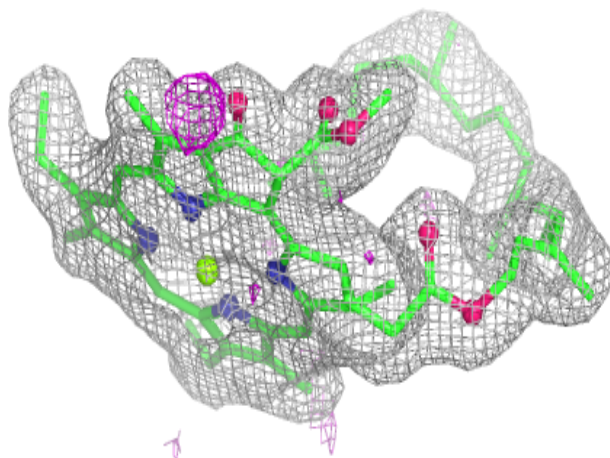
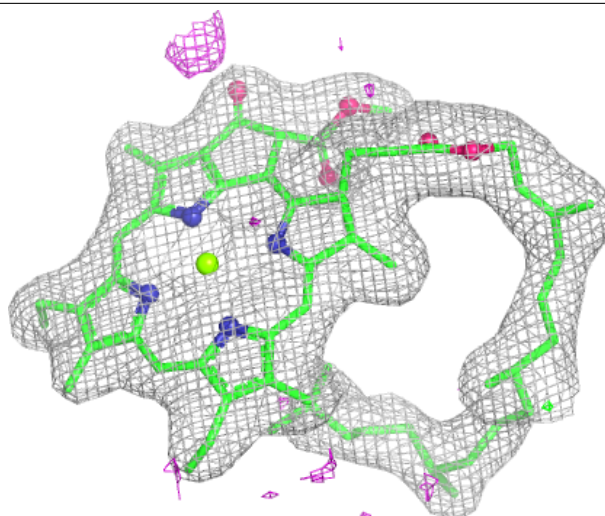
Electron density around CLA B 614:

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



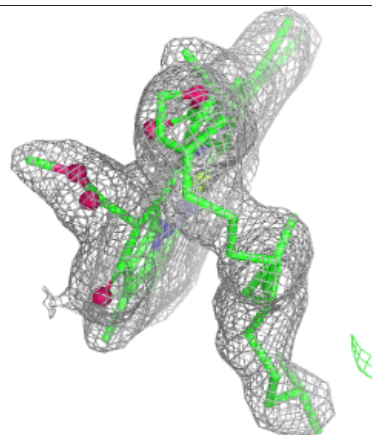
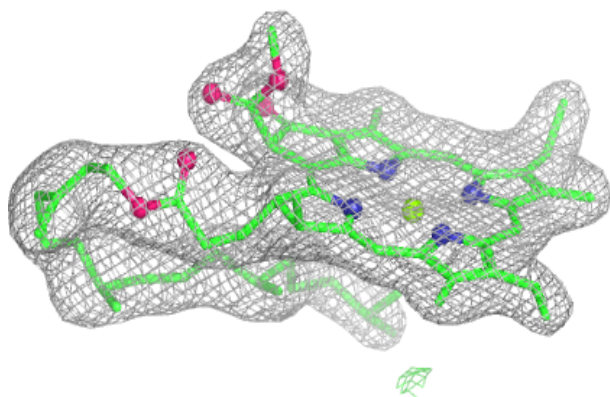
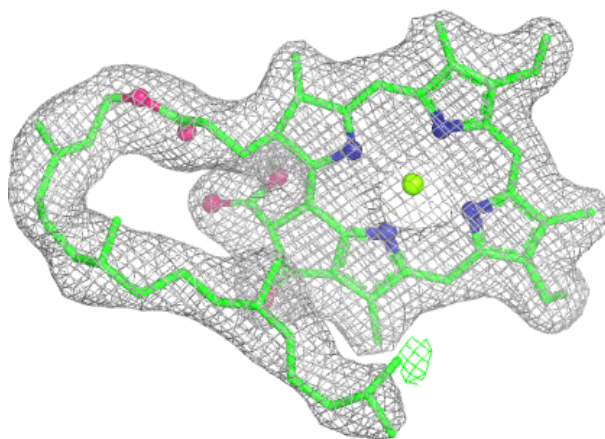
Electron density around CLA b 614:

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



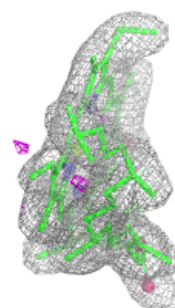
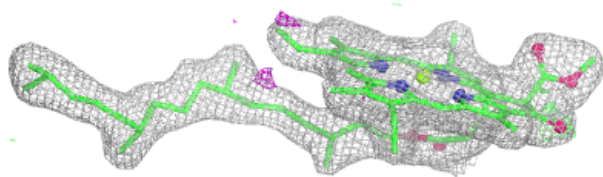
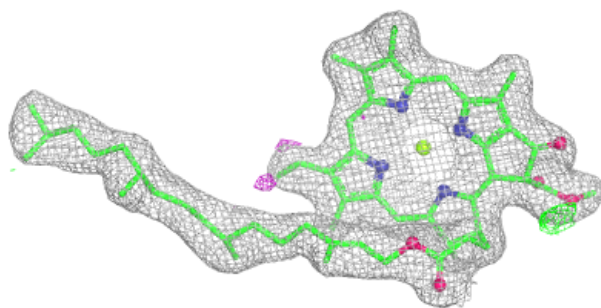
Electron density around CLA C 509:

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

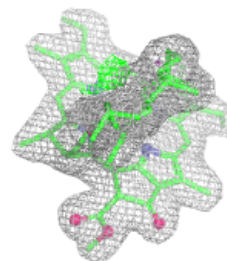
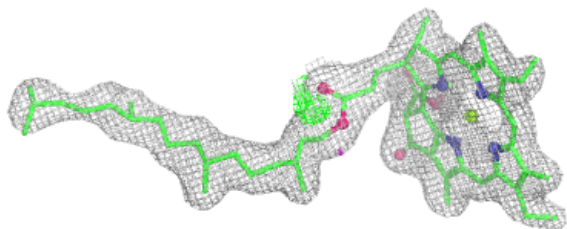
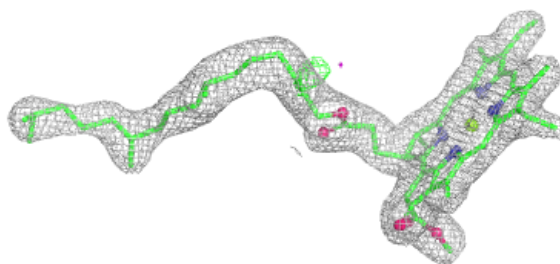


Electron density around CLA c 501:

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

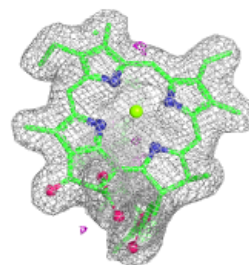
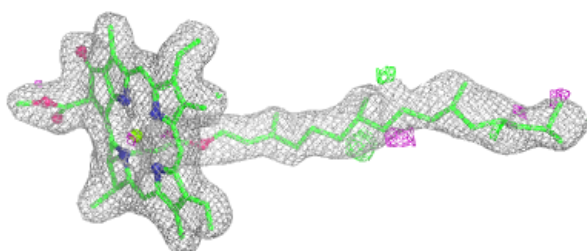
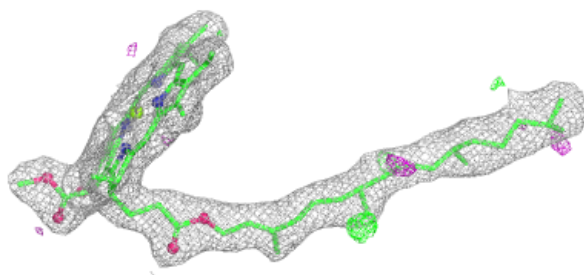
**Electron density around CLA c 502:**

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

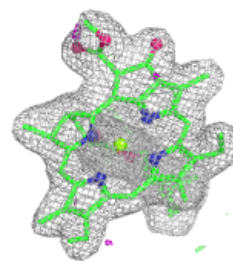
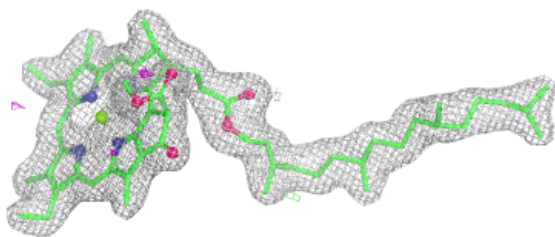
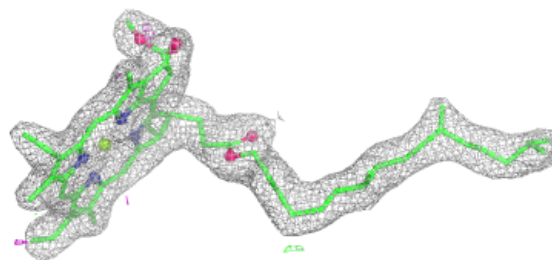


Electron density around CLA B 607:

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

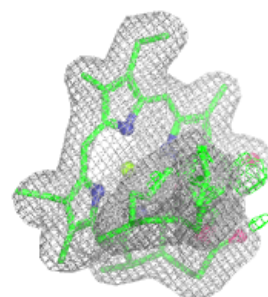
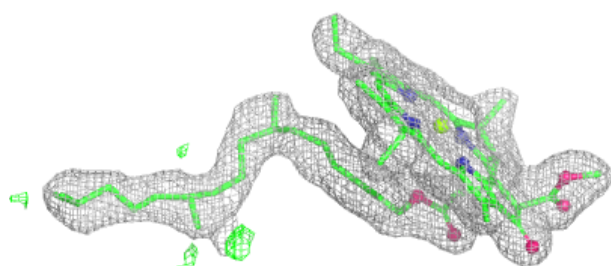
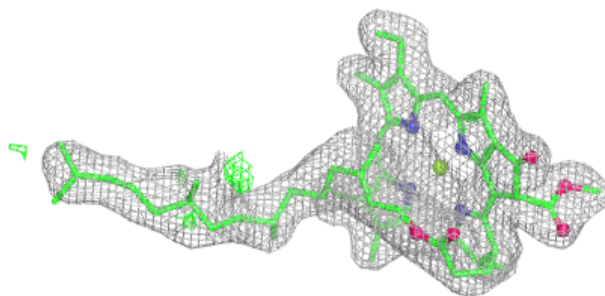
**Electron density around CLA C 502:**

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

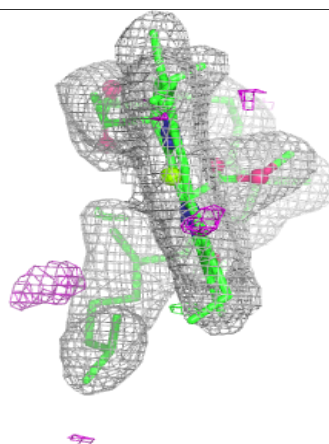
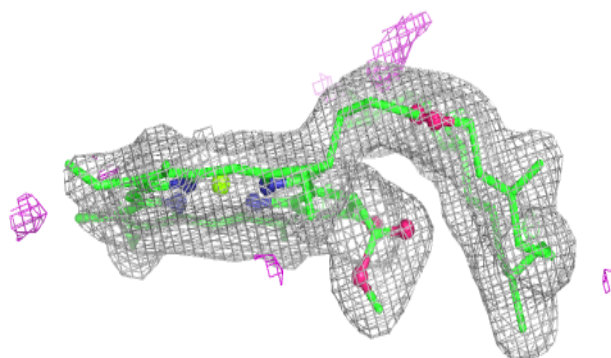
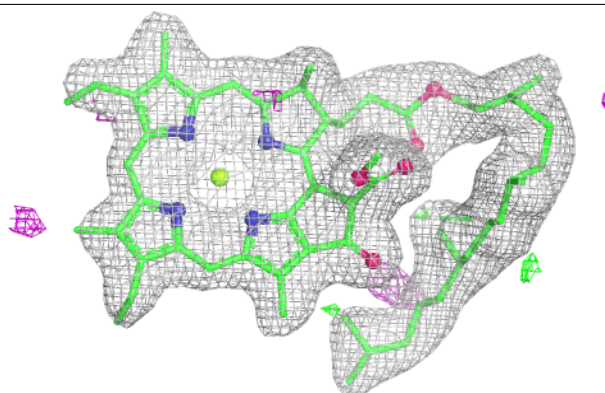


Electron density around CLA c 505:

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

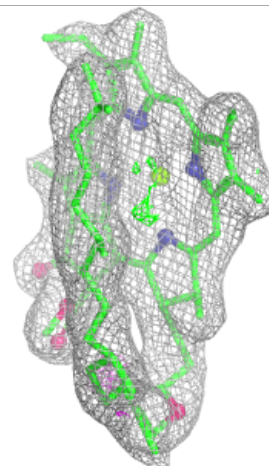
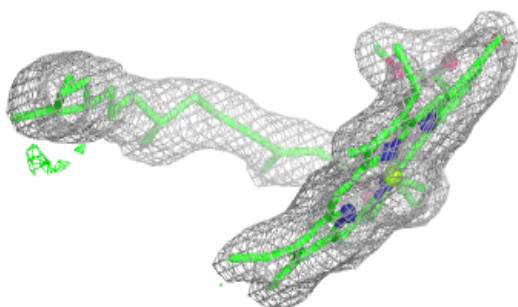
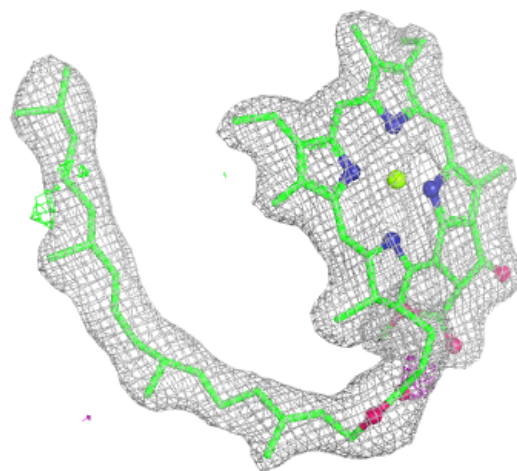
**Electron density around CLA B 610:**

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



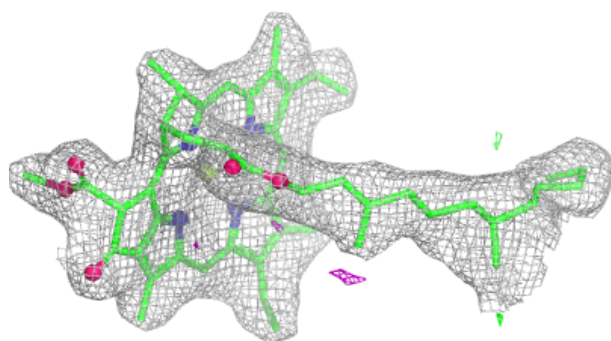
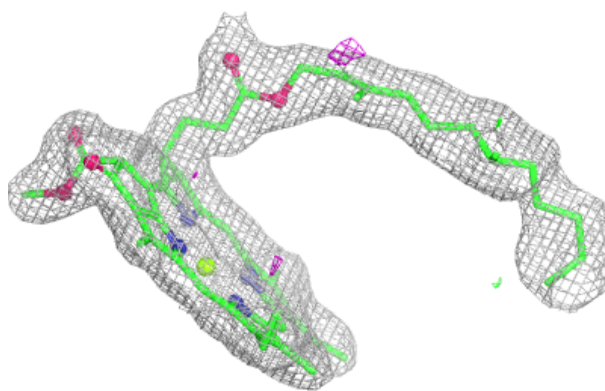
Electron density around CLA c 507:

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

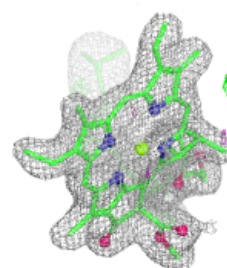
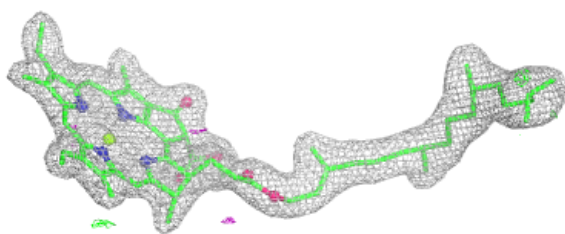
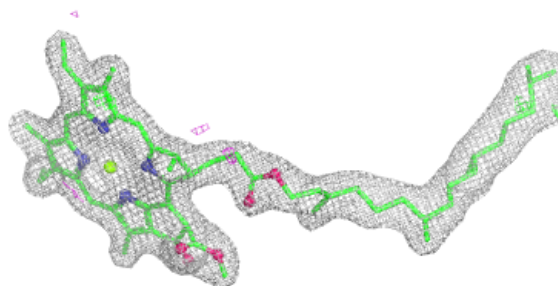


Electron density around CLA C 504:

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

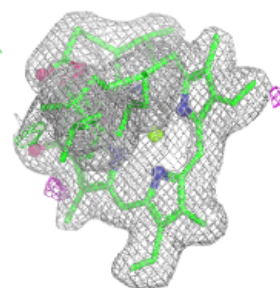
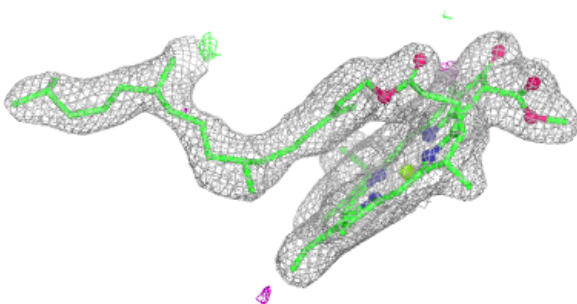
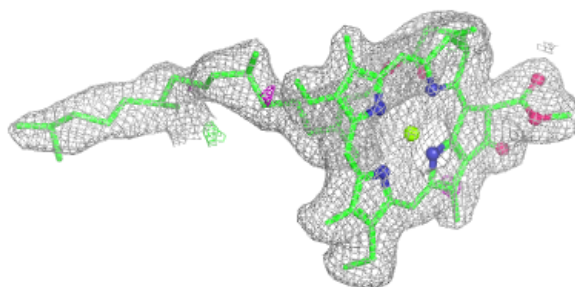
**Electron density around CLA a 607:**

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

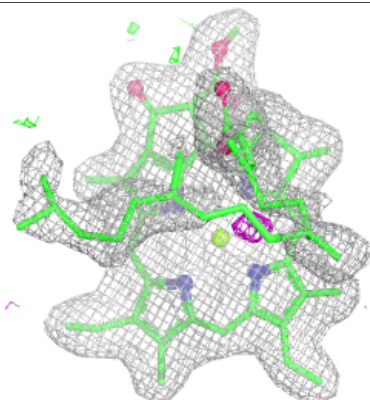
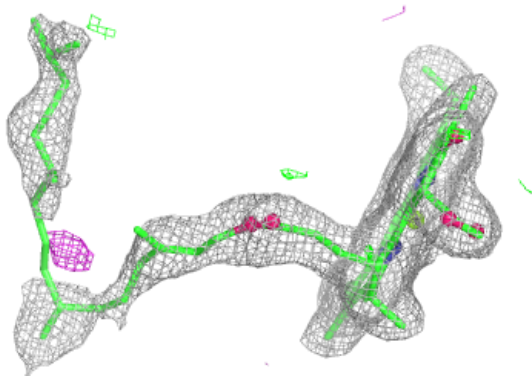
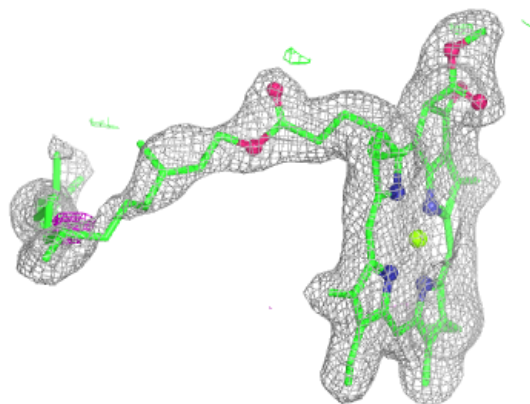


Electron density around CLA C 505:

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

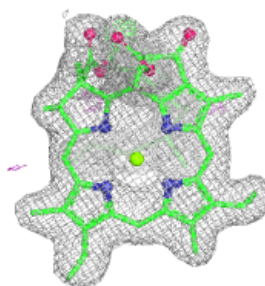
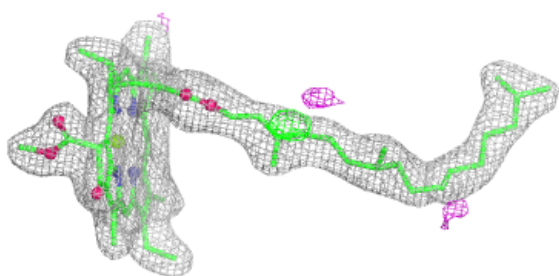
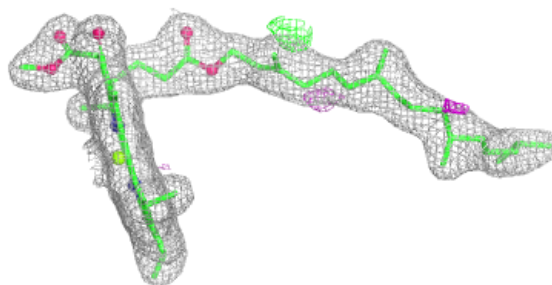
**Electron density around CLA a 610:**

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

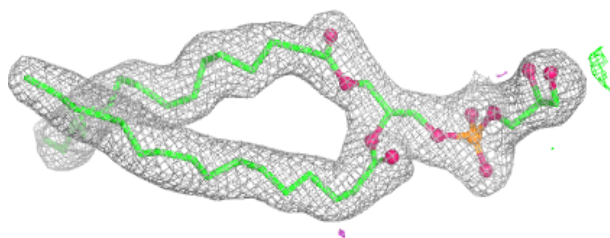
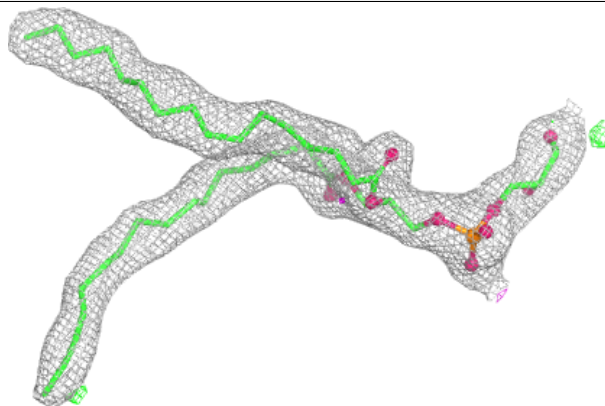


Electron density around CLA B 605:

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

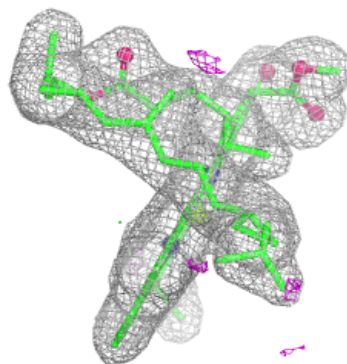
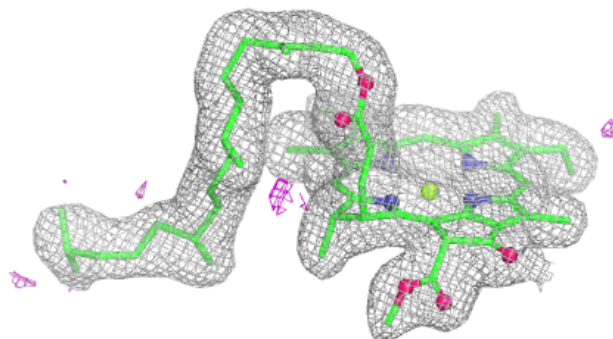
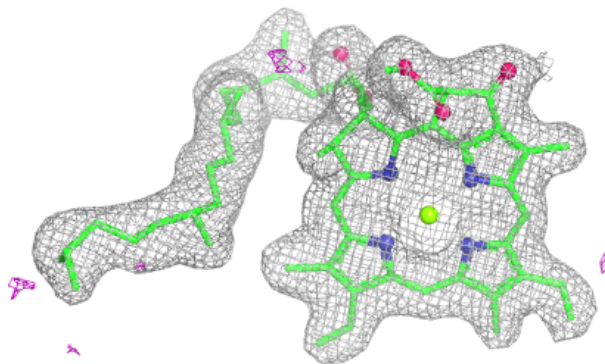
**Electron density around LHG D 408:**

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



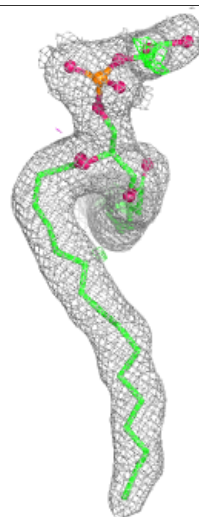
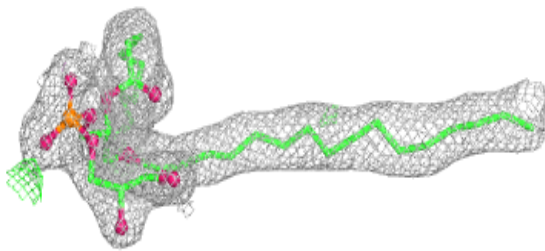
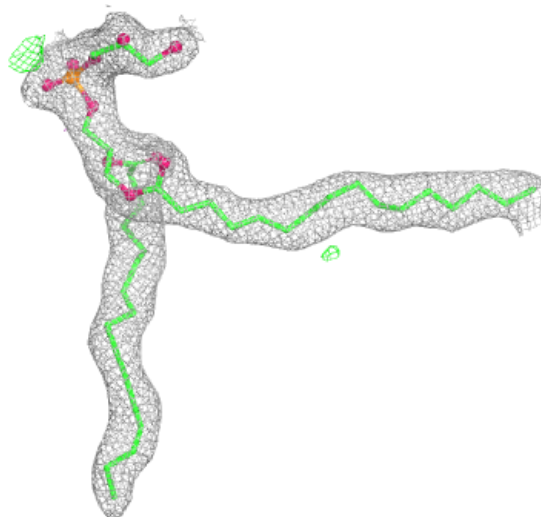
Electron density around CLA A 612:

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



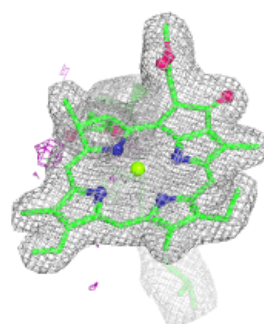
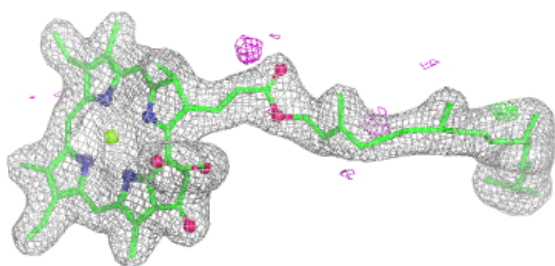
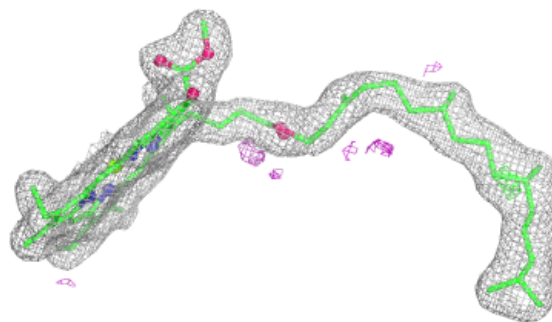
Electron density around LHG L 101:

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

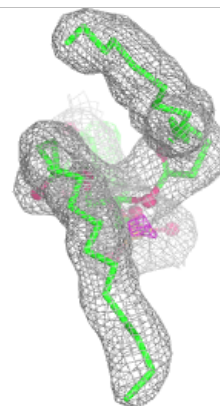
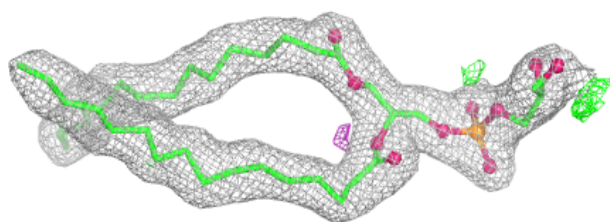
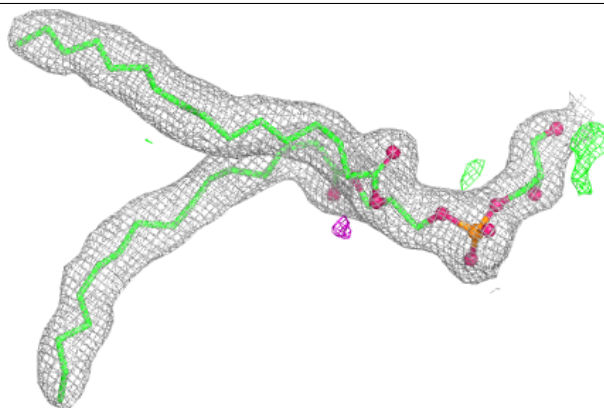


Electron density around CLA D 403:

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

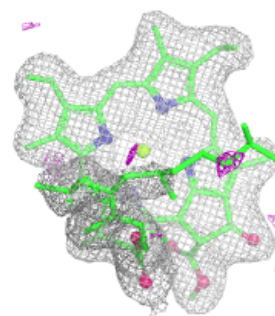
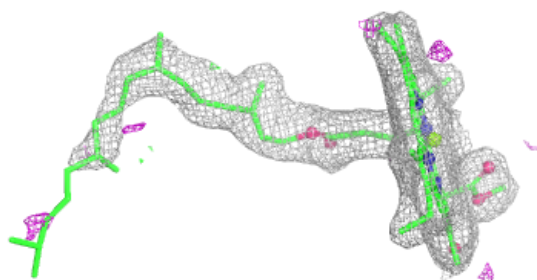
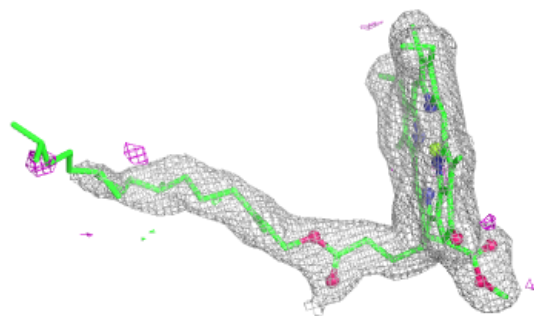
**Electron density around LHG d 406:**

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

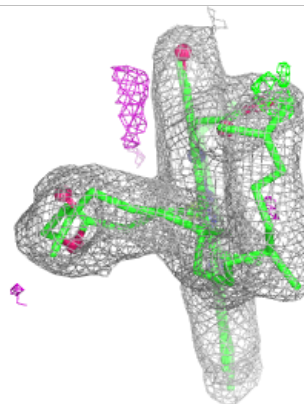
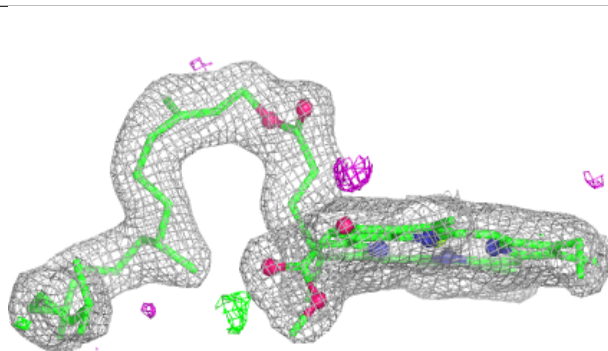
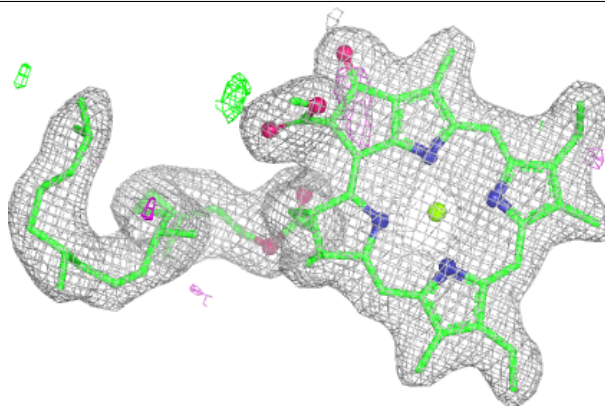


Electron density around CLA D 404:

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

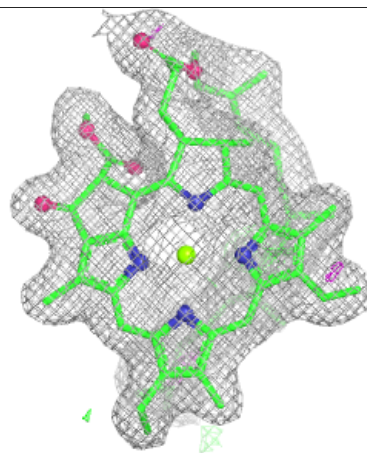
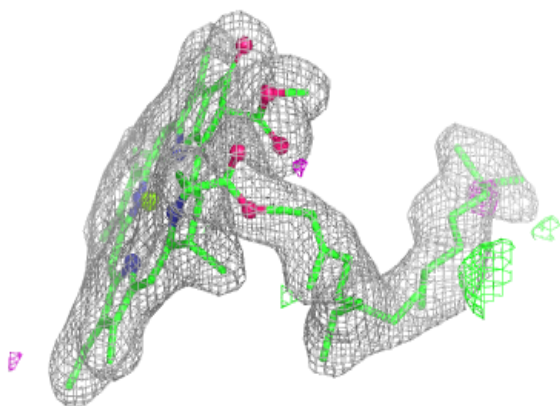
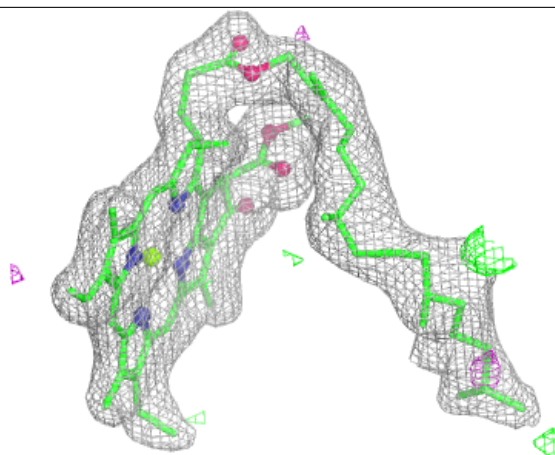
**Electron density around CLA B 612:**

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



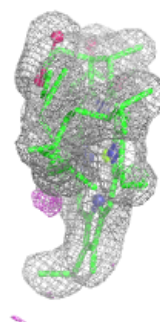
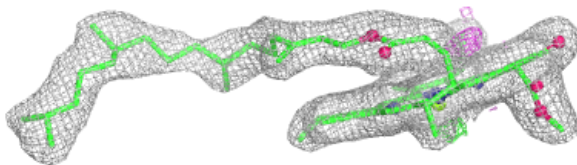
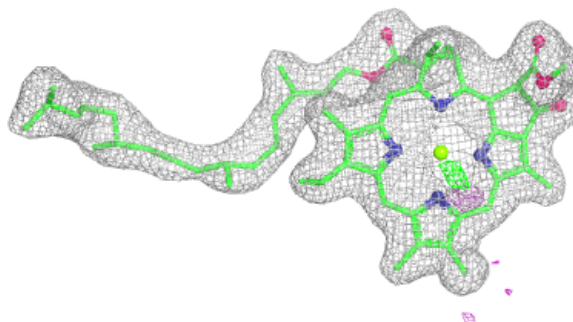
Electron density around CLA B 613:

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

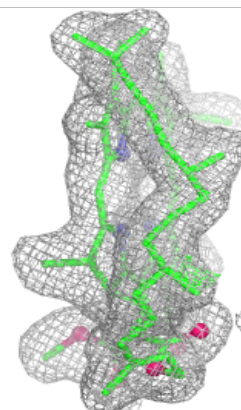
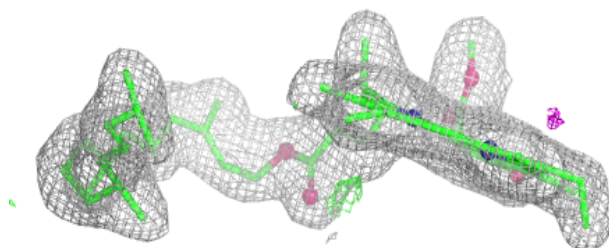
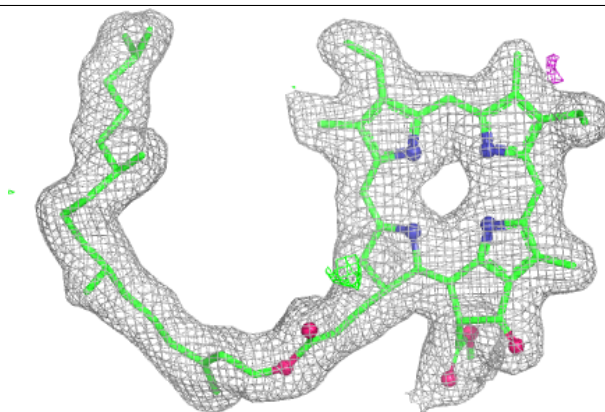


Electron density around CLA B 603:

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

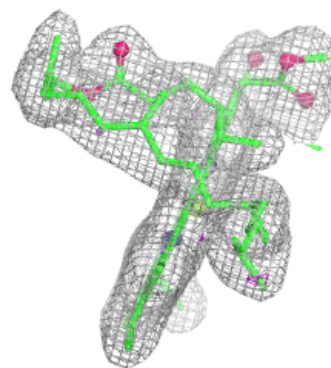
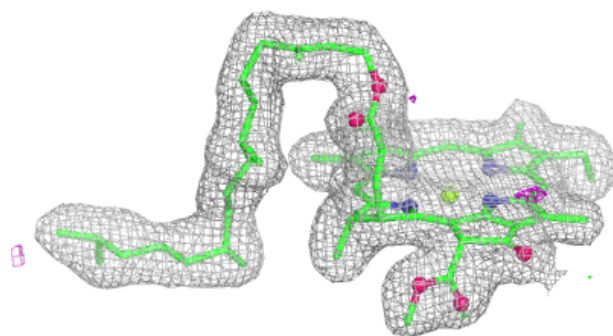
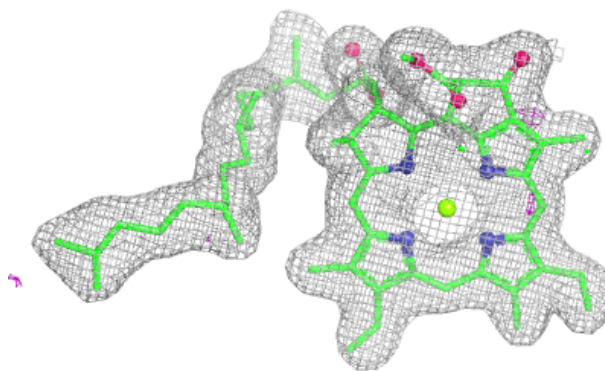
**Electron density around PHO A 608:**

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



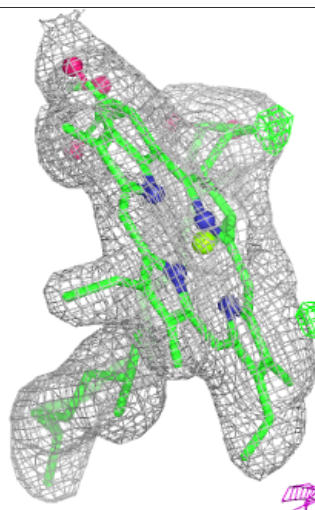
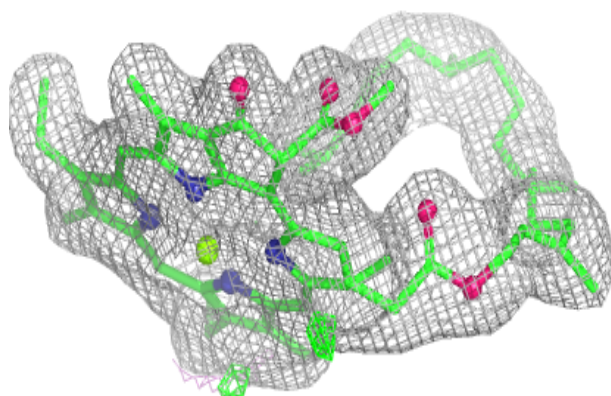
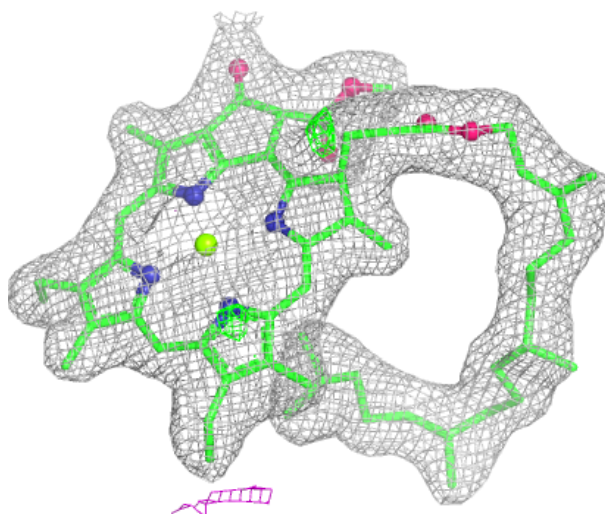
Electron density around CLA a 613:

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



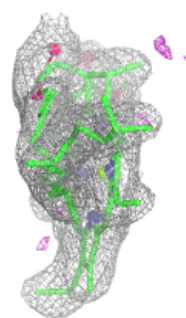
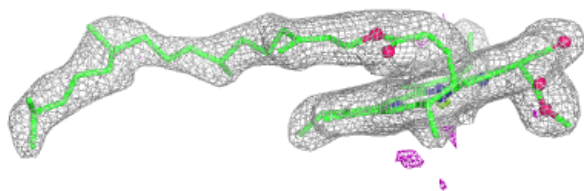
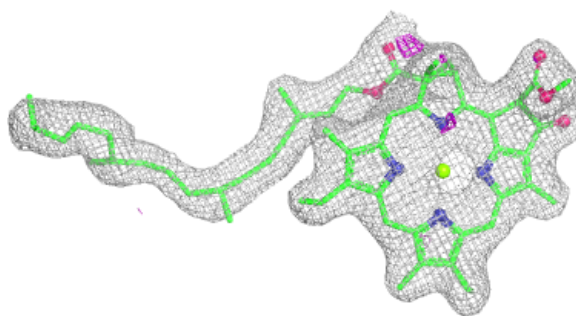
Electron density around CLA B 615:

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

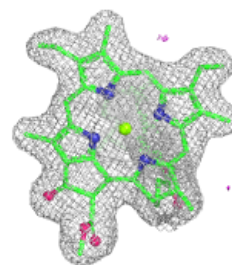
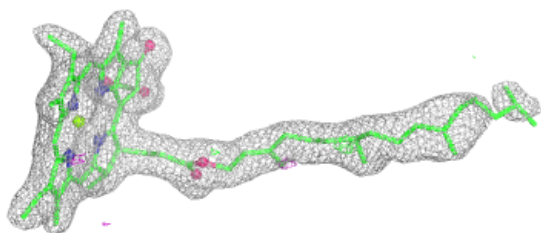
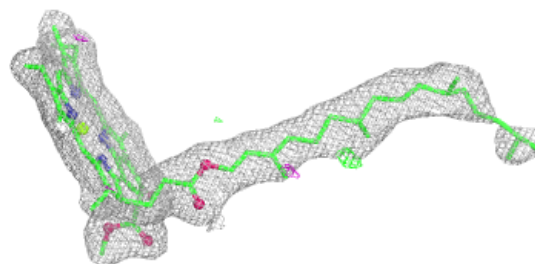


Electron density around CLA b 602:

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

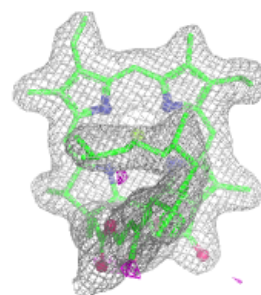
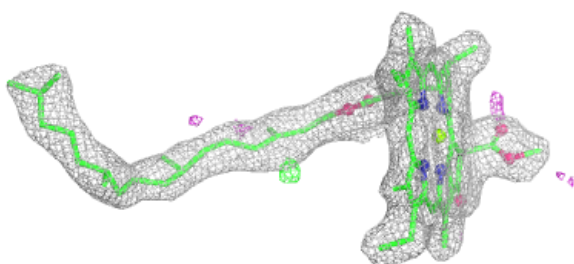
**Electron density around CLA b 603:**

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

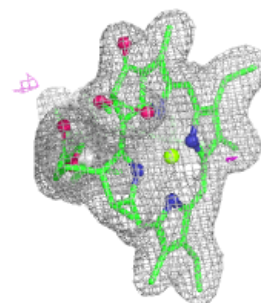
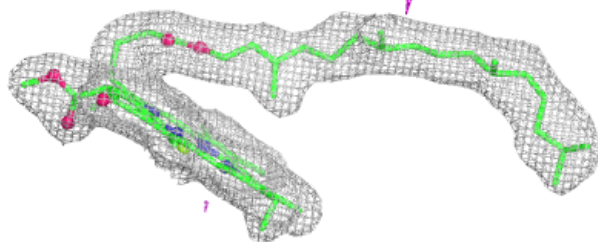
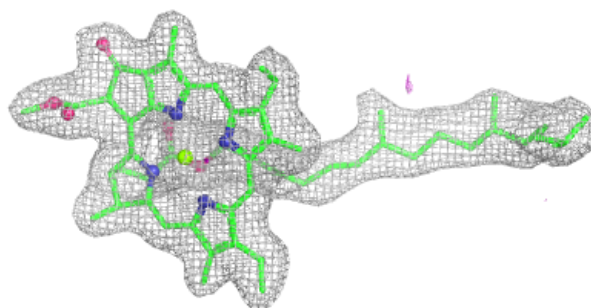


Electron density around CLA b 604:

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

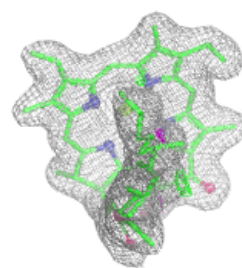
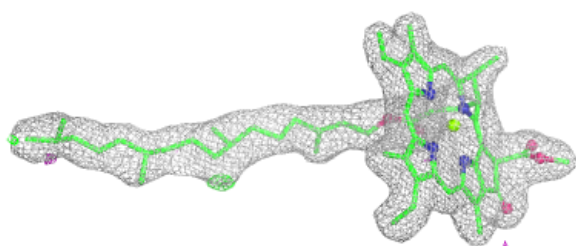
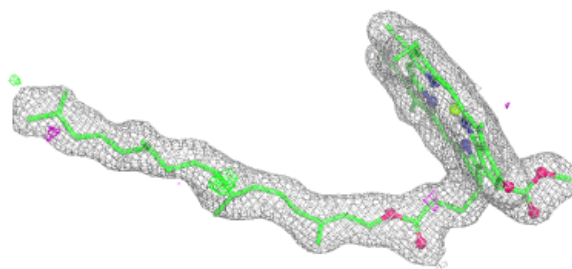
**Electron density around CLA B 608:**

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

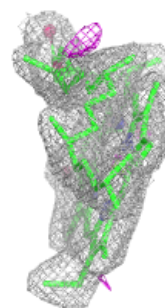
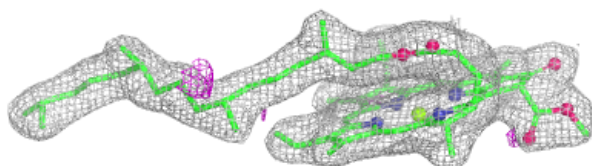
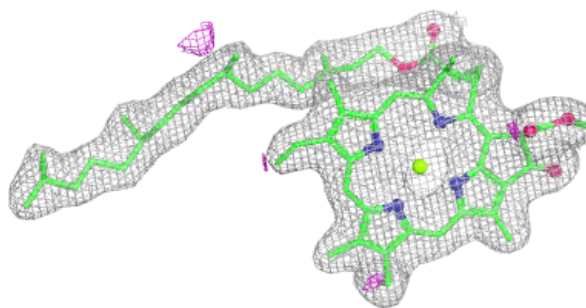


Electron density around CLA b 606:

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

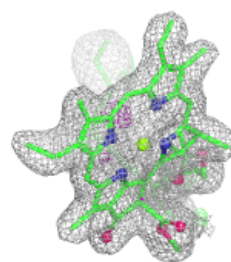
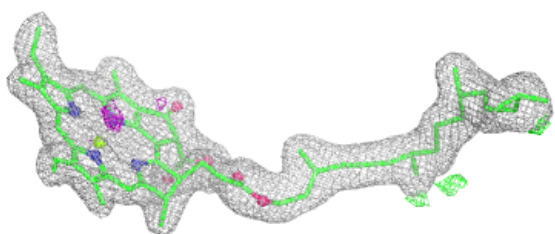
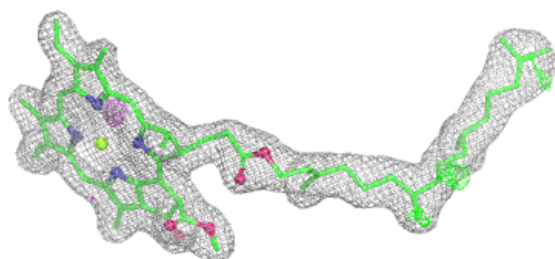
**Electron density around CLA C 501:**

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



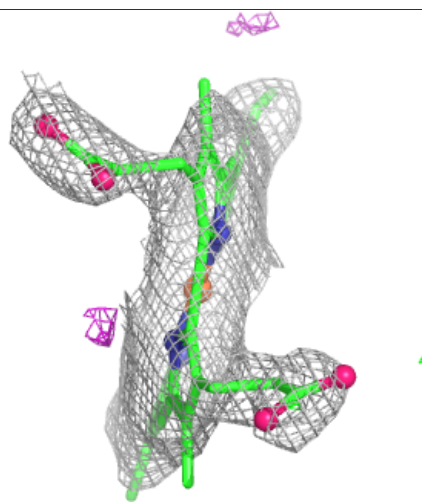
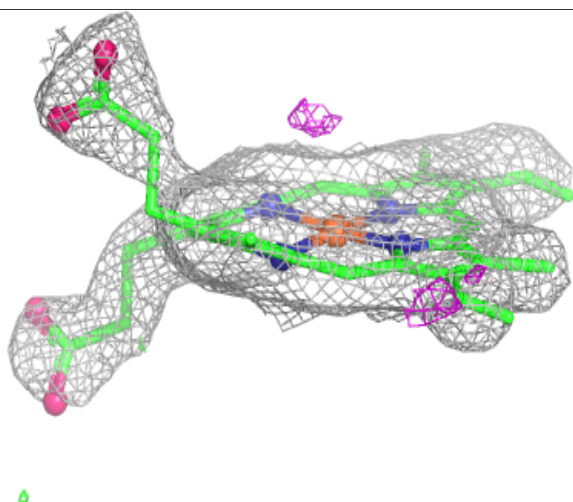
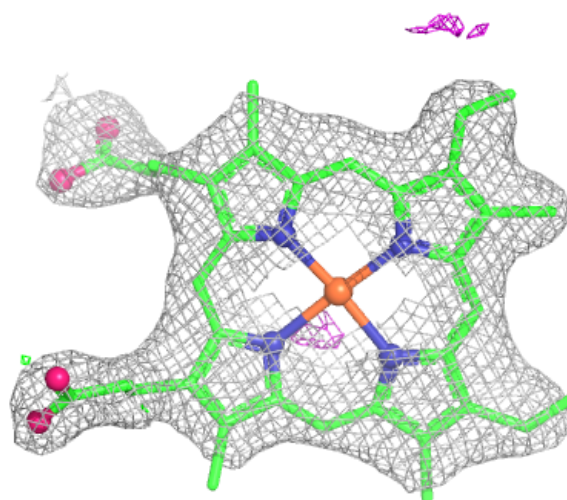
Electron density around CLA A 606:

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



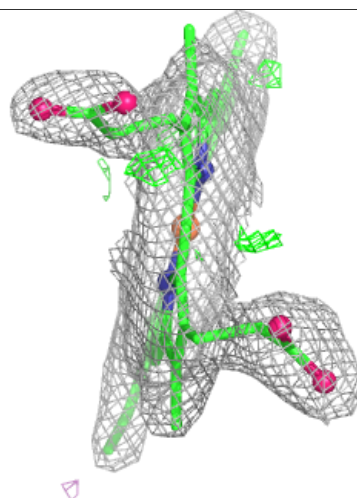
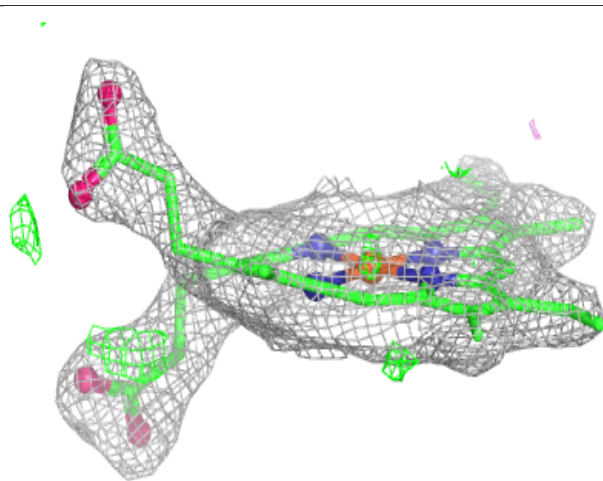
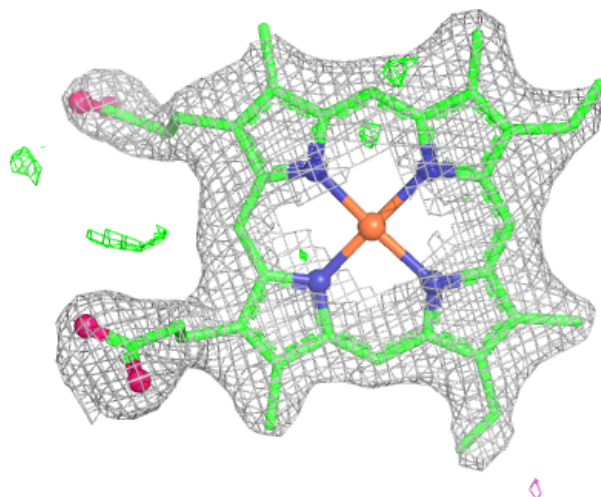
Electron density around HEM e 101:

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



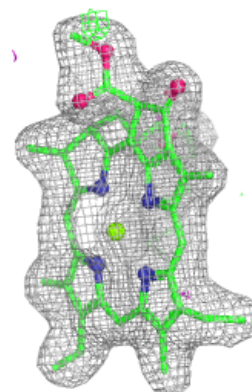
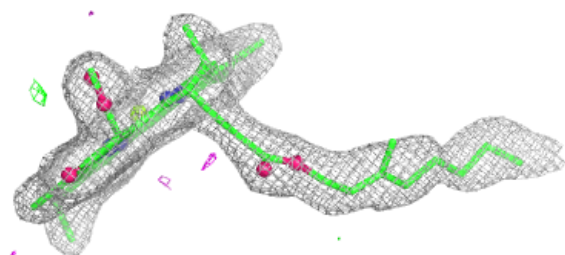
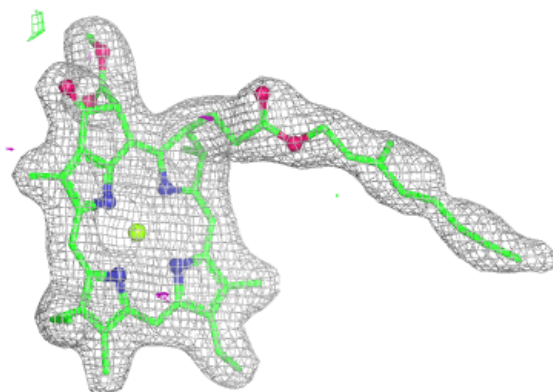
Electron density around HEM F 101:

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



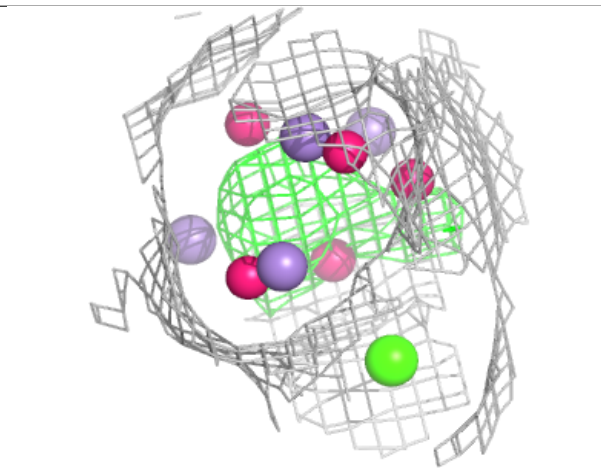
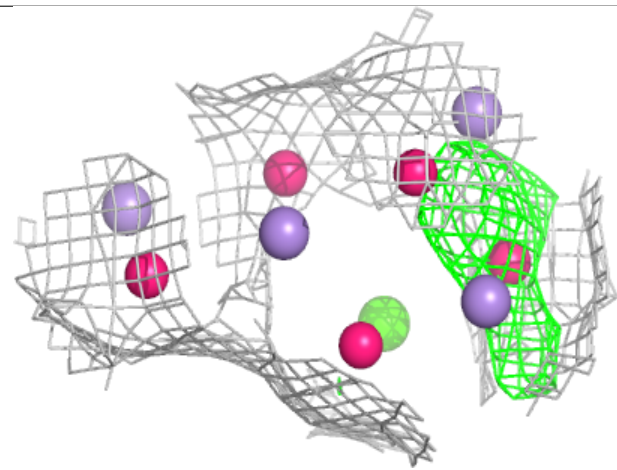
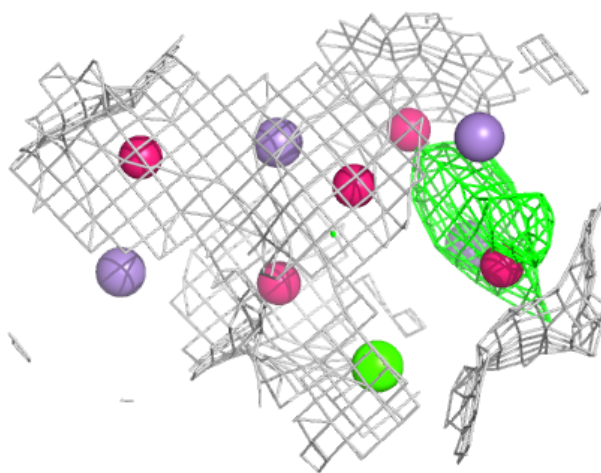
Electron density around CLA A 609:

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



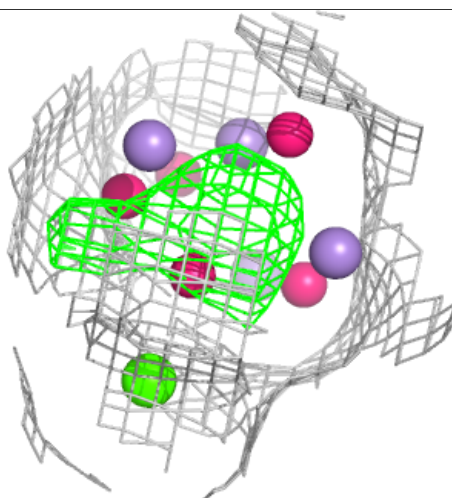
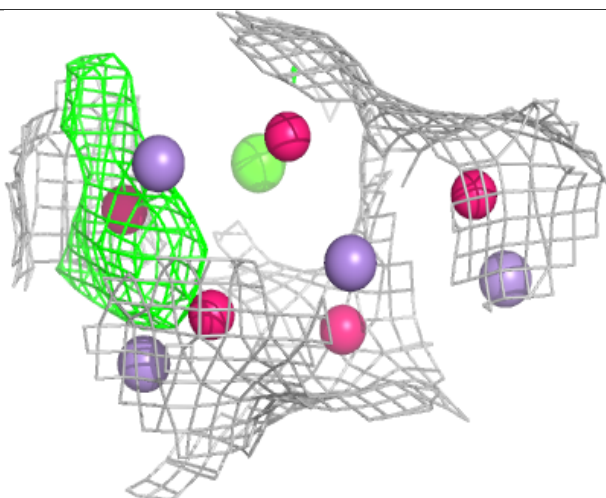
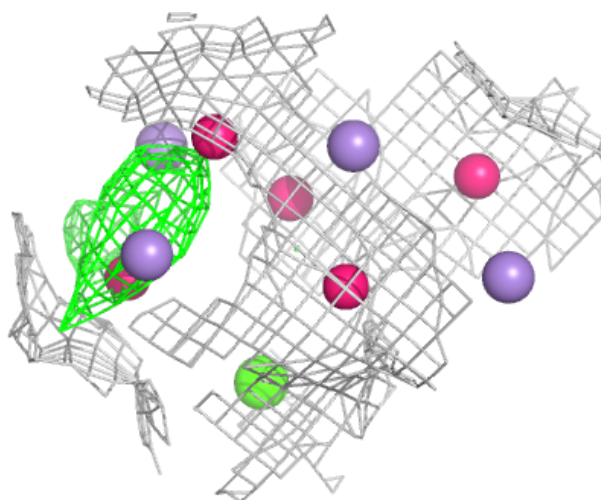
Electron density around OEX A 601 (B):

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



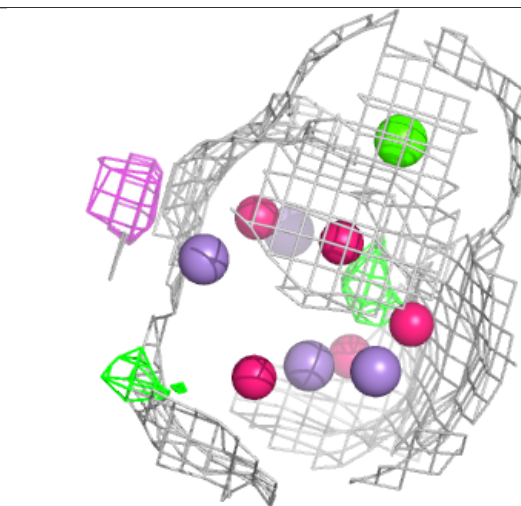
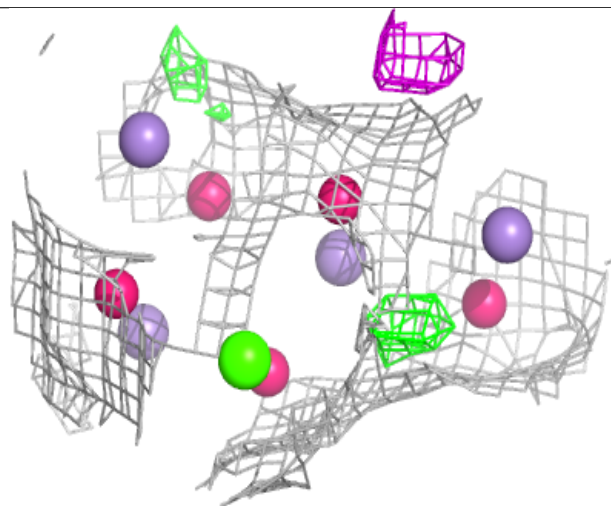
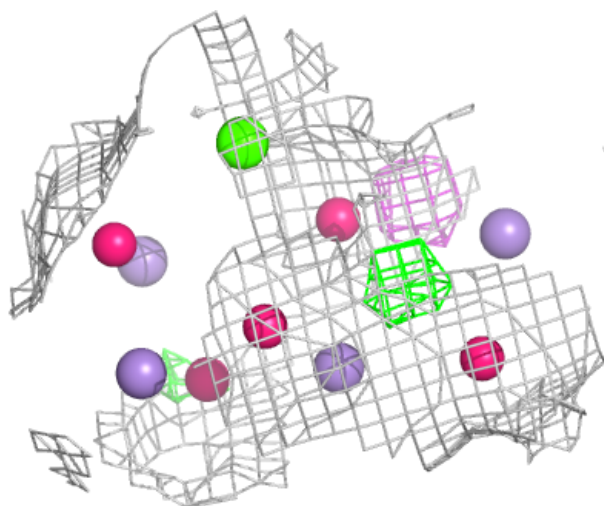
Electron density around OEX A 601 (C):

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



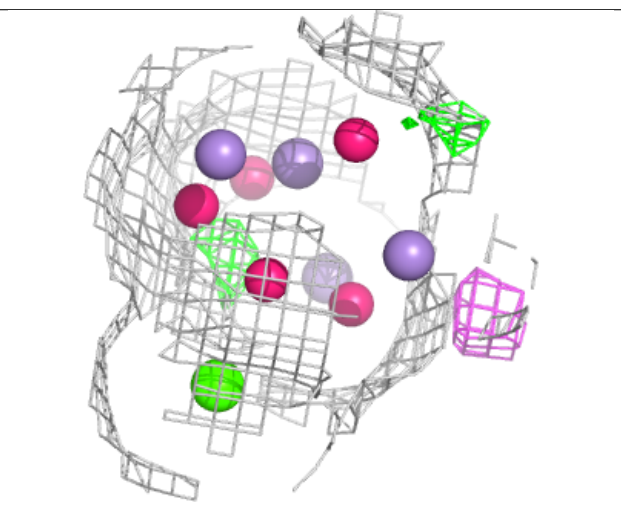
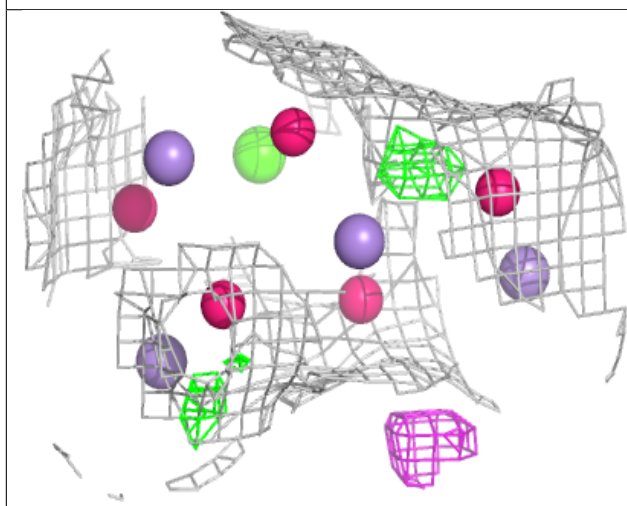
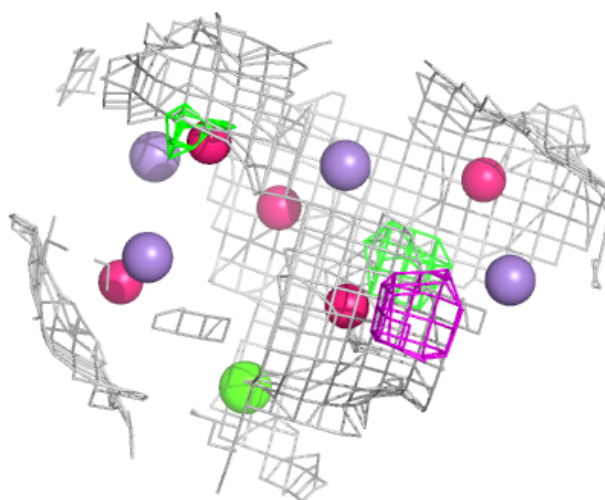
Electron density around OEX a 601 (B):

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



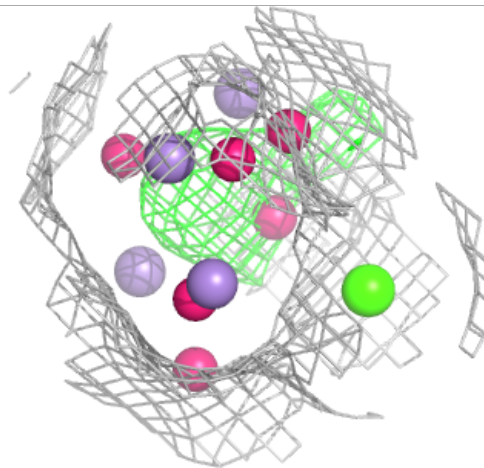
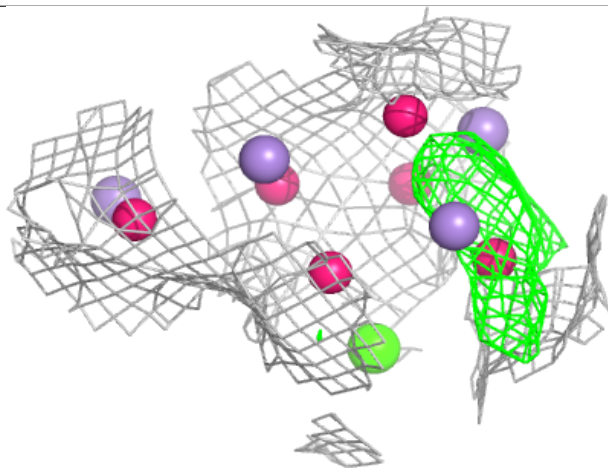
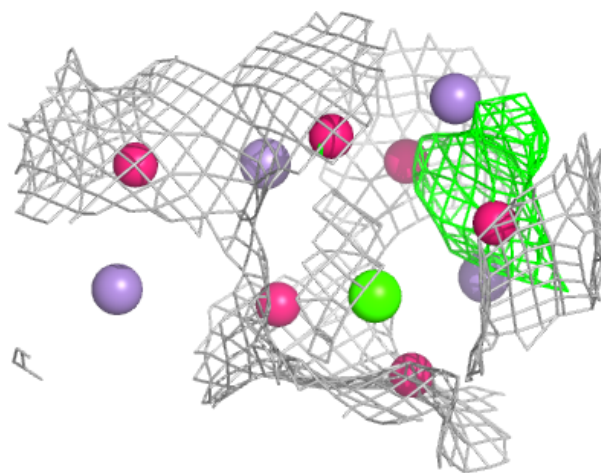
Electron density around OEX a 601 (C):

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



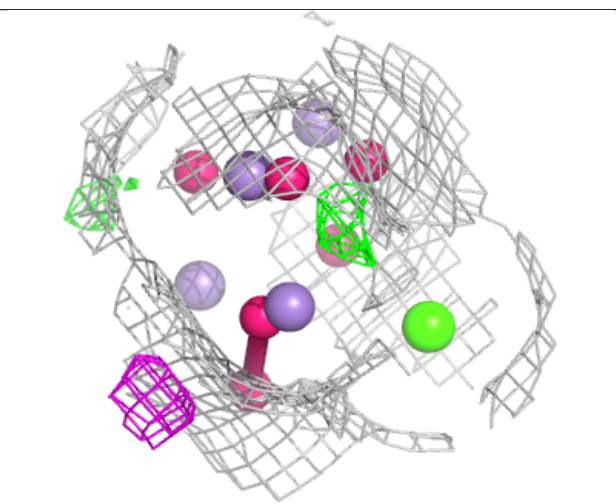
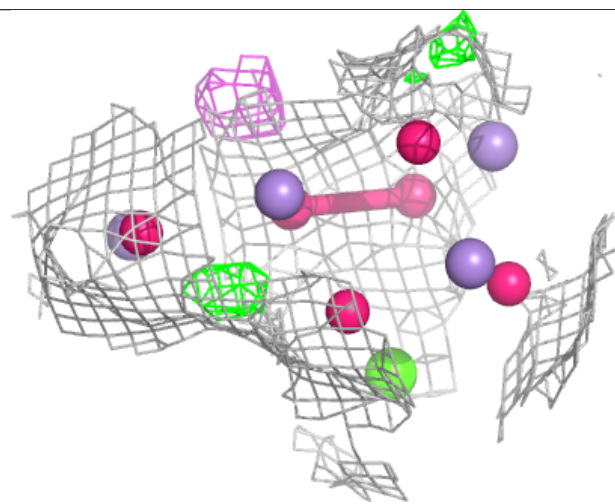
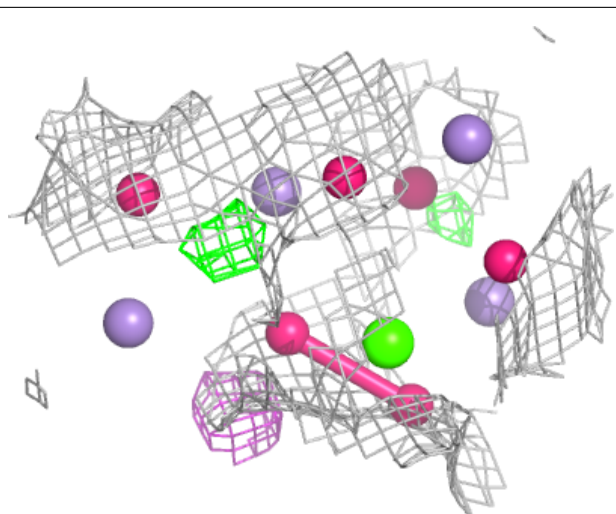
Electron density around OEY A 602 (A):

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



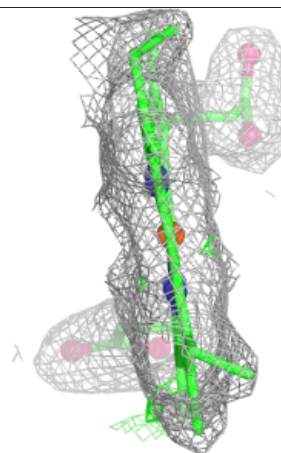
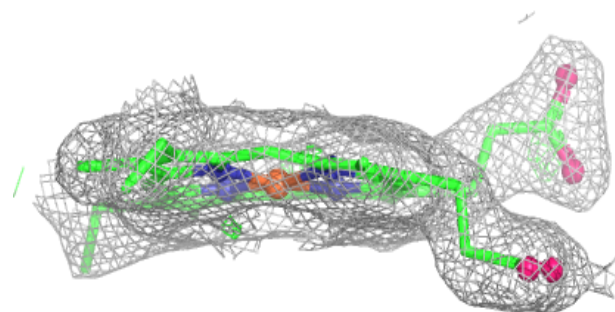
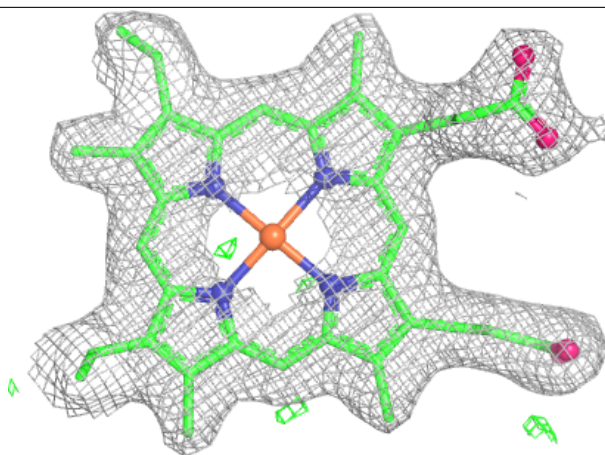
Electron density around OEY a 602 (A):

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



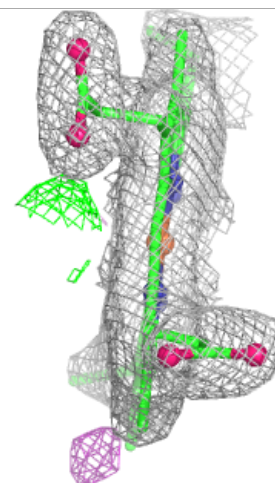
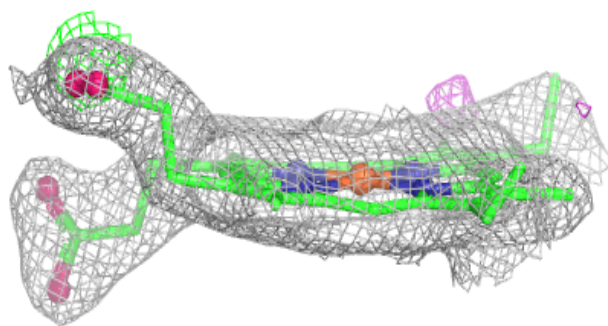
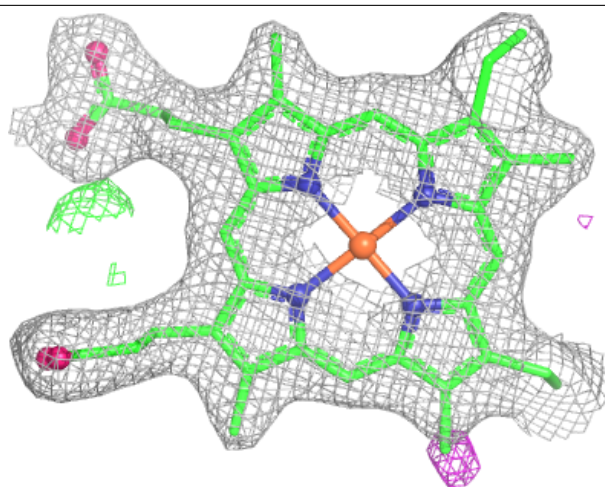
Electron density around HEC V 201:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.