



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 22, 2025 – 04:01 AM EDT

PDB ID : 8F4C / pdb_00008f4c
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.00 Angstrom resolution
Authors : Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2022-11-10
Resolution : 2.00 Å(reported)

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

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

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

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0

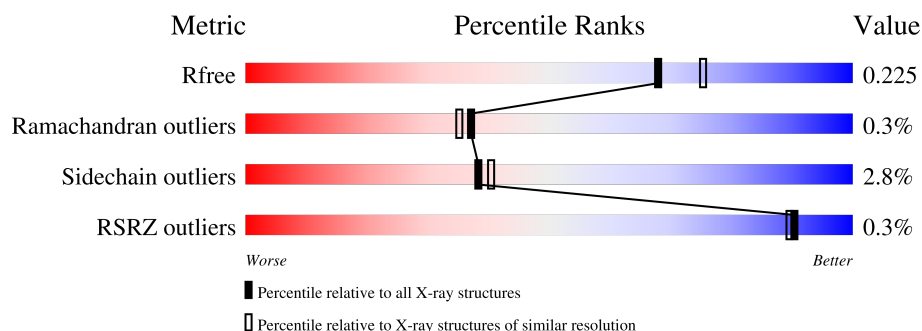
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

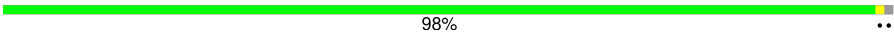
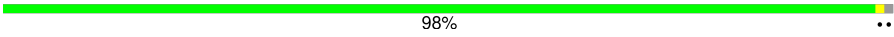
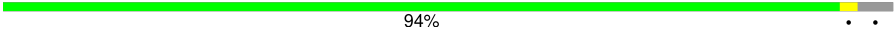
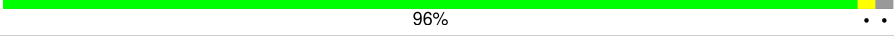
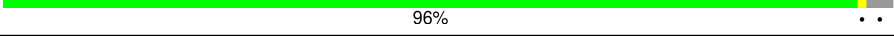
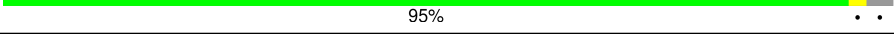

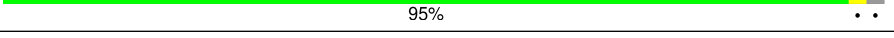
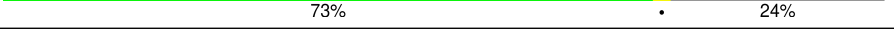

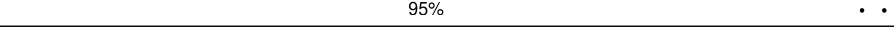
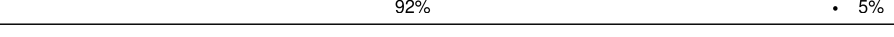
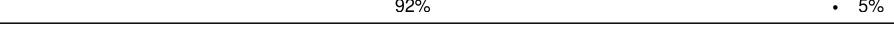
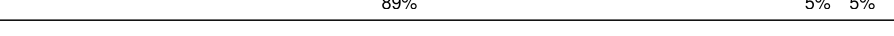


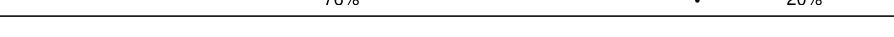

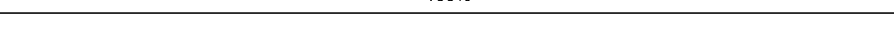






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	

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buster-report : 1.1.7 (2018)
 Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
 CCP4 : 9.0.006 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.42

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Mol	Chain	Length	Quality of chain
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	
14	T	32	

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Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	X	-	-	-
25	CLA	A	611	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
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25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 53435 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

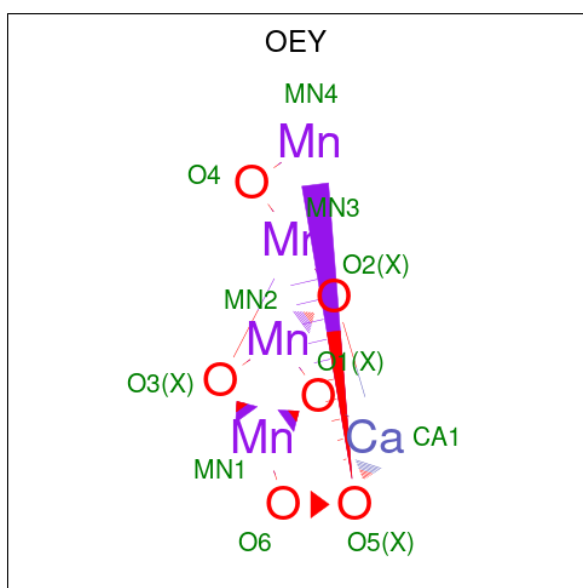
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

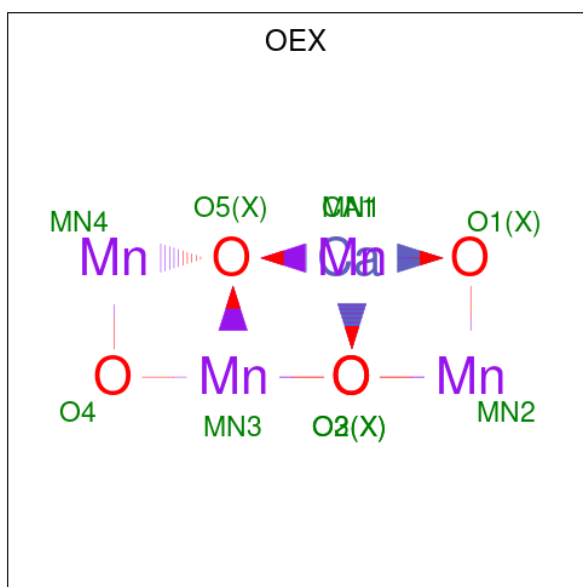
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
20	r	31	Total	C	N	O	0	0	0
			246	166	43	37			

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



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

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



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

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

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

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

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

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



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

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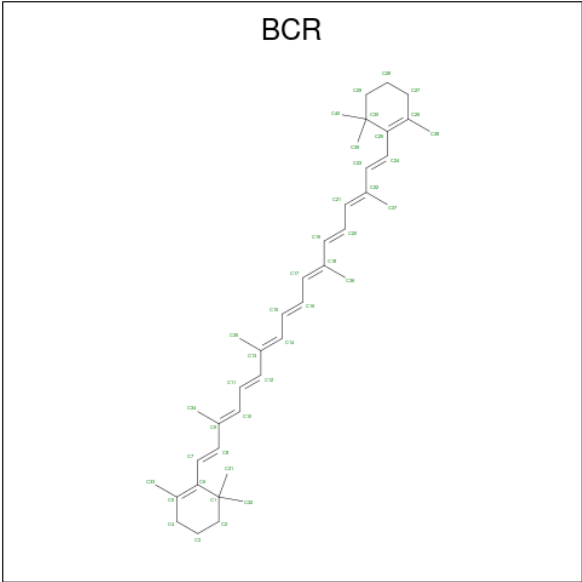
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total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

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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
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			64	54	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		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



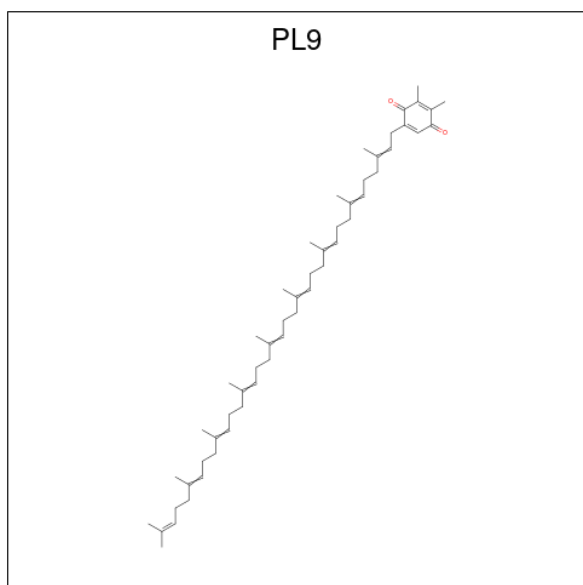
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Z	1	Total 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	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	x	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).



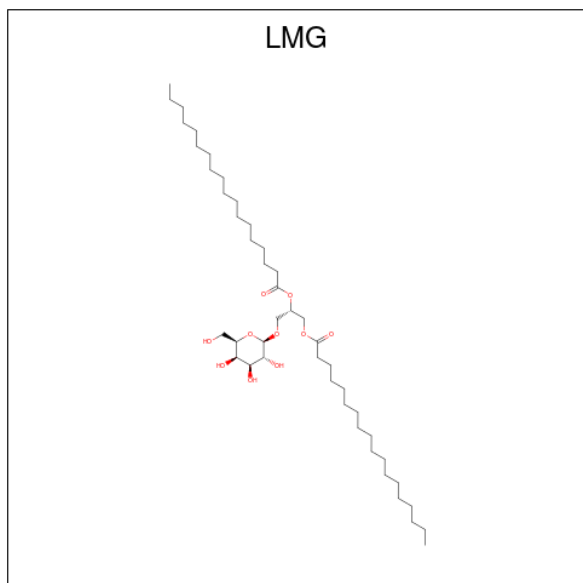
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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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		

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



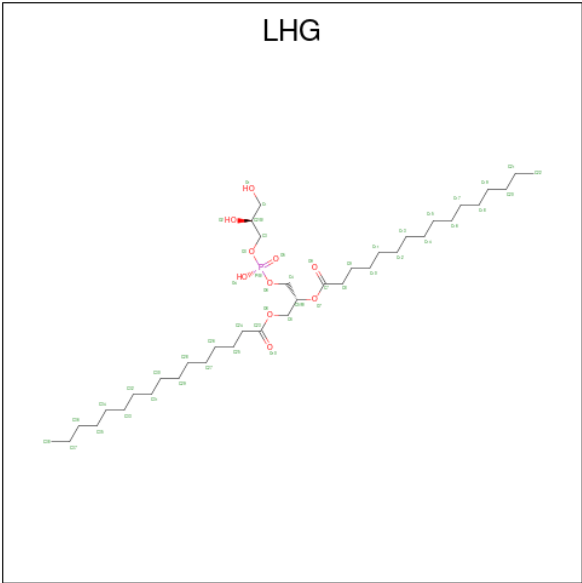
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			48	38	10		
28	B	1	Total	C	O	0	0
			28	24	4		
28	C	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			51	41	10		
28	D	1	Total	C	O	0	0
			33	27	6		
28	M	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



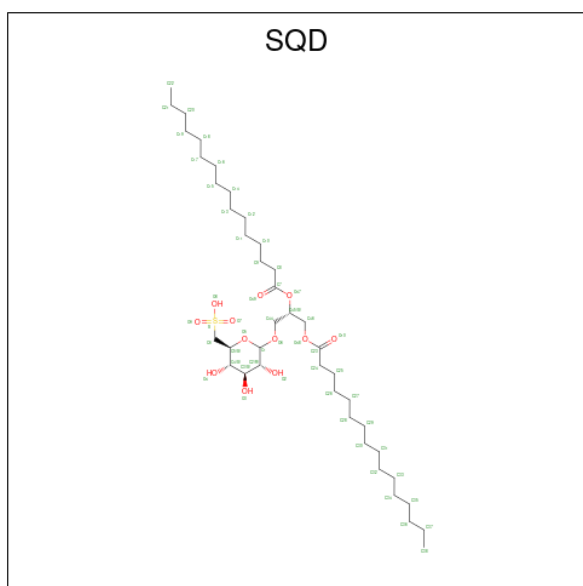
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			47	36	10	1		
29	B	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	E	1	Total	C	O	P	0	0
			49	38	10	1		
29	L	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0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

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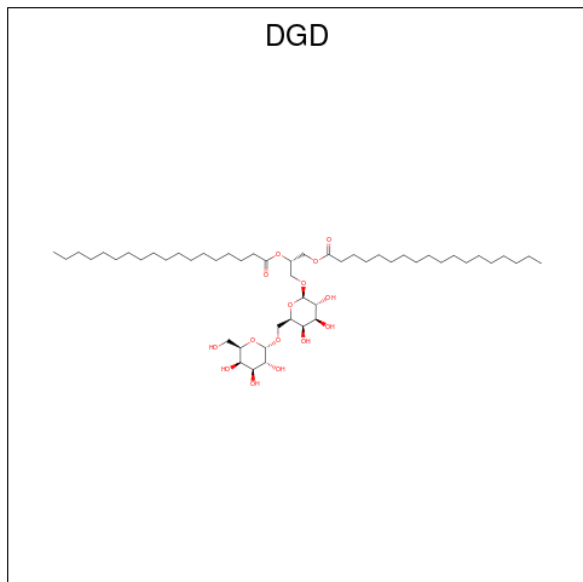
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	d	1	Total	C	O	P	0	0
			39	28	10	1		
29	e	1	Total	C	O	P	0	0
			42	31	10	1		
29	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



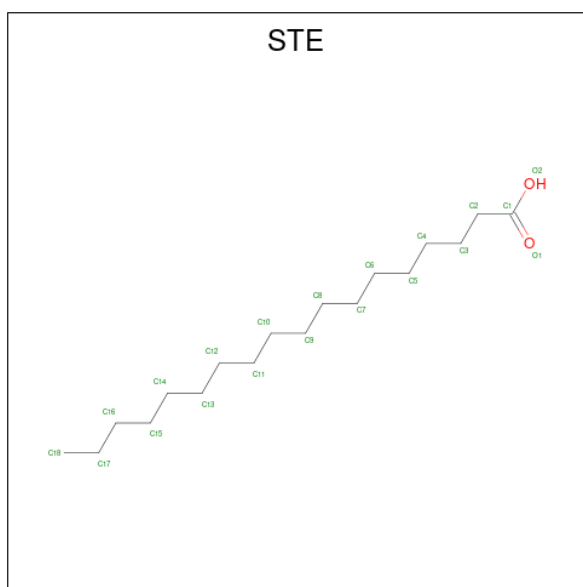
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			52	39	12	1		
30	A	1	Total	C	O		0	0
			39	35	4			
30	B	1	Total	C	O	S	0	0
			54	41	12	1		
30	D	1	Total	C	O	S	0	0
			36	25	10	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O		0	0
			36	31	5			
30	b	1	Total	C	O	S	0	0
			49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

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



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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



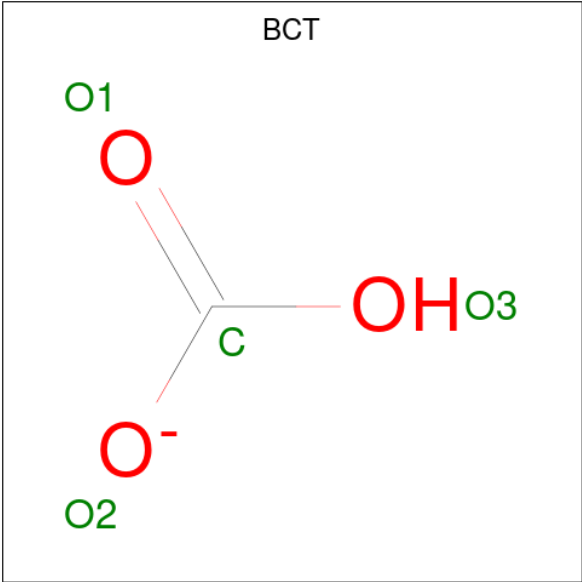
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total 17	C 15	O 2	0	0
32	B	1	Total 12	C 10	O 2	0	0
32	B	1	Total 18	C 16	O 2	0	0
32	B	1	Total 12	C 10	O 2	0	0
32	B	1	Total 16	C 16		0	0
32	C	1	Total 12	C 10	O 2	0	0
32	C	1	Total 12	C 10	O 2	0	0
32	C	1	Total 16	C 16		0	0
32	E	1	Total 12	C 10	O 2	0	0
32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

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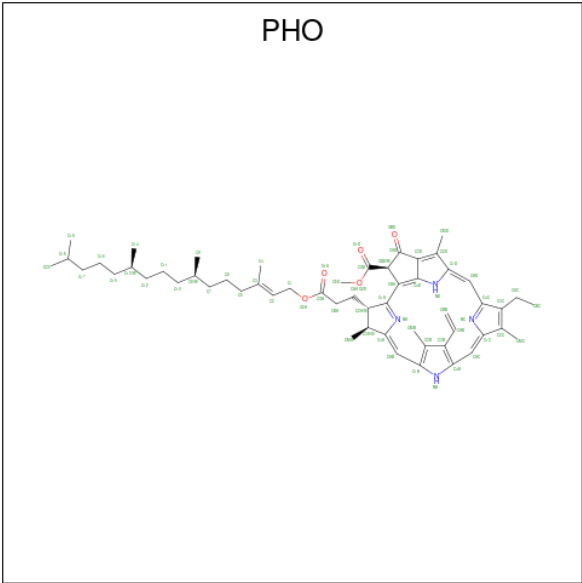
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	T	1	Total C 15 15	0	0
32	T	1	Total C O 20 18 2	0	0
32	X	1	Total C O 20 18 2	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C 16 16	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 2	0	0
32	c	1	Total C O 12 10 2	0	0
32	d	1	Total C O 17 15 2	0	0
32	d	1	Total C O 20 18 2	0	0
32	j	1	Total C O 12 10 2	0	0
32	l	1	Total C 18 18	0	0
32	m	1	Total C O 12 10 2	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 BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



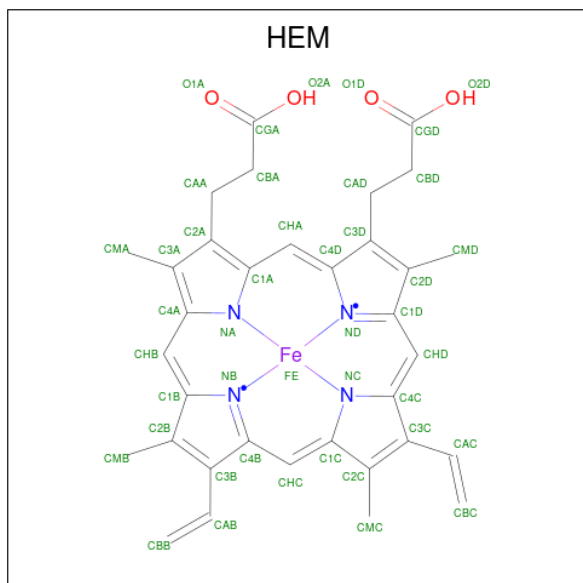
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	N	O	0	0
			64	55	4	5		
34	D	1	Total	C	N	O	0	0
			64	55	4	5		

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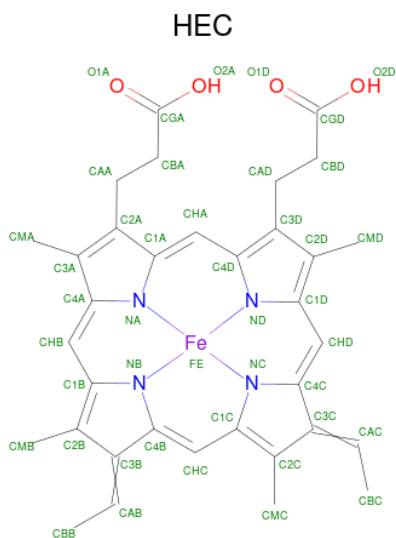
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	d	1	Total 64	C 55	N 4	O 5	0	0
34	d	1	Total 64	C 55	N 4	O 5	0	0

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



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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	140	Total O 144 144	0	4
37	B	208	Total O 208 208	0	0
37	C	199	Total O 199 199	0	0
37	D	134	Total O 134 134	0	0
37	E	31	Total O 31 31	0	0
37	F	8	Total O 8 8	0	0
37	H	30	Total O 30 30	0	0
37	I	16	Total O 16 16	0	0
37	J	12	Total O 12 12	0	0
37	K	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	9	Total 9	O 9	0	0
37	M	11	Total 11	O 11	0	0
37	O	85	Total 85	O 85	0	0
37	T	12	Total 12	O 12	0	0
37	U	41	Total 41	O 41	0	0
37	V	71	Total 71	O 71	0	0
37	Y	5	Total 5	O 5	0	0
37	X	9	Total 9	O 9	0	0
37	Z	5	Total 5	O 5	0	0
37	R	10	Total 10	O 10	0	0
37	a	133	Total 137	O 137	0	4
37	b	199	Total 199	O 199	0	0
37	c	172	Total 172	O 172	0	0
37	d	119	Total 119	O 119	0	0
37	e	32	Total 32	O 32	0	0
37	f	6	Total 6	O 6	0	0
37	h	27	Total 27	O 27	0	0
37	i	15	Total 15	O 15	0	0
37	j	9	Total 9	O 9	0	0
37	k	6	Total 6	O 6	0	0
37	l	9	Total 9	O 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	10	Total 10	O 10	0	0
37	o	102	Total 102	O 102	0	0
37	t	9	Total 9	O 9	0	0
37	u	53	Total 53	O 53	0	0
37	v	57	Total 57	O 57	0	0
37	y	5	Total 5	O 5	0	0
37	x	9	Total 9	O 9	0	0
37	z	3	Total 3	O 3	0	0
37	r	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1

Chain A:  96%



- Molecule 1: Photosystem II protein D1 1

Chain a:  94%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  98%



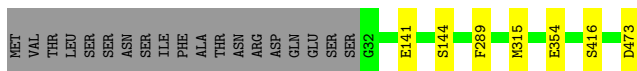
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  98%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  94%



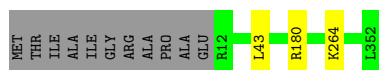
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  96%



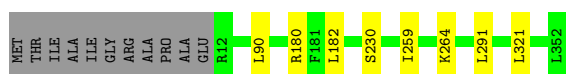
- Molecule 4: Photosystem II D2 protein

Chain D: 96%



- Molecule 4: Photosystem II D2 protein

Chain d: 95%



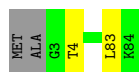
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 92%



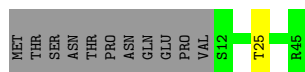
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 95%



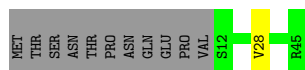
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 73%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 73%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 95%



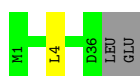
- Molecule 7: Photosystem II reaction center protein H

Chain h: 92% 5%



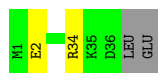
- Molecule 8: Photosystem II reaction center protein I

Chain I: 92% 5%



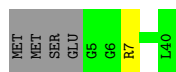
- Molecule 8: Photosystem II reaction center protein I

Chain i: 89% 5% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J: 88% 10%



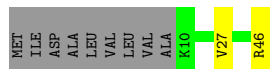
- Molecule 9: Photosystem II reaction center protein J

Chain j: 88% 10%



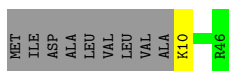
- Molecule 10: Photosystem II reaction center protein K

Chain K: 76% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 78% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 100%

There are no outlier residues recorded for this chain.

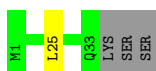
- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 8% . .



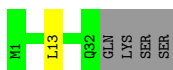
- Molecule 12: Photosystem II reaction center protein M

Chain M: 89% . 8%



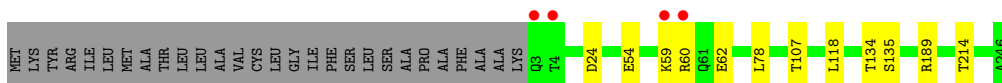
- Molecule 12: Photosystem II reaction center protein M

Chain m: 86% . 11%



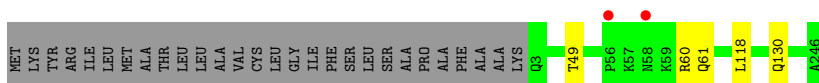
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 85% . 10%



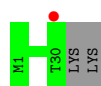
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 88% . 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 94% 6%



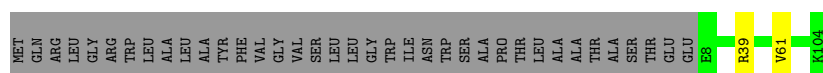
- Molecule 14: Photosystem II reaction center protein T

Chain t: 91% 6%



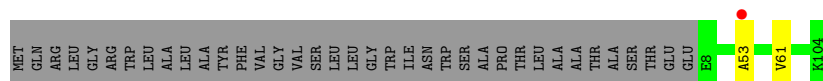
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 71% 28%



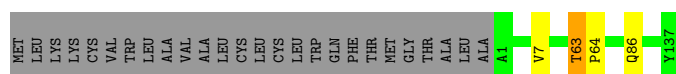
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 71% 28%



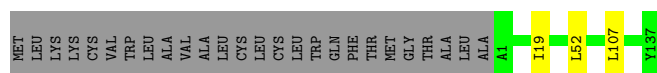
- Molecule 16: Cytochrome c-550

Chain V: 82% 16%



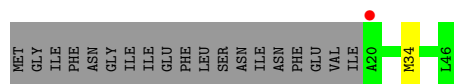
- Molecule 16: Cytochrome c-550

Chain v: 82% 16%



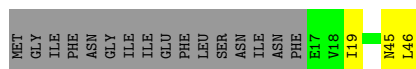
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 57% 2% 41%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 59% 7% 35%



- Molecule 18: Photosystem II reaction center X protein

Chain X: 90% 7%



- Molecule 18: Photosystem II reaction center X protein

Chain x: 90% 5% 5%



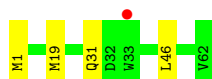
- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 85% 15% 3%



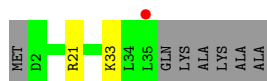
- Molecule 19: Photosystem II reaction center protein Z

Chain z: 94% 6% 2%



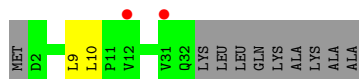
- Molecule 20: Photosystem II protein Y

Chain R: 78% 5% 17%



- Molecule 20: Photosystem II protein Y

Chain r: 71% 5% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.33Å 222.79Å 309.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.00 19.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.80-2.00) 85.5 (19.80-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.39 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.224 0.180 , 0.225	Depositor DCC
R_{free} test set	4804 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53435	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.43	0/3212	0.59	0/4376
1	a	0.42	0/3209	0.58	0/4372
2	B	0.40	0/4155	0.57	0/5661
2	b	0.39	0/4118	0.56	1/5611 (0.0%)
3	C	0.39	0/3625	0.54	0/4935
3	c	0.37	0/3705	0.54	0/5042
4	D	0.42	0/2825	0.57	0/3847
4	d	0.40	0/2834	0.57	0/3859
5	E	0.36	0/688	0.53	0/940
5	e	0.34	0/683	0.53	0/932
6	F	0.34	0/284	0.48	0/387
6	f	0.31	0/284	0.51	0/387
7	H	0.40	0/523	0.54	0/713
7	h	0.37	0/511	0.56	0/697
8	I	0.41	0/293	0.56	0/396
8	i	0.43	0/293	0.54	0/396
9	J	0.36	0/263	0.56	0/356
9	j	0.34	0/263	0.53	0/356
10	K	0.36	0/303	0.50	0/416
10	k	0.35	0/303	0.55	0/416
11	L	0.38	0/311	0.56	0/422
11	l	0.39	0/303	0.62	1/412 (0.2%)
12	M	0.36	0/249	0.51	0/341
12	m	0.39	0/244	0.51	0/334
13	O	0.38	0/1904	0.64	0/2585
13	o	0.38	0/1905	0.62	0/2583
14	T	0.46	0/257	0.59	0/349
14	t	0.41	0/255	0.52	0/346
15	U	0.33	0/785	0.57	0/1064
15	u	0.35	0/785	0.59	0/1064
16	V	0.34	0/1085	0.58	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.33	0/1085	0.55	0/1473
17	Y	0.30	0/197	0.53	0/264
17	y	0.28	0/219	0.50	0/294
18	X	0.35	0/284	0.50	0/384
18	x	0.32	0/289	0.43	0/391
19	Z	0.32	0/490	0.48	0/669
19	z	0.30	0/488	0.41	0/666
20	R	0.32	0/277	0.54	0/380
20	r	0.30	0/252	0.50	0/347
All	All	0.39	0/44038	0.56	3/59936 (0.0%)

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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	98	LEU	CA-CB-CG	5.55	128.08	115.30
16	V	63	THR	C-N-CD	-5.05	109.50	120.60
11	l	30	LEU	CA-CB-CG	5.02	126.84	115.30

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 ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/344 (115%)	389 (98%)	5 (1%)	1 (0%)	37	35
1	a	395/344 (115%)	388 (98%)	5 (1%)	2 (0%)	25	21
2	B	507/510 (99%)	498 (98%)	9 (2%)	0	100	100
2	b	503/510 (99%)	494 (98%)	8 (2%)	1 (0%)	44	42
3	C	451/461 (98%)	443 (98%)	7 (2%)	1 (0%)	44	42
3	c	461/461 (100%)	453 (98%)	7 (2%)	1 (0%)	44	42
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	231 (95%)	8 (3%)	4 (2%)	8	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	236 (98%)	5 (2%)	1 (0%)	30	27
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	12	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	19	14
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100	100
All	All	5386/5700 (94%)	5265 (98%)	107 (2%)	14 (0%)	37	35

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
9	J	7	ARG
13	O	60	ARG

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%)	320 (99%)	2 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	321/280 (115%)	310 (97%)	11 (3%)	32	32
2	B	407/407 (100%)	401 (98%)	6 (2%)	60	66
2	b	402/407 (99%)	398 (99%)	4 (1%)	73	78
3	C	353/362 (98%)	346 (98%)	7 (2%)	50	55
3	c	362/362 (100%)	352 (97%)	10 (3%)	38	40
4	D	277/283 (98%)	274 (99%)	3 (1%)	70	76
4	d	278/283 (98%)	270 (97%)	8 (3%)	37	39
5	E	72/73 (99%)	66 (92%)	6 (8%)	9	6
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	40
6	F	28/39 (72%)	27 (96%)	1 (4%)	30	30
6	f	28/39 (72%)	27 (96%)	1 (4%)	30	30
7	H	54/55 (98%)	52 (96%)	2 (4%)	29	29
7	h	53/55 (96%)	51 (96%)	2 (4%)	28	28
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	36
8	i	32/34 (94%)	30 (94%)	2 (6%)	15	12
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	25	24
10	K	30/37 (81%)	28 (93%)	2 (7%)	13	10
10	k	30/37 (81%)	29 (97%)	1 (3%)	33	33
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	4	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	30	30
12	m	28/32 (88%)	27 (96%)	1 (4%)	30	30
13	O	206/228 (90%)	198 (96%)	8 (4%)	27	27
13	o	207/228 (91%)	203 (98%)	4 (2%)	52	57
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	24 (96%)	1 (4%)	27	26
15	U	84/112 (75%)	82 (98%)	2 (2%)	44	47
15	u	84/112 (75%)	83 (99%)	1 (1%)	67	73
16	V	117/138 (85%)	115 (98%)	2 (2%)	56	61
16	v	117/138 (85%)	114 (97%)	3 (3%)	41	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	19/37 (51%)	18 (95%)	1 (5%)	19	16
17	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	35
18	x	31/34 (91%)	29 (94%)	2 (6%)	14	11
19	Z	52/52 (100%)	43 (83%)	9 (17%)	1	1
19	z	51/52 (98%)	47 (92%)	4 (8%)	10	7
20	R	28/33 (85%)	26 (93%)	2 (7%)	12	9
20	r	25/33 (76%)	23 (92%)	2 (8%)	10	6
All	All	4450/4654 (96%)	4327 (97%)	123 (3%)	38	40

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	28	LEU
16	v	52	LEU
3	c	72	LEU
16	v	19	ILE
19	z	19	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
18	x	33	GLN
20	r	30	GLN
1	a	234	ASN
2	b	409	GLN
2	b	490	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	0.95	0	8,9,11	0.85	0
14	FME	T	1	14	8,9,10	1.07	0	8,9,11	0.77	0
8	FME	i	1	8	8,9,10	0.95	0	8,9,11	0.94	0
8	FME	I	1	8	8,9,10	0.99	0	8,9,11	0.89	0
12	FME	M	1	12	8,9,10	1.01	0	8,9,11	0.82	0
14	FME	t	1	14	8,9,10	1.09	0	8,9,11	1.01	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	-	0/7/9/11	-
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	-
12	FME	M	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
35	HEM	f	101	6,5	42,50,50	1.48	5 (11%)	46,82,82	1.63	9 (19%)
25	CLA	a	609	-	63,73,73	1.43	7 (11%)	74,113,113	1.37	9 (12%)
26	BCR	a	610	-	41,41,41	0.91	1 (2%)	56,56,56	1.28	6 (10%)
26	BCR	Z	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	4 (7%)
25	CLA	C	512	-	63,73,73	1.48	7 (11%)	74,113,113	1.40	9 (12%)
25	CLA	a	607	-	63,73,73	1.65	9 (14%)	74,113,113	1.49	8 (10%)
25	CLA	b	613	-	63,73,73	1.43	7 (11%)	74,113,113	1.66	12 (16%)
29	LHG	A	613	-	46,46,48	0.86	2 (4%)	49,52,54	1.24	4 (8%)
25	CLA	a	612	37	63,73,73	1.72	6 (9%)	74,113,113	1.51	8 (10%)
25	CLA	b	607	37	63,73,73	1.37	7 (11%)	74,113,113	1.37	8 (10%)
26	BCR	c	514	-	41,41,41	1.15	3 (7%)	56,56,56	1.22	6 (10%)
32	STE	I	101	-	14,14,19	0.35	0	13,13,19	0.80	0
25	CLA	C	508	-	63,73,73	1.39	6 (9%)	74,113,113	1.52	12 (16%)
28	LMG	D	408	-	51,51,55	0.85	2 (3%)	59,59,63	1.32	5 (8%)
26	BCR	d	405	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	5 (8%)
27	PL9	d	406	-	55,55,55	1.20	4 (7%)	68,69,69	1.63	14 (20%)
25	CLA	b	610	37	63,73,73	1.40	6 (9%)	74,113,113	1.49	13 (17%)
26	BCR	A	609	-	41,41,41	0.94	2 (4%)	56,56,56	1.29	6 (10%)
22	OEX	A	602[A]	3,1,37	0,15,15	-	-	-	-	-
28	LMG	b	624	-	55,55,55	0.78	3 (5%)	63,63,63	1.41	10 (15%)
30	SQD	a	613	-	52,54,54	1.57	7 (13%)	62,65,65	1.83	12 (19%)
32	STE	B	627	-	15,15,19	0.37	0	14,14,19	0.78	0
29	LHG	L	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.19	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	608	-	52,62,73	1.44	4 (7%)	60,99,113	1.50	7 (11%)
25	CLA	b	615	-	63,73,73	1.60	7 (11%)	74,113,113	1.48	7 (9%)
25	CLA	c	508	-	62,72,73	1.42	6 (9%)	72,111,113	1.47	10 (13%)
32	STE	b	626	-	9,9,19	0.35	0	8,8,19	0.72	0
25	CLA	C	505	-	63,73,73	1.52	5 (7%)	74,113,113	1.45	8 (10%)
25	CLA	B	607	37	63,73,73	1.42	6 (9%)	74,113,113	1.47	8 (10%)
25	CLA	C	509	-	63,73,73	1.30	5 (7%)	74,113,113	1.40	8 (10%)
30	SQD	A	615	-	38,38,54	1.75	5 (13%)	40,40,65	1.24	3 (7%)
32	STE	b	625	-	15,15,19	0.73	0	15,15,19	0.93	0
32	STE	B	624	-	11,11,19	0.76	0	11,11,19	1.27	0
25	CLA	a	608	37	63,73,73	1.36	5 (7%)	74,113,113	1.35	9 (12%)
25	CLA	A	611	37	63,73,73	1.55	7 (11%)	74,113,113	1.43	8 (10%)
25	CLA	b	611	-	63,73,73	1.46	5 (7%)	74,113,113	1.42	9 (12%)
31	DGD	c	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.34	7 (9%)
25	CLA	A	606	-	63,73,73	1.59	6 (9%)	74,113,113	1.32	8 (10%)
25	CLA	C	504	37	57,67,73	1.44	6 (10%)	66,105,113	1.37	10 (15%)
32	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.07	0
28	LMG	c	520	-	48,48,55	0.98	5 (10%)	56,56,63	1.29	7 (12%)
29	LHG	D	410	-	48,48,48	0.82	2 (4%)	51,54,54	1.24	7 (13%)
25	CLA	B	601	37	63,73,73	1.57	7 (11%)	74,113,113	1.52	10 (13%)
30	SQD	A	614	-	50,52,54	1.57	8 (16%)	60,63,65	1.91	11 (18%)
25	CLA	b	614	-	63,73,73	1.39	6 (9%)	74,113,113	1.37	10 (13%)
25	CLA	c	505	-	63,73,73	1.38	7 (11%)	74,113,113	1.25	8 (10%)
25	CLA	B	608	-	63,73,73	1.32	5 (7%)	74,113,113	1.49	8 (10%)
25	CLA	D	404	-	63,73,73	1.49	4 (6%)	74,113,113	1.49	11 (14%)
32	STE	c	521	-	11,11,19	0.73	0	11,11,19	1.15	1 (9%)
25	CLA	c	502	-	63,73,73	1.28	6 (9%)	74,113,113	1.38	8 (10%)
32	STE	l	102	-	17,17,19	0.31	0	16,16,19	0.95	0
25	CLA	b	605	-	63,73,73	1.44	4 (6%)	74,113,113	1.44	10 (13%)
25	CLA	B	605	-	63,73,73	1.38	4 (6%)	74,113,113	1.35	9 (12%)
26	BCR	H	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.20	5 (8%)
25	CLA	c	504	37	58,68,73	1.37	4 (6%)	68,107,113	1.44	9 (13%)
32	STE	B	625	-	17,17,19	0.61	0	17,17,19	1.16	0
25	CLA	C	503	-	63,73,73	1.50	9 (14%)	74,113,113	1.71	11 (14%)
25	CLA	b	606	-	63,73,73	1.67	5 (7%)	74,113,113	1.53	6 (8%)
27	PL9	a	611	-	55,55,55	0.68	1 (1%)	68,69,69	1.53	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SQD	D	409	-	34,36,54	1.51	5 (14%)	42,45,65	3.17	12 (28%)
26	BCR	T	101	-	41,41,41	0.94	2 (4%)	56,56,56	1.25	7 (12%)
32	STE	M	102	-	14,14,19	0.76	0	14,14,19	1.05	0
22	OEX	a	602[A]	3,1,37	0,15,15	-	-	-		
25	CLA	b	604	-	63,73,73	1.28	6 (9%)	74,113,113	1.56	8 (10%)
34	PHO	d	401	-	50,69,69	0.98	2 (4%)	48,99,99	1.11	3 (6%)
32	STE	c	519	-	19,19,19	0.60	0	19,19,19	1.01	0
25	CLA	C	501	-	63,73,73	1.60	10 (15%)	74,113,113	1.37	5 (6%)
32	STE	C	519	-	11,11,19	0.69	0	11,11,19	1.44	1 (9%)
25	CLA	c	507	37	63,73,73	1.55	8 (12%)	74,113,113	1.51	9 (12%)
31	DGD	A	616	-	67,67,67	1.10	7 (10%)	81,81,81	1.31	8 (9%)
26	BCR	B	617	-	41,41,41	1.02	3 (7%)	56,56,56	1.20	5 (8%)
29	LHG	d	407	-	48,48,48	0.76	2 (4%)	51,54,54	1.34	6 (11%)
25	CLA	B	615	-	63,73,73	1.53	8 (12%)	74,113,113	1.28	7 (9%)
26	BCR	K	102	-	41,41,41	1.01	2 (4%)	56,56,56	1.06	3 (5%)
25	CLA	A	607	37	63,73,73	1.53	5 (7%)	74,113,113	1.46	11 (14%)
26	BCR	C	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	6 (10%)
29	LHG	E	101	-	48,48,48	0.77	2 (4%)	51,54,54	1.26	6 (11%)
32	STE	E	102	-	11,11,19	0.74	0	11,11,19	1.16	1 (9%)
25	CLA	b	616	-	58,68,73	1.52	5 (8%)	68,107,113	1.58	9 (13%)
29	LHG	e	101	-	41,41,48	0.76	1 (2%)	44,47,54	1.35	6 (13%)
32	STE	J	101	-	11,11,19	0.73	0	11,11,19	1.08	0
32	STE	C	520	-	11,11,19	0.72	0	11,11,19	1.19	1 (9%)
26	BCR	B	618	-	41,41,41	1.01	2 (4%)	56,56,56	1.20	6 (10%)
32	STE	d	412	-	16,16,19	0.58	0	16,16,19	1.23	1 (6%)
34	PHO	D	403	-	50,69,69	0.98	3 (6%)	48,99,99	1.31	6 (12%)
31	DGD	h	101	-	63,63,67	0.97	3 (4%)	77,77,81	1.40	11 (14%)
28	LMG	C	518	-	48,48,55	0.80	1 (2%)	56,56,63	1.33	8 (14%)
28	LMG	d	411	-	44,44,55	0.81	1 (2%)	52,52,63	1.33	6 (11%)
25	CLA	b	602	-	63,73,73	1.33	4 (6%)	74,113,113	1.48	10 (13%)
28	LMG	D	411	-	31,31,55	0.71	1 (3%)	33,33,63	1.25	3 (9%)
29	LHG	l	101	-	48,48,48	0.70	1 (2%)	51,54,54	1.22	4 (7%)
31	DGD	H	102	-	63,63,67	1.20	7 (11%)	77,77,81	1.37	10 (12%)
33	BCT	a	606	23	3,3,3	1.12	0	2,3,3	3.07	1 (50%)
25	CLA	B	612	-	63,73,73	1.23	4 (6%)	74,113,113	1.54	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	513	-	63,73,73	1.37	5 (7%)	74,113,113	1.38	7 (9%)
26	BCR	D	406	-	41,41,41	1.03	2 (4%)	56,56,56	1.08	3 (5%)
28	LMG	A	612	-	48,48,55	0.95	4 (8%)	56,56,63	1.23	3 (5%)
36	HEC	V	201	16	32,50,50	1.95	3 (9%)	30,82,82	2.54	8 (26%)
25	CLA	B	614	-	63,73,73	1.37	5 (7%)	74,113,113	1.51	10 (13%)
26	BCR	k	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.06	2 (3%)
25	CLA	B	616	-	58,68,73	1.48	6 (10%)	68,107,113	1.45	7 (10%)
25	CLA	c	511	3	63,73,73	1.70	6 (9%)	74,113,113	1.52	7 (9%)
25	CLA	B	604	-	63,73,73	1.55	5 (7%)	74,113,113	1.56	9 (12%)
30	SQD	b	620	-	47,49,54	1.63	9 (19%)	57,60,65	1.75	10 (17%)
32	STE	C	521	-	15,15,19	0.31	0	14,14,19	0.93	0
25	CLA	b	612	-	63,73,73	1.41	7 (11%)	74,113,113	1.57	10 (13%)
27	PL9	A	610	-	55,55,55	0.85	1 (1%)	68,69,69	1.47	12 (17%)
31	DGD	o	301	-	43,43,67	0.80	3 (6%)	45,45,81	1.43	6 (13%)
26	BCR	t	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	6 (10%)
26	BCR	x	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.23	5 (8%)
25	CLA	c	509	-	63,73,73	1.32	5 (7%)	74,113,113	1.54	9 (12%)
32	STE	H	103	-	17,17,19	0.36	0	16,16,19	0.88	0
34	PHO	d	402	-	50,69,69	0.92	1 (2%)	48,99,99	1.44	7 (14%)
33	BCT	D	401	23	3,3,3	1.00	0	2,3,3	3.32	1 (50%)
25	CLA	c	506	-	63,73,73	1.51	7 (11%)	74,113,113	1.37	9 (12%)
31	DGD	c	515	-	63,63,67	1.00	4 (6%)	77,77,81	1.40	12 (15%)
31	DGD	C	515	-	63,63,67	1.00	4 (6%)	77,77,81	1.36	8 (10%)
25	CLA	d	403	-	63,73,73	1.43	7 (11%)	74,113,113	1.31	7 (9%)
25	CLA	B	602	-	63,73,73	1.37	6 (9%)	74,113,113	1.46	10 (13%)
21	OEY	A	601[B]	3,1,37	0,16,16	-	-	-	-	-
25	CLA	b	603	-	63,73,73	1.39	8 (12%)	74,113,113	1.45	8 (10%)
25	CLA	c	503	-	63,73,73	1.45	8 (12%)	74,113,113	1.53	9 (12%)
29	LHG	B	622	-	48,48,48	0.80	1 (2%)	51,54,54	1.32	7 (13%)
25	CLA	c	510	-	63,73,73	1.57	6 (9%)	74,113,113	1.44	7 (9%)
32	STE	B	626	-	11,11,19	0.69	0	11,11,19	1.34	1 (9%)
25	CLA	C	510	-	63,73,73	1.33	6 (9%)	74,113,113	1.50	8 (10%)
26	BCR	k	103	-	41,41,41	1.05	2 (4%)	56,56,56	1.17	4 (7%)
25	CLA	C	507	37	63,73,73	1.40	5 (7%)	74,113,113	1.50	11 (14%)
29	LHG	d	408	-	48,48,48	0.70	1 (2%)	51,54,54	1.24	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	502	-	63,73,73	1.44	6 (9%)	74,113,113	1.33	7 (9%)
32	STE	T	102	-	14,14,19	0.31	0	13,13,19	0.99	0
25	CLA	B	609	-	63,73,73	1.46	7 (11%)	74,113,113	1.45	10 (13%)
25	CLA	c	512	-	63,73,73	1.38	6 (9%)	74,113,113	1.42	9 (12%)
26	BCR	b	617	-	41,41,41	1.02	3 (7%)	56,56,56	1.27	4 (7%)
32	STE	d	413	-	19,19,19	0.65	0	19,19,19	1.03	1 (5%)
25	CLA	b	608	-	63,73,73	1.46	7 (11%)	74,113,113	1.47	13 (17%)
28	LMG	B	621	-	26,26,55	0.68	1 (3%)	26,26,63	1.23	2 (7%)
31	DGD	C	517	-	63,63,67	0.92	2 (3%)	77,77,81	1.38	10 (12%)
30	SQD	B	623	-	52,54,54	1.59	9 (17%)	62,65,65	1.65	11 (17%)
25	CLA	D	405	-	63,73,73	1.33	8 (12%)	74,113,113	1.36	8 (10%)
28	LMG	b	622	-	51,51,55	0.87	1 (1%)	59,59,63	1.42	7 (11%)
31	DGD	C	516	-	63,63,67	1.06	6 (9%)	77,77,81	1.36	14 (18%)
28	LMG	c	522	-	49,49,55	0.89	4 (8%)	57,57,63	1.27	3 (5%)
31	DGD	c	516	-	63,63,67	1.01	2 (3%)	77,77,81	1.37	10 (12%)
26	BCR	B	619	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	4 (7%)
32	STE	b	621	-	15,15,19	0.35	0	14,14,19	0.82	0
30	SQD	a	614	-	35,35,54	1.69	5 (14%)	37,37,65	1.51	6 (16%)
25	CLA	B	611	-	63,73,73	1.53	6 (9%)	74,113,113	1.41	6 (8%)
28	LMG	c	518	-	37,37,55	0.99	3 (8%)	45,45,63	1.34	5 (11%)
25	CLA	C	513	-	63,73,73	1.38	6 (9%)	74,113,113	1.53	7 (9%)
35	HEM	F	101	6,5	42,50,50	1.54	5 (11%)	46,82,82	1.32	5 (10%)
32	STE	B	620	-	16,16,19	0.69	0	16,16,19	1.09	0
21	OEY	a	601[B]	3,1,37	0,16,16	-	-	-	-	-
26	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
26	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.14	5 (8%)
25	CLA	b	609	-	63,73,73	1.45	7 (11%)	74,113,113	1.42	6 (8%)
25	CLA	B	613	-	63,73,73	1.36	6 (9%)	74,113,113	1.53	9 (12%)
28	LMG	d	410	-	21,21,55	0.52	0	20,20,63	1.28	3 (15%)
32	STE	b	623	-	19,19,19	0.65	0	19,19,19	0.99	0
32	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.20	1 (7%)
25	CLA	d	404	-	63,73,73	1.41	9 (14%)	74,113,113	1.28	6 (8%)
27	PL9	D	407	-	55,55,55	0.93	3 (5%)	68,69,69	1.66	14 (20%)
36	HEC	v	201	16	32,50,50	2.11	4 (12%)	30,82,82	2.25	7 (23%)
26	BCR	K	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.16	5 (8%)
32	STE	t	103	-	9,9,19	0.36	0	8,8,19	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	606	-	63,73,73	1.72	6 (9%)	74,113,113	1.46	8 (10%)
32	STE	m	101	-	11,11,19	0.71	0	11,11,19	1.19	1 (9%)
34	PHO	D	402	-	50,69,69	0.98	3 (6%)	48,99,99	1.25	5 (10%)
32	STE	M	103	-	9,9,19	0.36	0	8,8,19	0.76	0
25	CLA	C	506	-	63,73,73	1.46	6 (9%)	74,113,113	1.27	8 (10%)
26	BCR	b	619	-	41,41,41	0.99	2 (4%)	56,56,56	1.12	3 (5%)
25	CLA	B	603	-	63,73,73	1.37	6 (9%)	74,113,113	1.43	9 (12%)
32	STE	a	615	-	11,11,19	0.80	0	11,11,19	1.16	1 (9%)
25	CLA	b	601	37	63,73,73	1.50	6 (9%)	74,113,113	1.47	7 (9%)
29	LHG	d	409	-	38,38,48	0.82	1 (2%)	41,44,54	1.09	2 (4%)
25	CLA	B	610	37	63,73,73	1.53	10 (15%)	74,113,113	1.36	10 (13%)
25	CLA	C	511	3	63,73,73	1.51	5 (7%)	74,113,113	1.51	10 (13%)
32	STE	T	103	-	19,19,19	0.59	0	19,19,19	1.07	1 (5%)
30	SQD	f	102	-	39,41,54	1.69	8 (20%)	49,52,65	1.69	11 (22%)
28	LMG	M	101	-	51,51,55	0.86	3 (5%)	59,59,63	1.36	5 (8%)
25	CLA	c	501	-	63,73,73	1.27	6 (9%)	74,113,113	1.46	8 (10%)
32	STE	X	101	-	19,19,19	0.59	0	19,19,19	1.17	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	f	101	6,5	-	4/12/54/54	-
25	CLA	a	609	-	1/1/15/20	7/37/115/115	-
26	BCR	a	610	-	-	1/29/63/63	0/2/2/2
26	BCR	Z	101	-	-	3/29/63/63	0/2/2/2
25	CLA	C	512	-	1/1/15/20	15/37/115/115	-
25	CLA	a	607	-	1/1/15/20	3/37/115/115	-
25	CLA	b	613	-	1/1/15/20	14/37/115/115	-
29	LHG	A	613	-	-	18/51/51/53	-
25	CLA	b	607	37	1/1/15/20	13/37/115/115	-
25	CLA	a	612	37	-	2/37/115/115	-
26	BCR	c	514	-	-	5/29/63/63	0/2/2/2
32	STE	I	101	-	-	3/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	508	-	-	6/37/115/115	-
28	LMG	D	408	-	-	18/46/66/70	0/1/1/1
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
27	PL9	d	406	-	-	13/53/73/73	0/1/1/1
25	CLA	b	610	37	1/1/15/20	4/37/115/115	-
26	BCR	A	609	-	-	1/29/63/63	0/2/2/2
28	LMG	b	624	-	-	24/50/70/70	0/1/1/1
30	SQD	a	613	-	-	24/49/69/69	0/1/1/1
32	STE	B	627	-	-	7/13/13/17	-
29	LHG	L	101	-	-	18/53/53/53	-
25	CLA	A	608	-	1/1/12/20	3/24/102/115	-
25	CLA	b	615	-	1/1/15/20	9/37/115/115	-
25	CLA	c	508	-	-	3/36/114/115	-
32	STE	b	626	-	-	5/7/7/17	-
25	CLA	C	505	-	1/1/15/20	10/37/115/115	-
25	CLA	B	607	37	1/1/15/20	5/37/115/115	-
25	CLA	C	509	-	1/1/15/20	14/37/115/115	-
30	SQD	A	615	-	-	12/39/39/69	-
32	STE	b	625	-	-	6/13/13/17	-
32	STE	B	624	-	-	5/9/9/17	-
25	CLA	a	608	37	-	8/37/115/115	-
25	CLA	A	611	37	1/1/15/20	5/37/115/115	-
25	CLA	b	611	-	1/1/15/20	4/37/115/115	-
31	DGD	c	517	-	-	23/51/91/95	0/2/2/2
25	CLA	A	606	-	1/1/15/20	4/37/115/115	-
25	CLA	C	504	37	1/1/13/20	6/30/108/115	-
32	STE	j	101	-	-	5/9/9/17	-
28	LMG	c	520	-	-	21/43/63/70	0/1/1/1
29	LHG	D	410	-	-	20/53/53/53	-
25	CLA	B	601	37	1/1/15/20	18/37/115/115	-
30	SQD	A	614	-	-	22/47/67/69	0/1/1/1
25	CLA	b	614	-	1/1/15/20	20/37/115/115	-
25	CLA	c	505	-	1/1/15/20	8/37/115/115	-
25	CLA	B	608	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	D	404	-	1/1/15/20	3/37/115/115	-
32	STE	c	521	-	-	4/9/9/17	-
25	CLA	c	502	-	1/1/15/20	2/37/115/115	-
32	STE	l	102	-	-	9/15/15/17	-
25	CLA	b	605	-	1/1/15/20	10/37/115/115	-
25	CLA	B	605	-	1/1/15/20	9/37/115/115	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
25	CLA	c	504	37	1/1/14/20	7/31/109/115	-
32	STE	B	625	-	-	9/15/15/17	-
25	CLA	C	503	-	1/1/15/20	3/37/115/115	-
25	CLA	b	606	-	1/1/15/20	5/37/115/115	-
27	PL9	a	611	-	-	15/53/73/73	0/1/1/1
30	SQD	D	409	-	-	13/28/48/69	0/1/1/1
26	BCR	T	101	-	-	6/29/63/63	0/2/2/2
32	STE	M	102	-	-	6/12/12/17	-
34	PHO	d	401	-	-	0/37/103/103	0/5/6/6
25	CLA	b	604	-	1/1/15/20	7/37/115/115	-
32	STE	c	519	-	-	10/17/17/17	-
25	CLA	C	501	-	1/1/15/20	4/37/115/115	-
32	STE	C	519	-	-	1/9/9/17	-
25	CLA	c	507	37	1/1/15/20	8/37/115/115	-
31	DGD	A	616	-	-	28/55/95/95	0/2/2/2
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
29	LHG	d	407	-	-	18/53/53/53	-
25	CLA	B	615	-	1/1/15/20	11/37/115/115	-
26	BCR	K	102	-	-	7/29/63/63	0/2/2/2
25	CLA	A	607	37	1/1/15/20	10/37/115/115	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
29	LHG	E	101	-	-	23/53/53/53	-
32	STE	E	102	-	-	6/9/9/17	-
25	CLA	b	616	-	1/1/14/20	5/31/109/115	-
29	LHG	e	101	-	-	26/46/46/53	-
32	STE	J	101	-	-	7/9/9/17	-
32	STE	C	520	-	-	4/9/9/17	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	d	412	-	-	10/14/14/17	-
34	PHO	D	403	-	-	1/37/103/103	0/5/6/6
31	DGD	h	101	-	-	14/51/91/95	0/2/2/2
28	LMG	C	518	-	-	20/43/63/70	0/1/1/1
28	LMG	d	411	-	-	13/39/59/70	0/1/1/1
25	CLA	b	602	-	1/1/15/20	9/37/115/115	-
28	LMG	D	411	-	-	14/33/33/70	-
29	LHG	l	101	-	-	15/53/53/53	-
31	DGD	H	102	-	-	17/51/91/95	0/2/2/2
25	CLA	B	612	-	1/1/15/20	9/37/115/115	-
25	CLA	c	513	-	1/1/15/20	5/37/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
28	LMG	A	612	-	-	17/43/63/70	0/1/1/1
36	HEC	V	201	16	-	2/10/54/54	-
25	CLA	B	614	-	1/1/15/20	7/37/115/115	-
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
25	CLA	B	616	-	1/1/14/20	7/31/109/115	-
25	CLA	c	511	3	1/1/15/20	7/37/115/115	-
25	CLA	B	604	-	1/1/15/20	11/37/115/115	-
30	SQD	b	620	-	-	20/44/64/69	0/1/1/1
32	STE	C	521	-	-	5/13/13/17	-
25	CLA	b	612	-	1/1/15/20	3/37/115/115	-
27	PL9	A	610	-	-	26/53/73/73	0/1/1/1
31	DGD	o	301	-	-	19/45/45/95	-
26	BCR	t	101	-	-	8/29/63/63	0/2/2/2
26	BCR	x	101	-	-	3/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	12/37/115/115	-
32	STE	H	103	-	-	10/15/15/17	-
34	PHO	d	402	-	-	5/37/103/103	0/5/6/6
25	CLA	c	506	-	1/1/15/20	15/37/115/115	-
31	DGD	c	515	-	-	26/51/91/95	0/2/2/2
31	DGD	C	515	-	-	24/51/91/95	0/2/2/2
25	CLA	d	403	-	1/1/15/20	6/37/115/115	-
25	CLA	B	602	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	603	-	1/1/15/20	13/37/115/115	-
25	CLA	c	503	-	1/1/15/20	7/37/115/115	-
29	LHG	B	622	-	-	18/53/53/53	-
25	CLA	c	510	-	1/1/15/20	8/37/115/115	-
32	STE	B	626	-	-	6/9/9/17	-
25	CLA	C	510	-	1/1/15/20	3/37/115/115	-
26	BCR	k	103	-	-	2/29/63/63	0/2/2/2
25	CLA	C	507	37	1/1/15/20	10/37/115/115	-
29	LHG	d	408	-	-	21/53/53/53	-
25	CLA	C	502	-	-	7/37/115/115	-
32	STE	T	102	-	-	9/12/12/17	-
25	CLA	B	609	-	-	2/37/115/115	-
25	CLA	c	512	-	1/1/15/20	20/37/115/115	-
26	BCR	b	617	-	-	4/29/63/63	0/2/2/2
32	STE	d	413	-	-	10/17/17/17	-
25	CLA	b	608	-	1/1/15/20	6/37/115/115	-
28	LMG	B	621	-	-	5/22/22/70	-
31	DGD	C	517	-	-	16/51/91/95	0/2/2/2
30	SQD	B	623	-	-	21/49/69/69	0/1/1/1
25	CLA	D	405	-	-	6/37/115/115	-
28	LMG	b	622	-	-	17/46/66/70	0/1/1/1
31	DGD	C	516	-	-	21/51/91/95	0/2/2/2
28	LMG	c	522	-	-	24/44/64/70	0/1/1/1
31	DGD	c	516	-	-	18/51/91/95	0/2/2/2
26	BCR	B	619	-	-	6/29/63/63	0/2/2/2
32	STE	b	621	-	-	10/13/13/17	-
30	SQD	a	614	-	-	18/37/37/69	-
25	CLA	B	611	-	1/1/15/20	5/37/115/115	-
28	LMG	c	518	-	-	12/31/51/70	0/1/1/1
25	CLA	C	513	-	1/1/15/20	11/37/115/115	-
35	HEM	F	101	6,5	-	2/12/54/54	-
32	STE	B	620	-	-	8/14/14/17	-
26	BCR	k	101	-	-	8/29/63/63	0/2/2/2
26	BCR	b	618	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	609	-	-	6/37/115/115	-
25	CLA	B	613	-	1/1/15/20	11/37/115/115	-
28	LMG	d	410	-	-	13/17/17/70	-
32	STE	b	623	-	-	12/17/17/17	-
32	STE	t	102	-	-	3/11/11/17	-
25	CLA	d	404	-	1/1/15/20	7/37/115/115	-
27	PL9	D	407	-	-	13/53/73/73	0/1/1/1
36	HEC	v	201	16	-	2/10/54/54	-
26	BCR	K	101	-	-	3/29/63/63	0/2/2/2
32	STE	t	103	-	-	3/7/7/17	-
25	CLA	B	606	-	1/1/15/20	13/37/115/115	-
32	STE	m	101	-	-	4/9/9/17	-
34	PHO	D	402	-	-	2/37/103/103	0/5/6/6
32	STE	M	103	-	-	5/7/7/17	-
25	CLA	C	506	-	1/1/15/20	11/37/115/115	-
26	BCR	b	619	-	-	1/29/63/63	0/2/2/2
25	CLA	B	603	-	1/1/15/20	5/37/115/115	-
32	STE	a	615	-	-	6/9/9/17	-
25	CLA	b	601	37	1/1/15/20	13/37/115/115	-
29	LHG	d	409	-	-	9/43/43/53	-
25	CLA	B	610	37	1/1/15/20	5/37/115/115	-
25	CLA	C	511	3	1/1/15/20	4/37/115/115	-
32	STE	T	103	-	-	8/17/17/17	-
30	SQD	f	102	-	-	17/36/56/69	0/1/1/1
28	LMG	M	101	-	-	23/46/66/70	0/1/1/1
25	CLA	c	501	-	1/1/15/20	5/37/115/115	-
32	STE	X	101	-	-	10/17/17/17	-

The worst 5 of 652 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	CHB-C4A	7.96	1.40	1.33
25	B	606	CLA	CHB-C4A	7.77	1.40	1.33
25	c	511	CLA	MG-NA	7.77	2.24	2.06
25	a	607	CLA	CHB-C4A	7.63	1.40	1.33
25	B	606	CLA	MG-NA	7.54	2.24	2.06

The worst 5 of 1120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409	SQD	O6-C1-C2	12.90	127.87	108.27
25	C	503	CLA	C4A-NA-C1A	9.31	110.92	106.68
25	c	511	CLA	C4A-NA-C1A	8.54	110.58	106.68
25	C	511	CLA	C4A-NA-C1A	8.24	110.44	106.68
30	D	409	SQD	C1-O5-C5	-8.23	97.65	113.72

5 of 62 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	608	CLA	ND
25	A	611	CLA	ND
25	B	601	CLA	ND

5 of 1686 torsion outliers are listed below:

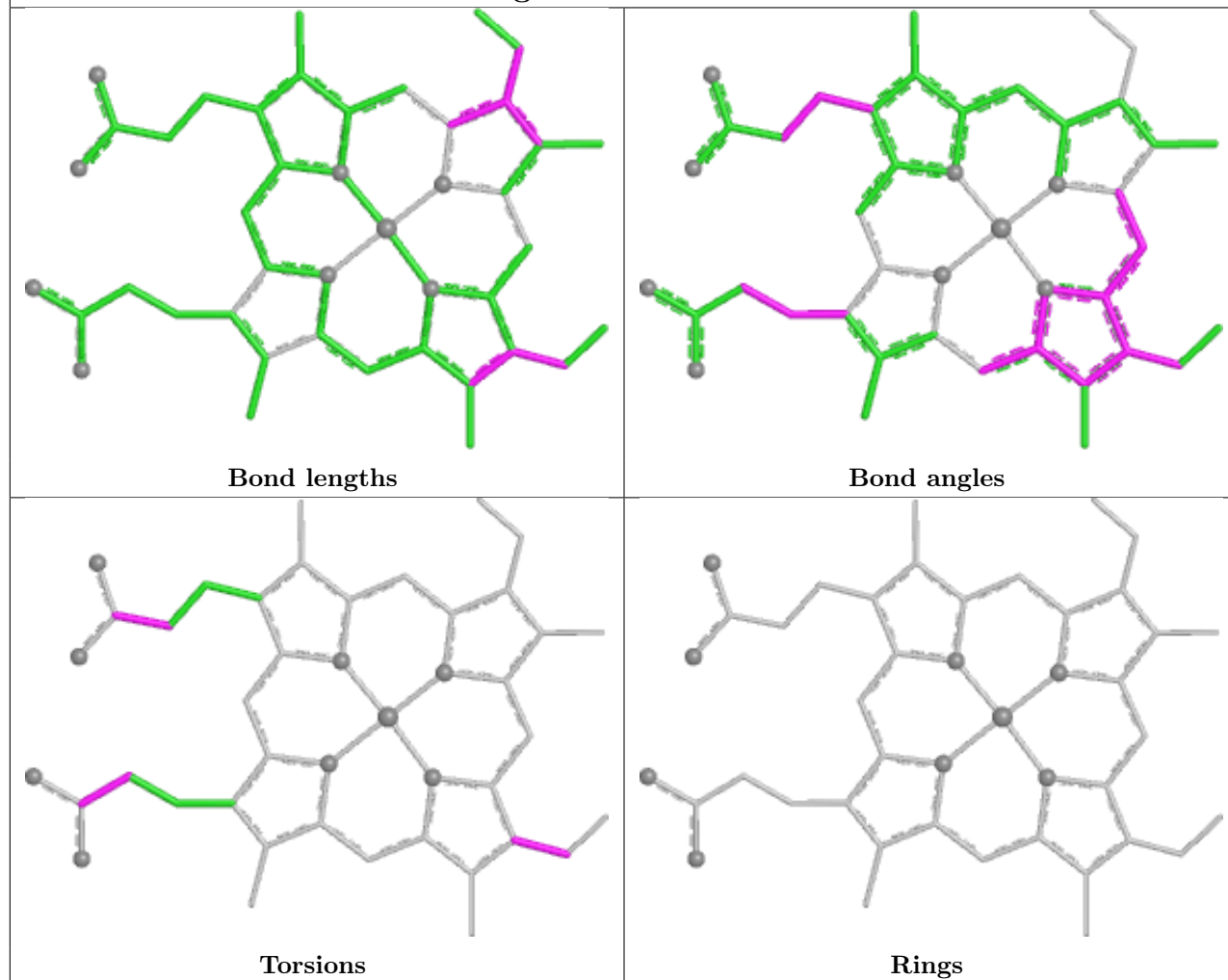
Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	602	CLA	C14-C13-C15-C16
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	C4-C3-C5-C6

There are no ring outliers.

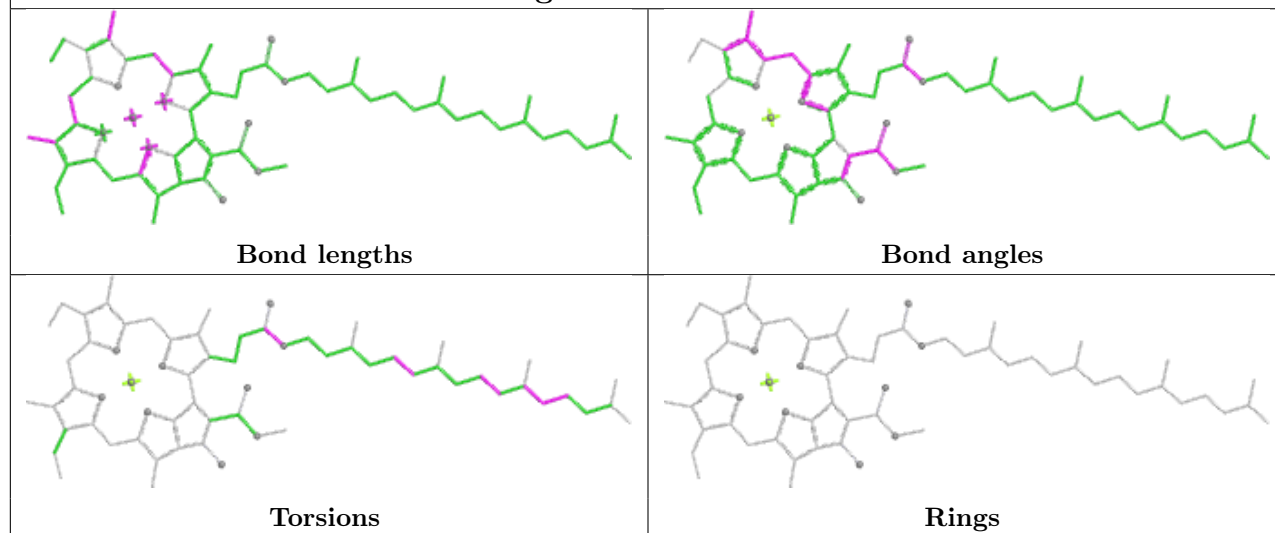
No monomer is involved in short contacts.

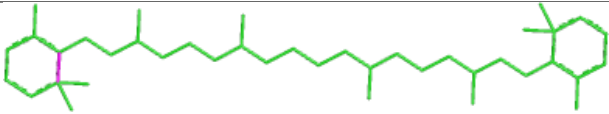
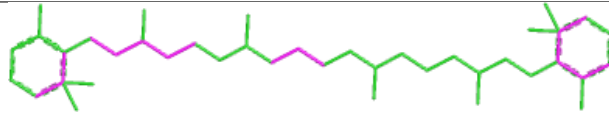
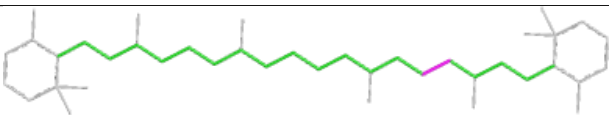
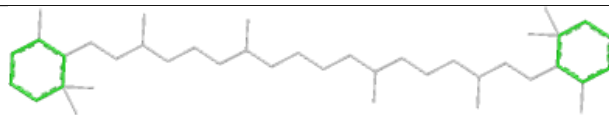

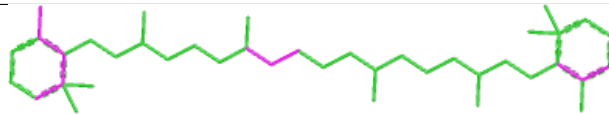
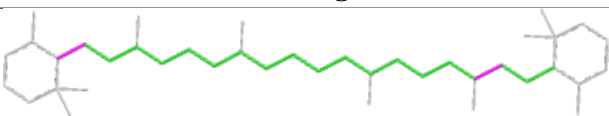
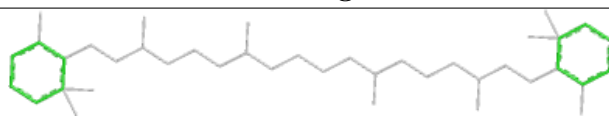
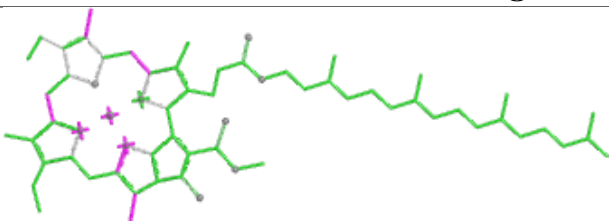
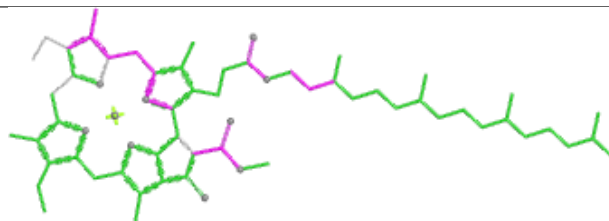
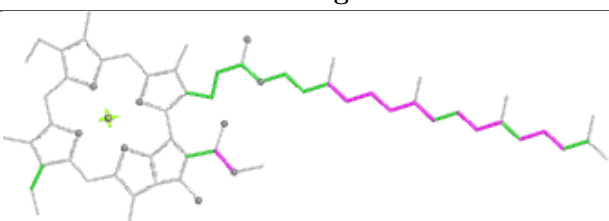
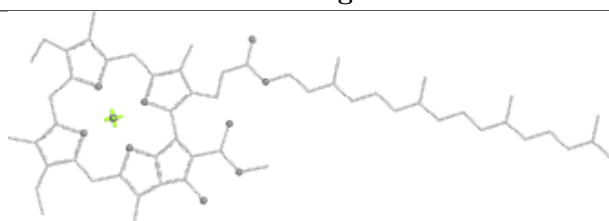
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

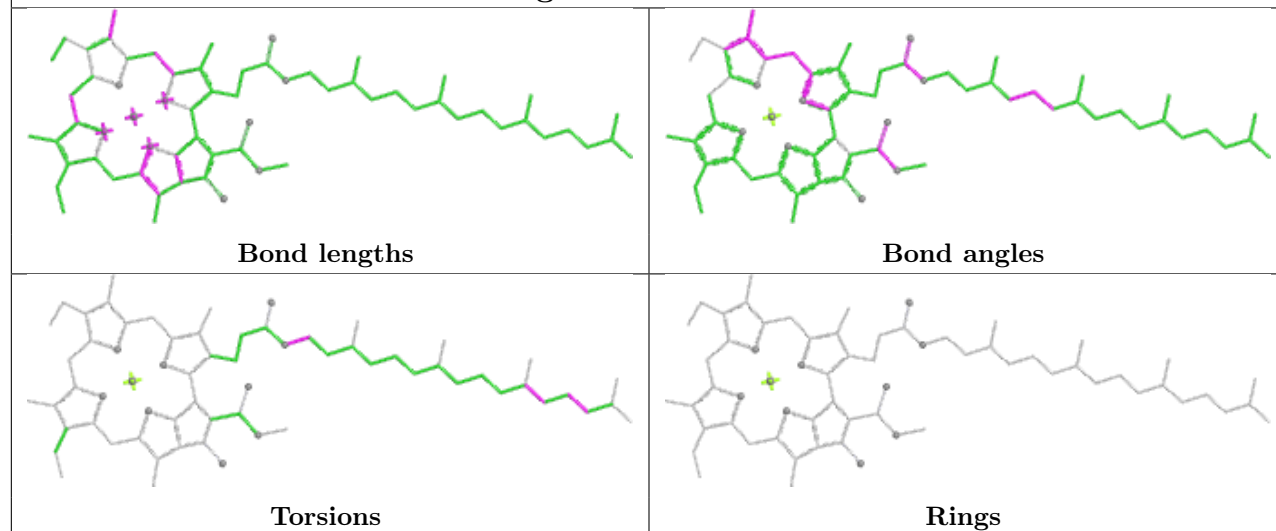
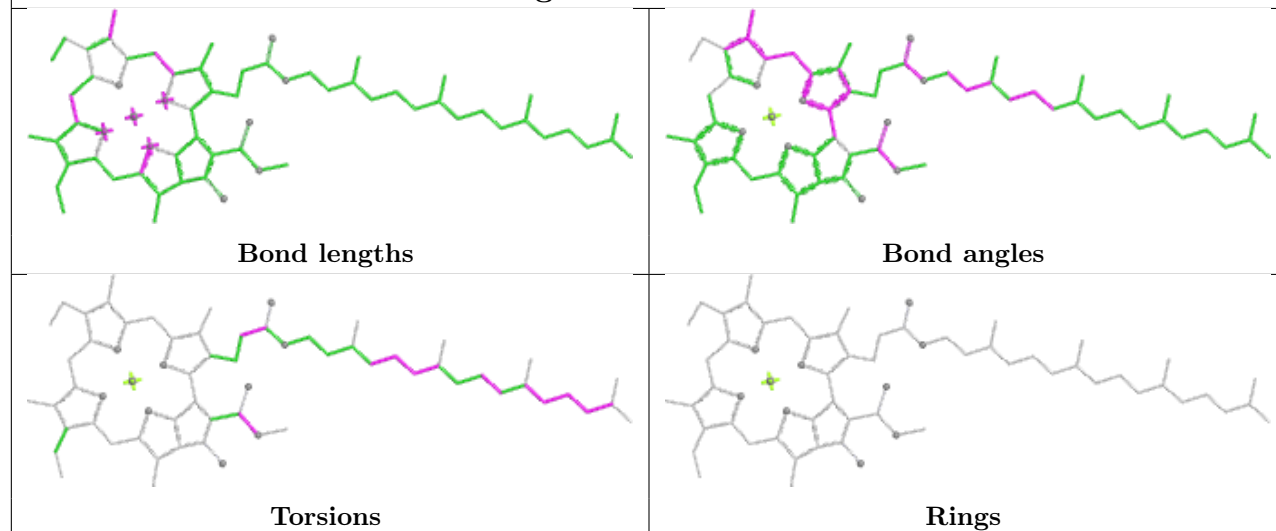
Ligand HEM f 101

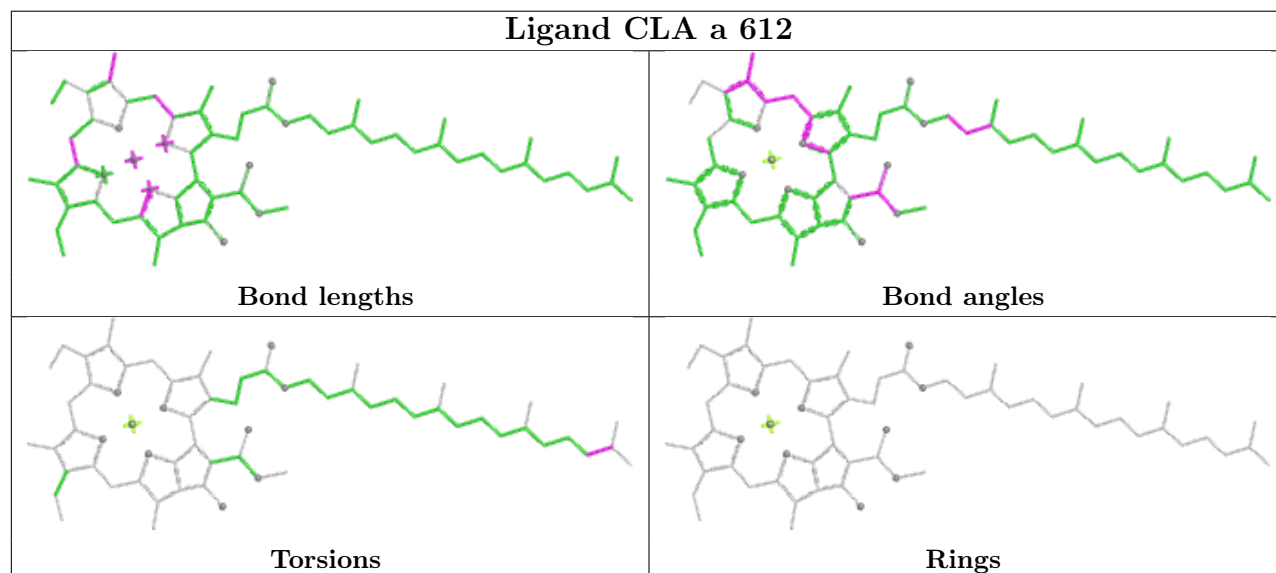
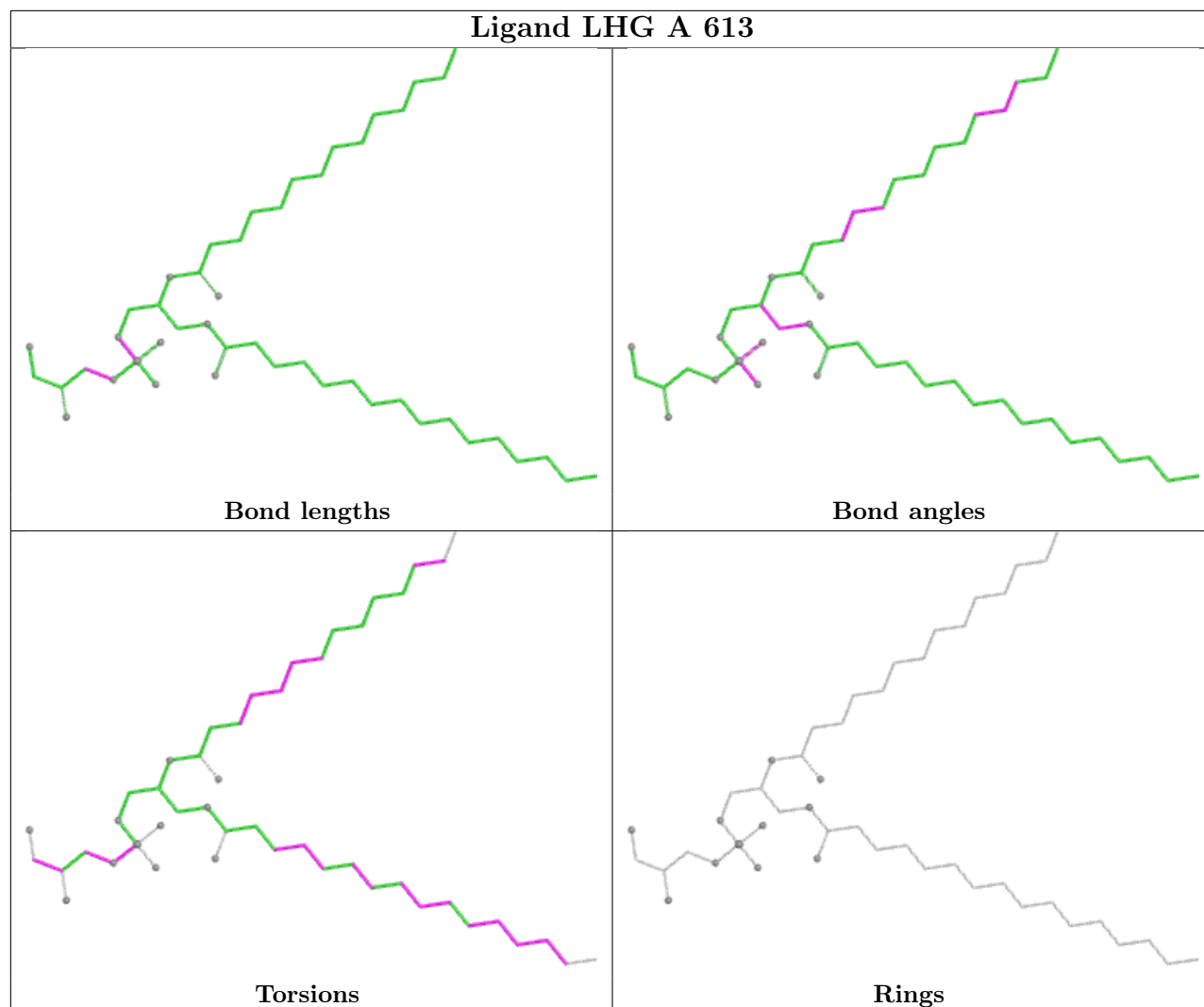


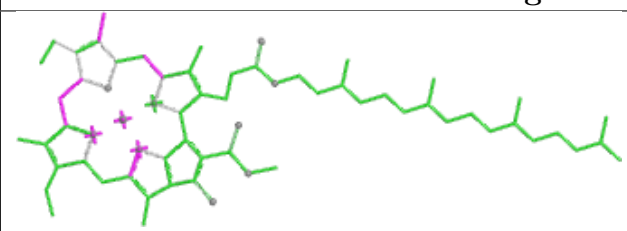
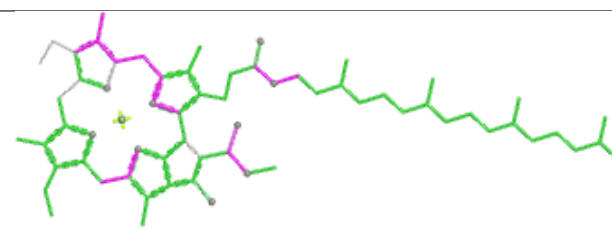
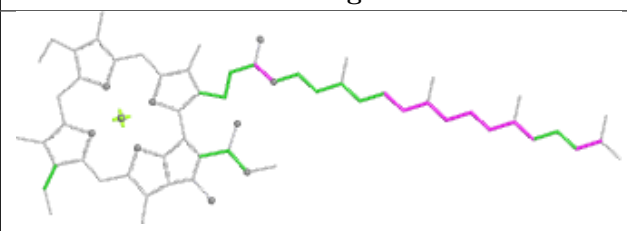
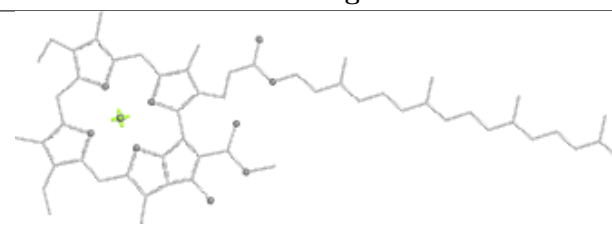
Ligand CLA a 609



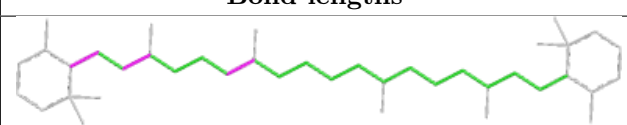
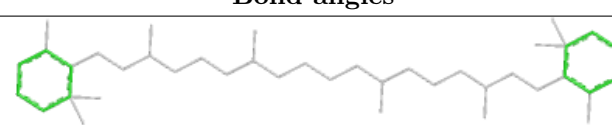




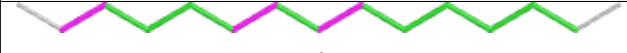

Ligand BCR a 610	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

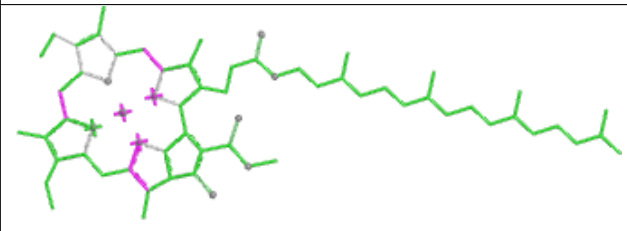
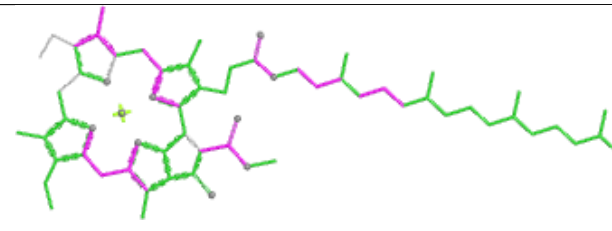
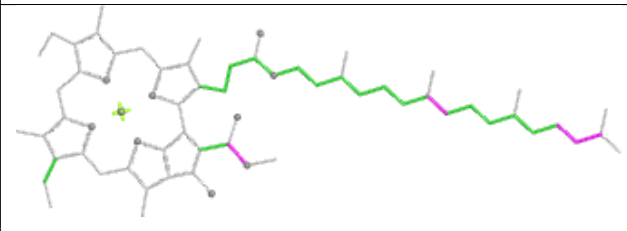
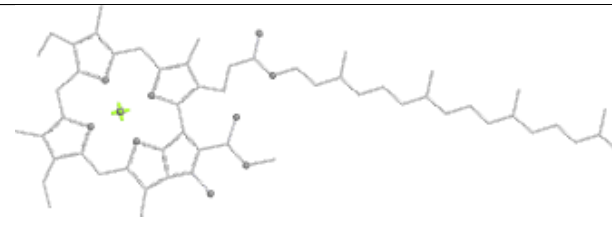
Ligand CLA a 607**Ligand CLA b 613**

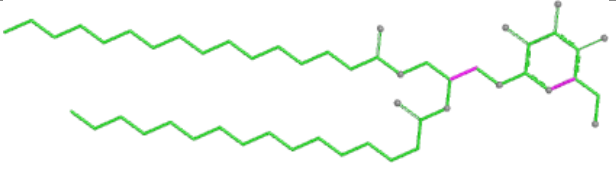
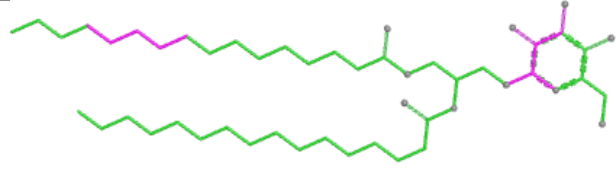
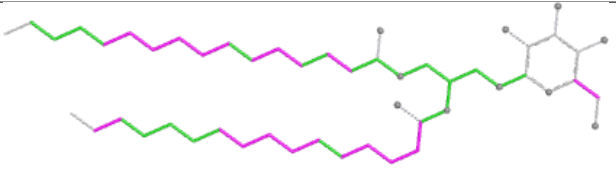
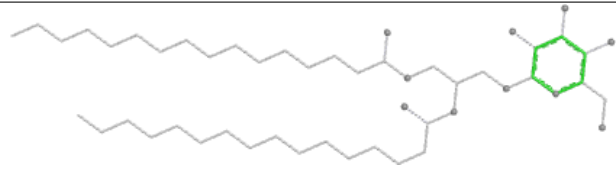


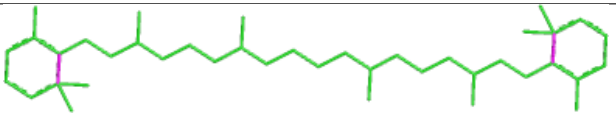
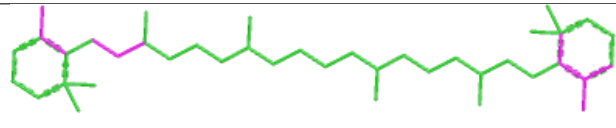
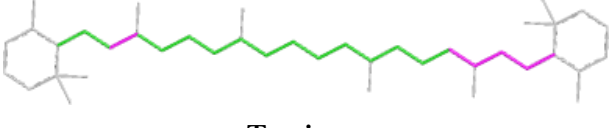
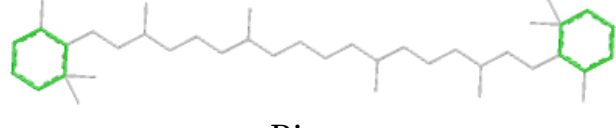
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings


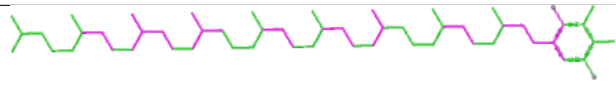

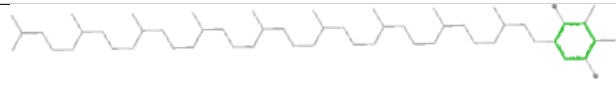
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

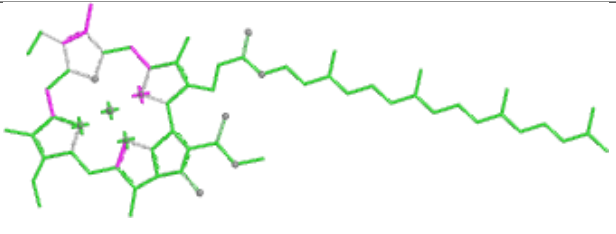
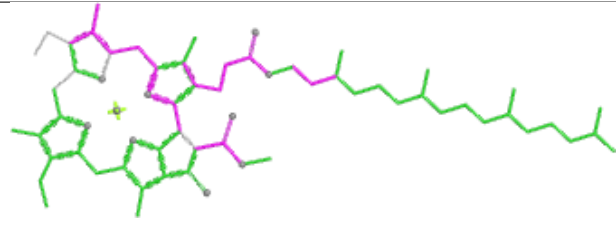
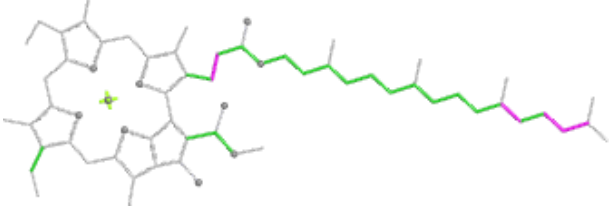
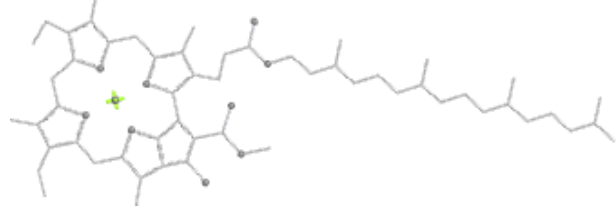
Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

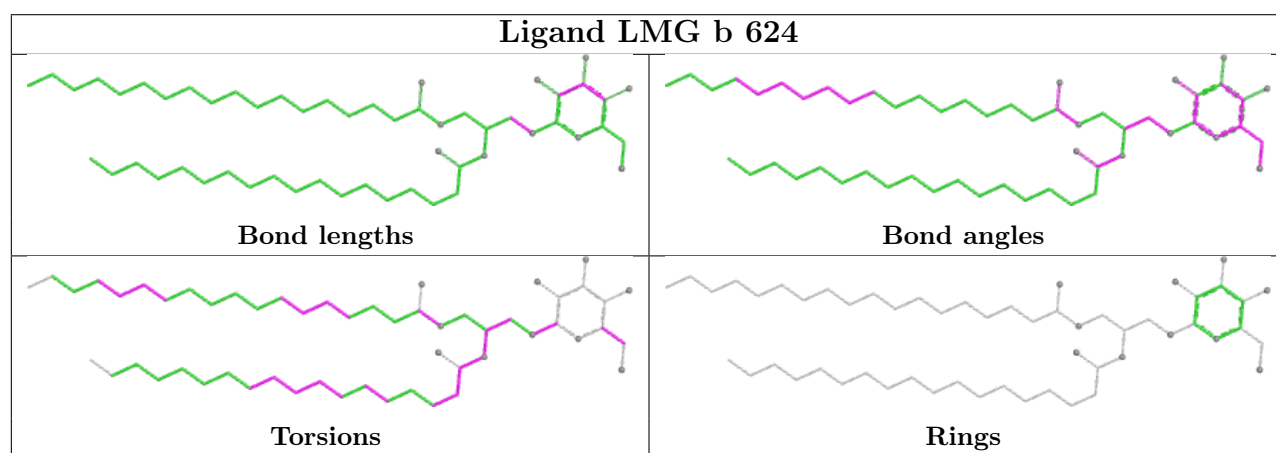
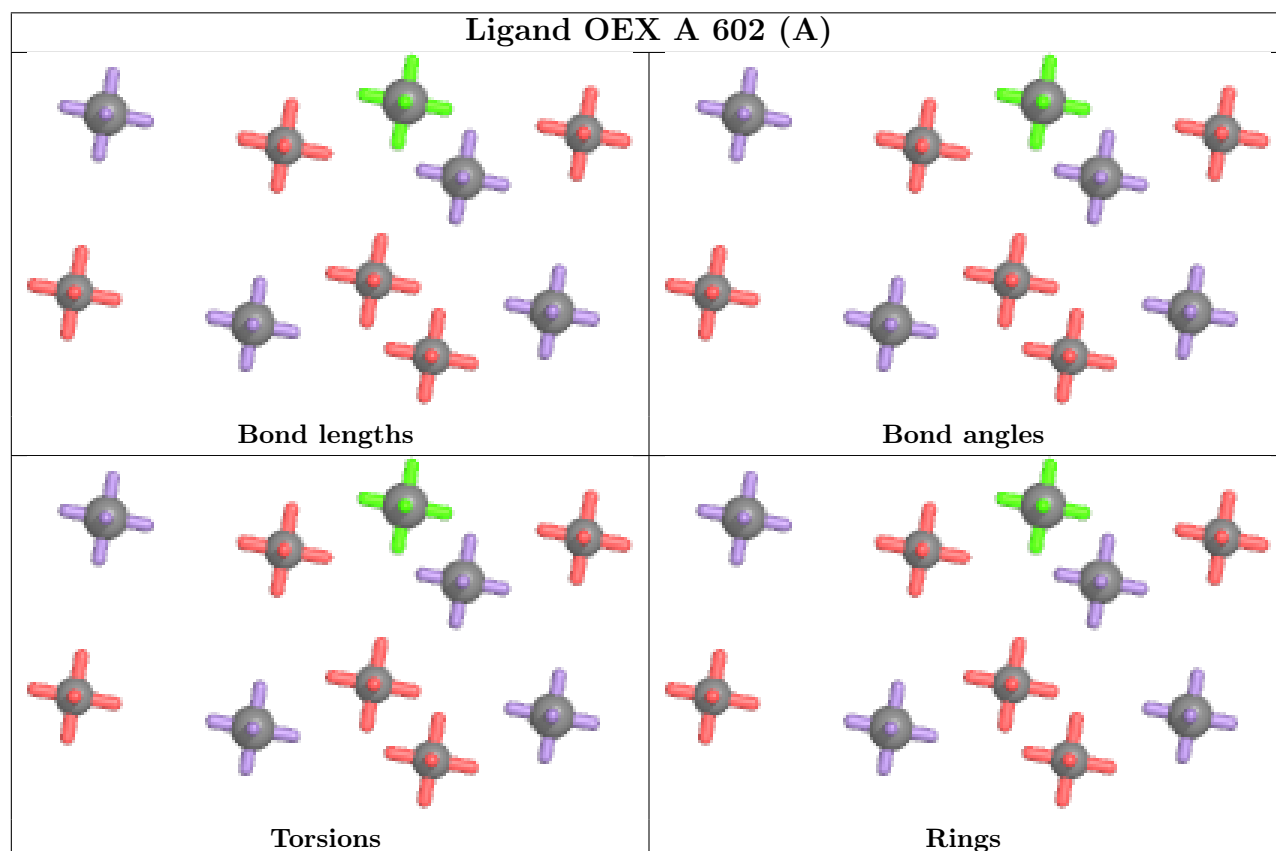
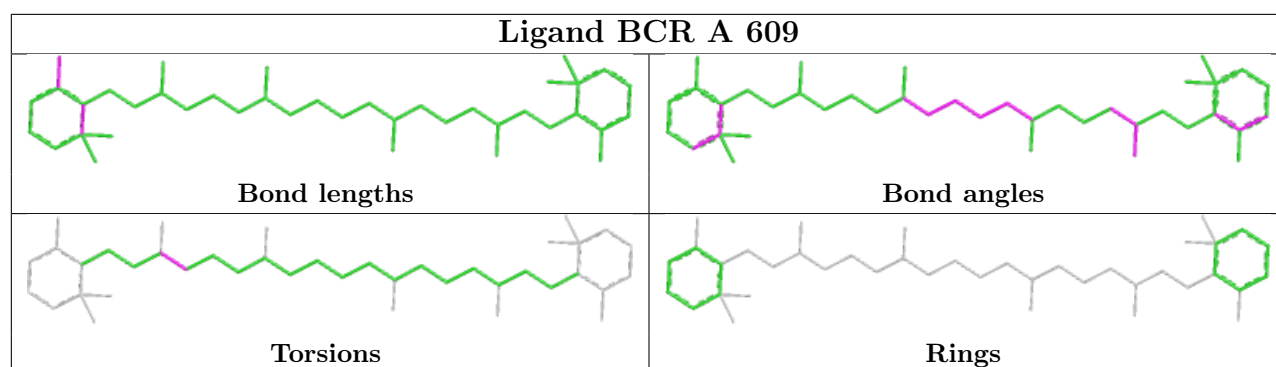
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

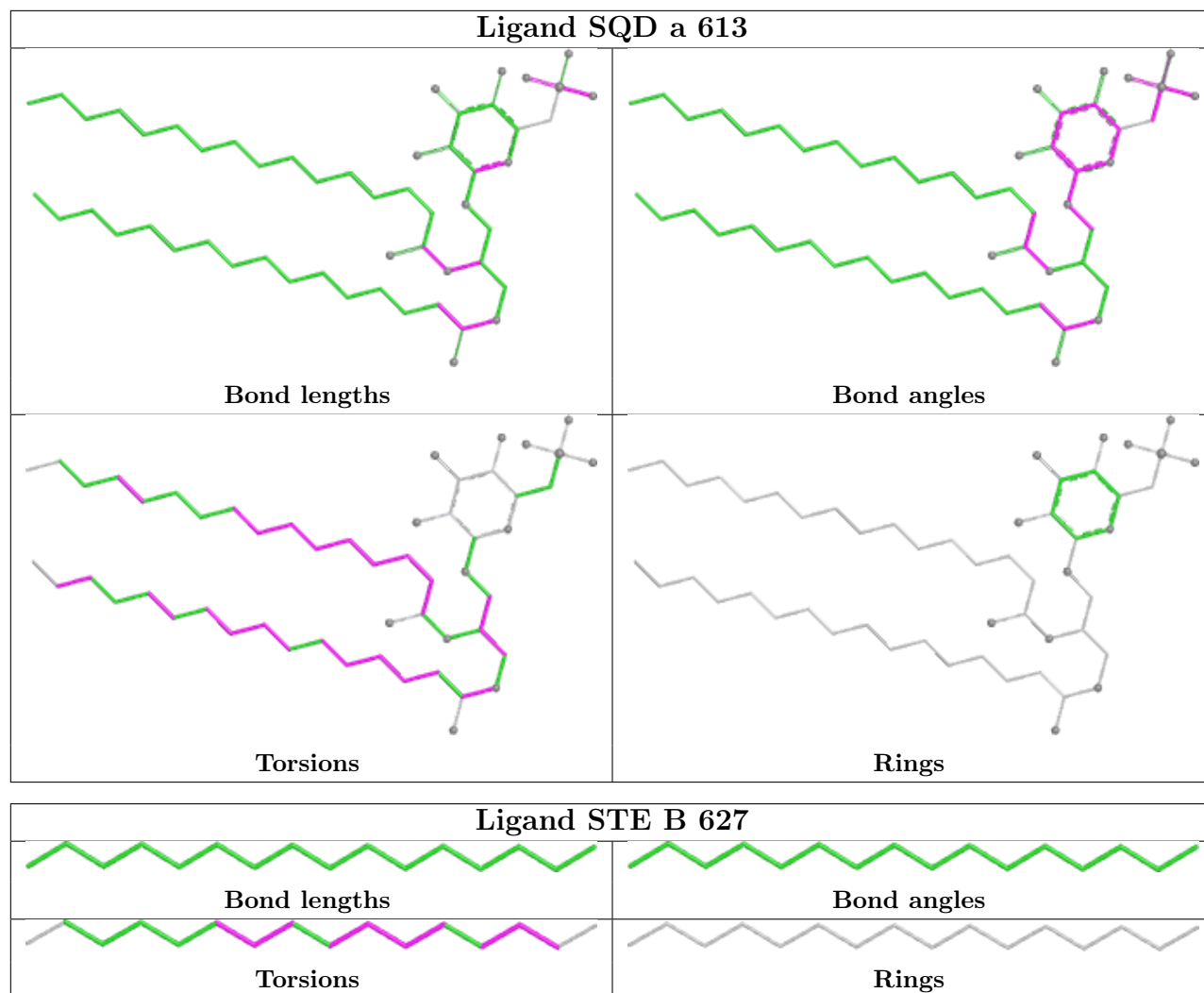
Ligand LMG D 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

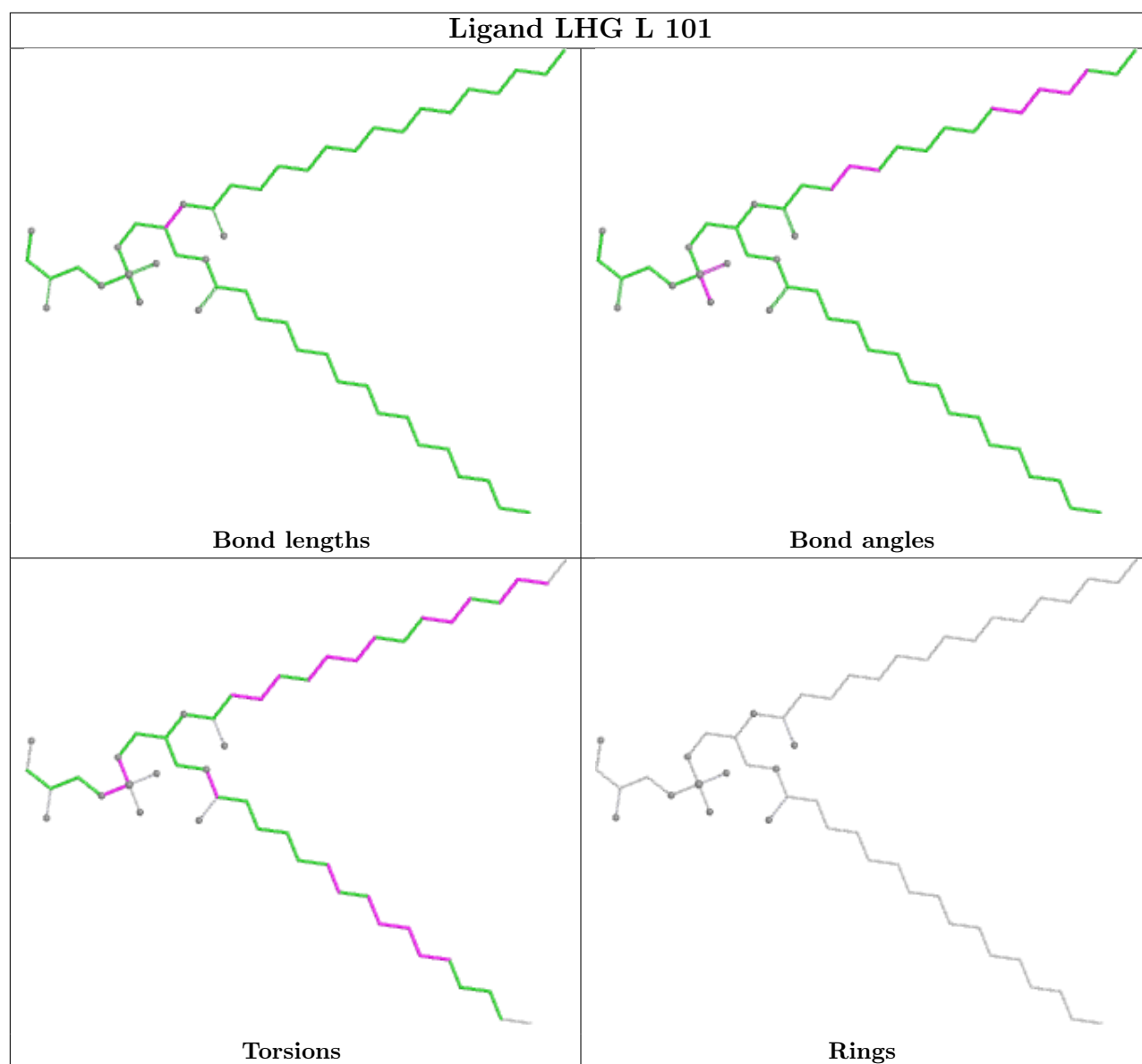
Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

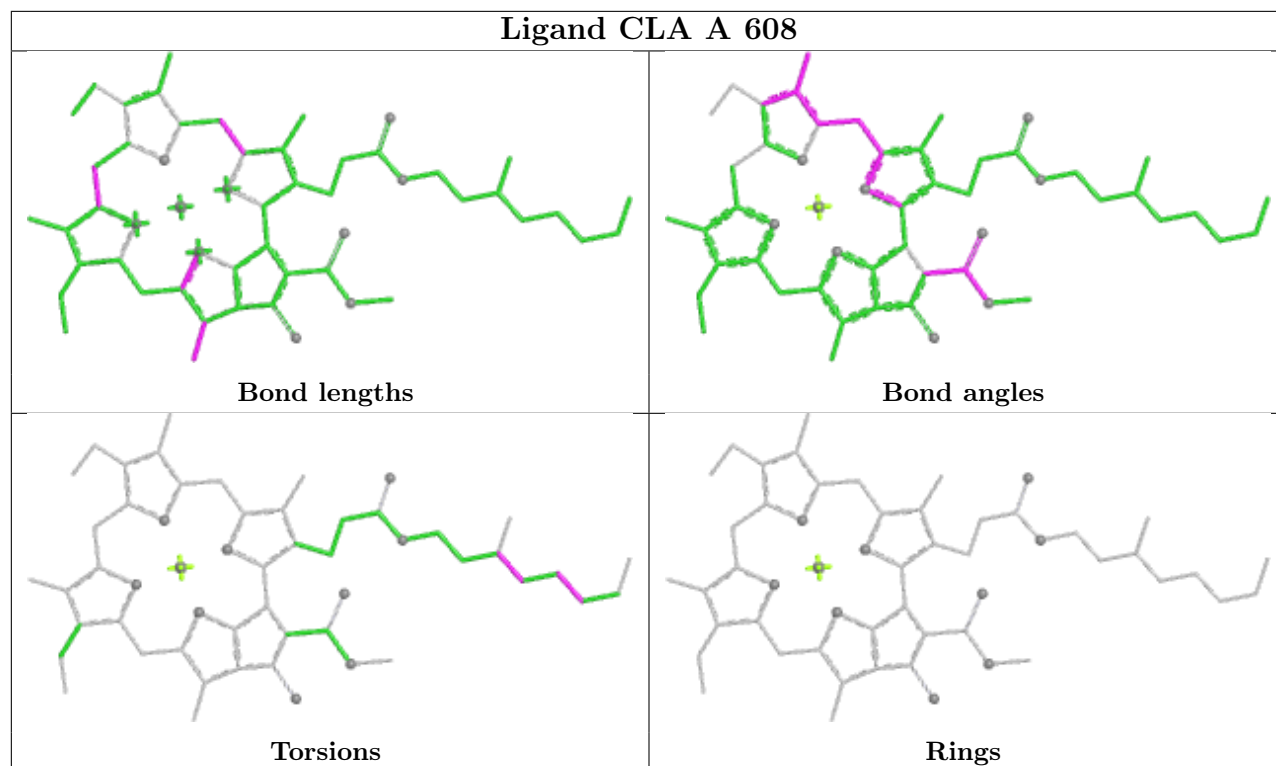
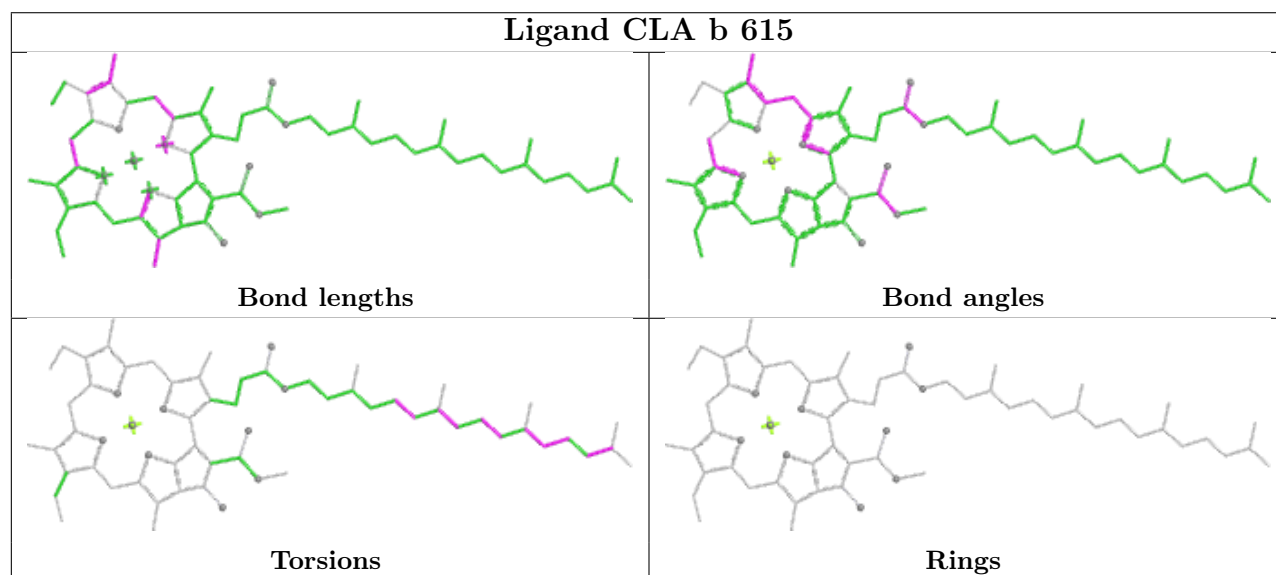
Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

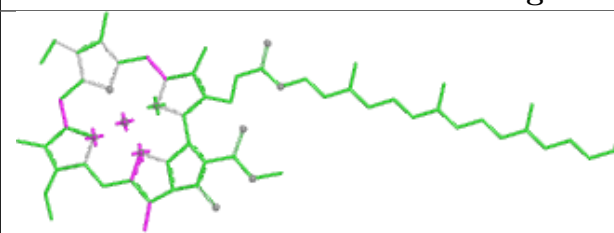
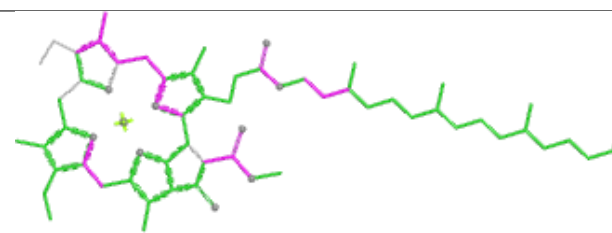
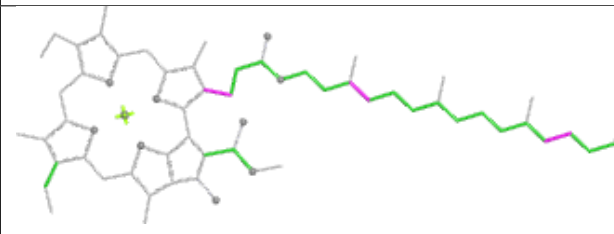
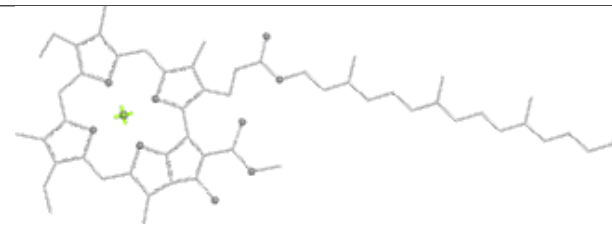




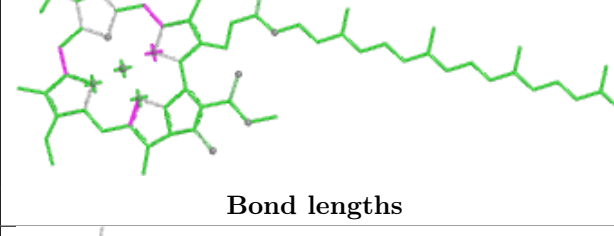
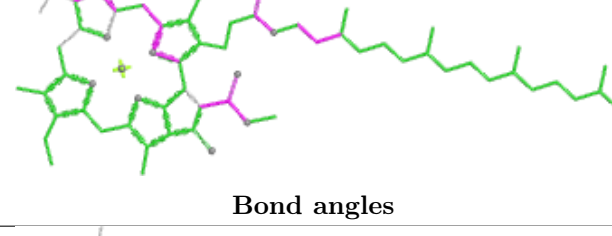
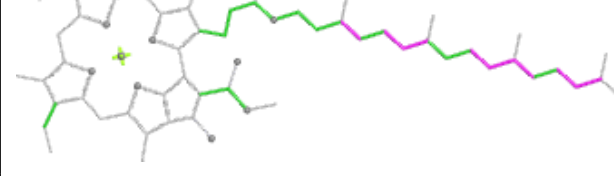
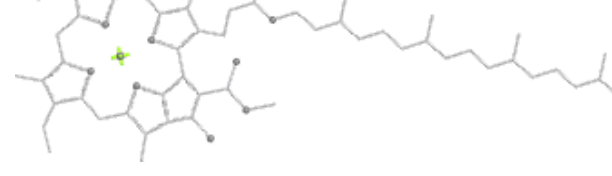
Ligand CLA b 610	
	
Bond lengths	Bond angles
	
Torsions	Rings



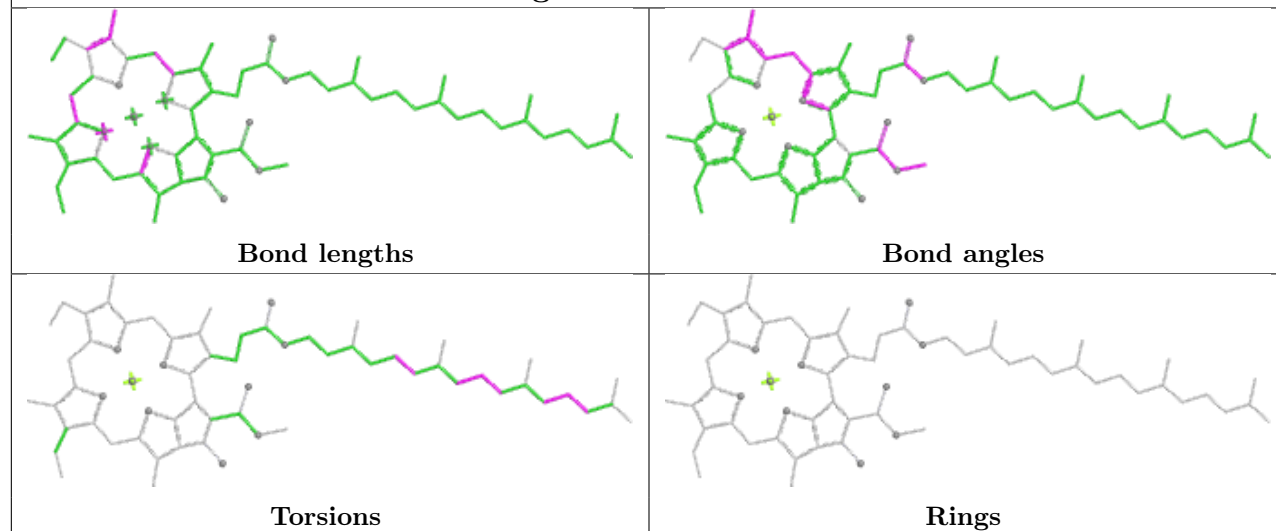




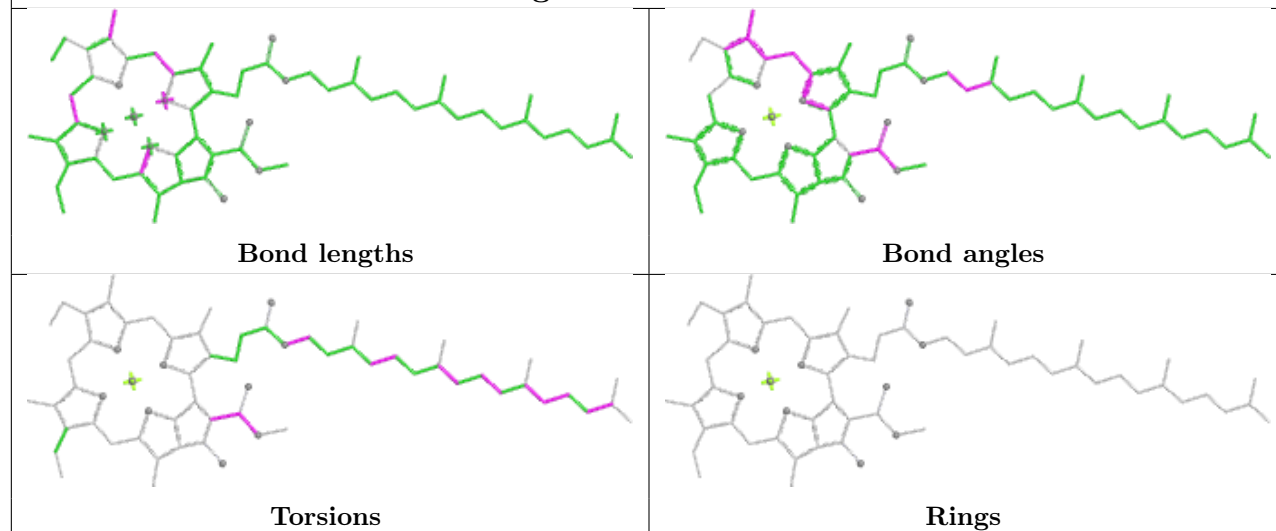
Ligand CLA A 608**Ligand CLA b 615**

Ligand CLA c 508	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE b 626	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA C 505	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

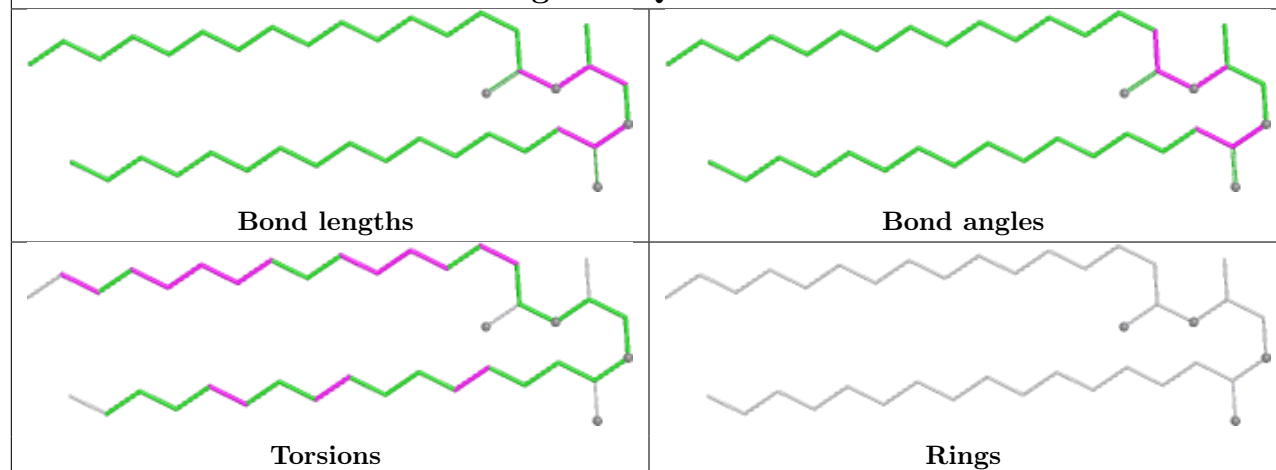
Ligand CLA B 607

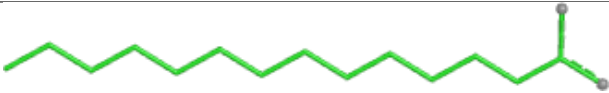
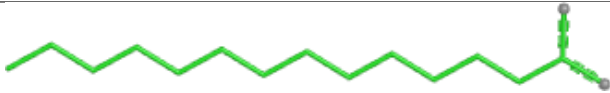
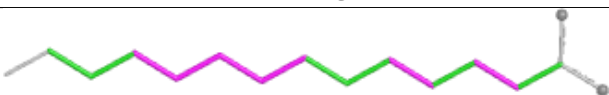
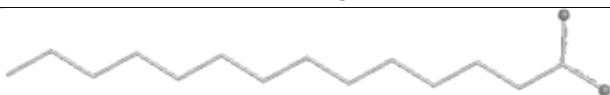






Ligand CLA C 509

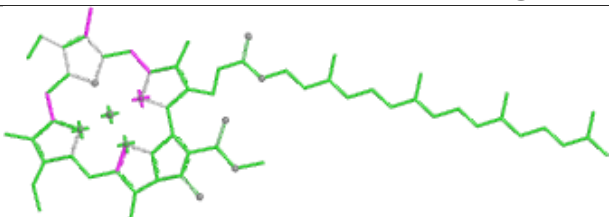
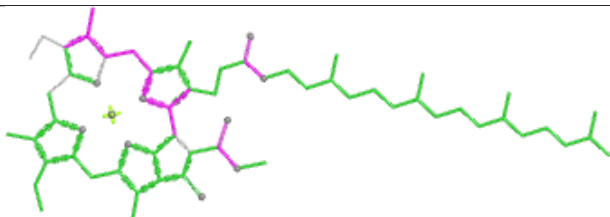
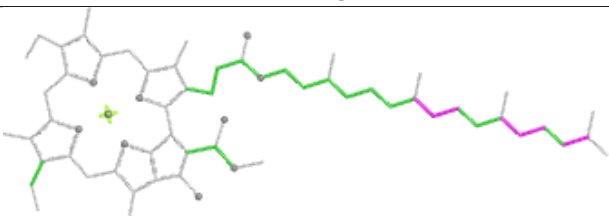
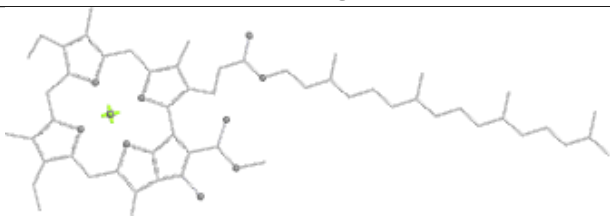


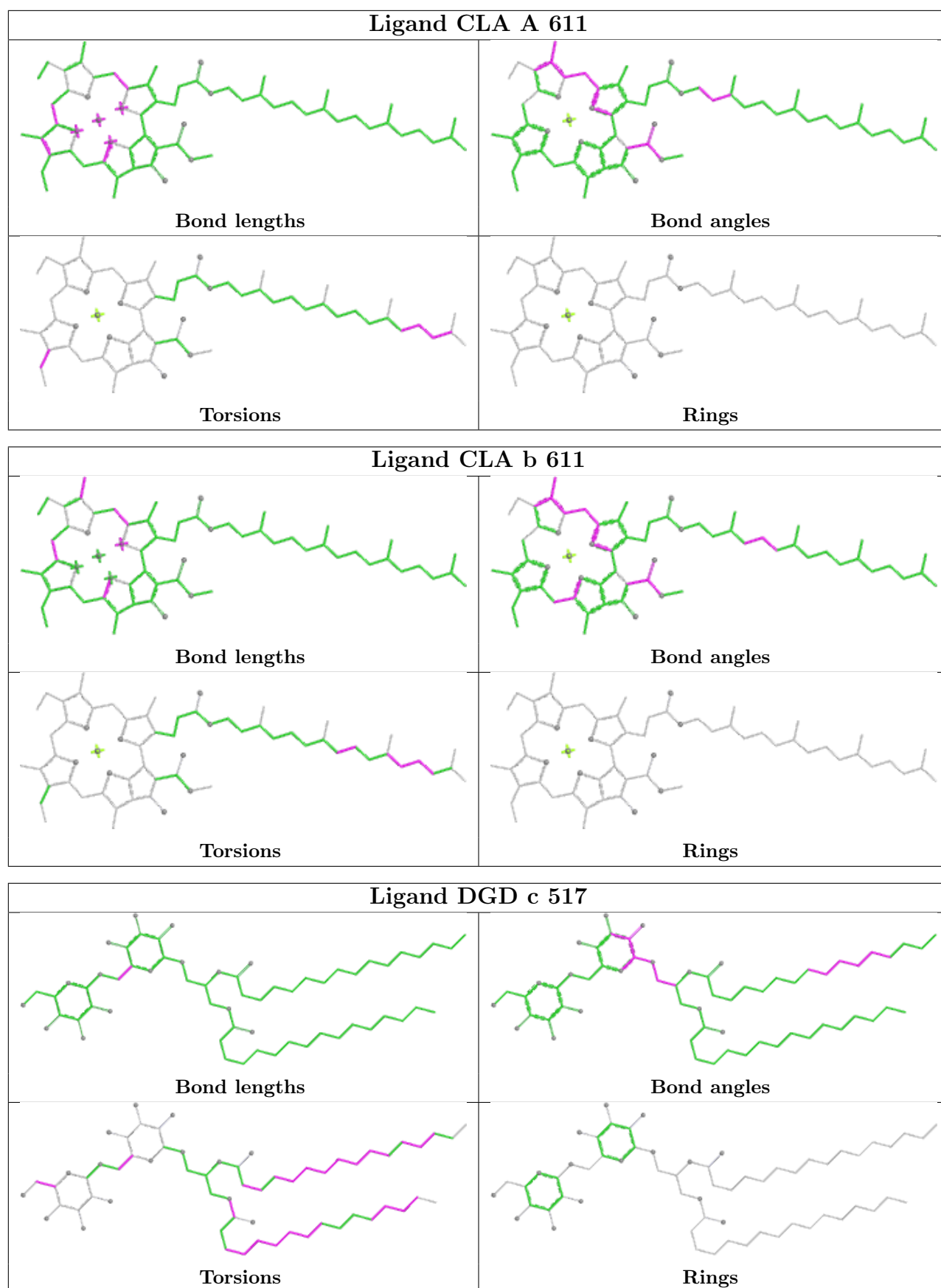
Ligand SQD A 615

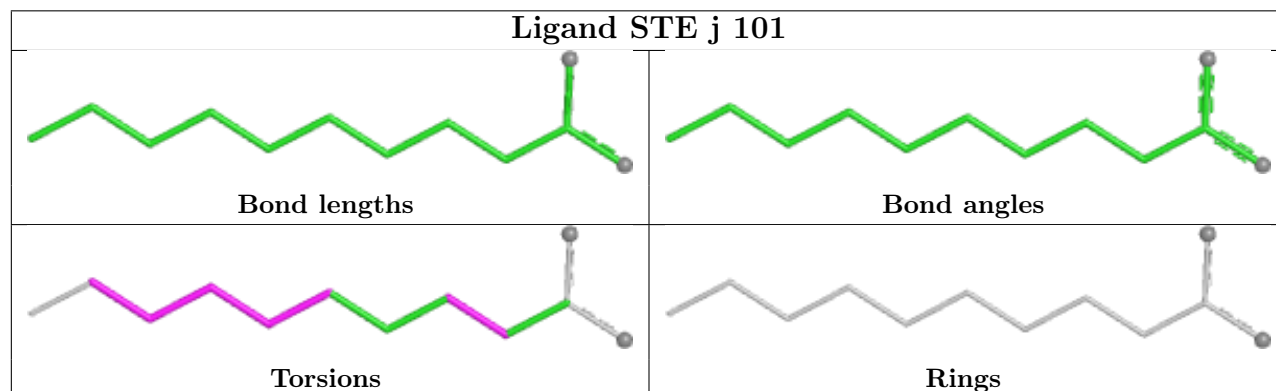
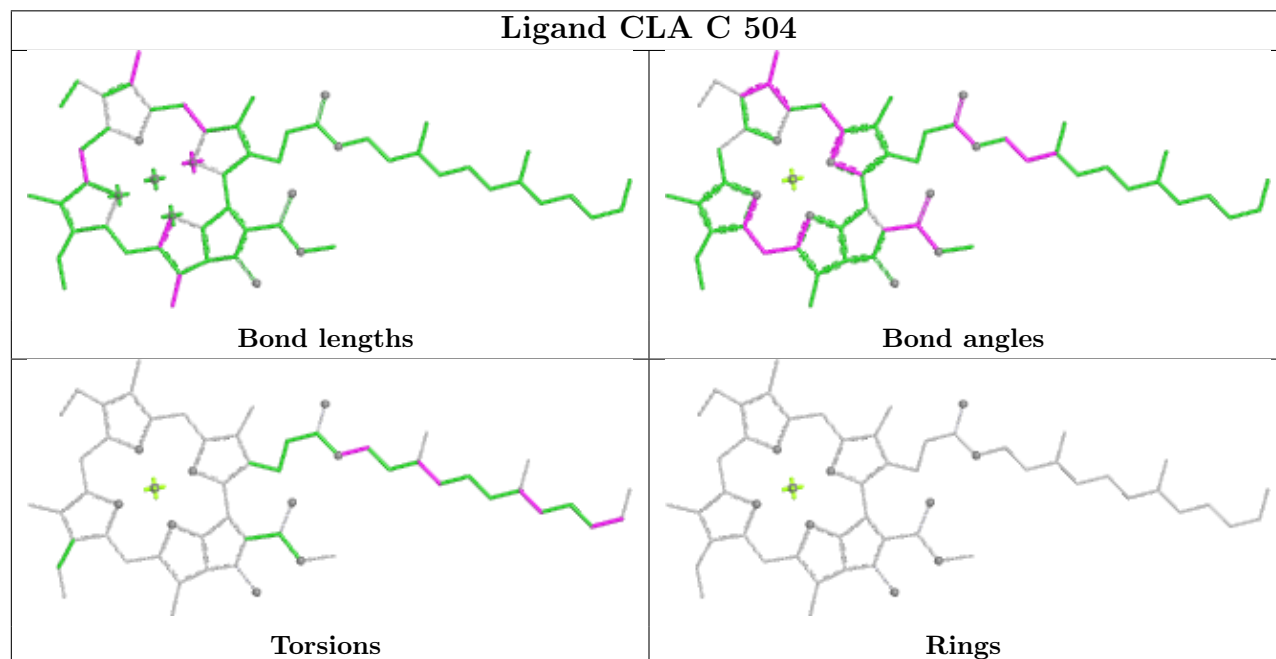
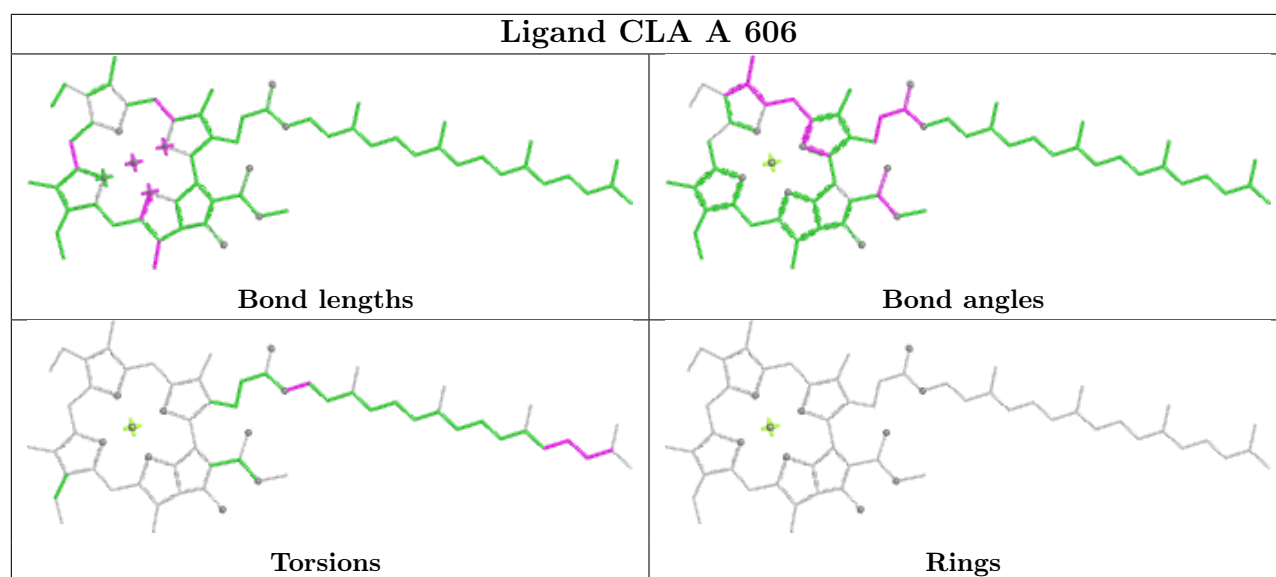


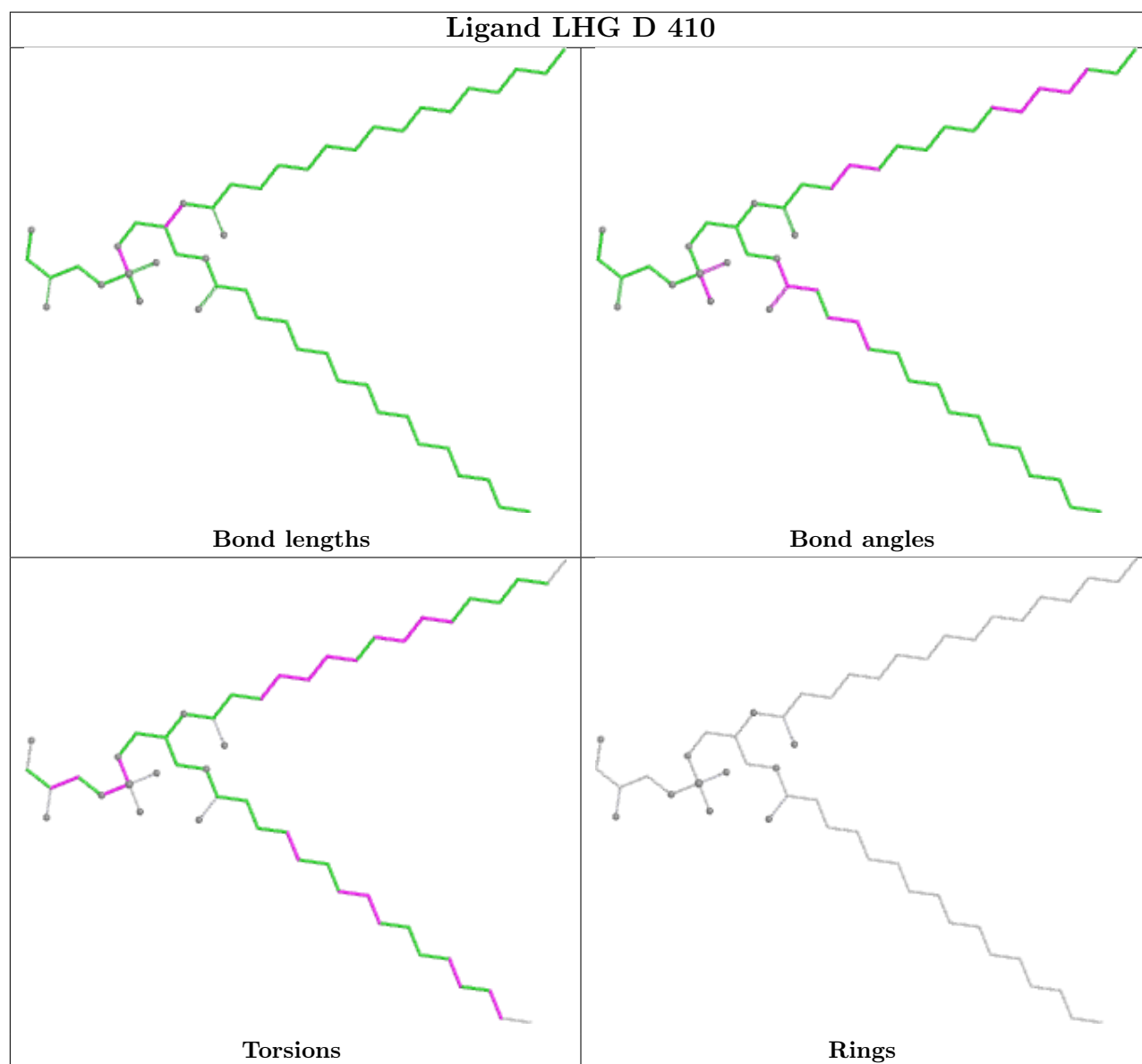
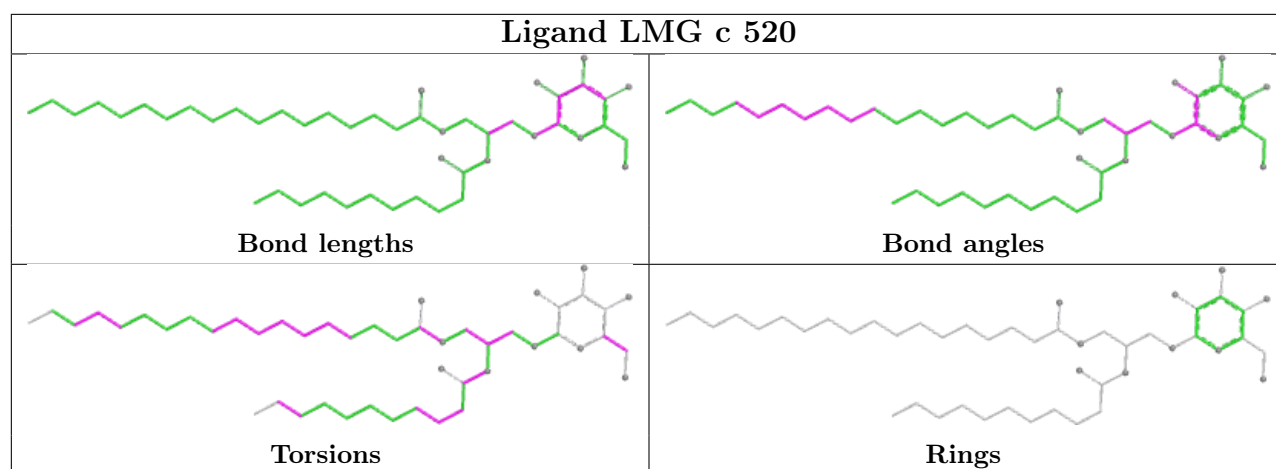
Ligand STE b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

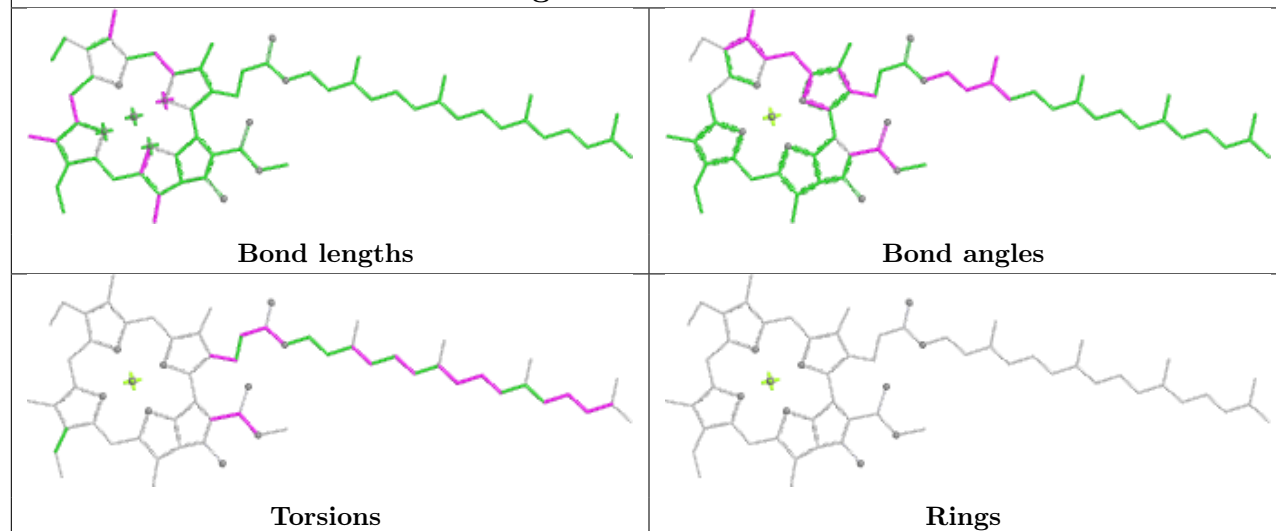
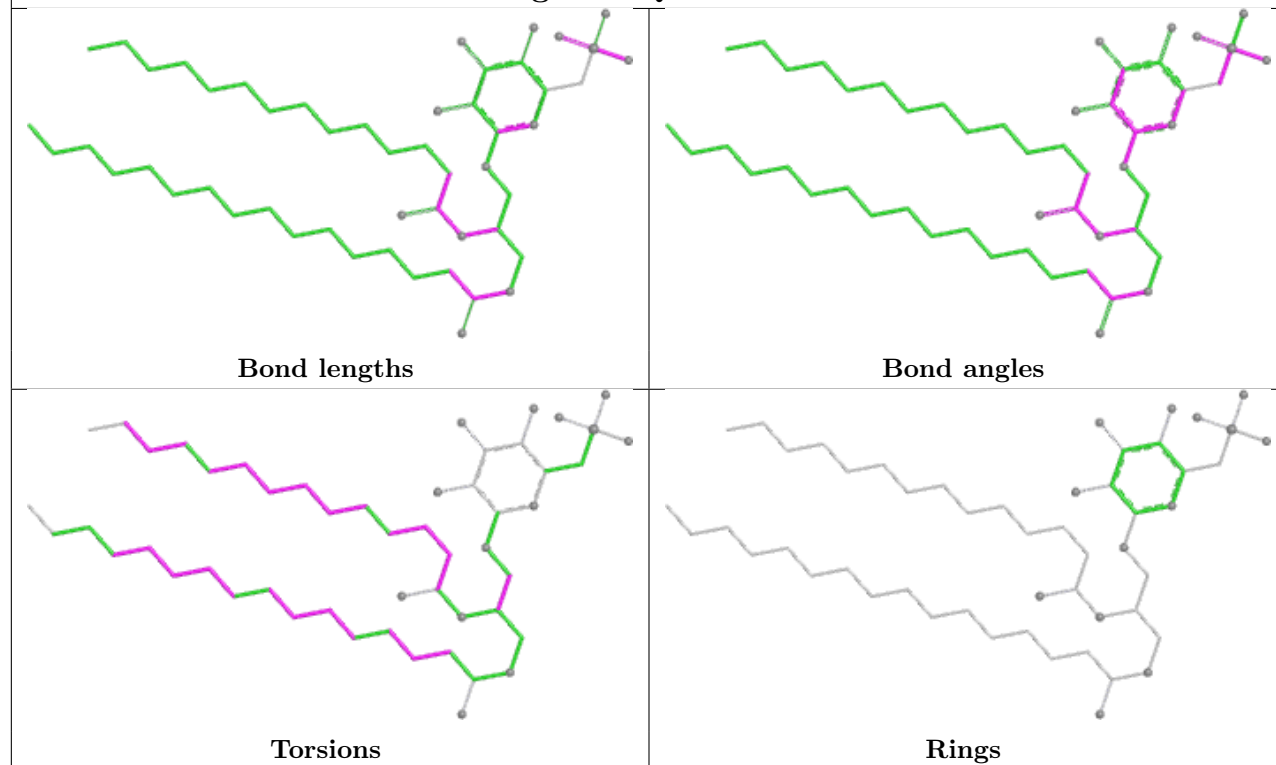
Ligand STE B 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

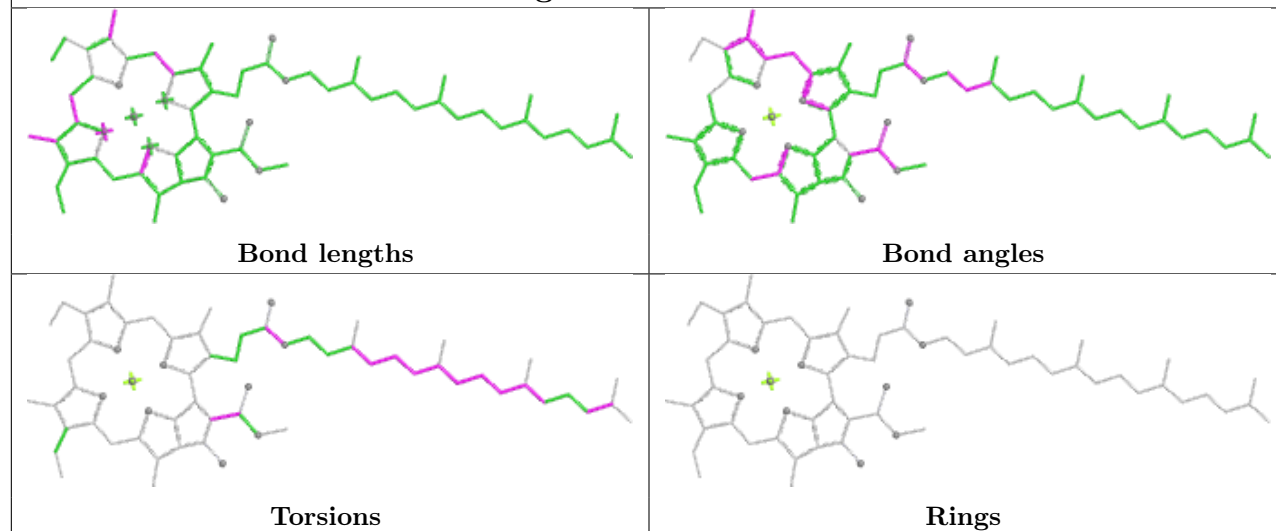
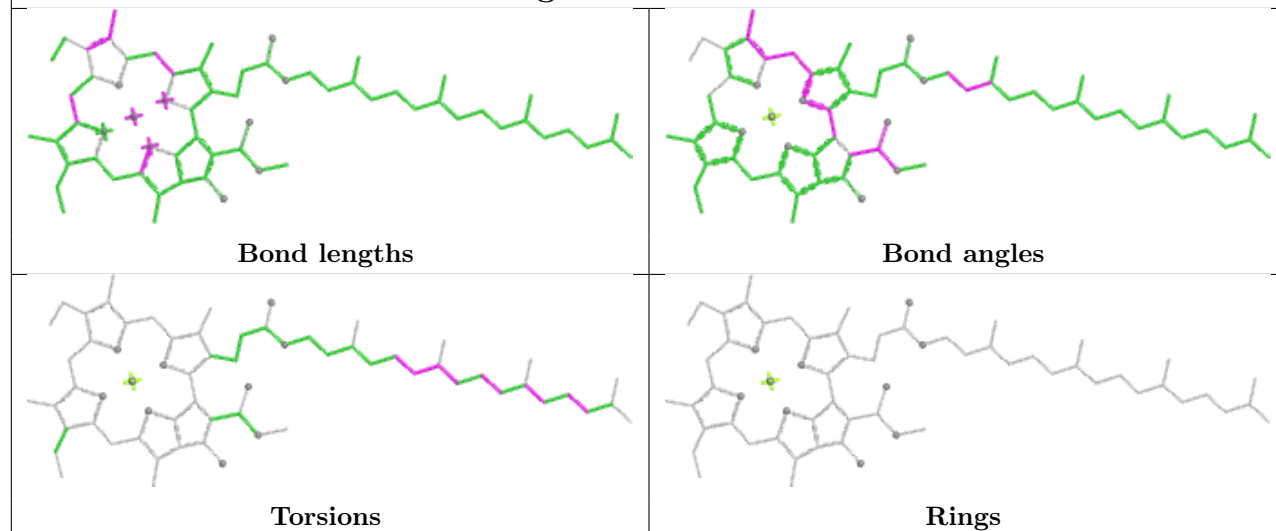
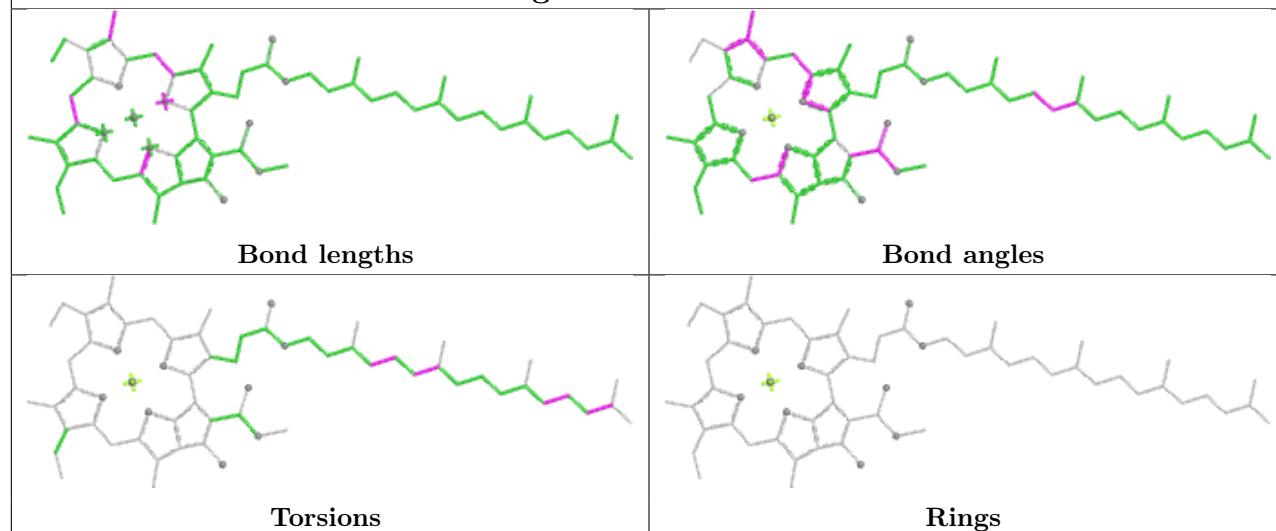
Ligand CLA a 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

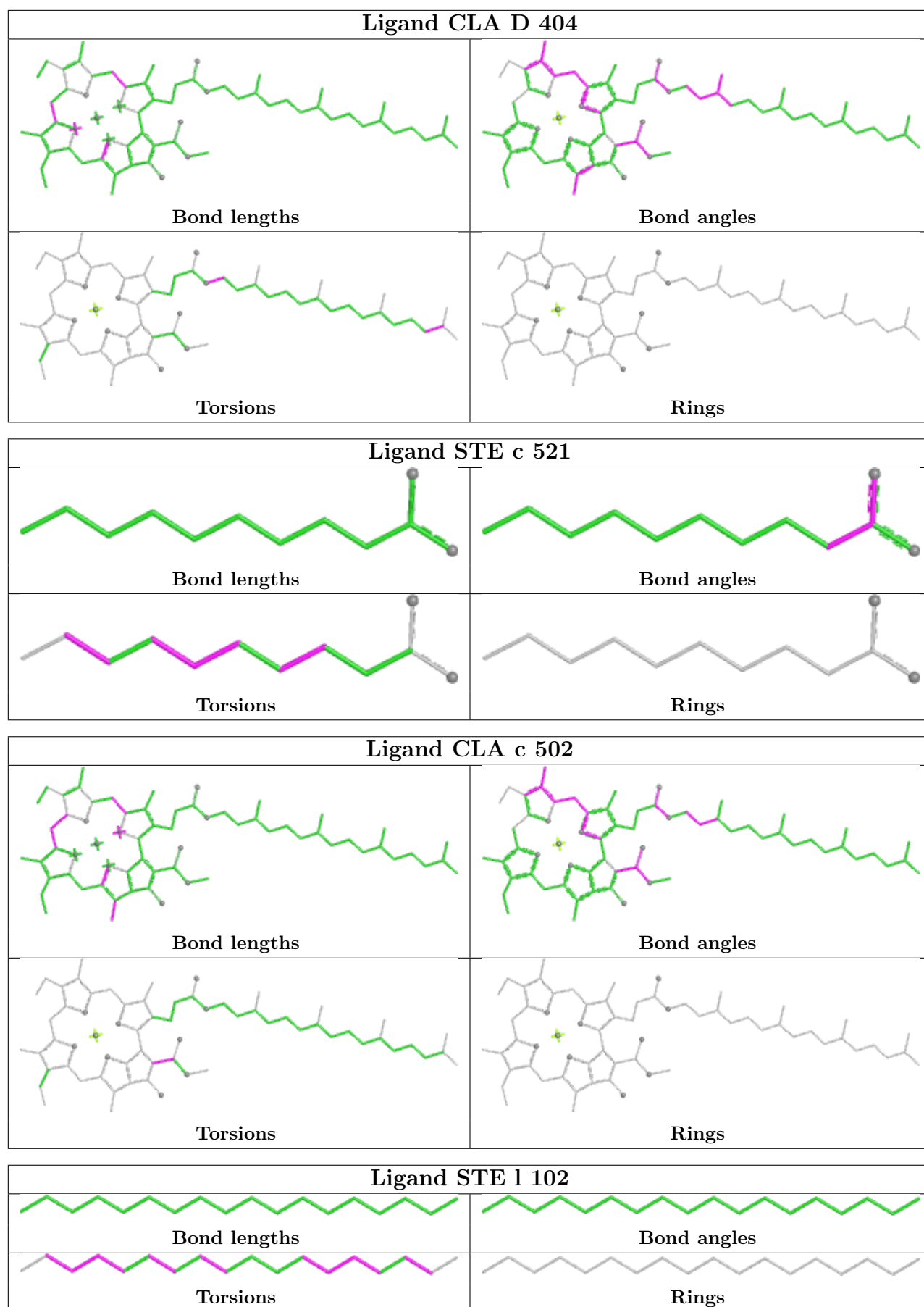


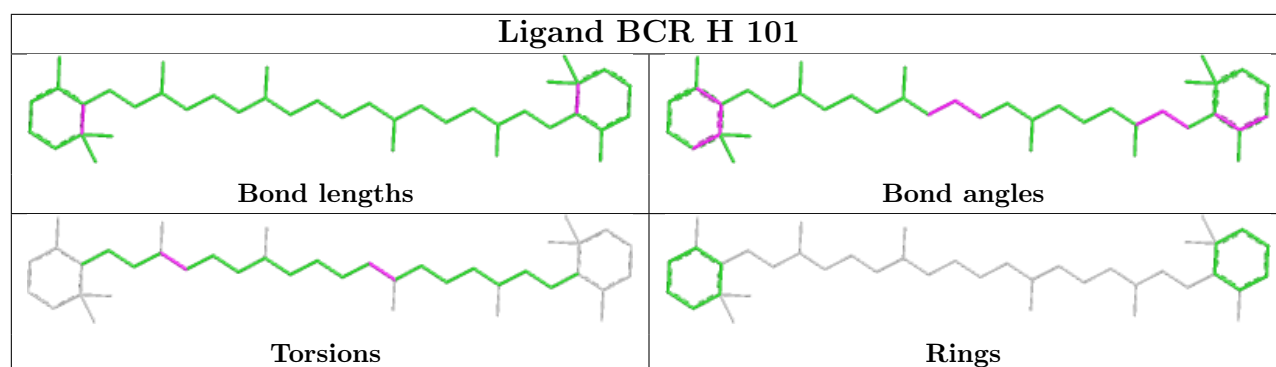
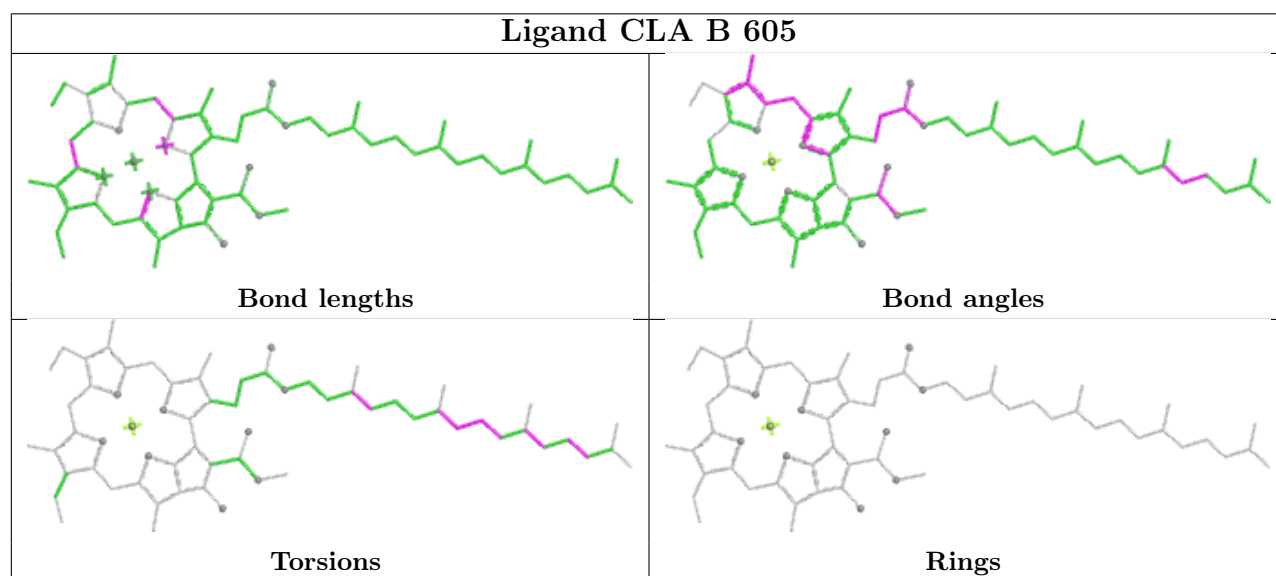
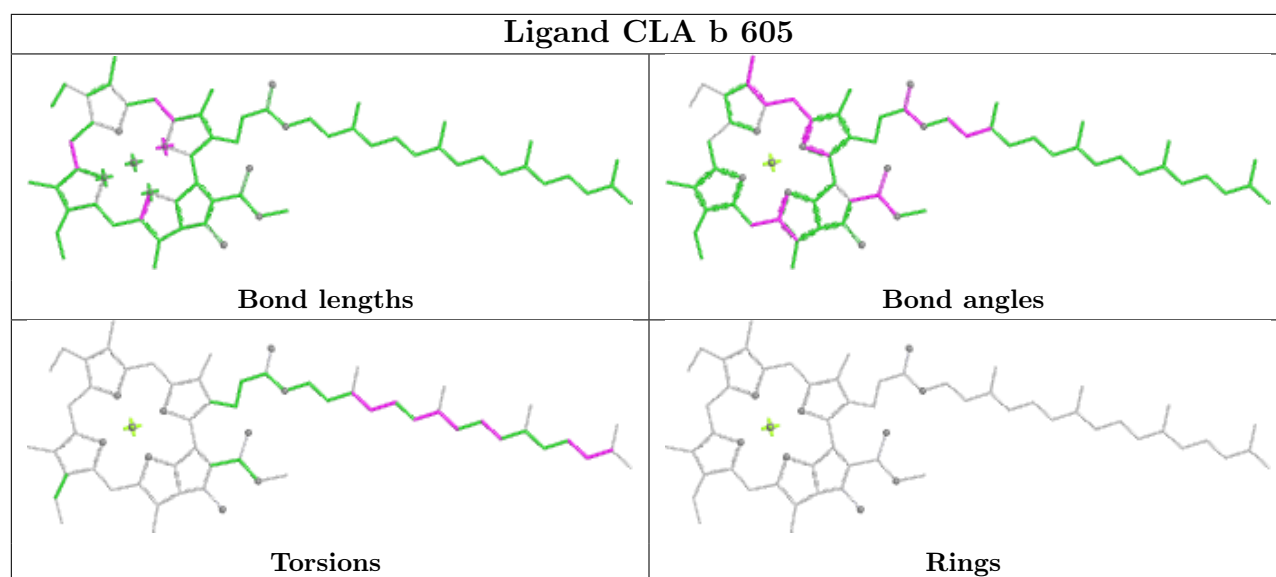




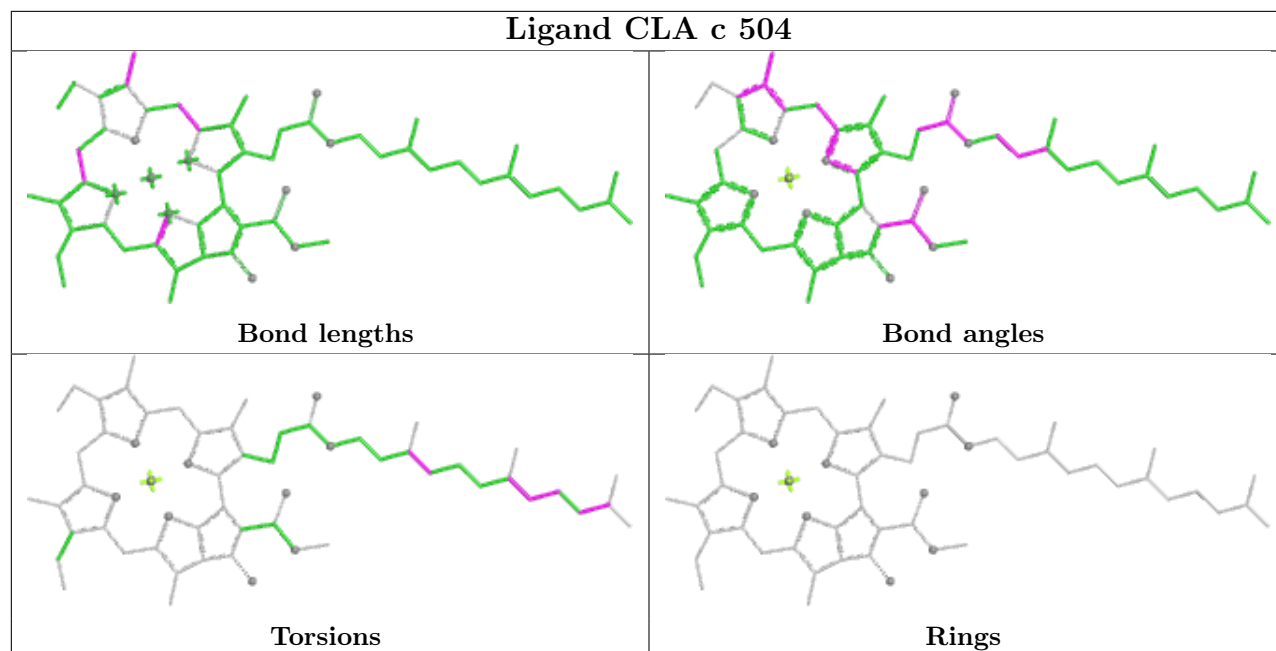
Ligand CLA B 601**Ligand SQD A 614**

Ligand CLA b 614**Ligand CLA c 505****Ligand CLA B 608**

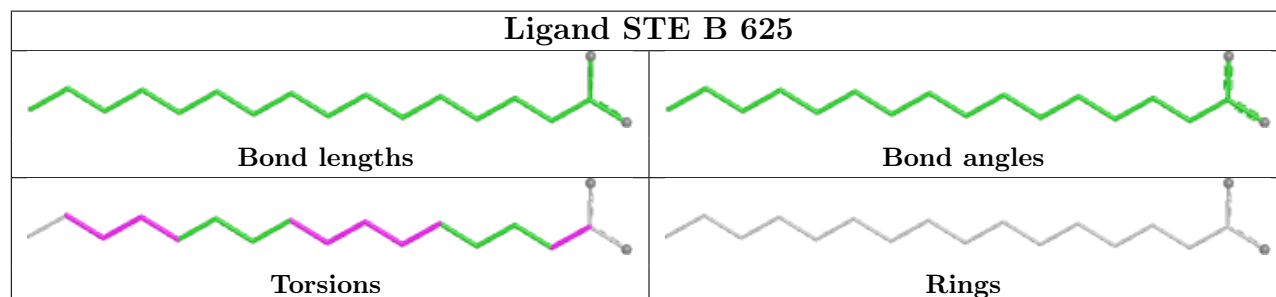




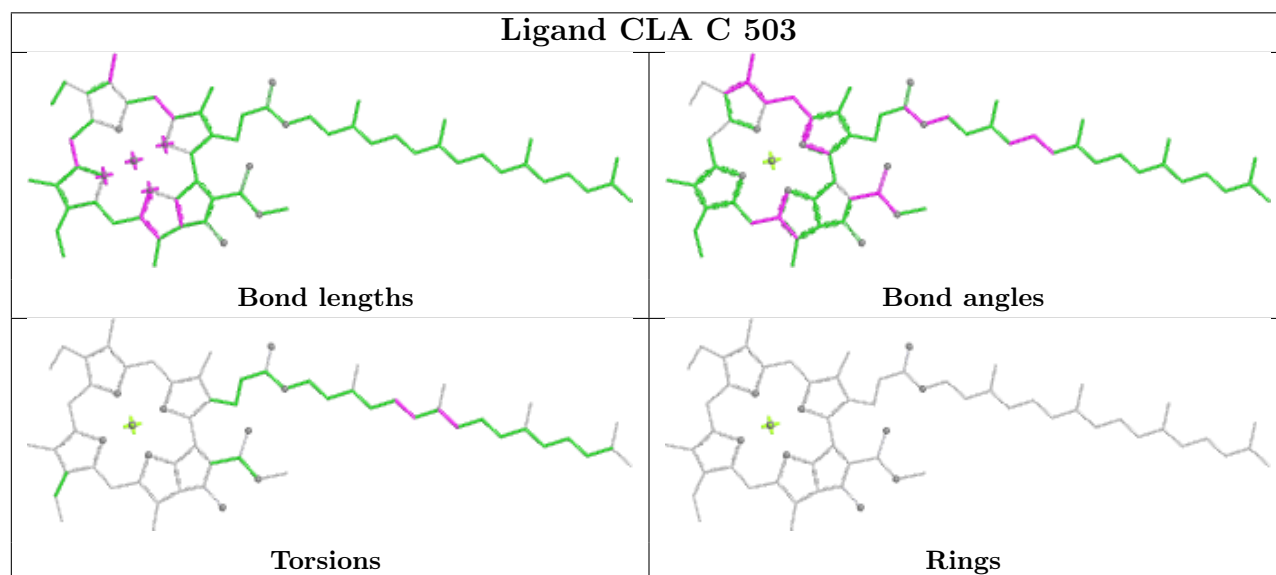
Ligand CLA c 504

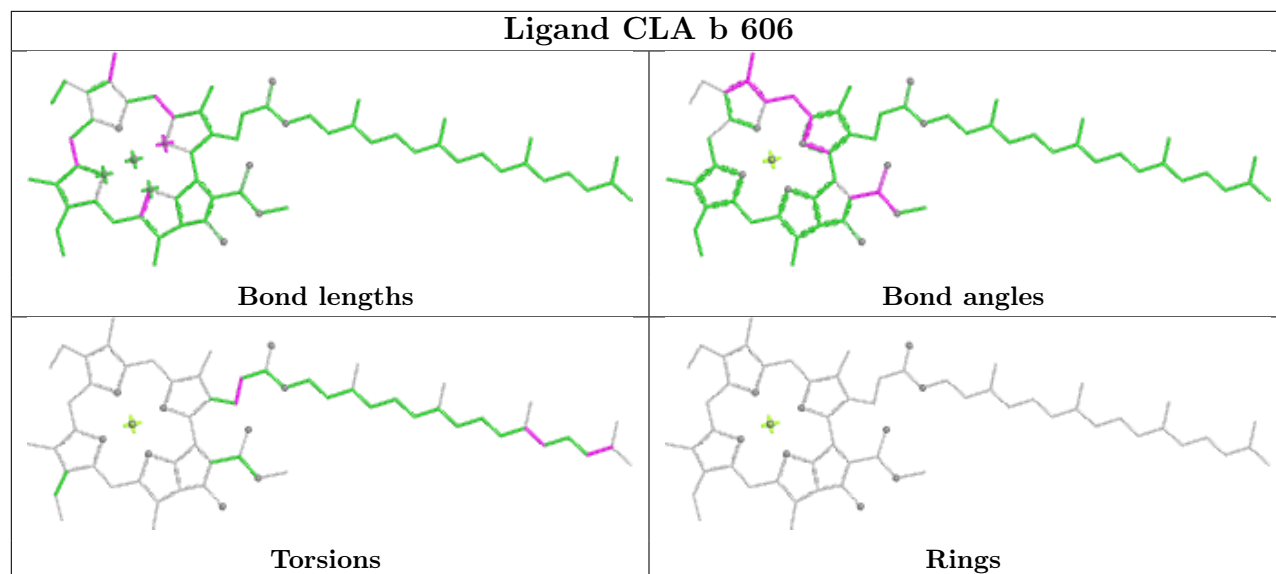
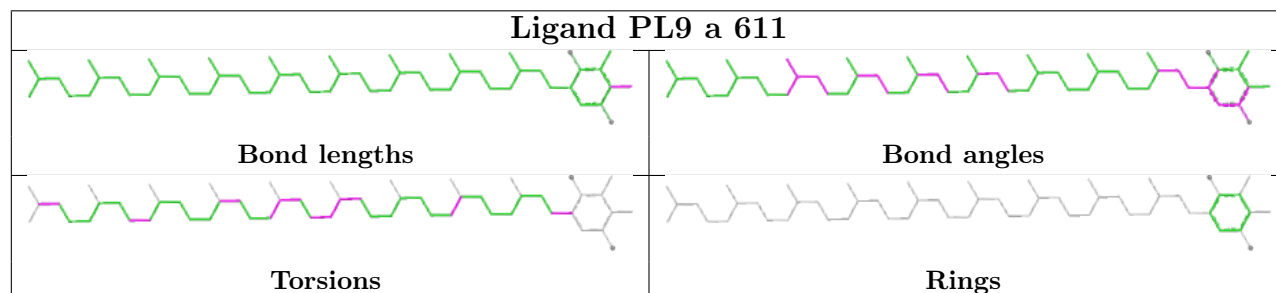
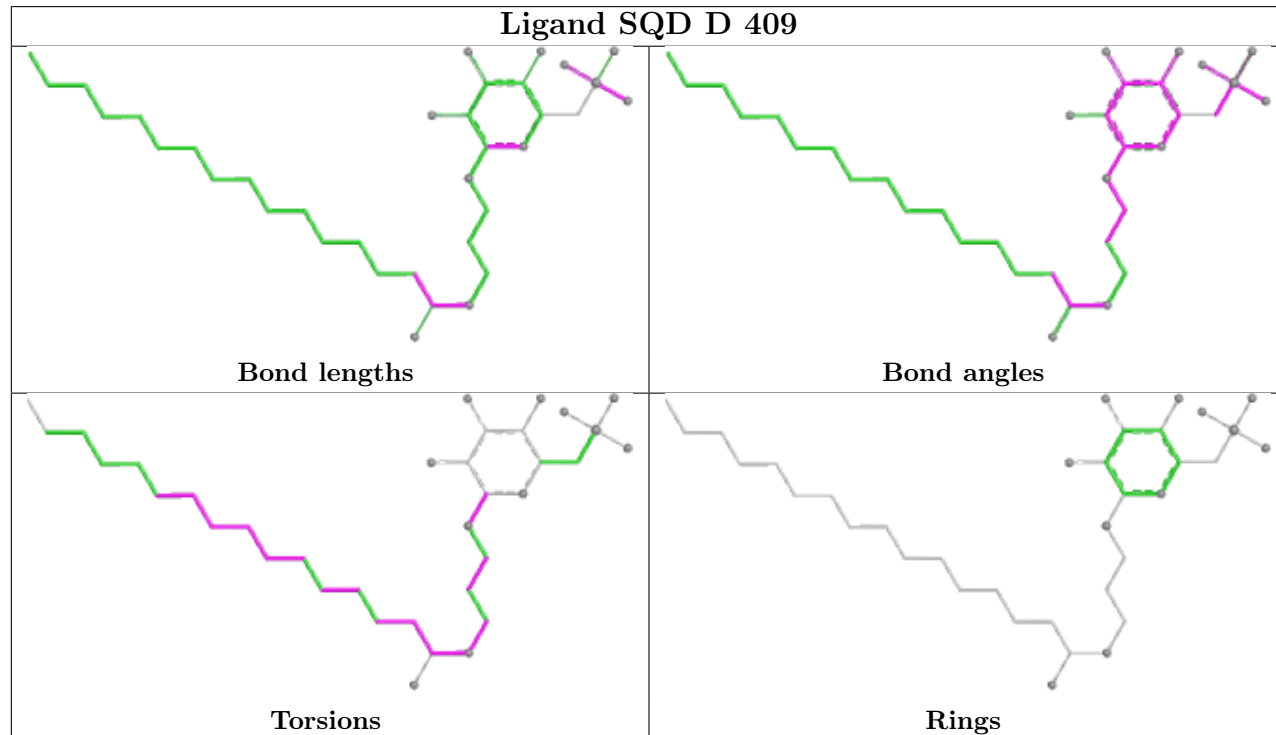


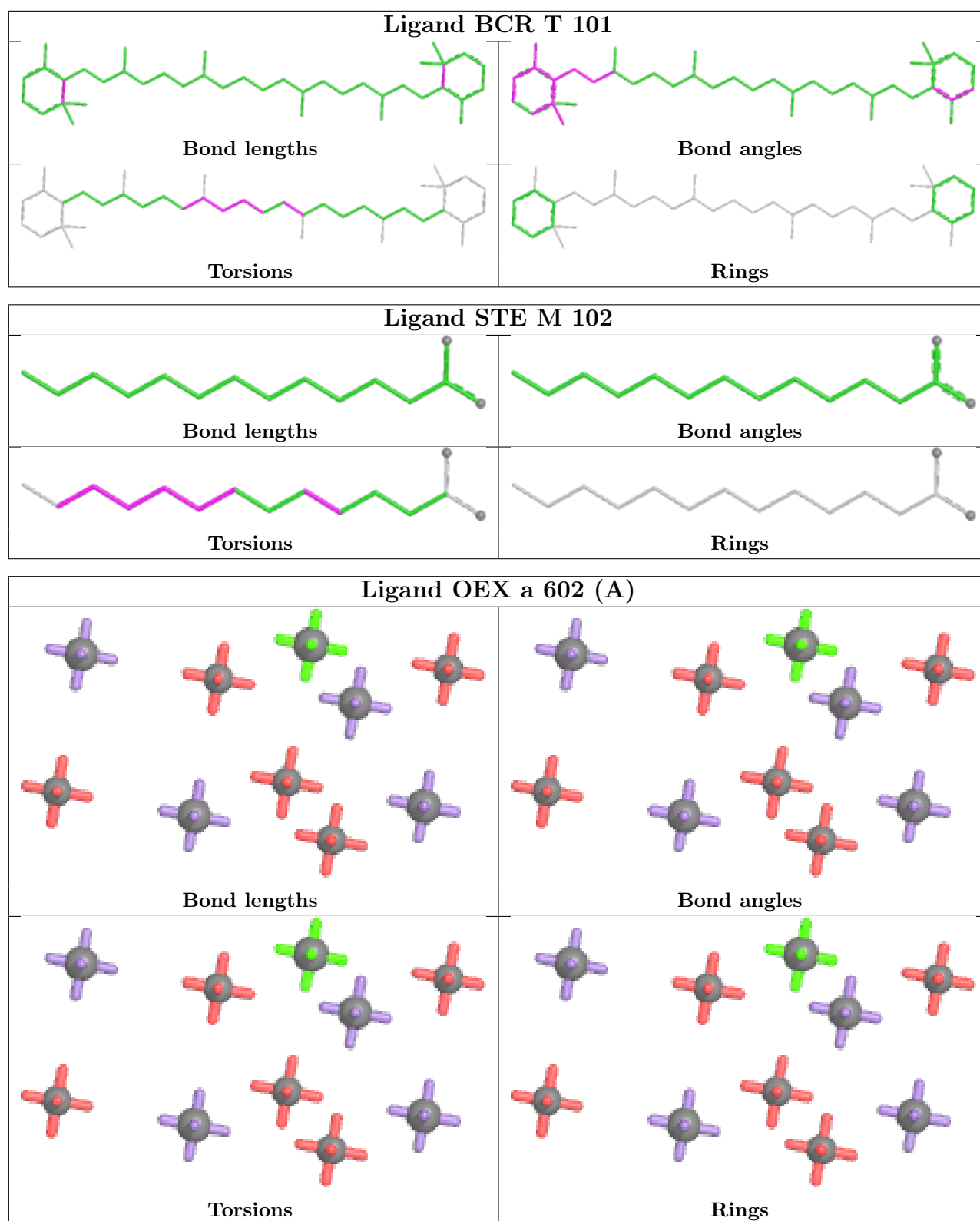
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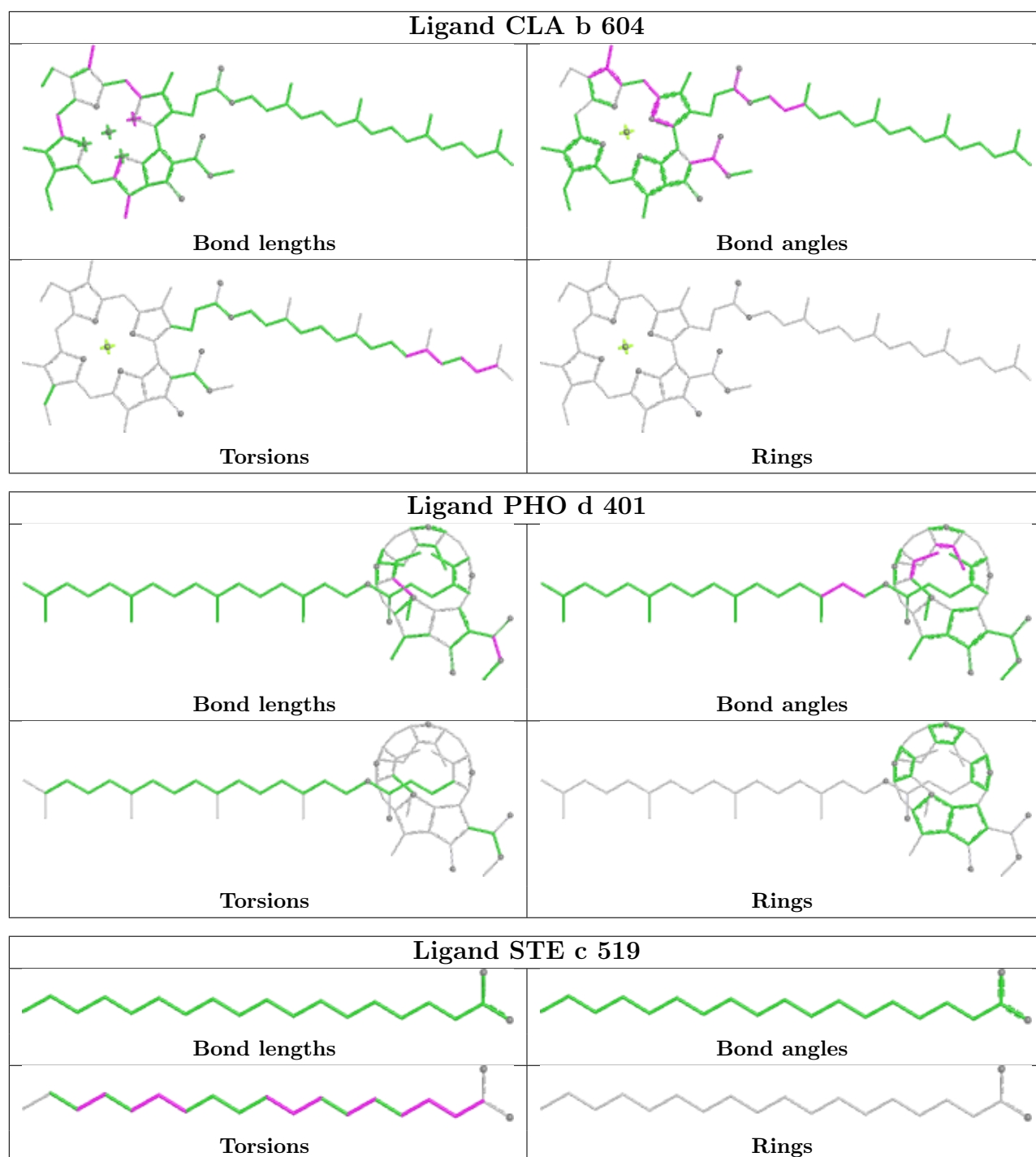


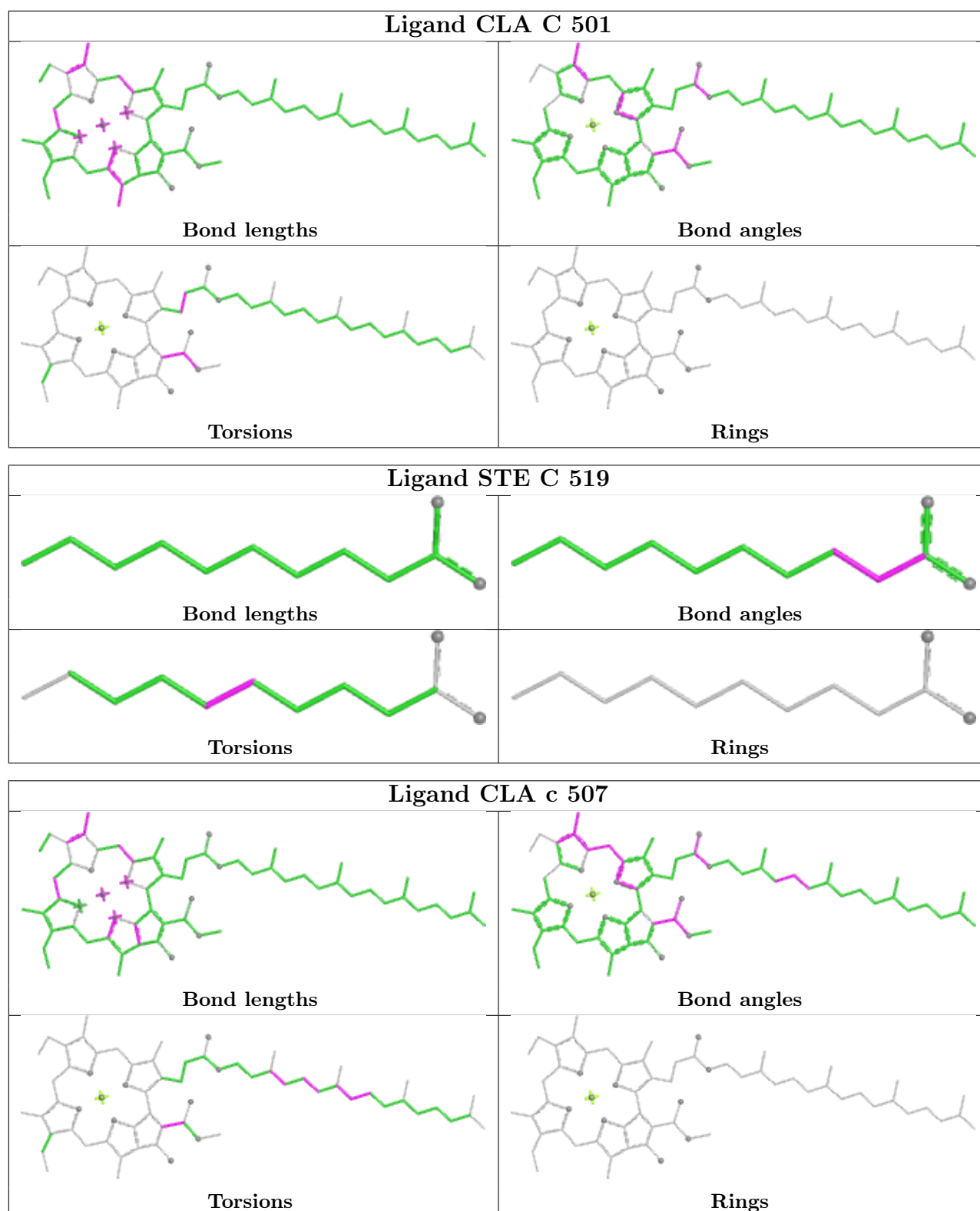
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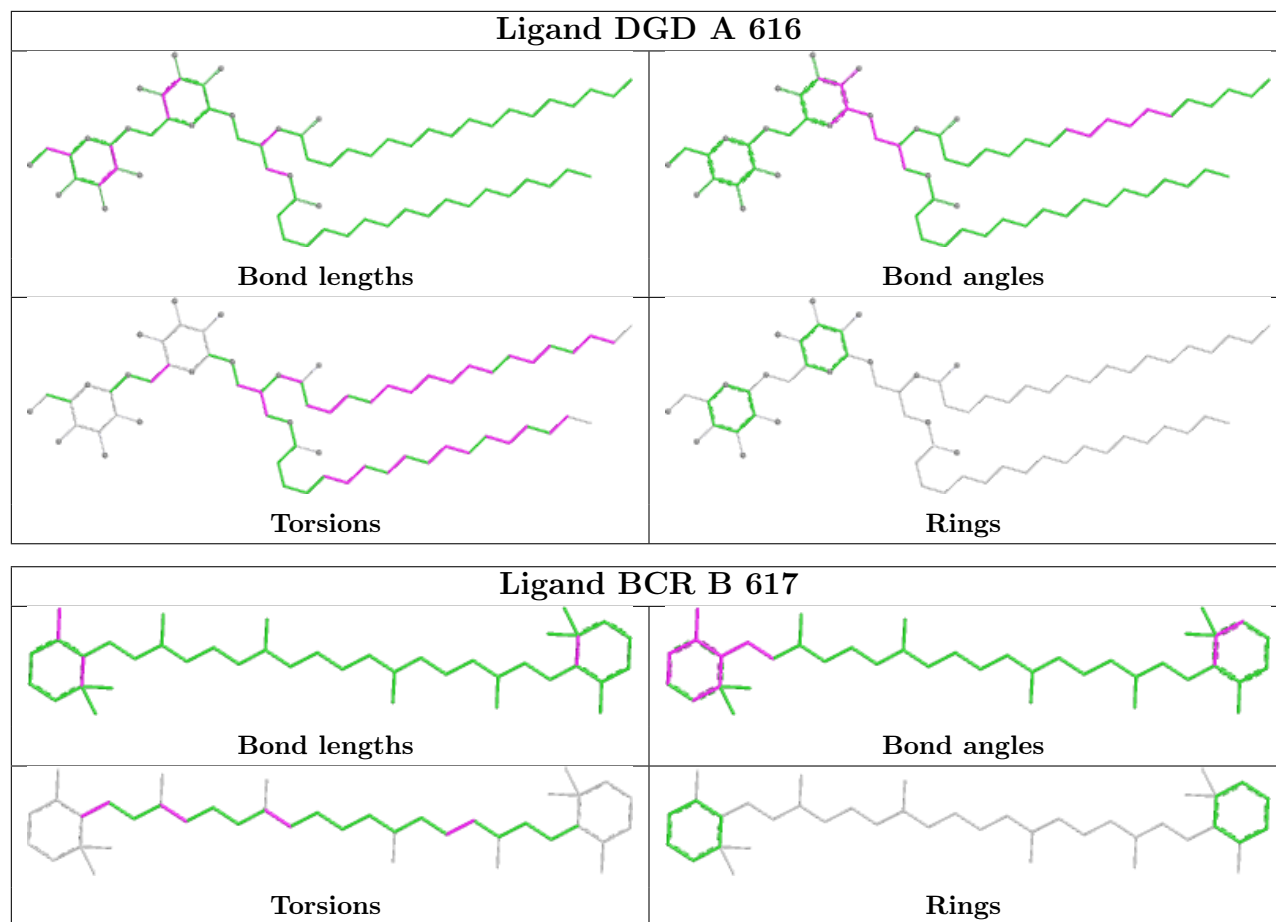


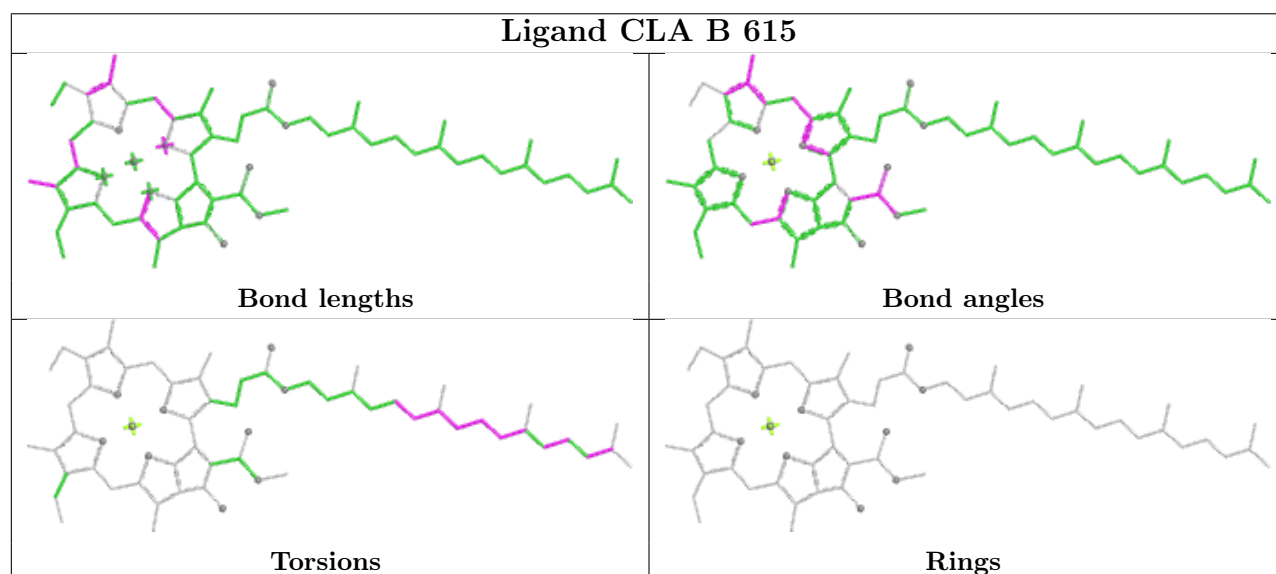
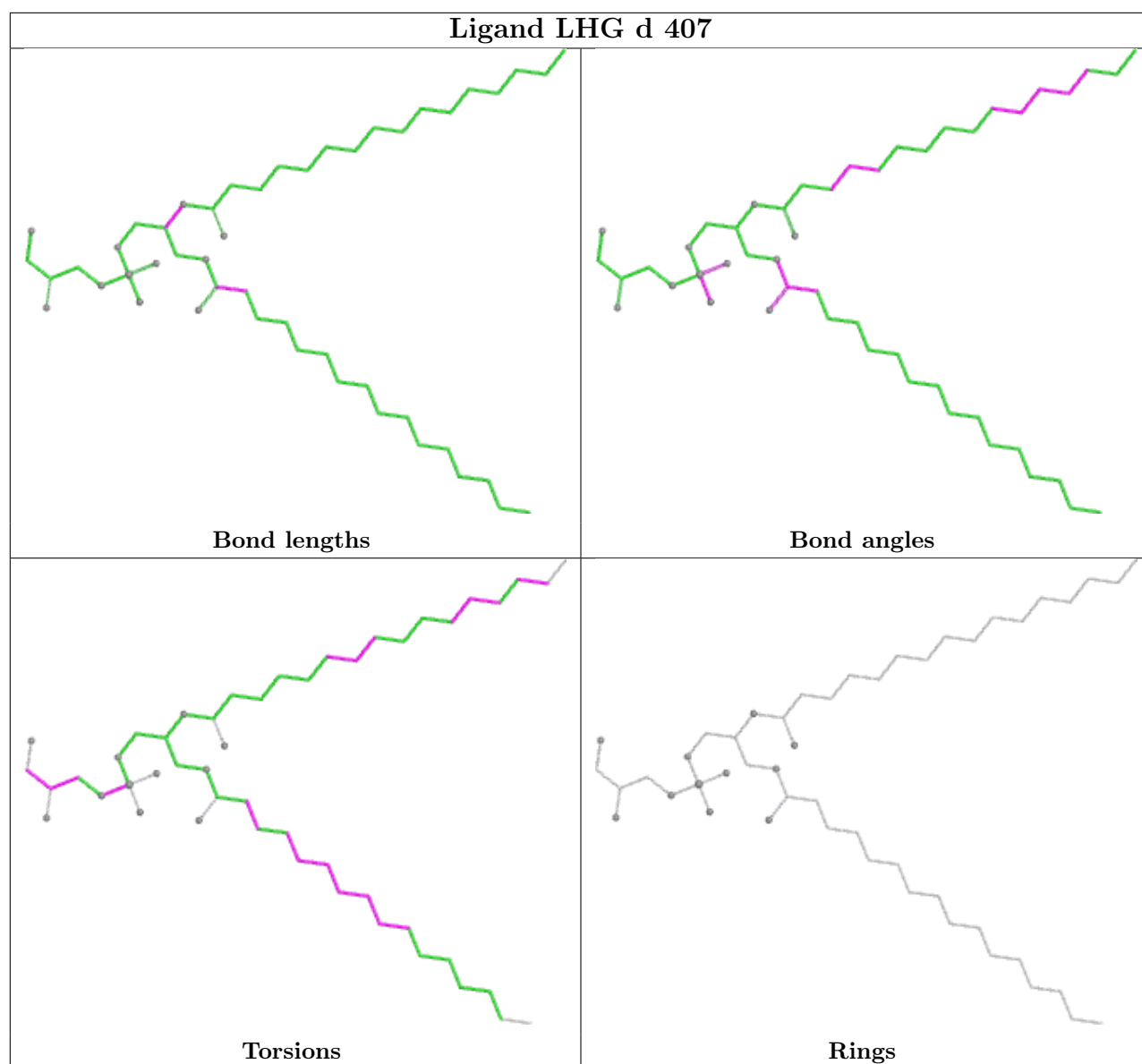
Ligand CLA b 606**Ligand PL9 a 611****Ligand SQD D 409**

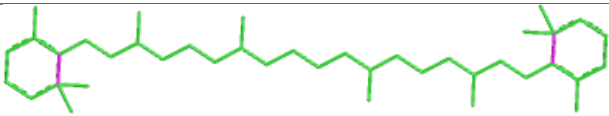
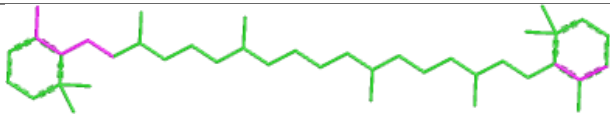
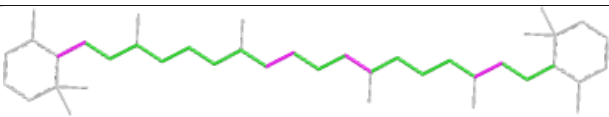
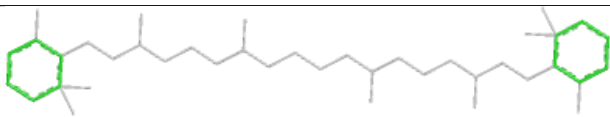


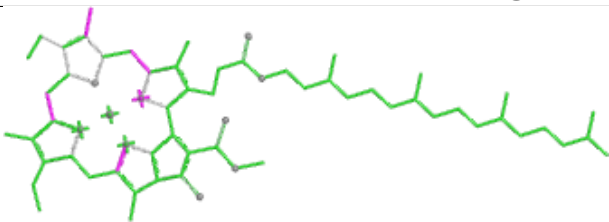
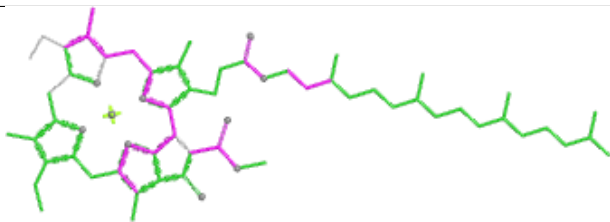
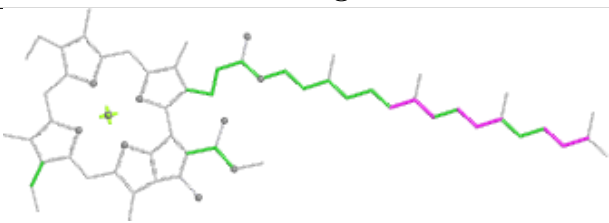
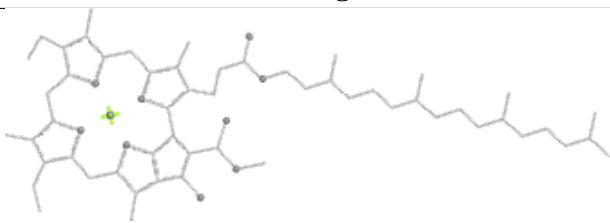


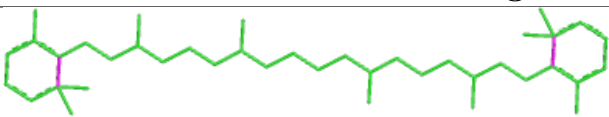
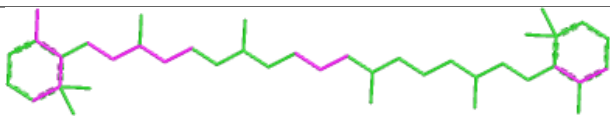
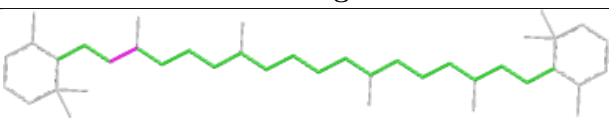
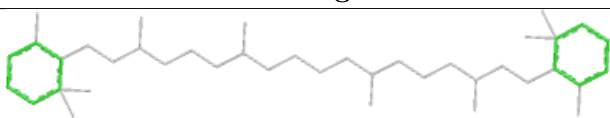


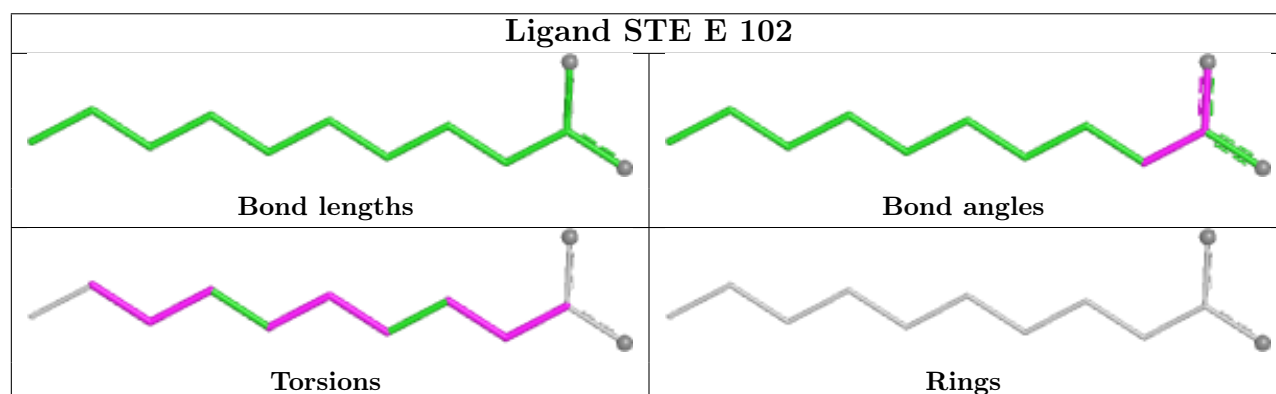
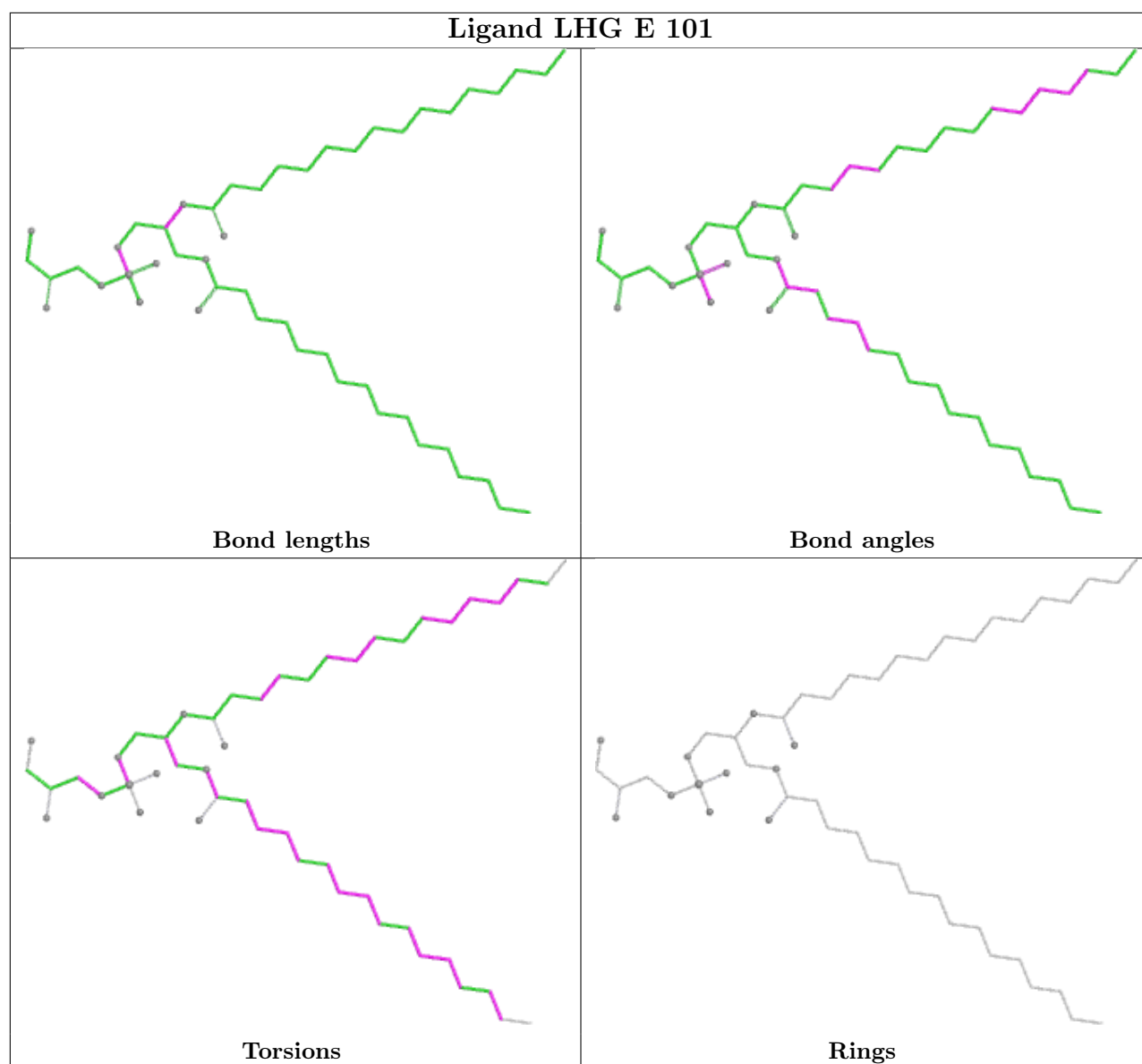


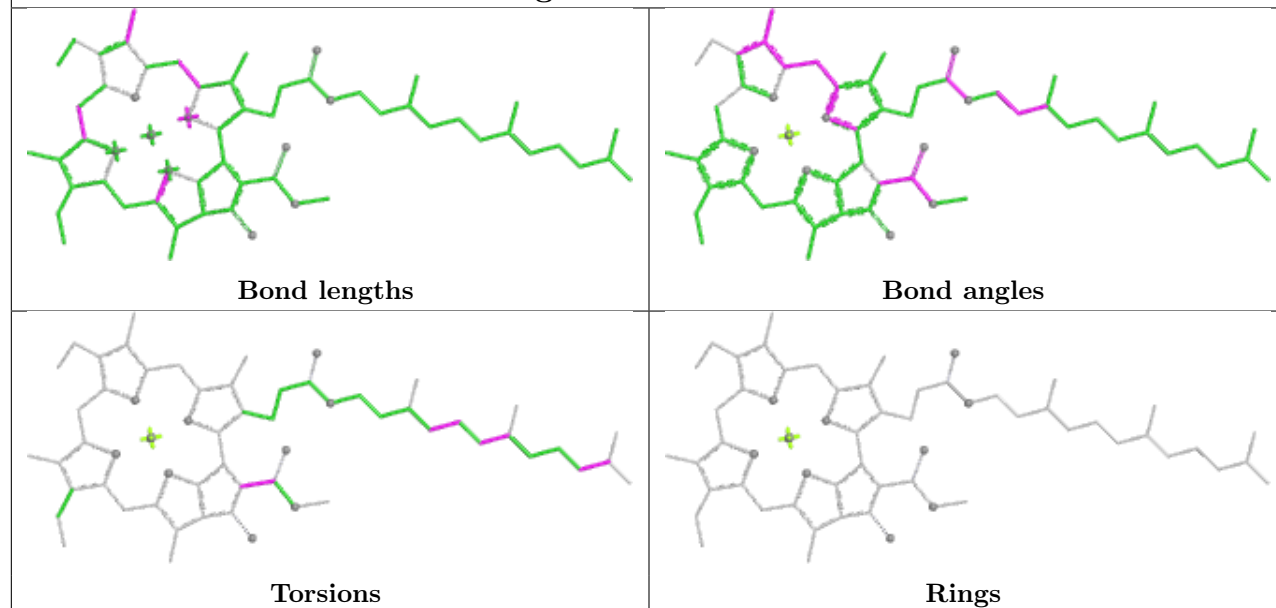
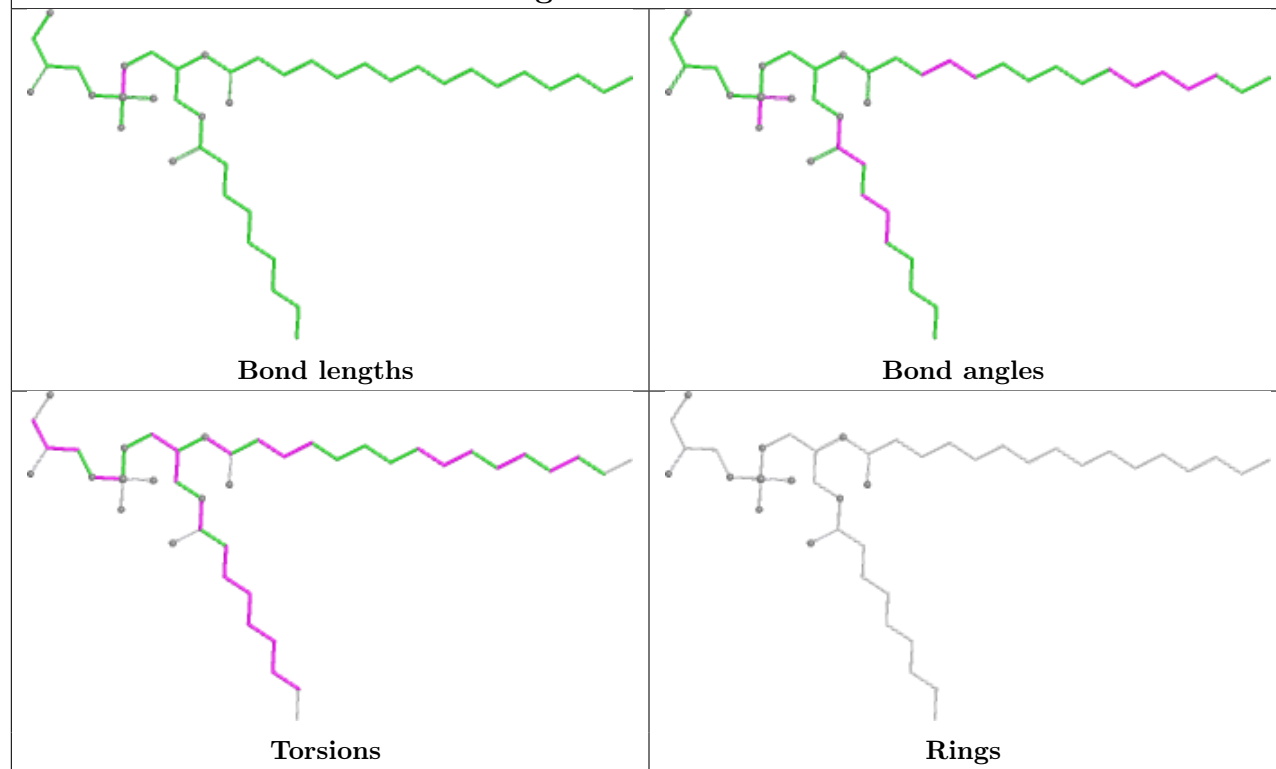


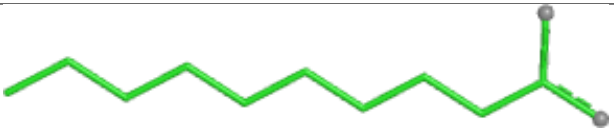
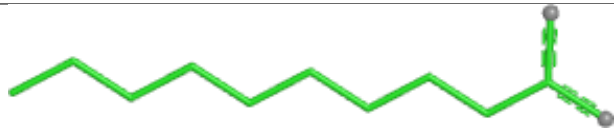
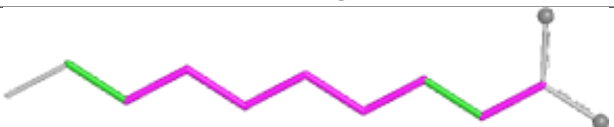
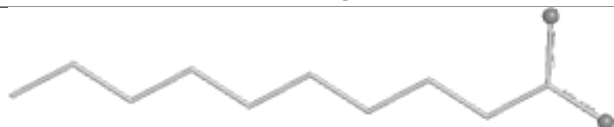
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

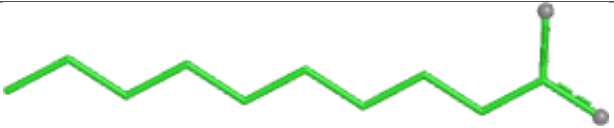
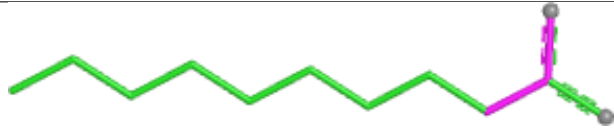
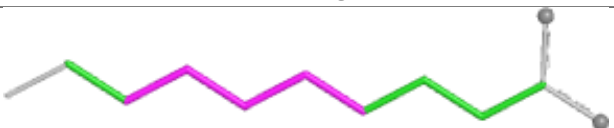
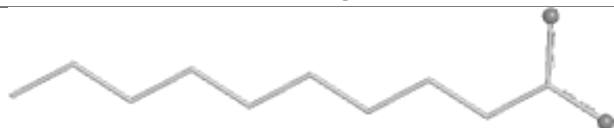
Ligand CLA A 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

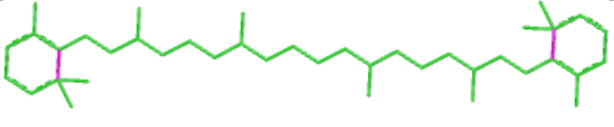
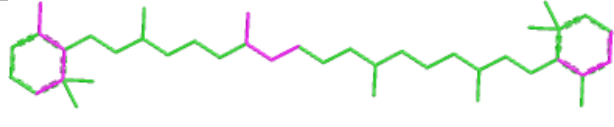
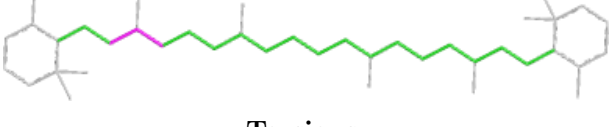
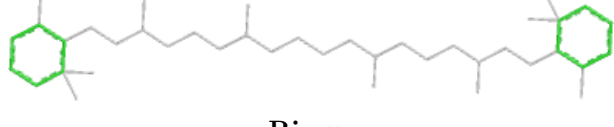
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

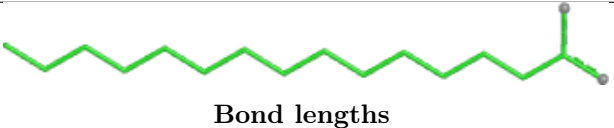
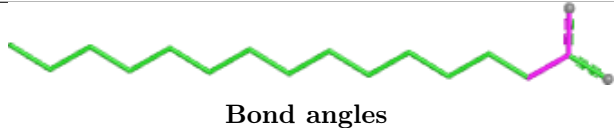




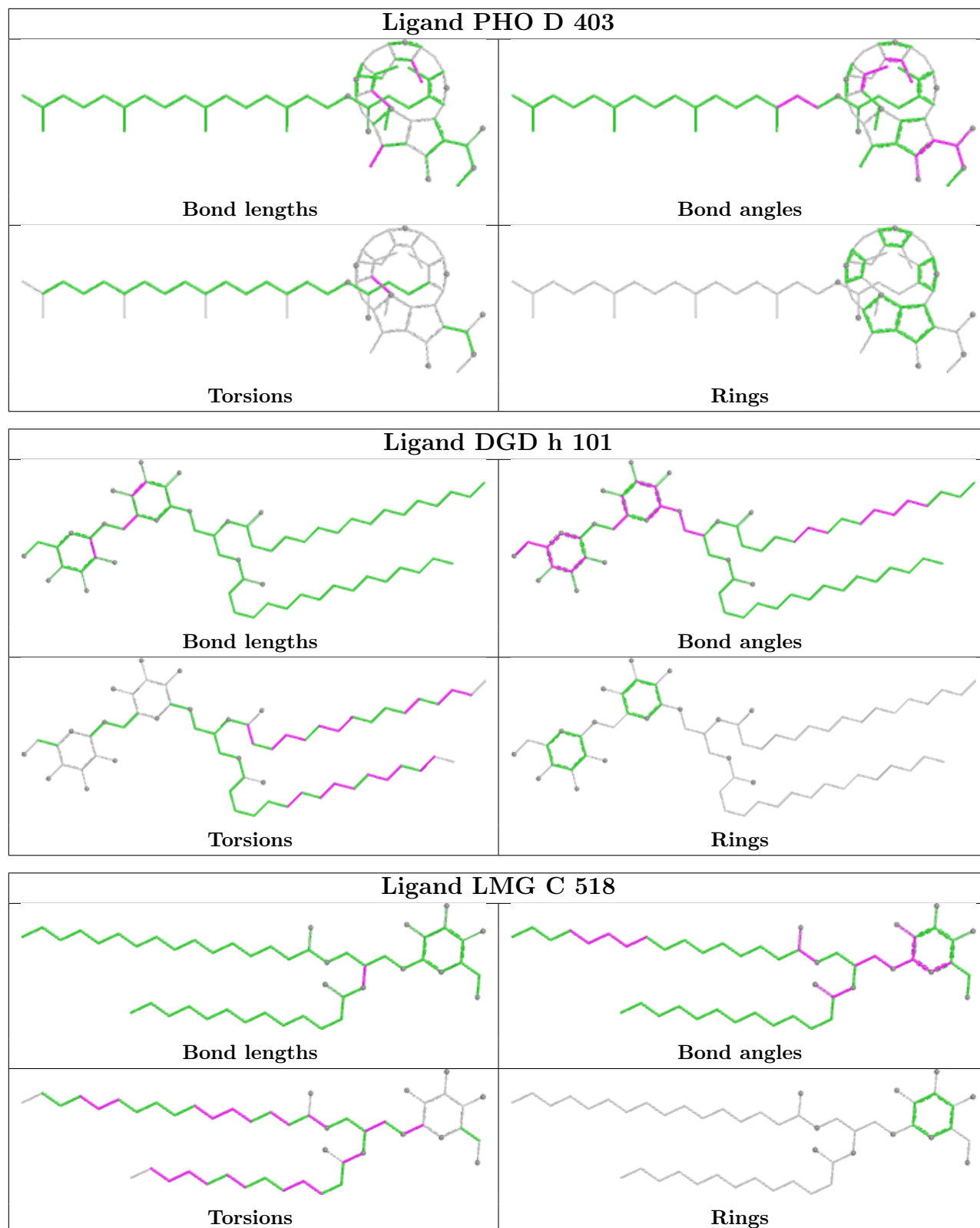
Ligand CLA b 616**Ligand LHG e 101**

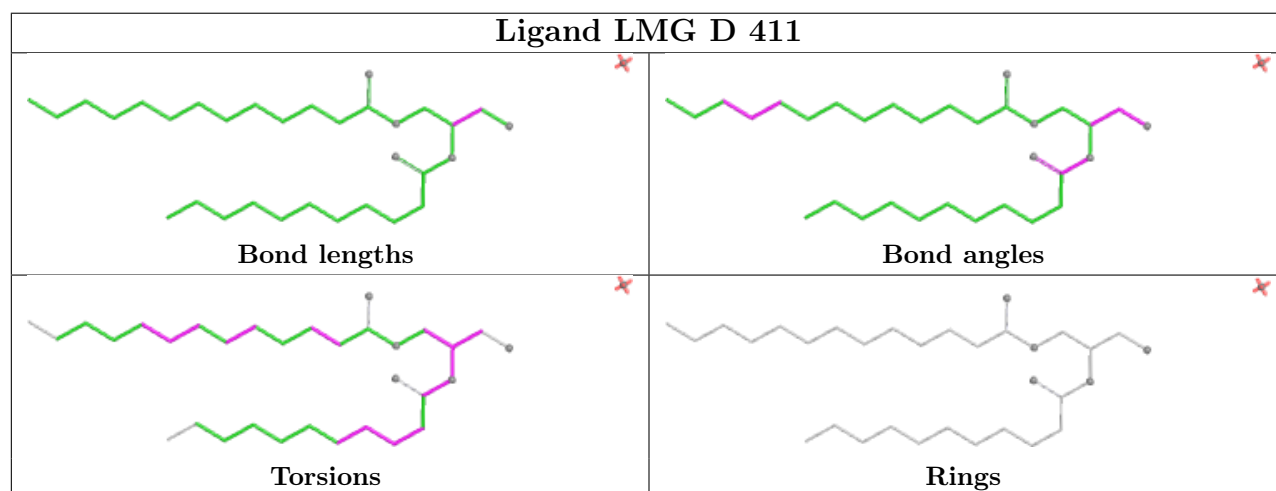
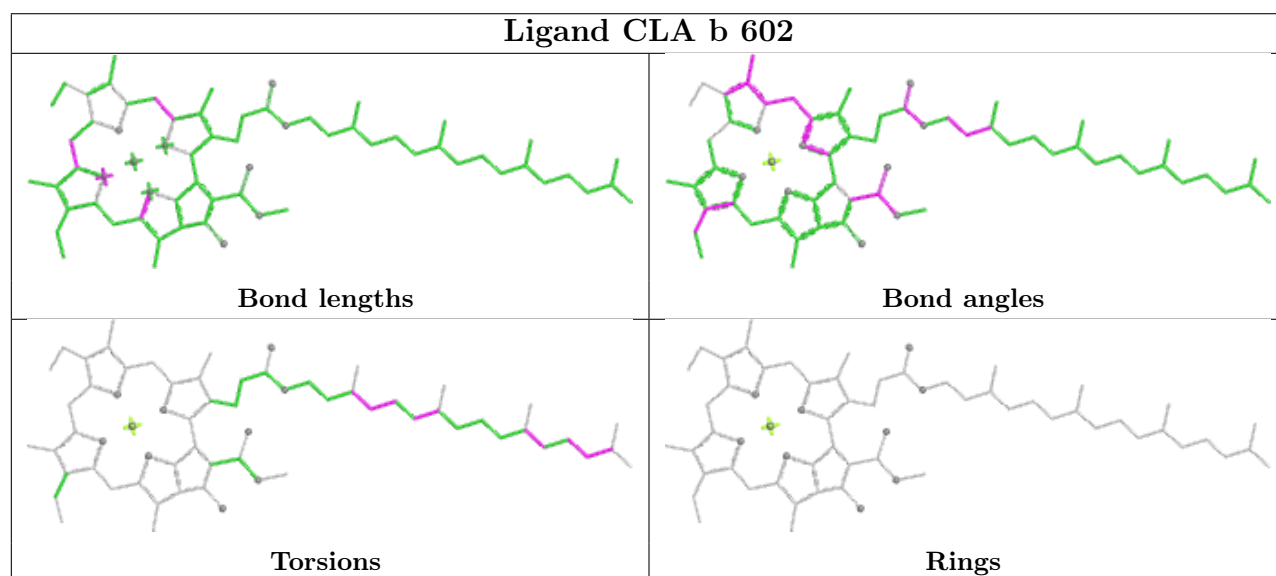
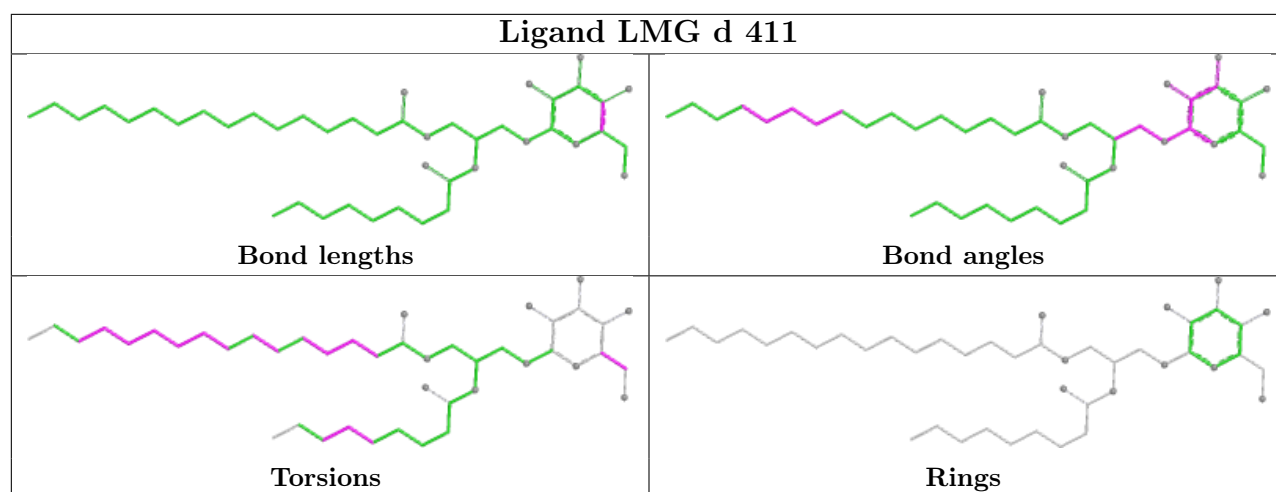
Ligand STE J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

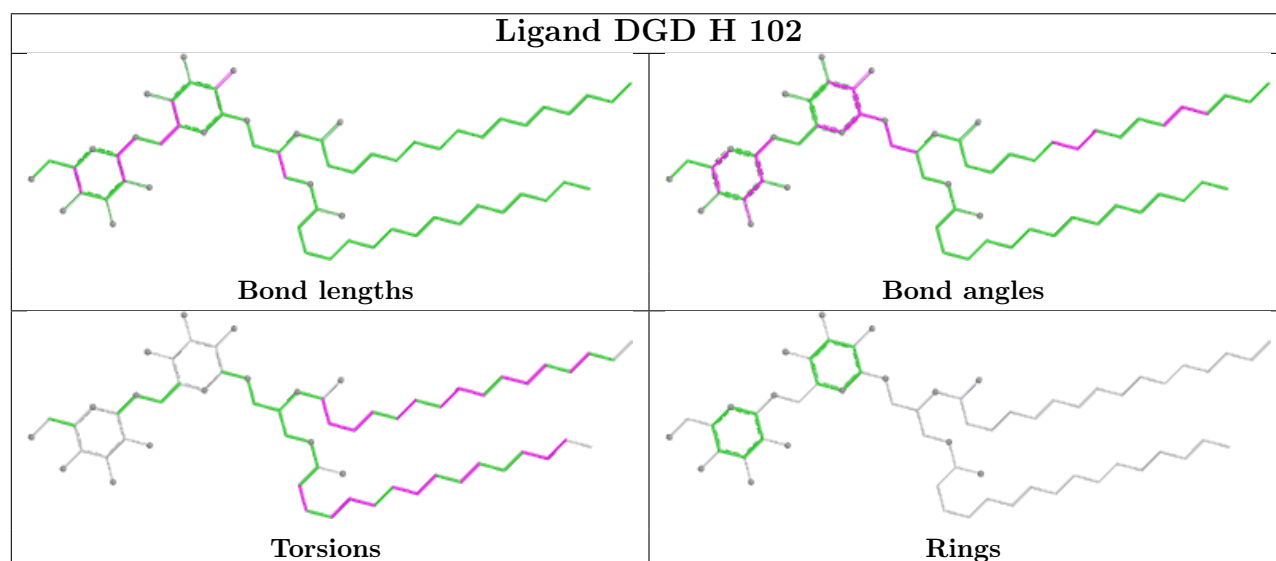
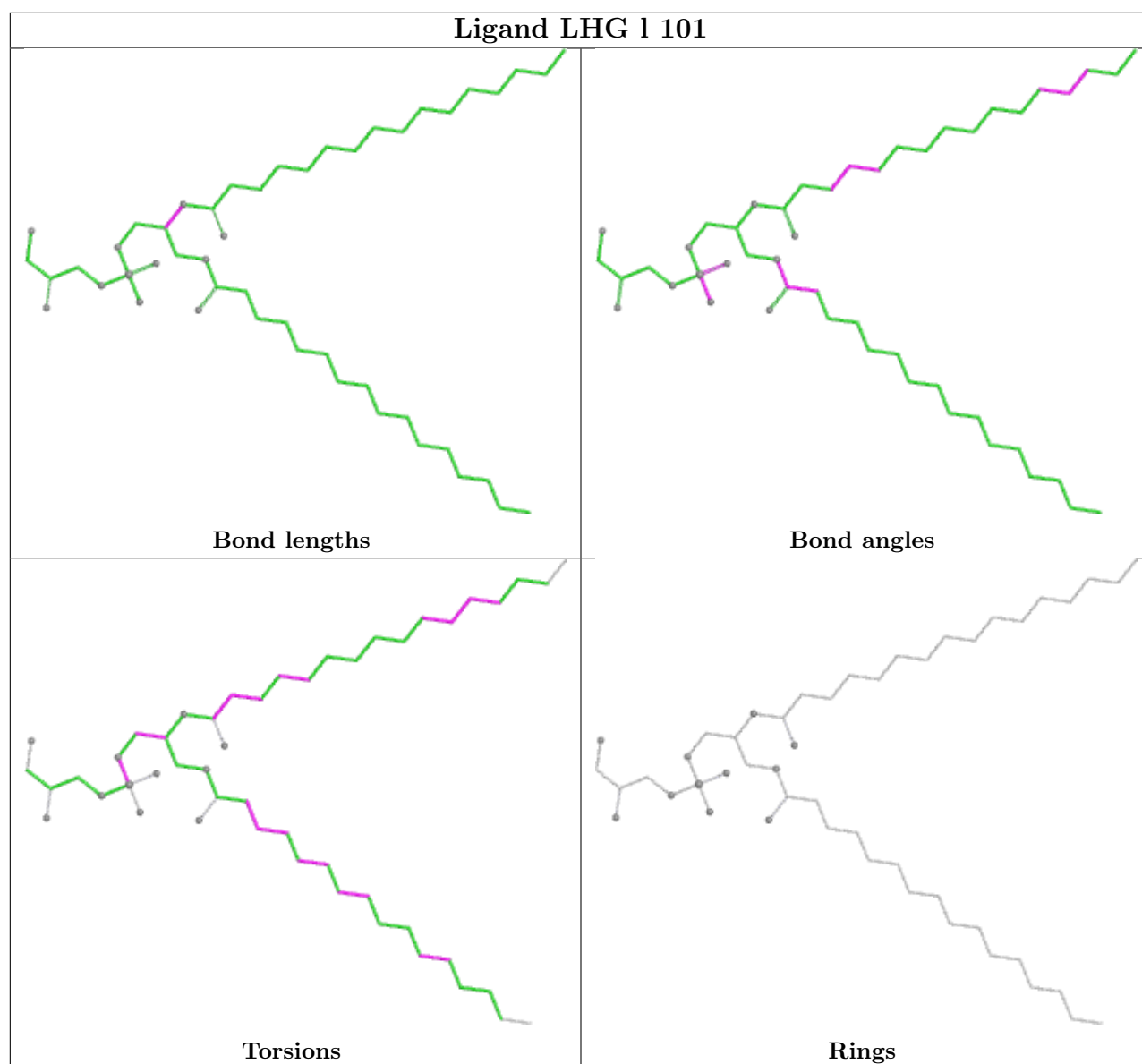
Ligand STE C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

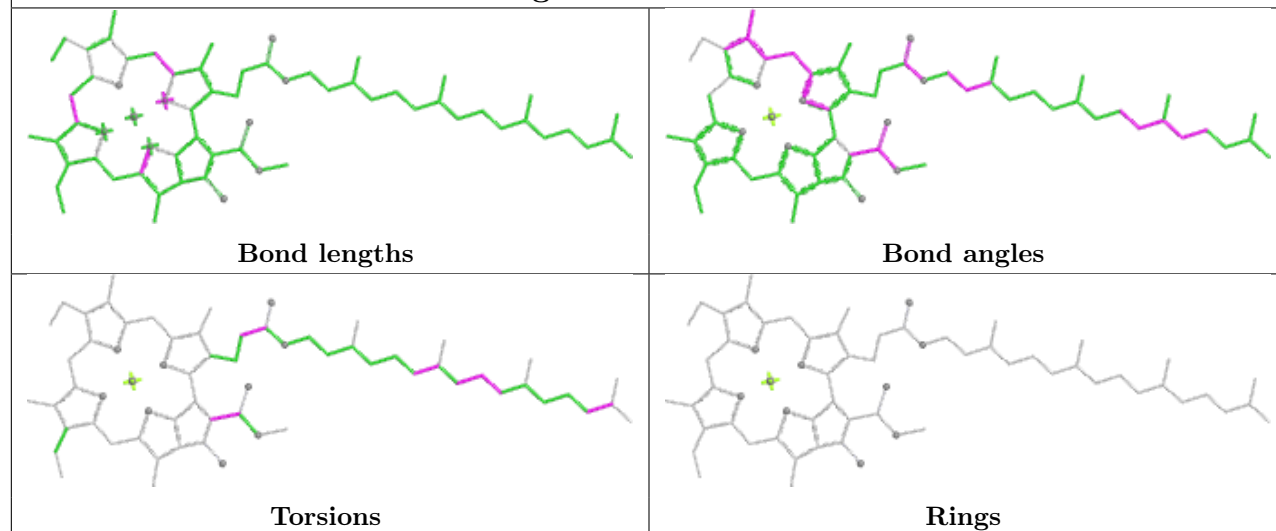
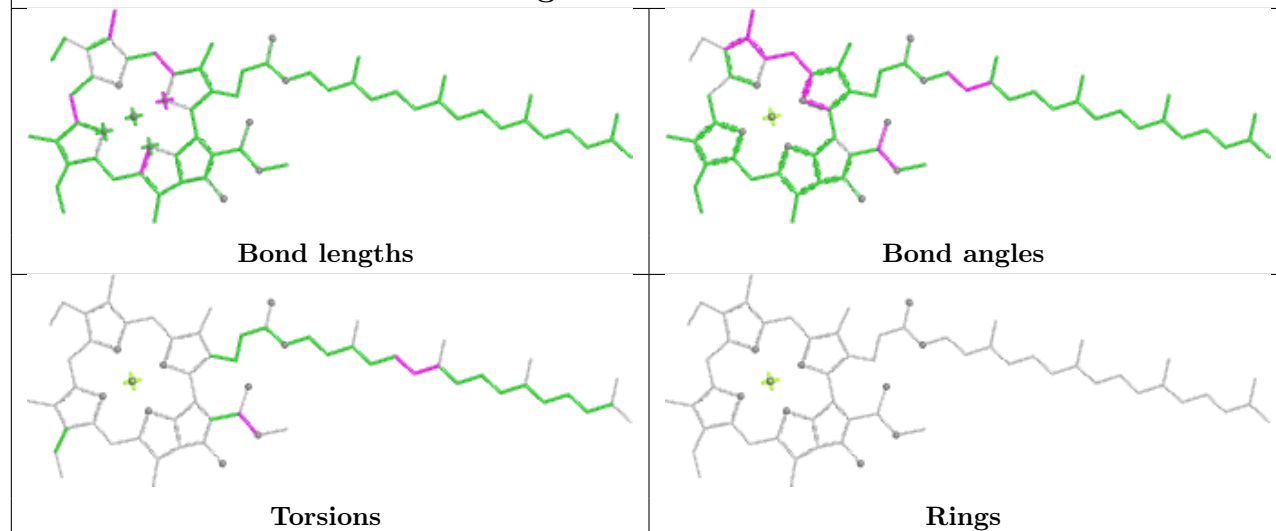
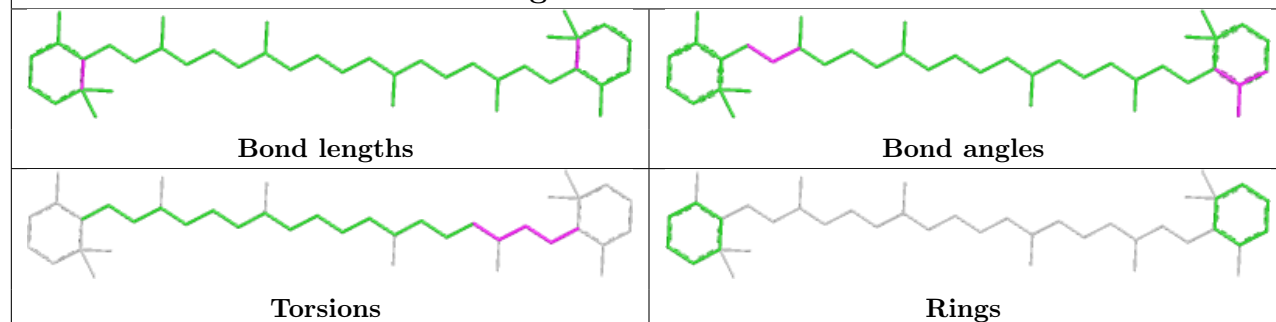
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

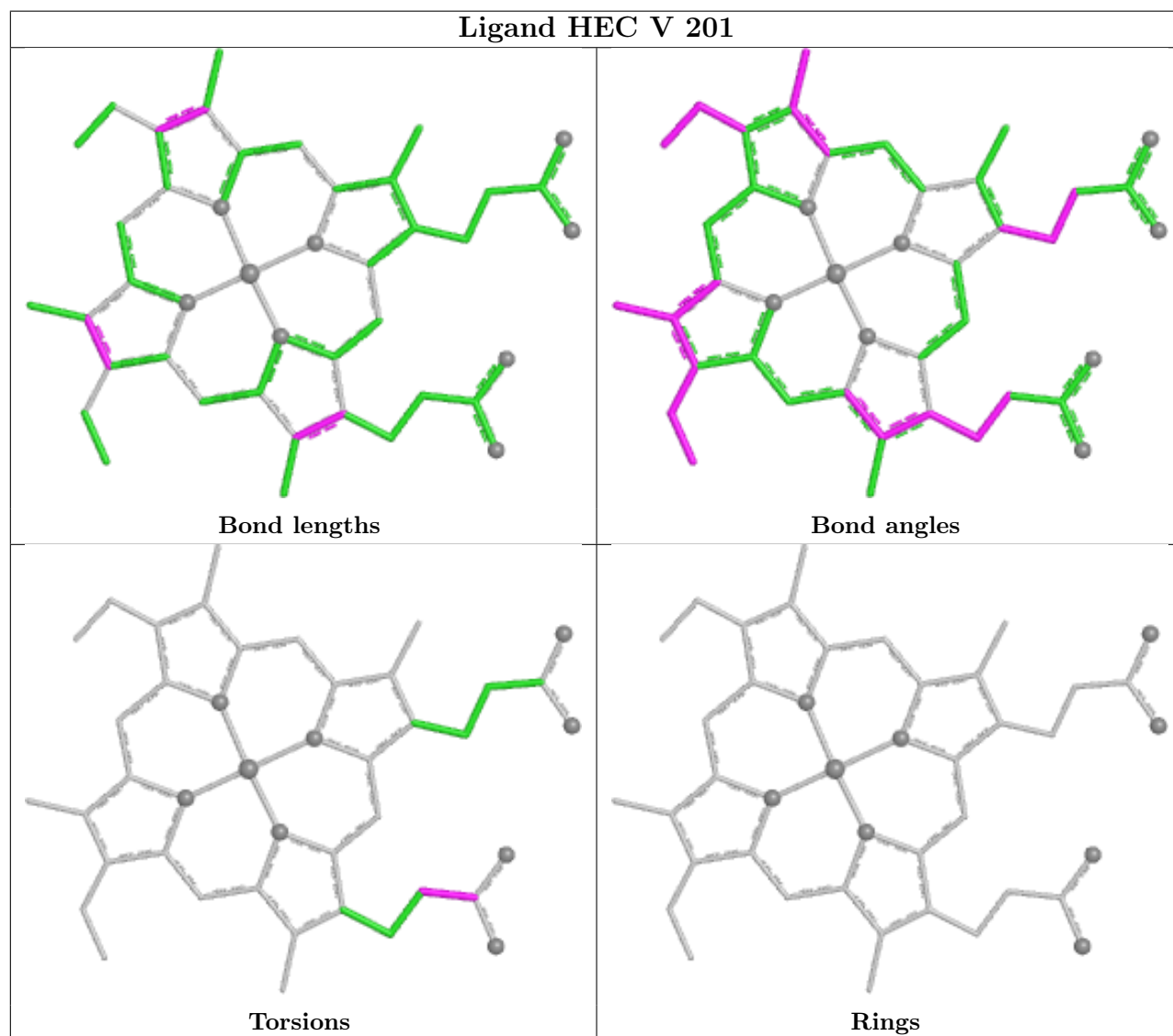
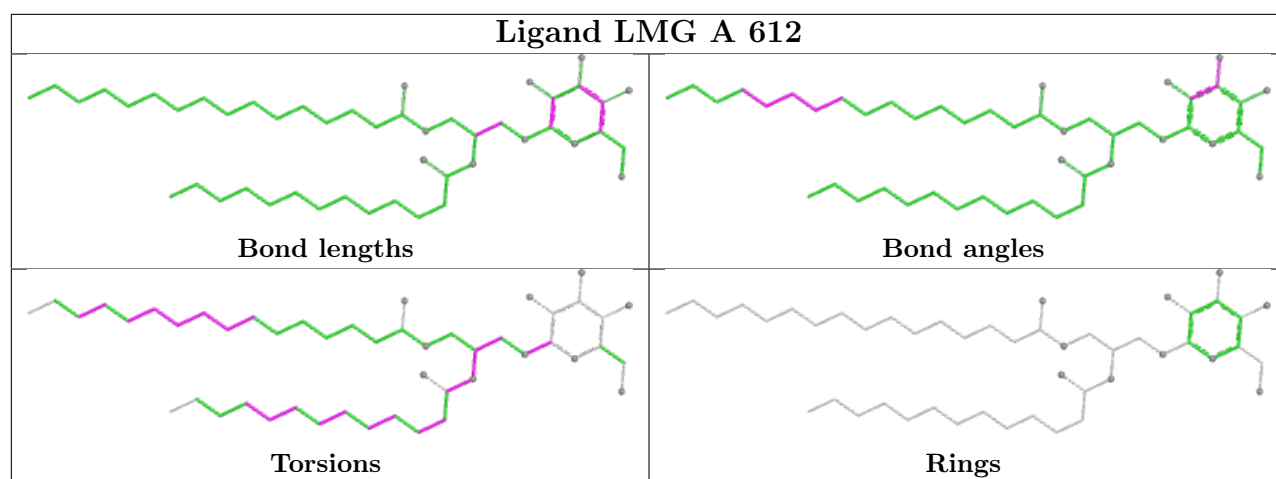
Ligand STE d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

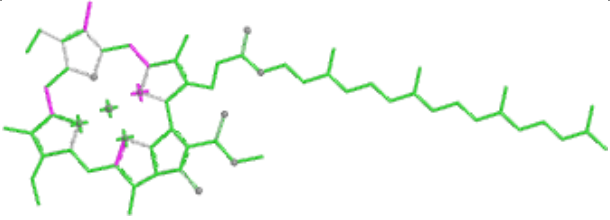
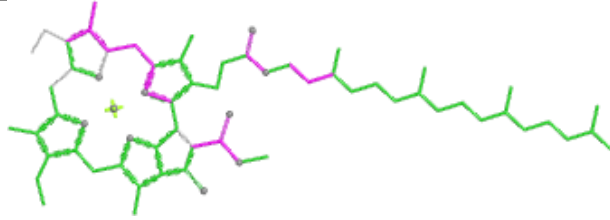
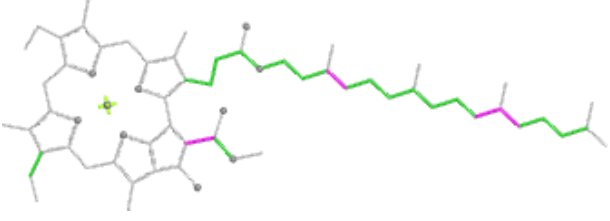
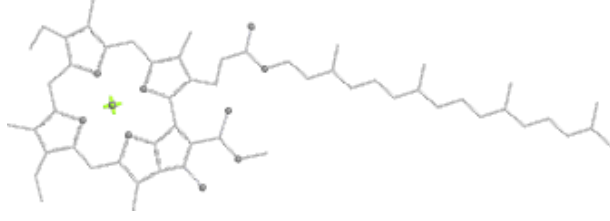
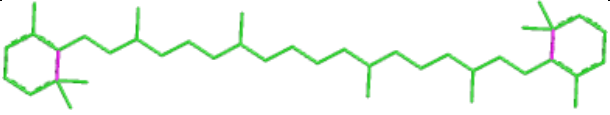
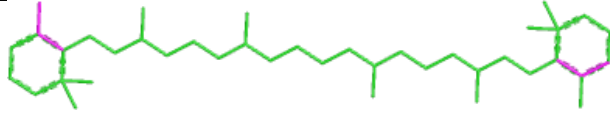
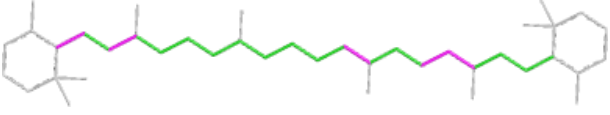
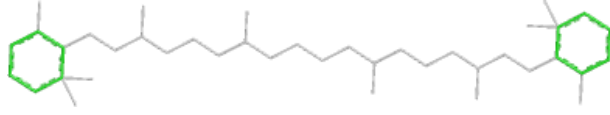
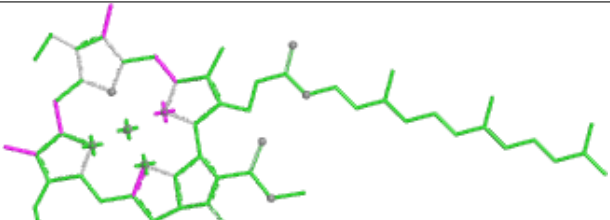
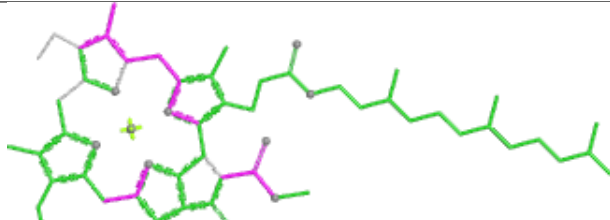
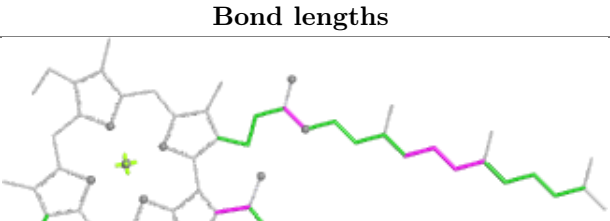
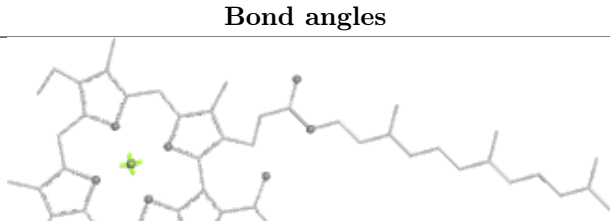


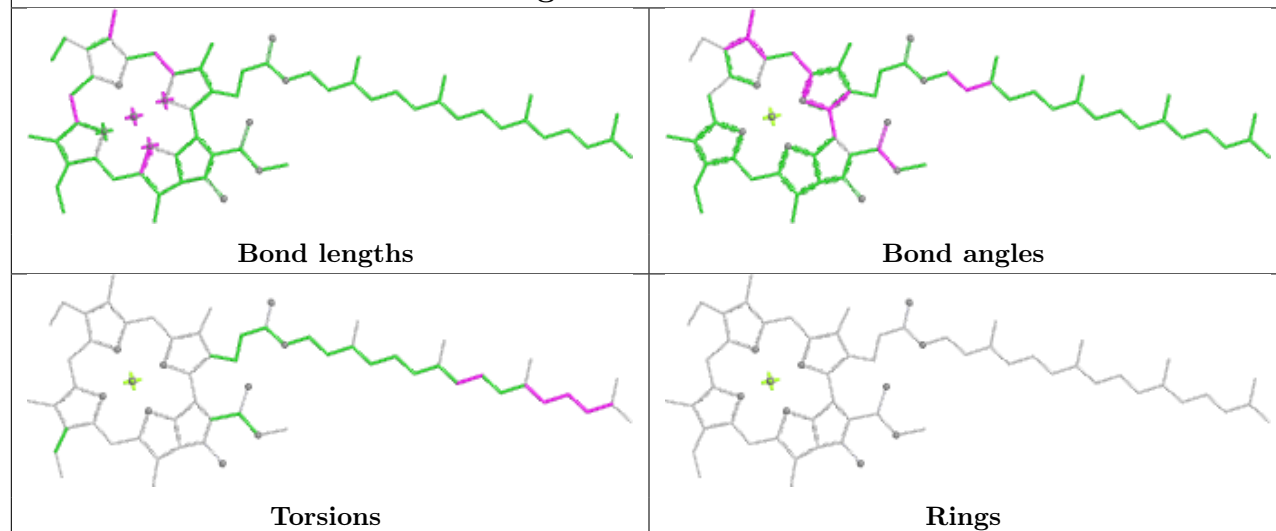
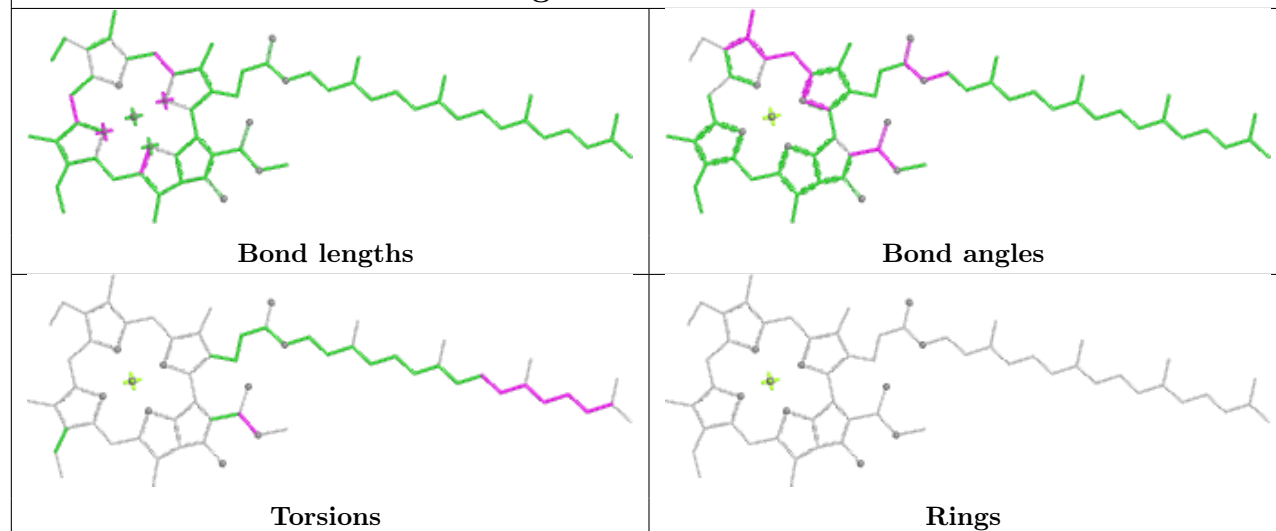


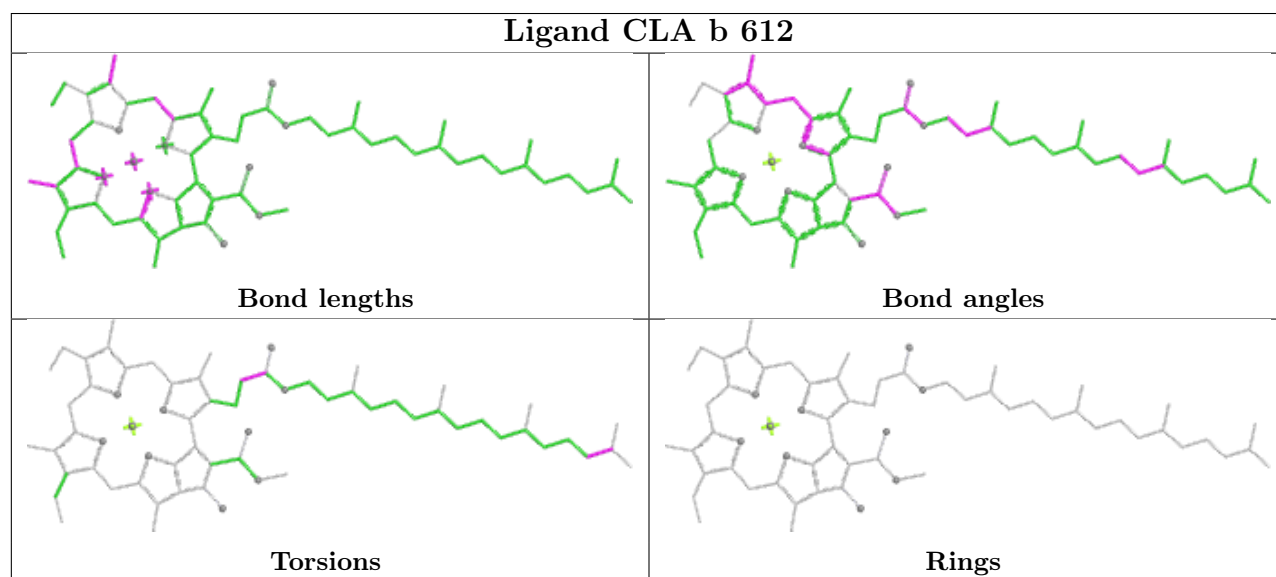
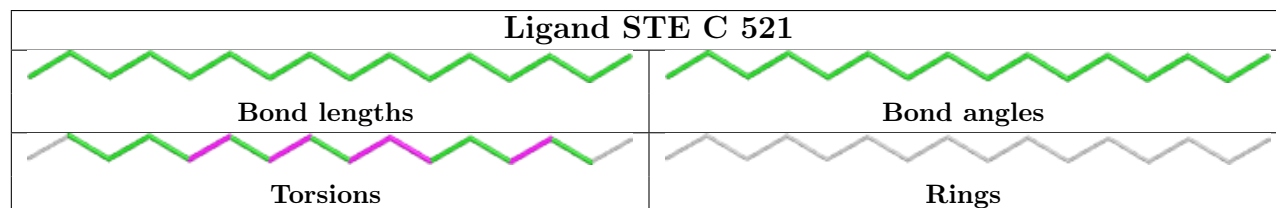
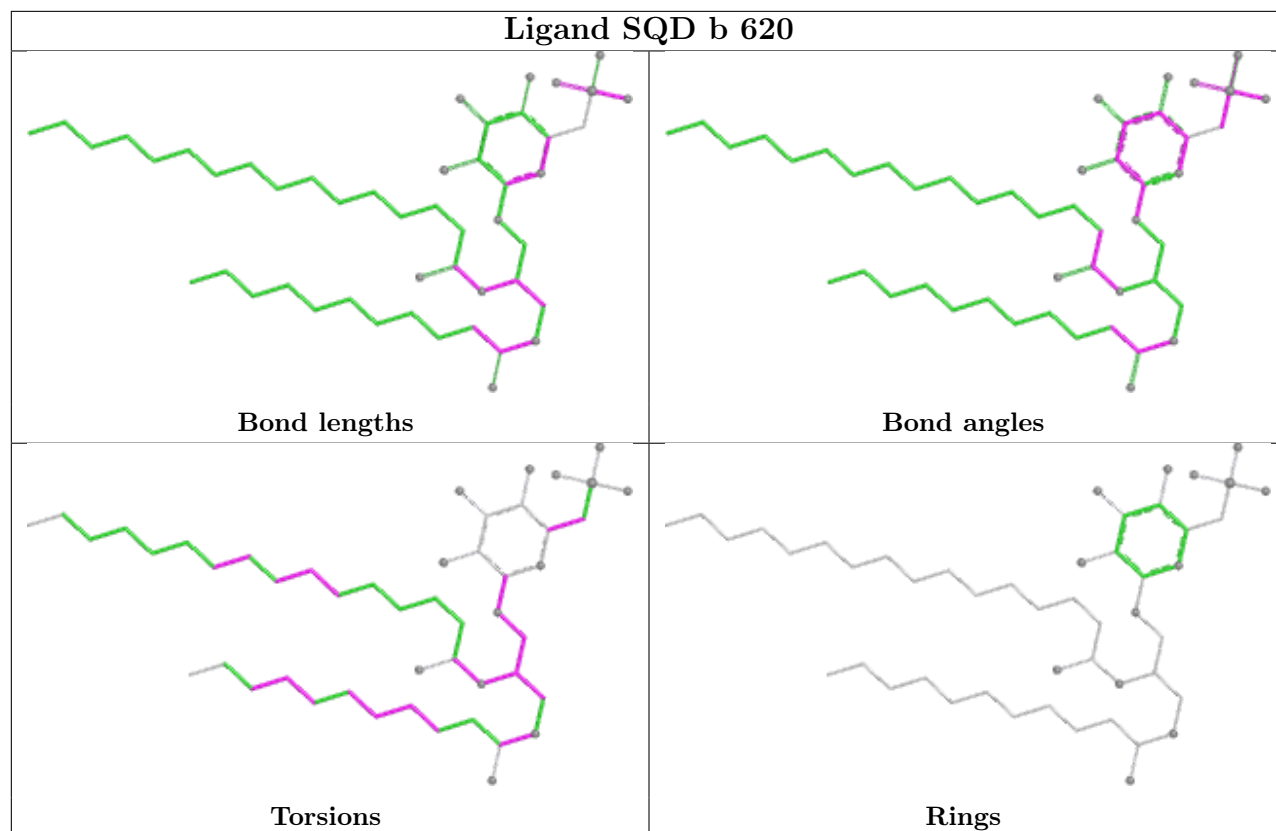


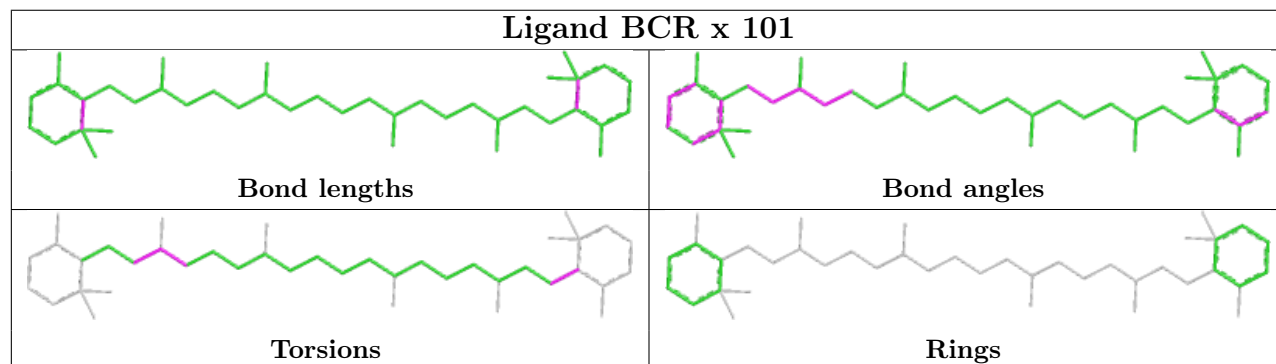
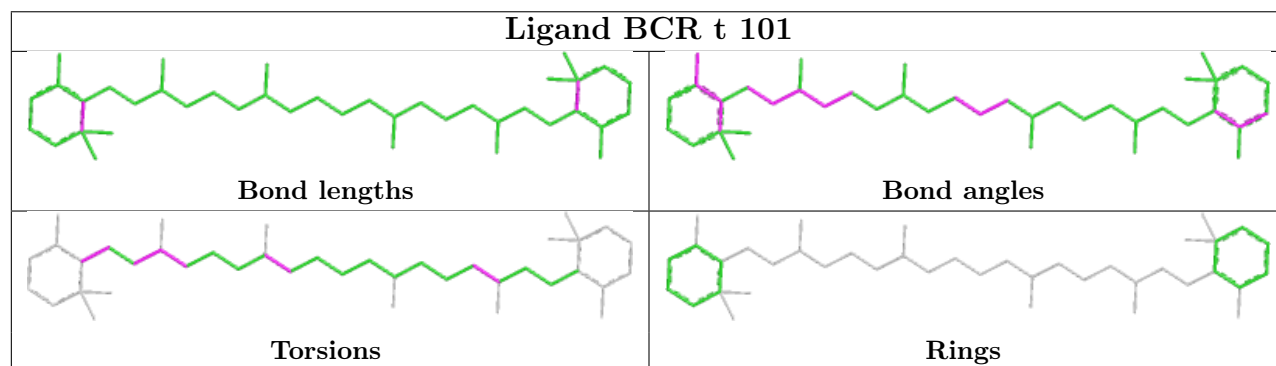
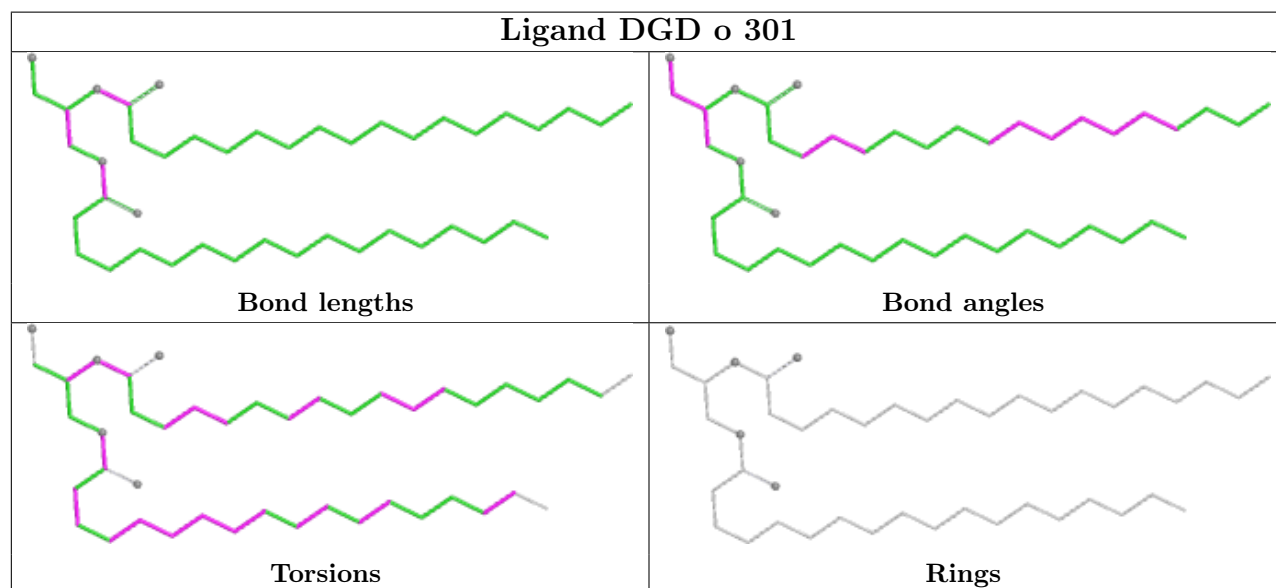
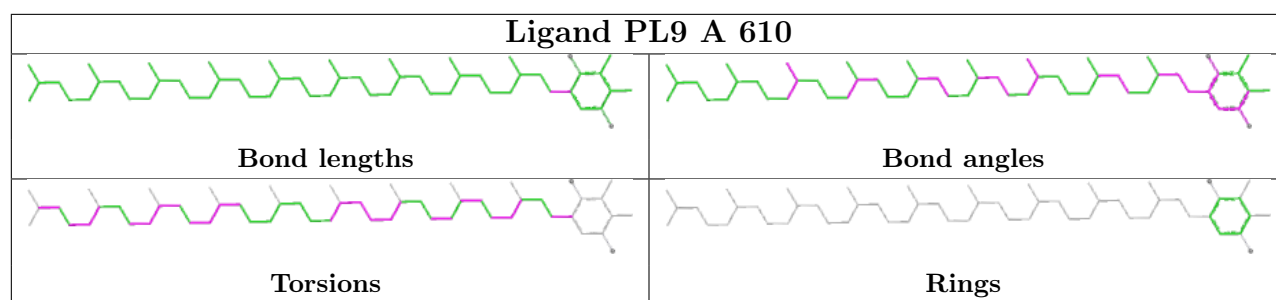
Ligand CLA B 612**Ligand CLA c 513****Ligand BCR D 406**

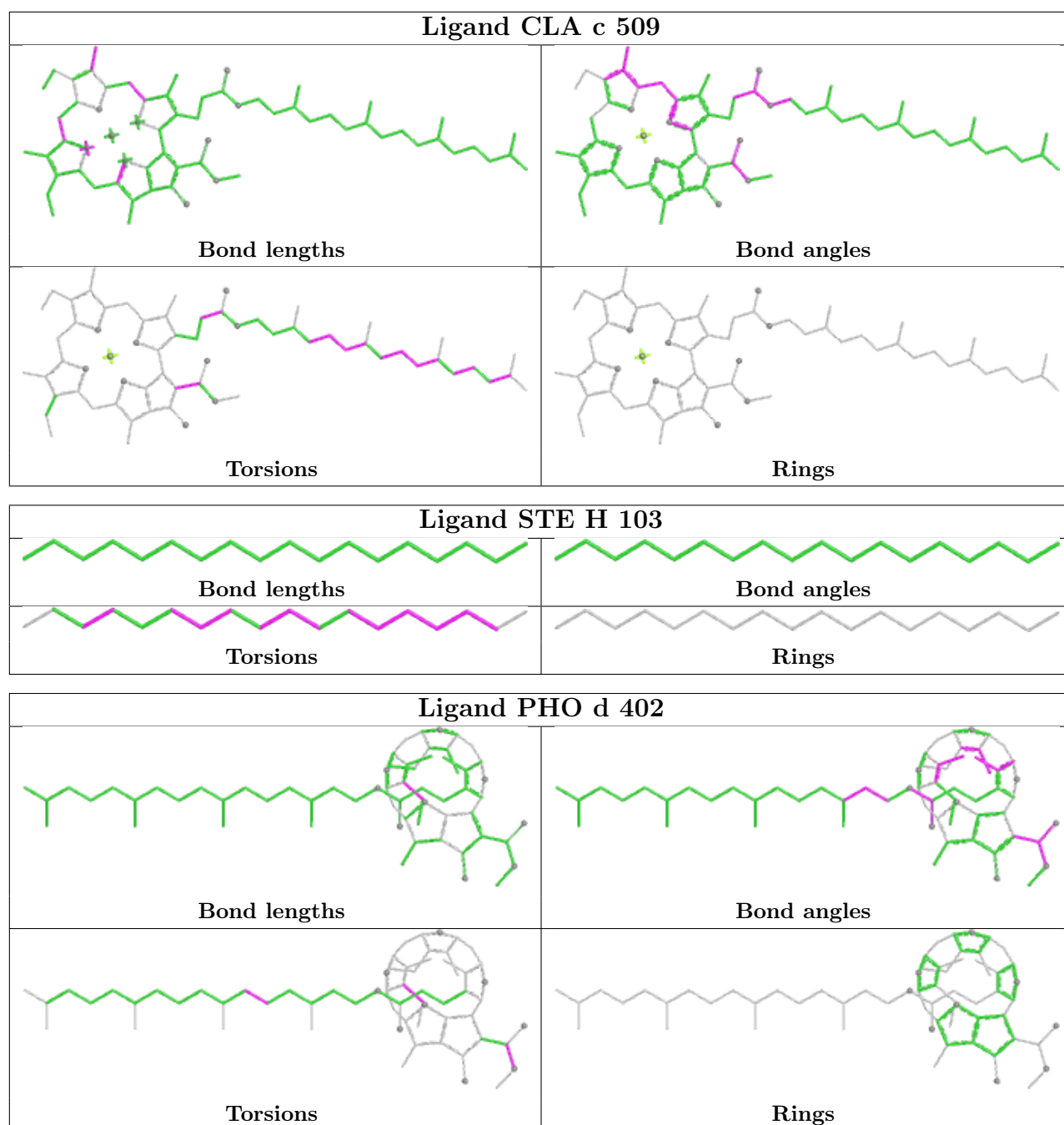


Ligand CLA B 614	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR k 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA B 616	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

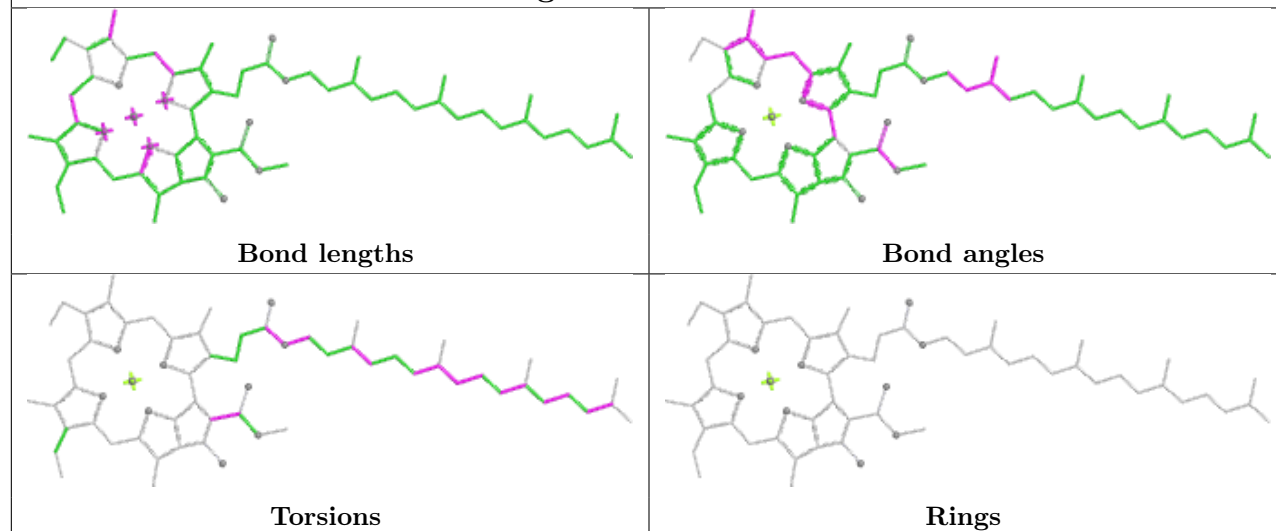
Ligand CLA c 511**Ligand CLA B 604**



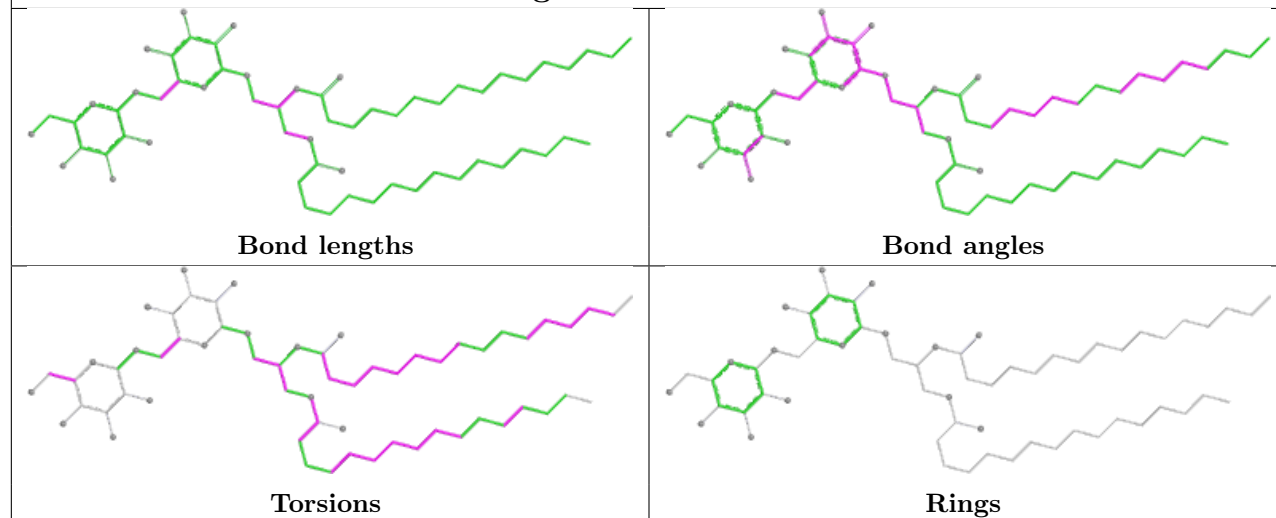




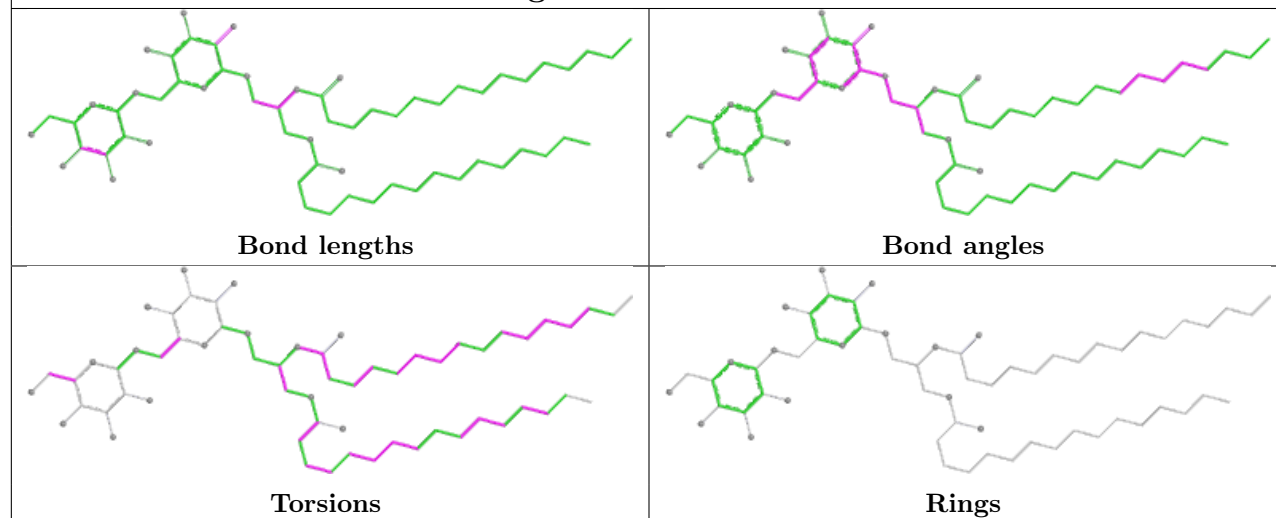
Ligand CLA c 506

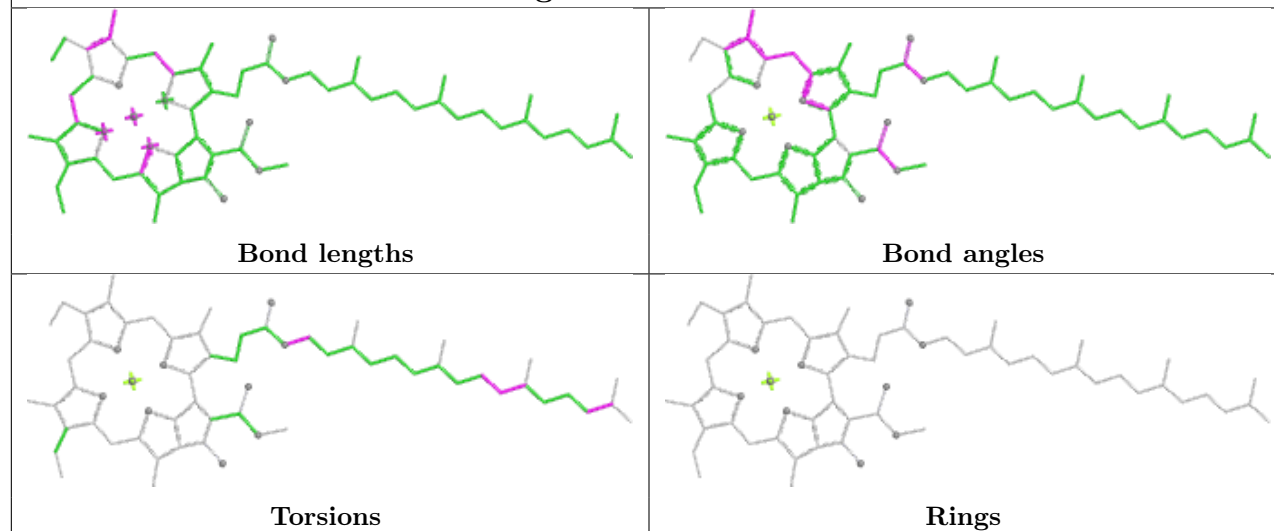
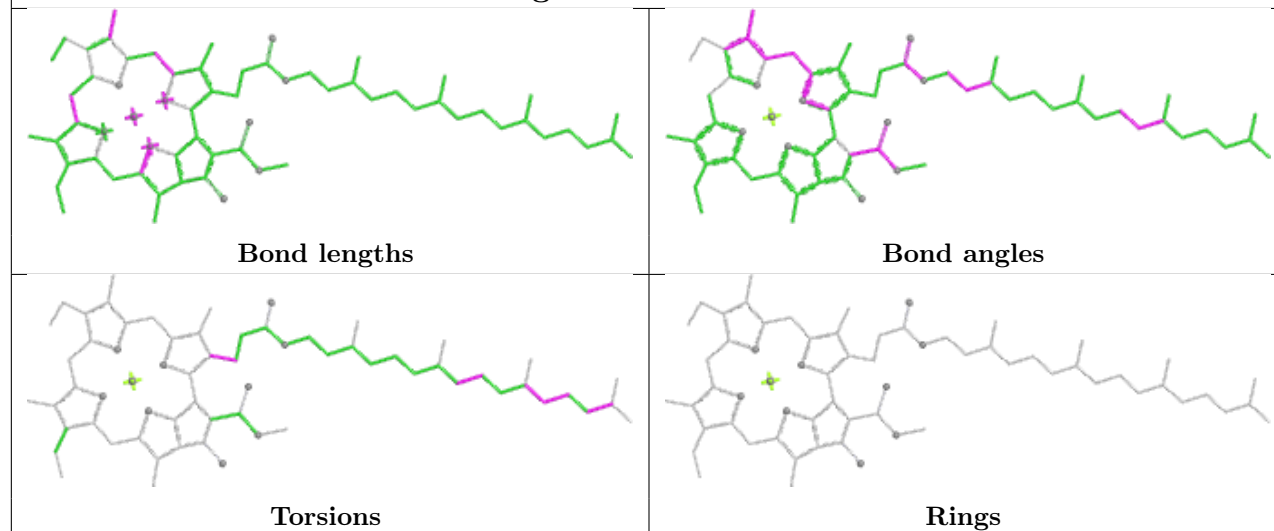


Ligand DGD c 515

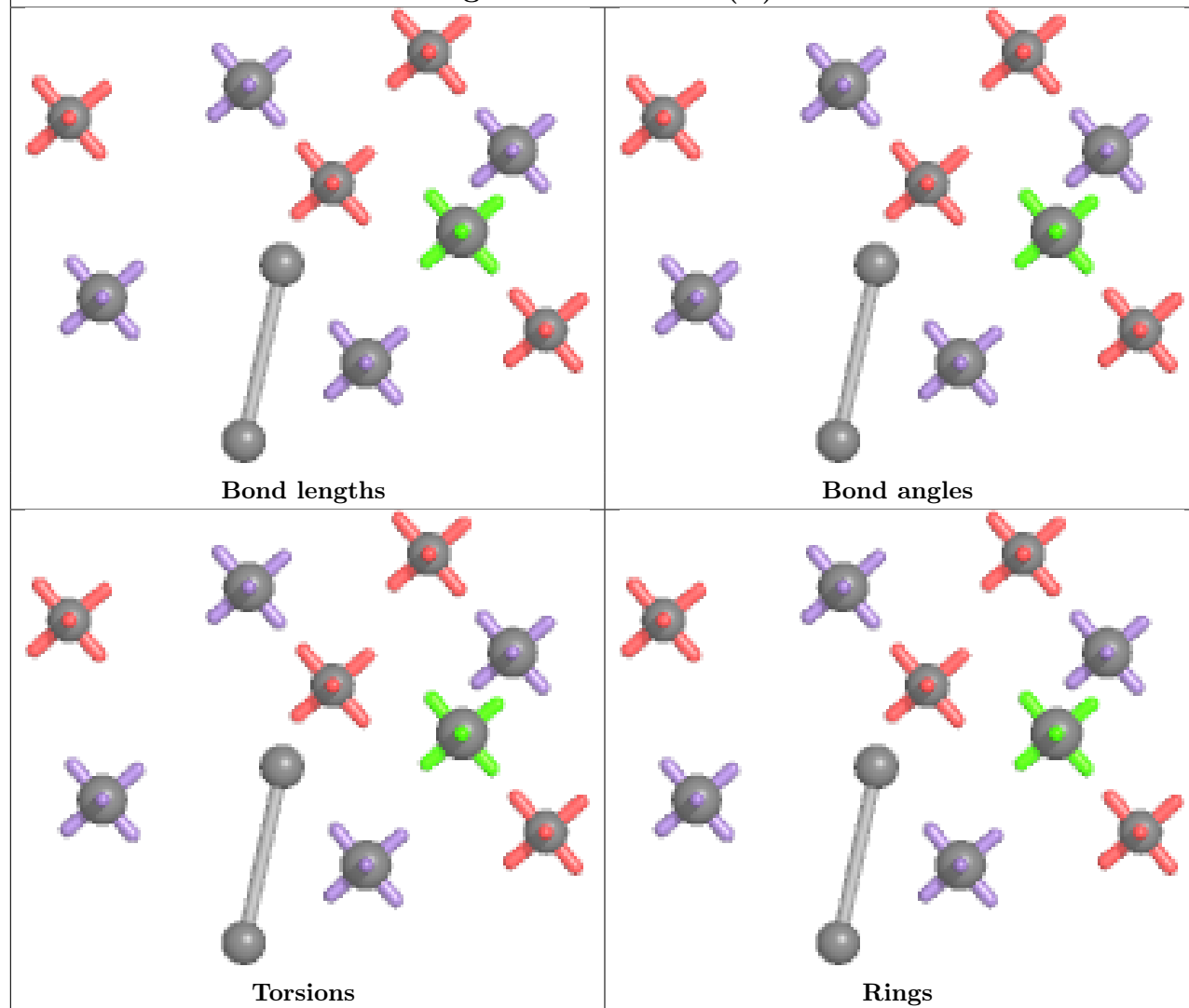


Ligand DGD C 515

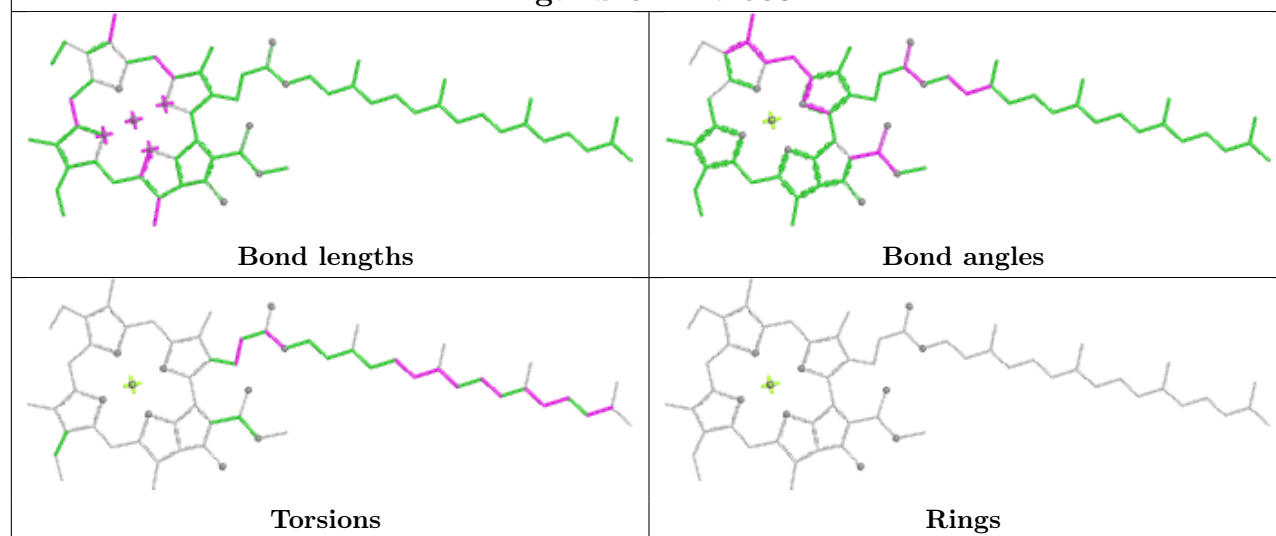


Ligand CLA d 403**Ligand CLA B 602**

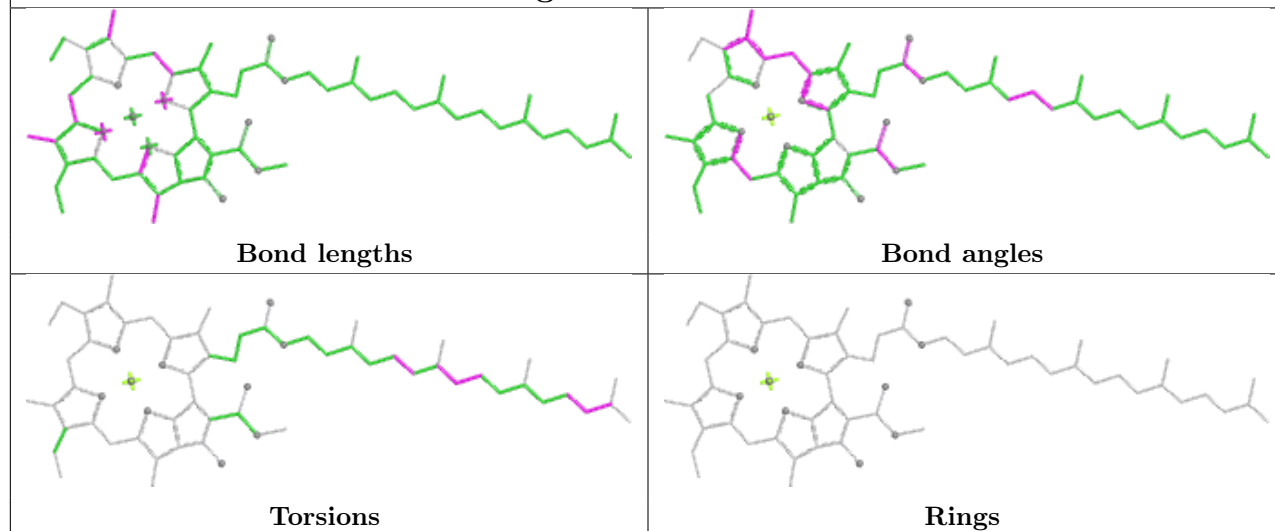
Ligand OEY A 601 (B)



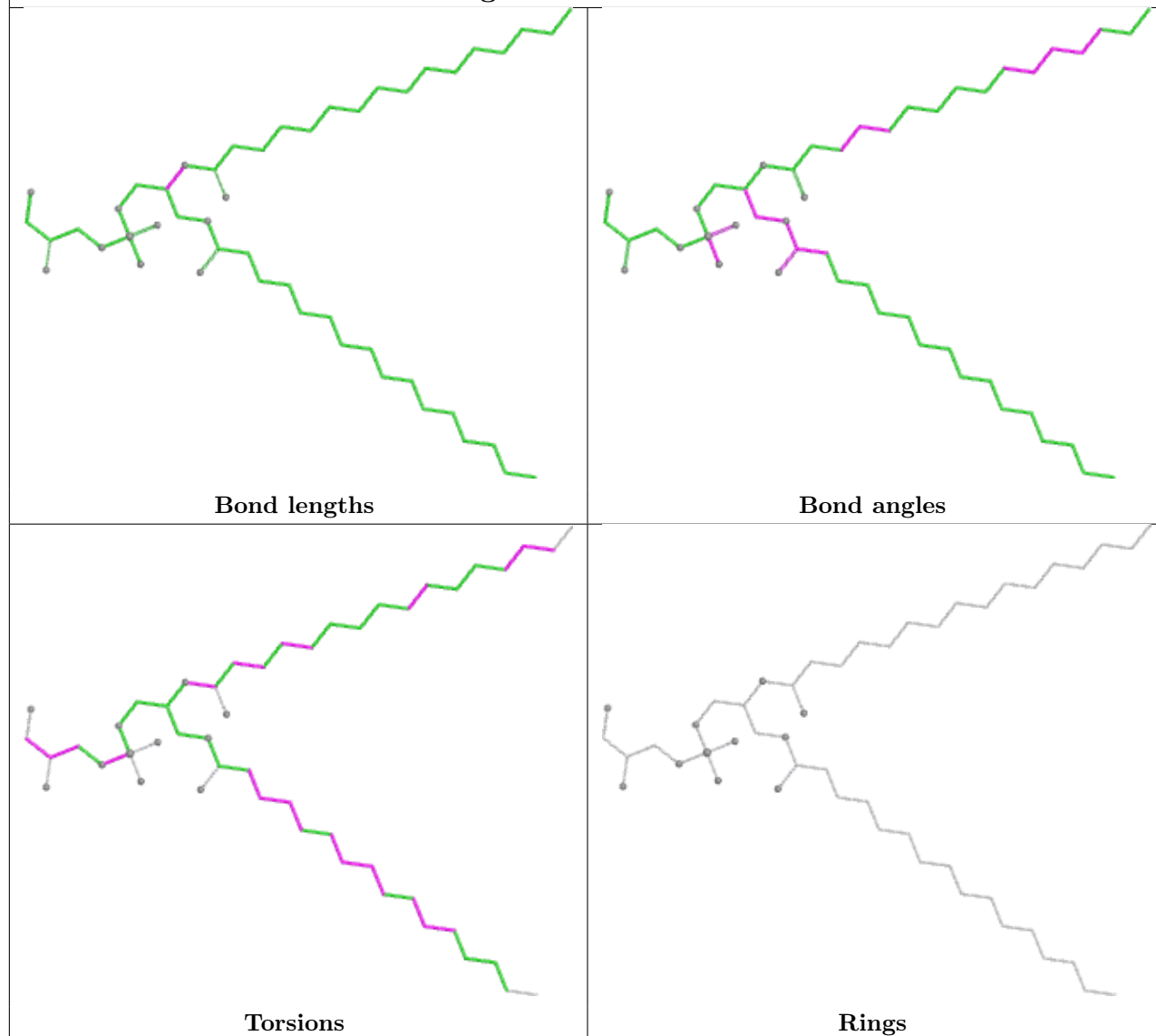
Ligand CLA b 603



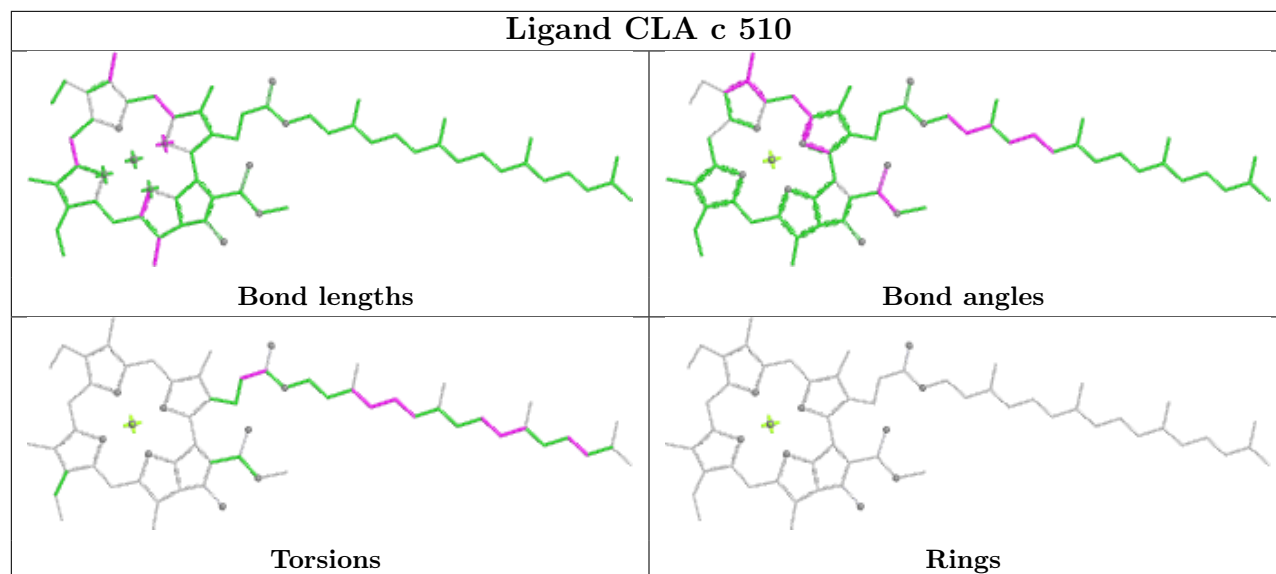
Ligand CLA c 503



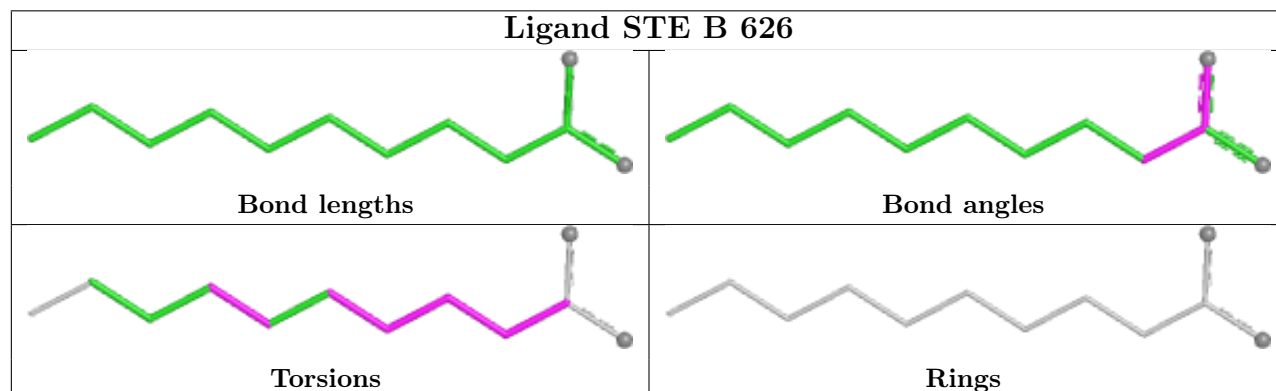
Ligand LHG B 622



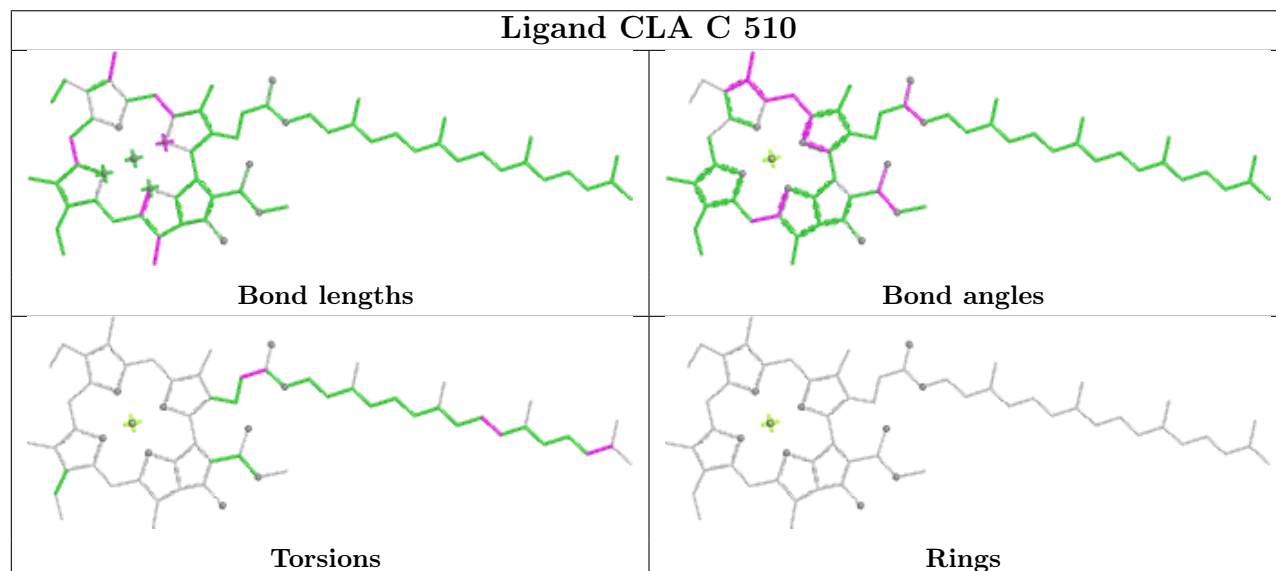
Ligand CLA c 510

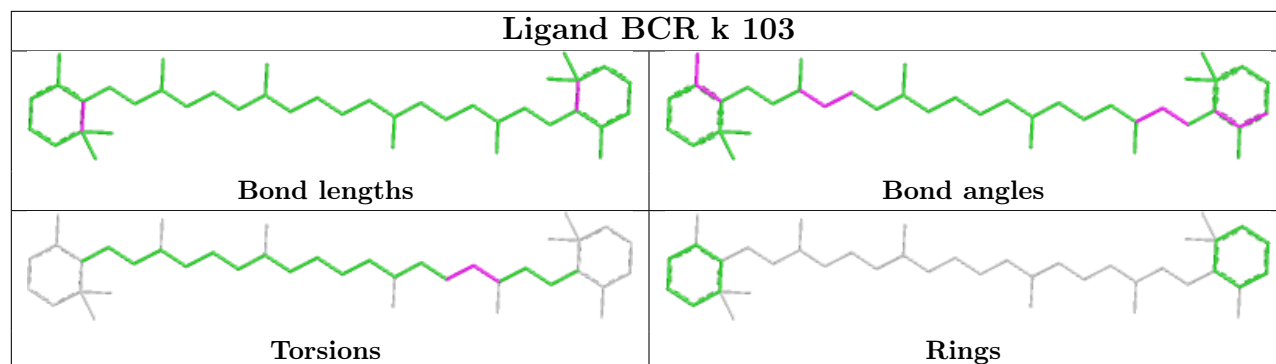
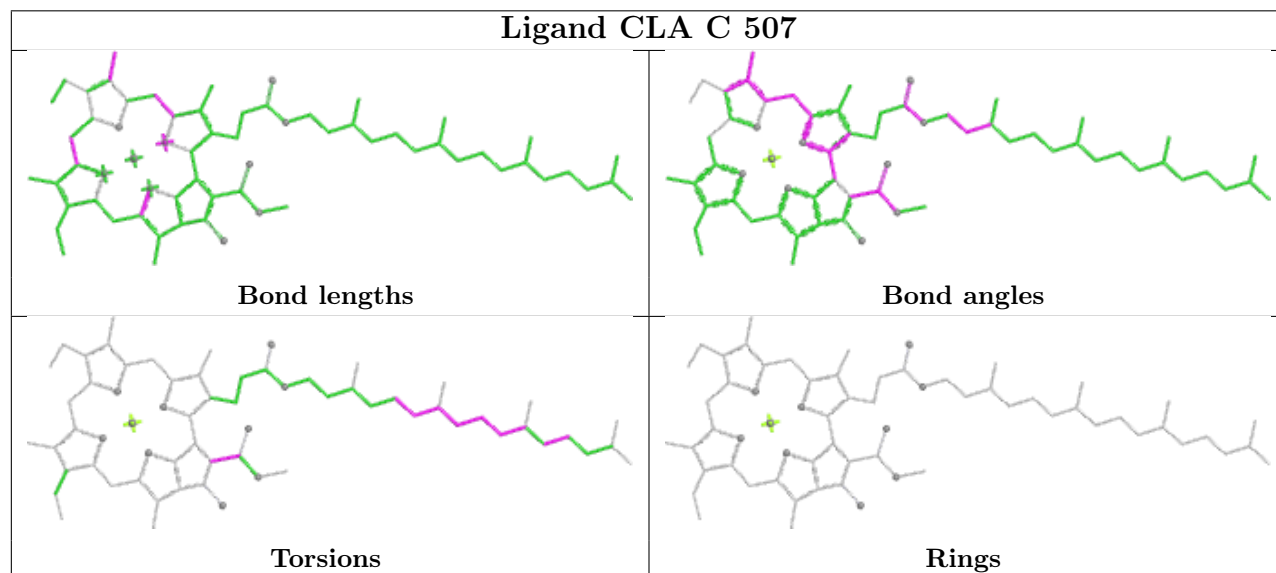


Ligand STE B 626

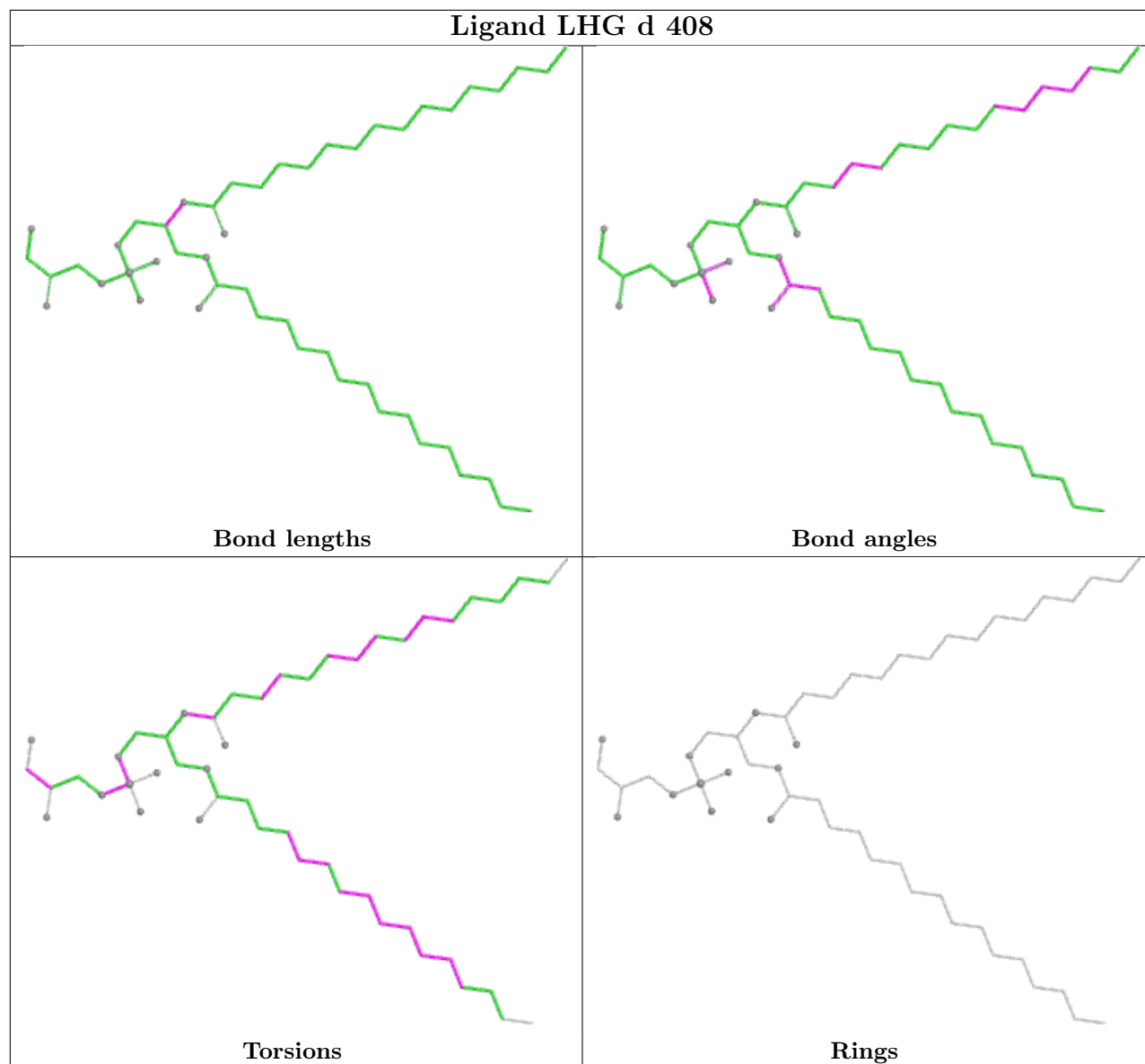


Ligand CLA C 510

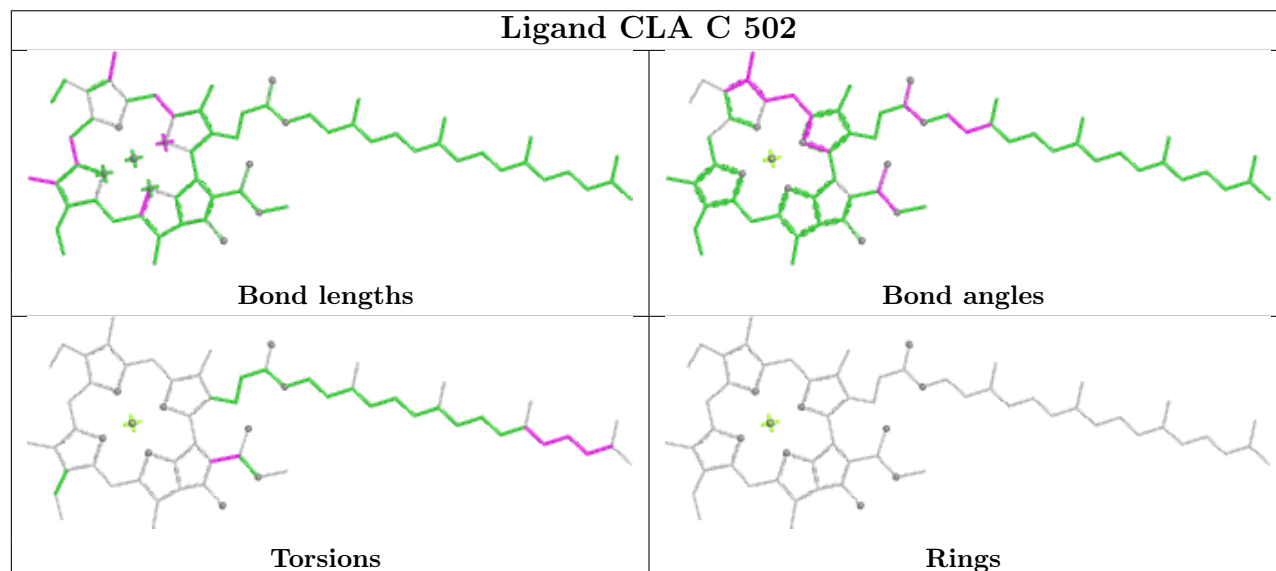


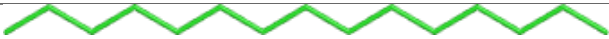
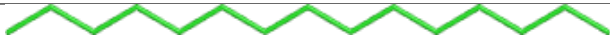


Ligand BCR k 103**Ligand CLA C 507**

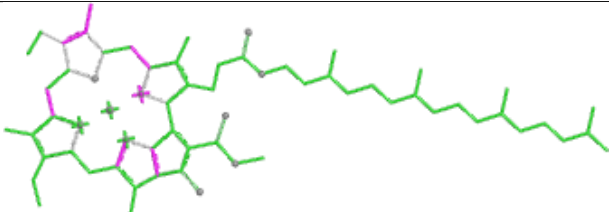
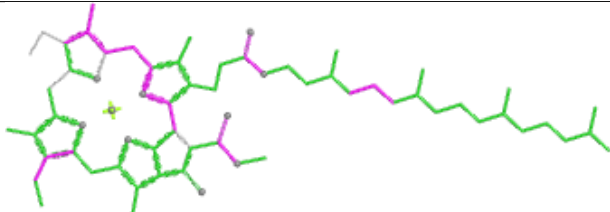
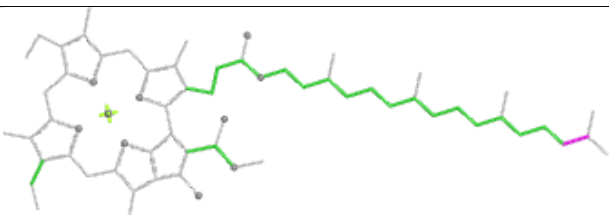
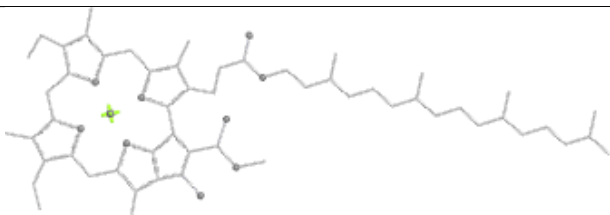
Ligand LHG d 408

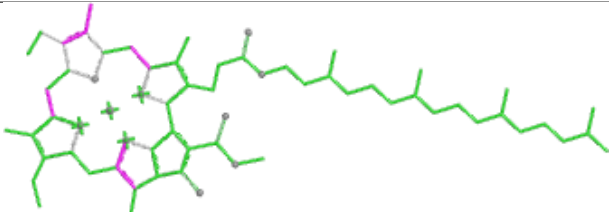
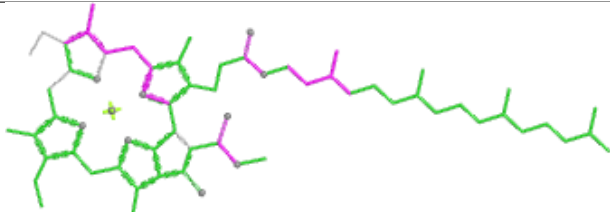
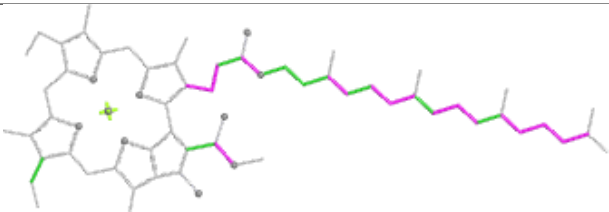
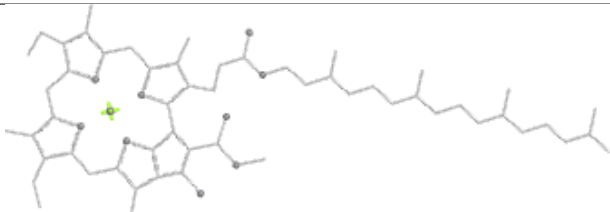


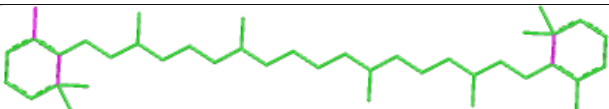
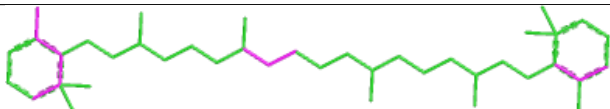

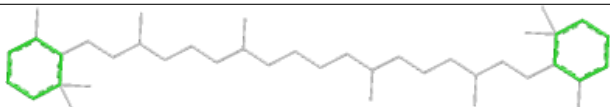
Ligand CLA C 502

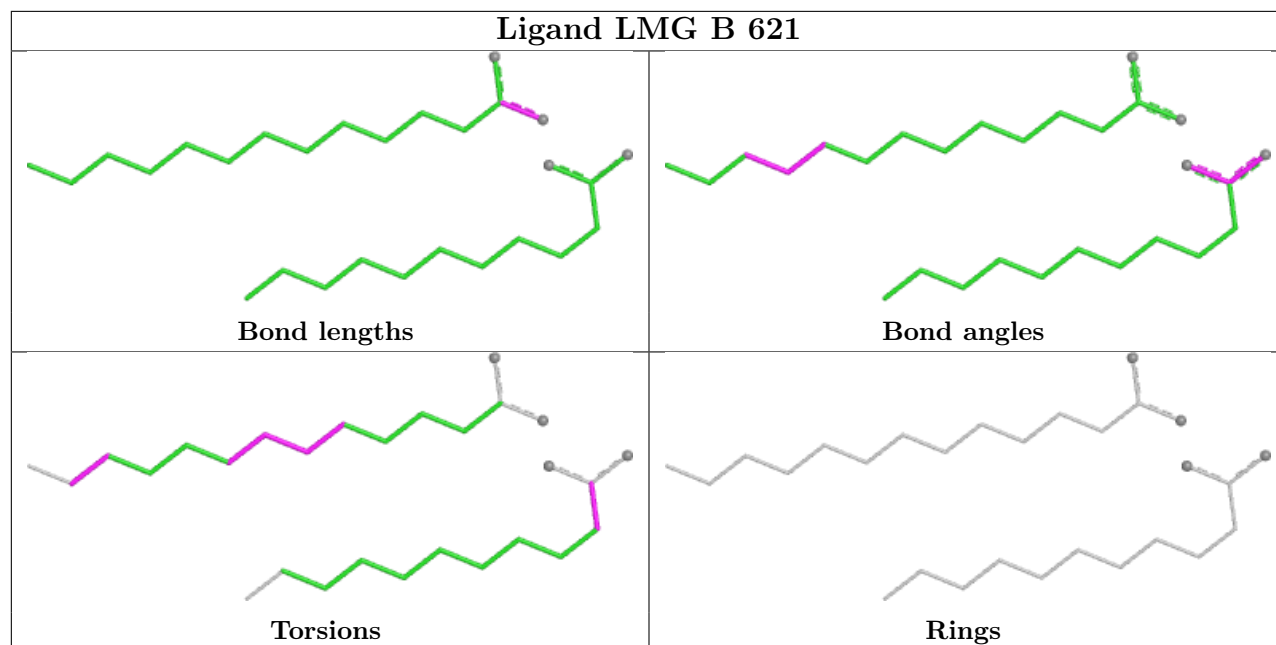
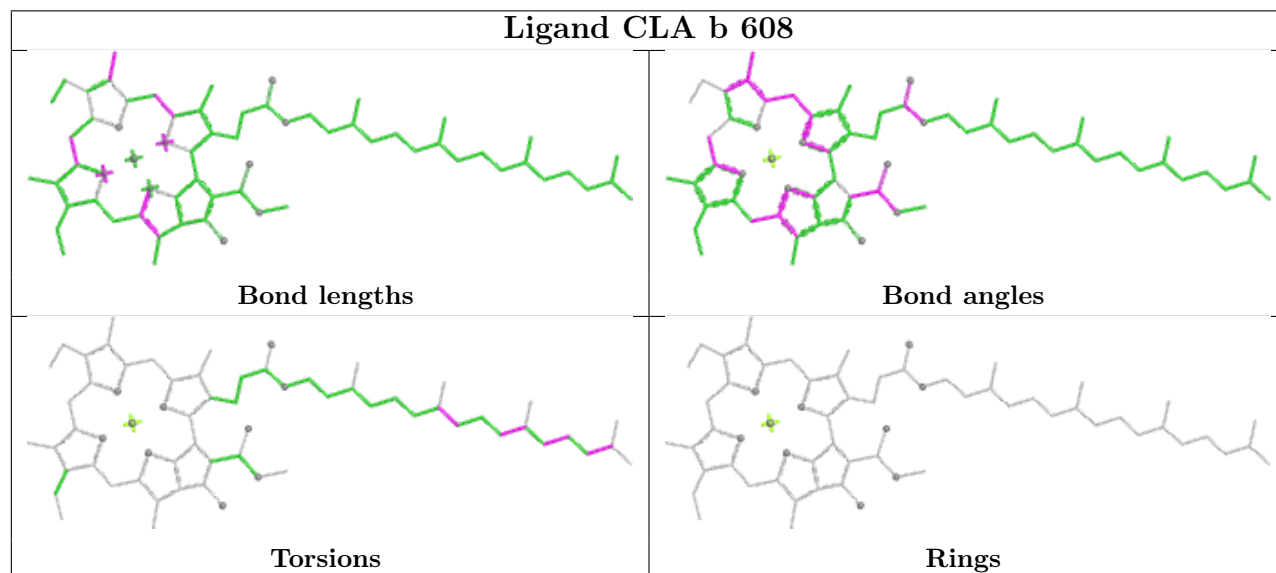
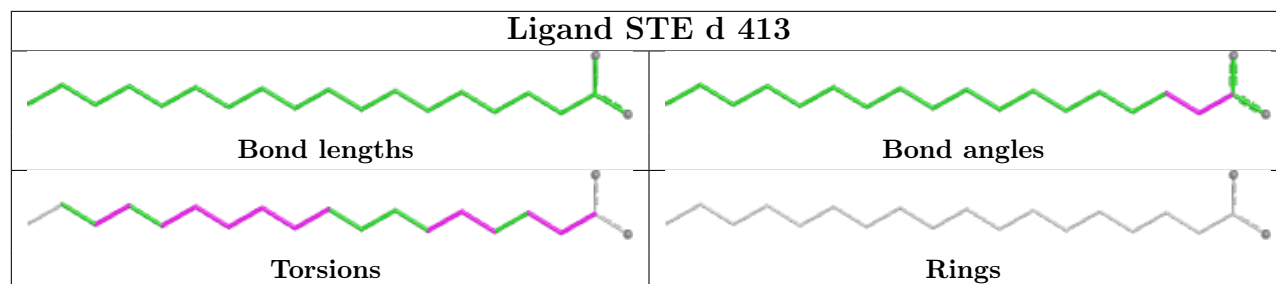


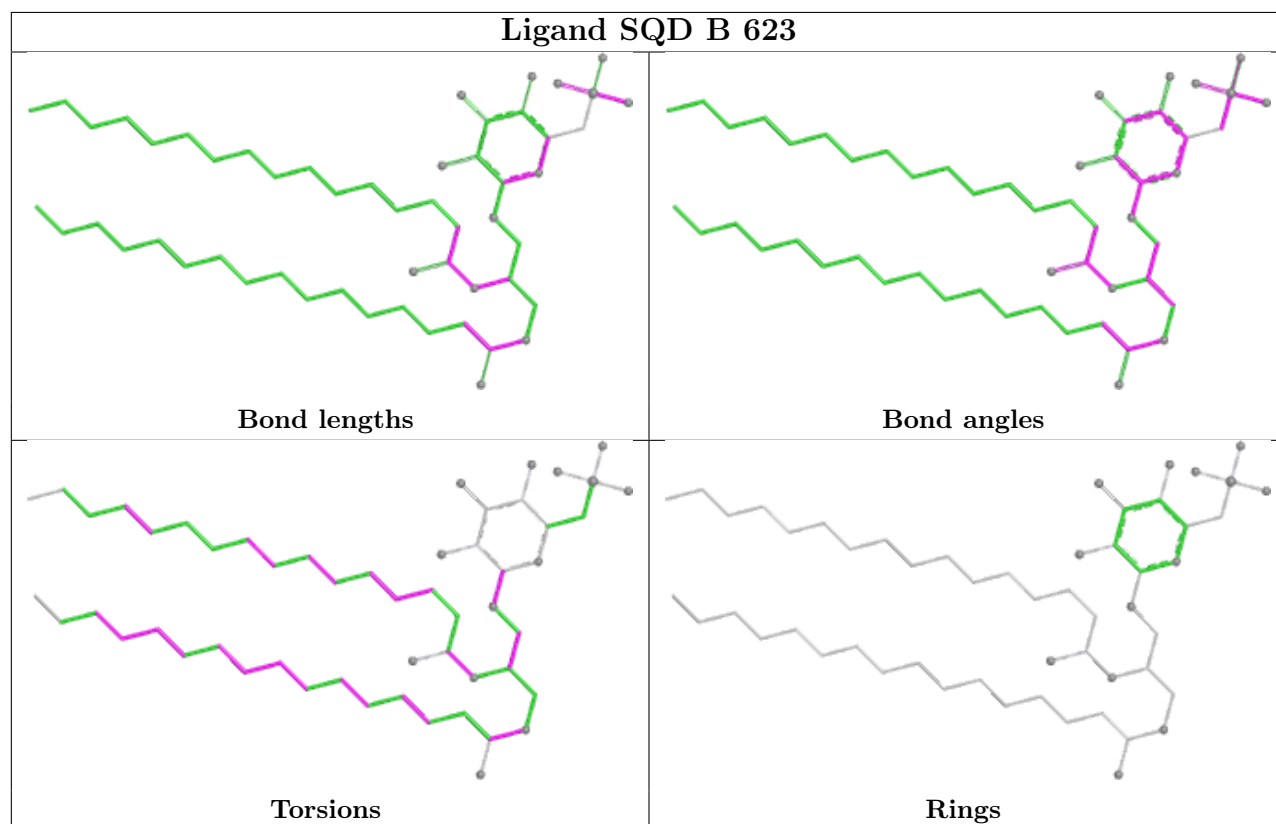
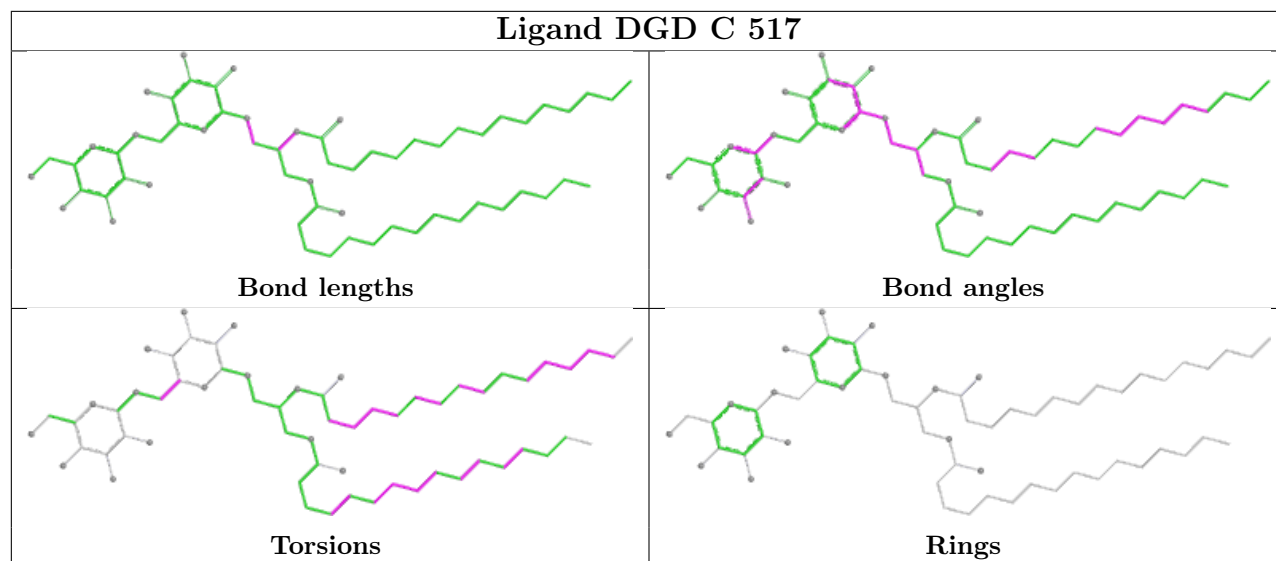
Ligand STE T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

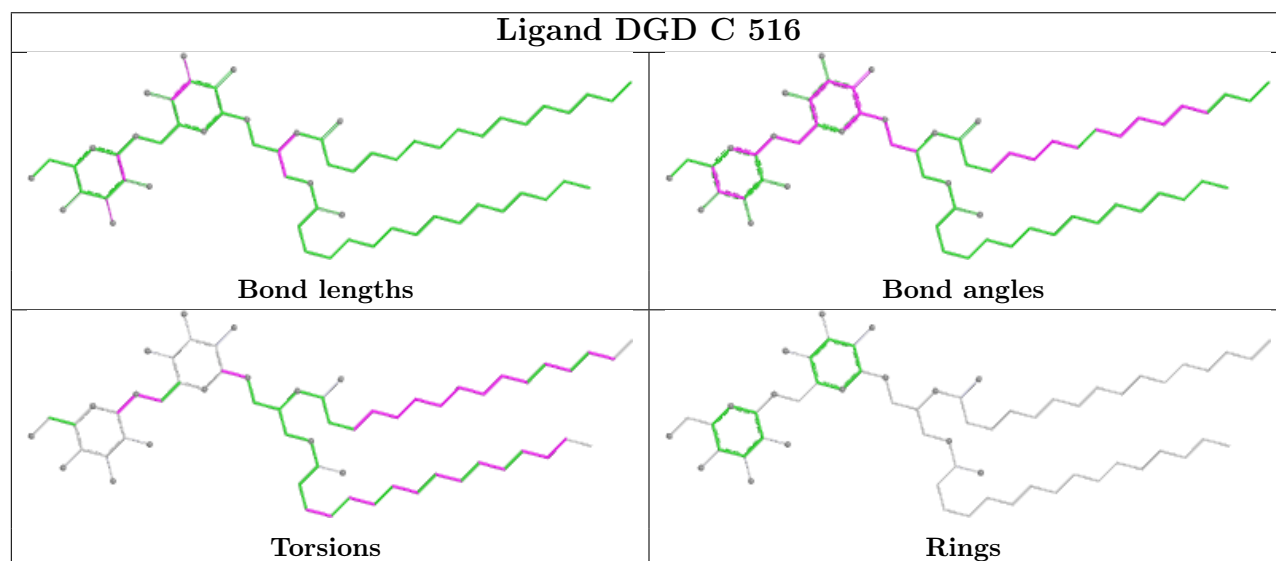
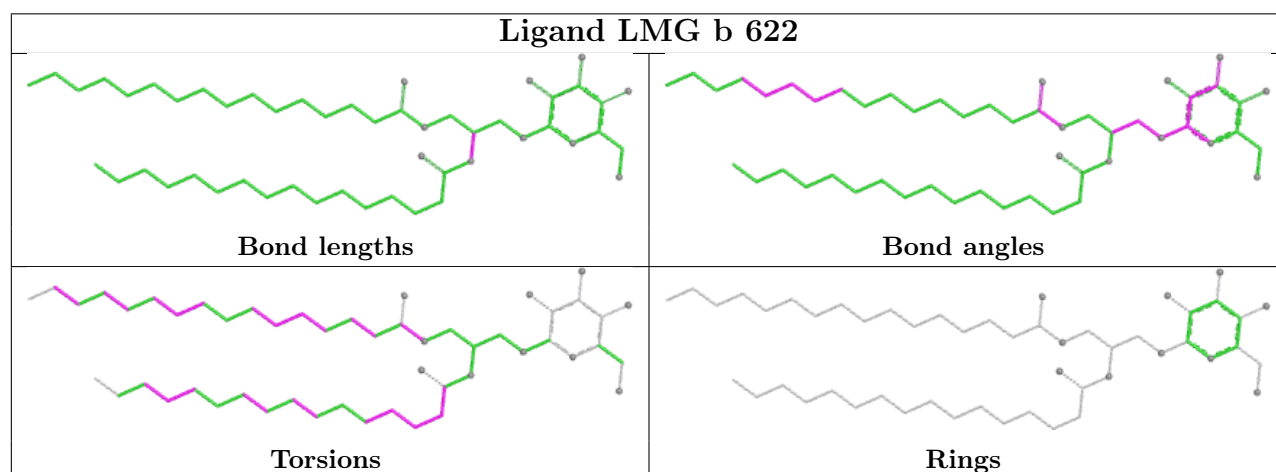
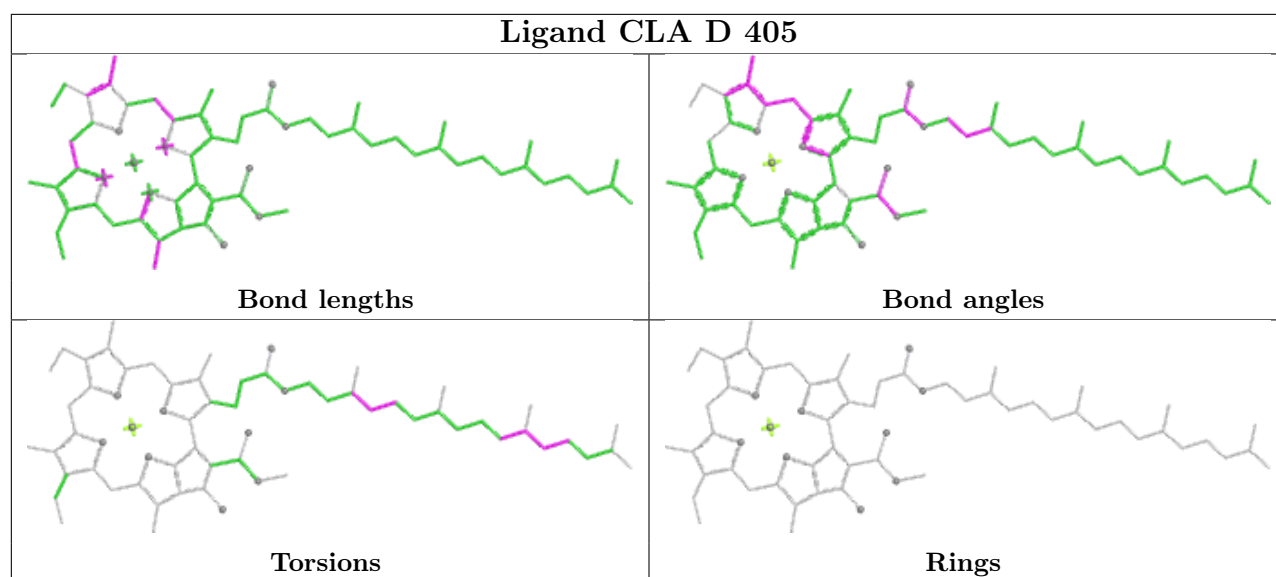
Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

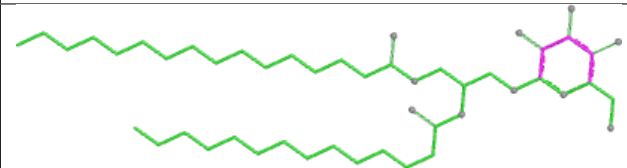
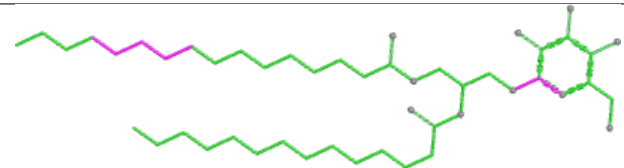
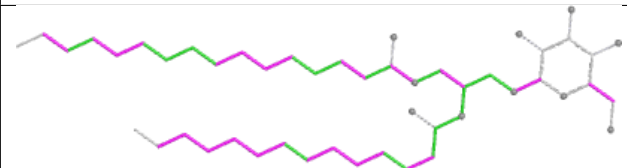
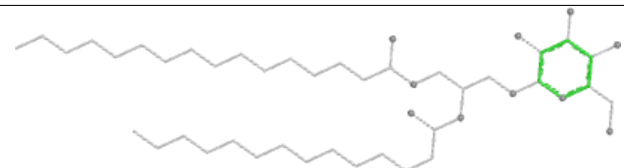
Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

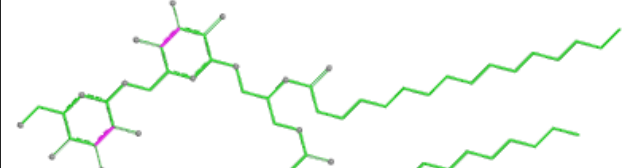
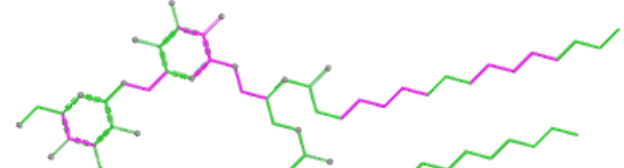
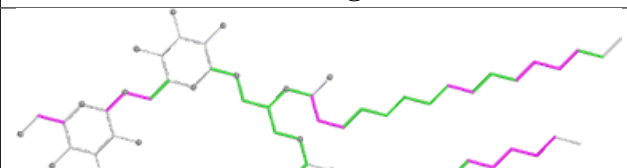
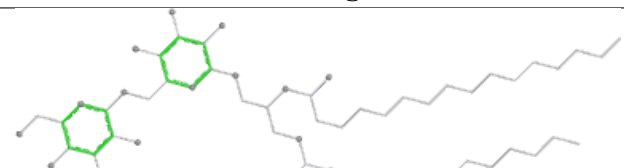
Ligand BCR b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

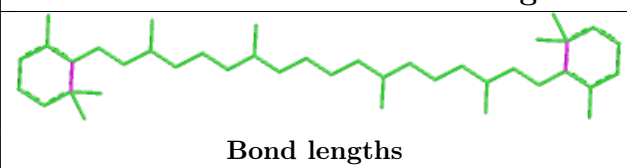
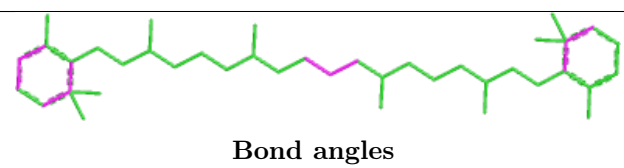

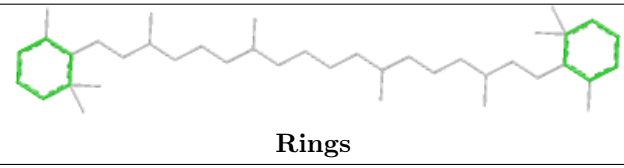




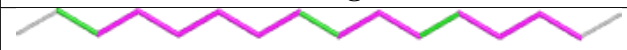



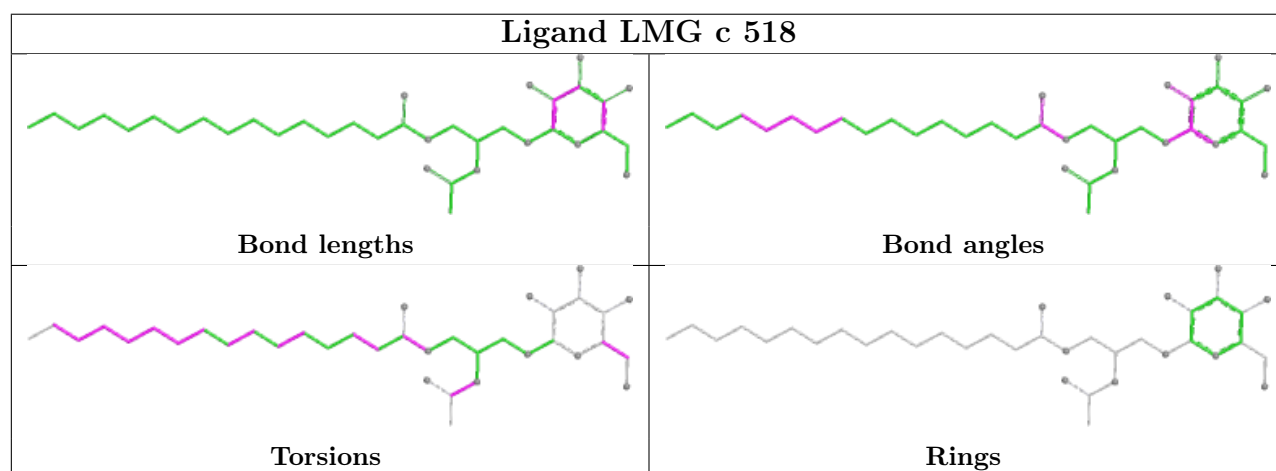
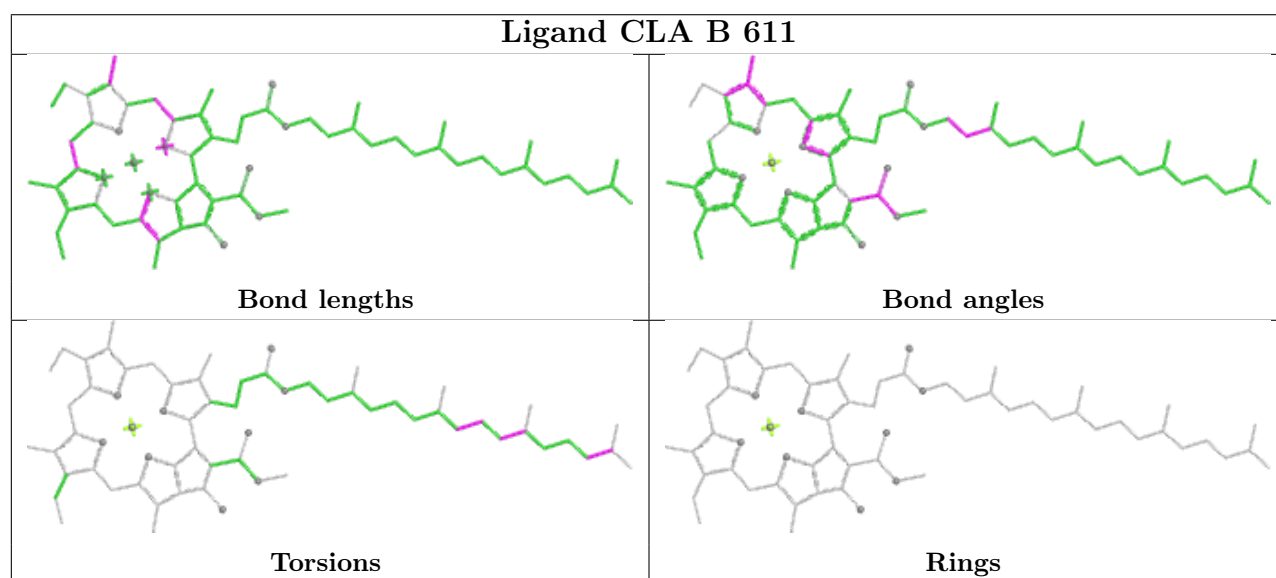
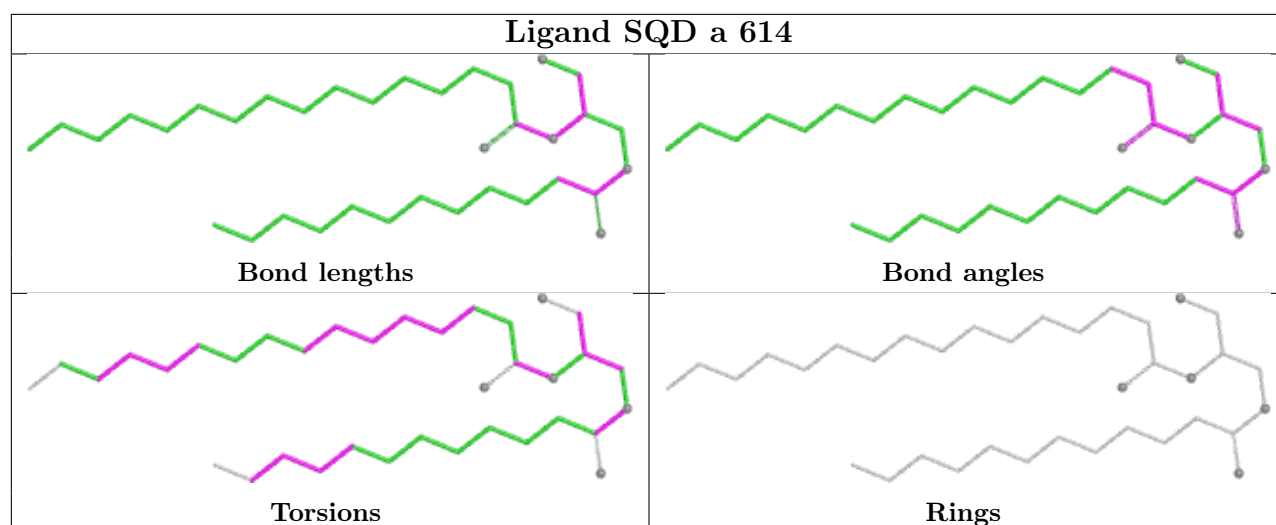


Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

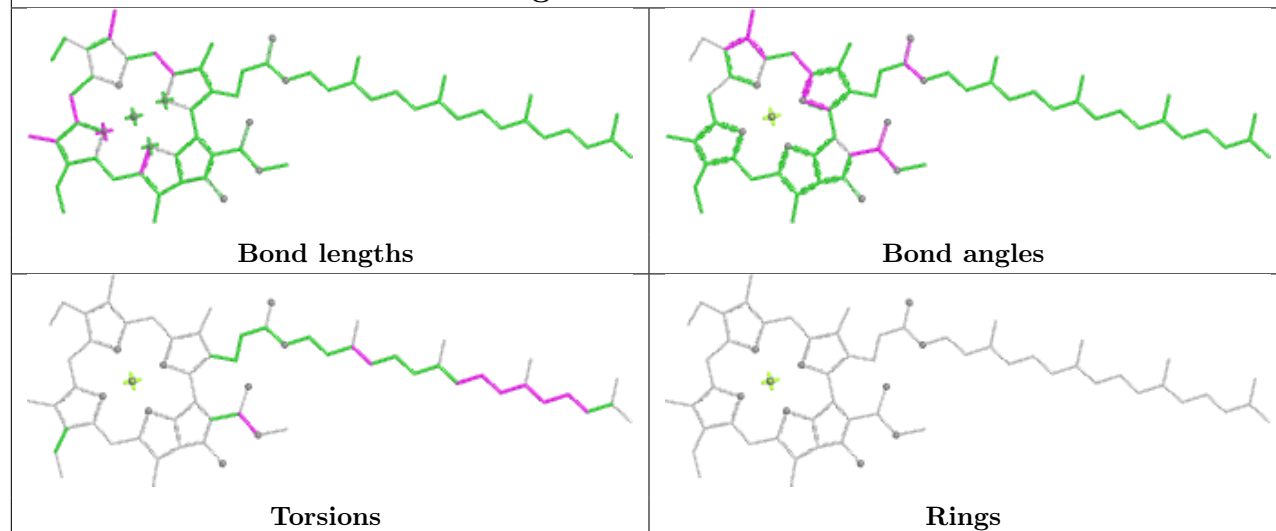
Ligand DGD c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

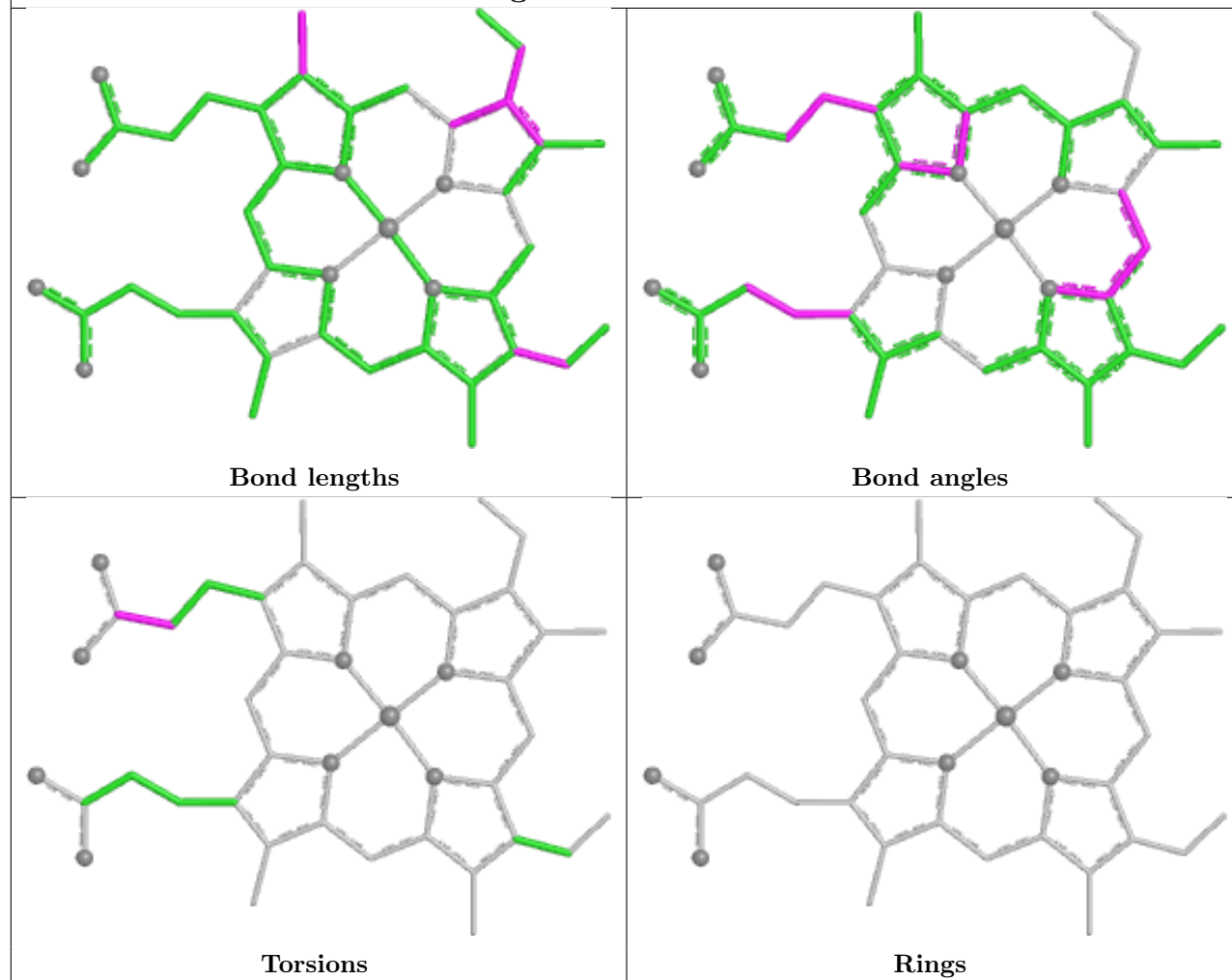
Ligand STE b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

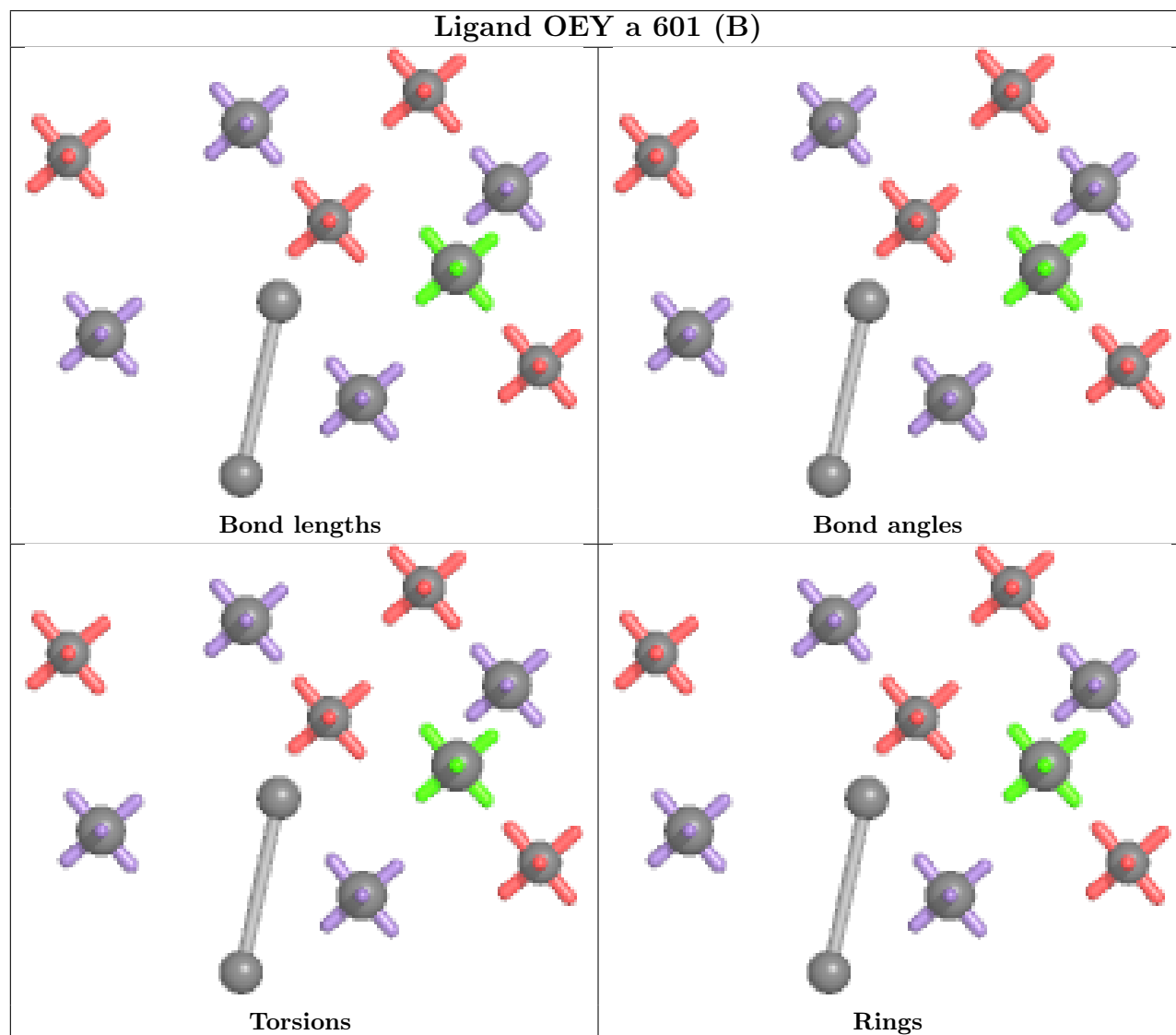
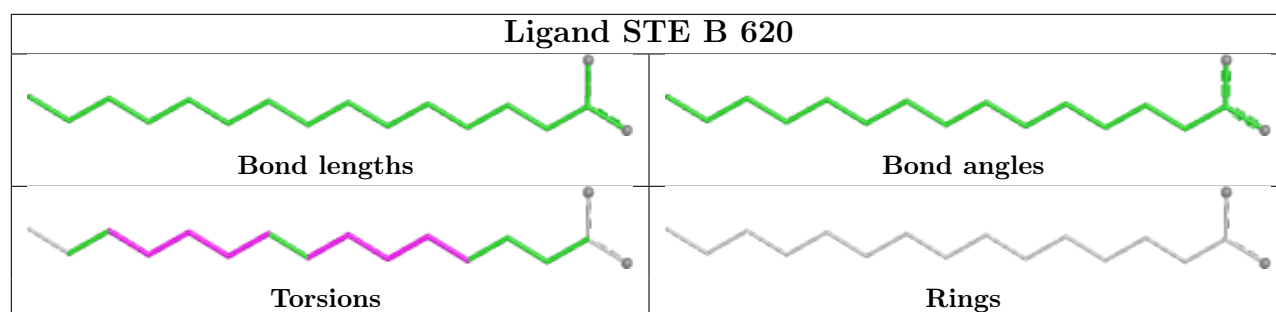


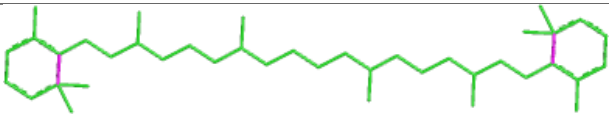
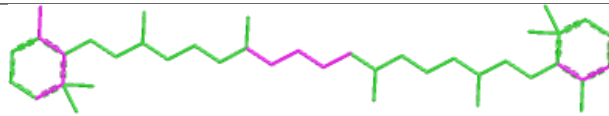
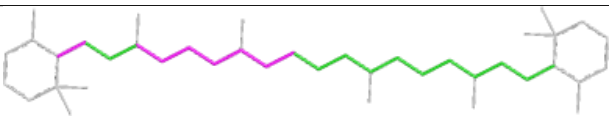
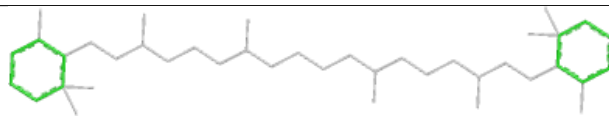
Ligand CLA C 513


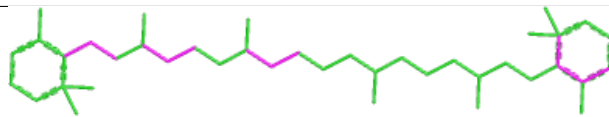
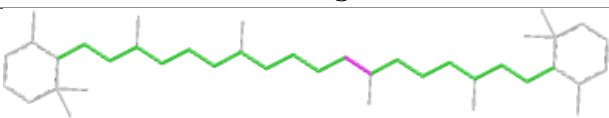
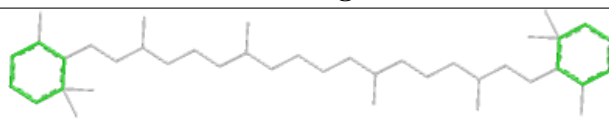


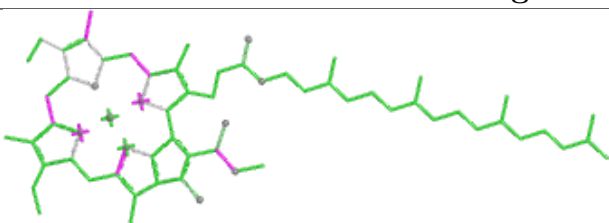
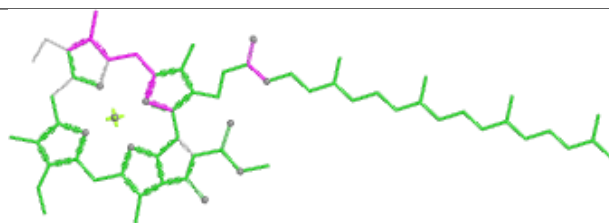
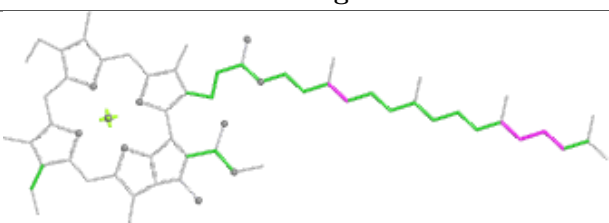
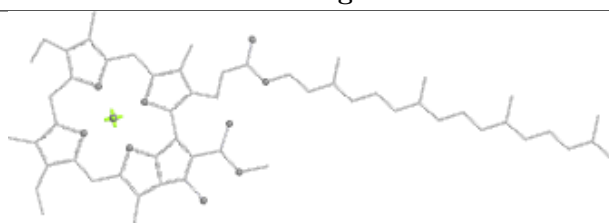
Ligand HEM F 101

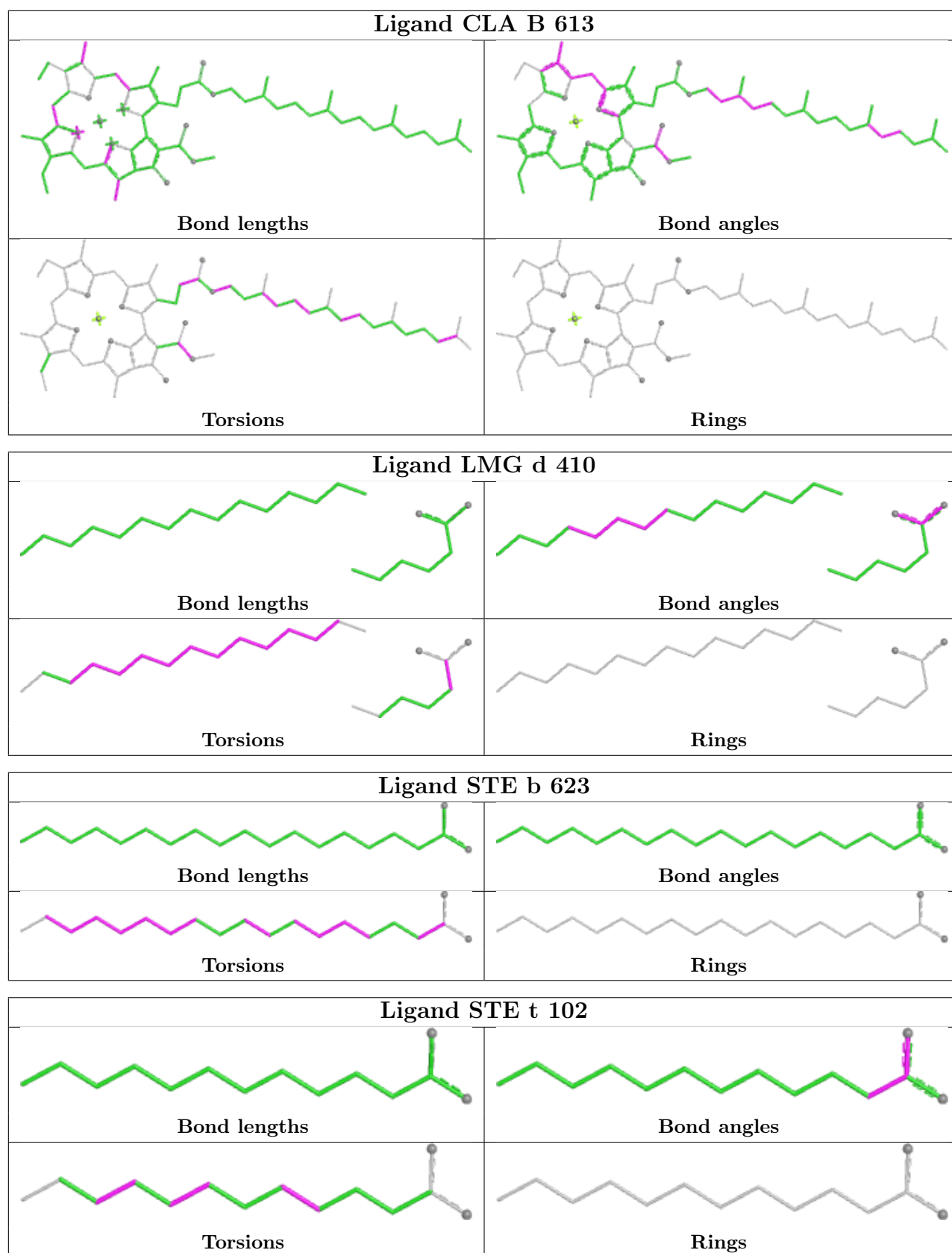


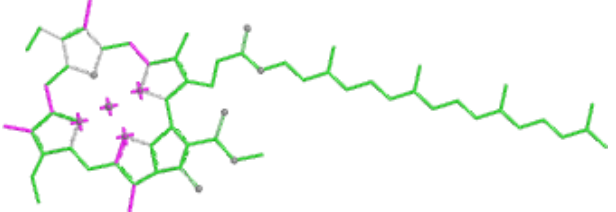
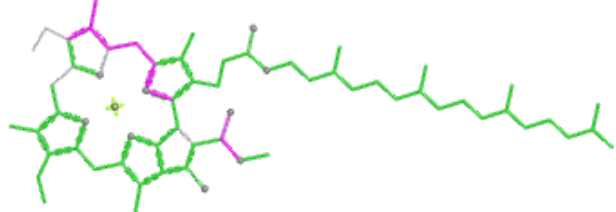
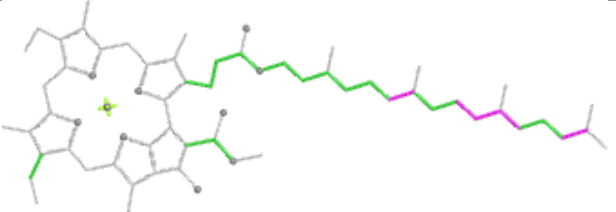
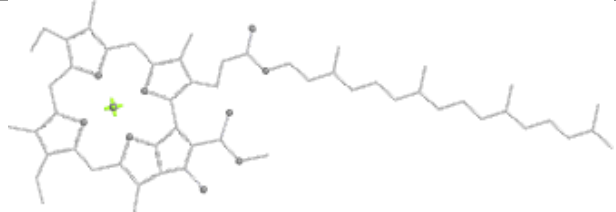


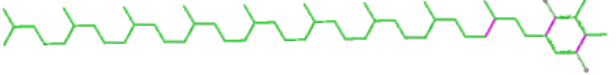
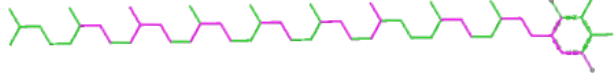
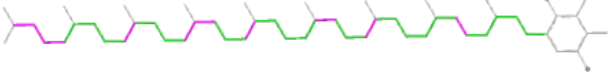
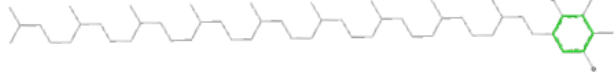
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

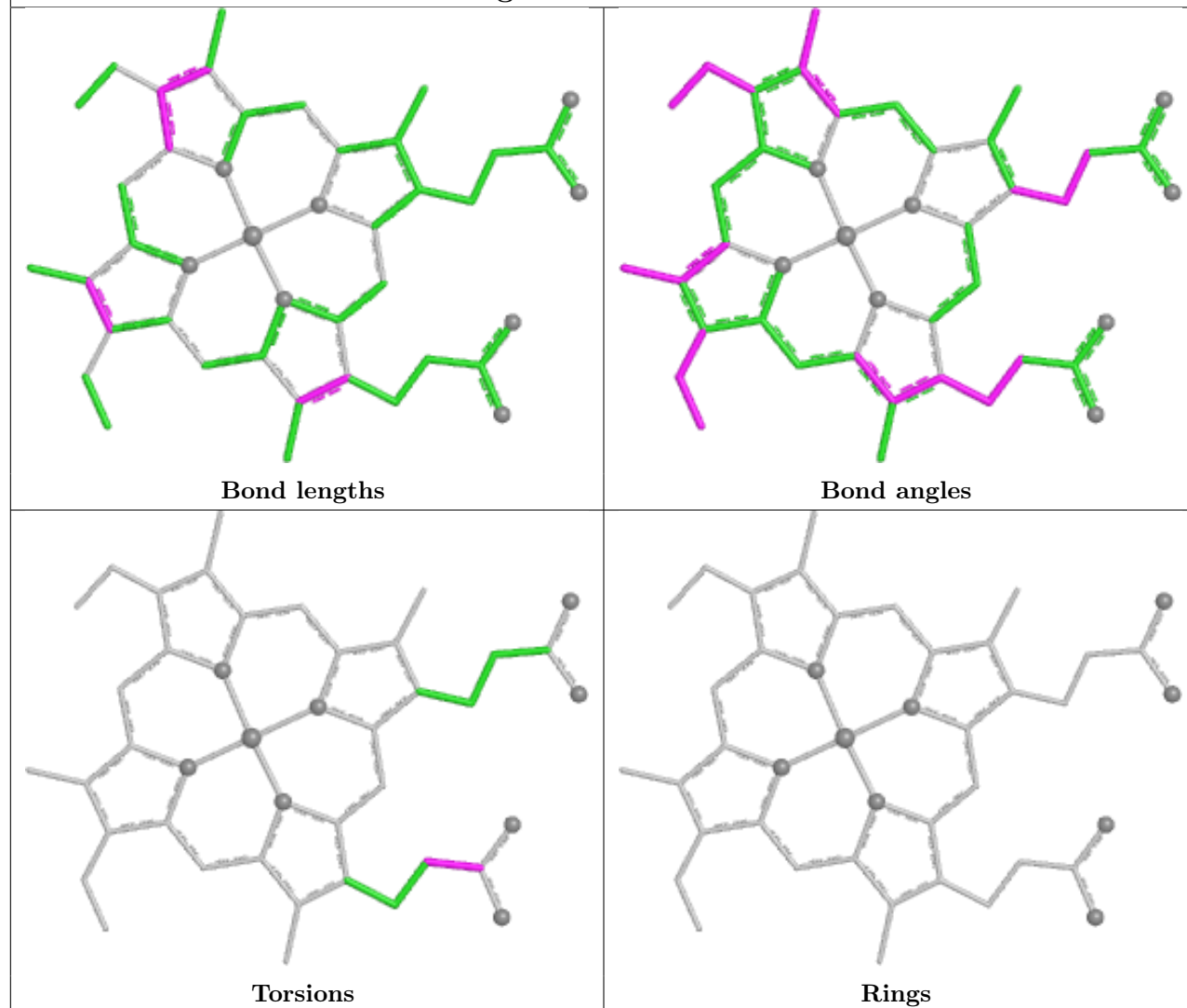
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings



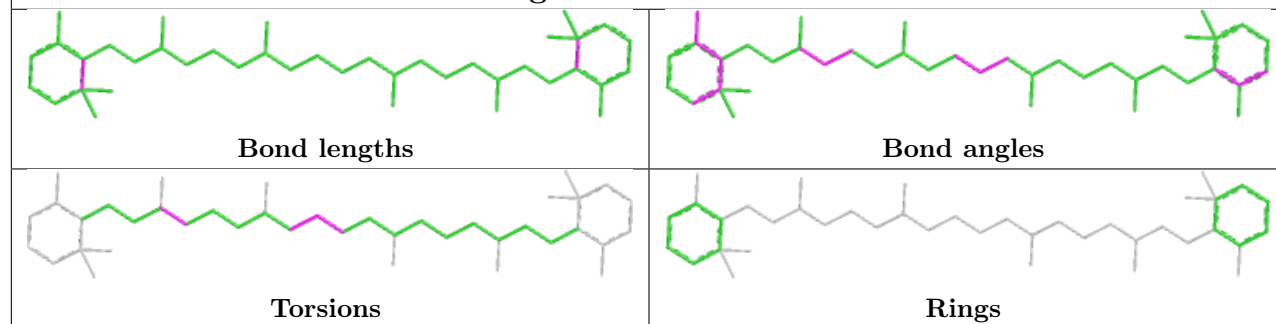
Ligand CLA d 404			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand PL9 D 407			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

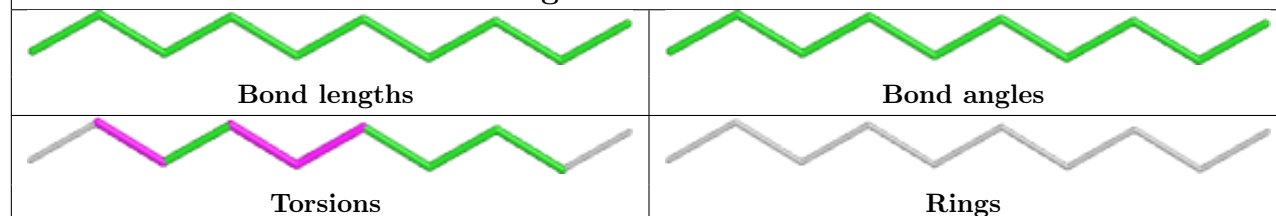
Ligand HEC v 201

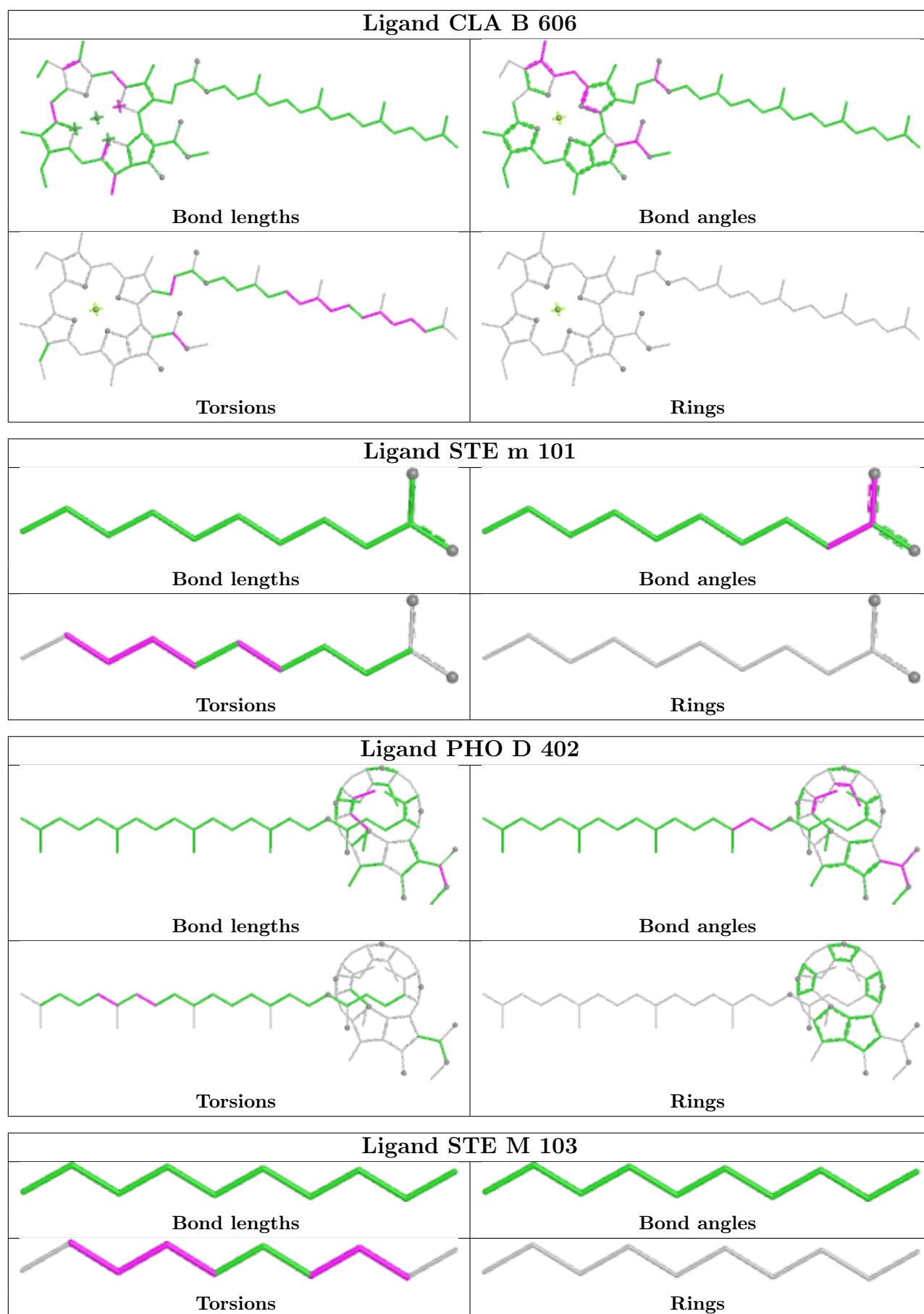


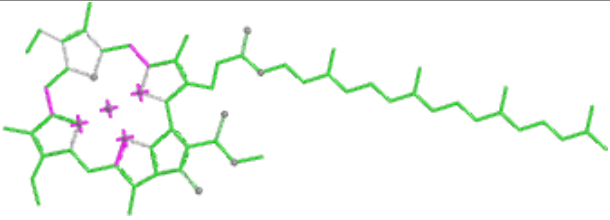
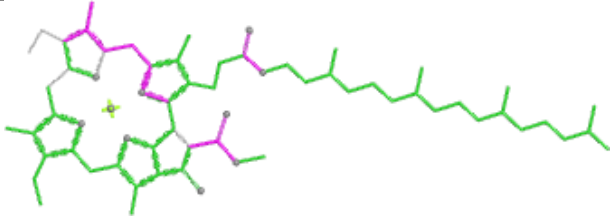
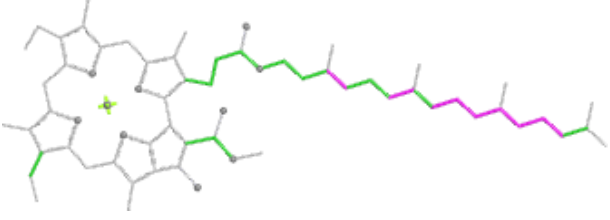
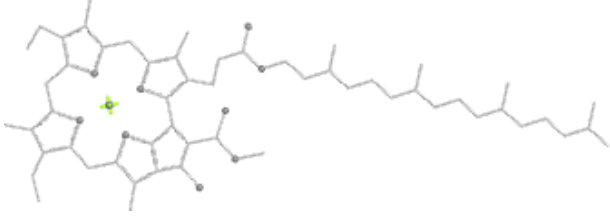
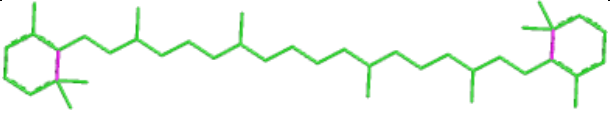

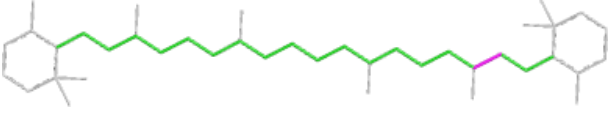
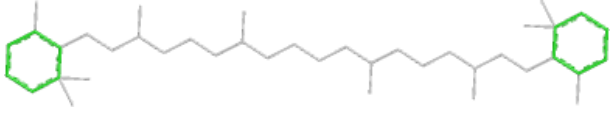
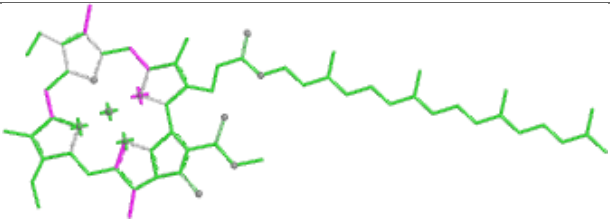
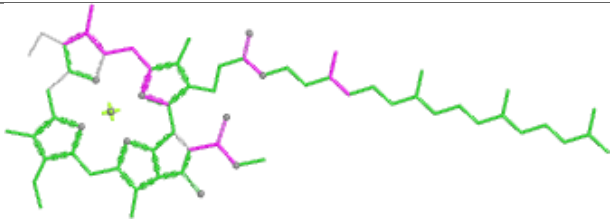
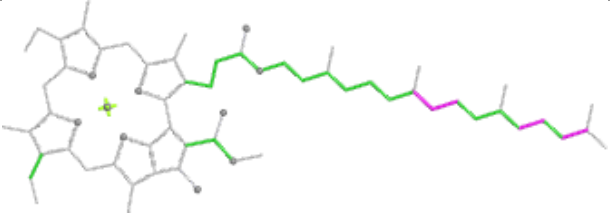
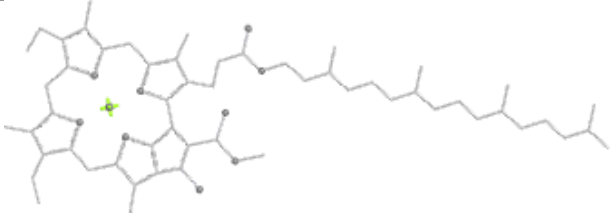
Ligand BCR K 101

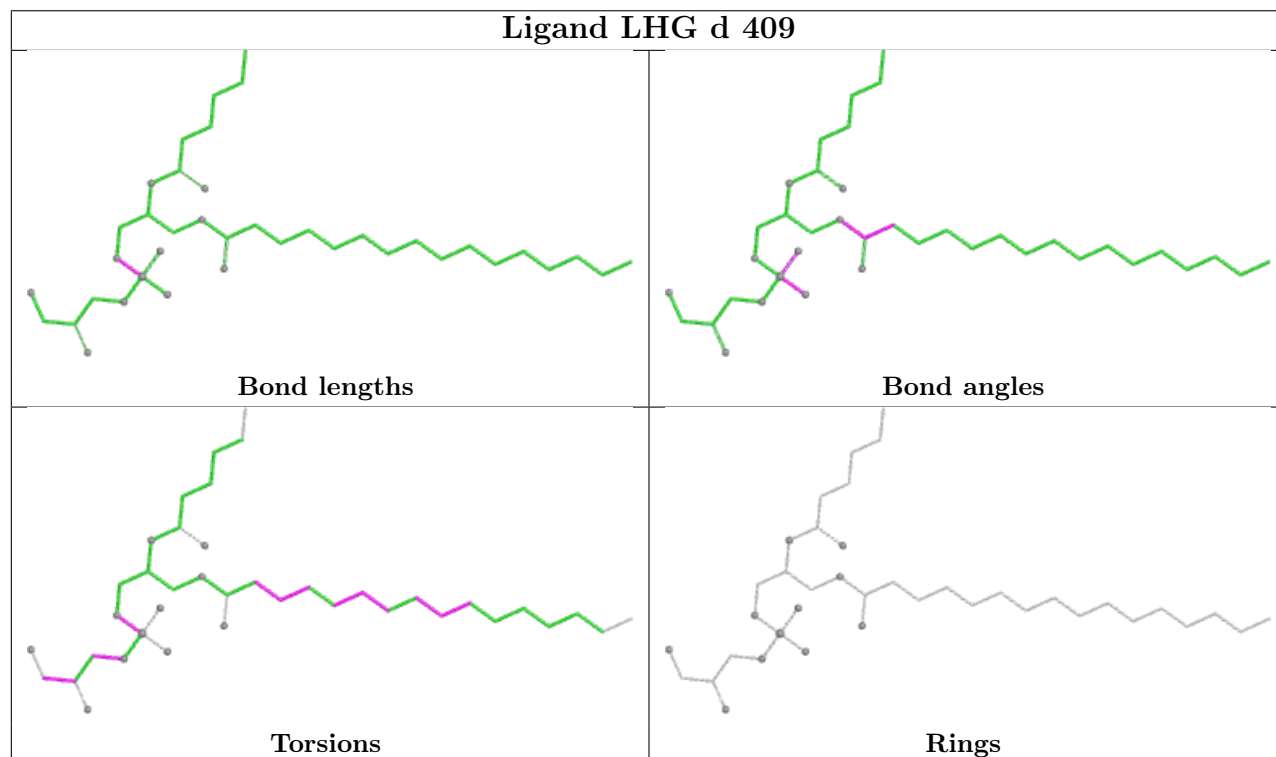
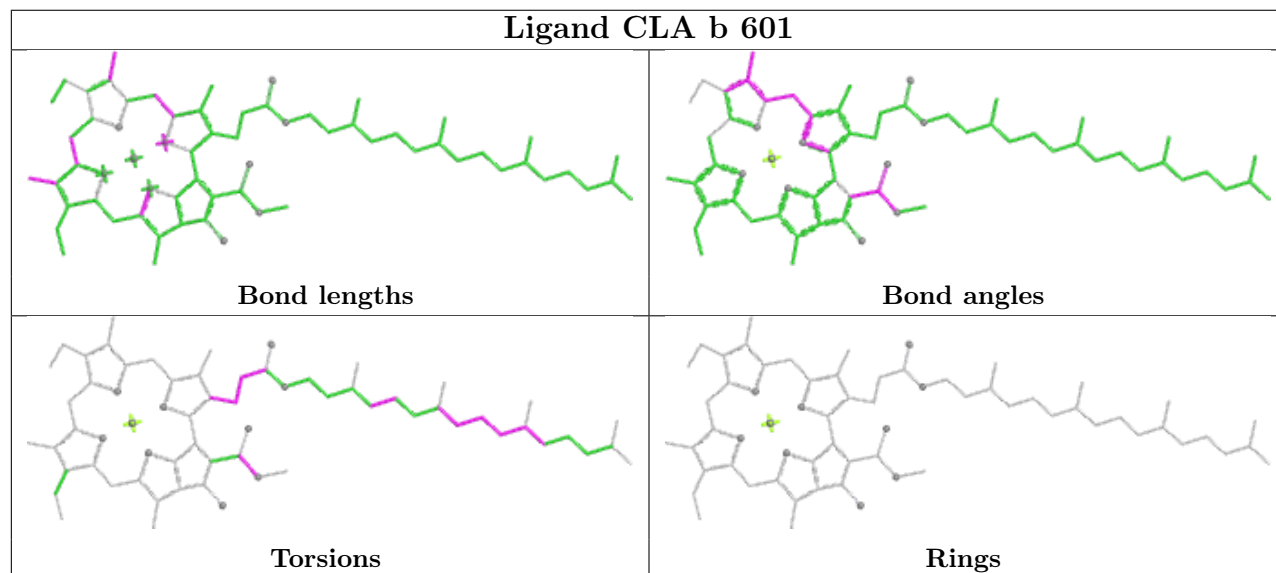
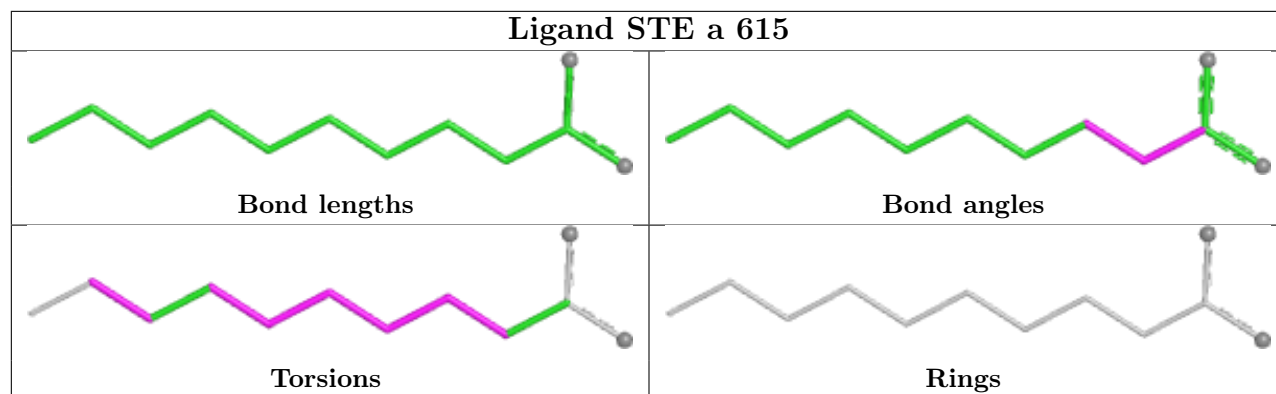


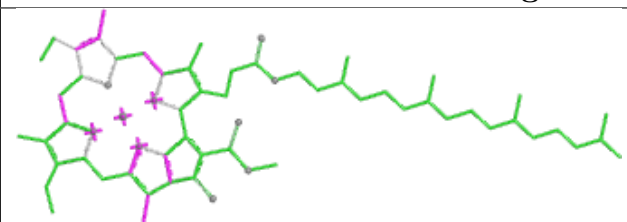
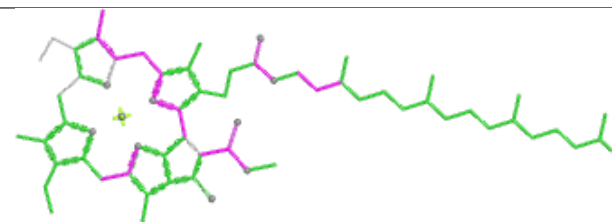
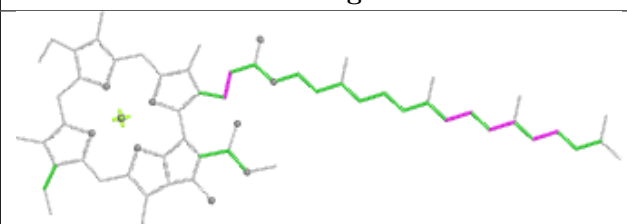
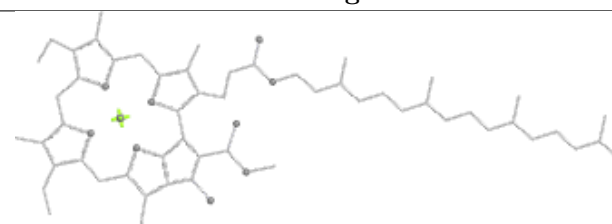
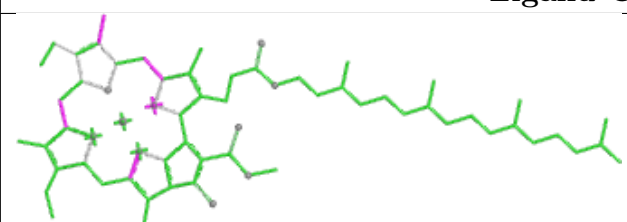
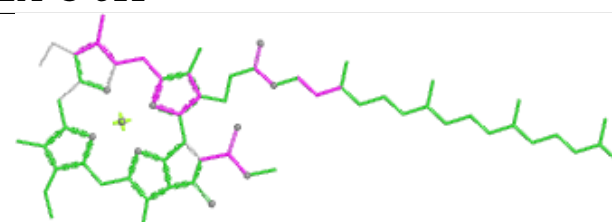
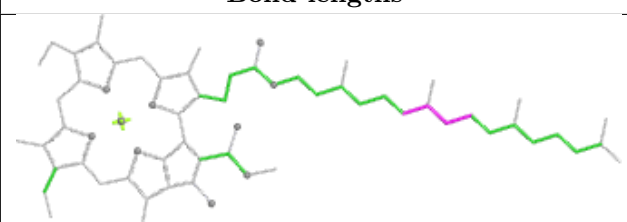
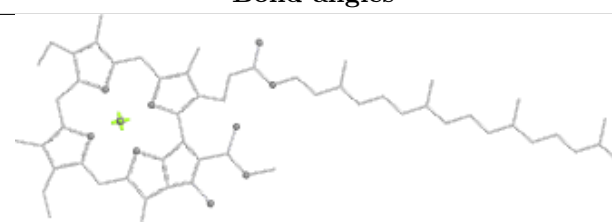
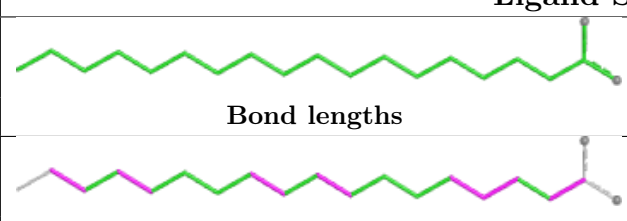
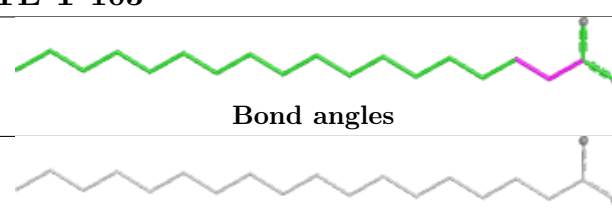

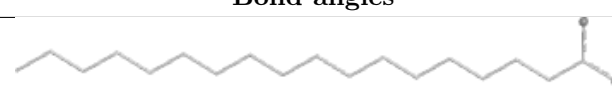
Ligand STE t 103

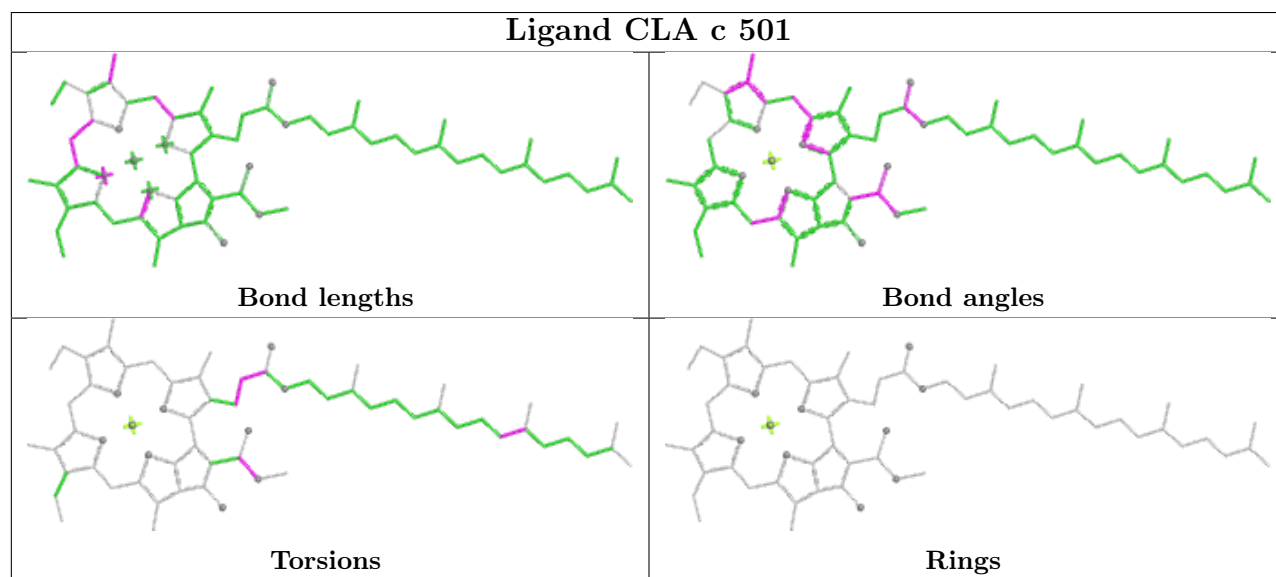
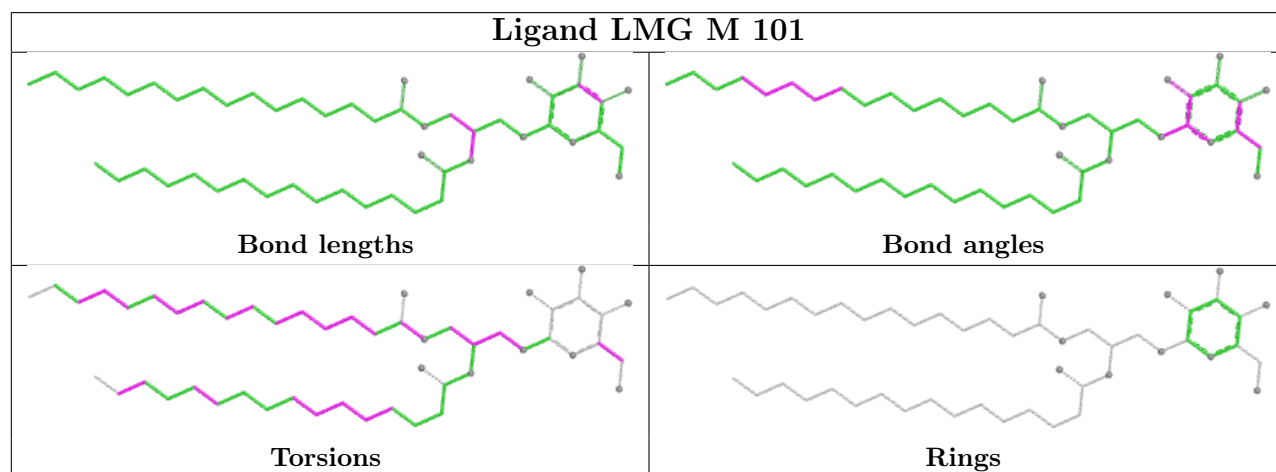
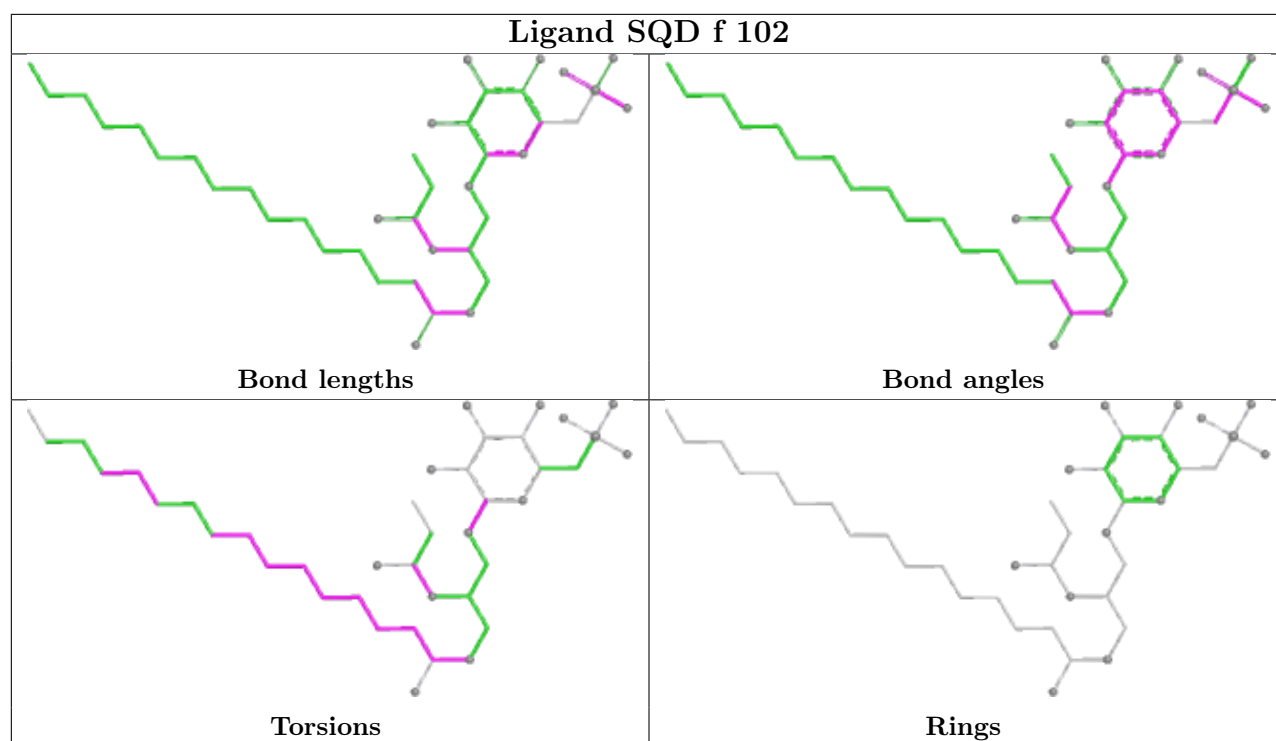


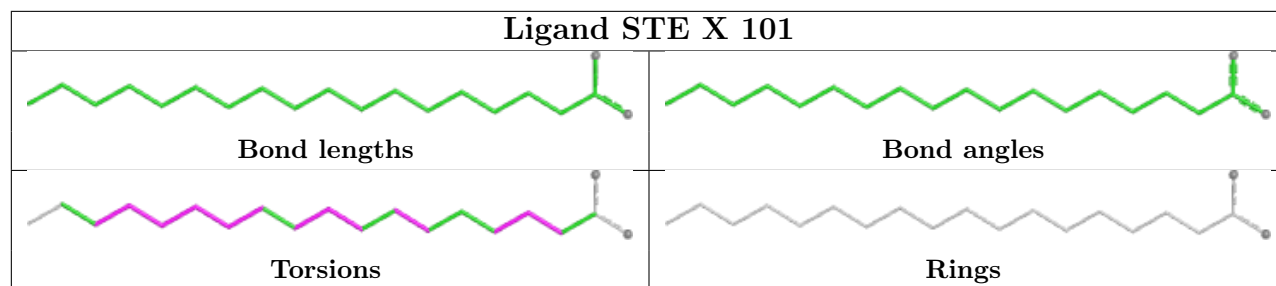


Ligand CLA C 506	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 619	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA B 603	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand STE T 103	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.81	0 100 100	11, 28, 45, 75	64 (19%)
1	a	334/344 (97%)	-0.74	0 100 100	11, 29, 54, 72	64 (19%)
2	B	505/510 (99%)	-0.66	0 100 100	17, 32, 57, 88	4 (0%)
2	b	505/510 (99%)	-0.57	1 (0%) 92 91	25, 35, 67, 99	0
3	C	442/461 (95%)	-0.70	0 100 100	13, 34, 50, 69	11 (2%)
3	c	451/461 (97%)	-0.56	0 100 100	13, 38, 57, 93	12 (2%)
4	D	341/352 (96%)	-0.84	0 100 100	14, 29, 44, 72	2 (0%)
4	d	341/352 (96%)	-0.72	0 100 100	14, 33, 55, 79	3 (0%)
5	E	82/84 (97%)	-0.15	0 100 100	31, 47, 66, 79	1 (1%)
5	e	82/84 (97%)	0.01	0 100 100	39, 54, 73, 84	0
6	F	34/45 (75%)	-0.36	0 100 100	34, 42, 57, 87	0
6	f	34/45 (75%)	-0.21	0 100 100	39, 48, 76, 83	0
7	H	65/66 (98%)	-0.40	0 100 100	32, 39, 54, 68	0
7	h	63/66 (95%)	-0.21	0 100 100	38, 49, 58, 61	0
8	I	35/38 (92%)	-0.52	0 100 100	33, 39, 62, 81	0
8	i	35/38 (92%)	-0.48	0 100 100	32, 39, 68, 86	0
9	J	36/40 (90%)	-0.35	0 100 100	32, 46, 70, 78	0
9	j	36/40 (90%)	-0.23	0 100 100	36, 51, 83, 93	0
10	K	37/46 (80%)	-0.44	0 100 100	38, 46, 61, 67	0
10	k	37/46 (80%)	-0.21	0 100 100	44, 52, 66, 74	0
11	L	37/37 (100%)	-0.68	0 100 100	25, 29, 59, 67	0
11	l	36/37 (97%)	-0.69	0 100 100	26, 29, 61, 80	0
12	M	32/36 (88%)	-0.69	0 100 100	27, 32, 57, 67	0
12	m	31/36 (86%)	-0.63	0 100 100	29, 34, 48, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.44	4 (1%) 70 69	26, 40, 75, 127	1 (0%)
13	o	244/272 (89%)	-0.44	2 (0%) 82 82	26, 40, 76, 115	0
14	T	29/32 (90%)	-0.73	1 (3%) 48 46	27, 30, 56, 71	0
14	t	29/32 (90%)	-0.69	0 100 100	26, 32, 68, 81	0
15	U	97/134 (72%)	-0.53	0 100 100	32, 41, 65, 91	0
15	u	97/134 (72%)	-0.53	1 (1%) 79 78	30, 38, 54, 83	0
16	V	137/163 (84%)	-0.59	0 100 100	29, 38, 52, 71	0
16	v	137/163 (84%)	-0.43	0 100 100	34, 45, 63, 79	0
17	Y	27/46 (58%)	0.42	1 (3%) 45 43	49, 64, 79, 87	0
17	y	30/46 (65%)	0.16	0 100 100	56, 66, 76, 90	0
18	X	38/41 (92%)	-0.27	0 100 100	40, 48, 64, 71	0
18	x	39/41 (95%)	0.06	1 (2%) 57 55	47, 59, 79, 91	0
19	Z	62/62 (100%)	0.40	2 (3%) 50 48	48, 62, 100, 113	0
19	z	62/62 (100%)	0.22	1 (1%) 70 69	55, 64, 104, 112	0
20	R	34/41 (82%)	0.45	1 (2%) 54 52	56, 65, 78, 79	0
20	r	31/41 (75%)	0.91	2 (6%) 26 24	67, 81, 97, 101	0
All	All	5302/5700 (93%)	-0.54	17 (0%) 90 89	11, 36, 68, 127	162 (3%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	35	LEU	4.1
18	x	37	VAL	3.2
19	Z	62	VAL	3.2
13	o	58	ASN	2.9
20	r	31	VAL	2.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.92	0.07	31,38,52,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	FME	M	1	10/11	0.93	0.09	36,46,59,62	0
14	FME	T	1	10/11	0.94	0.08	30,36,56,60	0
8	FME	I	1	10/11	0.95	0.06	38,44,50,50	0
12	FME	m	1	10/11	0.97	0.06	35,44,61,62	0
8	FME	i	1	10/11	0.98	0.06	37,45,47,48	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
32	STE	H	103	18/20	0.68	0.13	55,64,72,72	0
32	STE	a	615	12/20	0.75	0.10	51,57,70,73	0
32	STE	T	103	20/20	0.76	0.12	42,52,69,75	0
28	LMG	b	624	55/55	0.76	0.14	50,63,76,77	0
32	STE	b	625	16/20	0.77	0.11	49,56,68,71	0
29	LHG	e	101	42/49	0.78	0.12	56,75,91,95	0
32	STE	m	101	12/20	0.78	0.13	51,58,64,67	0
28	LMG	d	410	23/55	0.79	0.12	47,61,65,68	0
32	STE	c	521	12/20	0.79	0.12	57,66,70,71	0
29	LHG	E	101	49/49	0.79	0.12	40,69,89,97	0
32	STE	B	625	18/20	0.80	0.12	42,52,76,82	0
32	STE	B	627	16/20	0.80	0.12	46,56,68,68	0
28	LMG	c	520	48/55	0.80	0.12	52,68,80,83	0
31	DGD	o	301	44/66	0.80	0.12	36,50,67,70	0
32	STE	b	626	10/20	0.81	0.11	48,53,60,60	0
32	STE	T	102	15/20	0.81	0.13	43,50,65,66	0
32	STE	E	102	12/20	0.81	0.11	57,67,81,82	0
27	PL9	A	610	55/55	0.82	0.12	35,57,67,71	0
32	STE	B	626	12/20	0.82	0.10	50,54,67,69	0
31	DGD	A	616	66/66	0.82	0.10	45,55,63,68	0
28	LMG	D	411	33/55	0.82	0.10	38,51,70,71	0
32	STE	X	101	20/20	0.83	0.14	36,48,61,65	0
30	SQD	a	614	36/54	0.83	0.10	38,54,64,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	b	601	65/65	0.83	0.10	45,61,78,84	0
30	SQD	f	102	41/54	0.84	0.11	58,72,82,85	0
32	STE	J	101	12/20	0.84	0.10	46,52,61,63	0
30	SQD	A	615	39/54	0.84	0.10	41,51,74,77	0
27	PL9	a	611	55/55	0.84	0.12	39,60,70,76	0
32	STE	d	413	20/20	0.84	0.12	43,50,57,58	0
32	STE	B	620	17/20	0.84	0.11	36,47,60,64	0
32	STE	t	103	10/20	0.84	0.10	44,53,60,61	0
30	SQD	B	623	54/54	0.85	0.10	36,56,72,80	0
28	LMG	c	518	37/55	0.85	0.10	43,57,68,69	0
32	STE	I	101	15/20	0.85	0.10	42,50,56,56	0
28	LMG	A	612	48/55	0.85	0.09	41,54,62,65	0
32	STE	b	621	16/20	0.85	0.11	34,45,55,61	0
32	STE	t	102	14/20	0.85	0.09	40,44,57,58	0
32	STE	b	623	20/20	0.85	0.11	37,49,67,69	0
28	LMG	c	522	49/55	0.86	0.09	40,50,70,76	0
30	SQD	b	620	49/54	0.86	0.09	41,50,73,78	0
28	LMG	b	622	51/55	0.87	0.09	33,49,60,63	0
32	STE	C	519	12/20	0.87	0.10	39,44,58,59	0
32	STE	C	520	12/20	0.87	0.09	43,49,53,54	0
28	LMG	B	621	28/55	0.87	0.10	38,45,59,69	0
26	BCR	k	102	40/40	0.87	0.10	43,52,58,60	0
25	CLA	B	601	65/65	0.88	0.10	38,51,72,80	0
32	STE	j	101	12/20	0.88	0.09	46,52,58,58	0
32	STE	c	519	20/20	0.88	0.09	40,49,80,81	0
32	STE	B	624	12/20	0.88	0.11	44,53,58,60	0
32	STE	d	412	17/20	0.88	0.10	42,47,61,64	0
28	LMG	M	101	51/55	0.89	0.08	33,47,59,61	0
32	STE	M	103	10/20	0.89	0.09	40,43,49,51	0
28	LMG	C	518	48/55	0.89	0.09	38,59,70,72	0
26	BCR	x	101	40/40	0.90	0.09	38,50,63,64	0
26	BCR	K	102	40/40	0.90	0.09	38,44,53,55	0
32	STE	C	521	16/20	0.90	0.08	36,44,51,58	0
26	BCR	D	406	40/40	0.91	0.08	32,40,68,75	0
32	STE	l	102	18/20	0.91	0.09	35,45,60,62	0
30	SQD	a	613	54/54	0.91	0.10	37,54,73,77	0
25	CLA	C	513	65/65	0.91	0.08	41,51,72,76	0
26	BCR	d	405	40/40	0.91	0.08	38,44,70,72	0
31	DGD	c	516	62/66	0.92	0.07	34,45,68,72	0
26	BCR	k	101	40/40	0.92	0.08	42,52,57,60	0
32	STE	M	102	15/20	0.92	0.07	36,44,54,63	0
26	BCR	H	101	40/40	0.92	0.07	34,40,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	SQD	D	409	36/54	0.92	0.09	43,60,66,69	0
26	BCR	K	101	40/40	0.92	0.08	41,48,54,56	0
31	DGD	H	102	62/66	0.92	0.08	29,40,46,53	0
31	DGD	C	516	62/66	0.93	0.07	32,42,75,84	0
25	CLA	c	512	65/65	0.93	0.08	39,50,70,74	0
26	BCR	b	618	40/40	0.93	0.06	25,34,45,50	0
31	DGD	h	101	62/66	0.93	0.08	35,45,52,57	0
26	BCR	A	609	40/40	0.93	0.06	26,31,37,41	0
29	LHG	d	407	49/49	0.93	0.07	33,44,58,66	0
28	LMG	D	408	51/55	0.93	0.09	28,42,67,71	0
30	SQD	A	614	52/54	0.93	0.09	33,47,67,69	0
26	BCR	B	619	40/40	0.93	0.07	29,39,48,52	0
33	BCT	a	606	4/4	0.93	0.08	32,35,39,44	0
31	DGD	C	517	62/66	0.94	0.07	26,38,62,70	0
26	BCR	B	618	40/40	0.94	0.06	24,34,44,46	0
26	BCR	k	103	40/40	0.94	0.08	41,47,55,58	0
31	DGD	c	517	62/66	0.94	0.07	29,44,64,76	0
28	LMG	d	411	44/55	0.94	0.07	34,43,71,73	0
25	CLA	C	506	65/65	0.94	0.07	28,37,68,69	0
26	BCR	C	514	40/40	0.94	0.07	29,36,47,47	0
25	CLA	b	616	60/65	0.94	0.08	29,37,77,79	0
25	CLA	c	506	65/65	0.94	0.07	32,40,70,76	0
25	CLA	c	508	64/65	0.94	0.07	32,38,74,85	0
25	CLA	C	512	65/65	0.94	0.08	35,44,66,69	0
26	BCR	a	610	40/40	0.94	0.06	22,30,38,41	0
26	BCR	b	617	40/40	0.94	0.06	29,36,44,44	0
25	CLA	c	513	65/65	0.94	0.08	38,53,79,85	0
26	BCR	b	619	40/40	0.94	0.06	30,40,53,56	0
26	BCR	c	514	40/40	0.94	0.06	31,40,48,51	0
25	CLA	B	606	65/65	0.94	0.07	25,33,58,63	0
31	DGD	C	515	62/66	0.94	0.07	25,34,63,67	0
26	BCR	B	617	40/40	0.94	0.06	27,33,42,44	0
34	PHO	d	402	64/64	0.94	0.06	23,35,40,43	0
26	BCR	T	101	40/40	0.95	0.05	28,34,45,47	0
26	BCR	Z	101	40/40	0.95	0.07	34,42,53,54	0
25	CLA	C	508	65/65	0.95	0.06	28,34,75,82	0
29	LHG	A	613	47/49	0.95	0.08	27,39,64,68	0
29	LHG	B	622	49/49	0.95	0.07	30,39,53,55	0
25	CLA	c	503	65/65	0.95	0.06	31,39,43,50	0
25	CLA	c	504	60/65	0.95	0.06	29,38,70,72	0
25	CLA	C	510	65/65	0.95	0.06	27,35,46,51	0
29	LHG	l	101	49/49	0.95	0.06	32,39,46,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	c	507	65/65	0.95	0.07	29,37,46,49	0
25	CLA	C	511	65/65	0.95	0.07	30,41,54,56	0
25	CLA	c	509	65/65	0.95	0.07	31,38,52,55	0
25	CLA	c	510	65/65	0.95	0.07	32,40,51,53	0
25	CLA	c	511	65/65	0.95	0.07	36,47,58,62	0
26	BCR	t	101	40/40	0.95	0.05	25,36,46,48	0
25	CLA	C	501	65/65	0.95	0.06	26,31,43,47	0
25	CLA	C	503	65/65	0.95	0.06	30,36,40,48	0
25	CLA	d	403	65/65	0.95	0.07	22,29,47,56	0
27	PL9	d	406	55/55	0.95	0.06	25,31,36,38	0
25	CLA	d	404	65/65	0.95	0.08	30,38,76,78	0
25	CLA	a	607	65/65	0.95	0.06	21,27,37,45	0
25	CLA	a	608	65/65	0.95	0.07	27,34,72,79	0
31	DGD	c	515	62/66	0.95	0.07	22,35,58,66	0
25	CLA	B	609	65/65	0.95	0.06	27,34,47,54	0
25	CLA	b	602	65/65	0.95	0.07	29,36,49,55	0
25	CLA	b	606	65/65	0.95	0.07	29,35,61,64	0
25	CLA	b	608	65/65	0.95	0.06	27,36,53,59	0
25	CLA	b	609	65/65	0.95	0.07	29,38,56,66	0
33	BCT	D	401	4/4	0.95	0.06	29,32,34,35	0
25	CLA	b	610	65/65	0.95	0.07	27,34,41,47	0
25	CLA	b	614	65/65	0.95	0.06	26,35,62,66	0
29	LHG	L	101	49/49	0.96	0.06	28,35,46,55	0
25	CLA	D	405	65/65	0.96	0.07	27,33,74,84	0
29	LHG	d	408	49/49	0.96	0.06	30,37,48,50	0
29	LHG	d	409	39/49	0.96	0.07	33,38,53,55	0
25	CLA	B	616	60/65	0.96	0.07	25,33,69,74	0
25	CLA	B	602	65/65	0.96	0.06	24,32,47,50	0
25	CLA	a	609	65/65	0.96	0.08	22,28,62,68	0
25	CLA	a	612	65/65	0.96	0.05	22,27,38,44	0
25	CLA	C	502	65/65	0.96	0.06	26,32,44,50	0
25	CLA	B	604	65/65	0.96	0.06	22,28,57,59	0
27	PL9	D	407	55/55	0.96	0.05	22,28,37,39	0
25	CLA	b	603	65/65	0.96	0.06	26,31,52,61	0
25	CLA	C	504	59/65	0.96	0.06	28,34,67,70	0
25	CLA	b	607	65/65	0.96	0.06	23,30,54,57	0
25	CLA	C	505	65/65	0.96	0.06	26,35,56,62	0
25	CLA	A	607	65/65	0.96	0.06	22,28,73,79	0
25	CLA	B	607	65/65	0.96	0.06	21,28,49,55	0
25	CLA	b	611	65/65	0.96	0.05	25,30,43,50	0
25	CLA	b	612	65/65	0.96	0.06	23,30,38,45	0
25	CLA	b	613	65/65	0.96	0.06	19,28,60,65	0

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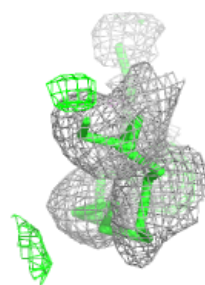
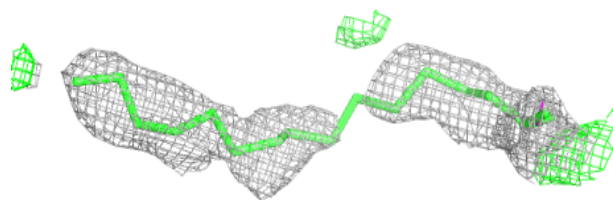
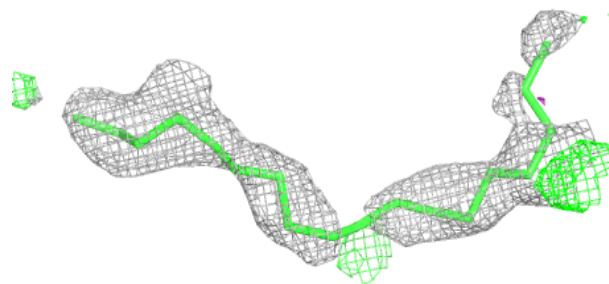
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CLA	C	509	65/65	0.96	0.07	24,33,50,54	0
25	CLA	b	615	65/65	0.96	0.06	28,36,50,57	0
25	CLA	A	606	65/65	0.96	0.05	18,25,38,47	0
25	CLA	c	501	65/65	0.96	0.06	29,35,45,52	0
25	CLA	c	502	65/65	0.96	0.06	25,35,47,51	0
25	CLA	B	610	65/65	0.96	0.06	23,29,36,39	0
25	CLA	B	613	65/65	0.96	0.06	21,26,55,61	0
25	CLA	c	505	65/65	0.96	0.06	29,35,56,65	0
34	PHO	D	402	64/64	0.96	0.05	19,26,33,37	0
34	PHO	D	403	64/64	0.96	0.05	22,30,34,37	0
25	CLA	B	614	65/65	0.96	0.06	20,32,57,62	0
25	CLA	C	507	65/65	0.97	0.06	25,34,47,50	0
25	CLA	B	605	65/65	0.97	0.05	22,27,37,39	0
25	CLA	B	603	65/65	0.97	0.06	21,27,50,56	0
25	CLA	B	611	65/65	0.97	0.05	21,27,41,47	0
25	CLA	B	612	65/65	0.97	0.06	21,27,37,42	0
25	CLA	A	611	65/65	0.97	0.05	21,25,40,46	0
25	CLA	B	608	65/65	0.97	0.05	25,30,46,53	0
25	CLA	b	604	65/65	0.97	0.06	24,29,65,75	0
25	CLA	b	605	65/65	0.97	0.05	23,30,42,45	0
25	CLA	D	404	65/65	0.97	0.05	20,24,43,50	0
29	LHG	D	410	49/49	0.97	0.06	27,34,44,48	0
34	PHO	d	401	64/64	0.97	0.05	24,28,33,36	0
25	CLA	B	615	65/65	0.97	0.05	23,32,52,60	0
35	HEM	F	101	43/43	0.97	0.08	39,44,55,61	0
35	HEM	f	101	43/43	0.97	0.08	46,52,65,78	0
25	CLA	A	608	54/65	0.98	0.05	21,26,53,57	0
24	CL	A	604	1/1	0.98	0.03	28,28,28,28	0
36	HEC	V	201	43/43	0.98	0.05	25,29,36,40	0
22	OEX	A	602[A]	10/10	0.99	0.04	21,29,33,33	10
22	OEX	a	602[A]	10/10	0.99	0.03	24,28,31,31	10
23	FE2	a	603	1/1	0.99	0.02	33,33,33,33	0
21	OEY	A	601[B]	11/11	0.99	0.03	24,27,30,30	11
24	CL	A	605	1/1	0.99	0.05	29,29,29,29	0
24	CL	a	604	1/1	0.99	0.04	30,30,30,30	0
24	CL	a	605	1/1	0.99	0.06	30,30,30,30	0
21	OEY	a	601[B]	11/11	0.99	0.03	26,29,32,32	11
36	HEC	v	201	43/43	0.99	0.05	29,33,40,44	0
23	FE2	A	603	1/1	1.00	0.01	27,27,27,27	0

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

orientation to approximate a three-dimensional view.

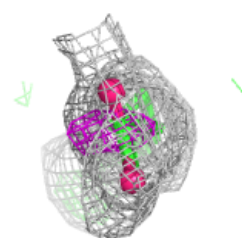
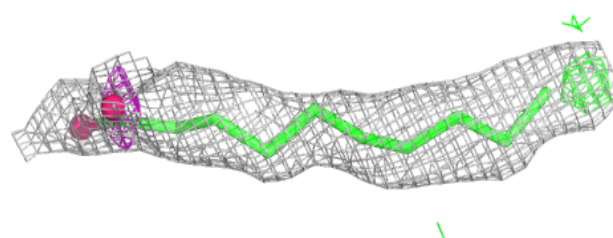
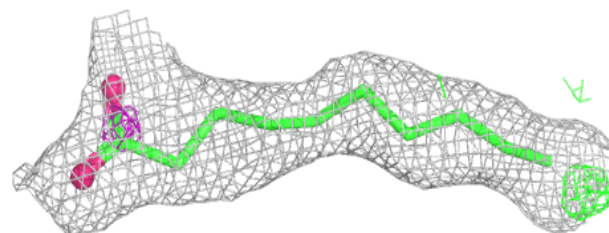
Electron density around STE H 103:

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



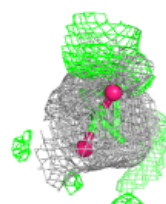
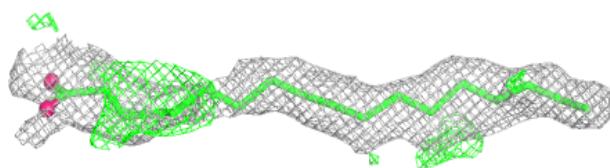
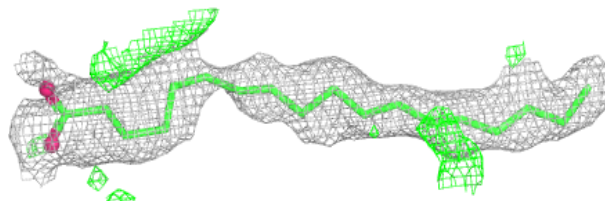
Electron density around STE a 615:

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

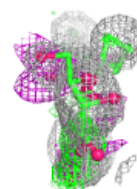
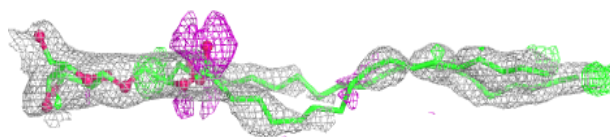
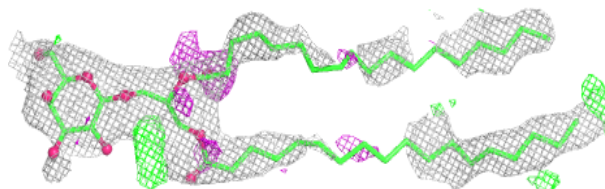


Electron density around STE T 103:

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

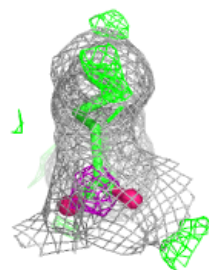
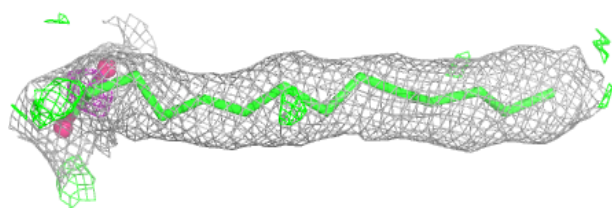
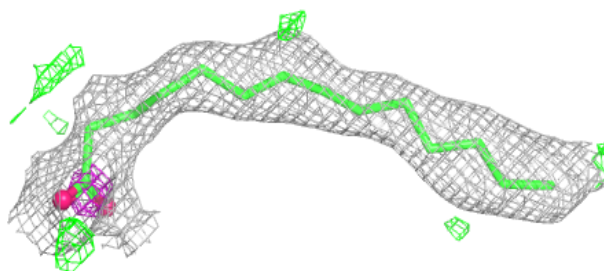
**Electron density around LMG b 624:**

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

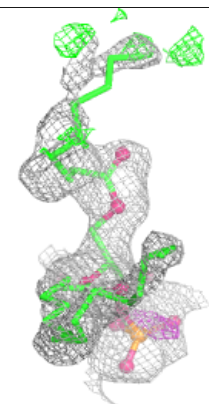
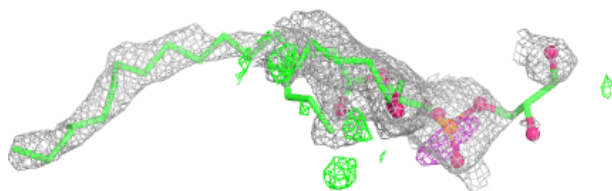
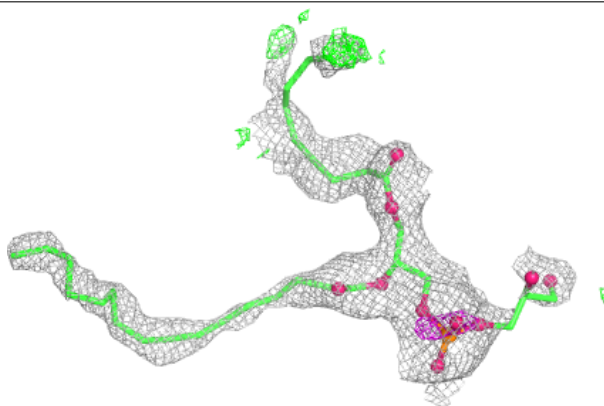


Electron density around STE b 625:

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

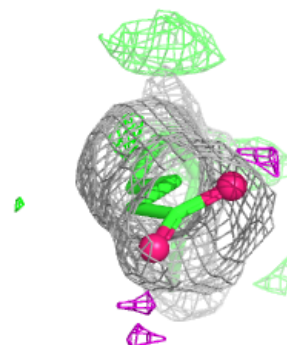
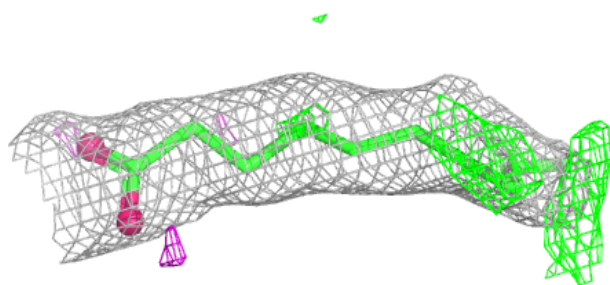
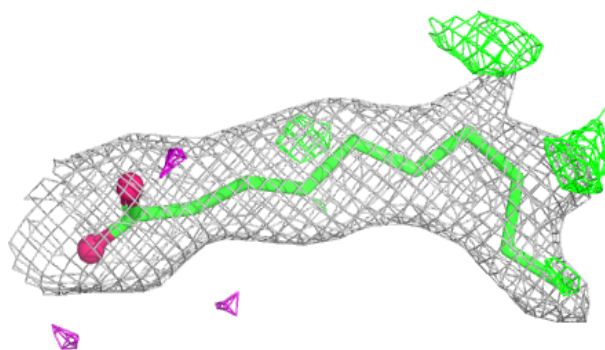
**Electron density around LHG e 101:**

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

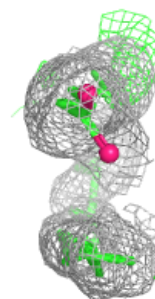
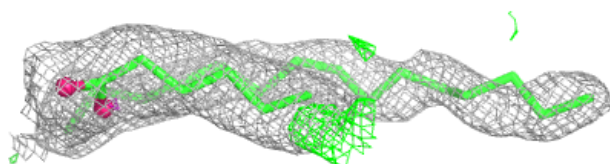
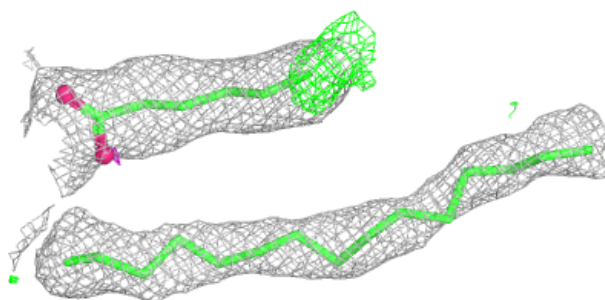


Electron density around STE m 101:

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

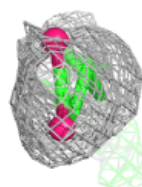
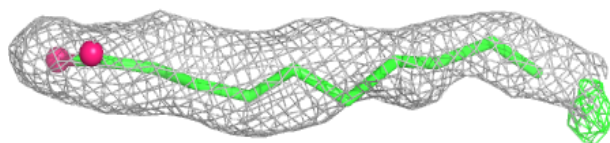
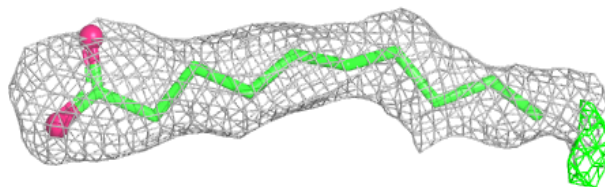
**Electron density around LMG d 410:**

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



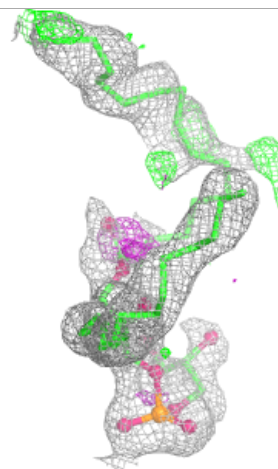
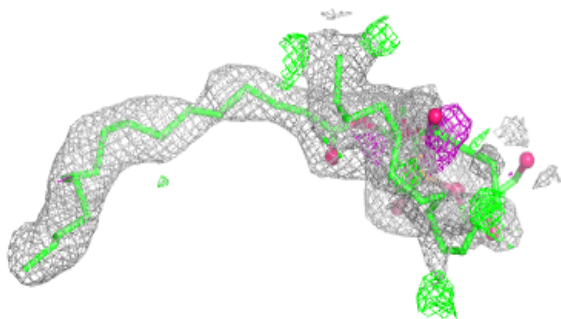
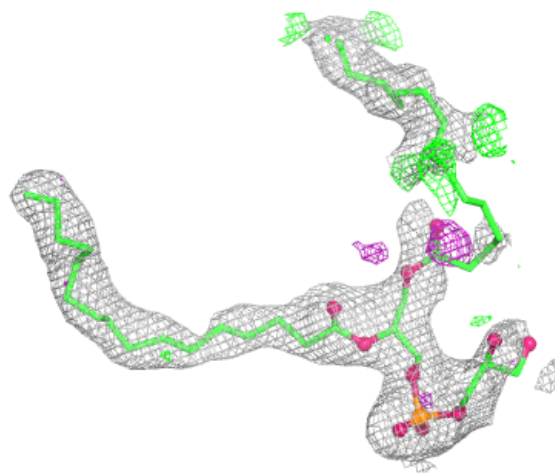
Electron density around STE c 521:

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



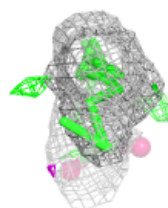
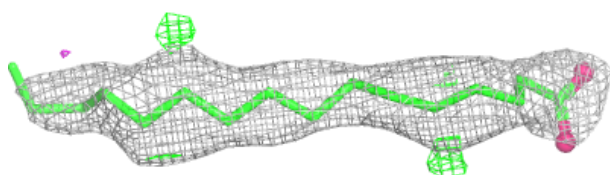
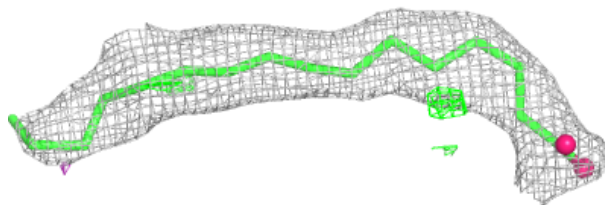
Electron density around LHG E 101:

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

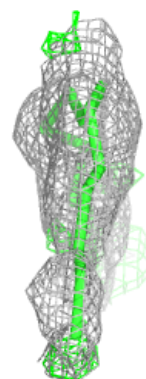
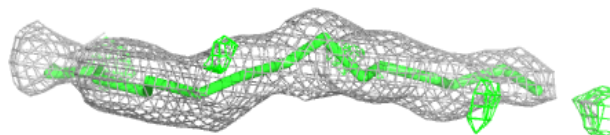


Electron density around STE B 625:

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

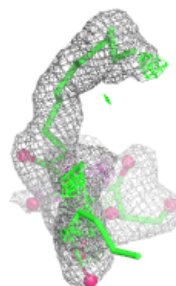
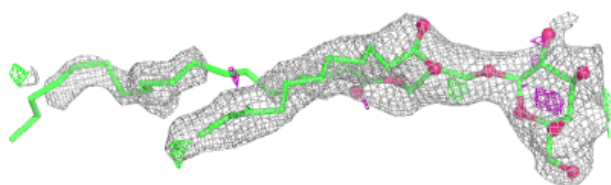
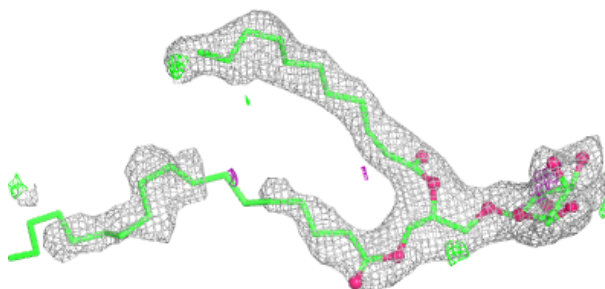
**Electron density around STE B 627:**

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

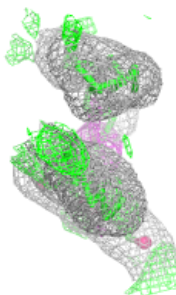
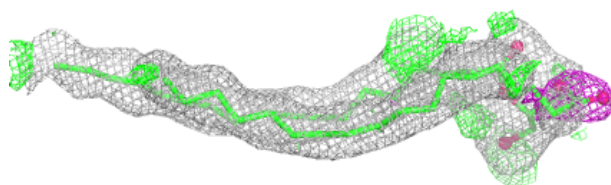
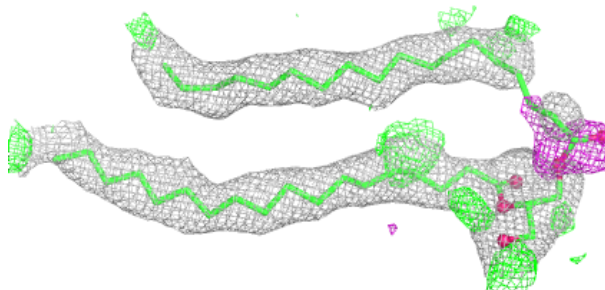


Electron density around LMG c 520:

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

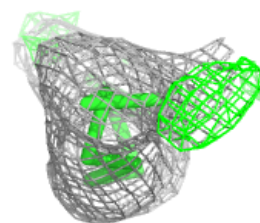
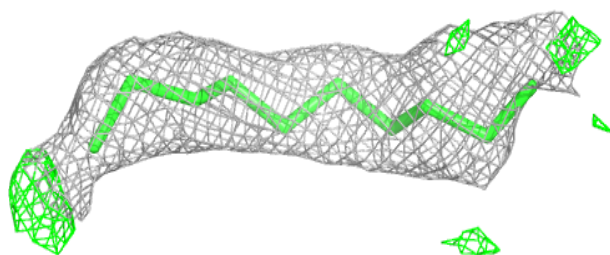
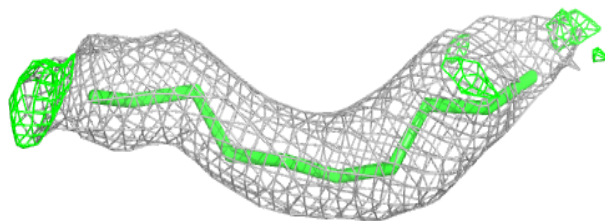
**Electron density around DGD o 301:**

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

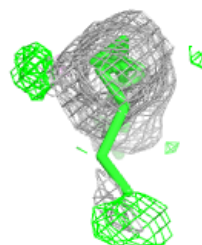
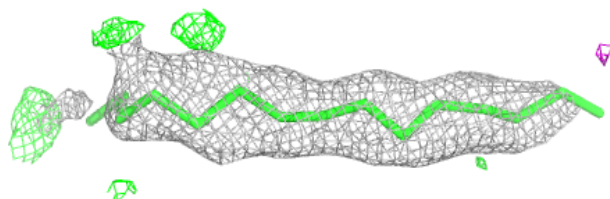
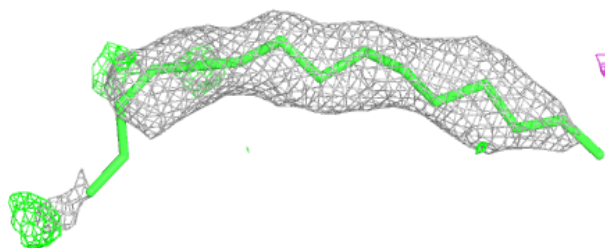


Electron density around STE b 626:

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

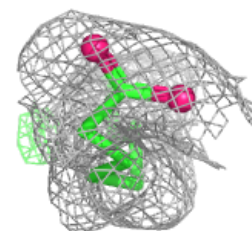
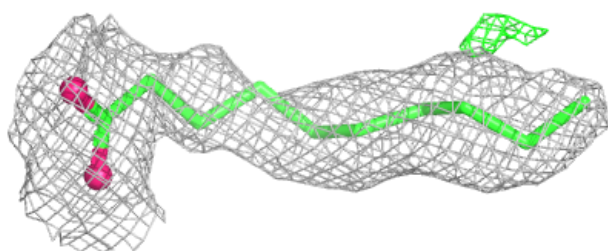
**Electron density around STE T 102:**

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

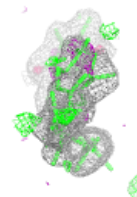
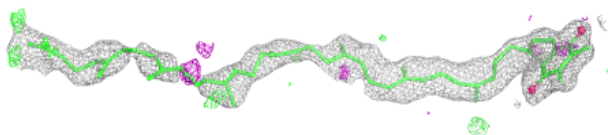
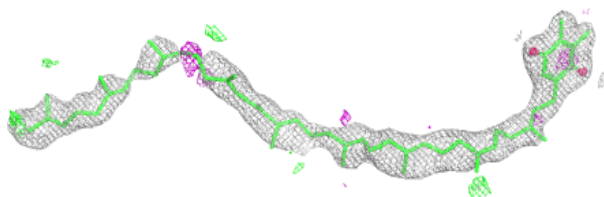


Electron density around STE E 102:

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

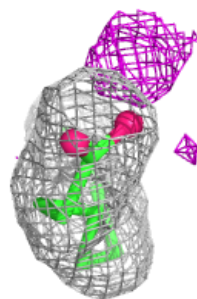
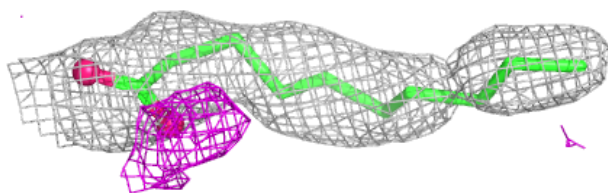
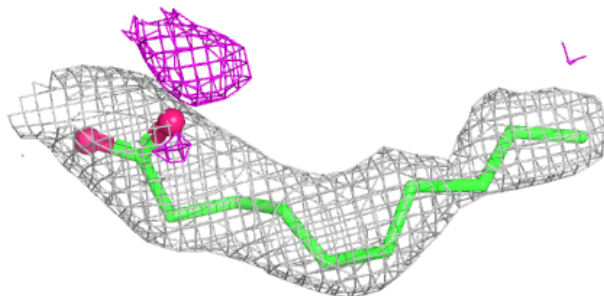
**Electron density around PL9 A 610:**

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

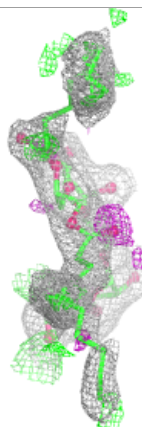
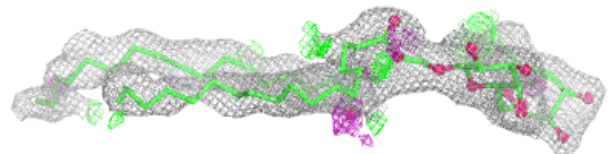
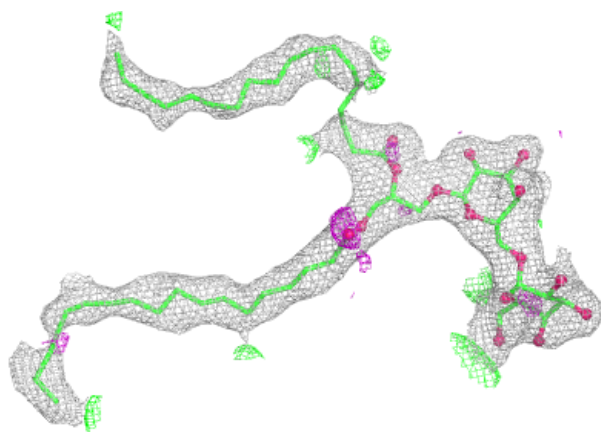


Electron density around STE B 626:

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

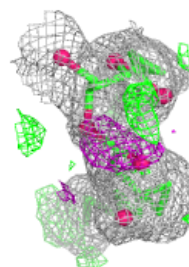
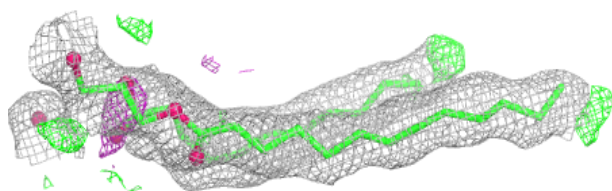
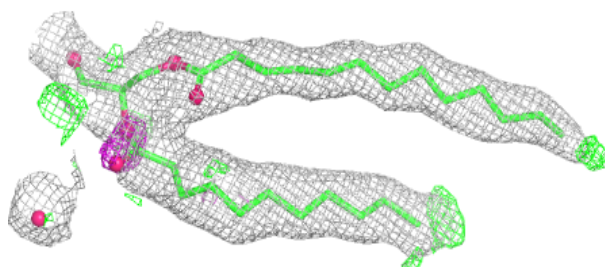
**Electron density around DGD A 616:**

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

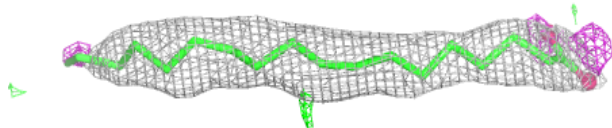
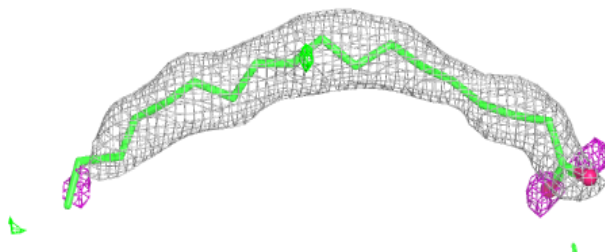


Electron density around LMG D 411:

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

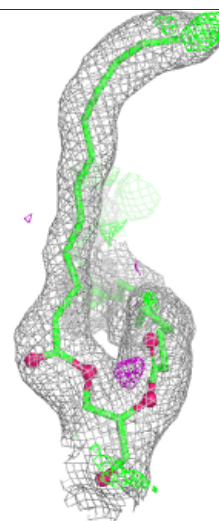
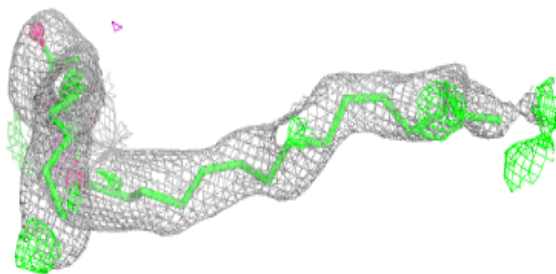
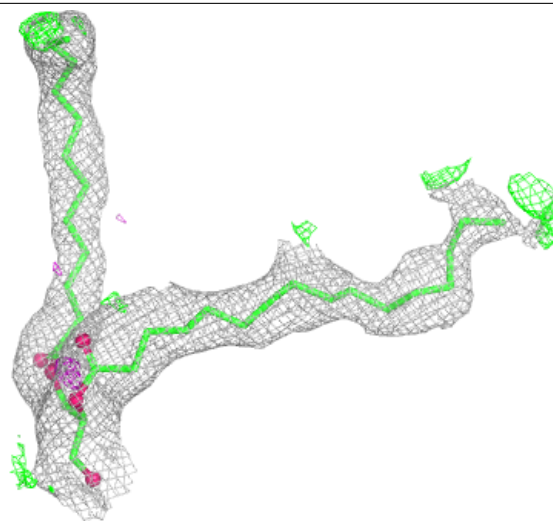
**Electron density around STE X 101:**

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



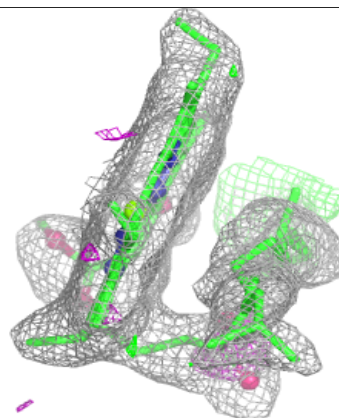
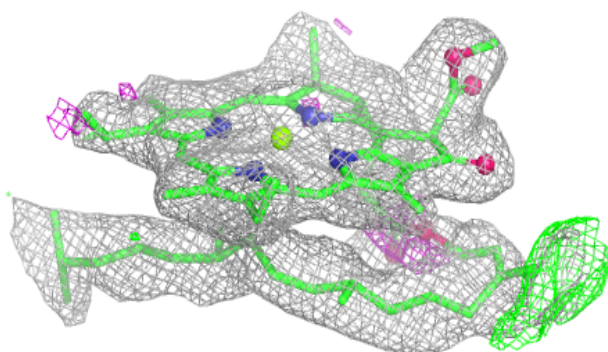
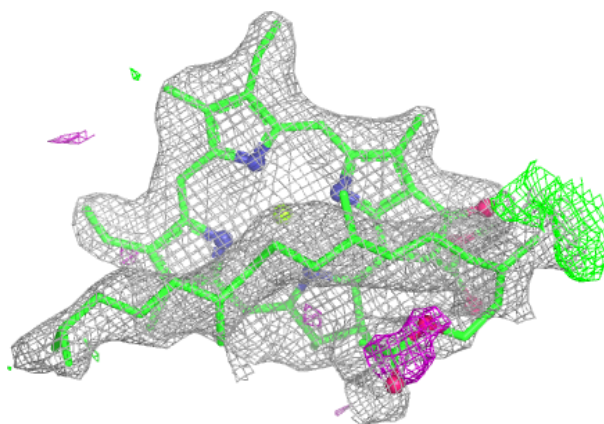
Electron density around SQD a 614:

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

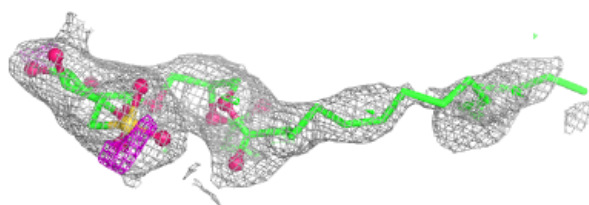
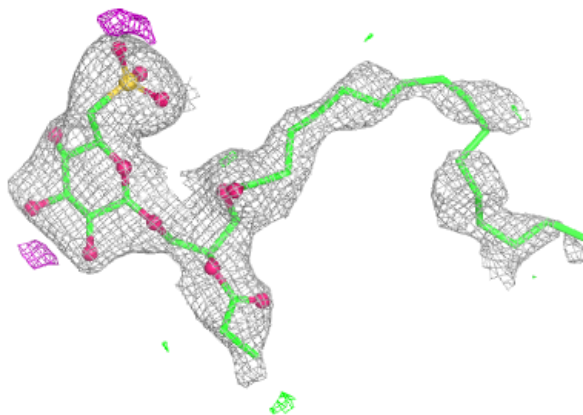


Electron density around CLA b 601:

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

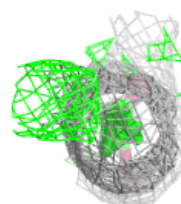
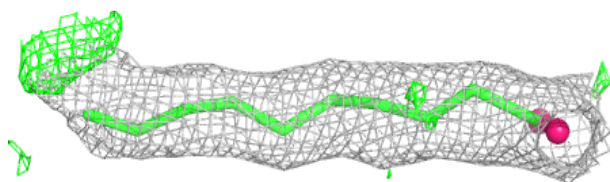
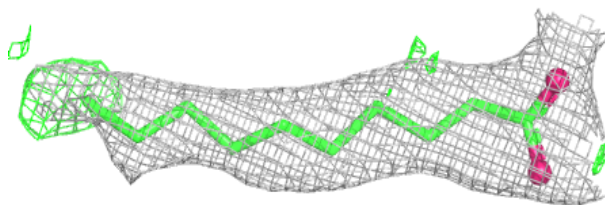
**Electron density around SQD f 102:**

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



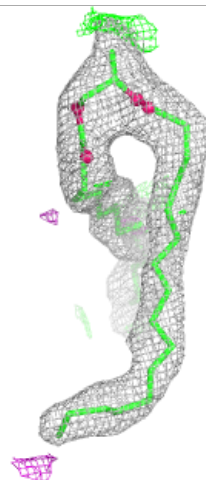
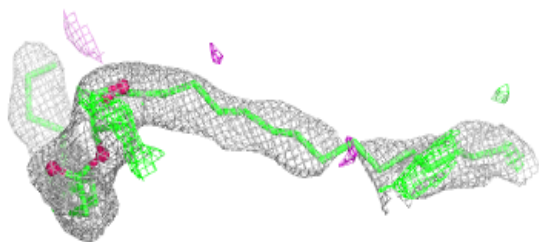
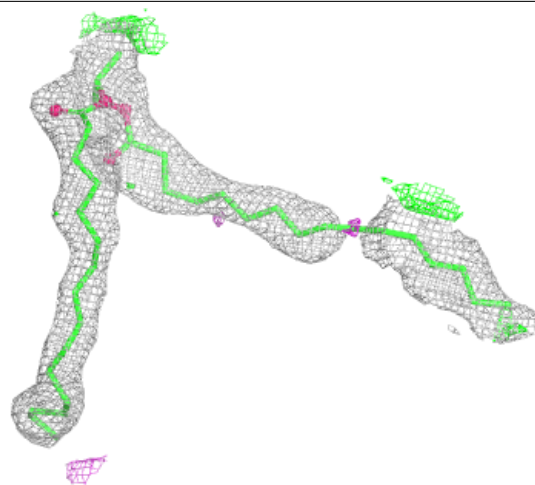
Electron density around STE J 101:

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



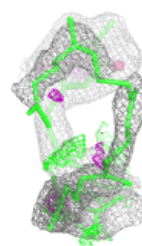
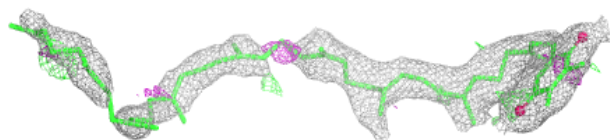
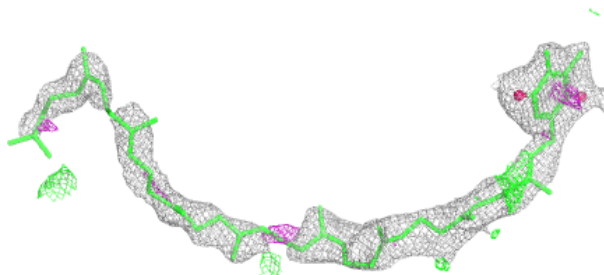
Electron density around SQD A 615:

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

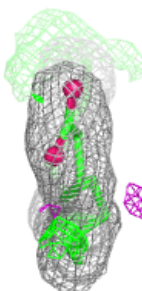
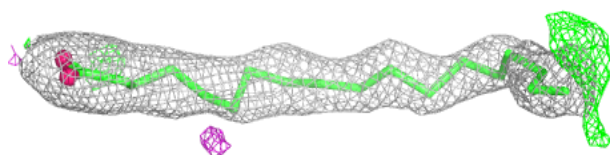
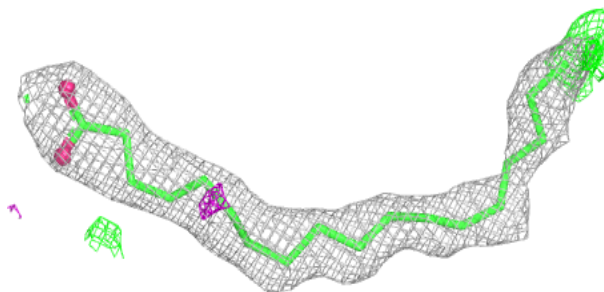


Electron density around PL9 a 611:

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

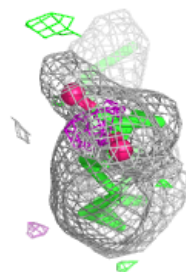
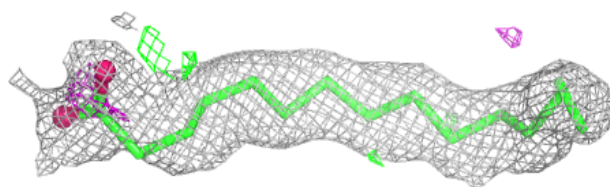
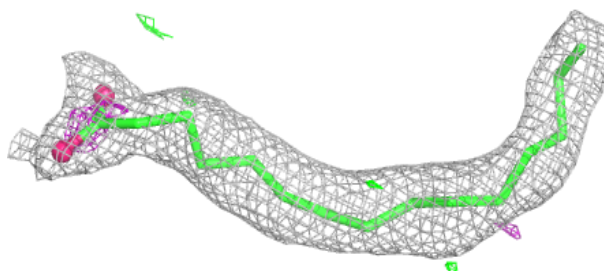
**Electron density around STE d 413:**

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

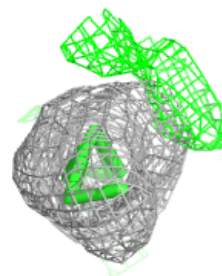
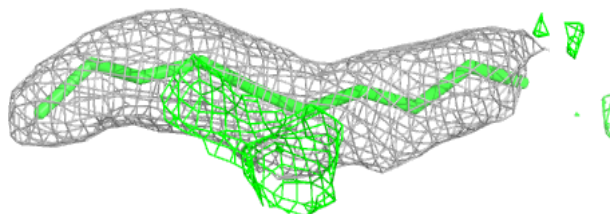
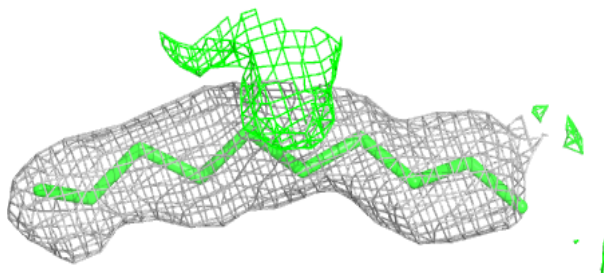


Electron density around STE B 620:

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

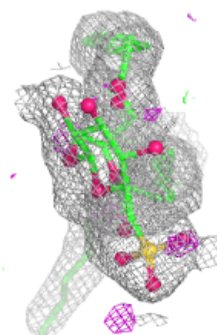
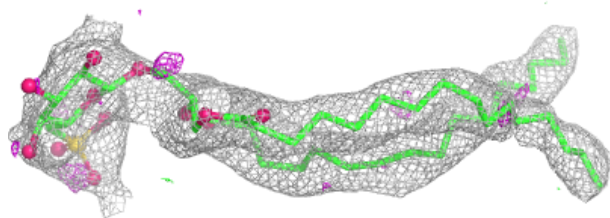
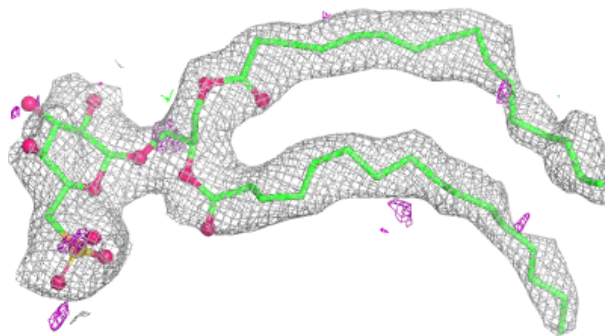
**Electron density around STE t 103:**

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

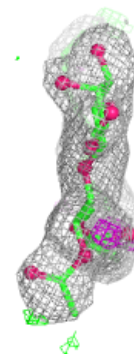
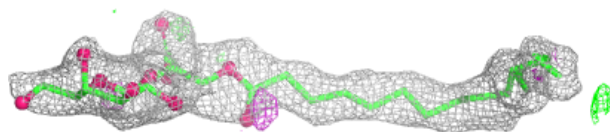
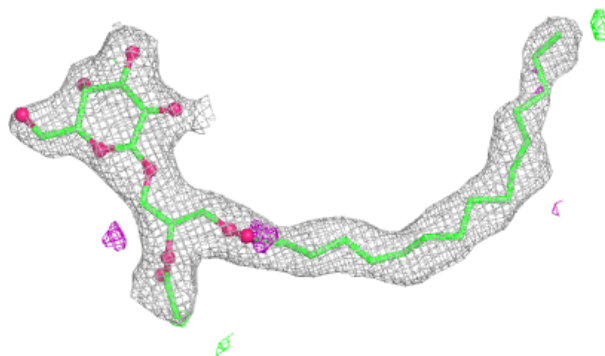


Electron density around SQD B 623:

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

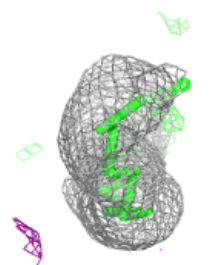
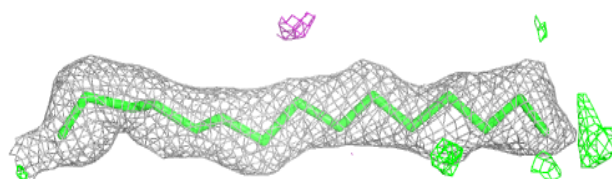
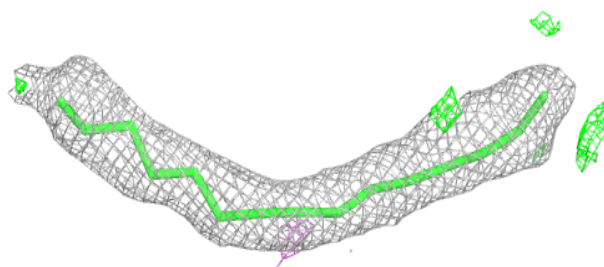
**Electron density around LMG c 518:**

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

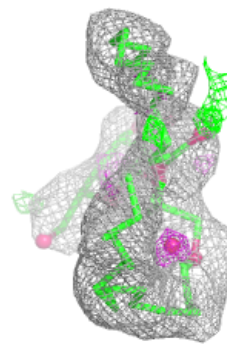
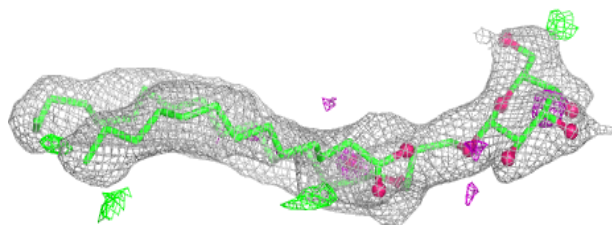
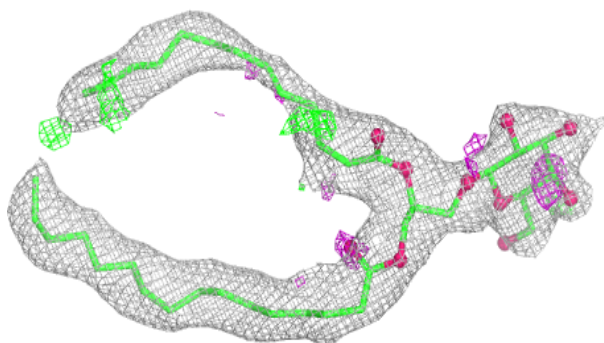


Electron density around STE I 101:

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

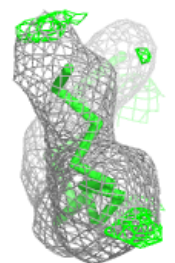
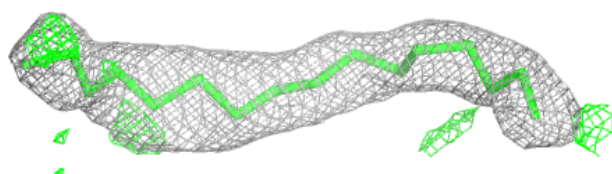
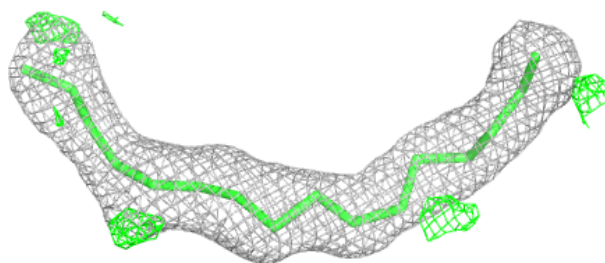
**Electron density around LMG A 612:**

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

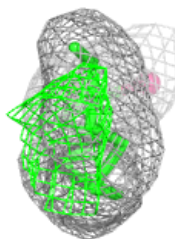
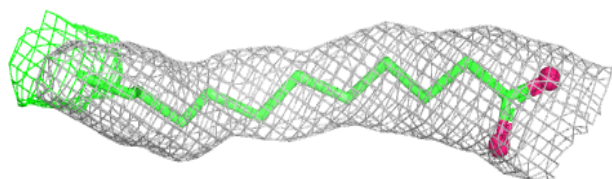
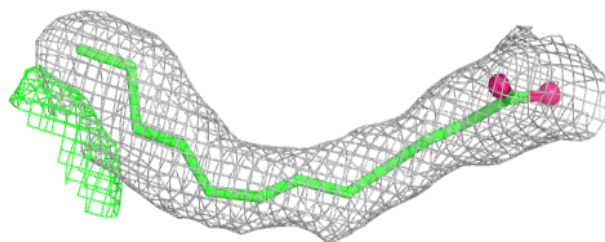


Electron density around STE b 621:

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

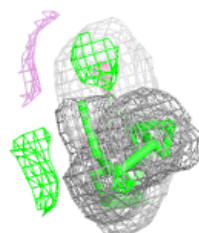
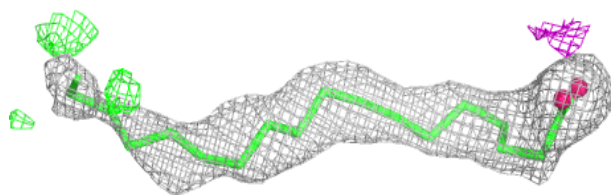
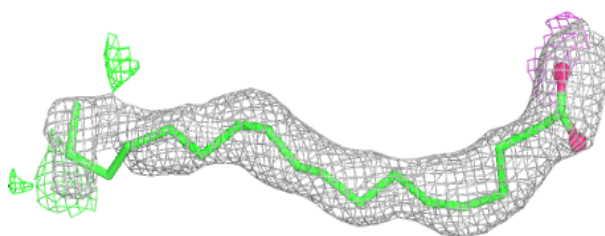
**Electron density around STE t 102:**

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

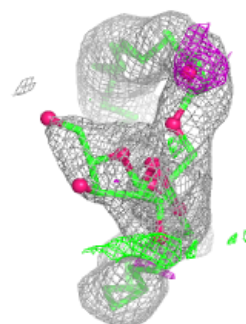
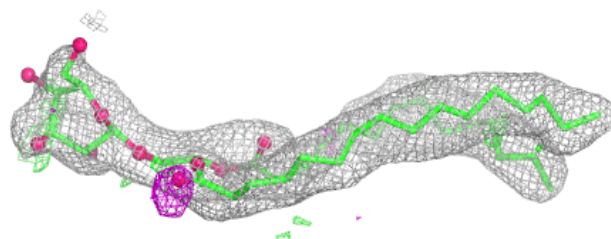
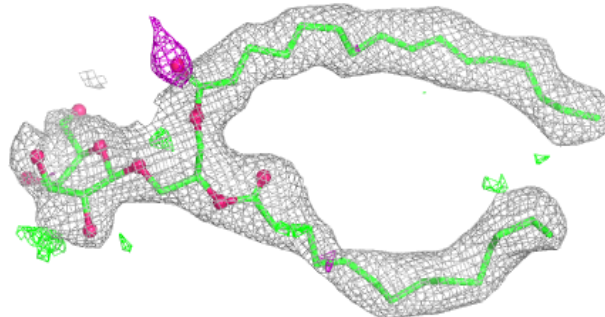


Electron density around STE b 623:

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

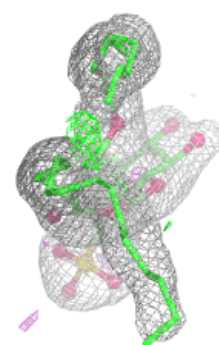
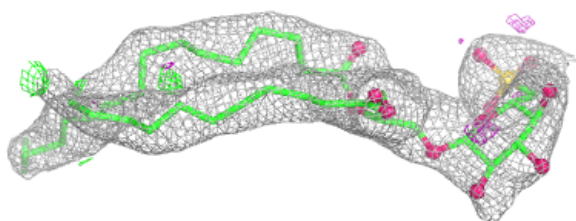
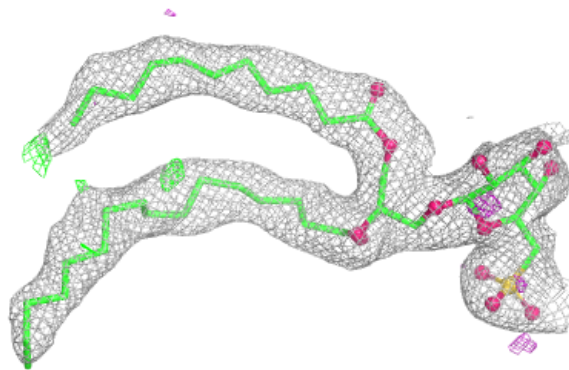
**Electron density around LMG c 522:**

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

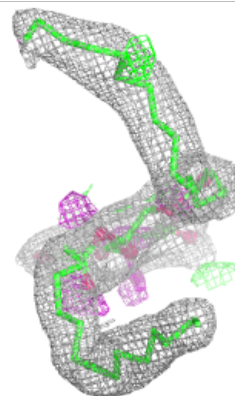
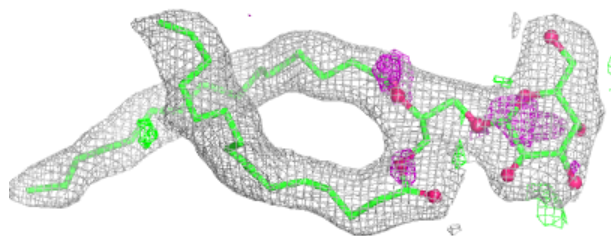
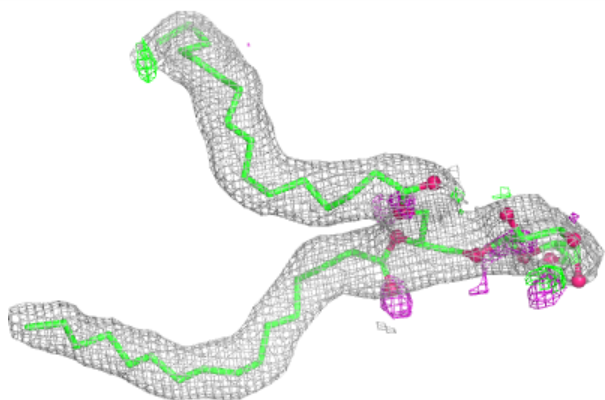


Electron density around SQD b 620:

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

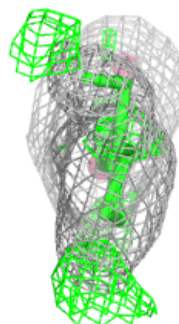
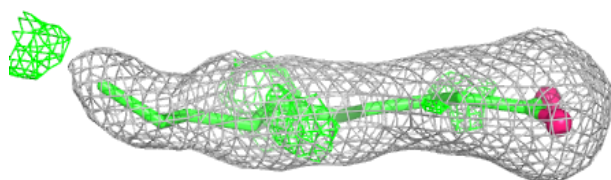
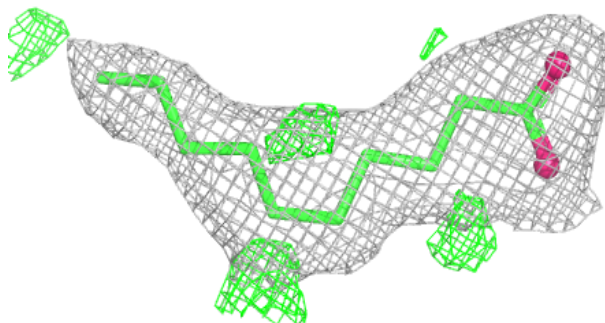
**Electron density around LMG b 622:**

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

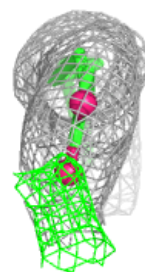
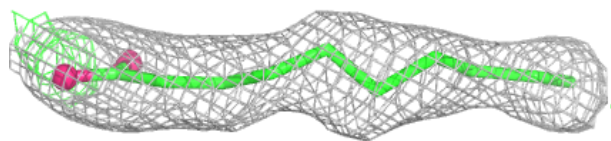
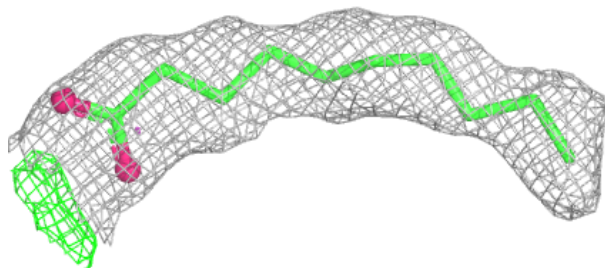


Electron density around STE C 519:

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

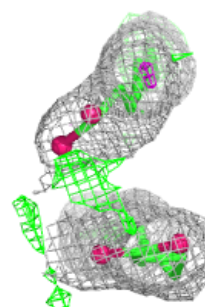
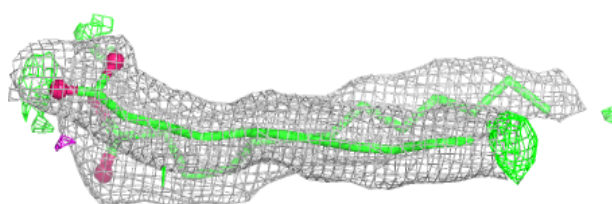
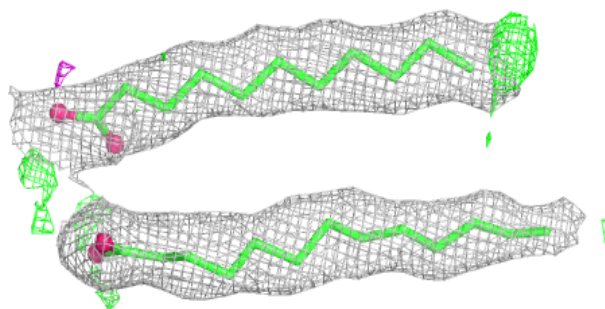
**Electron density around STE C 520:**

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

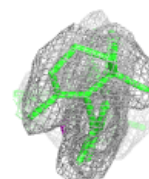
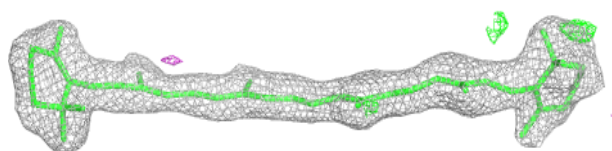
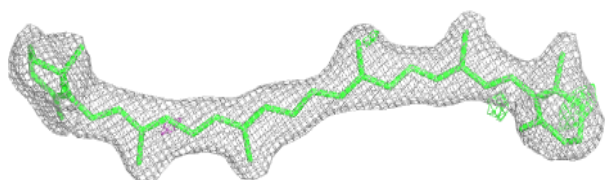


Electron density around LMG B 621:

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

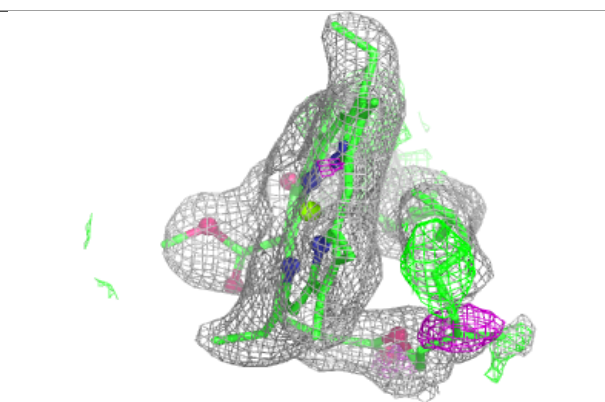
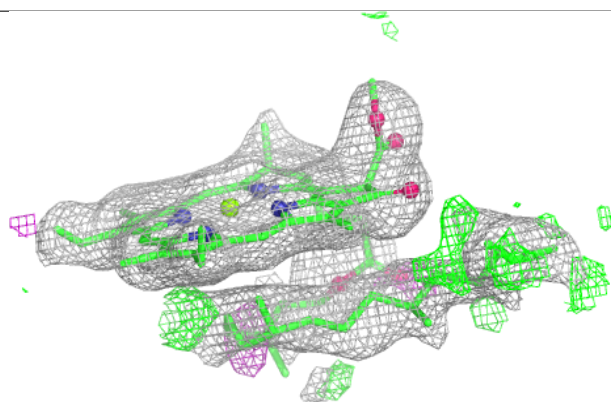
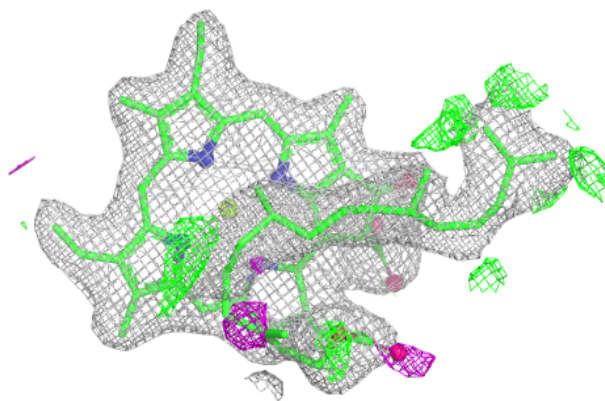
**Electron density around BCR k 102:**

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

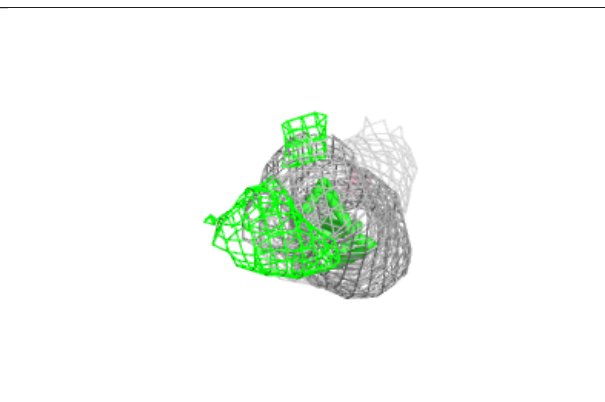
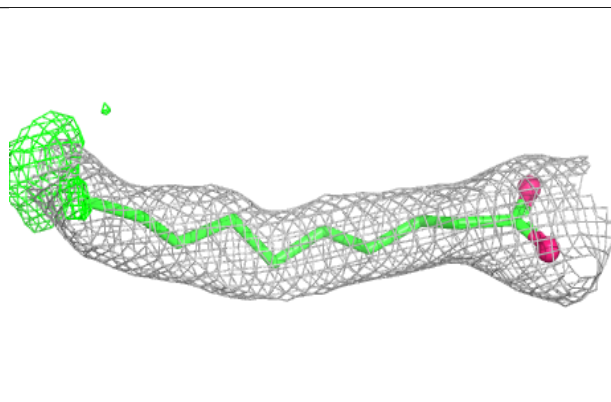
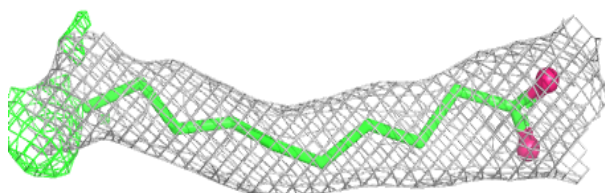


Electron density around CLA B 601:

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

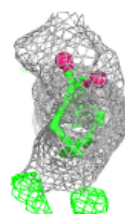
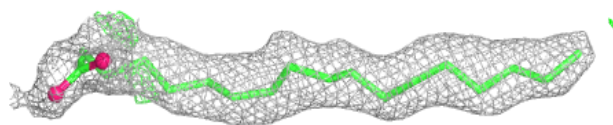
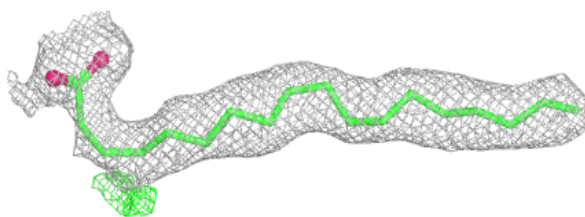
**Electron density around STE j 101:**

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

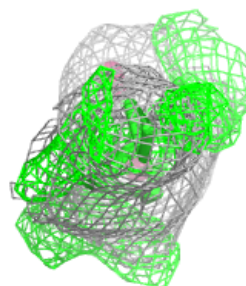
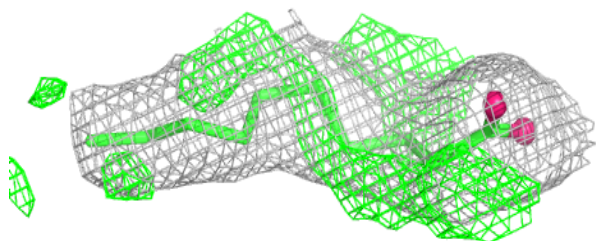
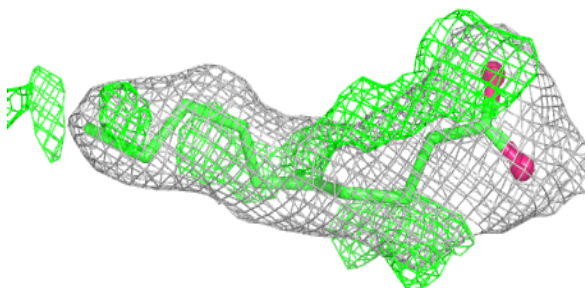


Electron density around STE c 519:

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

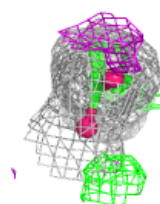
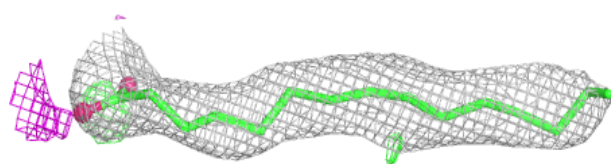
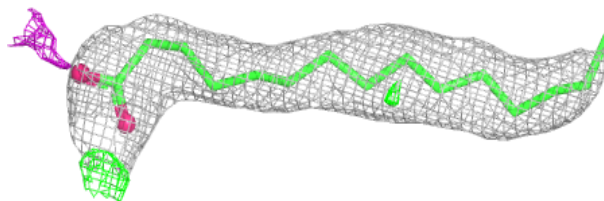
**Electron density around STE B 624:**

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

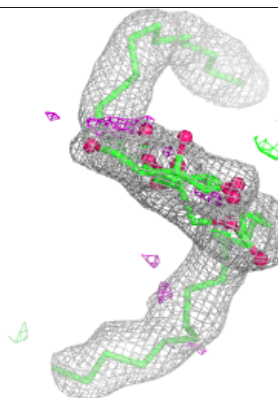
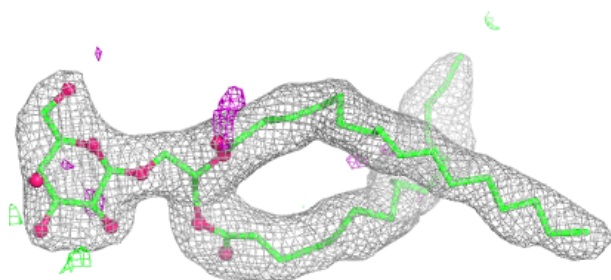
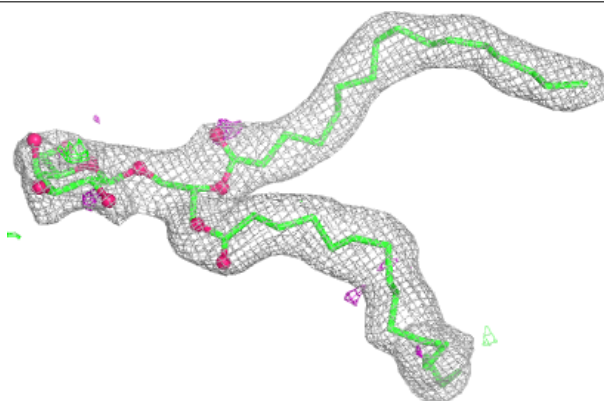


Electron density around STE d 412:

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

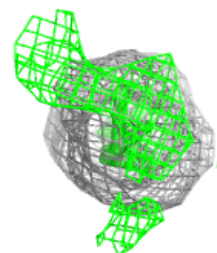
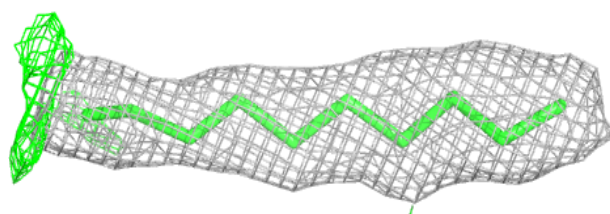
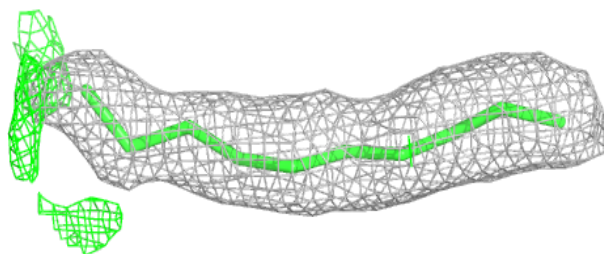
**Electron density around LMG M 101:**

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

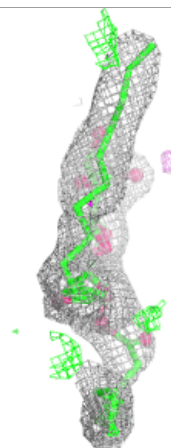
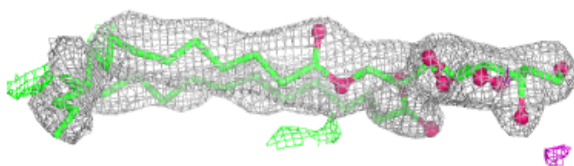
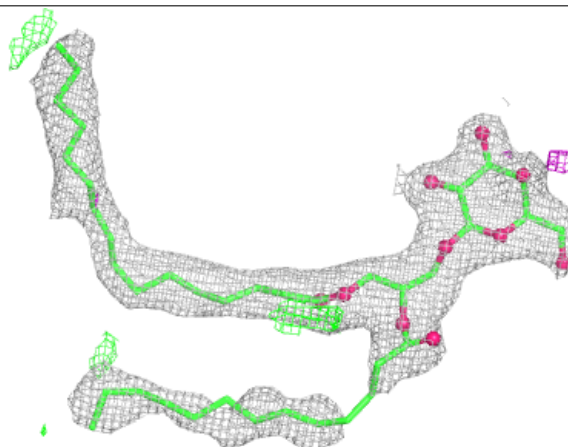


Electron density around STE M 103:

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

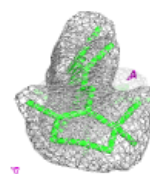
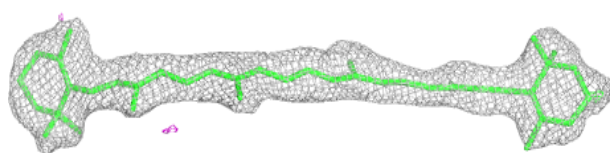
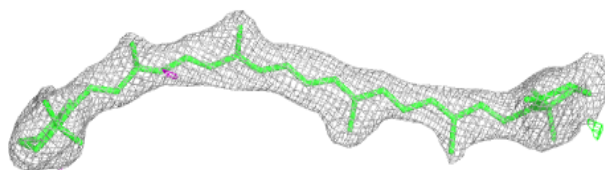
**Electron density around LMG C 518:**

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

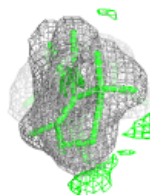
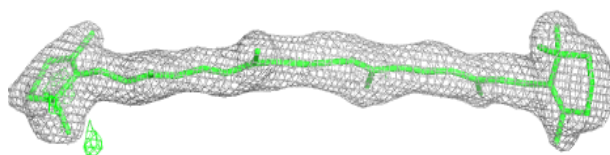
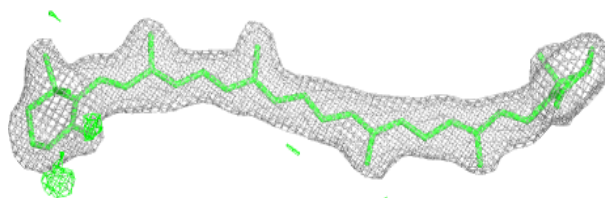


Electron density around BCR x 101:

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

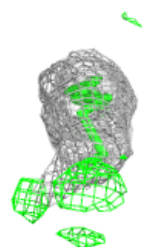
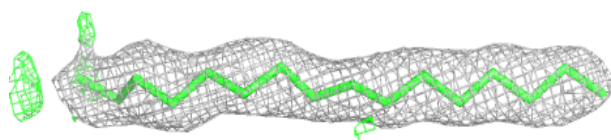
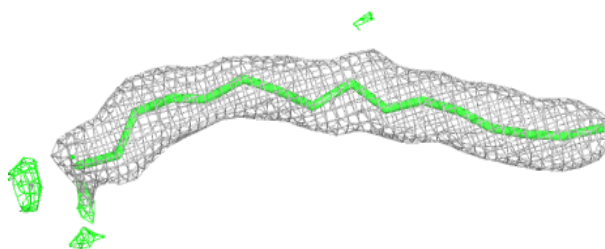
**Electron density around BCR K 102:**

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

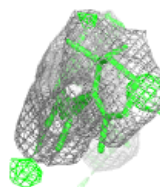
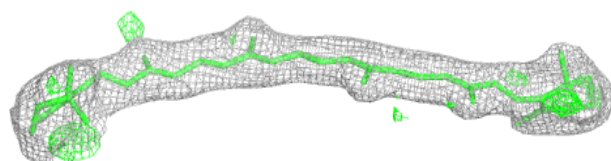
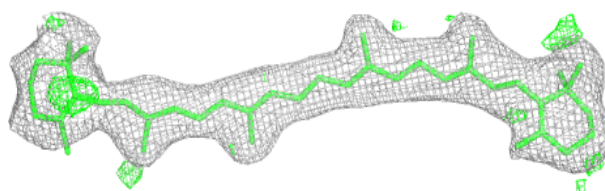


Electron density around STE C 521:

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

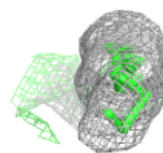
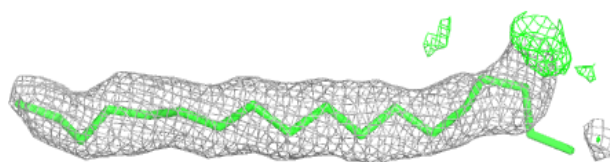
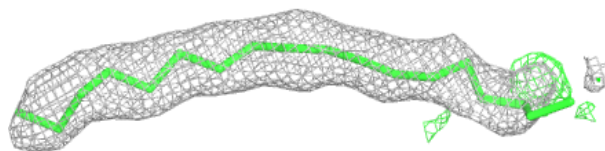
**Electron density around BCR D 406:**

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



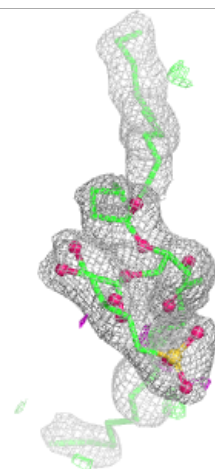
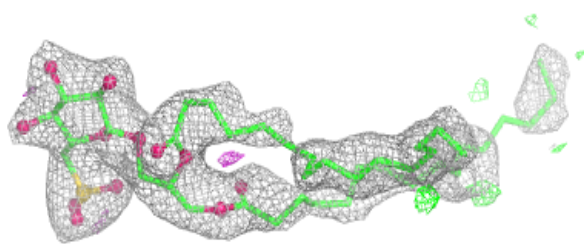
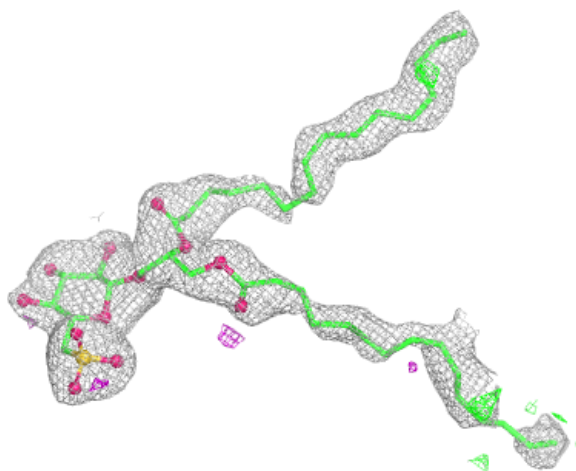
Electron density around STE 1 102:

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



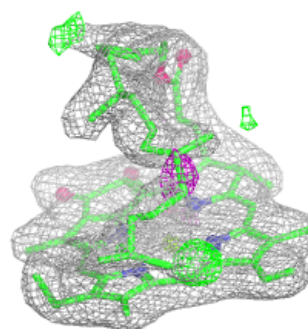
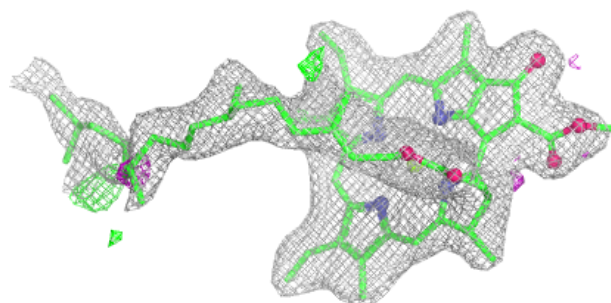
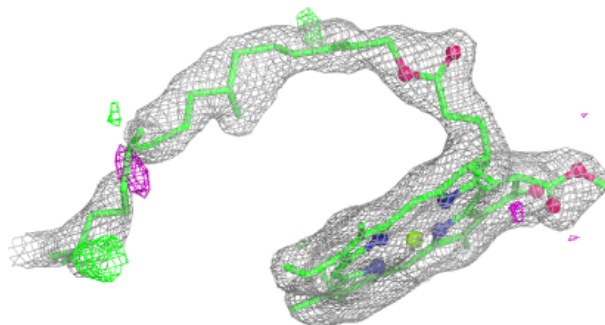
Electron density around SQD a 613:

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

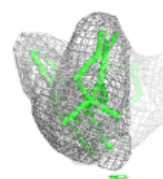
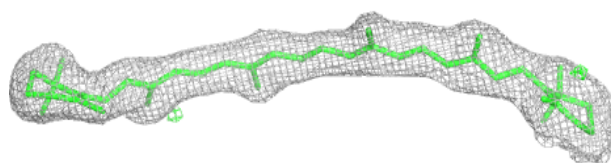
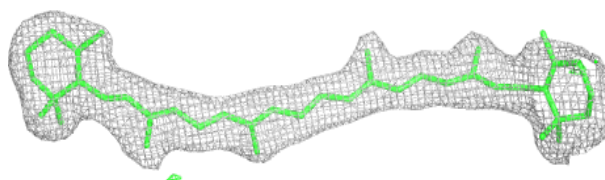


Electron density around CLA C 513:

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

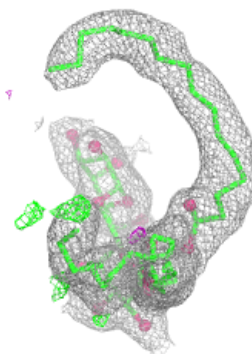
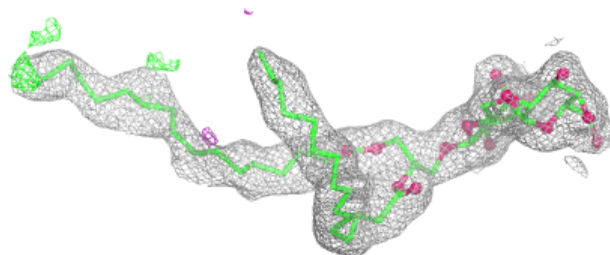
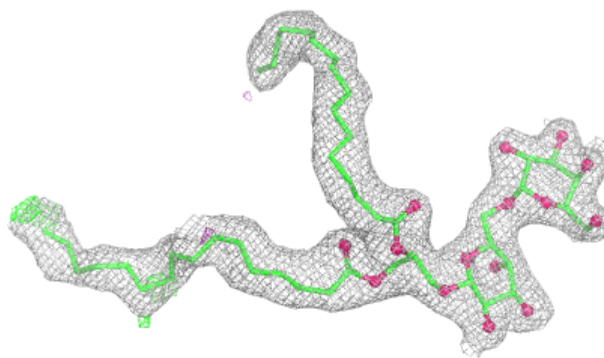
**Electron density around BCR d 405:**

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

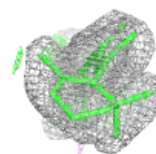
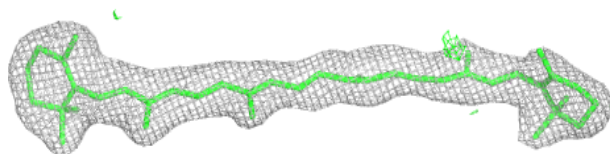
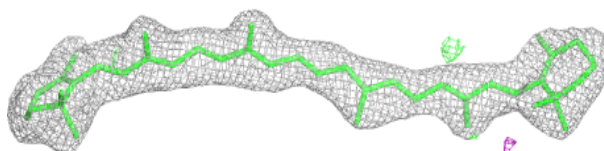


Electron density around DGD c 516:

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

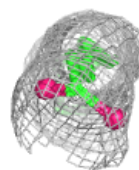
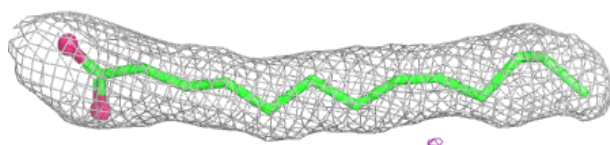
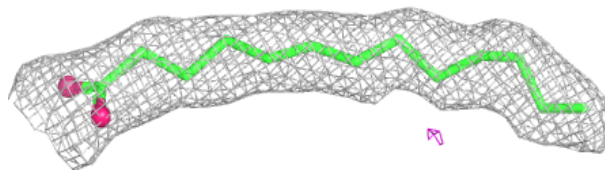
**Electron density around BCR k 101:**

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

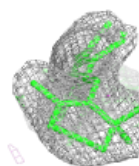
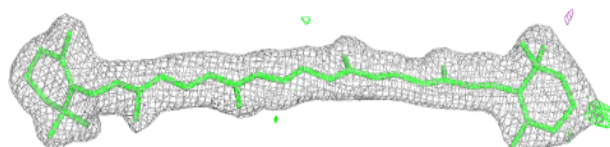
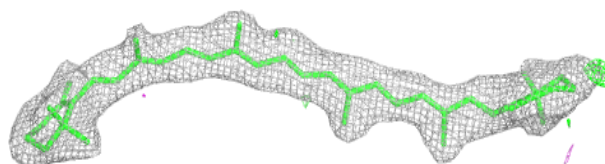


Electron density around STE M 102:

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

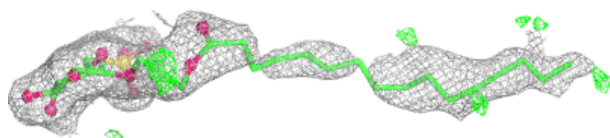
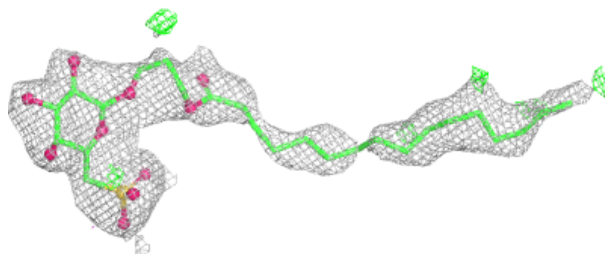
**Electron density around BCR H 101:**

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

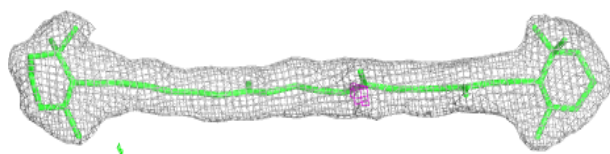
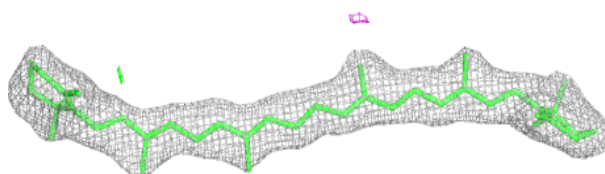


Electron density around SQD D 409:

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

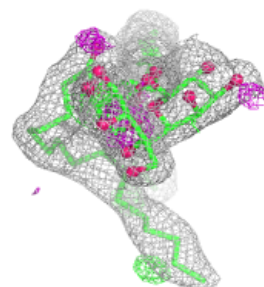
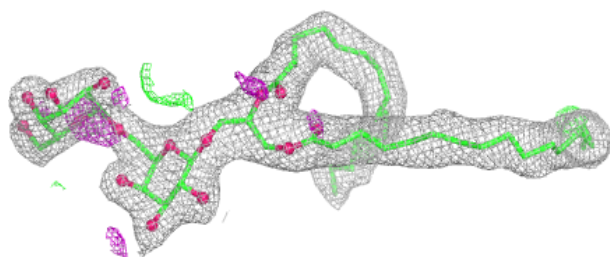
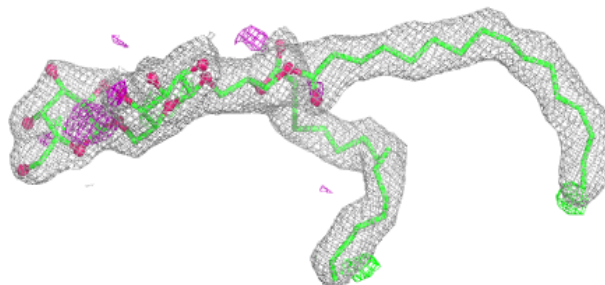
**Electron density around BCR K 101:**

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

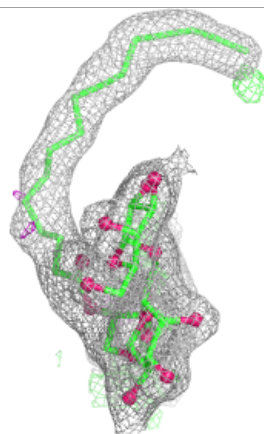
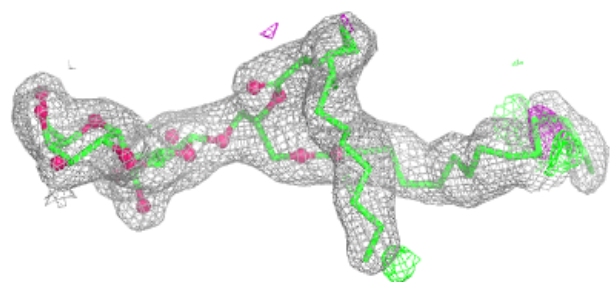
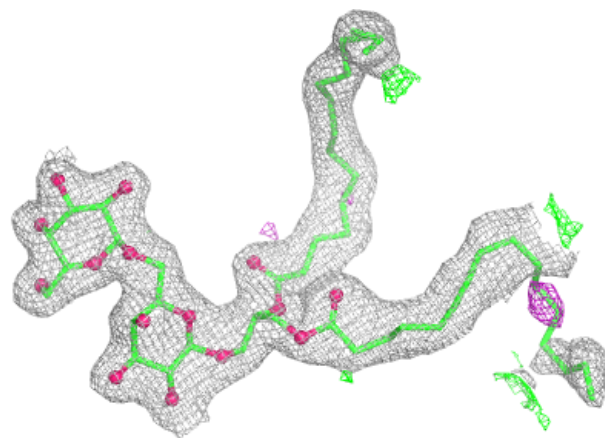


Electron density around DGD H 102:

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

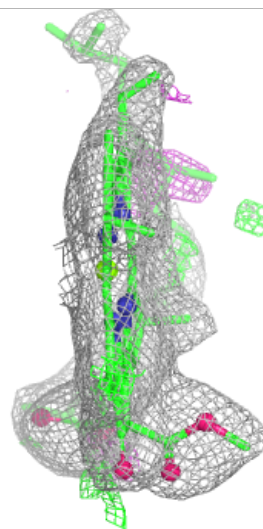
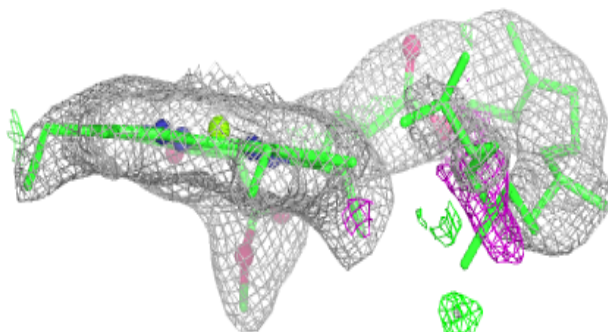
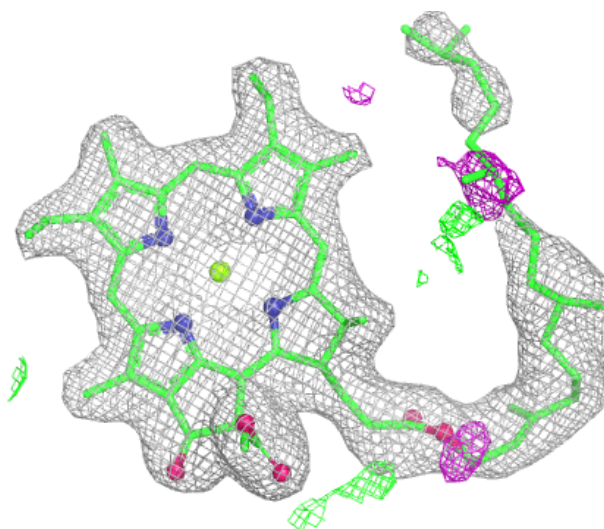
**Electron density around DGD C 516:**

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



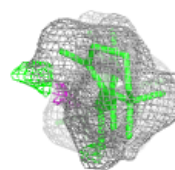
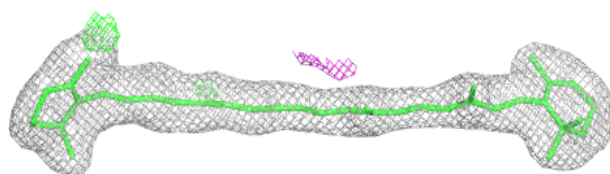
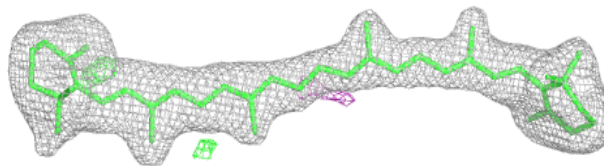
Electron density around CLA c 512:

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

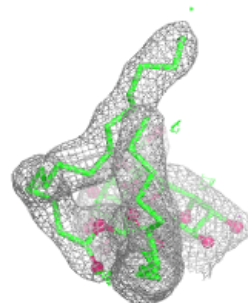
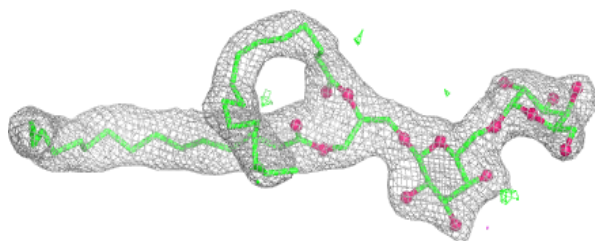
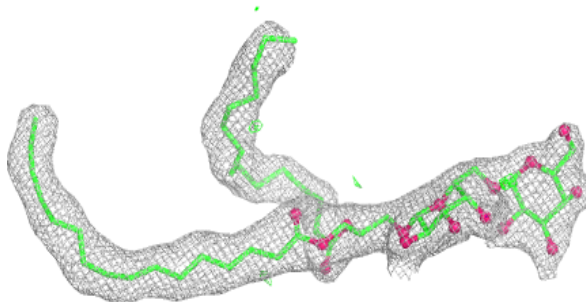


Electron density around BCR b 618:

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

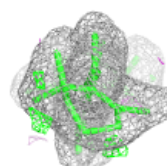
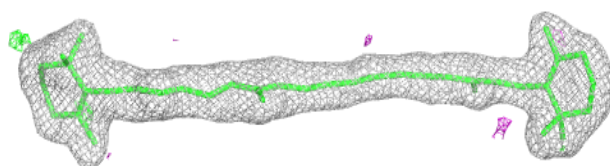
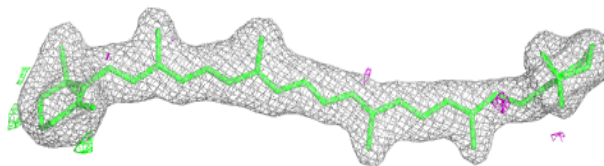
**Electron density around DGD h 101:**

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

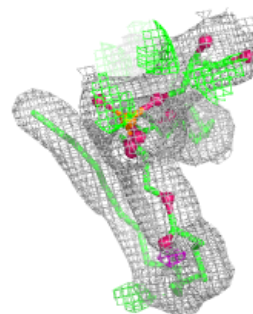
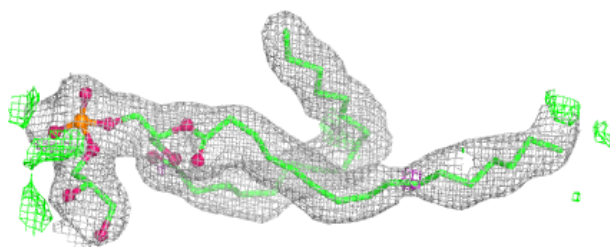
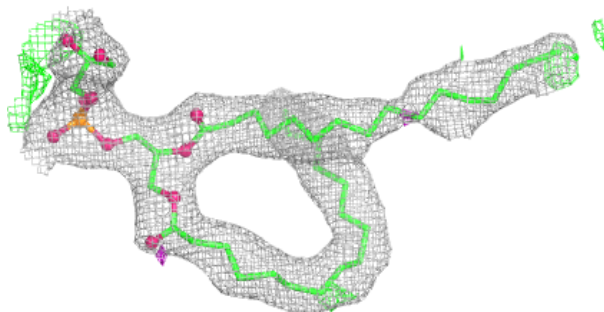


Electron density around BCR A 609:

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

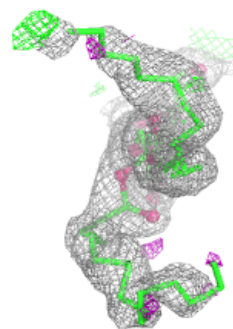
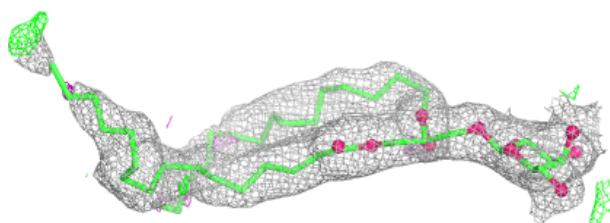
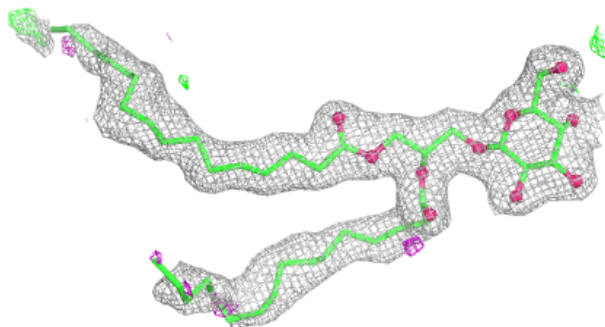
**Electron density around LHG d 407:**

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

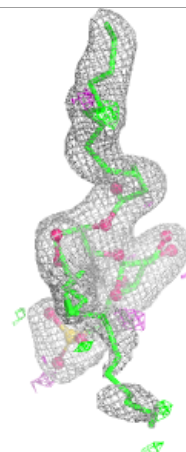
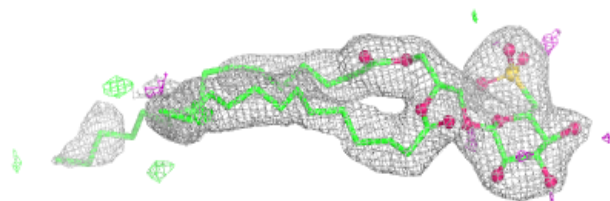
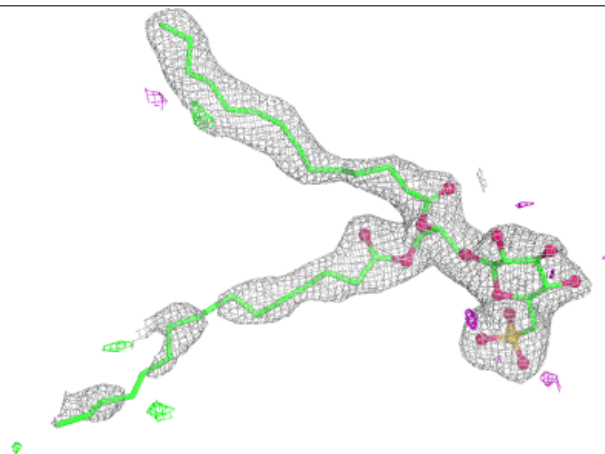


Electron density around LMG D 408:

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

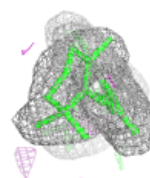
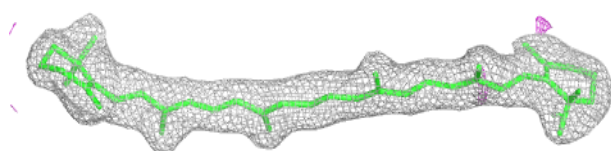
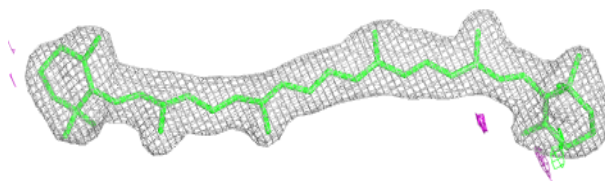
**Electron density around SQD A 614:**

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

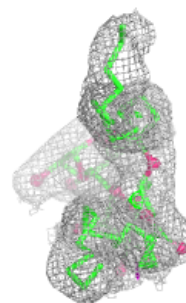
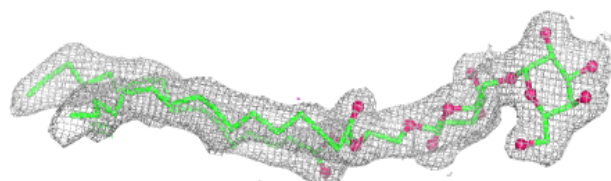
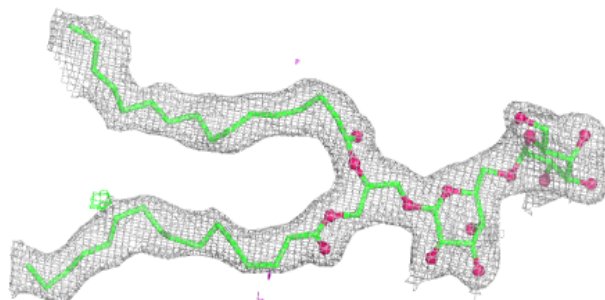


Electron density around BCR B 619:

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

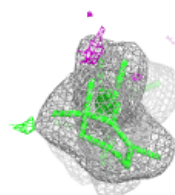
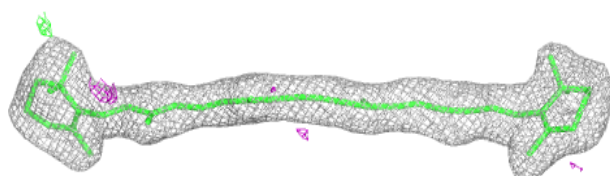
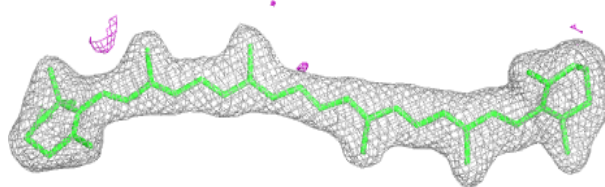
**Electron density around DGD C 517:**

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

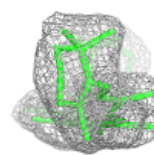
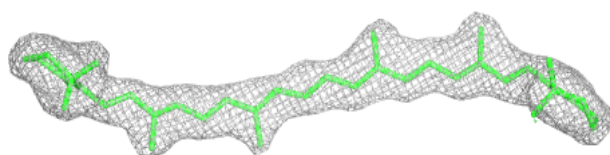
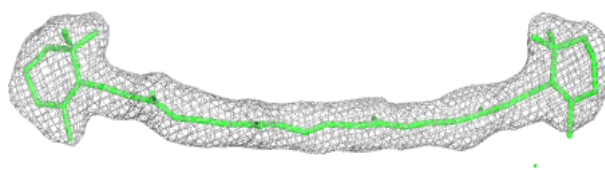


Electron density around BCR B 618:

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

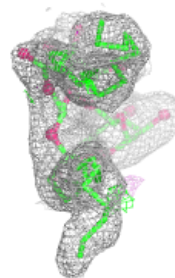
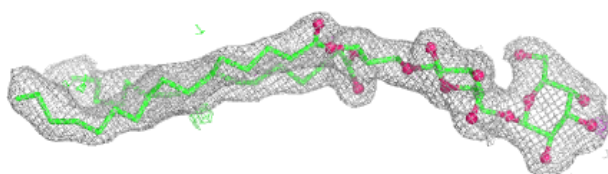
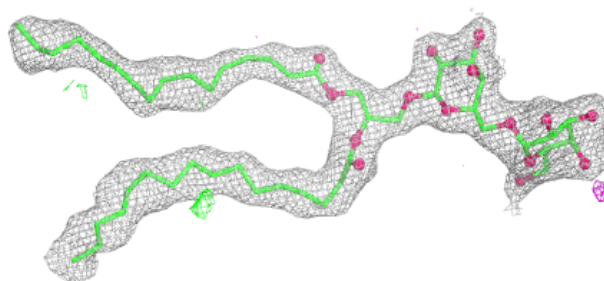
**Electron density around BCR k 103:**

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

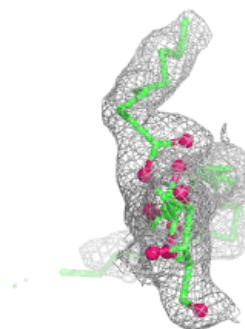
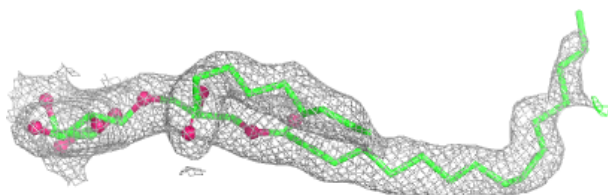
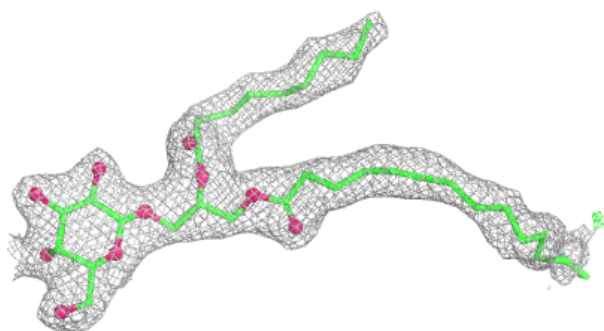


Electron density around DGD c 517:

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

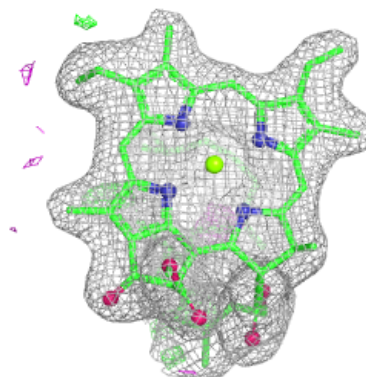
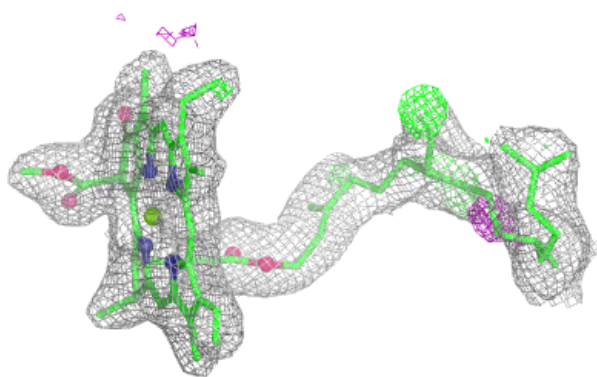
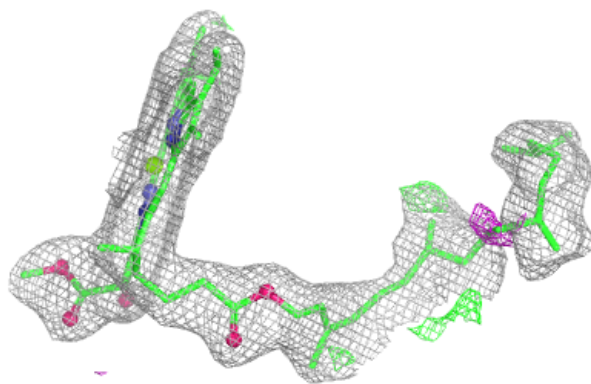
**Electron density around LMG d 411:**

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

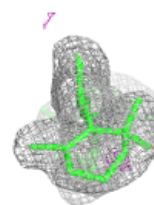
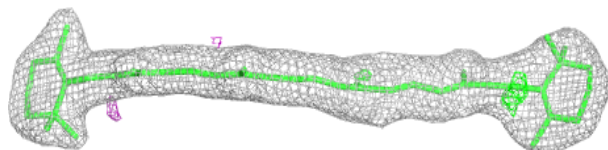
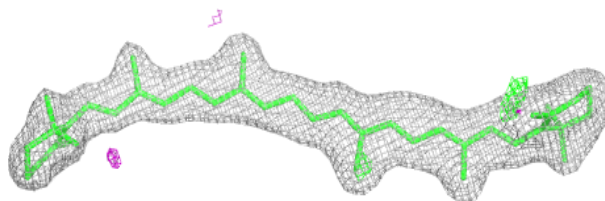


Electron density around CLA C 506:

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

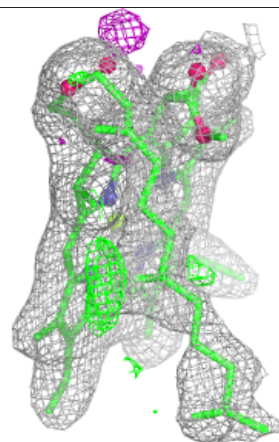
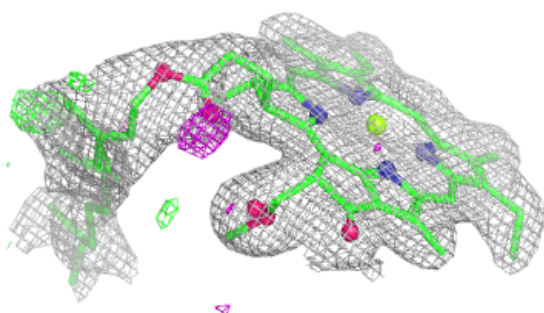
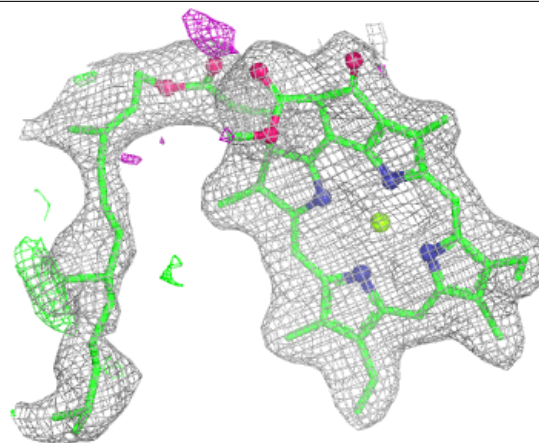
**Electron density around BCR C 514:**

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



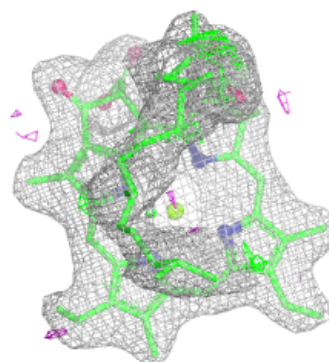
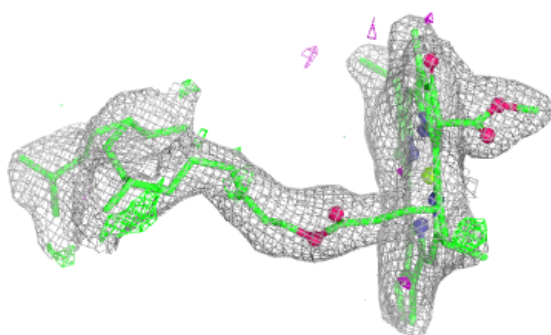
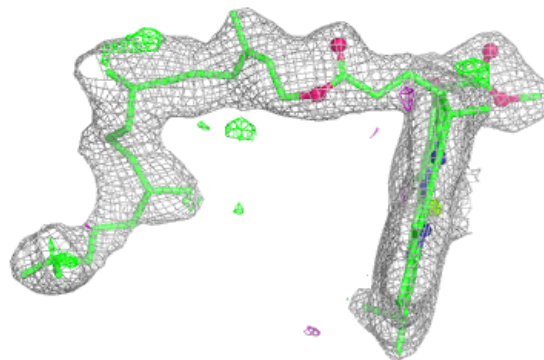
Electron density around CLA b 616:

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

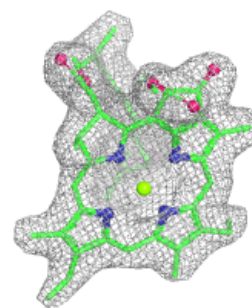
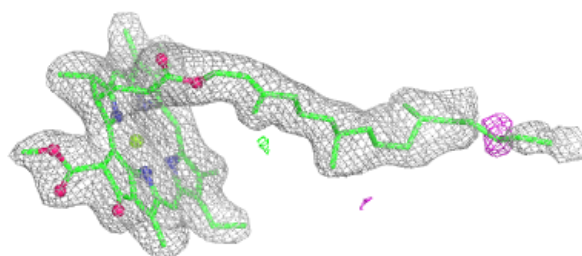
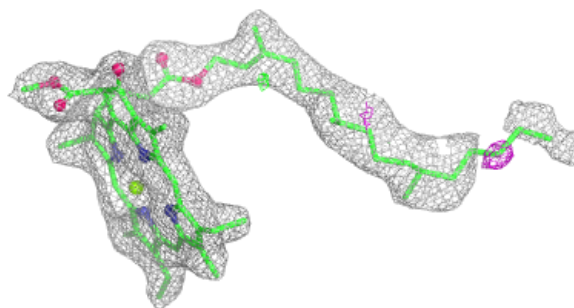


Electron density around CLA c 506:

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

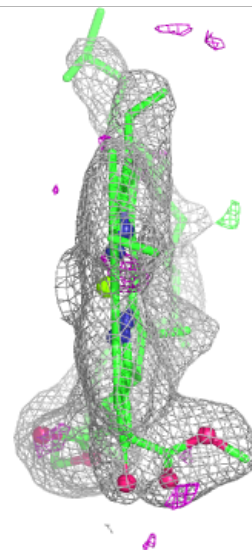
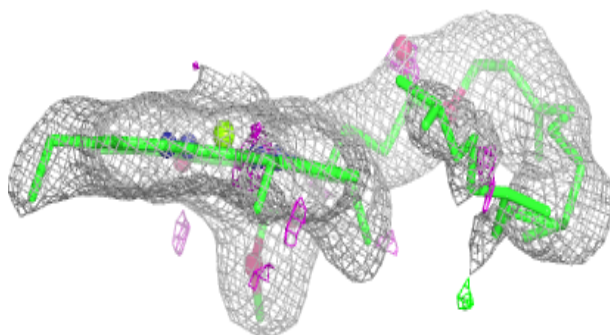
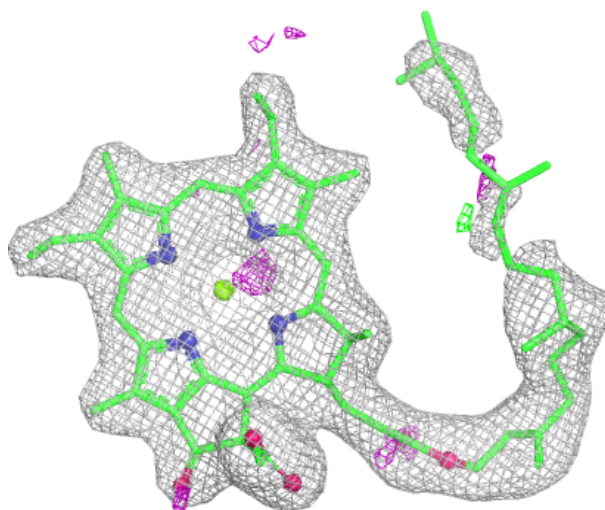
**Electron density around CLA c 508:**

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



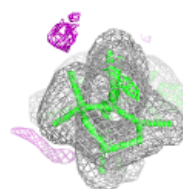
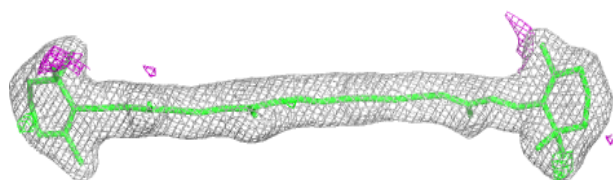
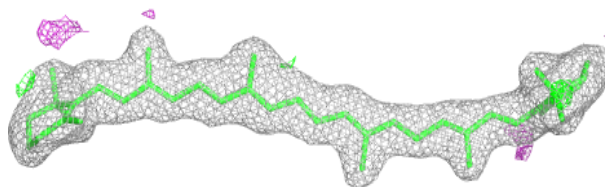
Electron density around CLA C 512:

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

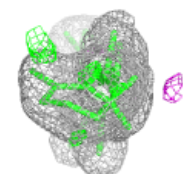
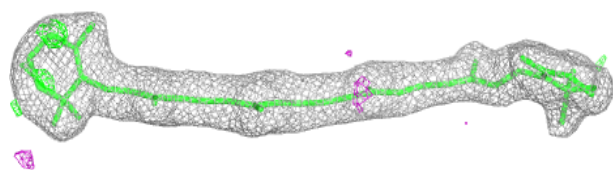
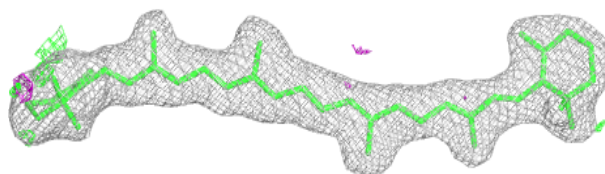


Electron density around BCR a 610:

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

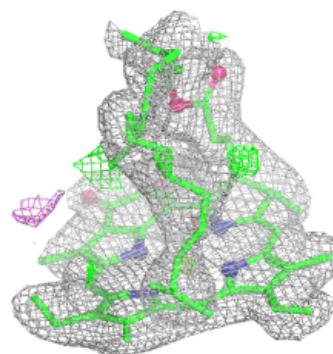
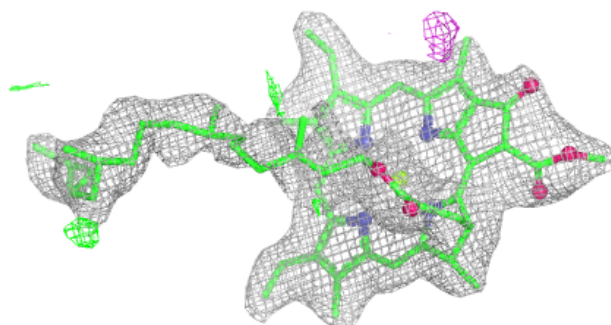
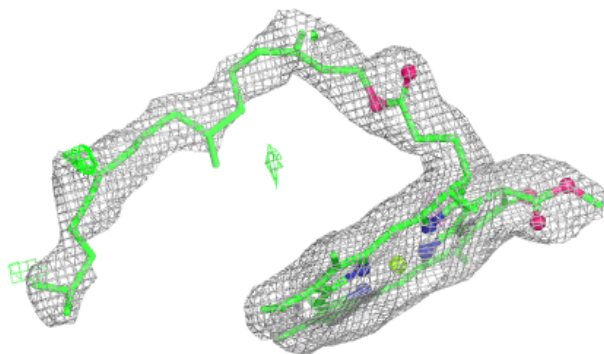
**Electron density around BCR b 617:**

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

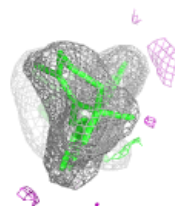
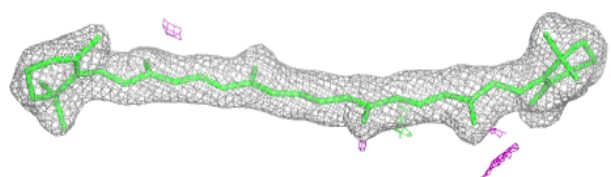
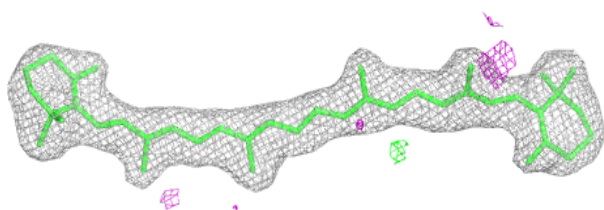


Electron density around CLA c 513:

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

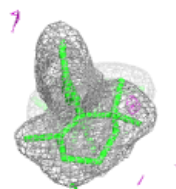
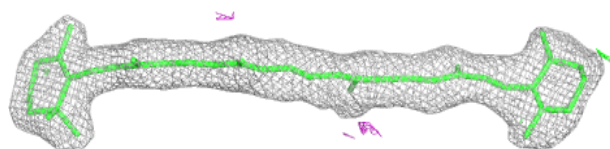
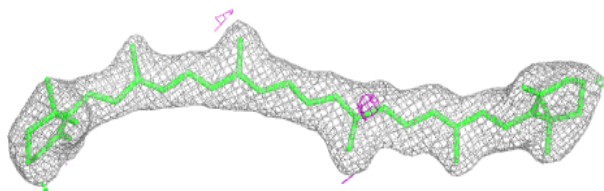
**Electron density around BCR b 619:**

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



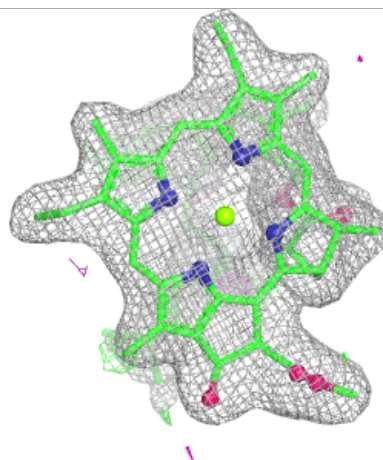
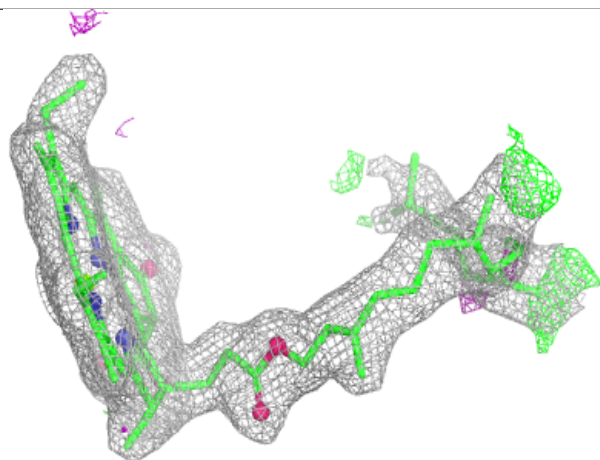
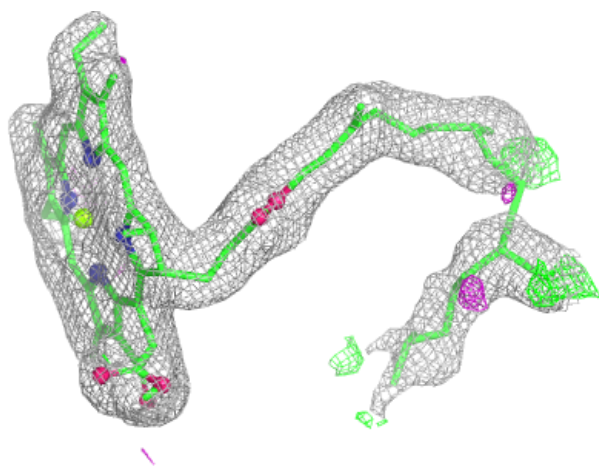
Electron density around BCR c 514:

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



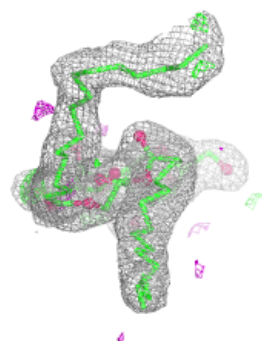
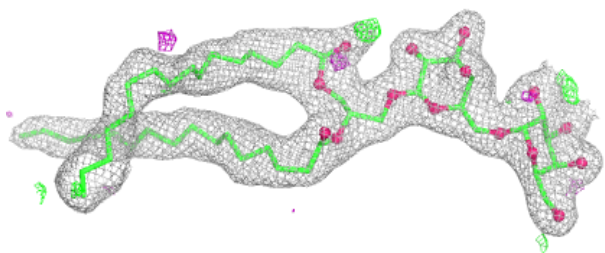
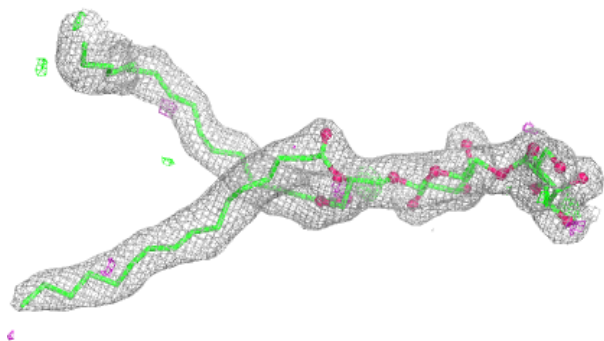
Electron density around CLA B 606:

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

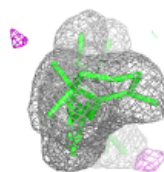
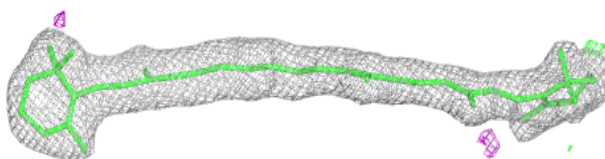
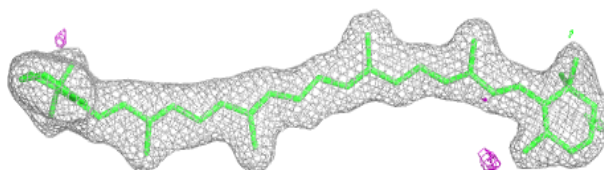


Electron density around DGD C 515:

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

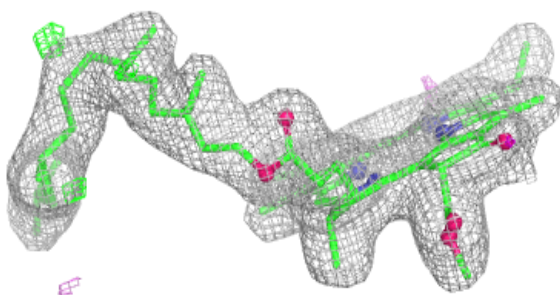
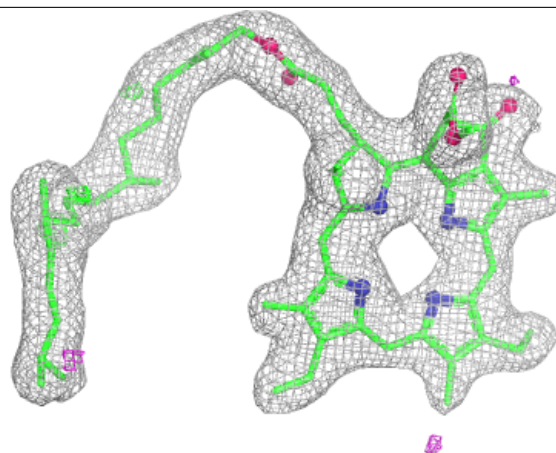
**Electron density around BCR B 617:**

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

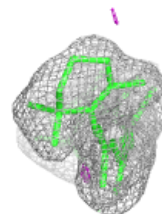
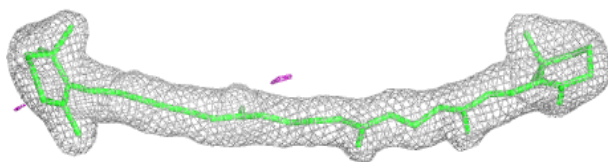
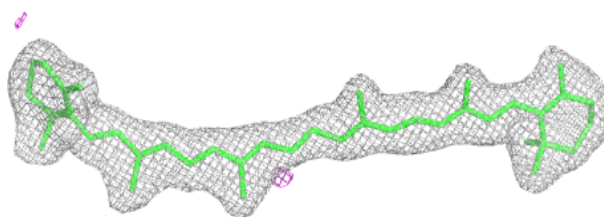


Electron density around PHO d 402:

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

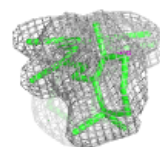
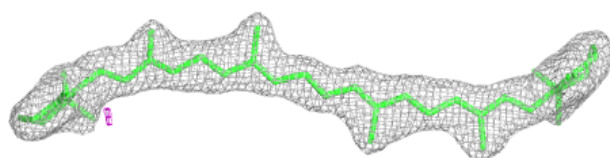
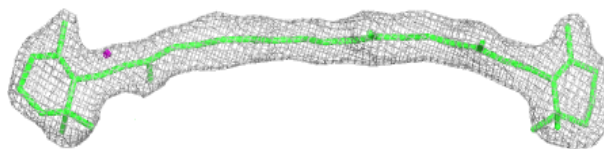
**Electron density around BCR T 101:**

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

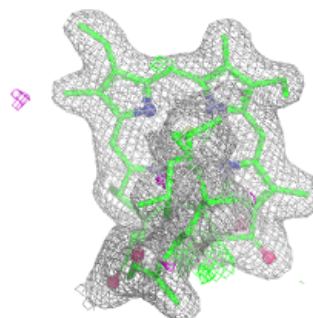
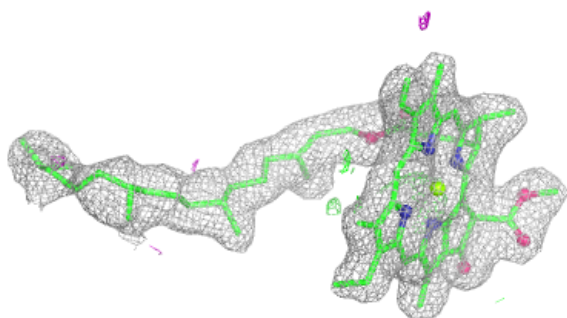
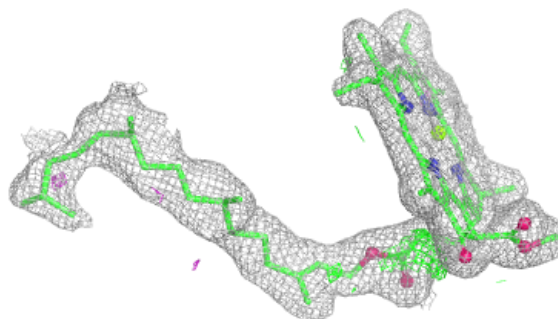


Electron density around BCR Z 101:

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

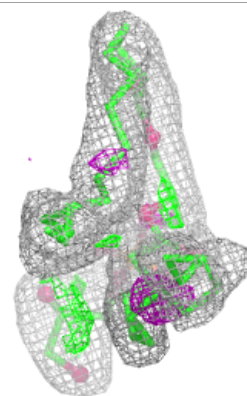
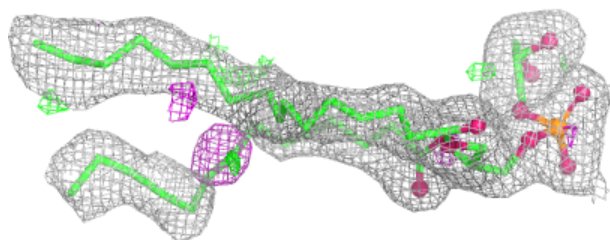
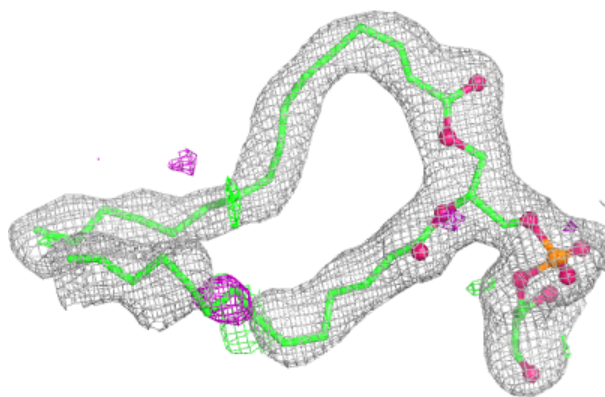
**Electron density around CLA C 508:**

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

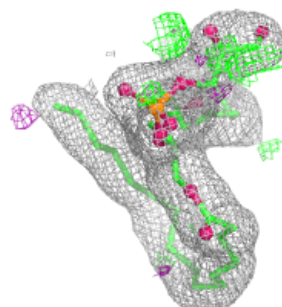
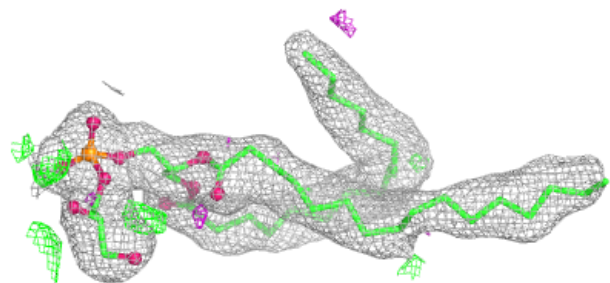
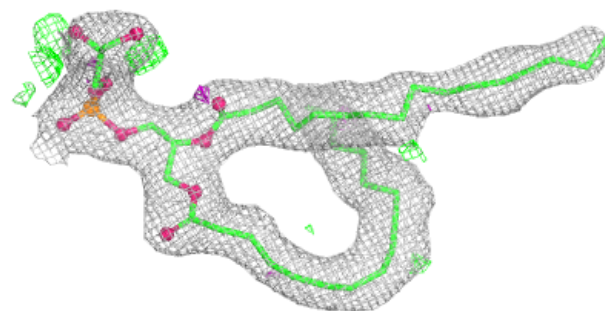


Electron density around LHG A 613:

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

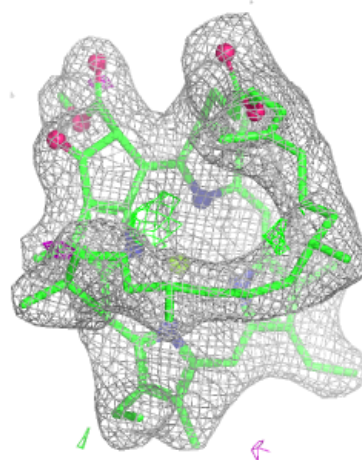
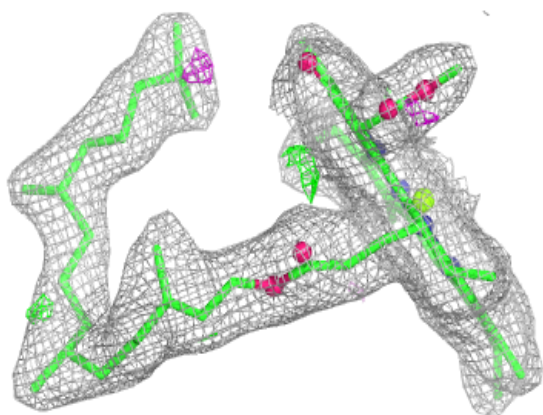
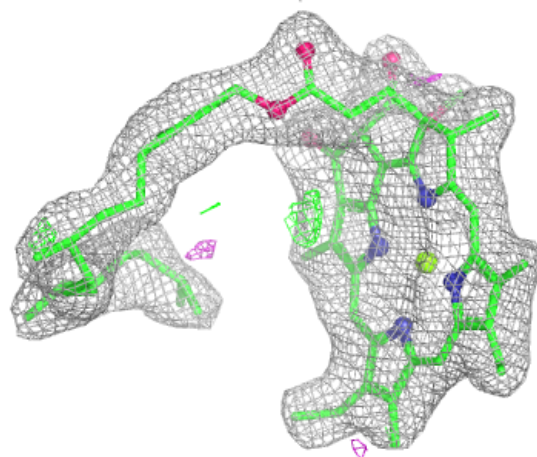
**Electron density around LHG B 622:**

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



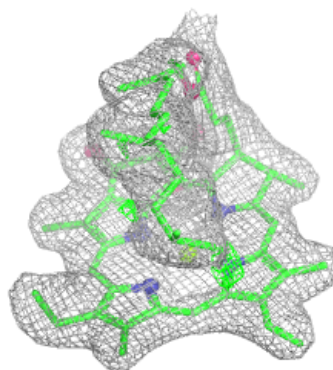
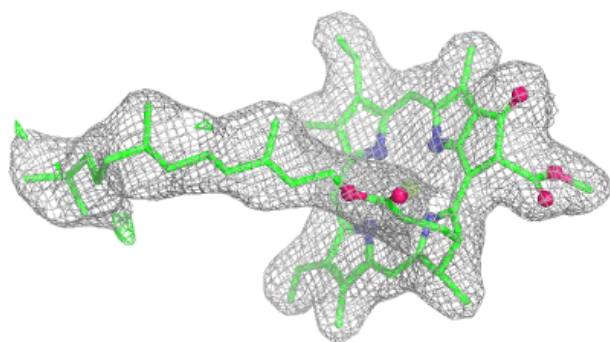
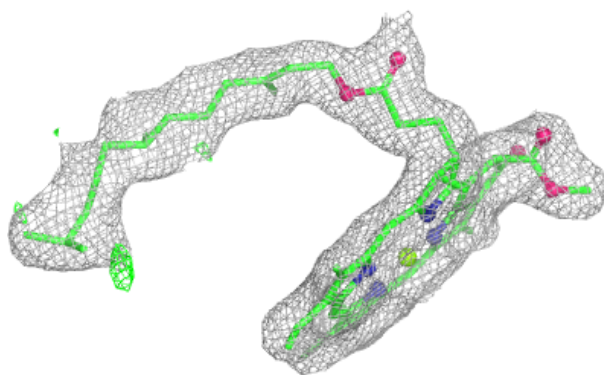
Electron density around CLA c 503:

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

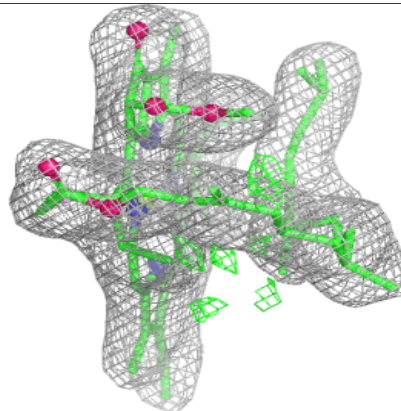
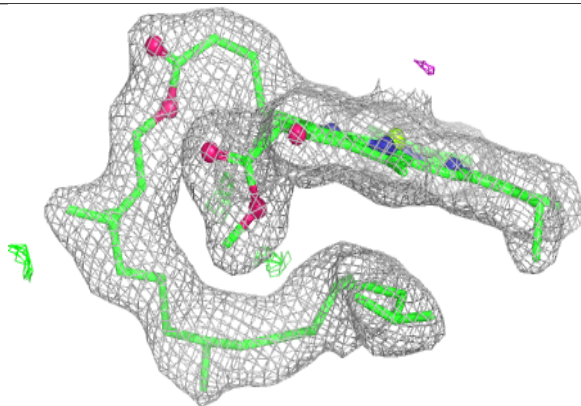
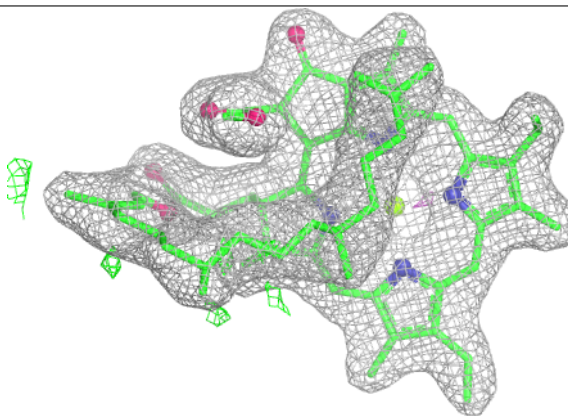


Electron density around CLA c 504:

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

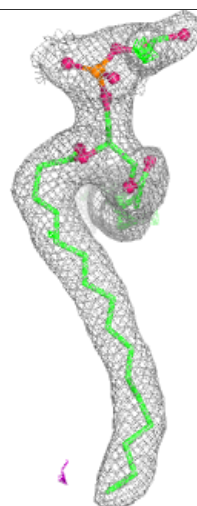
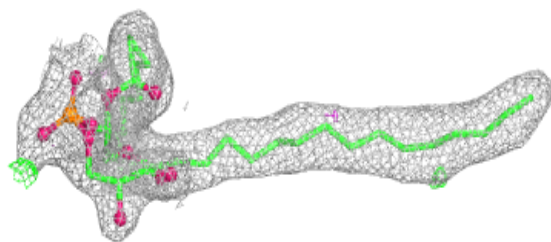
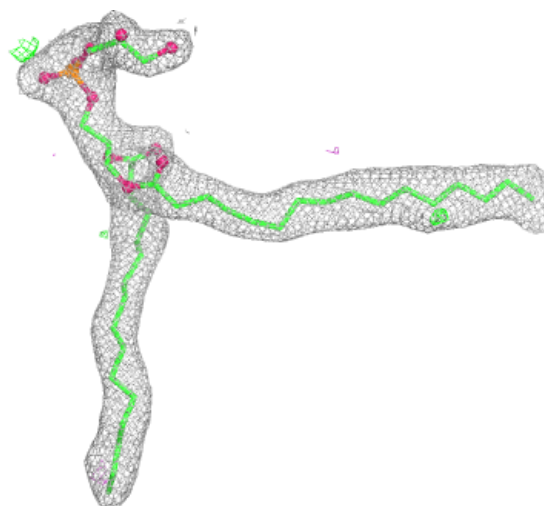
**Electron density around CLA C 510:**

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



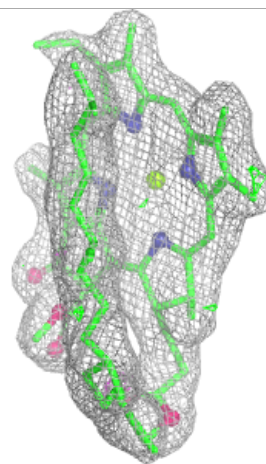
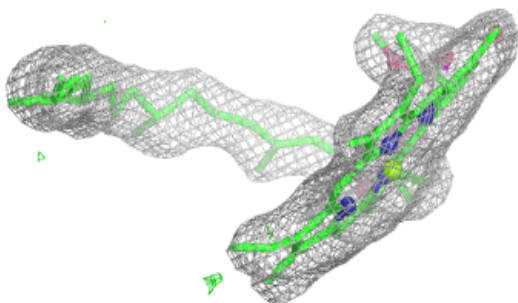
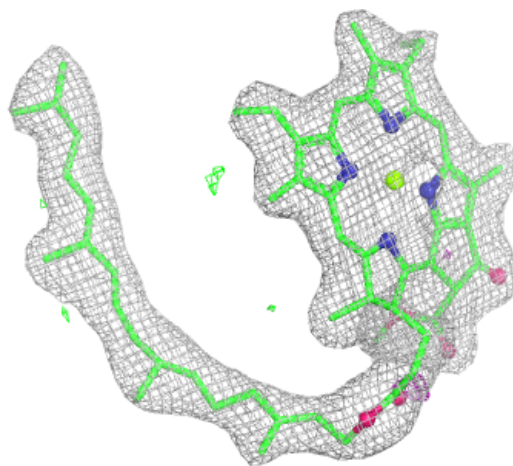
Electron density around LHG 1 101:

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



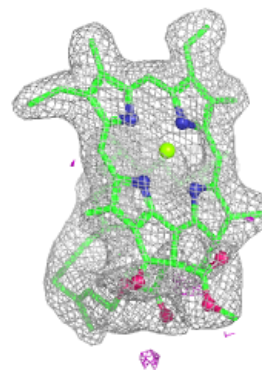
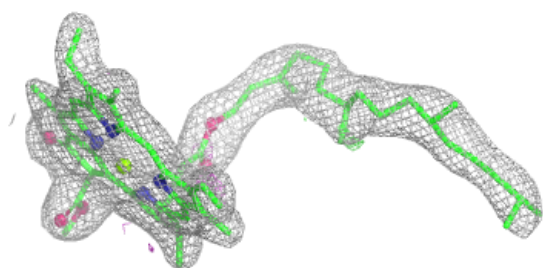
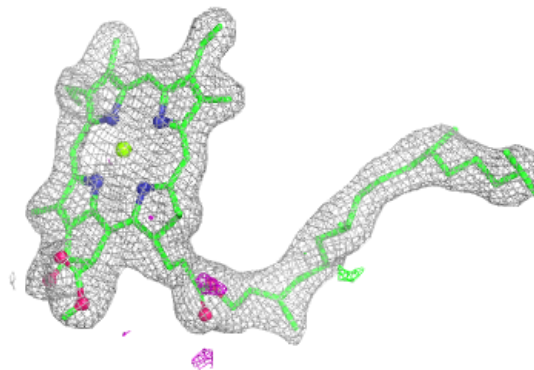
Electron density around CLA c 507:

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



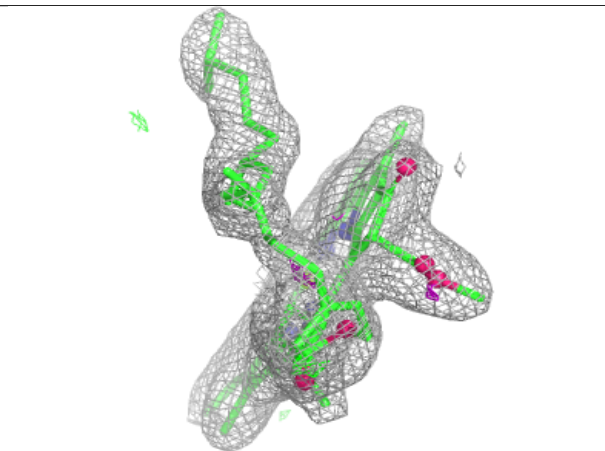
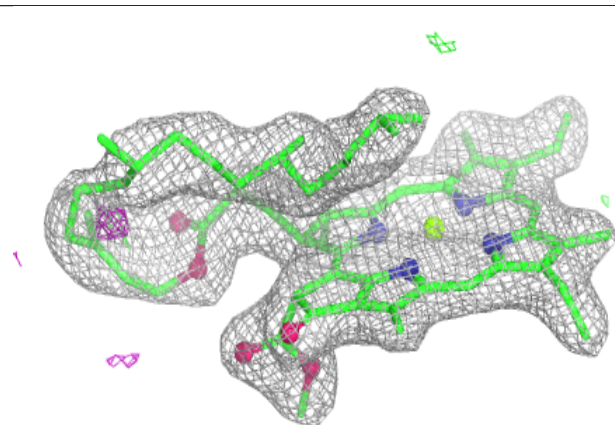
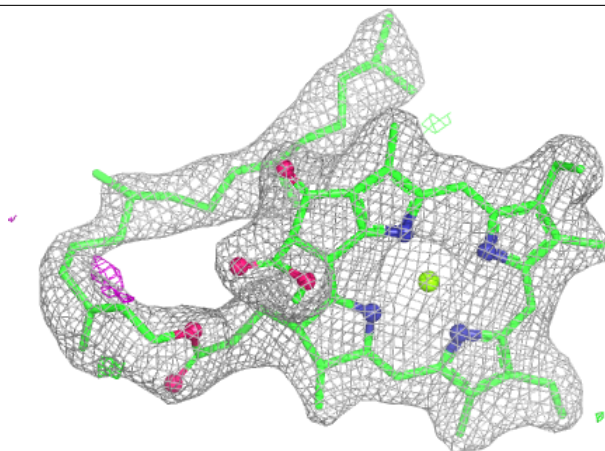
Electron density around CLA C 511:

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



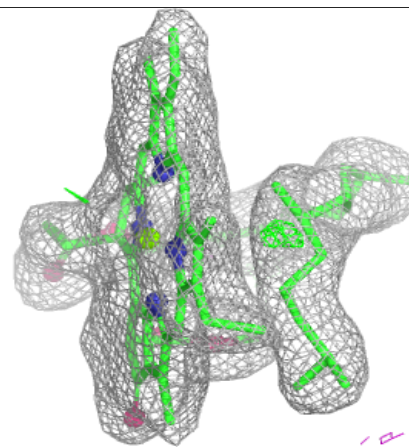
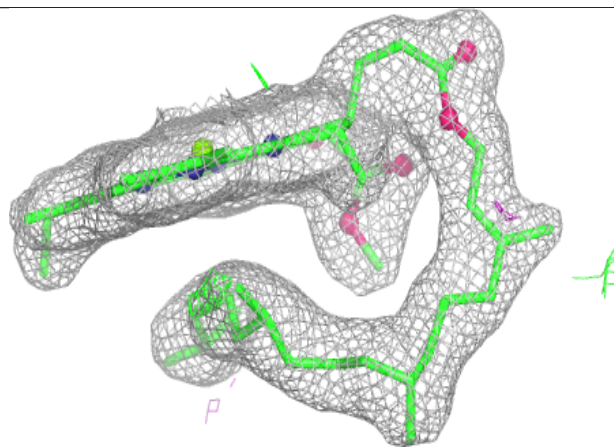
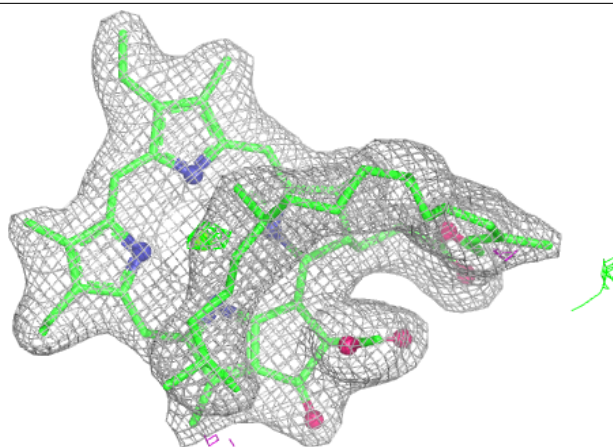
Electron density around CLA c 509:

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



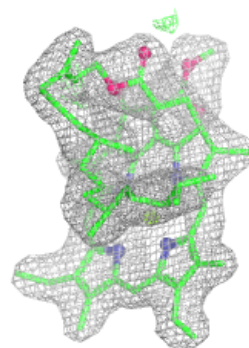
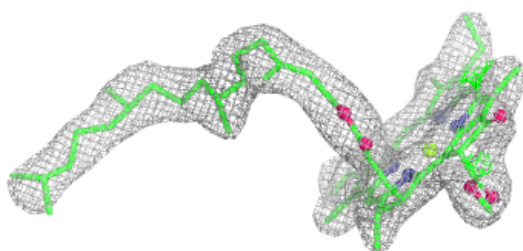
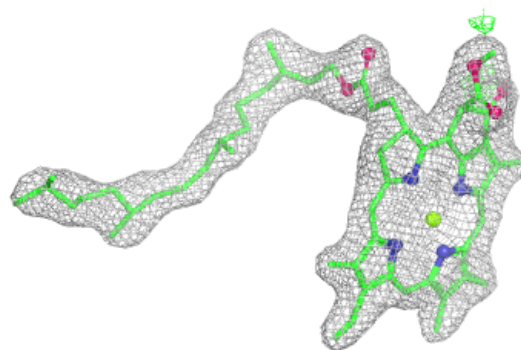
Electron density around CLA c 510:

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

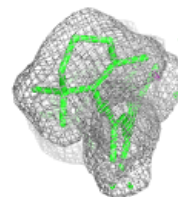
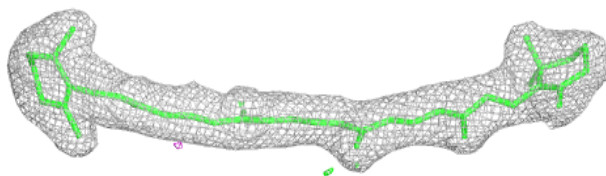
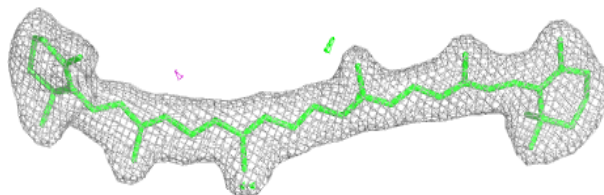


Electron density around CLA c 511:

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

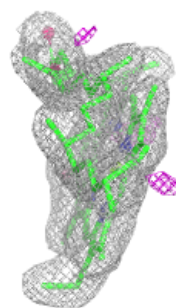
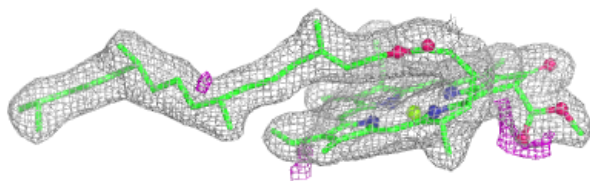
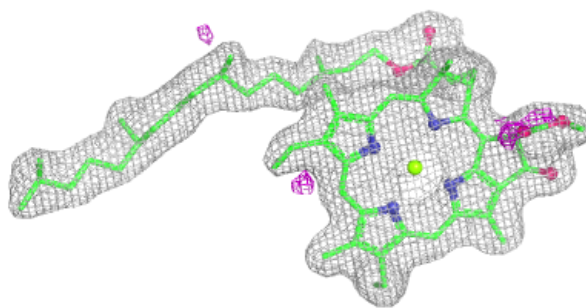
**Electron density around BCR t 101:**

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



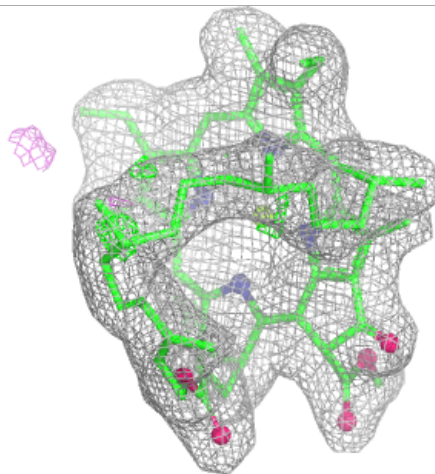
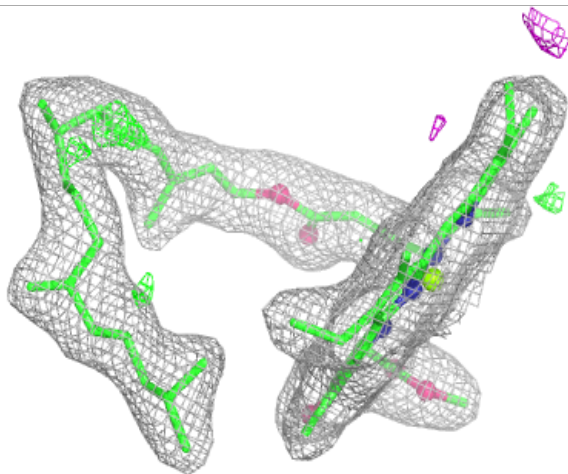
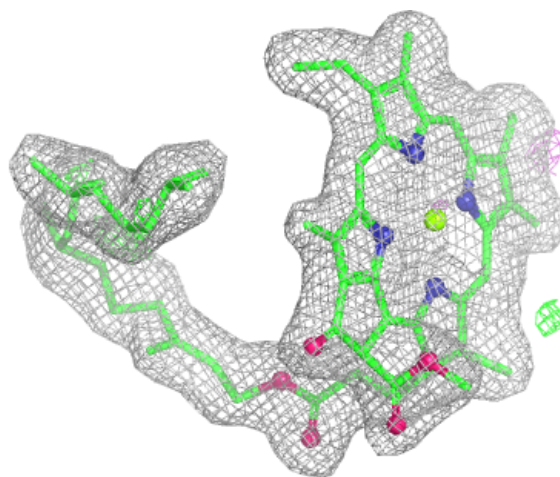
Electron density around CLA C 501:

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



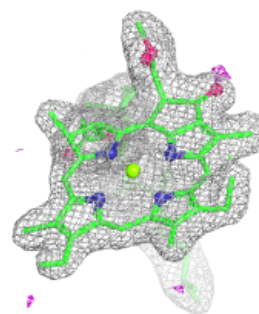
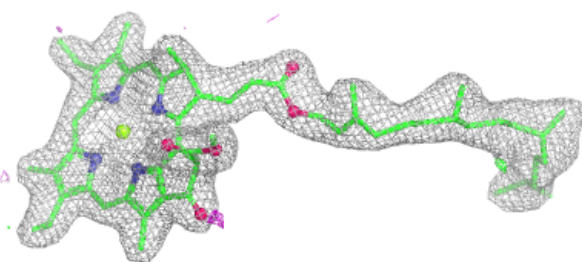
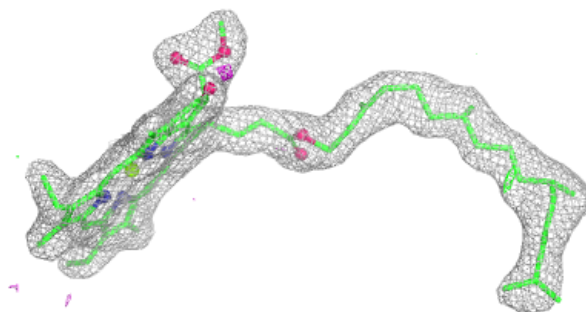
Electron density around CLA C 503:

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

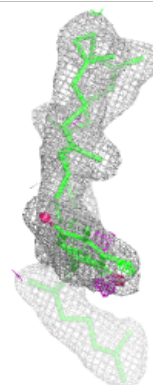
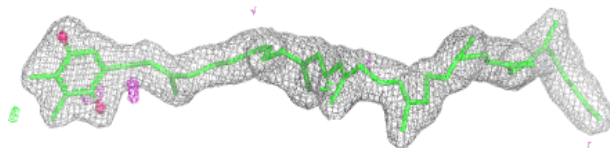
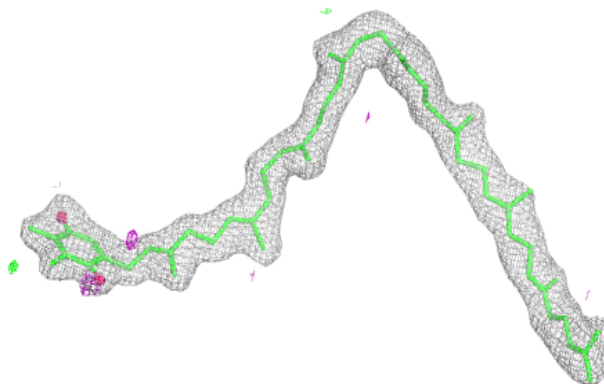


Electron density around CLA d 403:

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

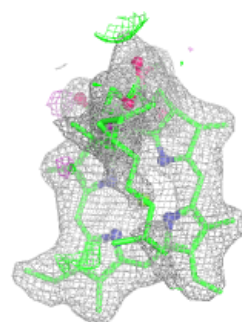
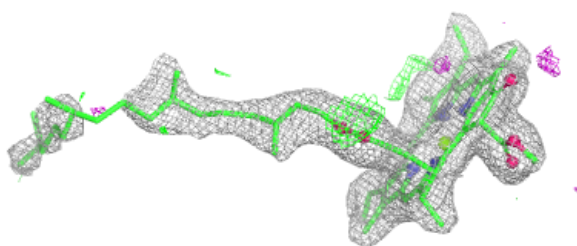
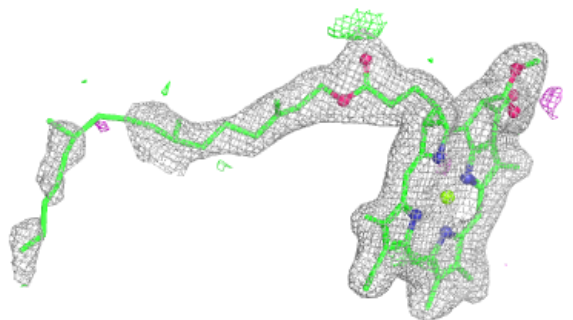
**Electron density around PL9 d 406:**

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

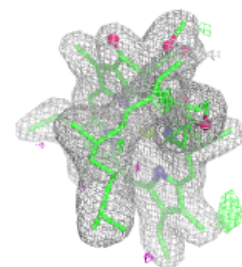
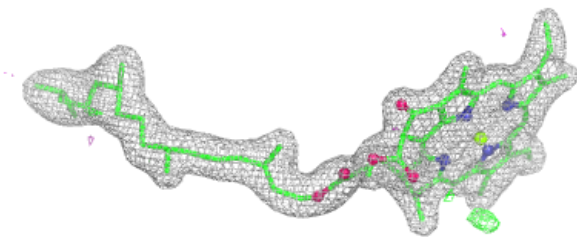
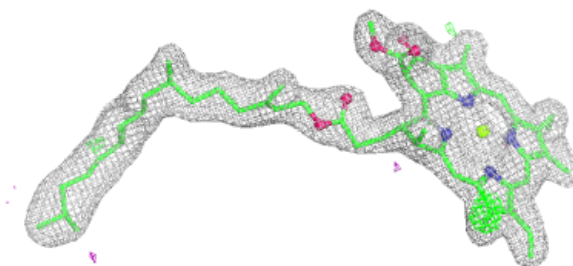


Electron density around CLA d 404:

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

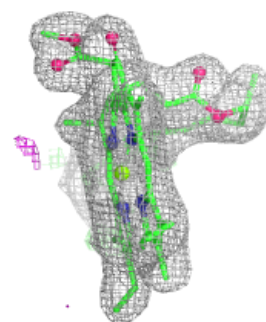
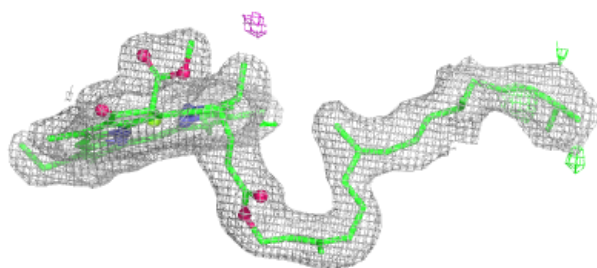
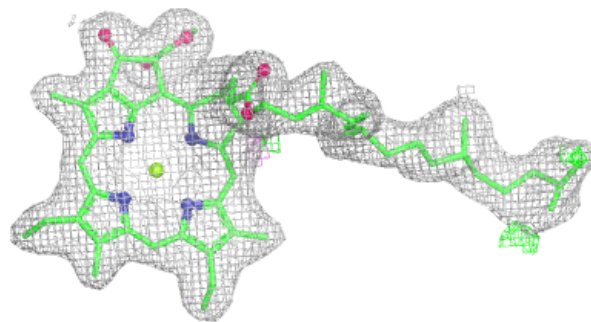
**Electron density around CLA a 607:**

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

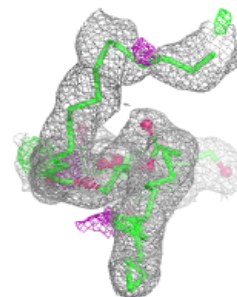
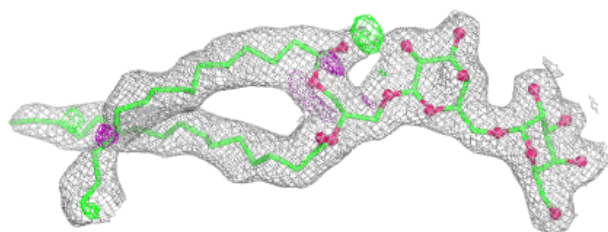
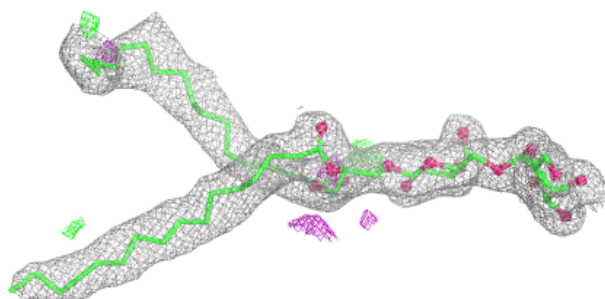


Electron density around CLA a 608:

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

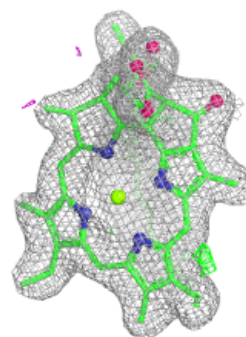
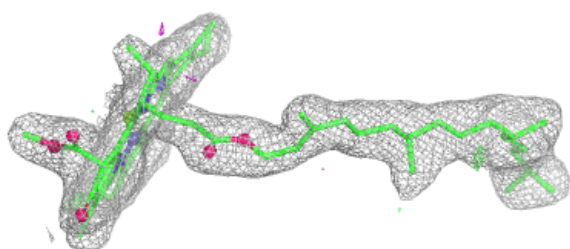
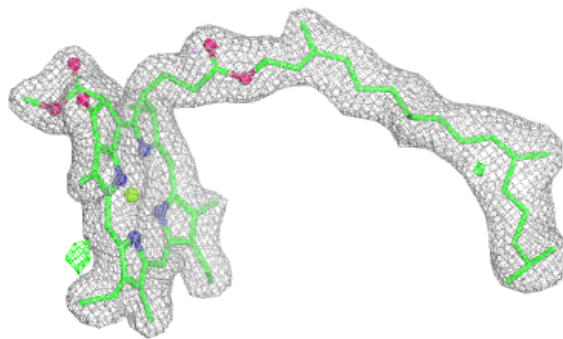
**Electron density around DGD c 515:**

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

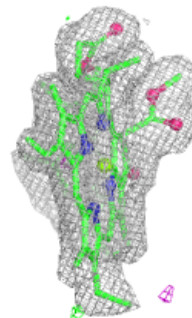
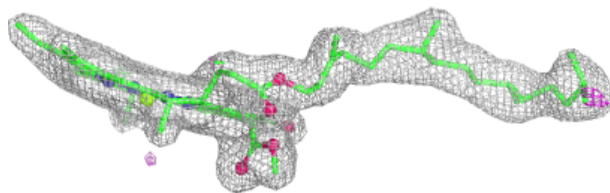
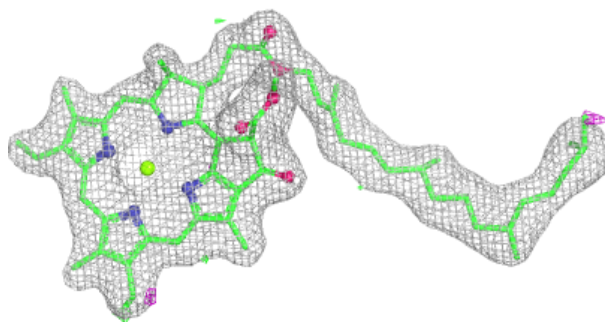


Electron density around CLA B 609:

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

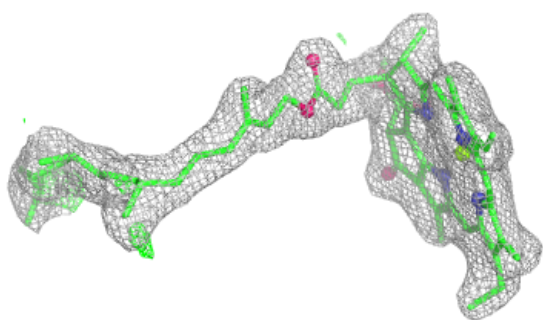
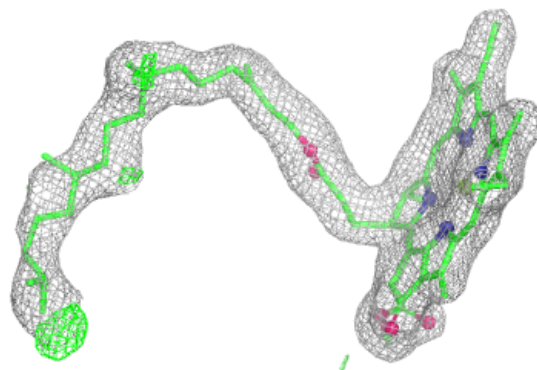
**Electron density around CLA b 602:**

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

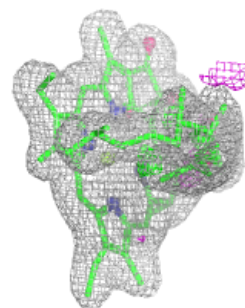
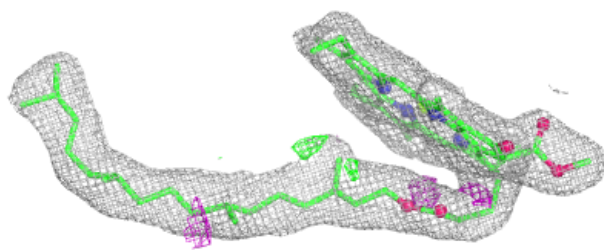
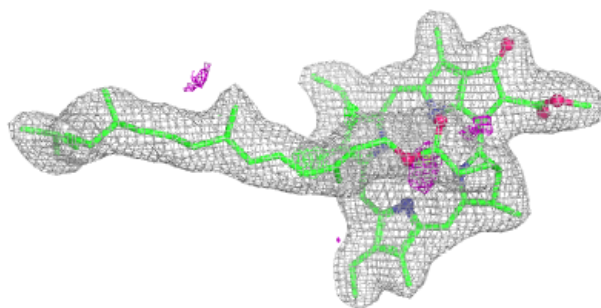


Electron density around CLA b 606:

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

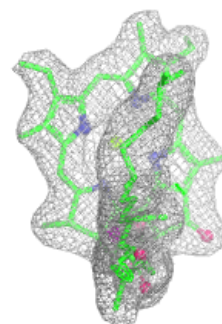
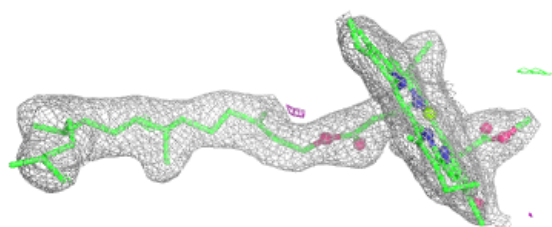
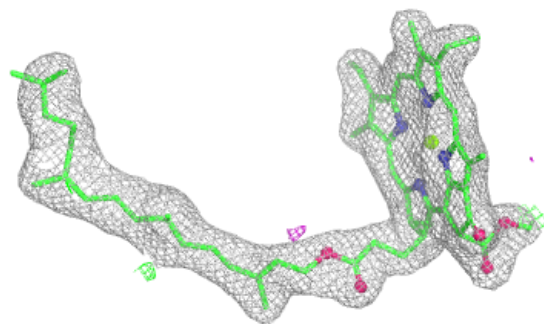
**Electron density around CLA b 608:**

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

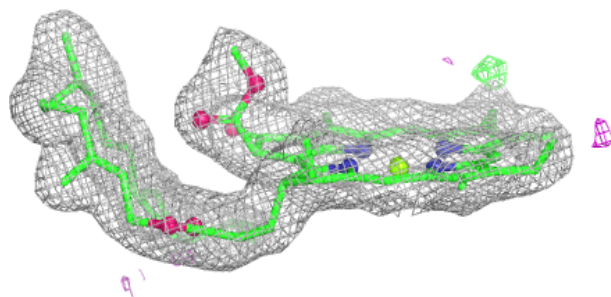
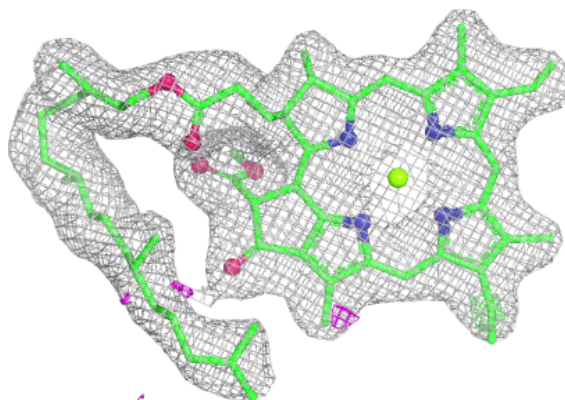


Electron density around CLA b 609:

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

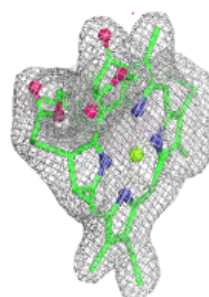
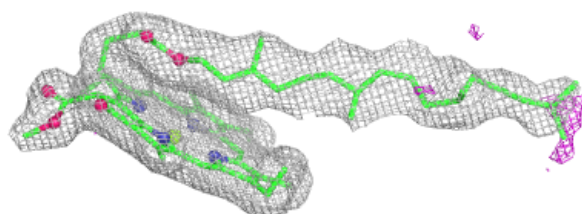
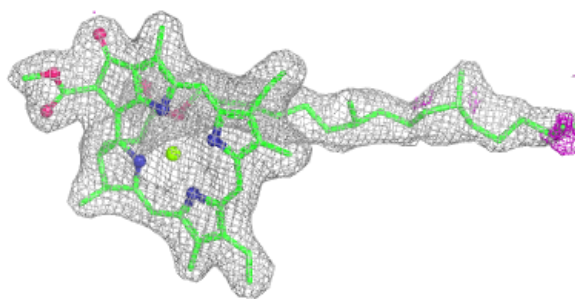
**Electron density around CLA b 610:**

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



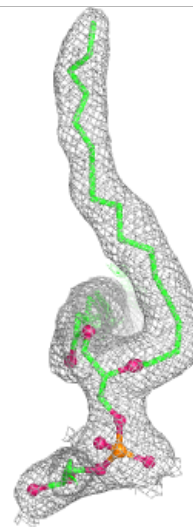
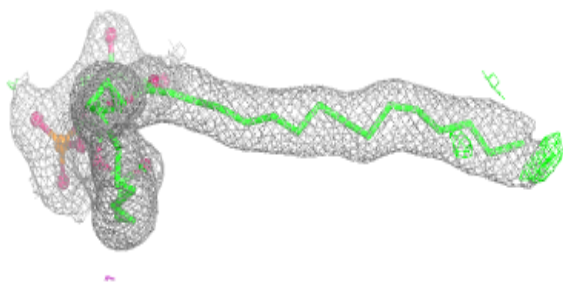
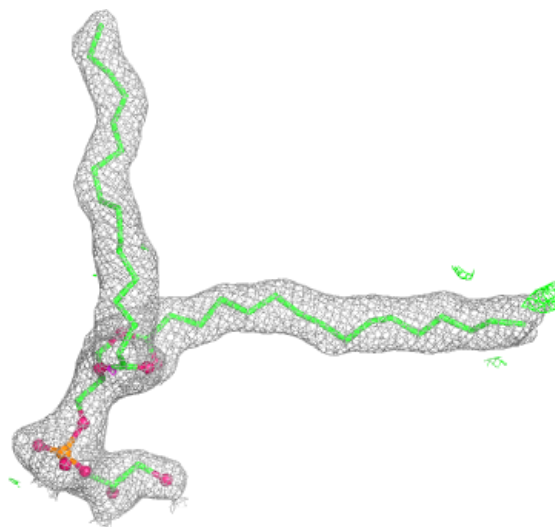
Electron density around CLA b 614:

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



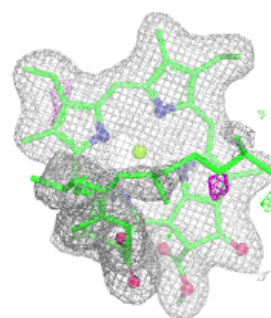
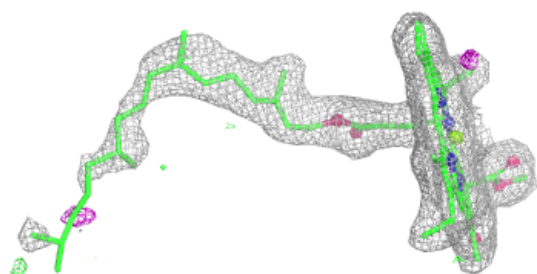
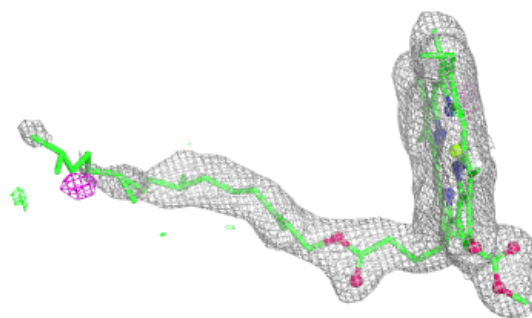
Electron density around LHG L 101:

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

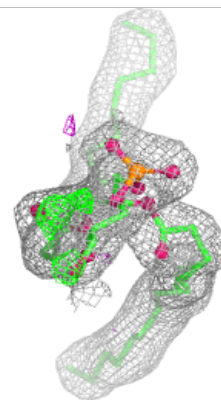
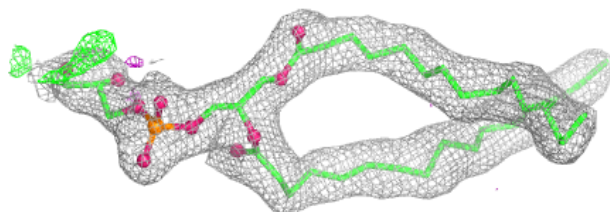
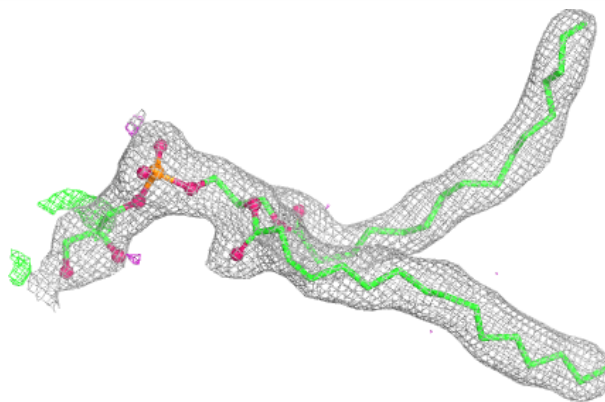


Electron density around CLA D 405:

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

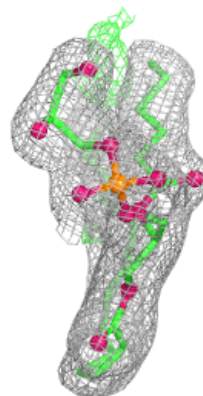
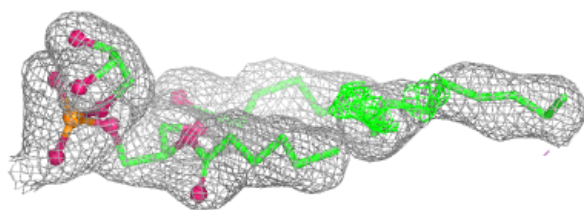
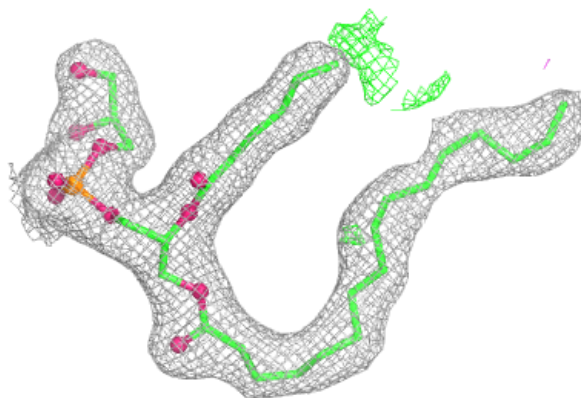
**Electron density around LHG d 408:**

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



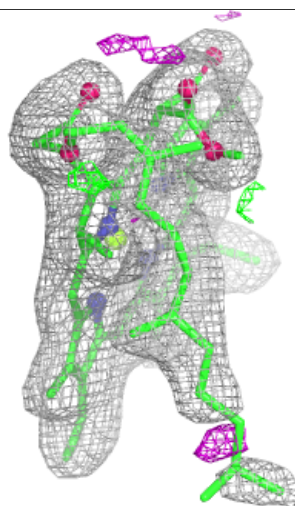
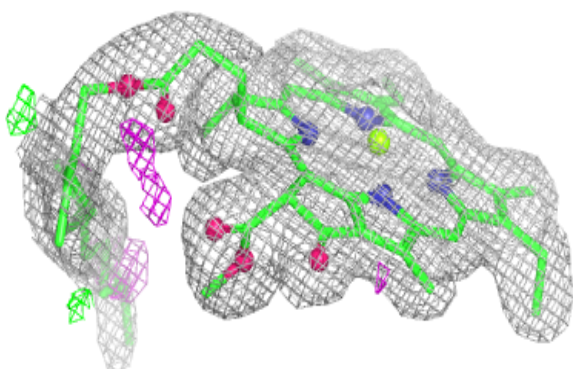
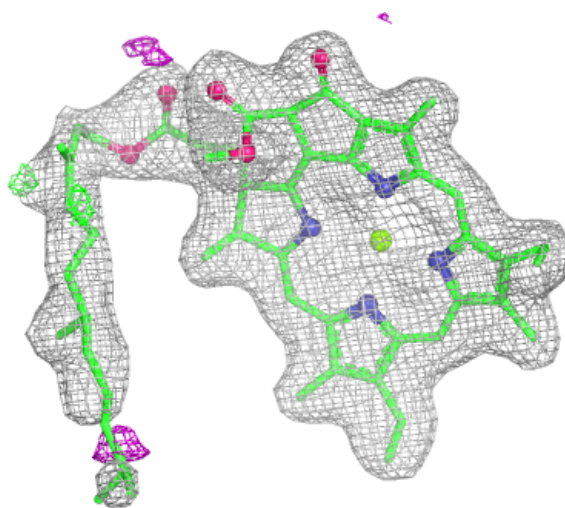
Electron density around LHG d 409:

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



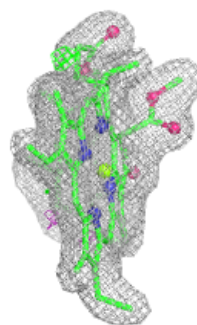
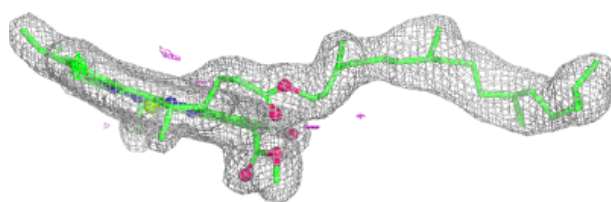
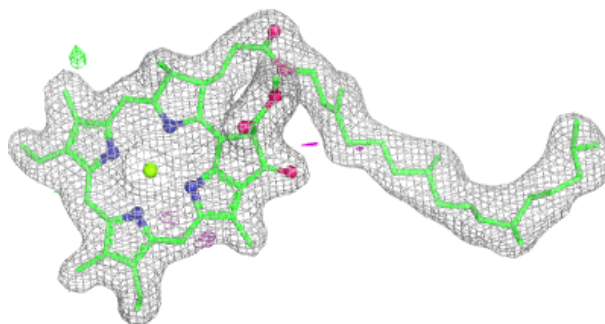
Electron density around CLA B 616:

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

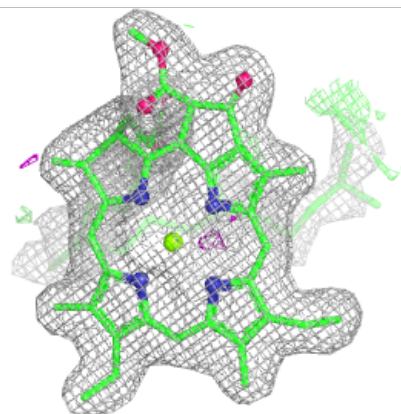
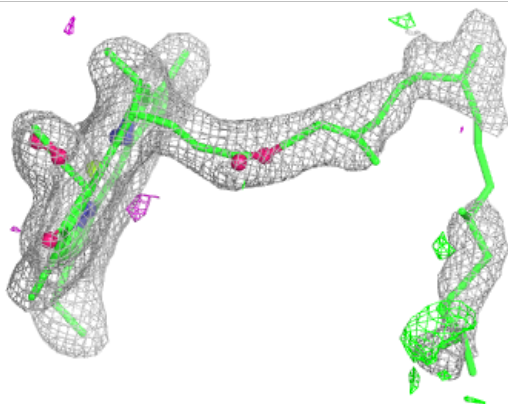
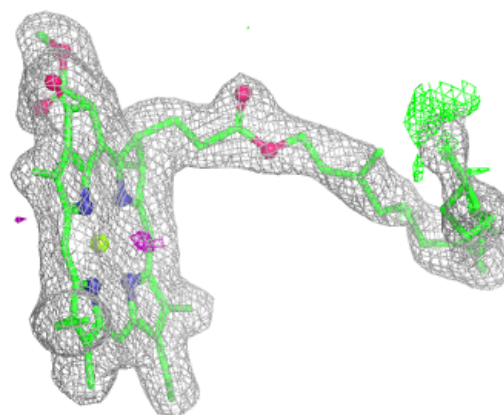


Electron density around CLA B 602:

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

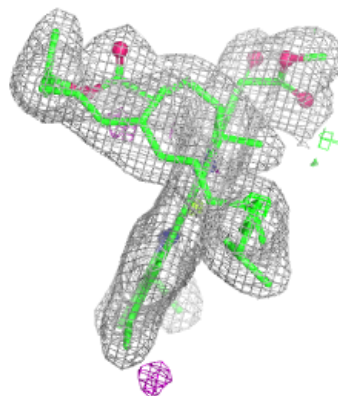
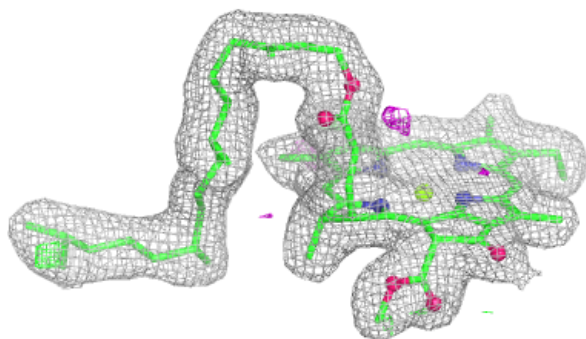
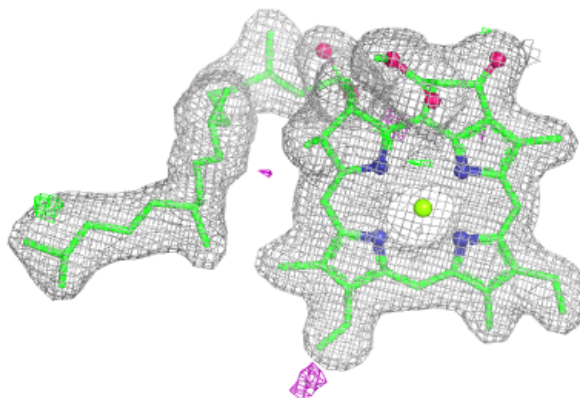
**Electron density around CLA a 609:**

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

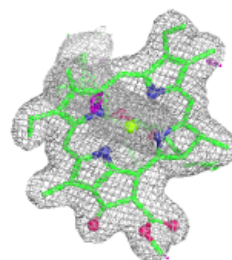
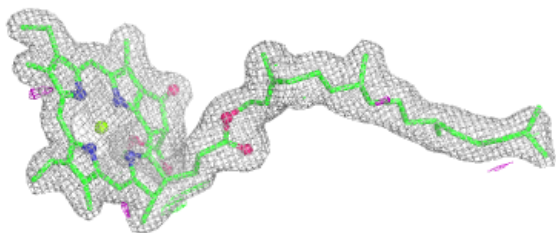
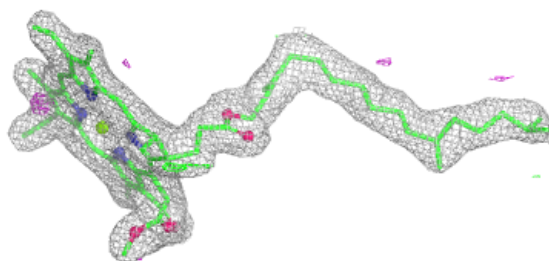


Electron density around CLA a 612:

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

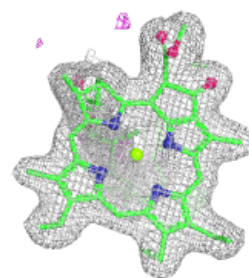
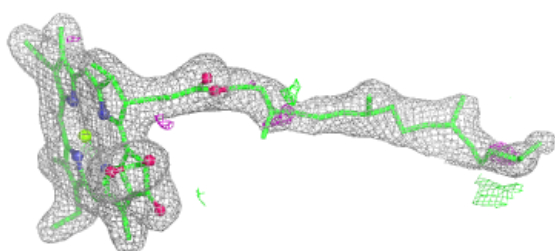
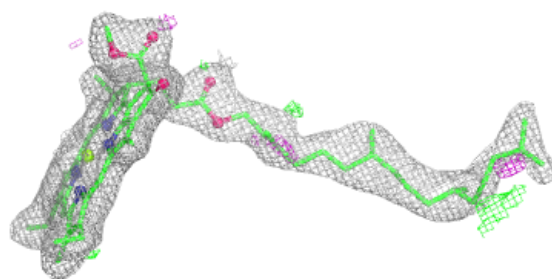
**Electron density around CLA C 502:**

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

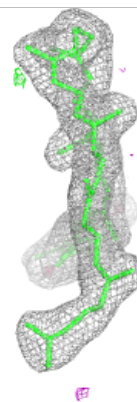
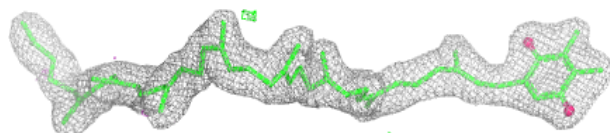
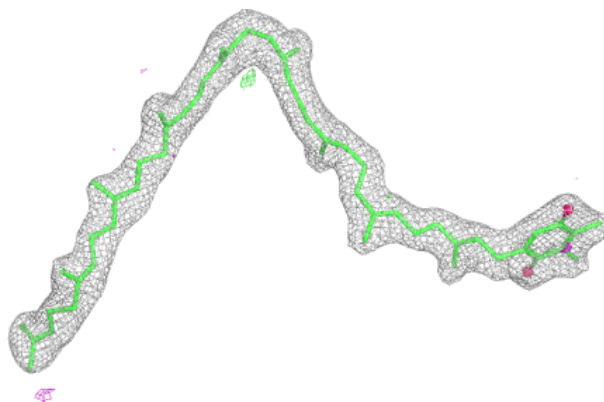


Electron density around CLA B 604:

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

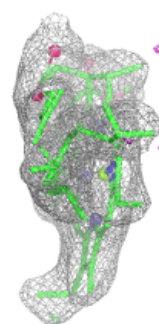
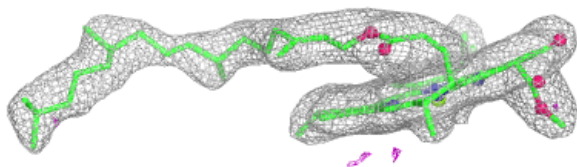
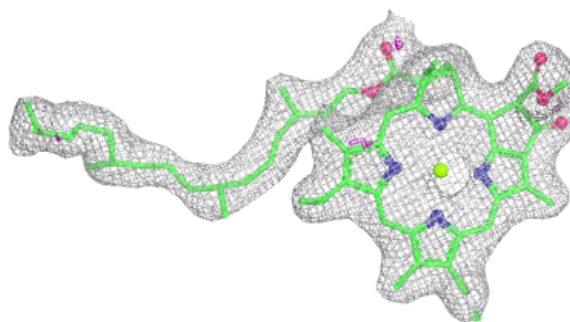
**Electron density around PL9 D 407:**

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

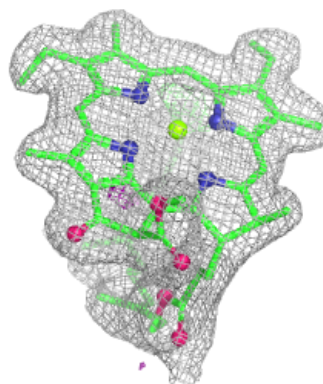
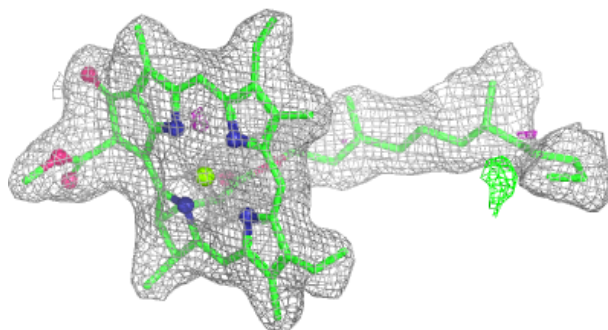
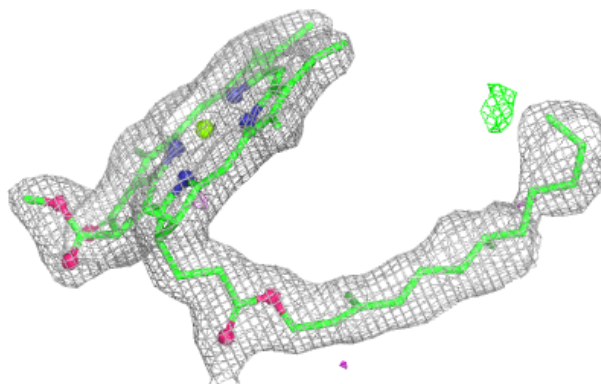


Electron density around CLA b 603:

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

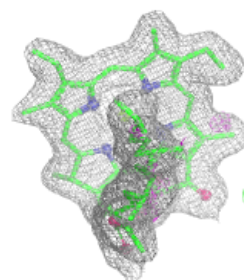
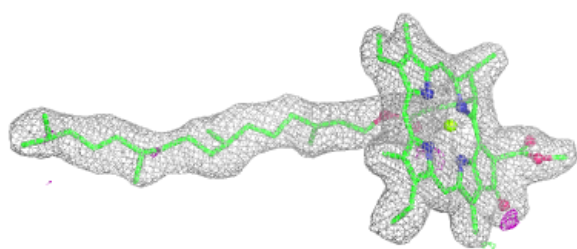
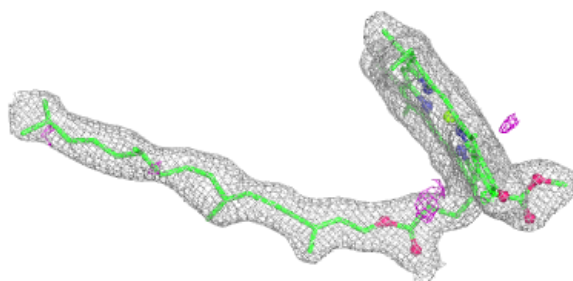
**Electron density around CLA C 504:**

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

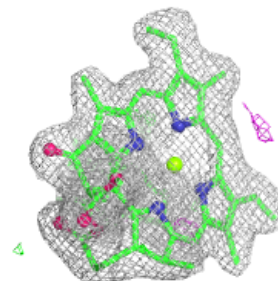
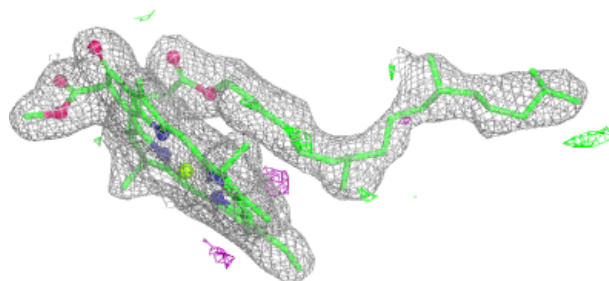
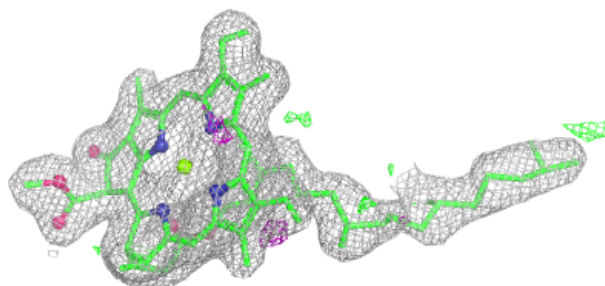


Electron density around CLA b 607:

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

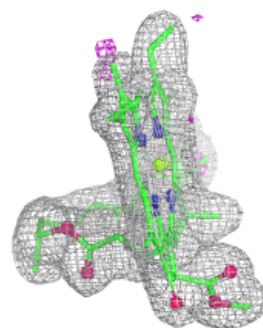
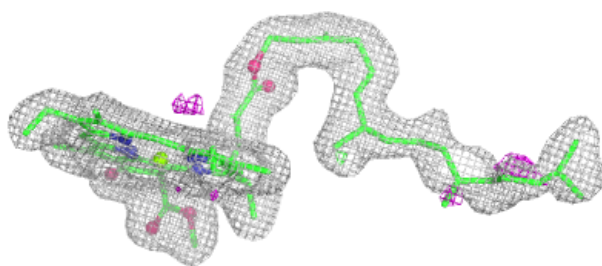
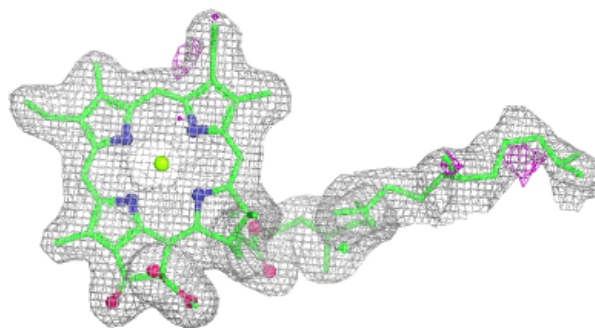
**Electron density around CLA C 505:**

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

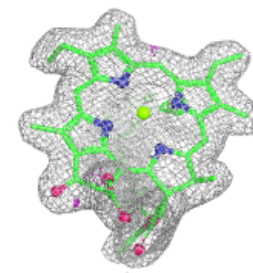
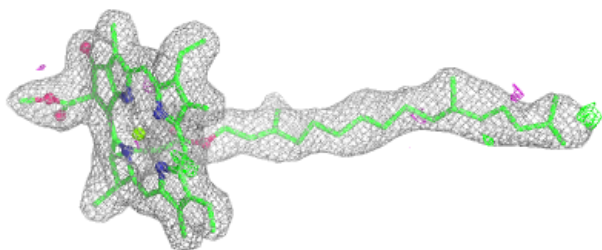
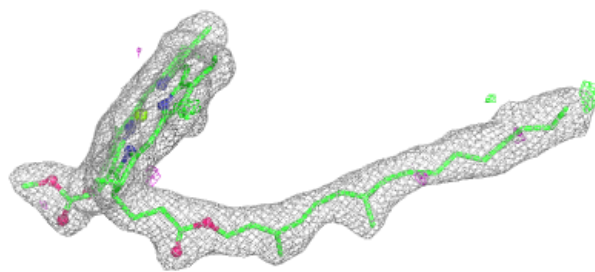


Electron density around CLA A 607:

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

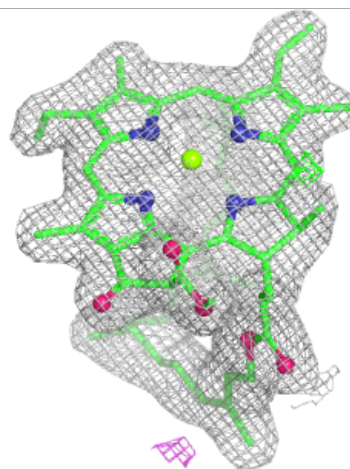
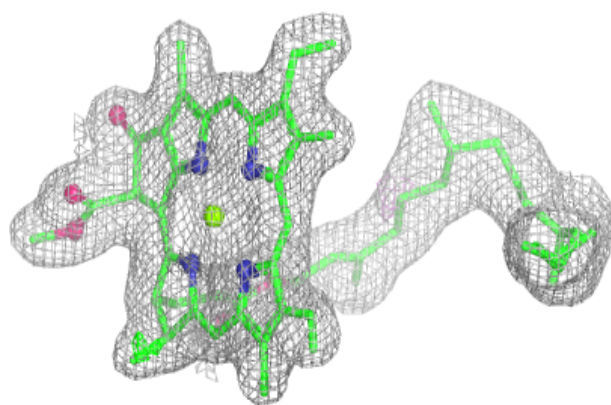
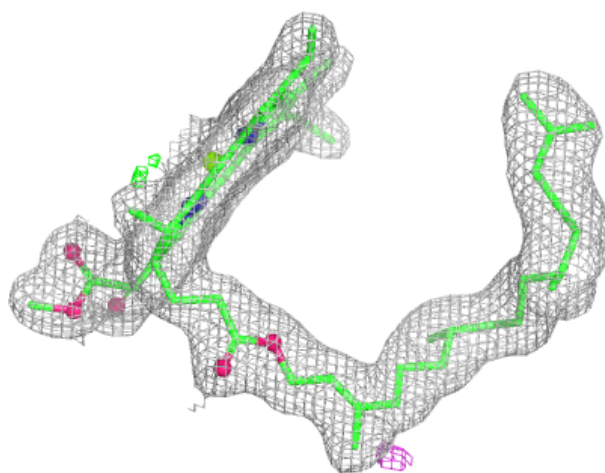
**Electron density around CLA B 607:**

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



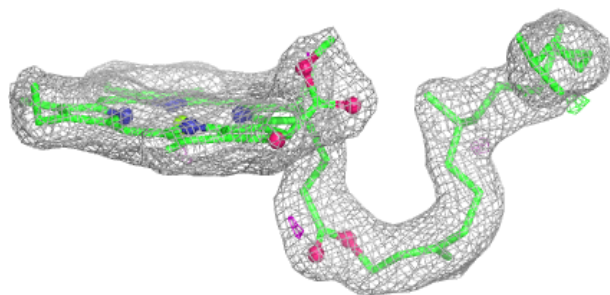
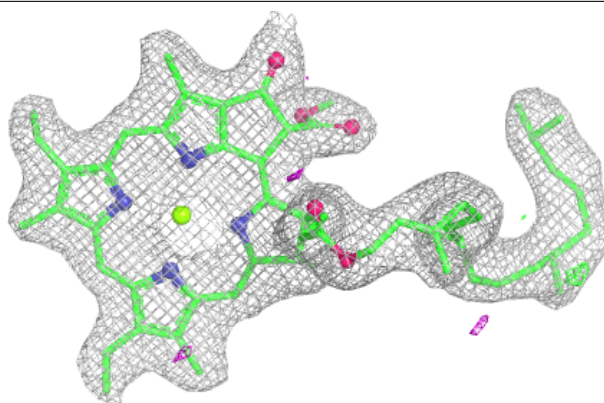
Electron density around CLA b 611:

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

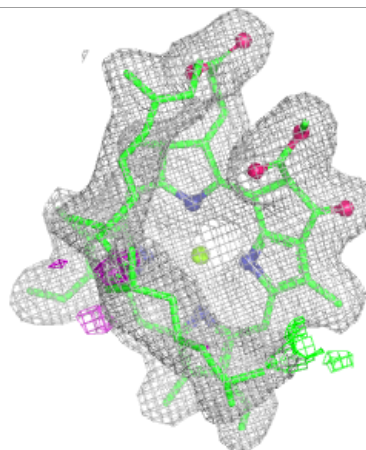
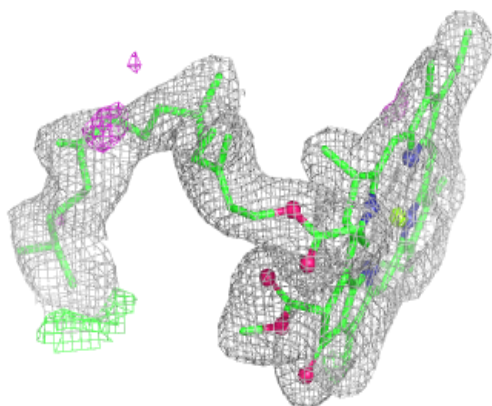
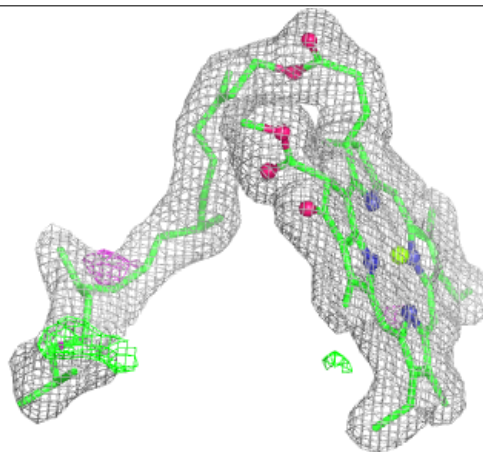


Electron density around CLA b 612:

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

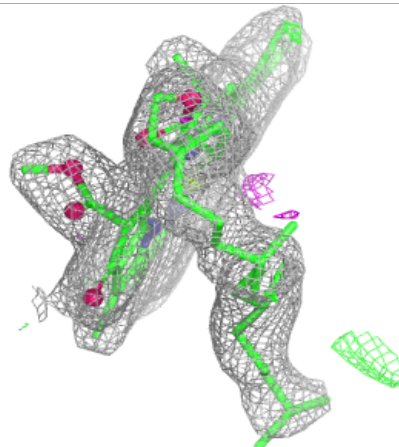
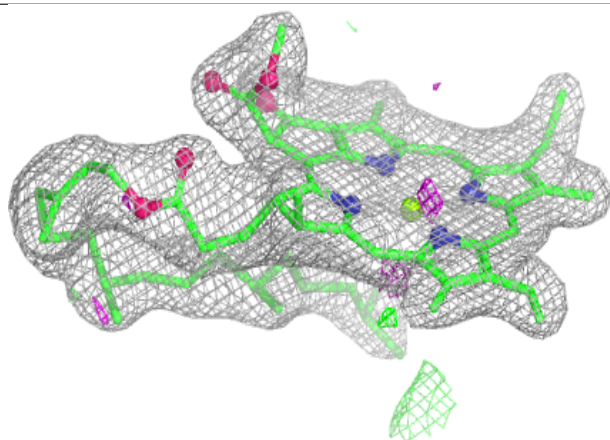
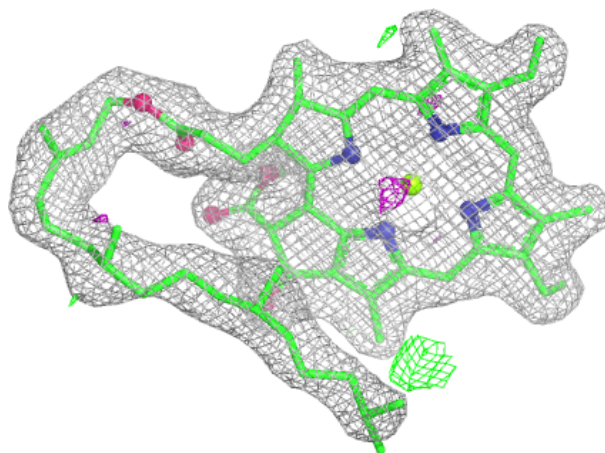
**Electron density around CLA b 613:**

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



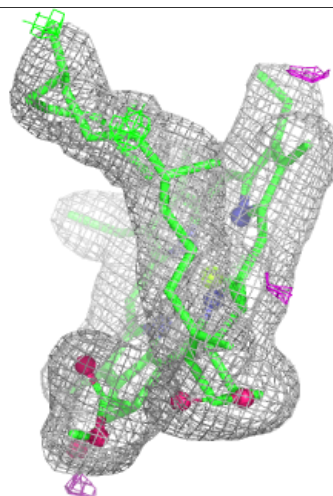
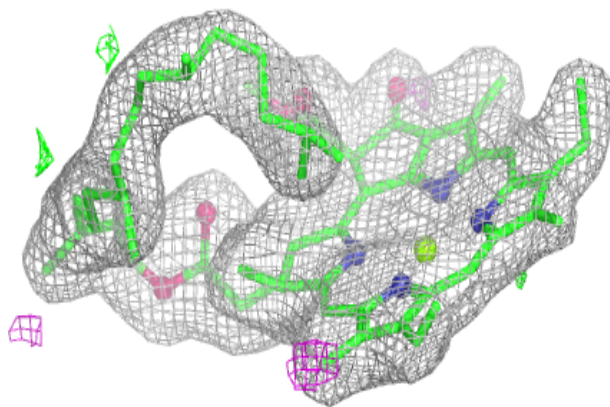
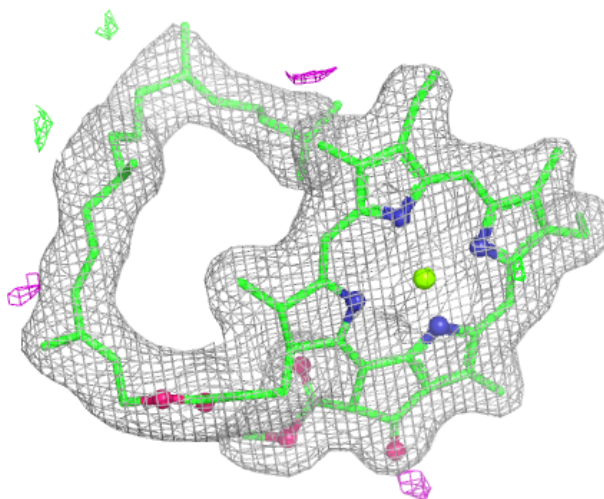
Electron density around CLA C 509:

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



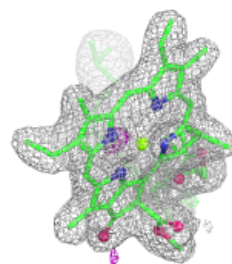
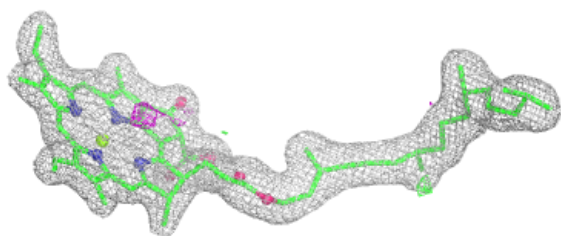
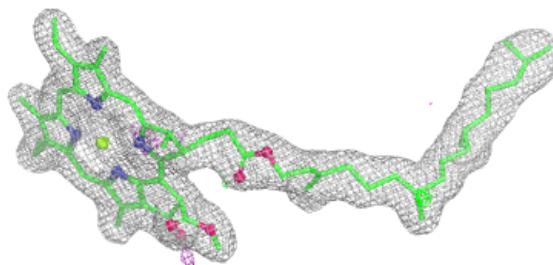
Electron density around CLA b 615:

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

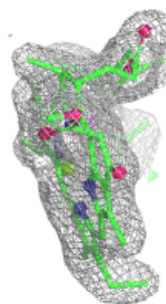
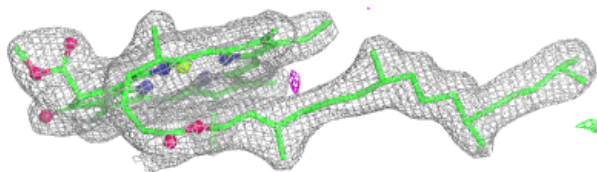
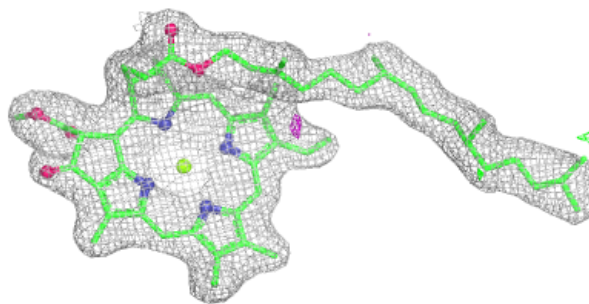


Electron density around CLA A 606:

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

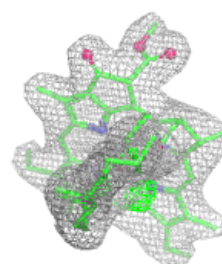
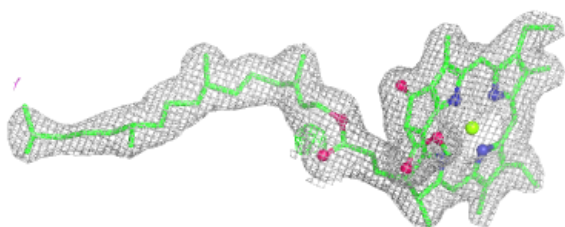
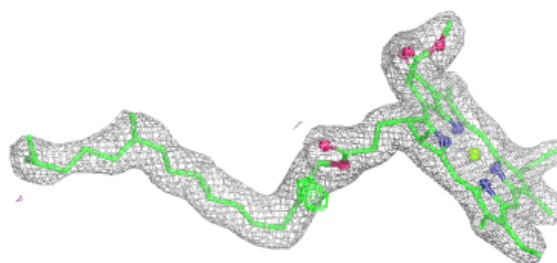
**Electron density around CLA c 501:**

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



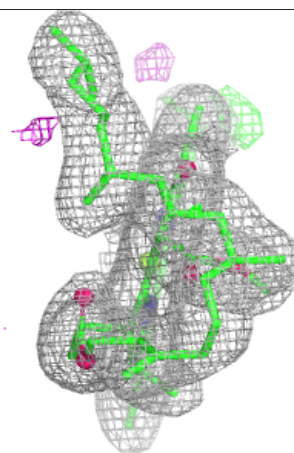
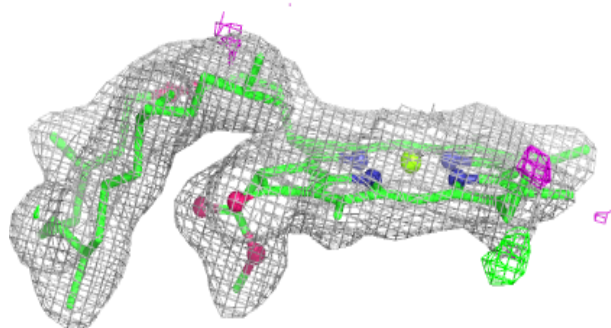
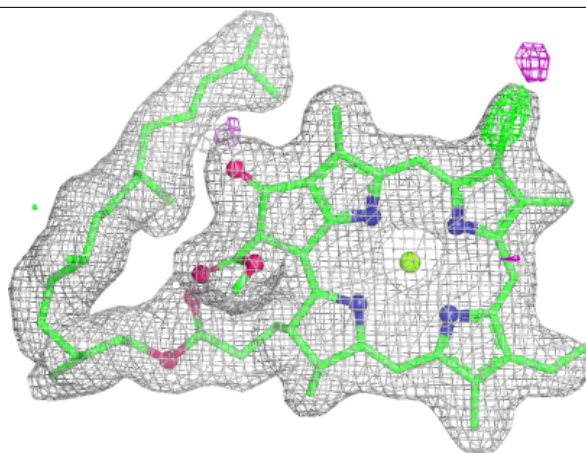
Electron density around CLA c 502:

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



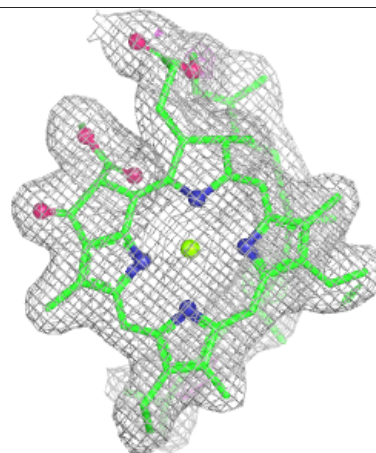
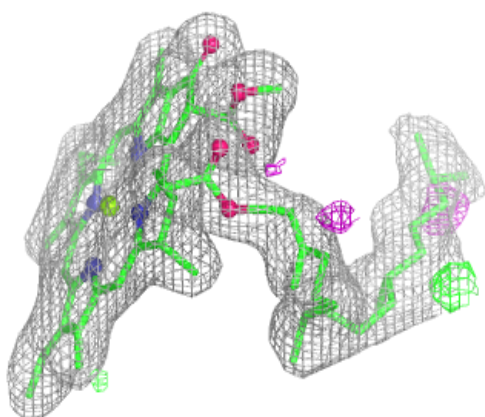
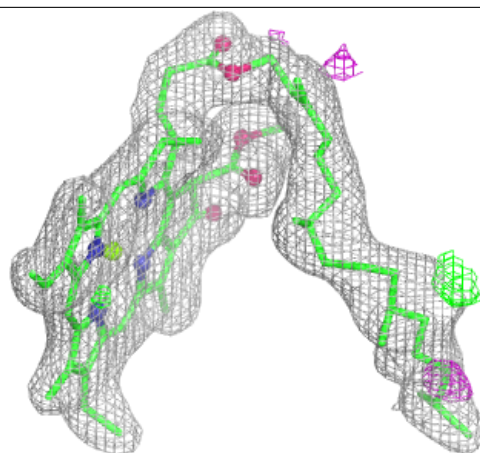
Electron density around CLA B 610:

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

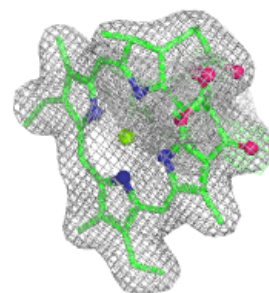
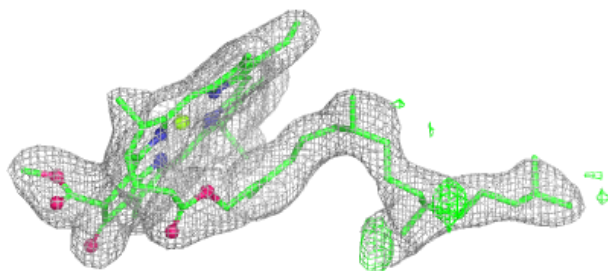
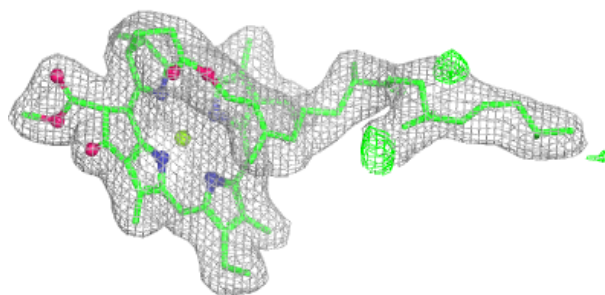


Electron density around CLA B 613:

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

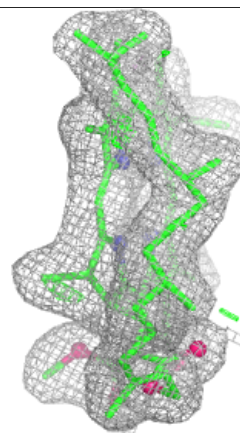
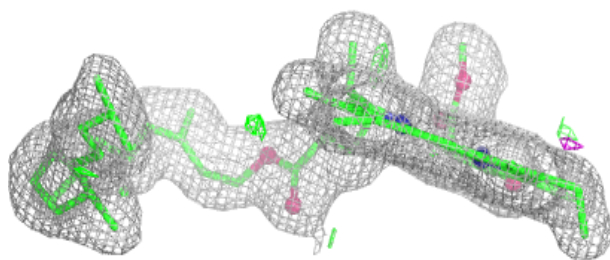
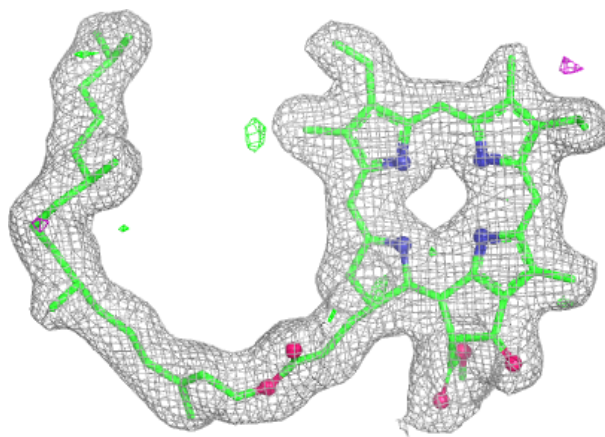
**Electron density around CLA c 505:**

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



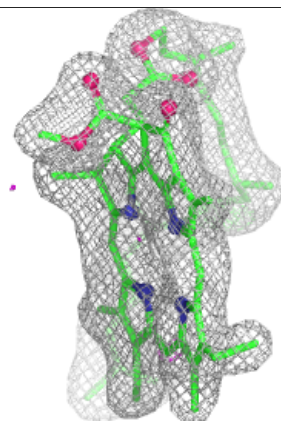
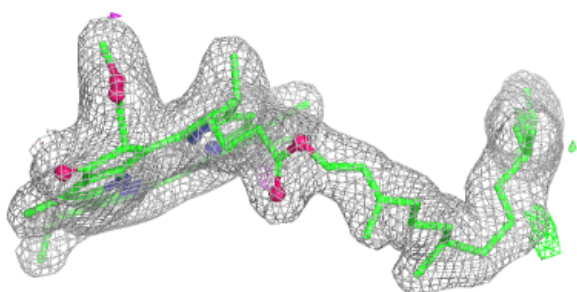
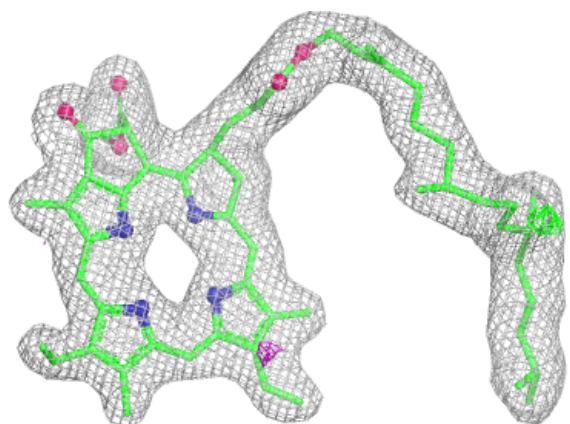
Electron density around PHO D 402:

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

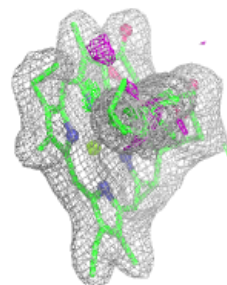
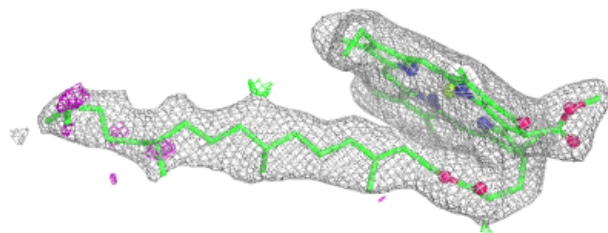
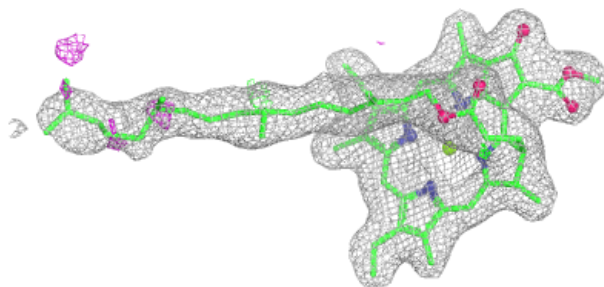


Electron density around PHO D 403:

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

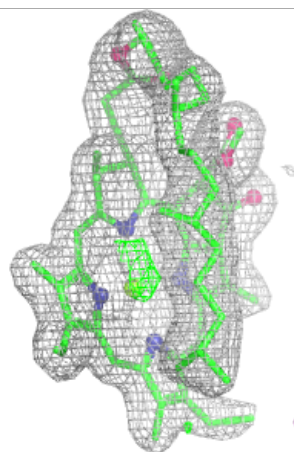
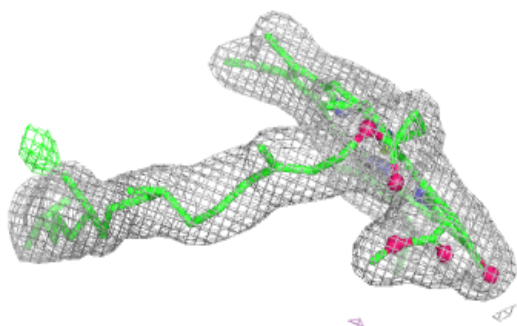
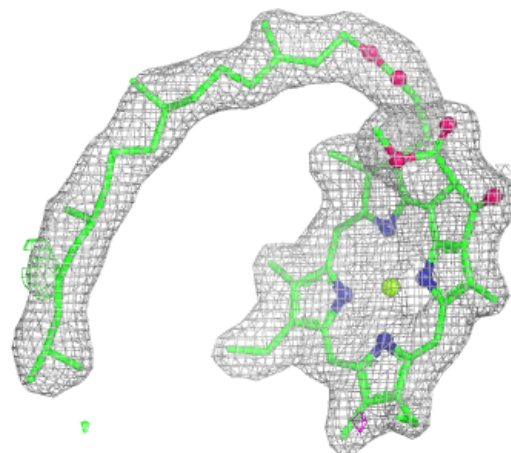
**Electron density around CLA B 614:**

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



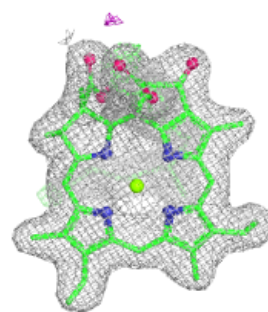
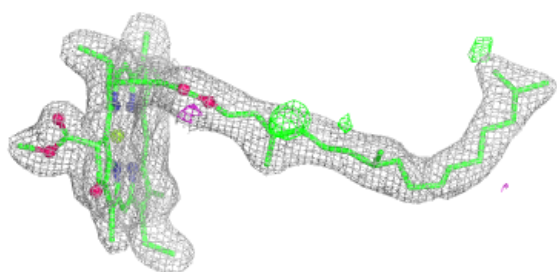
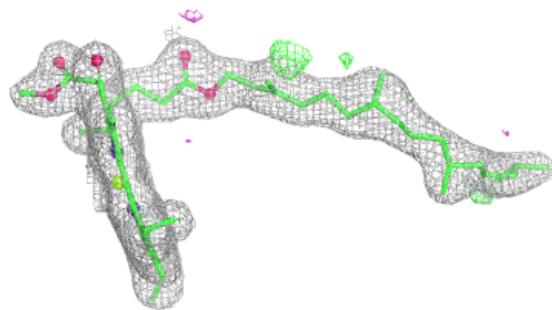
Electron density around CLA C 507:

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

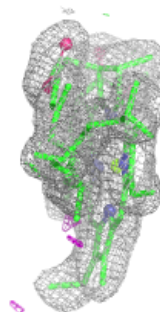
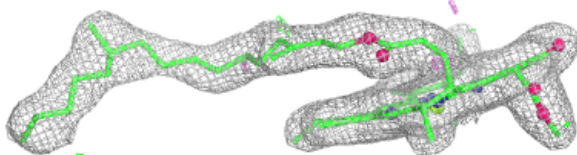
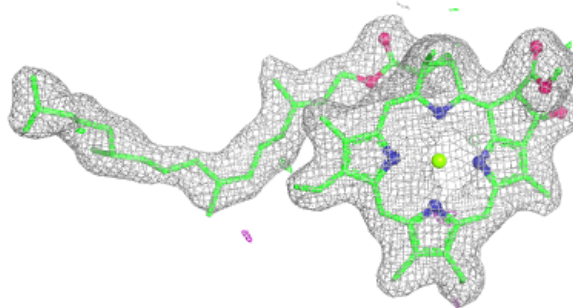


Electron density around CLA B 605:

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

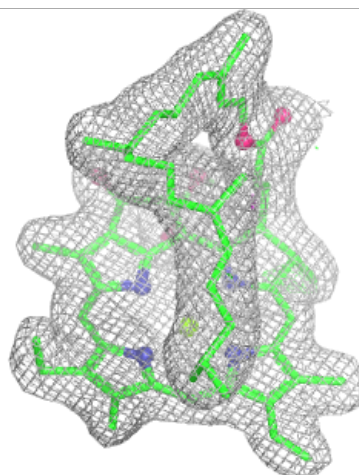
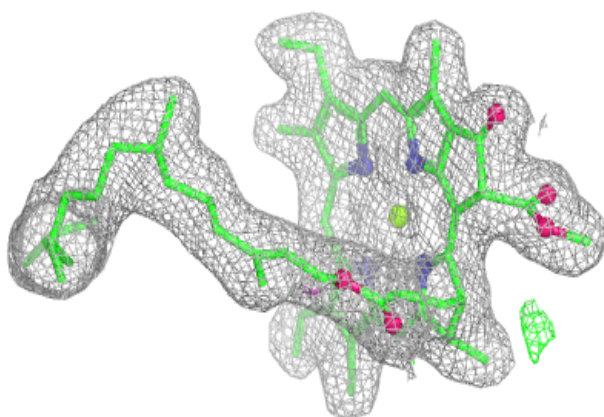
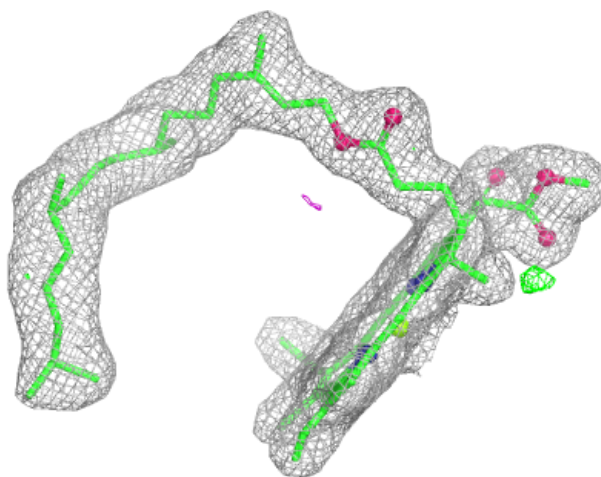
**Electron density around CLA B 603:**

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



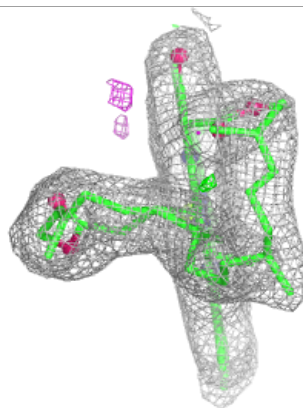
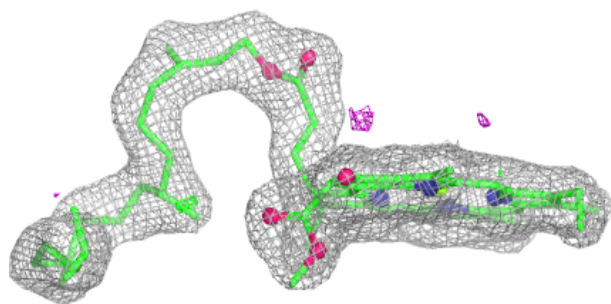
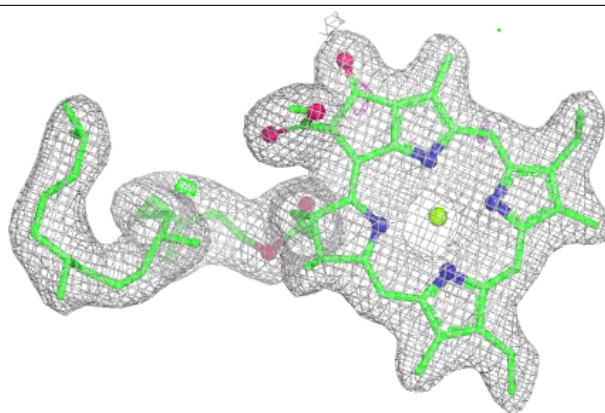
Electron density around CLA B 611:

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

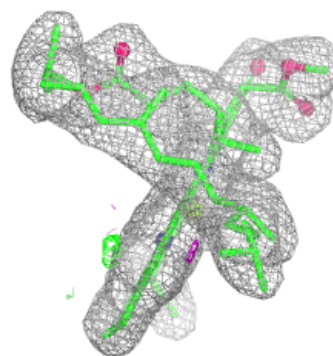
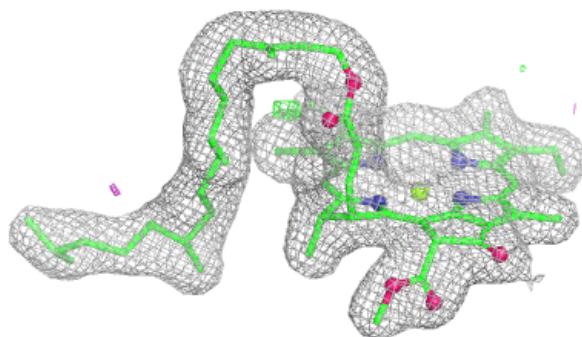
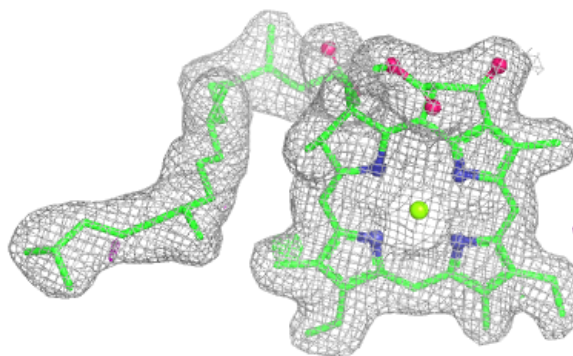


Electron density around CLA B 612:

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

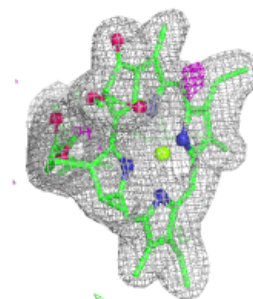
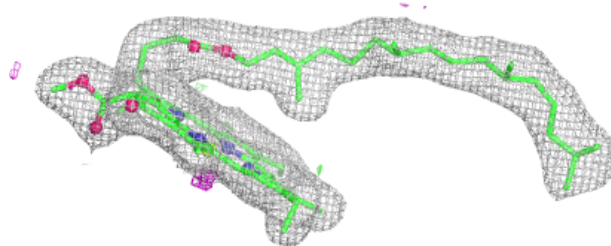
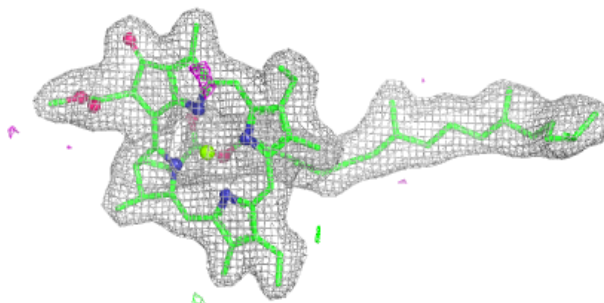
**Electron density around CLA A 611:**

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

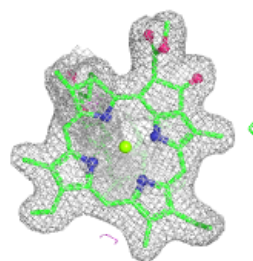
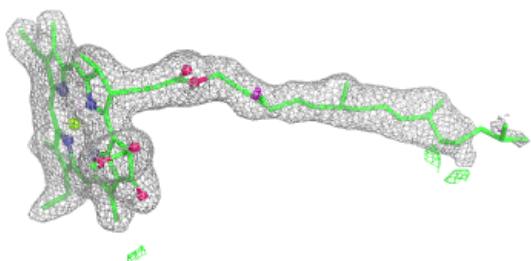
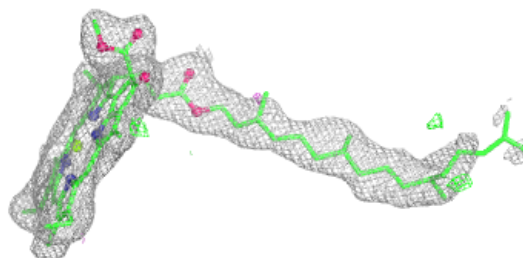


Electron density around CLA B 608:

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

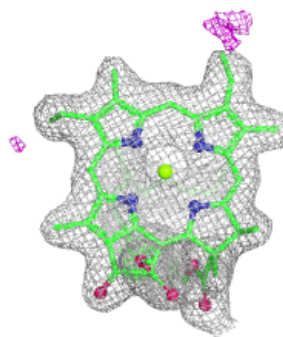
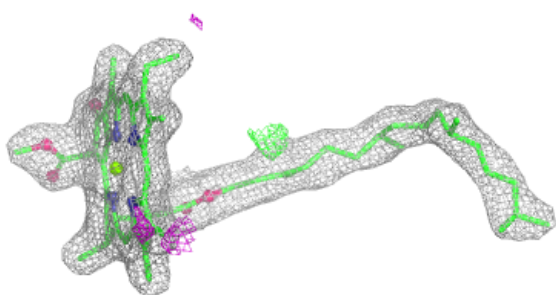
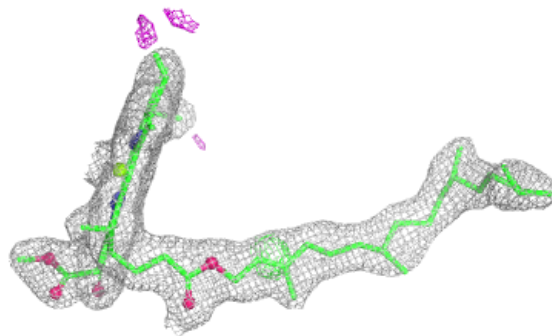
**Electron density around CLA b 604:**

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

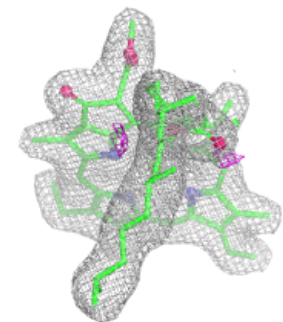
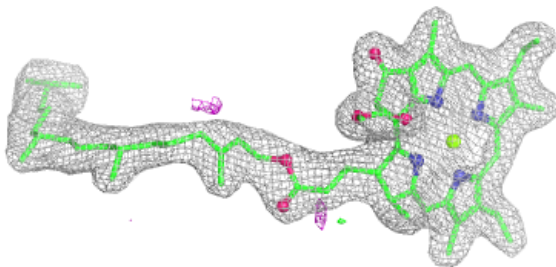
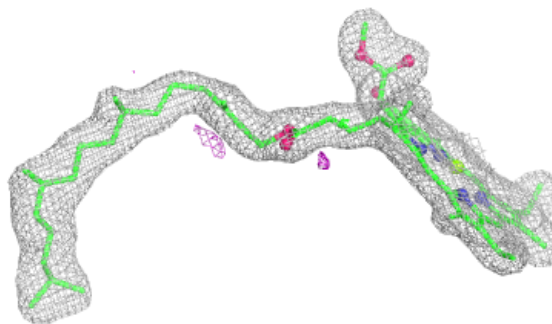


Electron density around CLA b 605:

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

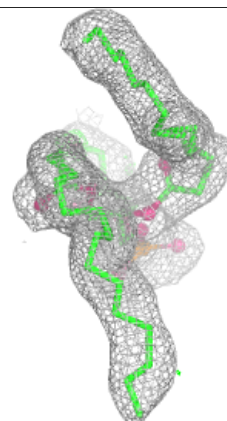
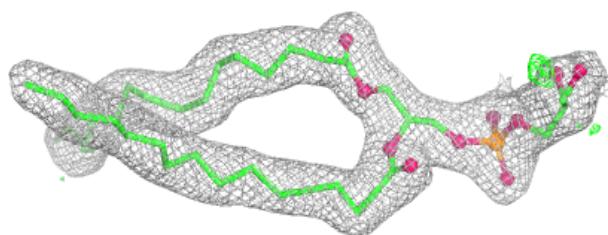
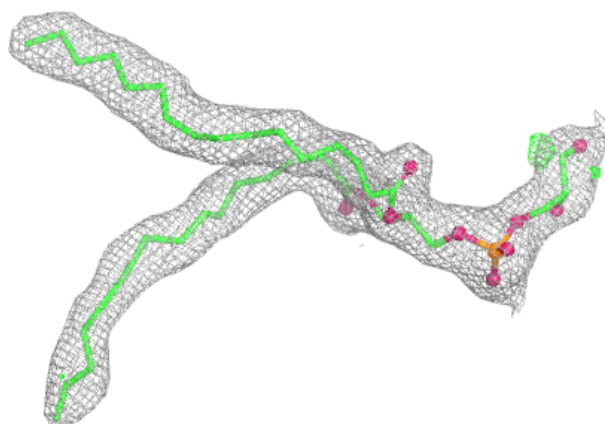
**Electron density around CLA D 404:**

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



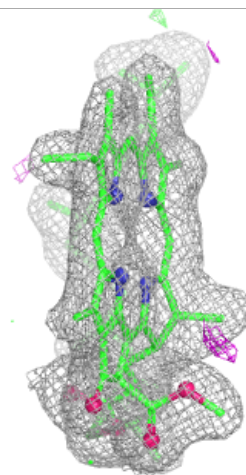
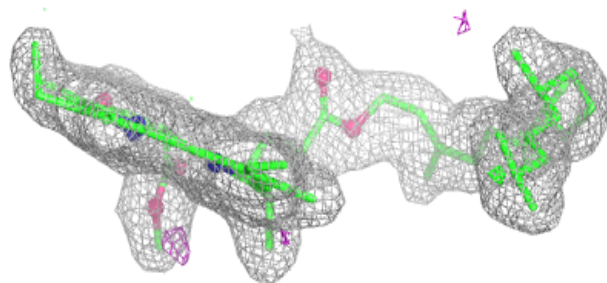
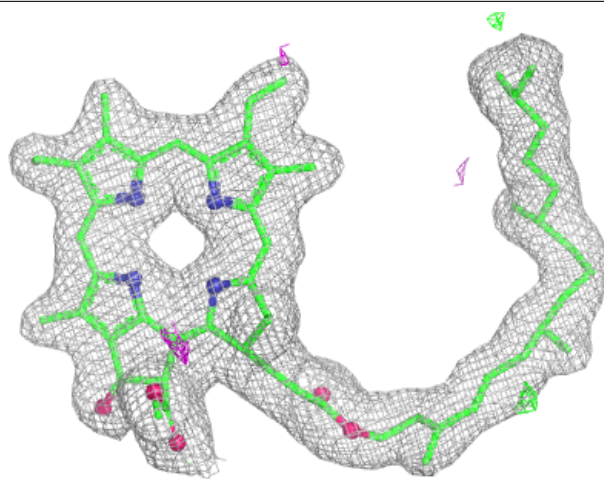
Electron density around LHG D 410:

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



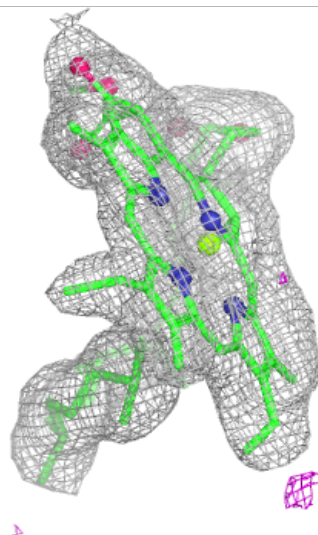
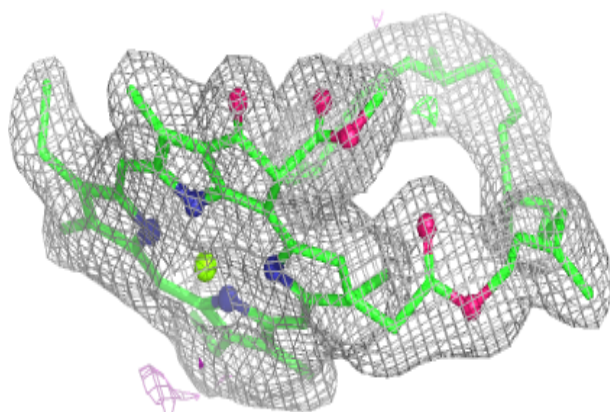
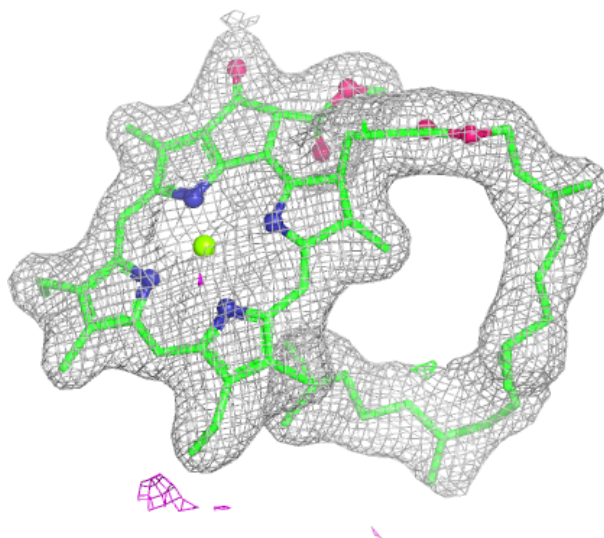
Electron density around PHO d 401:

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



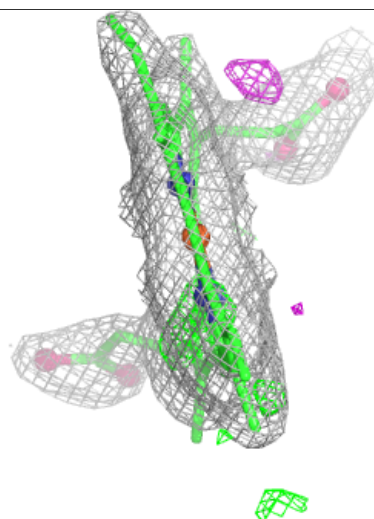
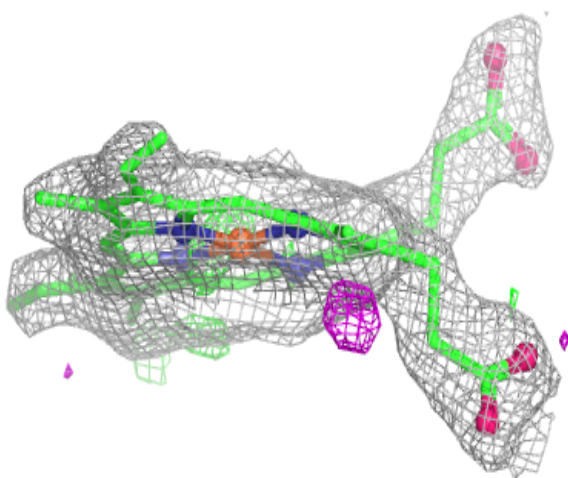
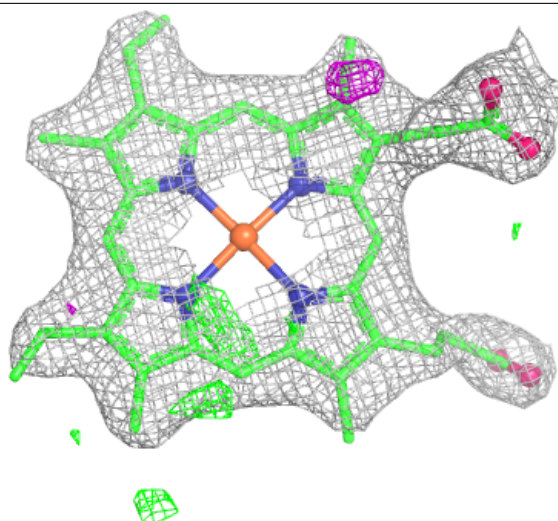
Electron density around CLA B 615:

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



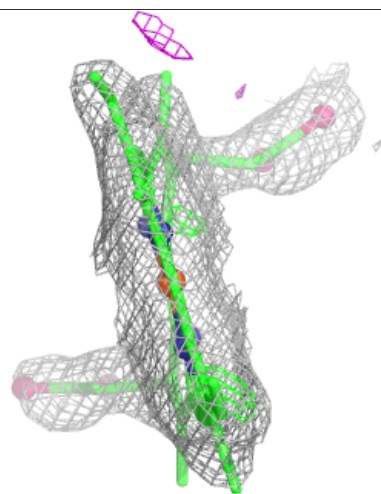
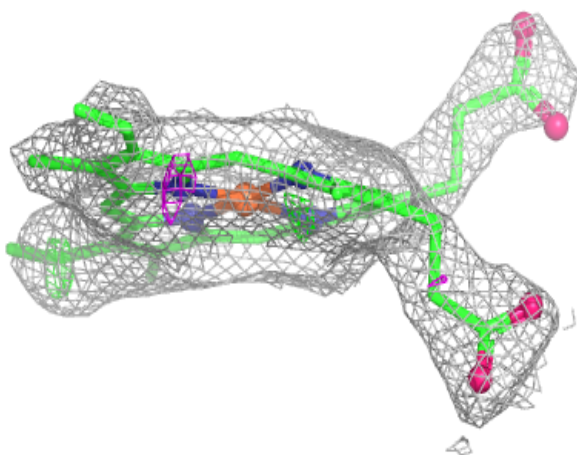
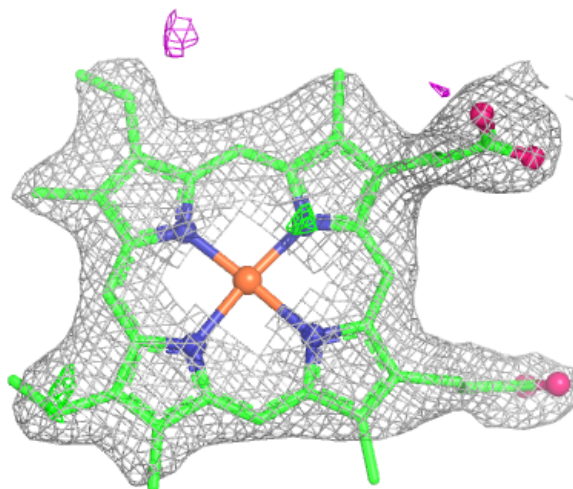
Electron density around HEM F 101:

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



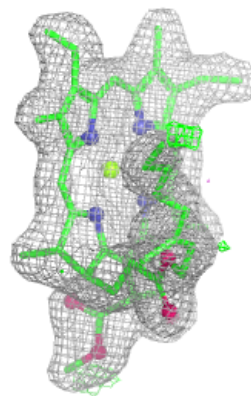
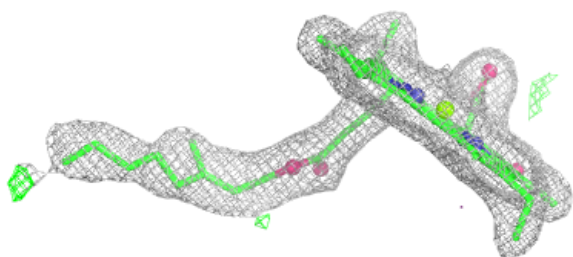
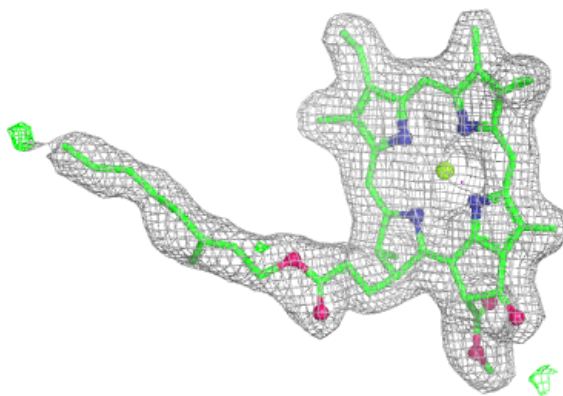
Electron density around HEM f 101:

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



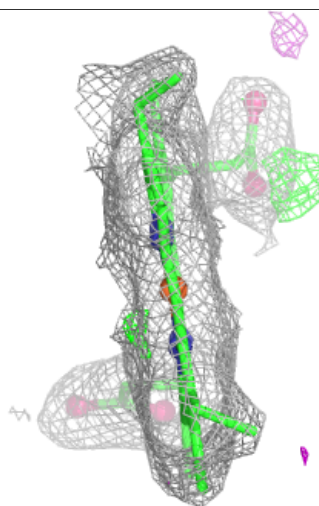
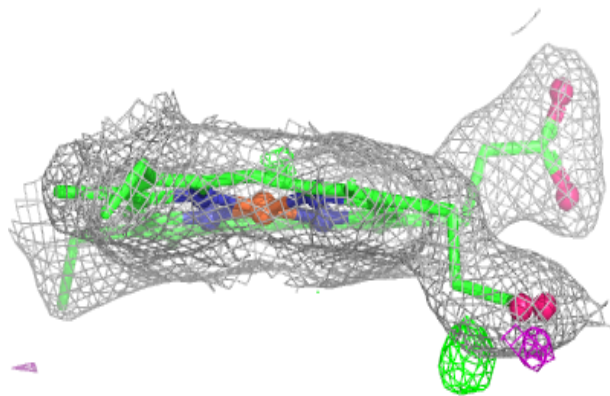
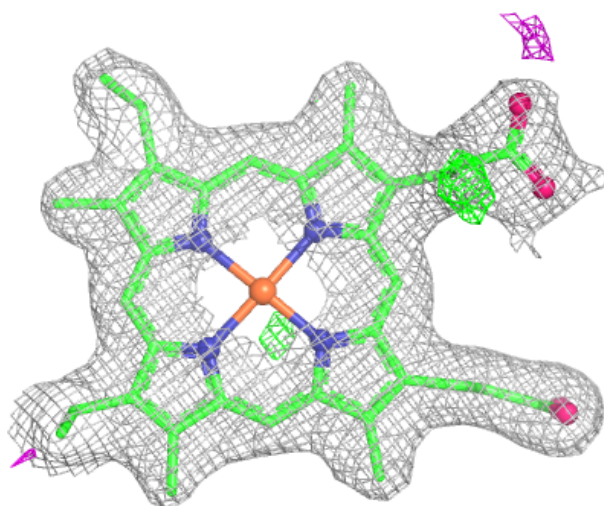
Electron density around CLA A 608:

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



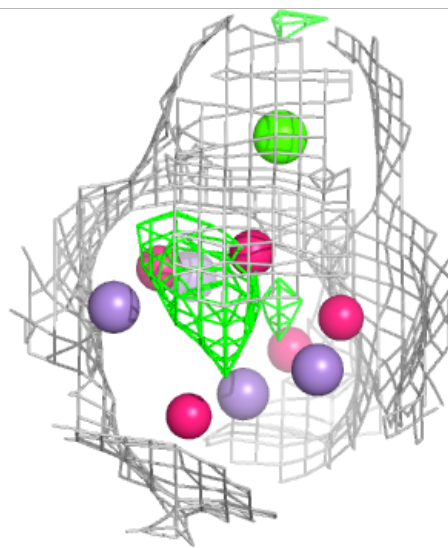
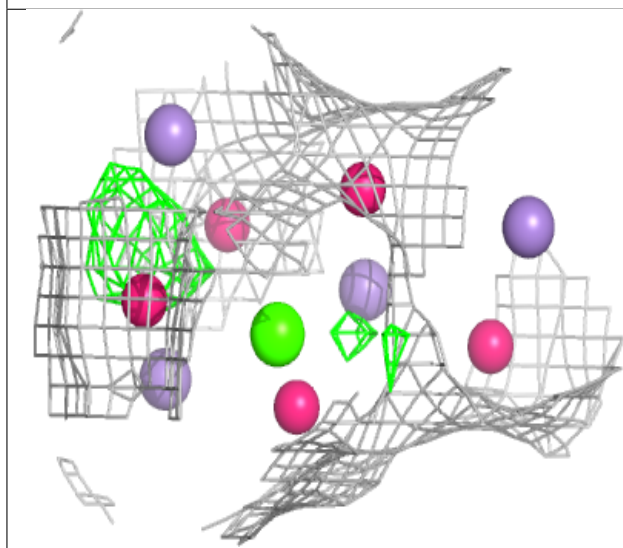
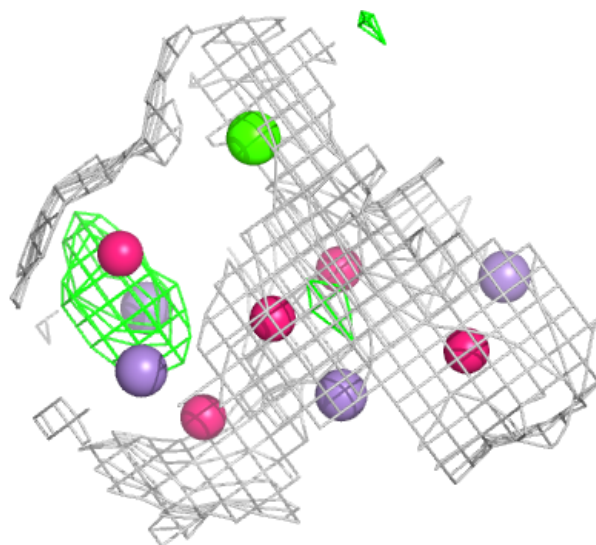
Electron density around HEC V 201:

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



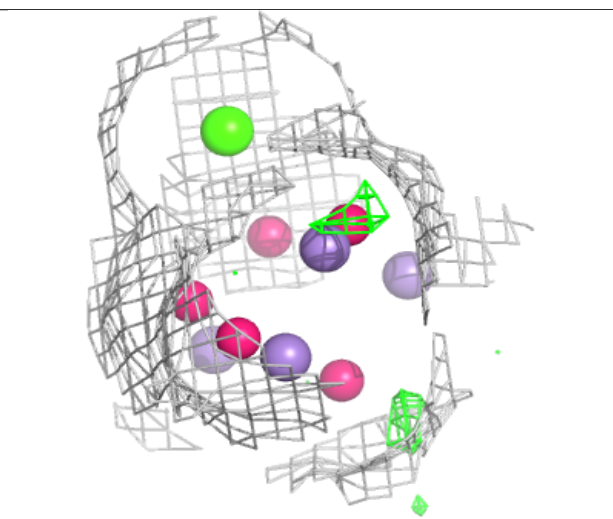
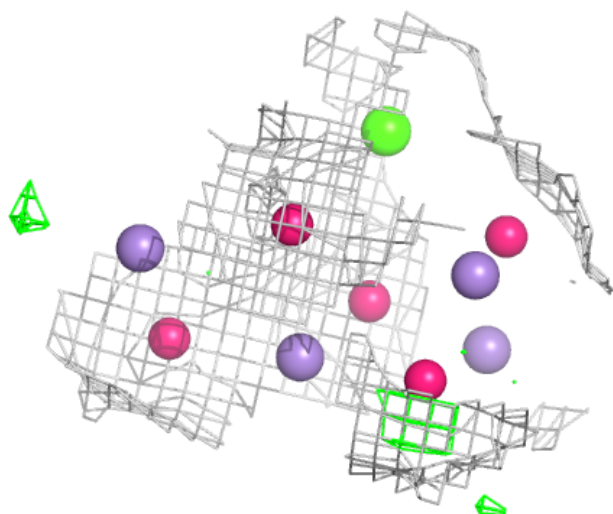
Electron density around OEX A 602 (A):

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



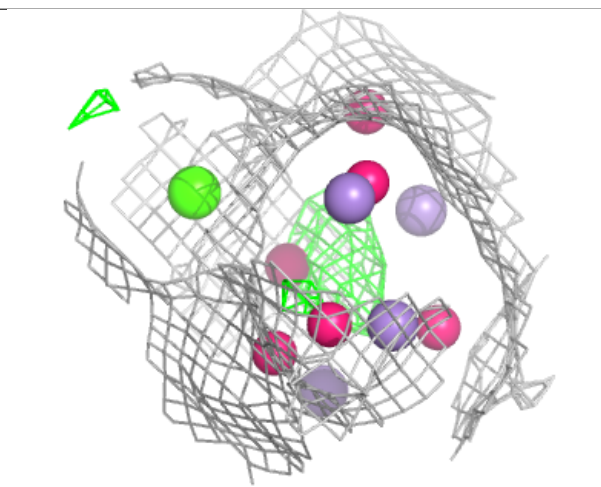
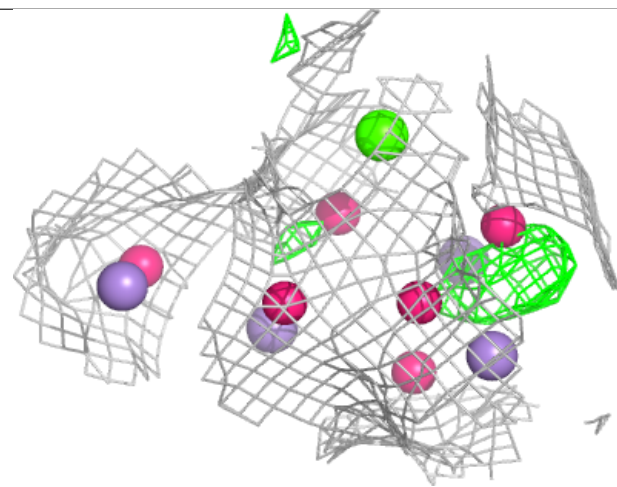
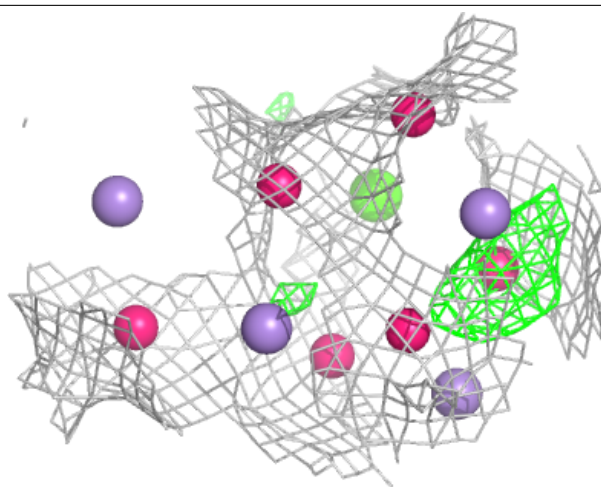
Electron density around OEX a 602 (A):

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



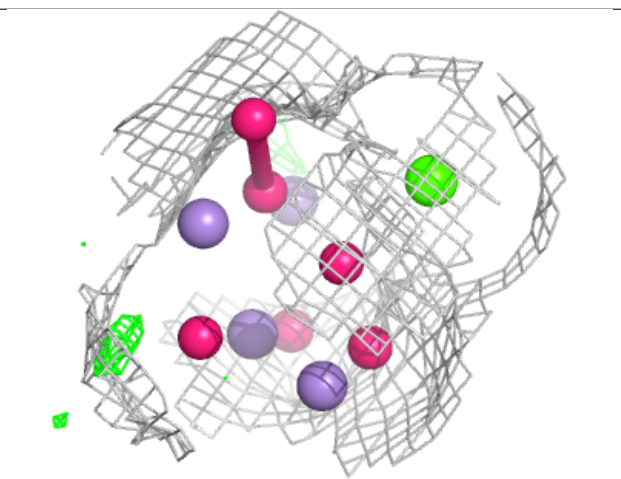
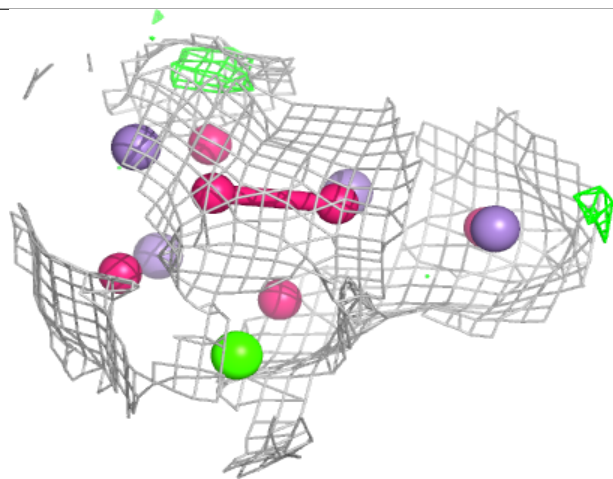
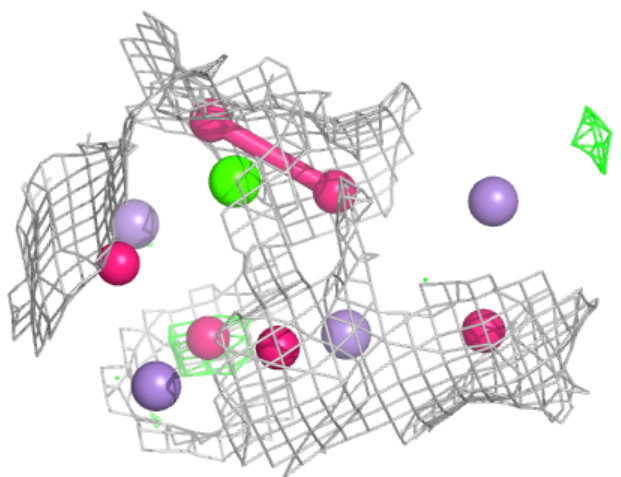
Electron density around OEY A 601 (B):

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



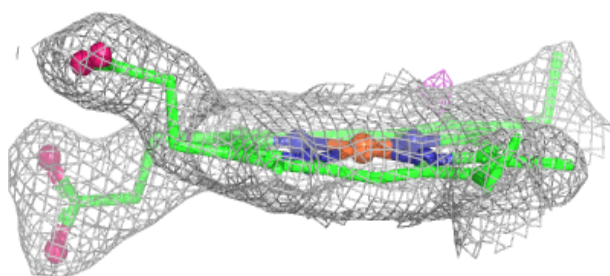
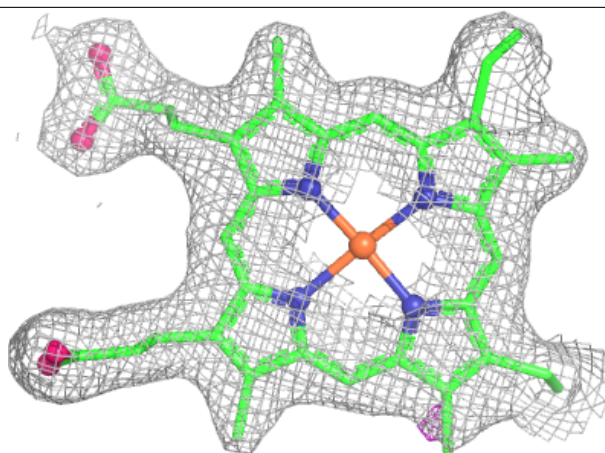
Electron density around OEY a 601 (B):

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.