



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:57 PM EDT

PDB ID : 8F4F / pdb_00008f4f
Title : RT XFEL structure of Photosystem II 500 microseconds after the third illumination at 2.03 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.03 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

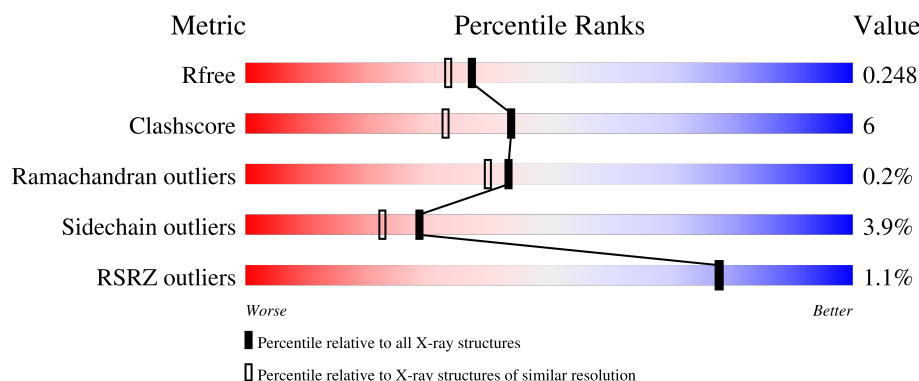
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	

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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
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 53209 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				

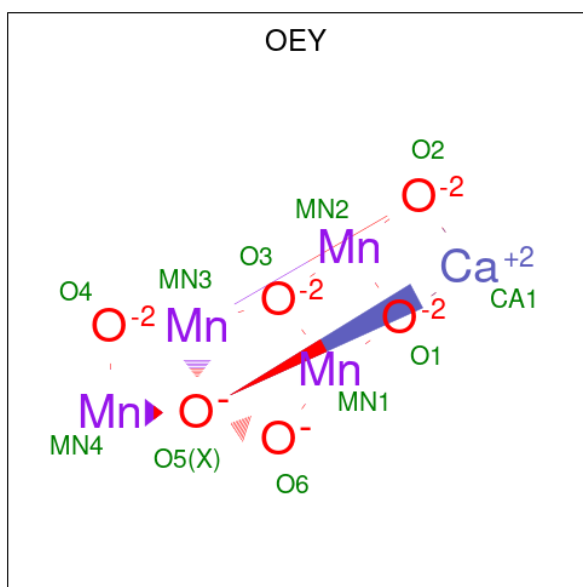
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			22	2	8	12		
21	a	1	Total	Ca	Mn	O	0	1
			22	2	8	12		

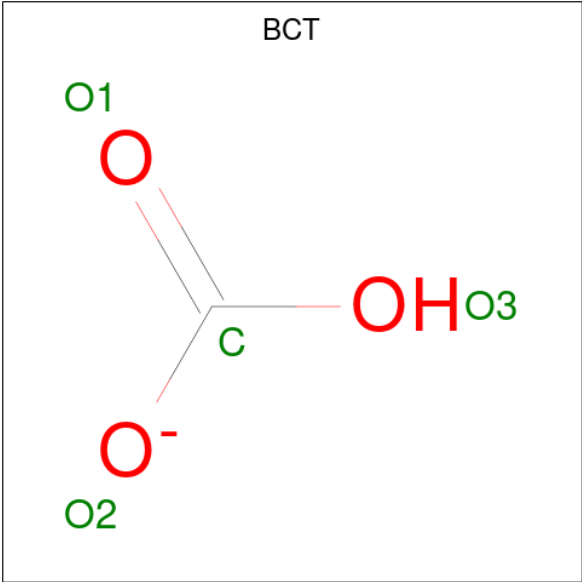
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

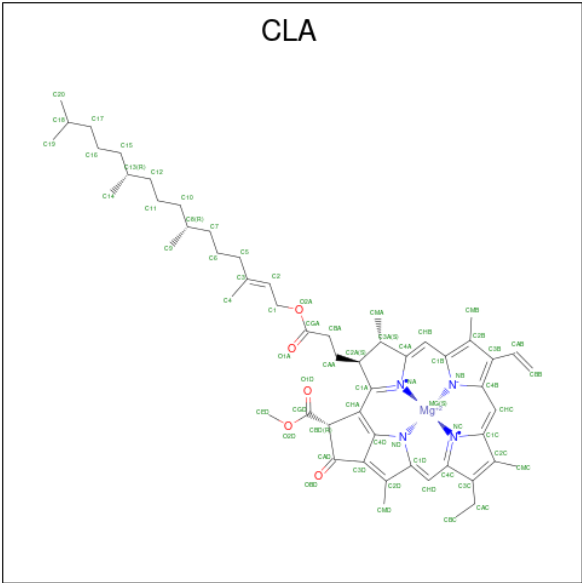
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O		0	0
			4	1	3			
24	d	1	Total	C	O		0	0
			4	1	3			

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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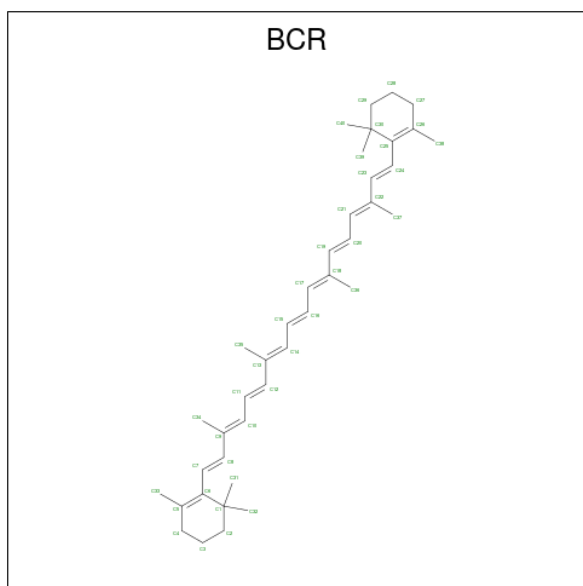
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N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

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



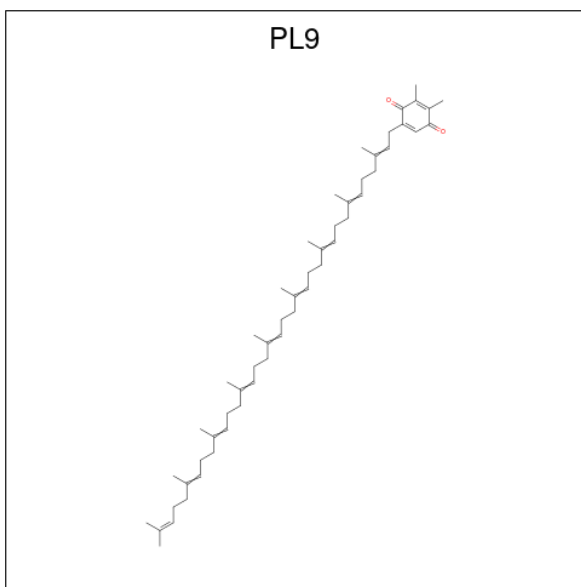
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		

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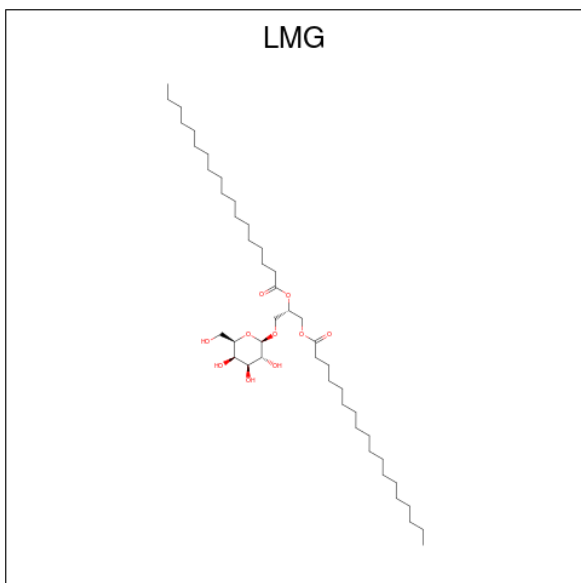
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

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



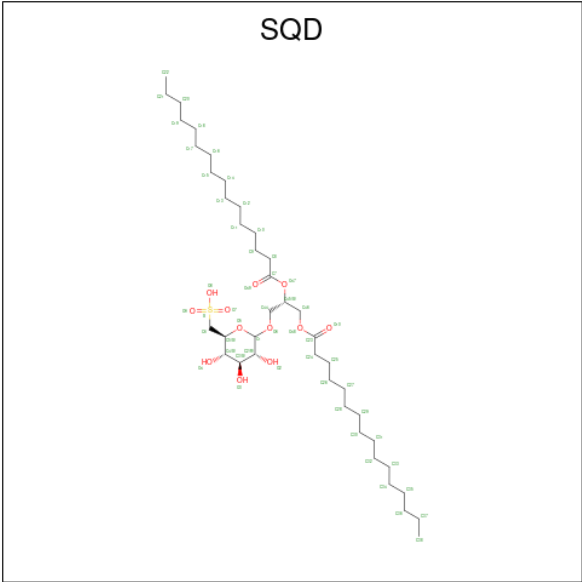
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



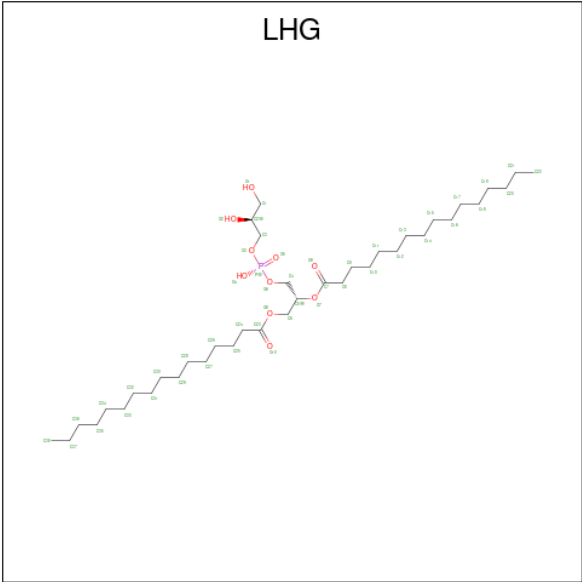
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			48	38	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			28	24	4		
28	C	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			51	41	10		
28	D	1	Total	C	O	0	0
			33	27	6		
28	b	1	Total	C	O	0	0
			55	45	10		
28	c	1	Total	C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

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



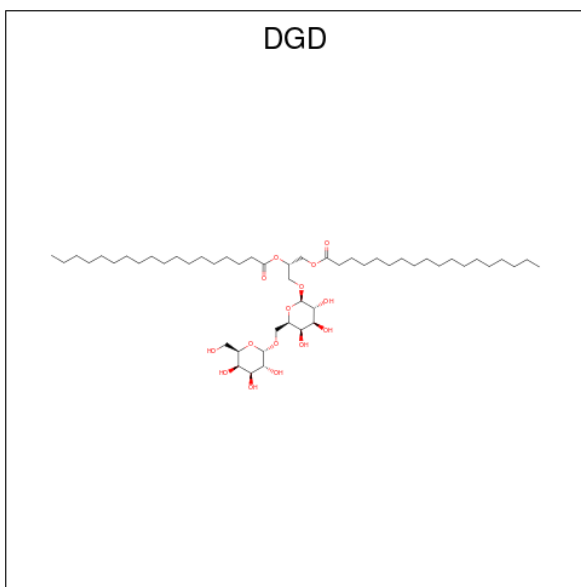
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			39	35	4			
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			36	25	10	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O		0	0
			36	31	5			
29	b	1	Total	C	O	S	0	0
			49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

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



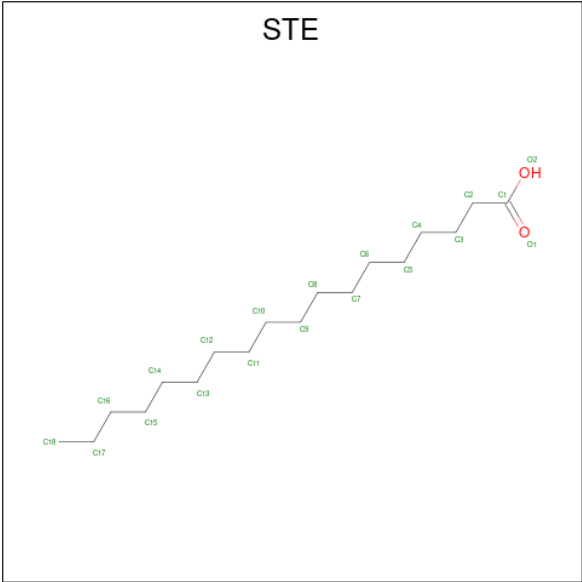
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			47	36	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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	H	1	Total	C	O	0	0
			62	47	15		
31	J	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: $C_{18}H_{36}O_2$).



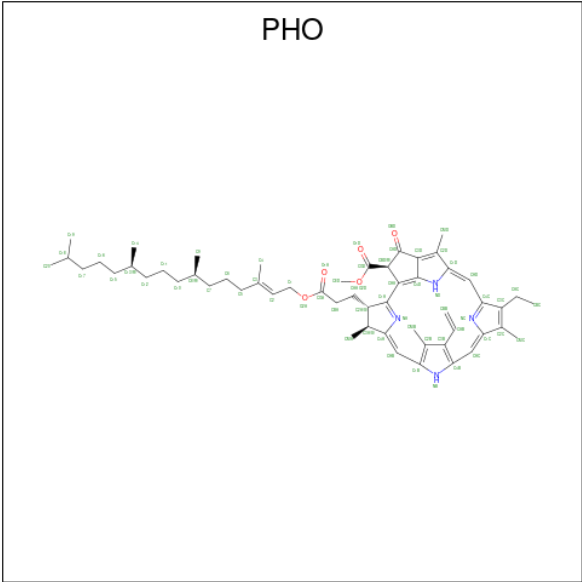
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			20	18	2		
32	B	1	Total	C	O	0	0
			17	15	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C	O	0	0
			18	16	2		
32	B	1	Total	C	O	0	0
			12	10	2		
32	B	1	Total	C		0	0
			16	16			
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C	O	0	0
			12	10	2		
32	C	1	Total	C		0	0
			16	16			
32	D	1	Total	C	O	0	0
			20	18	2		
32	E	1	Total	C	O	0	0
			12	10	2		
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		

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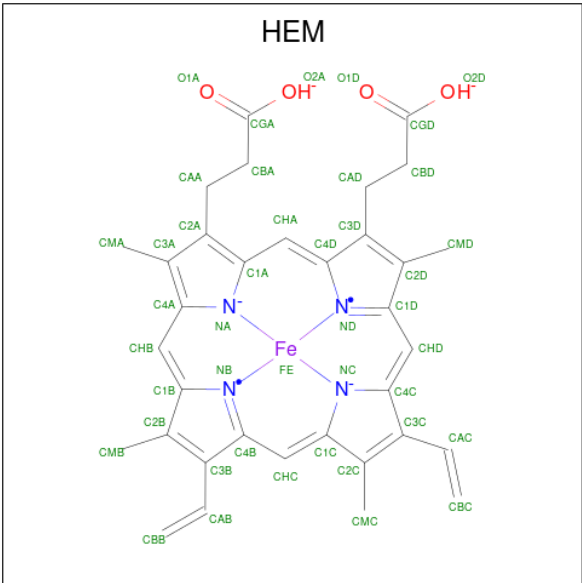
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	L	1	Total C O 12 10 2	0	0
32	M	1	Total C O 15 13 2	0	0
32	M	1	Total C 10 10	0	0
32	T	1	Total C 16 16	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 15 15	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 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	k	1	Total C O 12 10 2	0	0
32	m	1	Total C 18 18	0	0
32	t	1	Total C O 14 12 2	0	0
32	t	1	Total C 10 10	0	0

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



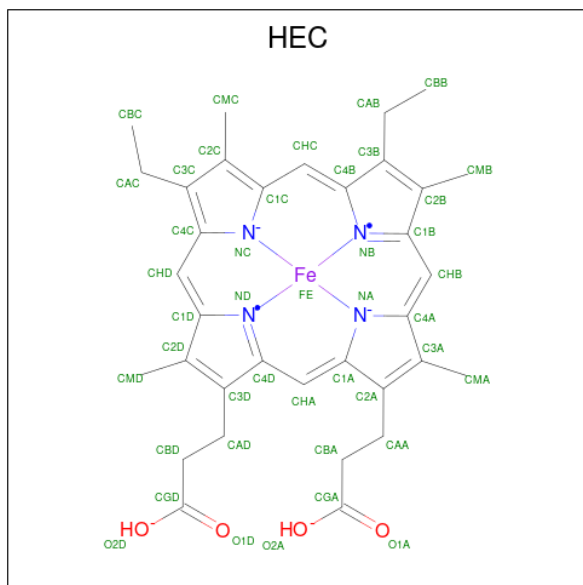
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	N	O	0	0
			64	55	4	5		
33	D	1	Total	C	N	O	0	0
			64	55	4	5		
33	a	1	Total	C	N	O	0	0
			64	55	4	5		
33	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	124	Total O 128 128	0	4
36	B	185	Total O 185 185	0	0
36	C	160	Total O 160 160	0	0
36	D	123	Total O 123 123	0	0
36	E	17	Total O 17 17	0	0
36	F	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	H	32	Total 32	O 32	0	0
36	I	9	Total 9	O 9	0	0
36	J	11	Total 11	O 11	0	0
36	K	10	Total 10	O 10	0	0
36	L	7	Total 7	O 7	0	0
36	M	8	Total 8	O 8	0	0
36	O	108	Total 108	O 108	0	0
36	T	9	Total 9	O 9	0	0
36	U	33	Total 33	O 33	0	0
36	V	74	Total 74	O 74	0	0
36	Y	10	Total 10	O 10	0	0
36	X	11	Total 11	O 11	0	0
36	Z	4	Total 4	O 4	0	0
36	R	4	Total 4	O 4	0	0
36	a	107	Total 111	O 111	0	4
36	b	171	Total 171	O 171	0	0
36	c	150	Total 150	O 150	0	0
36	d	94	Total 94	O 94	0	0
36	e	16	Total 16	O 16	0	0
36	f	3	Total 3	O 3	0	0
36	h	16	Total 16	O 16	0	0

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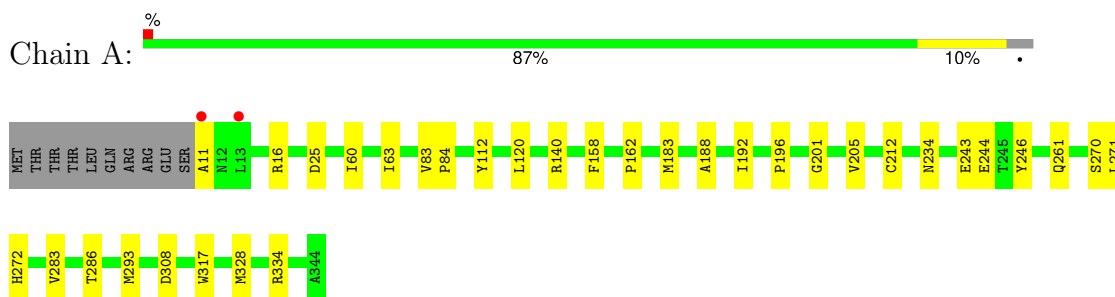
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	i	16	Total 16	O 16	0	0
36	j	11	Total 11	O 11	0	0
36	k	6	Total 6	O 6	0	0
36	l	14	Total 14	O 14	0	0
36	m	8	Total 8	O 8	0	0
36	o	96	Total 96	O 96	0	0
36	t	9	Total 9	O 9	0	0
36	u	58	Total 58	O 58	0	0
36	v	44	Total 44	O 44	0	0
36	y	11	Total 11	O 11	0	0
36	x	11	Total 11	O 11	0	0
36	r	10	Total 10	O 10	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.

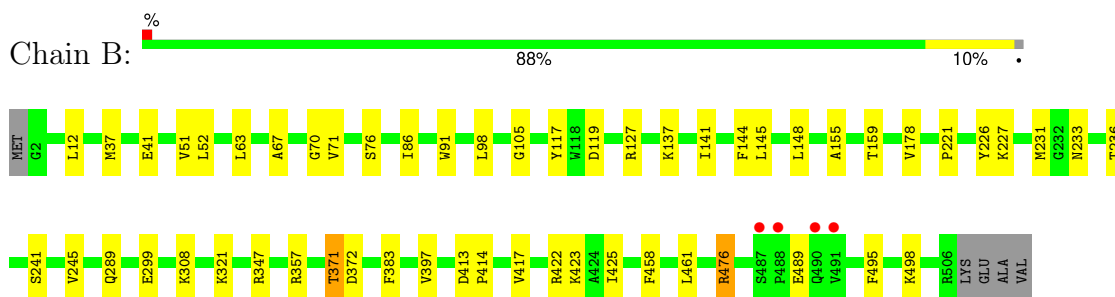
- Molecule 1: Photosystem II protein D1 1



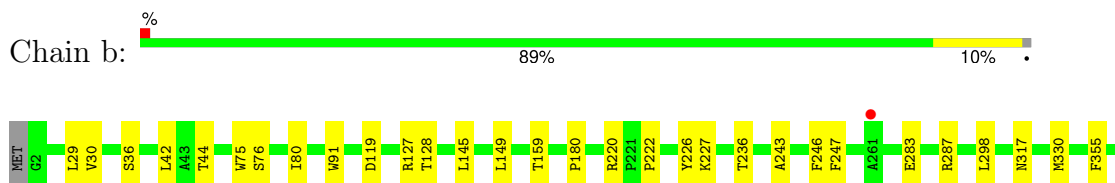
- Molecule 1: Photosystem II protein D1 1

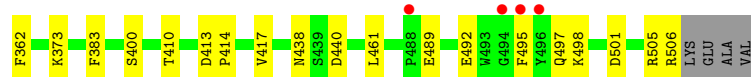


- Molecule 2: Photosystem II CP47 reaction center protein

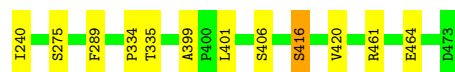


- Molecule 2: Photosystem II CP47 reaction center protein

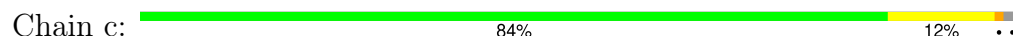




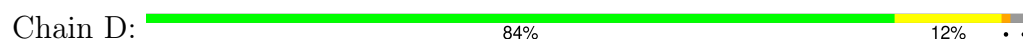
- Molecule 3: Photosystem II CP43 reaction center protein



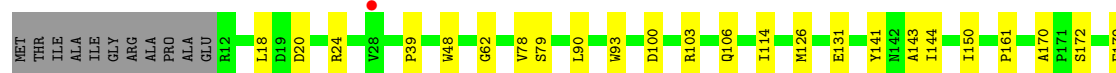
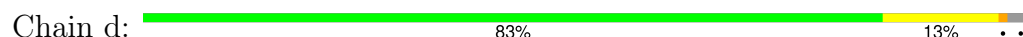
- Molecule 3: Photosystem II CP43 reaction center protein



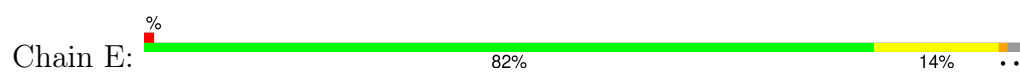
- Molecule 4: Photosystem II D2 protein



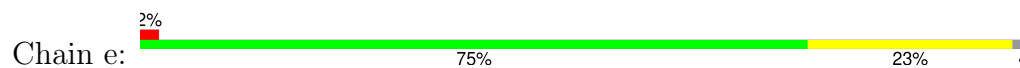
- Molecule 4: Photosystem II D2 protein



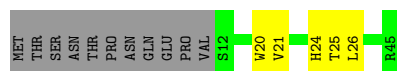
- Molecule 5: Cytochrome b559 subunit alpha



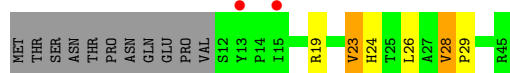
- Molecule 5: Cytochrome b559 subunit alpha



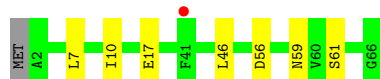
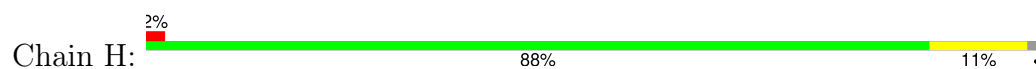
- Molecule 6: Cytochrome b559 subunit beta



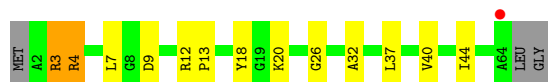
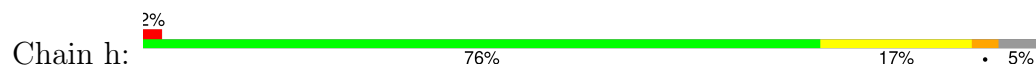
- Molecule 6: Cytochrome b559 subunit beta



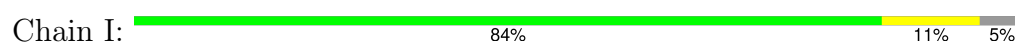
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  79% 16% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  2% 78% 12% 10%



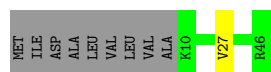
- Molecule 9: Photosystem II reaction center protein J

Chain j:  8% 65% 22% 10%



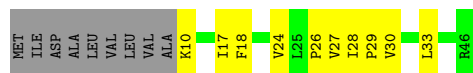
- Molecule 10: Photosystem II reaction center protein K

Chain K:  78% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  59% 22% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  84% 16%



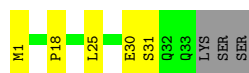
- Molecule 11: Photosystem II reaction center protein L

Chain l:  84% 8% 5% 5%



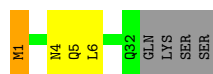
- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 14% 8%



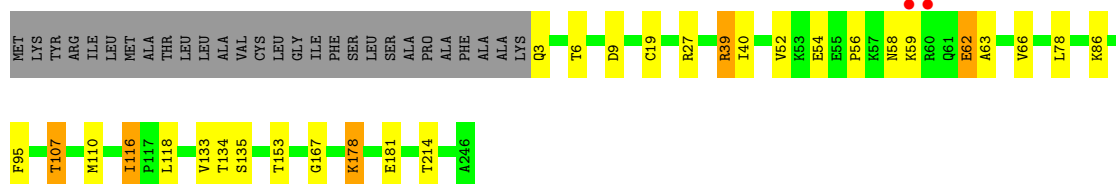
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 8% 11%



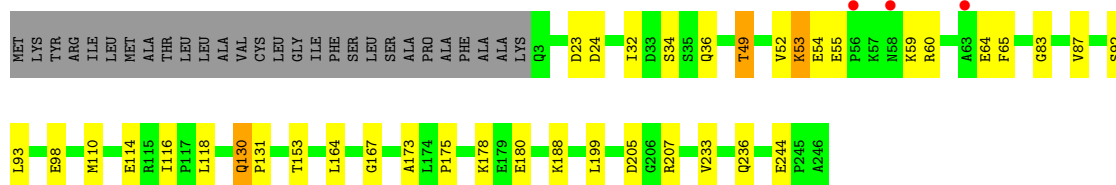
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  79% 9% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  75% 13% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 6% 6%



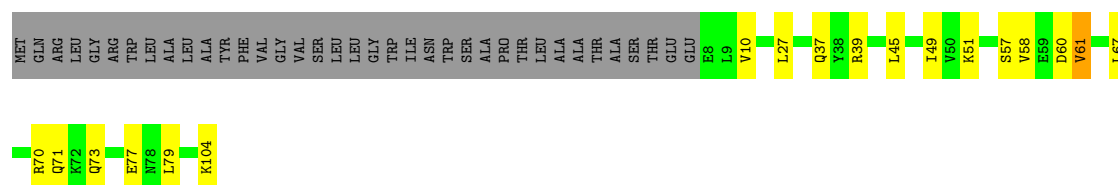
- Molecule 14: Photosystem II reaction center protein T

Chain t:  88% 6% 6%



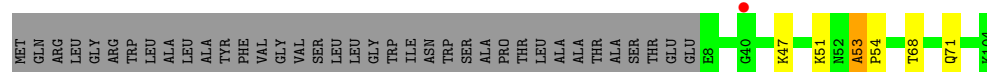
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 



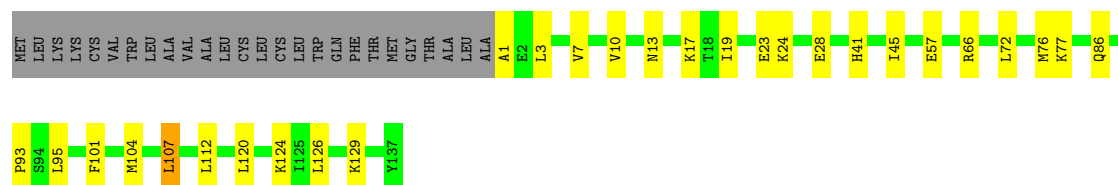
- Molecule 16: Cytochrome c-550

Chain V: 

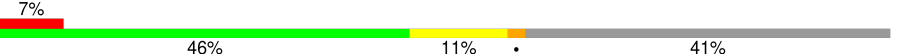


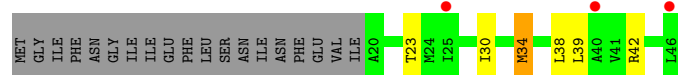
- Molecule 16: Cytochrome c-550

Chain v: 



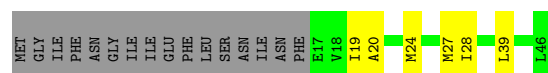
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 

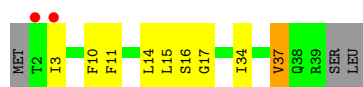


- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 



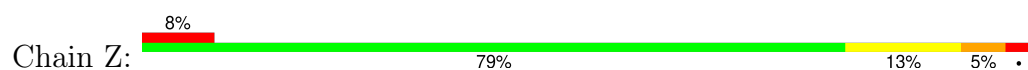
- Molecule 18: Photosystem II reaction center X protein



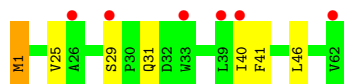
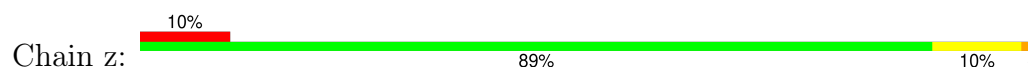
- Molecule 18: Photosystem II reaction center X protein



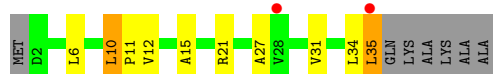
- Molecule 19: Photosystem II reaction center protein Z



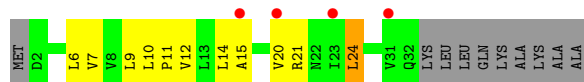
- Molecule 19: Photosystem II reaction center protein Z



- 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	117.53Å 222.83Å 309.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.23 – 2.03 31.23 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.9 (31.23-2.03) 85.2 (31.23-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.199 , 0.248 0.200 , 0.248	Depositor DCC
R_{free} test set	4617 reflections (0.74%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53209	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: DGD, LMG, HEM, BCR, LHG, SQD, CL, OEY, PHO, HEC, PL9, CLA, FE2, BCT, STE, FME

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	0.32	0/3212	0.49	0/4376
1	a	0.31	0/3209	0.48	0/4372
2	B	0.33	0/4155	0.48	0/5661
2	b	0.31	0/4118	0.46	0/5611
3	C	0.31	0/3625	0.47	0/4935
3	c	0.29	0/3705	0.45	0/5042
4	D	0.35	0/2825	0.50	0/3847
4	d	0.34	0/2834	0.51	0/3859
5	E	0.25	0/688	0.41	0/940
5	e	0.22	0/683	0.42	0/932
6	F	0.27	0/284	0.42	0/387
6	f	0.27	0/284	0.49	0/387
7	H	0.31	0/523	0.47	0/713
7	h	0.28	0/511	0.44	0/697
8	I	0.31	0/293	0.46	0/396
8	i	0.32	0/293	0.46	0/396
9	J	0.26	0/263	0.38	0/356
9	j	0.25	0/263	0.40	0/356
10	K	0.26	0/303	0.43	0/416
10	k	0.25	0/303	0.41	0/416
11	L	0.34	0/311	0.44	0/422
11	l	0.33	0/303	0.49	0/412
12	M	0.33	0/249	0.45	0/341
12	m	0.34	0/244	0.47	0/334
13	O	0.30	0/1904	0.52	0/2585
13	o	0.31	0/1905	0.50	0/2583
14	T	0.32	0/257	0.48	0/349
14	t	0.30	0/255	0.44	0/346
15	U	0.27	0/785	0.45	0/1064
15	u	0.31	0/785	0.49	0/1064
16	V	0.30	0/1085	0.50	0/1473
16	v	0.26	0/1085	0.43	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.25	0/197	0.38	0/264
17	y	0.19	0/219	0.40	0/294
18	X	0.25	0/284	0.39	0/384
18	x	0.22	0/289	0.28	0/391
19	Z	0.20	0/490	0.41	0/669
19	z	0.18	0/488	0.30	0/666
20	R	0.25	0/277	0.40	0/380
20	r	0.21	0/252	0.36	0/347
All	All	0.31	0/44038	0.47	0/59936

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	2981	29	0
1	a	3110	0	2972	36	0
2	B	4005	0	3871	36	0
2	b	3978	0	3836	38	0
3	C	3509	0	3426	22	0
3	c	3583	0	3499	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2731	0	2637	35	0
4	d	2737	0	2643	31	0
5	E	666	0	651	11	0
5	e	664	0	648	12	0
6	F	275	0	282	3	0
6	f	275	0	282	4	0
7	H	510	0	532	4	0
7	h	498	0	518	11	0
8	I	296	0	311	1	0
8	i	296	0	311	6	0
9	J	257	0	268	3	0
9	j	257	0	268	7	0
10	K	293	0	305	0	0
10	k	293	0	305	4	0
11	L	304	0	316	8	0
11	l	296	0	304	3	0
12	M	256	0	269	5	0
12	m	251	0	267	4	0
13	O	1870	0	1830	20	0
13	o	1874	0	1846	21	0
14	T	258	0	261	4	0
14	t	256	0	256	1	0
15	U	774	0	773	8	0
15	u	774	0	773	5	0
16	V	1064	0	1073	13	0
16	v	1064	0	1073	15	0
17	Y	196	0	217	4	0
17	y	218	0	241	4	0
18	X	281	0	312	6	0
18	x	286	0	314	9	0
19	Z	479	0	516	10	0
19	z	477	0	509	4	0
20	R	271	0	298	4	0
20	r	246	0	263	4	0
21	A	22	0	0	2	0
21	a	22	0	0	1	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	4	0	1	1	0
24	d	4	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	249	0	264	6	0
25	B	1035	0	1139	30	0
25	C	839	0	922	30	0
25	D	130	0	144	6	0
25	a	260	0	288	8	0
25	b	1035	0	1139	37	0
25	c	839	0	919	36	0
25	d	130	0	144	3	0
26	A	40	0	56	0	0
26	B	120	0	168	5	0
26	C	40	0	56	2	0
26	D	40	0	56	1	0
26	H	40	0	56	5	0
26	K	120	0	168	4	0
26	T	40	0	56	3	0
26	a	40	0	56	0	0
26	b	120	0	168	6	0
26	c	40	0	56	4	0
26	d	40	0	56	1	0
26	h	40	0	56	5	0
26	k	120	0	168	4	0
26	t	40	0	56	4	0
27	A	55	0	80	6	0
27	D	55	0	80	2	0
27	a	55	0	80	5	0
27	d	55	0	80	3	0
28	A	48	0	66	0	0
28	B	79	0	112	7	0
28	C	48	0	66	1	0
28	D	84	0	116	4	0
28	b	55	0	86	1	0
28	c	134	0	181	6	0
28	d	67	0	92	1	0
28	m	51	0	72	4	0
29	A	91	0	136	2	0
29	B	54	0	78	5	0
29	D	36	0	46	1	0
29	a	90	0	134	4	0
29	b	49	0	65	5	0
29	f	41	0	49	3	0
30	A	49	0	74	1	0
30	D	145	0	215	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	L	49	0	74	1	0
30	d	137	0	199	6	0
30	e	42	0	57	5	0
30	l	49	0	74	5	0
31	A	66	0	96	4	0
31	C	124	0	164	2	0
31	H	62	0	82	2	0
31	J	62	0	82	5	0
31	a	44	0	75	3	0
31	c	186	0	246	12	0
31	h	62	0	82	0	0
32	A	20	0	35	0	0
32	B	75	0	117	5	0
32	C	40	0	63	1	0
32	D	20	0	35	6	0
32	E	12	0	16	0	0
32	H	18	0	35	2	0
32	I	15	0	26	2	0
32	J	12	0	16	0	0
32	L	12	0	16	1	0
32	M	25	0	38	0	0
32	T	16	0	31	2	0
32	a	12	0	16	0	0
32	b	61	0	104	4	0
32	c	20	0	35	1	0
32	d	37	0	61	7	0
32	j	12	0	16	1	0
32	k	12	0	16	0	0
32	m	18	0	35	2	0
32	t	24	0	36	0	0
33	D	128	0	148	1	0
33	a	64	0	74	1	0
33	d	64	0	74	3	0
34	E	43	0	30	2	0
34	f	43	0	30	3	0
35	V	43	0	30	0	0
35	v	43	0	30	1	0
36	A	128	0	0	6	0
36	B	185	0	0	2	0
36	C	160	0	0	1	0
36	D	123	0	0	2	0
36	E	17	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	F	2	0	0	0	0
36	H	32	0	0	0	0
36	I	9	0	0	0	0
36	J	11	0	0	0	0
36	K	10	0	0	0	0
36	L	7	0	0	0	0
36	M	8	0	0	1	0
36	O	108	0	0	5	0
36	R	4	0	0	0	0
36	T	9	0	0	0	0
36	U	33	0	0	1	0
36	V	74	0	0	2	0
36	X	11	0	0	0	0
36	Y	10	0	0	1	0
36	Z	4	0	0	0	0
36	a	111	0	0	3	0
36	b	171	0	0	3	0
36	c	150	0	0	2	0
36	d	94	0	0	0	0
36	e	16	0	0	0	0
36	f	3	0	0	0	0
36	h	16	0	0	0	0
36	i	16	0	0	3	0
36	j	11	0	0	2	0
36	k	6	0	0	0	0
36	l	14	0	0	1	0
36	m	8	0	0	1	0
36	o	96	0	0	3	0
36	r	10	0	0	1	0
36	t	9	0	0	0	0
36	u	58	0	0	2	0
36	v	44	0	0	1	0
36	x	11	0	0	0	0
36	y	11	0	0	0	0
All	All	53209	0	52752	630	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 6.

The worst 5 of 630 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	1.93	0.85
32:D:413:STE:H142	18:X:17:GLY:HA2	1.60	0.83
25:C:513:CLA:HBB1	26:K:101:BCR:H24C	1.58	0.83
15:u:53:ALA:O	36:u:201:HOH:O	1.95	0.82
2:B:357:ARG:NH1	36:D:501:HOH:O	2.15	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%)	391 (99%)	4 (1%)	0	100	100
1	a	395/344 (115%)	390 (99%)	5 (1%)	0	100	100
2	B	507/510 (99%)	502 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	495 (98%)	8 (2%)	0	100	100
3	C	451/461 (98%)	439 (97%)	11 (2%)	1 (0%)	43	40
3	c	461/461 (100%)	448 (97%)	12 (3%)	1 (0%)	43	40
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	331 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	230 (95%)	10 (4%)	3 (1%)	10	4
13	o	242/272 (89%)	234 (97%)	8 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	5
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	10
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	3	1
19	z	60/62 (97%)	60 (100%)	0	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5386/5700 (94%)	5252 (98%)	125 (2%)	9 (0%)	43	40

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
19	Z	31	GLN
3	c	416	SER
13	O	59	LYS

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	73
1	a	321/280 (115%)	309 (96%)	12 (4%)	30	24
2	B	407/407 (100%)	399 (98%)	8 (2%)	48	48
2	b	402/407 (99%)	393 (98%)	9 (2%)	45	45
3	C	353/362 (98%)	347 (98%)	6 (2%)	53	53
3	c	362/362 (100%)	345 (95%)	17 (5%)	23	16
4	D	277/283 (98%)	271 (98%)	6 (2%)	45	45
4	d	278/283 (98%)	266 (96%)	12 (4%)	26	19
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	20
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	12
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	26
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	7
7	H	54/55 (98%)	52 (96%)	2 (4%)	30	24
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	11
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	9
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	5
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	29
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	34
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	1
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	26
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	206/228 (90%)	198 (96%)	8 (4%)	28	22
13	o	207/228 (91%)	195 (94%)	12 (6%)	18	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	23
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	22
15	U	84/112 (75%)	77 (92%)	7 (8%)	10	5
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	53
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	28
17	Y	19/37 (51%)	16 (84%)	3 (16%)	2	0
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	4
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	2
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	2
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2	0
19	z	51/52 (98%)	49 (96%)	2 (4%)	28	22
20	R	28/33 (85%)	23 (82%)	5 (18%)	2	0
20	r	25/33 (76%)	18 (72%)	7 (28%)	0	0
All	All	4450/4654 (96%)	4278 (96%)	172 (4%)	28	22

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	233	ARG
13	o	53	LYS
4	d	291	LEU
7	h	7	LEU
13	o	130	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	338	GLN
3	c	25	ASN
13	o	219	GLN
2	b	497	GLN
3	c	311	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	0.99	0	8,9,11	1.01	0
12	FME	m	1	12	8,9,10	1.04	1 (12%)	8,9,11	0.90	0
14	FME	t	1	14	8,9,10	1.10	0	8,9,11	0.80	0
14	FME	T	1	14	8,9,10	1.28	1 (12%)	8,9,11	1.10	1 (12%)
8	FME	i	1	8	8,9,10	1.00	0	8,9,11	1.04	1 (12%)
8	FME	I	1	8	8,9,10	1.06	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
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	3/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.87	1.42	1.46
8	I	1	FME	CA-N	-2.10	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	FME	CA-N	-2.04	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.58	114.48	109.50
8	i	1	FME	CA-N-CN	-2.01	119.73	122.82

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	1	0
12	m	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	606	2	69,73,73	1.36	7 (10%)	82,113,113	1.51	8 (9%)
35	HEC	v	201	16	50,50,50	1.80	7 (14%)	68,82,82	1.32	4 (5%)
25	CLA	b	610	36	69,73,73	1.26	6 (8%)	82,113,113	1.21	8 (9%)
28	LMG	D	411	-	31,31,55	0.69	1 (3%)	33,33,63	1.24	3 (9%)
29	SQD	a	613	-	35,35,54	1.73	5 (14%)	37,37,65	1.37	3 (8%)
25	CLA	b	616	2	64,68,73	1.30	8 (12%)	76,107,113	1.56	7 (9%)
25	CLA	b	615	2	69,73,73	1.40	7 (10%)	82,113,113	1.29	5 (6%)
25	CLA	C	504	36	63,67,73	1.50	10 (15%)	74,105,113	1.36	10 (13%)
25	CLA	C	511	3	69,73,73	1.34	8 (11%)	82,113,113	1.44	5 (6%)
31	DGD	a	614	-	43,43,67	0.69	2 (4%)	45,45,81	1.40	6 (13%)
25	CLA	b	608	2	69,73,73	1.26	9 (13%)	82,113,113	1.32	8 (9%)
25	CLA	C	502	3	69,73,73	1.12	6 (8%)	82,113,113	1.23	5 (6%)
32	STE	C	519	-	11,11,19	0.72	0	11,11,19	1.10	0
24	BCT	d	401	22	3,3,3	1.16	0	2,3,3	2.97	1 (50%)
26	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	7 (12%)
26	BCR	H	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.22	6 (10%)
32	STE	C	518	-	11,11,19	0.71	0	11,11,19	1.38	1 (9%)
28	LMG	B	620	-	51,51,55	0.83	2 (3%)	59,59,63	1.36	5 (8%)
21	OEY	A	601[A]	36,3,1	0,16,16	-	-	-	-	-
31	DGD	H	102	-	63,63,67	1.10	7 (11%)	77,77,81	1.44	9 (11%)
32	STE	b	625	-	9,9,19	0.40	0	8,8,19	0.63	0
28	LMG	c	518	-	37,37,55	0.95	2 (5%)	45,45,63	1.31	5 (11%)
25	CLA	B	601	36	69,73,73	1.34	7 (10%)	82,113,113	1.53	8 (9%)
25	CLA	C	513	3	69,73,73	1.39	9 (13%)	82,113,113	1.30	8 (9%)
32	STE	B	625	-	17,17,19	0.68	0	17,17,19	1.00	0
25	CLA	c	503	3	69,73,73	1.26	8 (11%)	82,113,113	1.49	7 (8%)
26	BCR	k	102	-	41,41,41	1.06	3 (7%)	56,56,56	1.09	2 (3%)
32	STE	C	520	-	15,15,19	0.38	0	14,14,19	0.80	0
29	SQD	A	613	-	50,52,54	1.58	7 (14%)	60,63,65	1.95	12 (20%)
31	DGD	A	616	-	67,67,67	1.09	9 (13%)	81,81,81	1.33	10 (12%)
29	SQD	D	408	-	34,36,54	1.50	6 (17%)	42,45,65	1.84	11 (26%)
28	LMG	c	520	-	48,48,55	0.82	1 (2%)	56,56,63	1.39	9 (16%)
26	BCR	a	609	-	41,41,41	0.96	2 (4%)	56,56,56	1.17	4 (7%)
32	STE	d	413	-	19,19,19	0.56	0	19,19,19	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	B	617	-	41,41,41	1.00	3 (7%)	56,56,56	1.24	3 (5%)
25	CLA	b	601	36	69,73,73	1.40	7 (10%)	82,113,113	1.40	9 (10%)
30	LHG	d	407	-	48,48,48	0.82	3 (6%)	51,54,54	1.30	5 (9%)
25	CLA	C	510	3	69,73,73	1.29	10 (14%)	82,113,113	1.48	7 (8%)
30	LHG	D	410	-	46,46,48	0.82	3 (6%)	49,52,54	1.28	6 (12%)
32	STE	B	621	-	16,16,19	0.70	0	16,16,19	1.04	0
31	DGD	c	517	-	63,63,67	0.92	3 (4%)	77,77,81	1.39	10 (12%)
25	CLA	b	606	2	69,73,73	1.29	7 (10%)	82,113,113	1.45	7 (8%)
26	BCR	b	619	-	41,41,41	0.97	2 (4%)	56,56,56	1.16	3 (5%)
25	CLA	d	403	4	69,73,73	1.20	8 (11%)	82,113,113	1.26	6 (7%)
25	CLA	c	506	3	69,73,73	1.33	8 (11%)	82,113,113	1.27	6 (7%)
29	SQD	A	615	-	38,38,54	1.74	5 (13%)	40,40,65	1.13	2 (5%)
26	BCR	k	103	-	41,41,41	1.02	2 (4%)	56,56,56	1.09	2 (3%)
25	CLA	a	611	36	69,73,73	1.39	7 (10%)	82,113,113	1.41	11 (13%)
27	PL9	A	610	-	55,55,55	0.71	0	68,69,69	1.50	10 (14%)
33	PHO	D	401	-	58,69,69	1.91	10 (17%)	55,99,99	1.39	4 (7%)
25	CLA	B	616	2	64,68,73	1.27	7 (10%)	76,107,113	1.36	6 (7%)
26	BCR	b	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
25	CLA	b	602	2	69,73,73	1.20	7 (10%)	82,113,113	1.34	8 (9%)
25	CLA	c	508	3	68,72,73	1.35	9 (13%)	80,111,113	1.30	7 (8%)
25	CLA	B	608	2	69,73,73	1.22	10 (14%)	82,113,113	1.35	7 (8%)
31	DGD	h	102	-	63,63,67	0.96	4 (6%)	77,77,81	1.45	12 (15%)
32	STE	B	627	-	15,15,19	0.33	0	14,14,19	0.87	0
25	CLA	D	403	4	69,73,73	1.20	7 (10%)	82,113,113	1.36	10 (12%)
25	CLA	c	505	3	69,73,73	1.29	8 (11%)	82,113,113	1.37	8 (9%)
25	CLA	a	608	1	69,73,73	1.23	6 (8%)	82,113,113	1.17	4 (4%)
21	OEY	A	601[B]	36,3,1	0,16,16	-	-	-	-	-
25	CLA	B	605	2	69,73,73	1.21	7 (10%)	82,113,113	1.32	9 (10%)
28	LMG	C	517	-	48,48,55	0.82	1 (2%)	56,56,63	1.33	6 (10%)
31	DGD	J	101	-	63,63,67	0.84	3 (4%)	77,77,81	1.41	11 (14%)
32	STE	J	102	-	11,11,19	0.72	0	11,11,19	1.16	0
32	STE	b	624	-	14,14,19	0.30	0	13,13,19	0.97	0
35	HEC	V	201	16	50,50,50	1.70	8 (16%)	68,82,82	1.37	8 (11%)
32	STE	d	412	-	16,16,19	0.65	0	16,16,19	1.10	0
25	CLA	d	404	4	69,73,73	1.22	9 (13%)	82,113,113	1.29	8 (9%)
26	BCR	B	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.37	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	t	102	-	13,13,19	0.70	0	13,13,19	1.16	2 (15%)
32	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.80	0
26	BCR	c	514	-	41,41,41	1.09	3 (7%)	56,56,56	1.17	5 (8%)
26	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.32	8 (14%)
30	LHG	d	409	-	38,38,48	0.71	1 (2%)	41,44,54	1.14	3 (7%)
26	BCR	K	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.16	2 (3%)
32	STE	D	413	-	19,19,19	0.59	0	19,19,19	1.14	0
32	STE	j	101	-	11,11,19	0.74	0	11,11,19	1.19	1 (9%)
25	CLA	C	501	3	69,73,73	1.49	10 (14%)	82,113,113	1.48	7 (8%)
27	PL9	D	406	-	55,55,55	0.98	4 (7%)	68,69,69	1.48	15 (22%)
28	LMG	d	410	-	21,21,55	0.52	0	20,20,63	1.19	2 (10%)
25	CLA	C	505	3	69,73,73	1.20	7 (10%)	82,113,113	1.21	7 (8%)
28	LMG	b	622	-	55,55,55	0.87	4 (7%)	63,63,63	1.43	11 (17%)
28	LMG	d	411	-	44,44,55	0.90	2 (4%)	52,52,63	1.33	6 (11%)
25	CLA	b	604	2	69,73,73	1.32	8 (11%)	82,113,113	1.49	11 (13%)
25	CLA	B	603	2	69,73,73	1.35	6 (8%)	82,113,113	1.37	9 (10%)
25	CLA	c	511	3	69,73,73	1.44	6 (8%)	82,113,113	1.46	7 (8%)
25	CLA	b	603	2	69,73,73	1.29	9 (13%)	82,113,113	1.33	10 (12%)
25	CLA	b	613	2	69,73,73	1.24	7 (10%)	82,113,113	1.34	10 (12%)
26	BCR	h	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.26	6 (10%)
28	LMG	B	622	-	26,26,55	0.76	2 (7%)	26,26,63	1.21	1 (3%)
25	CLA	C	512	3	69,73,73	1.36	9 (13%)	82,113,113	1.38	10 (12%)
33	PHO	a	607	-	58,69,69	2.03	10 (17%)	55,99,99	1.39	6 (10%)
28	LMG	A	612	-	48,48,55	0.70	0	56,56,63	1.36	6 (10%)
25	CLA	C	503	3	69,73,73	1.39	9 (13%)	82,113,113	1.54	10 (12%)
25	CLA	c	502	3	69,73,73	1.25	6 (8%)	82,113,113	1.31	7 (8%)
30	LHG	D	409	-	48,48,48	0.74	3 (6%)	51,54,54	1.25	7 (13%)
32	STE	T	102	-	15,15,19	0.38	0	14,14,19	0.75	0
25	CLA	B	614	2	69,73,73	1.38	9 (13%)	82,113,113	1.27	10 (12%)
30	LHG	l	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.23	4 (7%)
27	PL9	d	406	-	55,55,55	0.90	1 (1%)	68,69,69	1.58	14 (20%)
25	CLA	c	507	36	69,73,73	1.24	9 (13%)	82,113,113	1.37	7 (8%)
30	LHG	D	412	-	48,48,48	0.82	1 (2%)	51,54,54	1.38	7 (13%)
26	BCR	d	405	-	41,41,41	1.05	3 (7%)	56,56,56	1.17	5 (8%)
25	CLA	B	607	36	69,73,73	1.14	6 (8%)	82,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	504	36	64,68,73	1.32	7 (10%)	76,107,113	1.31	8 (10%)
21	OEY	a	601[A]	36,3,1	0,16,16	-	-	-		
30	LHG	e	101	-	41,41,48	0.78	1 (2%)	44,47,54	1.31	6 (13%)
25	CLA	b	614	2	69,73,73	1.38	7 (10%)	82,113,113	1.29	10 (12%)
26	BCR	A	609	-	41,41,41	0.92	1 (2%)	56,56,56	1.23	5 (8%)
32	STE	I	101	-	14,14,19	0.35	0	13,13,19	0.88	0
25	CLA	a	605	1	69,73,73	1.44	10 (14%)	82,113,113	1.46	8 (9%)
32	STE	M	101	-	14,14,19	0.67	0	14,14,19	1.25	1 (7%)
30	LHG	L	101	-	48,48,48	0.64	1 (2%)	51,54,54	1.27	4 (7%)
25	CLA	B	602	2	69,73,73	1.21	5 (7%)	82,113,113	1.36	8 (9%)
25	CLA	C	509	3	69,73,73	1.20	8 (11%)	82,113,113	1.28	8 (9%)
25	CLA	A	608	1	58,62,73	1.27	8 (13%)	68,99,113	1.40	12 (17%)
25	CLA	a	606	36	69,73,73	1.26	6 (8%)	82,113,113	1.37	9 (10%)
30	LHG	d	408	-	48,48,48	0.69	0	51,54,54	1.26	6 (11%)
25	CLA	b	611	2	69,73,73	1.33	6 (8%)	82,113,113	1.35	9 (10%)
25	CLA	c	501	3	69,73,73	1.31	9 (13%)	82,113,113	1.38	6 (7%)
26	BCR	C	514	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	6 (10%)
32	STE	B	626	-	11,11,19	0.66	0	11,11,19	1.55	2 (18%)
32	STE	c	519	-	19,19,19	0.64	0	19,19,19	0.89	0
26	BCR	K	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	3 (5%)
25	CLA	B	609	2	69,73,73	1.24	8 (11%)	82,113,113	1.36	6 (7%)
32	STE	M	102	-	9,9,19	0.37	0	8,8,19	0.83	0
34	HEM	E	101	5,6	50,50,50	1.54	6 (12%)	67,82,82	1.15	5 (7%)
25	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.51	11 (13%)
32	STE	k	104	-	11,11,19	0.76	0	11,11,19	1.07	0
32	STE	L	102	-	11,11,19	0.67	0	11,11,19	1.19	1 (9%)
26	BCR	T	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.27	6 (10%)
25	CLA	B	615	2	69,73,73	1.29	6 (8%)	82,113,113	1.41	7 (8%)
29	SQD	b	620	-	47,49,54	1.65	9 (19%)	57,60,65	1.88	11 (19%)
29	SQD	f	102	-	39,41,54	1.65	7 (17%)	49,52,65	1.70	10 (20%)
29	SQD	a	612	-	52,54,54	1.60	7 (13%)	62,65,65	1.77	9 (14%)
25	CLA	c	513	3	69,73,73	1.20	7 (10%)	82,113,113	1.24	6 (7%)
25	CLA	A	607	36	69,73,73	1.44	8 (11%)	82,113,113	1.41	14 (17%)
32	STE	a	615	-	11,11,19	0.80	0	11,11,19	1.01	0
32	STE	m	102	-	17,17,19	0.36	0	16,16,19	0.90	0
27	PL9	a	610	-	55,55,55	0.75	0	68,69,69	1.47	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	B	623	-	52,54,54	1.57	8 (15%)	62,65,65	1.56	8 (12%)
30	LHG	A	614	-	48,48,48	0.79	2 (4%)	51,54,54	1.20	5 (9%)
25	CLA	b	605	2	69,73,73	1.21	6 (8%)	82,113,113	1.35	10 (12%)
25	CLA	C	506	3	69,73,73	1.23	7 (10%)	82,113,113	1.35	7 (8%)
32	STE	b	623	-	15,15,19	0.67	0	15,15,19	1.12	0
31	DGD	C	515	-	63,63,67	1.02	5 (7%)	77,77,81	1.30	10 (12%)
32	STE	t	103	-	9,9,19	0.32	0	8,8,19	0.84	0
25	CLA	A	606	1	69,73,73	1.35	8 (11%)	82,113,113	1.34	7 (8%)
25	CLA	B	604	2	69,73,73	1.45	7 (10%)	82,113,113	1.58	9 (10%)
25	CLA	B	610	36	69,73,73	1.18	7 (10%)	82,113,113	1.39	10 (12%)
25	CLA	B	613	2	69,73,73	1.34	7 (10%)	82,113,113	1.41	6 (7%)
28	LMG	D	407	-	51,51,55	0.94	3 (5%)	59,59,63	1.36	8 (13%)
21	OEY	a	601[B]	36,3,1	0,16,16	-	-	-	-	-
26	BCR	D	405	-	41,41,41	0.99	2 (4%)	56,56,56	1.24	4 (7%)
28	LMG	c	521	-	49,49,55	0.89	3 (6%)	57,57,63	1.26	7 (12%)
31	DGD	c	515	-	63,63,67	0.99	4 (6%)	77,77,81	1.40	11 (14%)
25	CLA	B	612	2	69,73,73	1.24	8 (11%)	82,113,113	1.36	9 (10%)
32	STE	A	617	-	19,19,19	0.62	0	19,19,19	0.95	0
25	CLA	b	612	2	69,73,73	1.14	5 (7%)	82,113,113	1.37	11 (13%)
25	CLA	A	611	36	69,73,73	1.19	6 (8%)	82,113,113	1.41	7 (8%)
33	PHO	D	402	-	58,69,69	2.14	9 (15%)	55,99,99	1.48	6 (10%)
25	CLA	D	404	4	69,73,73	1.26	8 (11%)	82,113,113	1.20	4 (4%)
24	BCT	A	605	22	3,3,3	1.15	0	2,3,3	2.84	1 (50%)
25	CLA	b	609	2	69,73,73	1.27	7 (10%)	82,113,113	1.38	9 (10%)
26	BCR	b	617	-	41,41,41	1.07	3 (7%)	56,56,56	1.34	7 (12%)
34	HEM	f	101	5,6	50,50,50	1.58	11 (22%)	67,82,82	1.34	8 (11%)
25	CLA	b	607	36	69,73,73	1.10	5 (7%)	82,113,113	1.26	10 (12%)
32	STE	B	624	-	11,11,19	0.75	0	11,11,19	1.40	2 (18%)
32	STE	b	621	-	19,19,19	0.59	0	19,19,19	1.14	0
26	BCR	B	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	c	512	3	69,73,73	1.33	12 (17%)	82,113,113	1.35	7 (8%)
25	CLA	B	611	2	69,73,73	1.16	7 (10%)	82,113,113	1.40	9 (10%)
31	DGD	C	516	-	63,63,67	1.04	5 (7%)	77,77,81	1.36	10 (12%)
25	CLA	c	509	3	69,73,73	1.17	8 (11%)	82,113,113	1.47	7 (8%)
25	CLA	C	507	36	69,73,73	1.27	7 (10%)	82,113,113	1.48	9 (10%)
25	CLA	c	510	3	69,73,73	1.35	7 (10%)	82,113,113	1.26	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.28	6 (10%)
33	PHO	d	402	-	58,69,69	2.07	10 (17%)	55,99,99	1.54	8 (14%)
31	DGD	c	516	-	63,63,67	1.03	7 (11%)	77,77,81	1.45	15 (19%)
28	LMG	m	101	-	51,51,55	0.91	3 (5%)	59,59,63	1.39	7 (11%)
32	STE	E	102	-	11,11,19	0.77	0	11,11,19	1.13	1 (9%)

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	606	2	-	14/39/115/115	-
35	HEC	v	201	16	1/1/3/7	6/14/54/54	-
25	CLA	b	610	36	-	9/39/115/115	-
28	LMG	D	411	-	-	13/33/33/70	-
29	SQD	a	613	-	-	22/37/37/69	-
25	CLA	b	616	2	-	4/33/109/115	-
25	CLA	b	615	2	-	9/39/115/115	-
25	CLA	C	504	36	-	8/32/108/115	-
25	CLA	C	511	3	-	6/39/115/115	-
31	DGD	a	614	-	-	26/45/45/95	-
25	CLA	b	608	2	-	5/39/115/115	-
25	CLA	C	502	3	-	6/39/115/115	-
32	STE	C	519	-	-	5/9/9/17	-
26	BCR	k	101	-	-	7/29/63/63	0/2/2/2
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
32	STE	C	518	-	-	5/9/9/17	-
28	LMG	B	620	-	-	14/46/66/70	0/1/1/1
31	DGD	H	102	-	-	17/51/91/95	0/2/2/2
32	STE	b	625	-	-	4/7/7/17	-
28	LMG	c	518	-	-	13/31/51/70	0/1/1/1
25	CLA	B	601	36	-	18/39/115/115	-
25	CLA	C	513	3	-	13/39/115/115	-
32	STE	B	625	-	-	5/15/15/17	-
25	CLA	c	503	3	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
32	STE	C	520	-	-	5/13/13/17	-
29	SQD	A	613	-	-	19/47/67/69	0/1/1/1
31	DGD	A	616	-	-	28/55/95/95	0/2/2/2
29	SQD	D	408	-	-	15/28/48/69	0/1/1/1
28	LMG	c	520	-	-	20/43/63/70	0/1/1/1
26	BCR	a	609	-	-	0/29/63/63	0/2/2/2
32	STE	d	413	-	-	10/17/17/17	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
25	CLA	b	601	36	-	17/39/115/115	-
30	LHG	d	407	-	-	15/53/53/53	-
25	CLA	C	510	3	-	7/39/115/115	-
30	LHG	D	410	-	-	21/51/51/53	-
32	STE	B	621	-	-	6/14/14/17	-
31	DGD	c	517	-	-	22/51/91/95	0/2/2/2
25	CLA	b	606	2	-	12/39/115/115	-
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	CLA	d	403	4	-	10/39/115/115	-
25	CLA	c	506	3	-	11/39/115/115	-
29	SQD	A	615	-	-	15/39/39/69	-
26	BCR	k	103	-	-	5/29/63/63	0/2/2/2
25	CLA	a	611	36	-	3/39/115/115	-
27	PL9	A	610	-	-	20/53/73/73	0/1/1/1
33	PHO	D	401	-	-	3/37/103/103	0/5/6/6
25	CLA	B	616	2	-	12/33/109/115	-
26	BCR	b	618	-	-	5/29/63/63	0/2/2/2
25	CLA	b	602	2	-	9/39/115/115	-
25	CLA	c	508	3	-	8/38/114/115	-
25	CLA	B	608	2	-	1/39/115/115	-
31	DGD	h	102	-	-	16/51/91/95	0/2/2/2
32	STE	B	627	-	-	7/13/13/17	-
25	CLA	D	403	4	-	7/39/115/115	-
25	CLA	c	505	3	-	9/39/115/115	-
25	CLA	a	608	1	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	605	2	-	10/39/115/115	-
28	LMG	C	517	-	-	18/43/63/70	0/1/1/1
35	HEC	V	201	16	1/1/3/7	6/14/54/54	-
31	DGD	J	101	-	-	15/51/91/95	0/2/2/2
32	STE	J	102	-	-	3/9/9/17	-
32	STE	b	624	-	-	10/12/12/17	-
32	STE	d	412	-	-	8/14/14/17	-
25	CLA	d	404	4	-	7/39/115/115	-
26	BCR	B	619	-	-	3/29/63/63	0/2/2/2
32	STE	t	102	-	-	7/11/11/17	-
32	STE	H	103	-	-	11/15/15/17	-
26	BCR	c	514	-	-	2/29/63/63	0/2/2/2
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2
30	LHG	d	409	-	-	13/43/43/53	-
26	BCR	K	103	-	-	7/29/63/63	0/2/2/2
32	STE	D	413	-	-	12/17/17/17	-
32	STE	j	101	-	-	5/9/9/17	-
25	CLA	C	501	3	-	5/39/115/115	-
27	PL9	D	406	-	-	10/53/73/73	0/1/1/1
28	LMG	d	410	-	-	11/17/17/70	-
25	CLA	C	505	3	-	6/39/115/115	-
28	LMG	b	622	-	-	27/50/70/70	0/1/1/1
28	LMG	d	411	-	-	15/39/59/70	0/1/1/1
25	CLA	b	604	2	-	8/39/115/115	-
25	CLA	B	603	2	-	10/39/115/115	-
25	CLA	c	511	3	-	5/39/115/115	-
25	CLA	b	603	2	-	6/39/115/115	-
25	CLA	b	613	2	-	8/39/115/115	-
26	BCR	h	101	-	-	7/29/63/63	0/2/2/2
28	LMG	B	622	-	-	12/22/22/70	-
25	CLA	C	512	3	-	10/39/115/115	-
33	PHO	a	607	-	-	4/37/103/103	0/5/6/6
28	LMG	A	612	-	-	20/43/63/70	0/1/1/1
25	CLA	C	503	3	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	502	3	-	10/39/115/115	-
30	LHG	D	409	-	-	22/53/53/53	-
32	STE	T	102	-	-	8/13/13/17	-
25	CLA	B	614	2	-	16/39/115/115	-
30	LHG	l	101	-	-	15/53/53/53	-
27	PL9	d	406	-	-	13/53/73/73	0/1/1/1
25	CLA	c	507	36	-	10/39/115/115	-
30	LHG	D	412	-	-	14/53/53/53	-
26	BCR	d	405	-	-	7/29/63/63	0/2/2/2
25	CLA	B	607	36	-	9/39/115/115	-
25	CLA	c	504	36	-	7/33/109/115	-
30	LHG	e	101	-	-	22/46/46/53	-
25	CLA	b	614	2	-	13/39/115/115	-
26	BCR	A	609	-	-	4/29/63/63	0/2/2/2
32	STE	I	101	-	-	4/12/12/17	-
25	CLA	a	605	1	-	1/39/115/115	-
32	STE	M	101	-	-	3/12/12/17	-
30	LHG	L	101	-	-	15/53/53/53	-
25	CLA	B	602	2	-	10/39/115/115	-
25	CLA	C	509	3	-	13/39/115/115	-
25	CLA	A	608	1	-	5/26/102/115	-
25	CLA	a	606	36	-	8/39/115/115	-
30	LHG	d	408	-	-	19/53/53/53	-
25	CLA	b	611	2	-	11/39/115/115	-
25	CLA	c	501	3	-	4/39/115/115	-
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
32	STE	B	626	-	-	3/9/9/17	-
32	STE	c	519	-	-	11/17/17/17	-
26	BCR	K	102	-	-	7/29/63/63	0/2/2/2
25	CLA	B	609	2	-	7/39/115/115	-
32	STE	M	102	-	-	2/7/7/17	-
34	HEM	E	101	5,6	-	2/14/54/54	-
25	CLA	C	508	3	-	6/39/115/115	-
32	STE	k	104	-	-	4/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	L	102	-	-	4/9/9/17	-
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
25	CLA	B	615	2	-	7/39/115/115	-
29	SQD	b	620	-	-	22/44/64/69	0/1/1/1
29	SQD	f	102	-	-	14/36/56/69	0/1/1/1
29	SQD	a	612	-	-	29/49/69/69	0/1/1/1
25	CLA	c	513	3	-	12/39/115/115	-
25	CLA	A	607	36	-	7/39/115/115	-
32	STE	a	615	-	-	5/9/9/17	-
32	STE	m	102	-	-	8/15/15/17	-
27	PL9	a	610	-	-	16/53/73/73	0/1/1/1
29	SQD	B	623	-	-	25/49/69/69	0/1/1/1
30	LHG	A	614	-	-	24/53/53/53	-
25	CLA	b	605	2	-	8/39/115/115	-
25	CLA	C	506	3	-	12/39/115/115	-
32	STE	b	623	-	-	9/13/13/17	-
31	DGD	C	515	-	-	17/51/91/95	0/2/2/2
32	STE	t	103	-	-	5/7/7/17	-
25	CLA	A	606	1	-	3/39/115/115	-
25	CLA	B	604	2	-	13/39/115/115	-
25	CLA	B	610	36	-	7/39/115/115	-
25	CLA	B	613	2	-	13/39/115/115	-
28	LMG	D	407	-	-	19/46/66/70	0/1/1/1
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
28	LMG	c	521	-	-	27/44/64/70	0/1/1/1
31	DGD	c	515	-	-	27/51/91/95	0/2/2/2
25	CLA	B	612	2	-	10/39/115/115	-
32	STE	A	617	-	-	10/17/17/17	-
25	CLA	b	612	2	-	12/39/115/115	-
25	CLA	A	611	36	-	4/39/115/115	-
33	PHO	D	402	-	-	1/37/103/103	0/5/6/6
25	CLA	D	404	4	-	9/39/115/115	-
25	CLA	b	609	2	-	12/39/115/115	-
26	BCR	b	617	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HEM	f	101	5,6	-	2/14/54/54	-
25	CLA	b	607	36	-	11/39/115/115	-
32	STE	B	624	-	-	5/9/9/17	-
32	STE	b	621	-	-	11/17/17/17	-
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	CLA	c	512	3	-	16/39/115/115	-
25	CLA	B	611	2	-	2/39/115/115	-
31	DGD	C	516	-	-	17/51/91/95	0/2/2/2
25	CLA	c	509	3	-	13/39/115/115	-
25	CLA	C	507	36	-	9/39/115/115	-
25	CLA	c	510	3	-	11/39/115/115	-
26	BCR	t	101	-	-	4/29/63/63	0/2/2/2
33	PHO	d	402	-	-	11/37/103/103	0/5/6/6
31	DGD	c	516	-	-	23/51/91/95	0/2/2/2
28	LMG	m	101	-	-	24/46/66/70	0/1/1/1
32	STE	E	102	-	-	5/9/9/17	-

The worst 5 of 797 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	402	PHO	C1B-C2B	9.21	1.49	1.39
33	d	402	PHO	C1B-C2B	9.12	1.49	1.39
33	D	402	PHO	C3B-C4B	8.87	1.50	1.41
33	a	607	PHO	C1B-C2B	8.76	1.49	1.39
33	d	402	PHO	C3B-C4B	8.22	1.49	1.41

The worst 5 of 1086 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C4A-NA-C1A	9.64	111.08	106.68
25	b	616	CLA	C4A-NA-C1A	9.10	110.83	106.68
25	B	601	CLA	C4A-NA-C1A	9.04	110.80	106.68
25	c	511	CLA	C4A-NA-C1A	8.69	110.64	106.68
25	C	503	CLA	C4A-NA-C1A	8.49	110.55	106.68

All (2) chirality outliers are listed below:

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

5 of 1807 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C4-C3-C5-C6
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

149 monomers are involved in 312 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	606	CLA	1	0
35	v	201	HEC	1	0
25	b	610	CLA	1	0
28	D	411	LMG	2	0
29	a	613	SQD	4	0
25	b	616	CLA	3	0
25	b	615	CLA	4	0
25	C	504	CLA	3	0
25	C	511	CLA	4	0
31	a	614	DGD	3	0
25	b	608	CLA	3	0
25	C	502	CLA	4	0
26	k	101	BCR	2	0
26	H	101	BCR	5	0
32	C	518	STE	1	0
28	B	620	LMG	5	0
21	A	601[A]	OEY	1	0
31	H	102	DGD	2	0
28	c	518	LMG	2	0
25	B	601	CLA	6	0
25	C	513	CLA	4	0
32	B	625	STE	2	0
25	c	503	CLA	5	0
26	k	102	BCR	1	0
29	A	613	SQD	1	0
31	A	616	DGD	4	0
29	D	408	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	c	520	LMG	1	0
32	d	413	STE	6	0
26	B	617	BCR	1	0
25	b	601	CLA	4	0
30	d	407	LHG	4	0
25	C	510	CLA	2	0
32	B	621	STE	2	0
31	c	517	DGD	6	0
25	b	606	CLA	3	0
26	b	619	BCR	3	0
25	d	403	CLA	1	0
25	c	506	CLA	3	0
29	A	615	SQD	1	0
26	k	103	BCR	1	0
25	a	611	CLA	3	0
27	A	610	PL9	6	0
25	B	616	CLA	1	0
26	b	618	BCR	2	0
25	b	602	CLA	3	0
25	c	508	CLA	3	0
25	D	403	CLA	3	0
25	c	505	CLA	3	0
25	a	608	CLA	1	0
21	A	601[B]	OEY	1	0
25	B	605	CLA	1	0
28	C	517	LMG	1	0
31	J	101	DGD	5	0
32	d	412	STE	1	0
25	d	404	CLA	2	0
26	B	619	BCR	2	0
32	H	103	STE	2	0
26	c	514	BCR	4	0
26	K	101	BCR	2	0
26	K	103	BCR	1	0
32	D	413	STE	6	0
32	j	101	STE	1	0
25	C	501	CLA	1	0
27	D	406	PL9	2	0
28	d	410	LMG	1	0
25	C	505	CLA	2	0
28	b	622	LMG	1	0
25	b	604	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	603	CLA	1	0
25	c	511	CLA	4	0
25	b	603	CLA	3	0
25	b	613	CLA	1	0
26	h	101	BCR	5	0
28	B	622	LMG	2	0
25	C	512	CLA	3	0
33	a	607	PHO	1	0
25	c	502	CLA	3	0
30	D	409	LHG	2	0
32	T	102	STE	2	0
25	B	614	CLA	7	0
30	l	101	LHG	5	0
27	d	406	PL9	3	0
25	c	507	CLA	3	0
30	D	412	LHG	5	0
26	d	405	BCR	1	0
25	B	607	CLA	3	0
25	c	504	CLA	2	0
30	e	101	LHG	5	0
25	b	614	CLA	5	0
32	I	101	STE	2	0
25	a	605	CLA	4	0
30	L	101	LHG	1	0
25	B	602	CLA	2	0
25	C	509	CLA	2	0
25	A	608	CLA	1	0
25	a	606	CLA	2	0
30	d	408	LHG	2	0
25	b	611	CLA	2	0
25	c	501	CLA	3	0
26	C	514	BCR	2	0
32	c	519	STE	1	0
26	K	102	BCR	1	0
25	B	609	CLA	2	0
34	E	101	HEM	2	0
25	C	508	CLA	5	0
32	L	102	STE	1	0
26	T	101	BCR	3	0
25	B	615	CLA	2	0
29	b	620	SQD	5	0
29	f	102	SQD	3	0

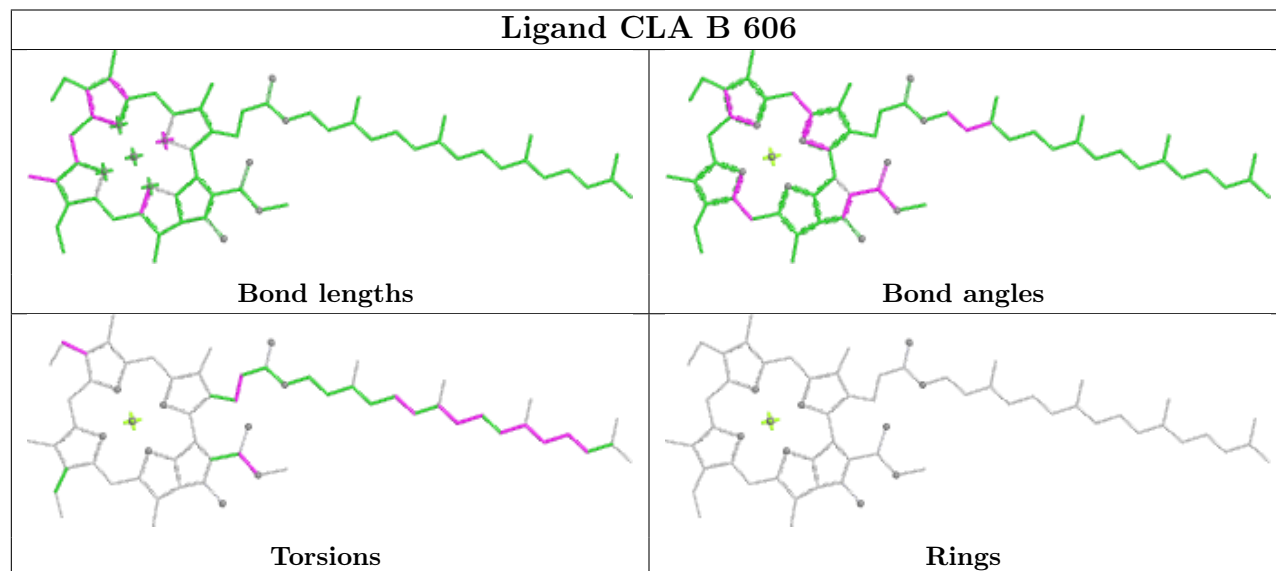
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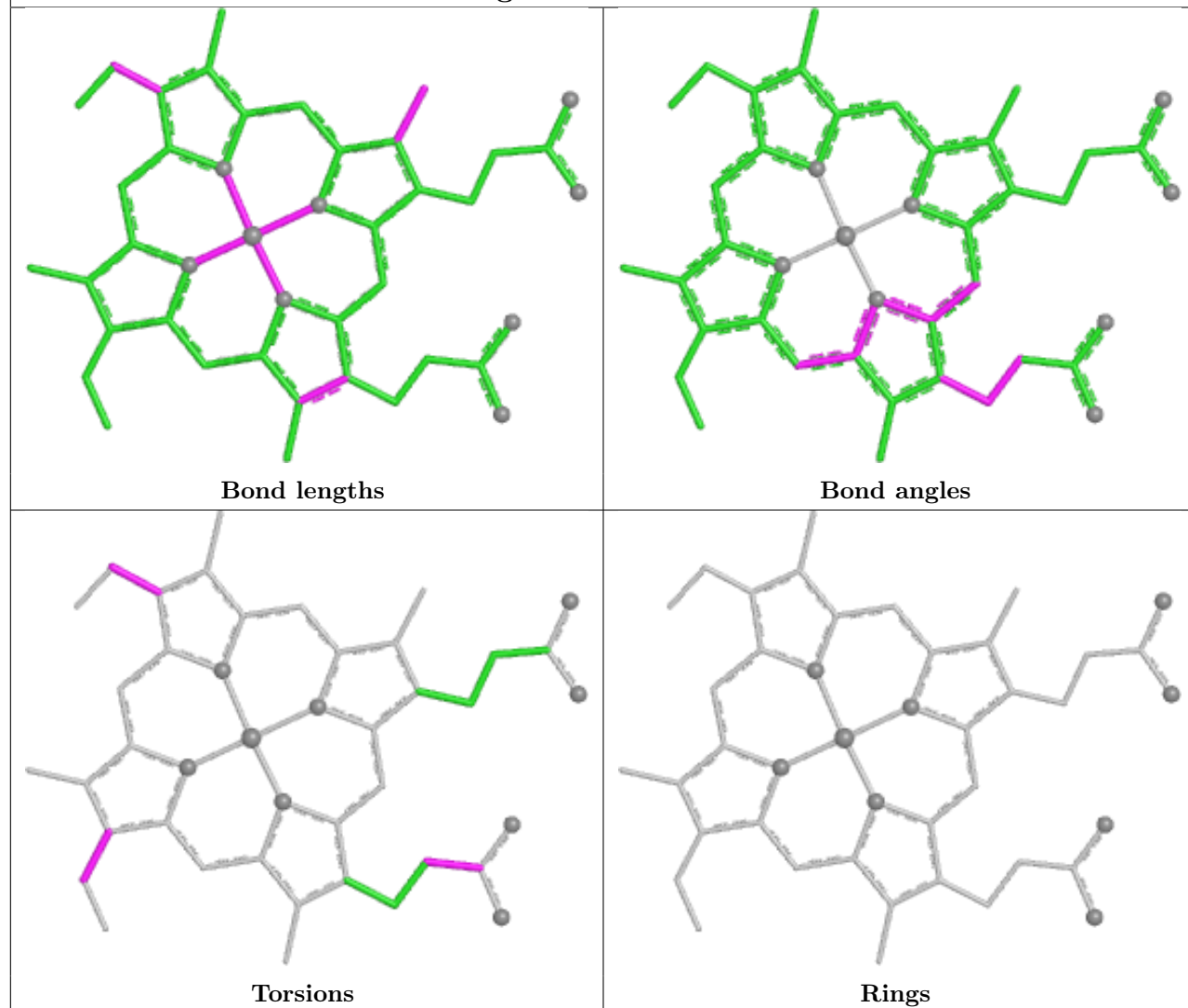
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	513	CLA	3	0
25	A	607	CLA	2	0
32	m	102	STE	2	0
27	a	610	PL9	5	0
29	B	623	SQD	5	0
30	A	614	LHG	1	0
25	b	605	CLA	4	0
25	C	506	CLA	4	0
25	A	606	CLA	3	0
25	B	604	CLA	1	0
25	B	613	CLA	3	0
28	D	407	LMG	2	0
21	a	601[B]	OEY	1	0
26	D	405	BCR	1	0
28	c	521	LMG	3	0
31	c	515	DGD	3	0
25	B	612	CLA	2	0
25	b	612	CLA	3	0
33	D	402	PHO	1	0
25	D	404	CLA	3	0
24	A	605	BCT	1	0
25	b	609	CLA	3	0
26	b	617	BCR	1	0
34	f	101	HEM	3	0
25	b	607	CLA	1	0
32	B	624	STE	1	0
32	b	621	STE	4	0
26	B	618	BCR	2	0
25	c	512	CLA	5	0
25	B	611	CLA	1	0
31	C	516	DGD	2	0
25	c	509	CLA	5	0
25	C	507	CLA	2	0
25	c	510	CLA	4	0
26	t	101	BCR	4	0
33	d	402	PHO	3	0
31	c	516	DGD	4	0
28	m	101	LMG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

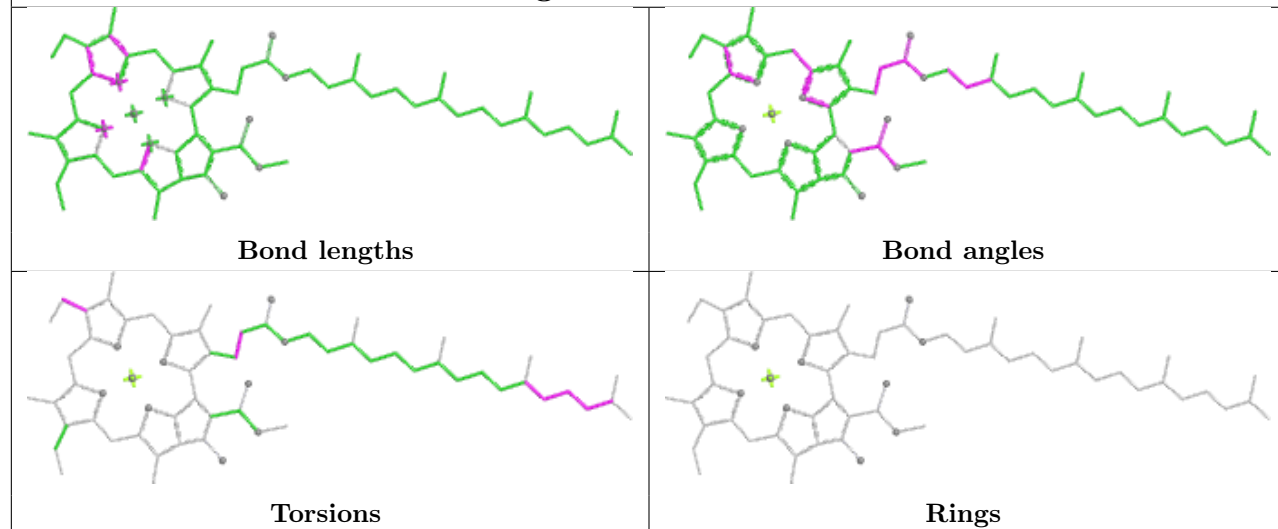
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

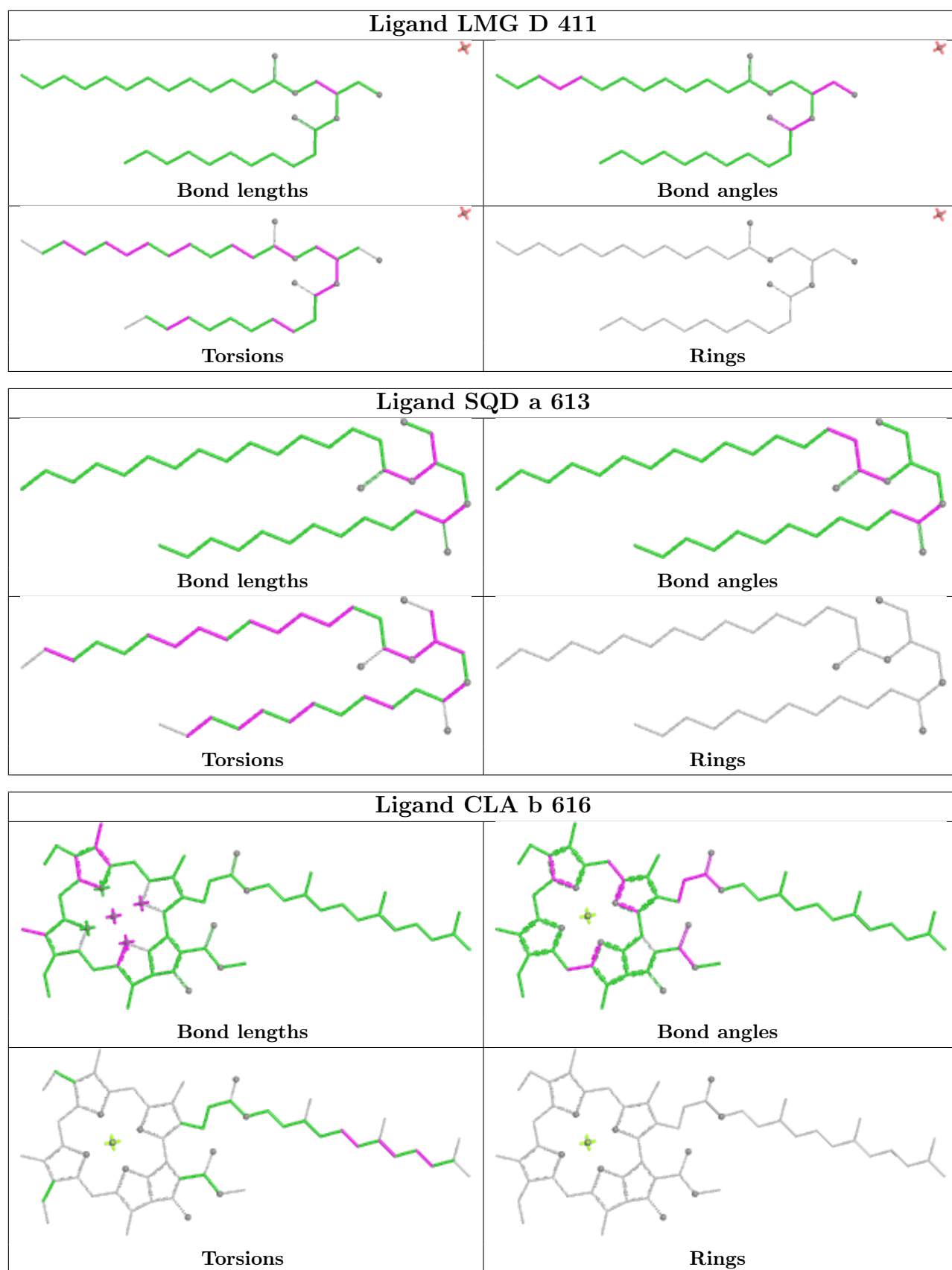


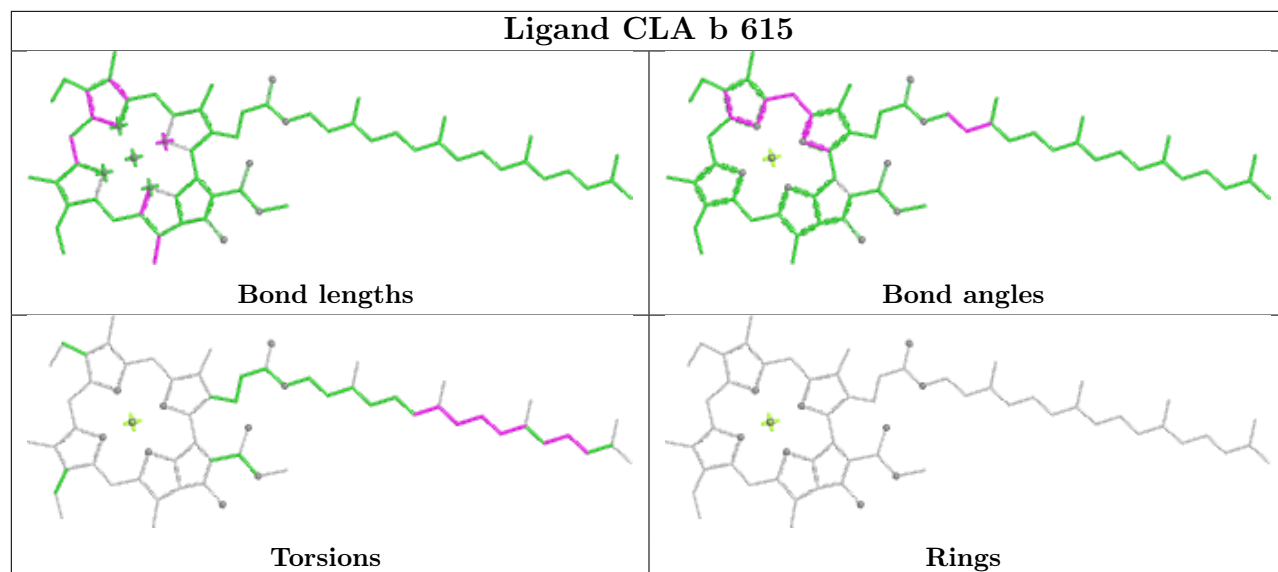
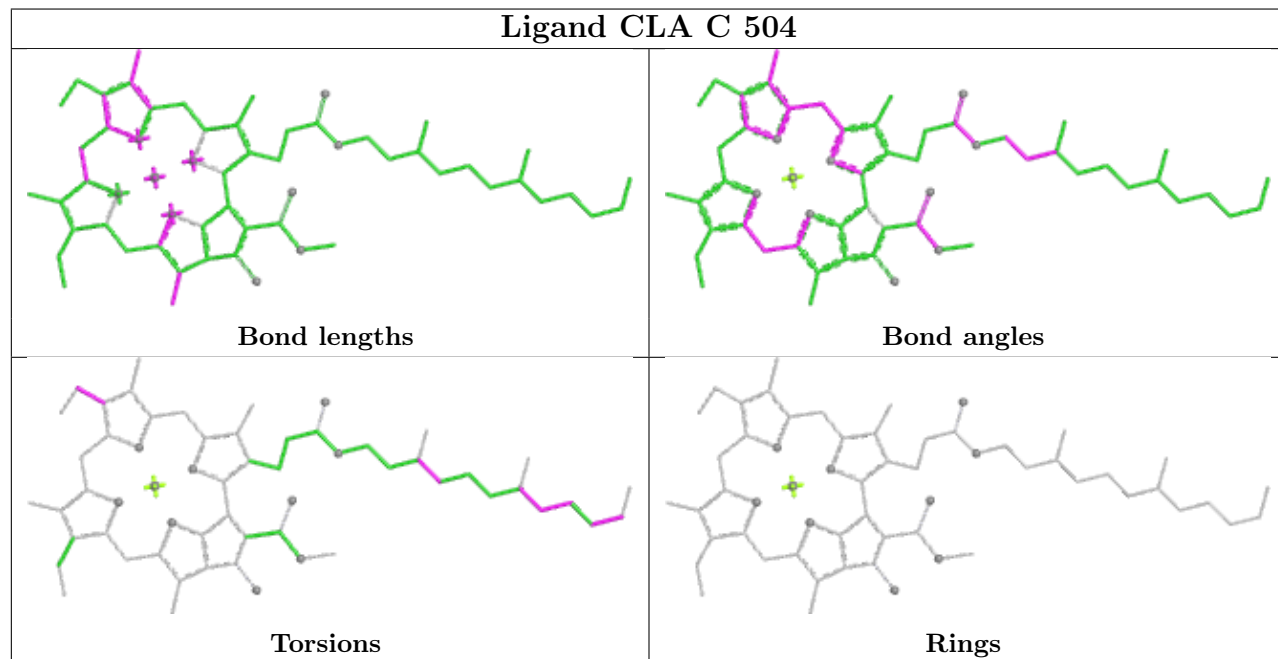
Ligand HEC v 201

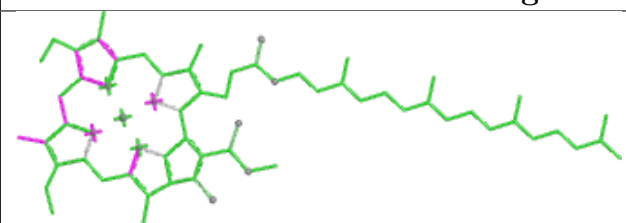
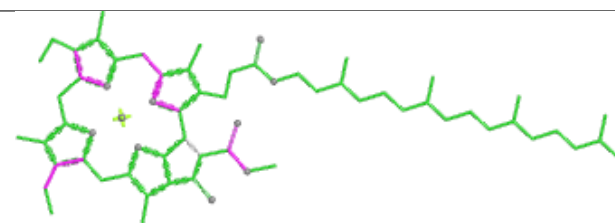
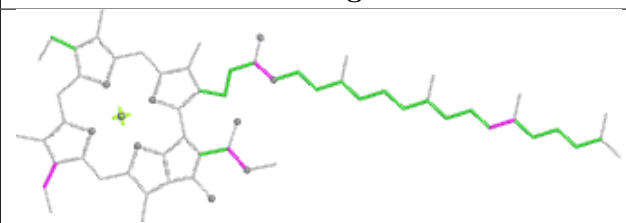
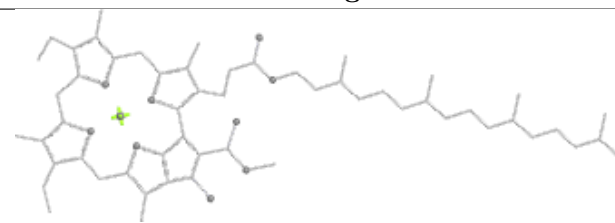


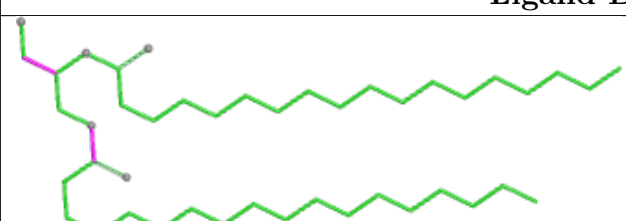
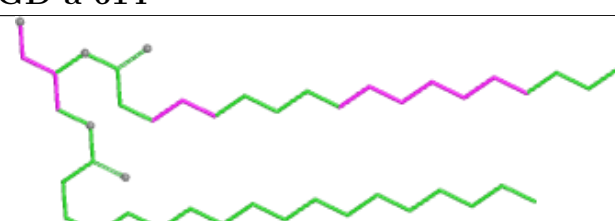
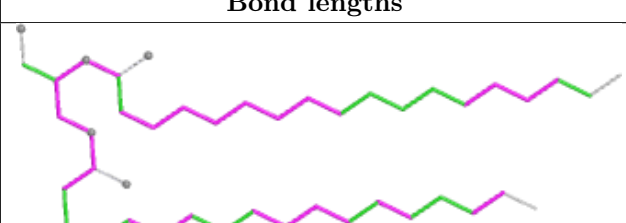
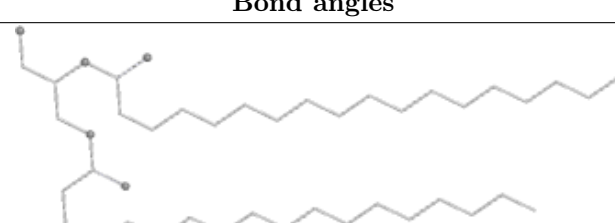
Ligand CLA b 610

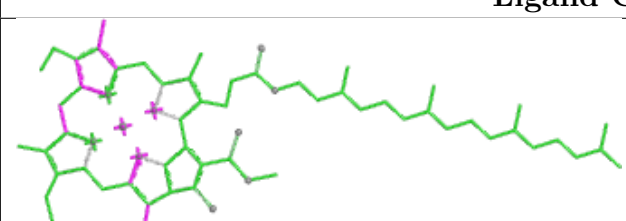
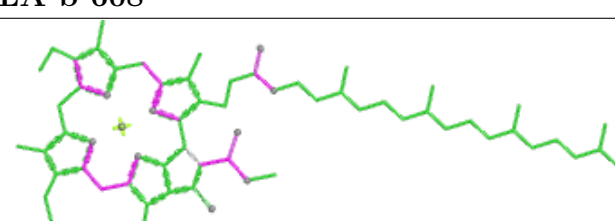
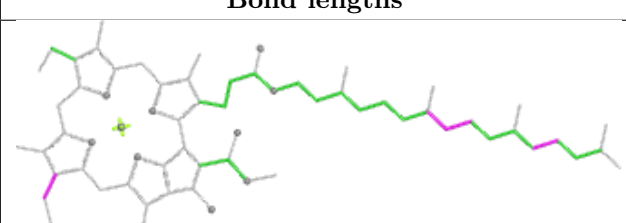
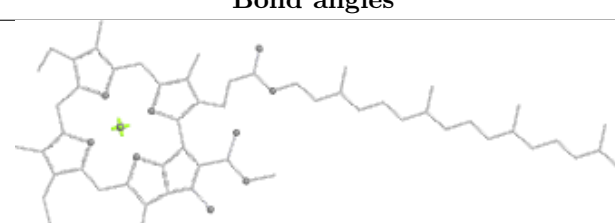


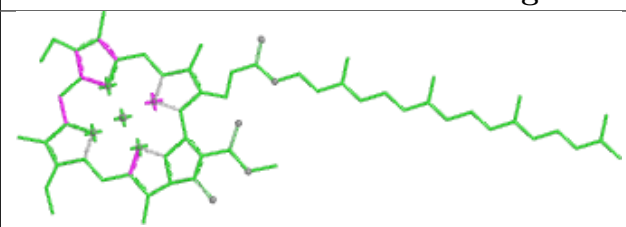
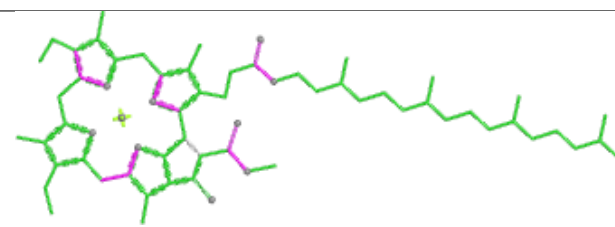
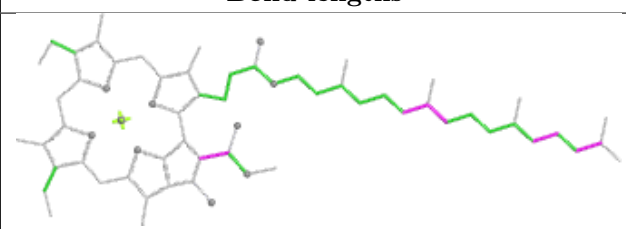
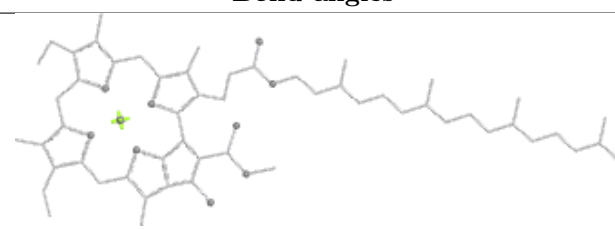


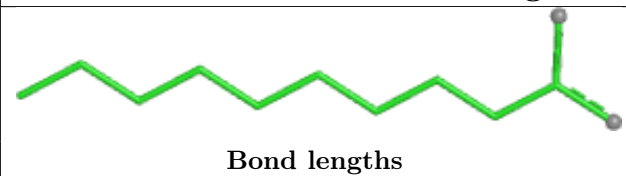
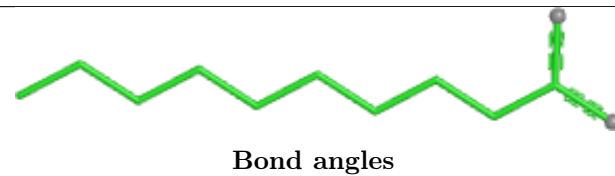
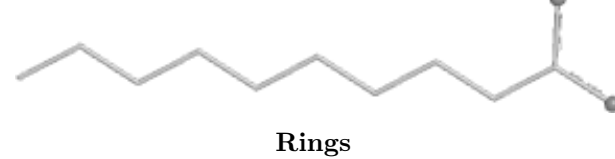
Ligand CLA b 615**Ligand CLA C 504**

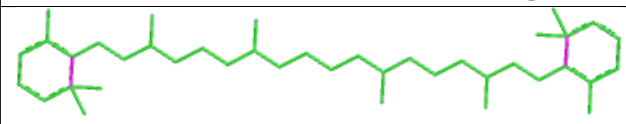
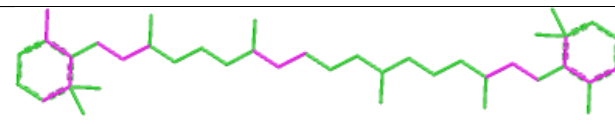
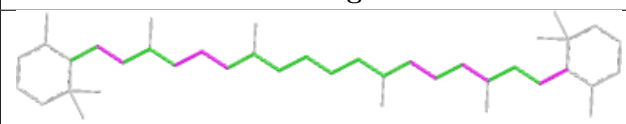
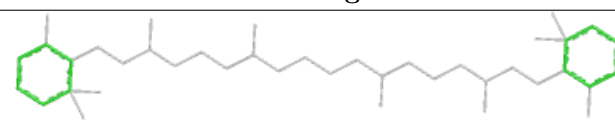
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

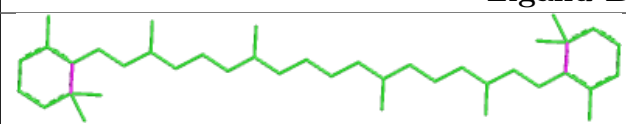
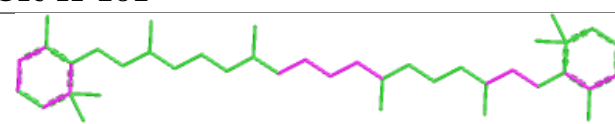
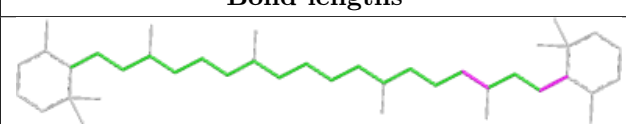
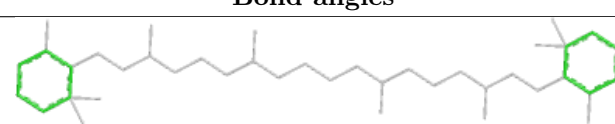
Ligand DGD a 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

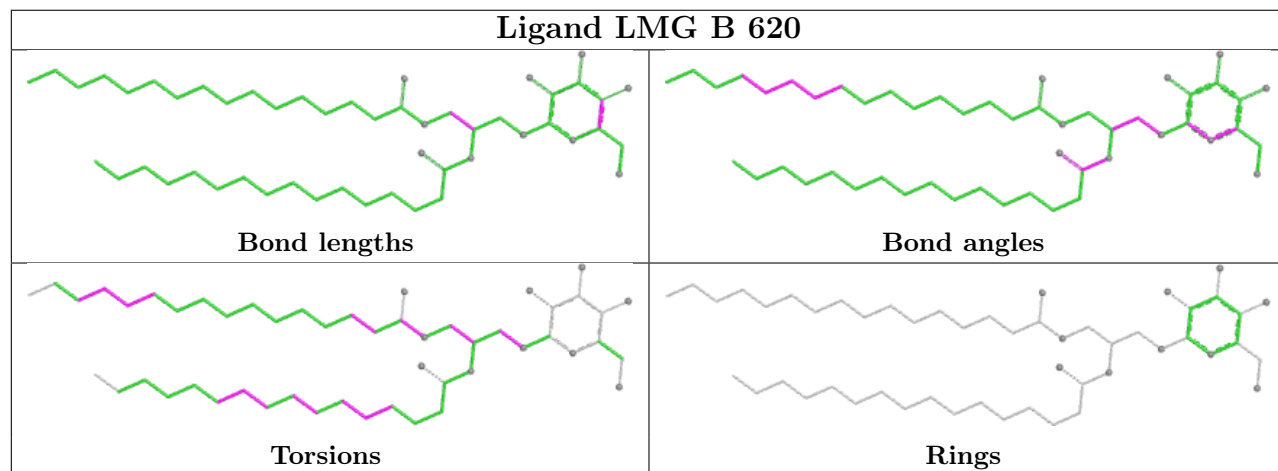
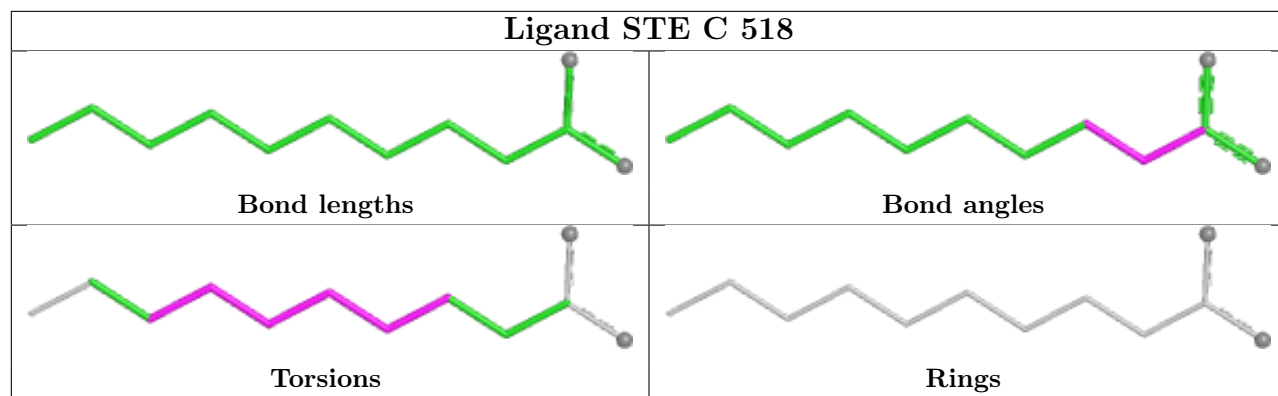
Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

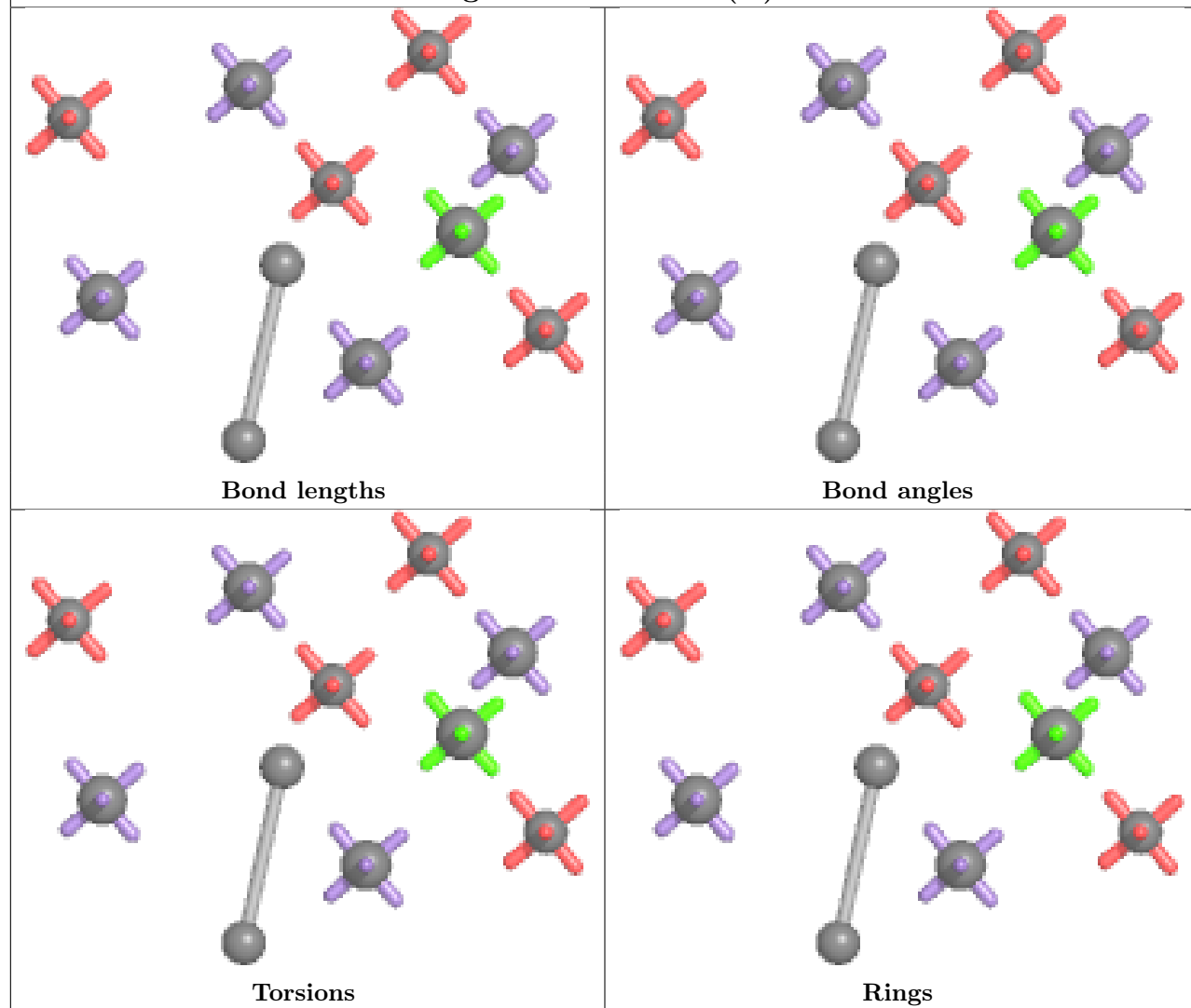
Ligand STE C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

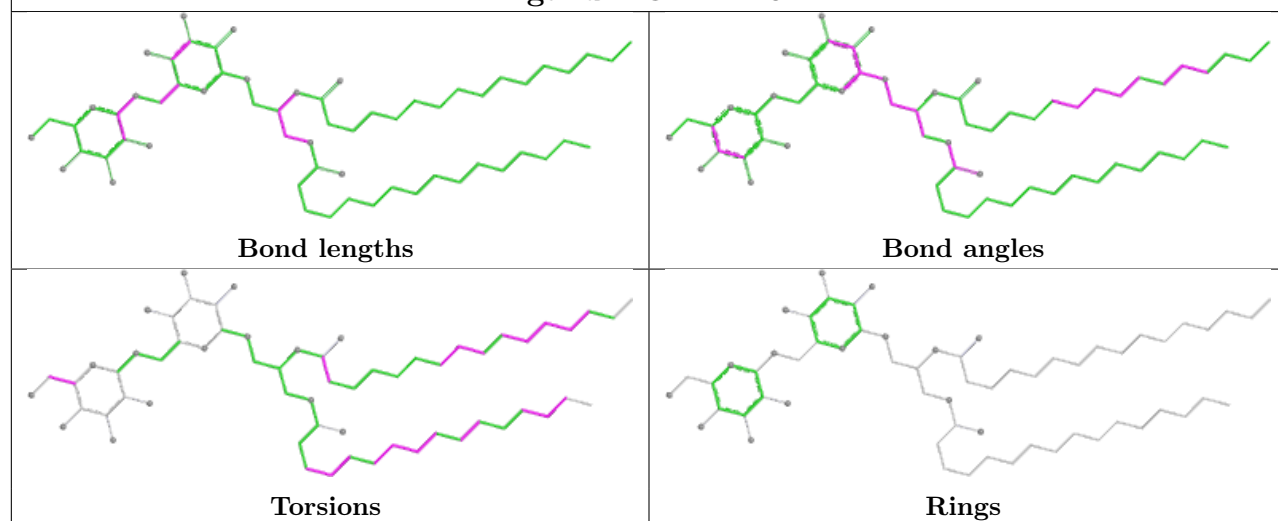
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



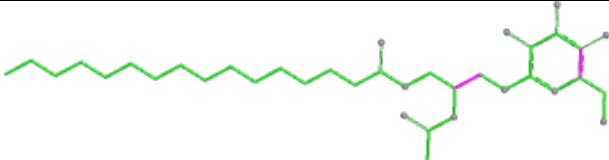
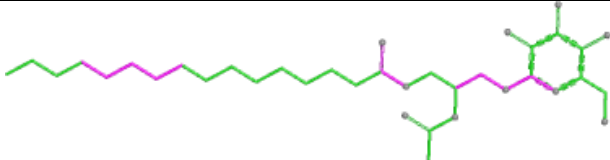
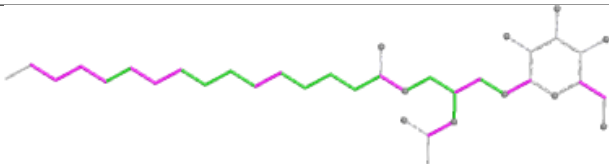
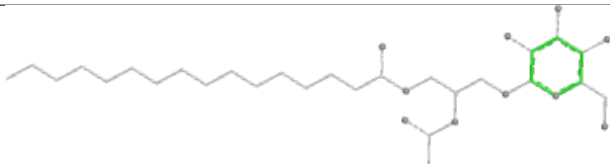
Ligand OEY A 601 (A)

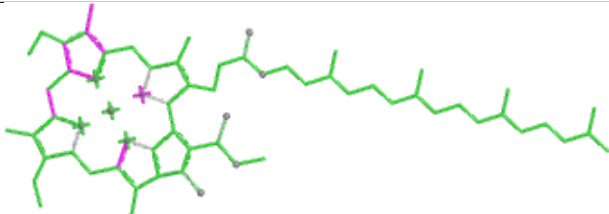
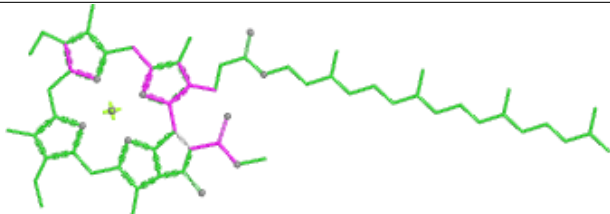
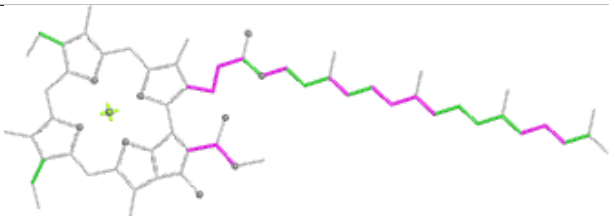
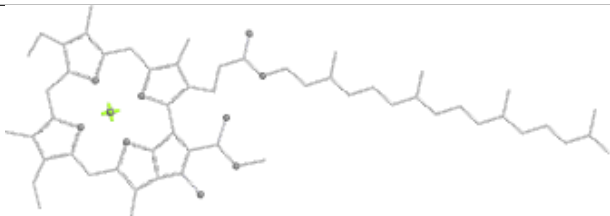


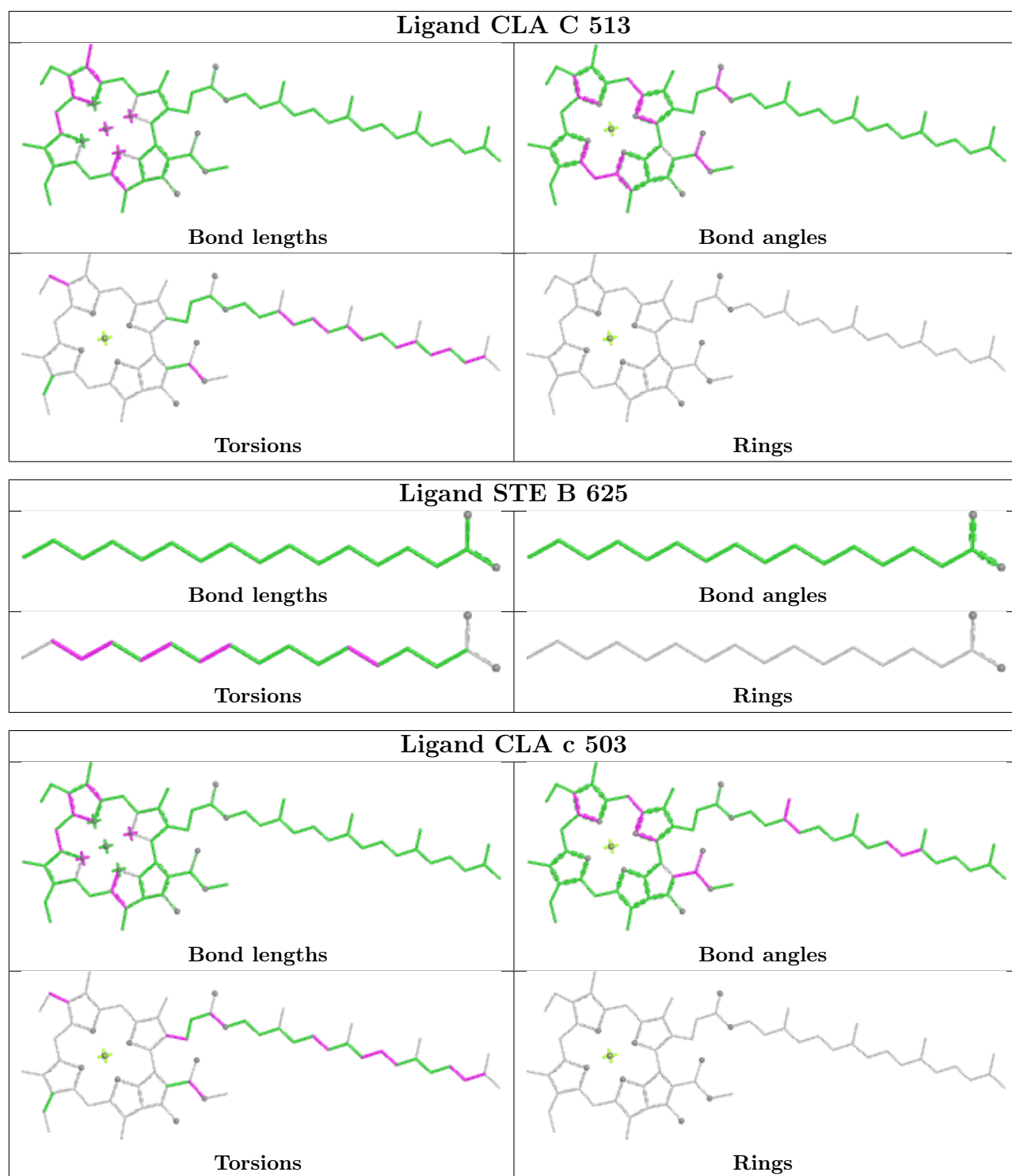
Ligand DGD H 102

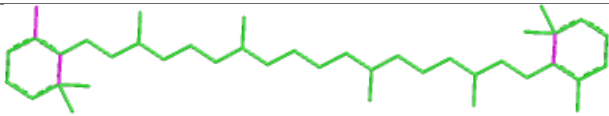
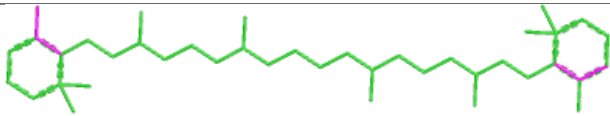
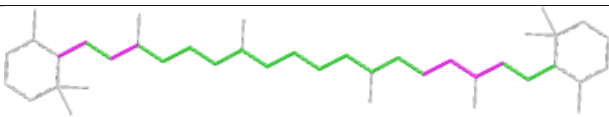
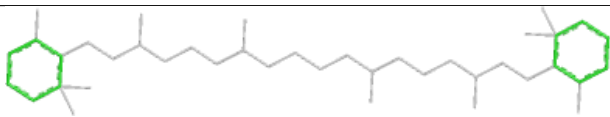


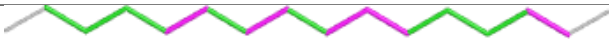
Ligand STE b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

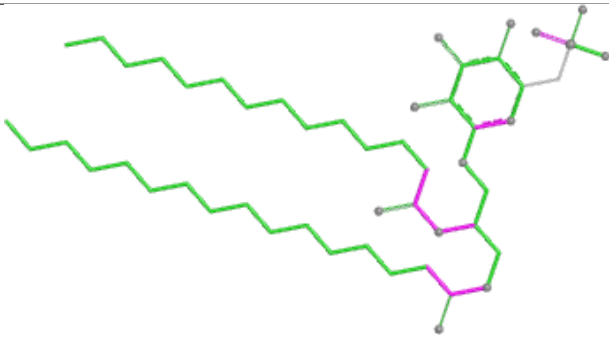
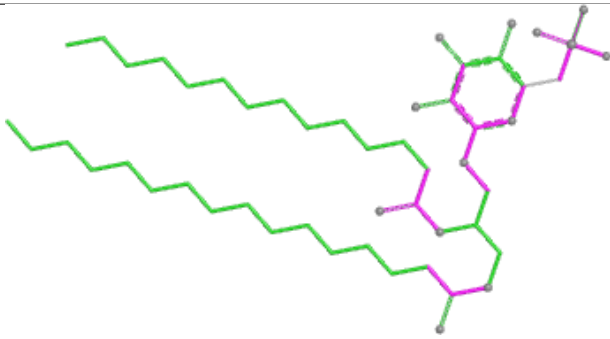
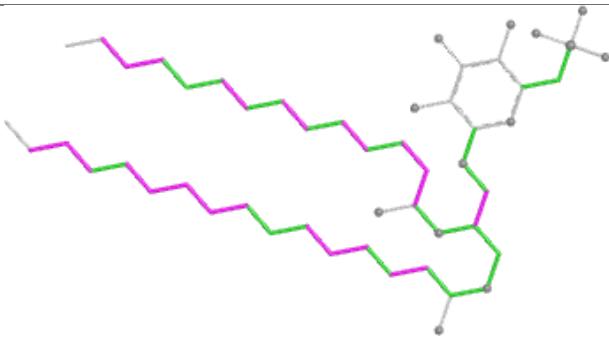
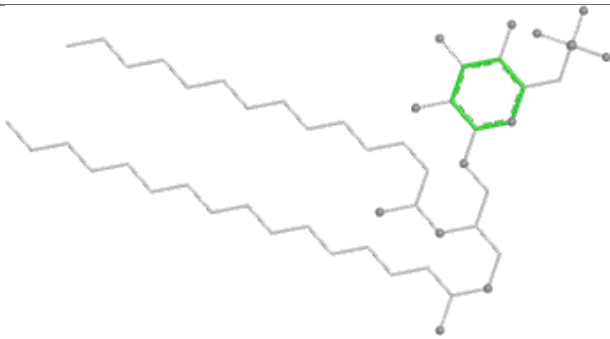
Ligand LMG c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

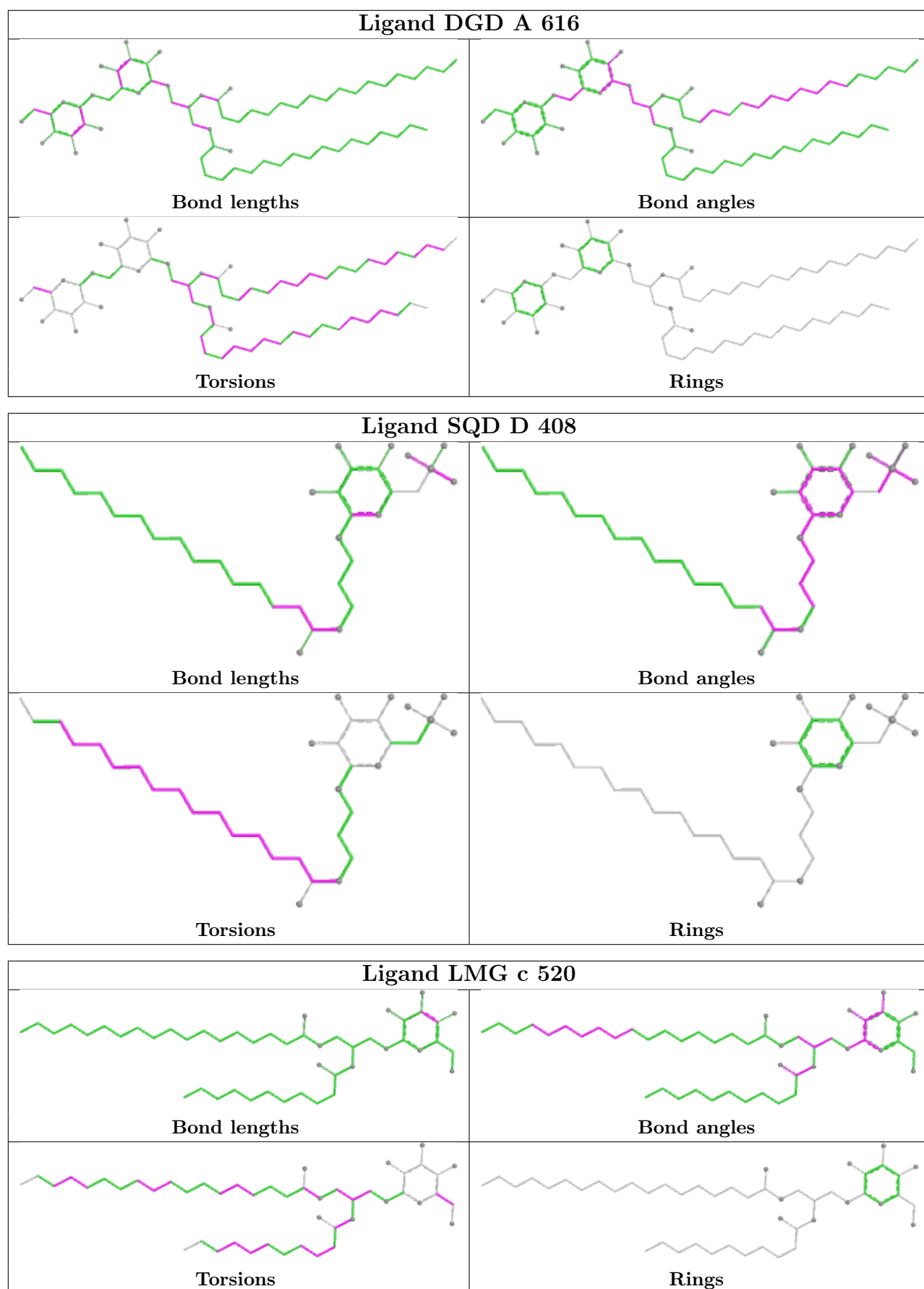
Ligand CLA B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

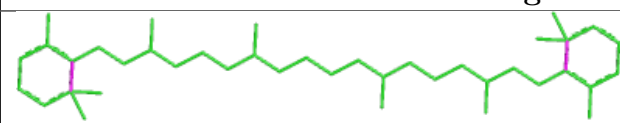
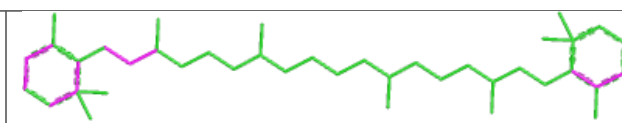
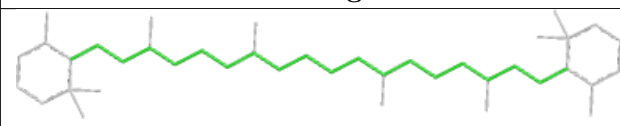
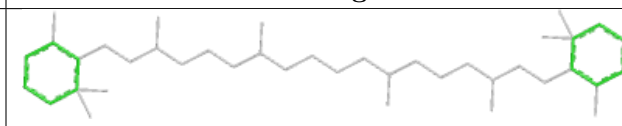


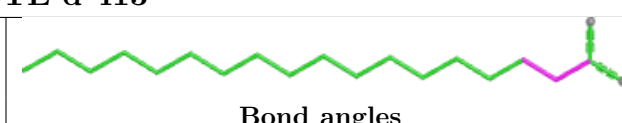
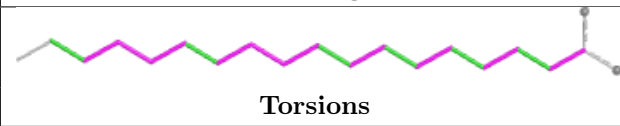
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

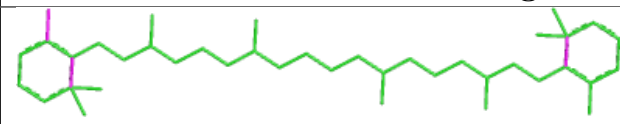
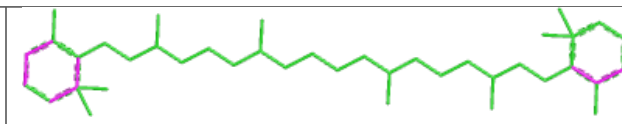
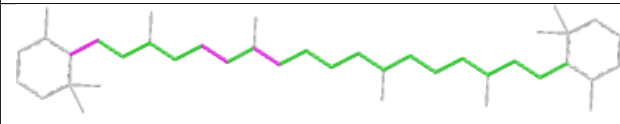
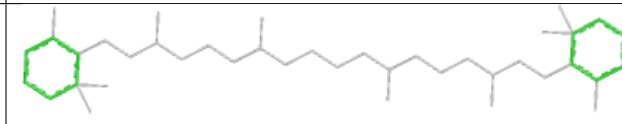
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Bond lengths	Bond angles
	
Torsions	Rings

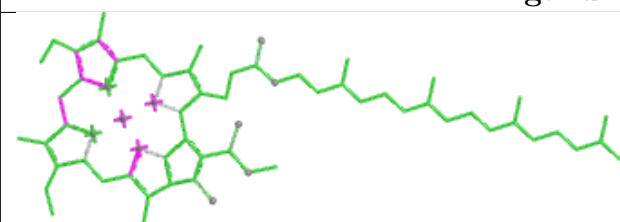
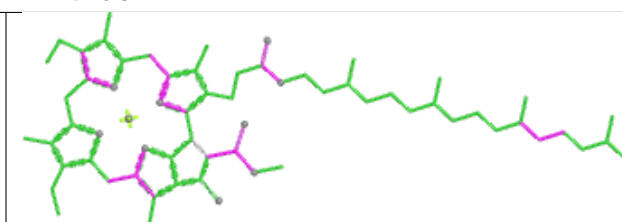
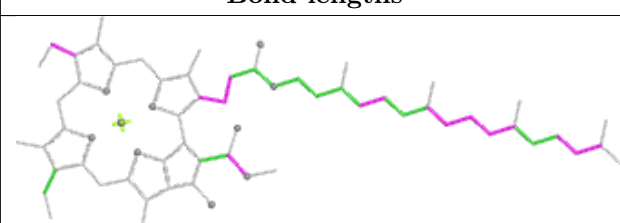
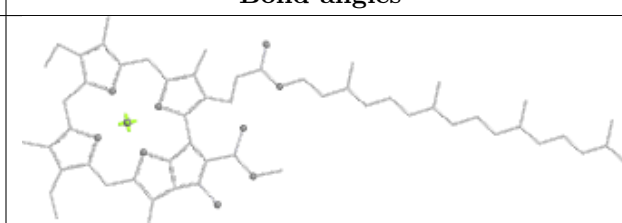
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Bond lengths	Bond angles
	
Torsions	Rings

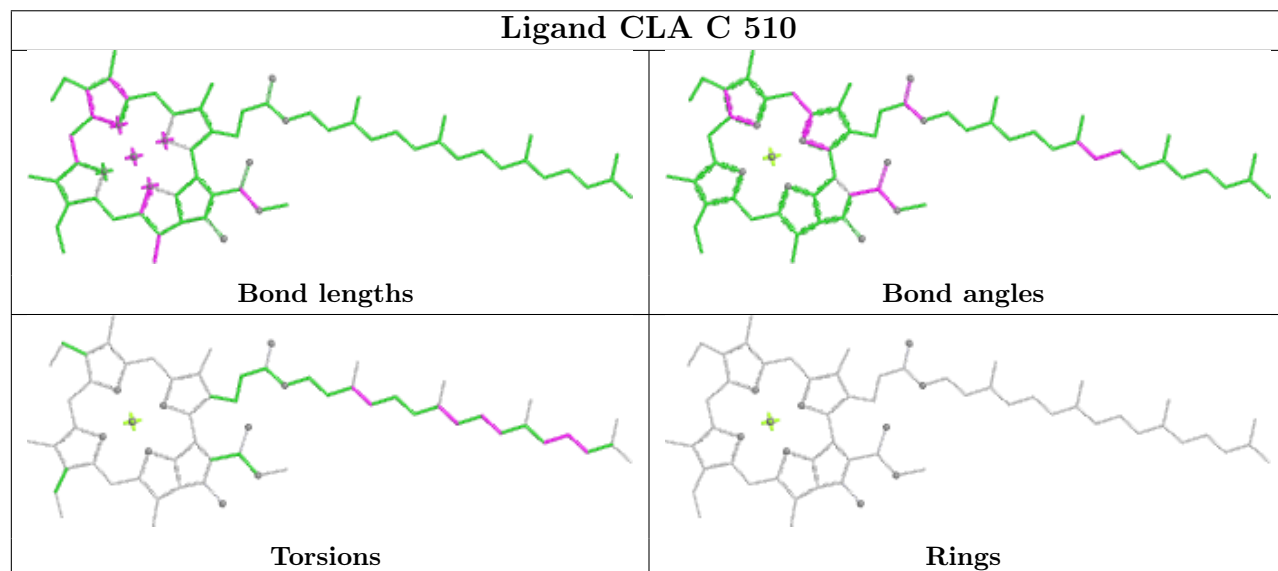
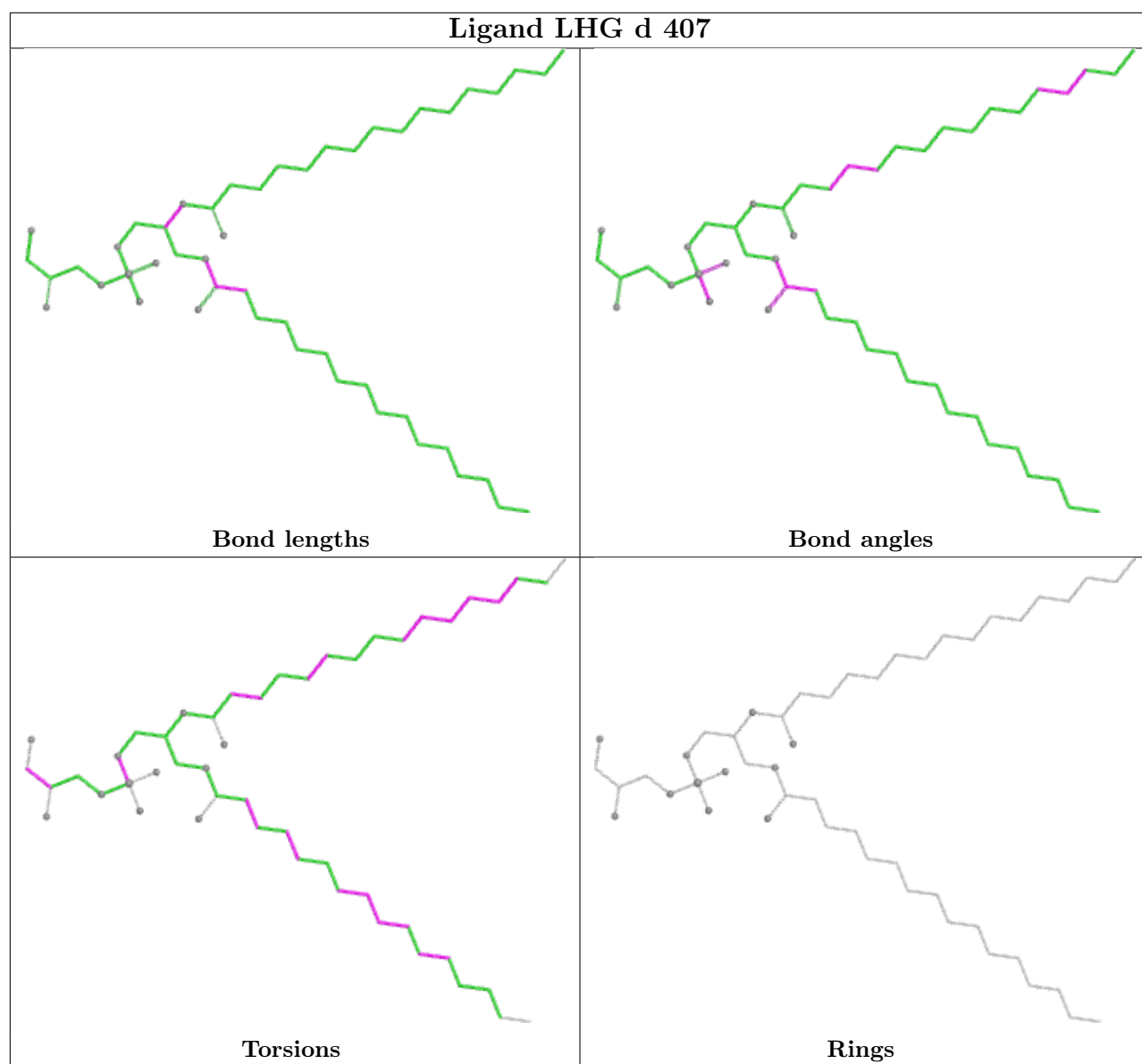


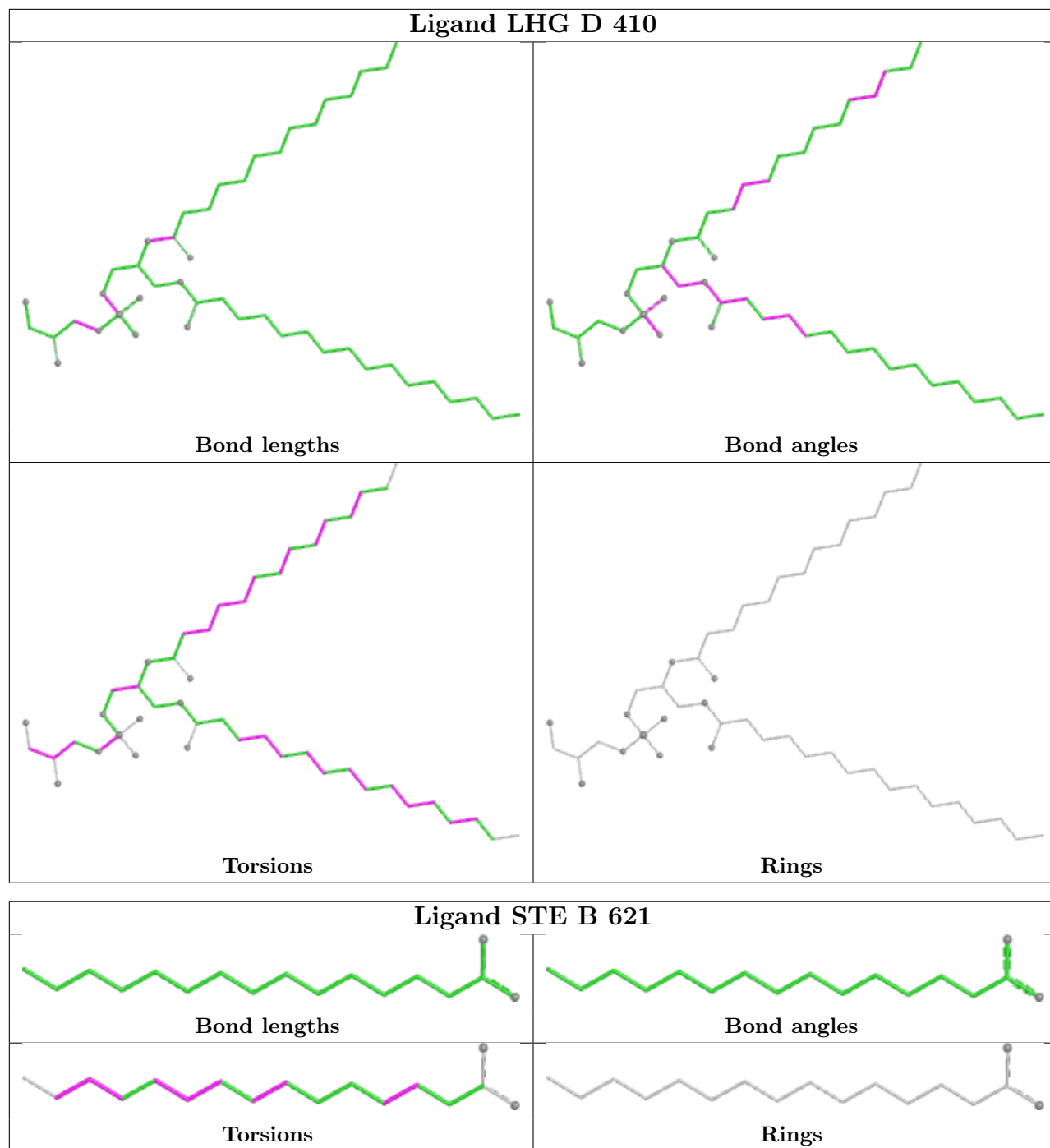
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Bond lengths	Bond angles
	
Torsions	Rings

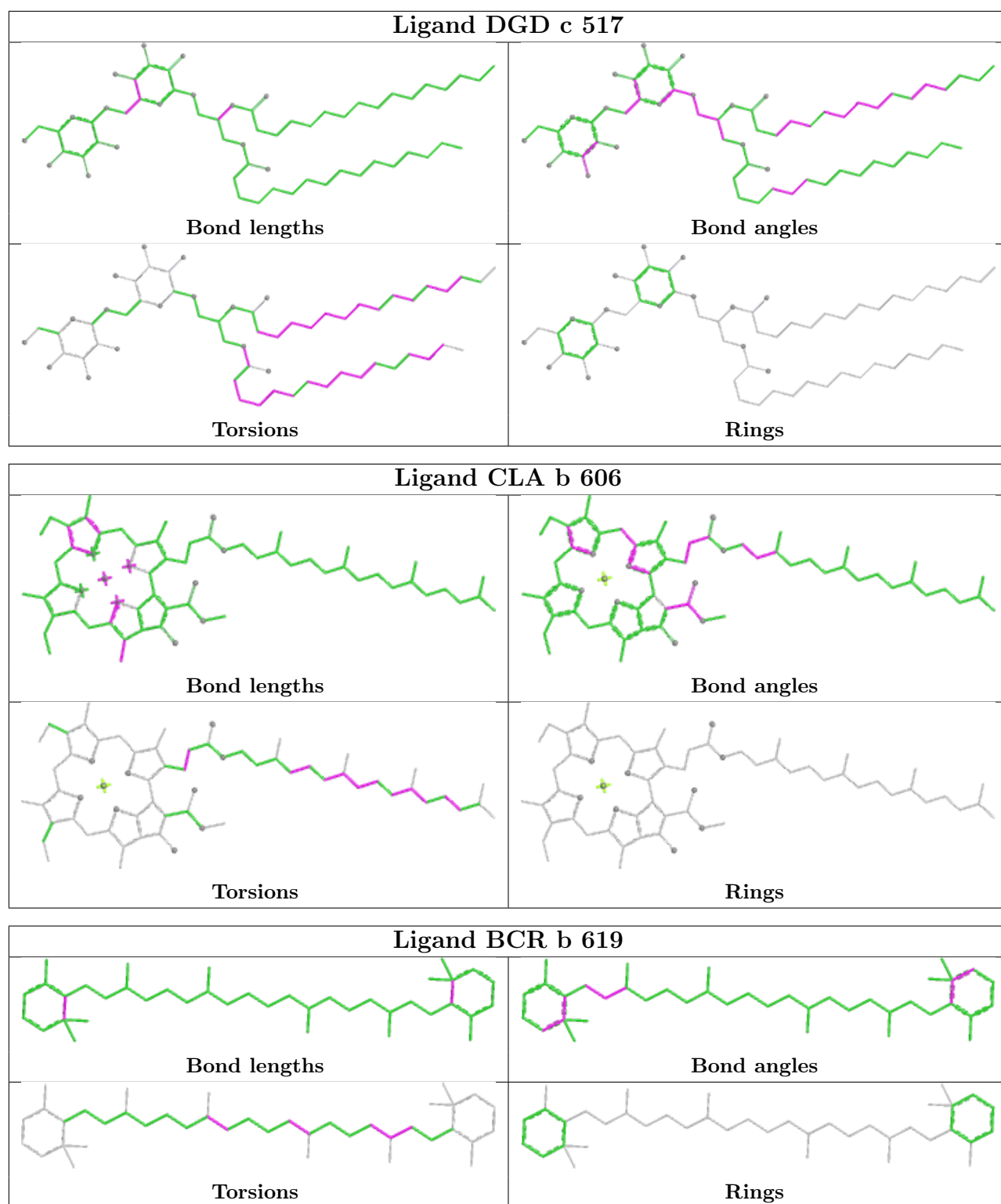
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

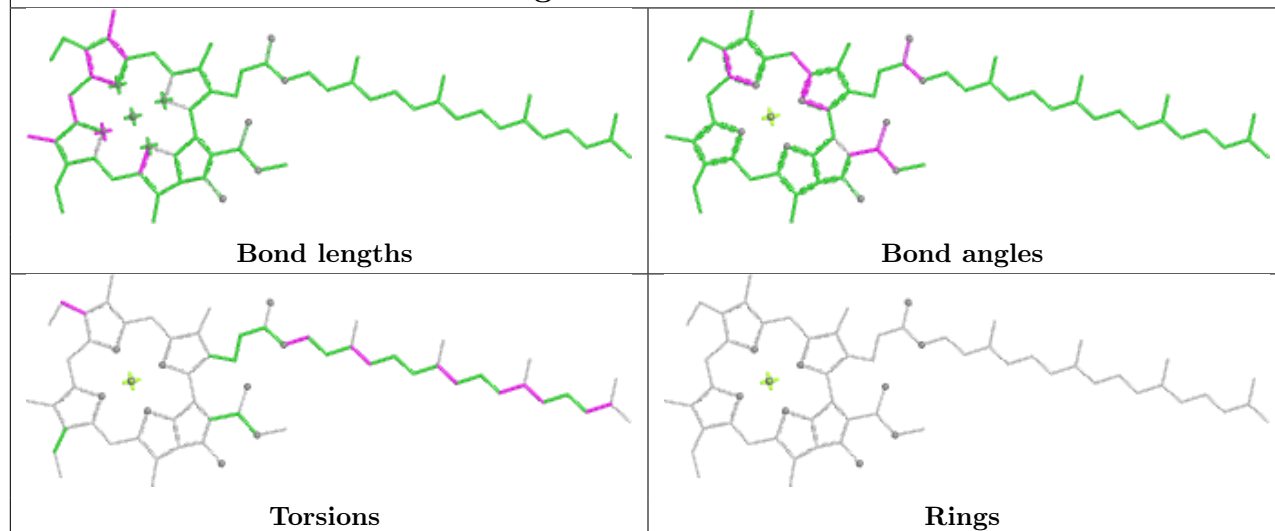
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Bond lengths	Bond angles
	
Torsions	Rings



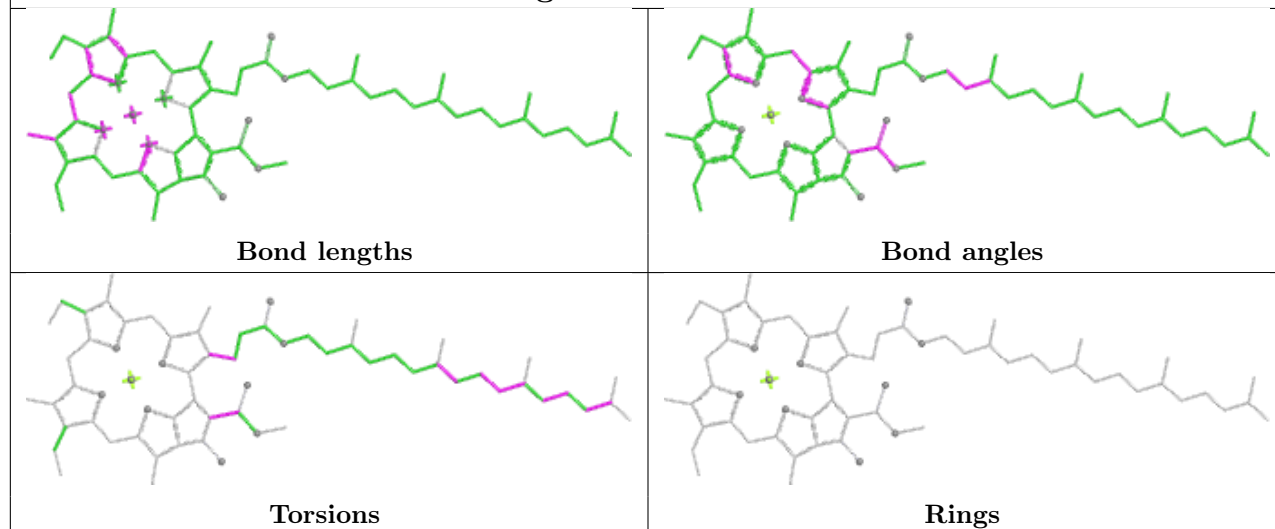




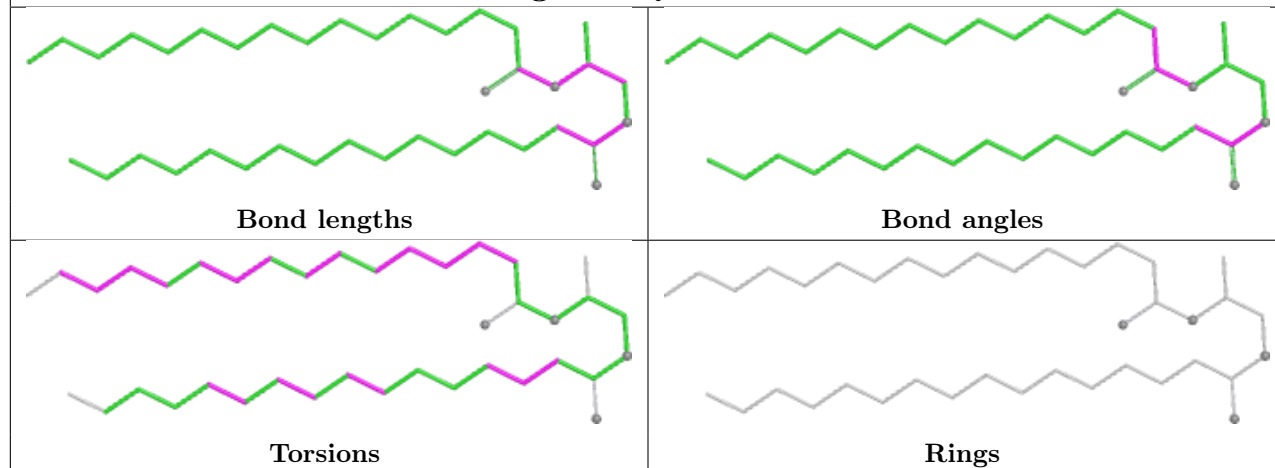
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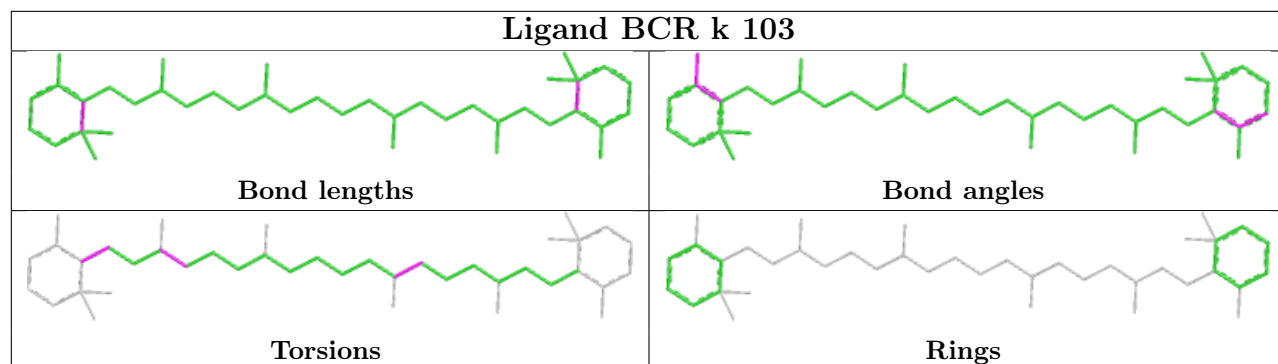
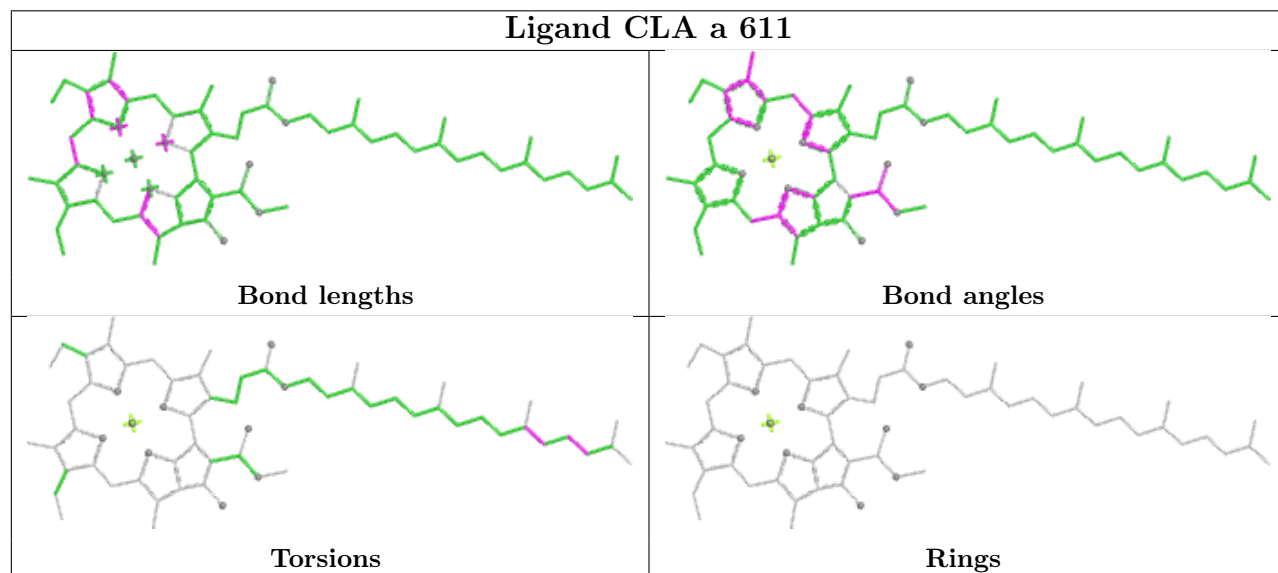
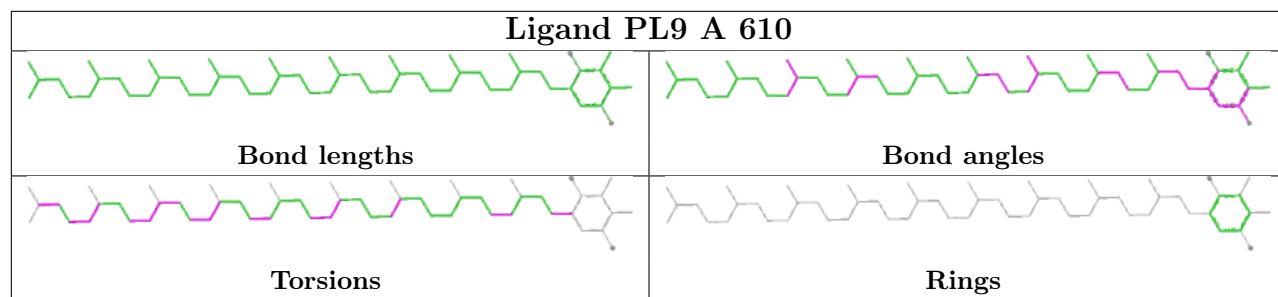
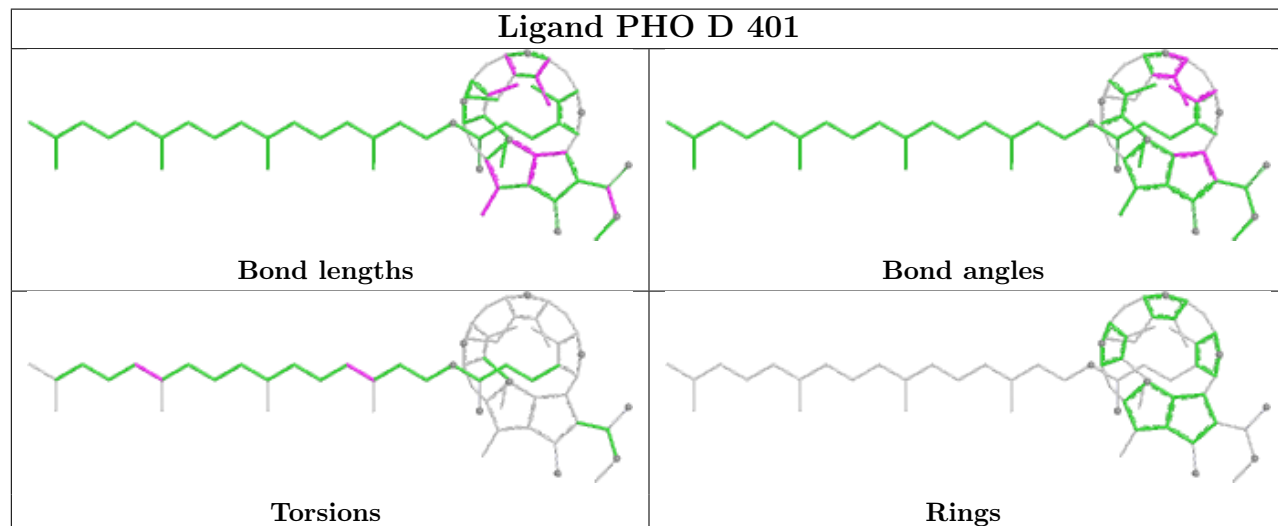


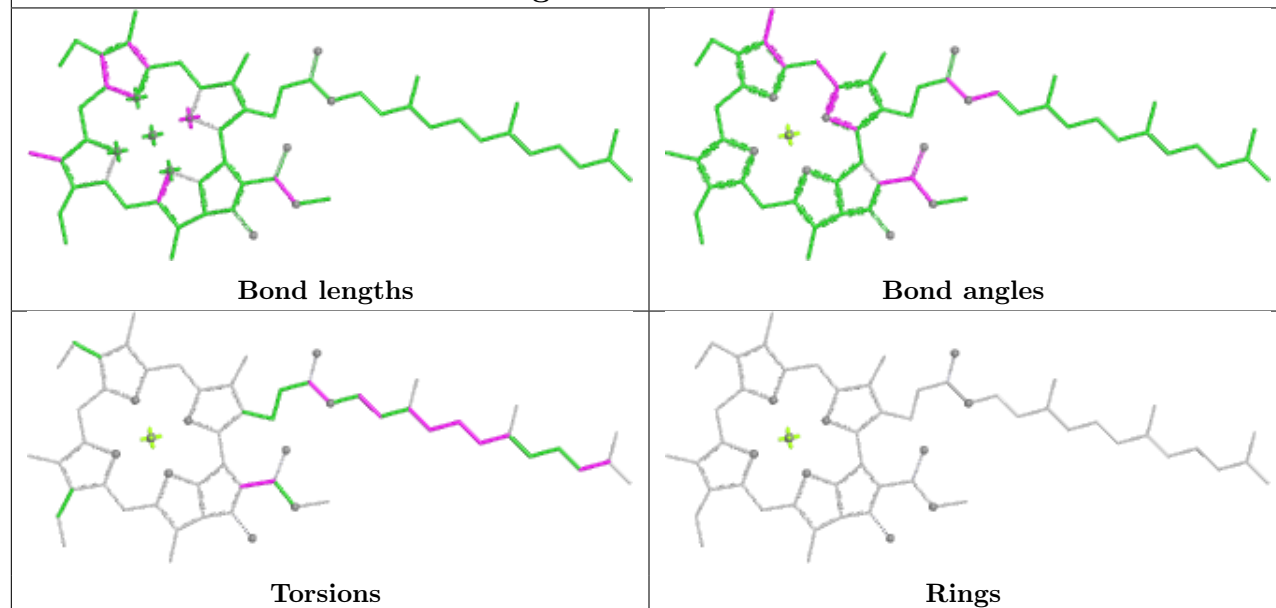
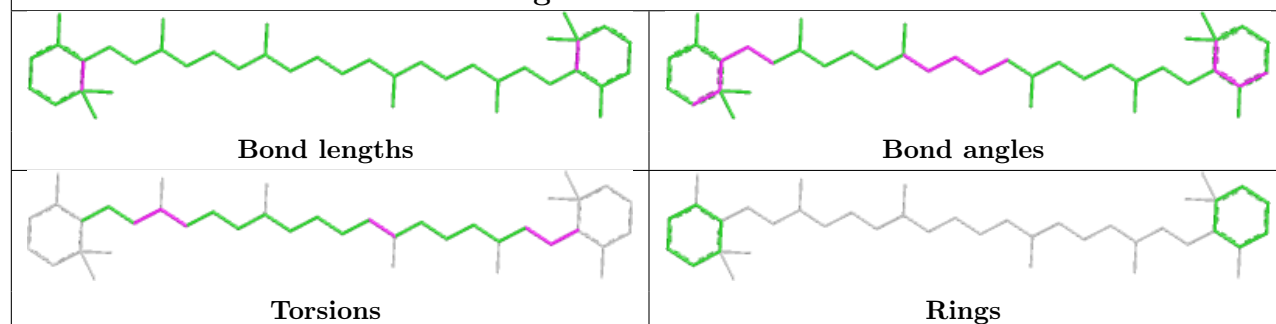
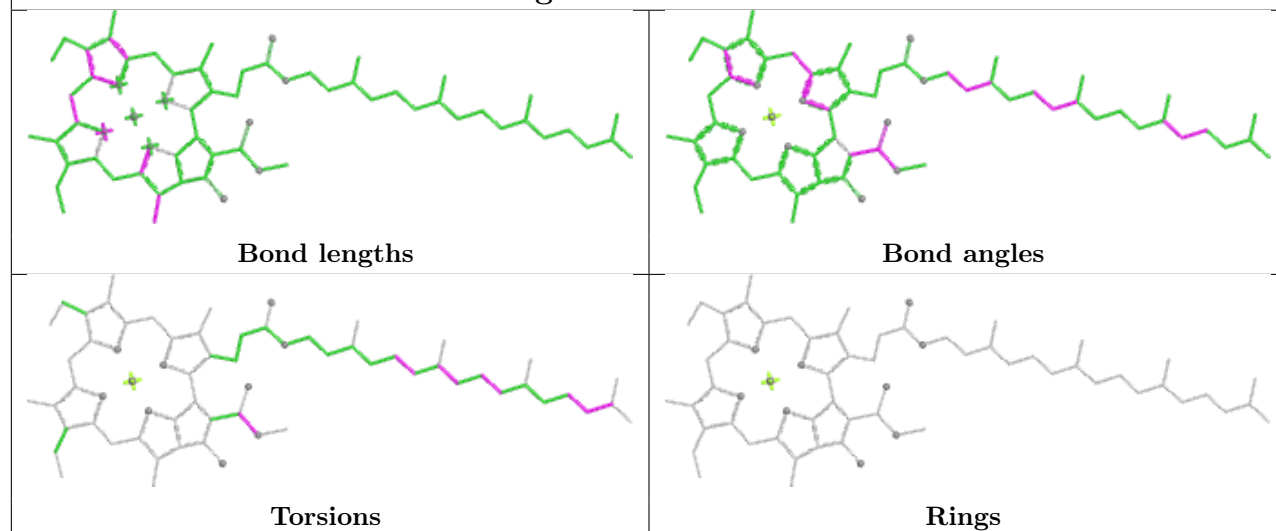
Ligand CLA c 506

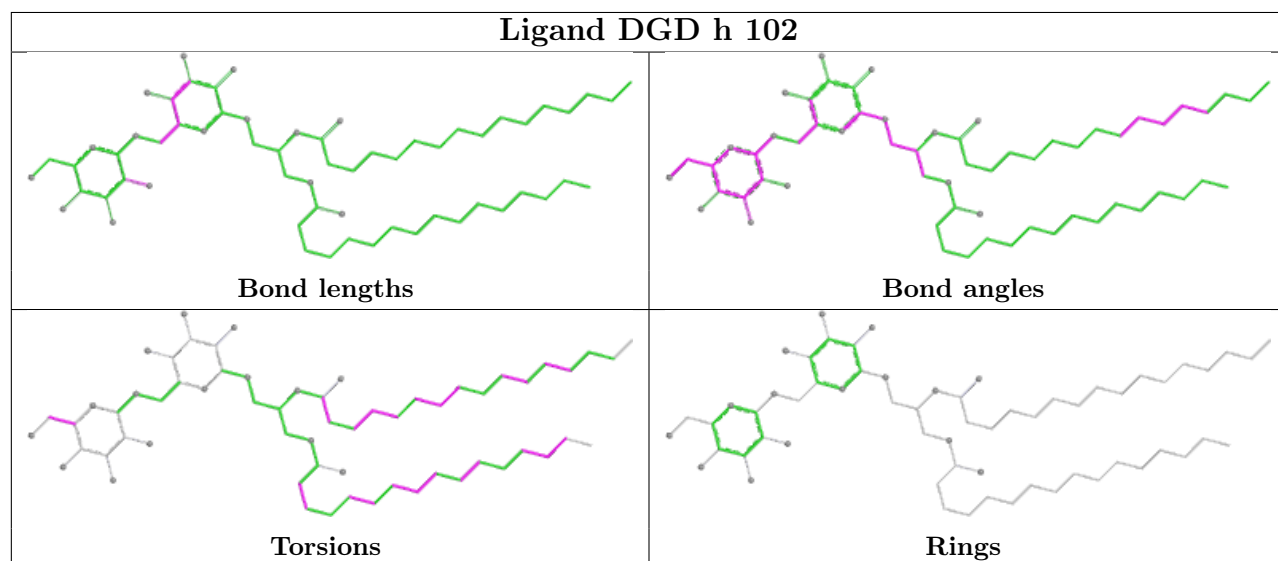
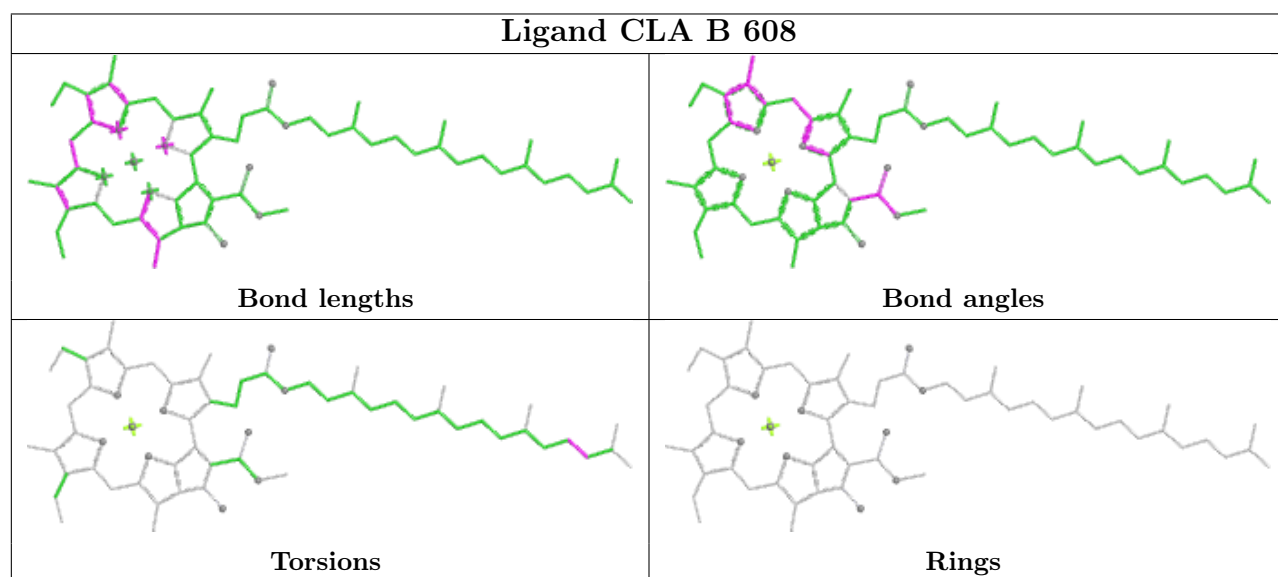
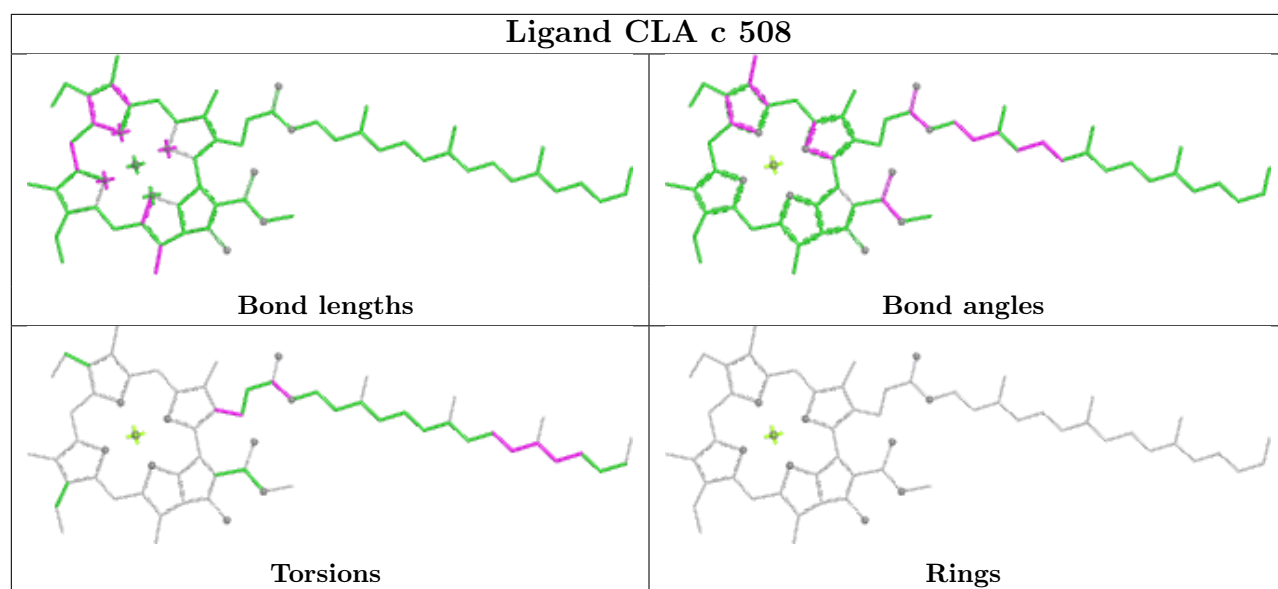


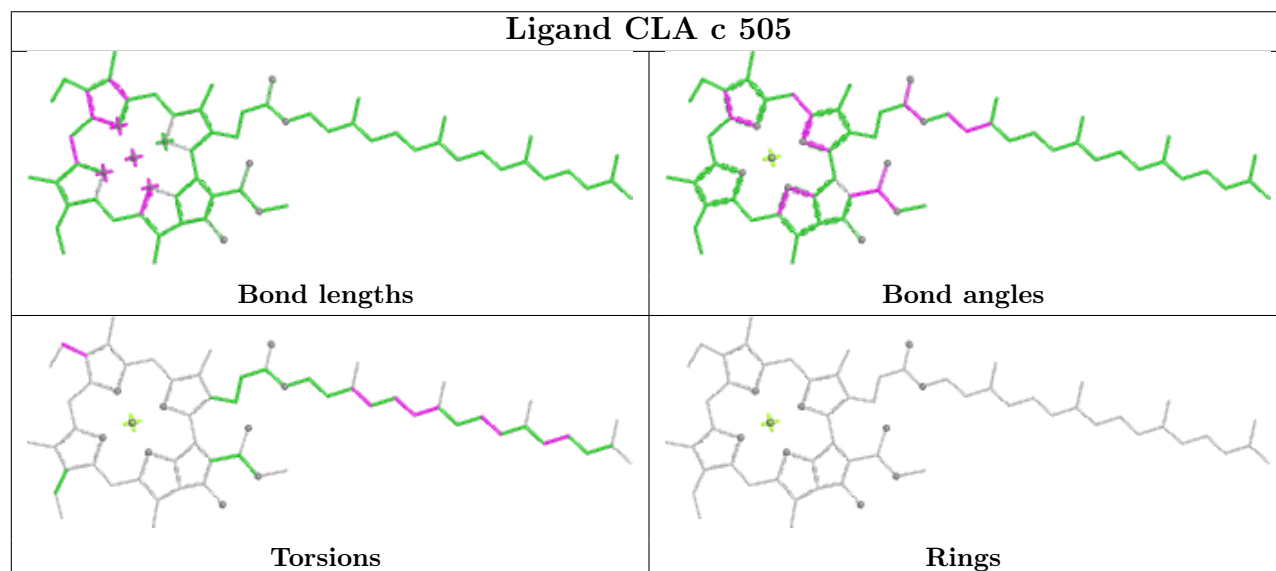
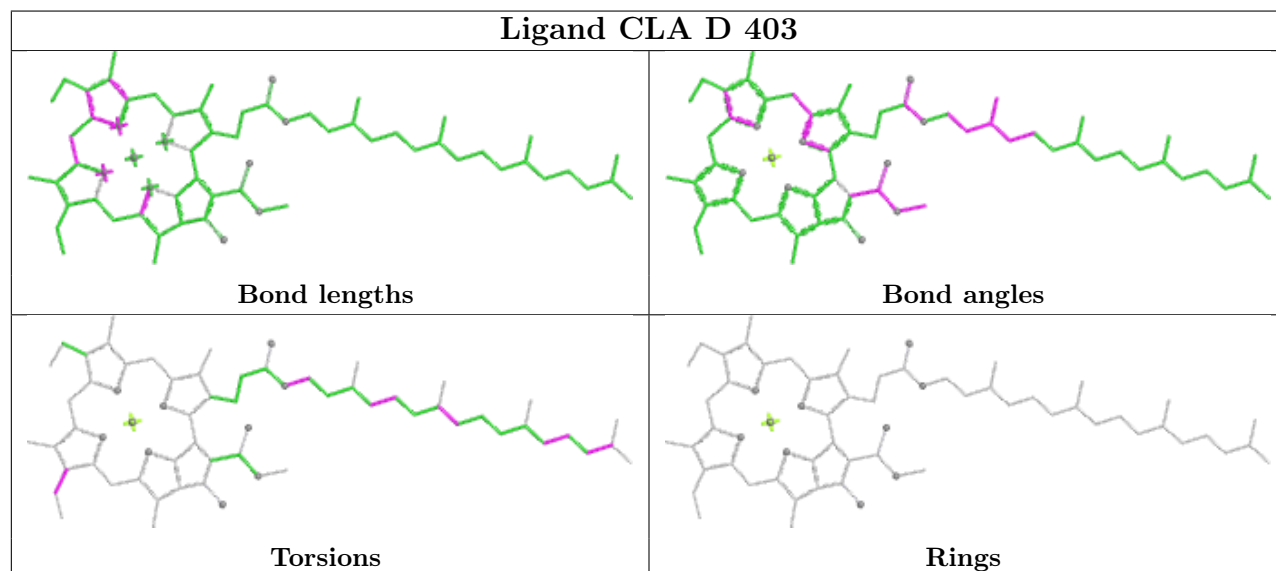
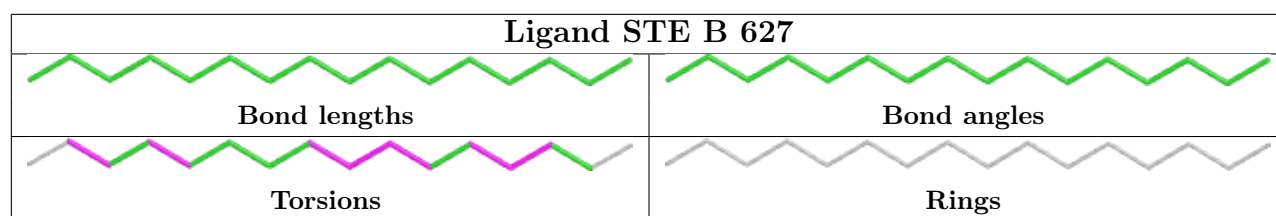
Ligand SQD A 615



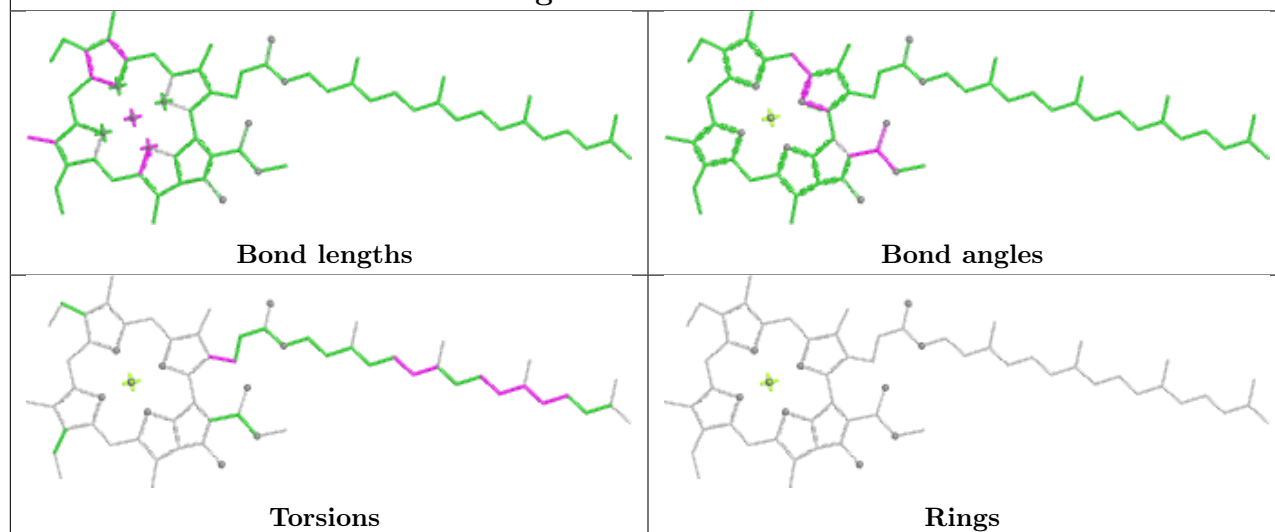
Ligand BCR k 103**Ligand CLA a 611****Ligand PL9 A 610****Ligand PHO D 401**

Ligand CLA B 616**Ligand BCR b 618****Ligand CLA b 602**

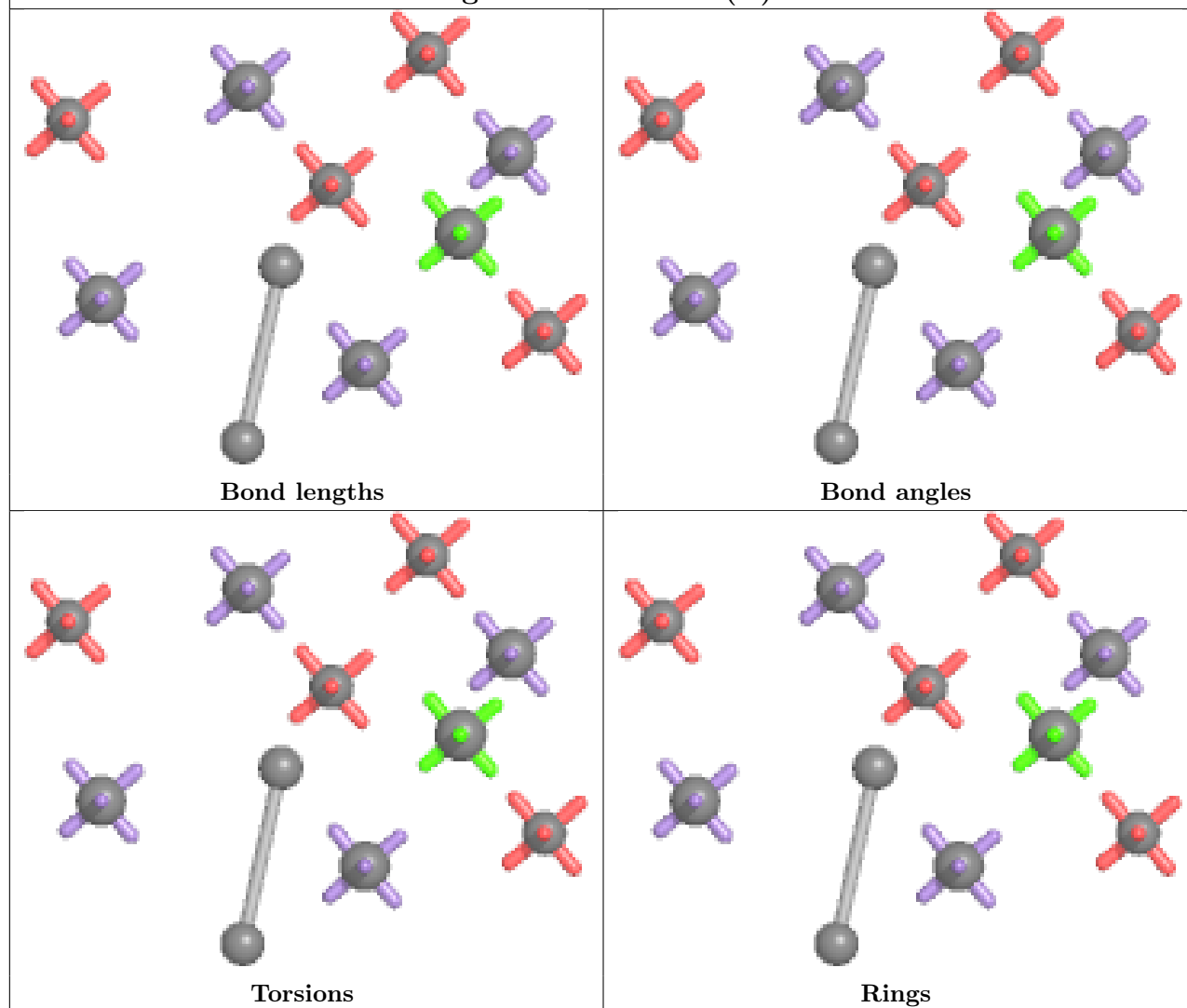




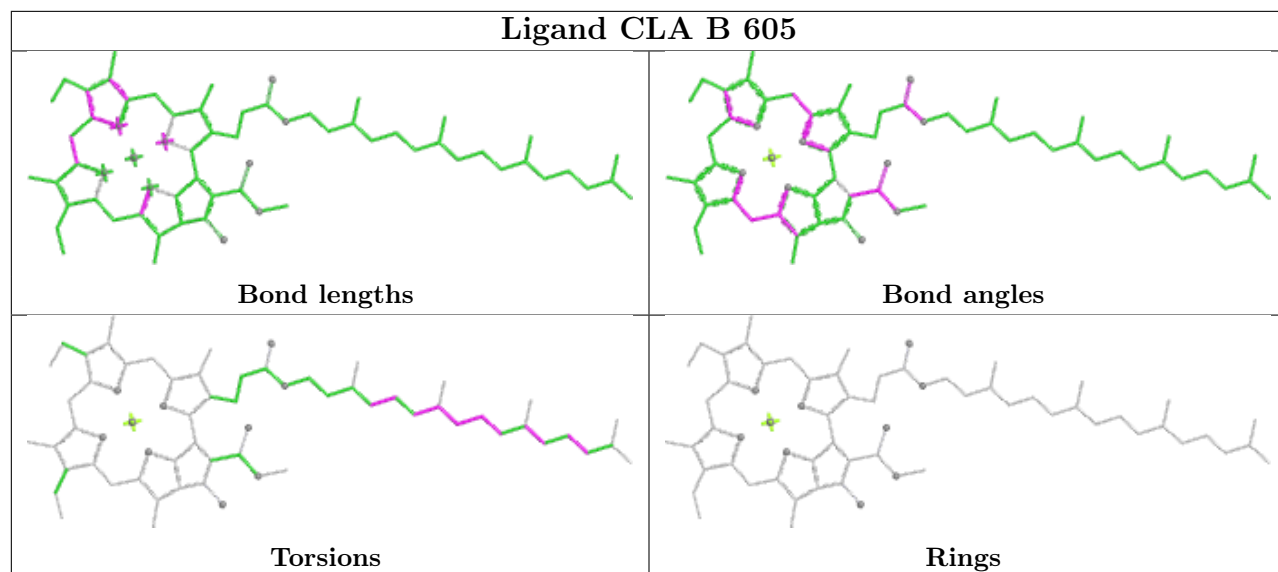
Ligand CLA a 608



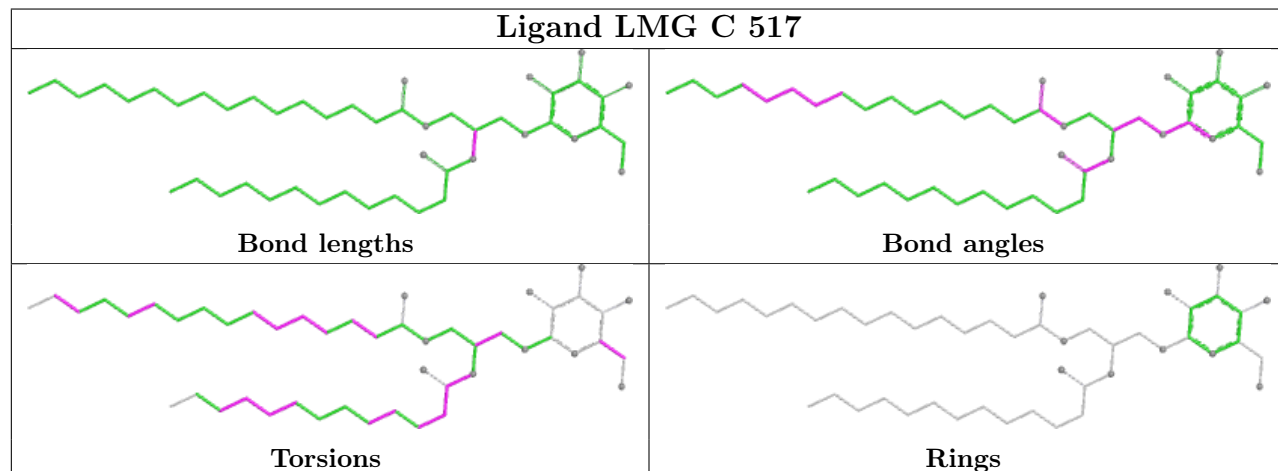
Ligand OEY A 601 (B)



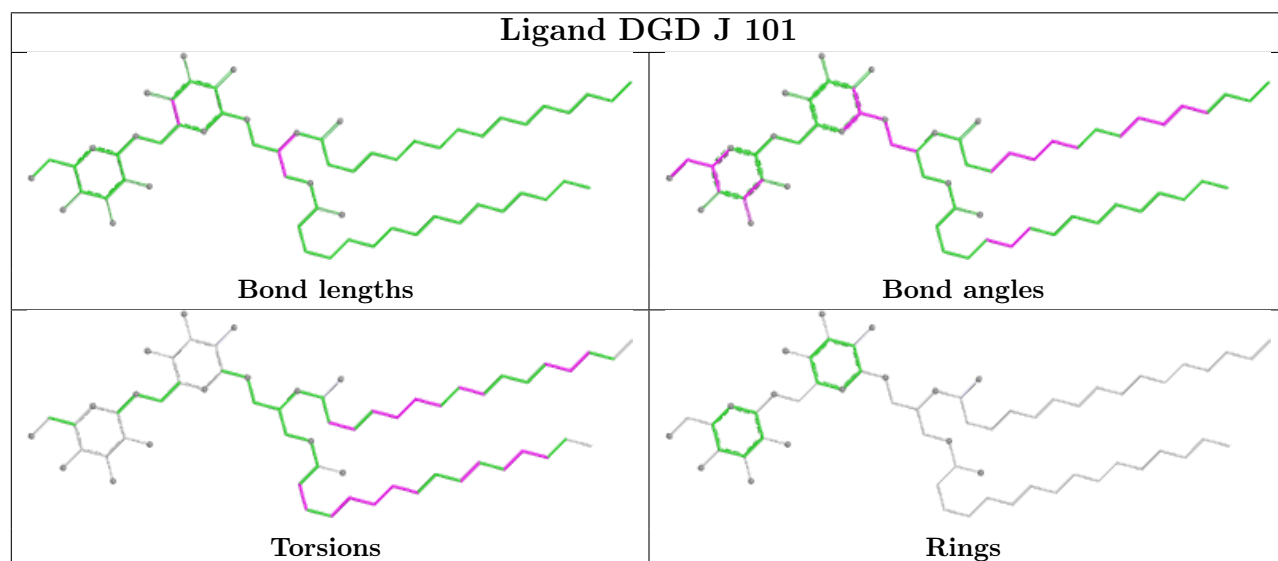
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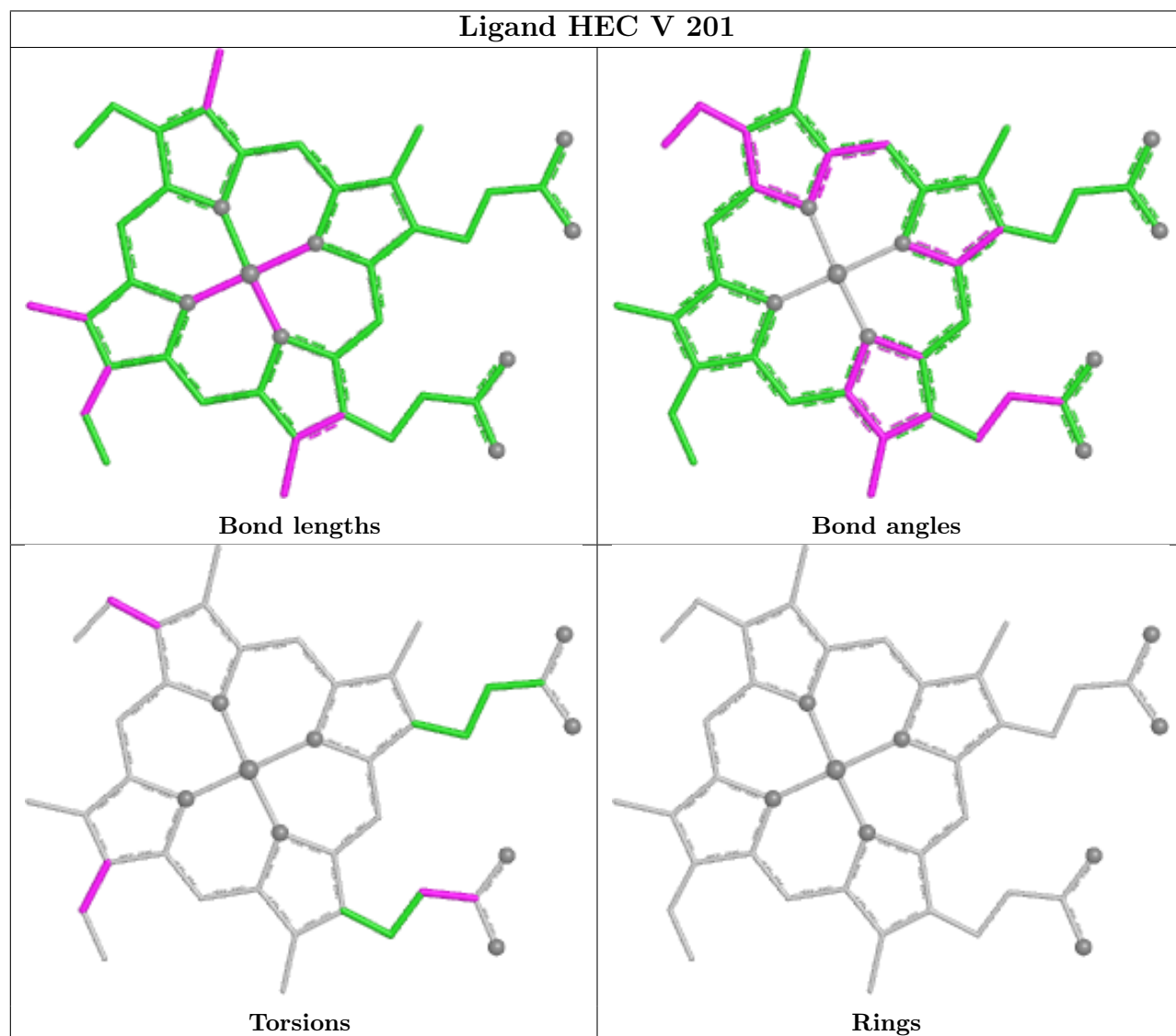
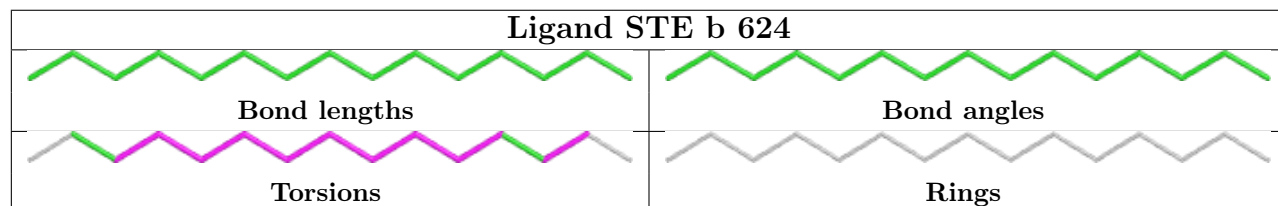
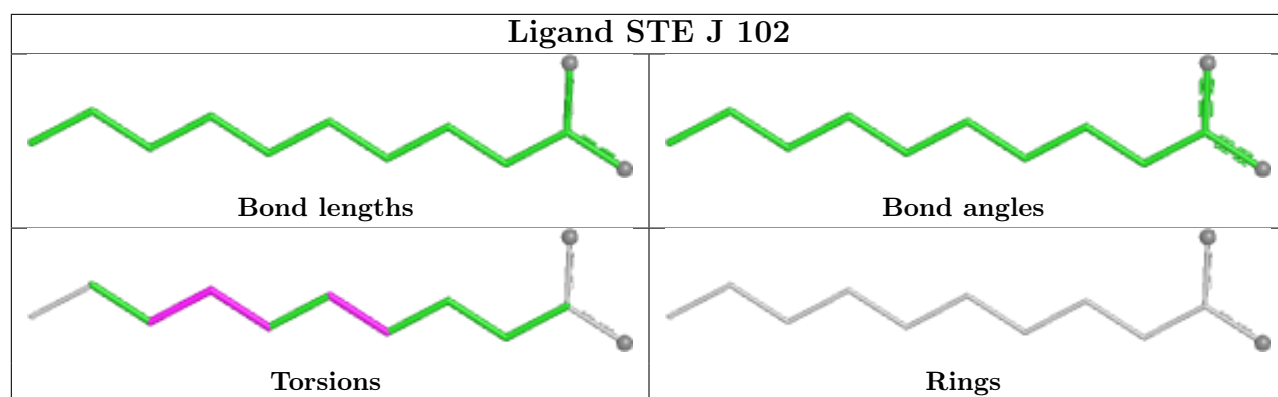


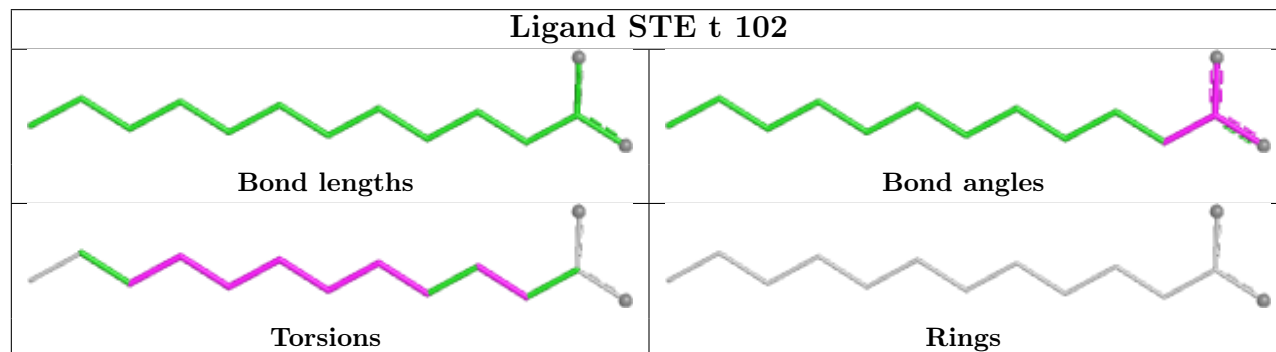
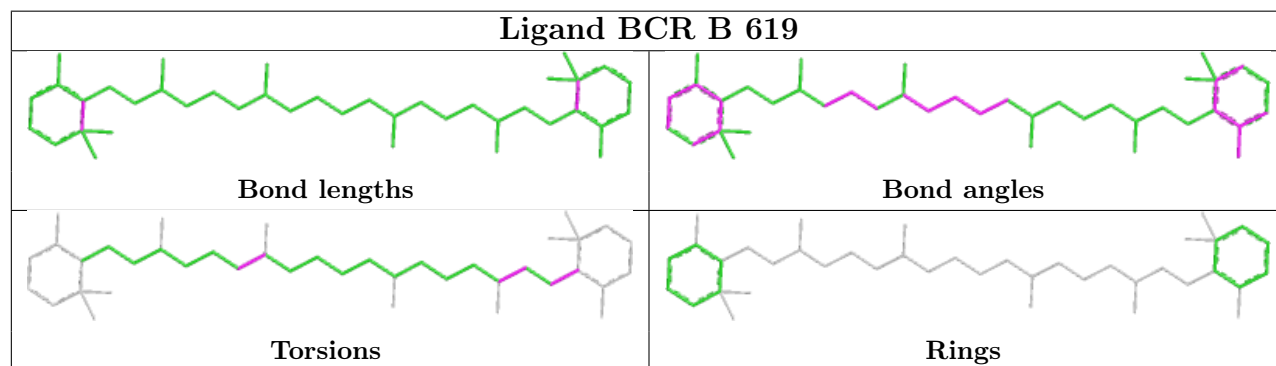
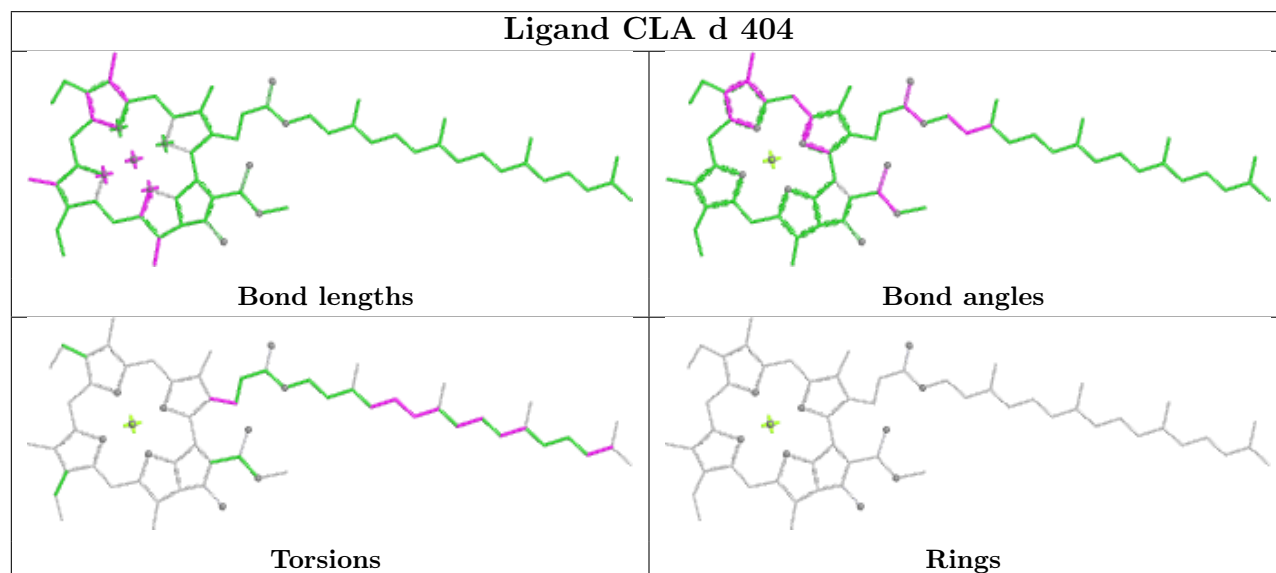
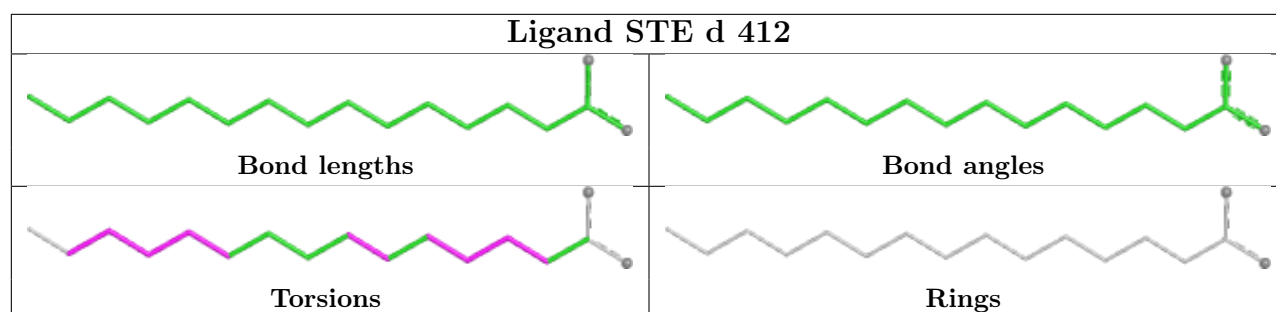
Ligand LMG C 517

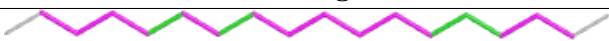
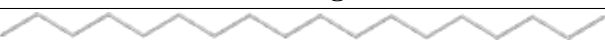


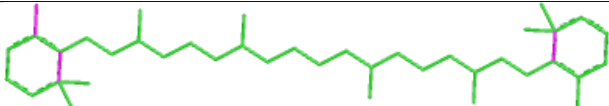
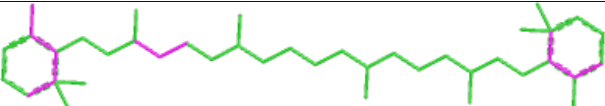
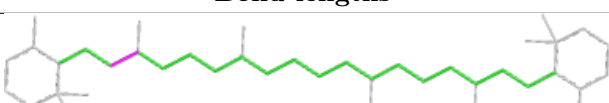
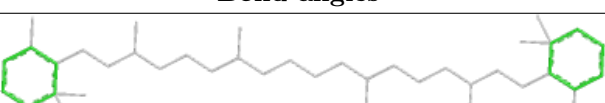
Ligand DGD J 101

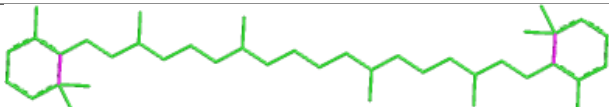
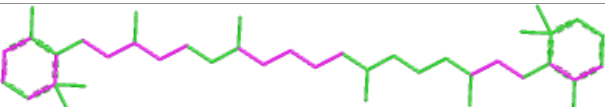
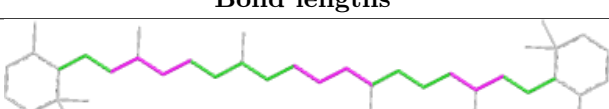
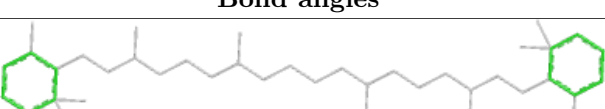


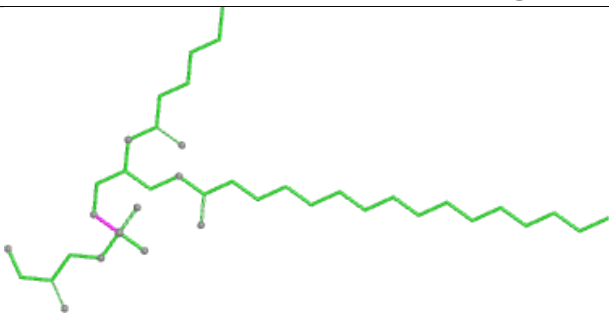
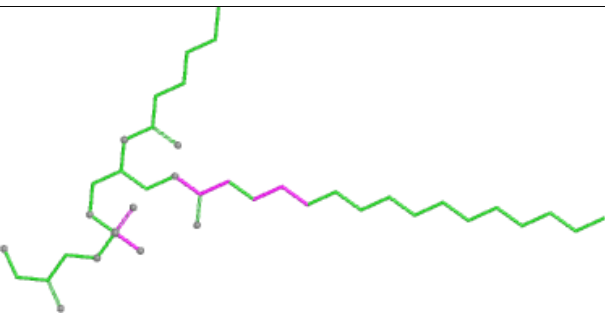
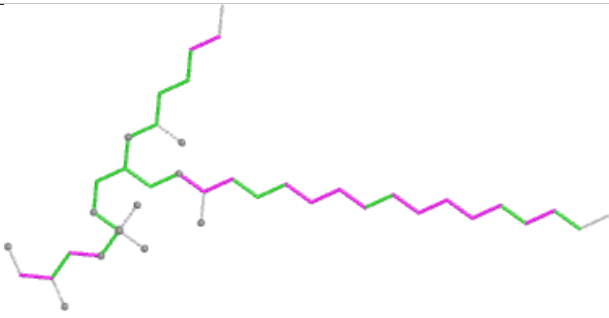
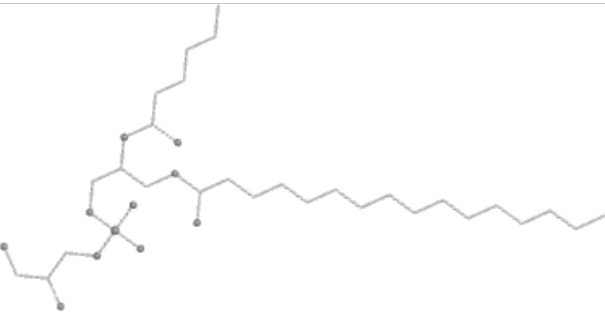


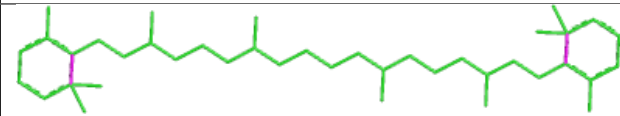
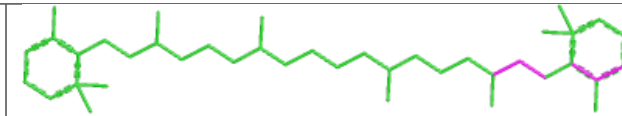
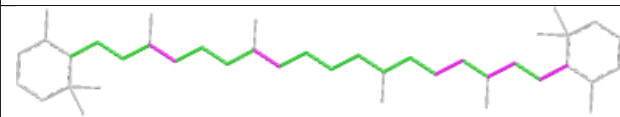
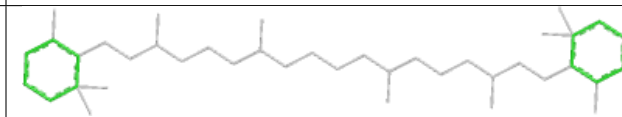


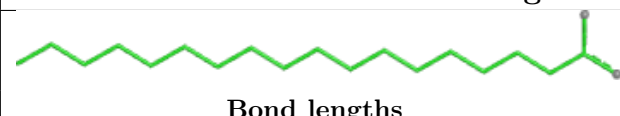
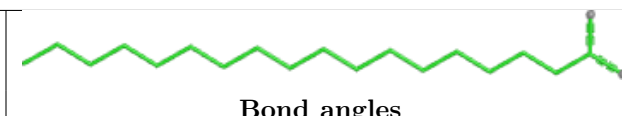
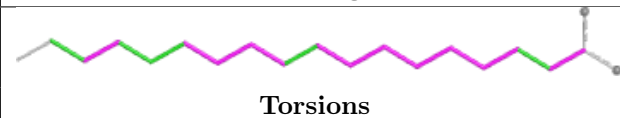
Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

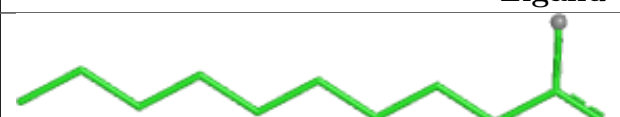
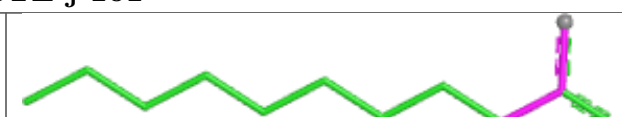
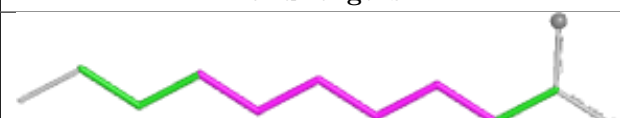
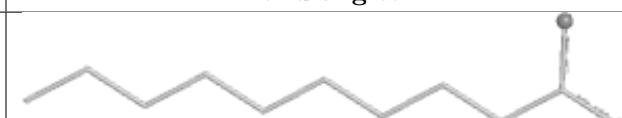
Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

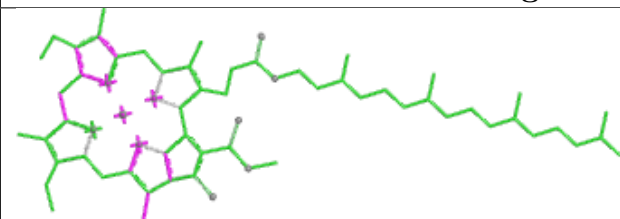
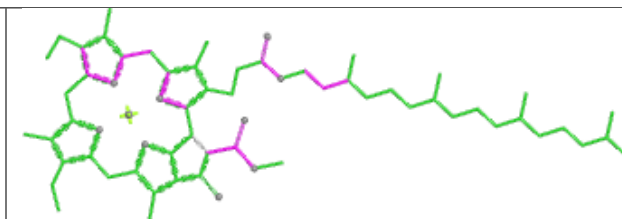
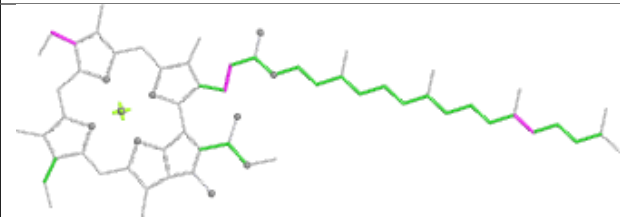
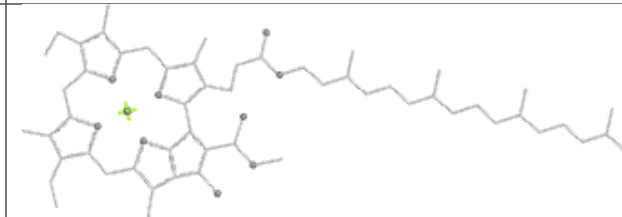
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

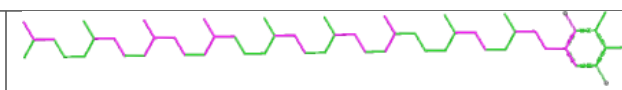
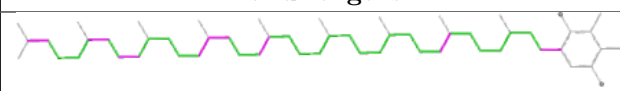
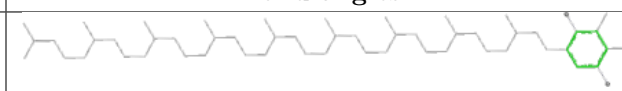
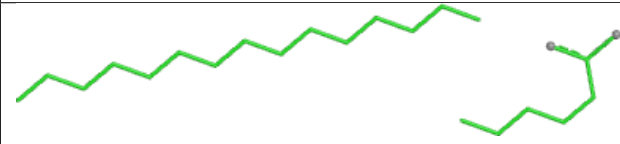
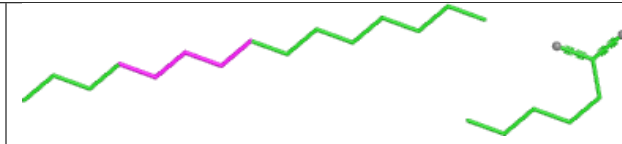
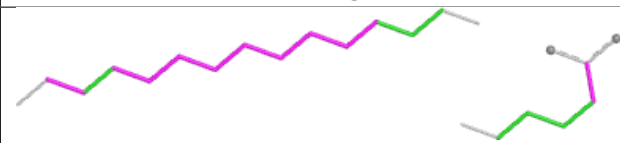
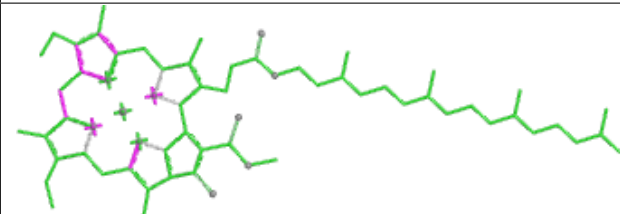
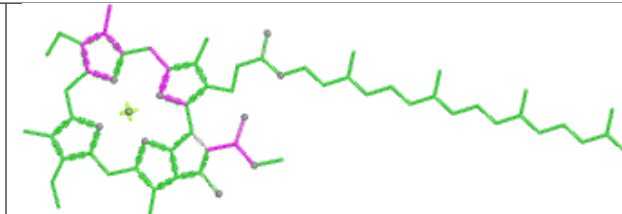
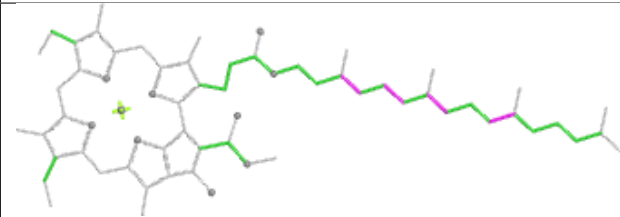
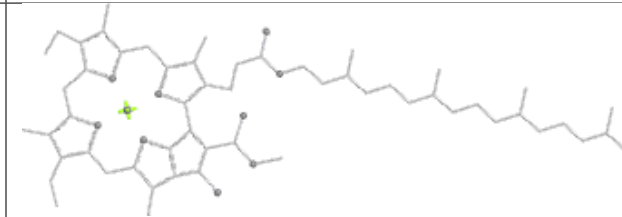
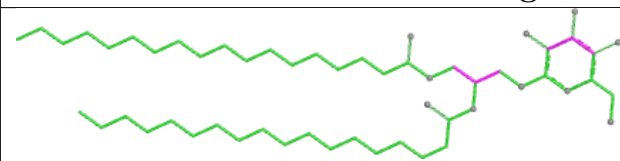
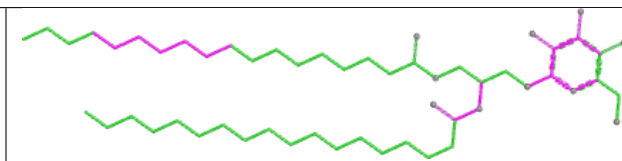
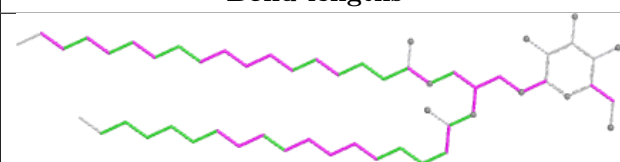
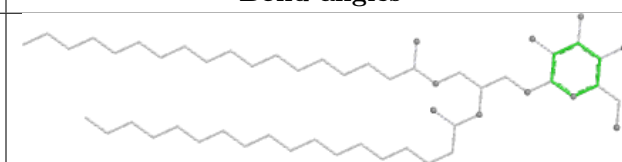
Ligand LHG d 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

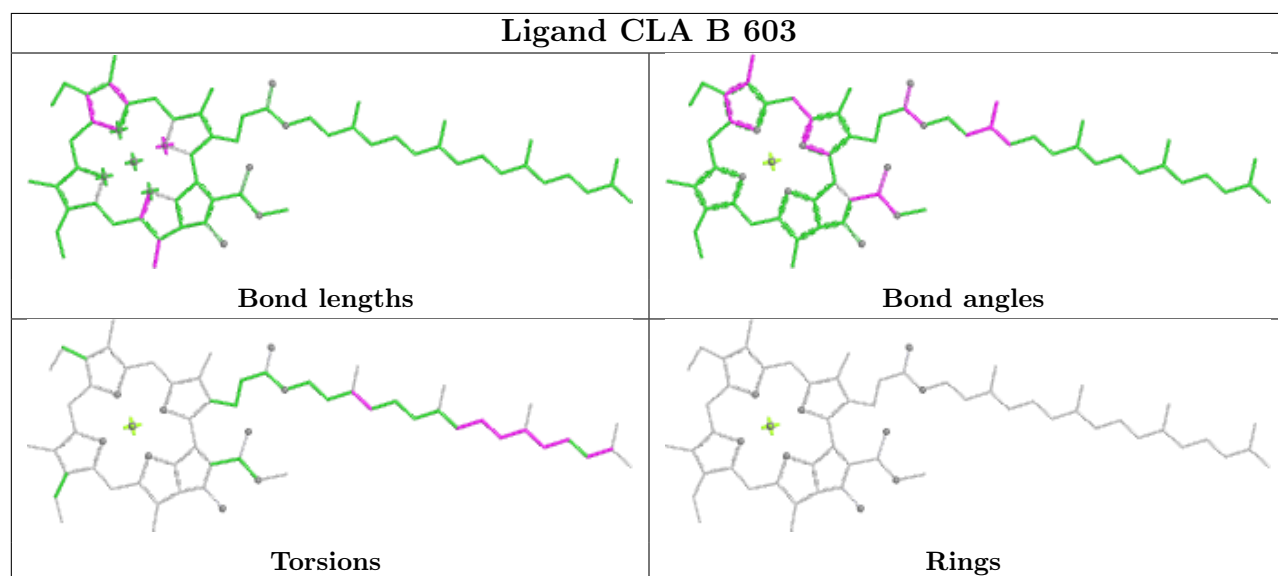
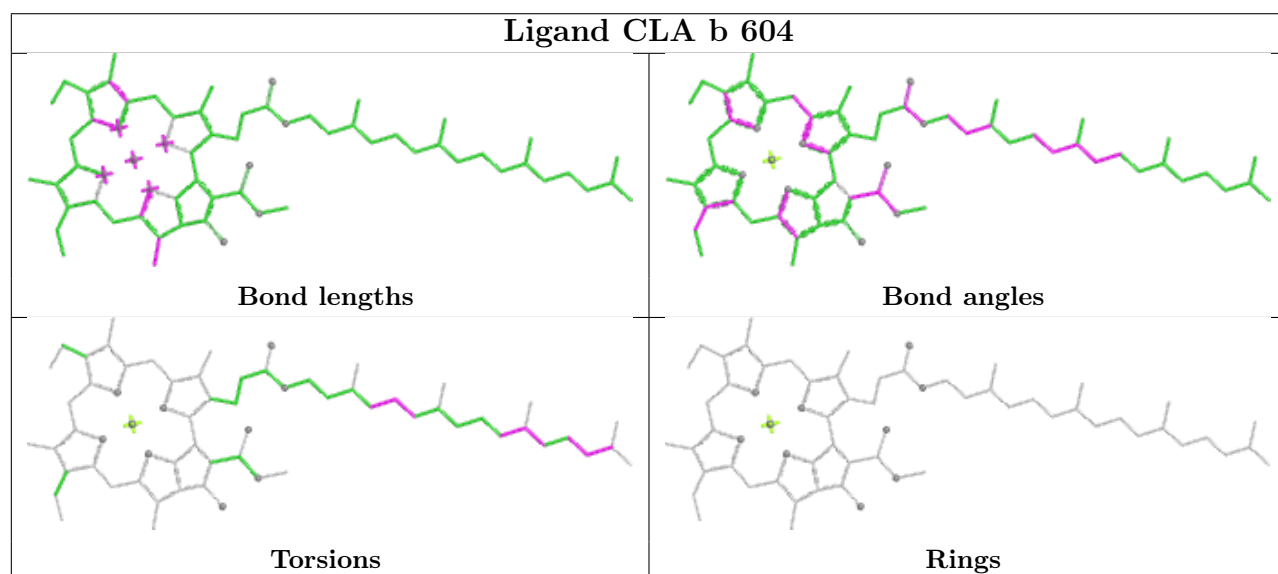
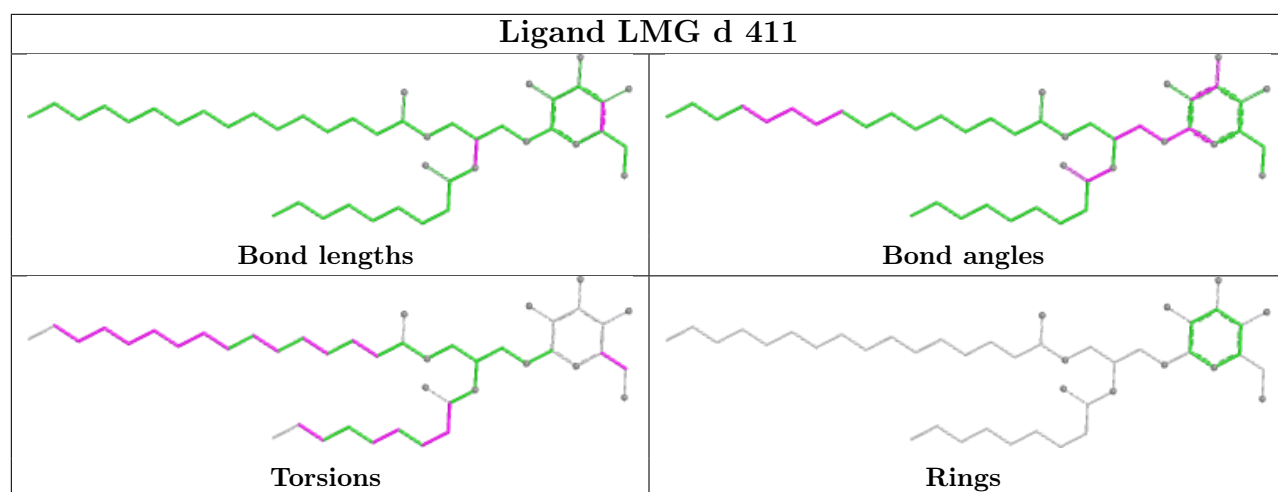
Ligand BCR K 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

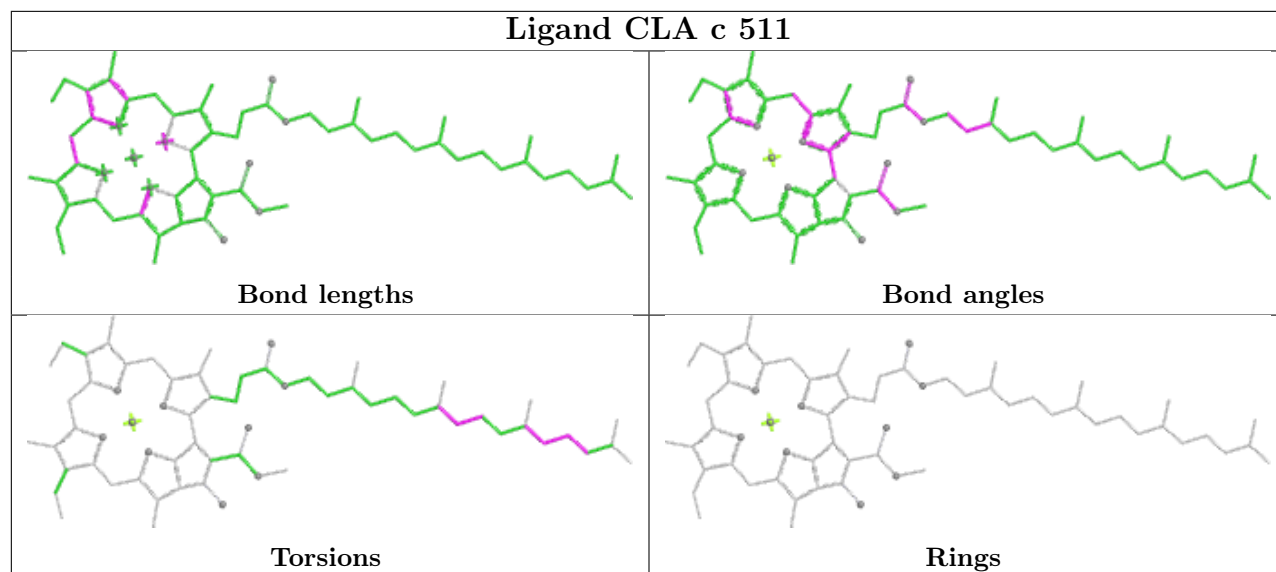
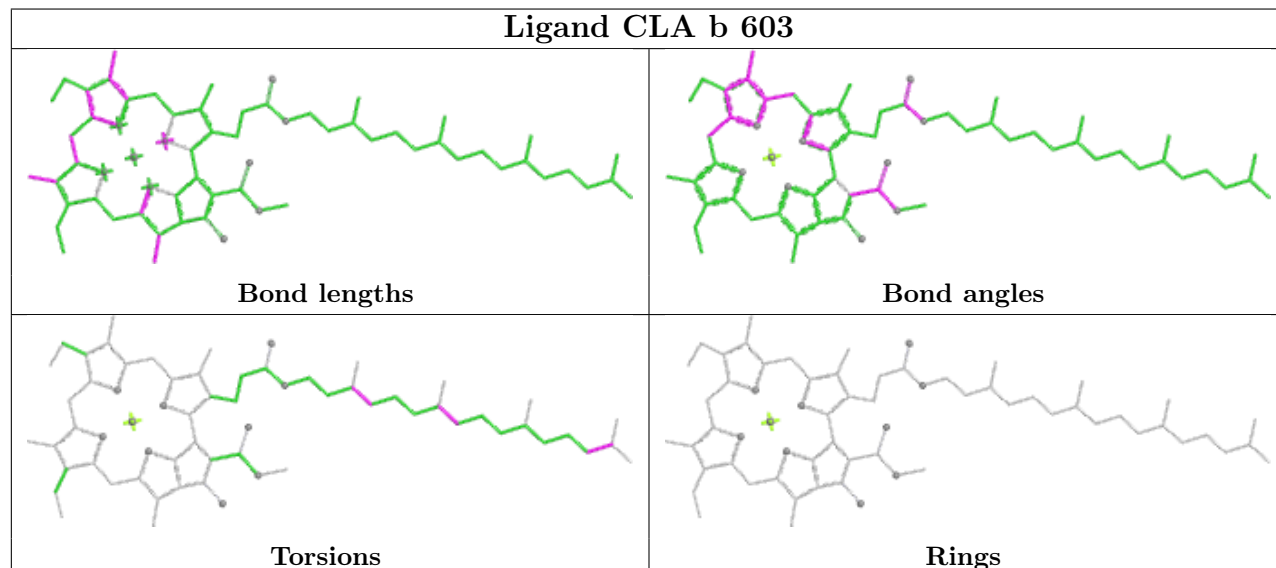
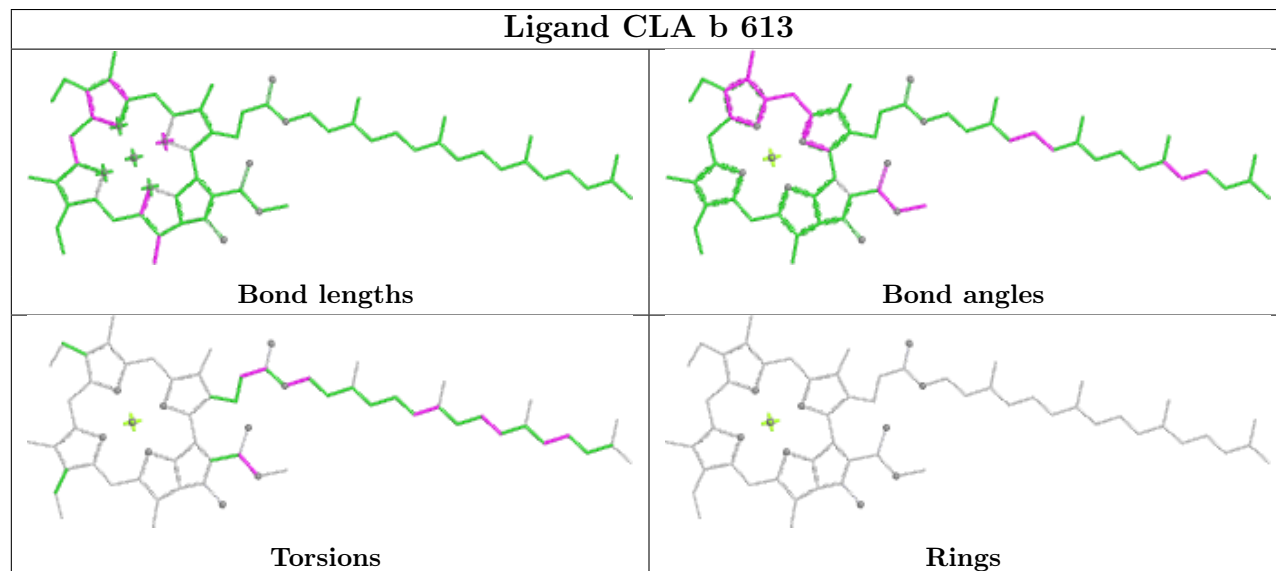
Ligand STE D 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

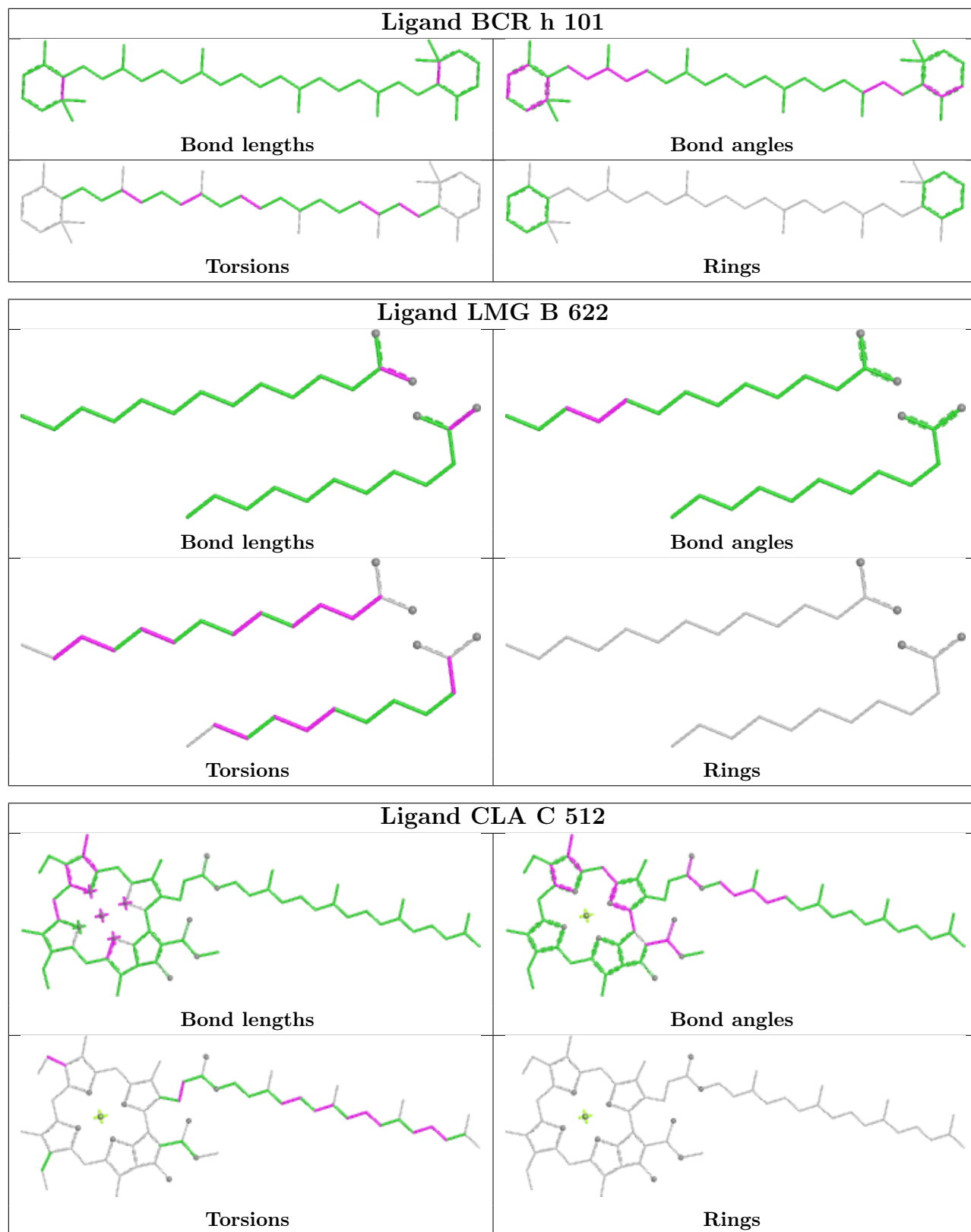
Ligand STE j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

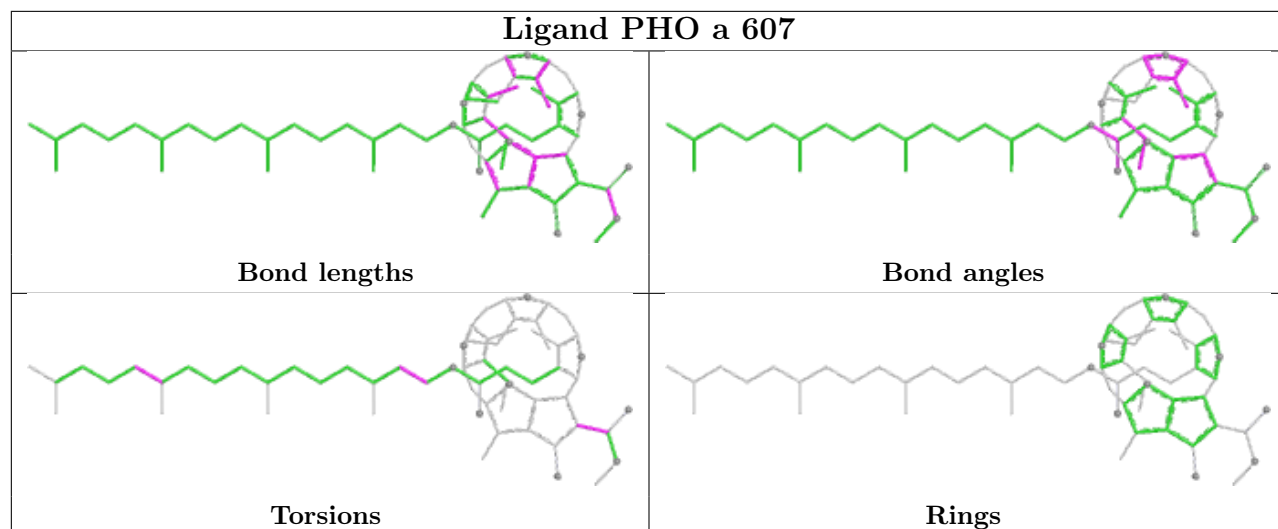
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG d 410	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings



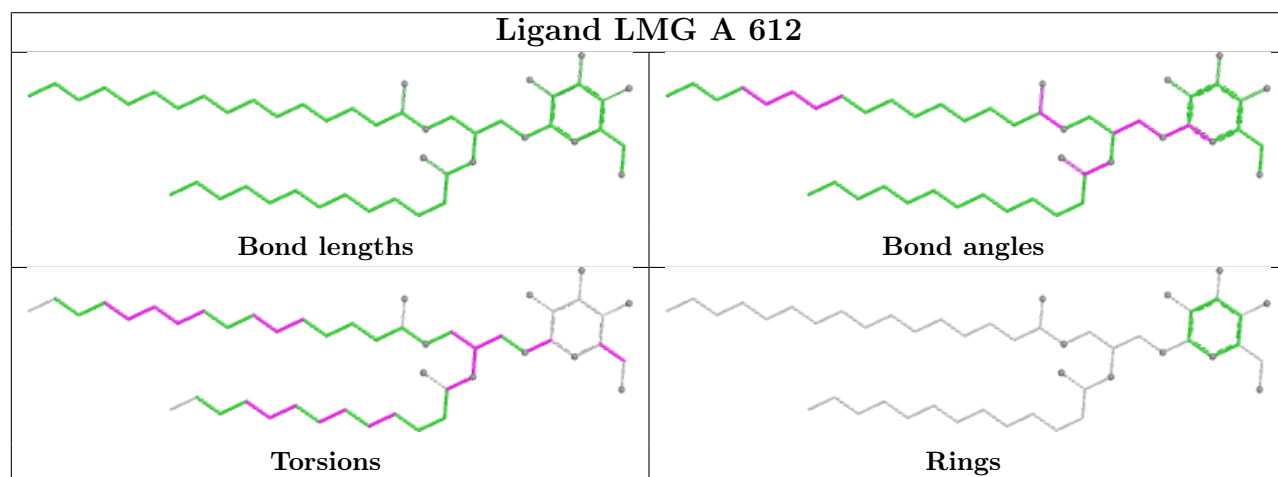
Ligand CLA c 511**Ligand CLA b 603****Ligand CLA b 613**



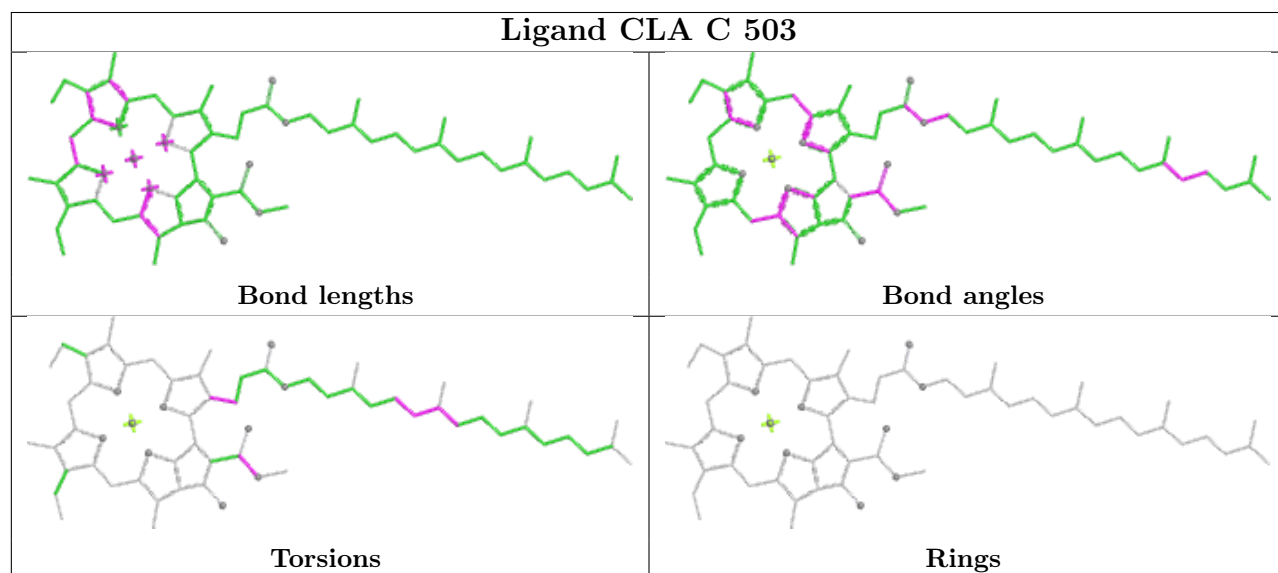
Ligand PHO a 607

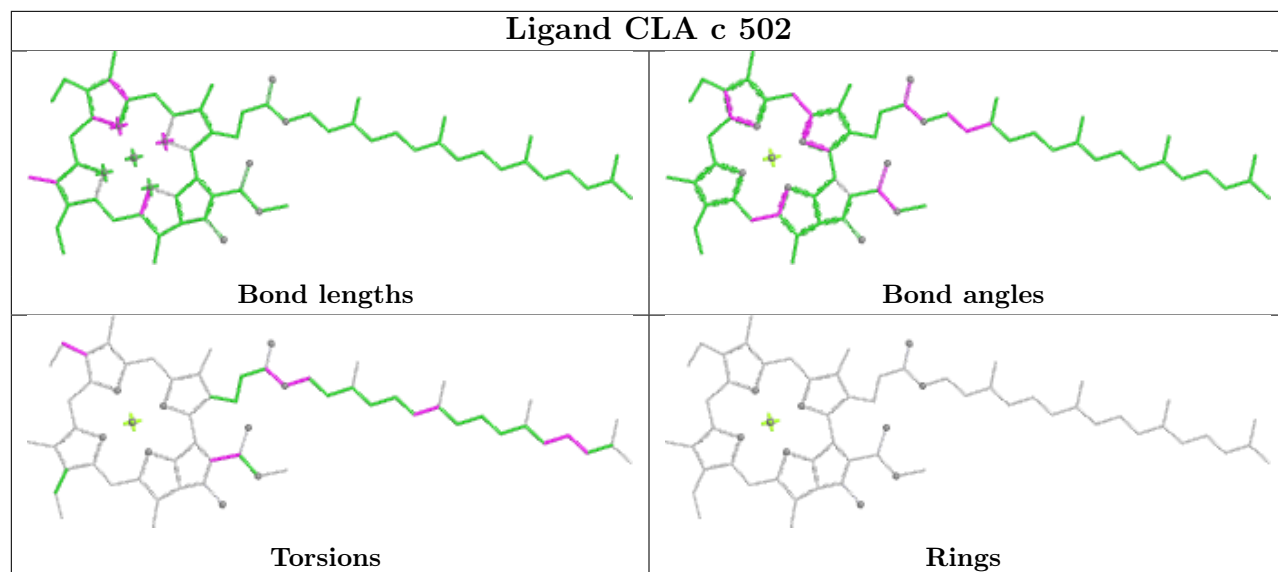
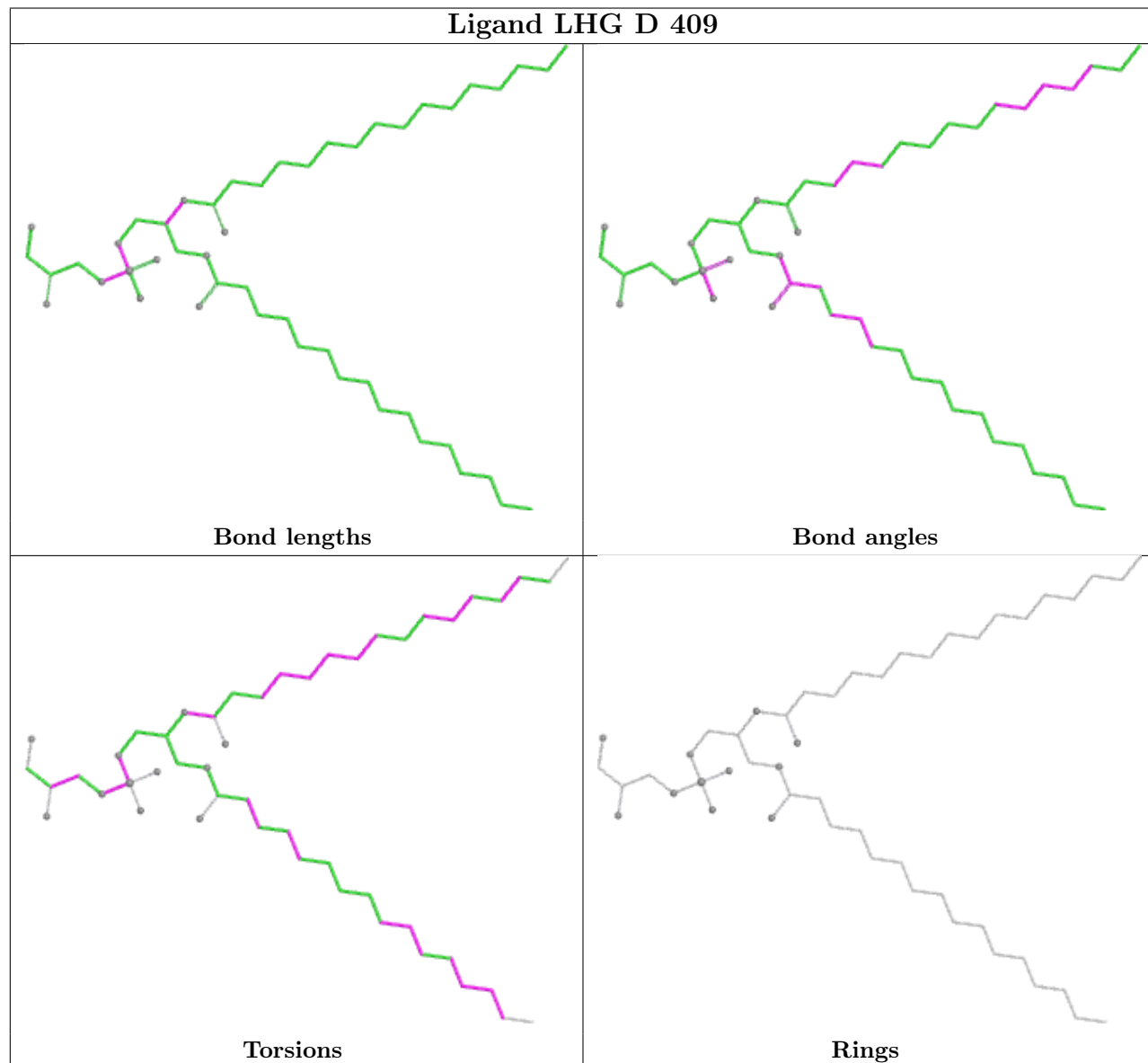


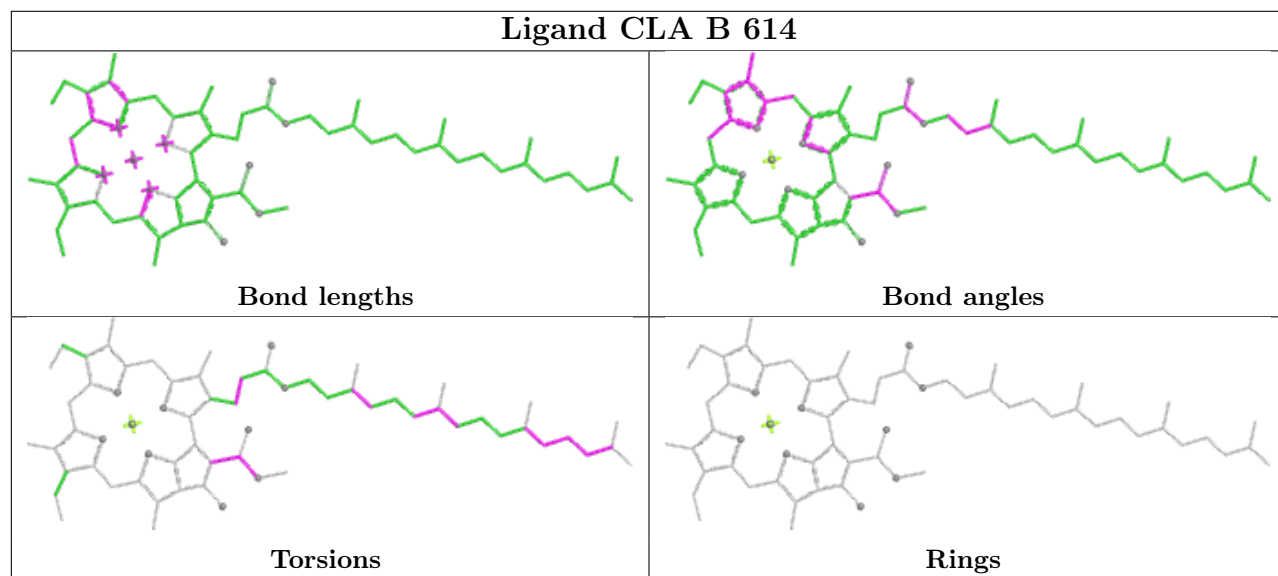
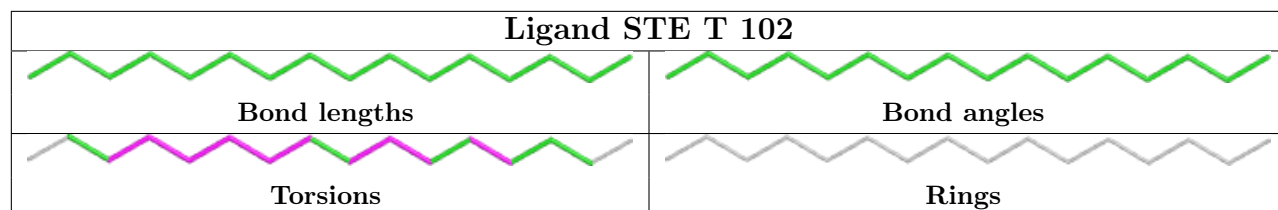
Ligand LMG A 612

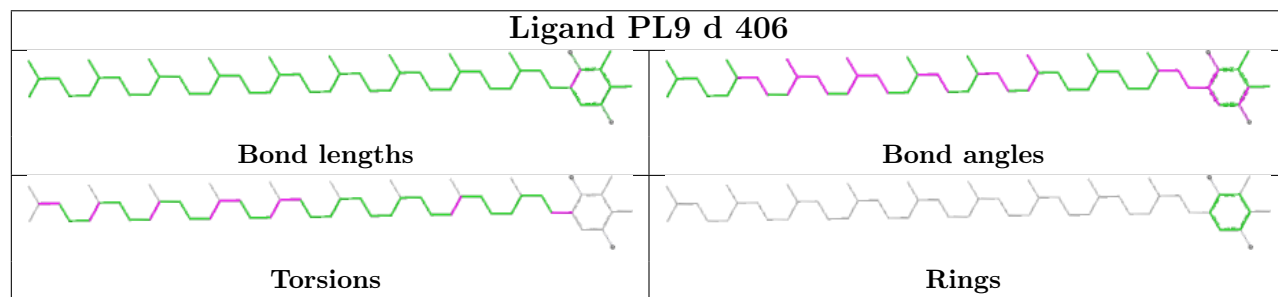
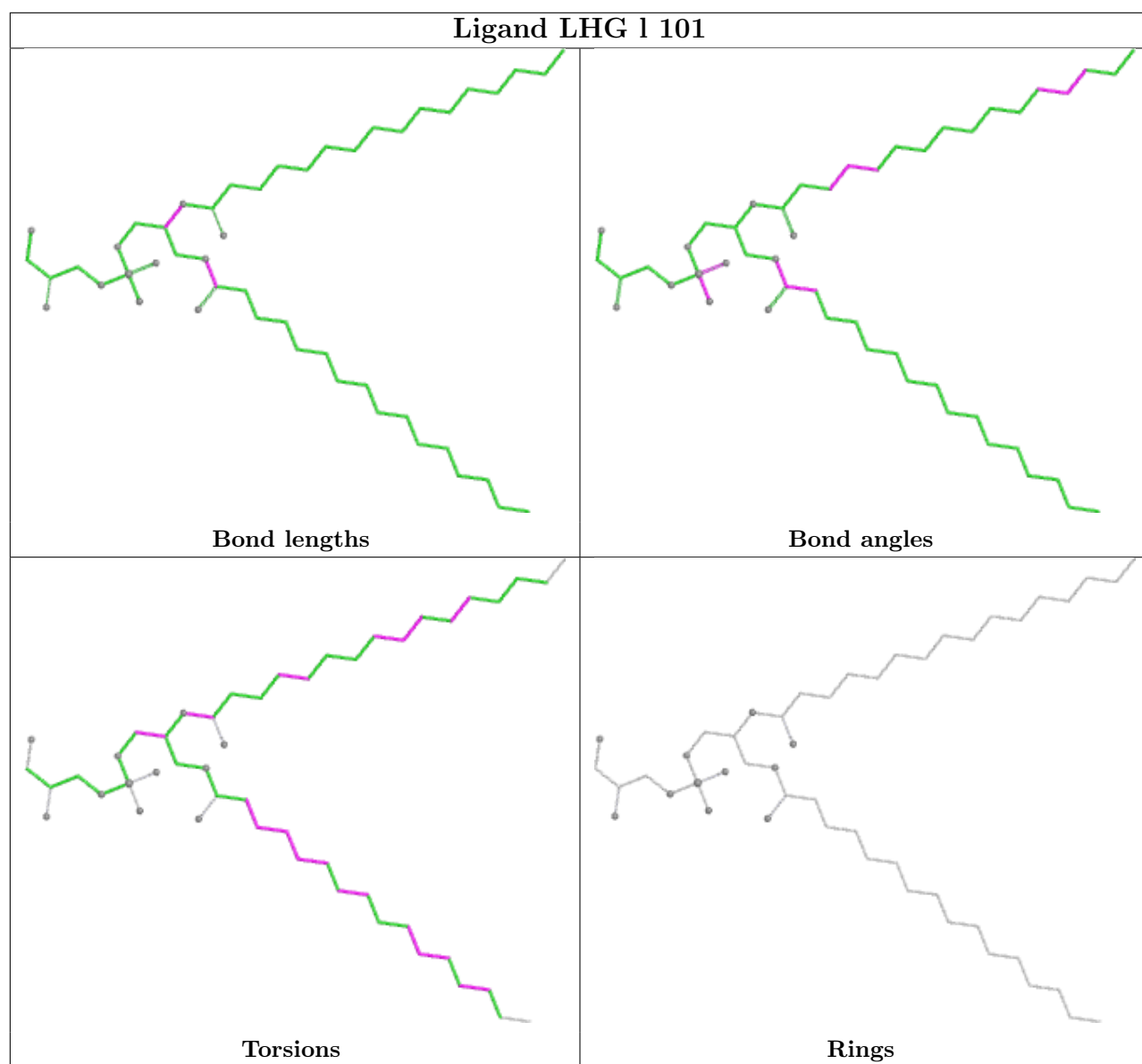


Ligand CLA C 503

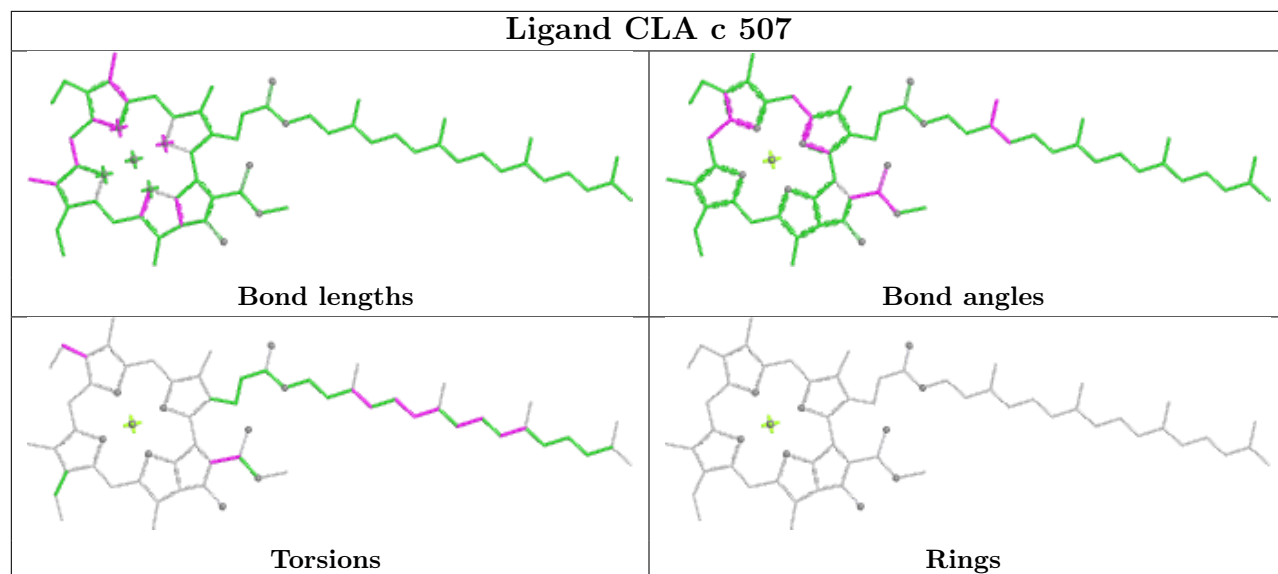


Ligand CLA c 502**Ligand LHG D 409**

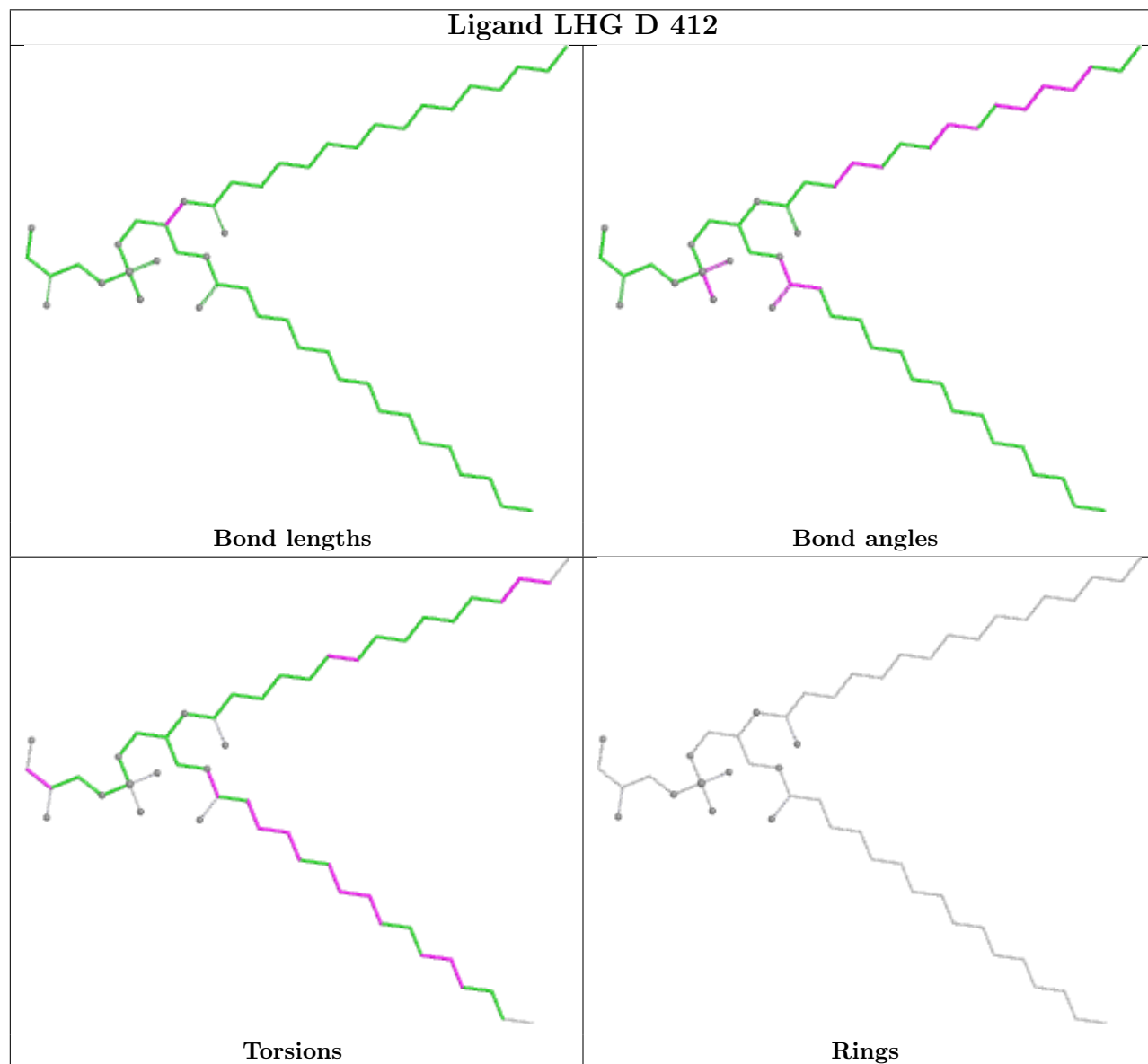




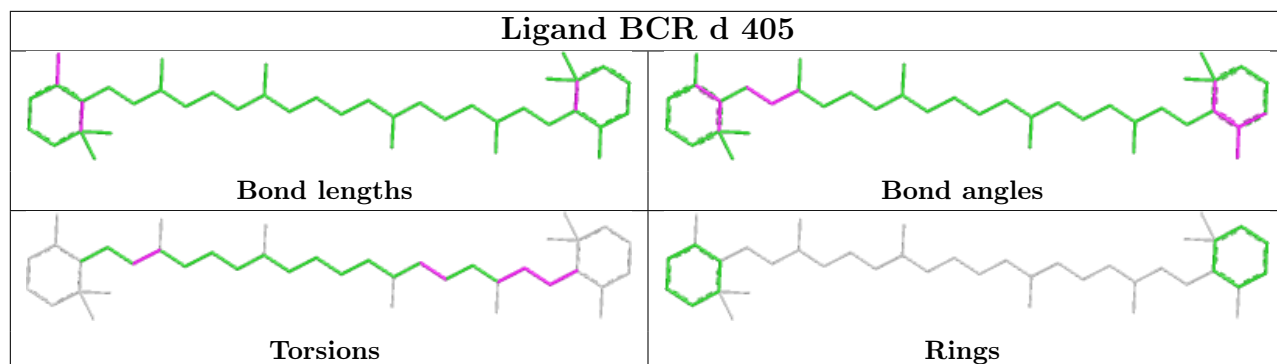
Ligand CLA c 507



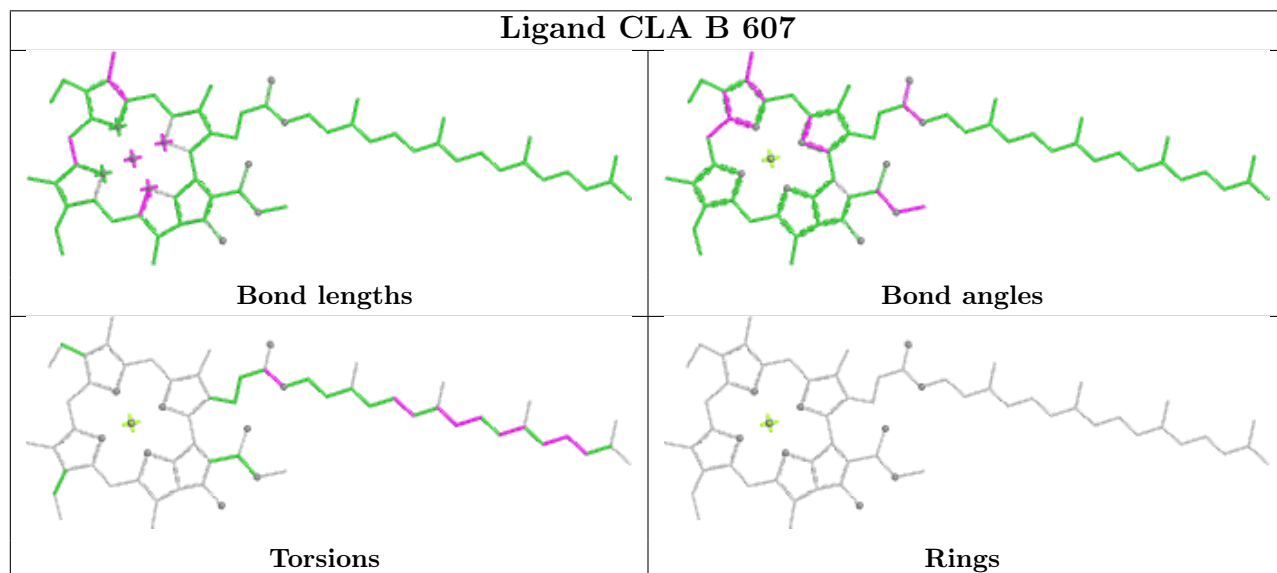
Ligand LHG D 412



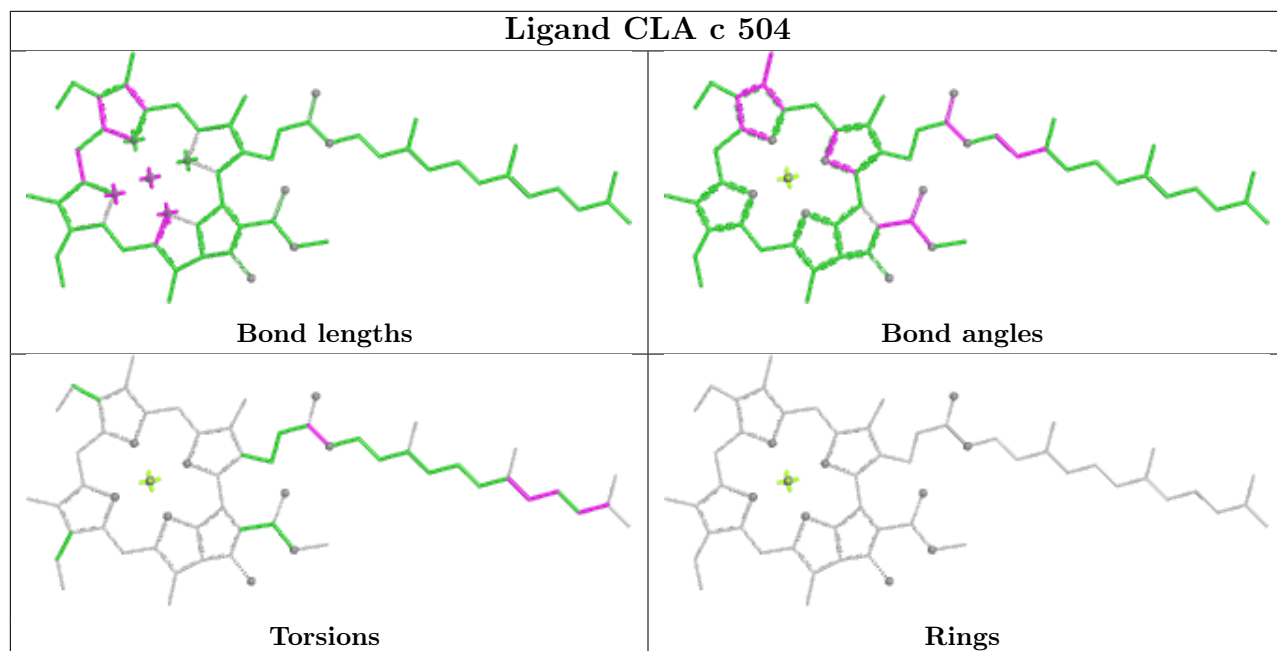
Ligand BCR d 405

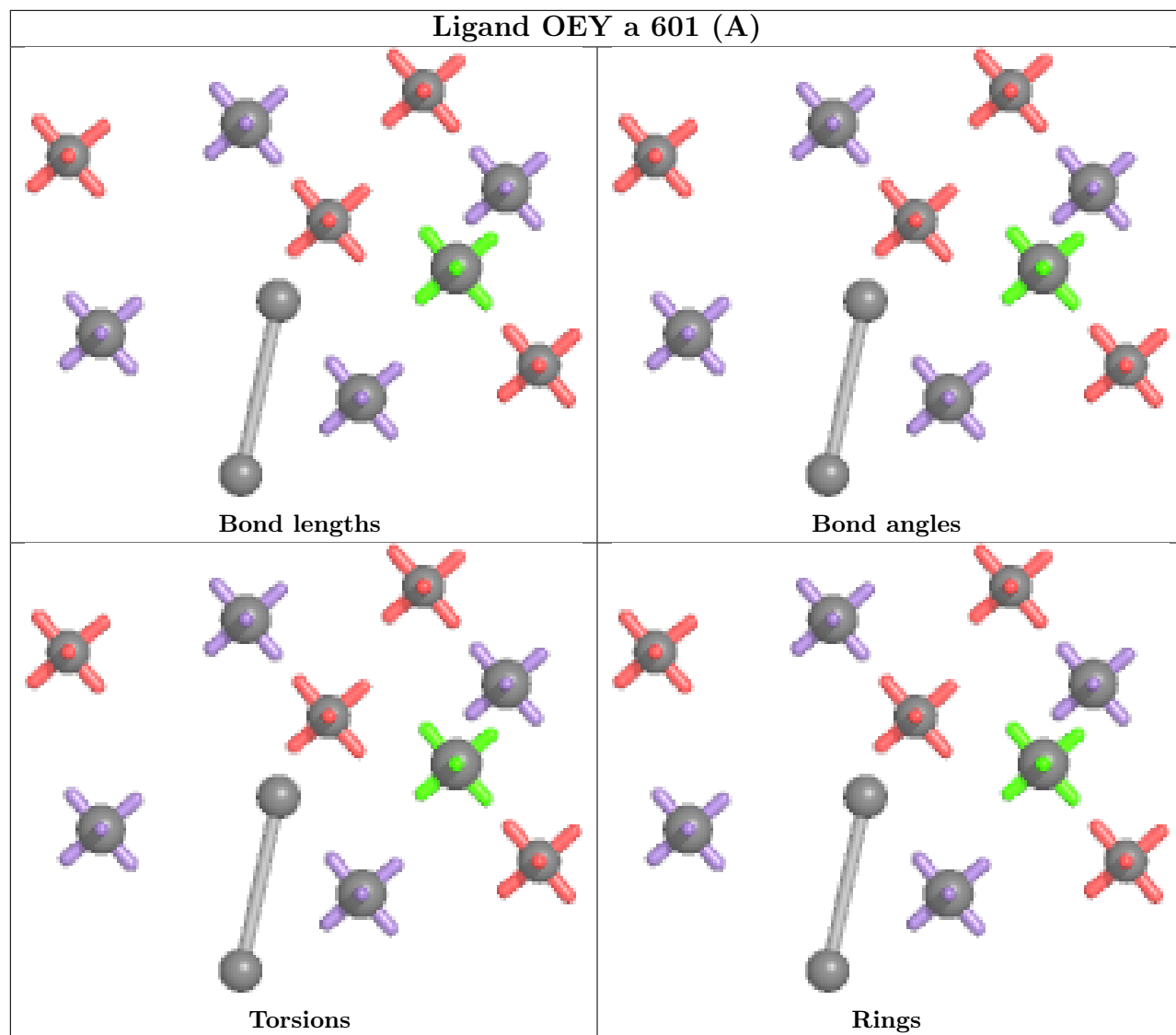


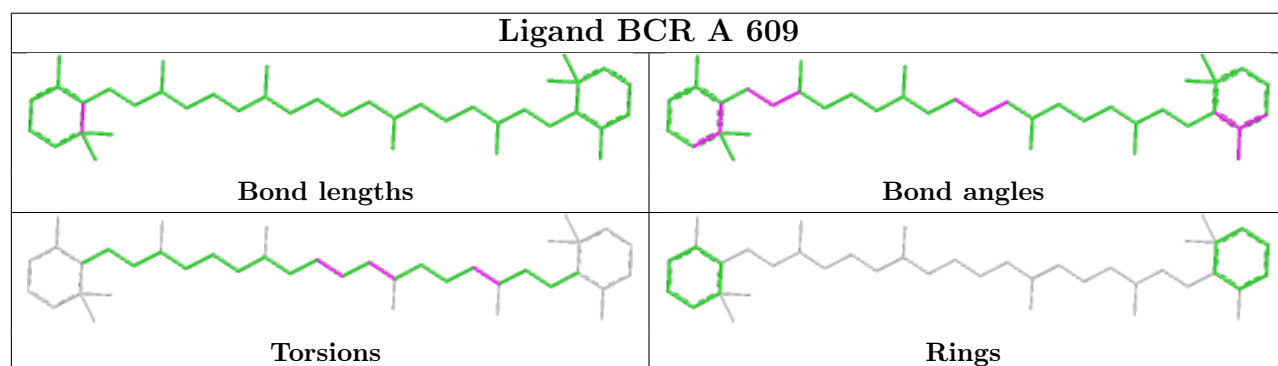
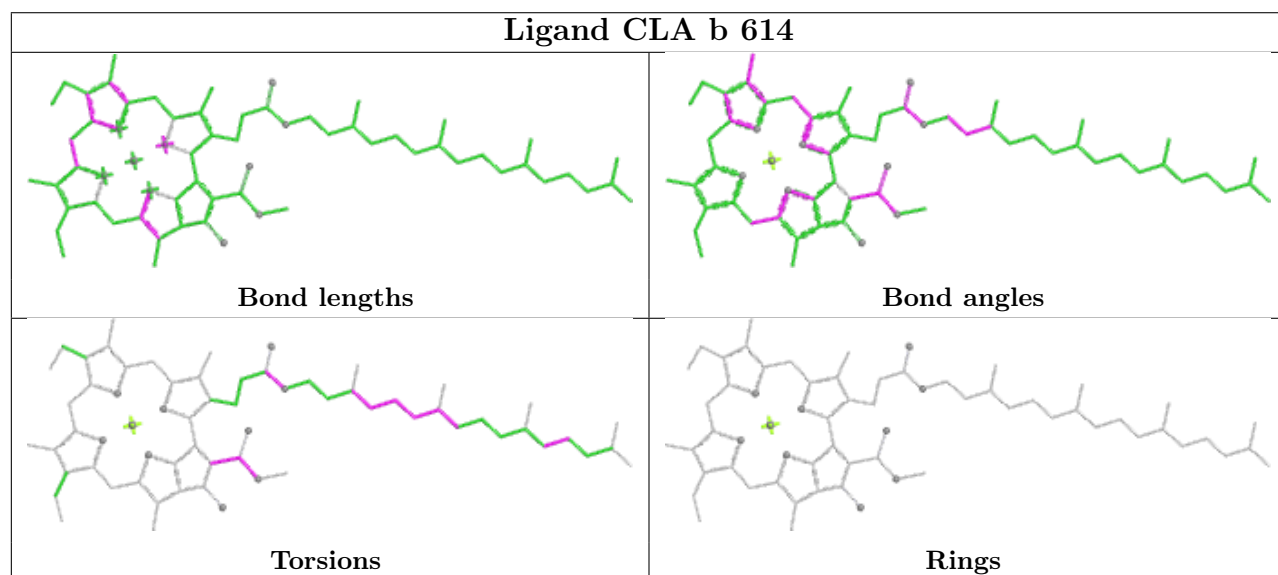
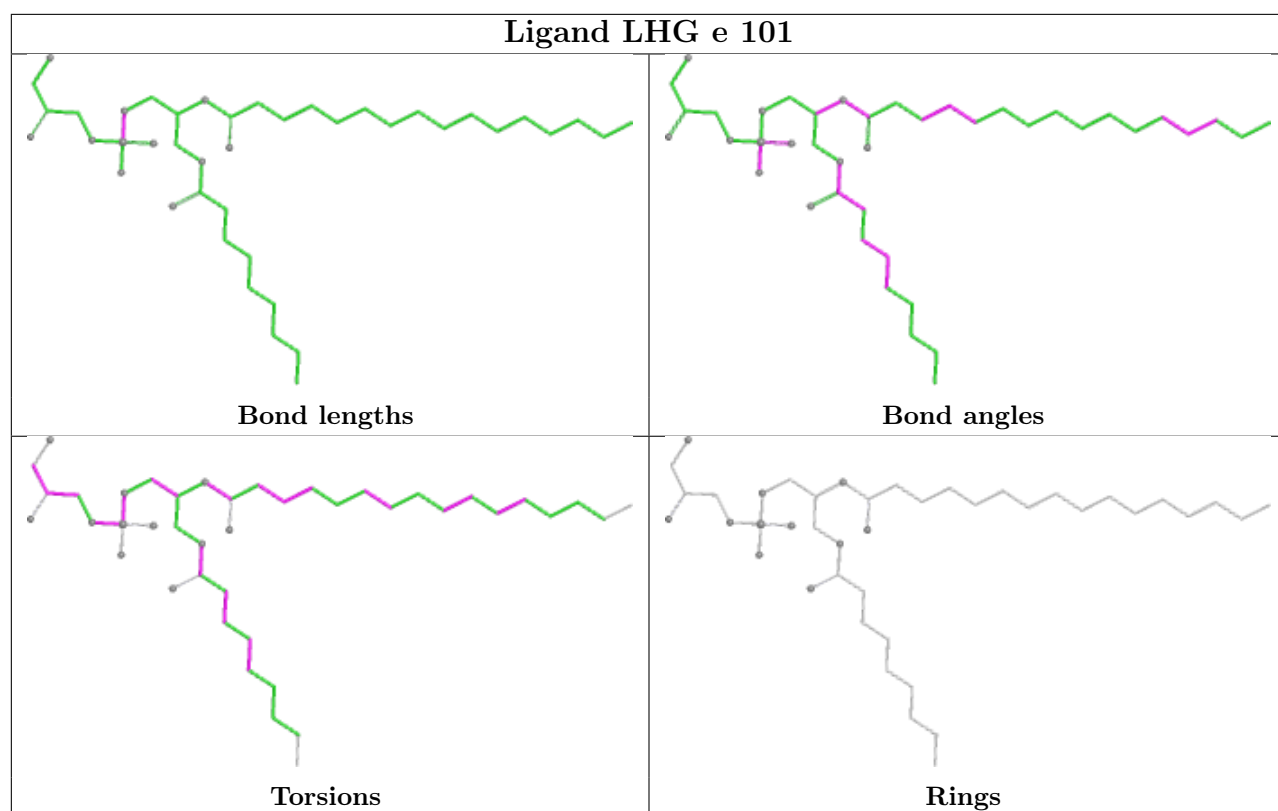
Ligand CLA B 607

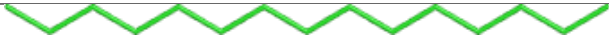
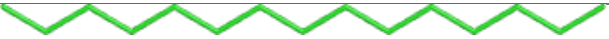
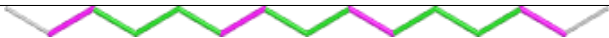


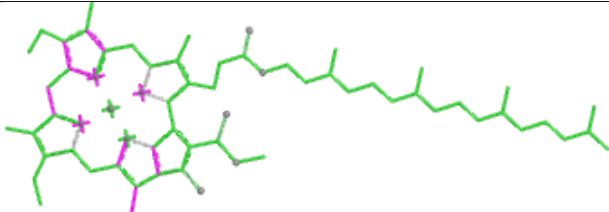
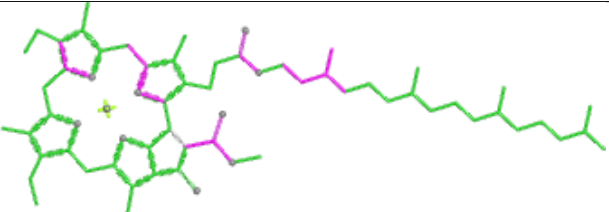
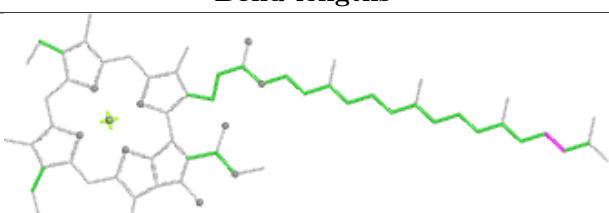
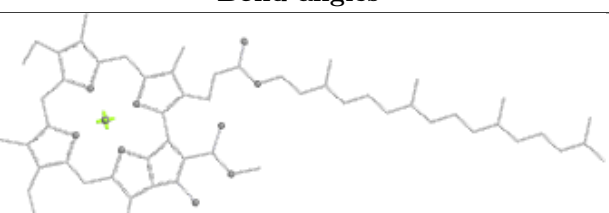
Ligand CLA c 504

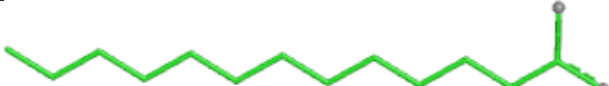
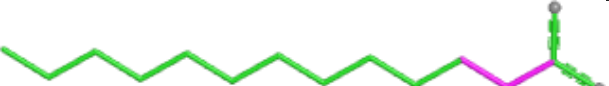
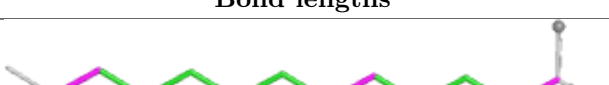




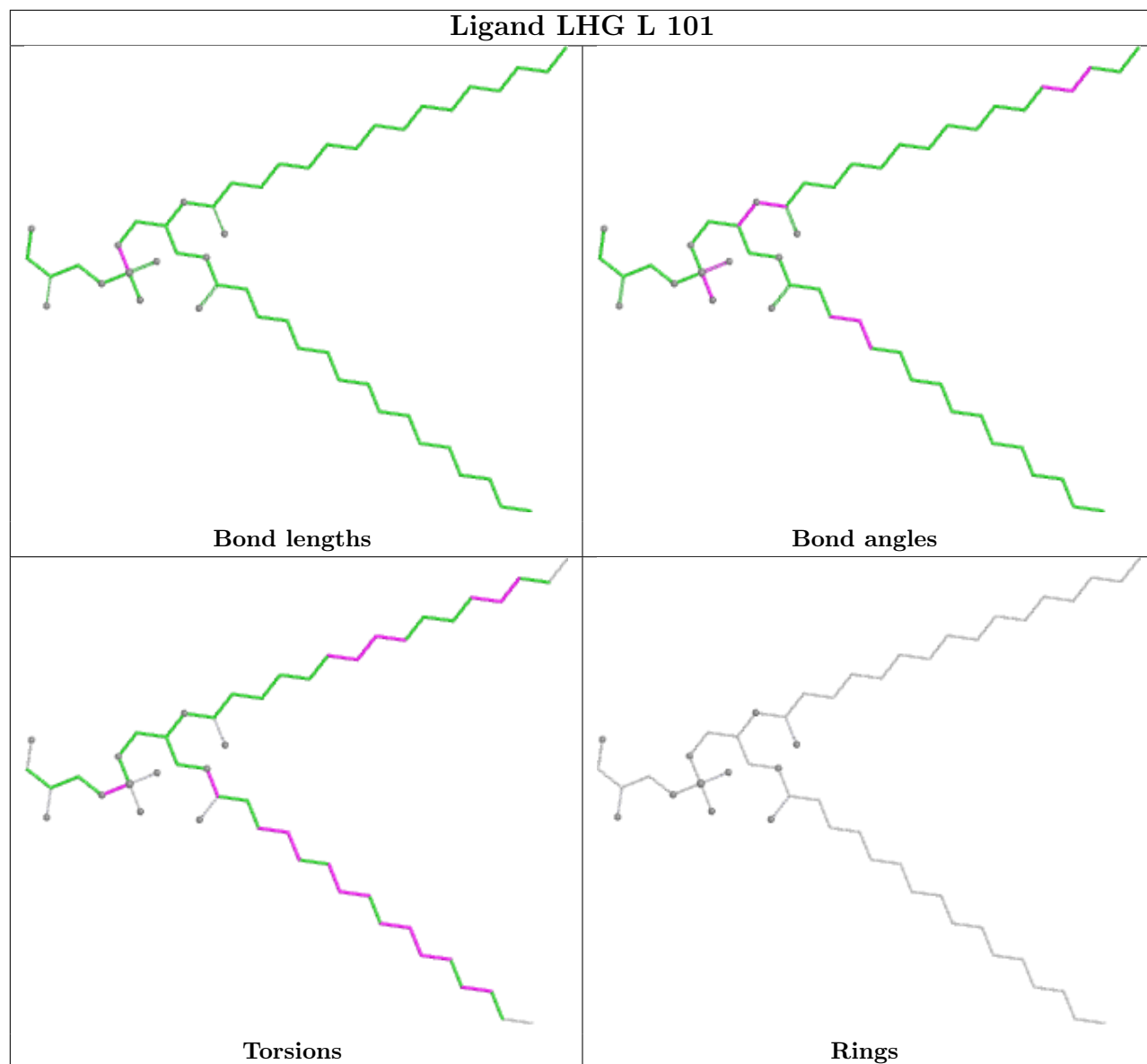


Ligand STE I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

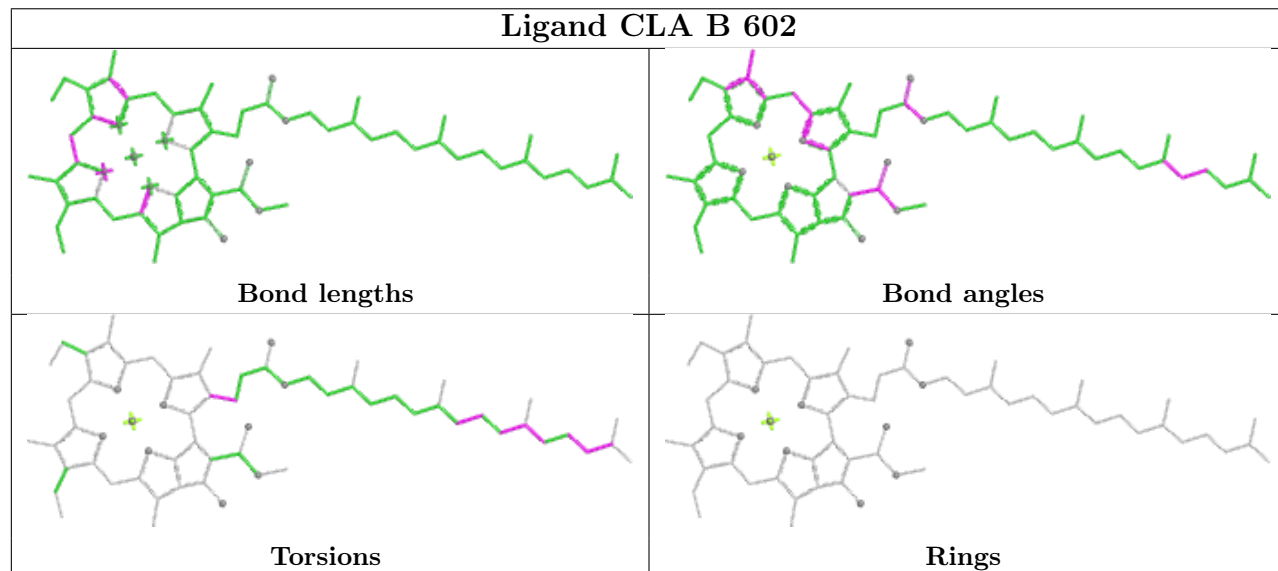
Ligand CLA a 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

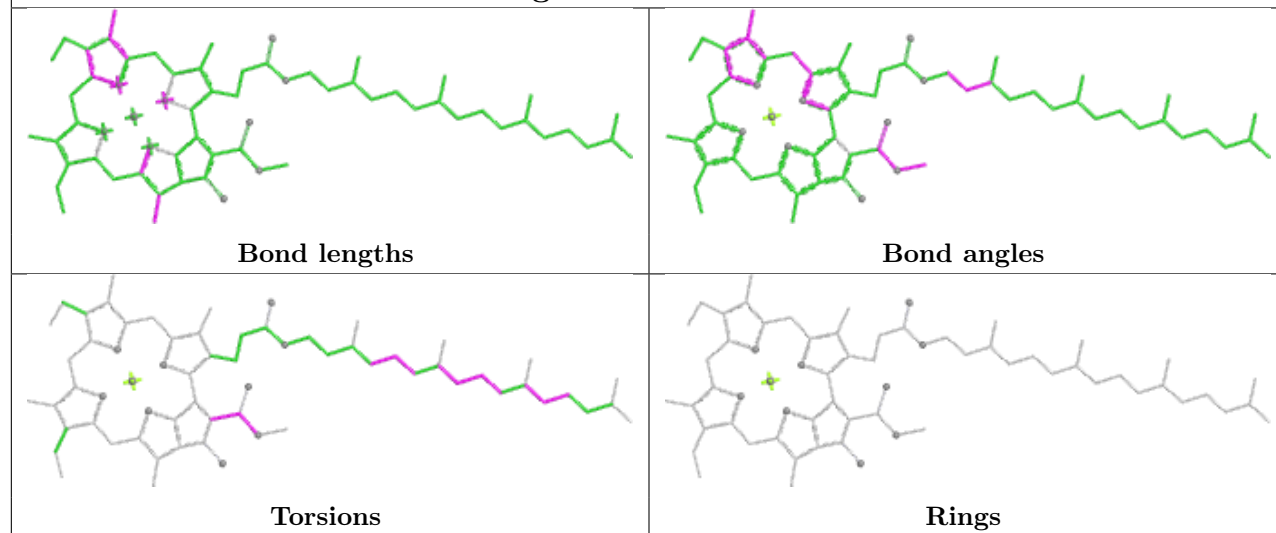
Ligand LHG L 101



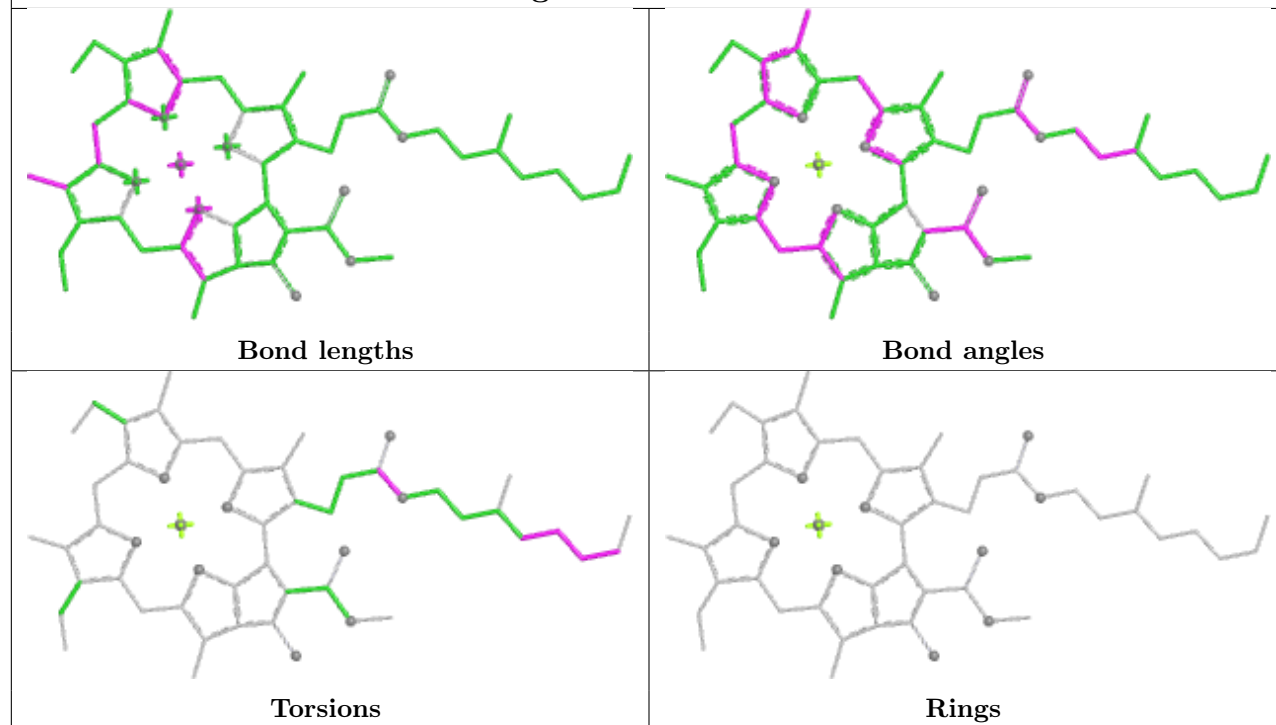
Ligand CLA B 602

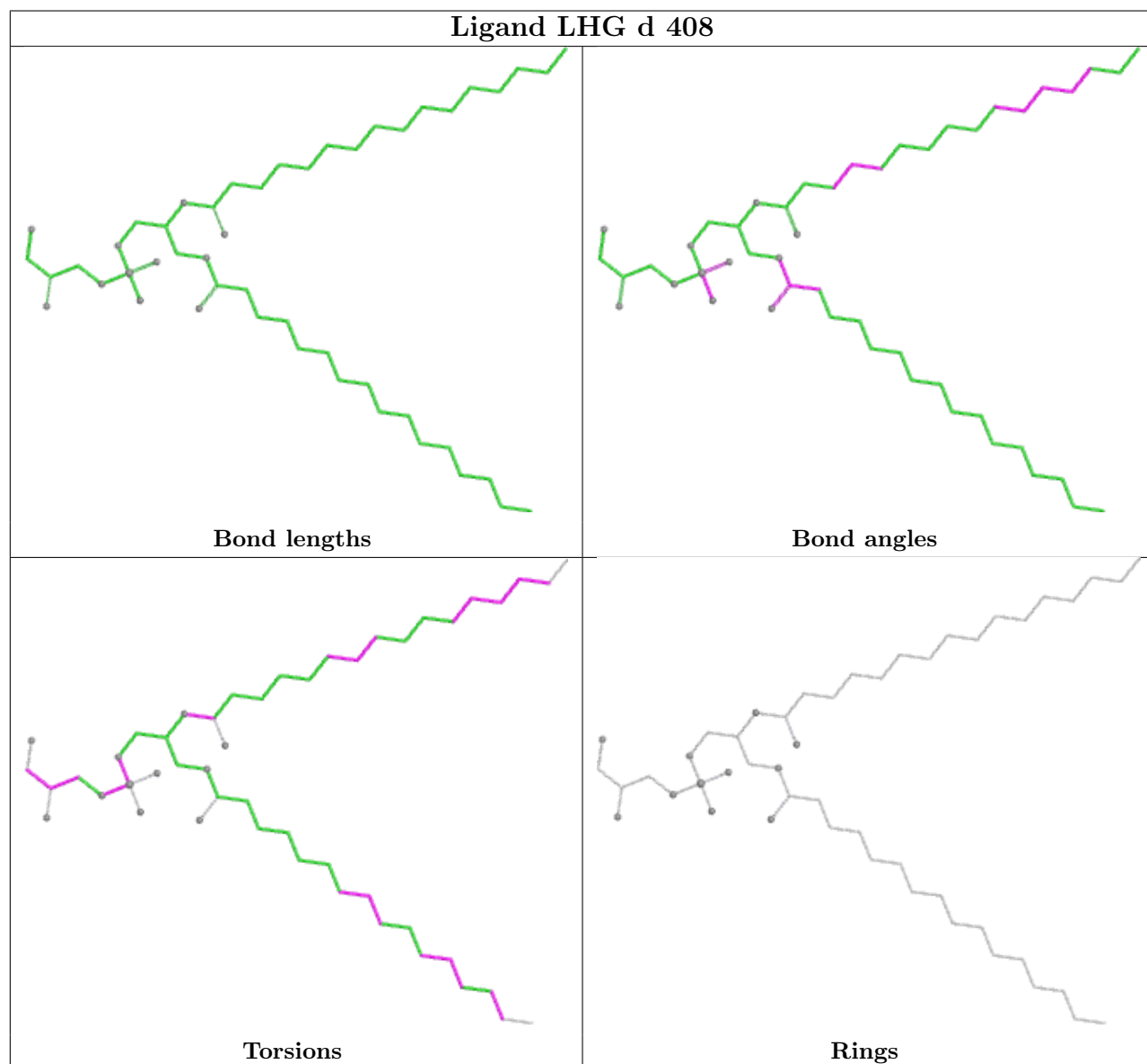
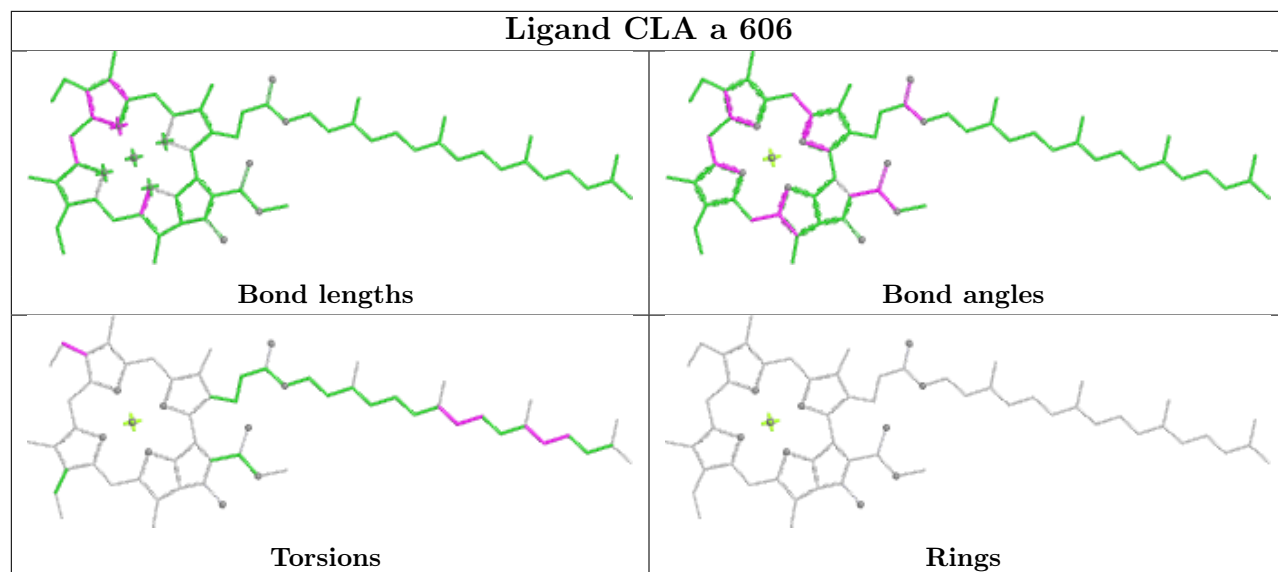


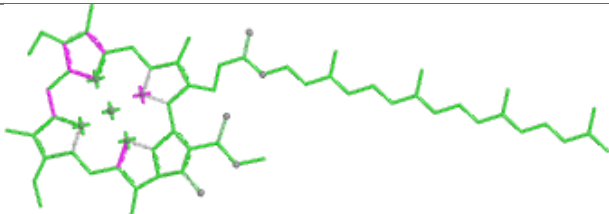
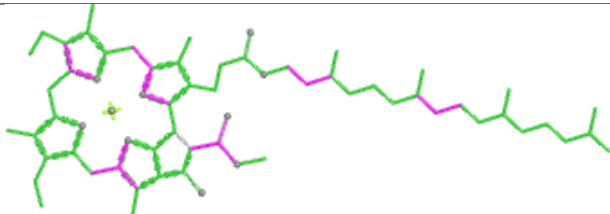
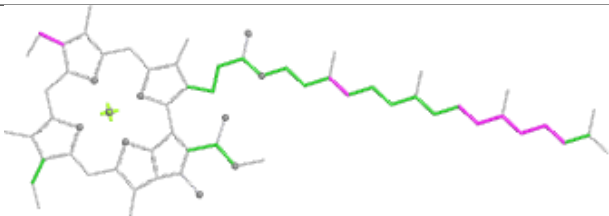
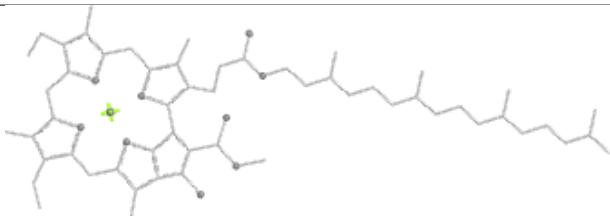
Ligand CLA C 509

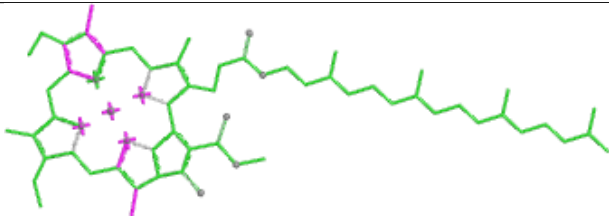
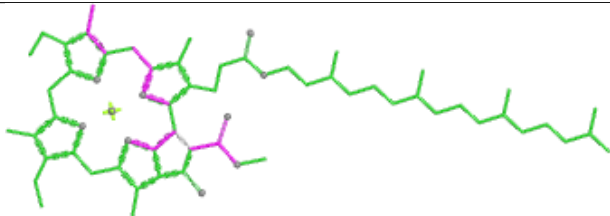
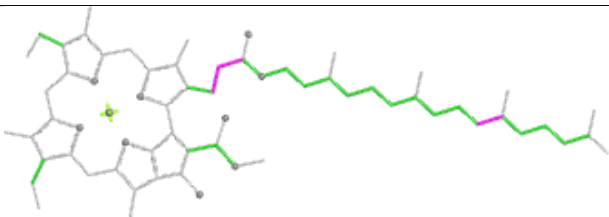
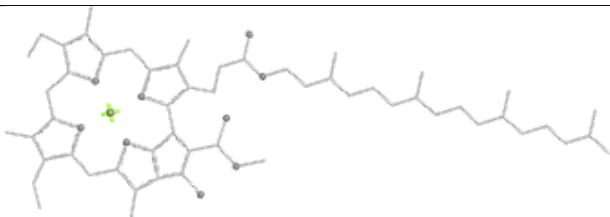


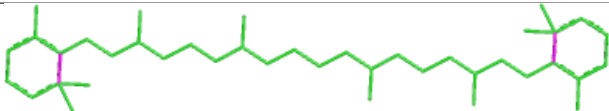
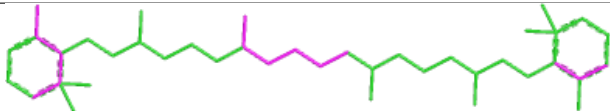
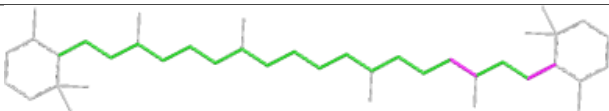
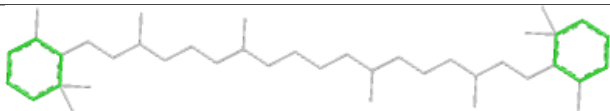
Ligand CLA A 608

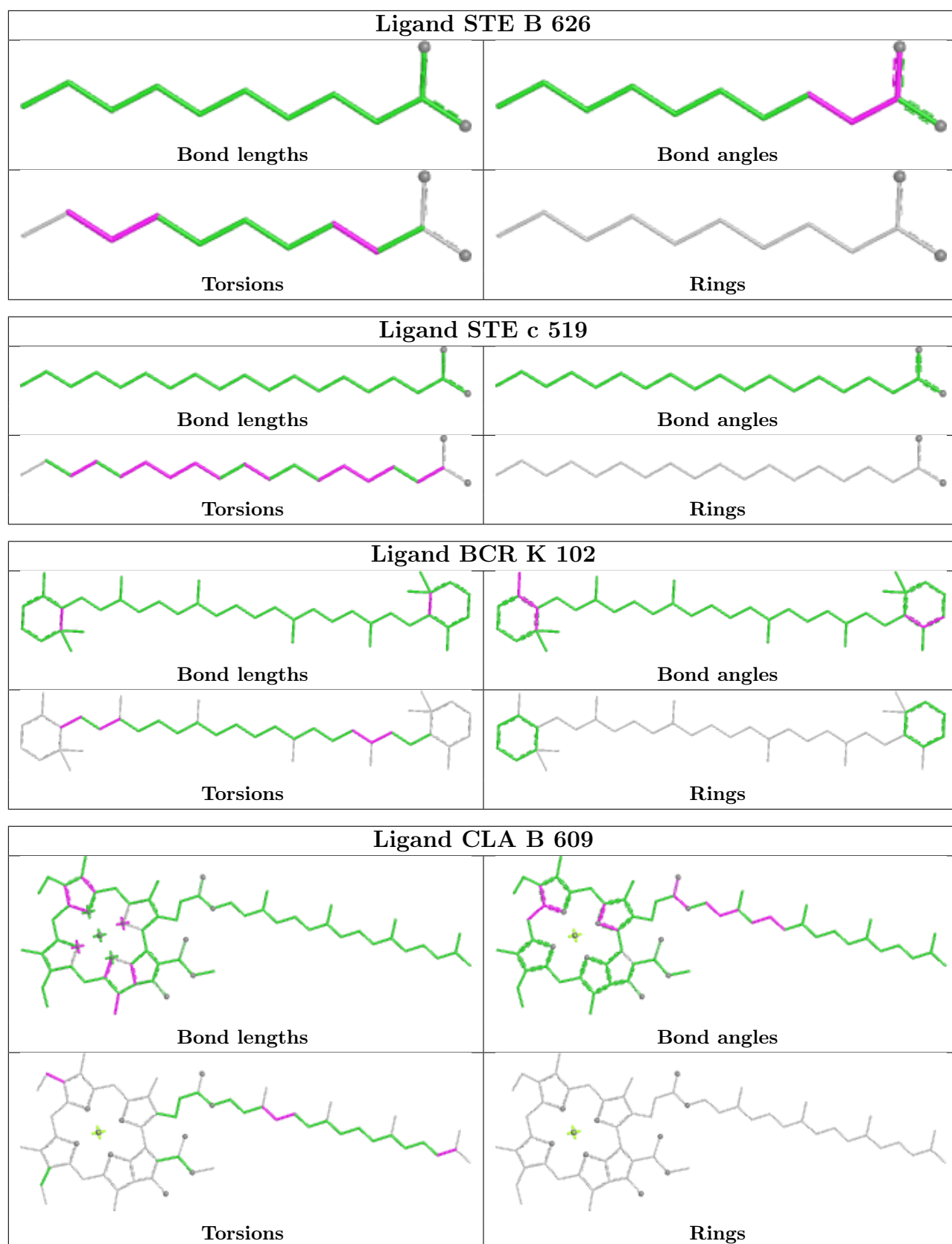


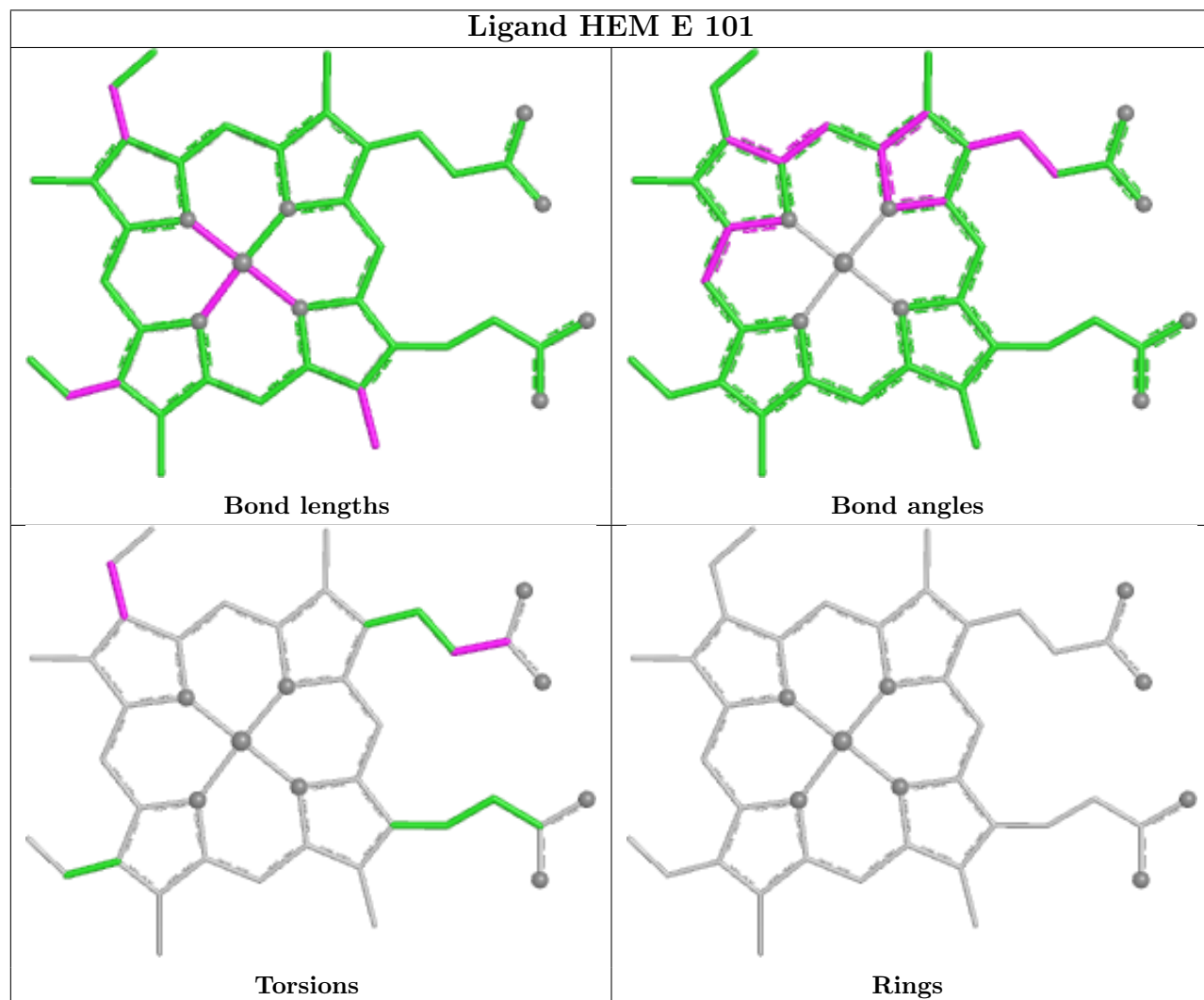
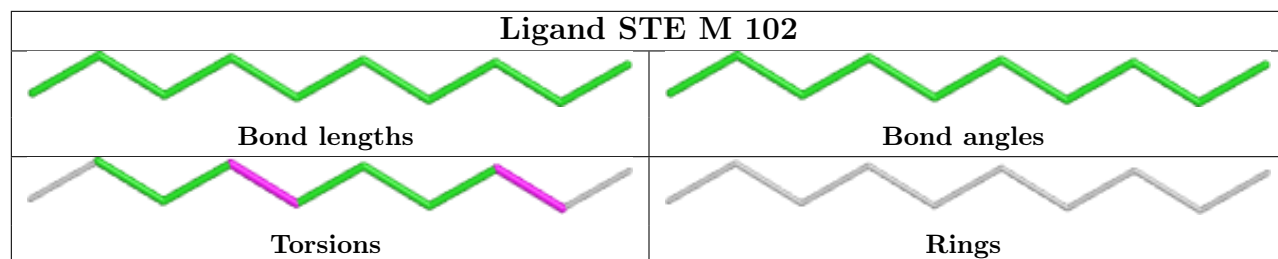


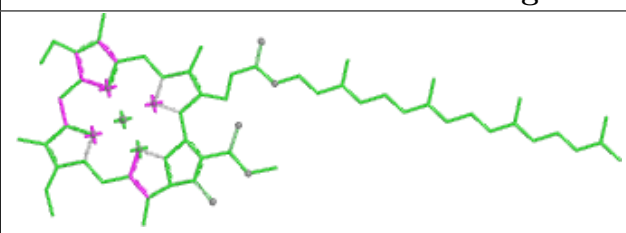
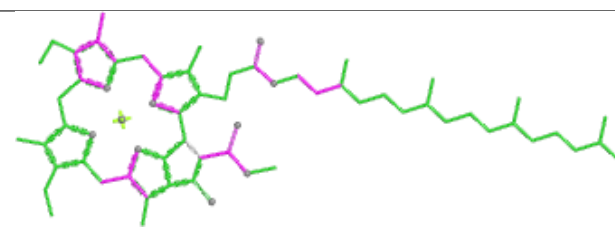
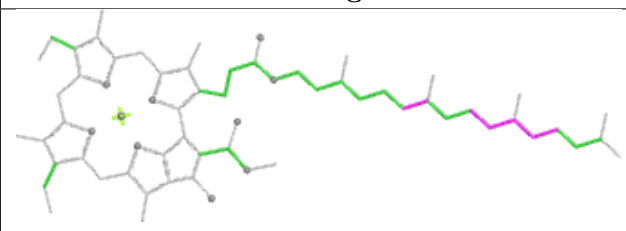
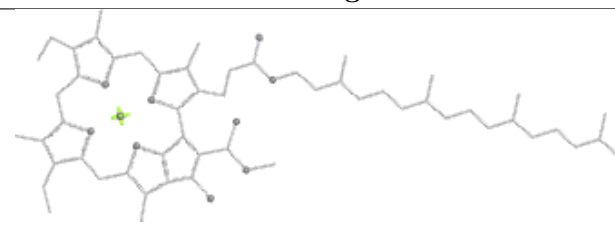
Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

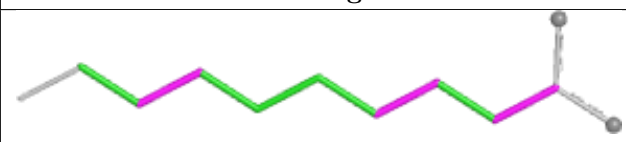
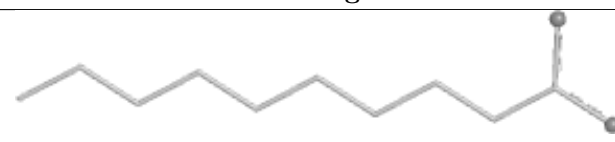
Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

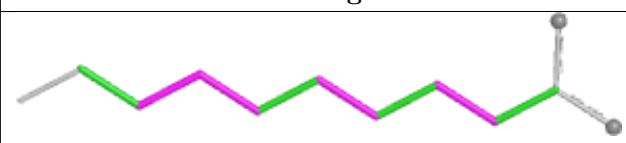
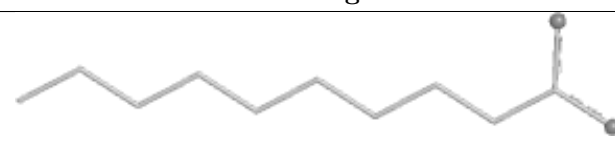
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

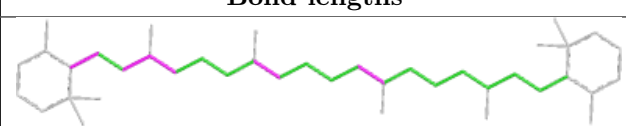
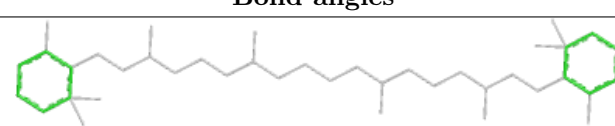


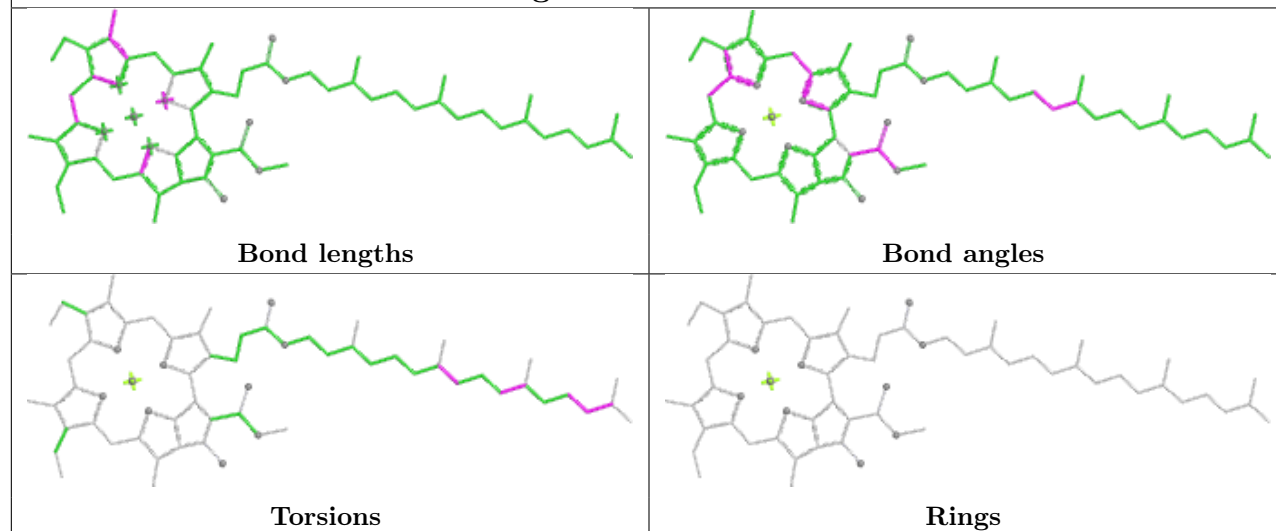
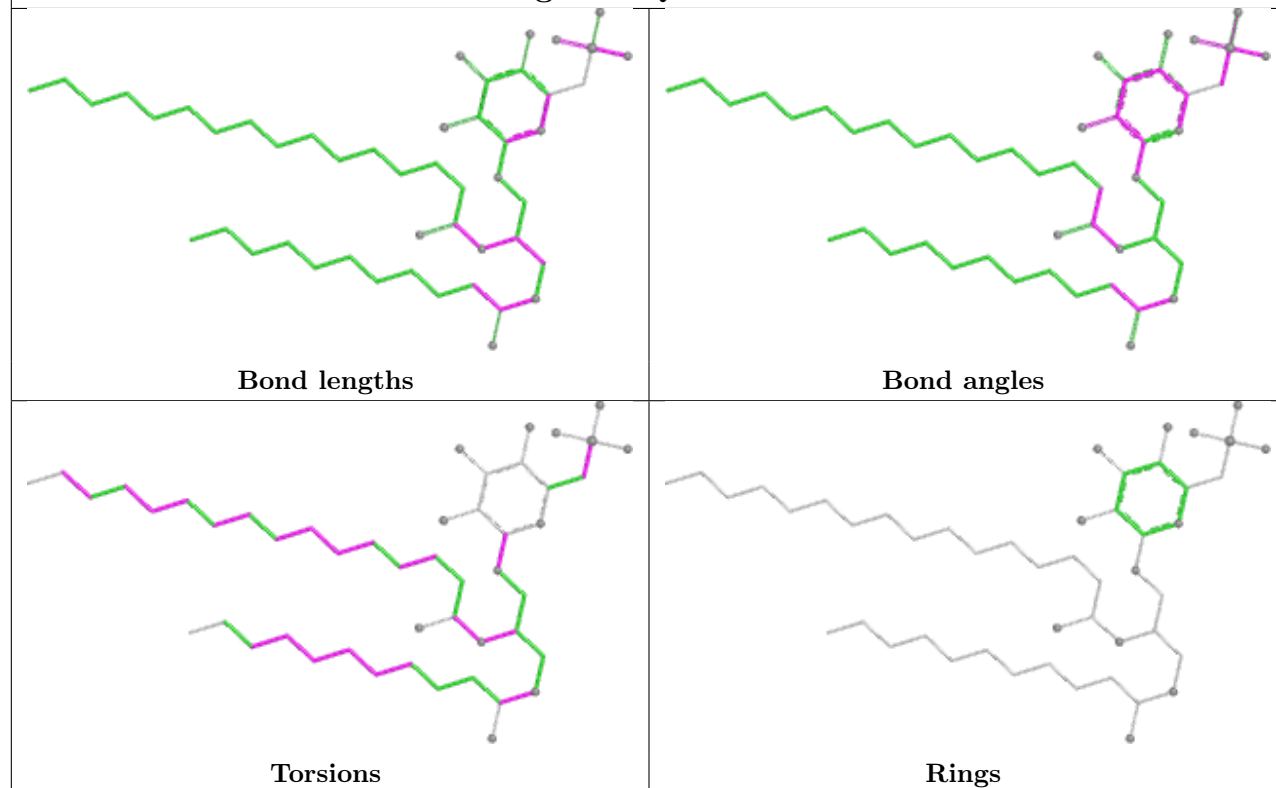


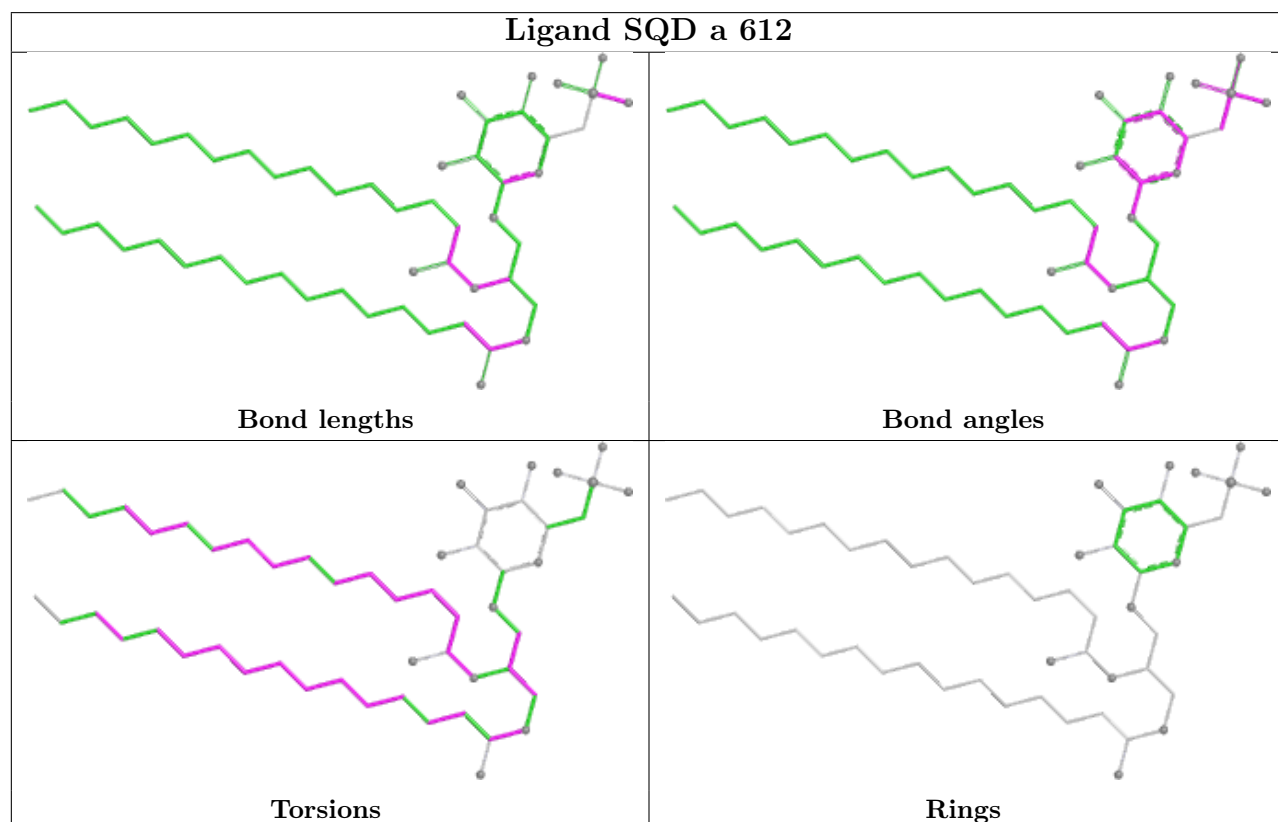
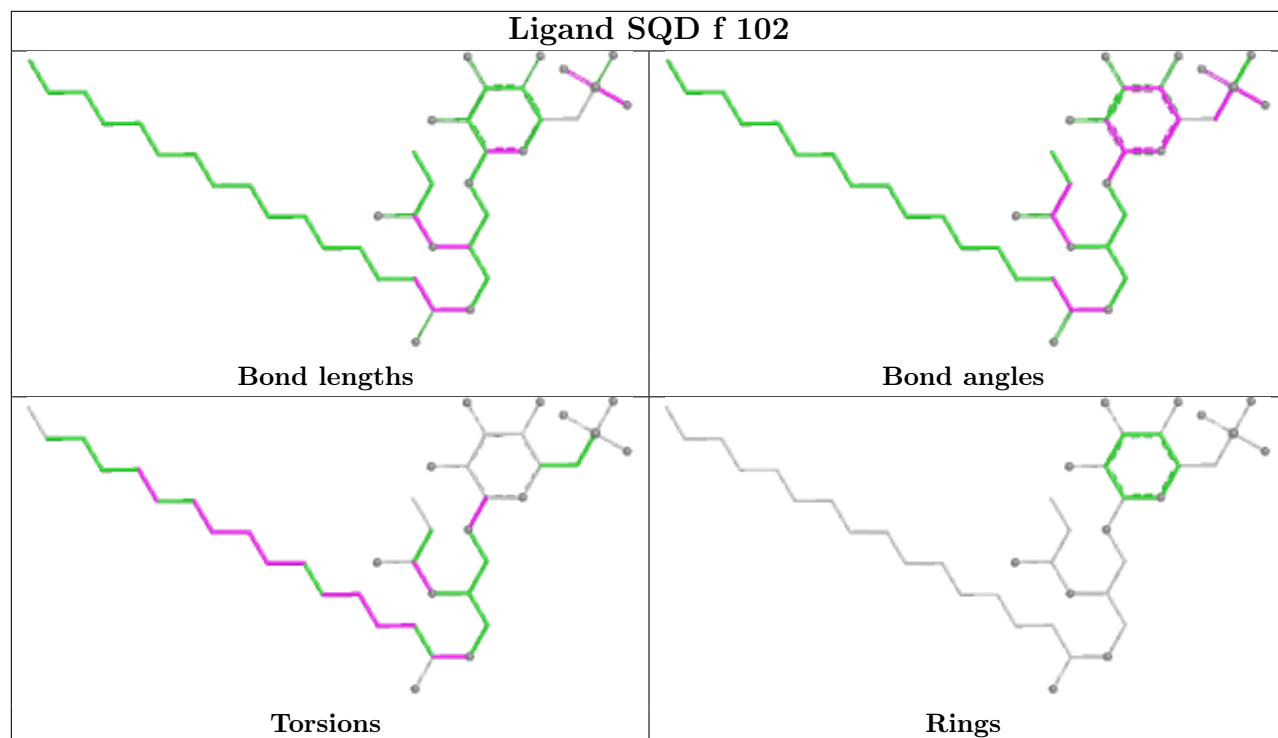
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE k 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

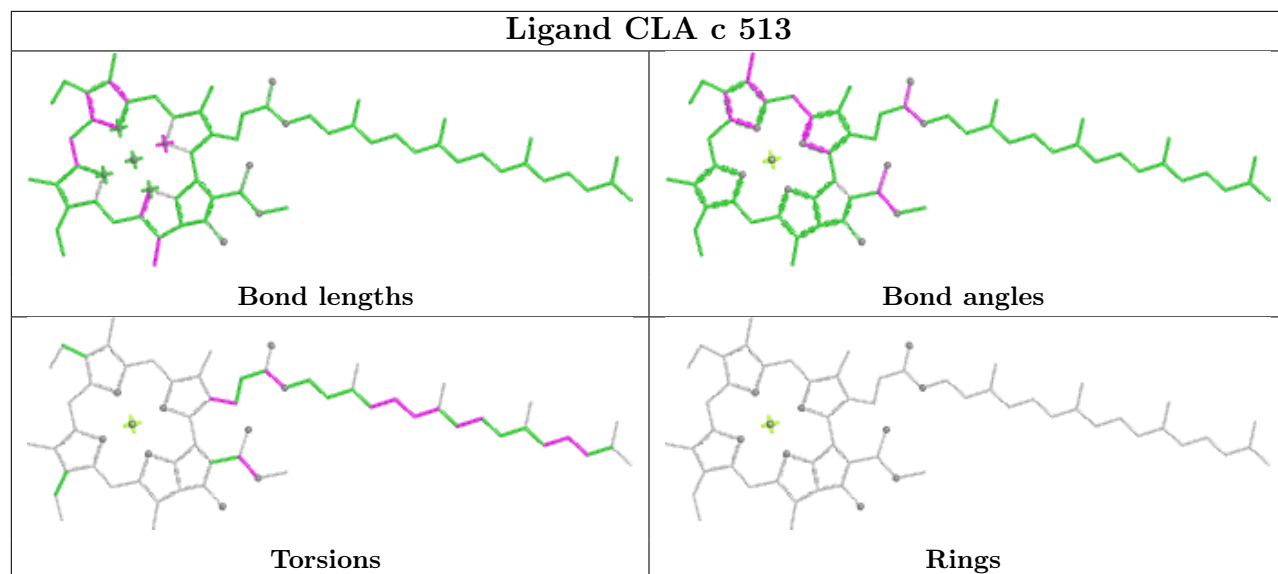
Ligand STE L 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

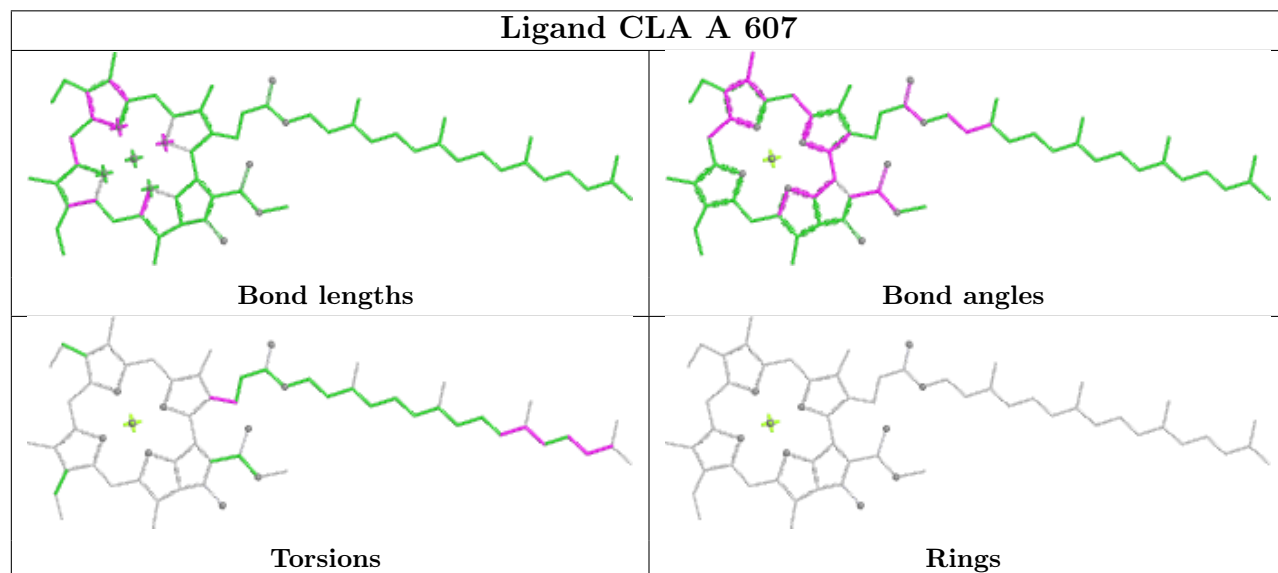
Ligand CLA B 615**Ligand SQD b 620**



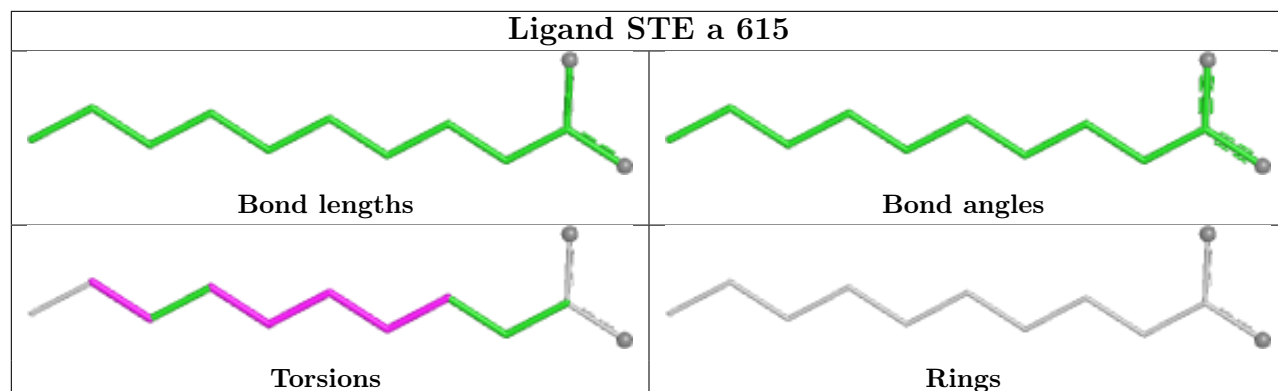
Ligand CLA c 513



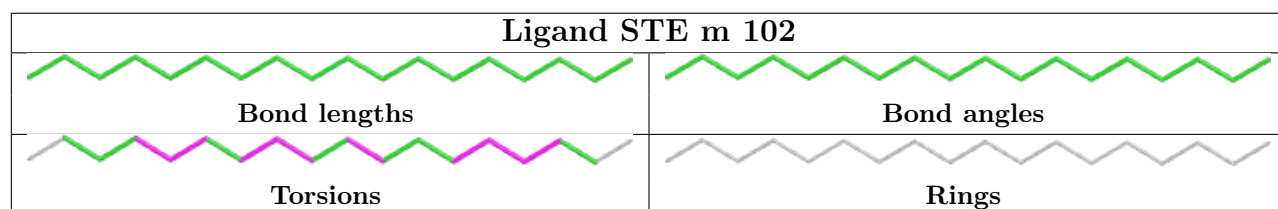
Ligand CLA A 607

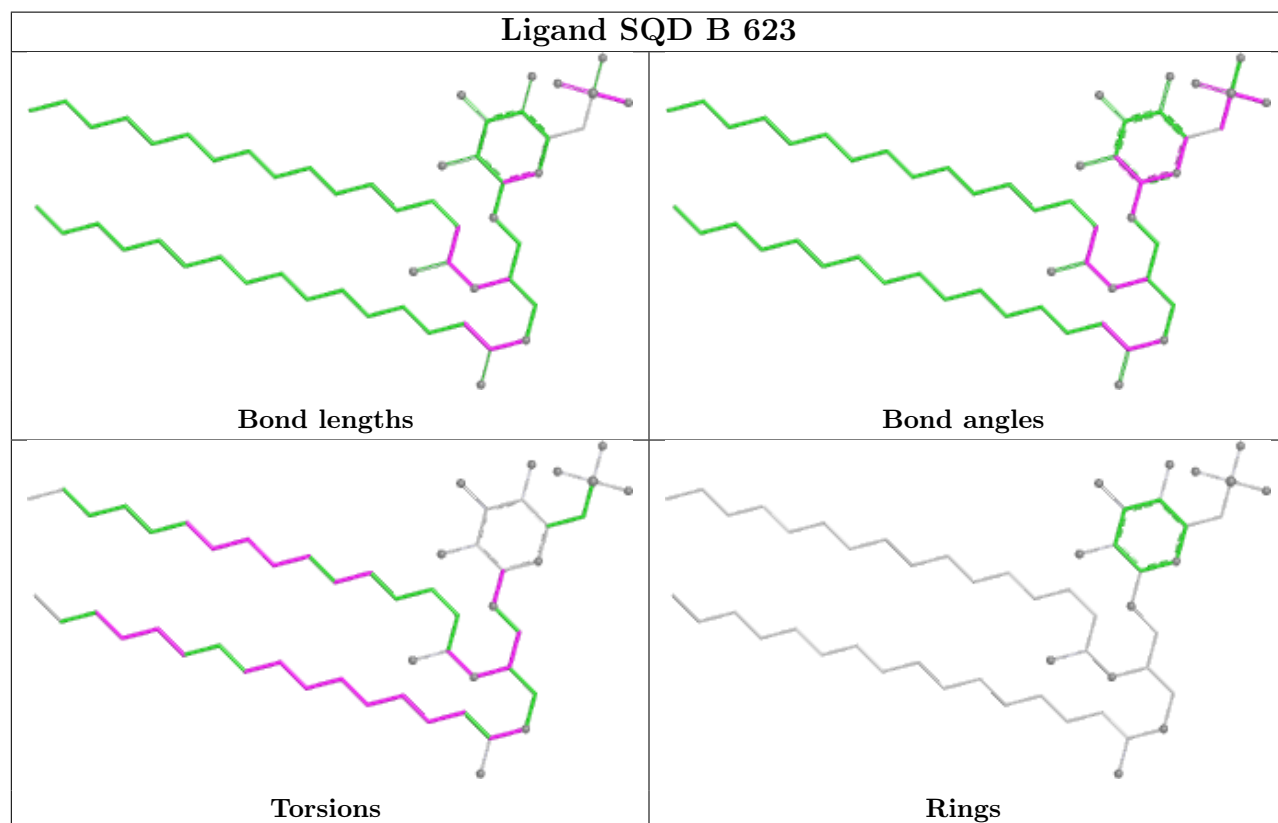
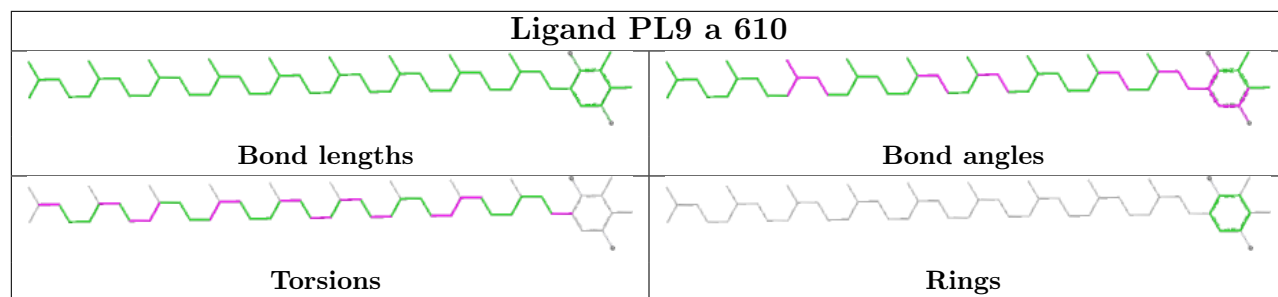


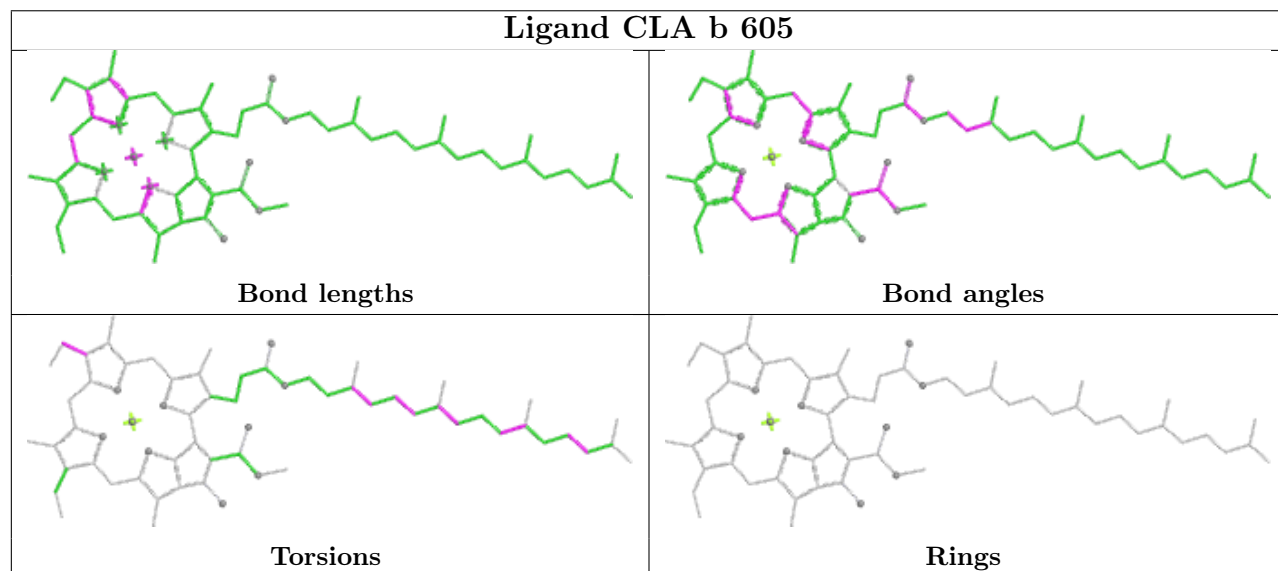
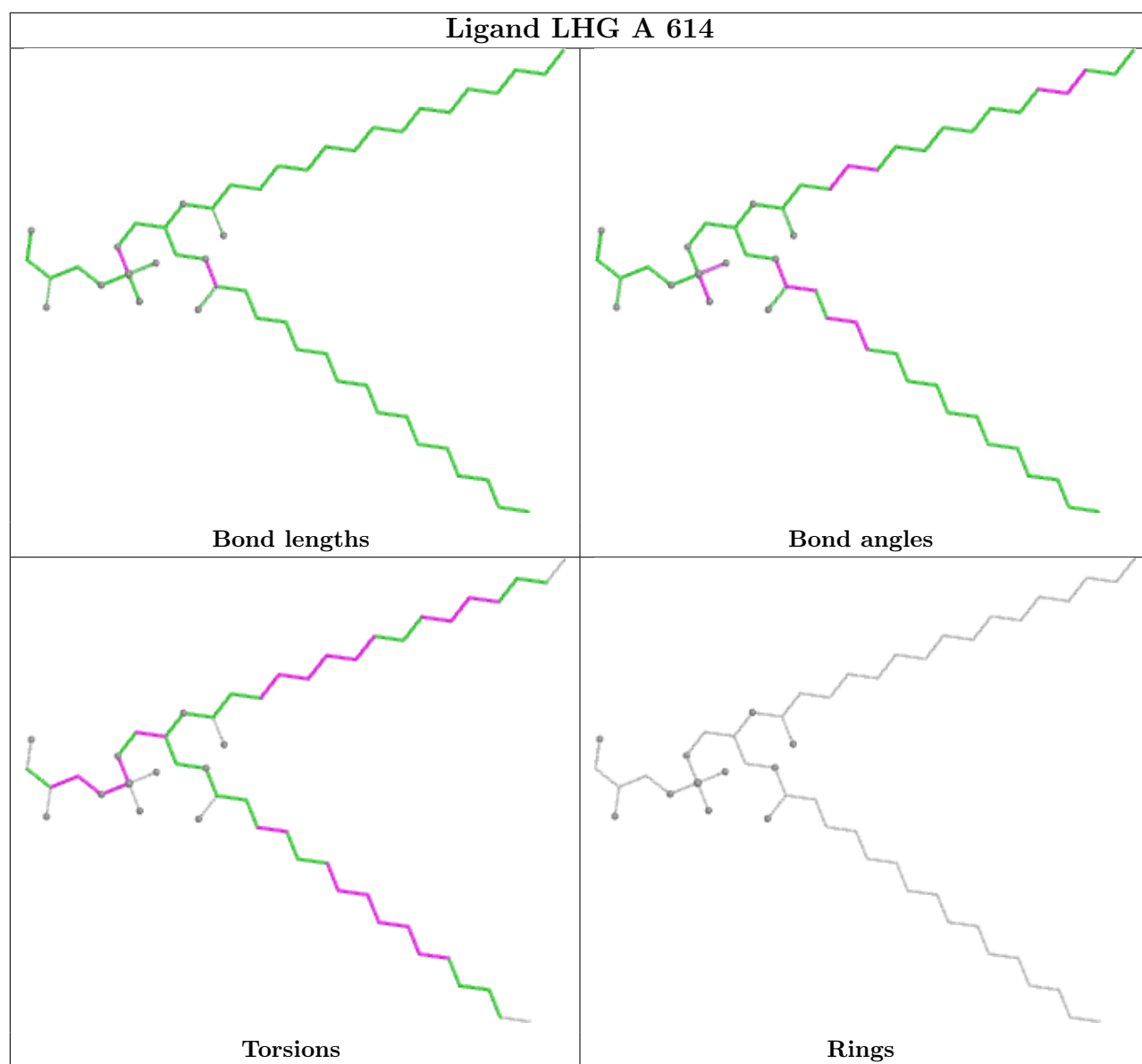
Ligand STE a 615



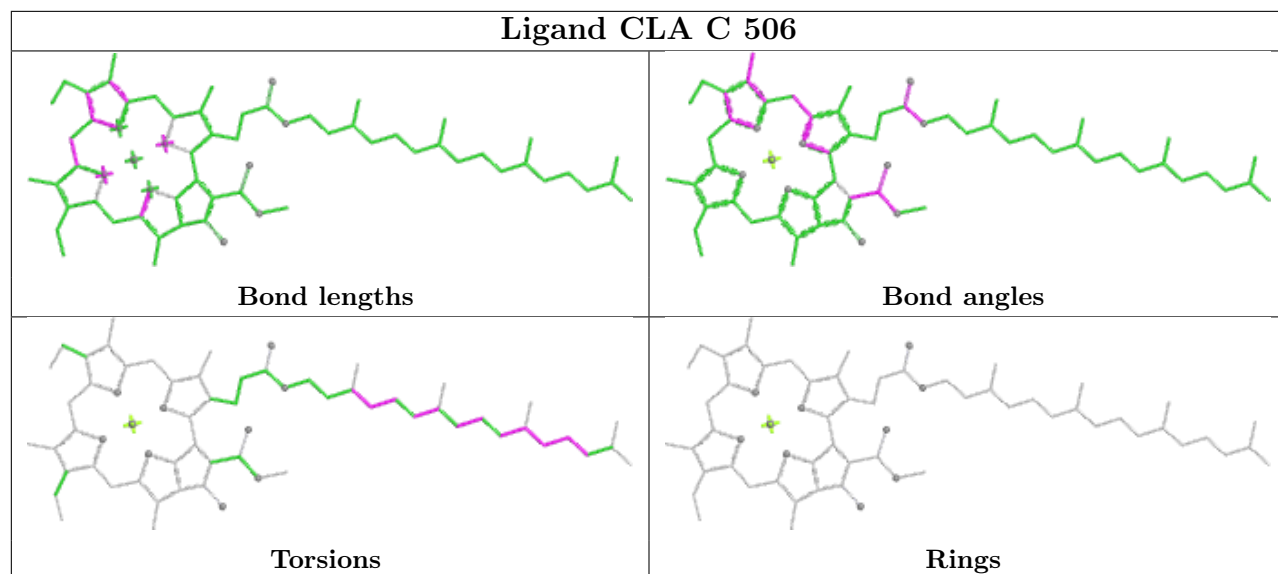
Ligand STE m 102



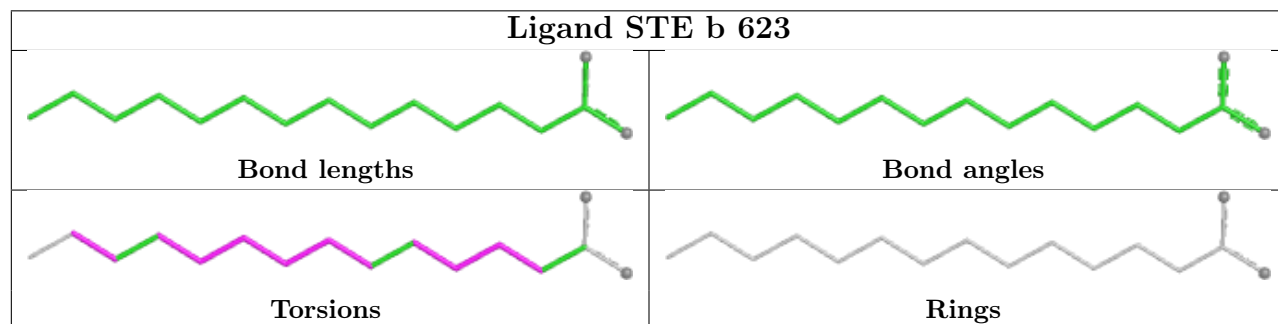




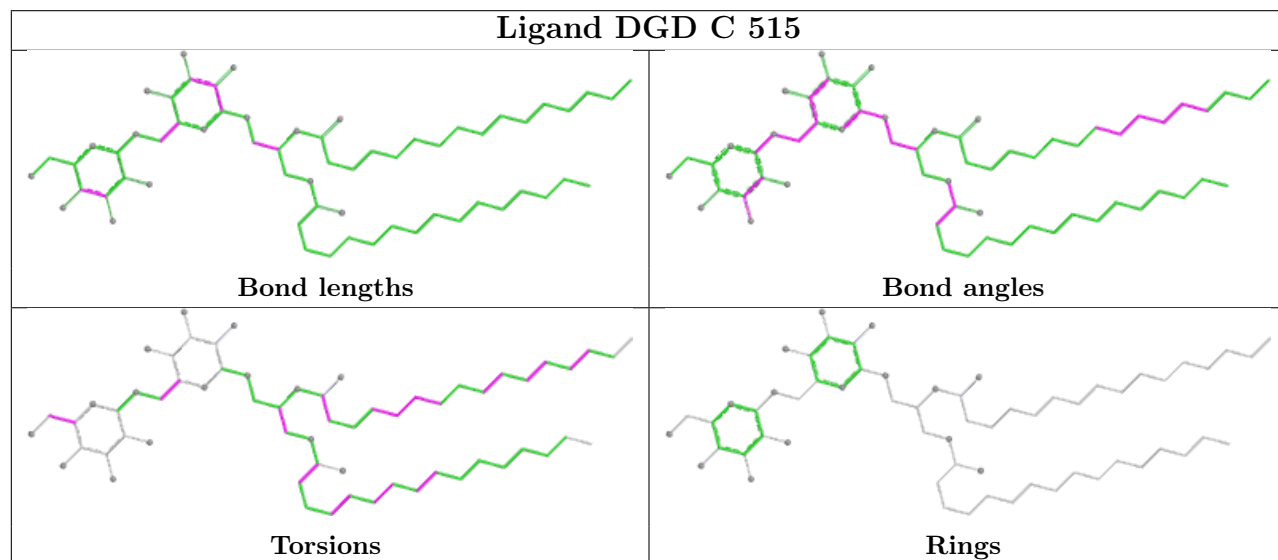
Ligand CLA C 506



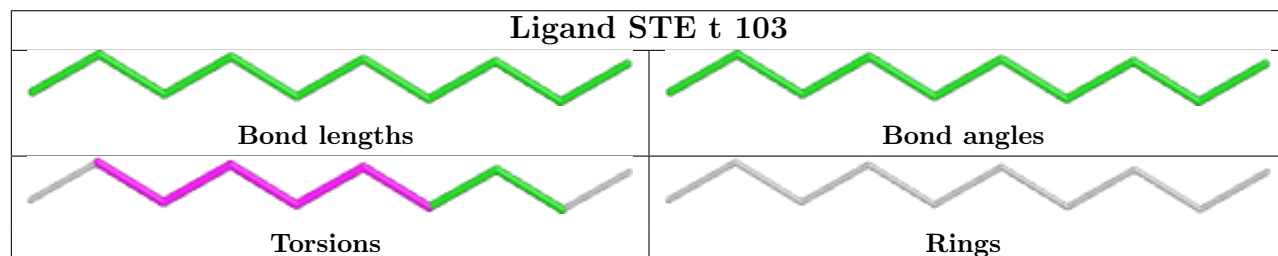
Ligand STE b 623

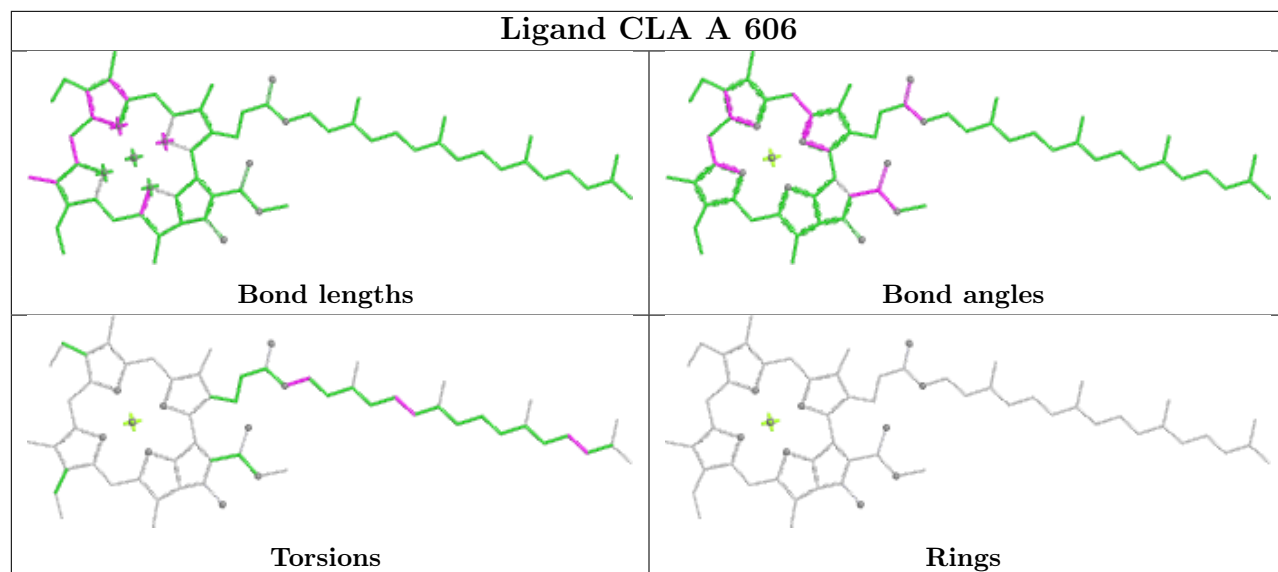
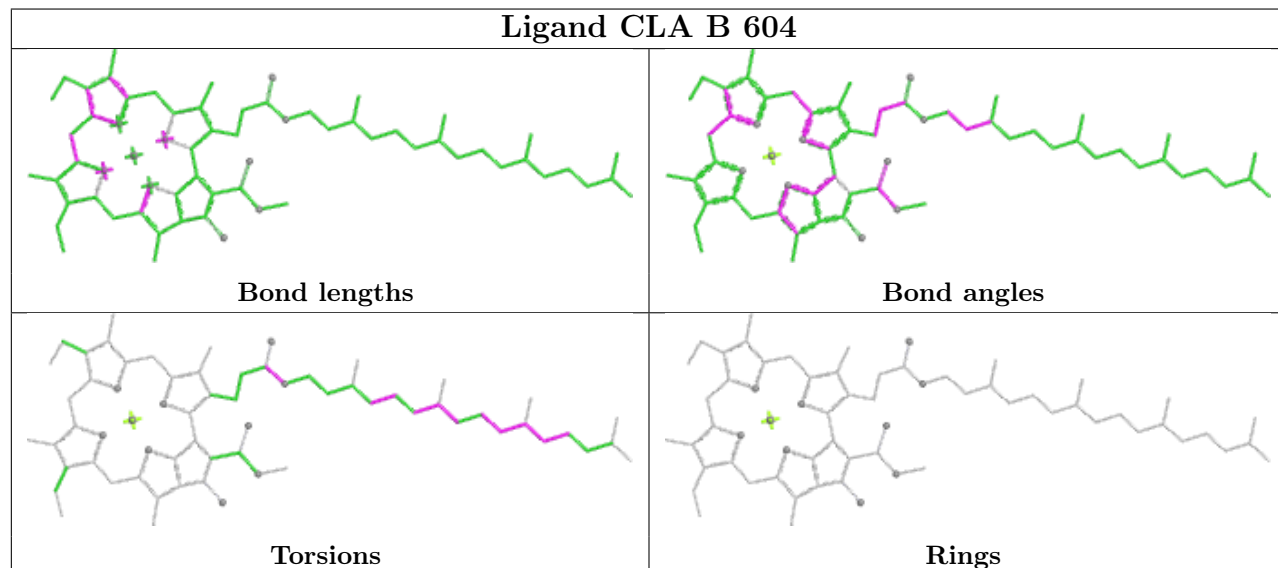
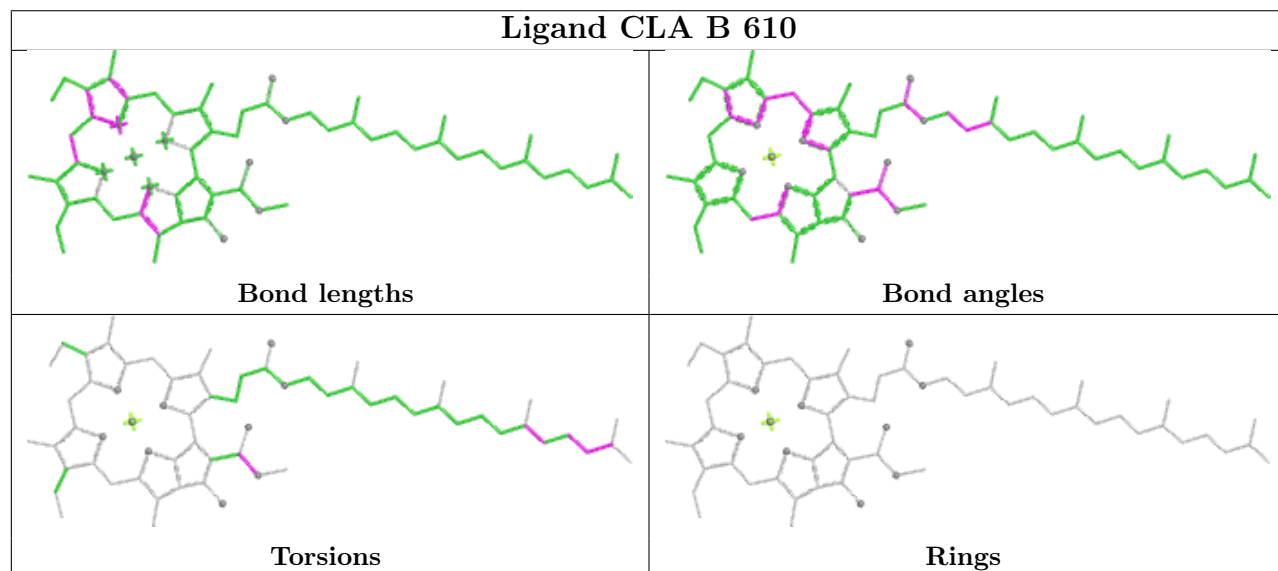


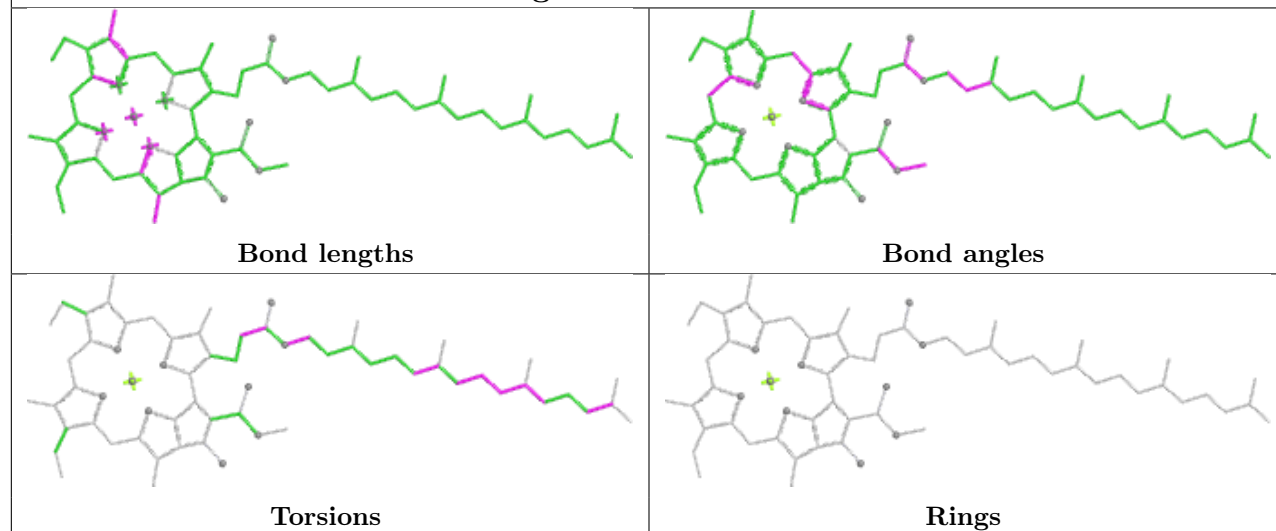
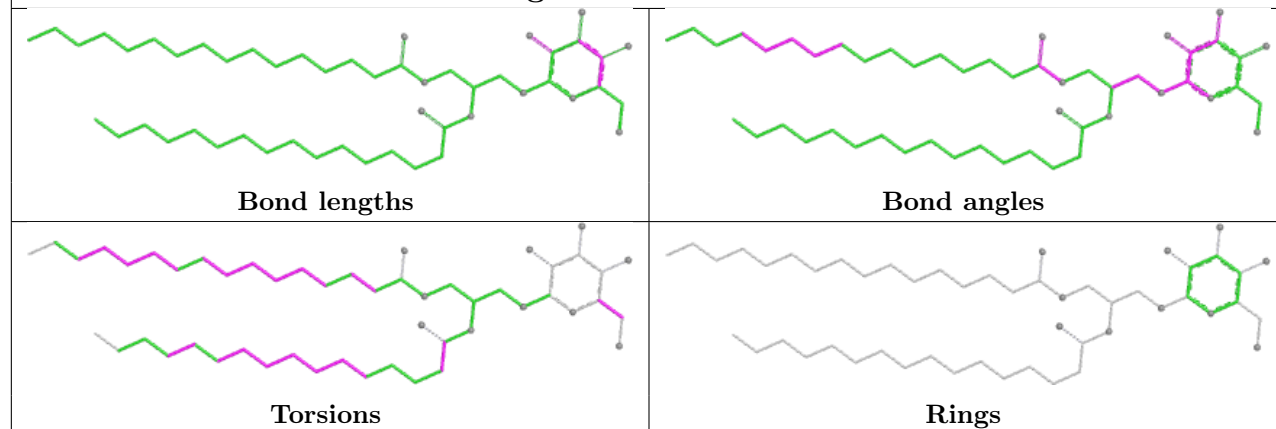
Ligand DGD C 515



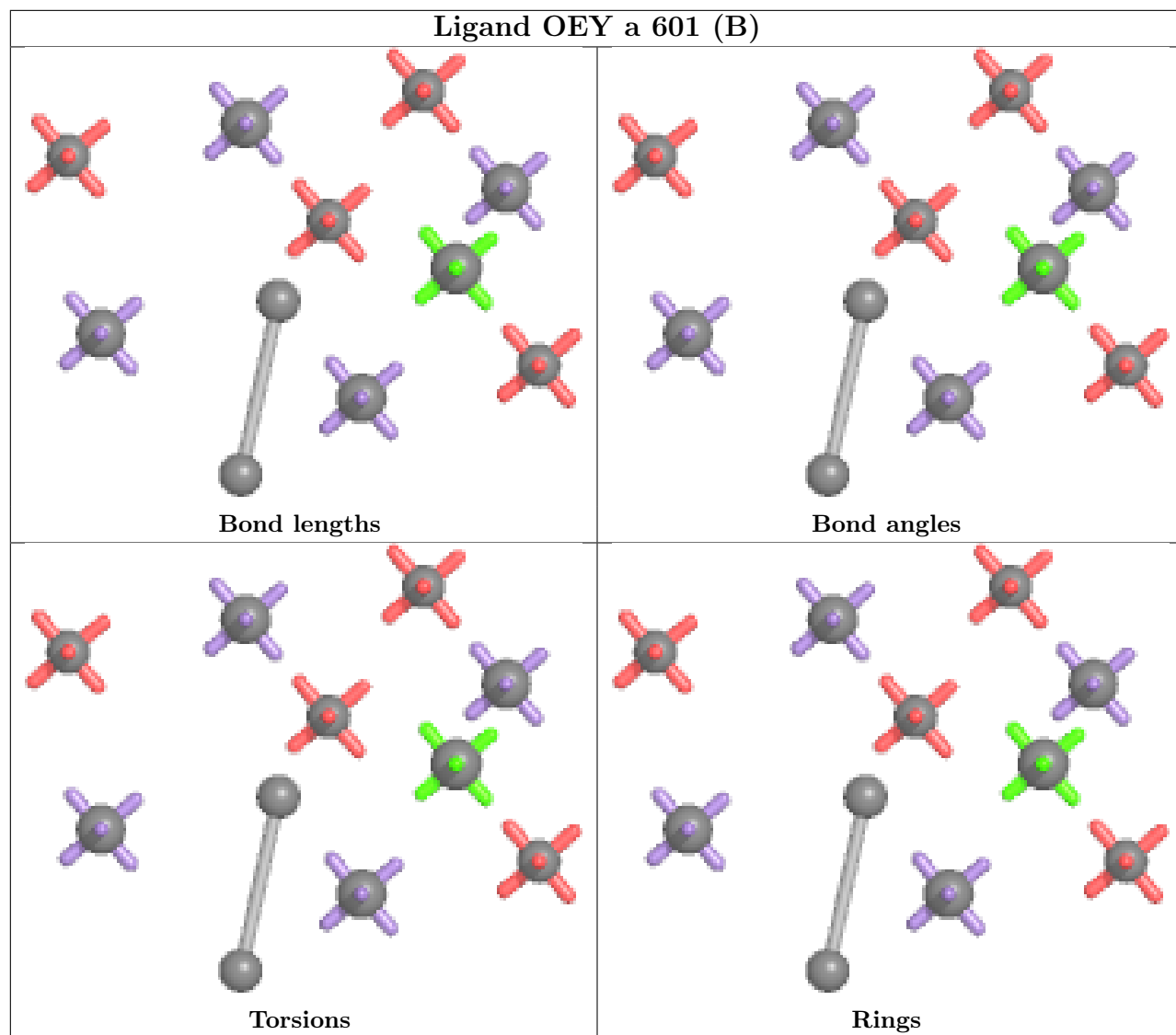
Ligand STE t 103



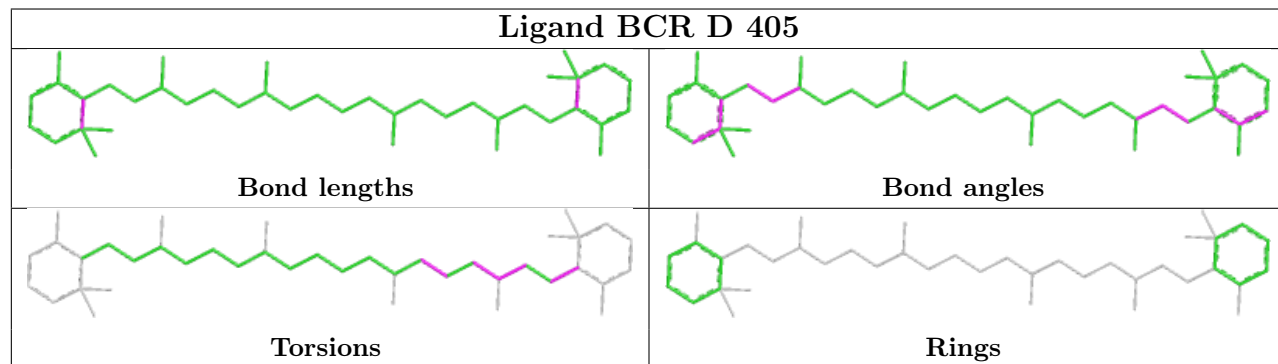
Ligand CLA A 606**Ligand CLA B 604****Ligand CLA B 610**

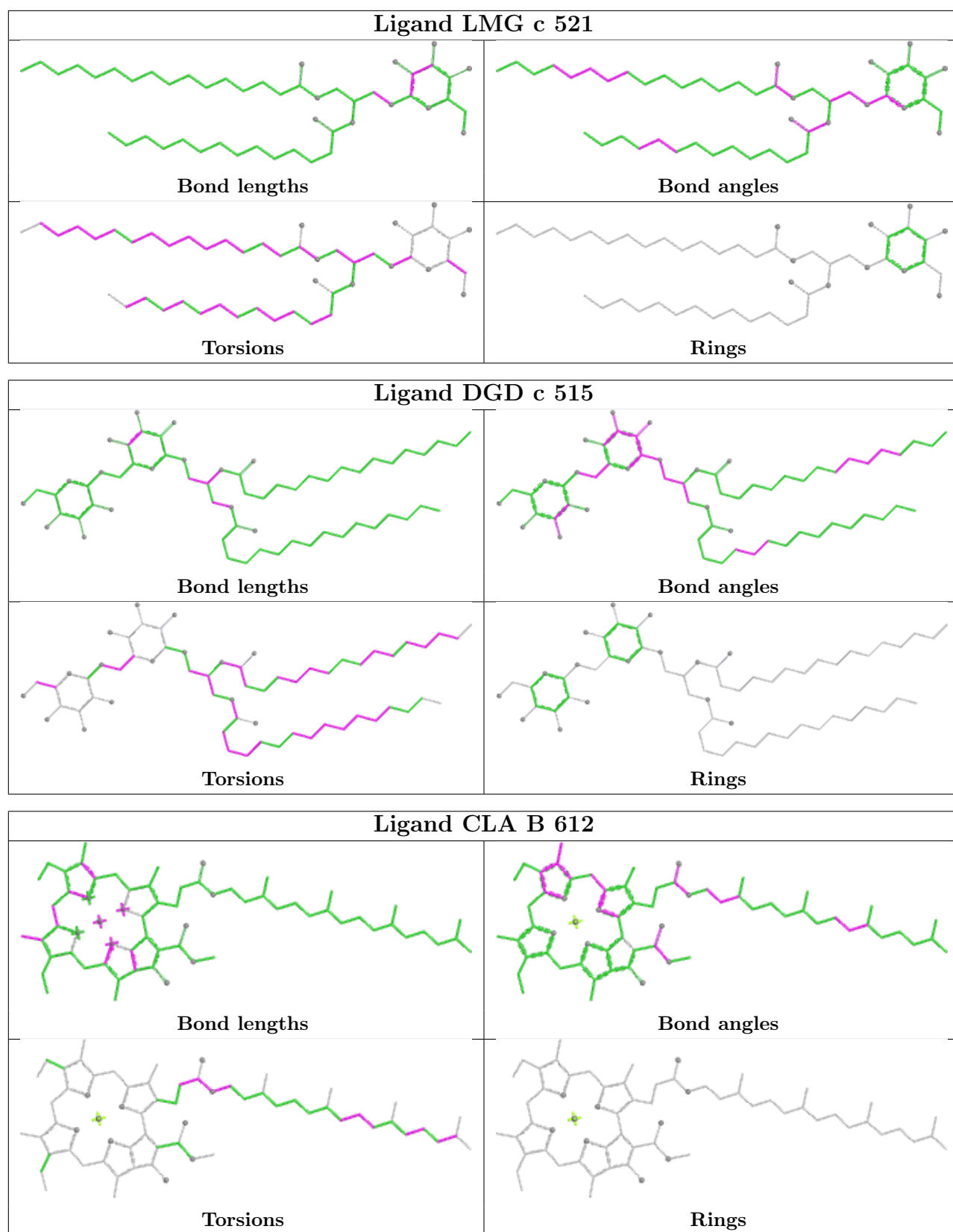
Ligand CLA B 613**Ligand LMG D 407**

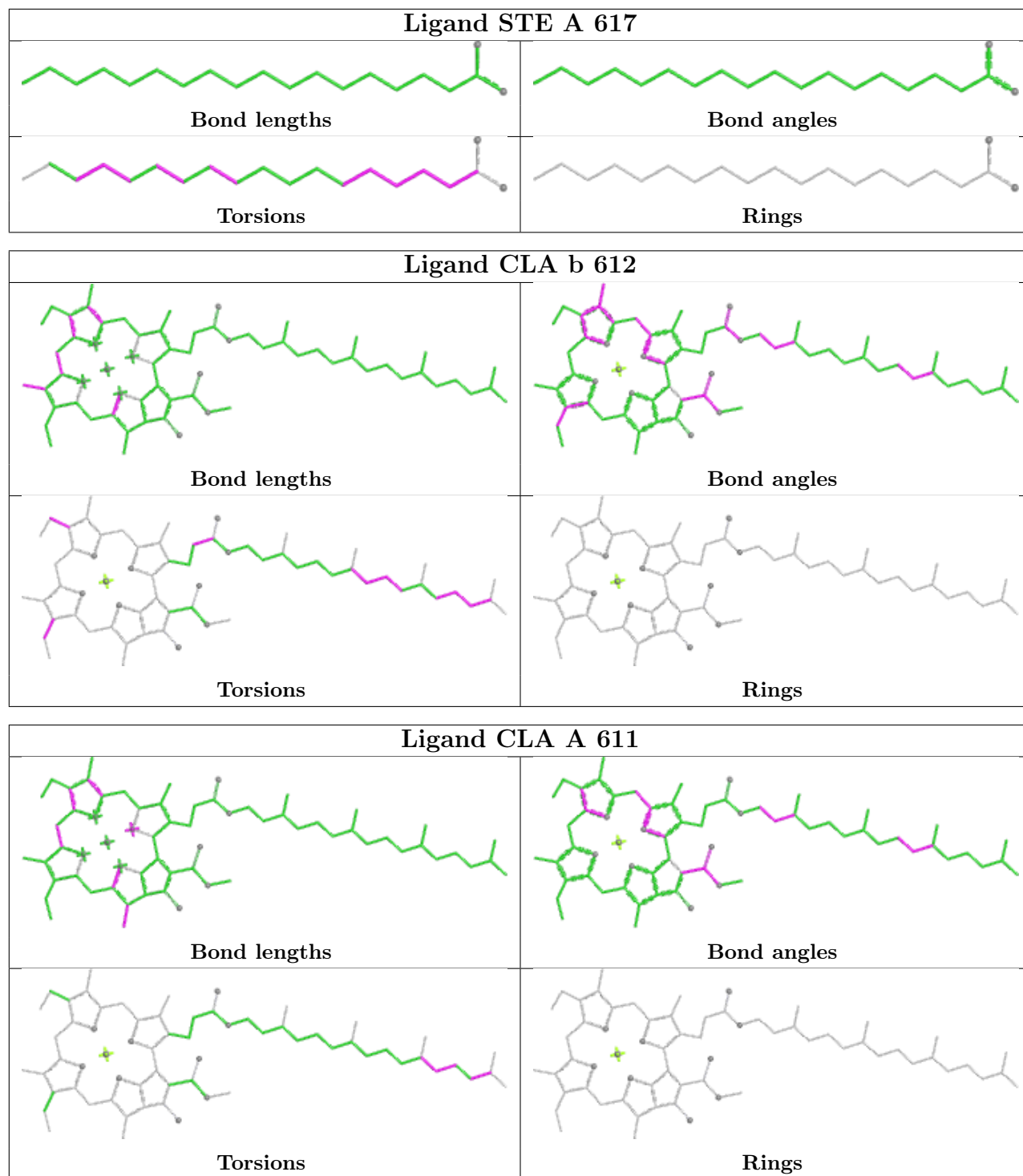
Ligand OEY a 601 (B)

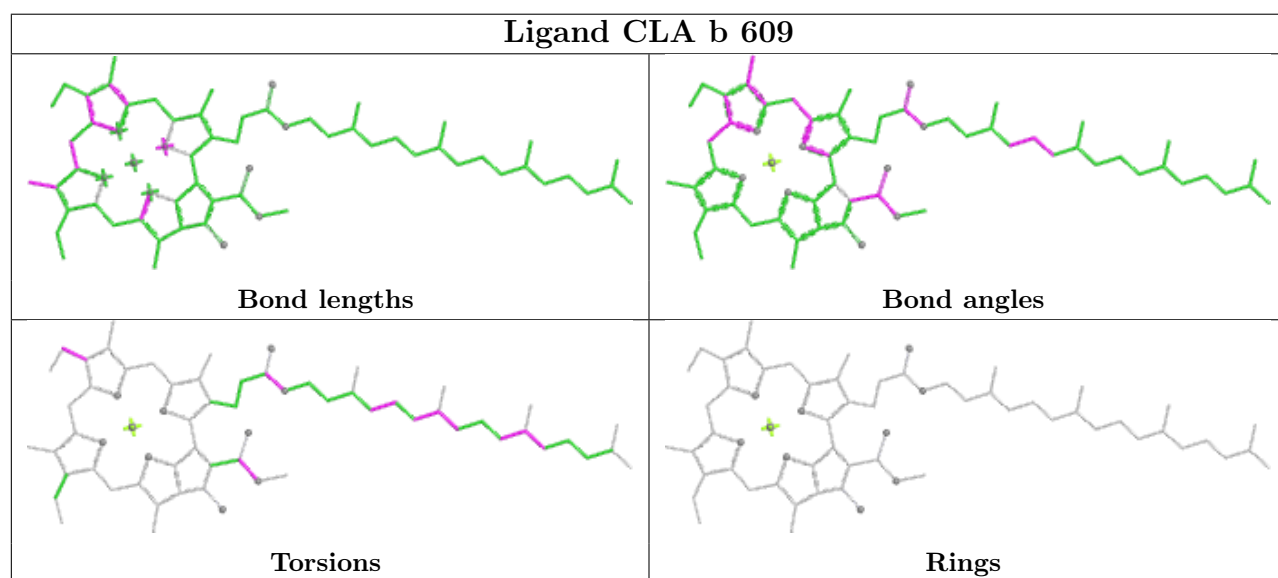
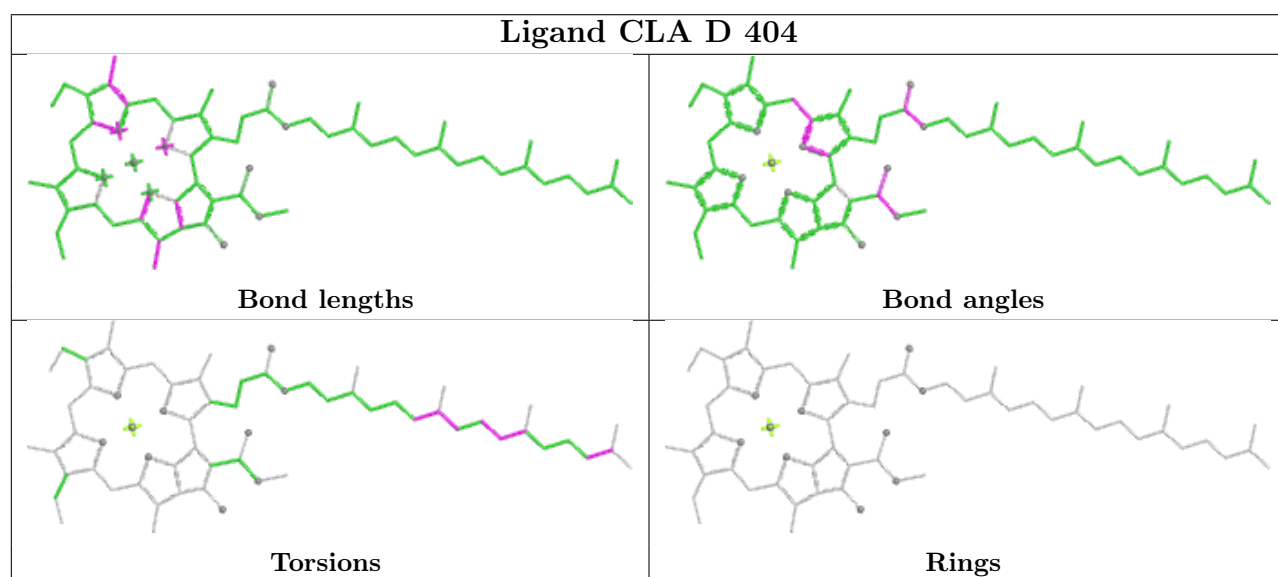
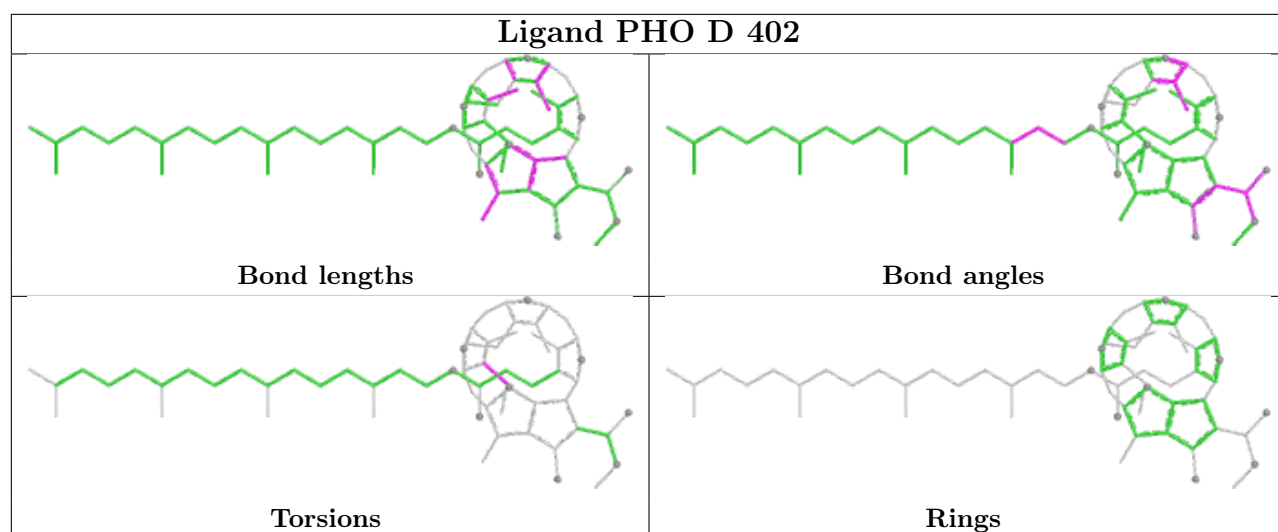


Ligand BCR D 405

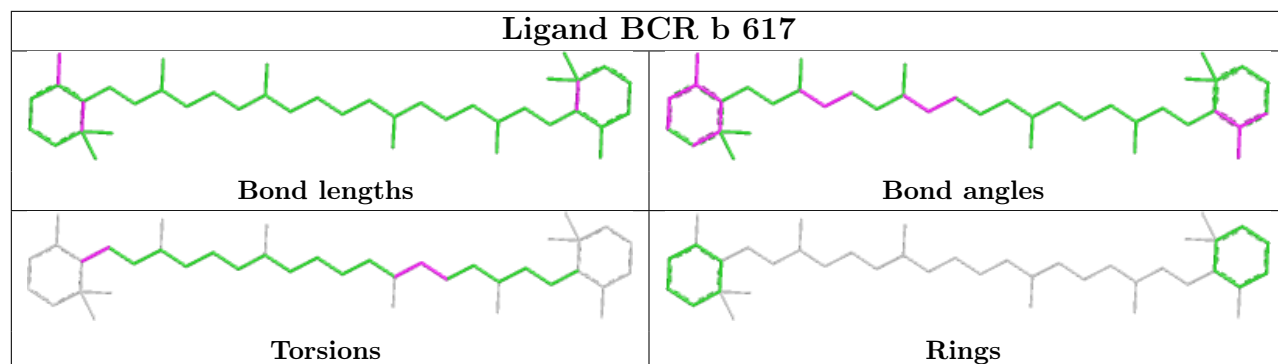




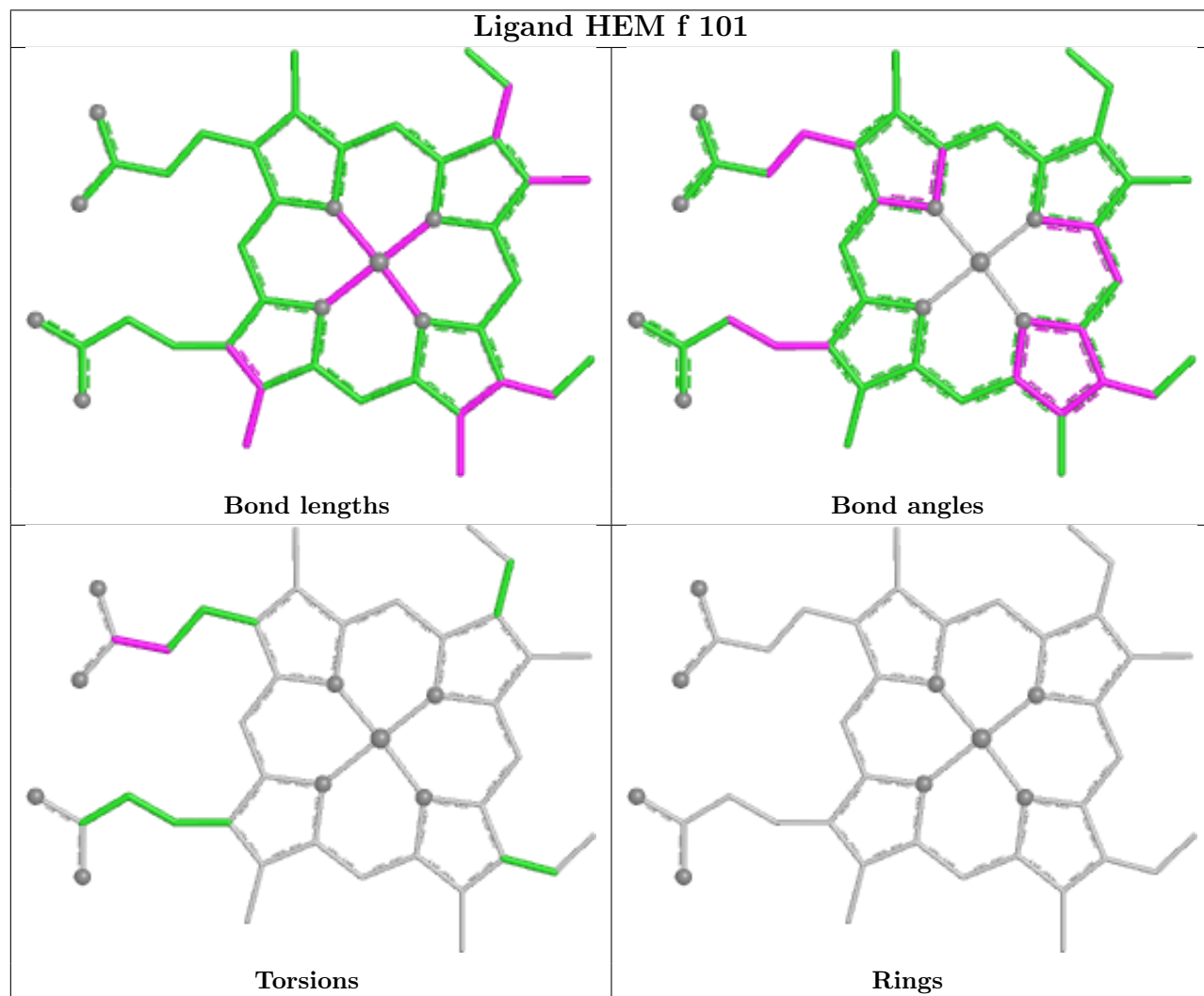


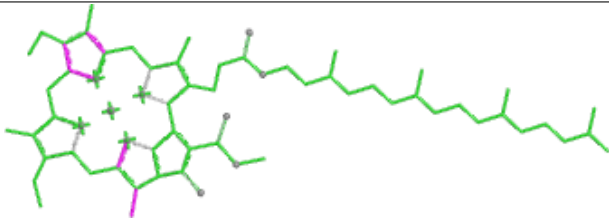
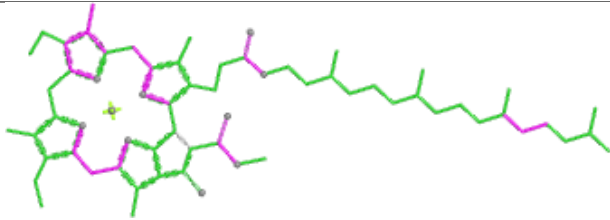
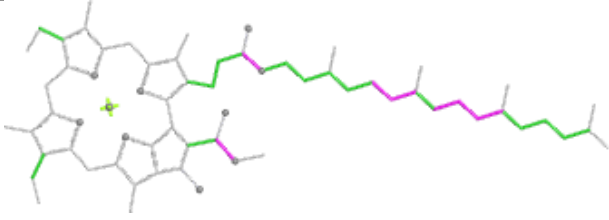
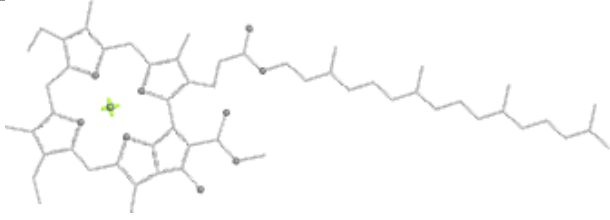


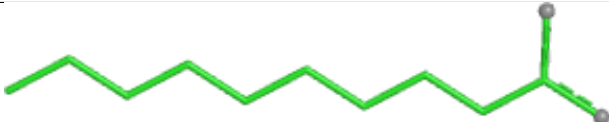
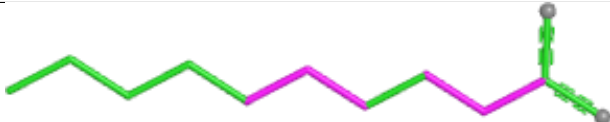
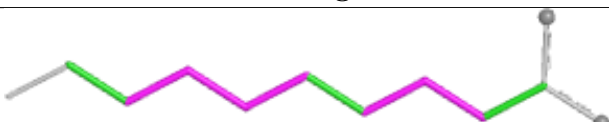
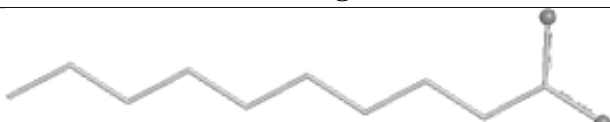
Ligand BCR b 617

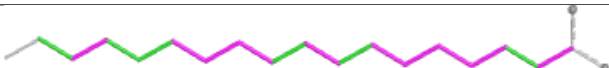
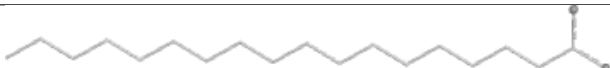


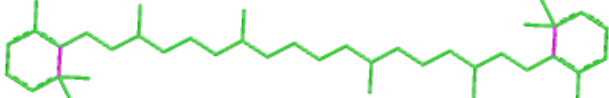
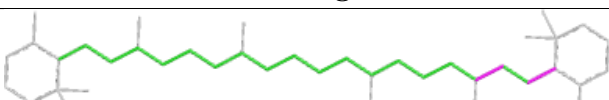
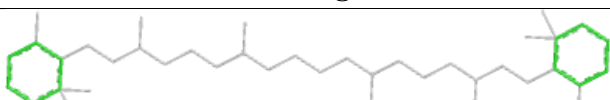
Ligand HEM f 101



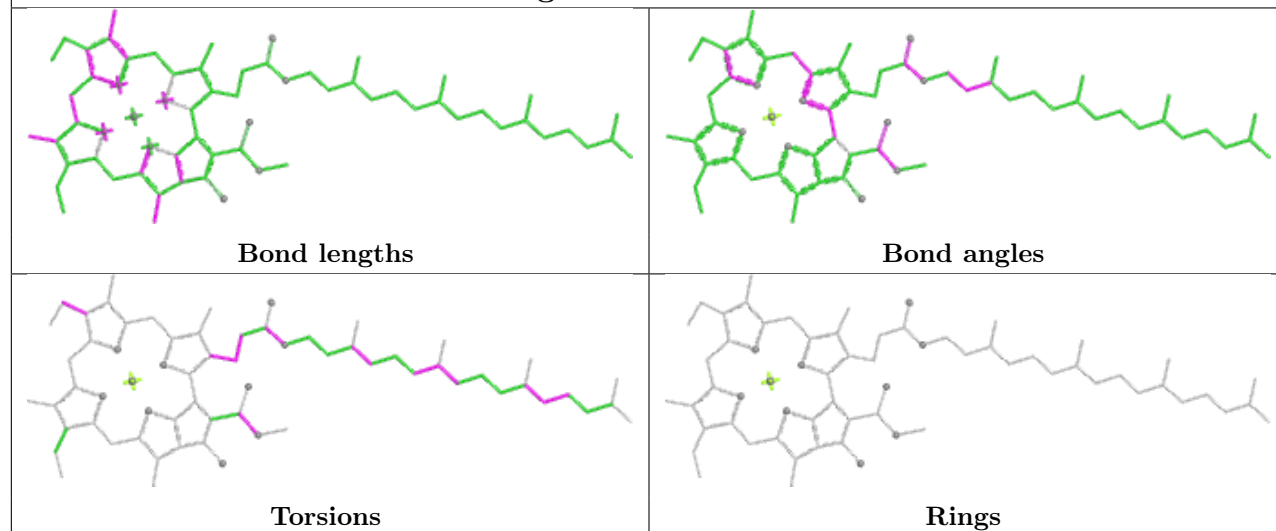
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

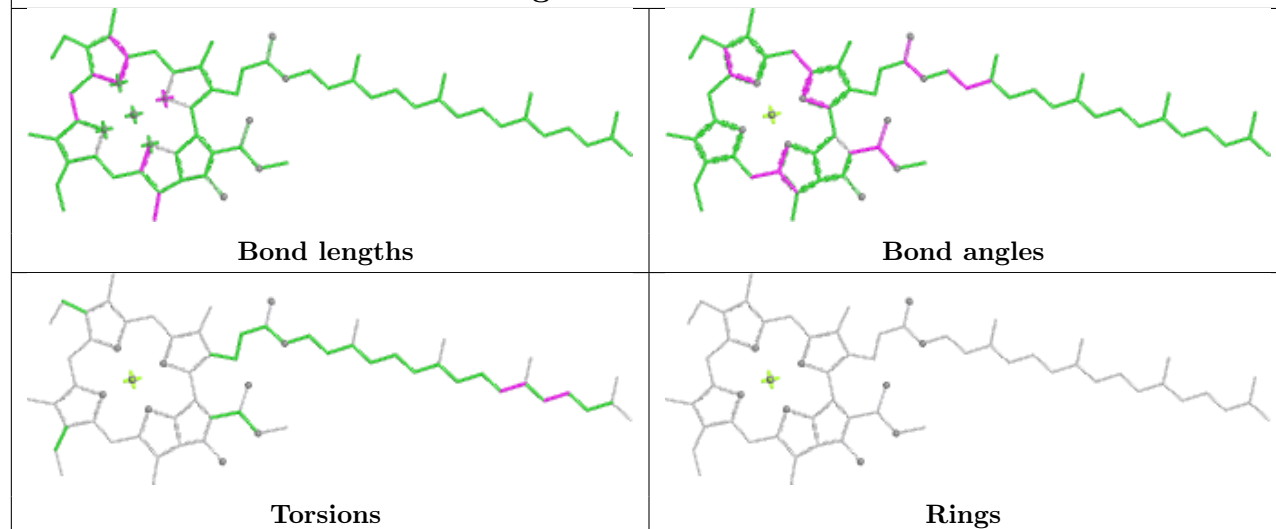
Ligand STE b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

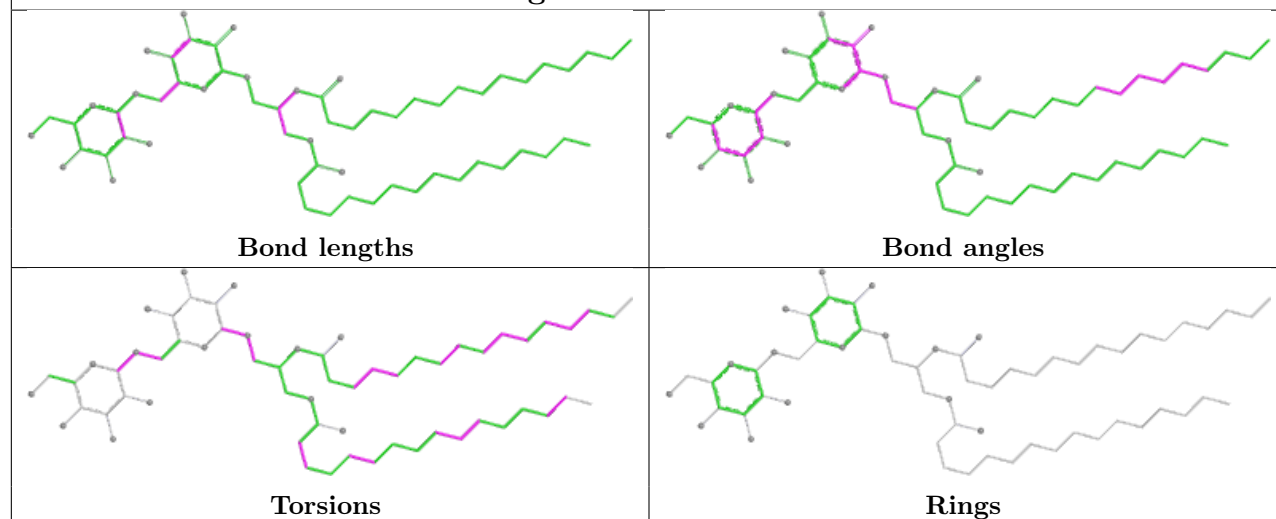
Ligand CLA c 512



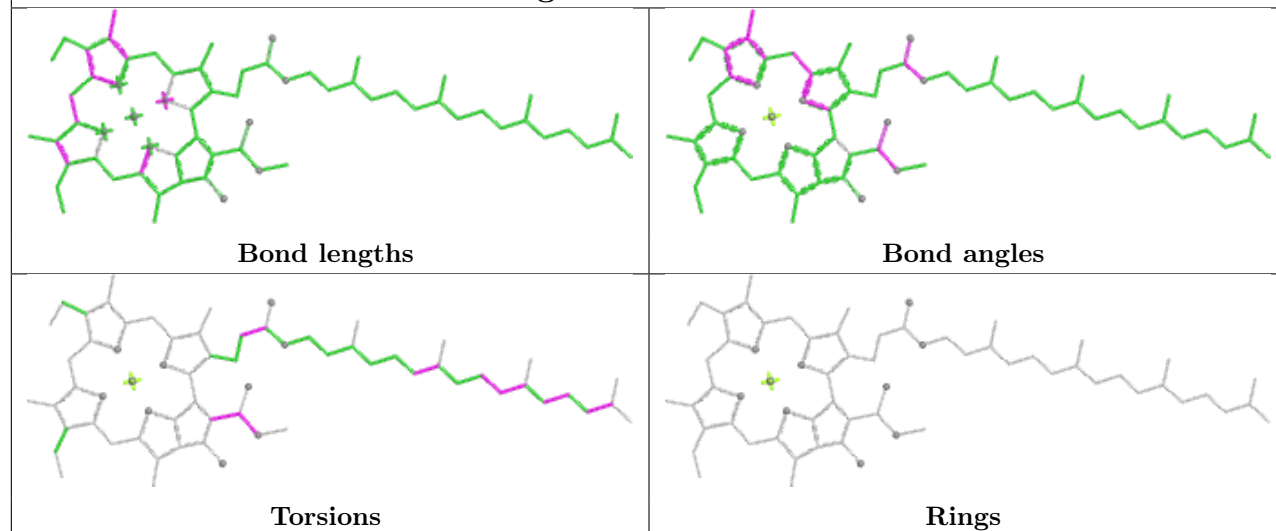
Ligand CLA B 611



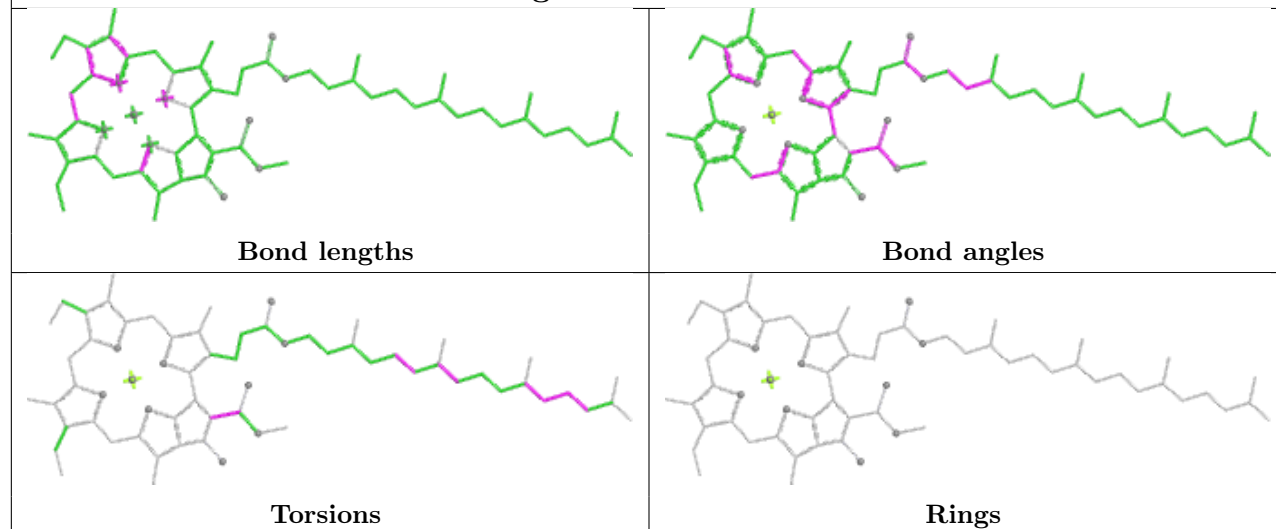
Ligand DGD C 516



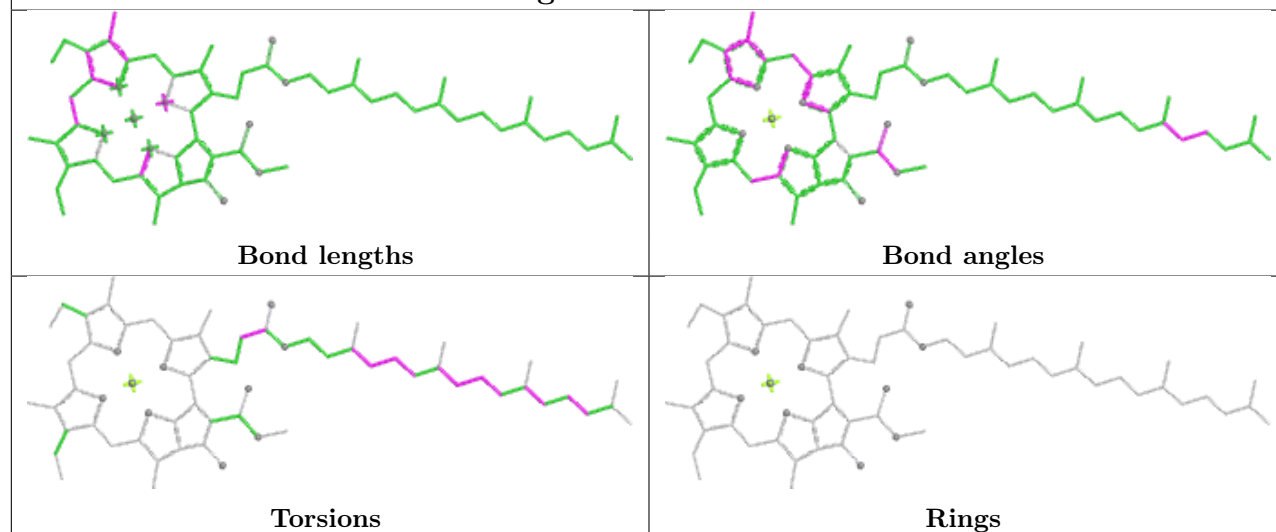
Ligand CLA c 509

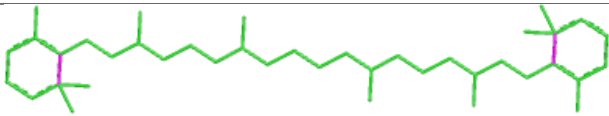
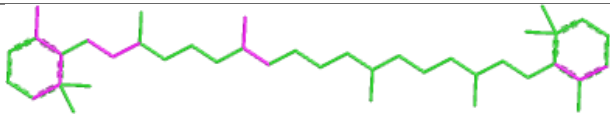
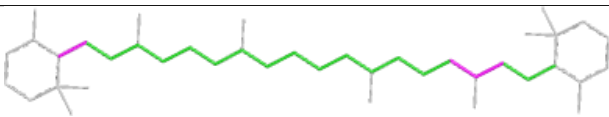
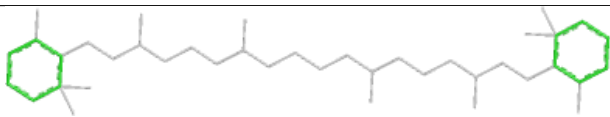


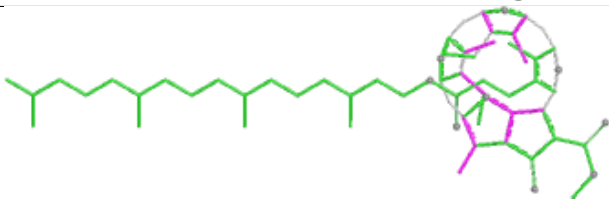
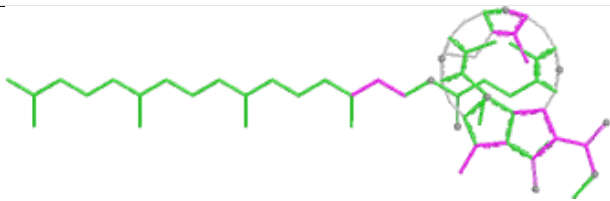
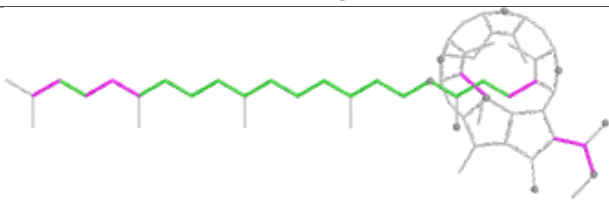
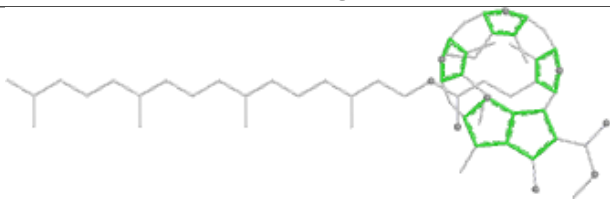
Ligand CLA C 507

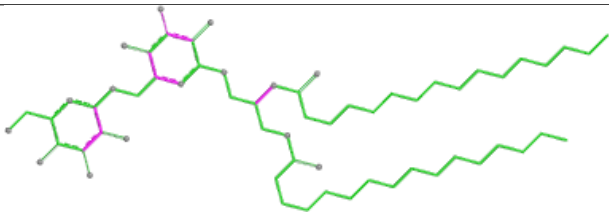
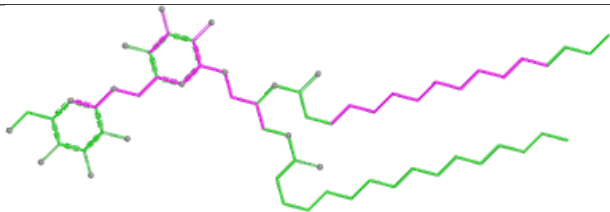
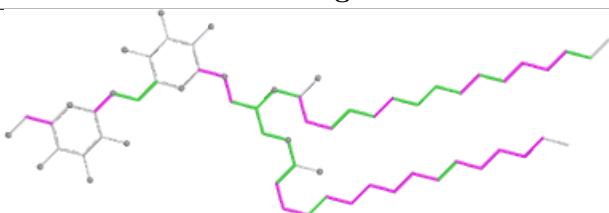
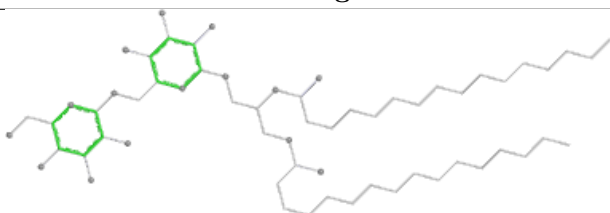


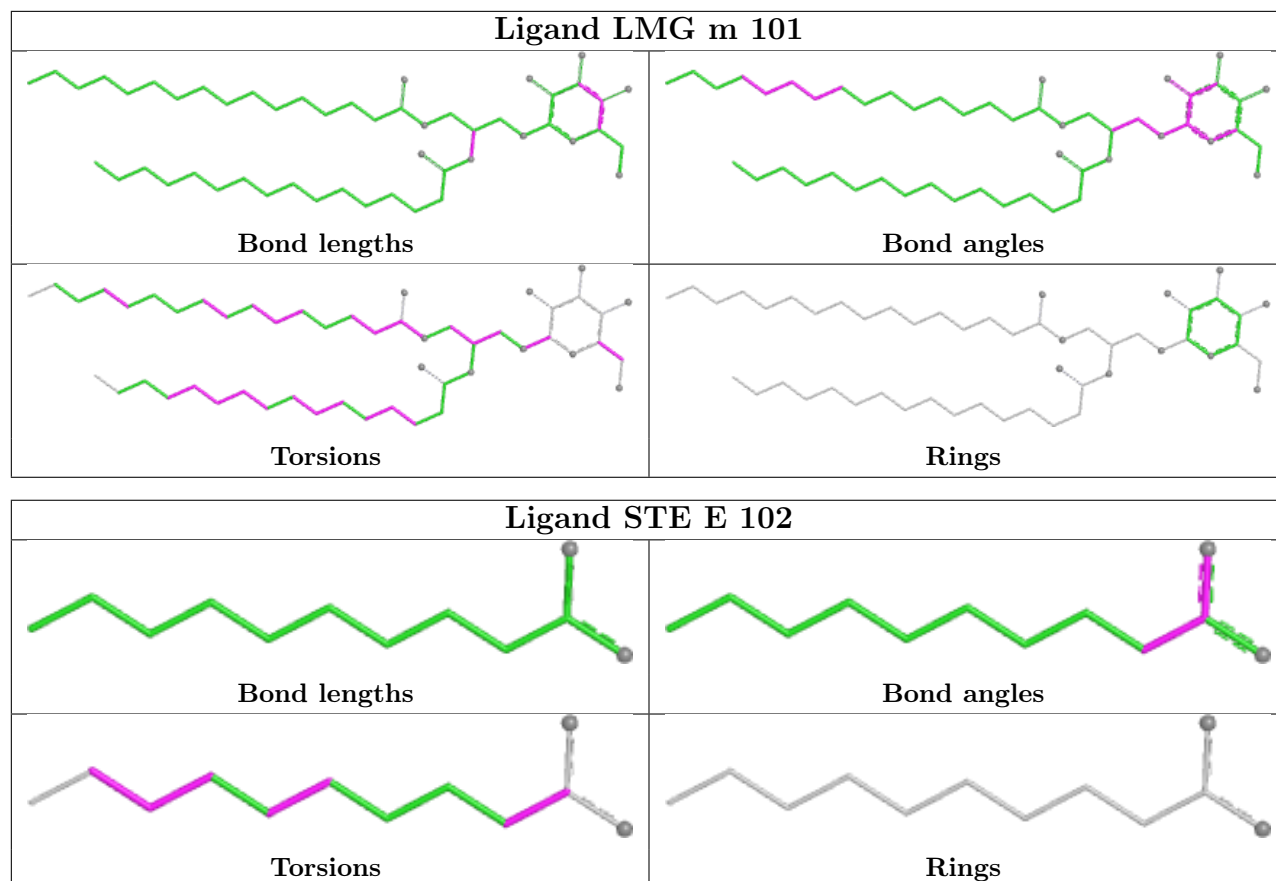
Ligand CLA c 510



Ligand BCR t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 516	
	
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%)	-0.33	2 (0%) 85 86	11, 28, 49, 77	64 (19%)
1	a	334/344 (97%)	-0.22	2 (0%) 85 86	11, 31, 57, 73	64 (19%)
2	B	505/510 (99%)	-0.21	4 (0%) 82 83	18, 32, 60, 86	4 (0%)
2	b	505/510 (99%)	-0.11	5 (0%) 79 80	26, 36, 69, 98	0
3	C	442/461 (95%)	-0.18	1 (0%) 91 91	13, 35, 50, 72	11 (2%)
3	c	451/461 (97%)	-0.03	1 (0%) 91 91	13, 40, 61, 86	12 (2%)
4	D	341/352 (96%)	-0.36	1 (0%) 90 90	14, 30, 47, 77	2 (0%)
4	d	341/352 (96%)	-0.21	1 (0%) 90 90	15, 34, 58, 75	3 (0%)
5	E	82/84 (97%)	0.43	1 (1%) 76 76	32, 50, 68, 82	1 (1%)
5	e	82/84 (97%)	0.70	2 (2%) 59 60	42, 61, 76, 84	0
6	F	34/45 (75%)	0.06	0 100 100	35, 42, 61, 80	0
6	f	34/45 (75%)	0.48	2 (5%) 28 27	43, 50, 77, 96	0
7	H	65/66 (98%)	0.05	1 (1%) 72 72	32, 41, 53, 68	0
7	h	63/66 (95%)	0.34	1 (1%) 70 70	40, 52, 60, 65	0
8	I	35/38 (92%)	-0.01	0 100 100	31, 38, 60, 73	0
8	i	35/38 (92%)	-0.02	0 100 100	30, 40, 64, 78	0
9	J	36/40 (90%)	0.38	1 (2%) 55 54	34, 49, 72, 83	0
9	j	36/40 (90%)	0.54	3 (8%) 17 16	39, 55, 88, 88	0
10	K	37/46 (80%)	0.20	0 100 100	41, 51, 65, 70	0
10	k	37/46 (80%)	0.43	0 100 100	49, 57, 75, 84	0
11	L	37/37 (100%)	-0.33	0 100 100	25, 29, 58, 66	0
11	l	36/37 (97%)	-0.41	0 100 100	27, 30, 58, 73	0
12	M	32/36 (88%)	-0.25	0 100 100	26, 33, 56, 69	0
12	m	31/36 (86%)	-0.28	0 100 100	29, 33, 52, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.03	2 (0%) 82 83	26, 41, 74, 127	1 (0%)
13	o	244/272 (89%)	0.03	3 (1%) 76 76	26, 40, 73, 103	0
14	T	29/32 (90%)	-0.40	1 (3%) 48 47	26, 31, 52, 67	0
14	t	29/32 (90%)	-0.31	0 100 100	26, 32, 65, 78	0
15	U	97/134 (72%)	0.02	0 100 100	33, 42, 69, 83	0
15	u	97/134 (72%)	-0.02	1 (1%) 79 80	30, 40, 54, 78	0
16	V	137/163 (84%)	-0.11	1 (0%) 84 84	29, 40, 53, 69	0
16	v	137/163 (84%)	0.13	0 100 100	34, 47, 69, 90	0
17	Y	27/46 (58%)	1.00	3 (11%) 10 9	51, 72, 91, 99	0
17	y	30/46 (65%)	0.91	0 100 100	64, 74, 87, 93	0
18	X	38/41 (92%)	0.31	2 (5%) 32 31	41, 51, 74, 75	0
18	x	39/41 (95%)	0.56	1 (2%) 57 57	50, 60, 82, 95	0
19	Z	62/62 (100%)	0.87	5 (8%) 18 17	51, 64, 102, 110	0
19	z	62/62 (100%)	1.04	6 (9%) 13 12	62, 74, 108, 118	0
20	R	34/41 (82%)	0.90	2 (5%) 28 27	56, 67, 76, 80	0
20	r	31/41 (75%)	1.20	4 (12%) 7 6	65, 78, 95, 98	0
All	All	5302/5700 (93%)	-0.04	59 (1%) 78 78	11, 38, 72, 127	162 (3%)

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	4.1
19	Z	33	TRP	4.0
20	R	35	LEU	3.7
13	o	58	ASN	3.4
2	B	488	PRO	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
14	FME	t	1	10/11	0.89	0.10	32,34,49,55	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	0.92	0.09	39,45,59,60	0
14	FME	T	1	10/11	0.95	0.09	28,32,52,66	0
8	FME	i	1	10/11	0.95	0.07	36,44,49,52	0
12	FME	m	1	10/11	0.95	0.08	34,47,55,64	0
8	FME	I	1	10/11	0.95	0.08	38,43,50,50	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
30	LHG	A	614	49/49	0.72	0.17	50,74,90,93	0
32	STE	H	103	18/20	0.72	0.17	48,62,67,71	0
32	STE	k	104	12/20	0.74	0.14	61,66,72,82	0
32	STE	L	102	12/20	0.76	0.19	50,55,63,64	0
27	PL9	A	610	55/55	0.77	0.16	35,58,68,70	0
28	LMG	c	520	48/55	0.77	0.15	45,66,74,78	0
32	STE	a	615	12/20	0.78	0.14	52,57,68,69	0
28	LMG	d	410	23/55	0.79	0.18	48,57,66,67	0
28	LMG	b	622	55/55	0.79	0.16	46,59,69,72	0
32	STE	d	412	17/20	0.79	0.15	46,51,67,67	0
25	CLA	b	601	65/65	0.79	0.14	47,66,83,86	0
32	STE	b	621	20/20	0.80	0.13	40,48,67,73	0
32	STE	b	625	10/20	0.80	0.18	44,53,65,68	0
31	DGD	a	614	44/66	0.80	0.14	37,49,60,70	0
29	SQD	a	613	36/54	0.80	0.14	41,53,65,70	0
32	STE	b	624	15/20	0.81	0.16	45,48,60,69	0
28	LMG	D	411	33/55	0.81	0.14	37,53,72,74	0
32	STE	B	625	18/20	0.82	0.16	39,52,69,76	0
32	STE	b	623	16/20	0.82	0.15	48,59,75,76	0
28	LMG	c	518	37/55	0.82	0.12	49,62,78,80	0
32	STE	B	621	17/20	0.83	0.13	36,47,63,65	0
32	STE	B	624	12/20	0.83	0.15	40,51,59,60	0
31	DGD	A	616	66/66	0.83	0.12	42,54,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	B	626	12/20	0.83	0.14	47,54,63,63	0
32	STE	D	413	20/20	0.83	0.13	37,45,67,73	0
32	STE	c	519	20/20	0.83	0.14	41,49,76,82	0
27	PL9	a	610	55/55	0.83	0.15	42,61,72,74	0
32	STE	A	617	20/20	0.83	0.12	41,50,64,64	0
32	STE	B	627	16/20	0.84	0.14	42,49,60,61	0
32	STE	d	413	20/20	0.84	0.12	42,50,63,64	0
28	LMG	A	612	48/55	0.84	0.11	37,50,62,73	0
32	STE	C	518	12/20	0.85	0.13	36,44,54,57	0
32	STE	C	519	12/20	0.85	0.12	46,54,59,62	0
28	LMG	B	622	28/55	0.85	0.13	38,45,55,60	0
32	STE	E	102	12/20	0.85	0.13	51,63,72,74	0
32	STE	j	101	12/20	0.85	0.12	47,53,58,58	0
30	LHG	e	101	42/49	0.85	0.12	58,74,88,99	0
29	SQD	b	620	49/54	0.86	0.11	38,50,70,73	0
29	SQD	f	102	41/54	0.86	0.13	55,72,85,88	0
28	LMG	c	521	49/55	0.86	0.11	37,50,74,82	0
26	BCR	d	405	40/40	0.86	0.11	39,49,75,79	0
28	LMG	m	101	51/55	0.86	0.11	33,47,59,61	0
29	SQD	A	615	39/54	0.86	0.13	36,51,71,75	0
28	LMG	C	517	48/55	0.86	0.12	44,61,67,69	0
32	STE	t	102	14/20	0.86	0.11	37,43,50,53	0
32	STE	t	103	10/20	0.86	0.11	46,54,55,57	0
28	LMG	B	620	51/55	0.87	0.11	31,46,58,63	0
26	BCR	k	102	40/40	0.87	0.12	51,61,68,73	0
26	BCR	h	101	40/40	0.87	0.12	40,53,63,65	0
32	STE	T	102	16/20	0.87	0.13	39,47,55,57	0
26	BCR	k	101	40/40	0.88	0.11	45,56,63,66	0
32	STE	I	101	15/20	0.89	0.13	46,50,59,60	0
32	STE	J	102	12/20	0.89	0.11	48,53,60,61	0
25	CLA	B	601	65/65	0.89	0.10	41,53,69,75	0
26	BCR	D	405	40/40	0.89	0.10	34,42,66,71	0
32	STE	C	520	16/20	0.89	0.10	39,46,51,52	0
31	DGD	H	102	62/66	0.89	0.11	34,42,51,57	0
32	STE	m	102	18/20	0.89	0.14	32,42,61,63	0
29	SQD	B	623	54/54	0.89	0.10	39,52,71,82	0
29	SQD	D	408	36/54	0.89	0.12	44,60,68,70	0
29	SQD	a	612	54/54	0.90	0.10	38,57,66,72	0
26	BCR	K	101	40/40	0.90	0.11	44,50,59,62	0
31	DGD	c	516	62/66	0.90	0.10	36,45,70,78	0
26	BCR	k	103	40/40	0.90	0.13	45,51,62,64	0
26	BCR	K	102	40/40	0.90	0.10	41,47,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	c	512	65/65	0.90	0.11	47,53,65,72	0
26	BCR	B	618	40/40	0.90	0.09	24,37,45,45	0
25	CLA	C	513	65/65	0.90	0.10	41,52,73,76	0
28	LMG	D	407	51/55	0.91	0.11	32,44,66,69	0
26	BCR	b	619	40/40	0.91	0.09	29,43,57,60	0
25	CLA	c	513	65/65	0.91	0.10	43,60,78,84	0
26	BCR	H	101	40/40	0.91	0.09	31,40,52,53	0
31	DGD	C	516	62/66	0.91	0.10	30,43,72,87	0
26	BCR	B	619	40/40	0.91	0.08	28,37,51,56	0
32	STE	M	101	15/20	0.91	0.10	38,45,56,65	0
32	STE	M	102	10/20	0.91	0.12	41,44,53,54	0
26	BCR	C	514	40/40	0.91	0.09	26,35,47,48	0
26	BCR	T	101	40/40	0.91	0.08	29,36,47,50	0
31	DGD	h	102	62/66	0.91	0.10	35,44,54,56	0
29	SQD	A	613	52/54	0.92	0.10	34,50,68,75	0
30	LHG	d	407	49/49	0.92	0.10	34,43,59,64	0
26	BCR	t	101	40/40	0.92	0.08	29,35,45,49	0
25	CLA	C	512	65/65	0.92	0.09	35,46,70,72	0
26	BCR	b	618	40/40	0.92	0.07	26,35,44,49	0
25	CLA	c	511	65/65	0.93	0.10	42,52,60,67	0
25	CLA	C	508	65/65	0.93	0.09	25,35,67,76	0
30	LHG	d	409	39/49	0.93	0.10	35,40,54,55	0
26	BCR	K	103	40/40	0.93	0.11	37,47,58,59	0
24	BCT	d	401	4/4	0.93	0.08	33,34,43,43	0
26	BCR	b	617	40/40	0.93	0.08	28,40,45,48	0
26	BCR	A	609	40/40	0.93	0.07	22,31,36,37	0
25	CLA	B	606	65/65	0.93	0.09	25,33,54,60	0
26	BCR	c	514	40/40	0.93	0.09	31,44,51,55	0
31	DGD	c	517	62/66	0.93	0.09	32,45,62,72	0
25	CLA	C	503	65/65	0.93	0.08	29,36,42,53	0
25	CLA	b	614	65/65	0.93	0.09	28,35,59,64	0
25	CLA	c	503	65/65	0.93	0.09	34,41,47,52	0
25	CLA	c	510	65/65	0.93	0.08	33,42,51,55	0
25	CLA	C	501	65/65	0.94	0.07	24,32,43,44	0
30	LHG	D	410	47/49	0.94	0.09	28,39,59,63	0
30	LHG	D	412	49/49	0.94	0.09	28,38,53,55	0
24	BCT	A	605	4/4	0.94	0.07	28,32,34,34	0
25	CLA	C	506	65/65	0.94	0.09	29,37,64,72	0
25	CLA	b	606	65/65	0.94	0.08	26,37,56,69	0
30	LHG	l	101	49/49	0.94	0.09	33,40,48,54	0
26	BCR	B	617	40/40	0.94	0.08	28,37,45,46	0
31	DGD	C	515	62/66	0.94	0.09	23,33,60,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	609	65/65	0.94	0.09	34,42,56,64	0
25	CLA	B	616	60/65	0.94	0.10	26,34,63,70	0
31	DGD	J	101	62/66	0.94	0.09	28,39,66,75	0
25	CLA	b	616	60/65	0.94	0.09	31,39,71,75	0
31	DGD	c	515	62/66	0.94	0.09	24,37,60,72	0
28	LMG	d	411	44/55	0.94	0.09	37,47,70,72	0
25	CLA	C	510	65/65	0.94	0.08	28,37,47,57	0
25	CLA	c	504	60/65	0.94	0.09	31,40,63,68	0
25	CLA	c	505	65/65	0.94	0.08	27,36,50,52	0
27	PL9	D	406	55/55	0.94	0.07	20,29,37,39	0
25	CLA	c	508	64/65	0.94	0.09	32,40,73,83	0
27	PL9	d	406	55/55	0.94	0.07	25,32,39,40	0
25	CLA	c	509	65/65	0.94	0.09	33,43,54,58	0
25	CLA	C	511	65/65	0.94	0.10	34,45,57,63	0
26	BCR	a	609	40/40	0.94	0.07	22,30,39,44	0
33	PHO	d	402	64/64	0.94	0.07	28,37,43,45	0
25	CLA	a	606	65/65	0.95	0.08	25,35,74,77	0
25	CLA	a	608	65/65	0.95	0.09	22,30,63,67	0
25	CLA	d	403	65/65	0.95	0.07	22,28,48,53	0
25	CLA	d	404	65/65	0.95	0.09	28,38,73,79	0
25	CLA	B	610	65/65	0.95	0.07	22,28,37,39	0
25	CLA	b	602	65/65	0.95	0.08	29,38,49,55	0
25	CLA	C	504	59/65	0.95	0.07	28,37,67,70	0
25	CLA	b	608	65/65	0.95	0.07	29,39,54,57	0
25	CLA	C	505	65/65	0.95	0.07	26,34,53,59	0
25	CLA	b	610	65/65	0.95	0.08	29,35,43,46	0
25	CLA	b	613	65/65	0.95	0.08	23,30,58,67	0
25	CLA	B	611	65/65	0.95	0.06	23,28,38,44	0
25	CLA	b	615	65/65	0.95	0.07	29,37,49,52	0
25	CLA	C	507	65/65	0.95	0.08	26,34,46,52	0
25	CLA	c	501	65/65	0.95	0.07	29,36,47,53	0
25	CLA	c	502	65/65	0.95	0.07	31,36,48,52	0
25	CLA	B	614	65/65	0.95	0.08	23,34,58,63	0
25	CLA	C	509	65/65	0.95	0.09	27,35,52,54	0
25	CLA	B	615	65/65	0.95	0.08	27,33,50,55	0
25	CLA	c	506	65/65	0.95	0.08	35,42,67,73	0
25	CLA	c	507	65/65	0.95	0.08	32,39,48,51	0
25	CLA	B	602	65/65	0.95	0.07	23,32,51,55	0
25	CLA	B	607	65/65	0.95	0.08	20,27,51,56	0
25	CLA	C	502	65/65	0.95	0.07	25,33,46,55	0
33	PHO	a	607	64/64	0.95	0.07	21,28,34,37	0
25	CLA	a	605	65/65	0.95	0.07	22,28,36,43	0

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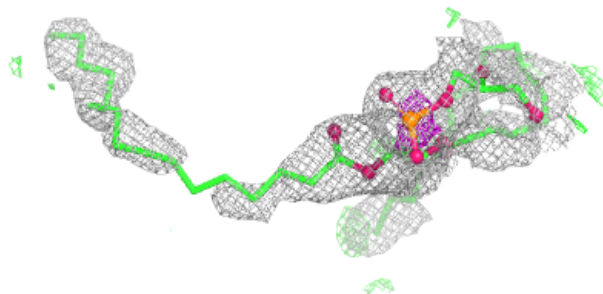
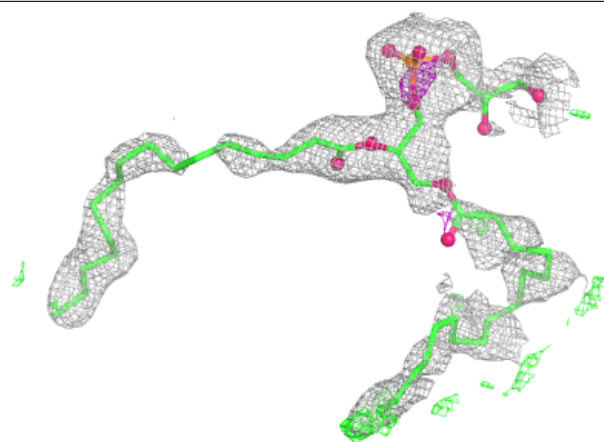
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	B	604	65/65	0.96	0.07	21,27,59,65	0
25	CLA	a	611	65/65	0.96	0.06	19,28,39,46	0
25	CLA	B	605	65/65	0.96	0.07	20,28,40,44	0
25	CLA	A	611	65/65	0.96	0.06	17,25,34,37	0
25	CLA	b	603	65/65	0.96	0.07	21,31,53,59	0
25	CLA	b	604	65/65	0.96	0.07	22,30,56,61	0
25	CLA	b	605	65/65	0.96	0.07	23,31,39,43	0
25	CLA	A	606	65/65	0.96	0.06	19,26,36,44	0
25	CLA	b	607	65/65	0.96	0.07	22,30,52,58	0
25	CLA	B	608	65/65	0.96	0.07	25,31,49,59	0
25	CLA	B	609	65/65	0.96	0.07	23,34,52,58	0
30	LHG	L	101	49/49	0.96	0.07	28,36,43,55	0
25	CLA	A	607	65/65	0.96	0.09	22,29,77,81	0
30	LHG	d	408	49/49	0.96	0.08	27,37,44,50	0
25	CLA	b	611	65/65	0.96	0.07	24,30,42,49	0
25	CLA	b	612	65/65	0.96	0.07	24,32,40,46	0
25	CLA	D	403	65/65	0.96	0.07	19,25,41,56	0
25	CLA	D	404	65/65	0.96	0.08	27,33,73,82	0
33	PHO	D	401	64/64	0.96	0.06	19,26,33,38	0
33	PHO	D	402	64/64	0.96	0.06	24,31,35,37	0
25	CLA	B	603	65/65	0.96	0.07	20,27,49,55	0
25	CLA	B	612	65/65	0.96	0.06	21,27,38,41	0
34	HEM	E	101	43/43	0.96	0.09	38,45,55,63	0
34	HEM	f	101	43/43	0.96	0.09	47,56,67,76	0
25	CLA	A	608	54/65	0.97	0.06	19,26,50,54	0
30	LHG	D	409	49/49	0.97	0.07	24,35,44,49	0
25	CLA	B	613	65/65	0.97	0.06	20,26,54,58	0
35	HEC	V	201	43/43	0.98	0.06	24,30,38,43	0
35	HEC	v	201	43/43	0.98	0.06	29,35,42,46	0
23	CL	a	603	1/1	0.99	0.03	31,31,31,31	0
23	CL	a	604	1/1	0.99	0.09	32,32,32,32	0
21	OEY	A	601[A]	11/11	0.99	0.03	29,32,36,36	11
21	OEY	A	601[B]	11/11	0.99	0.03	23,28,31,31	11
21	OEY	a	601[A]	11/11	0.99	0.03	28,31,33,35	11
21	OEY	a	601[B]	11/11	0.99	0.03	24,29,29,31	11
22	FE2	A	602	1/1	0.99	0.01	29,29,29,29	0
22	FE2	a	602	1/1	0.99	0.02	32,32,32,32	0
23	CL	A	603	1/1	0.99	0.04	27,27,27,27	0
23	CL	A	604	1/1	0.99	0.02	29,29,29,29	0

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

orientation to approximate a three-dimensional view.

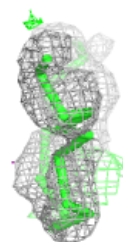
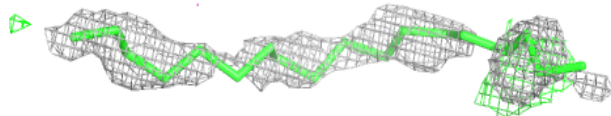
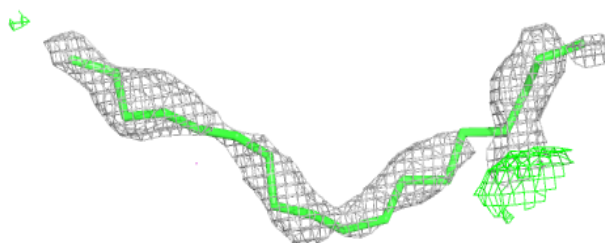
Electron density around LHG A 614:

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

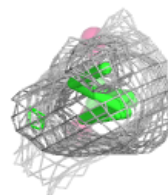
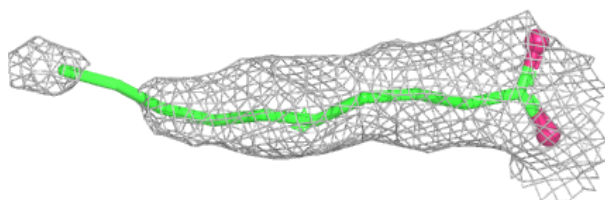


Electron density around STE H 103:

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

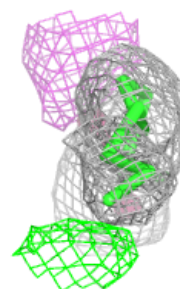
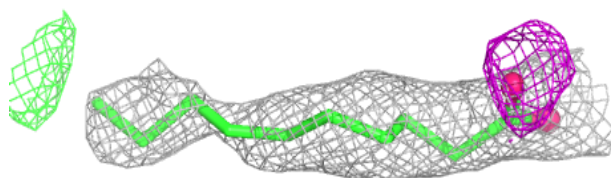
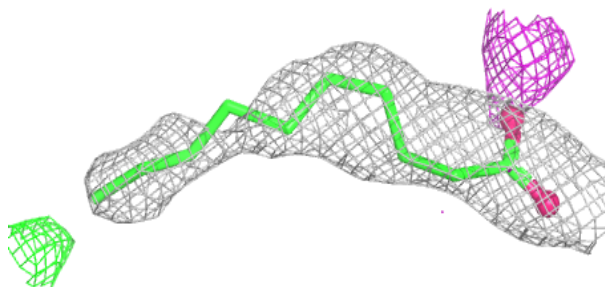
**Electron density around STE k 104:**

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

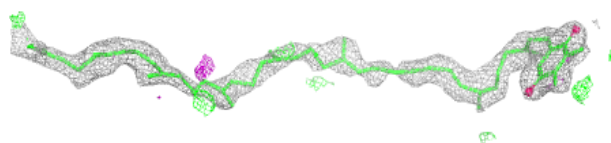
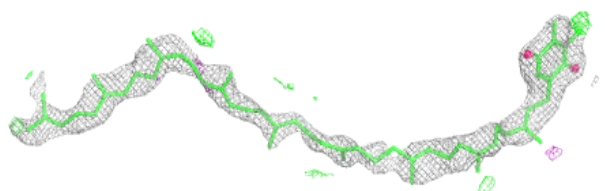


Electron density around STE L 102:

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

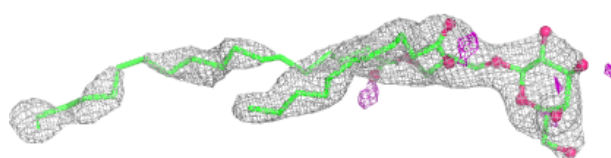
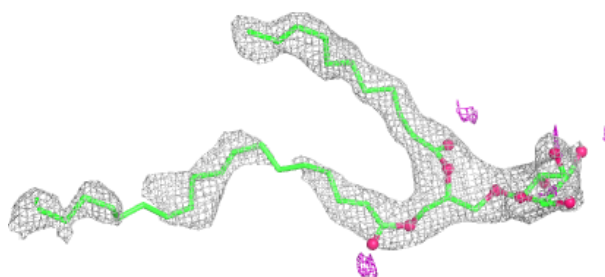
**Electron density around PL9 A 610:**

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

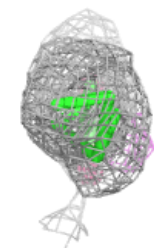
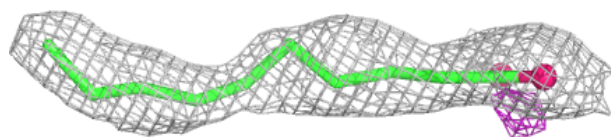
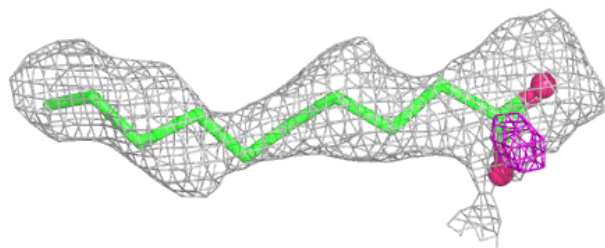


Electron density around LMG c 520:

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

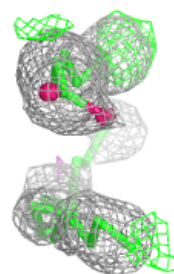
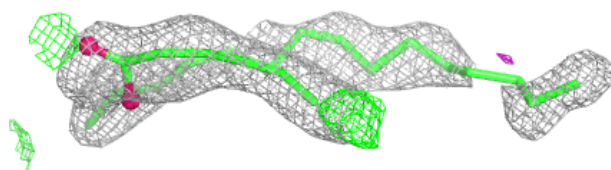
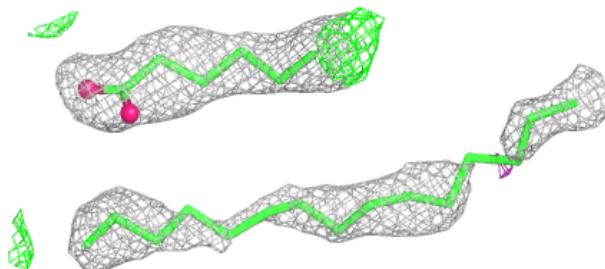
**Electron density around STE a 615:**

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

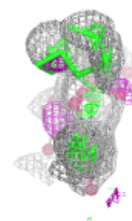
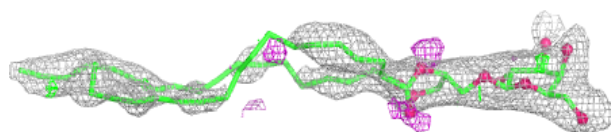
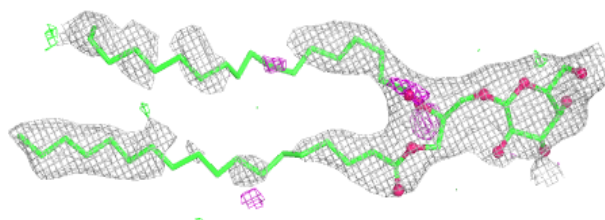


Electron density around LMG d 410:

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

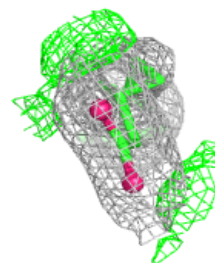
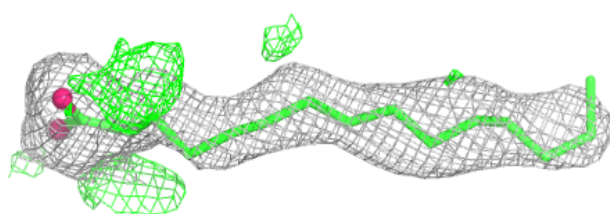
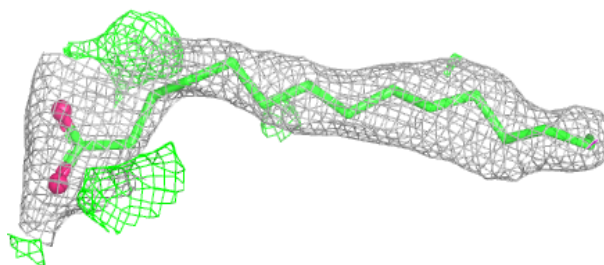
**Electron density around LMG b 622:**

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

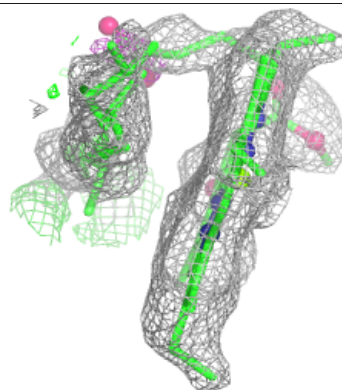
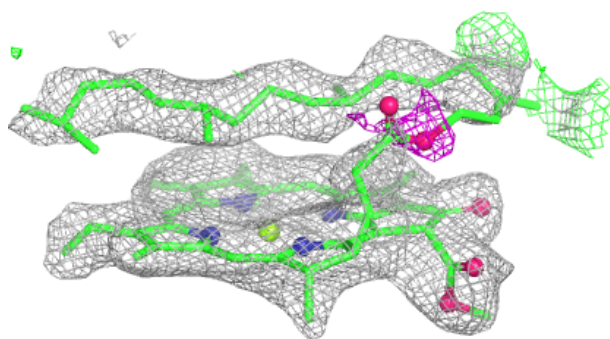
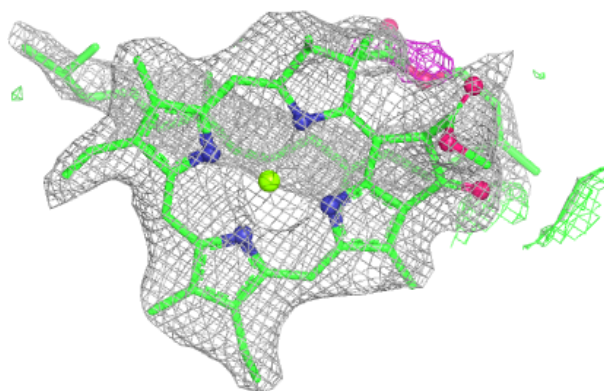


Electron density around STE d 412:

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

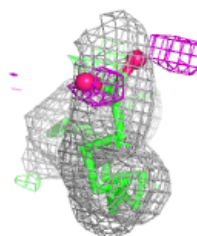
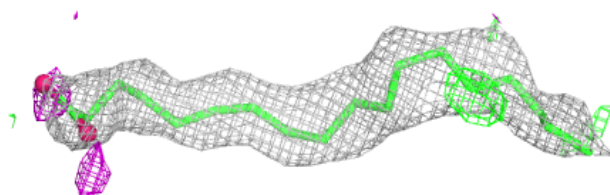
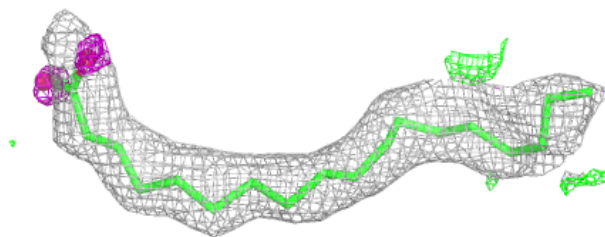
**Electron density around CLA b 601:**

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

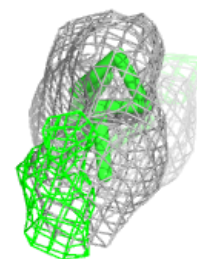
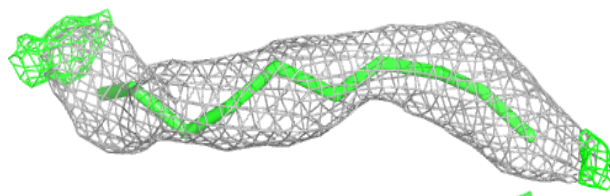
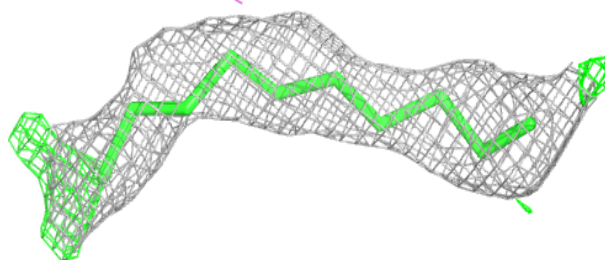


Electron density around STE b 621:

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

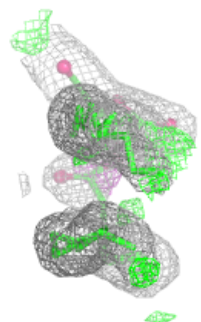
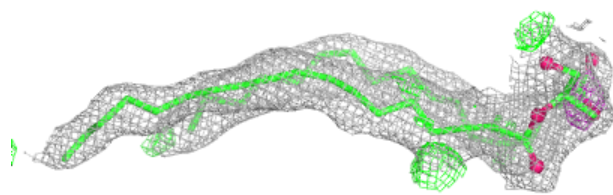
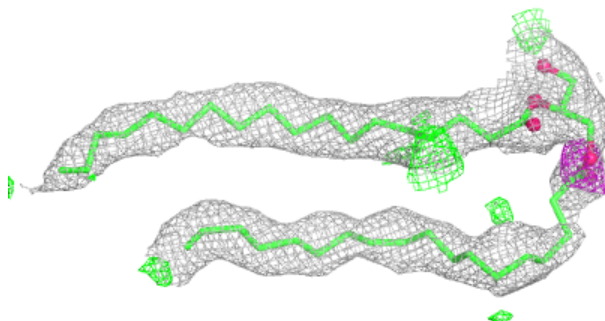
**Electron density around STE b 625:**

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



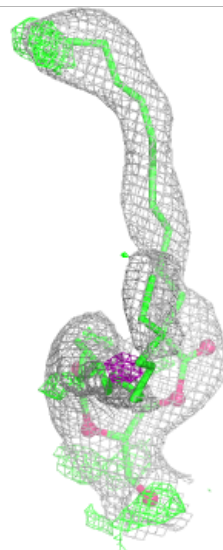
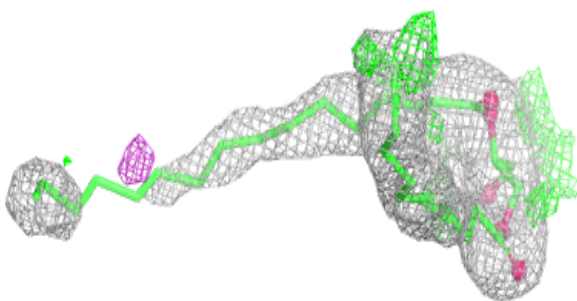
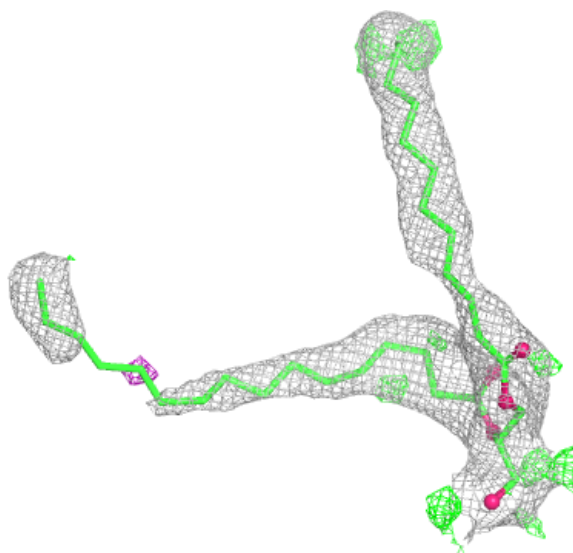
Electron density around DGD a 614:

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



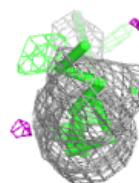
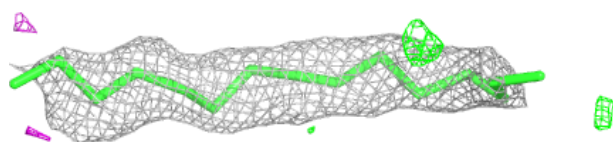
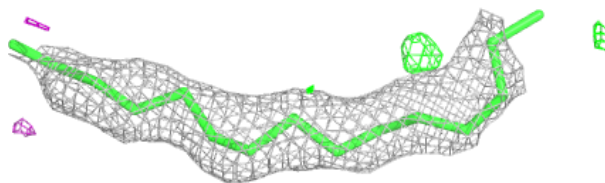
Electron density around SQD a 613:

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

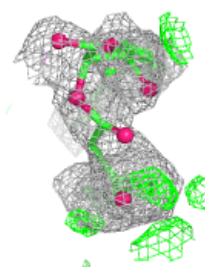
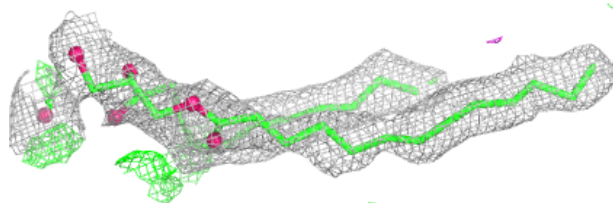
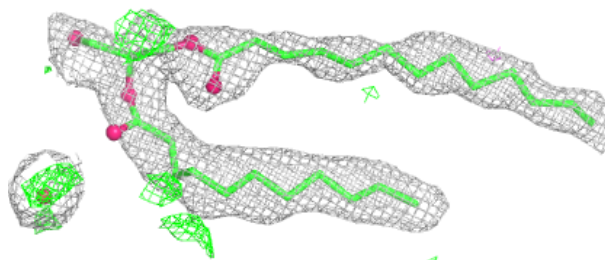


Electron density around STE b 624:

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

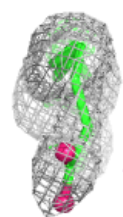
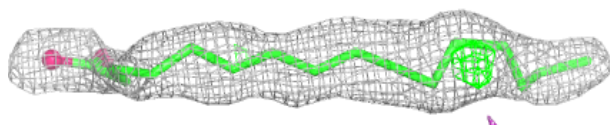
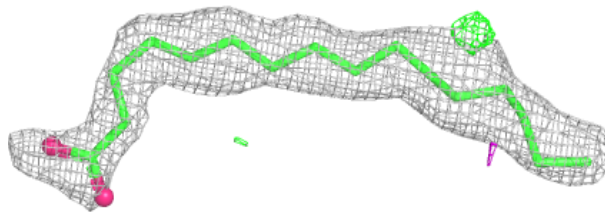
**Electron density around LMG D 411:**

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

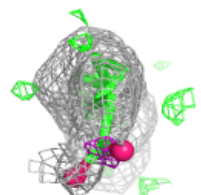
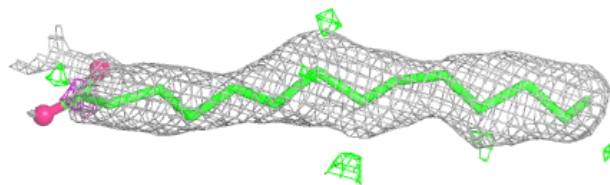
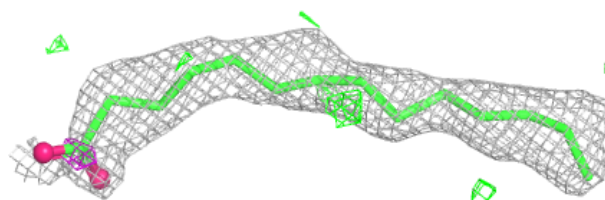


Electron density around STE B 625:

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

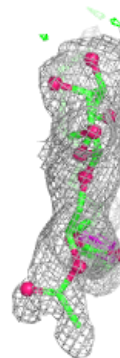
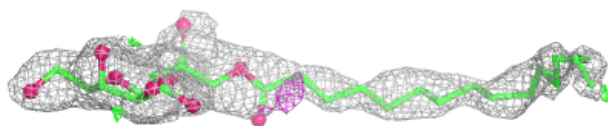
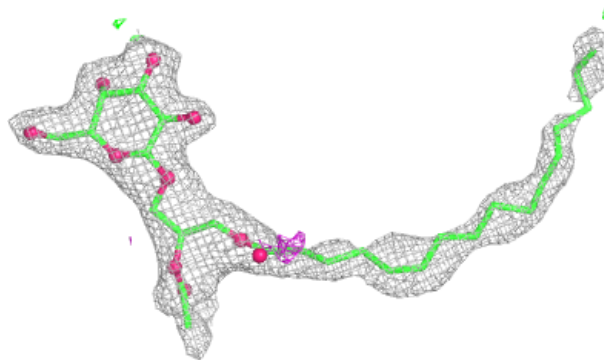
**Electron density around STE b 623:**

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

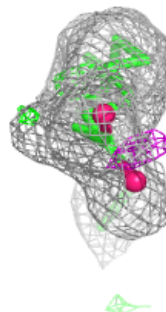
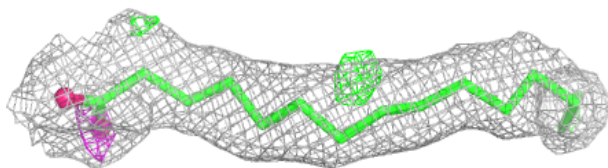
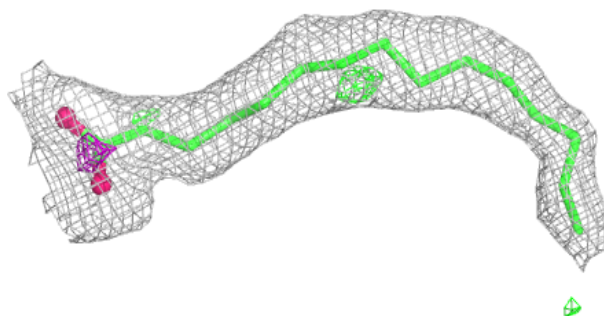


Electron density around LMG c 518:

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

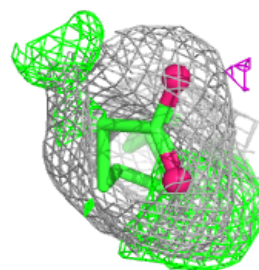
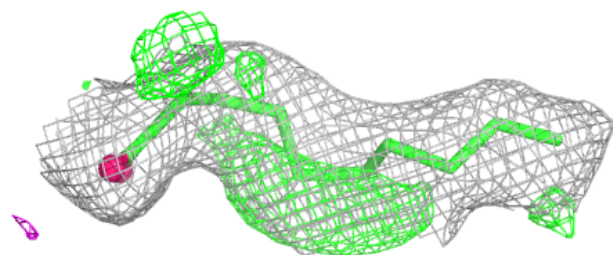
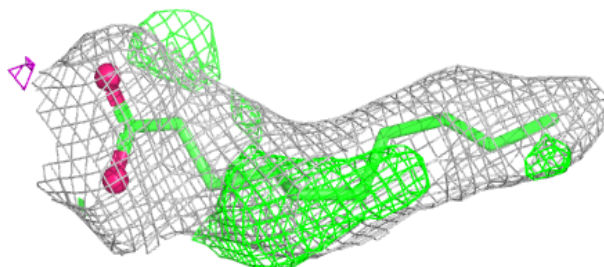
**Electron density around STE B 621:**

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

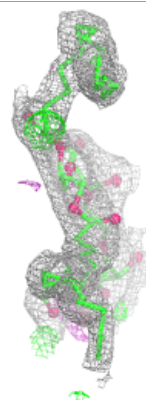
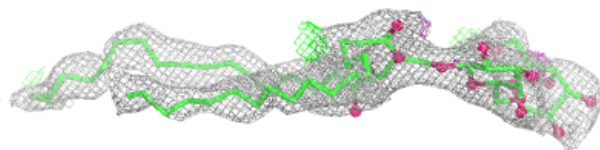
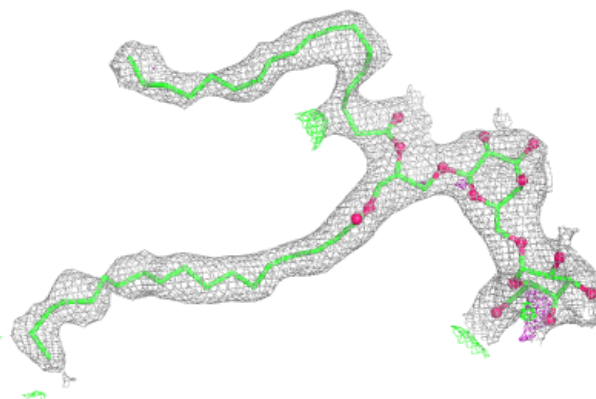


Electron density around STE B 624:

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

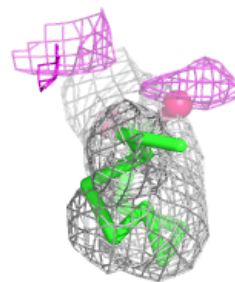
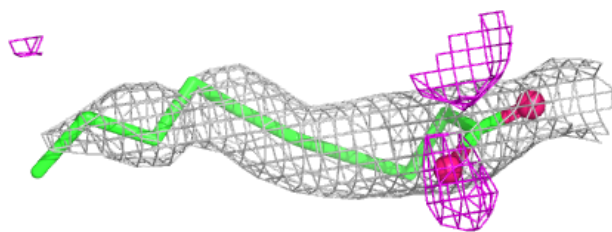
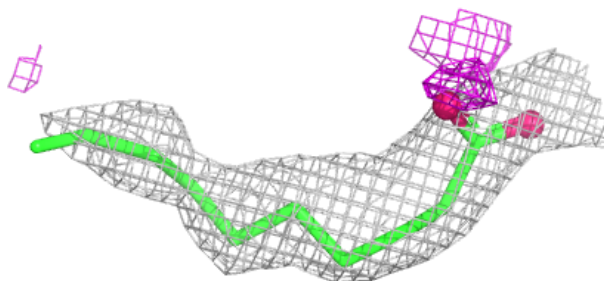
**Electron density around DGD A 616:**

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

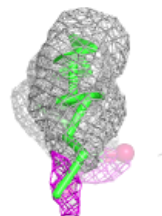
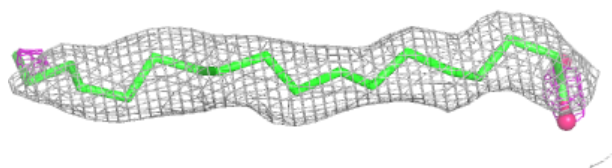
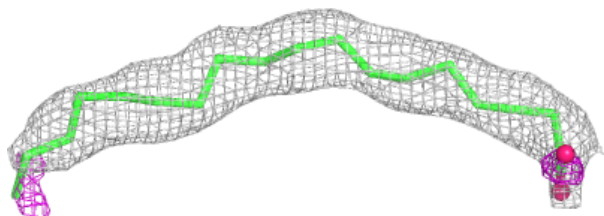


Electron density around STE B 626:

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

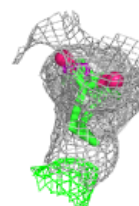
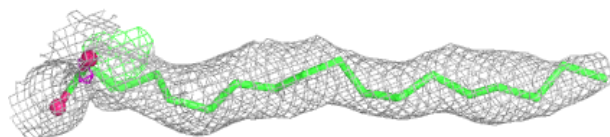
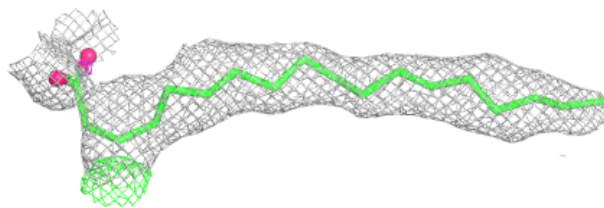
**Electron density around STE D 413:**

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

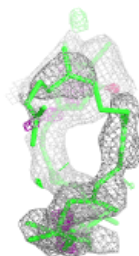
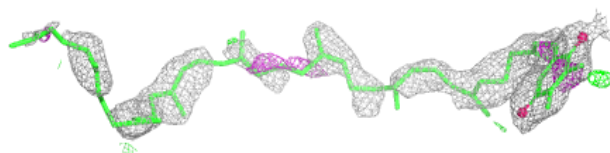
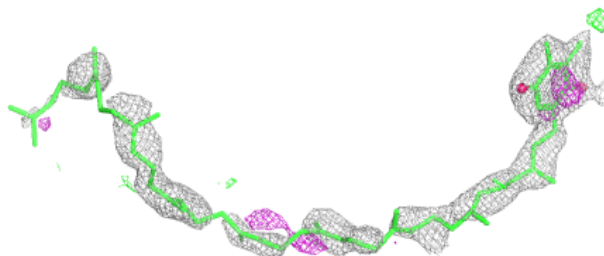


Electron density around STE c 519:

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

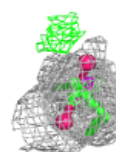
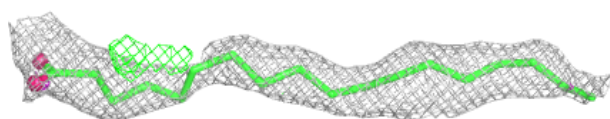
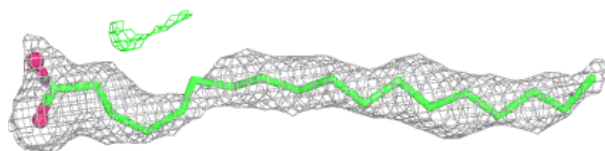
**Electron density around PL9 a 610:**

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

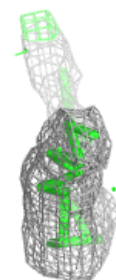
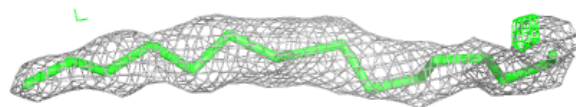
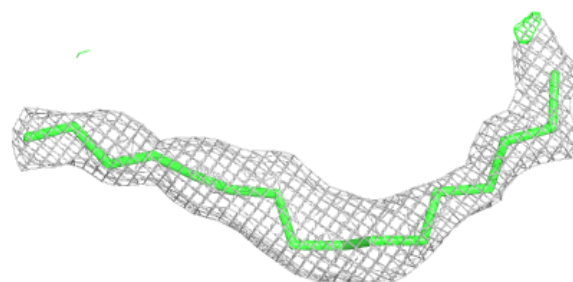


Electron density around STE A 617:

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

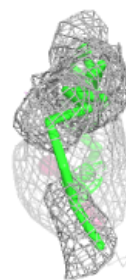
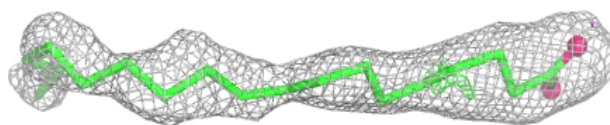
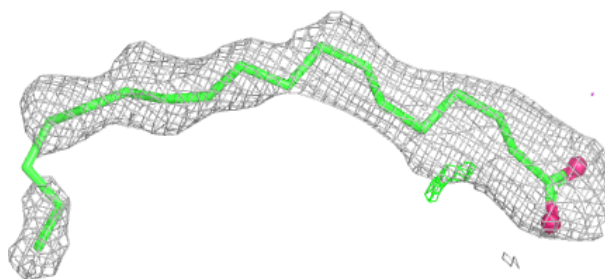
**Electron density around STE B 627:**

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

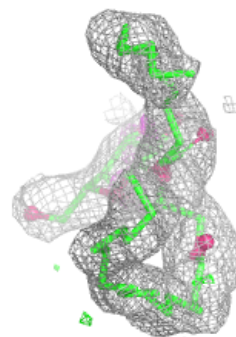
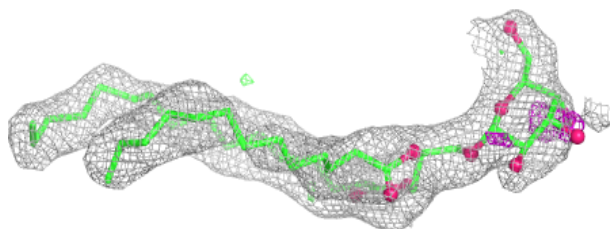
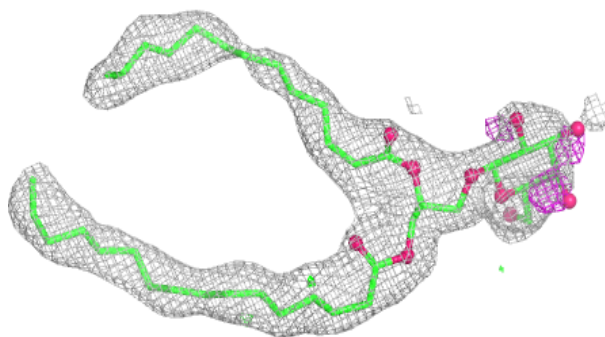


Electron density around STE d 413:

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

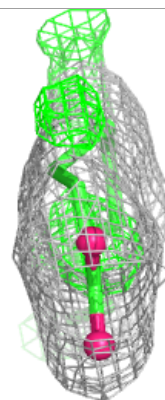
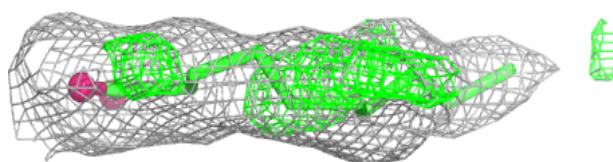
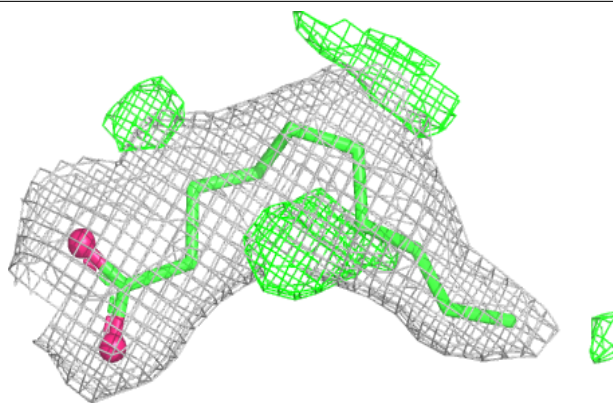
**Electron density around LMG A 612:**

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

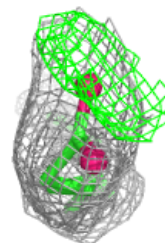
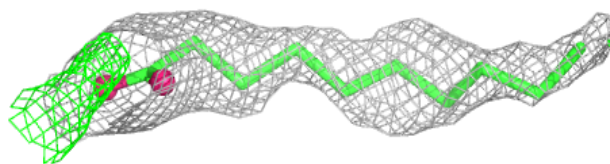
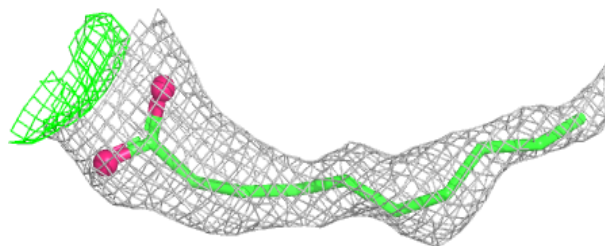


Electron density around STE C 518:

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

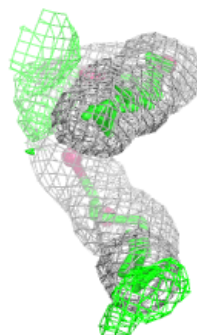
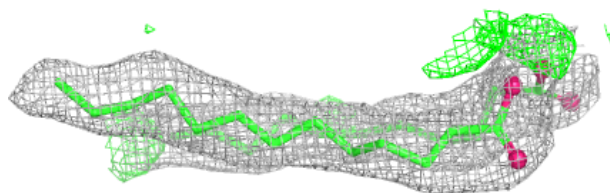
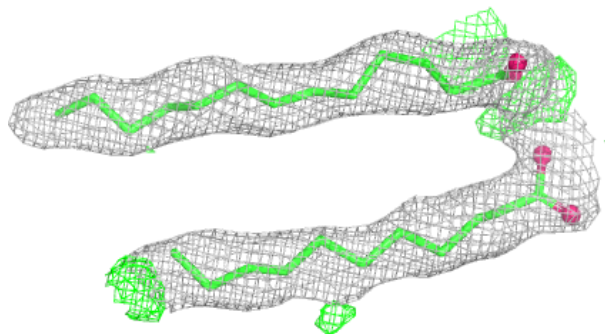
**Electron density around STE C 519:**

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

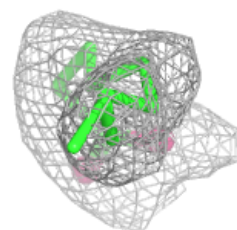
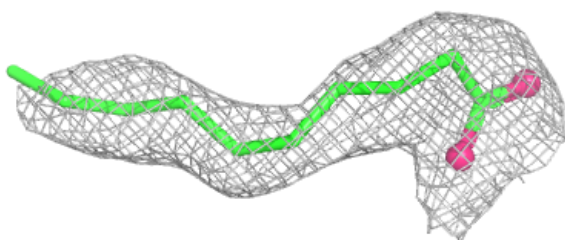
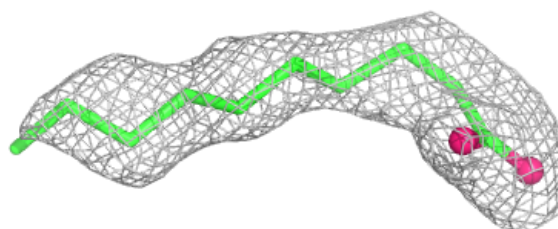


Electron density around LMG B 622:

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

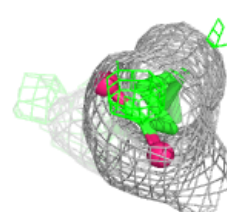
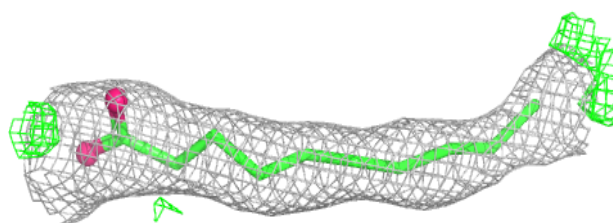
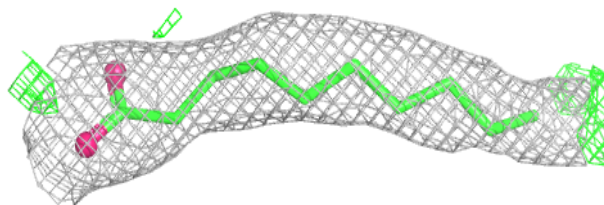
**Electron density around STE E 102:**

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

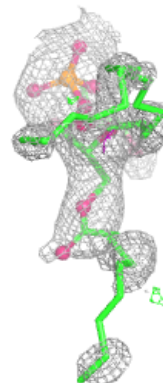
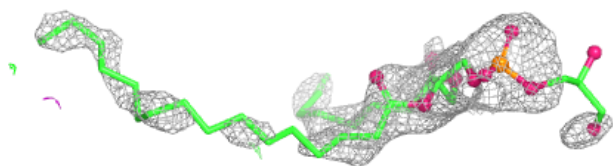
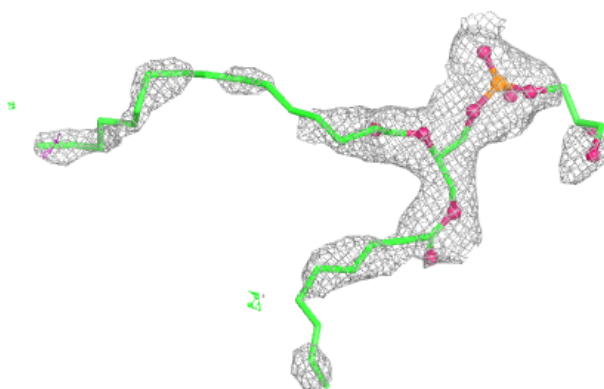


Electron density around STE j 101:

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

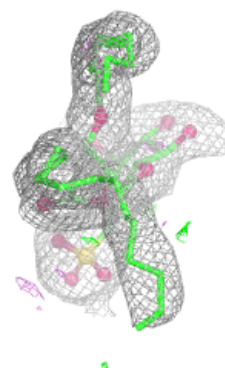
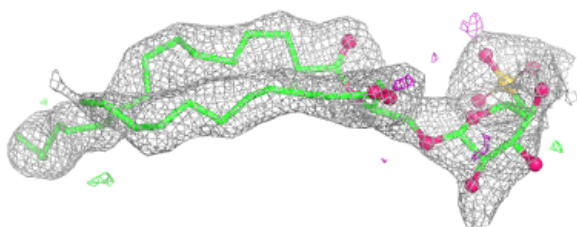
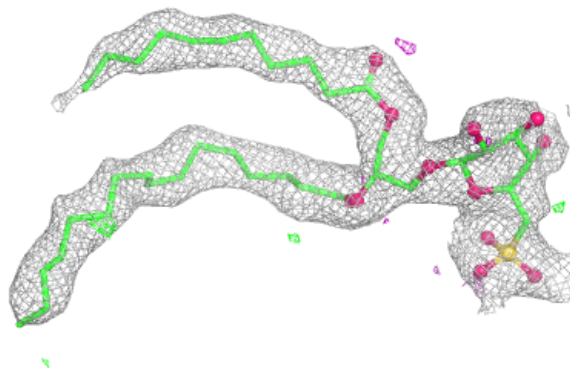
**Electron density around LHG e 101:**

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

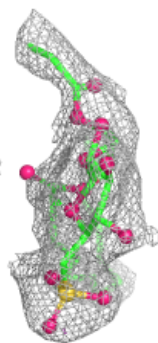
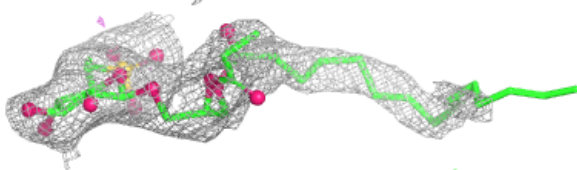
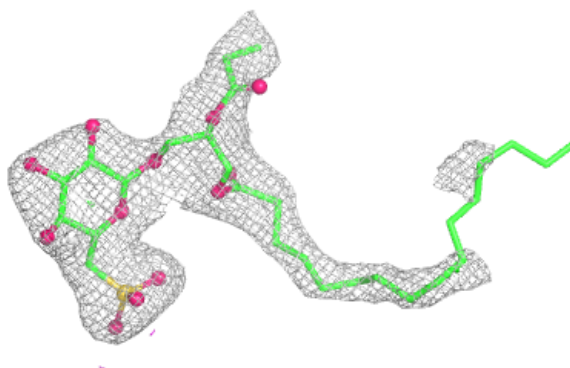


Electron density around SQD b 620:

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

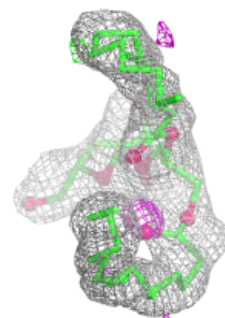
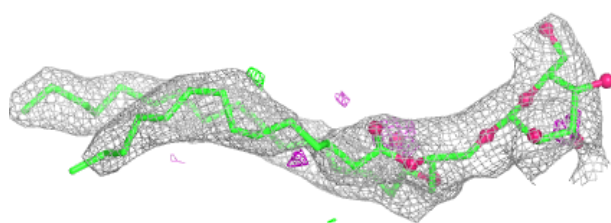
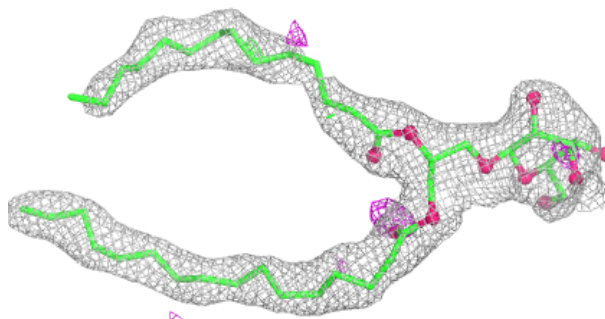
**Electron density around SQD f 102:**

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

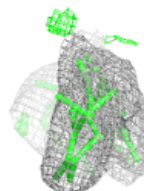
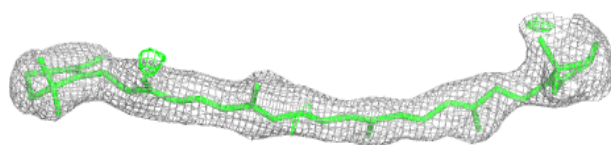
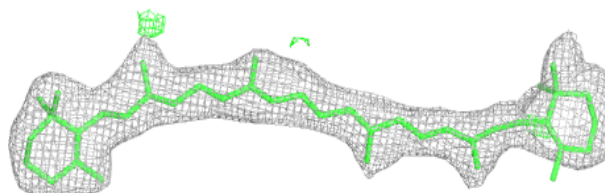


Electron density around LMG c 521:

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

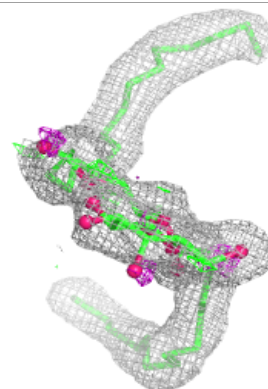
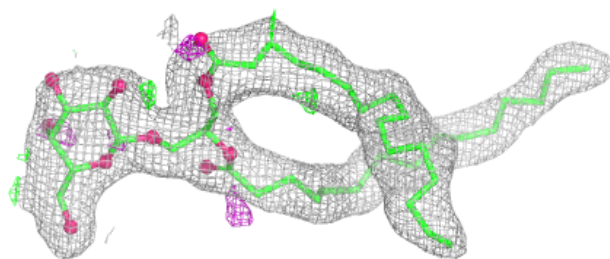
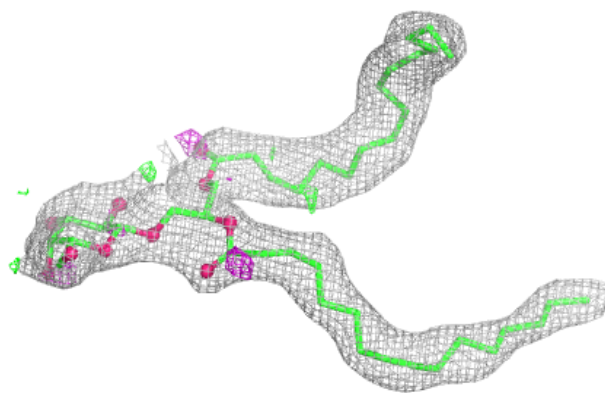
**Electron density around BCR d 405:**

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



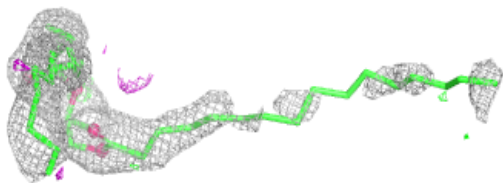
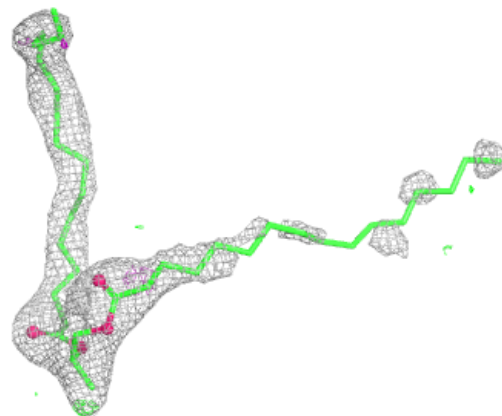
Electron density around LMG m 101:

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



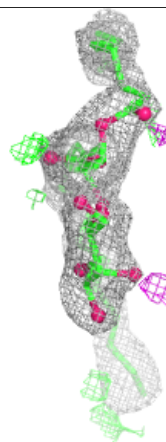
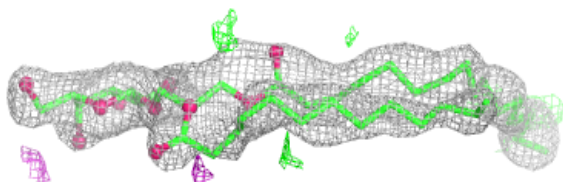
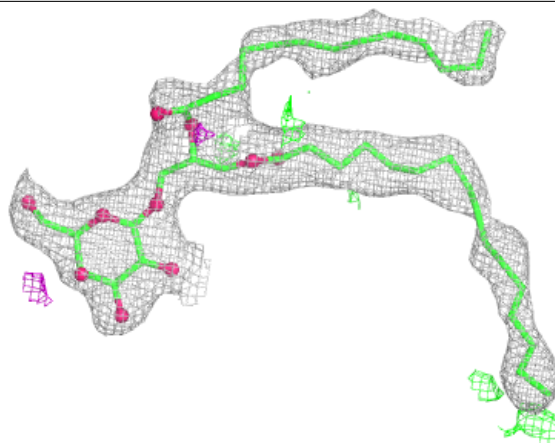
Electron density around SQD A 615:

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

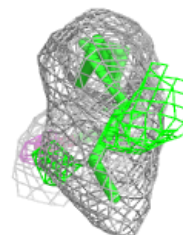
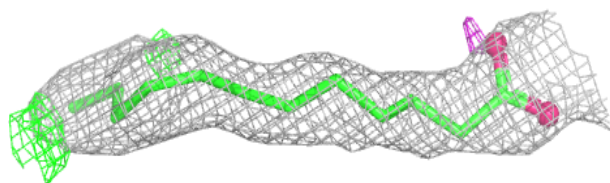
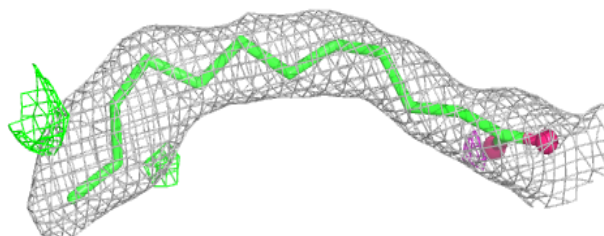


Electron density around LMG C 517:

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

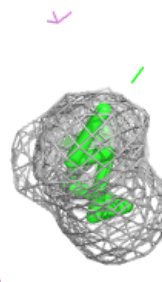
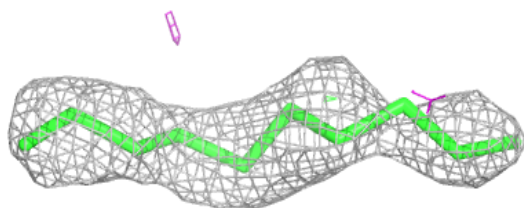
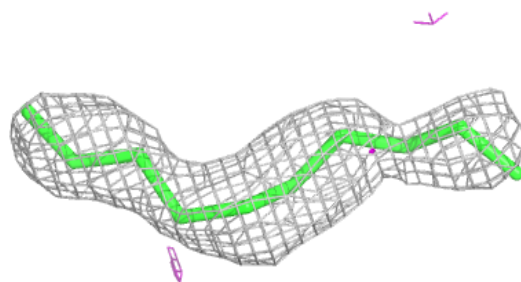
**Electron density around STE t 102:**

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

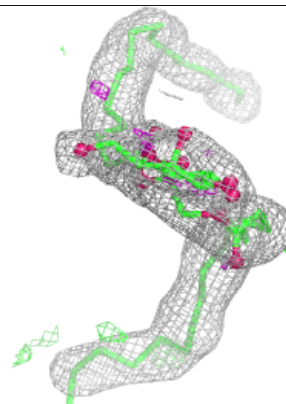
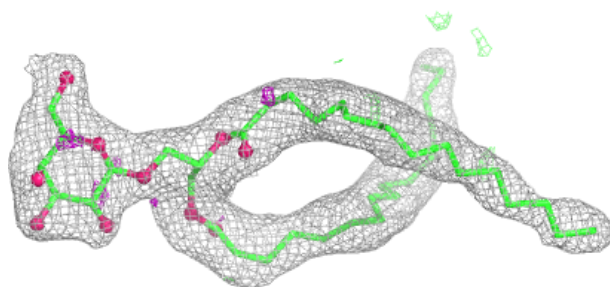
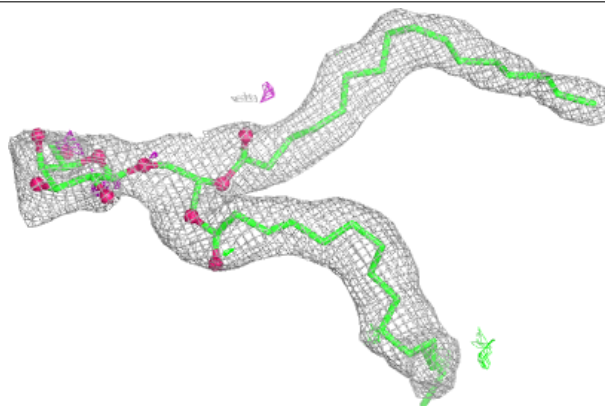


Electron density around STE t 103:

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

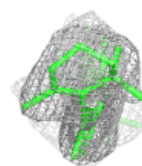
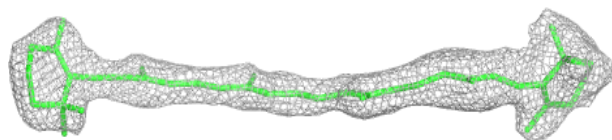
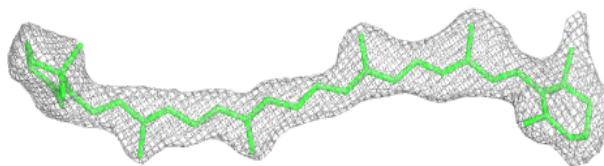
**Electron density around LMG B 620:**

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

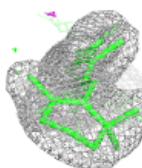
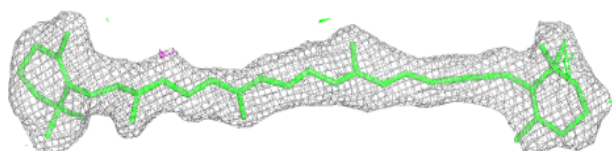
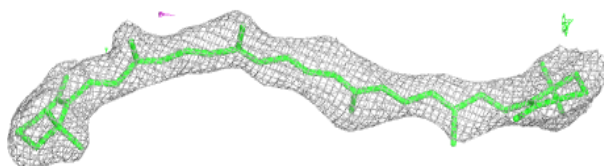


Electron density around BCR k 102:

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

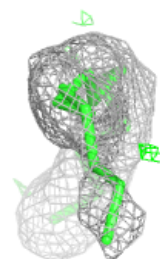
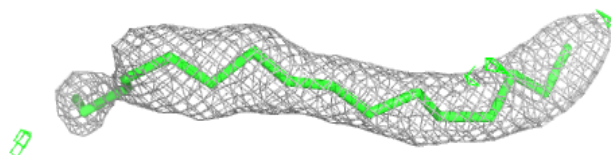
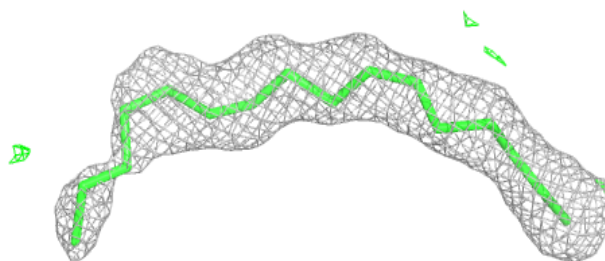
**Electron density around BCR h 101:**

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

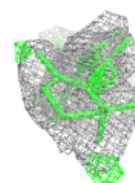
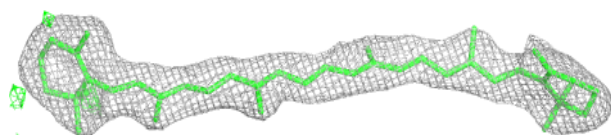
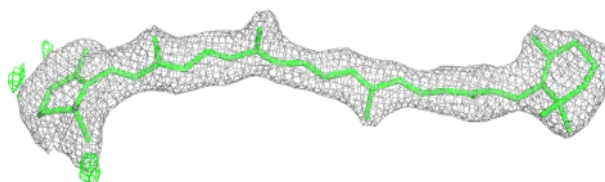


Electron density around STE T 102:

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

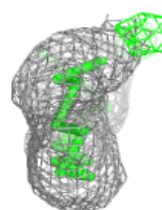
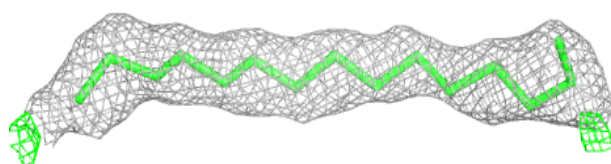
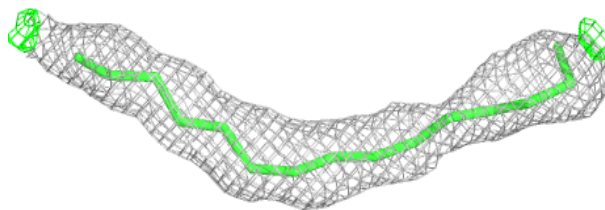
**Electron density around BCR k 101:**

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

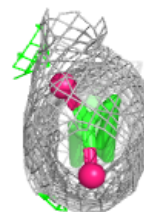
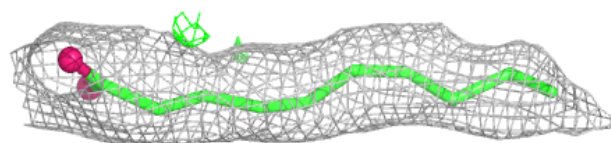
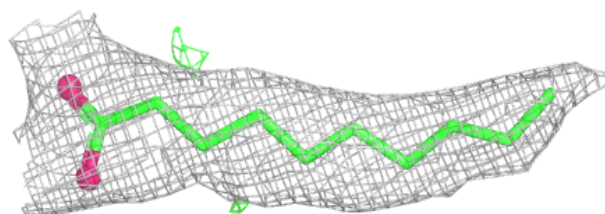


Electron density around STE I 101:

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

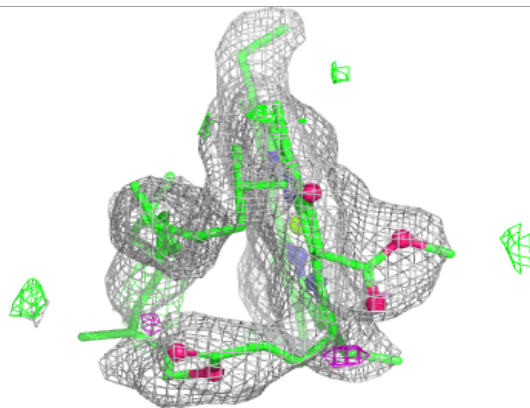
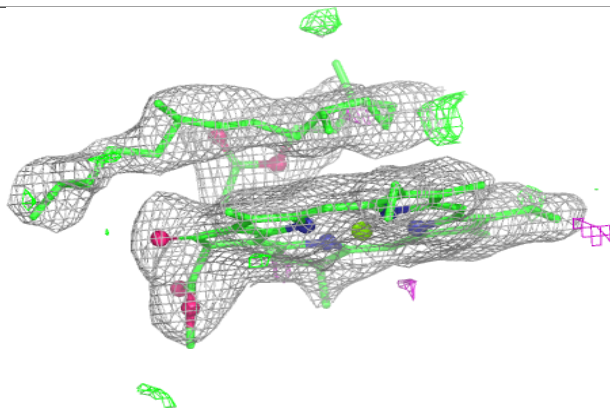
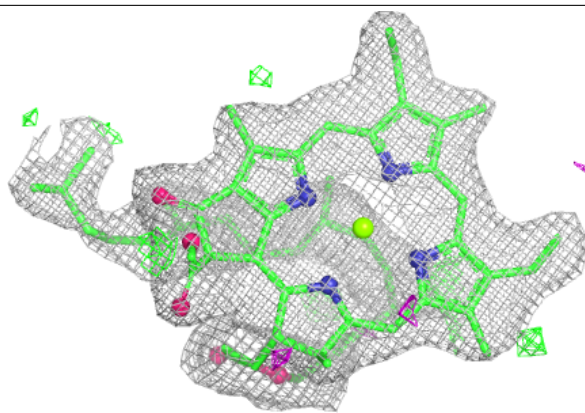
**Electron density around STE J 102:**

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

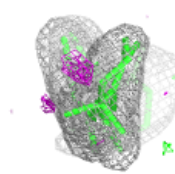
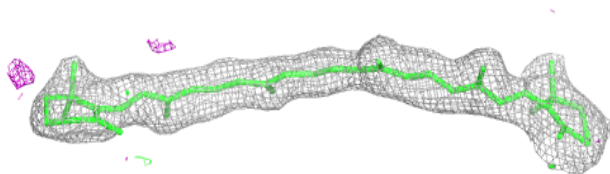
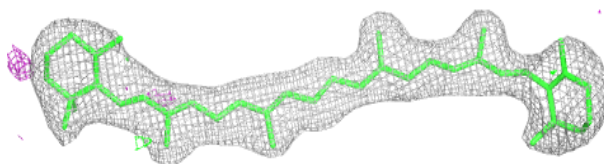


Electron density around CLA B 601:

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

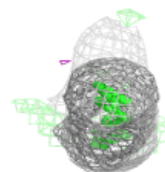
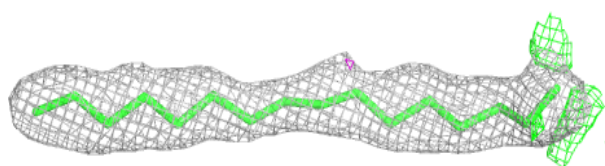
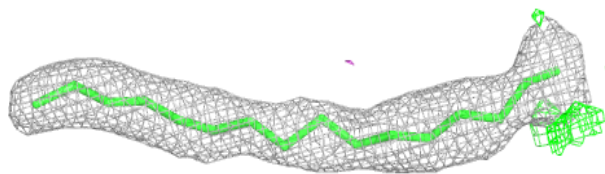
**Electron density around BCR D 405:**

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

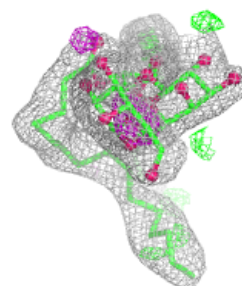
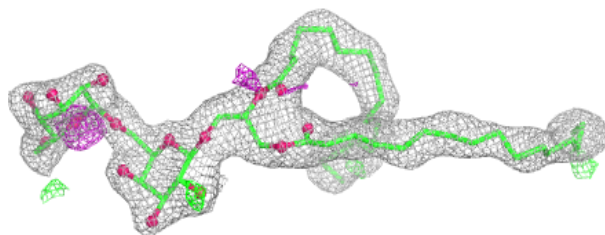
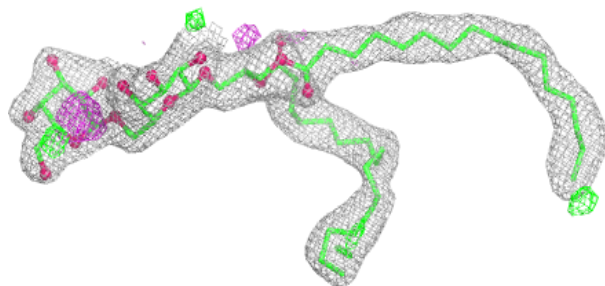


Electron density around STE C 520:

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

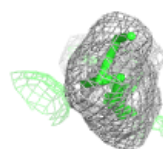
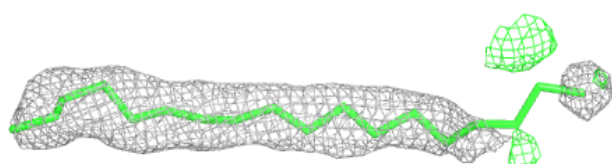
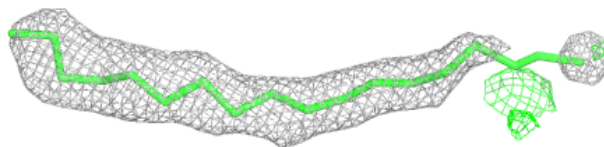
**Electron density around DGD H 102:**

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

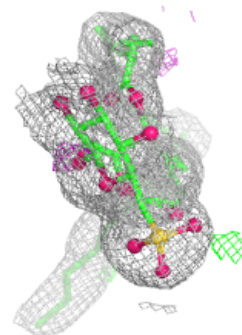
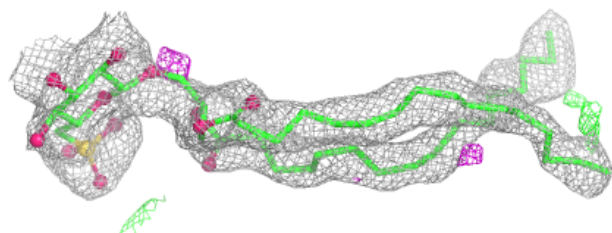
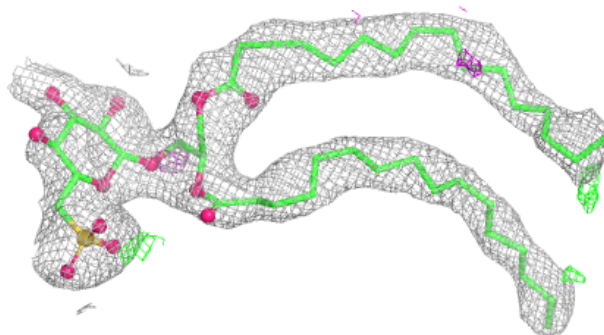


Electron density around STE m 102:

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

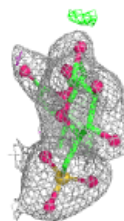
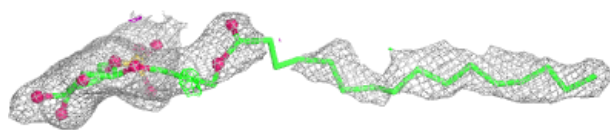
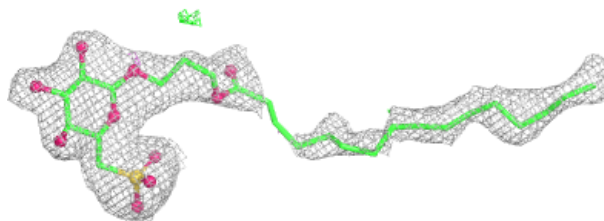
**Electron density around SQD B 623:**

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



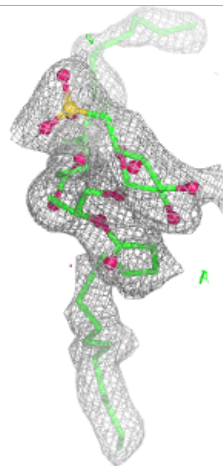
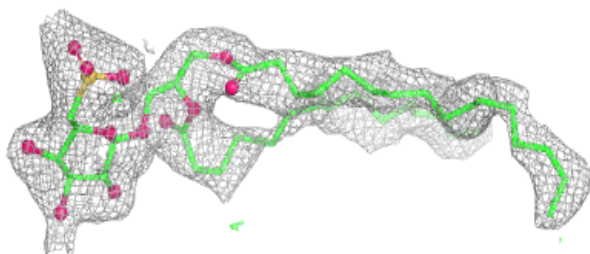
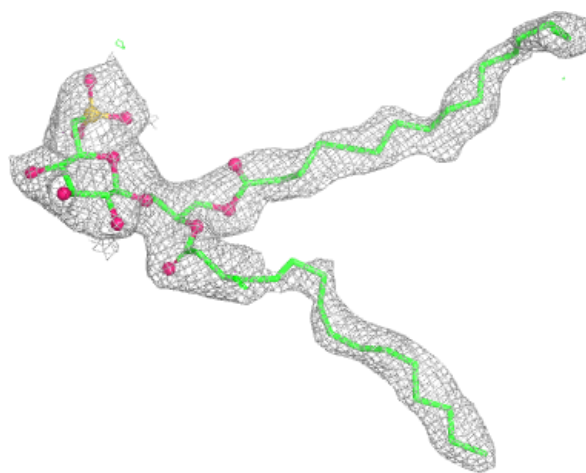
Electron density around SQD D 408:

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



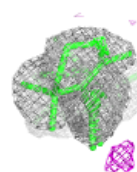
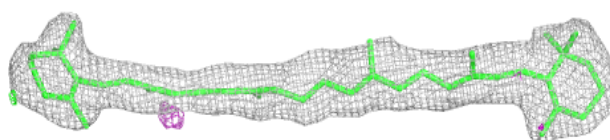
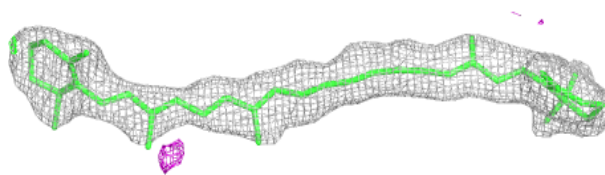
Electron density around SQD a 612:

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

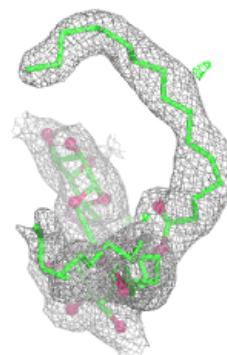
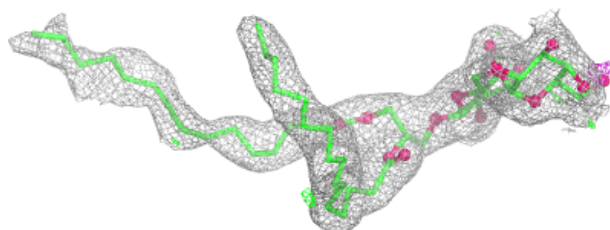
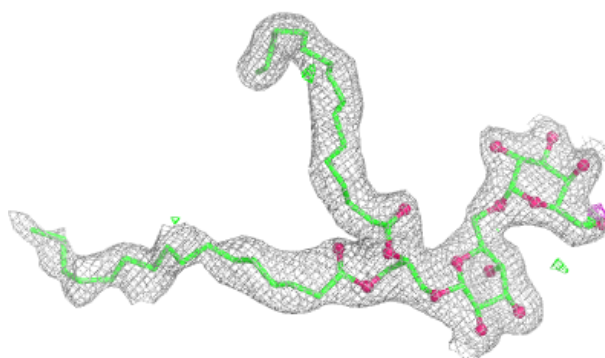


Electron density around BCR K 101:

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

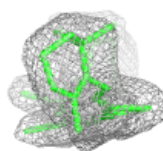
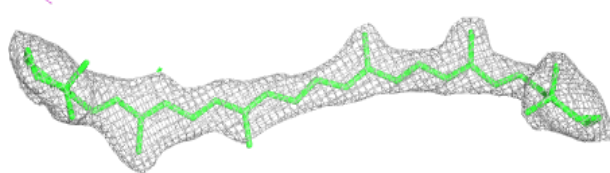
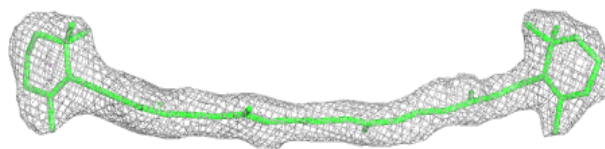
**Electron density around DGD c 516:**

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

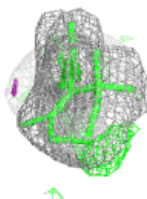
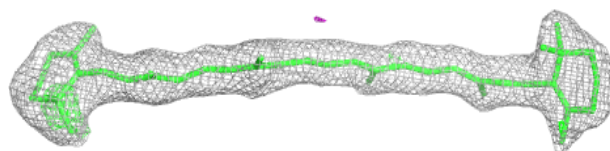
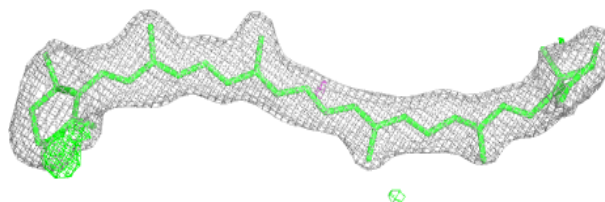


Electron density around BCR k 103:

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

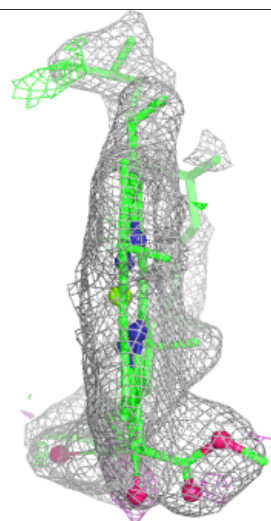
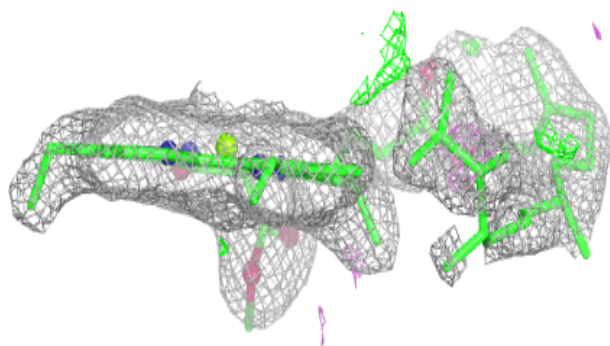
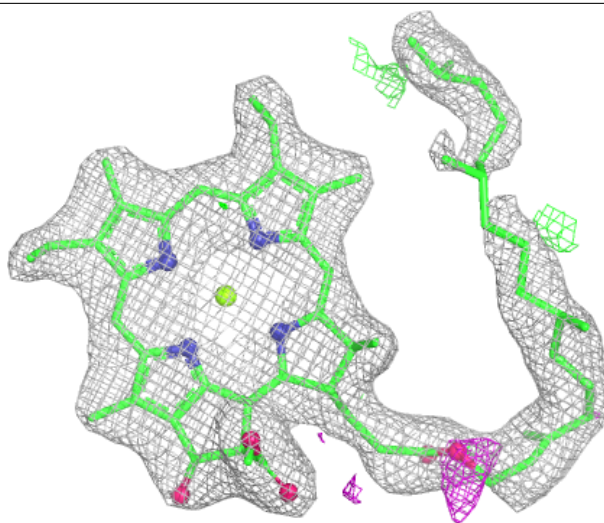
**Electron density around BCR K 102:**

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



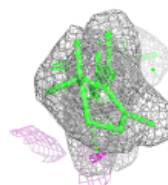
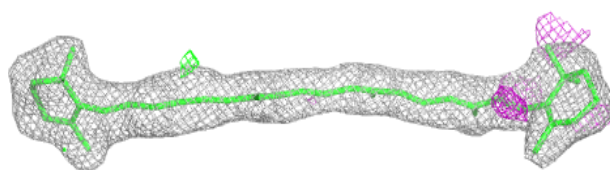
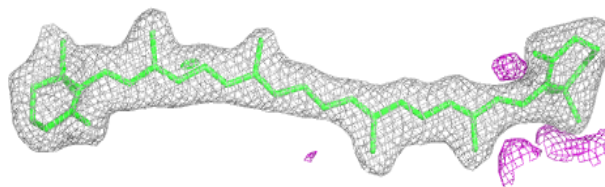
Electron density around CLA c 512:

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

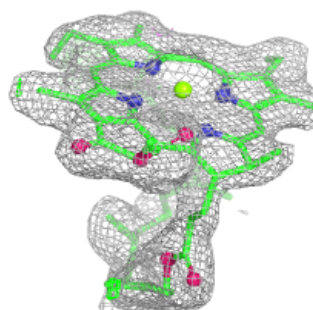
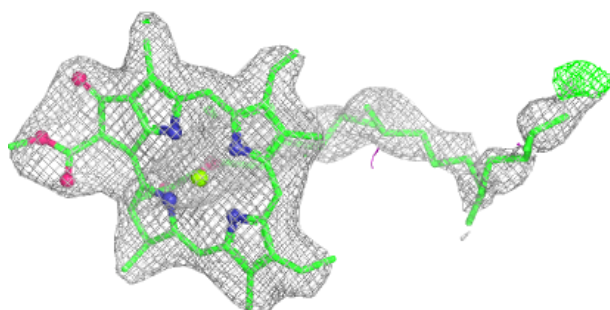
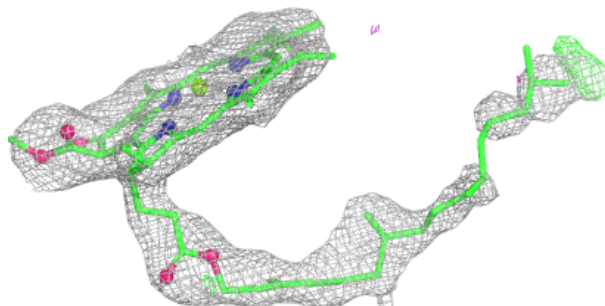


Electron density around BCR B 618:

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

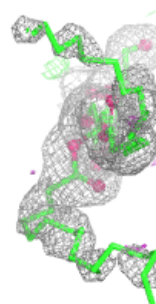
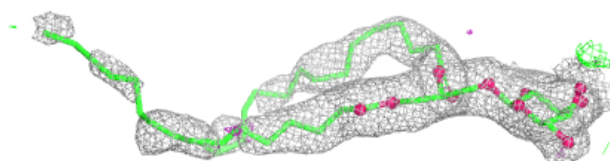
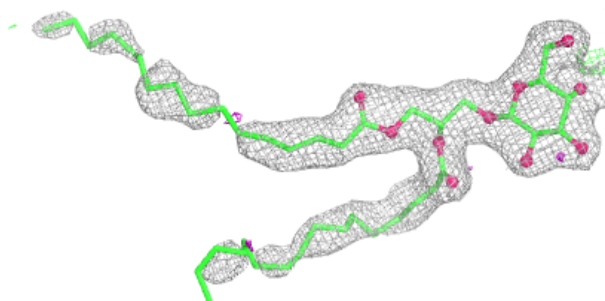
**Electron density around CLA C 513:**

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

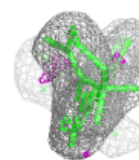
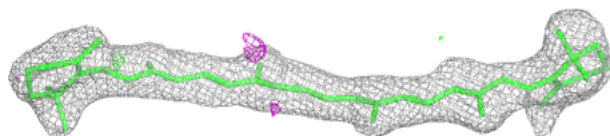
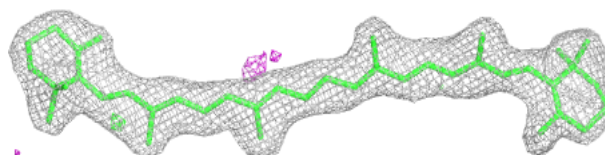


Electron density around LMG D 407:

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

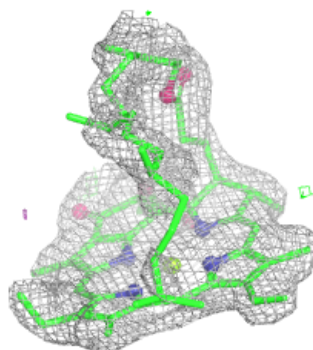
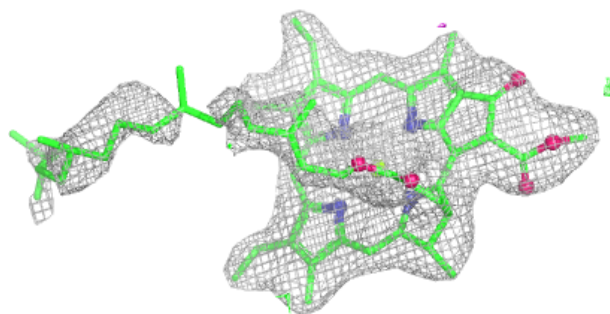
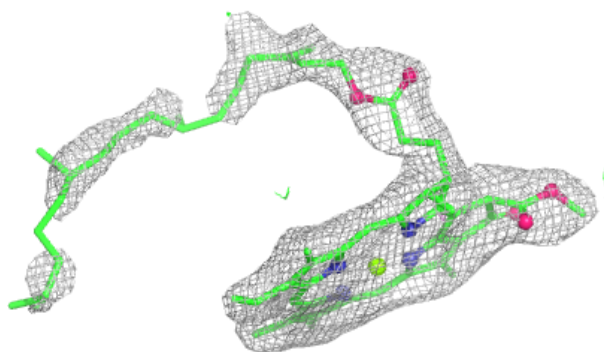
**Electron density around BCR b 619:**

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

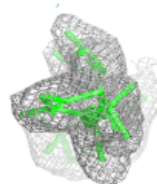
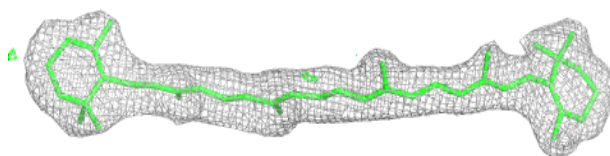
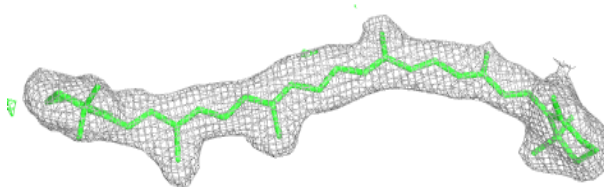


Electron density around CLA c 513:

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

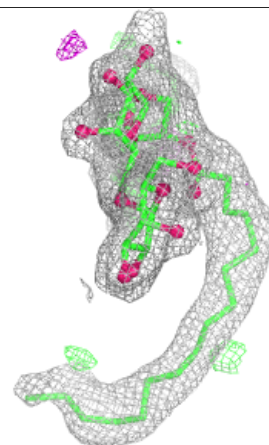
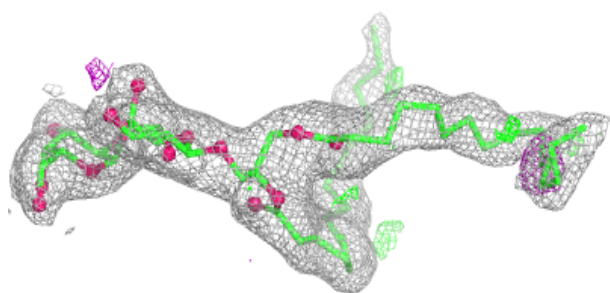
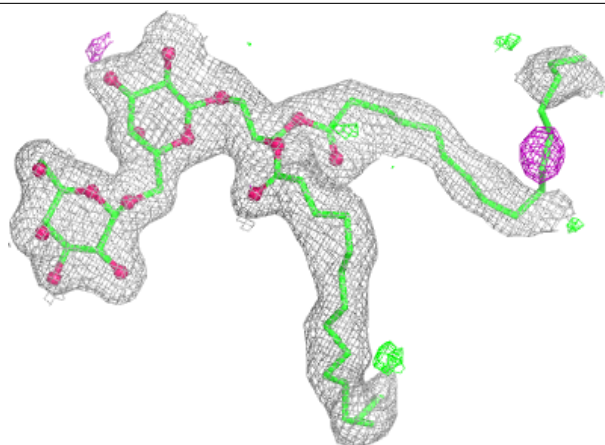
**Electron density around BCR H 101:**

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

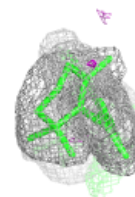
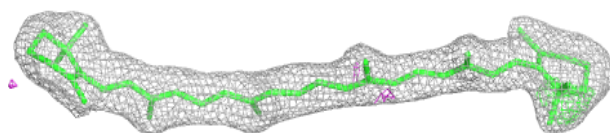
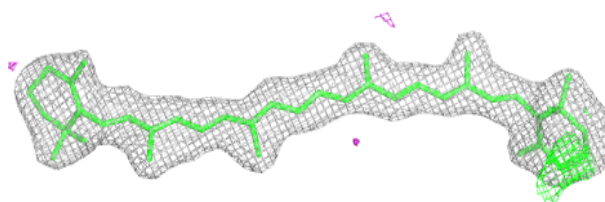


Electron density around DGD C 516:

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

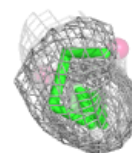
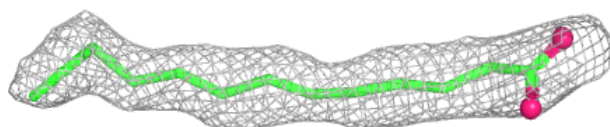
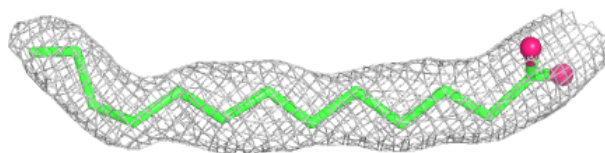
**Electron density around BCR B 619:**

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

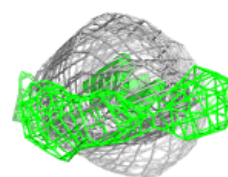
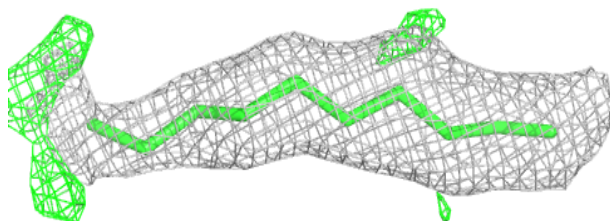
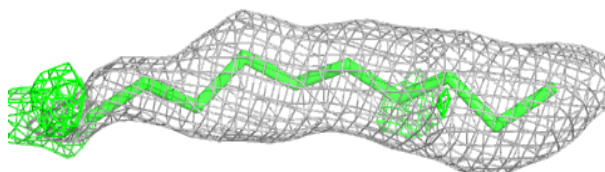


Electron density around STE M 101:

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

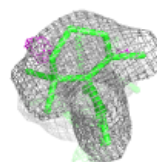
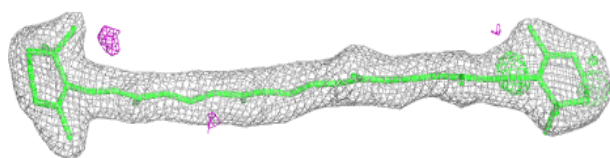
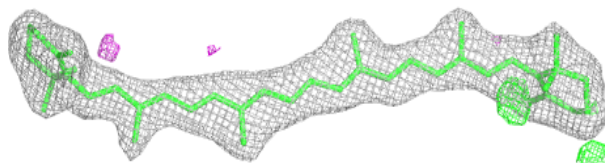
**Electron density around STE M 102:**

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

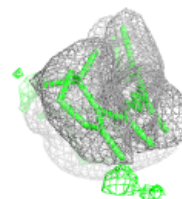
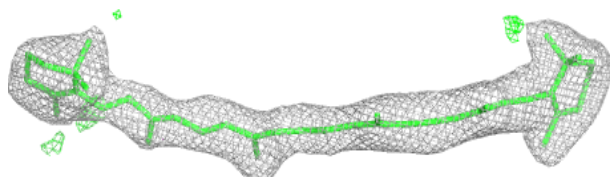
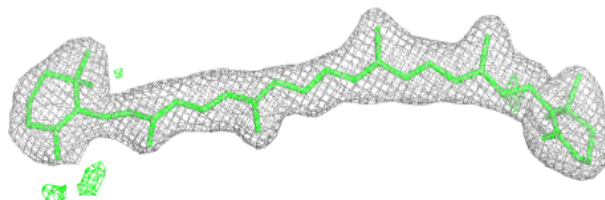


Electron density around BCR C 514:

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

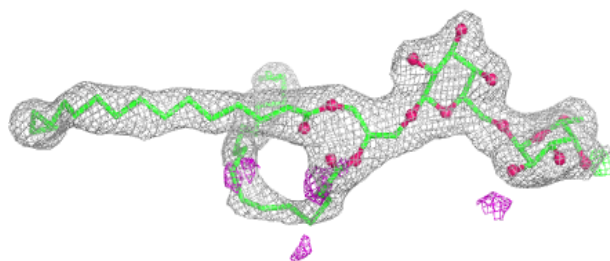
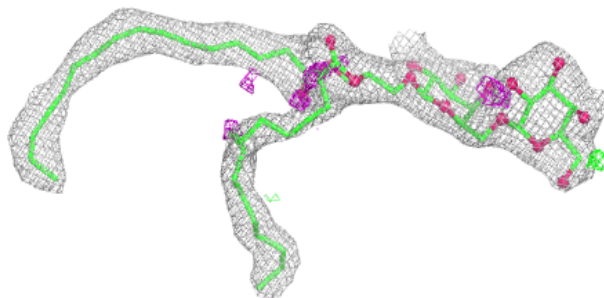
**Electron density around BCR T 101:**

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



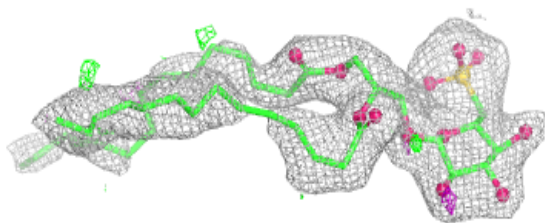
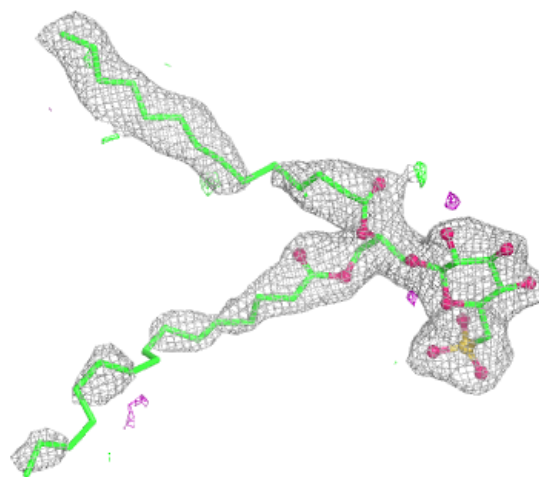
Electron density around DGD h 102:

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



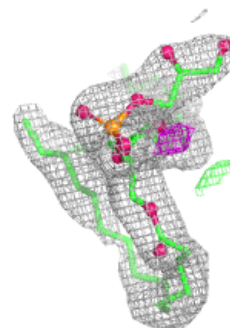
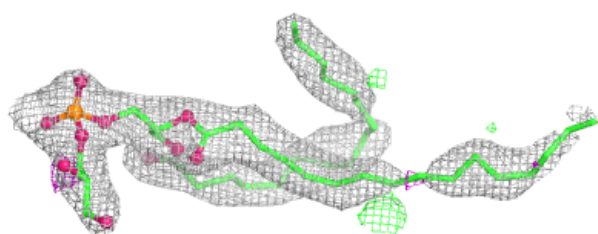
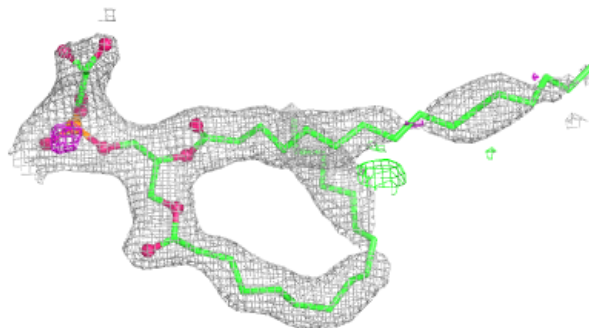
Electron density around SQD A 613:

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

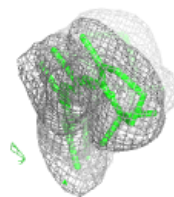
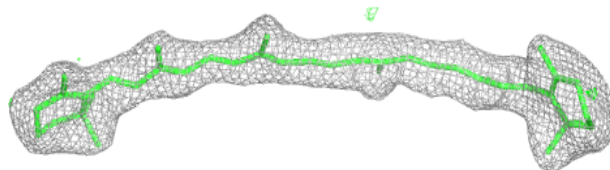
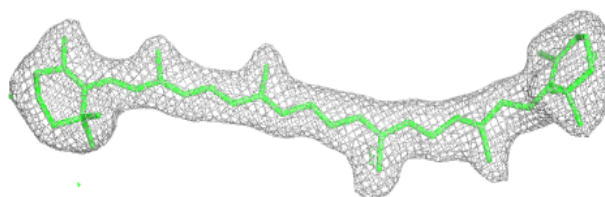


Electron density around LHG d 407:

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

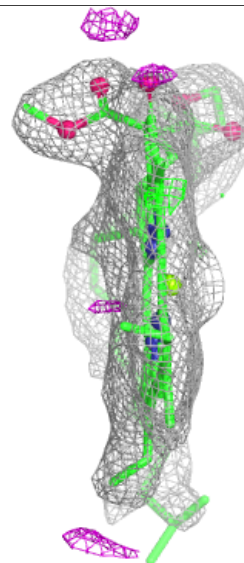
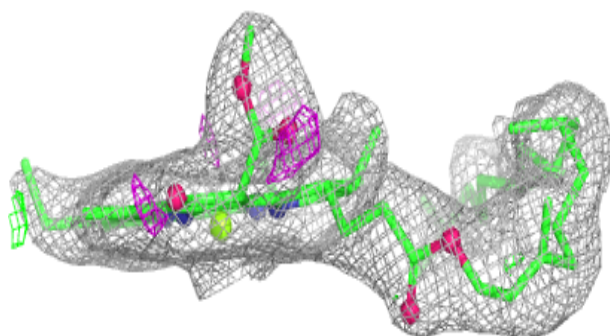
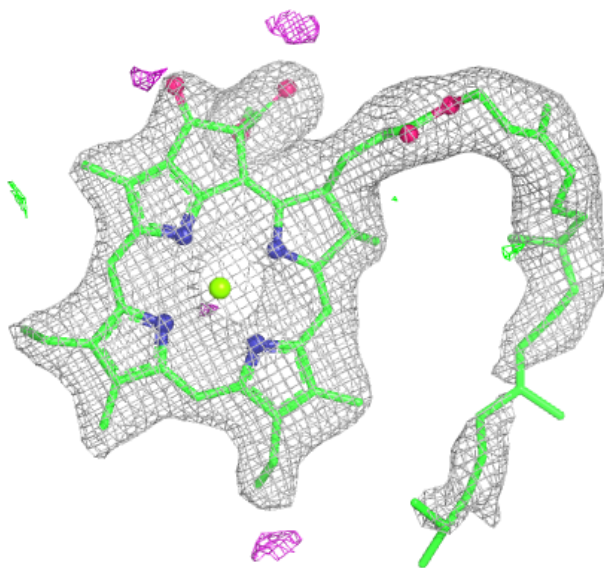
**Electron density around BCR t 101:**

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



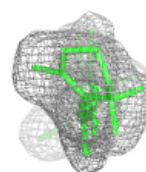
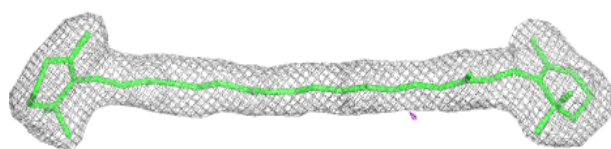
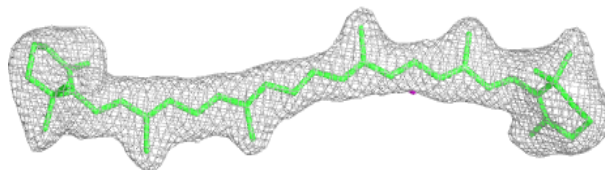
Electron density around CLA C 512:

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

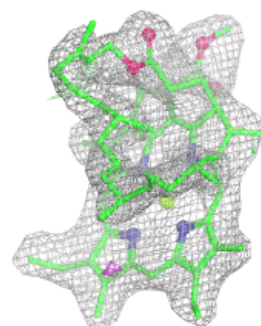
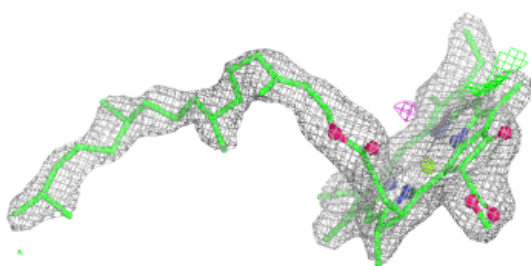
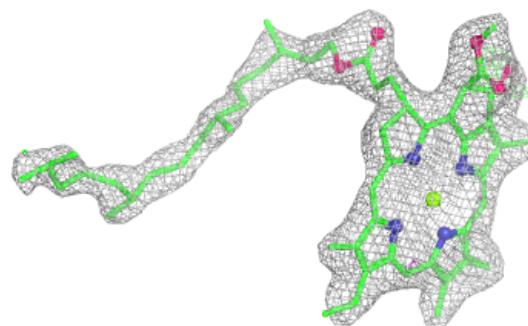


Electron density around BCR b 618:

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

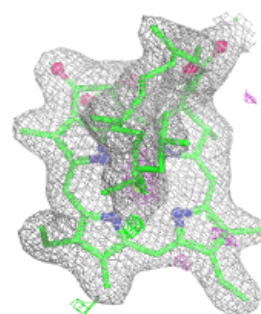
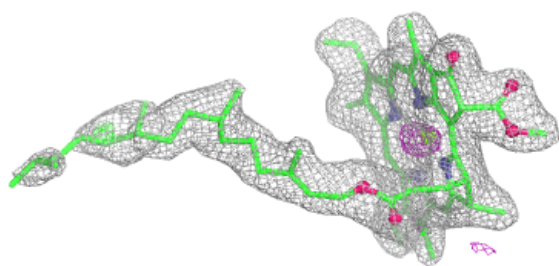
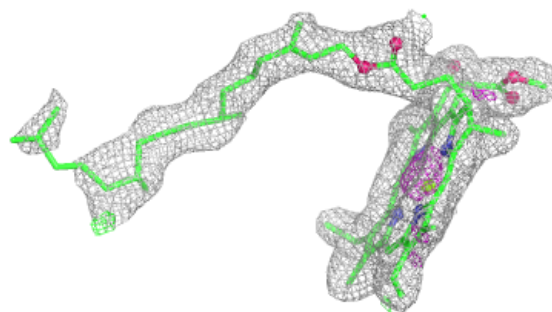
**Electron density around CLA c 511:**

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

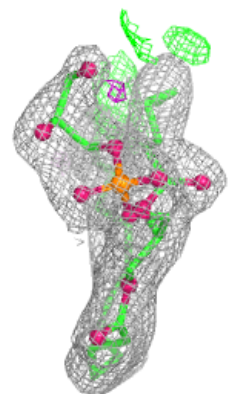
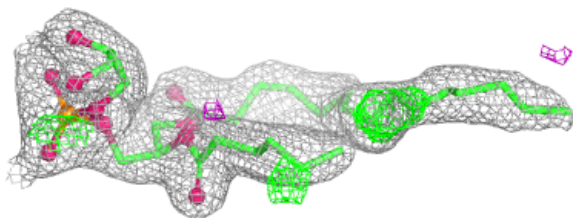
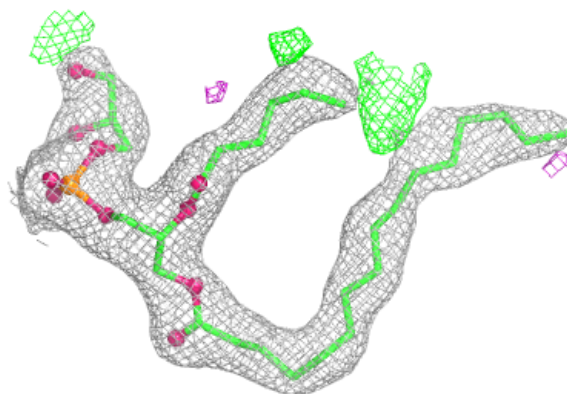


Electron density around CLA C 508:

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

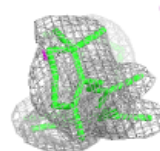
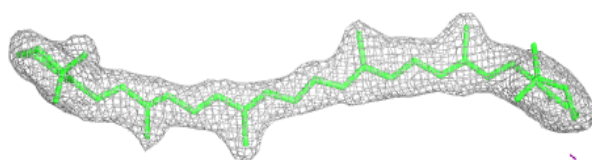
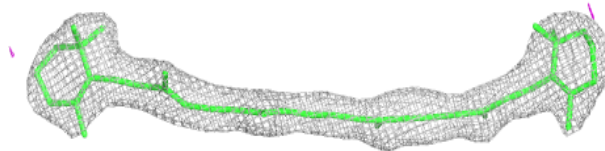
**Electron density around LHG d 409:**

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

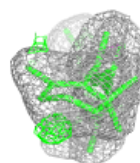
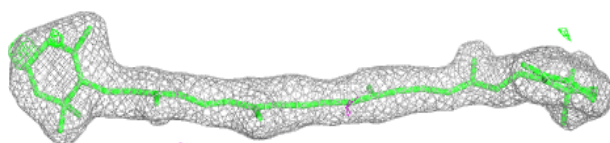
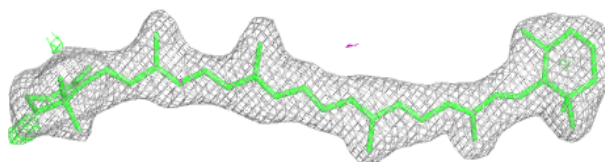


Electron density around BCR K 103:

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

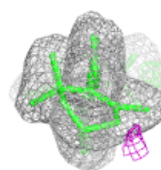
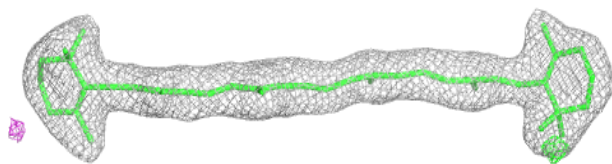
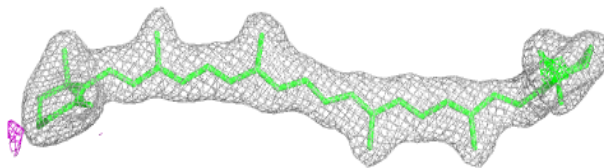
**Electron density around BCR b 617:**

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



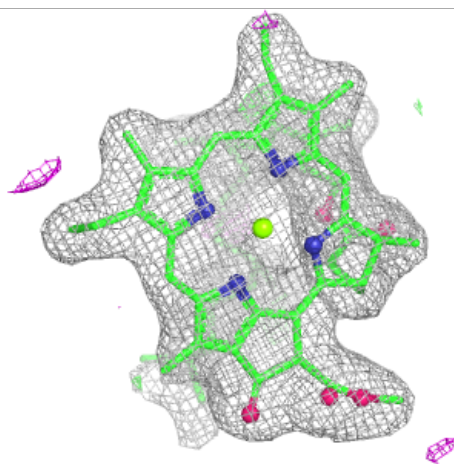
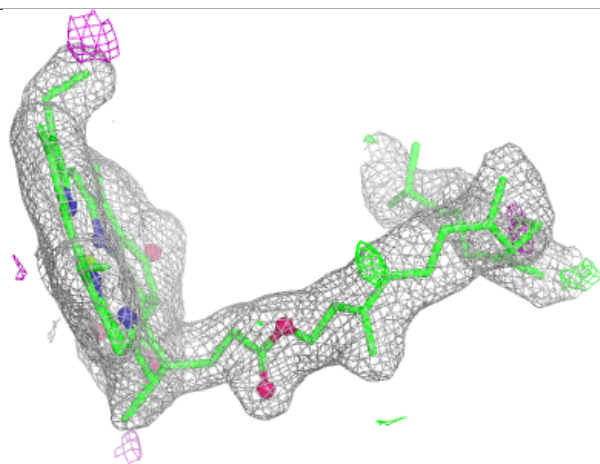
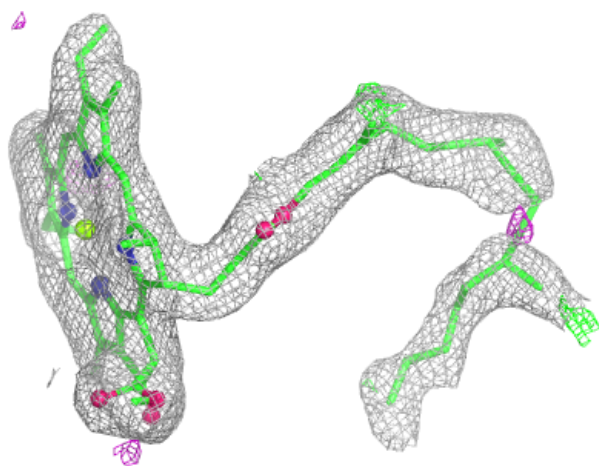
Electron density around BCR A 609:

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



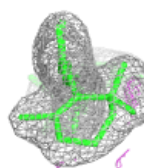
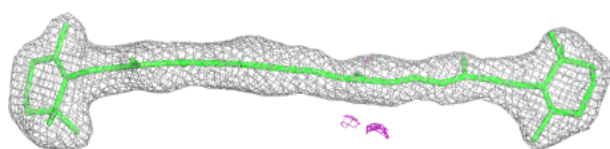
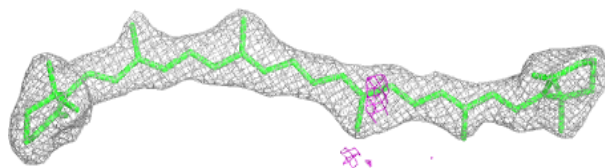
Electron density around CLA B 606:

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

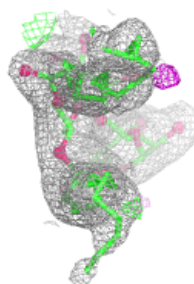
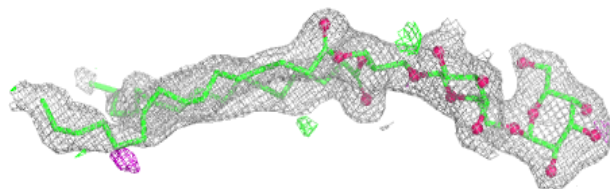
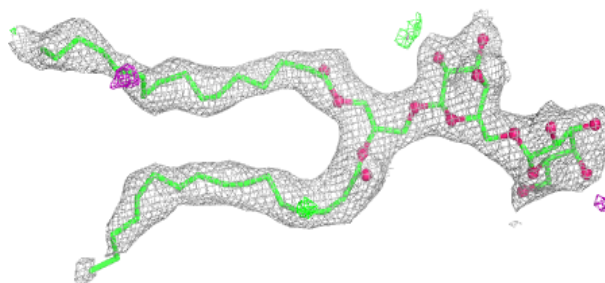


Electron density around BCR c 514:

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

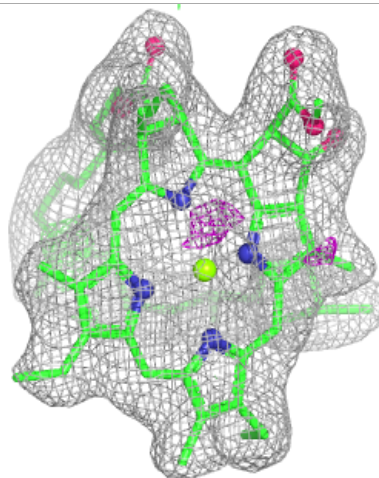
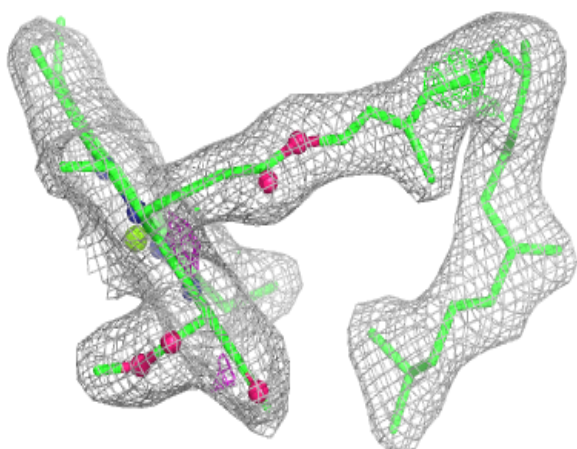
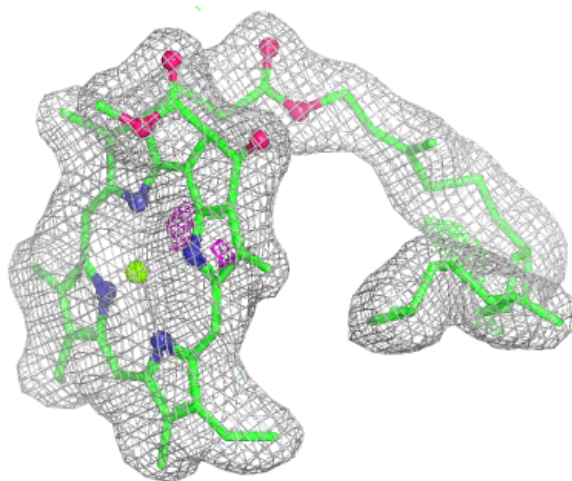
**Electron density around DGD c 517:**

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



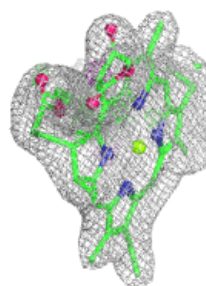
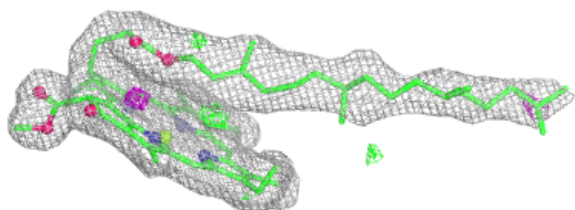
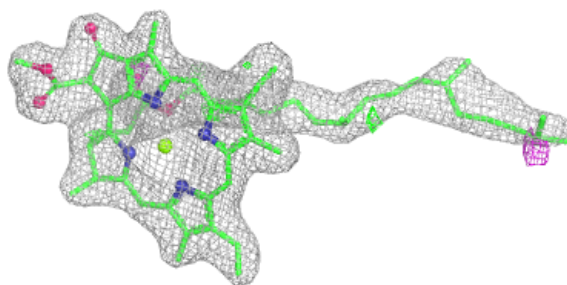
Electron density around CLA C 503:

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



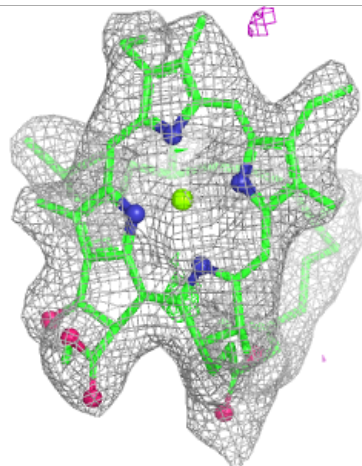
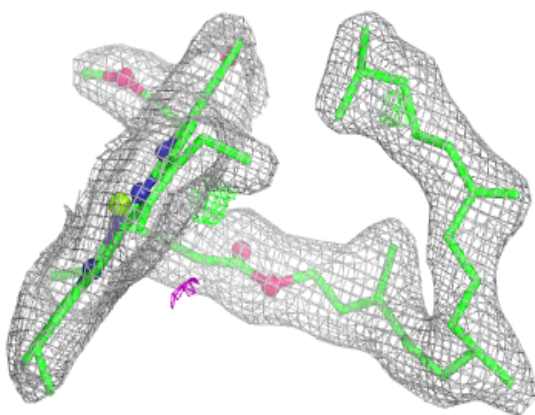
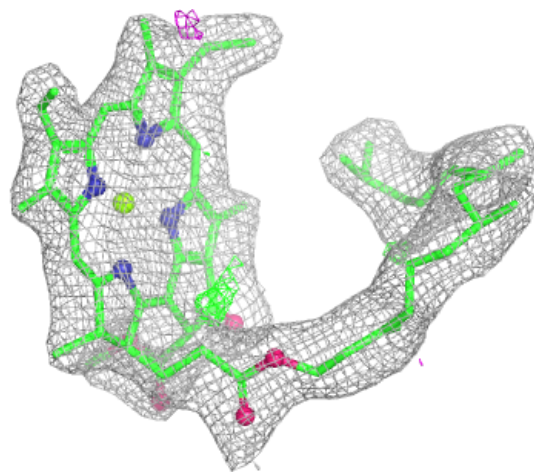
Electron density around CLA b 614:

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



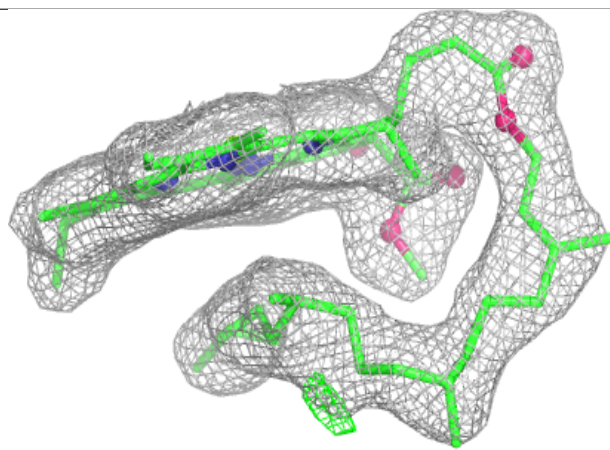
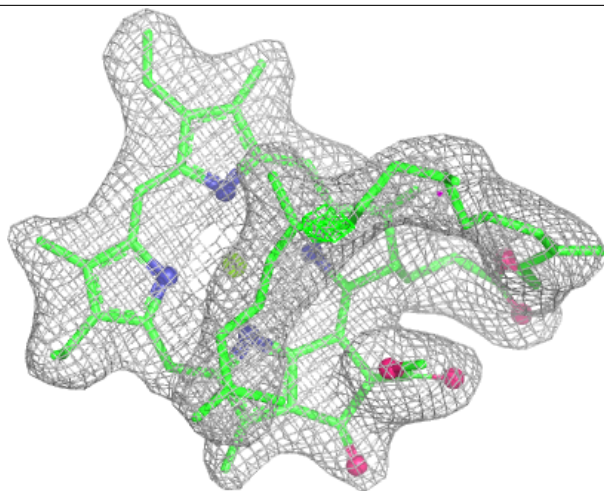
Electron density around CLA c 503:

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



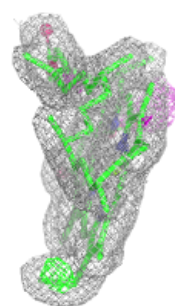
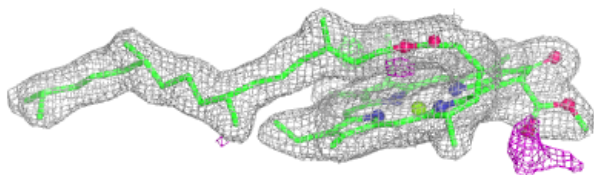
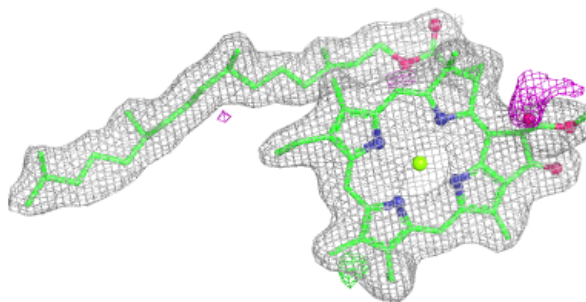
Electron density around CLA c 510:

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

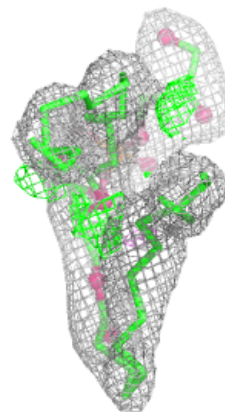
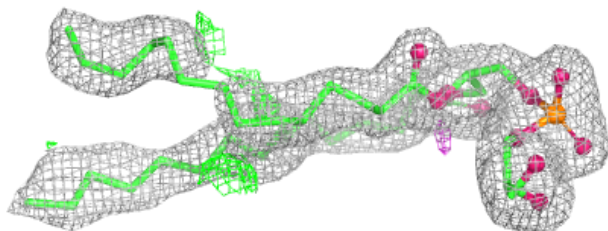
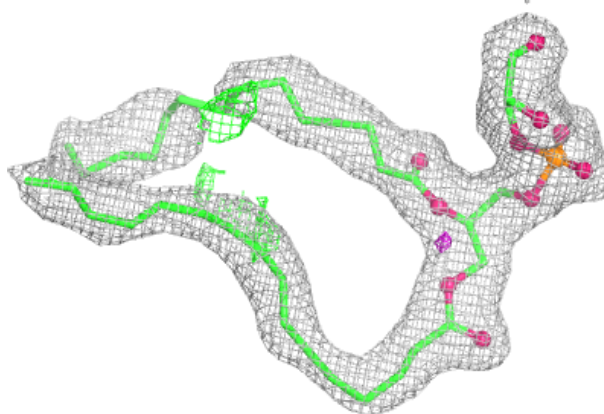


Electron density around CLA C 501:

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

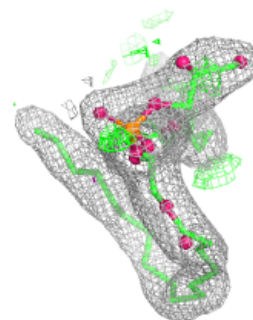
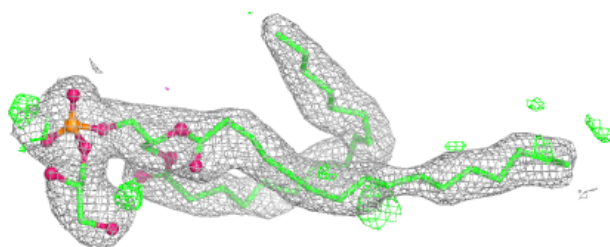
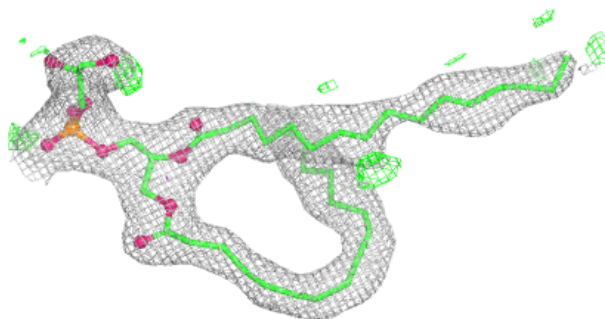
**Electron density around LHG D 410:**

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

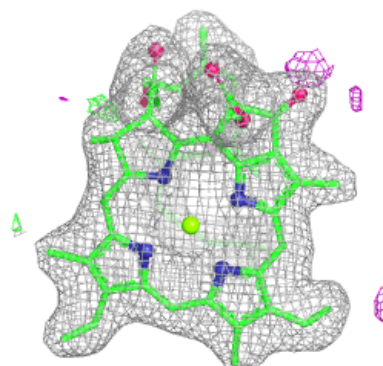
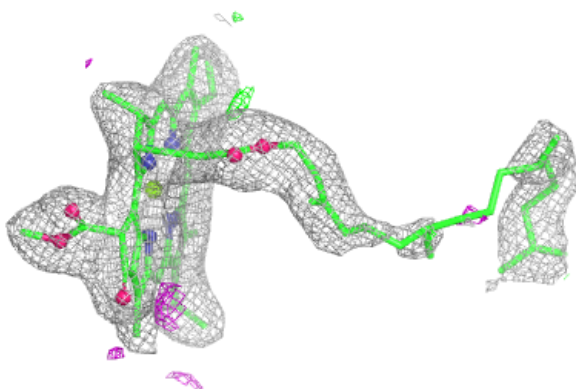
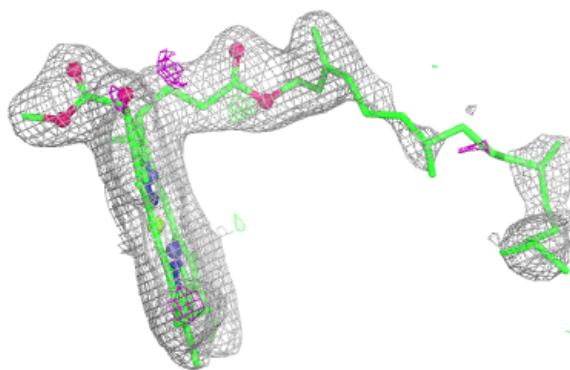


Electron density around LHG D 412:

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

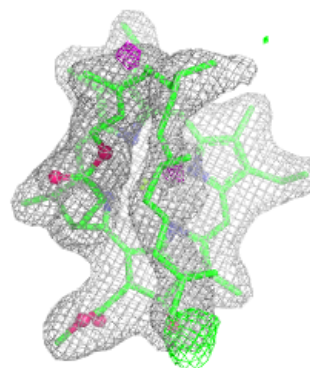
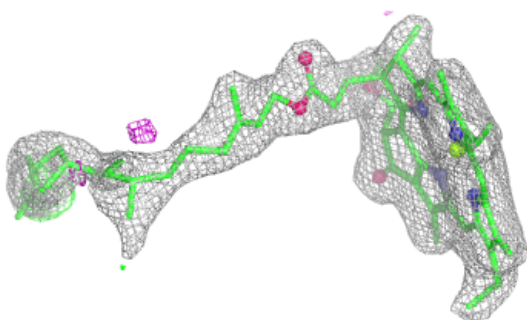
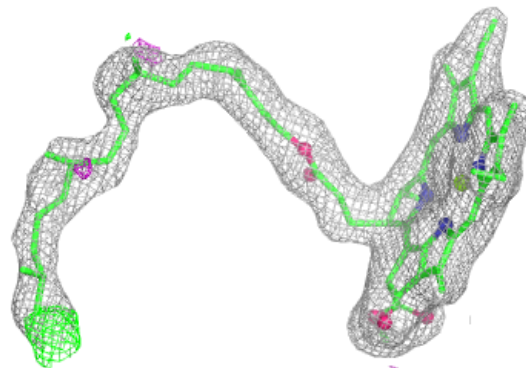
**Electron density around CLA C 506:**

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



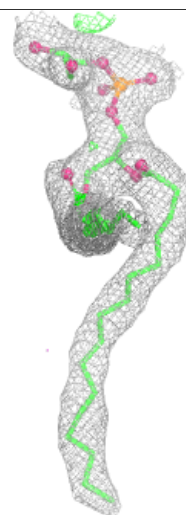
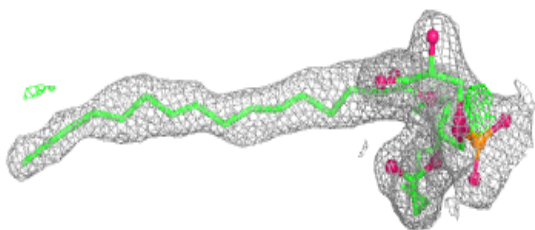
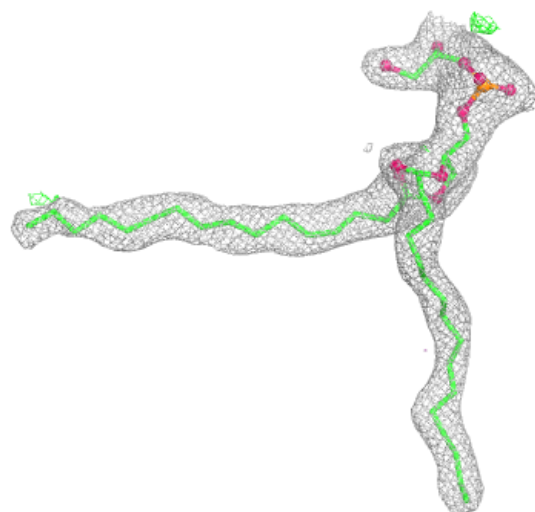
Electron density around CLA b 606:

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



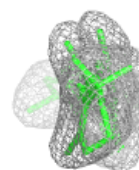
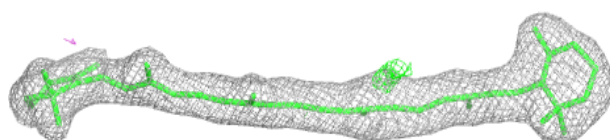
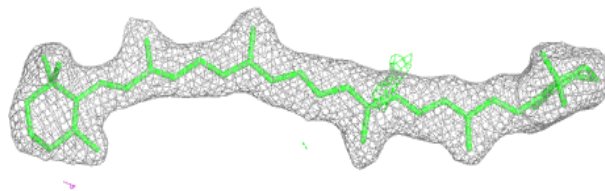
Electron density around LHG 1 101:

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

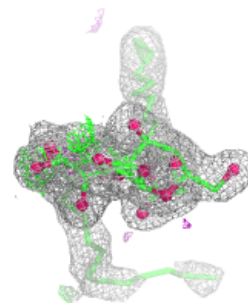
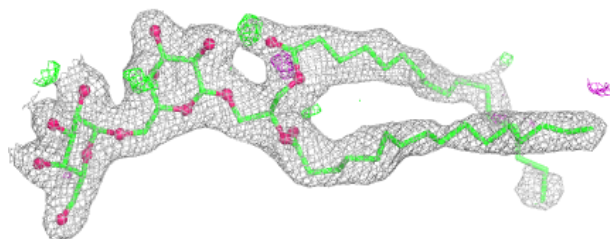
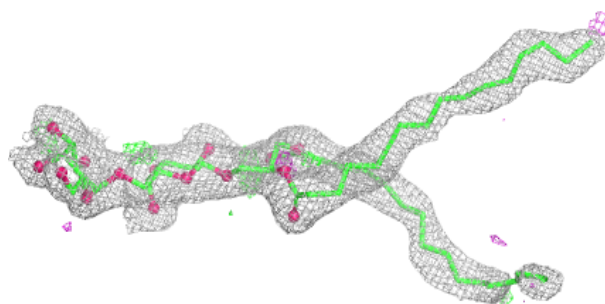


Electron density around BCR B 617:

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

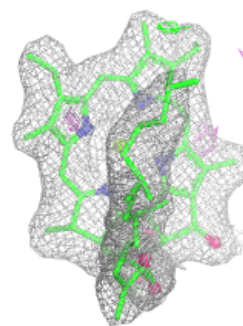
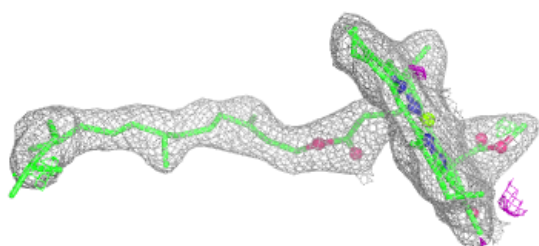
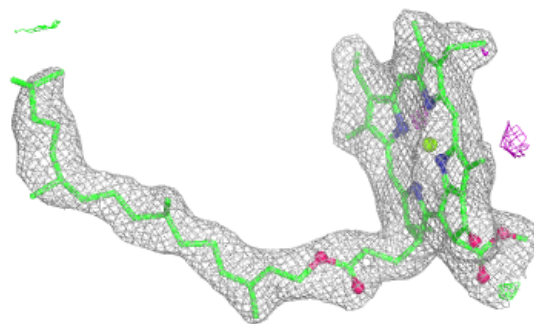
**Electron density around DGD C 515:**

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



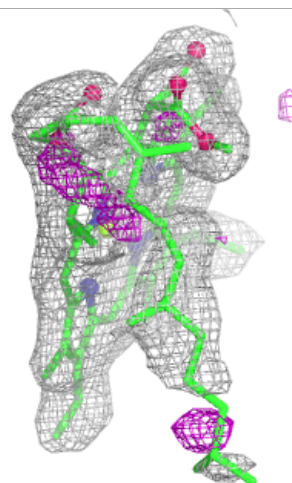
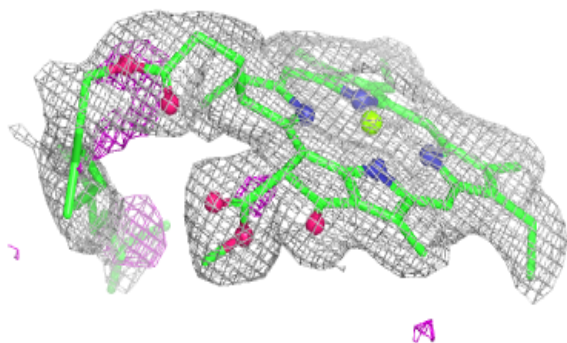
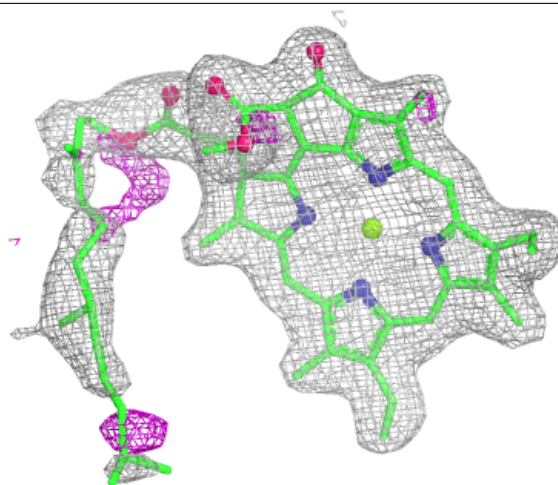
Electron density around CLA b 609:

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



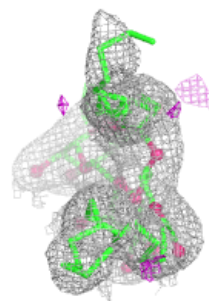
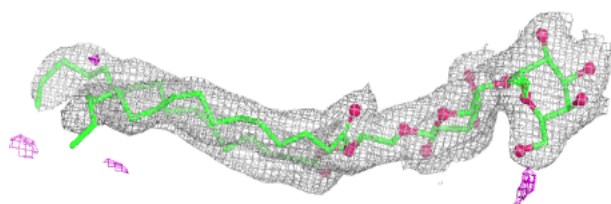
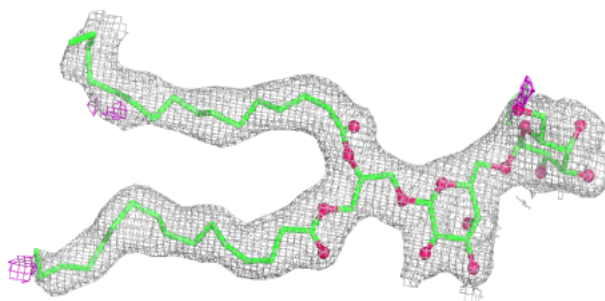
Electron density around CLA B 616:

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



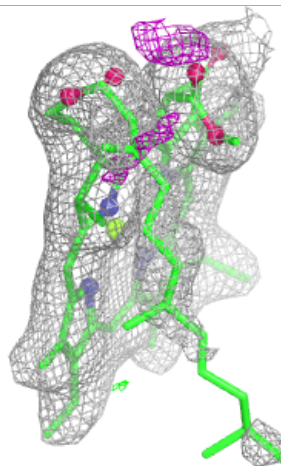
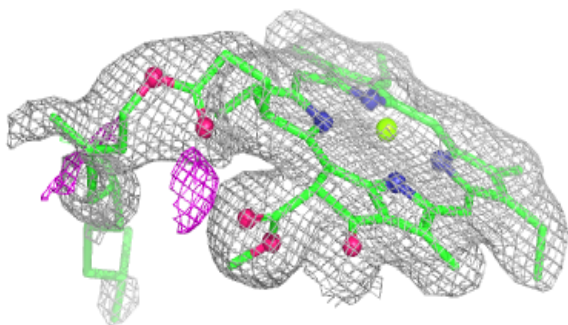
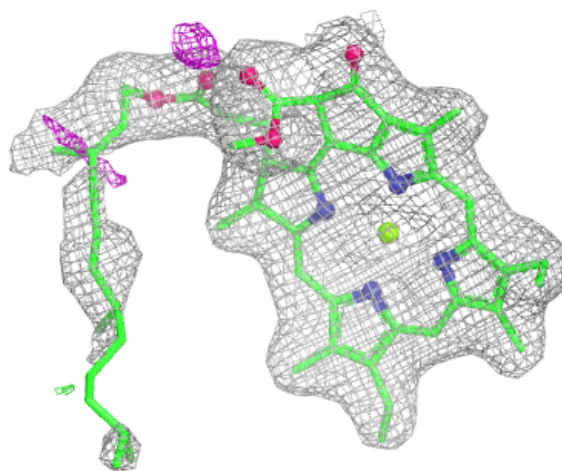
Electron density around DGD J 101:

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



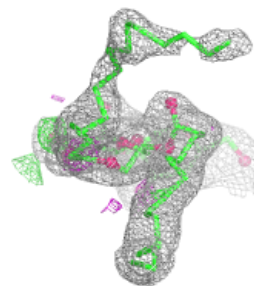
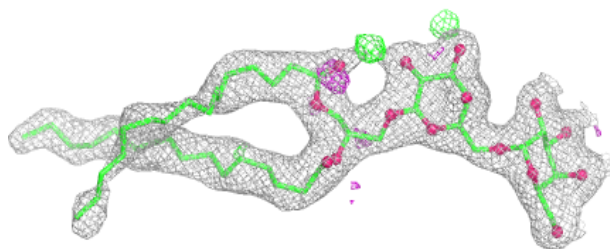
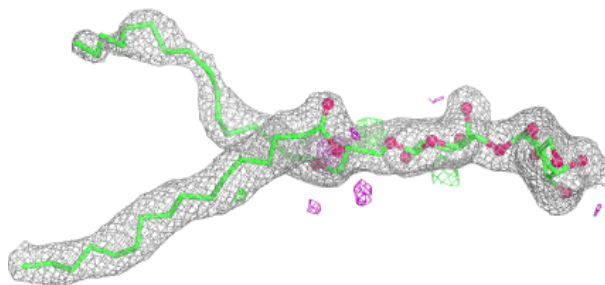
Electron density around CLA b 616:

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

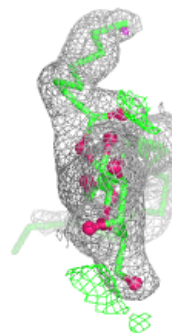
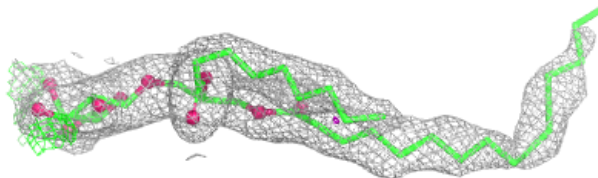
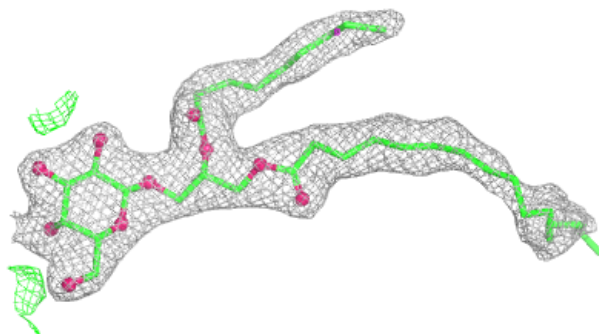


Electron density around DGD c 515:

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

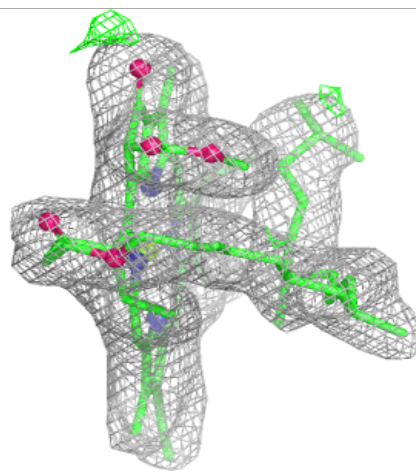
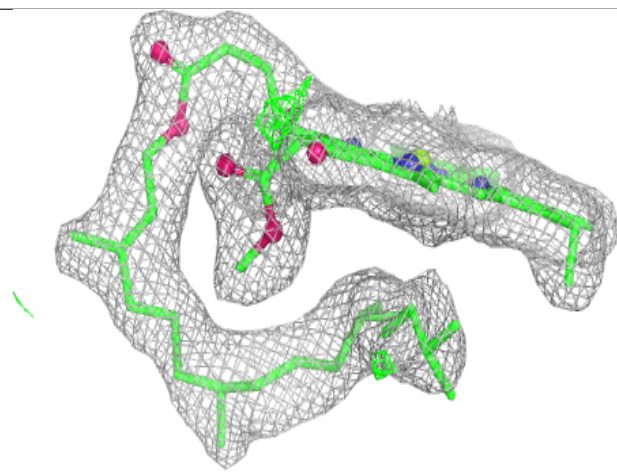
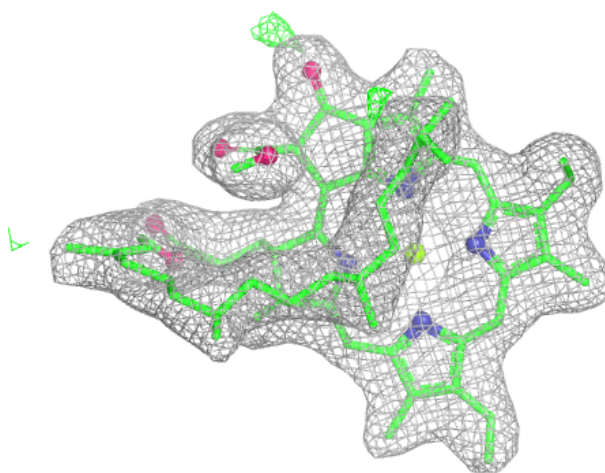
**Electron density around LMG d 411:**

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



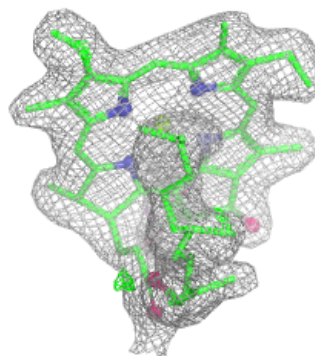
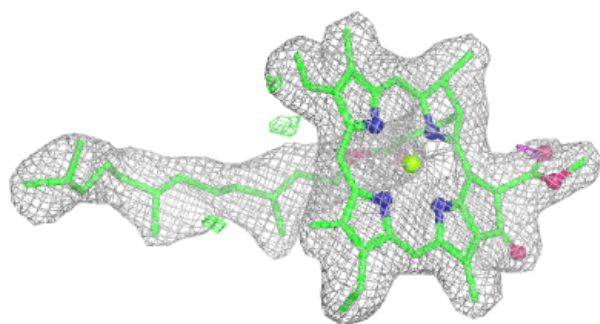
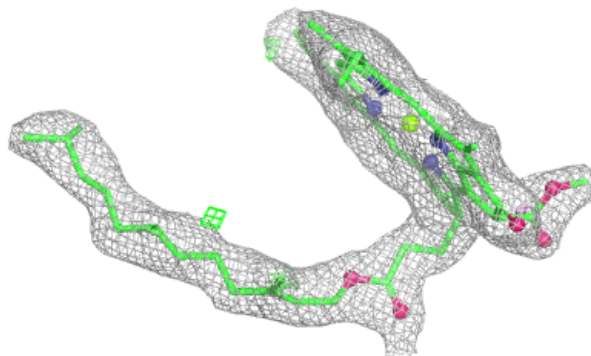
Electron density around CLA C 510:

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

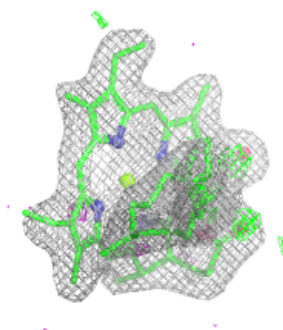
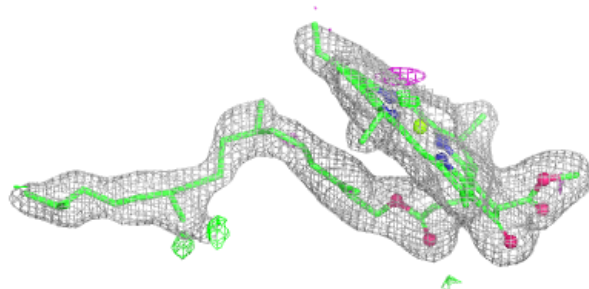
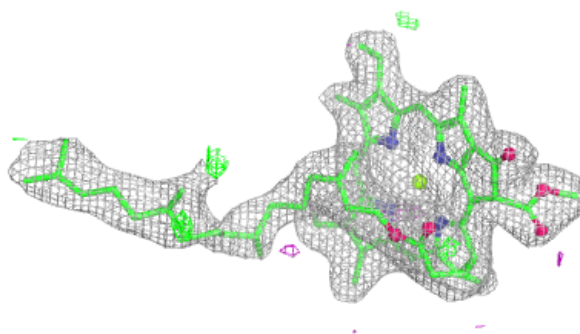


Electron density around CLA c 504:

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

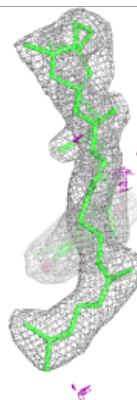
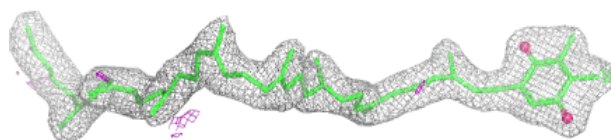
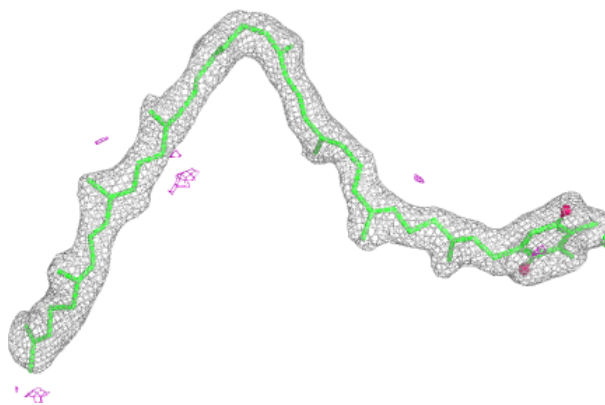
**Electron density around CLA c 505:**

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

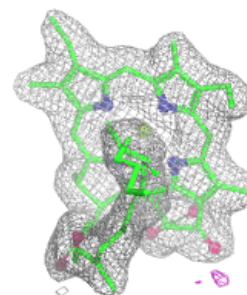
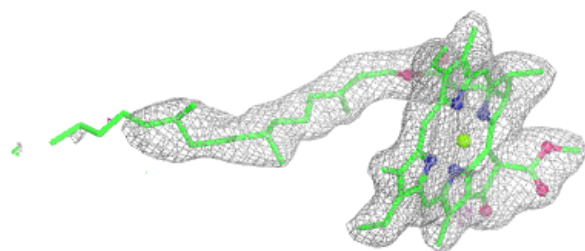
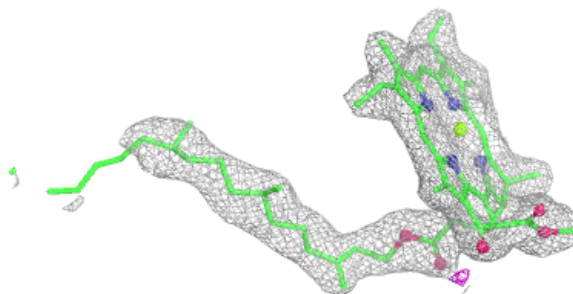


Electron density around PL9 D 406:

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

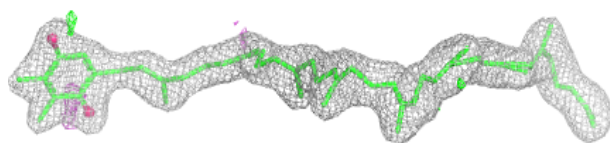
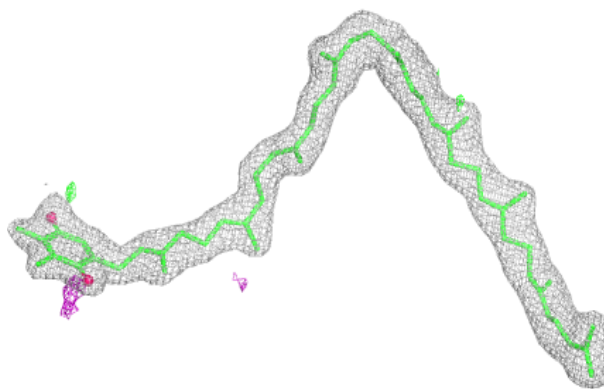
**Electron density around CLA c 508:**

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

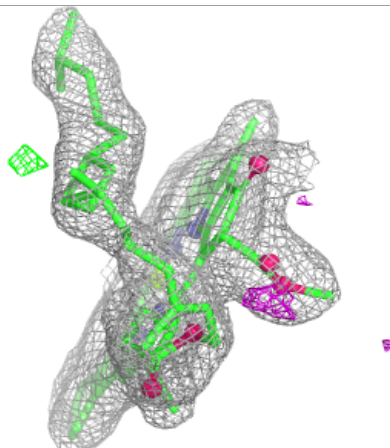
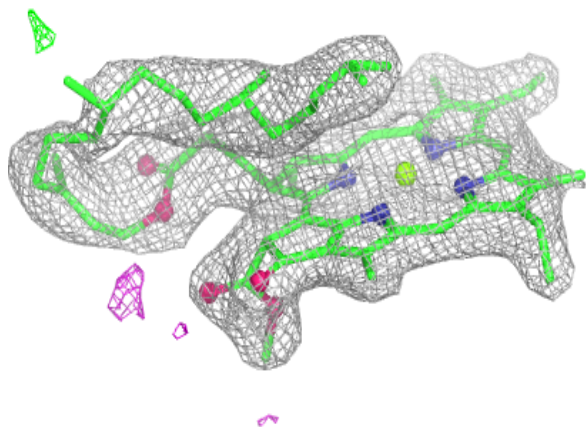
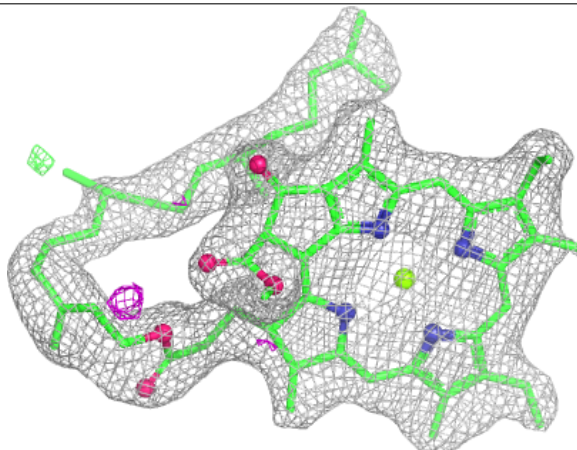


Electron density around PL9 d 406:

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

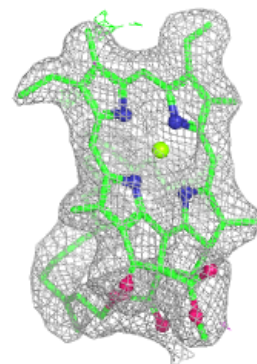
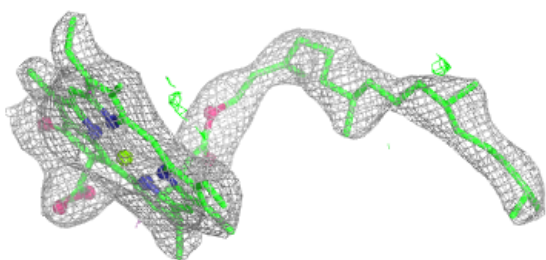
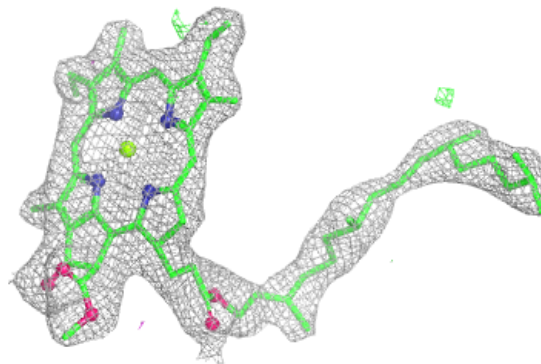
**Electron density around CLA c 509:**

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

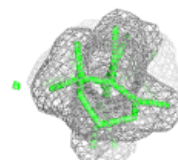
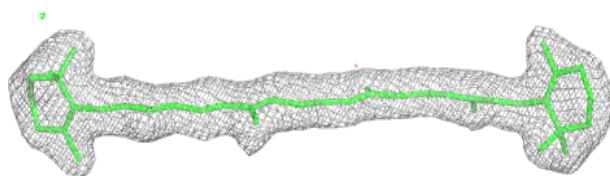
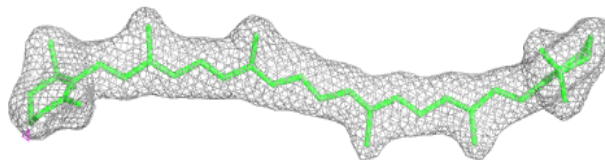


Electron density around CLA C 511:

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

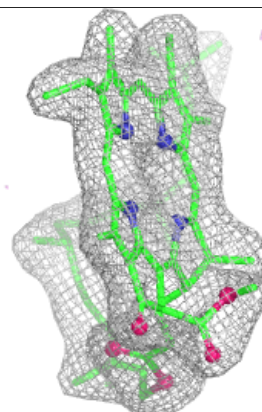
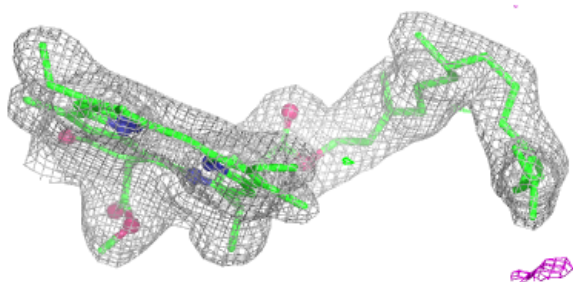
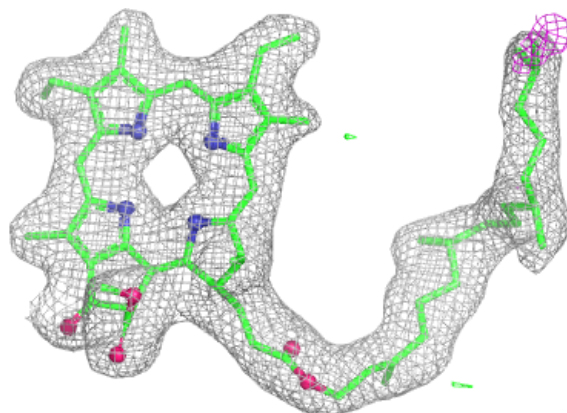
**Electron density around BCR a 609:**

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

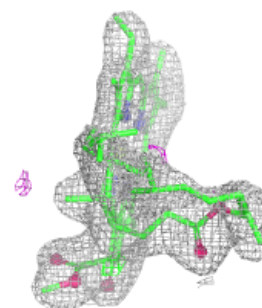
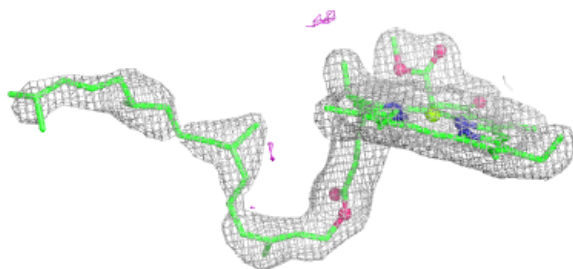
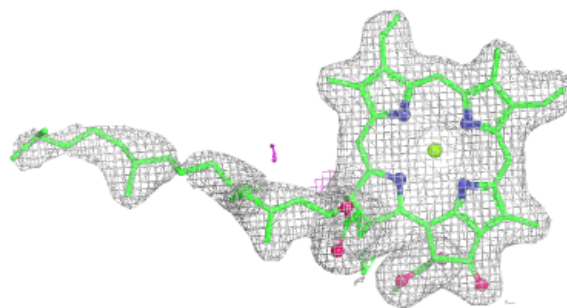


Electron density around PHO d 402:

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

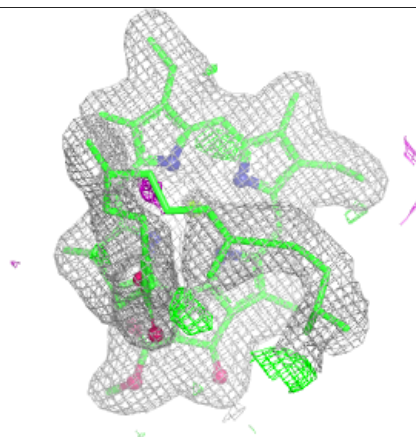
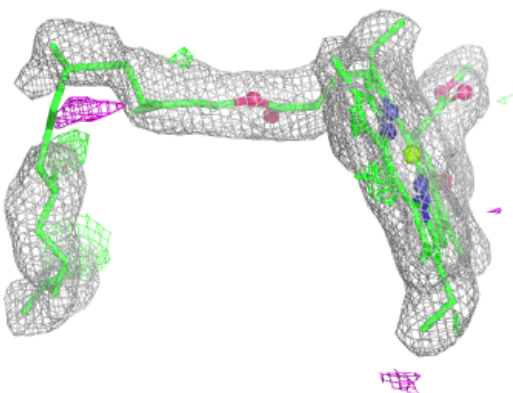
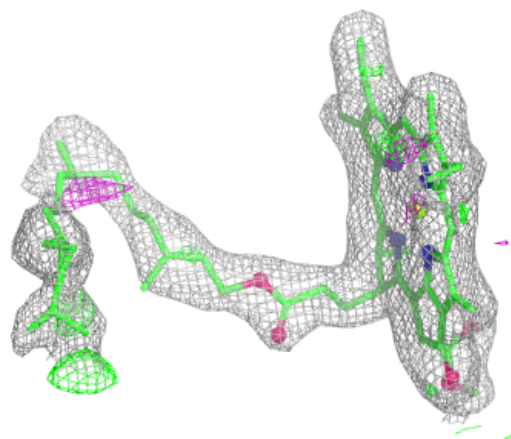
**Electron density around CLA a 606:**

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



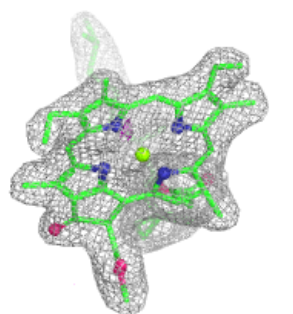
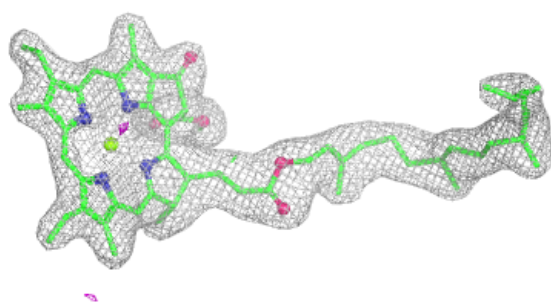
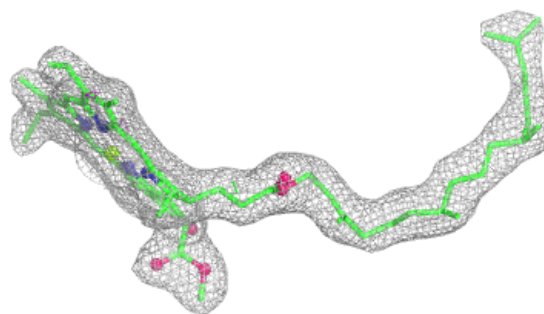
Electron density around CLA a 608:

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

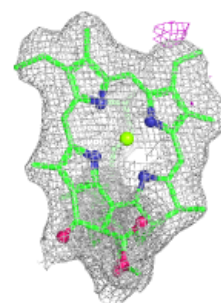
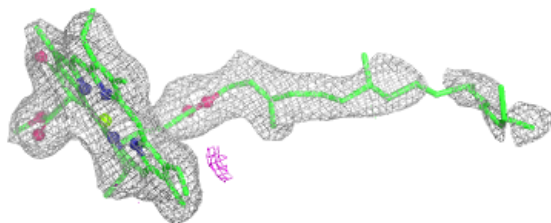
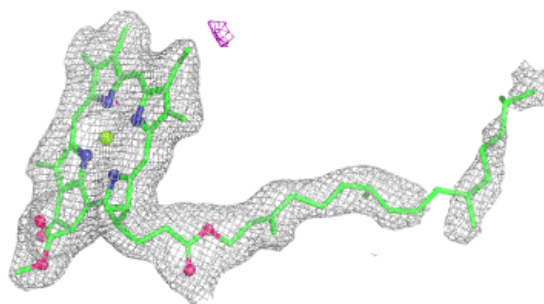


Electron density around CLA d 403:

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

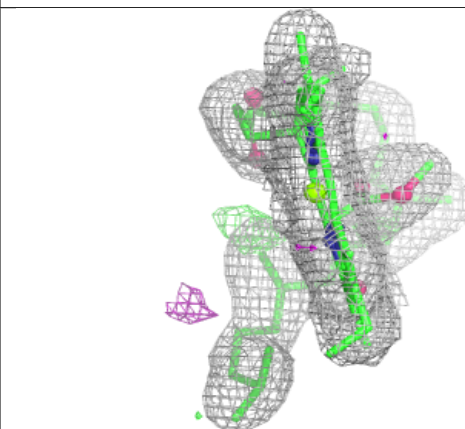
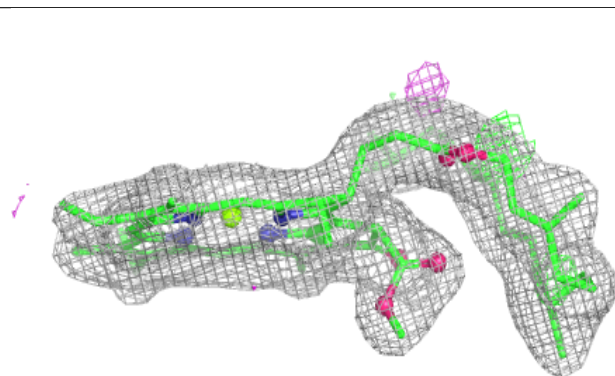
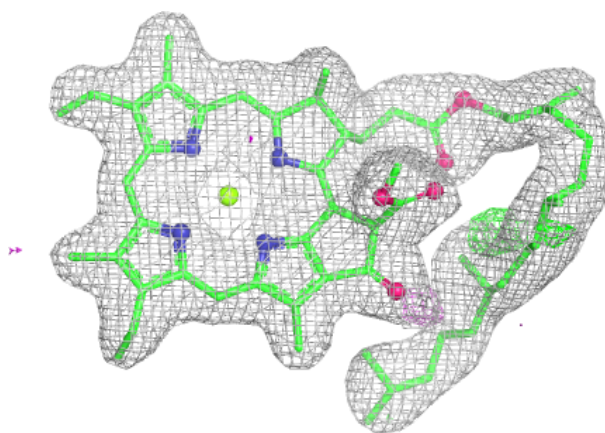
**Electron density around CLA d 404:**

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

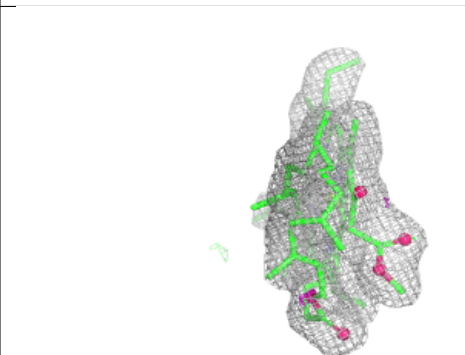
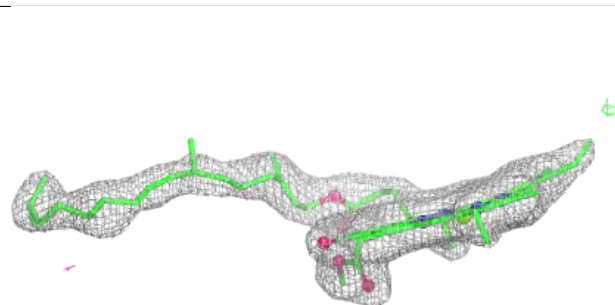
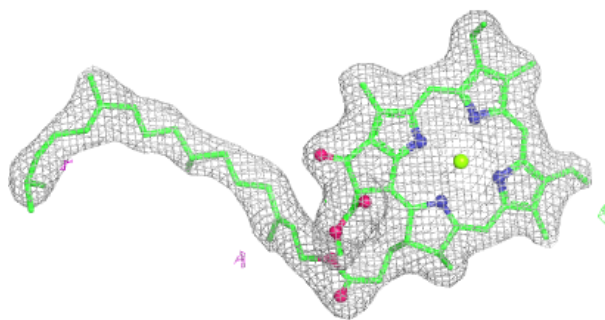


Electron density around CLA B 610:

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

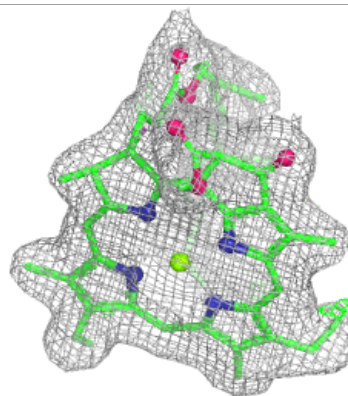
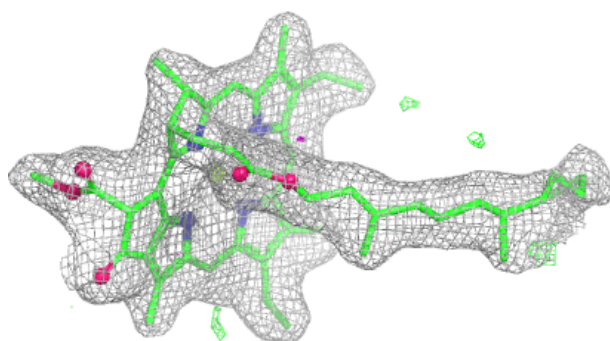
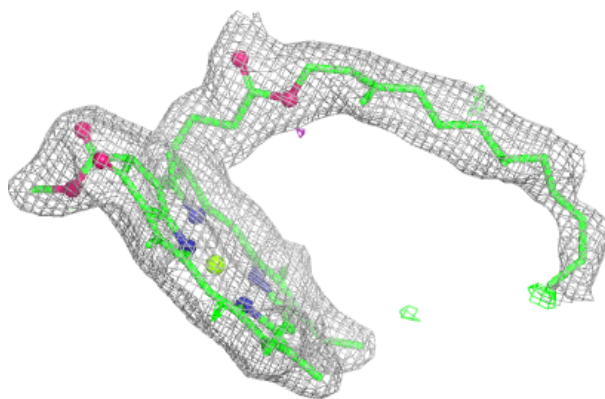
**Electron density around CLA b 602:**

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

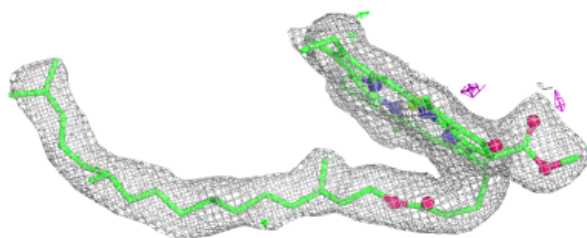
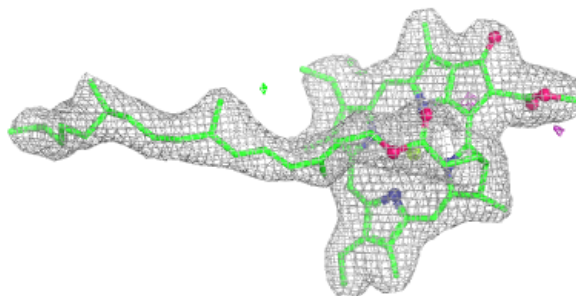


Electron density around CLA C 504:

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

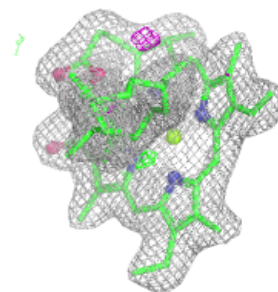
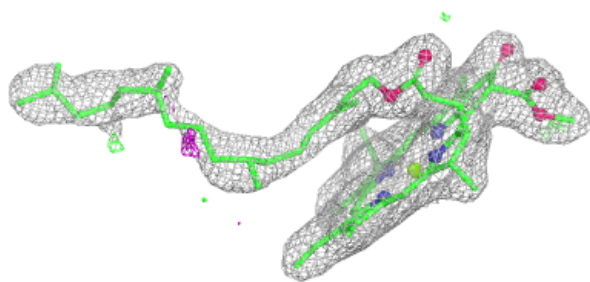
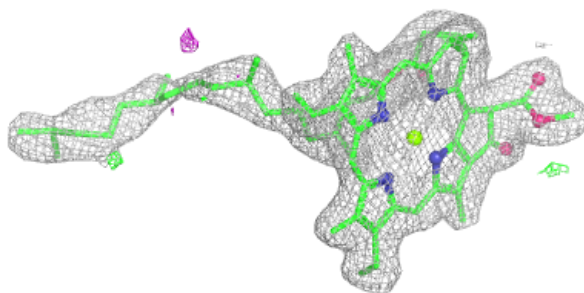
**Electron density around CLA b 608:**

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



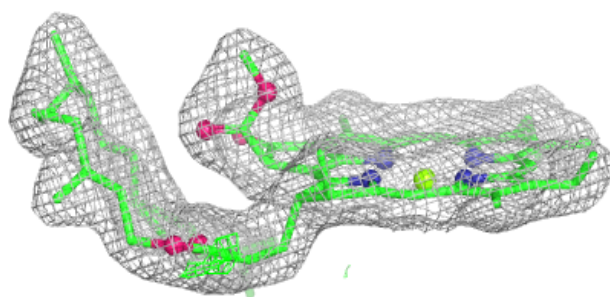
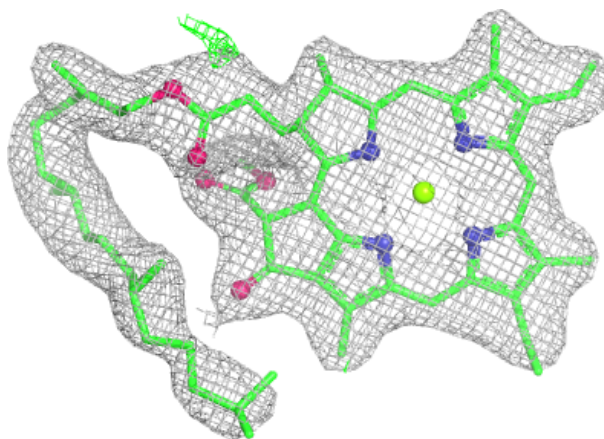
Electron density around CLA C 505:

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



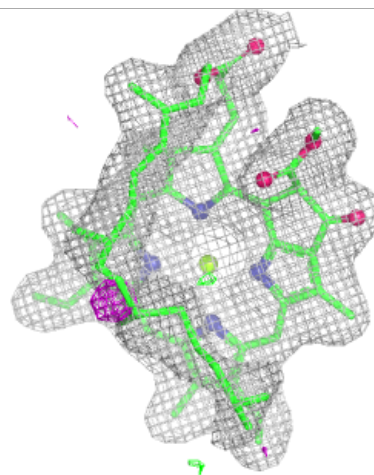
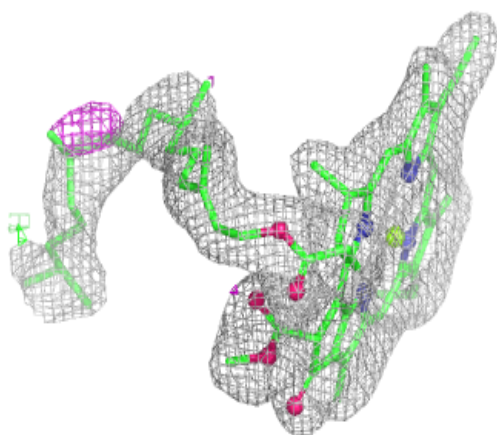
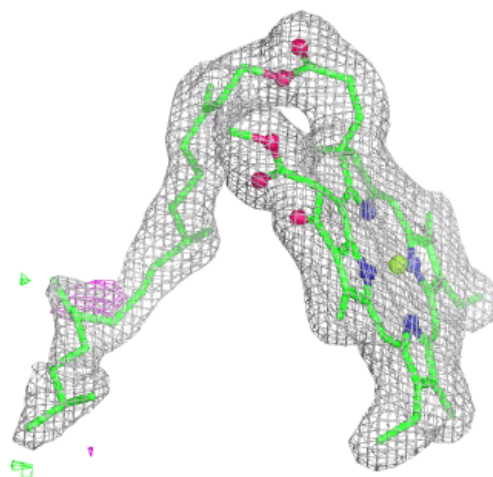
Electron density around CLA b 610:

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



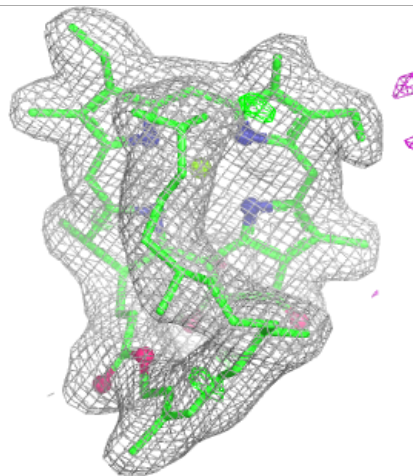
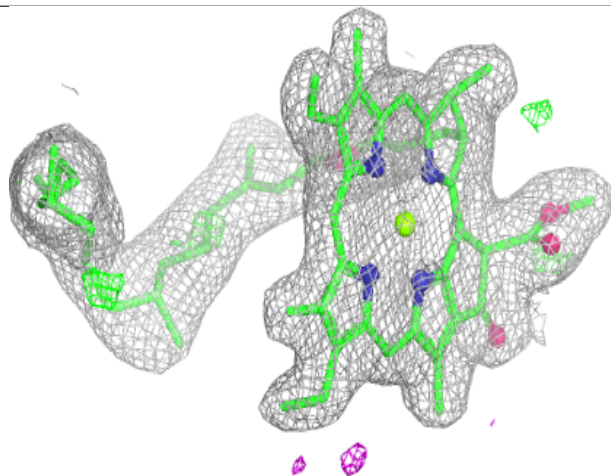
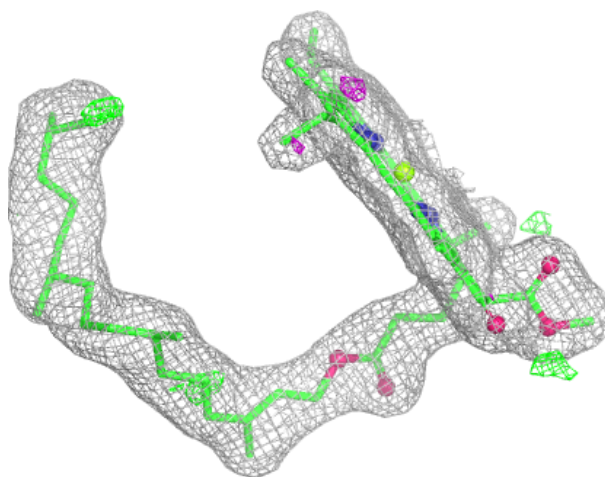
Electron density around CLA b 613:

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



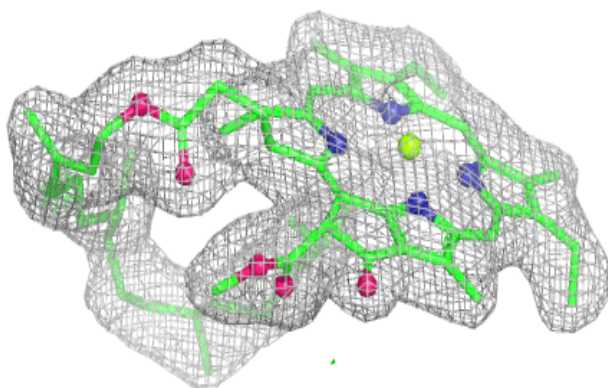
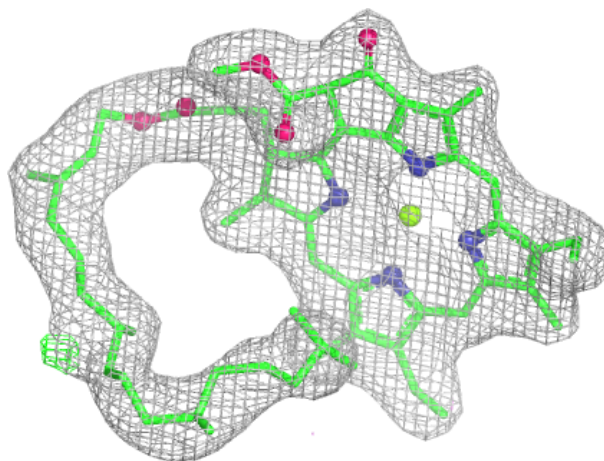
Electron density around CLA B 611:

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



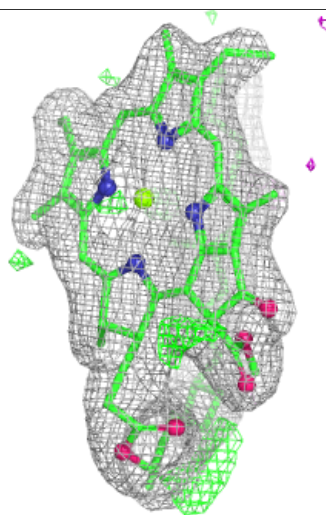
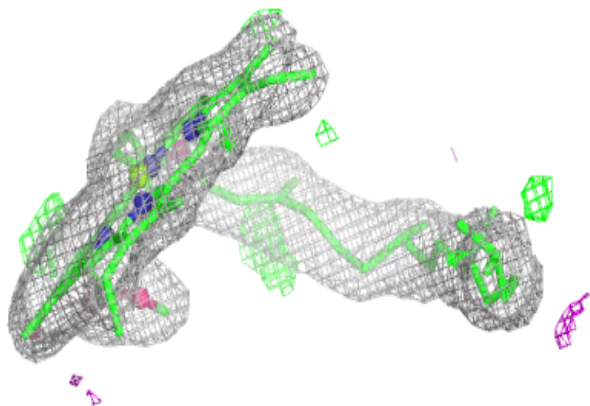
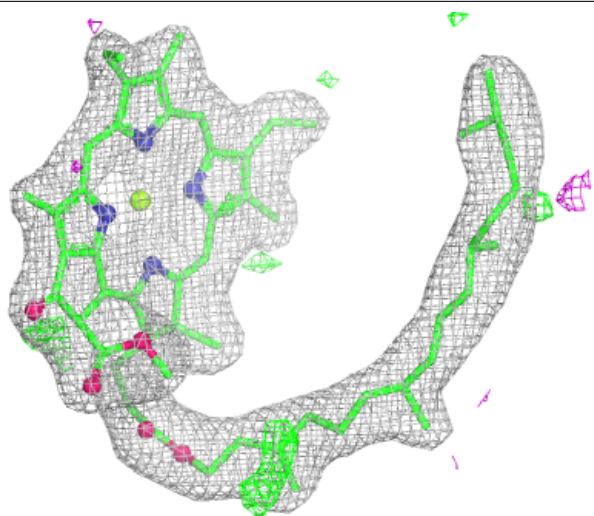
Electron density around CLA b 615:

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



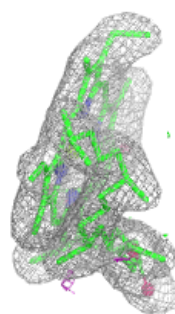
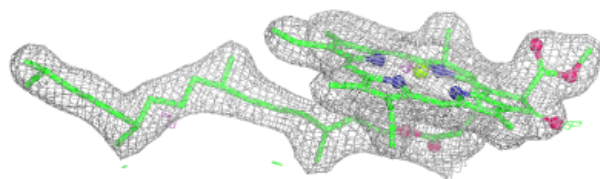
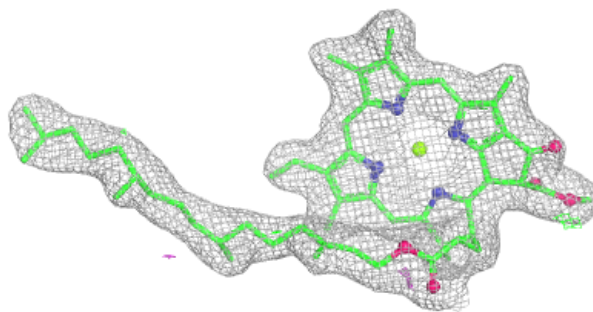
Electron density around CLA C 507:

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

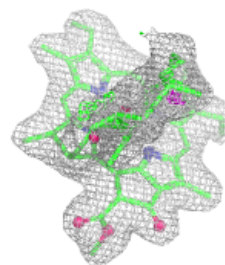
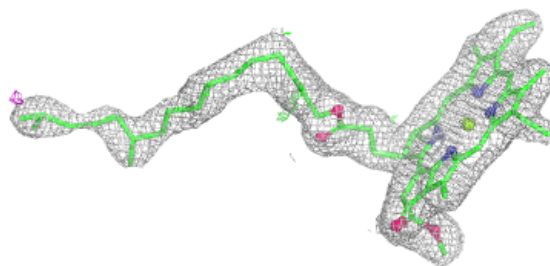


Electron density around CLA c 501:

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

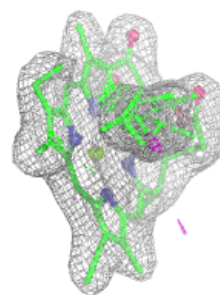
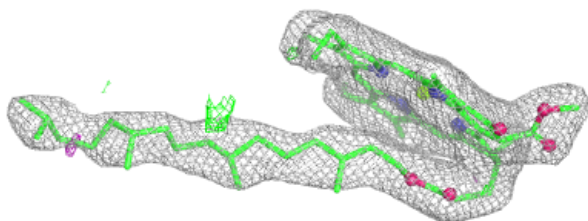
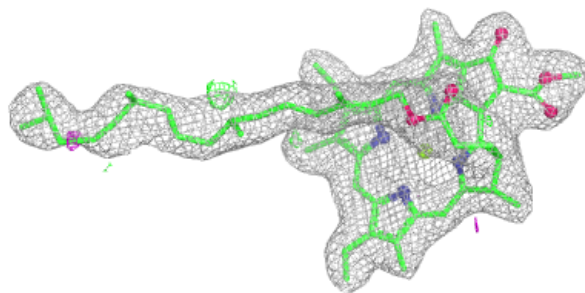
**Electron density around CLA c 502:**

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



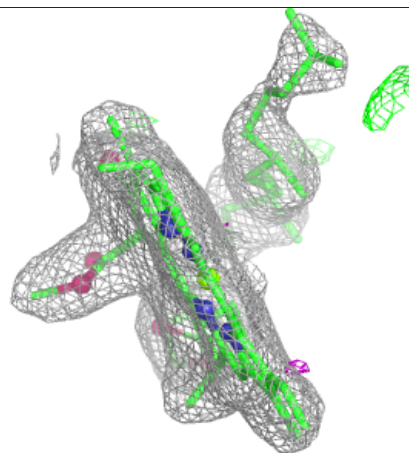
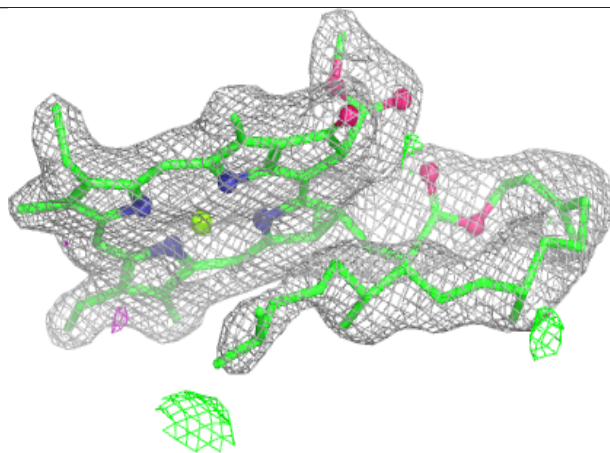
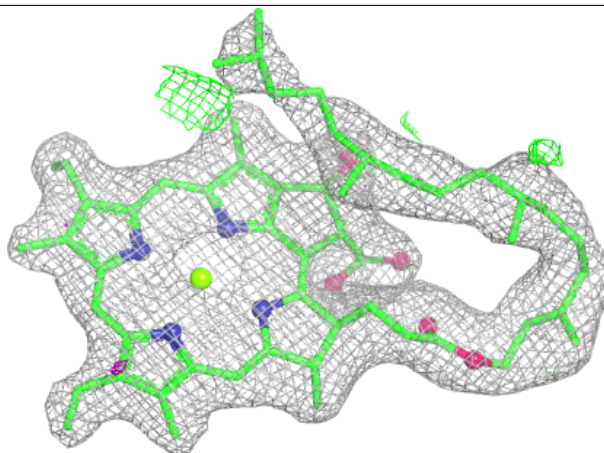
Electron density around CLA B 614:

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



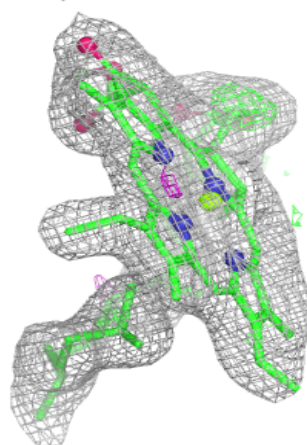
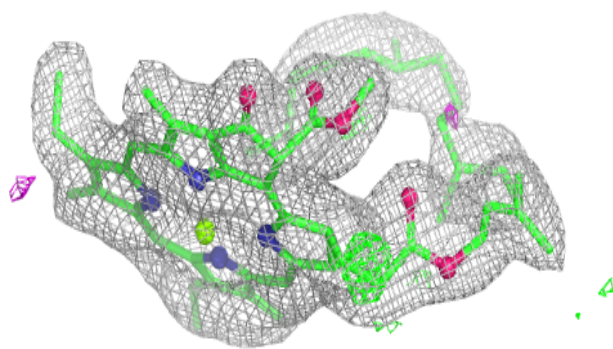
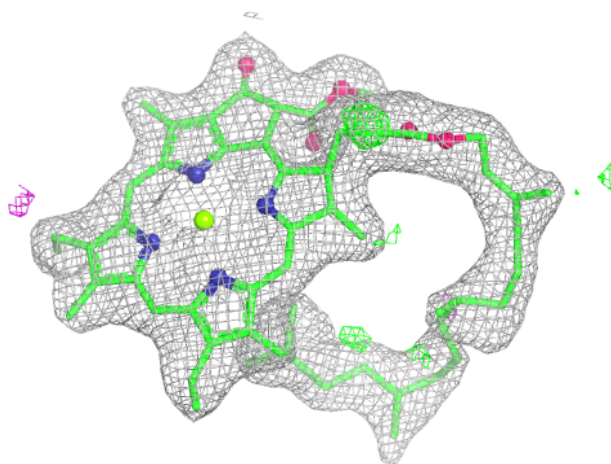
Electron density around CLA C 509:

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



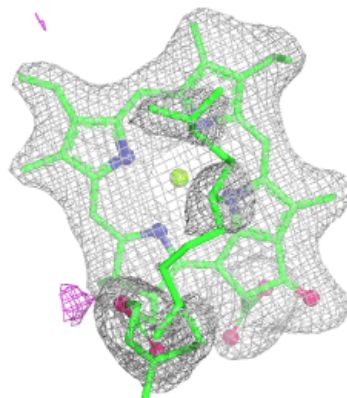
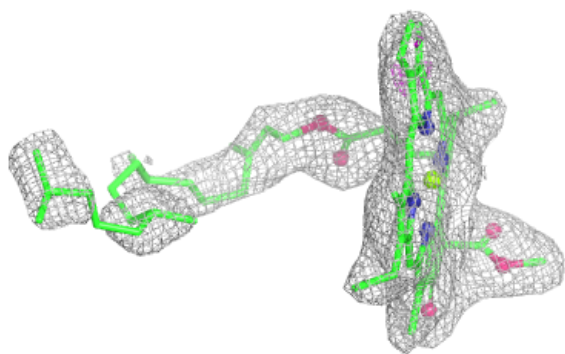
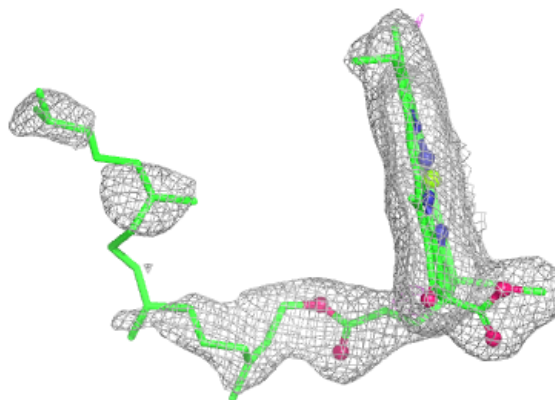
Electron density around CLA B 615:

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



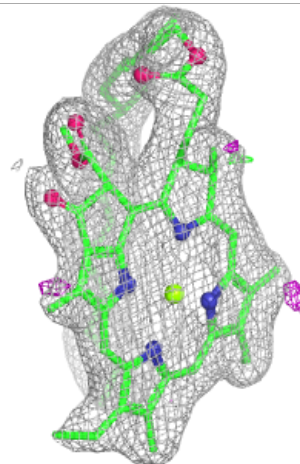
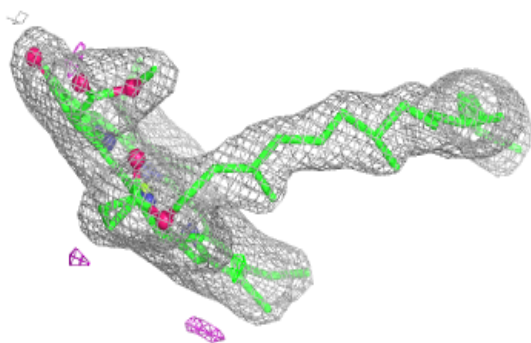
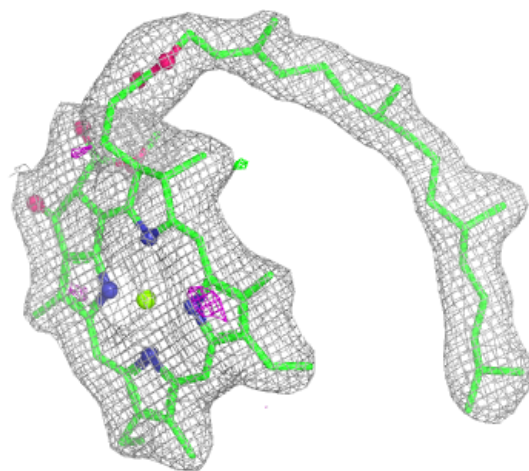
Electron density around CLA c 506:

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



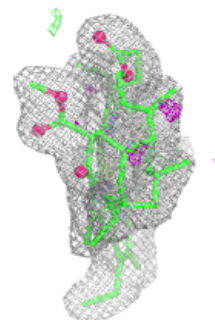
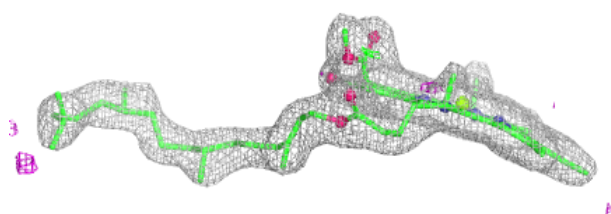
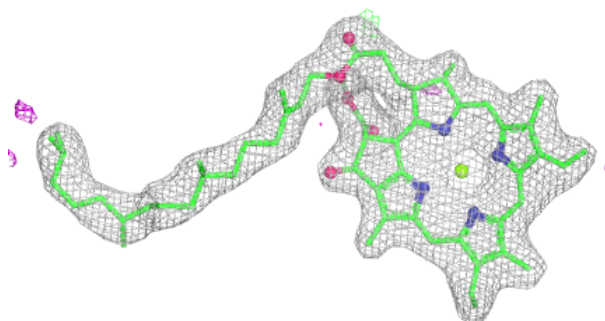
Electron density around CLA c 507:

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

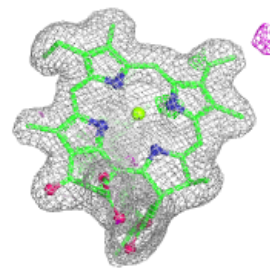
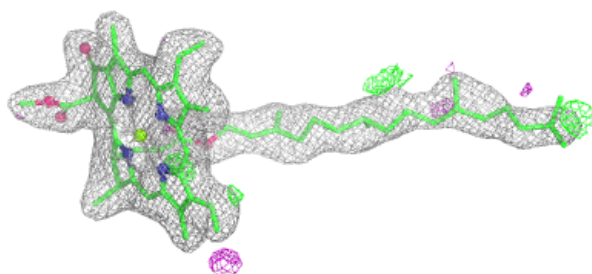
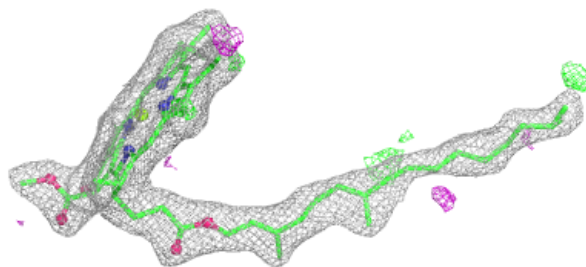


Electron density around CLA B 602:

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

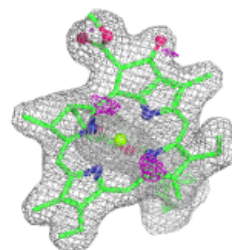
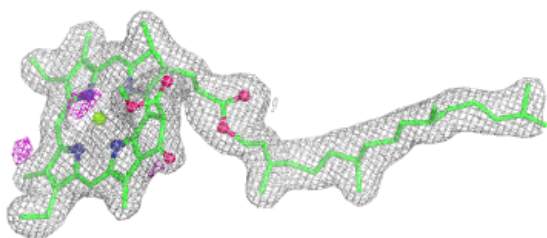
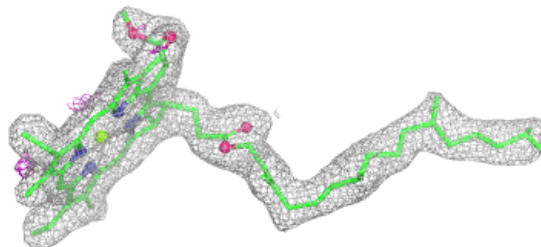
**Electron density around CLA B 607:**

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



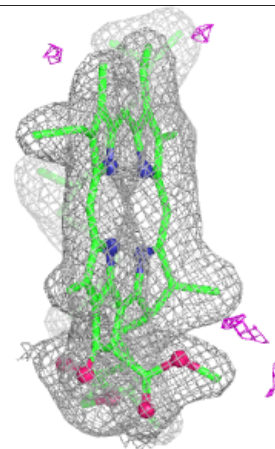
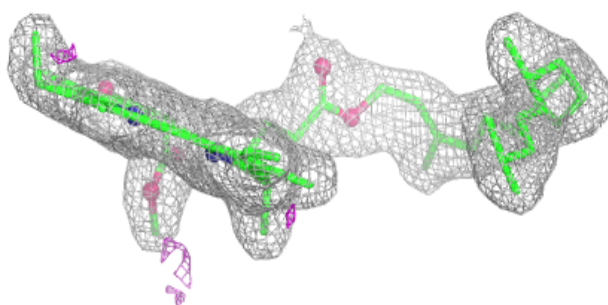
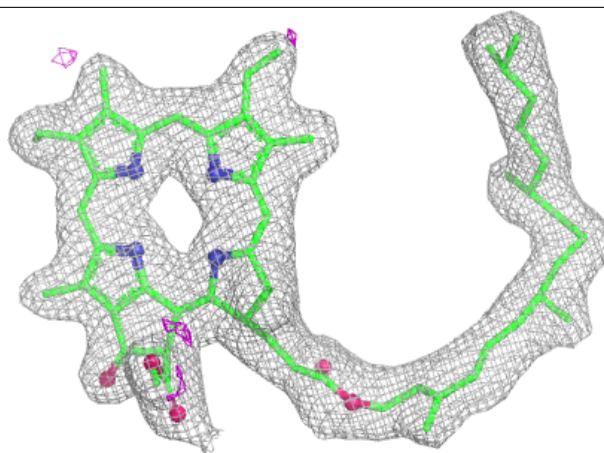
Electron density around CLA C 502:

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



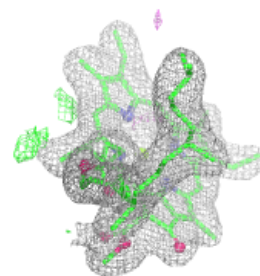
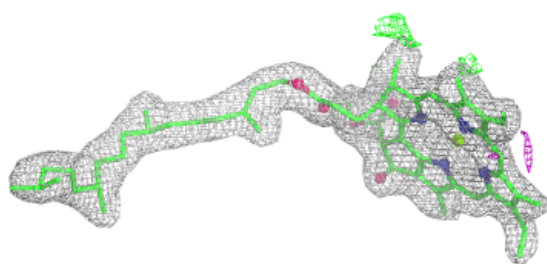
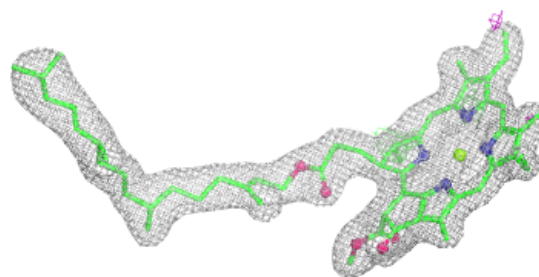
Electron density around PHO a 607:

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

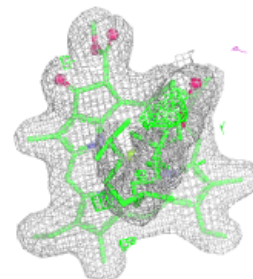
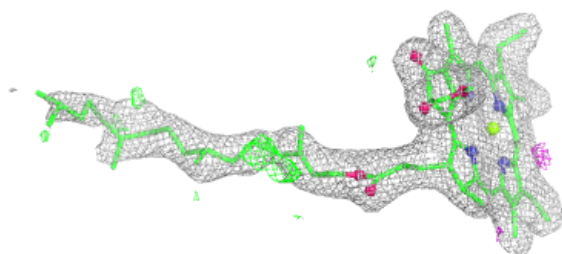
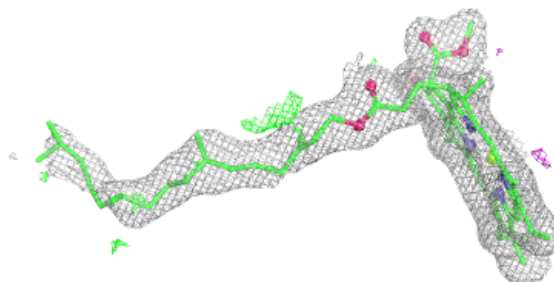


Electron density around CLA a 605:

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

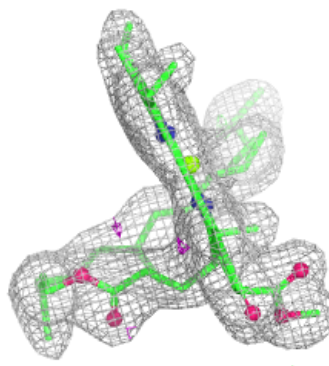
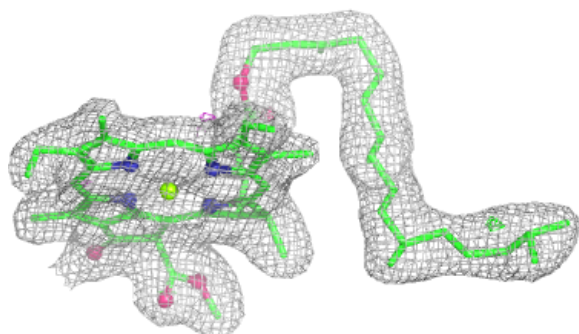
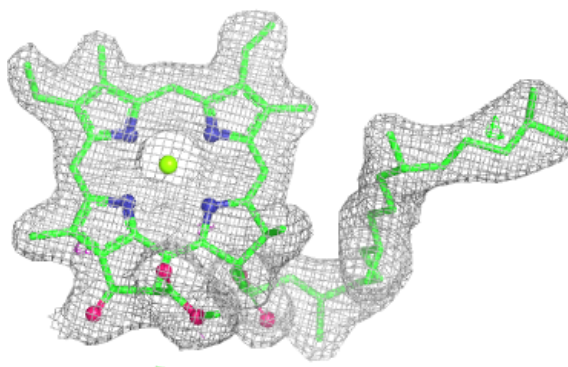
**Electron density around CLA B 604:**

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

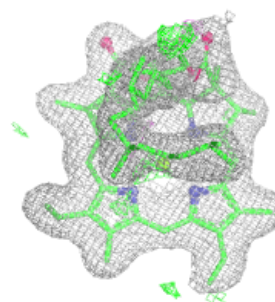
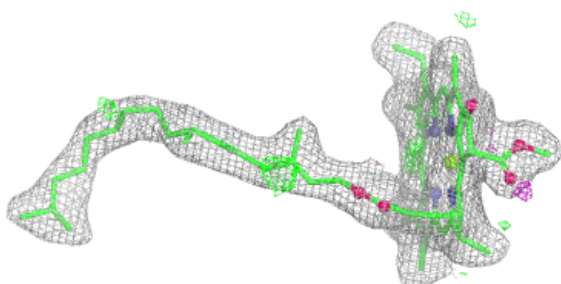
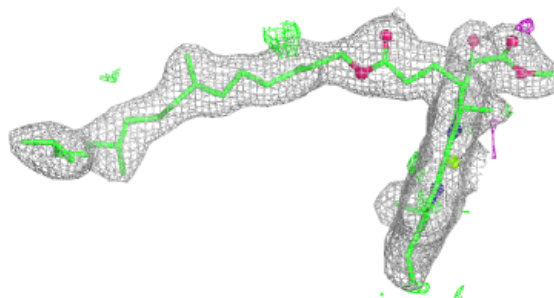


Electron density around CLA a 611:

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

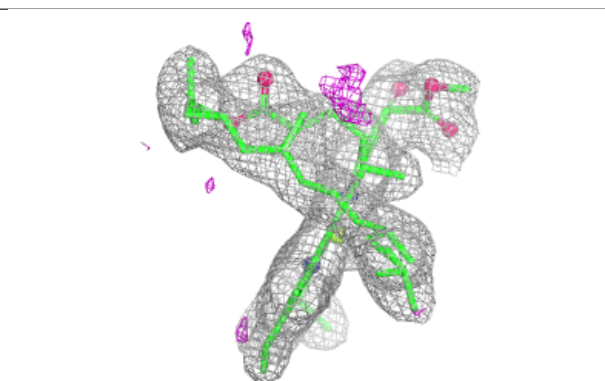
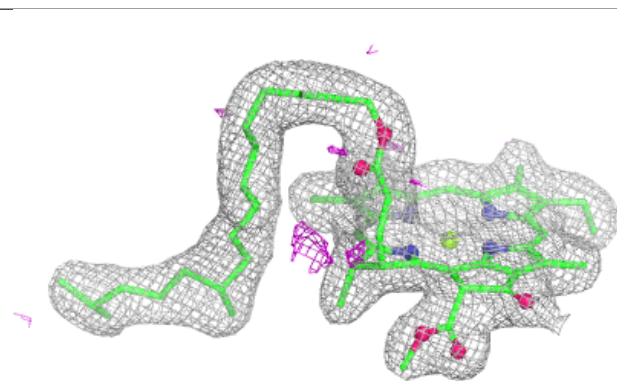
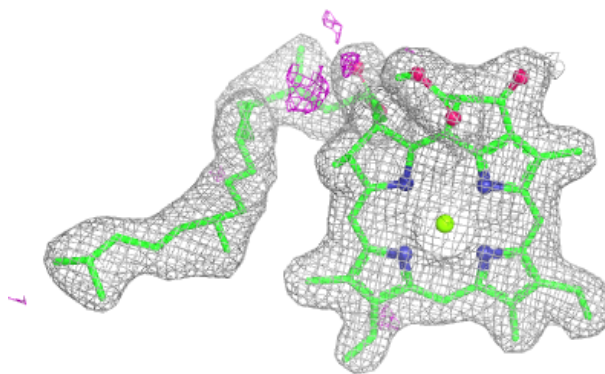
**Electron density around CLA B 605:**

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

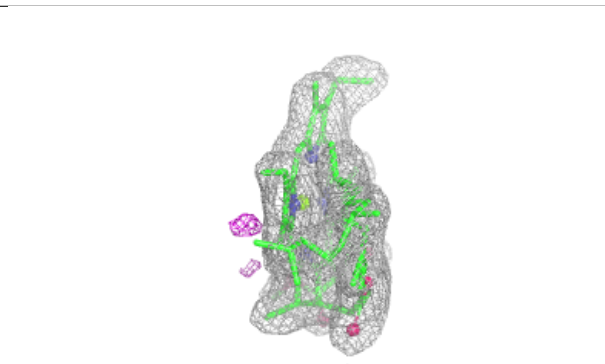
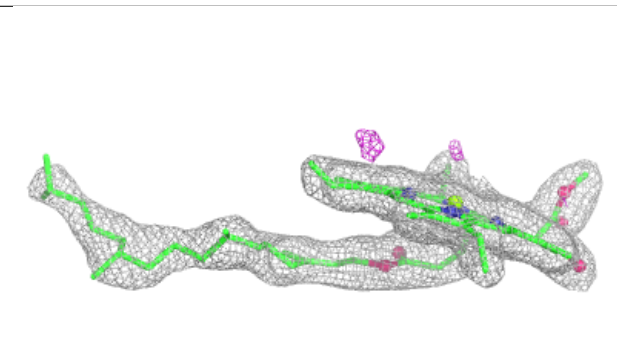
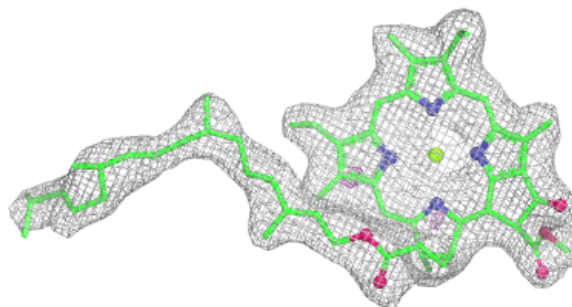


Electron density around CLA A 611:

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

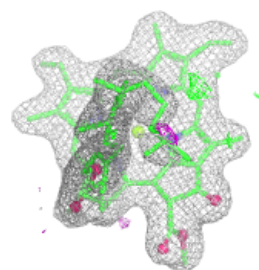
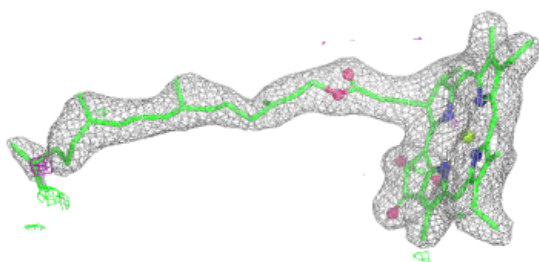
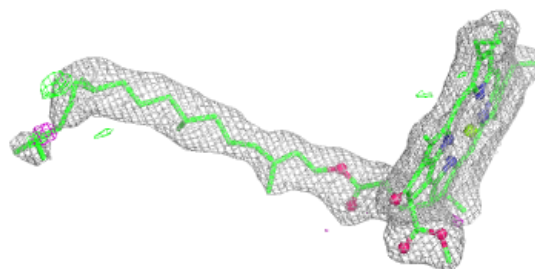
**Electron density around CLA b 603:**

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

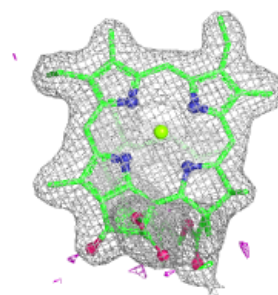
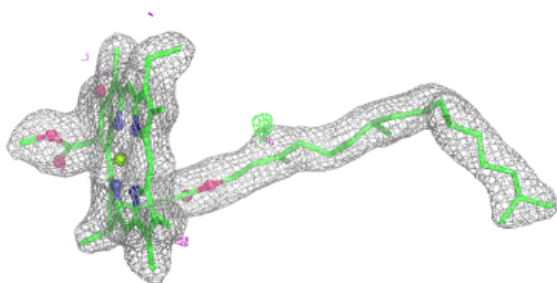
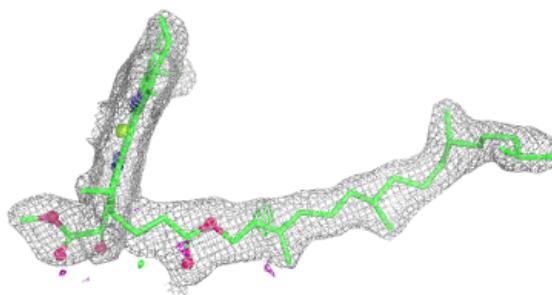


Electron density around CLA b 604:

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

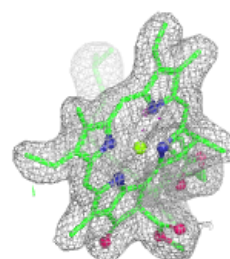
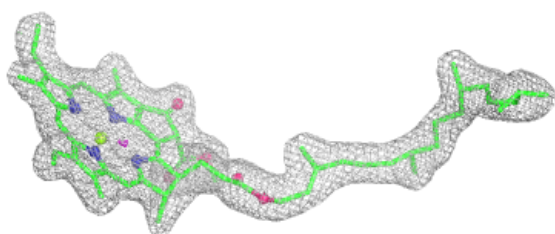
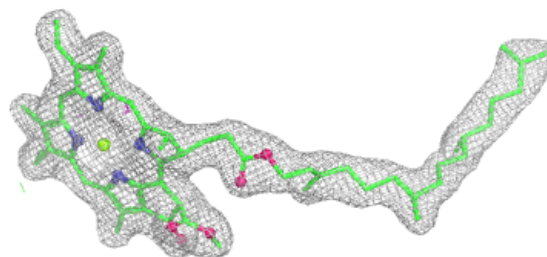
**Electron density around CLA b 605:**

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

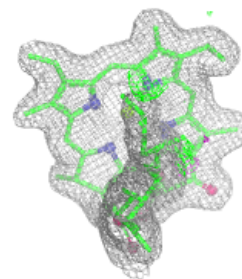
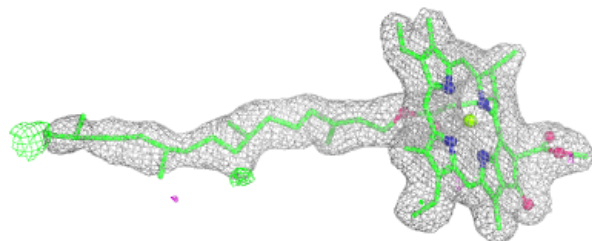
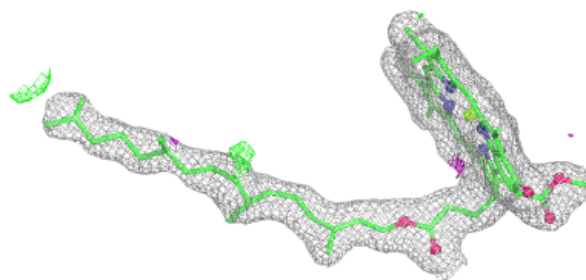


Electron density around CLA A 606:

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

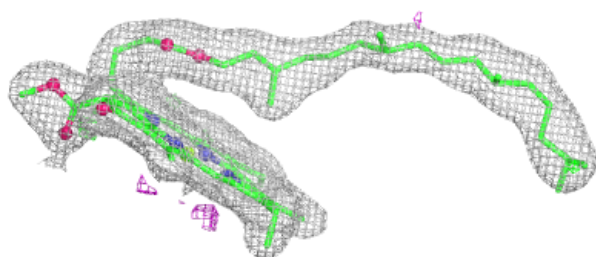
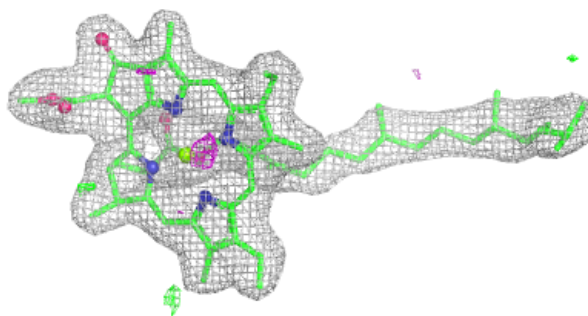
**Electron density around CLA b 607:**

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

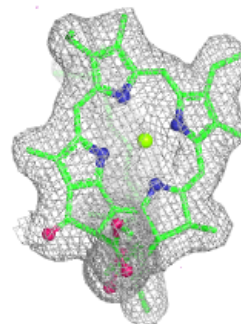
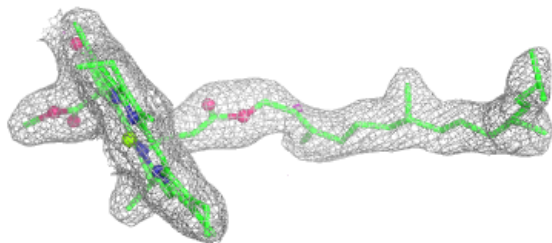
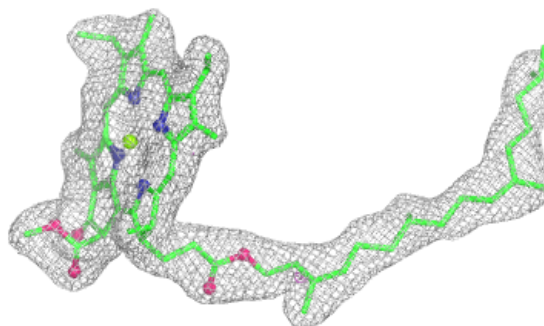


Electron density around CLA B 608:

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

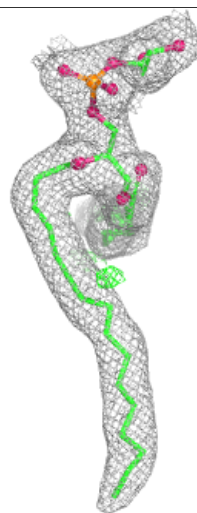
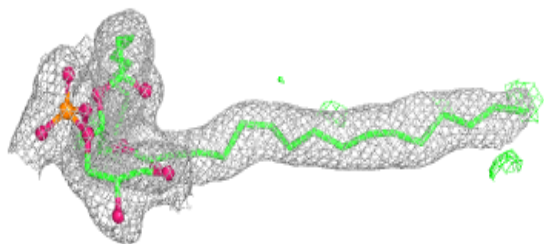
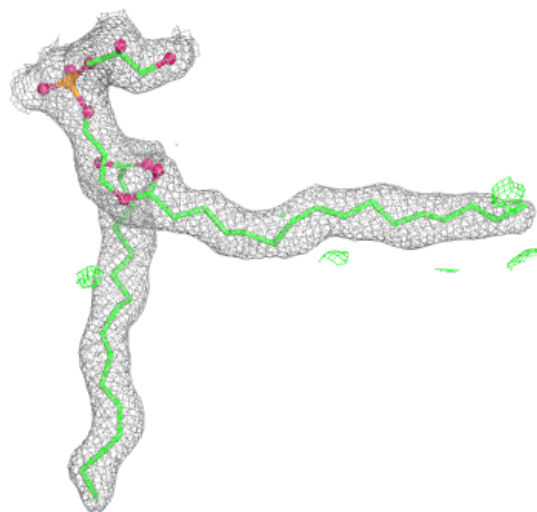
**Electron density around CLA B 609:**

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



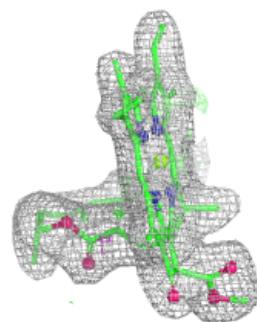
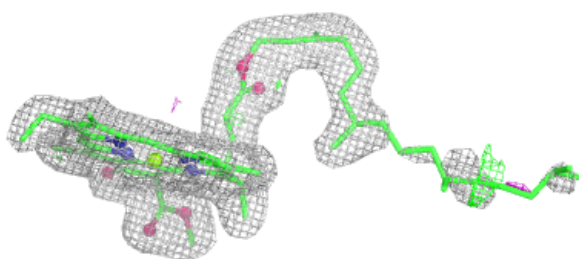
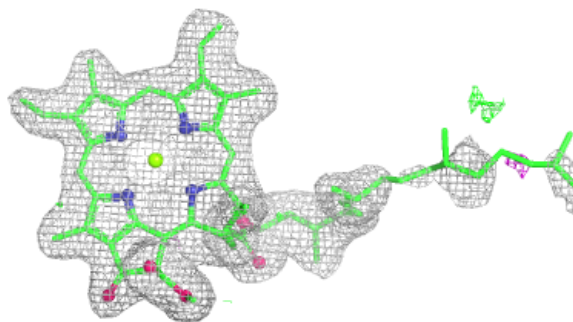
Electron density around LHG L 101:

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

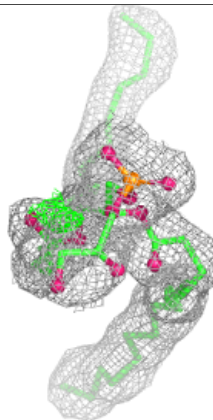
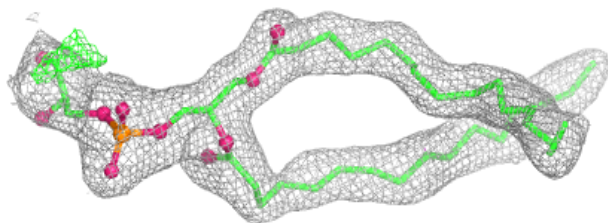
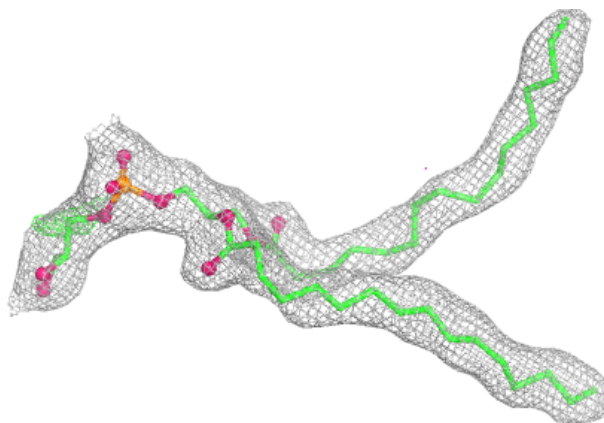


Electron density around CLA A 607:

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

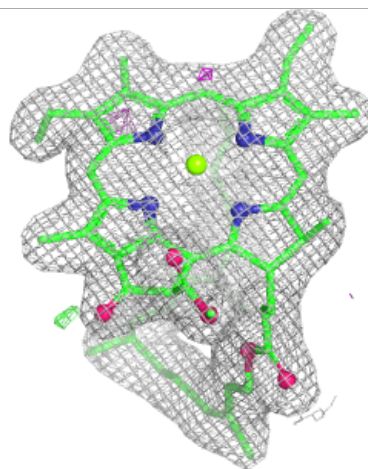
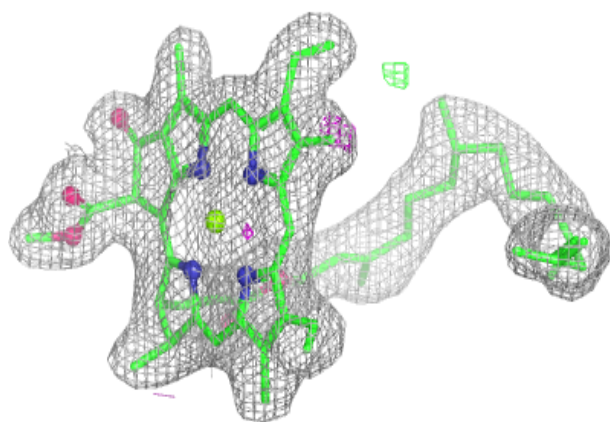
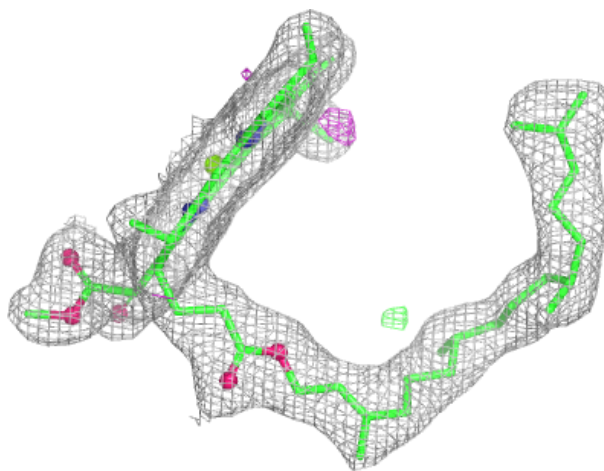
**Electron density around LHG d 408:**

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



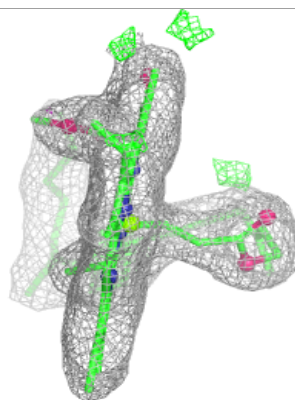
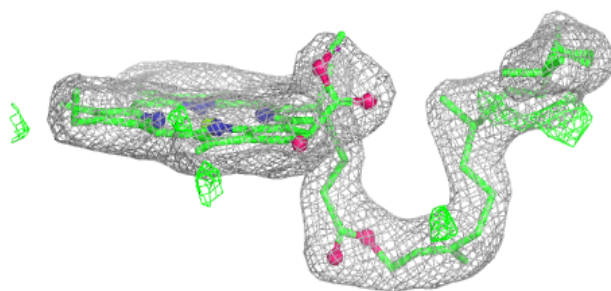
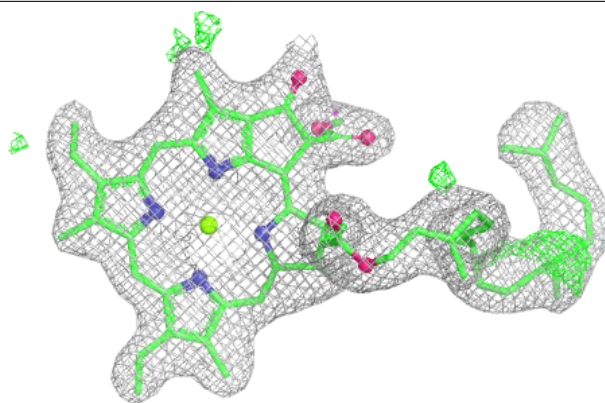
Electron density around CLA b 611:

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

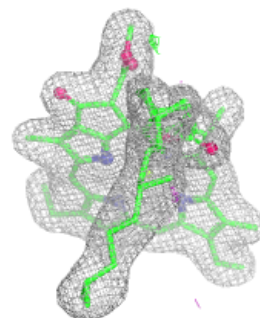
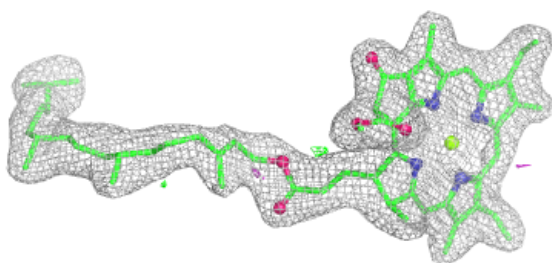
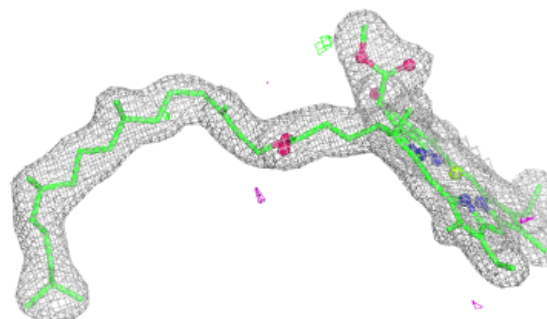


Electron density around CLA b 612:

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

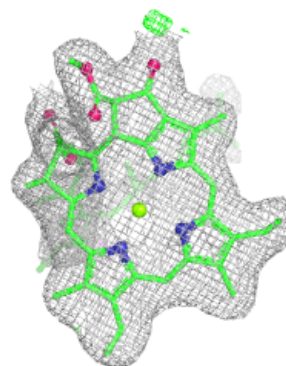
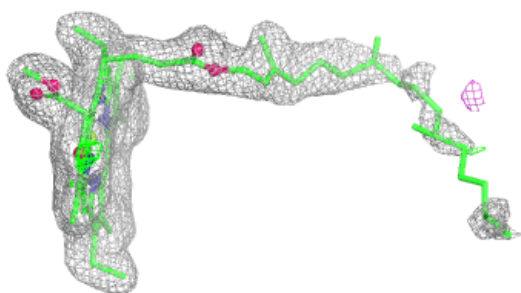
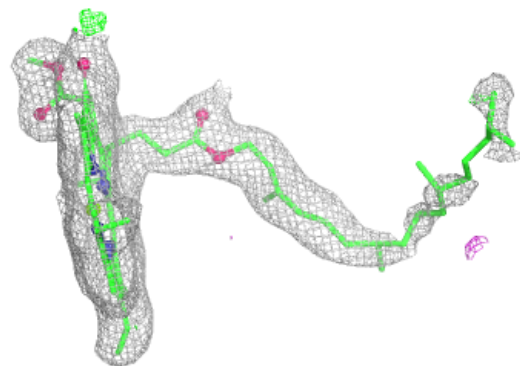
**Electron density around CLA D 403:**

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

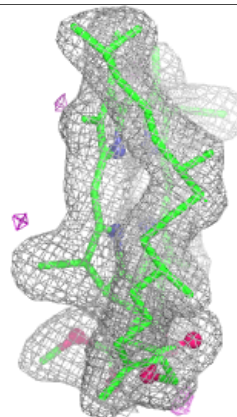
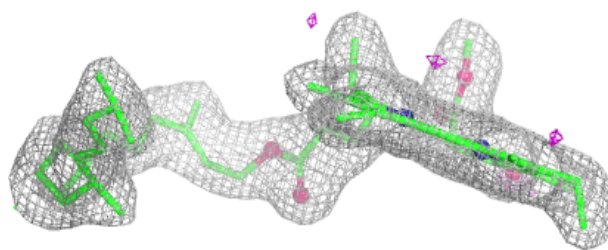
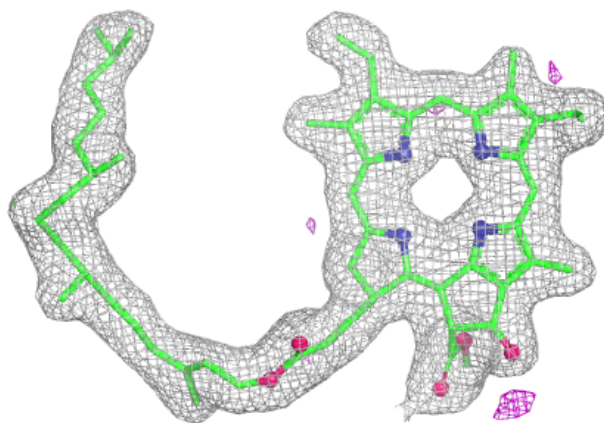


Electron density around CLA D 404:

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

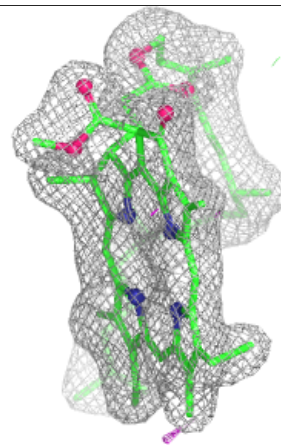
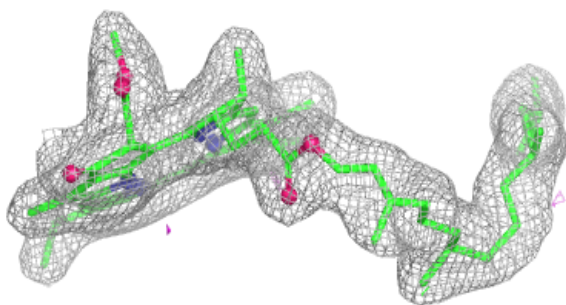
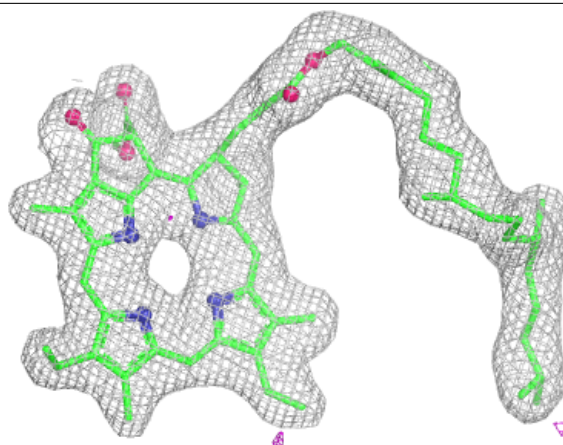
**Electron density around PHO D 401:**

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



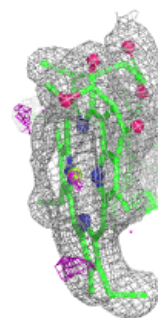
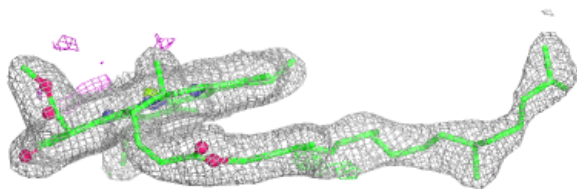
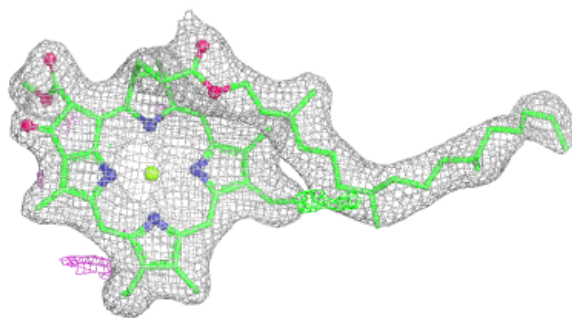
Electron density around PHO D 402:

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

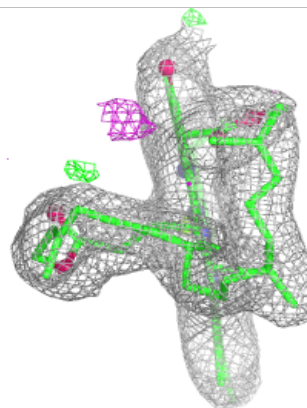
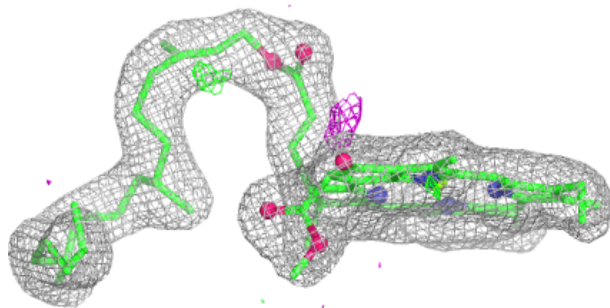
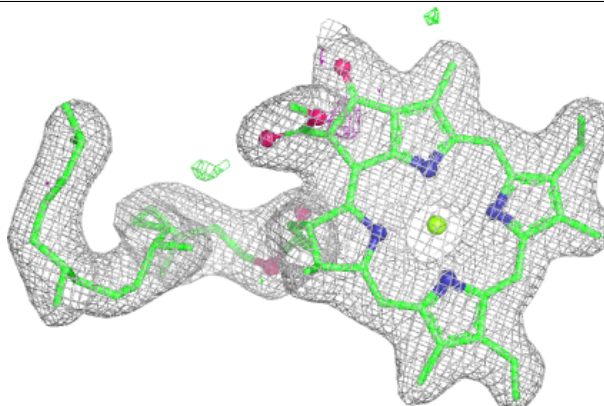


Electron density around CLA B 603:

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

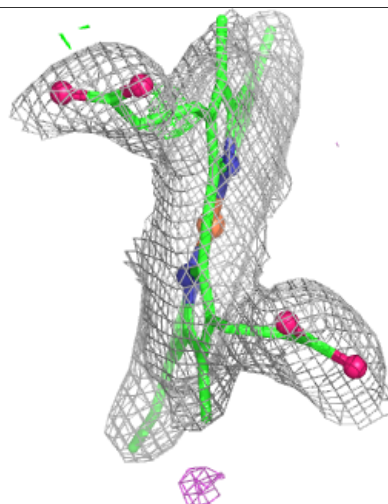
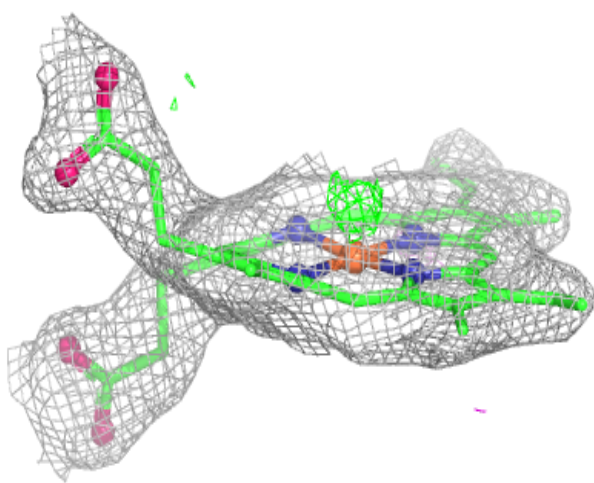
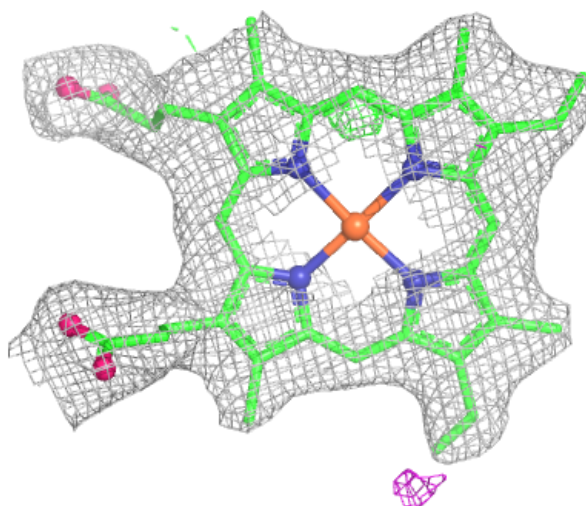
**Electron density around CLA B 612:**

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



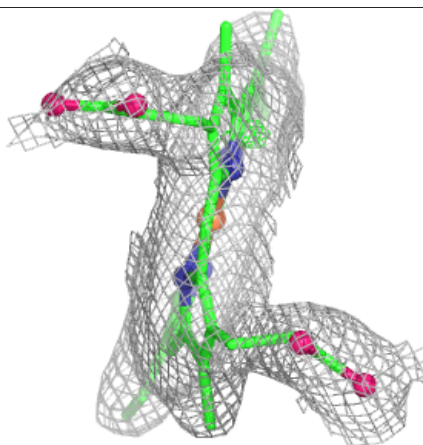
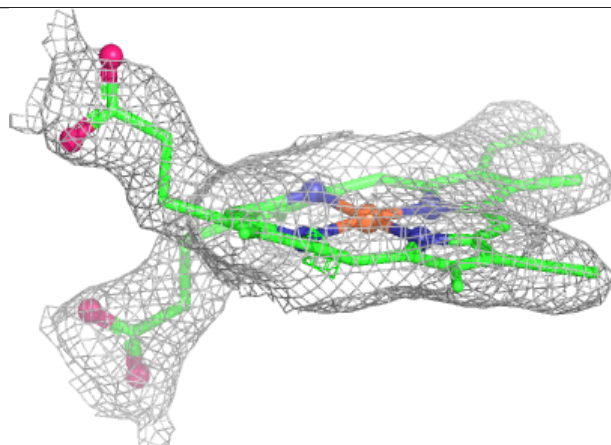
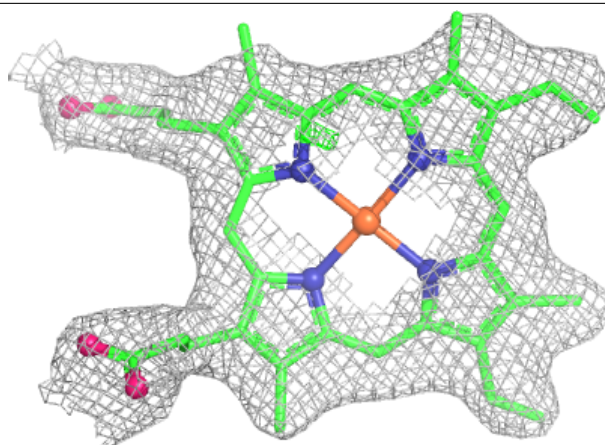
Electron density around HEM E 101:

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



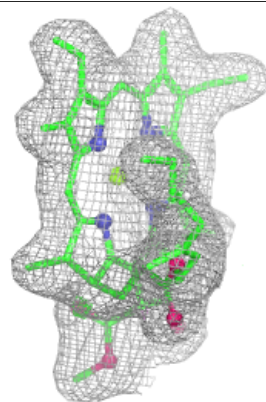
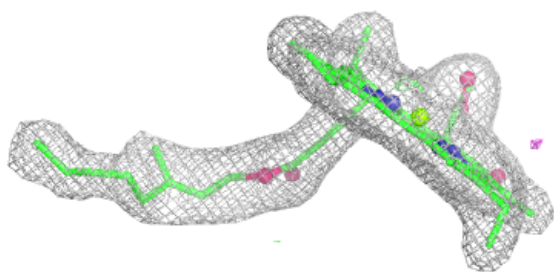
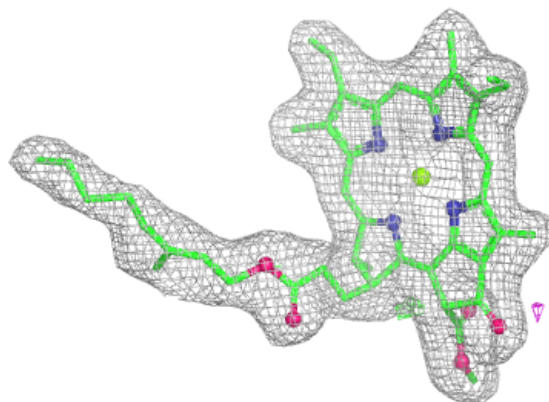
Electron density around HEM f 101:

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

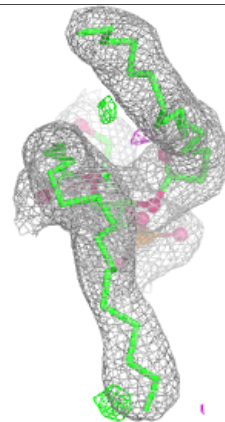
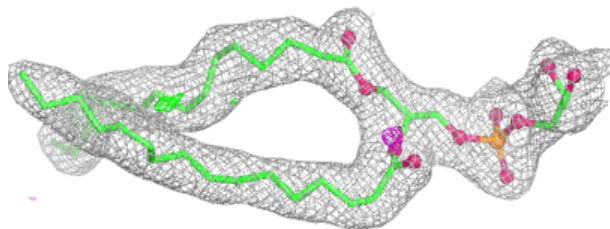
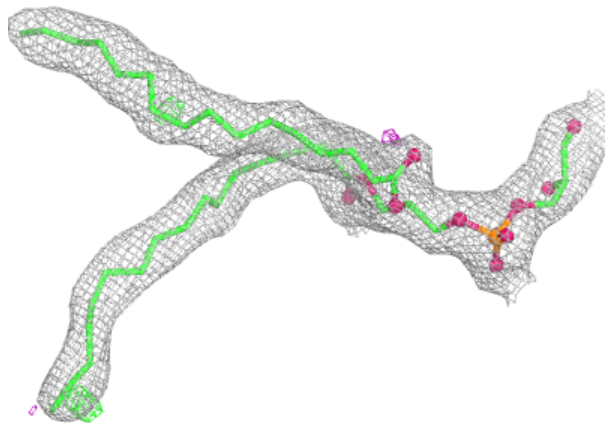


Electron density around CLA A 608:

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

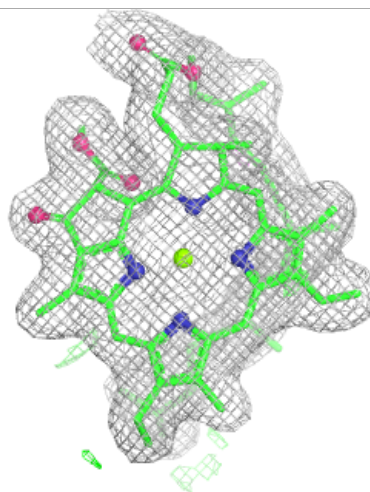
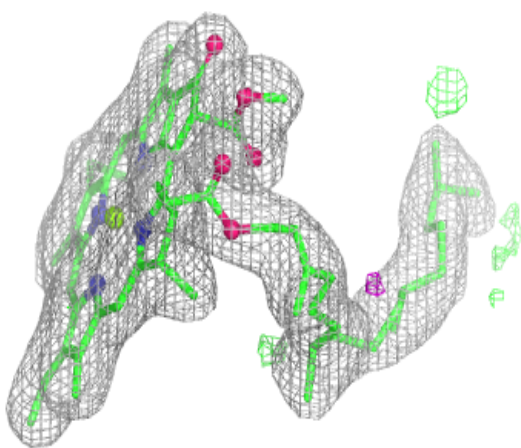
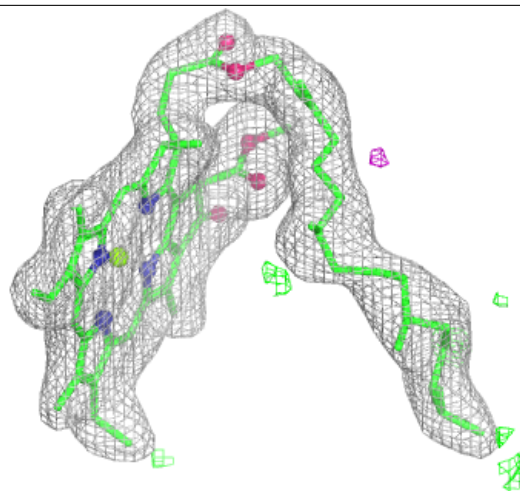
**Electron density around LHG D 409:**

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



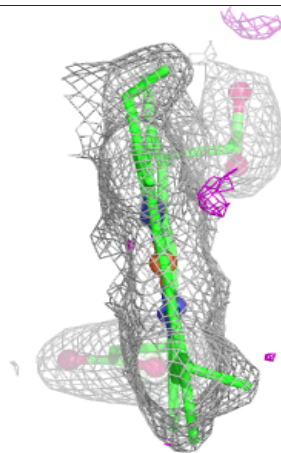
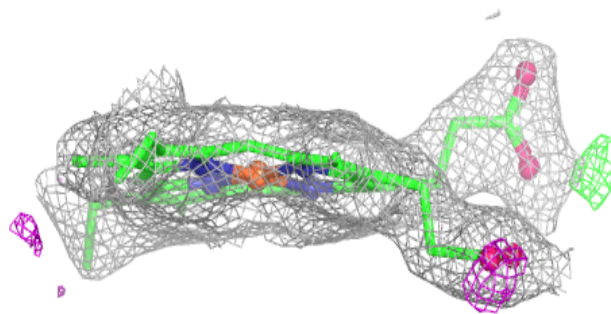
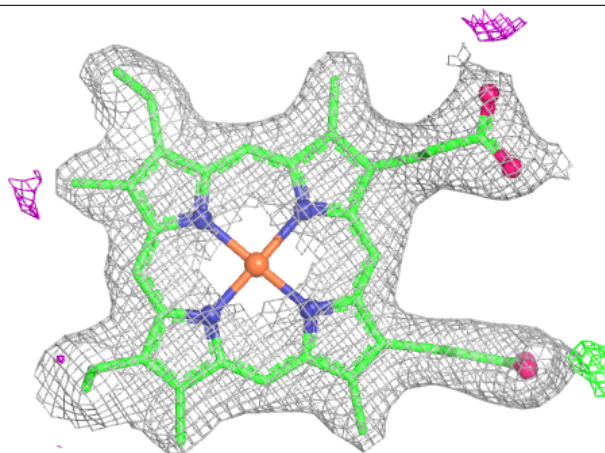
Electron density around CLA B 613:

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



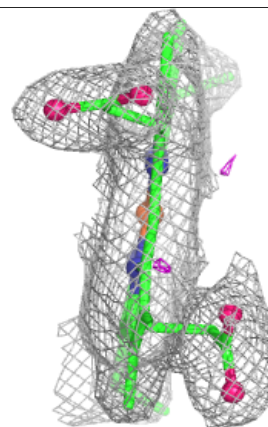
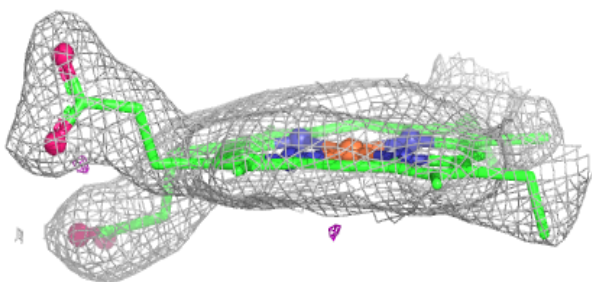
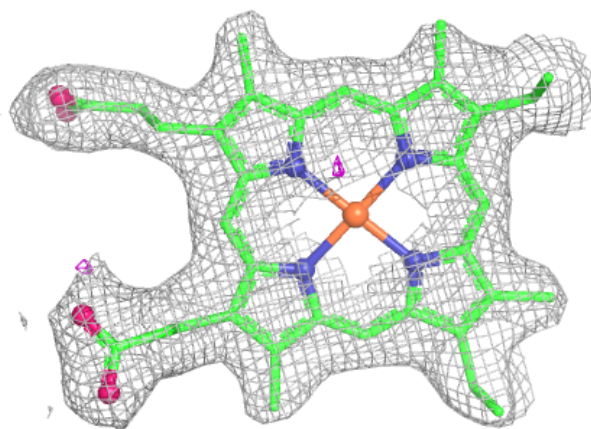
Electron density around HEC V 201:

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



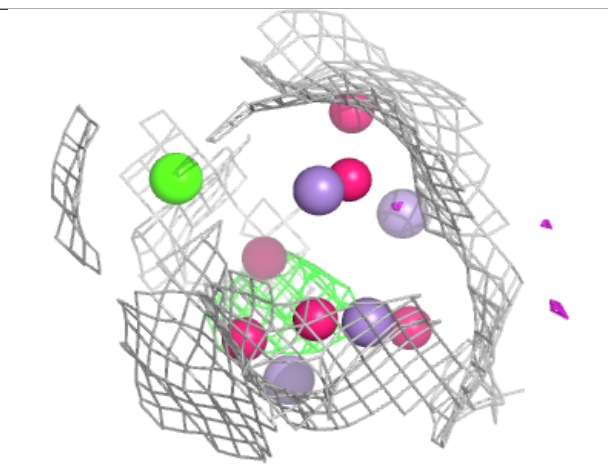
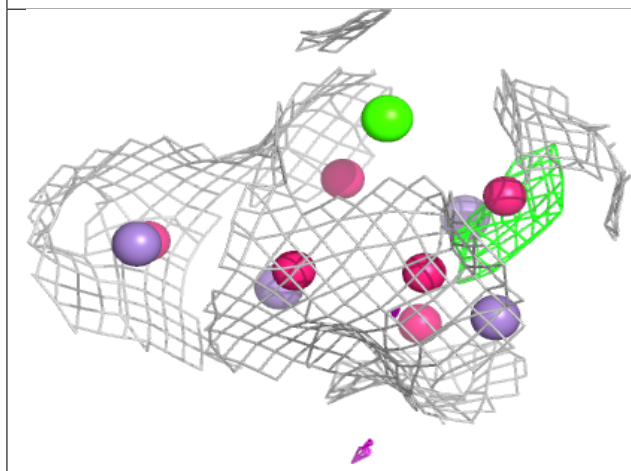
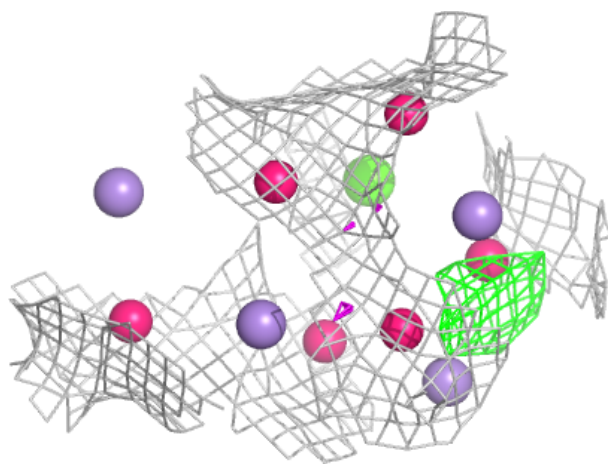
Electron density around HEC v 201:

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



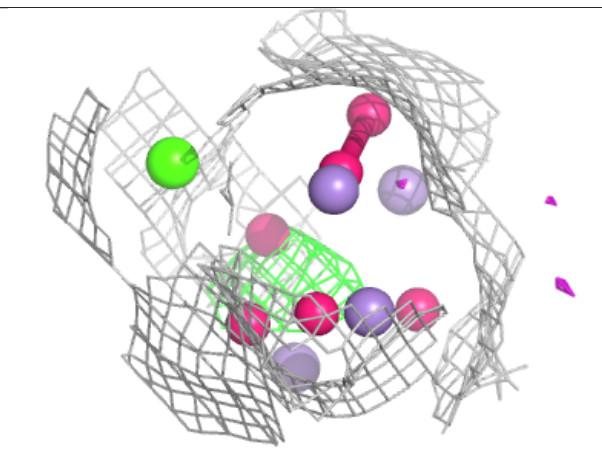
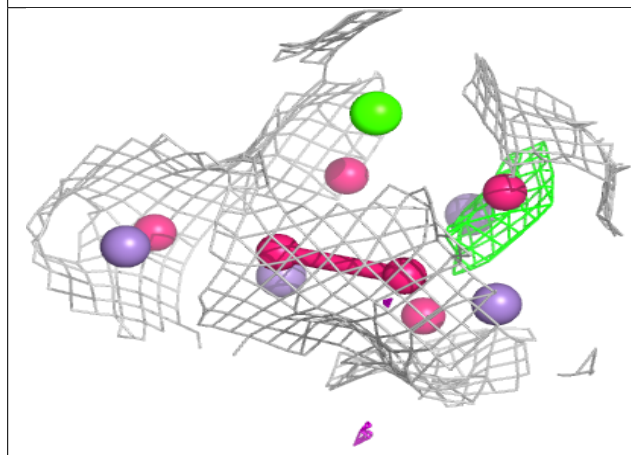
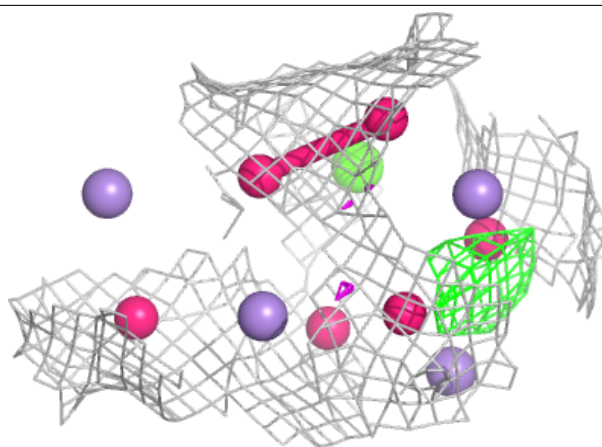
Electron density around OEY A 601 (A):

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



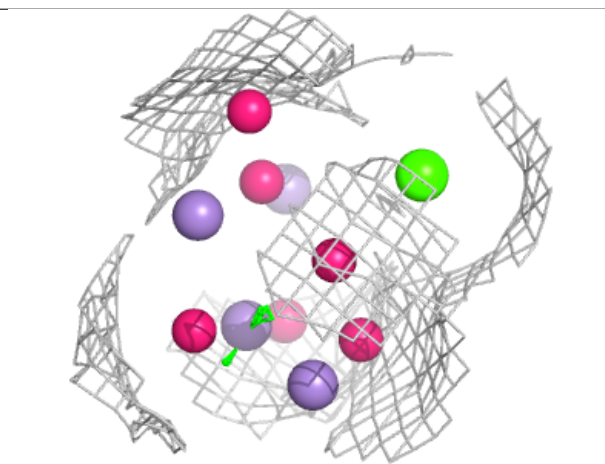
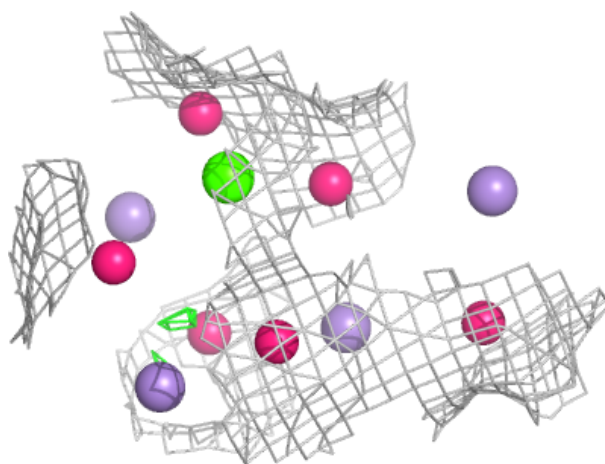
Electron density around OEY A 601 (B):

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



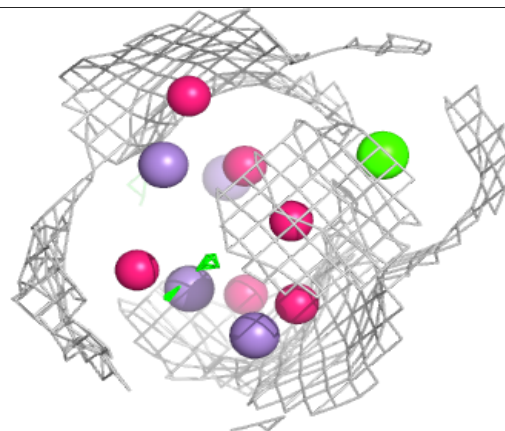
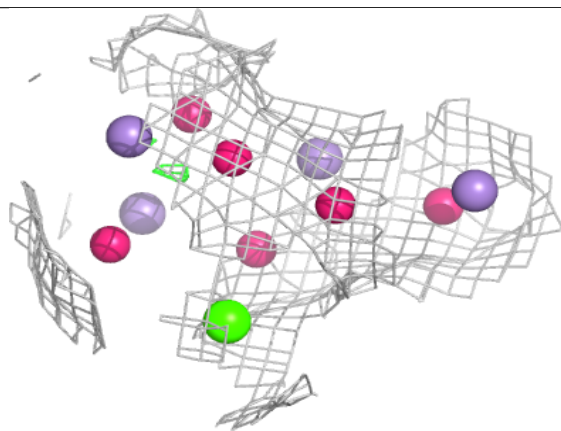
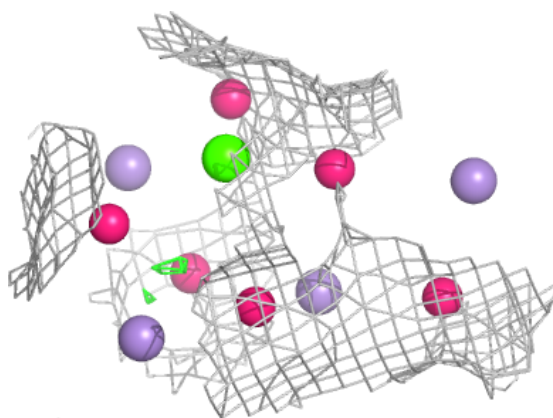
Electron density around OEY a 601 (A):

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



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.