



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 10:59 PM EDT

PDB ID : 8F4D / pdb_00008f4d
Title : RT XFEL structure of Photosystem II 50 microseconds after the third illumination at 2.15 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 : 2.15 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

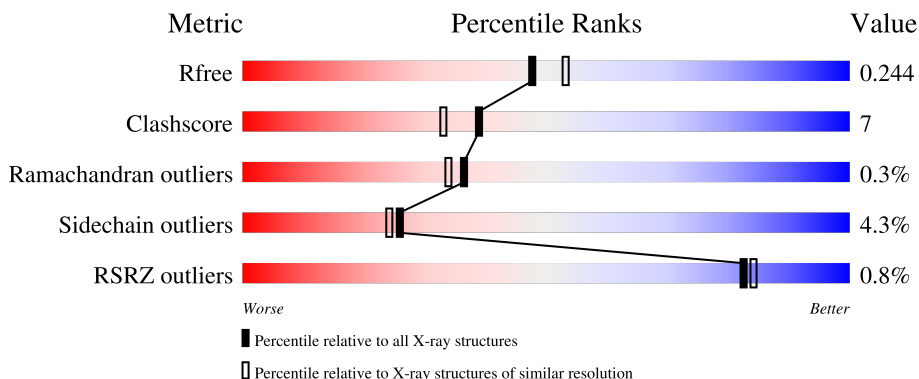
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

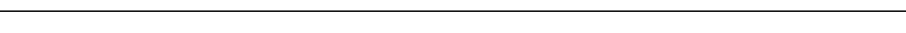
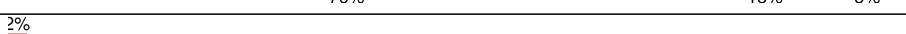
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	

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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 52853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	64	0
			3113	2030	513	551	19			
1	a	334	Total	C	N	O	S	0	64	0
			3110	2027	513	551	19			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3509	2302	586	607	14			
3	c	451	Total	C	N	O	S	0	12	0
			3583	2343	602	624	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2731	1809	446	464	12			
4	d	341	Total	C	N	O	S	0	3	0
			2737	1813	446	466	12			

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

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

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

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

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

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

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

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

- 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		0	0	0
			281	188	45	48				
18	x	39	Total	C	N	O		0	0	0
			286	191	46	49				

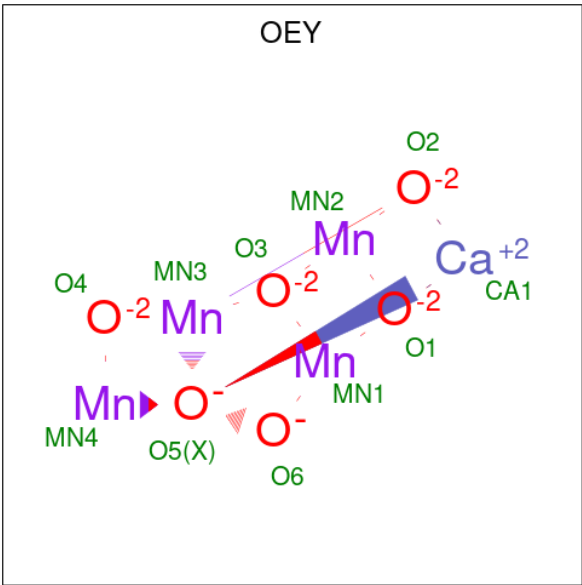
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			477	326	72	77	2			

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

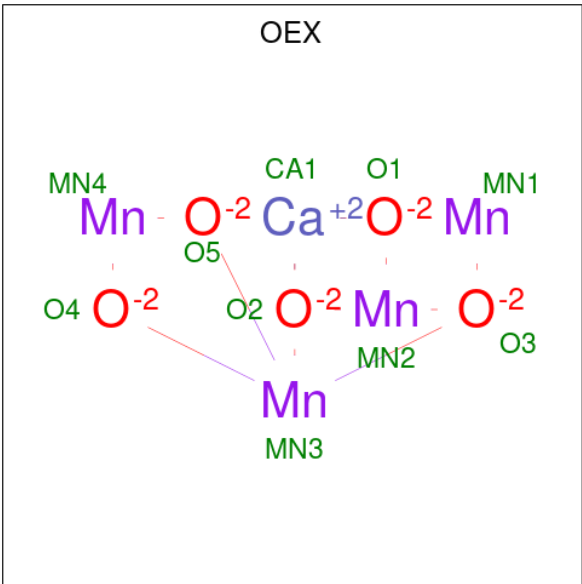
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			271	184	47	40				
20	r	31	Total	C	N	O		0	0	0
			246	166	43	37				

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



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

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



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

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

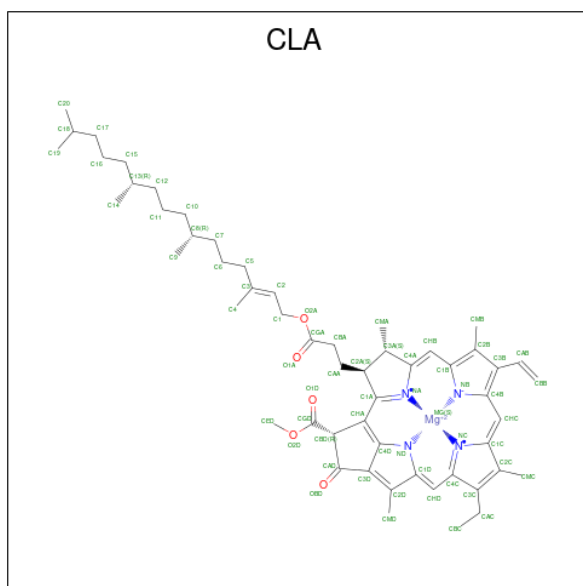
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

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



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

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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	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
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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

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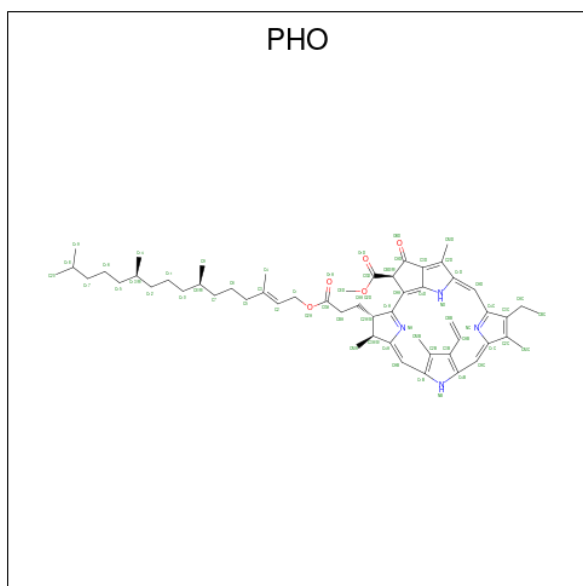
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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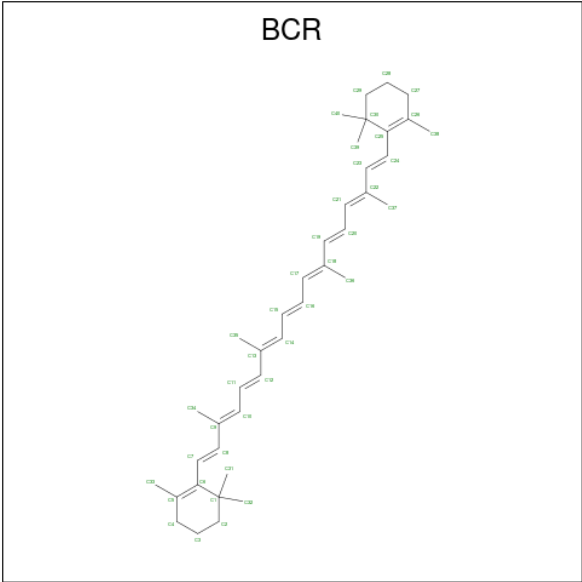
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



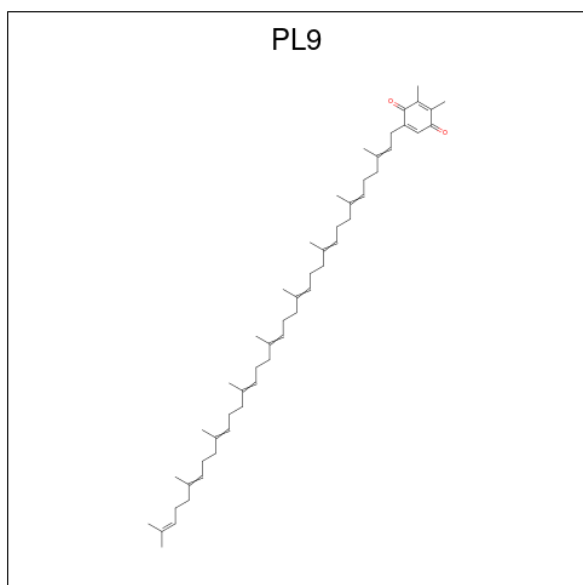
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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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).



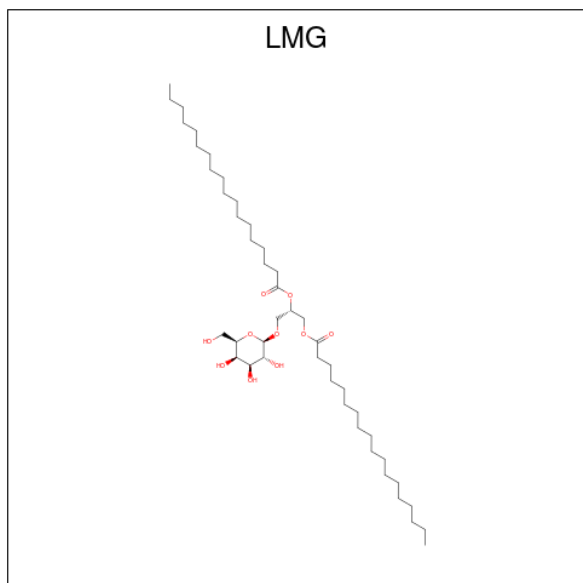
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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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: $C_{45}H_{86}O_{10}$).



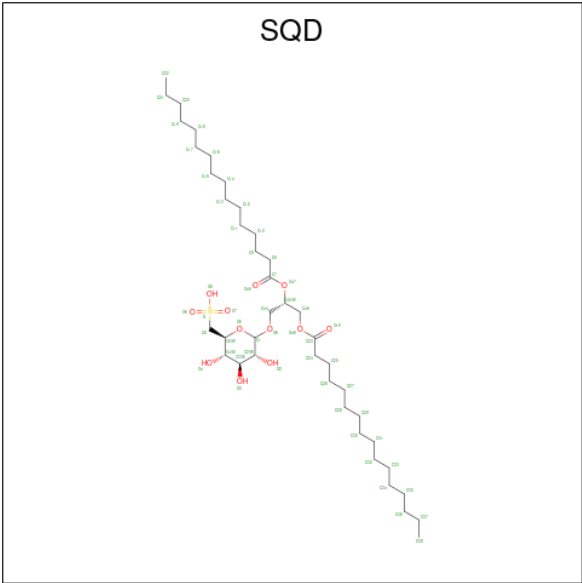
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			28	24	4		
29	C	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			33	27	6		
29	M	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			55	45	10		
29	c	1	Total	C	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-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



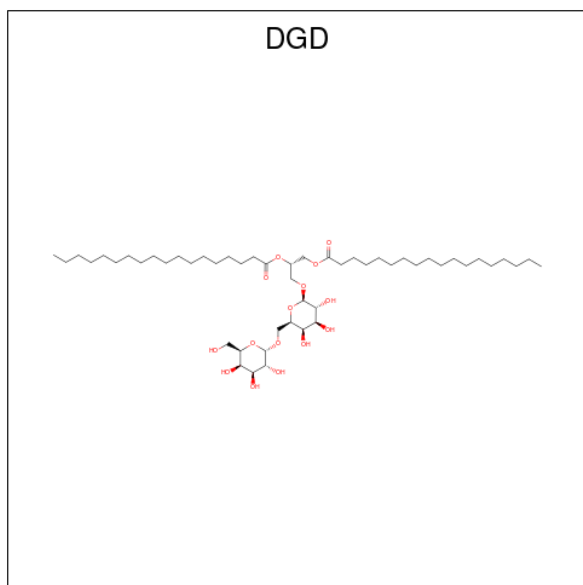
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	L	1	Total	C	O	S	0	0
			49	36	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	f	1	Total	C	O	S	0	0
		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

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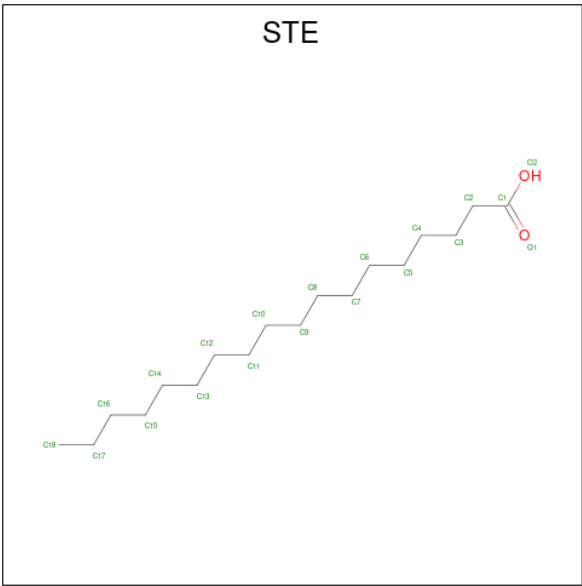
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	t	1	Total	C	O	0	0
			36	31	5		

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



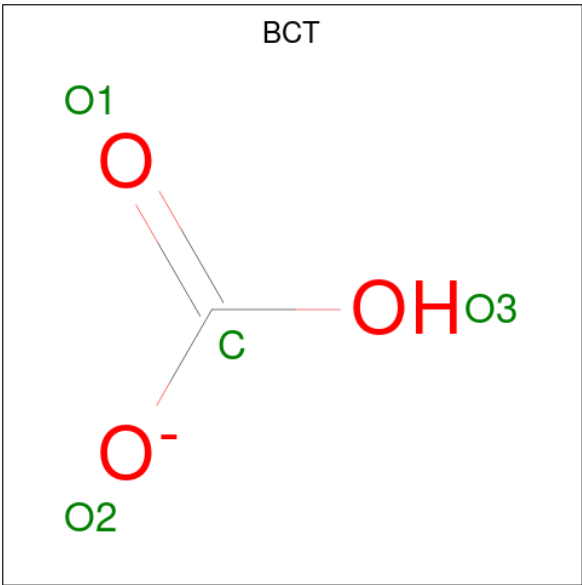
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			17	15	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C		0	0
			16	16			
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C		0	0
			16	16			
32	H	1	Total	C		0	0
			18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

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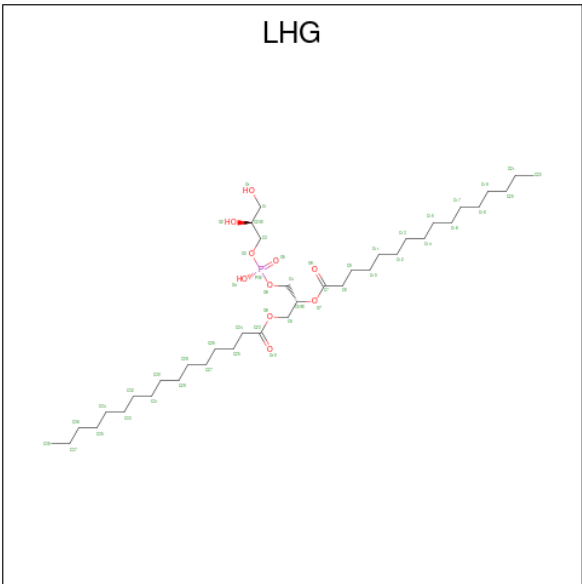
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 20 18 2	0	0
32	R	1	Total C O 12 10 2	0	0
32	a	1	Total C 10 10	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C 16 16	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 15 15	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total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

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



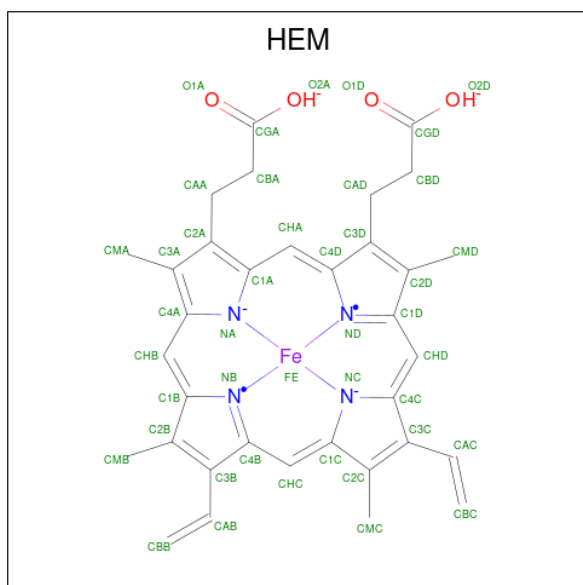
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	O	P	0	0
			49	38	10	1		

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

- 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
35	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- # HEC
-
- The chemical structure of HEC (Hexaethylchlorin) is a complex macrocyclic molecule. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including ethyl, propyl, butyl, and pentyl groups, as well as two carboxylic acid groups (HO-C(=O)-). The structure is labeled with various atoms and bonds, including C, H, N, O, and Fe, and is identified as HEC.

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 37 | A | 120 | Total O
124 124 | 0 | 4 |
| 37 | B | 165 | Total O
165 165 | 0 | 0 |
| 37 | C | 112 | Total O
112 112 | 0 | 0 |
| 37 | D | 94 | Total O
94 94 | 0 | 0 |
| 37 | E | 22 | Total O
22 22 | 0 | 0 |
| 37 | F | 5 | Total O
5 5 | 0 | 0 |
| 37 | H | 24 | Total O
24 24 | 0 | 0 |
| 37 | I | 18 | Total O
18 18 | 0 | 0 |
| 37 | J | 8 | Total O
8 8 | 0 | 0 |



WORLD WIDE
PDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	K	2	Total 2	O 2	0	0
37	L	8	Total 8	O 8	0	0
37	M	7	Total 7	O 7	0	0
37	O	66	Total 66	O 66	0	0
37	T	6	Total 6	O 6	0	0
37	U	30	Total 30	O 30	0	0
37	V	45	Total 45	O 45	0	0
37	Y	6	Total 6	O 6	0	0
37	X	10	Total 10	O 10	0	0
37	Z	5	Total 5	O 5	0	0
37	R	9	Total 9	O 9	0	0
37	a	103	Total 107	O 107	0	4
37	b	132	Total 132	O 132	0	0
37	c	128	Total 128	O 128	0	0
37	d	77	Total 77	O 77	0	0
37	e	14	Total 14	O 14	0	0
37	f	2	Total 2	O 2	0	0
37	h	20	Total 20	O 20	0	0
37	i	10	Total 10	O 10	0	0
37	j	7	Total 7	O 7	0	0
37	k	5	Total 5	O 5	0	0

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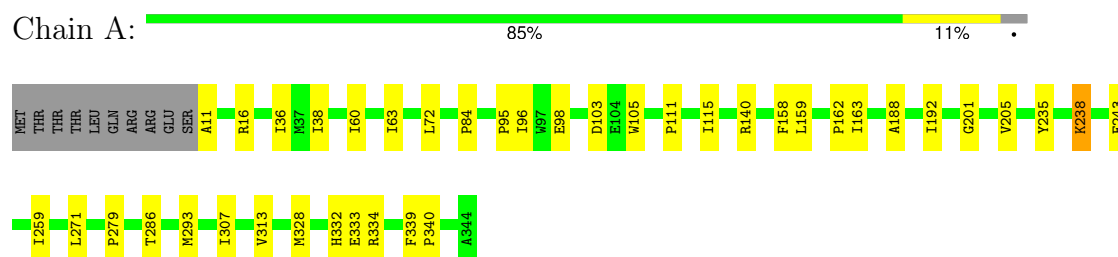
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	l	7	Total 7	O 7	0	0
37	m	3	Total 3	O 3	0	0
37	o	76	Total 76	O 76	0	0
37	t	7	Total 7	O 7	0	0
37	u	34	Total 34	O 34	0	0
37	v	39	Total 39	O 39	0	0
37	y	2	Total 2	O 2	0	0
37	x	4	Total 4	O 4	0	0
37	z	1	Total 1	O 1	0	0
37	r	5	Total 5	O 5	0	0

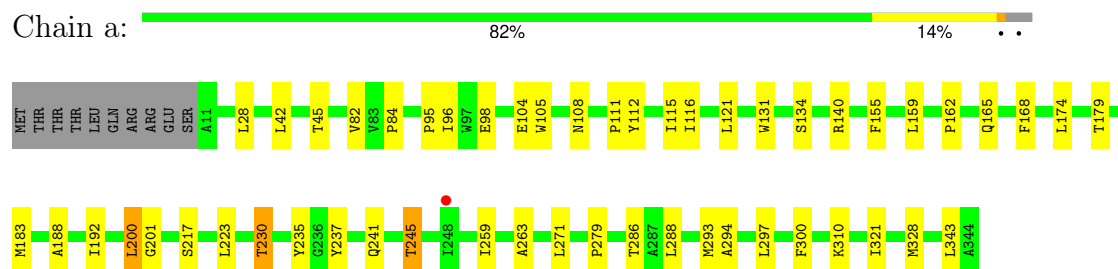
3 Residue-property plots [i](#)

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

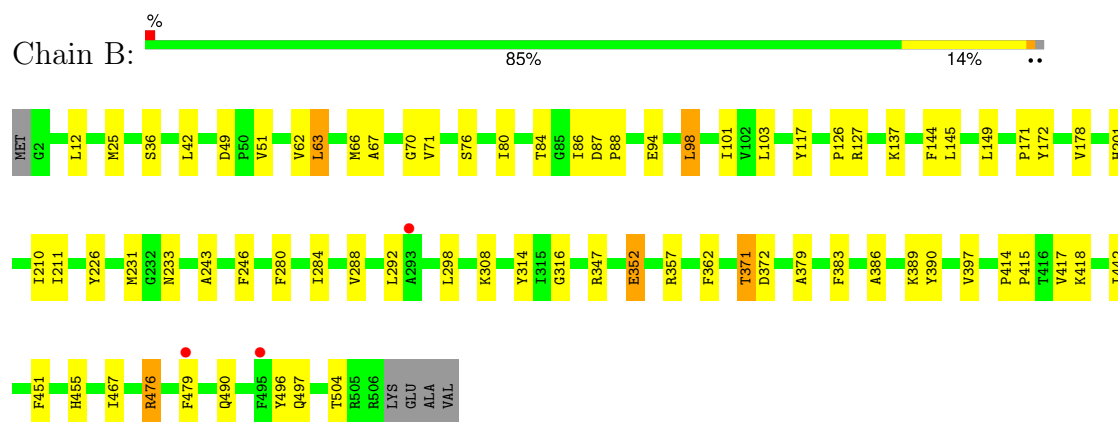
- Molecule 1: Photosystem II protein D1 1



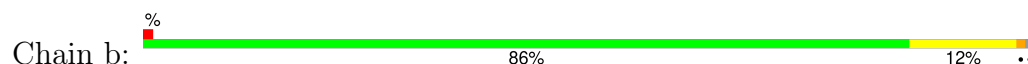
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



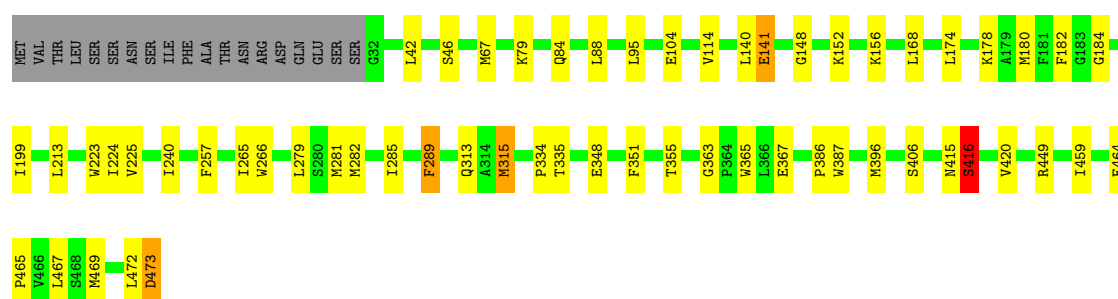
- Molecule 2: Photosystem II CP47 reaction center protein





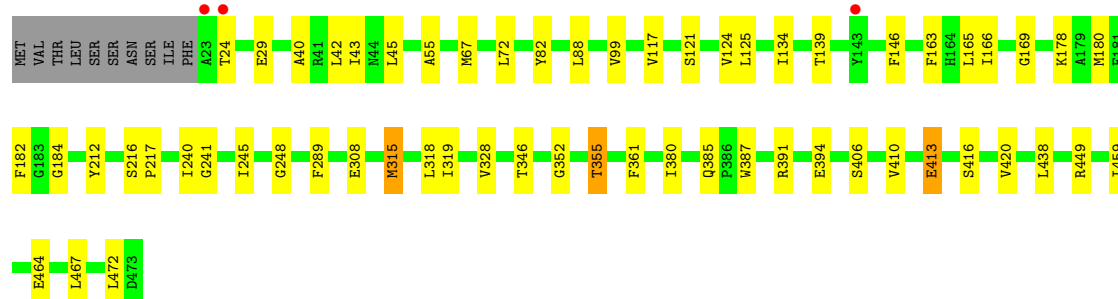
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 83% 12% ..



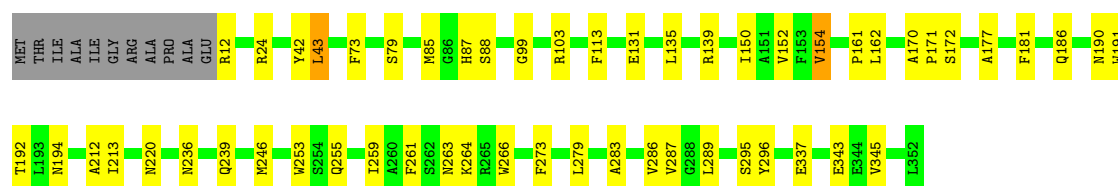
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 85% 12% ..



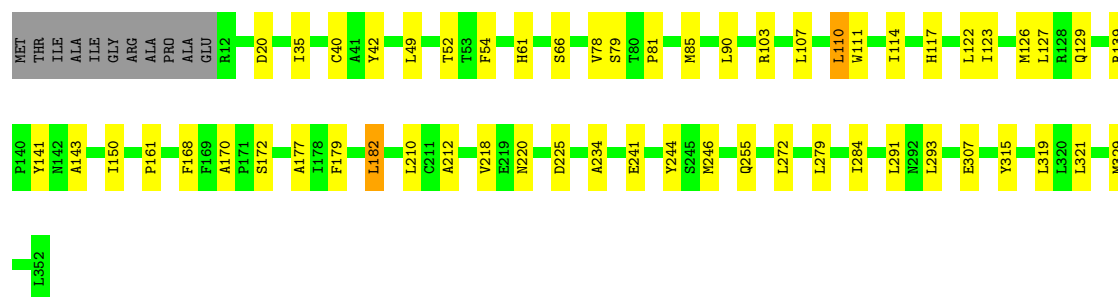
• Molecule 4: Photosystem II D2 protein

Chain D: 82% 15% ..



• Molecule 4: Photosystem II D2 protein

Chain d:  81% 15% ..



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  4% 73% 23% ..



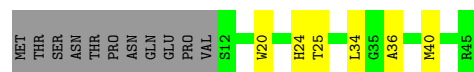
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  4% 74% 21% ..



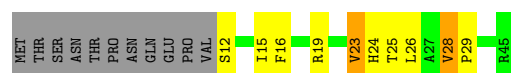
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  62% 13% 24%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  53% 18% 24%

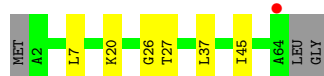
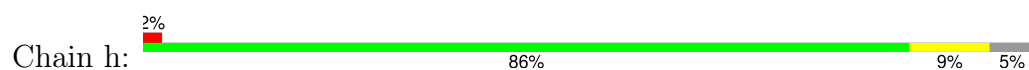


- Molecule 7: Photosystem II reaction center protein H

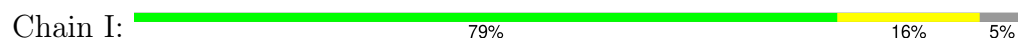
Chain H:  3% 86% 12% .



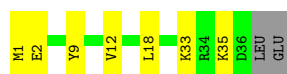
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

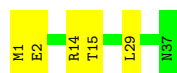


- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 14%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  84% 11% . .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 17% 8%



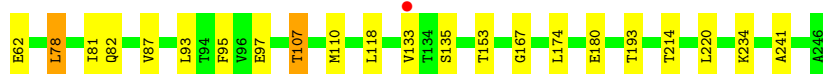
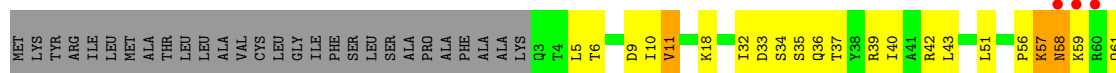
- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 17% 11%



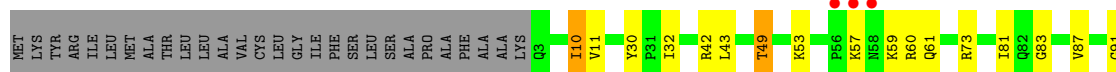
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  74% 14% . 10%

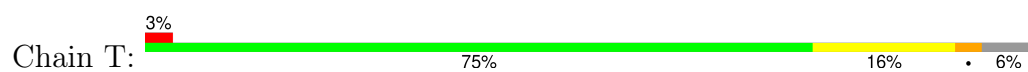


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

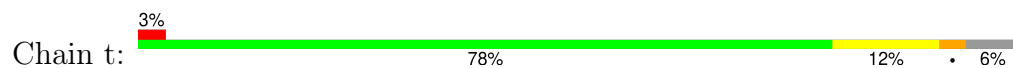
Chain o:  75% 14% . 10%



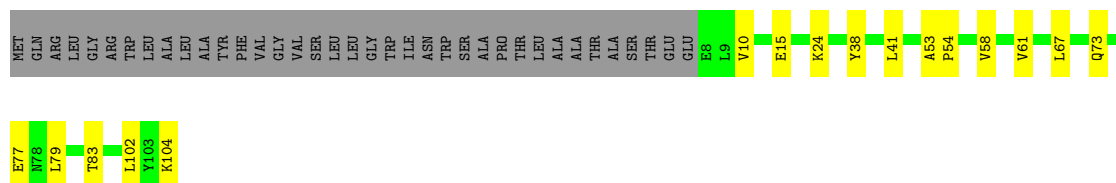
- Molecule 14: Photosystem II reaction center protein T



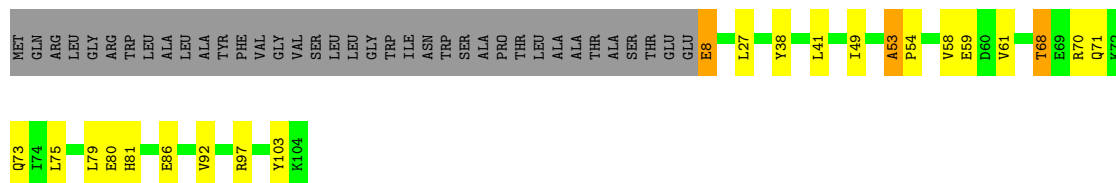
- Molecule 14: Photosystem II reaction center protein T



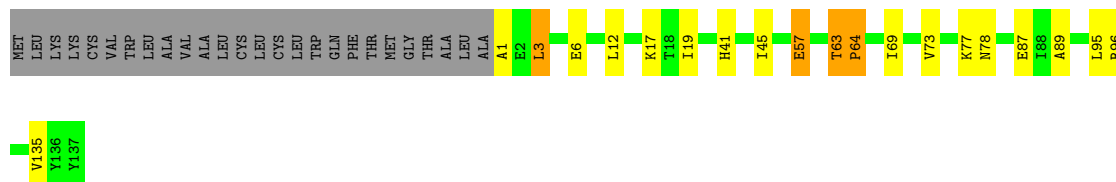
- Molecule 15: Photosystem II 12 kDa extrinsic protein



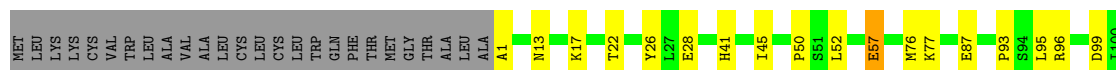
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

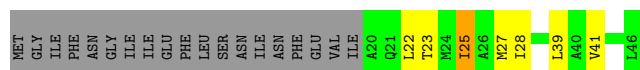


- Molecule 16: Cytochrome c-550

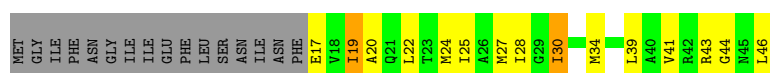
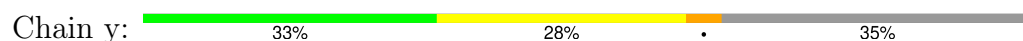




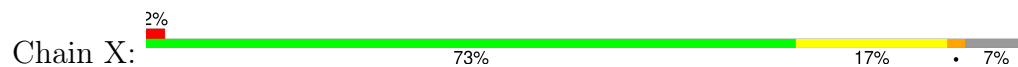
- Molecule 17: Photosystem II reaction center protein Ycf12



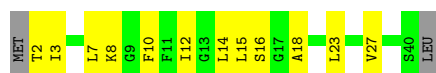
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



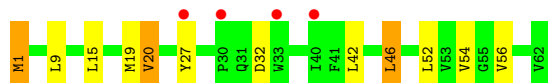
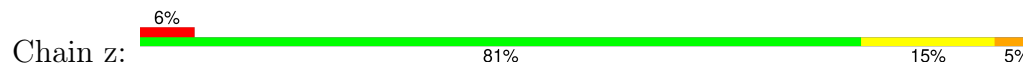
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z

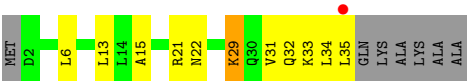


- Molecule 19: Photosystem II reaction center protein Z

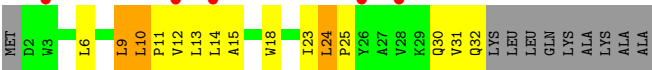


- Molecule 20: Photosystem II protein Y





● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.10Å 222.20Å 308.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.74 – 2.15 33.74 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.74-2.15) 85.0 (33.74-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.42 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.243 0.188 , 0.244	Depositor DCC
R_{free} test set	3853 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52853	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/3212	0.51	0/4376
1	a	0.30	0/3209	0.48	0/4372
2	B	0.34	0/4155	0.50	0/5661
2	b	0.31	0/4118	0.47	0/5611
3	C	0.32	0/3625	0.47	0/4935
3	c	0.30	0/3705	0.46	0/5042
4	D	0.35	0/2825	0.50	0/3847
4	d	0.34	0/2834	0.51	0/3859
5	E	0.27	0/688	0.45	0/940
5	e	0.24	0/683	0.44	0/932
6	F	0.30	0/284	0.48	0/387
6	f	0.26	0/284	0.49	0/387
7	H	0.33	0/523	0.50	0/713
7	h	0.31	0/511	0.49	0/697
8	I	0.33	0/293	0.47	0/396
8	i	0.34	0/293	0.46	0/396
9	J	0.28	0/263	0.46	0/356
9	j	0.26	0/263	0.39	0/356
10	K	0.28	0/303	0.44	0/416
10	k	0.26	0/303	0.51	0/416
11	L	0.37	0/311	0.45	0/422
11	l	0.32	0/303	0.43	0/412
12	M	0.33	0/249	0.54	0/341
12	m	0.35	0/244	0.52	0/334
13	O	0.32	0/1904	0.50	0/2585
13	o	0.32	0/1905	0.51	0/2583
14	T	0.36	0/257	0.54	0/349
14	t	0.32	0/255	0.48	0/346
15	U	0.29	0/785	0.46	0/1064
15	u	0.31	0/785	0.51	0/1064
16	V	0.30	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.29	0/1085	0.47	0/1473
17	Y	0.23	0/197	0.36	0/264
17	y	0.20	0/219	0.43	0/294
18	X	0.26	0/284	0.40	0/384
18	x	0.23	0/289	0.35	0/391
19	Z	0.22	0/490	0.43	0/669
19	z	0.19	0/488	0.33	0/666
20	R	0.27	0/277	0.53	0/380
20	r	0.23	0/252	0.40	0/347
All	All	0.31	0/44038	0.48	0/59936

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	2981	28	0
1	a	3110	0	2972	36	0
2	B	4005	0	3871	48	0
2	b	3978	0	3836	46	0
3	C	3509	0	3426	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3583	0	3499	35	0
4	D	2731	0	2637	41	0
4	d	2737	0	2643	41	0
5	E	666	0	651	13	0
5	e	664	0	648	15	0
6	F	275	0	282	5	0
6	f	275	0	282	9	0
7	H	510	0	532	6	0
7	h	498	0	518	3	0
8	I	296	0	311	2	0
8	i	296	0	311	4	0
9	J	257	0	268	5	0
9	j	257	0	268	5	0
10	K	293	0	305	3	0
10	k	293	0	305	8	0
11	L	304	0	316	4	0
11	l	296	0	304	2	0
12	M	256	0	269	5	0
12	m	251	0	267	4	0
13	O	1870	0	1830	27	0
13	o	1874	0	1846	20	0
14	T	258	0	261	4	0
14	t	256	0	256	3	0
15	U	774	0	773	8	0
15	u	774	0	773	14	0
16	V	1064	0	1073	15	0
16	v	1064	0	1073	15	0
17	Y	196	0	217	4	0
17	y	218	0	241	11	0
18	X	281	0	312	7	0
18	x	286	0	314	8	0
19	Z	479	0	516	13	0
19	z	477	0	509	6	0
20	R	271	0	298	3	0
20	r	246	0	263	10	0
21	A	11	0	0	1	0
21	a	11	0	0	1	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	184	0	192	5	0
25	B	1035	0	1139	42	0
25	C	839	0	922	31	0
25	D	195	0	216	6	0
25	a	260	0	288	6	0
25	b	1035	0	1139	42	0
25	c	839	0	919	23	0
25	d	130	0	144	5	0
26	A	64	0	74	1	0
26	D	64	0	74	1	0
26	a	64	0	74	1	0
26	d	64	0	74	4	0
27	A	40	0	56	0	0
27	B	120	0	168	6	0
27	C	80	0	112	6	0
27	D	40	0	56	0	0
27	H	40	0	56	0	0
27	K	80	0	112	1	0
27	T	40	0	56	5	0
27	a	40	0	56	2	0
27	b	120	0	168	7	0
27	c	80	0	112	5	0
27	d	40	0	56	2	0
27	h	40	0	56	2	0
27	k	80	0	112	5	0
27	t	40	0	56	3	0
28	A	55	0	80	8	0
28	D	55	0	80	1	0
28	a	55	0	80	7	0
28	d	55	0	80	2	0
29	A	48	0	66	0	0
29	B	28	0	40	1	0
29	C	48	0	66	2	0
29	D	84	0	117	4	0
29	M	51	0	72	1	0
29	b	55	0	86	3	0
29	c	134	0	181	11	0
29	d	67	0	92	1	0
29	m	51	0	72	3	0
30	A	91	0	136	7	0
30	B	54	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D	36	0	46	0	0
30	L	49	0	65	4	0
30	a	54	0	78	3	0
30	f	41	0	49	0	0
30	t	36	0	56	3	0
31	A	66	0	96	6	0
31	C	186	0	246	8	0
31	H	62	0	82	3	0
31	a	44	0	75	1	0
31	c	186	0	245	9	0
31	h	62	0	82	1	0
32	B	57	0	89	2	0
32	C	40	0	63	3	0
32	H	18	0	35	3	0
32	I	15	0	26	3	0
32	J	12	0	16	1	0
32	L	12	0	16	1	0
32	M	25	0	38	0	0
32	R	12	0	16	0	0
32	X	20	0	35	4	0
32	a	22	0	32	0	0
32	b	97	0	170	5	0
32	c	32	0	51	2	0
32	d	37	0	61	3	0
32	j	12	0	16	0	0
32	l	18	0	35	2	0
32	t	32	0	48	1	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	D	145	0	215	10	0
34	E	49	0	74	4	0
34	L	49	0	74	3	0
34	d	137	0	199	7	0
34	e	42	0	57	4	0
34	l	49	0	74	2	0
35	F	43	0	30	4	0
35	e	43	0	30	2	0
36	V	43	0	30	0	0
36	v	43	0	30	0	0
37	A	124	0	0	2	0
37	B	165	0	0	0	0
37	C	112	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	94	0	0	0	0
37	E	22	0	0	1	0
37	F	5	0	0	0	0
37	H	24	0	0	0	0
37	I	18	0	0	0	0
37	J	8	0	0	1	0
37	K	2	0	0	0	0
37	L	8	0	0	0	0
37	M	7	0	0	0	0
37	O	66	0	0	2	0
37	R	9	0	0	0	0
37	T	6	0	0	0	0
37	U	30	0	0	1	0
37	V	45	0	0	2	0
37	X	10	0	0	0	0
37	Y	6	0	0	0	0
37	Z	5	0	0	1	0
37	a	107	0	0	1	0
37	b	132	0	0	1	0
37	c	128	0	0	1	0
37	d	77	0	0	0	0
37	e	14	0	0	0	0
37	f	2	0	0	1	0
37	h	20	0	0	0	0
37	i	10	0	0	0	0
37	j	7	0	0	0	0
37	k	5	0	0	1	0
37	l	7	0	0	0	0
37	m	3	0	0	0	0
37	o	76	0	0	1	0
37	r	5	0	0	0	0
37	t	7	0	0	1	0
37	u	34	0	0	3	0
37	v	39	0	0	0	0
37	x	4	0	0	0	0
37	y	2	0	0	0	0
37	z	1	0	0	0	0
All	All	52853	0	52752	707	0

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

The worst 5 of 707 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)
25:B:601:CLA:H92	32:H:103:STE:H162	1.61	0.82
12:m:4:ASN:ND2	29:m:101:LMG:O10	2.13	0.81
5:E:3:GLY:N	37:E:201:HOH:O	2.14	0.80
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.62	0.80
15:u:53:ALA:O	37:u:201:HOH:O	2.01	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/344 (115%)	389 (98%)	5 (1%)	1 (0%)	36	34
1	a	395/344 (115%)	388 (98%)	6 (2%)	1 (0%)	36	34
2	B	507/510 (99%)	502 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	495 (98%)	7 (1%)	1 (0%)	43	44
3	C	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	43	44
3	c	461/461 (100%)	447 (97%)	13 (3%)	1 (0%)	43	44
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	78 (96%)	2 (2%)	1 (1%)	10	5
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	30 (88%)	4 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	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	5
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	30	26
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	7
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	13
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	26 (93%)	2 (7%)	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%)	57 (95%)	2 (3%)	1 (2%)	7	2
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5386/5700 (94%)	5242 (97%)	130 (2%)	14 (0%)	36	34

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	O	59	LYS
13	O	62	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/280 (115%)	319 (99%)	3 (1%)	70	77
1	a	321/280 (115%)	310 (97%)	11 (3%)	32	33
2	B	407/407 (100%)	393 (97%)	14 (3%)	32	33
2	b	402/407 (99%)	389 (97%)	13 (3%)	34	36
3	C	353/362 (98%)	343 (97%)	10 (3%)	38	40
3	c	362/362 (100%)	346 (96%)	16 (4%)	25	23
4	D	277/283 (98%)	272 (98%)	5 (2%)	51	58
4	d	278/283 (98%)	270 (97%)	8 (3%)	37	39
5	E	72/73 (99%)	65 (90%)	7 (10%)	8	4
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	9
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	56
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	14
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	11
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	37
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	6
10	K	30/37 (81%)	26 (87%)	4 (13%)	4	1
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	39
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	31
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	19
13	o	207/228 (91%)	198 (96%)	9 (4%)	26	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	26/28 (93%)	24 (92%)	2 (8%)	12	7
14	t	25/28 (89%)	23 (92%)	2 (8%)	11	7
15	U	84/112 (75%)	81 (96%)	3 (4%)	31	31
15	u	84/112 (75%)	81 (96%)	3 (4%)	31	31
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	60
16	v	117/138 (85%)	112 (96%)	5 (4%)	26	24
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6	3
17	y	22/37 (60%)	18 (82%)	4 (18%)	2	0
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	11
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	11
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
19	z	51/52 (98%)	45 (88%)	6 (12%)	5	2
20	R	28/33 (85%)	20 (71%)	8 (29%)	0	0
20	r	25/33 (76%)	20 (80%)	5 (20%)	1	0
All	All	4450/4654 (96%)	4258 (96%)	192 (4%)	26	24

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	216	SER
8	i	2	GLU
3	c	346	THR
4	d	321	LEU
10	k	35	LEU

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

Mol	Chain	Res	Type
13	o	80	GLN
13	o	155	ASN
17	y	45	ASN
18	X	38	GLN
15	U	37	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	1.18	1 (12%)	8,9,11	0.89	0
8	FME	I	1	8	8,9,10	1.04	0	8,9,11	1.44	1 (12%)
12	FME	M	1	12	8,9,10	1.04	1 (12%)	8,9,11	1.10	0
14	FME	T	1	14	8,9,10	1.06	1 (12%)	8,9,11	1.03	0
8	FME	i	1	8	8,9,10	1.08	1 (12%)	8,9,11	0.83	0
12	FME	m	1	12	8,9,10	1.04	1 (12%)	8,9,11	0.69	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	-	4/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.36	1.43	1.46
12	M	1	FME	CA-N	-2.15	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.09	1.43	1.46
12	m	1	FME	CA-N	-2.08	1.43	1.46
8	i	1	FME	CA-N	-2.01	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CA-N-CN	-3.18	117.93	122.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	t	1	FME	1	0
14	T	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	CLA	B	611	2	69,73,73	1.17	6 (8%)	82,113,113	1.49	7 (8%)
25	CLA	C	504	37	63,67,73	1.40	12 (19%)	74,105,113	1.32	11 (14%)
32	STE	M	102	-	14,14,19	0.73	0	14,14,19	1.09	1 (7%)
25	CLA	C	505	3	69,73,73	1.43	7 (10%)	82,113,113	1.33	11 (13%)
25	CLA	b	606	2	69,73,73	1.38	7 (10%)	82,113,113	1.48	9 (10%)
34	LHG	d	408	-	48,48,48	0.63	0	51,54,54	1.34	7 (13%)
25	CLA	C	511	3	69,73,73	1.41	7 (10%)	82,113,113	1.28	3 (3%)
25	CLA	a	609	1	69,73,73	1.24	7 (10%)	82,113,113	1.20	8 (9%)
30	SQD	D	409	-	34,36,54	1.52	5 (14%)	42,45,65	3.01	11 (26%)
25	CLA	b	601	37	69,73,73	1.32	7 (10%)	82,113,113	1.34	6 (7%)
34	LHG	D	411	-	46,46,48	0.92	2 (4%)	49,52,54	1.27	4 (8%)
21	OEY	a	601[B]	1,3,37	0,16,16	-	-	-	-	-
32	STE	d	412	-	16,16,19	0.66	0	16,16,19	1.11	1 (6%)
31	DGD	c	518	-	63,63,67	0.92	3 (4%)	77,77,81	1.46	14 (18%)
32	STE	I	101	-	14,14,19	0.40	0	13,13,19	0.66	0
25	CLA	b	614	2	69,73,73	1.26	9 (13%)	82,113,113	1.23	9 (10%)
25	CLA	B	615	2	69,73,73	1.27	8 (11%)	82,113,113	1.25	6 (7%)
25	CLA	b	603	2	69,73,73	1.36	10 (14%)	82,113,113	1.44	12 (14%)
27	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.35	6 (10%)
25	CLA	B	604	2	69,73,73	1.30	7 (10%)	82,113,113	1.64	9 (10%)
29	LMG	d	411	-	44,44,55	0.83	2 (4%)	52,52,63	1.33	6 (11%)
26	PHO	D	402	-	58,69,69	2.10	11 (18%)	55,99,99	1.65	11 (20%)
34	LHG	d	407	-	48,48,48	0.81	2 (4%)	51,54,54	1.35	7 (13%)
28	PL9	D	407	-	55,55,55	0.99	3 (5%)	68,69,69	1.48	14 (20%)
34	LHG	d	409	-	38,38,48	0.72	1 (2%)	41,44,54	1.17	3 (7%)
25	CLA	C	502	3	69,73,73	1.39	8 (11%)	82,113,113	1.10	8 (9%)
30	SQD	a	613	-	52,54,54	1.55	6 (11%)	62,65,65	1.98	12 (19%)
25	CLA	D	404	4	69,73,73	1.21	6 (8%)	82,113,113	1.35	7 (8%)
27	BCR	b	618	-	41,41,41	1.13	3 (7%)	56,56,56	1.26	6 (10%)
25	CLA	B	601	37	69,73,73	1.39	9 (13%)	82,113,113	1.32	11 (13%)
35	HEM	e	101	5,6	50,50,50	1.62	8 (16%)	67,82,82	1.32	9 (13%)
27	BCR	B	617	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	7 (12%)
25	CLA	A	606	1	69,73,73	1.22	7 (10%)	82,113,113	1.34	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OEY	A	601[B]	1,3,37	0,16,16	-	-	-		
25	CLA	C	510	3	69,73,73	1.20	8 (11%)	82,113,113	1.31	7 (8%)
29	LMG	b	622	-	55,55,55	0.81	1 (1%)	63,63,63	1.38	6 (9%)
27	BCR	T	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.22	5 (8%)
32	STE	c	522	-	11,11,19	0.74	0	11,11,19	1.22	1 (9%)
31	DGD	A	615	-	67,67,67	1.04	7 (10%)	81,81,81	1.41	16 (19%)
34	LHG	e	102	-	41,41,48	0.79	1 (2%)	44,47,54	1.33	6 (13%)
32	STE	J	101	-	11,11,19	0.74	0	11,11,19	1.35	2 (18%)
29	LMG	m	101	-	51,51,55	0.90	3 (5%)	59,59,63	1.47	9 (15%)
25	CLA	c	503	3	69,73,73	1.32	8 (11%)	82,113,113	1.44	8 (9%)
25	CLA	c	513	3	69,73,73	1.27	9 (13%)	82,113,113	1.08	5 (6%)
25	CLA	A	609	1	58,62,73	1.22	5 (8%)	68,99,113	1.32	8 (11%)
25	CLA	B	603	2	69,73,73	1.47	9 (13%)	82,113,113	1.35	8 (9%)
31	DGD	H	102	-	63,63,67	1.16	4 (6%)	77,77,81	1.43	11 (14%)
27	BCR	D	406	-	41,41,41	1.16	3 (7%)	56,56,56	1.29	6 (10%)
27	BCR	k	102	-	41,41,41	1.07	4 (9%)	56,56,56	1.22	6 (10%)
27	BCR	d	405	-	41,41,41	1.08	3 (7%)	56,56,56	1.12	3 (5%)
28	PL9	d	406	-	55,55,55	1.04	3 (5%)	68,69,69	1.68	16 (23%)
27	BCR	H	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	4 (7%)
32	STE	B	623	-	11,11,19	0.77	0	11,11,19	1.13	1 (9%)
25	CLA	B	609	2	69,73,73	1.12	7 (10%)	82,113,113	1.24	8 (9%)
32	STE	B	620	-	16,16,19	0.69	0	16,16,19	1.11	0
34	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.28	8 (15%)
26	PHO	A	608	-	58,69,69	1.92	10 (17%)	55,99,99	1.57	7 (12%)
25	CLA	c	502	3	69,73,73	1.26	10 (14%)	82,113,113	1.41	7 (8%)
32	STE	C	521	-	11,11,19	0.74	0	11,11,19	1.17	1 (9%)
25	CLA	c	508	3	68,72,73	1.28	9 (13%)	80,111,113	1.29	9 (11%)
27	BCR	t	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
32	STE	t	104	-	17,17,19	0.57	0	17,17,19	1.20	1 (5%)
32	STE	L	103	-	11,11,19	0.66	0	11,11,19	1.38	1 (9%)
25	CLA	B	605	2	69,73,73	1.26	9 (13%)	82,113,113	1.23	7 (8%)
25	CLA	B	602	2	69,73,73	1.36	8 (11%)	82,113,113	1.37	8 (9%)
25	CLA	C	503	3	69,73,73	1.48	12 (17%)	82,113,113	1.36	7 (8%)
27	BCR	B	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	7 (12%)
29	LMG	A	612	-	48,48,55	0.97	3 (6%)	56,56,63	1.31	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	D	412	-	31,31,55	0.67	1 (3%)	33,33,63	1.20	2 (6%)
30	SQD	f	101	-	39,41,54	1.70	8 (20%)	49,52,65	1.77	11 (22%)
32	STE	X	101	-	19,19,19	0.65	0	19,19,19	1.06	0
25	CLA	b	616	2	64,68,73	1.14	6 (9%)	76,107,113	1.47	6 (7%)
25	CLA	b	607	37	69,73,73	1.32	9 (13%)	82,113,113	1.22	10 (12%)
32	STE	c	520	-	19,19,19	0.64	0	19,19,19	0.98	0
30	SQD	t	102	-	35,35,54	1.71	5 (14%)	37,37,65	1.50	5 (13%)
25	CLA	c	509	3	69,73,73	1.06	4 (5%)	82,113,113	1.51	8 (9%)
25	CLA	b	610	37	69,73,73	1.31	6 (8%)	82,113,113	1.26	8 (9%)
30	SQD	L	101	-	47,49,54	1.63	10 (21%)	57,60,65	1.93	13 (22%)
25	CLA	b	609	2	69,73,73	1.24	9 (13%)	82,113,113	1.36	8 (9%)
32	STE	b	625	-	19,19,19	0.61	0	19,19,19	1.01	1 (5%)
26	PHO	a	608	-	58,69,69	2.03	10 (17%)	55,99,99	1.54	8 (14%)
25	CLA	b	608	2	69,73,73	1.36	9 (13%)	82,113,113	1.50	11 (13%)
29	LMG	c	523	-	49,49,55	0.84	2 (4%)	57,57,63	1.30	4 (7%)
22	OEX	a	602[A]	1,3,37	0,14,14	-	-	-	-	-
27	BCR	b	619	-	41,41,41	1.02	2 (4%)	56,56,56	1.20	3 (5%)
34	LHG	D	410	-	48,48,48	0.79	1 (2%)	51,54,54	1.34	7 (13%)
34	LHG	D	413	-	48,48,48	0.92	2 (4%)	51,54,54	1.40	6 (11%)
29	LMG	c	519	-	37,37,55	1.02	4 (10%)	45,45,63	1.33	6 (13%)
25	CLA	C	512	3	69,73,73	1.45	10 (14%)	82,113,113	1.38	9 (10%)
32	STE	H	103	-	17,17,19	0.37	0	16,16,19	0.80	0
32	STE	C	522	-	15,15,19	0.41	0	14,14,19	0.69	0
36	HEC	V	201	16	50,50,50	1.64	6 (12%)	68,82,82	1.38	9 (13%)
25	CLA	d	403	4	69,73,73	1.11	7 (10%)	82,113,113	1.19	6 (7%)
25	CLA	C	507	37	69,73,73	1.19	8 (11%)	82,113,113	1.41	8 (9%)
26	PHO	d	402	-	58,69,69	2.13	9 (15%)	55,99,99	1.66	8 (14%)
25	CLA	D	405	4	69,73,73	1.32	7 (10%)	82,113,113	1.28	6 (7%)
25	CLA	a	607	37	69,73,73	1.16	7 (10%)	82,113,113	1.29	8 (9%)
25	CLA	d	404	4	69,73,73	1.21	8 (11%)	82,113,113	1.17	9 (10%)
32	STE	j	101	-	11,11,19	0.80	0	11,11,19	1.16	0
25	CLA	C	508	3	69,73,73	1.26	7 (10%)	82,113,113	1.46	11 (13%)
31	DGD	c	516	-	63,63,67	1.07	8 (12%)	77,77,81	1.39	10 (12%)
25	CLA	c	510	3	69,73,73	1.22	8 (11%)	82,113,113	1.41	9 (10%)
25	CLA	c	511	3	69,73,73	1.33	6 (8%)	82,113,113	1.33	6 (7%)
25	CLA	C	506	3	69,73,73	1.21	8 (11%)	82,113,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DGD	h	102	-	63,63,67	0.91	2 (3%)	77,77,81	1.50	14 (18%)
22	OEX	A	602[A]	1,3,37	0,14,14	-	-	-		
29	LMG	C	519	-	48,48,55	0.86	2 (4%)	56,56,63	1.34	6 (10%)
32	STE	b	626	-	9,9,19	0.35	0	8,8,19	0.74	0
31	DGD	a	614	-	43,43,67	0.73	2 (4%)	45,45,81	1.46	6 (13%)
32	STE	M	103	-	9,9,19	0.39	0	8,8,19	0.67	0
25	CLA	c	512	3	69,73,73	1.28	9 (13%)	82,113,113	1.35	8 (9%)
25	CLA	b	613	2	69,73,73	1.40	9 (13%)	82,113,113	1.47	13 (15%)
27	BCR	k	101	-	41,41,41	1.07	4 (9%)	56,56,56	1.13	3 (5%)
32	STE	b	623	-	15,15,19	0.80	0	15,15,19	0.89	0
33	BCT	d	401	23	3,3,3	1.16	0	2,3,3	2.97	1 (50%)
30	SQD	A	614	-	38,38,54	1.78	5 (13%)	40,40,65	1.27	3 (7%)
25	CLA	c	505	3	69,73,73	1.28	7 (10%)	82,113,113	1.33	9 (10%)
32	STE	d	413	-	19,19,19	0.71	0	19,19,19	0.85	1 (5%)
25	CLA	a	612	37	69,73,73	1.42	10 (14%)	82,113,113	1.23	7 (8%)
25	CLA	B	608	2	69,73,73	1.18	7 (10%)	82,113,113	1.32	7 (8%)
25	CLA	B	607	37	69,73,73	1.34	7 (10%)	82,113,113	1.43	10 (12%)
32	STE	t	103	-	13,13,19	0.67	0	13,13,19	1.25	2 (15%)
25	CLA	b	615	2	69,73,73	1.26	8 (11%)	82,113,113	1.42	4 (4%)
30	SQD	A	613	-	50,52,54	1.58	8 (16%)	60,63,65	2.01	13 (21%)
34	LHG	E	101	-	48,48,48	0.78	2 (4%)	51,54,54	1.23	6 (11%)
25	CLA	b	612	2	69,73,73	1.23	8 (11%)	82,113,113	1.39	12 (14%)
31	DGD	C	518	-	63,63,67	0.83	3 (4%)	77,77,81	1.45	12 (15%)
27	BCR	h	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	8 (14%)
30	SQD	B	622	-	52,54,54	1.58	8 (15%)	62,65,65	1.76	11 (17%)
25	CLA	b	611	2	69,73,73	1.27	9 (13%)	82,113,113	1.39	5 (6%)
25	CLA	b	605	2	69,73,73	1.11	5 (7%)	82,113,113	1.38	8 (9%)
27	BCR	a	610	-	41,41,41	0.96	3 (7%)	56,56,56	1.26	4 (7%)
25	CLA	A	607	37	69,73,73	1.18	9 (13%)	82,113,113	1.34	10 (12%)
25	CLA	B	614	2	69,73,73	1.39	7 (10%)	82,113,113	1.24	9 (10%)
32	STE	b	621	-	19,19,19	0.61	0	19,19,19	1.09	1 (5%)
31	DGD	C	517	-	63,63,67	0.96	6 (9%)	77,77,81	1.42	9 (11%)
29	LMG	M	101	-	51,51,55	0.84	4 (7%)	59,59,63	1.38	7 (11%)
33	BCT	D	401	23	3,3,3	1.13	0	2,3,3	2.86	1 (50%)
25	CLA	D	403	37	69,73,73	1.23	7 (10%)	82,113,113	1.27	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	c	521	-	48,48,55	0.96	4 (8%)	56,56,63	1.31	7 (12%)
25	CLA	B	610	37	69,73,73	1.19	10 (14%)	82,113,113	1.41	10 (12%)
32	STE	l	102	-	17,17,19	0.33	0	16,16,19	0.95	0
32	STE	a	615	-	9,9,19	0.43	0	8,8,19	0.60	0
25	CLA	B	616	2	64,68,73	1.25	7 (10%)	76,107,113	1.29	4 (5%)
31	DGD	C	516	-	63,63,67	1.05	3 (4%)	77,77,81	1.35	10 (12%)
25	CLA	c	501	3	69,73,73	1.20	5 (7%)	82,113,113	1.39	5 (6%)
25	CLA	a	606	1	69,73,73	1.30	9 (13%)	82,113,113	1.30	7 (8%)
27	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	3 (5%)
32	STE	a	616	-	11,11,19	0.84	0	11,11,19	0.86	0
28	PL9	A	611	-	55,55,55	0.91	2 (3%)	68,69,69	1.47	10 (14%)
29	LMG	D	408	-	51,51,55	0.78	1 (1%)	59,59,63	1.24	6 (10%)
25	CLA	b	604	2	69,73,73	1.24	8 (11%)	82,113,113	1.55	12 (14%)
32	STE	R	101	-	11,11,19	0.71	0	11,11,19	1.15	1 (9%)
34	LHG	L	102	-	48,48,48	0.72	0	51,54,54	1.25	5 (9%)
25	CLA	C	513	3	69,73,73	1.30	6 (8%)	82,113,113	1.28	6 (7%)
36	HEC	v	201	16	50,50,50	1.72	6 (12%)	68,82,82	1.43	6 (8%)
31	DGD	c	517	-	63,63,67	1.00	5 (7%)	77,77,81	1.46	12 (15%)
35	HEM	F	101	5,6	50,50,50	1.37	8 (16%)	67,82,82	1.17	1 (1%)
25	CLA	B	606	2	69,73,73	1.27	5 (7%)	82,113,113	1.39	9 (10%)
25	CLA	c	504	37	64,68,73	1.21	6 (9%)	76,107,113	1.21	5 (6%)
25	CLA	c	506	3	69,73,73	1.27	8 (11%)	82,113,113	1.32	4 (4%)
27	BCR	K	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
27	BCR	b	617	-	41,41,41	0.99	3 (7%)	56,56,56	1.26	5 (8%)
29	LMG	d	410	-	21,21,55	0.61	0	20,20,63	1.15	0
27	BCR	c	514	-	41,41,41	1.07	3 (7%)	56,56,56	1.28	8 (14%)
25	CLA	c	507	37	69,73,73	1.26	7 (10%)	82,113,113	1.26	7 (8%)
32	STE	B	624	-	11,11,19	0.68	0	11,11,19	1.22	2 (18%)
32	STE	b	620	-	15,15,19	0.39	0	14,14,19	0.88	0
28	PL9	a	611	-	55,55,55	0.76	1 (1%)	68,69,69	1.52	11 (16%)
29	LMG	B	621	-	26,26,55	0.77	2 (7%)	26,26,63	1.19	1 (3%)
27	BCR	c	515	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	4 (7%)
27	BCR	K	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.39	9 (16%)
32	STE	B	625	-	15,15,19	0.36	0	14,14,19	0.84	0
25	CLA	b	602	2	69,73,73	1.39	10 (14%)	82,113,113	1.45	8 (9%)
27	BCR	A	610	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	613	2	69,73,73	1.20	7 (10%)	82,113,113	1.36	10 (12%)
32	STE	C	520	-	11,11,19	0.68	0	11,11,19	1.52	1 (9%)
32	STE	b	624	-	14,14,19	0.29	0	13,13,19	0.98	0
25	CLA	C	509	3	69,73,73	1.37	10 (14%)	82,113,113	1.34	9 (10%)
27	BCR	C	514	-	41,41,41	1.15	3 (7%)	56,56,56	1.27	8 (14%)
25	CLA	C	501	3	69,73,73	1.32	10 (14%)	82,113,113	1.42	8 (9%)
25	CLA	B	612	2	69,73,73	1.17	9 (13%)	82,113,113	1.38	11 (13%)

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
25	CLA	B	611	2	-	8/39/115/115	-
25	CLA	C	504	37	-	7/32/108/115	-
32	STE	M	102	-	-	8/12/12/17	-
25	CLA	C	505	3	-	12/39/115/115	-
25	CLA	b	606	2	-	7/39/115/115	-
34	LHG	d	408	-	-	20/53/53/53	-
25	CLA	C	511	3	-	6/39/115/115	-
25	CLA	a	609	1	-	6/39/115/115	-
30	SQD	D	409	-	-	14/28/48/69	0/1/1/1
25	CLA	b	601	37	-	21/39/115/115	-
34	LHG	D	411	-	-	19/51/51/53	-
32	STE	d	412	-	-	7/14/14/17	-
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
32	STE	I	101	-	-	5/12/12/17	-
25	CLA	b	614	2	-	18/39/115/115	-
25	CLA	B	615	2	-	10/39/115/115	-
25	CLA	b	603	2	-	7/39/115/115	-
27	BCR	B	619	-	-	8/29/63/63	0/2/2/2
25	CLA	B	604	2	-	16/39/115/115	-
29	LMG	d	411	-	-	10/39/59/70	0/1/1/1
26	PHO	D	402	-	-	2/37/103/103	0/5/6/6
34	LHG	d	407	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	D	407	-	-	15/53/73/73	0/1/1/1
34	LHG	d	409	-	-	12/43/43/53	-
25	CLA	C	502	3	-	11/39/115/115	-
30	SQD	a	613	-	-	23/49/69/69	0/1/1/1
25	CLA	D	404	4	-	17/39/115/115	-
27	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	CLA	B	601	37	-	23/39/115/115	-
35	HEM	e	101	5,6	-	3/14/54/54	-
27	BCR	B	617	-	-	4/29/63/63	0/2/2/2
25	CLA	A	606	1	-	3/39/115/115	-
25	CLA	C	510	3	-	9/39/115/115	-
29	LMG	b	622	-	-	24/50/70/70	0/1/1/1
27	BCR	T	101	-	-	7/29/63/63	0/2/2/2
32	STE	c	522	-	-	5/9/9/17	-
31	DGD	A	615	-	-	22/55/95/95	0/2/2/2
34	LHG	e	102	-	-	22/46/46/53	-
32	STE	J	101	-	-	3/9/9/17	-
29	LMG	m	101	-	-	20/46/66/70	0/1/1/1
25	CLA	c	503	3	-	15/39/115/115	-
25	CLA	c	513	3	-	11/39/115/115	-
25	CLA	A	609	1	-	5/26/102/115	-
25	CLA	B	603	2	-	9/39/115/115	-
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
27	BCR	D	406	-	-	7/29/63/63	0/2/2/2
27	BCR	k	102	-	-	5/29/63/63	0/2/2/2
27	BCR	d	405	-	-	9/29/63/63	0/2/2/2
28	PL9	d	406	-	-	16/53/73/73	0/1/1/1
27	BCR	H	101	-	-	4/29/63/63	0/2/2/2
32	STE	B	623	-	-	5/9/9/17	-
25	CLA	B	609	2	-	7/39/115/115	-
32	STE	B	620	-	-	10/14/14/17	-
34	LHG	l	101	-	-	20/53/53/53	-
26	PHO	A	608	-	-	9/37/103/103	0/5/6/6
25	CLA	c	502	3	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	C	521	-	-	5/9/9/17	-
25	CLA	c	508	3	-	6/38/114/115	-
27	BCR	t	101	-	-	7/29/63/63	0/2/2/2
32	STE	t	104	-	-	9/15/15/17	-
32	STE	L	103	-	-	6/9/9/17	-
25	CLA	B	605	2	-	11/39/115/115	-
25	CLA	B	602	2	-	9/39/115/115	-
25	CLA	C	503	3	-	11/39/115/115	-
27	BCR	B	618	-	-	8/29/63/63	0/2/2/2
29	LMG	A	612	-	-	19/43/63/70	0/1/1/1
29	LMG	D	412	-	-	19/33/33/70	-
30	SQD	f	101	-	-	15/36/56/69	0/1/1/1
32	STE	X	101	-	-	11/17/17/17	-
25	CLA	b	616	2	-	13/33/109/115	-
25	CLA	b	607	37	-	14/39/115/115	-
32	STE	c	520	-	-	14/17/17/17	-
30	SQD	t	102	-	-	19/37/37/69	-
25	CLA	c	509	3	-	5/39/115/115	-
25	CLA	b	610	37	-	9/39/115/115	-
30	SQD	L	101	-	-	25/44/64/69	0/1/1/1
25	CLA	b	609	2	-	8/39/115/115	-
32	STE	b	625	-	-	11/17/17/17	-
26	PHO	a	608	-	-	4/37/103/103	0/5/6/6
25	CLA	b	608	2	-	7/39/115/115	-
29	LMG	c	523	-	-	28/44/64/70	0/1/1/1
27	BCR	b	619	-	-	6/29/63/63	0/2/2/2
34	LHG	D	410	-	-	19/53/53/53	-
34	LHG	D	413	-	-	23/53/53/53	-
29	LMG	c	519	-	-	10/31/51/70	0/1/1/1
25	CLA	C	512	3	-	10/39/115/115	-
32	STE	H	103	-	-	10/15/15/17	-
32	STE	C	522	-	-	5/13/13/17	-
36	HEC	V	201	16	1/1/3/7	4/14/54/54	-
25	CLA	d	403	4	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	507	37	-	11/39/115/115	-
26	PHO	d	402	-	-	5/37/103/103	0/5/6/6
25	CLA	D	405	4	-	6/39/115/115	-
25	CLA	a	607	37	-	16/39/115/115	-
25	CLA	d	404	4	-	7/39/115/115	-
32	STE	j	101	-	-	5/9/9/17	-
25	CLA	C	508	3	-	5/39/115/115	-
31	DGD	c	516	-	-	26/51/91/95	0/2/2/2
25	CLA	c	510	3	-	13/39/115/115	-
25	CLA	c	511	3	-	16/39/115/115	-
25	CLA	C	506	3	-	13/39/115/115	-
31	DGD	h	102	-	-	14/51/91/95	0/2/2/2
29	LMG	C	519	-	-	18/43/63/70	0/1/1/1
32	STE	b	626	-	-	2/7/7/17	-
31	DGD	a	614	-	-	26/45/45/95	-
32	STE	M	103	-	-	3/7/7/17	-
25	CLA	c	512	3	-	20/39/115/115	-
25	CLA	b	613	2	-	11/39/115/115	-
27	BCR	k	101	-	-	8/29/63/63	0/2/2/2
32	STE	b	623	-	-	8/13/13/17	-
30	SQD	A	614	-	-	14/39/39/69	-
25	CLA	c	505	3	-	11/39/115/115	-
32	STE	d	413	-	-	11/17/17/17	-
25	CLA	a	612	37	-	2/39/115/115	-
25	CLA	B	608	2	-	5/39/115/115	-
25	CLA	B	607	37	-	16/39/115/115	-
32	STE	t	103	-	-	3/11/11/17	-
25	CLA	b	615	2	-	17/39/115/115	-
30	SQD	A	613	-	-	19/47/67/69	0/1/1/1
34	LHG	E	101	-	-	29/53/53/53	-
25	CLA	b	612	2	-	10/39/115/115	-
31	DGD	C	518	-	-	14/51/91/95	0/2/2/2
27	BCR	h	101	-	-	4/29/63/63	0/2/2/2
30	SQD	B	622	-	-	24/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	611	2	-	8/39/115/115	-
25	CLA	b	605	2	-	9/39/115/115	-
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2
25	CLA	A	607	37	-	7/39/115/115	-
25	CLA	B	614	2	-	18/39/115/115	-
32	STE	b	621	-	-	10/17/17/17	-
31	DGD	C	517	-	-	21/51/91/95	0/2/2/2
29	LMG	M	101	-	-	20/46/66/70	0/1/1/1
25	CLA	D	403	37	-	2/39/115/115	-
29	LMG	c	521	-	-	25/43/63/70	0/1/1/1
25	CLA	B	610	37	-	5/39/115/115	-
32	STE	l	102	-	-	7/15/15/17	-
32	STE	a	615	-	-	5/7/7/17	-
25	CLA	B	616	2	-	8/33/109/115	-
31	DGD	C	516	-	-	23/51/91/95	0/2/2/2
25	CLA	c	501	3	-	4/39/115/115	-
25	CLA	a	606	1	-	3/39/115/115	-
27	BCR	C	515	-	-	6/29/63/63	0/2/2/2
32	STE	a	616	-	-	4/9/9/17	-
28	PL9	A	611	-	-	21/53/73/73	0/1/1/1
29	LMG	D	408	-	-	21/46/66/70	0/1/1/1
25	CLA	b	604	2	-	7/39/115/115	-
32	STE	R	101	-	-	4/9/9/17	-
34	LHG	L	102	-	-	20/53/53/53	-
25	CLA	C	513	3	-	13/39/115/115	-
36	HEC	v	201	16	1/1/3/7	6/14/54/54	-
31	DGD	c	517	-	-	19/51/91/95	0/2/2/2
35	HEM	F	101	5,6	-	2/14/54/54	-
25	CLA	B	606	2	-	12/39/115/115	-
25	CLA	c	504	37	-	8/33/109/115	-
25	CLA	c	506	3	-	12/39/115/115	-
27	BCR	K	102	-	-	6/29/63/63	0/2/2/2
27	BCR	b	617	-	-	6/29/63/63	0/2/2/2
29	LMG	d	410	-	-	13/17/17/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	c	514	-	-	7/29/63/63	0/2/2/2
25	CLA	c	507	37	-	13/39/115/115	-
32	STE	B	624	-	-	4/9/9/17	-
32	STE	b	620	-	-	5/13/13/17	-
28	PL9	a	611	-	-	23/53/73/73	0/1/1/1
29	LMG	B	621	-	-	14/22/22/70	-
27	BCR	c	515	-	-	3/29/63/63	0/2/2/2
27	BCR	K	101	-	-	7/29/63/63	0/2/2/2
32	STE	B	625	-	-	2/13/13/17	-
25	CLA	b	602	2	-	8/39/115/115	-
27	BCR	A	610	-	-	2/29/63/63	0/2/2/2
25	CLA	B	613	2	-	15/39/115/115	-
32	STE	C	520	-	-	3/9/9/17	-
32	STE	b	624	-	-	9/12/12/17	-
25	CLA	C	509	3	-	13/39/115/115	-
27	BCR	C	514	-	-	7/29/63/63	0/2/2/2
25	CLA	C	501	3	-	7/39/115/115	-
25	CLA	B	612	2	-	12/39/115/115	-

The worst 5 of 821 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	402	PHO	C1B-C2B	9.20	1.49	1.39
26	d	402	PHO	C3B-C4B	9.00	1.50	1.41
26	a	608	PHO	C1B-C2B	8.90	1.49	1.39
26	D	402	PHO	C1B-C2B	8.81	1.49	1.39
26	D	402	PHO	C3B-C4B	8.52	1.50	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O6-C1-C2	13.59	128.91	108.27
25	B	604	CLA	C4A-NA-C1A	9.23	110.89	106.68
25	c	509	CLA	C4A-NA-C1A	8.52	110.57	106.68
25	C	507	CLA	C4A-NA-C1A	7.94	110.30	106.68
25	b	615	CLA	C4A-NA-C1A	7.84	110.25	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 1937 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	601	CLA	CAD-CBD-CGD-O2D
25	B	601	CLA	C11-C12-C13-C14
25	B	605	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

148 monomers are involved in 314 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	611	CLA	3	0
25	C	504	CLA	2	0
25	C	505	CLA	3	0
25	b	606	CLA	3	0
25	C	511	CLA	2	0
25	a	609	CLA	2	0
25	b	601	CLA	3	0
34	D	411	LHG	2	0
21	a	601[B]	OEY	1	0
32	d	412	STE	1	0
31	c	518	DGD	5	0
32	I	101	STE	3	0
25	b	614	CLA	5	0
25	B	615	CLA	5	0
25	b	603	CLA	1	0
27	B	619	BCR	2	0
25	B	604	CLA	6	0
29	d	411	LMG	1	0
26	D	402	PHO	1	0
34	d	407	LHG	5	0
28	D	407	PL9	1	0
34	d	409	LHG	2	0
25	C	502	CLA	3	0
30	a	613	SQD	3	0
25	D	404	CLA	3	0
27	b	618	BCR	2	0
25	B	601	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	e	101	HEM	2	0
27	B	617	BCR	2	0
25	A	606	CLA	2	0
21	A	601[B]	OEY	1	0
29	b	622	LMG	3	0
27	T	101	BCR	5	0
31	A	615	DGD	6	0
34	e	102	LHG	4	0
32	J	101	STE	1	0
29	m	101	LMG	3	0
25	c	503	CLA	3	0
25	c	513	CLA	2	0
25	A	609	CLA	1	0
25	B	603	CLA	3	0
31	H	102	DGD	3	0
27	k	102	BCR	4	0
27	d	405	BCR	2	0
28	d	406	PL9	2	0
25	B	609	CLA	2	0
34	l	101	LHG	2	0
26	A	608	PHO	1	0
25	c	508	CLA	1	0
27	t	101	BCR	3	0
32	t	104	STE	1	0
32	L	103	STE	1	0
25	B	605	CLA	7	0
25	B	602	CLA	3	0
25	C	503	CLA	5	0
27	B	618	BCR	2	0
29	D	412	LMG	1	0
32	X	101	STE	4	0
25	b	616	CLA	2	0
25	b	607	CLA	1	0
32	c	520	STE	2	0
30	t	102	SQD	3	0
25	c	509	CLA	2	0
25	b	610	CLA	2	0
30	L	101	SQD	4	0
25	b	609	CLA	3	0
26	a	608	PHO	1	0
25	b	608	CLA	4	0
29	c	523	LMG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	619	BCR	3	0
34	D	410	LHG	6	0
34	D	413	LHG	2	0
29	c	519	LMG	2	0
25	C	512	CLA	3	0
32	H	103	STE	3	0
32	C	522	STE	2	0
25	d	403	CLA	2	0
25	C	507	CLA	1	0
26	d	402	PHO	4	0
25	D	405	CLA	1	0
25	d	404	CLA	3	0
25	C	508	CLA	4	0
31	c	516	DGD	2	0
25	c	510	CLA	3	0
25	c	511	CLA	4	0
25	C	506	CLA	3	0
31	h	102	DGD	1	0
29	C	519	LMG	2	0
31	a	614	DGD	1	0
25	c	512	CLA	3	0
25	b	613	CLA	3	0
27	k	101	BCR	2	0
32	b	623	STE	1	0
30	A	614	SQD	5	0
25	c	505	CLA	4	0
32	d	413	STE	2	0
25	a	612	CLA	4	0
25	B	608	CLA	1	0
25	B	607	CLA	1	0
25	b	615	CLA	3	0
30	A	613	SQD	2	0
34	E	101	LHG	4	0
25	b	612	CLA	3	0
31	C	518	DGD	2	0
27	h	101	BCR	2	0
30	B	622	SQD	2	0
25	b	611	CLA	1	0
25	b	605	CLA	4	0
27	a	610	BCR	2	0
25	A	607	CLA	2	0
25	B	614	CLA	4	0

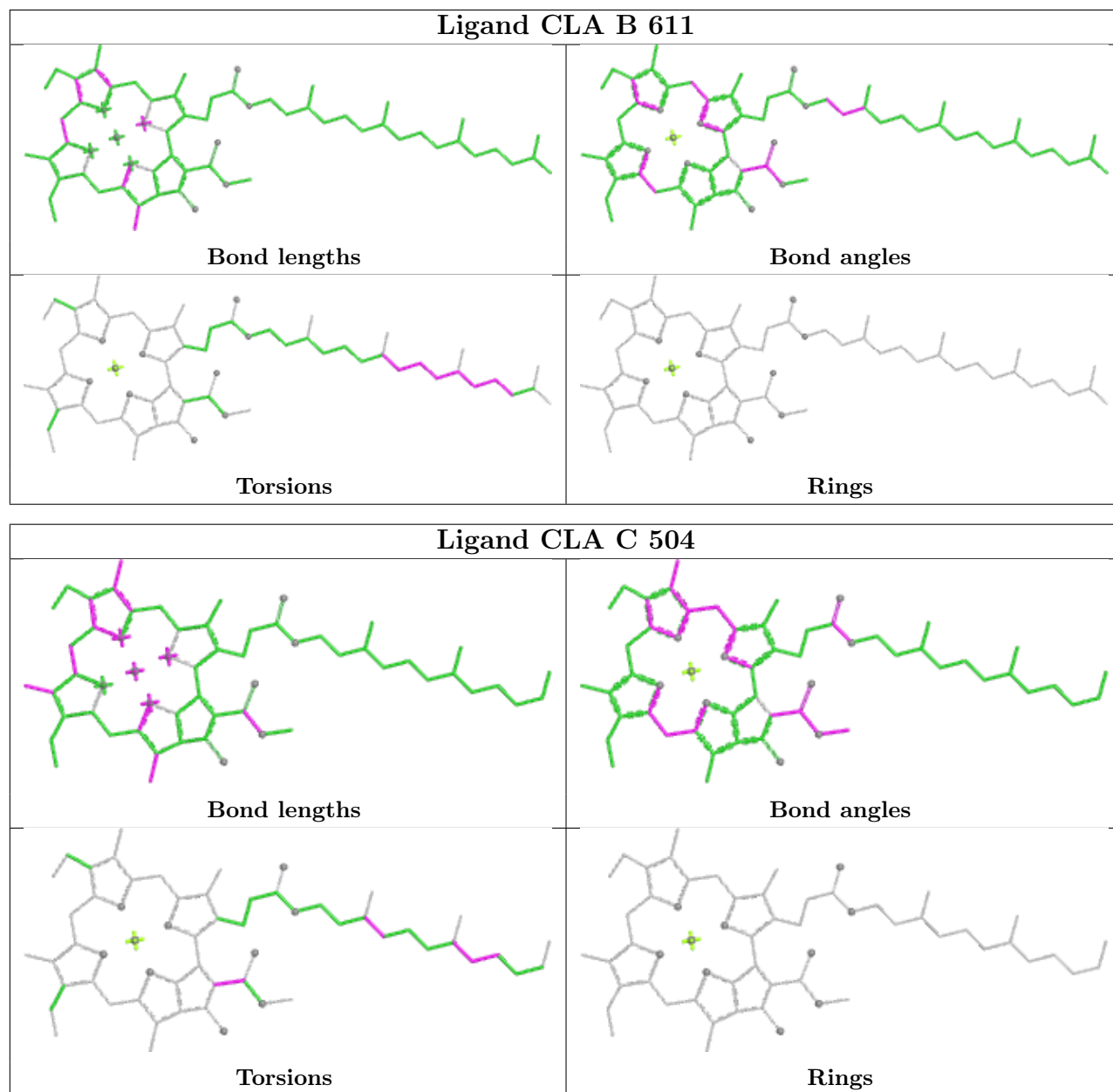
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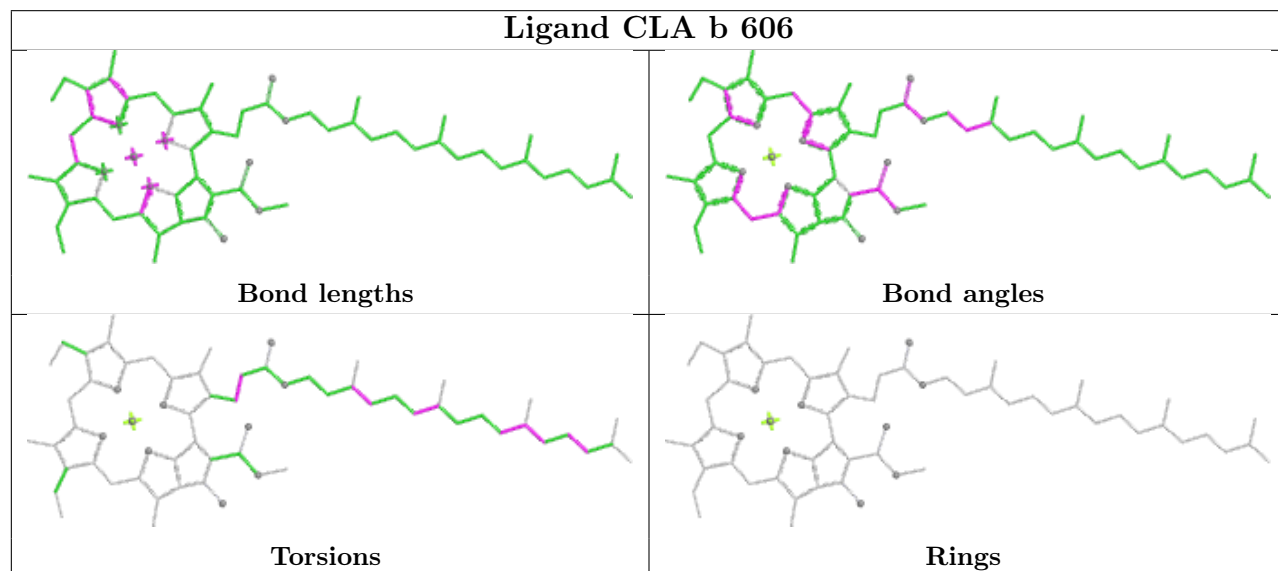
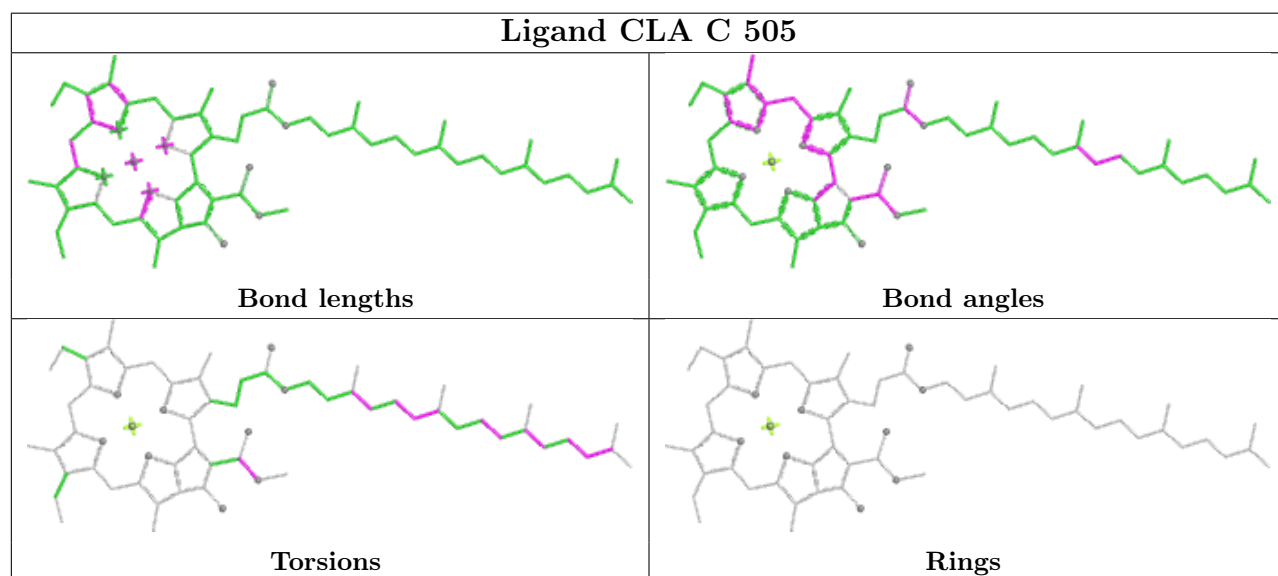
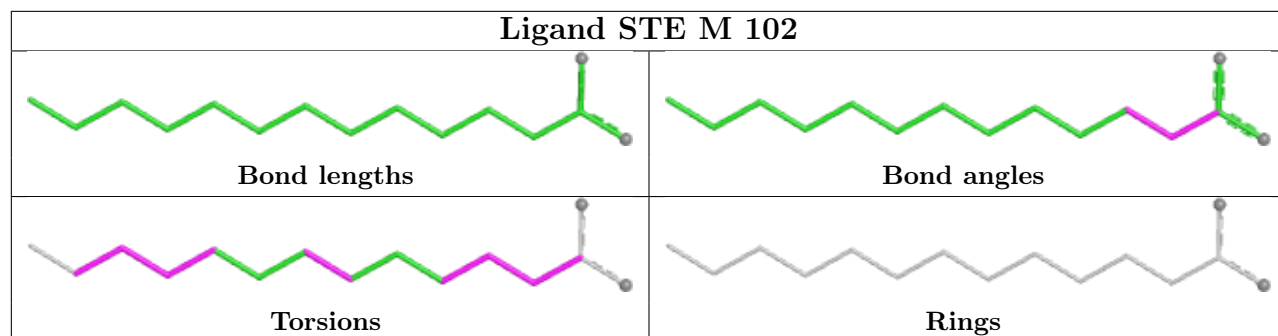
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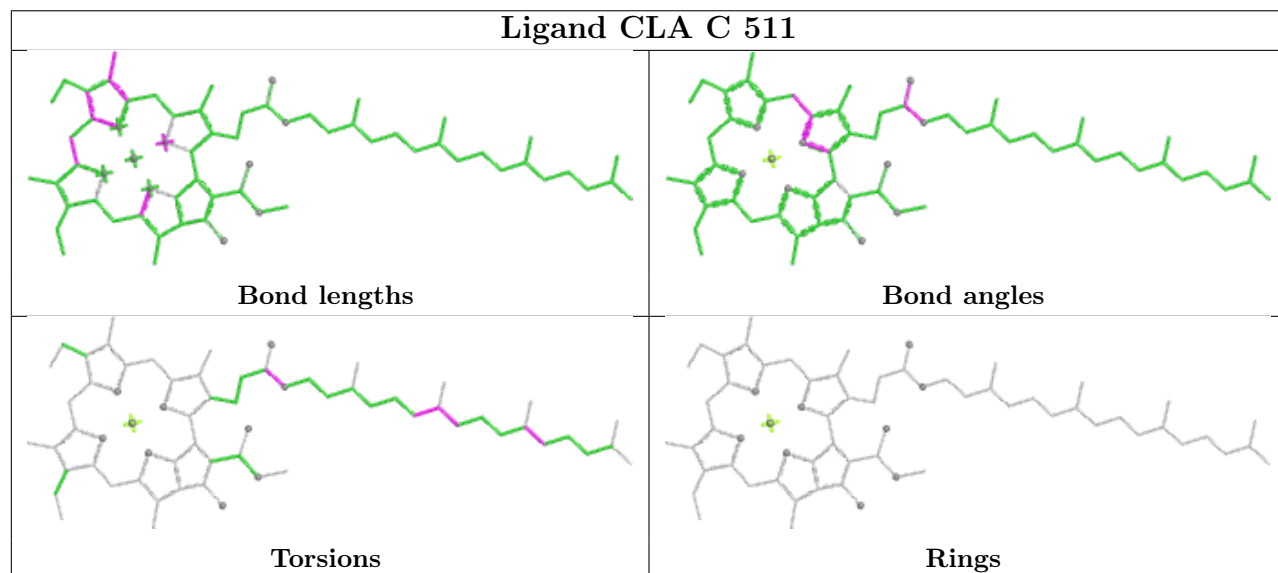
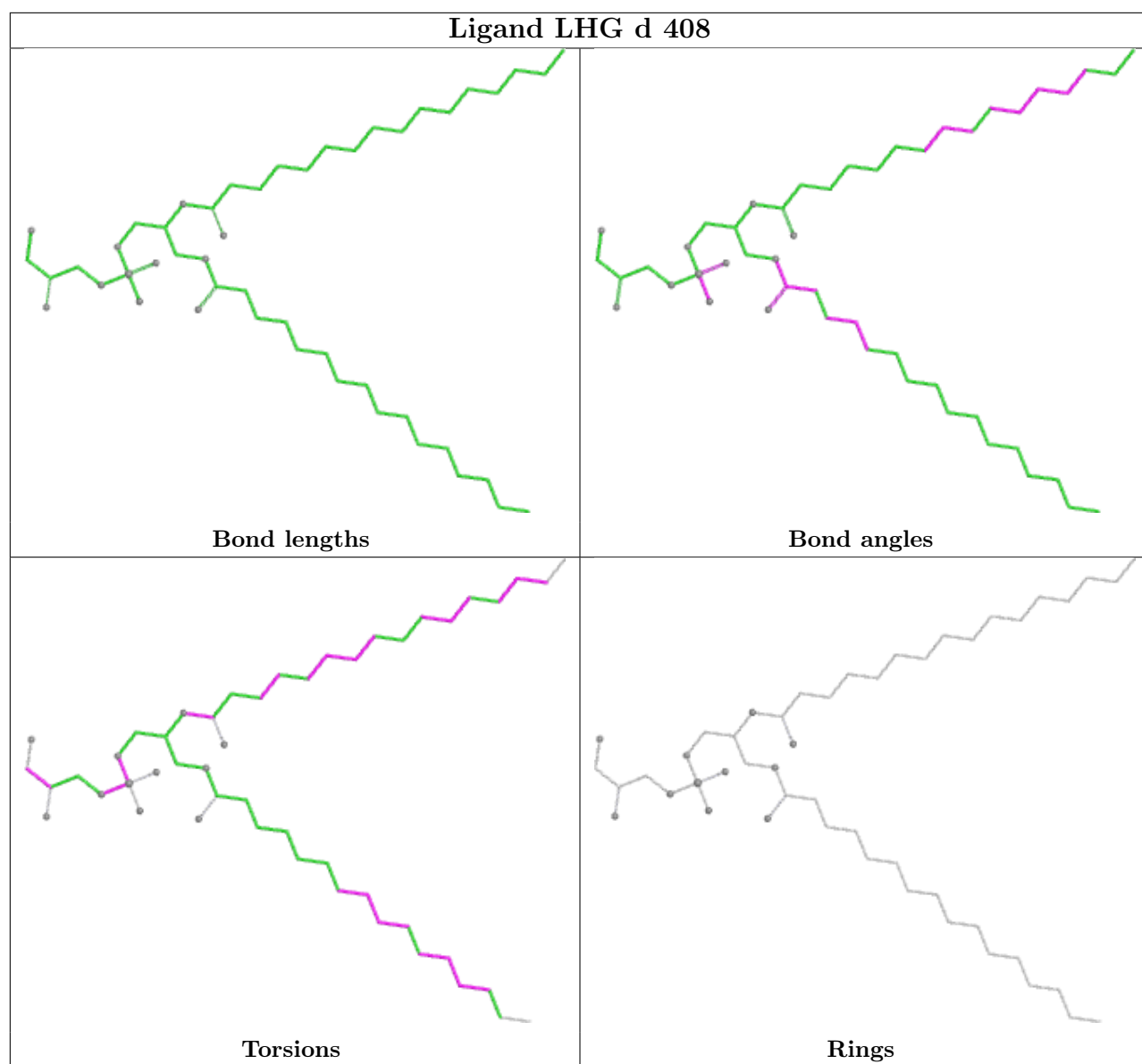
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	b	621	STE	1	0
31	C	517	DGD	5	0
29	M	101	LMG	1	0
25	D	403	CLA	2	0
29	c	521	LMG	4	0
25	B	610	CLA	1	0
32	l	102	STE	2	0
31	C	516	DGD	1	0
25	c	501	CLA	4	0
25	a	606	CLA	2	0
27	C	515	BCR	1	0
28	A	611	PL9	8	0
29	D	408	LMG	3	0
25	b	604	CLA	5	0
34	L	102	LHG	3	0
25	C	513	CLA	3	0
31	c	517	DGD	3	0
35	F	101	HEM	4	0
25	B	606	CLA	4	0
27	b	617	BCR	2	0
27	c	514	BCR	1	0
25	c	507	CLA	3	0
32	B	624	STE	2	0
32	b	620	STE	2	0
28	a	611	PL9	7	0
29	B	621	LMG	1	0
27	c	515	BCR	4	0
27	K	101	BCR	1	0
32	B	625	STE	1	0
25	b	602	CLA	4	0
25	B	613	CLA	3	0
32	C	520	STE	1	0
32	b	624	STE	2	0
25	C	509	CLA	3	0
27	C	514	BCR	5	0
25	C	501	CLA	3	0
25	B	612	CLA	3	0

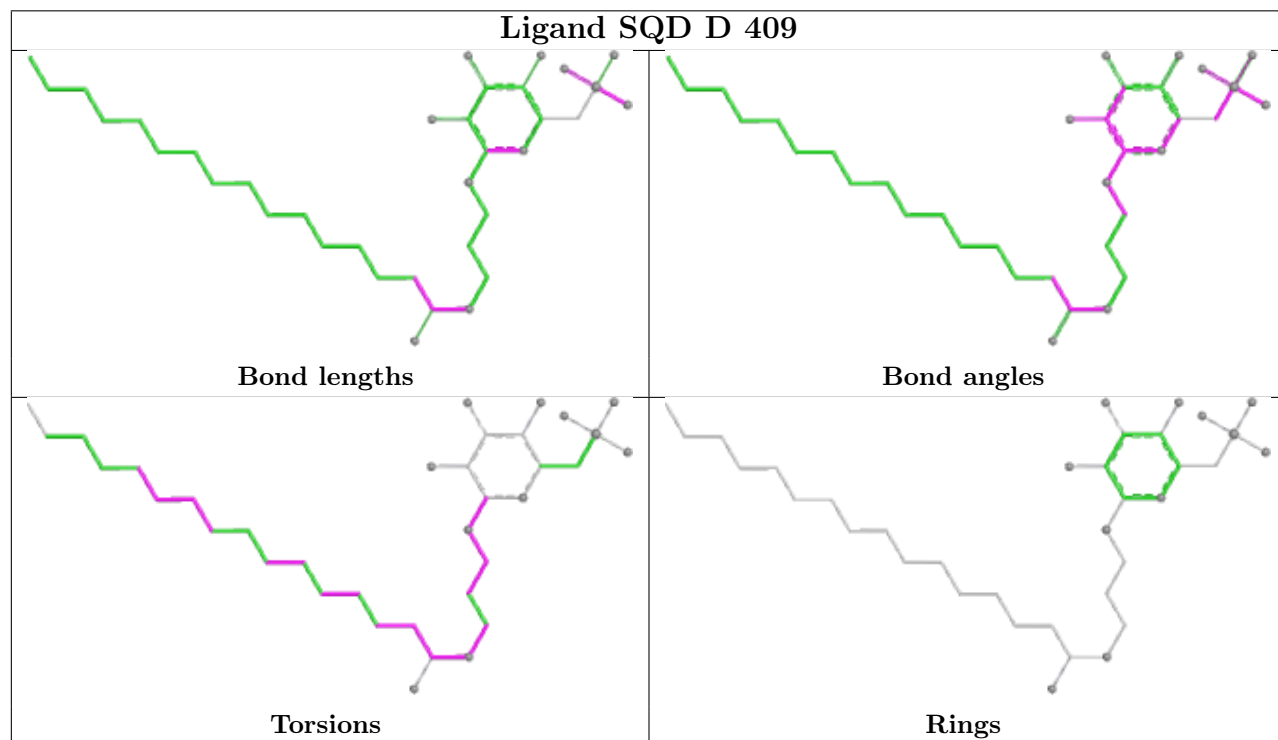
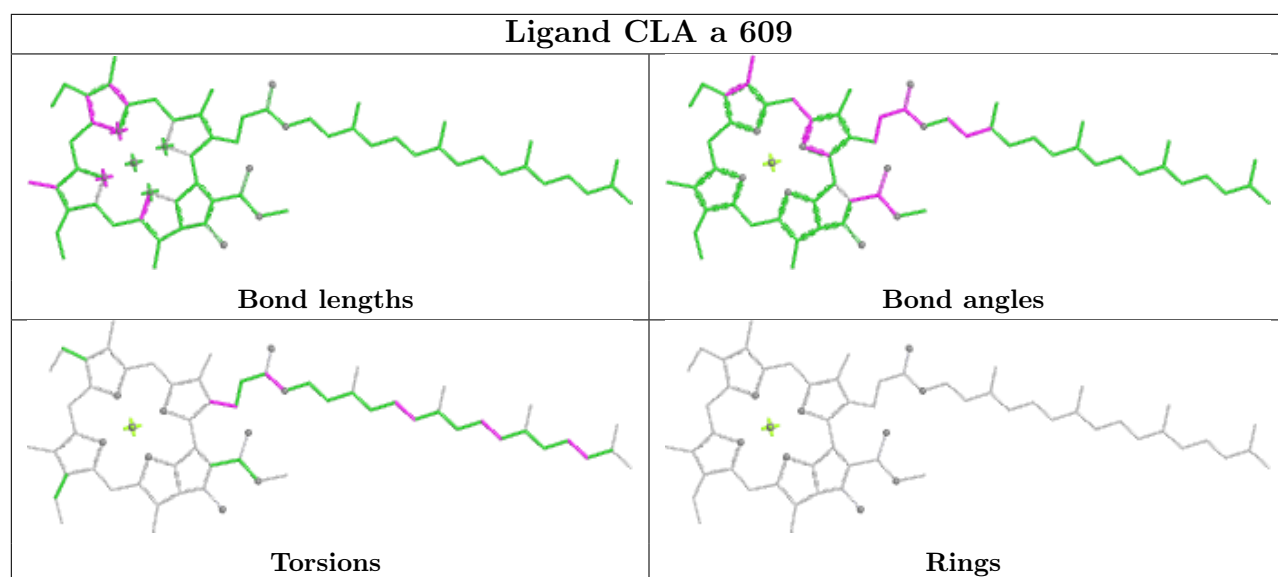
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

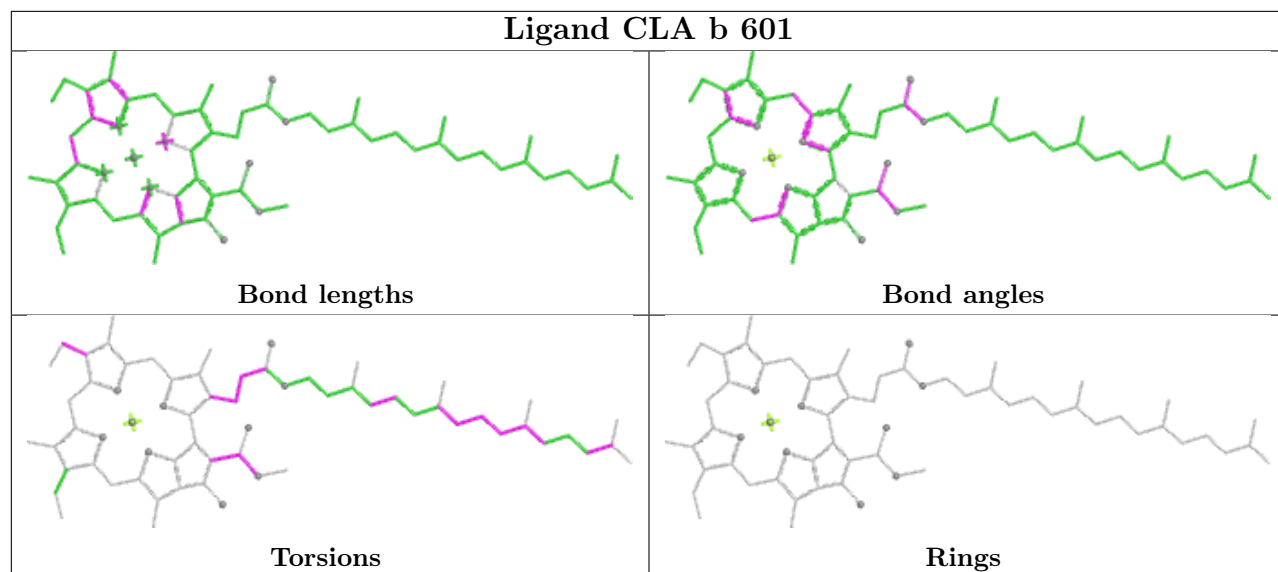




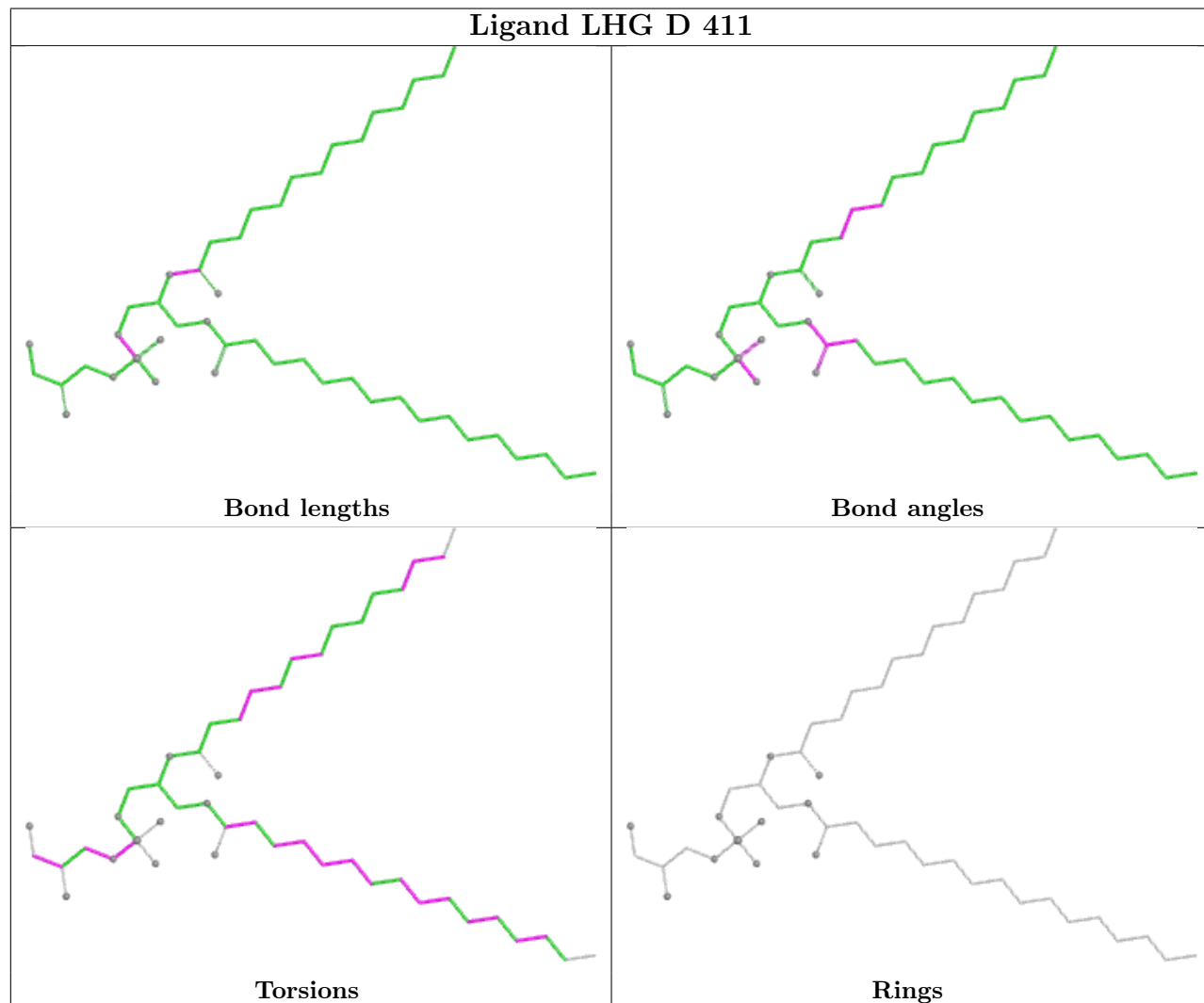


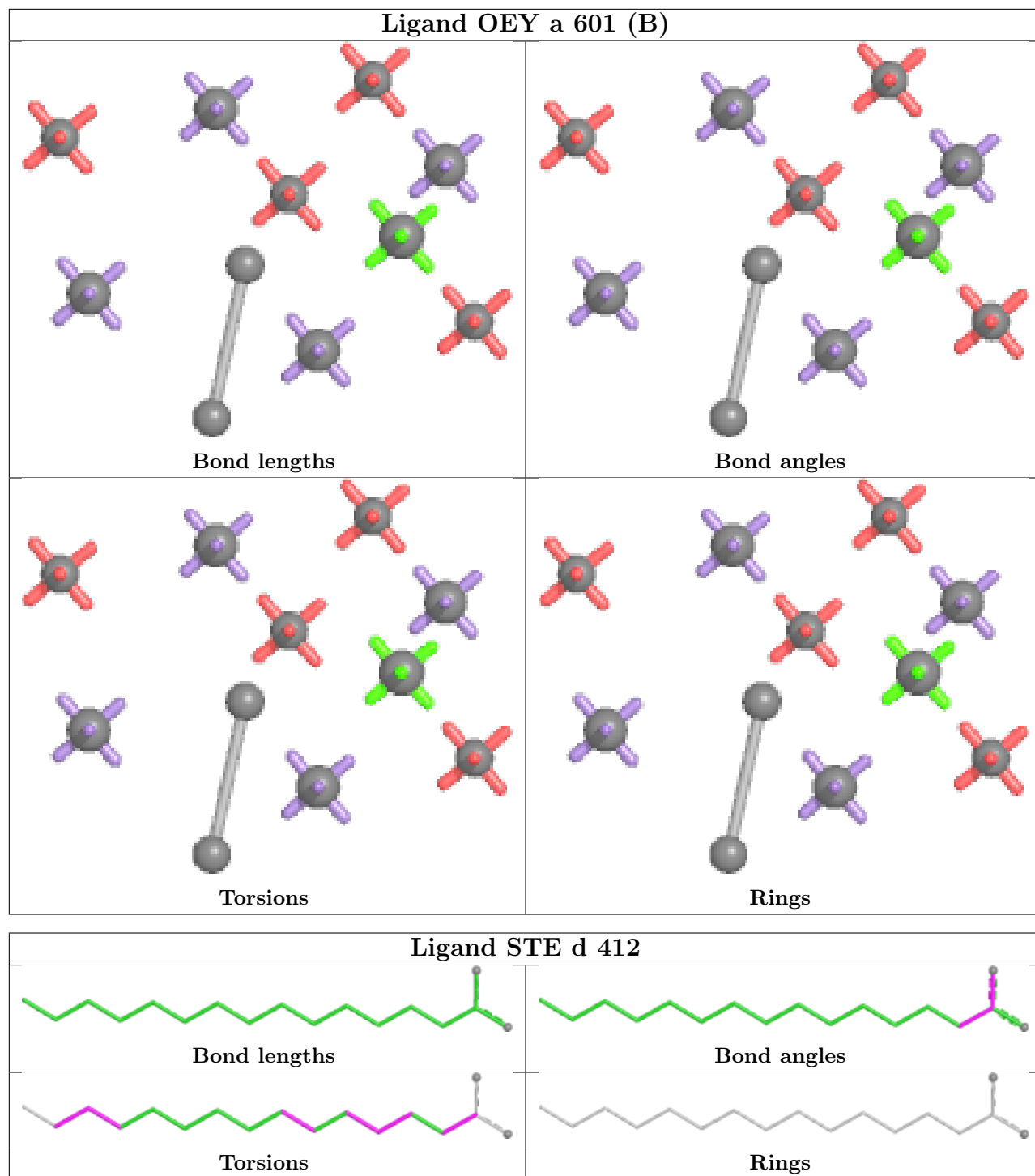


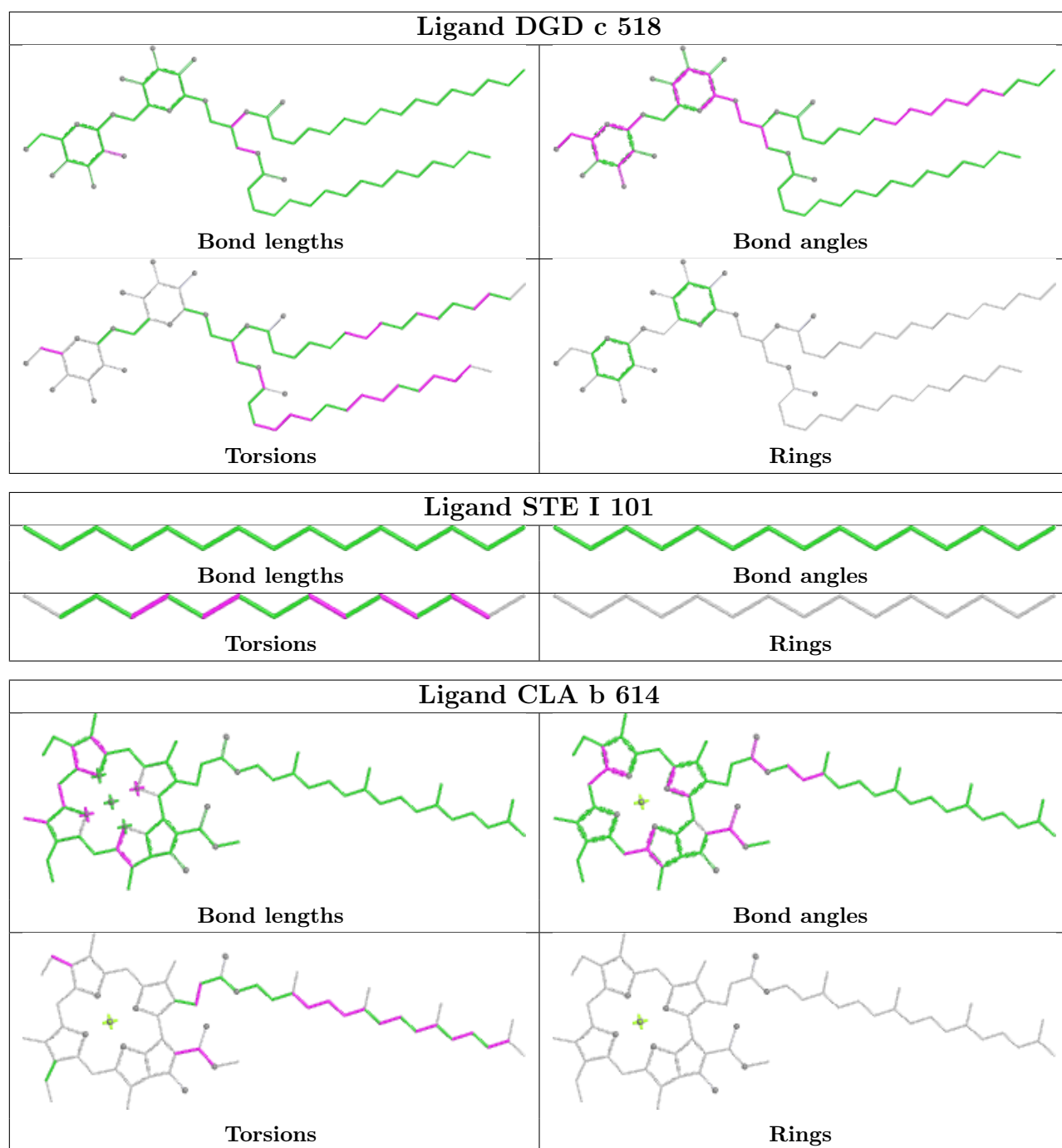
Ligand CLA b 601

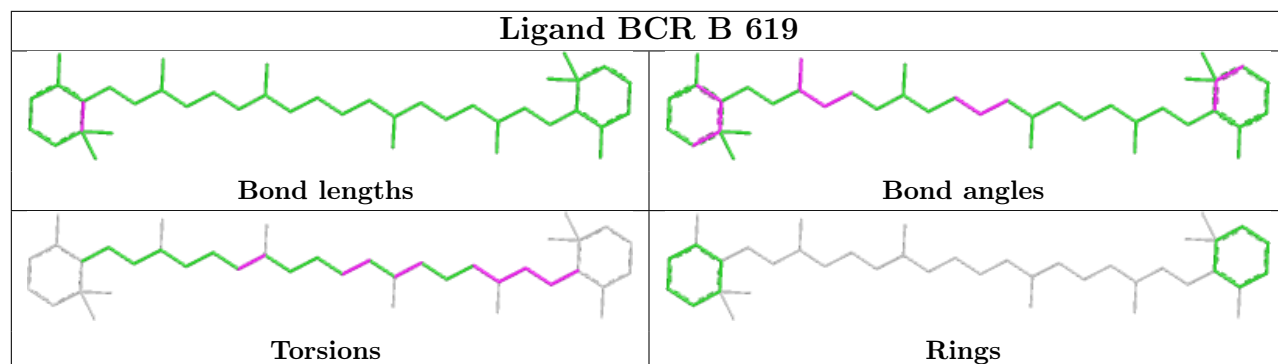
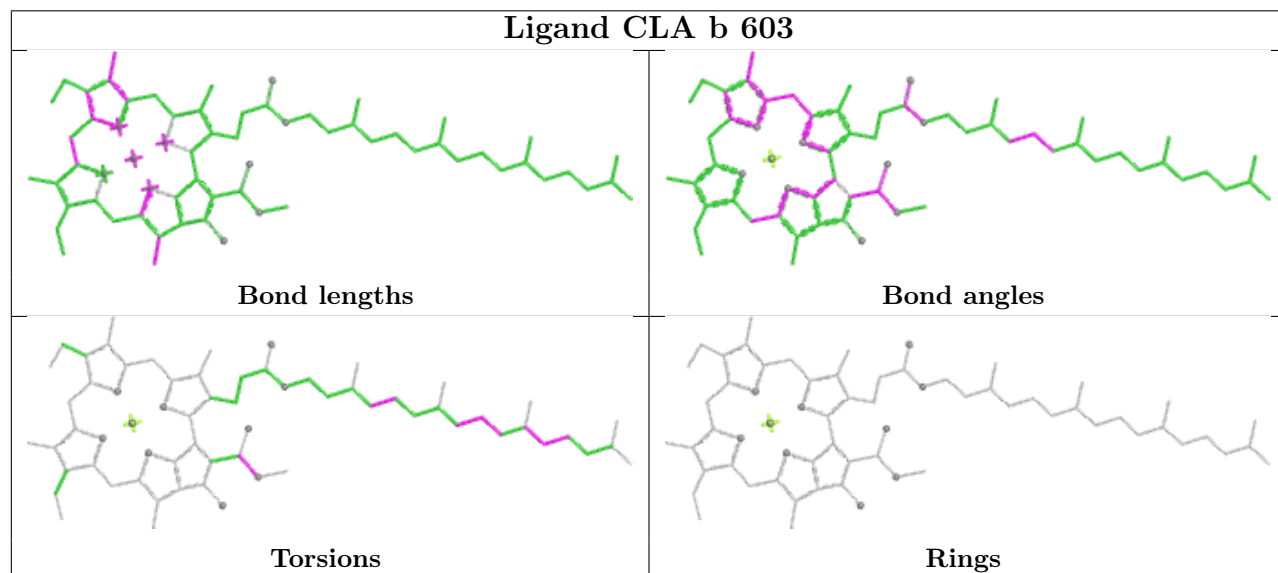
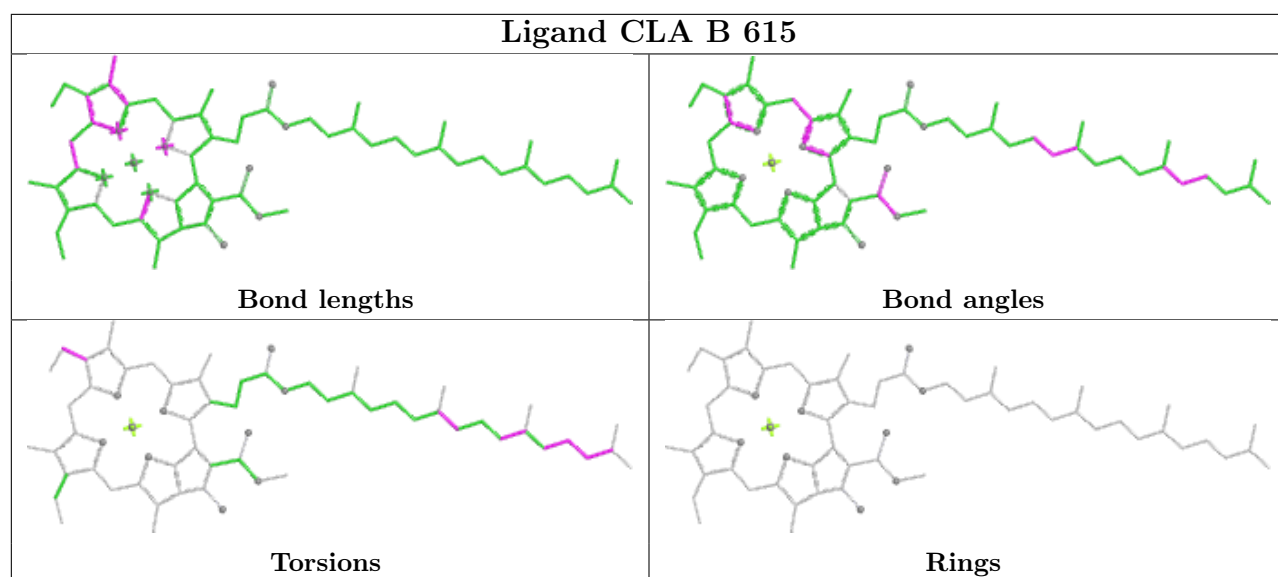


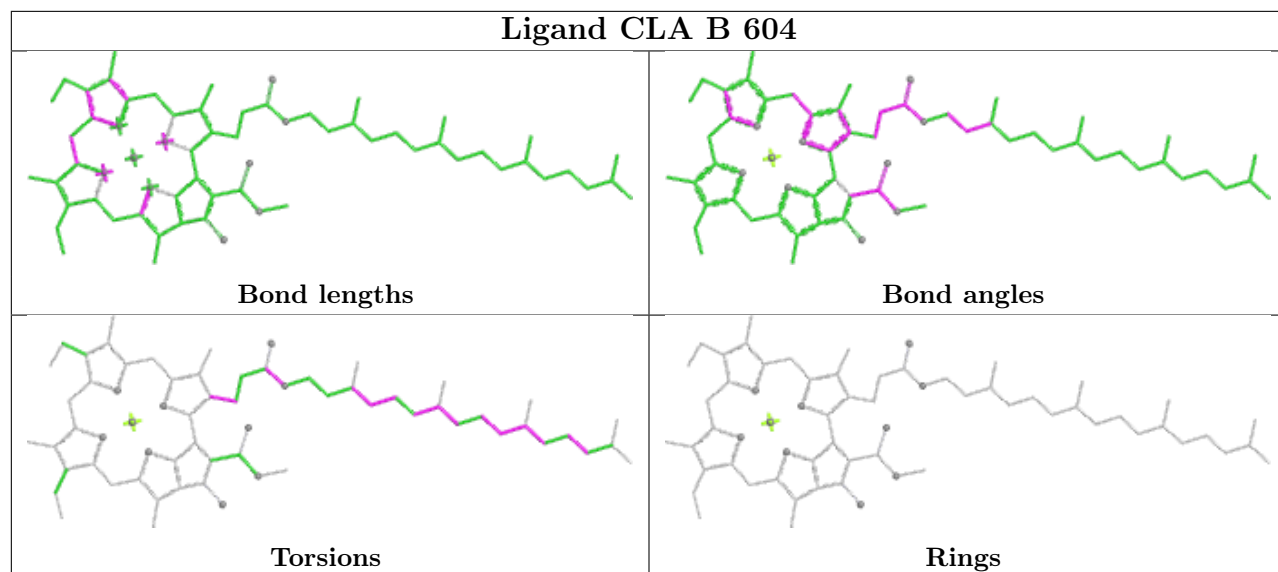
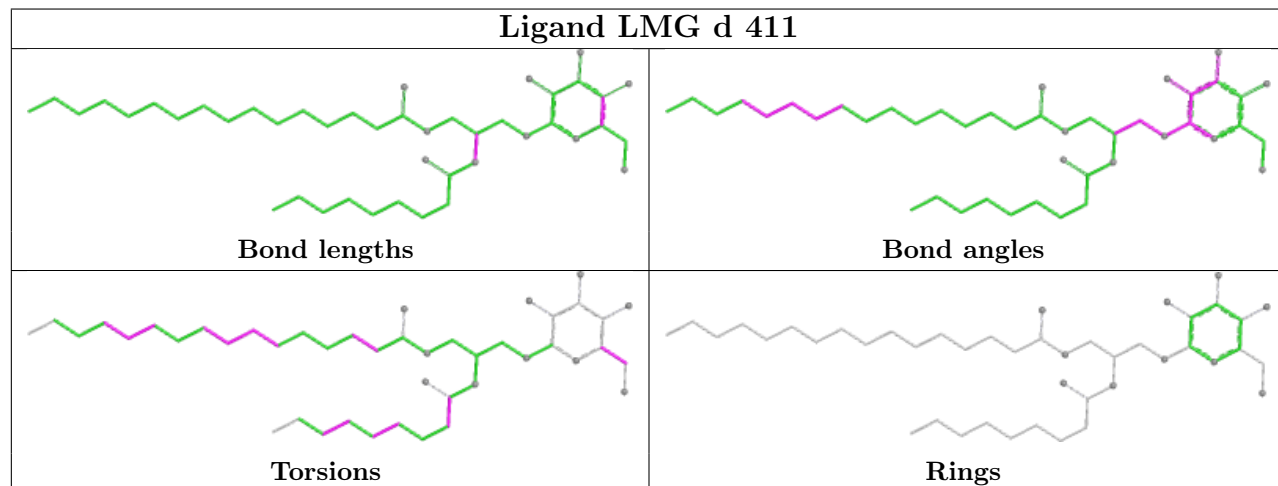
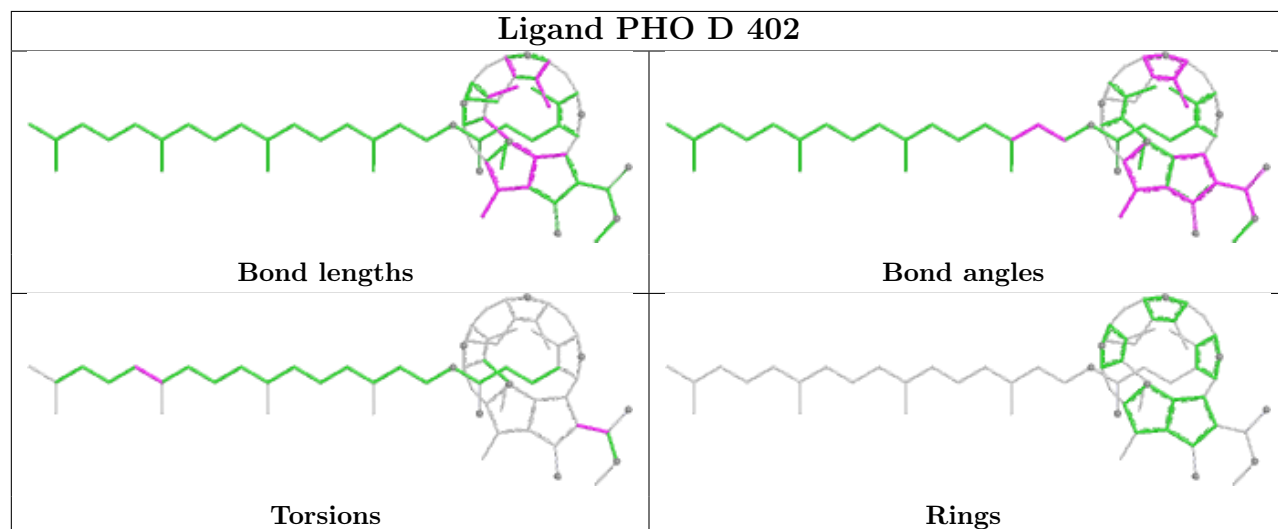
Ligand LHG D 411

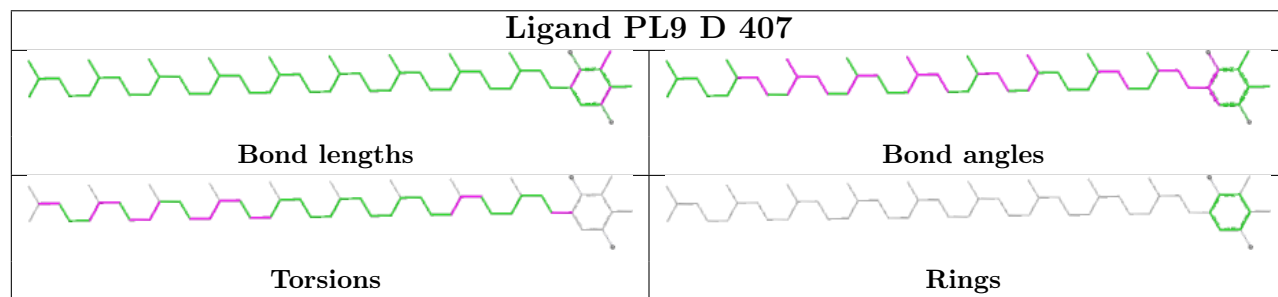
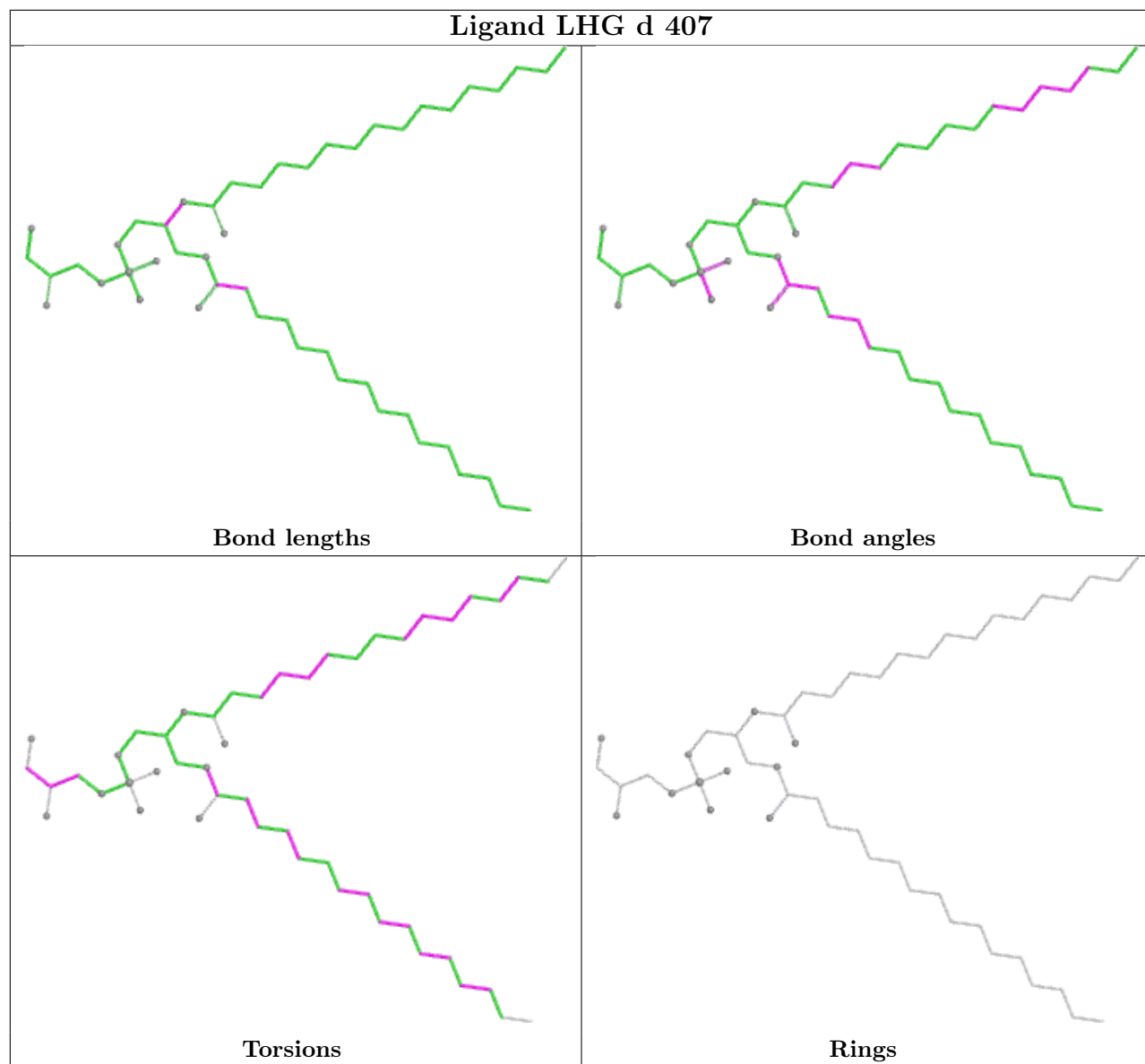


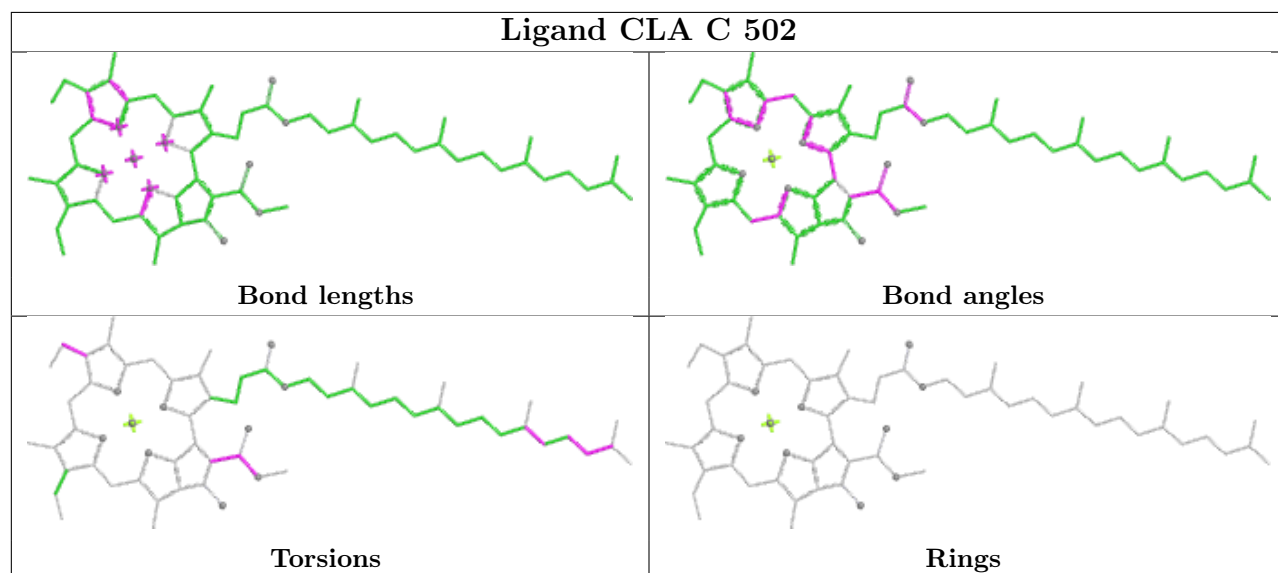
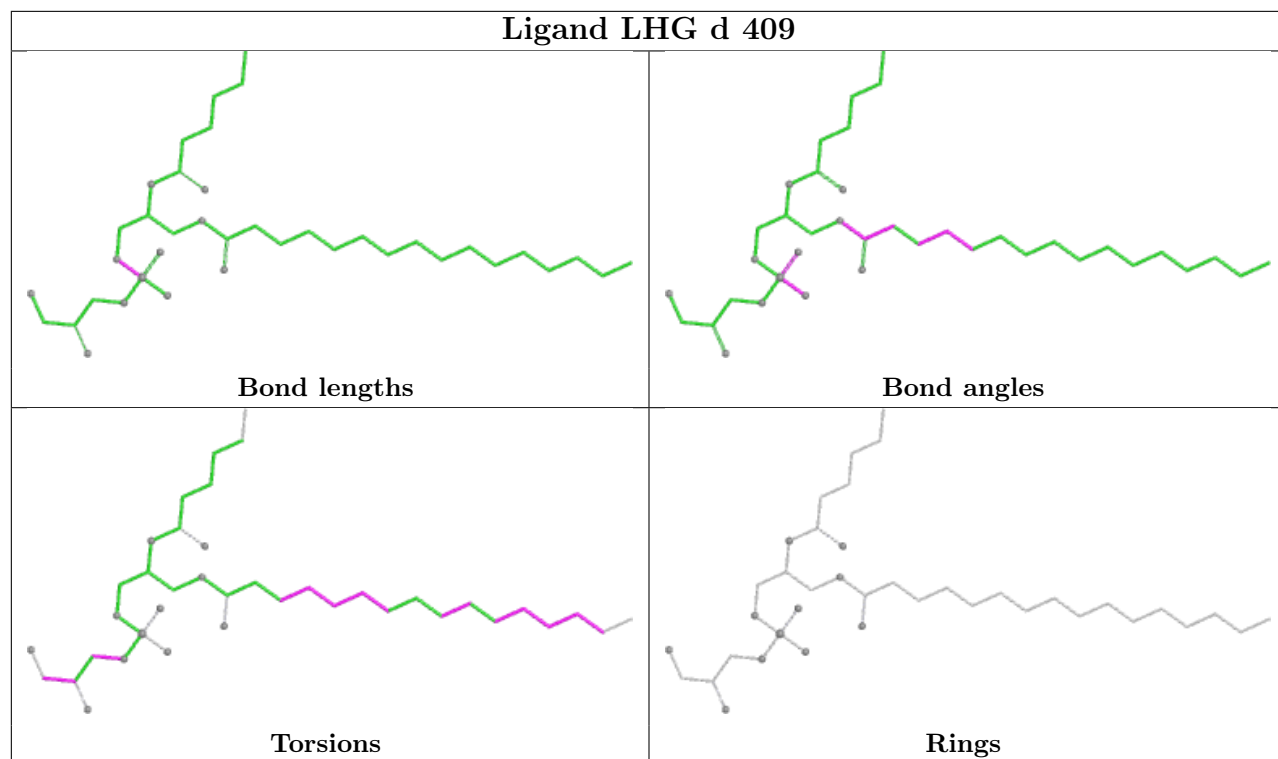


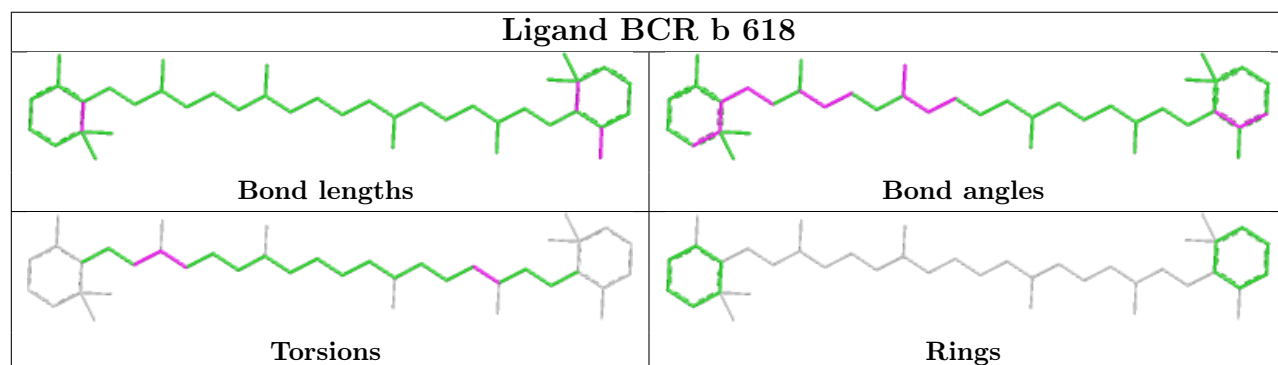
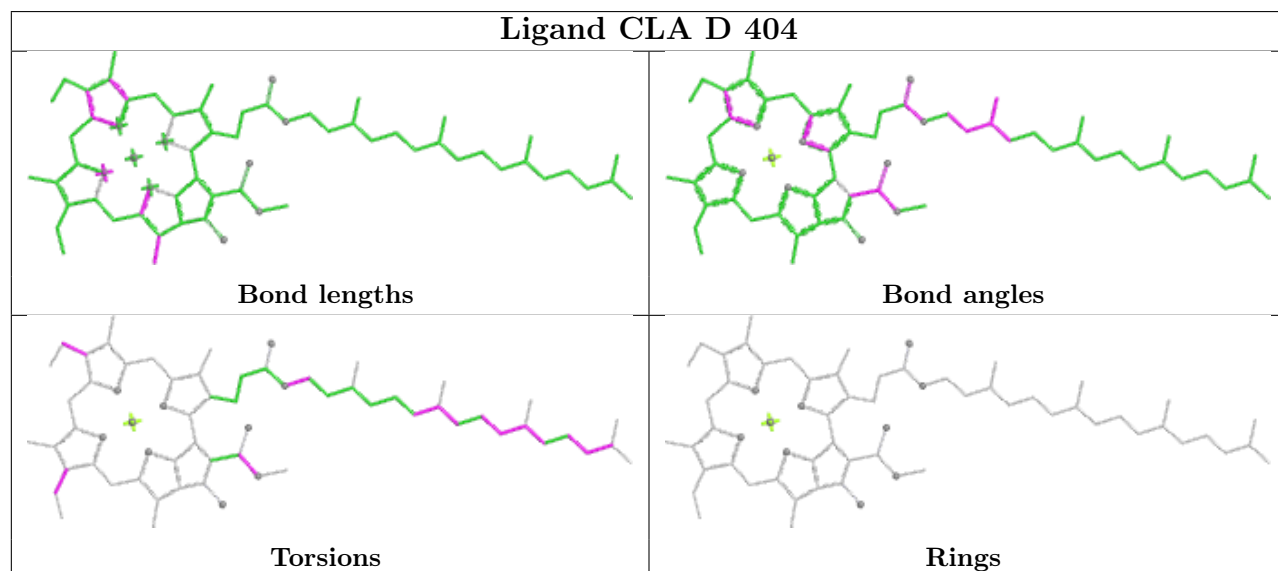
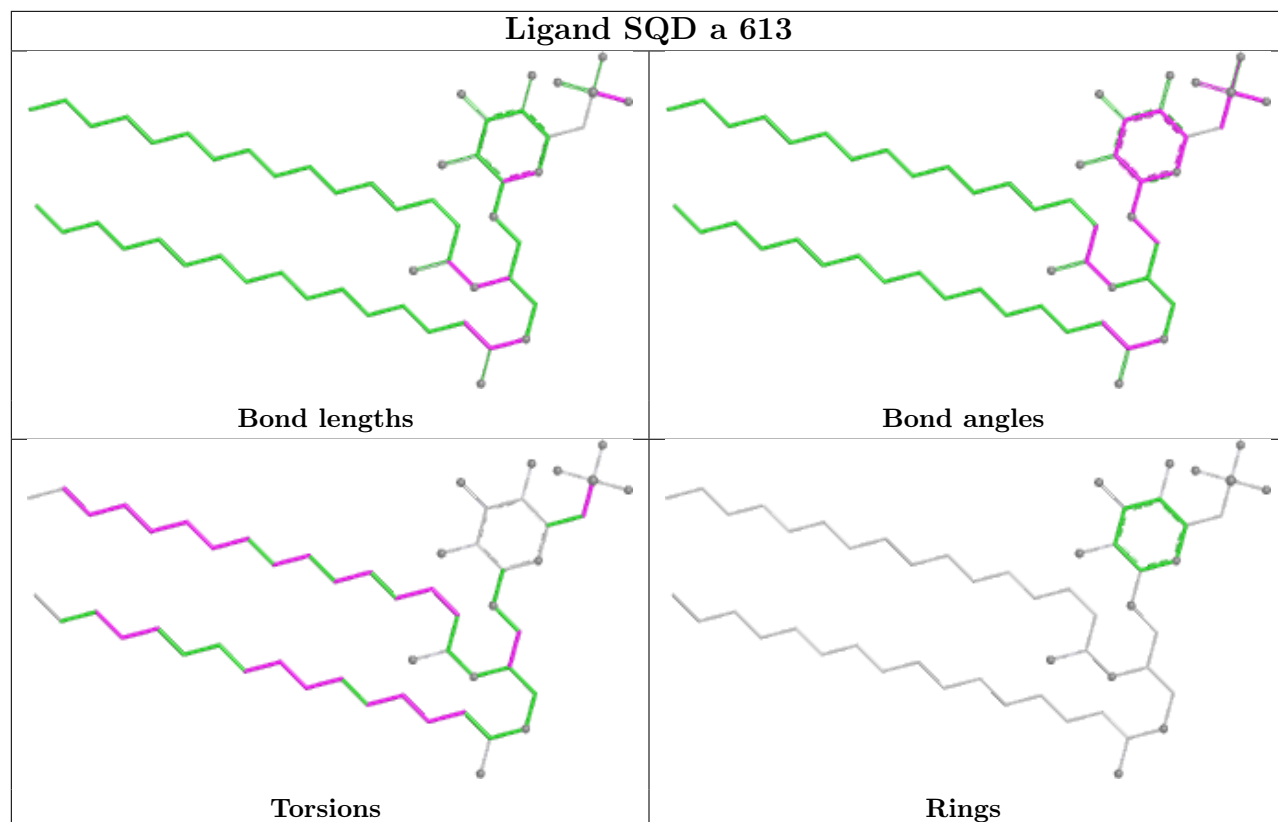




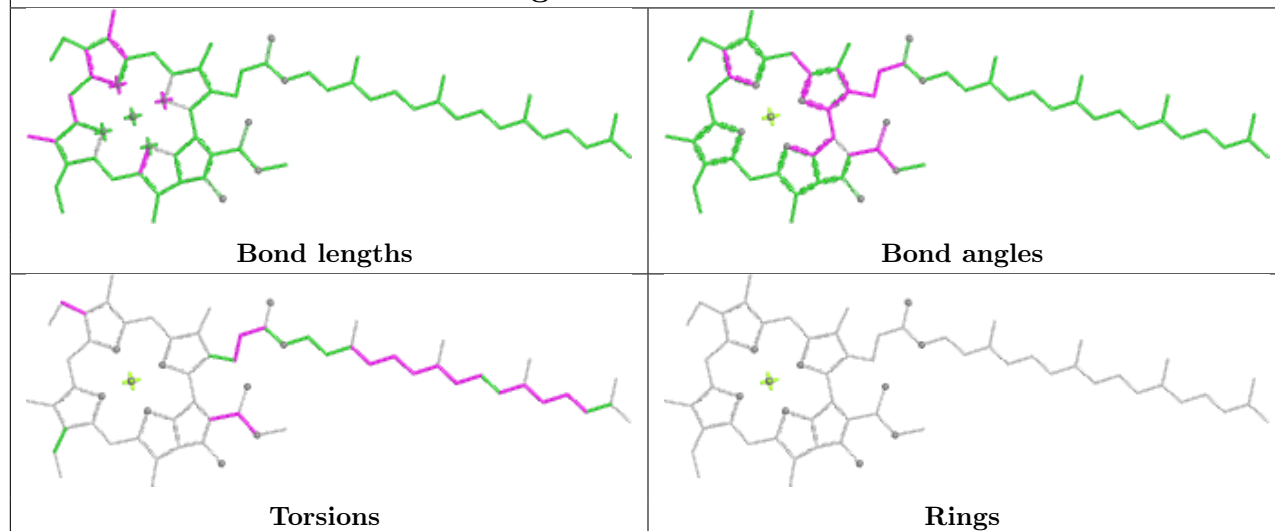
Ligand CLA B 604**Ligand LMG d 411****Ligand PHO D 402**



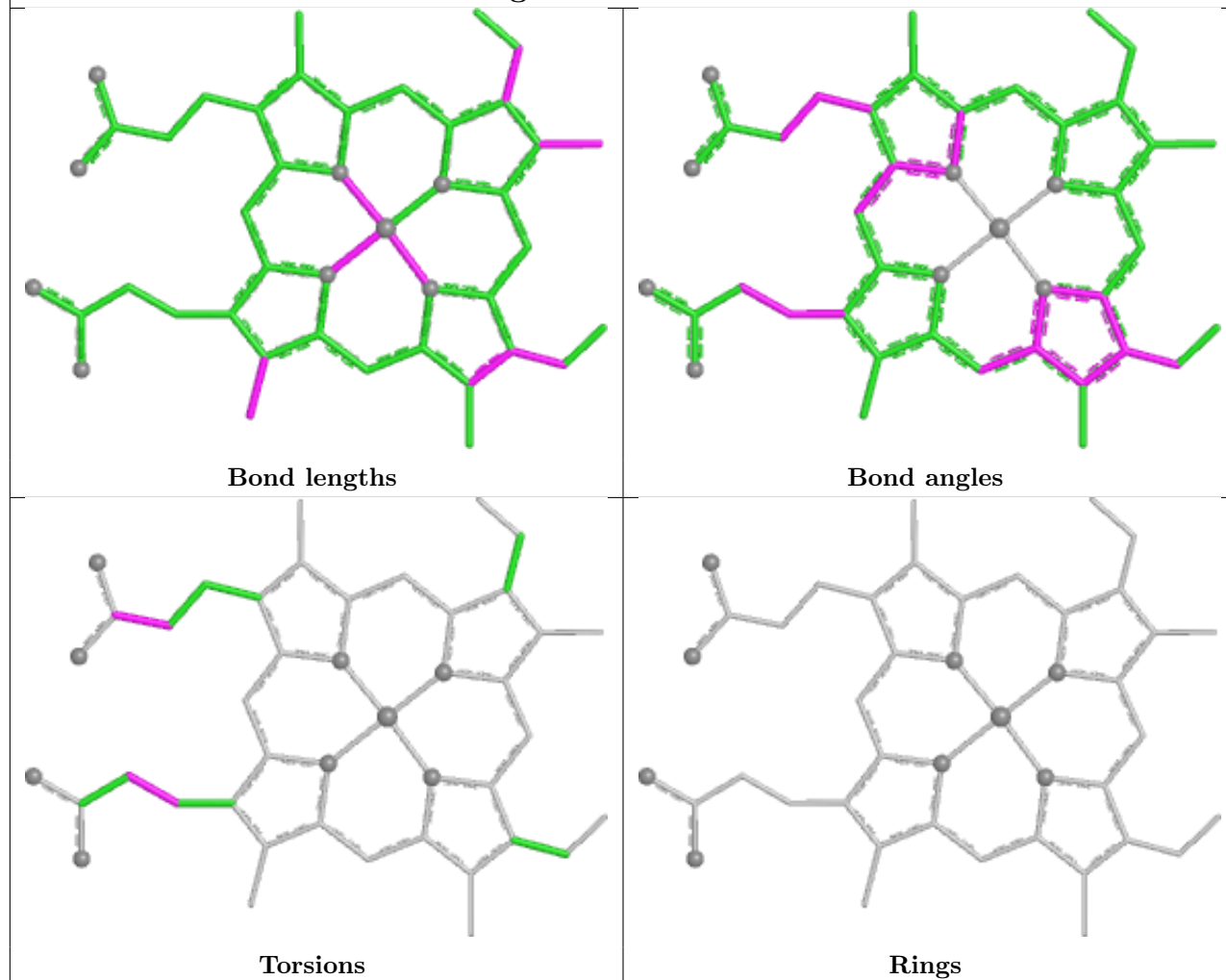


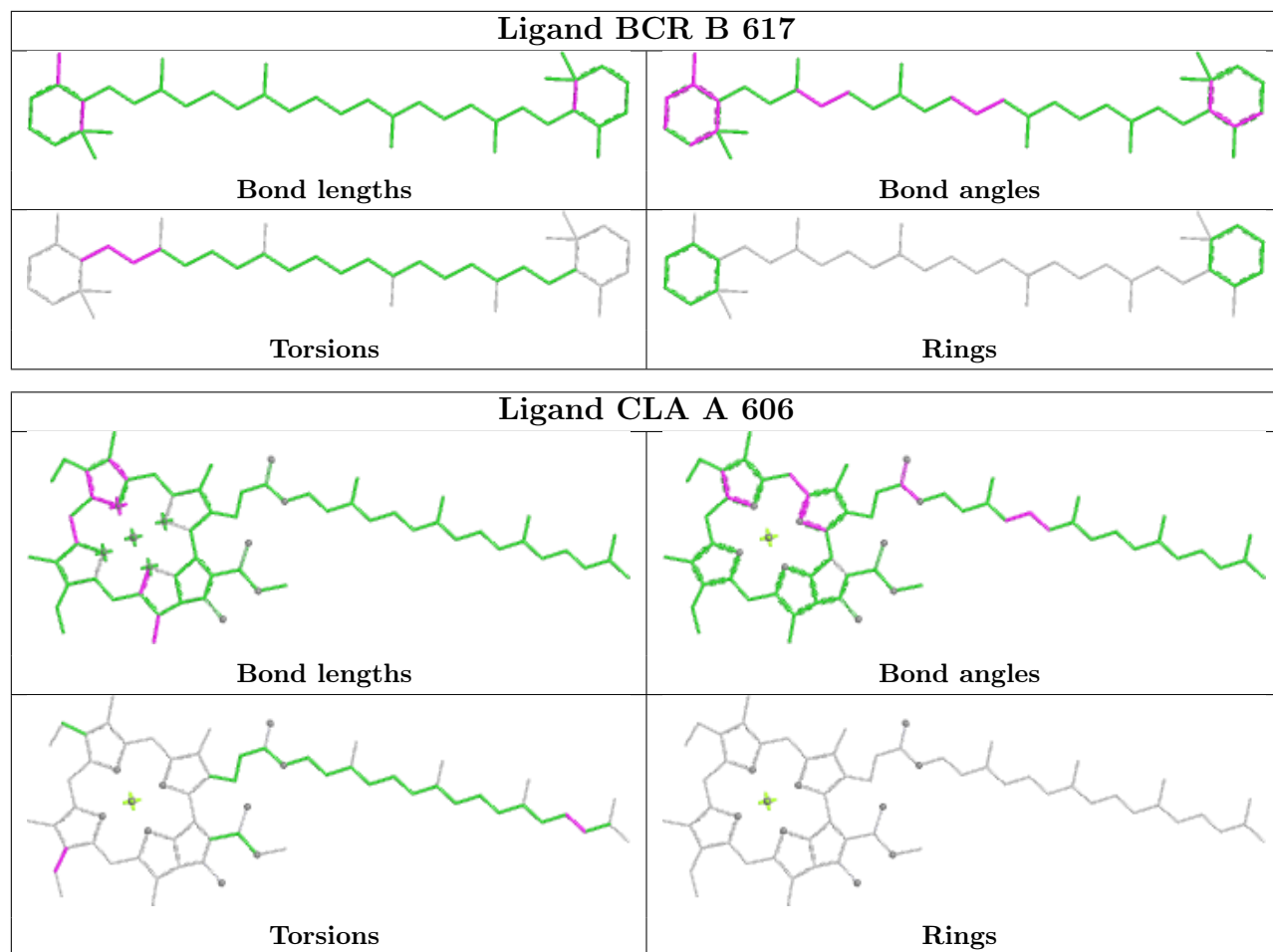


Ligand CLA B 601

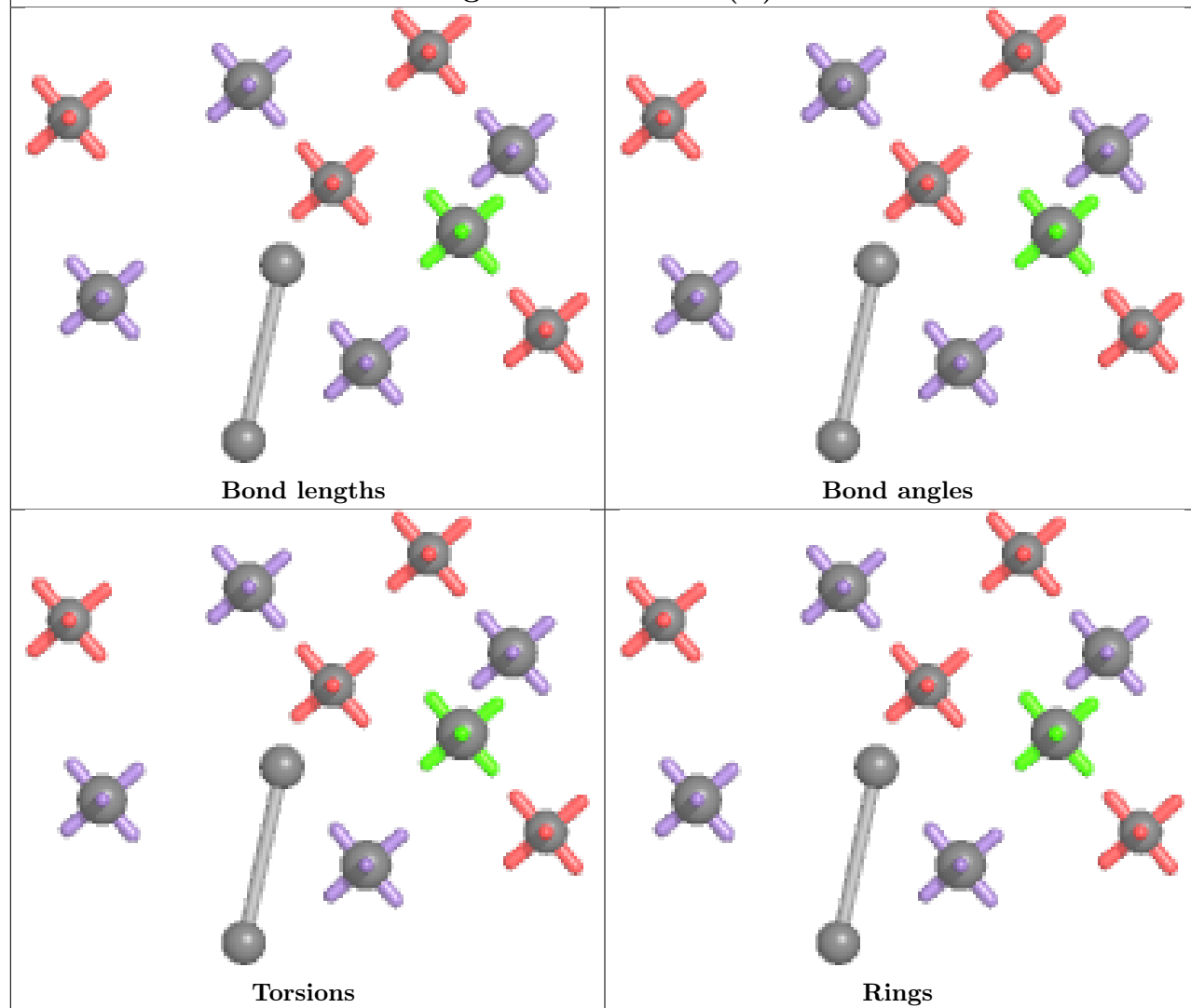


Ligand HEM e 101

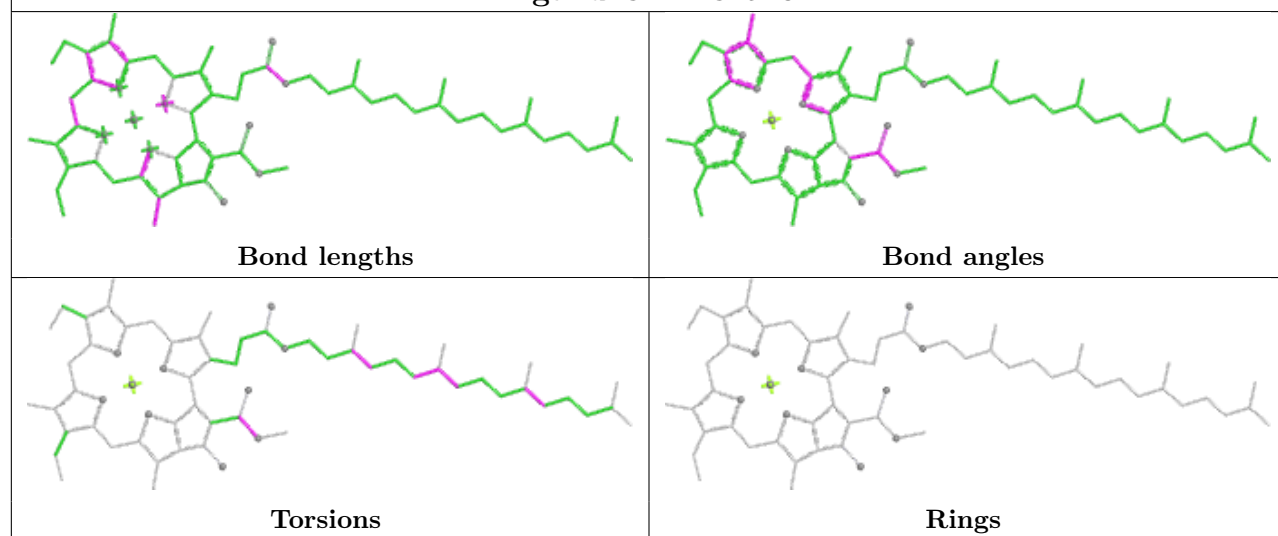


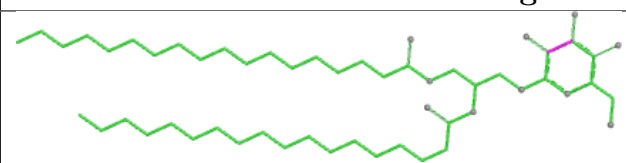
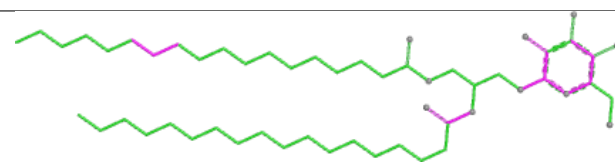
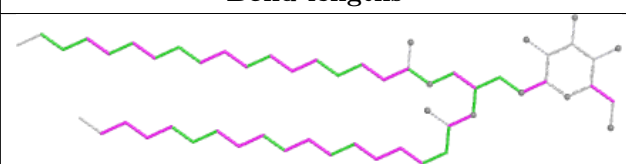
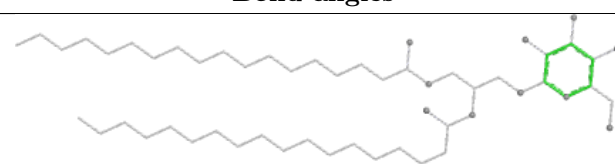


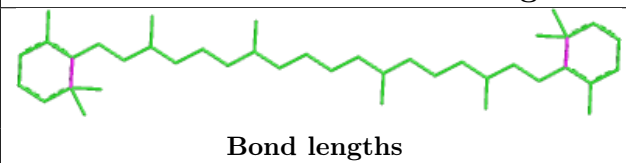
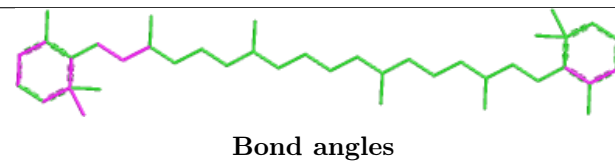
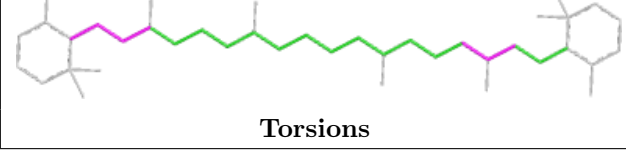
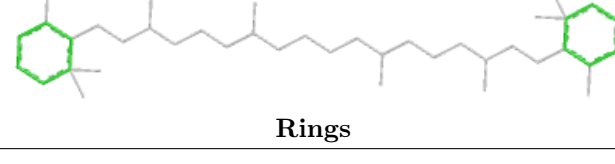
Ligand OEY A 601 (B)

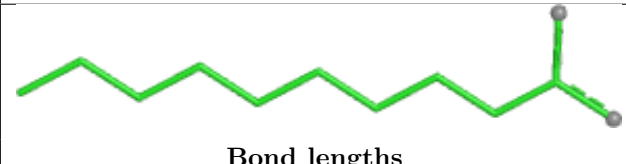
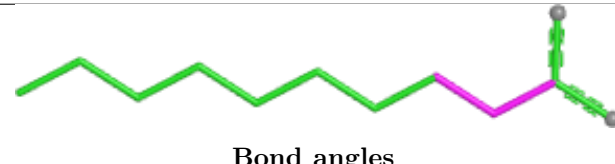
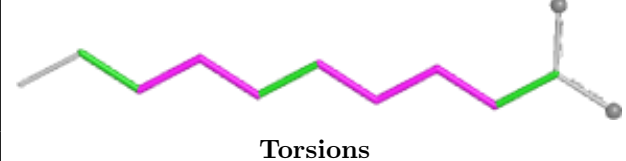
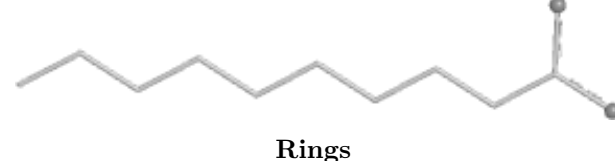


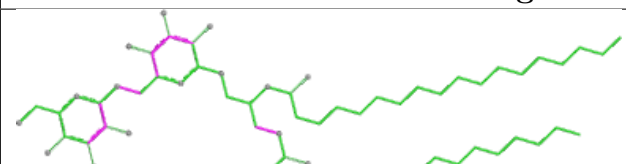
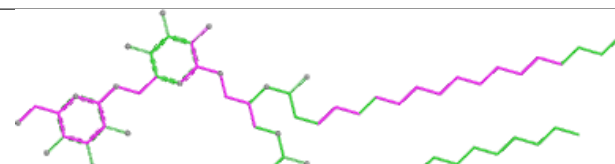
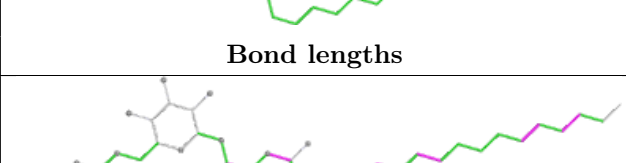
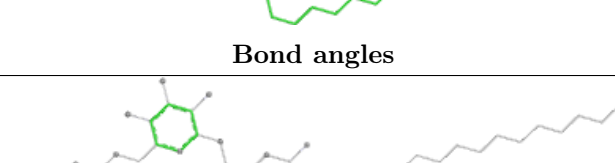
Ligand CLA C 510

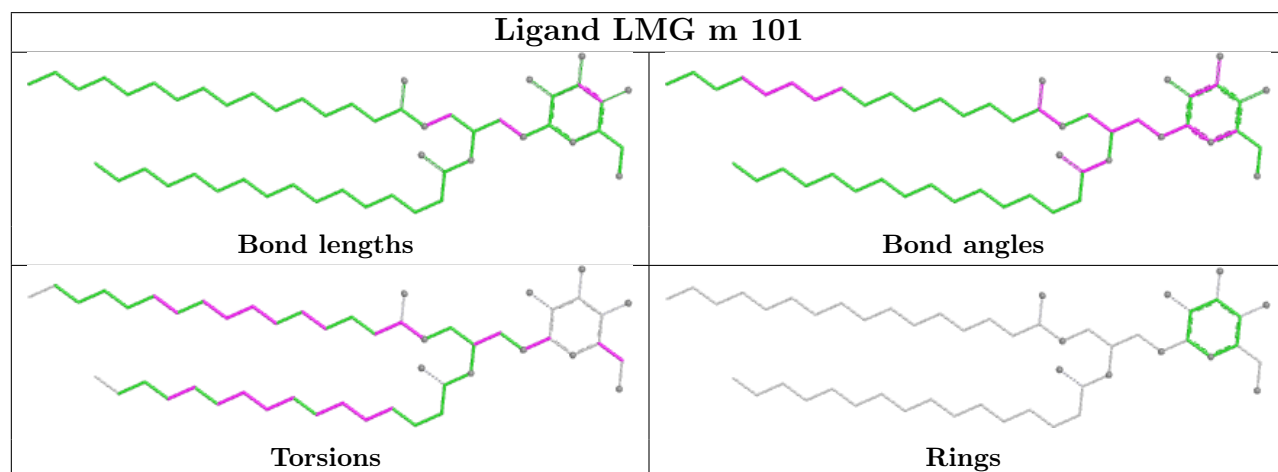
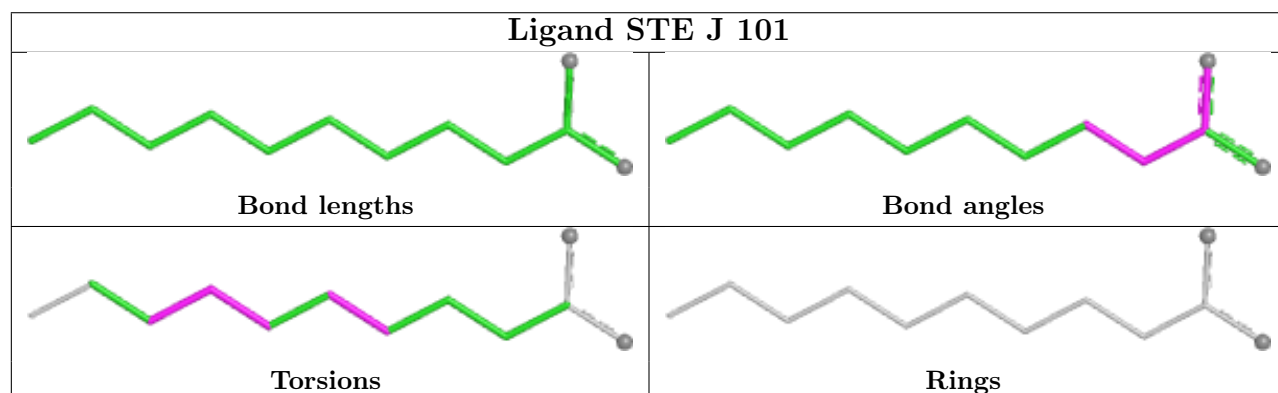
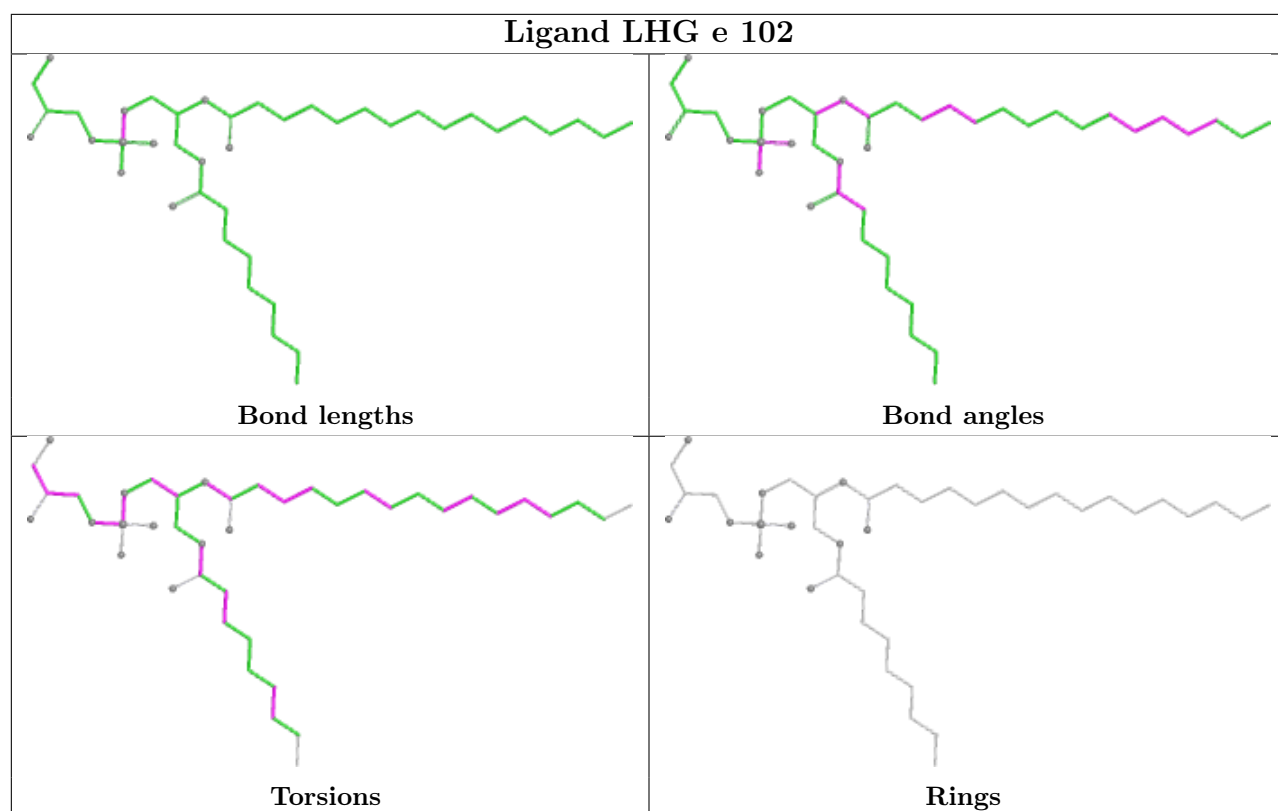


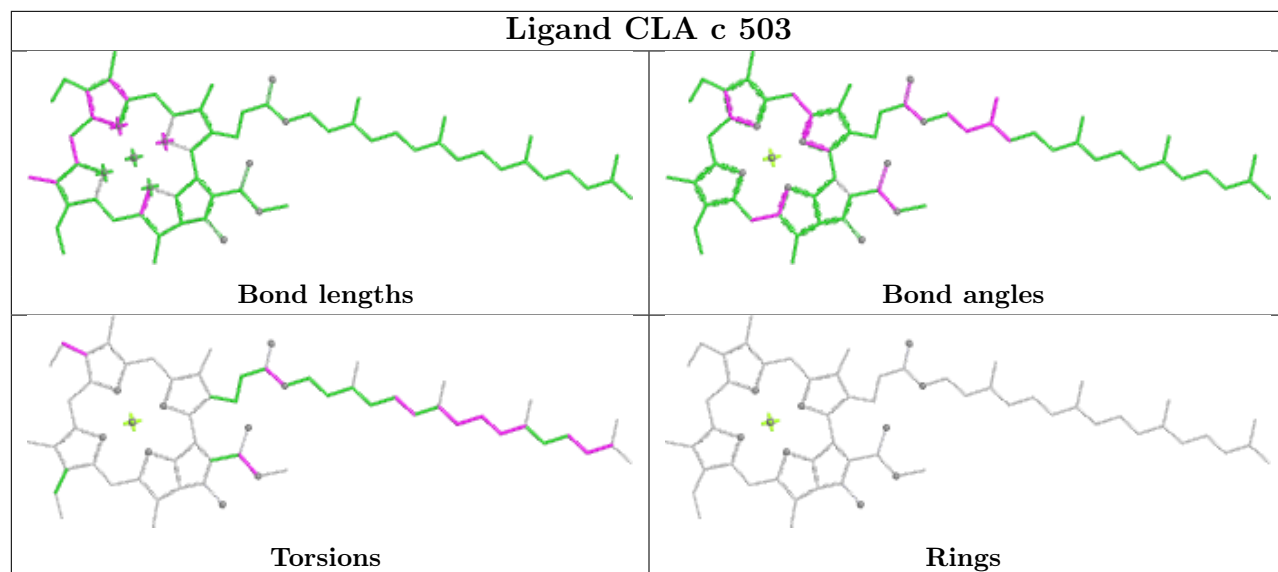
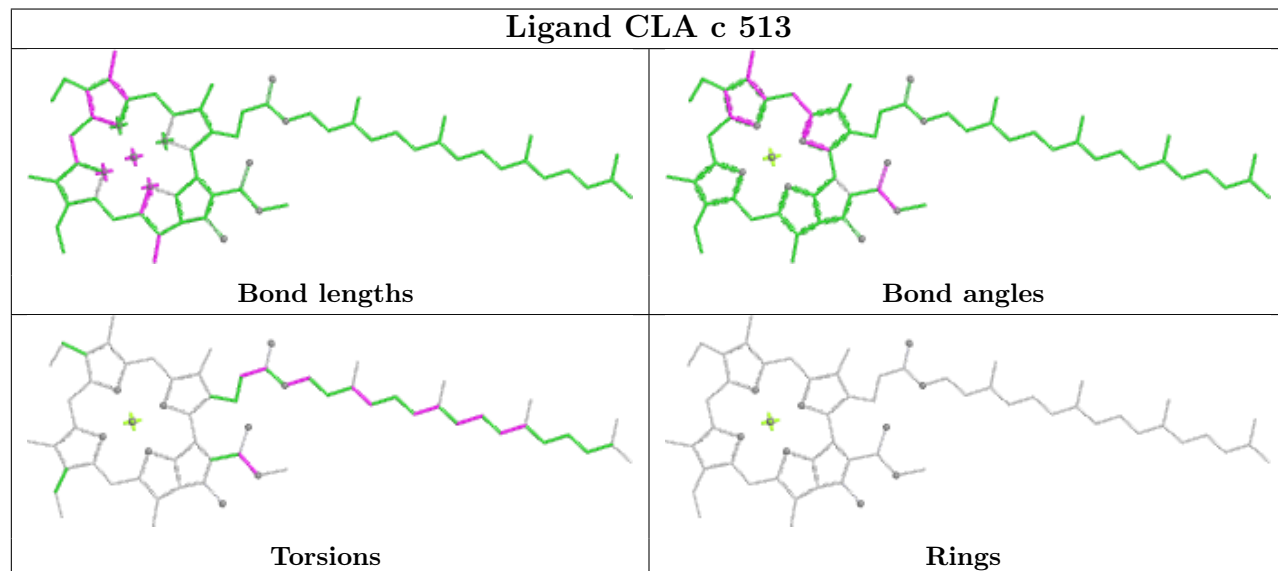
Ligand LMG b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

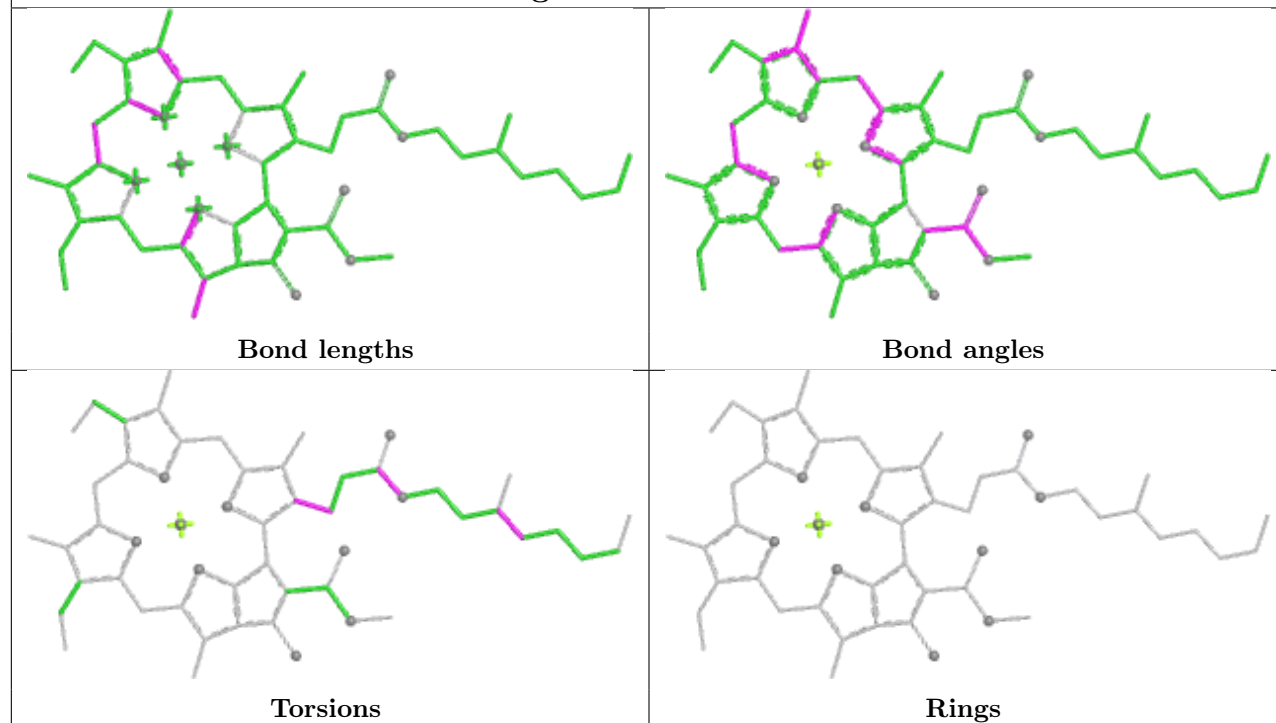
Ligand STE c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD A 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

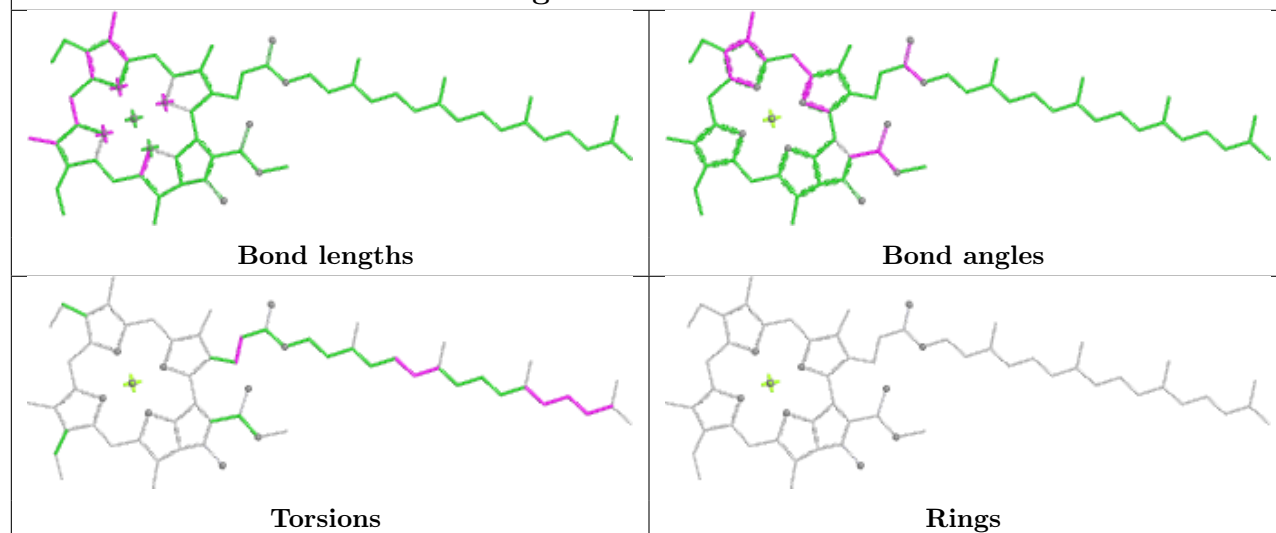


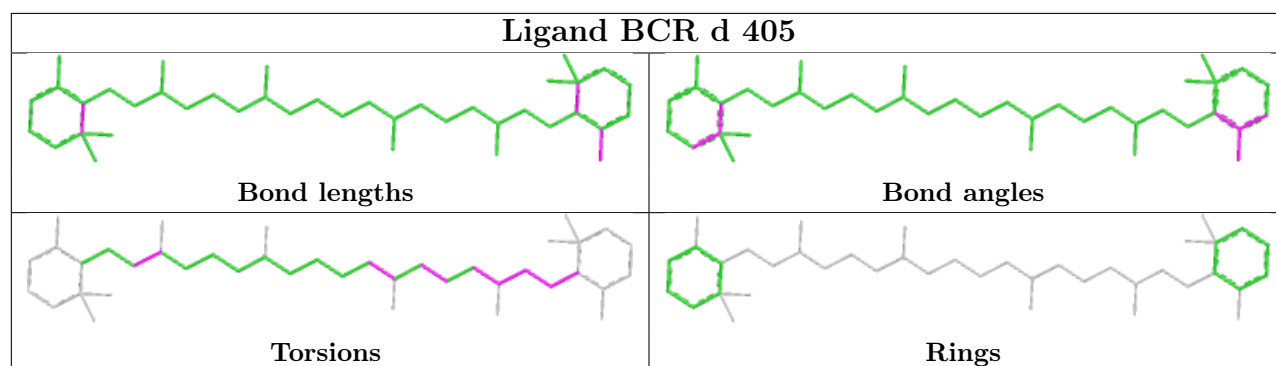
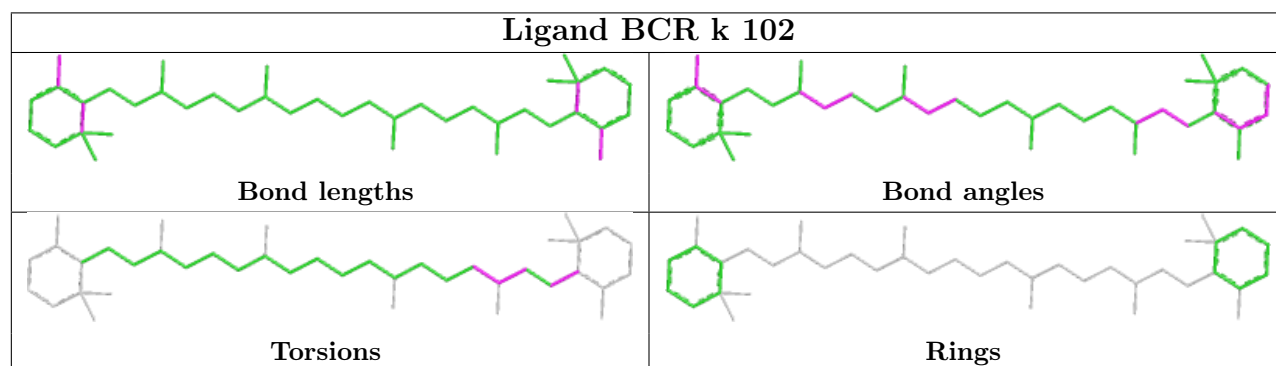
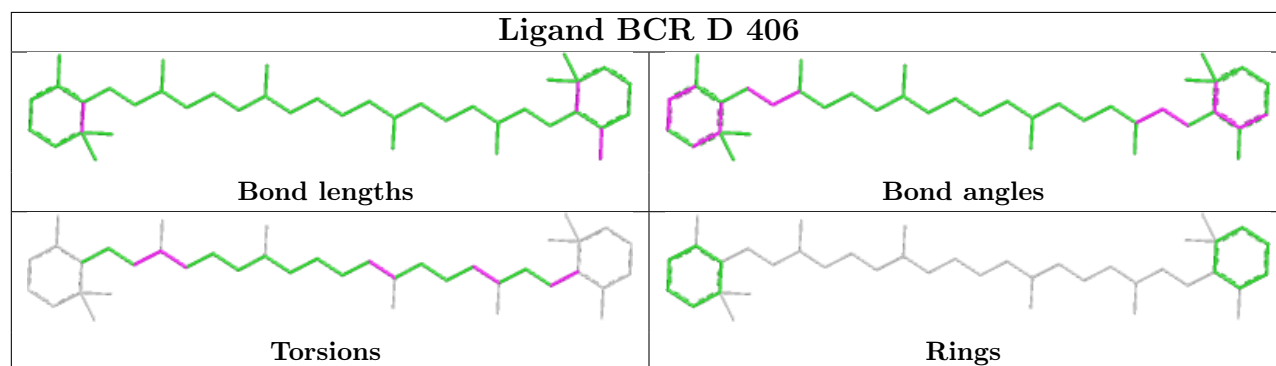
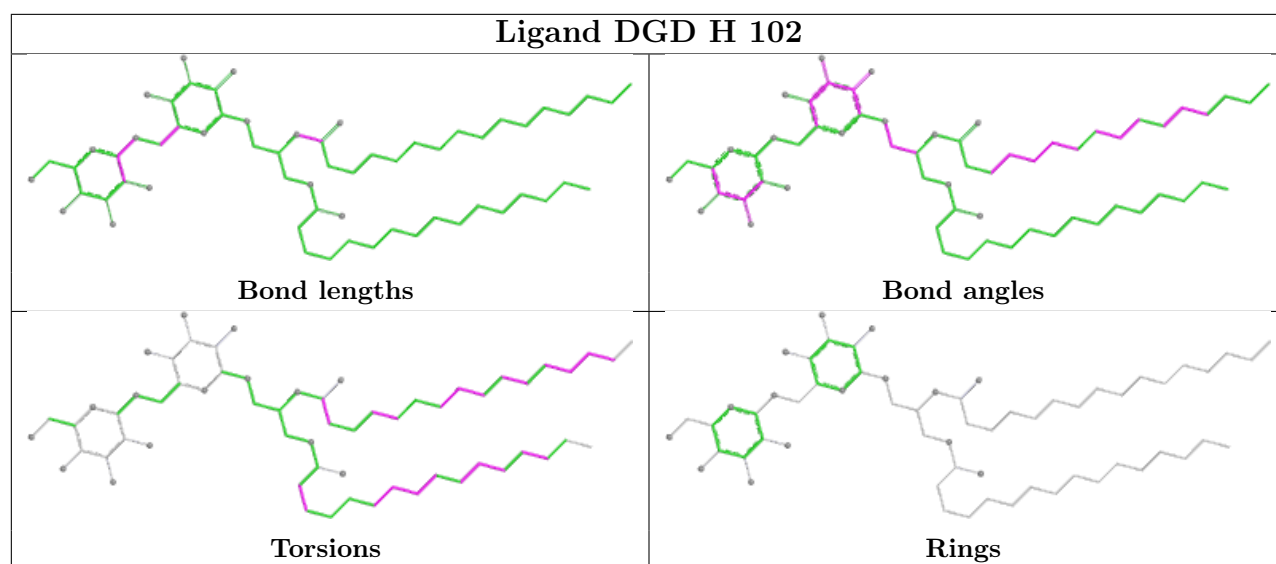
Ligand CLA c 503**Ligand CLA c 513**

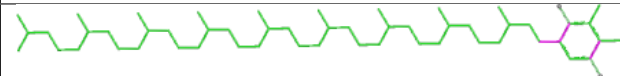
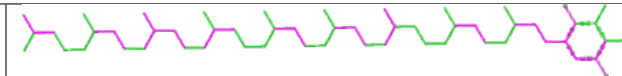
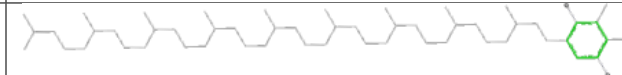
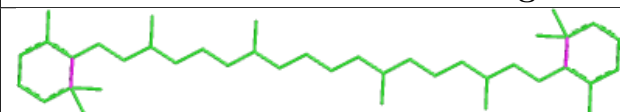
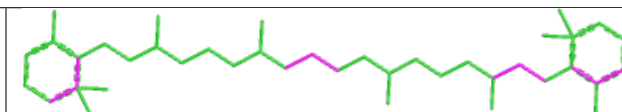
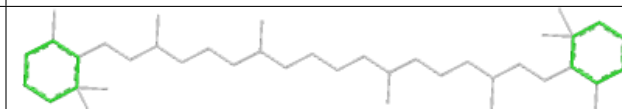
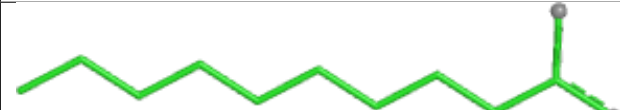
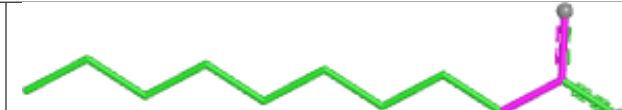
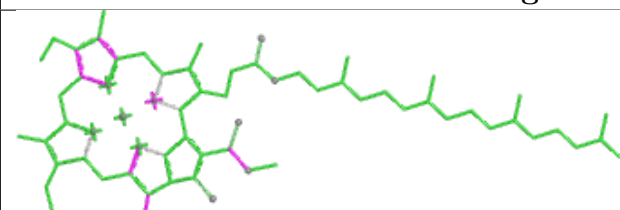
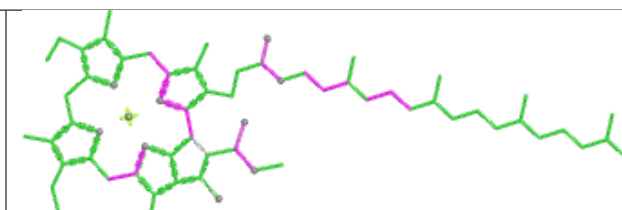
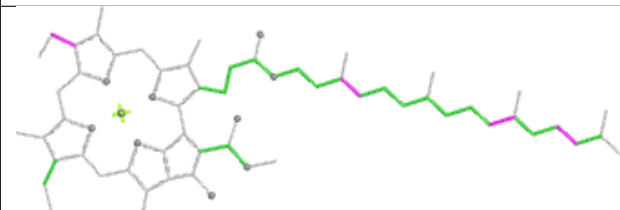
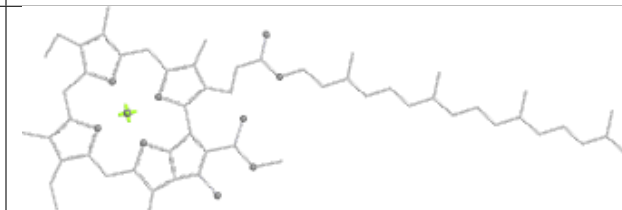
Ligand CLA A 609

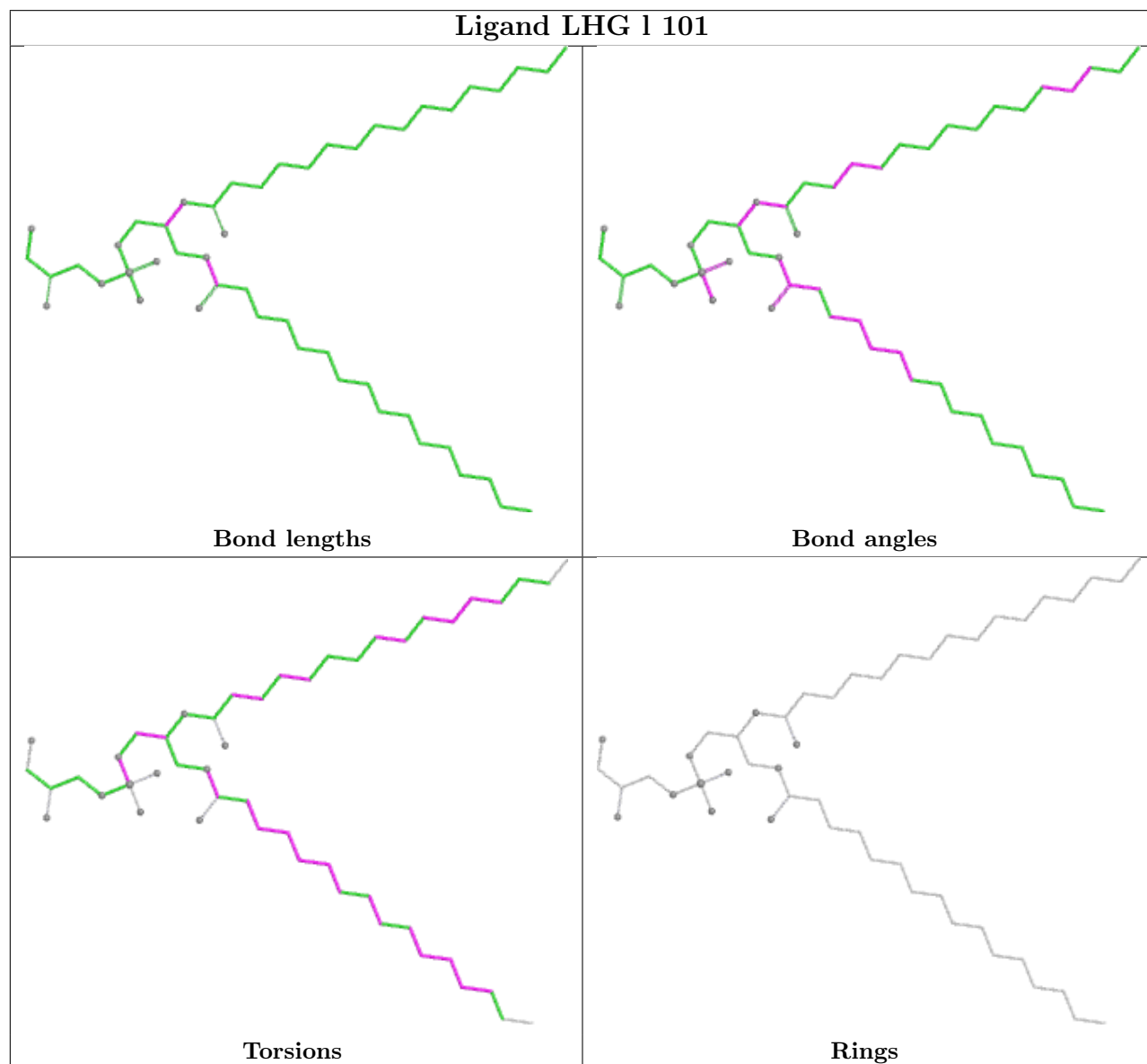
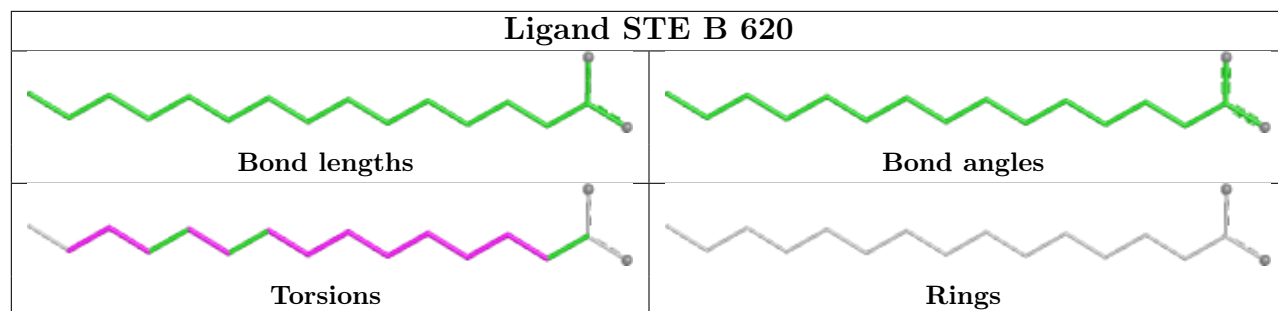


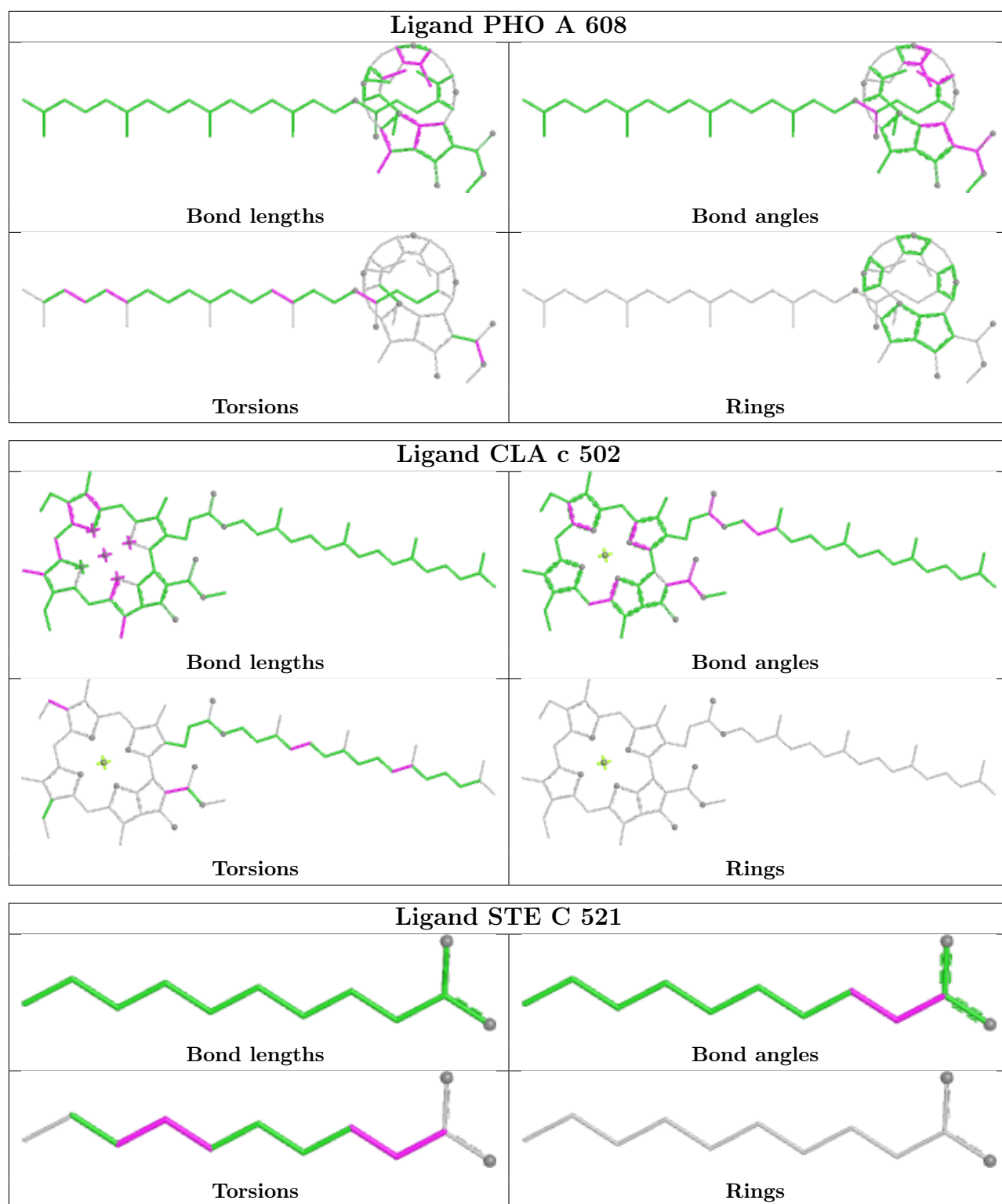
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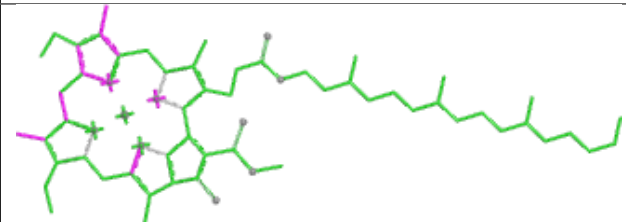
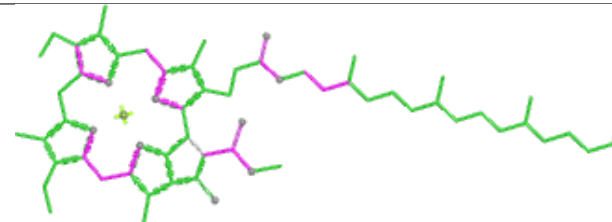
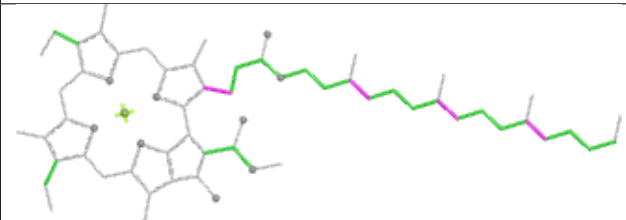
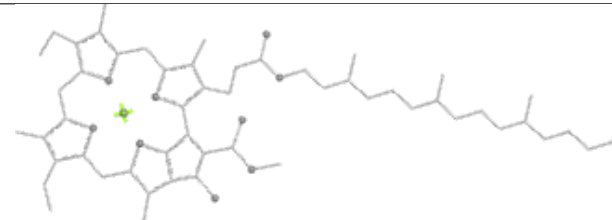


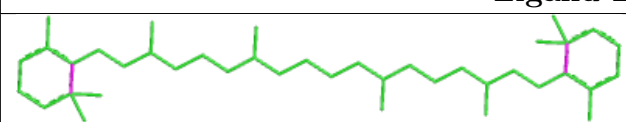
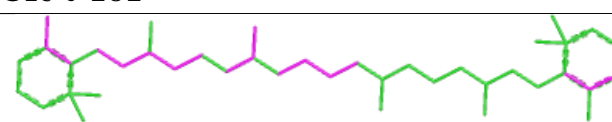
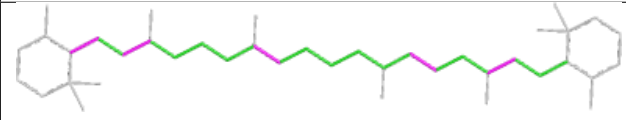
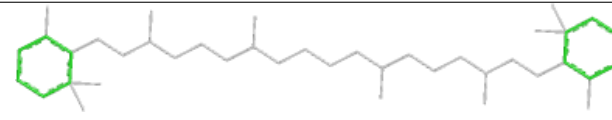


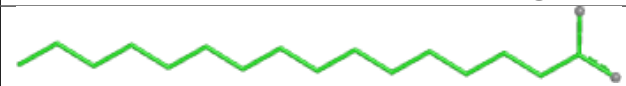
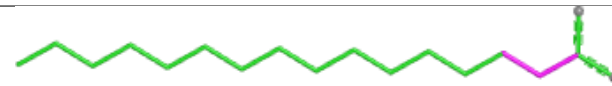
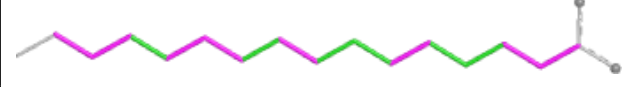
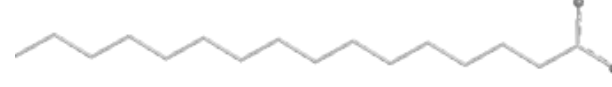
Ligand PL9 d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

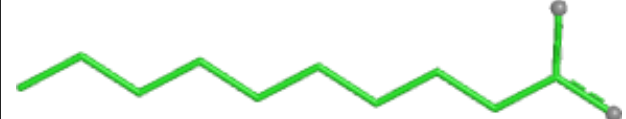
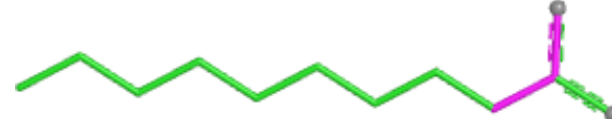
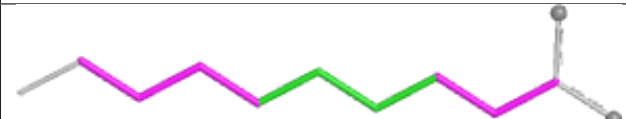
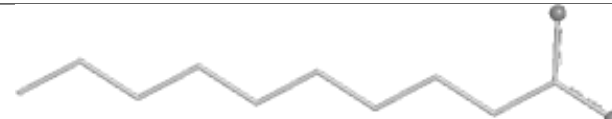


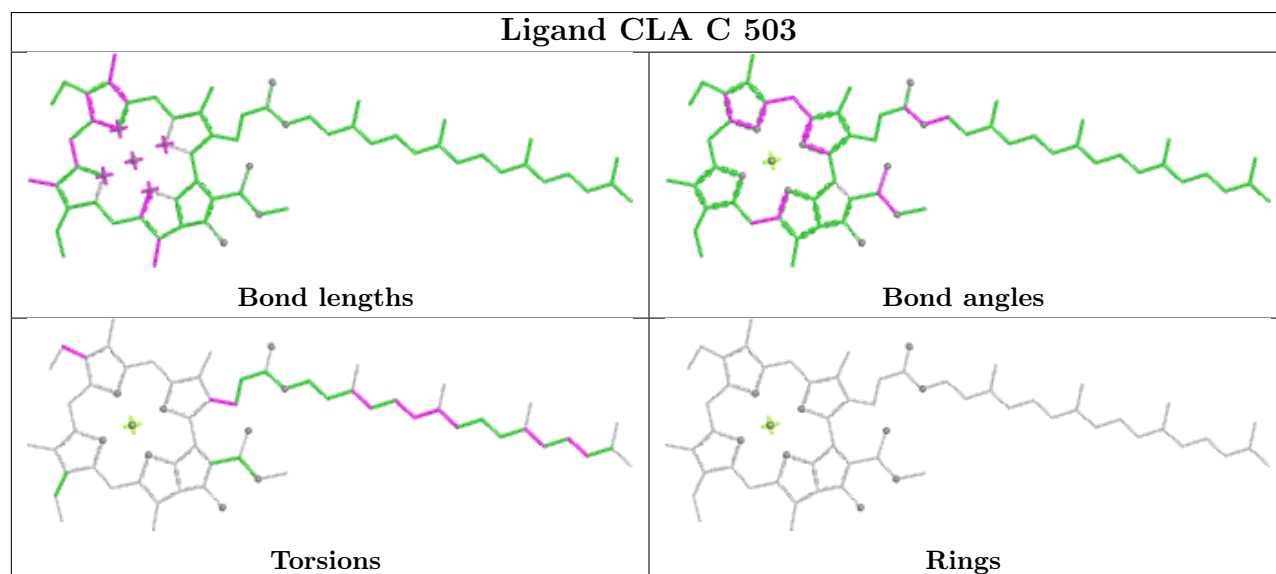
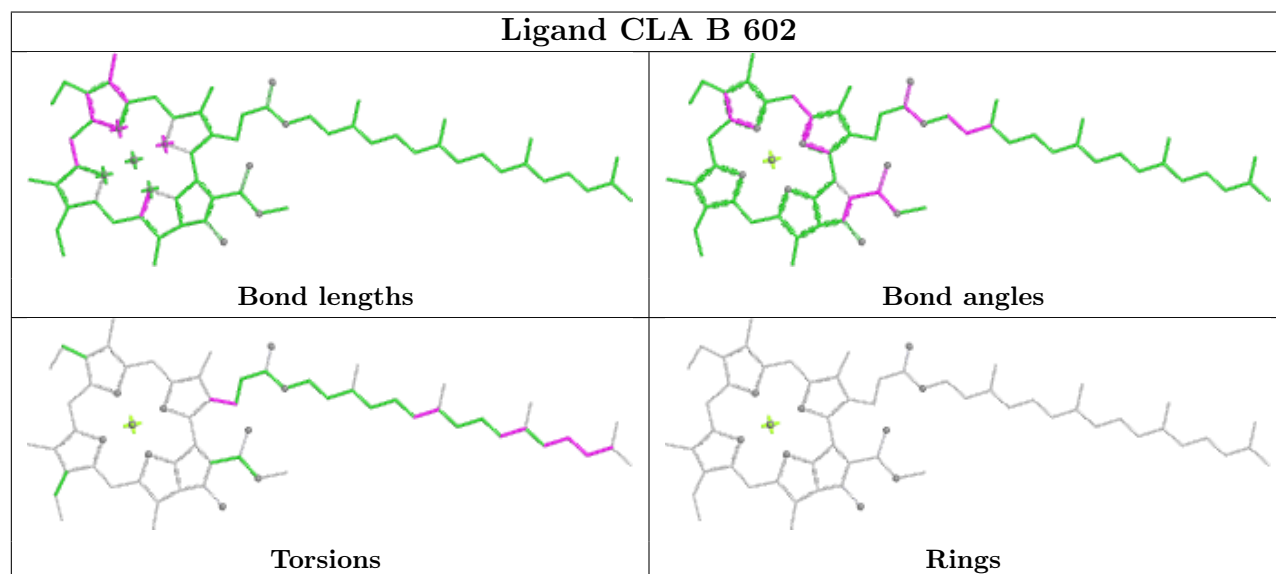
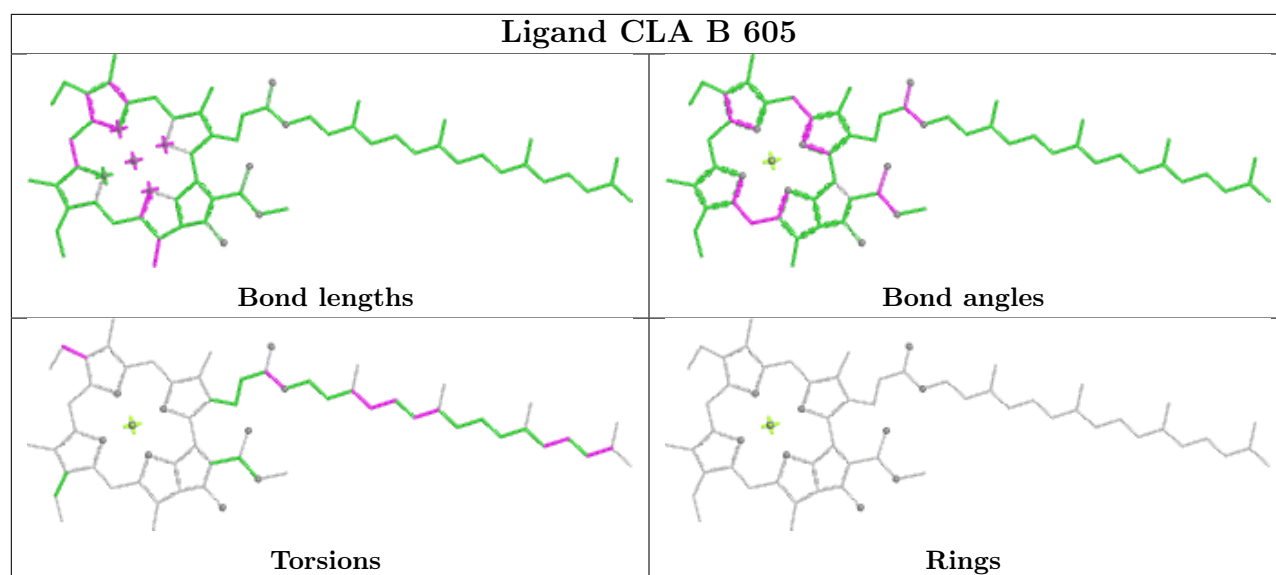


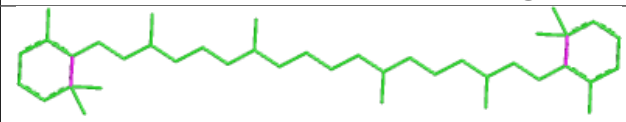
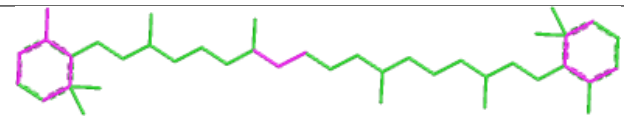
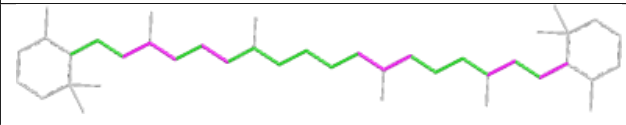
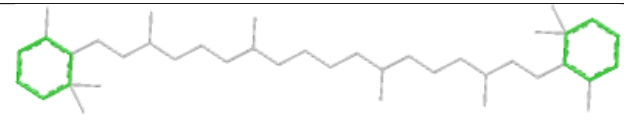
Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

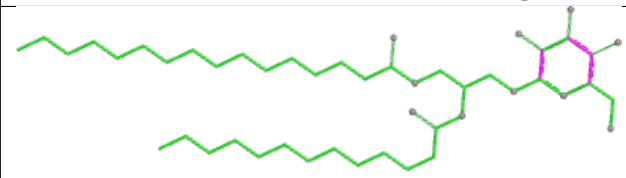
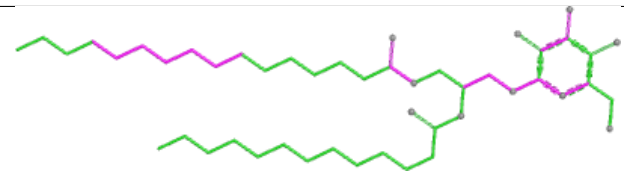
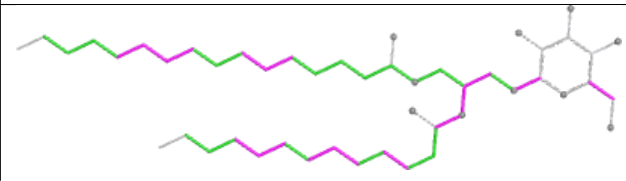
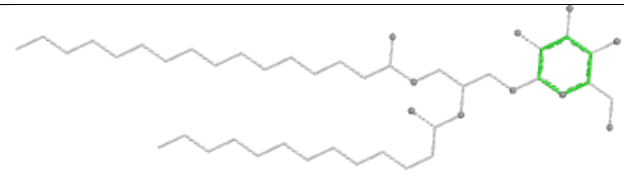
Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

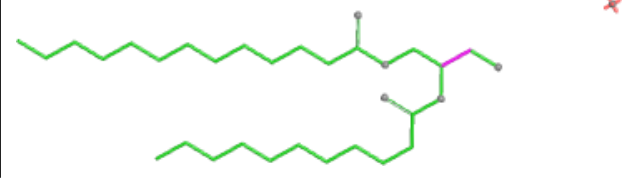
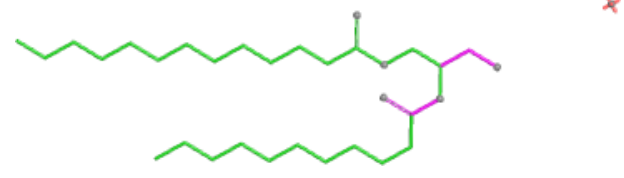
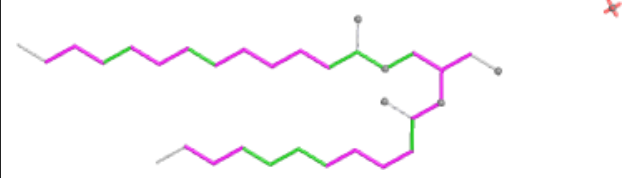
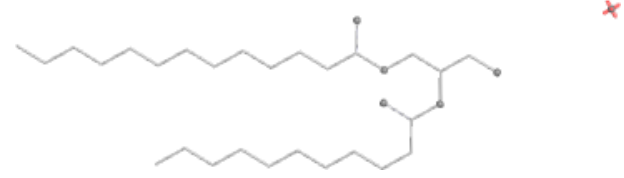
Ligand STE t 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

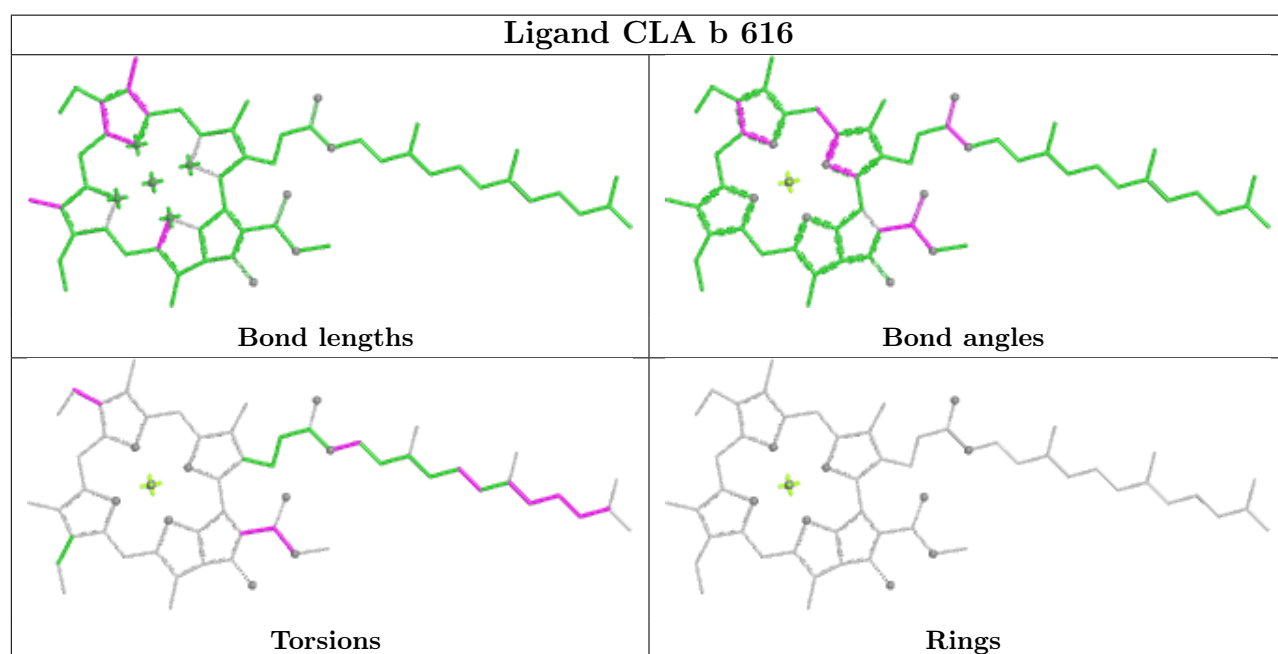
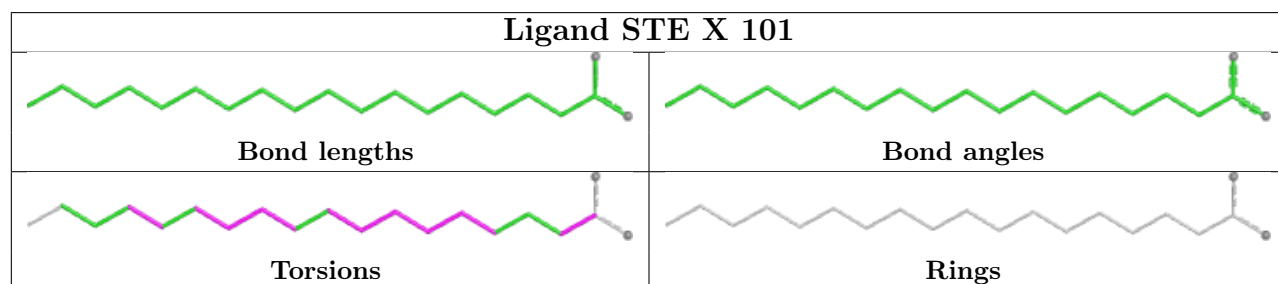
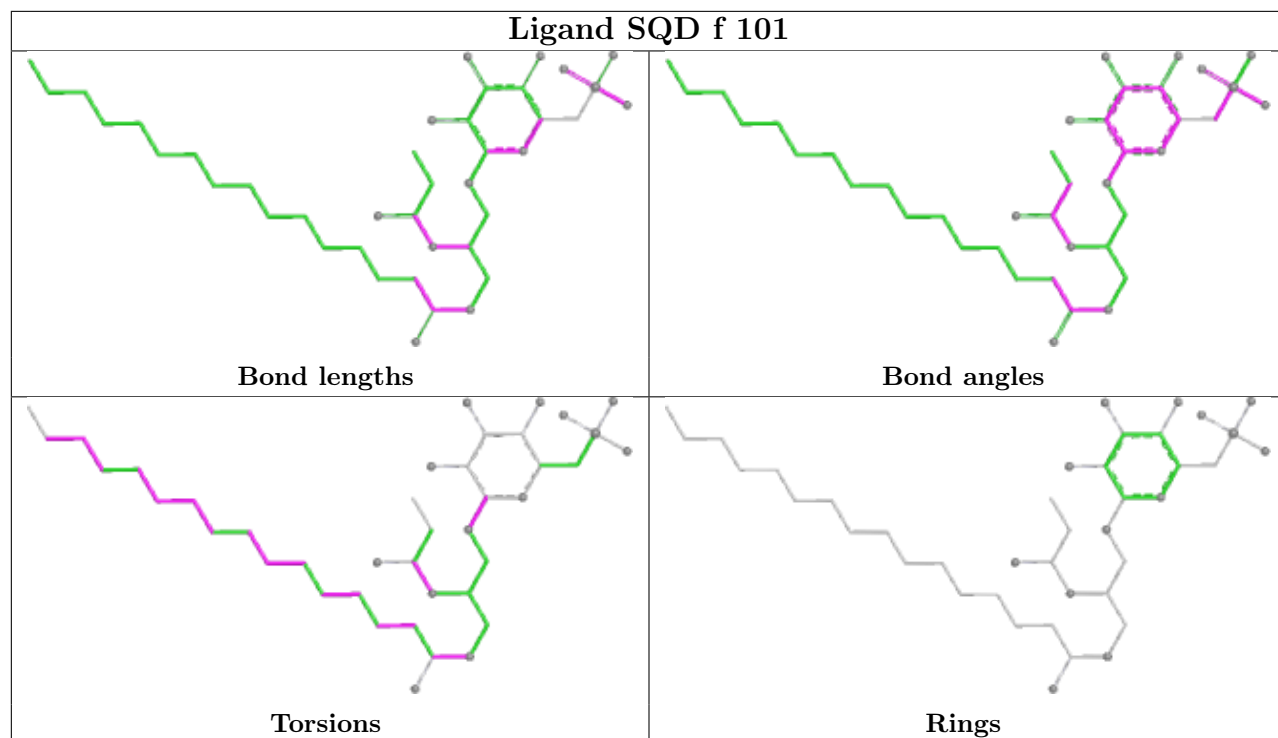
Ligand STE L 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

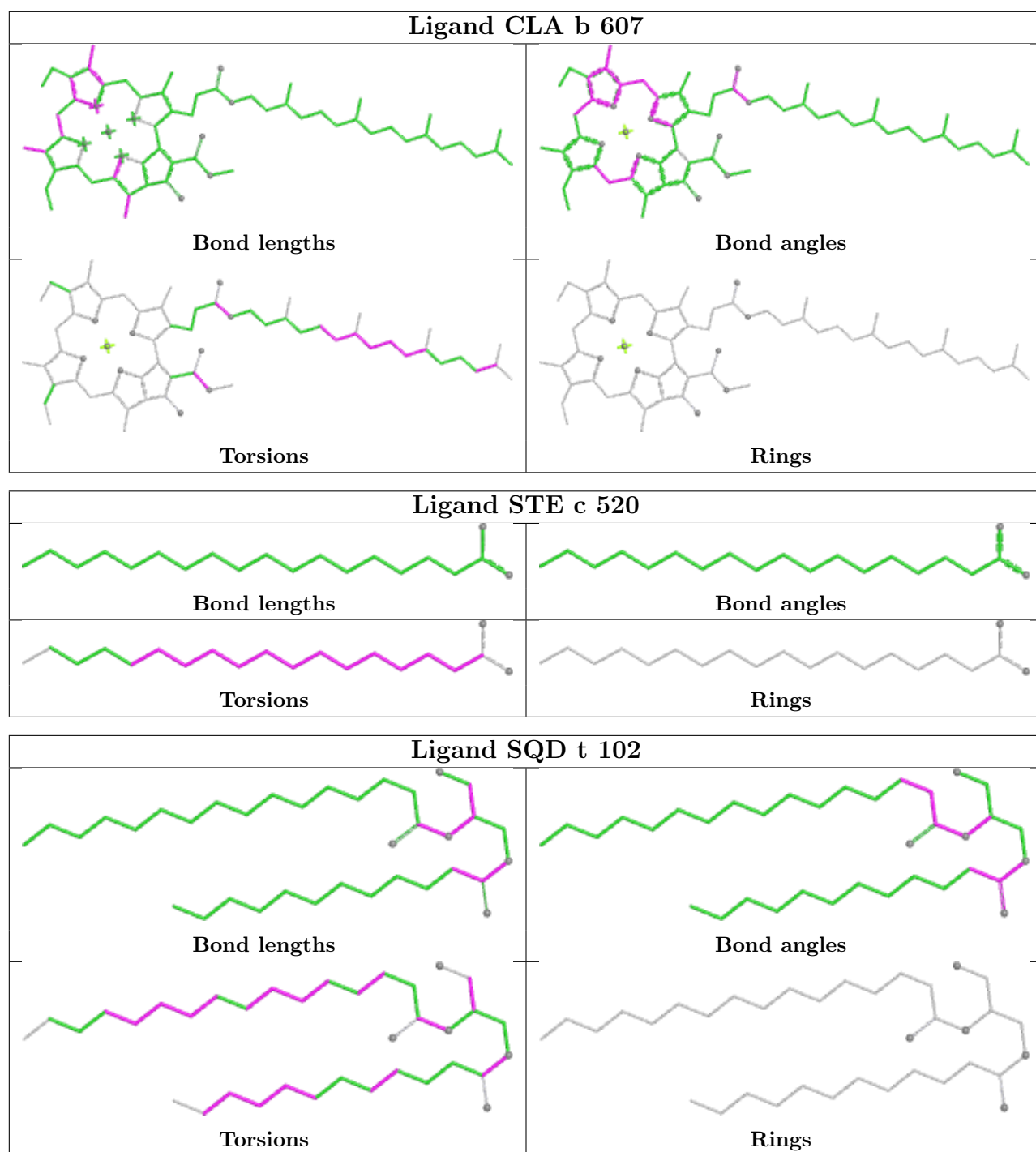


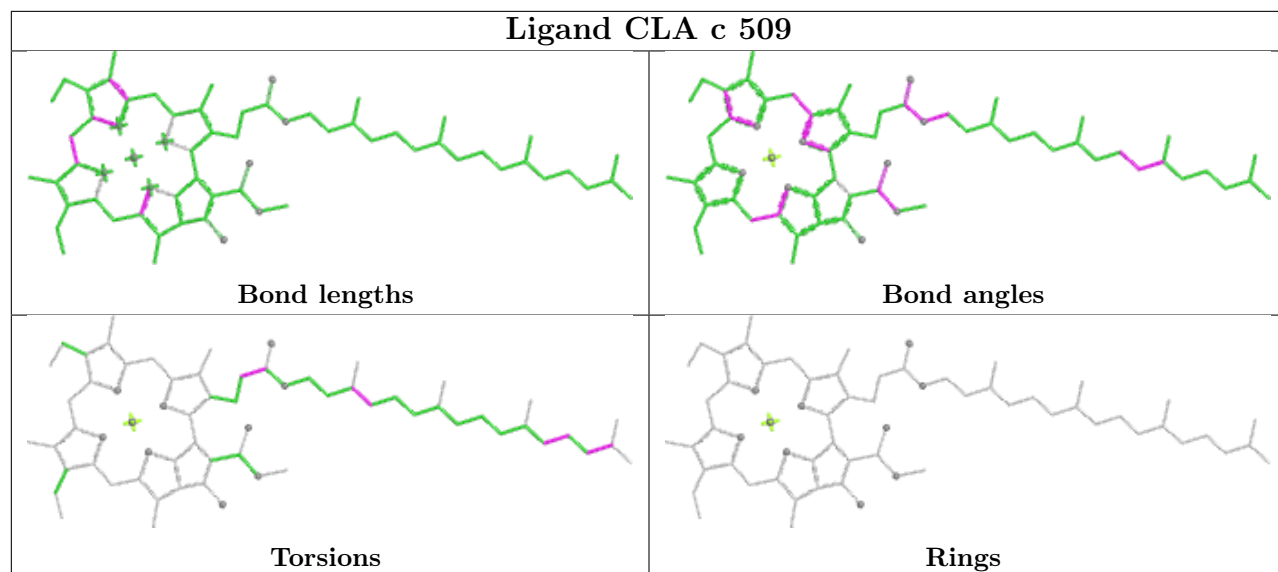
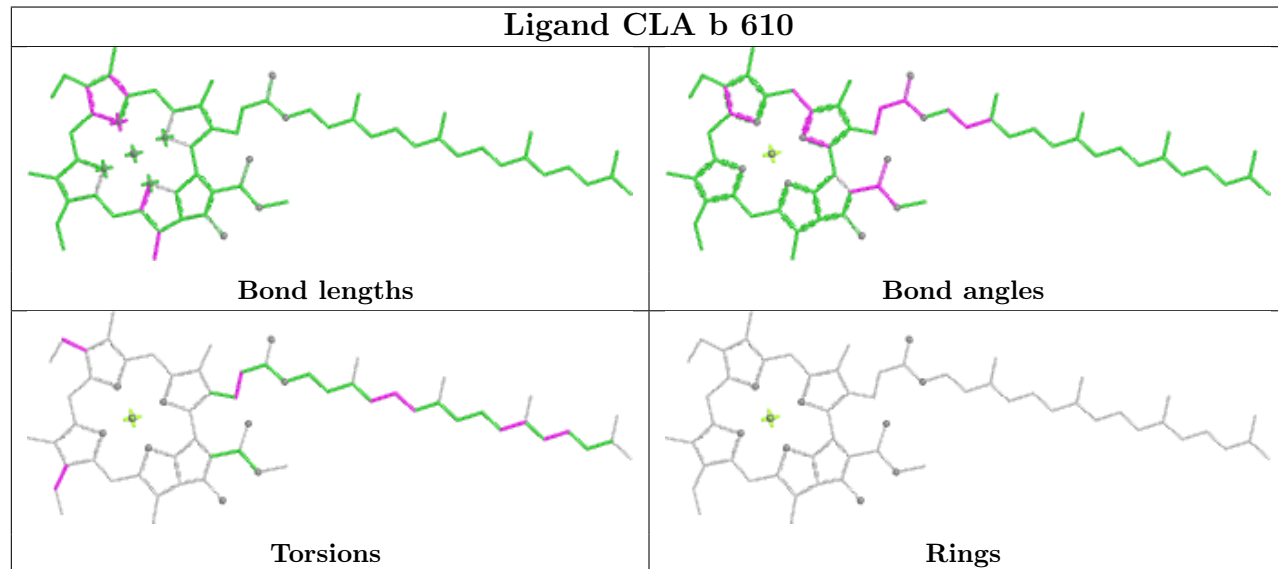
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

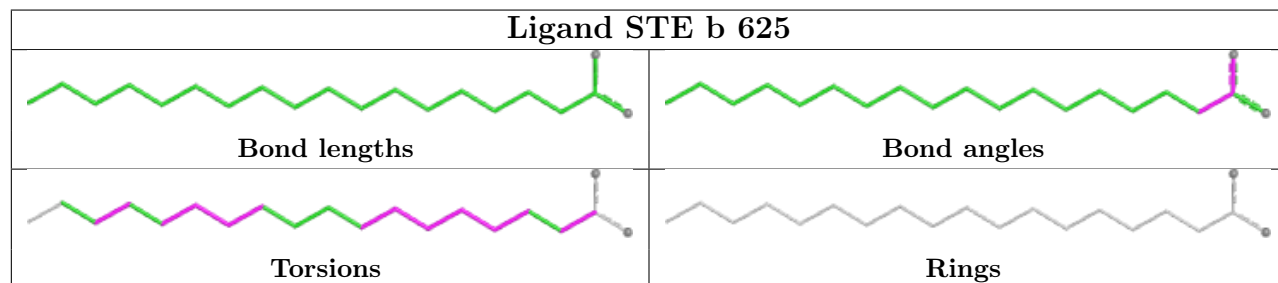
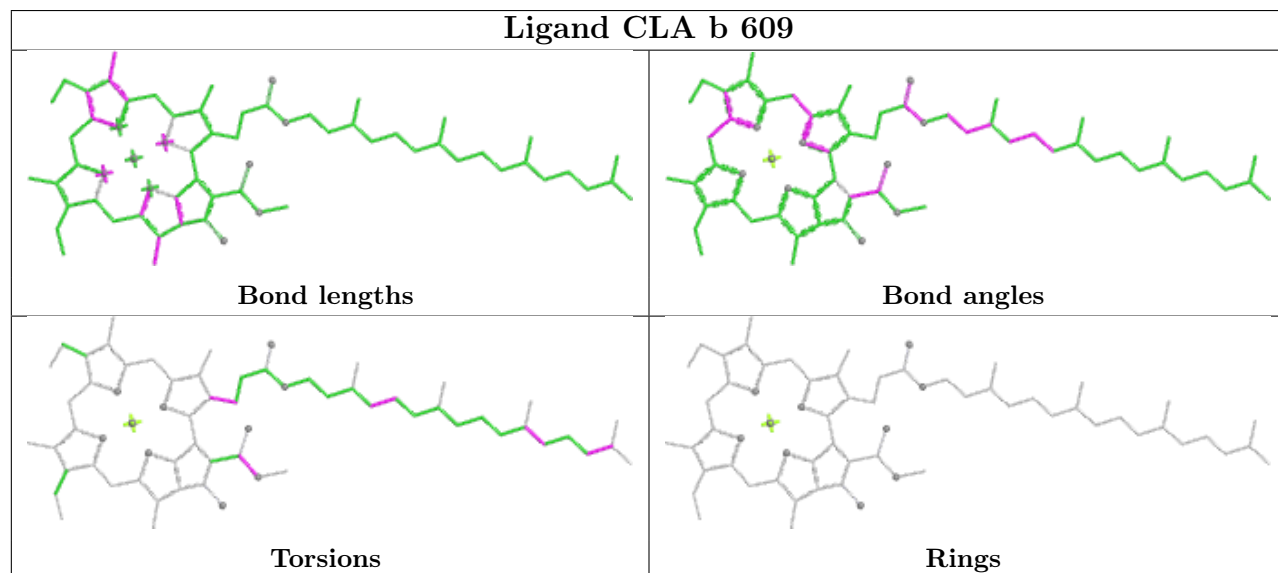
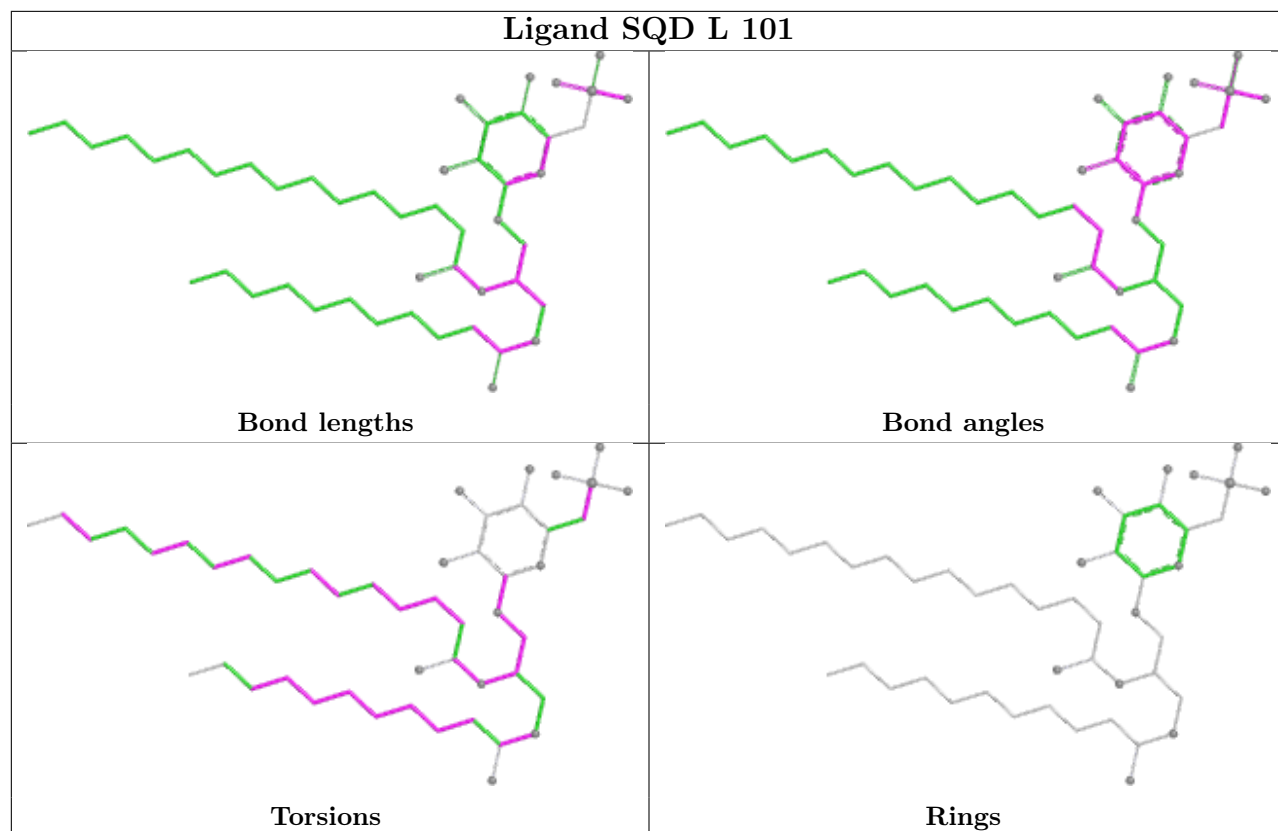
Ligand LMG A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

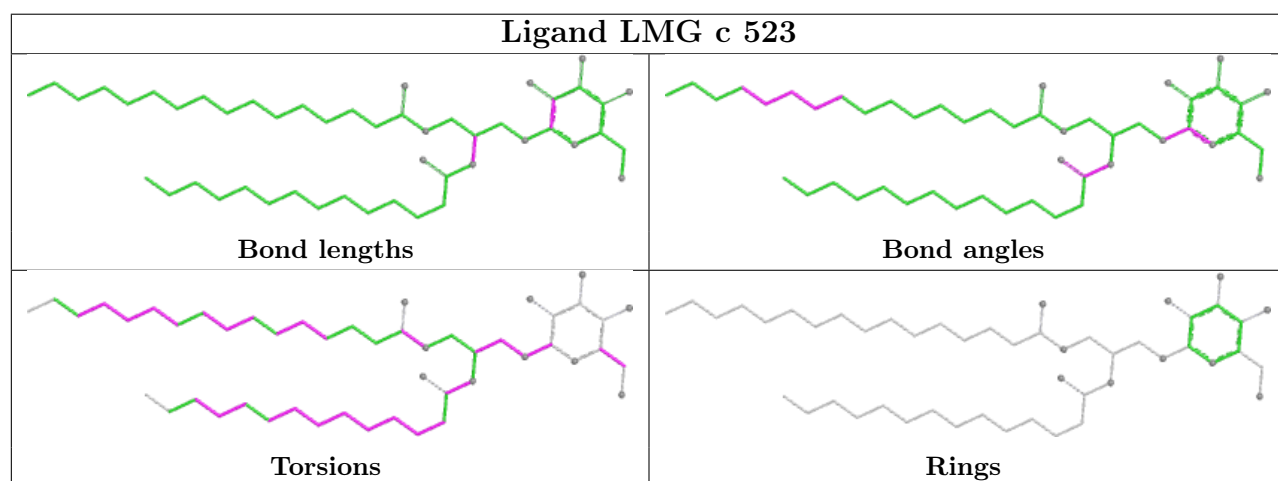
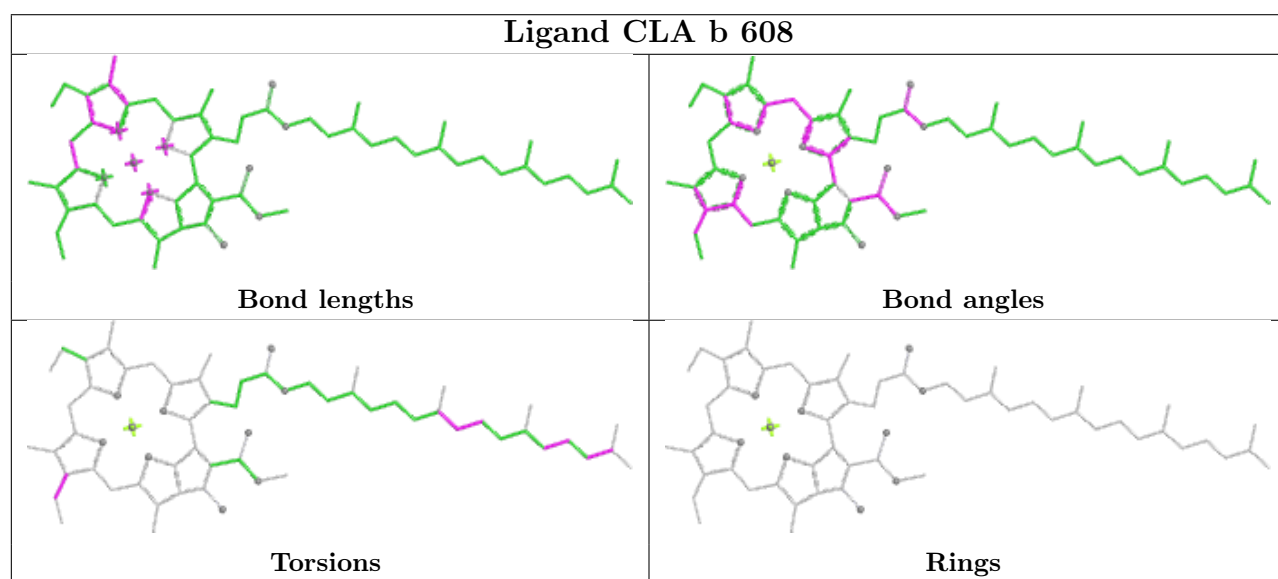
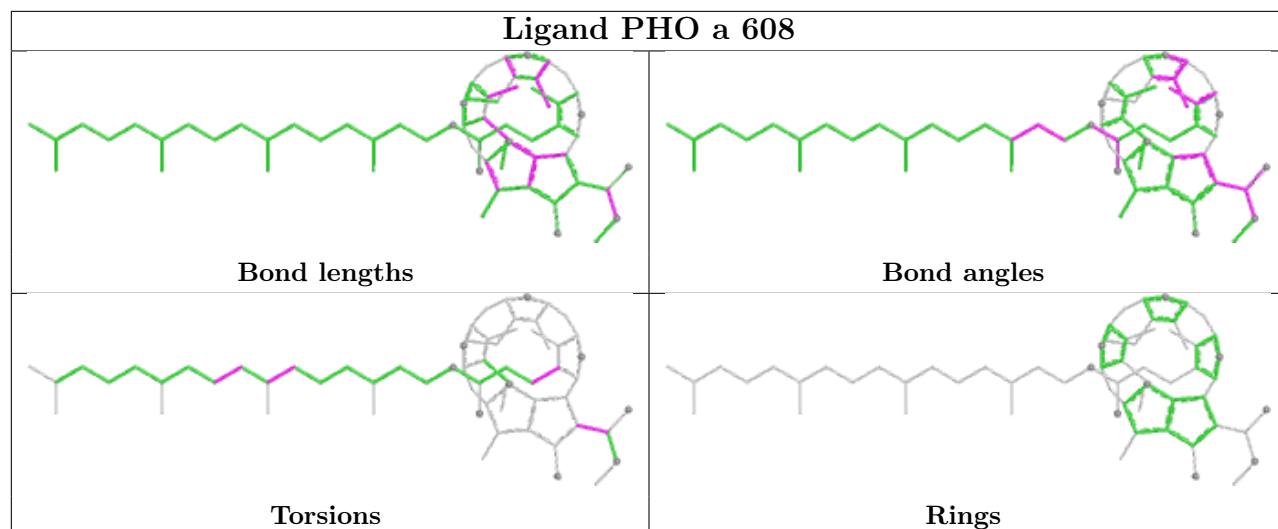
Ligand LMG D 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

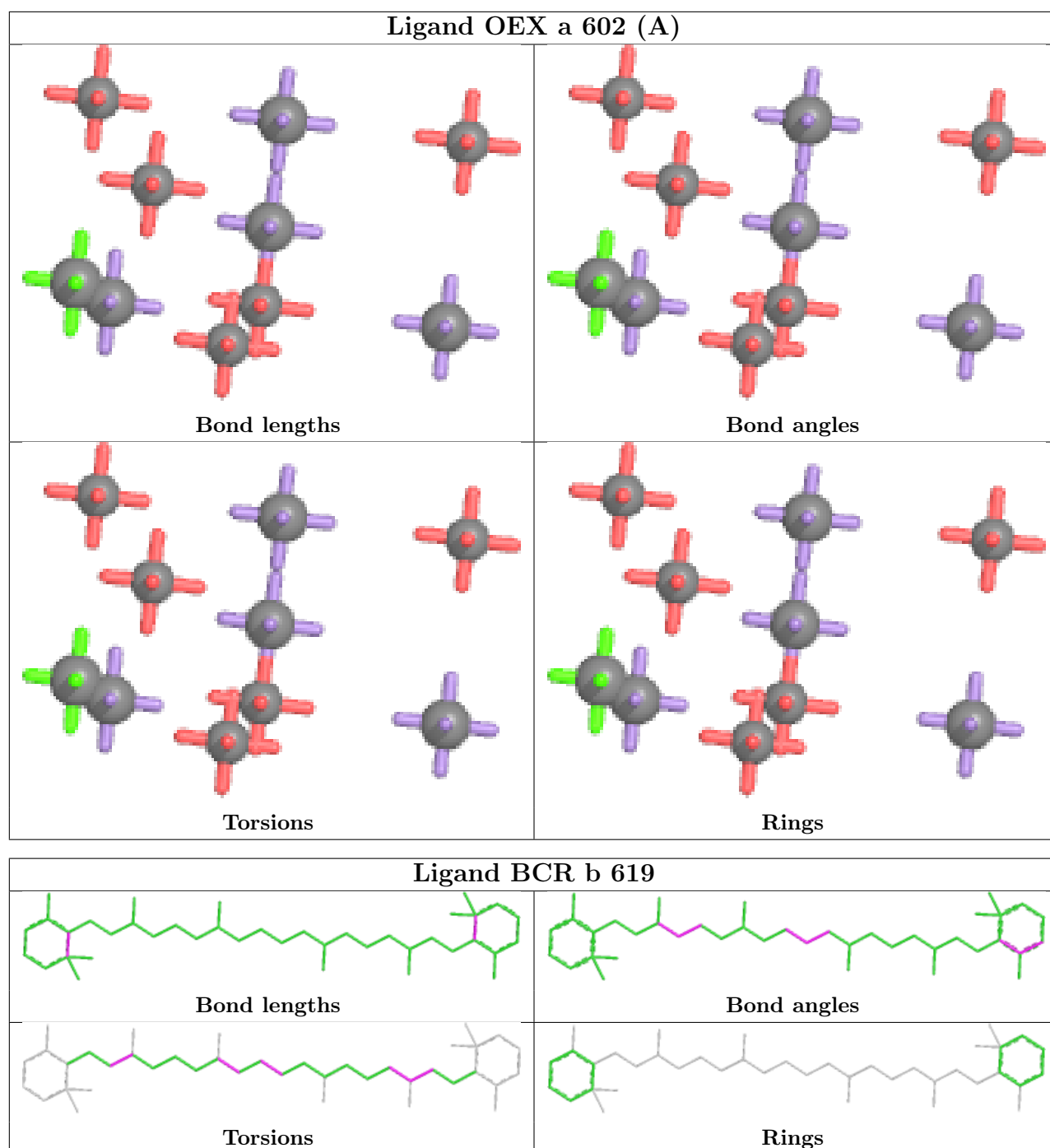


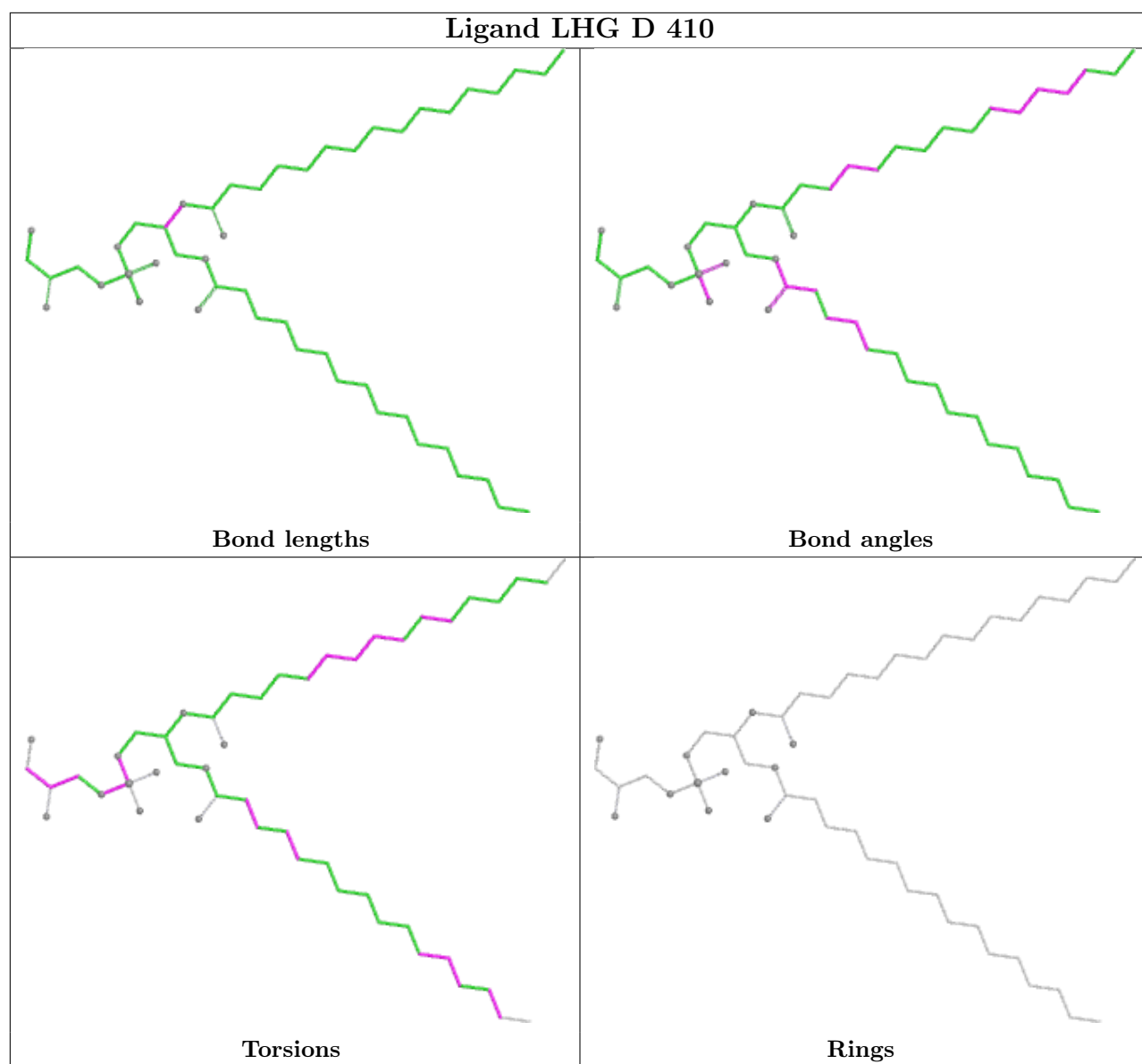


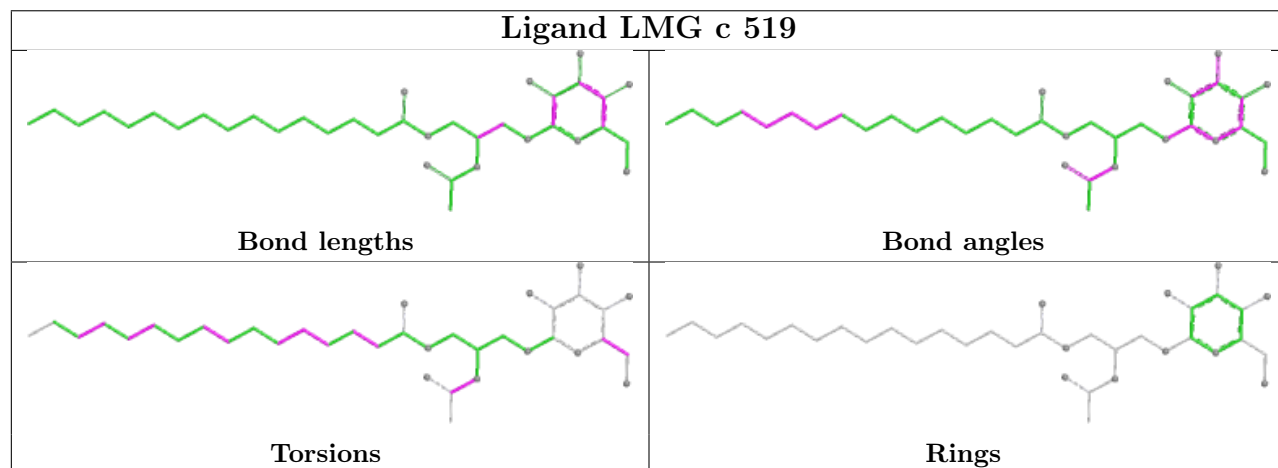
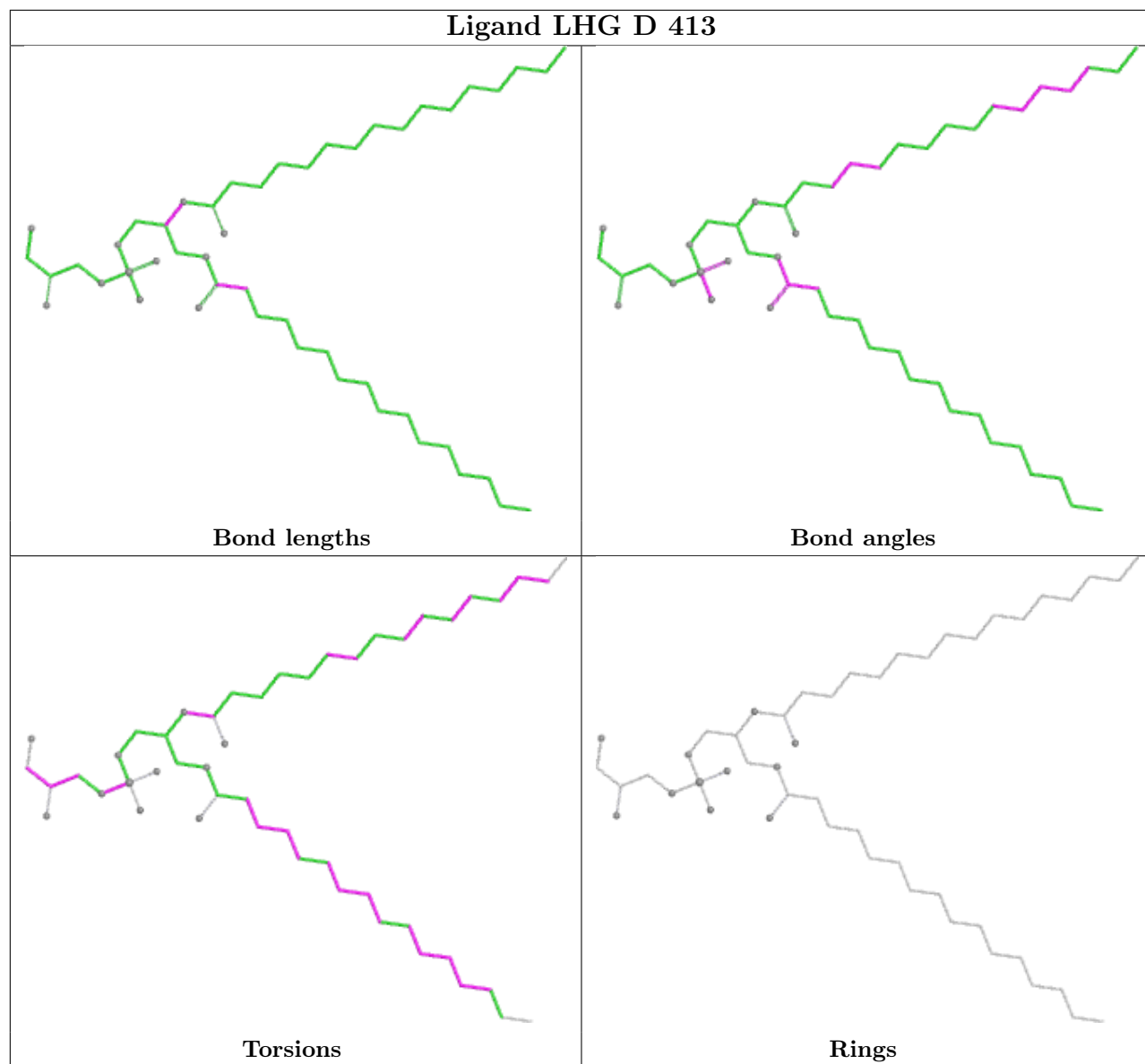
Ligand CLA c 509**Ligand CLA b 610**

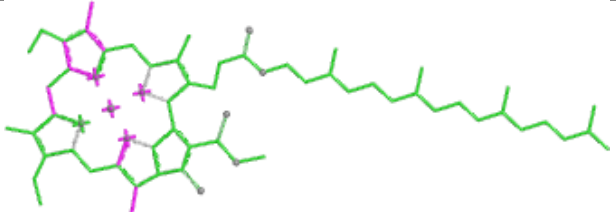
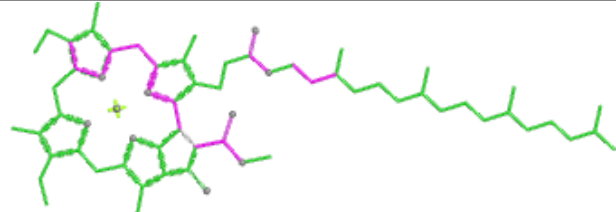
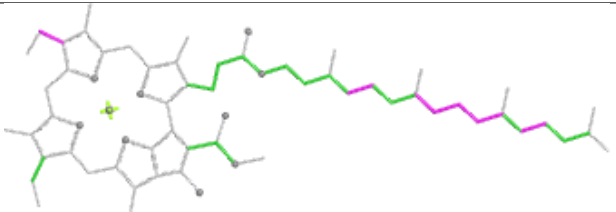
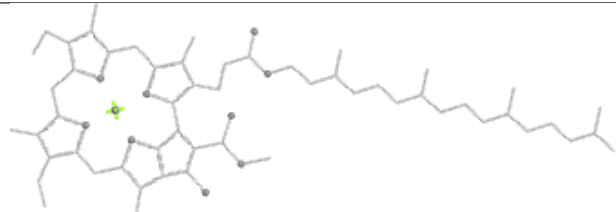




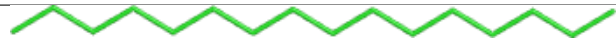
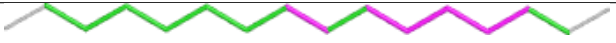




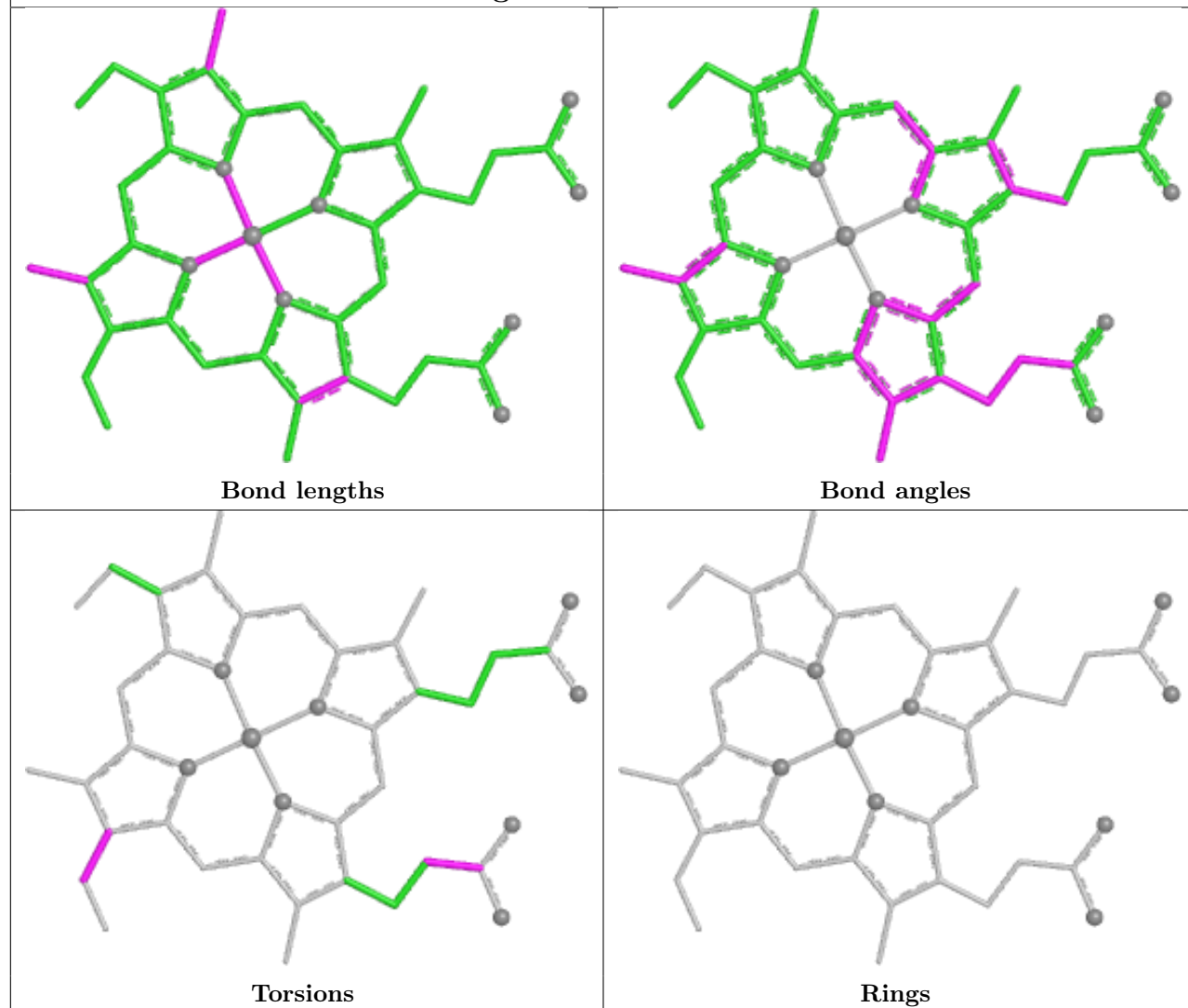


Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

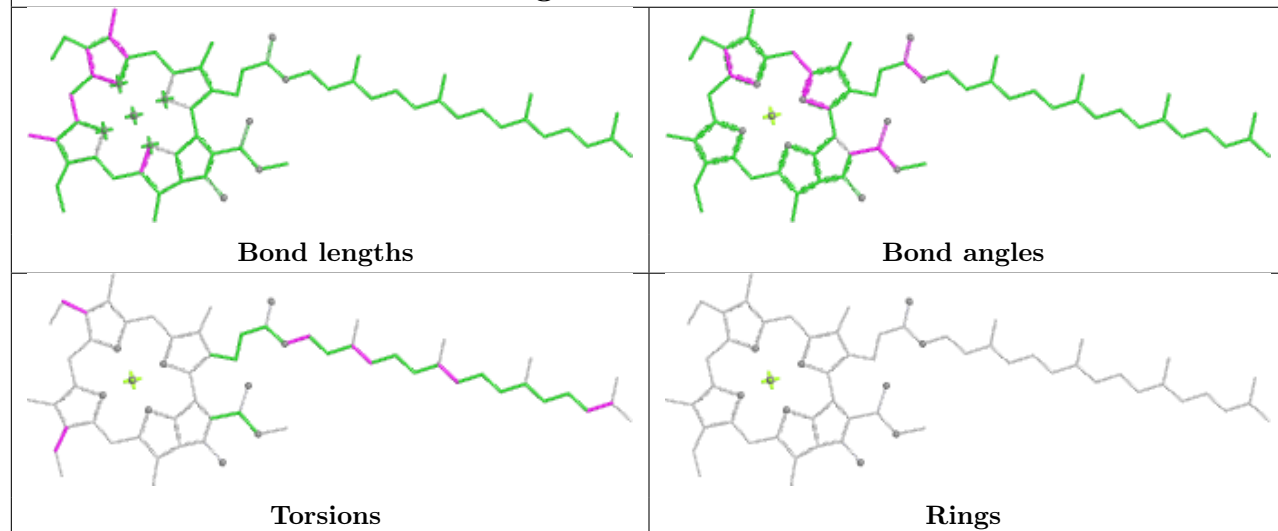
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

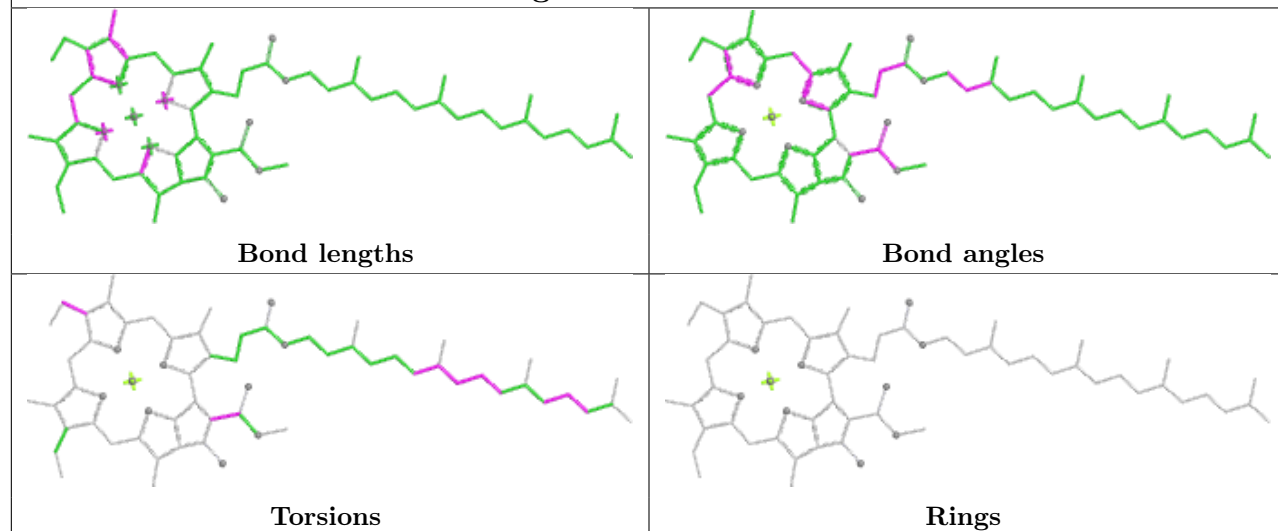
Ligand HEC V 201



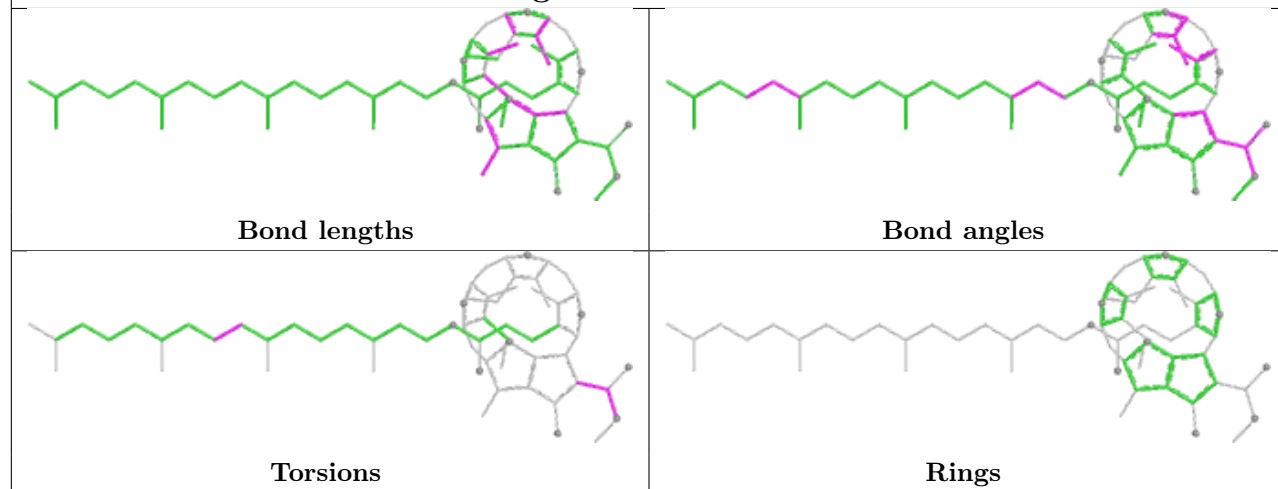
Ligand CLA d 403



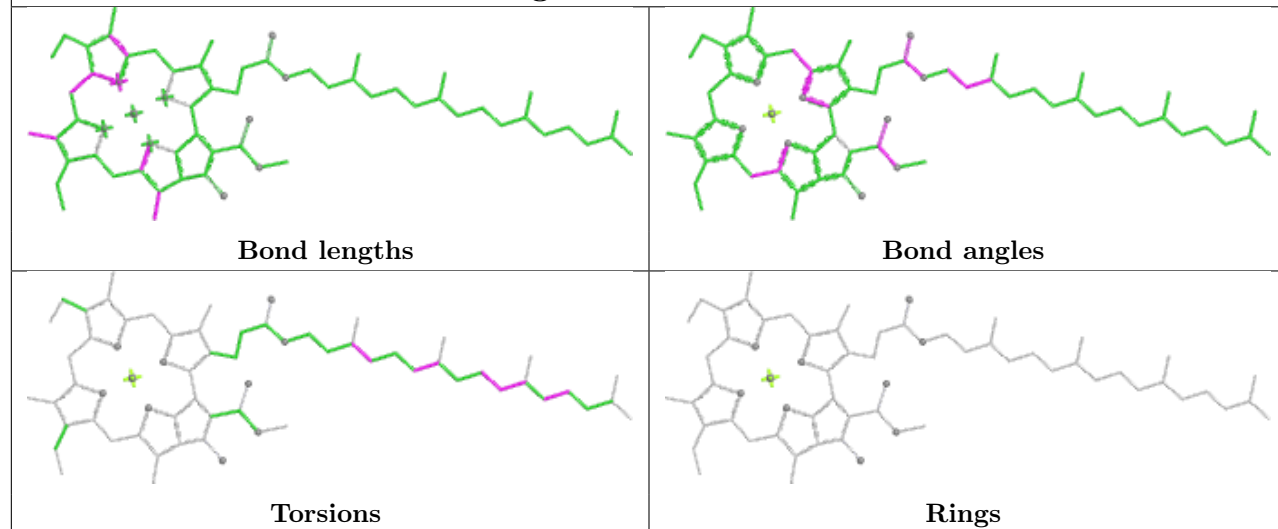
Ligand CLA C 507



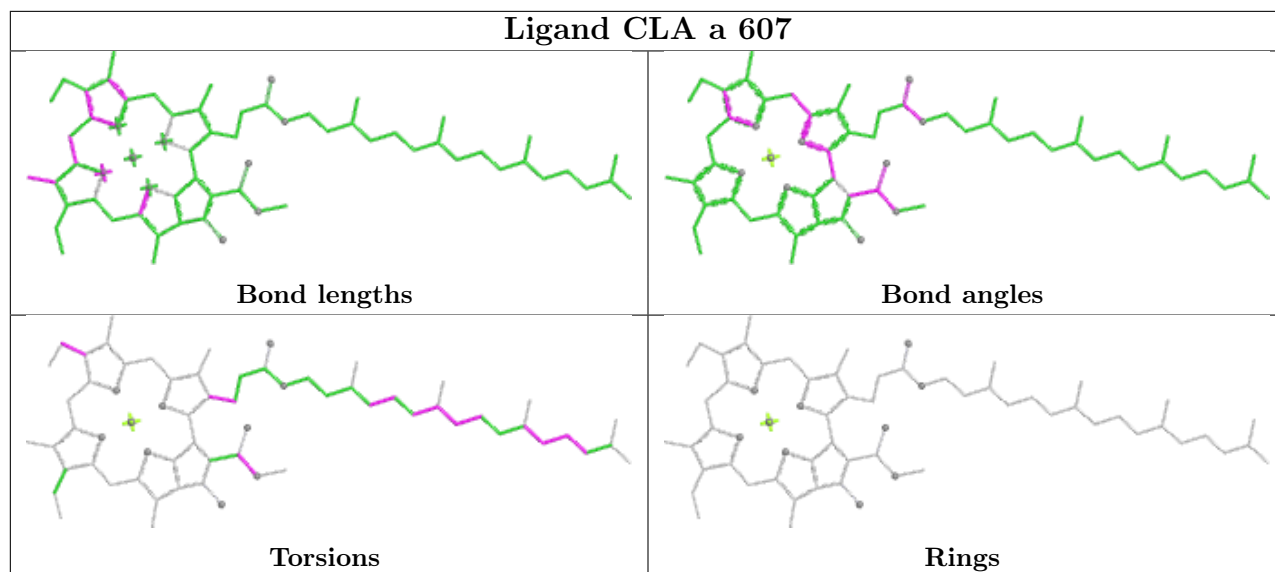
Ligand PHO d 402



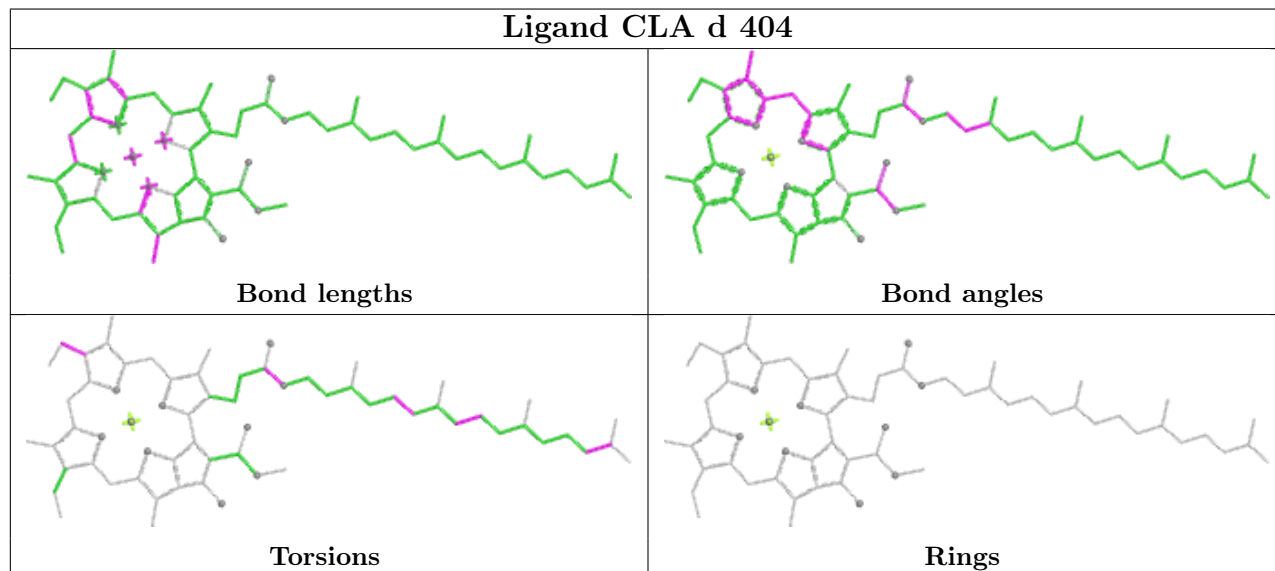
Ligand CLA D 405



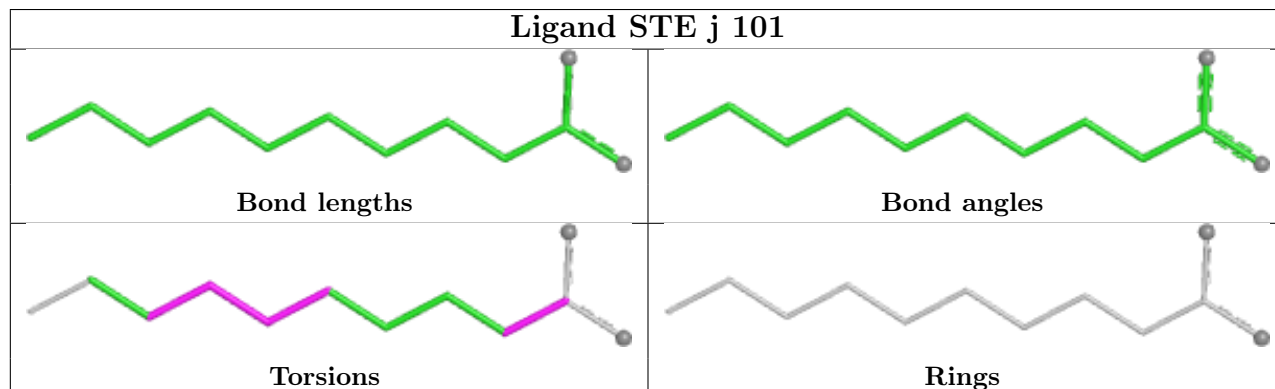
Ligand CLA a 607

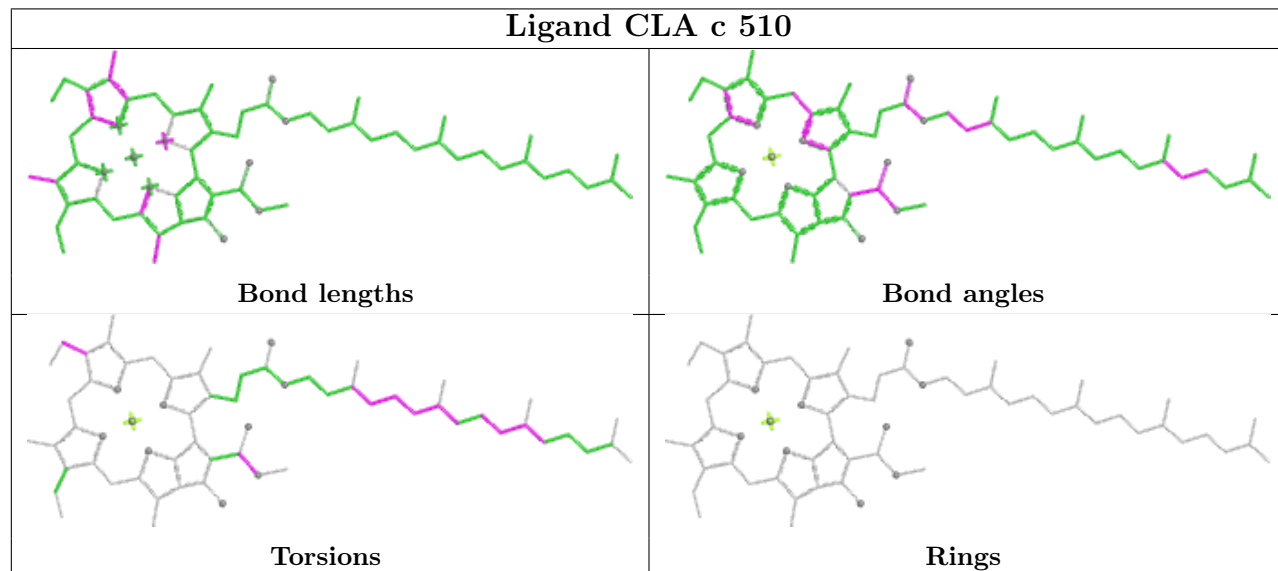
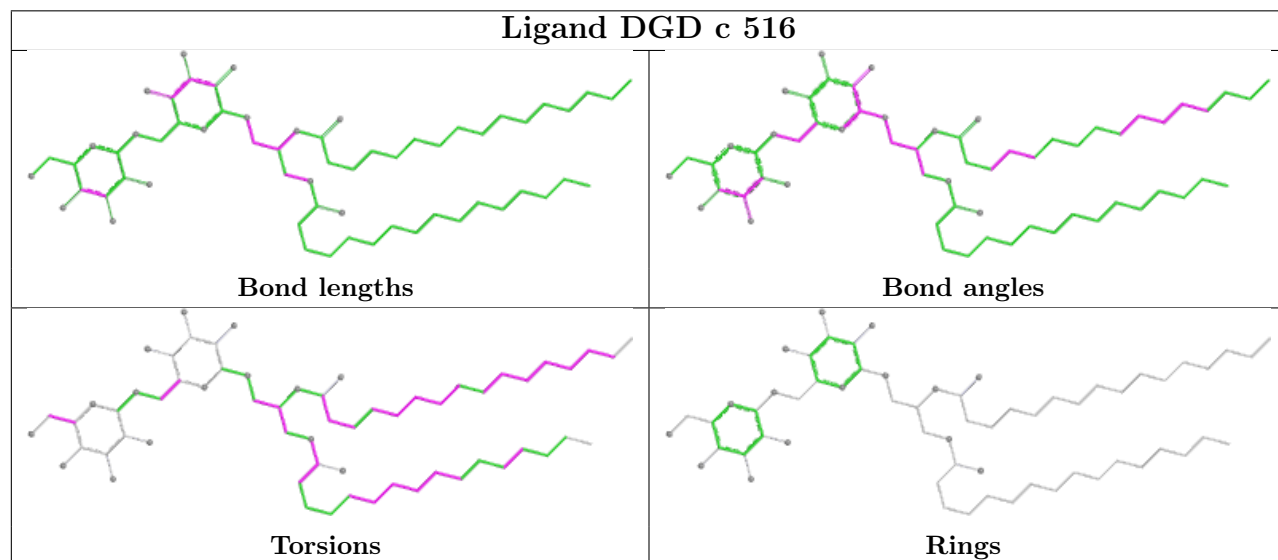
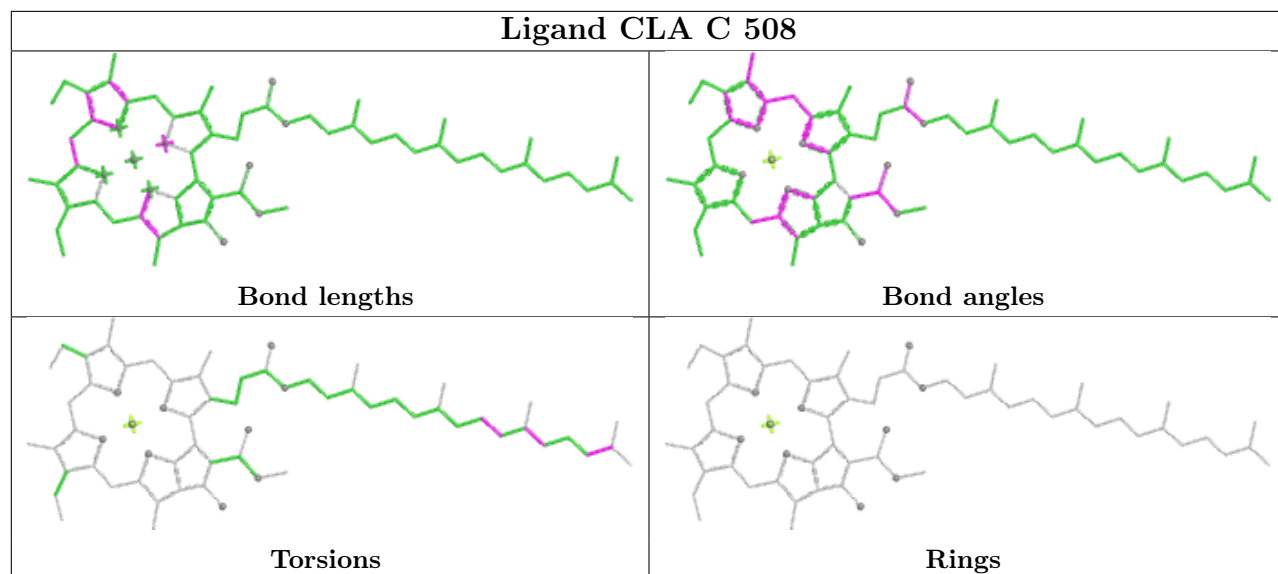


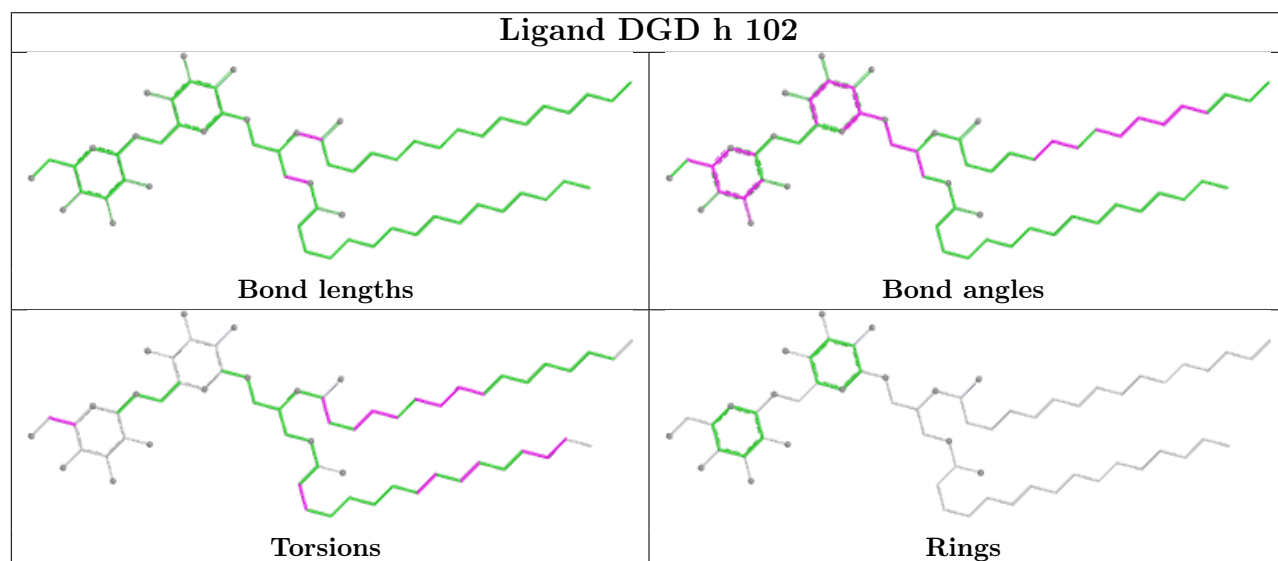
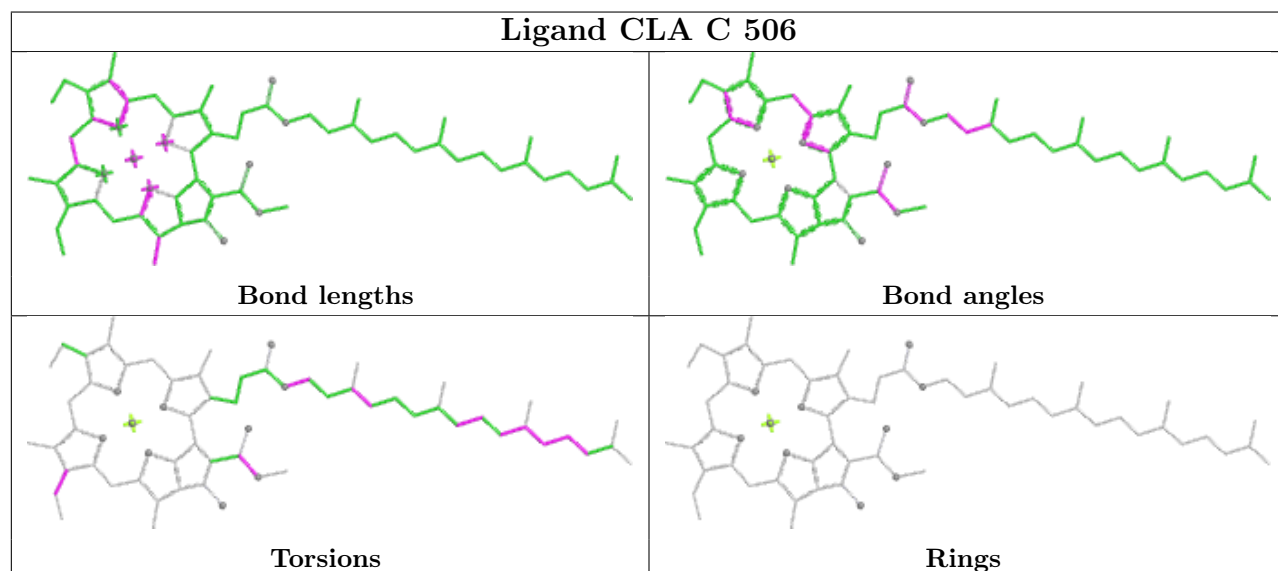
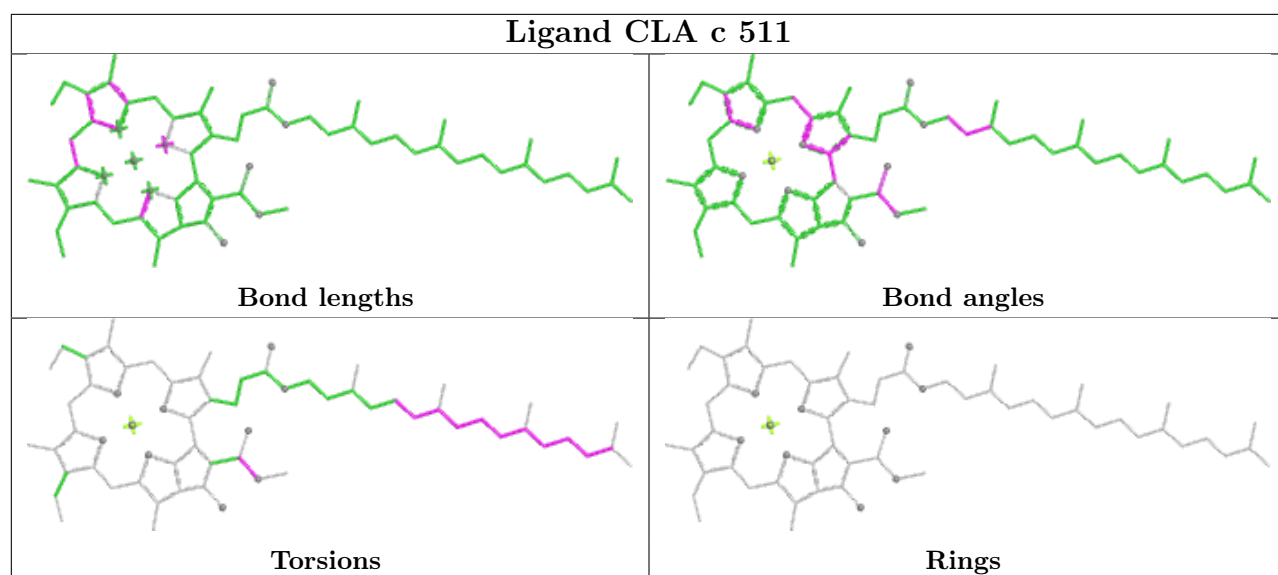
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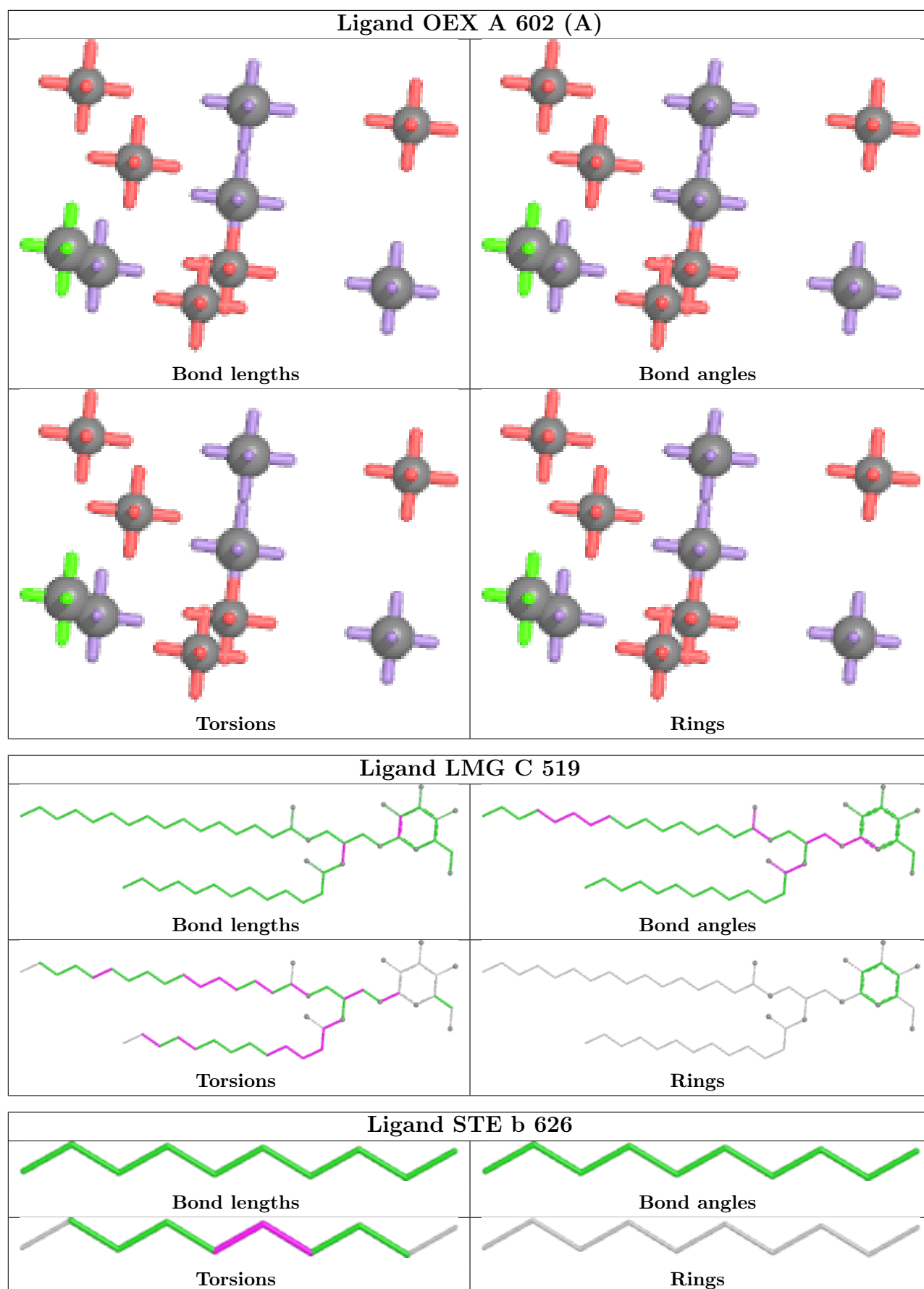


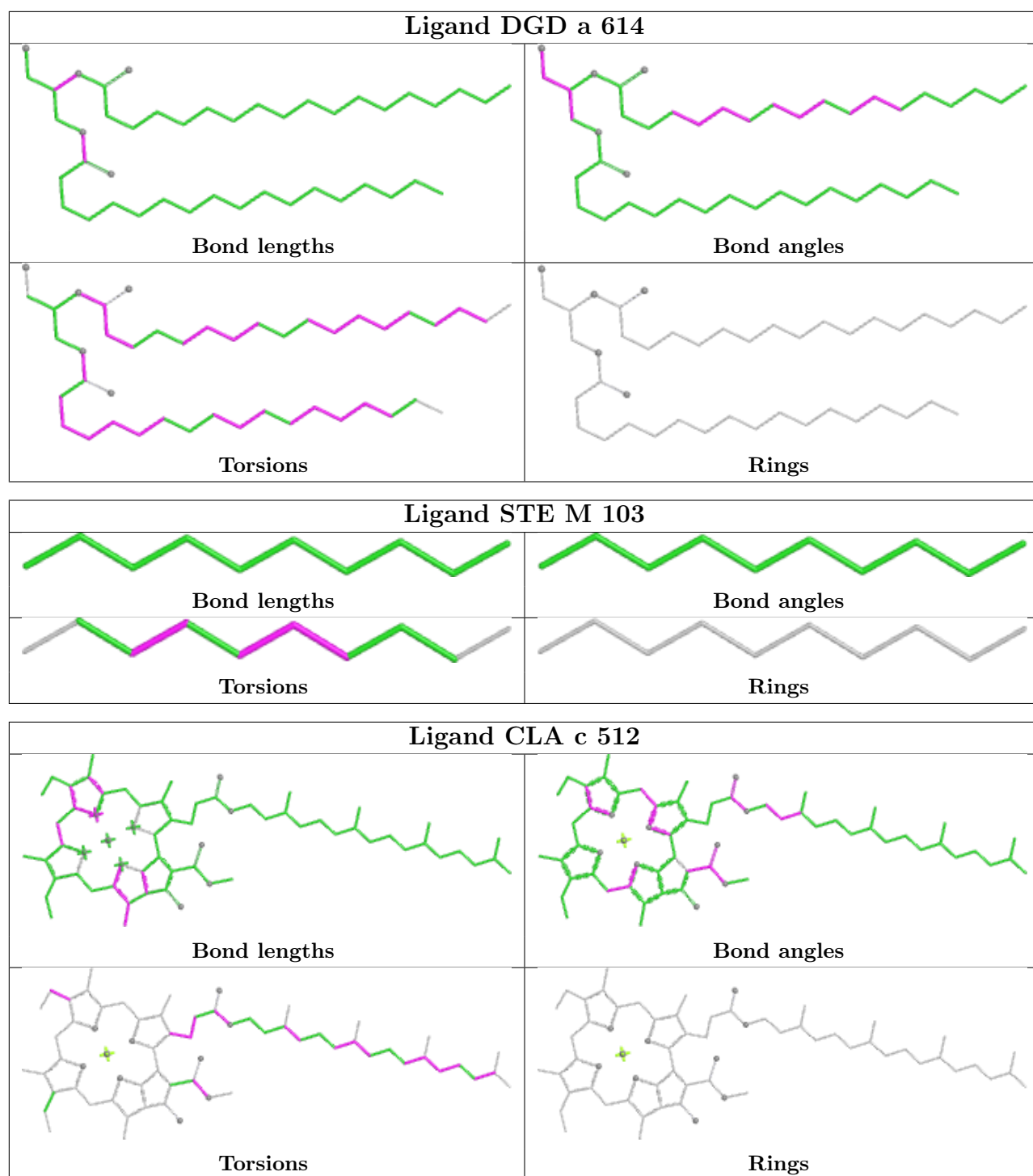
Ligand STE j 101

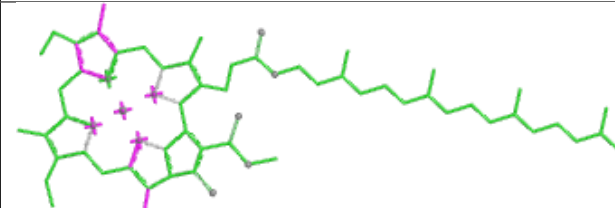
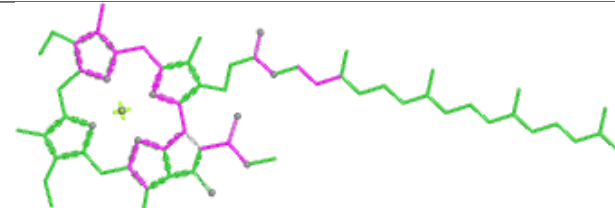
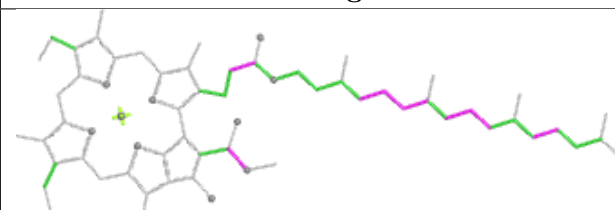
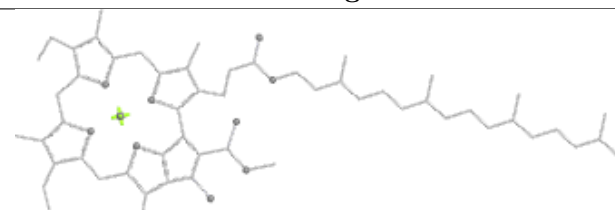


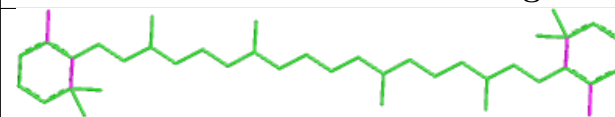
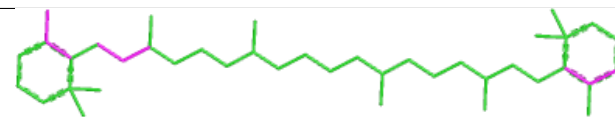
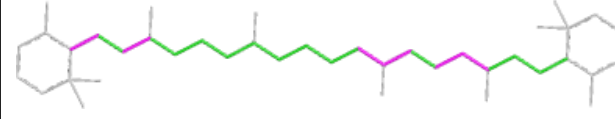
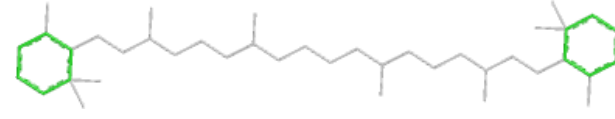


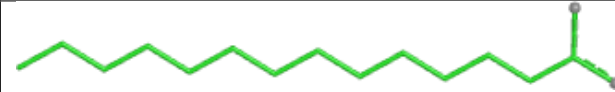
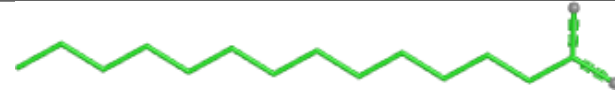
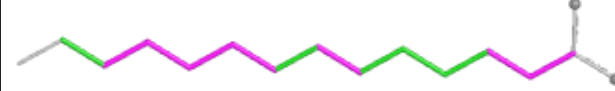
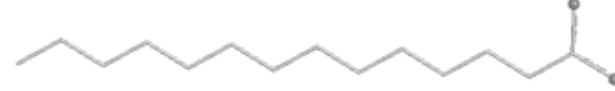


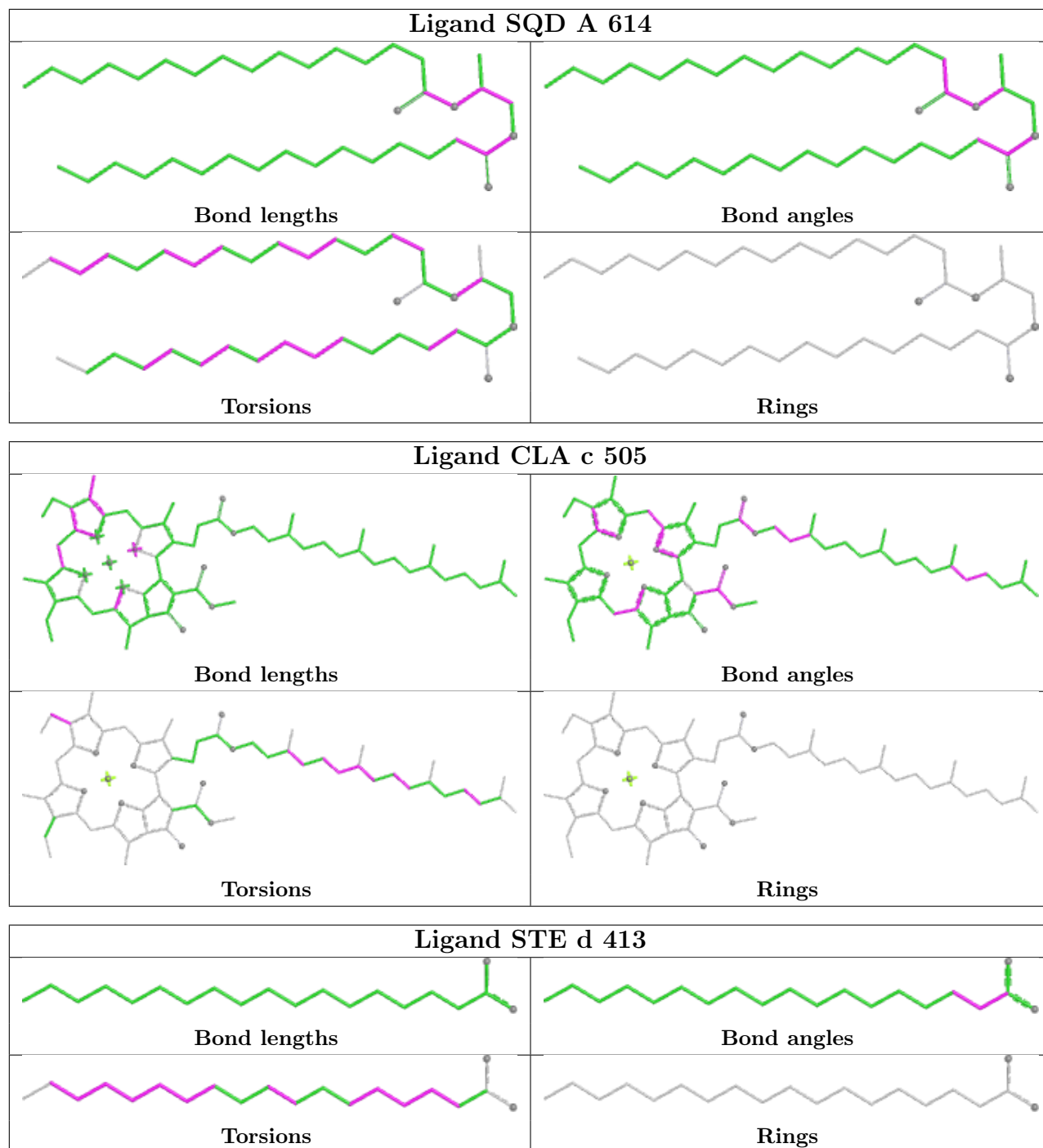


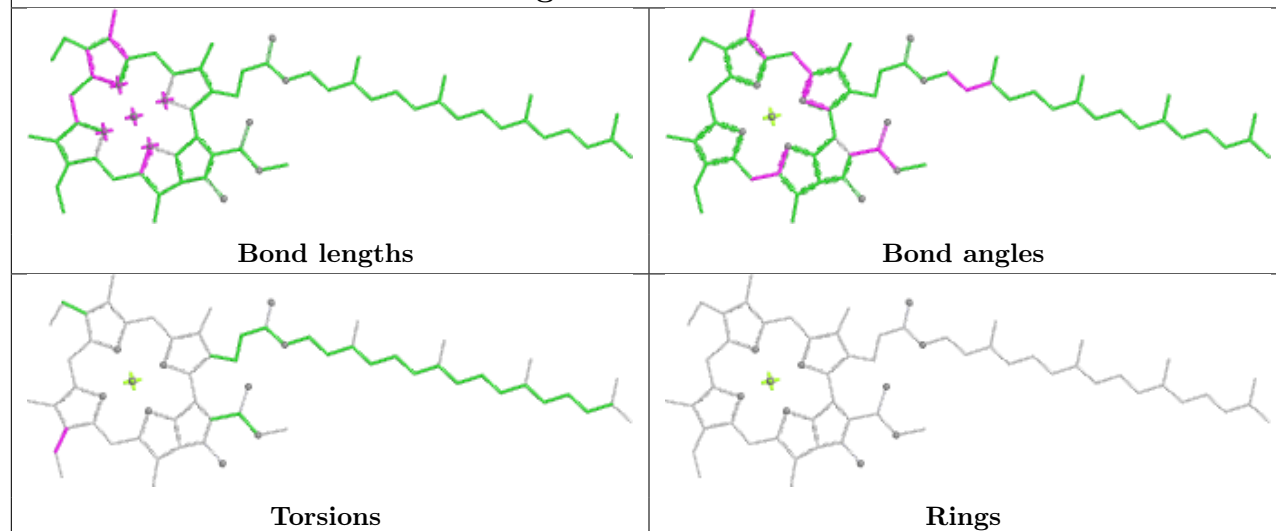
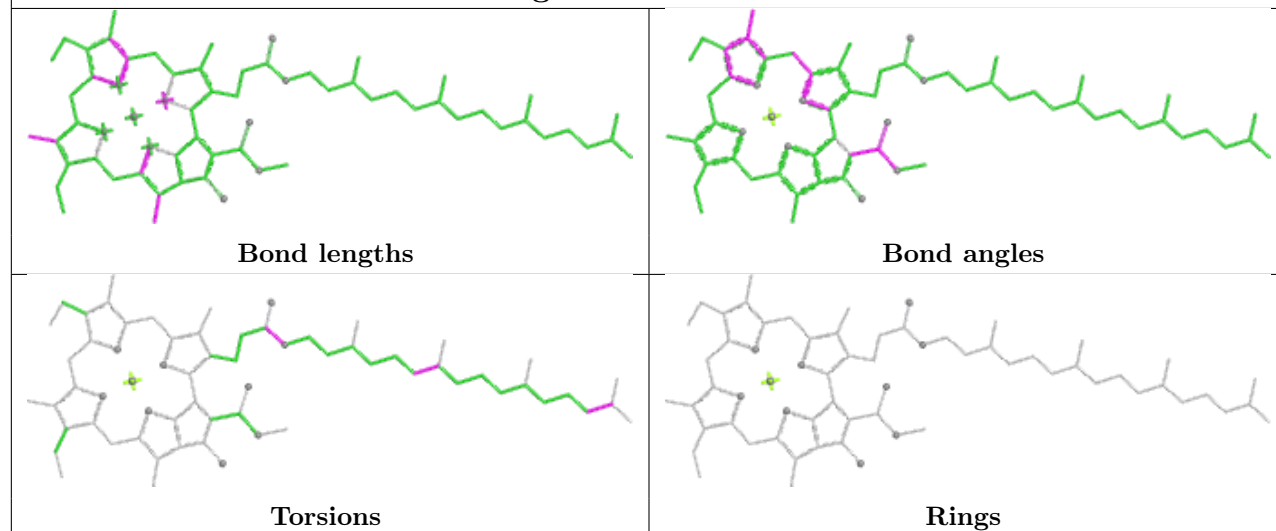
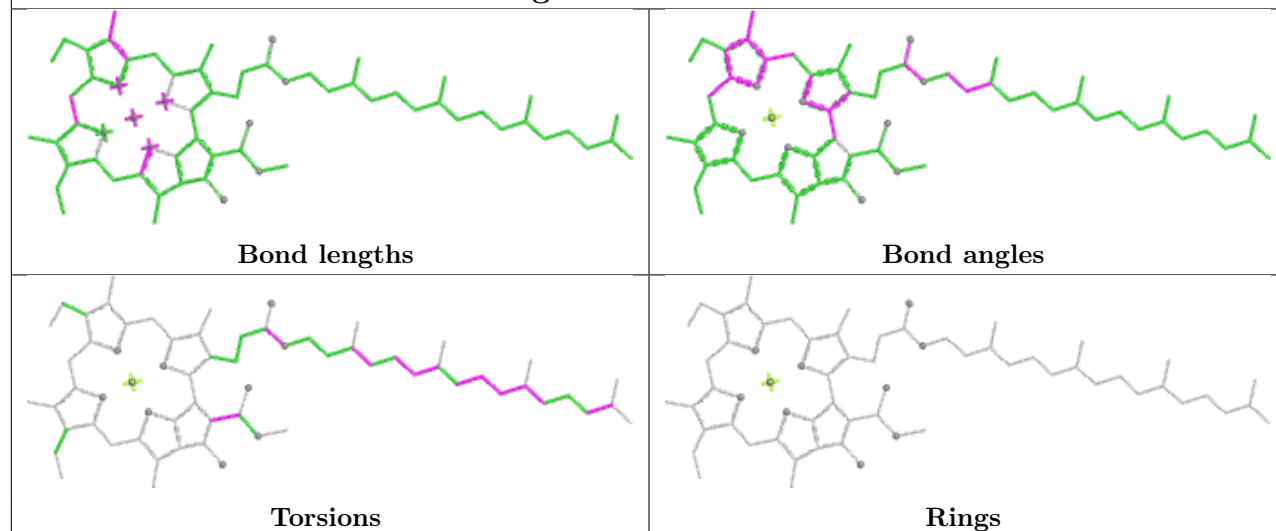


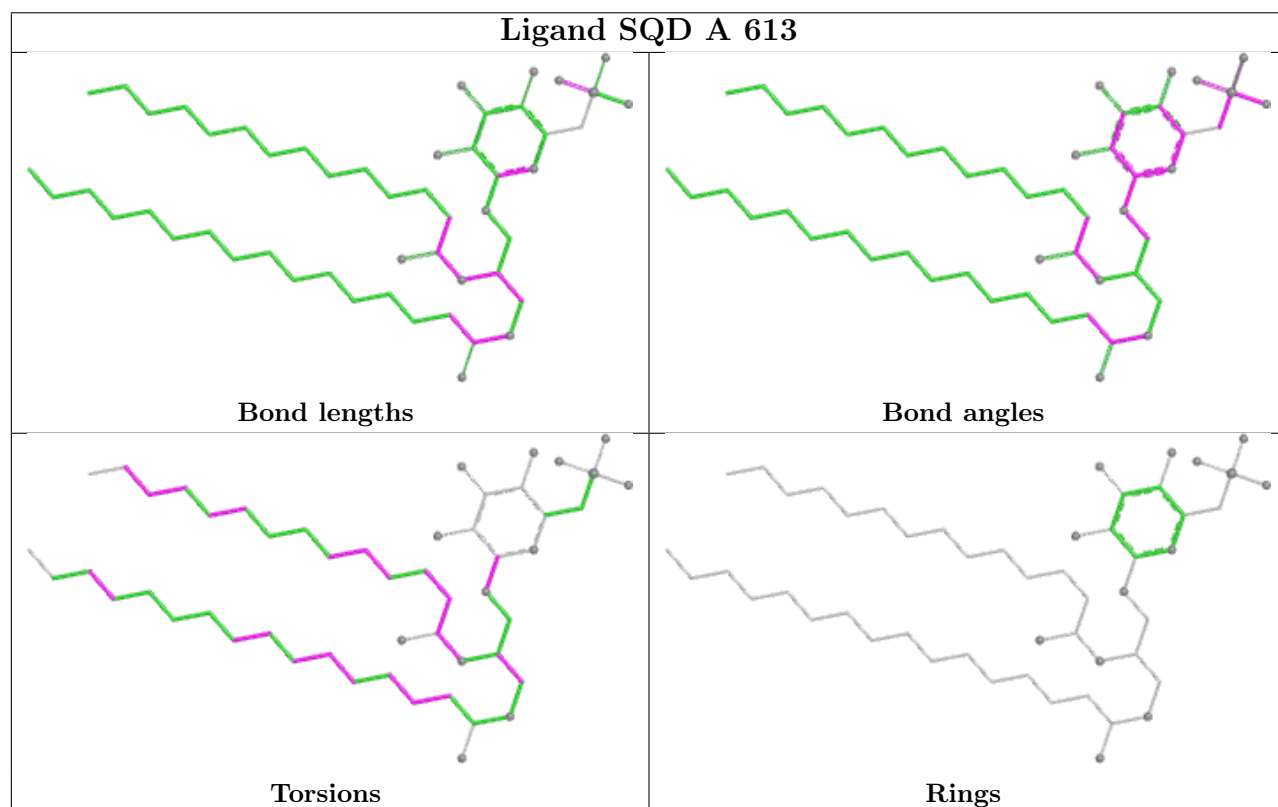
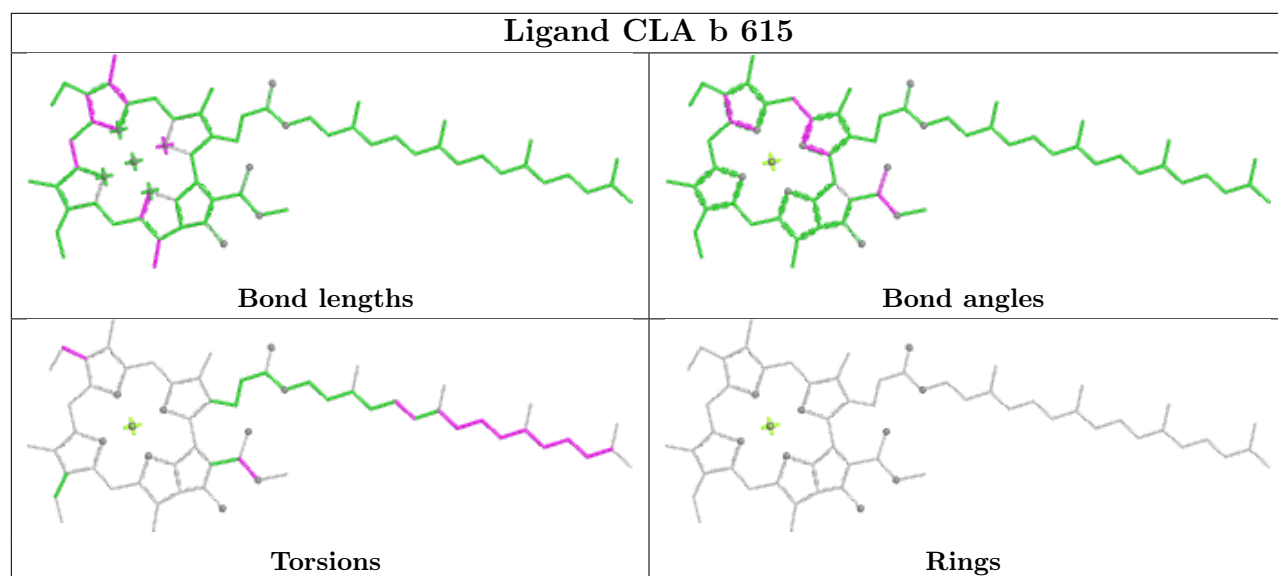
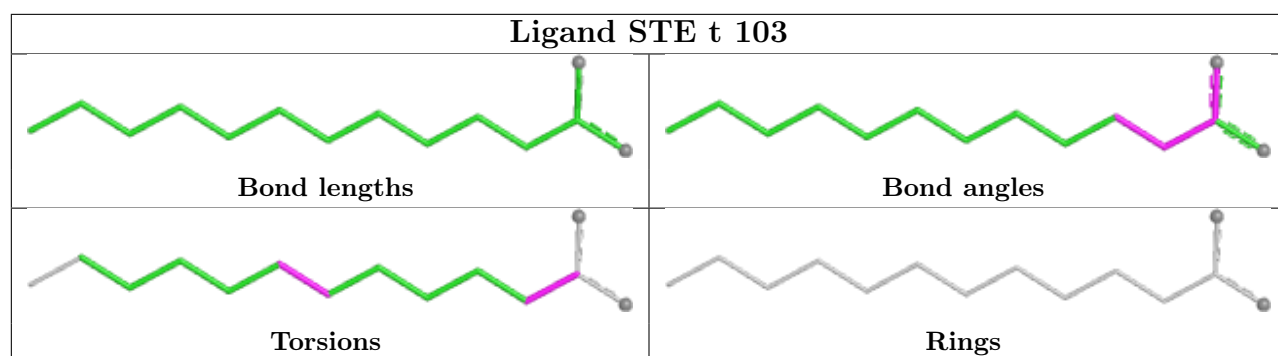
Ligand CLA b 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

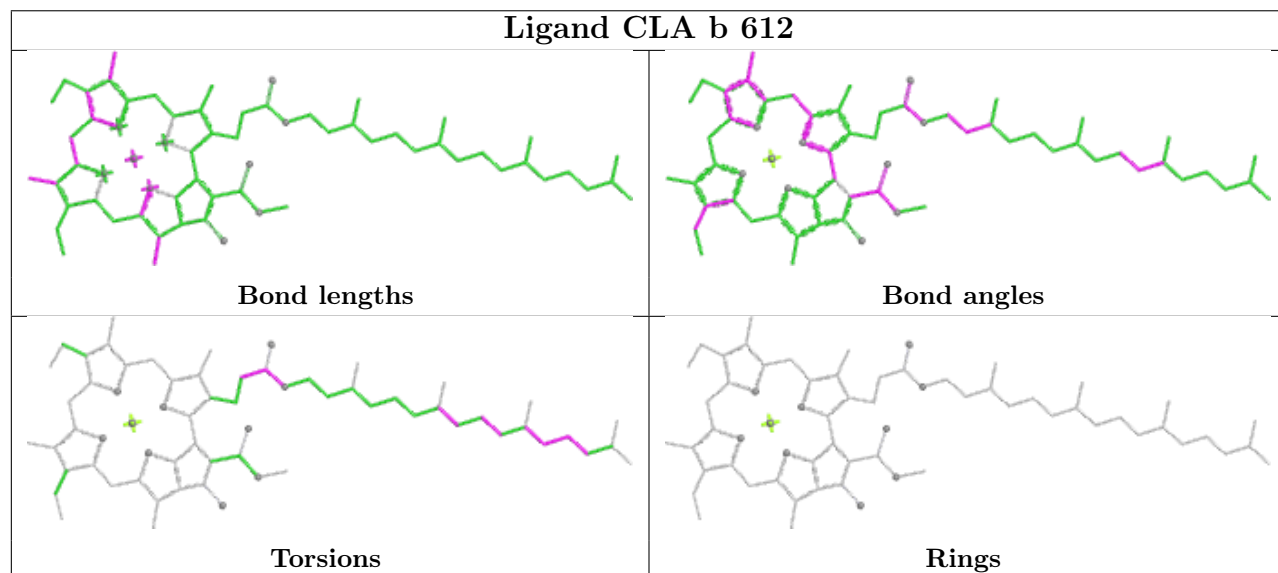
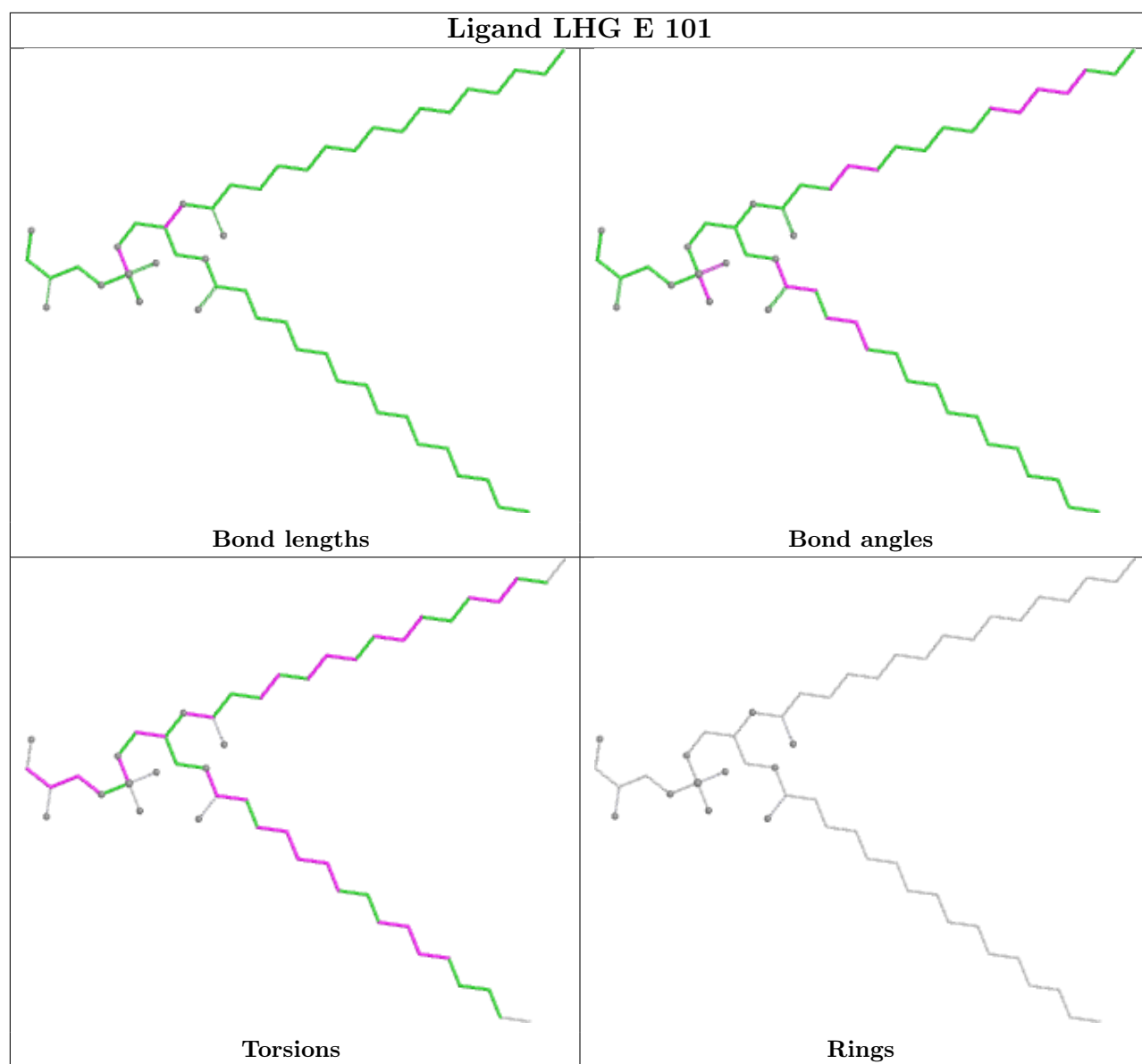
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

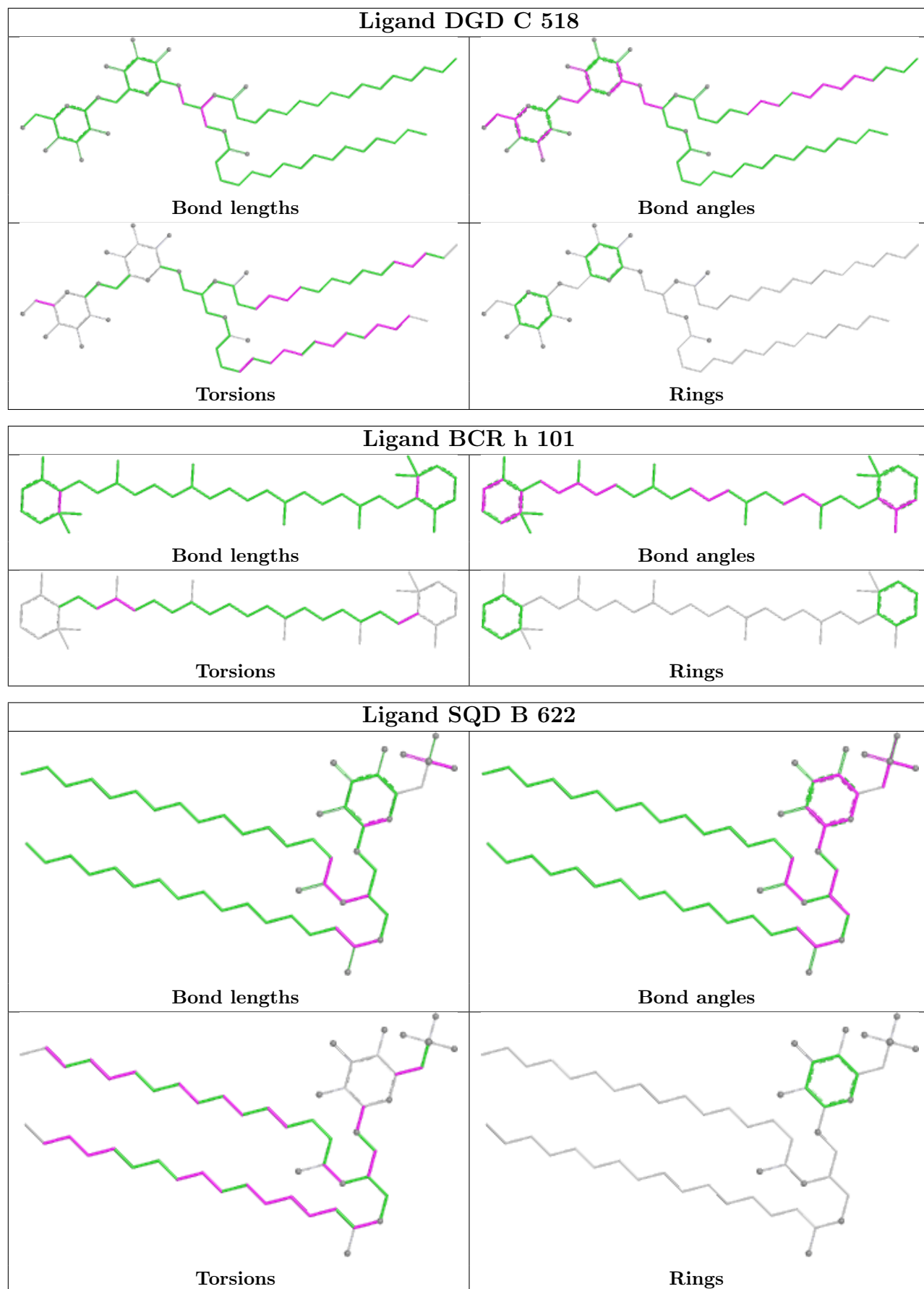
Ligand STE b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

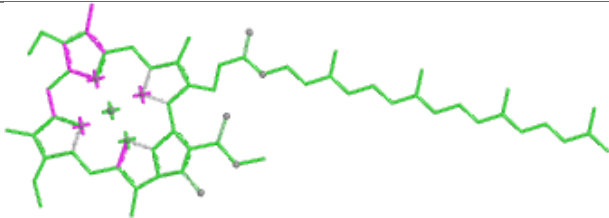
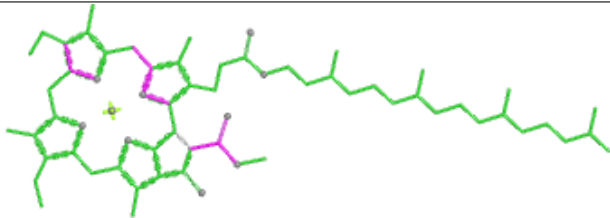
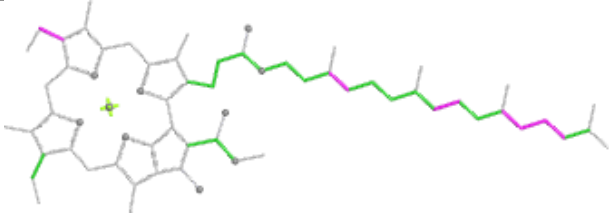
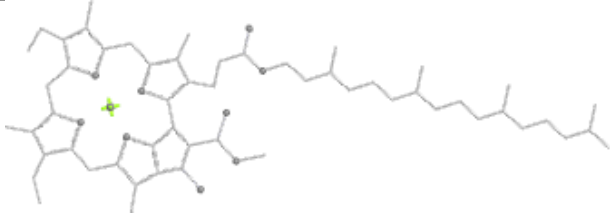


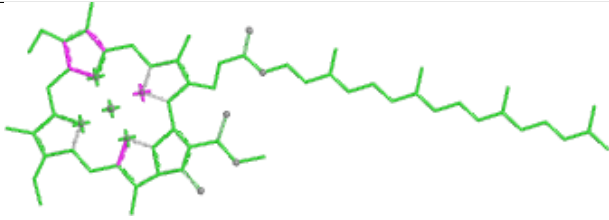
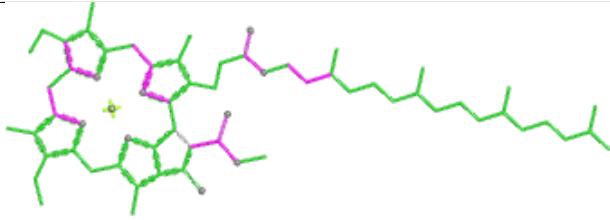
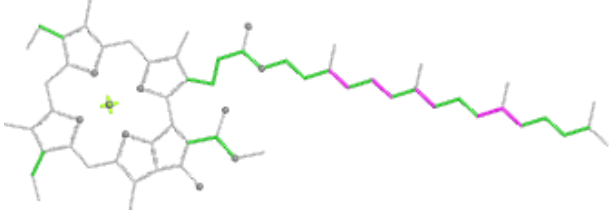
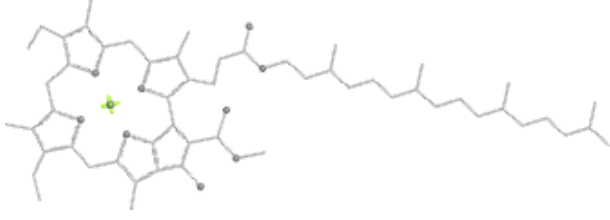
Ligand CLA a 612**Ligand CLA B 608****Ligand CLA B 607**

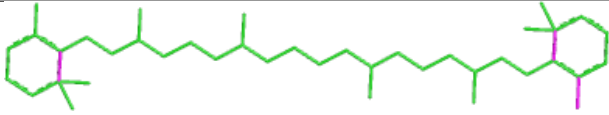
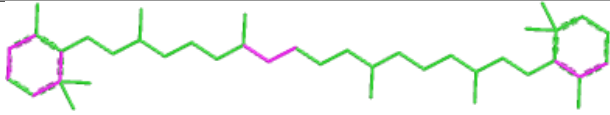
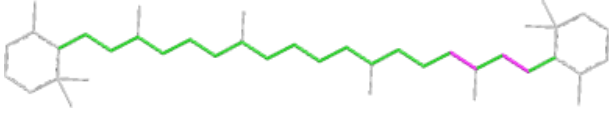
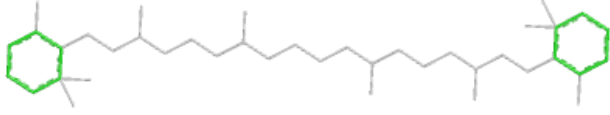


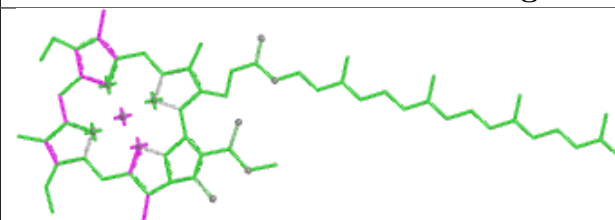
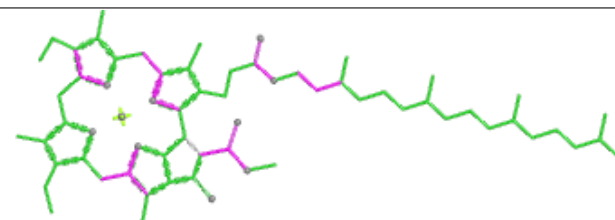
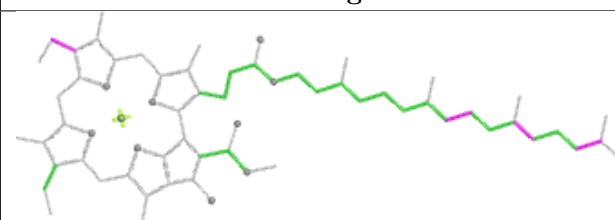
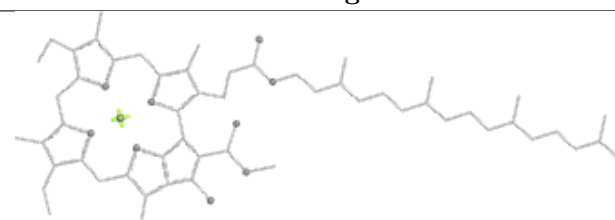


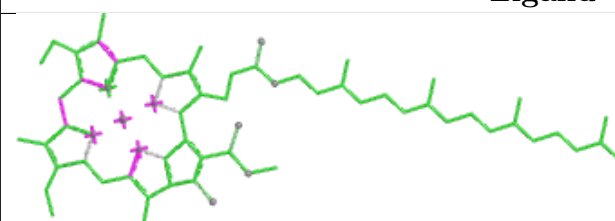
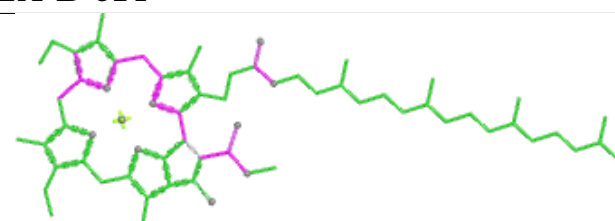
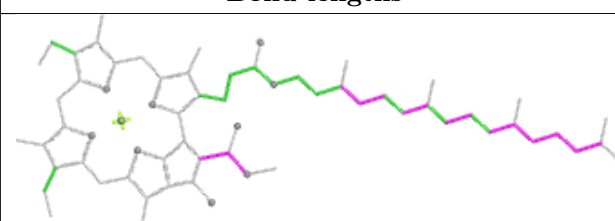
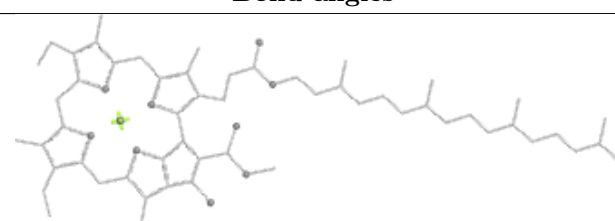


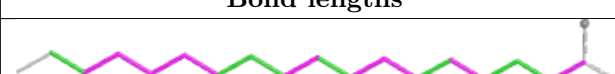
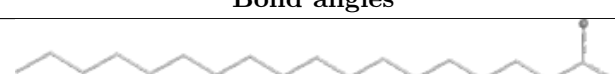
Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

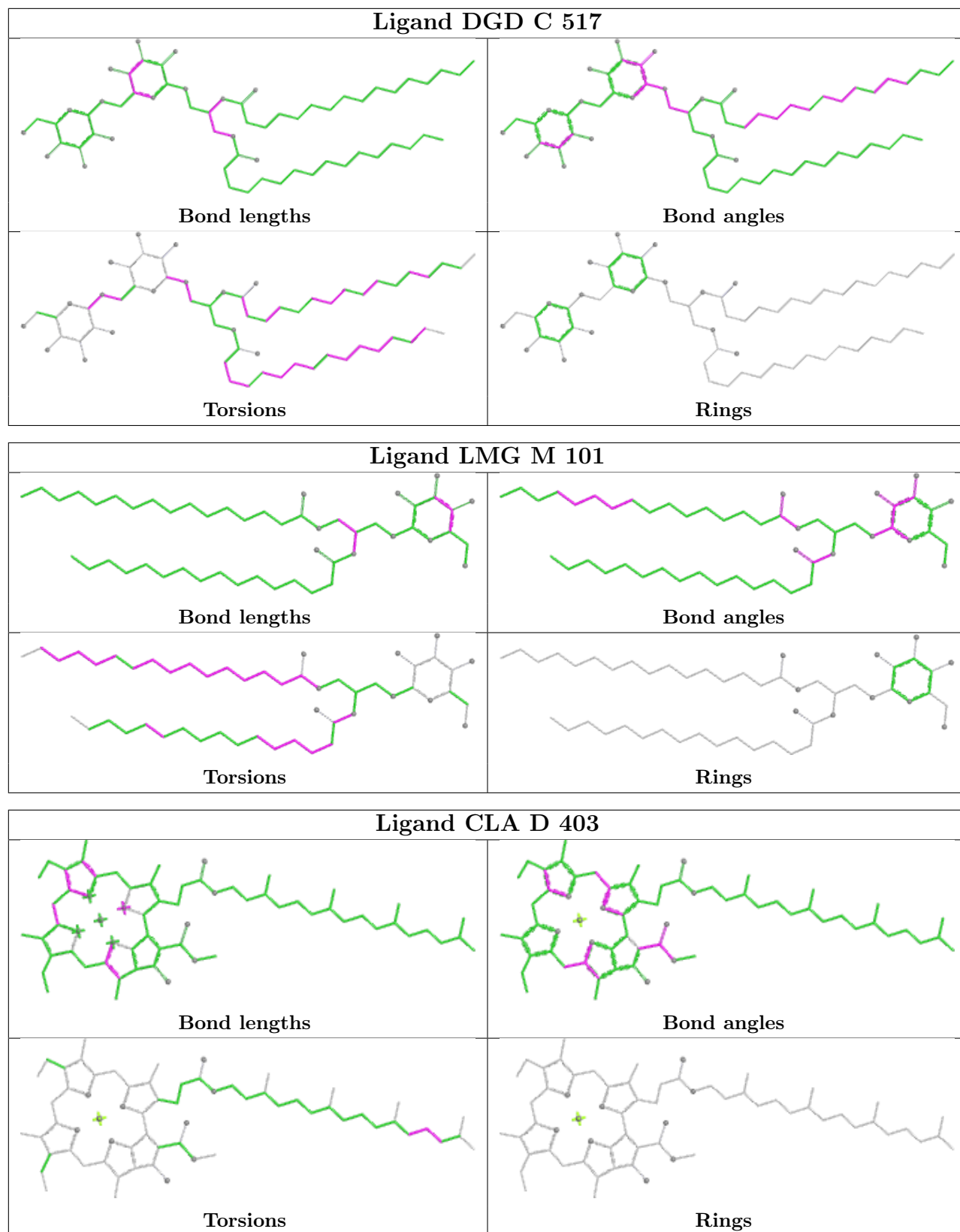
Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

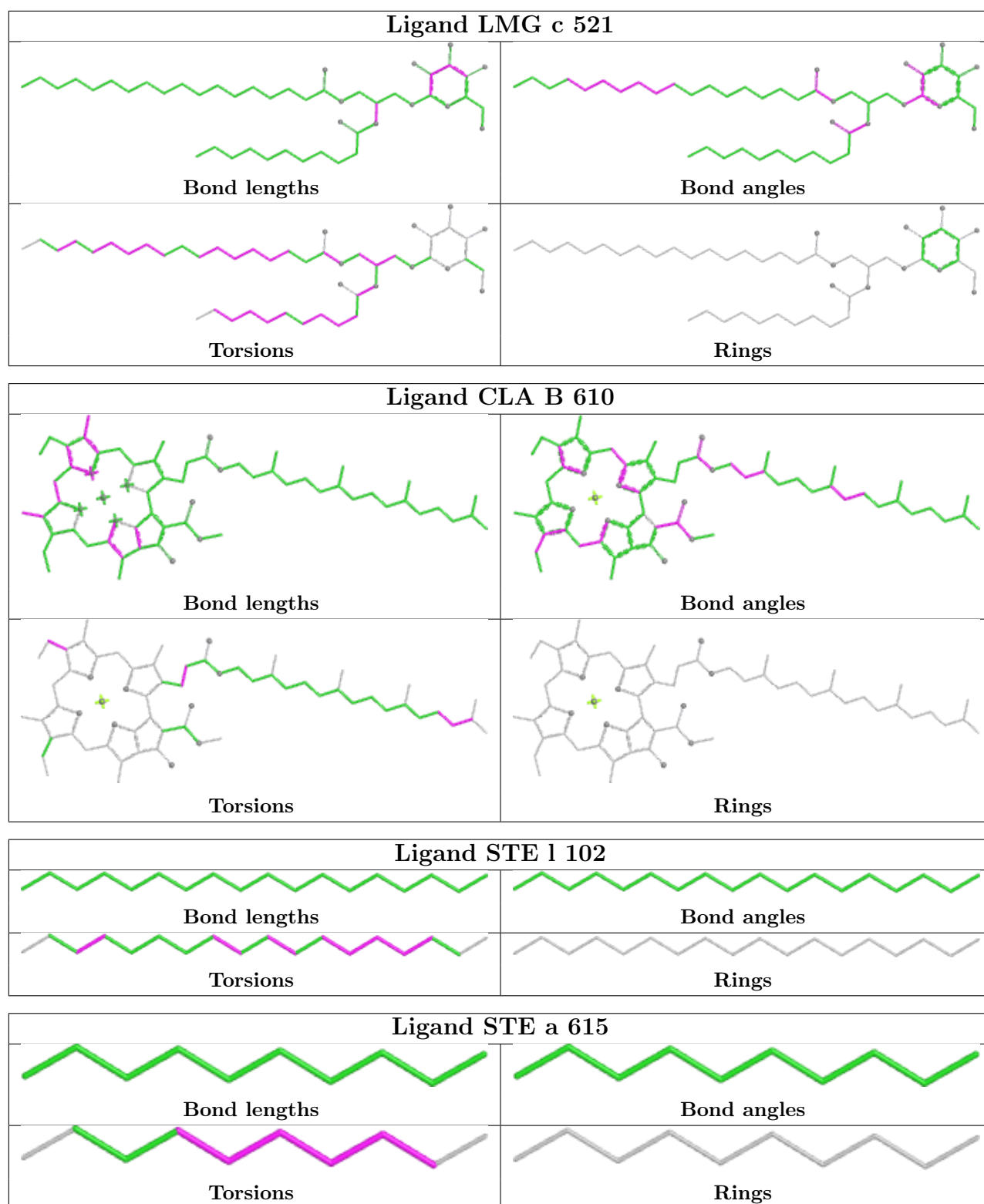
Ligand BCR a 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

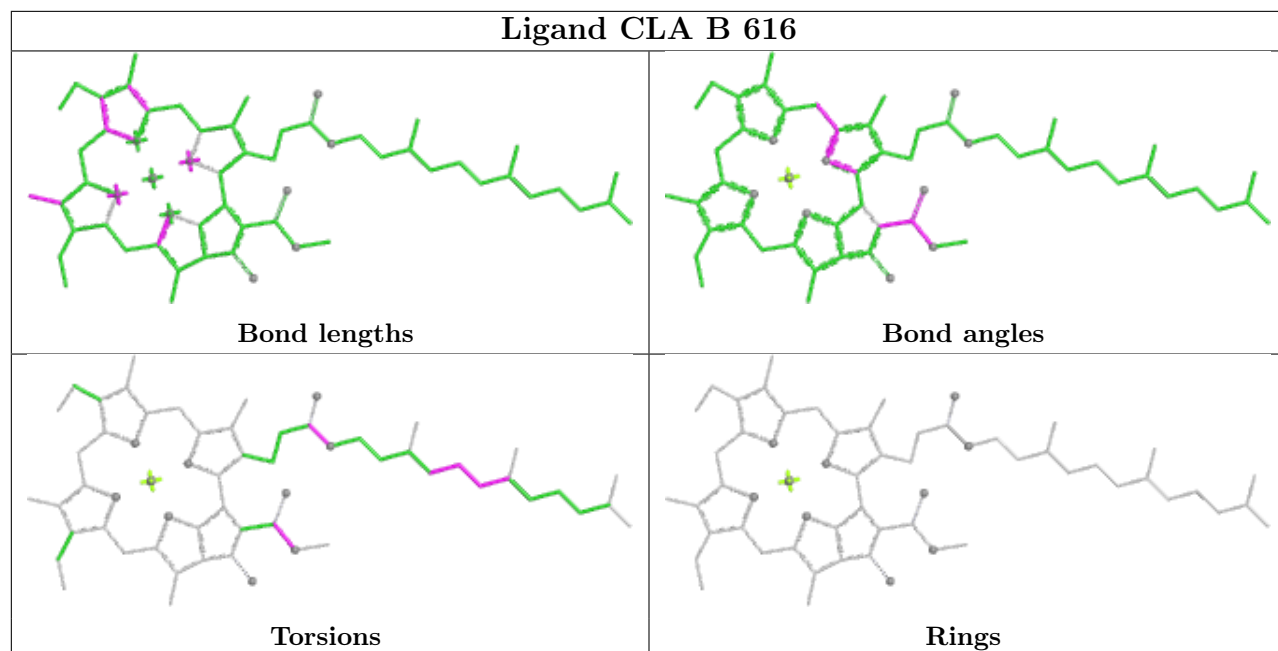
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

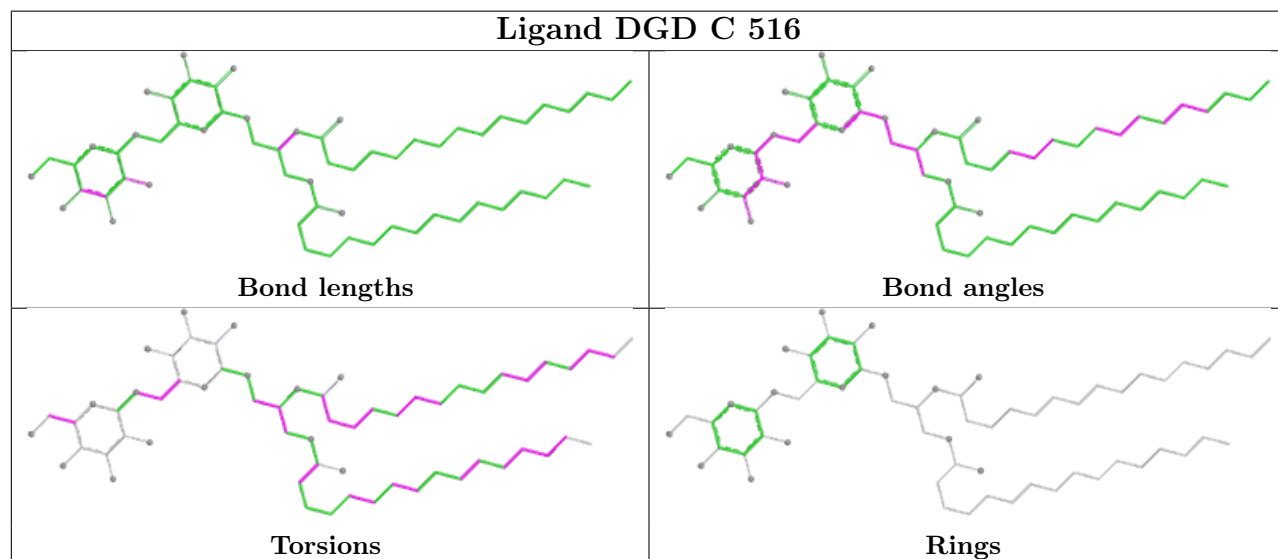




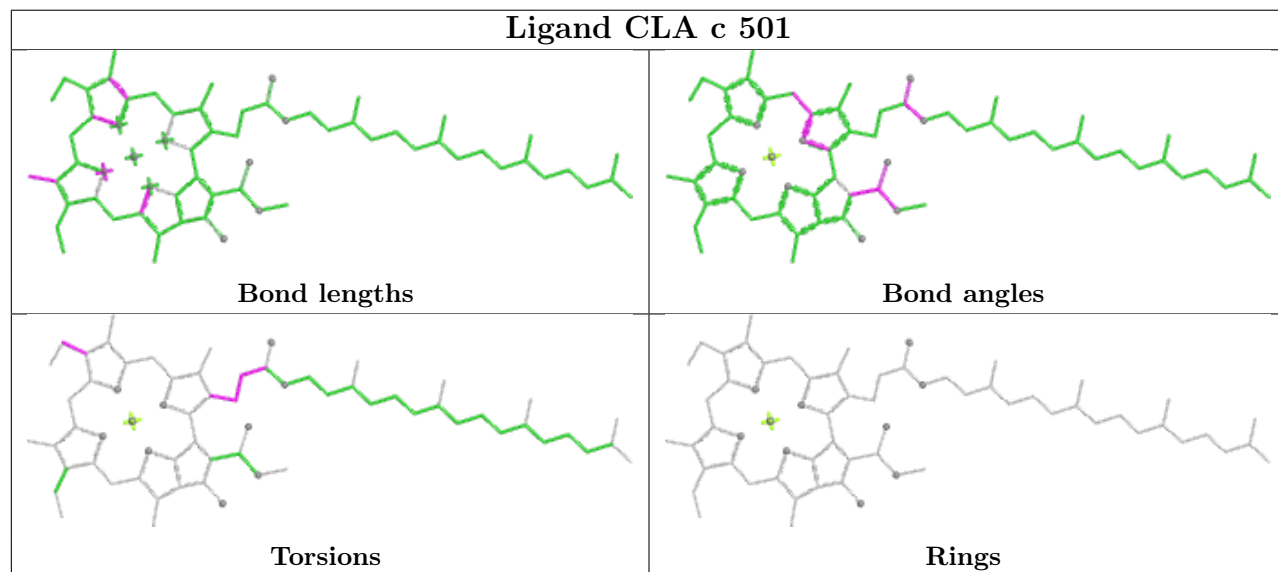
Ligand CLA B 616



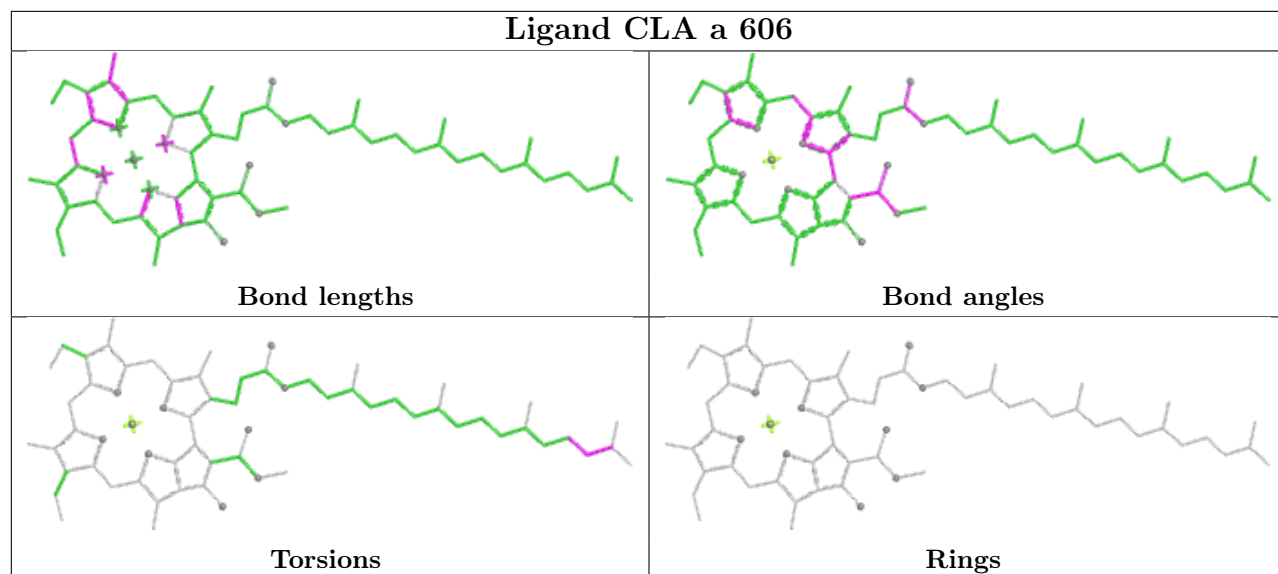
Ligand DGD C 516



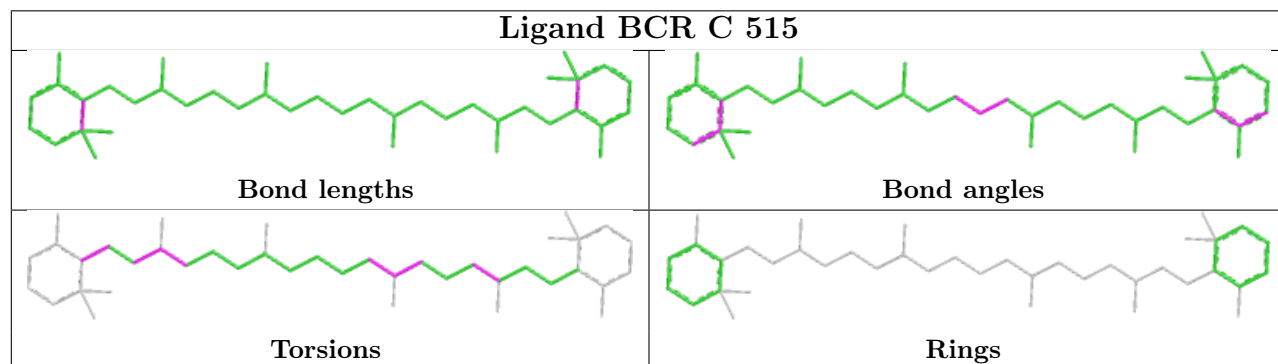
Ligand CLA c 501



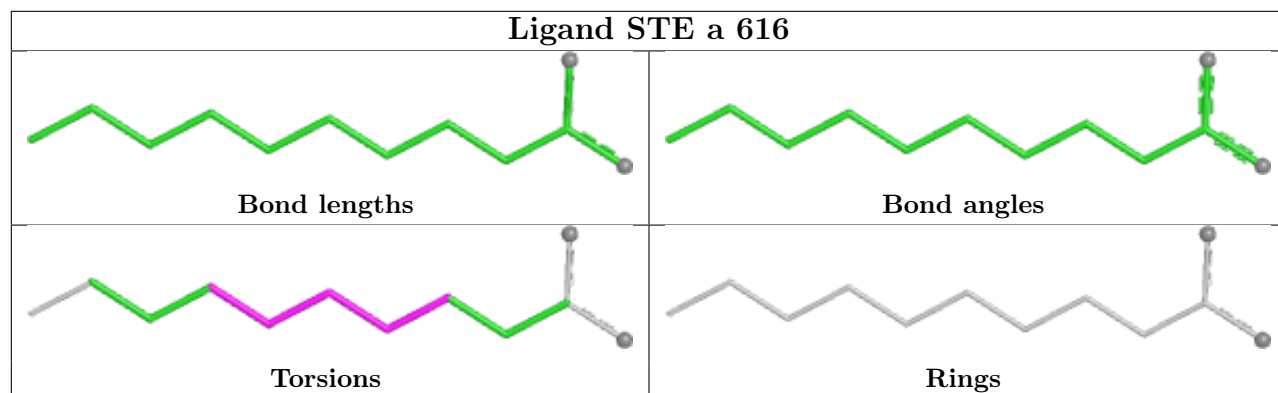
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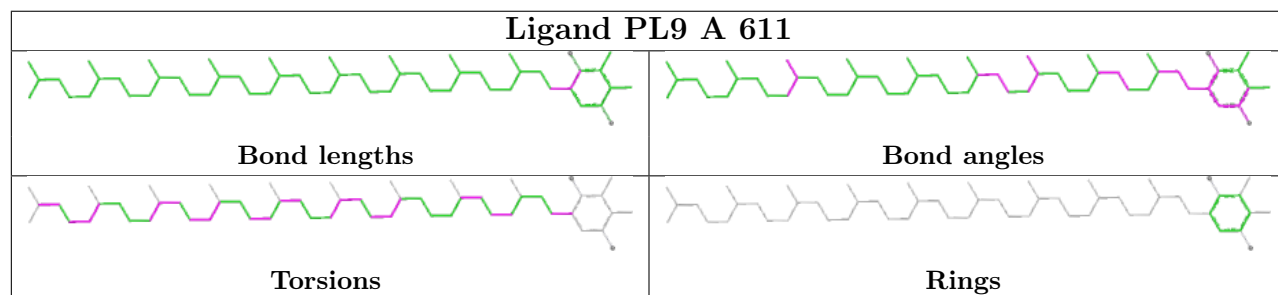
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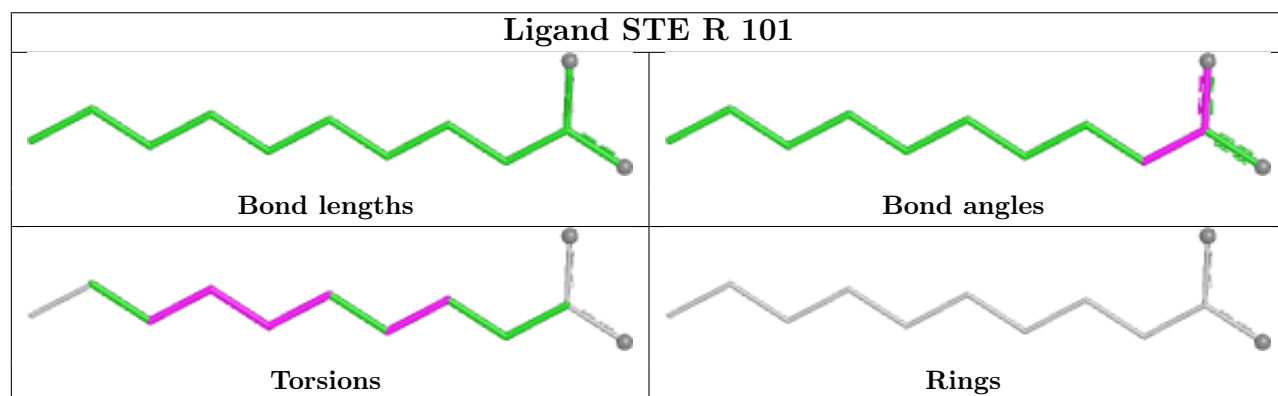
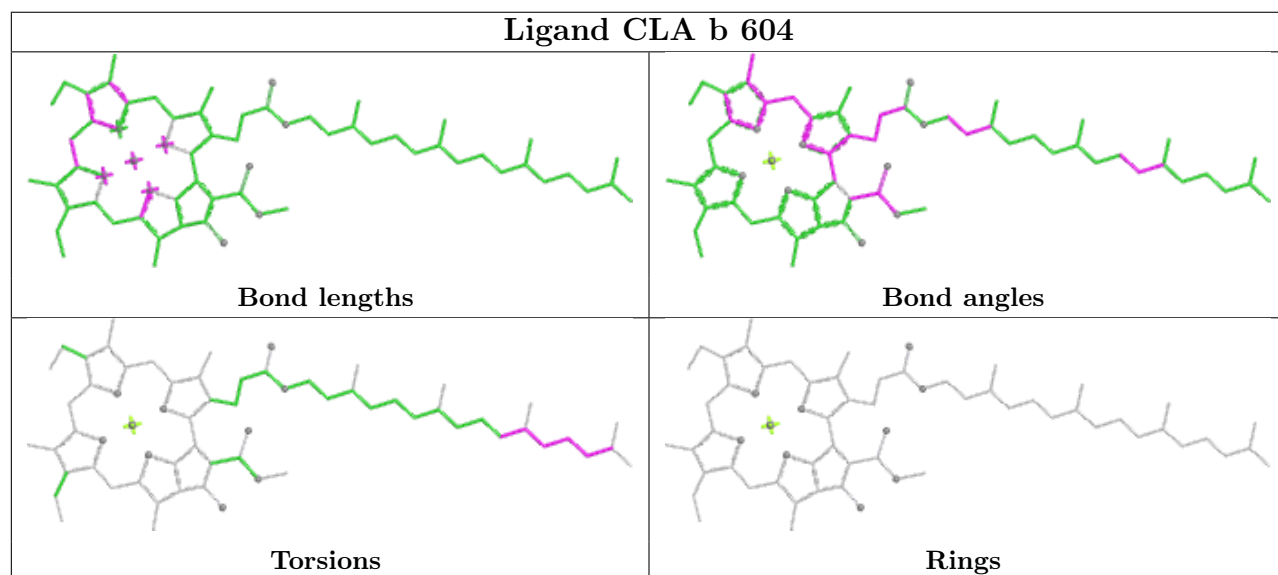
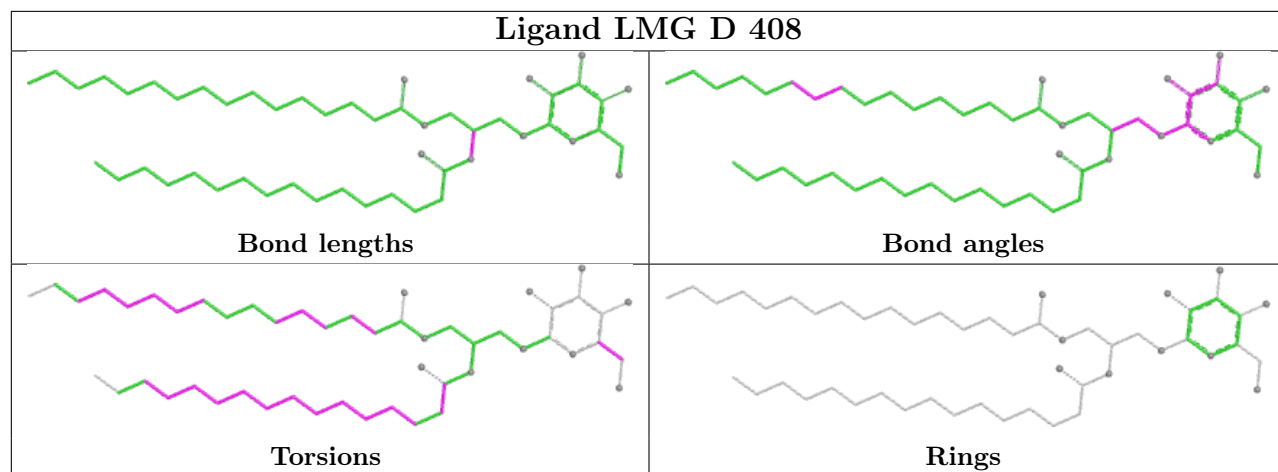


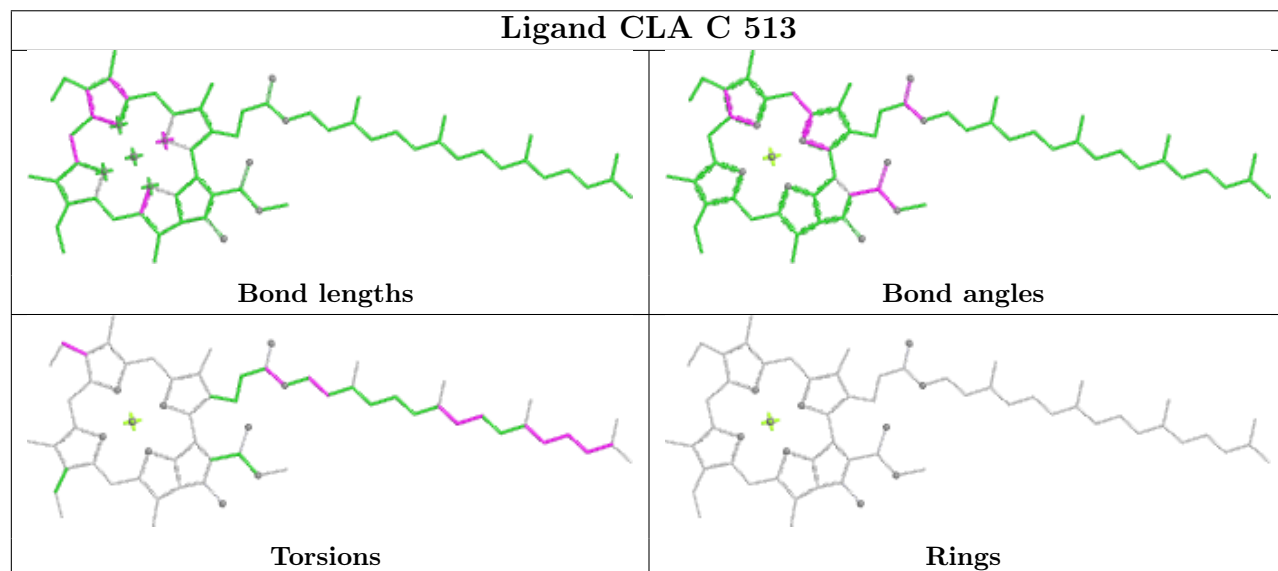
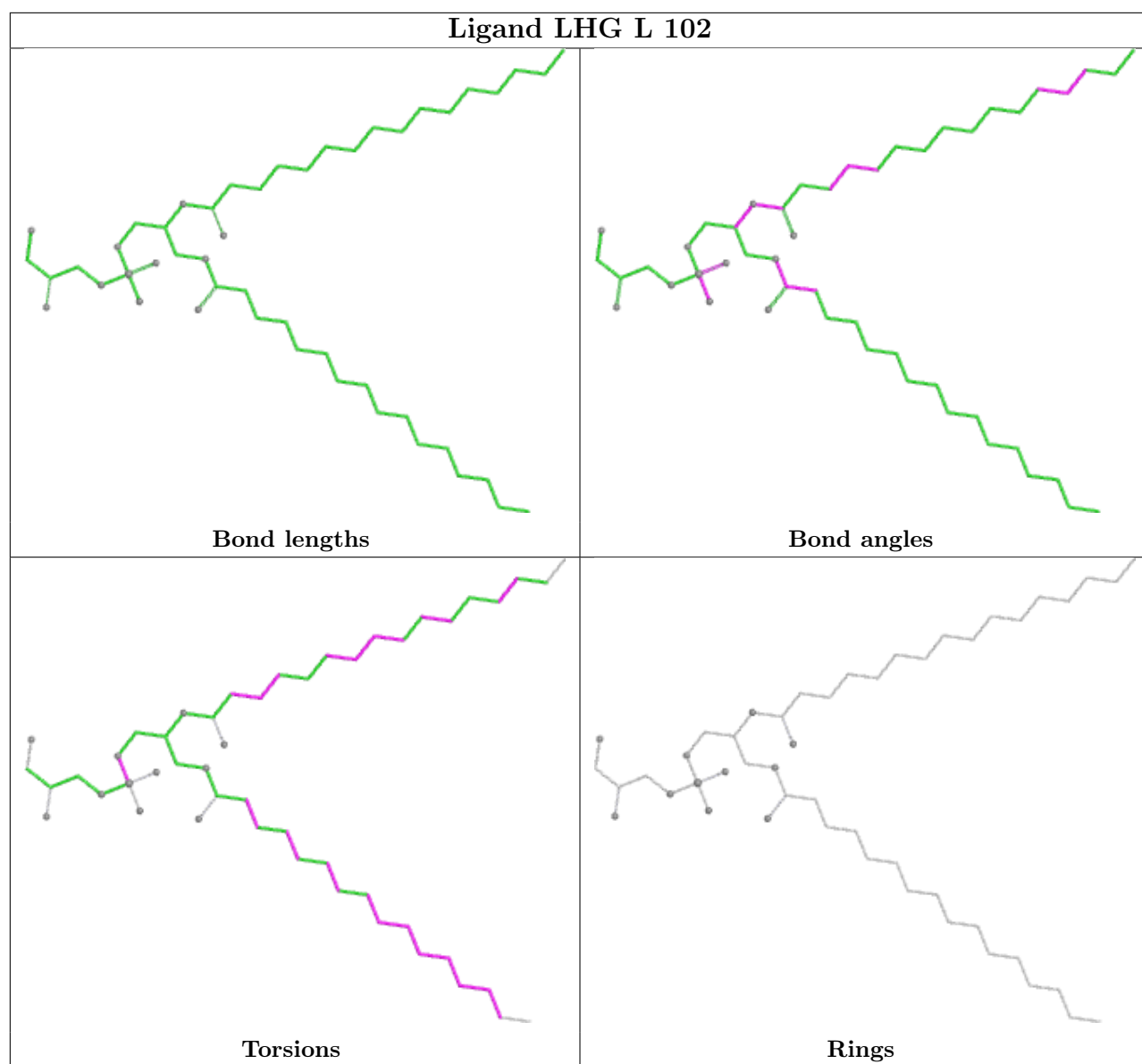
Ligand STE a 616



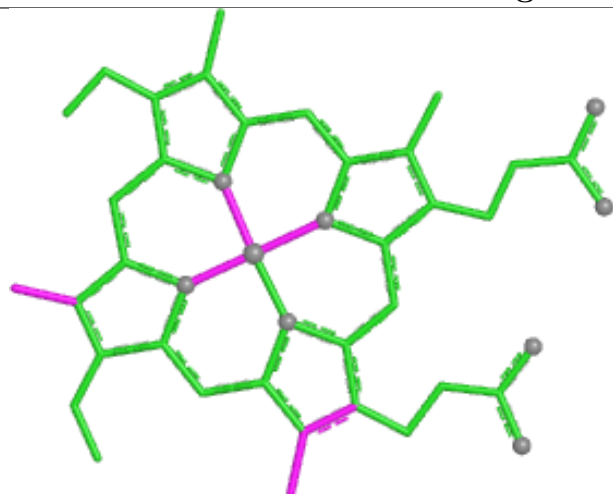
Ligand PL9 A 611



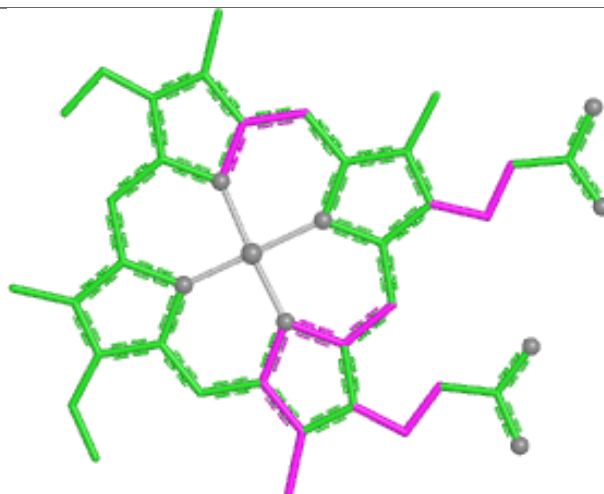




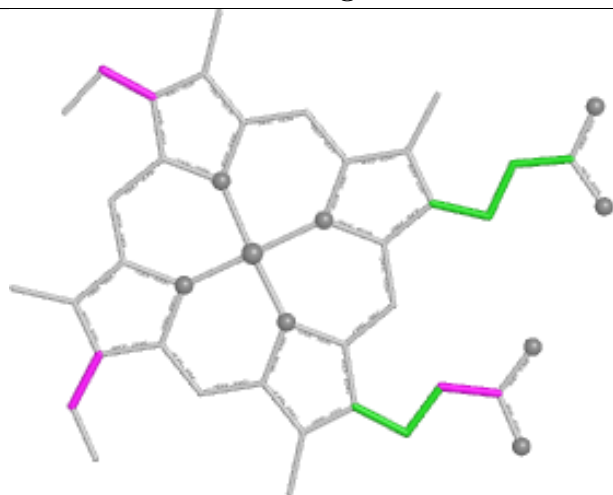
Ligand HEC v 201



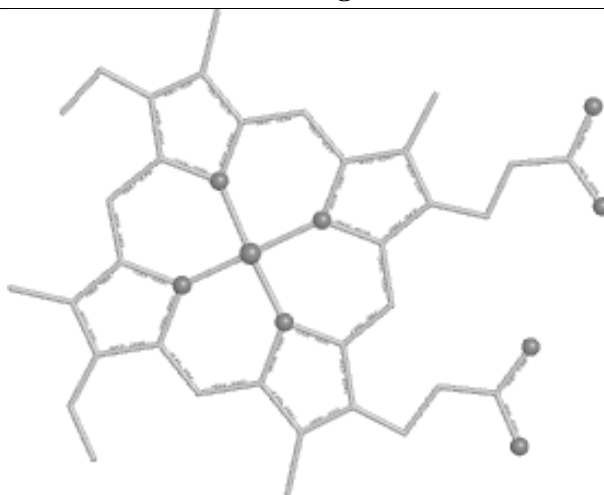
Bond lengths



Bond angles

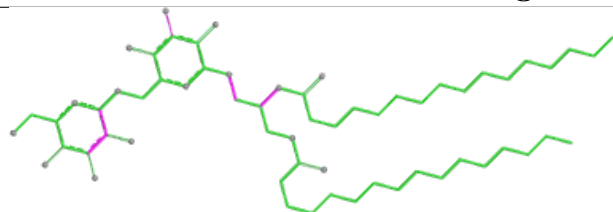


Torsions

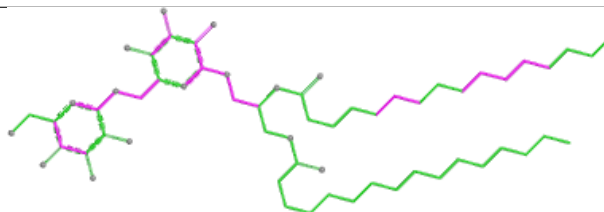


Rings

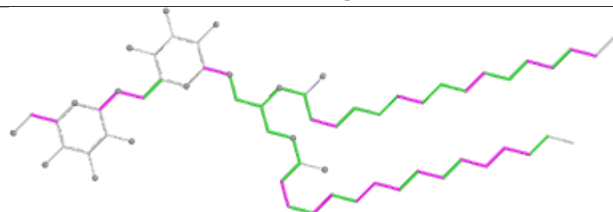
Ligand DGD c 517



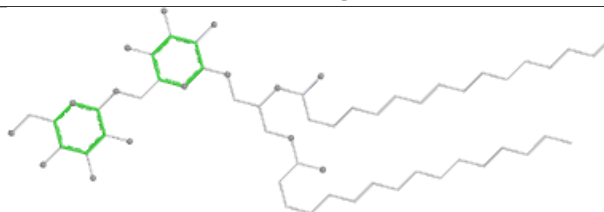
Bond lengths



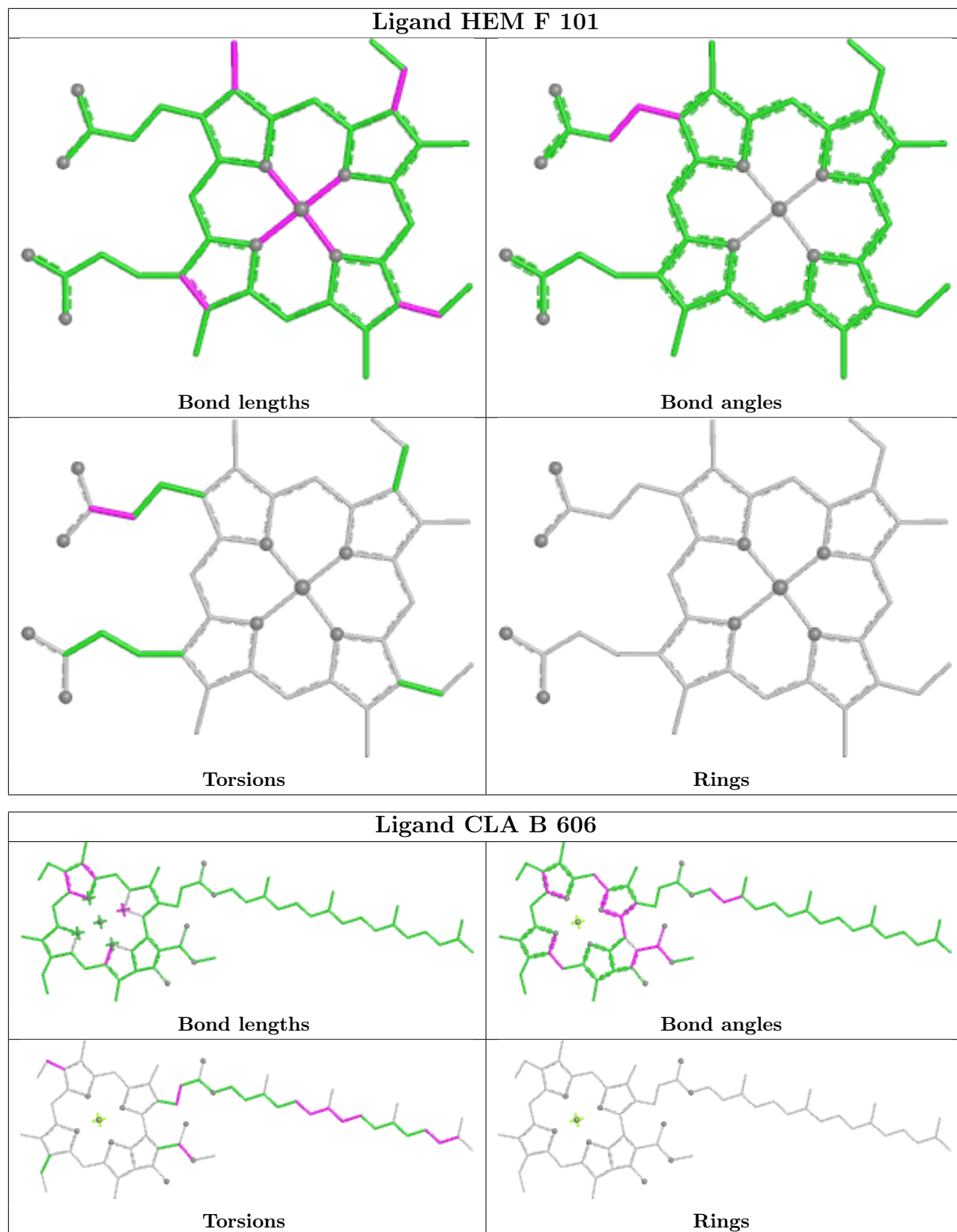
Bond angles



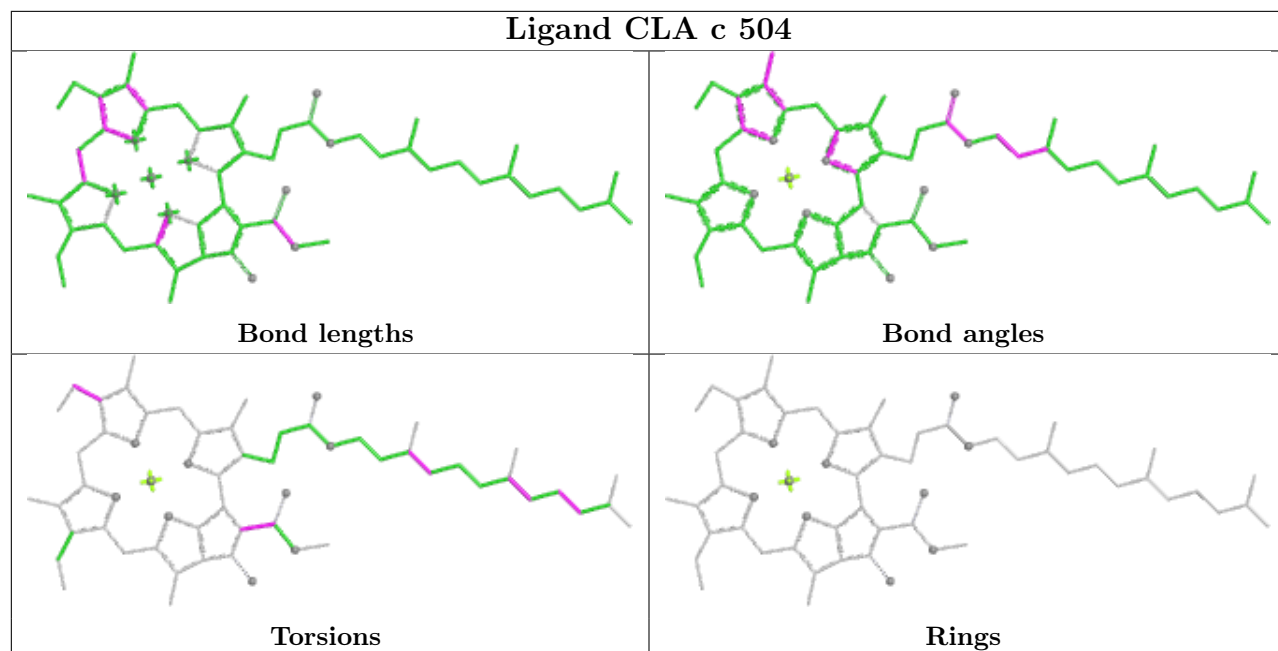
Torsions



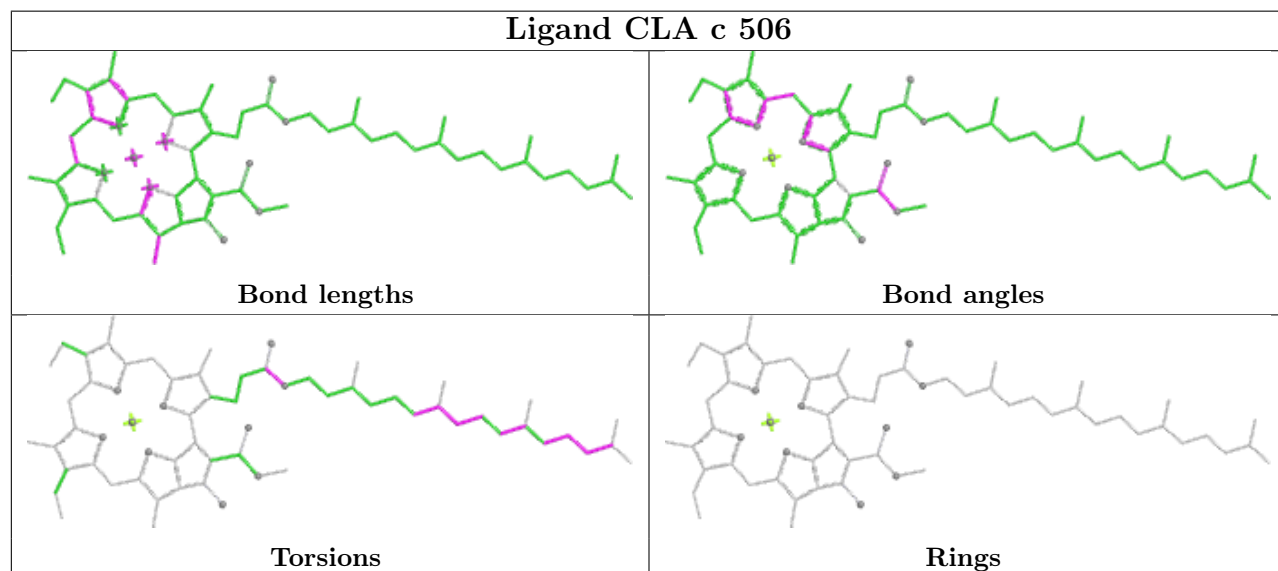
Rings



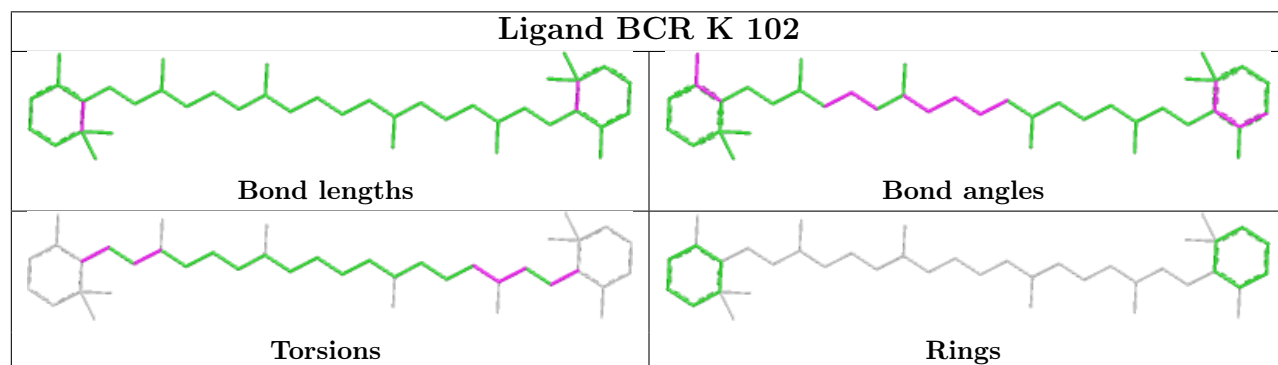
Ligand CLA c 504

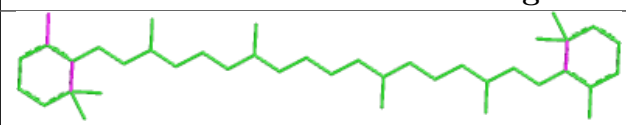
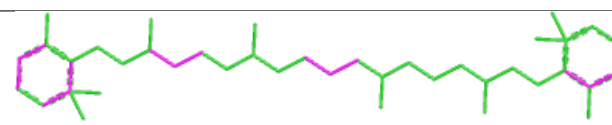
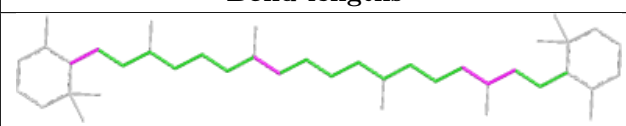
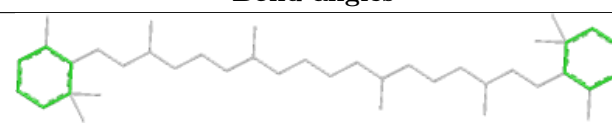


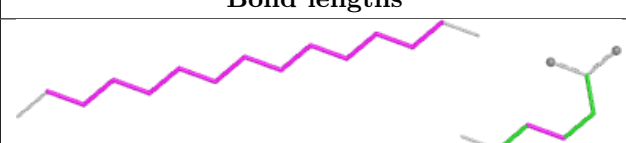
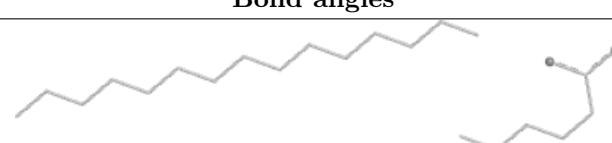
Ligand CLA c 506

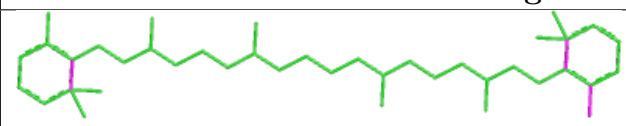
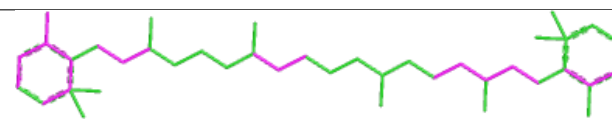
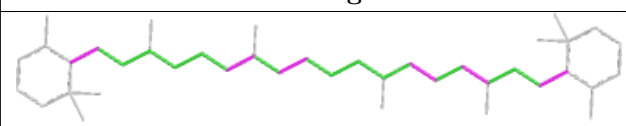
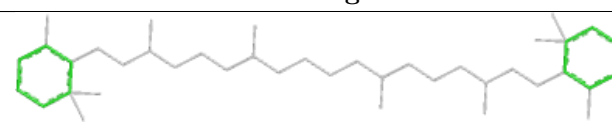


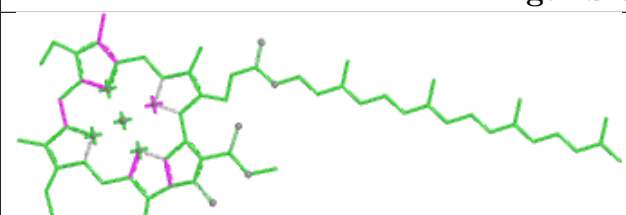
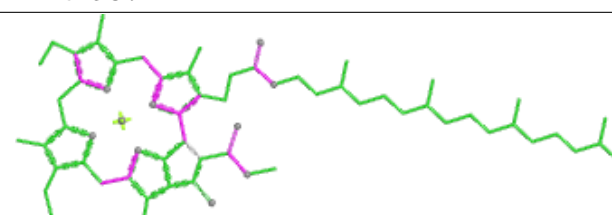
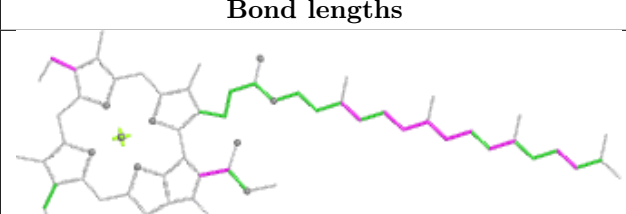
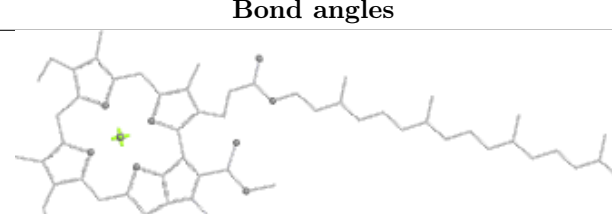
Ligand BCR K 102

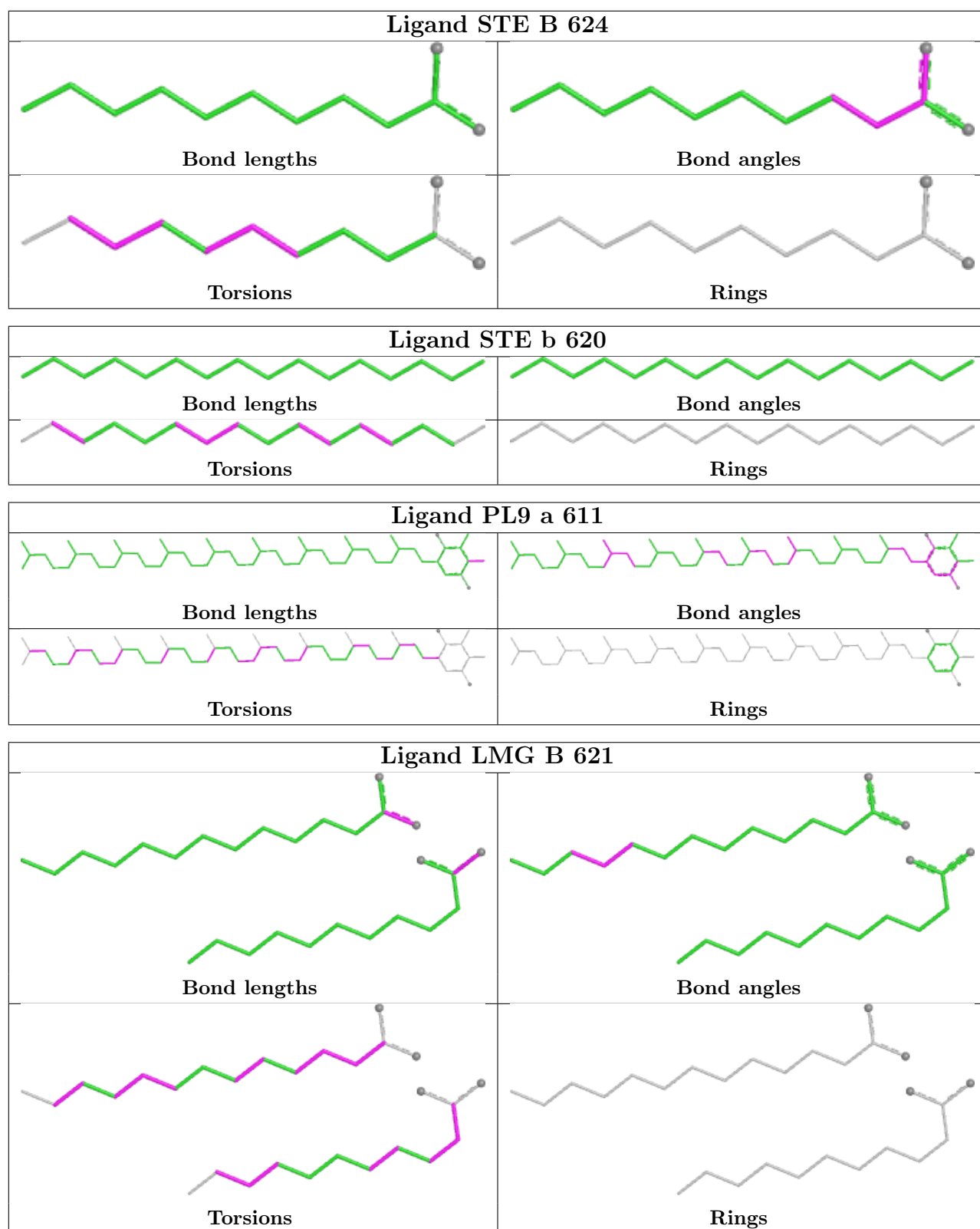


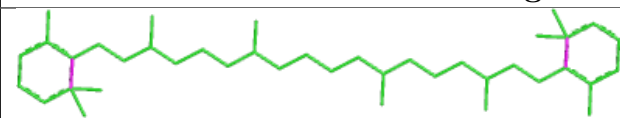
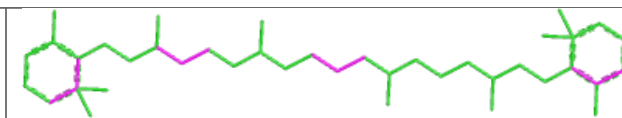
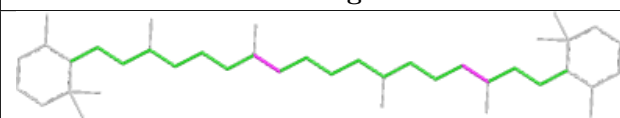
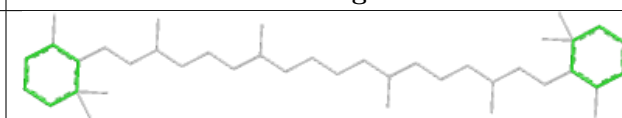
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

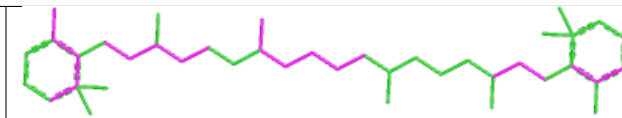
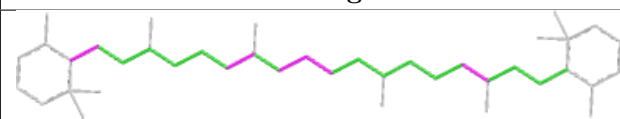
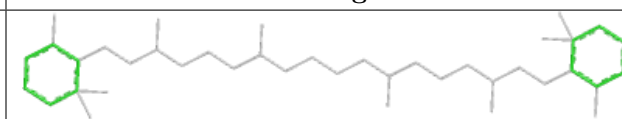
Ligand LMG d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

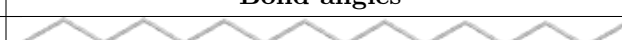
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

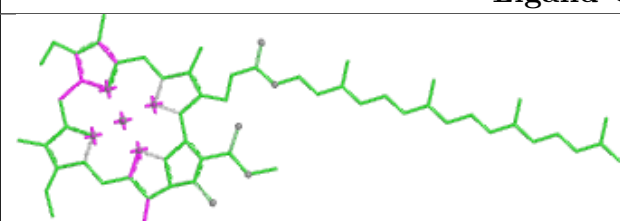
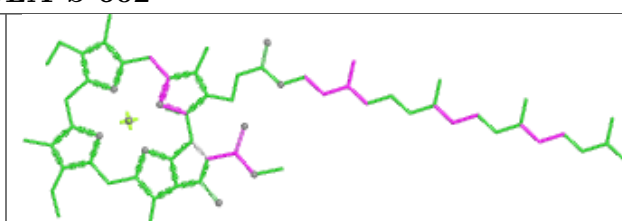
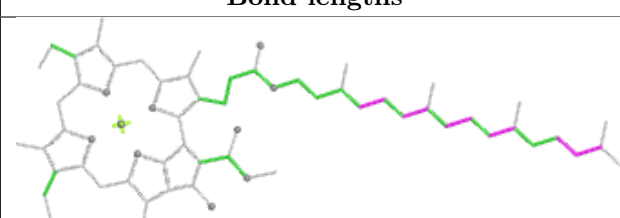
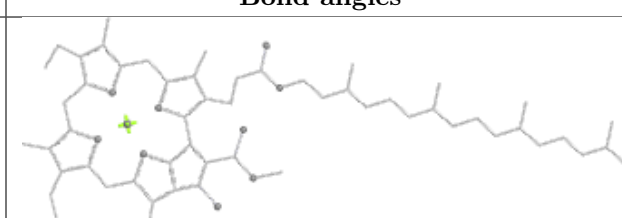
Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

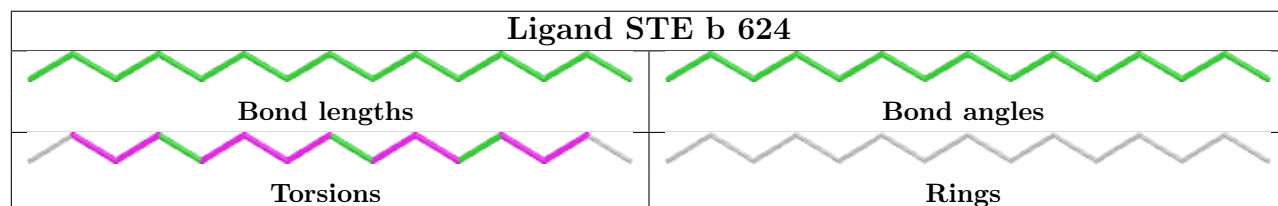
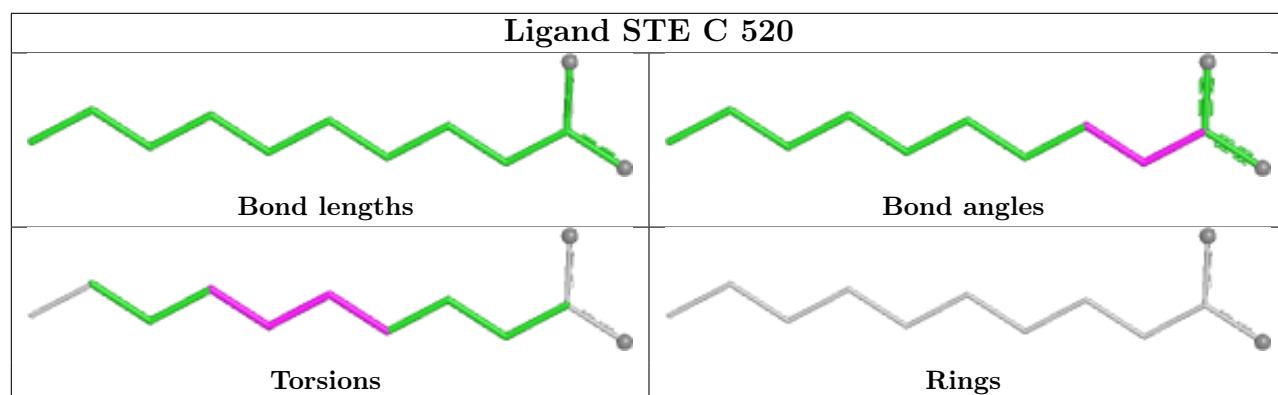
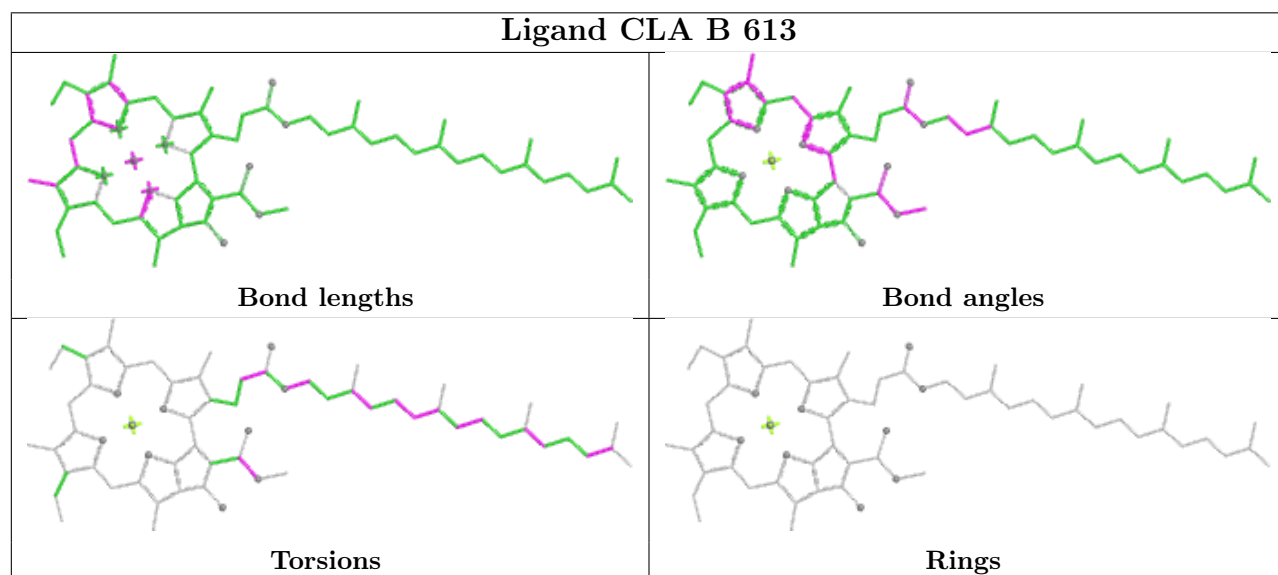
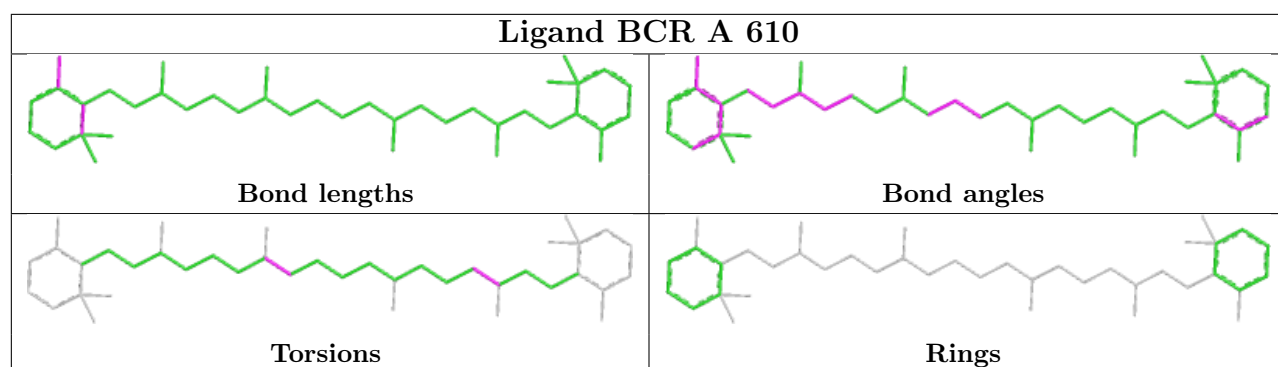


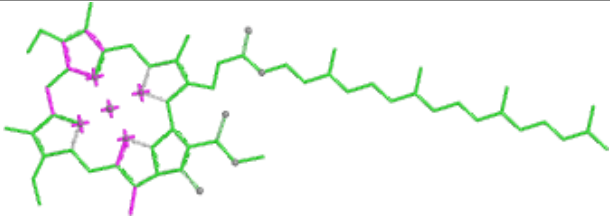
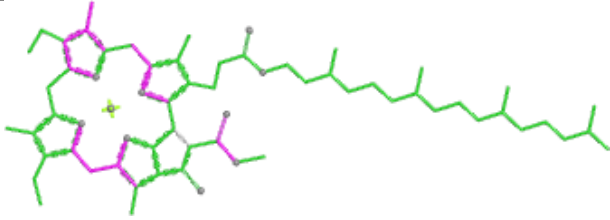
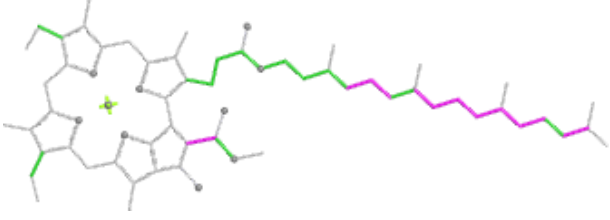
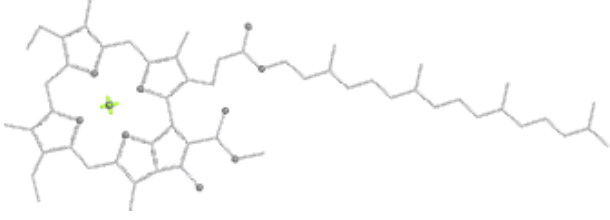
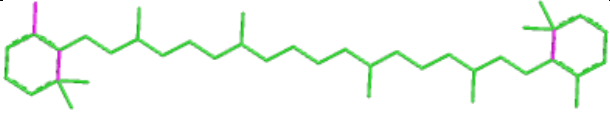
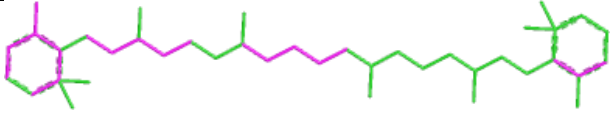
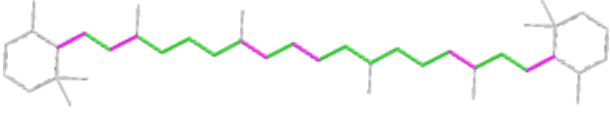
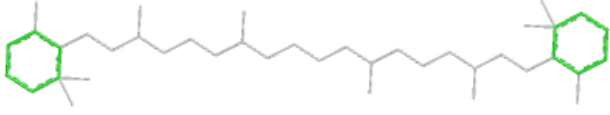
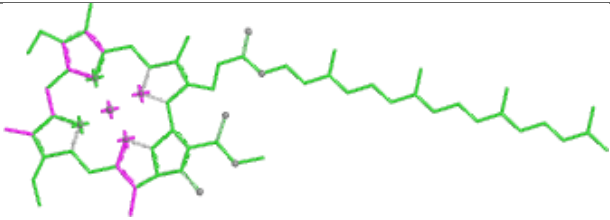
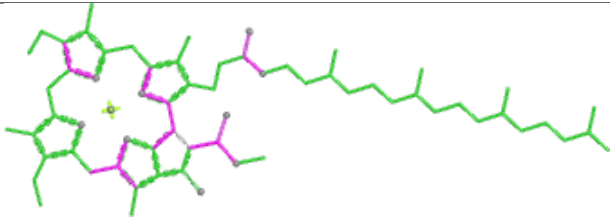
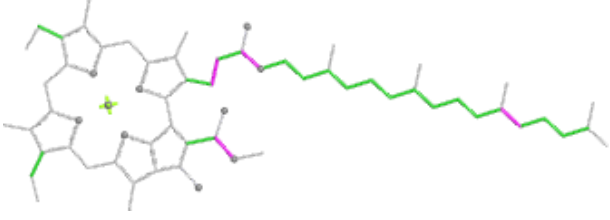
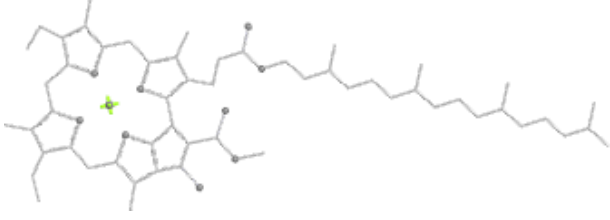
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

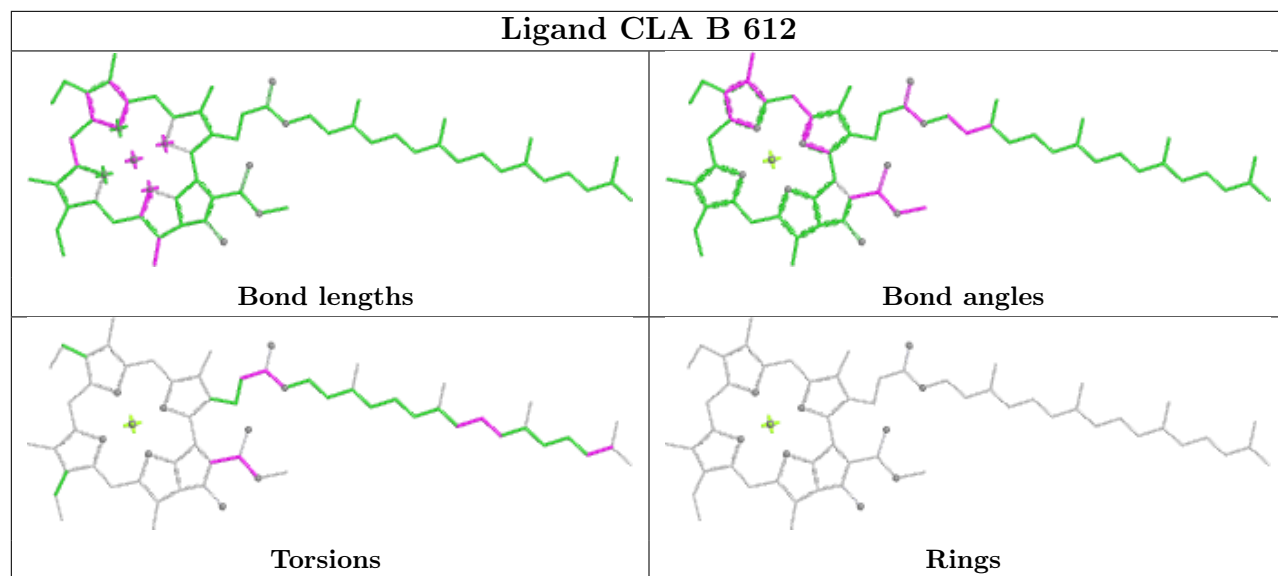
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings



Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 501	
 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%)	-0.37	0 100 100	12, 31, 50, 83	64 (19%)
1	a	334/344 (97%)	-0.26	1 (0%) 90 91	14, 33, 59, 81	64 (19%)
2	B	505/510 (99%)	-0.25	3 (0%) 85 87	21, 35, 63, 86	4 (0%)
2	b	505/510 (99%)	-0.14	4 (0%) 82 84	28, 39, 70, 108	0
3	C	442/461 (95%)	-0.22	0 100 100	15, 38, 54, 78	11 (2%)
3	c	451/461 (97%)	-0.08	3 (0%) 84 85	15, 42, 63, 101	12 (2%)
4	D	341/352 (96%)	-0.39	0 100 100	16, 33, 49, 81	2 (0%)
4	d	341/352 (96%)	-0.25	0 100 100	17, 37, 60, 83	3 (0%)
5	E	82/84 (97%)	0.35	3 (3%) 45 49	35, 53, 70, 84	1 (1%)
5	e	82/84 (97%)	0.48	1 (1%) 76 79	41, 60, 81, 90	0
6	F	34/45 (75%)	-0.04	0 100 100	38, 46, 62, 86	0
6	f	34/45 (75%)	0.25	0 100 100	45, 53, 79, 90	0
7	H	65/66 (98%)	-0.03	2 (3%) 51 55	34, 42, 57, 74	0
7	h	63/66 (95%)	0.28	1 (1%) 70 74	43, 53, 64, 67	0
8	I	35/38 (92%)	-0.14	0 100 100	34, 41, 66, 78	0
8	i	35/38 (92%)	-0.03	0 100 100	35, 42, 70, 89	0
9	J	36/40 (90%)	0.22	1 (2%) 55 59	36, 50, 82, 91	0
9	j	36/40 (90%)	0.35	2 (5%) 30 34	40, 57, 91, 102	0
10	K	37/46 (80%)	0.16	0 100 100	44, 52, 66, 72	0
10	k	37/46 (80%)	0.28	0 100 100	53, 57, 76, 83	0
11	L	37/37 (100%)	-0.35	0 100 100	27, 32, 61, 64	0
11	l	36/37 (97%)	-0.43	0 100 100	28, 33, 72, 92	0
12	M	32/36 (88%)	-0.33	0 100 100	30, 35, 62, 72	0
12	m	31/36 (86%)	-0.36	0 100 100	30, 36, 57, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.01	4 (1%) 70 74	29, 45, 82, 141	1 (0%)
13	o	244/272 (89%)	-0.01	3 (1%) 76 79	30, 44, 79, 131	0
14	T	29/32 (90%)	-0.38	1 (3%) 48 52	29, 34, 60, 78	0
14	t	29/32 (90%)	-0.32	1 (3%) 48 52	31, 35, 70, 88	0
15	U	97/134 (72%)	-0.03	0 100 100	34, 46, 71, 98	0
15	u	97/134 (72%)	-0.12	0 100 100	34, 43, 58, 83	0
16	V	137/163 (84%)	-0.16	0 100 100	32, 43, 56, 76	0
16	v	137/163 (84%)	0.12	0 100 100	37, 49, 71, 88	0
17	Y	27/46 (58%)	0.98	0 100 100	52, 71, 95, 98	0
17	y	30/46 (65%)	0.85	0 100 100	64, 77, 85, 100	0
18	X	38/41 (92%)	0.13	1 (2%) 57 61	44, 52, 68, 71	0
18	x	39/41 (95%)	0.32	0 100 100	50, 61, 85, 100	0
19	Z	62/62 (100%)	0.90	4 (6%) 25 28	55, 69, 112, 127	0
19	z	62/62 (100%)	0.92	4 (6%) 25 28	63, 77, 115, 117	0
20	R	34/41 (82%)	0.94	1 (2%) 53 57	61, 70, 81, 89	0
20	r	31/41 (75%)	1.30	5 (16%) 4 5	72, 88, 113, 121	0
All	All	5302/5700 (93%)	-0.09	45 (0%) 82 84	12, 40, 75, 141	162 (3%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.8
20	R	35	LEU	4.0
5	e	79	PHE	3.7
14	T	30	THR	3.4
19	Z	33	TRP	3.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.93	0.12	41,53,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	m	1	10/11	0.93	0.10	32,53,69,70	0
14	FME	t	1	10/11	0.93	0.09	35,42,63,65	0
8	FME	i	1	10/11	0.95	0.08	38,52,60,65	0
8	FME	I	1	10/11	0.95	0.07	39,52,59,61	0
14	FME	T	1	10/11	0.95	0.08	36,44,53,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	H	103	18/20	0.75	0.18	56,63,72,72	0
29	LMG	b	622	55/55	0.78	0.17	53,66,81,85	0
32	STE	L	103	12/20	0.79	0.18	48,53,65,67	0
32	STE	a	616	12/20	0.79	0.13	41,57,67,73	0
32	STE	b	621	20/20	0.79	0.15	42,56,70,72	0
29	LMG	d	410	23/55	0.80	0.18	51,61,75,75	0
32	STE	b	625	20/20	0.80	0.14	49,58,70,73	0
25	CLA	b	601	65/65	0.81	0.13	46,66,83,93	0
28	PL9	A	611	55/55	0.81	0.17	43,59,72,76	0
31	DGD	a	614	44/66	0.81	0.15	40,54,74,82	0
32	STE	b	623	16/20	0.81	0.16	50,60,78,82	0
28	PL9	a	611	55/55	0.81	0.17	45,63,78,82	0
32	STE	c	522	12/20	0.81	0.12	58,68,79,85	0
34	LHG	E	101	49/49	0.81	0.15	46,74,91,94	0
29	LMG	c	521	48/55	0.82	0.15	41,68,89,92	0
32	STE	d	413	20/20	0.82	0.14	45,55,66,67	0
32	STE	t	104	18/20	0.82	0.14	43,52,77,83	0
32	STE	b	626	10/20	0.82	0.14	47,49,57,58	0
32	STE	I	101	15/20	0.83	0.14	43,53,69,73	0
32	STE	B	625	16/20	0.83	0.16	46,60,71,71	0
32	STE	a	615	10/20	0.83	0.14	43,51,57,58	0
29	LMG	D	412	33/55	0.83	0.14	36,52,75,79	0
32	STE	J	101	12/20	0.84	0.13	50,59,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LHG	e	102	42/49	0.84	0.13	62,79,89,95	0
32	STE	B	620	17/20	0.85	0.11	39,49,62,64	0
31	DGD	A	615	66/66	0.85	0.12	47,59,68,71	0
32	STE	b	620	16/20	0.85	0.17	38,49,62,63	0
29	LMG	c	519	37/55	0.85	0.12	47,62,72,74	0
32	STE	C	520	12/20	0.86	0.13	38,44,61,64	0
32	STE	C	521	12/20	0.86	0.12	44,51,56,56	0
32	STE	X	101	20/20	0.86	0.12	38,48,68,69	0
32	STE	R	101	12/20	0.86	0.13	61,68,87,87	0
30	SQD	f	101	41/54	0.87	0.13	63,74,84,88	0
32	STE	c	520	20/20	0.87	0.11	50,54,77,81	0
32	STE	B	624	12/20	0.87	0.12	51,55,65,71	0
32	STE	d	412	17/20	0.87	0.13	44,54,69,70	0
30	SQD	t	102	36/54	0.87	0.12	34,53,67,70	0
32	STE	t	103	14/20	0.87	0.11	39,46,53,62	0
29	LMG	C	519	48/55	0.87	0.12	44,62,77,82	0
30	SQD	A	614	39/54	0.87	0.12	39,53,69,74	0
32	STE	C	522	16/20	0.87	0.13	44,49,57,59	0
25	CLA	B	601	65/65	0.88	0.11	38,54,75,79	0
30	SQD	B	622	54/54	0.88	0.11	38,58,78,81	0
32	STE	B	623	12/20	0.88	0.12	37,49,57,59	0
30	SQD	L	101	49/54	0.88	0.10	37,53,76,83	0
32	STE	j	101	12/20	0.88	0.12	51,59,64,67	0
32	STE	l	102	18/20	0.88	0.14	32,44,65,68	0
29	LMG	c	523	49/55	0.88	0.10	36,50,78,82	0
32	STE	b	624	15/20	0.88	0.13	45,52,70,74	0
29	LMG	A	612	48/55	0.88	0.11	43,54,65,71	0
29	LMG	m	101	51/55	0.88	0.11	33,47,64,67	0
29	LMG	B	621	28/55	0.89	0.12	37,49,60,61	0
27	BCR	k	101	40/40	0.89	0.13	52,61,69,72	0
27	BCR	K	102	40/40	0.89	0.11	40,50,58,62	0
29	LMG	M	101	51/55	0.89	0.10	30,49,64,69	0
27	BCR	d	405	40/40	0.90	0.11	43,49,83,87	0
27	BCR	h	101	40/40	0.90	0.11	40,52,63,66	0
30	SQD	D	409	36/54	0.90	0.12	45,62,74,79	0
32	STE	M	103	10/20	0.91	0.12	30,45,53,58	0
25	CLA	c	512	65/65	0.91	0.11	41,55,79,83	0
27	BCR	c	514	40/40	0.91	0.10	48,57,63,67	0
30	SQD	a	613	54/54	0.91	0.11	38,55,77,82	0
27	BCR	B	618	40/40	0.91	0.09	28,38,49,52	0
27	BCR	D	406	40/40	0.91	0.11	32,43,69,72	0
27	BCR	H	101	40/40	0.91	0.10	33,44,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	BCR	b	619	40/40	0.92	0.10	33,47,61,63	0
29	LMG	d	411	44/55	0.92	0.10	43,52,72,79	0
25	CLA	c	513	65/65	0.92	0.10	48,62,83,88	0
25	CLA	C	513	65/65	0.92	0.10	48,56,82,87	0
31	DGD	C	517	62/66	0.92	0.10	35,46,84,99	0
31	DGD	H	102	62/66	0.92	0.09	31,41,52,54	0
27	BCR	K	101	40/40	0.92	0.11	37,54,60,63	0
31	DGD	c	517	62/66	0.92	0.09	42,48,78,81	0
27	BCR	B	619	40/40	0.92	0.08	31,40,53,54	0
29	LMG	D	408	51/55	0.92	0.11	34,46,66,70	0
27	BCR	T	101	40/40	0.93	0.07	31,40,46,50	0
27	BCR	b	617	40/40	0.93	0.08	35,43,49,51	0
27	BCR	b	618	40/40	0.93	0.08	25,36,47,48	0
31	DGD	h	102	62/66	0.93	0.08	32,44,53,56	0
27	BCR	k	102	40/40	0.93	0.12	49,53,60,67	0
27	BCR	t	101	40/40	0.93	0.08	27,38,45,48	0
25	CLA	C	512	65/65	0.93	0.10	35,46,77,84	0
30	SQD	A	613	52/54	0.93	0.10	36,52,71,78	0
34	LHG	d	407	49/49	0.93	0.10	33,46,62,63	0
34	LHG	d	409	39/49	0.93	0.10	36,43,58,59	0
27	BCR	C	514	40/40	0.93	0.09	31,39,45,54	0
25	CLA	B	606	65/65	0.94	0.08	27,37,57,68	0
31	DGD	c	518	62/66	0.94	0.09	34,46,69,77	0
25	CLA	C	501	65/65	0.94	0.07	27,35,44,46	0
27	BCR	C	515	40/40	0.94	0.10	35,47,57,62	0
25	CLA	C	502	65/65	0.94	0.08	31,38,46,54	0
25	CLA	b	616	60/65	0.94	0.09	31,42,75,83	0
25	CLA	c	503	65/65	0.94	0.08	36,44,48,54	0
25	CLA	c	504	60/65	0.94	0.08	29,43,64,72	0
25	CLA	c	505	65/65	0.94	0.08	32,38,54,55	0
25	CLA	c	506	65/65	0.94	0.09	40,46,72,75	0
25	CLA	c	511	65/65	0.94	0.10	41,55,63,66	0
25	CLA	C	503	65/65	0.94	0.07	34,42,46,51	0
25	CLA	C	510	65/65	0.94	0.07	31,42,51,67	0
31	DGD	C	516	62/66	0.94	0.09	26,34,66,70	0
32	STE	M	102	15/20	0.94	0.09	40,46,55,60	0
33	BCT	d	401	4/4	0.94	0.08	36,36,40,46	0
34	LHG	D	411	47/49	0.94	0.10	30,42,63,74	0
27	BCR	c	515	40/40	0.94	0.09	33,45,54,56	0
31	DGD	C	518	62/66	0.94	0.08	33,43,68,70	0
27	BCR	B	617	40/40	0.94	0.07	26,39,45,49	0
25	CLA	C	511	65/65	0.94	0.09	31,46,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	614	65/65	0.95	0.08	30,38,66,71	0
25	CLA	b	615	65/65	0.95	0.07	28,38,50,54	0
25	CLA	C	506	65/65	0.95	0.09	32,43,72,77	0
25	CLA	c	502	65/65	0.95	0.07	33,40,48,57	0
25	CLA	C	508	65/65	0.95	0.08	32,38,86,92	0
25	CLA	C	509	65/65	0.95	0.08	32,39,52,56	0
25	CLA	B	610	65/65	0.95	0.07	23,31,38,41	0
25	CLA	B	612	65/65	0.95	0.07	24,31,37,46	0
25	CLA	c	507	65/65	0.95	0.08	34,41,51,56	0
25	CLA	c	508	64/65	0.95	0.08	35,43,81,94	0
25	CLA	c	509	65/65	0.95	0.09	37,45,57,59	0
25	CLA	c	510	65/65	0.95	0.07	36,45,51,58	0
25	CLA	B	616	60/65	0.95	0.09	28,36,71,73	0
25	CLA	C	504	59/65	0.95	0.07	31,38,68,74	0
25	CLA	a	606	65/65	0.95	0.07	23,30,37,48	0
28	PL9	D	407	55/55	0.95	0.07	23,31,40,43	0
25	CLA	d	404	65/65	0.95	0.08	33,41,71,83	0
31	DGD	c	516	62/66	0.95	0.09	30,41,60,64	0
28	PL9	d	406	55/55	0.95	0.07	23,34,38,42	0
26	PHO	D	402	64/64	0.95	0.07	27,34,39,41	0
26	PHO	a	608	64/64	0.95	0.07	24,30,36,41	0
26	PHO	d	402	64/64	0.95	0.07	32,38,44,46	0
27	BCR	A	610	40/40	0.95	0.07	24,33,38,41	0
33	BCT	D	401	4/4	0.95	0.07	35,35,38,38	0
25	CLA	a	607	65/65	0.95	0.09	28,38,82,87	0
25	CLA	a	609	65/65	0.95	0.08	23,30,69,73	0
34	LHG	D	413	49/49	0.95	0.09	30,39,58,61	0
25	CLA	C	505	65/65	0.95	0.08	23,36,60,62	0
25	CLA	b	602	65/65	0.95	0.08	30,40,52,56	0
25	CLA	b	606	65/65	0.95	0.08	30,38,62,71	0
25	CLA	b	609	65/65	0.95	0.08	30,42,55,66	0
34	LHG	l	101	49/49	0.95	0.08	28,41,49,52	0
35	HEM	e	101	43/43	0.95	0.10	53,59,76,87	0
27	BCR	a	610	40/40	0.96	0.06	23,33,43,49	0
25	CLA	B	615	65/65	0.96	0.07	28,36,53,59	0
25	CLA	B	603	65/65	0.96	0.07	23,31,46,51	0
25	CLA	D	403	65/65	0.96	0.06	21,29,38,41	0
25	CLA	D	404	65/65	0.96	0.07	22,28,48,52	0
25	CLA	B	604	65/65	0.96	0.07	24,31,59,63	0
25	CLA	B	605	65/65	0.96	0.07	25,31,42,46	0
25	CLA	A	607	65/65	0.96	0.08	23,33,70,78	0
25	CLA	a	612	65/65	0.96	0.06	24,31,38,46	0

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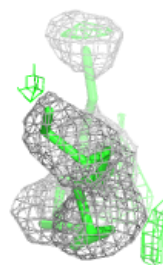
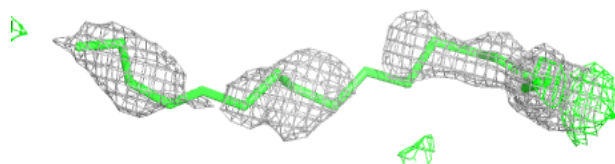
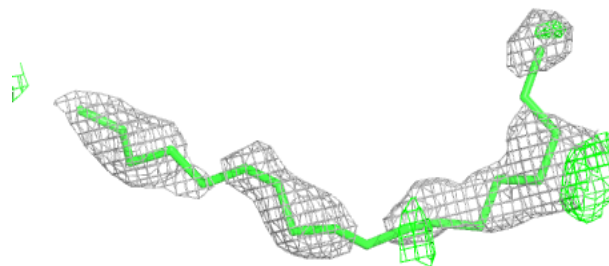
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	607	65/65	0.96	0.07	21,30,55,65	0
25	CLA	B	608	65/65	0.96	0.06	26,32,48,53	0
25	CLA	b	603	65/65	0.96	0.07	26,32,58,66	0
25	CLA	d	403	65/65	0.96	0.07	25,33,49,61	0
25	CLA	b	604	65/65	0.96	0.07	26,33,58,73	0
26	PHO	A	608	64/64	0.96	0.06	23,29,35,38	0
25	CLA	b	605	65/65	0.96	0.07	24,34,43,50	0
25	CLA	B	609	65/65	0.96	0.07	27,38,47,55	0
25	CLA	b	607	65/65	0.96	0.07	23,31,58,62	0
25	CLA	b	608	65/65	0.96	0.07	33,39,54,58	0
25	CLA	C	507	65/65	0.96	0.07	29,37,49,56	0
25	CLA	b	610	65/65	0.96	0.08	29,36,44,53	0
34	LHG	D	410	49/49	0.96	0.07	30,36,46,55	0
25	CLA	b	611	65/65	0.96	0.06	25,33,48,51	0
25	CLA	b	612	65/65	0.96	0.07	21,34,39,47	0
25	CLA	b	613	65/65	0.96	0.08	25,31,66,71	0
34	LHG	L	102	49/49	0.96	0.08	30,38,48,57	0
25	CLA	A	606	65/65	0.96	0.06	20,28,39,42	0
34	LHG	d	408	49/49	0.96	0.08	30,39,46,48	0
25	CLA	B	611	65/65	0.96	0.06	23,30,43,47	0
25	CLA	B	602	65/65	0.96	0.07	30,37,48,56	0
25	CLA	c	501	65/65	0.96	0.07	32,37,48,50	0
25	CLA	B	614	65/65	0.96	0.08	25,33,63,67	0
25	CLA	D	405	65/65	0.97	0.07	27,33,90,96	0
25	CLA	A	609	54/65	0.97	0.06	25,30,57,59	0
35	HEM	F	101	43/43	0.97	0.08	37,49,58,66	0
25	CLA	B	613	65/65	0.97	0.06	22,29,60,64	0
24	CL	a	605	1/1	0.98	0.07	38,38,38,38	0
24	CL	A	604	1/1	0.98	0.04	36,36,36,36	0
24	CL	a	604	1/1	0.98	0.05	38,38,38,38	0
36	HEC	V	201	43/43	0.98	0.06	28,34,39,49	0
36	HEC	v	201	43/43	0.98	0.06	32,38,45,48	0
21	OEY	a	601[B]	11/11	0.99	0.02	28,32,34,35	11
22	OEX	A	602[A]	10/10	0.99	0.03	26,36,38,39	10
22	OEX	a	602[A]	10/10	0.99	0.03	29,35,38,43	10
21	OEY	A	601[B]	11/11	0.99	0.03	29,32,34,34	11
24	CL	A	605	1/1	0.99	0.06	36,36,36,36	0
23	FE2	A	603	1/1	1.00	0.01	34,34,34,34	0
23	FE2	a	603	1/1	1.00	0.02	36,36,36,36	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.

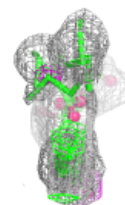
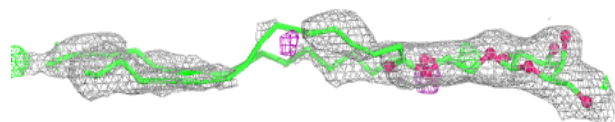
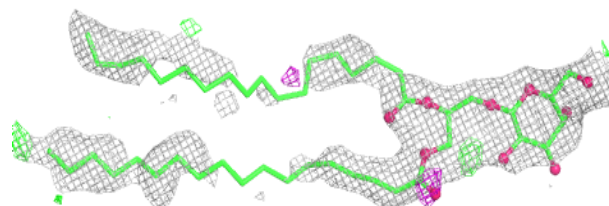
Electron density around STE H 103:

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



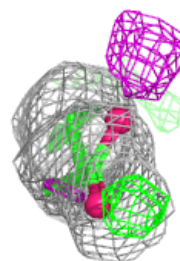
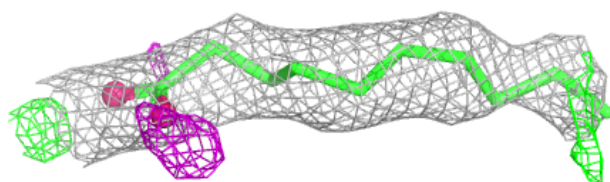
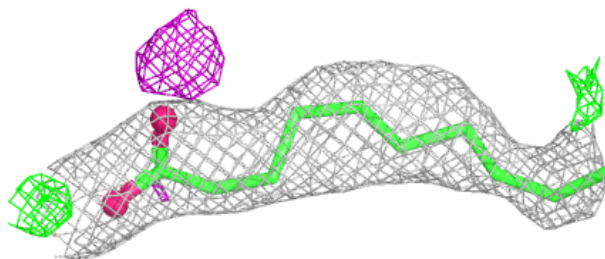
Electron density around LMG b 622:

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

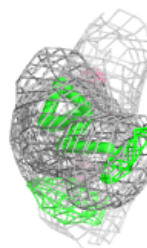
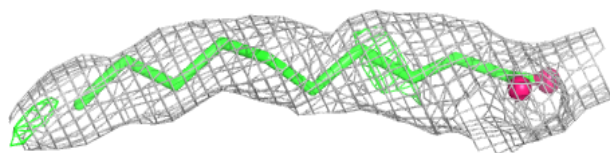
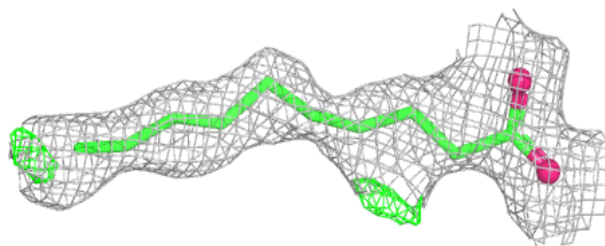


Electron density around STE L 103:

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

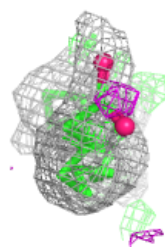
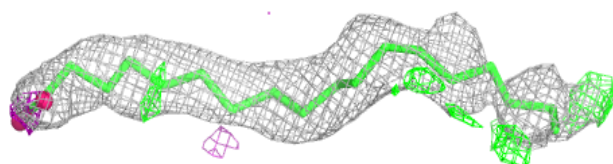
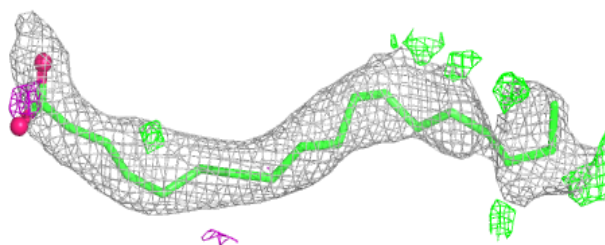
**Electron density around STE a 616:**

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

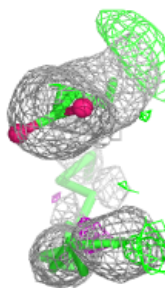
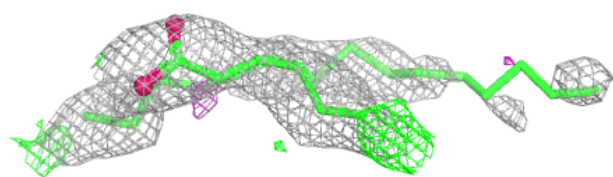
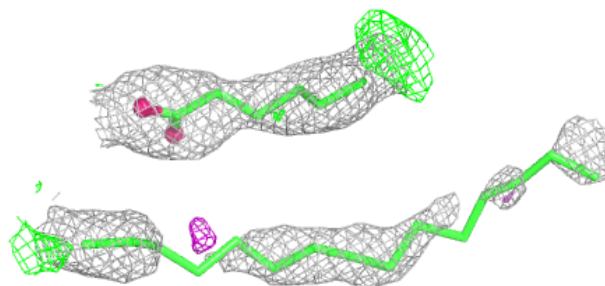


Electron density around STE b 621:

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

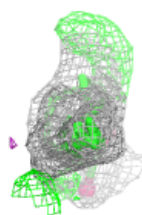
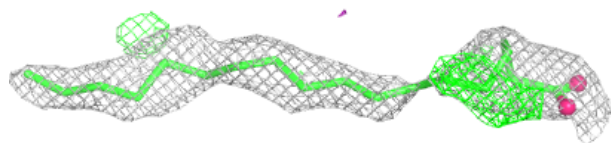
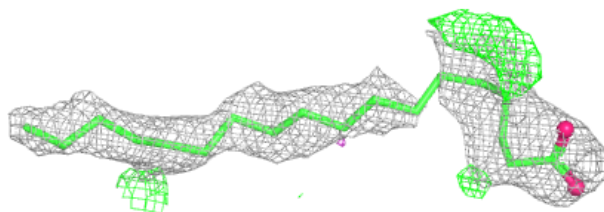
**Electron density around LMG d 410:**

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

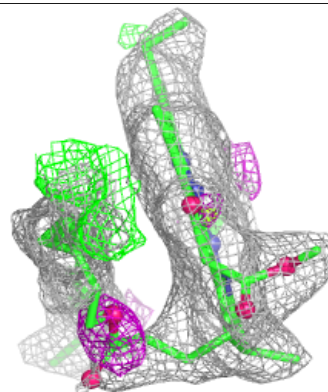
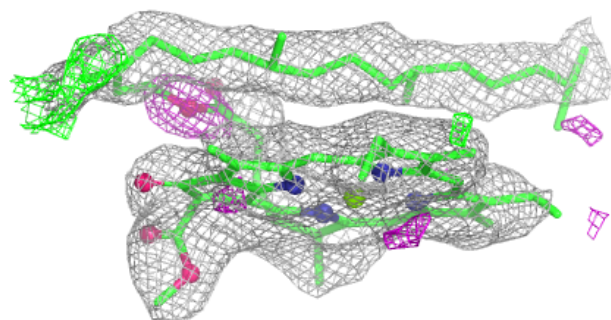
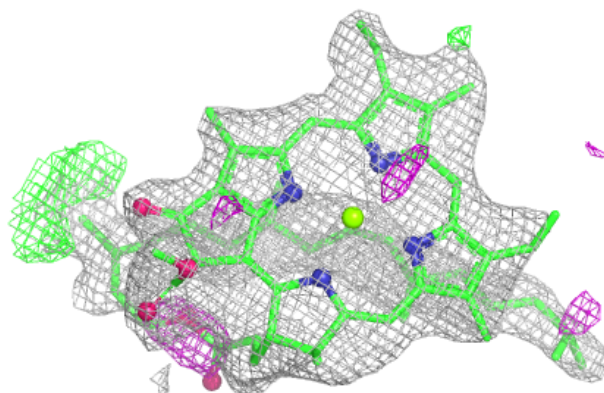


Electron density around STE b 625:

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

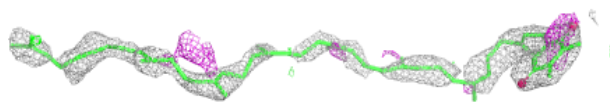
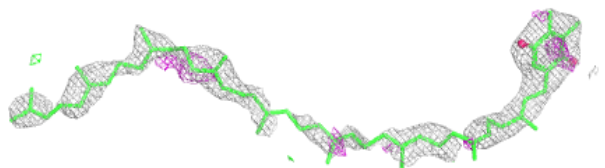
**Electron density around CLA b 601:**

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

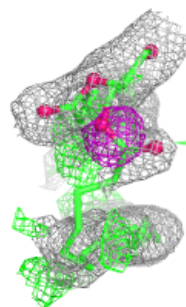
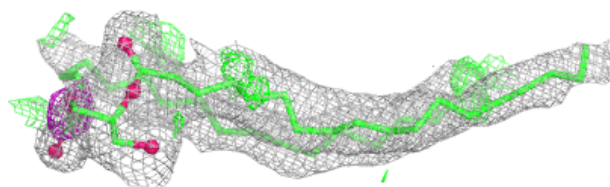
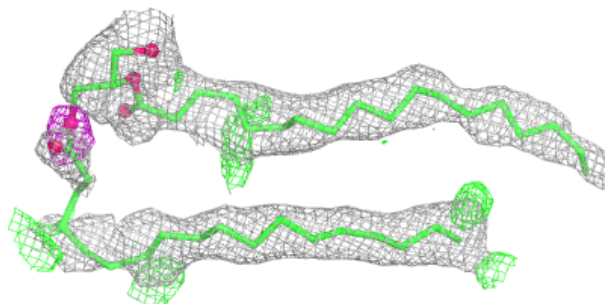


Electron density around PL9 A 611:

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

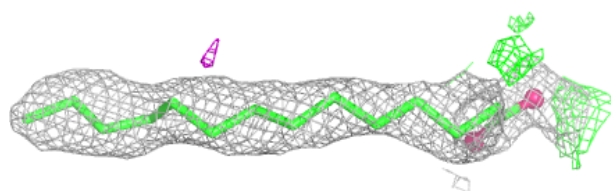
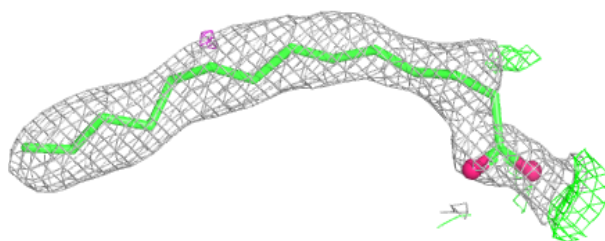
**Electron density around DGD a 614:**

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

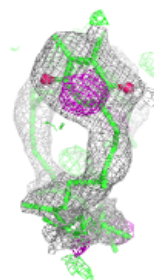
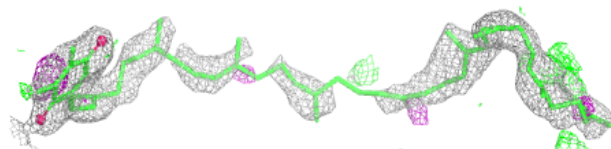
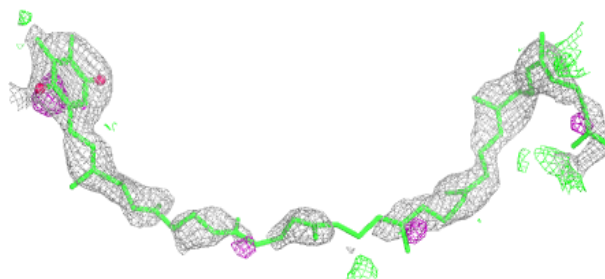


Electron density around STE b 623:

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

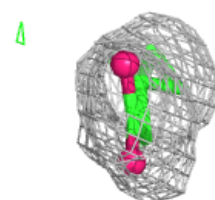
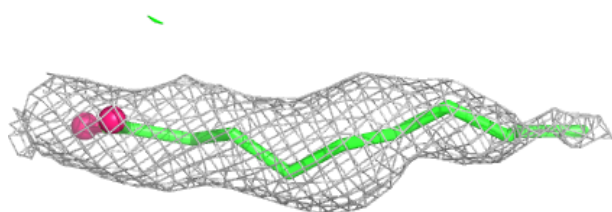
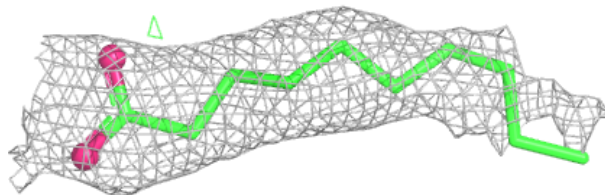
**Electron density around PL9 a 611:**

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

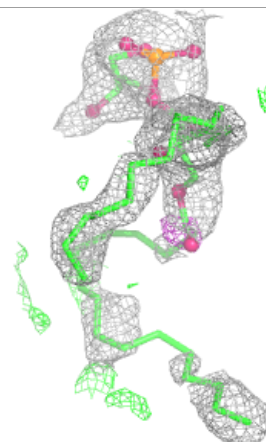
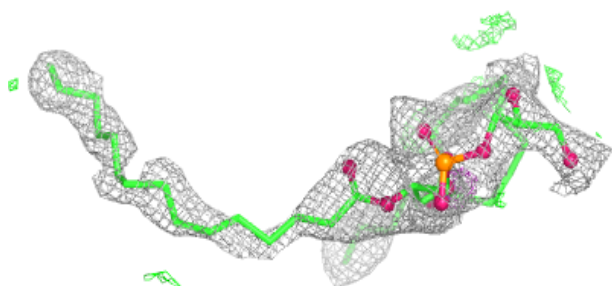
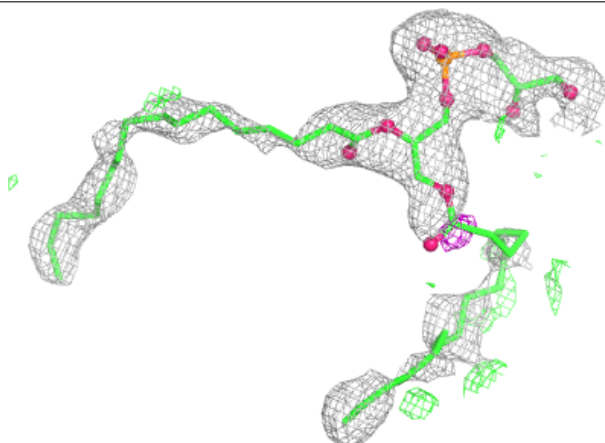


Electron density around STE c 522:

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

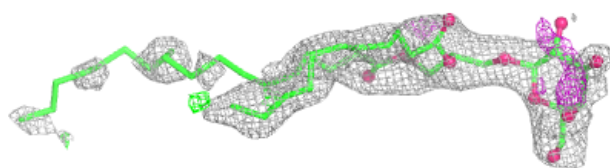
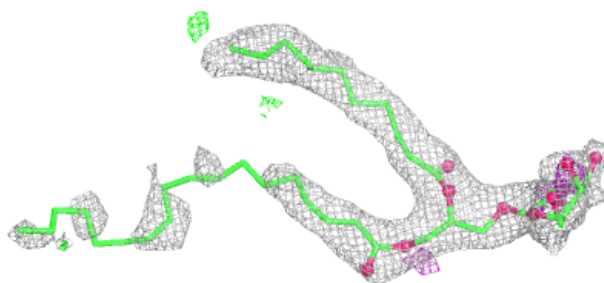
**Electron density around LHG E 101:**

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

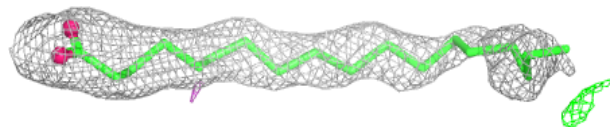
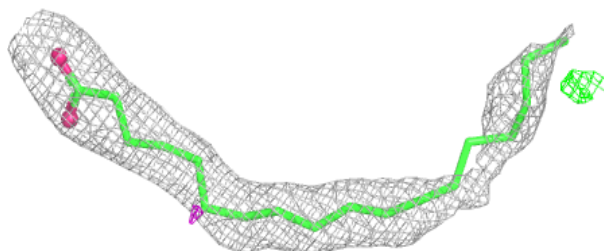


Electron density around LMG c 521:

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

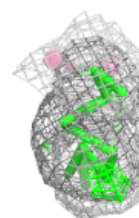
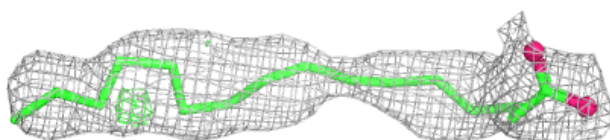
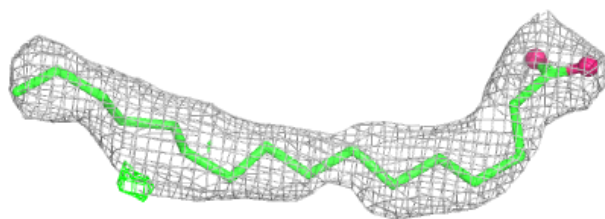
**Electron density around STE d 413:**

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

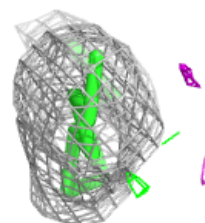
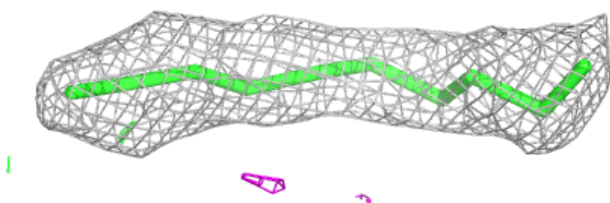
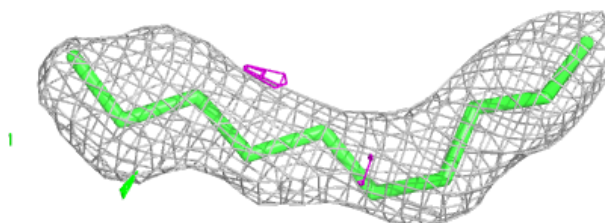


Electron density around STE t 104:

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

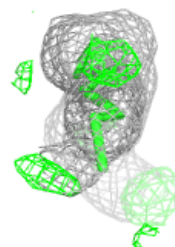
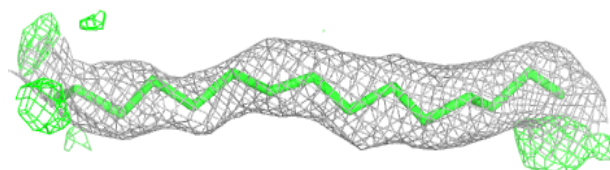
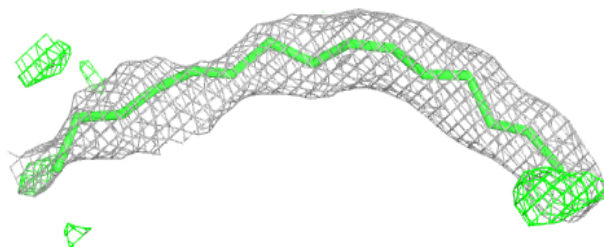
**Electron density around STE b 626:**

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

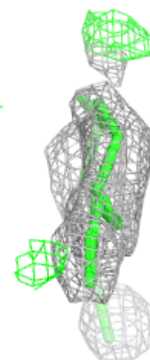
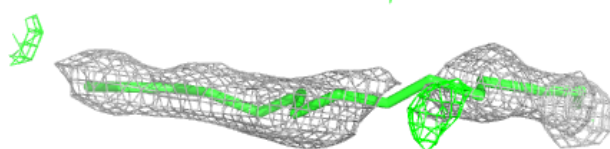
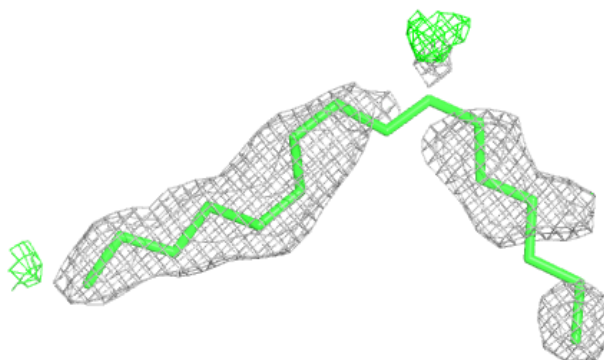


Electron density around STE I 101:

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

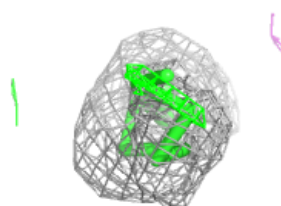
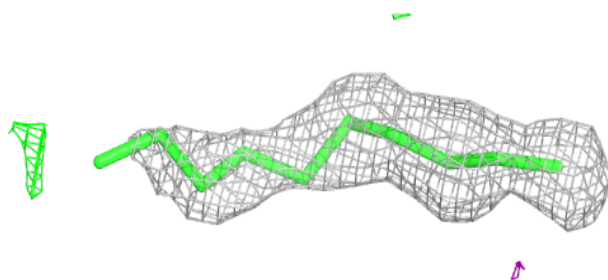
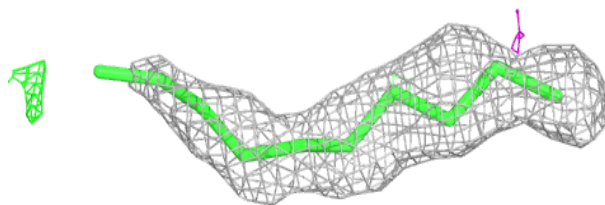
**Electron density around STE B 625:**

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

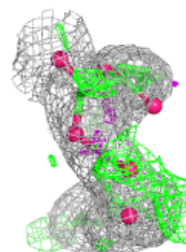
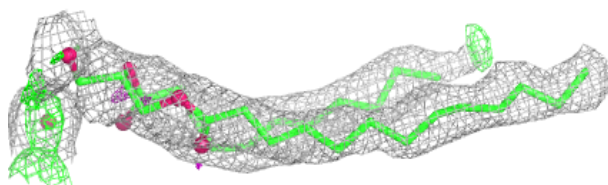
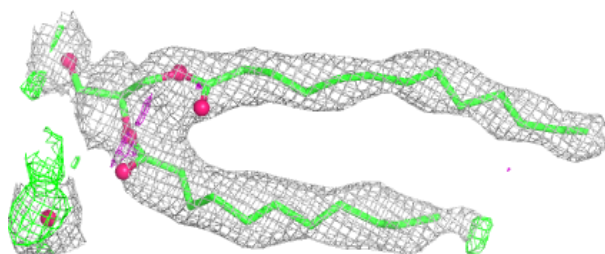


Electron density around STE a 615:

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

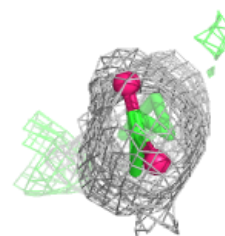
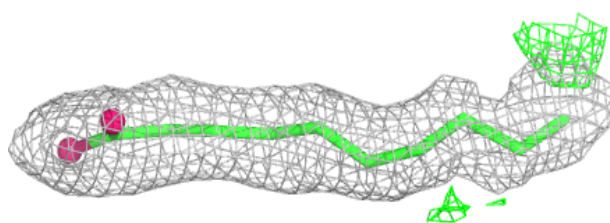
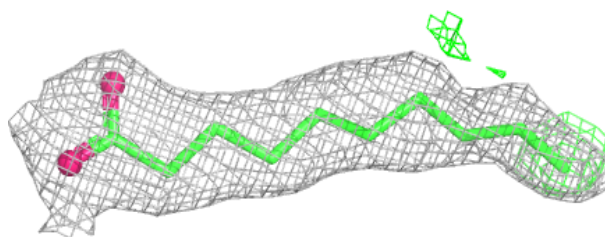
**Electron density around LMG D 412:**

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

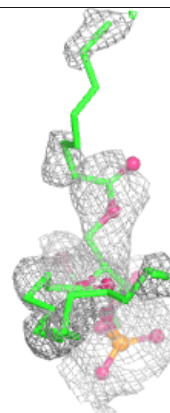
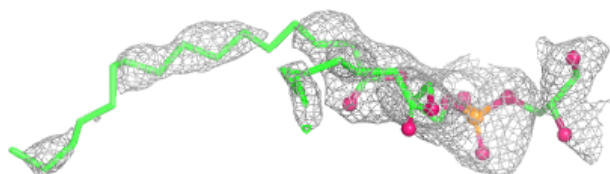
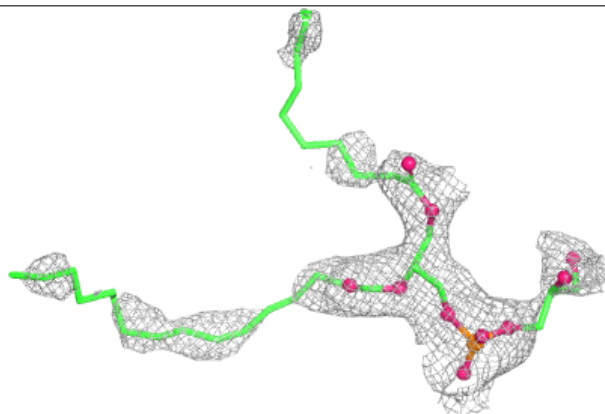


Electron density around STE J 101:

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

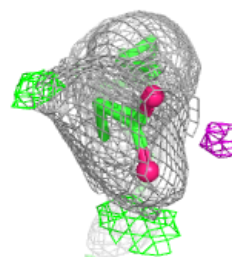
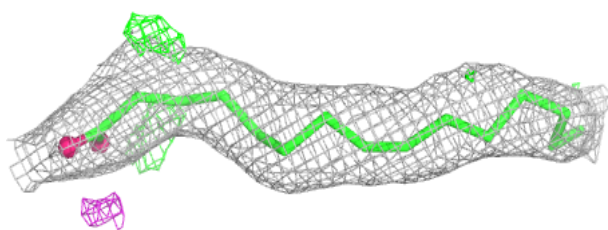
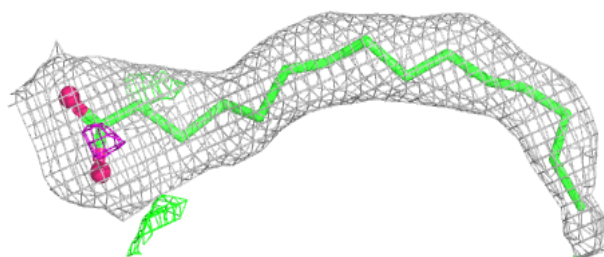
**Electron density around LHG e 102:**

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

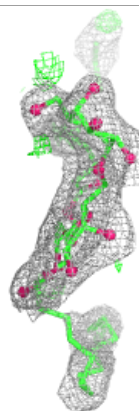
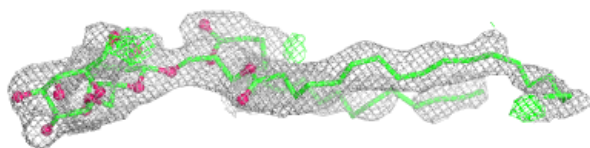
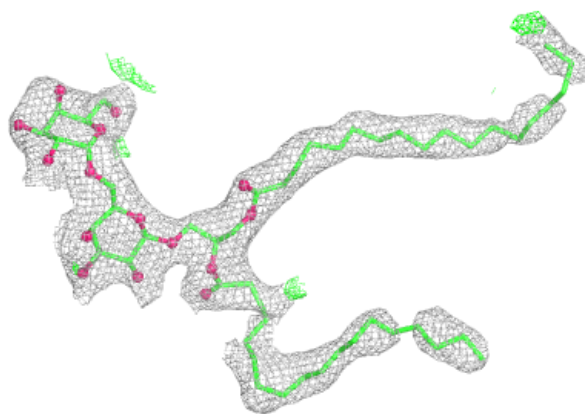


Electron density around STE B 620:

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

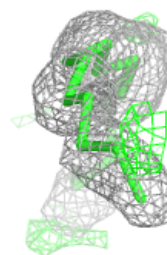
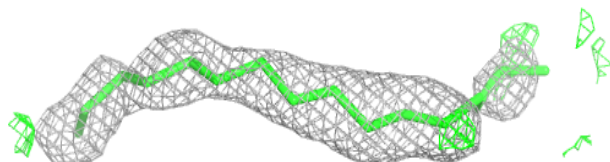
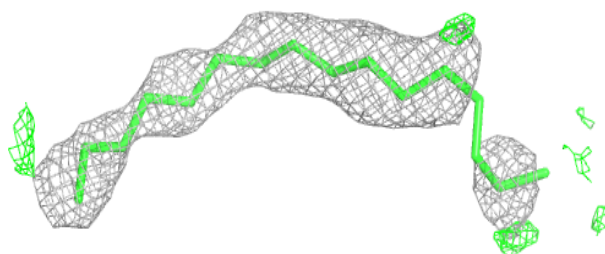
**Electron density around DGD A 615:**

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

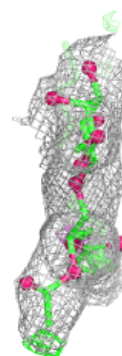
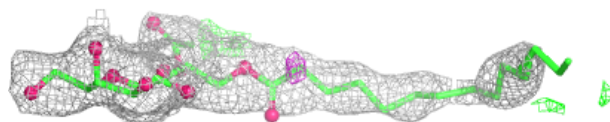
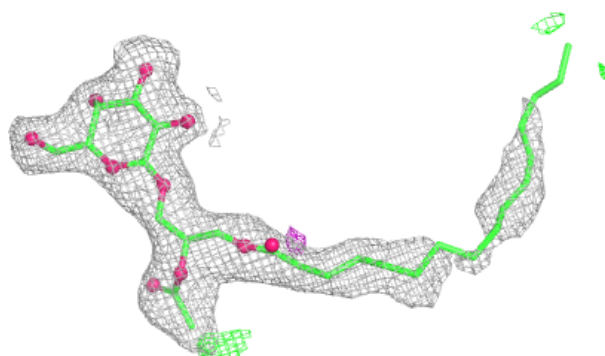


Electron density around STE b 620:

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

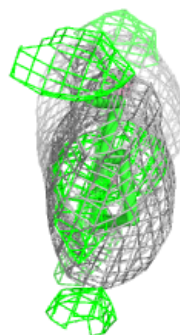
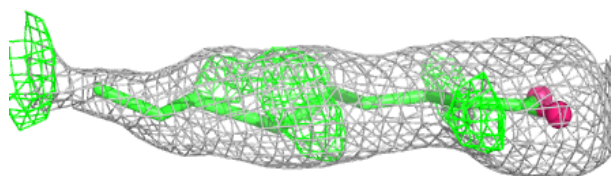
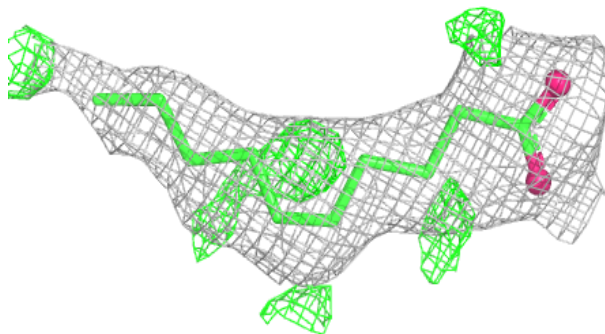
**Electron density around LMG c 519:**

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

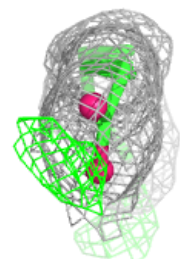
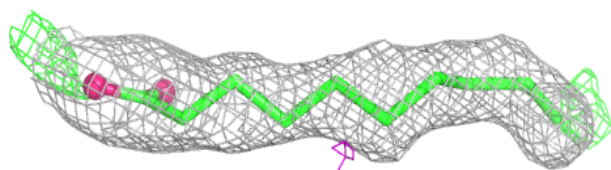
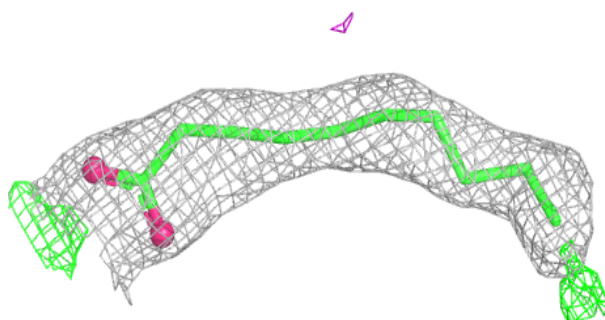


Electron density around STE C 520:

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

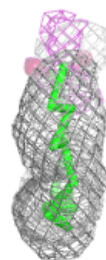
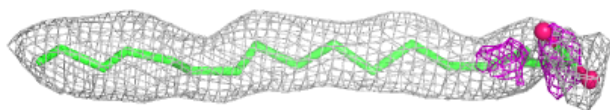
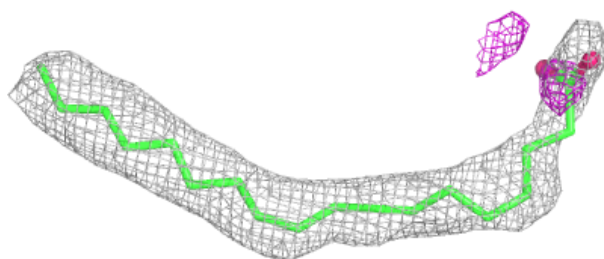
**Electron density around STE C 521:**

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

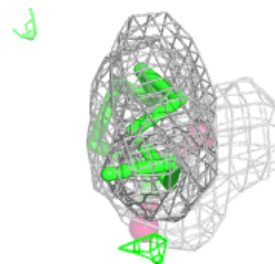
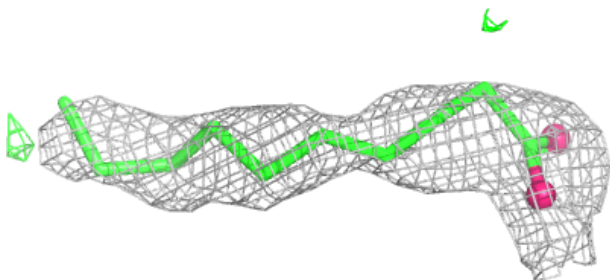
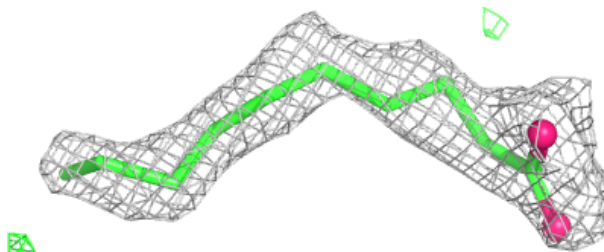


Electron density around STE X 101:

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

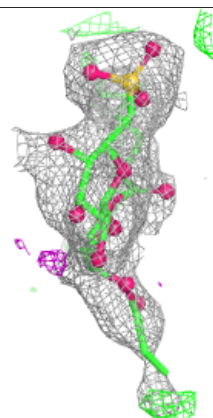
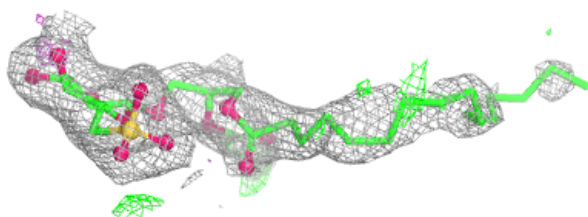
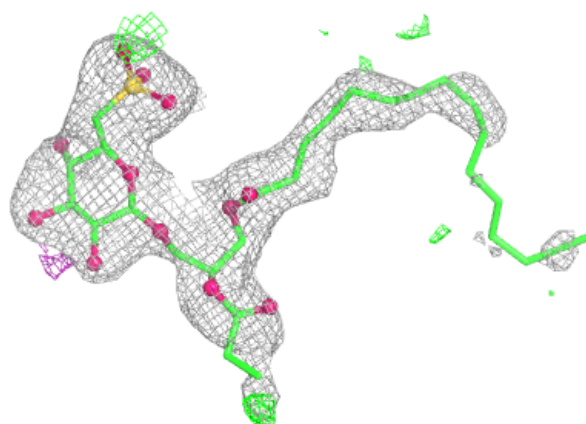
**Electron density around STE R 101:**

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

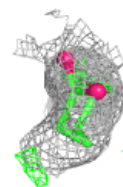
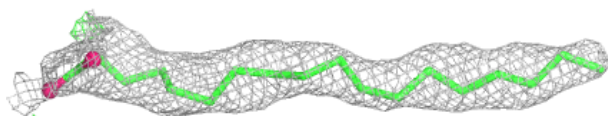
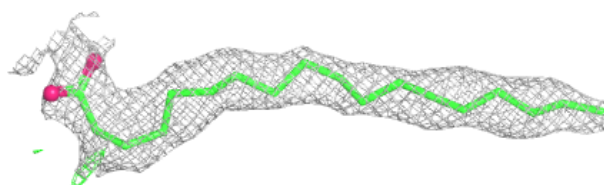


Electron density around SQD f 101:

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

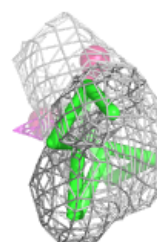
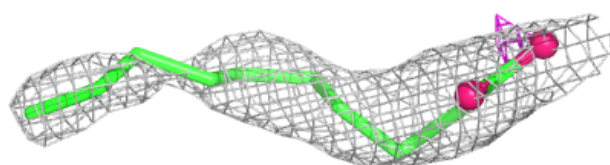
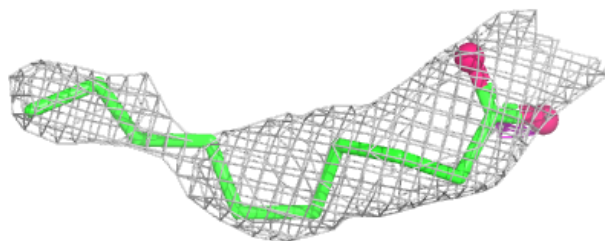
**Electron density around STE c 520:**

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

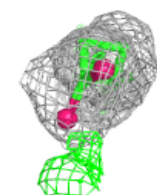
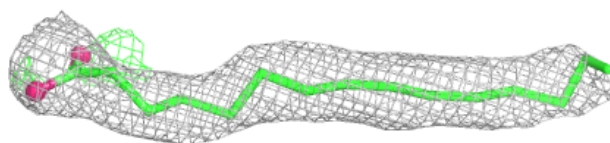
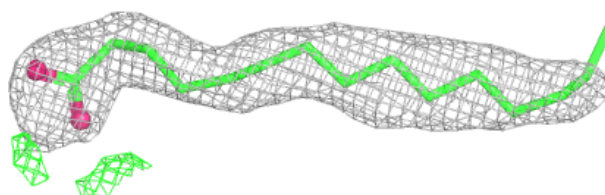


Electron density around STE B 624:

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

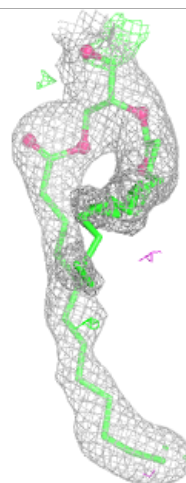
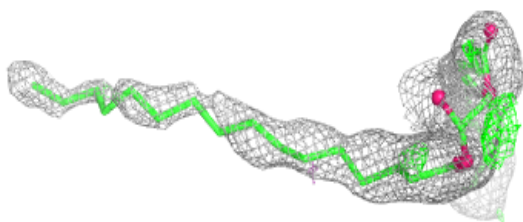
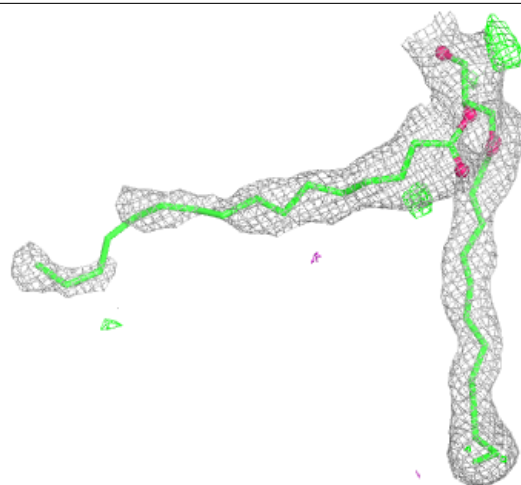
**Electron density around STE d 412:**

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



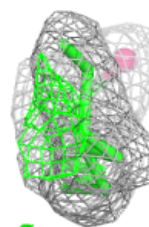
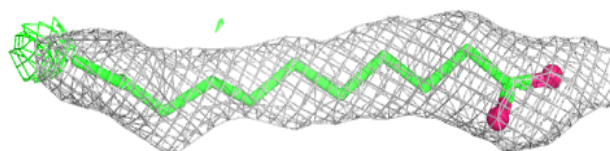
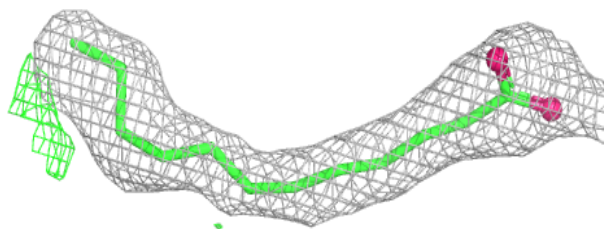
Electron density around SQD t 102:

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

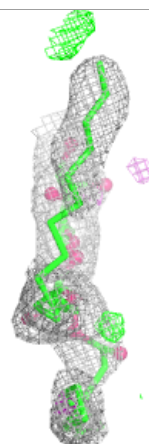
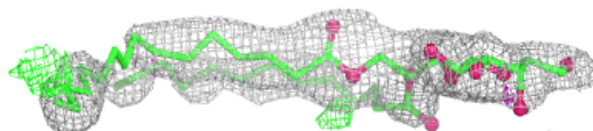
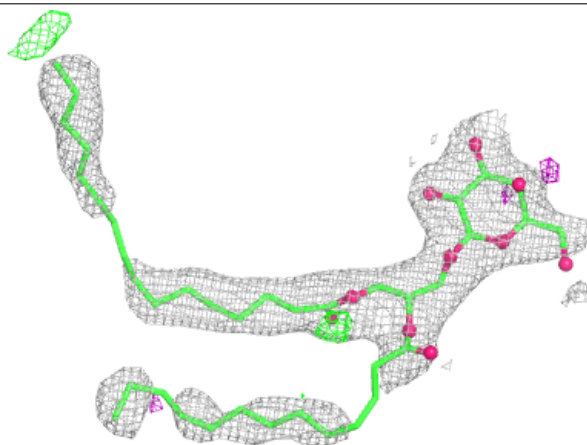


Electron density around STE t 103:

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

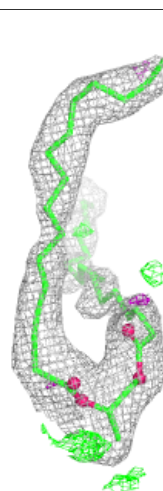
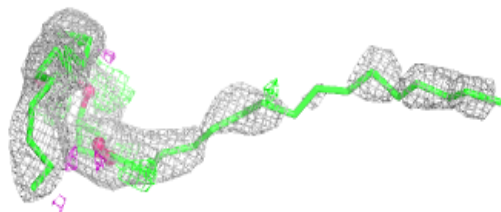
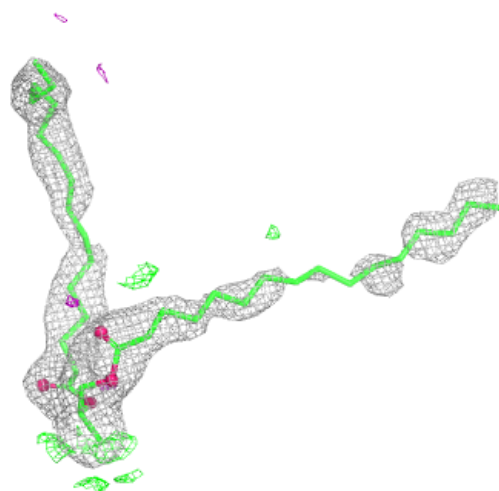
**Electron density around LMG C 519:**

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



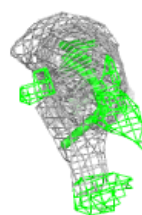
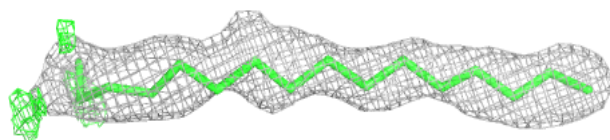
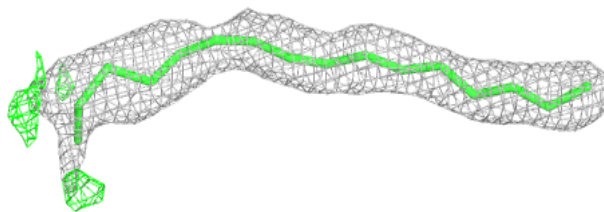
Electron density around SQD A 614:

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



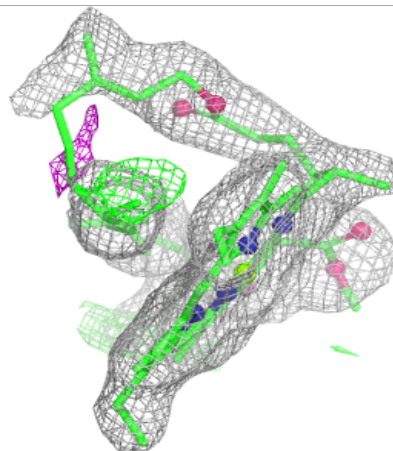
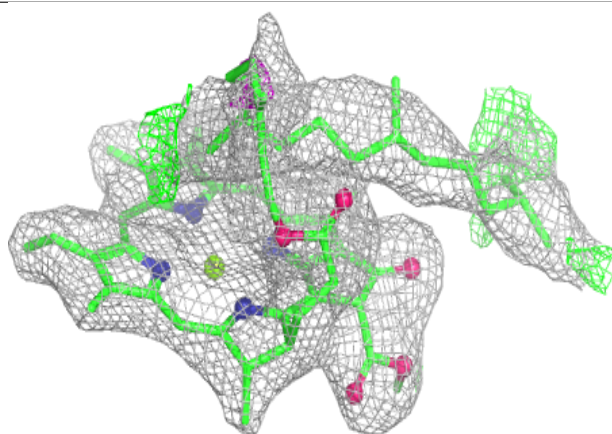
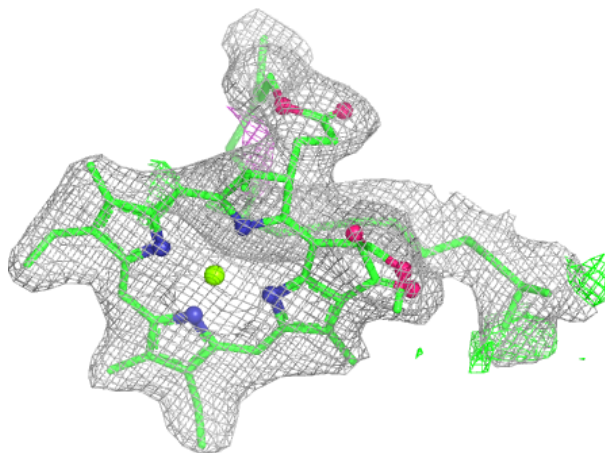
Electron density around STE C 522:

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



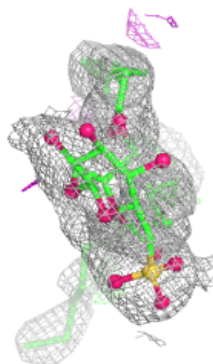
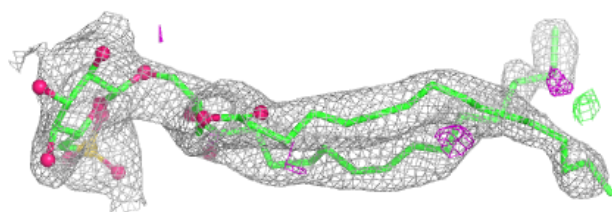
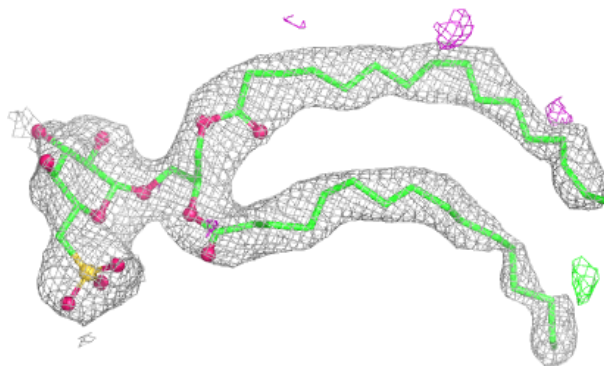
Electron density around CLA B 601:

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

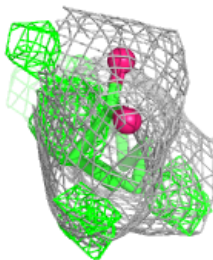
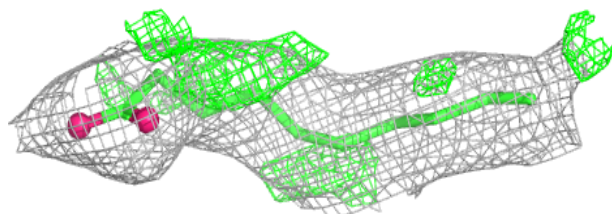
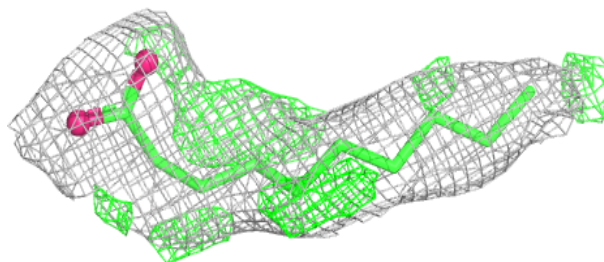


Electron density around SQD B 622:

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

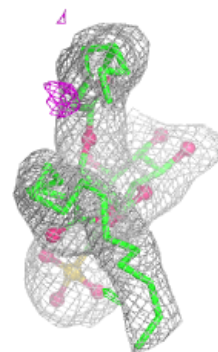
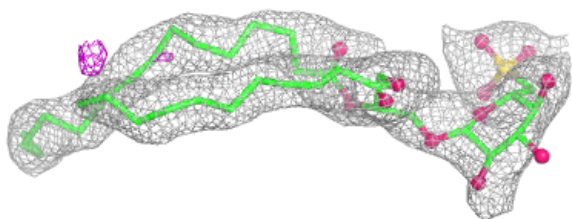
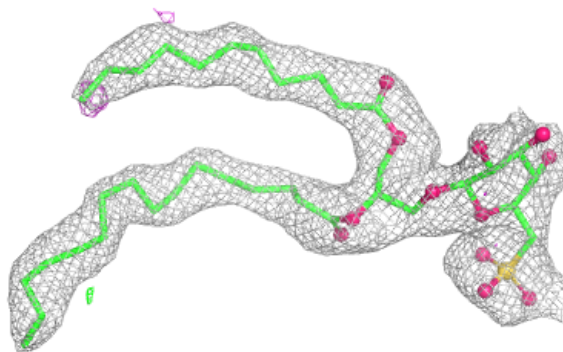
**Electron density around STE B 623:**

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

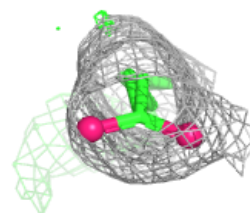
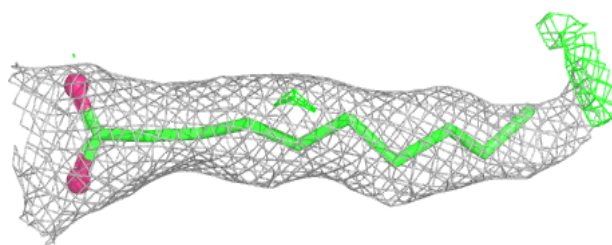
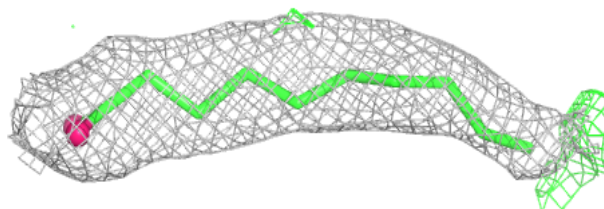


Electron density around SQD L 101:

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

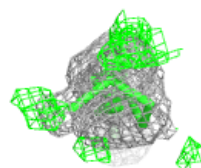
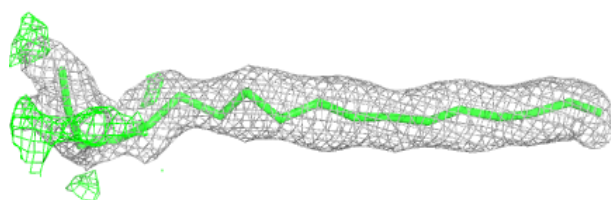
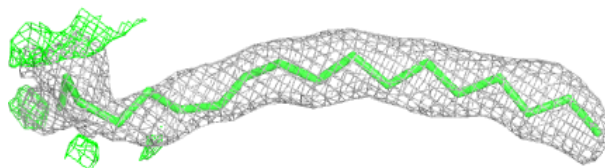
**Electron density around STE j 101:**

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

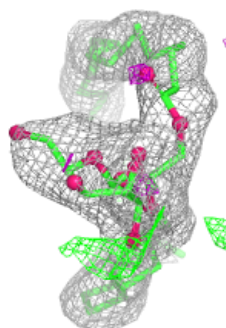
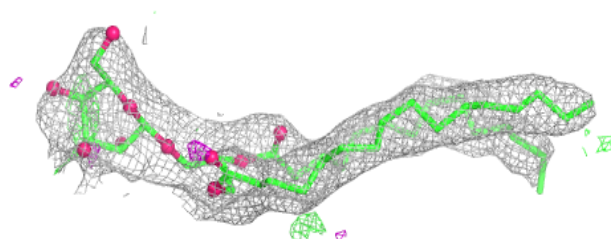
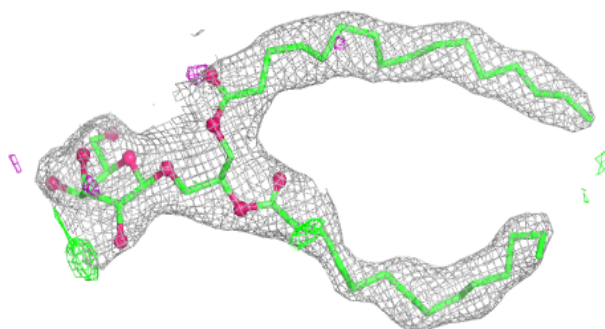


Electron density around STE 1 102:

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

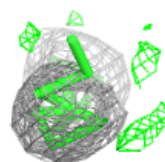
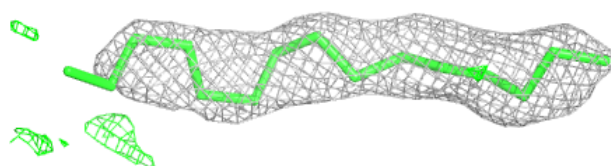
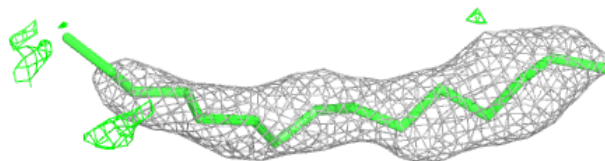
**Electron density around LMG c 523:**

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

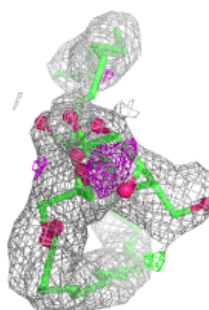
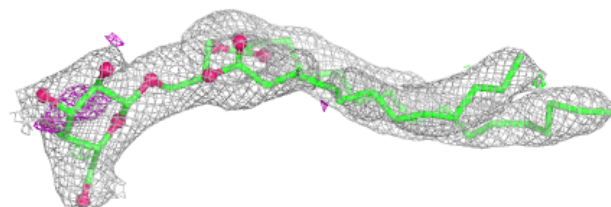
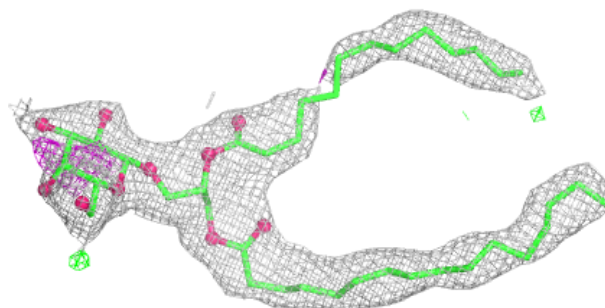


Electron density around STE b 624:

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

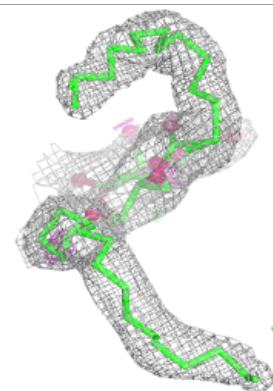
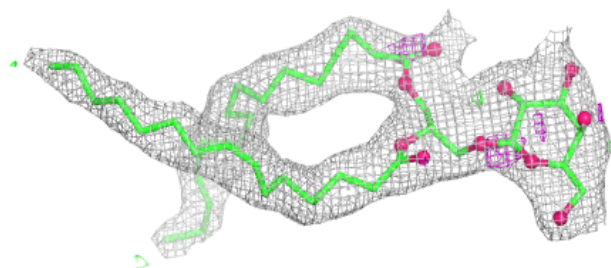
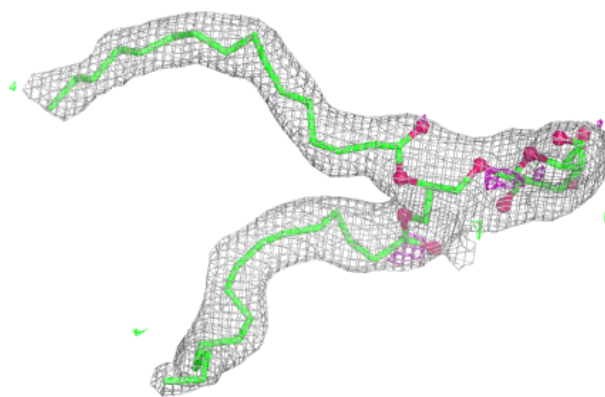
**Electron density around LMG A 612:**

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

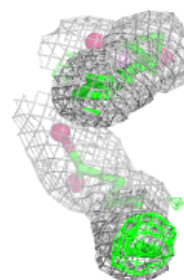
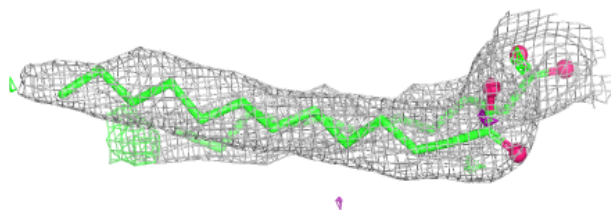
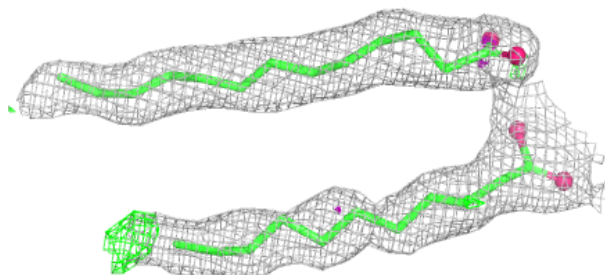


Electron density around LMG m 101:

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

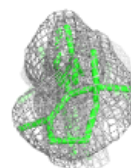
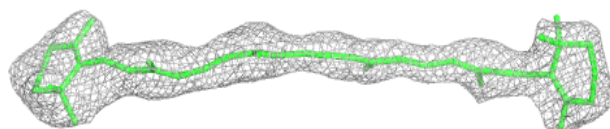
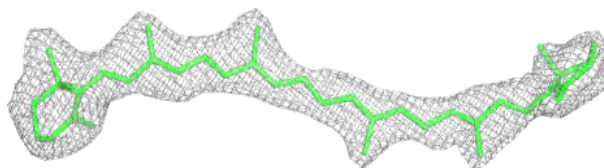
**Electron density around LMG B 621:**

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

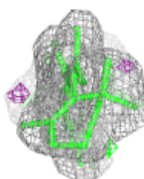
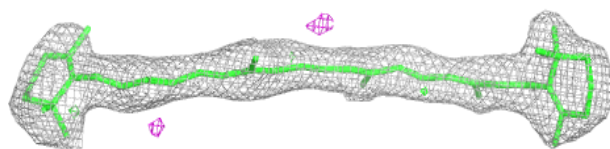


Electron density around BCR k 101:

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

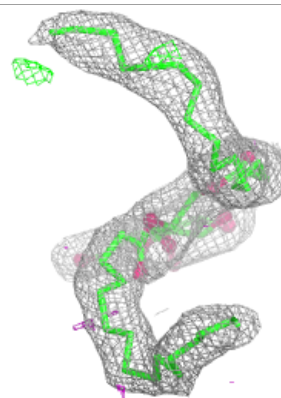
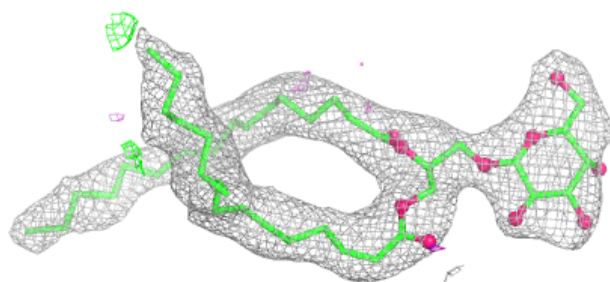
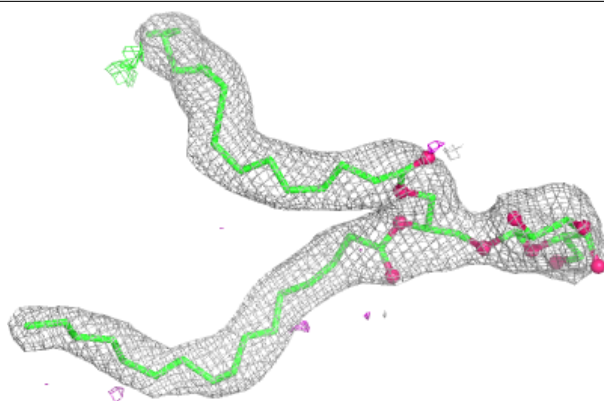
**Electron density around BCR K 102:**

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

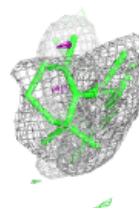
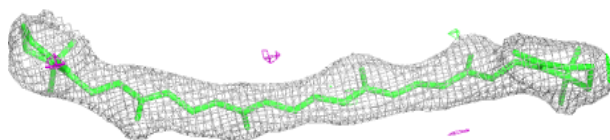
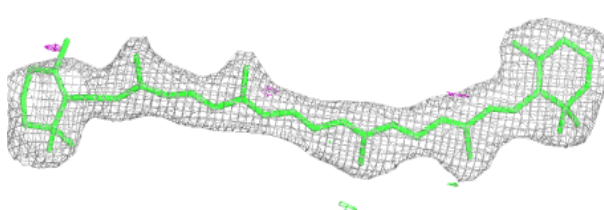


Electron density around LMG M 101:

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

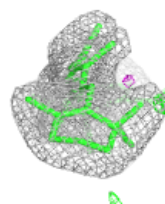
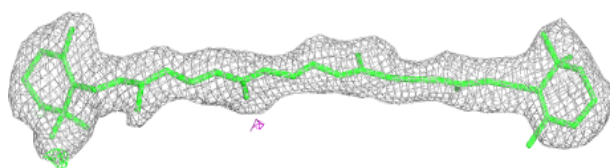
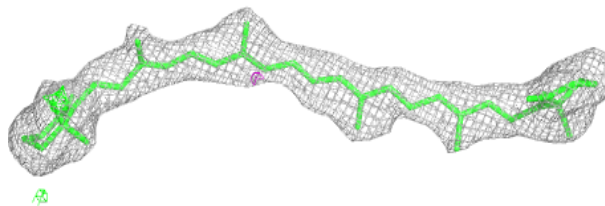
**Electron density around BCR d 405:**

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

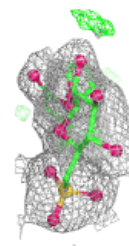
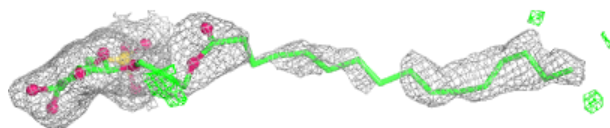
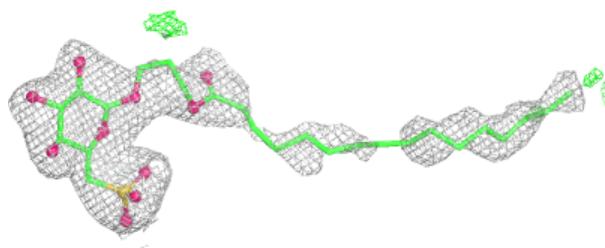


Electron density around BCR h 101:

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

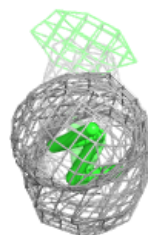
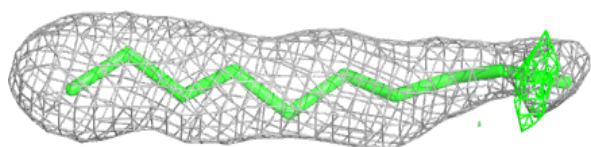
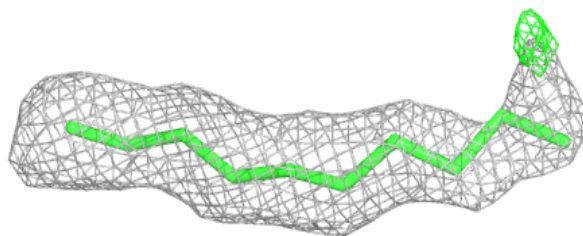
**Electron density around SQD D 409:**

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



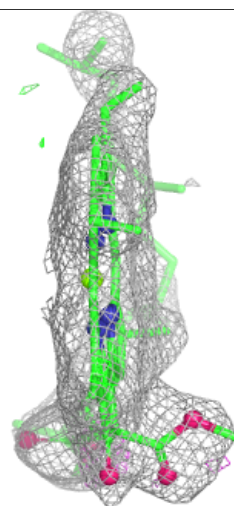
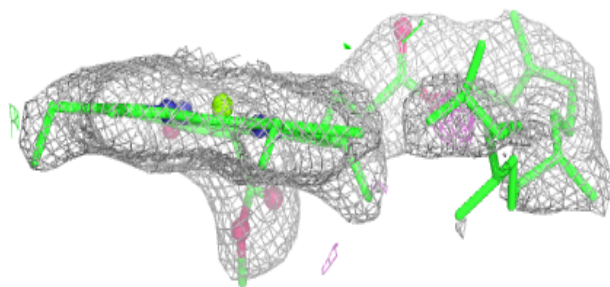
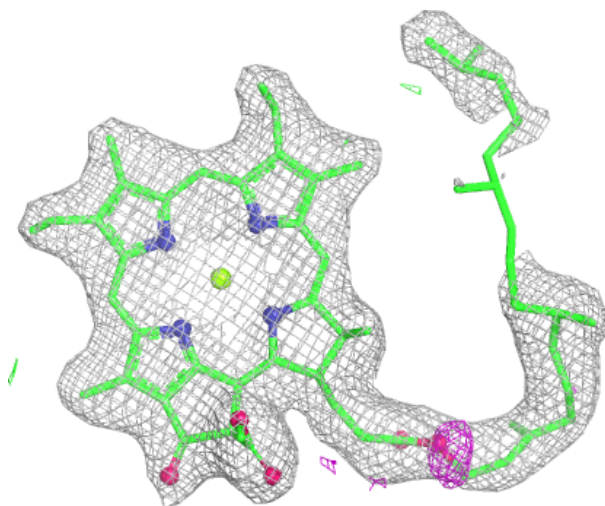
Electron density around STE M 103:

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



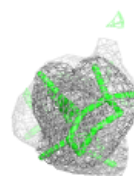
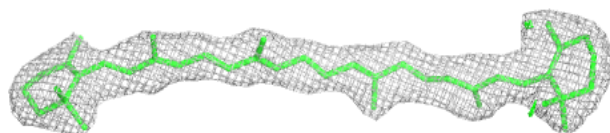
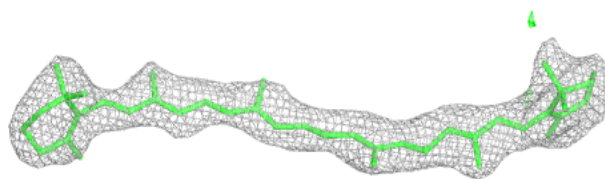
Electron density around CLA c 512:

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

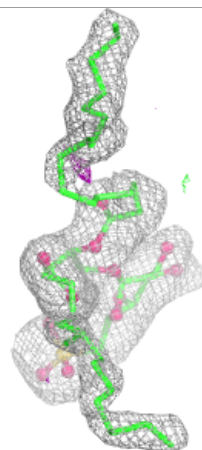
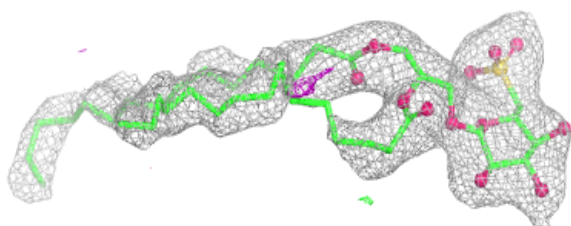
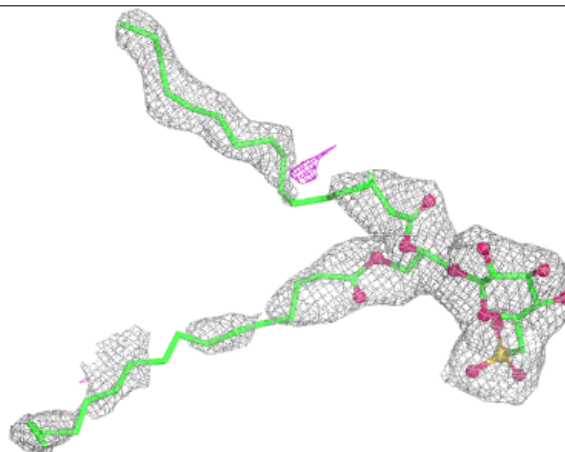


Electron density around BCR c 514:

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

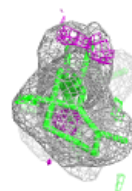
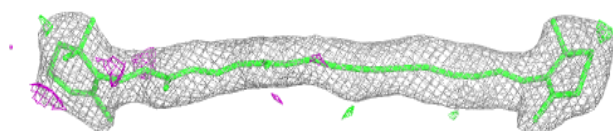
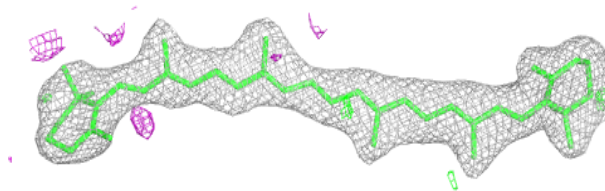
**Electron density around SQD a 613:**

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

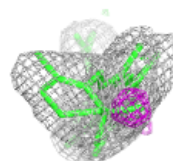
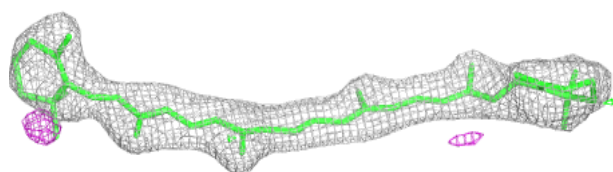
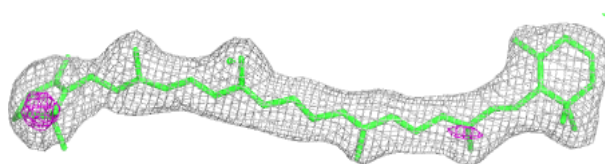


Electron density around BCR B 618:

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

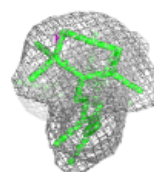
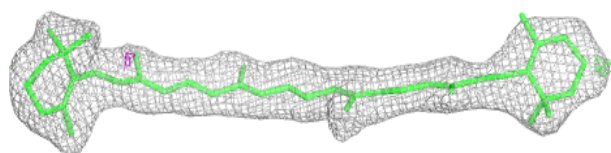
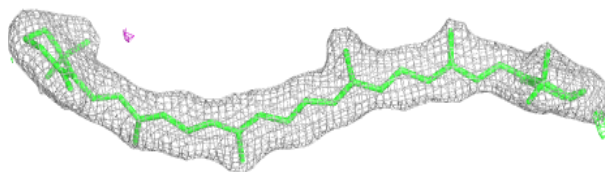
**Electron density around BCR D 406:**

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

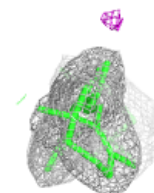
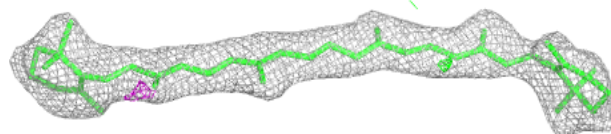
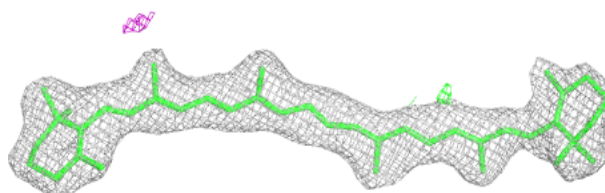


Electron density around BCR H 101:

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

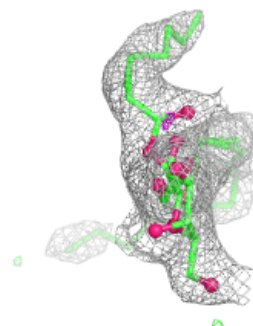
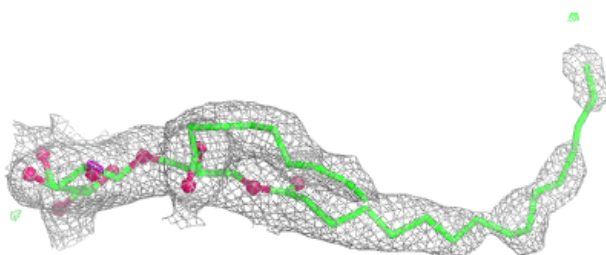
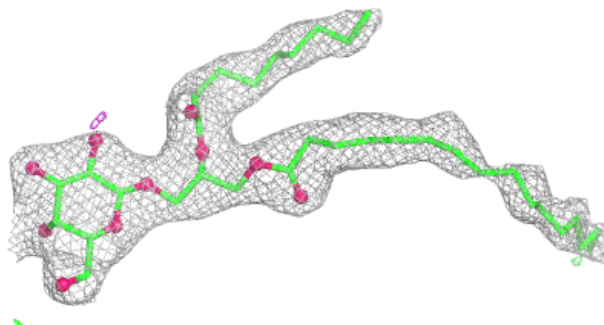
**Electron density around BCR b 619:**

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

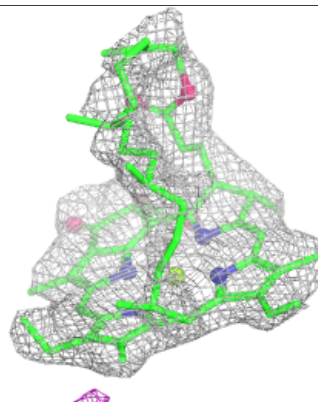
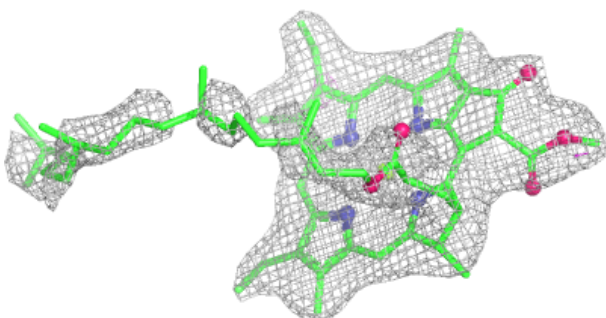
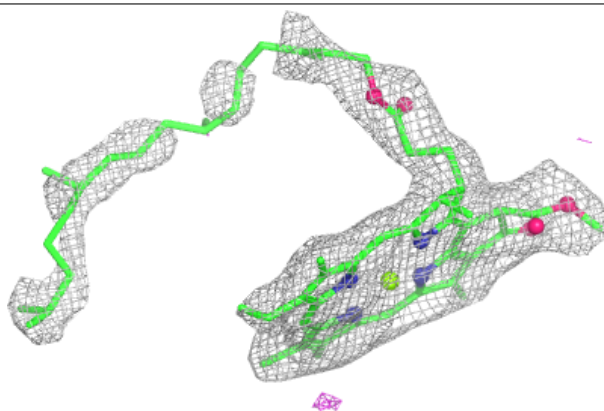


Electron density around LMG d 411:

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

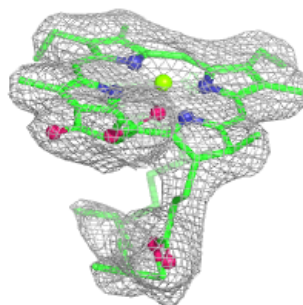
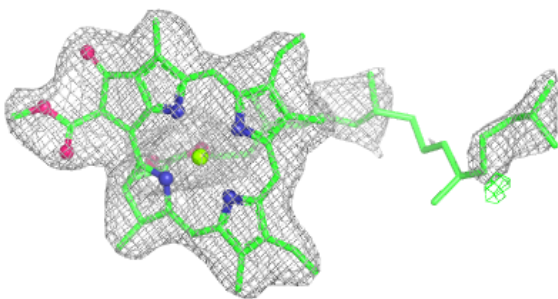
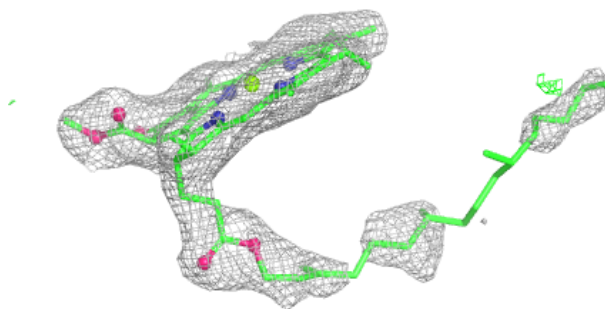
**Electron density around CLA c 513:**

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

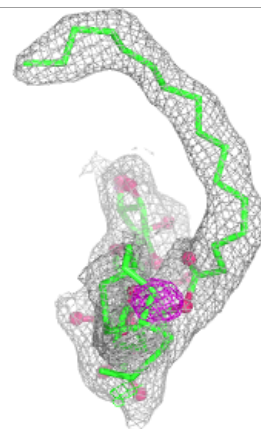
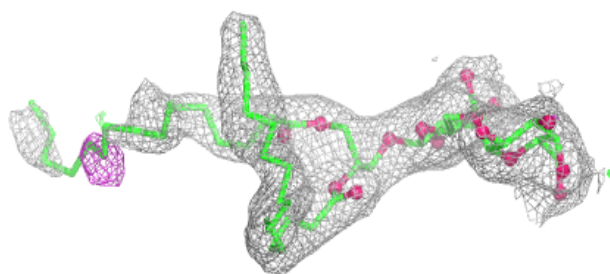
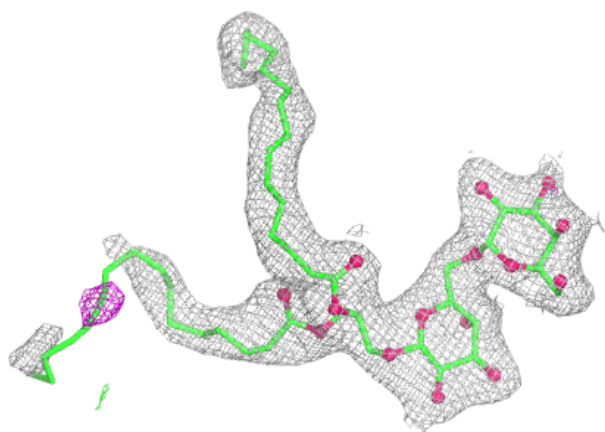


Electron density around CLA C 513:

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

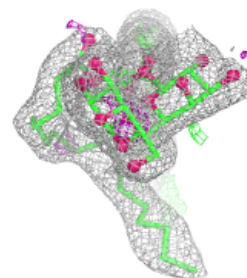
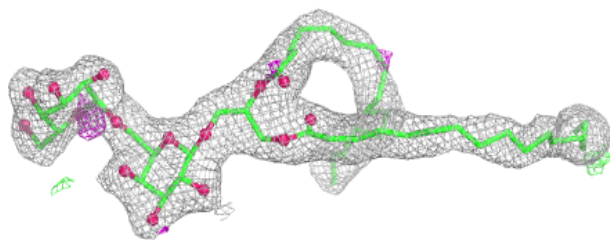
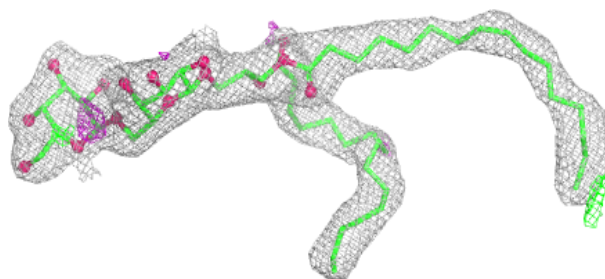
**Electron density around DGD C 517:**

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

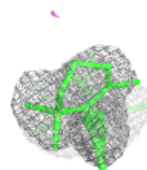
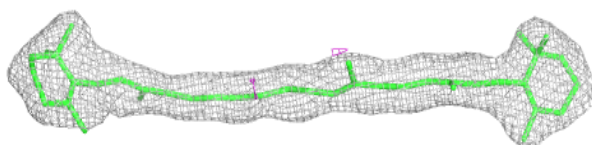
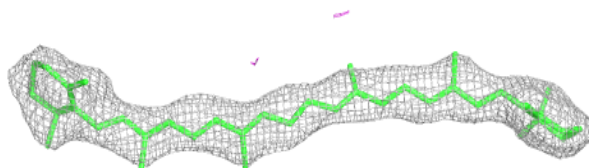


Electron density around DGD H 102:

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

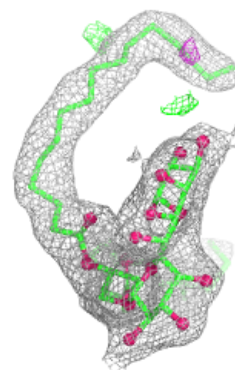
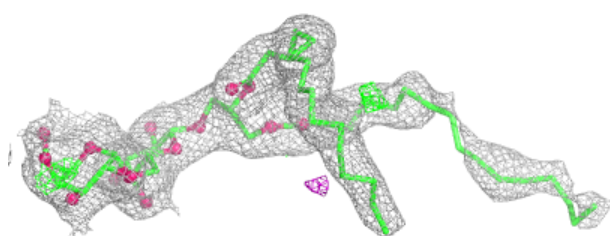
**Electron density around BCR K 101:**

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

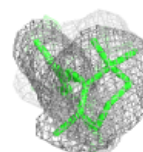
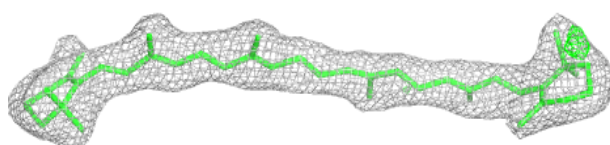
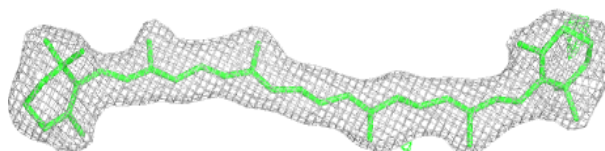


Electron density around DGD c 517:

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

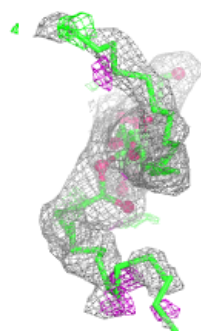
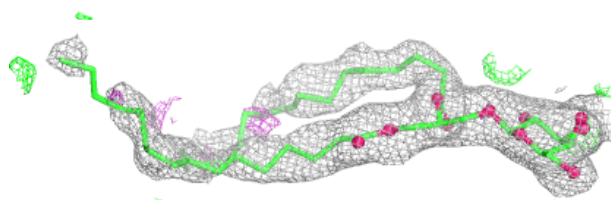
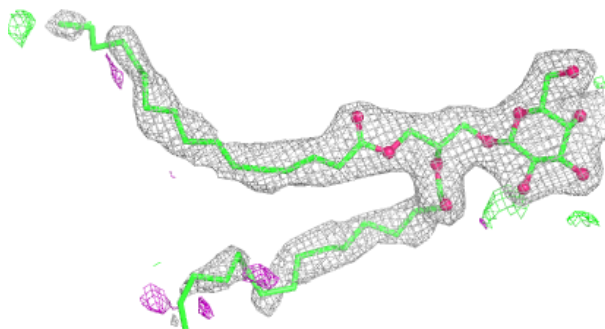
**Electron density around BCR B 619:**

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

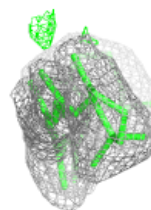
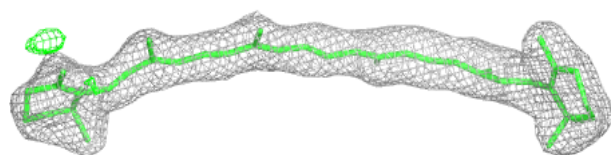
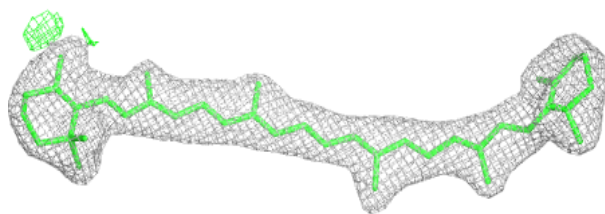


Electron density around LMG D 408:

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

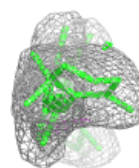
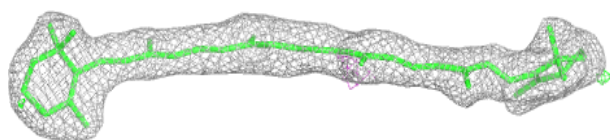
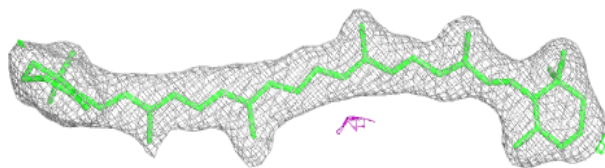
**Electron density around BCR T 101:**

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

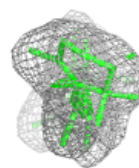
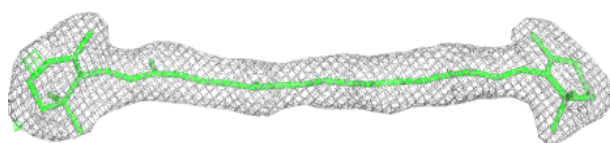
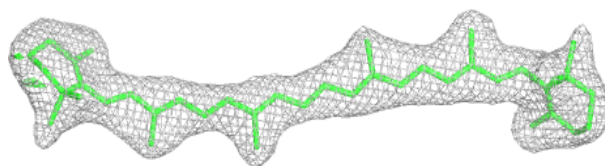


Electron density around BCR b 617:

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

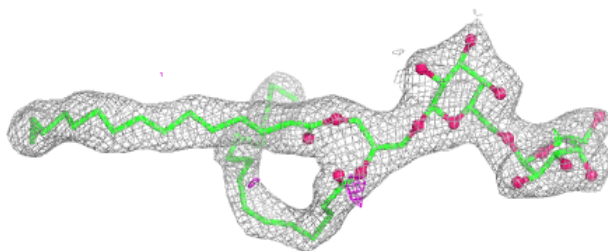
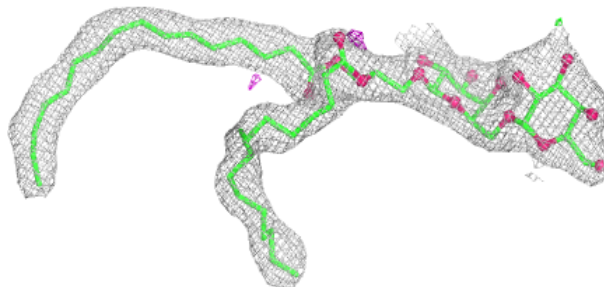
**Electron density around BCR b 618:**

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

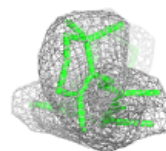
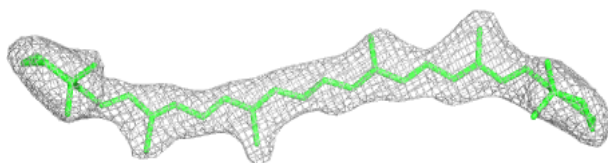
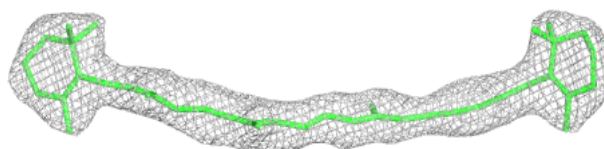


Electron density around DGD h 102:

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

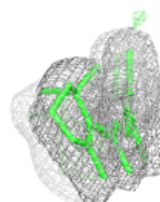
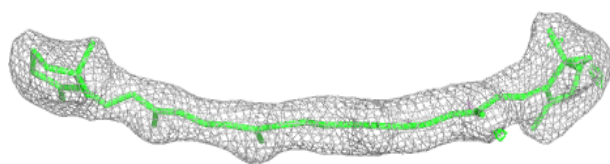
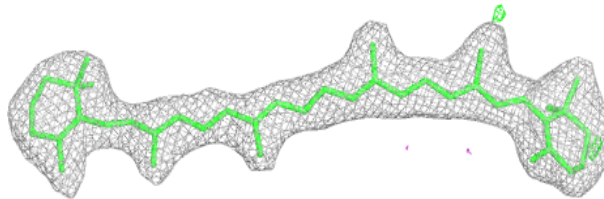
**Electron density around BCR k 102:**

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



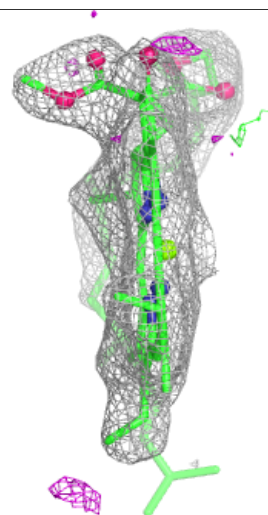
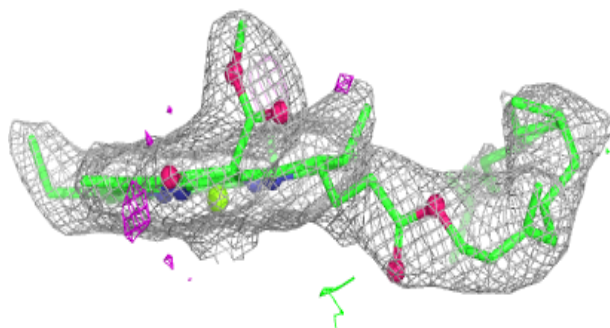
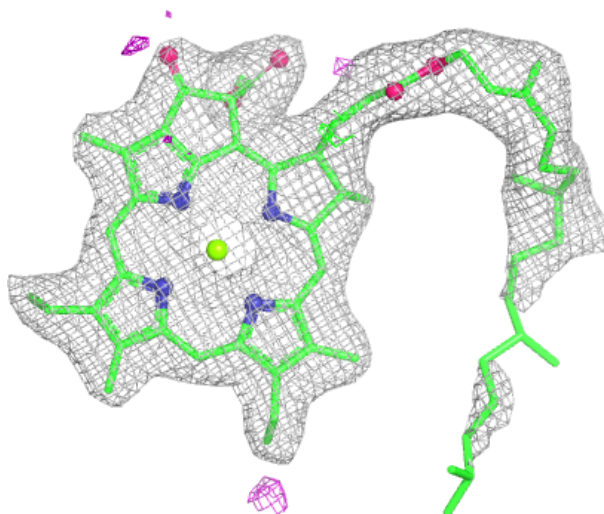
Electron density around BCR t 101:

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



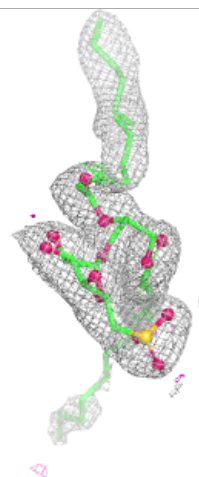
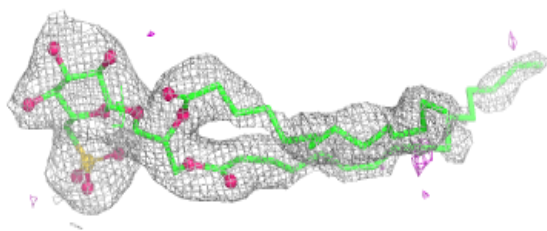
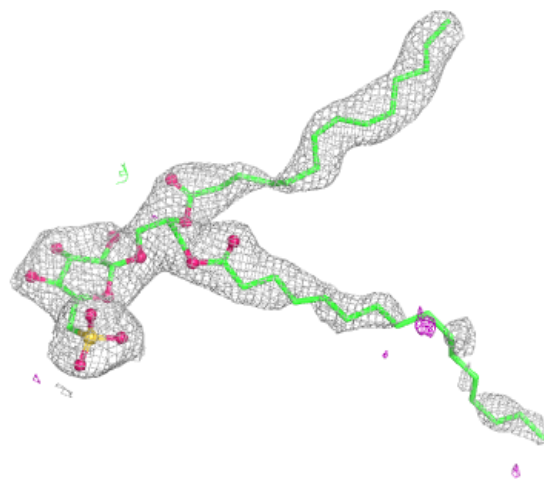
Electron density around CLA C 512:

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



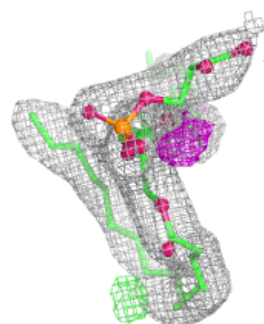
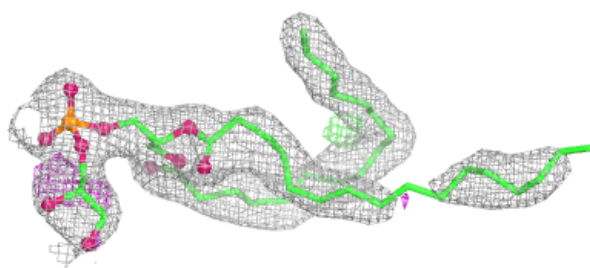
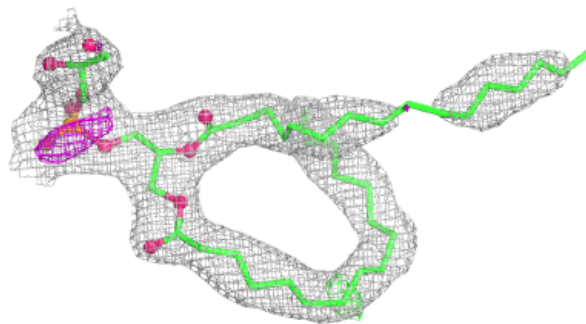
Electron density around SQD A 613:

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

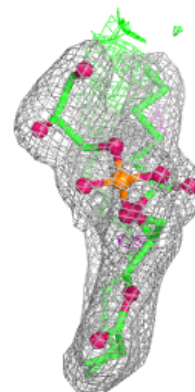
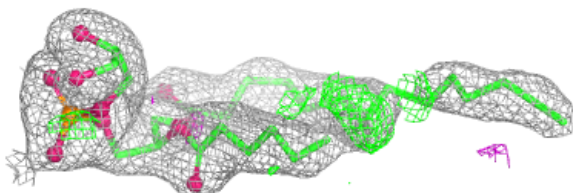
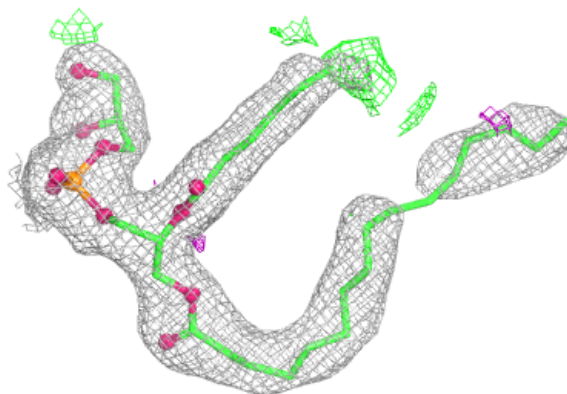


Electron density around LHG d 407:

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

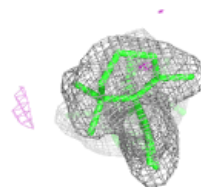
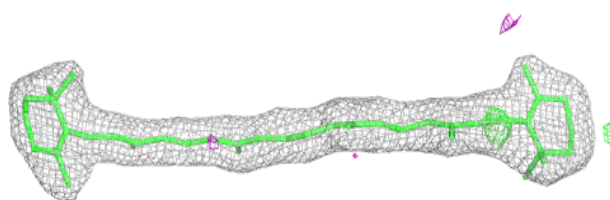
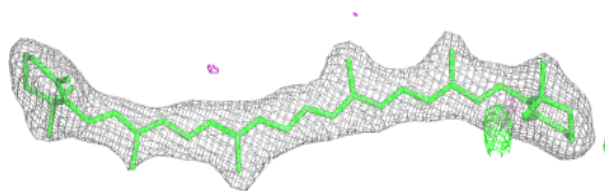
**Electron density around LHG d 409:**

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



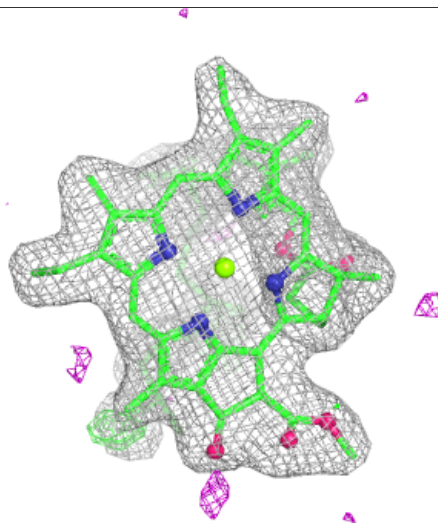
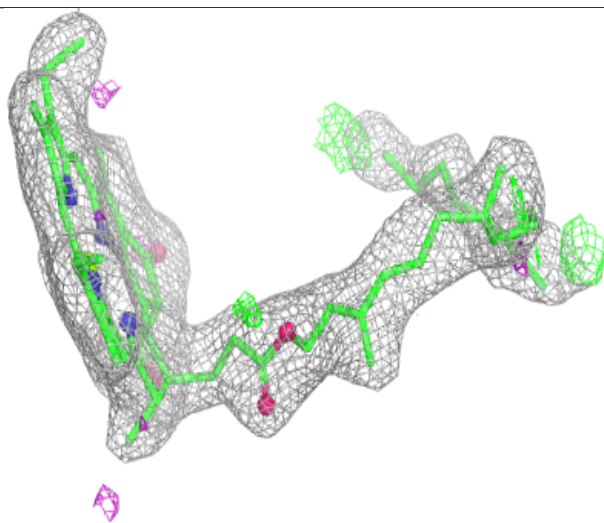
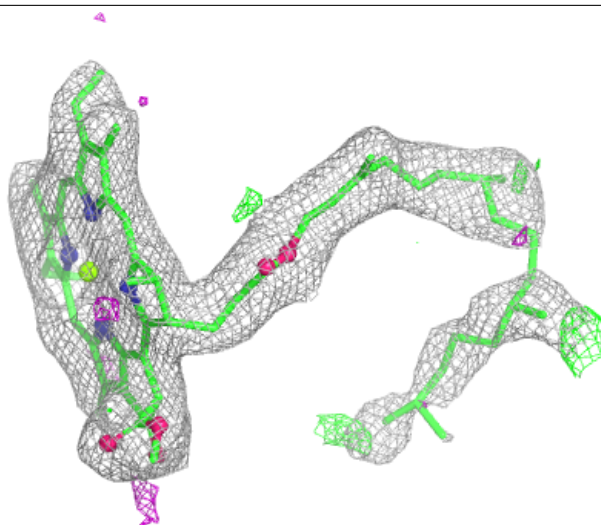
Electron density around BCR C 514:

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



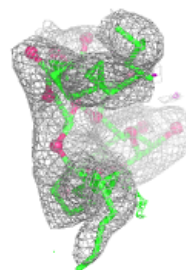
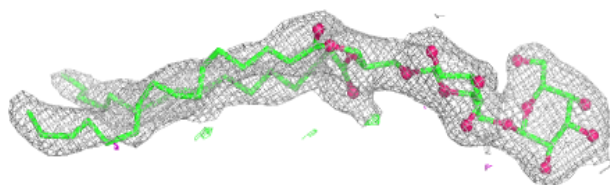
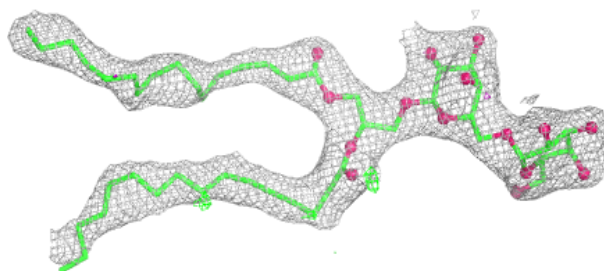
Electron density around CLA B 606:

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

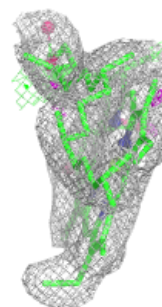
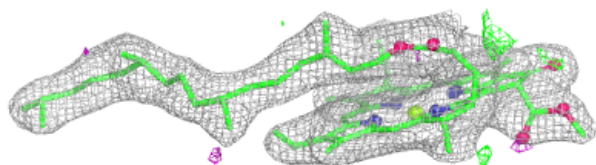
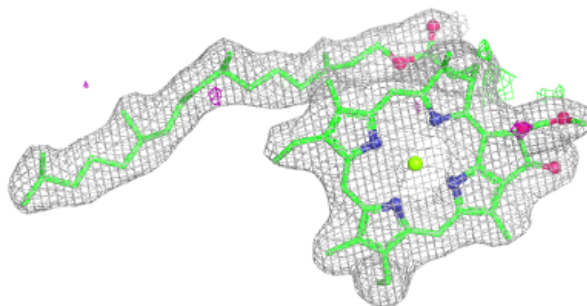


Electron density around DGD c 518:

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

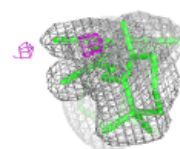
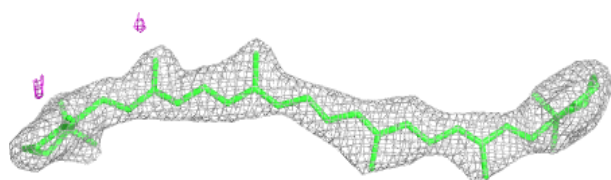
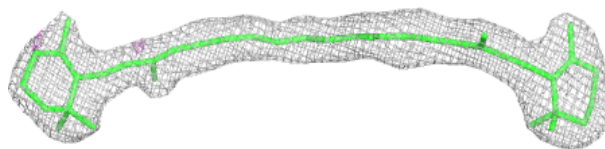
**Electron density around CLA C 501:**

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

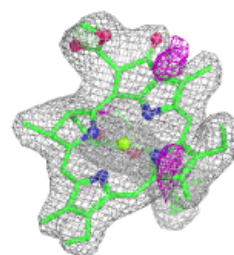
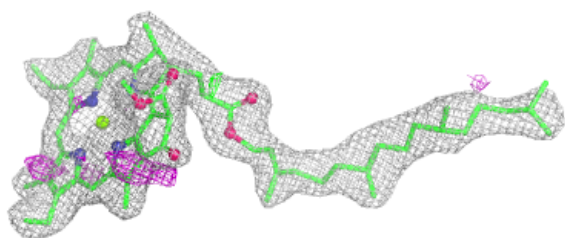
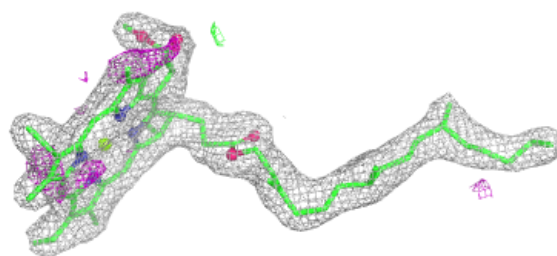


Electron density around BCR C 515:

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

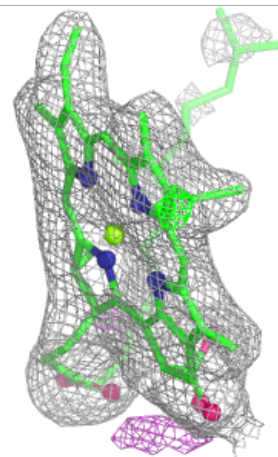
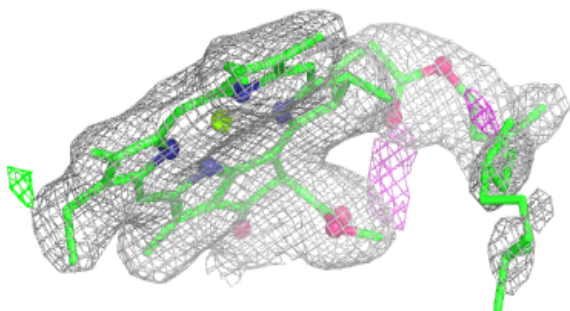
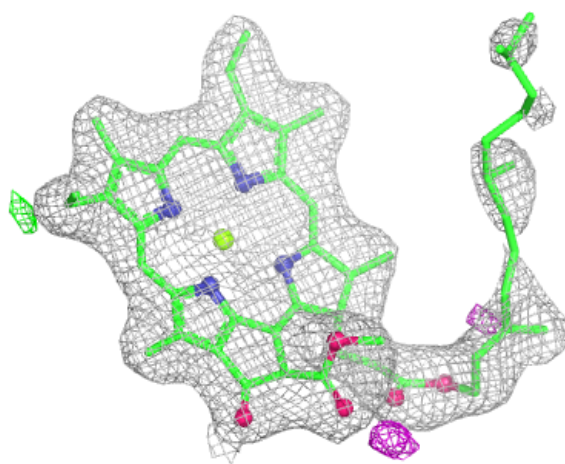
**Electron density around CLA C 502:**

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



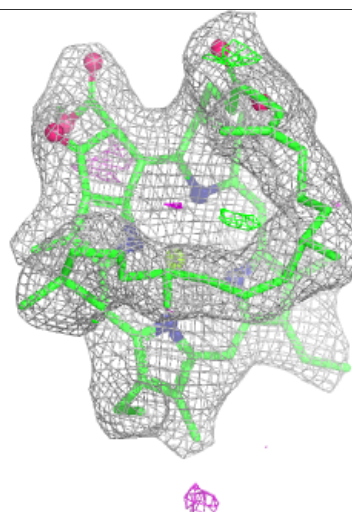
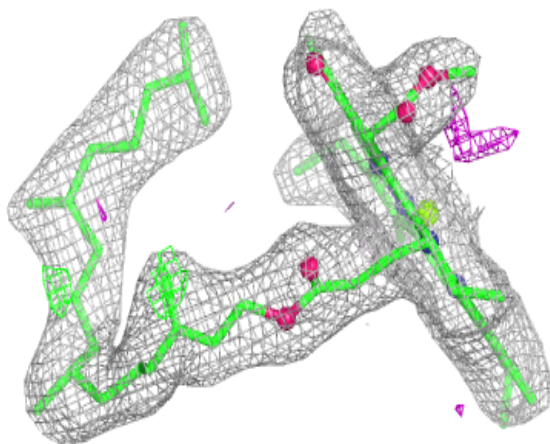
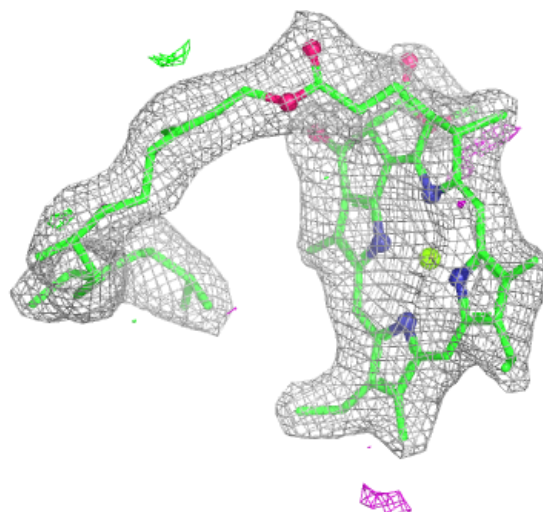
Electron density around CLA b 616:

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



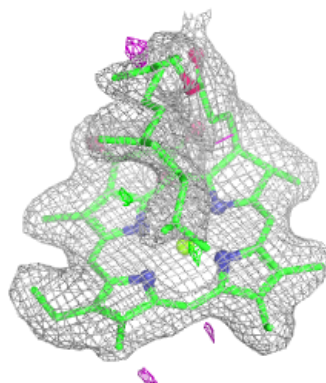
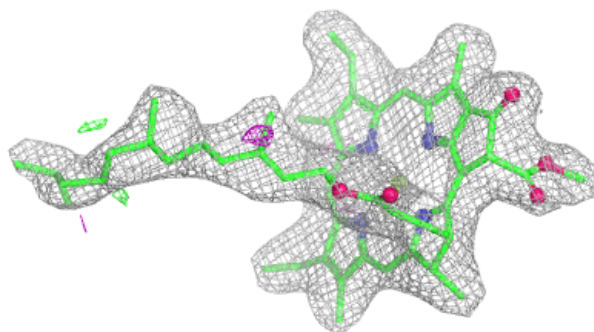
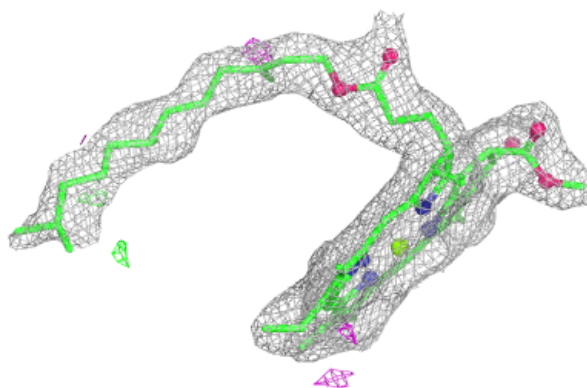
Electron density around CLA c 503:

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

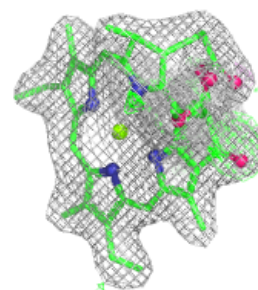
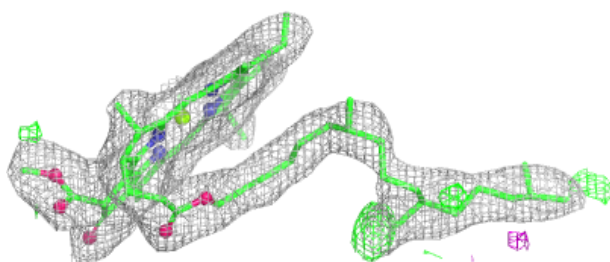
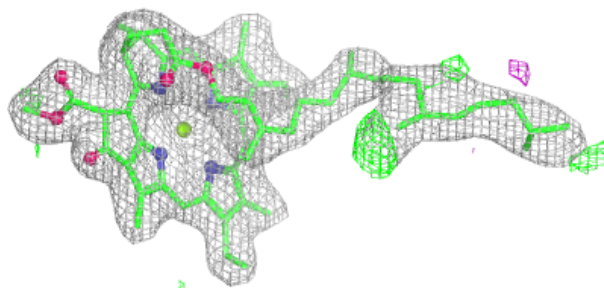


Electron density around CLA c 504:

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

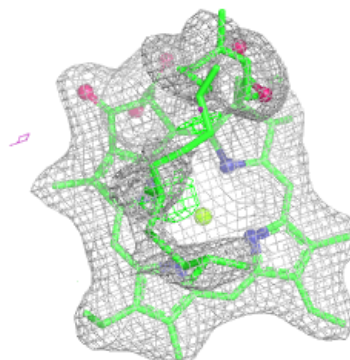
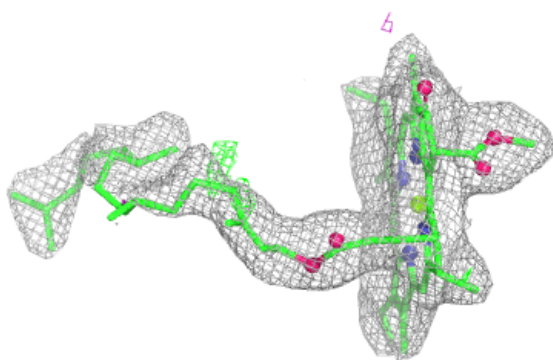
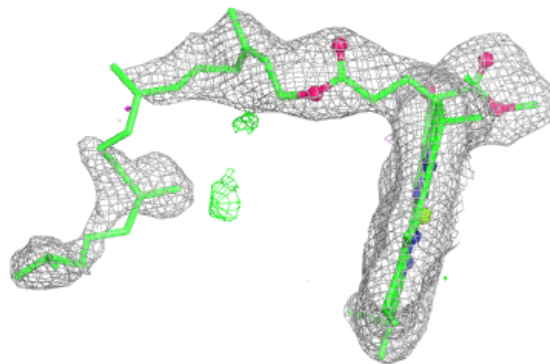
**Electron density around CLA c 505:**

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

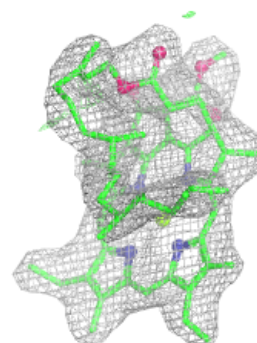
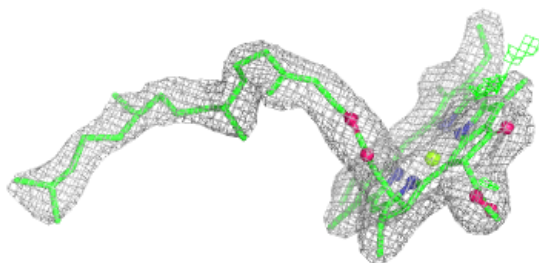
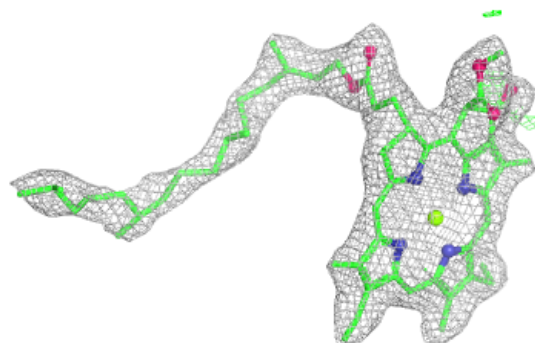


Electron density around CLA c 506:

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

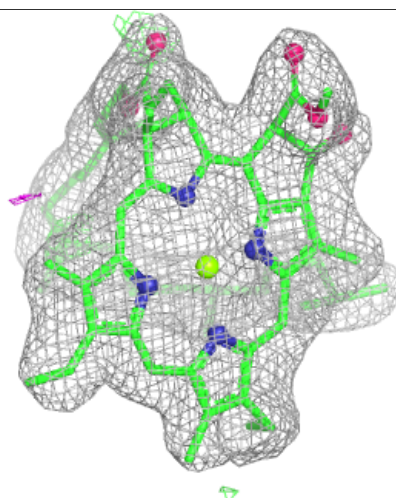
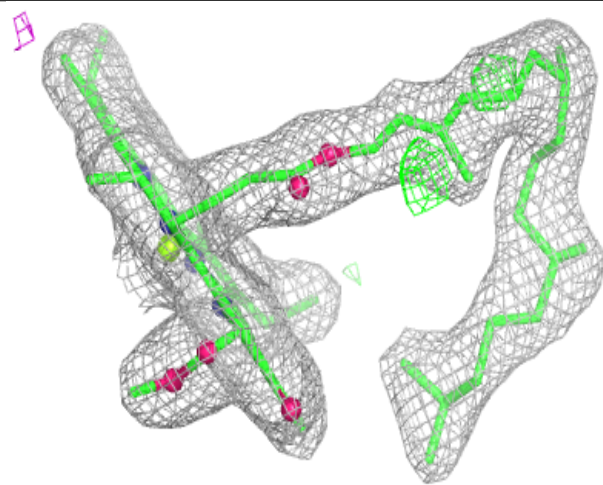
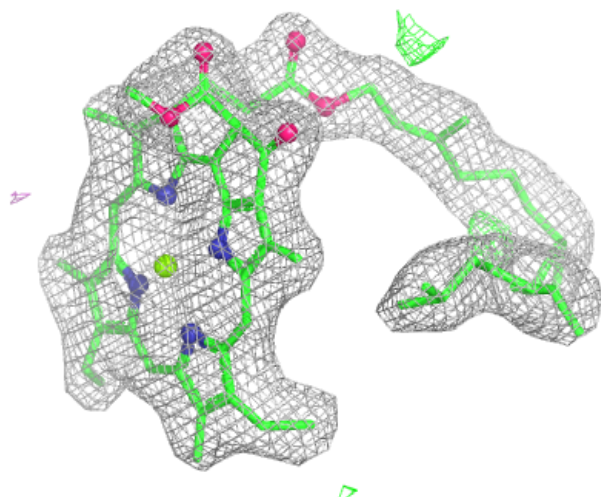
**Electron density around CLA c 511:**

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



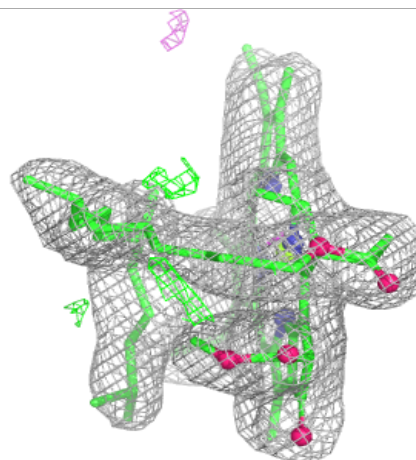
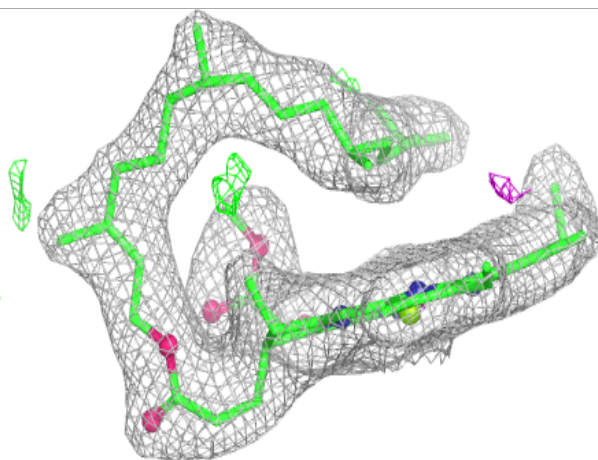
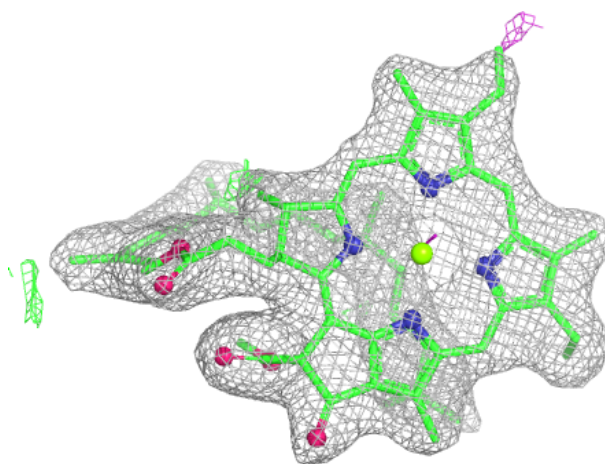
Electron density around CLA C 503:

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



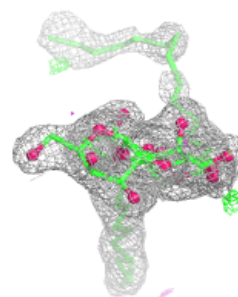
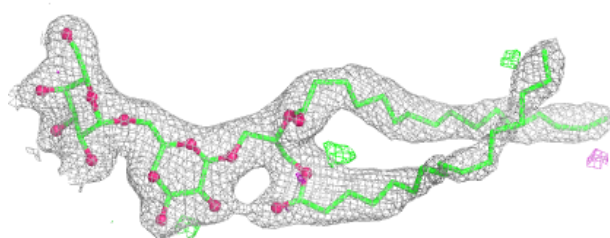
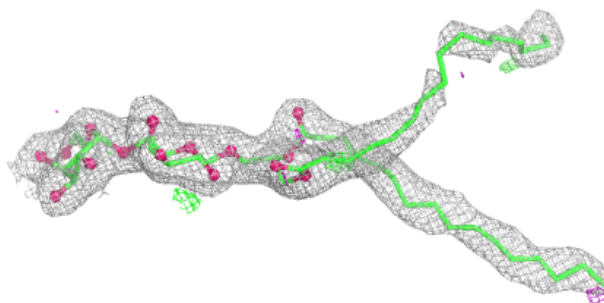
Electron density around CLA C 510:

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

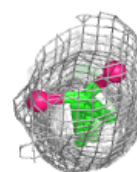
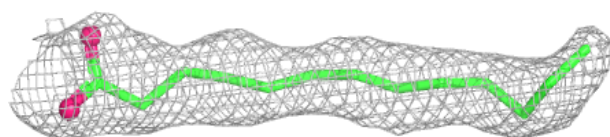
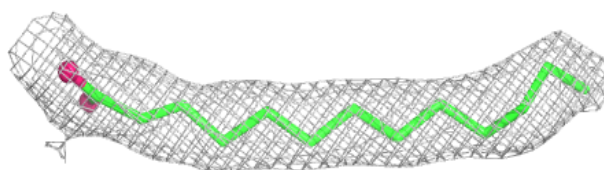


Electron density around DGD C 516:

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

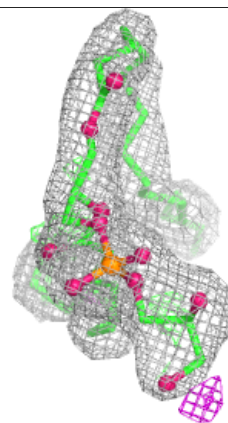
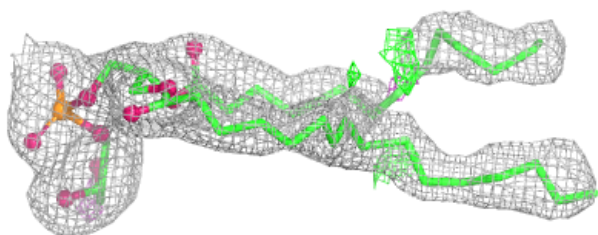
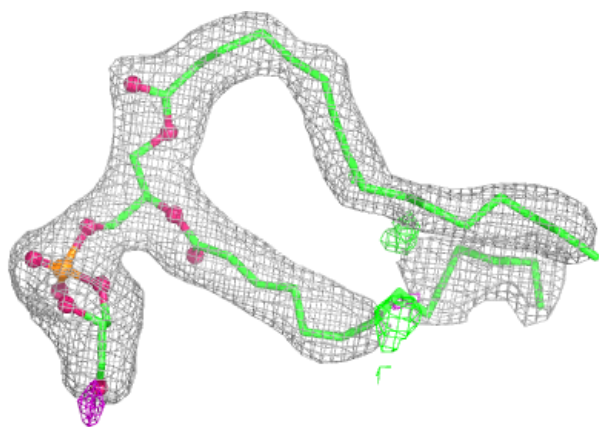
**Electron density around STE M 102:**

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

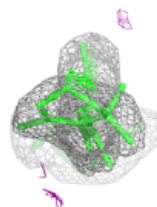
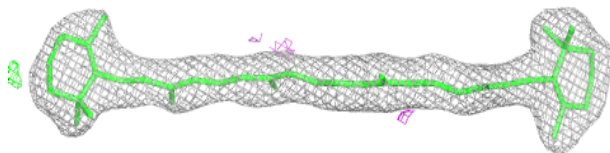
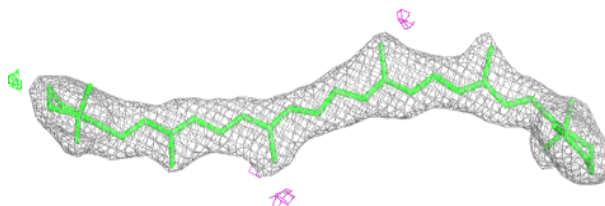


Electron density around LHG D 411:

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

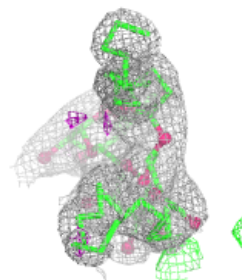
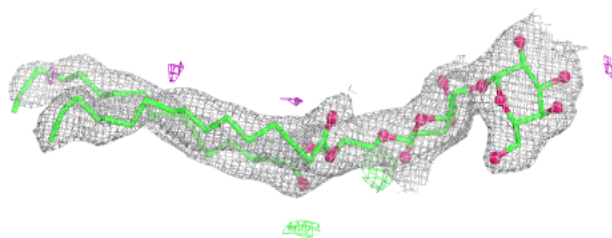
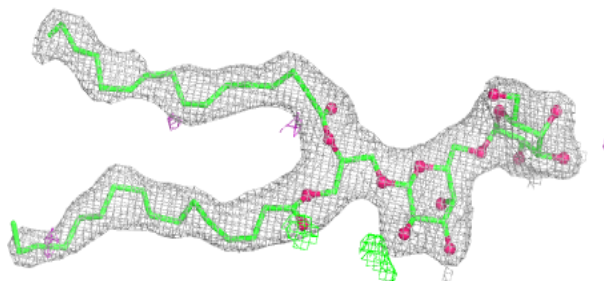
**Electron density around BCR c 515:**

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

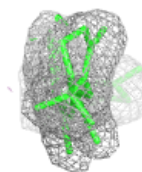
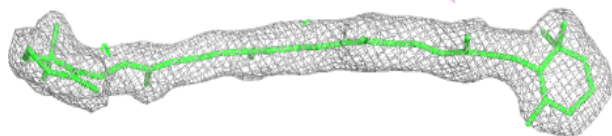
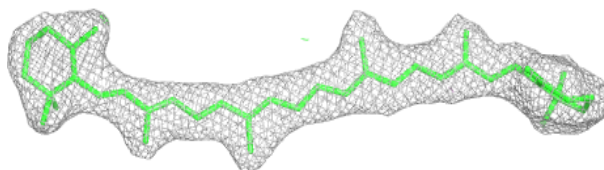


Electron density around DGD C 518:

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

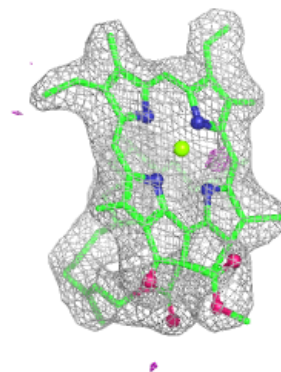
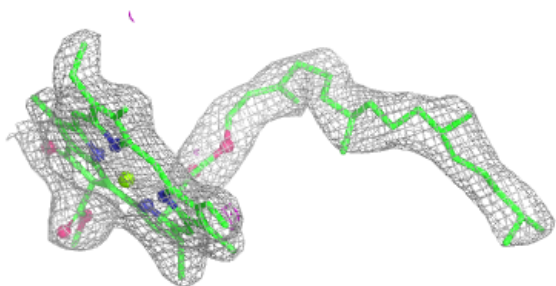
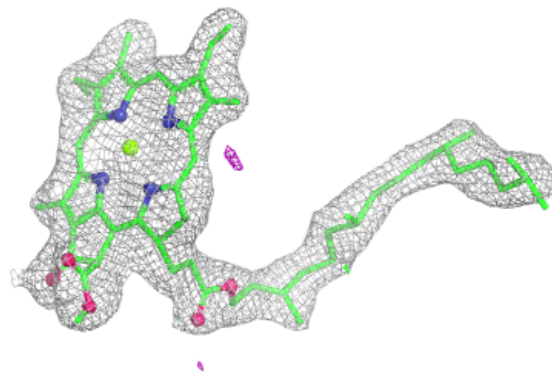
**Electron density around BCR B 617:**

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

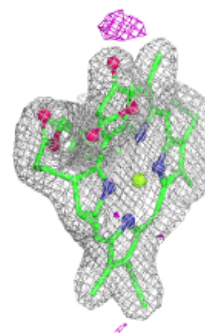
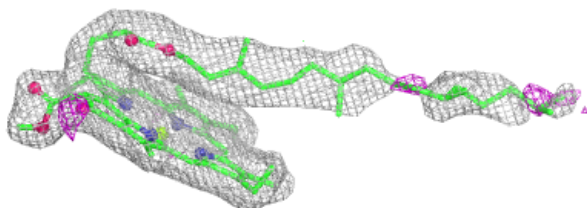
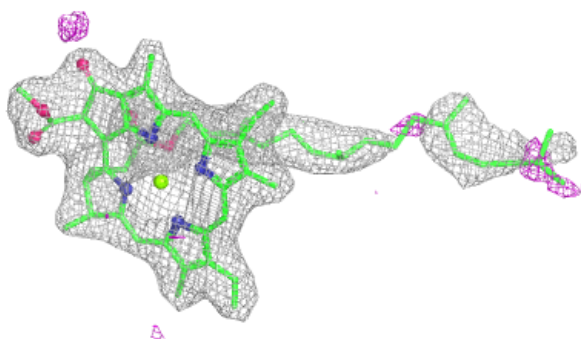


Electron density around CLA C 511:

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

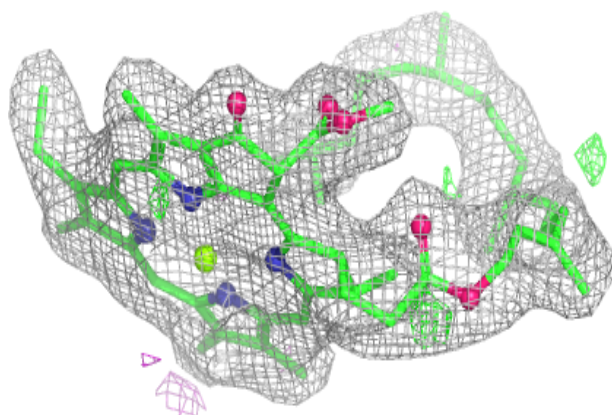
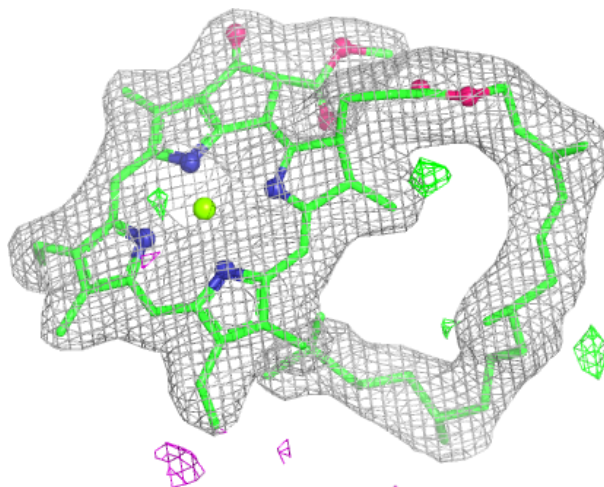
**Electron density around CLA b 614:**

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



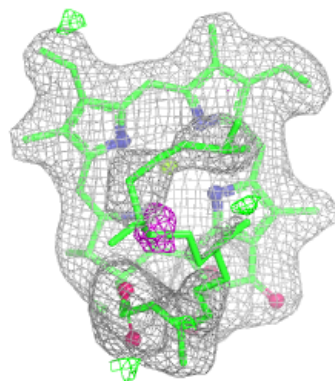
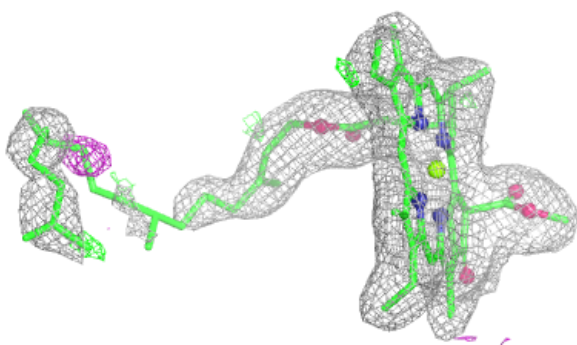
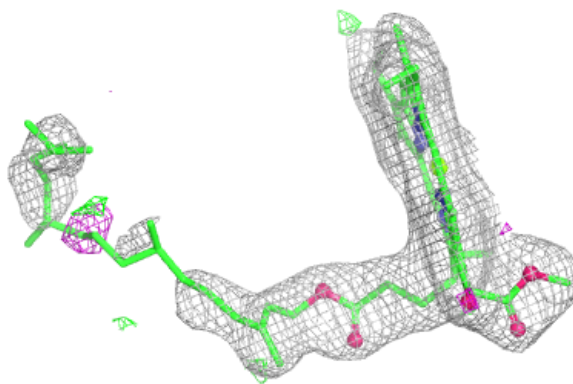
Electron density around CLA b 615:

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

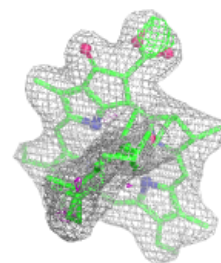
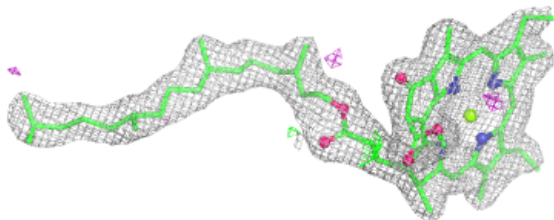
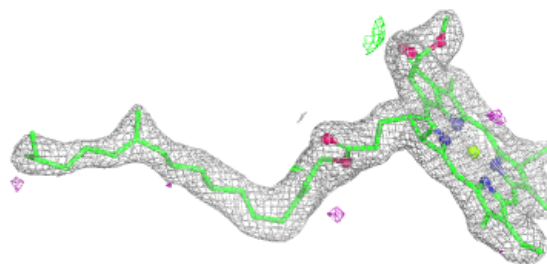


Electron density around CLA C 506:

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

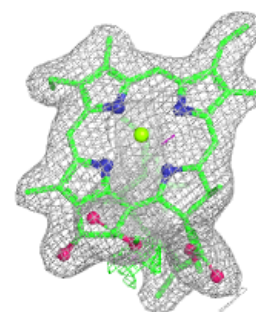
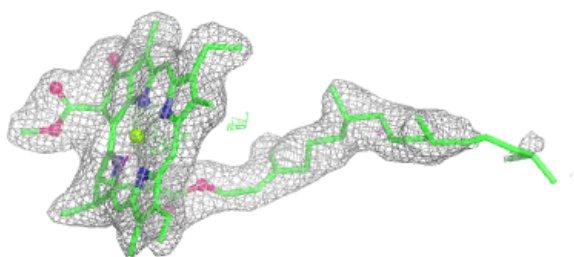
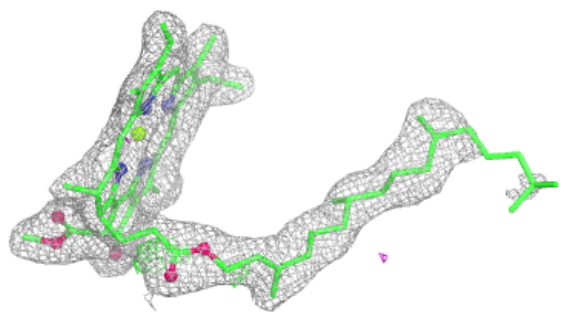
**Electron density around CLA c 502:**

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



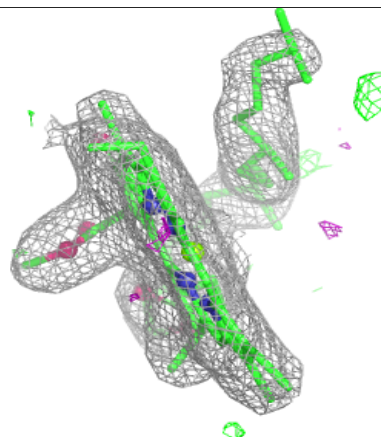
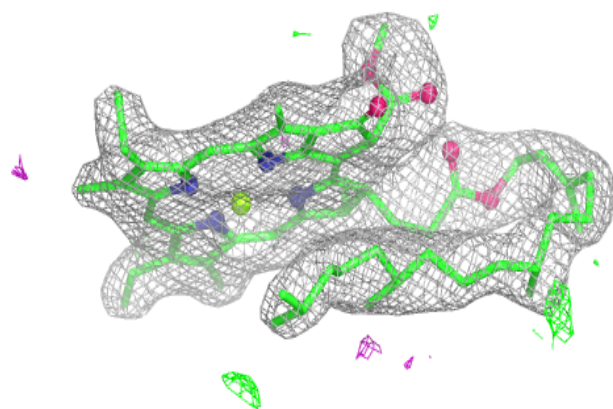
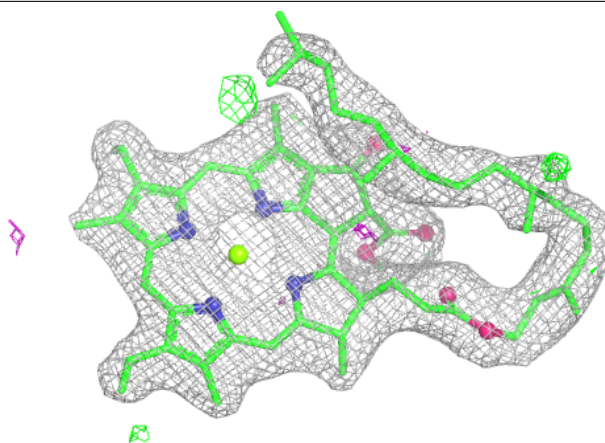
Electron density around CLA C 508:

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



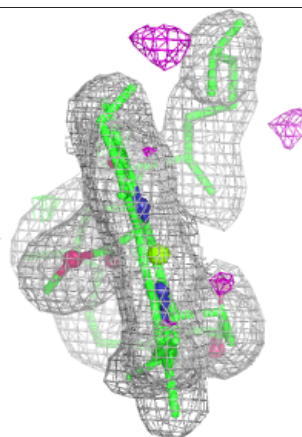
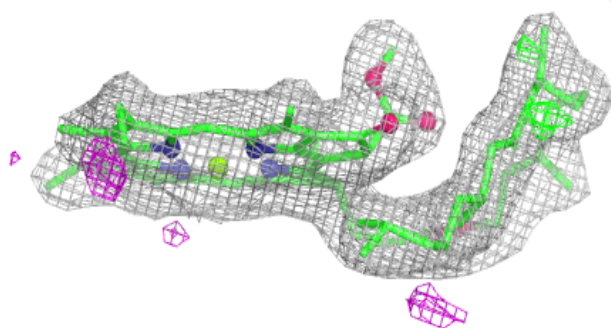
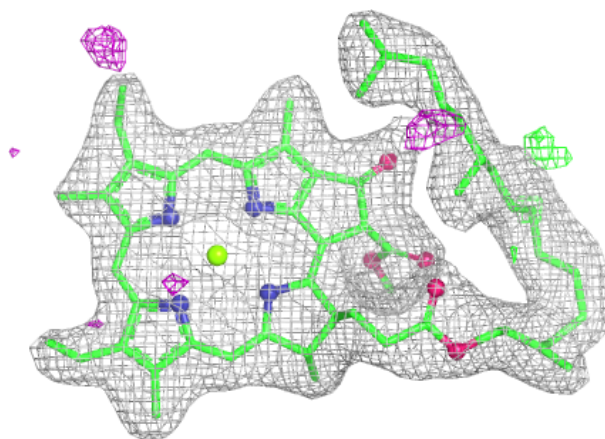
Electron density around CLA C 509:

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

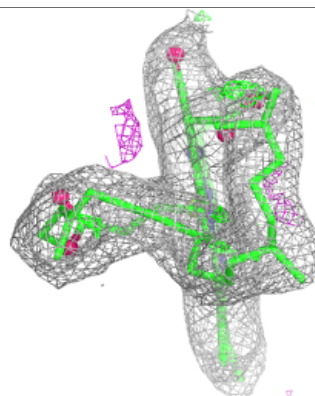
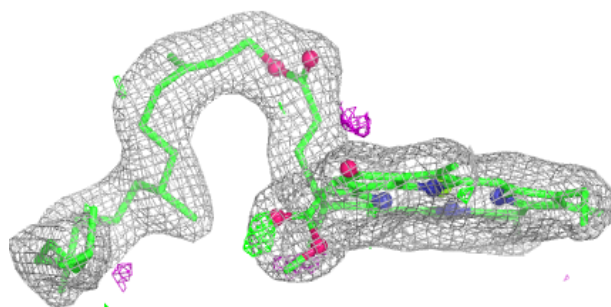
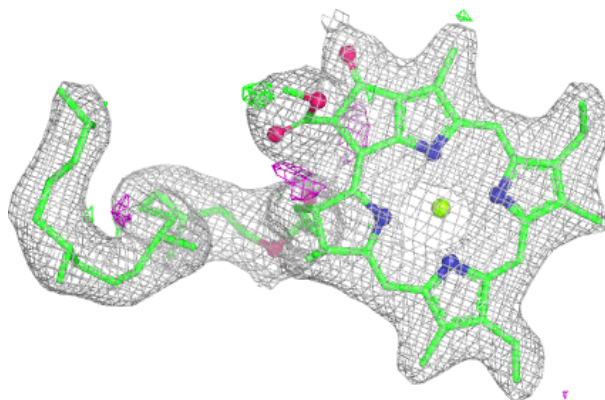


Electron density around CLA B 610:

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

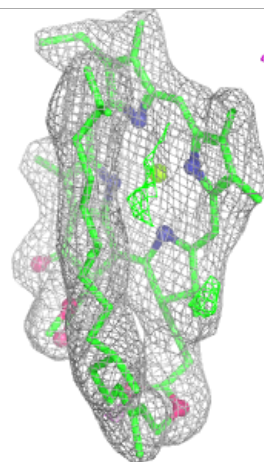
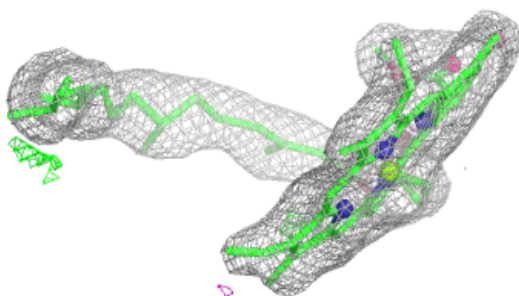
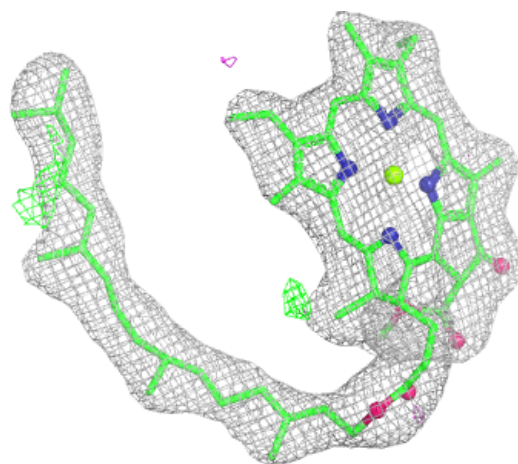
**Electron density around CLA B 612:**

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



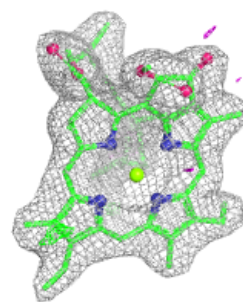
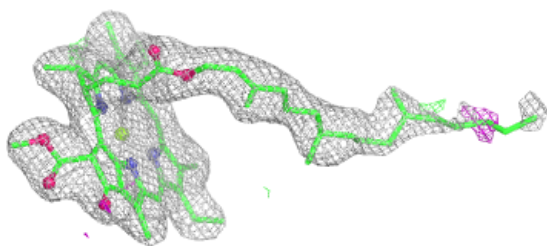
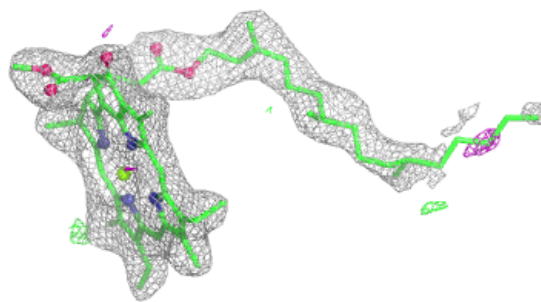
Electron density around CLA c 507:

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



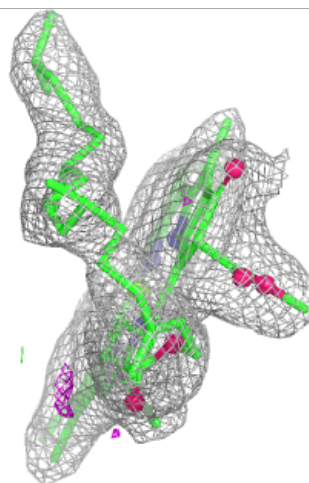
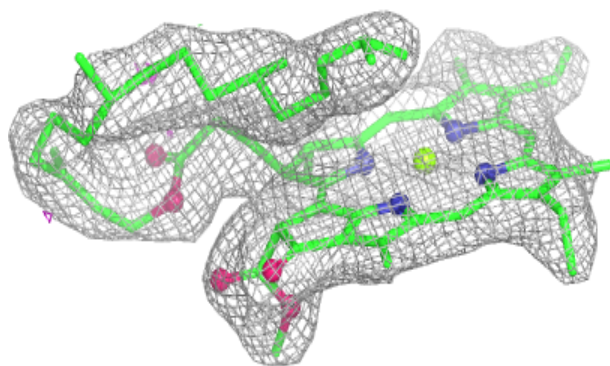
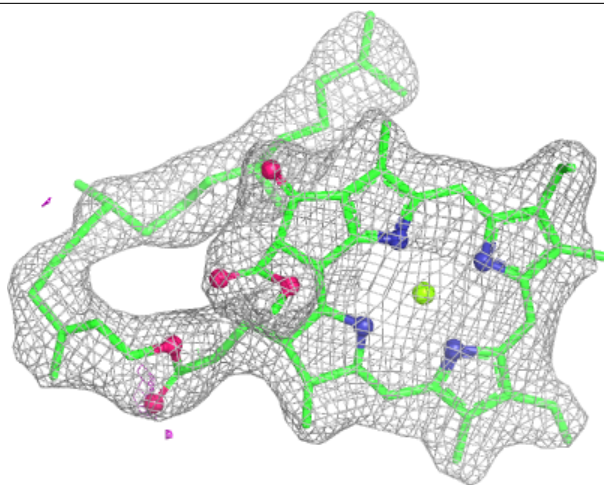
Electron density around CLA c 508:

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



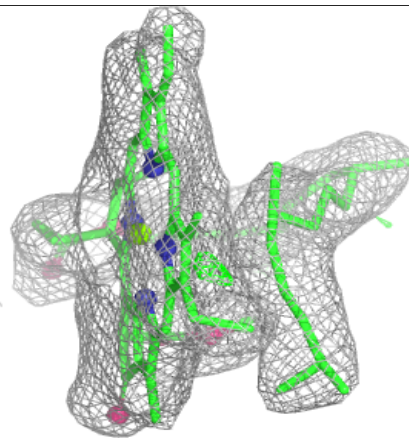
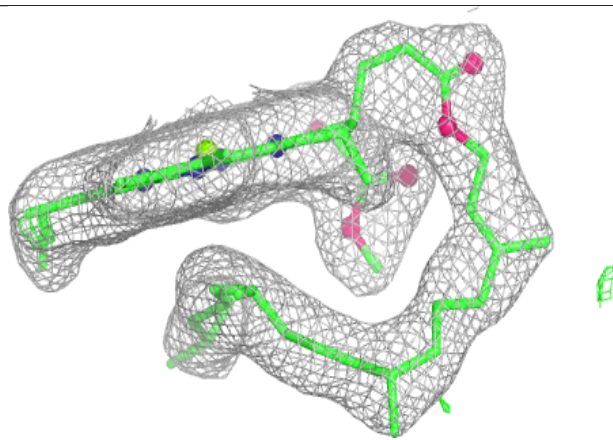
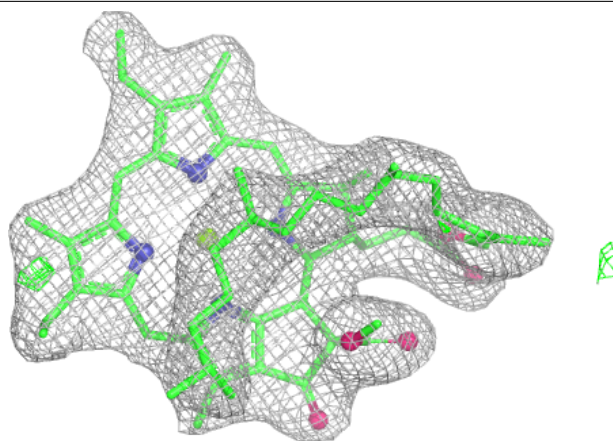
Electron density around CLA c 509:

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



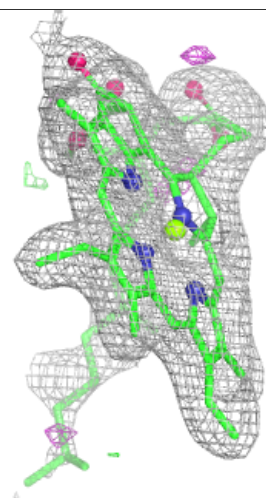
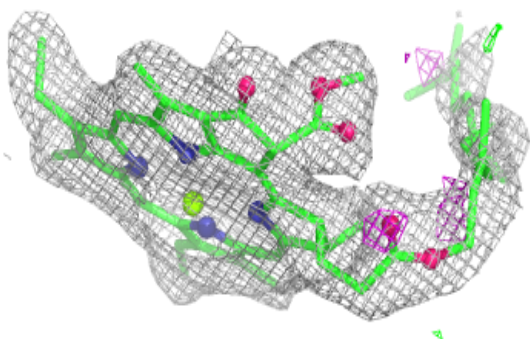
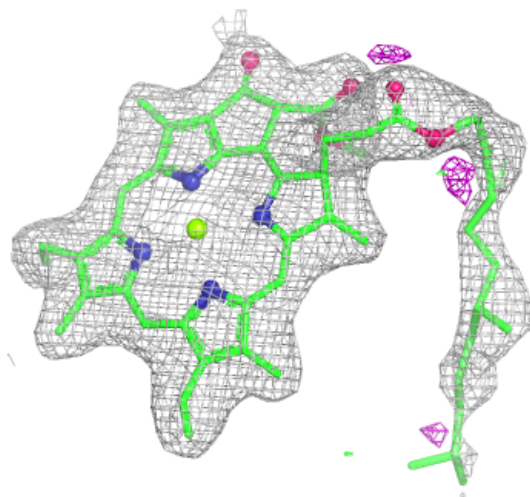
Electron density around CLA c 510:

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



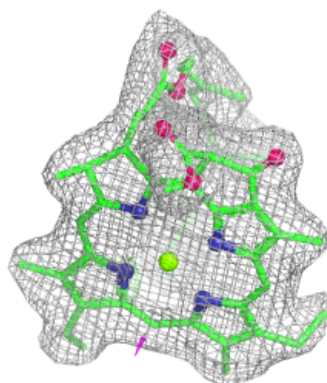
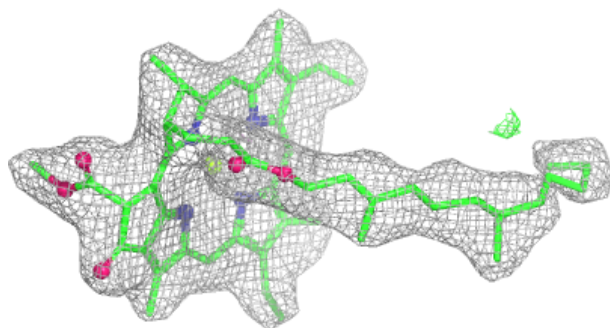
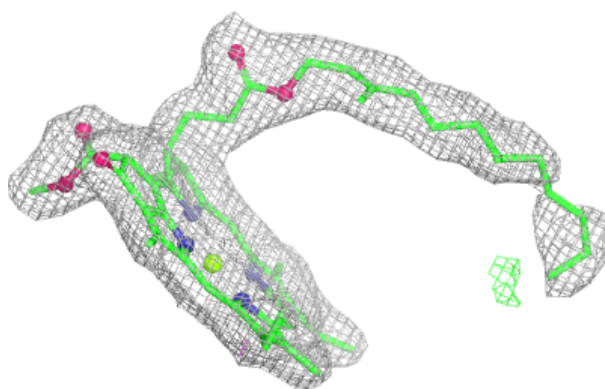
Electron density around CLA B 616:

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

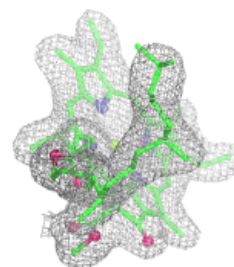
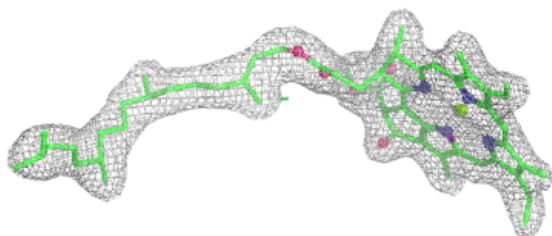
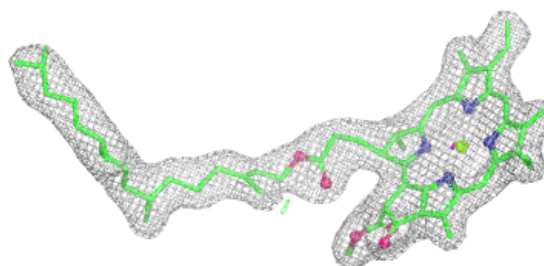


Electron density around CLA C 504:

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

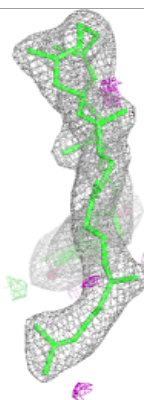
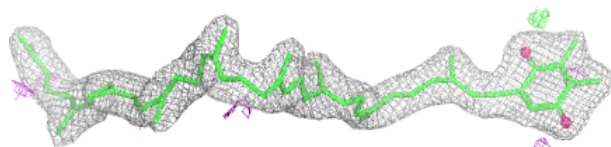
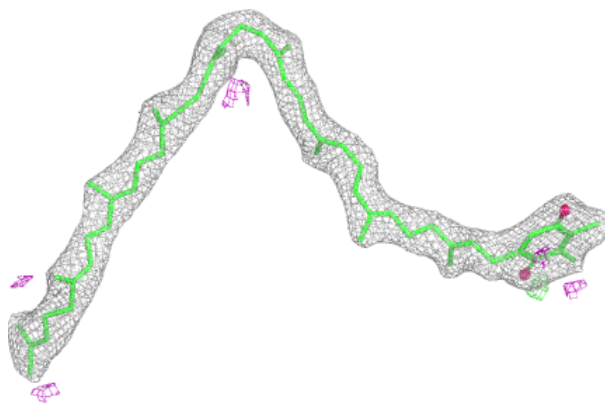
**Electron density around CLA a 606:**

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

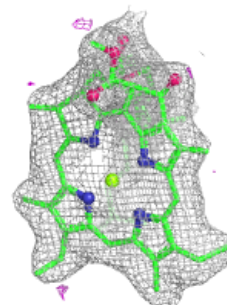
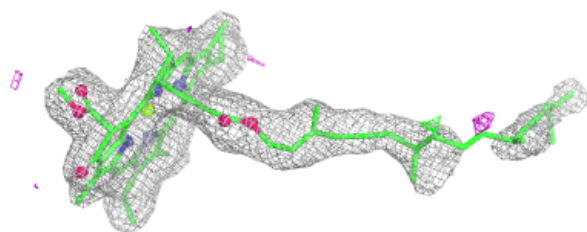
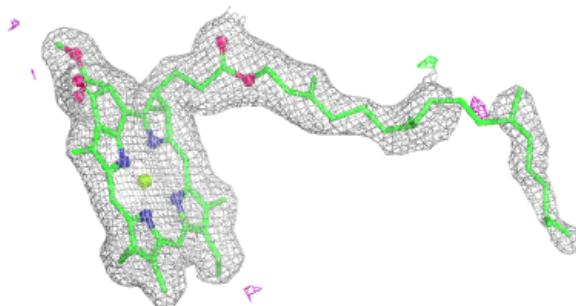


Electron density around PL9 D 407:

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

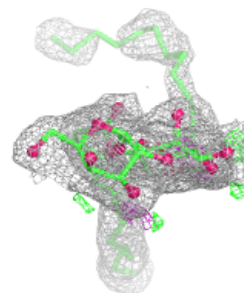
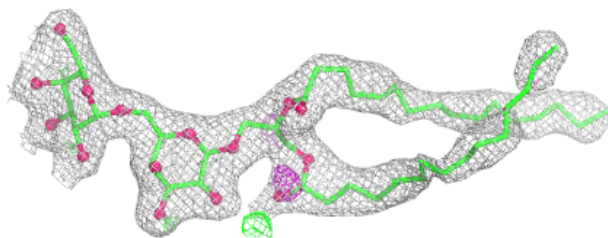
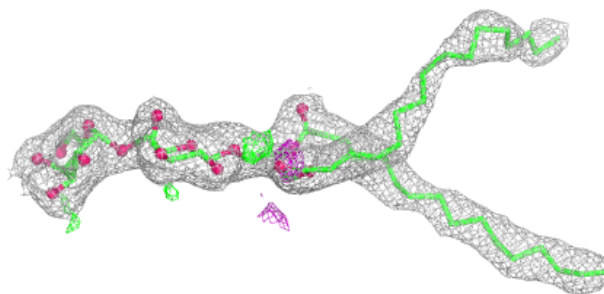
**Electron density around CLA d 404:**

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

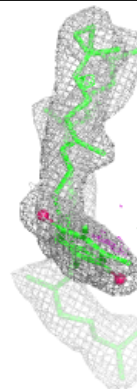
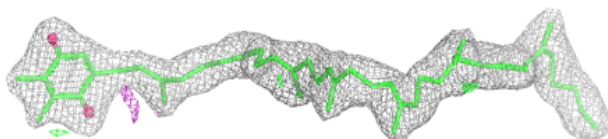
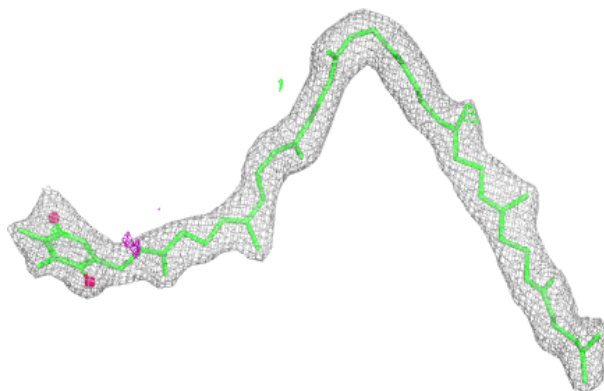


Electron density around DGD c 516:

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

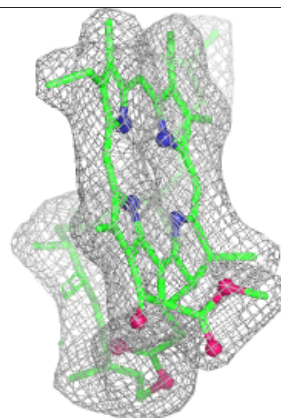
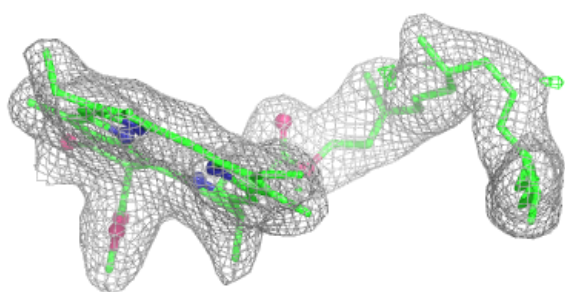
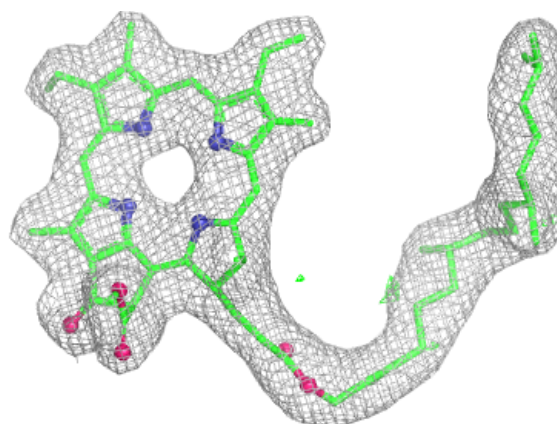
**Electron density around PL9 d 406:**

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



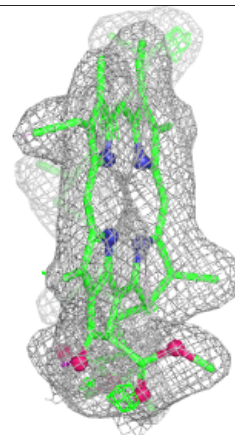
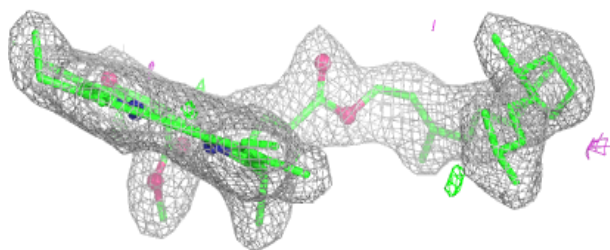
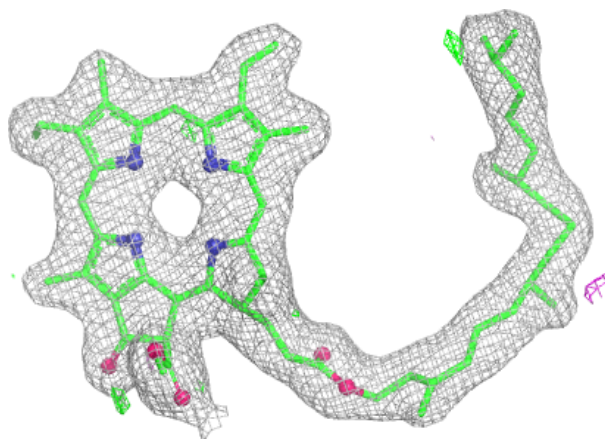
Electron density around PHO D 402:

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



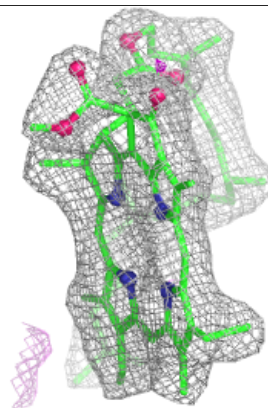
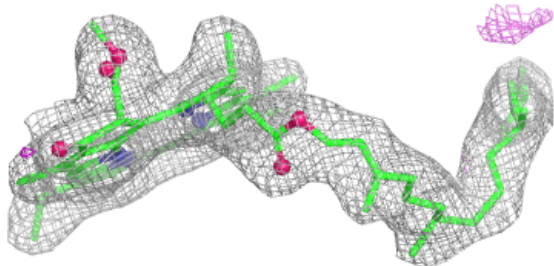
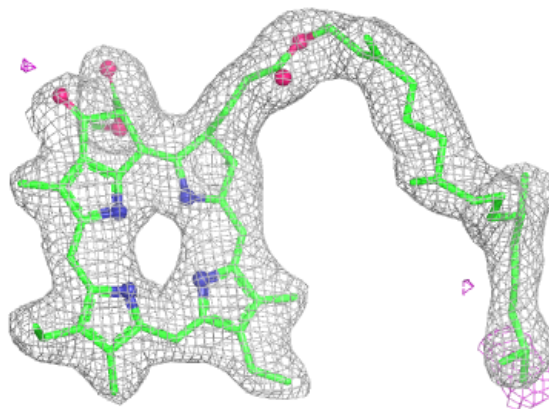
Electron density around PHO a 608:

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

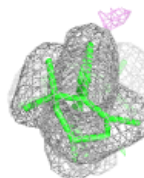
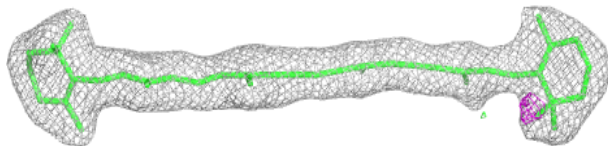
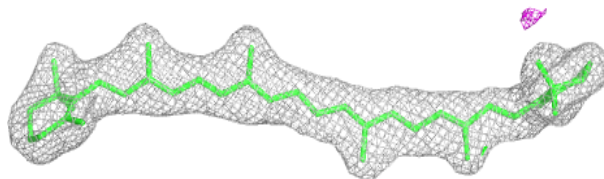


Electron density around PHO d 402:

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

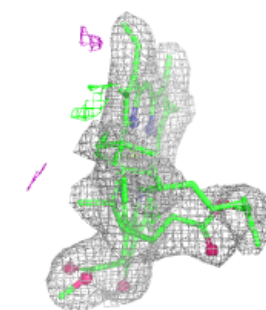
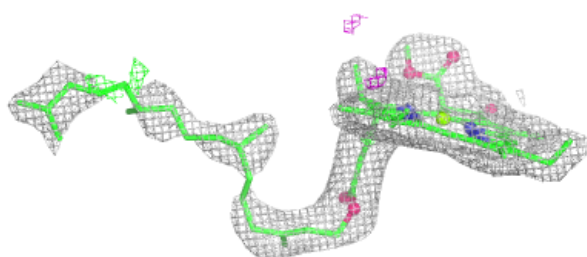
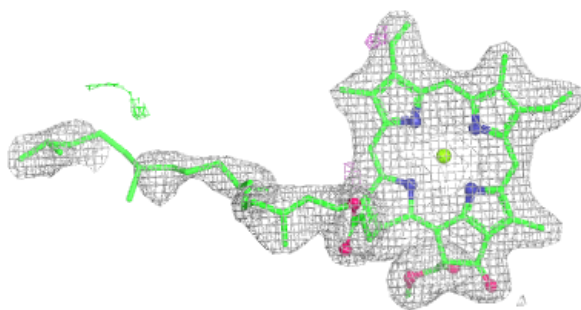
**Electron density around BCR A 610:**

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

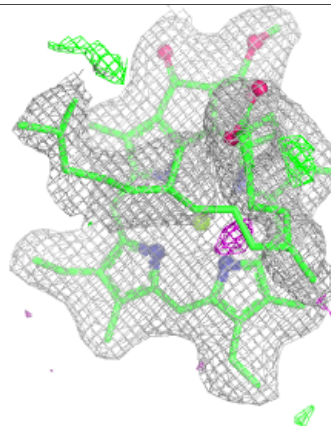
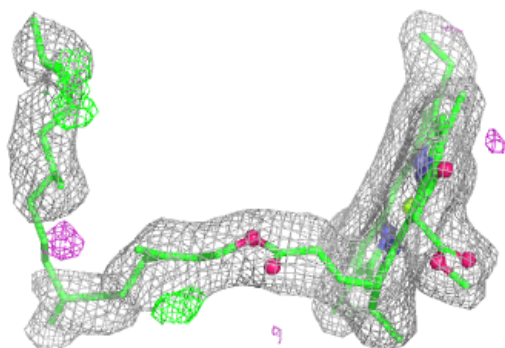
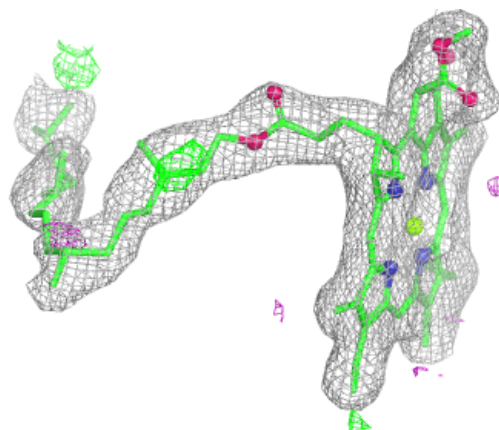


Electron density around CLA a 607:

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

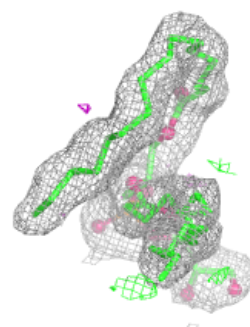
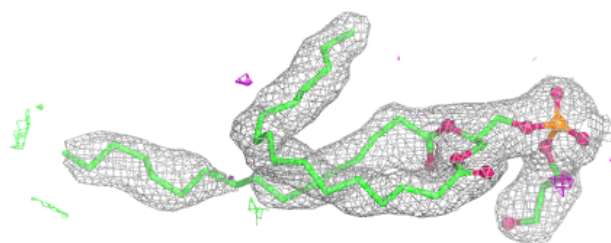
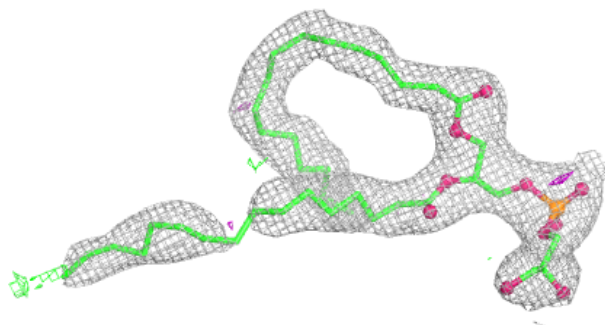
**Electron density around CLA a 609:**

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

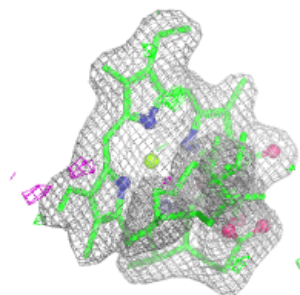
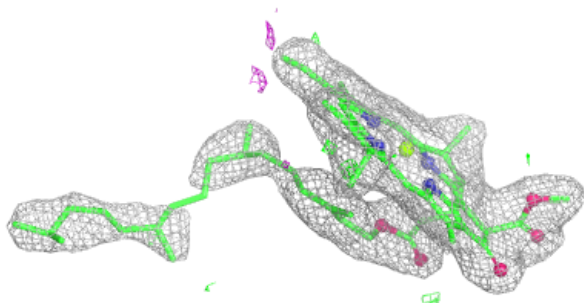
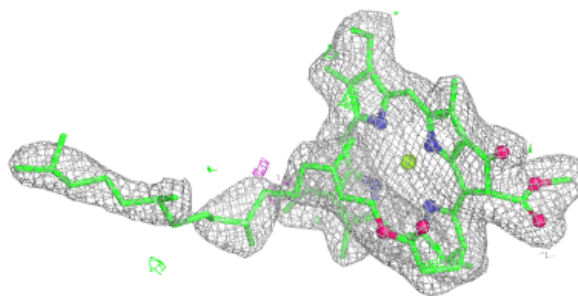


Electron density around LHG D 413:

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

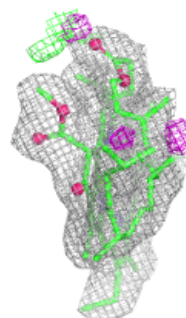
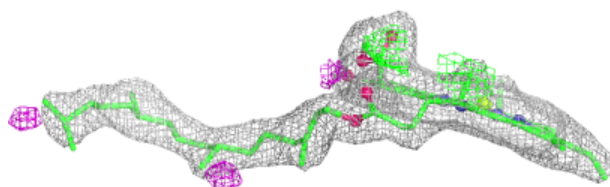
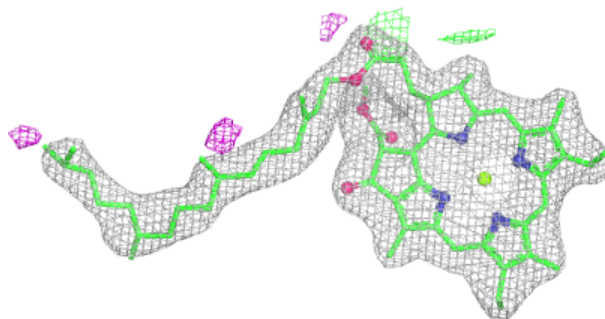
**Electron density around CLA C 505:**

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

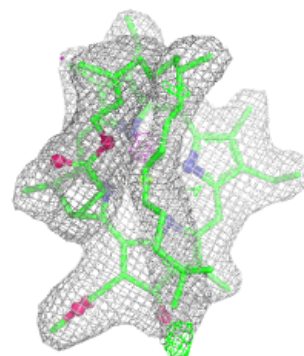
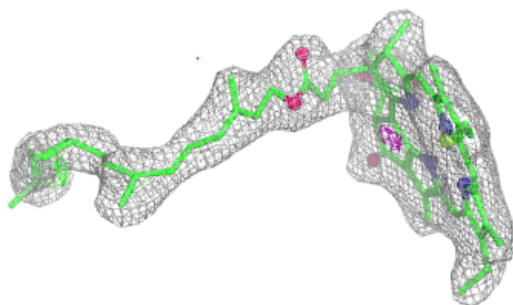
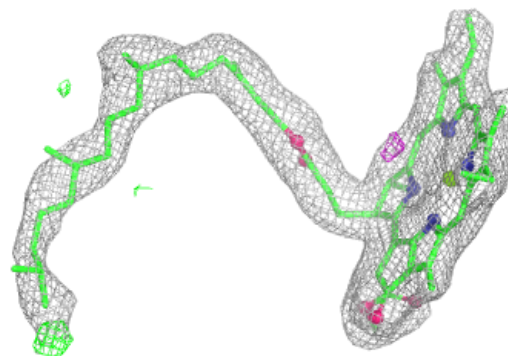


Electron density around CLA b 602:

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

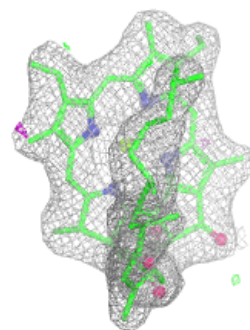
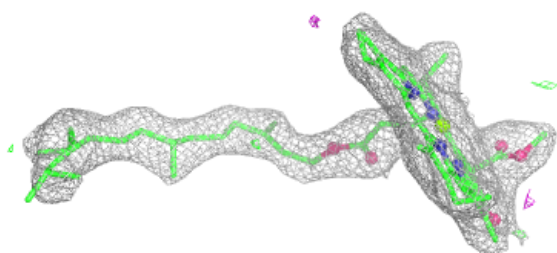
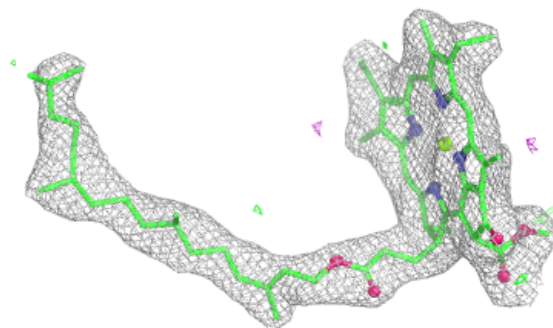
**Electron density around CLA b 606:**

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



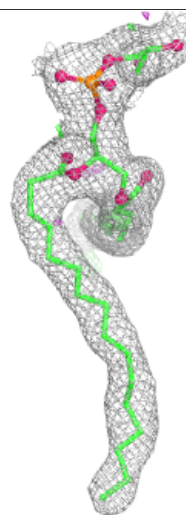
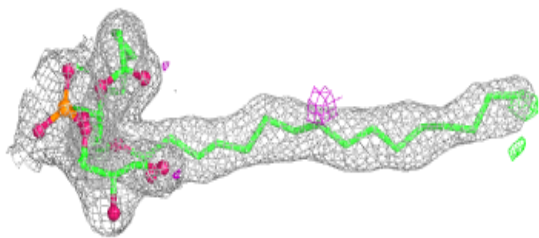
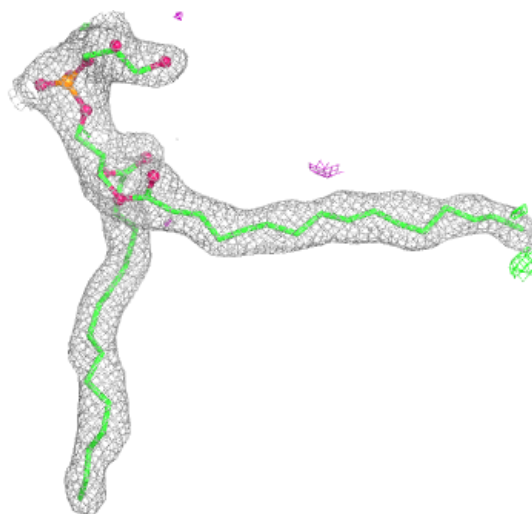
Electron density around CLA b 609:

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



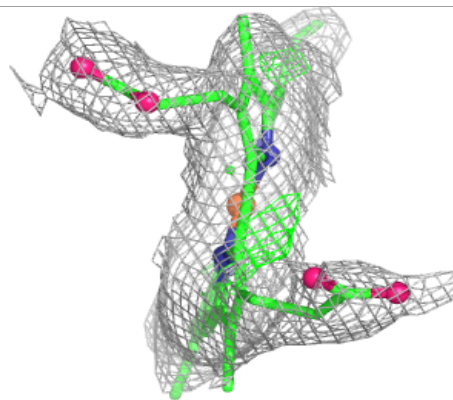
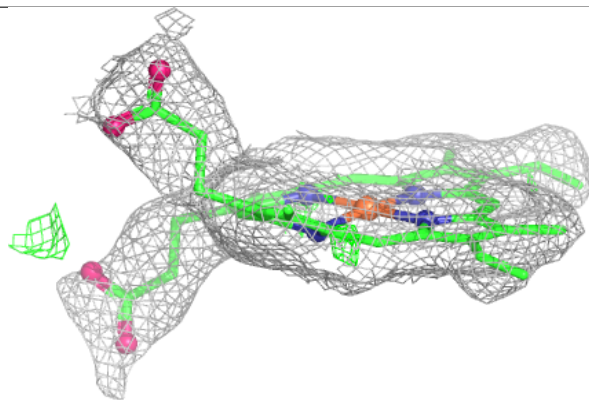
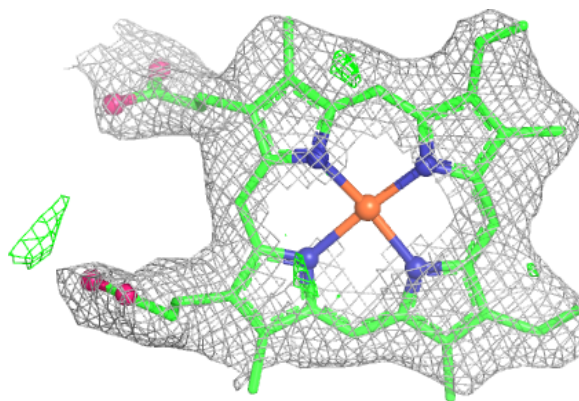
Electron density around LHG 1 101:

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

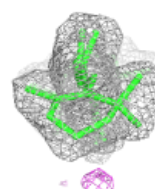
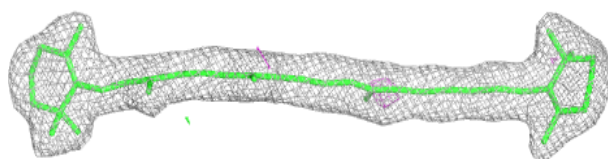
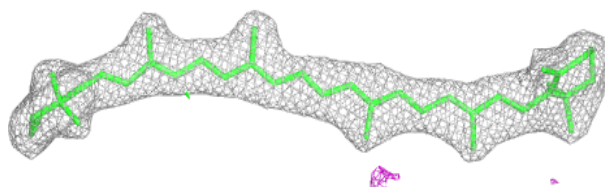


Electron density around HEM e 101:

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

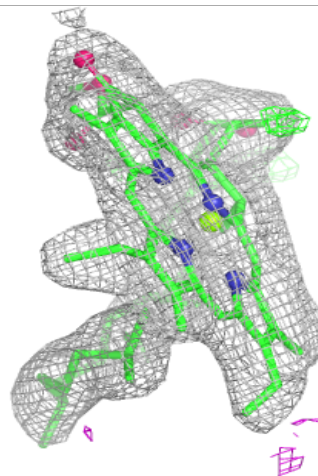
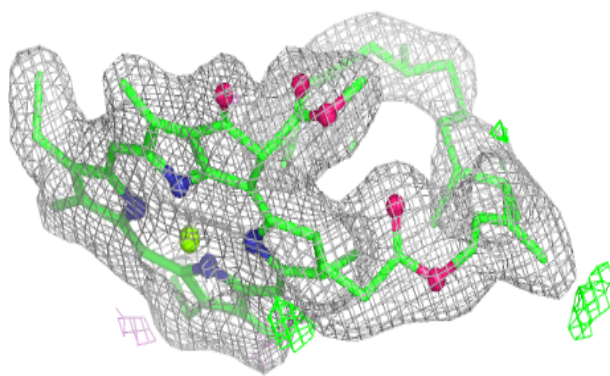
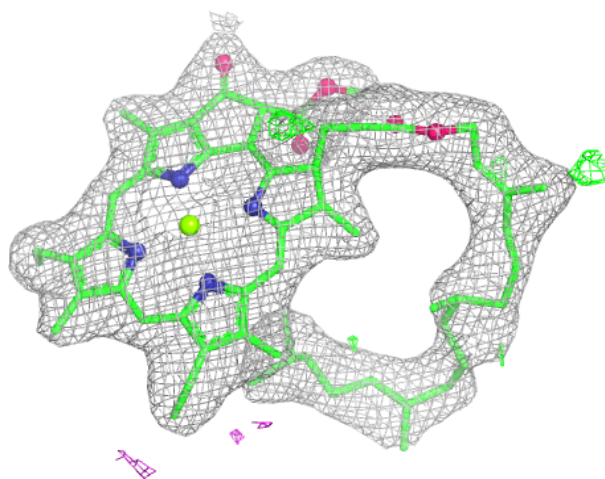
**Electron density around BCR a 610:**

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



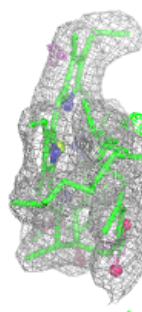
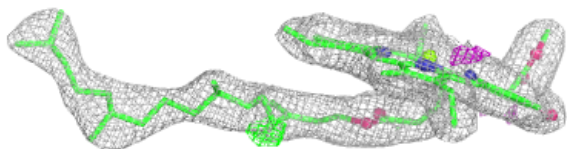
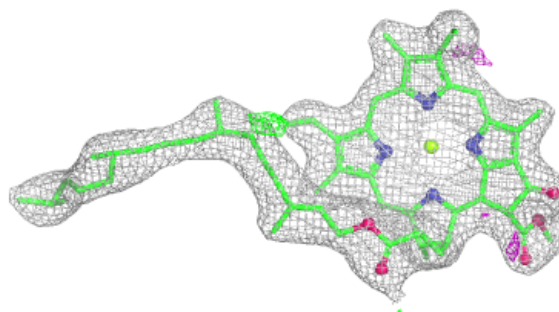
Electron density around CLA B 615:

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

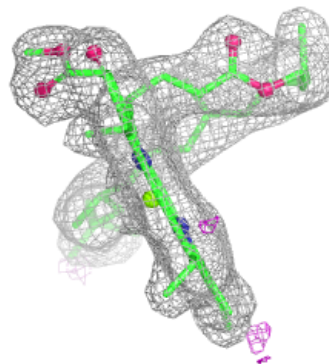
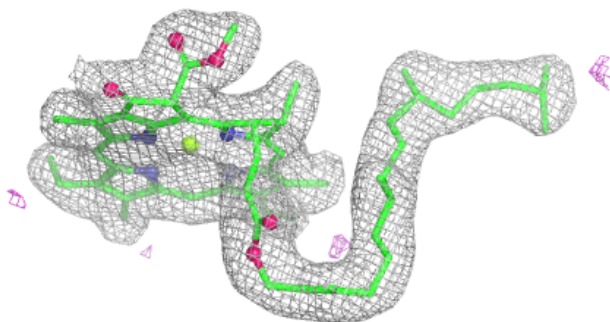
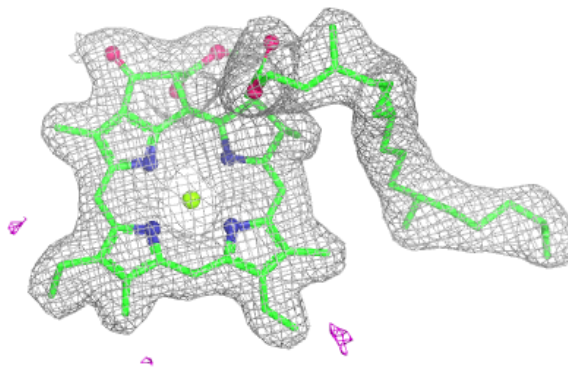


Electron density around CLA B 603:

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

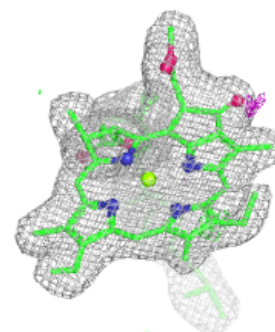
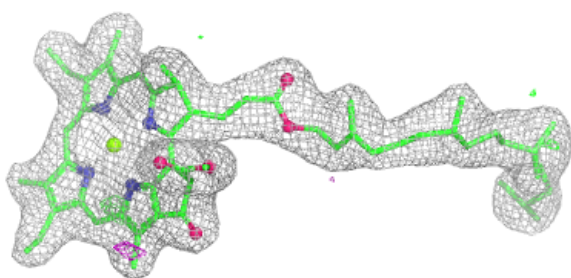
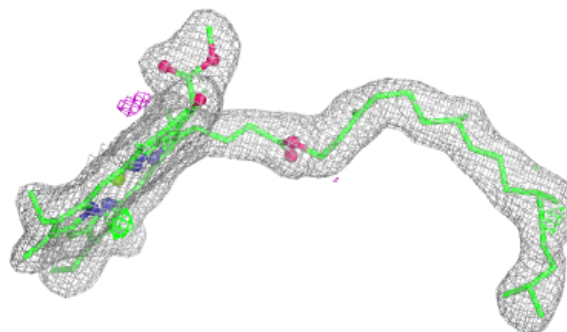
**Electron density around CLA D 403:**

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

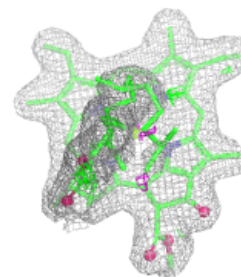
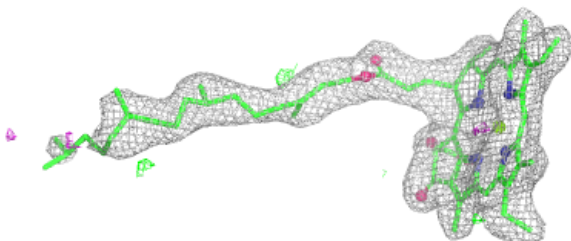
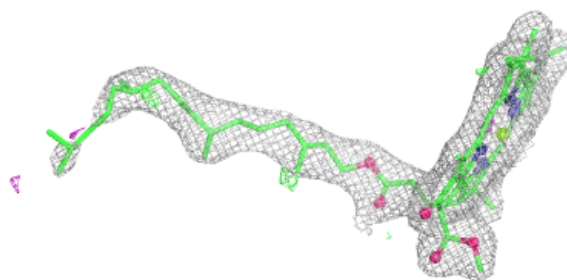


Electron density around CLA D 404:

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

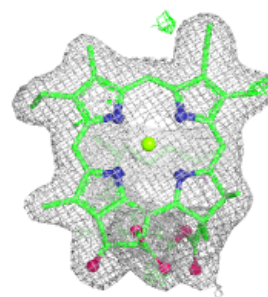
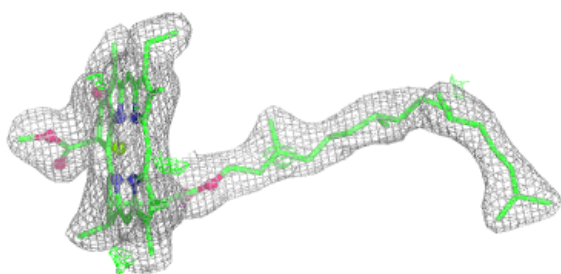
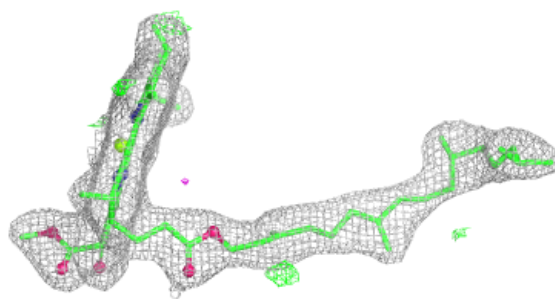
**Electron density around CLA B 604:**

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

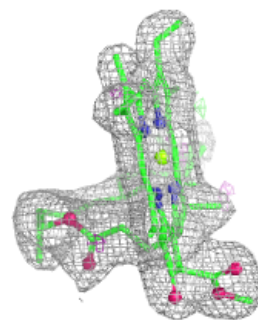
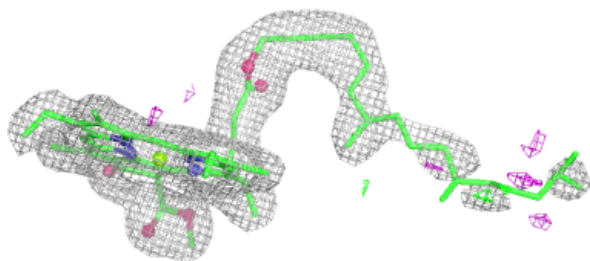
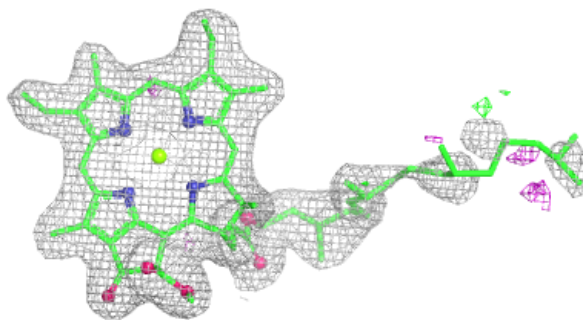


Electron density around CLA B 605:

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

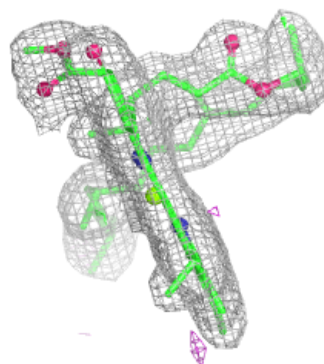
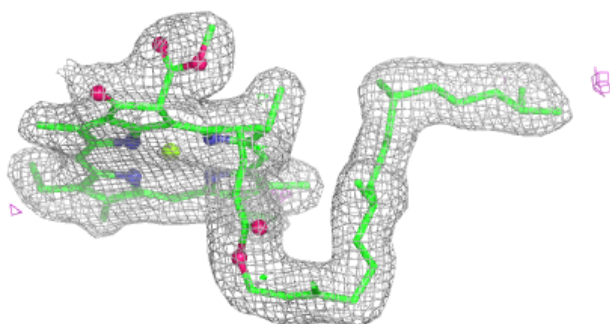
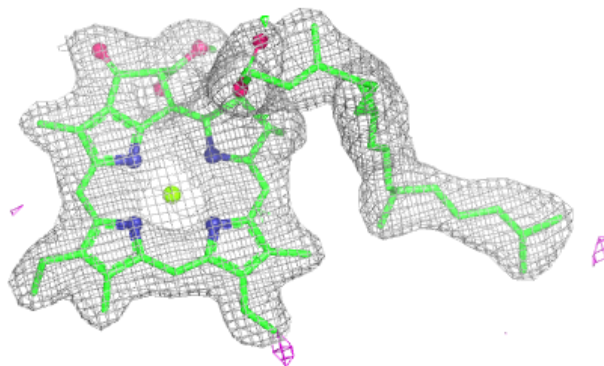
**Electron density around CLA A 607:**

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

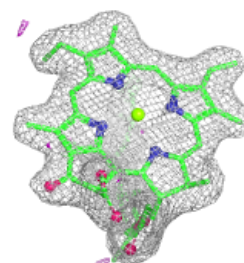
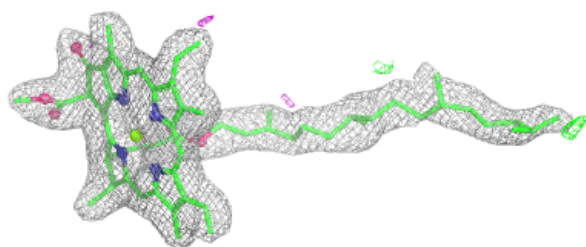
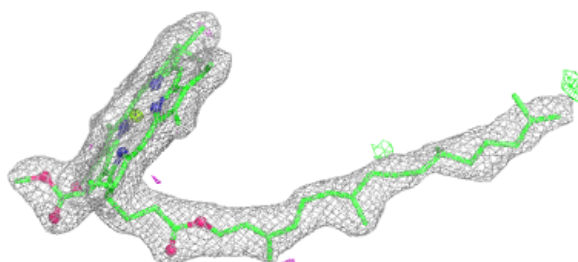


Electron density around CLA a 612:

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

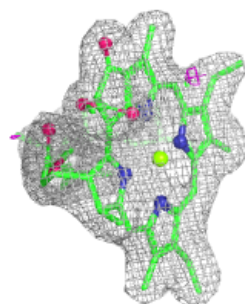
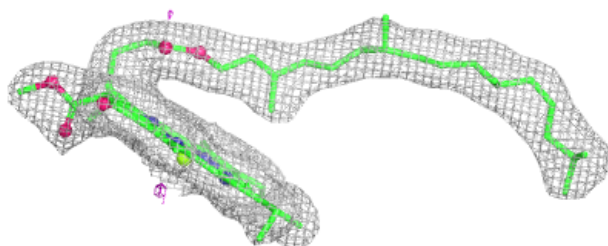
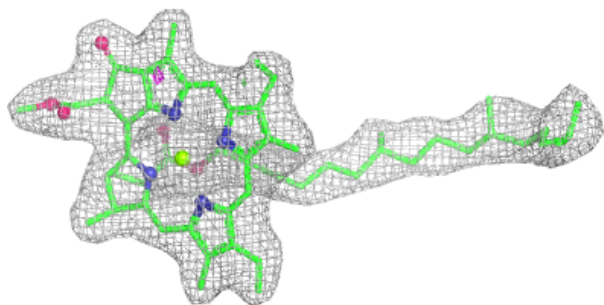
**Electron density around CLA B 607:**

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

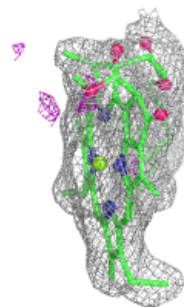
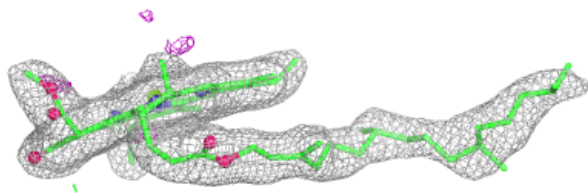
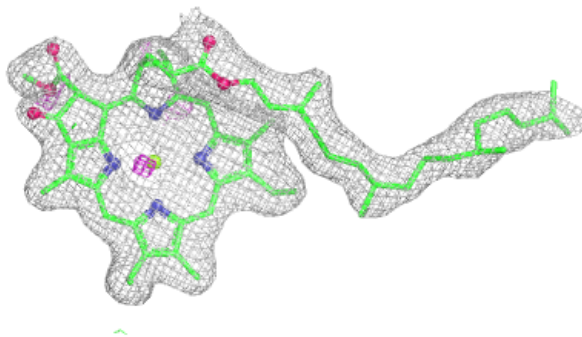


Electron density around CLA B 608:

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

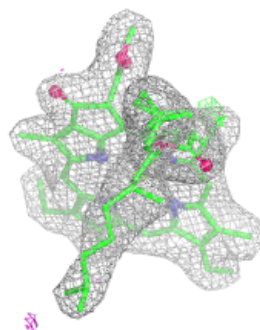
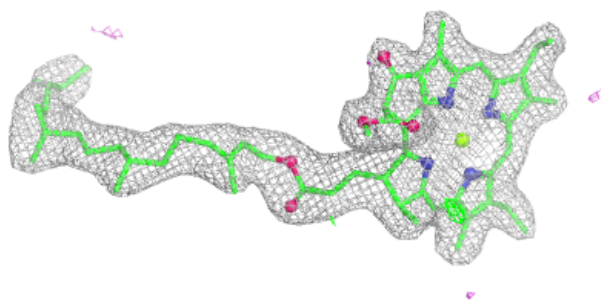
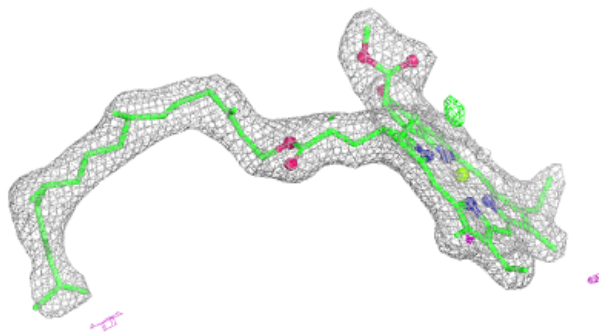
**Electron density around CLA b 603:**

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

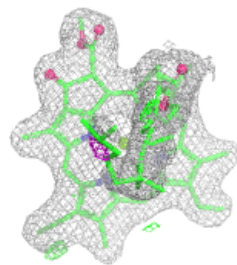
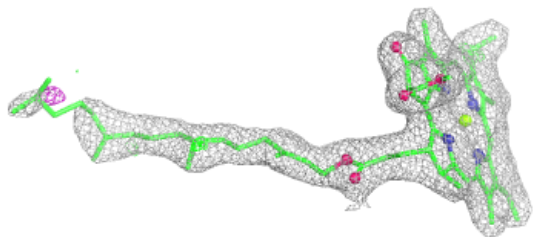
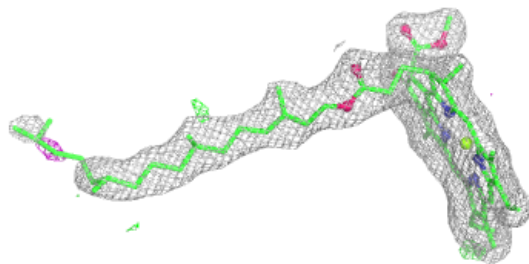


Electron density around CLA d 403:

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

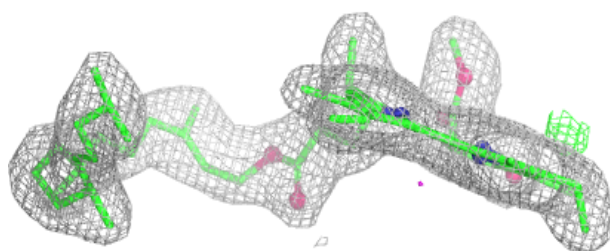
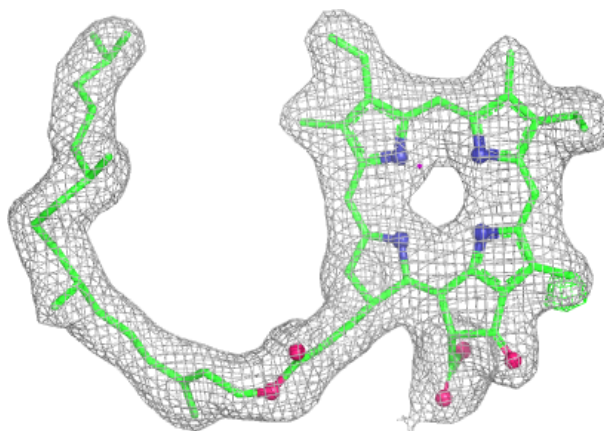
**Electron density around CLA b 604:**

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

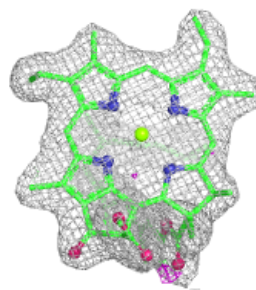
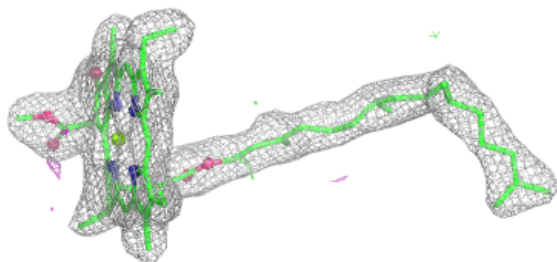
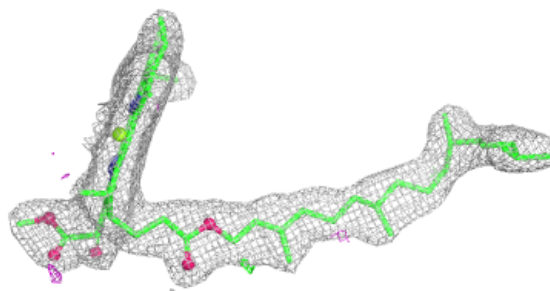


Electron density around PHO A 608:

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

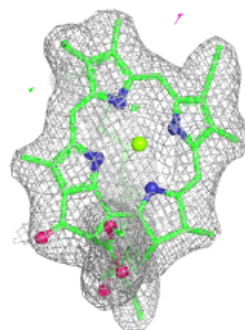
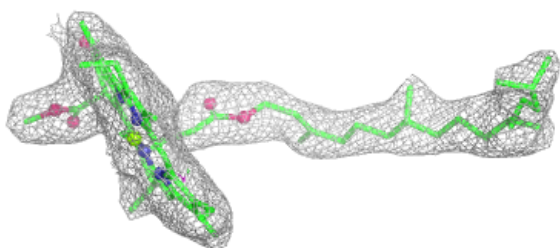
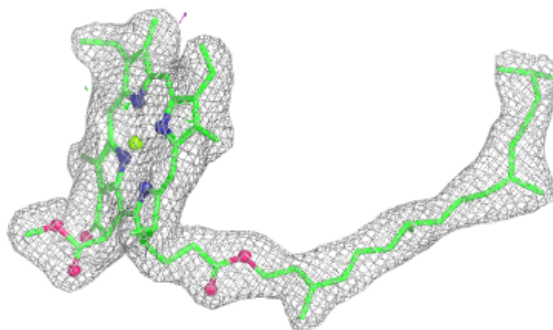
**Electron density around CLA b 605:**

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

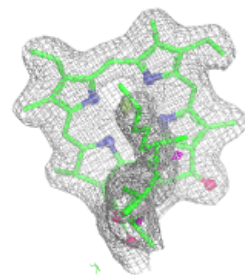
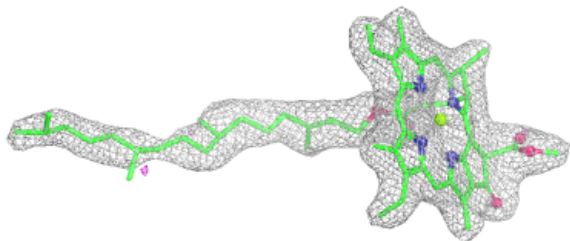
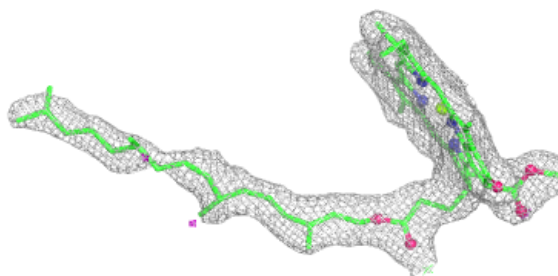


Electron density around CLA B 609:

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

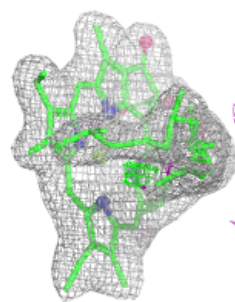
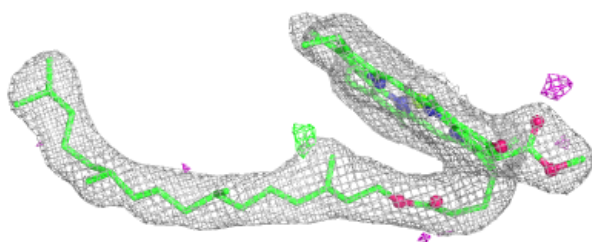
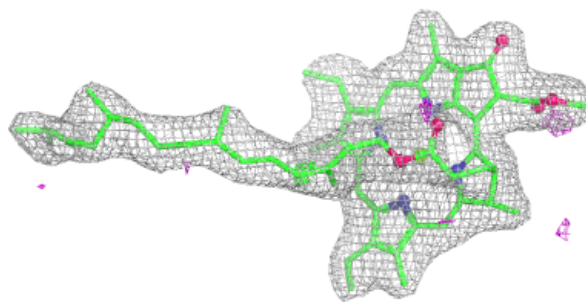
**Electron density around CLA b 607:**

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



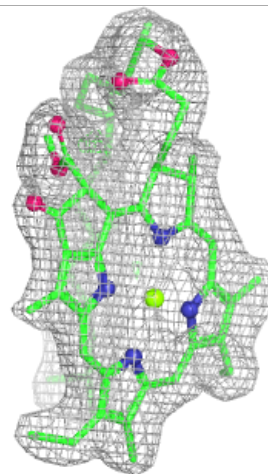
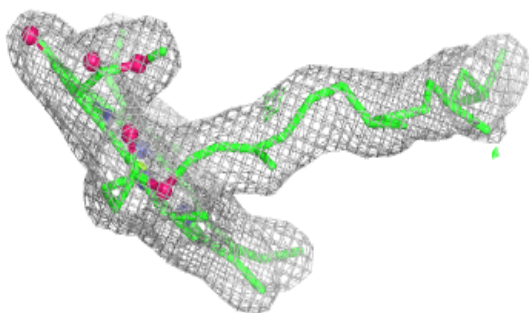
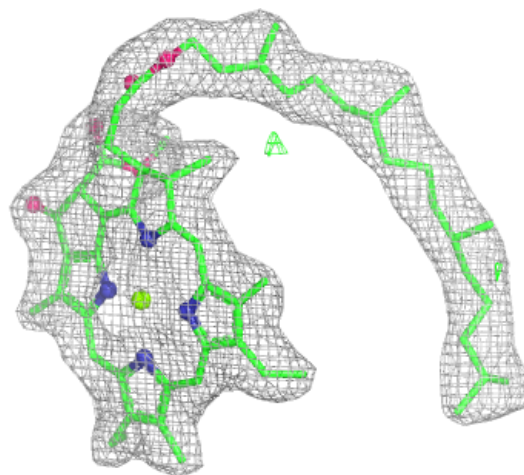
Electron density around CLA b 608:

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



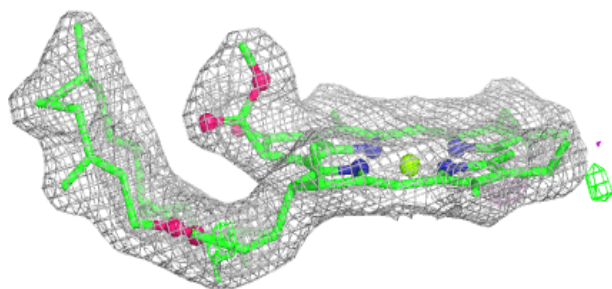
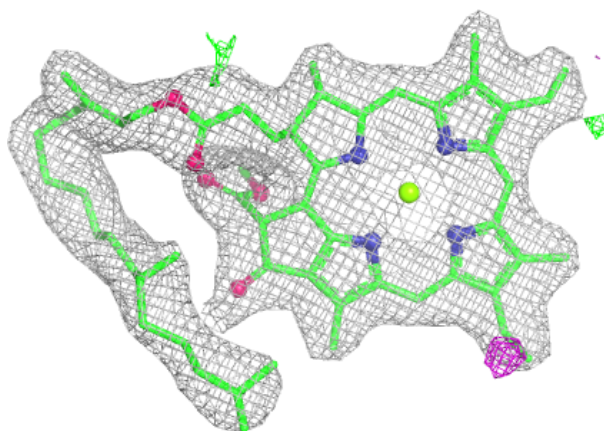
Electron density around CLA C 507:

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



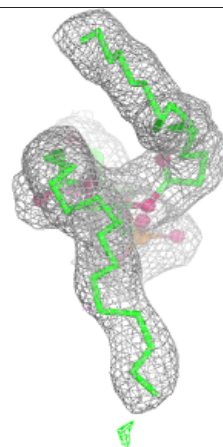
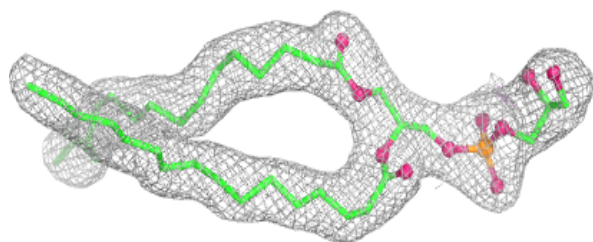
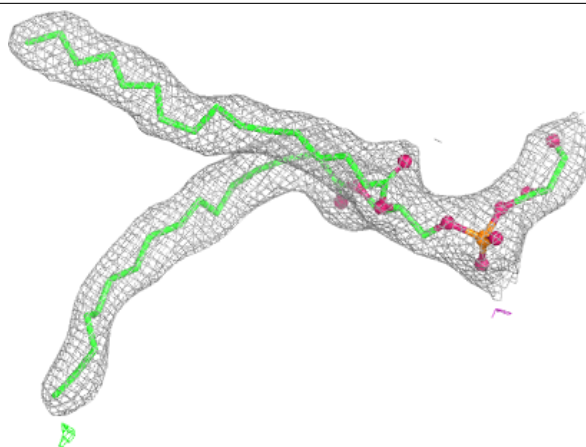
Electron density around CLA b 610:

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



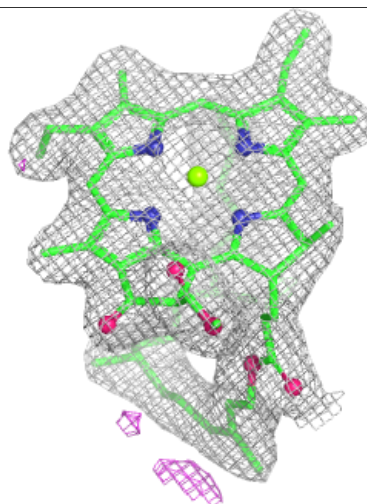
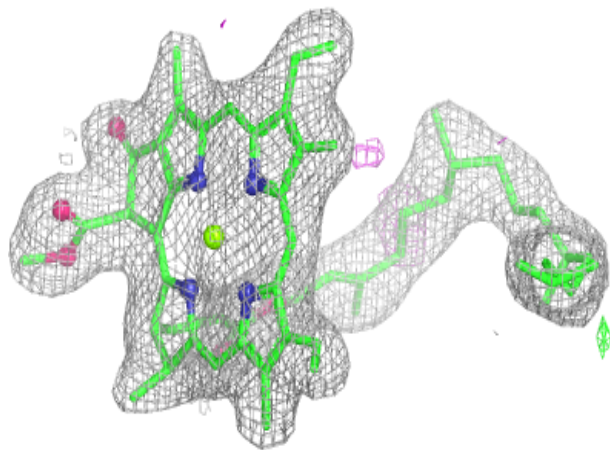
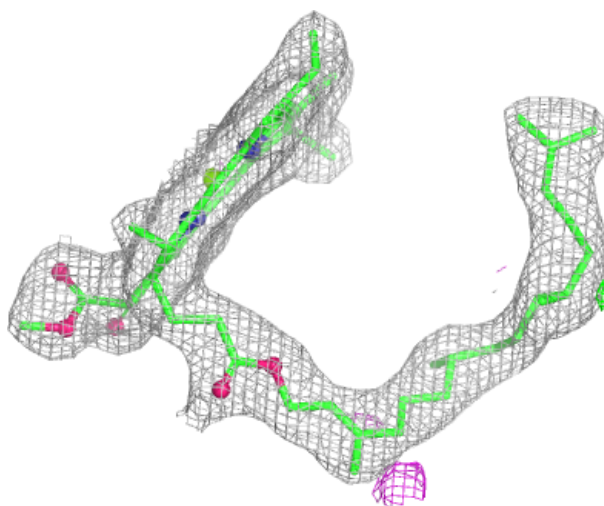
Electron density around LHG D 410:

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



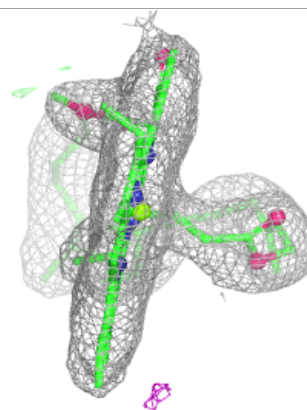
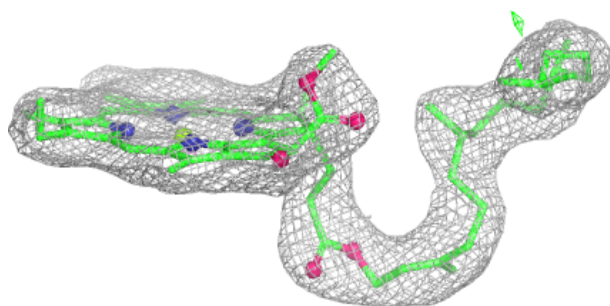
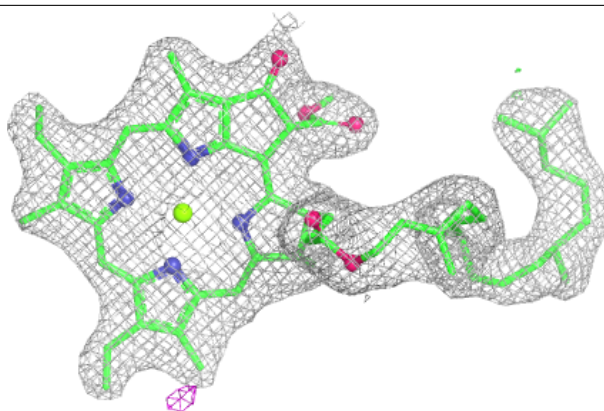
Electron density around CLA b 611:

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



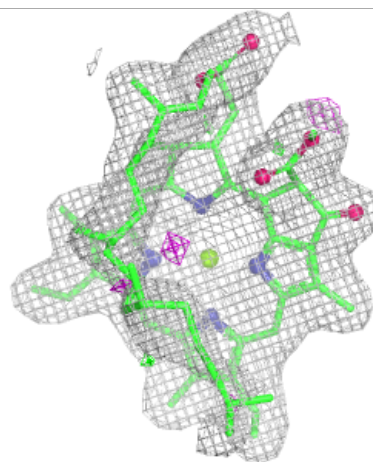
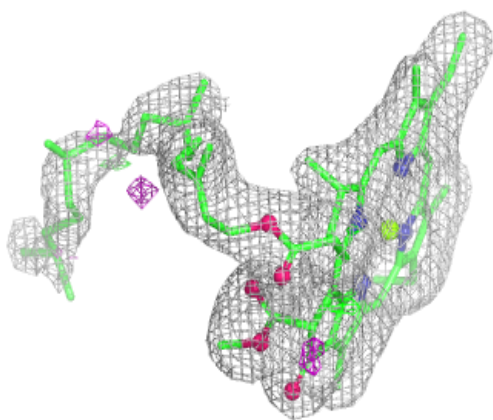
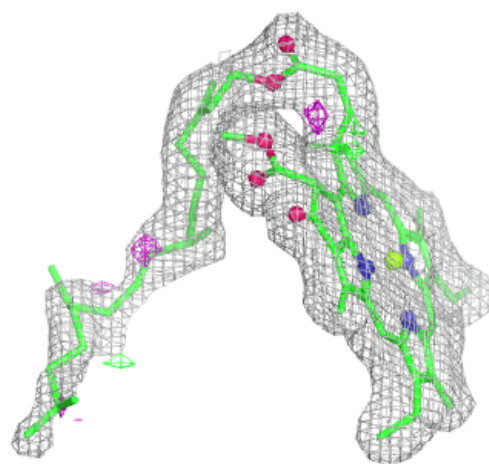
Electron density around CLA b 612:

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



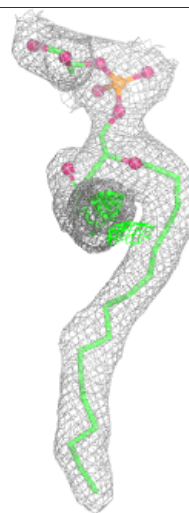
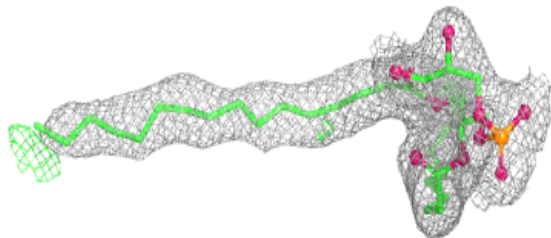
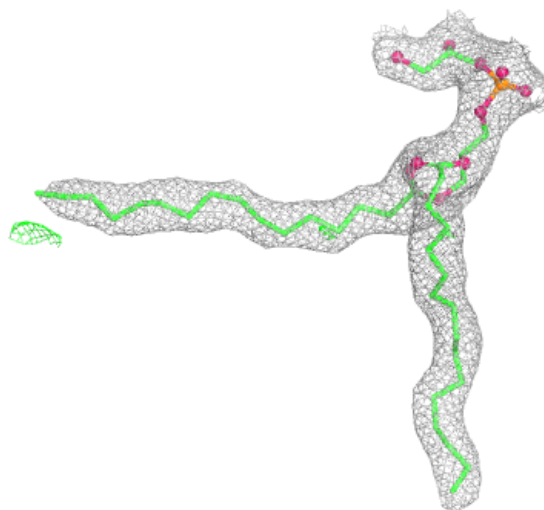
Electron density around CLA b 613:

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



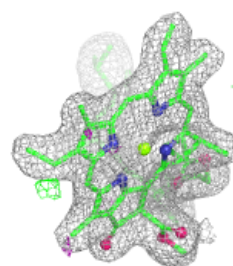
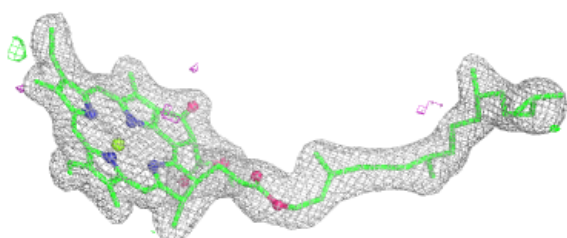
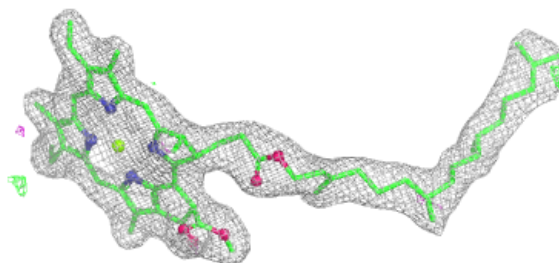
Electron density around LHG L 102:

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

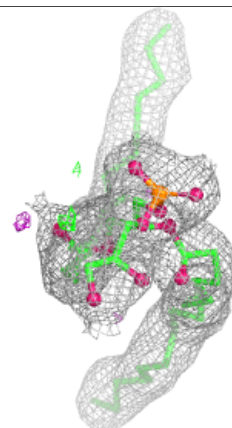
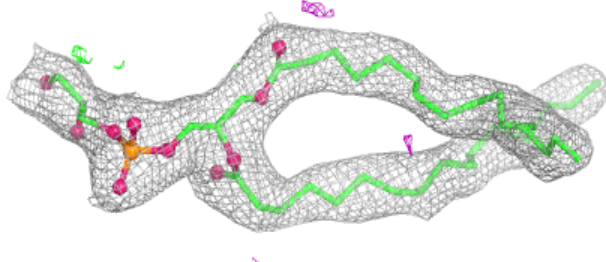
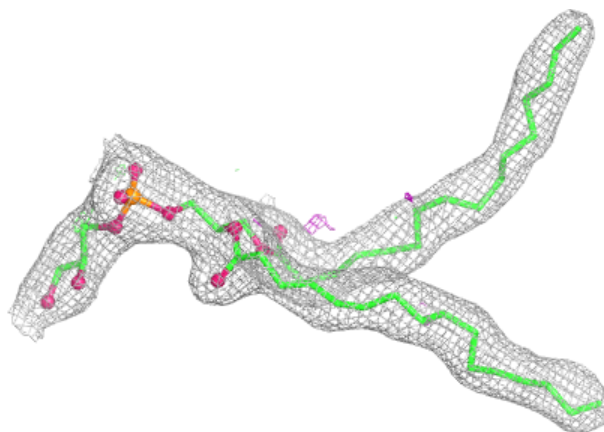


Electron density around CLA A 606:

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

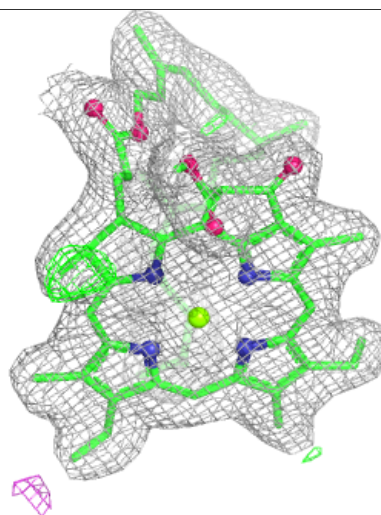
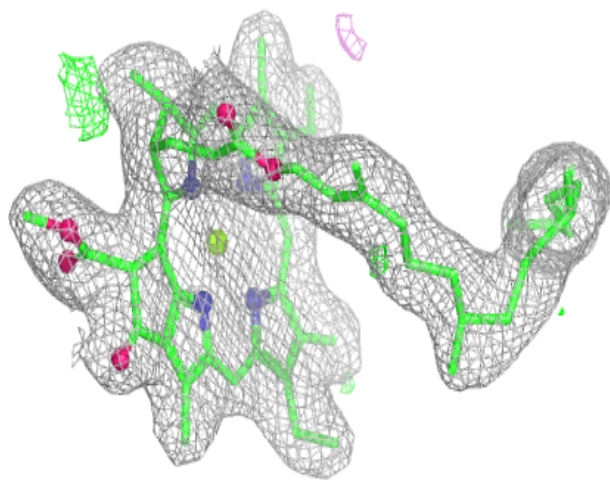
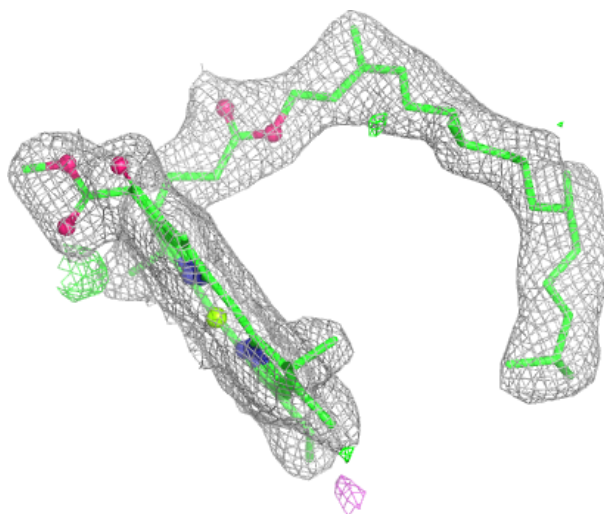
**Electron density around LHG d 408:**

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



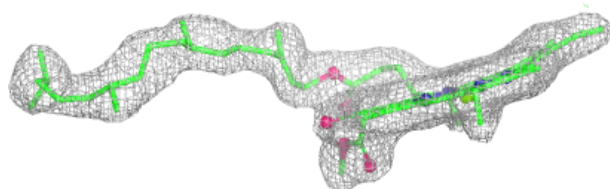
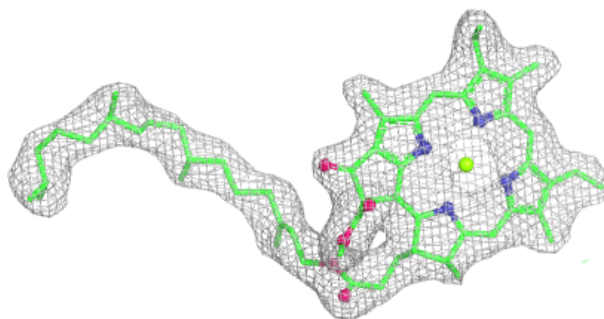
Electron density around CLA B 611:

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

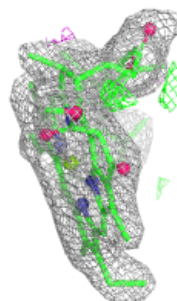
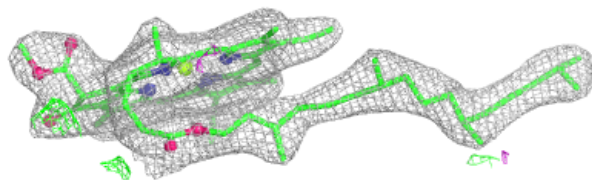
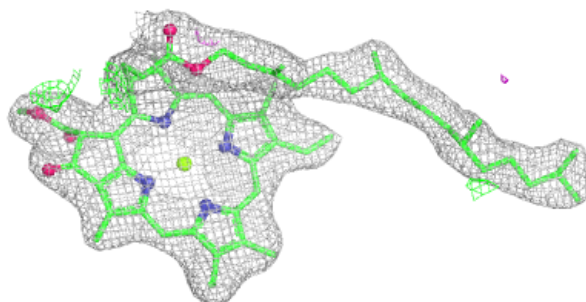


Electron density around CLA B 602:

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

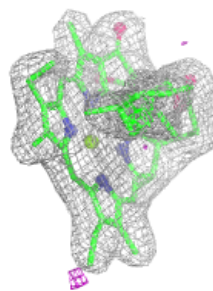
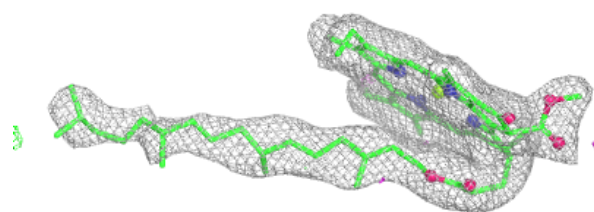
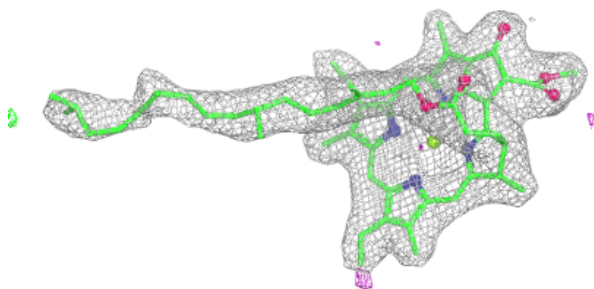
**Electron density around CLA c 501:**

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

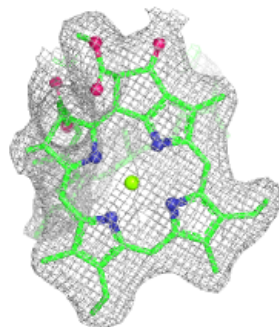
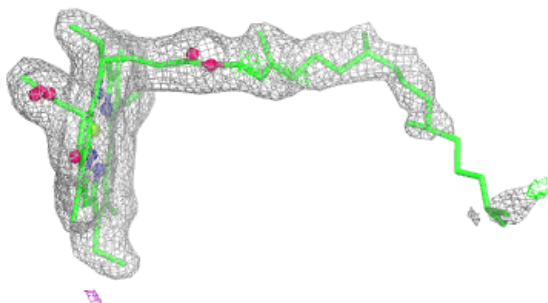
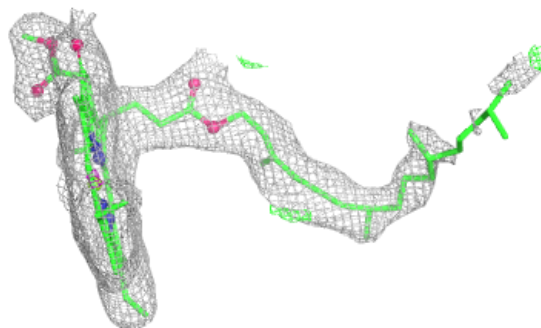


Electron density around CLA B 614:

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

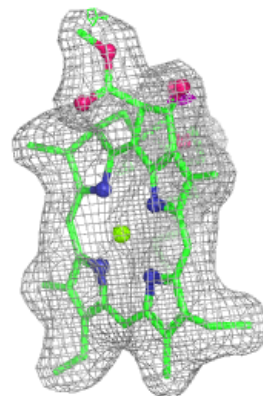
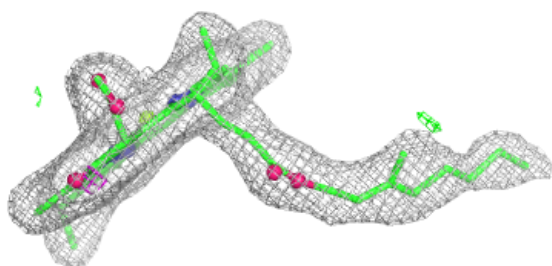
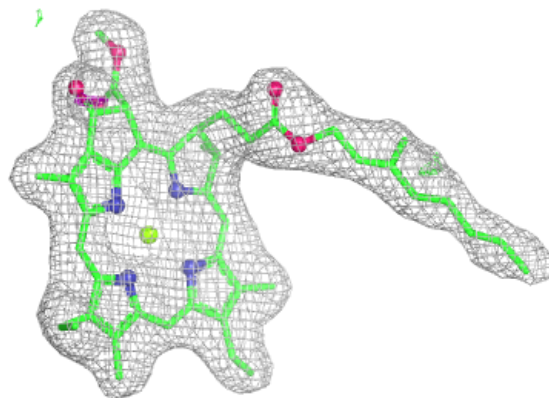
**Electron density around CLA D 405:**

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



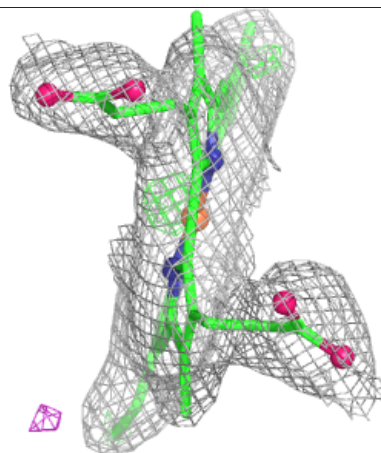
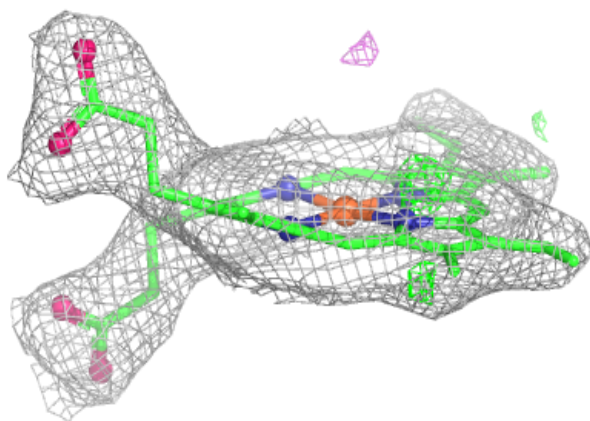
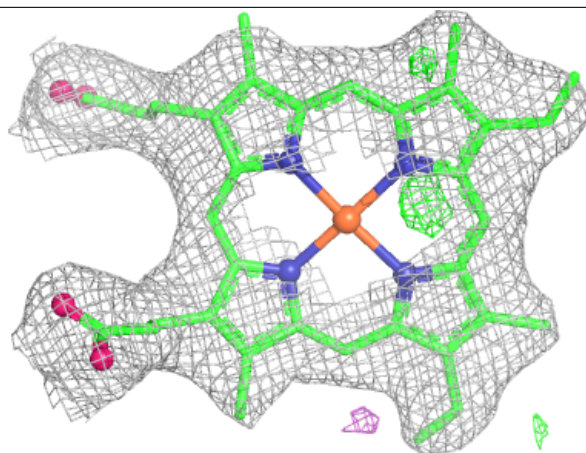
Electron density around CLA A 609:

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



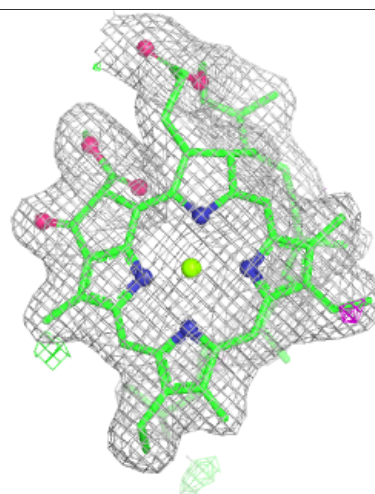
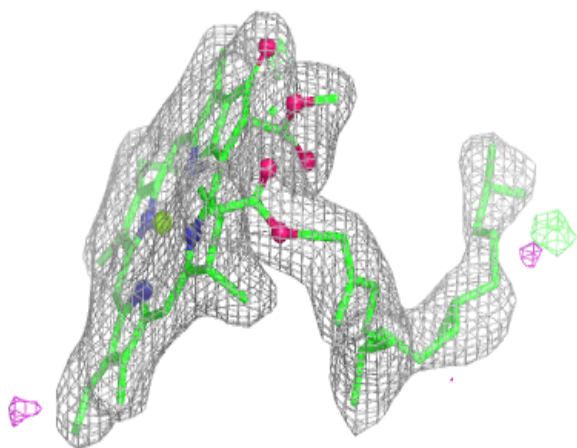
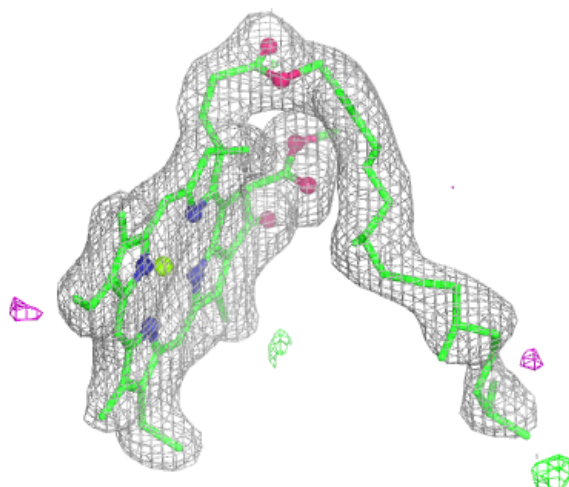
Electron density around HEM F 101:

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



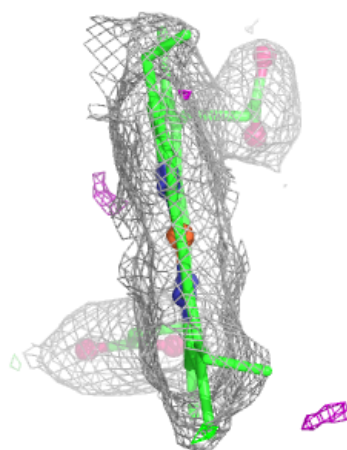
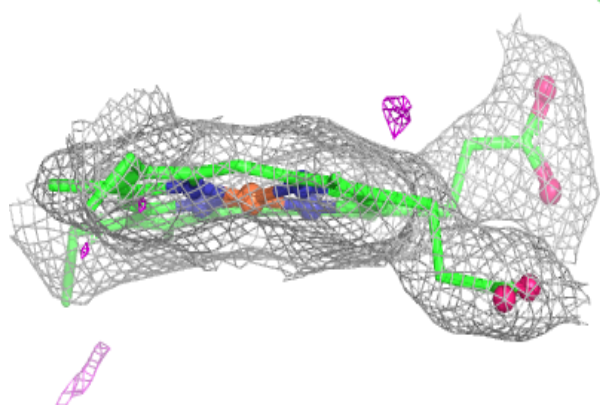
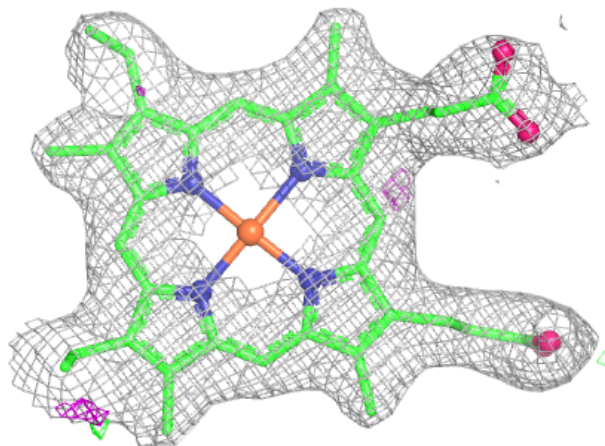
Electron density around CLA B 613:

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



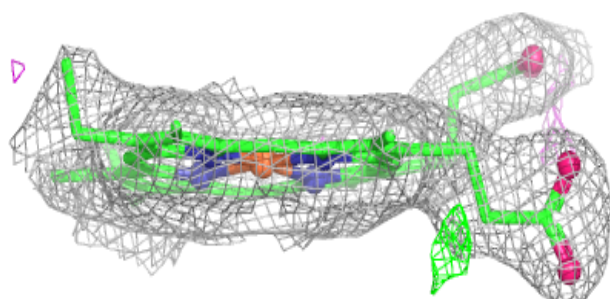
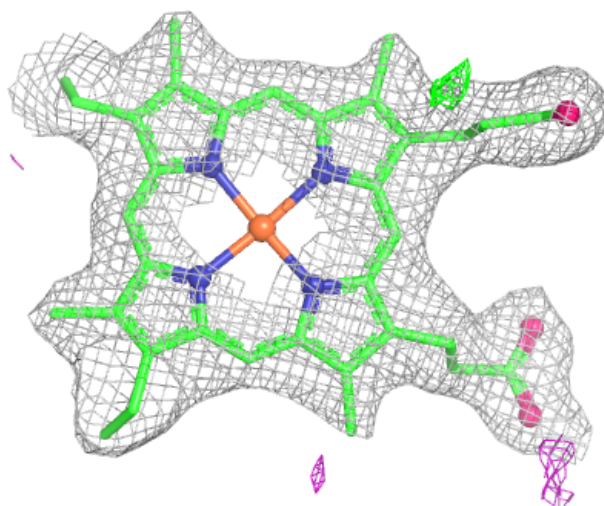
Electron density around HEC V 201:

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



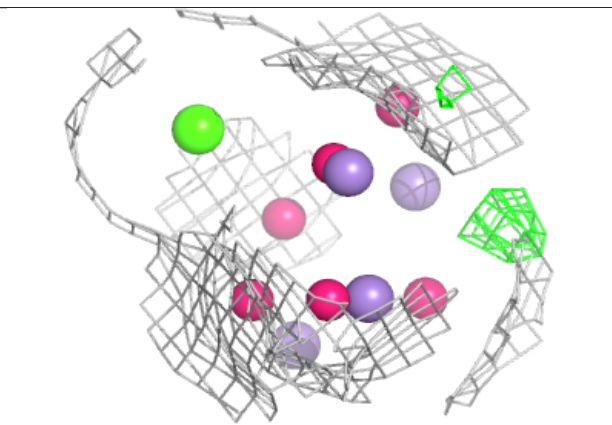
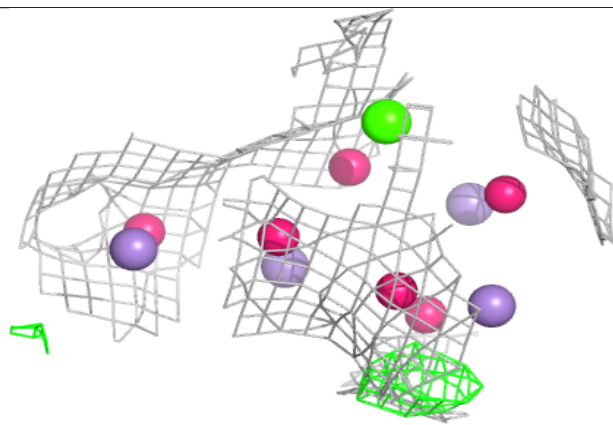
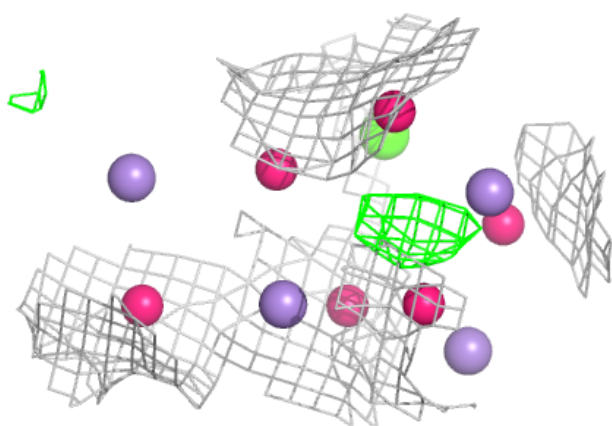
Electron density around HEC v 201:

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



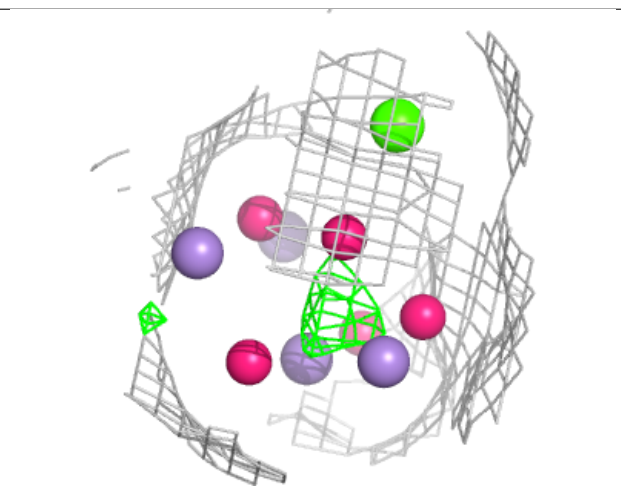
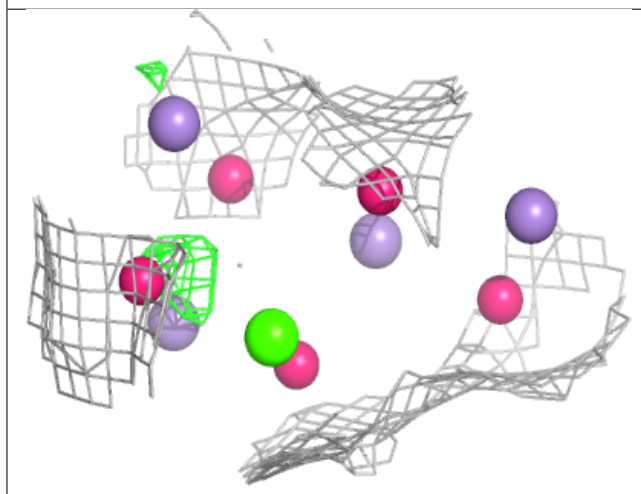
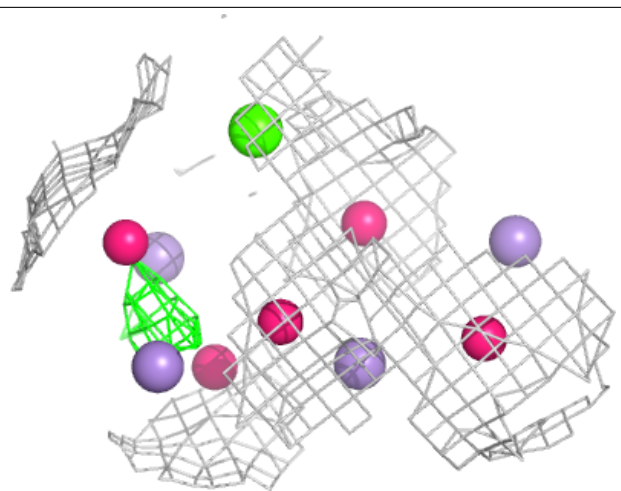
Electron density around OEY a 601 (B):

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



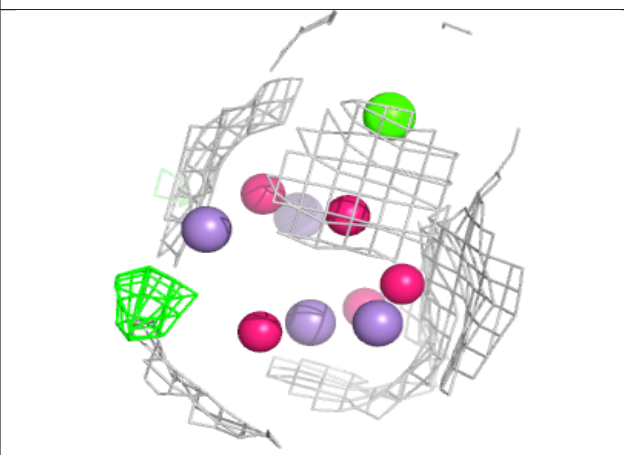
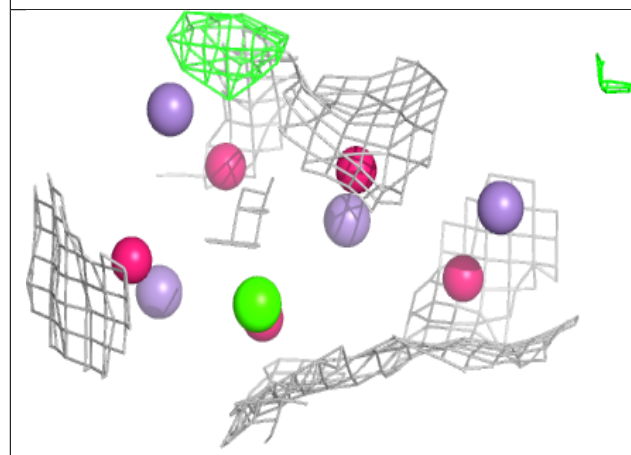
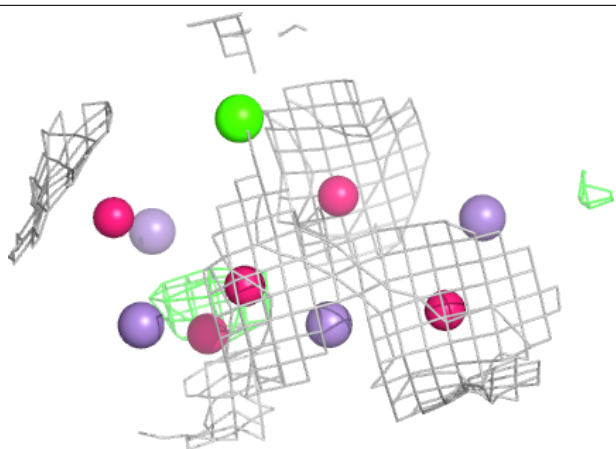
Electron density around OEX A 602 (A):

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



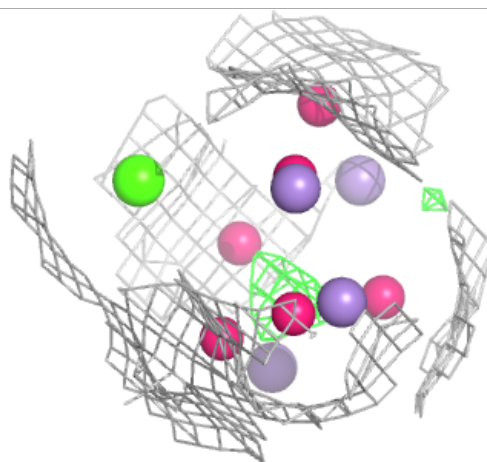
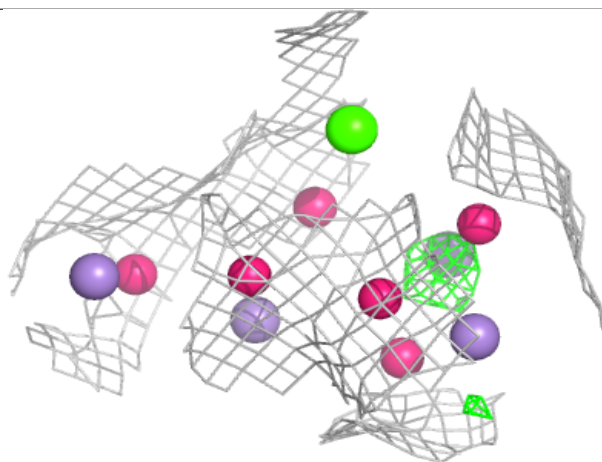
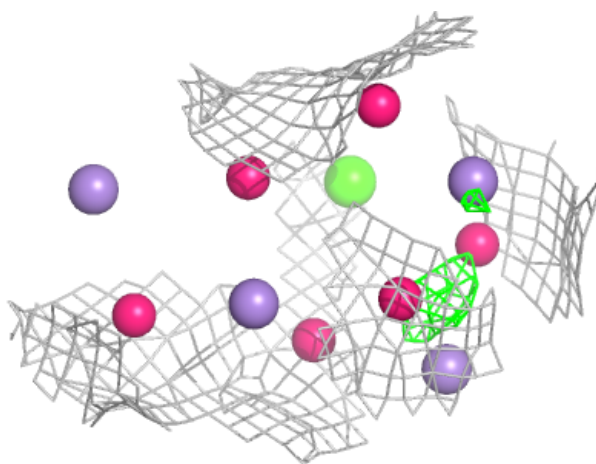
Electron density around OEX a 602 (Å):

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



Electron density around OEY A 601 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.