



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 09:17 AM BST

PDB ID : 5GTH
Title : Native XFEL structure of photosystem II (dark dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-08-20
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

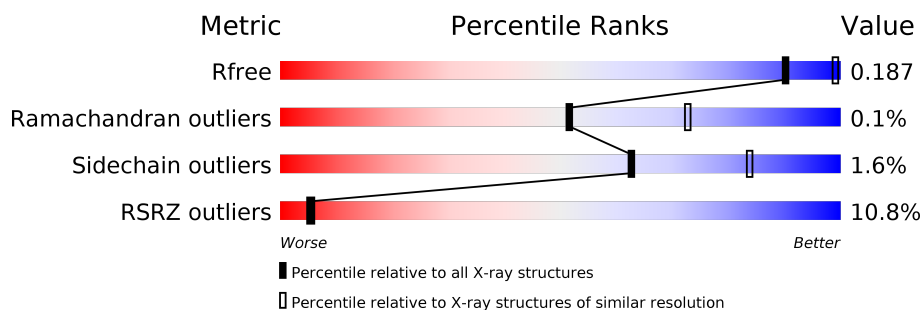
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
1	a	344	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
2	B	505	<div> <div>10%</div> <div>98%</div> <div>.</div> </div>
2	b	505	<div> <div>11%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>14%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>10%</div> <div>98%</div> <div>.</div> </div>
4	D	342	<div> <div>2%</div> <div>100%</div> <div></div> </div>

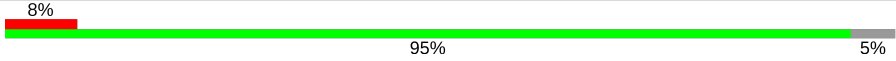
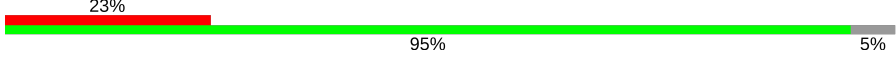
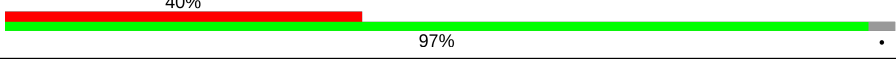
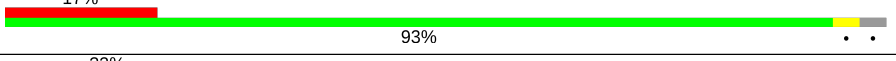
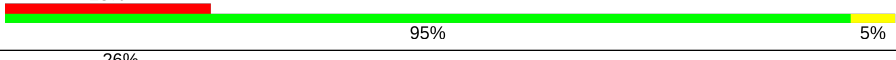
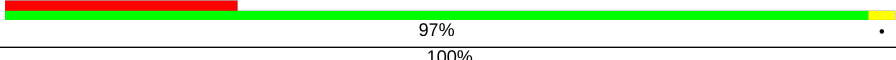

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

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
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	401	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
29	PL9	A	414	-	-	-	X
30	UNL	A	415	-	-	-	X
30	UNL	a	415	-	-	-	X
30	UNL	b	626	-	-	-	X
30	UNL	i	101	-	-	-	X
31	LHG	e	101	-	-	-	X
33	LMG	Z	101	-	-	-	X
34	HTG	B	624	-	-	-	X
34	HTG	C	521	-	-	-	X
34	HTG	C	522	-	-	-	X
34	HTG	D	412	-	-	-	X
34	HTG	b	622	-	-	-	X
34	HTG	b	623	-	-	-	X
34	HTG	c	522	-	-	-	X
35	LMT	B	630	-	-	-	X
35	LMT	E	102	-	-	-	X
35	LMT	I	101	-	-	-	X
35	LMT	e	102	-	-	-	X
35	LMT	m	102	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52773 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	5	0
			2639	1732	431	461	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	5	0
			3537	2317	589	618	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

- 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	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	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	1	0
			265	178	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

- 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
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
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 X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

- 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
			479	328	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
			273	186	47	40			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		

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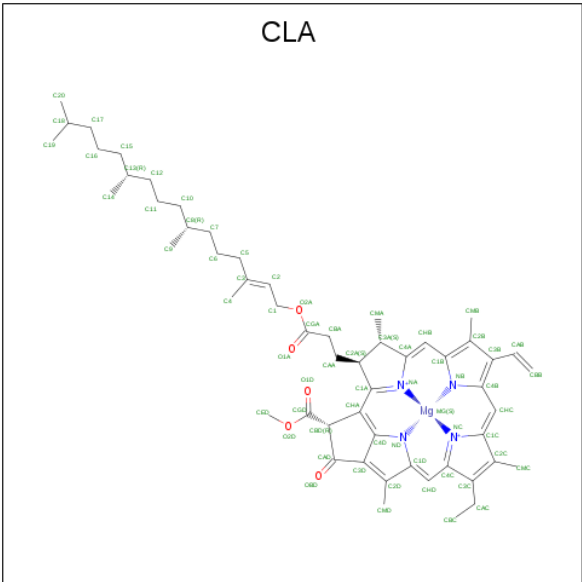
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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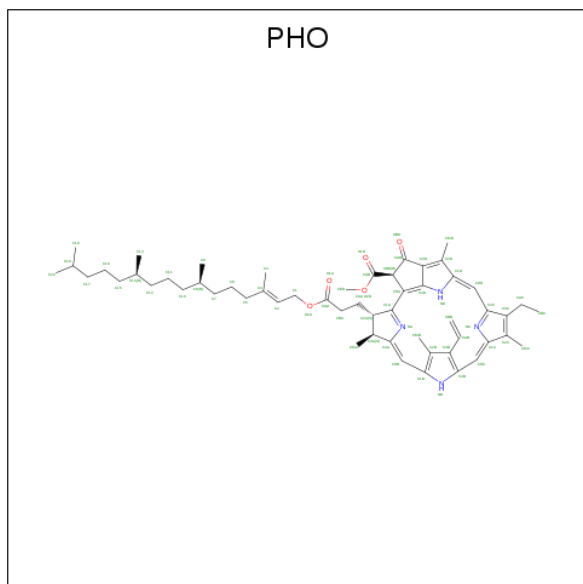
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

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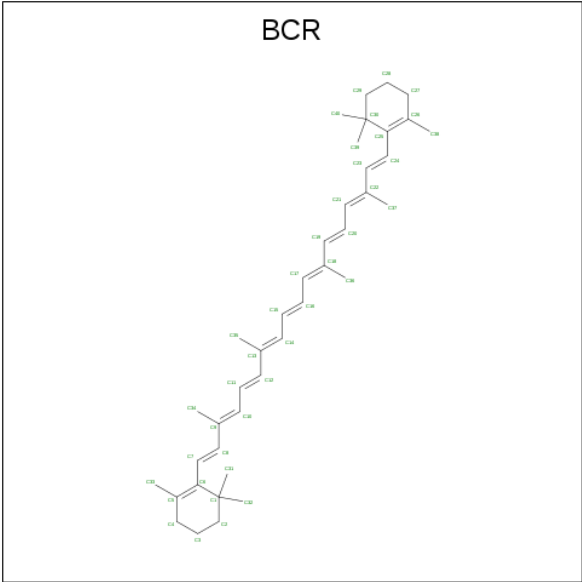
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



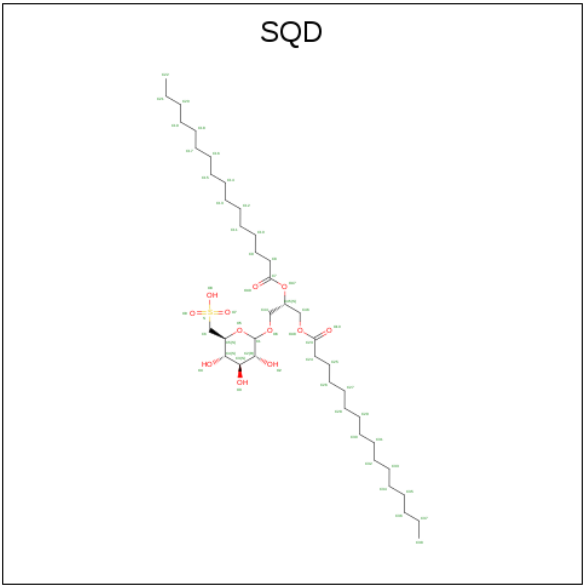
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



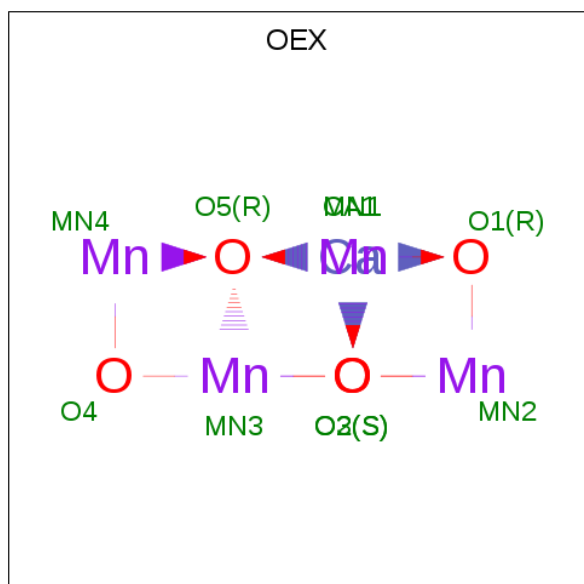
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

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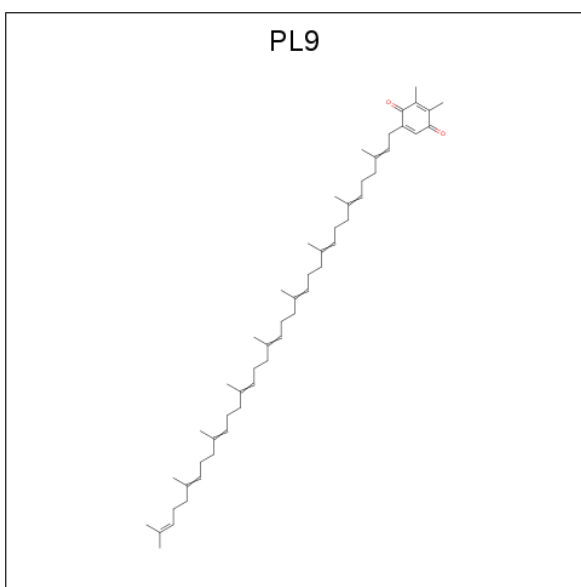
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	d	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 29 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 (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

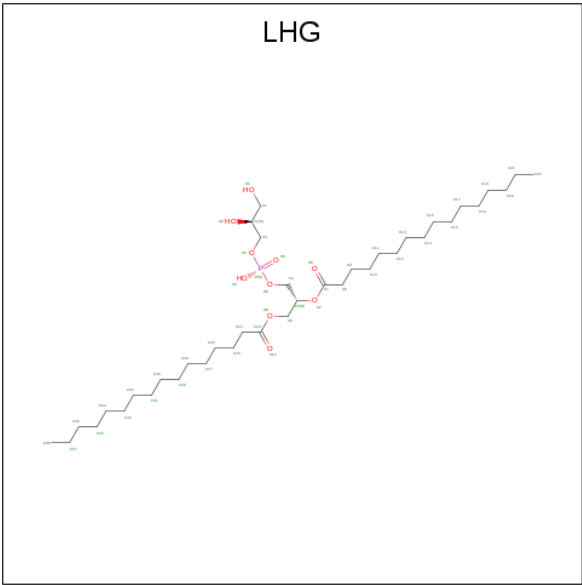
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	J	1	Total	C		0	0
			10	10			
30	i	1	Total	C	O	0	0
			40	35	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	K	1	Total	C	O	0	0
			34	29	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	I	1	Total	C	O	0	0
			40	35	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	a	1	Total	C	O	0	0
			30	25	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	x	1	Total C O 18 16 2	0	0
30	A	1	Total C O 28 23 5	0	0
30	j	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0
30	d	1	Total C O 17 16 1	0	0
30	m	1	Total C 10 10	0	0
30	b	2	Total C O 69 59 10	0	0
30	M	1	Total C 10 10	0	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



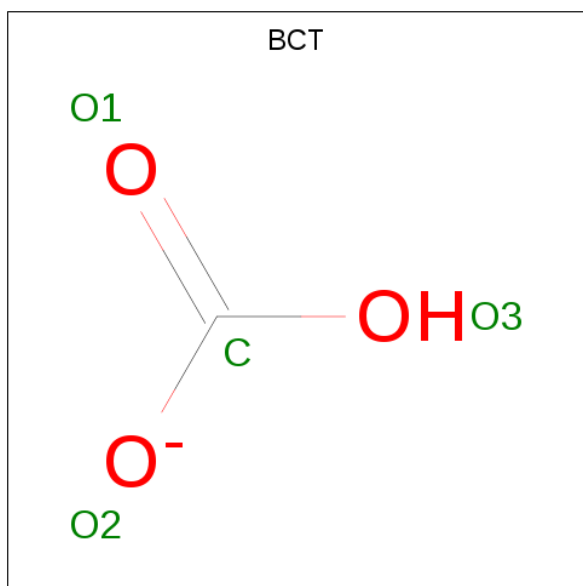
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O P 49 38 10 1	0	0
31	A	1	Total C O P 49 38 10 1	0	0
31	D	1	Total C O P 49 38 10 1	0	0

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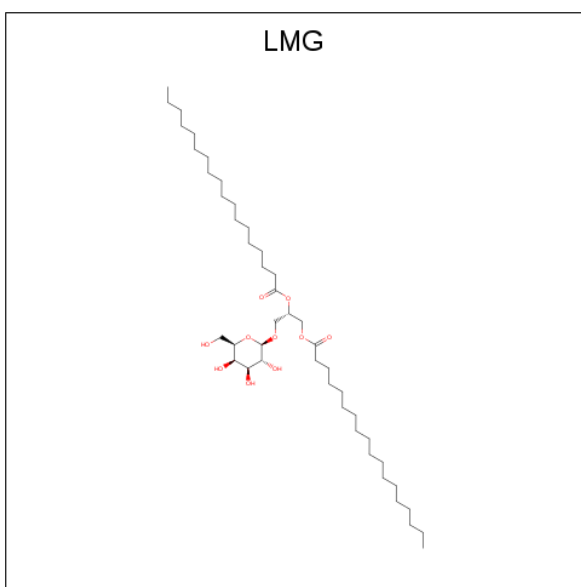
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0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

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



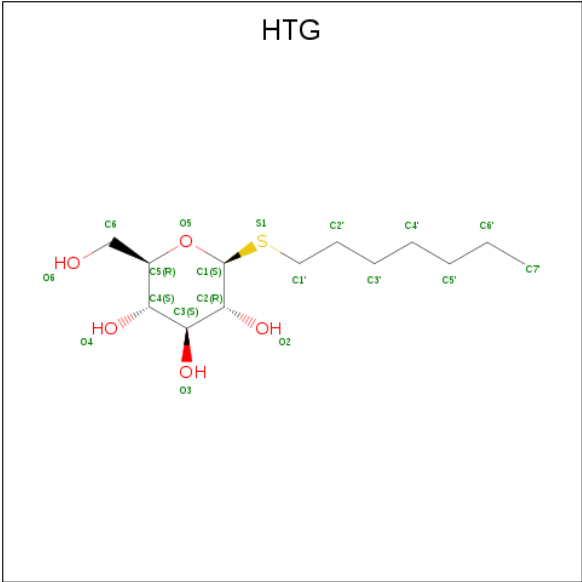
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



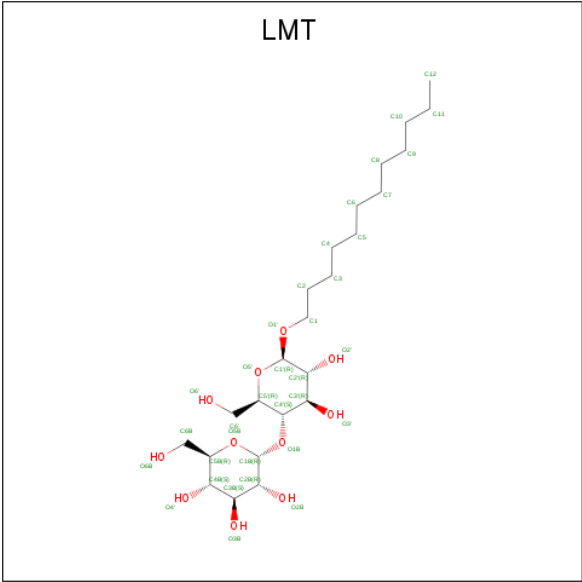
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16	10	5	1		
34	V	1	Total	C	O		0	0
			11	6	5			
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	c	1	Total	C	O	S	0	0
			19	13	5	1		
34	c	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	d	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



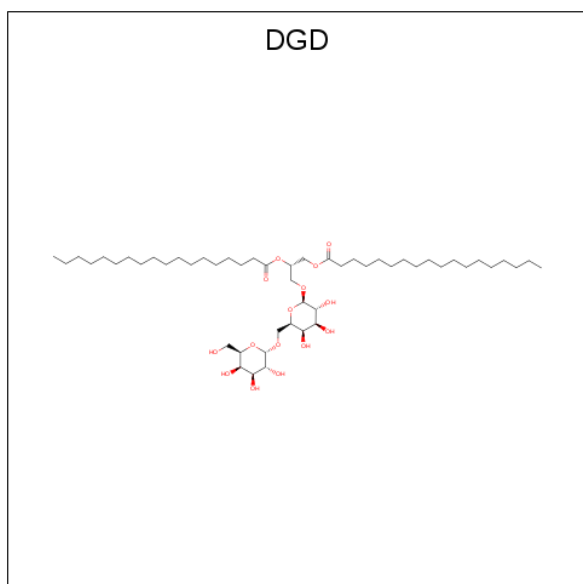
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O		0	0
			25	19	6			
35	B	1	Total	C	O		0	0
			35	24	11			
35	B	1	Total	C	O		0	0
			26	19	7			
35	D	1	Total	C	O		0	0
			35	24	11			
35	D	1	Total	C	O		0	0
			35	24	11			
35	E	1	Total	C	O		0	0
			35	24	11			
35	I	1	Total	C	O		0	0
			35	24	11			
35	M	1	Total	C	O		0	0
			35	24	11			
35	M	1	Total	C	O		0	0
			35	24	11			
35	a	1	Total	C	O		0	0
			35	24	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	b	1	Total	C	O	0	0
			25	19	6		
35	b	1	Total	C	O	0	0
			25	19	6		
35	e	1	Total	C	O	0	0
			35	24	11		
35	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		

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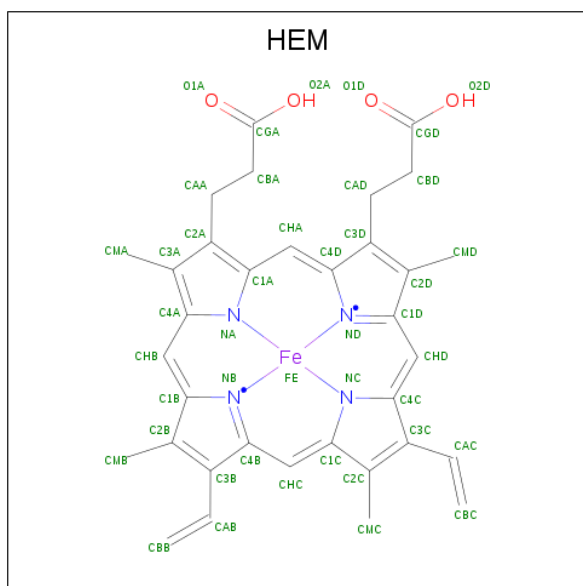
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	o	1	Total	Ca	0	0
			1	1		
37	O	1	Total	Ca	0	0
			1	1		
37	C	1	Total	Ca	0	0
			1	1		
37	V	1	Total	Ca	0	0
			1	1		
37	c	2	Total	Ca	0	0
			2	2		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

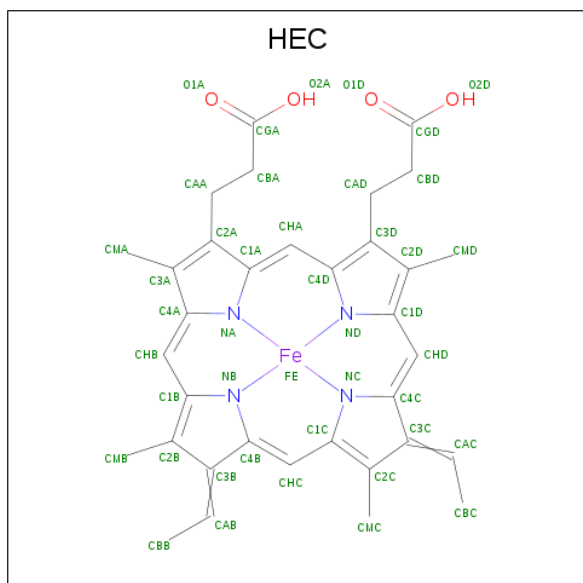


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
38	e	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	J	1	Total Mg 1 1	0	0
39	j	1	Total Mg 1 1	0	0

- Molecule 40 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	127	Total O 127 127	0	0
41	B	175	Total O 175 175	0	0
41	C	148	Total O 148 148	0	0
41	D	111	Total O 111 111	0	0
41	E	18	Total O 18 18	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	F	5	Total 5	O 5	0	0
41	H	19	Total 19	O 19	0	0
41	I	6	Total 6	O 6	0	0
41	J	5	Total 5	O 5	0	0
41	K	6	Total 6	O 6	0	0
41	L	9	Total 9	O 9	0	0
41	M	14	Total 14	O 14	0	0
41	O	100	Total 100	O 100	0	0
41	T	10	Total 10	O 10	0	0
41	U	46	Total 46	O 46	0	0
41	V	78	Total 79	O 79	0	1
41	X	3	Total 3	O 3	0	0
41	Y	1	Total 1	O 1	0	0
41	a	130	Total 130	O 130	0	0
41	b	192	Total 192	O 192	0	0
41	c	136	Total 136	O 136	0	0
41	d	108	Total 108	O 108	0	0
41	e	15	Total 15	O 15	0	0
41	f	5	Total 5	O 5	0	0
41	h	28	Total 28	O 28	0	0
41	i	4	Total 4	O 4	0	0

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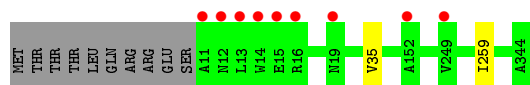
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	j	3	Total 3	O 3	0	0
41	k	4	Total 4	O 4	0	0
41	l	7	Total 7	O 7	0	0
41	m	11	Total 11	O 11	0	0
41	o	109	Total 109	O 109	0	0
41	t	7	Total 7	O 7	0	0
41	u	64	Total 64	O 64	0	0
41	v	71	Total 71	O 71	0	0
41	x	4	Total 4	O 4	0	0
41	y	2	Total 2	O 2	0	0

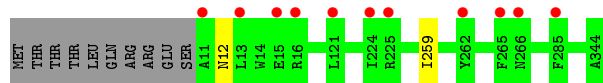
3 Residue-property plots [i](#)

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.

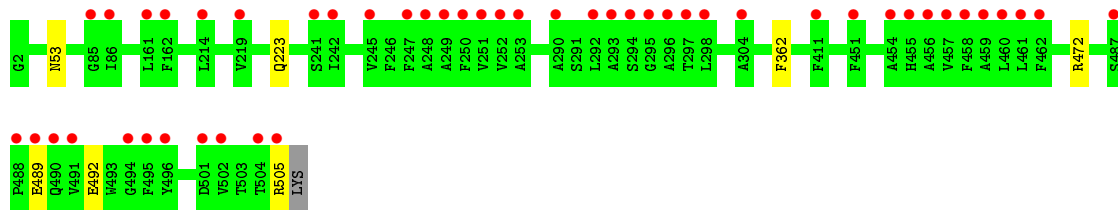
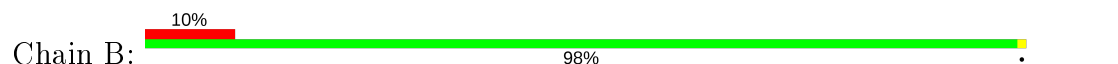
- Molecule 1: Photosystem II protein D1



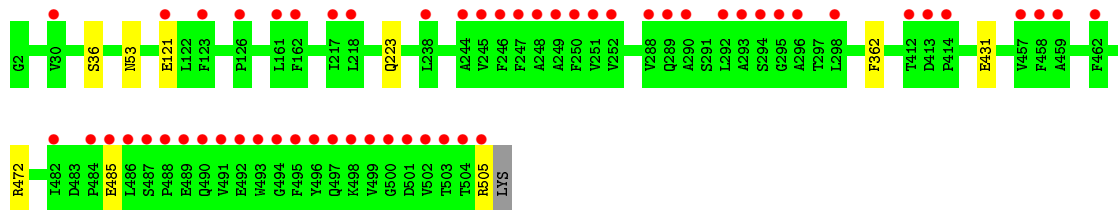
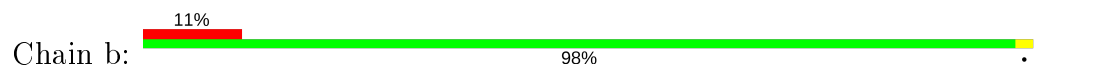
- Molecule 1: Photosystem II protein D1



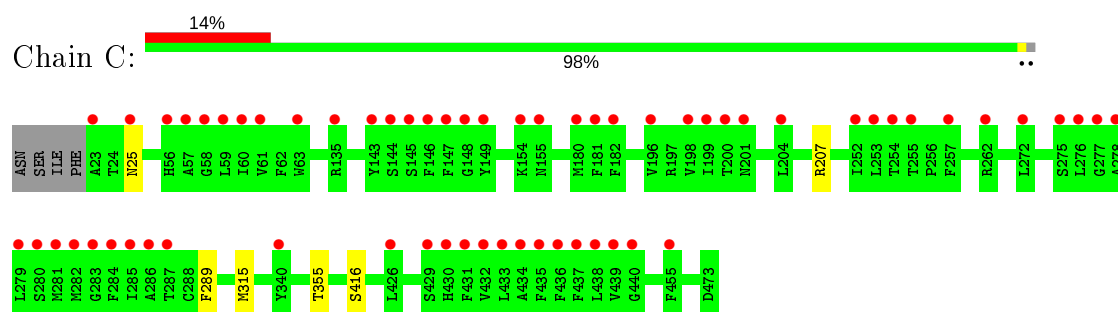
- Molecule 2: Photosystem II CP47 reaction center protein



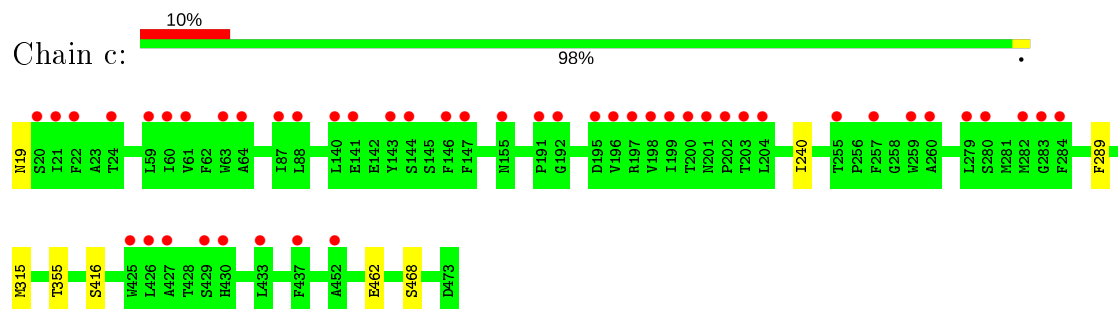
- Molecule 2: Photosystem II CP47 reaction center protein



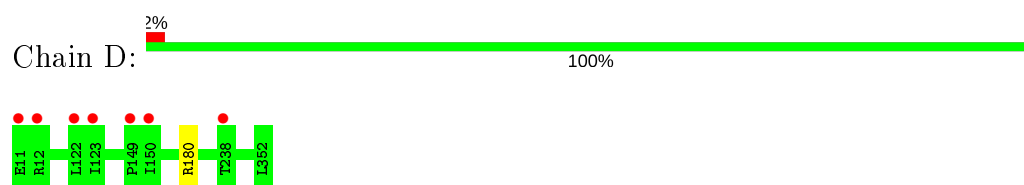
- Molecule 3: Photosystem II CP43 reaction center protein



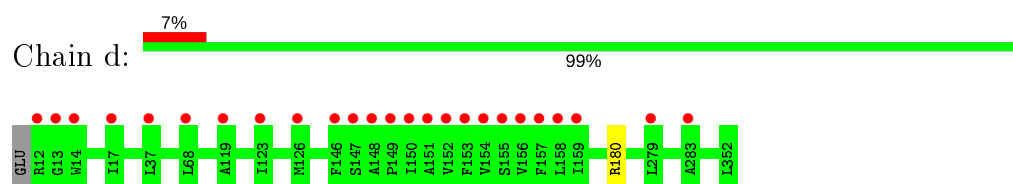
- Molecule 3: Photosystem II CP43 reaction center protein



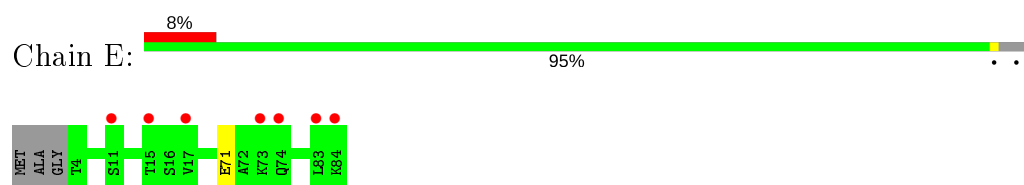
- Molecule 4: Photosystem II D2 protein



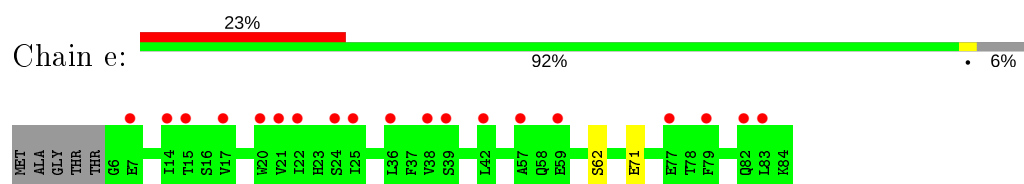
- Molecule 4: Photosystem II D2 protein




- Molecule 5: Cytochrome b559 subunit alpha

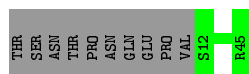


- Molecule 5: Cytochrome b559 subunit alpha



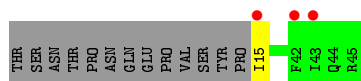
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  77% 23%



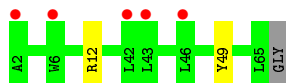
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  7% 68% 30%



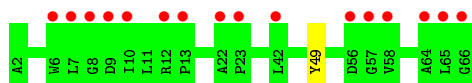
- Molecule 7: Photosystem II reaction center protein H

Chain H:  8% 95%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  25% 98%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  18% 95% 5%



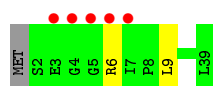
- Molecule 8: Photosystem II reaction center protein I

Chain i:  8% 92% 5%

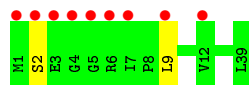


- Molecule 9: Photosystem II reaction center protein J

Chain J:  13% 92% 5%



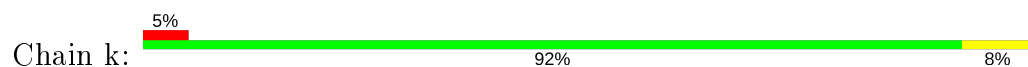
- Molecule 9: Photosystem II reaction center protein J



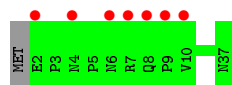
- Molecule 10: Photosystem II reaction center protein K



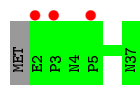
- Molecule 10: Photosystem II reaction center protein K



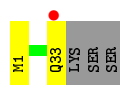
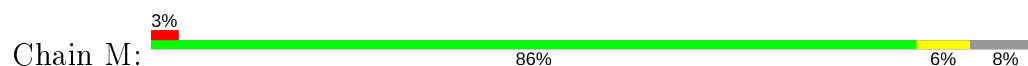
- Molecule 11: Photosystem II reaction center protein L



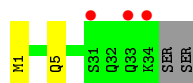
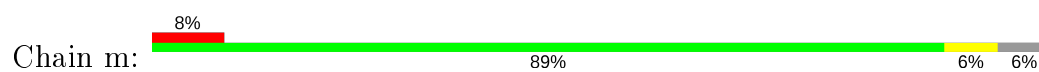
- Molecule 11: Photosystem II reaction center protein L



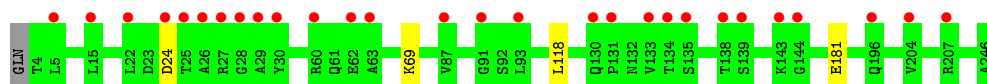
- Molecule 12: Photosystem II reaction center protein M



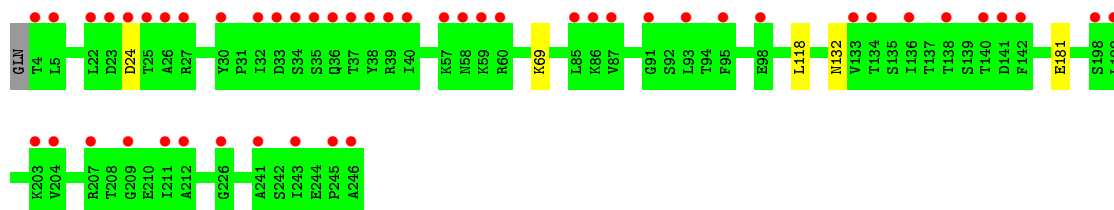
- Molecule 12: Photosystem II reaction center protein M



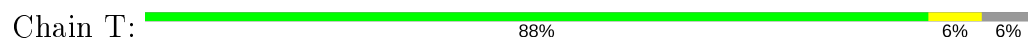
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



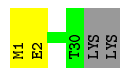
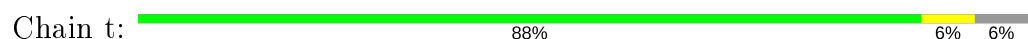
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



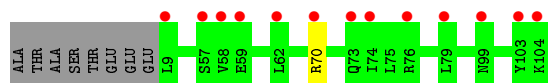
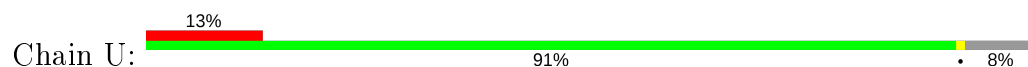
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

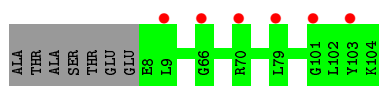


- Molecule 15: Photosystem II 12 kDa extrinsic protein

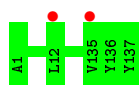


- Molecule 15: Photosystem II 12 kDa extrinsic protein





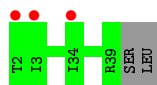
- Molecule 16: Cytochrome c-550



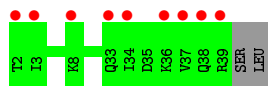
- Molecule 16: Cytochrome c-550



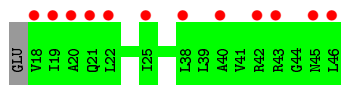
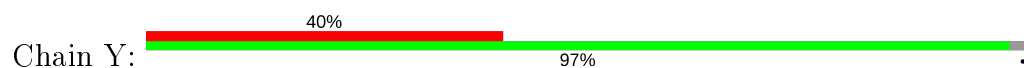
- Molecule 17: Photosystem II reaction center protein X



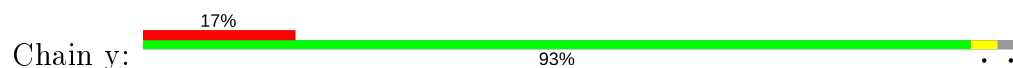
- Molecule 17: Photosystem II reaction center protein X



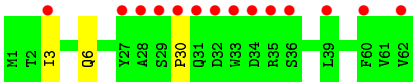
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center protein Ycf12



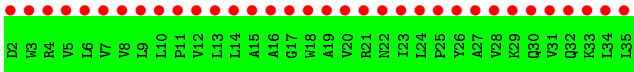
- Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 46.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 100.0 (46.51-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.186 0.142 , 0.187	Depositor DCC
R_{free} test set	14614 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.4	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	0.97	EDS
Total number of atoms	52773	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/2728	0.56	0/3719
1	a	0.45	0/2739	0.56	0/3735
2	B	0.42	0/4171	0.55	0/5683
2	b	0.42	0/4138	0.55	0/5640
3	C	0.40	0/3626	0.53	0/4936
3	c	0.41	0/3670	0.53	0/4996
4	D	0.45	0/2827	0.55	0/3852
4	d	0.45	0/2818	0.53	0/3840
5	E	0.34	0/687	0.53	0/936
5	e	0.34	0/667	0.50	0/908
6	F	0.34	0/284	0.47	0/387
6	f	0.38	0/257	0.48	0/349
7	H	0.35	0/530	0.51	0/723
7	h	0.34	0/524	0.50	0/713
8	I	0.37	0/311	0.49	0/419
8	i	0.37	0/311	0.52	0/419
9	J	0.36	0/278	0.48	0/376
9	j	0.37	0/283	0.50	0/383
10	K	0.36	0/303	0.54	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.43	0/311	0.48	0/423
11	l	0.39	0/311	0.50	0/423
12	M	0.44	0/261	0.55	0/357
12	m	0.44	0/262	0.60	0/357
13	O	0.37	0/1935	0.57	0/2623
13	o	0.37	0/1910	0.56	0/2589
14	T	0.51	0/257	0.56	0/349
14	t	0.52	0/257	0.52	0/349
15	U	0.40	0/776	0.58	0/1052
15	u	0.40	0/785	0.57	0/1064
16	V	0.38	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.37	0/1085	0.52	0/1473
17	X	0.35	0/284	0.48	0/384
17	x	0.31	0/284	0.49	0/384
18	Y	0.30	0/216	0.45	0/289
18	y	0.32	0/216	0.52	0/289
19	Z	0.32	0/490	0.45	0/669
19	z	0.34	0/490	0.45	0/669
20	R	0.28	0/279	0.43	0/383
All	All	0.41	0/42949	0.54	0/58445

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	41	61
1	a	337/344 (98%)	330 (98%)	6 (2%)	1 (0%)	41	61
2	B	510/505 (101%)	504 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	499 (99%)	7 (1%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	34	54
3	c	458/455 (101%)	445 (97%)	11 (2%)	2 (0%)	34	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	341/342 (100%)	332 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	7
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	238 (97%)	8 (3%)	0	100	100
13	o	243/244 (100%)	234 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	9	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	16
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5255/5384 (98%)	5126 (98%)	120 (2%)	9 (0%)	51	68

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER

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	272/279 (98%)	271 (100%)	1 (0%)	91	97
1	a	274/279 (98%)	273 (100%)	1 (0%)	91	97
2	B	410/403 (102%)	403 (98%)	7 (2%)	60	82
2	b	406/403 (101%)	397 (98%)	9 (2%)	52	77
3	C	356/356 (100%)	351 (99%)	5 (1%)	67	86
3	c	361/356 (101%)	353 (98%)	8 (2%)	52	77
4	D	278/277 (100%)	277 (100%)	1 (0%)	91	97
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	97
5	E	73/73 (100%)	72 (99%)	1 (1%)	67	86
5	e	70/73 (96%)	68 (97%)	2 (3%)	42	69
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	31	56
7	H	55/54 (102%)	52 (94%)	3 (6%)	21	41
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	69
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	37
9	J	26/27 (96%)	24 (92%)	2 (8%)	13	25
9	j	26/27 (96%)	24 (92%)	2 (8%)	13	25
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	15
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	15
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	29 (97%)	1 (3%)	38	64
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	64
13	O	211/207 (102%)	207 (98%)	4 (2%)	57	80
13	o	208/207 (100%)	203 (98%)	5 (2%)	49	74
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	58
14	t	26/28 (93%)	25 (96%)	1 (4%)	33	58
15	U	83/89 (93%)	82 (99%)	1 (1%)	71	88
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	117 (100%)	0	100	100
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	21 (96%)	1 (4%)	27	51
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	58
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	80
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4360/4403 (99%)	4288 (98%)	72 (2%)	62	82

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	6	GLN
2	b	472	ARG
13	o	118	LEU

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Mol	Chain	Res	Type
1	a	12	ASN
2	b	121	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	81	HIS
2	b	14	ASN
13	o	124	ASN
17	X	33	GLN
2	b	53	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	M	1	12	8,9,10	0.58	0	7,9,11	1.50	2 (28%)
14	FME	T	1	14	8,9,10	0.62	0	7,9,11	1.31	1 (14%)
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.09	1 (14%)
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.37	1 (14%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	1.85	3 (42%)
12	FME	m	1	12	8,9,10	0.58	0	7,9,11	1.38	2 (28%)

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	-	3/7/9/11	-
14	FME	T	1	14	-	4/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.73	117.62	124.78
14	t	1	FME	CA-N-CN	-2.63	118.77	122.82
12	M	1	FME	CA-N-CN	-2.31	119.27	122.82
8	I	1	FME	O-C-CA	-2.29	118.77	124.78
14	T	1	FME	O-C-CA	-2.25	118.88	124.78

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
14	T	1	FME	N-CA-CB-CG
14	T	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 214 ligands modelled in this entry, 18 are unknown and 14 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$
23	CLA	a	408	1	59,73,73	2.02	14 (23%)	67,113,113	2.22	25 (37%)
27	GOL	C	523	-	5,5,5	0.40	0	5,5,5	0.25	0
23	CLA	d	404	4	59,73,73	2.05	12 (20%)	67,113,113	2.16	26 (38%)
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.00	6 (7%)
23	CLA	B	608	2	59,73,73	1.96	12 (20%)	67,113,113	2.19	23 (34%)
38	HEM	e	103	5,6	27,50,50	0.81	1 (3%)	17,82,82	1.89	3 (17%)
23	CLA	B	603	2	59,73,73	1.99	13 (22%)	67,113,113	2.26	21 (31%)
23	CLA	b	607	41	59,73,73	1.96	14 (23%)	67,113,113	2.13	20 (29%)
23	CLA	C	502	3	59,73,73	1.96	13 (22%)	67,113,113	2.32	24 (35%)
33	LMG	j	101	39	51,51,55	0.88	2 (3%)	59,59,63	1.07	5 (8%)
31	LHG	l	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	C	514	3	59,73,73	2.02	13 (22%)	67,113,113	2.11	20 (29%)
31	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	5 (9%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
23	CLA	c	513	3	59,73,73	2.04	13 (22%)	67,113,113	2.24	21 (31%)
23	CLA	b	613	2	59,73,73	2.04	13 (22%)	67,113,113	2.19	23 (34%)
25	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.73	13 (23%)
24	PHO	D	401	-	67,69,69	2.13	19 (28%)	85,99,99	2.10	24 (28%)
23	CLA	A	406	41	59,73,73	2.02	13 (22%)	67,113,113	2.05	22 (32%)
23	CLA	D	405	4	59,73,73	1.99	12 (20%)	67,113,113	2.25	22 (32%)
31	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.96	3 (5%)
33	LMG	Z	101	-	51,51,55	0.99	2 (3%)	59,59,63	1.27	5 (8%)
23	CLA	b	605	2	59,73,73	2.02	14 (23%)	67,113,113	2.21	20 (29%)
23	CLA	B	616	2	59,73,73	2.05	13 (22%)	67,113,113	2.22	19 (28%)
31	LHG	d	409	-	48,48,48	0.97	2 (4%)	51,54,54	1.00	3 (5%)
31	LHG	d	408	-	48,48,48	0.89	2 (4%)	51,54,54	0.91	3 (5%)
23	CLA	B	613	2	59,73,73	2.06	13 (22%)	67,113,113	2.26	25 (37%)
23	CLA	C	508	41	59,73,73	2.00	12 (20%)	67,113,113	2.22	23 (34%)
27	GOL	a	411	-	5,5,5	0.38	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	510	3	59,73,73	1.92	13 (22%)	67,113,113	2.25	26 (38%)
23	CLA	B	605	2	59,73,73	1.99	14 (23%)	67,113,113	2.11	21 (31%)
34	HTG	B	624	-	19,19,19	1.00	1 (5%)	23,24,24	1.74	3 (13%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
23	CLA	c	512	3	59,73,73	2.00	13 (22%)	67,113,113	2.22	20 (29%)
23	CLA	B	604	2	59,73,73	1.96	13 (22%)	67,113,113	2.22	22 (32%)
29	PL9	A	414	-	55,55,55	0.65	2 (3%)	68,69,69	1.95	21 (30%)
25	BCR	d	405	-	41,41,41	1.09	1 (2%)	56,56,56	1.86	14 (25%)
23	CLA	a	404	1	59,73,73	2.00	12 (20%)	67,113,113	2.30	26 (38%)
23	CLA	c	508	3	59,73,73	2.09	13 (22%)	67,113,113	2.27	21 (31%)
23	CLA	C	507	3	59,73,73	2.01	13 (22%)	67,113,113	2.22	25 (37%)
25	BCR	c	514	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	13 (23%)
27	GOL	B	625	-	5,5,5	0.37	0	5,5,5	0.37	0
35	LMT	M	103	-	36,36,36	0.47	0	47,47,47	0.77	1 (2%)
25	BCR	a	409	-	41,41,41	0.95	1 (2%)	56,56,56	1.51	12 (21%)
23	CLA	B	615	2	59,73,73	1.98	11 (18%)	67,113,113	2.15	22 (32%)
23	CLA	C	509	3	59,73,73	2.12	14 (23%)	67,113,113	2.26	21 (31%)
35	LMT	b	627	-	25,25,36	0.56	1 (4%)	30,30,47	1.07	3 (10%)
23	CLA	C	513	3	59,73,73	2.02	13 (22%)	67,113,113	2.23	26 (38%)
23	CLA	c	503	3	59,73,73	1.98	13 (22%)	67,113,113	2.18	20 (29%)
33	LMG	a	416	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	3 (5%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.68	11 (19%)
26	SQD	L	101	-	53,54,54	1.02	3 (5%)	62,65,65	1.53	9 (14%)
31	LHG	A	416	-	48,48,48	0.90	3 (6%)	51,54,54	1.10	4 (7%)
23	CLA	B	611	2	59,73,73	2.01	13 (22%)	67,113,113	2.16	22 (32%)
23	CLA	b	616	2	59,73,73	2.01	12 (20%)	67,113,113	2.29	23 (34%)
31	LHG	D	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	4 (7%)
35	LMT	E	102	-	36,36,36	0.53	1 (2%)	47,47,47	0.84	0
25	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.39	10 (17%)
24	PHO	A	407	-	67,69,69	2.15	17 (25%)	85,99,99	2.04	25 (29%)
35	LMT	B	631	-	26,26,36	0.50	0	31,31,47	0.81	1 (3%)
23	CLA	C	511	3	59,73,73	2.00	13 (22%)	67,113,113	2.18	22 (32%)
35	LMT	m	102	-	36,36,36	0.51	0	47,47,47	0.92	2 (4%)
33	LMG	c	520	-	51,51,55	0.97	3 (5%)	59,59,63	1.24	6 (10%)
29	PL9	d	406	-	55,55,55	0.63	1 (1%)	68,69,69	1.82	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	6 (7%)
33	LMG	c	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	3 (5%)
35	LMT	B	629	-	25,25,36	0.46	0	30,30,47	0.70	0
25	BCR	C	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.58	9 (16%)
34	HTG	B	622	-	19,19,19	1.01	1 (5%)	23,24,24	1.44	4 (17%)
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
23	CLA	B	612	2	59,73,73	2.00	13 (22%)	67,113,113	2.25	23 (34%)
38	HEM	E	103	5,6	27,50,50	0.81	0	17,82,82	2.19	4 (23%)
33	LMG	Z	102	-	37,37,55	1.01	3 (8%)	45,45,63	1.64	9 (20%)
25	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.73	16 (28%)
40	HEC	v	201	16	26,50,50	1.60	4 (15%)	18,82,82	1.60	4 (22%)
34	HTG	c	521	-	19,19,19	0.91	1 (5%)	23,24,24	1.51	1 (4%)
23	CLA	A	408	1	59,73,73	1.98	14 (23%)	67,113,113	2.26	23 (34%)
23	CLA	b	615	2	59,73,73	1.93	12 (20%)	67,113,113	2.13	21 (31%)
23	CLA	D	404	4	59,73,73	2.00	12 (20%)	67,113,113	2.37	23 (34%)
23	CLA	b	609	2	59,73,73	2.00	13 (22%)	67,113,113	2.23	21 (31%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.70	17 (30%)
25	BCR	D	406	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	14 (25%)
23	CLA	C	503	3	59,73,73	2.00	12 (20%)	67,113,113	2.10	20 (29%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)
35	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.07	3 (6%)
23	CLA	C	506	3	59,73,73	1.97	13 (22%)	67,113,113	2.26	21 (31%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.48	10 (16%)
35	LMT	b	621	-	25,25,36	0.46	0	30,30,47	0.66	0
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.67	13 (23%)
23	CLA	c	501	3	59,73,73	1.96	13 (22%)	67,113,113	2.15	21 (31%)
23	CLA	b	601	41	59,73,73	2.07	13 (22%)	67,113,113	2.15	21 (31%)
23	CLA	C	505	41	59,73,73	2.08	13 (22%)	67,113,113	2.22	24 (35%)
32	BCT	a	418	21	0,3,3	0.00	-	0,3,3	0.00	-
27	GOL	d	402	-	5,5,5	0.32	0	5,5,5	0.55	0
23	CLA	B	609	2	59,73,73	1.97	12 (20%)	67,113,113	2.14	19 (28%)
27	GOL	B	626	-	5,5,5	0.52	0	5,5,5	0.40	0
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
25	BCR	b	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.69	13 (23%)
23	CLA	c	507	41	59,73,73	2.00	13 (22%)	67,113,113	2.11	22 (32%)
23	CLA	b	614	2	59,73,73	2.00	13 (22%)	67,113,113	2.21	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	4 (6%)
23	CLA	c	505	3	59,73,73	1.97	13 (22%)	67,113,113	2.13	20 (29%)
23	CLA	d	401	41	59,73,73	2.04	12 (20%)	67,113,113	2.25	25 (37%)
36	DGD	h	102	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	5 (6%)
23	CLA	c	509	3	59,73,73	2.08	13 (22%)	67,113,113	2.17	20 (29%)
35	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.02	2 (4%)
34	HTG	V	203	-	11,11,19	0.25	0	15,15,24	1.12	2 (13%)
23	CLA	b	612	2	59,73,73	2.06	13 (22%)	67,113,113	2.16	20 (29%)
34	HTG	B	623	-	19,19,19	0.84	1 (5%)	23,24,24	1.67	1 (4%)
23	CLA	c	502	3	59,73,73	2.02	12 (20%)	67,113,113	2.22	21 (31%)
23	CLA	C	510	3	59,73,73	2.08	13 (22%)	67,113,113	2.16	22 (32%)
35	LMT	a	417	-	36,36,36	0.46	0	47,47,47	0.77	1 (2%)
31	LHG	A	417	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	2 (3%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.52	11 (19%)
23	CLA	B	610	41	59,73,73	2.06	13 (22%)	67,113,113	2.24	24 (35%)
34	HTG	C	522	-	19,19,19	1.05	2 (10%)	23,24,24	1.89	5 (21%)
27	GOL	b	624	-	5,5,5	0.33	0	5,5,5	0.45	0
36	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.16	6 (7%)
23	CLA	A	405	41	59,73,73	2.06	12 (20%)	67,113,113	2.20	25 (37%)
23	CLA	b	606	2	59,73,73	1.94	12 (20%)	67,113,113	2.23	24 (35%)
34	HTG	D	412	-	16,16,19	1.04	2 (12%)	20,21,24	1.45	1 (5%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.72	3 (13%)
35	LMT	D	402	-	36,36,36	0.64	1 (2%)	47,47,47	1.26	4 (8%)
34	HTG	B	627	-	19,19,19	0.97	2 (10%)	23,24,24	1.40	2 (8%)
25	BCR	K	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	9 (16%)
23	CLA	b	602	2	59,73,73	2.05	13 (22%)	67,113,113	2.31	27 (40%)
35	LMT	D	403	-	36,36,36	0.44	0	47,47,47	1.32	7 (14%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.58	12 (21%)
25	BCR	b	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	8 (14%)
34	HTG	b	628	-	19,19,19	1.01	1 (5%)	23,24,24	1.83	4 (17%)
32	BCT	A	418	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	b	608	2	59,73,73	2.07	14 (23%)	67,113,113	2.20	22 (32%)
35	LMT	B	630	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
23	CLA	a	405	41	59,73,73	2.04	13 (22%)	67,113,113	2.09	24 (35%)
23	CLA	d	403	4	59,73,73	2.03	14 (23%)	67,113,113	2.19	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	e	101	-	41,41,48	1.03	2 (4%)	44,47,54	0.95	2 (4%)
23	CLA	b	611	2	59,73,73	2.04	13 (22%)	67,113,113	2.22	21 (31%)
26	SQD	D	413	-	42,43,54	1.15	3 (7%)	51,54,65	1.78	12 (23%)
29	PL9	a	414	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	20 (29%)
26	SQD	a	412	-	53,54,54	1.06	3 (5%)	62,65,65	1.24	7 (11%)
24	PHO	a	407	-	67,69,69	2.18	15 (22%)	85,99,99	1.98	19 (22%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.07	5 (6%)
23	CLA	c	506	3	59,73,73	2.01	14 (23%)	67,113,113	2.16	25 (37%)
34	HTG	d	411	-	16,16,19	1.12	2 (12%)	20,21,24	1.50	1 (5%)
25	BCR	B	617	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	10 (17%)
23	CLA	b	610	41	59,73,73	2.11	13 (22%)	67,113,113	2.27	23 (34%)
24	PHO	a	406	-	67,69,69	2.10	17 (25%)	85,99,99	1.94	24 (28%)
26	SQD	a	410	-	53,54,54	0.96	3 (5%)	62,65,65	1.73	12 (19%)
23	CLA	B	601	41	59,73,73	2.07	13 (22%)	67,113,113	2.17	21 (31%)
33	LMG	b	620	-	51,51,55	0.86	2 (3%)	59,59,63	1.26	8 (13%)
34	HTG	c	522	-	19,19,19	0.96	2 (10%)	23,24,24	1.49	3 (13%)
29	PL9	D	407	-	55,55,55	0.65	1 (1%)	68,69,69	1.74	21 (30%)
36	DGD	c	518	-	63,63,67	0.86	3 (4%)	77,77,81	1.09	6 (7%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.10	6 (9%)
40	HEC	V	202	16	26,50,50	1.58	4 (15%)	18,82,82	1.60	3 (16%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.11	5 (11%)
23	CLA	B	614	2	59,73,73	1.97	14 (23%)	67,113,113	2.29	24 (35%)
28	OEX	a	413	1,3,41	0,15,15	0.00	-	-	-	-
26	SQD	A	410	-	53,54,54	0.97	3 (5%)	62,65,65	1.86	12 (19%)
23	CLA	C	512	3	59,73,73	2.03	13 (22%)	67,113,113	2.13	22 (32%)
23	CLA	B	607	41	59,73,73	2.01	13 (22%)	67,113,113	2.20	22 (32%)
23	CLA	b	604	2	59,73,73	1.99	12 (20%)	67,113,113	2.23	20 (29%)
23	CLA	A	404	1	59,73,73	2.07	14 (23%)	67,113,113	2.22	26 (38%)
23	CLA	C	504	3	59,73,73	1.95	12 (20%)	67,113,113	2.06	19 (28%)
26	SQD	f	101	-	42,43,54	1.19	3 (7%)	51,54,65	1.38	7 (13%)
28	OEX	A	413	1,3,41	0,15,15	0.00	-	-	-	-
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	11 (19%)
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	13 (23%)
23	CLA	c	511	3	59,73,73	2.06	13 (22%)	67,113,113	2.15	20 (29%)
27	GOL	A	411	-	5,5,5	0.40	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	e	102	-	36,36,36	0.50	0	47,47,47	0.81	2 (4%)
33	LMG	J	101	39	51,51,55	0.91	2 (3%)	59,59,63	0.98	5 (8%)
34	HTG	b	623	-	19,19,19	1.07	2 (10%)	23,24,24	1.81	3 (13%)
25	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.57	10 (17%)
34	HTG	b	622	-	19,19,19	0.96	1 (5%)	23,24,24	1.52	3 (13%)
23	CLA	c	504	41	59,73,73	2.06	13 (22%)	67,113,113	2.15	24 (35%)
23	CLA	b	603	2	59,73,73	2.04	14 (23%)	67,113,113	2.18	19 (28%)
23	CLA	B	606	2	59,73,73	1.97	12 (20%)	67,113,113	2.26	21 (31%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.75	13 (23%)
36	DGD	c	517	-	63,63,67	0.91	3 (4%)	77,77,81	0.99	6 (7%)
23	CLA	B	602	2	59,73,73	2.05	13 (22%)	67,113,113	2.20	25 (37%)
34	HTG	C	521	-	19,19,19	0.92	1 (5%)	23,24,24	1.44	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	408	1	3/3/20/25	8/37/135/135	-
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	d	404	4	3/3/20/25	12/37/135/135	-
36	DGD	H	102	-	-	14/51/91/95	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	B	608	2	3/3/20/25	4/37/135/135	-
38	HEM	e	103	5,6	-	0/6/54/54	-
23	CLA	B	603	2	3/3/20/25	4/37/135/135	-
23	CLA	b	607	41	3/3/20/25	4/37/135/135	-
23	CLA	C	502	3	3/3/20/25	8/37/135/135	-
33	LMG	j	101	39	-	12/46/66/70	0/1/1/1
35	LMT	B	631	-	-	7/17/38/61	0/1/1/2
35	LMT	E	102	-	-	11/21/61/61	0/2/2/2
31	LHG	d	407	-	-	14/53/53/53	-
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
23	CLA	c	513	3	3/3/20/25	1/37/135/135	-
23	CLA	b	613	2	3/3/20/25	10/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
24	PHO	D	401	-	-	6/53/103/103	0/5/6/6
23	CLA	A	406	41	3/3/20/25	11/37/135/135	-
23	CLA	D	405	4	3/3/20/25	11/37/135/135	-
31	LHG	D	408	-	-	15/53/53/53	-
33	LMG	Z	101	-	-	9/46/66/70	0/1/1/1
23	CLA	b	605	2	3/3/20/25	10/37/135/135	-
23	CLA	B	616	2	3/3/20/25	8/37/135/135	-
31	LHG	d	409	-	-	16/53/53/53	-
31	LHG	d	408	-	-	20/53/53/53	-
23	CLA	B	613	2	3/3/20/25	6/37/135/135	-
23	CLA	C	508	41	3/3/20/25	6/37/135/135	-
27	GOL	a	411	-	-	2/4/4/4	-
23	CLA	c	510	3	3/3/20/25	10/37/135/135	-
23	CLA	B	605	2	3/3/20/25	9/37/135/135	-
34	HTG	B	624	-	-	4/10/30/30	0/1/1/1
23	CLA	b	606	2	3/3/20/25	12/37/135/135	-
23	CLA	c	512	3	3/3/20/25	12/37/135/135	-
23	CLA	B	604	2	3/3/20/25	11/37/135/135	-
29	PL9	A	414	-	-	11/53/73/73	0/1/1/1
25	BCR	d	405	-	-	6/29/63/63	0/2/2/2
23	CLA	a	404	1	3/3/20/25	10/37/135/135	-
23	CLA	c	508	3	3/3/20/25	5/37/135/135	-
23	CLA	C	507	3	3/3/20/25	13/37/135/135	-
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	GOL	B	625	-	-	3/4/4/4	-
35	LMT	M	103	-	-	11/21/61/61	0/2/2/2
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	2	3/3/20/25	12/37/135/135	-
23	CLA	C	509	3	3/3/20/25	5/37/135/135	-
35	LMT	b	627	-	-	6/17/37/61	0/1/1/2
23	CLA	C	513	3	3/3/20/25	8/37/135/135	-
23	CLA	c	503	3	3/3/20/25	2/37/135/135	-
33	LMG	a	416	-	-	15/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	B	629	-	-	10/17/37/61	0/1/1/2
26	SQD	L	101	-	-	23/49/69/69	0/1/1/1
31	LHG	A	416	-	-	11/53/53/53	-
23	CLA	B	611	2	3/3/20/25	3/37/135/135	-
23	CLA	b	616	2	3/3/20/25	13/37/135/135	-
31	LHG	D	409	-	-	15/53/53/53	-
23	CLA	C	514	3	2/2/20/25	11/37/135/135	-
23	CLA	B	607	41	3/3/20/25	2/37/135/135	-
24	PHO	A	407	-	-	2/53/103/103	0/5/6/6
31	LHG	l	101	-	-	19/53/53/53	-
23	CLA	C	511	3	3/3/20/25	14/37/135/135	-
35	LMT	m	102	-	-	7/21/61/61	0/2/2/2
33	LMG	c	520	-	-	7/46/66/70	0/1/1/1
29	PL9	d	406	-	-	6/53/73/73	0/1/1/1
36	DGD	C	519	-	-	15/51/91/95	0/2/2/2
33	LMG	c	519	-	-	13/46/66/70	0/1/1/1
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
36	DGD	C	518	-	-	13/51/91/95	0/2/2/2
23	CLA	B	612	2	3/3/20/25	9/37/135/135	-
38	HEM	E	103	5,6	-	0/6/54/54	-
33	LMG	C	520	-	-	15/46/66/70	0/1/1/1
33	LMG	Z	102	-	-	14/31/51/70	0/1/1/1
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
40	HEC	v	201	16	-	0/6/54/54	-
34	HTG	c	521	-	-	7/10/30/30	0/1/1/1
23	CLA	A	408	1	3/3/20/25	11/37/135/135	-
23	CLA	b	615	2	3/3/20/25	6/37/135/135	-
23	CLA	D	404	4	1/1/20/25	2/37/135/135	-
23	CLA	b	609	2	3/3/20/25	6/37/135/135	-
36	DGD	c	516	-	-	13/51/91/95	0/2/2/2
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
25	BCR	D	406	-	-	7/29/63/63	0/2/2/2
23	CLA	C	503	3	3/3/20/25	7/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	B	621	-	-	13/46/66/70	0/1/1/1
35	LMT	I	101	-	-	10/21/61/61	0/2/2/2
23	CLA	C	506	3	1/1/20/25	8/37/135/135	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
35	LMT	b	621	-	-	7/17/37/61	0/1/1/2
23	CLA	B	606	2	3/3/20/25	7/37/135/135	-
23	CLA	c	501	3	3/3/20/25	6/37/135/135	-
23	CLA	b	601	41	3/3/20/25	15/37/135/135	-
23	CLA	C	505	41	3/3/20/25	7/37/135/135	-
27	GOL	d	402	-	-	2/4/4/4	-
23	CLA	B	609	2	3/3/20/25	6/37/135/135	-
27	GOL	B	626	-	-	3/4/4/4	-
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	c	507	41	3/3/20/25	7/37/135/135	-
23	CLA	b	614	2	3/3/20/25	16/37/135/135	-
33	LMG	C	501	-	-	9/46/66/70	0/1/1/1
23	CLA	c	505	3	1/1/20/25	10/37/135/135	-
23	CLA	d	401	41	3/3/20/25	6/37/135/135	-
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	c	509	3	3/3/20/25	12/37/135/135	-
35	LMT	M	101	-	-	2/21/61/61	0/2/2/2
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
23	CLA	b	612	2	3/3/20/25	8/37/135/135	-
34	HTG	B	623	-	-	6/10/30/30	0/1/1/1
23	CLA	c	502	3	3/3/20/25	6/37/135/135	-
23	CLA	C	510	3	3/3/20/25	6/37/135/135	-
35	LMT	a	417	-	-	4/21/61/61	0/2/2/2
31	LHG	A	417	-	-	21/53/53/53	-
23	CLA	B	610	41	3/3/20/25	8/37/135/135	-
34	HTG	C	522	-	-	2/10/30/30	0/1/1/1
27	GOL	b	624	-	-	1/4/4/4	-
23	CLA	b	604	2	3/3/20/25	13/37/135/135	-
23	CLA	A	405	41	3/3/20/25	7/37/135/135	-
35	LMT	e	102	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HTG	D	412	-	-	0/7/27/30	0/1/1/1
34	HTG	b	625	-	-	6/10/30/30	0/1/1/1
35	LMT	D	402	-	-	6/21/61/61	0/2/2/2
34	HTG	B	627	-	-	2/10/30/30	0/1/1/1
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	b	602	2	3/3/20/25	6/37/135/135	-
35	LMT	D	403	-	-	9/21/61/61	0/2/2/2
25	BCR	A	409	-	-	2/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
34	HTG	b	628	-	-	6/10/30/30	0/1/1/1
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	b	608	2	2/2/20/25	4/37/135/135	-
35	LMT	B	630	-	-	7/21/61/61	0/2/2/2
23	CLA	a	405	41	2/2/20/25	5/37/135/135	-
23	CLA	d	403	4	1/1/20/25	3/37/135/135	-
31	LHG	e	101	-	-	14/46/46/53	-
23	CLA	b	611	2	3/3/20/25	6/37/135/135	-
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
29	PL9	a	414	-	-	13/53/73/73	0/1/1/1
26	SQD	a	412	-	-	11/49/69/69	0/1/1/1
24	PHO	a	407	-	-	4/53/103/103	0/5/6/6
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
23	CLA	c	506	3	2/2/20/25	8/37/135/135	-
34	HTG	d	411	-	-	3/7/27/30	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	b	610	41	3/3/20/25	5/37/135/135	-
24	PHO	a	406	-	-	4/53/103/103	0/5/6/6
26	SQD	a	410	-	-	12/49/69/69	0/1/1/1
23	CLA	B	601	41	3/3/20/25	13/37/135/135	-
33	LMG	b	620	-	-	14/46/66/70	0/1/1/1
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
29	PL9	D	407	-	-	11/53/73/73	0/1/1/1
36	DGD	c	518	-	-	5/51/91/95	0/2/2/2
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
40	HEC	V	202	16	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	E	101	-	-	20/46/46/53	-
23	CLA	B	614	2	3/3/20/25	13/37/135/135	-
26	SQD	A	410	-	-	13/49/69/69	0/1/1/1
23	CLA	C	512	3	3/3/20/25	4/37/135/135	-
23	CLA	A	404	1	3/3/20/25	6/37/135/135	-
23	CLA	C	504	3	2/2/20/25	2/37/135/135	-
26	SQD	f	101	-	-	16/38/58/69	0/1/1/1
25	BCR	y	101	-	-	7/29/63/63	0/2/2/2
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	511	3	3/3/20/25	3/37/135/135	-
27	GOL	A	411	-	-	2/4/4/4	-
33	LMG	J	101	39	-	9/46/66/70	0/1/1/1
34	HTG	b	623	-	-	3/10/30/30	0/1/1/1
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
34	HTG	b	622	-	-	2/10/30/30	0/1/1/1
23	CLA	c	504	41	3/3/20/25	7/37/135/135	-
23	CLA	b	603	2	2/2/20/25	10/37/135/135	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
36	DGD	c	517	-	-	14/51/91/95	0/2/2/2
23	CLA	B	602	2	3/3/20/25	6/37/135/135	-
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1

The worst 5 of 1126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3B-C2B	6.82	1.49	1.40
23	C	509	CLA	C3B-C2B	6.72	1.49	1.40
23	C	510	CLA	C3B-C2B	6.65	1.49	1.40
23	C	502	CLA	C3B-C2B	6.54	1.49	1.40
23	b	612	CLA	C3B-C2B	6.53	1.49	1.40

The worst 5 of 2293 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	PHO	CMD-C2D-C1D	8.00	137.38	125.06
24	A	407	PHO	CMD-C2D-C1D	7.45	136.53	125.06
23	B	606	CLA	C4A-NA-C1A	-7.40	103.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	PHO	CMD-C2D-C1D	7.33	136.36	125.06
23	C	504	CLA	C4A-NA-C1A	-7.18	103.48	106.71

5 of 196 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	a	408	CLA	NC
23	a	408	CLA	ND
23	a	408	CLA	NA
23	d	404	CLA	NC
23	d	404	CLA	ND

5 of 1331 torsion outliers are listed below:

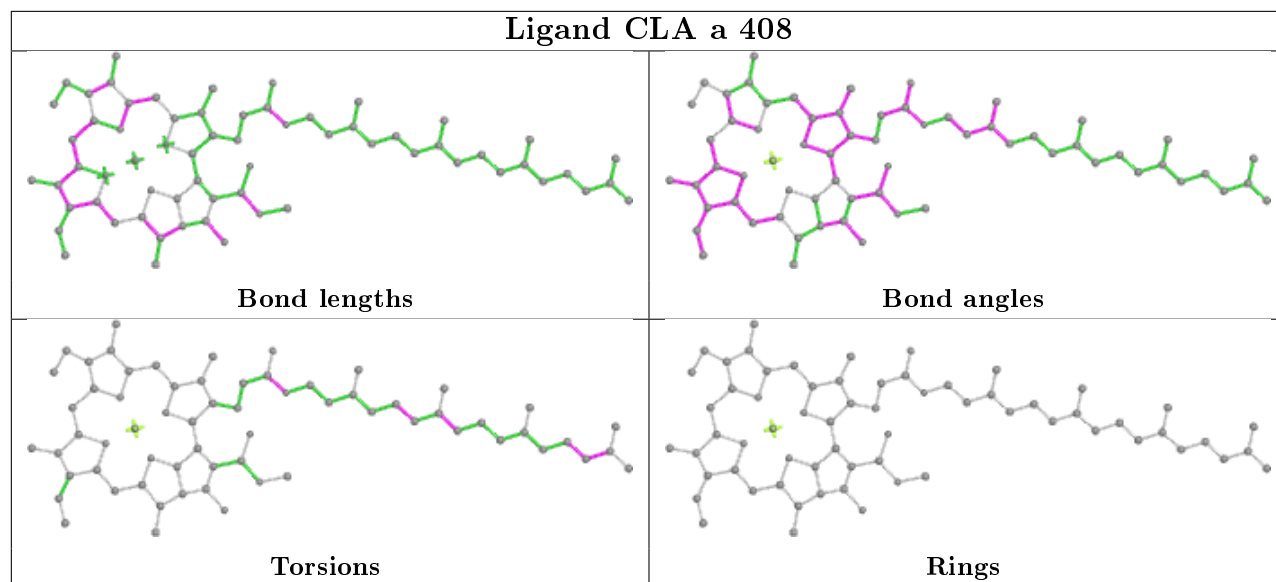
Mol	Chain	Res	Type	Atoms
27	C	523	GOL	O1-C1-C2-O2
27	C	523	GOL	O1-C1-C2-C3
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
31	l	101	LHG	C4-O6-P-O4

There are no ring outliers.

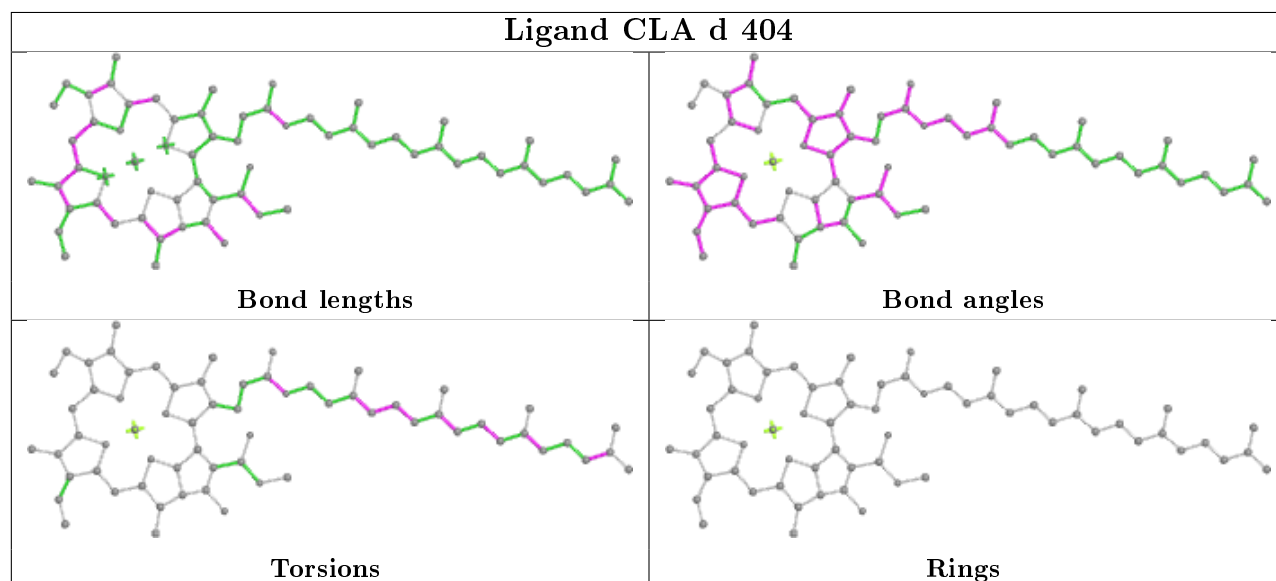
No monomer is involved in short contacts.

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.

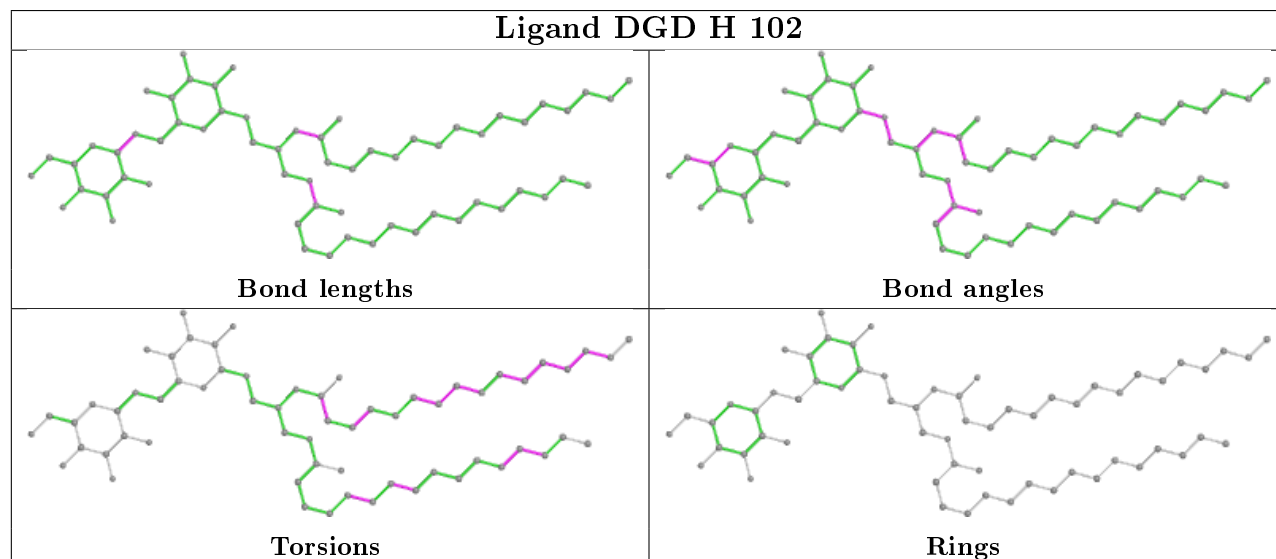
Ligand CLA a 408



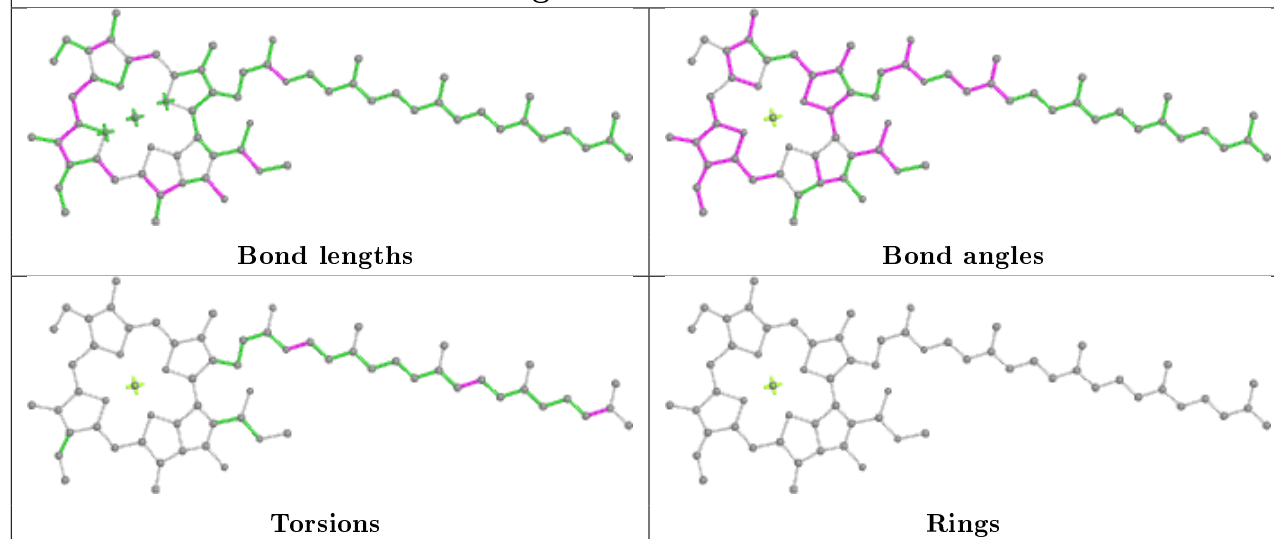
Ligand CLA d 404



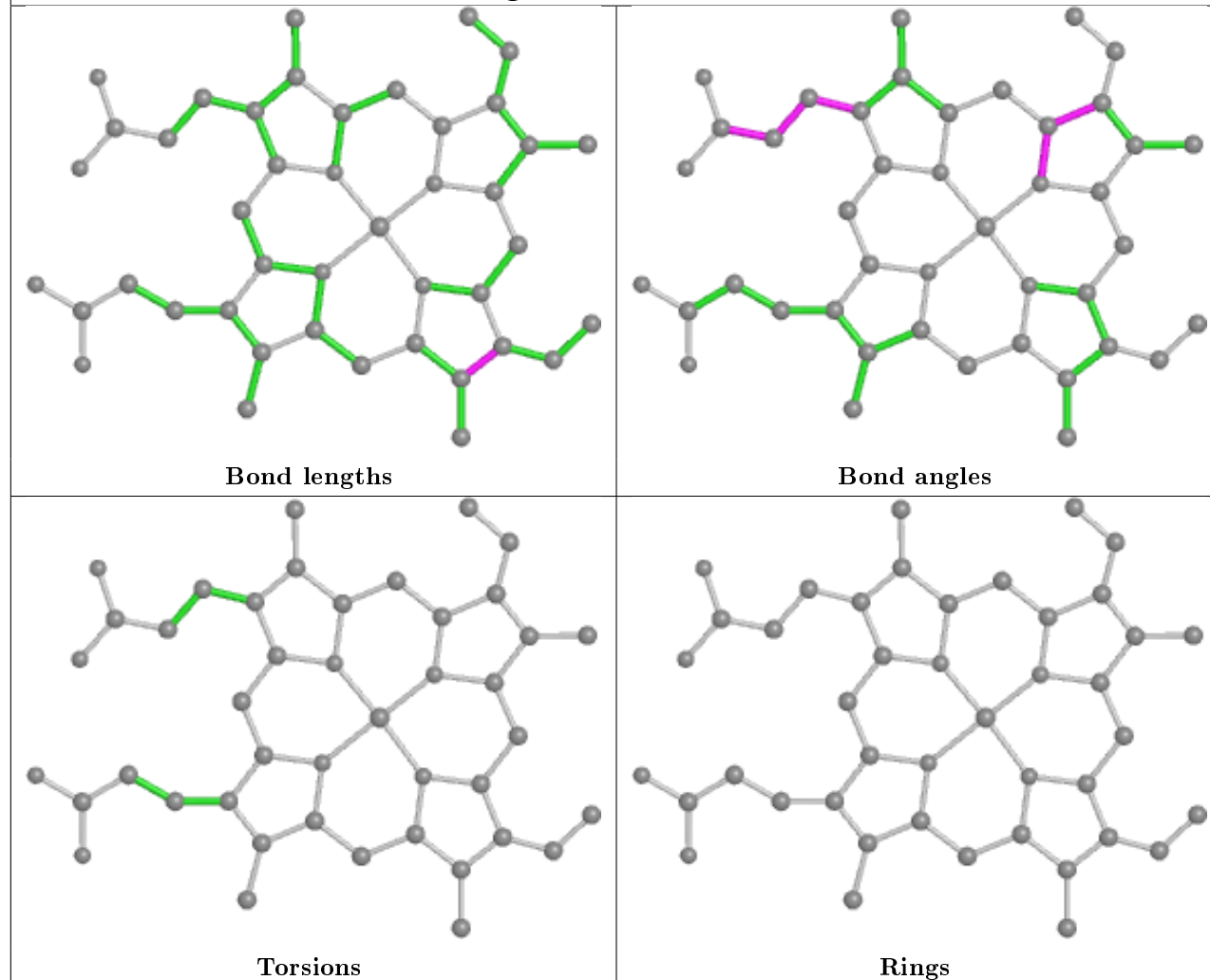
Ligand DGD H 102

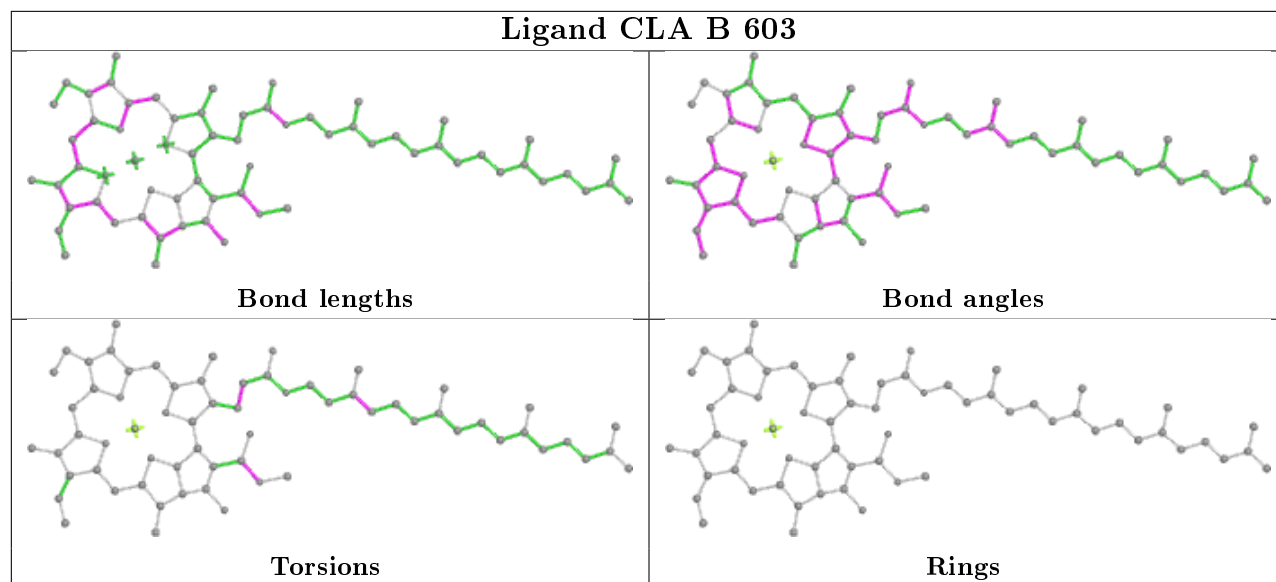
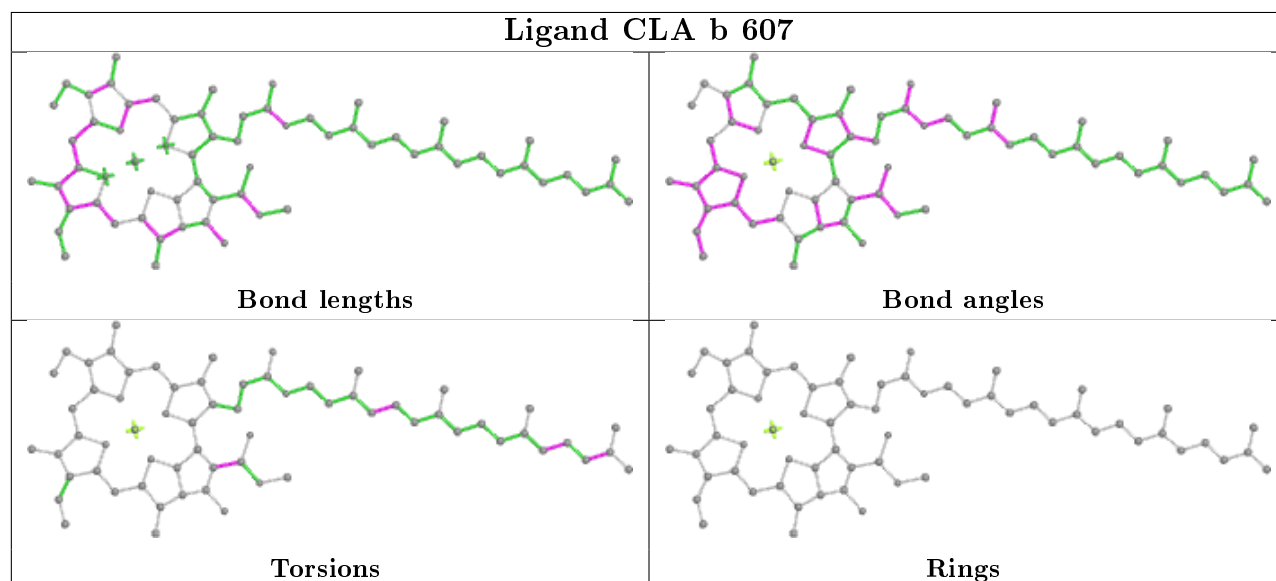
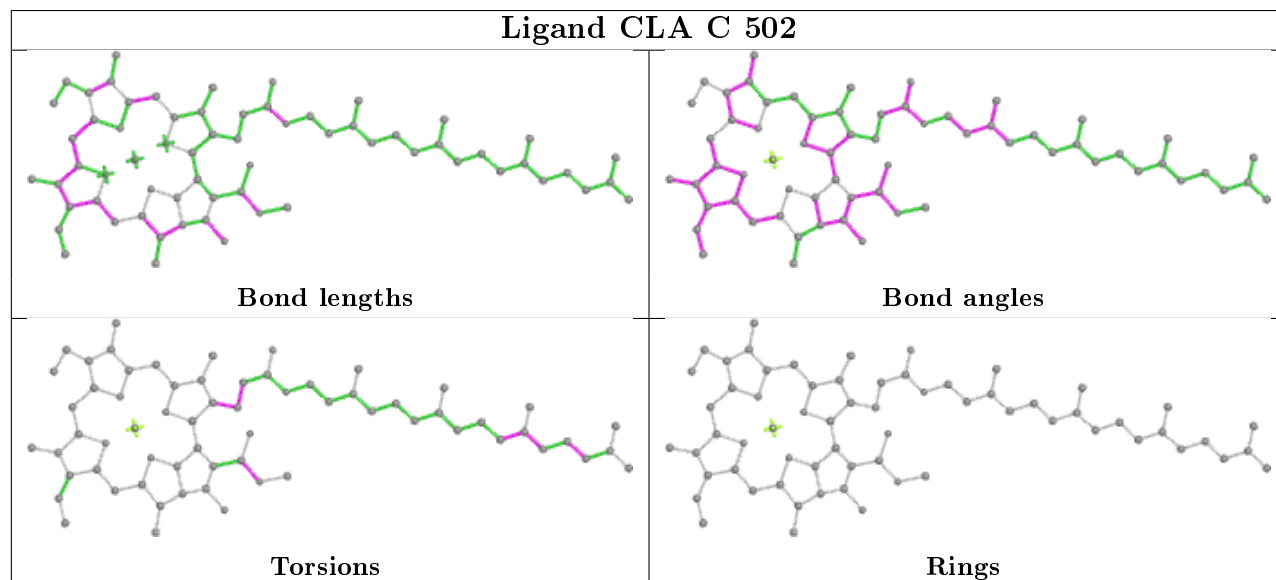


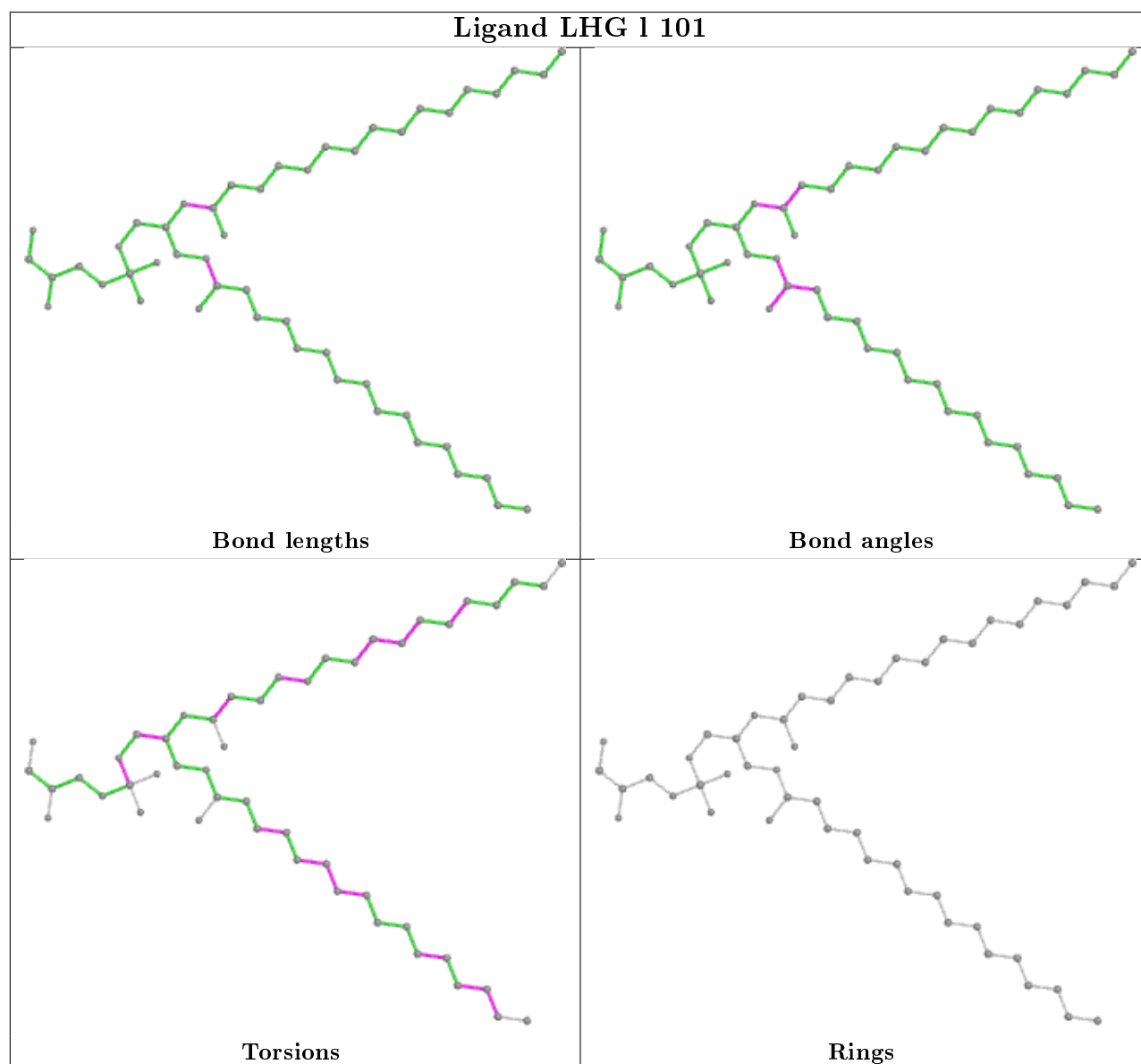
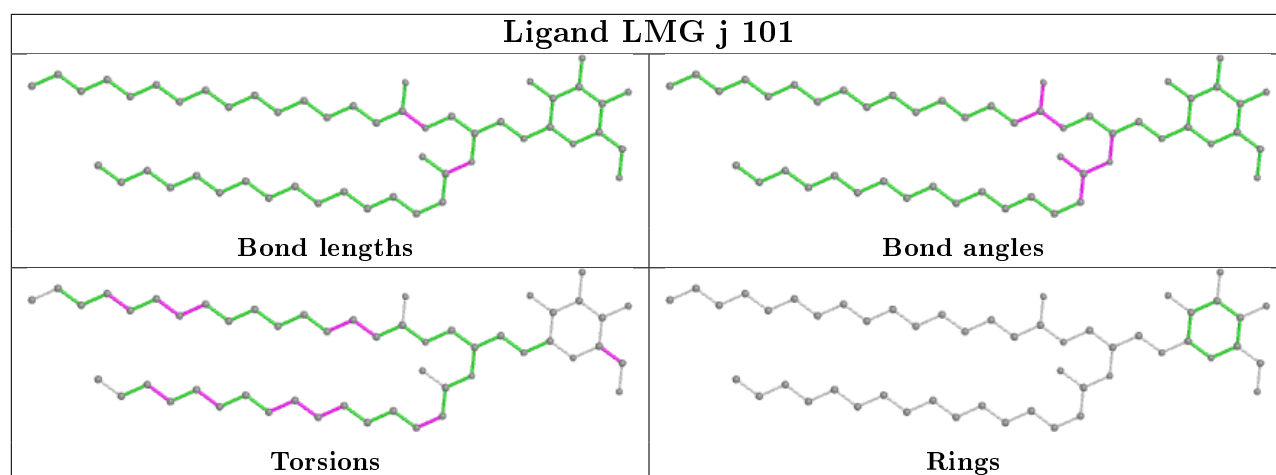
Ligand CLA B 608

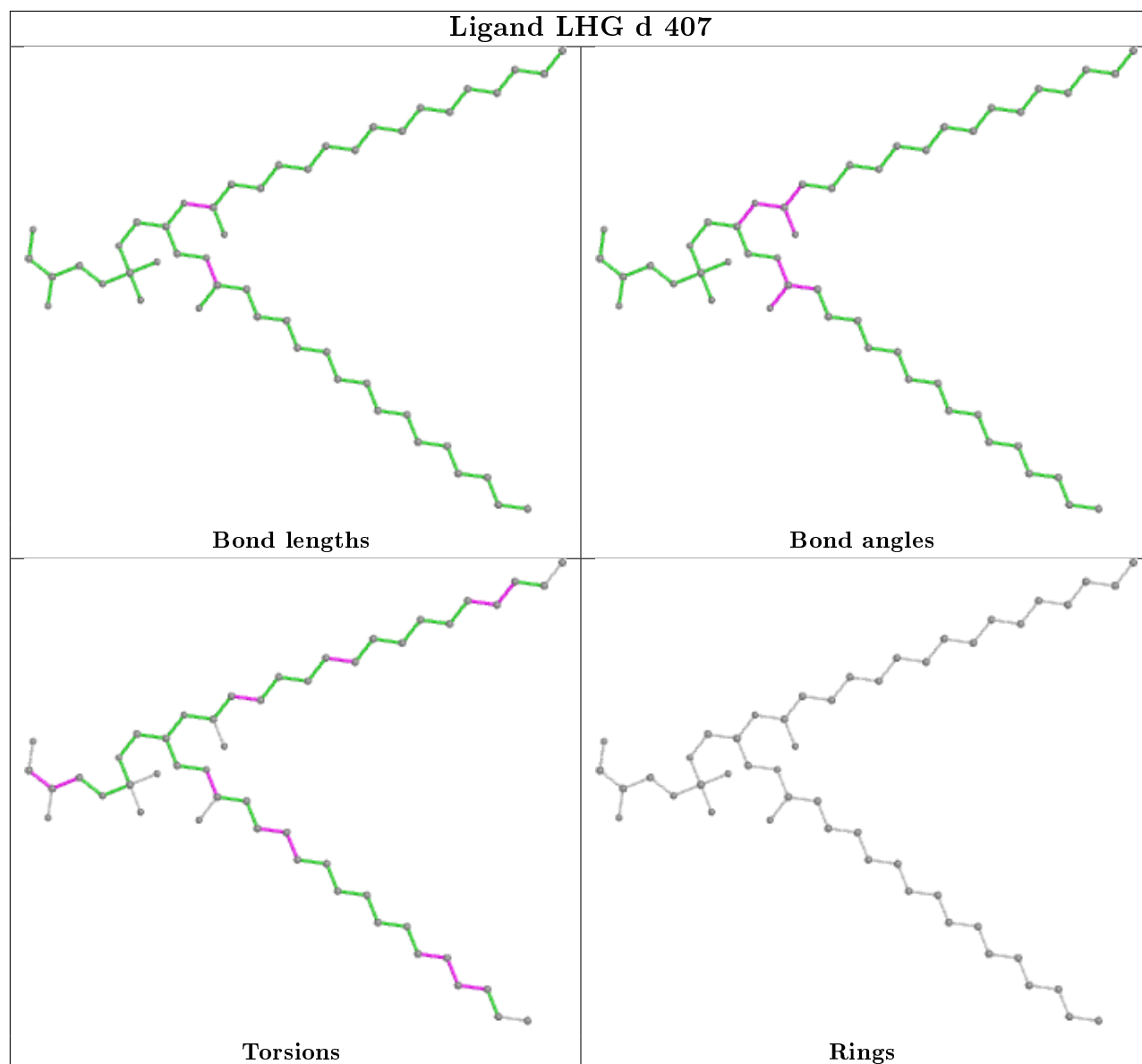
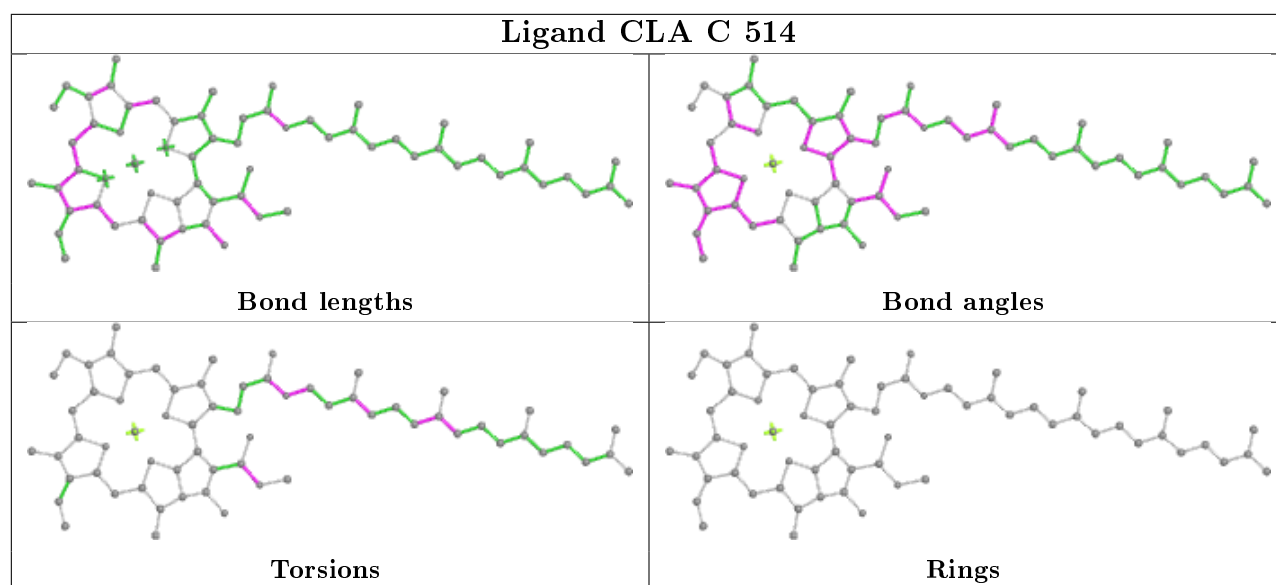


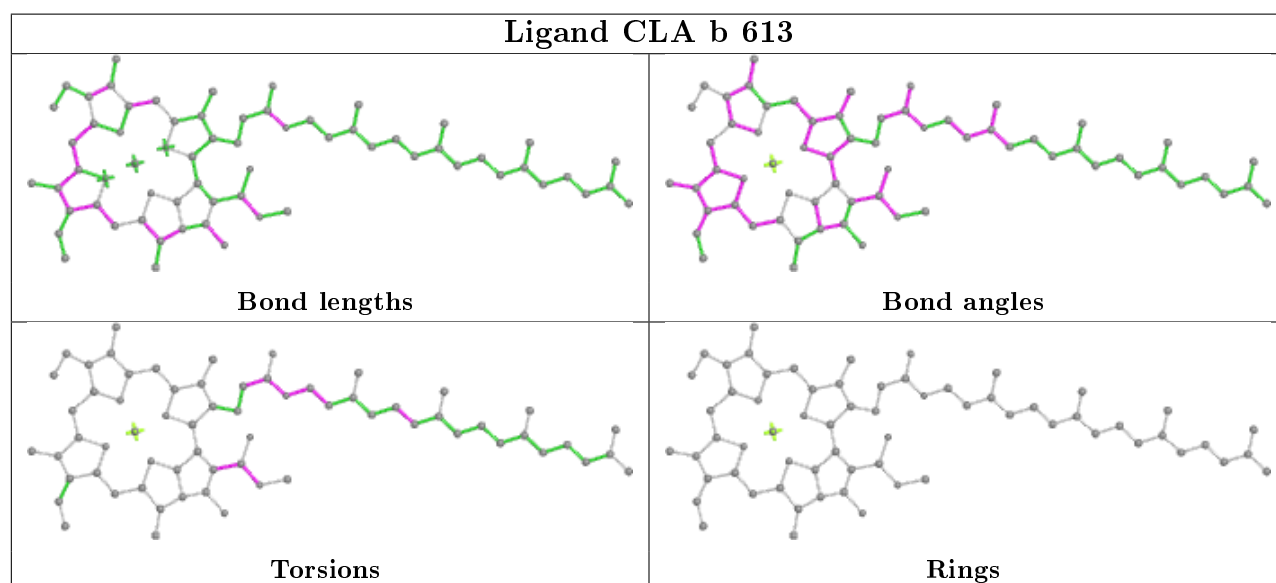
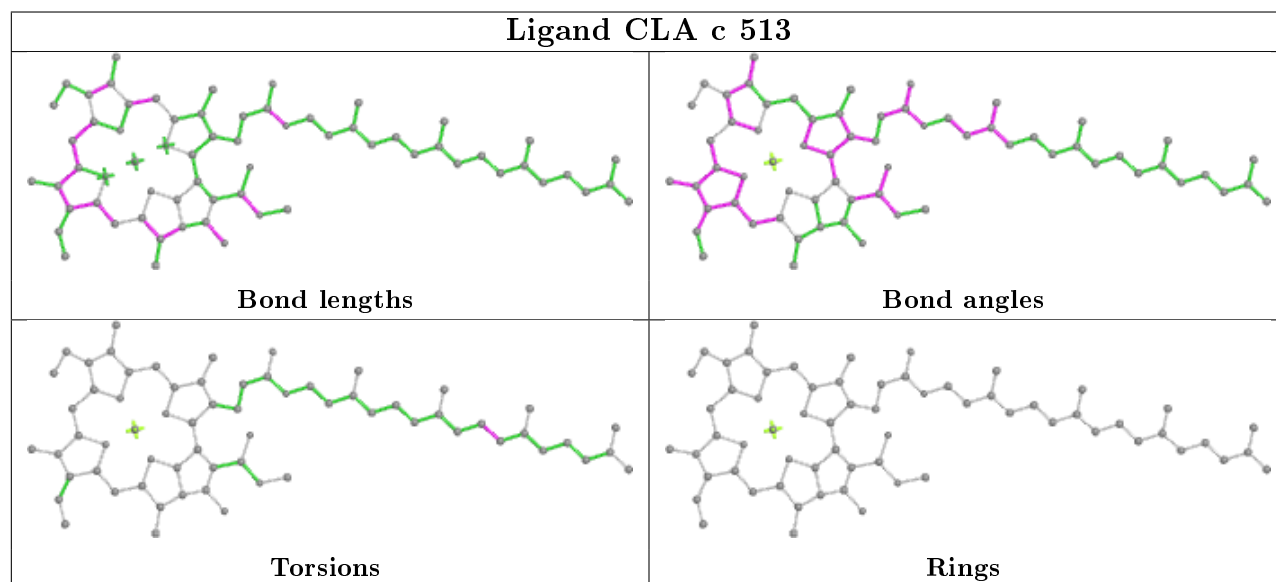
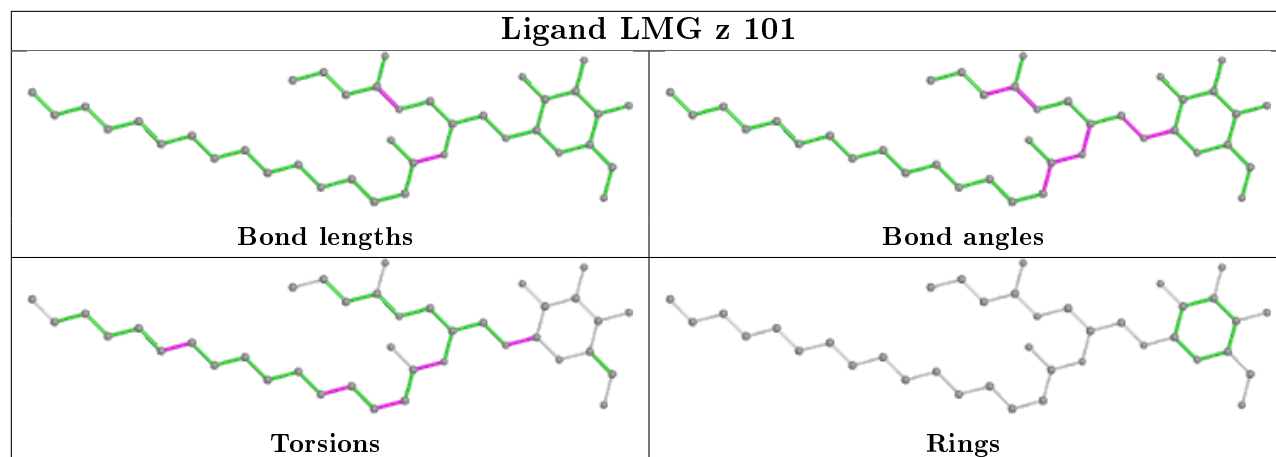
Ligand HEM e 103

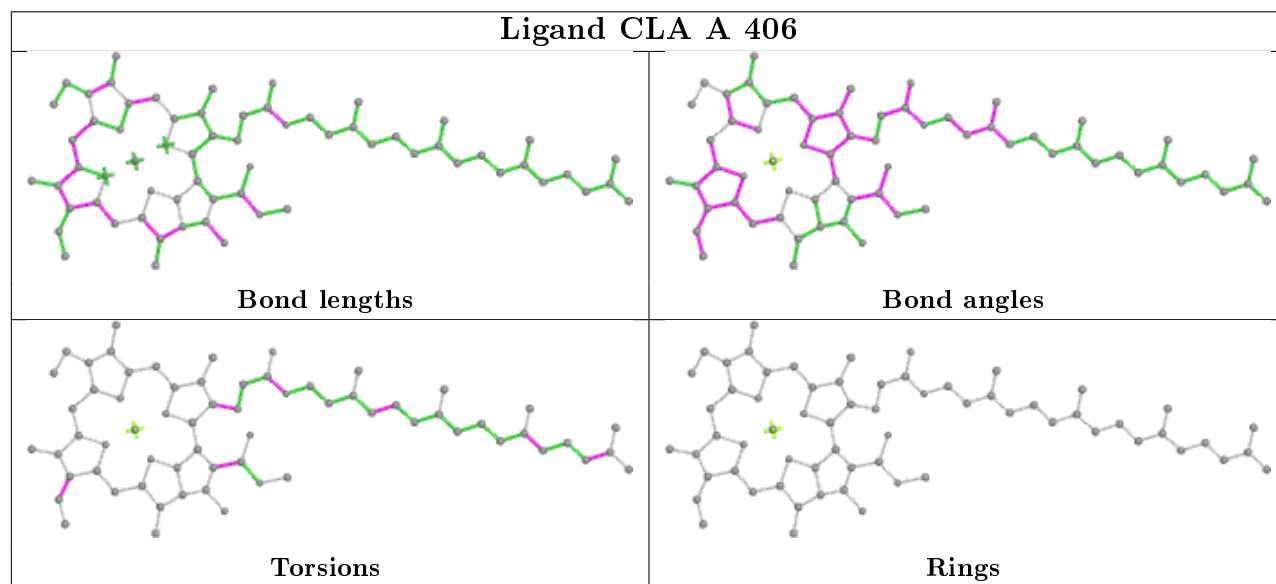
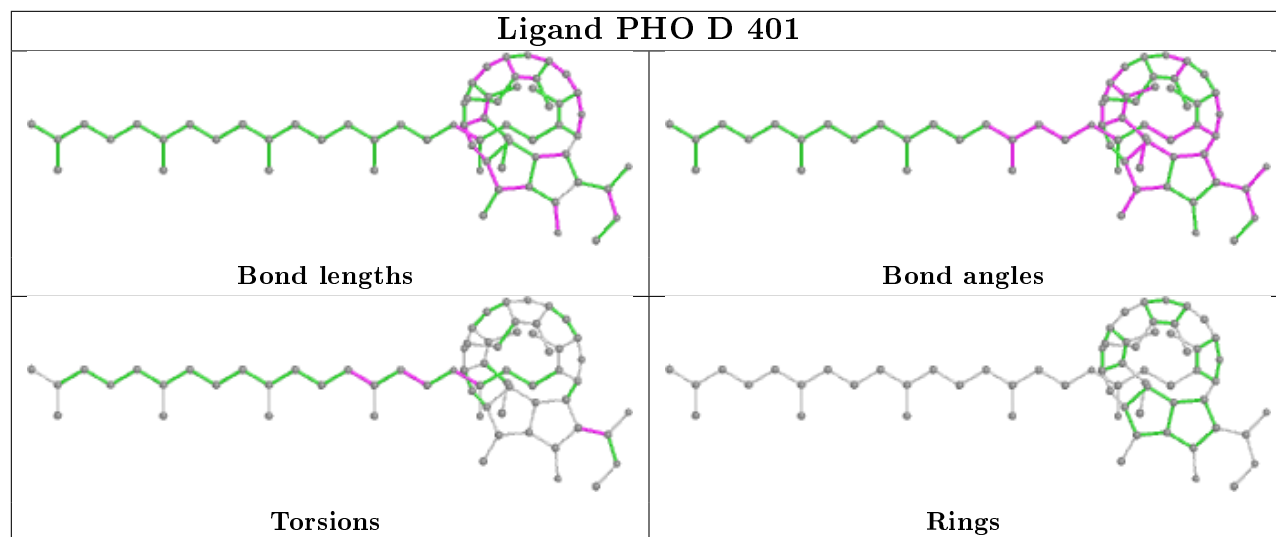
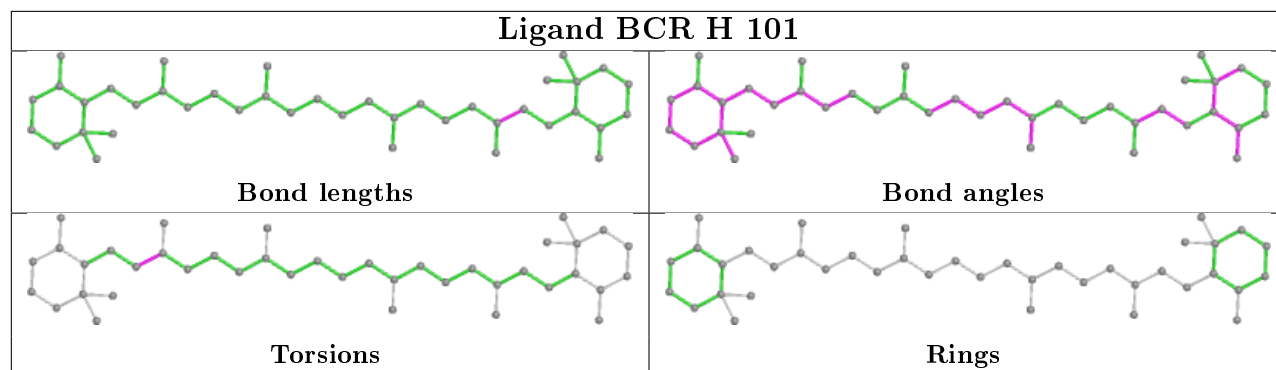


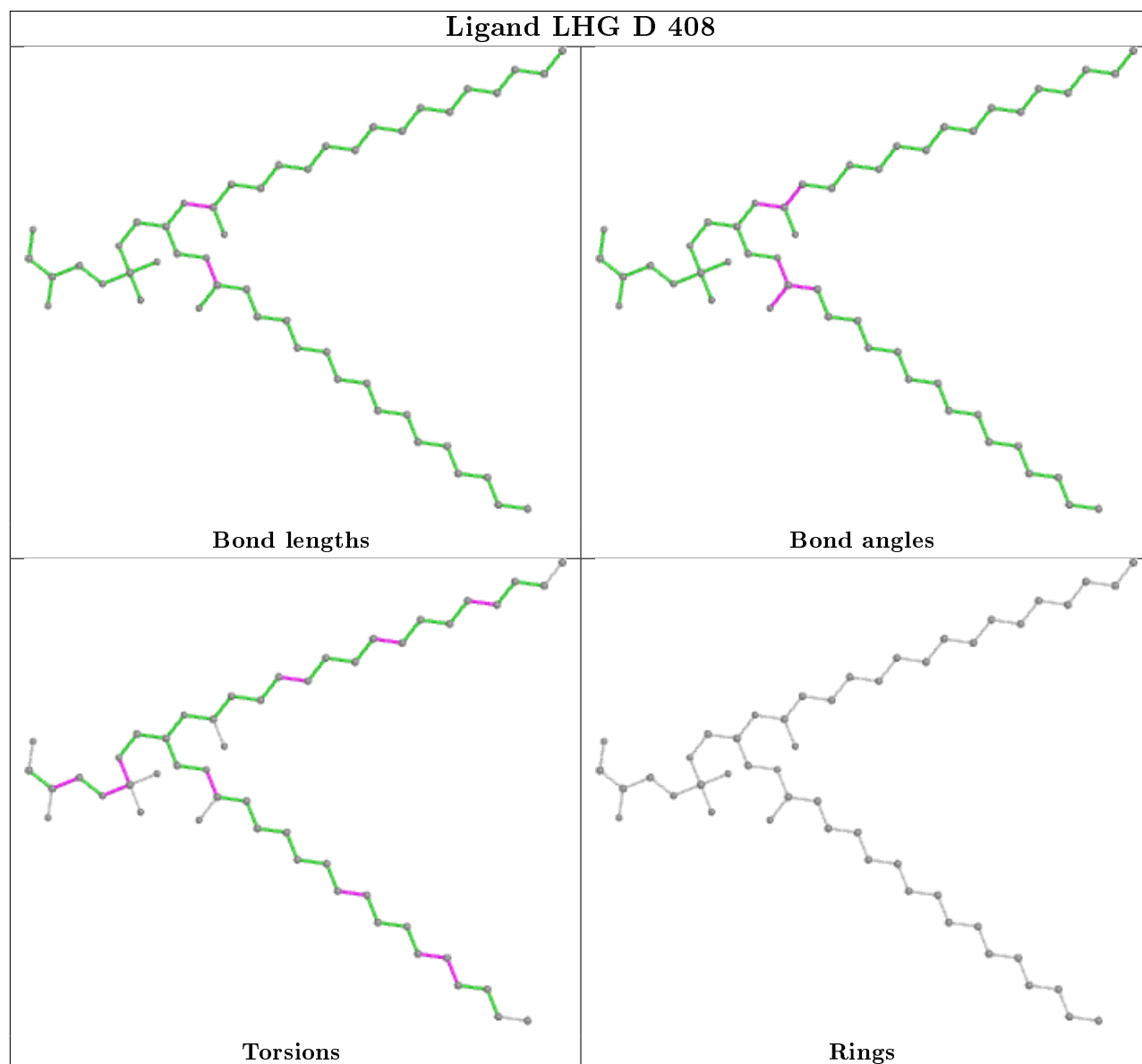
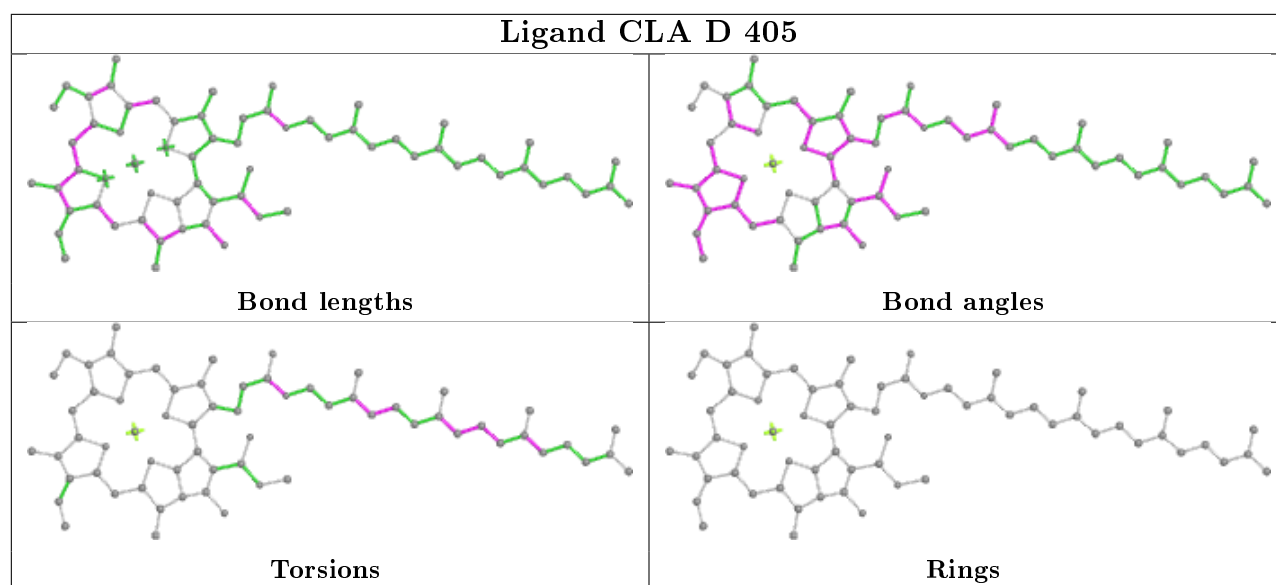
Ligand CLA B 603**Ligand CLA b 607****Ligand CLA C 502**

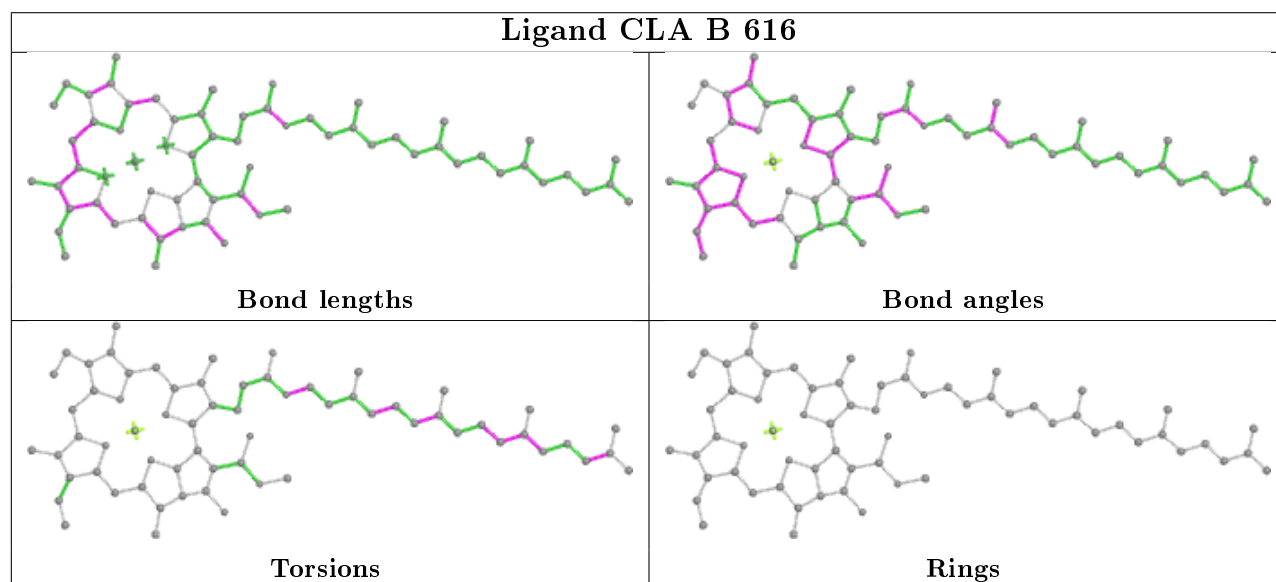
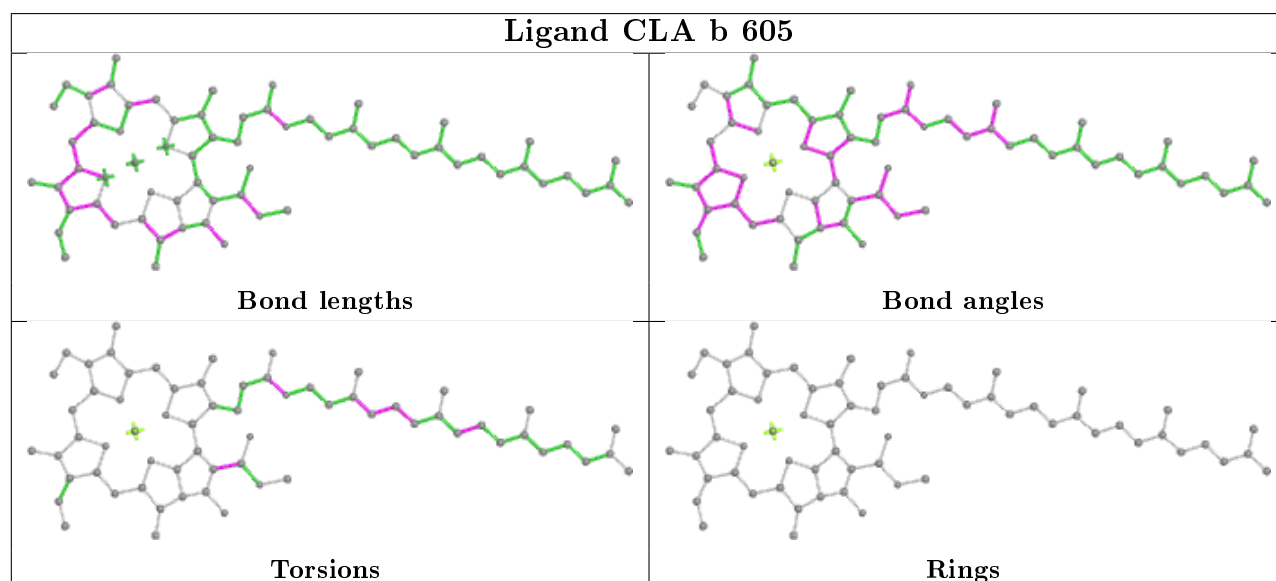
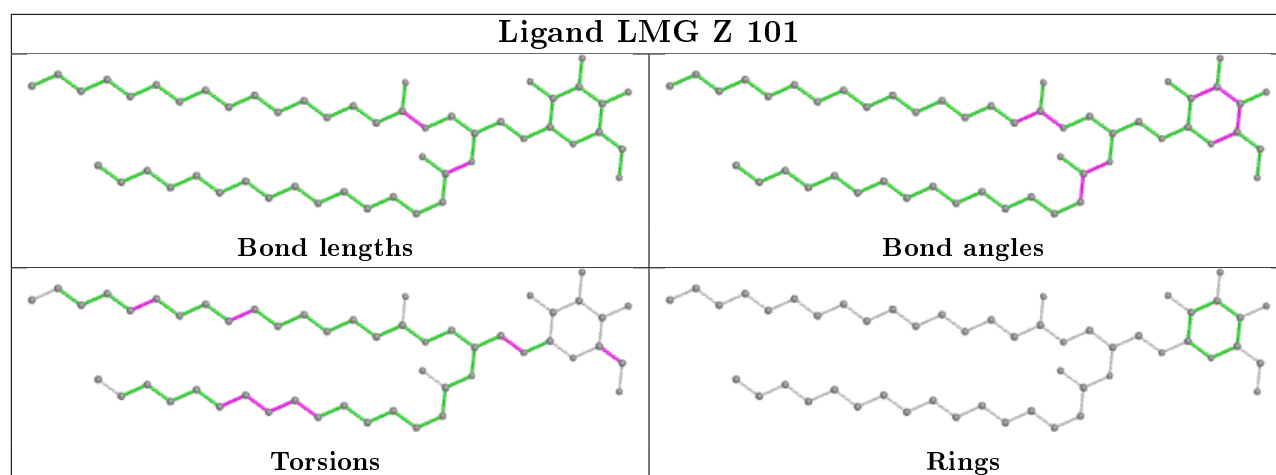


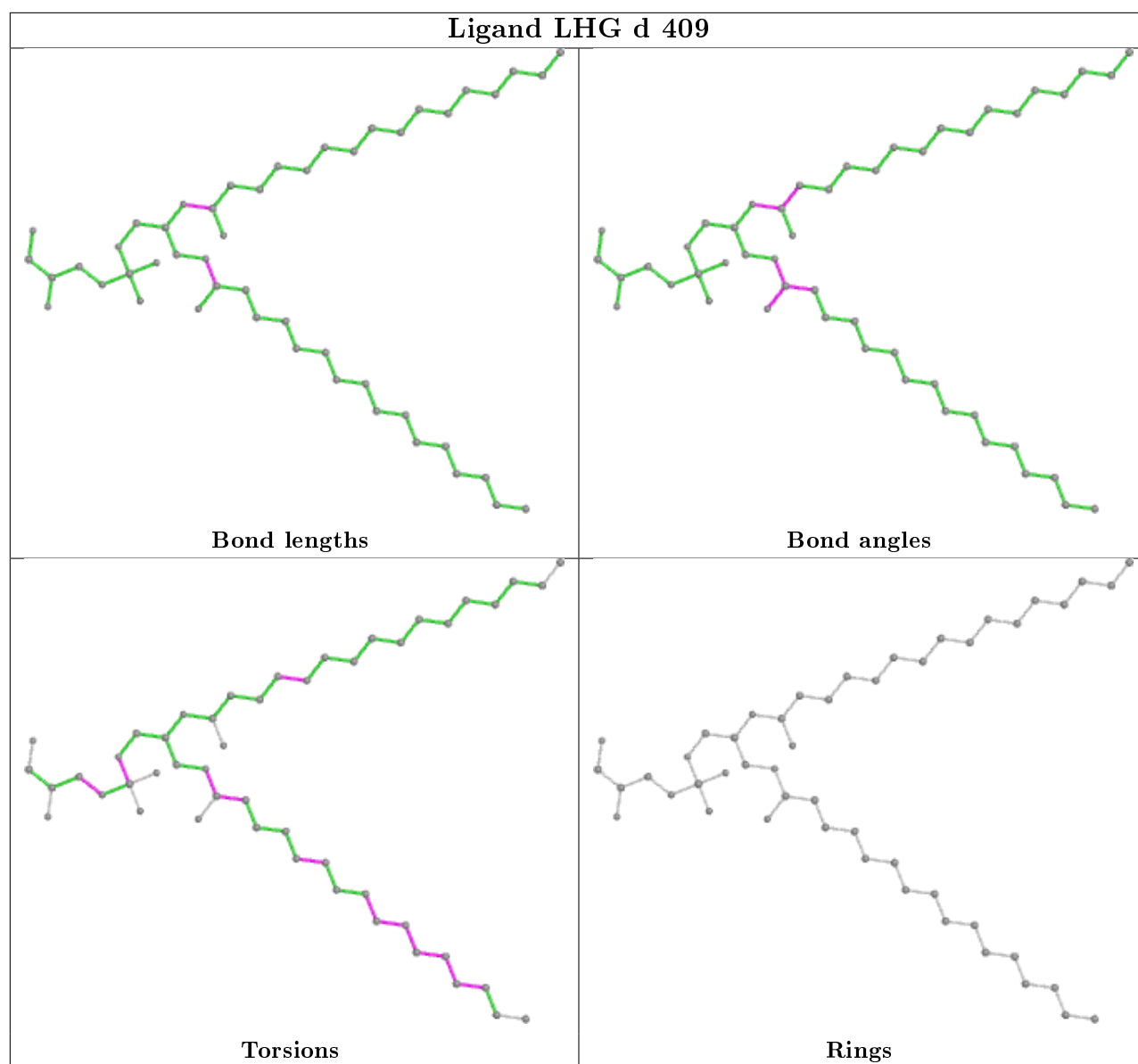


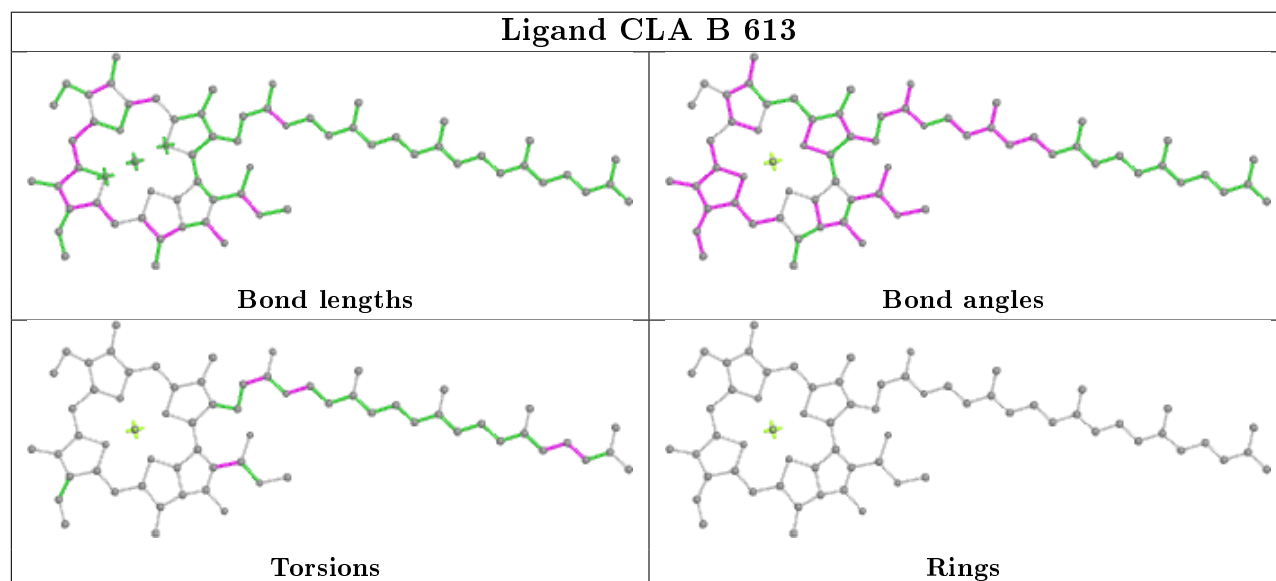
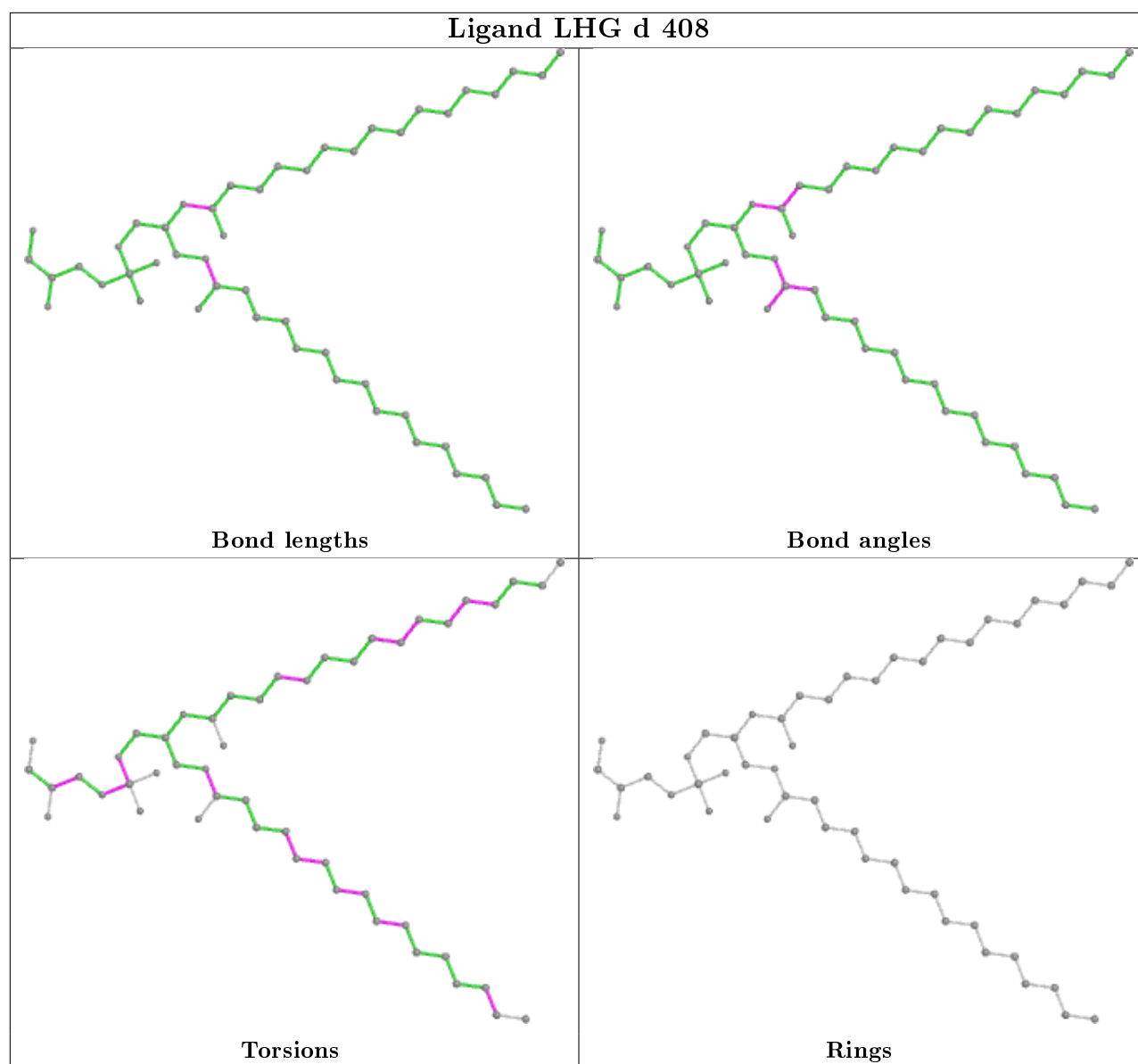


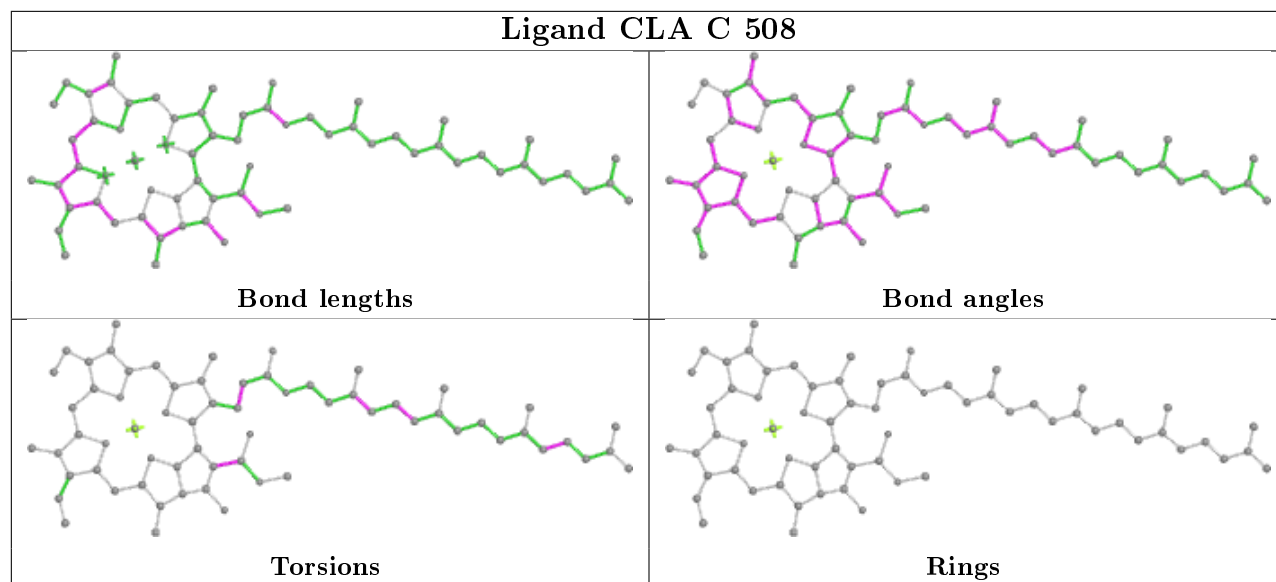
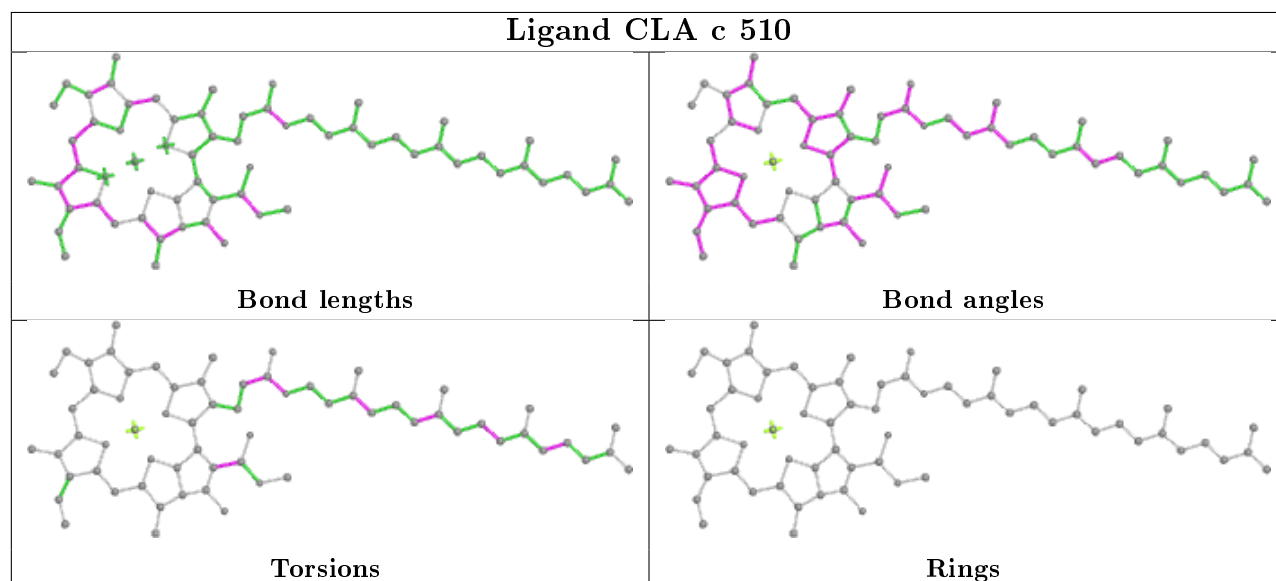
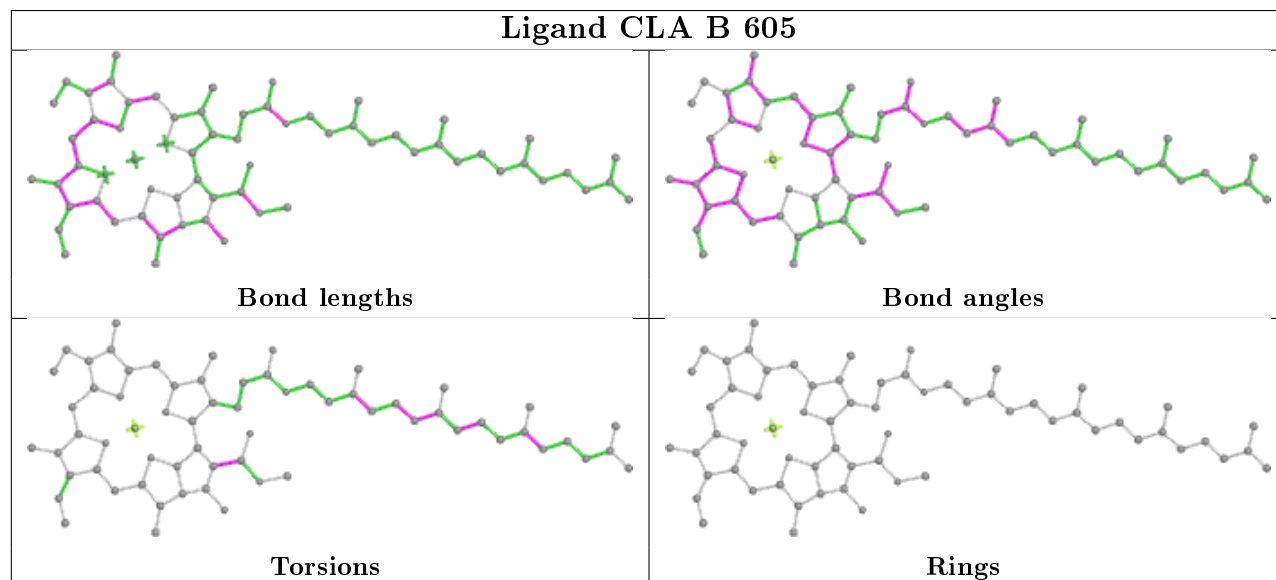


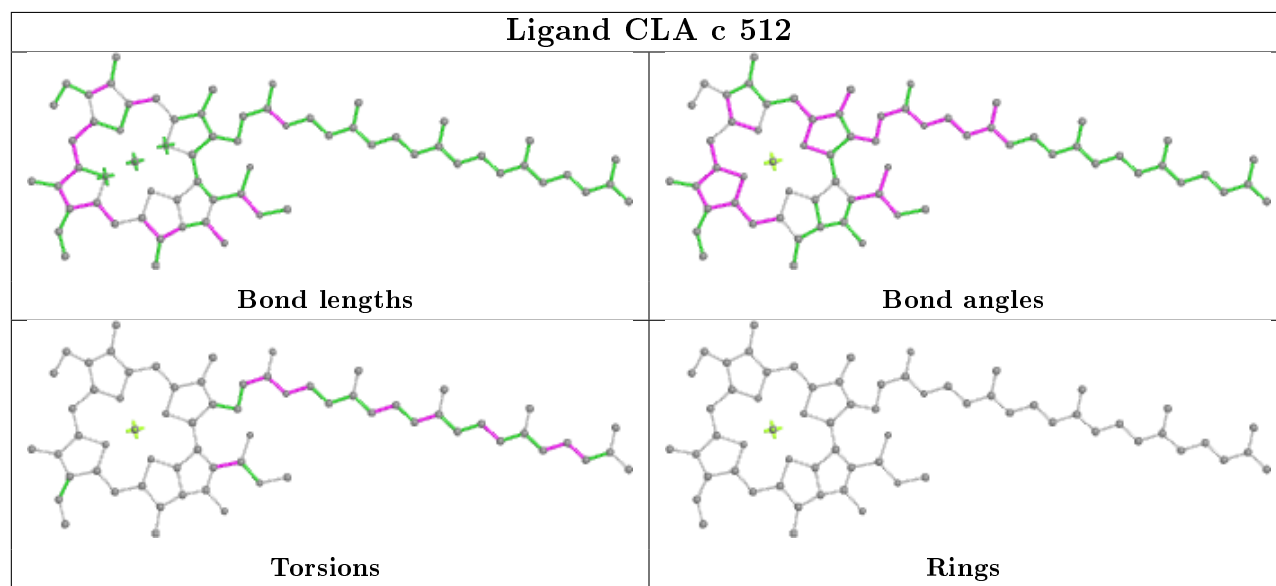
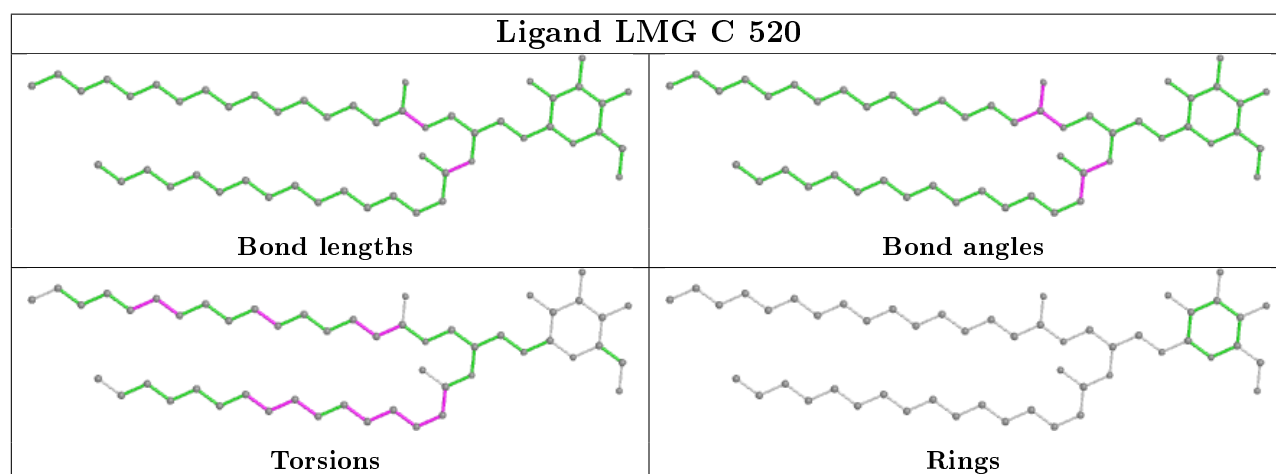
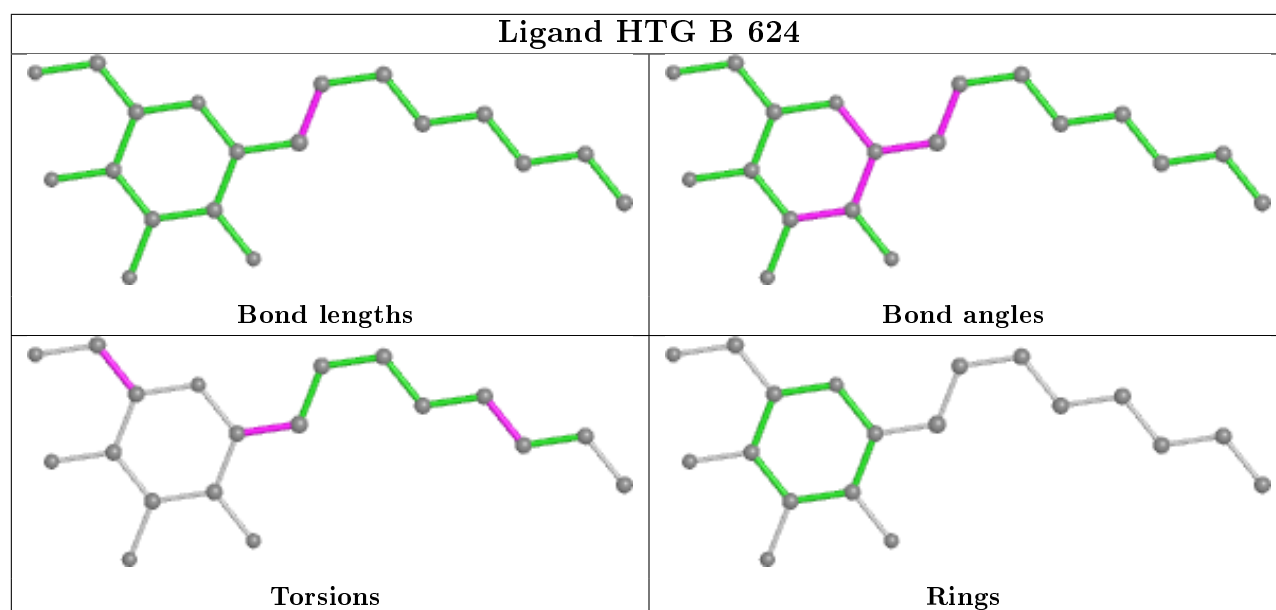


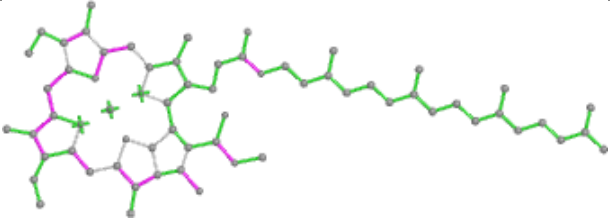
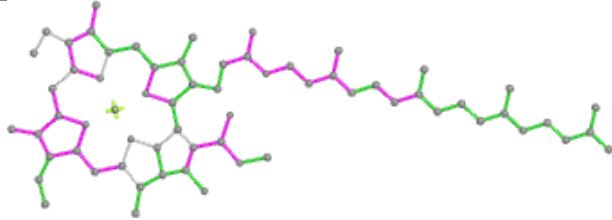
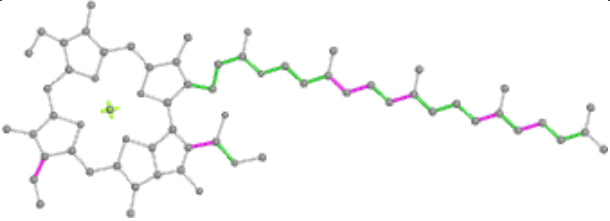
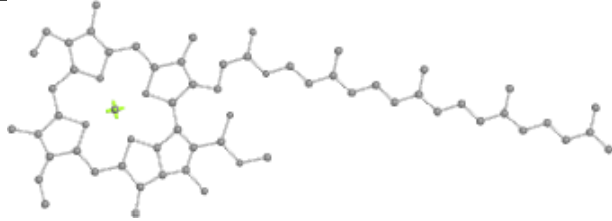
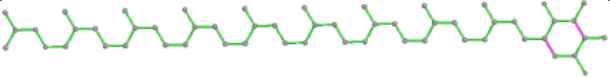
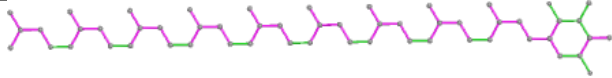
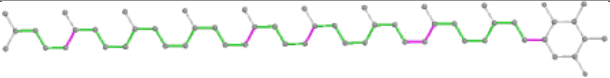
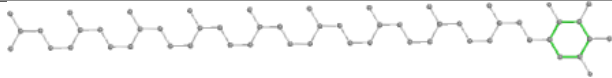
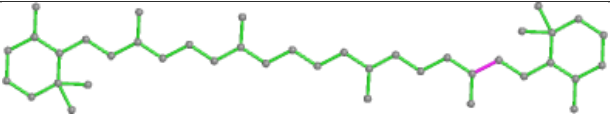
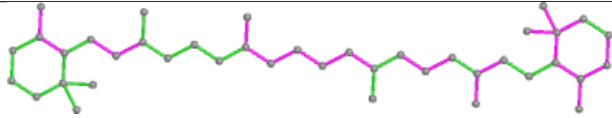
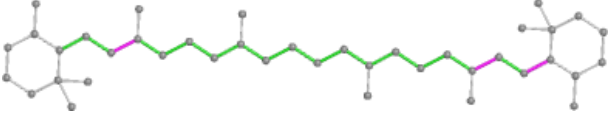
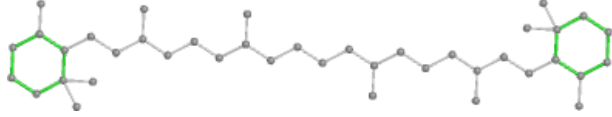


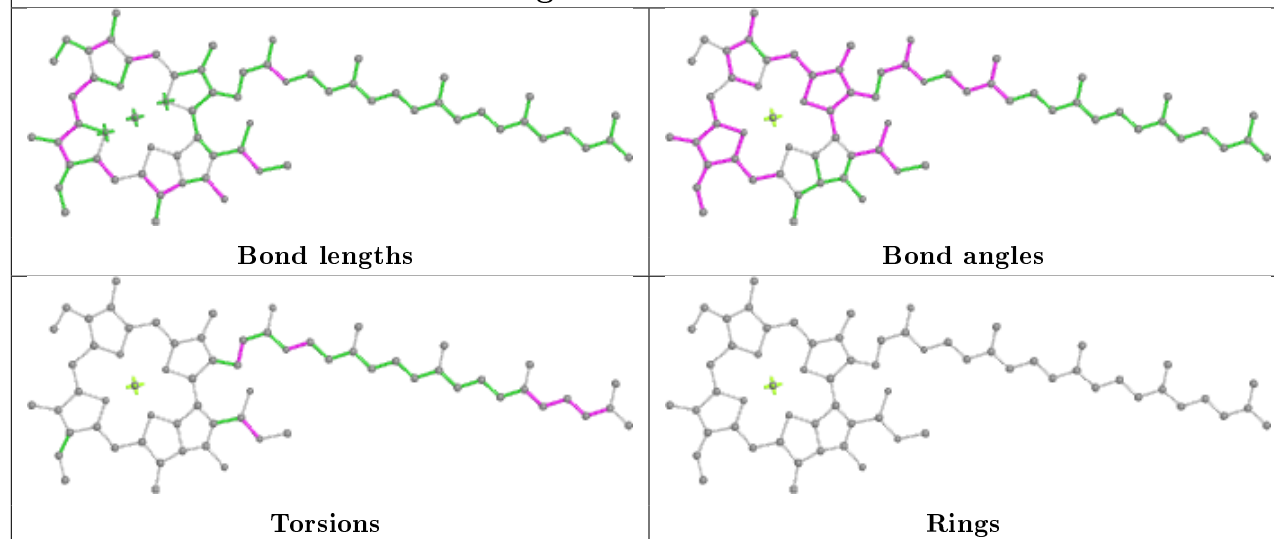
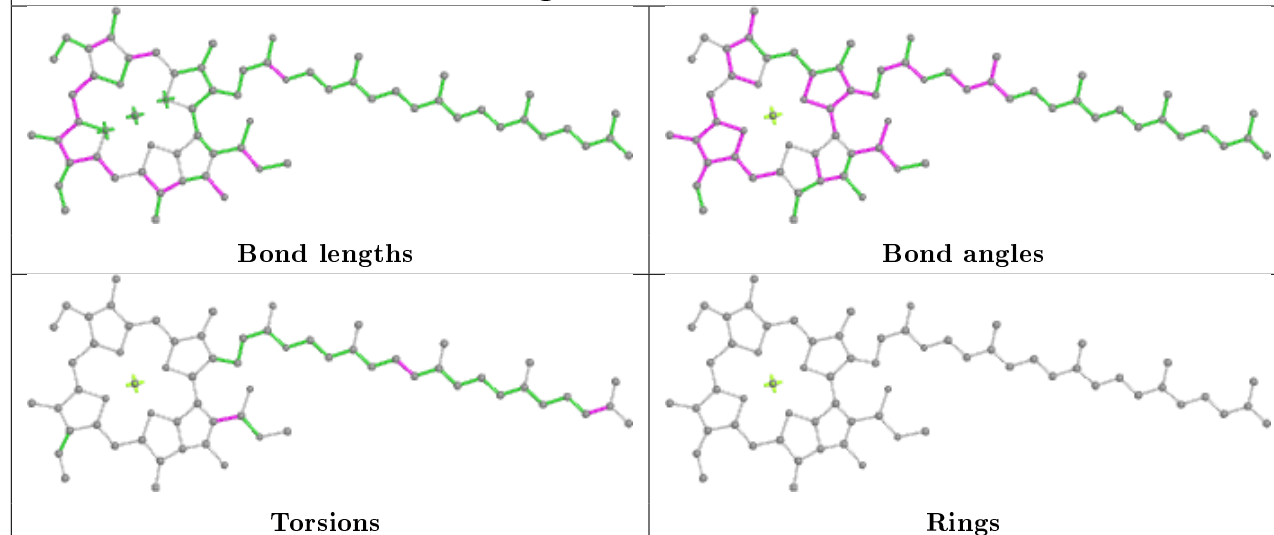
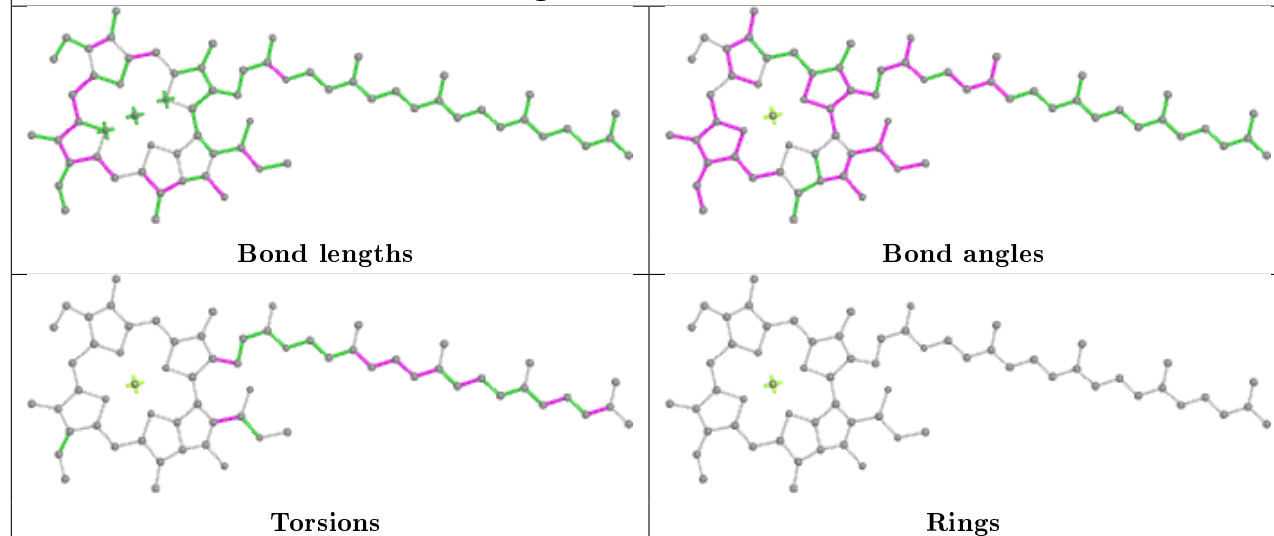


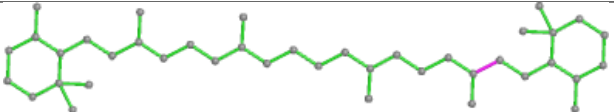
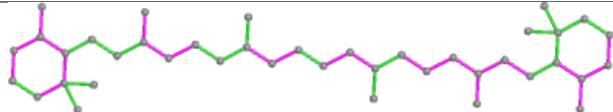
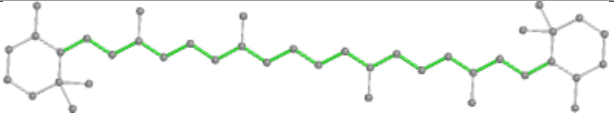
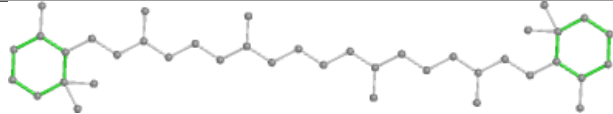


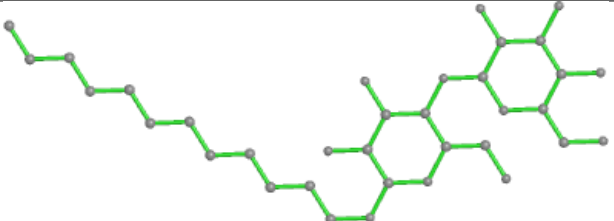
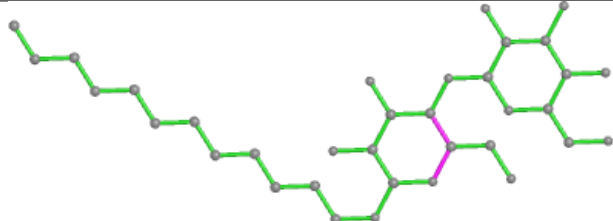
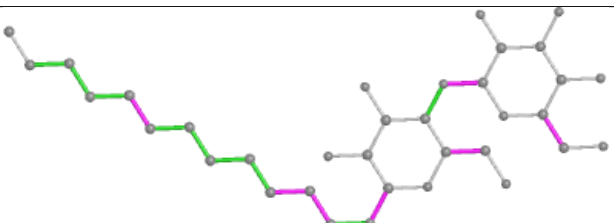
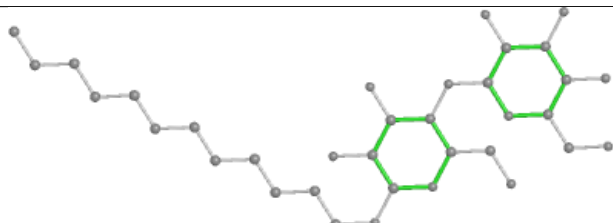
Ligand CLA C 508**Ligand CLA c 510****Ligand CLA B 605**

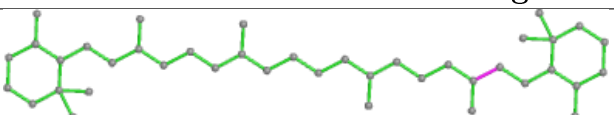
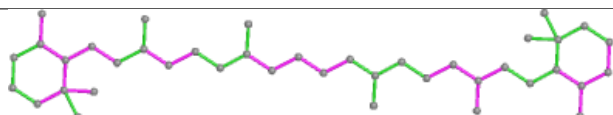
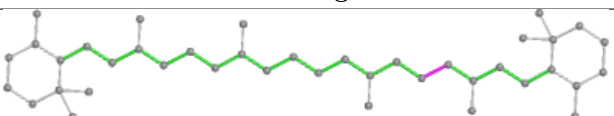
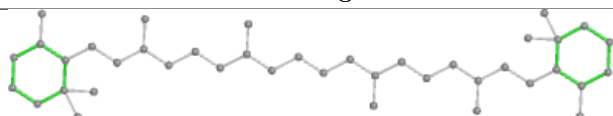


Ligand CLA B 604	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 A 414	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR d 405	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

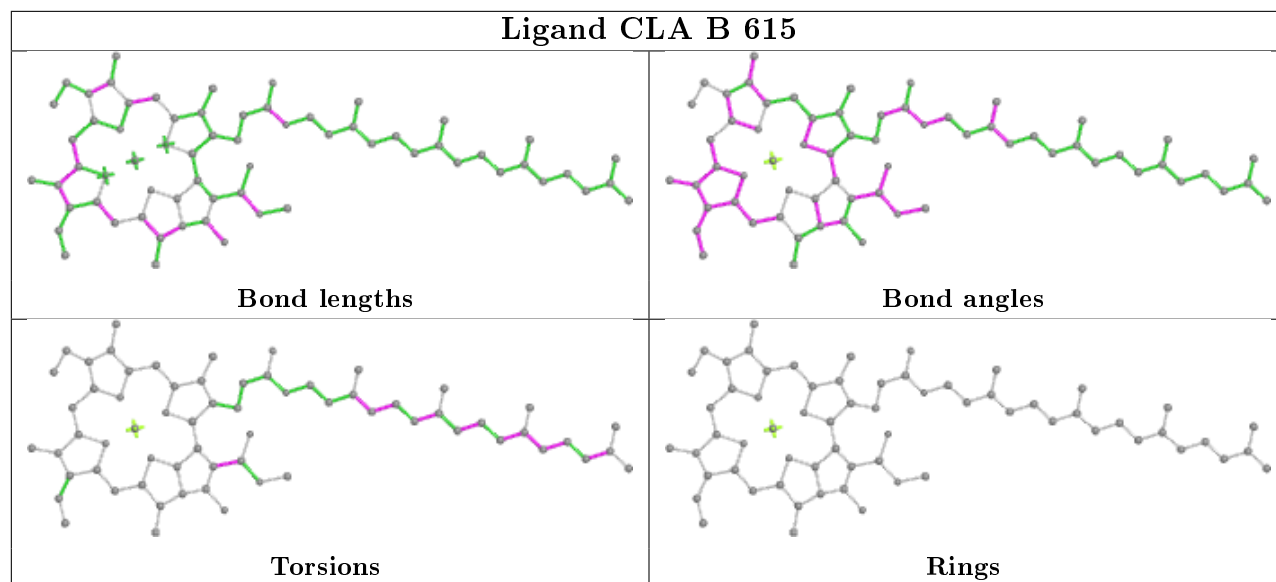
Ligand CLA a 404**Ligand CLA c 508****Ligand CLA C 507**

Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

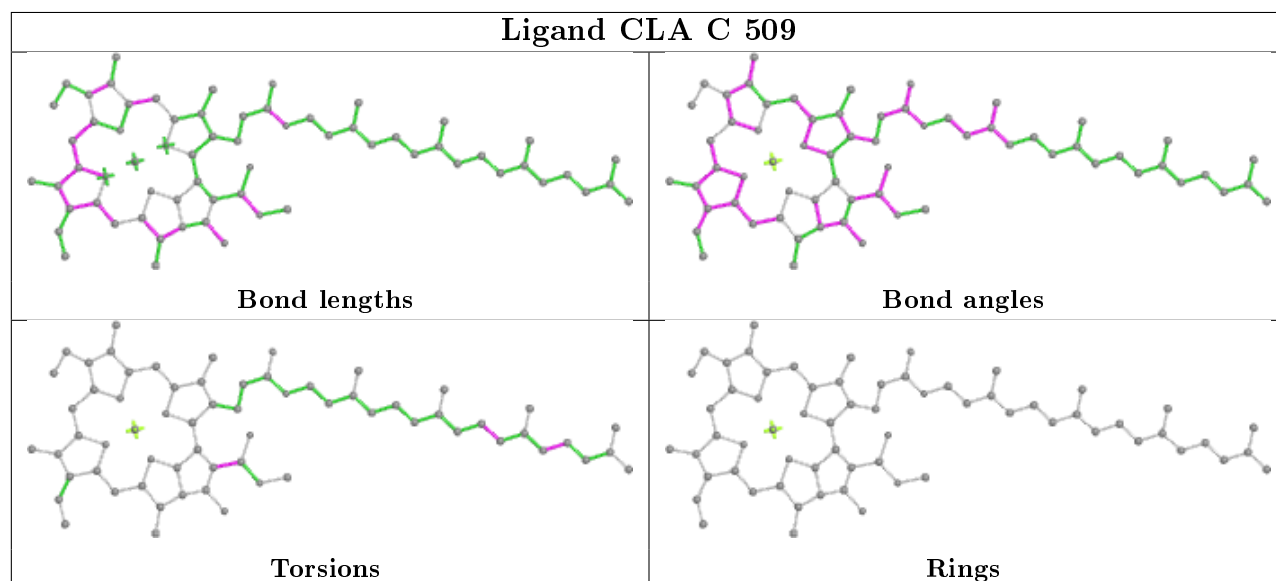
Ligand LMT M 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

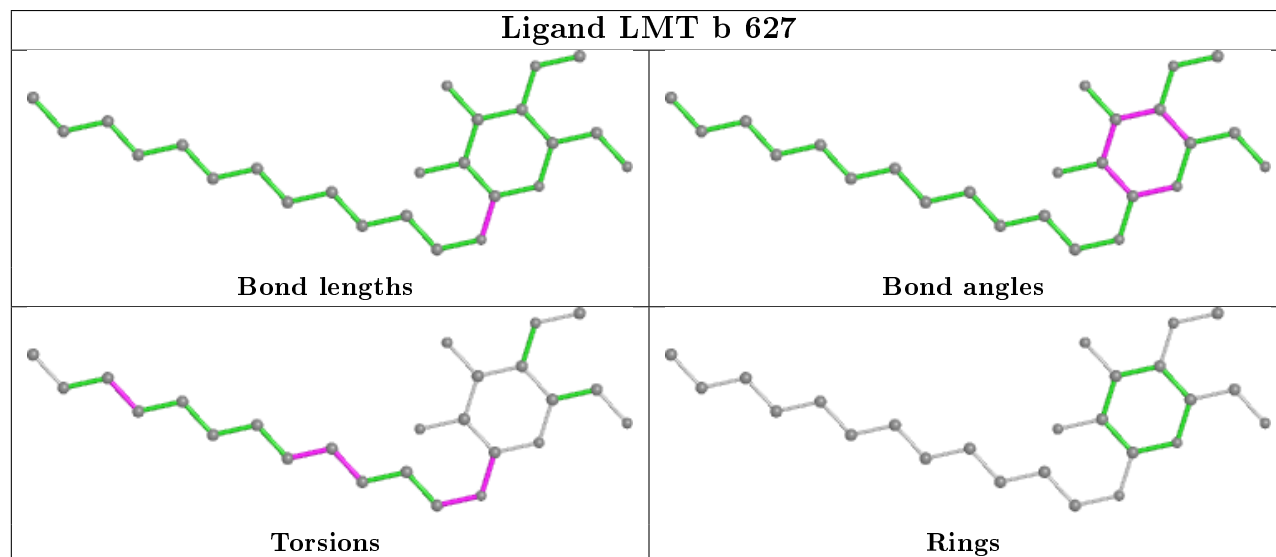
Ligand CLA B 615

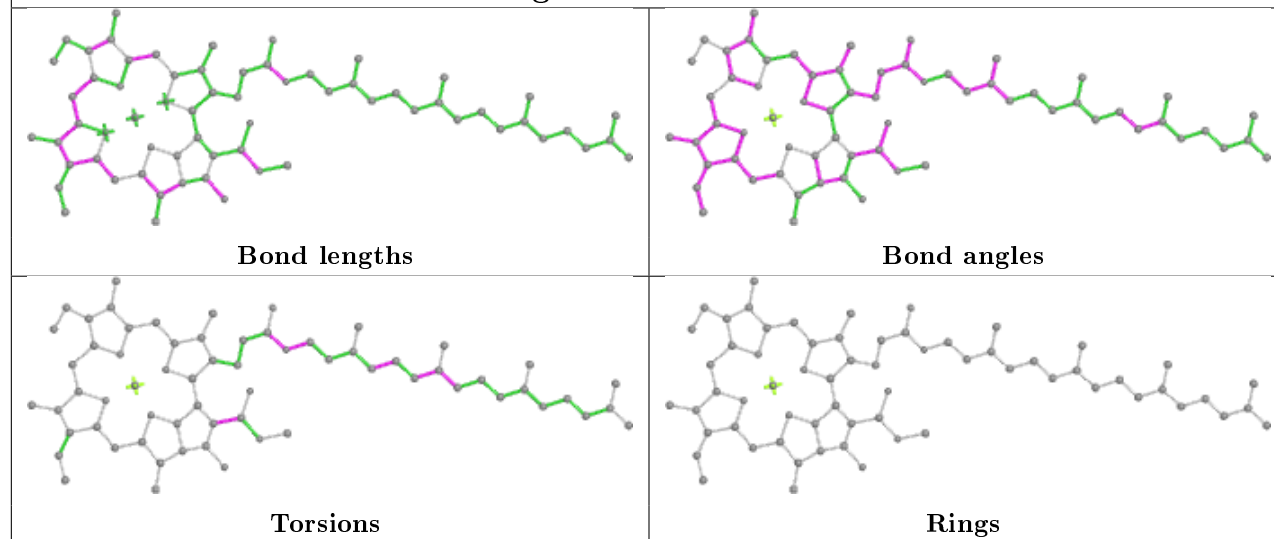
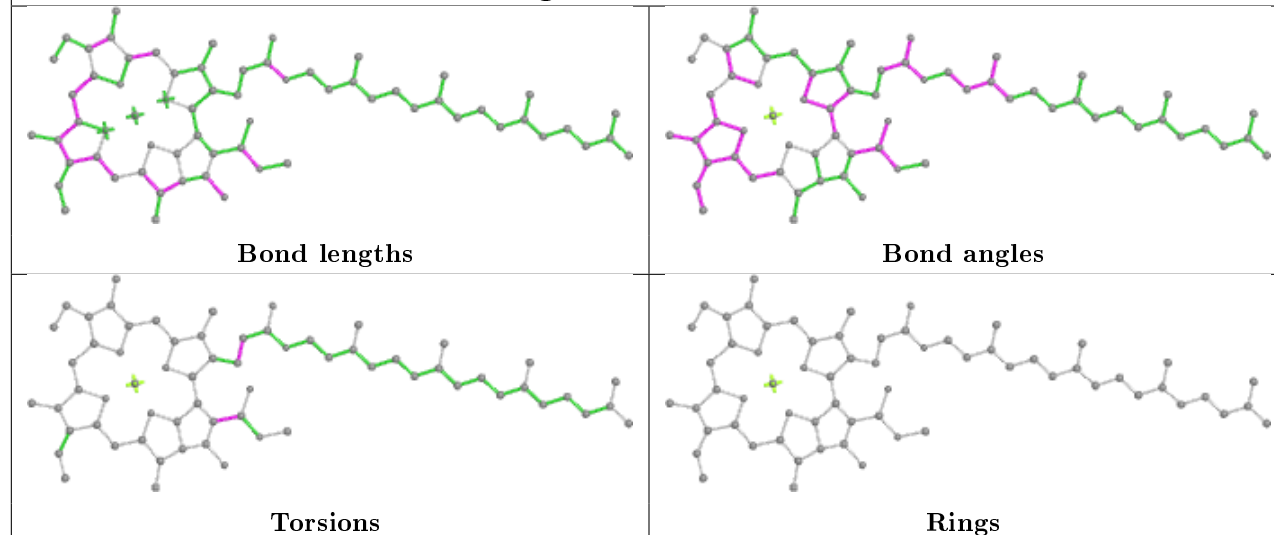
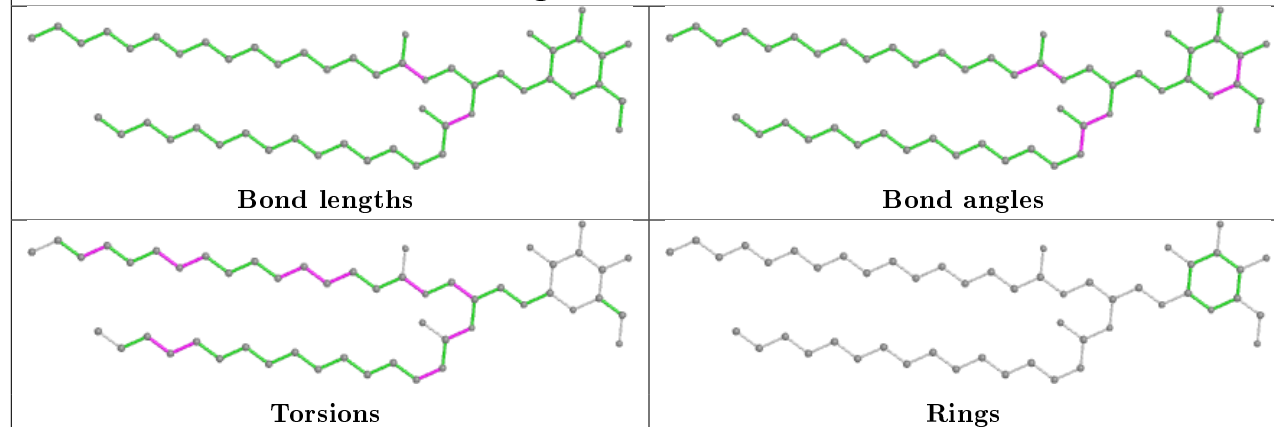


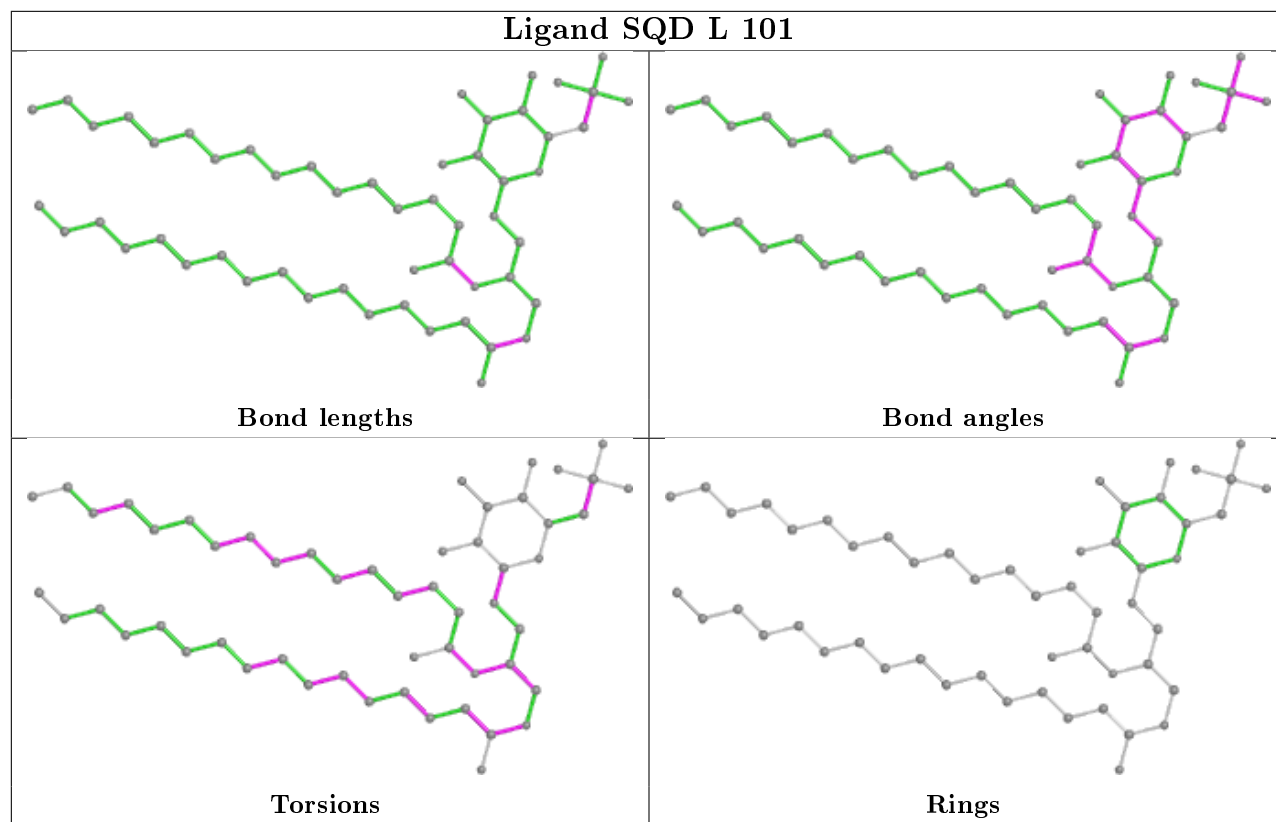
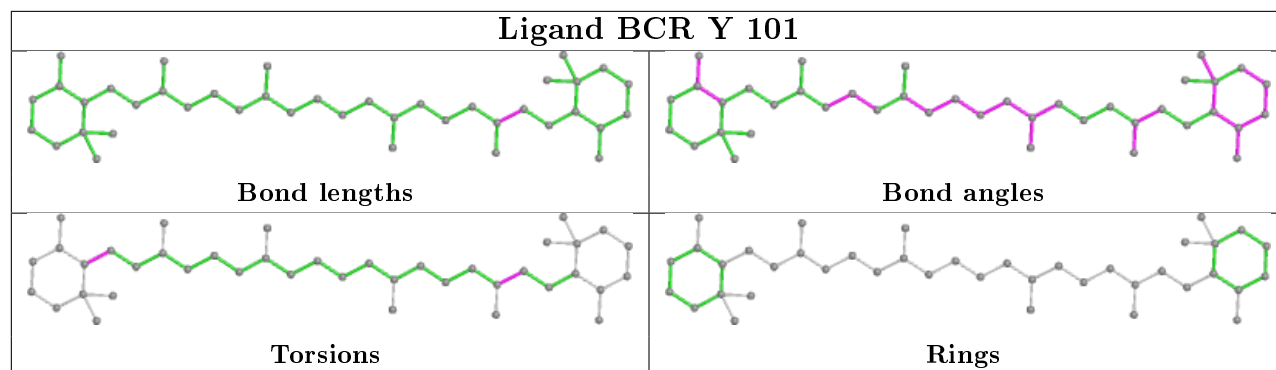
Ligand CLA C 509

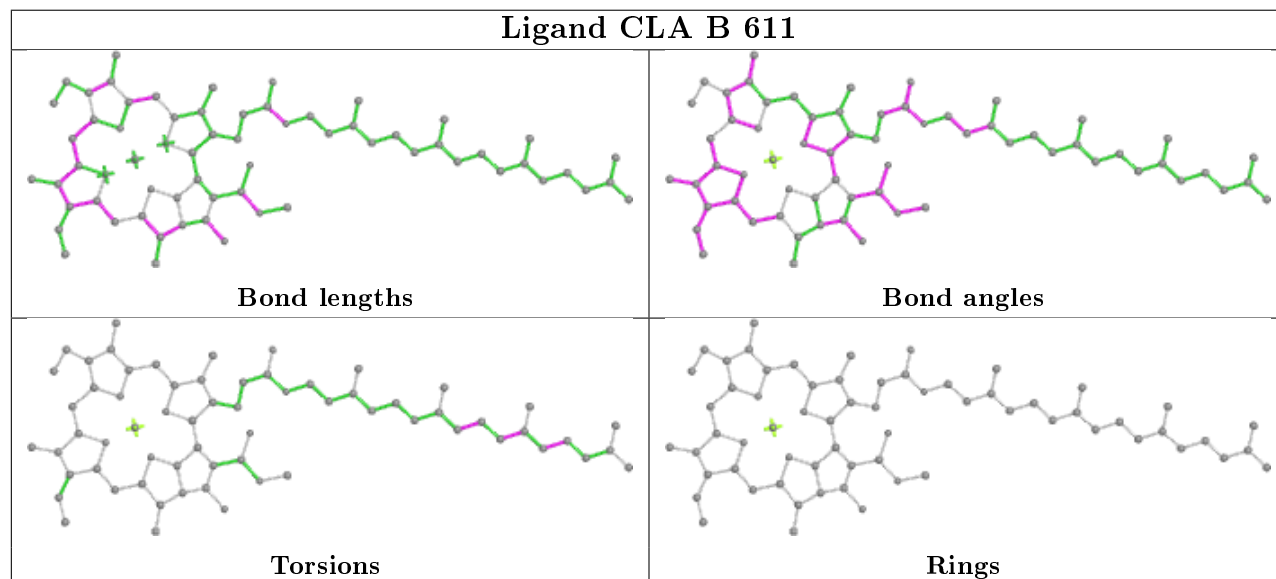
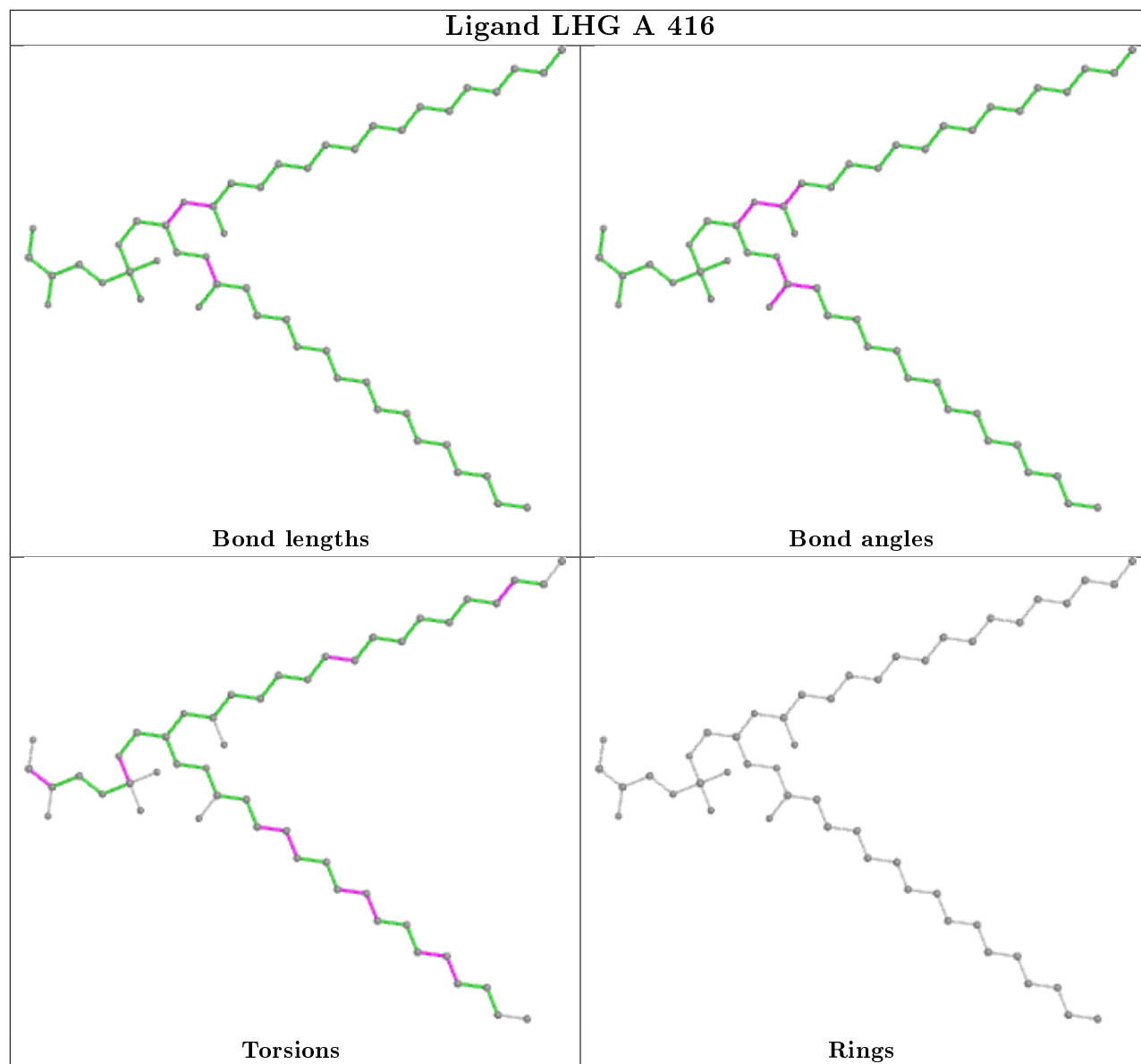


Ligand LMT b 627

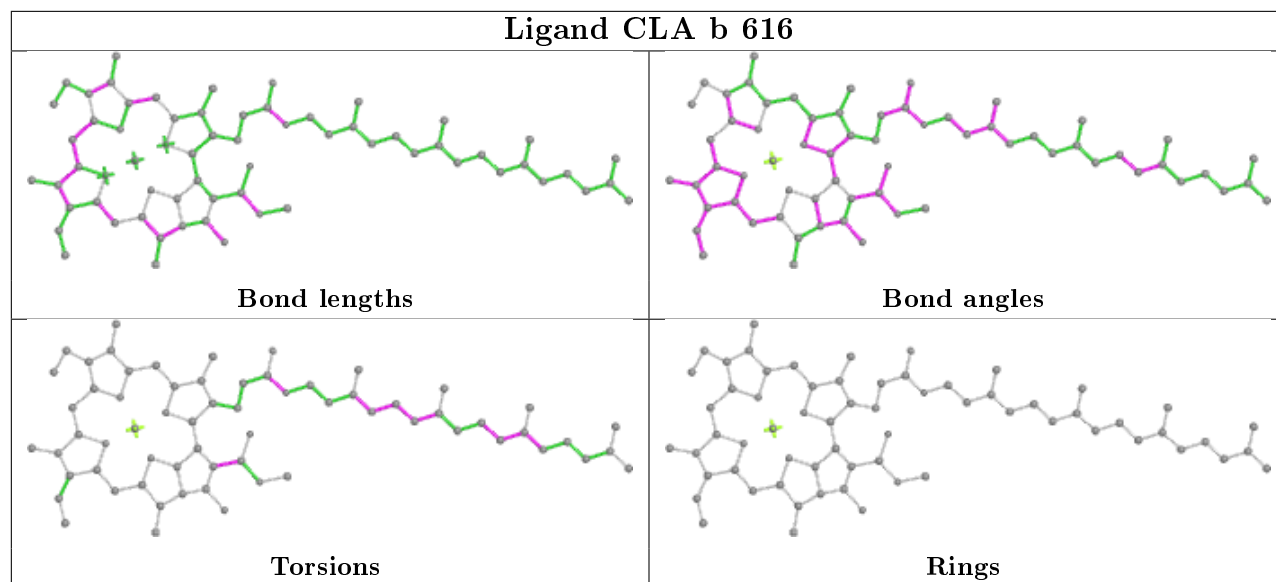


Ligand CLA C 513**Ligand CLA c 503****Ligand LMG a 416**

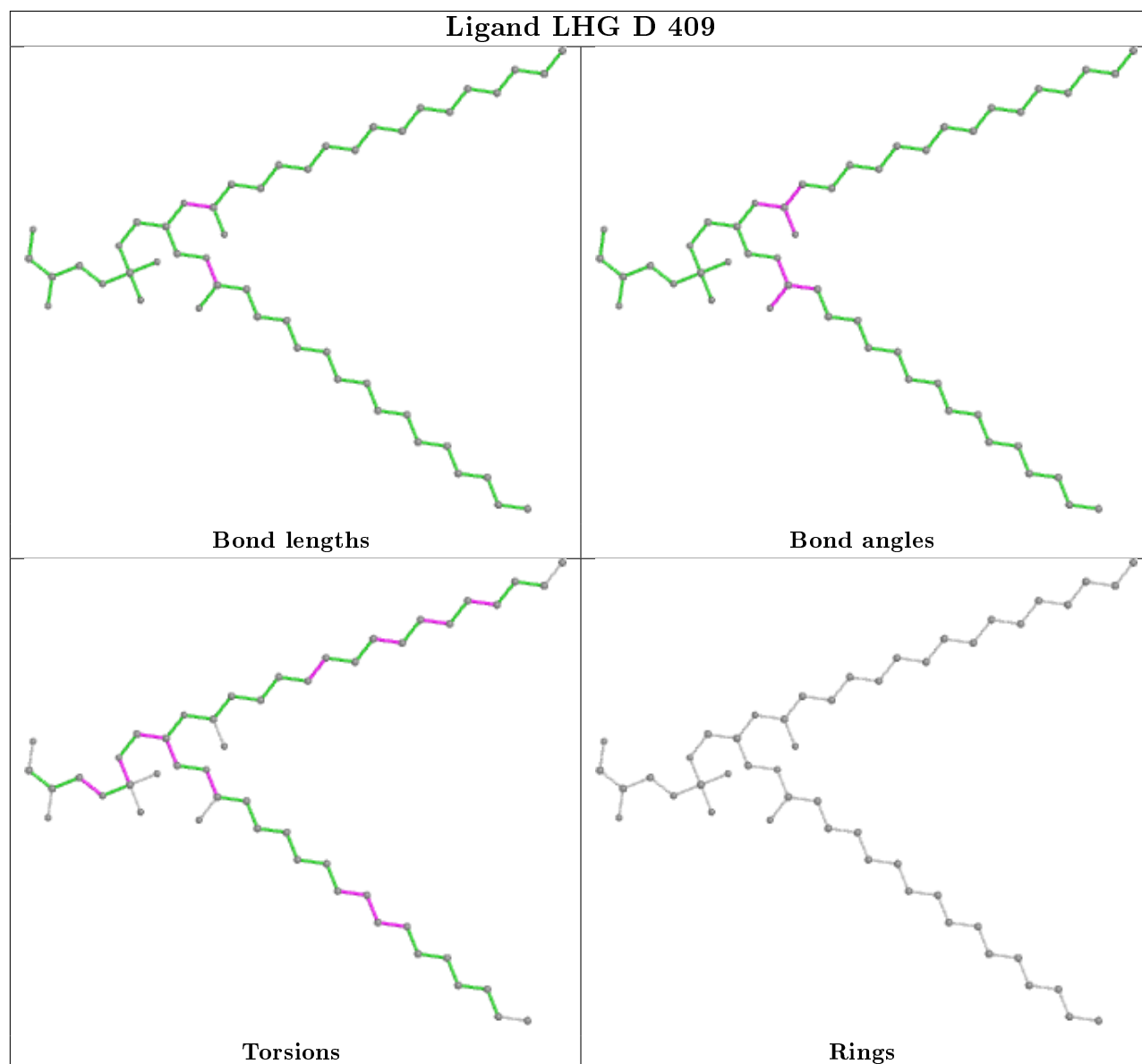


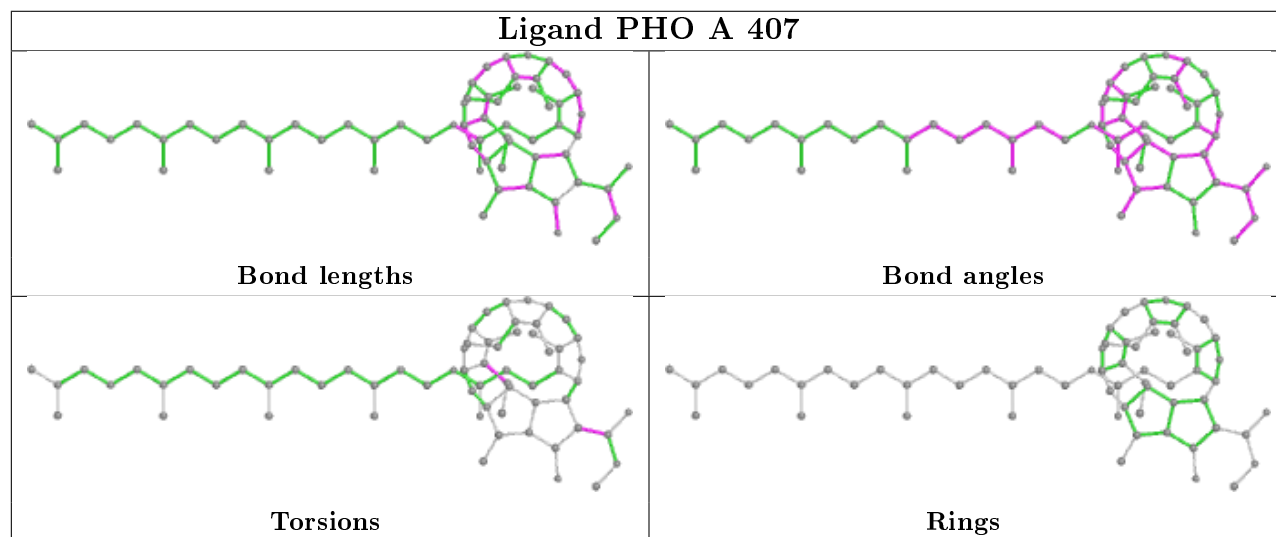
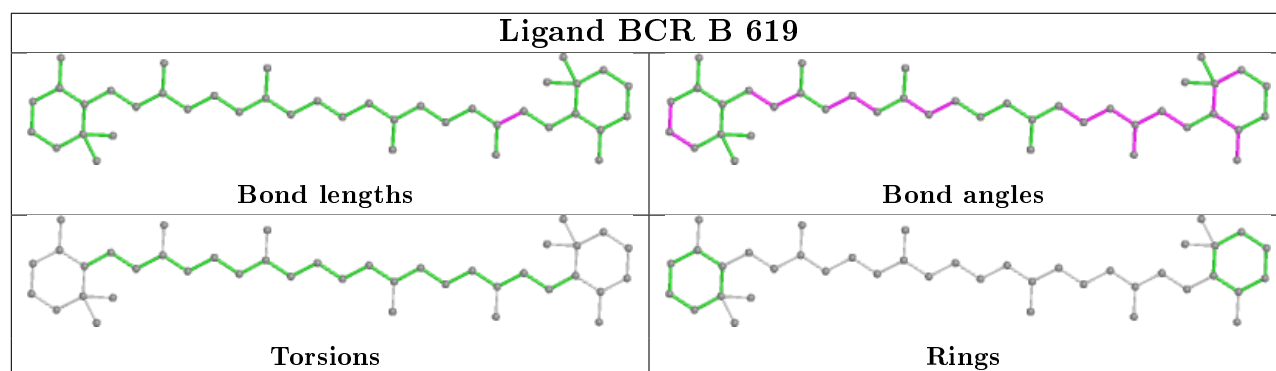
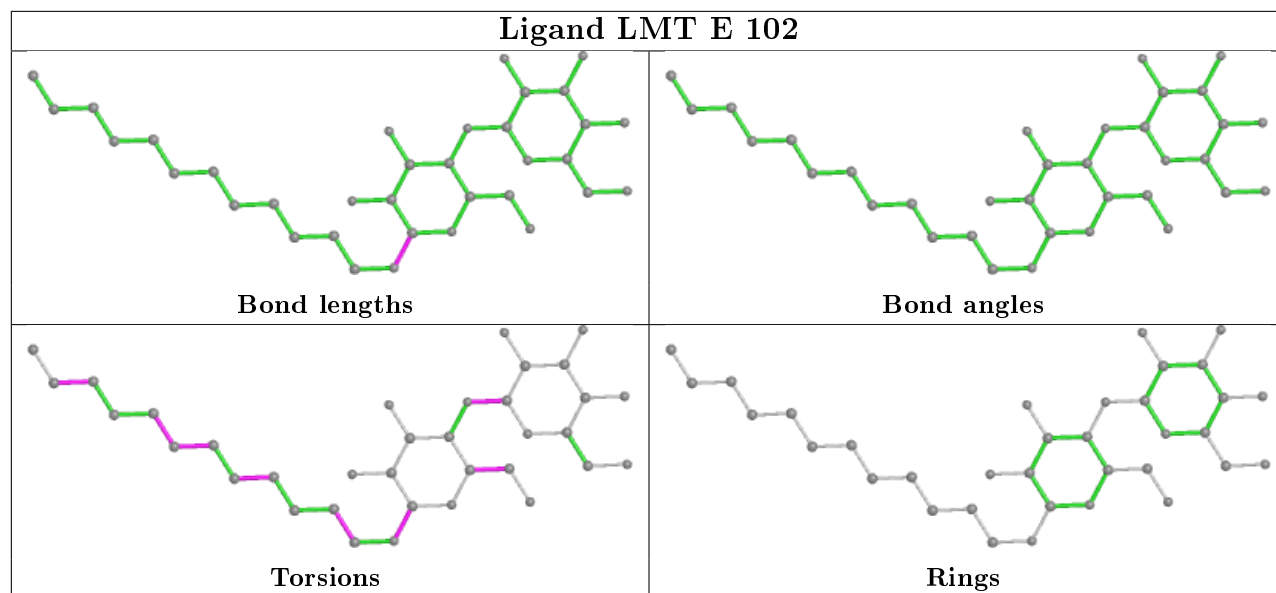


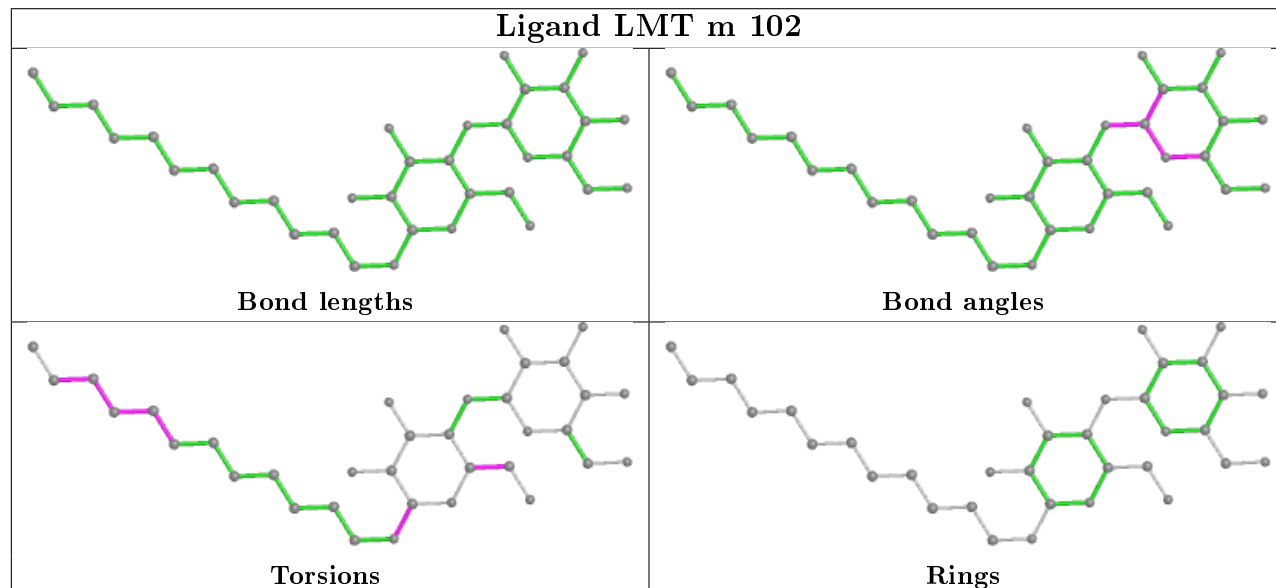
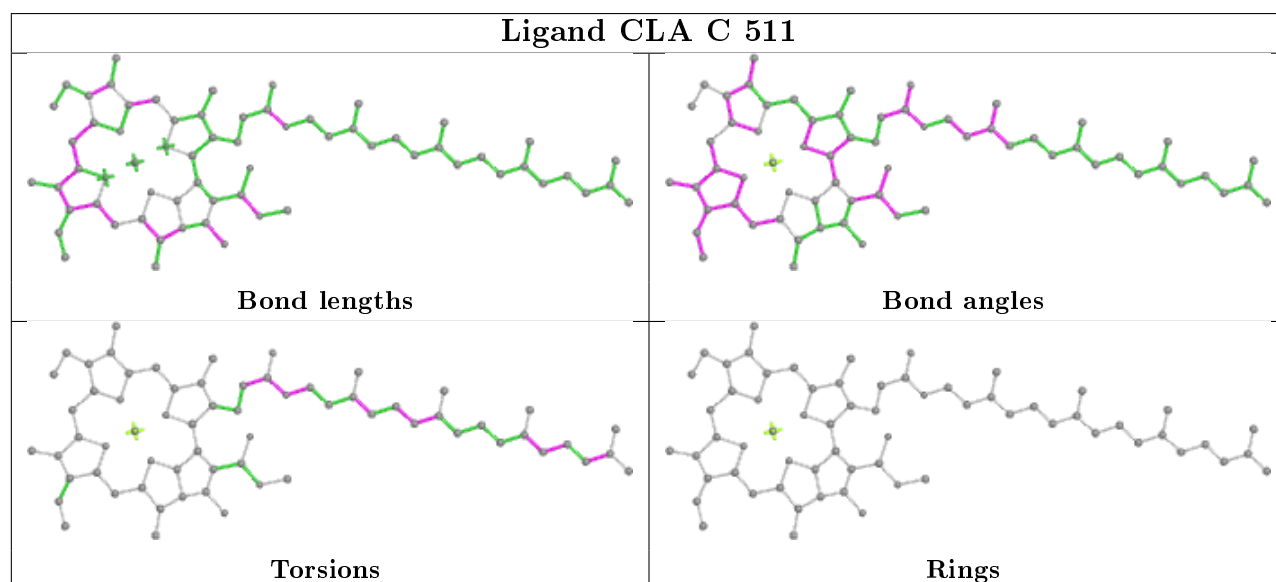
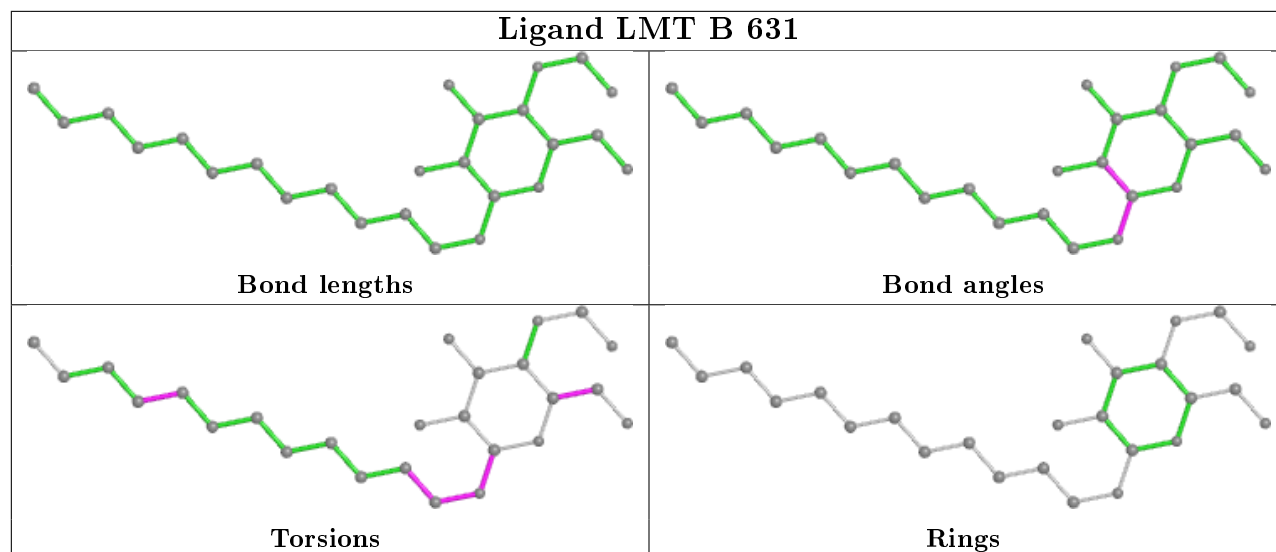
Ligand CLA b 616

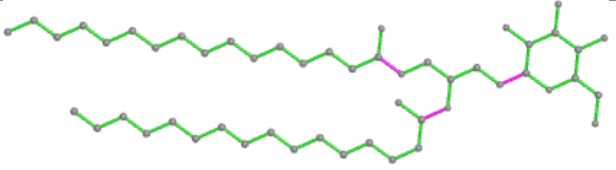
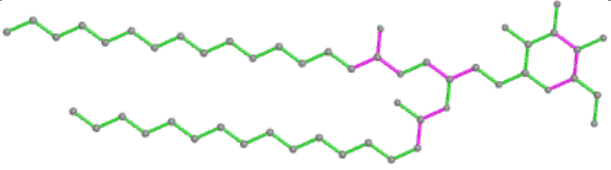
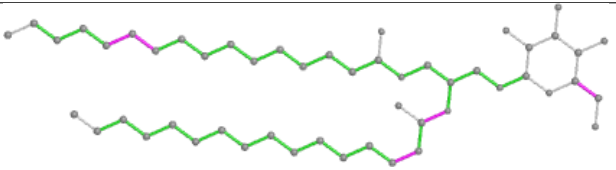
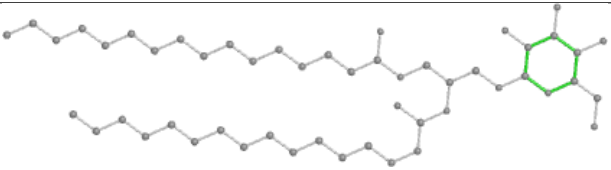
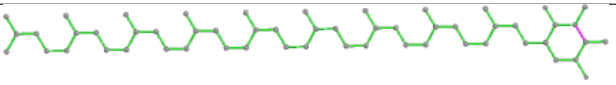
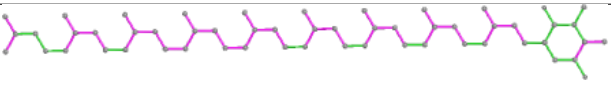
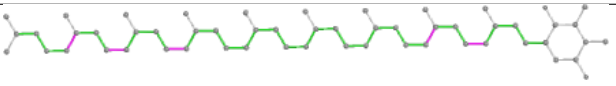
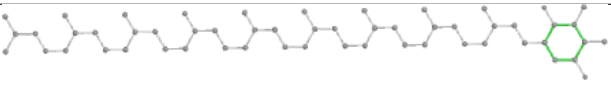
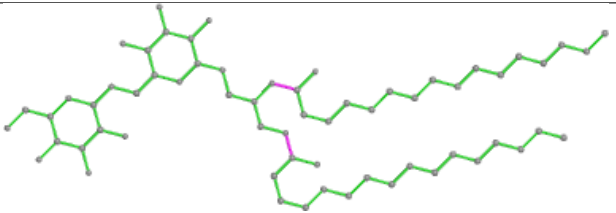
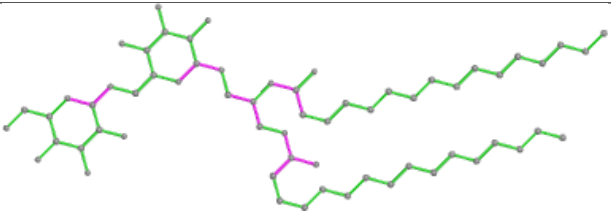
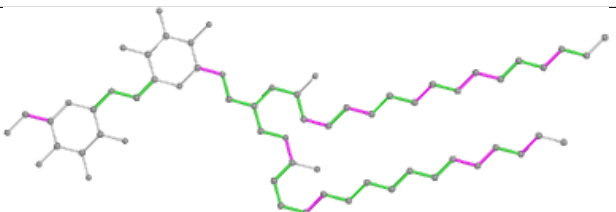
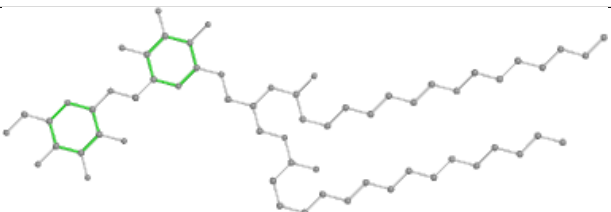


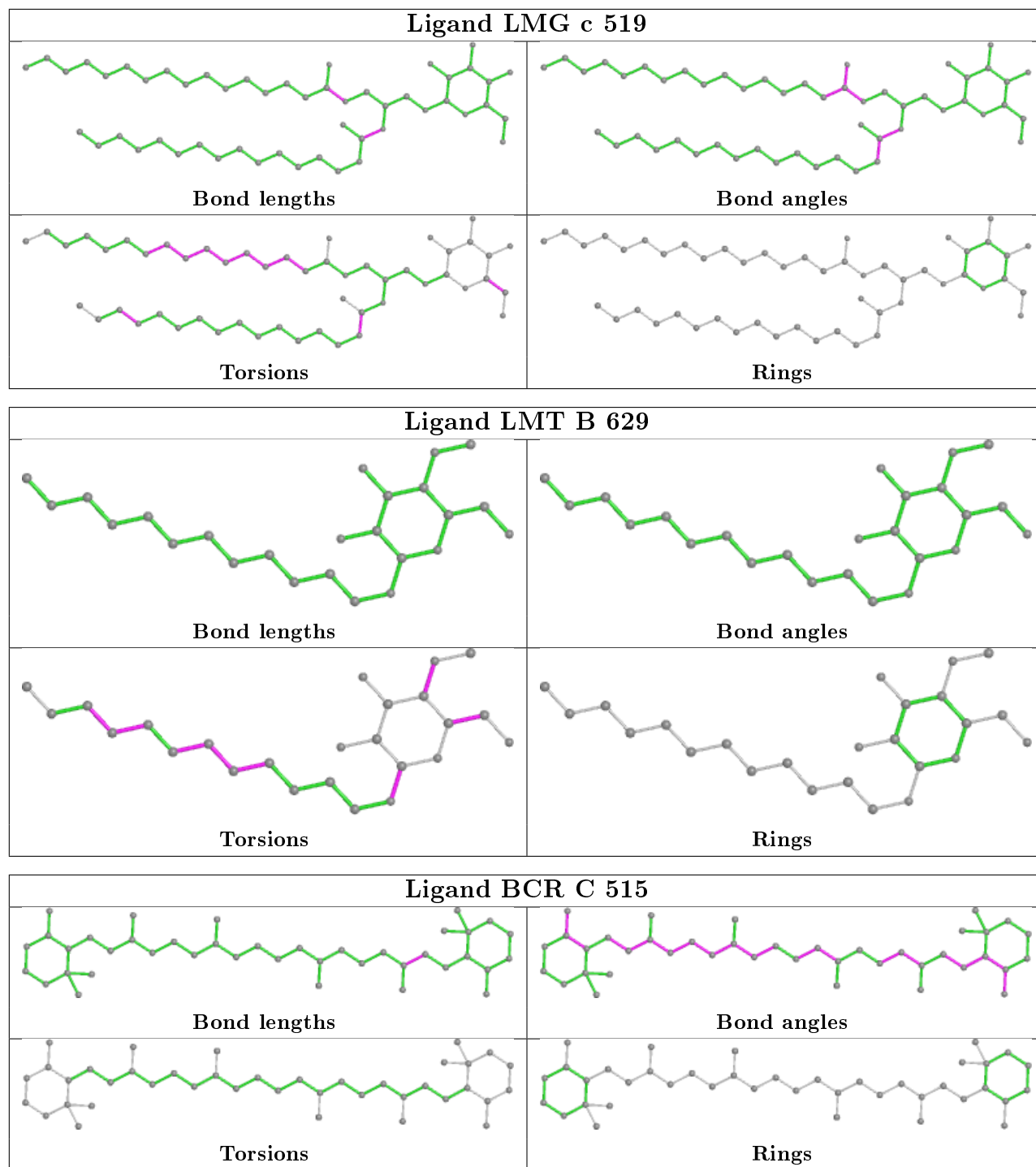
Ligand LHG D 409

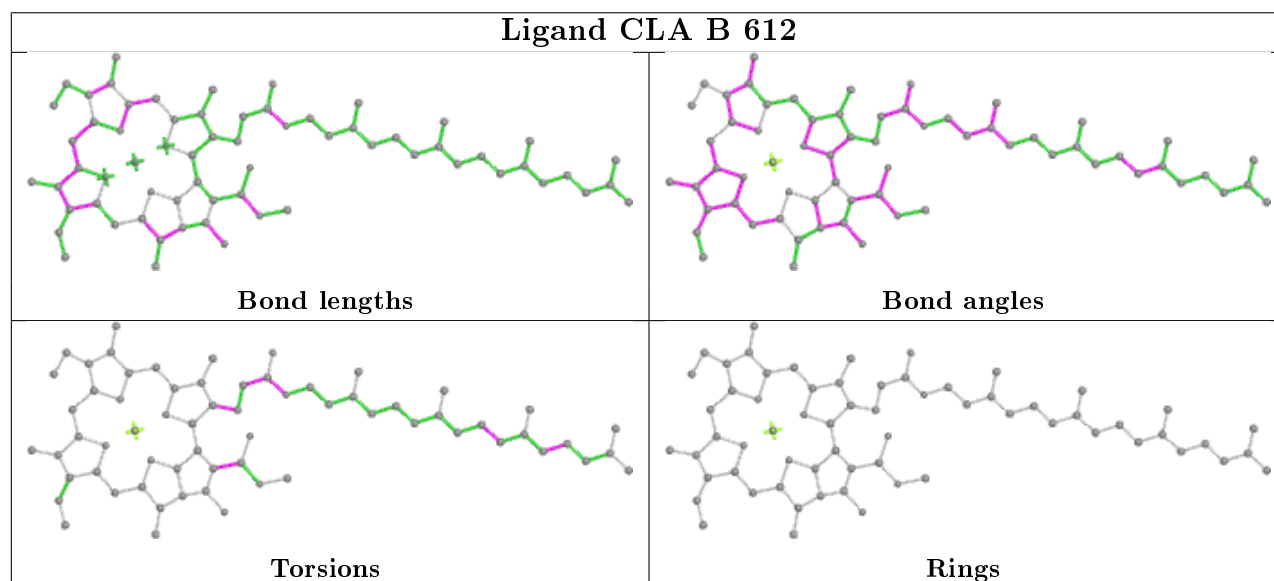
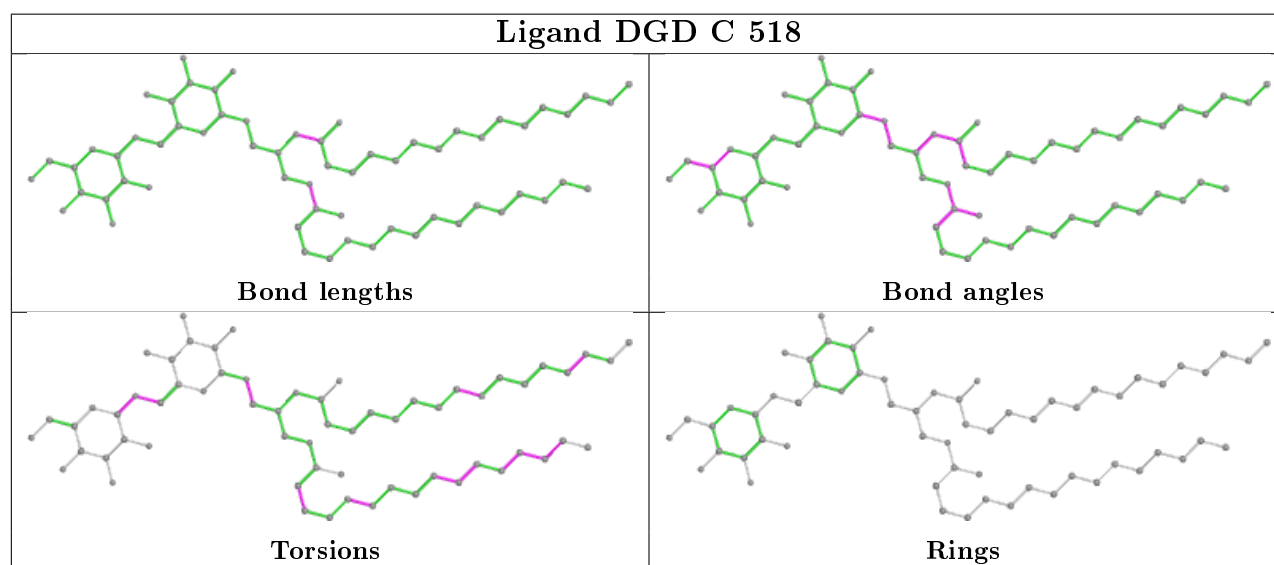
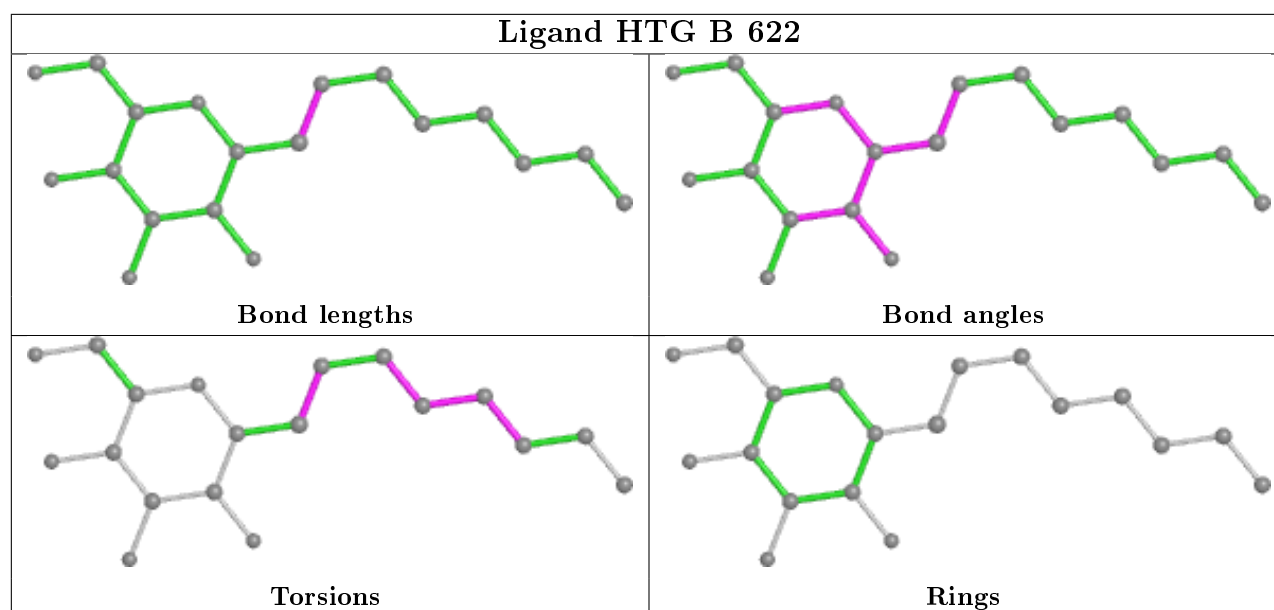


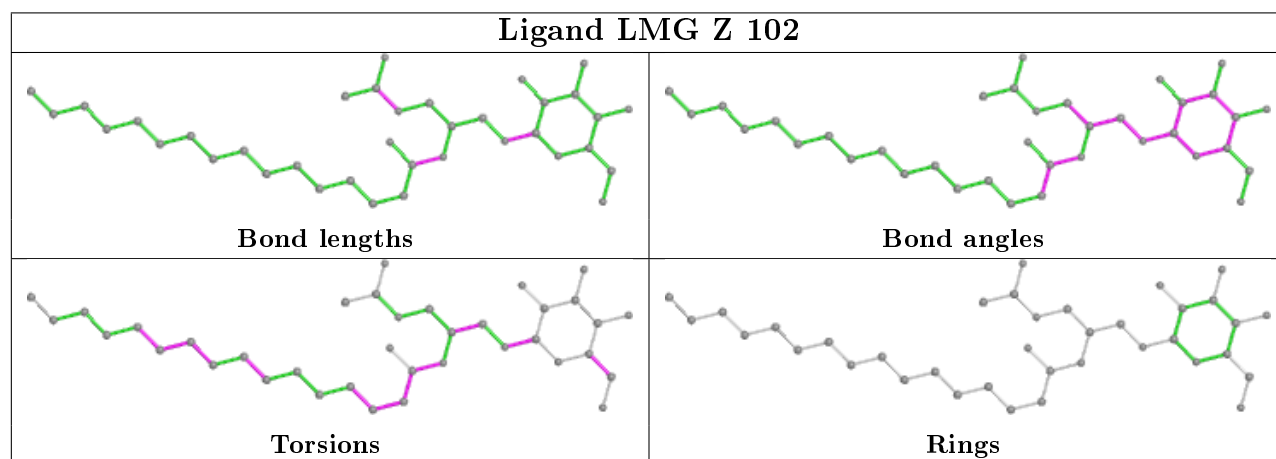
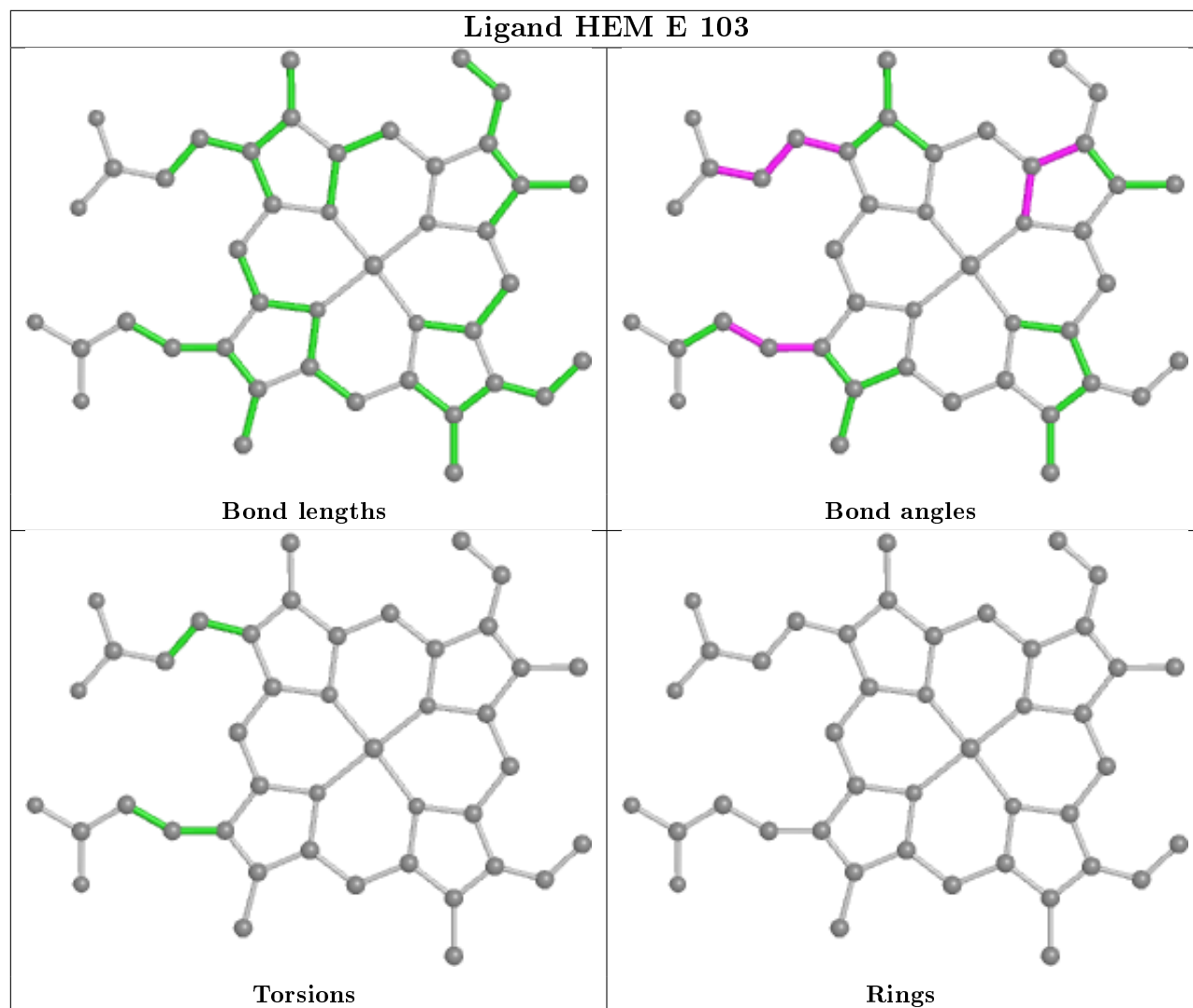


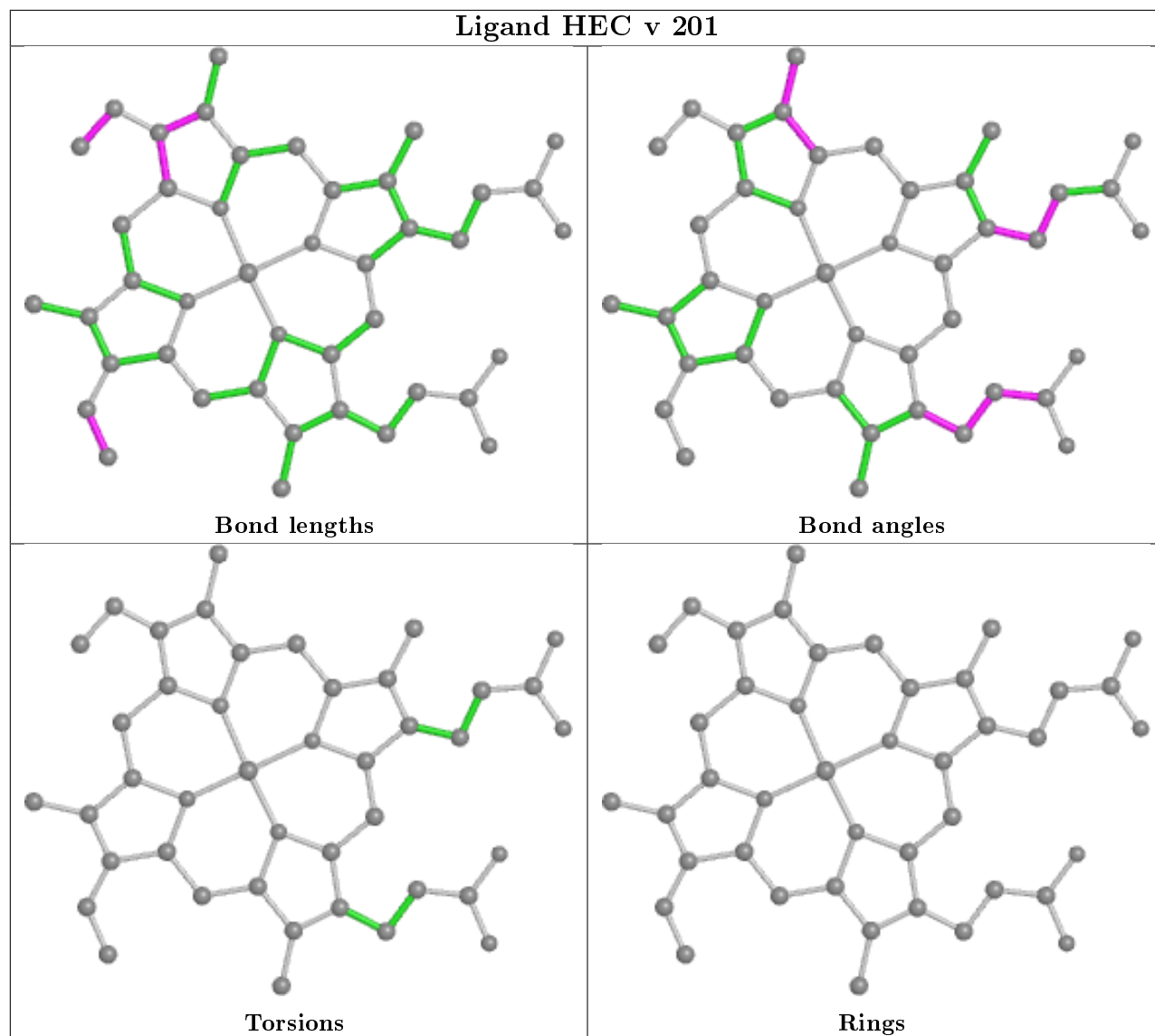
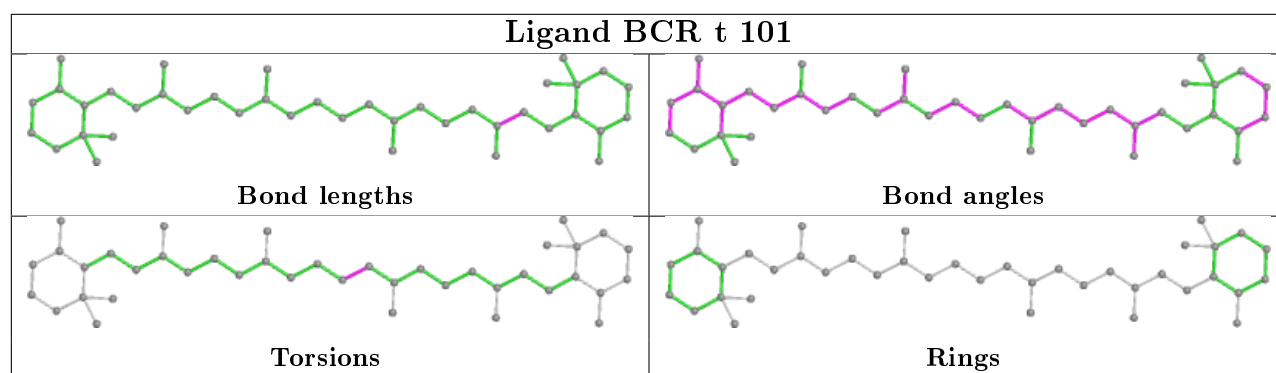


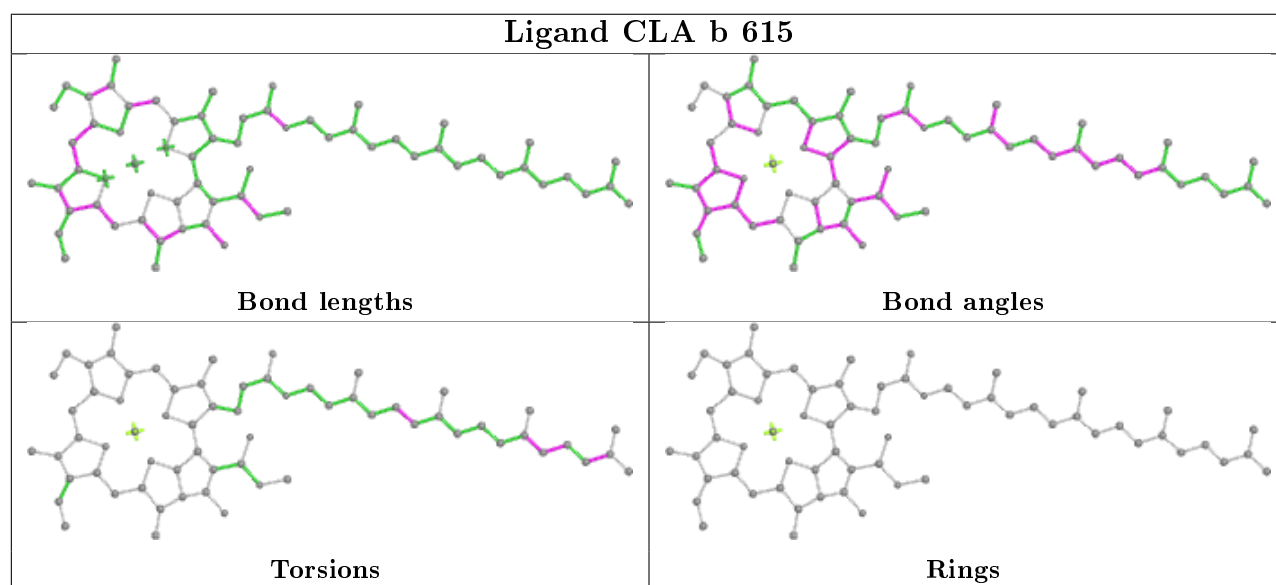
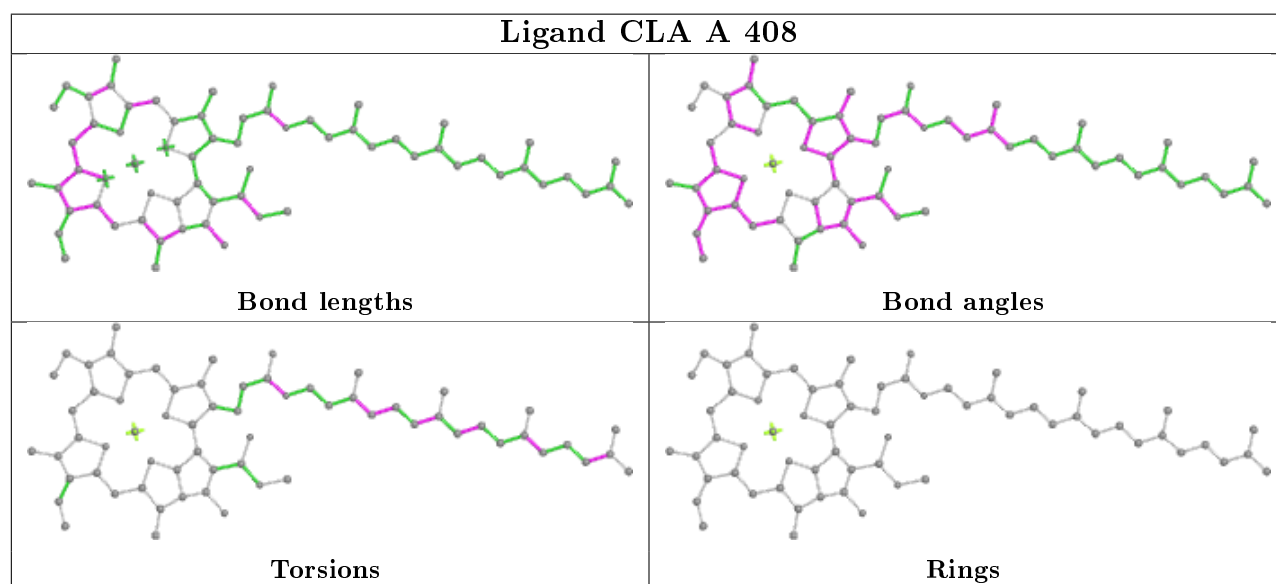
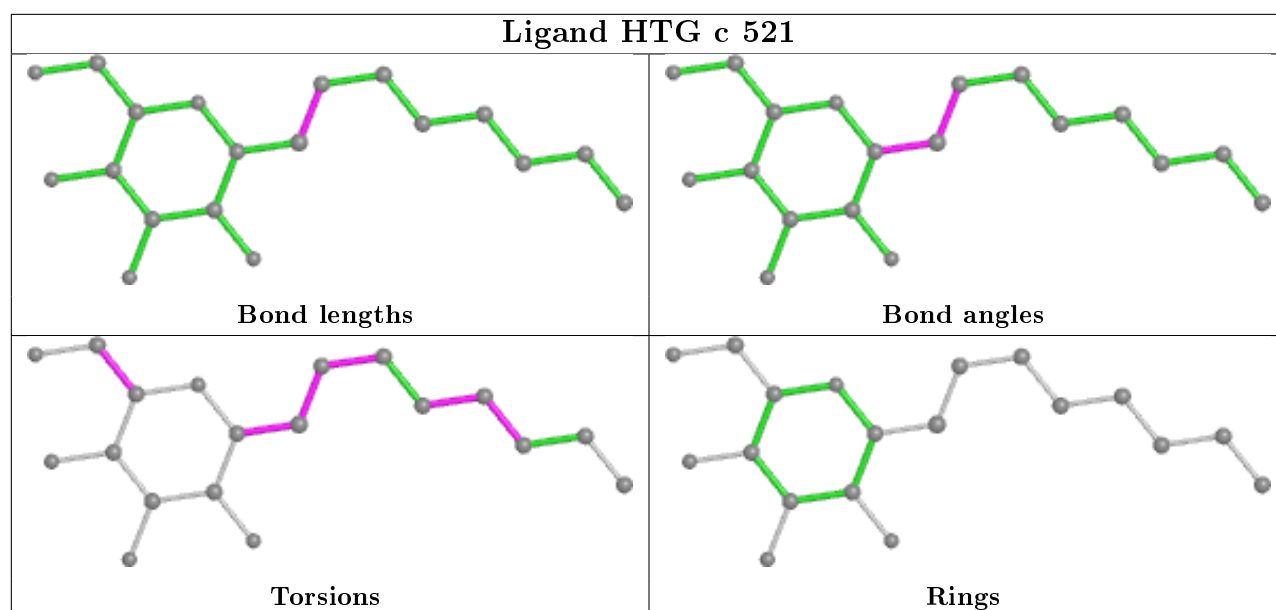
Ligand LMG c 520	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 d 406	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGD C 519	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



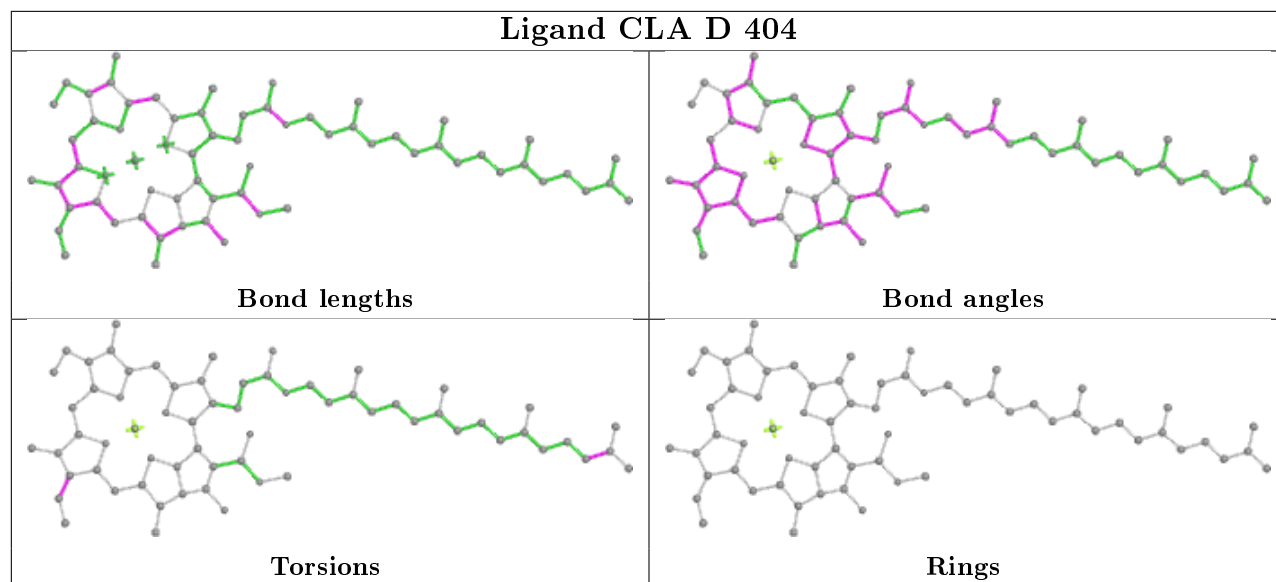




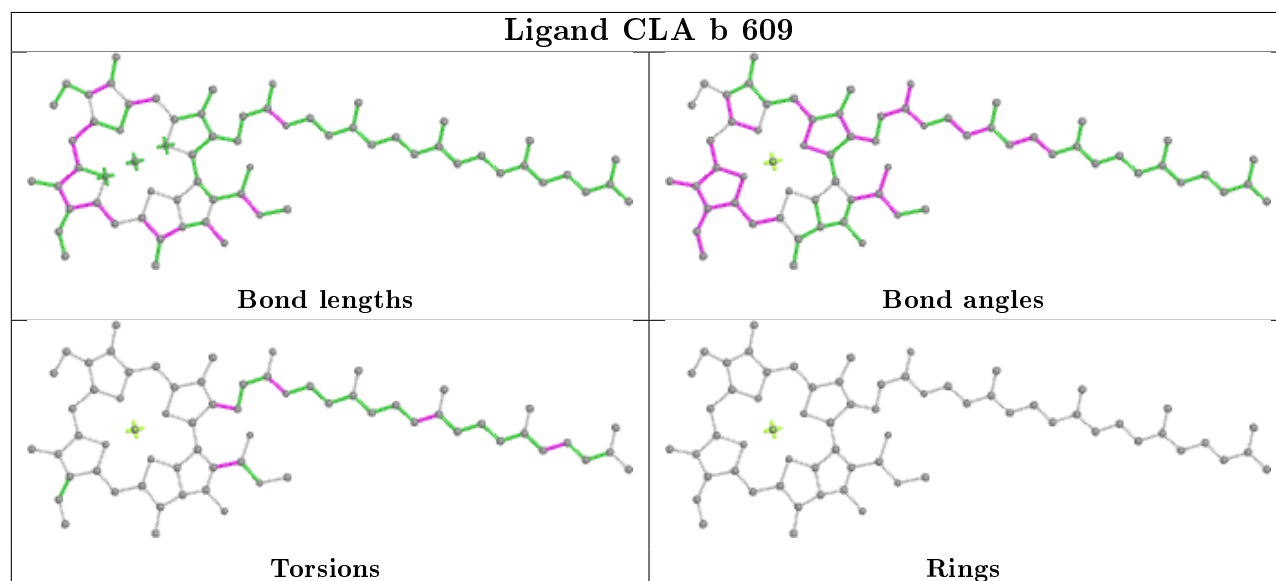




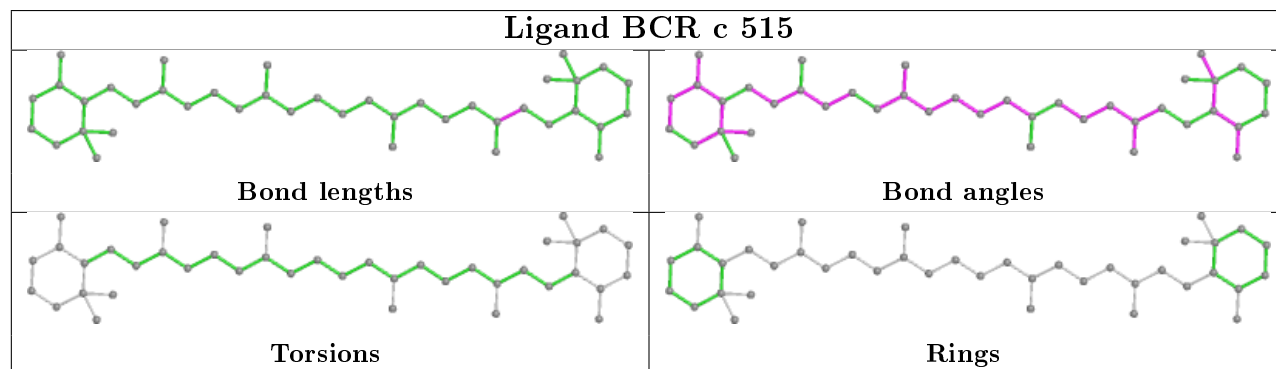
Ligand CLA D 404

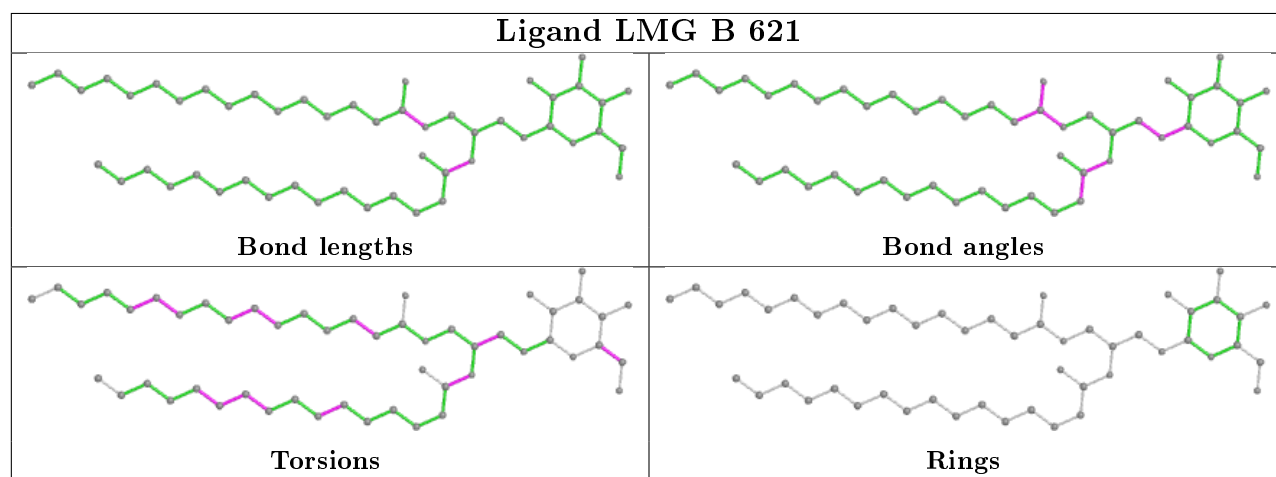
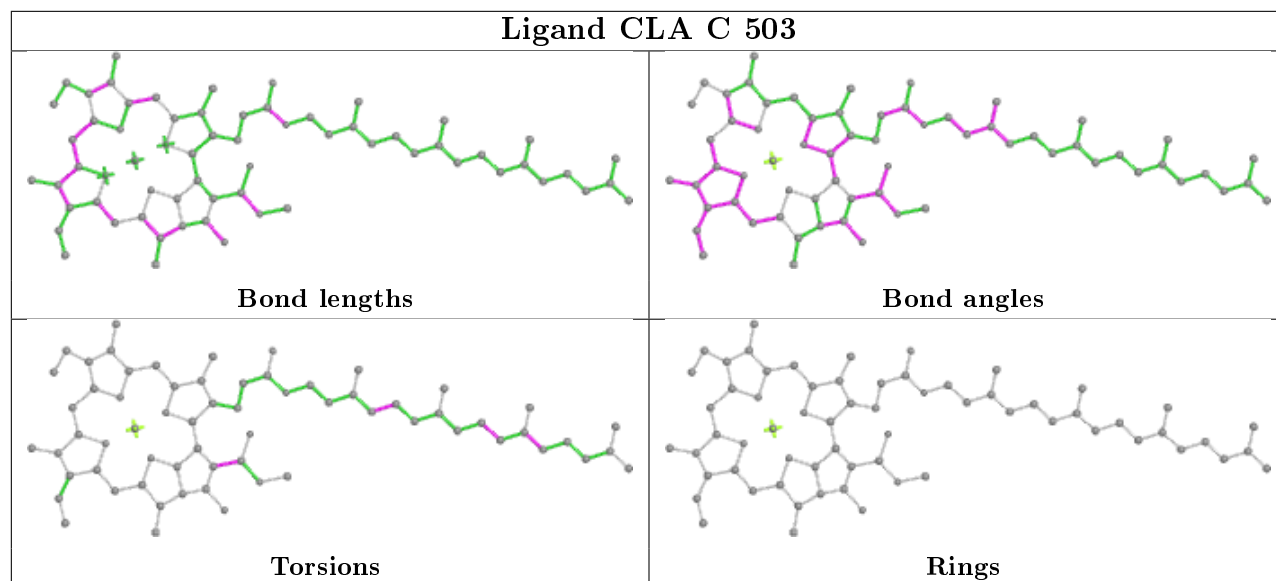
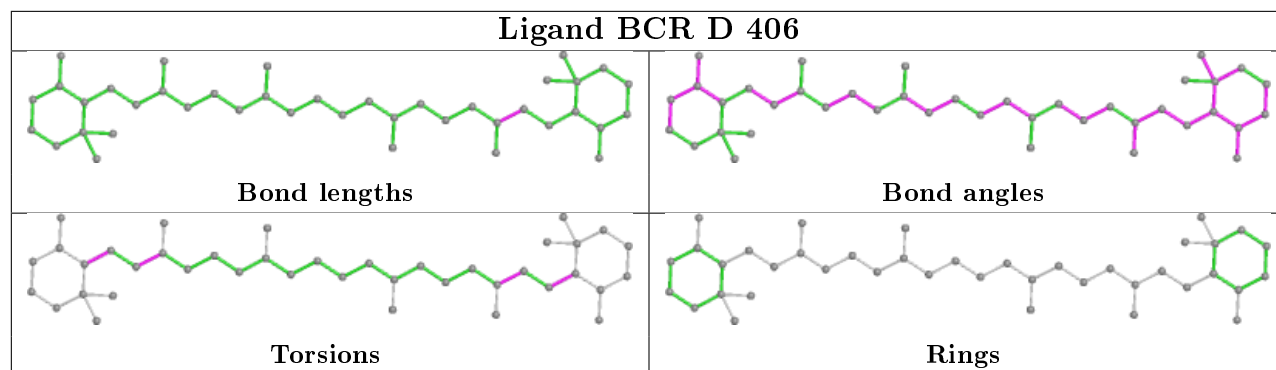


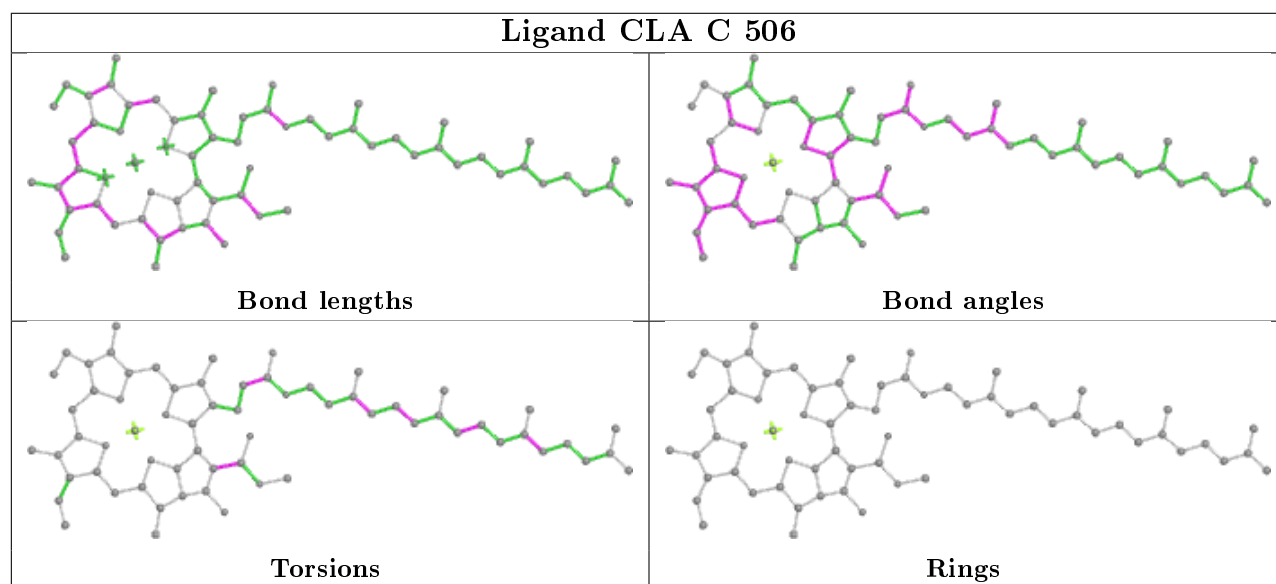
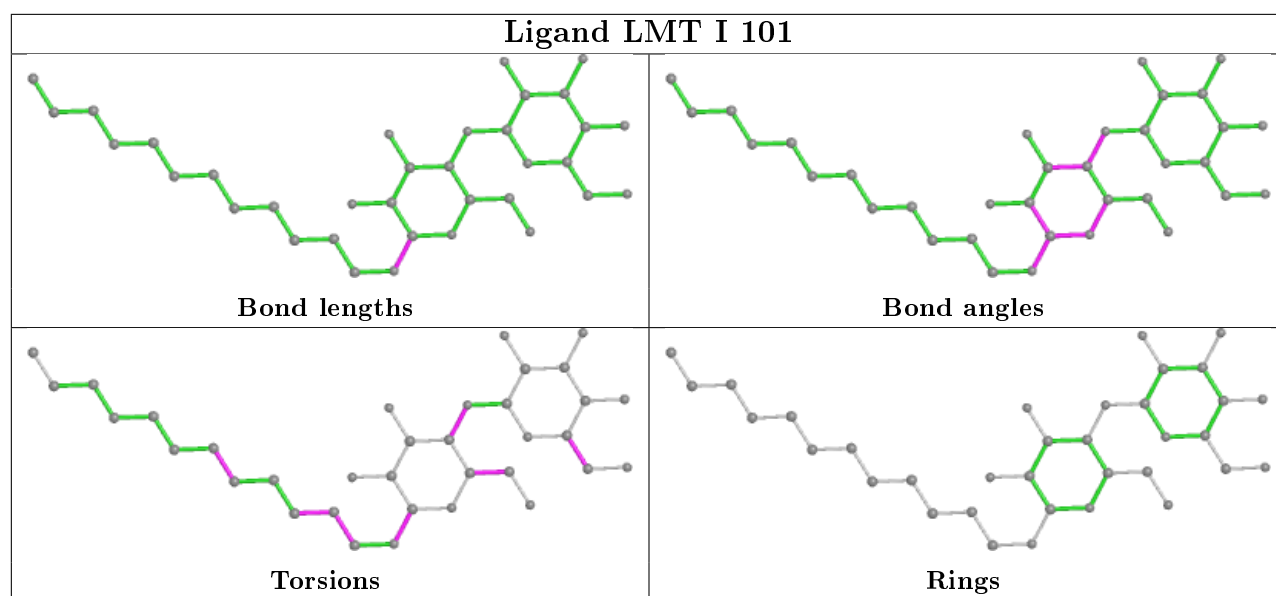
Ligand CLA b 609

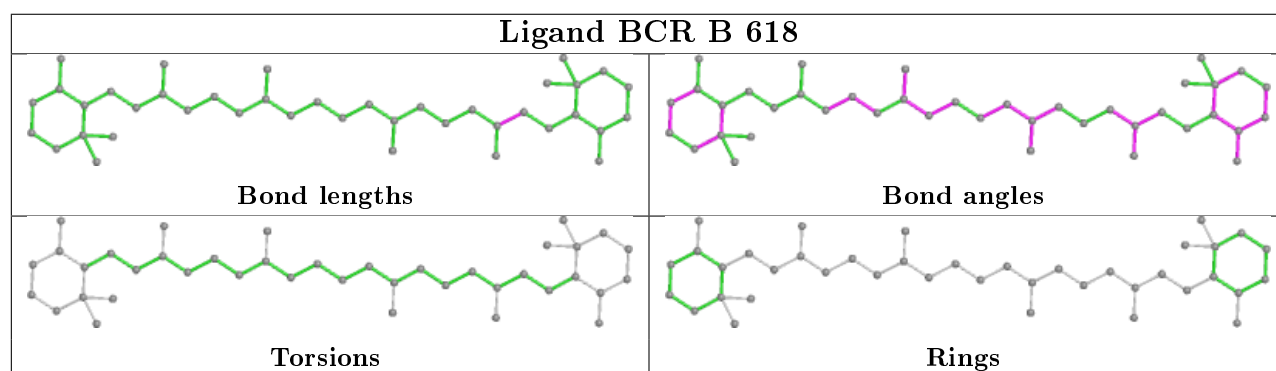
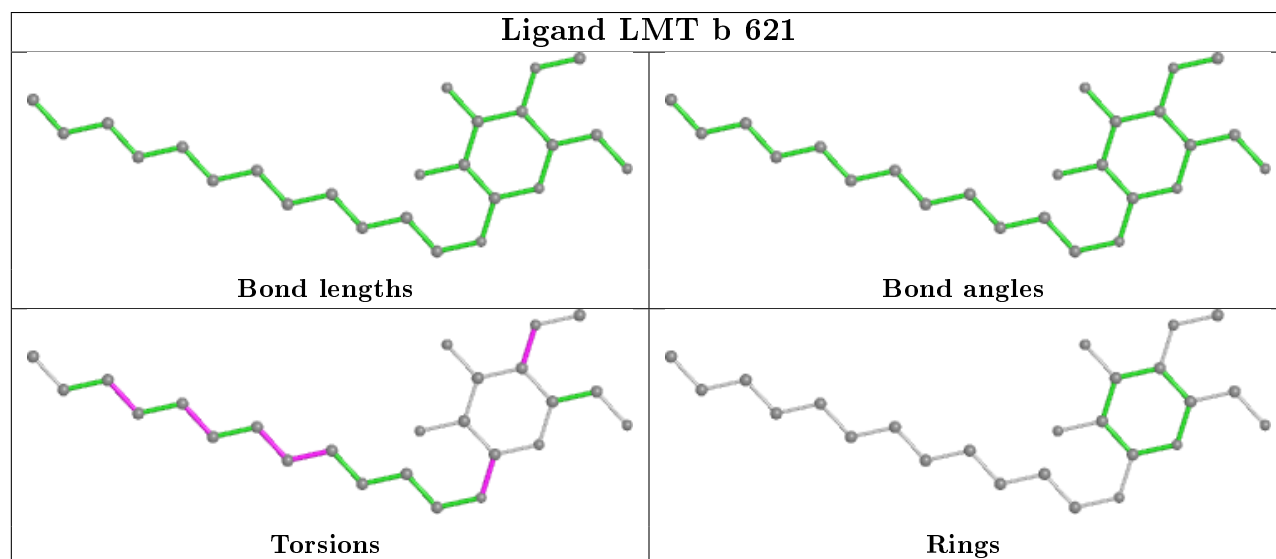
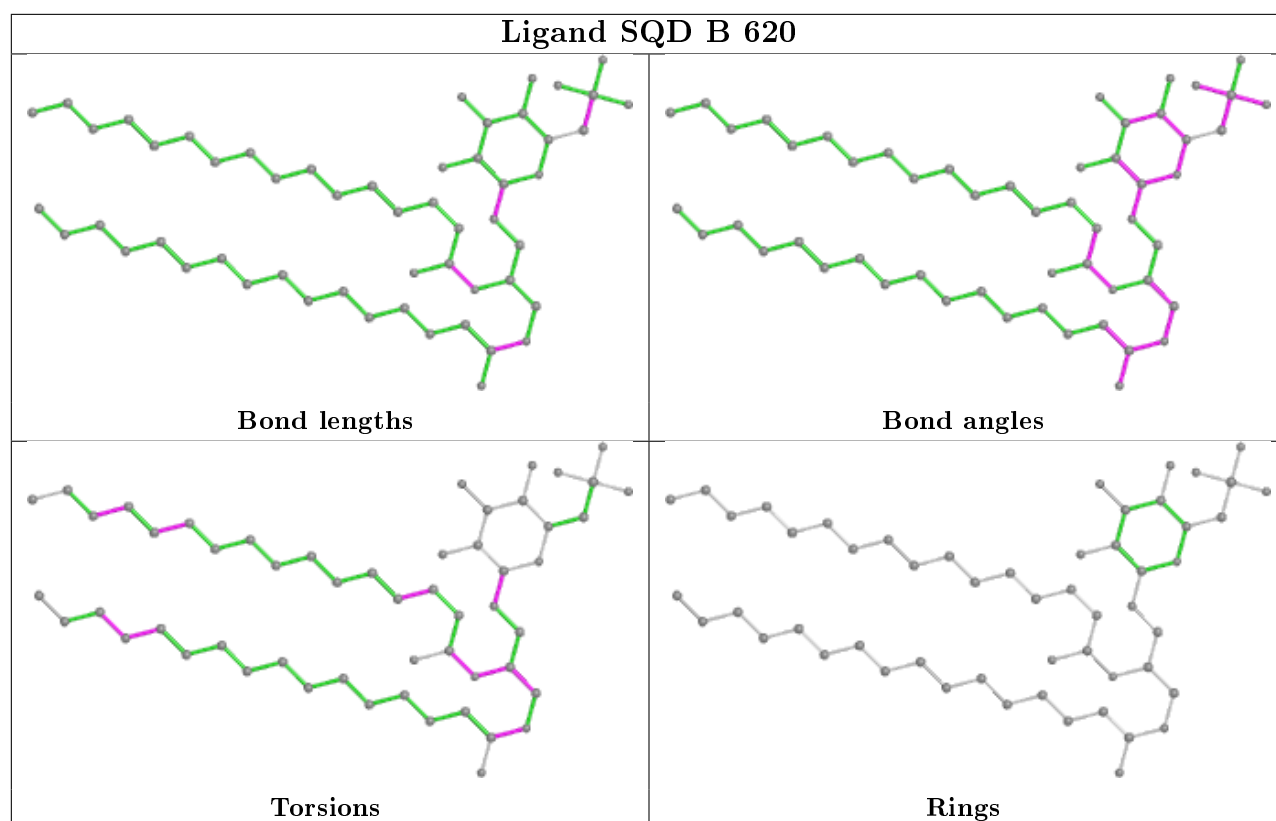


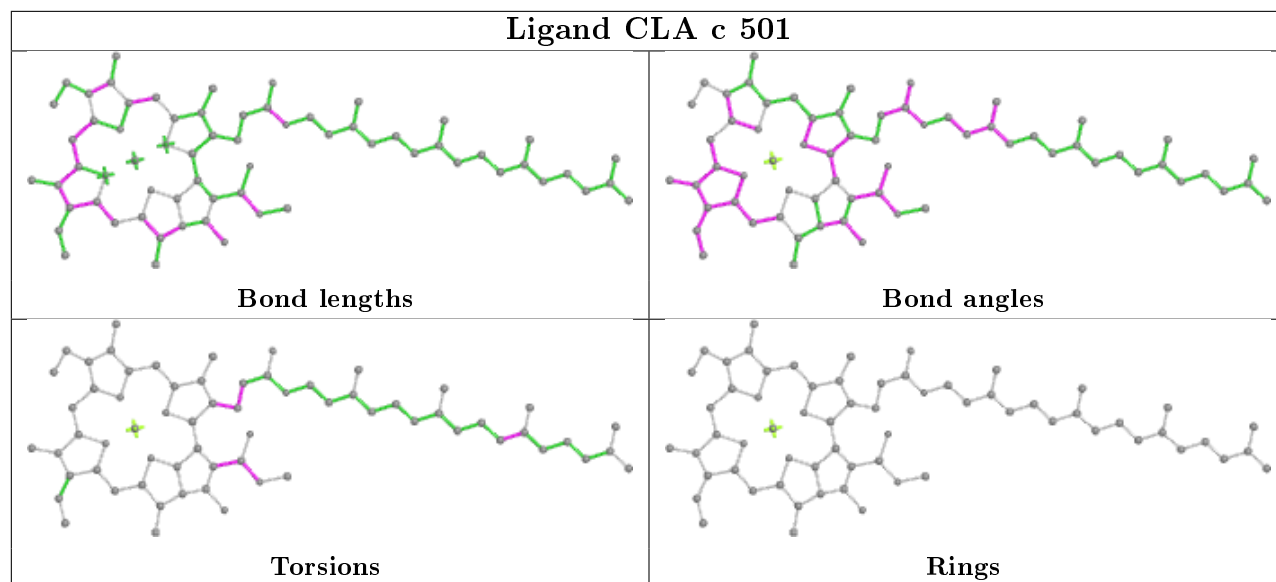
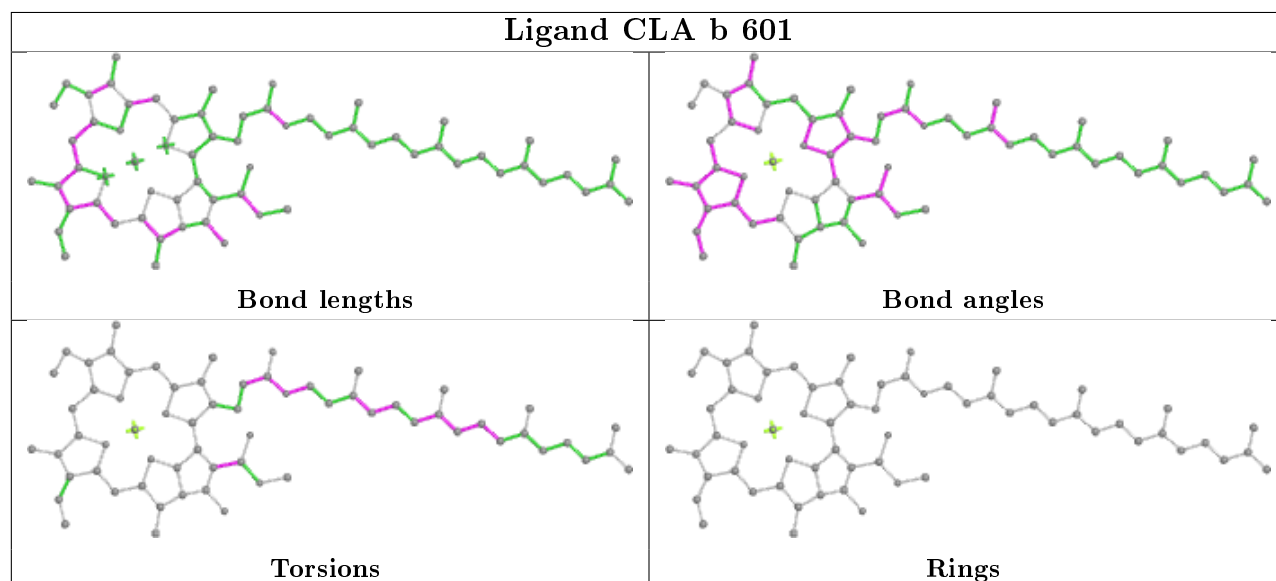
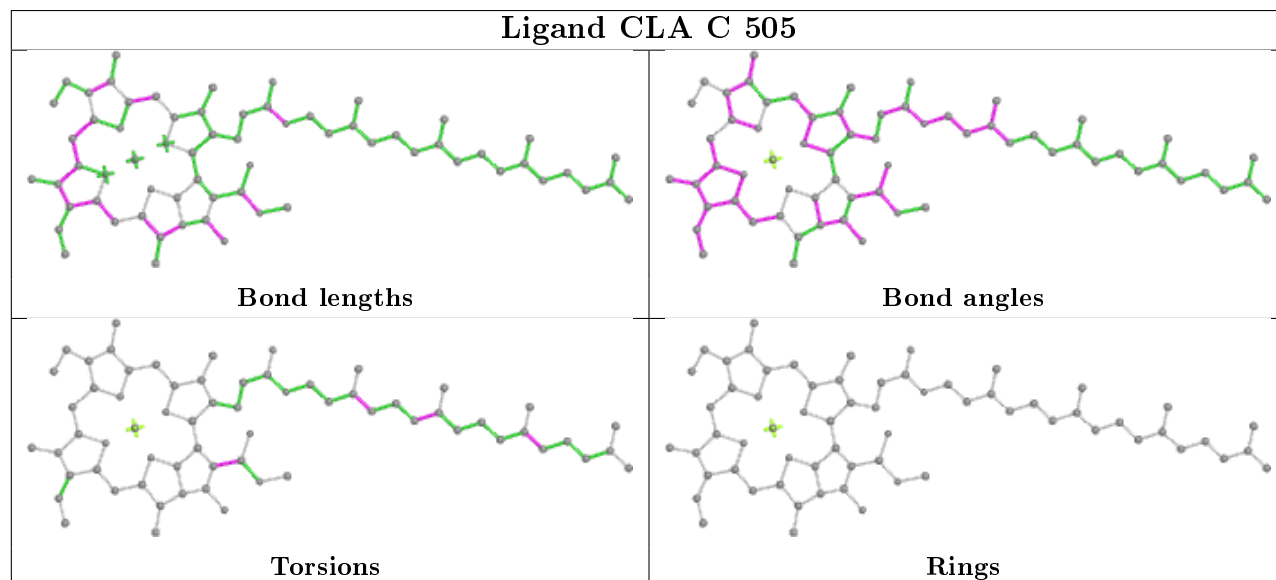
Ligand BCR c 515

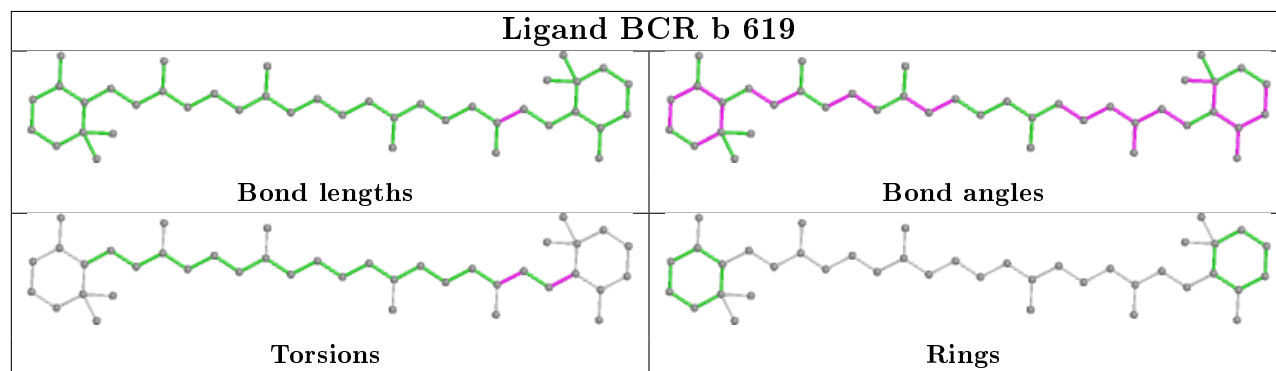
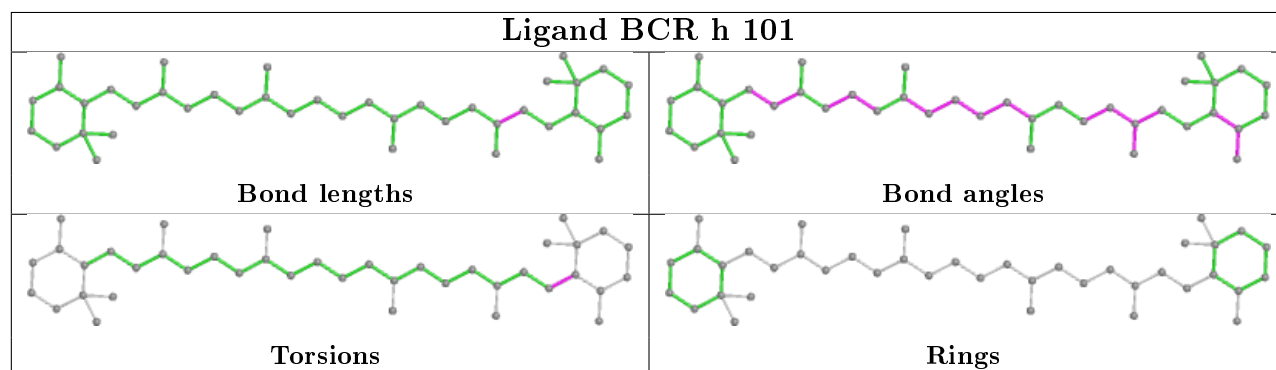
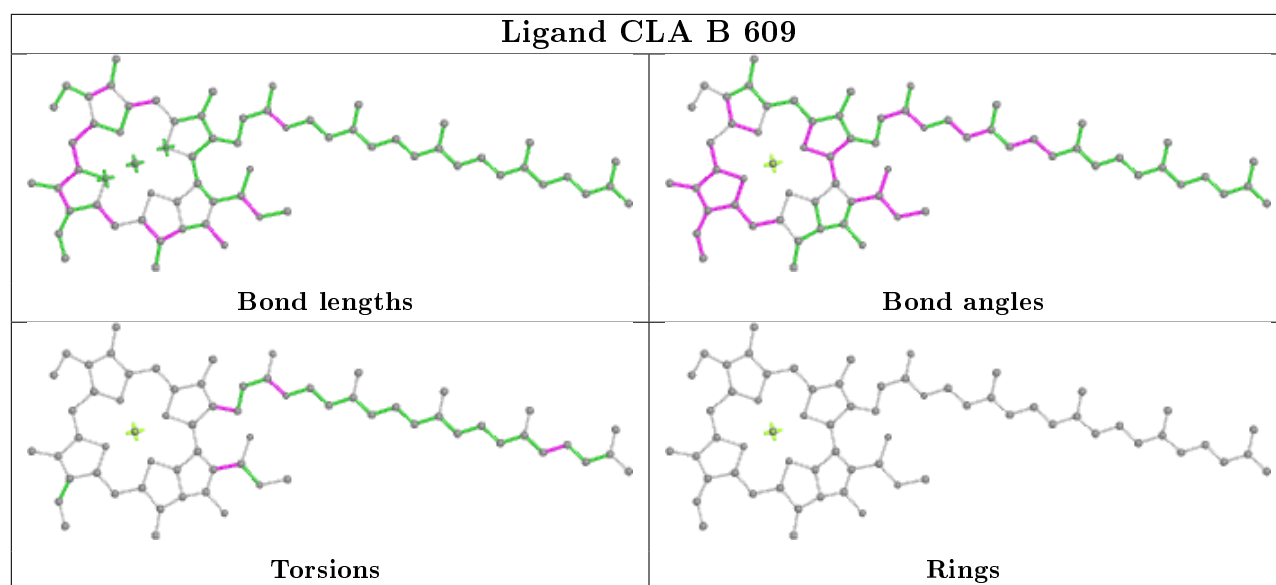


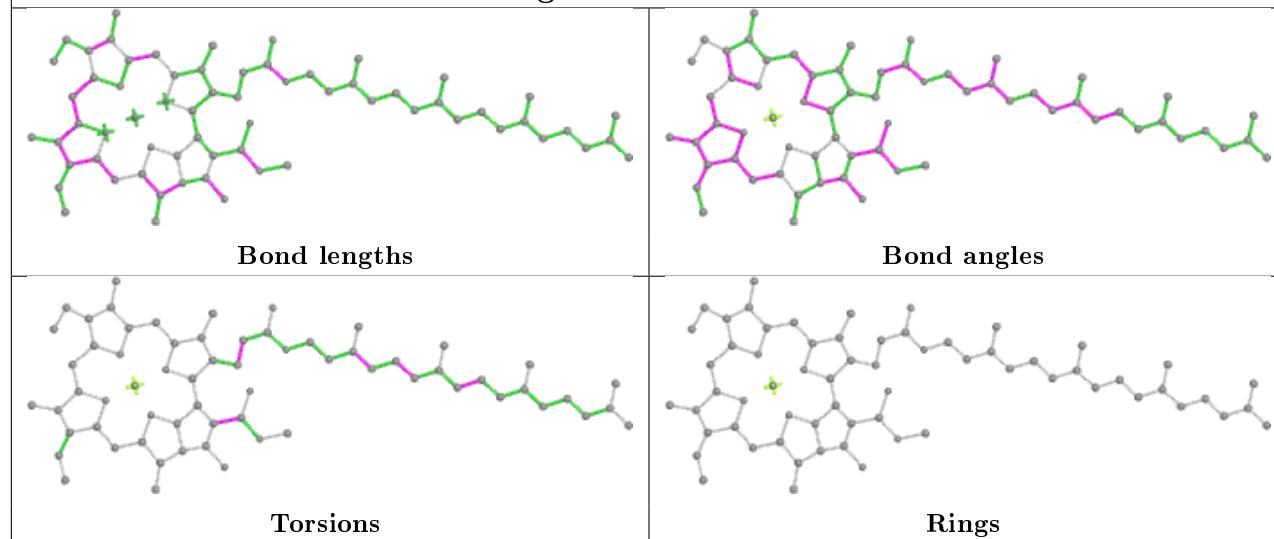
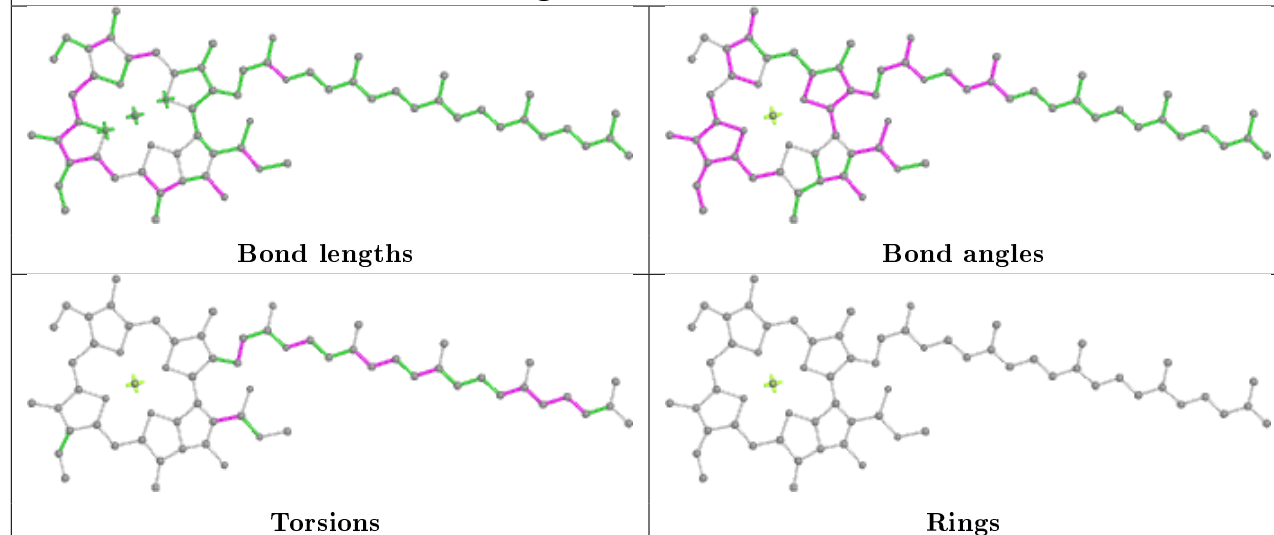
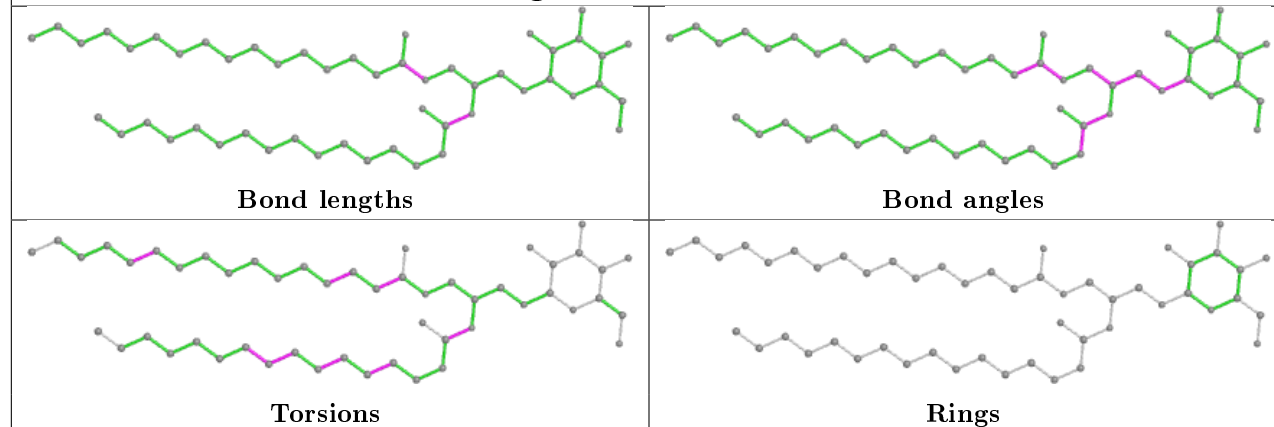




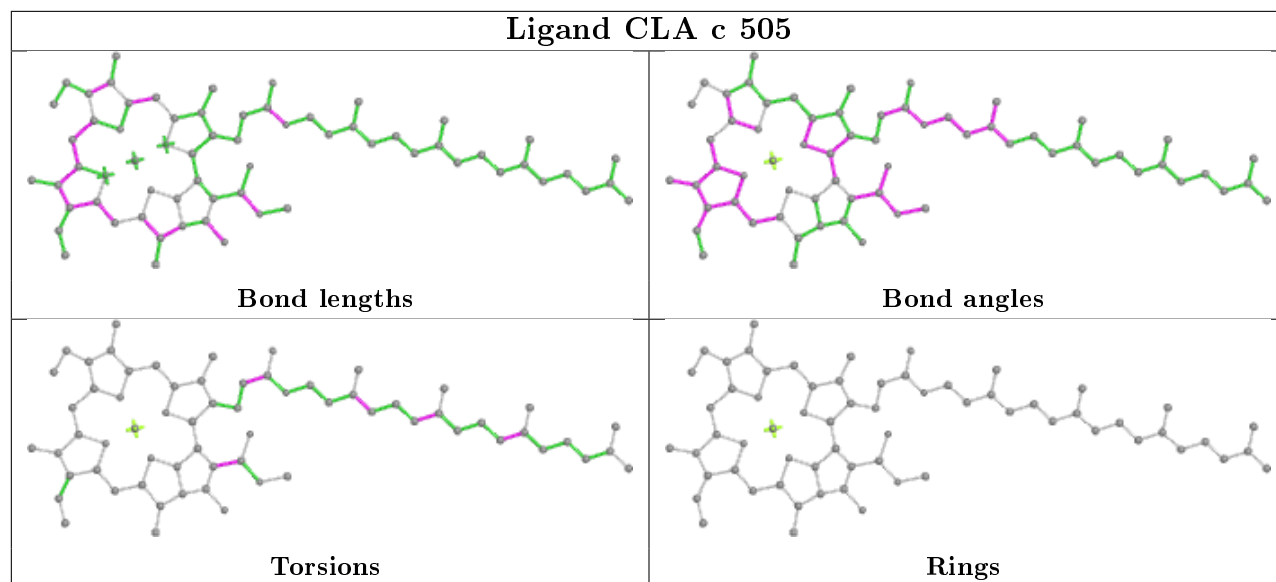


Ligand CLA c 501**Ligand CLA b 601****Ligand CLA C 505**

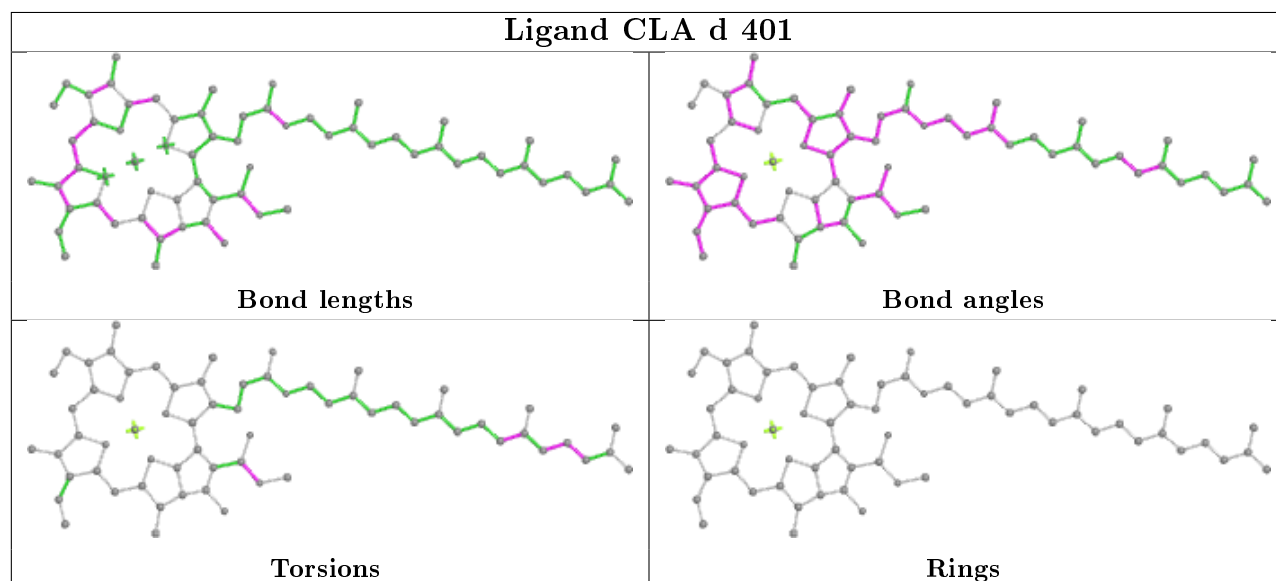


Ligand CLA c 507**Ligand CLA b 614****Ligand LMG C 501**

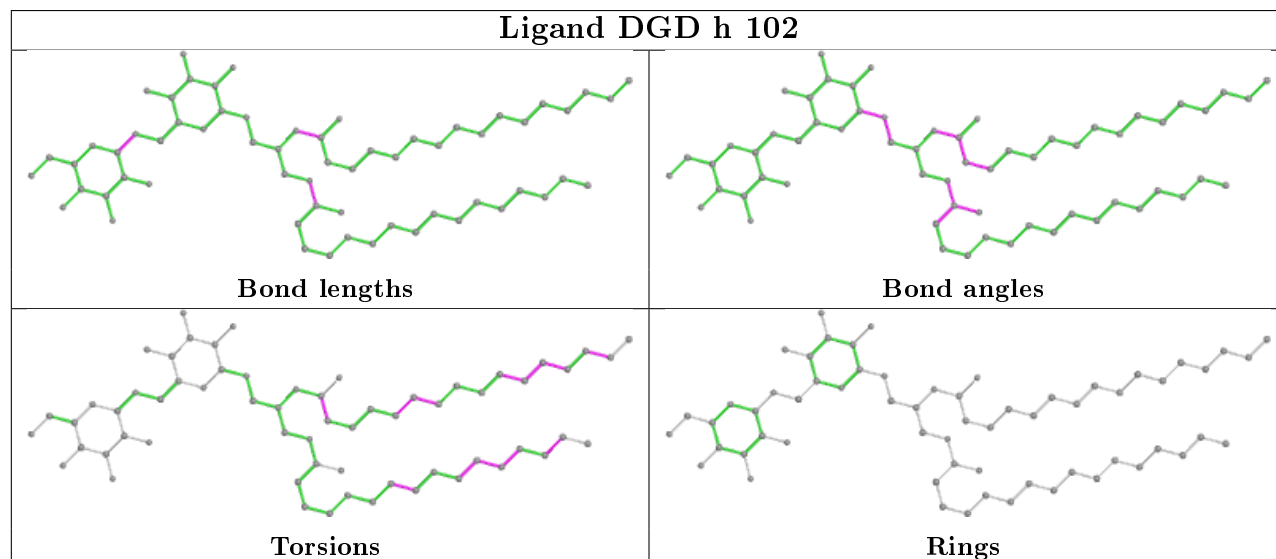
Ligand CLA c 505



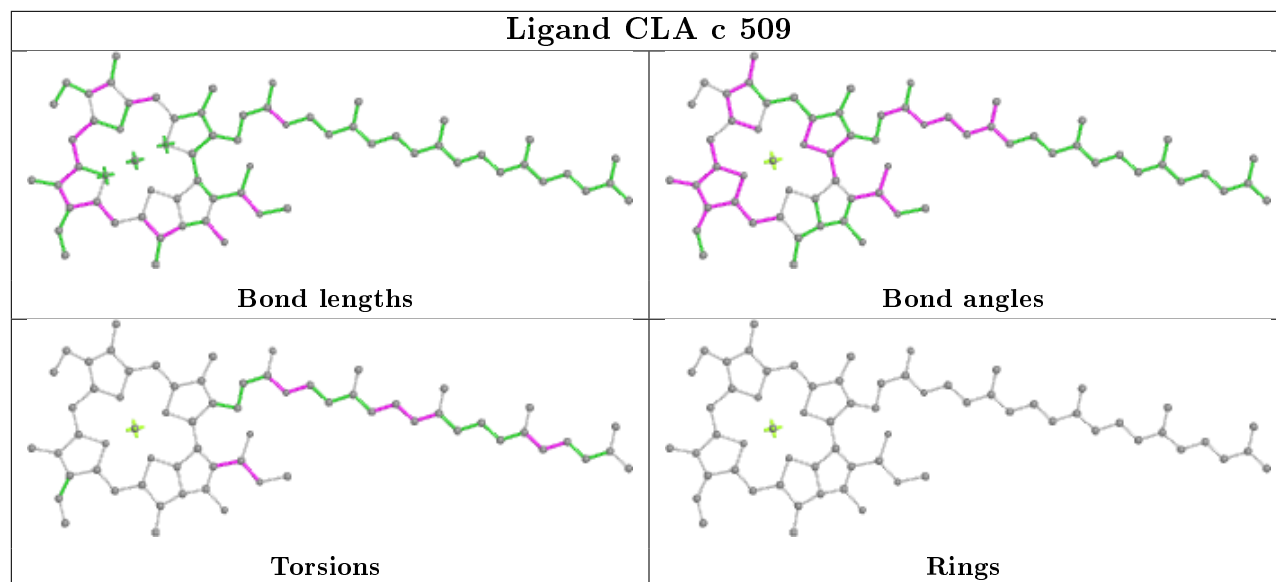
Ligand CLA d 401



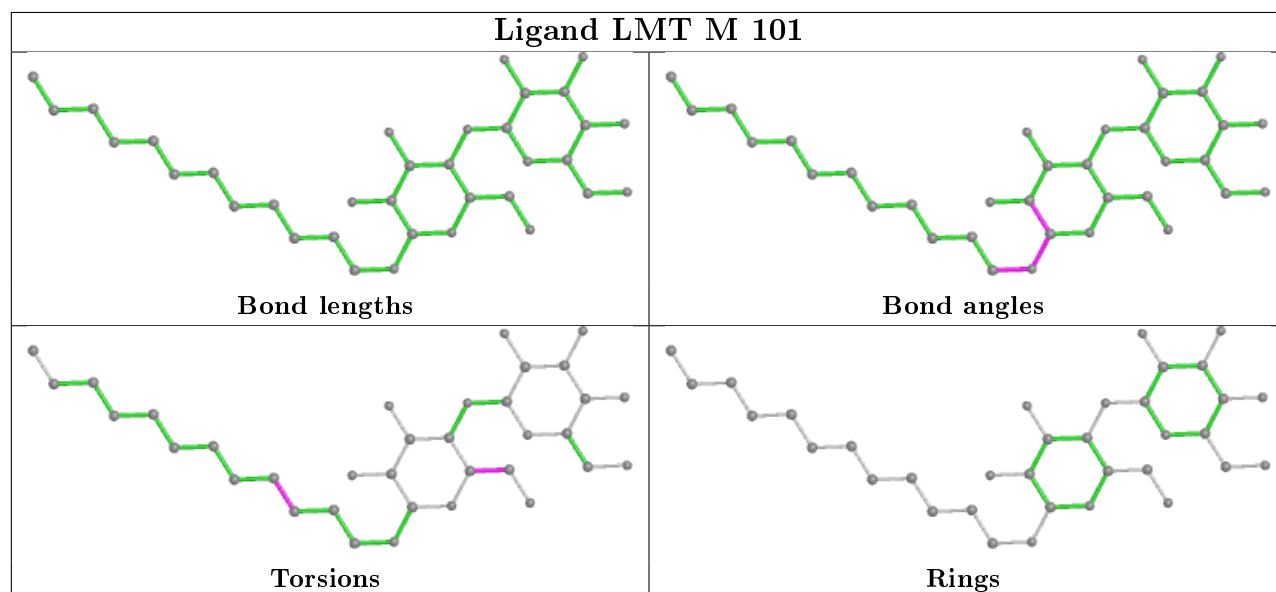
Ligand DGD h 102

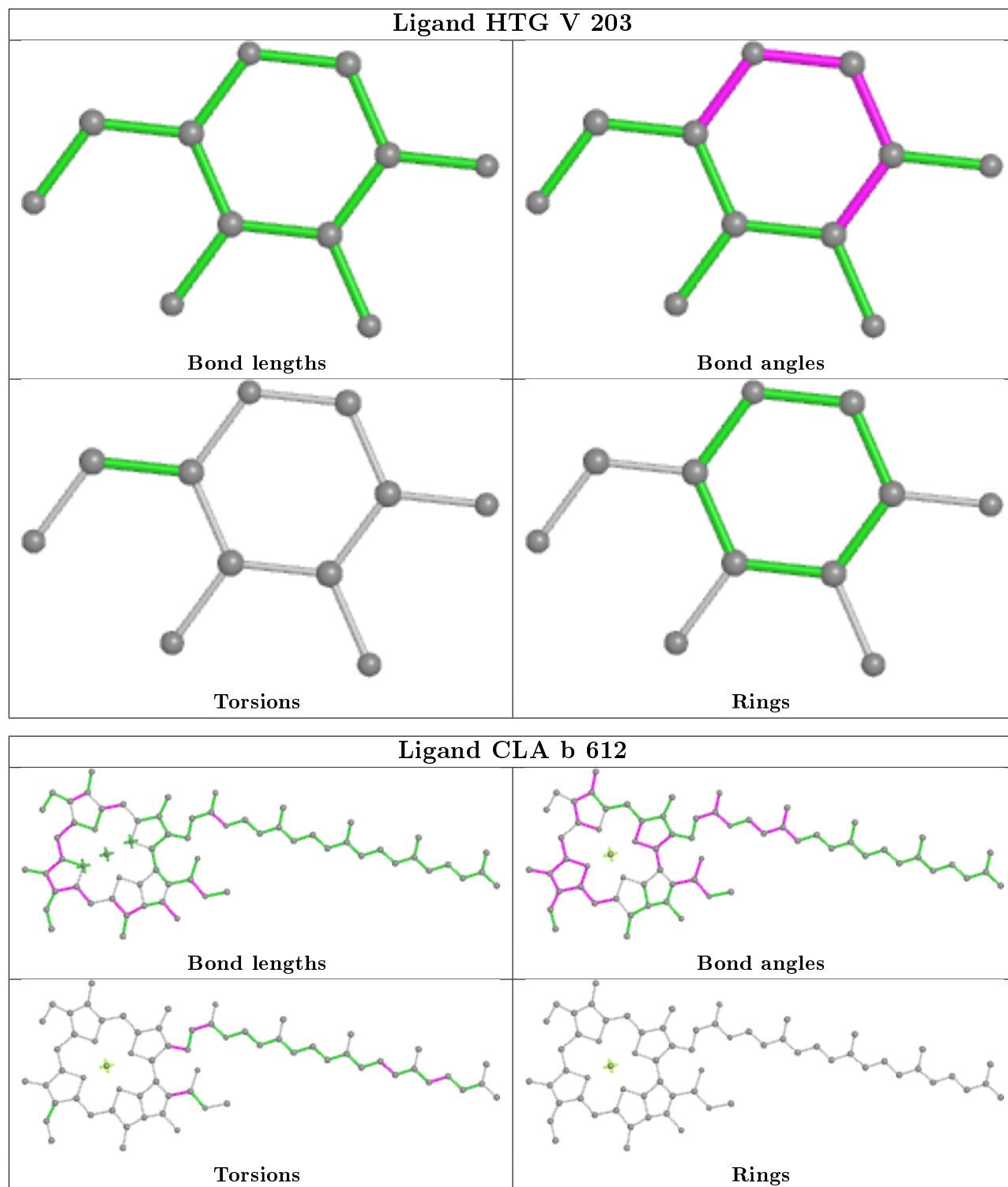


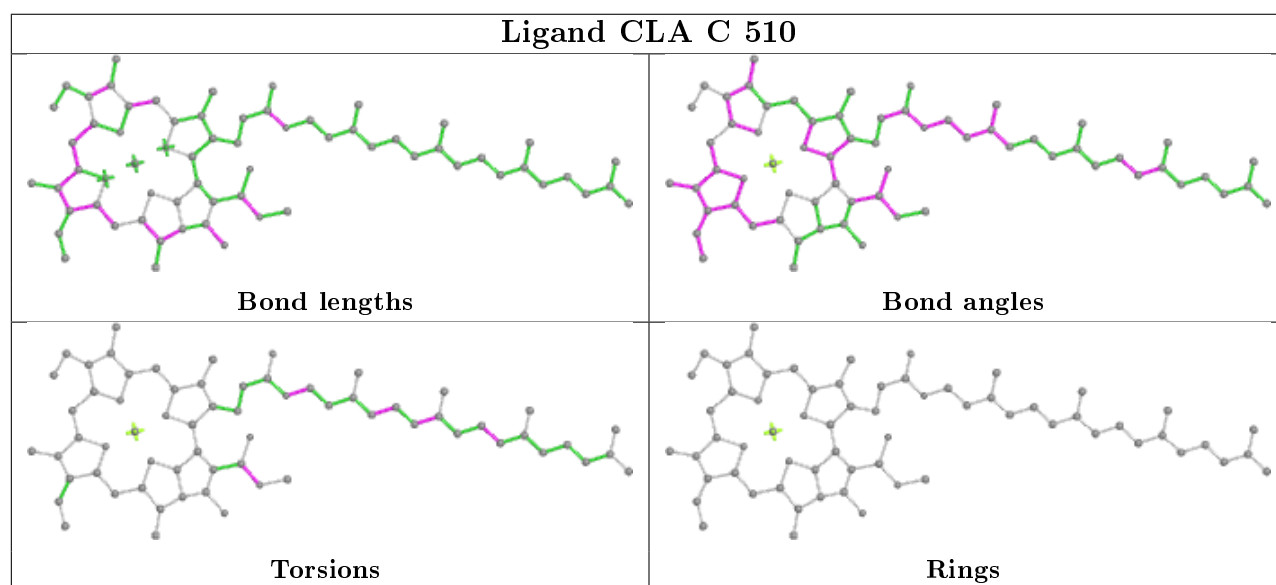
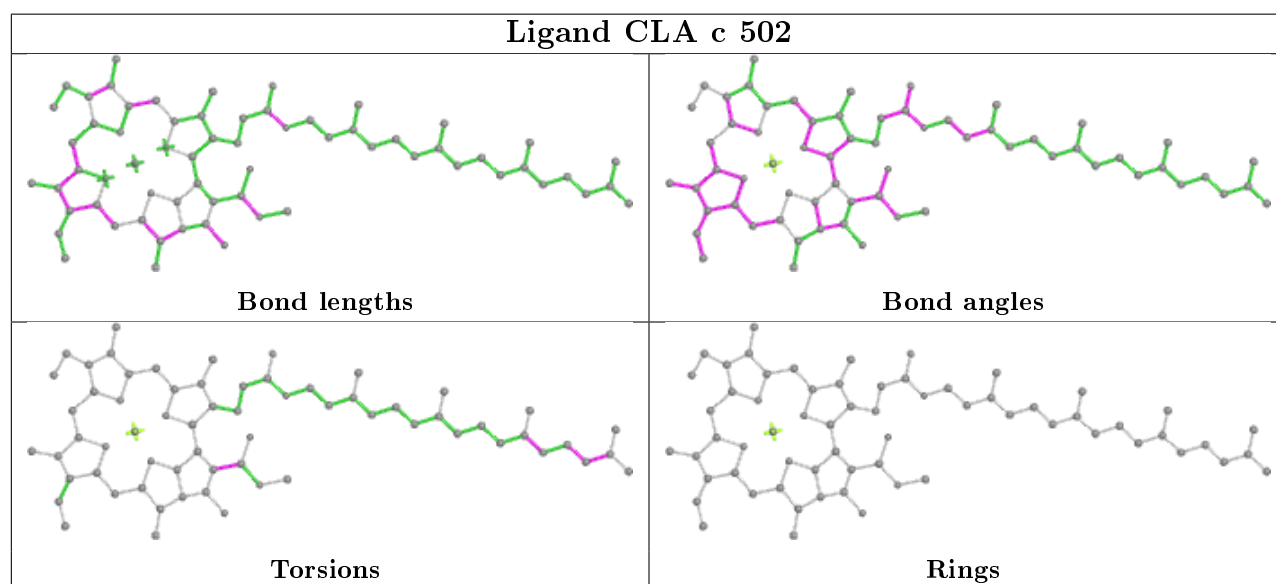
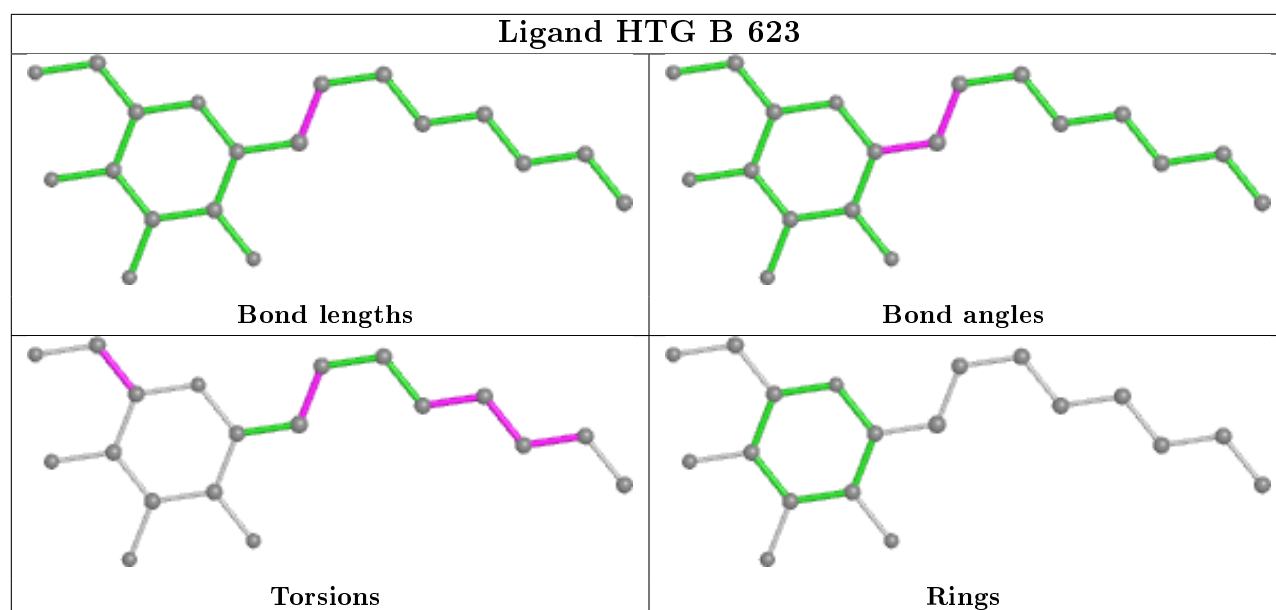
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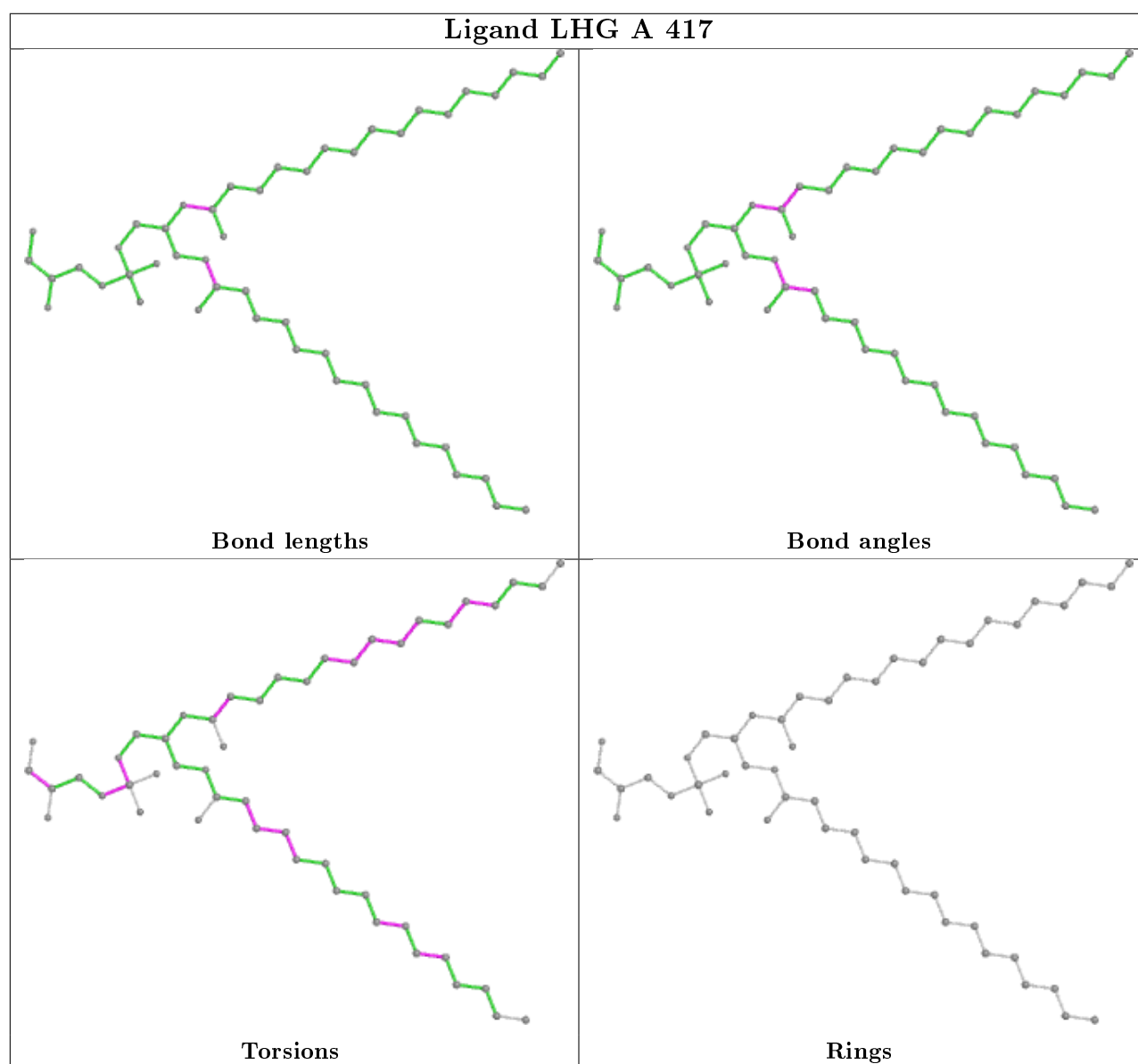
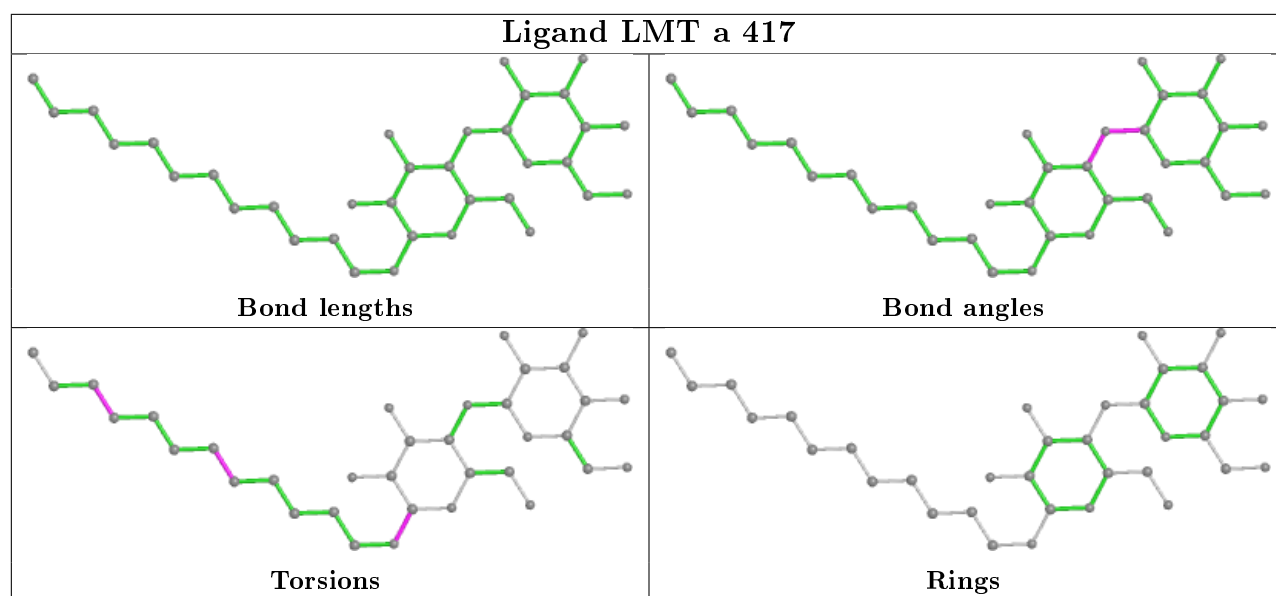


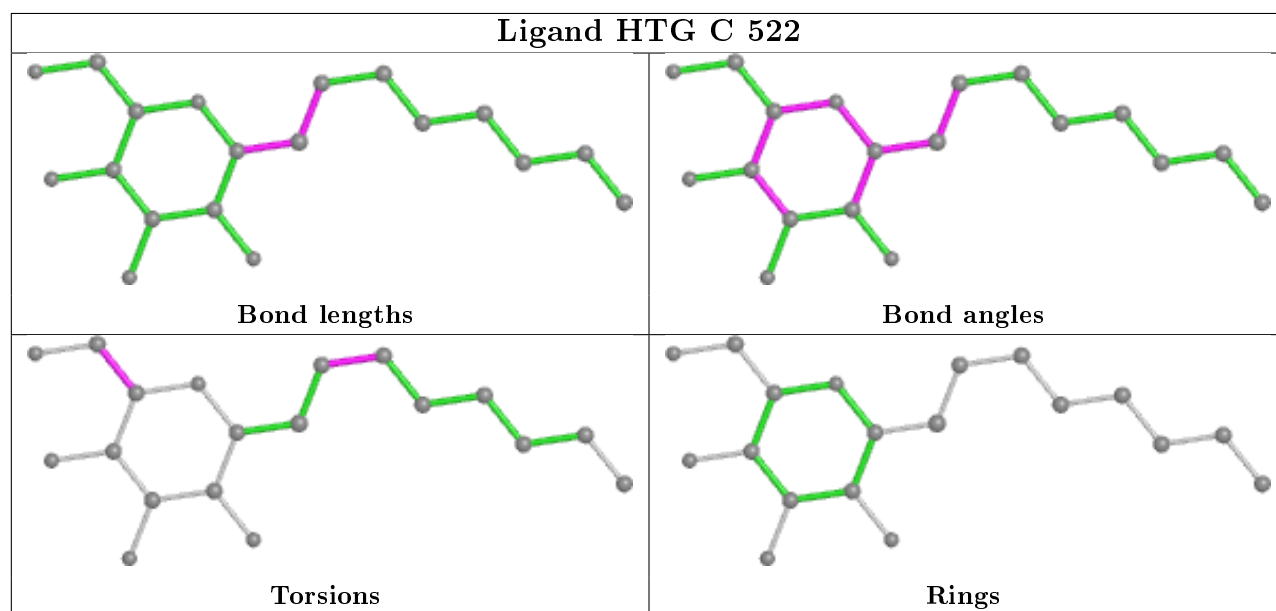
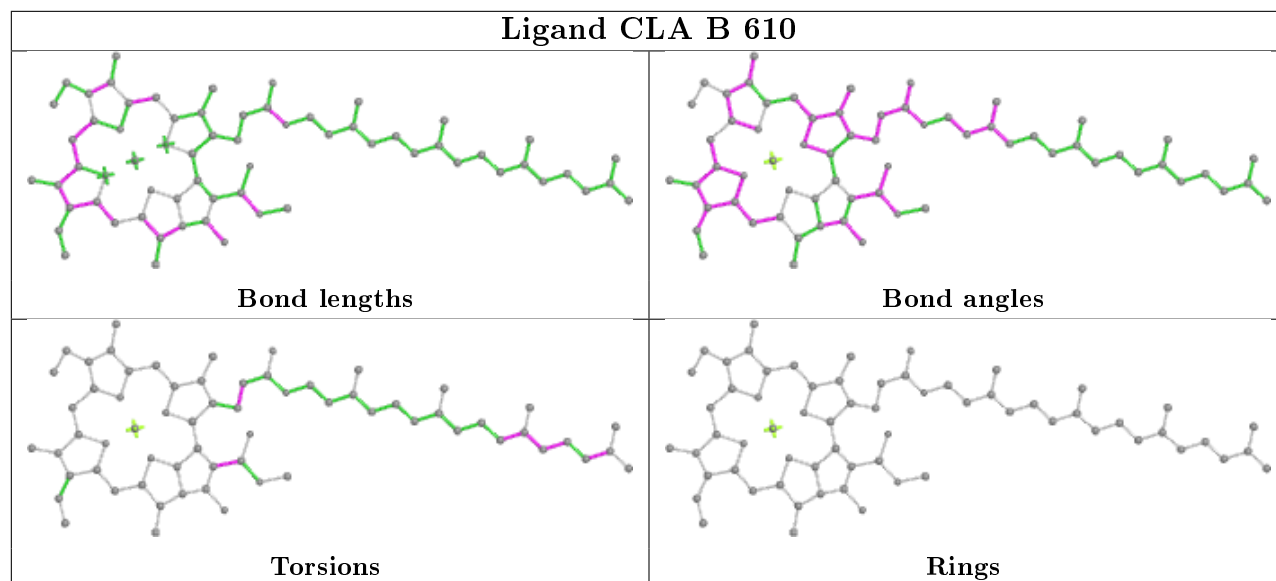
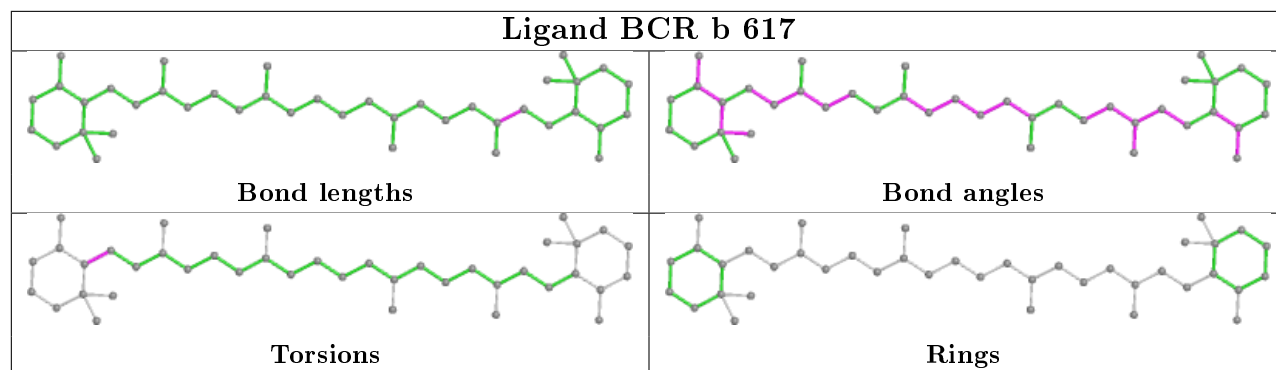
Ligand LMT M 101



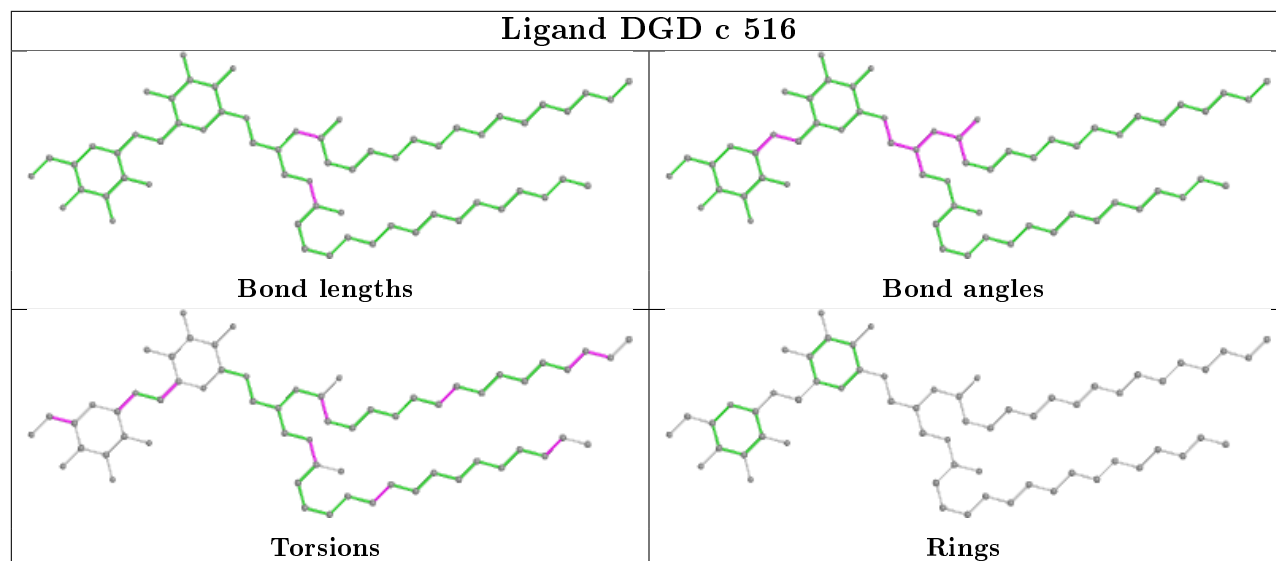




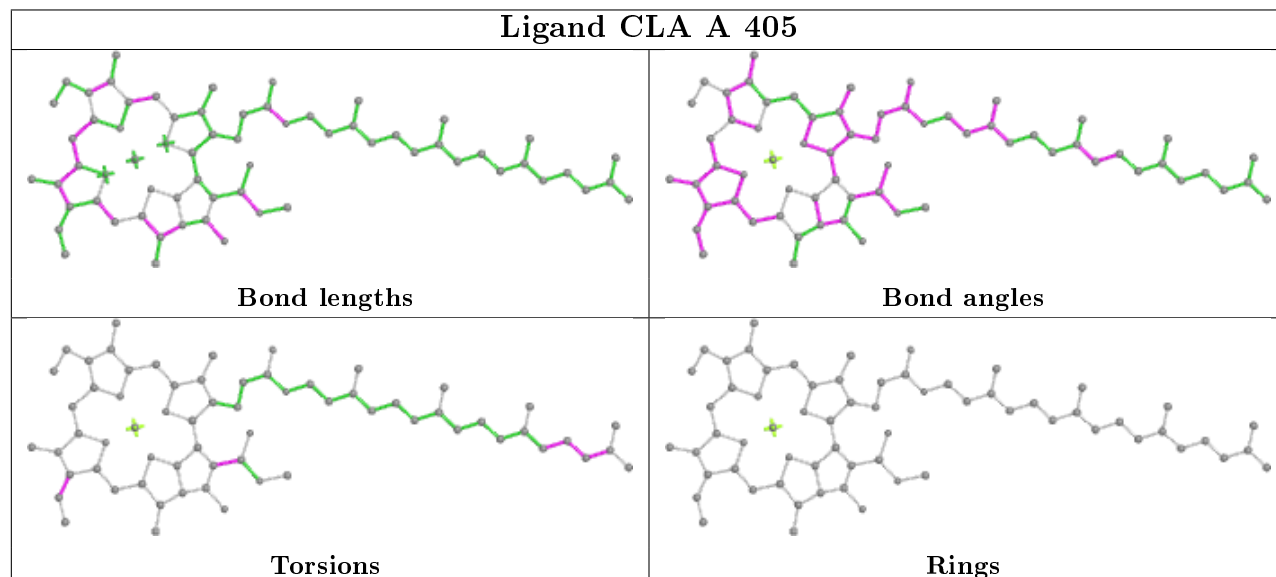




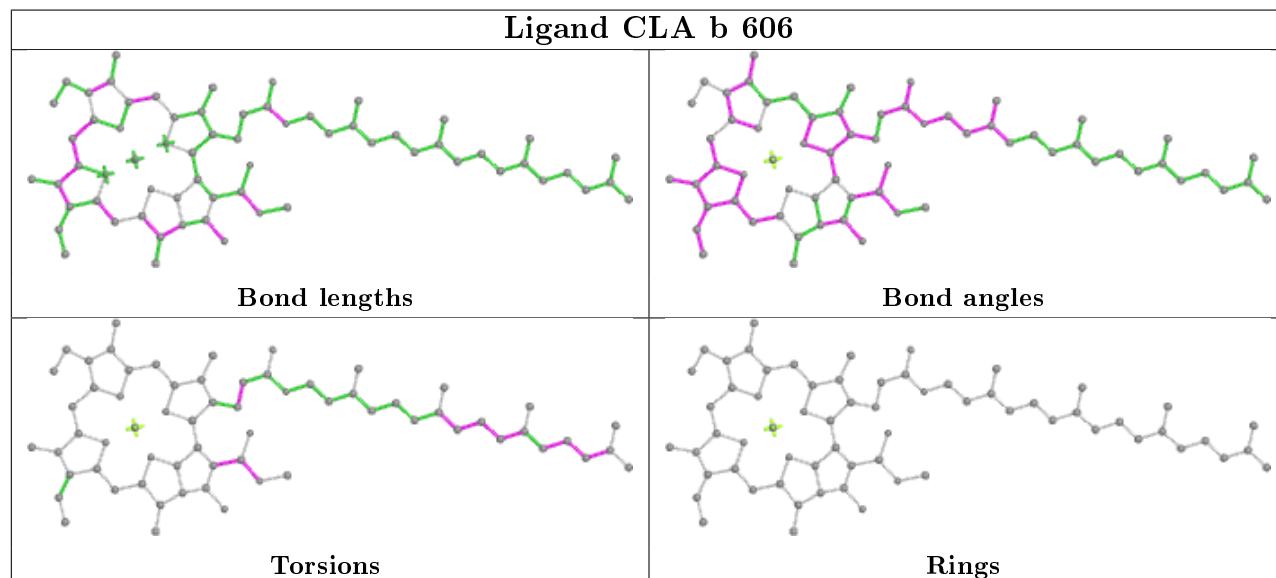
Ligand DGD c 516

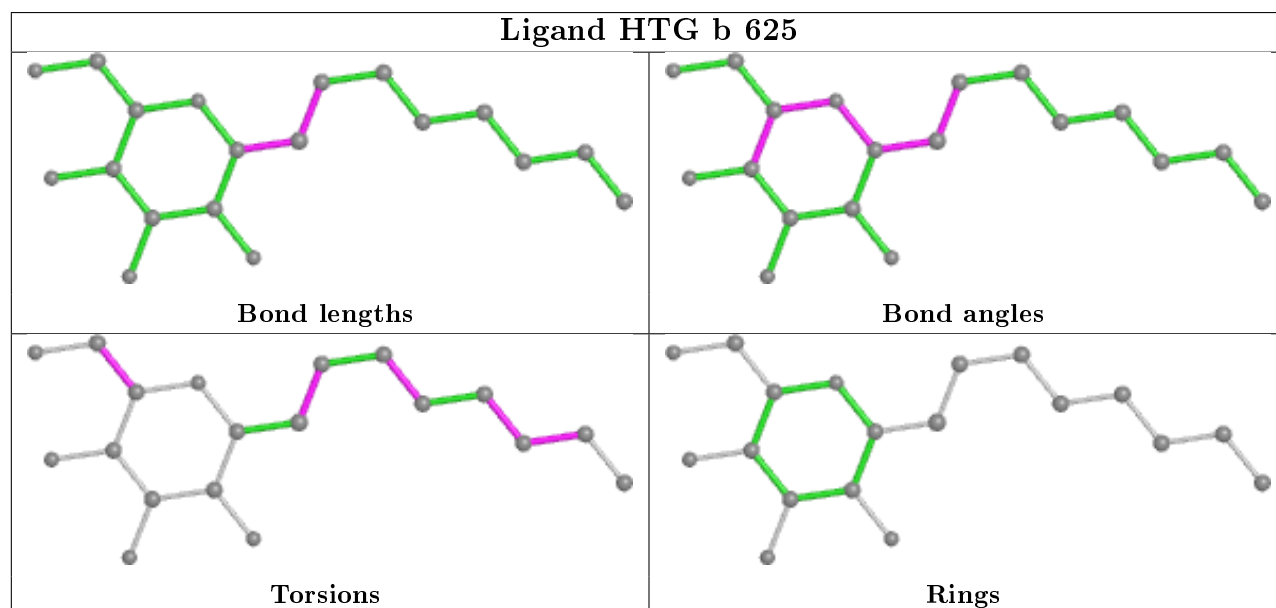
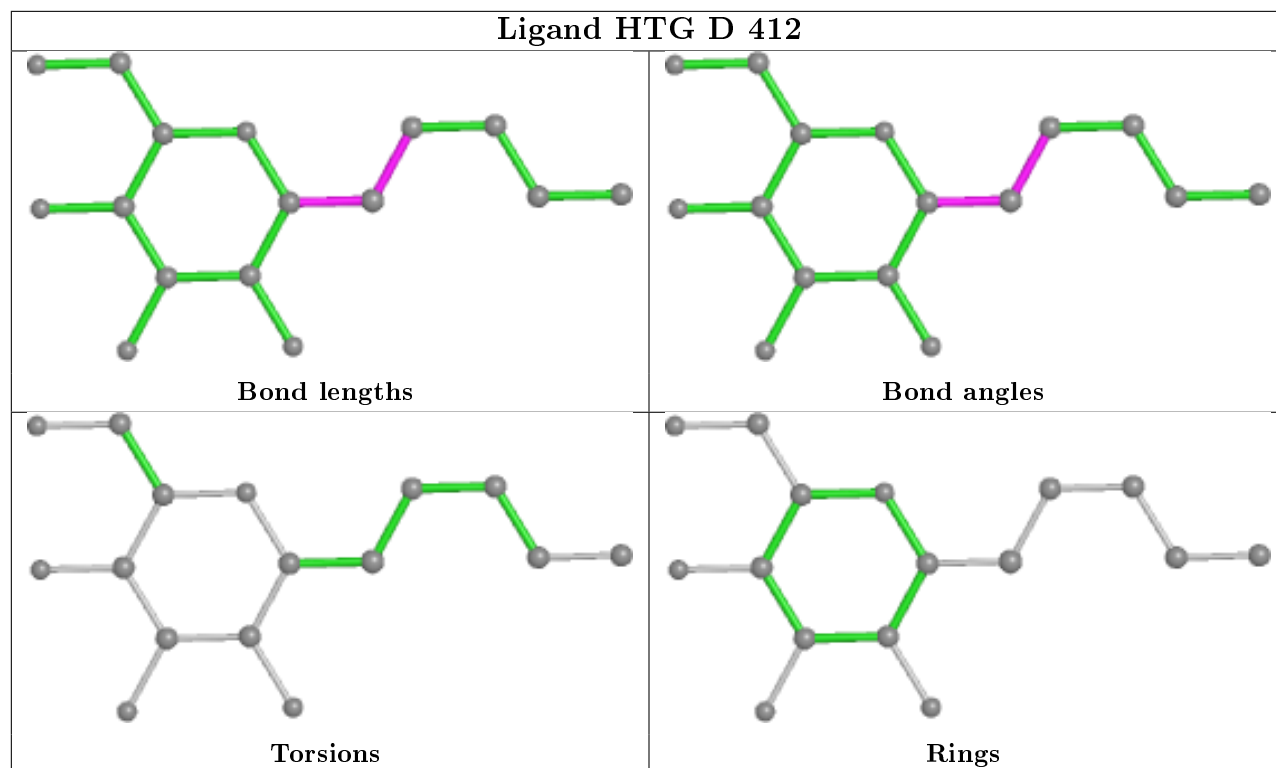


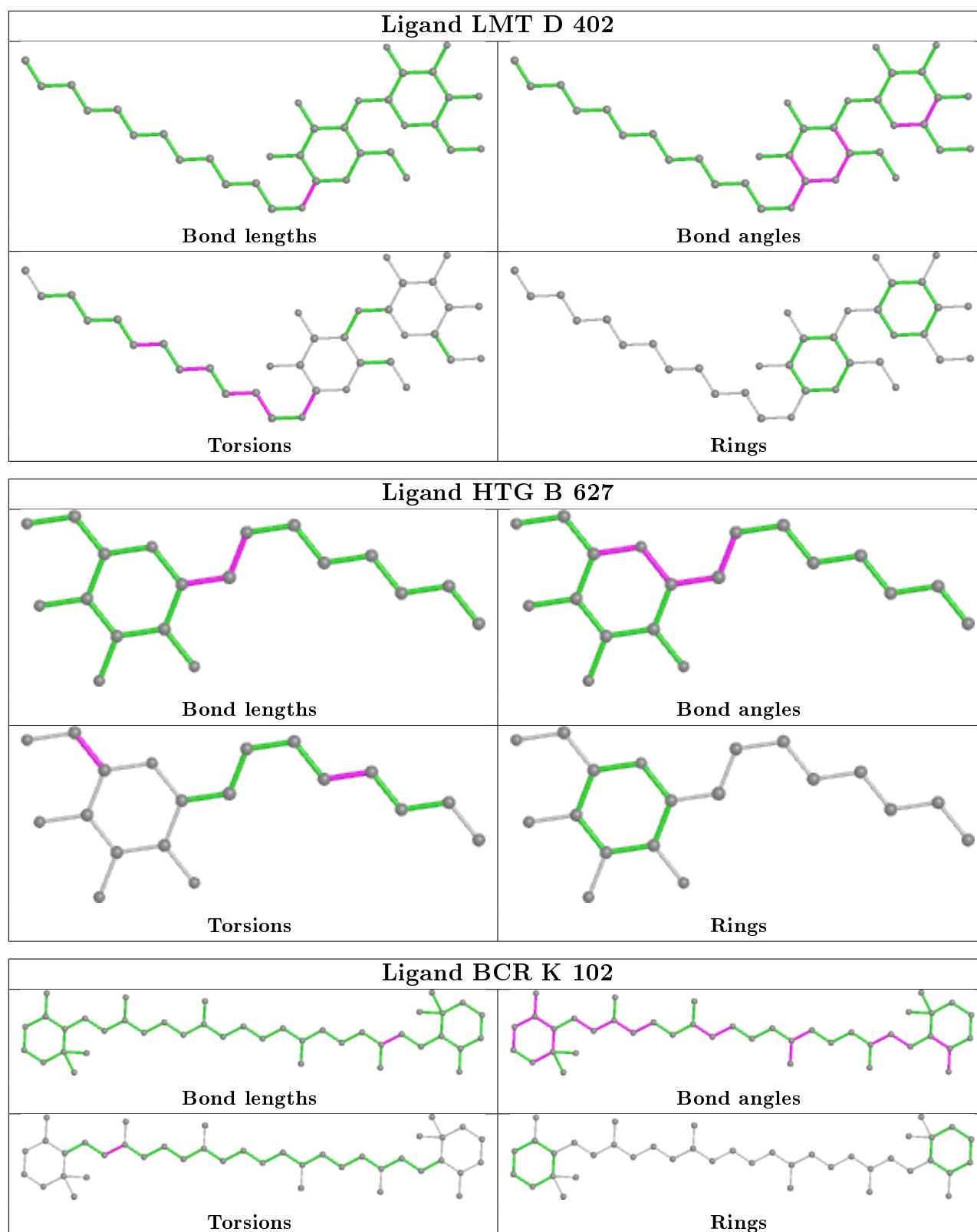
Ligand CLA A 405

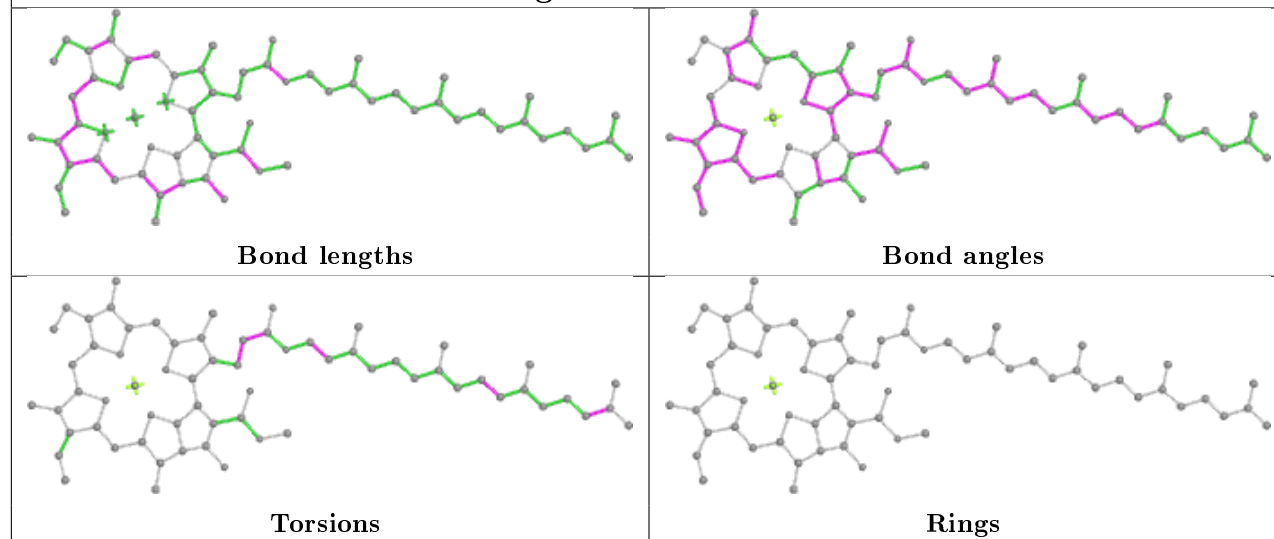
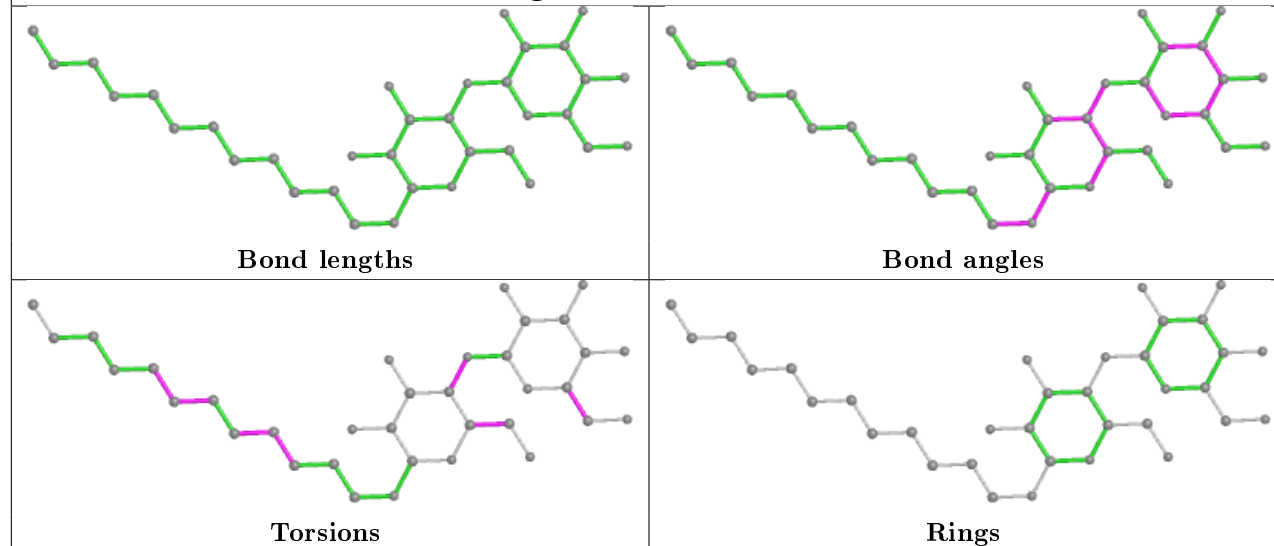
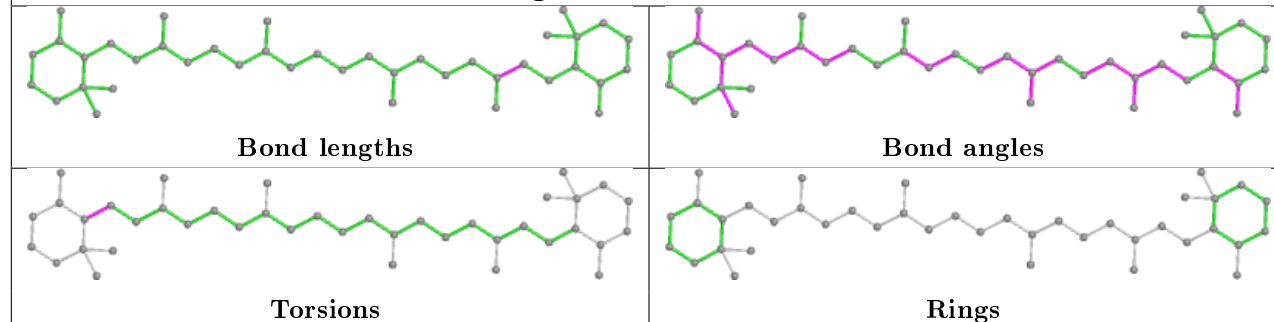


Ligand CLA b 606

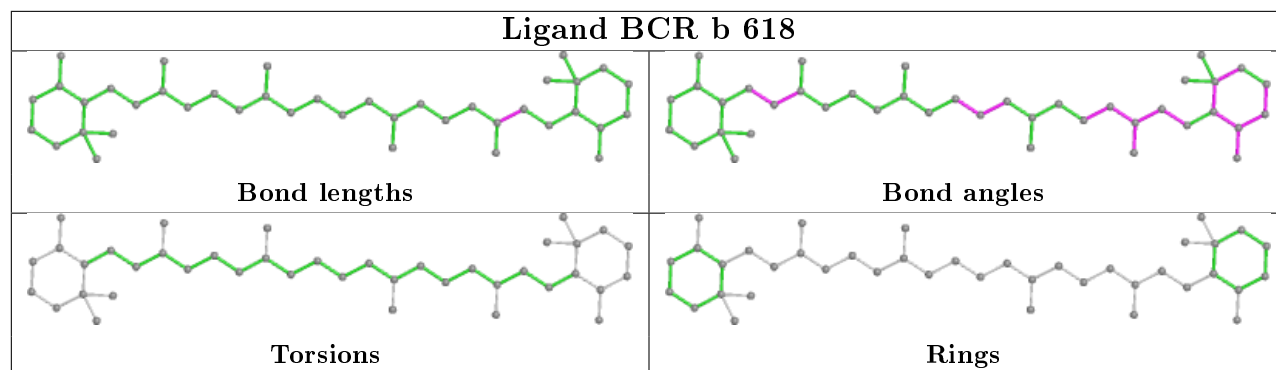




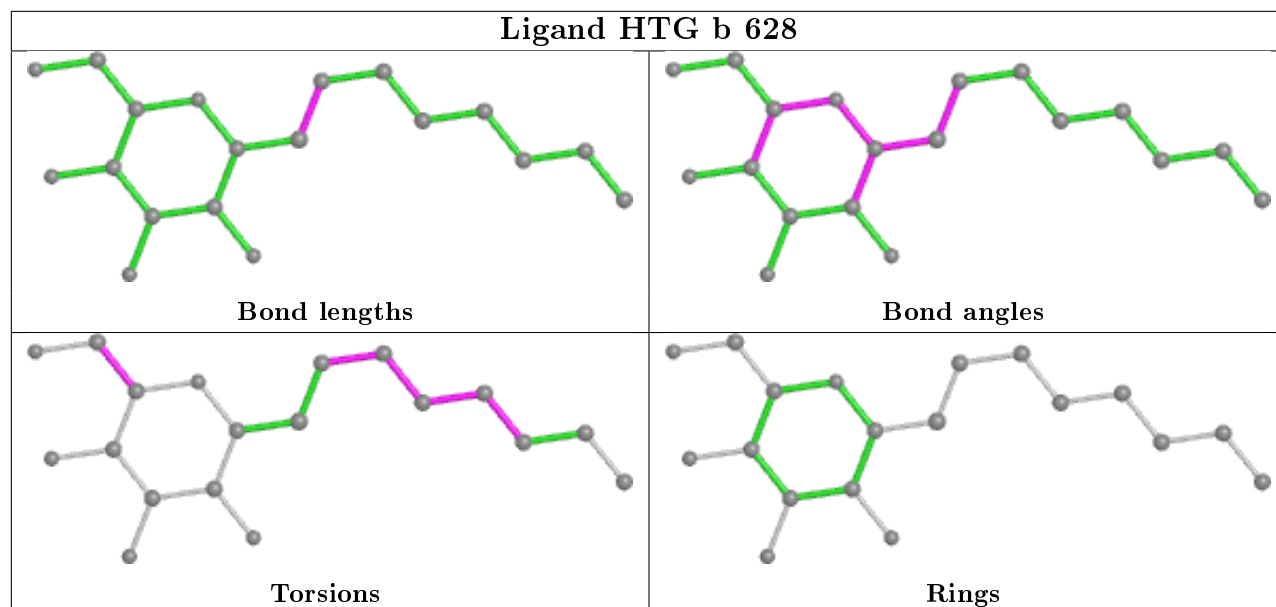


Ligand CLA b 602**Ligand LMT D 403****Ligand BCR A 409**

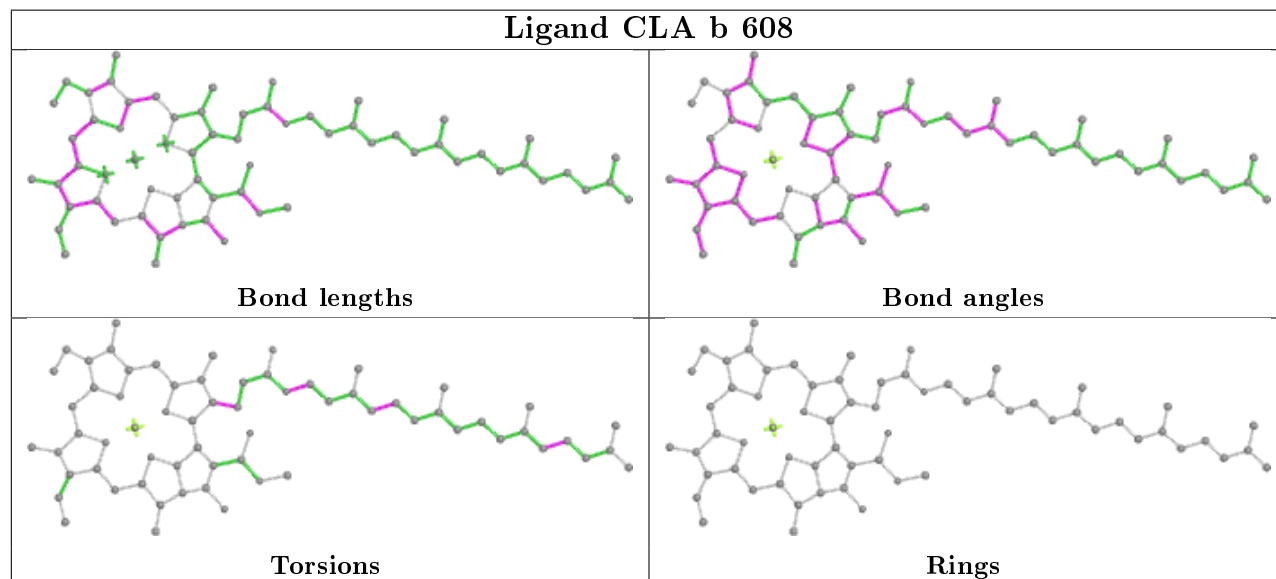
Ligand BCR b 618

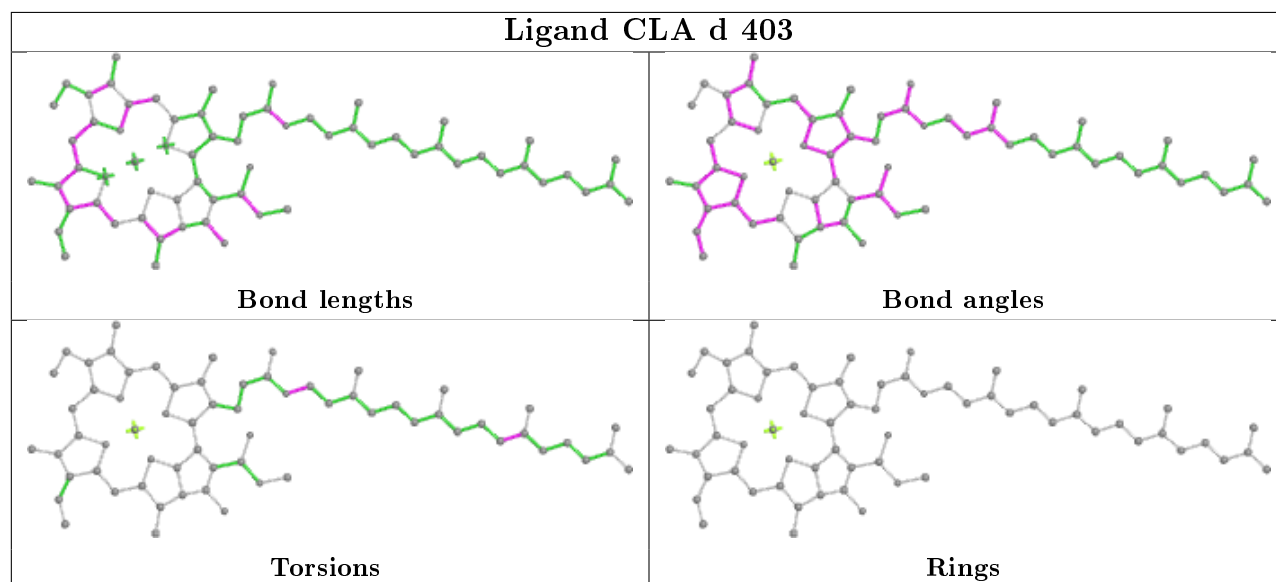
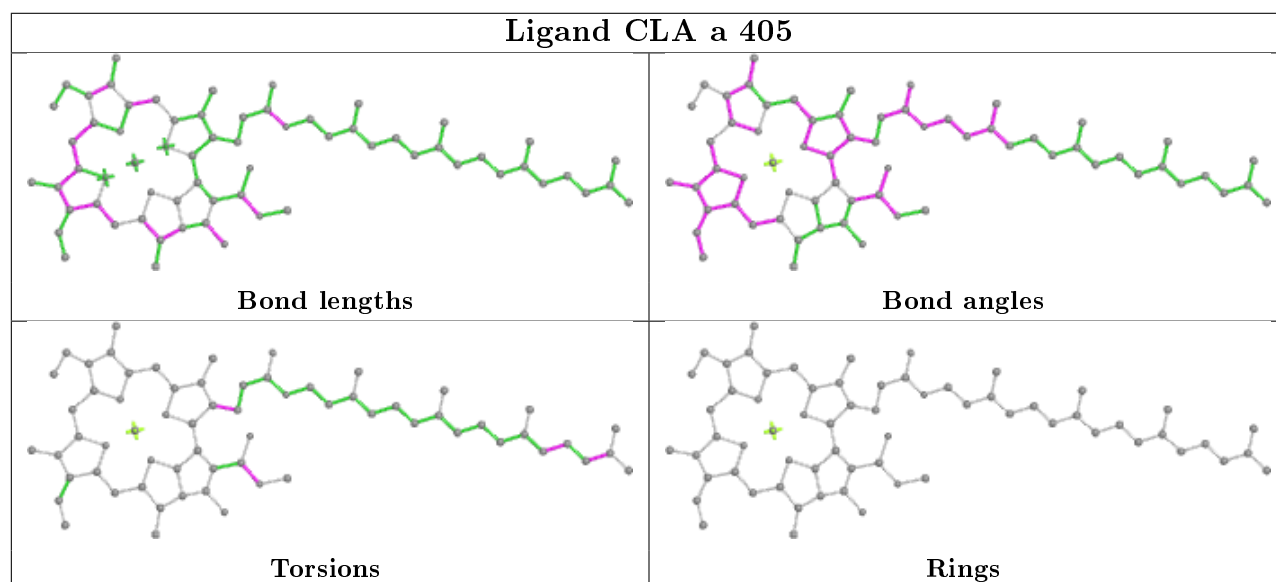
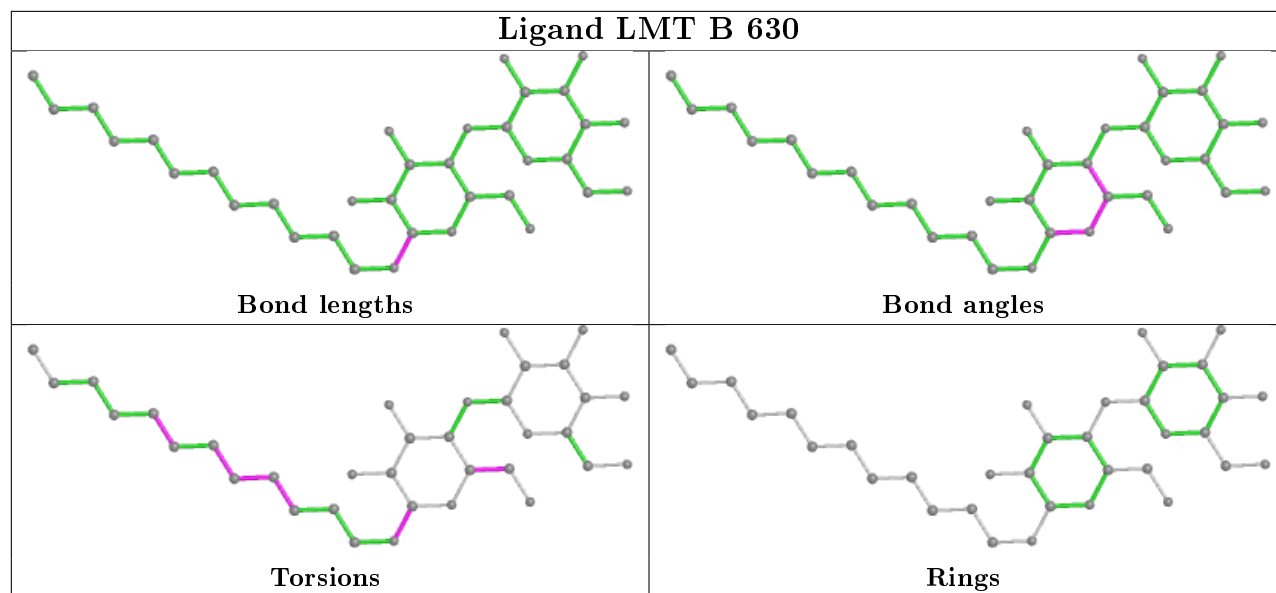


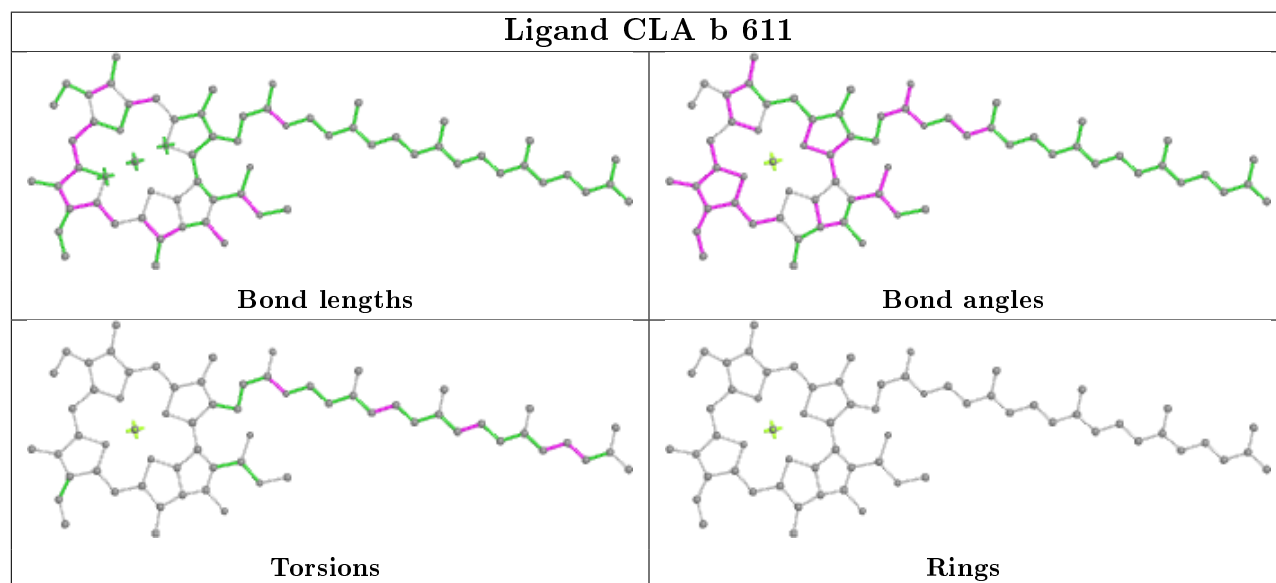
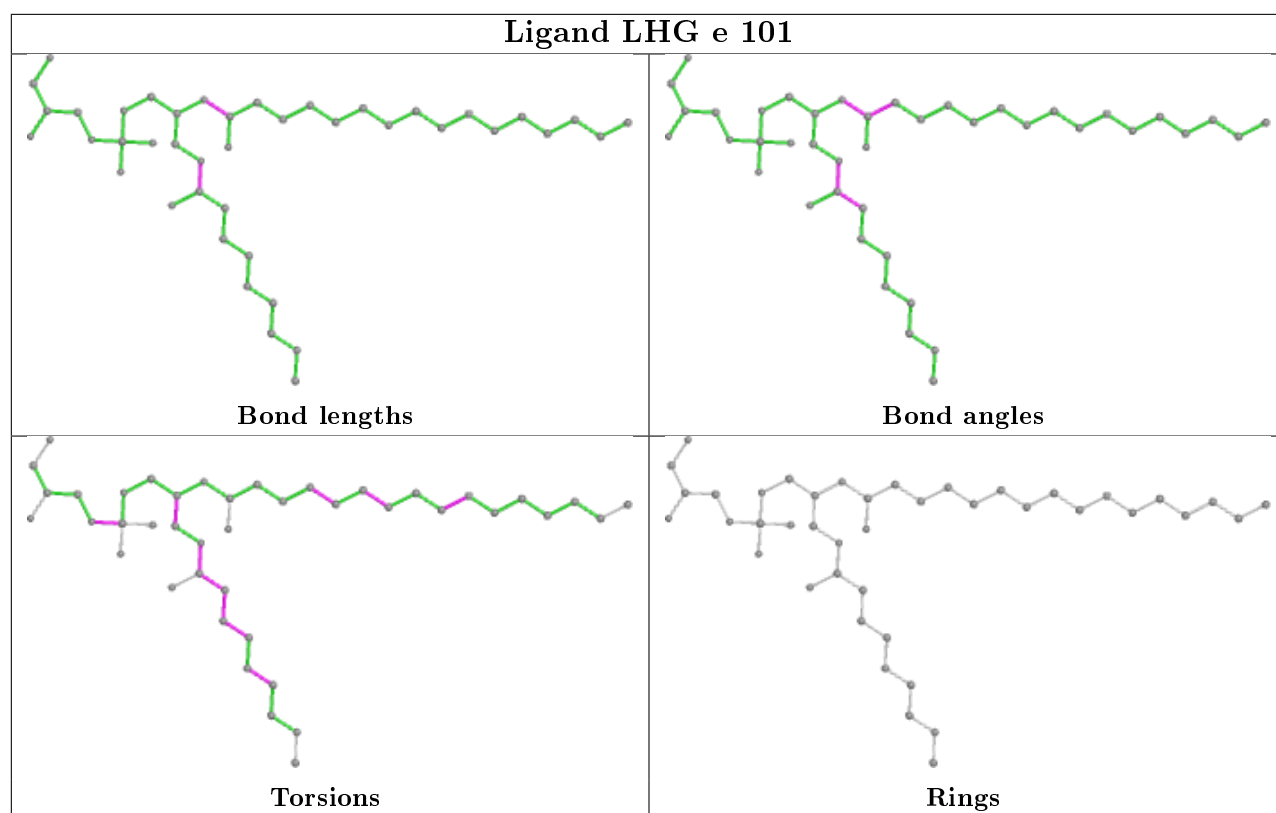
Ligand HTG b 628

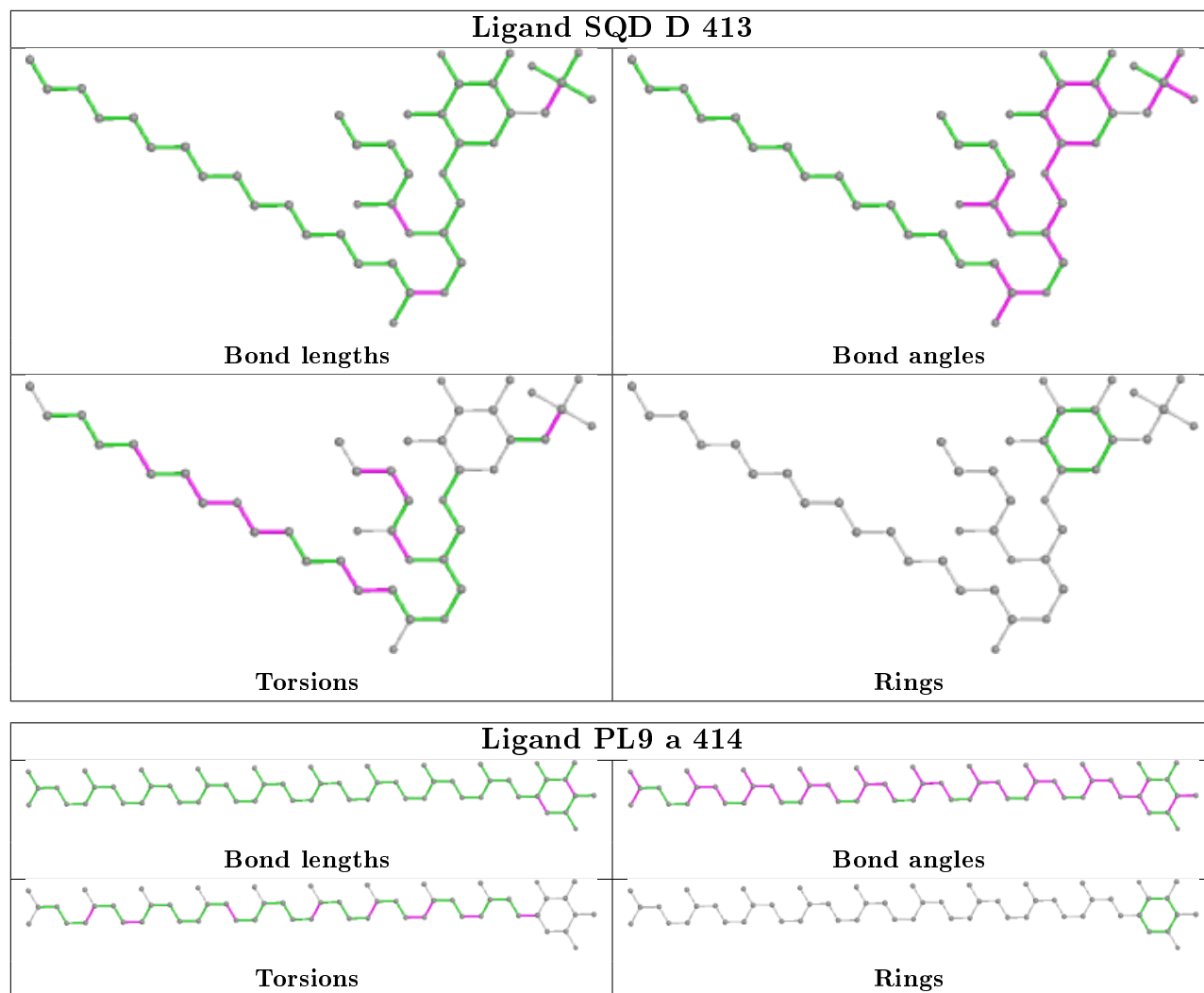


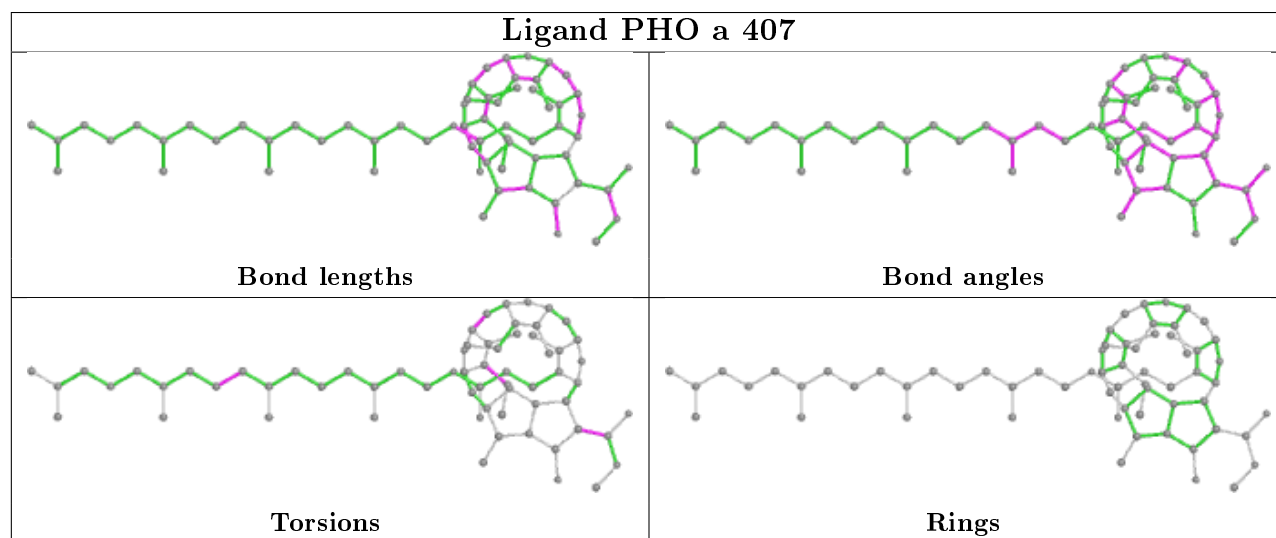
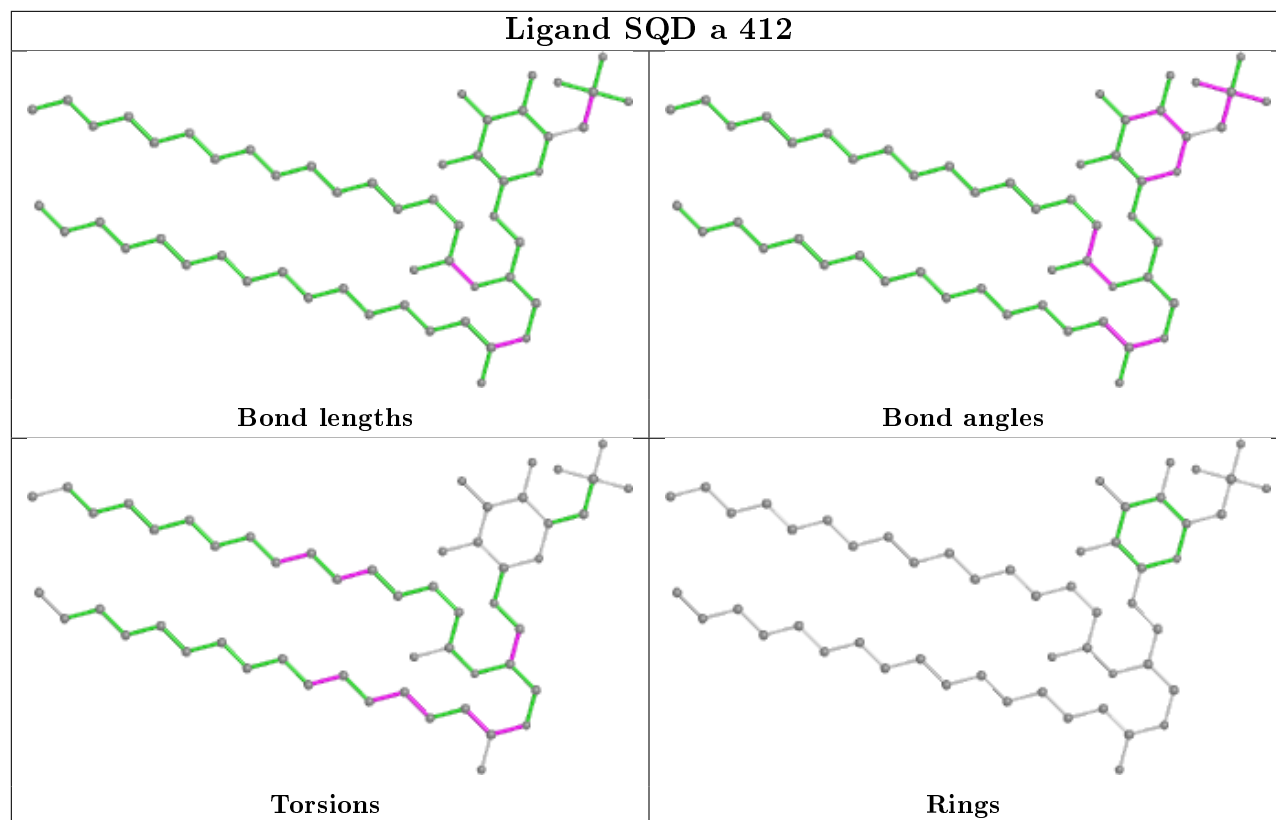
Ligand CLA b 608

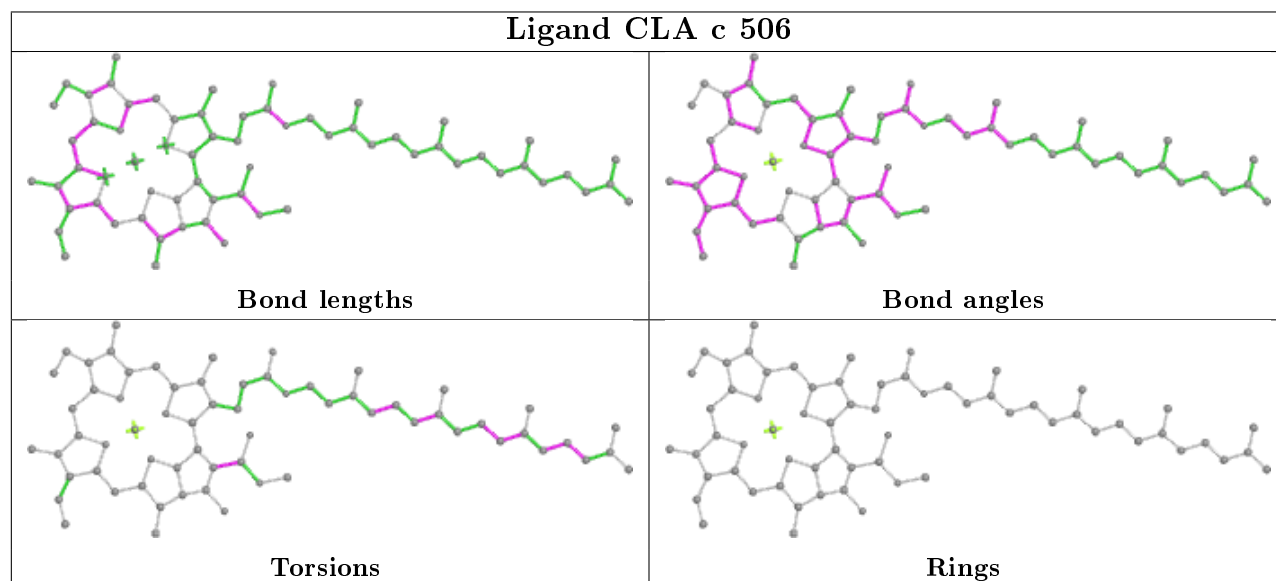
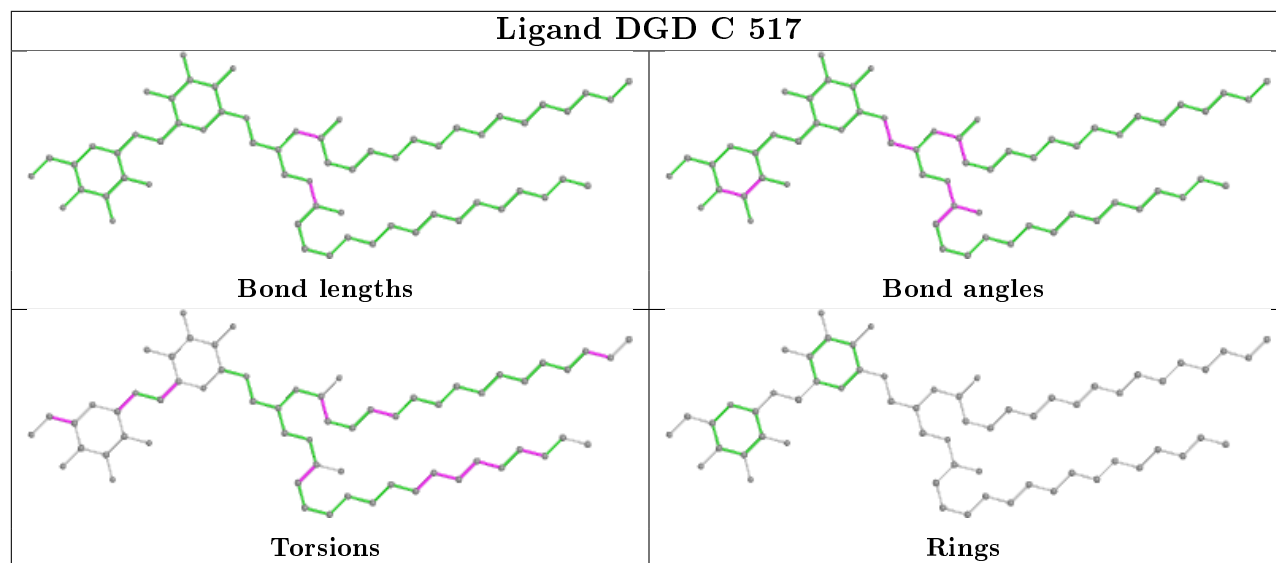


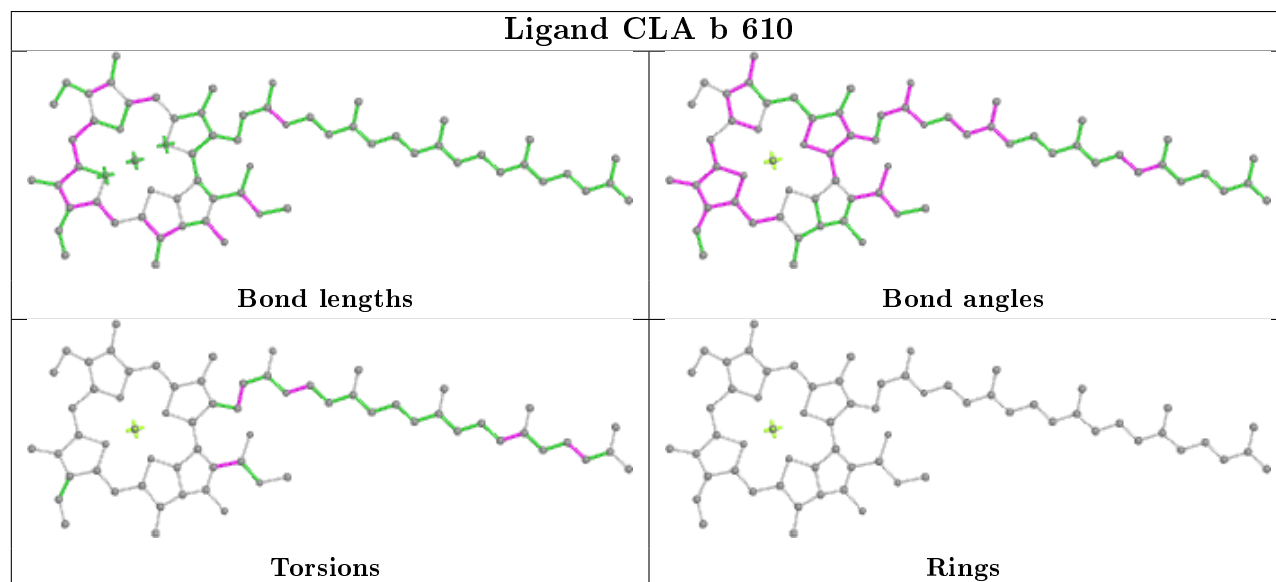
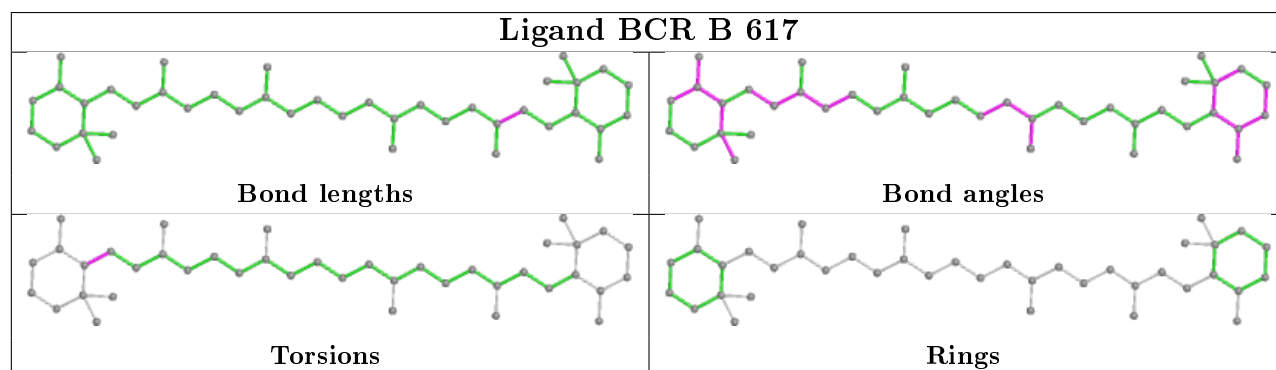
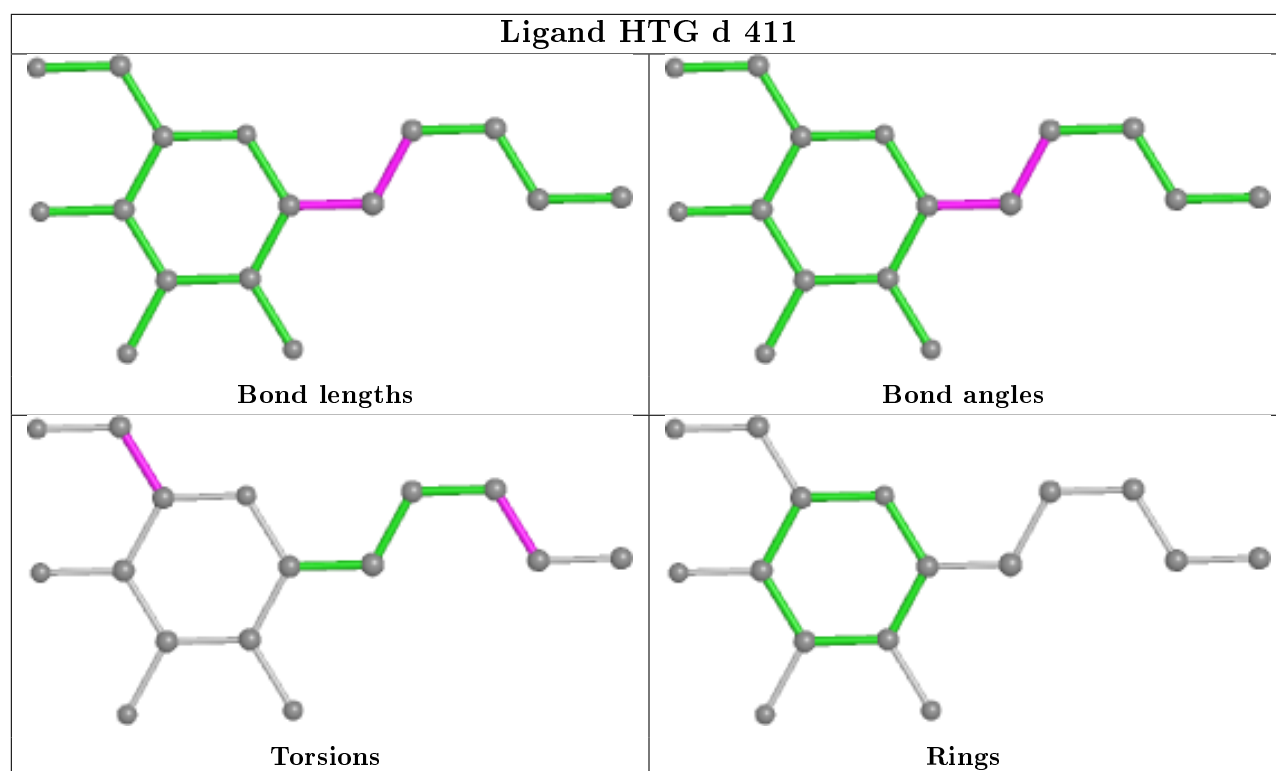


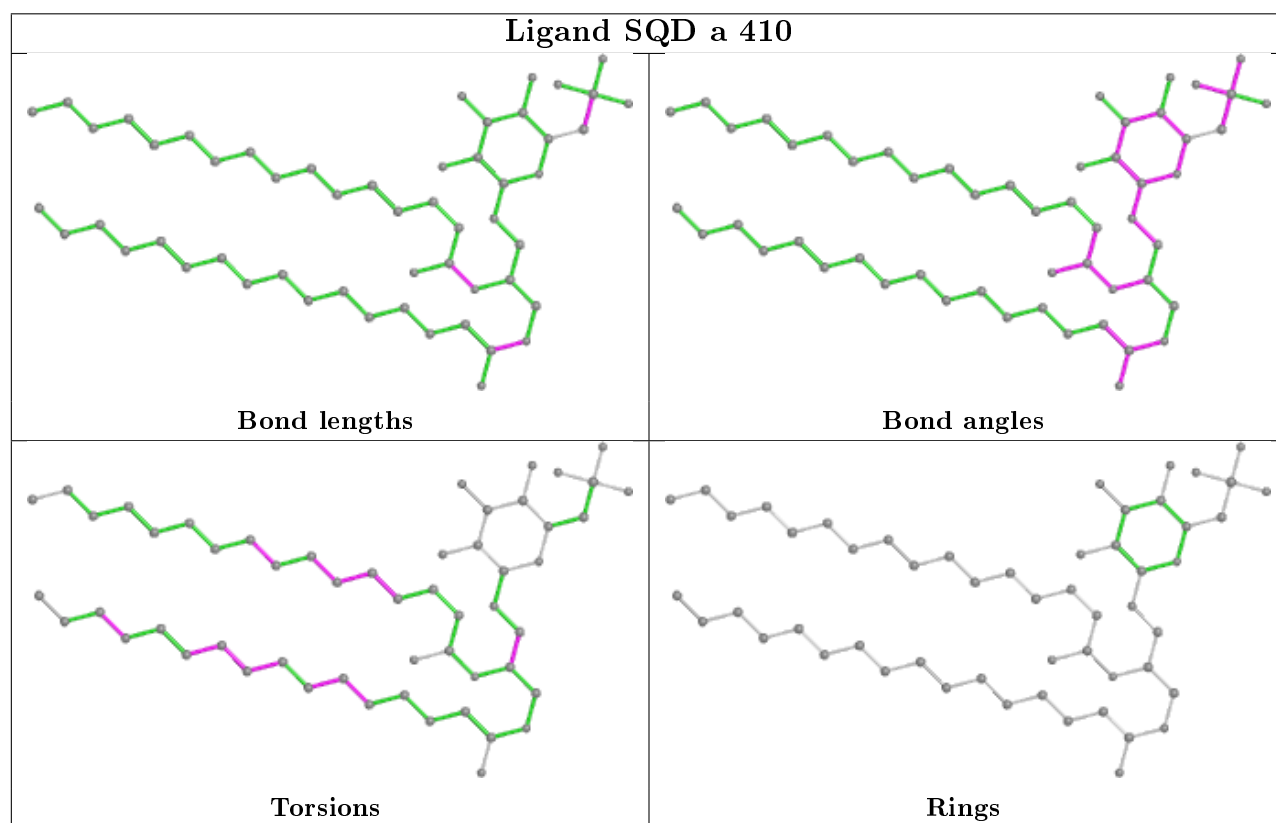
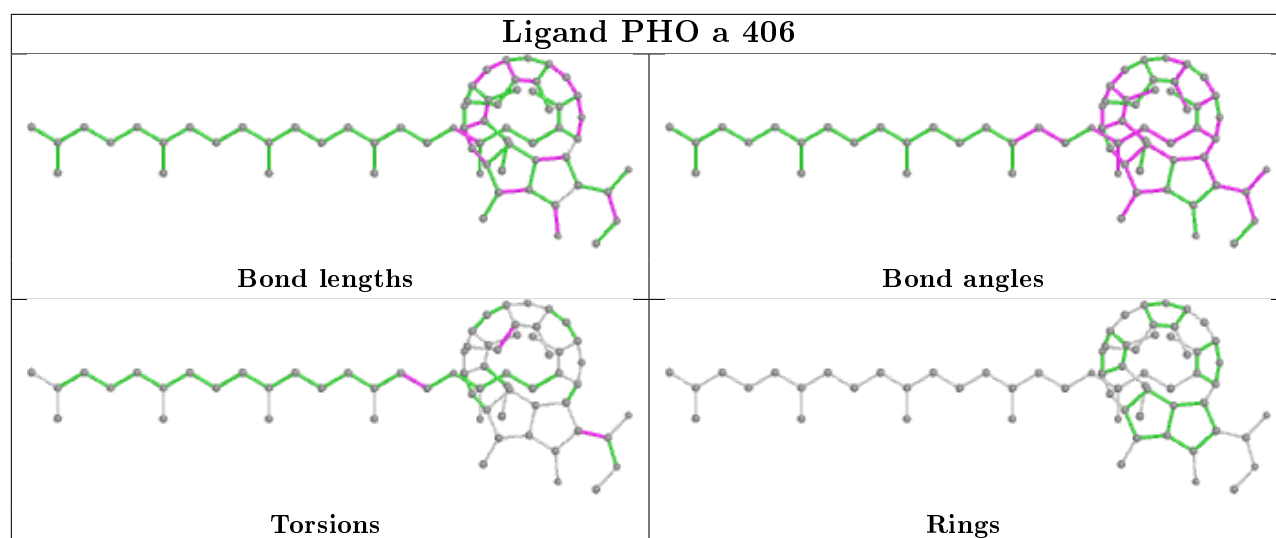




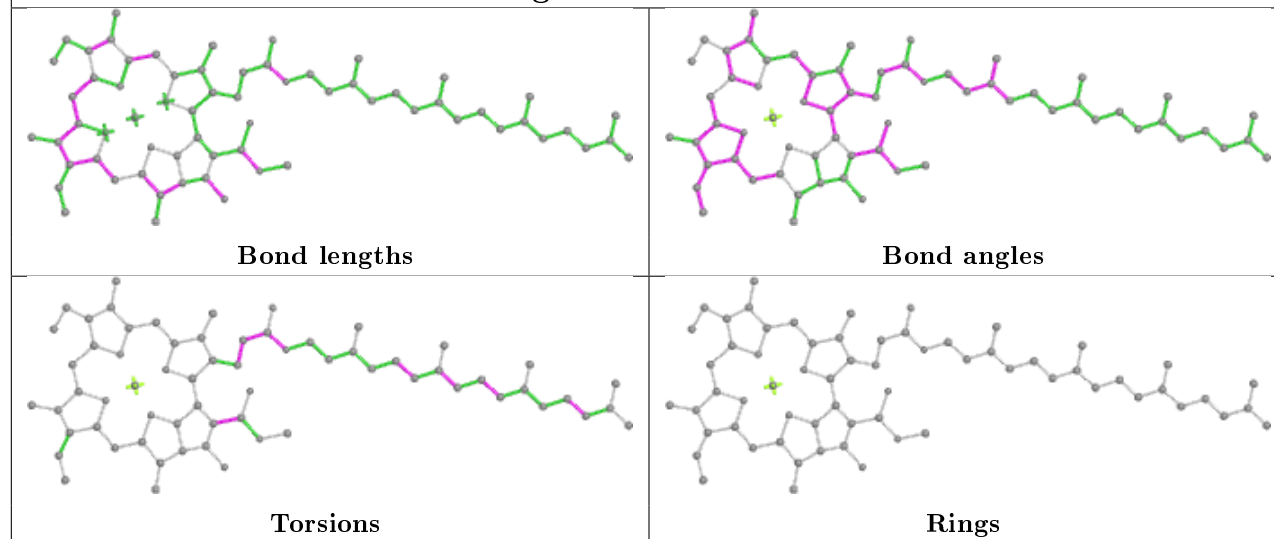




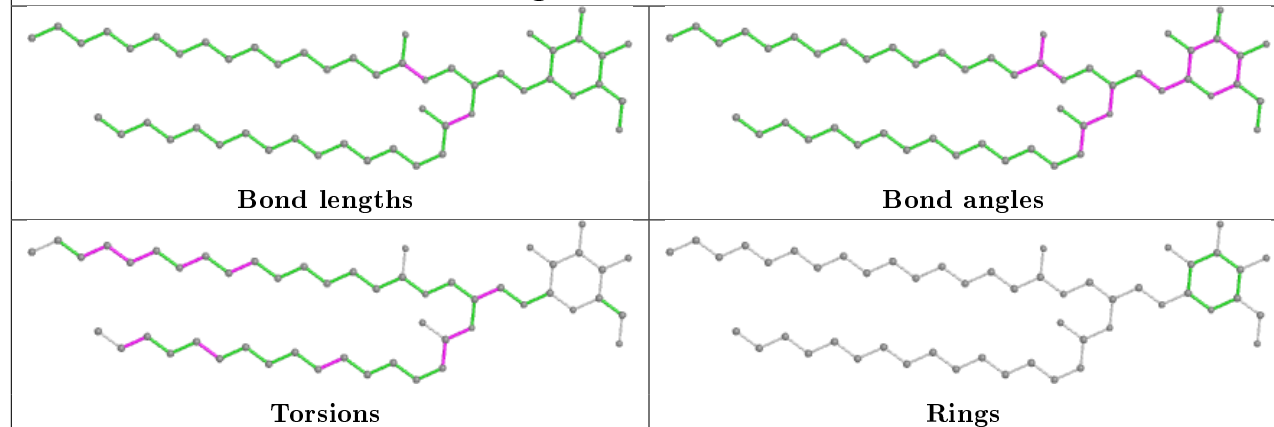




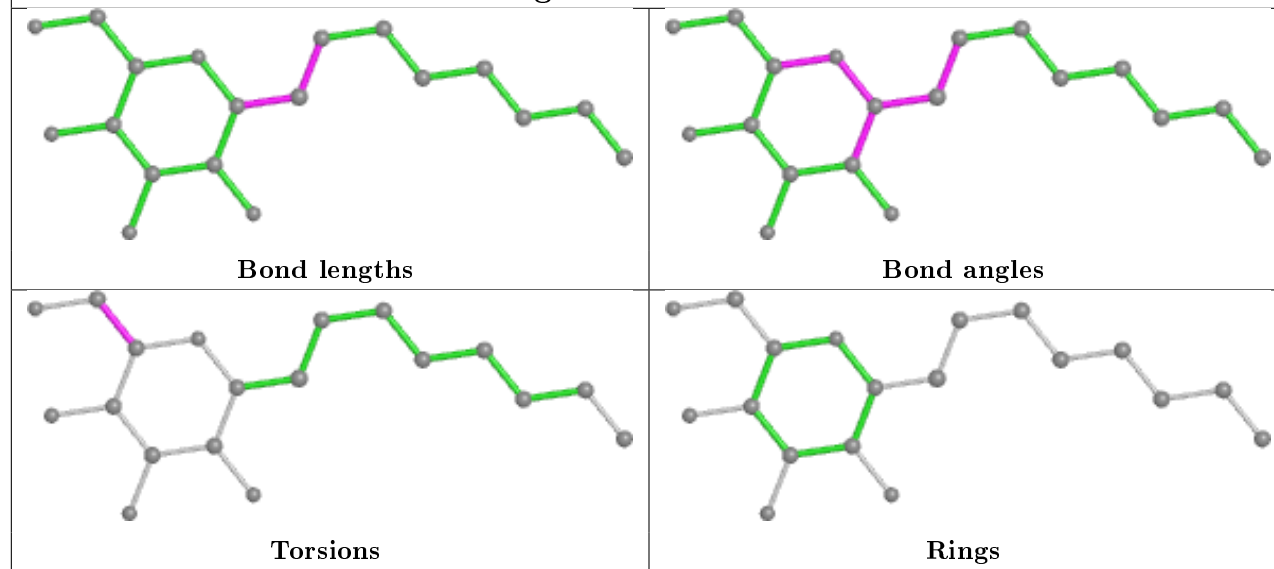
Ligand CLA B 601

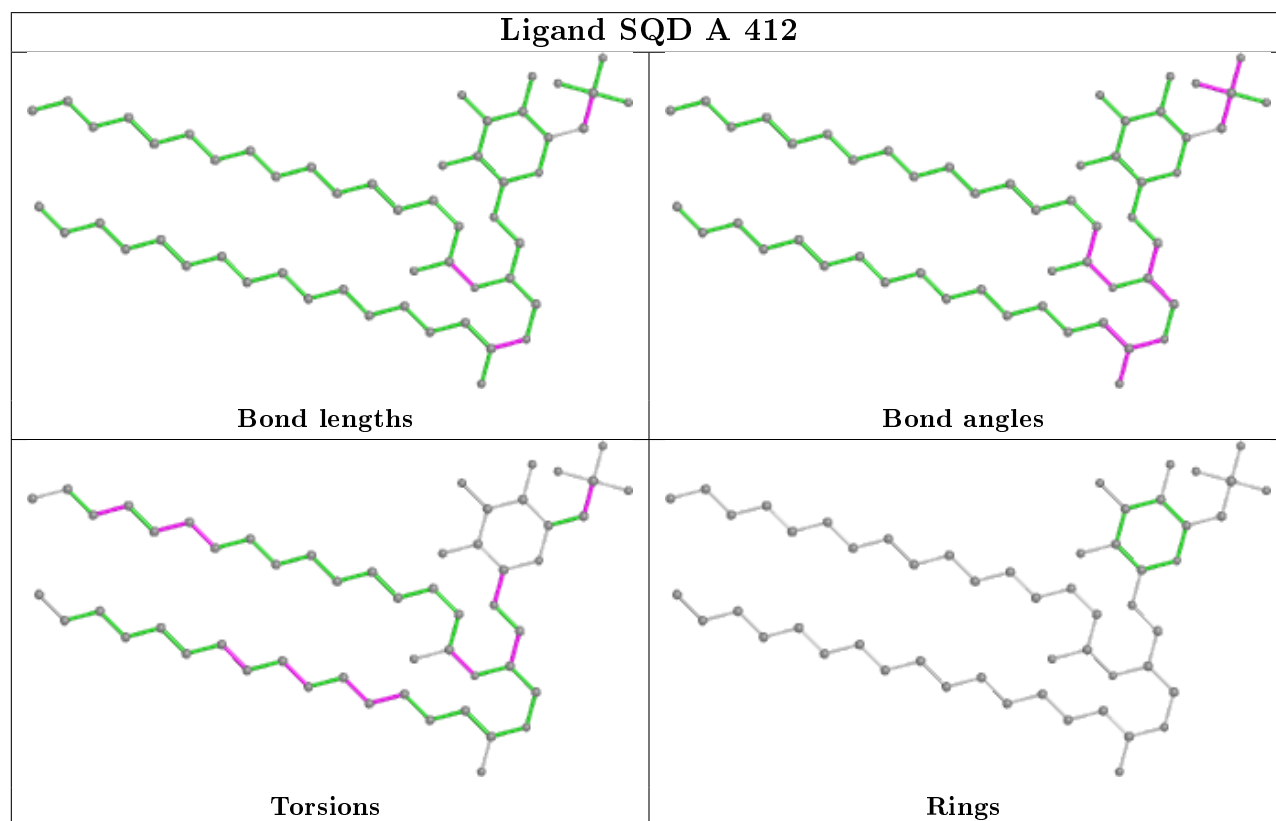
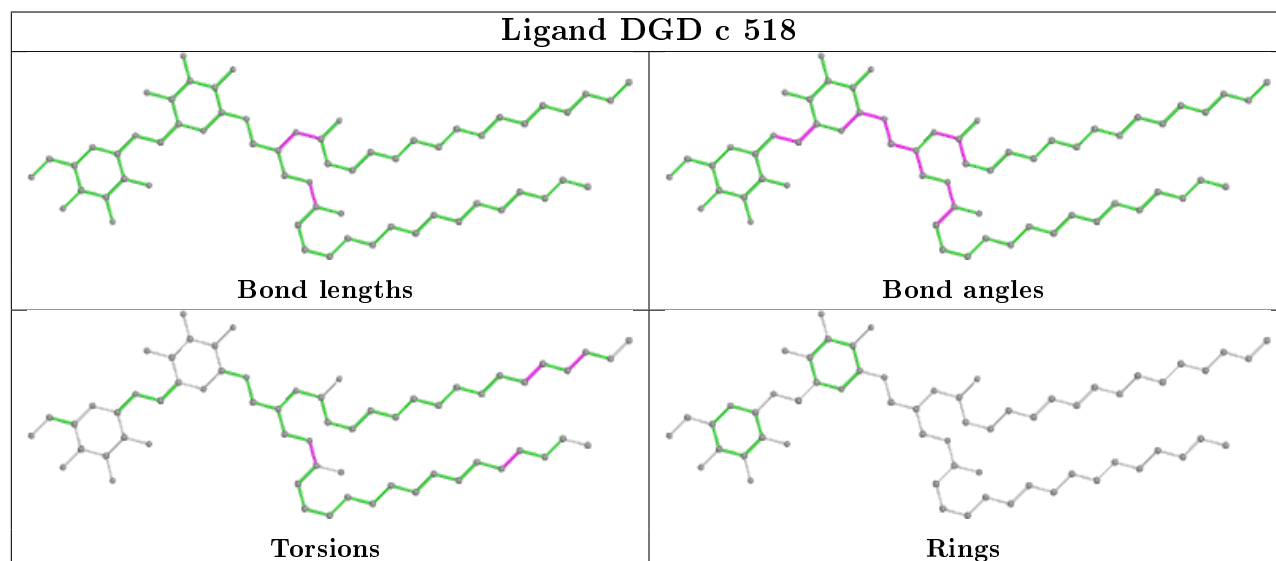
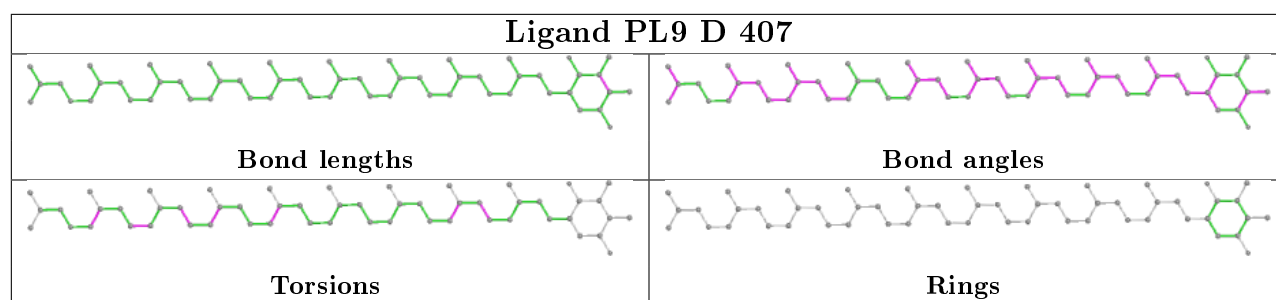


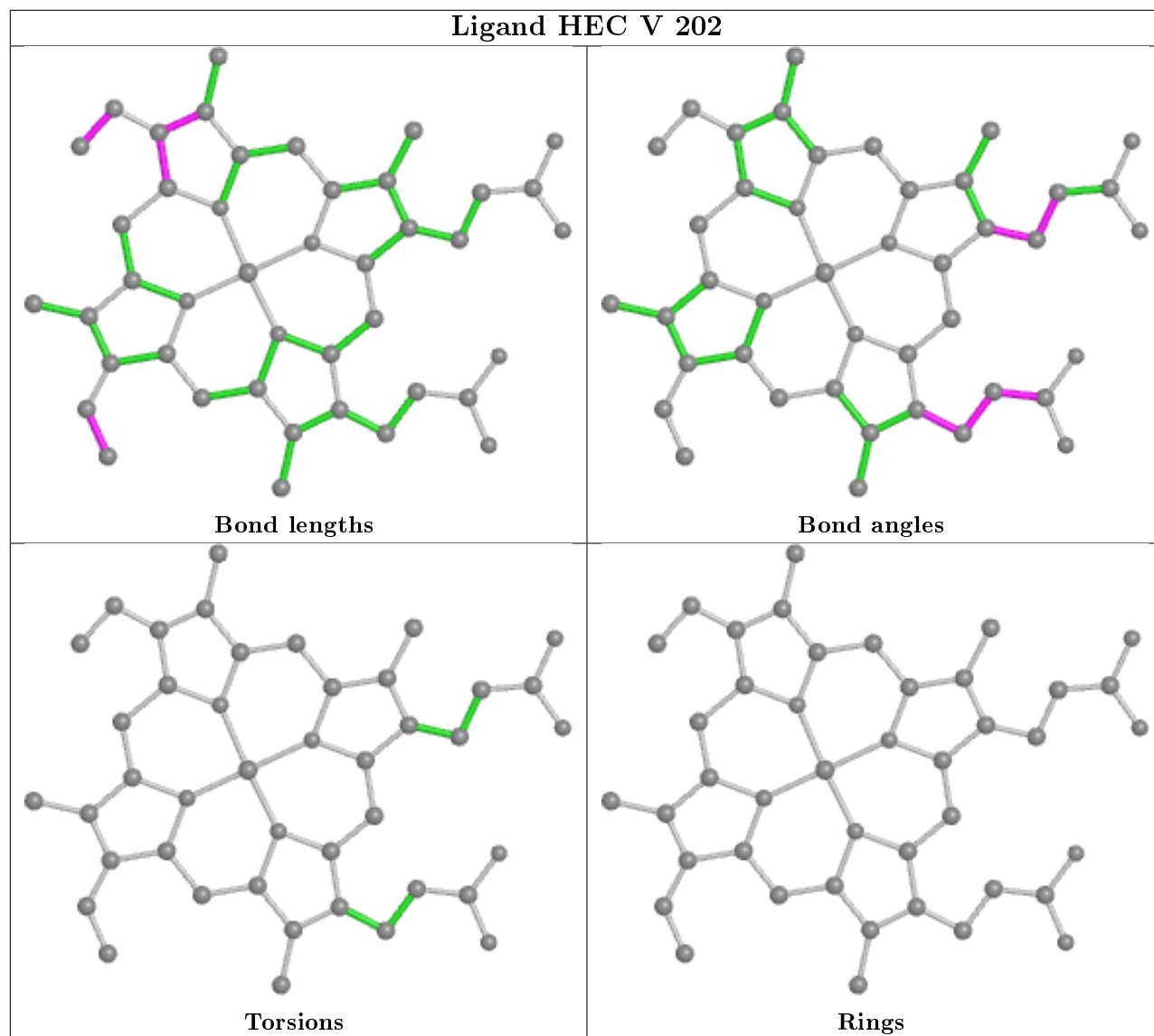
Ligand LMG b 620

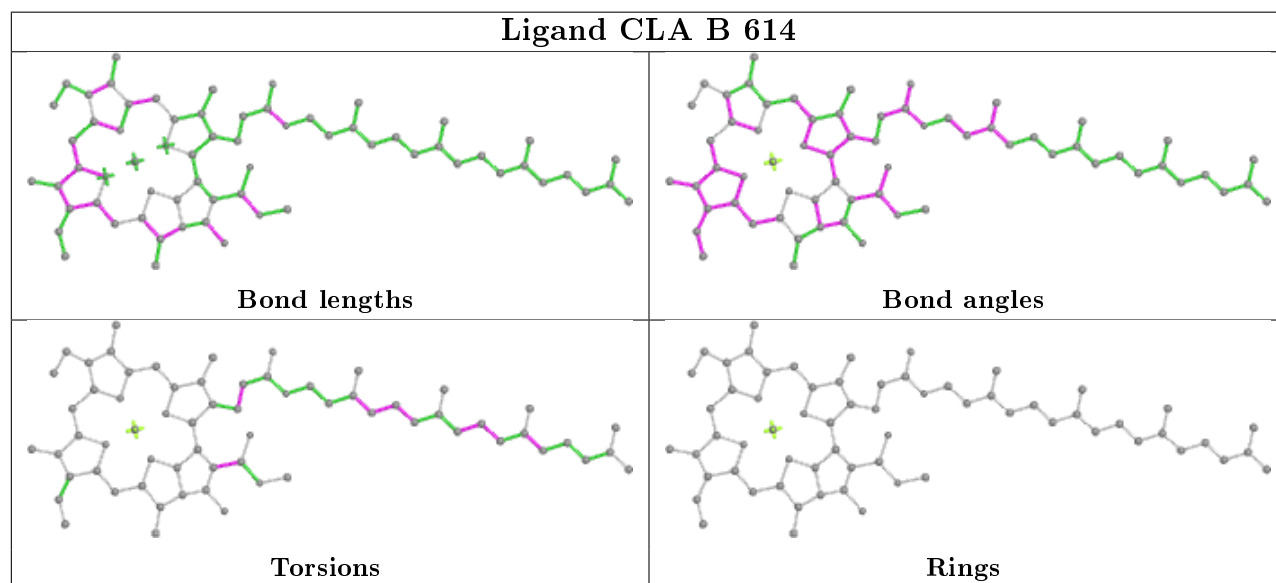
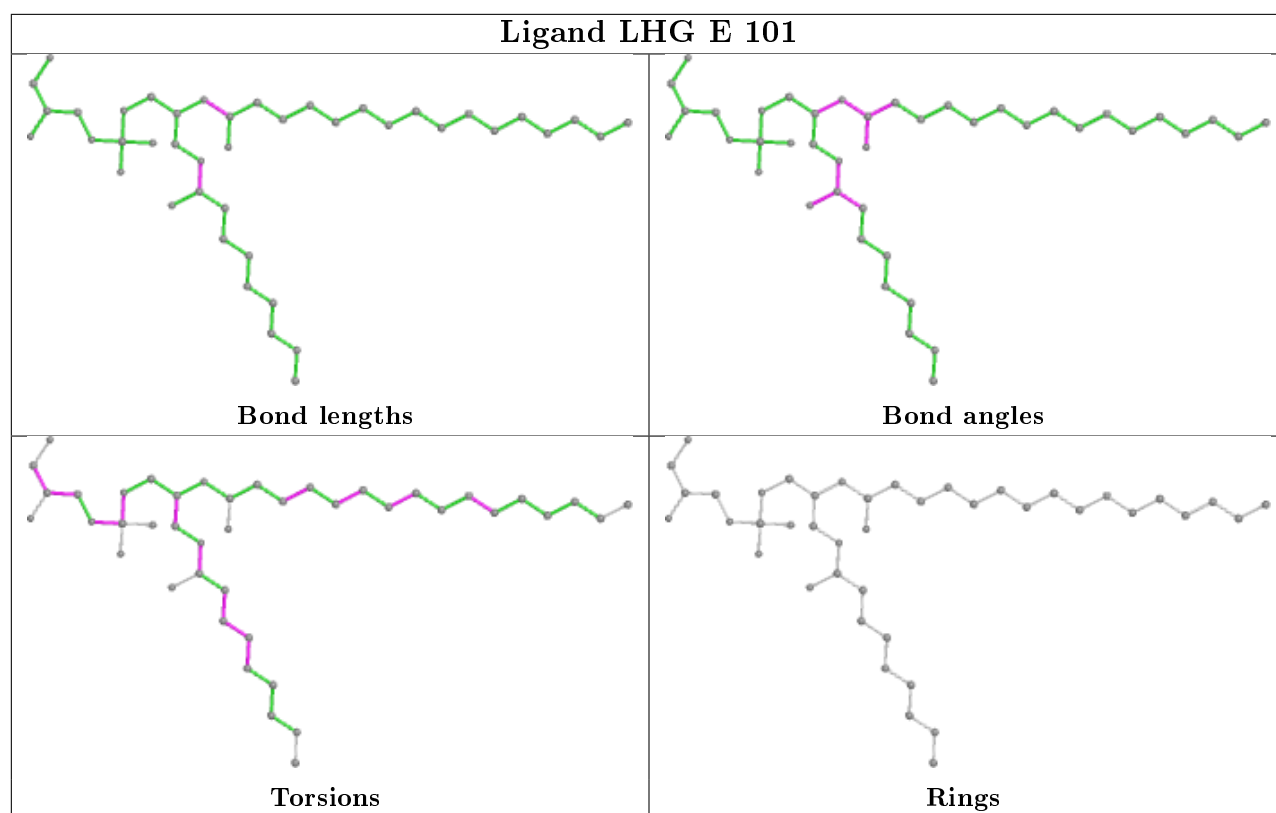


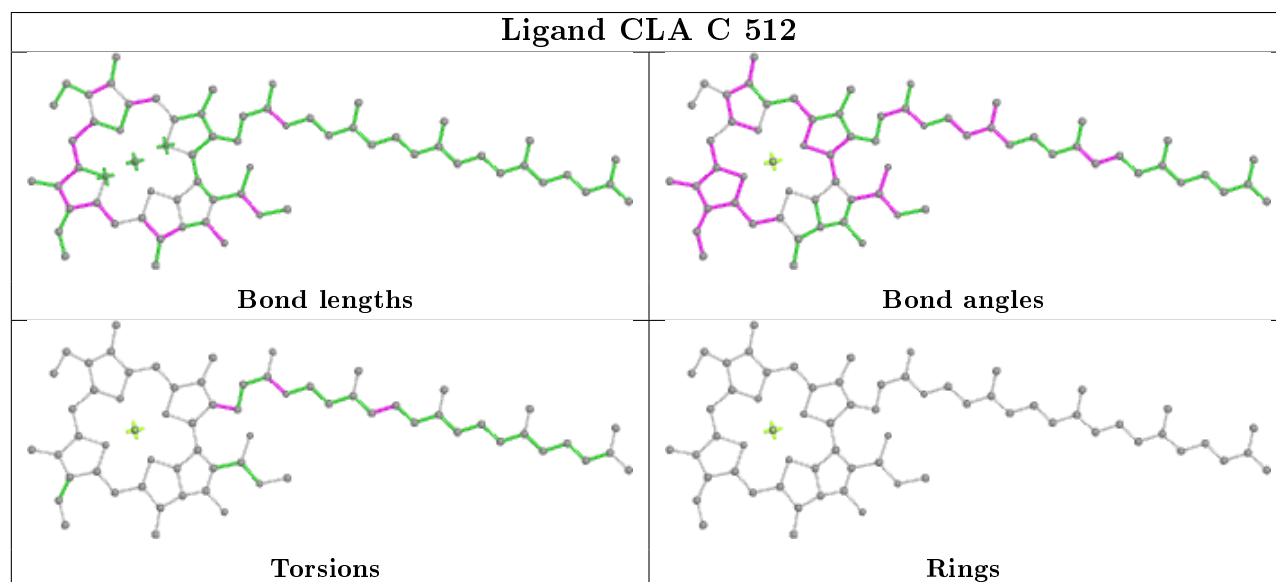
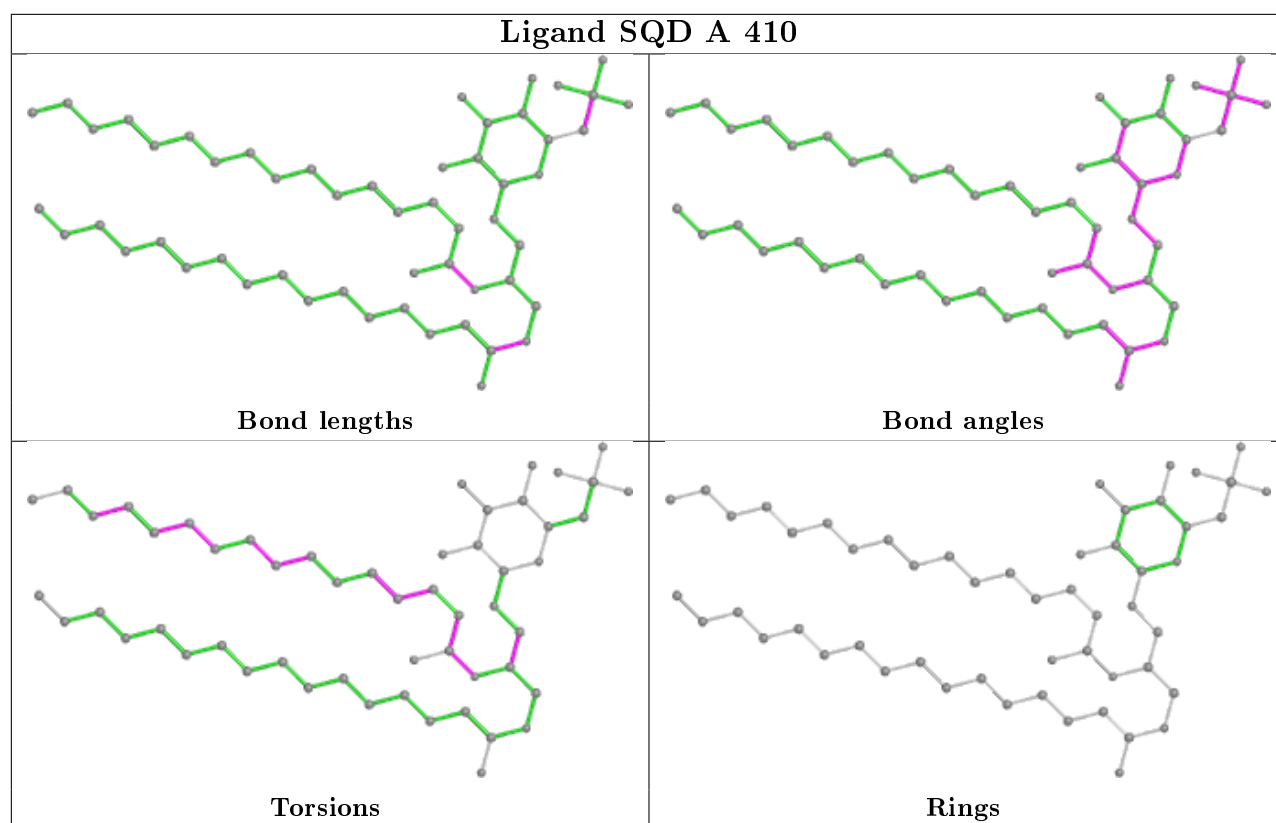
Ligand HTG c 522

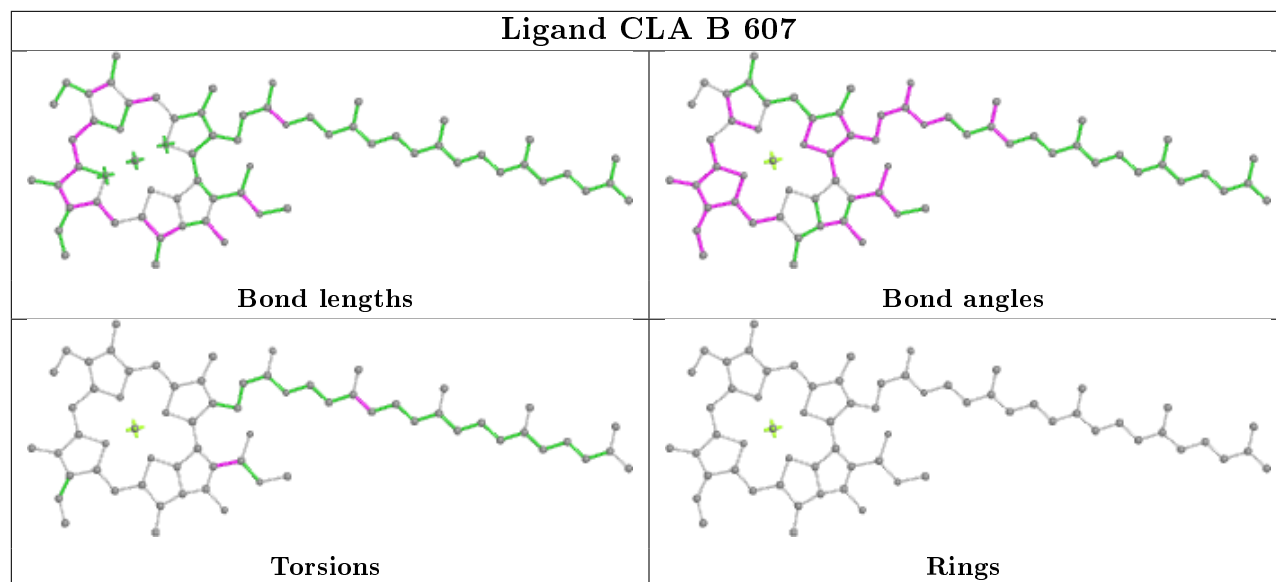
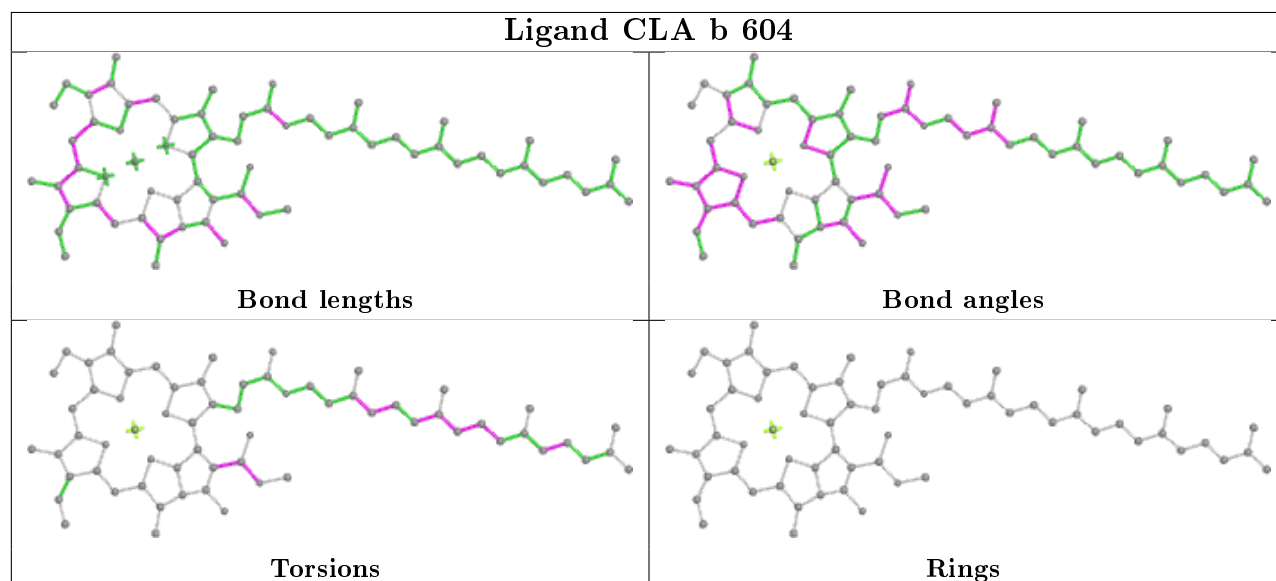
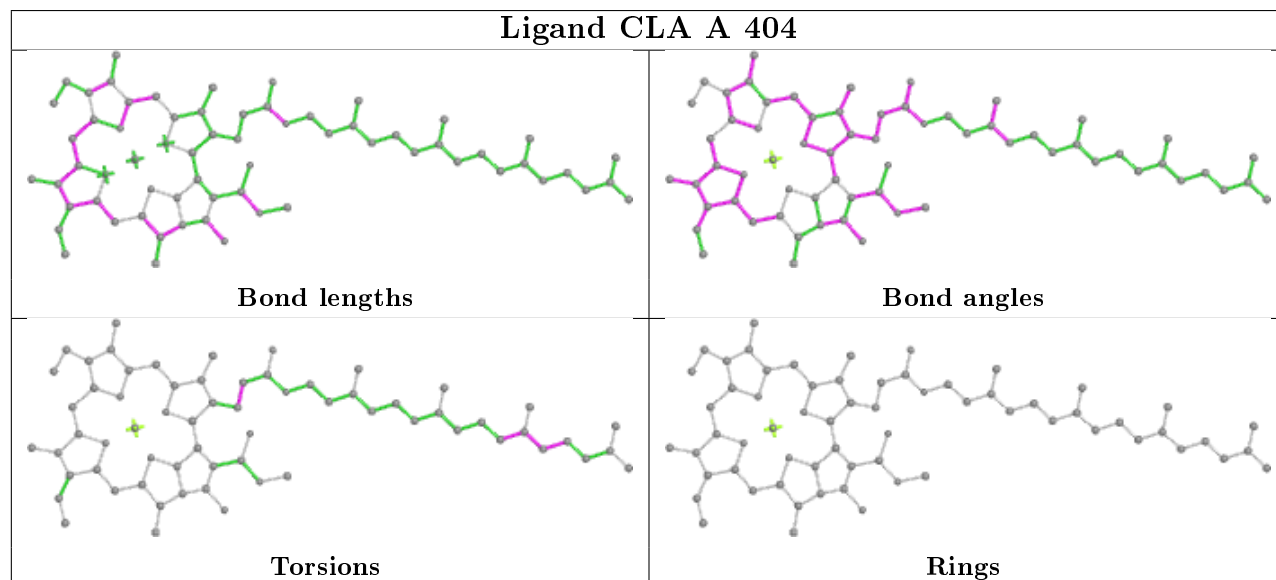




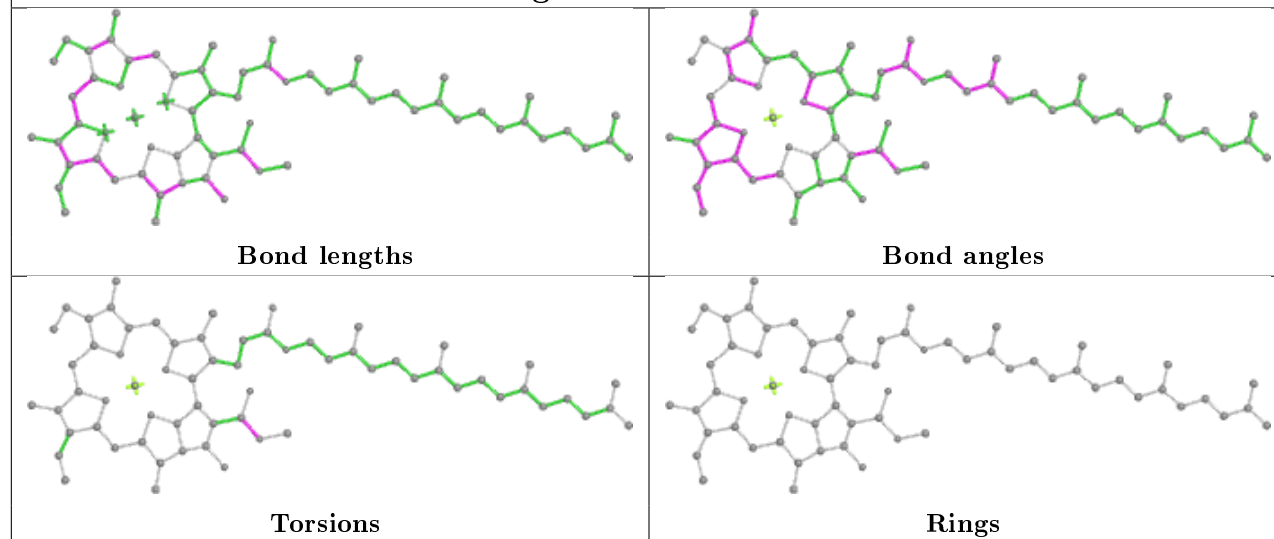




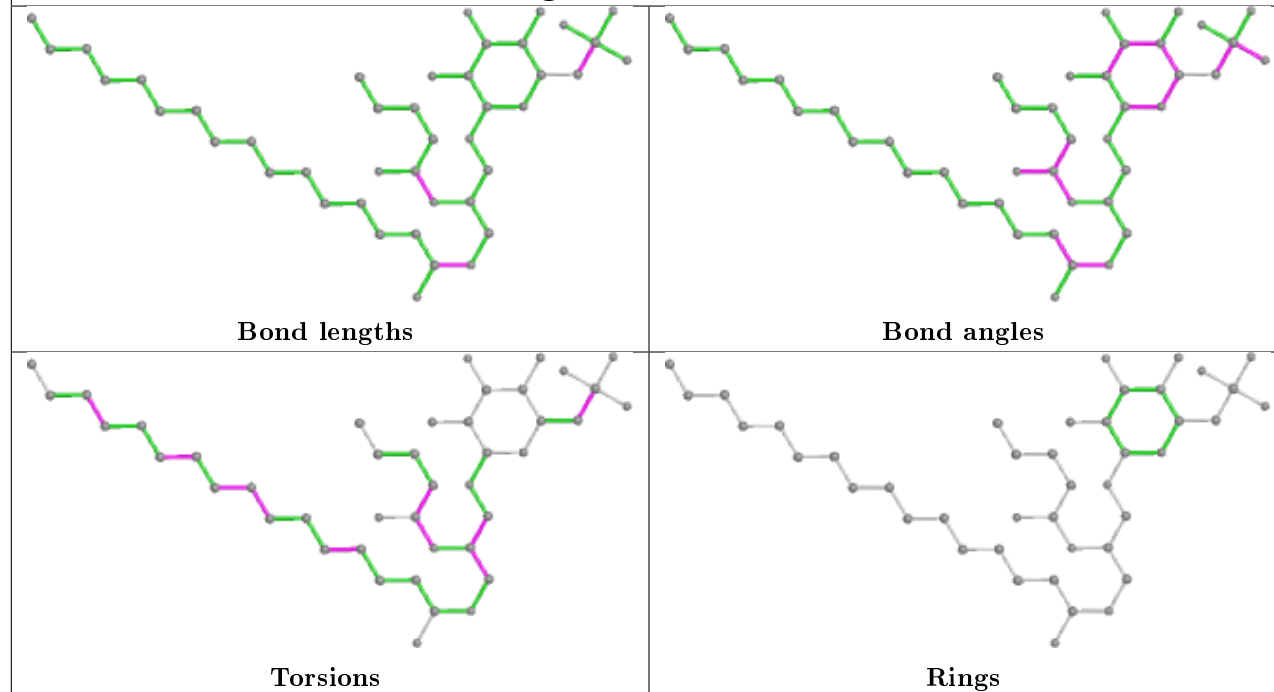


Ligand CLA B 607**Ligand CLA b 604****Ligand CLA A 404**

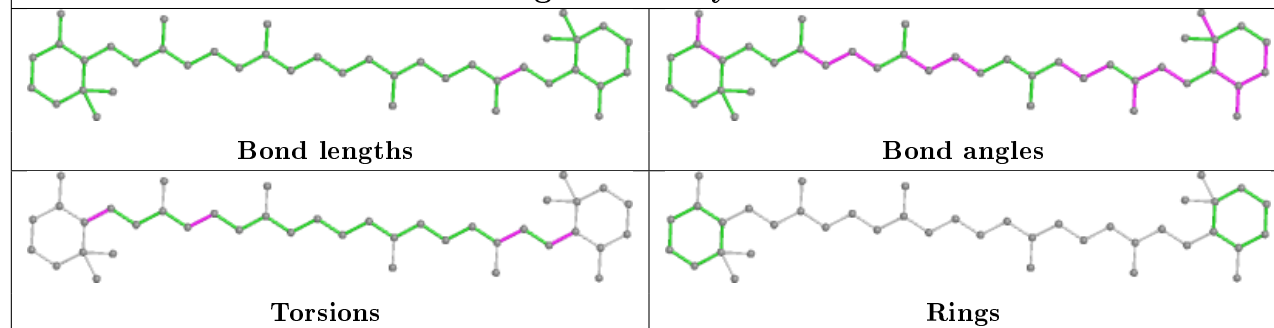
Ligand CLA C 504

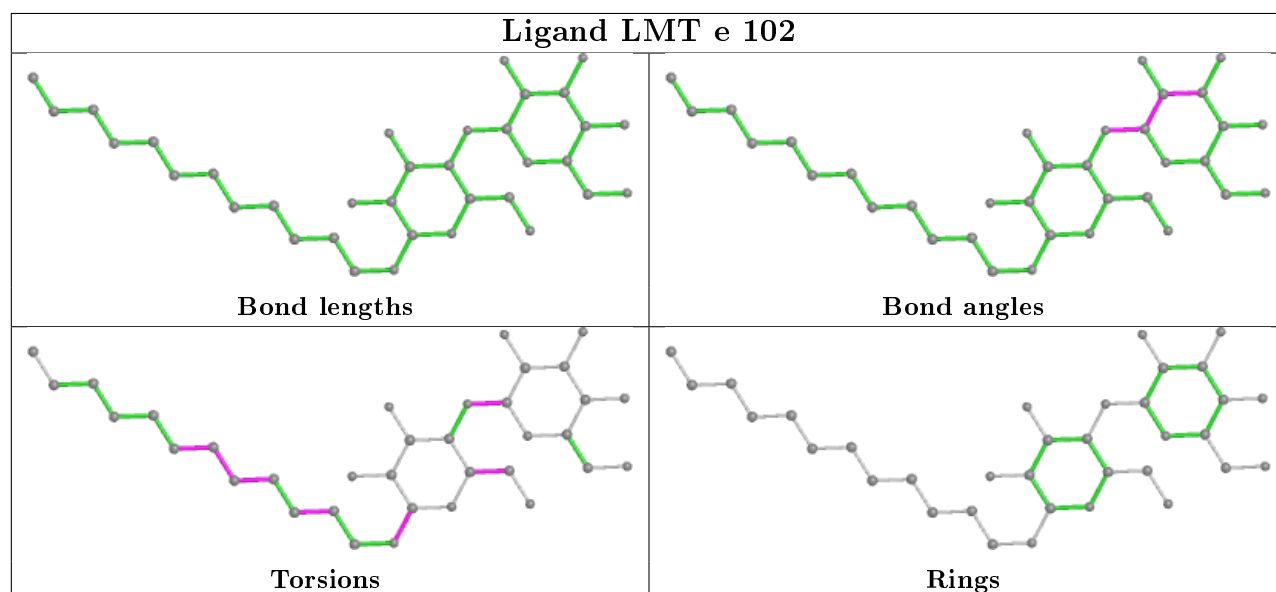
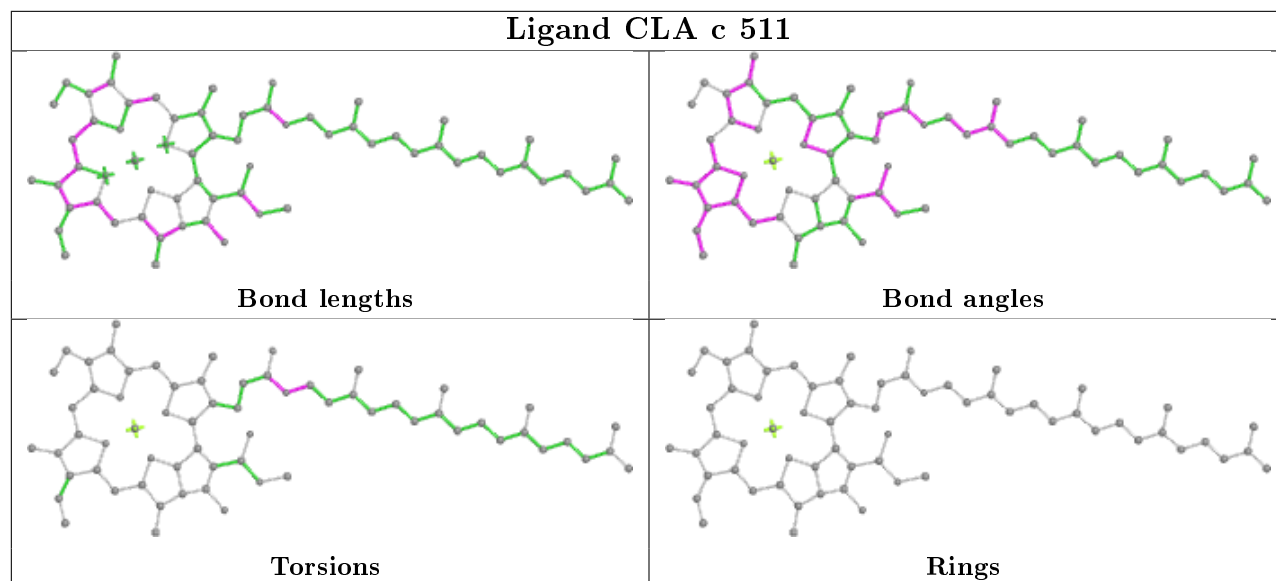
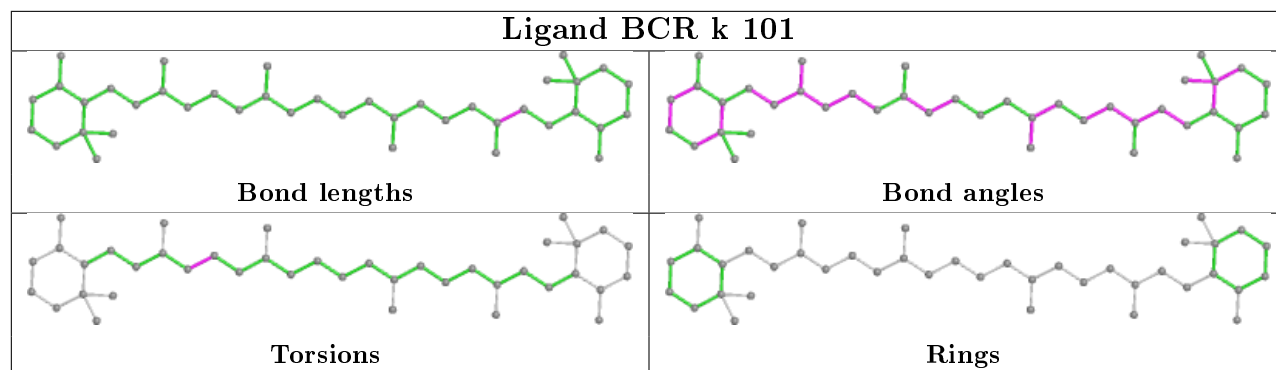


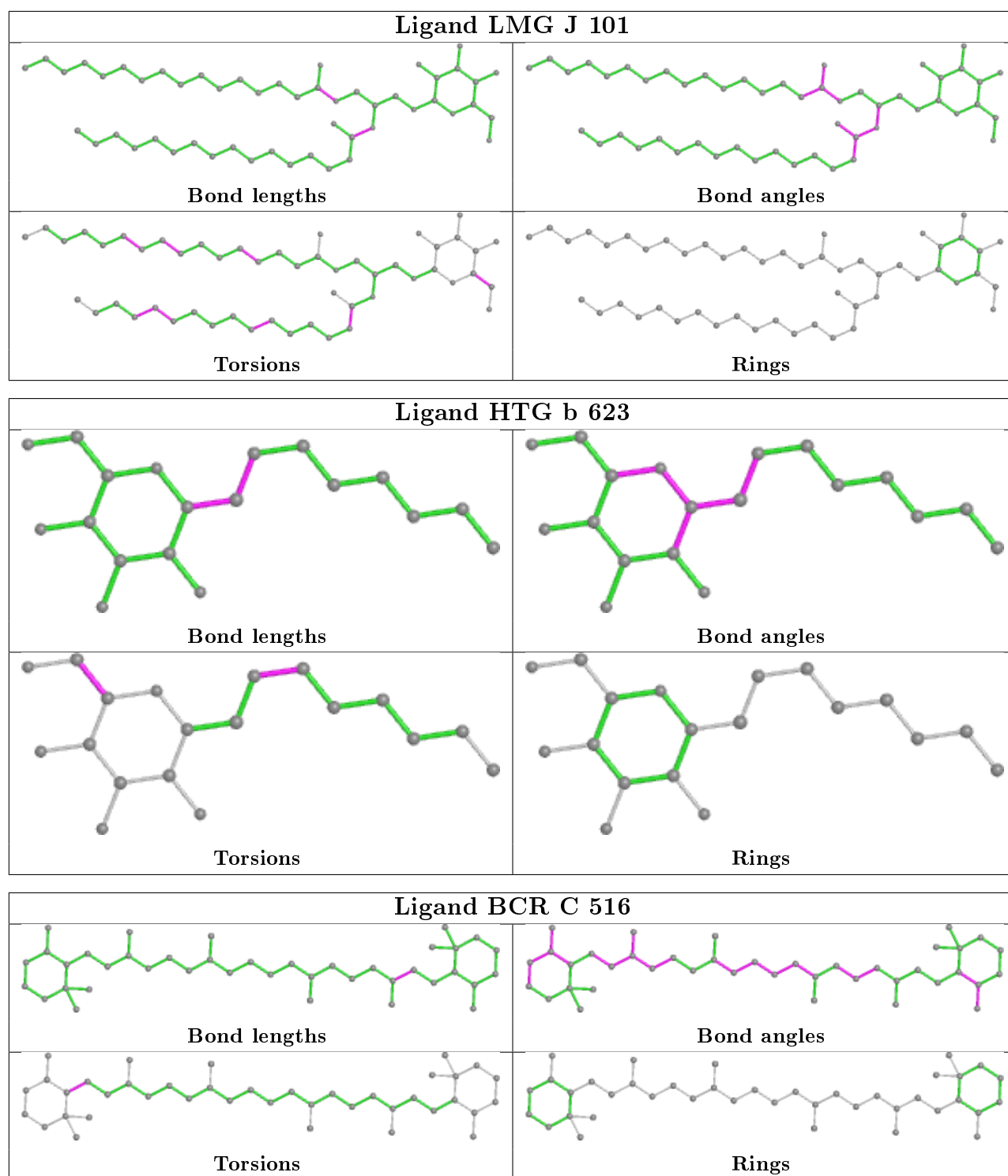
Ligand SQD f 101

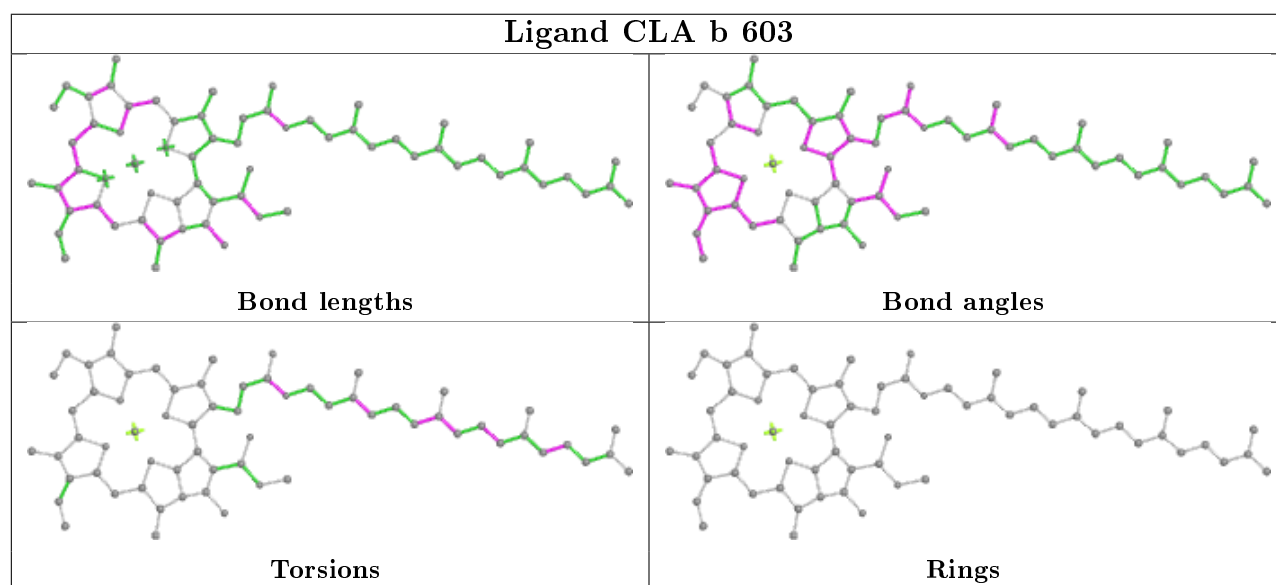
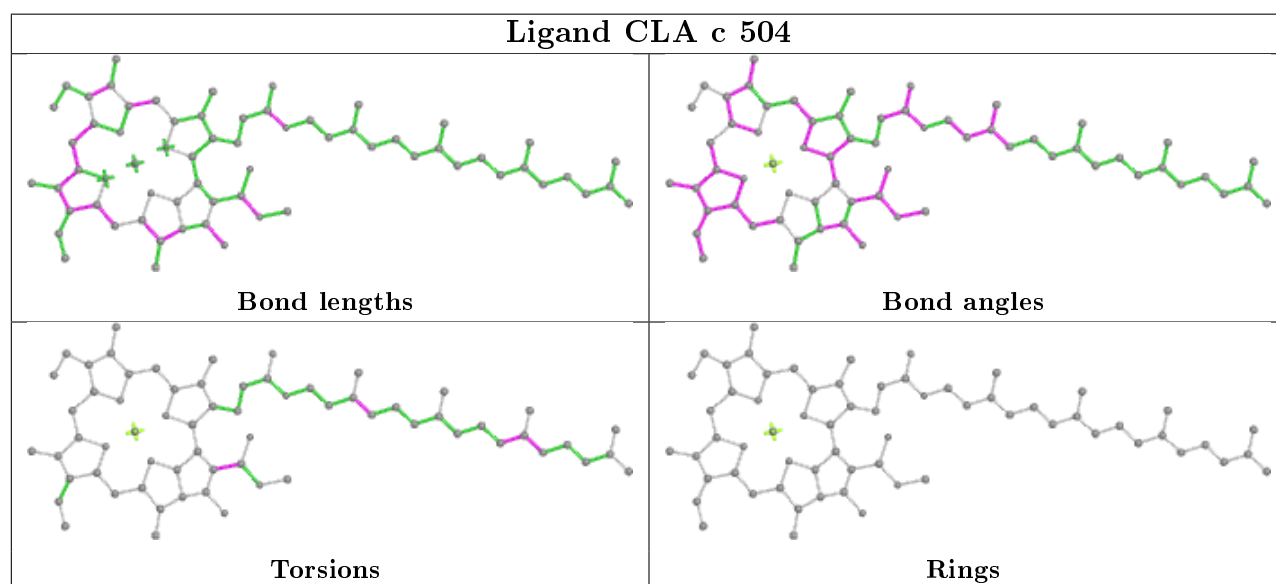
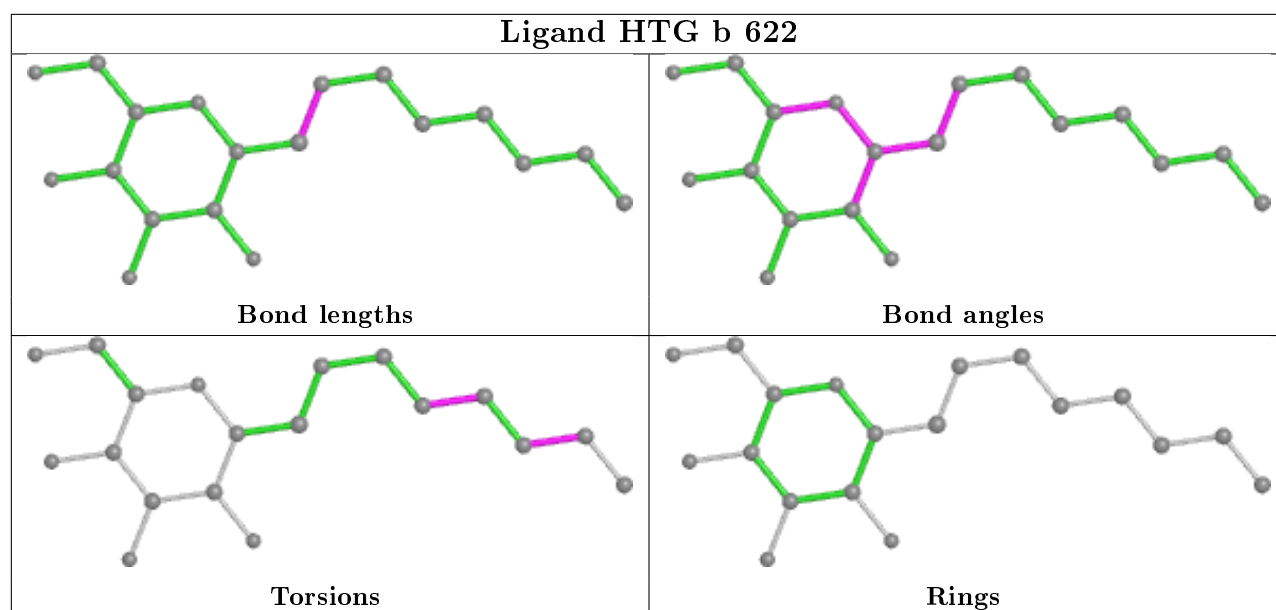


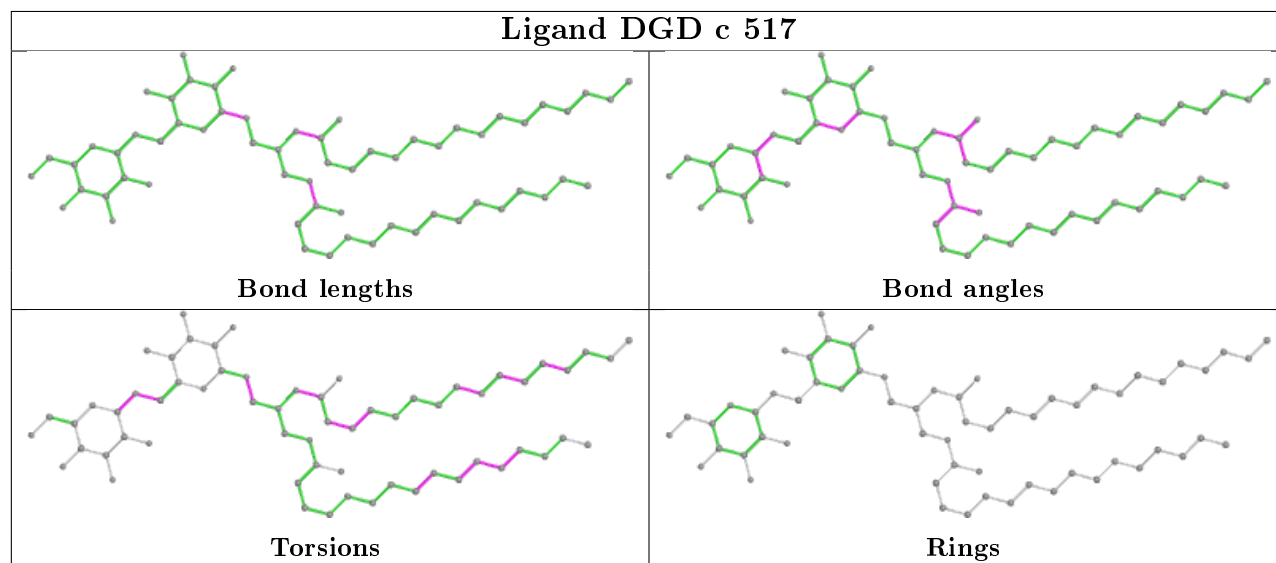
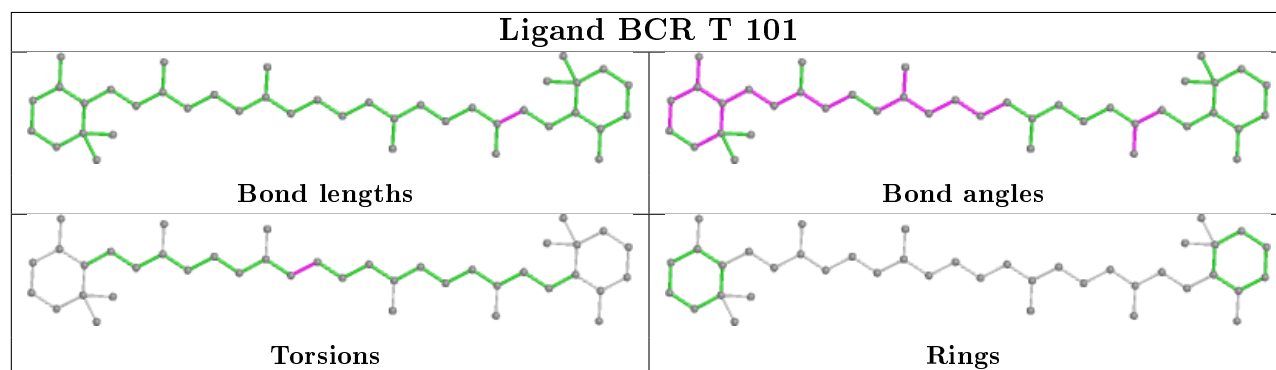
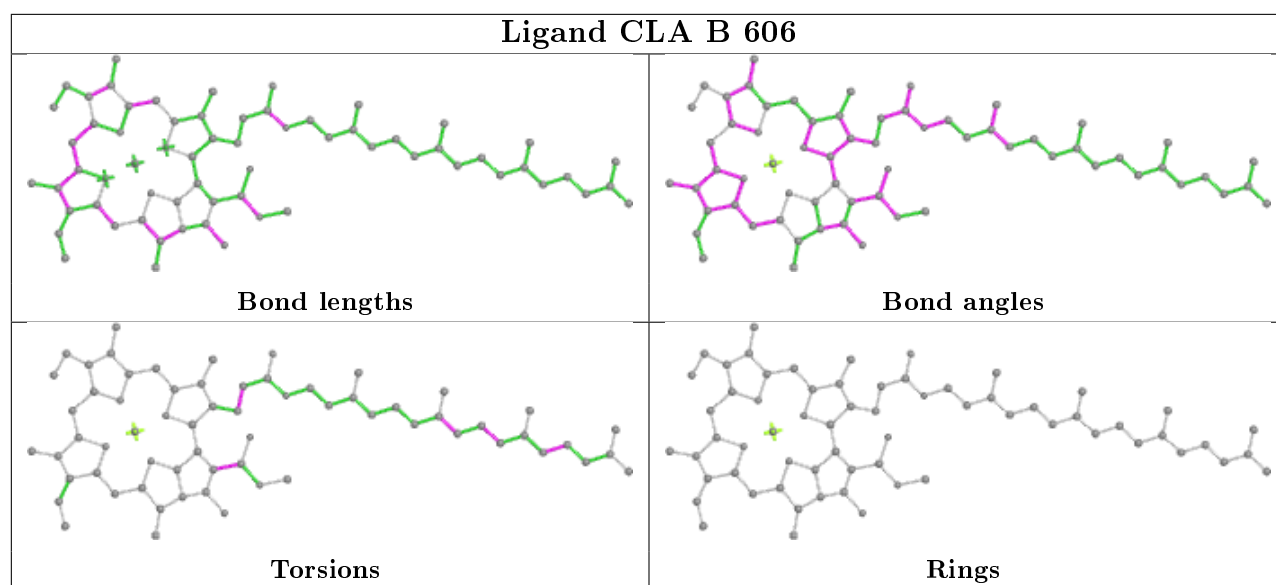
Ligand BCR y 101

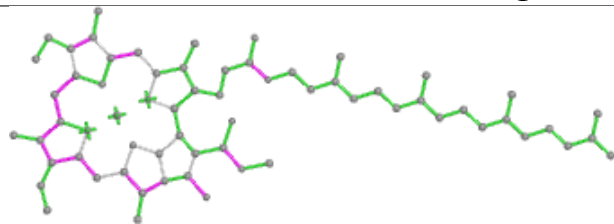
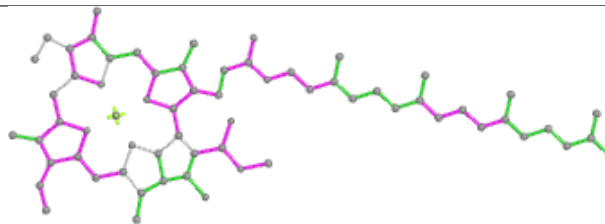
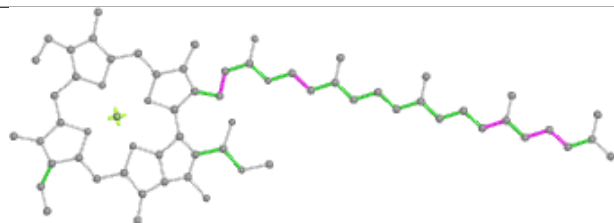
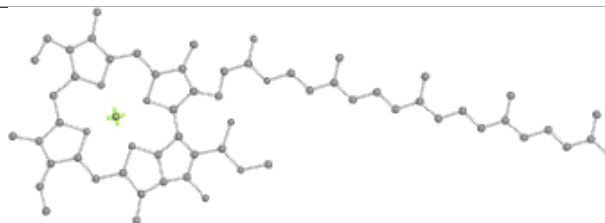
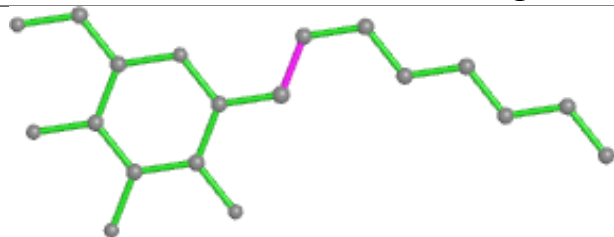
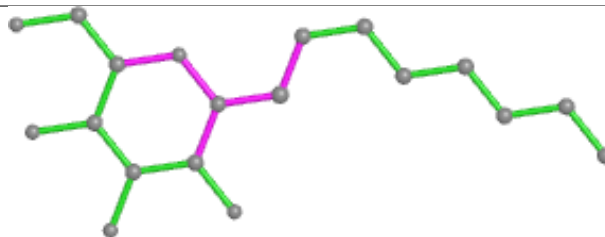
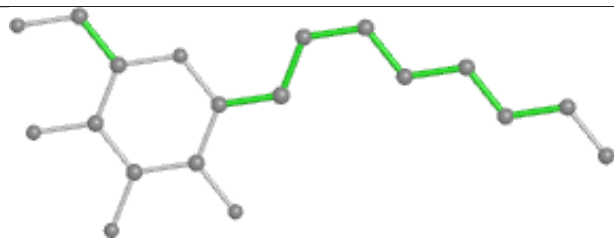
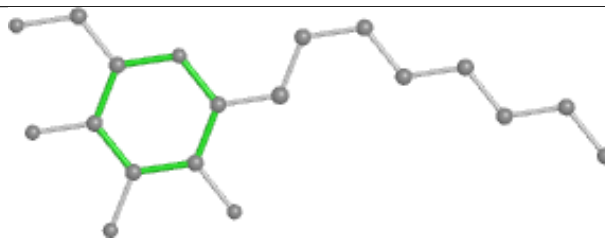


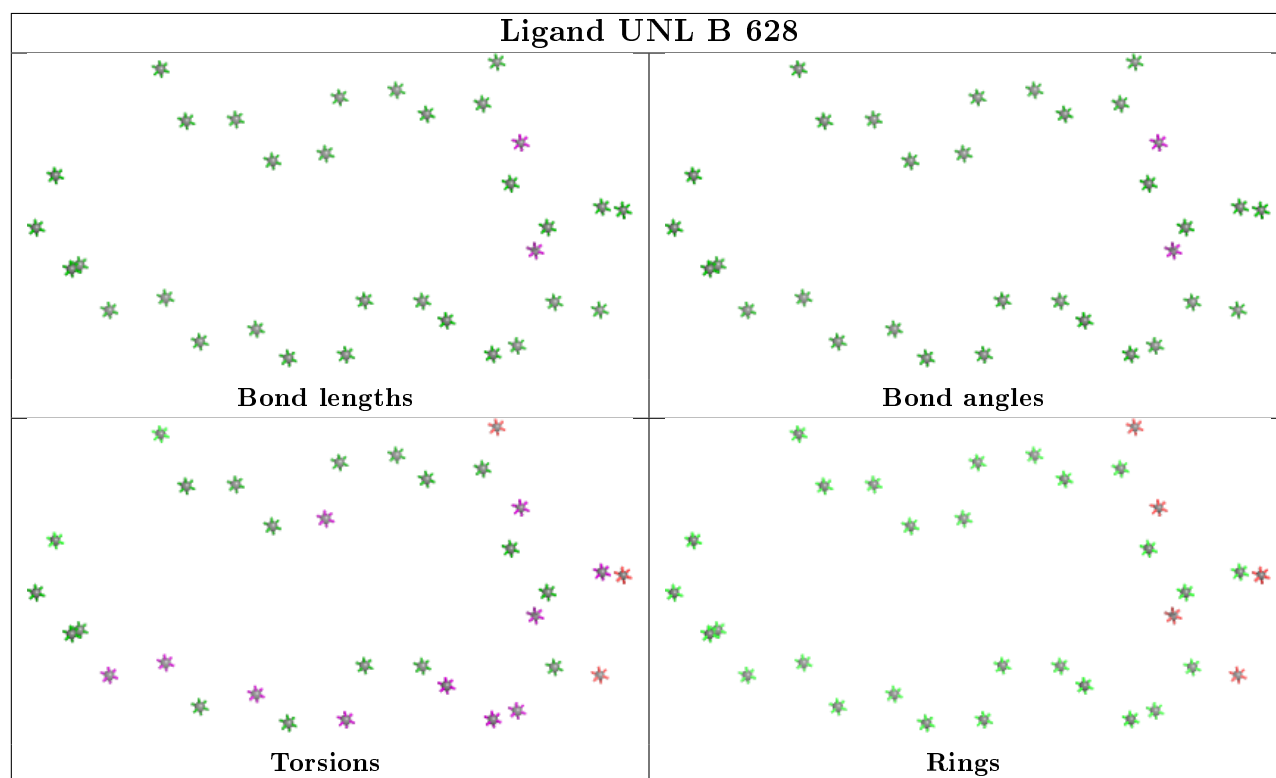
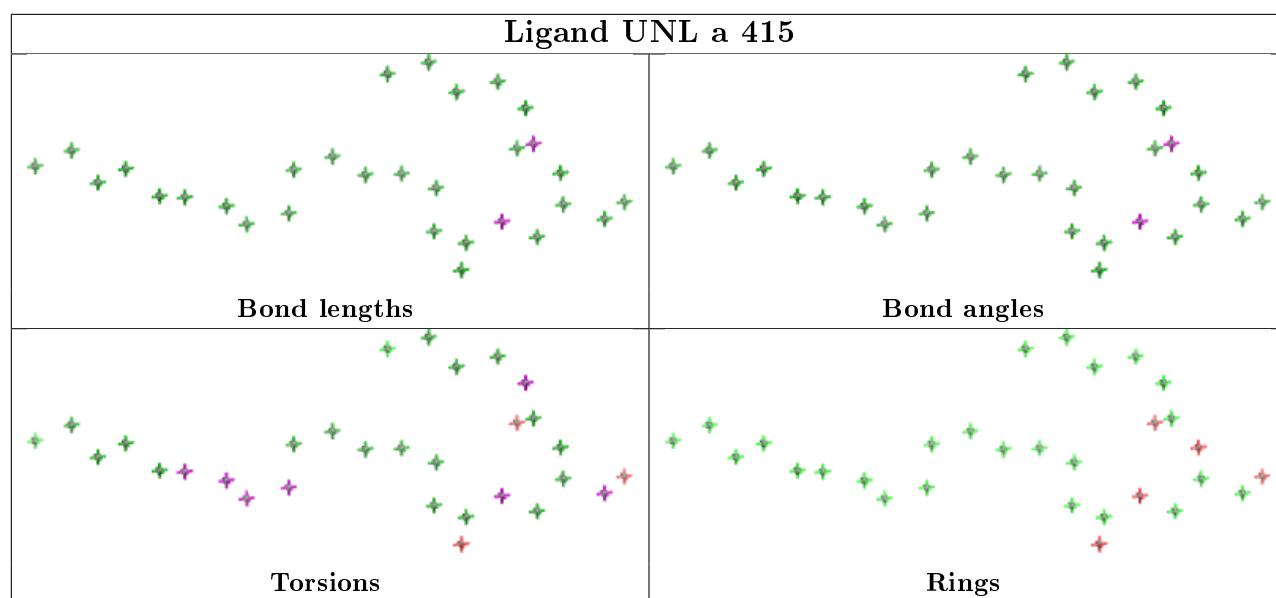


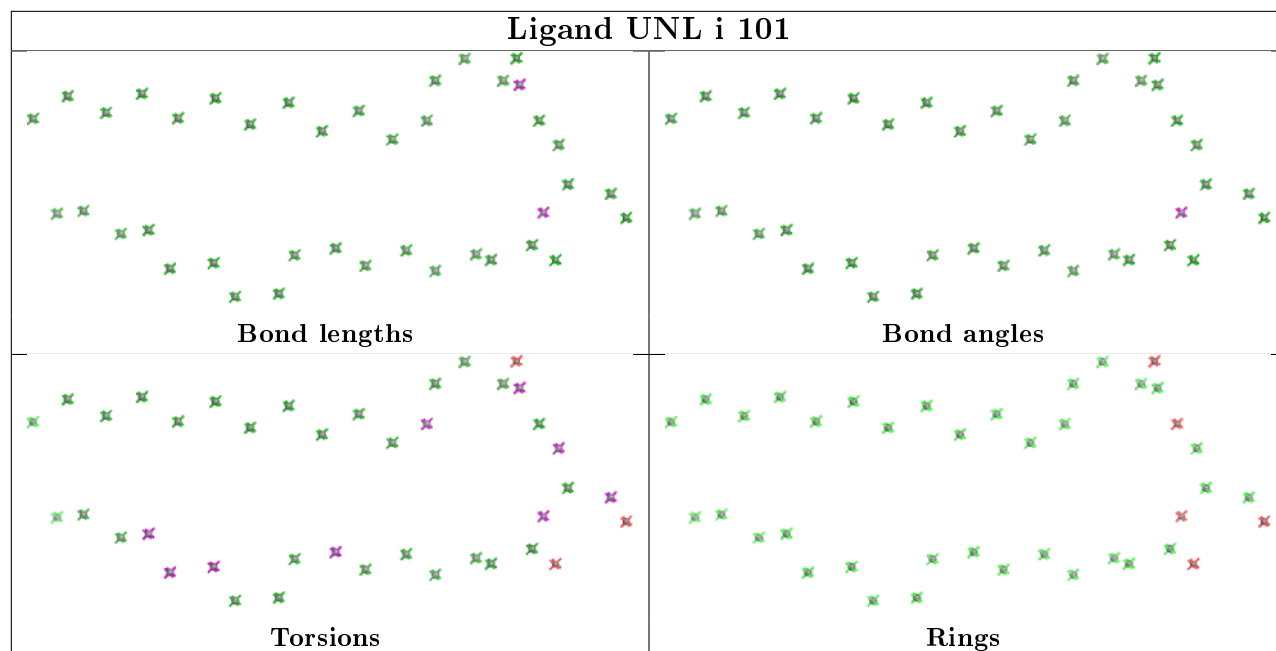
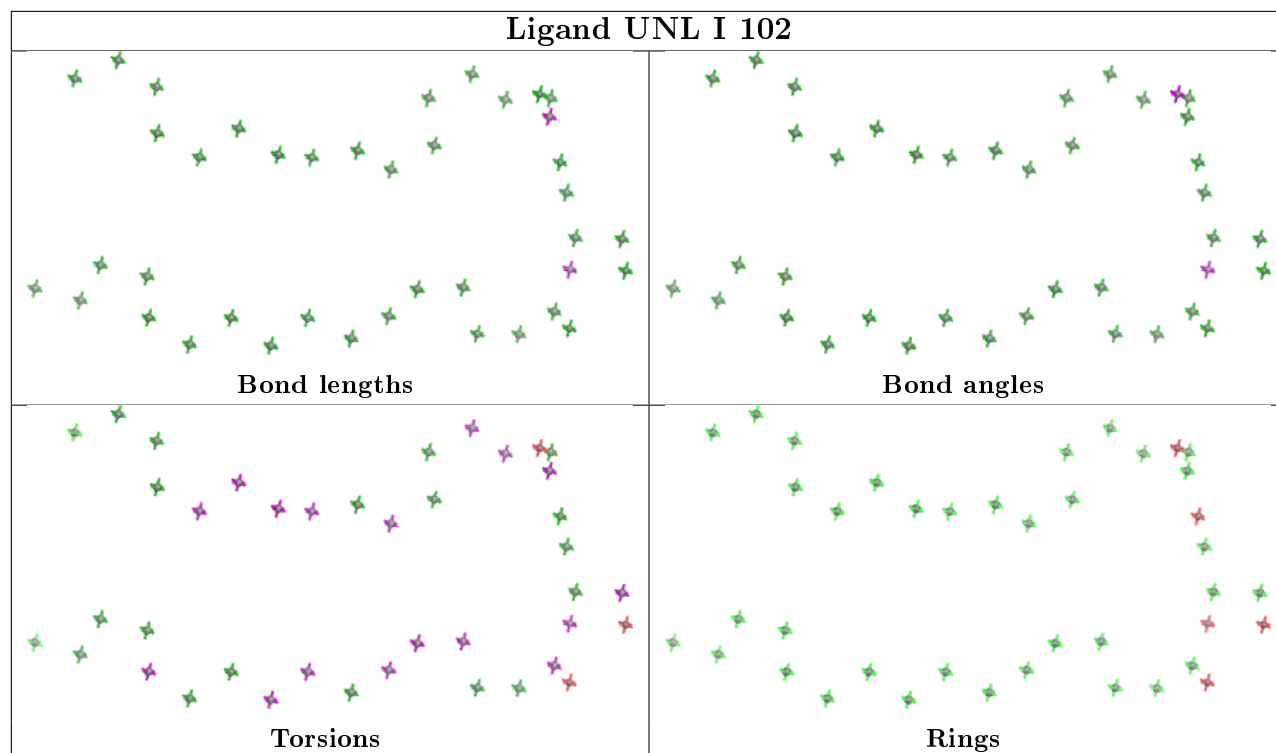


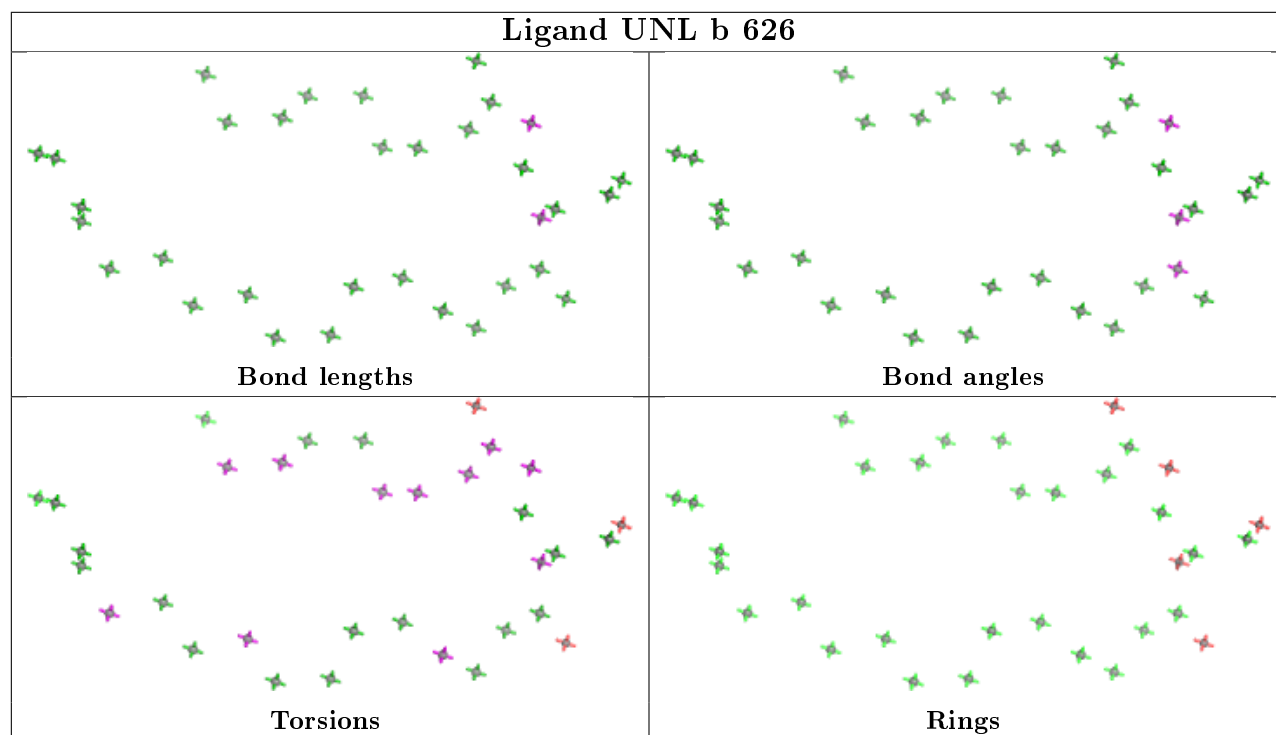
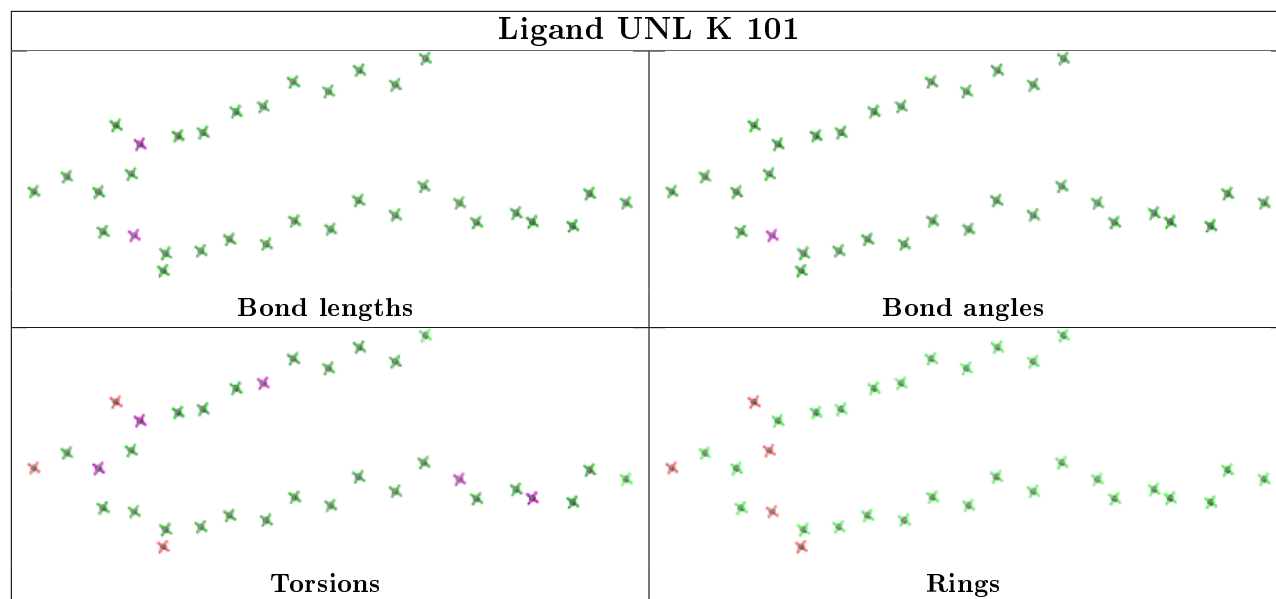


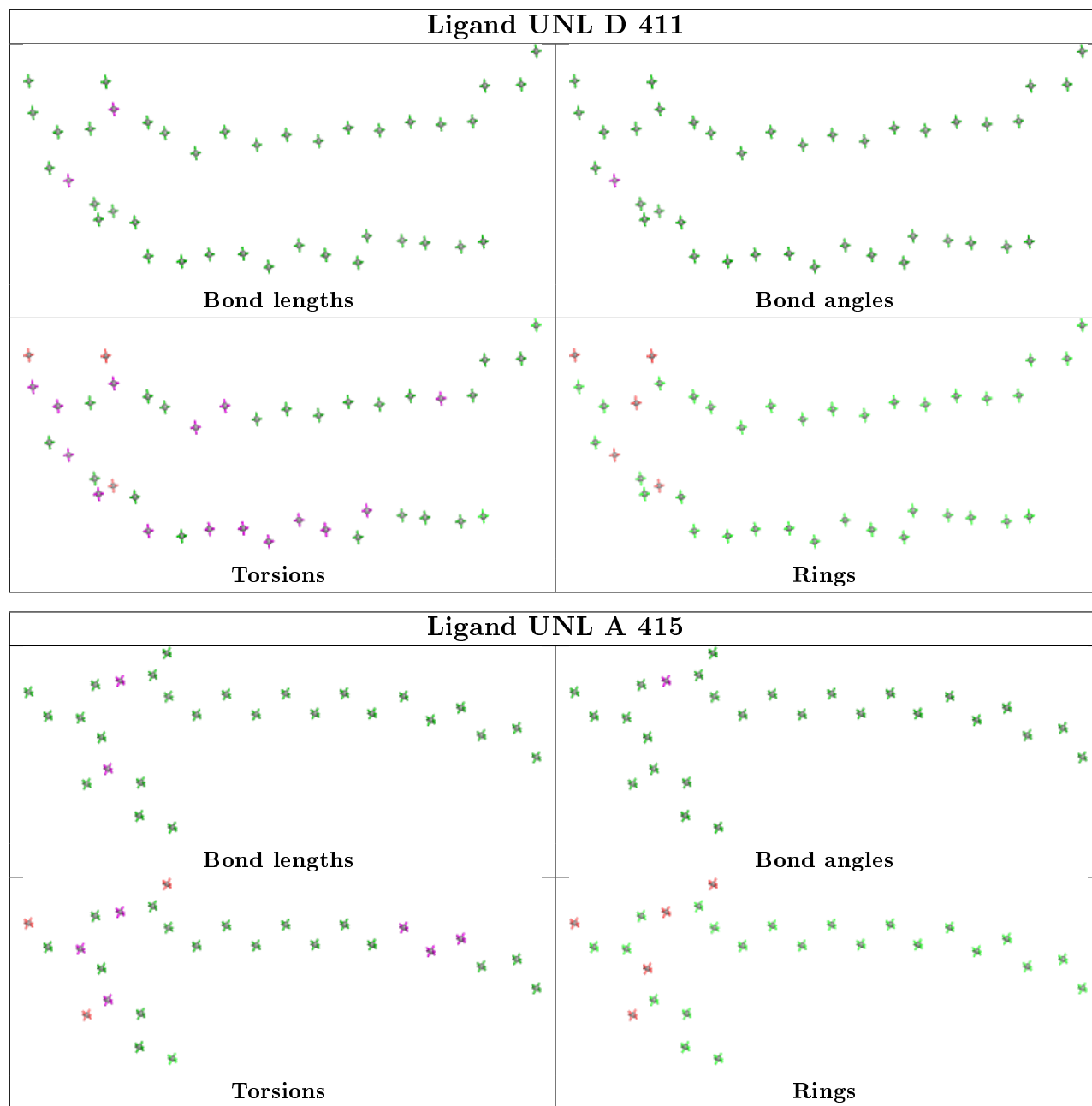


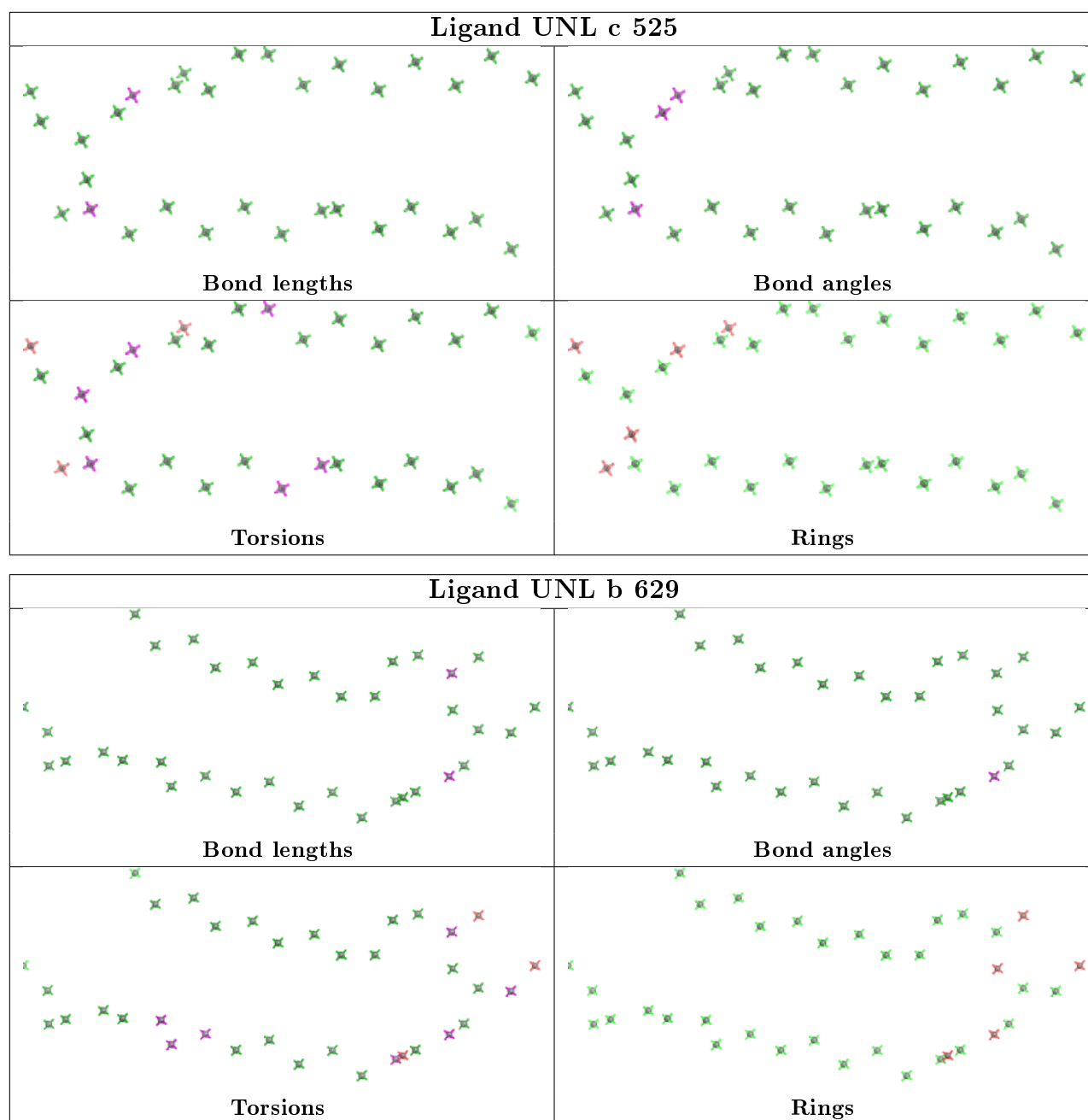
Ligand CLA B 602**Bond lengths****Bond angles****Torsions****Rings****Ligand HTG C 521****Bond lengths****Bond angles****Torsions****Rings**











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%)	-0.07	9 (2%) 54 58	21, 31, 53, 100	0
1	a	334/344 (97%)	0.08	11 (3%) 46 50	23, 33, 62, 108	0
2	B	504/505 (99%)	0.20	48 (9%) 8 8	21, 36, 65, 109	0
2	b	504/505 (99%)	0.35	57 (11%) 5 4	23, 37, 74, 118	0
3	C	451/455 (99%)	0.51	63 (13%) 2 2	26, 45, 67, 117	0
3	c	455/455 (100%)	0.31	47 (10%) 6 6	30, 48, 69, 109	0
4	D	342/342 (100%)	-0.04	7 (2%) 65 68	21, 32, 53, 108	0
4	d	341/342 (99%)	0.21	25 (7%) 15 15	23, 36, 54, 123	0
5	E	81/84 (96%)	0.20	7 (8%) 10 10	37, 54, 82, 120	0
5	e	79/84 (94%)	1.05	19 (24%) 0 0	42, 58, 97, 120	0
6	F	34/44 (77%)	-0.22	0 100 100	38, 46, 78, 92	0
6	f	31/44 (70%)	-0.20	3 (9%) 7 7	44, 50, 86, 122	0
7	H	64/65 (98%)	0.26	5 (7%) 13 13	34, 47, 68, 101	0
7	h	65/65 (100%)	1.07	16 (24%) 0 0	37, 51, 74, 141	0
8	I	37/38 (97%)	0.42	7 (18%) 1 1	37, 46, 88, 130	0
8	i	37/38 (97%)	0.22	3 (8%) 12 12	38, 46, 93, 135	0
9	J	38/39 (97%)	0.20	5 (13%) 3 3	32, 52, 106, 147	0
9	j	39/39 (100%)	0.73	9 (23%) 0 0	40, 51, 107, 129	0
10	K	37/37 (100%)	0.01	3 (8%) 12 12	44, 53, 76, 91	0
10	k	37/37 (100%)	0.29	2 (5%) 25 27	47, 54, 78, 93	0
11	L	36/37 (97%)	0.56	7 (19%) 1 1	20, 26, 89, 129	0
11	l	36/37 (97%)	0.21	3 (8%) 11 11	22, 28, 87, 128	0
12	M	32/36 (88%)	-0.04	1 (3%) 49 52	22, 29, 49, 117	0
12	m	33/36 (91%)	-0.25	3 (9%) 9 9	24, 29, 72, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.25	28 (11%) 4 4	22, 45, 100, 157	0
13	o	243/244 (99%)	0.61	49 (20%) 1 0	24, 46, 99, 144	0
14	T	29/32 (90%)	0.21	0 100 100	23, 28, 60, 96	0
14	t	29/32 (90%)	-0.14	0 100 100	23, 29, 61, 97	0
15	U	96/104 (92%)	0.46	13 (13%) 3 2	31, 40, 66, 84	0
15	u	97/104 (93%)	-0.17	6 (6%) 20 21	32, 43, 68, 101	0
16	V	137/137 (100%)	0.08	2 (1%) 73 75	29, 43, 70, 100	0
16	v	137/137 (100%)	0.45	20 (14%) 2 2	34, 50, 74, 101	0
17	X	38/40 (95%)	0.20	3 (7%) 12 12	44, 56, 82, 110	0
17	x	38/40 (95%)	1.14	9 (23%) 0 0	47, 58, 83, 112	0
18	Y	29/30 (96%)	1.74	12 (41%) 0 0	56, 71, 112, 114	0
18	y	29/30 (96%)	0.94	5 (17%) 1 1	58, 70, 110, 114	0
19	Z	62/62 (100%)	1.06	14 (22%) 0 0	57, 72, 117, 152	0
19	z	62/62 (100%)	1.32	16 (25%) 0 0	60, 74, 117, 153	0
20	R	34/34 (100%)	6.04	34 (100%) 0 0	89, 108, 128, 135	0
All	All	5284/5384 (98%)	0.33	571 (10%) 5 5	20, 41, 82, 157	0

The worst 5 of 571 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	10.4
20	R	35	LEU	9.1
20	R	20	VAL	8.8
20	R	19	ALA	8.7
9	J	5	GLY	8.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	m	1	10/11	0.96	0.11	30,42,63,78	0
8	FME	i	1	10/11	0.97	0.09	37,49,57,62	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	0.97	0.16	18,38,70,79	0
14	FME	T	1	10/11	0.98	0.08	18,32,46,47	0
14	FME	t	1	10/11	0.98	0.10	21,32,41,71	0
8	FME	I	1	10/11	0.98	0.22	31,47,56,62	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
30	UNL	A	415	28/-	0.19	0.56	67,87,108,112	0
35	LMT	B	630	35/35	0.55	0.46	33,105,126,134	0
34	HTG	D	412	16/19	0.55	0.43	48,115,128,130	0
30	UNL	b	626	33/-	0.58	0.44	44,78,131,135	0
33	LMG	Z	101	51/55	0.59	0.43	46,105,140,150	0
35	LMT	I	101	35/35	0.59	0.65	74,108,131,141	0
30	UNL	a	415	30/-	0.61	0.50	72,90,111,118	0
34	HTG	b	623	19/19	0.62	0.65	71,109,141,169	0
34	HTG	B	624	19/19	0.63	0.68	57,104,140,144	0
35	LMT	D	402	35/35	0.65	0.37	31,97,113,115	0
35	LMT	e	102	35/35	0.66	0.79	76,134,147,156	0
29	PL9	a	414	55/55	0.67	0.40	57,93,112,120	0
34	HTG	C	522	19/19	0.67	0.91	58,139,157,179	0
30	UNL	B	628	33/-	0.67	0.28	29,76,136,139	0
35	LMT	M	103	35/35	0.68	0.34	40,120,148,154	0
35	LMT	M	101	35/35	0.69	0.35	39,80,103,109	0
35	LMT	m	102	35/35	0.70	0.47	34,78,102,109	0
25	BCR	h	101	40/40	0.70	0.27	39,50,64,77	0
33	LMG	c	520	51/55	0.70	0.36	51,102,132,138	0
29	PL9	A	414	55/55	0.71	0.40	41,88,105,119	0
30	UNL	J	102	10/-	0.71	0.39	55,64,89,90	0
30	UNL	i	101	40/-	0.71	0.42	48,88,140,147	0
30	UNL	K	101	34/-	0.72	0.34	55,96,114,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	LMT	E	102	35/35	0.72	0.55	78,120,147,150	0
30	UNL	I	102	40/-	0.73	0.31	40,85,135,142	0
31	LHG	e	101	42/49	0.73	0.41	81,118,142,148	0
30	UNL	j	102	10/-	0.74	0.30	60,75,88,89	0
34	HTG	c	522	19/19	0.74	0.85	79,124,142,146	0
30	UNL	m	101	10/-	0.74	0.30	40,50,55,56	0
33	LMG	Z	102	37/55	0.74	0.38	47,97,129,137	0
30	UNL	c	525	32/-	0.75	0.30	71,97,113,119	0
34	HTG	B	623	19/19	0.76	0.40	60,84,110,115	0
34	HTG	b	622	19/19	0.76	0.88	74,95,125,130	0
26	SQD	f	101	43/54	0.77	0.36	85,111,157,164	0
26	SQD	L	101	54/54	0.77	0.27	47,71,116,121	0
34	HTG	d	411	16/19	0.77	0.38	81,112,121,122	0
35	LMT	b	621	25/35	0.78	0.24	60,99,144,148	0
34	HTG	c	521	19/19	0.78	0.36	68,112,134,140	0
34	HTG	C	521	19/19	0.79	0.41	66,101,116,120	0
27	GOL	d	402	6/6	0.80	0.59	33,50,65,68	0
31	LHG	E	101	42/49	0.81	0.26	41,93,108,124	0
30	UNL	b	629	36/-	0.81	0.29	49,80,131,138	0
35	LMT	D	403	35/35	0.81	0.32	48,91,116,117	0
30	UNL	x	101	18/-	0.82	0.29	44,63,91,92	0
34	HTG	V	203	11/19	0.82	0.56	71,92,107,108	0
33	LMG	C	520	51/55	0.83	0.28	37,69,104,121	0
35	LMT	b	627	25/35	0.83	0.25	29,61,134,139	0
30	UNL	D	411	40/-	0.83	0.24	40,77,117,122	0
35	LMT	B	629	25/35	0.83	0.24	34,68,124,125	0
25	BCR	H	101	40/40	0.84	0.23	33,42,63,67	0
35	LMT	a	417	35/35	0.84	0.55	78,114,130,131	0
33	LMG	C	501	51/55	0.84	0.28	35,74,98,102	0
23	CLA	C	513	65/65	0.84	0.26	43,59,94,101	0
33	LMG	a	416	51/55	0.84	0.25	41,77,102,118	0
34	HTG	b	628	19/19	0.85	0.25	34,65,115,119	0
30	UNL	M	102	10/-	0.85	0.26	33,52,59,69	0
26	SQD	B	620	54/54	0.86	0.21	41,73,108,113	0
27	GOL	B	626	6/6	0.86	0.32	38,51,55,62	0
33	LMG	z	101	39/55	0.88	0.24	63,112,140,147	0
33	LMG	c	519	51/55	0.88	0.27	43,77,114,124	0
26	SQD	a	412	54/54	0.88	0.21	44,73,125,133	0
26	SQD	A	412	54/54	0.89	0.21	39,65,102,118	0
23	CLA	C	514	65/65	0.89	0.23	46,64,87,95	0
36	DGD	h	102	62/66	0.89	0.27	31,46,62,73	0
33	LMG	B	621	51/55	0.89	0.21	32,49,79,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	LMG	b	620	51/55	0.90	0.19	29,50,88,106	0
36	DGD	C	518	62/66	0.90	0.21	29,46,103,110	0
23	CLA	c	513	65/65	0.90	0.22	52,73,115,119	0
35	LMT	B	631	26/35	0.90	0.17	52,80,105,109	0
23	CLA	C	512	65/65	0.90	0.18	36,52,73,84	0
23	CLA	C	508	65/65	0.91	0.25	36,47,60,70	0
23	CLA	c	502	65/65	0.91	0.41	37,48,68,73	0
23	CLA	c	512	65/65	0.91	0.20	48,64,90,96	0
34	HTG	B	627	19/19	0.91	0.17	45,63,74,75	0
26	SQD	D	413	43/54	0.91	0.27	64,97,112,116	0
27	GOL	a	411	6/6	0.91	0.20	52,60,62,66	0
30	UNL	X	101	18/-	0.91	0.19	40,53,83,90	0
36	DGD	H	102	62/66	0.92	0.25	26,40,58,66	0
25	BCR	y	101	40/40	0.92	0.16	44,54,70,72	0
23	CLA	B	609	65/65	0.92	0.17	29,39,53,63	0
33	LMG	j	101	51/55	0.92	0.18	37,53,102,123	0
23	CLA	b	609	65/65	0.92	0.17	36,44,63,82	0
23	CLA	B	614	65/65	0.92	0.18	21,31,82,100	0
23	CLA	c	507	65/65	0.92	0.18	41,53,65,68	0
34	HTG	B	622	19/19	0.92	0.21	34,61,127,132	0
31	LHG	l	101	49/49	0.92	0.17	25,38,55,60	0
23	CLA	c	511	65/65	0.92	0.21	43,56,74,82	0
33	LMG	J	101	51/55	0.92	0.18	30,51,88,99	0
23	CLA	c	509	65/65	0.92	0.24	43,52,66,73	0
31	LHG	A	416	49/49	0.92	0.32	26,44,61,77	0
23	CLA	b	602	65/65	0.92	0.23	32,44,60,68	0
36	DGD	c	517	62/66	0.92	0.22	38,53,112,129	0
23	CLA	B	602	65/65	0.92	0.23	29,37,55,67	0
23	CLA	b	616	65/65	0.92	0.18	31,46,98,105	0
25	BCR	d	405	40/40	0.93	0.16	40,50,74,81	0
23	CLA	C	507	65/65	0.93	0.15	39,55,102,106	0
30	UNL	D	410	17/-	0.93	0.29	44,56,91,100	0
23	CLA	b	601	65/65	0.93	0.24	43,69,99,126	0
27	GOL	C	523	6/6	0.93	0.23	44,54,59,60	0
23	CLA	C	510	65/65	0.93	0.29	36,47,67,69	0
34	HTG	b	625	19/19	0.93	0.11	43,56,83,93	0
37	CA	O	301	1/1	0.93	0.11	87,87,87,87	0
23	CLA	b	615	65/65	0.93	0.17	29,40,66,81	0
37	CA	V	201	1/1	0.93	0.15	93,93,93,93	0
36	DGD	C	519	62/66	0.93	0.17	28,44,71,95	0
23	CLA	D	405	65/65	0.93	0.19	31,46,99,111	0
25	BCR	C	516	40/40	0.93	0.21	36,48,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	C	503	65/65	0.93	0.35	31,42,55,73	0
36	DGD	C	517	62/66	0.93	0.23	27,36,81,92	0
31	LHG	d	408	49/49	0.93	0.22	24,35,53,70	0
23	CLA	c	503	65/65	0.93	0.41	40,51,63,78	0
26	SQD	a	410	54/54	0.93	0.18	41,64,98,105	0
23	CLA	B	601	65/65	0.94	0.22	39,57,88,119	0
25	BCR	Y	101	40/40	0.94	0.15	37,49,59,62	0
25	BCR	K	102	40/40	0.94	0.17	39,47,62,65	0
23	CLA	B	604	65/65	0.94	0.30	21,29,92,104	0
23	CLA	d	404	65/65	0.94	0.17	38,48,98,109	0
23	CLA	B	616	65/65	0.94	0.21	30,45,113,124	0
25	BCR	C	515	40/40	0.94	0.15	46,61,72,73	0
26	SQD	A	410	54/54	0.94	0.15	38,62,99,105	0
23	CLA	b	612	65/65	0.94	0.23	25,35,48,59	0
23	CLA	c	508	65/65	0.94	0.19	35,48,107,118	0
23	CLA	C	504	65/65	0.94	0.27	36,44,65,75	0
23	CLA	C	505	65/65	0.94	0.21	30,41,79,104	0
25	BCR	k	101	40/40	0.94	0.16	47,55,79,81	0
31	LHG	d	409	49/49	0.94	0.20	33,50,98,110	0
37	CA	c	523	1/1	0.94	0.17	68,68,68,68	0
23	CLA	C	502	65/65	0.94	0.22	34,41,60,77	0
29	PL9	d	406	55/55	0.94	0.19	23,30,41,58	0
27	GOL	b	624	6/6	0.94	0.13	58,76,78,86	0
25	BCR	B	619	40/40	0.94	0.15	28,42,63,67	0
23	CLA	B	606	65/65	0.94	0.15	26,35,76,99	0
25	BCR	b	619	40/40	0.94	0.15	32,45,61,69	0
23	CLA	B	611	65/65	0.94	0.24	23,30,41,45	0
25	BCR	D	406	40/40	0.94	0.17	32,42,87,90	0
23	CLA	c	505	65/65	0.94	0.20	32,45,68,86	0
37	CA	o	301	1/1	0.95	0.10	85,85,85,85	0
23	CLA	c	501	65/65	0.95	0.23	38,49,64,71	0
23	CLA	b	606	65/65	0.95	0.14	27,42,77,106	0
30	UNL	d	410	17/-	0.95	0.29	42,57,85,90	0
23	CLA	B	612	65/65	0.95	0.23	24,29,42,51	0
31	LHG	d	407	49/49	0.95	0.21	25,44,72,87	0
36	DGD	c	516	62/66	0.95	0.23	33,43,73,95	0
25	BCR	c	514	40/40	0.95	0.13	52,65,76,79	0
23	CLA	a	408	65/65	0.95	0.19	28,40,107,115	0
31	LHG	D	409	49/49	0.95	0.19	29,47,107,124	0
23	CLA	B	615	65/65	0.95	0.14	27,34,61,68	0
23	CLA	b	614	65/65	0.95	0.14	23,34,76,89	0
29	PL9	D	407	55/55	0.95	0.23	20,31,45,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	504	65/65	0.95	0.27	37,50,89,111	0
36	DGD	c	518	62/66	0.95	0.19	36,46,77,96	0
31	LHG	A	417	49/49	0.95	0.23	23,37,55,66	0
27	GOL	B	625	6/6	0.95	0.29	48,76,85,89	0
23	CLA	C	509	65/65	0.95	0.29	30,43,102,115	0
23	CLA	b	604	65/65	0.95	0.31	23,31,85,96	0
23	CLA	A	404	65/65	0.96	0.16	20,23,41,58	0
23	CLA	D	404	65/65	0.96	0.17	20,26,46,52	0
23	CLA	B	605	65/65	0.96	0.20	22,30,44,48	0
31	LHG	D	408	49/49	0.96	0.23	22,34,51,68	0
23	CLA	B	607	65/65	0.96	0.22	18,27,54,66	0
25	BCR	c	515	40/40	0.96	0.14	37,52,65,75	0
23	CLA	b	607	65/65	0.96	0.17	20,31,53,63	0
23	CLA	C	511	65/65	0.96	0.42	33,44,57,61	0
23	CLA	b	605	65/65	0.96	0.23	24,34,52,97	0
25	BCR	b	618	40/40	0.96	0.20	21,34,49,55	0
39	MG	j	103	1/1	0.96	0.14	51,51,51,51	0
23	CLA	b	603	65/65	0.96	0.24	30,40,53,74	0
23	CLA	c	506	65/65	0.96	0.14	44,58,90,111	0
23	CLA	c	510	65/65	0.96	0.31	39,47,62,66	0
25	BCR	T	101	40/40	0.96	0.22	20,36,45,53	0
25	BCR	b	617	40/40	0.96	0.15	20,34,41,44	0
23	CLA	b	610	65/65	0.96	0.20	30,42,51,60	0
23	CLA	C	506	65/65	0.96	0.26	31,40,71,78	0
24	PHO	a	407	64/64	0.97	0.26	28,35,50,52	0
25	BCR	B	618	40/40	0.97	0.23	21,36,54,69	0
25	BCR	a	409	40/40	0.97	0.14	24,35,45,49	0
23	CLA	B	603	65/65	0.97	0.26	26,39,52,57	0
25	BCR	A	409	40/40	0.97	0.15	22,34,46,49	0
23	CLA	B	610	65/65	0.97	0.23	27,36,52,69	0
23	CLA	d	401	65/65	0.97	0.15	23,26,48,75	0
27	GOL	A	411	6/6	0.97	0.12	50,58,65,79	0
23	CLA	a	404	65/65	0.97	0.17	25,30,50,60	0
23	CLA	b	608	65/65	0.97	0.28	32,41,60,68	0
25	BCR	t	101	40/40	0.97	0.23	19,42,59,62	0
23	CLA	a	405	65/65	0.97	0.22	27,36,105,111	0
23	CLA	d	403	65/65	0.97	0.22	25,29,49,62	0
37	CA	c	524	1/1	0.97	0.09	66,66,66,66	0
24	PHO	A	407	64/64	0.97	0.21	23,31,46,51	0
23	CLA	A	405	65/65	0.97	0.16	19,23,41,47	0
23	CLA	b	611	65/65	0.97	0.19	25,34,49,61	0
23	CLA	B	608	65/65	0.97	0.23	27,37,51,55	0

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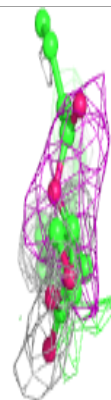
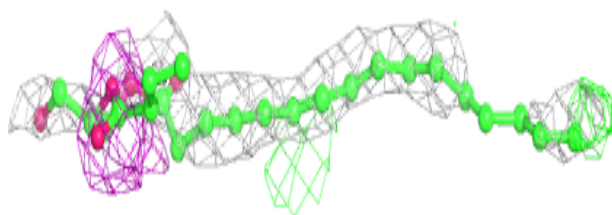
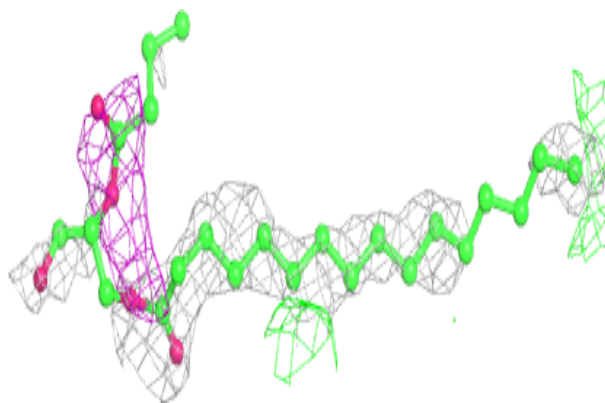
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	A	408	65/65	0.97	0.14	26,36,101,109	0
23	CLA	A	406	65/65	0.97	0.14	22,29,80,89	0
23	CLA	b	613	65/65	0.97	0.23	22,33,67,78	0
23	CLA	B	613	65/65	0.97	0.32	21,29,68,78	0
38	HEM	E	103	43/43	0.98	0.09	40,54,66,73	0
40	HEC	V	202	43/43	0.98	0.11	30,33,44,53	0
24	PHO	a	406	64/64	0.98	0.20	22,31,40,51	0
38	HEM	e	103	43/43	0.98	0.19	48,73,98,105	0
37	CA	C	524	1/1	0.98	0.24	62,62,62,62	0
25	BCR	B	617	40/40	0.98	0.16	22,31,46,49	0
24	PHO	D	401	64/64	0.98	0.18	21,27,35,45	0
22	CL	a	403	1/1	0.98	0.19	34,34,34,34	0
39	MG	J	103	1/1	0.98	0.15	39,39,39,39	0
40	HEC	v	201	43/43	0.98	0.13	40,50,59,66	0
32	BCT	a	418	4/4	0.99	0.10	45,52,54,59	0
21	FE2	A	401	1/1	0.99	0.04	42,42,42,42	0
22	CL	a	402	1/1	0.99	0.10	31,31,31,31	0
28	OEX	A	413	10/10	0.99	0.09	22,30,43,45	0
32	BCT	A	418	4/4	0.99	0.08	34,39,47,65	0
21	FE2	a	401	1/1	0.99	0.06	45,45,45,45	0
22	CL	A	402	1/1	0.99	0.07	24,24,24,24	0
22	CL	A	403	1/1	1.00	0.24	27,27,27,27	0
28	OEX	a	413	10/10	1.00	0.09	27,34,45,53	0

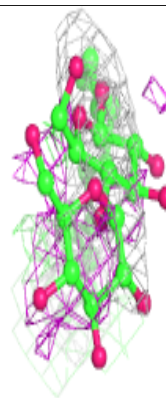
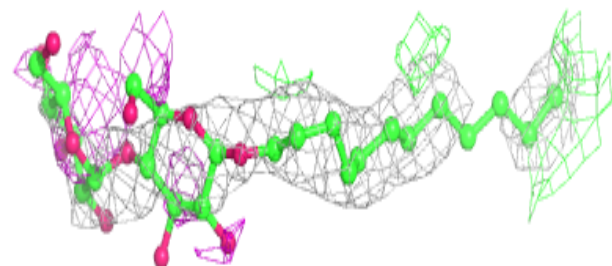
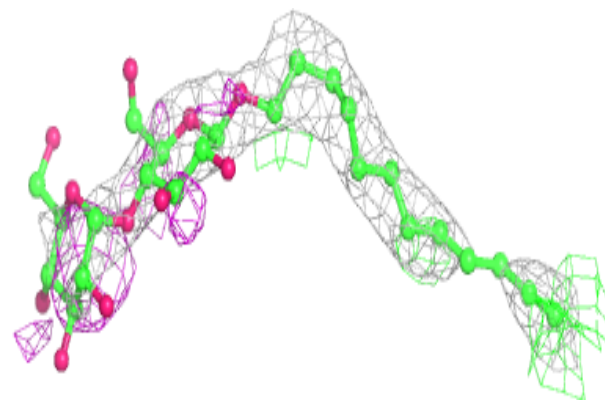
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UNL A 415:

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

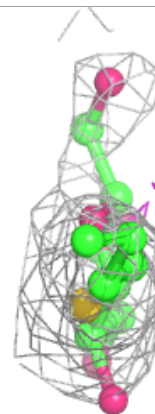
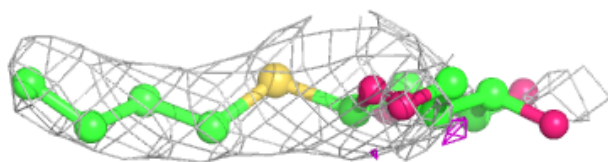
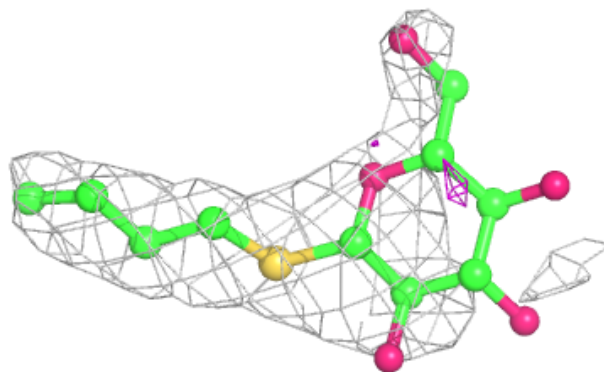
**Electron density around LMT B 630:**

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

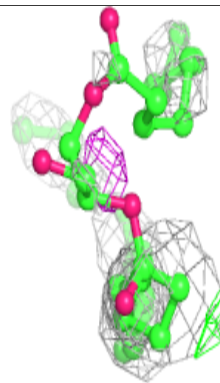
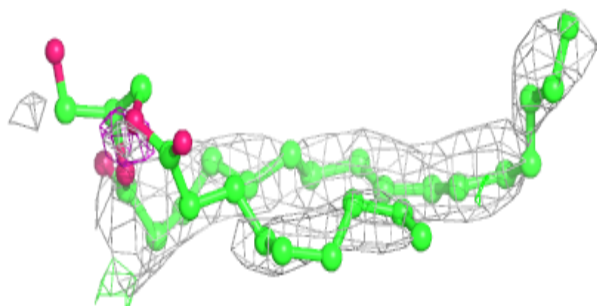
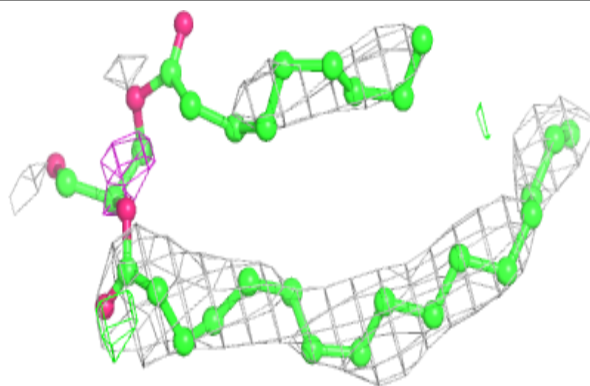


Electron density around HTG D 412:

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

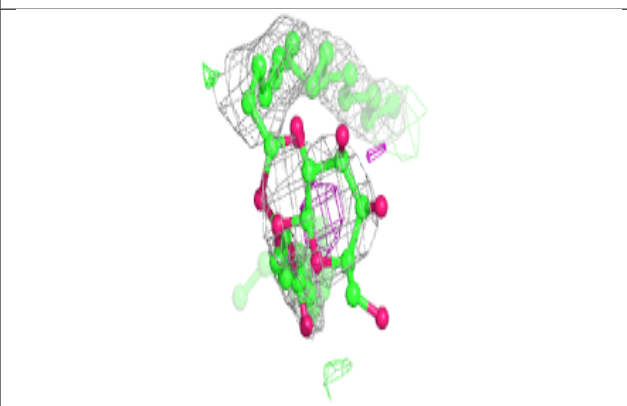
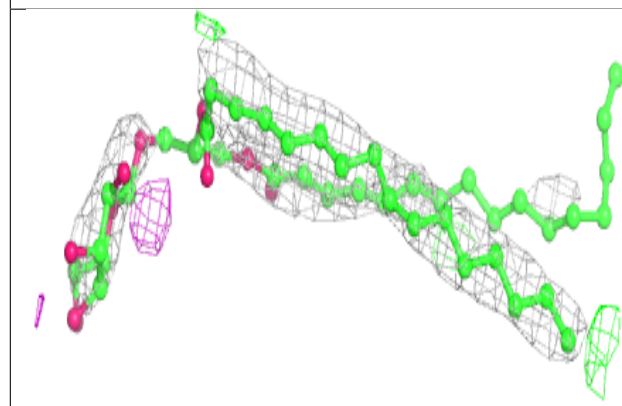
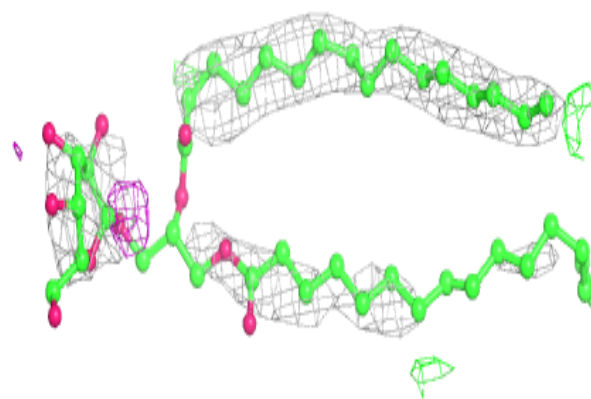
**Electron density around UNL b 626:**

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

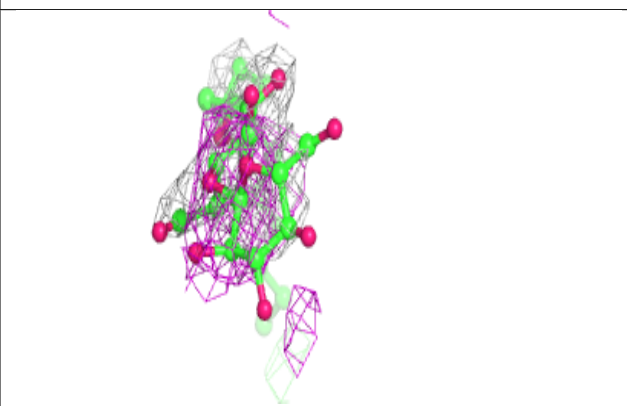
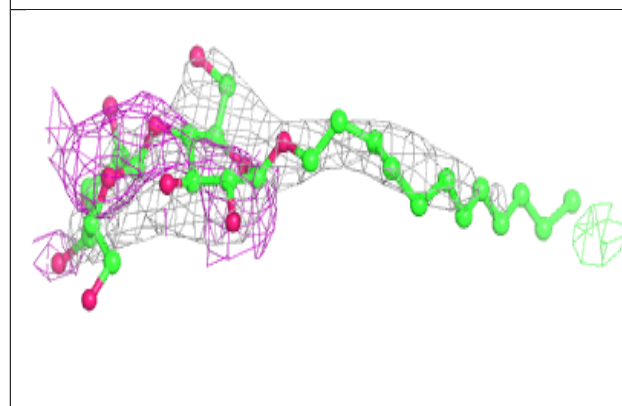
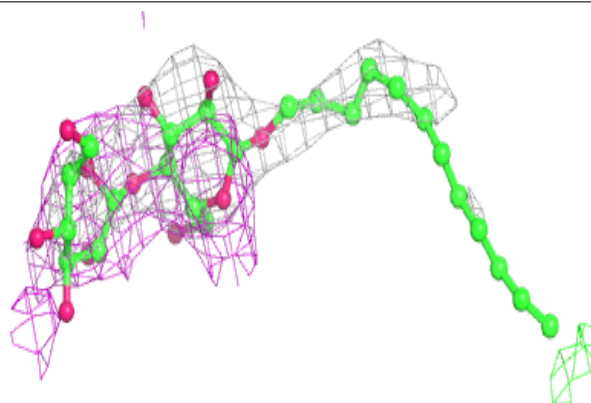


Electron density around LMG Z 101:

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

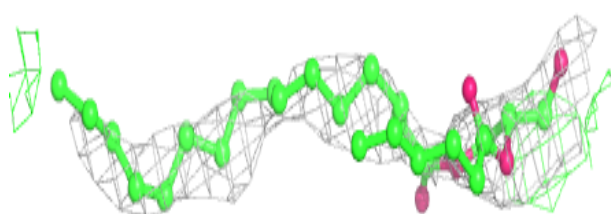
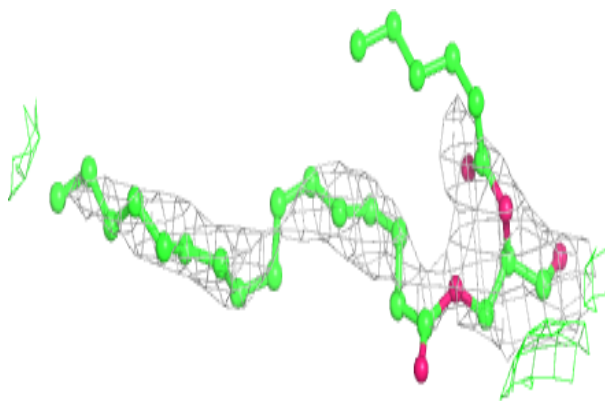
**Electron density around LMT I 101:**

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

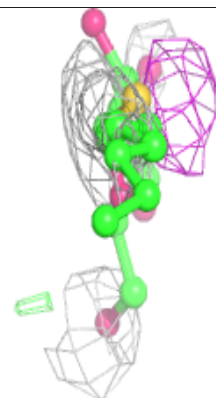
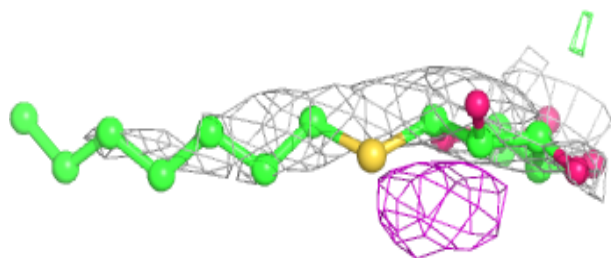
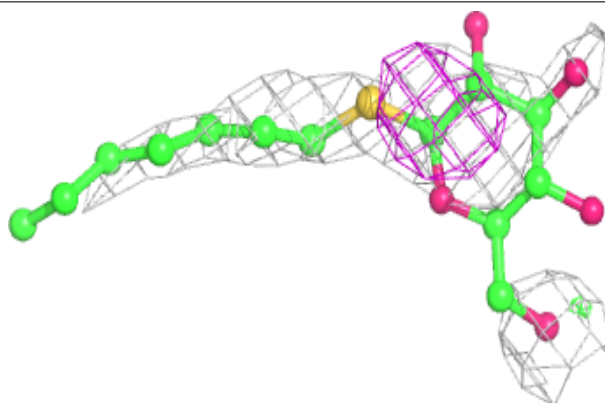


Electron density around UNL a 415:

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

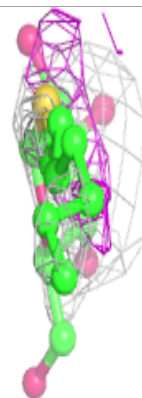
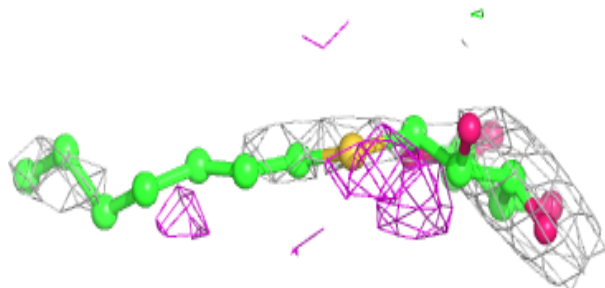
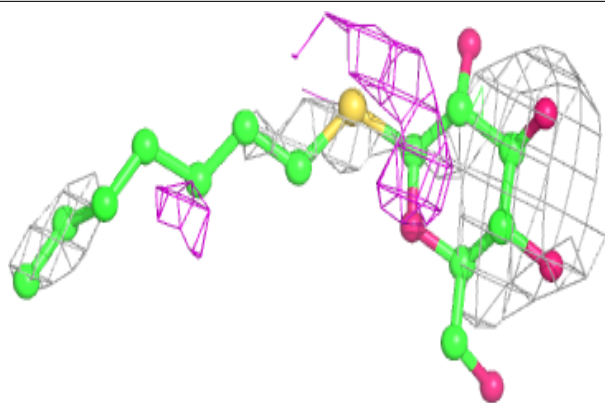
**Electron density around HTG b 623:**

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

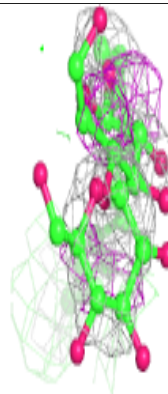
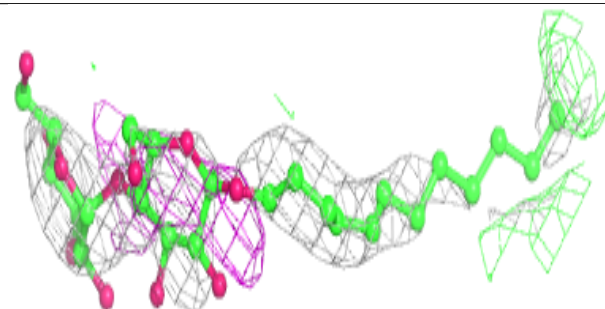
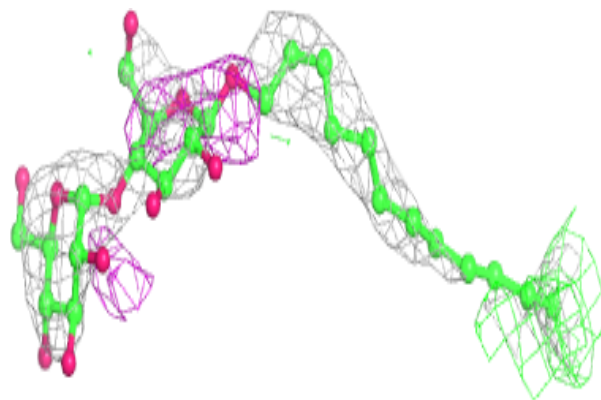


Electron density around HTG B 624:

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

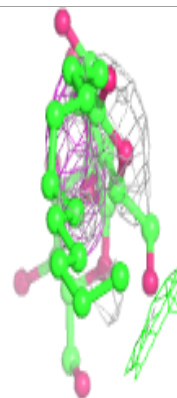
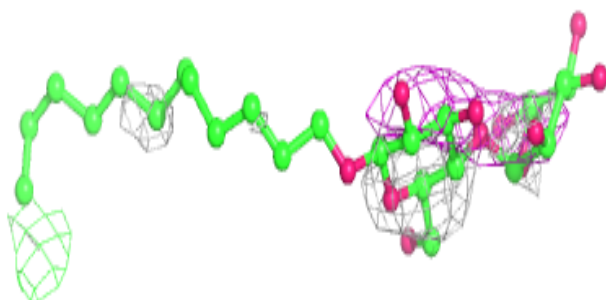
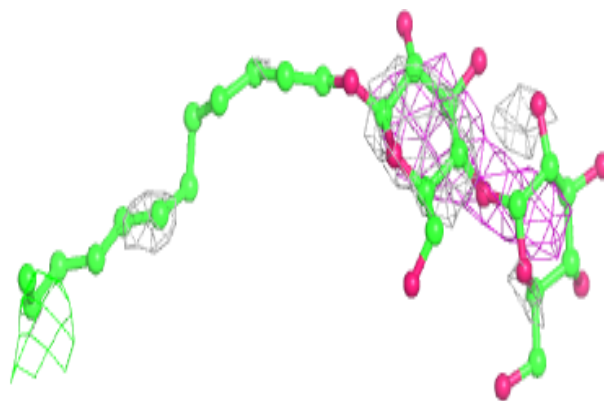
**Electron density around LMT D 402:**

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

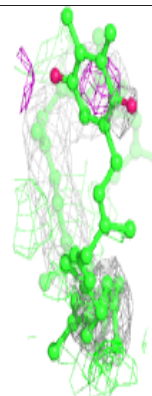
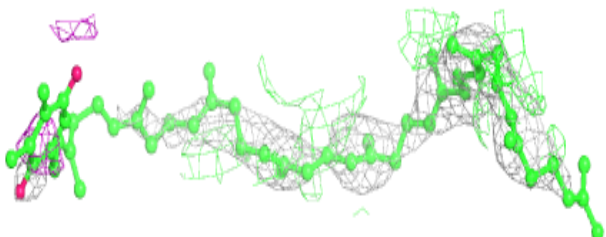
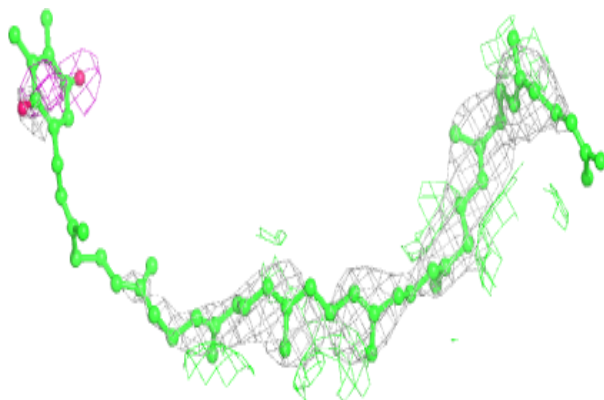


Electron density around LMT e 102:

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

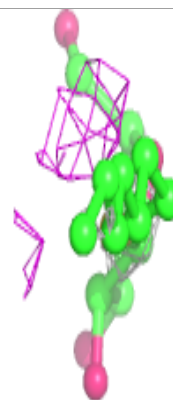
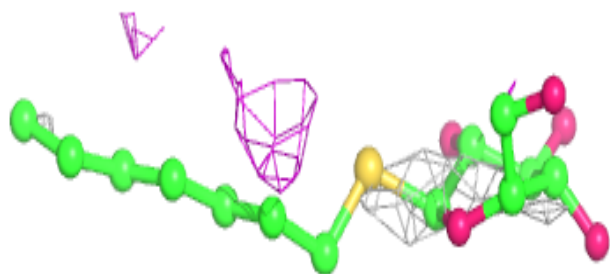
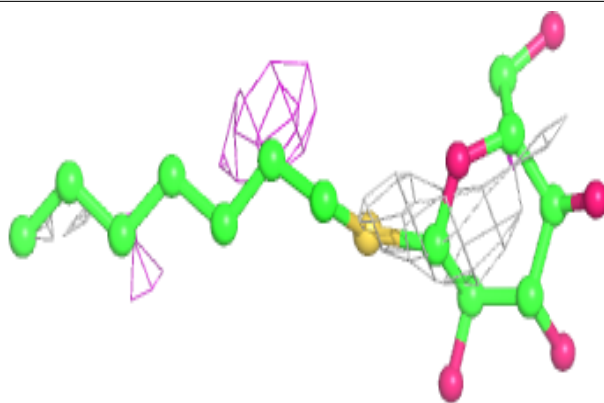
**Electron density around PL9 a 414:**

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

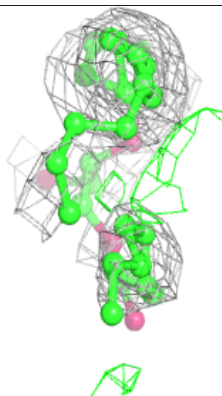
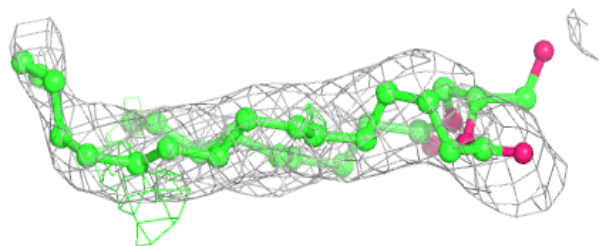
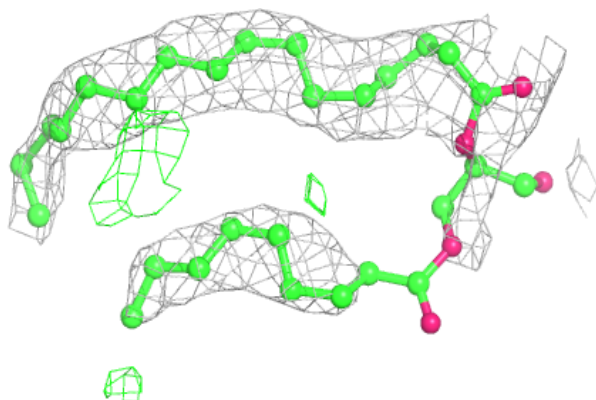


Electron density around HTG C 522:

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

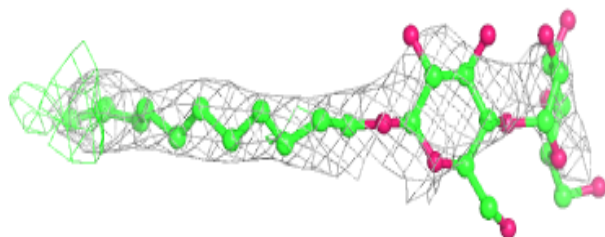
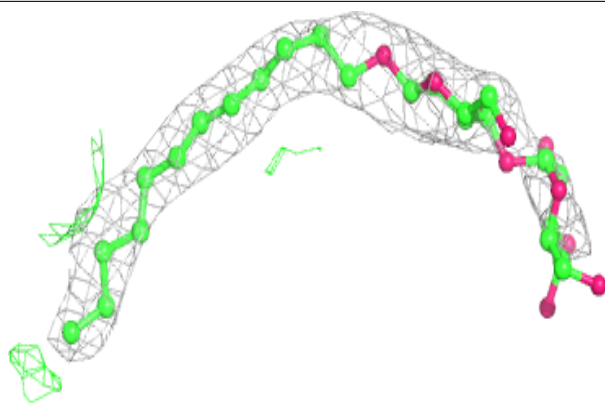
**Electron density around UNL B 628:**

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

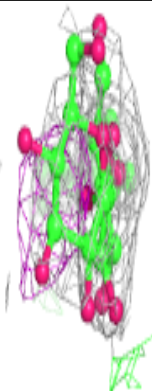
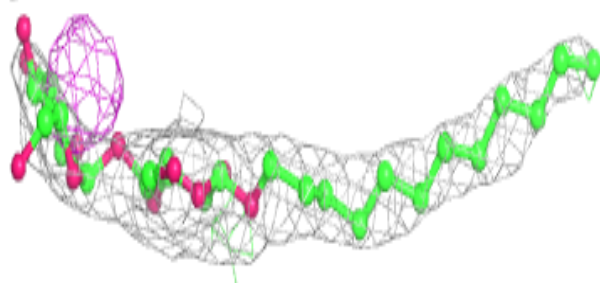
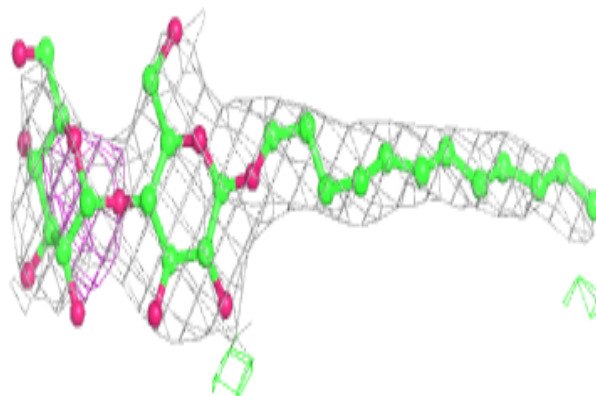


Electron density around LMT M 103:

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

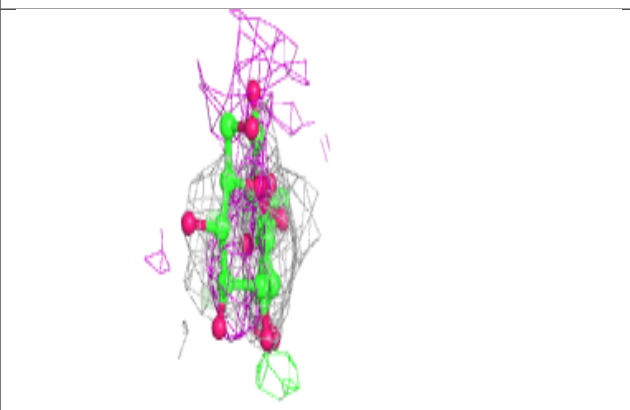
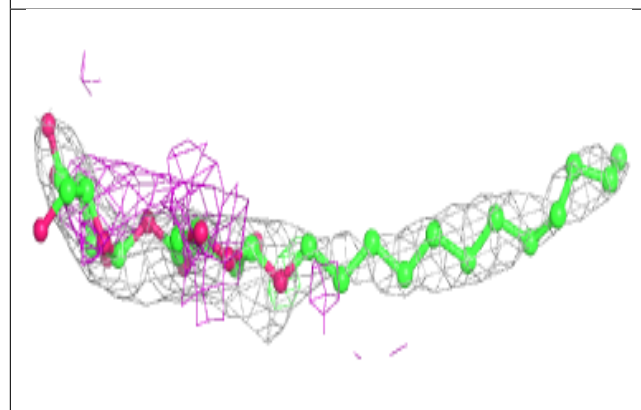
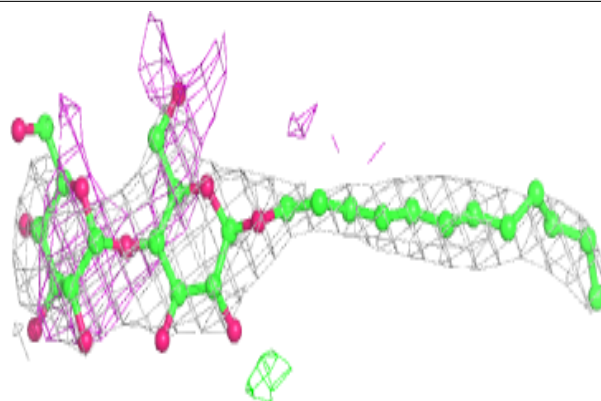
**Electron density around LMT M 101:**

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

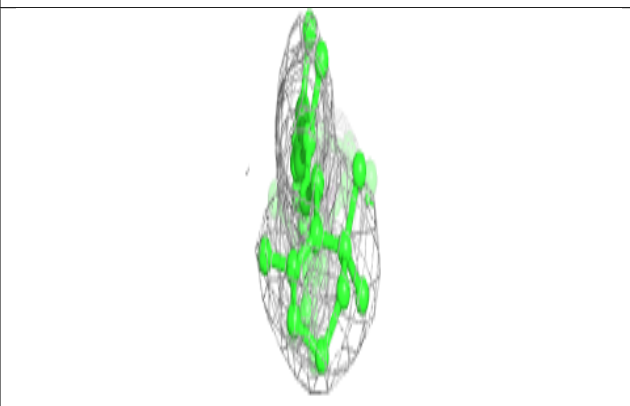
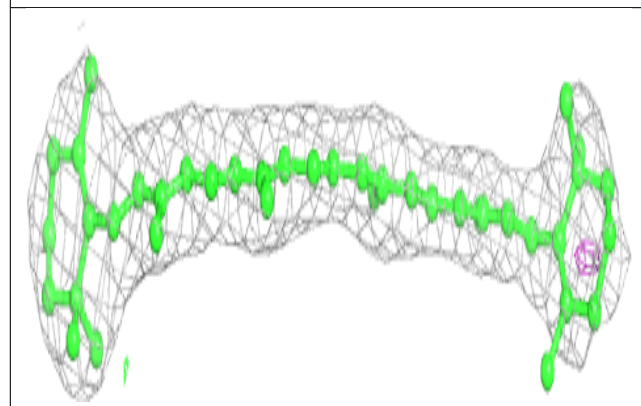
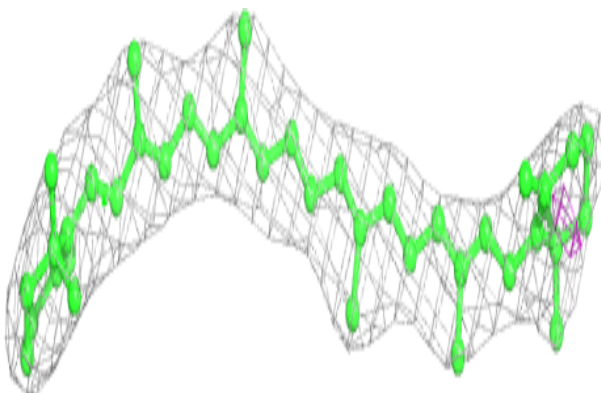


Electron density around LMT m 102:

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

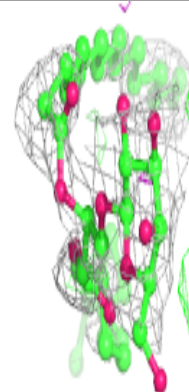
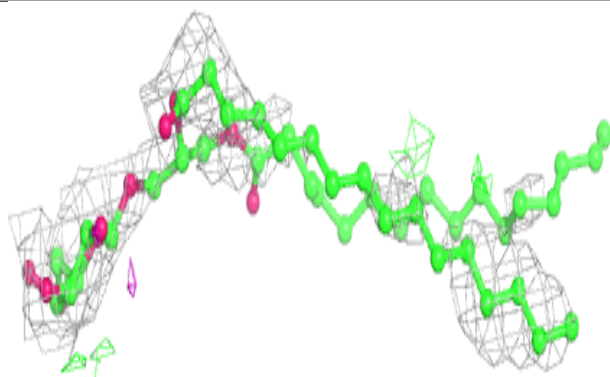
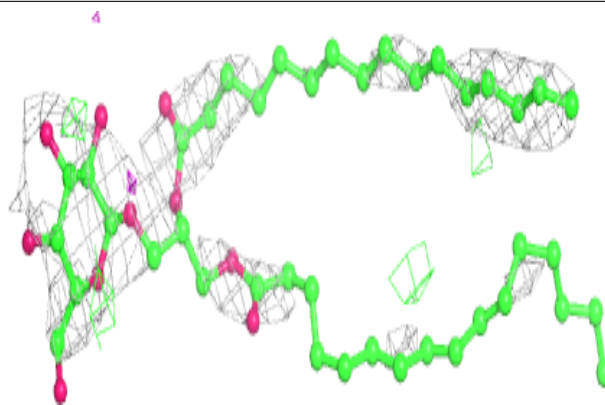
**Electron density around BCR h 101:**

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

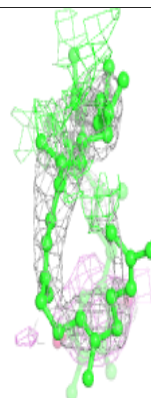
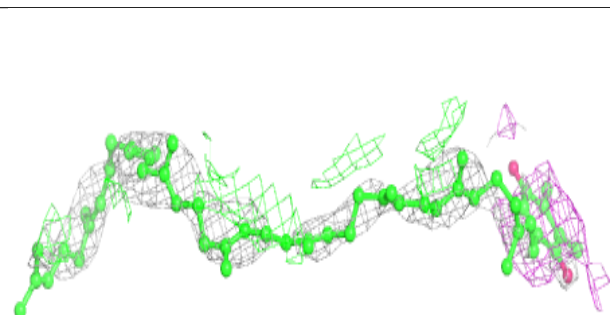
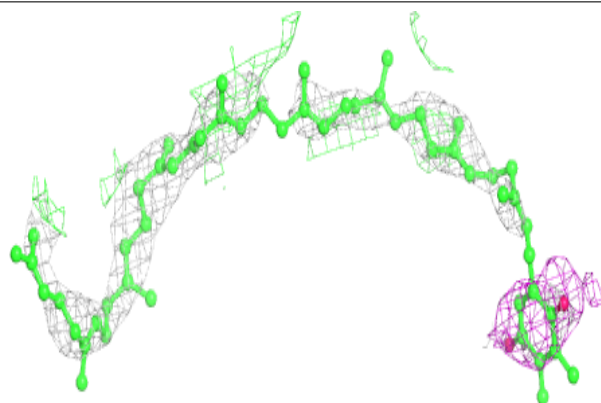


Electron density around LMG c 520:

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

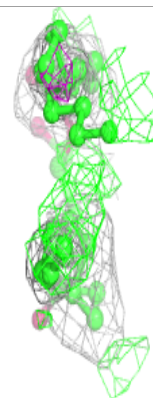
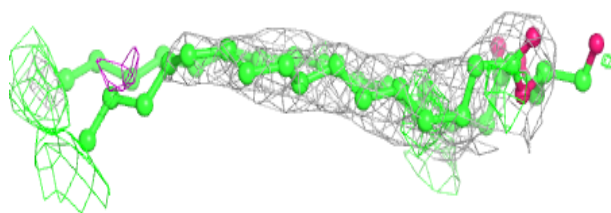
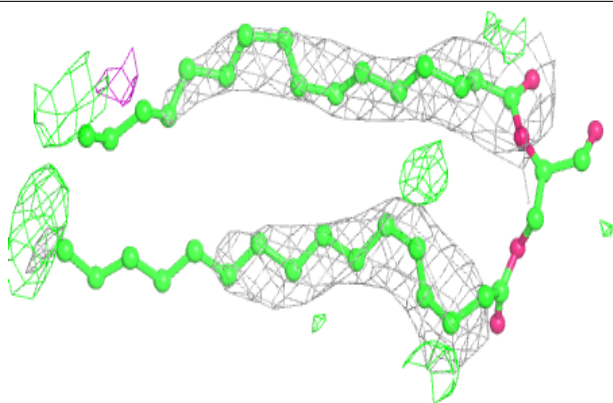
**Electron density around PL9 A 414:**

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

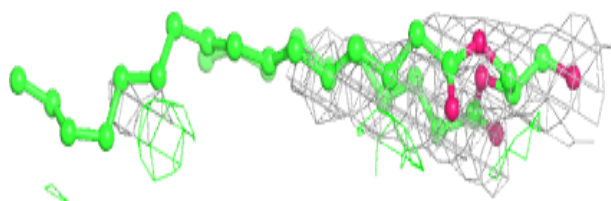
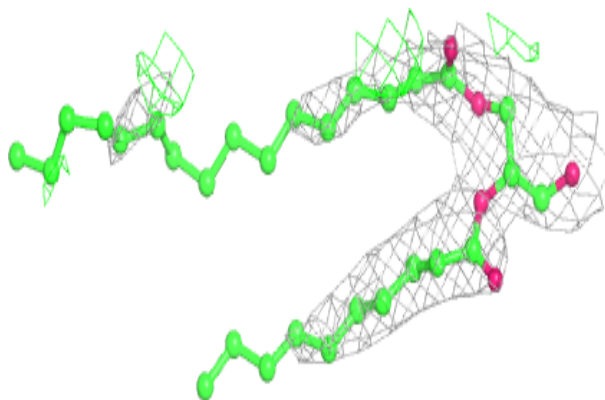


Electron density around UNL i 101:

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

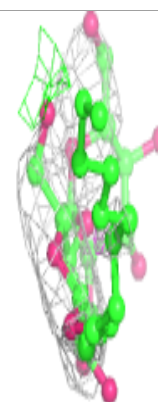
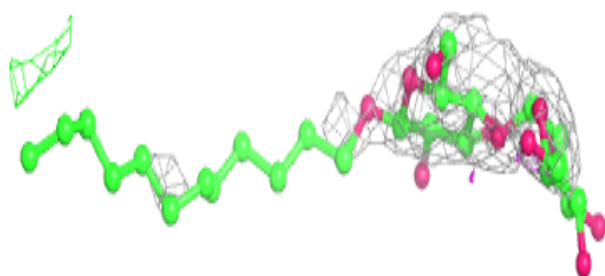
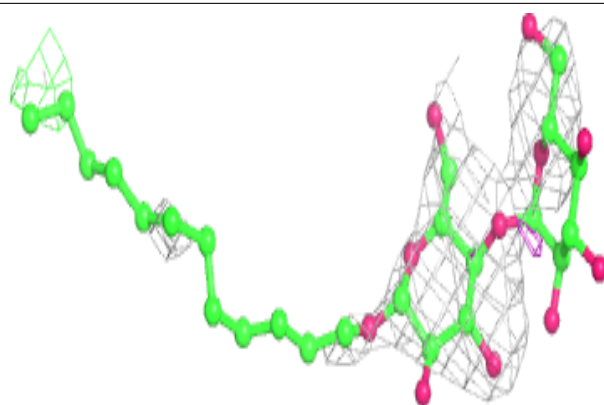
**Electron density around UNL K 101:**

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

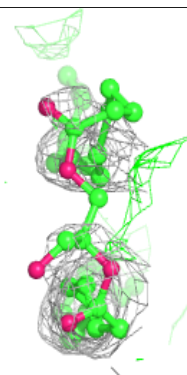
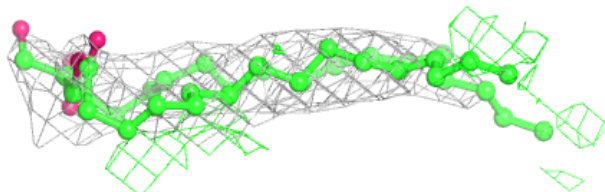
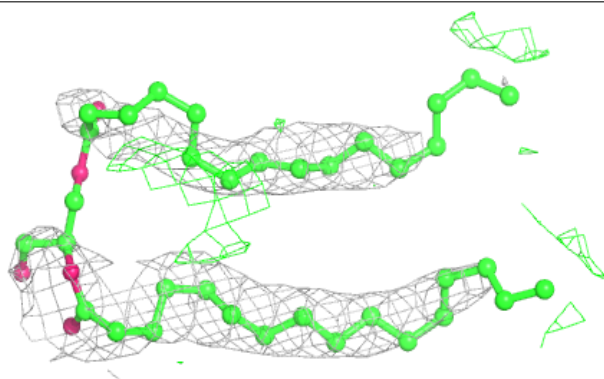


Electron density around LMT E 102:

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

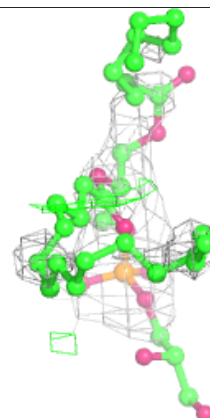
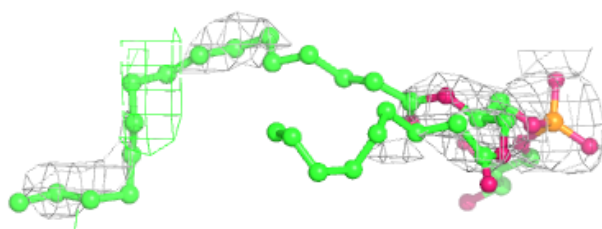
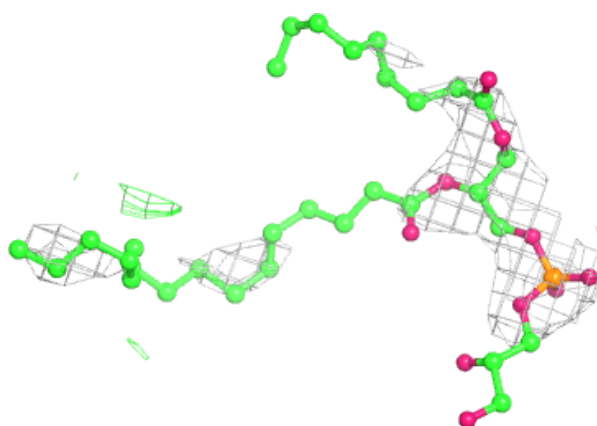
**Electron density around UNL I 102:**

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

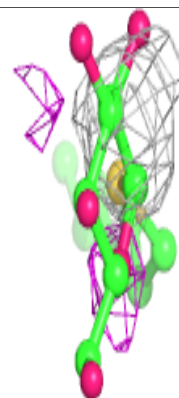
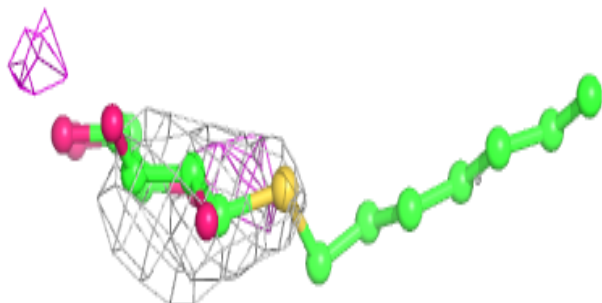
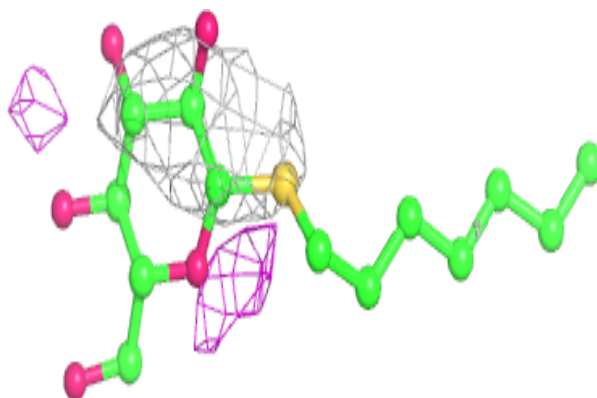


Electron density around LHG e 101:

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

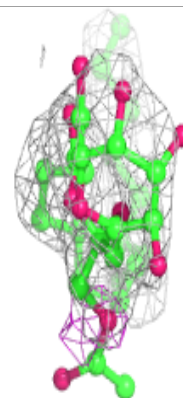
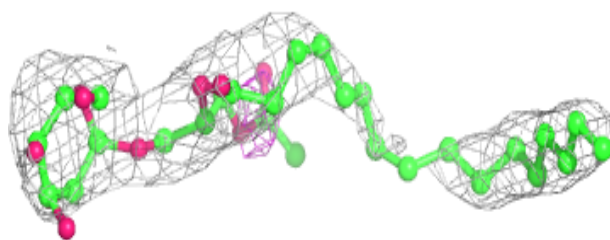
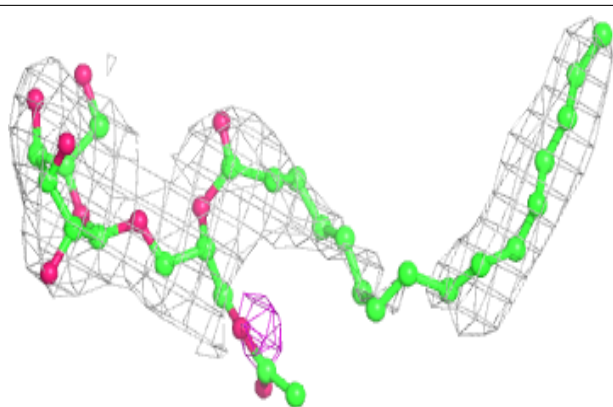
**Electron density around HTG c 522:**

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

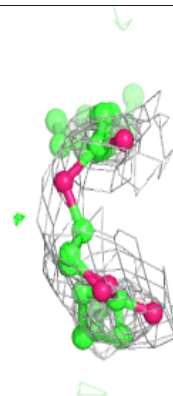
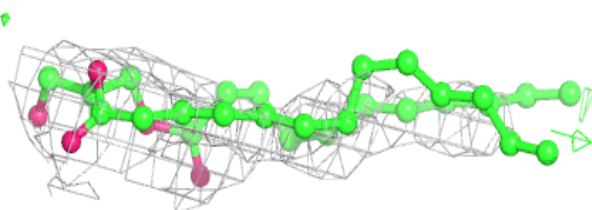
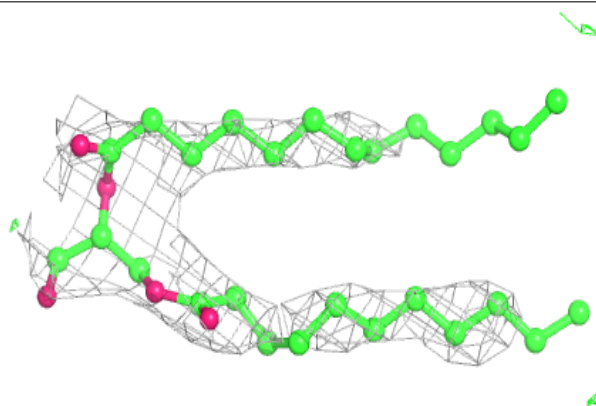


Electron density around LMG Z 102:

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

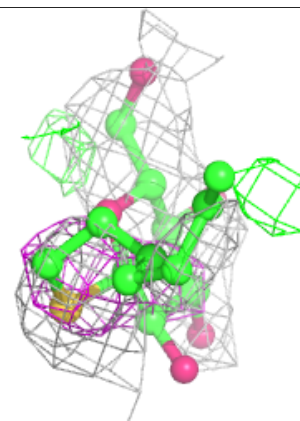
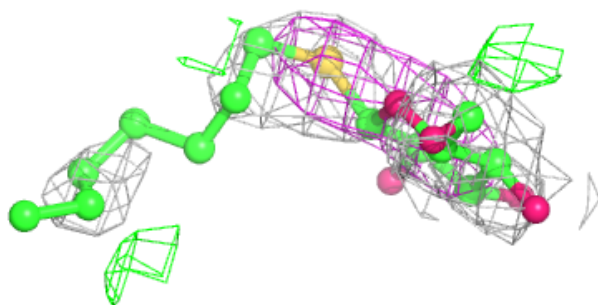
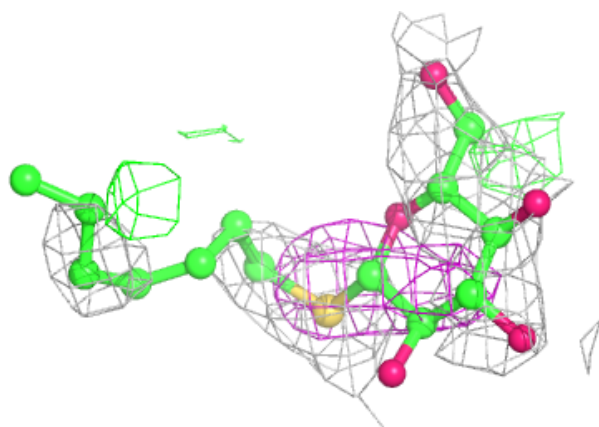
**Electron density around UNL c 525:**

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

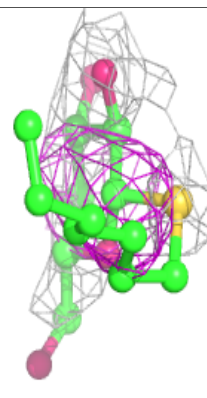
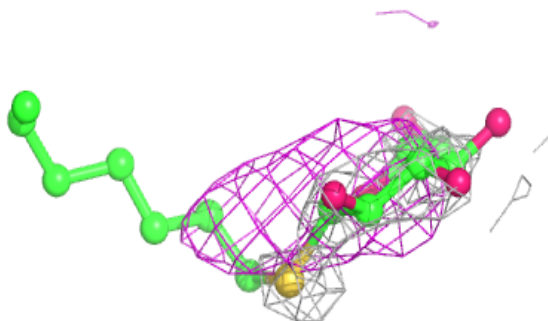
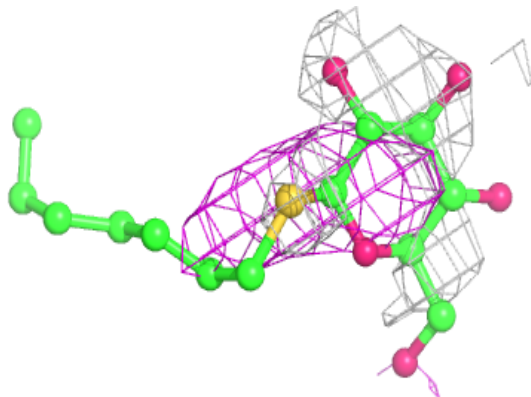


Electron density around HTG B 623:

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

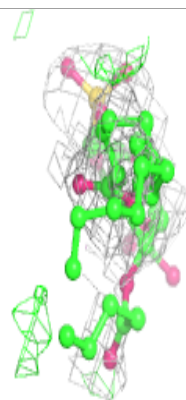
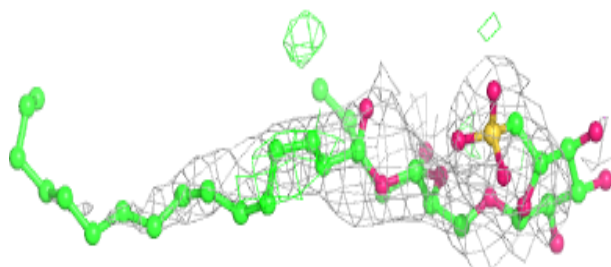
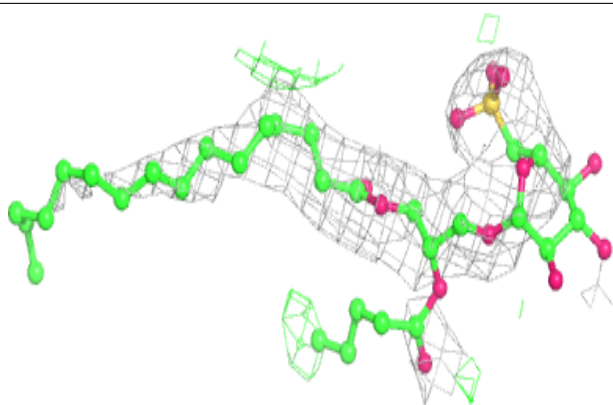
**Electron density around HTG b 622:**

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

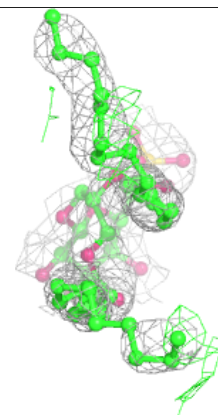
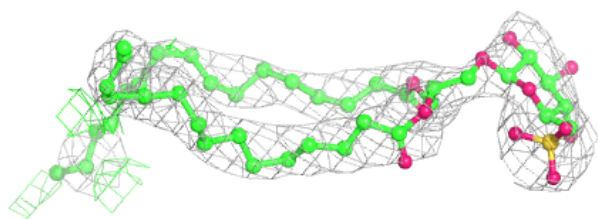
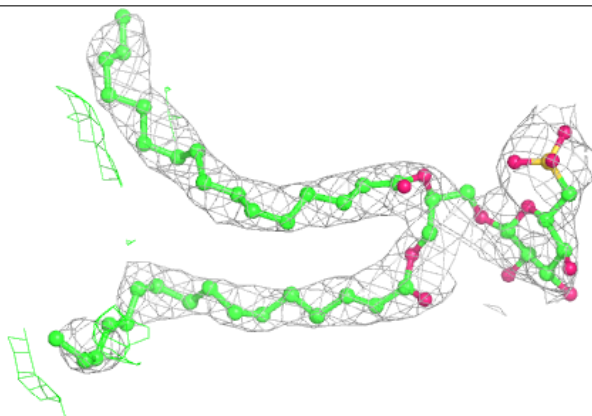


Electron density around SQD f 101:

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

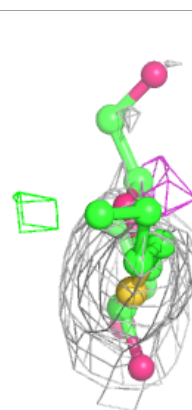
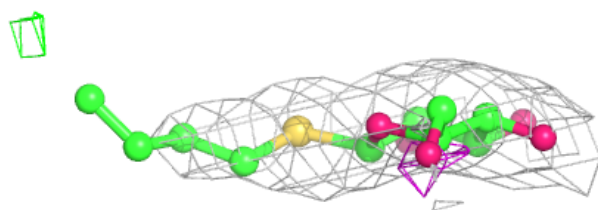
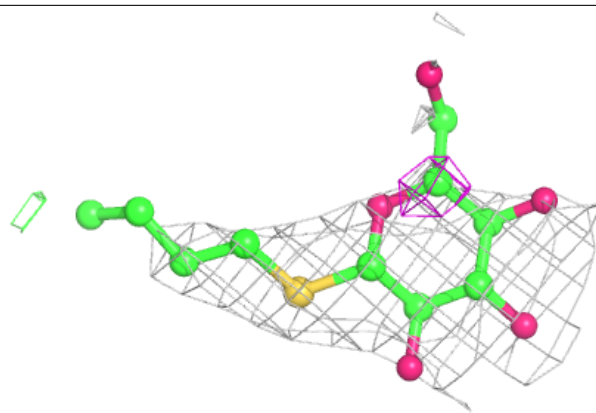
**Electron density around SQD L 101:**

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

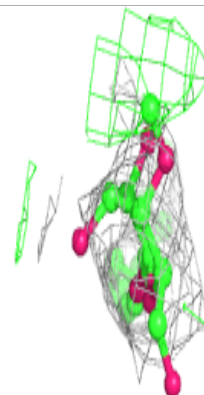
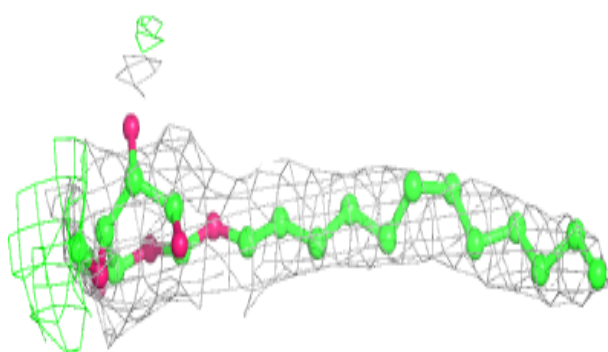
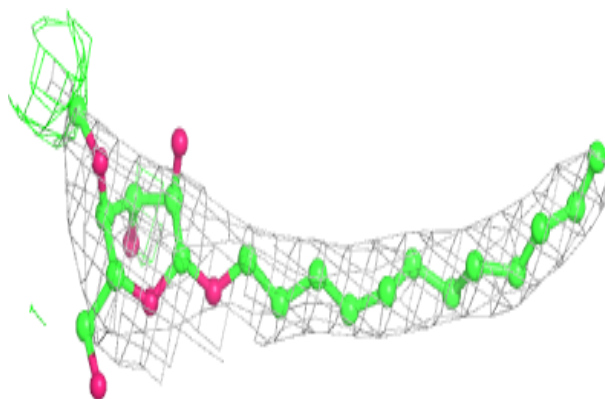


Electron density around HTG d 411:

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

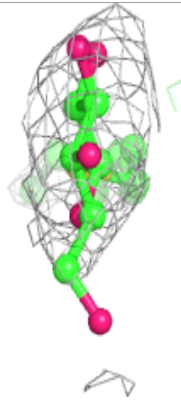
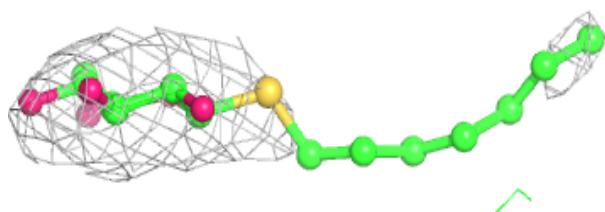
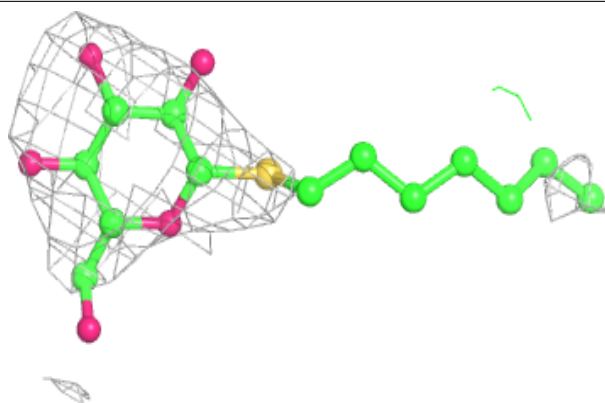
**Electron density around LMT b 621:**

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

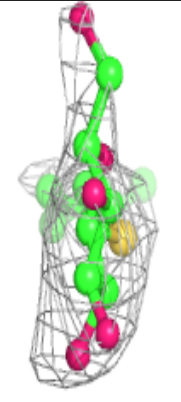
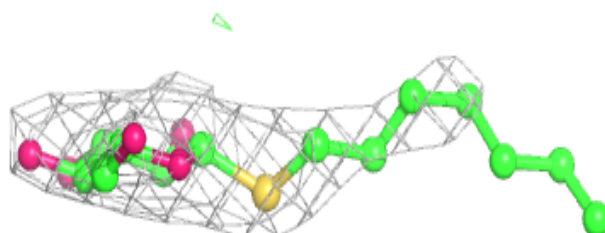
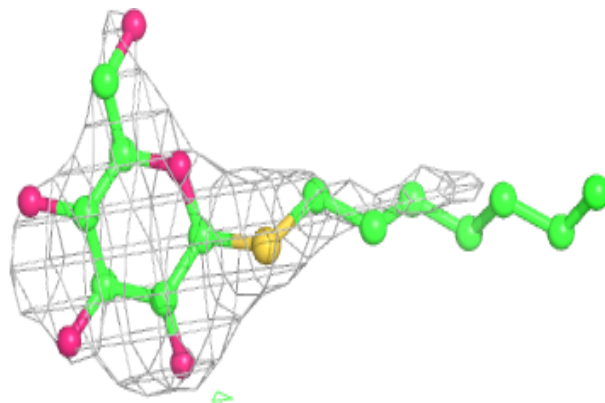


Electron density around HTG c 521:

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

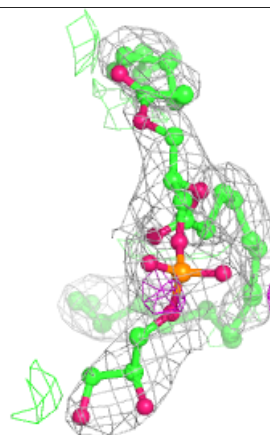
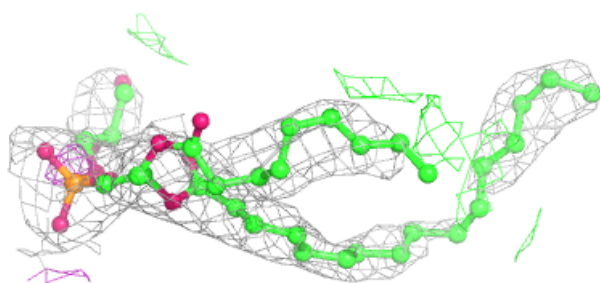
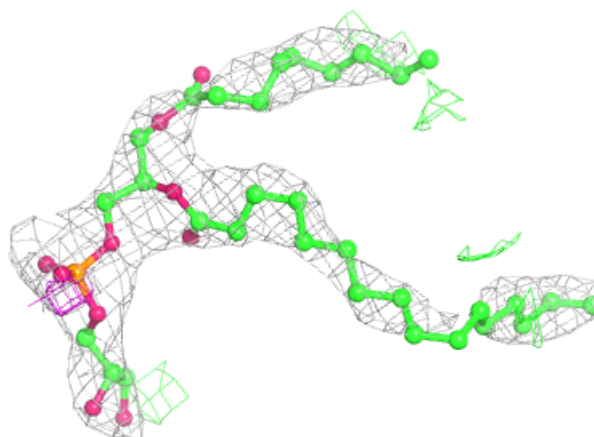
**Electron density around HTG C 521:**

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

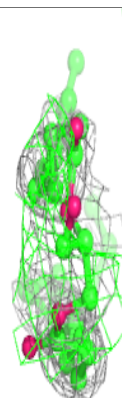
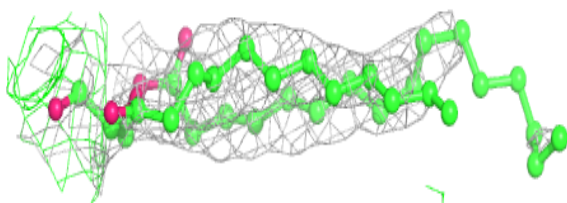
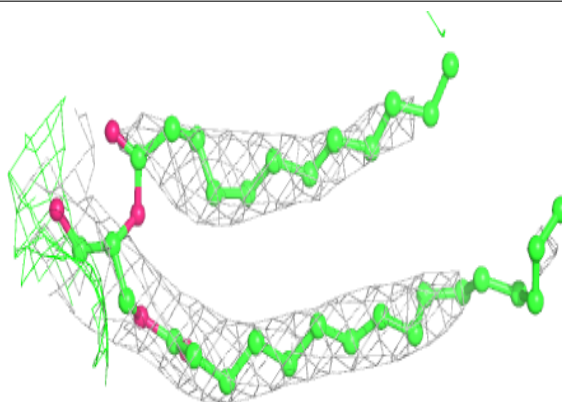


Electron density around LHG E 101:

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

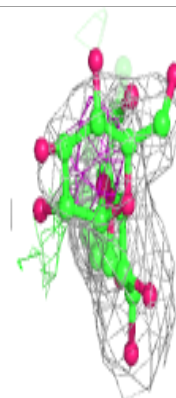
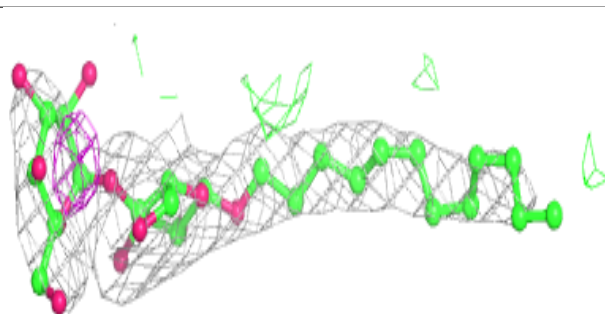
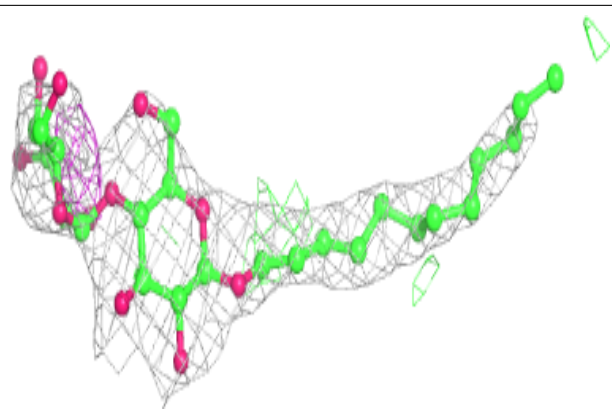
**Electron density around UNL b 629:**

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



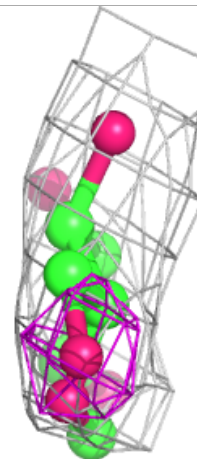
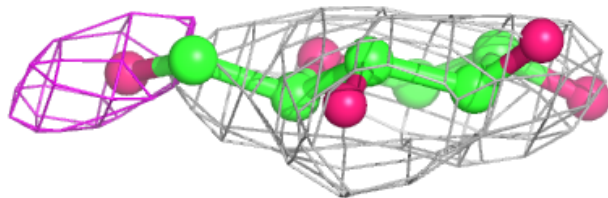
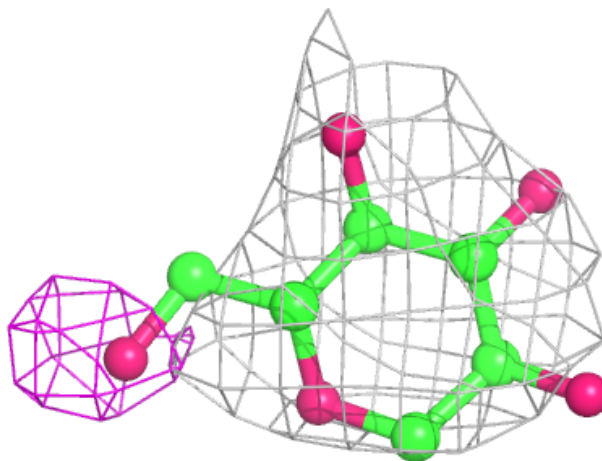
Electron density around LMT D 403:

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



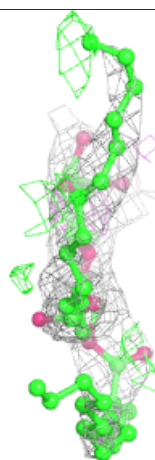
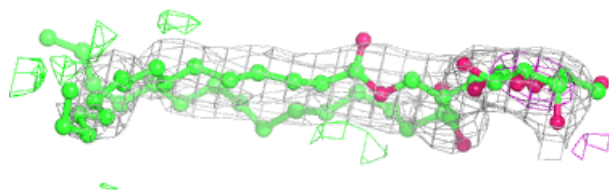
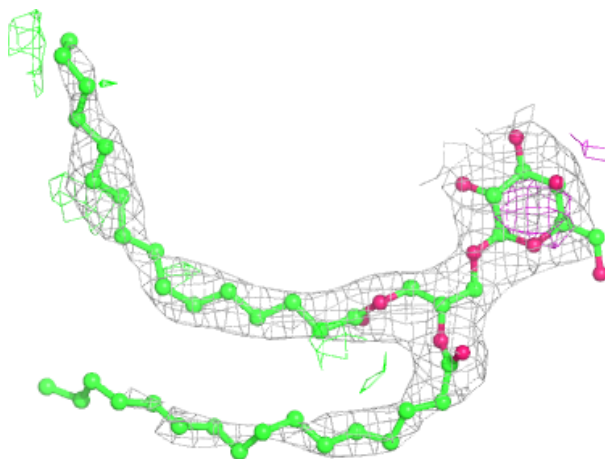
Electron density around HTG V 203:

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



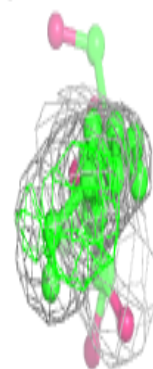
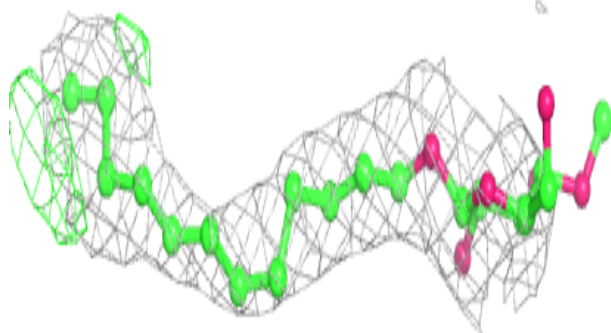
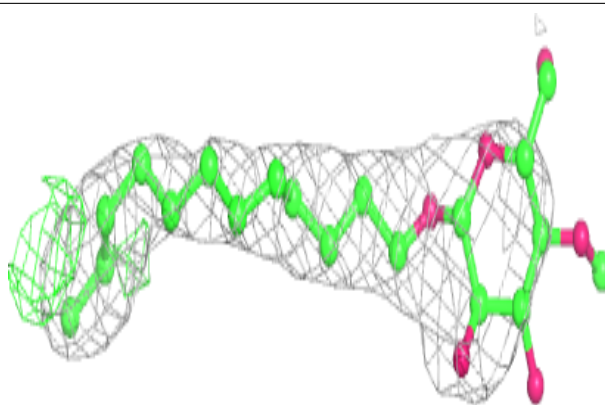
Electron density around LMG C 520:

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

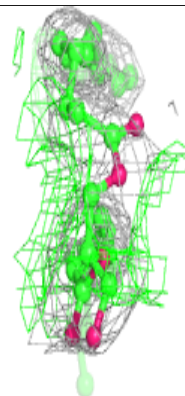
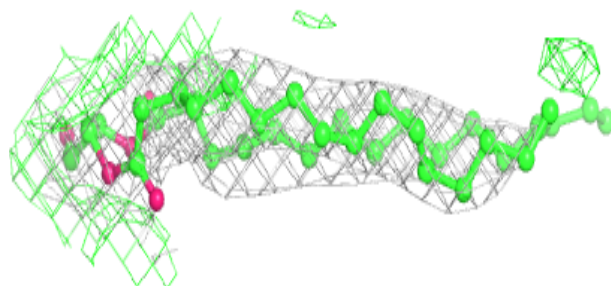
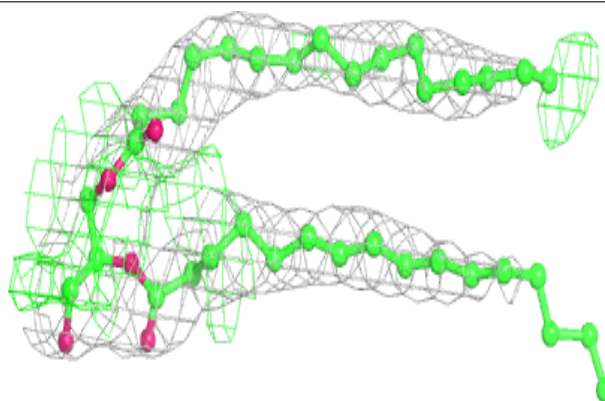


Electron density around LMT b 627:

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

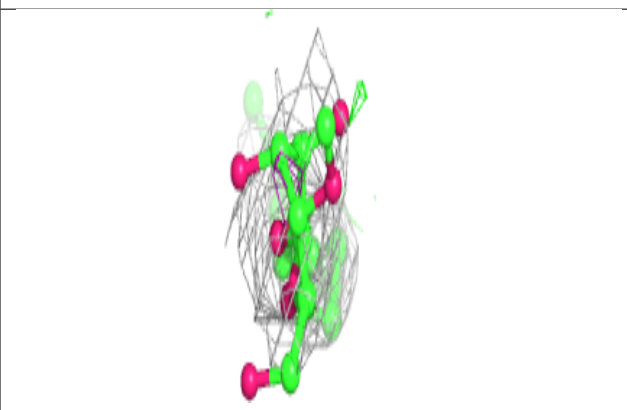
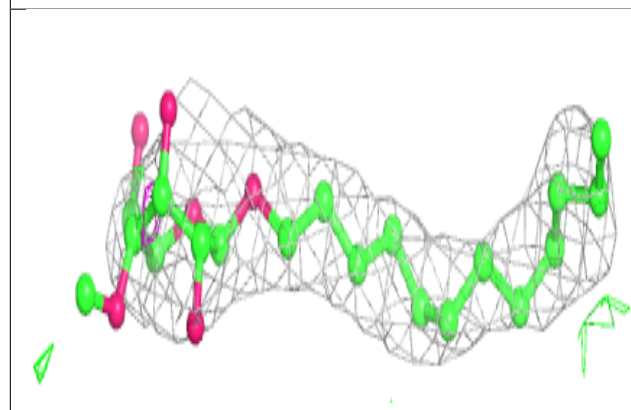
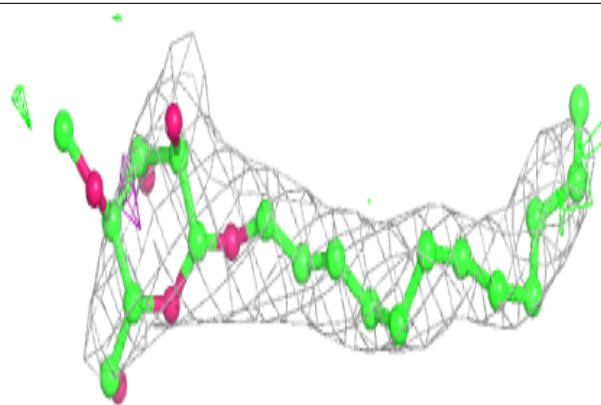
**Electron density around UNL D 411:**

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

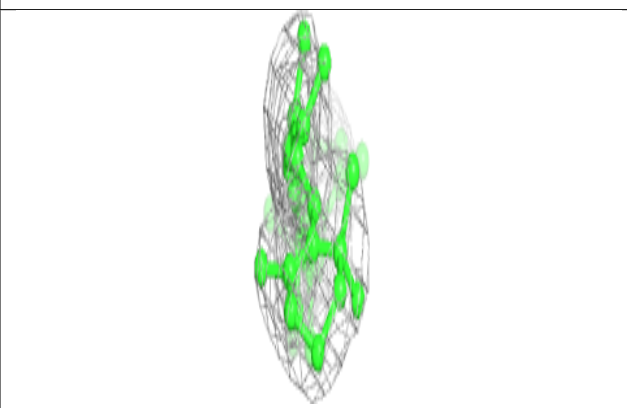
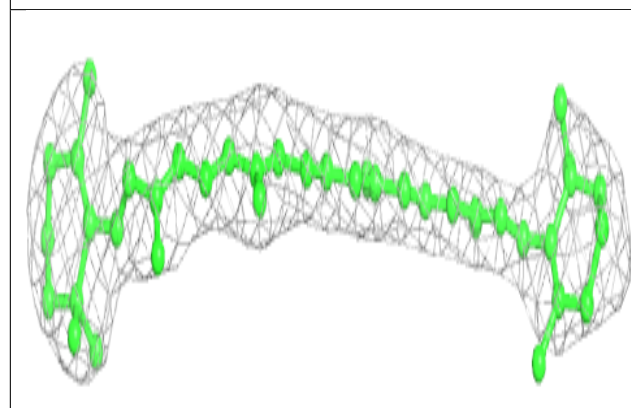
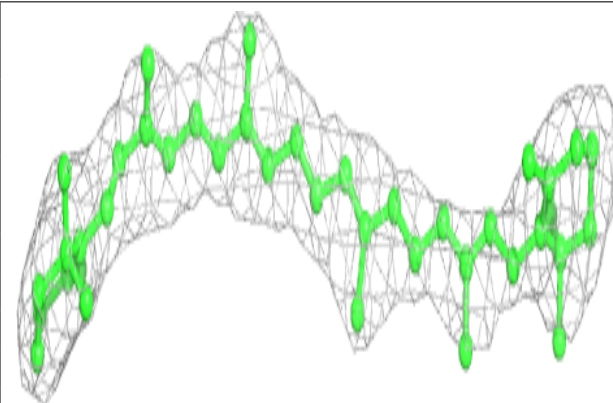


Electron density around LMT B 629:

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

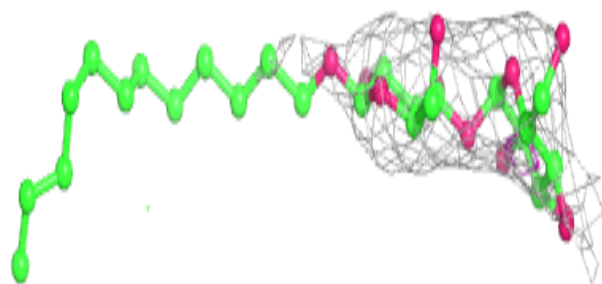
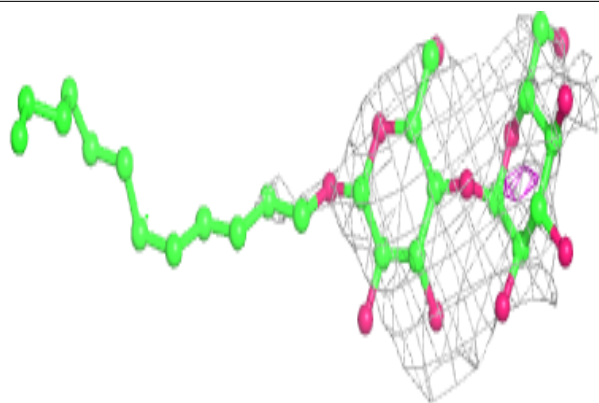
**Electron density around BCR H 101:**

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

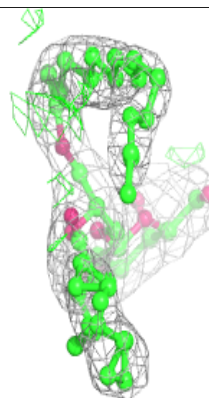
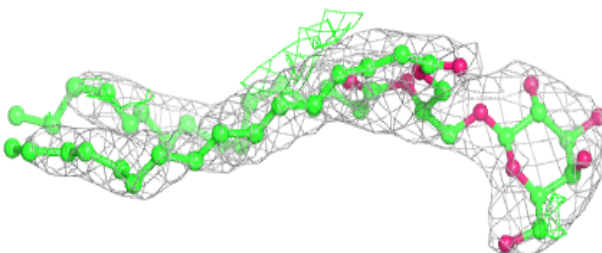
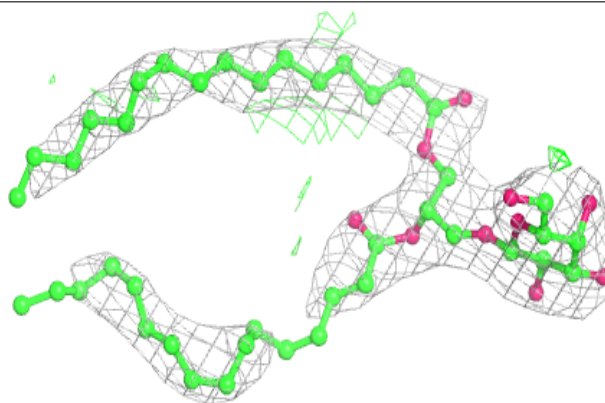


Electron density around LMT a 417:

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

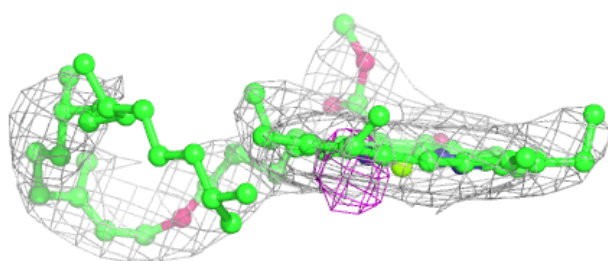
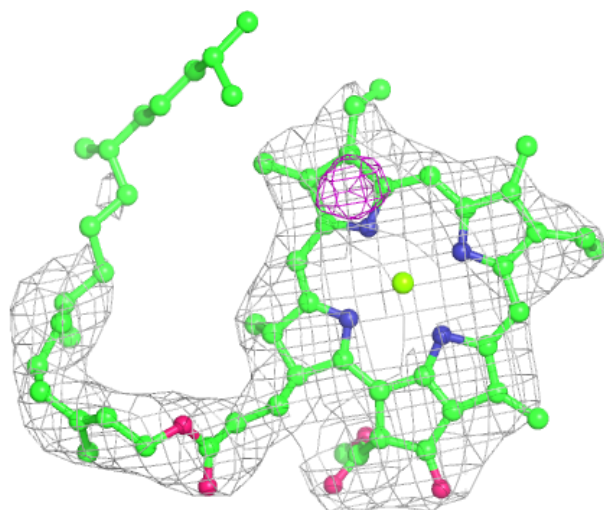
**Electron density around LMG C 501:**

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



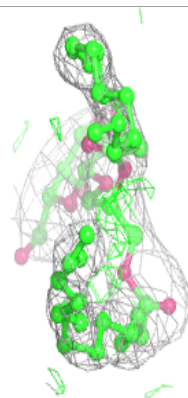
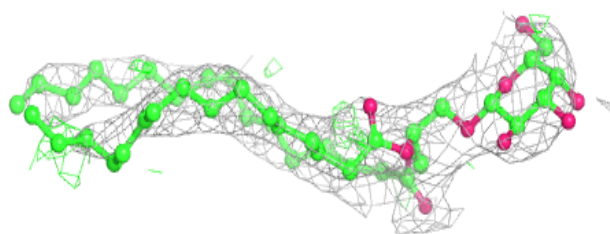
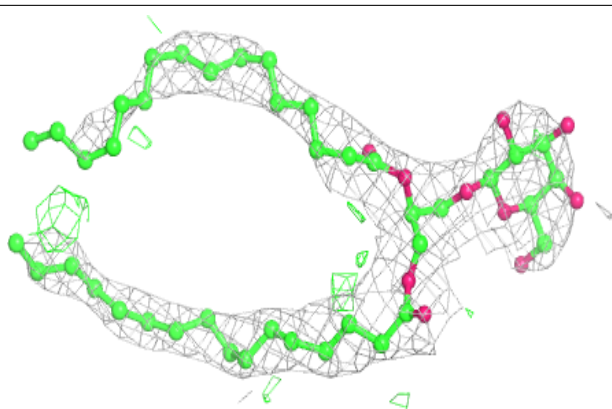
Electron density around CLA C 513:

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

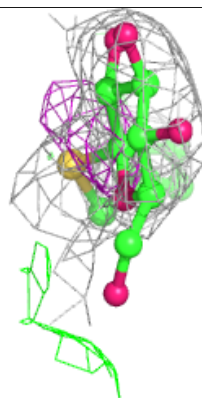
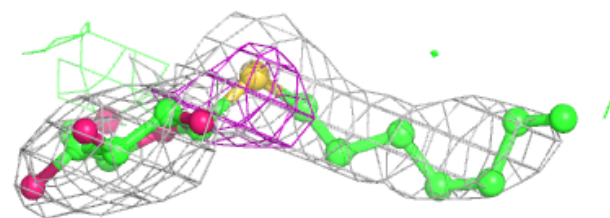
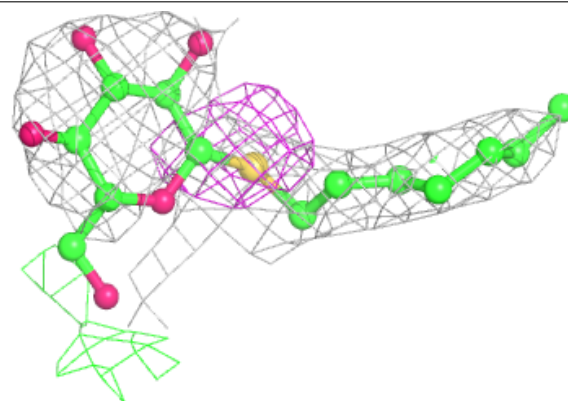


Electron density around LMG a 416:

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

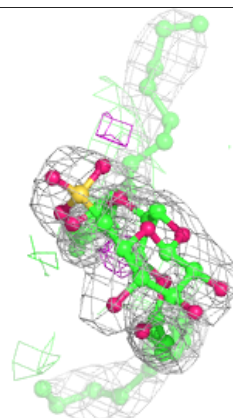
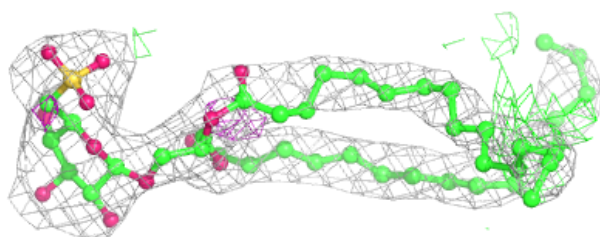
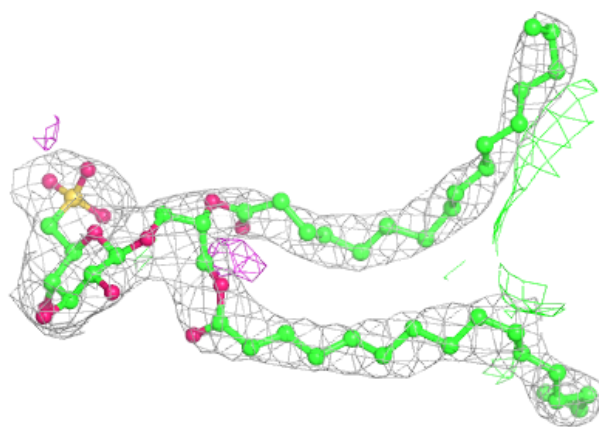
**Electron density around HTG b 628:**

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

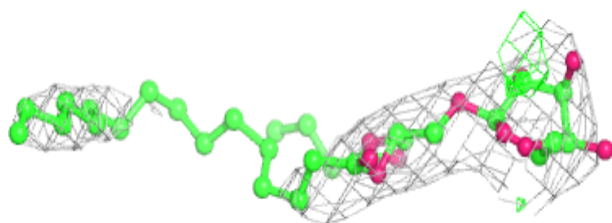
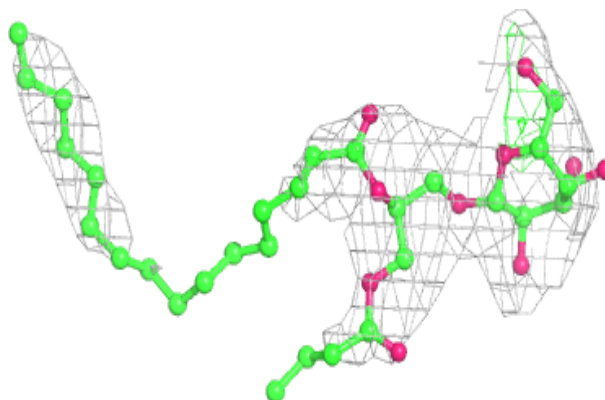


Electron density around SQD B 620:

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

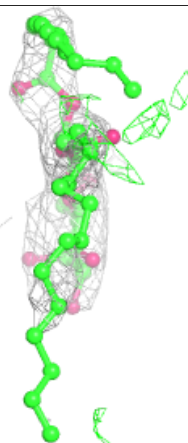
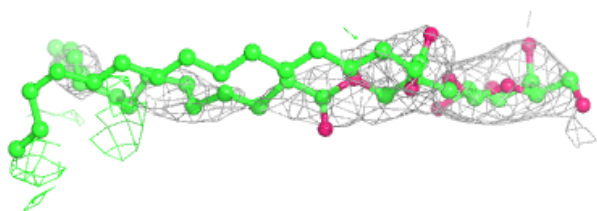
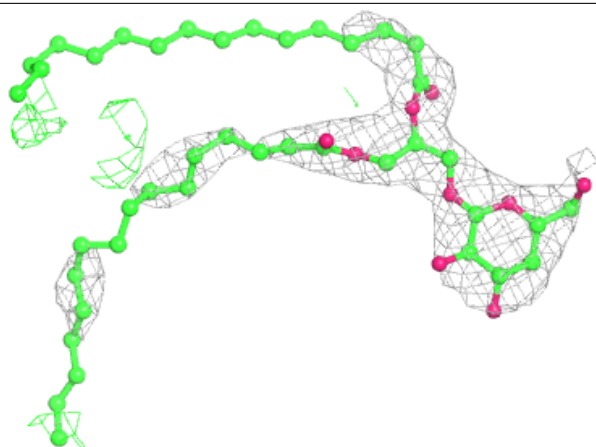
**Electron density around LMG z 101:**

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

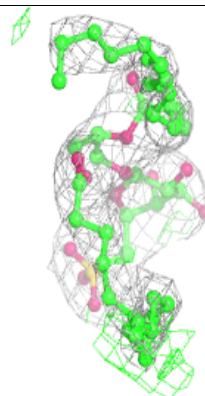
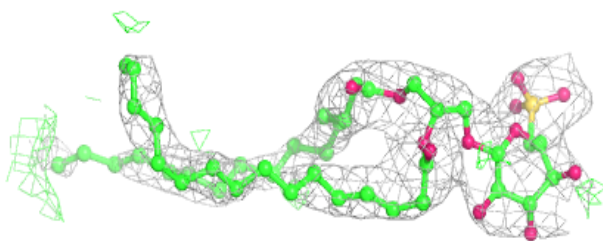
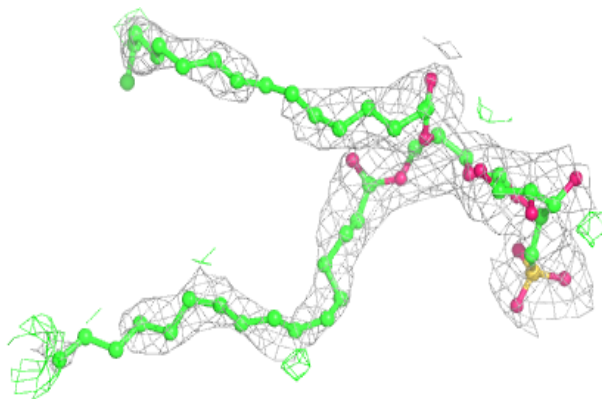


Electron density around LMG c 519:

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

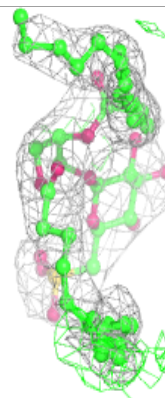
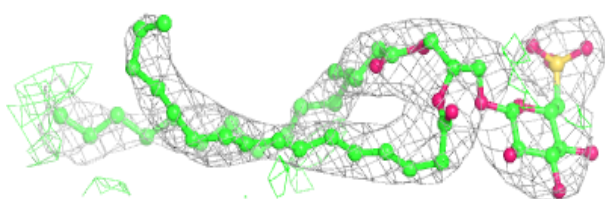
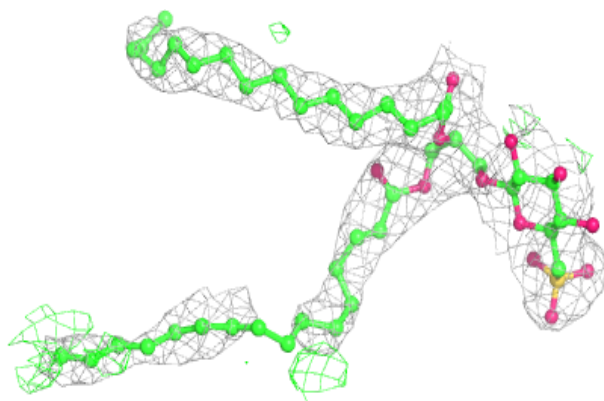
**Electron density around SQD a 412:**

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

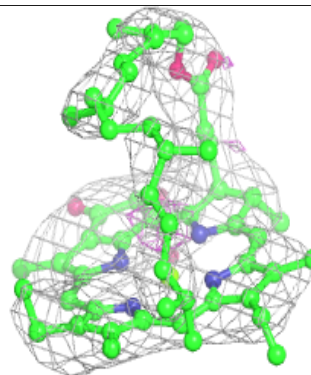
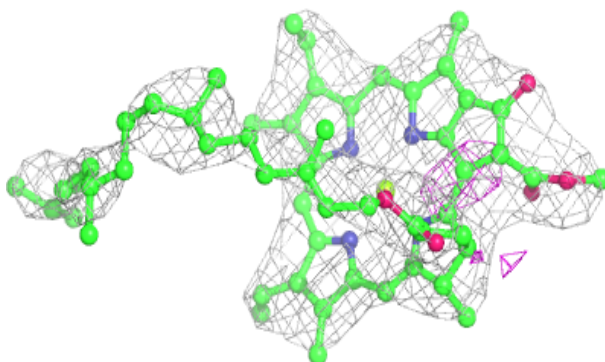
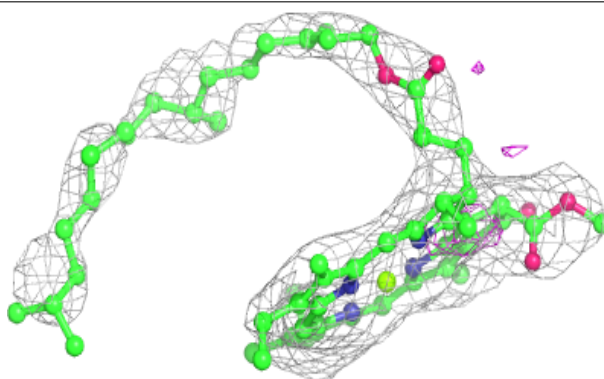


Electron density around SQD A 412:

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

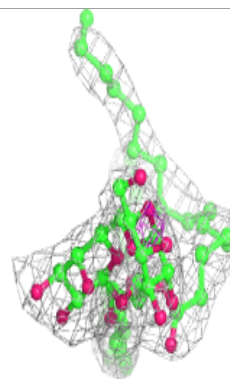
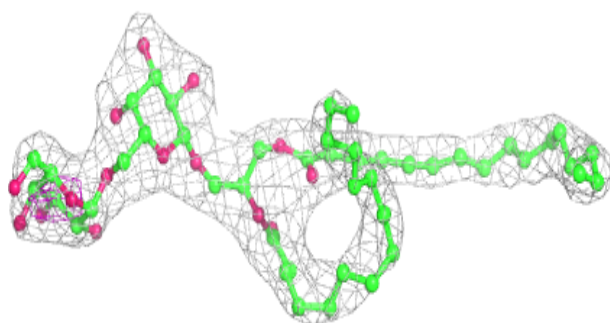
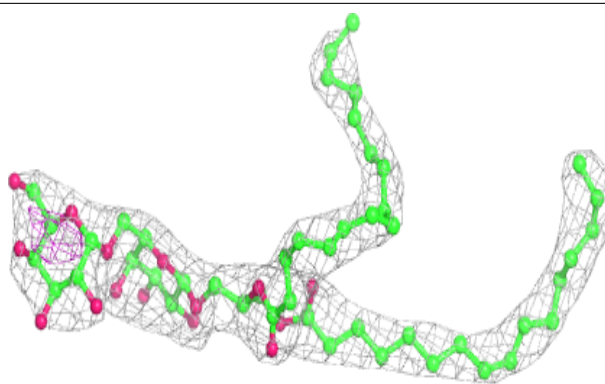
**Electron density around CLA C 514:**

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

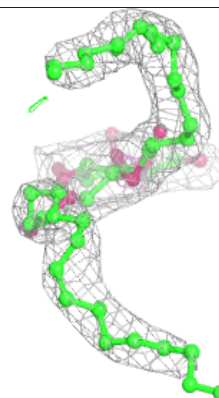
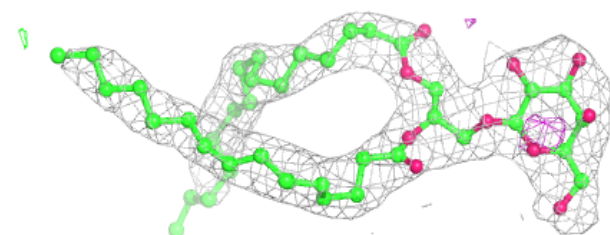
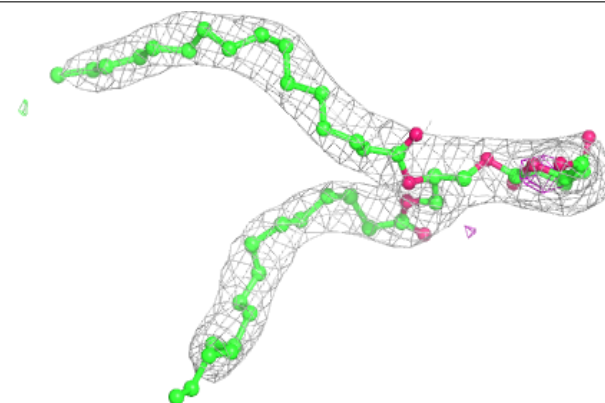


Electron density around DGD h 102:

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

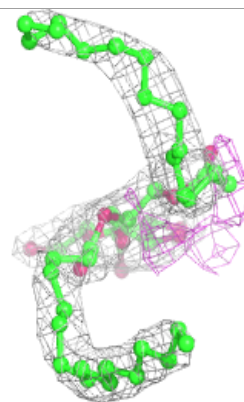
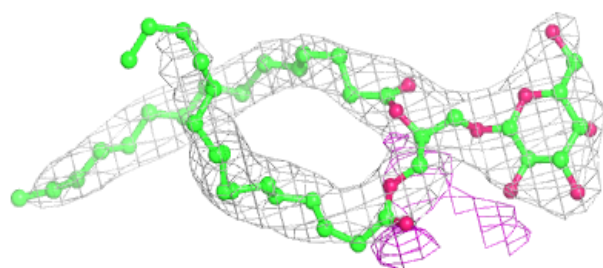
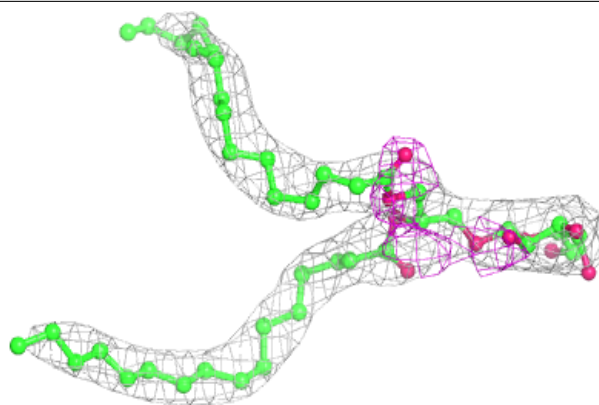
**Electron density around LMG B 621:**

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

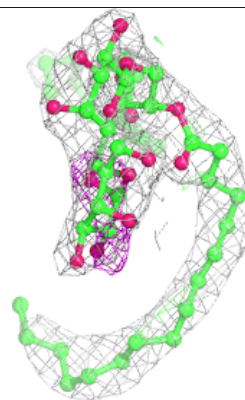
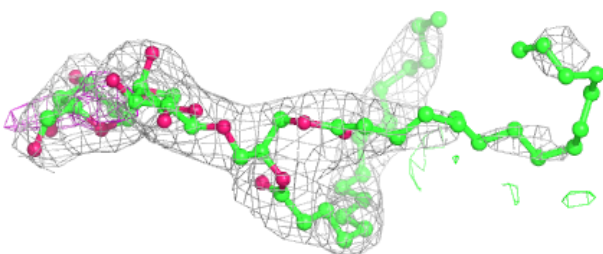
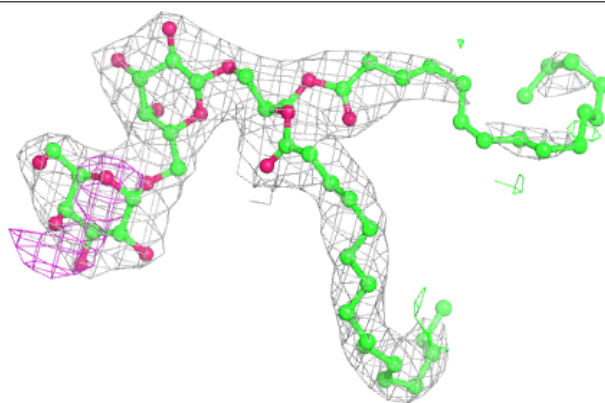


Electron density around LMG b 620:

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

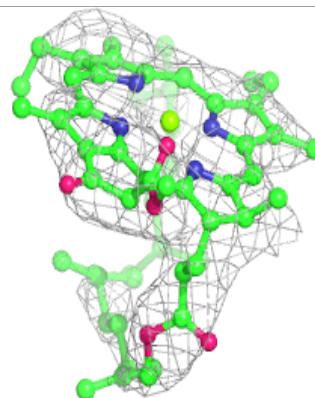
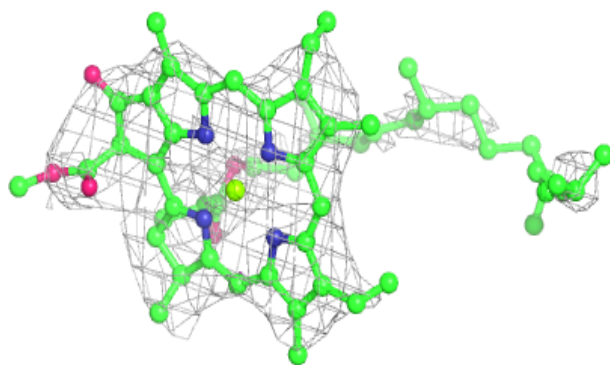
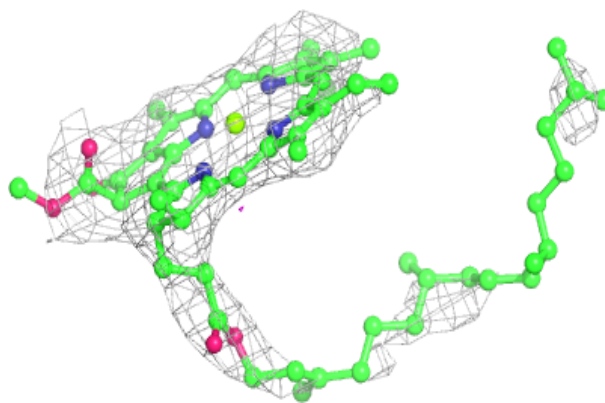
**Electron density around DGD C 518:**

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

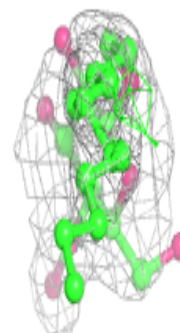
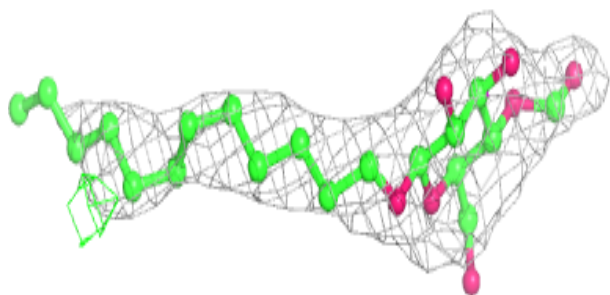
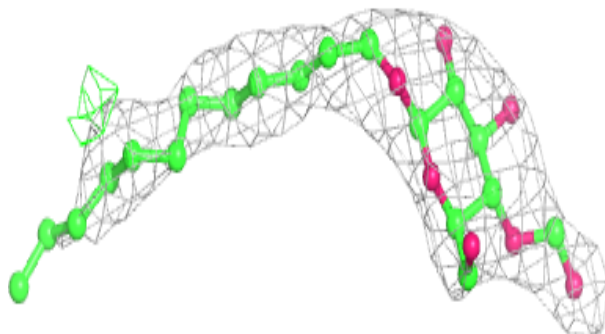


Electron density around CLA c 513:

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

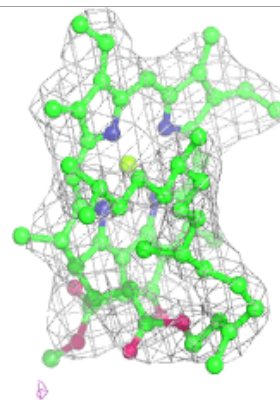
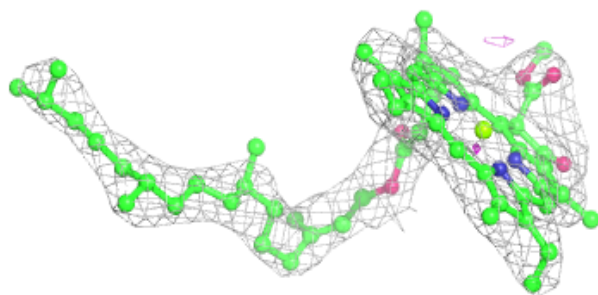
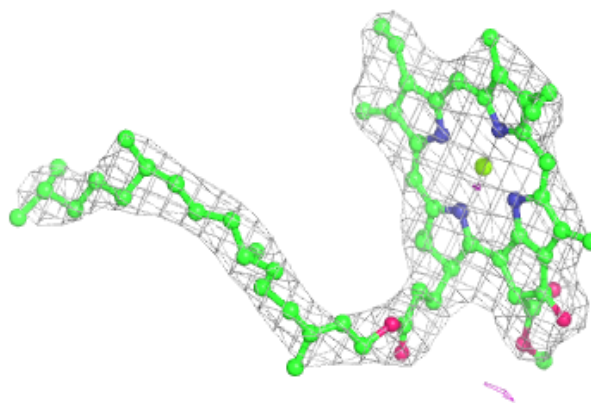
**Electron density around LMT B 631:**

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



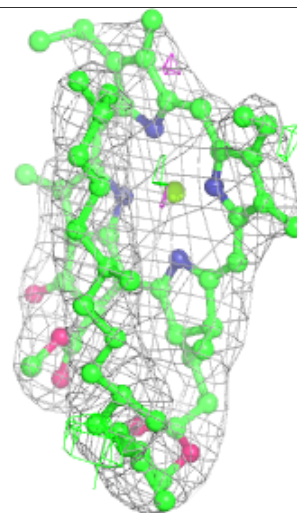
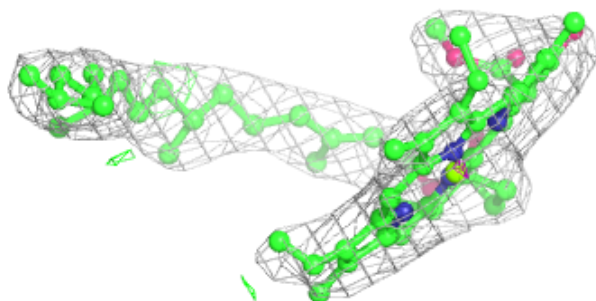
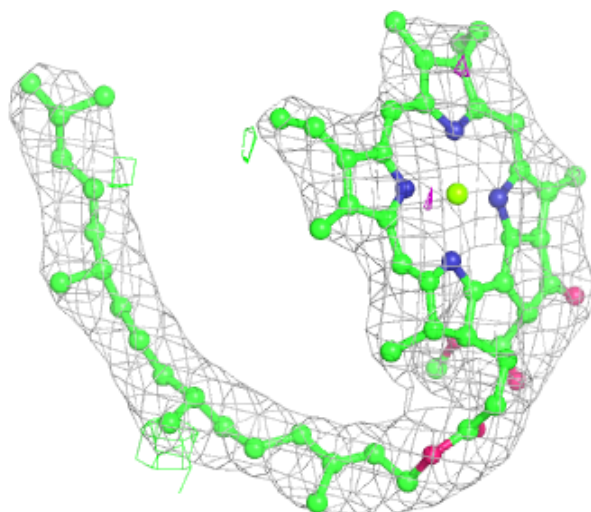
Electron density around CLA C 512:

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



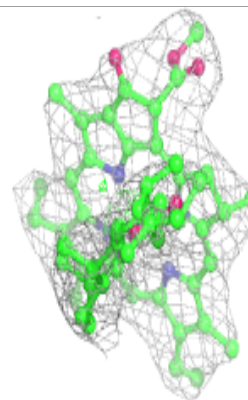
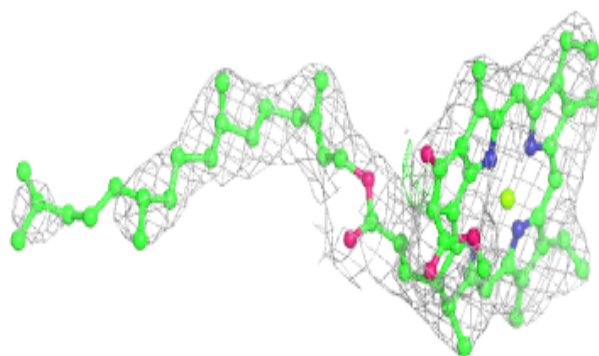
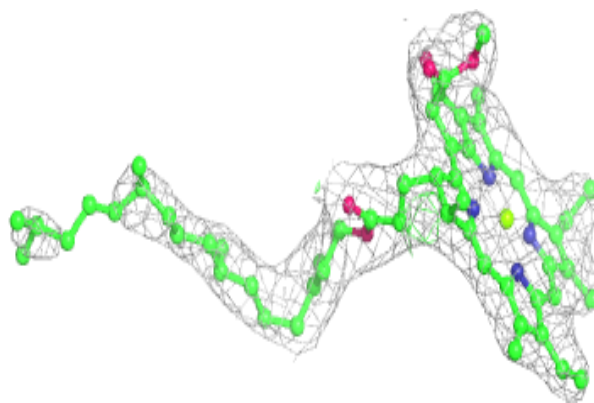
Electron density around CLA C 508:

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



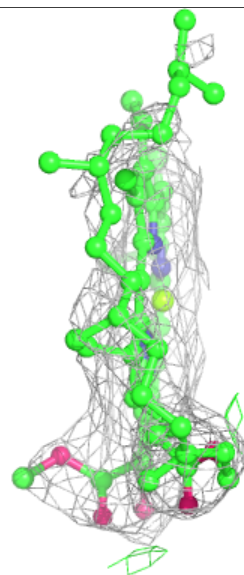
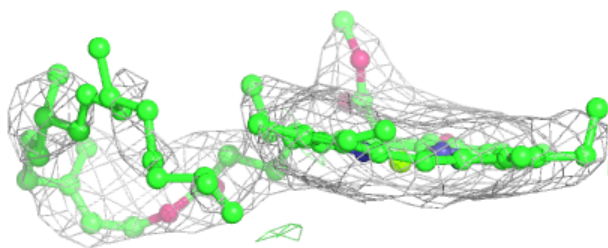
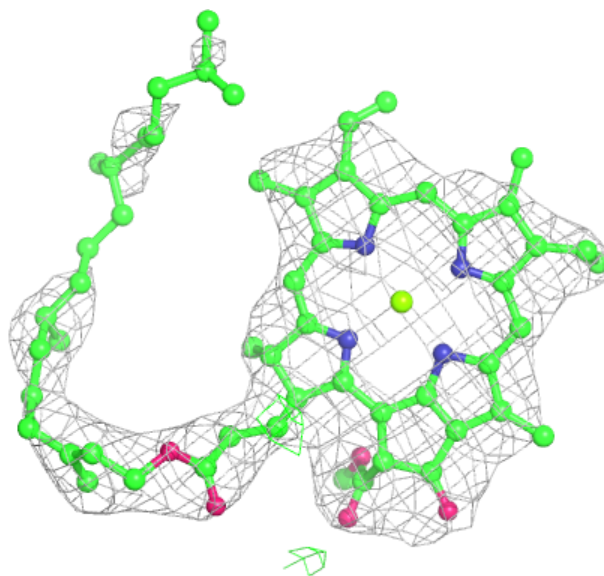
Electron density around CLA c 502:

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



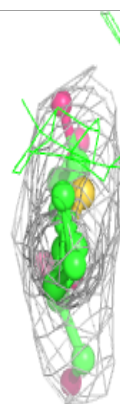
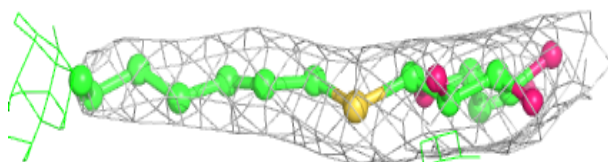
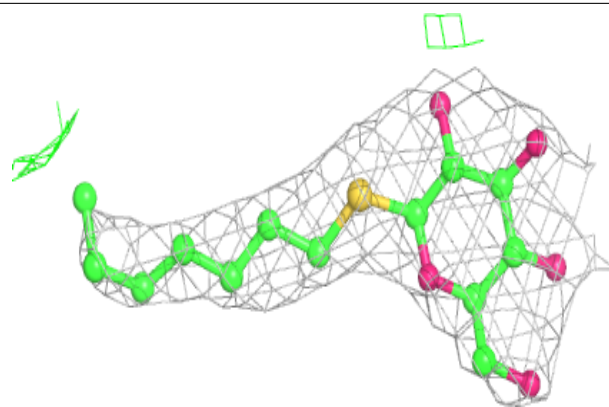
Electron density around CLA c 512:

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

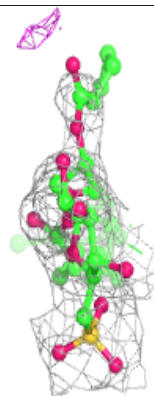
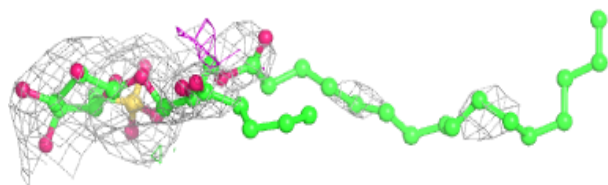
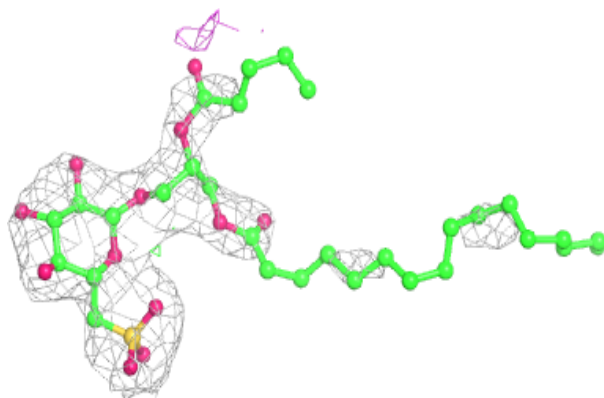


Electron density around HTG B 627:

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

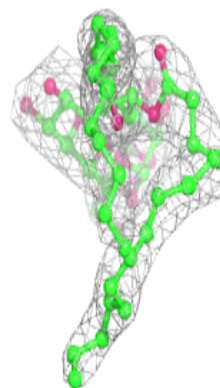
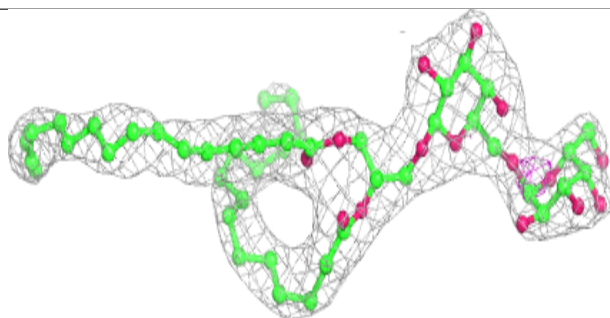
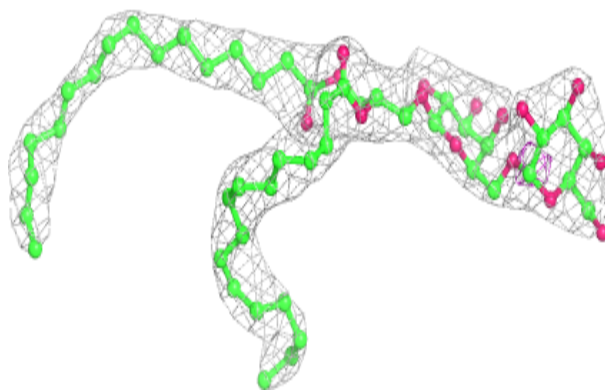
**Electron density around SQD D 413:**

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

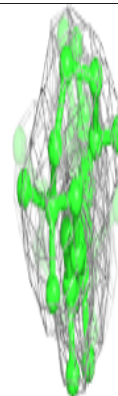
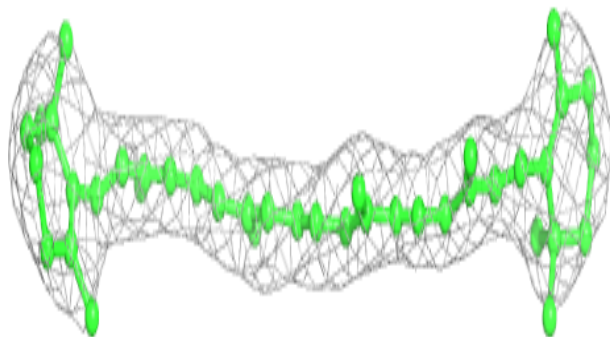
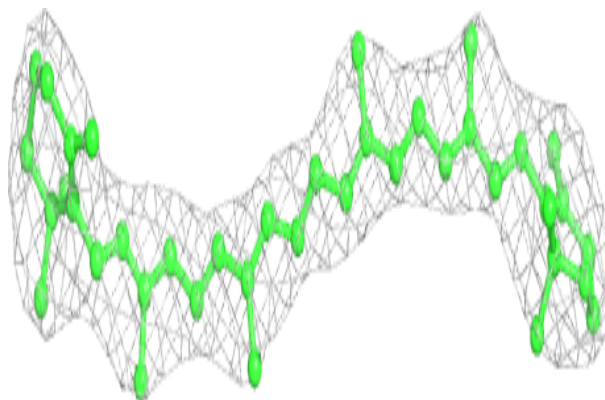


Electron density around DGD H 102:

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

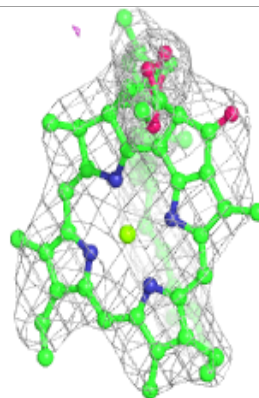
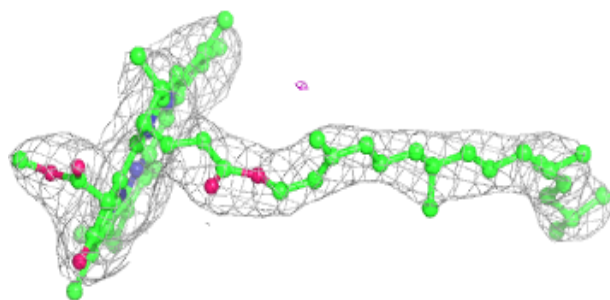
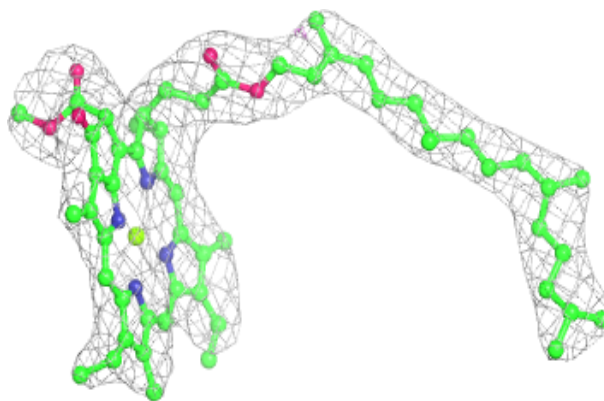
**Electron density around BCR y 101:**

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

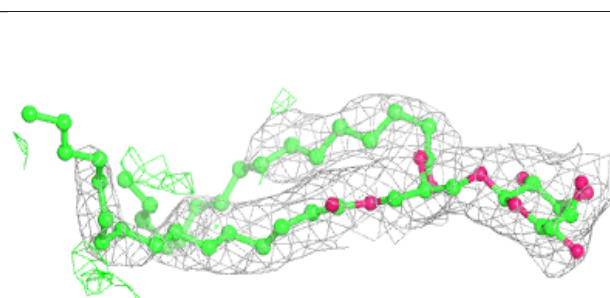
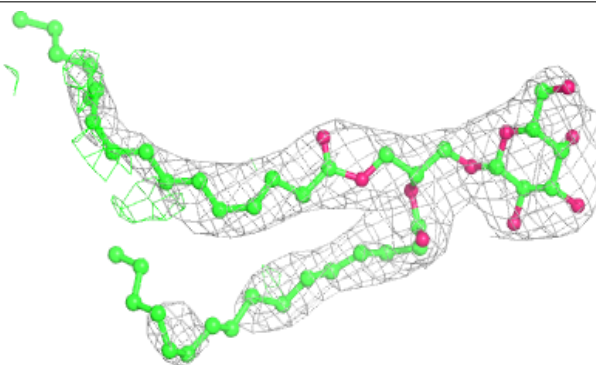


Electron density around CLA B 609:

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

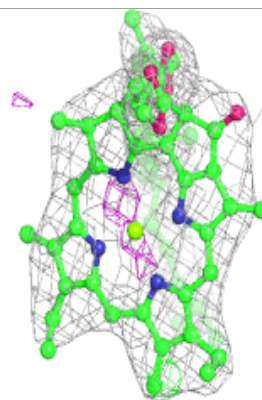
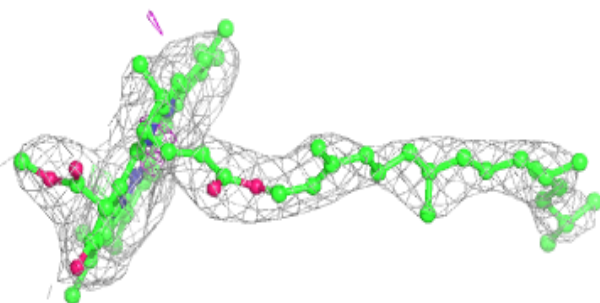
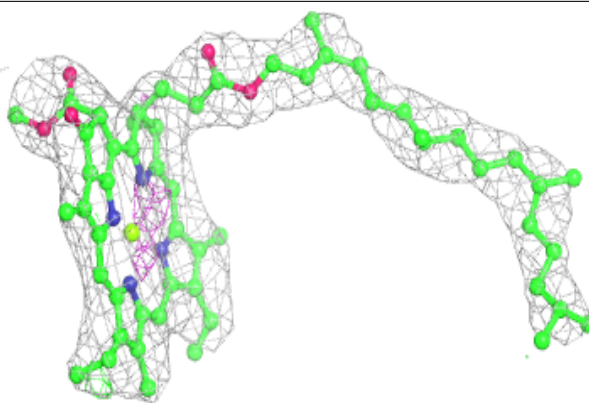
**Electron density around LMG j 101:**

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

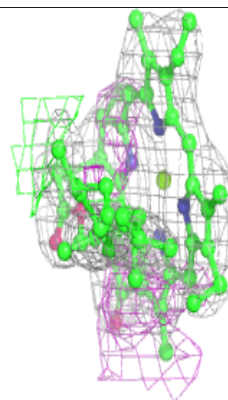
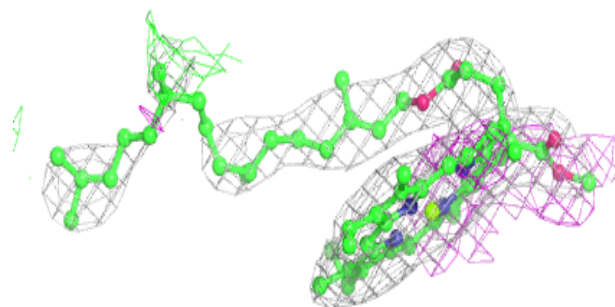
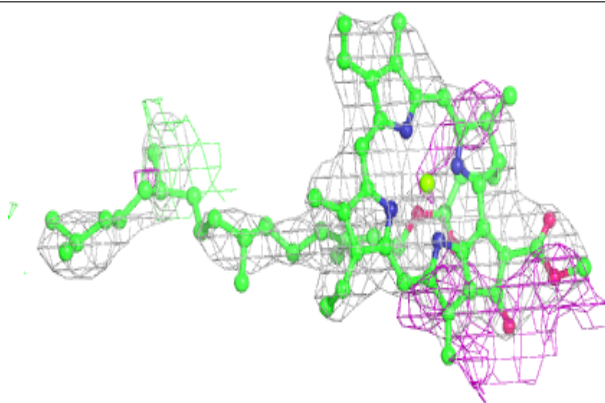


Electron density around CLA b 609:

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

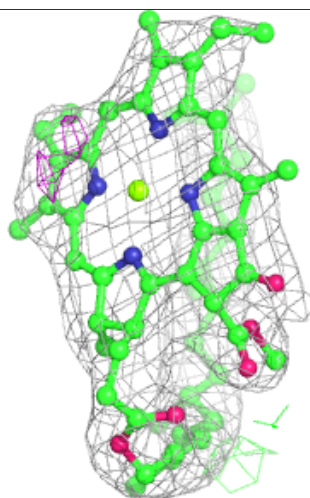
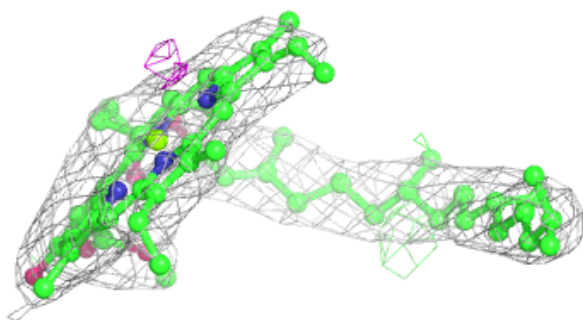
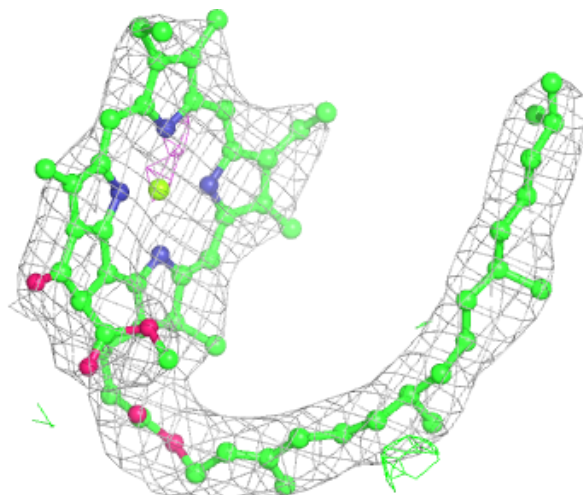
**Electron density around CLA B 614:**

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



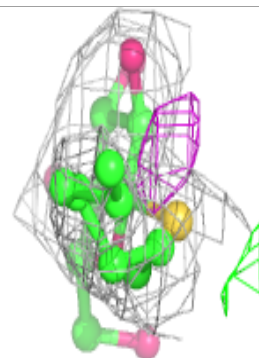
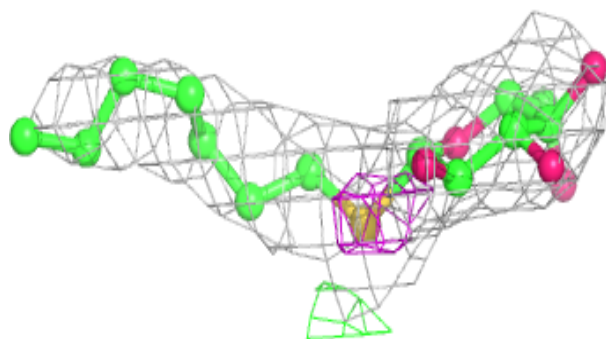
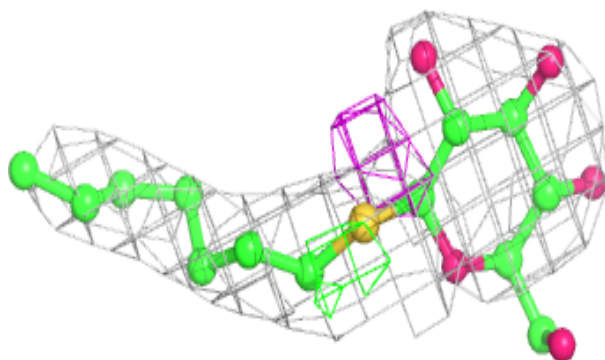
Electron density around CLA c 507:

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



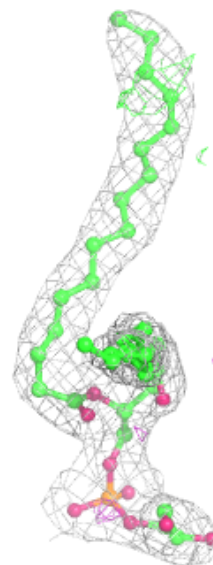
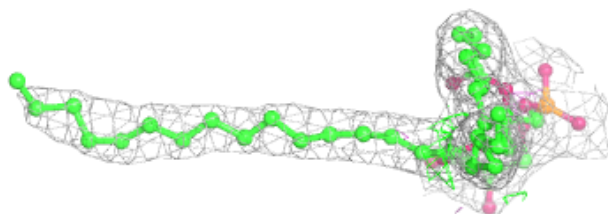
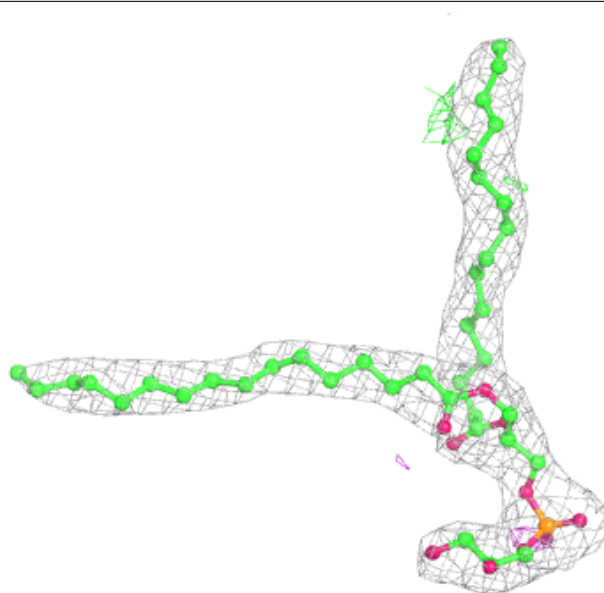
Electron density around HTG B 622:

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



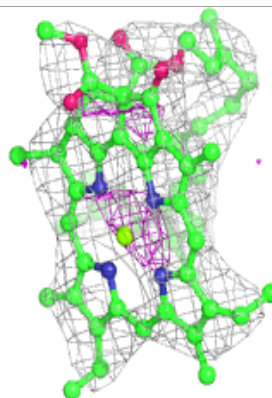
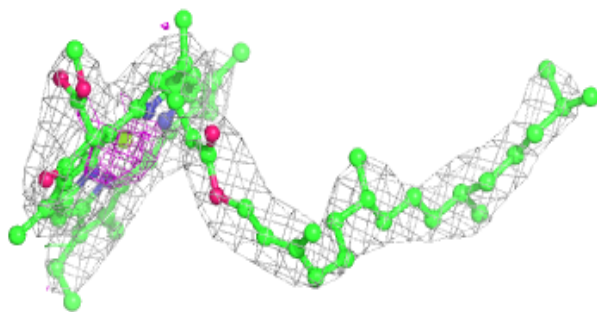
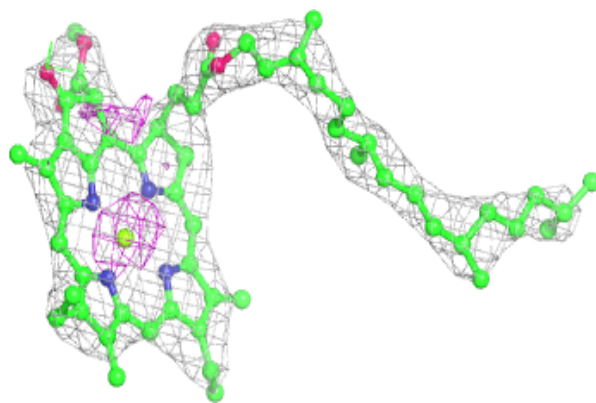
Electron density around LHG 1 101:

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

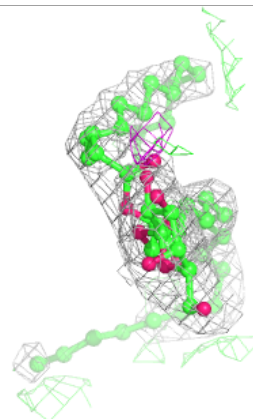
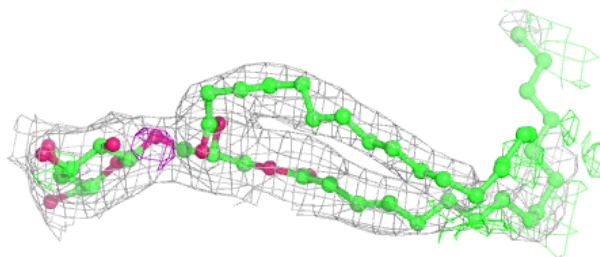
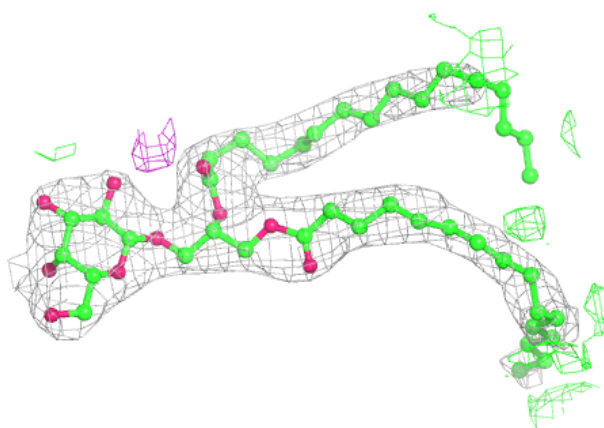


Electron density around CLA c 511:

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

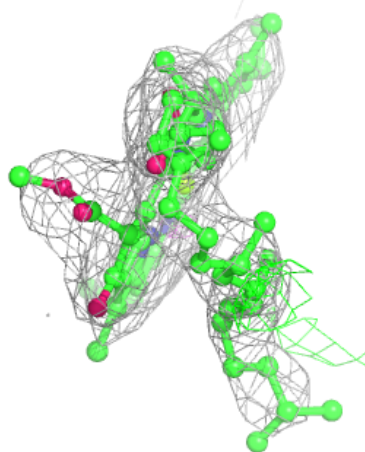
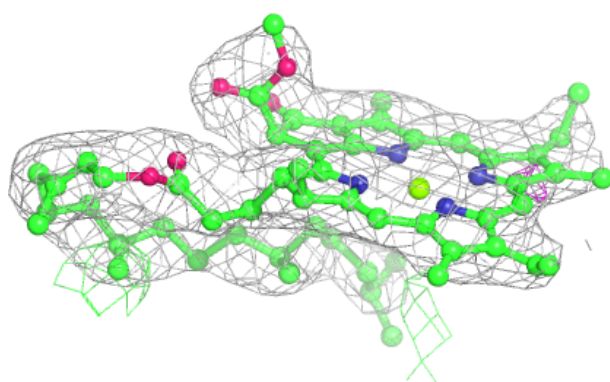
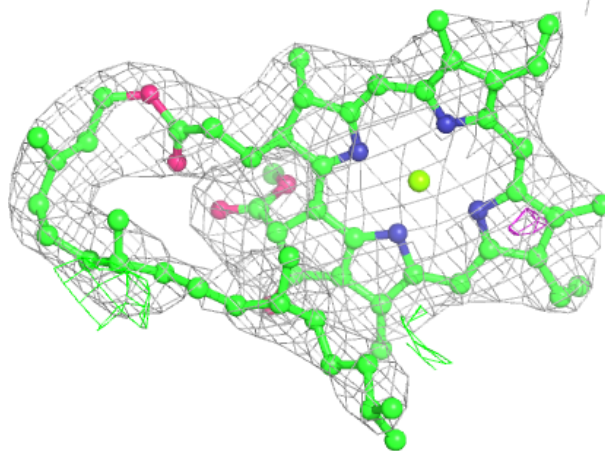
**Electron density around LMG J 101:**

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



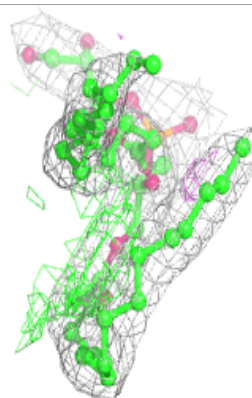
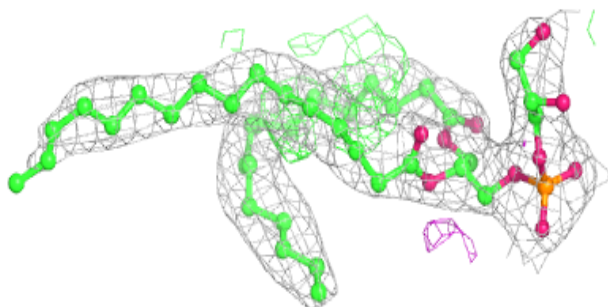
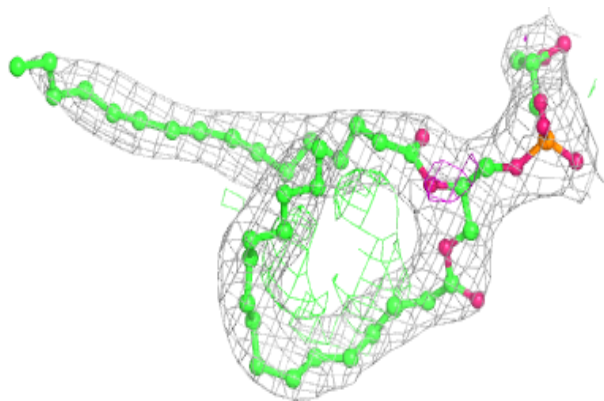
Electron density around CLA c 509:

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

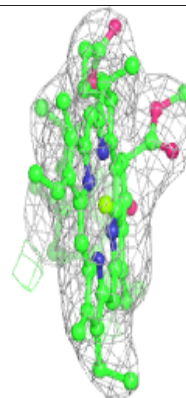
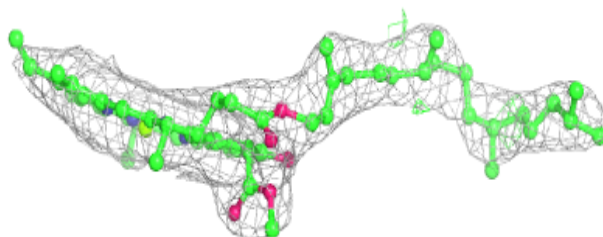
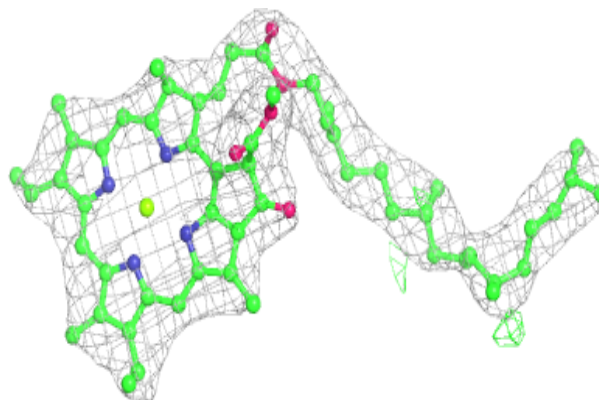


Electron density around LHG A 416:

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

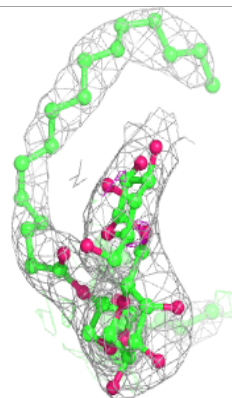
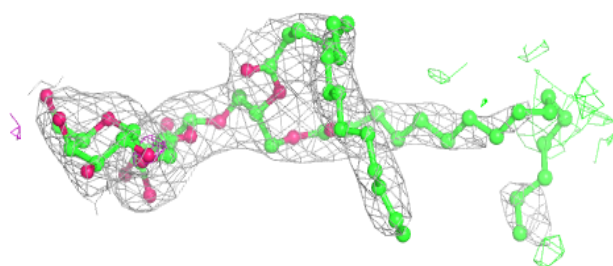
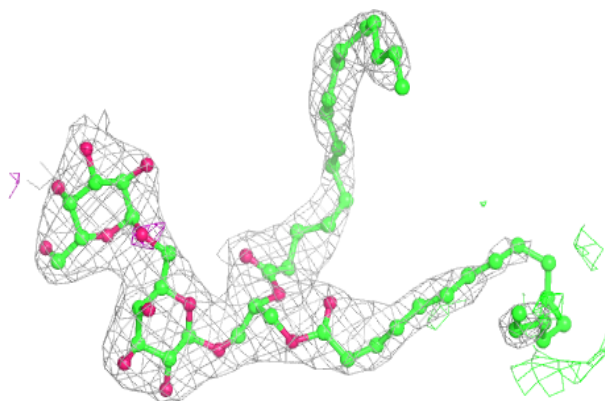
**Electron density around CLA b 602:**

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

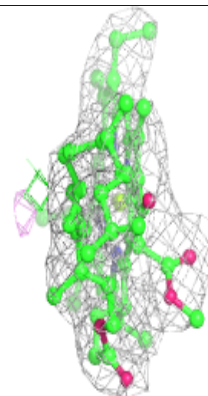
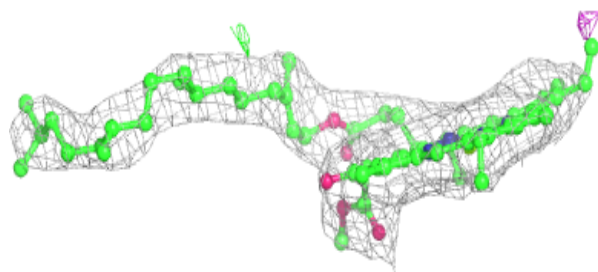
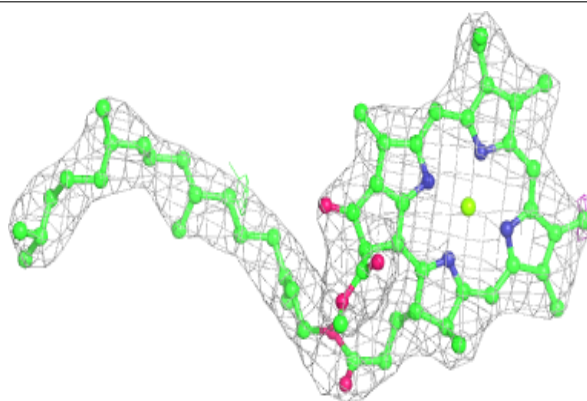


Electron density around DGD c 517:

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

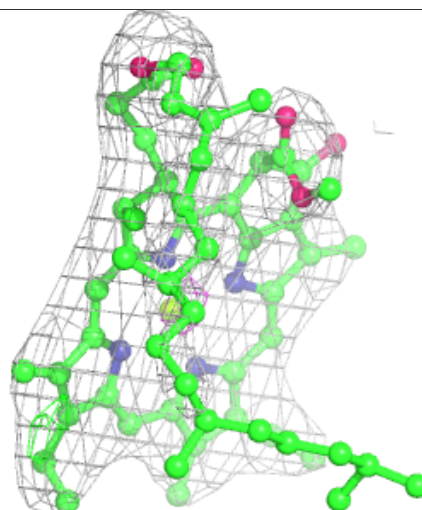
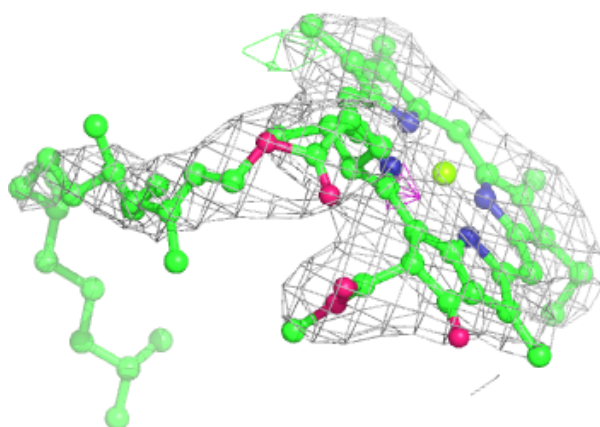
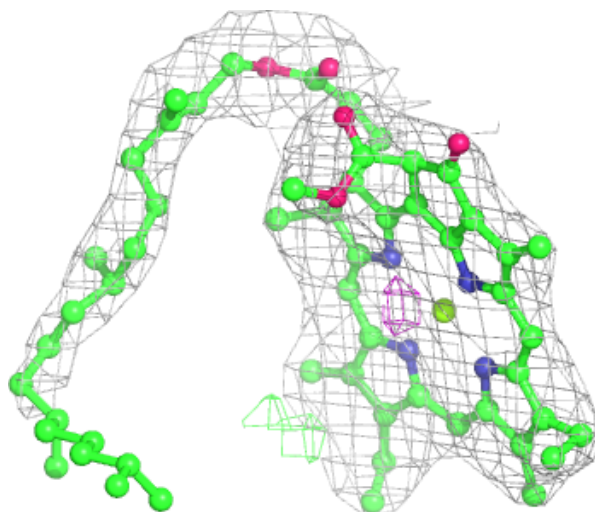
**Electron density around CLA B 602:**

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



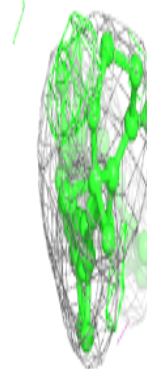
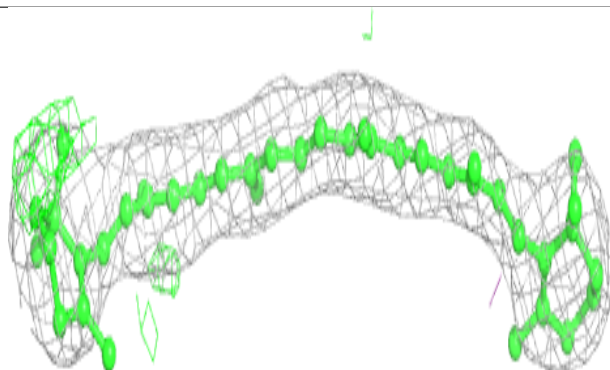
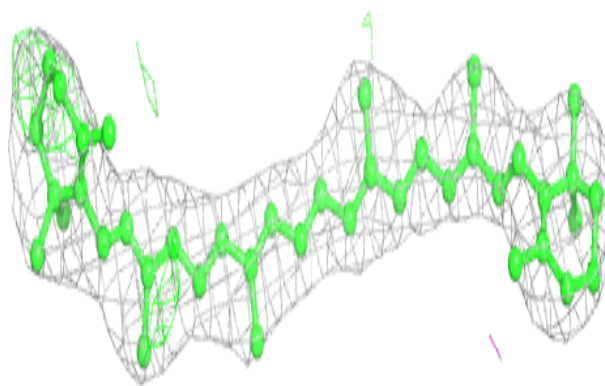
Electron density around CLA b 616:

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

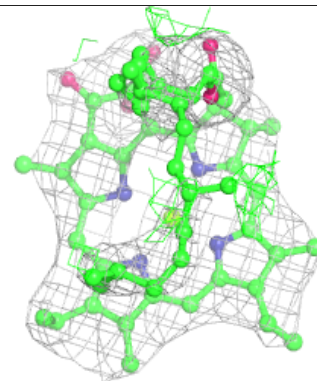
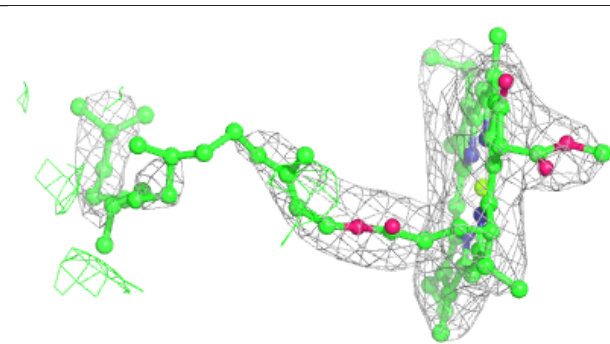
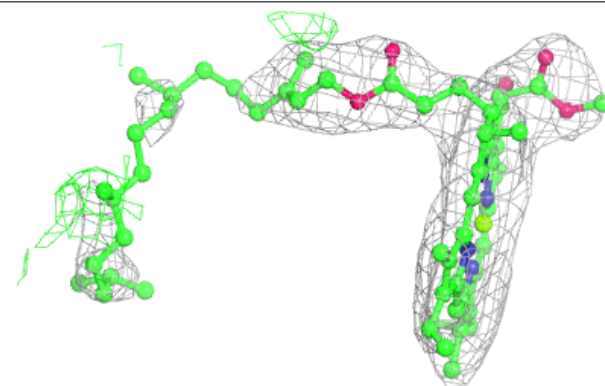


Electron density around BCR d 405:

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

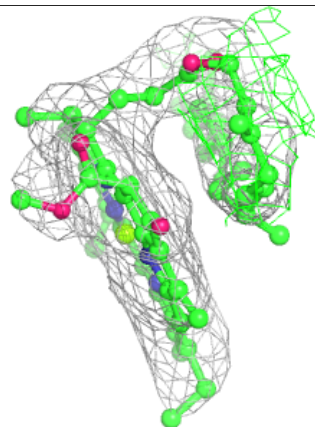
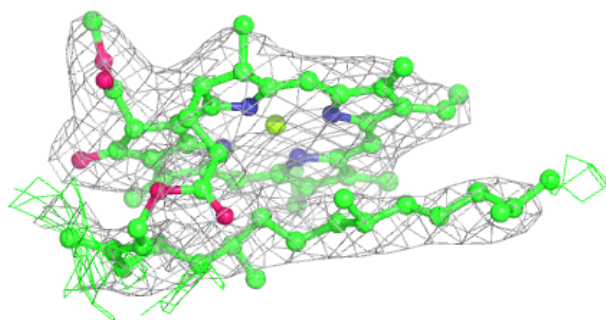
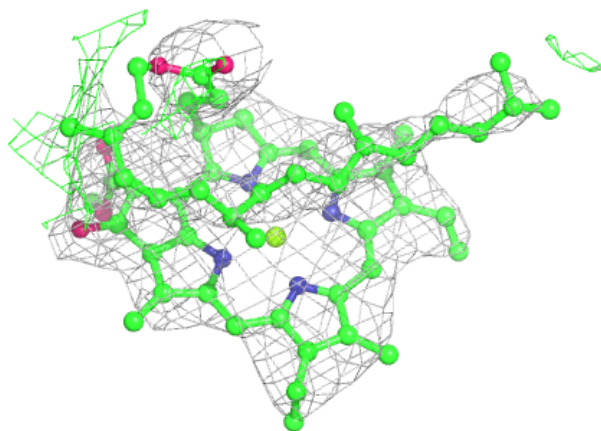
**Electron density around CLA C 507:**

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



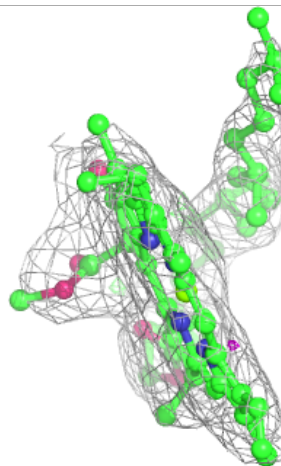
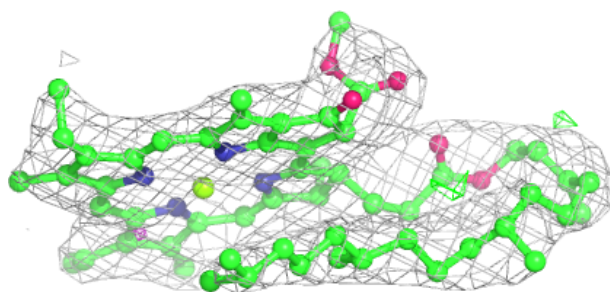
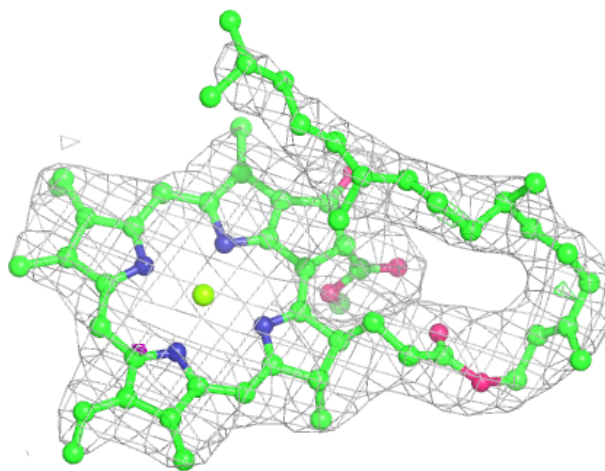
Electron density around CLA b 601:

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



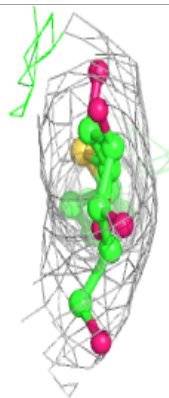
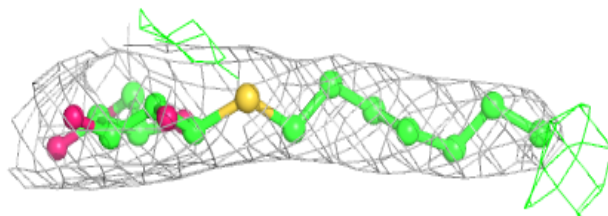
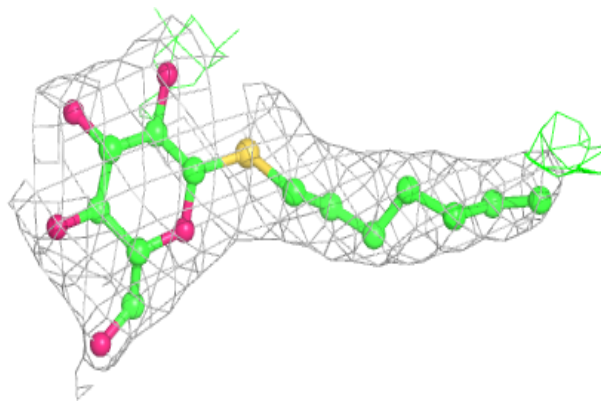
Electron density around CLA C 510:

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



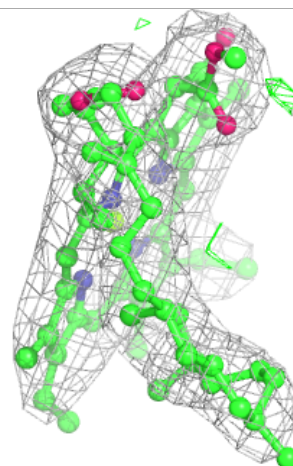
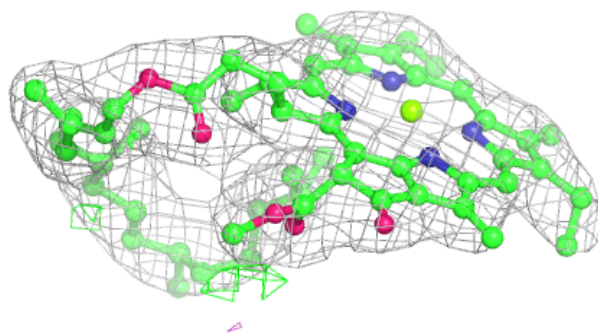
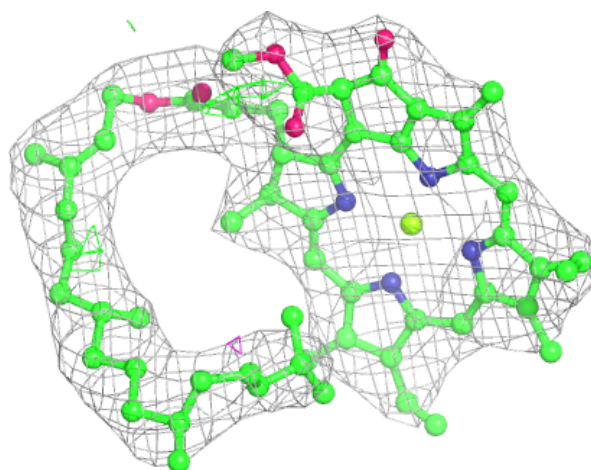
Electron density around HTG b 625:

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



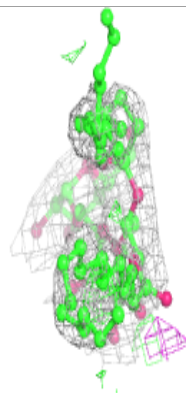
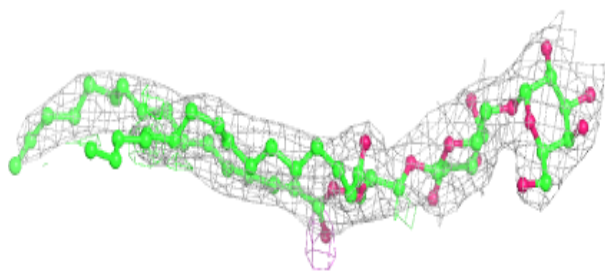
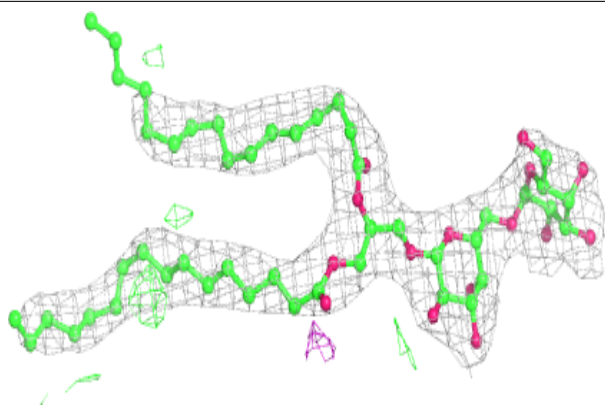
Electron density around CLA b 615:

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

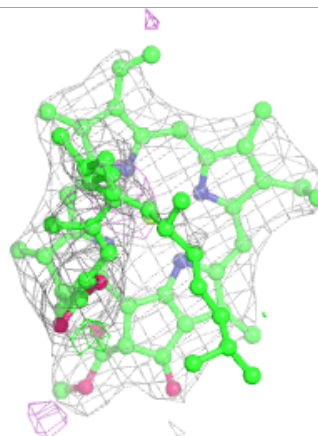
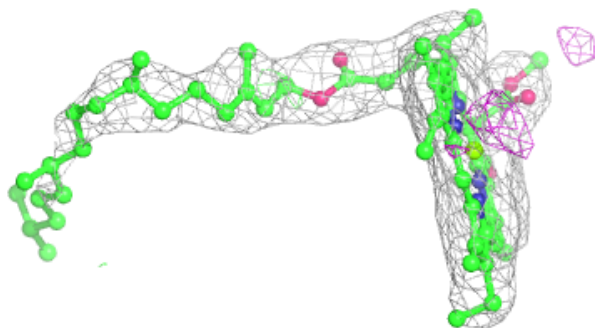
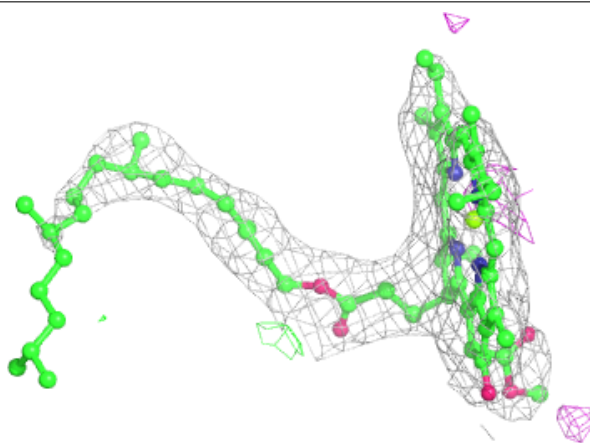


Electron density around DGD C 519:

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

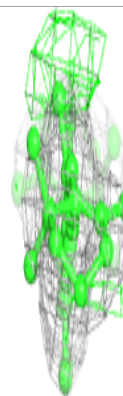
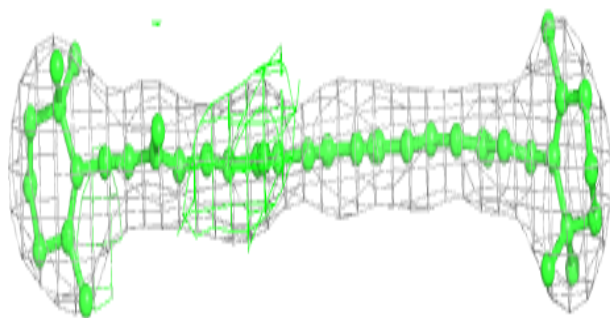
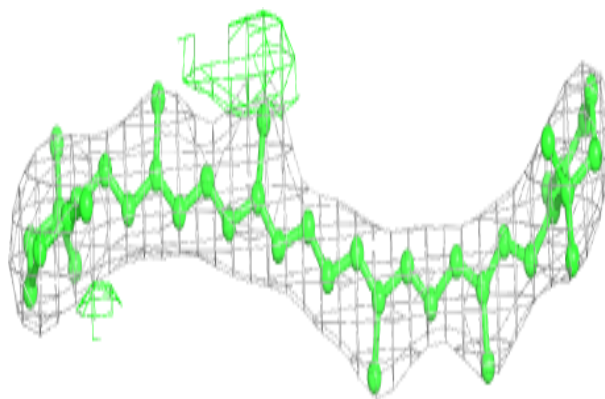
**Electron density around CLA D 405:**

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

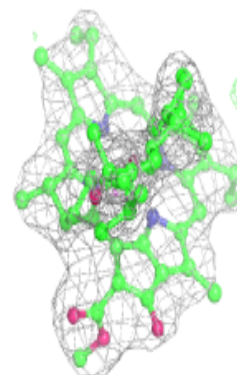
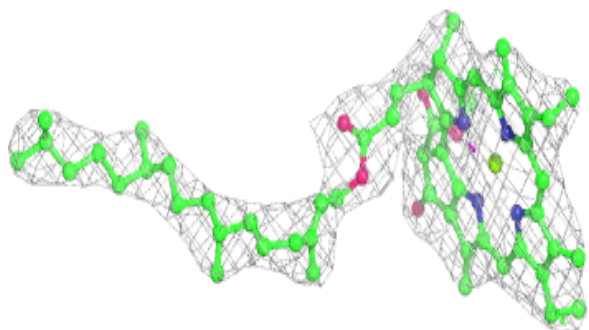
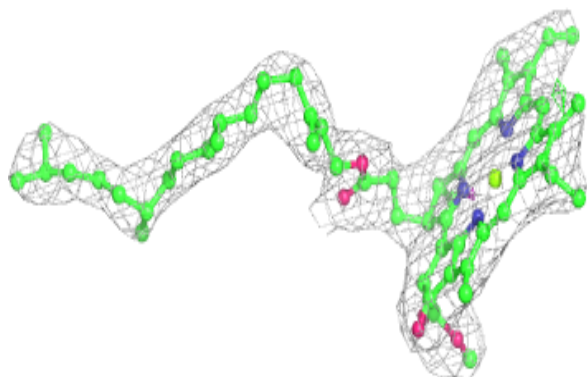


Electron density around BCR C 516:

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

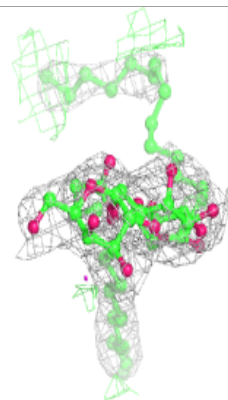
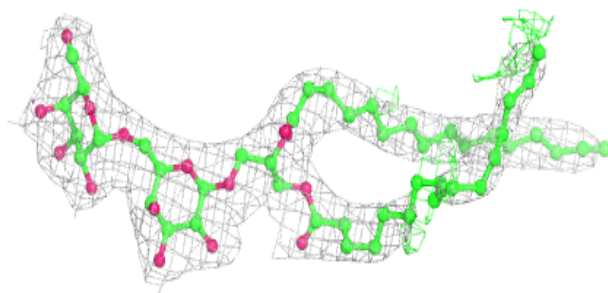
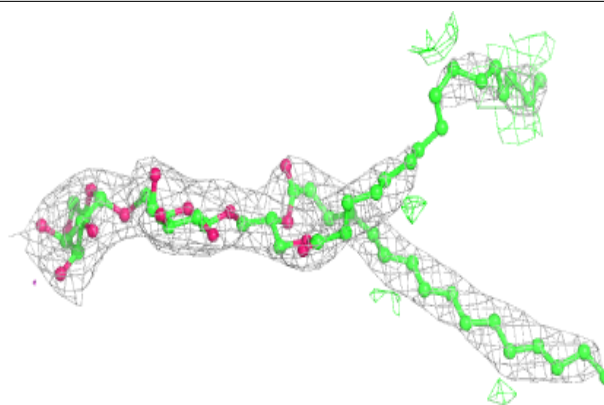
**Electron density around CLA C 503:**

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



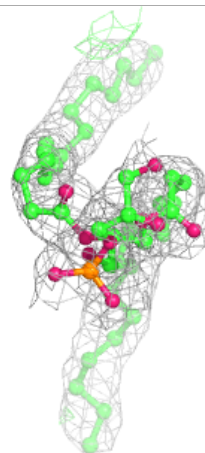
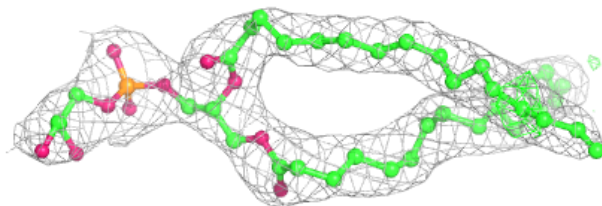
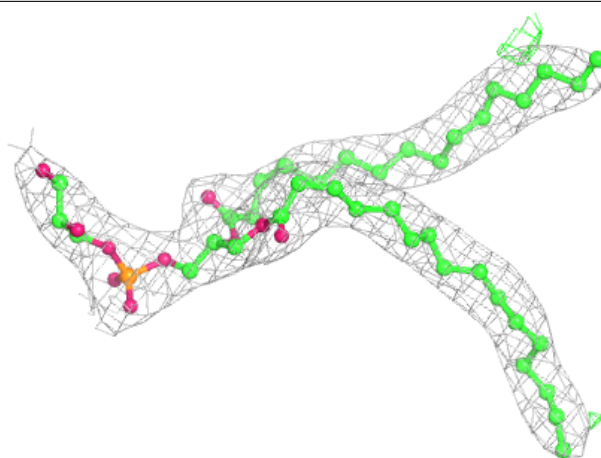
Electron density around DGD C 517:

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



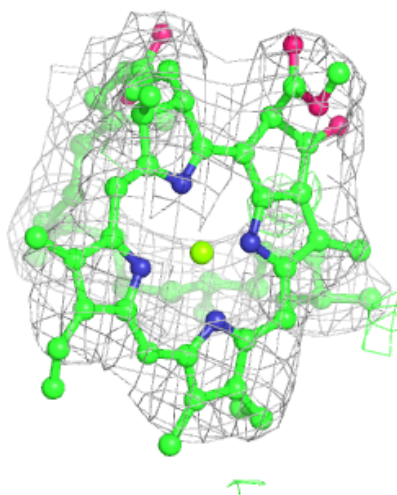
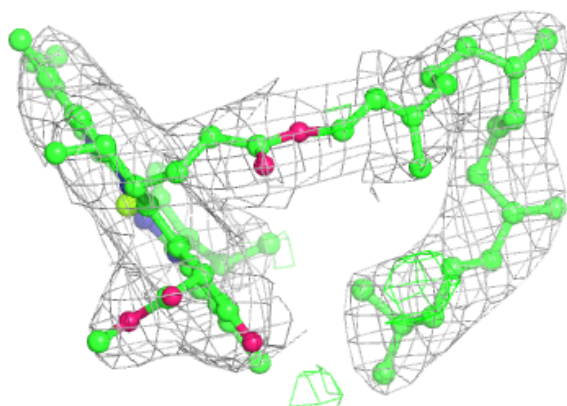
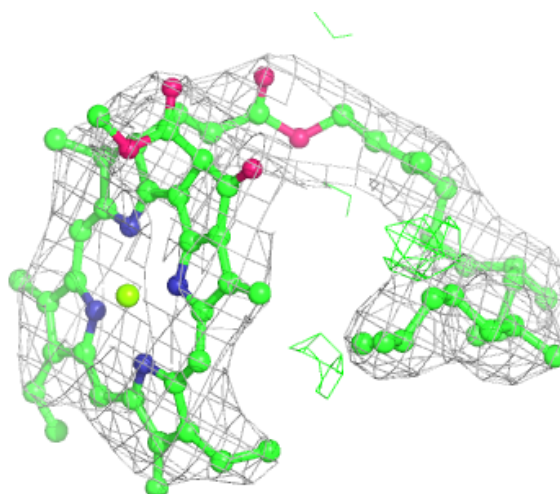
Electron density around LHG d 408:

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



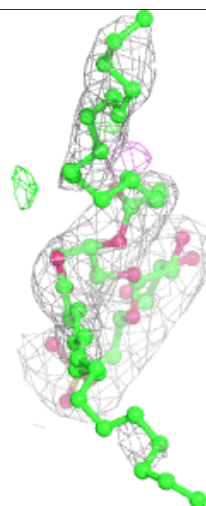
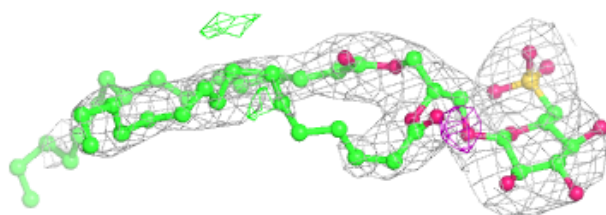
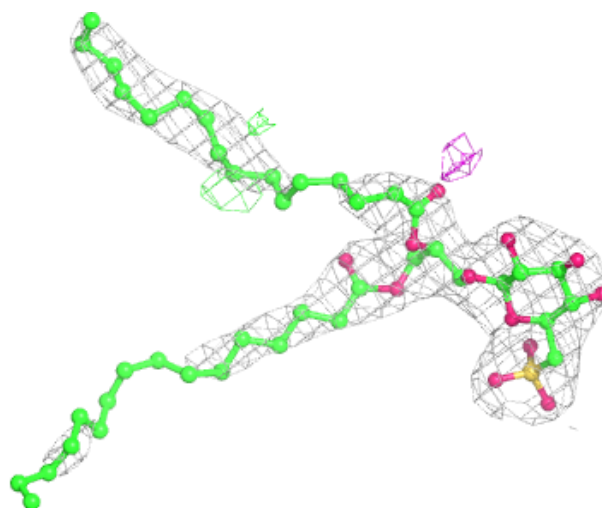
Electron density around CLA c 503:

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



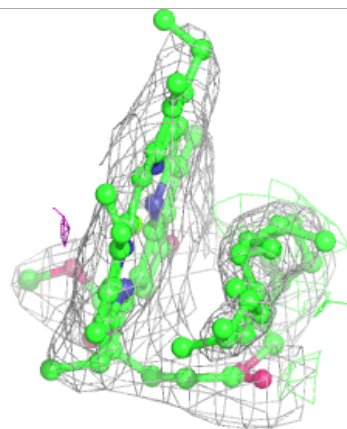
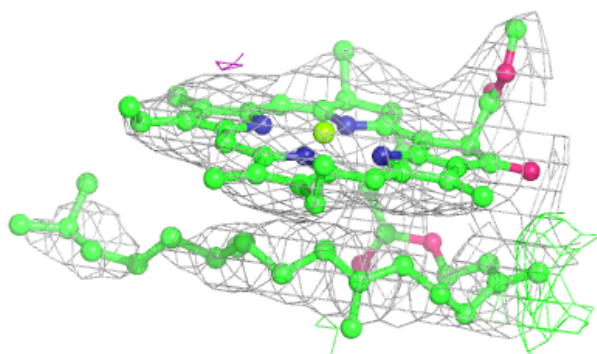
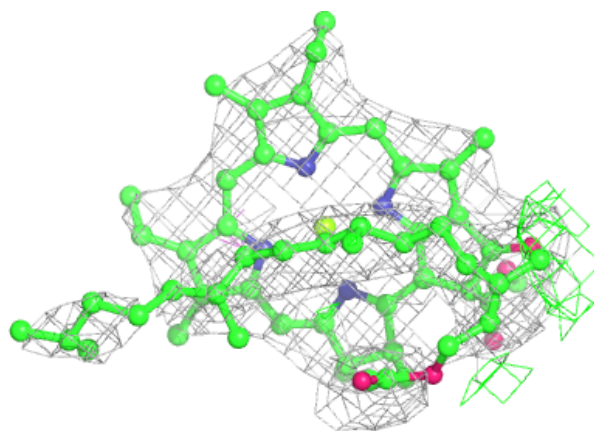
Electron density around SQD a 410:

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



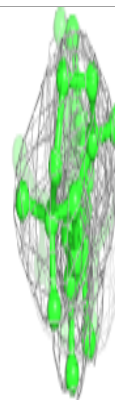
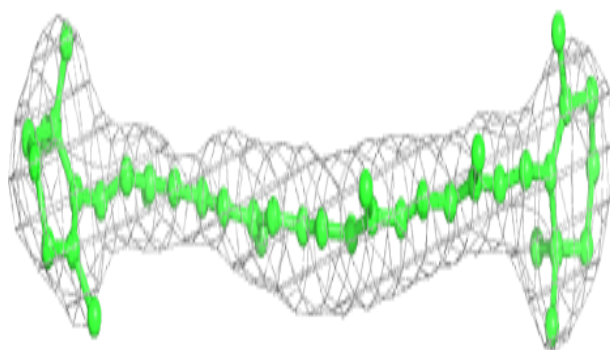
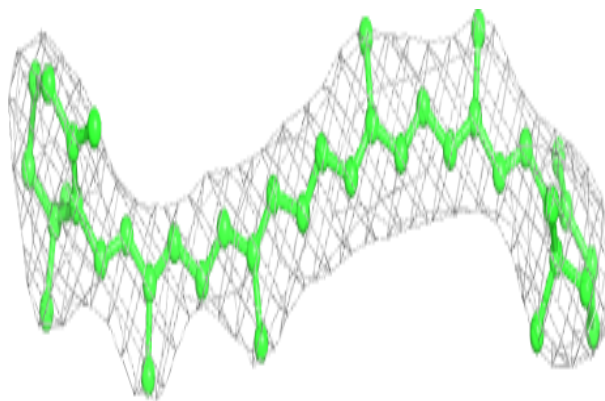
Electron density around CLA B 601:

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

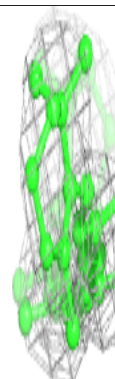
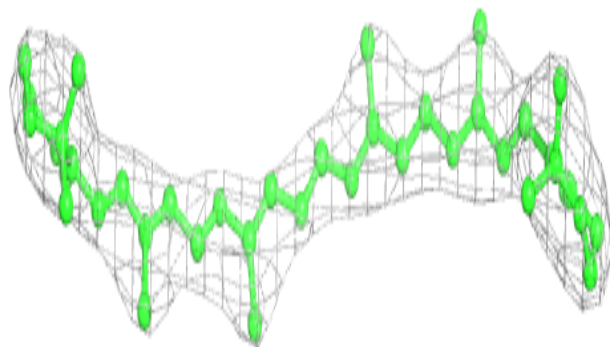
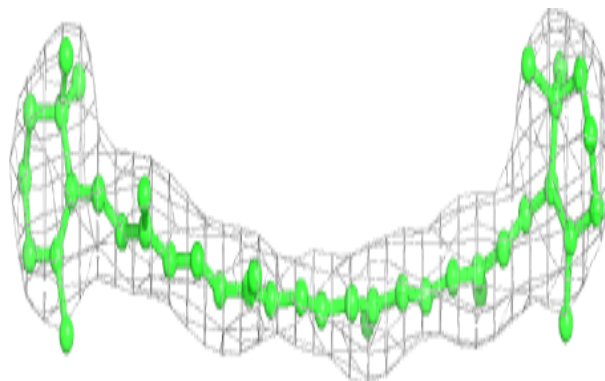


Electron density around BCR Y 101:

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

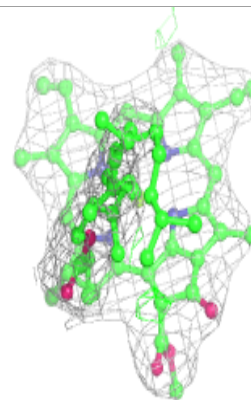
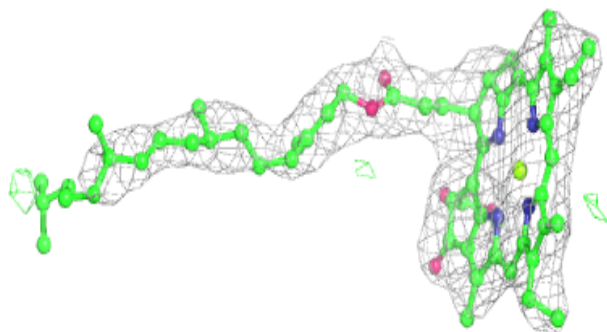
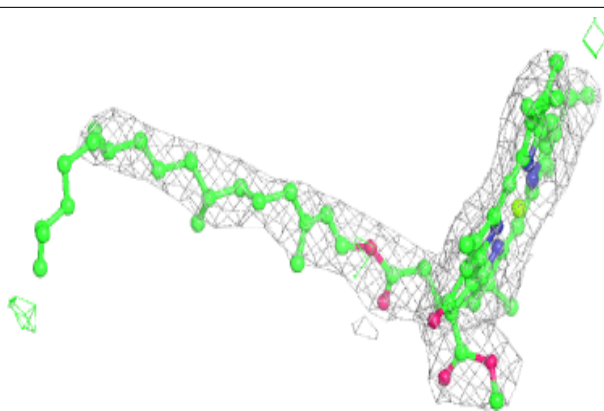
**Electron density around BCR K 102:**

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

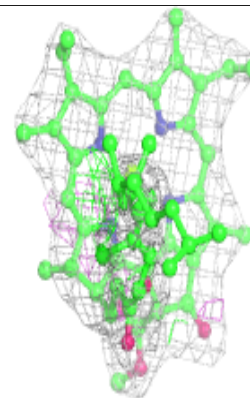
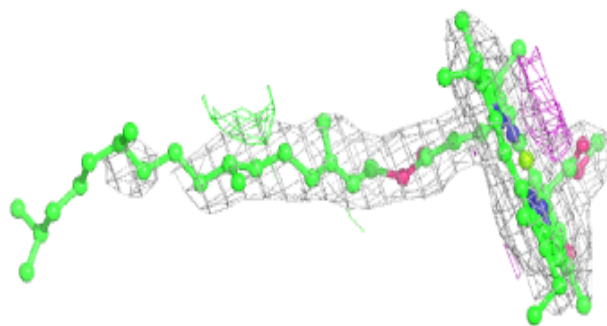
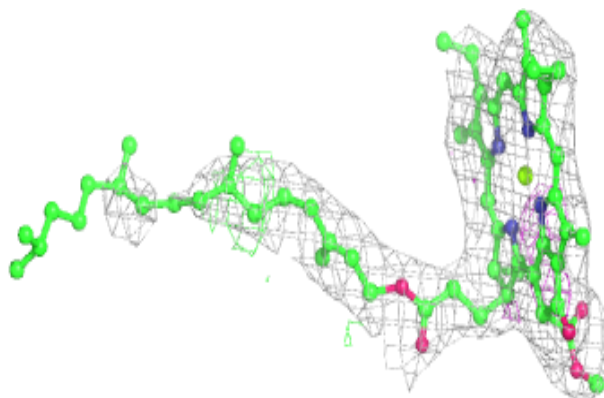


Electron density around CLA B 604:

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

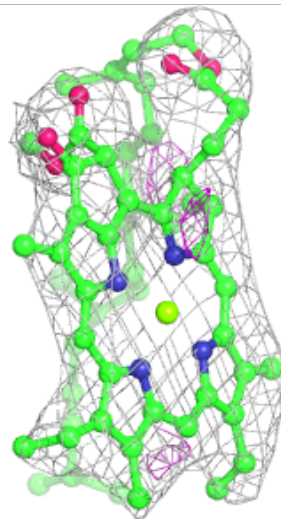
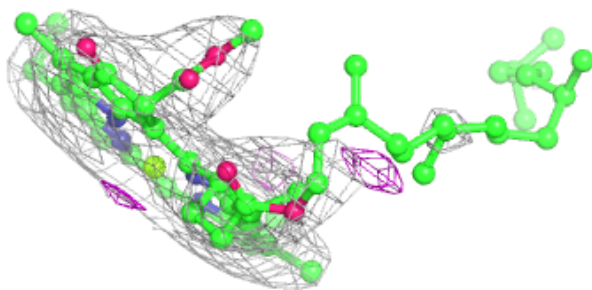
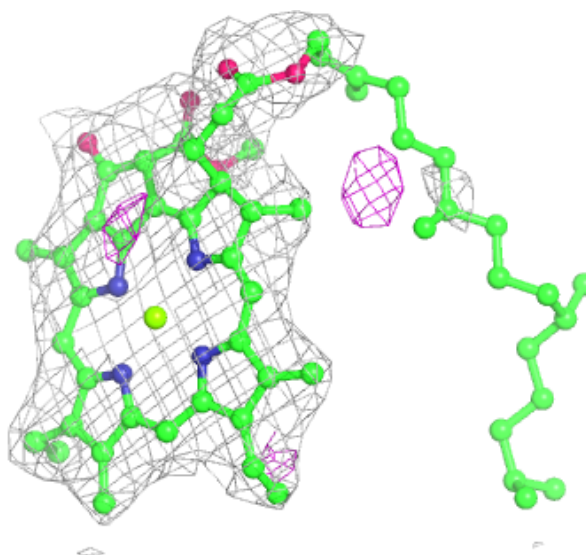
**Electron density around CLA d 404:**

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



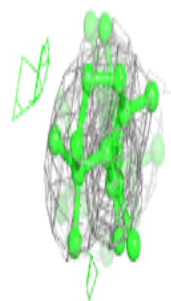
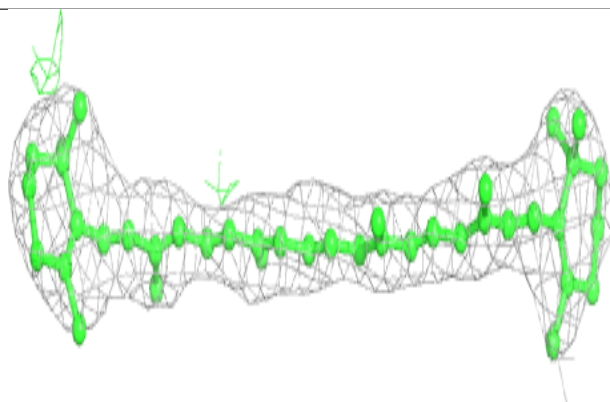
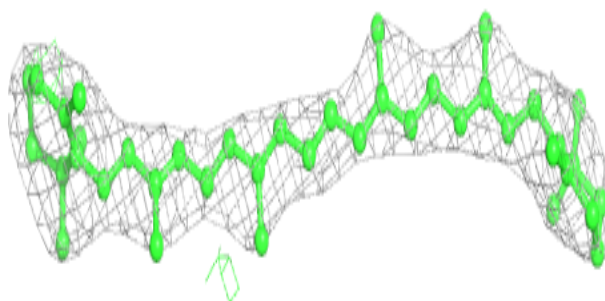
Electron density around CLA B 616:

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



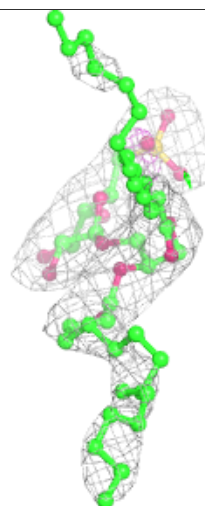
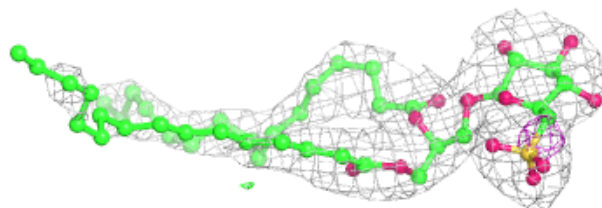
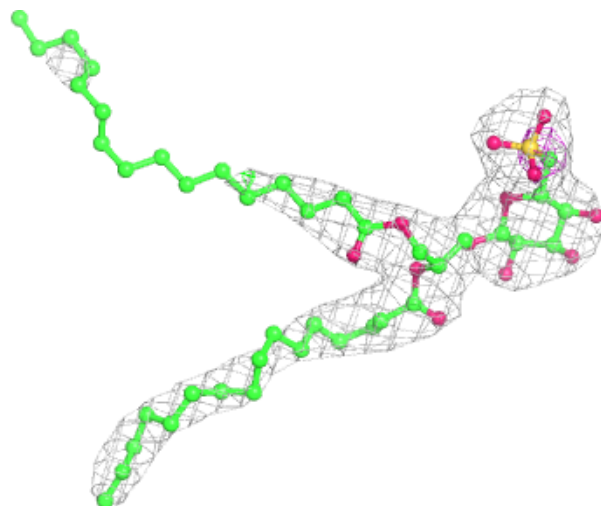
Electron density around BCR C 515:

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



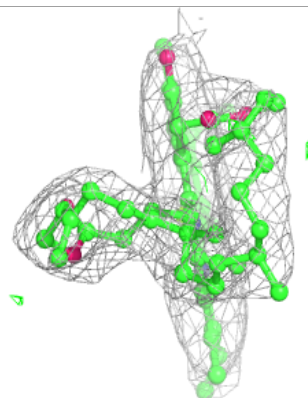
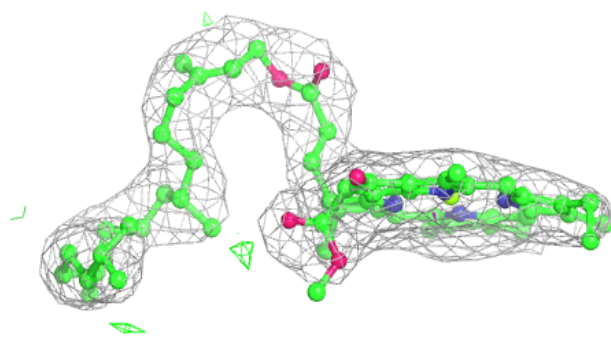
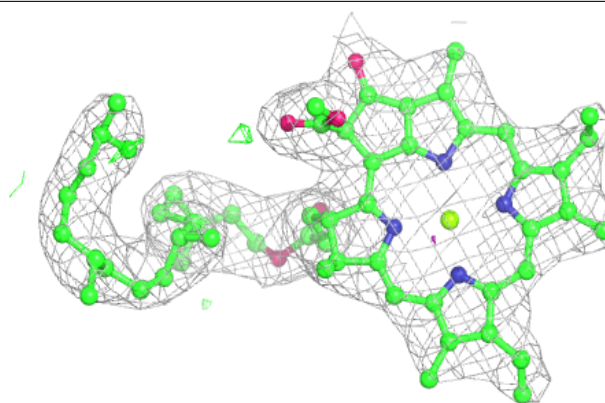
Electron density around SQD A 410:

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

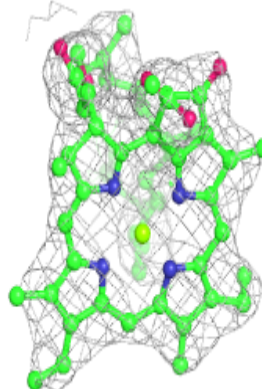
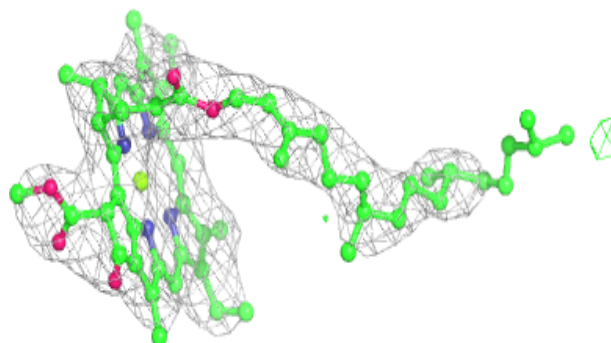
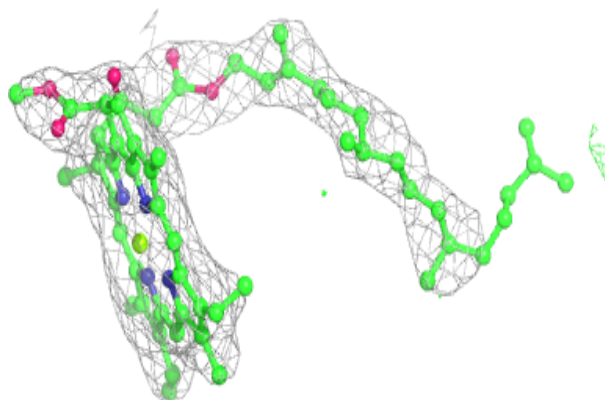


Electron density around CLA b 612:

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

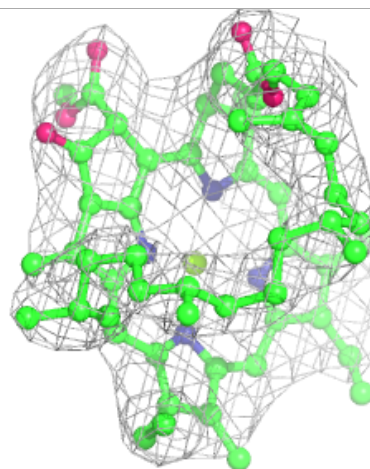
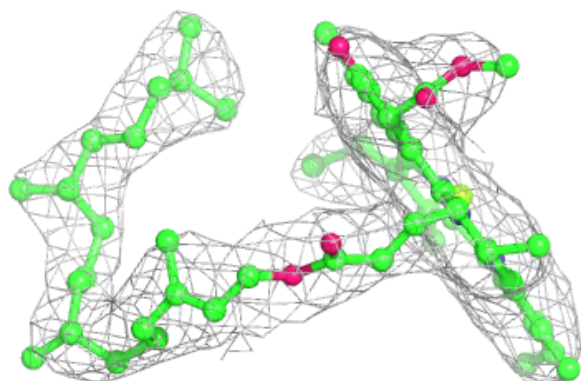
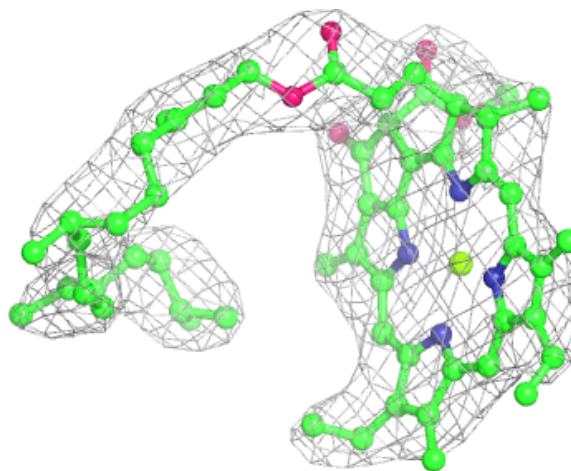
**Electron density around CLA c 508:**

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



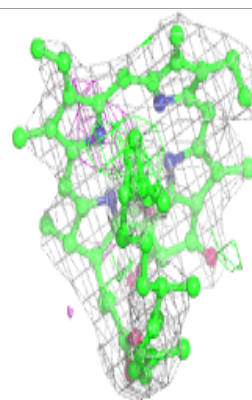
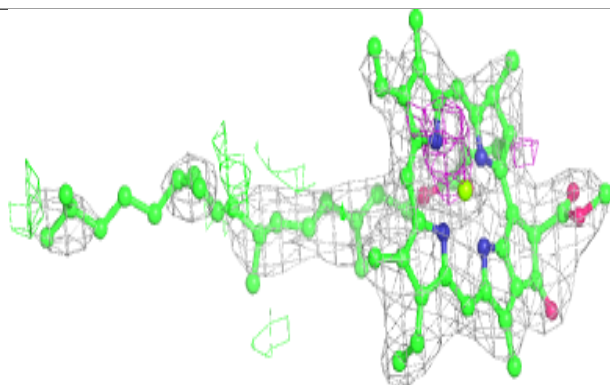
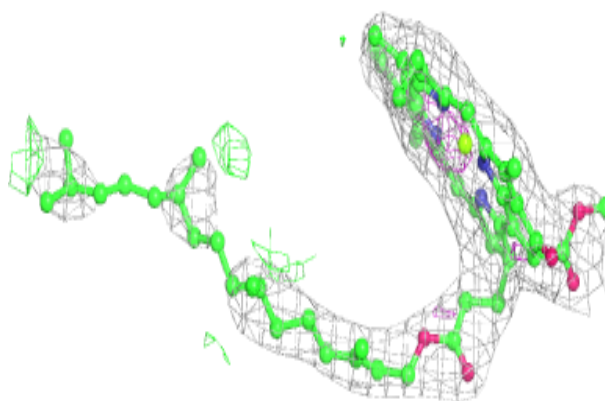
Electron density around CLA C 504:

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

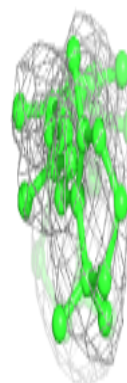
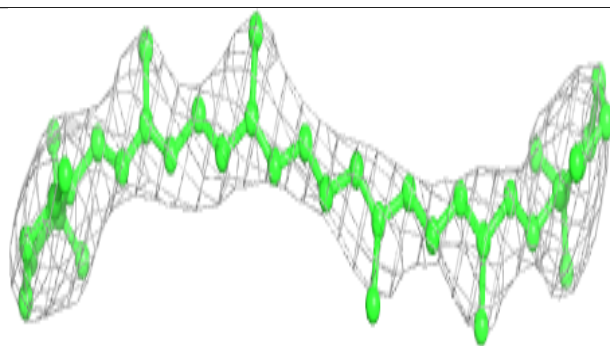
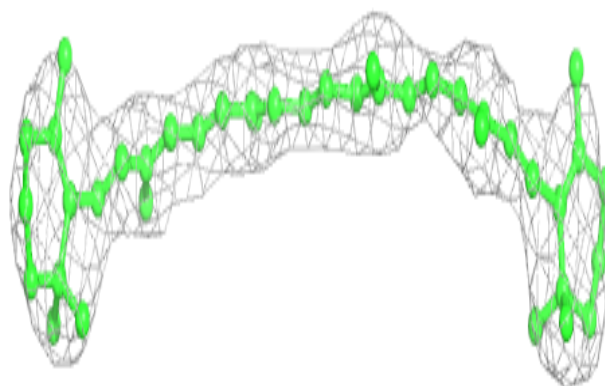


Electron density around CLA C 505:

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

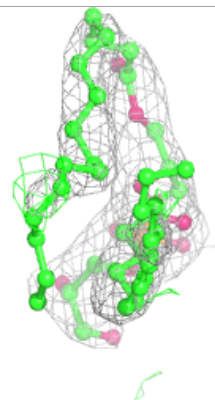
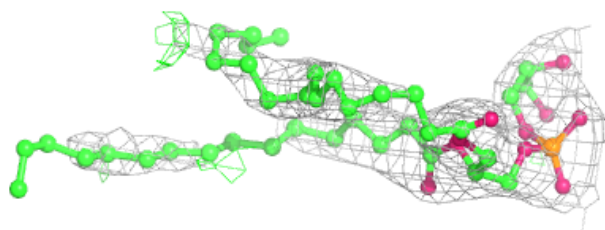
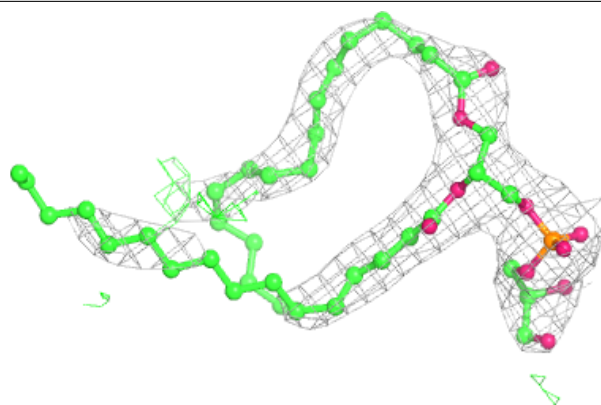
**Electron density around BCR k 101:**

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

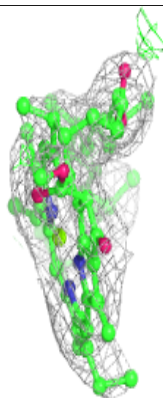
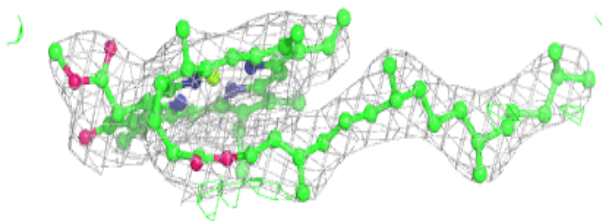
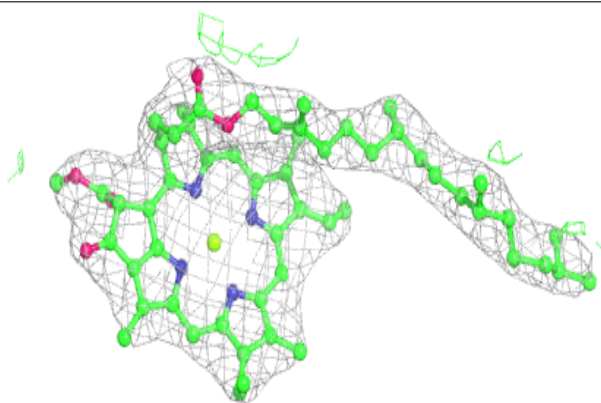


Electron density around LHG d 409:

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

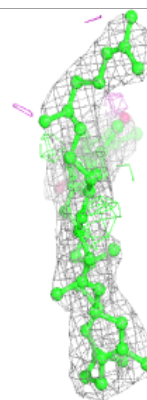
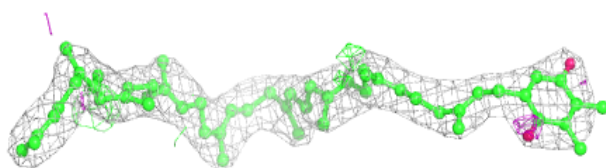
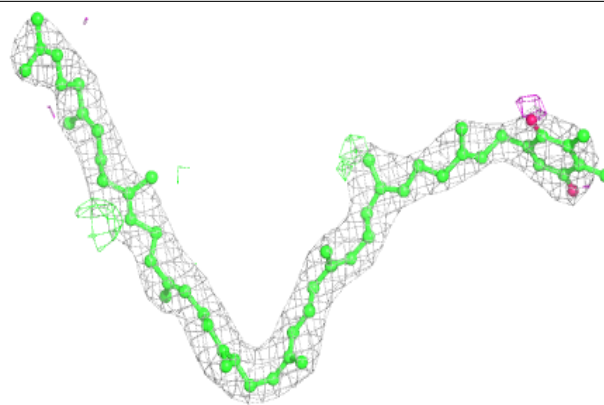
**Electron density around CLA C 502:**

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

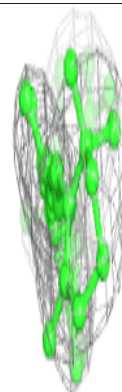
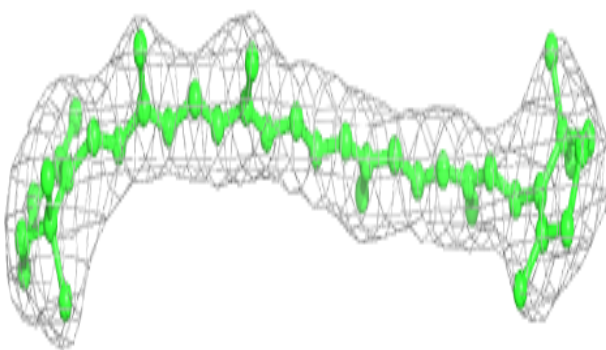
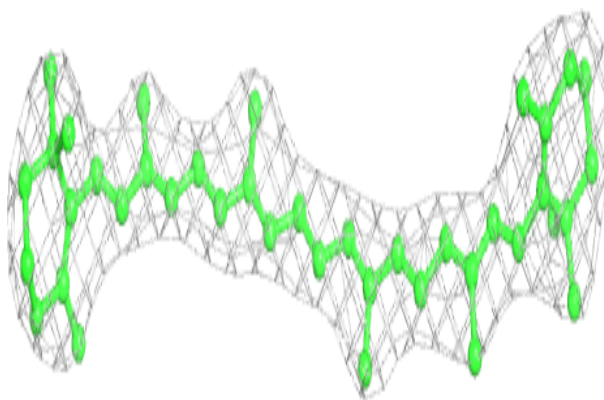


Electron density around PL9 d 406:

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

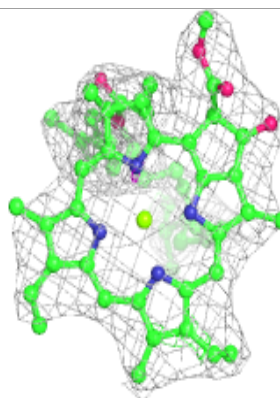
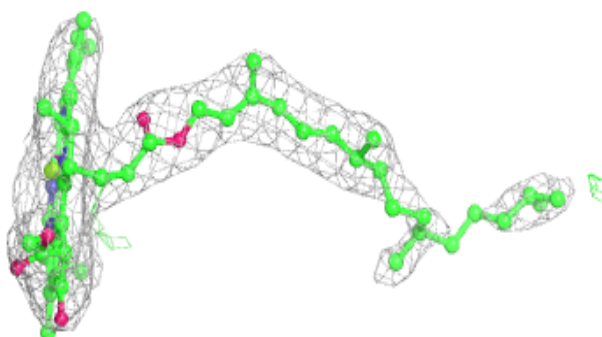
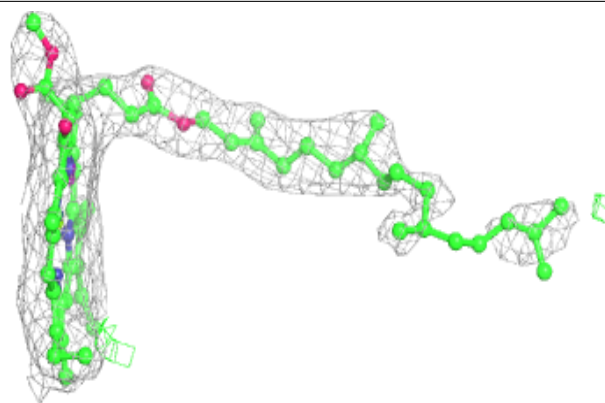
**Electron density around BCR B 619:**

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

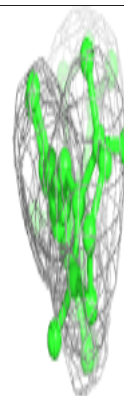
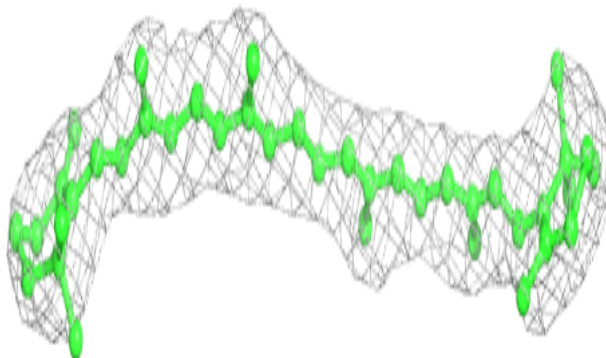
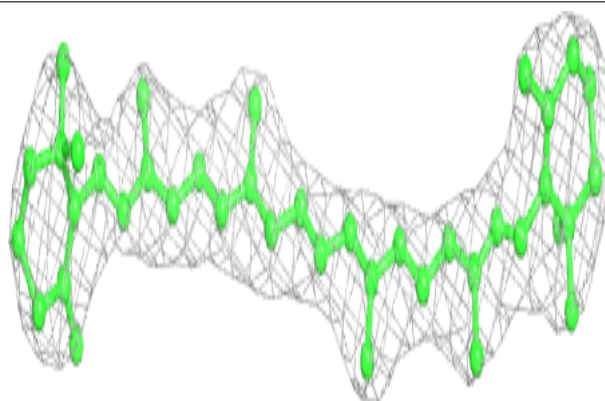


Electron density around CLA B 606:

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

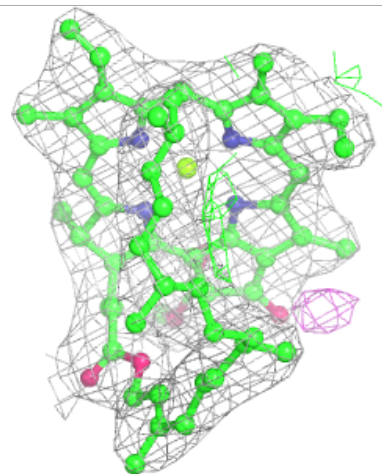
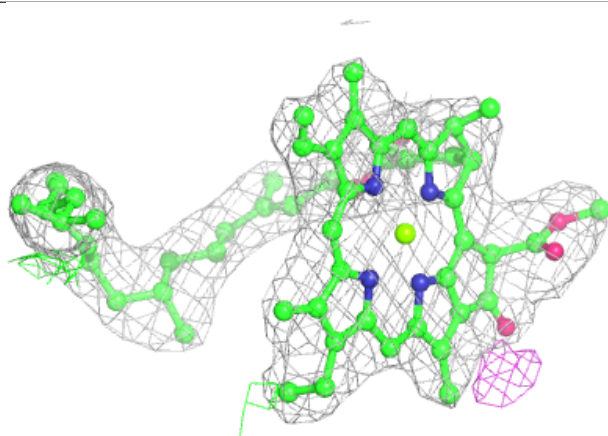
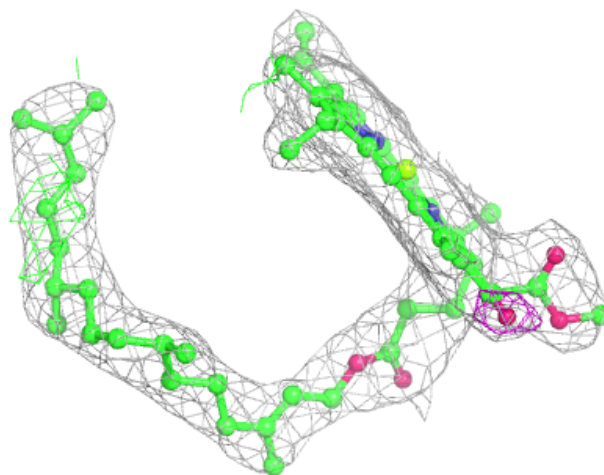
**Electron density around BCR b 619:**

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



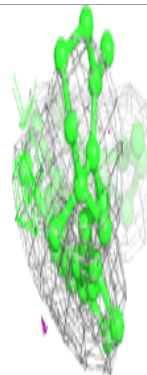
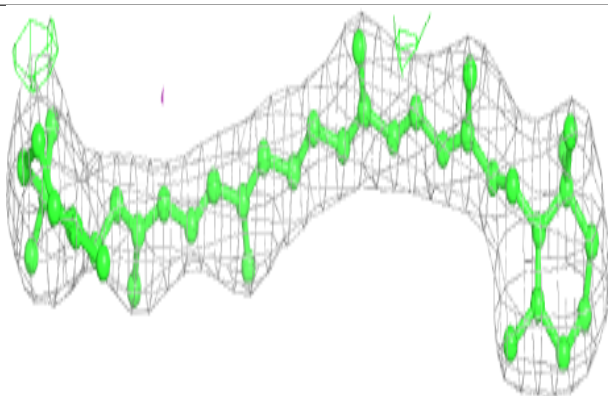
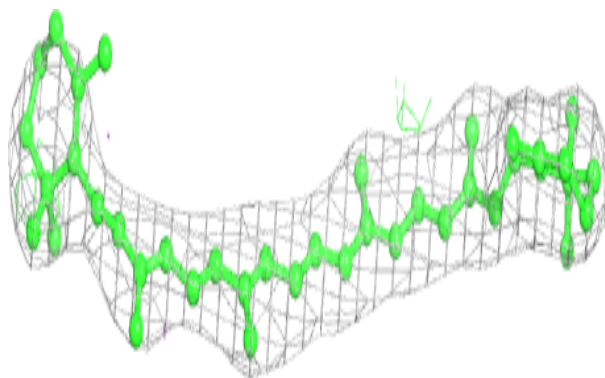
Electron density around CLA B 611:

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

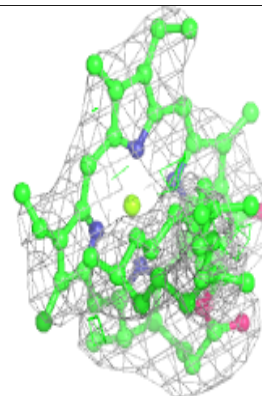
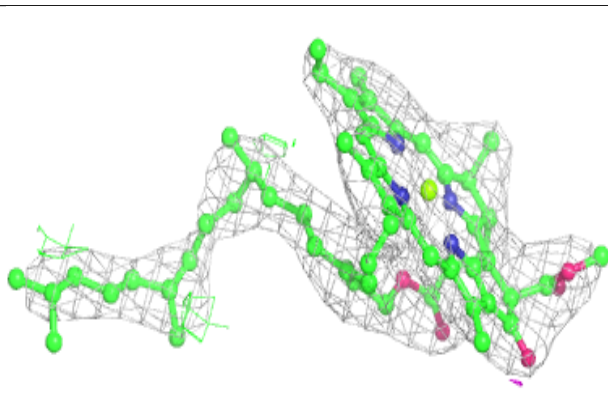
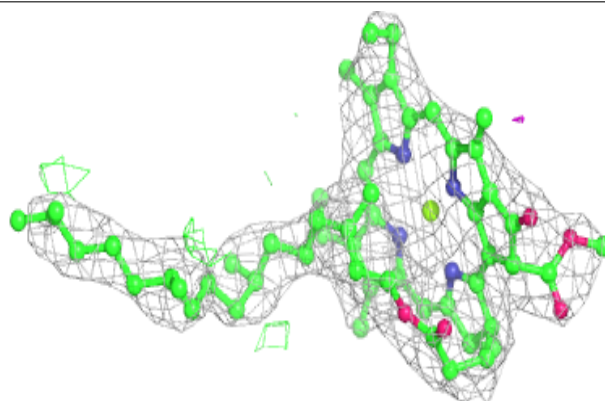


Electron density around BCR D 406:

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

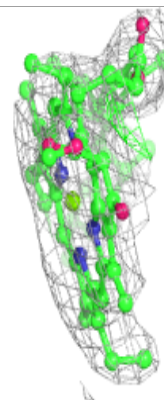
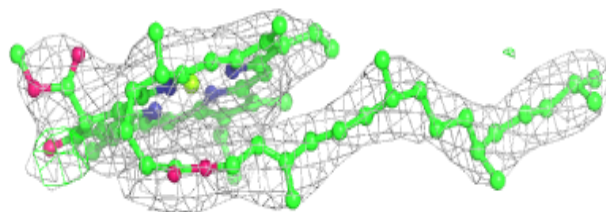
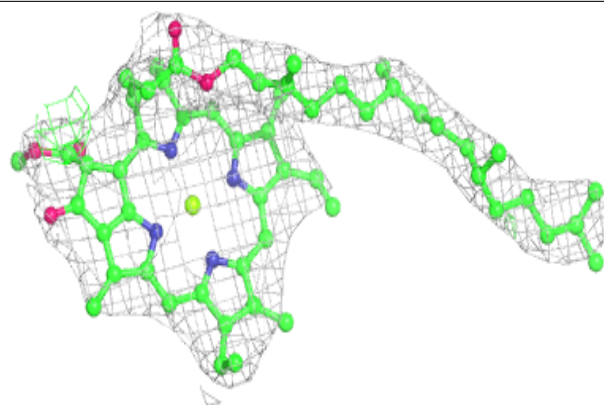
**Electron density around CLA c 505:**

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

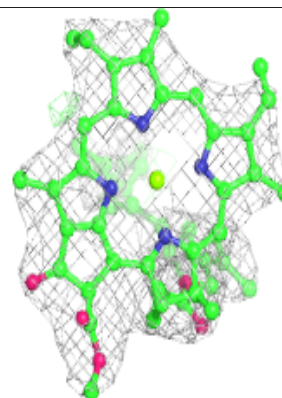
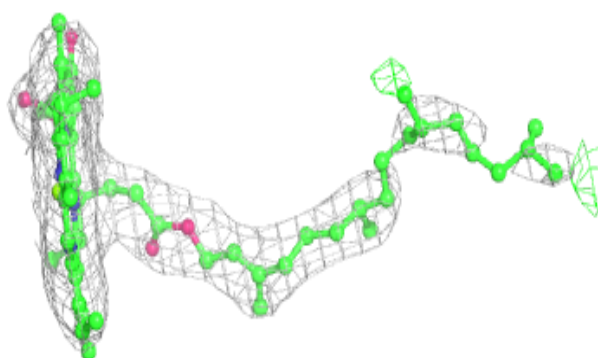
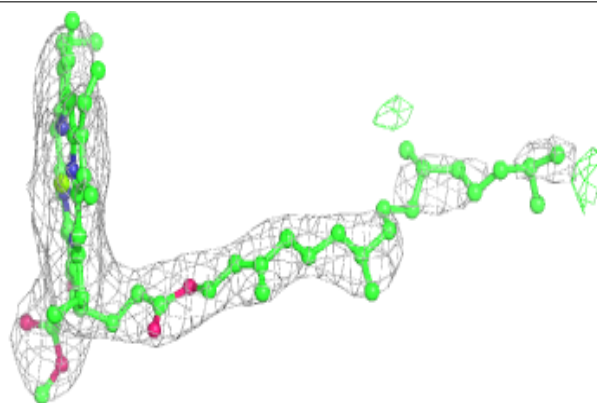


Electron density around CLA c 501:

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

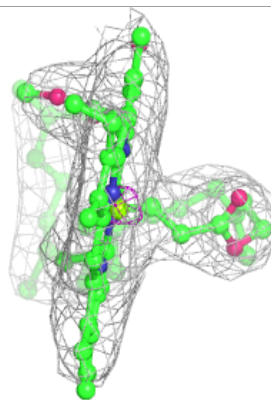
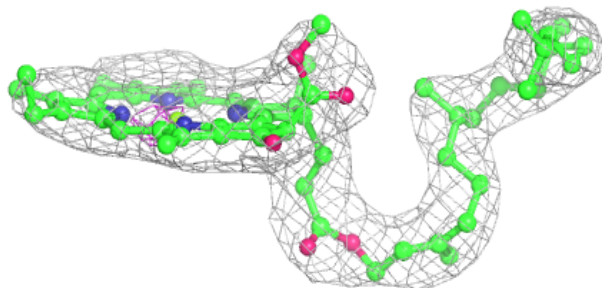
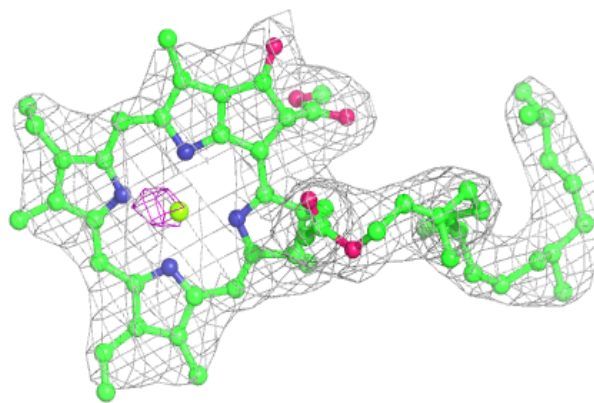
**Electron density around CLA b 606:**

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

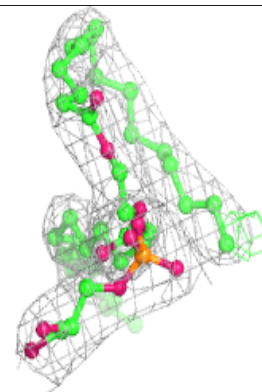
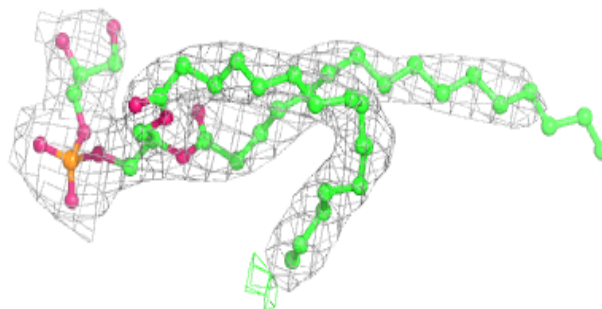
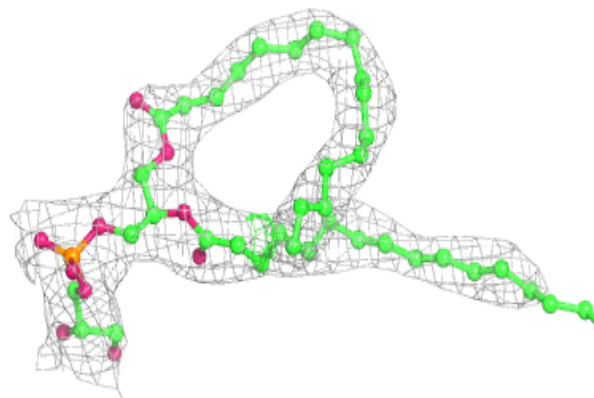


Electron density around CLA B 612:

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

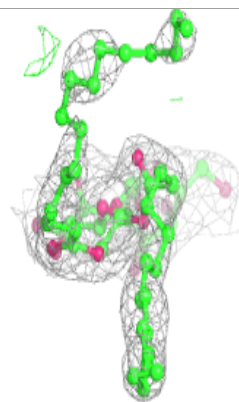
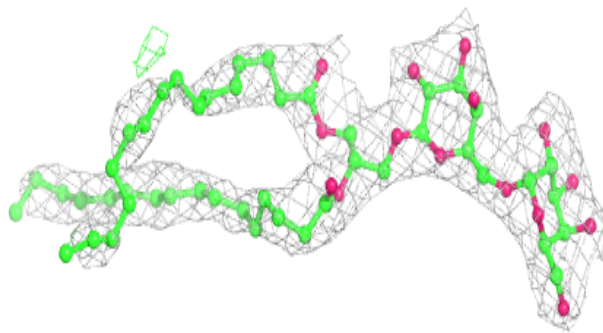
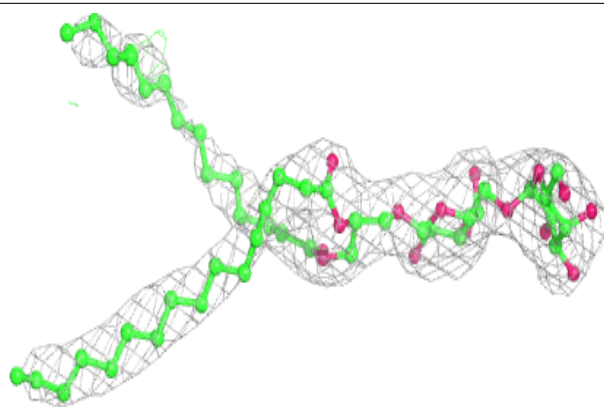
**Electron density around LHG d 407:**

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

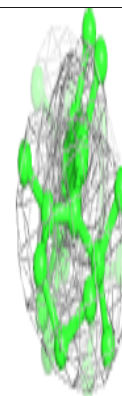
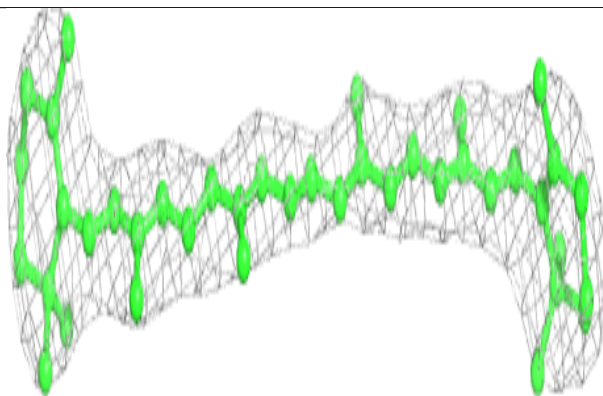
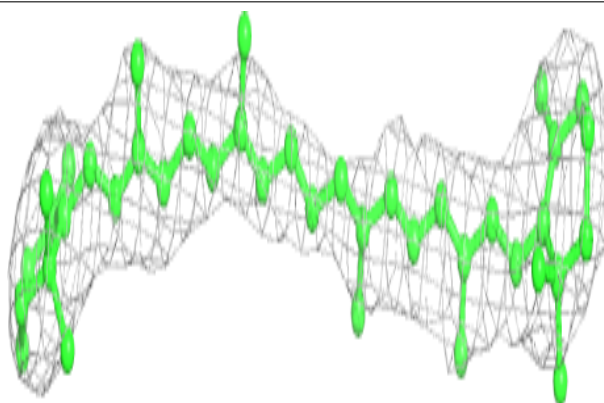


Electron density around DGD c 516:

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

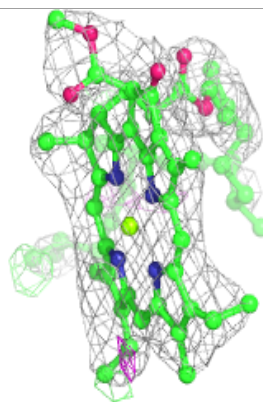
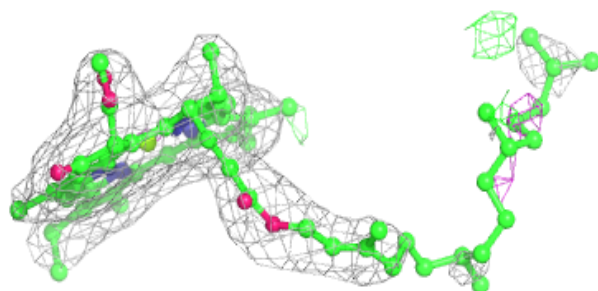
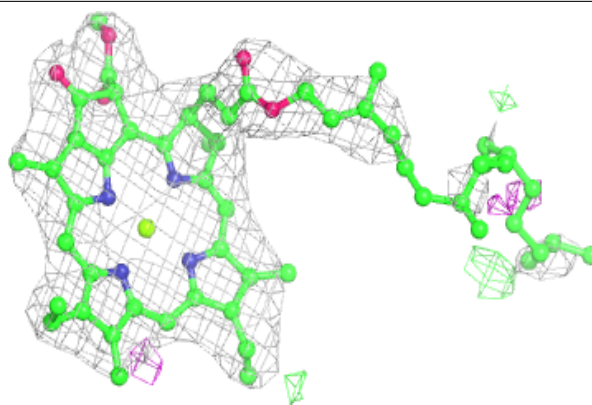
**Electron density around BCR c 514:**

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

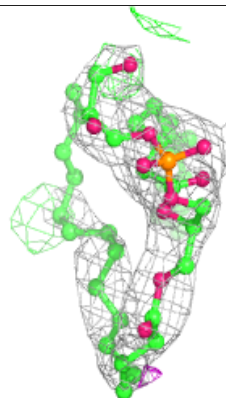
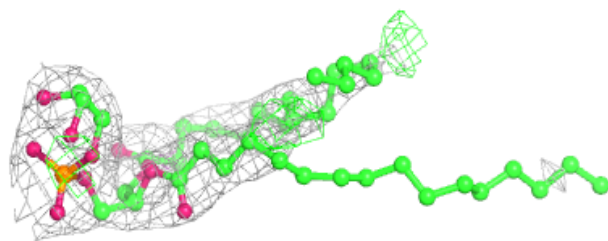
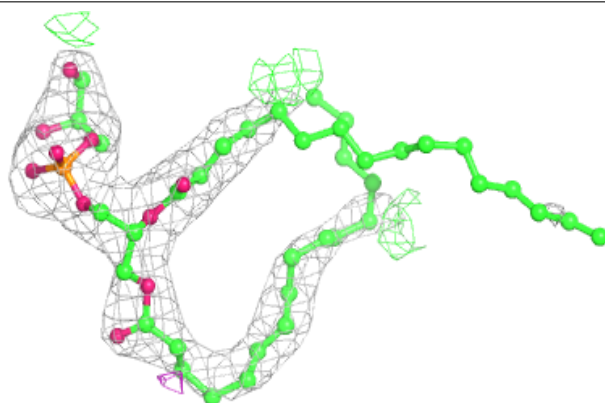


Electron density around CLA a 408:

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

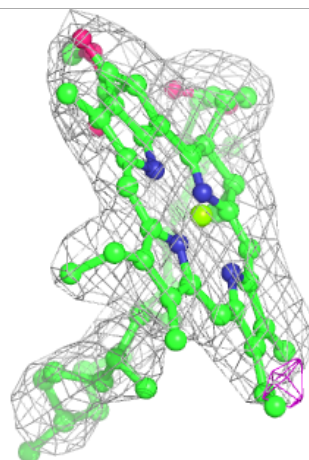
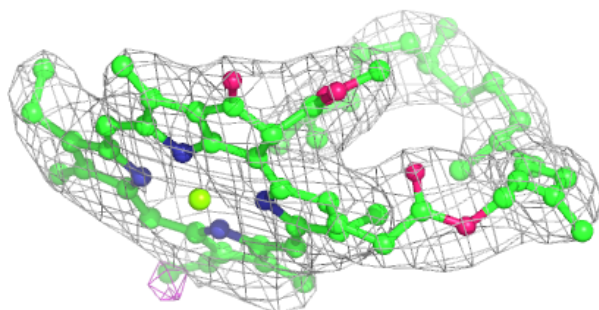
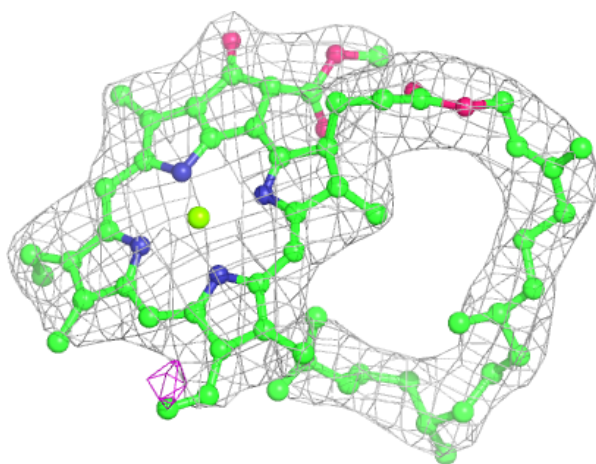
**Electron density around LHG D 409:**

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



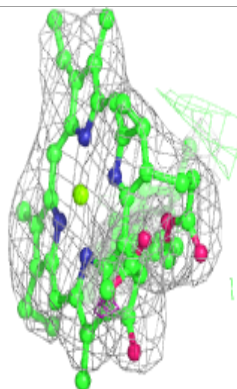
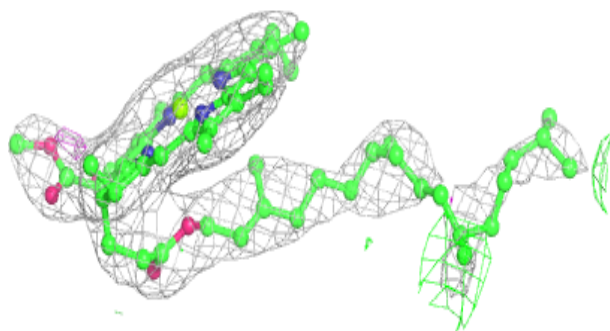
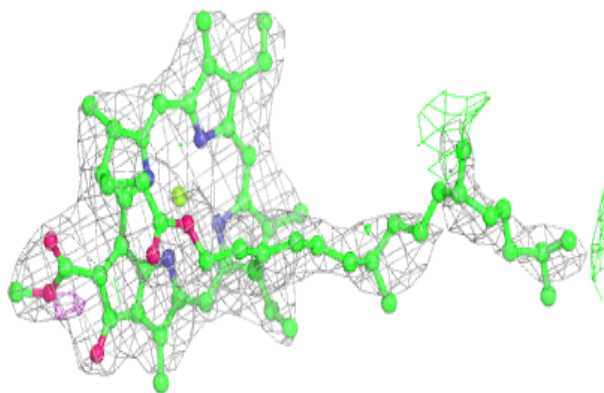
Electron density around CLA B 615:

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

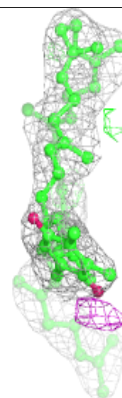
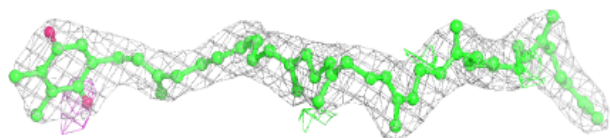
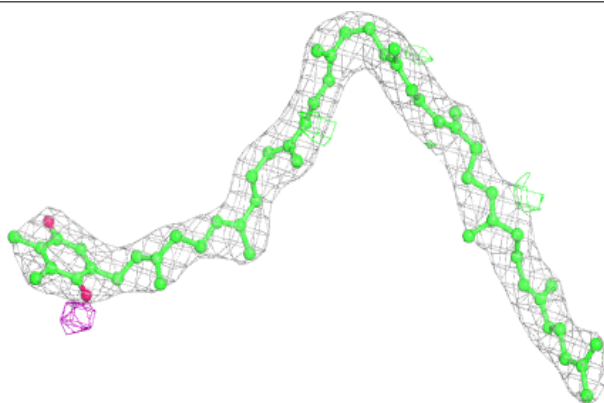


Electron density around CLA b 614:

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

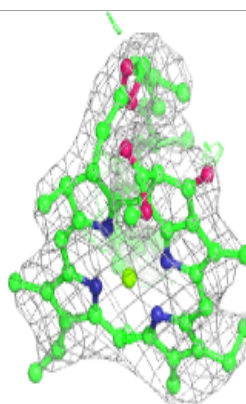
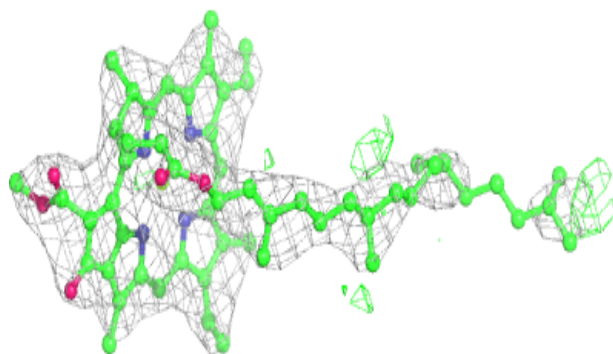
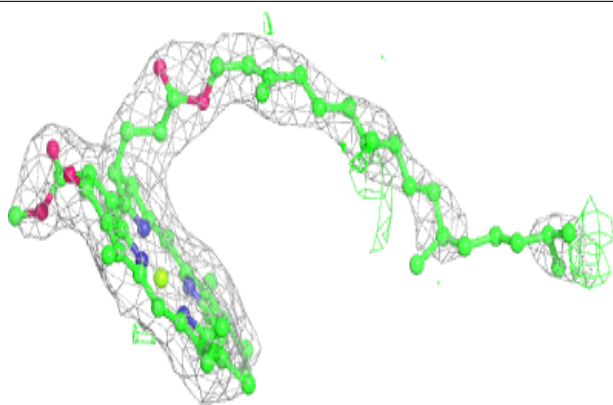
**Electron density around PL9 D 407:**

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

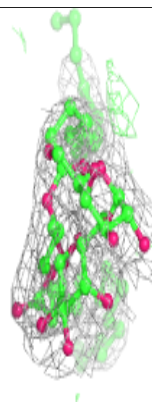
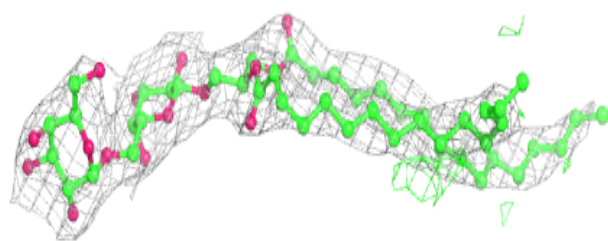
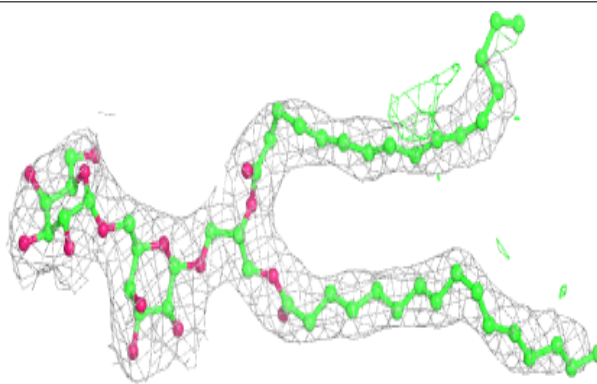


Electron density around CLA c 504:

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

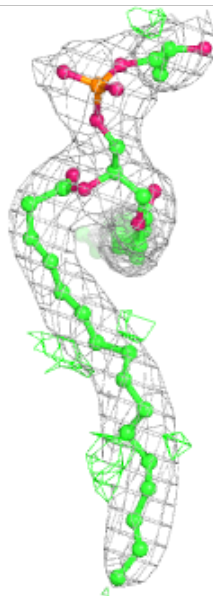
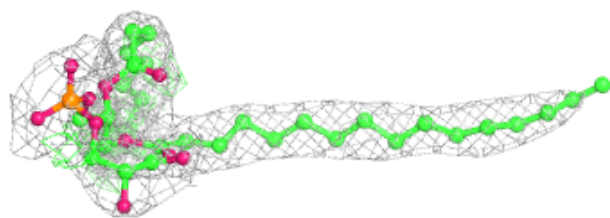
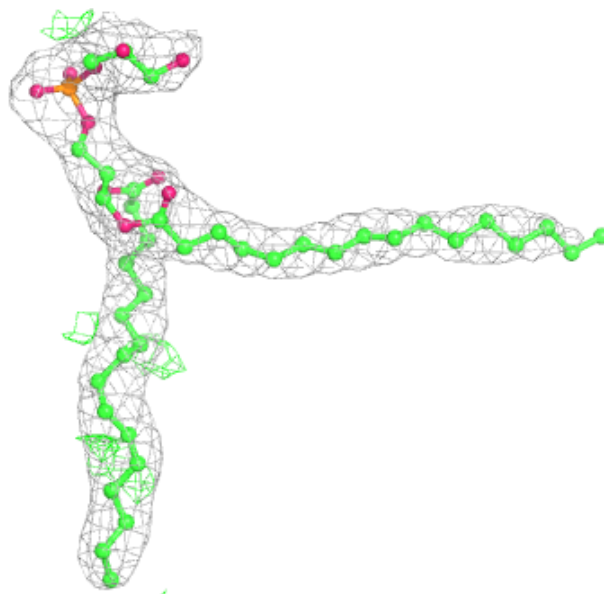
**Electron density around DGD c 518:**

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



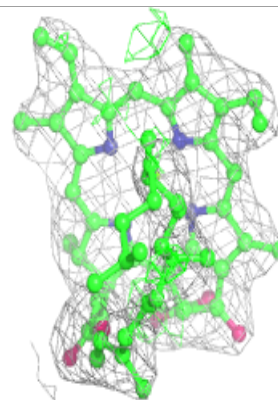
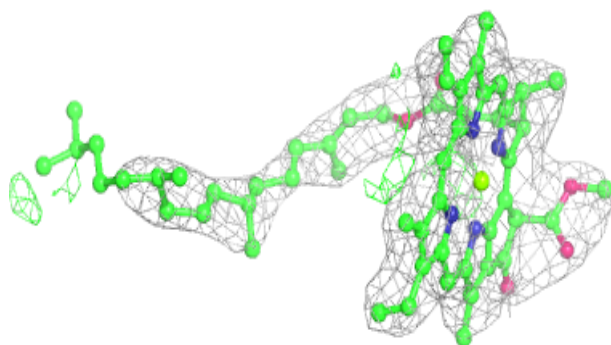
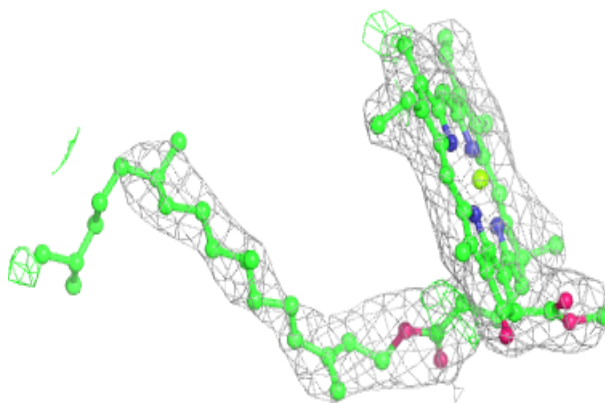
Electron density around LHG A 417:

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

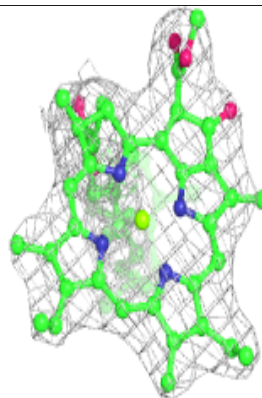
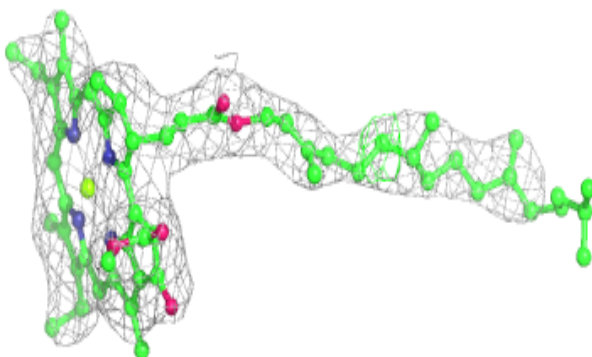
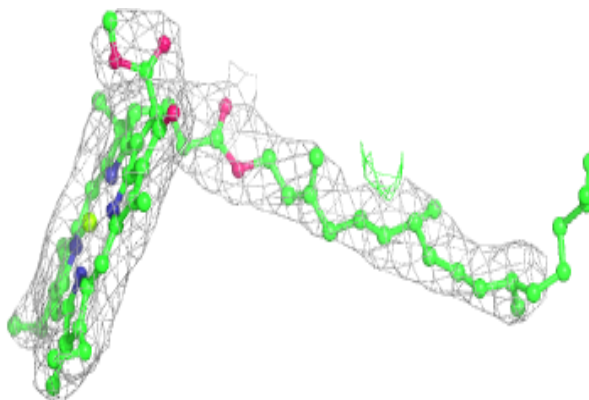


Electron density around CLA C 509:

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

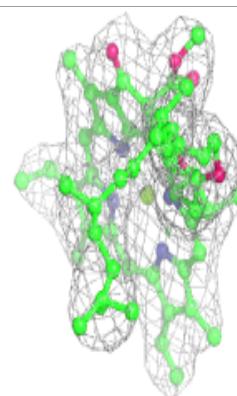
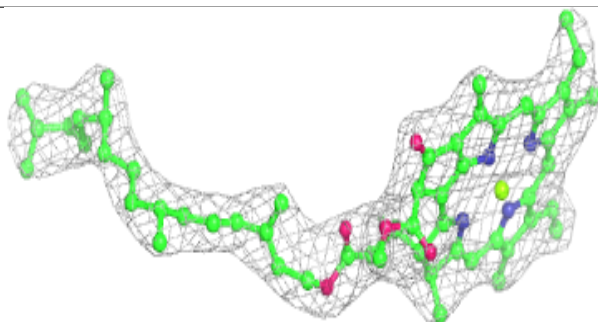
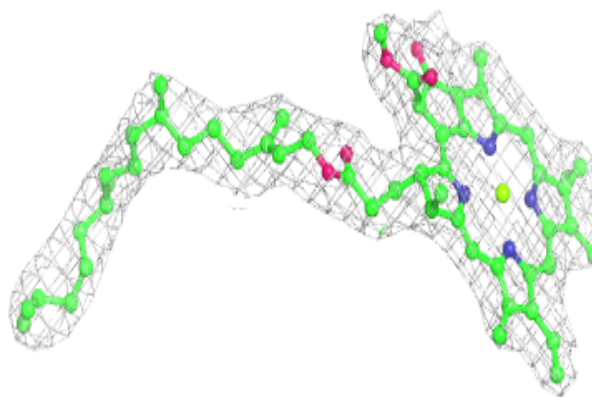
**Electron density around CLA b 604:**

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

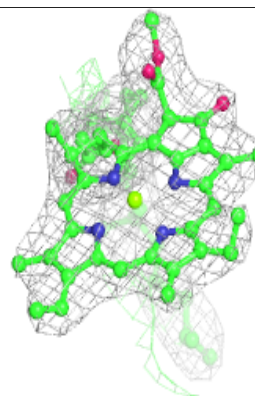
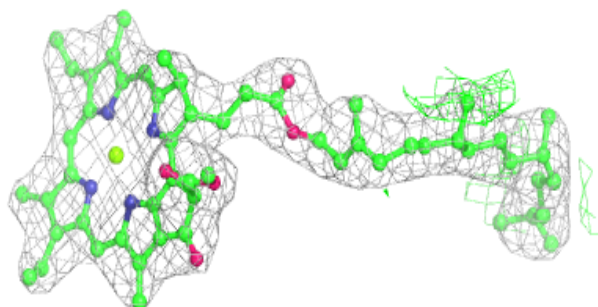
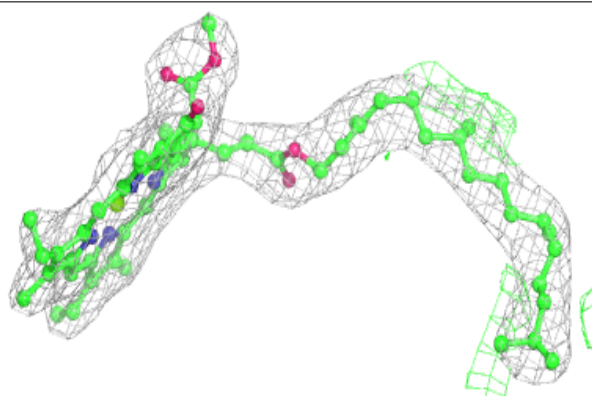


Electron density around CLA A 404:

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

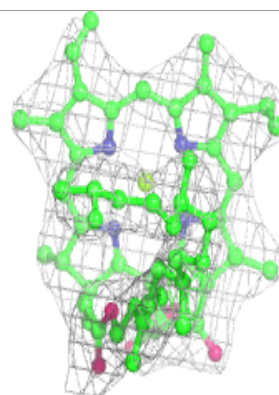
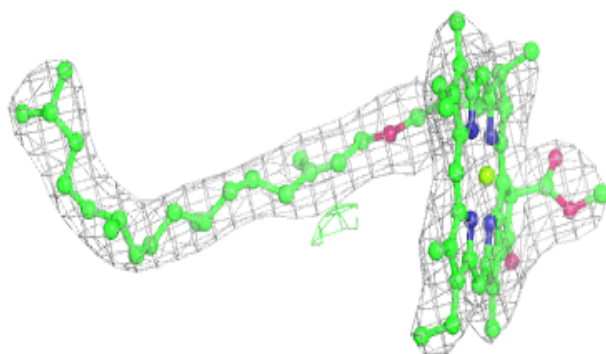
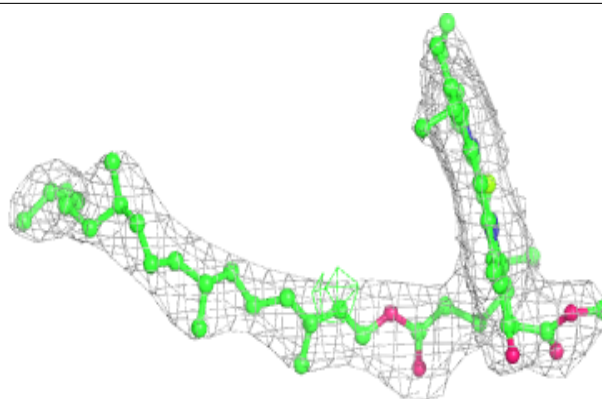
**Electron density around CLA D 404:**

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

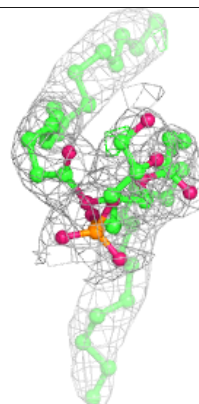
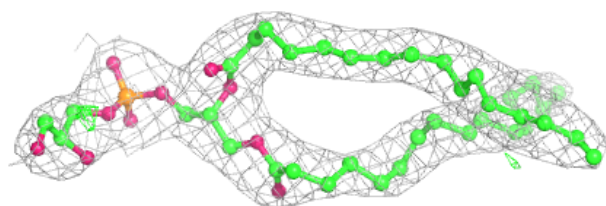
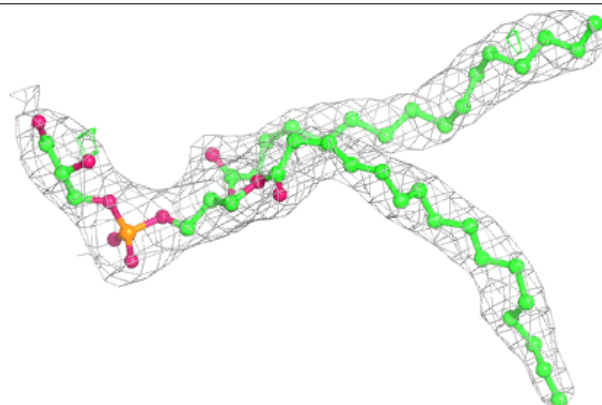


Electron density around CLA B 605:

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

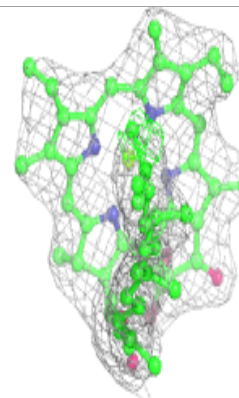
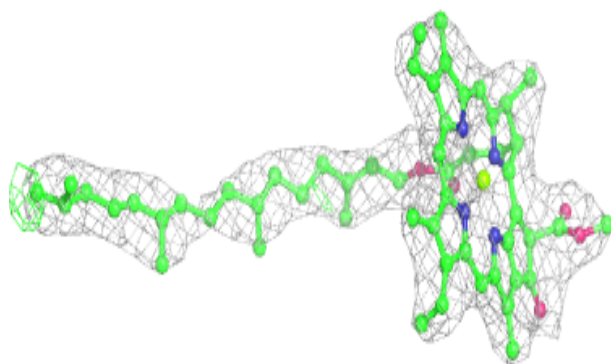
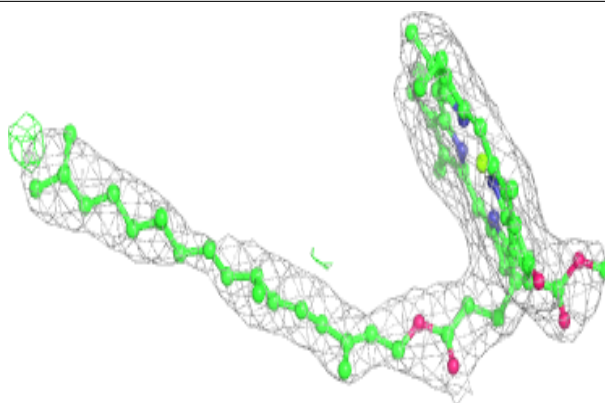
**Electron density around LHG D 408:**

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

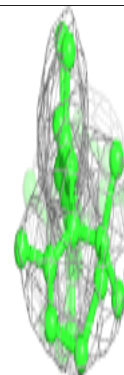
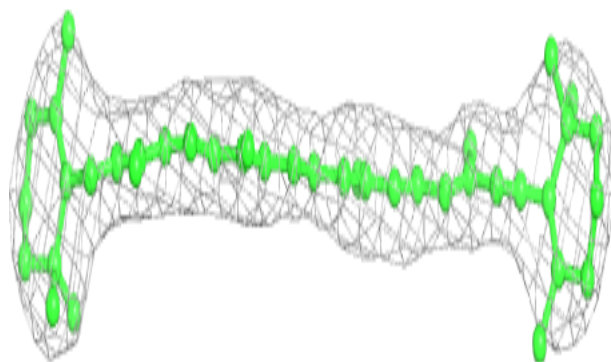
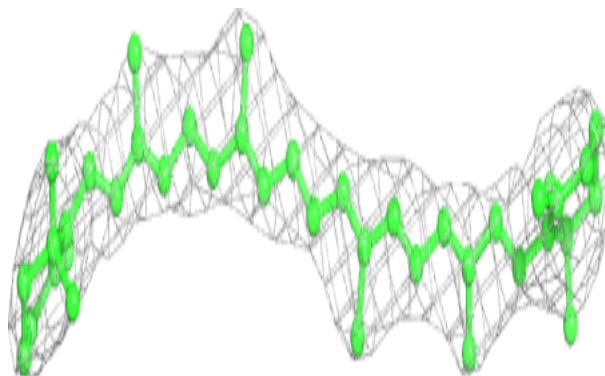


Electron density around CLA B 607:

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

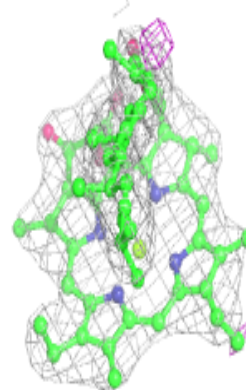
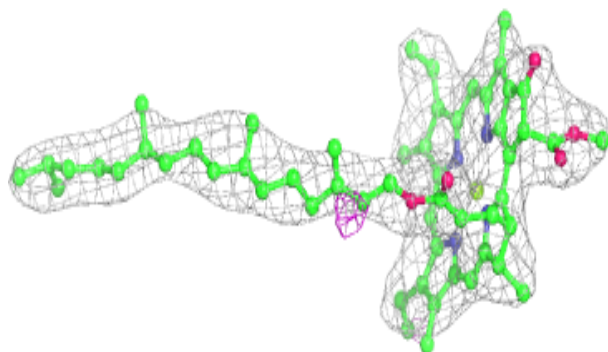
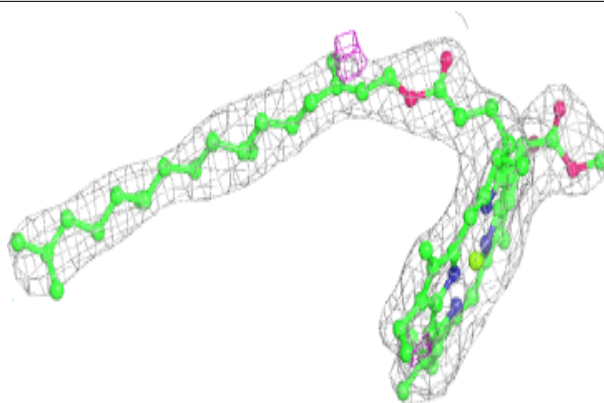
**Electron density around BCR c 515:**

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

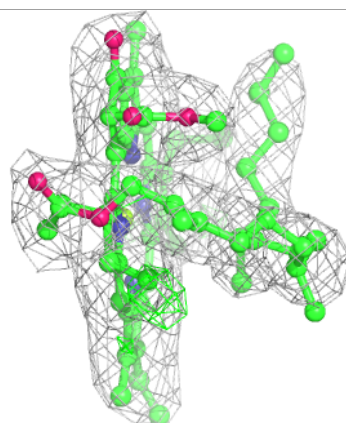
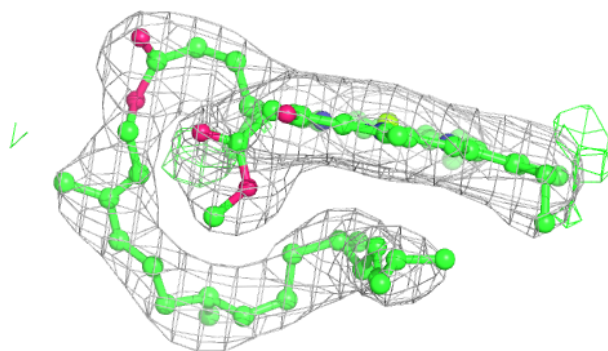
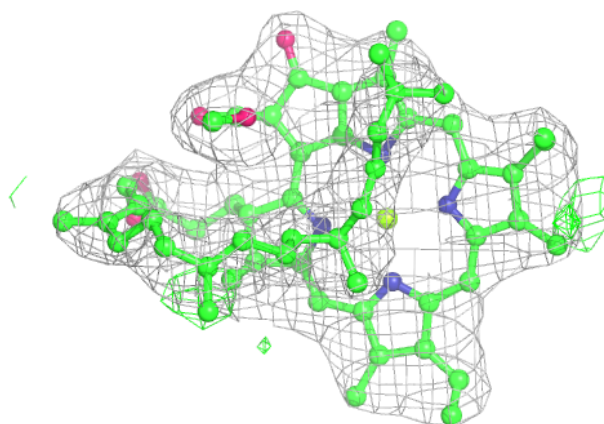


Electron density around CLA b 607:

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

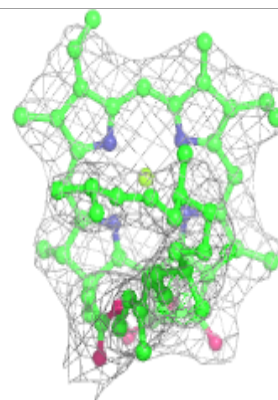
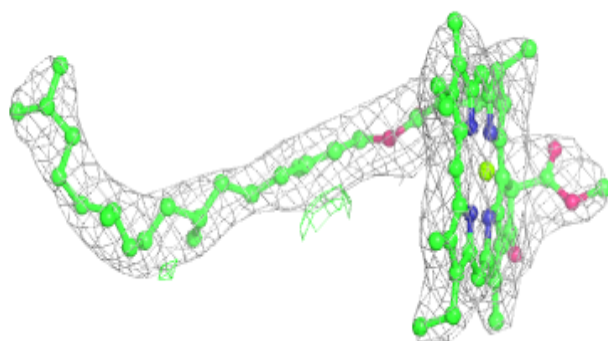
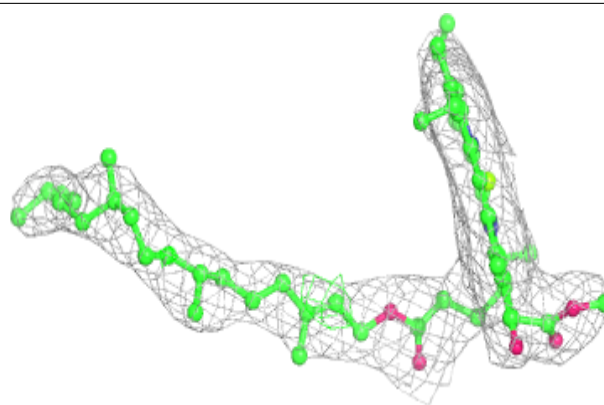
**Electron density around CLA C 511:**

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

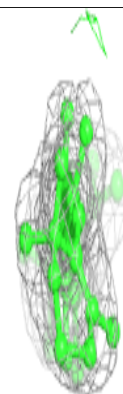
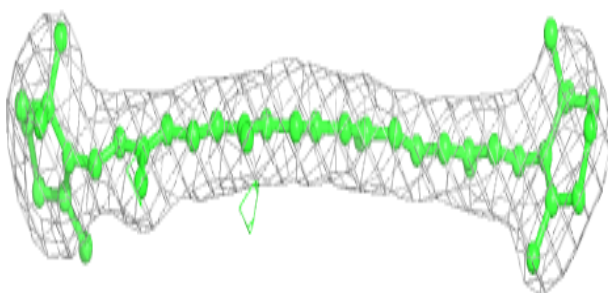
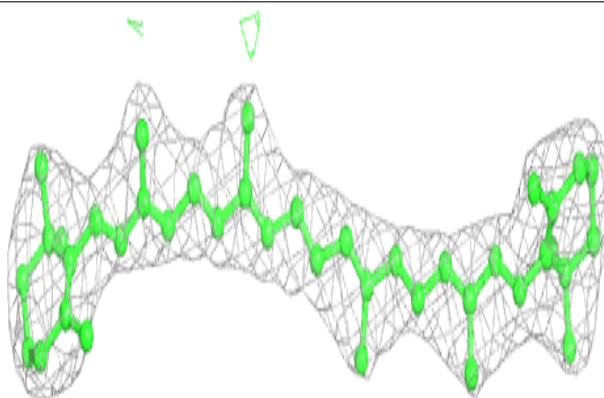


Electron density around CLA b 605:

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

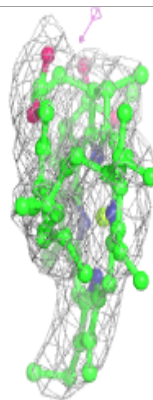
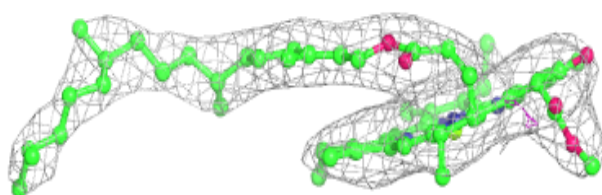
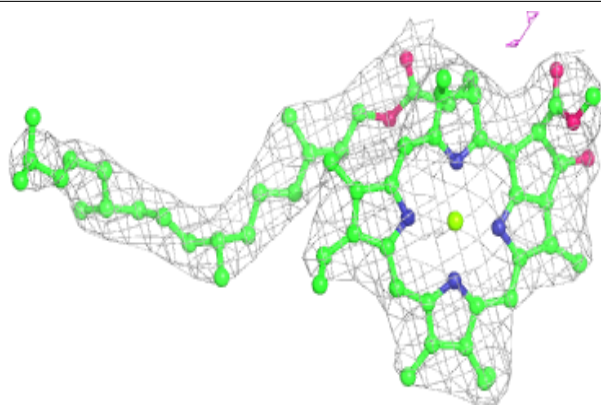
**Electron density around BCR b 618:**

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

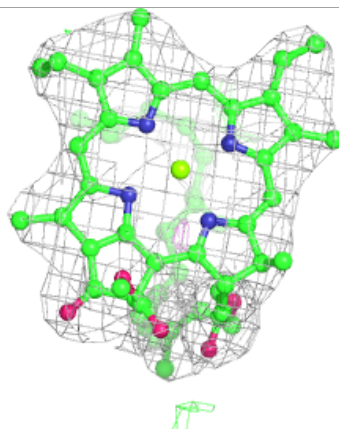
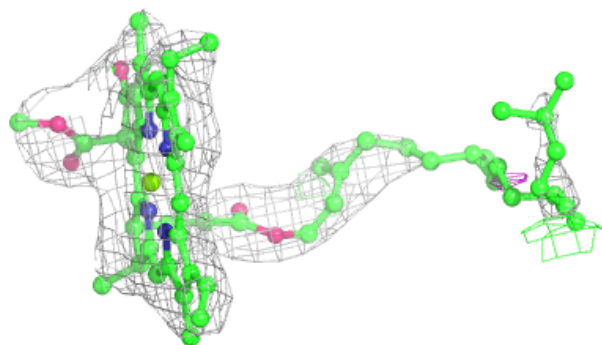
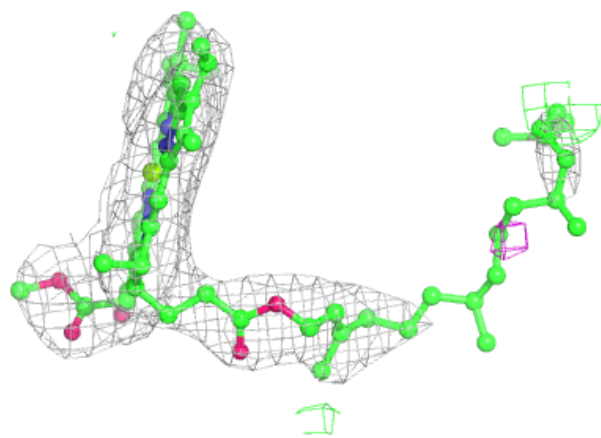


Electron density around CLA b 603:

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

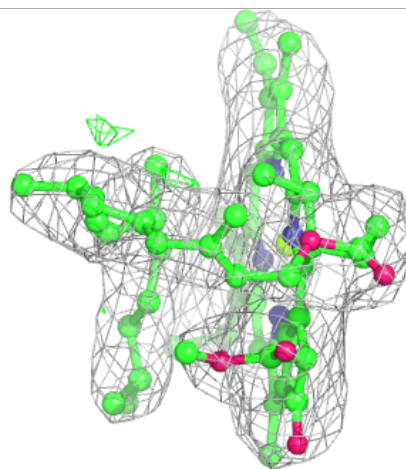
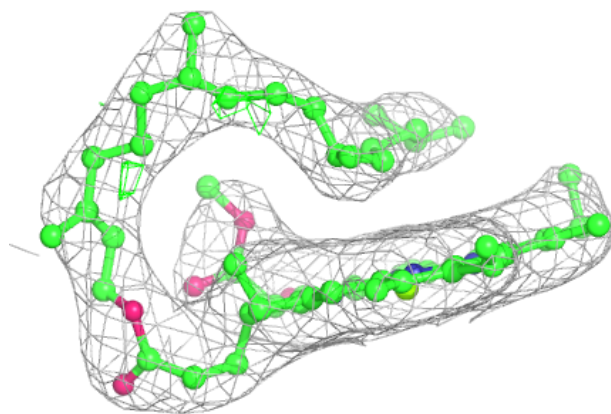
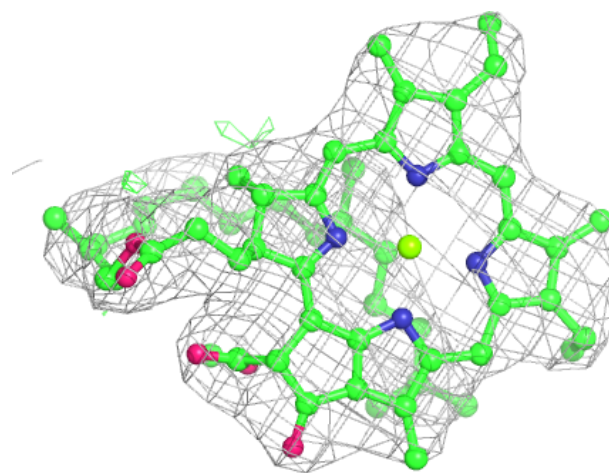
**Electron density around CLA c 506:**

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



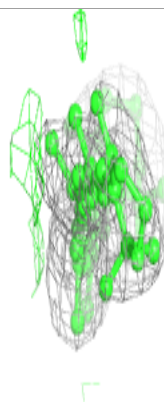
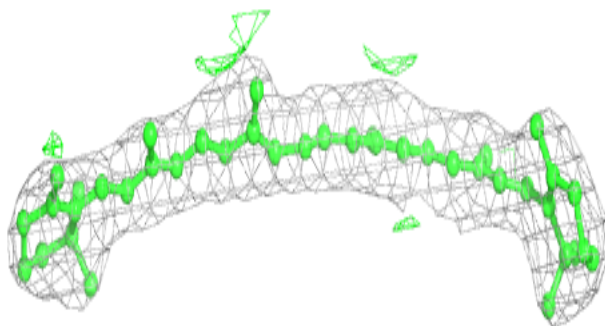
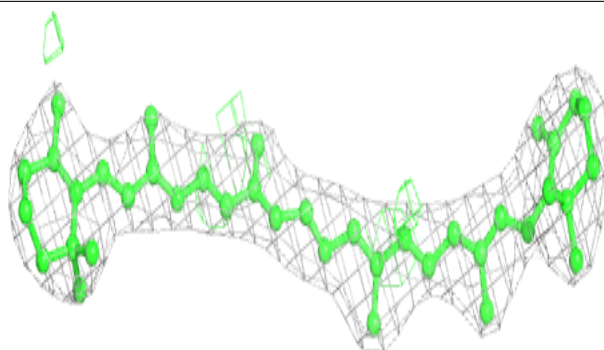
Electron density around CLA c 510:

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

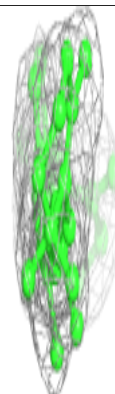
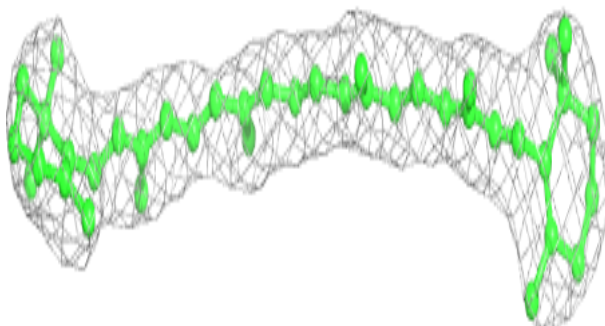
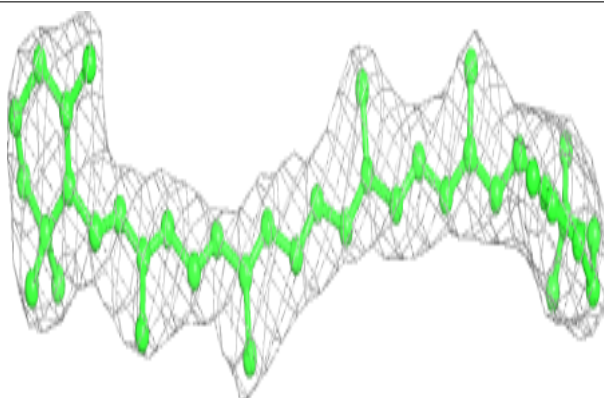


Electron density around BCR T 101:

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

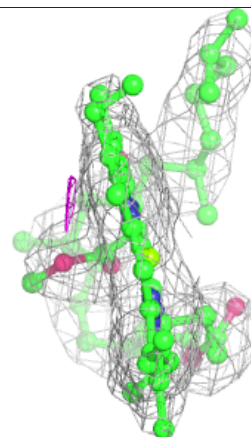
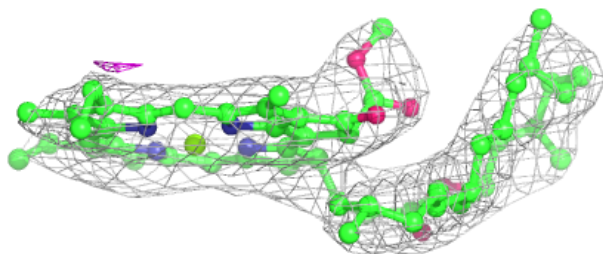
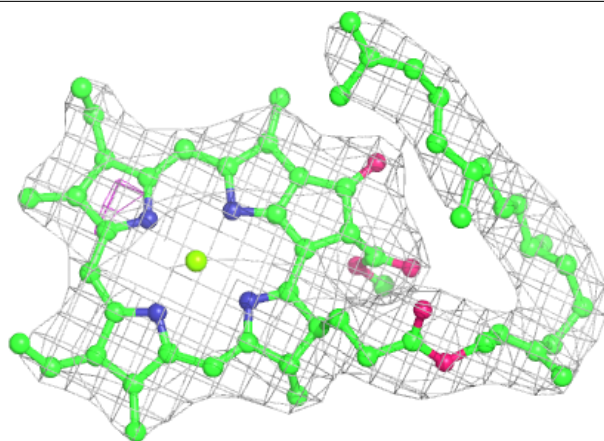
**Electron density around BCR b 617:**

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

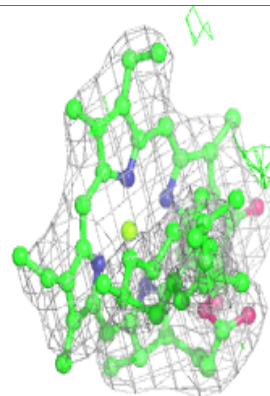
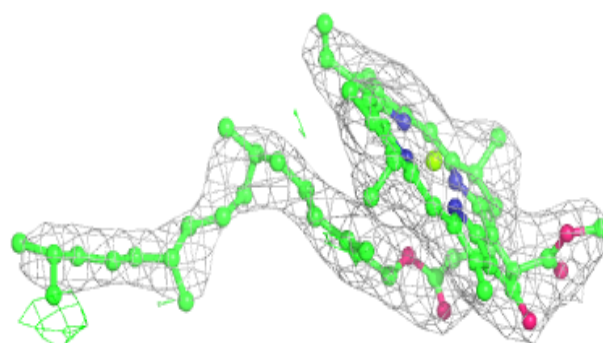
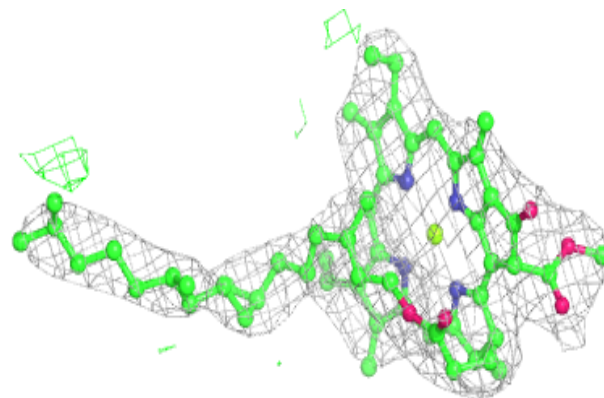


Electron density around CLA b 610:

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

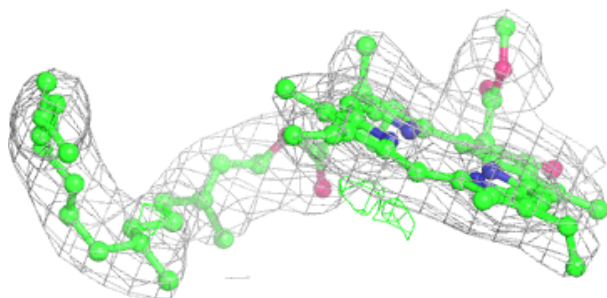
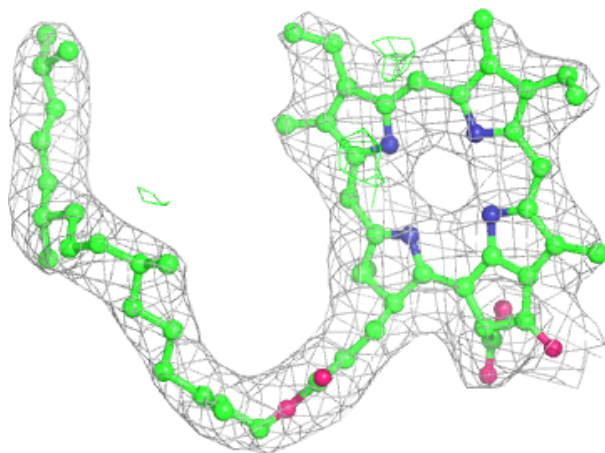
**Electron density around CLA C 506:**

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



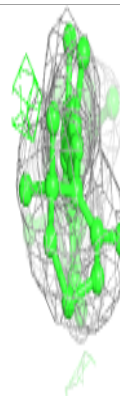
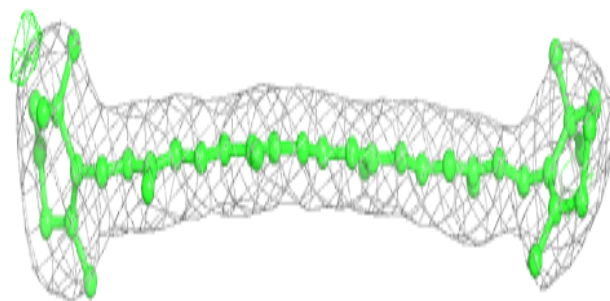
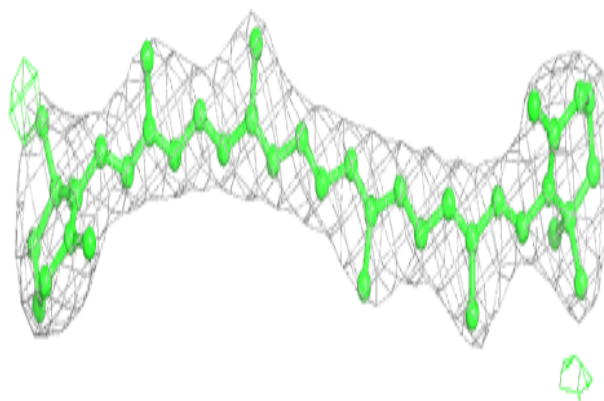
Electron density around PHO a 407:

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

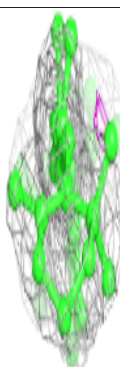
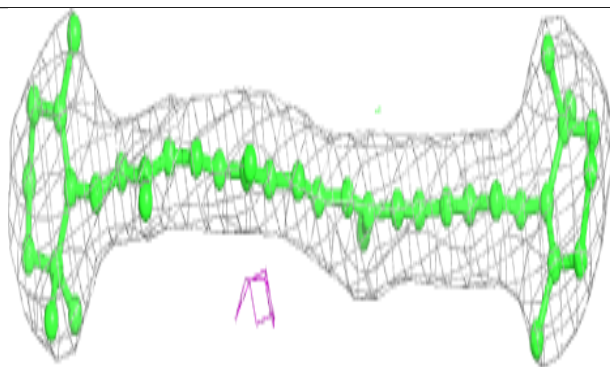
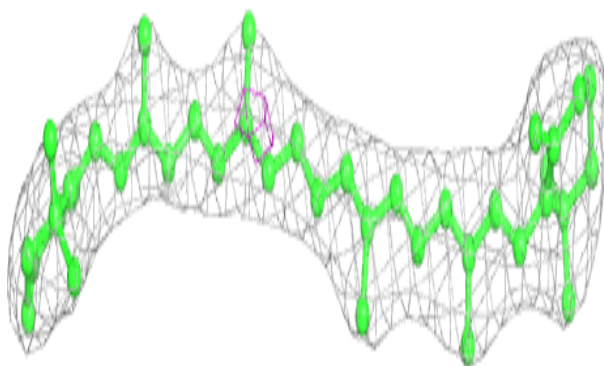


Electron density around BCR B 618:

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

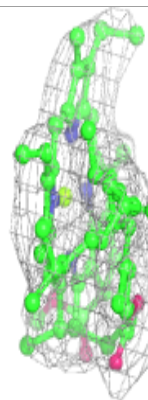
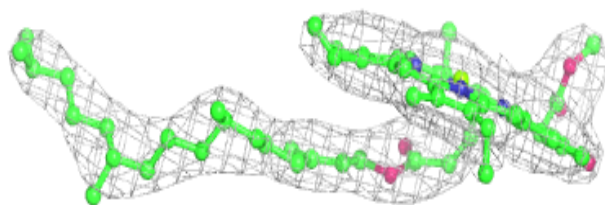
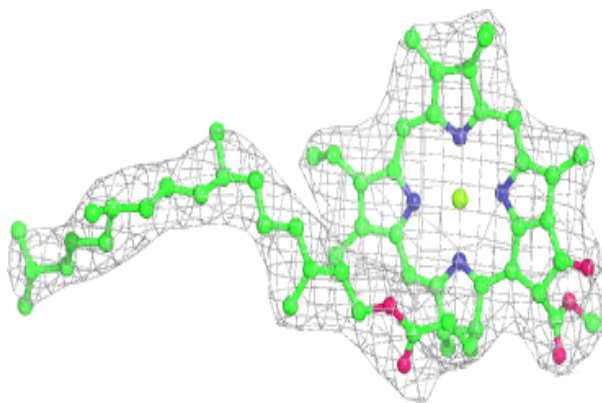
**Electron density around BCR a 409:**

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

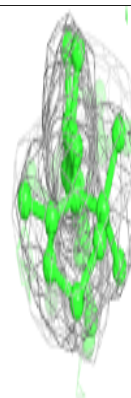
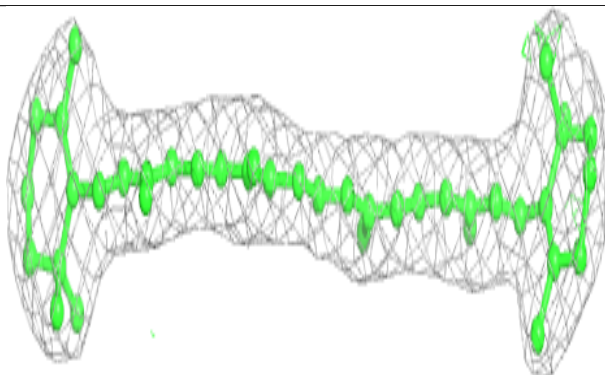
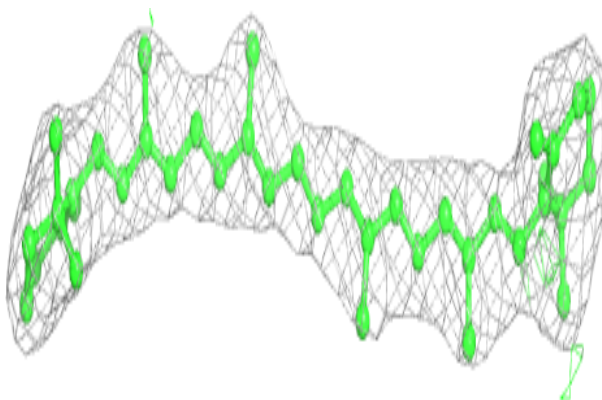


Electron density around CLA B 603:

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

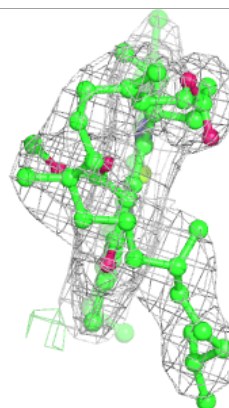
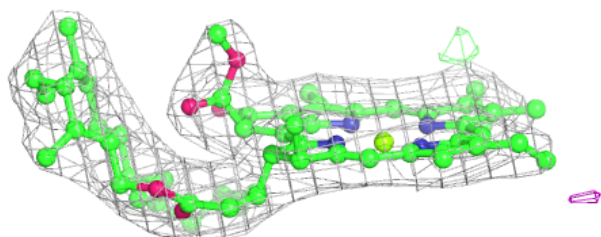
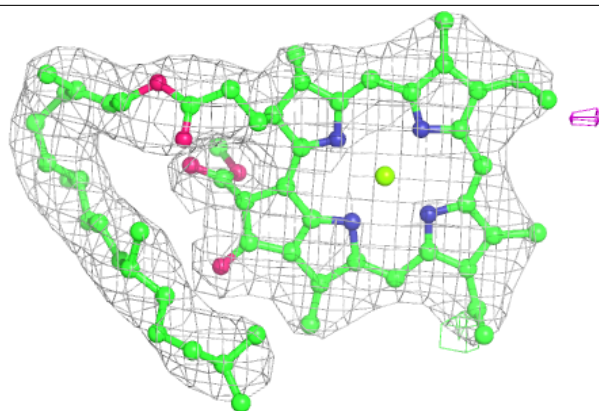
**Electron density around BCR A 409:**

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

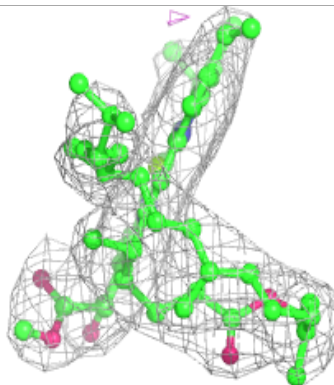
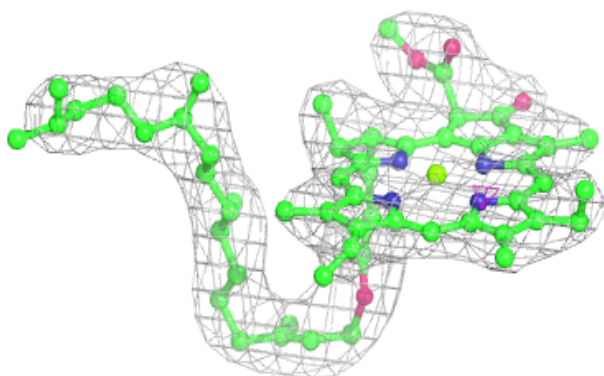
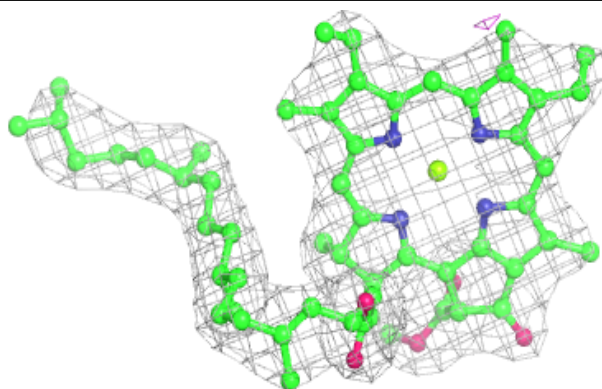


Electron density around CLA B 610:

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

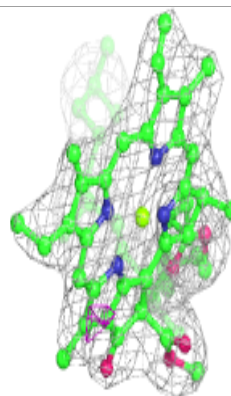
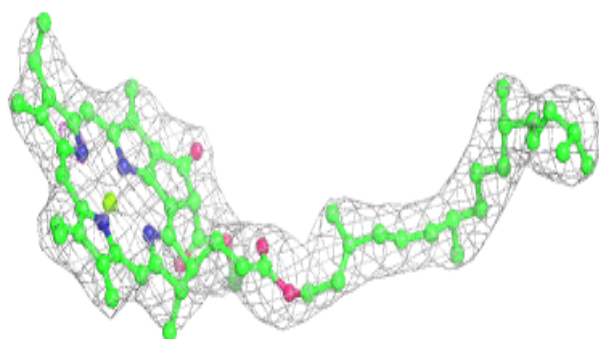
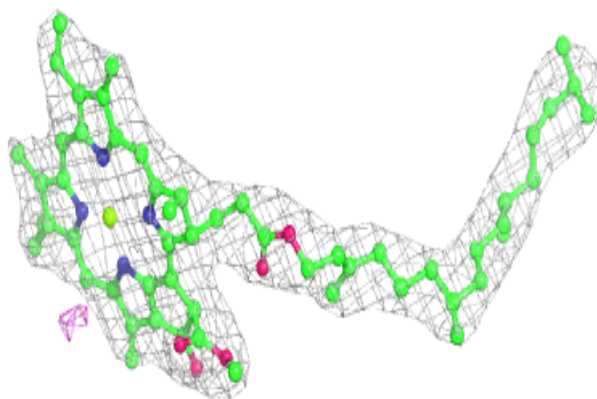
**Electron density around CLA d 401:**

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

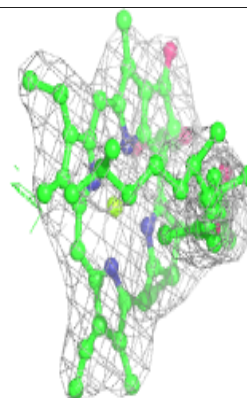
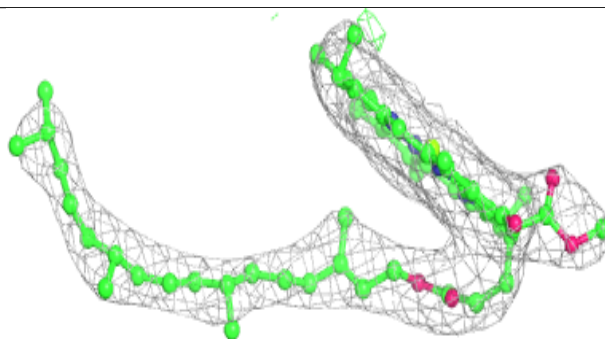
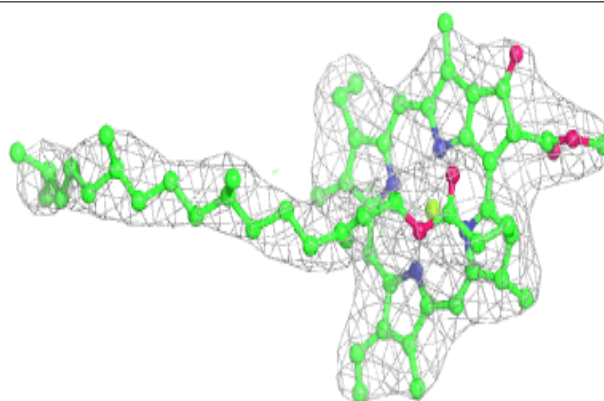


Electron density around CLA a 404:

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

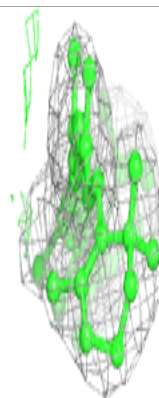
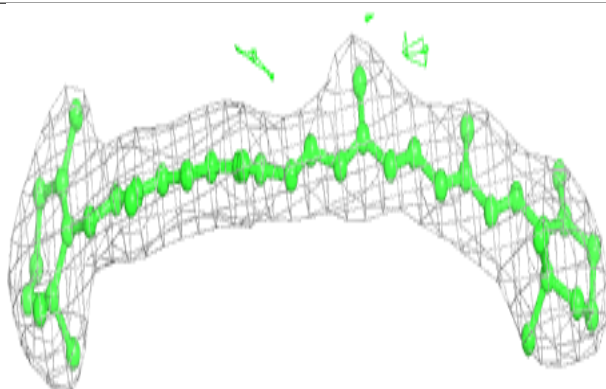
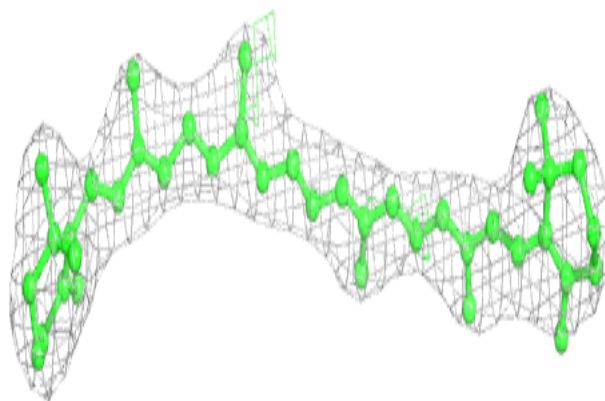
**Electron density around CLA b 608:**

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

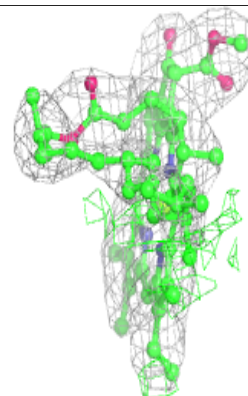
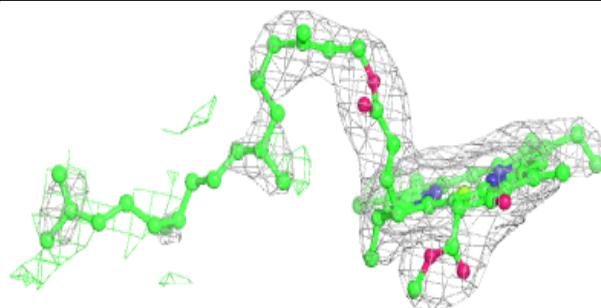
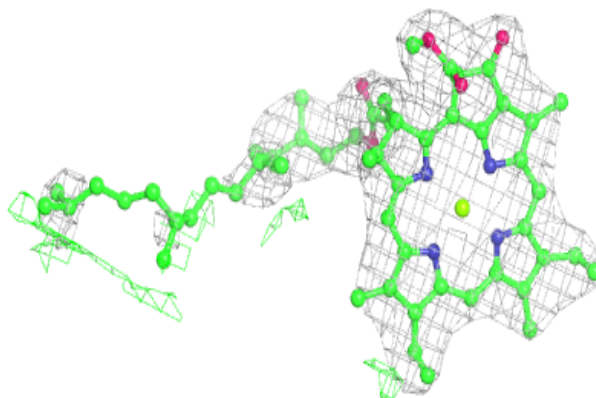


Electron density around BCR t 101:

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

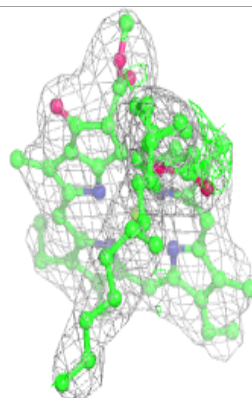
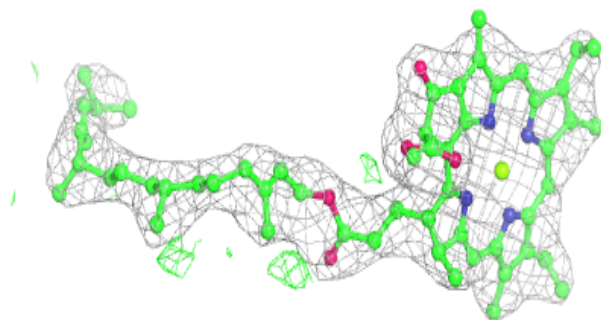
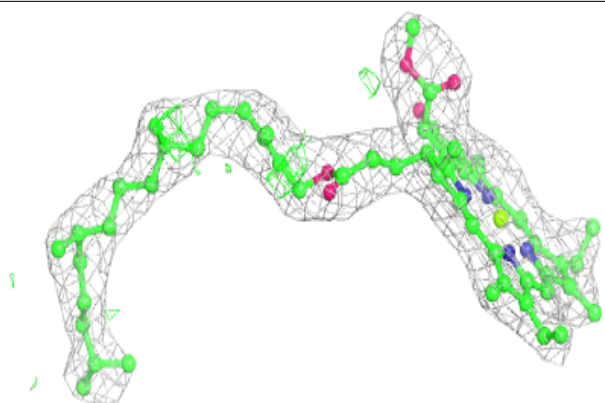
**Electron density around CLA a 405:**

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

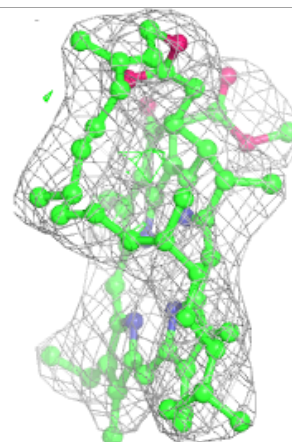
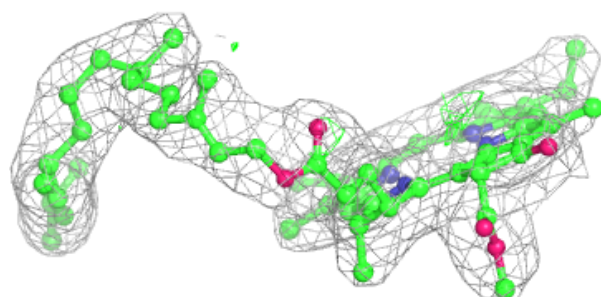
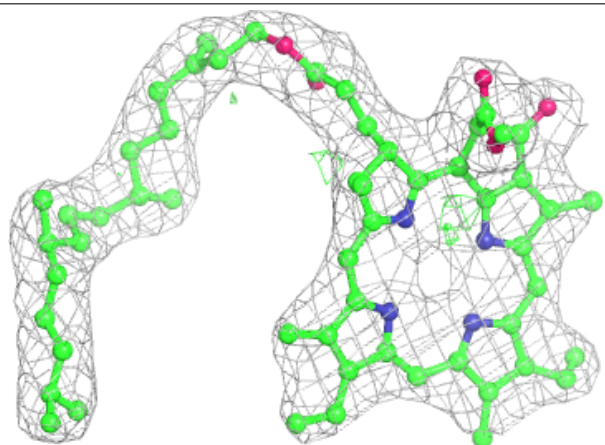


Electron density around CLA d 403:

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

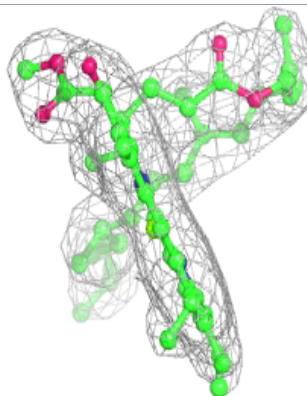
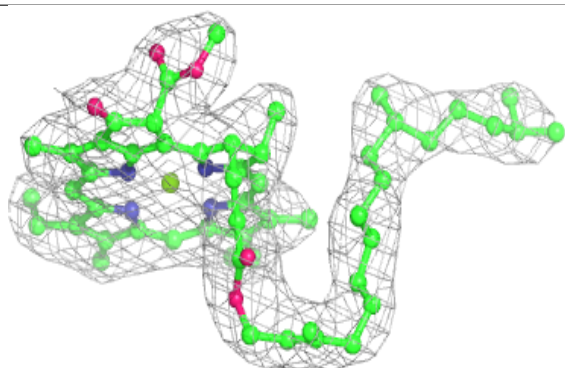
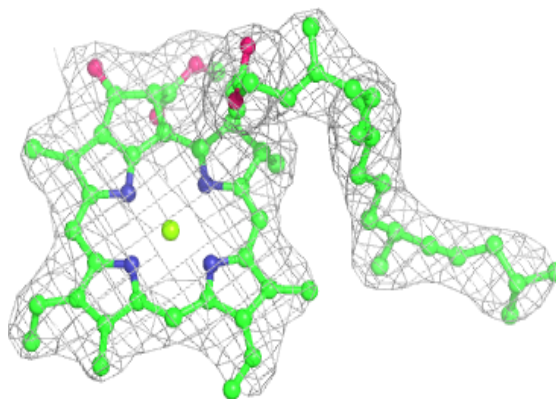
**Electron density around PHO A 407:**

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



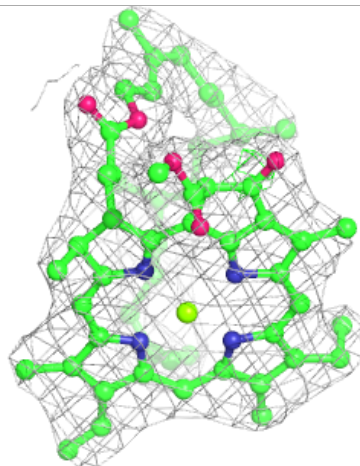
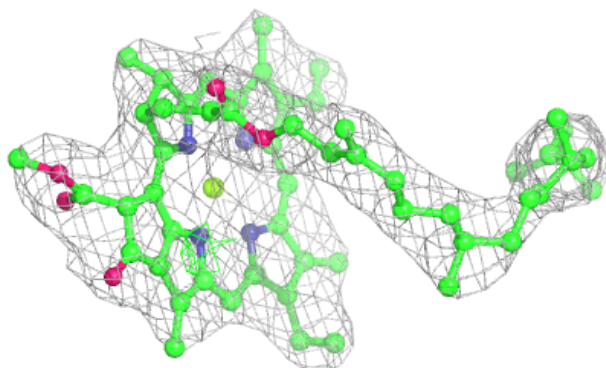
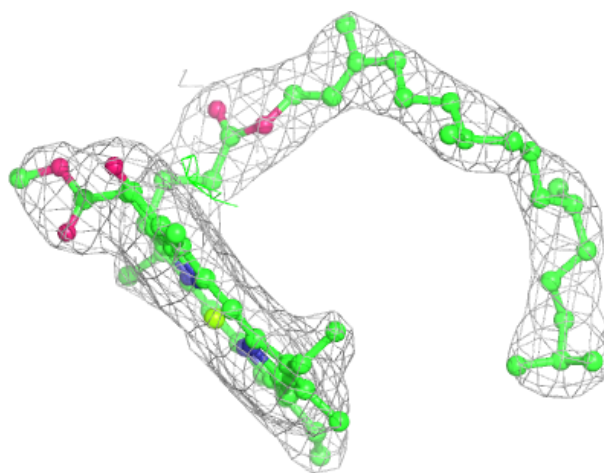
Electron density around CLA A 405:

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



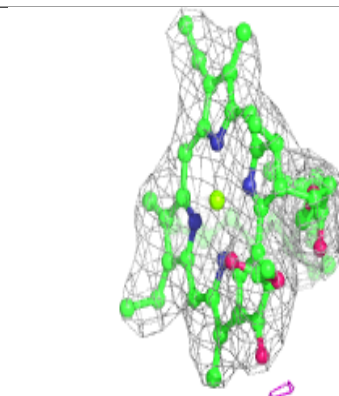
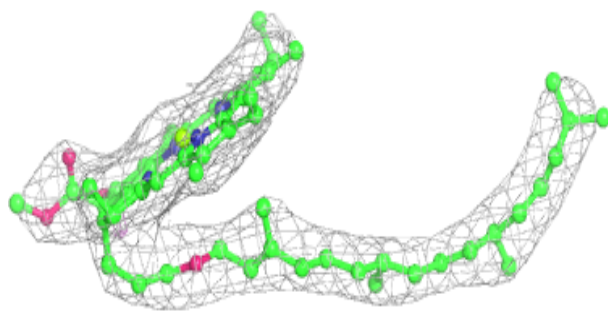
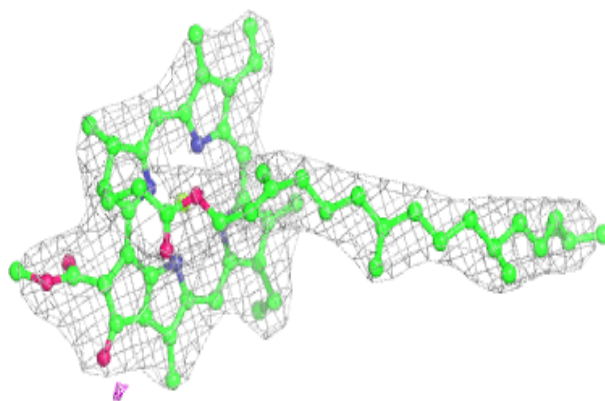
Electron density around CLA b 611:

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

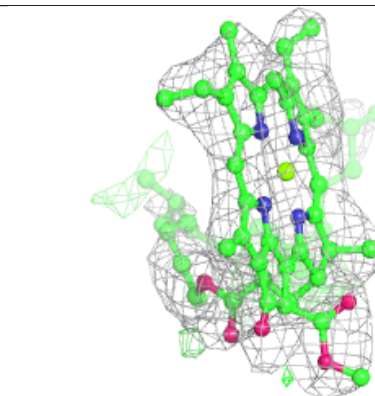
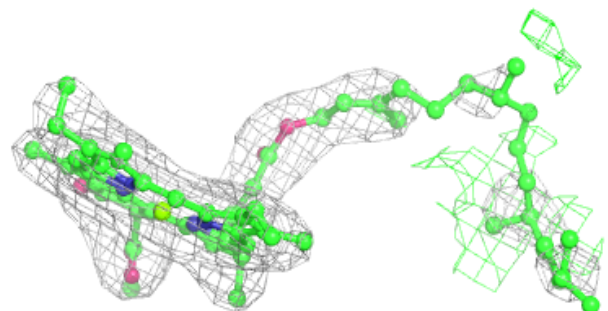
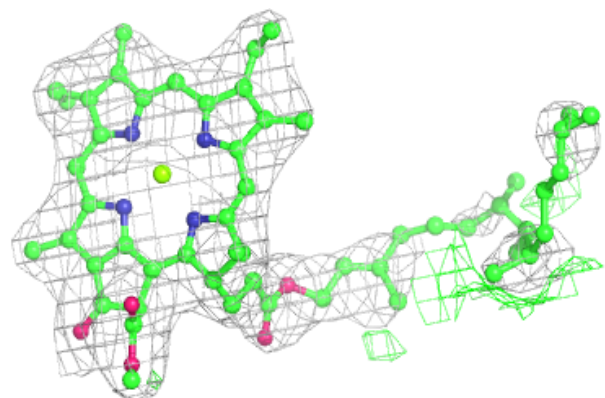


Electron density around CLA B 608:

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

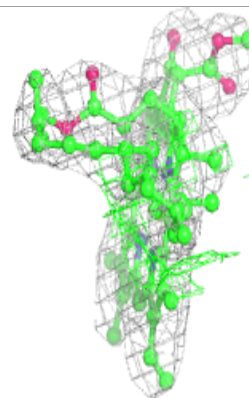
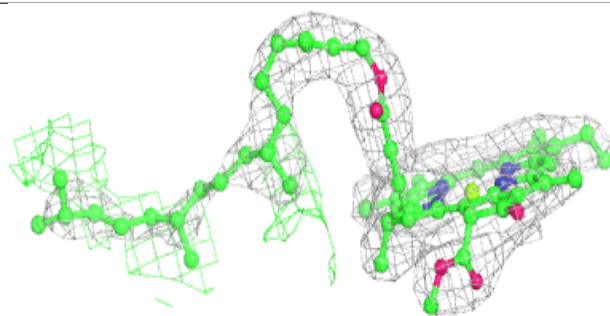
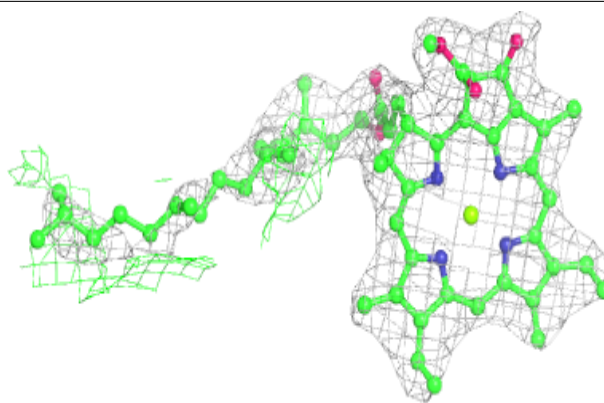
**Electron density around CLA A 408:**

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



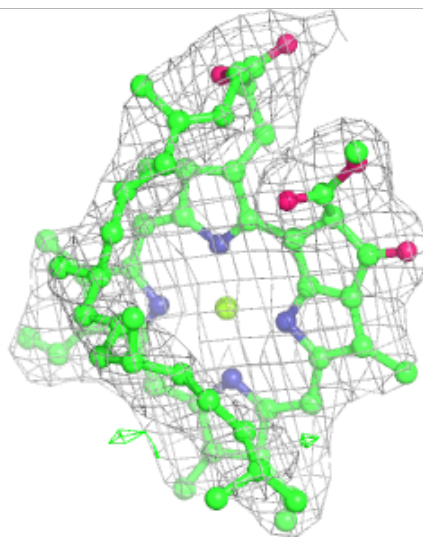
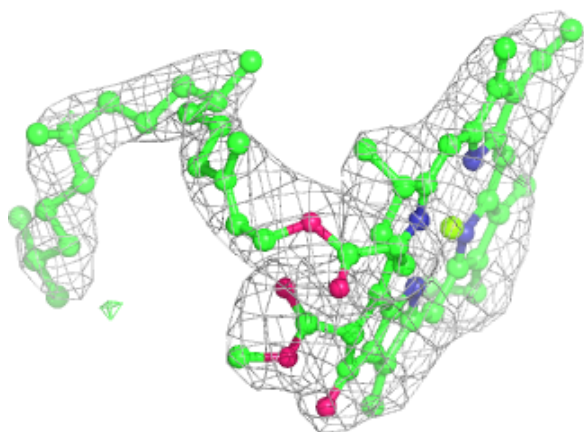
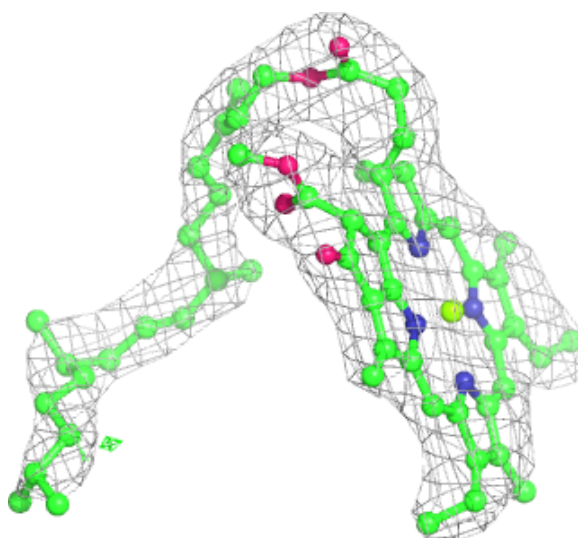
Electron density around CLA A 406:

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



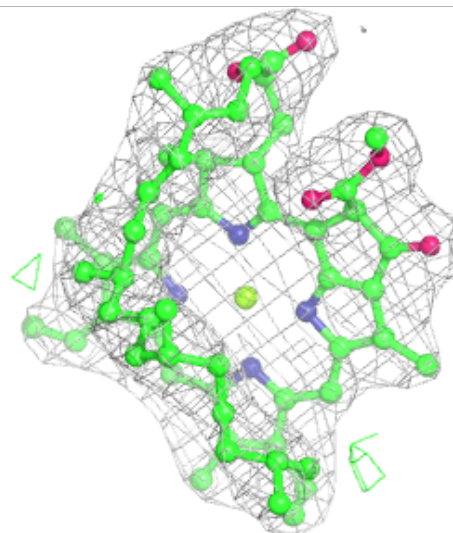
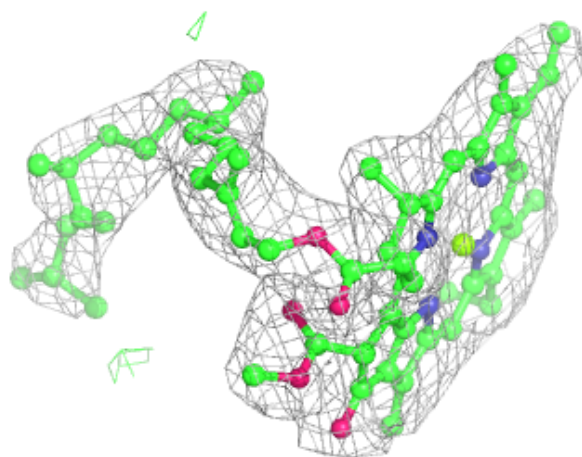
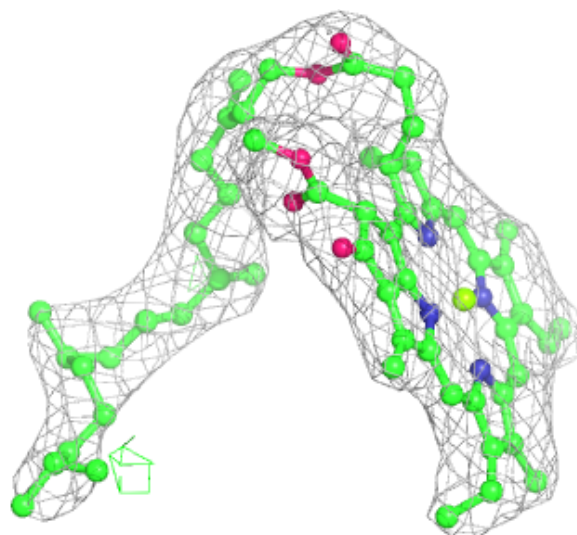
Electron density around CLA b 613:

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



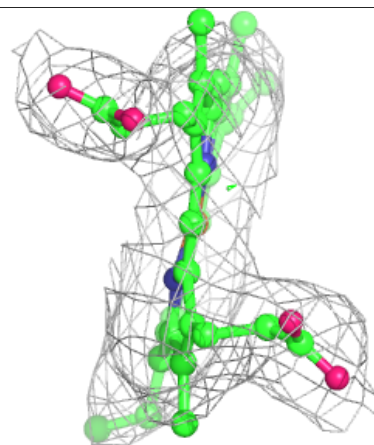
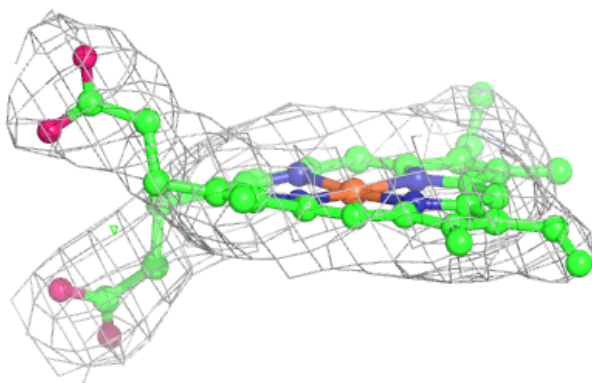
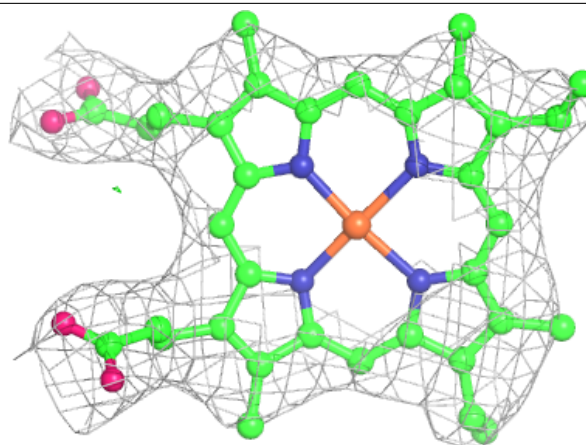
Electron density around CLA B 613:

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



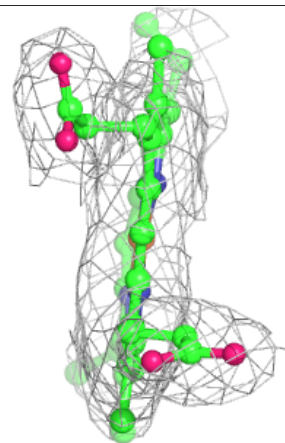
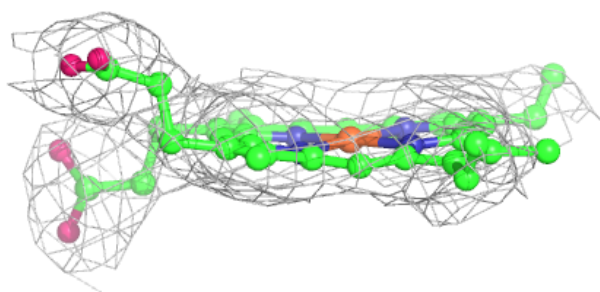
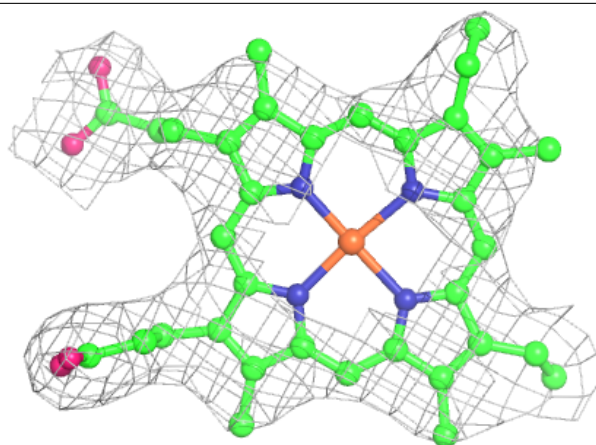
Electron density around HEM E 103:

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



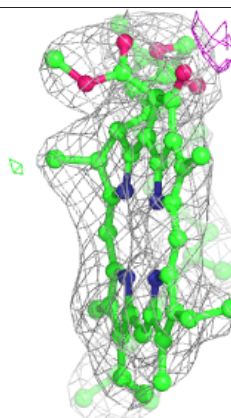
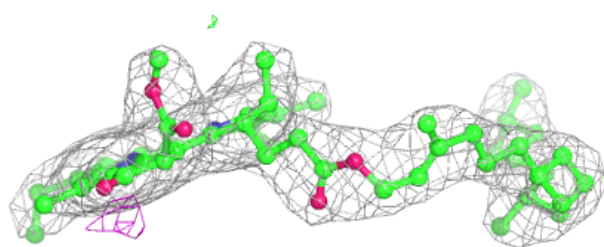
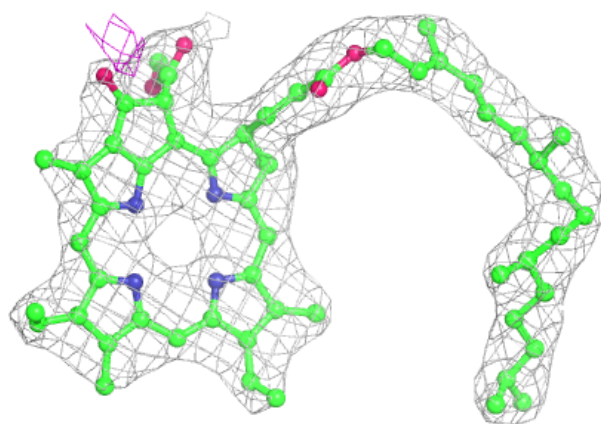
Electron density around HEC V 202:

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



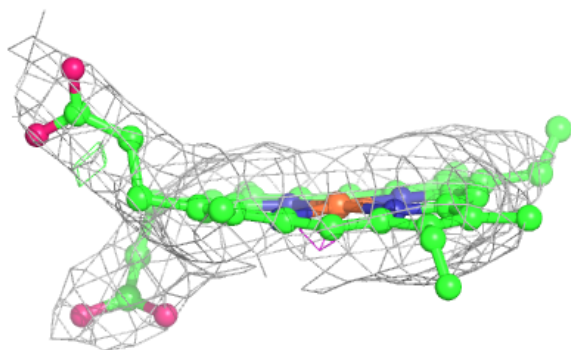
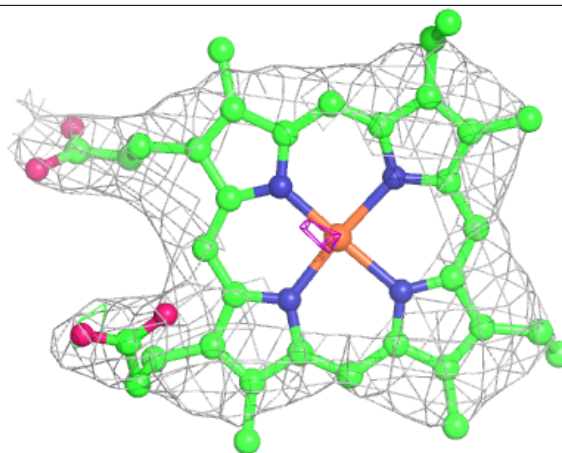
Electron density around PHO a 406:

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

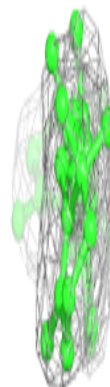
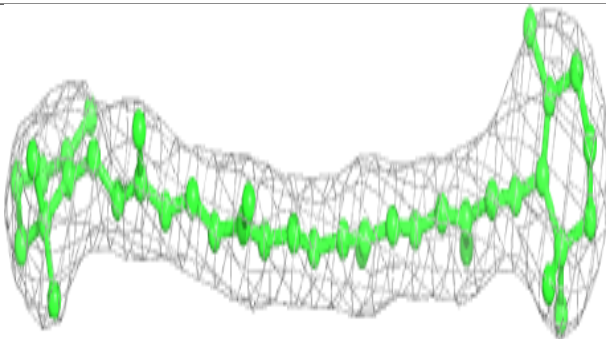
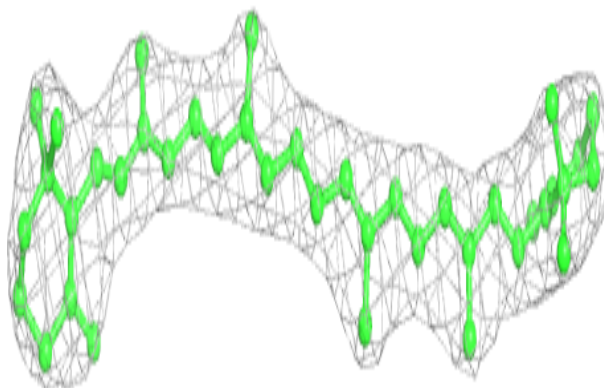


Electron density around HEM e 103:

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

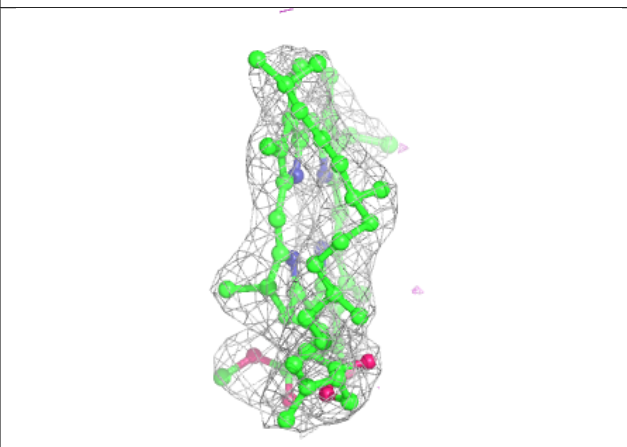
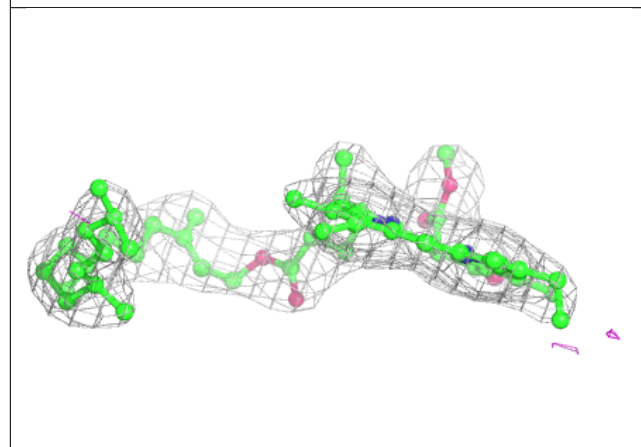
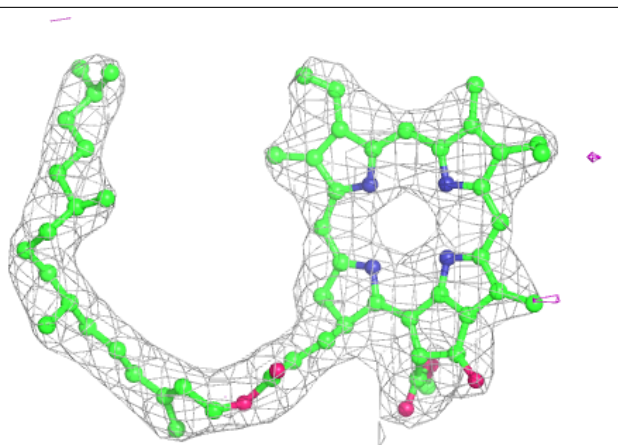
**Electron density around BCR B 617:**

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



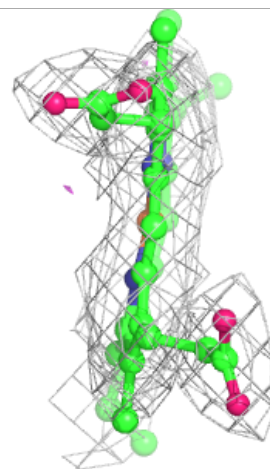
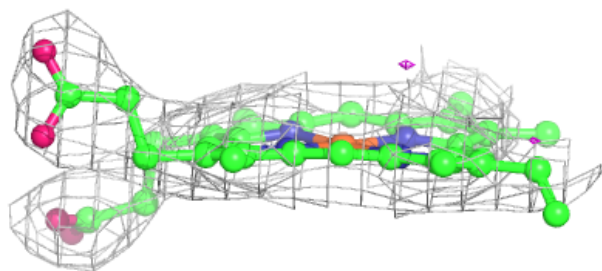
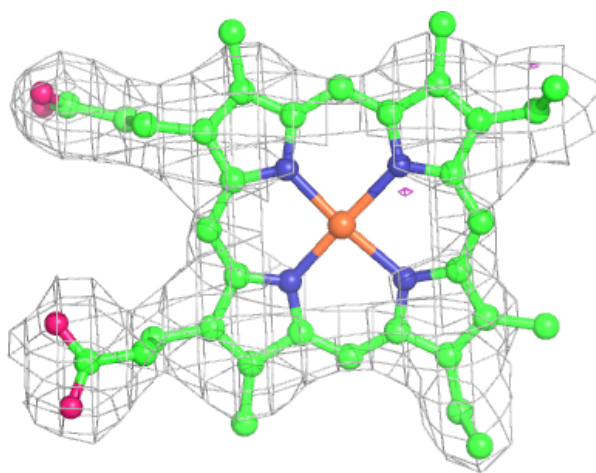
Electron density around PHO D 401:

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



Electron density around 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.