



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 20, 2021 – 10:31 PM JST

PDB ID : 7CJJ
Title : Photosystem II structure in the S2 state
Authors : Li, H.; Shen, J.-R.; Suga, M.
Deposited on : 2020-07-11
Resolution : 2.40 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 : 2.18
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) : 2.18

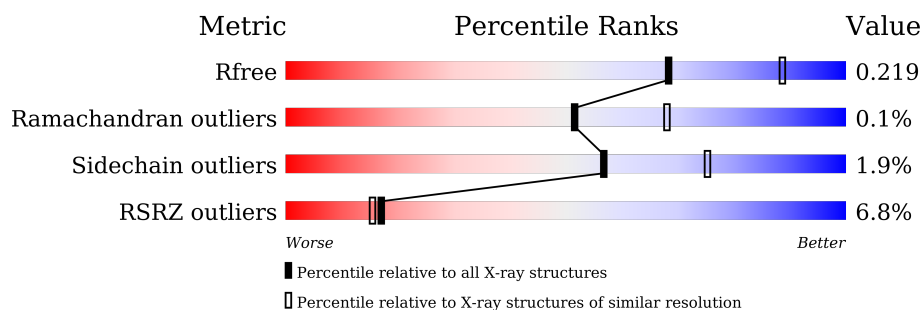
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

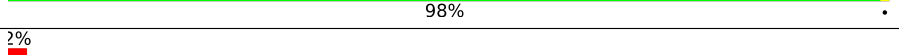
The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	344	 2% 96% ..
1	a	344	 3% 96% ..
2	B	505	 5% 99% .
2	b	505	 9% 98% .
3	C	455	 4% 98% ..
3	c	455	 5% 98% .
4	D	342	 2% 99% .

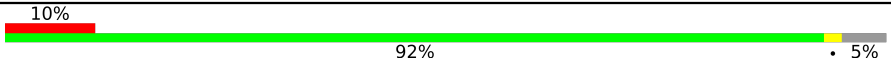
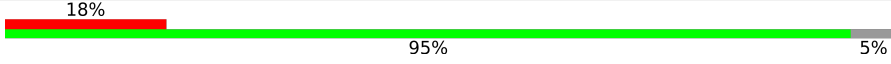
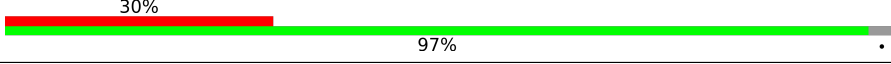
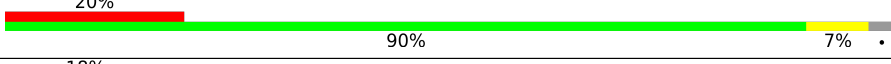
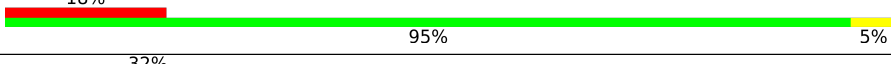
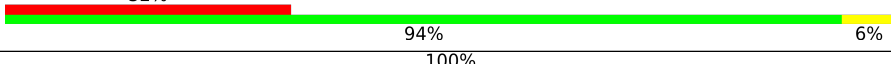

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	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	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	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	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	C	515	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	407	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	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	-	-	-
23	CLA	c	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	515	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
26	SQD	f	101	-	-	-	X
30	UNL	A	414	-	-	-	X
32	HTG	b	622	-	-	-	X
33	LMT	C	526	-	-	-	X
33	LMT	F	101	-	-	-	X
33	LMT	a	418	-	-	-	X
33	LMT	e	101	-	-	-	X
34	LMG	C	522	-	-	-	X
34	LMG	c	522	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53612 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	18	0
			2773	1805	459	494	15			
1	a	334	Total	C	N	O	S	0	19	0
			2781	1811	460	495	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

- 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	10	0
			4050	2650	677	710	13			
2	b	504	Total	C	N	O	S	0	4	0
			3998	2622	665	698	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	5	0
			3522	2300	589	620	13			
3	c	455	Total	C	N	O	S	0	3	0
			3543	2316	592	622	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	UNP D0VWR7

- 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	4	0
			2764	1828	454	470	12			
4	d	341	Total	C	N	O	S	0	4	0
			2755	1823	453	467	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
			668	435	108	125			
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
			517	345	85	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	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			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	UNP P19054

- 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
			304	203	48	53			
11	l	36	Total	C	N	O	0	1	0
			304	203	48	53			

- 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
			268	179	39	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

- 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	3	0
			1886	1177	318	386	5			
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	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	1
			2	2		
21	a	1	Total	Fe	0	1
			2	2		

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

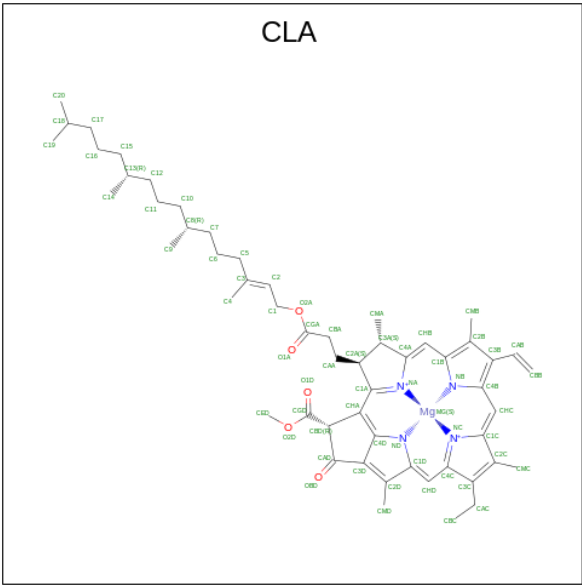
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Cl	0	0
			1	1		
22	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	1	Total	Cl	0	0
			1	1		
22	c	1	Total	Cl	0	0
			1	1		

- 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
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	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

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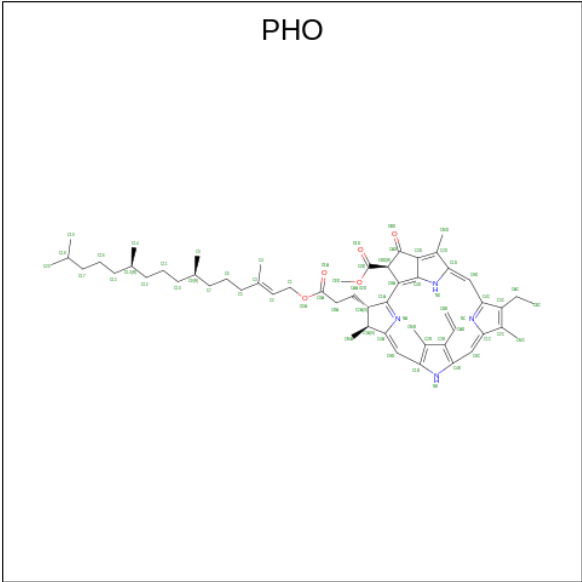
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23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	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
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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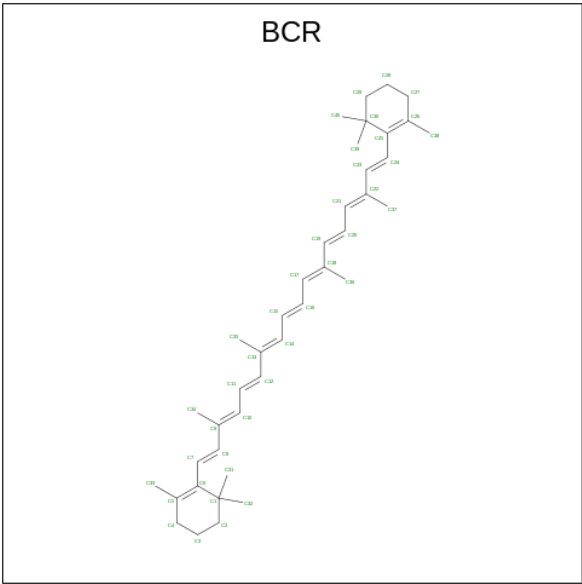
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: C₅₅H₇₄N₄O₅).



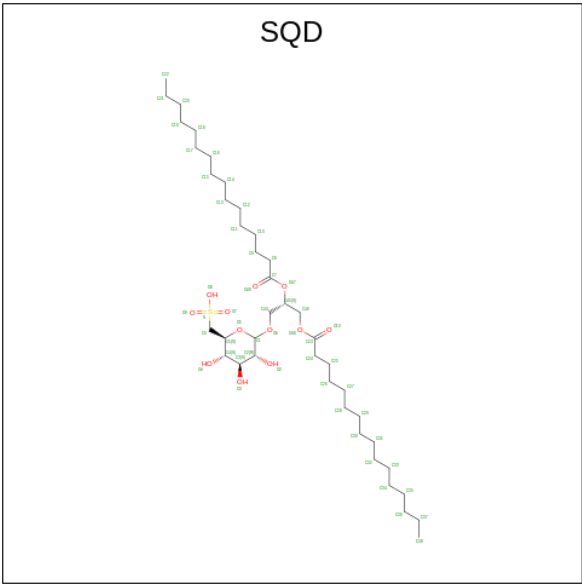
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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	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
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	k	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).



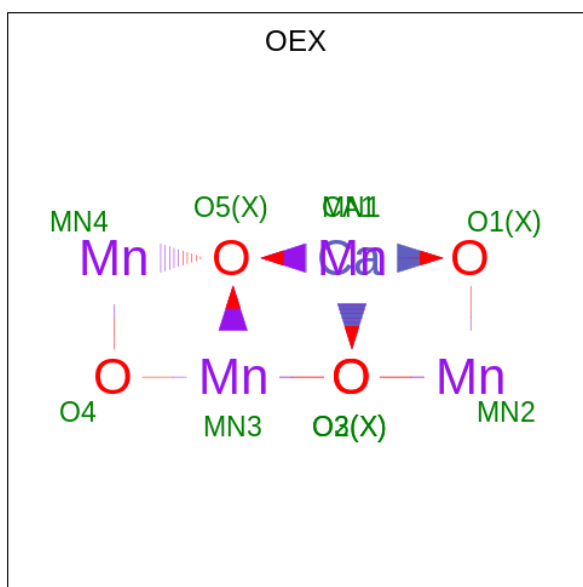
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			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: C₃H₈O₃).



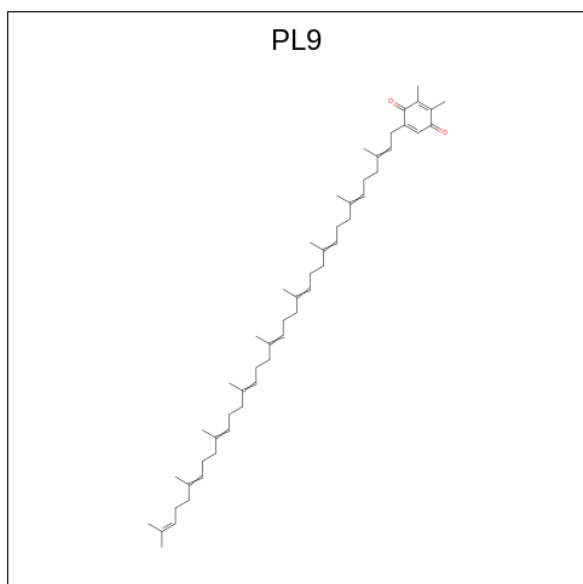
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	v	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	1
			20	2	8	10		
28	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- 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: $C_{53}H_{80}O_2$).



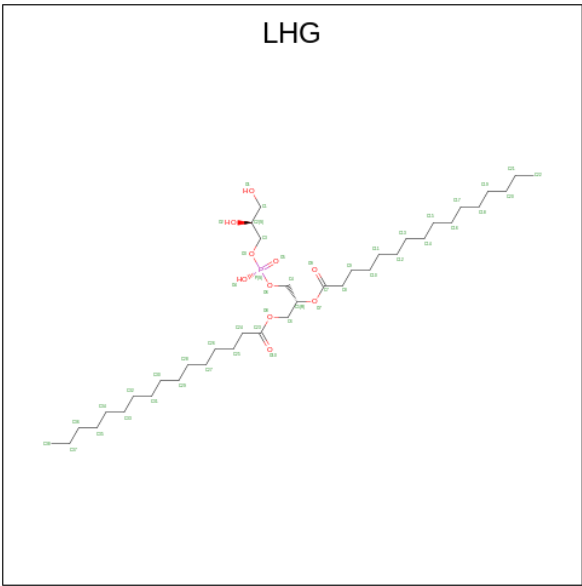
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	1
			110	106	4		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	1
			110	106	4		
29	d	1	Total	C	O	0	0
			55	53	2		

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	C	1	Total	C	O	0	0
			34	29	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	3	Total	C	O	0	0
			71	63	8		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	l	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			

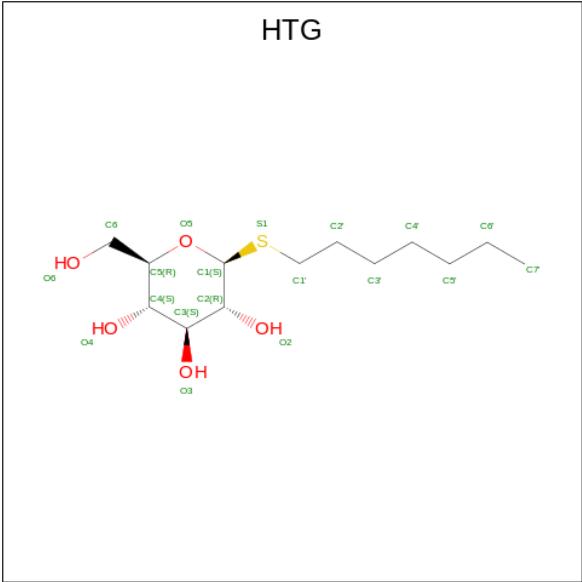
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: C₃₈H₇₅O₁₀P).



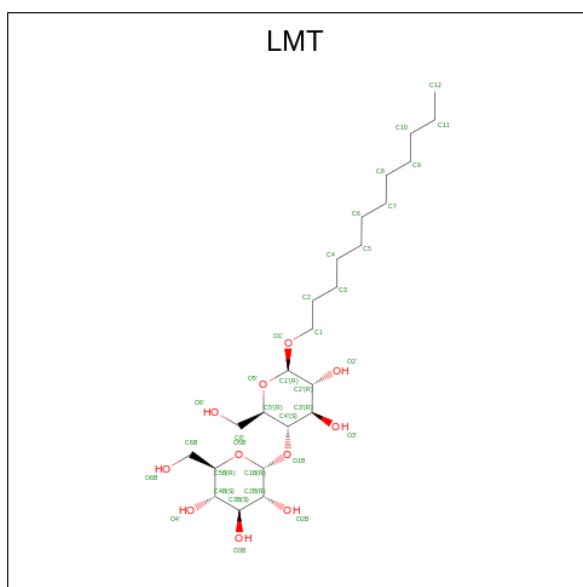
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	b	1	Total	C	O	P	0	0
			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	d	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



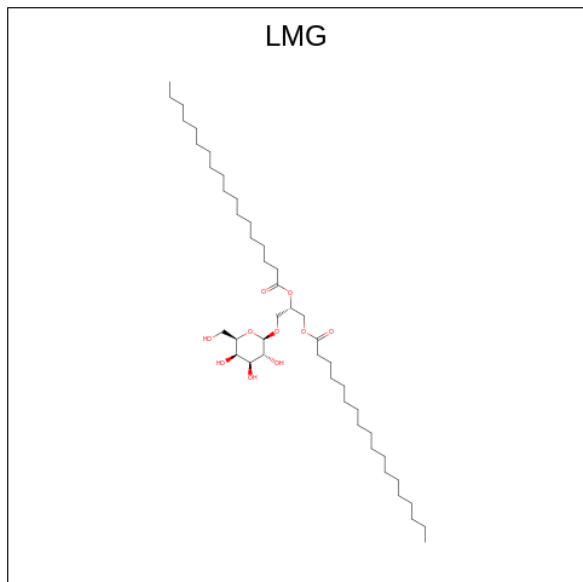
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	D	1	Total	C	O	S	0	0
			16	10	5	1		
32	V	1	Total	C	O		0	0
			11	6	5			
32	b	1	Total	C	O	S	0	0
			19	13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

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



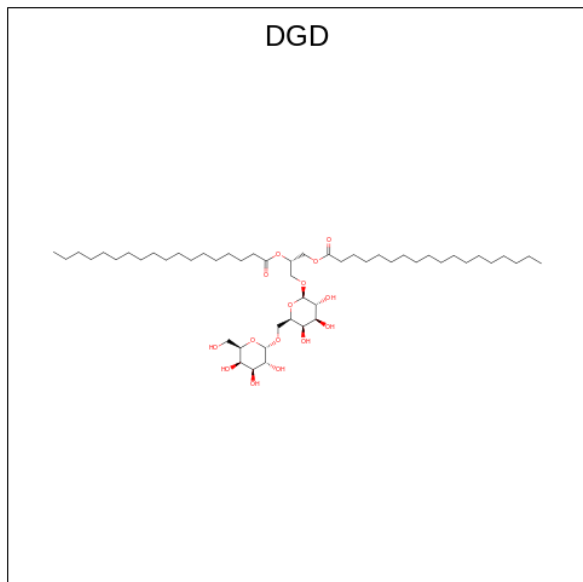
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total 35	C 24	O 11	0	0
33	B	1	Total 25	C 19	O 6	0	0
33	B	1	Total 26	C 19	O 7	0	0
33	C	1	Total 35	C 24	O 11	0	0
33	D	1	Total 35	C 24	O 11	0	0
33	F	1	Total 35	C 24	O 11	0	0
33	M	1	Total 35	C 24	O 11	0	0
33	M	1	Total 35	C 24	O 11	0	0
33	a	1	Total 35	C 24	O 11	0	0
33	a	1	Total 35	C 24	O 11	0	0
33	b	1	Total 25	C 19	O 6	0	0
33	b	1	Total 25	C 19	O 6	0	0
33	e	1	Total 35	C 24	O 11	0	0
33	m	1	Total 35	C 24	O 11	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	M	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

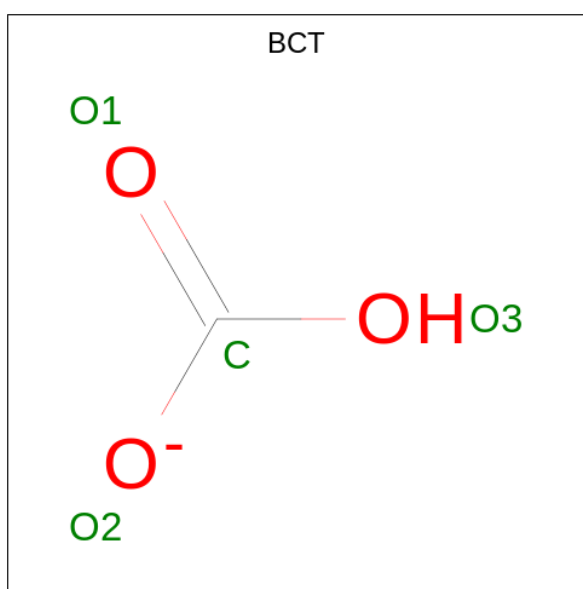
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		

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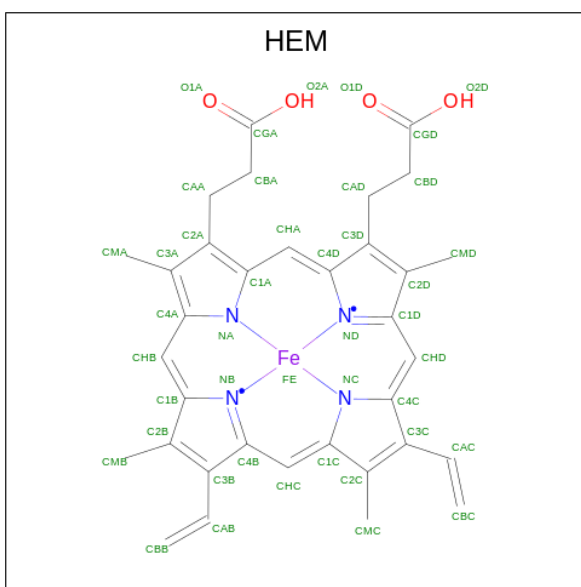
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Ca	0	0
			1	1		
36	a	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	o	1	Total	Ca	0	0
			1	1		

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	1
			8	2	6		
37	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).

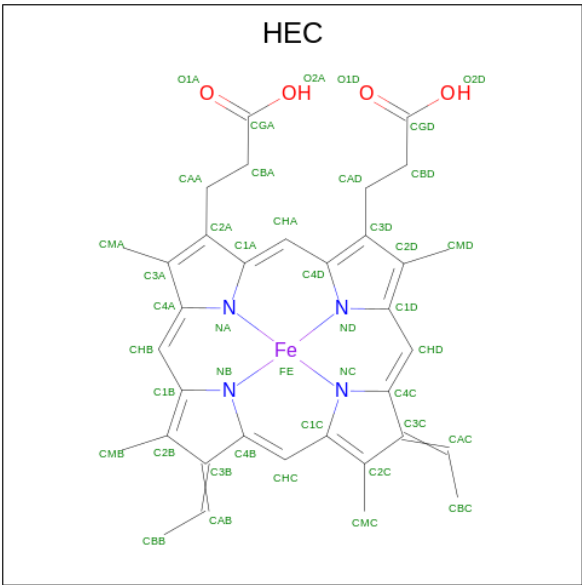


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	147	Total	O	0	11
			157	157		
41	B	218	Total	O	0	0
			218	218		
41	C	188	Total	O	0	4
			191	191		
41	D	124	Total	O	0	2
			126	126		
41	E	24	Total	O	0	0
			24	24		
41	F	8	Total	O	0	0
			8	8		
41	H	28	Total	O	0	0
			28	28		
41	I	4	Total	O	0	0
			4	4		
41	J	6	Total	O	0	0
			6	6		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	8	Total O 8 8	0	0
41	M	18	Total O 18 18	0	0
41	O	118	Total O 118 118	0	0
41	T	14	Total O 14 14	0	0
41	U	56	Total O 56 56	0	0
41	V	95	Total O 95 95	0	0
41	X	10	Total O 10 10	0	0
41	Y	1	Total O 1 1	0	0
41	R	1	Total O 1 1	0	0
41	a	139	Total O 150 150	0	12
41	b	220	Total O 220 220	0	0
41	c	169	Total O 172 172	0	4
41	d	129	Total O 129 129	0	0
41	e	15	Total O 15 15	0	0
41	f	5	Total O 5 5	0	0
41	h	22	Total O 22 22	0	0
41	i	1	Total O 1 1	0	0
41	j	4	Total O 4 4	0	0
41	k	5	Total O 5 5	0	0
41	l	8	Total O 8 8	0	0
41	m	10	Total O 10 10	0	0

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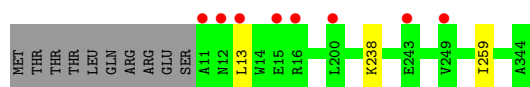
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	99	Total 99	O 99	0	0
41	t	10	Total 10	O 10	0	0
41	u	68	Total 68	O 68	0	0
41	v	57	Total 57	O 57	0	0
41	x	10	Total 10	O 10	0	0
41	y	4	Total 4	O 4	0	0

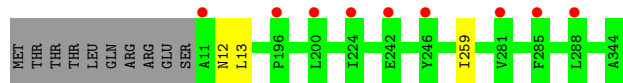
3 Residue-property plots [i](#)

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

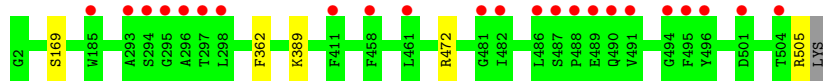
- Molecule 1: Photosystem II protein D1



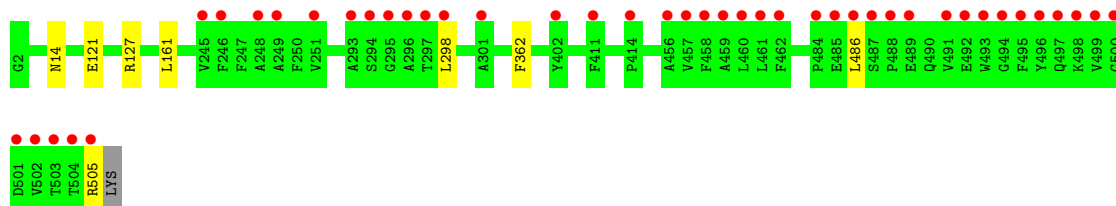
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

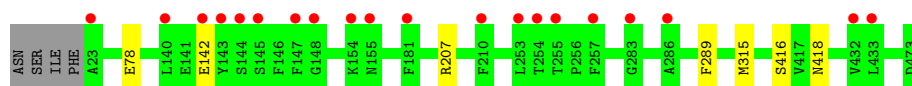


- Molecule 2: Photosystem II CP47 reaction center protein

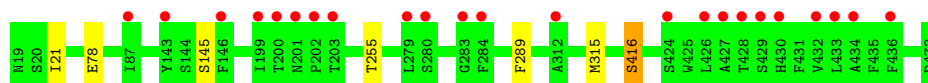


- Molecule 3: Photosystem II CP43 reaction center protein

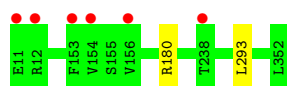




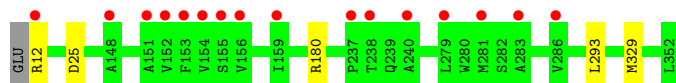
- Molecule 3: Photosystem II CP43 reaction center protein



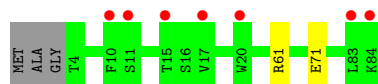
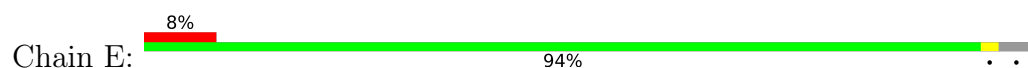
- Molecule 4: Photosystem II D2 protein



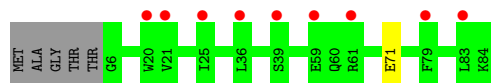
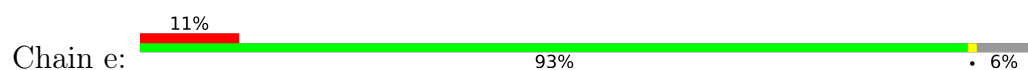
- Molecule 4: Photosystem II D2 protein



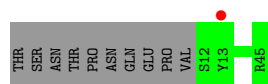
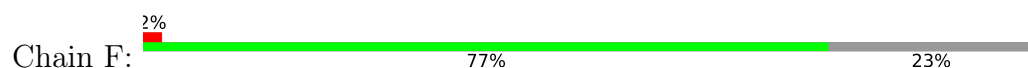
- Molecule 5: Cytochrome b559 subunit alpha



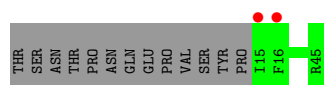
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



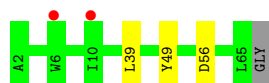
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



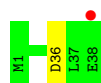
- Molecule 7: Photosystem II reaction center protein H



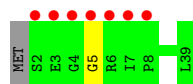
- Molecule 8: Photosystem II reaction center protein I



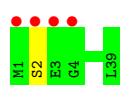
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

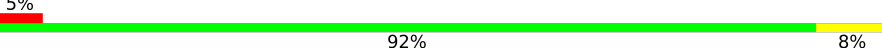


- Molecule 10: Photosystem II reaction center protein K

Chain K:  92% 8%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  5% 92% 8%



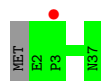
- Molecule 11: Photosystem II reaction center protein L

Chain L:  97% .



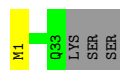
- Molecule 11: Photosystem II reaction center protein L

Chain l:  3% 97% .




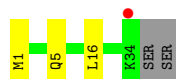
- Molecule 12: Photosystem II reaction center protein M

Chain M:  89% . 8%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  3% 86% 8% 6%

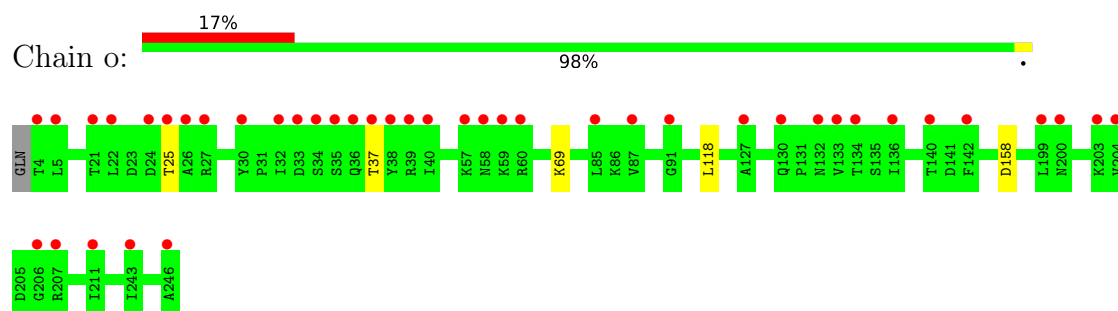


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

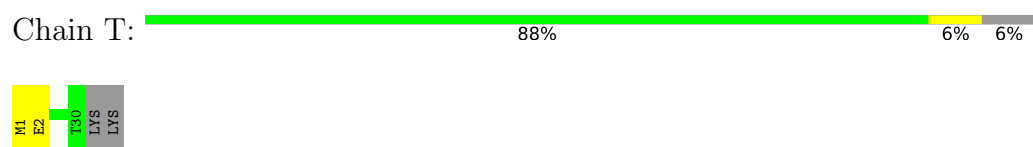
Chain O:  9% 98% .



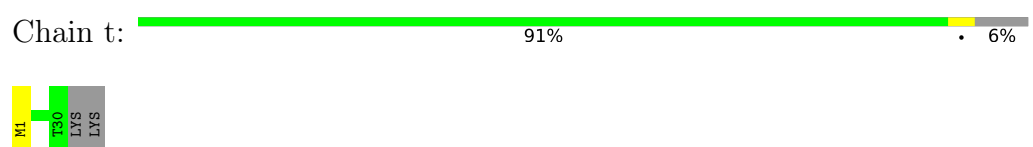
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



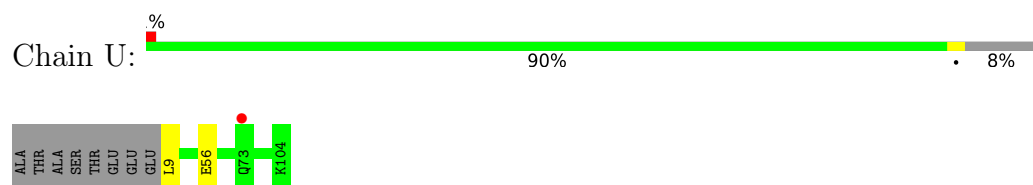
- Molecule 14: Photosystem II reaction center protein T



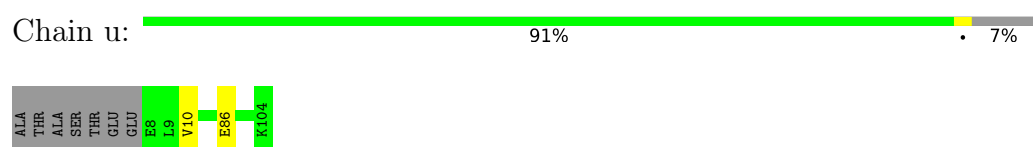
- Molecule 14: Photosystem II reaction center protein T



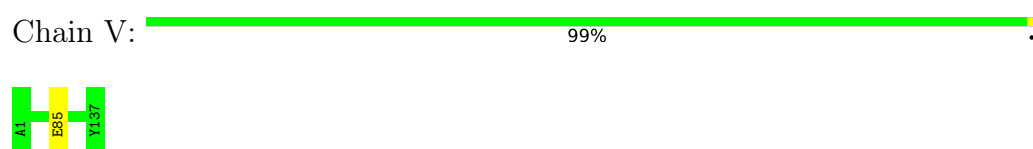
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

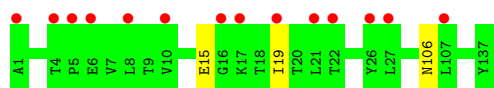


- Molecule 16: Cytochrome c-550

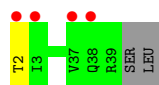
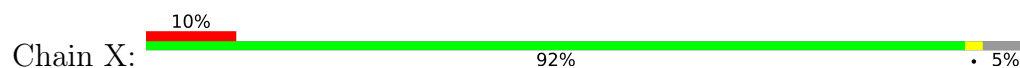


- Molecule 16: Cytochrome c-550

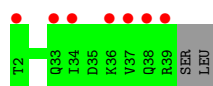




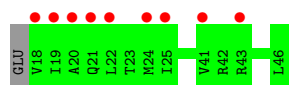
- Molecule 17: Photosystem II reaction center protein X



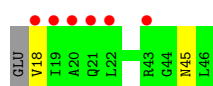
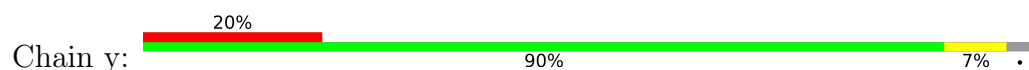
- Molecule 17: Photosystem II reaction center protein X



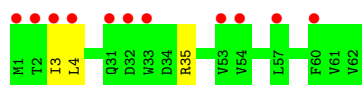
- Molecule 18: Photosystem II reaction center protein Ycf12



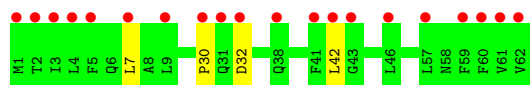
- Molecule 18: Photosystem II reaction center protein Ycf12



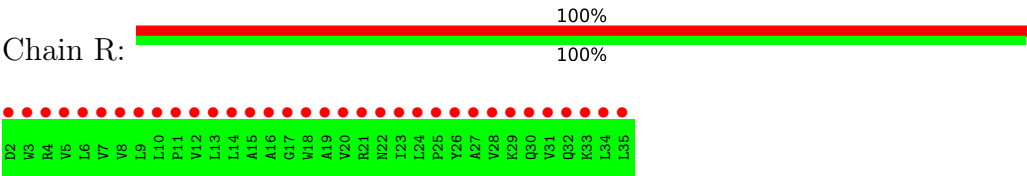
- Molecule 19: Photosystem II reaction center protein Z



- 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	125.75Å 231.63Å 288.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.40 52.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.90-2.40) 82.1 (52.70-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.168 , 0.218 0.169 , 0.219	Depositor DCC
R_{free} test set	16450 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 77.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53612	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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: PL9, CL, CLA, SQD, MG, FME, BCR, HTG, LMG, UNL, LMT, GOL, DGD, FE2, LHG, CA, HEM, BCT, OEX, HEC, PHO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/2861	0.56	0/3897
1	a	0.40	0/2869	0.54	0/3908
2	B	0.41	0/4190	0.55	0/5708
2	b	0.40	0/4138	0.53	0/5640
3	C	0.39	0/3635	0.51	0/4948
3	c	0.36	0/3657	0.49	0/4978
4	D	0.43	0/2861	0.55	0/3897
4	d	0.41	0/2852	0.54	0/3885
5	E	0.34	0/687	0.50	0/936
5	e	0.36	0/667	0.47	0/908
6	F	0.38	0/284	0.48	0/387
6	f	0.32	0/257	0.47	0/349
7	H	0.35	0/530	0.56	0/723
7	h	0.34	0/519	0.55	0/708
8	I	0.35	0/311	0.50	0/419
8	i	0.34	0/311	0.49	0/419
9	J	0.33	0/278	0.51	0/376
9	j	0.32	0/283	0.52	0/383
10	K	0.35	0/303	0.51	0/416
10	k	0.35	0/303	0.50	0/416
11	L	0.44	0/311	0.51	0/423
11	l	0.42	0/311	0.51	0/423
12	M	0.45	0/261	0.54	0/357
12	m	0.39	0/262	0.51	0/357
13	O	0.40	0/1917	0.58	0/2599
13	o	0.37	0/1910	0.59	1/2589 (0.0%)
14	T	0.46	0/257	0.50	0/349
14	t	0.45	0/257	0.44	0/349
15	U	0.38	0/776	0.55	0/1052
15	u	0.36	0/785	0.58	0/1064
16	V	0.37	0/1085	0.53	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.34	0/1085	0.52	0/1473
17	X	0.31	0/284	0.48	0/384
17	x	0.30	0/284	0.45	0/384
18	Y	0.29	0/216	0.45	0/289
18	y	0.30	0/216	0.44	0/289
19	Z	0.31	0/490	0.40	0/669
19	z	0.31	0/490	0.41	0/669
20	R	0.28	0/279	0.46	0/383
All	All	0.39	0/43272	0.53	1/58876 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/344 (102%)	345 (99%)	3 (1%)	1 (0%)	41	55
1	a	350/344 (102%)	345 (99%)	4 (1%)	1 (0%)	41	55
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	496 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	454/455 (100%)	447 (98%)	5 (1%)	2 (0%)	34	48
3	c	456/455 (100%)	445 (98%)	10 (2%)	1 (0%)	47	62
4	D	344/342 (101%)	334 (97%)	10 (3%)	0	100	100
4	d	343/342 (100%)	331 (96%)	12 (4%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	74 (96%)	3 (4%)	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%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	32 (89%)	3 (8%)	1 (3%)	5	4
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%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	244/244 (100%)	236 (97%)	7 (3%)	1 (0%)	34	48
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	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%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	11
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5286/5384 (98%)	5165 (98%)	113 (2%)	8 (0%)	51	62

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
13	O	61	GLN
19	z	30	PRO

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	286/279 (102%)	284 (99%)	2 (1%)	84	92
1	a	287/279 (103%)	285 (99%)	2 (1%)	84	92
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	85
2	b	406/403 (101%)	398 (98%)	8 (2%)	55	74
3	C	357/356 (100%)	351 (98%)	6 (2%)	60	78
3	c	359/356 (101%)	352 (98%)	7 (2%)	57	75
4	D	281/277 (101%)	279 (99%)	2 (1%)	84	92
4	d	280/277 (101%)	275 (98%)	5 (2%)	59	76
5	E	73/73 (100%)	71 (97%)	2 (3%)	44	65
5	e	70/73 (96%)	69 (99%)	1 (1%)	67	82
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	55/54 (102%)	50 (91%)	5 (9%)	9	14
7	h	54/54 (100%)	51 (94%)	3 (6%)	21	34
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	62
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	51
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	11
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	11
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%)	30 (100%)	0	100	100
12	m	30/32 (94%)	28 (93%)	2 (7%)	16	26
13	O	209/207 (101%)	205 (98%)	4 (2%)	57	75
13	o	208/207 (100%)	204 (98%)	4 (2%)	57	75
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	51
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	68
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	68
16	V	117/117 (100%)	116 (99%)	1 (1%)	78	90
16	v	117/117 (100%)	114 (97%)	3 (3%)	46	66
17	X	31/33 (94%)	30 (97%)	1 (3%)	39	59
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%)	20 (91%)	2 (9%)	9	14
19	Z	52/52 (100%)	49 (94%)	3 (6%)	20	32
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	32
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4392/4403 (100%)	4308 (98%)	84 (2%)	57	75

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	293	LEU

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Mol	Chain	Res	Type
13	o	37	THR
5	e	71	GLU
10	k	10	LYS
15	u	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
13	O	80	GLN
13	o	88	ASN
13	o	196	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.61	0	7,9,11	1.18	1 (14%)
8	FME	I	1	8	8,9,10	0.63	0	7,9,11	1.14	1 (14%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.21	1 (14%)
14	FME	t	1	14	8,9,10	0.61	0	7,9,11	1.50	2 (28%)
8	FME	i	1	8	8,9,10	0.59	0	7,9,11	0.93	0
12	FME	M	1	12	8,9,10	0.59	0	7,9,11	1.55	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	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	O-C-CA	-2.72	117.65	124.78
12	M	1	FME	CA-N-CN	-2.68	118.70	122.82
14	t	1	FME	O-C-CA	-2.56	118.08	124.78
14	t	1	FME	CA-N-CN	-2.42	119.10	122.82
12	M	1	FME	O-C-CA	-2.21	118.99	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN

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 224 ligands modelled in this entry, 17 are monoatomic and 18 are unknown - leaving 189 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	B	601	41	59,73,73	2.08	14 (23%)	67,113,113	2.10	21 (31%)
31	LHG	D	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
24	PHO	a	406	-	67,69,69	2.13	16 (23%)	85,99,99	1.91	23 (27%)
29	PL9	A	413[B]	-	55,55,55	0.63	2 (3%)	68,69,69	2.02	23 (33%)
23	CLA	a	407	-	59,73,73	1.96	14 (23%)	67,113,113	2.29	24 (35%)
25	BCR	b	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.65	13 (23%)
23	CLA	B	607	41	59,73,73	1.98	13 (22%)	67,113,113	2.20	21 (31%)
26	SQD	B	620	-	53,54,54	1.01	3 (5%)	62,65,65	1.51	9 (14%)
34	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.49	6 (13%)
35	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	1.09	5 (6%)
25	BCR	C	517	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	11 (19%)
27	GOL	A	410	-	5,5,5	1.09	0	5,5,5	0.90	0
25	BCR	k	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.59	13 (23%)
23	CLA	C	514	-	59,73,73	2.07	13 (22%)	67,113,113	2.24	22 (32%)
34	LMG	d	411	39	51,51,55	0.91	2 (3%)	59,59,63	0.92	1 (1%)
23	CLA	b	606	-	59,73,73	1.92	12 (20%)	67,113,113	2.28	23 (34%)
25	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.66	11 (19%)
26	SQD	A	411	-	53,54,54	1.05	3 (5%)	62,65,65	1.28	8 (12%)
33	LMT	b	620	-	25,25,36	0.51	0	30,30,47	0.61	0
32	HTG	b	621	-	19,19,19	1.01	2 (10%)	23,24,24	1.35	4 (17%)
23	CLA	b	603	-	59,73,73	2.08	13 (22%)	67,113,113	2.27	21 (31%)
27	GOL	v	201	-	5,5,5	1.19	0	5,5,5	0.85	0
24	PHO	A	406	-	67,69,69	2.13	16 (23%)	85,99,99	1.90	23 (27%)
33	LMT	B	630	-	26,26,36	0.51	0	31,31,47	1.00	1 (3%)
34	LMG	D	412	39	51,51,55	0.87	3 (5%)	59,59,63	1.08	5 (8%)
23	CLA	C	509	41	59,73,73	2.01	13 (22%)	67,113,113	2.17	20 (29%)
25	BCR	d	404	-	41,41,41	1.19	2 (4%)	56,56,56	1.81	14 (25%)
27	GOL	a	410	-	5,5,5	0.89	0	5,5,5	1.04	0
32	HTG	c	523	-	19,19,19	0.99	2 (10%)	23,24,24	1.33	1 (4%)
34	LMG	C	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	2 (3%)
23	CLA	C	512	-	59,73,73	1.99	14 (23%)	67,113,113	2.21	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	608	-	59,73,73	2.02	13 (22%)	67,113,113	2.21	26 (38%)
23	CLA	B	611	-	59,73,73	2.02	14 (23%)	67,113,113	2.31	23 (34%)
23	CLA	b	613	-	59,73,73	2.02	12 (20%)	67,113,113	2.26	24 (35%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.05	2 (4%)
23	CLA	c	503	-	59,73,73	1.98	14 (23%)	67,113,113	2.16	24 (35%)
27	GOL	C	524	-	5,5,5	1.10	0	5,5,5	1.09	0
23	CLA	b	610	41	59,73,73	1.95	14 (23%)	67,113,113	2.33	25 (37%)
31	LHG	d	406	-	48,48,48	0.90	2 (4%)	51,54,54	1.12	5 (9%)
23	CLA	c	512	-	59,73,73	1.95	13 (22%)	67,113,113	2.22	24 (35%)
33	LMT	M	103	-	36,36,36	0.52	0	47,47,47	1.07	3 (6%)
33	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.93	2 (4%)
26	SQD	a	411	-	53,54,54	1.04	3 (5%)	62,65,65	1.25	7 (11%)
23	CLA	C	511	-	59,73,73	2.08	14 (23%)	67,113,113	2.20	21 (31%)
23	CLA	C	505	-	59,73,73	2.00	13 (22%)	67,113,113	2.20	20 (29%)
25	BCR	B	618	-	41,41,41	0.92	1 (2%)	56,56,56	1.59	12 (21%)
27	GOL	b	623	-	5,5,5	0.95	0	5,5,5	1.10	0
27	GOL	B	628	-	5,5,5	1.05	0	5,5,5	0.91	0
23	CLA	B	602	-	59,73,73	2.01	13 (22%)	67,113,113	2.34	24 (35%)
25	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.44	8 (14%)
25	BCR	A	408	-	41,41,41	1.10	1 (2%)	56,56,56	1.38	6 (10%)
28	OEX	A	412[A]	3,1,41	0,15,15	0.00	-	-	-	-
33	LMT	D	402	-	36,36,36	0.55	1 (2%)	47,47,47	0.77	0
23	CLA	c	513	3	59,73,73	1.97	13 (22%)	67,113,113	2.21	25 (37%)
23	CLA	a	405	41	59,73,73	1.96	12 (20%)	67,113,113	2.18	23 (34%)
37	BCT	D	401[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
25	BCR	h	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	9 (16%)
23	CLA	b	612	-	59,73,73	2.04	13 (22%)	67,113,113	2.35	23 (34%)
34	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.09	4 (6%)
33	LMT	a	412	-	36,36,36	0.64	1 (2%)	47,47,47	1.29	5 (10%)
27	GOL	b	627	-	5,5,5	0.98	0	5,5,5	1.02	0
27	GOL	c	527	-	5,5,5	0.81	0	5,5,5	1.07	0
34	LMG	M	101	-	51,51,55	1.03	2 (3%)	59,59,63	1.07	3 (5%)
29	PL9	a	414[B]	-	55,55,55	0.67	2 (3%)	68,69,69	1.94	19 (27%)
23	CLA	B	608	-	59,73,73	1.98	13 (22%)	67,113,113	2.21	25 (37%)
37	BCT	d	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	C	508	-	59,73,73	1.99	13 (22%)	67,113,113	2.17	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	504	-	59,73,73	2.03	12 (20%)	67,113,113	2.10	20 (29%)
26	SQD	a	409	-	53,54,54	1.00	3 (5%)	62,65,65	1.68	11 (17%)
28	OEX	a	413[A]	3,1,41	0,15,15	0.00	-	-		
25	BCR	b	617	-	41,41,41	1.11	1 (2%)	56,56,56	1.48	8 (14%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.47	11 (19%)
23	CLA	A	407	-	59,73,73	2.00	13 (22%)	67,113,113	2.20	24 (35%)
23	CLA	c	509	41	59,73,73	2.02	13 (22%)	67,113,113	2.17	20 (29%)
23	CLA	A	404	41	59,73,73	1.95	14 (23%)	67,113,113	2.20	25 (37%)
23	CLA	c	511	-	59,73,73	2.12	14 (23%)	67,113,113	2.26	23 (34%)
23	CLA	D	404	-	59,73,73	2.01	12 (20%)	67,113,113	2.18	23 (34%)
32	HTG	D	411	-	16,16,19	1.05	2 (12%)	20,21,24	1.41	1 (5%)
34	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.20	6 (10%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.06	4 (5%)
33	LMT	e	101	-	36,36,36	0.52	1 (2%)	47,47,47	0.92	3 (6%)
27	GOL	B	623	-	5,5,5	0.87	0	5,5,5	1.04	0
23	CLA	b	601	41	59,73,73	2.07	13 (22%)	67,113,113	2.23	22 (32%)
23	CLA	c	506	41	59,73,73	2.13	14 (23%)	67,113,113	2.20	24 (35%)
23	CLA	b	611	-	59,73,73	1.94	13 (22%)	67,113,113	2.21	20 (29%)
34	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.06	5 (8%)
24	PHO	A	415	-	67,69,69	2.10	17 (25%)	85,99,99	2.04	20 (23%)
23	CLA	b	605	-	59,73,73	1.98	14 (23%)	67,113,113	2.25	22 (32%)
23	CLA	b	604	-	59,73,73	1.97	13 (22%)	67,113,113	2.21	21 (31%)
33	LMT	m	103	-	36,36,36	0.46	0	47,47,47	1.06	3 (6%)
38	HEM	E	102	5,6	27,50,50	0.85	1 (3%)	17,82,82	2.14	4 (23%)
23	CLA	A	405	41	59,73,73	1.99	11 (18%)	67,113,113	2.10	18 (26%)
34	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.20	7 (11%)
35	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.13	5 (6%)
33	LMT	F	101	-	36,36,36	0.55	1 (2%)	47,47,47	1.18	5 (10%)
23	CLA	c	510	-	59,73,73	2.11	14 (23%)	67,113,113	2.39	22 (32%)
26	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.64	9 (14%)
40	HEC	v	202	16	26,50,50	2.24	3 (11%)	18,82,82	2.03	5 (27%)
26	SQD	A	409	-	53,54,54	0.96	3 (5%)	62,65,65	2.05	11 (17%)
23	CLA	B	605	-	59,73,73	2.00	12 (20%)	67,113,113	2.29	21 (31%)
23	CLA	C	510	-	59,73,73	2.09	14 (23%)	67,113,113	2.32	21 (31%)
23	CLA	c	514	-	59,73,73	2.01	13 (22%)	67,113,113	2.23	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	504	-	59,73,73	2.01	13 (22%)	67,113,113	2.09	21 (31%)
33	LMT	B	629	-	25,25,36	0.42	0	30,30,47	1.11	2 (6%)
33	LMT	B	627	-	36,36,36	0.43	0	47,47,47	1.14	4 (8%)
24	PHO	a	416	-	67,69,69	2.14	19 (28%)	85,99,99	2.10	23 (27%)
29	PL9	D	406	-	55,55,55	0.68	2 (3%)	68,69,69	1.67	20 (29%)
32	HTG	b	624	-	19,19,19	1.03	2 (10%)	23,24,24	1.40	4 (17%)
31	LHG	L	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	5 (9%)
23	CLA	C	503	-	59,73,73	1.95	13 (22%)	67,113,113	2.25	23 (34%)
25	BCR	c	517	-	41,41,41	1.07	1 (2%)	56,56,56	1.60	12 (21%)
27	GOL	c	502	-	5,5,5	1.05	0	5,5,5	0.91	0
25	BCR	D	405	-	41,41,41	1.01	1 (2%)	56,56,56	1.78	17 (30%)
23	CLA	B	610	41	59,73,73	2.03	13 (22%)	67,113,113	2.24	23 (34%)
29	PL9	A	413[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
33	LMT	b	626	-	25,25,36	0.56	1 (4%)	30,30,47	1.12	3 (10%)
35	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.01	4 (5%)
23	CLA	B	614	-	59,73,73	1.94	13 (22%)	67,113,113	2.33	25 (37%)
23	CLA	B	616	-	59,73,73	1.96	13 (22%)	67,113,113	2.21	20 (29%)
23	CLA	b	602	-	59,73,73	2.05	13 (22%)	67,113,113	2.35	25 (37%)
28	OEX	A	412[B]	3,1,41	0,15,15	0.00	-	-	-	-
32	HTG	h	101	-	16,16,19	1.16	2 (12%)	20,21,24	2.03	7 (35%)
25	BCR	a	408	-	41,41,41	1.05	1 (2%)	56,56,56	1.48	9 (16%)
23	CLA	c	515	-	59,73,73	2.03	13 (22%)	67,113,113	2.16	23 (34%)
26	SQD	D	413	-	42,43,54	1.15	3 (7%)	51,54,65	1.87	11 (21%)
33	LMT	C	526	-	36,36,36	0.52	1 (2%)	47,47,47	1.12	3 (6%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.74	16 (28%)
37	BCT	D	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
34	LMG	C	522	-	51,51,55	1.04	3 (5%)	59,59,63	1.38	7 (11%)
34	LMG	C	521	-	51,51,55	0.98	2 (3%)	59,59,63	1.02	3 (5%)
35	DGD	c	520	-	63,63,67	0.87	2 (3%)	77,77,81	1.05	7 (9%)
23	CLA	b	607	41	59,73,73	1.96	15 (25%)	67,113,113	2.20	20 (29%)
40	HEC	V	201	16	26,50,50	2.17	4 (15%)	18,82,82	2.28	7 (38%)
23	CLA	B	606	-	59,73,73	1.96	13 (22%)	67,113,113	2.30	23 (34%)
23	CLA	C	513	3	59,73,73	2.06	14 (23%)	67,113,113	2.11	22 (32%)
23	CLA	b	609	-	59,73,73	2.02	13 (22%)	67,113,113	2.20	23 (34%)
23	CLA	c	507	-	59,73,73	2.03	13 (22%)	67,113,113	2.19	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	OEX	a	413[B]	3,1,41	0,15,15	0.00	-	-		
32	HTG	b	622	-	19,19,19	1.02	1 (5%)	23,24,24	1.62	2 (8%)
32	HTG	B	624	-	19,19,19	1.12	2 (10%)	23,24,24	1.41	3 (13%)
23	CLA	c	508	-	59,73,73	2.02	14 (23%)	67,113,113	2.21	23 (34%)
23	CLA	b	615	-	59,73,73	1.97	12 (20%)	67,113,113	2.09	21 (31%)
33	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.97	2 (4%)
27	GOL	O	302	-	5,5,5	0.89	0	5,5,5	0.98	0
23	CLA	C	507	-	59,73,73	1.93	13 (22%)	67,113,113	2.16	21 (31%)
23	CLA	B	603	-	59,73,73	2.05	14 (23%)	67,113,113	2.28	22 (32%)
23	CLA	A	403	-	59,73,73	1.99	13 (22%)	67,113,113	2.23	27 (40%)
26	SQD	f	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.28	6 (11%)
23	CLA	B	609	-	59,73,73	1.93	13 (22%)	67,113,113	2.10	18 (26%)
23	CLA	a	404	41	59,73,73	2.01	13 (22%)	67,113,113	2.26	26 (38%)
23	CLA	C	506	41	59,73,73	2.02	13 (22%)	67,113,113	2.24	28 (41%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.09	3 (6%)
23	CLA	b	614	-	59,73,73	1.98	14 (23%)	67,113,113	2.33	23 (34%)
23	CLA	b	616	-	59,73,73	1.94	13 (22%)	67,113,113	2.49	25 (37%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.47	8 (14%)
23	CLA	B	604	-	59,73,73	2.00	14 (23%)	67,113,113	2.34	21 (31%)
32	HTG	B	622	-	19,19,19	0.85	1 (5%)	23,24,24	1.39	1 (4%)
23	CLA	D	403	-	59,73,73	1.97	13 (22%)	67,113,113	2.26	22 (32%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	10 (17%)
35	DGD	C	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.16	4 (5%)
25	BCR	B	631	-	41,41,41	1.06	1 (2%)	56,56,56	1.44	11 (19%)
23	CLA	d	403	-	59,73,73	2.04	13 (22%)	67,113,113	2.21	22 (32%)
25	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.15	5 (8%)
23	CLA	B	613	-	59,73,73	2.00	14 (23%)	67,113,113	2.17	21 (31%)
23	CLA	d	402	-	59,73,73	1.93	12 (20%)	67,113,113	2.29	27 (40%)
27	GOL	B	626	-	5,5,5	0.87	0	5,5,5	1.13	0
23	CLA	B	612	-	59,73,73	1.98	12 (20%)	67,113,113	2.41	22 (32%)
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.10	5 (9%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.53	10 (17%)
31	LHG	D	407	-	48,48,48	0.89	3 (6%)	51,54,54	0.98	3 (5%)
29	PL9	a	414[A]	-	55,55,55	0.64	1 (1%)	68,69,69	2.01	21 (30%)
23	CLA	C	515	-	59,73,73	1.98	13 (22%)	67,113,113	2.19	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	403	-	59,73,73	2.01	13 (22%)	67,113,113	2.36	27 (40%)
37	BCT	d	401[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	c	505	-	59,73,73	1.91	13 (22%)	67,113,113	2.19	22 (32%)
31	LHG	d	407	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	4 (7%)
31	LHG	b	628	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
32	HTG	B	621	-	19,19,19	0.98	1 (5%)	23,24,24	1.60	4 (17%)
23	CLA	B	615	-	59,73,73	1.97	12 (20%)	67,113,113	2.31	23 (34%)
29	PL9	d	405	-	55,55,55	0.70	2 (3%)	68,69,69	1.63	18 (26%)
38	HEM	e	102	5,6	27,50,50	0.92	1 (3%)	17,82,82	2.08	3 (17%)
35	DGD	H	102	-	63,63,67	0.84	3 (4%)	77,77,81	1.07	7 (9%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.02	4 (5%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.34	8 (14%)
32	HTG	V	202	-	11,11,19	0.19	0	15,15,24	1.21	1 (6%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.85	15 (26%)
32	HTG	C	523	-	19,19,19	0.92	1 (5%)	23,24,24	1.47	2 (8%)
31	LHG	A	416	-	48,48,48	0.88	2 (4%)	51,54,54	1.22	5 (9%)
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.96	2 (4%)

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	B	601	41	3/3/20/25	11/37/135/135	-
31	LHG	D	408	-	-	11/53/53/53	-
24	PHO	a	406	-	-	8/53/103/103	0/5/6/6
29	PL9	A	413[B]	-	-	15/53/73/73	0/1/1/1
23	CLA	a	407	-	3/3/20/25	11/37/135/135	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	B	607	41	3/3/20/25	3/37/135/135	-
26	SQD	B	620	-	-	19/49/69/69	0/1/1/1
34	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
35	DGD	c	518	-	-	18/51/91/95	0/2/2/2
25	BCR	C	517	-	-	3/29/63/63	0/2/2/2
27	GOL	A	410	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	C	514	-	3/3/20/25	16/37/135/135	-
34	LMG	d	411	39	-	9/46/66/70	0/1/1/1
23	CLA	b	606	-	3/3/20/25	11/37/135/135	-
25	BCR	k	102	-	-	5/29/63/63	0/2/2/2
26	SQD	A	411	-	-	14/49/69/69	0/1/1/1
33	LMT	b	620	-	-	6/17/37/61	0/1/1/2
32	HTG	b	621	-	-	5/10/30/30	0/1/1/1
23	CLA	b	603	-	2/2/20/25	5/37/135/135	-
27	GOL	v	201	-	-	2/4/4/4	-
24	PHO	A	406	-	-	2/53/103/103	0/5/6/6
33	LMT	B	630	-	-	8/17/38/61	0/1/1/2
34	LMG	D	412	39	-	9/46/66/70	0/1/1/1
23	CLA	C	509	41	3/3/20/25	5/37/135/135	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
27	GOL	a	410	-	-	4/4/4/4	-
32	HTG	c	523	-	-	4/10/30/30	0/1/1/1
34	LMG	C	502	-	-	24/46/66/70	0/1/1/1
23	CLA	C	512	-	3/3/20/25	10/37/135/135	-
23	CLA	b	608	-	3/3/20/25	5/37/135/135	-
23	CLA	B	611	-	3/3/20/25	2/37/135/135	-
23	CLA	b	613	-	3/3/20/25	2/37/135/135	-
31	LHG	E	101	-	-	17/46/46/53	-
23	CLA	c	503	-	3/3/20/25	6/37/135/135	-
27	GOL	C	524	-	-	0/4/4/4	-
23	CLA	b	610	41	3/3/20/25	8/37/135/135	-
31	LHG	d	406	-	-	20/53/53/53	-
23	CLA	c	512	-	3/3/20/25	9/37/135/135	-
33	LMT	M	103	-	-	9/21/61/61	0/2/2/2
33	LMT	M	102	-	-	7/21/61/61	0/2/2/2
26	SQD	a	411	-	-	17/49/69/69	0/1/1/1
23	CLA	C	511	-	3/3/20/25	3/37/135/135	-
23	CLA	C	505	-	3/3/20/25	5/37/135/135	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	b	623	-	-	2/4/4/4	-
27	GOL	B	628	-	-	0/4/4/4	-
23	CLA	B	602	-	3/3/20/25	10/37/135/135	-
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
33	LMT	D	402	-	-	10/21/61/61	0/2/2/2
23	CLA	c	513	3	3/3/20/25	6/37/135/135	-
23	CLA	a	405	41	2/2/20/25	8/37/135/135	-
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
23	CLA	b	612	-	3/3/20/25	6/37/135/135	-
34	LMG	m	101	-	-	11/46/66/70	0/1/1/1
33	LMT	a	412	-	-	7/21/61/61	0/2/2/2
27	GOL	b	627	-	-	0/4/4/4	-
27	GOL	c	527	-	-	0/4/4/4	-
34	LMG	M	101	-	-	18/46/66/70	0/1/1/1
29	PL9	a	414[B]	-	-	16/53/73/73	0/1/1/1
23	CLA	B	608	-	2/2/20/25	2/37/135/135	-
23	CLA	C	508	-	3/3/20/25	12/37/135/135	-
23	CLA	C	504	-	2/2/20/25	8/37/135/135	-
26	SQD	a	409	-	-	12/49/69/69	0/1/1/1
25	BCR	b	617	-	-	4/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	A	407	-	3/3/20/25	8/37/135/135	-
23	CLA	c	509	41	3/3/20/25	8/37/135/135	-
23	CLA	A	404	41	3/3/20/25	6/37/135/135	-
23	CLA	c	511	-	3/3/20/25	12/37/135/135	-
23	CLA	D	404	-	3/3/20/25	9/37/135/135	-
32	HTG	D	411	-	-	2/7/27/30	0/1/1/1
34	LMG	c	522	-	-	9/46/66/70	0/1/1/1
35	DGD	h	103	-	-	11/51/91/95	0/2/2/2
33	LMT	e	101	-	-	9/21/61/61	0/2/2/2
27	GOL	B	623	-	-	2/4/4/4	-
23	CLA	b	601	41	3/3/20/25	15/37/135/135	-
23	CLA	c	506	41	3/3/20/25	4/37/135/135	-
23	CLA	b	611	-	3/3/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
24	PHO	A	415	-	-	3/53/103/103	0/5/6/6
23	CLA	b	605	-	3/3/20/25	5/37/135/135	-
23	CLA	b	604	-	3/3/20/25	13/37/135/135	-
33	LMT	m	103	-	-	6/21/61/61	0/2/2/2
38	HEM	E	102	5,6	-	0/6/54/54	-
23	CLA	A	405	41	2/2/20/25	5/37/135/135	-
34	LMG	a	417	-	-	12/46/66/70	0/1/1/1
35	DGD	C	518	-	-	16/51/91/95	0/2/2/2
33	LMT	F	101	-	-	5/21/61/61	0/2/2/2
23	CLA	c	510	-	3/3/20/25	10/37/135/135	-
26	SQD	L	102	-	-	19/49/69/69	0/1/1/1
40	HEC	v	202	16	-	0/6/54/54	-
26	SQD	A	409	-	-	15/49/69/69	0/1/1/1
23	CLA	B	605	-	2/2/20/25	8/37/135/135	-
23	CLA	C	510	-	3/3/20/25	7/37/135/135	-
23	CLA	c	514	-	3/3/20/25	9/37/135/135	-
23	CLA	c	504	-	3/3/20/25	3/37/135/135	-
33	LMT	B	629	-	-	4/17/37/61	0/1/1/2
33	LMT	B	627	-	-	9/21/61/61	0/2/2/2
24	PHO	a	416	-	-	5/53/103/103	0/5/6/6
29	PL9	D	406	-	-	7/53/73/73	0/1/1/1
32	HTG	b	624	-	-	2/10/30/30	0/1/1/1
31	LHG	L	101	-	-	16/53/53/53	-
23	CLA	C	503	-	3/3/20/25	5/37/135/135	-
25	BCR	c	517	-	-	2/29/63/63	0/2/2/2
27	GOL	c	502	-	-	0/4/4/4	-
25	BCR	D	405	-	-	8/29/63/63	0/2/2/2
23	CLA	B	610	41	3/3/20/25	8/37/135/135	-
29	PL9	A	413[A]	-	-	17/53/73/73	0/1/1/1
33	LMT	b	626	-	-	9/17/37/61	0/1/1/2
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
23	CLA	B	614	-	3/3/20/25	11/37/135/135	-
23	CLA	B	616	-	3/3/20/25	7/37/135/135	-
23	CLA	b	602	-	2/2/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	h	101	-	-	3/7/27/30	0/1/1/1
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
23	CLA	c	515	-	3/3/20/25	9/37/135/135	-
26	SQD	D	413	-	-	12/38/58/69	0/1/1/1
33	LMT	C	526	-	-	8/21/61/61	0/2/2/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
34	LMG	C	522	-	-	11/46/66/70	0/1/1/1
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	b	607	41	3/3/20/25	1/37/135/135	-
40	HEC	V	201	16	-	0/6/54/54	-
23	CLA	B	606	-	3/3/20/25	12/37/135/135	-
23	CLA	C	513	3	3/3/20/25	5/37/135/135	-
23	CLA	b	609	-	3/3/20/25	8/37/135/135	-
23	CLA	c	507	-	1/1/20/25	5/37/135/135	-
32	HTG	b	622	-	-	2/10/30/30	0/1/1/1
32	HTG	B	624	-	-	5/10/30/30	0/1/1/1
23	CLA	c	508	-	3/3/20/25	10/37/135/135	-
23	CLA	b	615	-	3/3/20/25	11/37/135/135	-
33	LMT	a	418	-	-	4/21/61/61	0/2/2/2
27	GOL	O	302	-	-	4/4/4/4	-
23	CLA	C	507	-	1/1/20/25	6/37/135/135	-
23	CLA	B	603	-	2/2/20/25	6/37/135/135	-
23	CLA	A	403	-	3/3/20/25	3/37/135/135	-
26	SQD	f	101	-	-	14/38/58/69	0/1/1/1
23	CLA	B	609	-	2/2/20/25	6/37/135/135	-
23	CLA	a	404	41	3/3/20/25	11/37/135/135	-
23	CLA	C	506	41	3/3/20/25	6/37/135/135	-
34	LMG	z	101	-	-	7/34/54/70	0/1/1/1
23	CLA	b	614	-	3/3/20/25	13/37/135/135	-
23	CLA	b	616	-	3/3/20/25	10/37/135/135	-
25	BCR	c	516	-	-	2/29/63/63	0/2/2/2
23	CLA	B	604	-	3/3/20/25	8/37/135/135	-
23	CLA	D	403	-	1/1/20/25	4/37/135/135	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	C	519	-	-	17/51/91/95	0/2/2/2
25	BCR	B	631	-	-	4/29/63/63	0/2/2/2
23	CLA	d	403	-	3/3/20/25	8/37/135/135	-
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
23	CLA	B	613	-	3/3/20/25	9/37/135/135	-
23	CLA	d	402	-	1/1/20/25	3/37/135/135	-
27	GOL	B	626	-	-	3/4/4/4	-
23	CLA	B	612	-	3/3/20/25	7/37/135/135	-
31	LHG	d	408	-	-	9/53/53/53	-
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
31	LHG	D	407	-	-	15/53/53/53	-
29	PL9	a	414[A]	-	-	18/53/73/73	0/1/1/1
23	CLA	C	515	-	3/3/20/25	7/37/135/135	-
23	CLA	a	403	-	3/3/20/25	6/37/135/135	-
23	CLA	c	505	-	3/3/20/25	3/37/135/135	-
31	LHG	d	407	-	-	23/53/53/53	-
31	LHG	b	628	-	-	13/53/53/53	-
32	HTG	B	621	-	-	5/10/30/30	0/1/1/1
23	CLA	B	615	-	3/3/20/25	8/37/135/135	-
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
38	HEM	e	102	5,6	-	0/6/54/54	-
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
35	DGD	C	520	-	-	7/51/91/95	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
32	HTG	V	202	-	-	1/2/19/30	0/1/1/1
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
32	HTG	C	523	-	-	2/10/30/30	0/1/1/1
31	LHG	A	416	-	-	16/53/53/53	-
31	LHG	a	419	-	-	19/46/46/53	-

The worst 5 of 1146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C3B-C2B	7.24	1.50	1.40
23	c	506	CLA	C3B-C2B	7.17	1.50	1.40
23	a	403	CLA	C3B-C2B	6.92	1.50	1.40
23	A	403	CLA	C3B-C2B	6.89	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C3B-C2B	6.89	1.49	1.40

The worst 5 of 2318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	C4A-NA-C1A	-8.14	103.05	106.71
23	b	616	CLA	C4A-NA-C1A	-7.71	103.24	106.71
23	B	615	CLA	CHD-C4C-C3C	-7.46	113.88	124.84
23	B	602	CLA	C4A-NA-C1A	-7.41	103.38	106.71
24	A	415	PHO	CMD-C2D-C1D	7.41	136.47	125.06

5 of 193 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	NA
23	A	403	CLA	NC
23	A	403	CLA	ND
23	A	404	CLA	NA
23	A	404	CLA	NC

5 of 1338 torsion outliers are listed below:

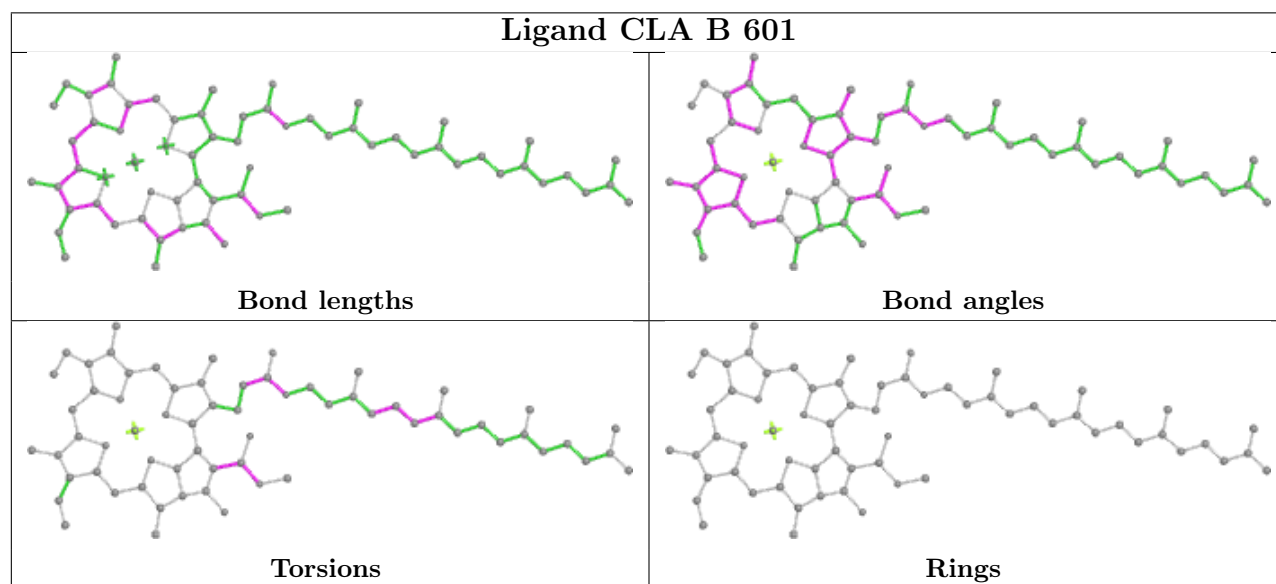
Mol	Chain	Res	Type	Atoms
23	A	407	CLA	C2-C3-C5-C6
23	A	407	CLA	C4-C3-C5-C6
23	B	605	CLA	C6-C7-C8-C9
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D

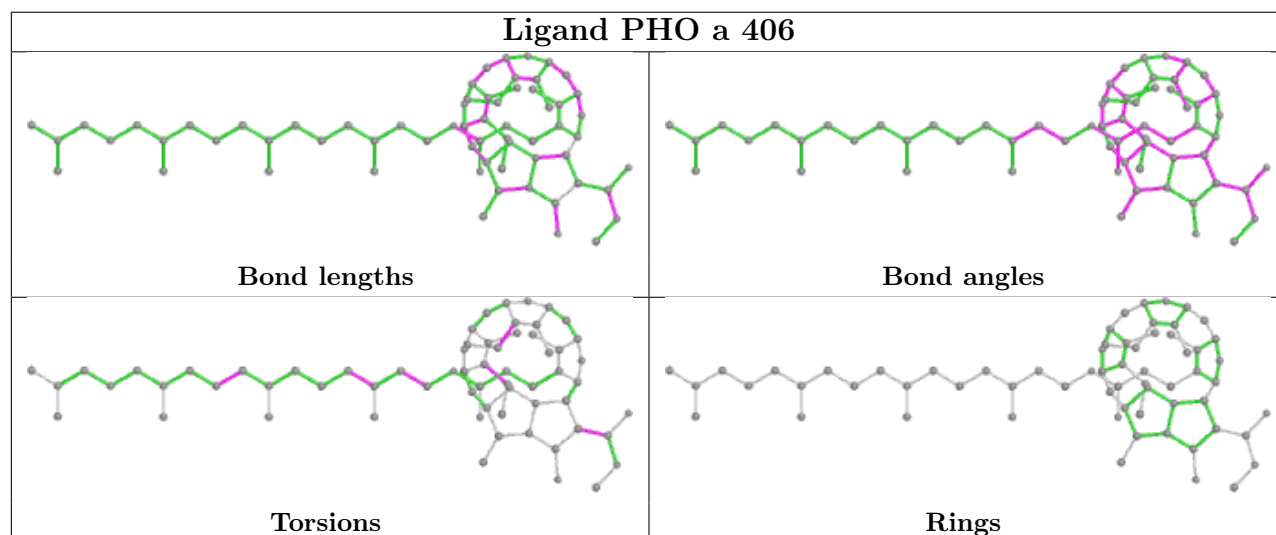
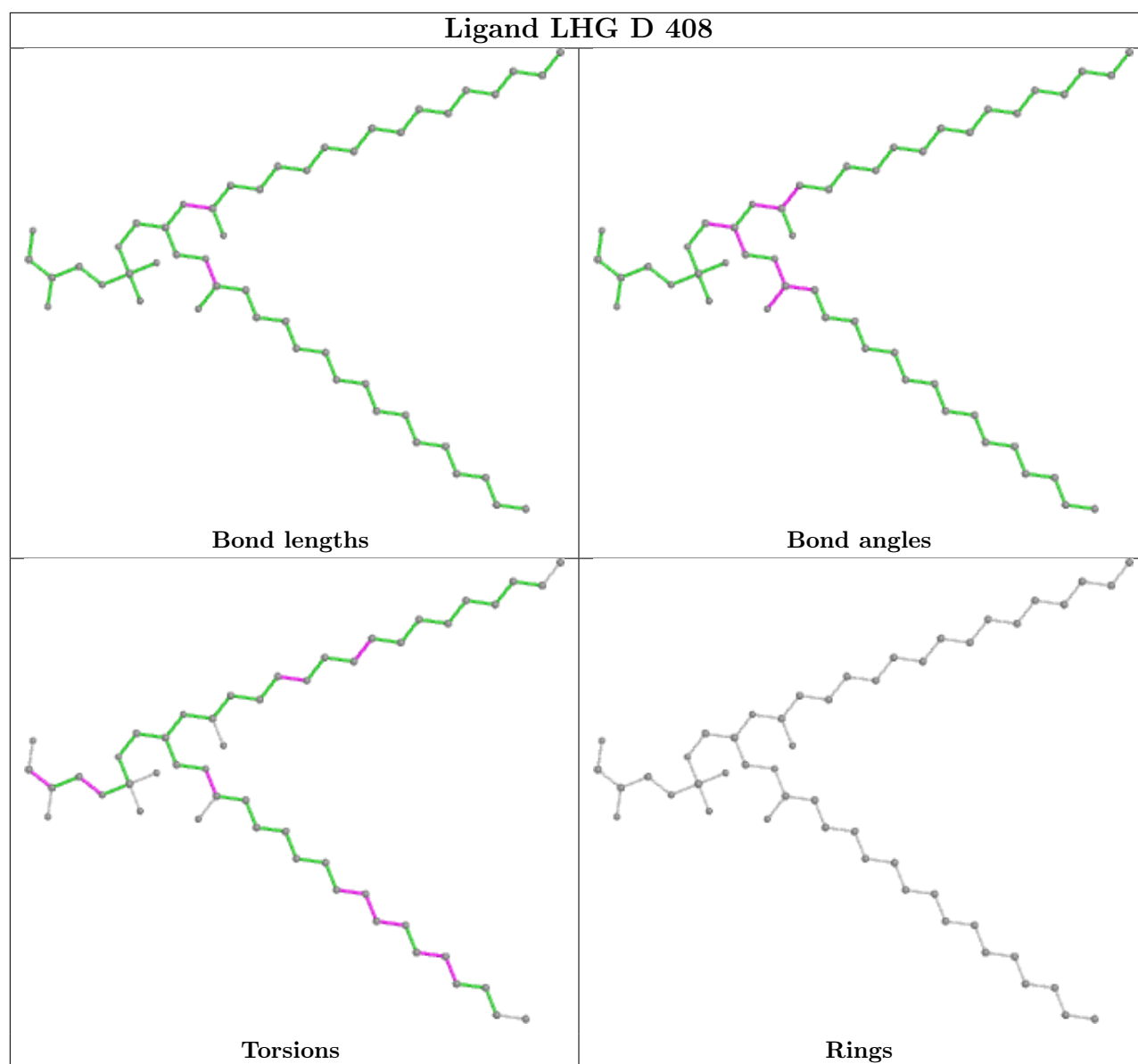
There are no ring outliers.

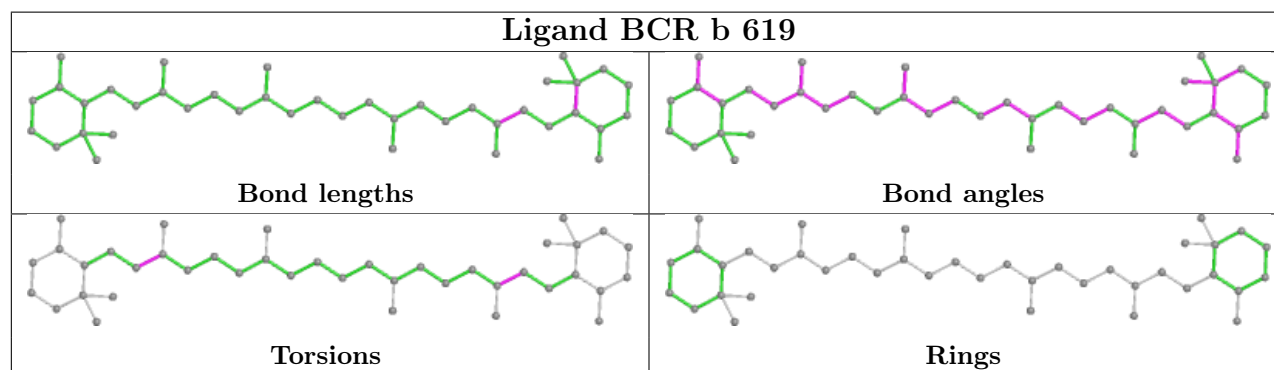
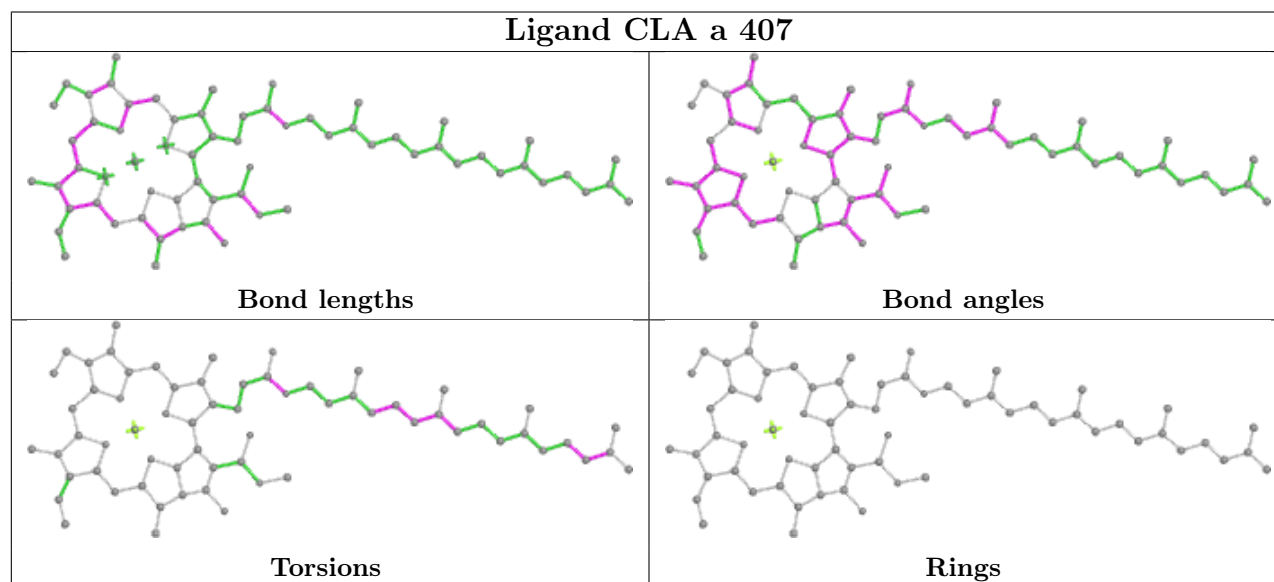
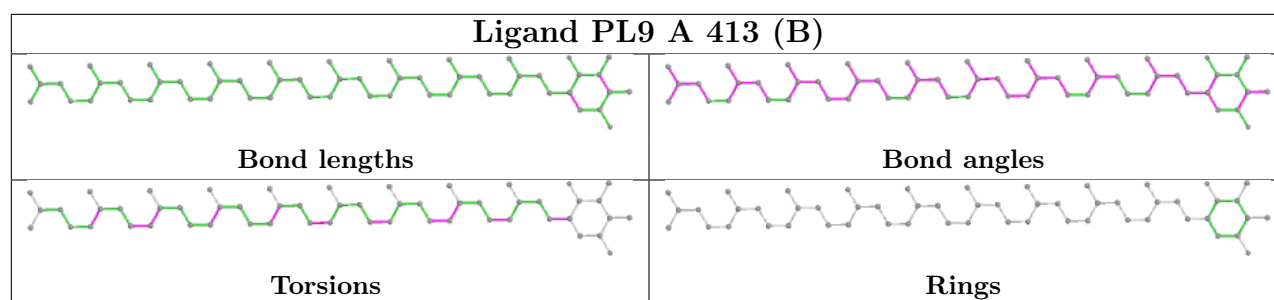
No monomer is involved in short contacts.

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.

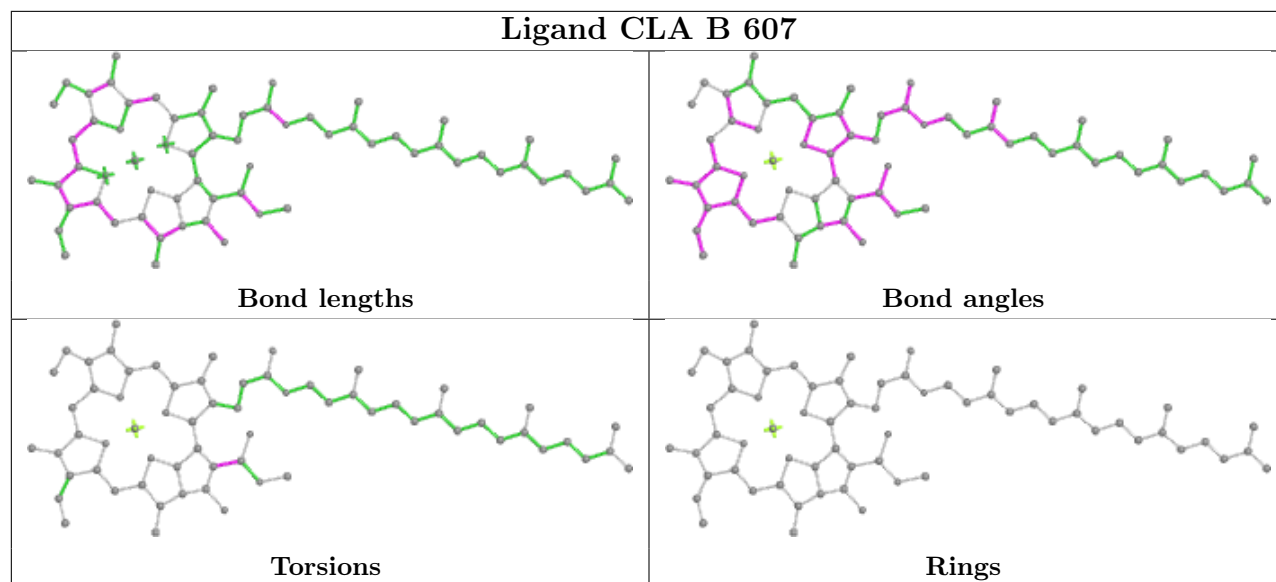
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



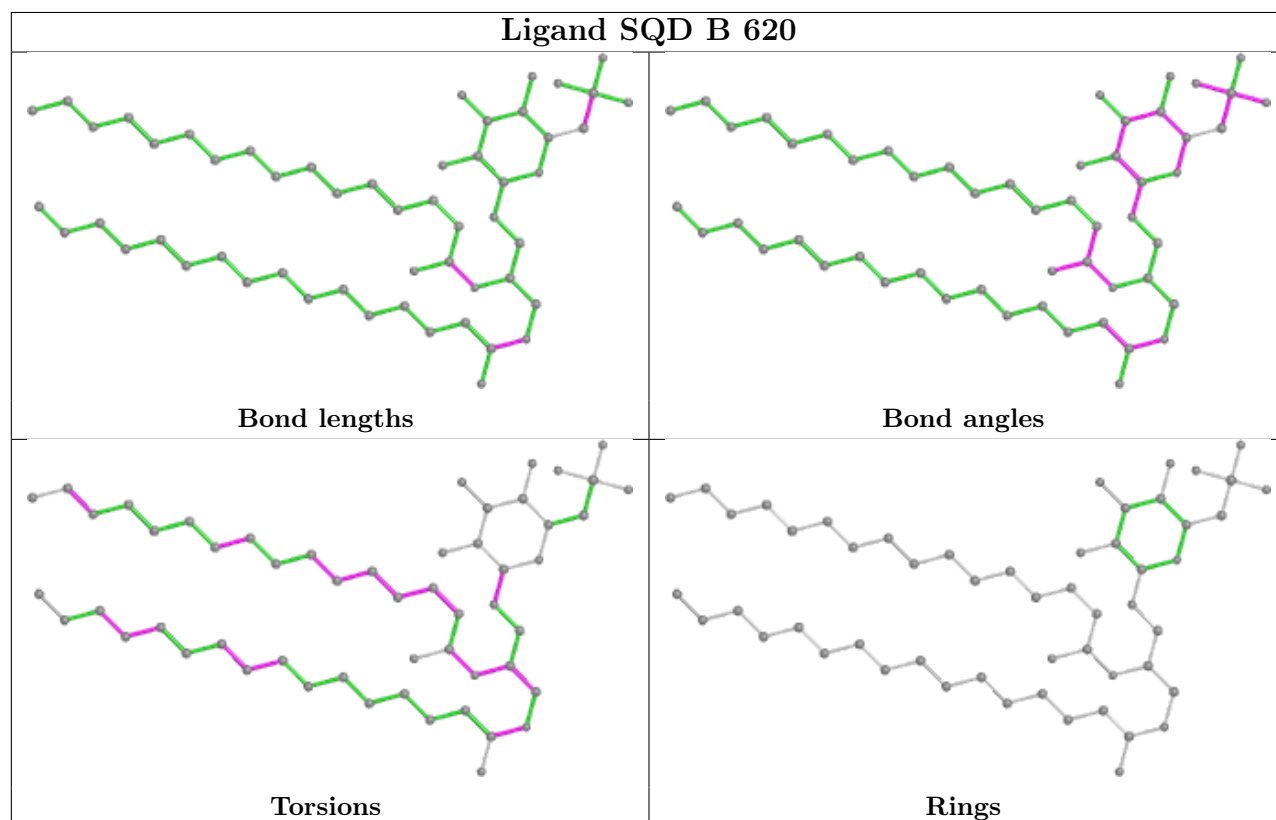


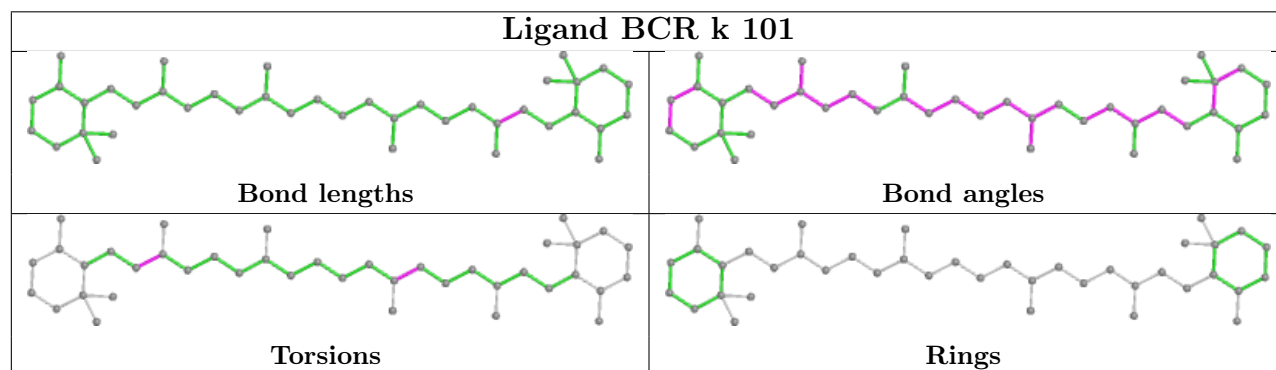
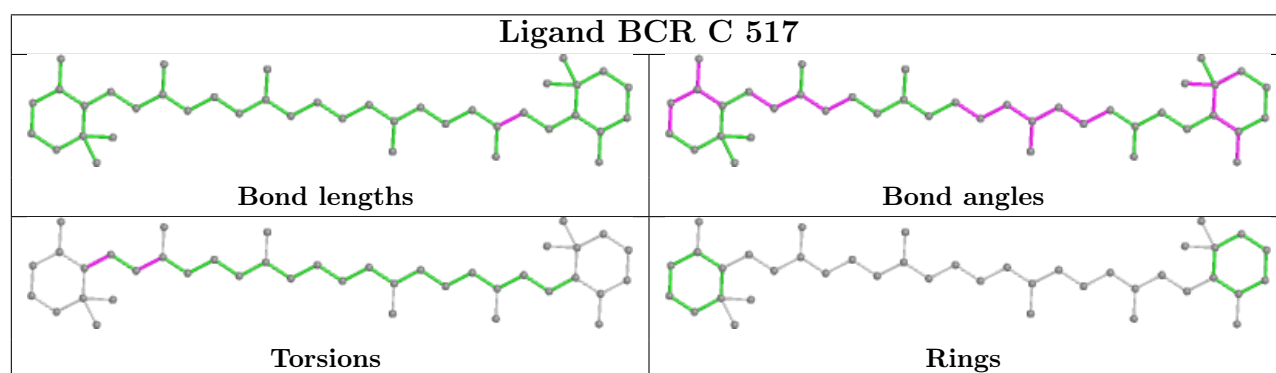
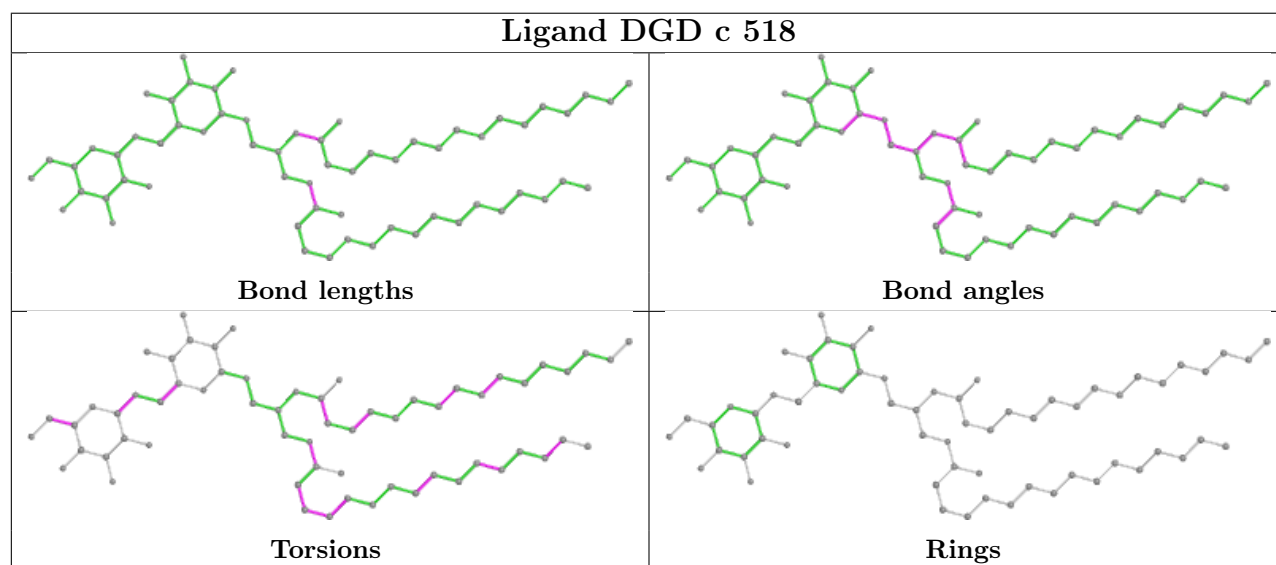
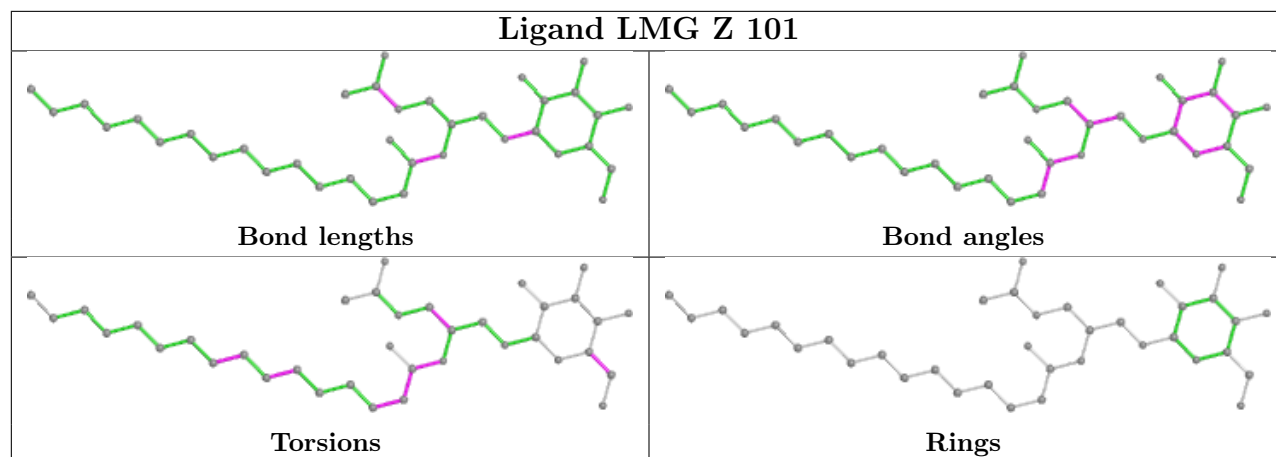


Ligand CLA B 607

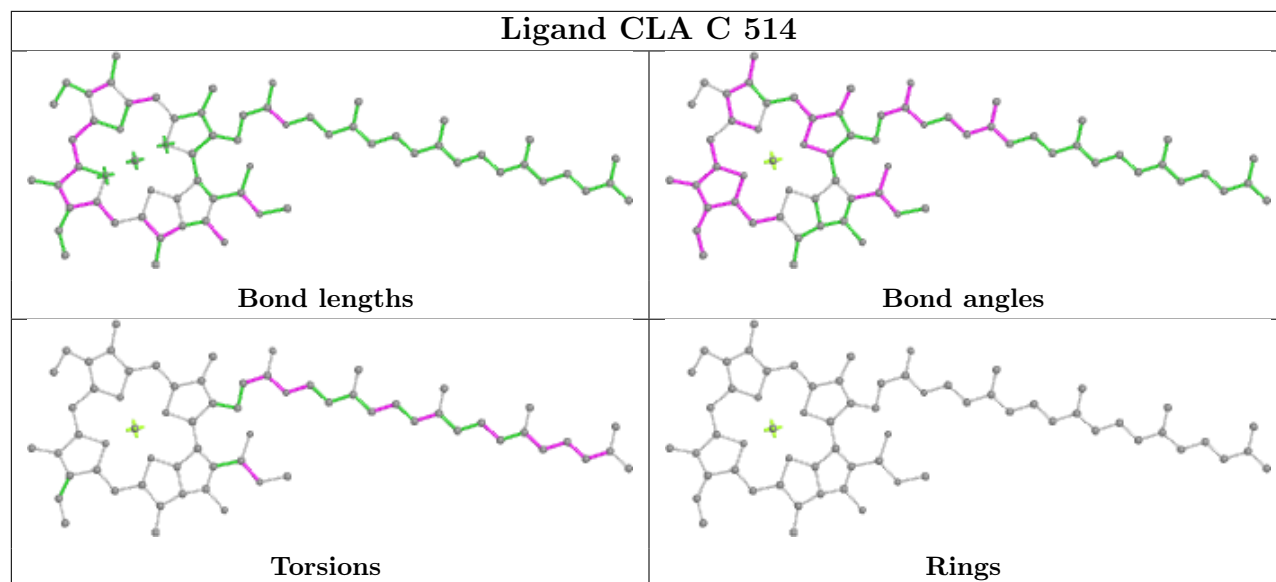


Ligand SQD B 620

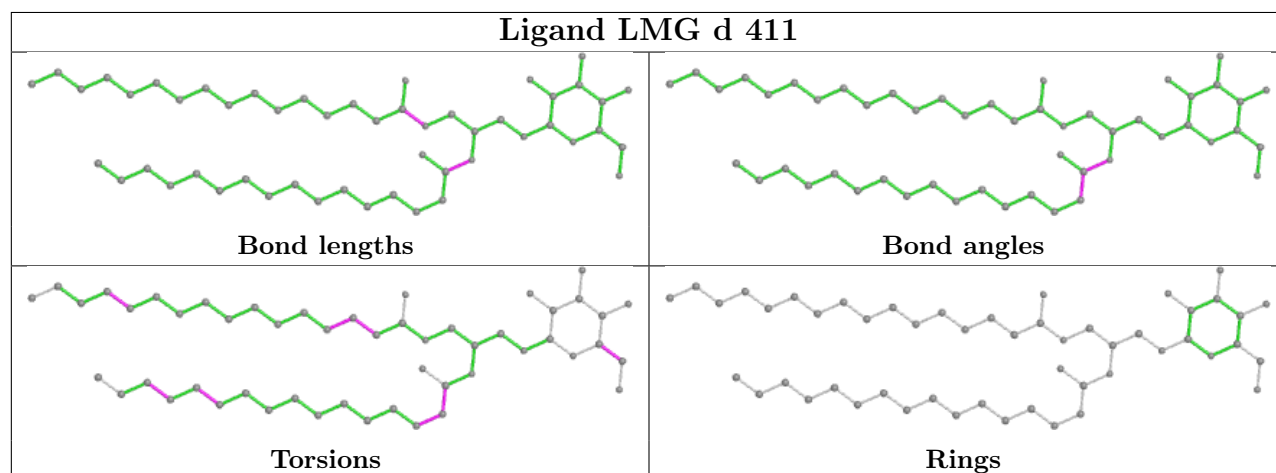




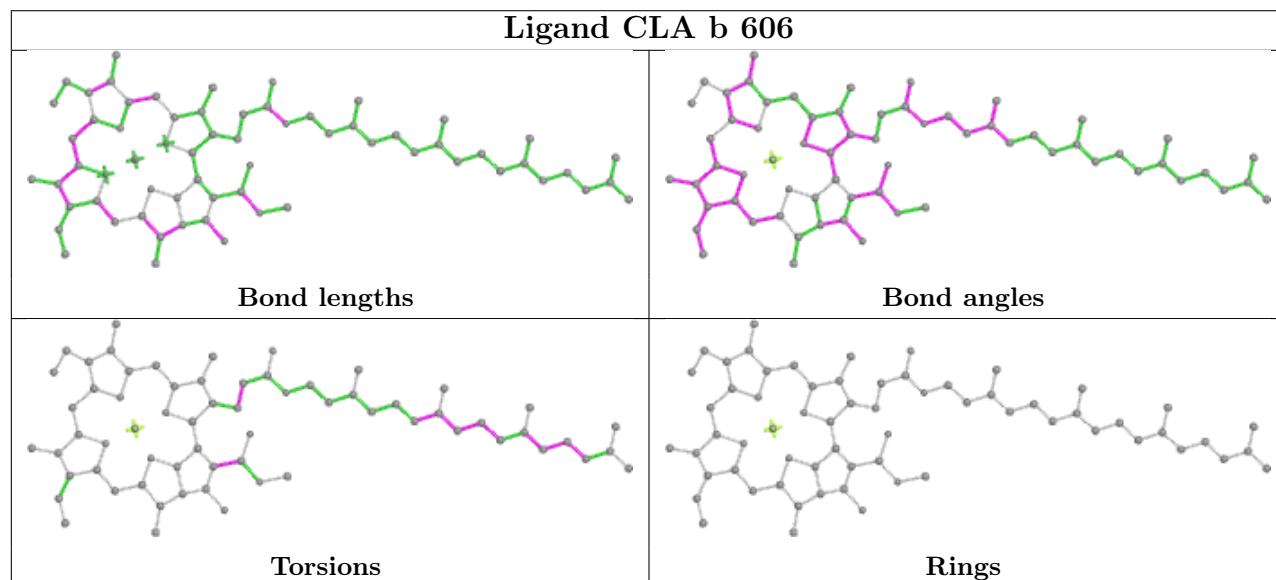
Ligand CLA C 514

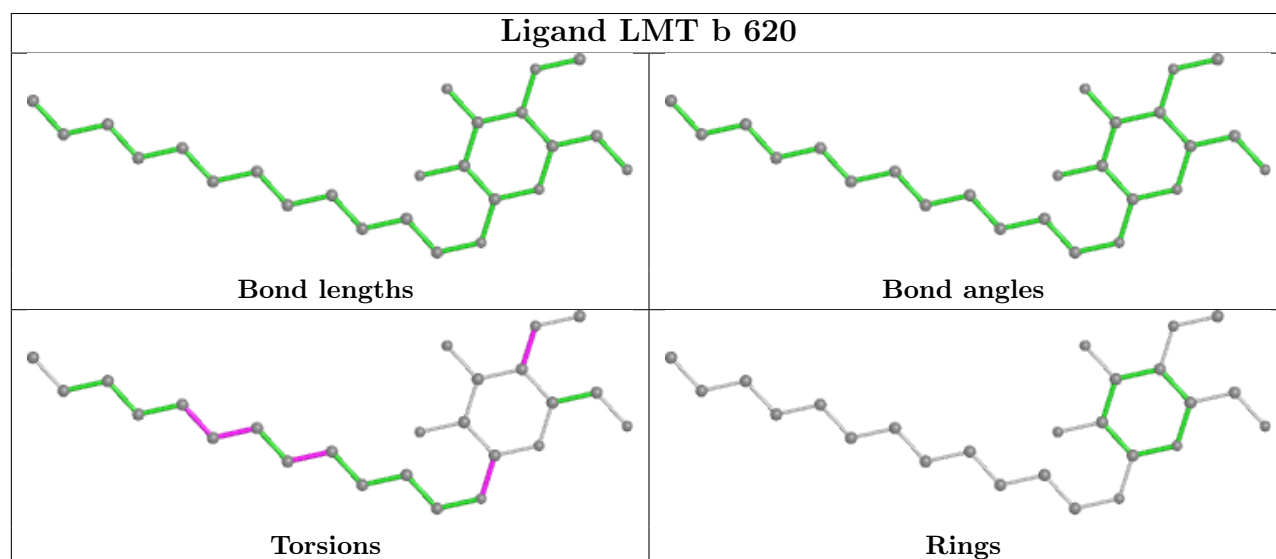
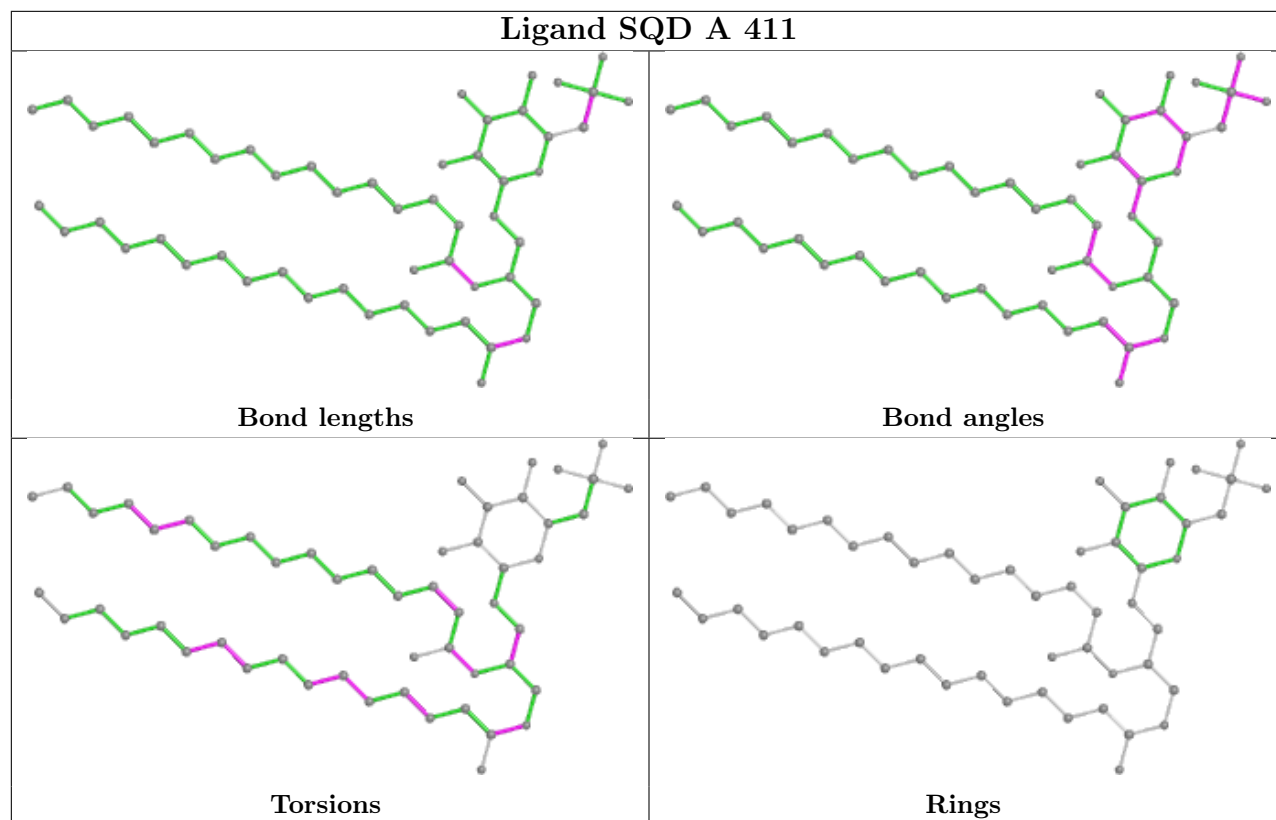
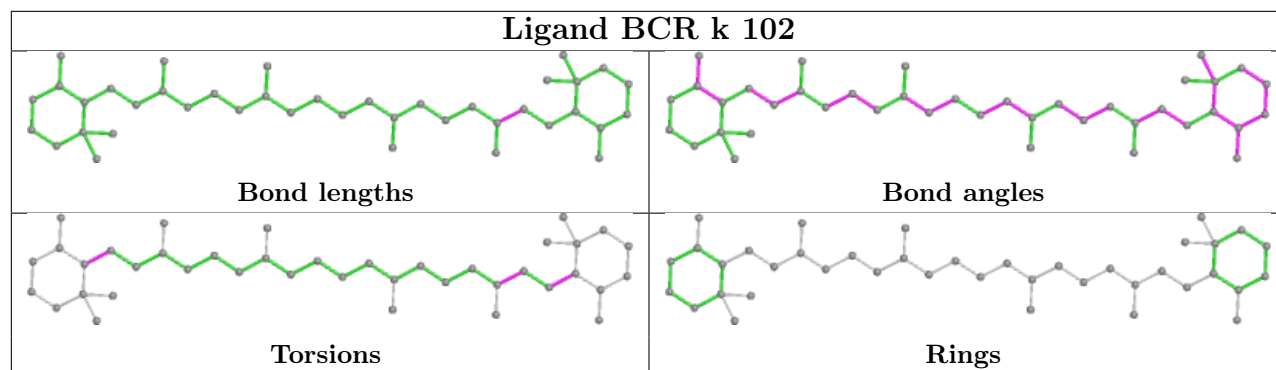


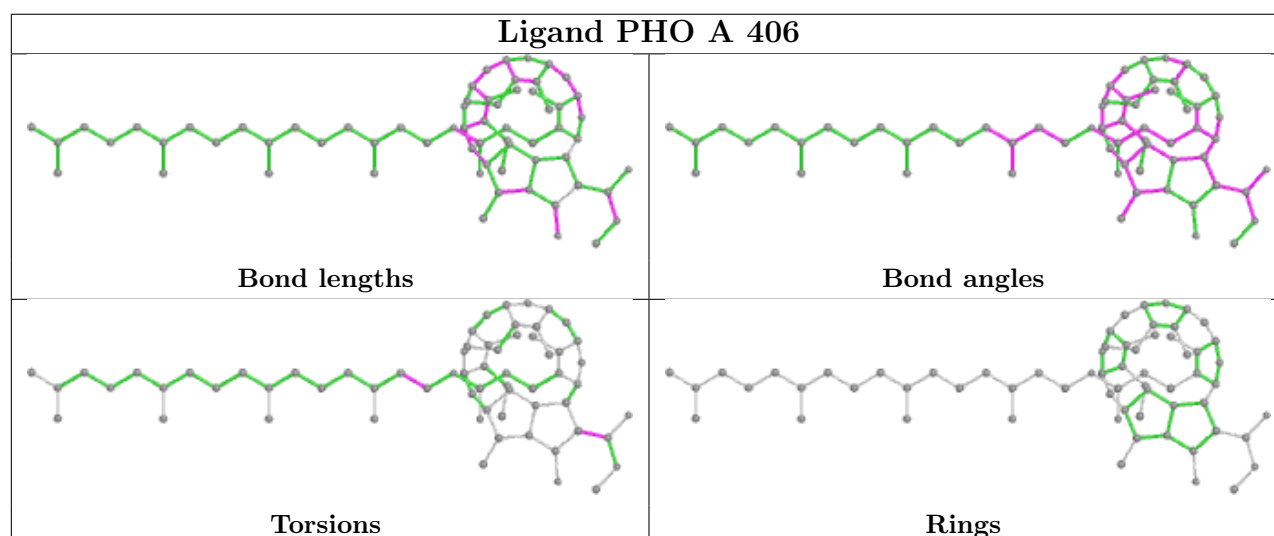
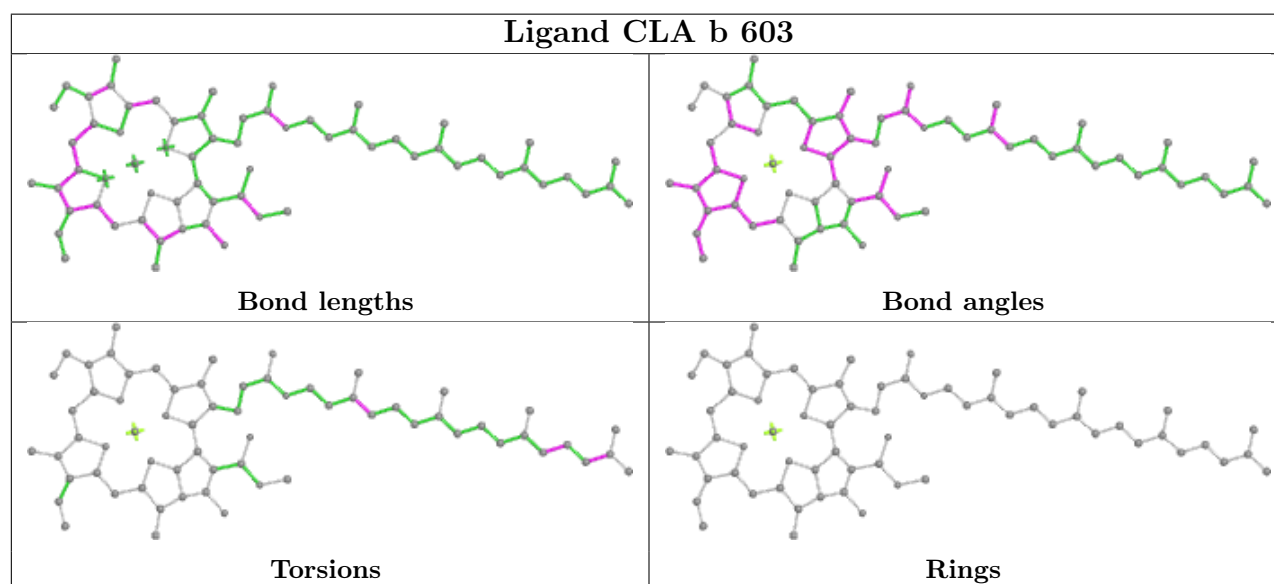
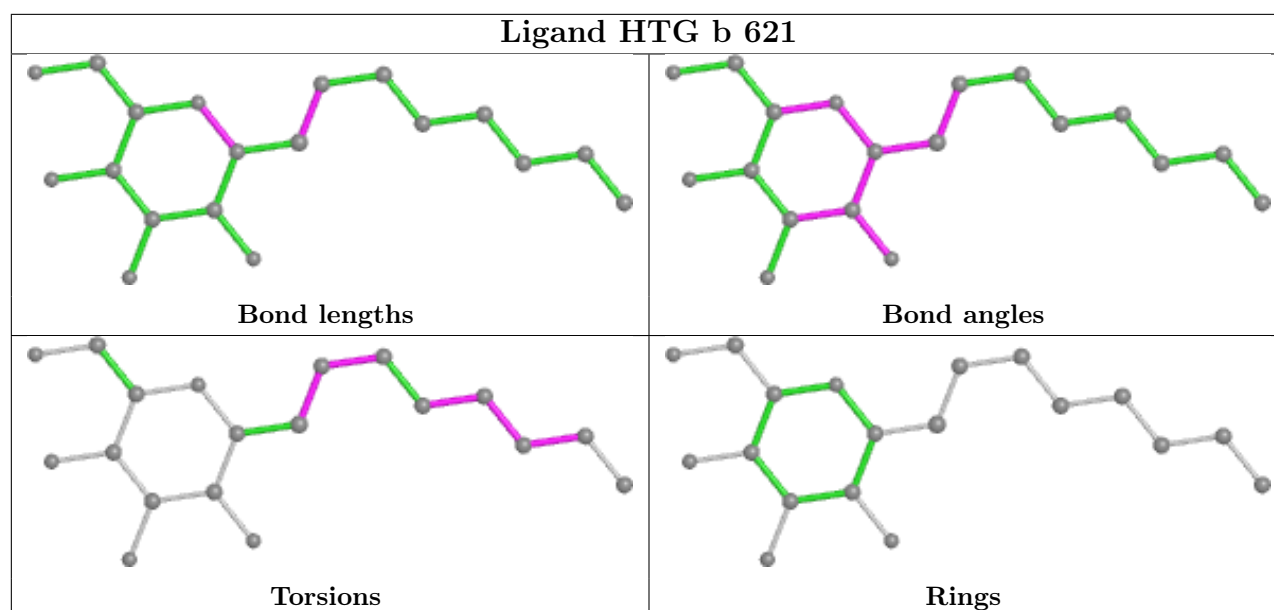
Ligand LMG d 411

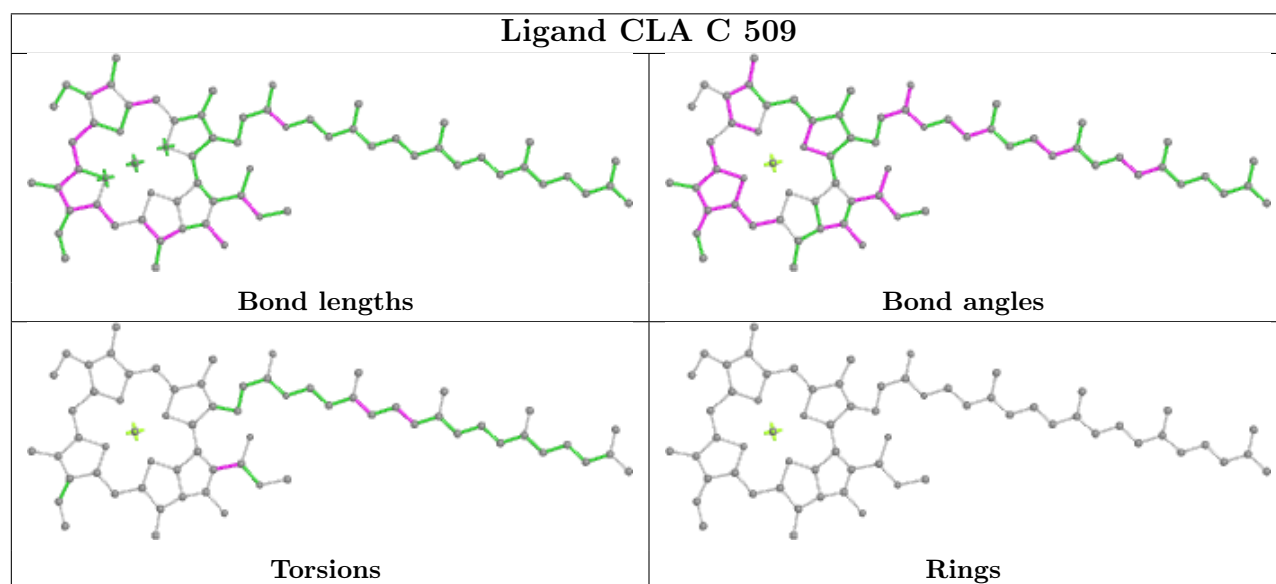
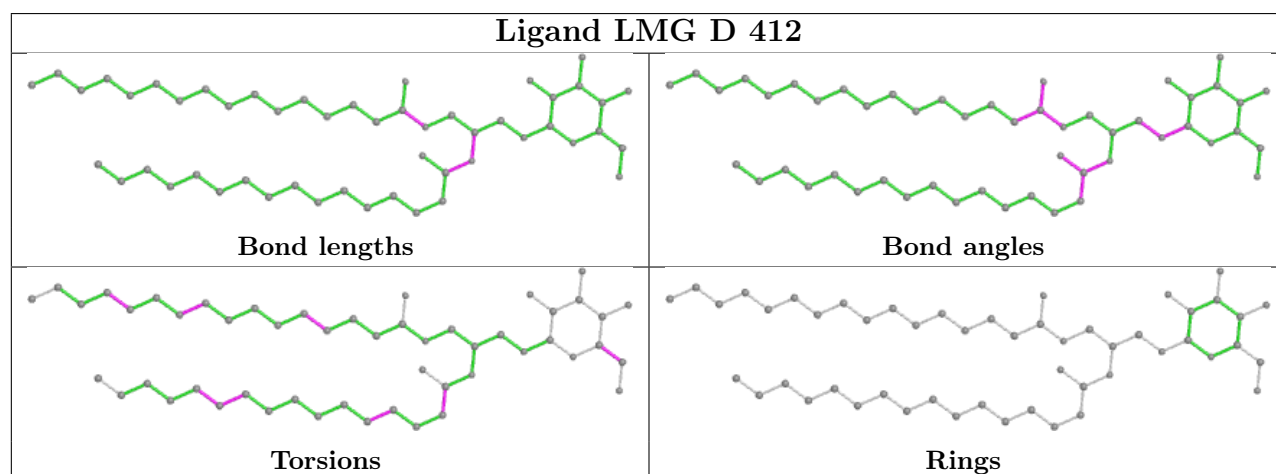
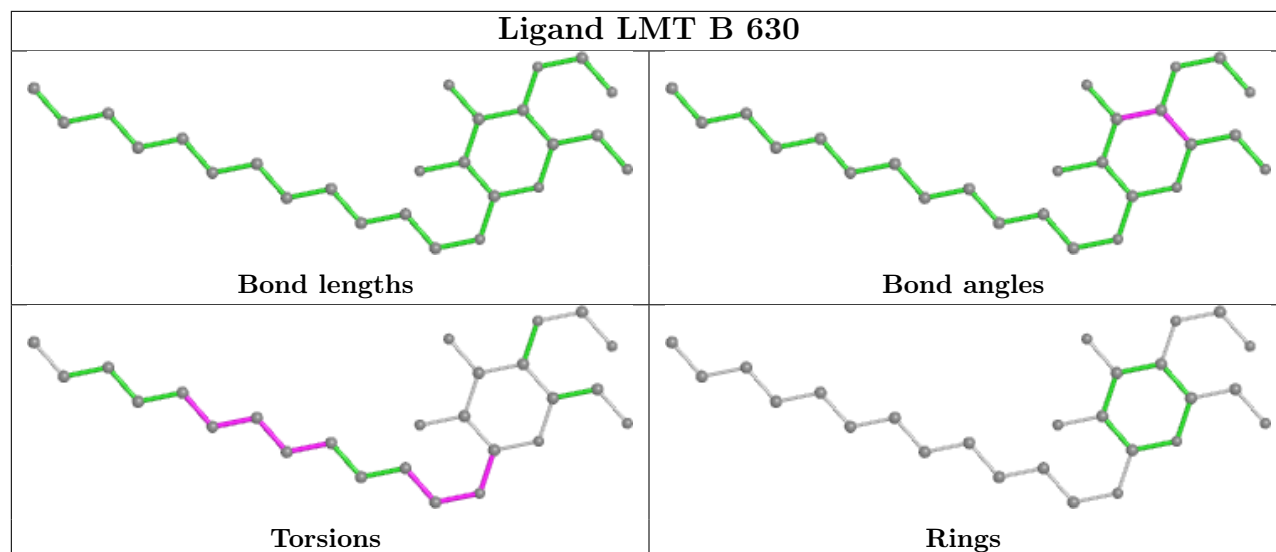


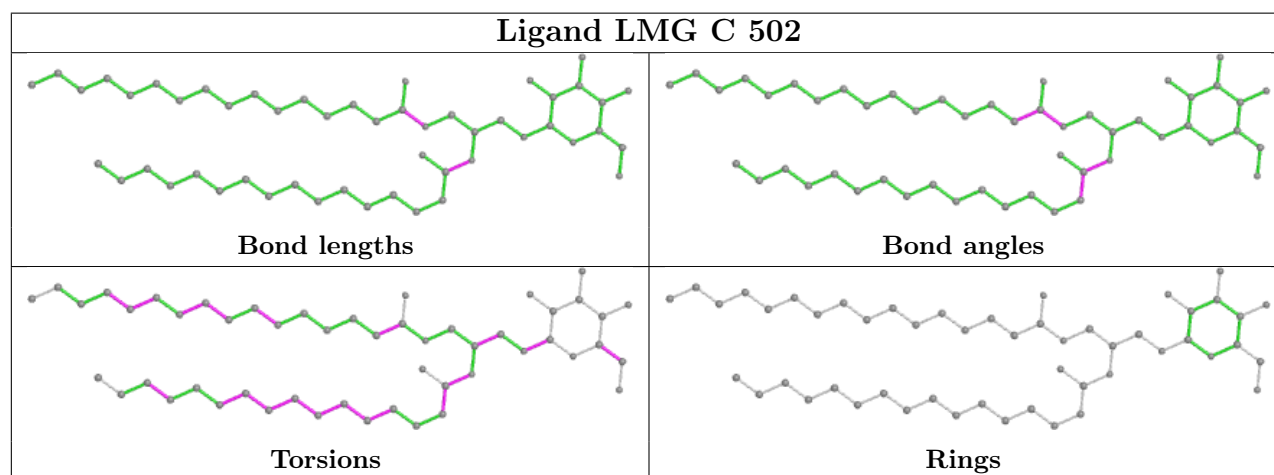
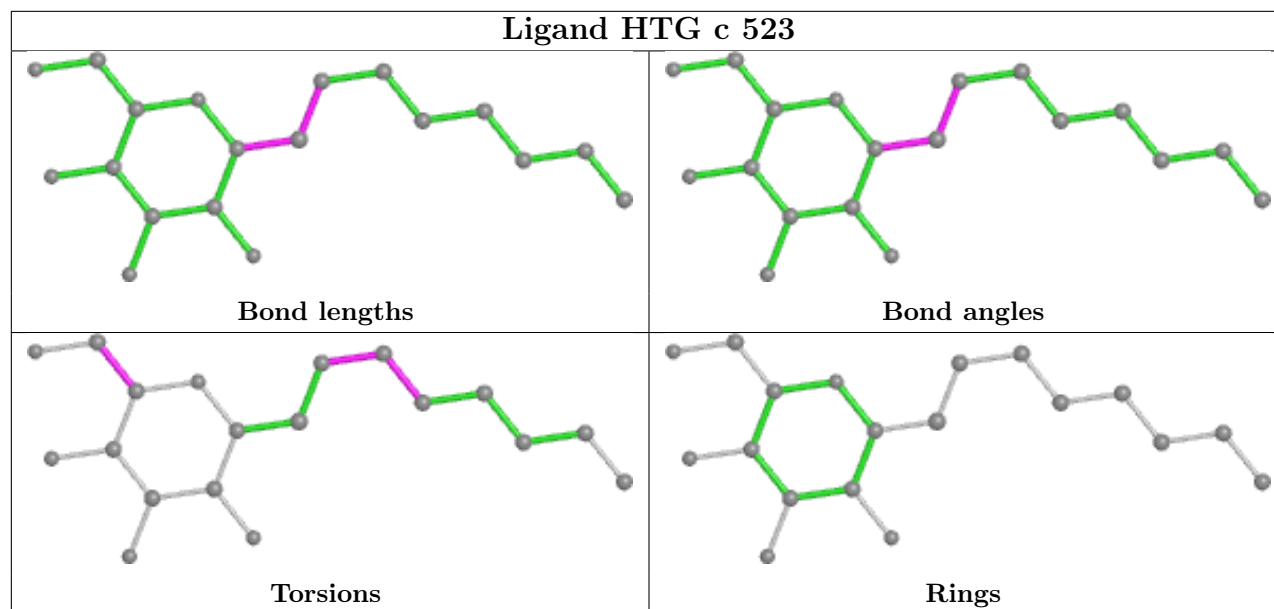
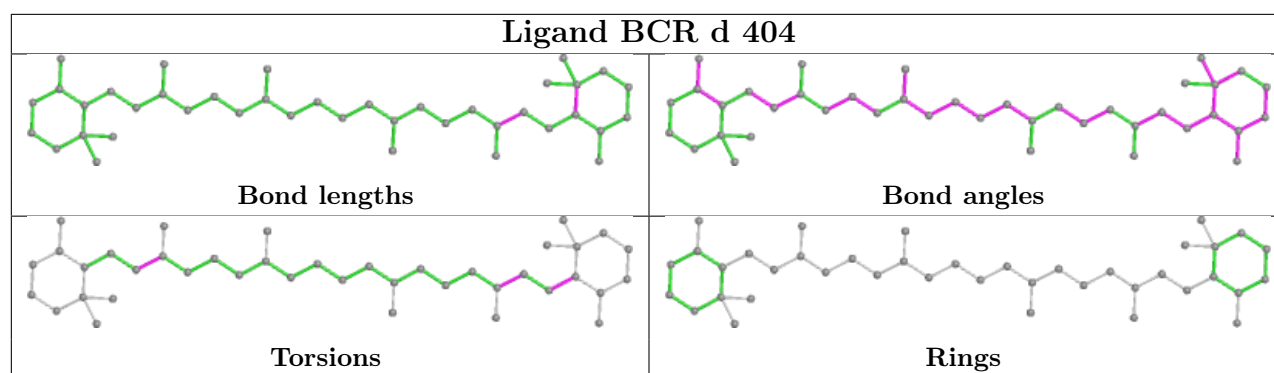
Ligand CLA b 606

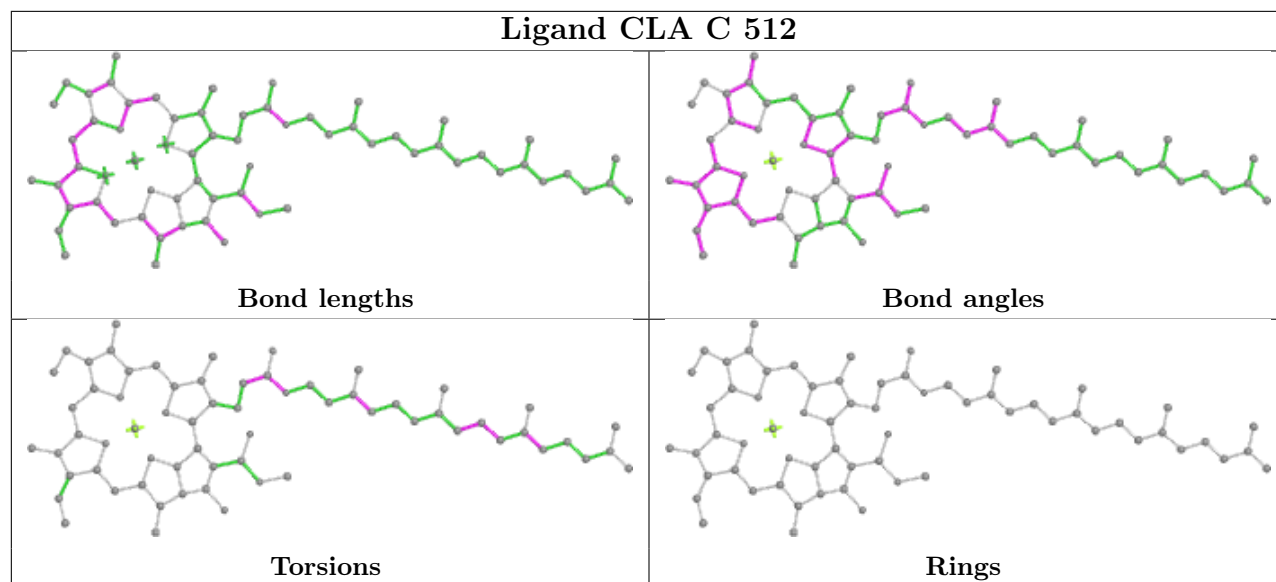
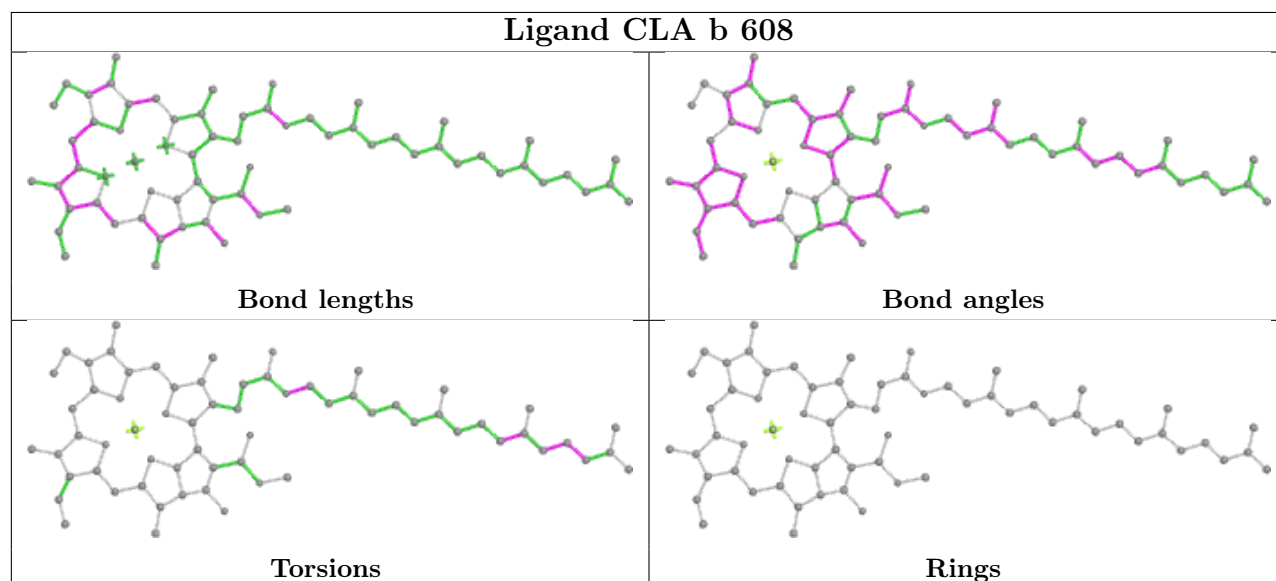
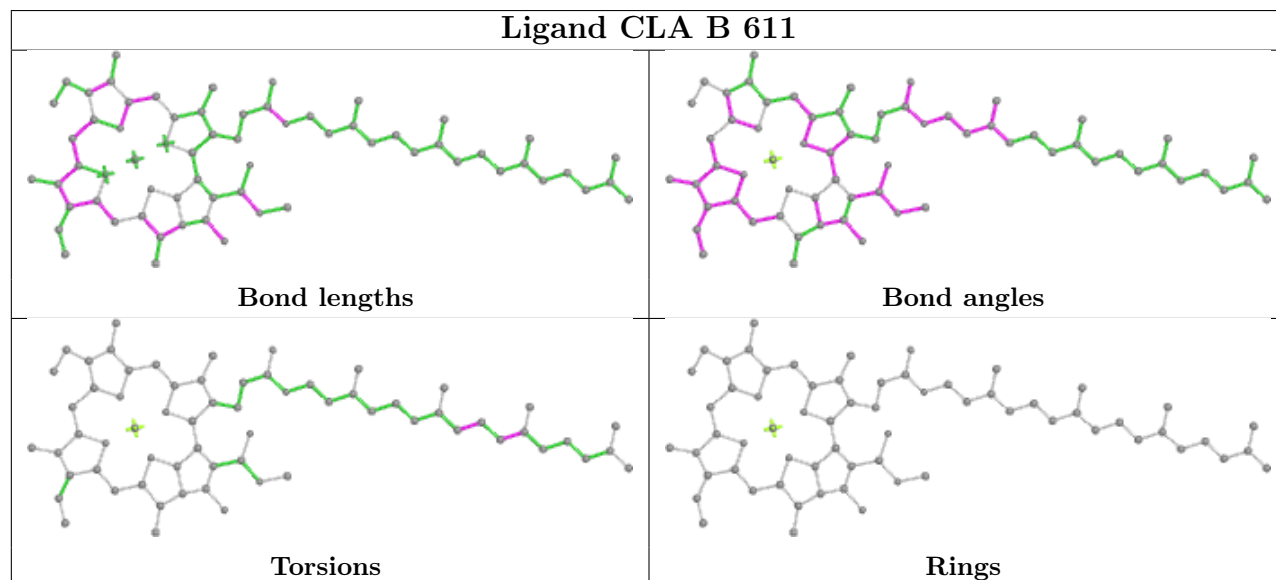


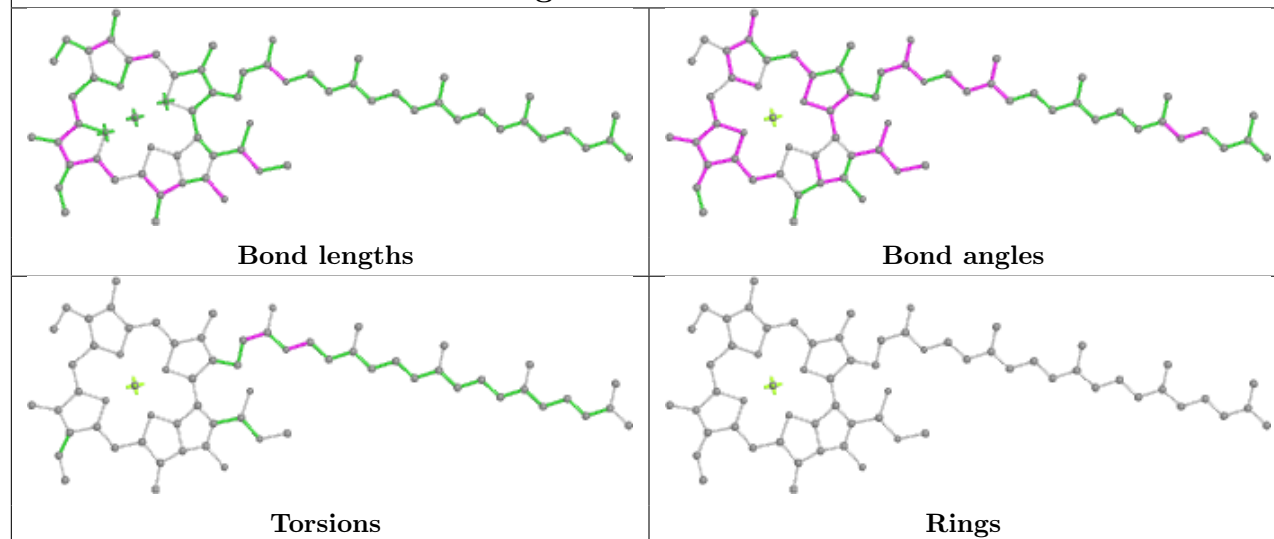
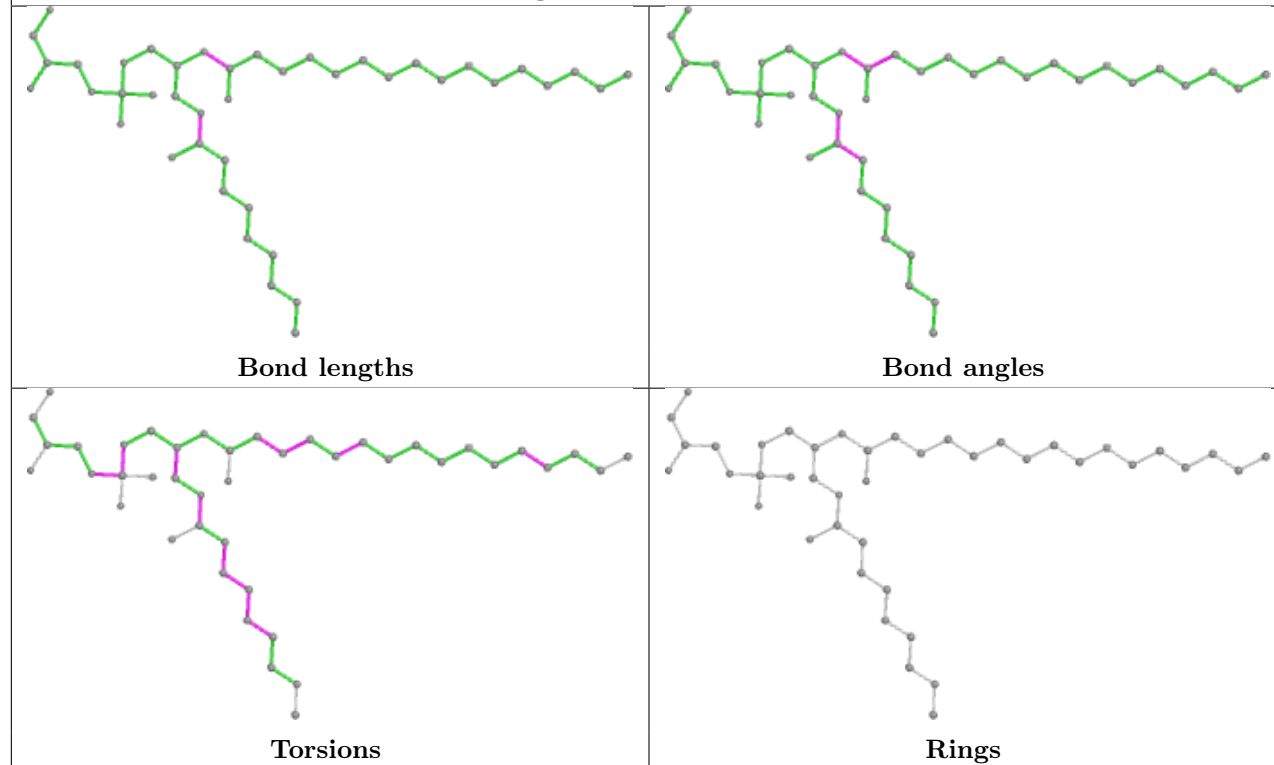


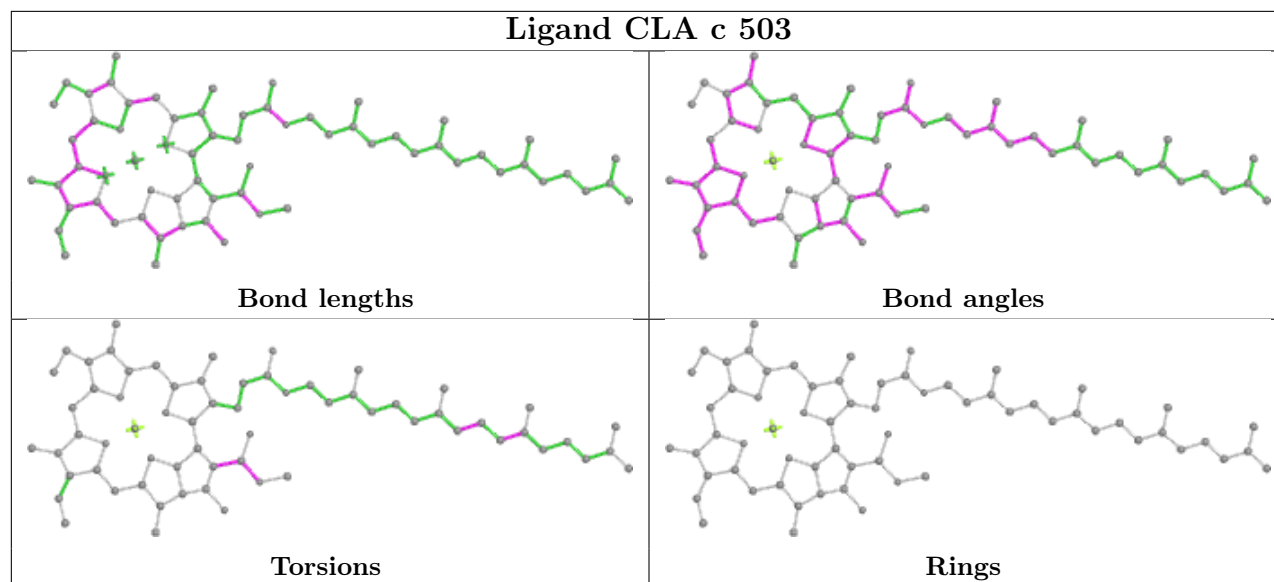
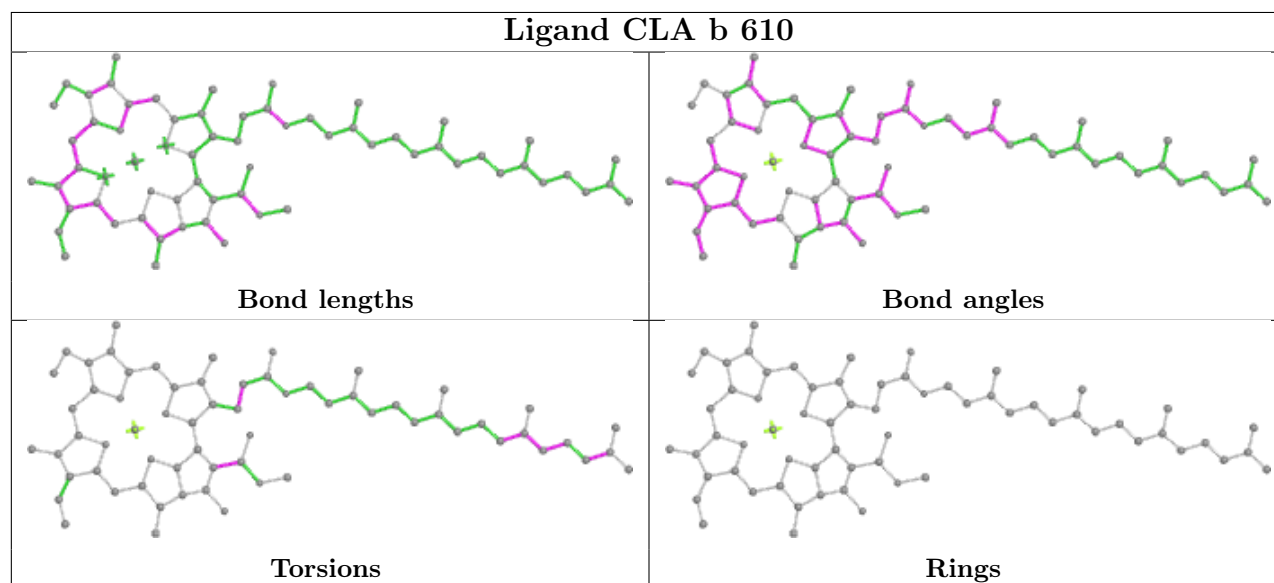


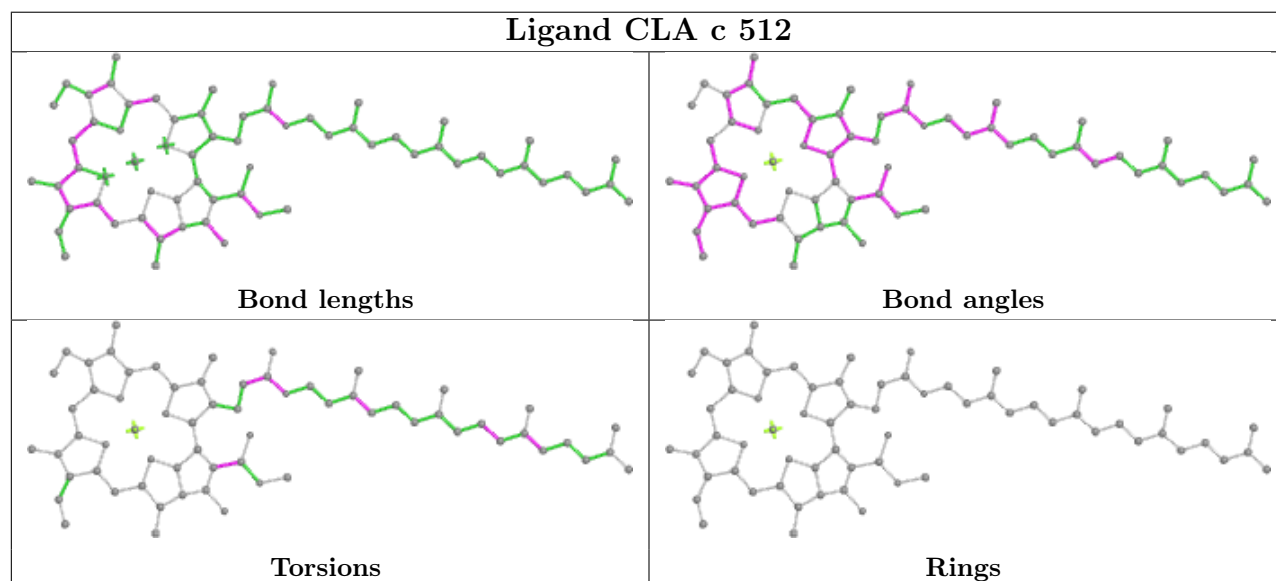
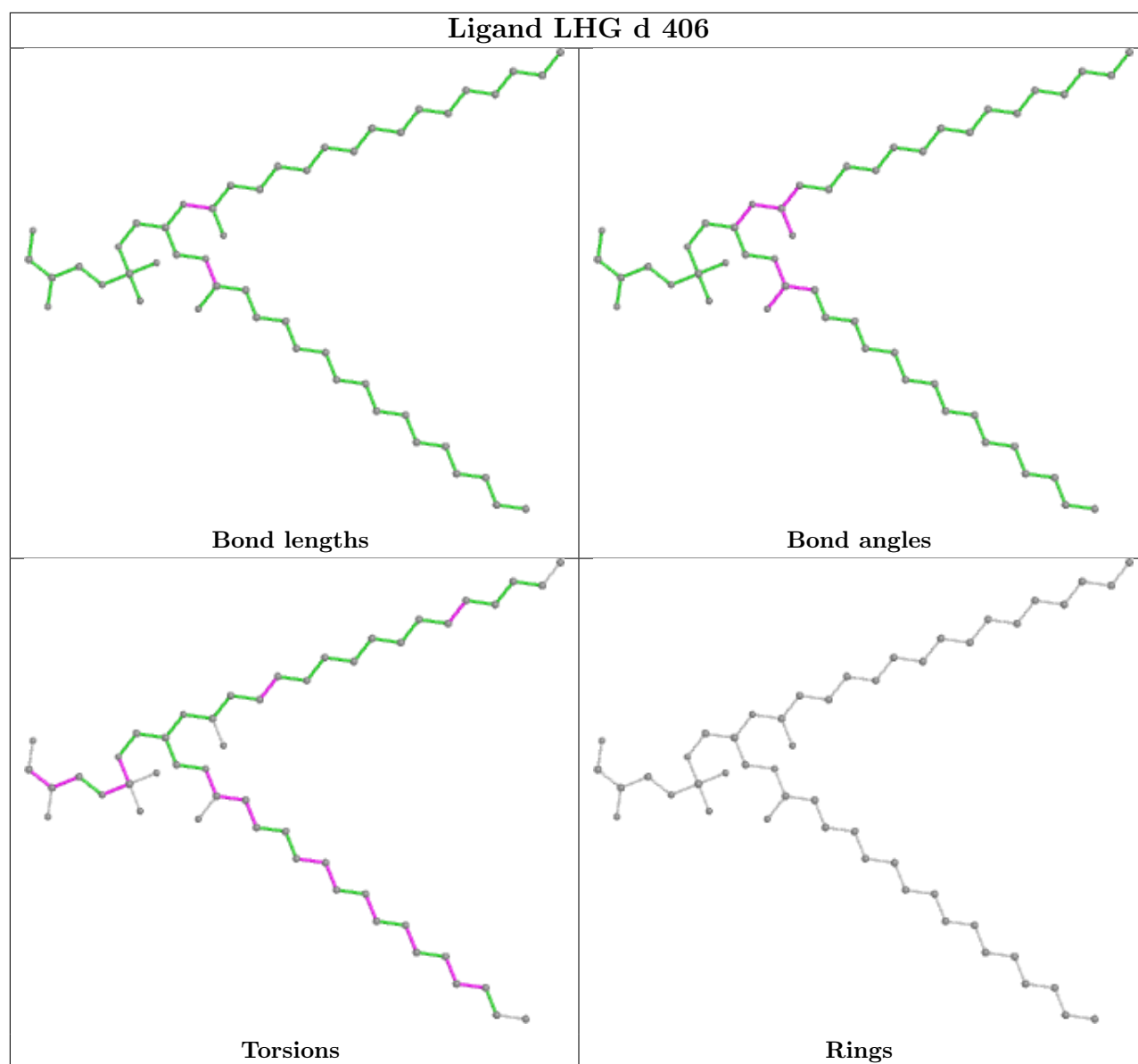


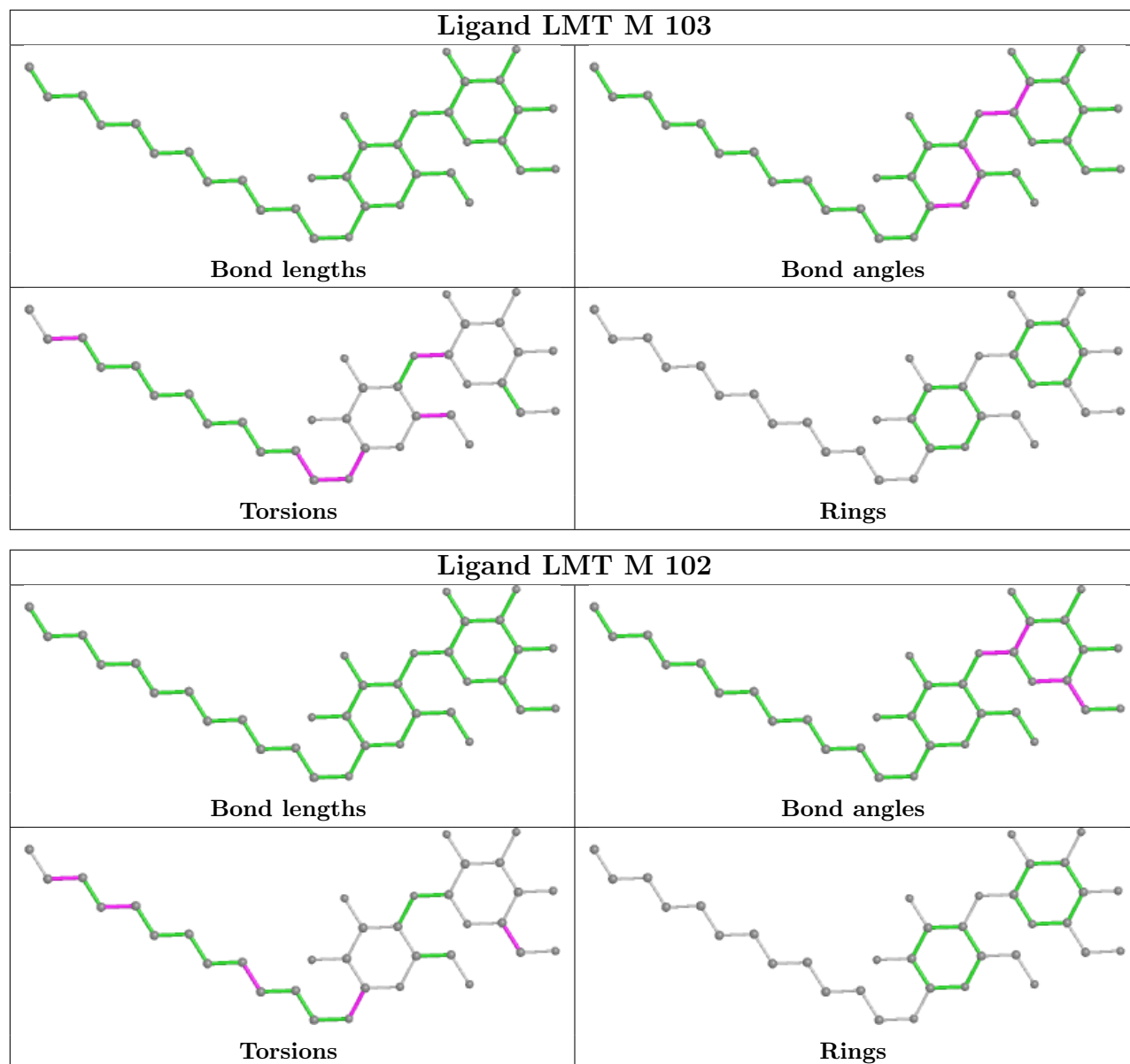


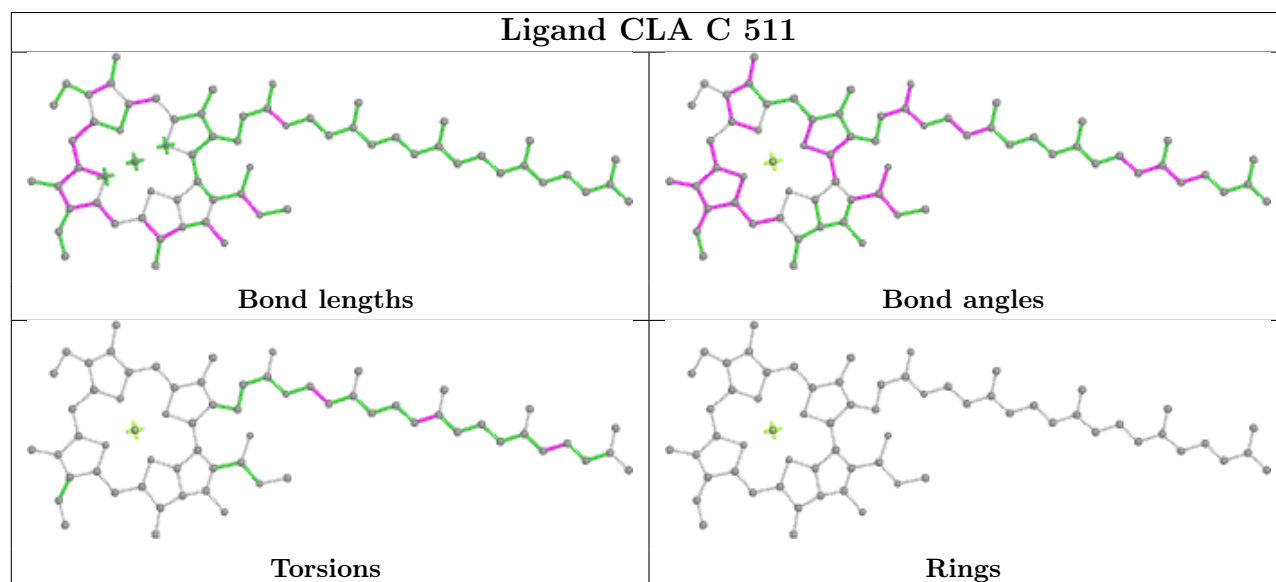
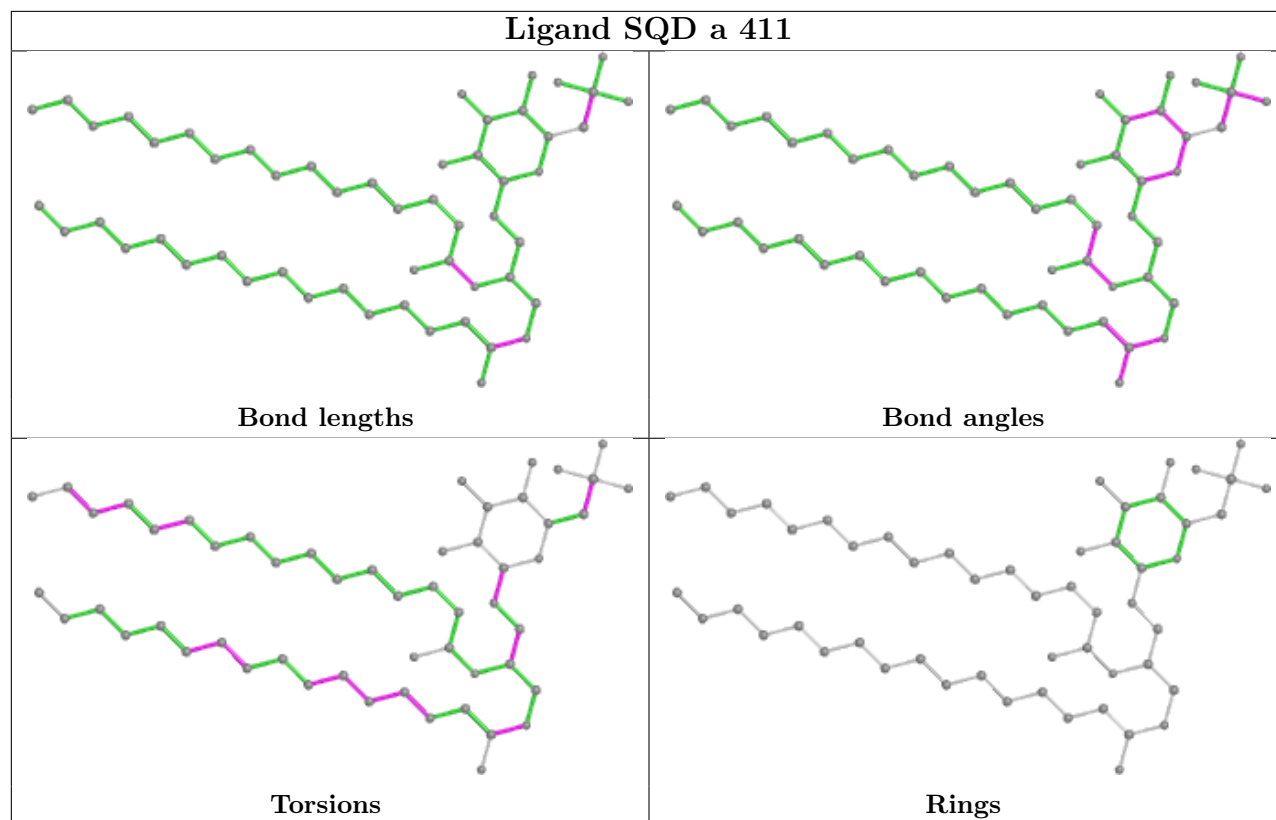
Ligand CLA C 512**Ligand CLA b 608****Ligand CLA B 611**

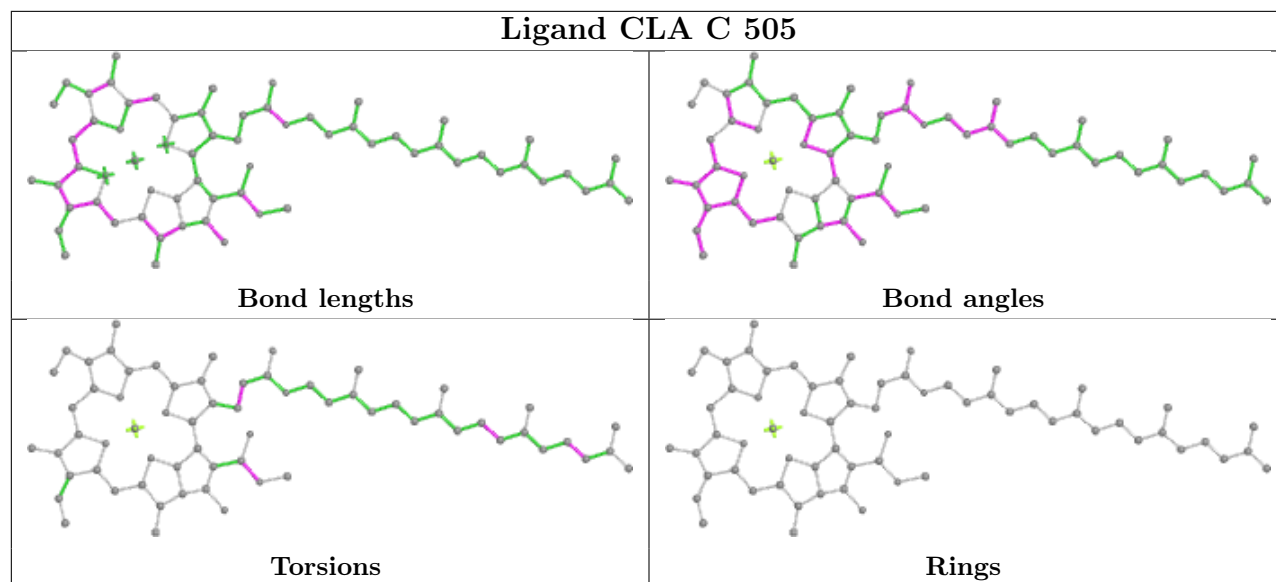
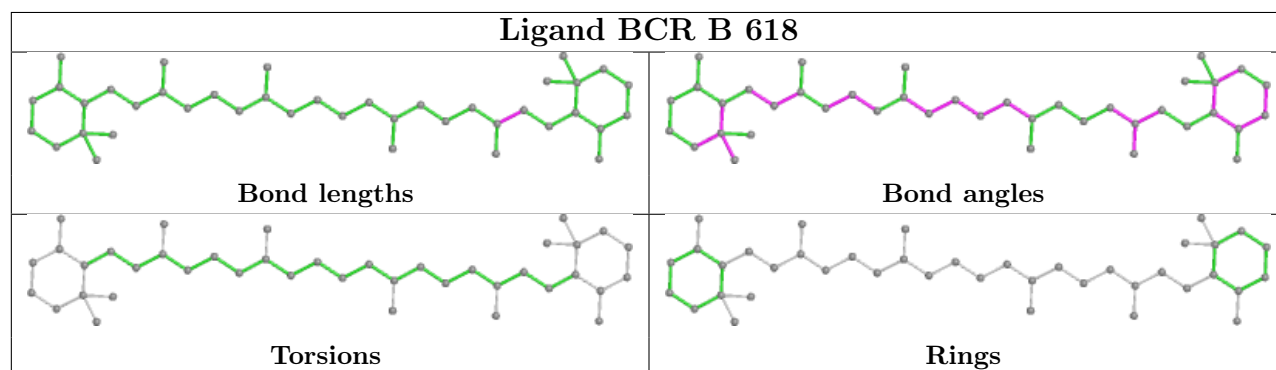
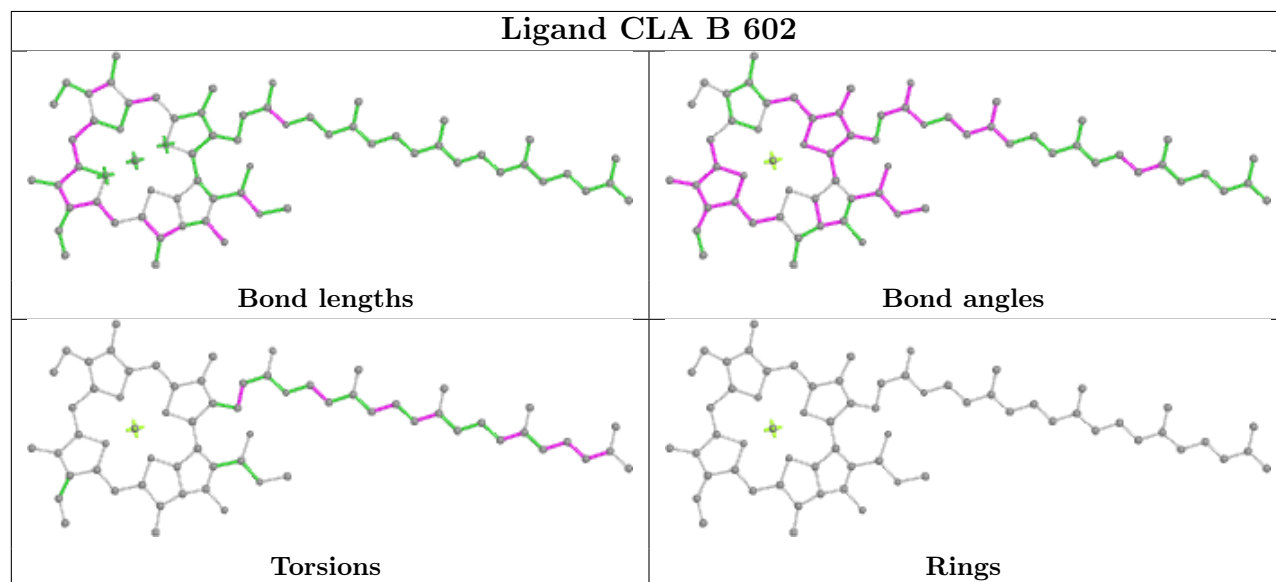
Ligand CLA b 613**Ligand LHG E 101**

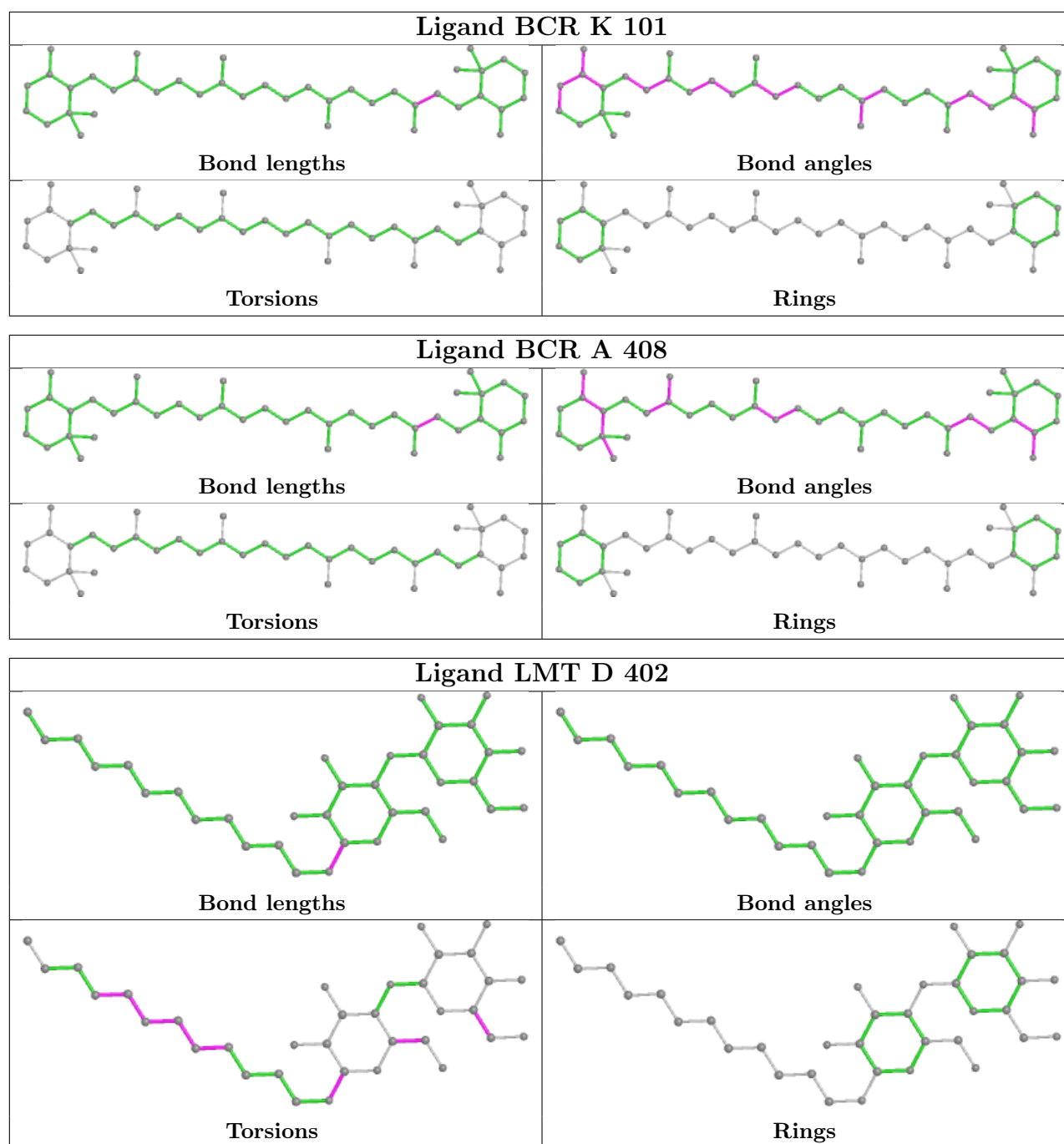
Ligand CLA c 503**Ligand CLA b 610**



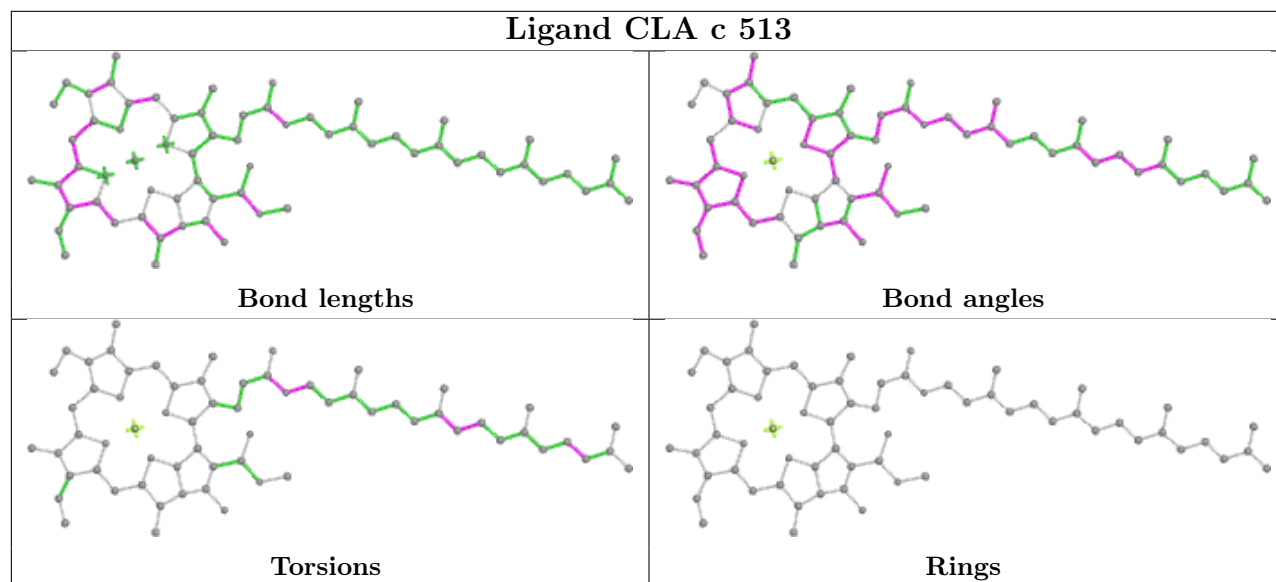




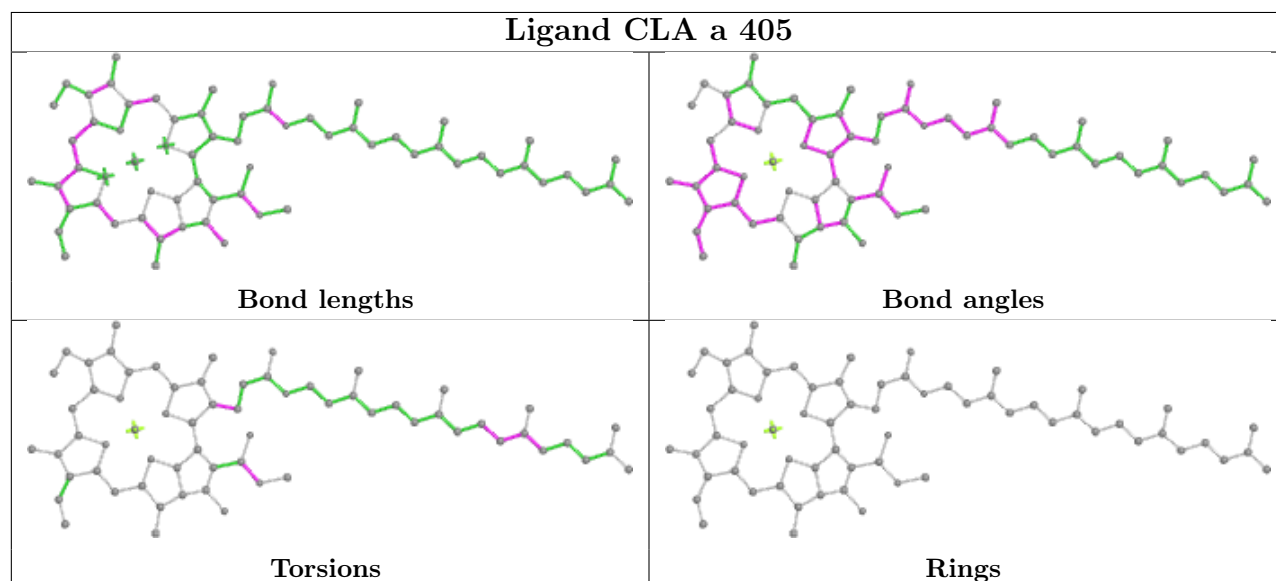
Ligand CLA C 505**Ligand BCR B 618****Ligand CLA B 602**



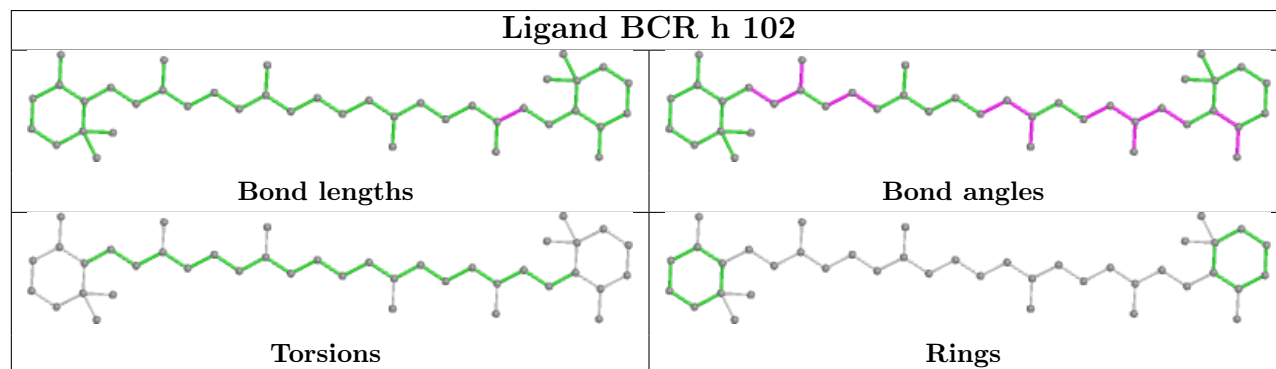
Ligand CLA c 513



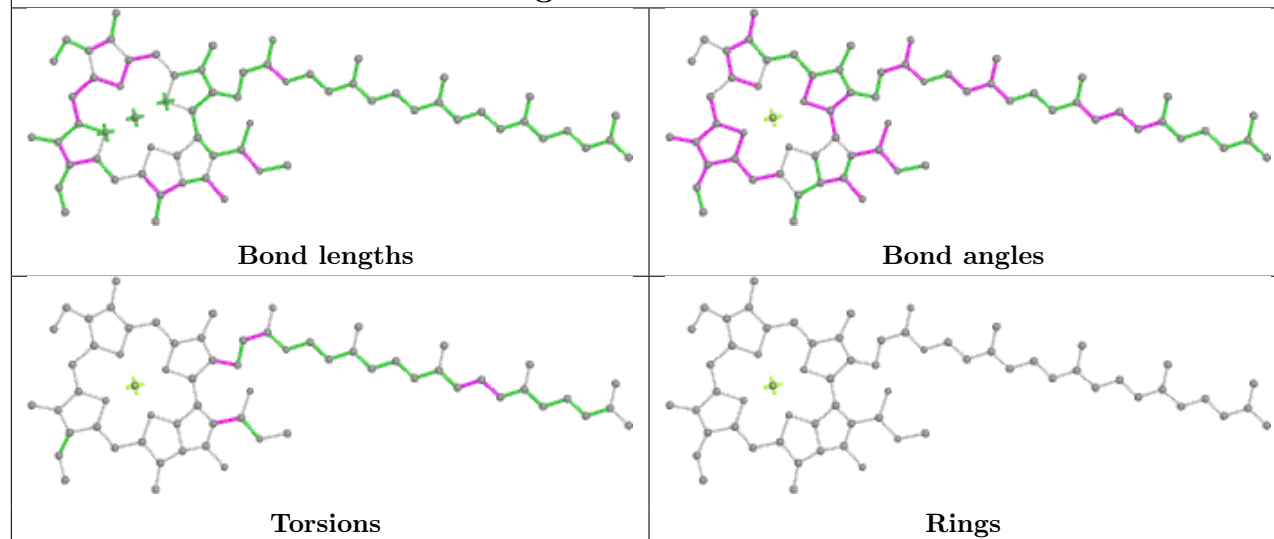
Ligand CLA a 405



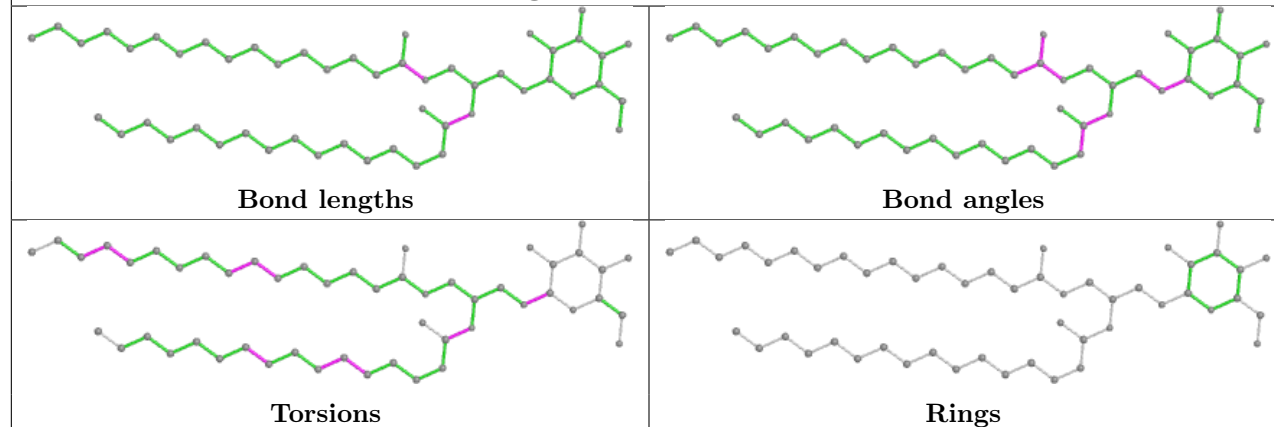
Ligand BCR h 102



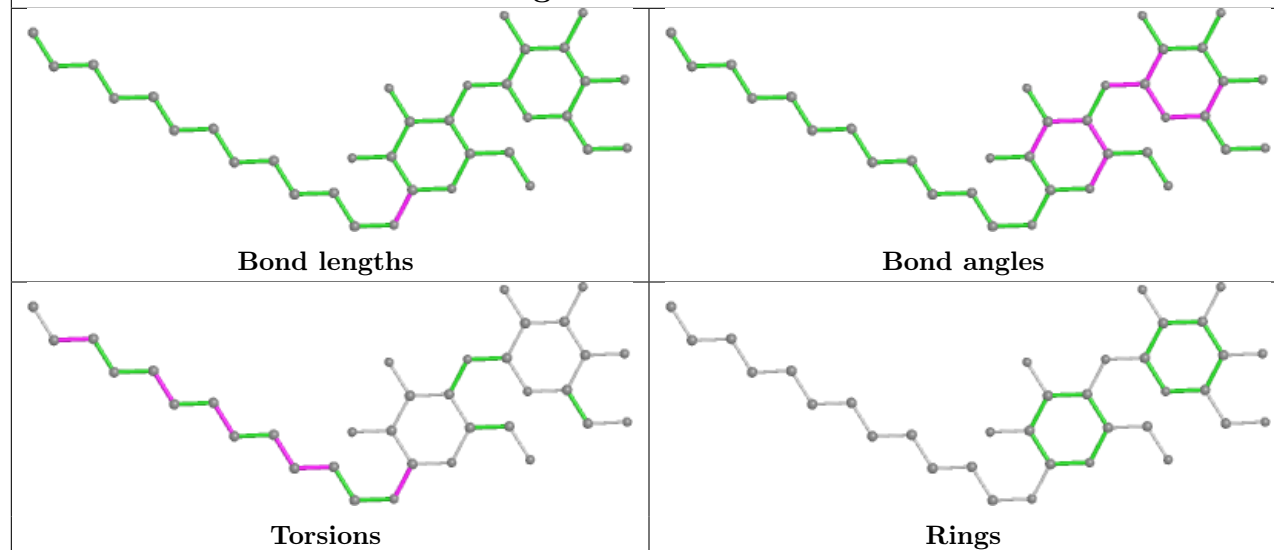
Ligand CLA b 612

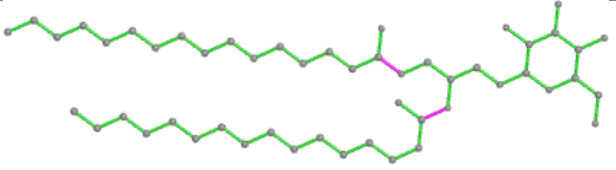
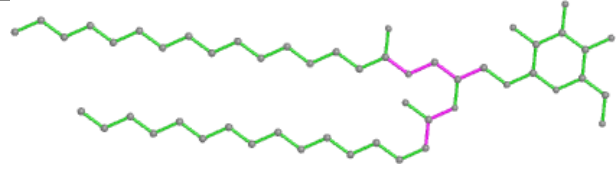
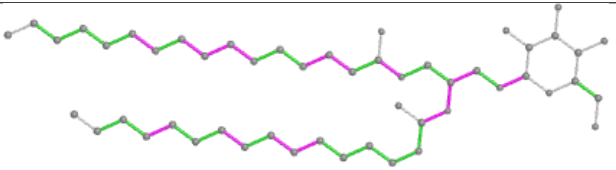
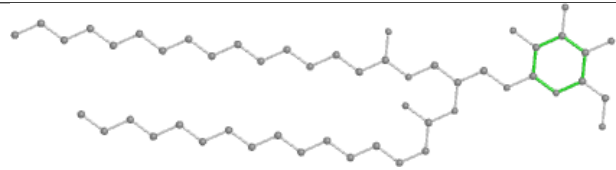


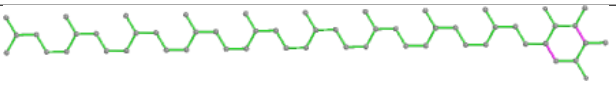
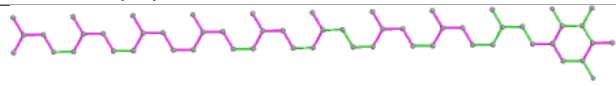
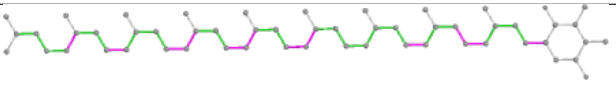
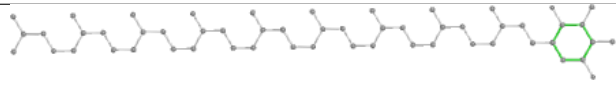
Ligand LMG m 101

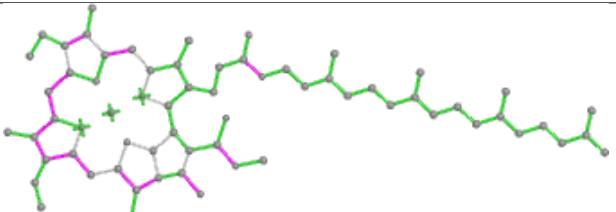
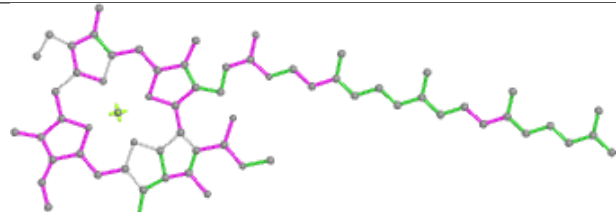
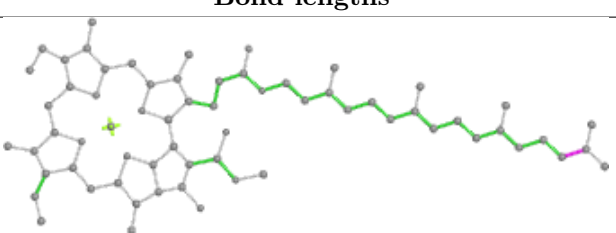
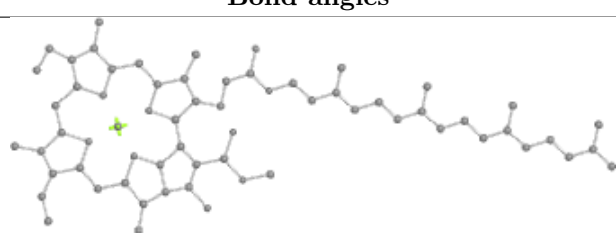


Ligand LMT a 412

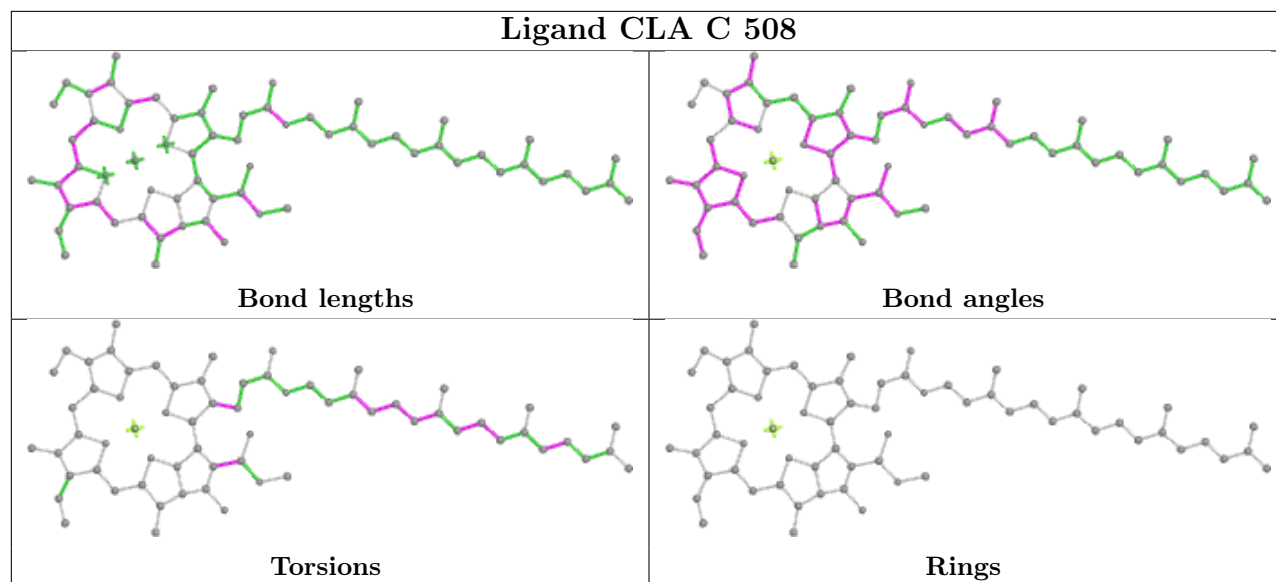


Ligand LMG M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

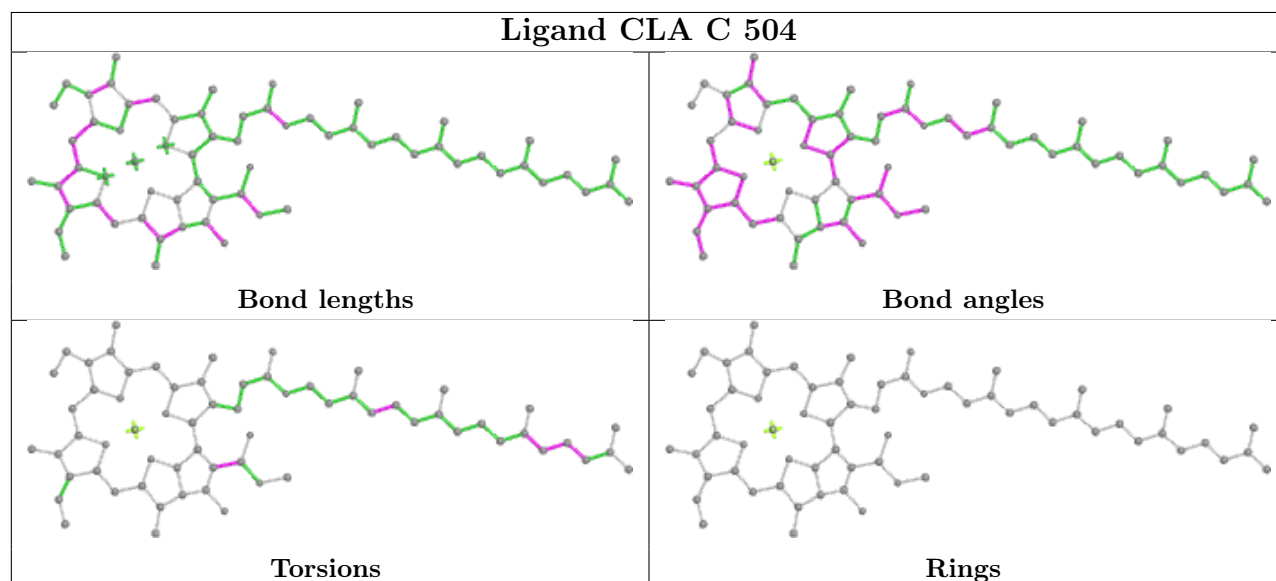
Ligand PL9 a 414 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

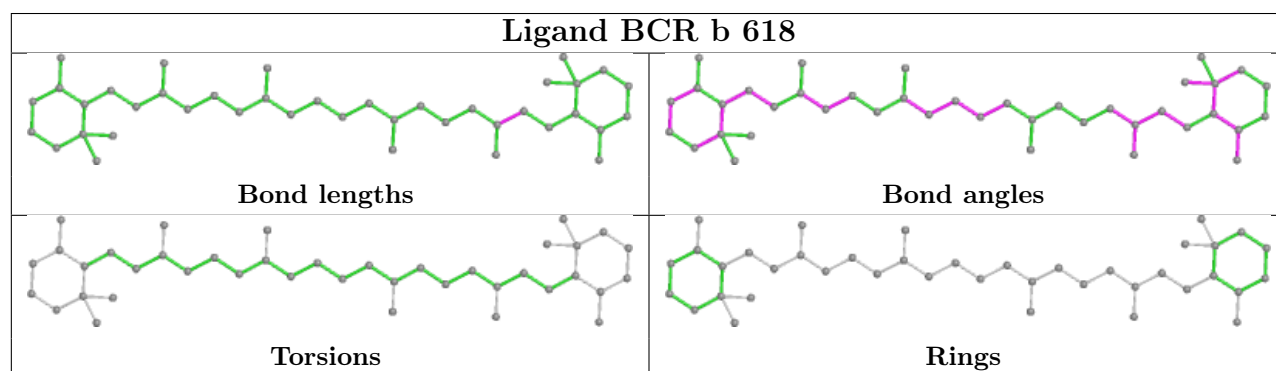
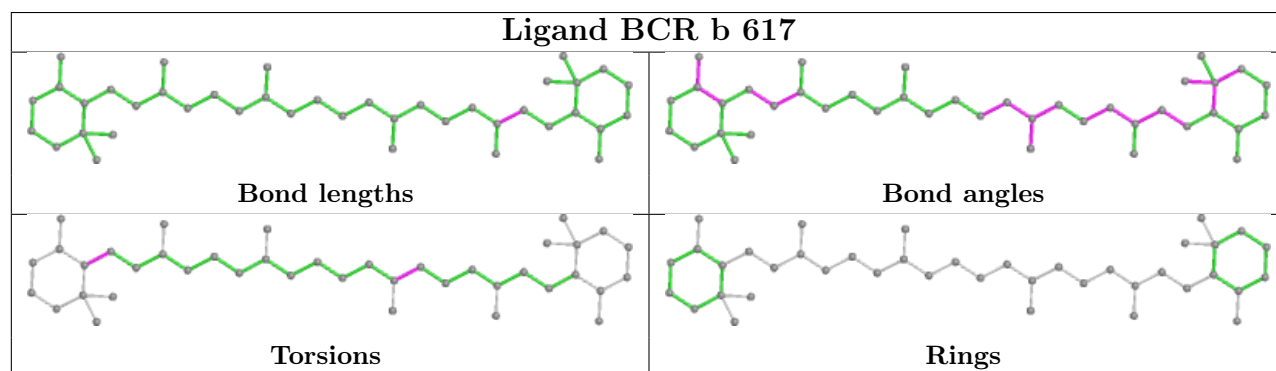
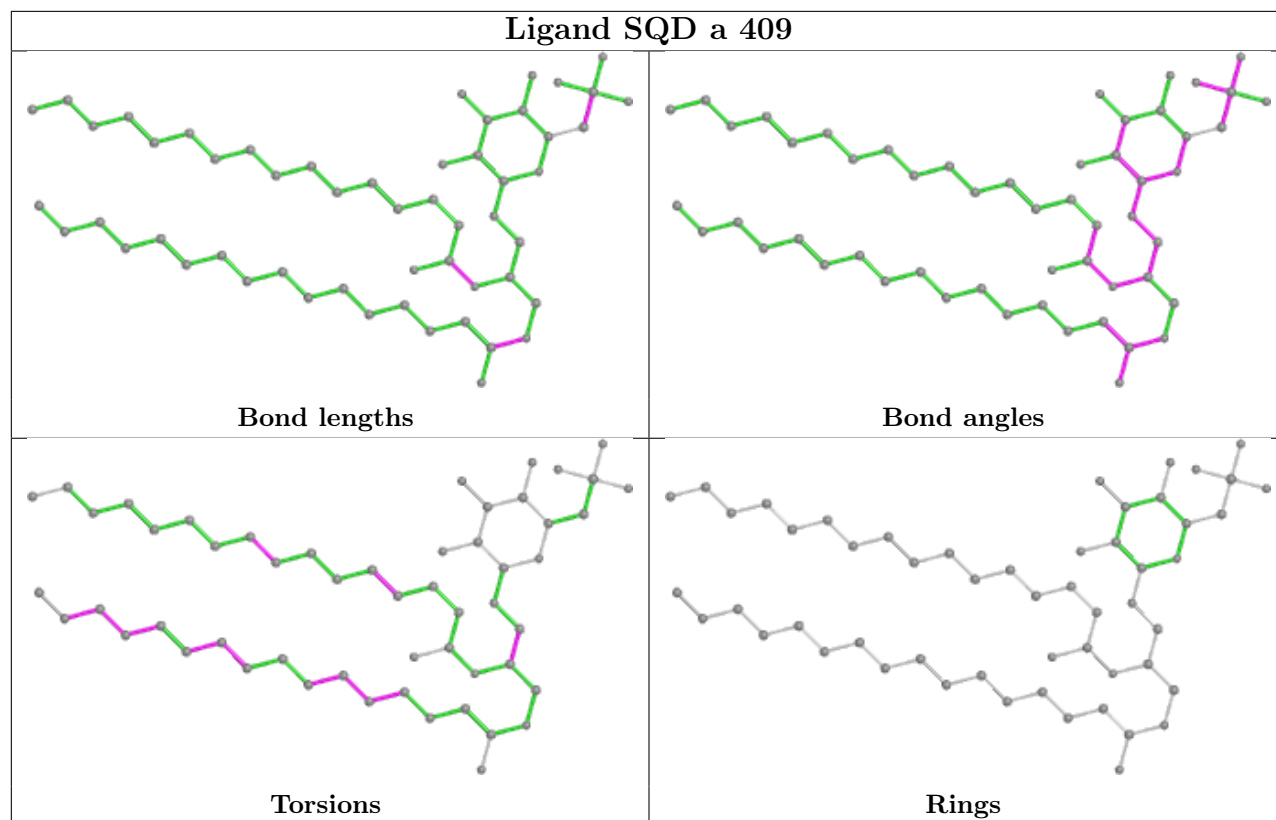
Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 508

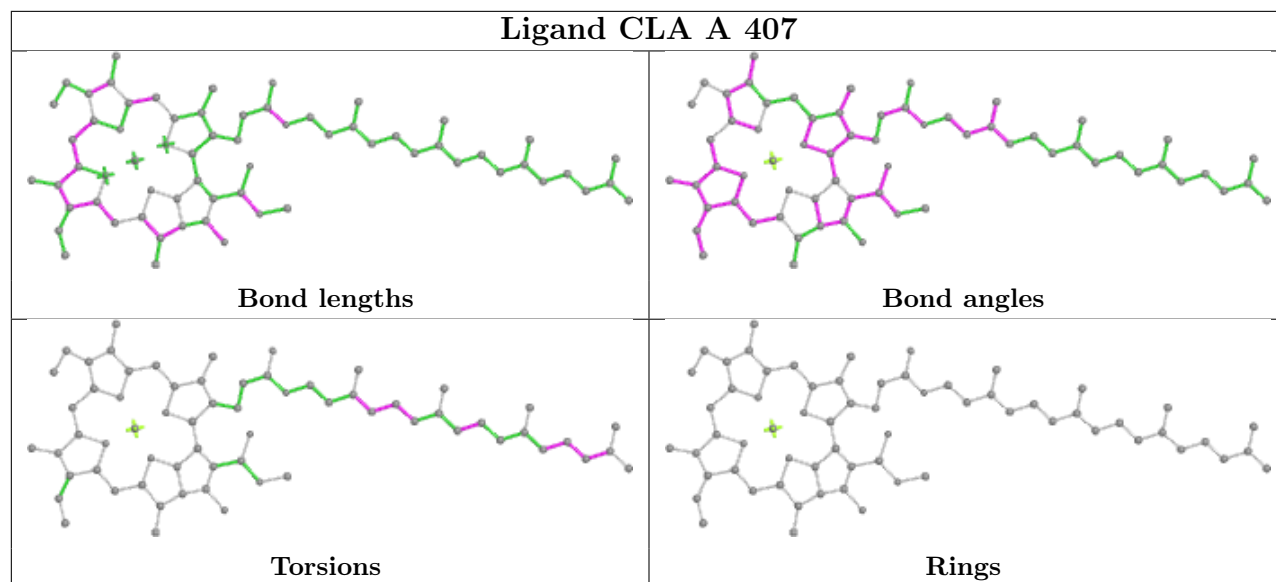


Ligand CLA C 504

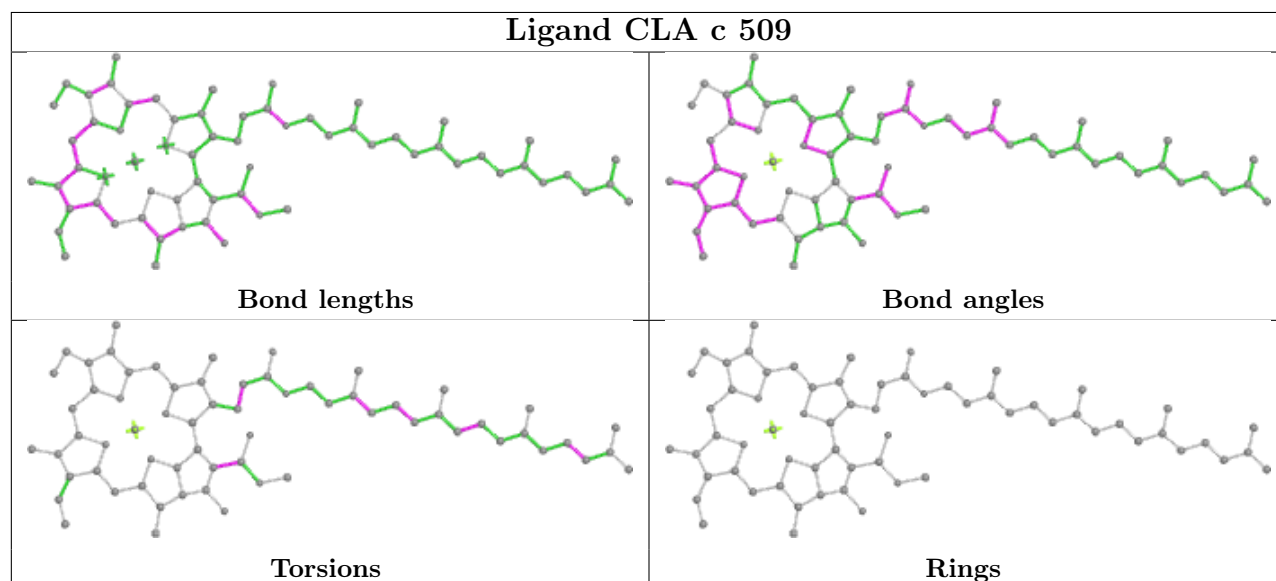




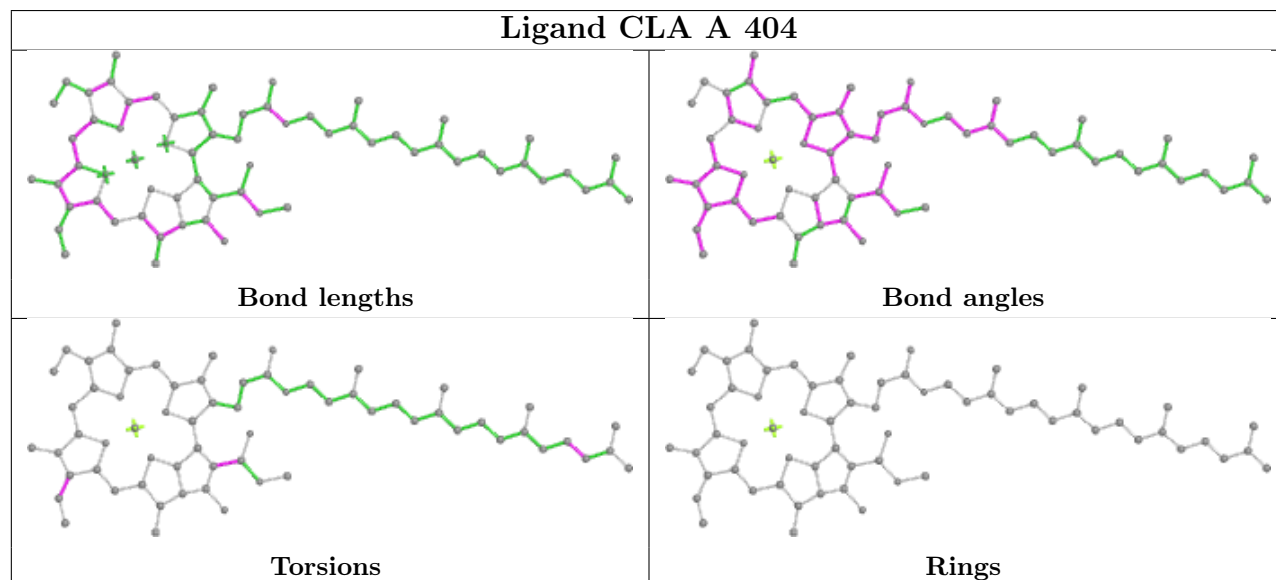
Ligand CLA A 407

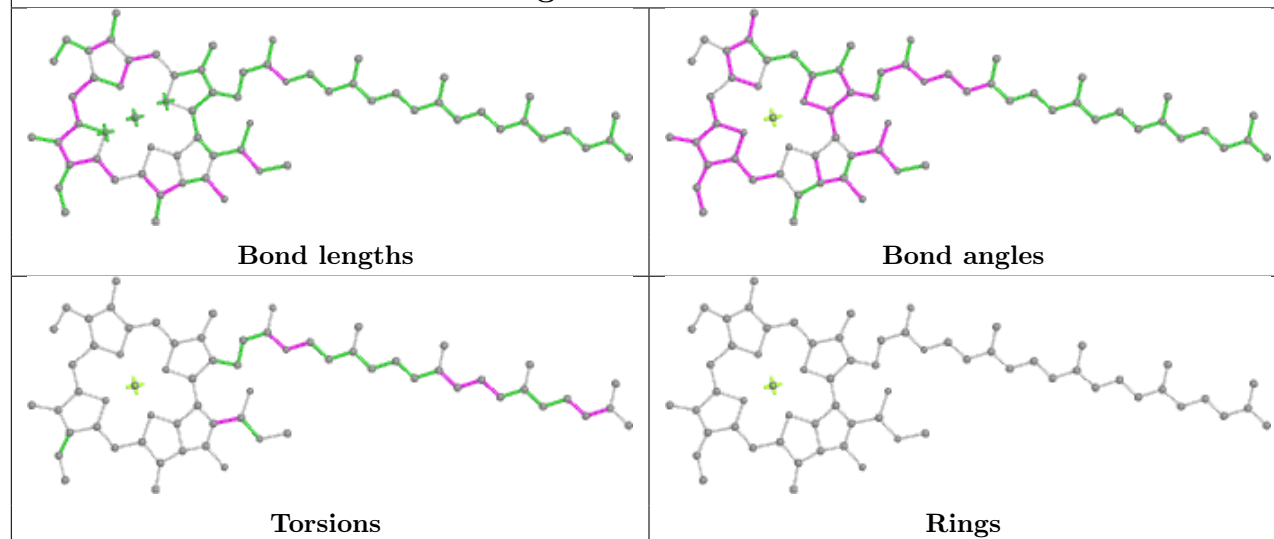
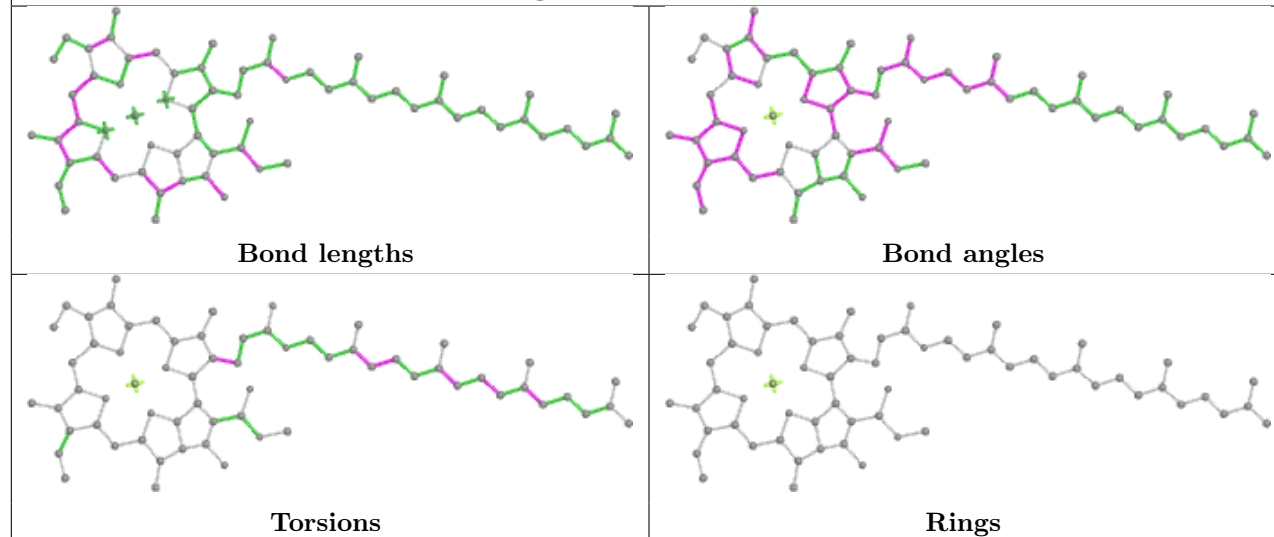


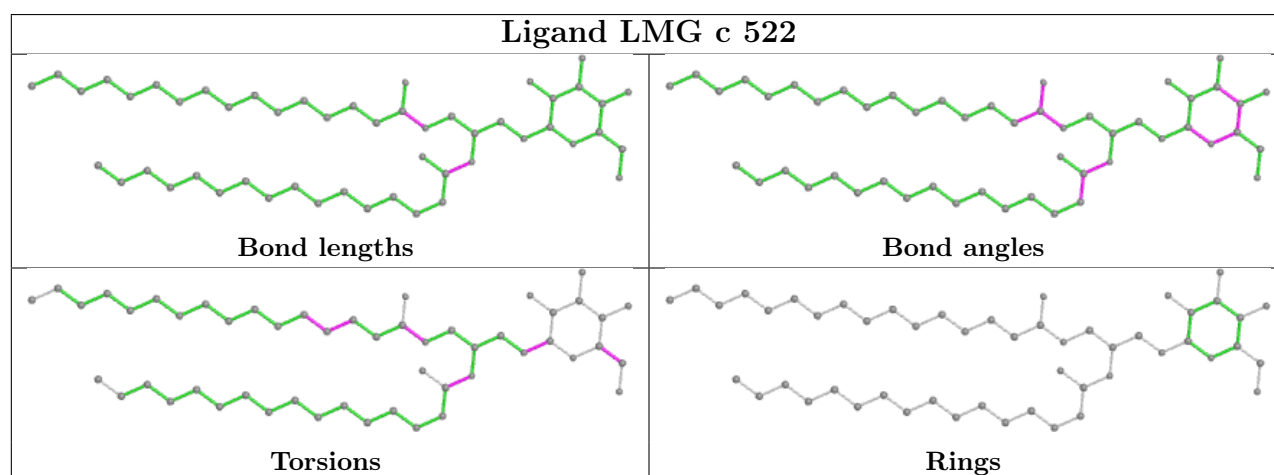
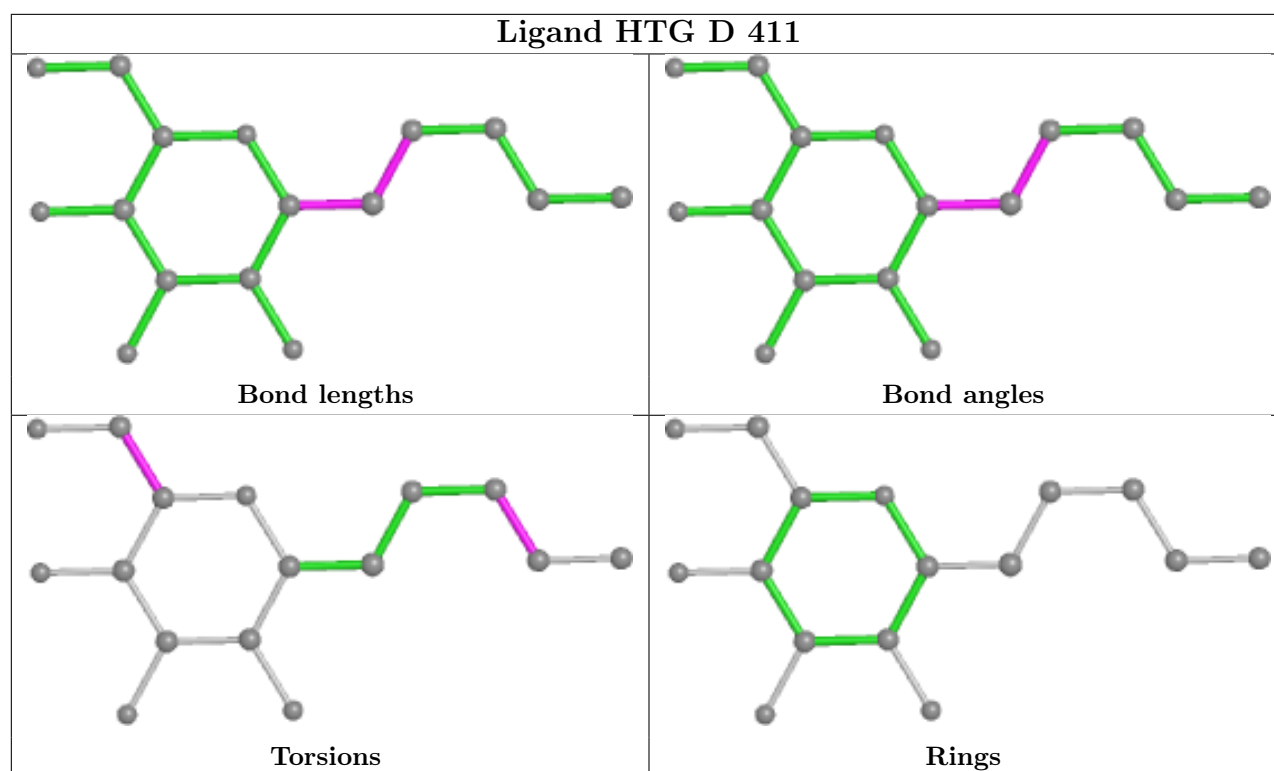
Ligand CLA c 509

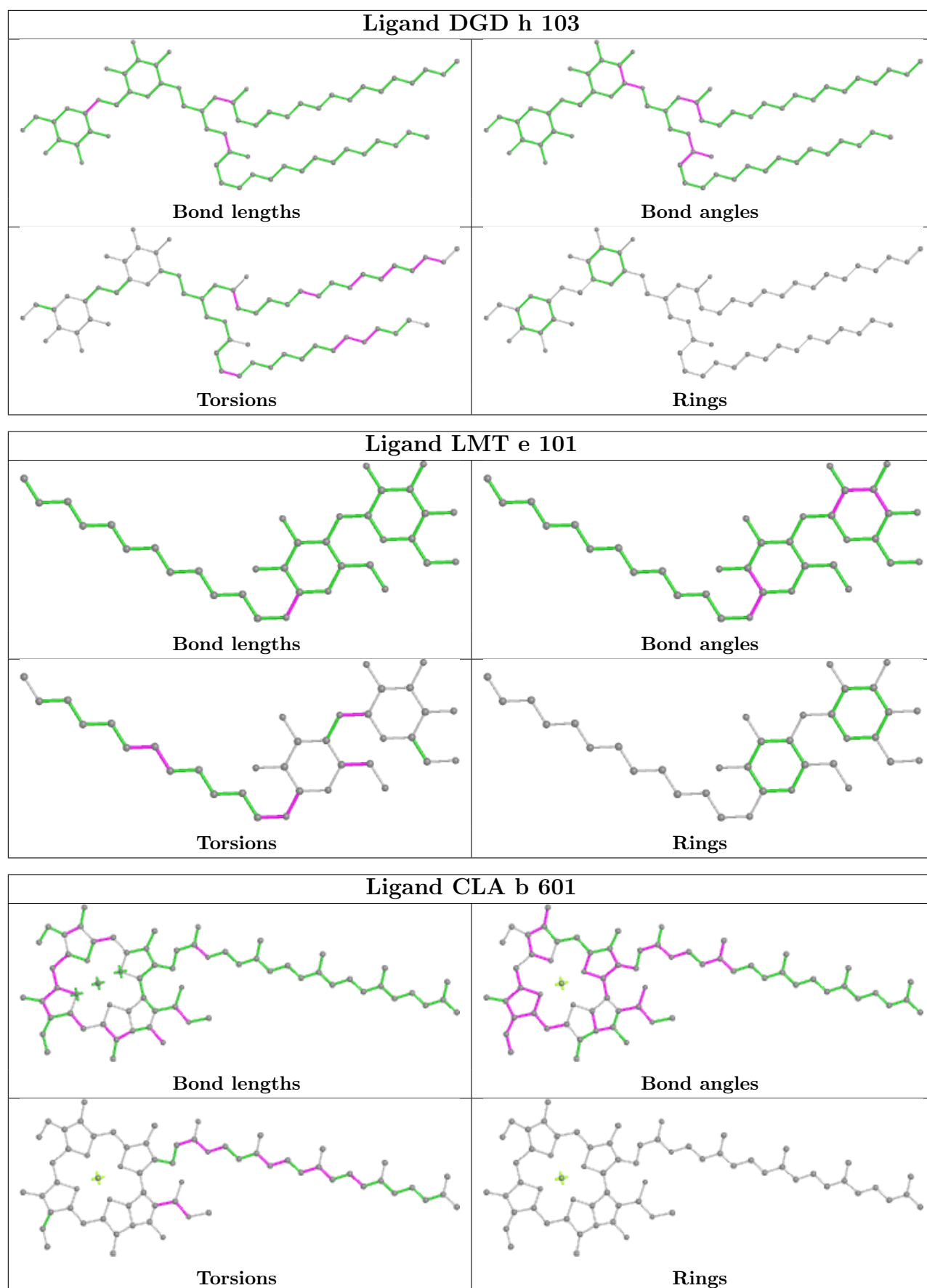


Ligand CLA A 404

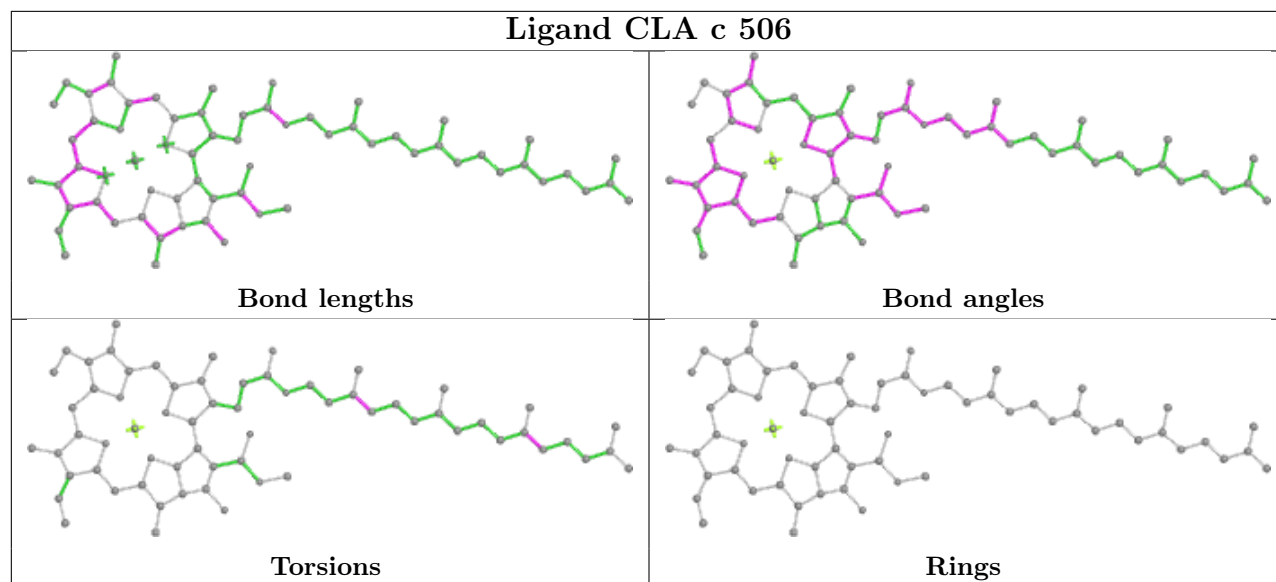


Ligand CLA c 511**Ligand CLA D 404**

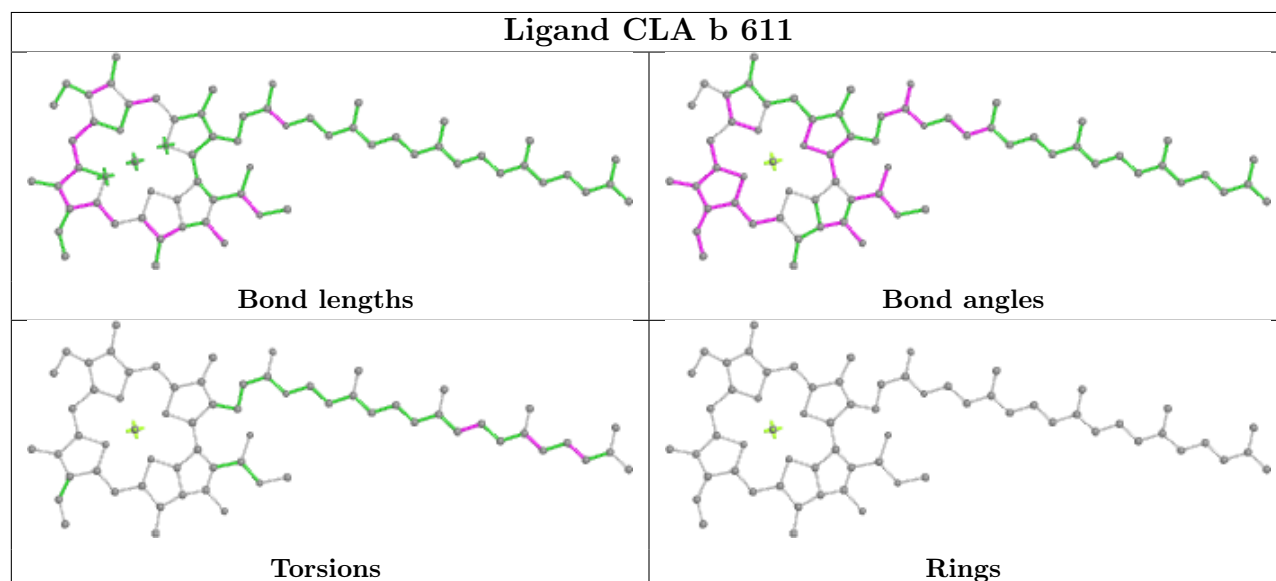




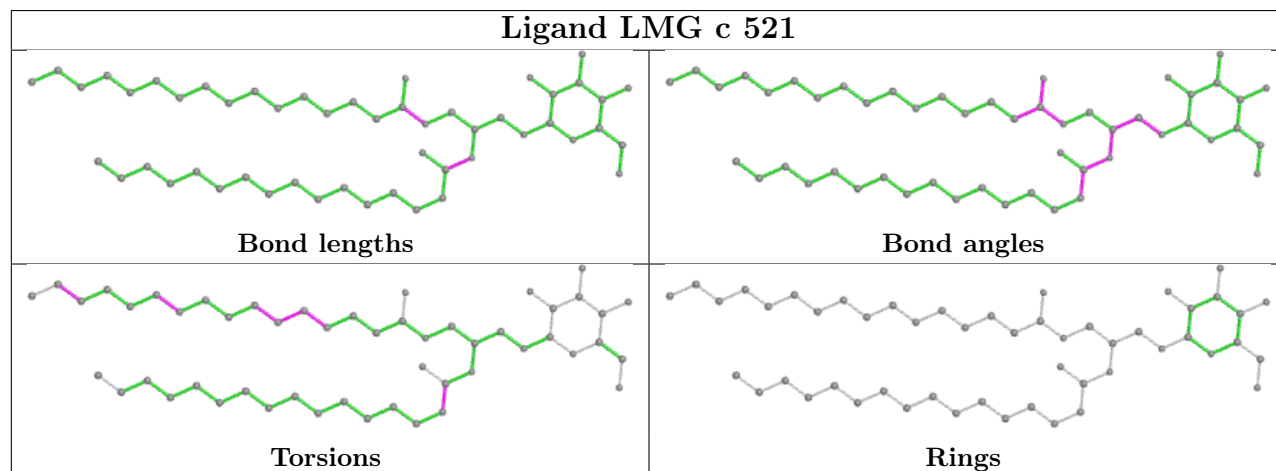
Ligand CLA c 506

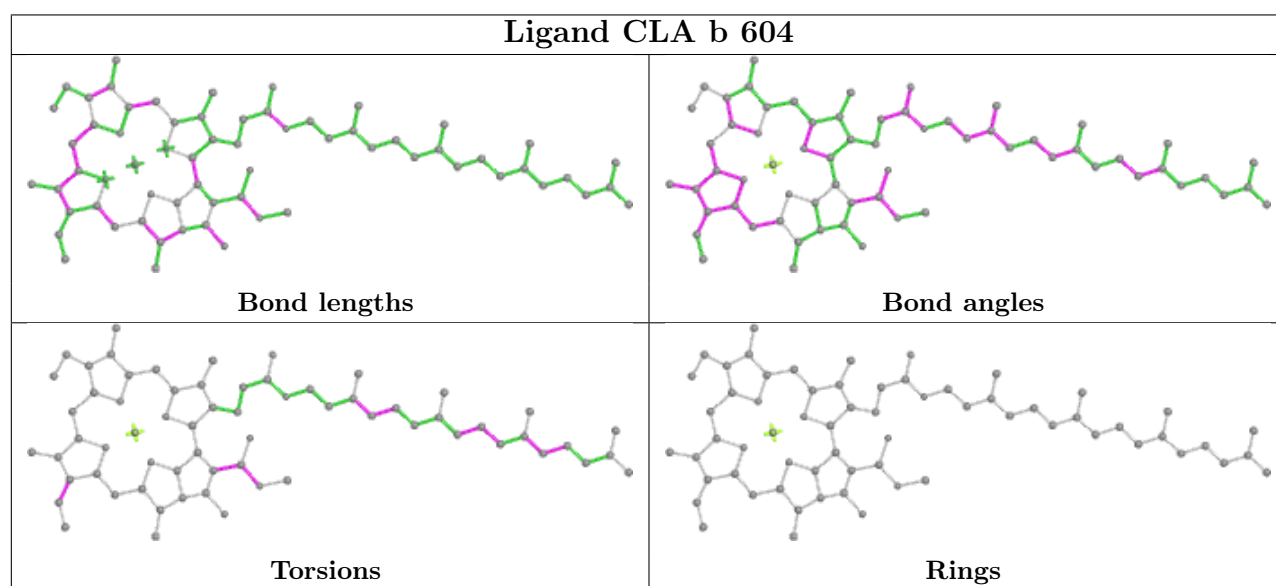
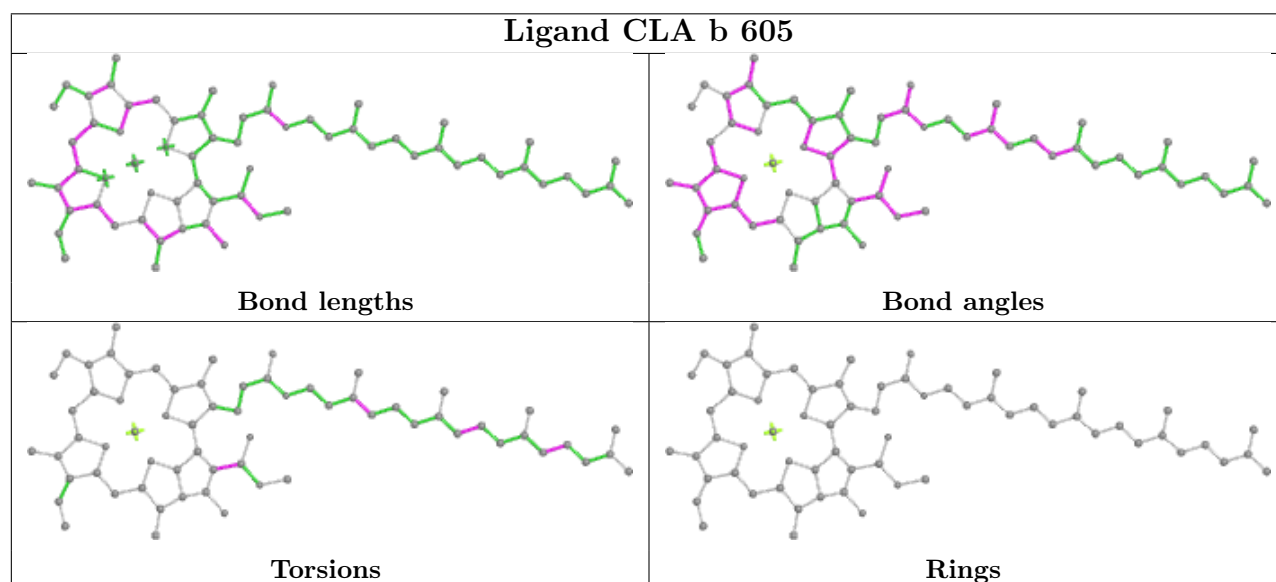
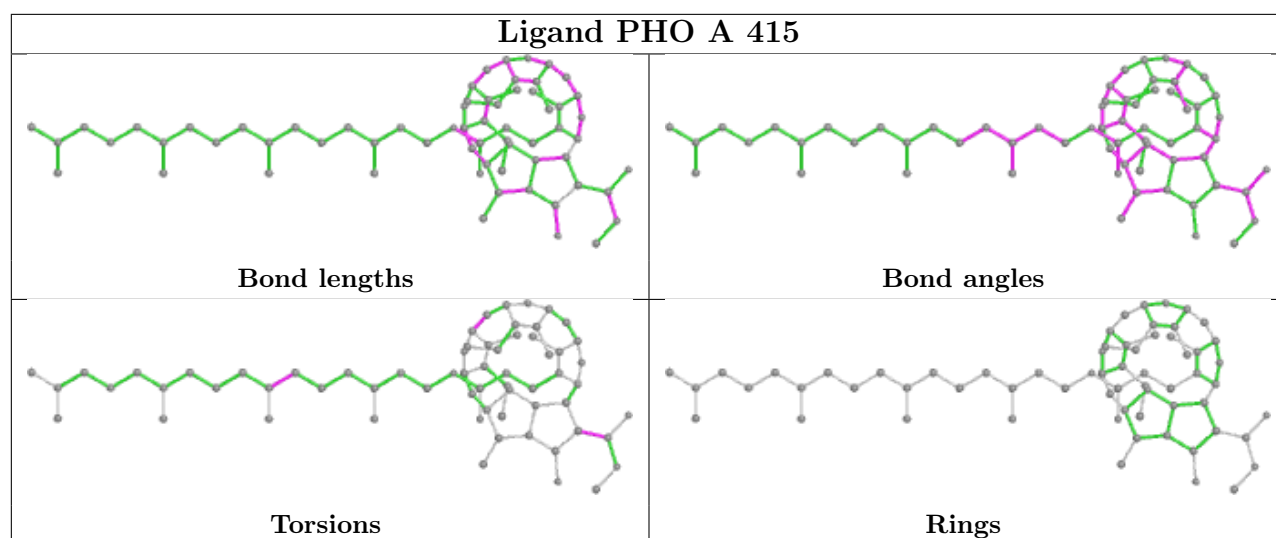


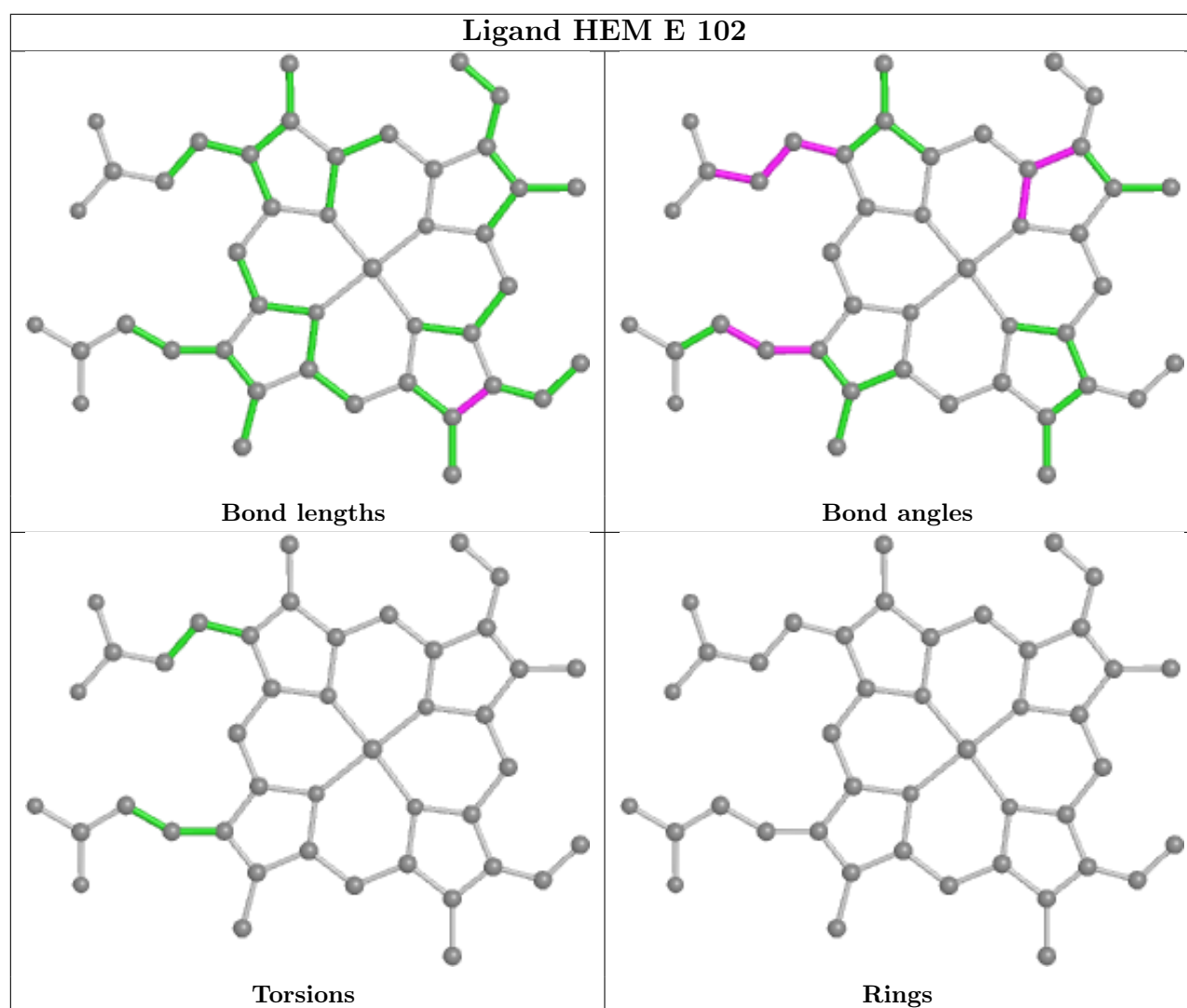
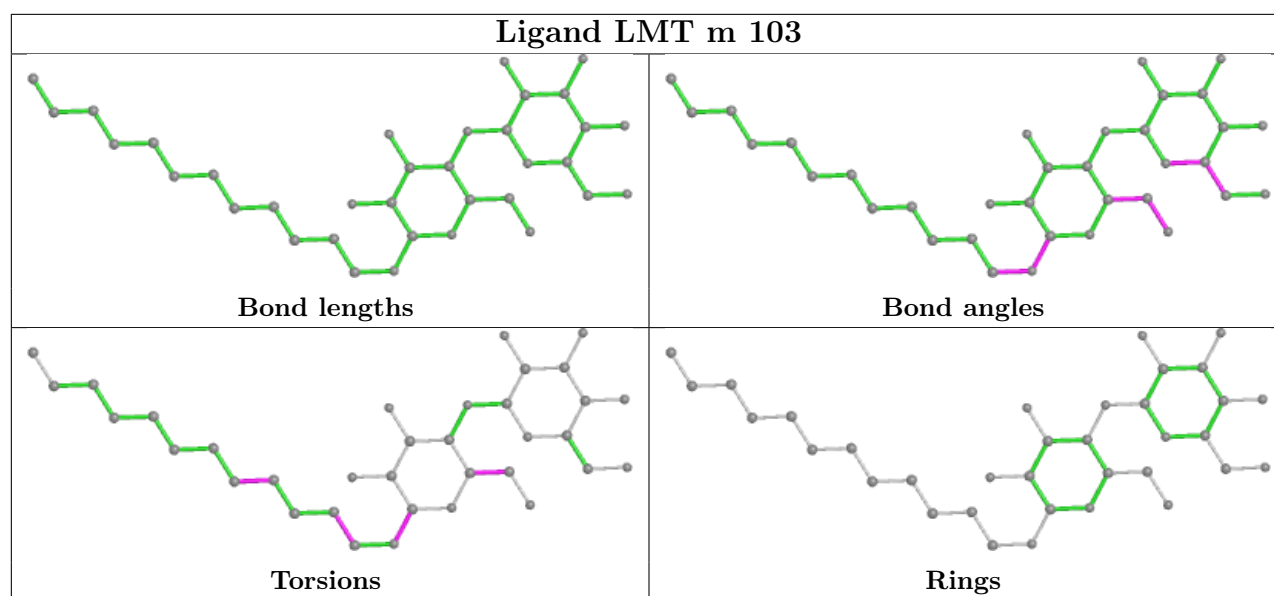
Ligand CLA b 611

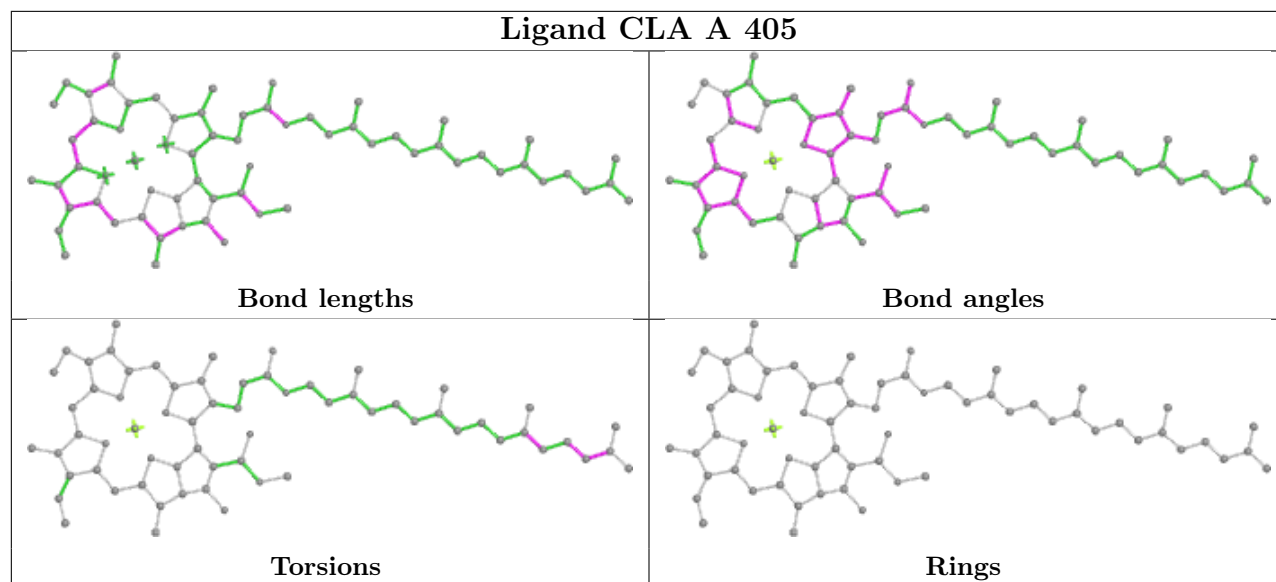
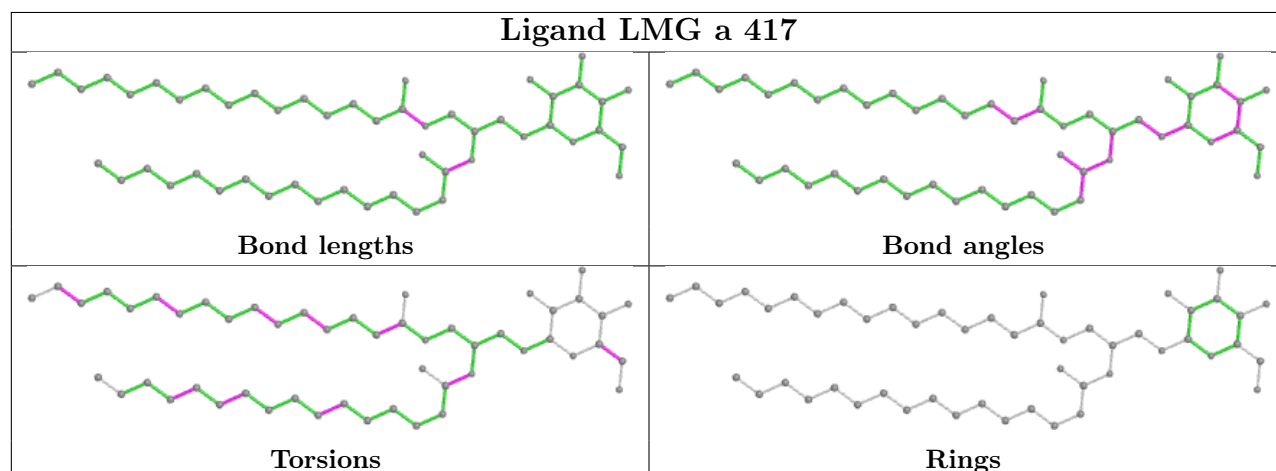
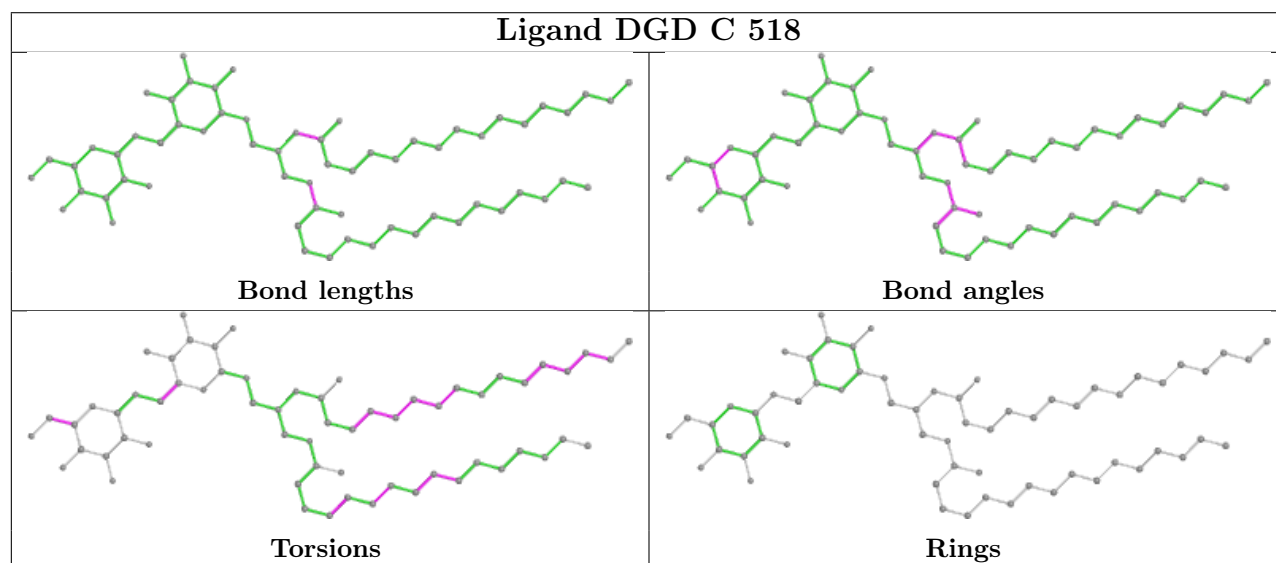


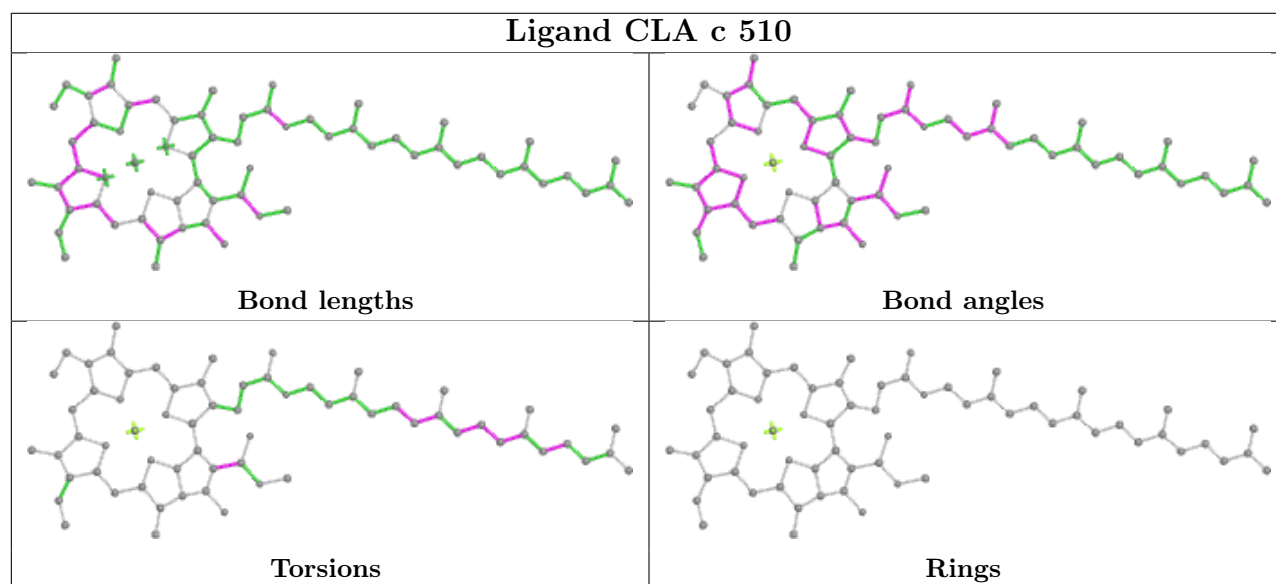
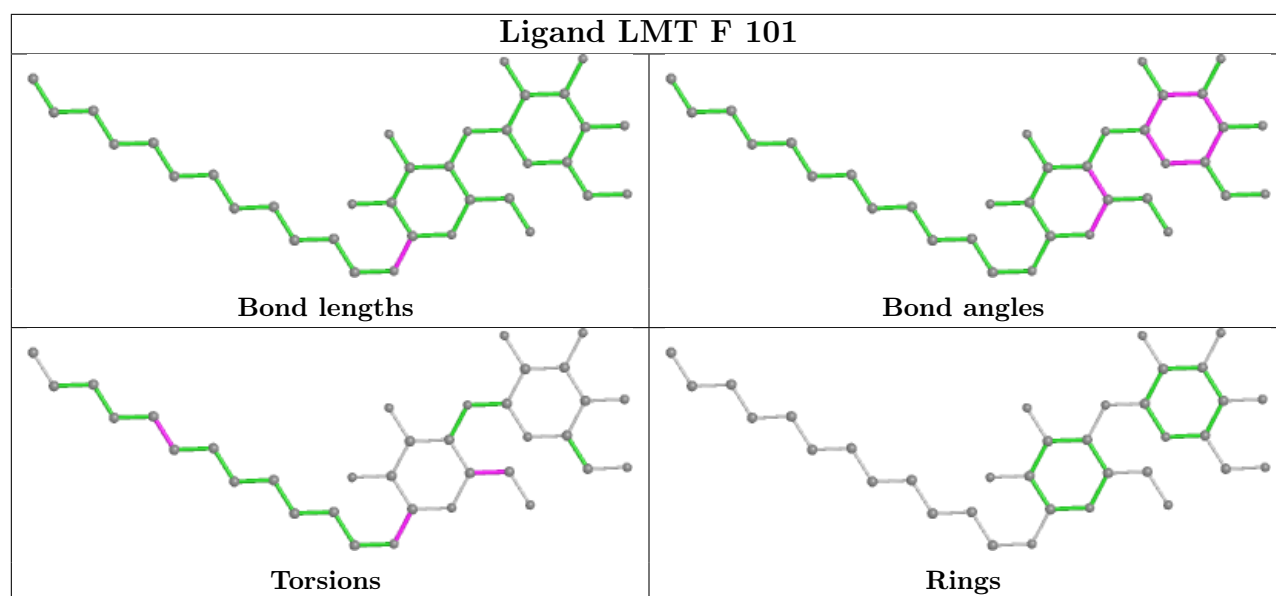
Ligand LMG c 521

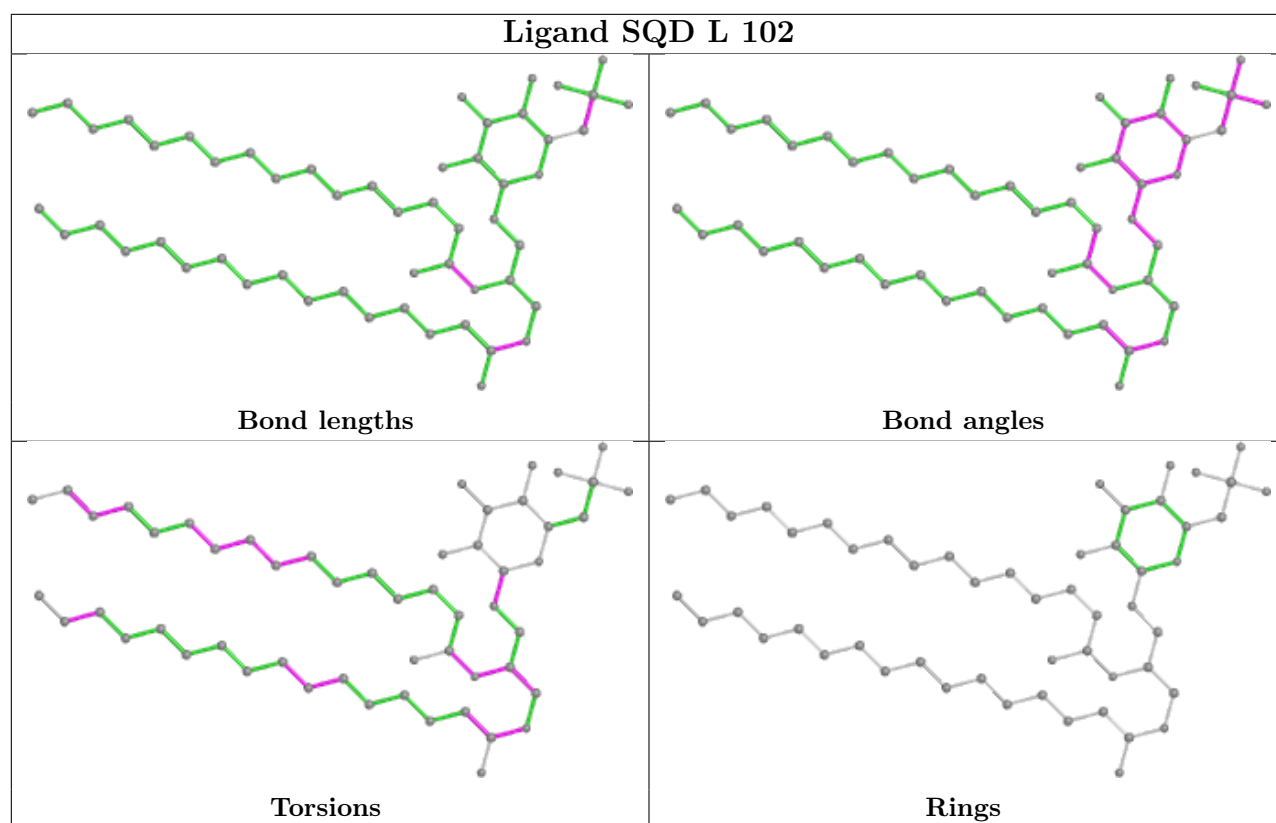


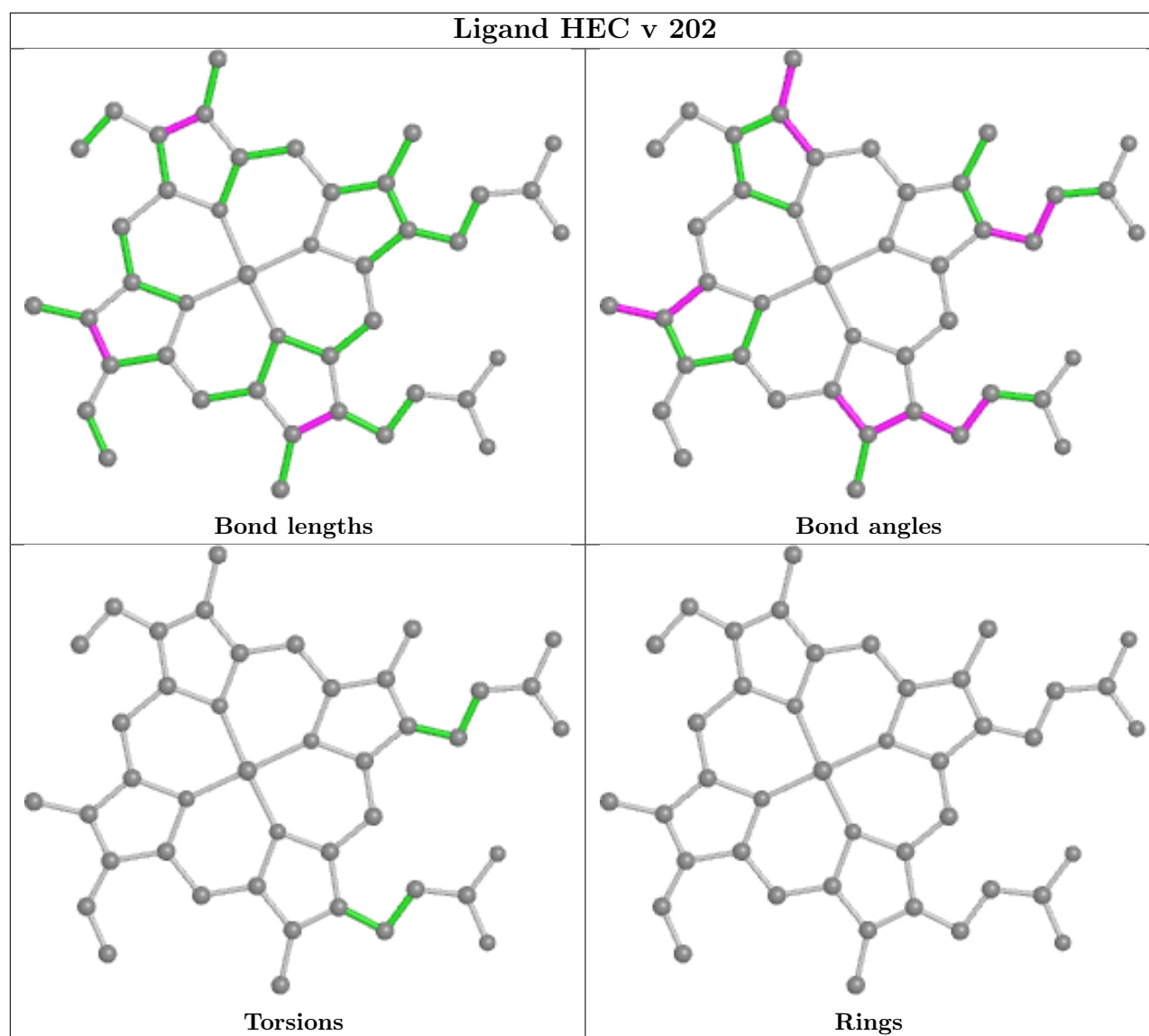


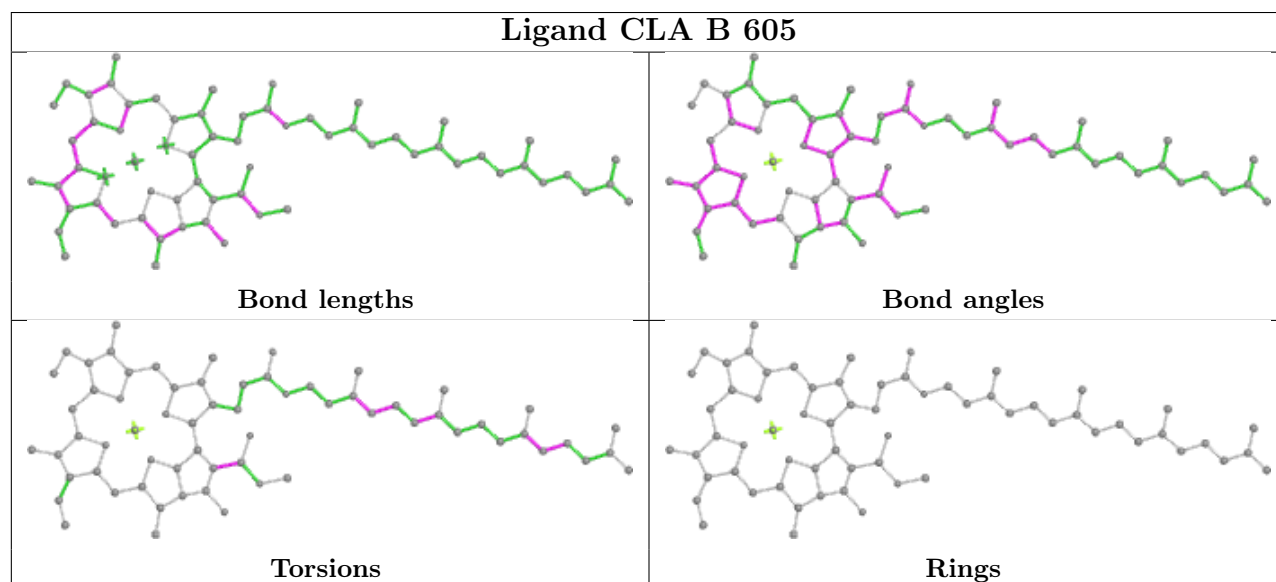
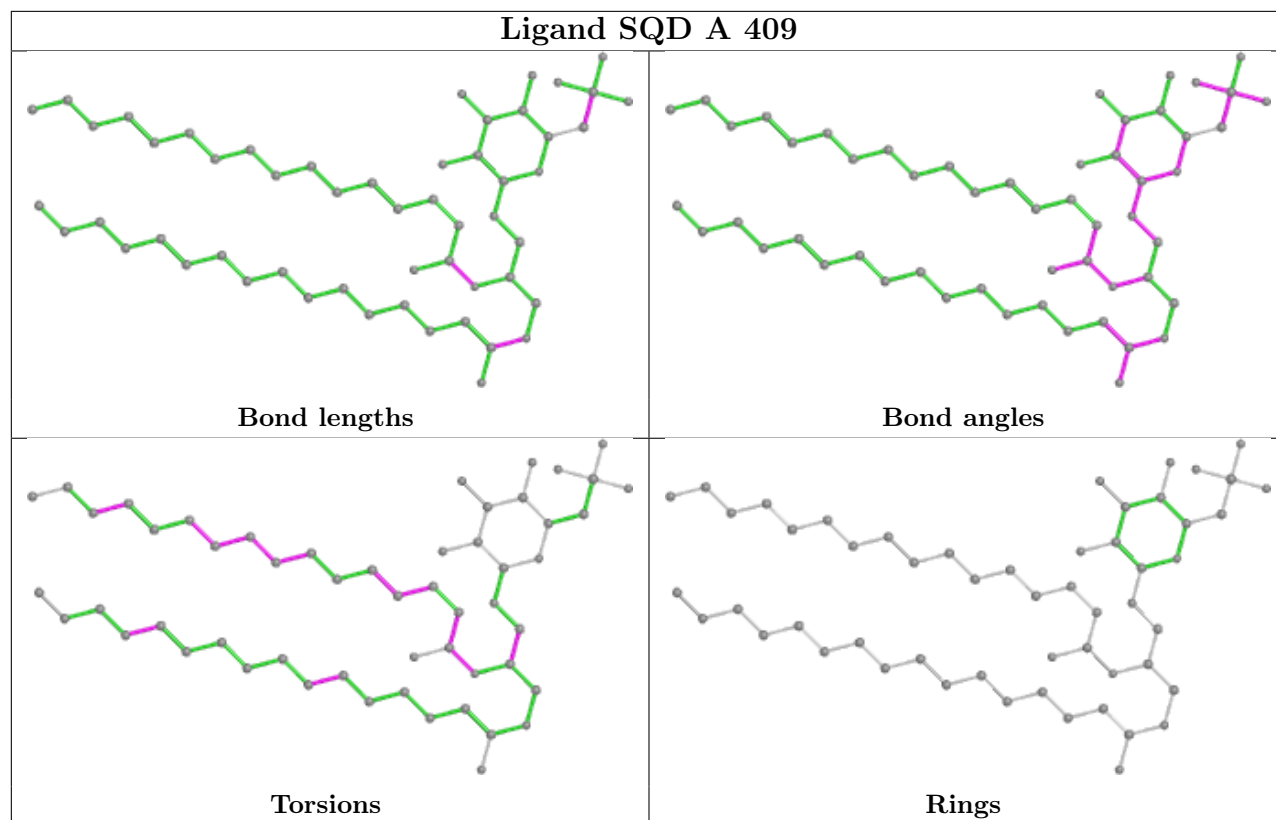


Ligand CLA A 405**Ligand LMG a 417****Ligand DGD C 518**

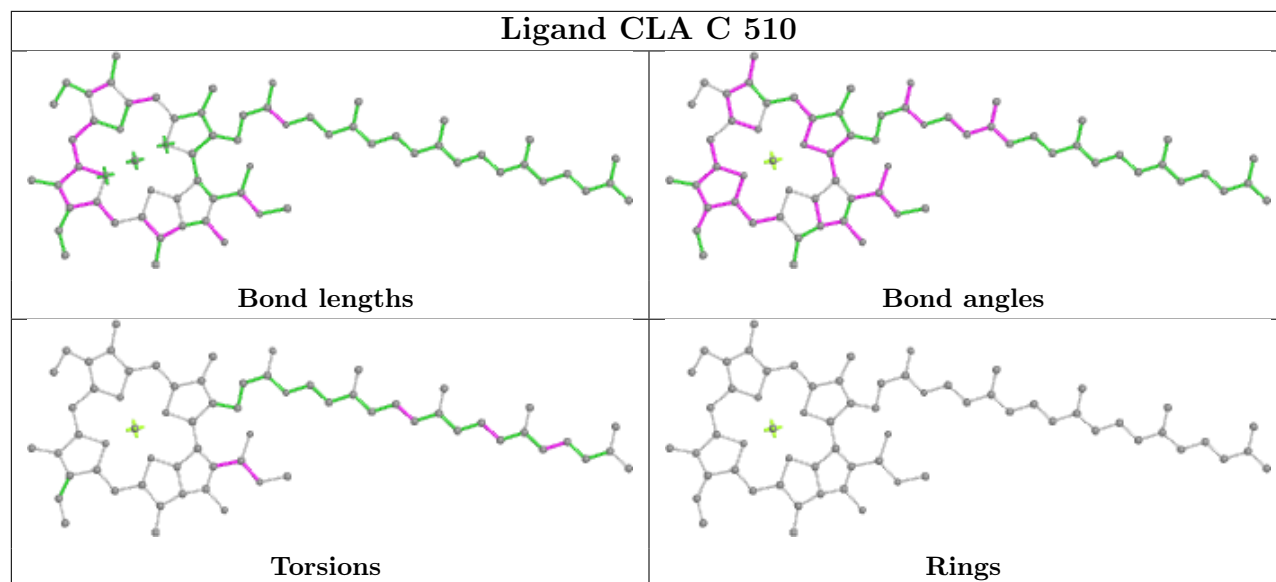




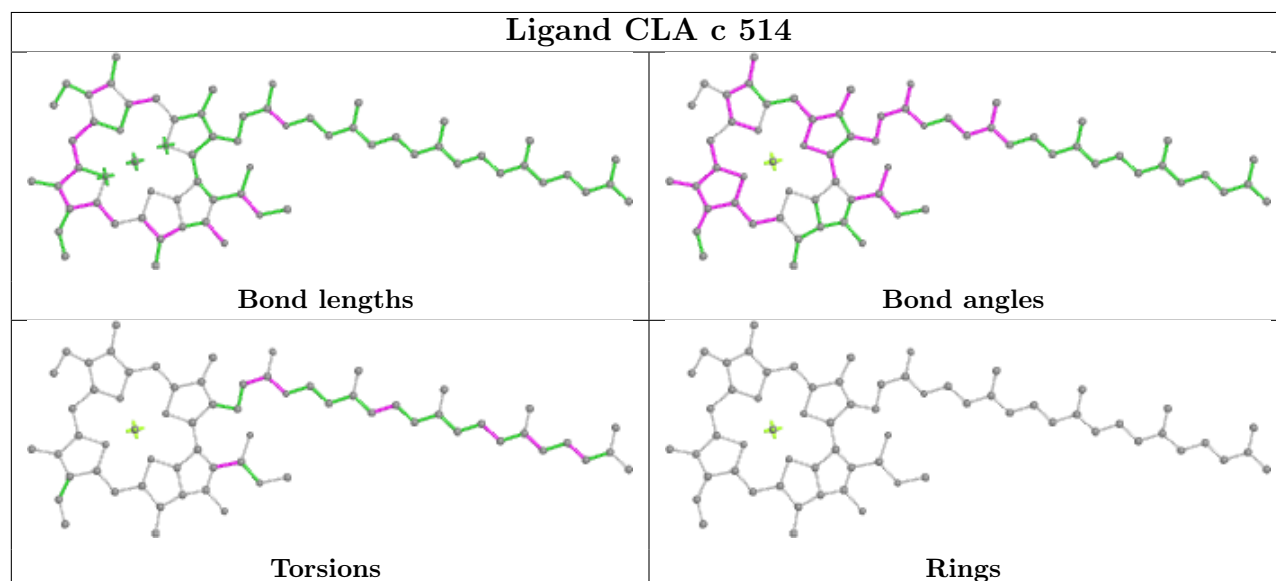




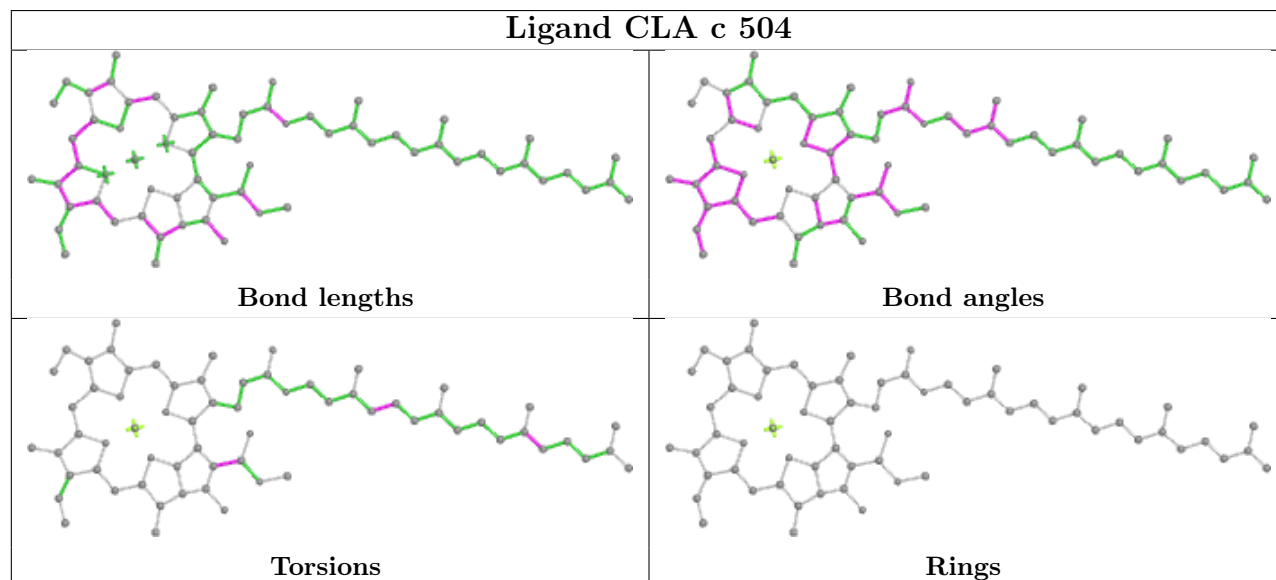
Ligand CLA C 510

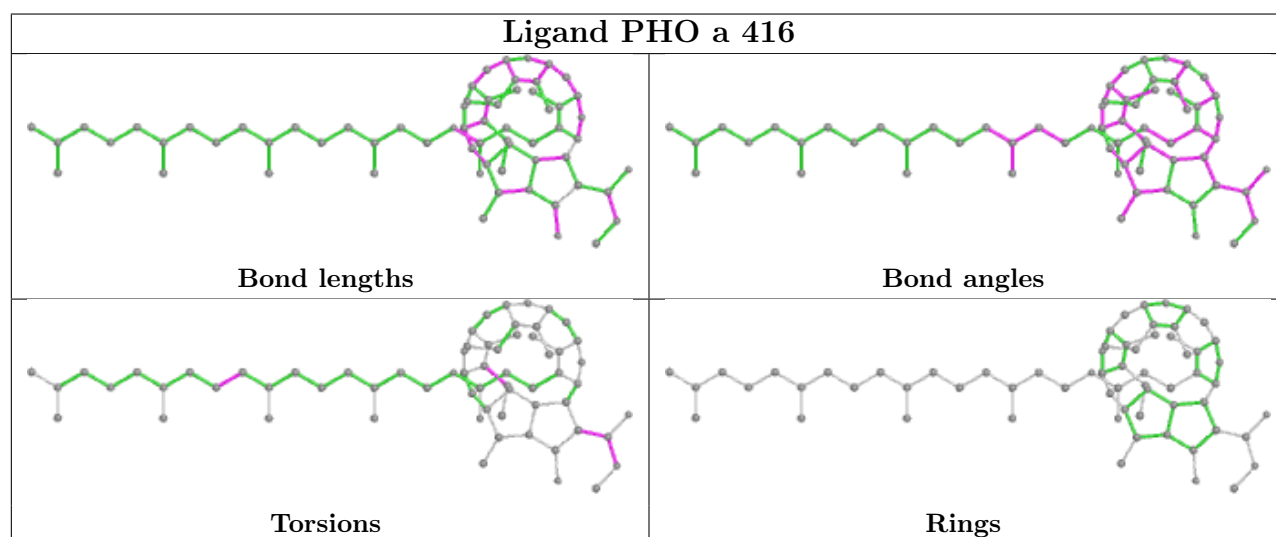
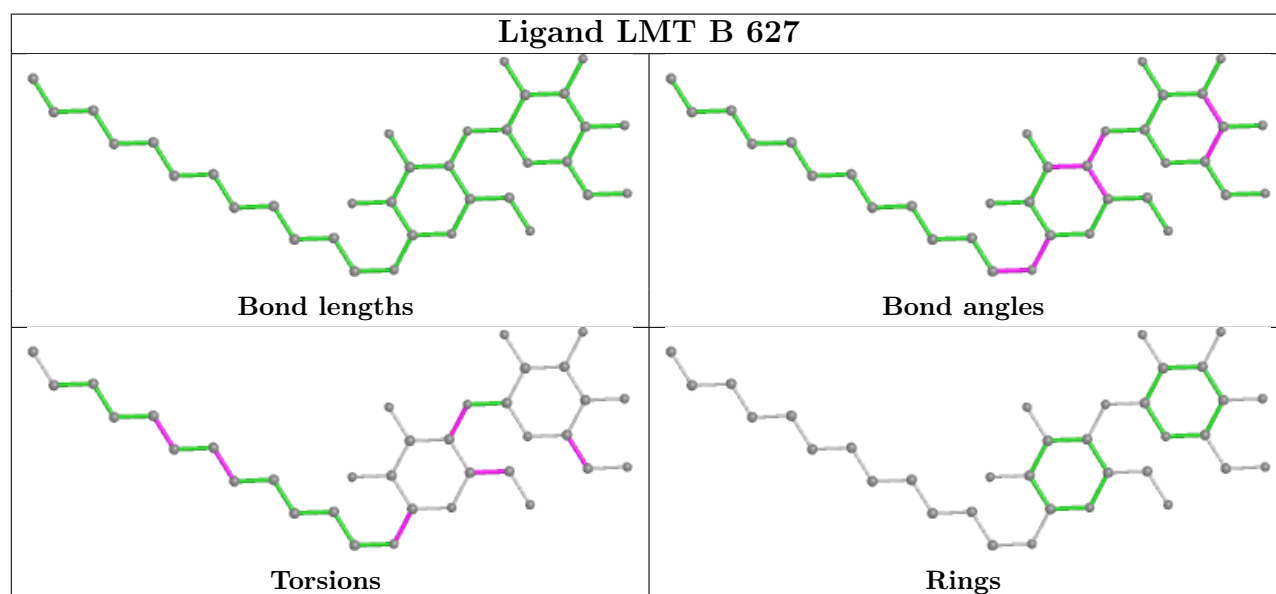
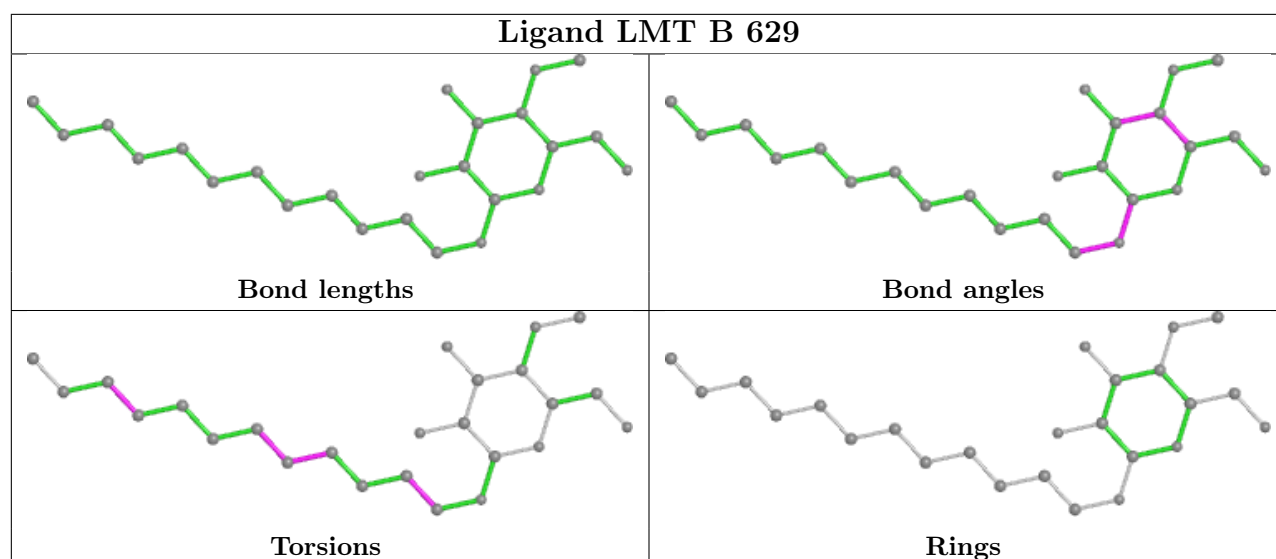


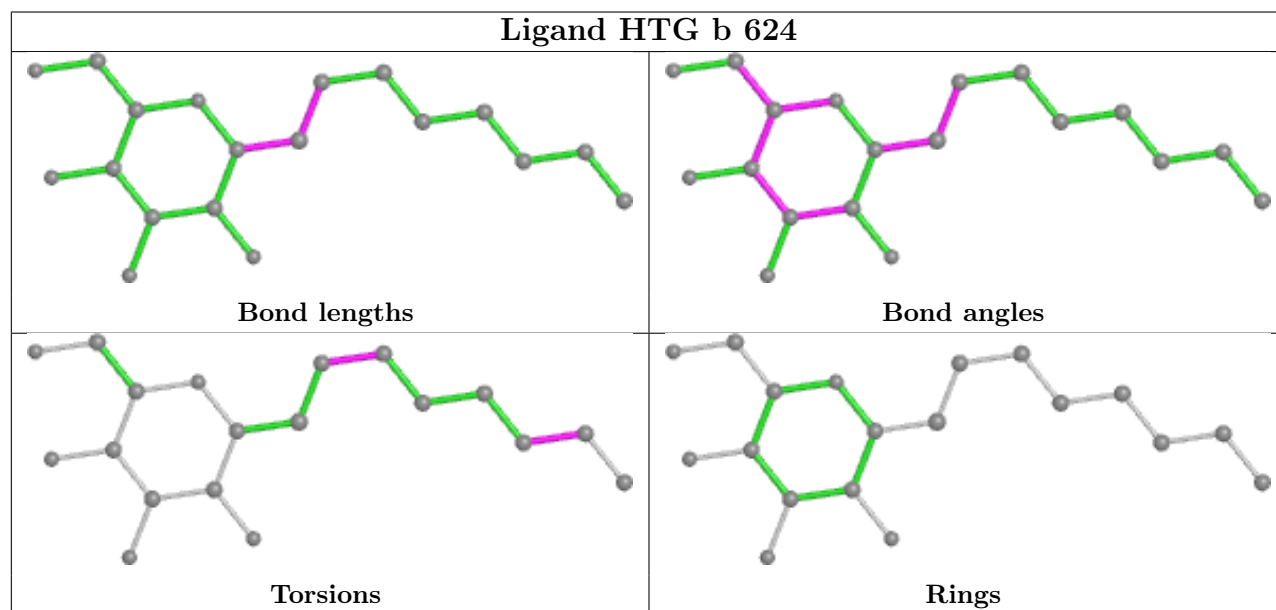
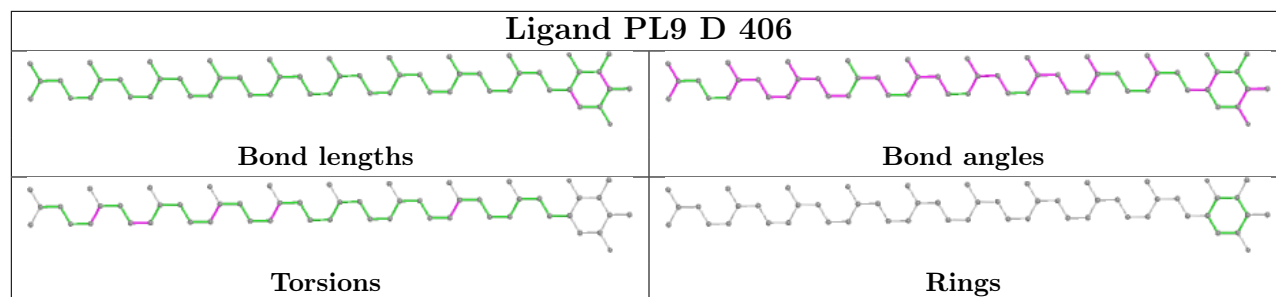
Ligand CLA c 514



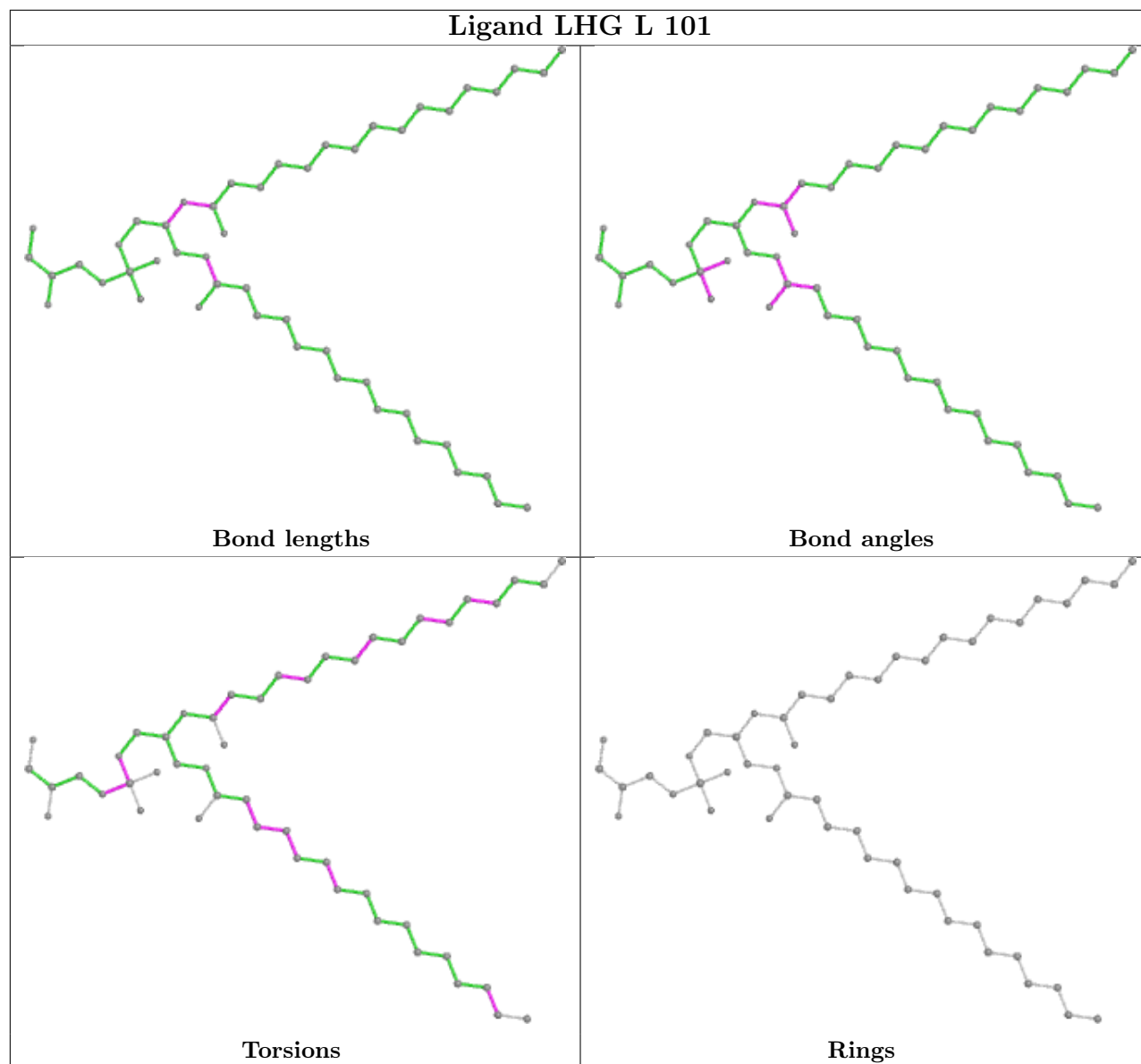
Ligand CLA c 504



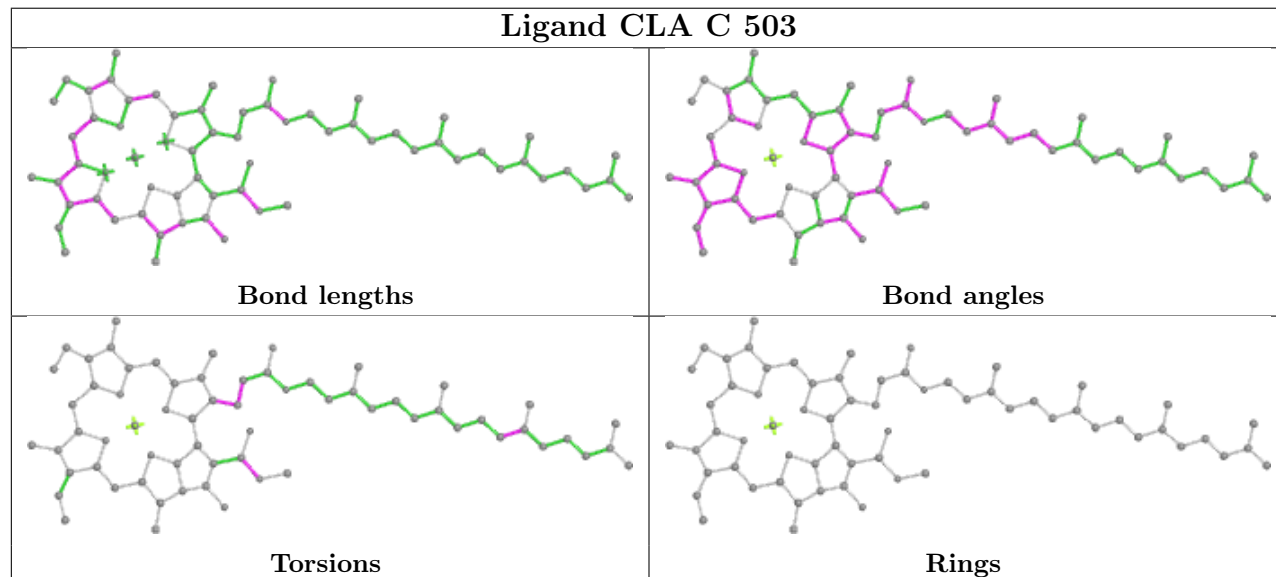


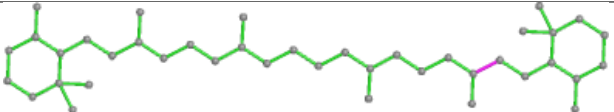
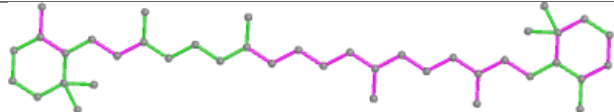
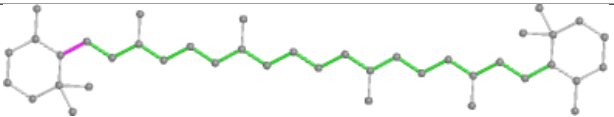
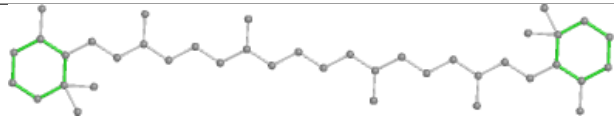


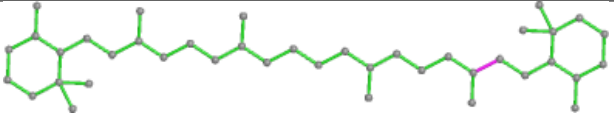
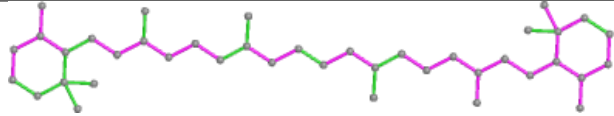
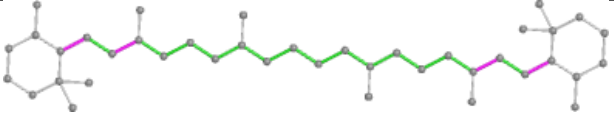
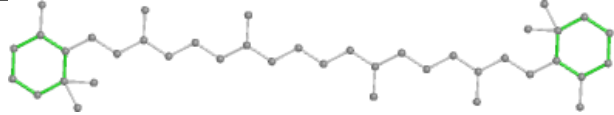
Ligand LHG L 101

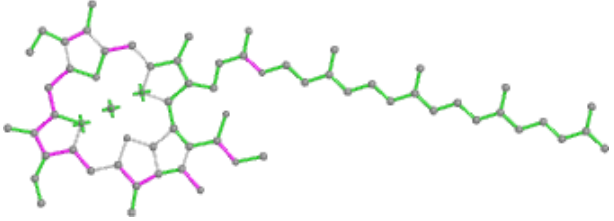
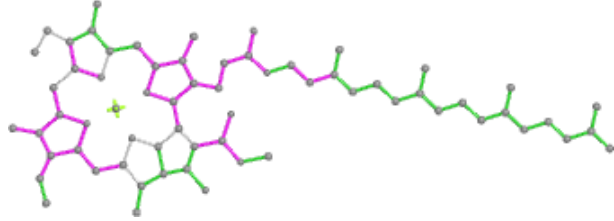
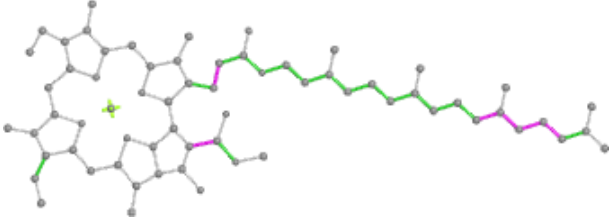
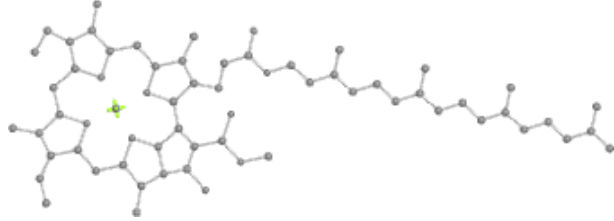


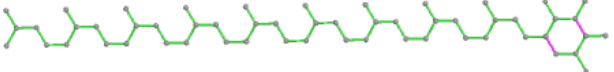
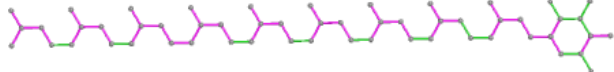
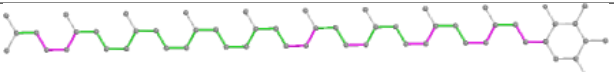
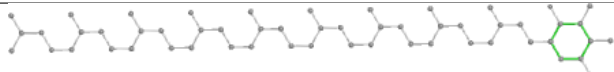
Ligand CLA C 503

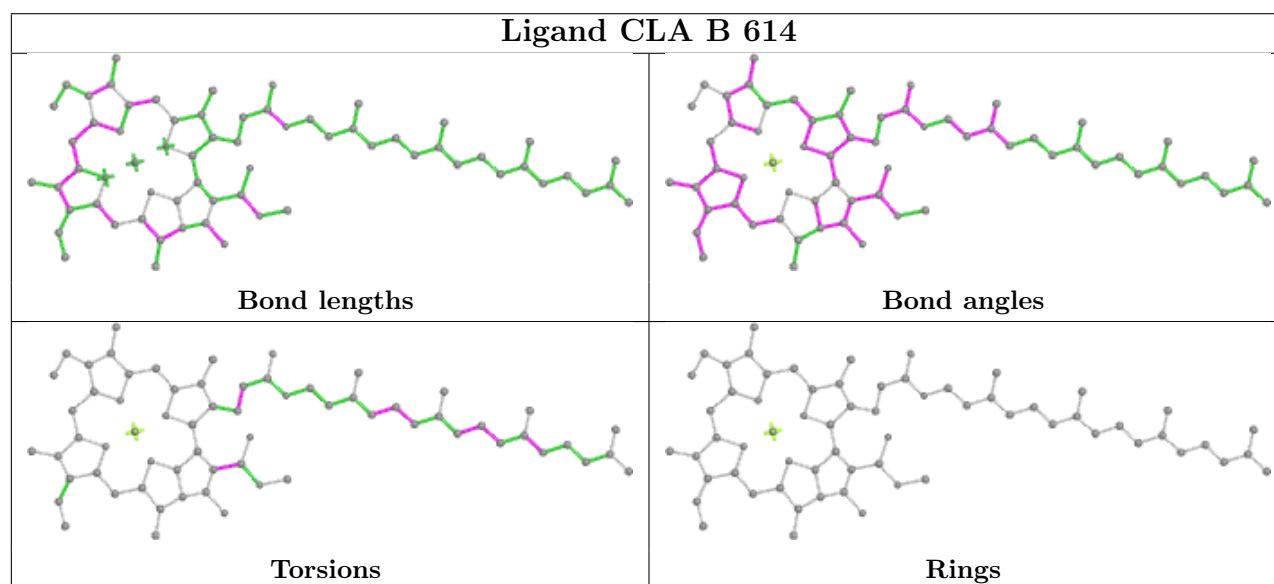
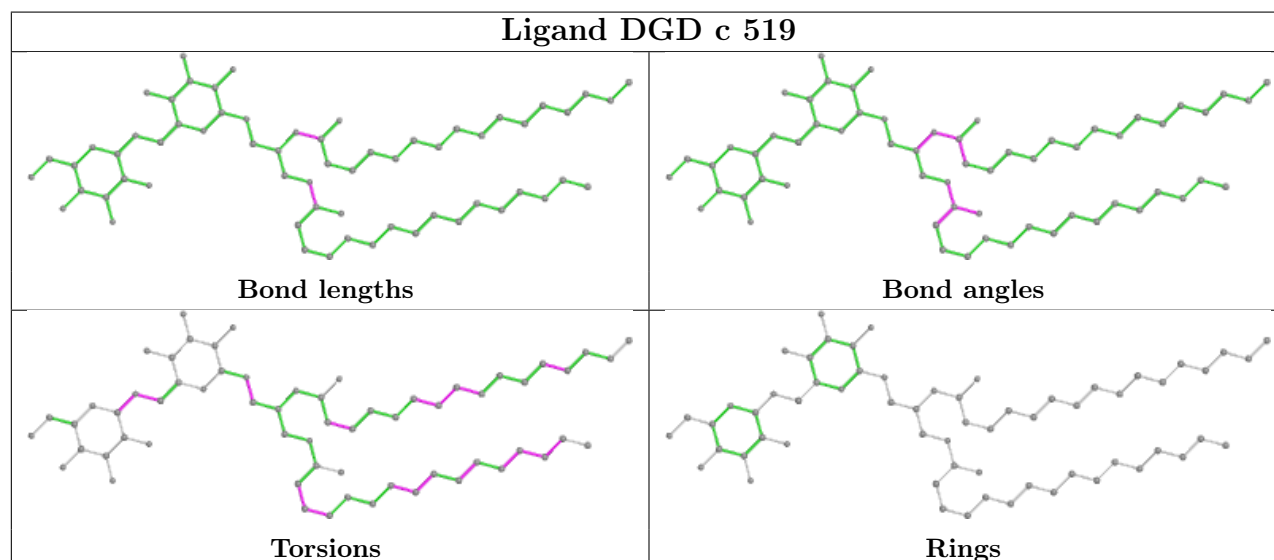
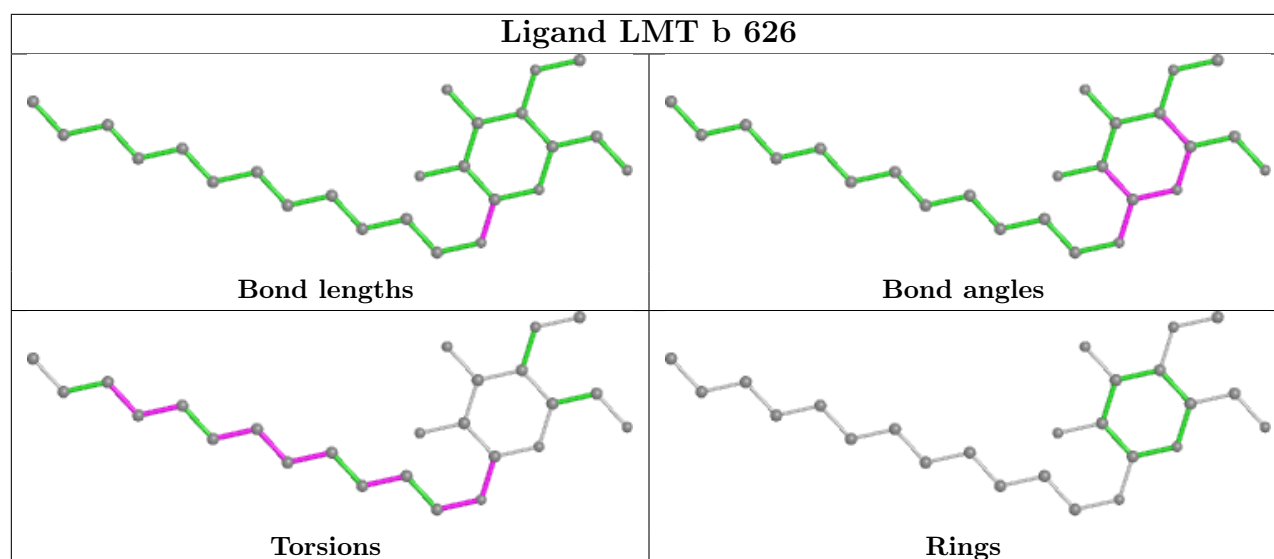


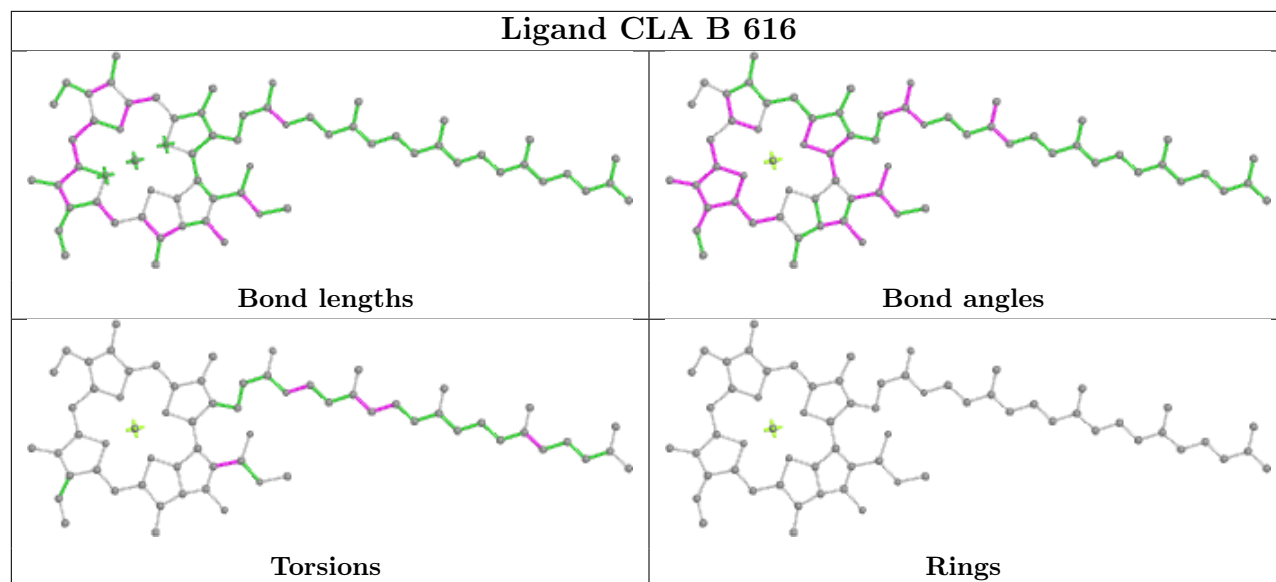
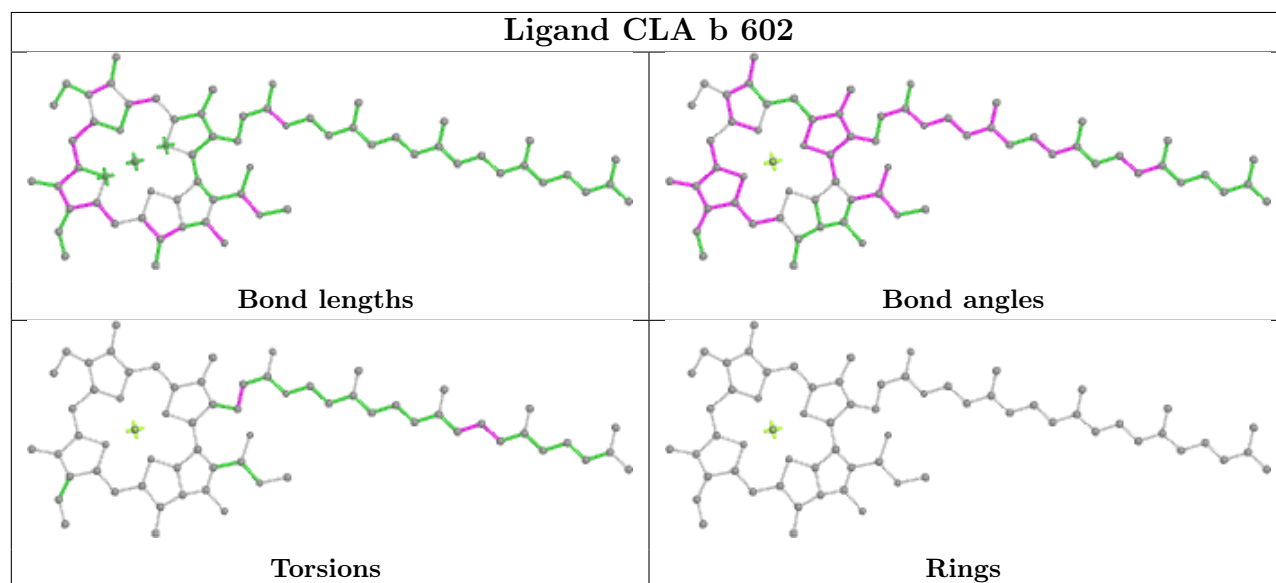
Ligand BCR c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

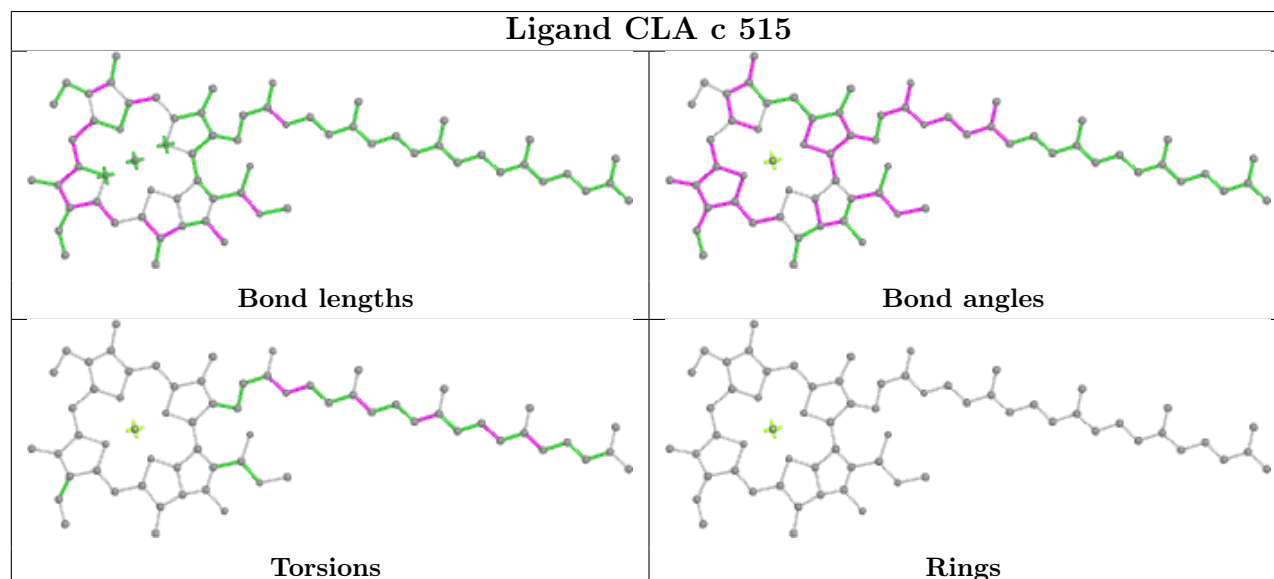
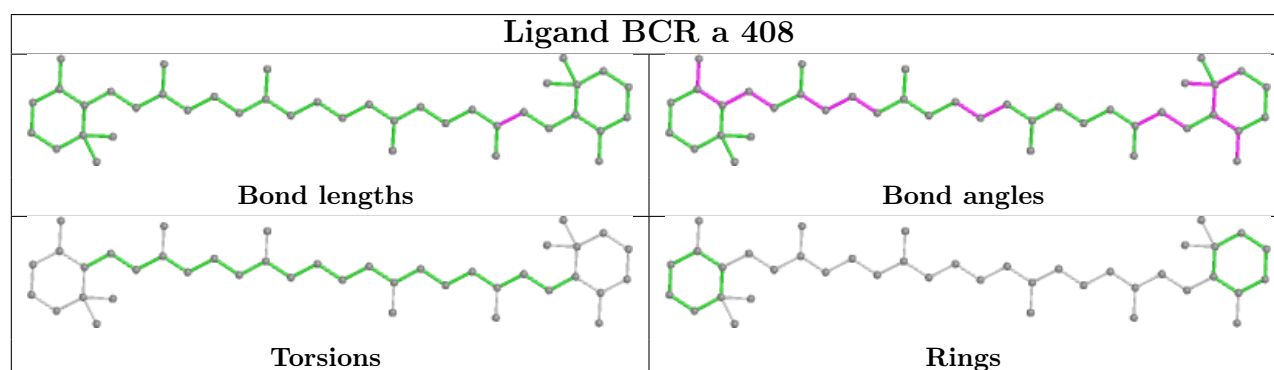
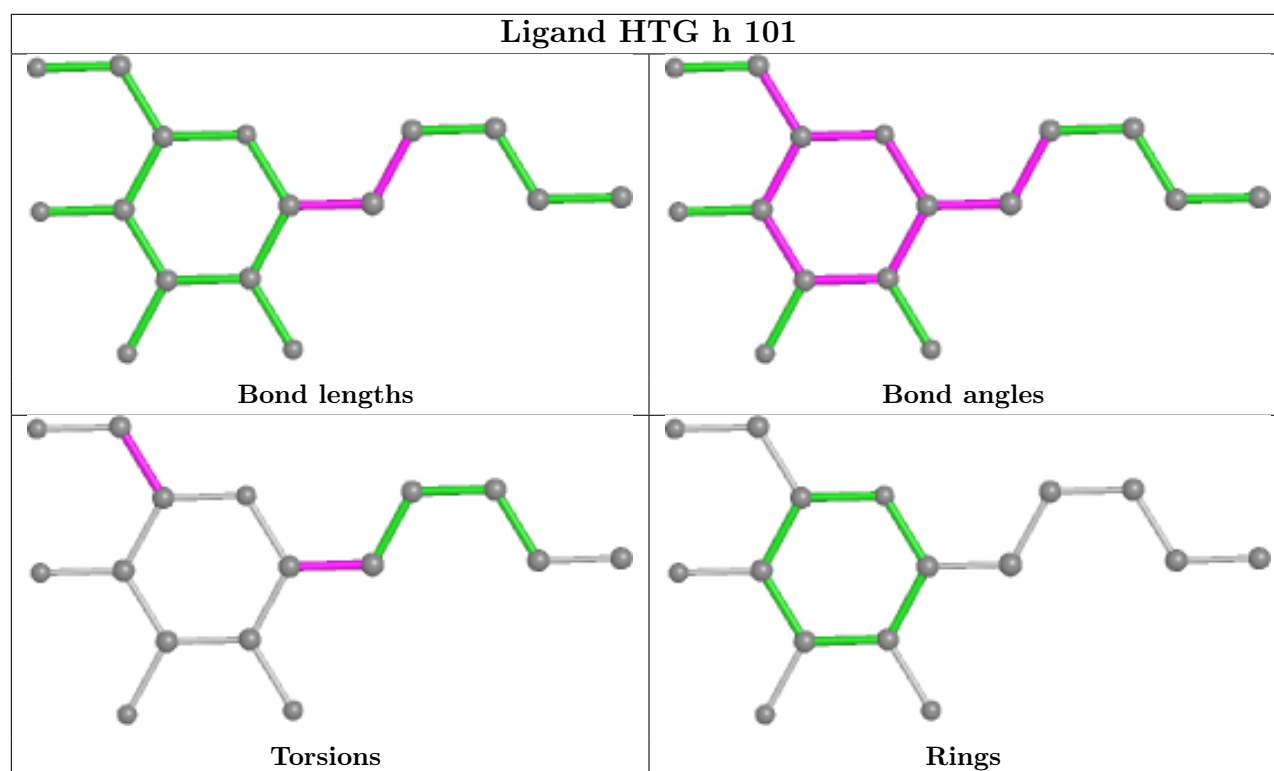
Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

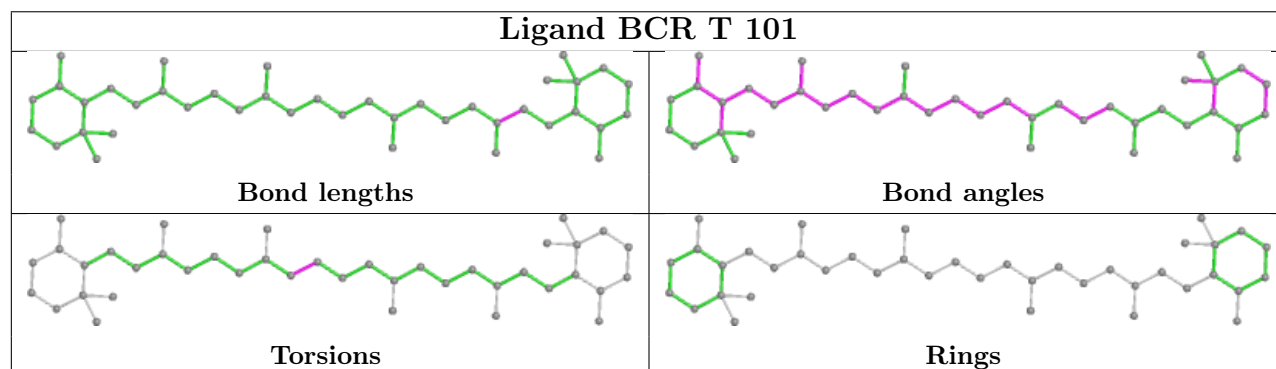
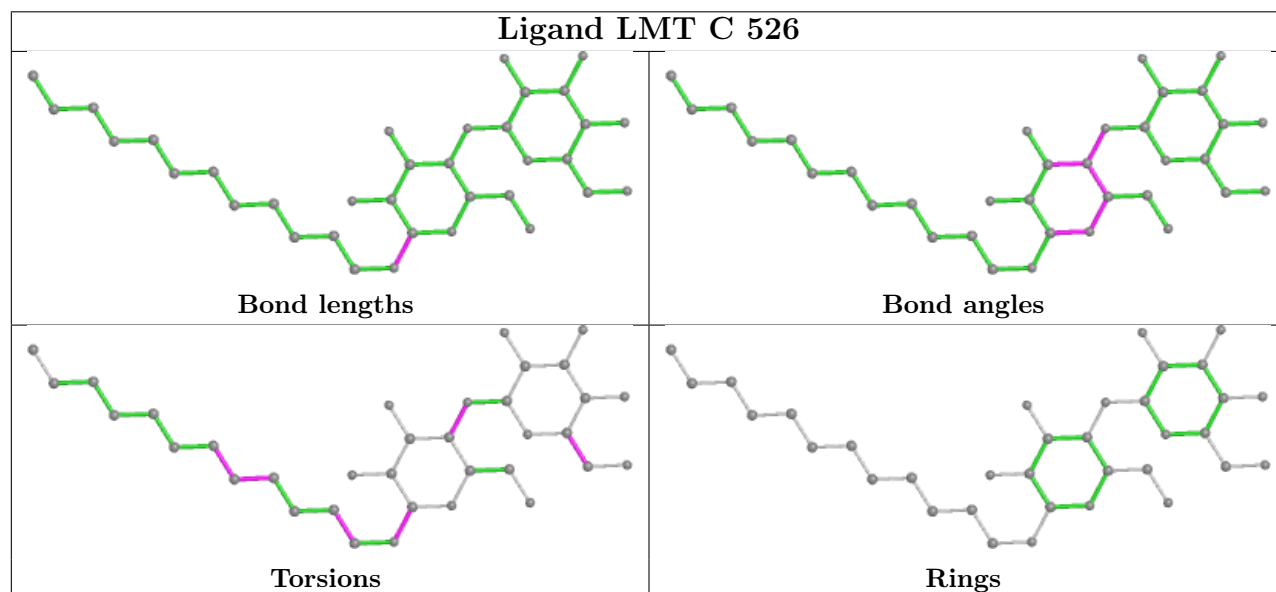
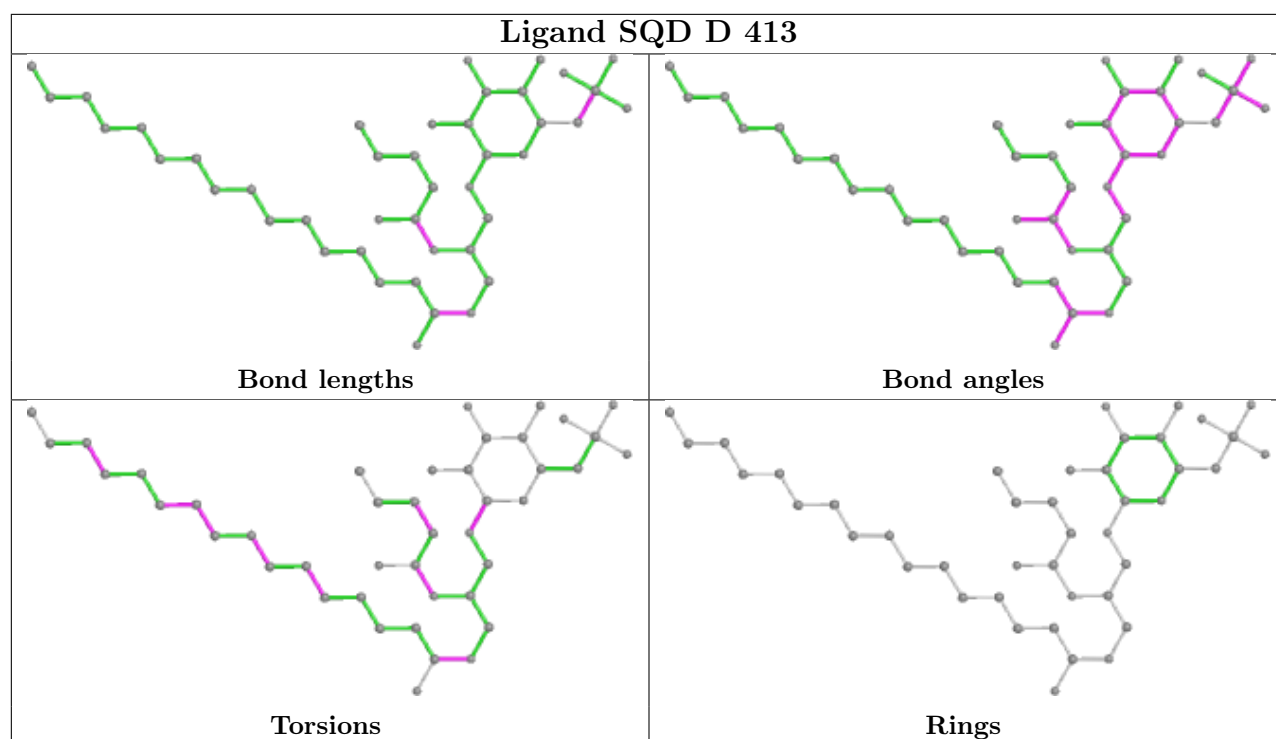
Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

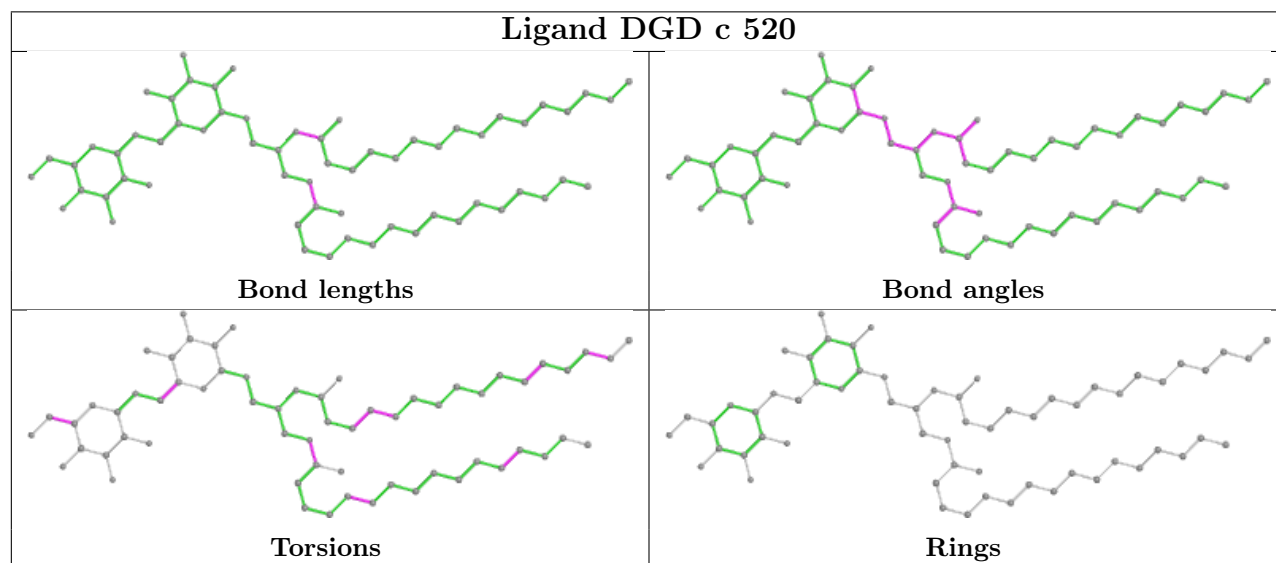
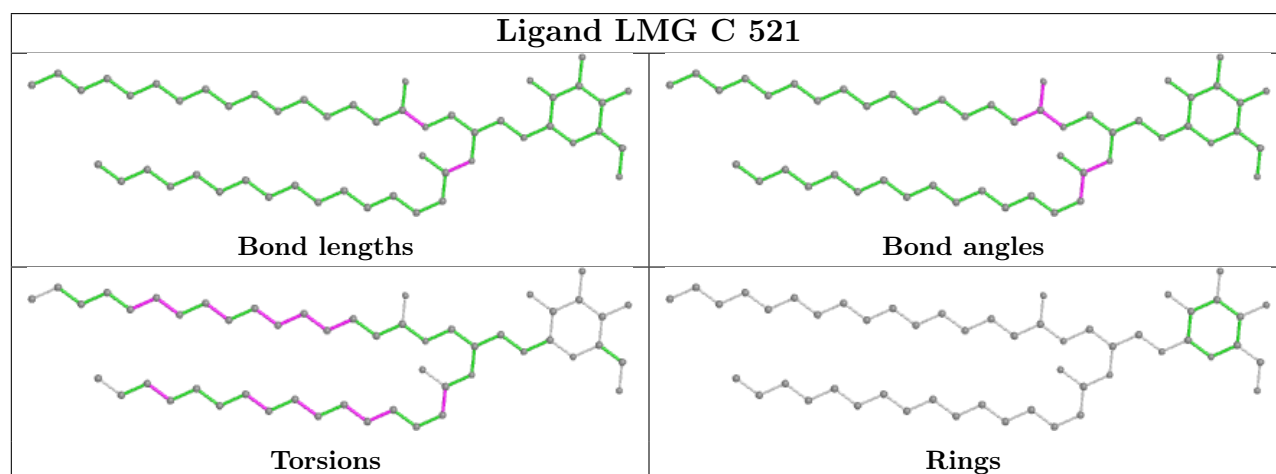
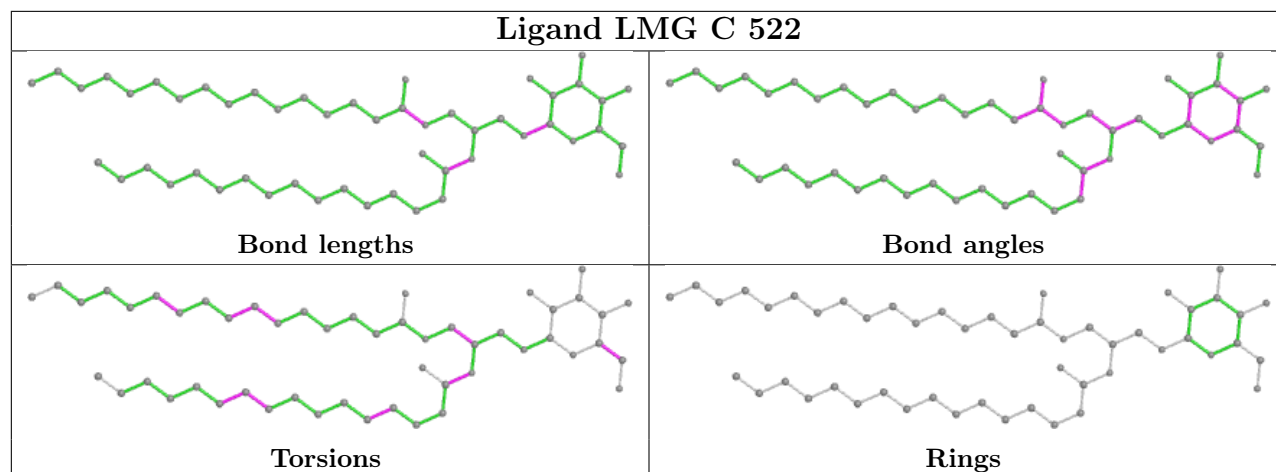
Ligand PL9 A 413 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings



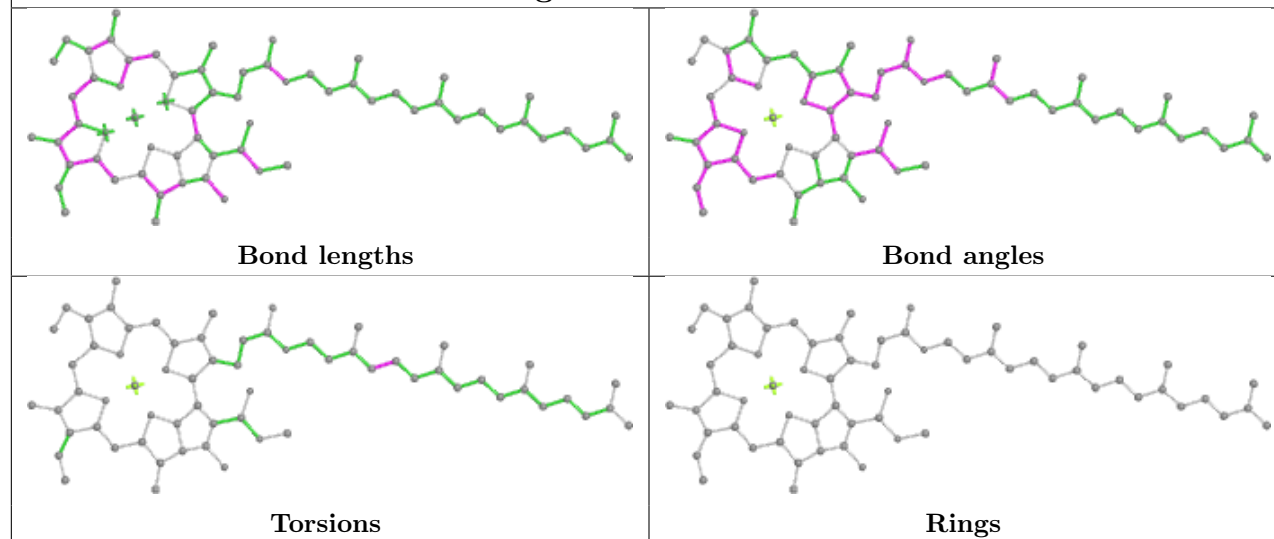
Ligand CLA B 616**Ligand CLA b 602**



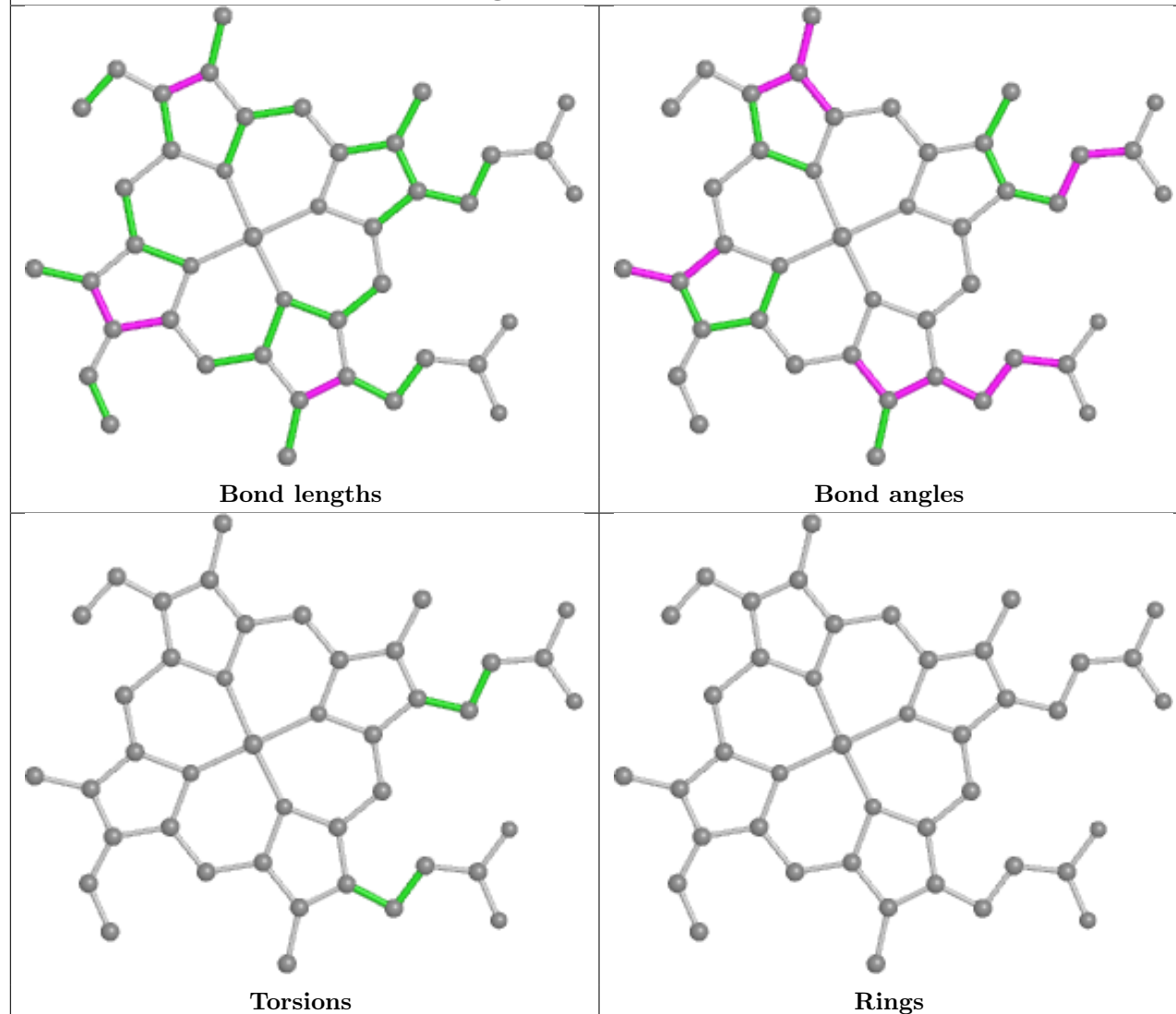


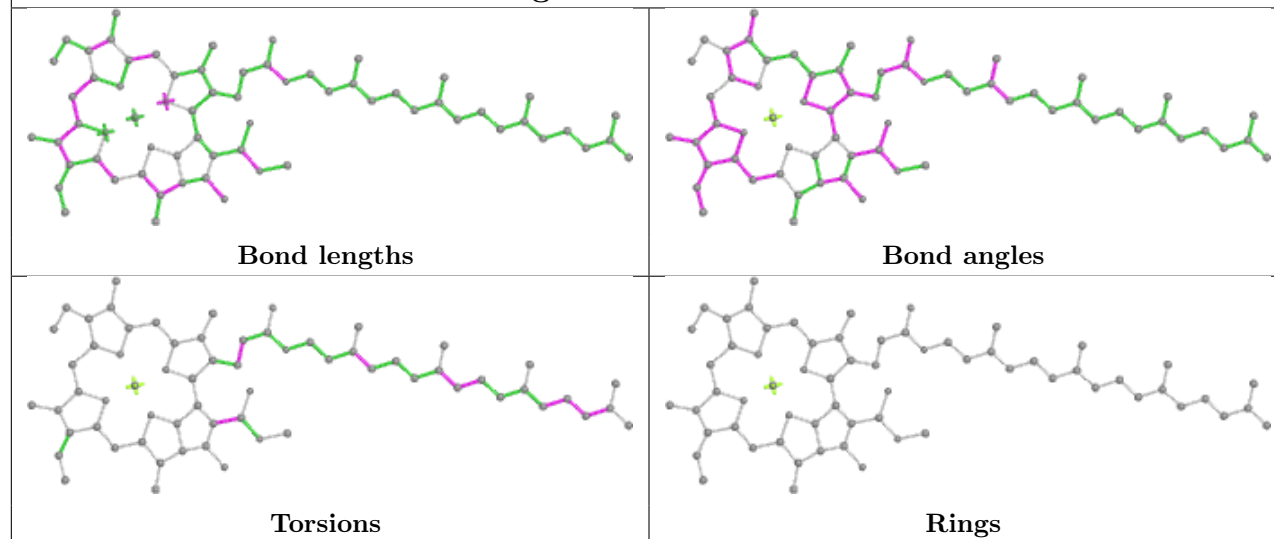
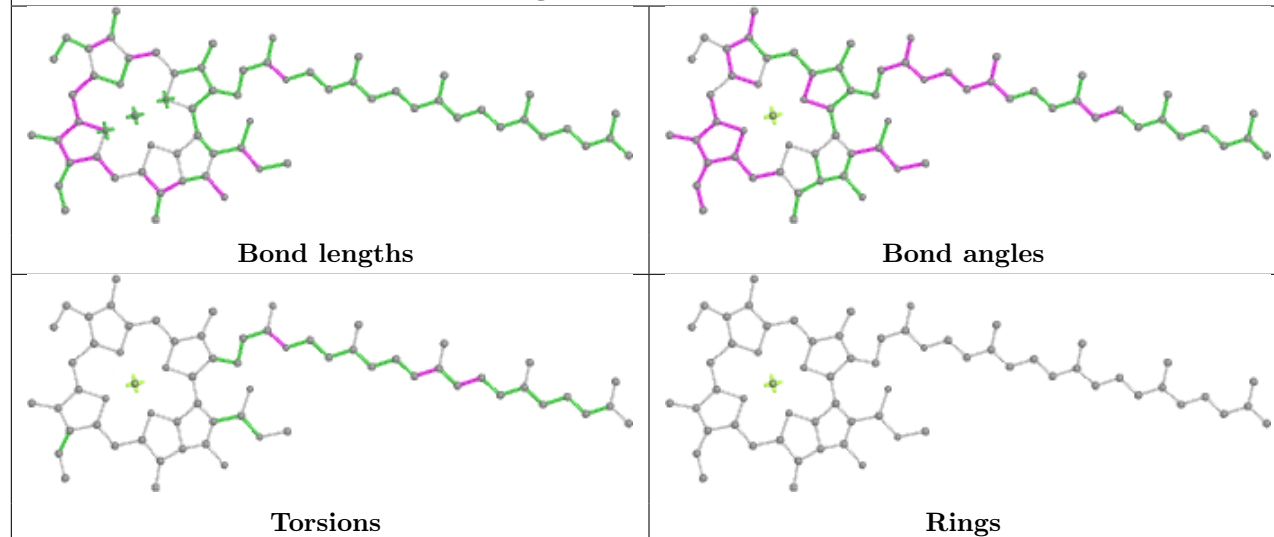
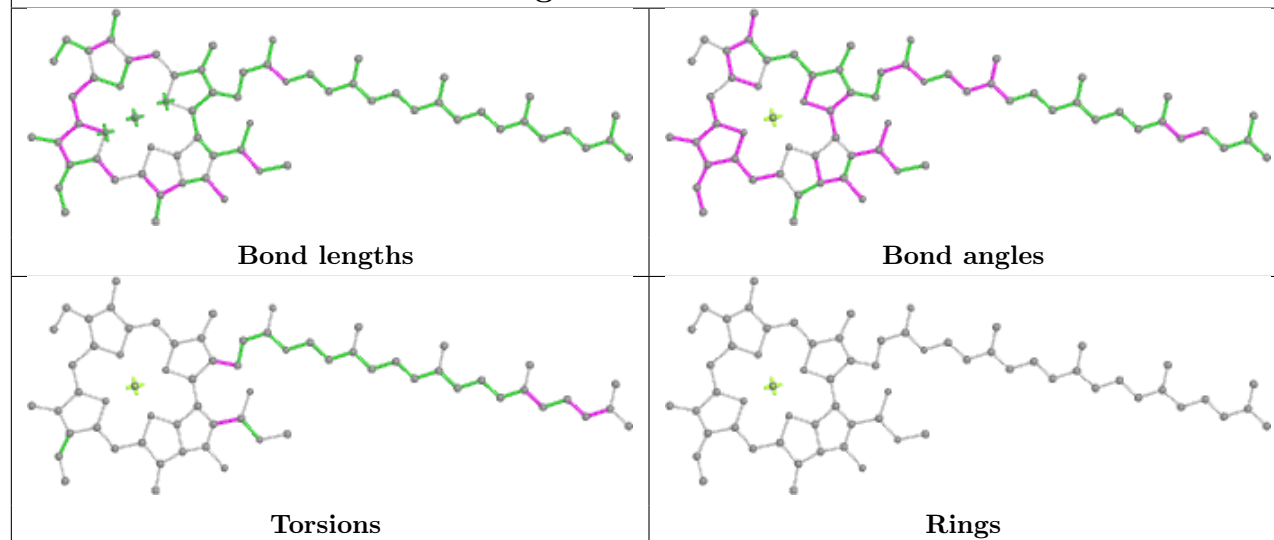


Ligand CLA b 607

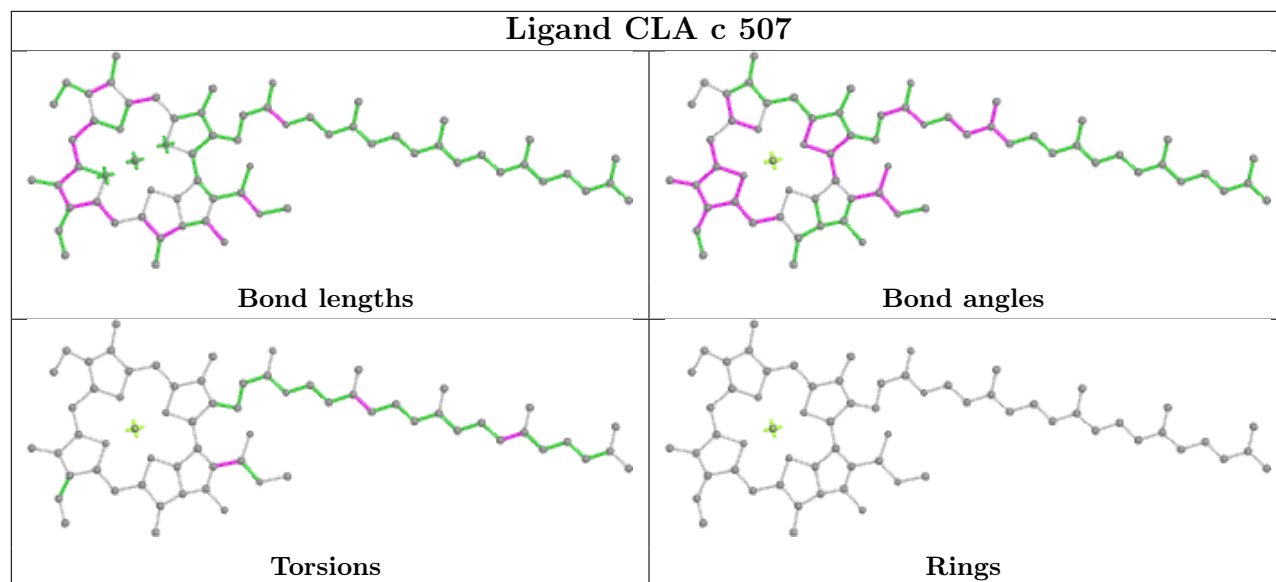


Ligand HEC V 201

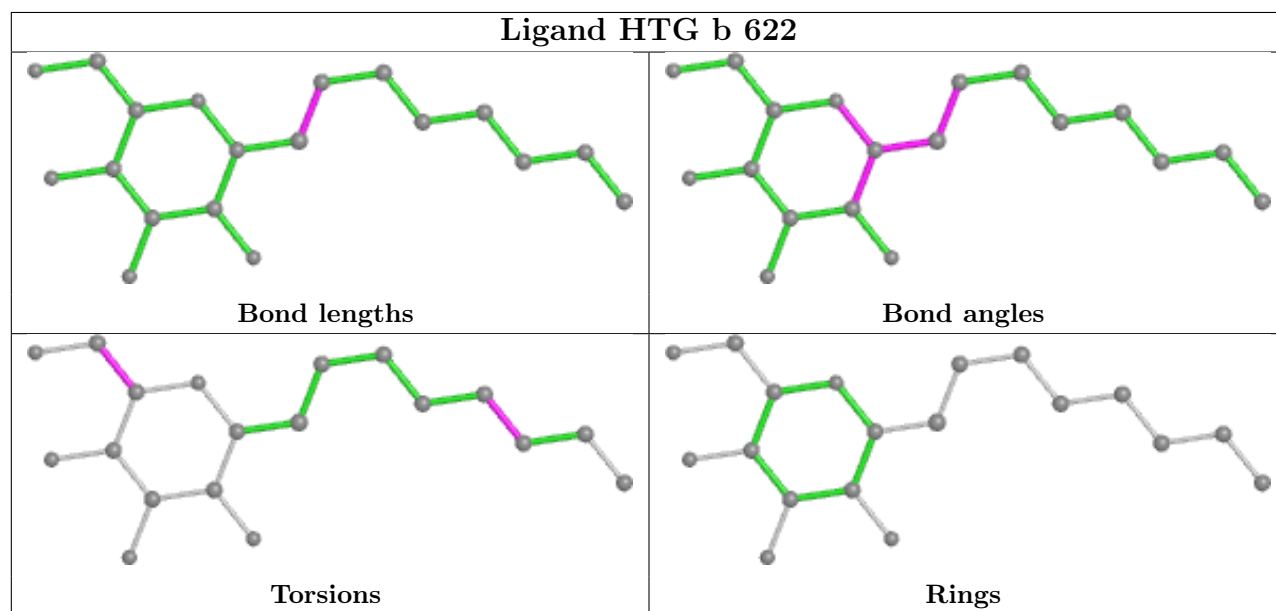


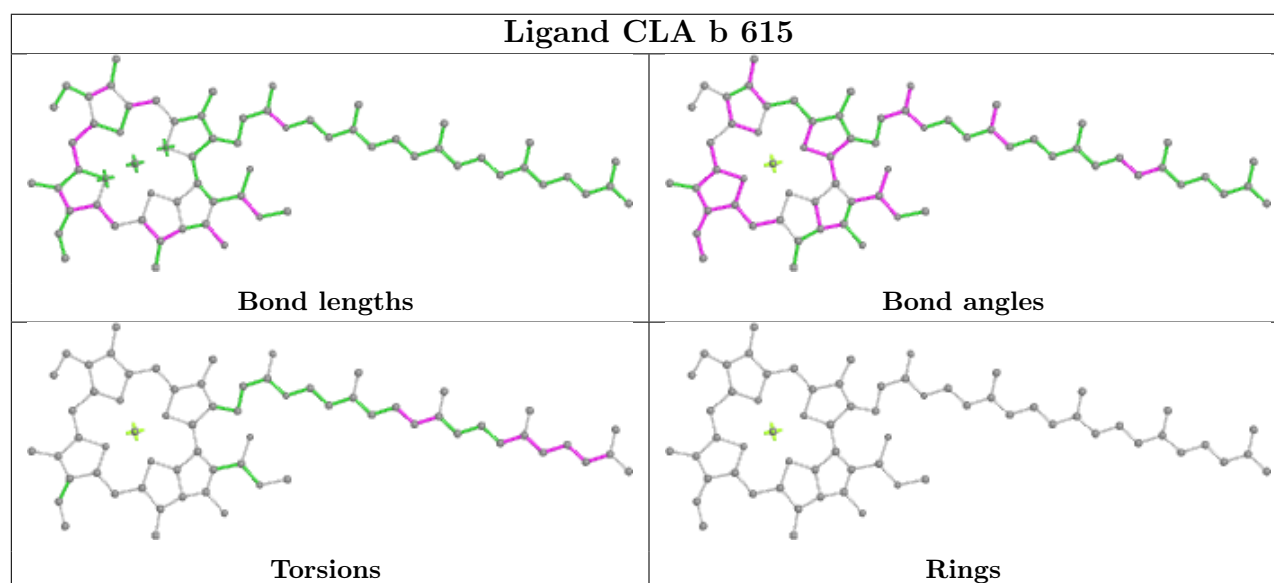
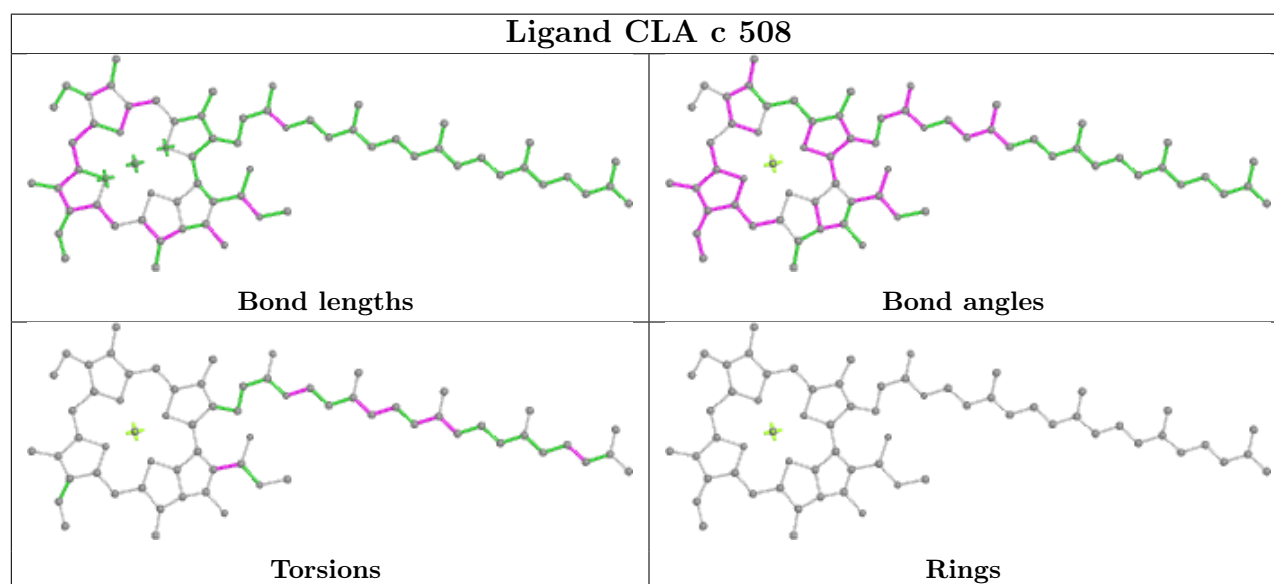
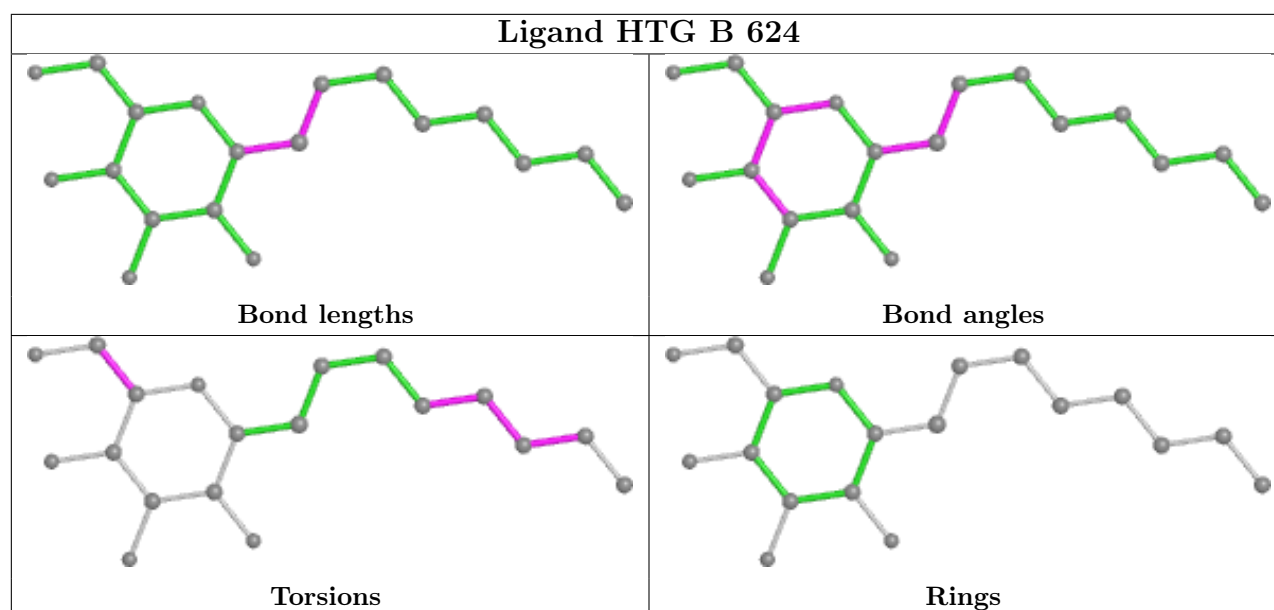
Ligand CLA B 606**Ligand CLA C 513****Ligand CLA b 609**

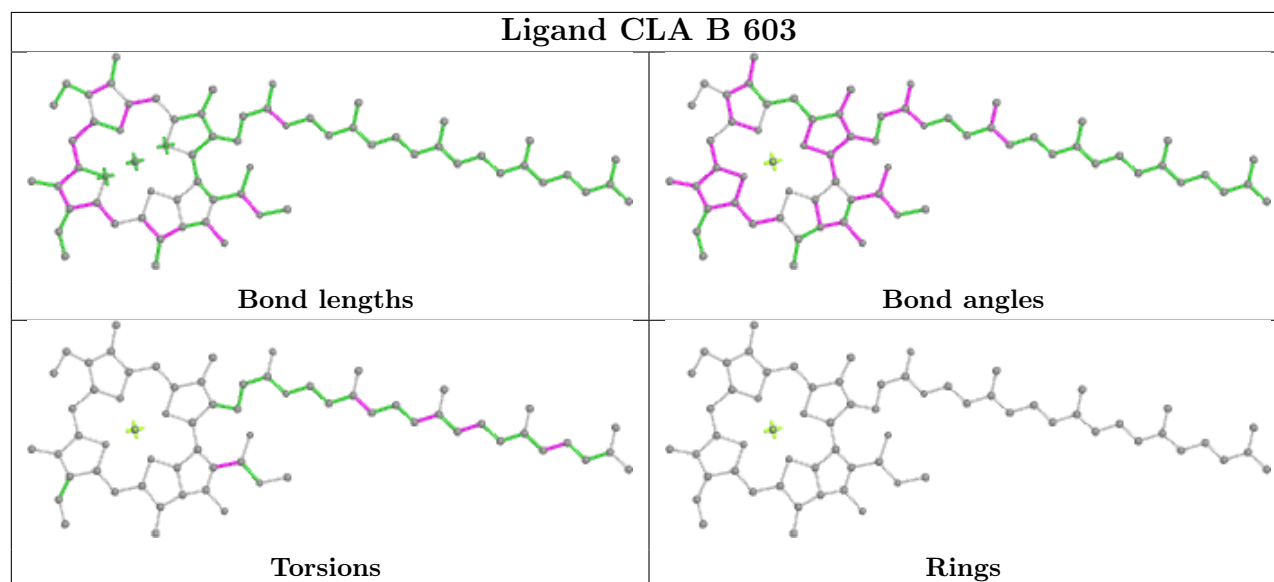
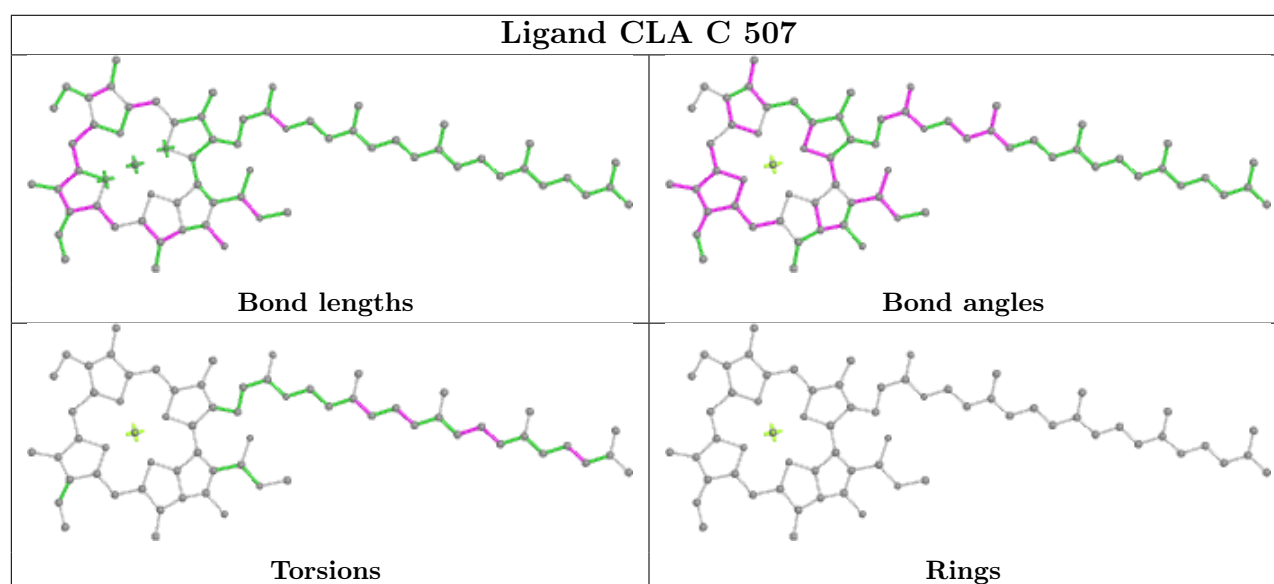
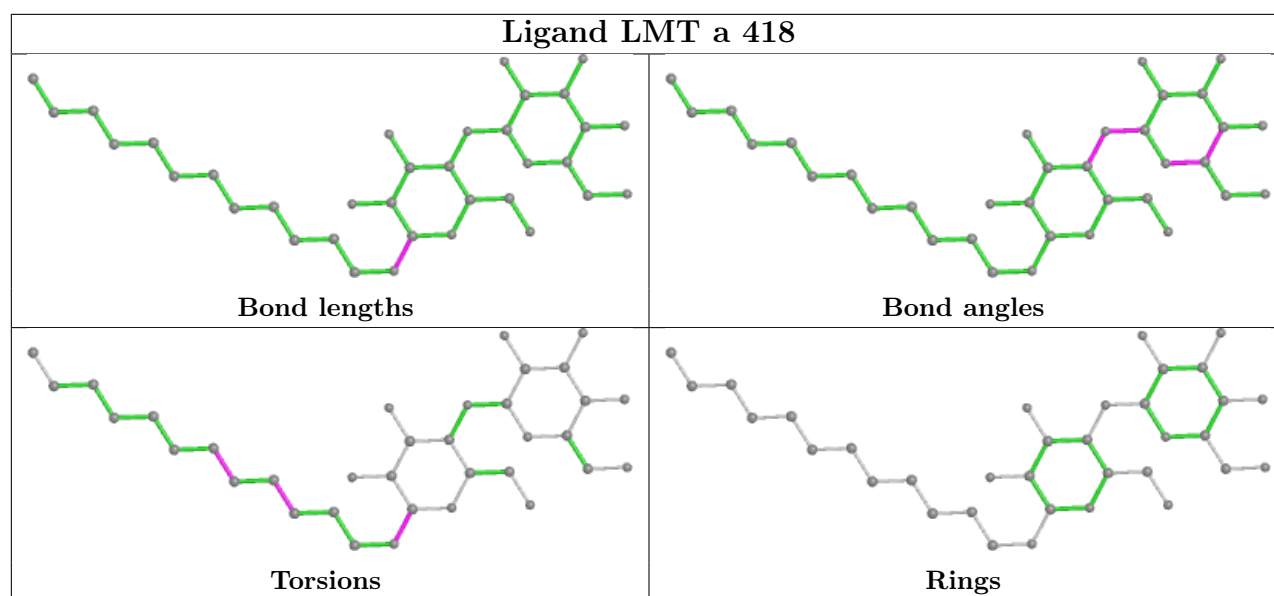
Ligand CLA c 507

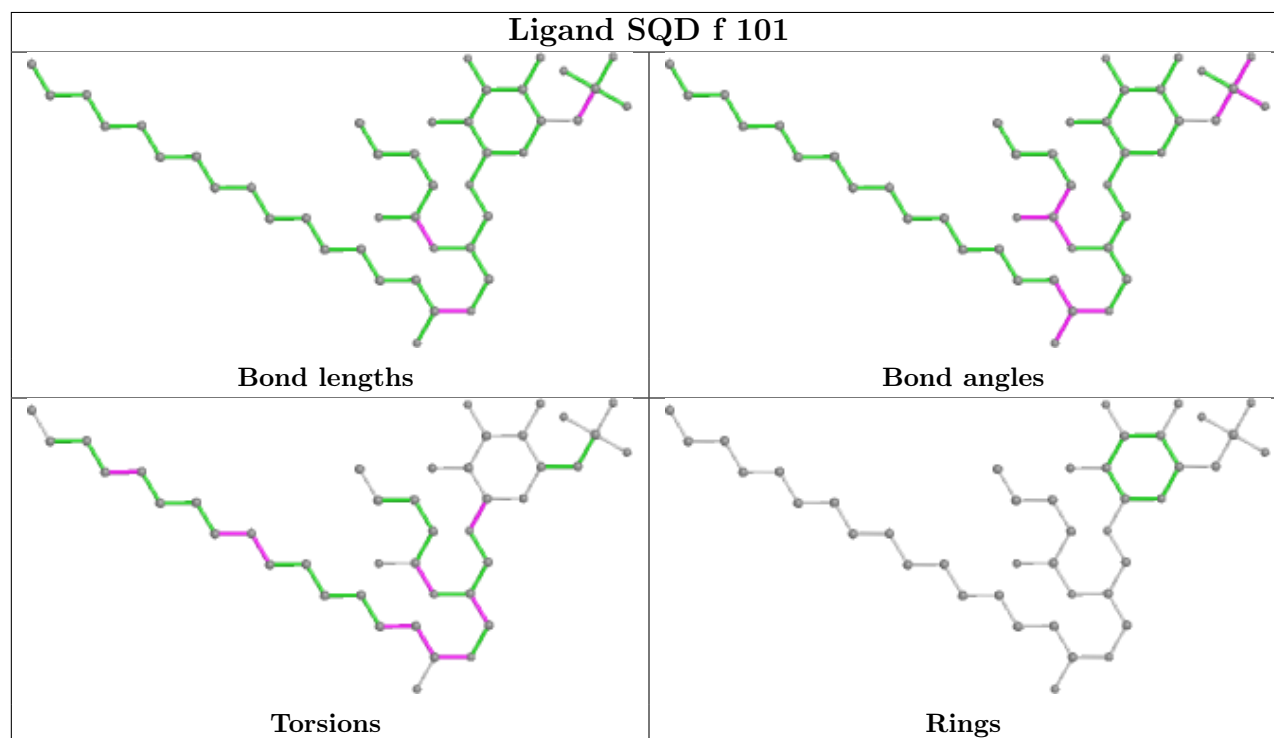
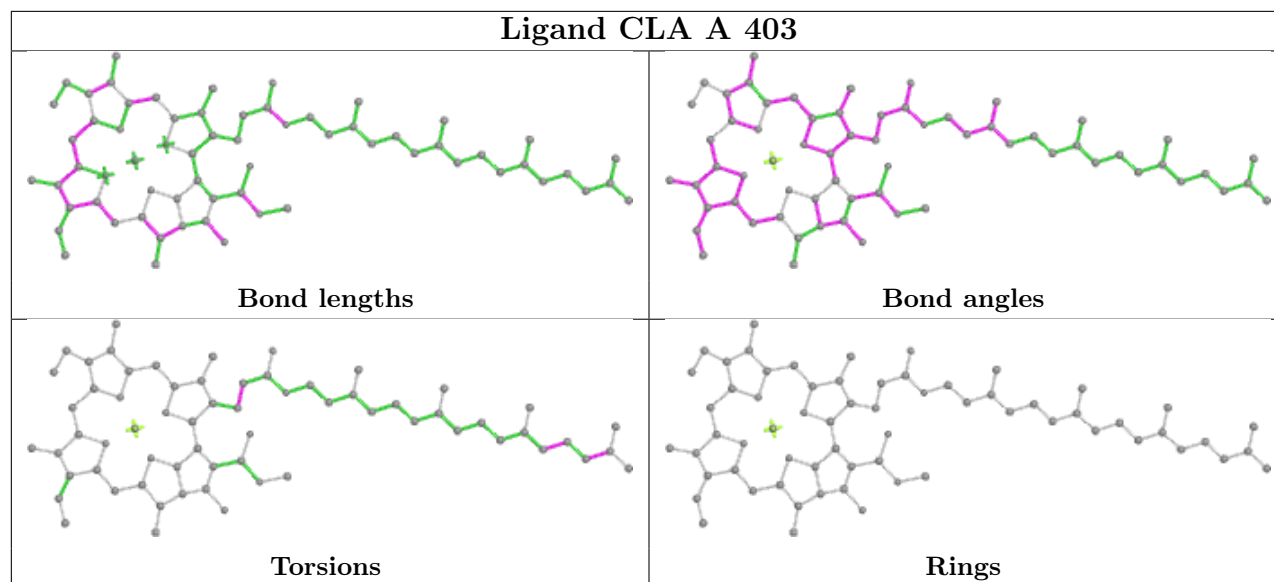


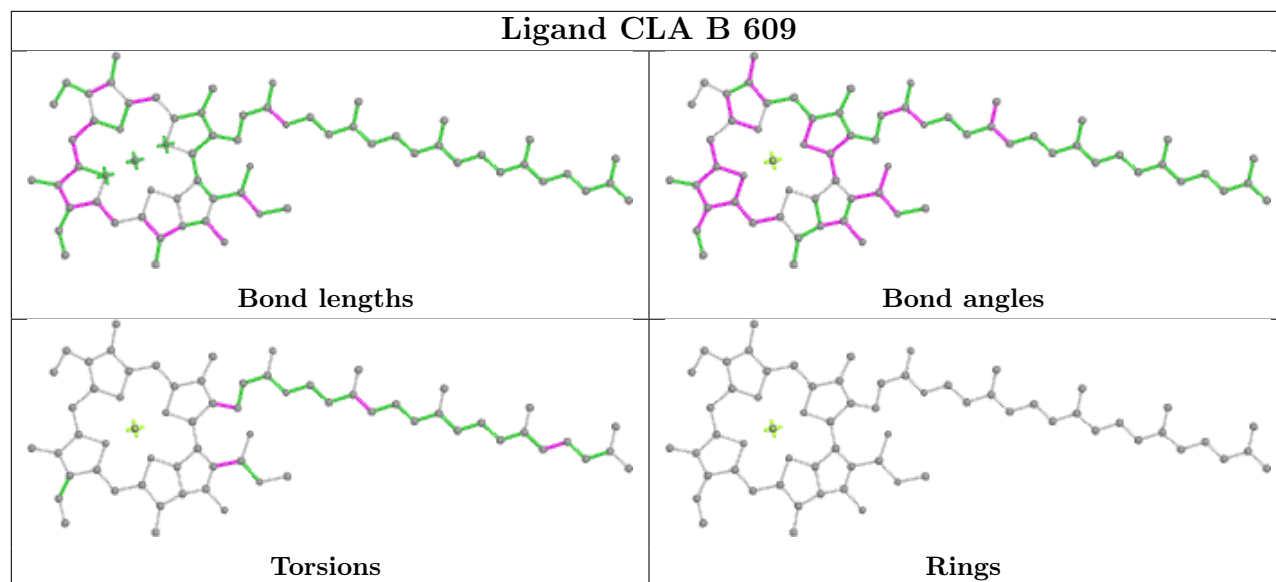
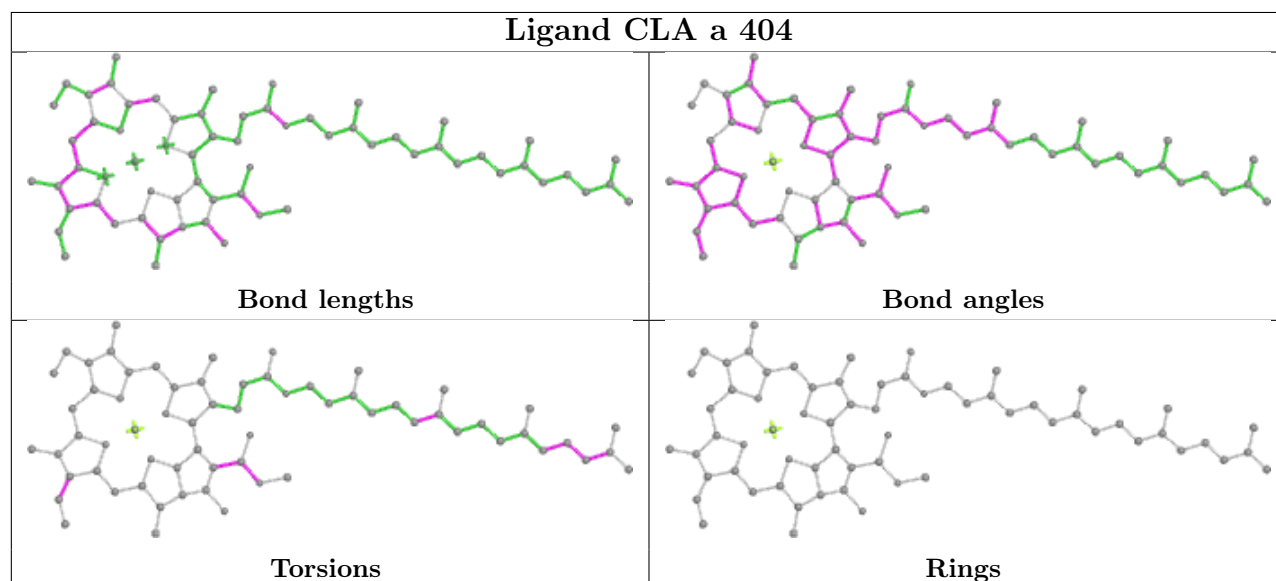
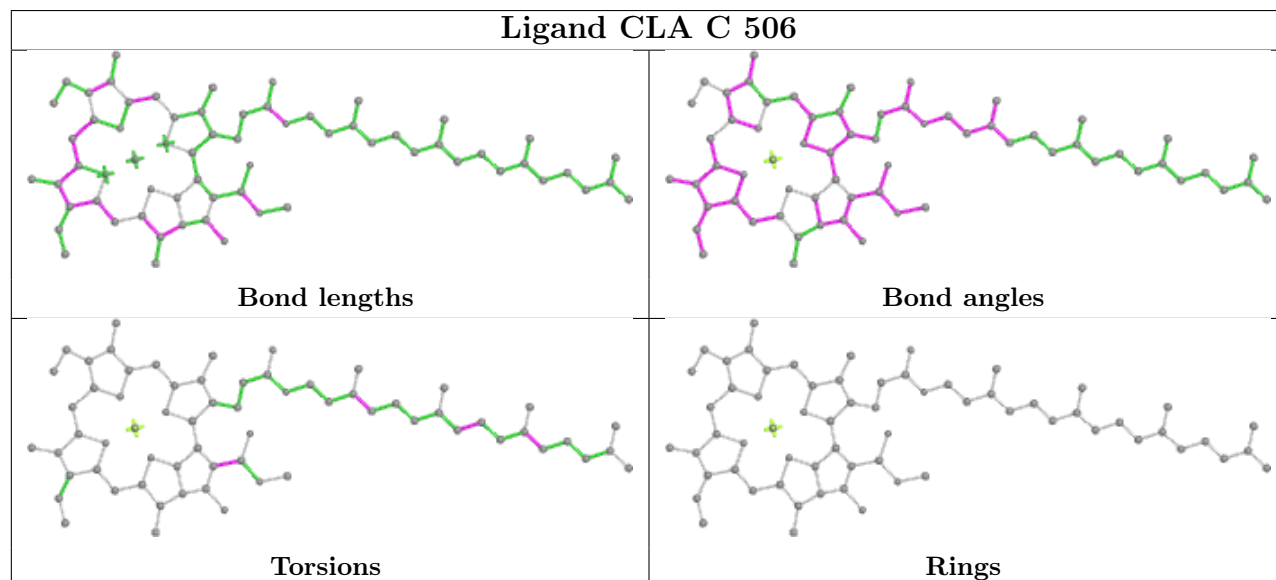
Ligand HTG b 622

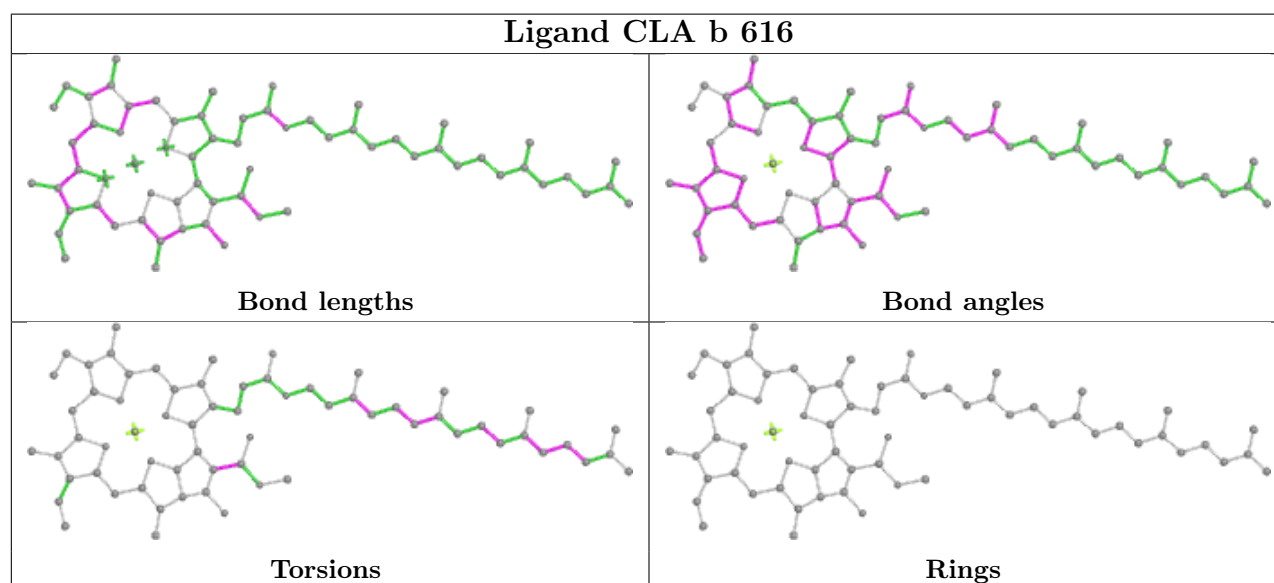
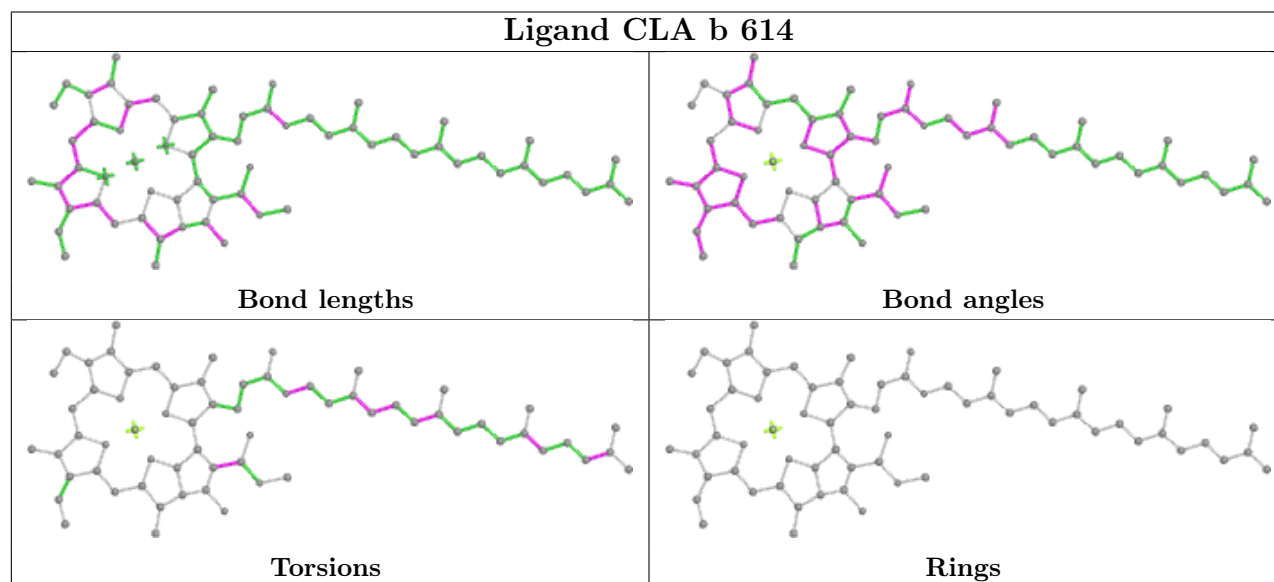
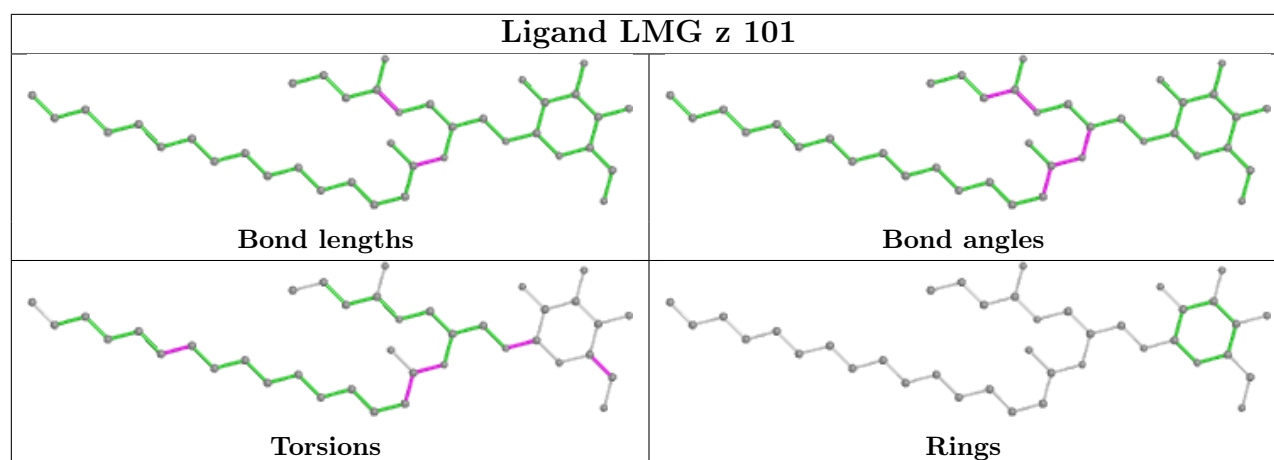


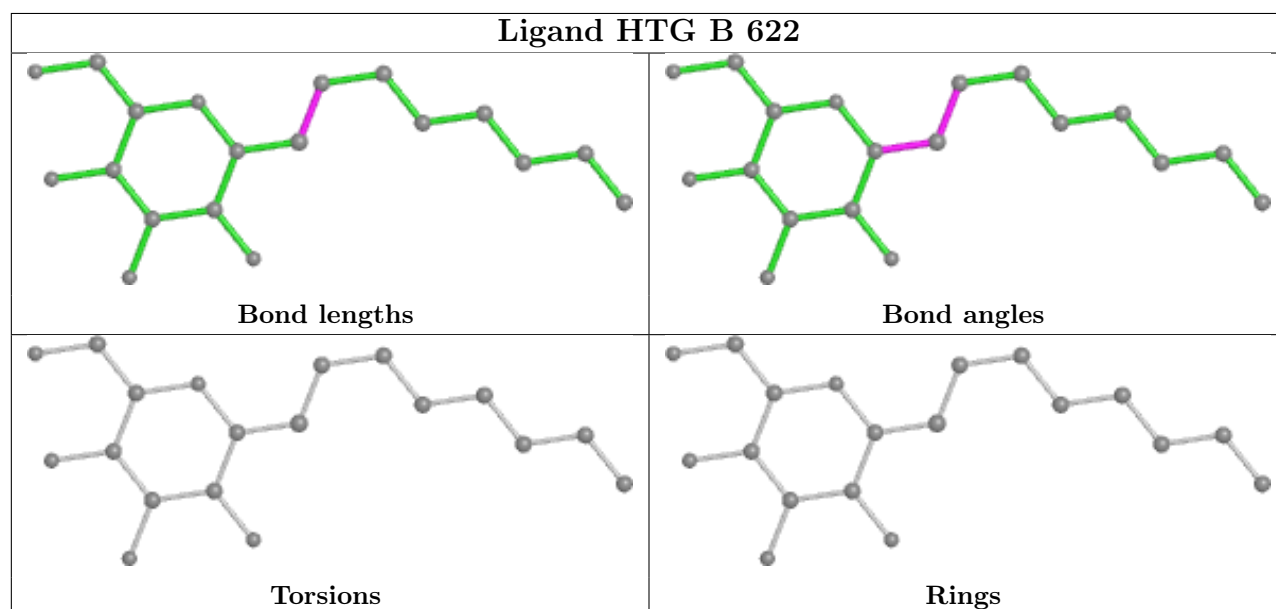
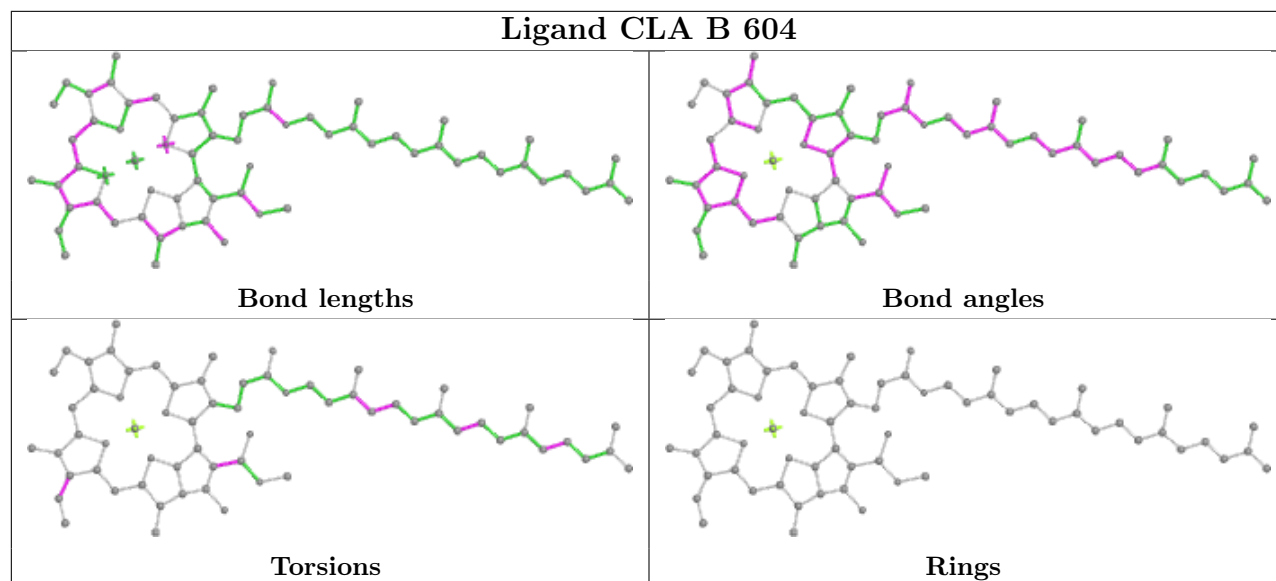
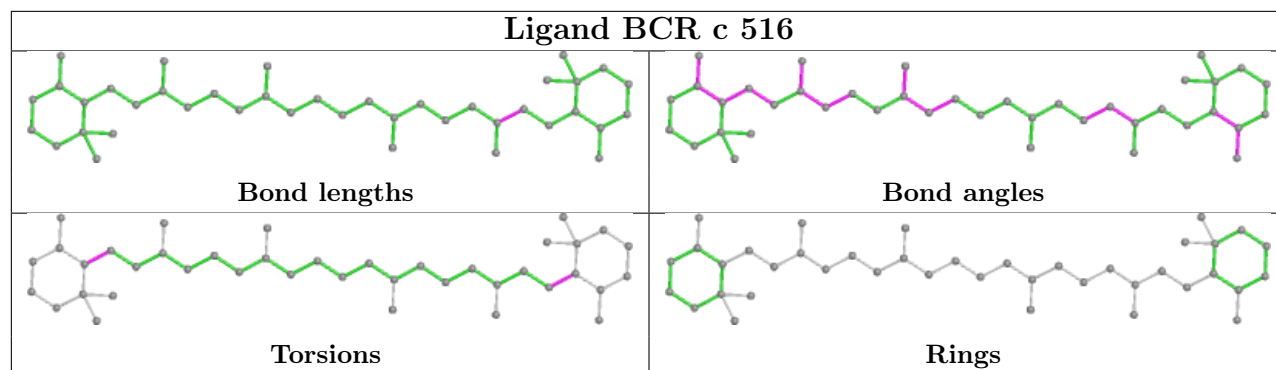


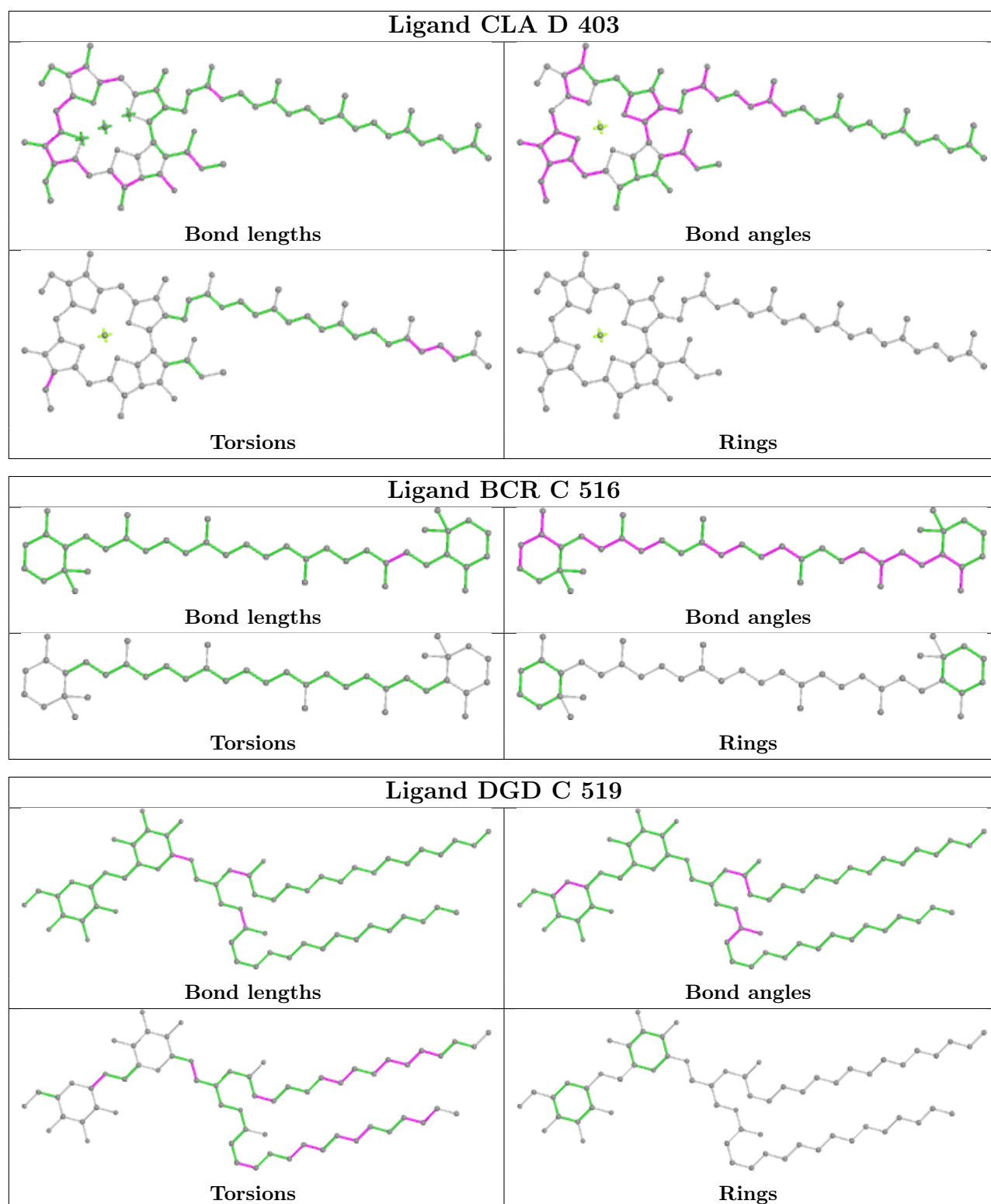


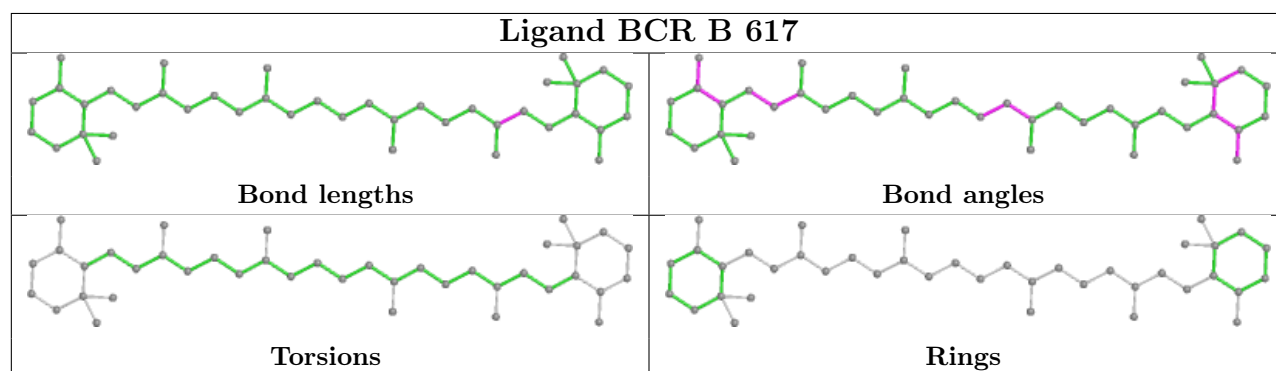
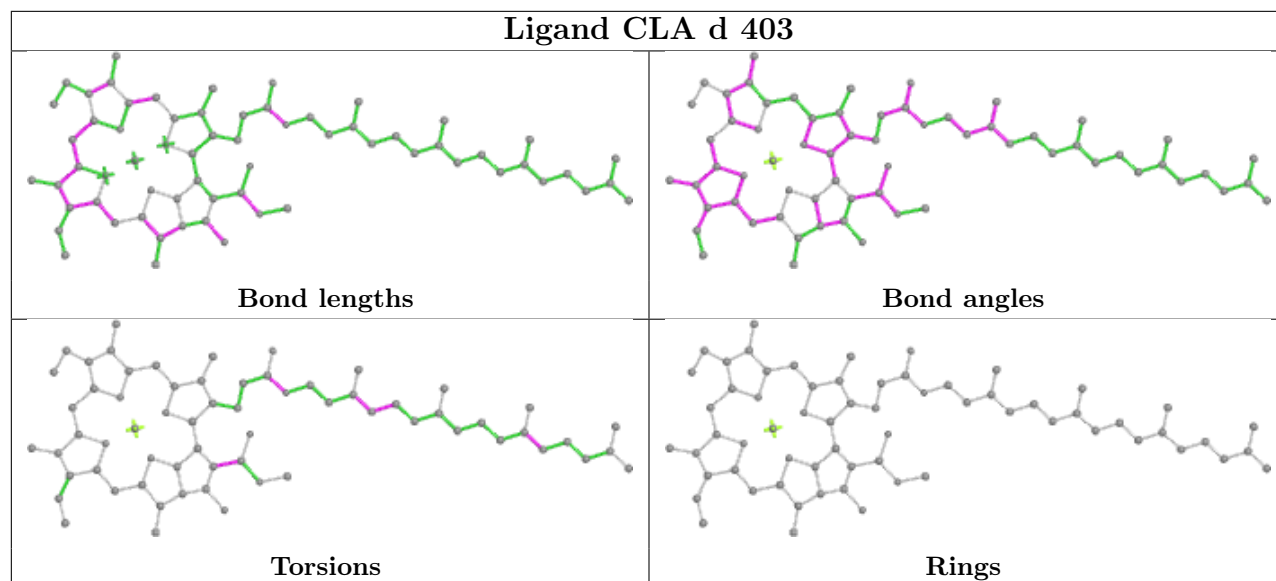
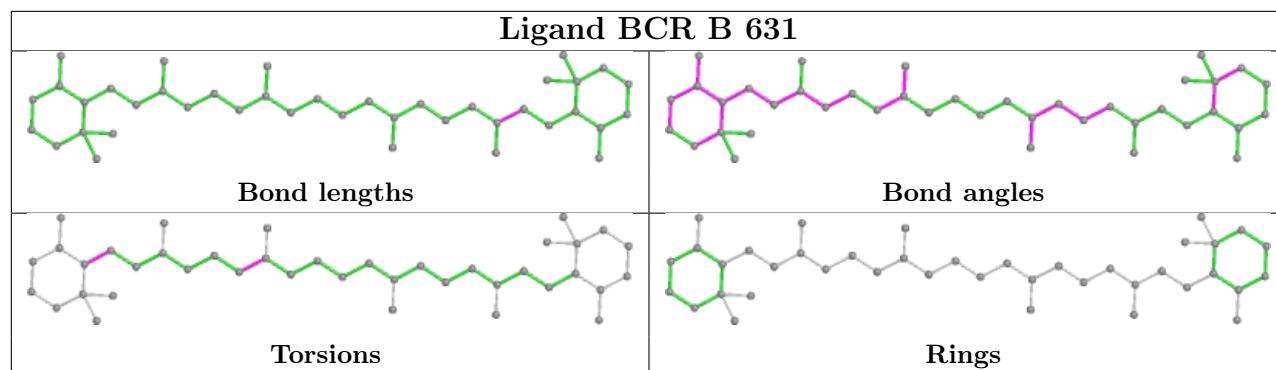


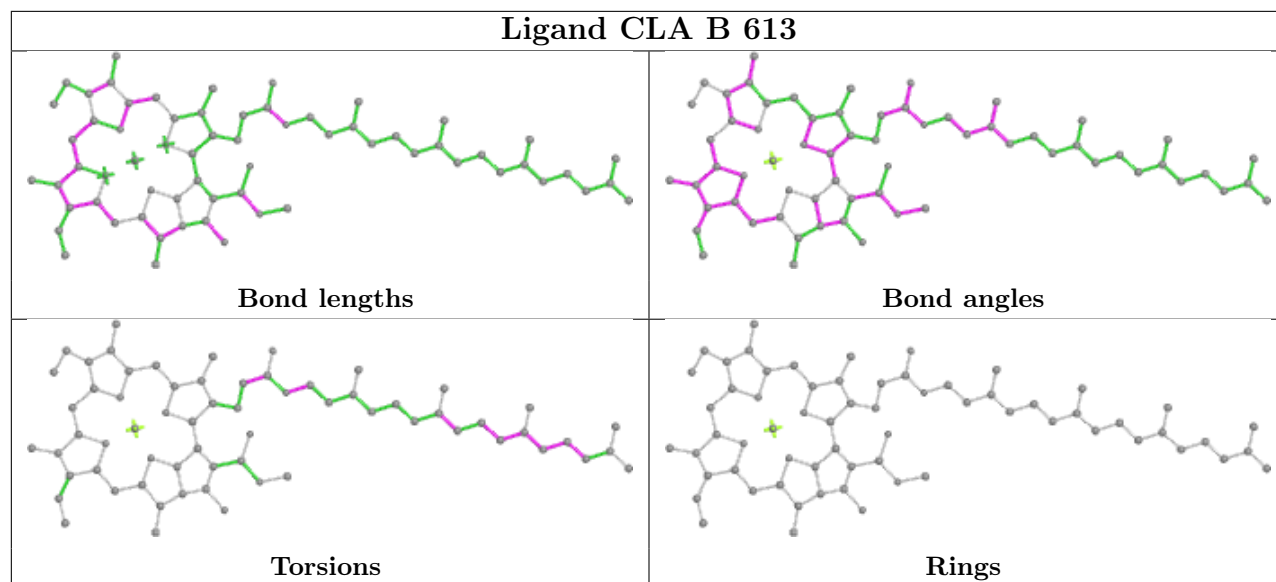
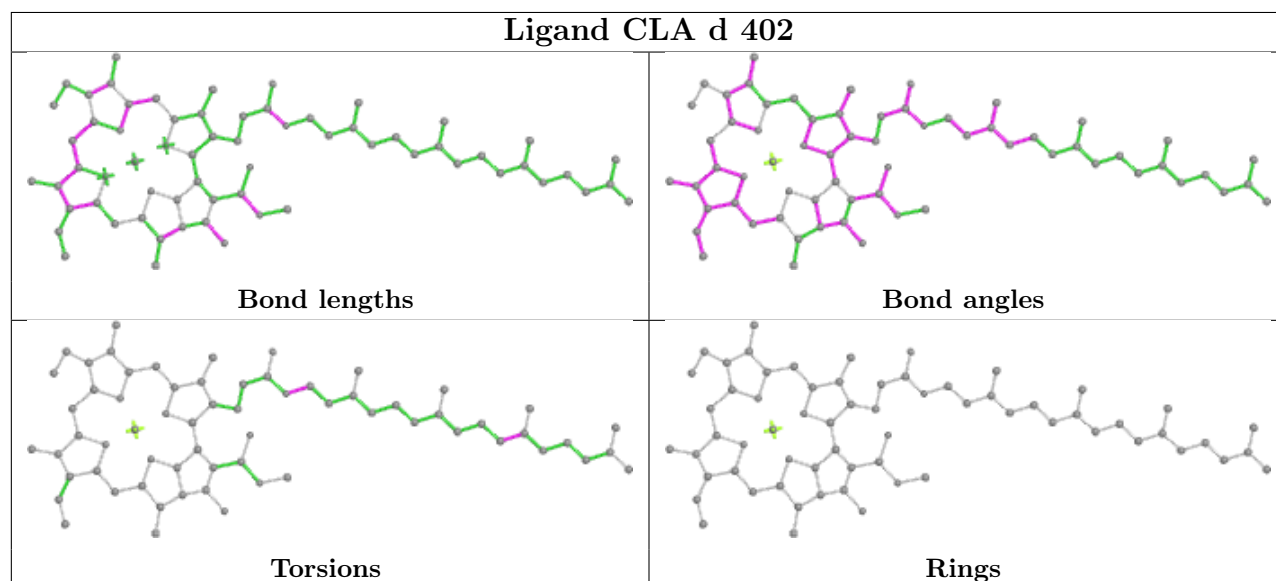
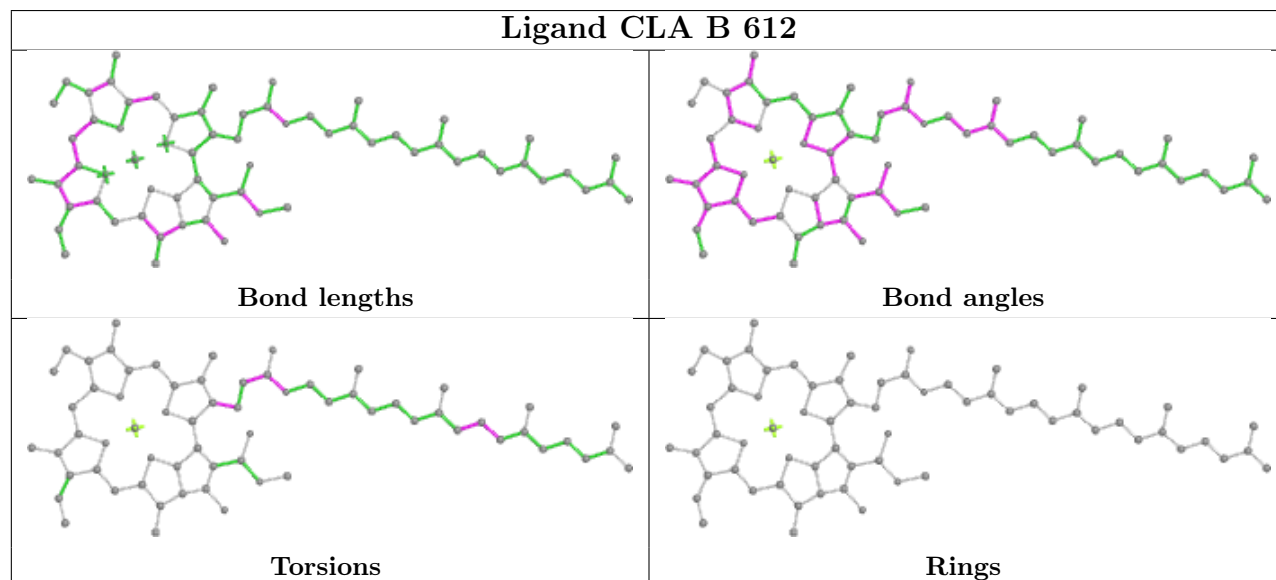
Ligand CLA B 609**Ligand CLA a 404****Ligand CLA C 506**



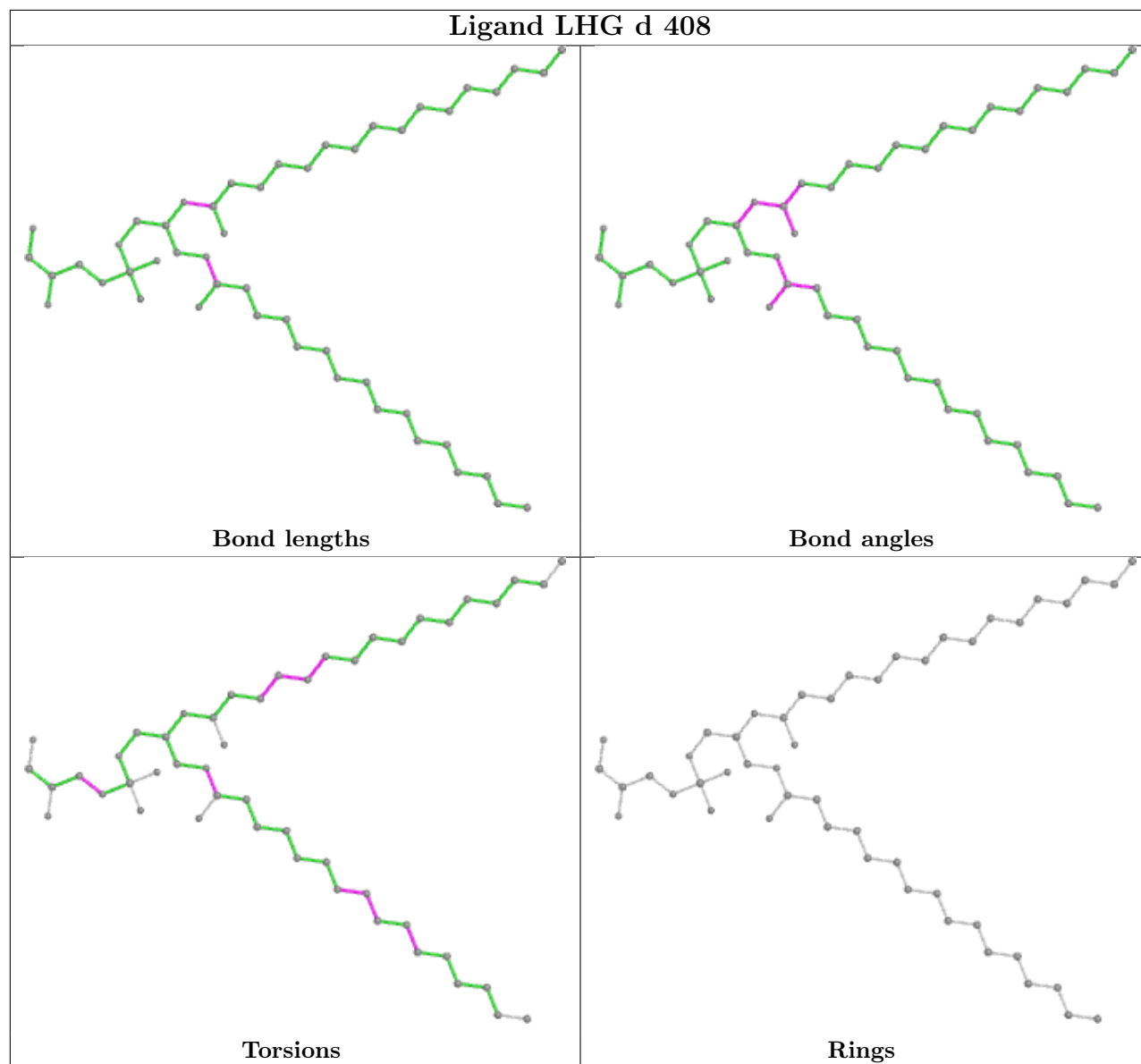




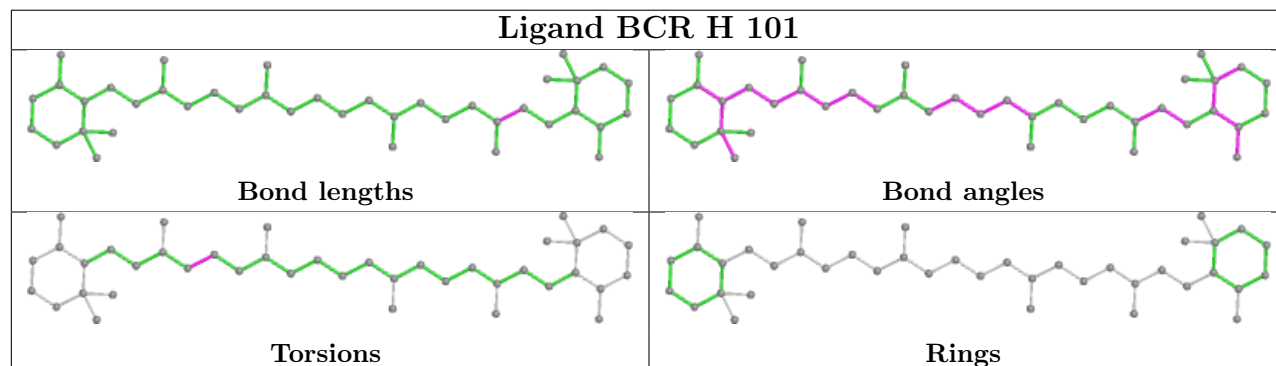


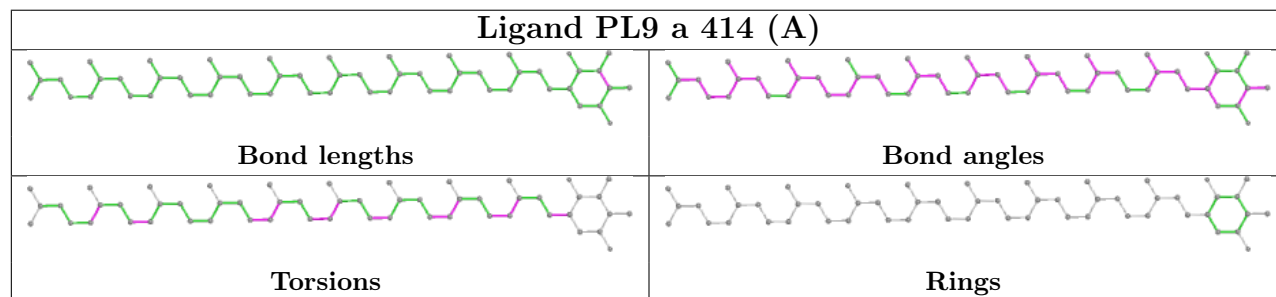
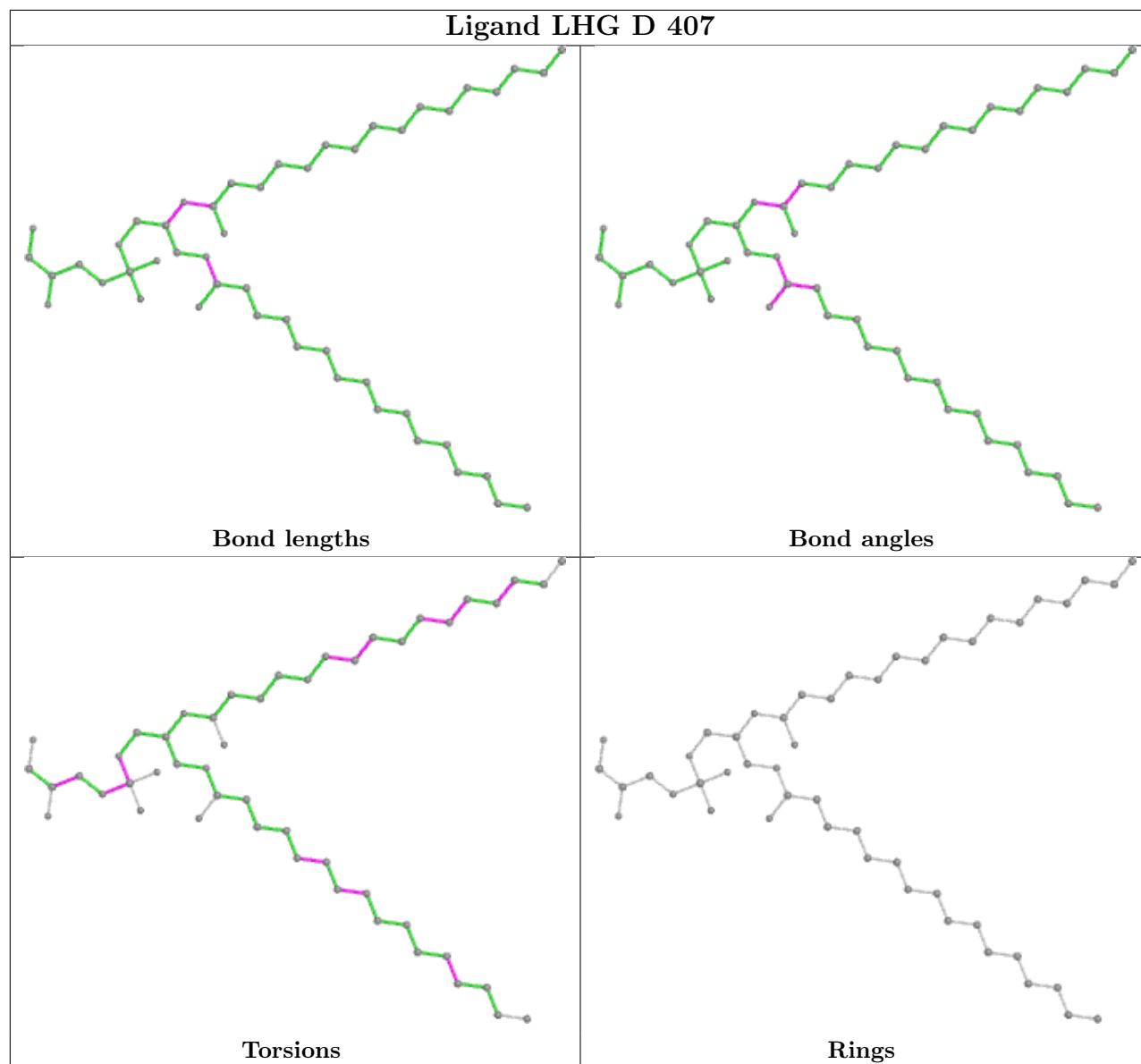
Ligand CLA B 613**Ligand CLA d 402****Ligand CLA B 612**

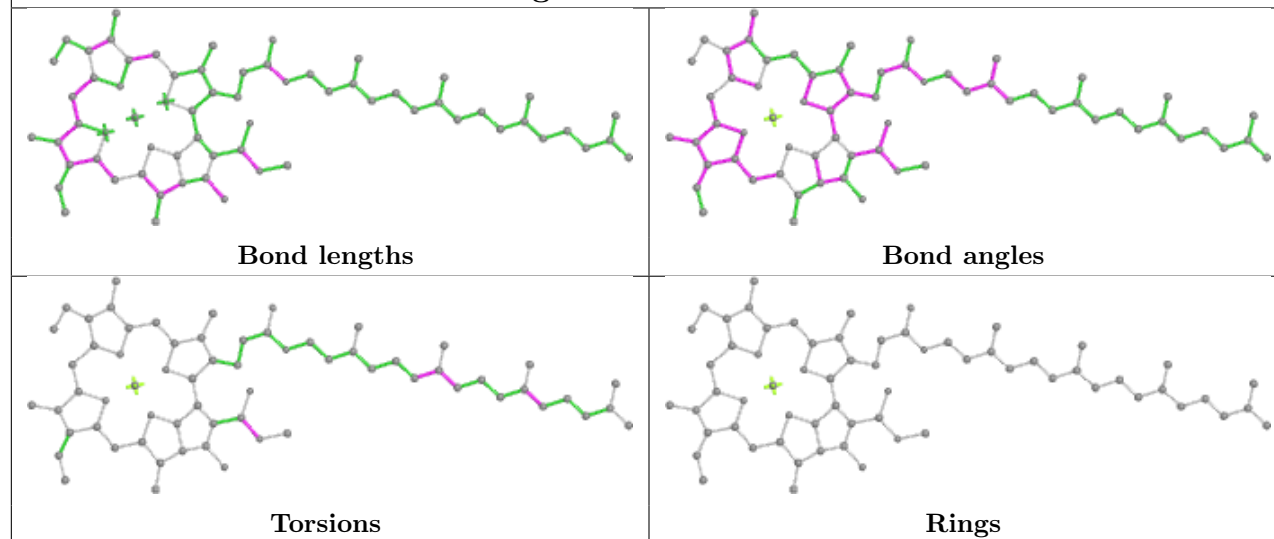
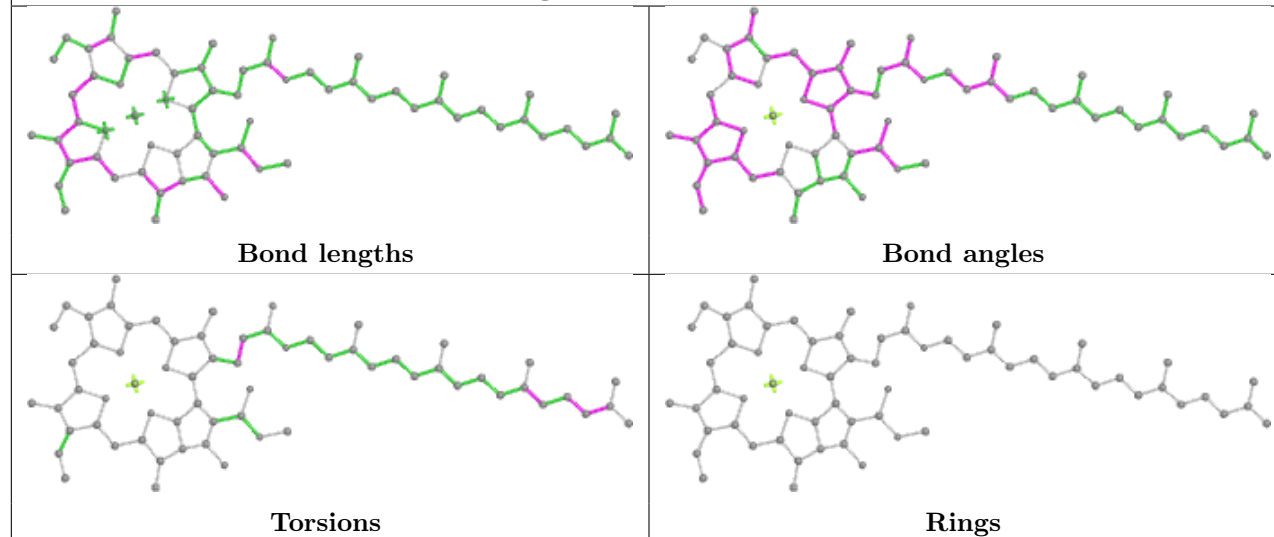
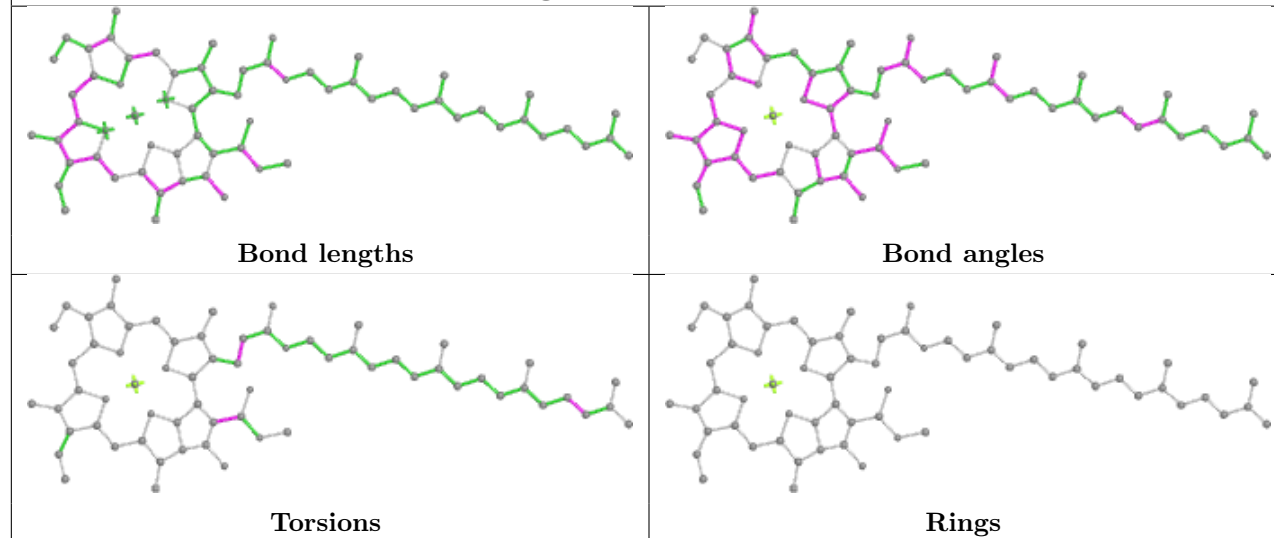
Ligand LHG d 408

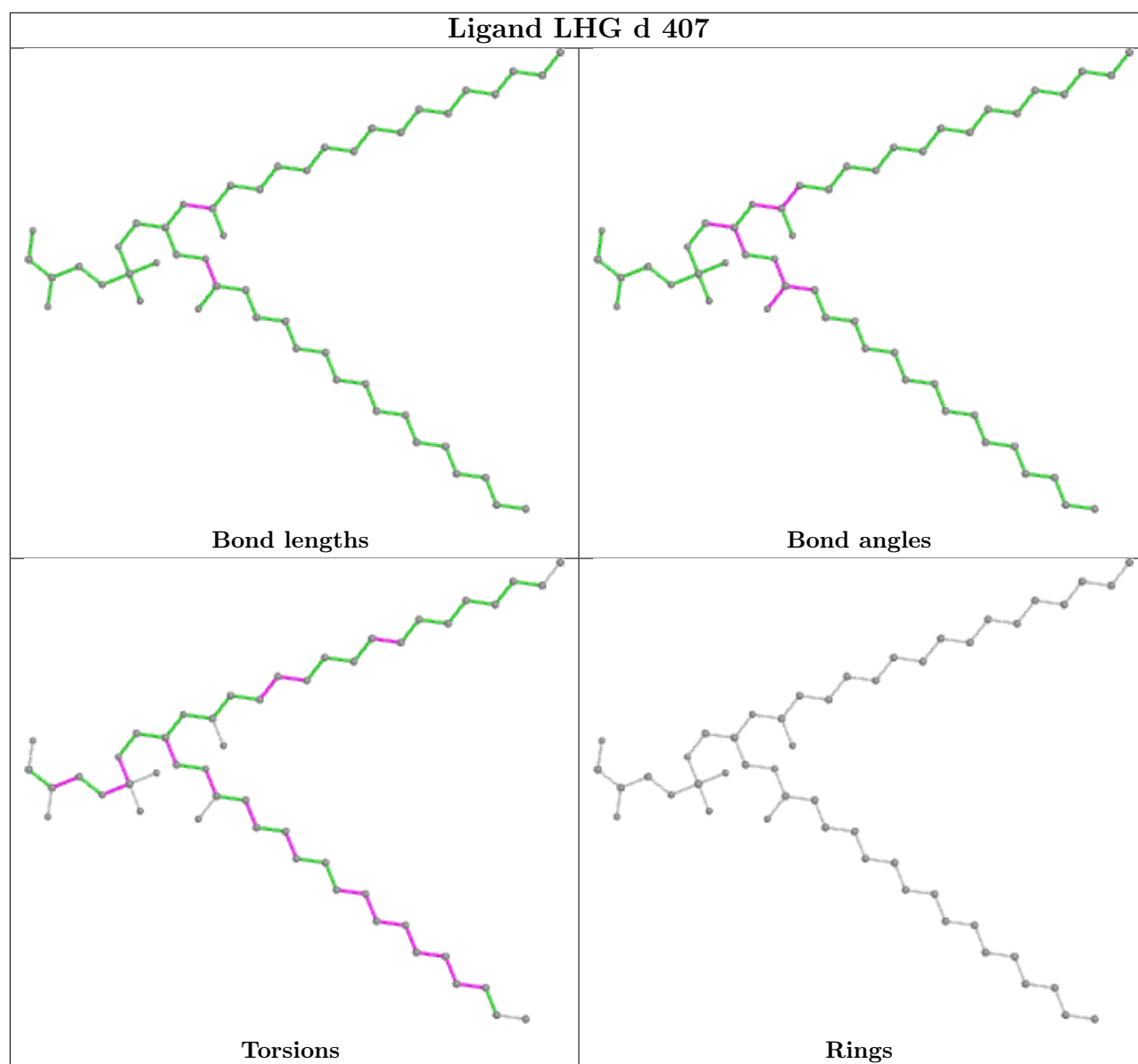


Ligand BCR H 101

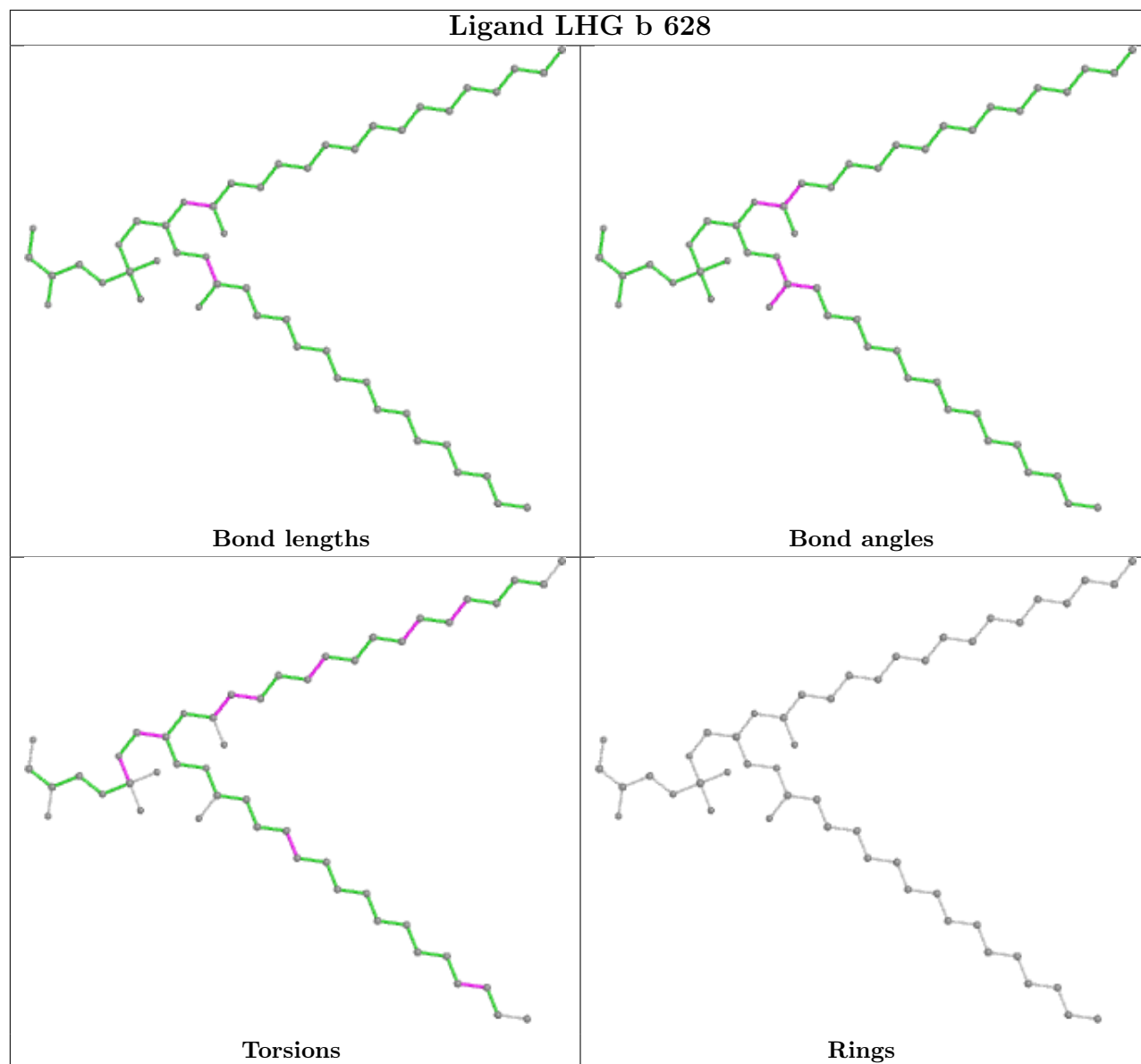




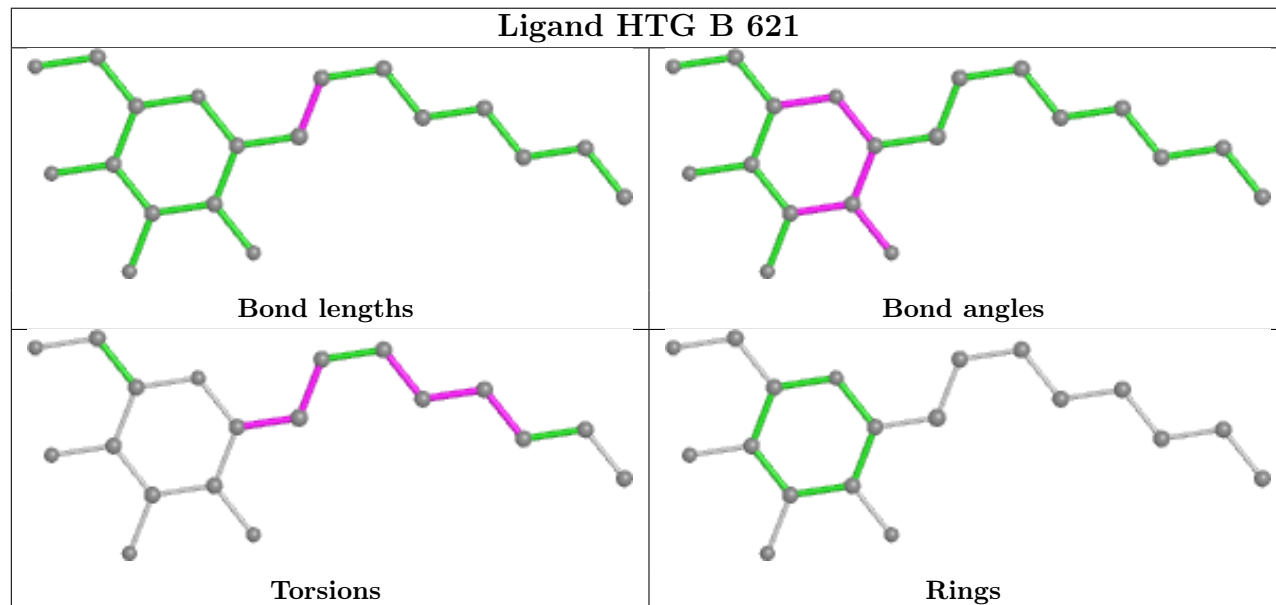
Ligand CLA C 515**Ligand CLA a 403****Ligand CLA c 505**

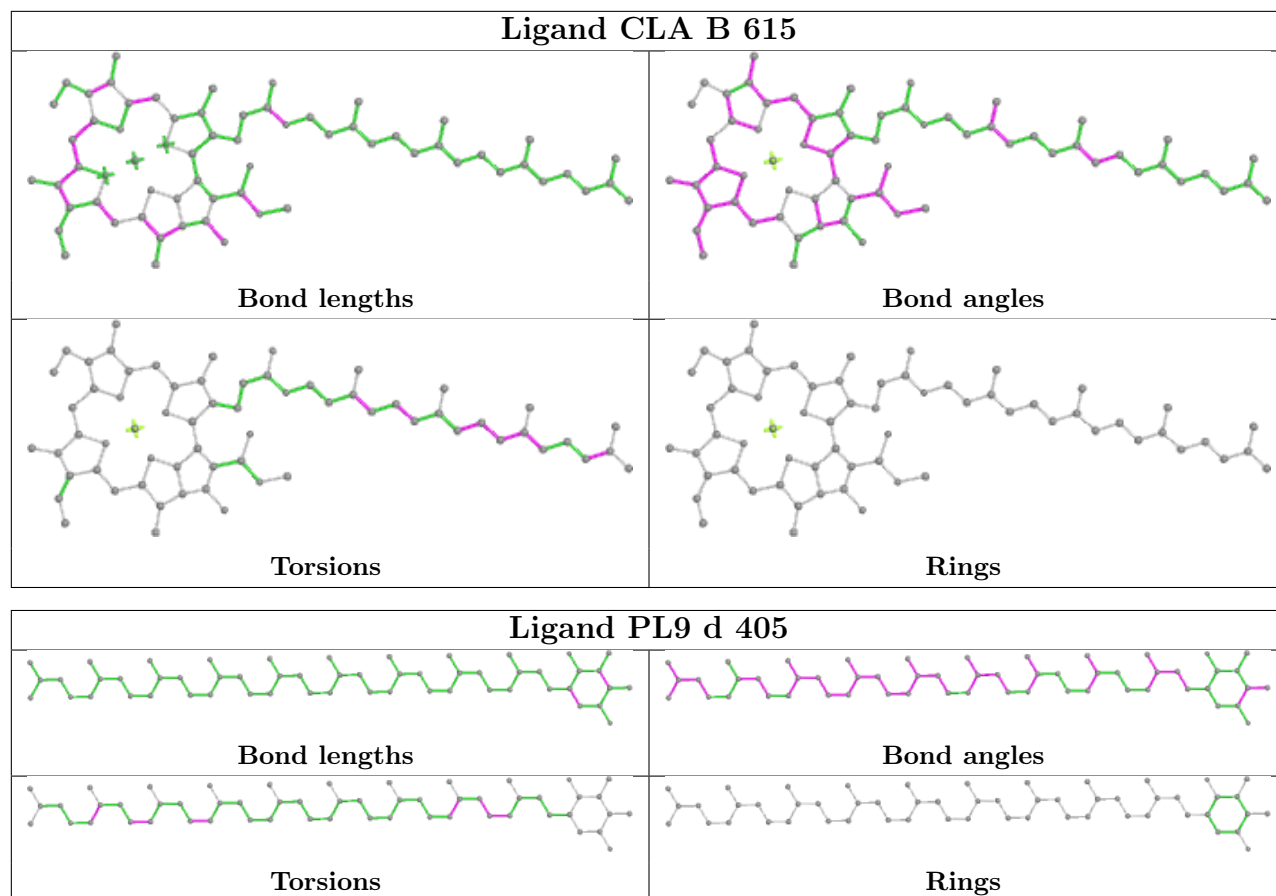


Ligand LHG b 628

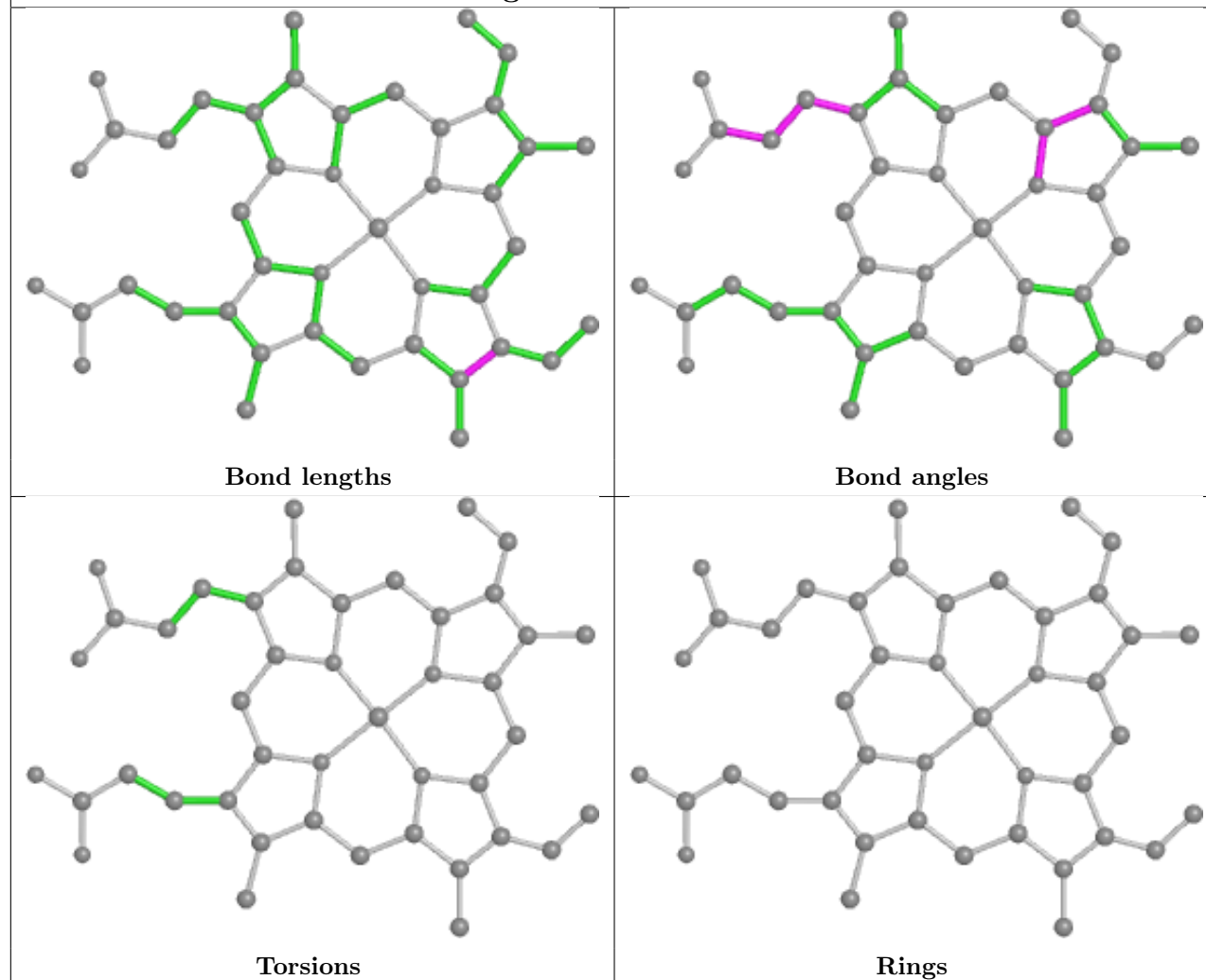


Ligand HTG B 621

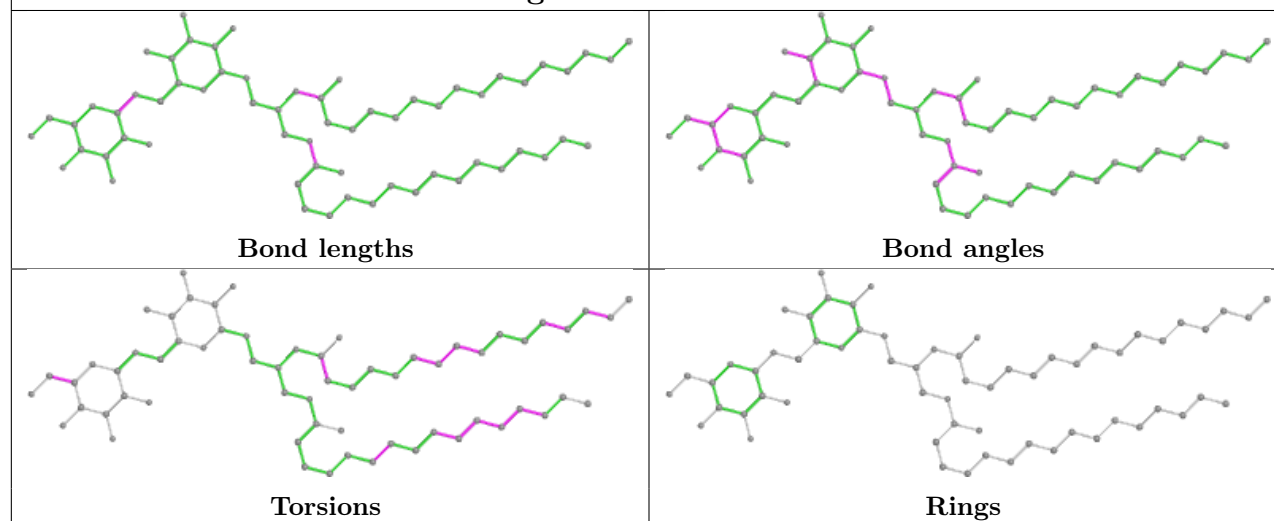


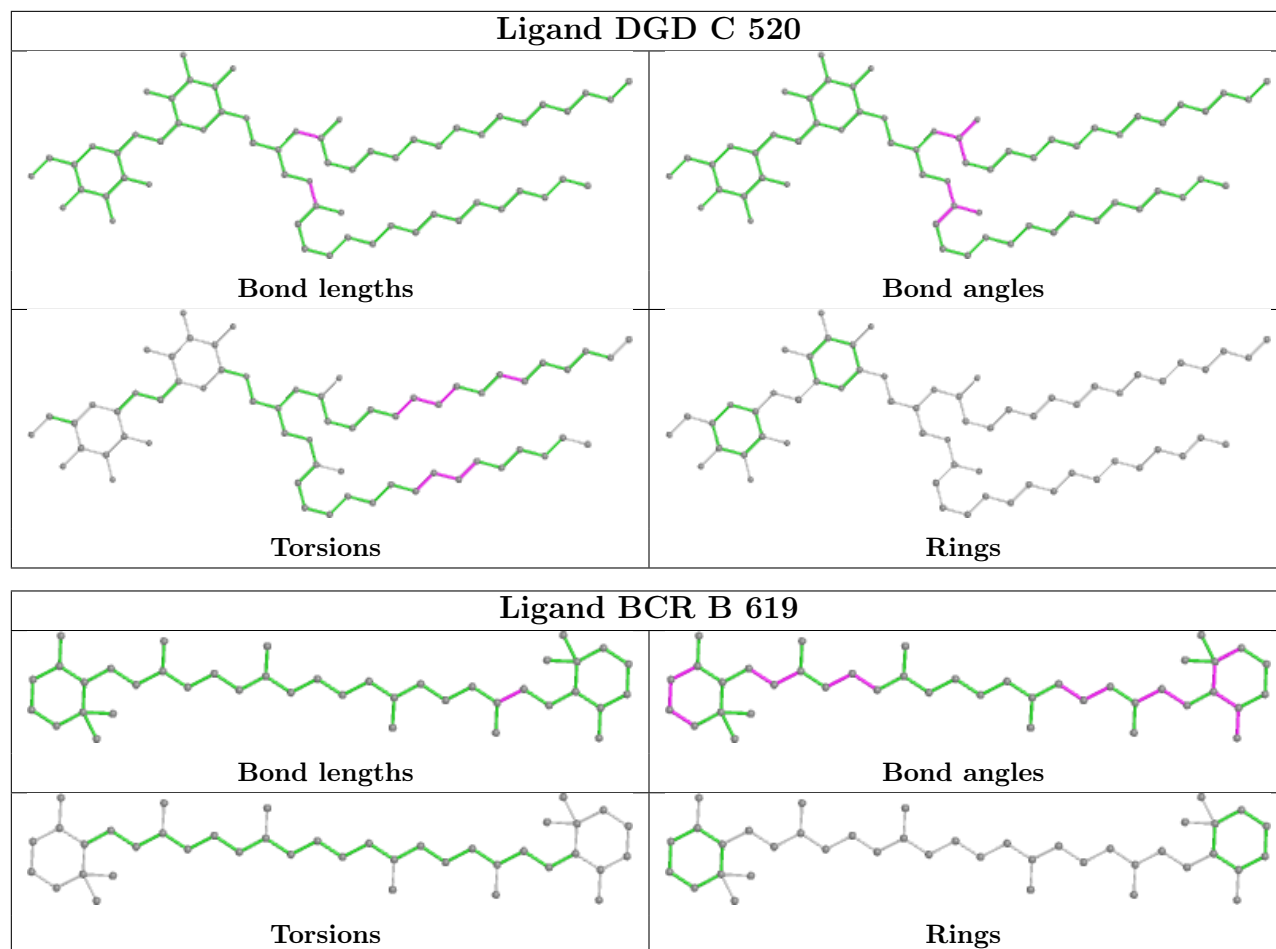


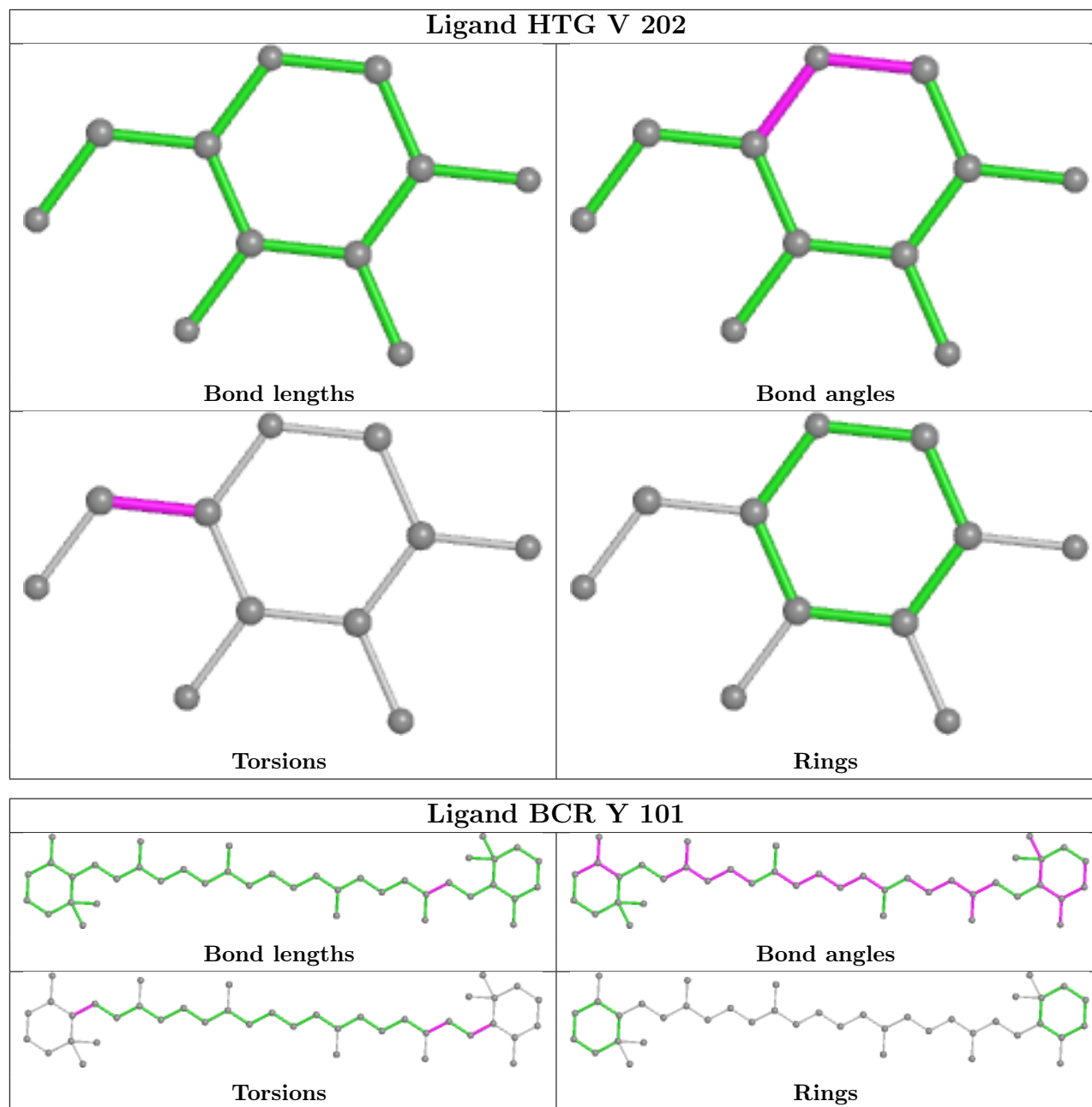
Ligand HEM e 102

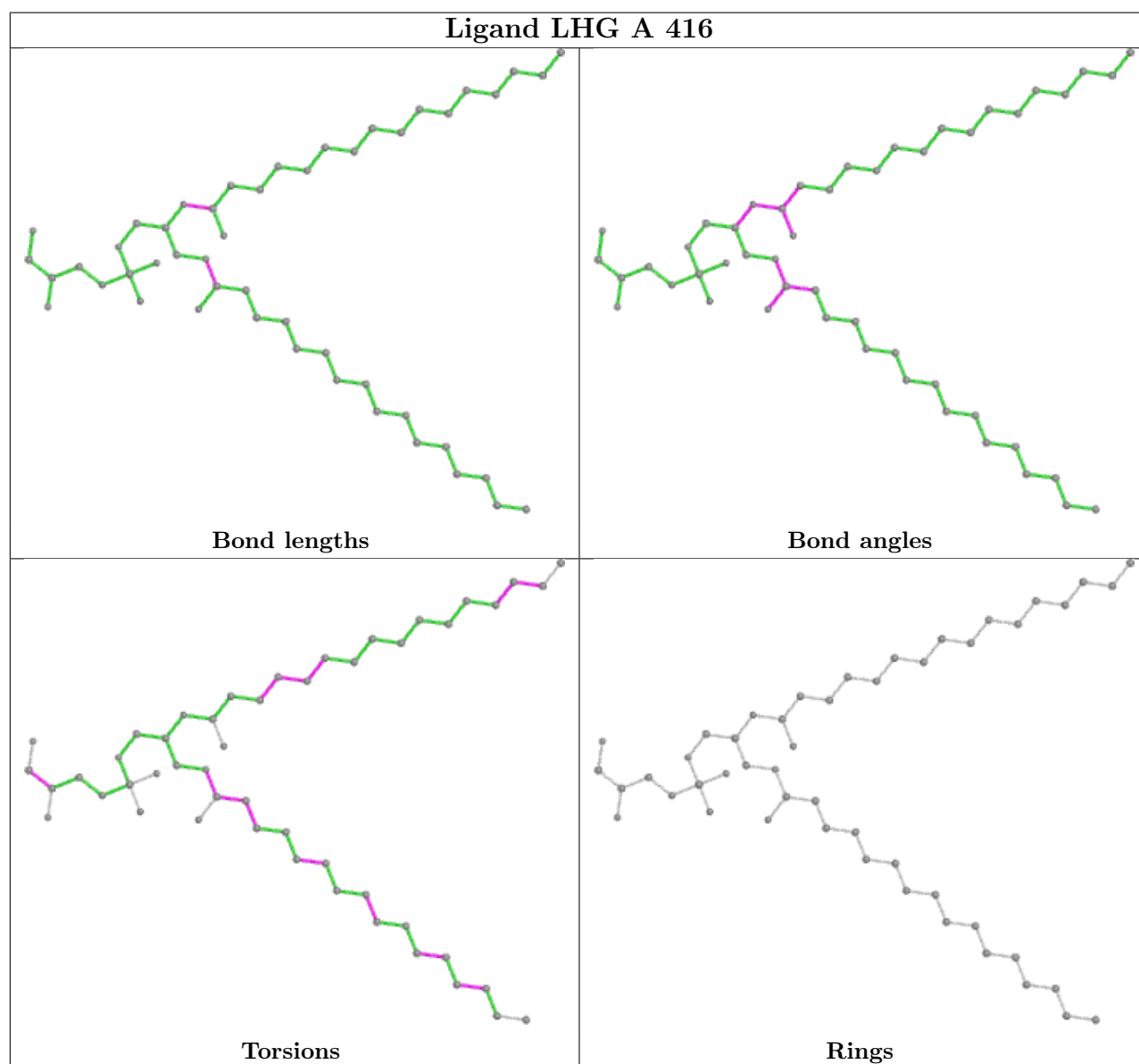
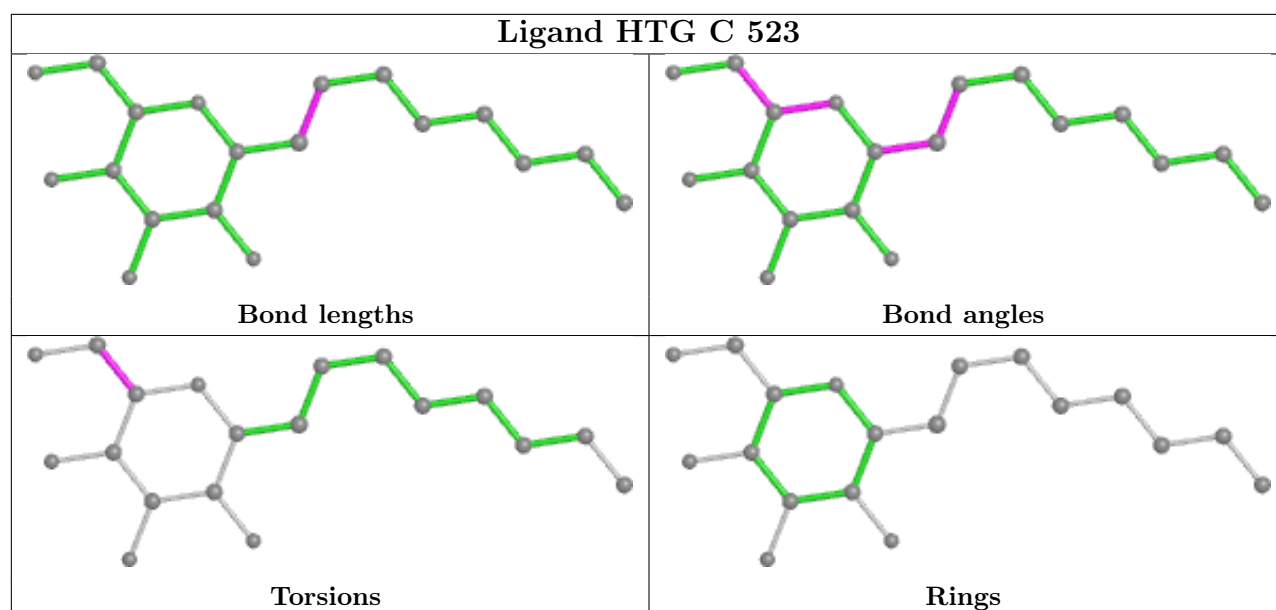


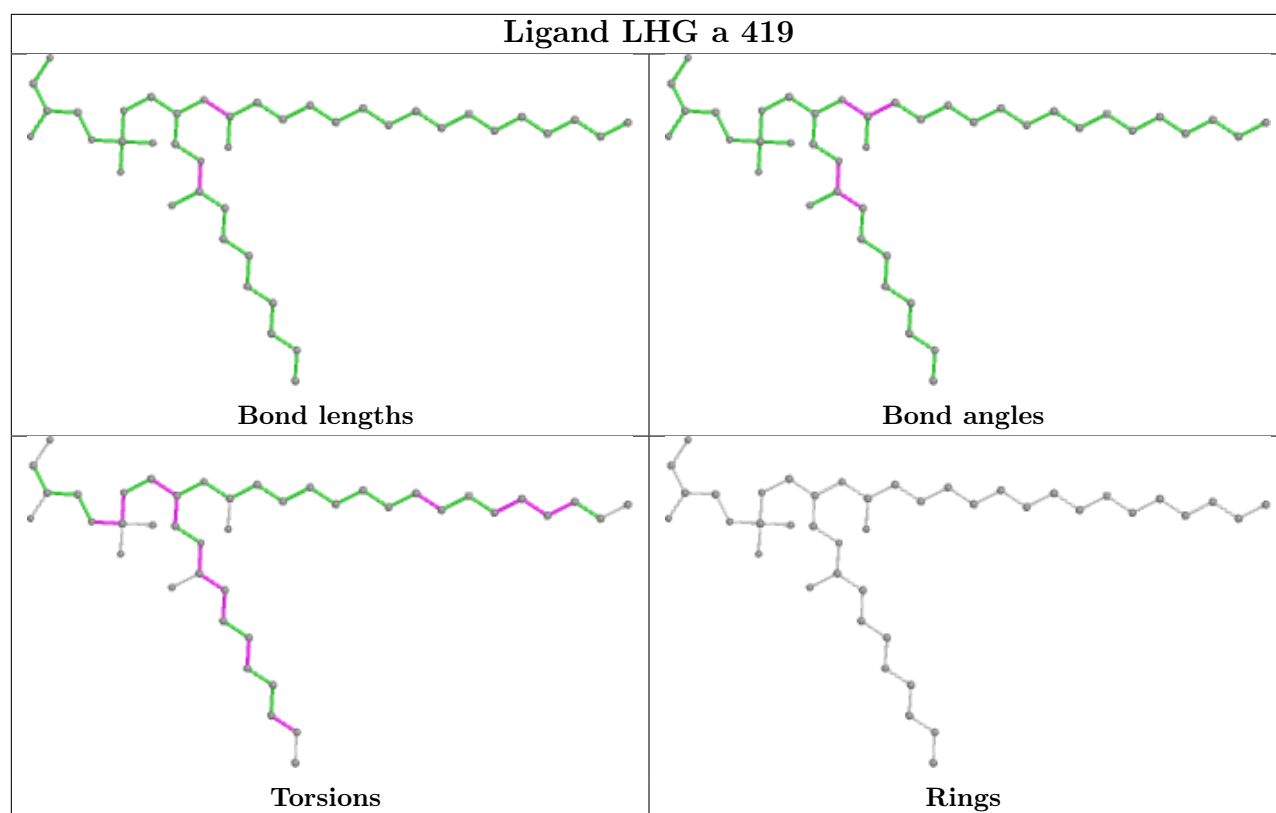
Ligand DGD H 102











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.11	8 (2%) 59 57	34, 44, 69, 128	0
1	a	334/344 (97%)	-0.02	9 (2%) 54 52	37, 48, 78, 110	0
2	B	504/505 (99%)	-0.32	23 (4%) 32 31	37, 49, 81, 127	0
2	b	504/505 (99%)	-0.11	43 (8%) 10 10	39, 53, 92, 158	0
3	C	451/455 (99%)	-0.24	20 (4%) 34 33	40, 56, 82, 156	0
3	c	455/455 (100%)	-0.05	23 (5%) 28 26	44, 64, 86, 133	0
4	D	342/342 (100%)	-0.22	6 (1%) 68 66	35, 45, 68, 139	0
4	d	341/342 (99%)	-0.18	16 (4%) 31 30	38, 50, 73, 129	0
5	E	81/84 (96%)	0.24	7 (8%) 10 9	51, 70, 96, 139	0
5	e	79/84 (94%)	0.30	9 (11%) 5 4	59, 74, 116, 157	0
6	F	34/44 (77%)	-0.35	1 (2%) 51 50	50, 62, 85, 108	0
6	f	31/44 (70%)	-0.19	2 (6%) 18 17	58, 67, 92, 144	0
7	H	64/65 (98%)	-0.54	1 (1%) 72 70	43, 59, 81, 133	0
7	h	64/65 (98%)	0.05	2 (3%) 49 47	52, 65, 91, 105	0
8	I	37/38 (97%)	-0.28	2 (5%) 25 24	49, 60, 124, 148	0
8	i	37/38 (97%)	-0.44	1 (2%) 54 52	52, 60, 114, 145	0
9	J	38/39 (97%)	0.31	7 (18%) 1 1	50, 70, 131, 177	0
9	j	39/39 (100%)	0.08	4 (10%) 6 6	58, 73, 125, 165	0
10	K	37/37 (100%)	-0.62	0 100 100	58, 67, 89, 113	0
10	k	37/37 (100%)	-0.10	2 (5%) 25 24	66, 73, 95, 113	0
11	L	36/37 (97%)	-0.32	0 100 100	35, 41, 93, 140	0
11	l	36/37 (97%)	-0.15	1 (2%) 53 51	37, 42, 105, 134	0
12	M	32/36 (88%)	-0.34	0 100 100	38, 44, 73, 146	0
12	m	33/36 (91%)	-0.35	1 (3%) 50 49	38, 44, 82, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.03	22 (9%) 9 8	35, 60, 113, 178	0
13	o	243/244 (99%)	0.42	42 (17%) 1 1	40, 61, 119, 171	0
14	T	29/32 (90%)	-0.53	0 100 100	38, 43, 83, 104	0
14	t	29/32 (90%)	-0.42	0 100 100	38, 46, 74, 139	0
15	U	96/104 (92%)	-0.38	1 (1%) 82 80	44, 56, 88, 92	0
15	u	97/104 (93%)	-0.59	0 100 100	48, 61, 80, 129	0
16	V	137/137 (100%)	-0.51	0 100 100	43, 55, 80, 112	0
16	v	137/137 (100%)	0.10	14 (10%) 6 6	50, 69, 103, 131	0
17	X	38/40 (95%)	-0.09	4 (10%) 6 5	54, 69, 91, 110	0
17	x	38/40 (95%)	0.57	7 (18%) 1 1	60, 74, 124, 157	0
18	Y	29/30 (96%)	1.57	9 (31%) 0 0	67, 89, 136, 169	0
18	y	29/30 (96%)	0.45	6 (20%) 1 0	75, 87, 113, 116	0
19	Z	62/62 (100%)	0.76	11 (17%) 1 1	69, 83, 138, 186	0
19	z	62/62 (100%)	1.43	20 (32%) 0 0	76, 95, 137, 185	0
20	R	34/34 (100%)	4.62	34 (100%) 0 0	91, 106, 138, 142	0
All	All	5283/5384 (98%)	-0.06	358 (6%) 17 15	34, 56, 99, 186	0

The worst 5 of 358 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Y	19	ILE	9.3
17	x	38	GLN	8.9
20	R	6	LEU	8.0
1	A	11	ALA	6.6
20	R	5	VAL	6.2

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	0.13	31,59,83,93	0
8	FME	I	1	10/11	0.97	0.14	46,67,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	FME	T	1	10/11	0.97	0.09	39,48,63,64	0
8	FME	i	1	10/11	0.97	0.11	52,62,75,81	0
12	FME	m	1	10/11	0.98	0.08	38,52,79,90	0
14	FME	t	1	10/11	0.98	0.08	35,44,61,70	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
34	LMG	C	522	51/55	0.47	0.44	76,125,159,161	0
33	LMT	C	526	35/35	0.53	0.55	93,147,159,160	0
33	LMT	a	412	35/35	0.54	0.39	63,131,144,146	0
33	LMT	F	101	35/35	0.54	0.41	105,152,164,167	0
32	HTG	D	411	16/19	0.60	0.33	82,116,129,129	0
33	LMT	M	103	35/35	0.60	0.32	75,140,160,163	0
30	UNL	A	414	28/-	0.61	0.46	88,103,120,121	0
34	LMG	c	522	51/55	0.62	0.41	80,125,151,152	0
33	LMT	D	402	35/35	0.63	0.35	75,130,140,142	0
32	HTG	b	622	19/19	0.63	0.57	86,138,148,150	0
30	UNL	C	527	34/-	0.63	0.36	83,110,123,129	0
33	LMT	m	103	35/35	0.64	0.38	59,97,109,113	0
30	UNL	I	101	40/-	0.65	0.28	74,108,148,149	0
30	UNL	j	101	10/-	0.65	0.34	81,90,102,103	0
30	UNL	b	625	33/-	0.66	0.36	65,94,146,147	0
33	LMT	e	101	35/35	0.68	0.62	121,173,177,179	0
30	UNL	a	415	30/-	0.69	0.31	100,110,133,140	0
31	LHG	E	101	42/49	0.70	0.26	74,114,131,133	0
33	LMT	M	102	35/35	0.71	0.27	54,105,130,138	0
30	UNL	i	101	40/-	0.73	0.31	72,97,151,154	0
33	LMT	b	620	25/35	0.73	0.24	90,129,147,148	0
27	GOL	B	626	6/6	0.73	0.27	82,99,100,103	0
34	LMG	Z	101	37/55	0.74	0.32	73,129,162,169	0
33	LMT	B	627	35/35	0.74	0.28	68,112,127,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	PL9	A	413[A]	55/55	0.75	0.32	89,97,103,104	55
30	UNL	d	410	36/-	0.75	0.26	72,92,117,120	0
30	UNL	J	101	10/-	0.75	0.29	69,84,88,90	0
29	PL9	A	413[B]	55/55	0.75	0.32	88,97,104,104	55
31	LHG	a	419	42/49	0.76	0.34	86,136,170,174	0
33	LMT	a	418	35/35	0.76	0.51	113,144,152,153	0
30	UNL	B	625	33/-	0.76	0.24	56,105,148,152	0
30	UNL	c	526	32/-	0.76	0.37	91,111,125,129	0
27	GOL	c	527	6/6	0.77	0.37	105,109,114,116	0
26	SQD	f	101	43/54	0.77	0.45	111,129,159,160	0
33	LMT	B	629	25/35	0.78	0.22	56,79,132,133	0
30	UNL	m	102	10/-	0.79	0.23	59,67,88,90	0
32	HTG	B	622	19/19	0.79	0.35	79,89,99,100	0
33	LMT	b	626	25/35	0.79	0.22	46,70,129,135	0
27	GOL	O	302	6/6	0.79	0.27	78,84,85,85	0
29	PL9	a	414[A]	55/55	0.80	0.29	93,104,111,112	55
33	LMT	B	630	26/35	0.80	0.24	78,117,140,143	0
32	HTG	h	101	16/19	0.80	0.30	99,134,140,142	0
29	PL9	a	414[B]	55/55	0.80	0.29	92,104,111,112	55
34	LMG	a	417	51/55	0.81	0.22	59,90,115,128	0
32	HTG	b	621	19/19	0.81	0.20	61,78,111,112	0
27	GOL	B	628	6/6	0.82	0.41	90,102,105,109	0
32	HTG	c	523	19/19	0.82	0.30	119,131,139,141	0
26	SQD	L	102	54/54	0.82	0.21	55,91,118,119	0
36	CA	F	102	1/1	0.82	0.07	103,103,103,103	0
34	LMG	z	101	39/55	0.83	0.29	81,136,147,148	0
30	UNL	l	101	10/-	0.83	0.24	63,74,83,85	0
32	HTG	V	202	11/19	0.84	0.39	109,114,122,124	0
32	HTG	B	621	19/19	0.84	0.23	72,87,118,120	0
34	LMG	c	521	51/55	0.84	0.30	66,93,123,128	0
30	UNL	D	410	40/-	0.85	0.23	52,87,126,132	0
25	BCR	h	102	40/40	0.85	0.18	50,66,74,75	0
36	CA	c	525	1/1	0.85	0.05	81,81,81,81	0
34	LMG	C	521	51/55	0.86	0.22	59,84,115,118	0
26	SQD	A	411	54/54	0.87	0.17	60,84,125,128	0
32	HTG	C	523	19/19	0.87	0.33	108,122,132,133	0
27	GOL	b	623	6/6	0.87	0.18	87,92,94,102	0
26	SQD	B	620	54/54	0.87	0.17	60,89,121,127	0
35	DGD	h	103	62/66	0.87	0.25	46,62,73,78	0
34	LMG	M	101	51/55	0.87	0.19	48,69,87,101	0
23	CLA	C	515	65/65	0.87	0.22	59,76,108,109	0
30	UNL	d	412	18/-	0.88	0.20	72,81,121,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	SQD	a	411	54/54	0.88	0.16	63,89,126,130	0
25	BCR	H	101	40/40	0.88	0.18	47,59,77,80	0
30	UNL	D	409	17/-	0.88	0.30	60,78,113,114	0
30	UNL	X	101	18/-	0.88	0.15	57,74,95,98	0
31	LHG	A	416	49/49	0.88	0.24	41,61,78,84	0
27	GOL	v	201	6/6	0.89	0.21	59,82,83,86	0
36	CA	O	301	1/1	0.89	0.18	118,118,118,118	0
34	LMG	m	101	51/55	0.89	0.22	53,69,98,101	0
35	DGD	C	519	62/66	0.90	0.18	45,64,116,121	0
35	DGD	c	519	62/66	0.90	0.20	51,73,114,122	0
23	CLA	C	514	65/65	0.90	0.18	55,69,119,122	0
25	BCR	k	102	40/40	0.90	0.17	58,72,89,92	0
34	LMG	C	502	51/55	0.90	0.20	58,89,113,120	0
30	UNL	d	409	17/-	0.90	0.22	68,84,106,108	0
26	SQD	D	413	43/54	0.91	0.22	70,105,125,136	0
23	CLA	c	514	65/65	0.91	0.17	62,80,117,125	0
23	CLA	B	602	65/65	0.91	0.16	40,51,74,84	0
35	DGD	C	520	62/66	0.91	0.19	43,57,92,104	0
35	DGD	H	102	62/66	0.91	0.22	41,57,76,80	0
36	CA	o	301	1/1	0.91	0.10	104,104,104,104	0
29	PL9	d	405	55/55	0.92	0.19	36,47,56,65	0
27	GOL	b	627	6/6	0.92	0.29	91,93,95,97	0
23	CLA	C	508	65/65	0.92	0.14	51,69,117,126	0
27	GOL	A	410	6/6	0.92	0.17	65,67,74,83	0
23	CLA	b	609	65/65	0.92	0.14	49,57,76,98	0
23	CLA	c	504	65/65	0.92	0.26	49,58,73,89	0
25	BCR	k	101	40/40	0.92	0.16	60,73,84,87	0
23	CLA	c	505	65/65	0.92	0.19	52,65,75,81	0
26	SQD	A	409	54/54	0.93	0.17	57,74,105,111	0
23	CLA	c	515	65/65	0.93	0.26	68,85,111,112	0
23	CLA	C	506	65/65	0.93	0.17	43,53,92,102	0
34	LMG	D	412	51/55	0.93	0.18	46,69,108,116	0
31	LHG	b	628	49/49	0.93	0.18	42,54,68,80	0
25	BCR	d	404	40/40	0.93	0.13	52,64,87,93	0
27	GOL	a	410	6/6	0.93	0.20	60,70,83,86	0
23	CLA	B	609	65/65	0.93	0.13	45,54,72,80	0
23	CLA	D	404	65/65	0.93	0.17	43,55,120,122	0
23	CLA	b	601	65/65	0.93	0.22	58,80,119,128	0
23	CLA	d	403	65/65	0.94	0.15	49,60,108,119	0
26	SQD	a	409	54/54	0.94	0.20	62,81,108,113	0
29	PL9	D	406	55/55	0.94	0.18	32,44,58,67	0
32	HTG	b	624	19/19	0.94	0.13	64,77,95,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	BCR	C	516	40/40	0.94	0.13	64,80,88,91	0
23	CLA	b	616	65/65	0.94	0.17	41,58,112,116	0
25	BCR	b	618	40/40	0.94	0.22	39,53,69,75	0
27	GOL	B	623	6/6	0.94	0.21	79,89,96,98	0
23	CLA	C	509	65/65	0.94	0.12	48,57,78,86	0
34	LMG	d	411	51/55	0.94	0.14	53,67,107,116	0
23	CLA	b	602	65/65	0.94	0.18	48,56,68,81	0
23	CLA	c	506	65/65	0.94	0.26	51,59,100,110	0
31	LHG	L	101	49/49	0.94	0.16	41,52,63,88	0
23	CLA	c	509	65/65	0.94	0.14	55,65,78,87	0
23	CLA	c	510	65/65	0.94	0.25	48,59,116,123	0
31	LHG	d	407	49/49	0.94	0.15	39,51,69,80	0
35	DGD	c	520	62/66	0.94	0.16	49,60,97,101	0
31	LHG	d	408	49/49	0.94	0.21	56,66,109,120	0
23	CLA	c	513	65/65	0.94	0.14	56,66,80,83	0
27	GOL	c	502	6/6	0.94	0.25	67,70,80,85	0
23	CLA	B	601	65/65	0.94	0.26	54,73,118,127	0
23	CLA	b	612	65/65	0.94	0.18	38,47,59,75	0
23	CLA	B	603	65/65	0.95	0.14	38,49,65,68	0
23	CLA	c	507	65/65	0.95	0.14	44,57,80,84	0
23	CLA	a	407	65/65	0.95	0.16	40,51,124,127	0
23	CLA	B	611	65/65	0.95	0.17	35,41,60,68	0
23	CLA	B	616	65/65	0.95	0.17	45,56,134,137	0
23	CLA	b	604	65/65	0.95	0.24	35,46,105,111	0
23	CLA	C	510	65/65	0.95	0.19	44,55,118,130	0
23	CLA	b	610	65/65	0.95	0.16	44,52,66,73	0
23	CLA	C	512	65/65	0.95	0.21	47,57,77,83	0
25	BCR	C	517	40/40	0.95	0.13	50,61,74,79	0
31	LHG	D	407	49/49	0.95	0.15	41,50,67,84	0
31	LHG	D	408	49/49	0.95	0.19	43,60,115,123	0
35	DGD	C	518	62/66	0.95	0.23	41,57,98,102	0
23	CLA	b	614	65/65	0.95	0.14	36,45,103,107	0
25	BCR	K	101	40/40	0.95	0.14	57,69,78,81	0
25	BCR	Y	101	40/40	0.95	0.12	53,67,77,84	0
25	BCR	b	617	40/40	0.95	0.15	39,49,57,59	0
31	LHG	d	406	49/49	0.95	0.25	50,62,82,94	0
23	CLA	C	513	65/65	0.95	0.13	51,65,83,84	0
25	BCR	c	516	40/40	0.95	0.16	68,85,89,95	0
23	CLA	C	503	65/65	0.95	0.14	47,56,66,81	0
36	CA	a	420	1/1	0.95	0.27	108,108,108,108	0
36	CA	c	524	1/1	0.95	0.07	75,75,75,75	0
23	CLA	C	505	65/65	0.95	0.13	48,58,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	HTG	B	624	19/19	0.95	0.11	63,79,90,90	0
23	CLA	b	611	65/65	0.96	0.22	38,47,70,82	0
24	PHO	A	415	64/64	0.96	0.24	36,46,53,54	0
25	BCR	A	408	40/40	0.96	0.12	35,46,55,56	0
25	BCR	B	618	40/40	0.96	0.17	39,53,64,68	0
25	BCR	B	619	40/40	0.96	0.10	43,55,74,76	0
25	BCR	B	631	40/40	0.96	0.15	36,57,68,70	0
23	CLA	B	614	65/65	0.96	0.14	34,44,96,103	0
23	CLA	a	405	65/65	0.96	0.21	40,50,112,117	0
25	BCR	D	405	40/40	0.96	0.15	48,57,94,99	0
23	CLA	b	615	65/65	0.96	0.11	41,52,73,79	0
23	CLA	B	607	65/65	0.96	0.16	32,42,62,72	0
25	BCR	T	101	40/40	0.96	0.14	35,51,63,63	0
23	CLA	c	503	65/65	0.96	0.13	56,63,75,79	0
25	BCR	a	408	40/40	0.96	0.11	38,48,56,59	0
23	CLA	A	407	65/65	0.96	0.12	39,47,109,116	0
23	CLA	C	504	65/65	0.96	0.18	44,57,77,85	0
35	DGD	c	518	62/66	0.96	0.20	46,59,90,92	0
23	CLA	b	603	65/65	0.96	0.16	41,53,74,81	0
25	BCR	c	517	40/40	0.96	0.12	54,67,73,75	0
23	CLA	B	610	65/65	0.96	0.15	42,50,63,75	0
23	CLA	c	508	65/65	0.96	0.13	56,69,122,127	0
23	CLA	b	605	65/65	0.96	0.16	36,47,67,70	0
23	CLA	b	606	65/65	0.96	0.13	40,52,114,120	0
23	CLA	b	607	65/65	0.96	0.18	33,43,72,80	0
23	CLA	B	604	65/65	0.96	0.19	34,41,98,103	0
23	CLA	C	507	65/65	0.96	0.15	43,52,86,87	0
37	BCT	d	401[A]	4/4	0.96	0.12	55,59,59,60	4
37	BCT	d	401[B]	4/4	0.96	0.12	53,58,60,67	4
39	MG	J	102	1/1	0.96	0.14	56,56,56,56	0
24	PHO	A	406	64/64	0.97	0.15	33,41,49,58	0
23	CLA	C	511	65/65	0.97	0.13	49,58,76,83	0
24	PHO	a	416	64/64	0.97	0.18	40,48,55,63	0
25	BCR	b	619	40/40	0.97	0.11	46,55,77,86	0
23	CLA	B	613	65/65	0.97	0.23	36,43,86,93	0
25	BCR	B	617	40/40	0.97	0.14	38,47,58,61	0
27	GOL	C	524	6/6	0.97	0.16	49,58,63,63	0
23	CLA	B	608	65/65	0.97	0.18	39,49,66,67	0
23	CLA	B	615	65/65	0.97	0.12	40,47,75,84	0
23	CLA	b	613	65/65	0.97	0.26	34,45,80,86	0
23	CLA	B	605	65/65	0.97	0.12	37,43,59,71	0
23	CLA	c	511	65/65	0.97	0.19	54,63,79,88	0

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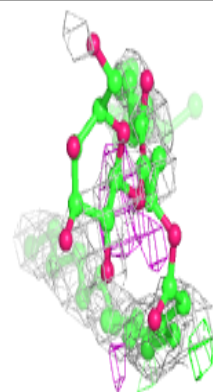
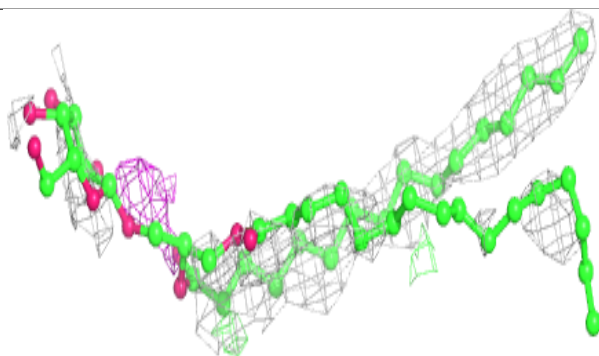
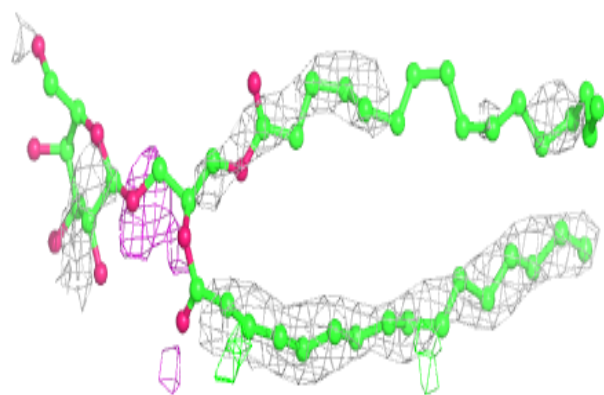
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	512	65/65	0.97	0.29	52,61,74,79	0
23	CLA	B	606	65/65	0.97	0.12	39,50,95,104	0
23	CLA	a	403	65/65	0.97	0.19	37,43,66,74	0
23	CLA	A	405	65/65	0.97	0.21	34,46,107,111	0
38	HEM	e	102	43/43	0.97	0.19	63,77,113,121	0
23	CLA	b	608	65/65	0.97	0.21	45,53,68,73	0
39	MG	j	102	1/1	0.97	0.08	61,61,61,61	0
40	HEC	v	202	43/43	0.97	0.12	53,60,67,72	0
23	CLA	a	404	65/65	0.98	0.15	35,43,52,58	0
23	CLA	A	403	65/65	0.98	0.21	34,38,63,71	0
37	BCT	D	401[A]	4/4	0.98	0.09	57,57,60,62	4
37	BCT	D	401[B]	4/4	0.98	0.09	59,59,61,64	4
23	CLA	d	402	65/65	0.98	0.22	37,44,70,78	0
36	CA	C	525	1/1	0.98	0.21	68,68,68,68	0
38	HEM	E	102	43/43	0.98	0.13	58,65,82,93	0
23	CLA	D	403	65/65	0.98	0.24	33,40,57,69	0
23	CLA	B	612	65/65	0.98	0.15	36,44,58,67	0
23	CLA	A	404	65/65	0.98	0.18	32,40,51,56	0
40	HEC	V	201	43/43	0.98	0.09	44,51,55,56	0
24	PHO	a	406	64/64	0.98	0.14	35,44,51,58	0
21	FE2	a	401[A]	1/1	0.99	0.02	56,56,56,56	1
21	FE2	a	401[B]	1/1	0.99	0.02	63,63,63,63	1
22	CL	C	501	1/1	0.99	0.12	43,43,43,43	0
22	CL	c	501	1/1	0.99	0.11	46,46,46,46	0
28	OEX	A	412[A]	10/10	0.99	0.10	42,45,49,49	10
28	OEX	A	412[B]	10/10	0.99	0.10	39,46,51,51	10
22	CL	a	402	1/1	1.00	0.08	46,46,46,46	0
21	FE2	A	401[B]	1/1	1.00	0.03	57,57,57,57	1
22	CL	A	402	1/1	1.00	0.09	39,39,39,39	0
21	FE2	A	401[A]	1/1	1.00	0.03	54,54,54,54	1
28	OEX	a	413[A]	10/10	1.00	0.10	46,48,52,56	10
28	OEX	a	413[B]	10/10	1.00	0.10	44,50,54,54	10

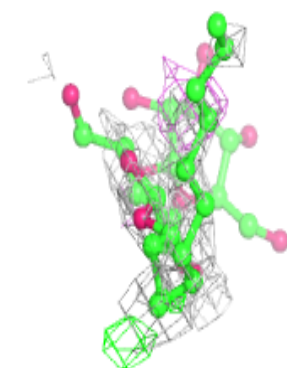
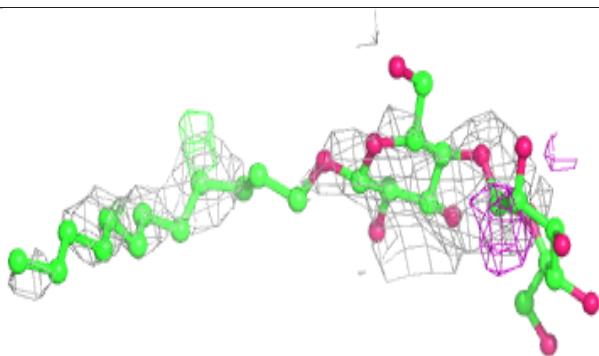
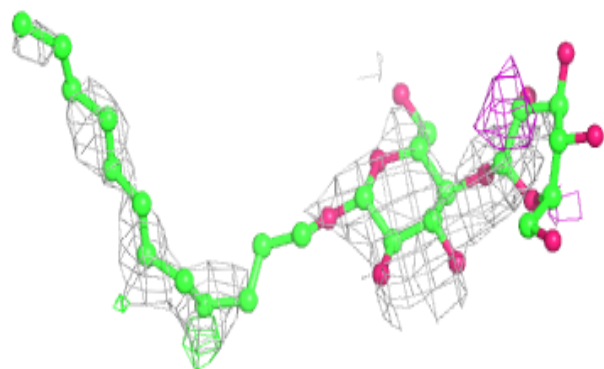
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMG C 522:

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

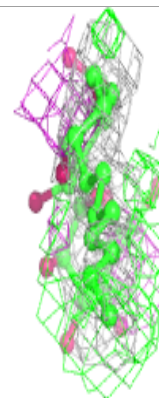
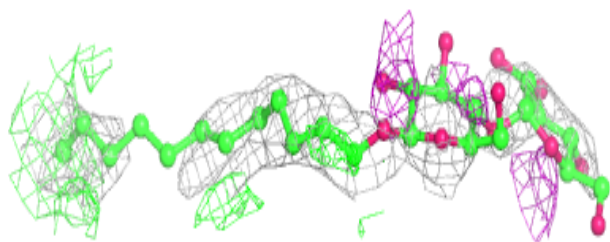
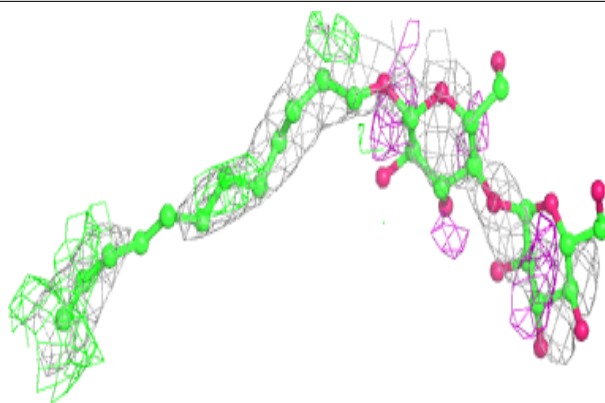
**Electron density around LMT C 526:**

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

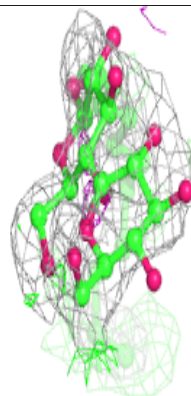
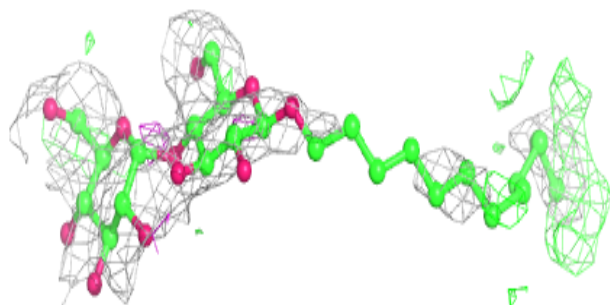
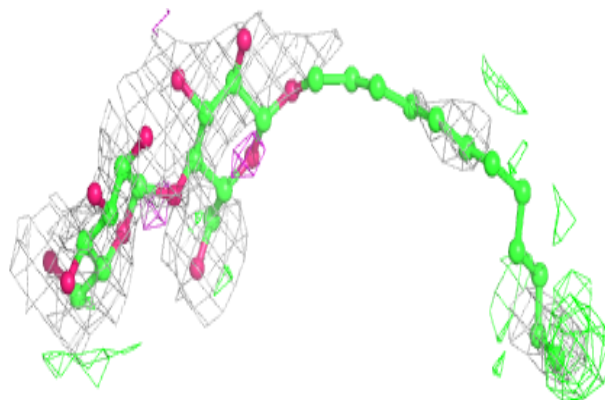


Electron density around LMT a 412:

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

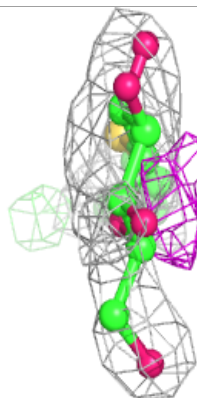
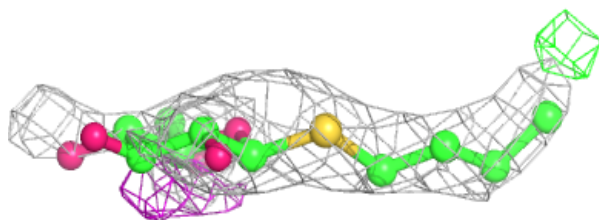
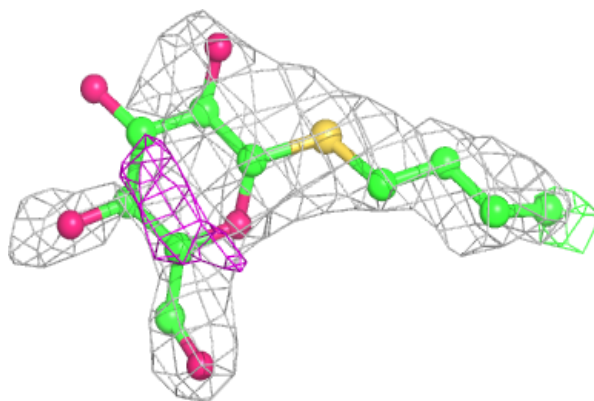
**Electron density around LMT F 101:**

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

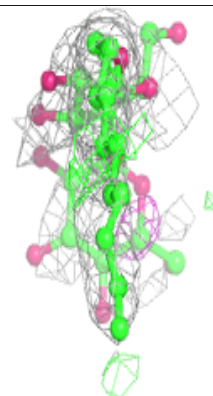
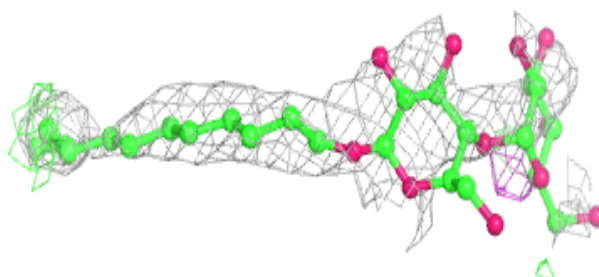
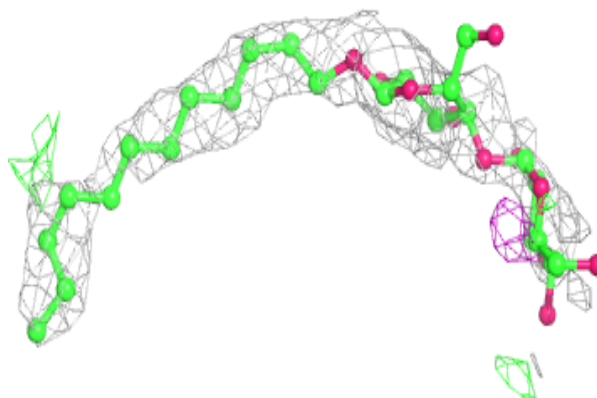


Electron density around HTG D 411:

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

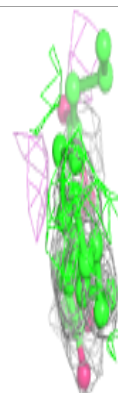
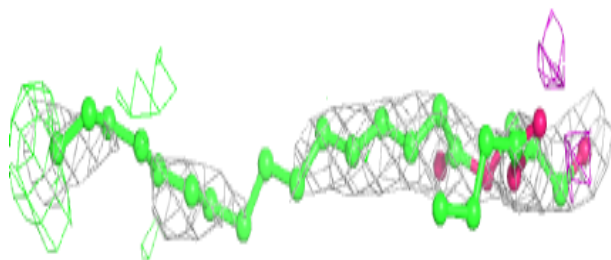
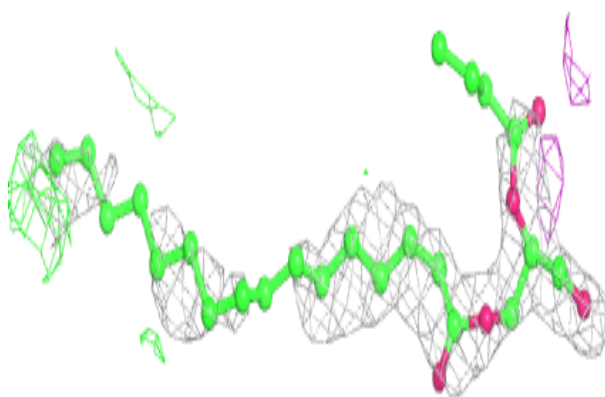
**Electron density around LMT M 103:**

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

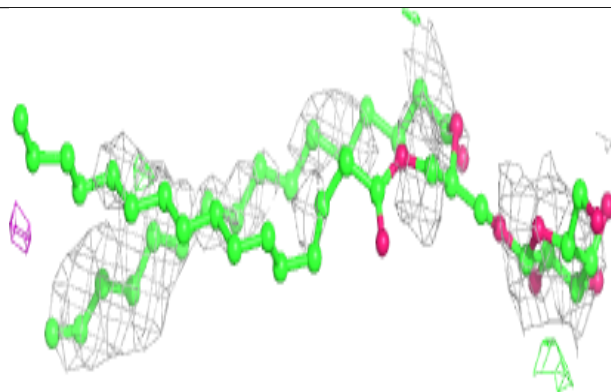
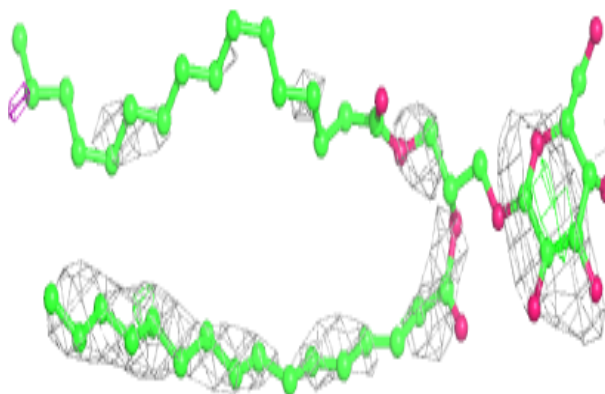


Electron density around UNL A 414:

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

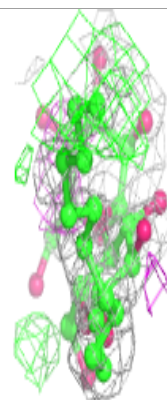
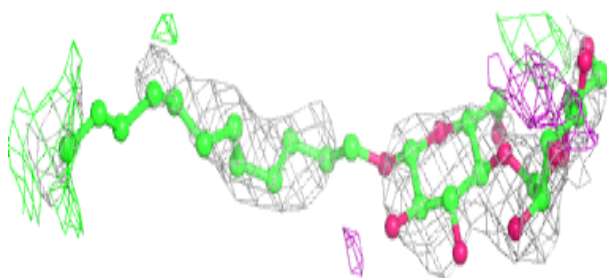
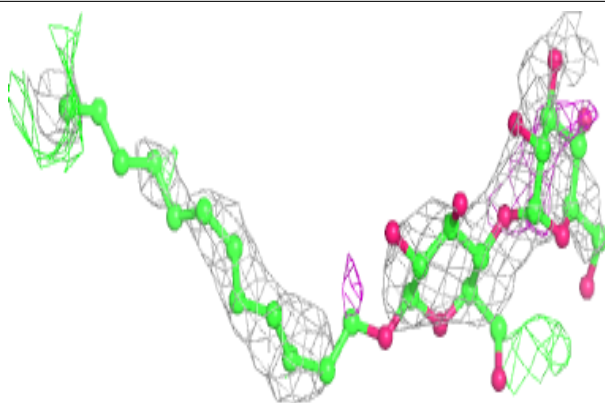
**Electron density around LMG c 522:**

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

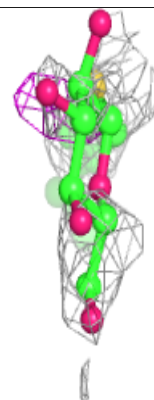
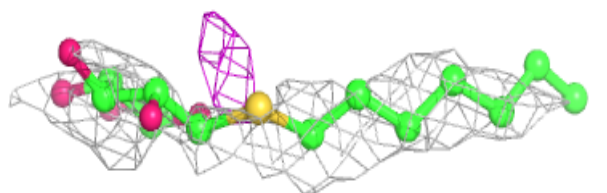
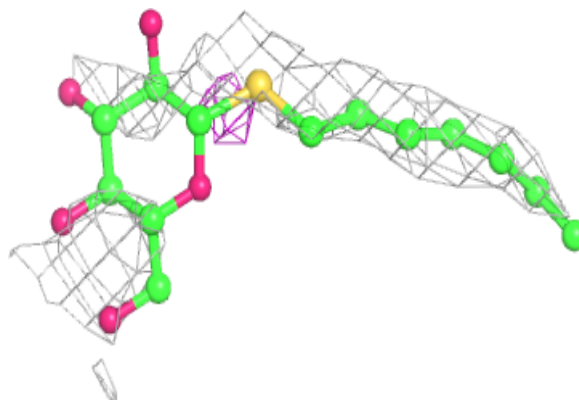


Electron density around LMT D 402:

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

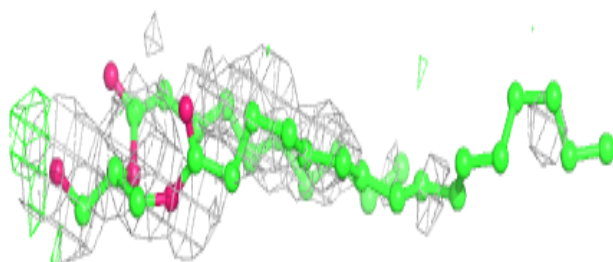
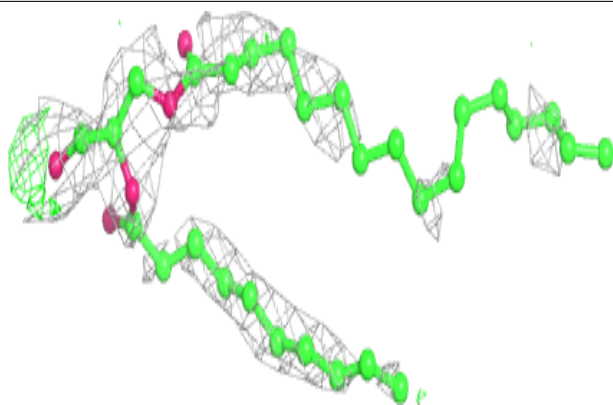
**Electron density around HTG b 622:**

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

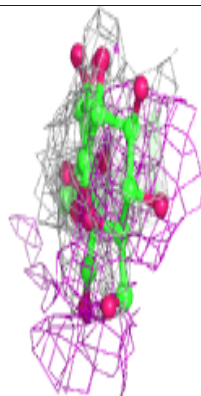
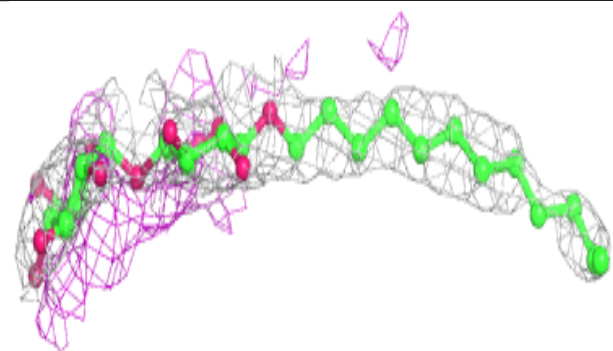
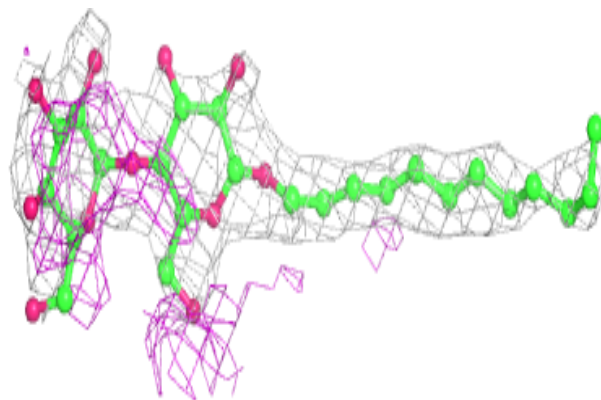


Electron density around UNL C 527:

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

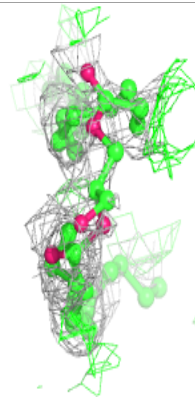
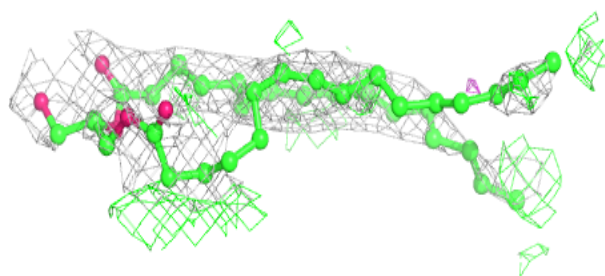
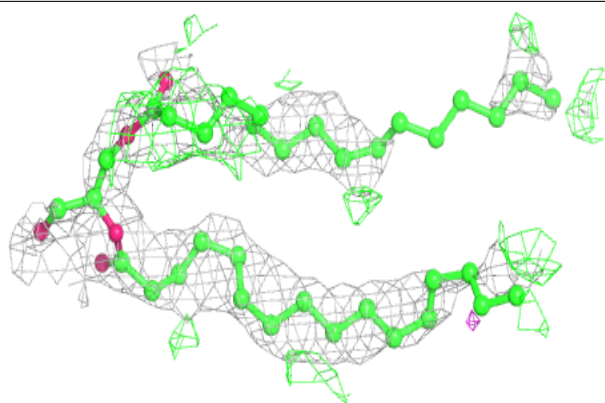
**Electron density around LMT m 103:**

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

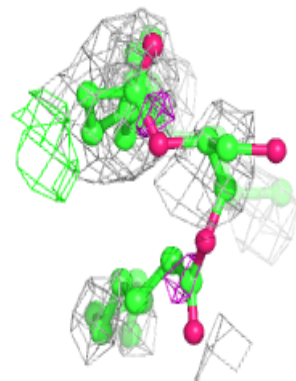
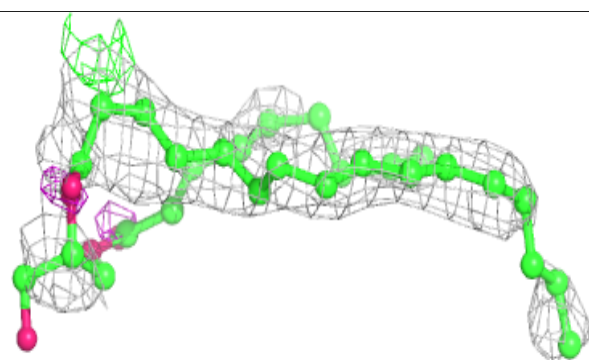
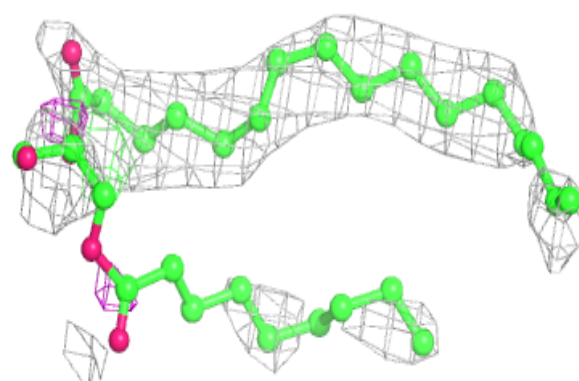


Electron density around UNL I 101:

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

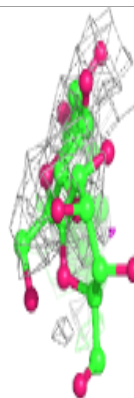
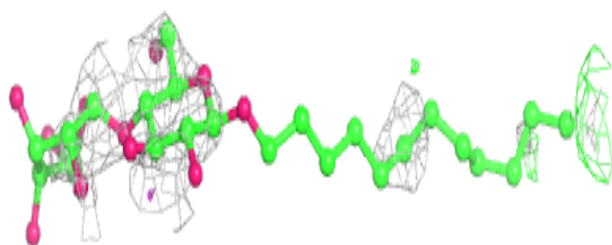
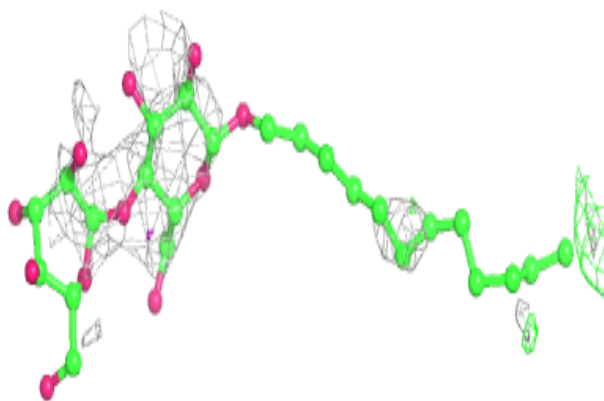
**Electron density around UNL b 625:**

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

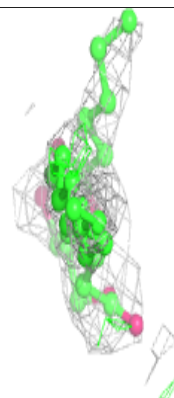
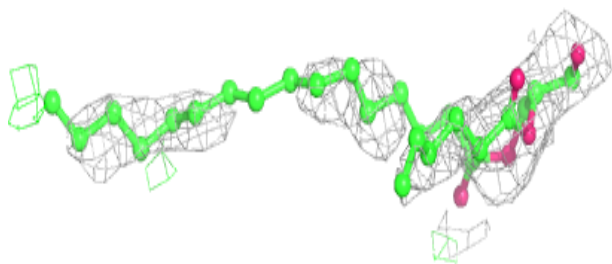
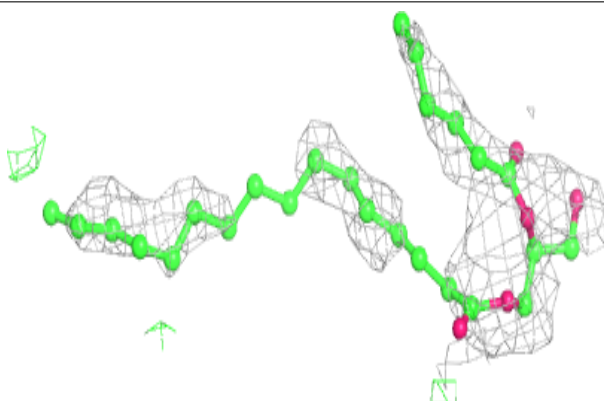


Electron density around LMT e 101:

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

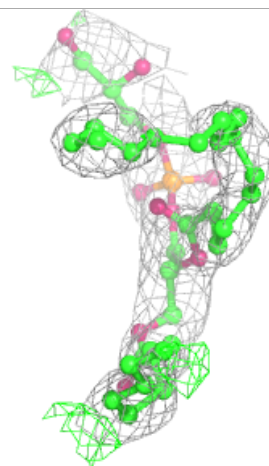
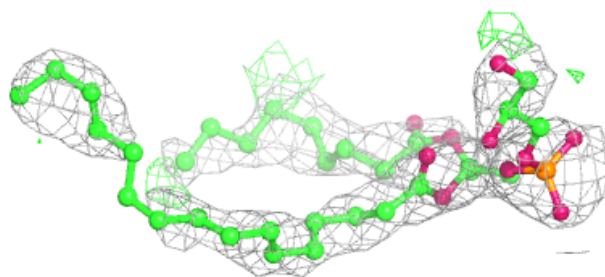
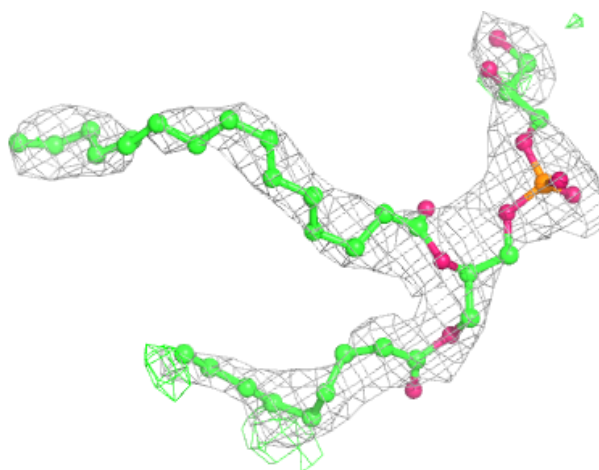
**Electron density around UNL a 415:**

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



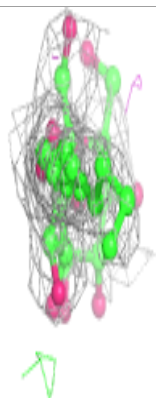
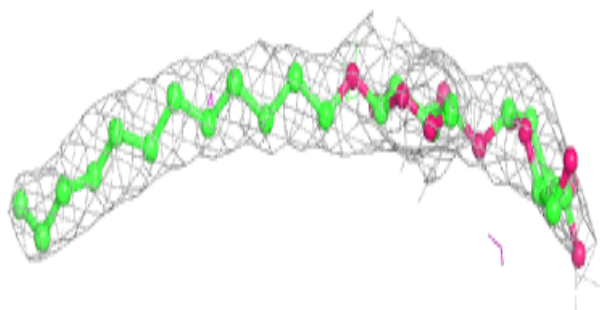
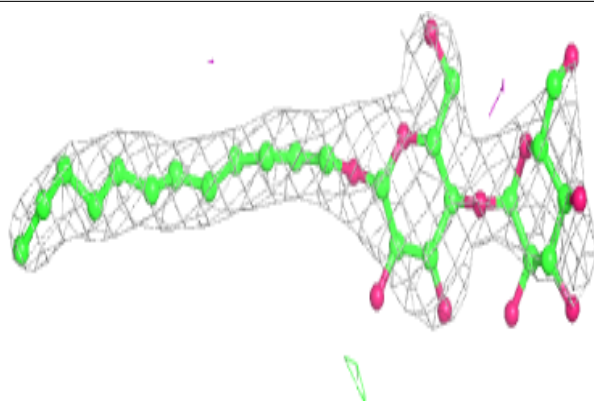
Electron density around LHG E 101:

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

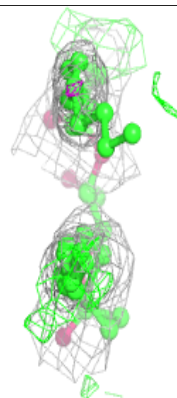
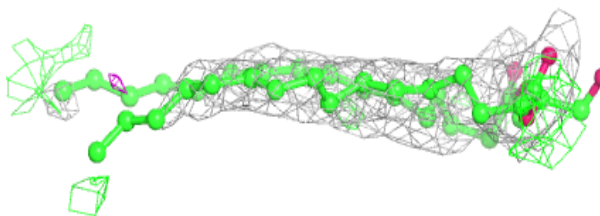
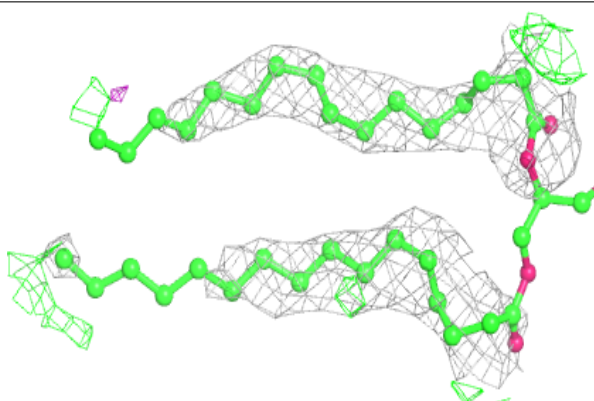


Electron density around LMT M 102:

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

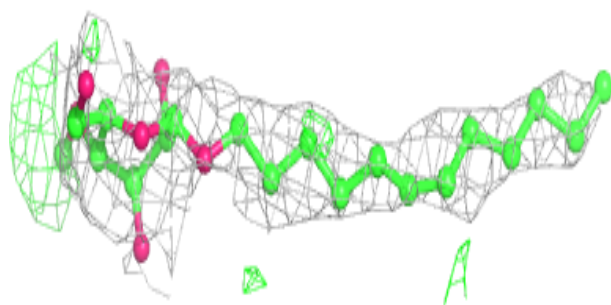
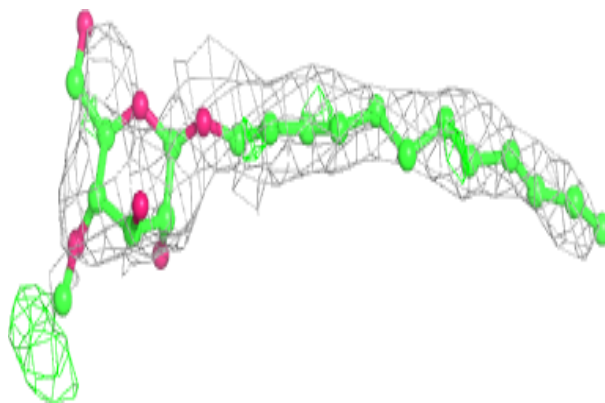
**Electron density around UNL i 101:**

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

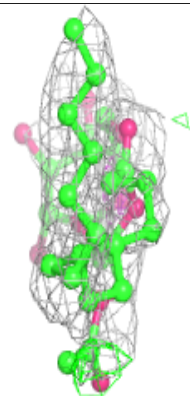
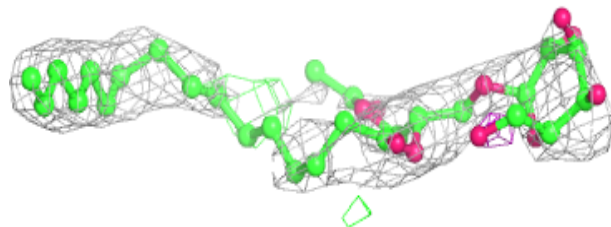
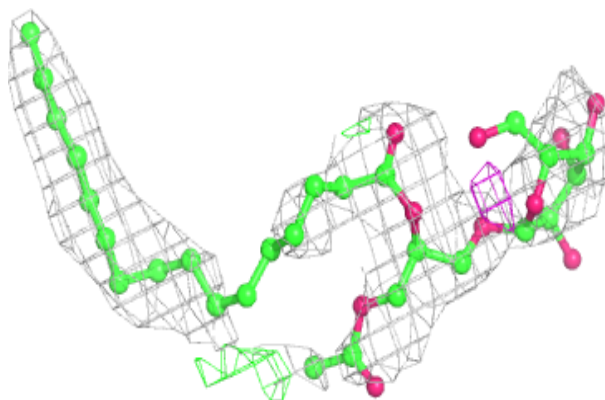


Electron density around LMT b 620:

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

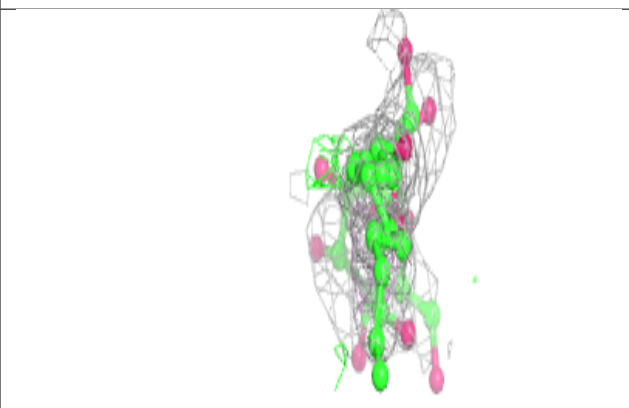
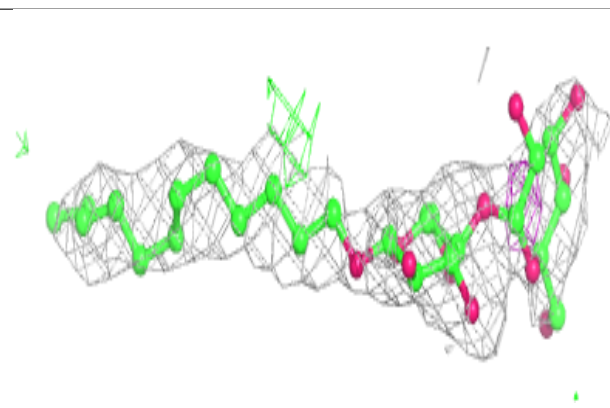
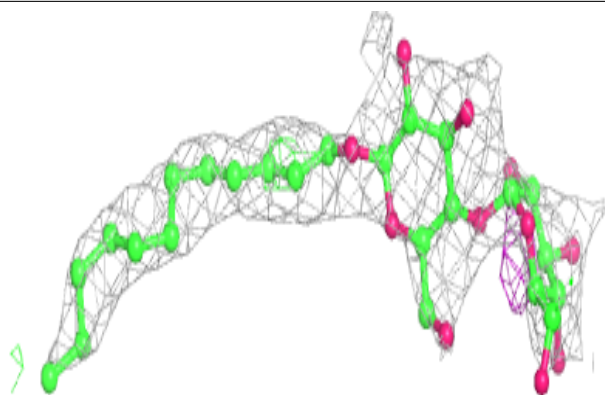
**Electron density around LMG Z 101:**

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

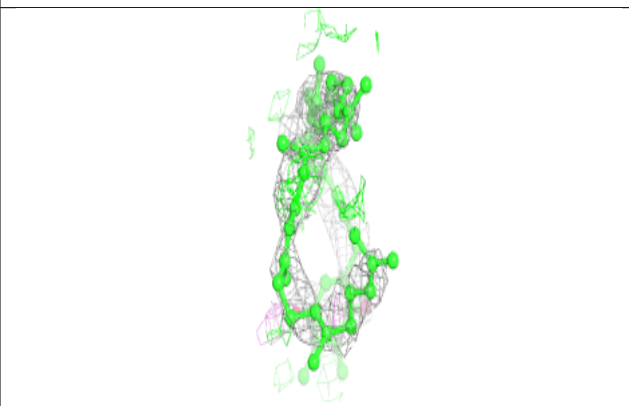
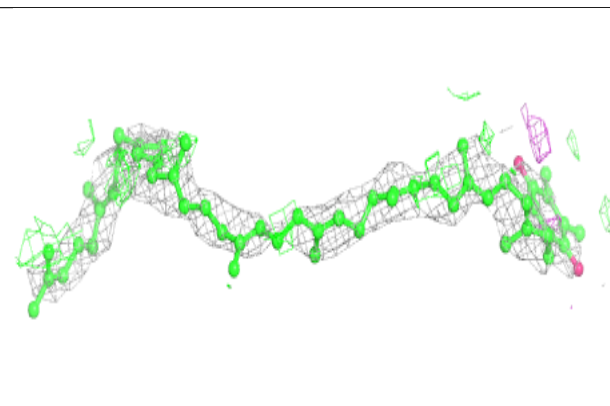
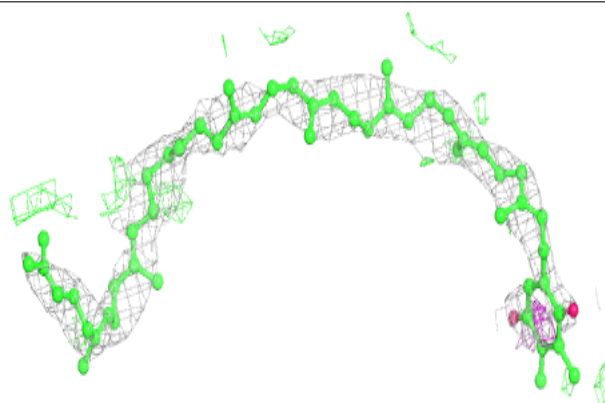


Electron density around LMT B 627:

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

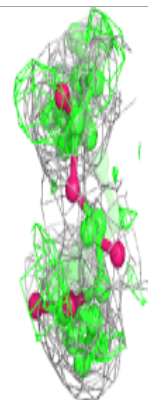
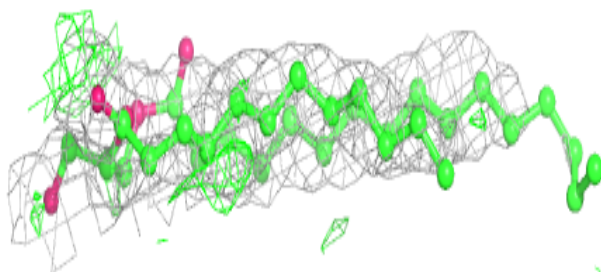
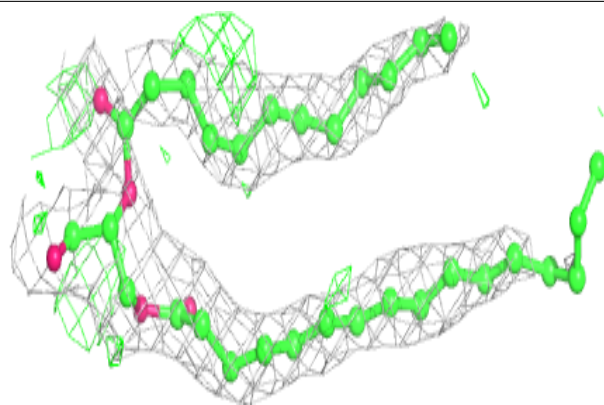
**Electron density around PL9 A 413 (A):**

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

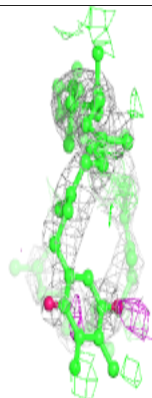
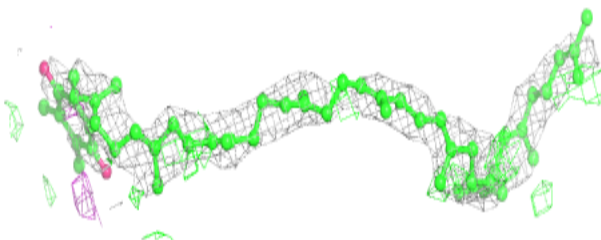
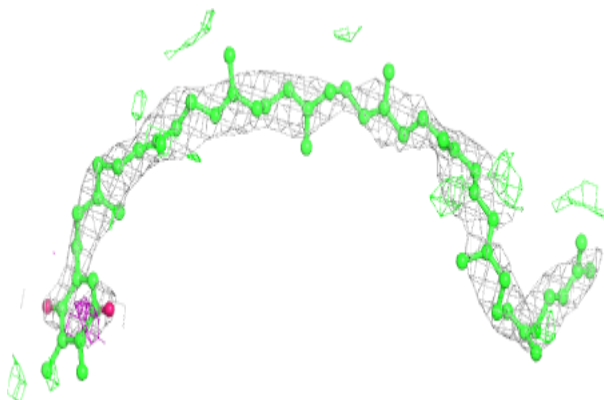


Electron density around UNL d 410:

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

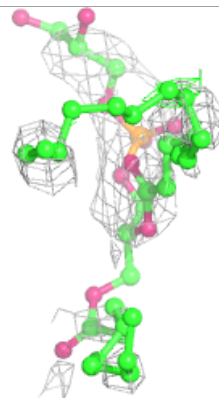
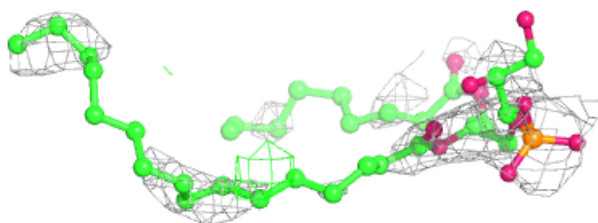
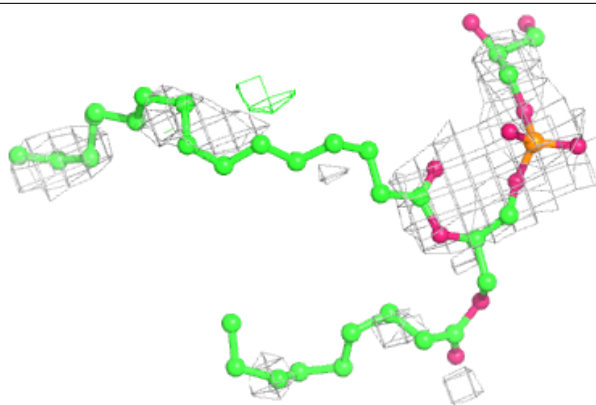
**Electron density around PL9 A 413 (B):**

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

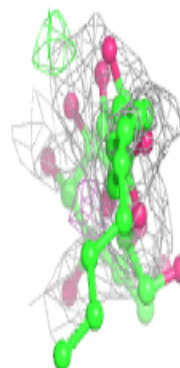
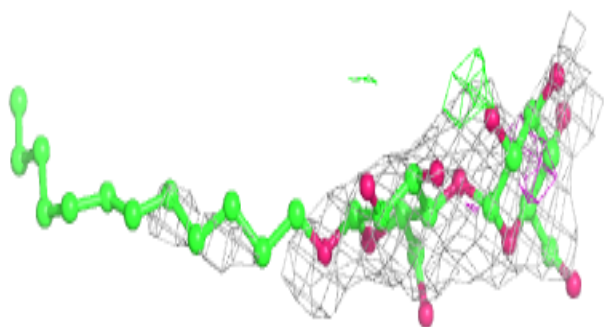
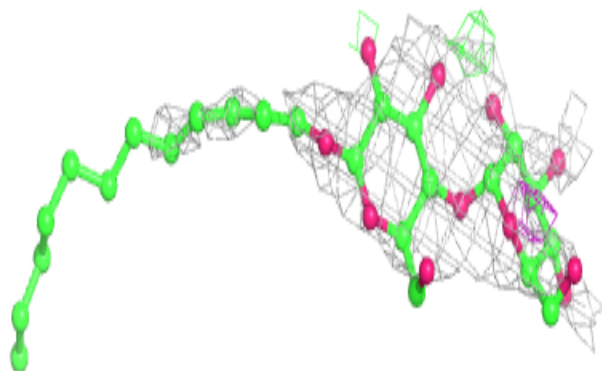


Electron density around LHG a 419:

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

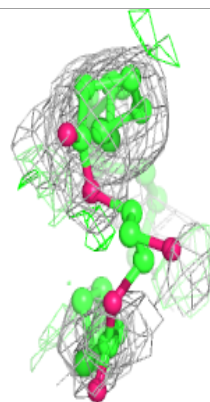
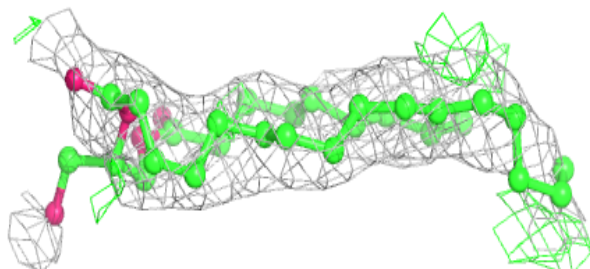
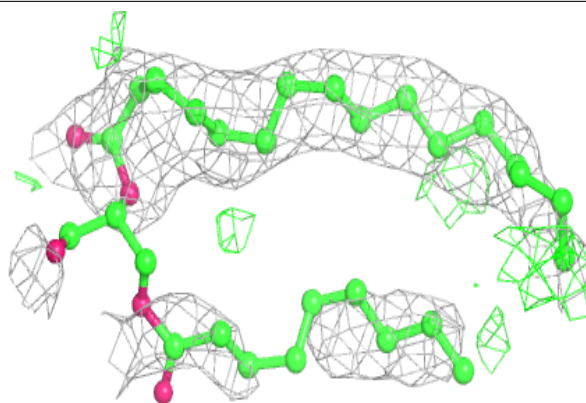
**Electron density around LMT a 418:**

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

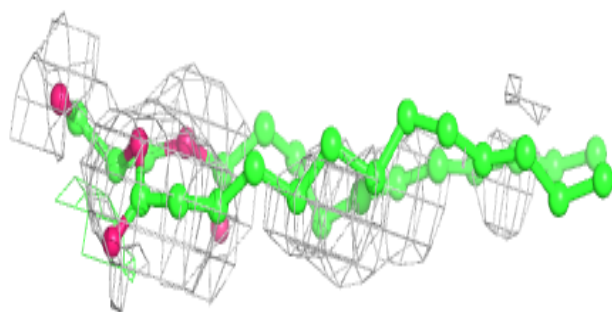
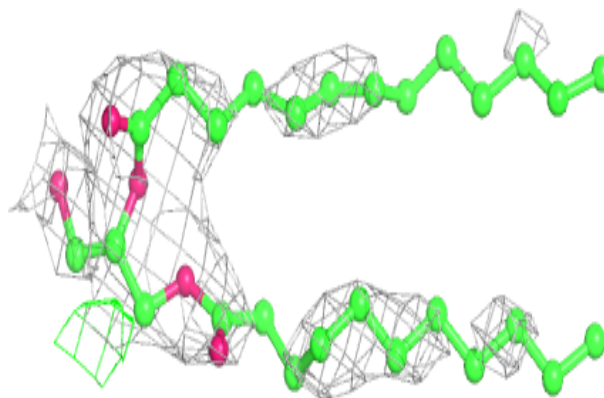


Electron density around UNL B 625:

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

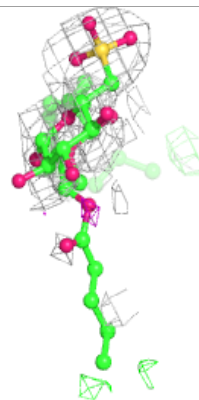
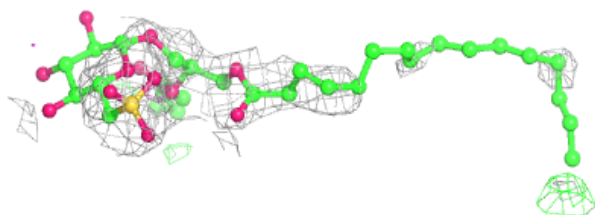
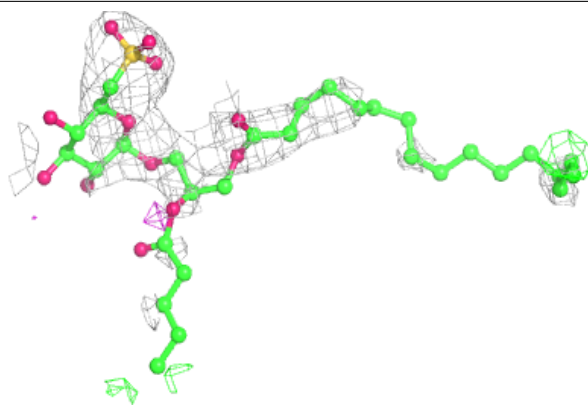
**Electron density around UNL c 526:**

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

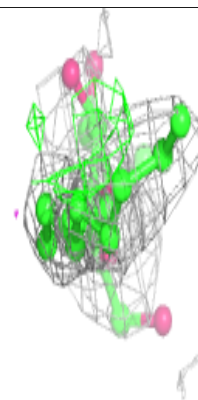
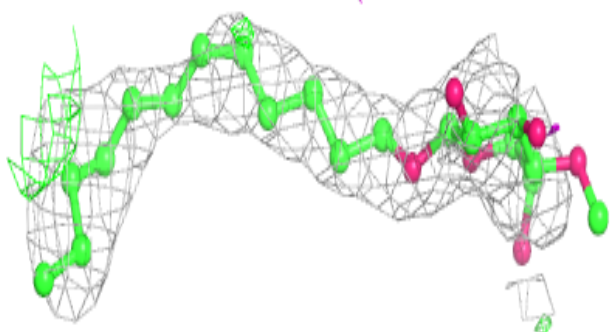
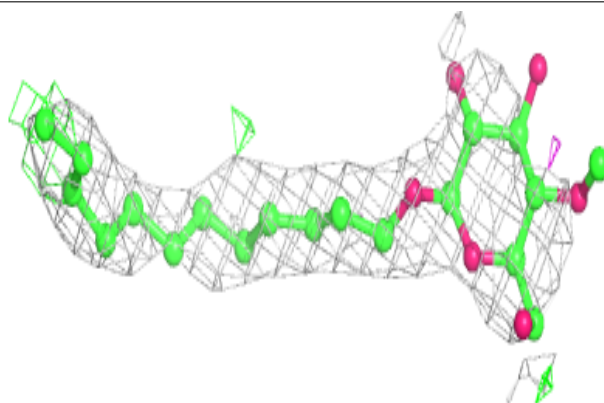


Electron density around SQD f 101:

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

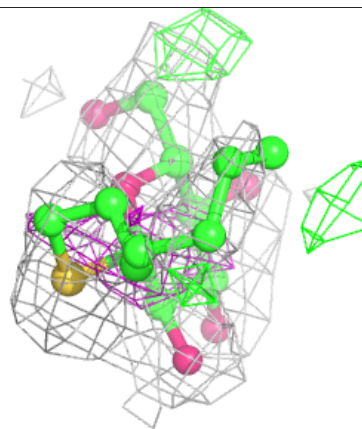
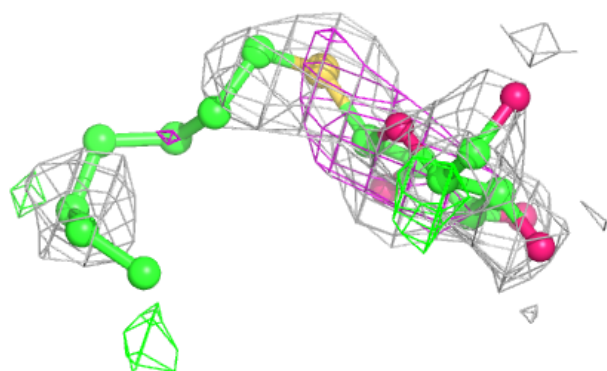
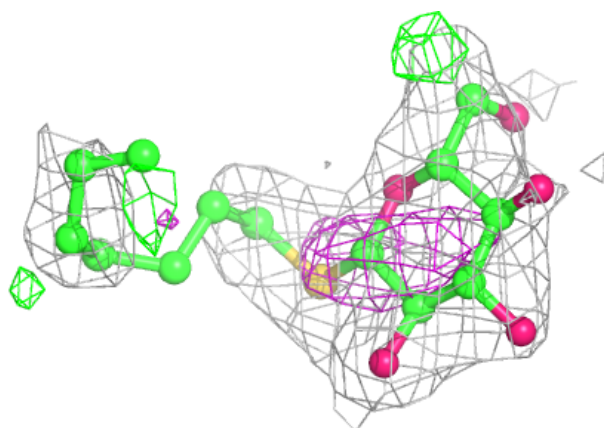
**Electron density around LMT B 629:**

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

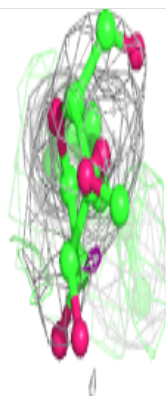
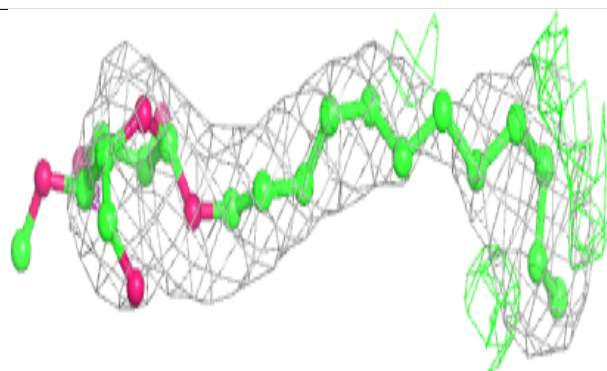
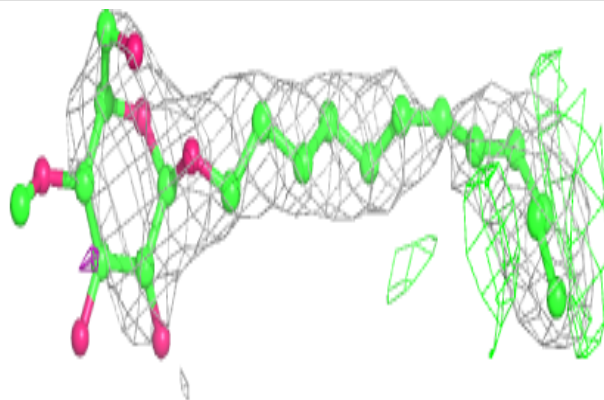


Electron density around HTG B 622:

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

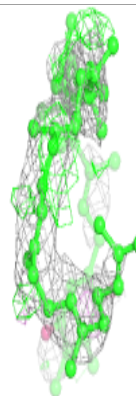
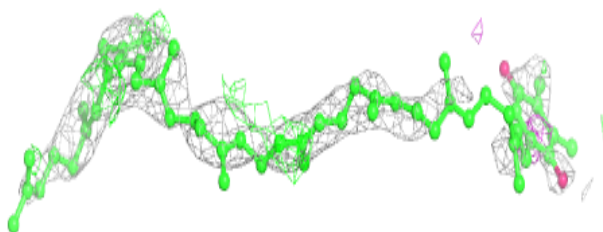
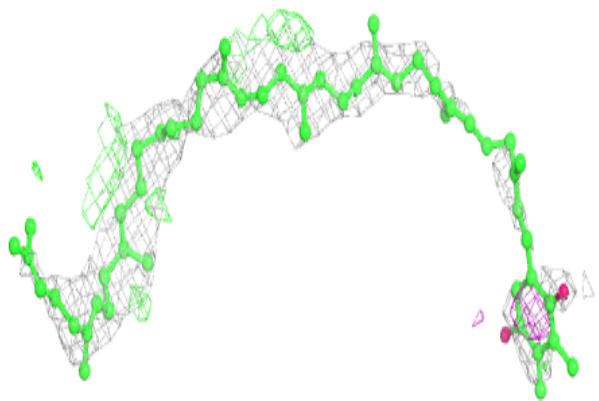
**Electron density around LMT b 626:**

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

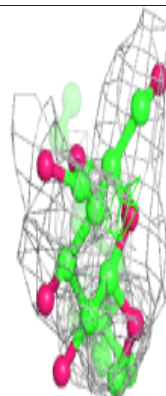
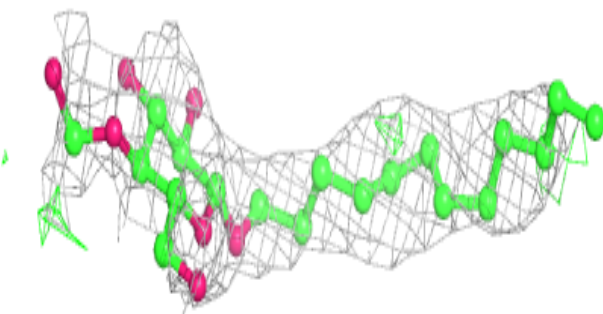
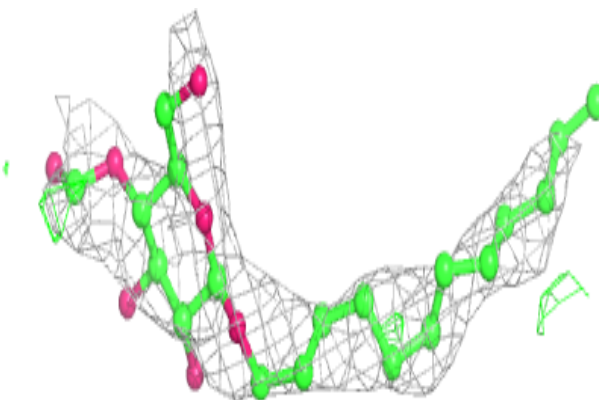


Electron density around PL9 a 414 (A):

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

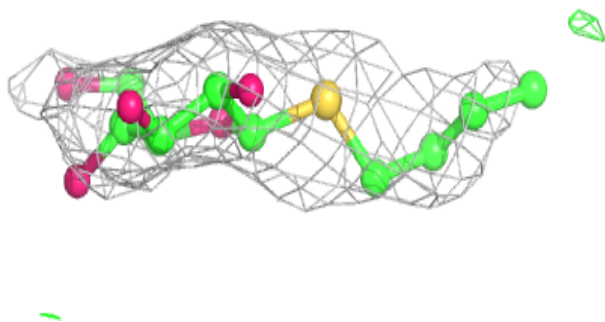
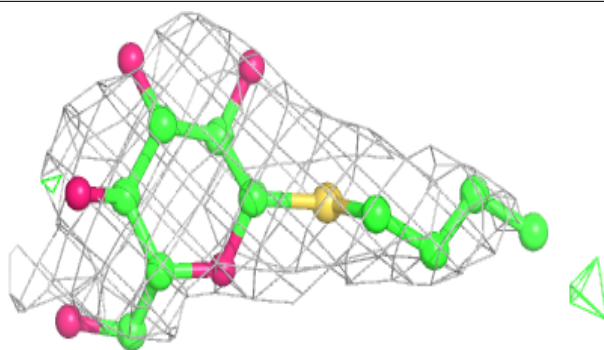
**Electron density around LMT B 630:**

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

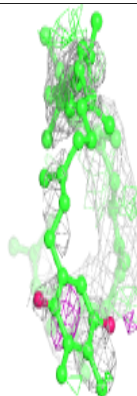
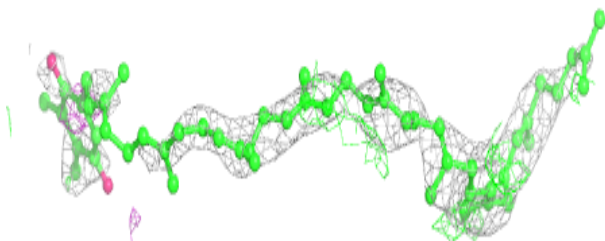
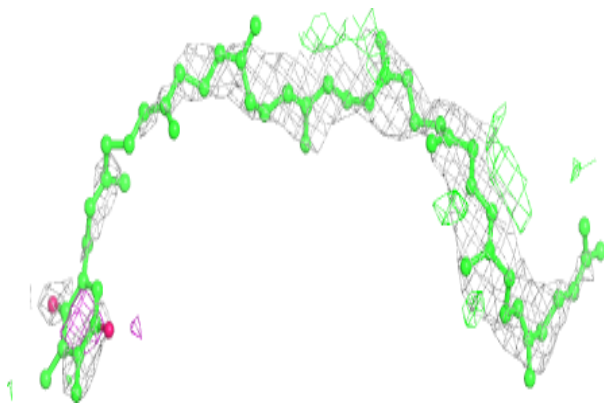


Electron density around HTG h 101:

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

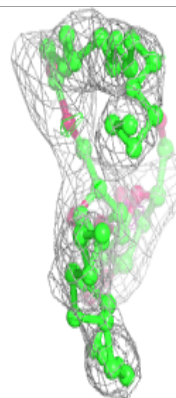
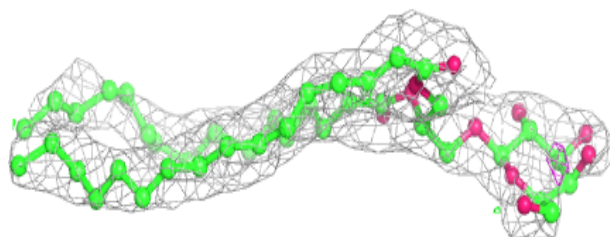
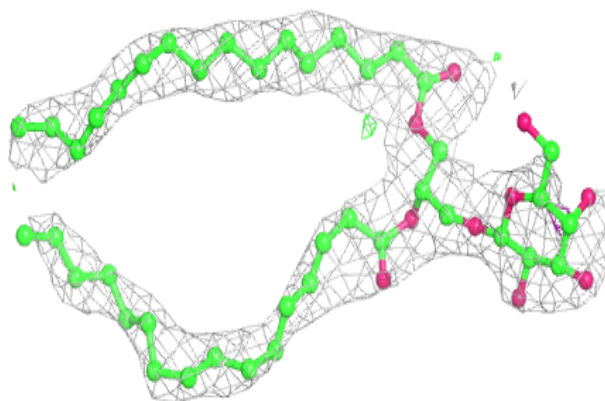
**Electron density around PL9 a 414 (B):**

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

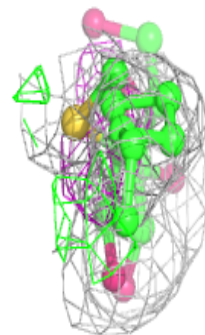
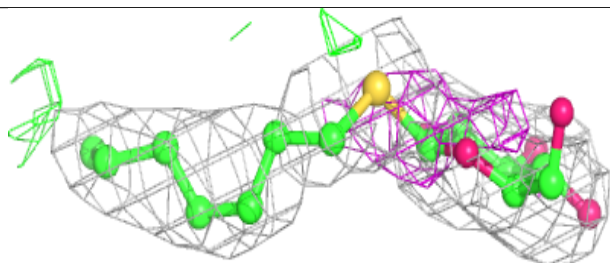
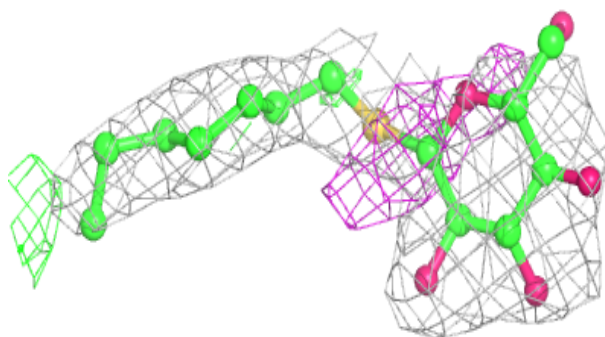


Electron density around LMG a 417:

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

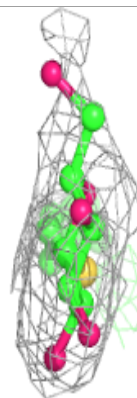
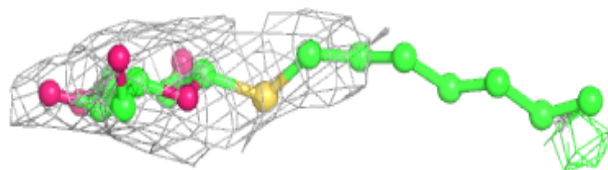
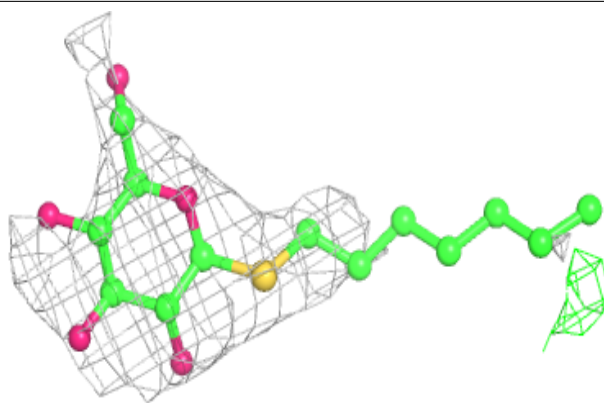
**Electron density around HTG b 621:**

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

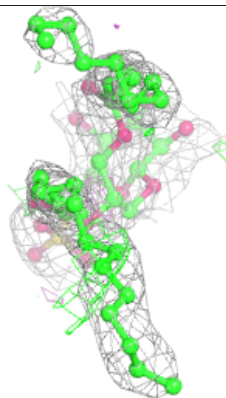
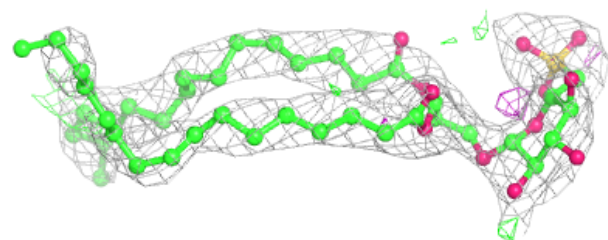
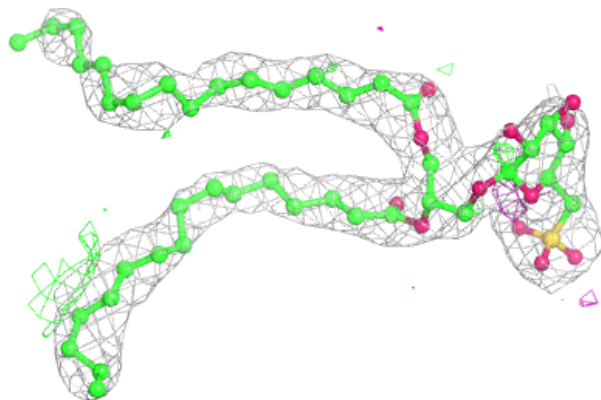


Electron density around HTG c 523:

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

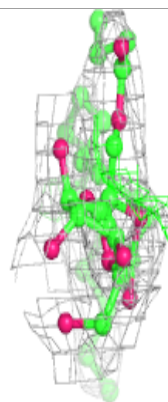
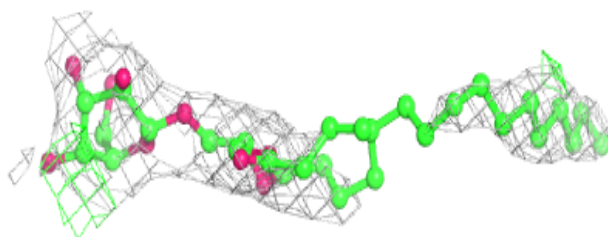
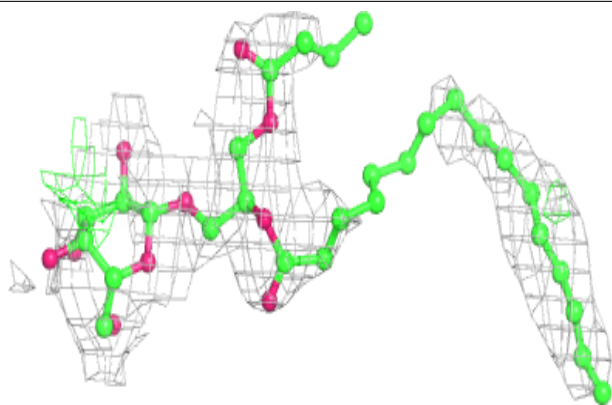
**Electron density around SQD L 102:**

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



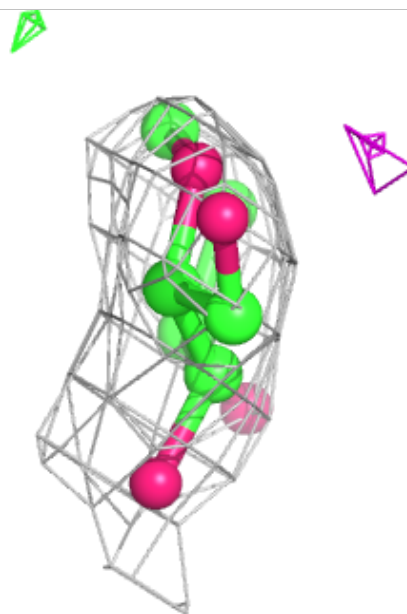
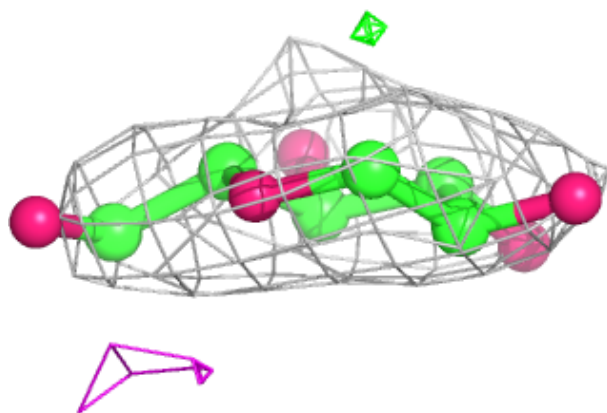
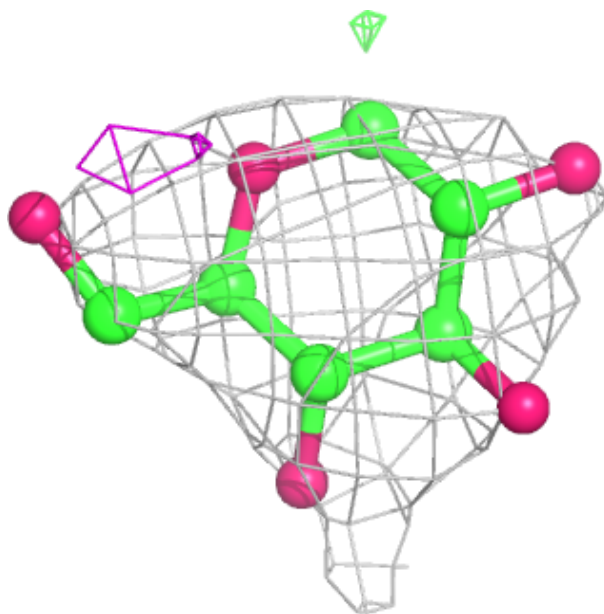
Electron density around LMG z 101:

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



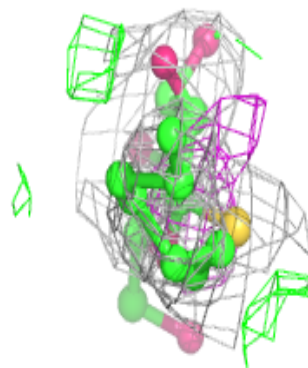
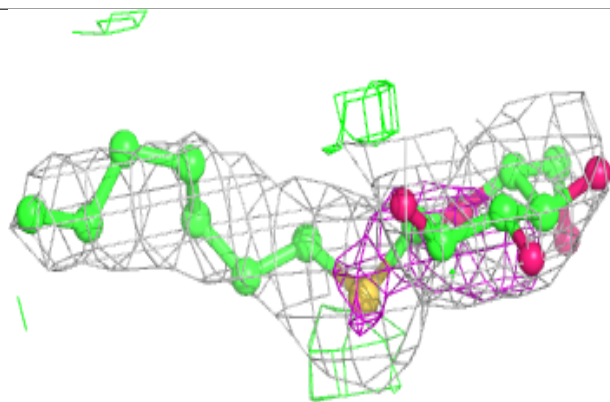
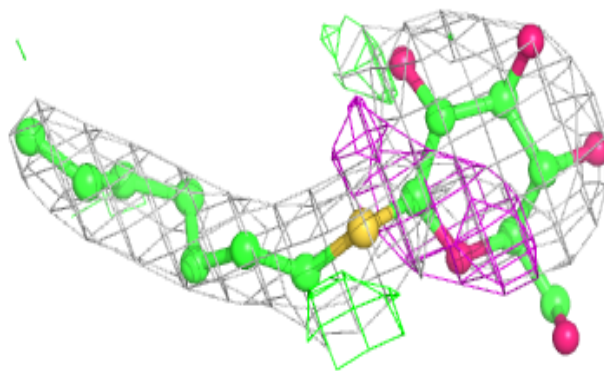
Electron density around HTG V 202:

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



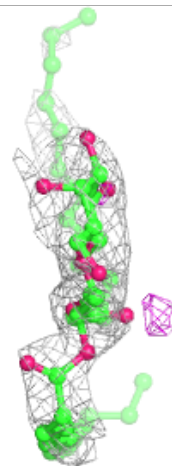
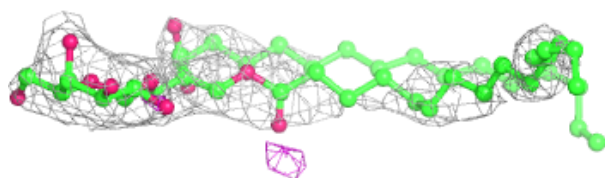
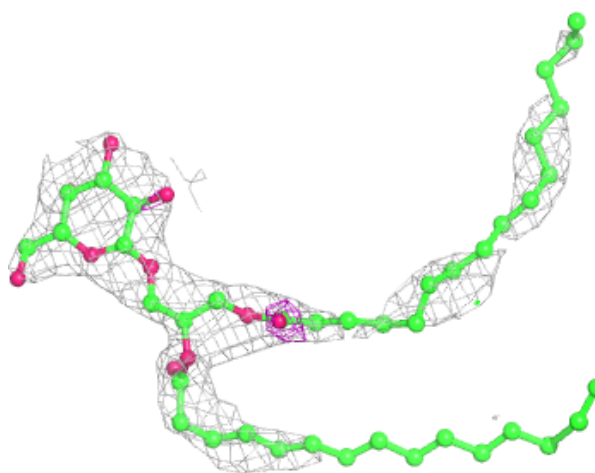
Electron density around HTG B 621:

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



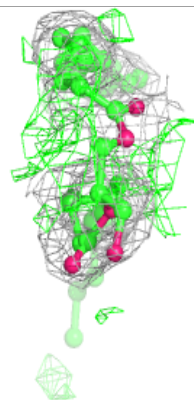
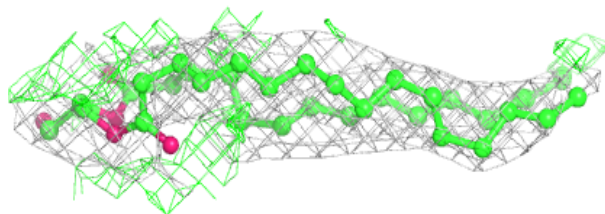
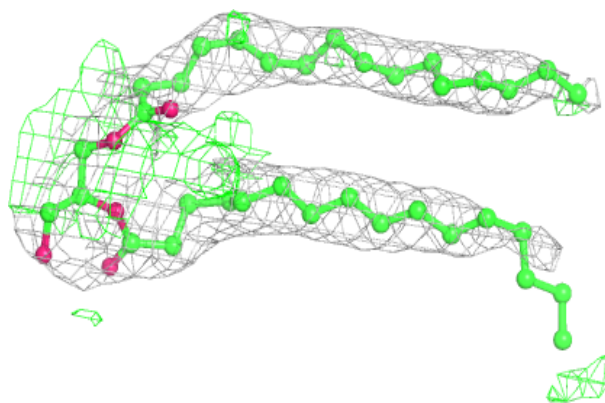
Electron density around LMG c 521:

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

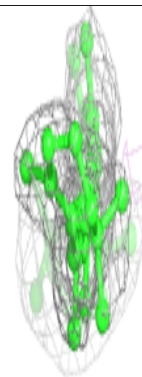
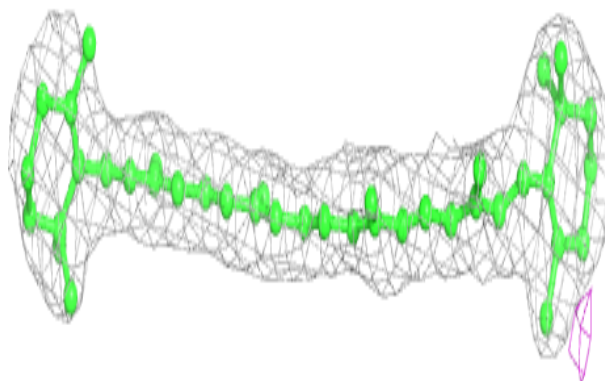
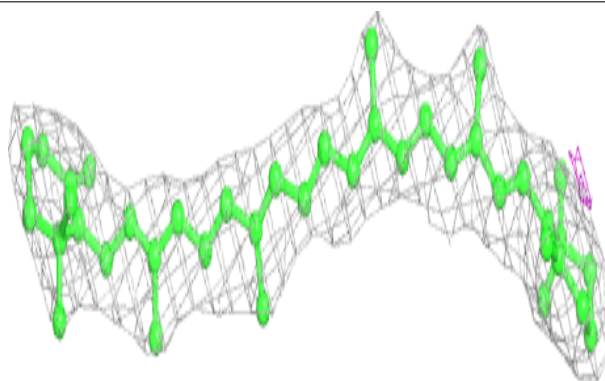


Electron density around UNL D 410:

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

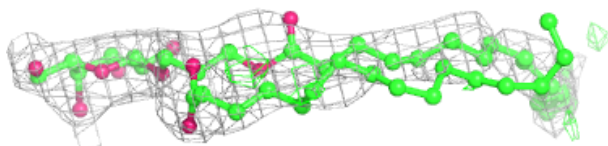
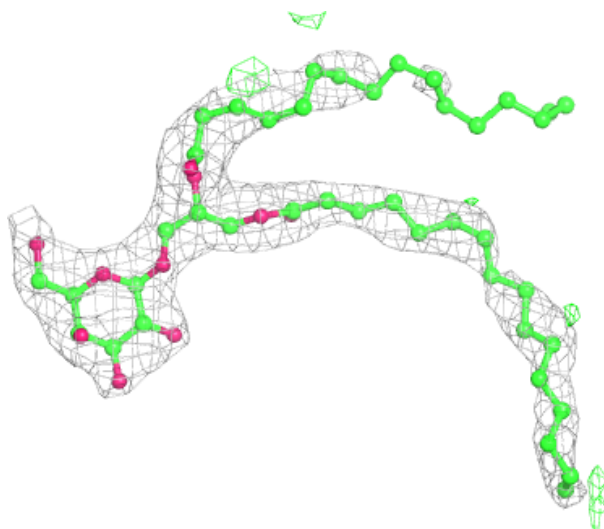
**Electron density around BCR h 102:**

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



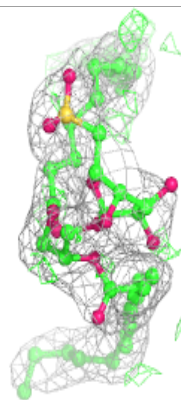
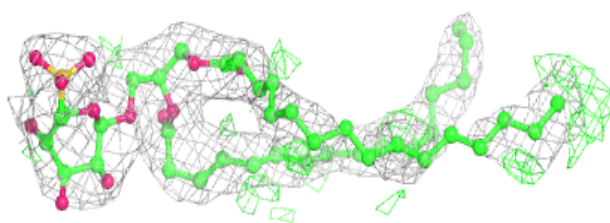
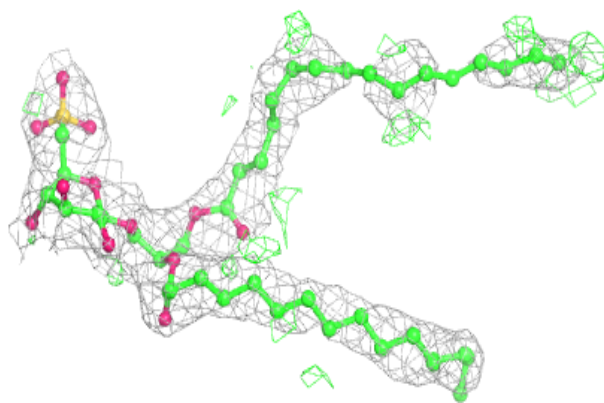
Electron density around LMG C 521:

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

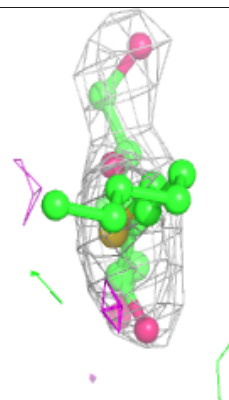
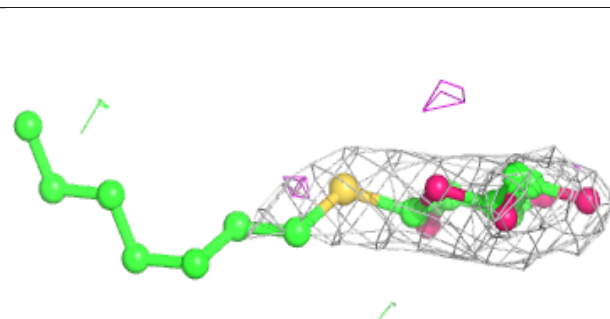
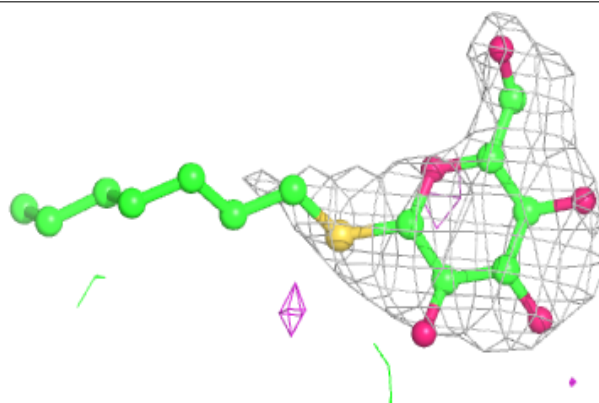


Electron density around SQD A 411:

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

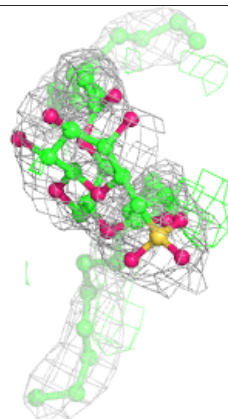
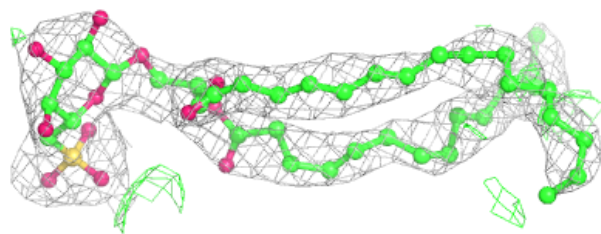
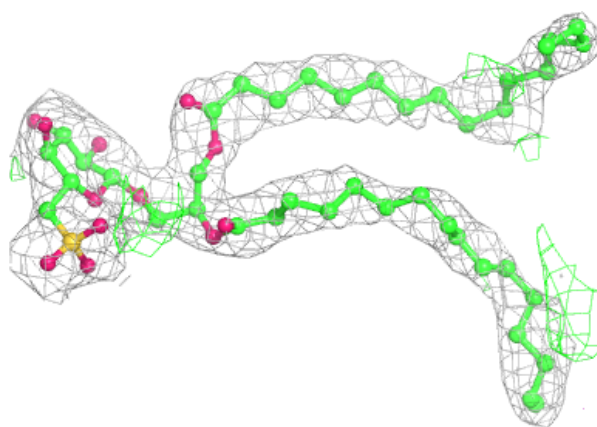
**Electron density around HTG C 523:**

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

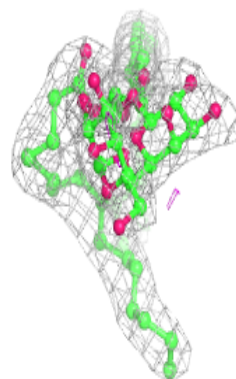
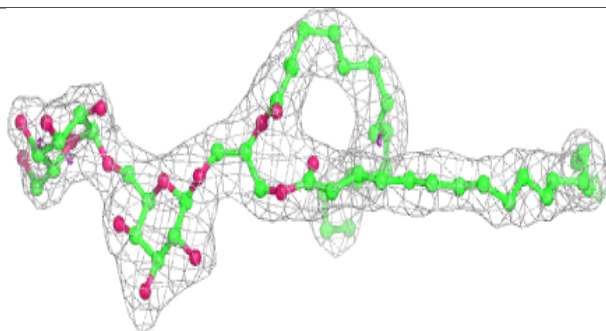
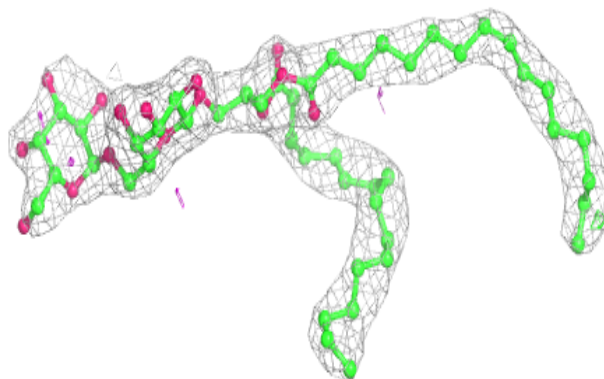


Electron density around SQD B 620:

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

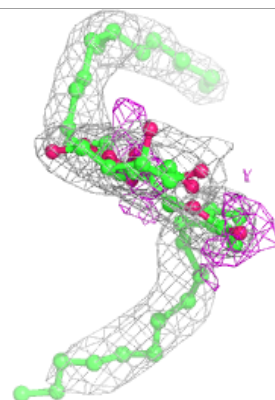
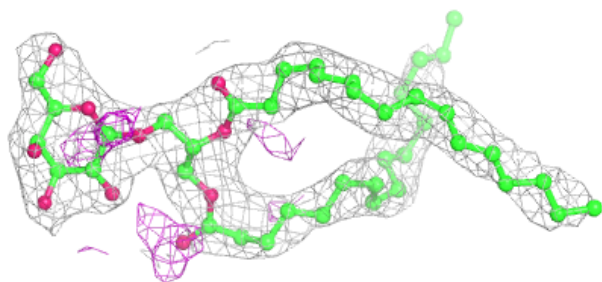
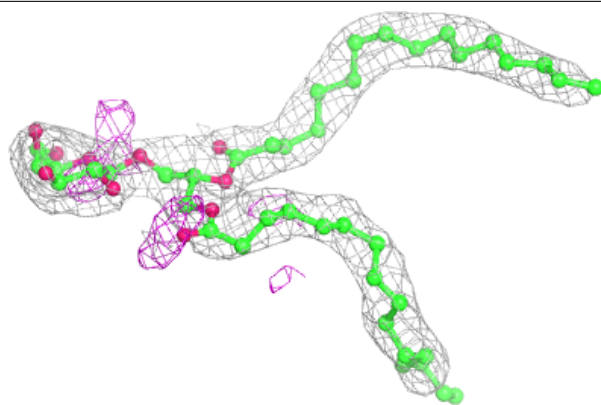
**Electron density around DGD h 103:**

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

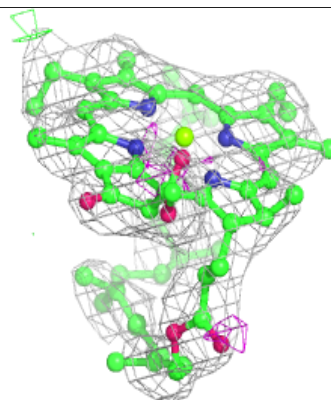
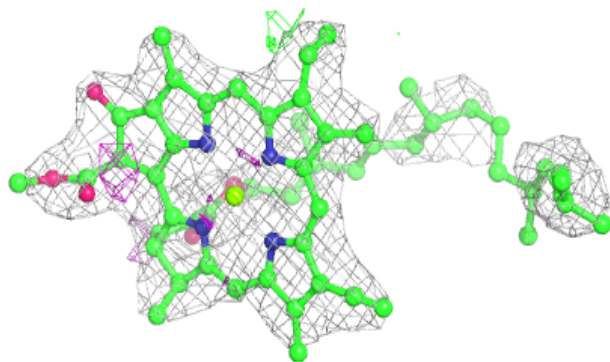
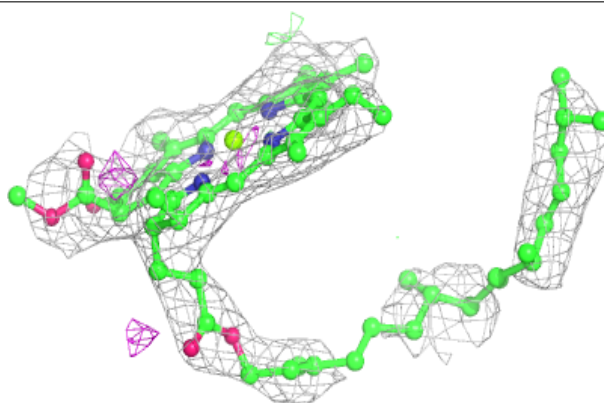


Electron density around LMG M 101:

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

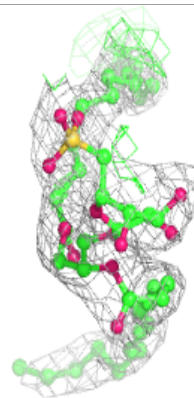
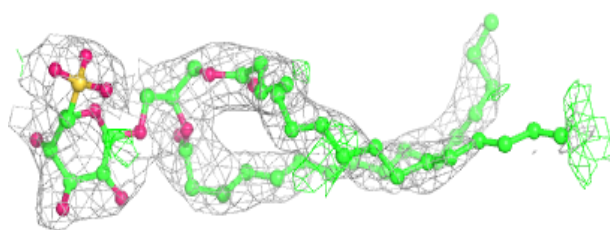
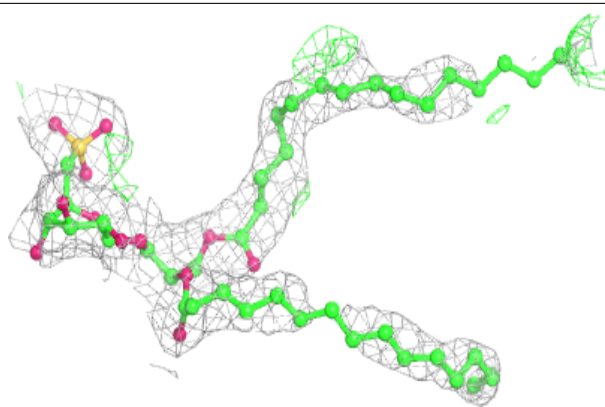
**Electron density around CLA C 515:**

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

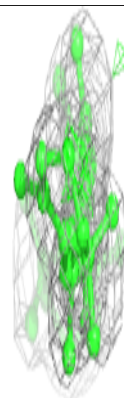
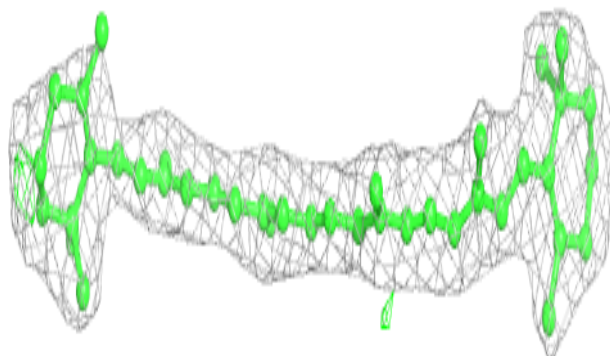
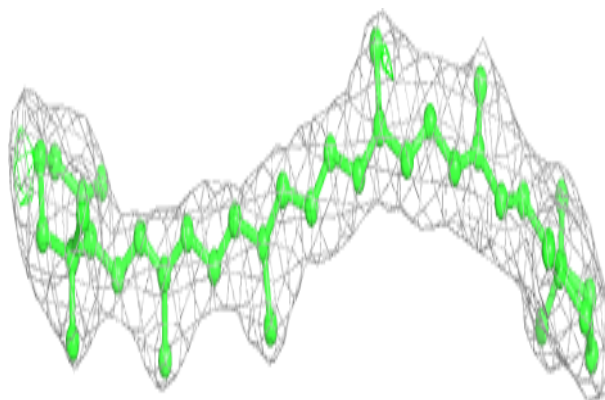


Electron density around SQD a 411:

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

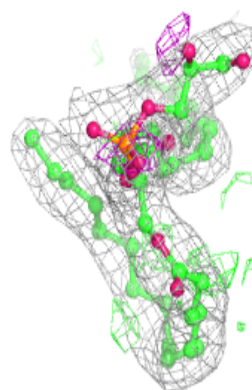
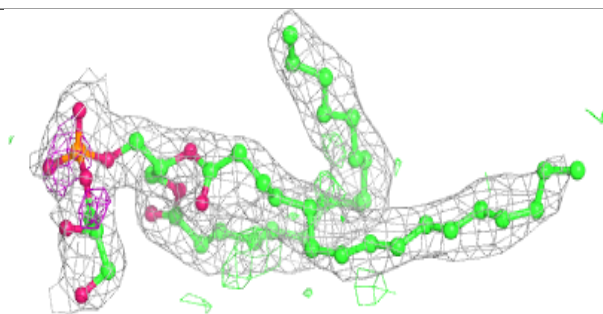
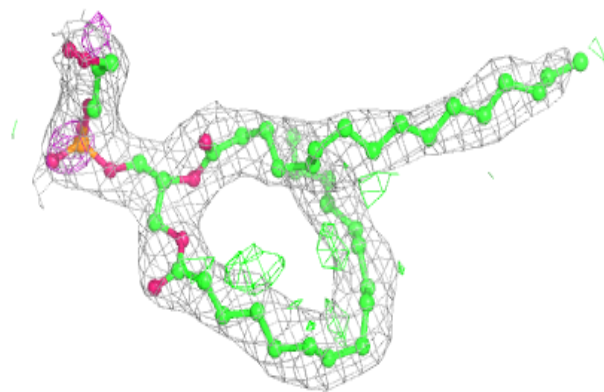
**Electron density around BCR H 101:**

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

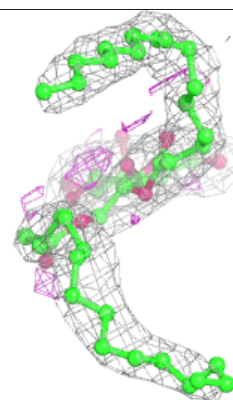
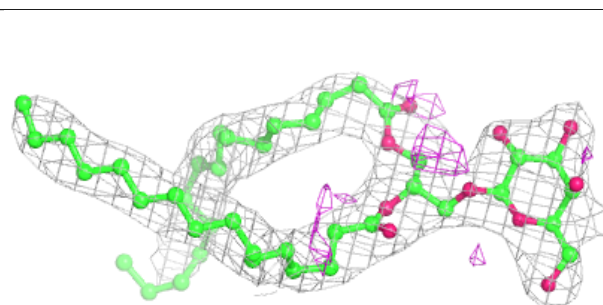
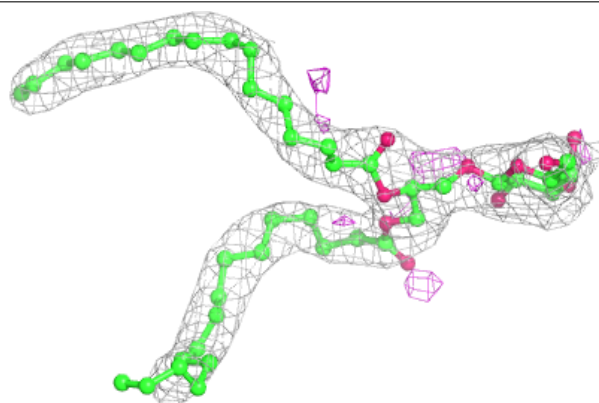


Electron density around LHG A 416:

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

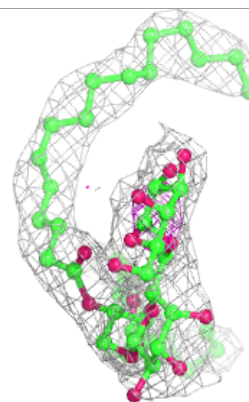
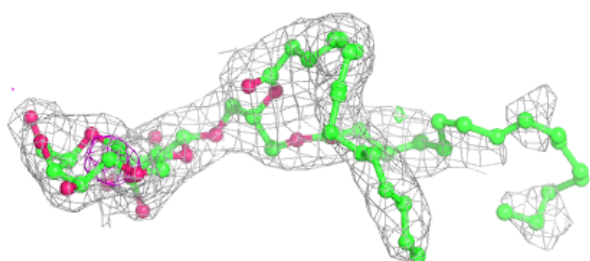
**Electron density around LMG m 101:**

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

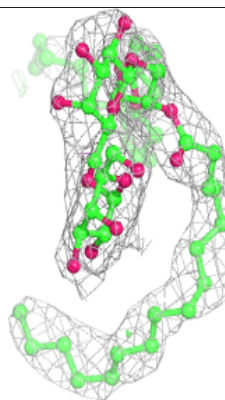
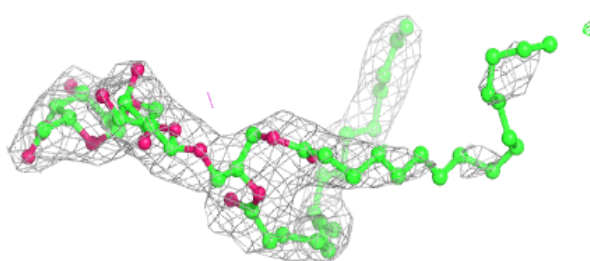
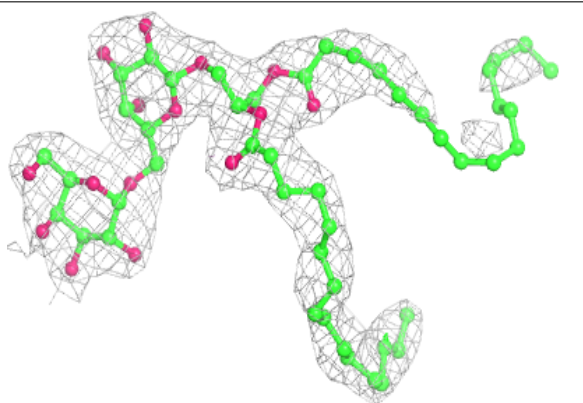


Electron density around DGD C 519:

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

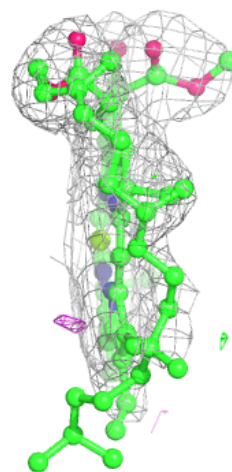
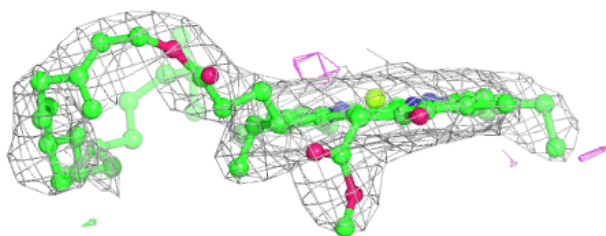
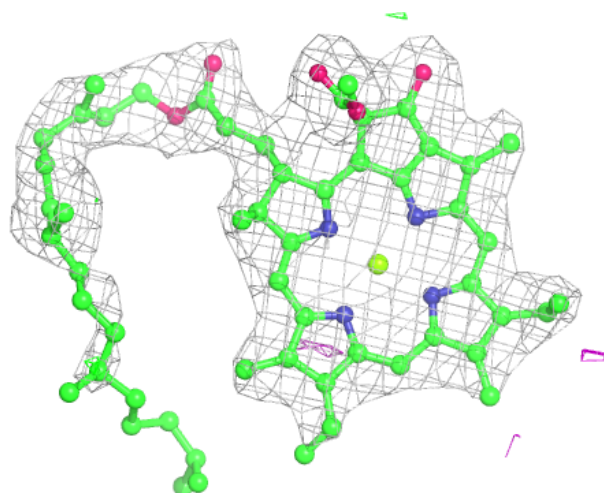
**Electron density around DGD c 519:**

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



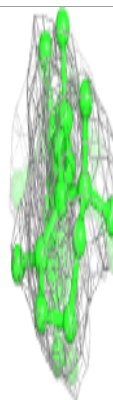
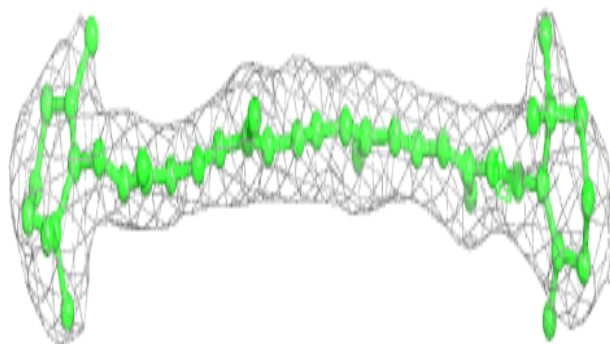
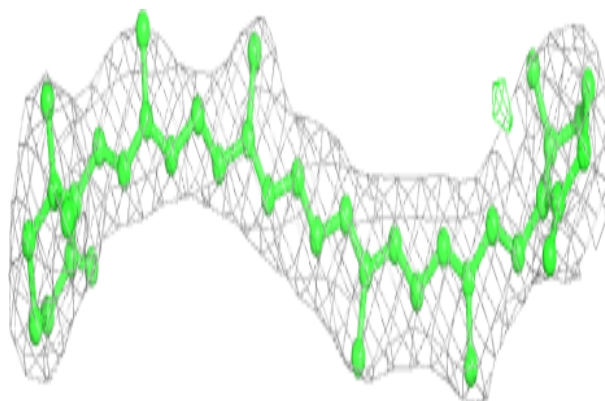
Electron density around CLA C 514:

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

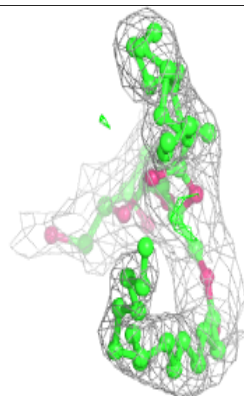
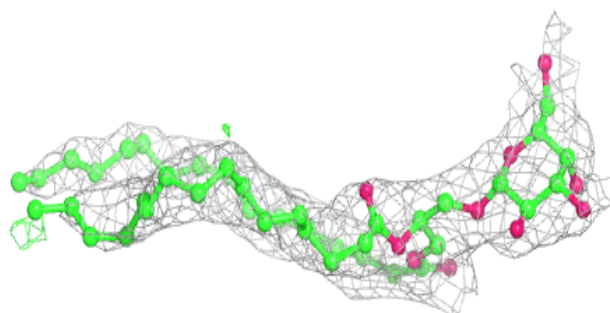
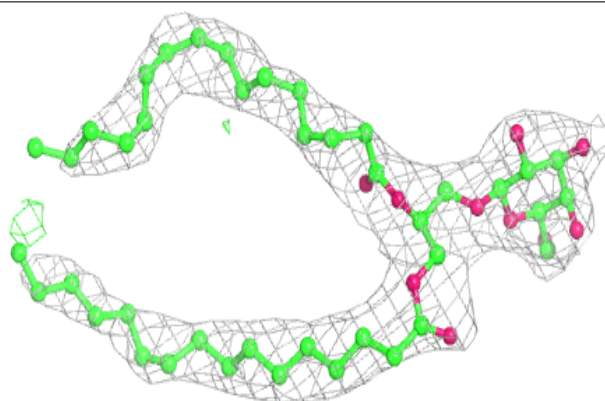


Electron density around BCR k 102:

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

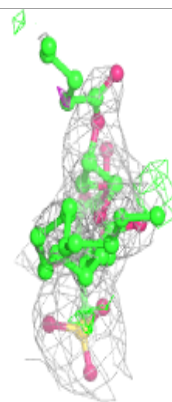
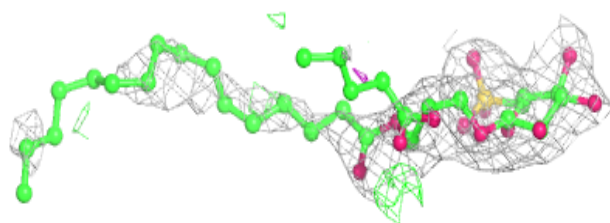
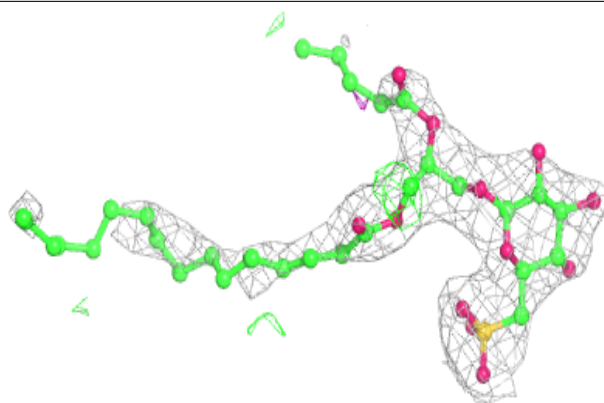
**Electron density around LMG C 502:**

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



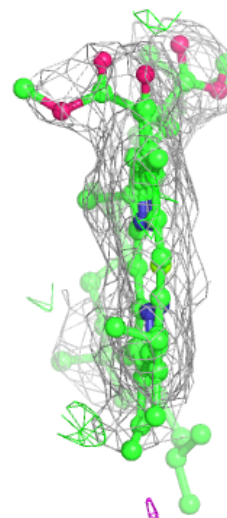
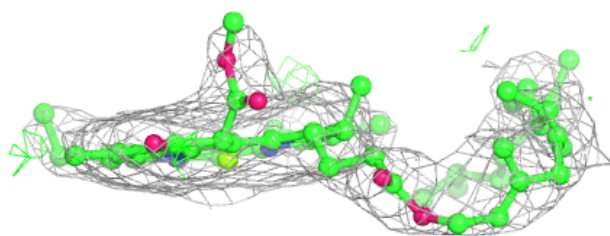
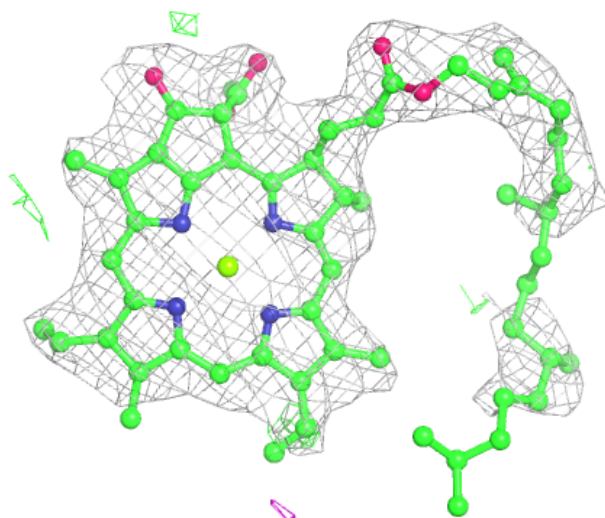
Electron density around SQD D 413:

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



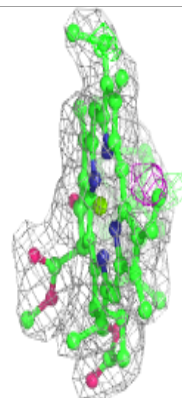
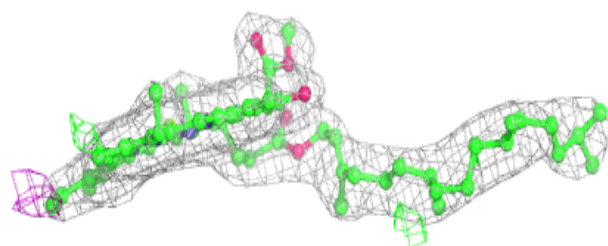
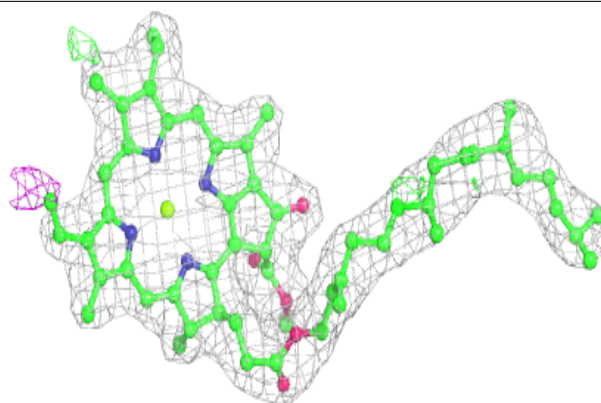
Electron density around CLA c 514:

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

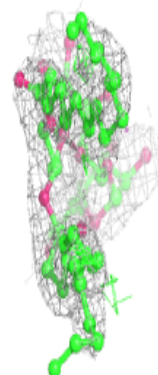
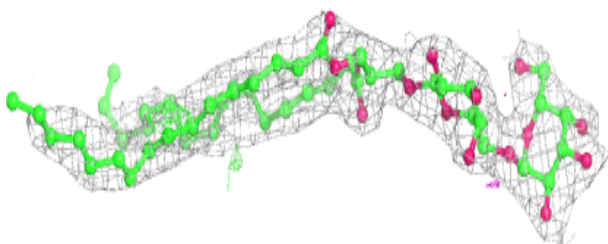
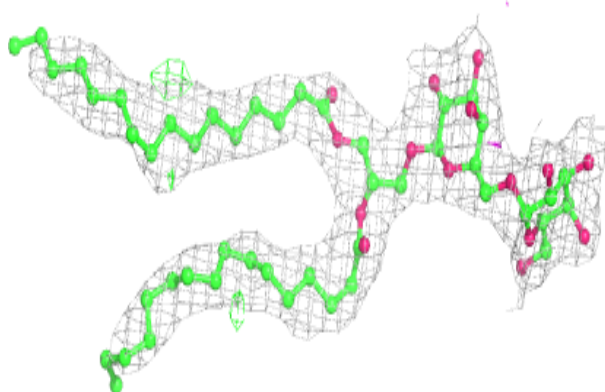


Electron density around CLA B 602:

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

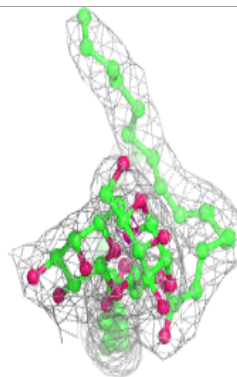
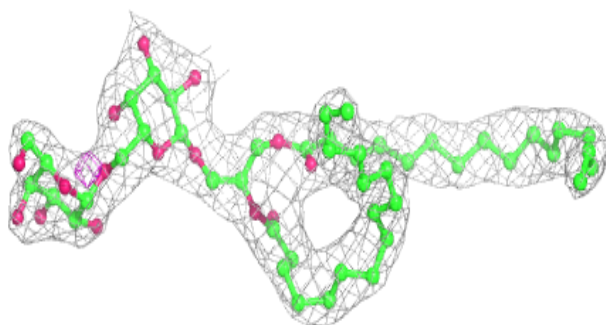
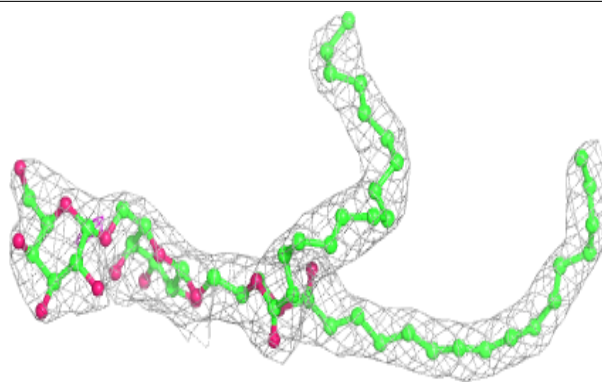
**Electron density around DGD C 520:**

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

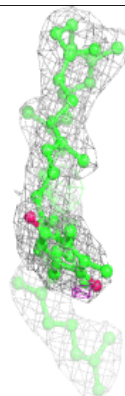
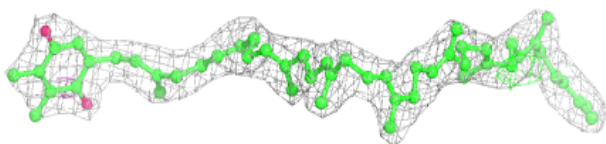
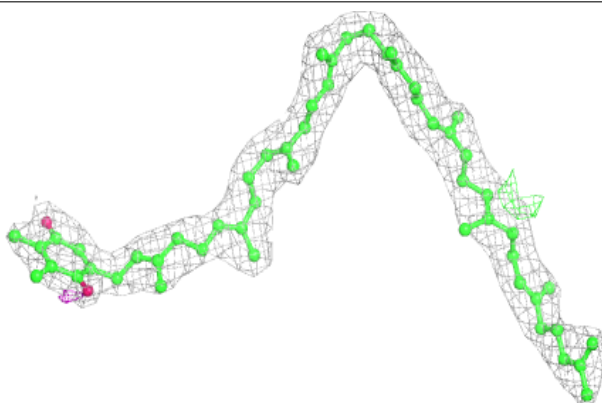


Electron density around DGD H 102:

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

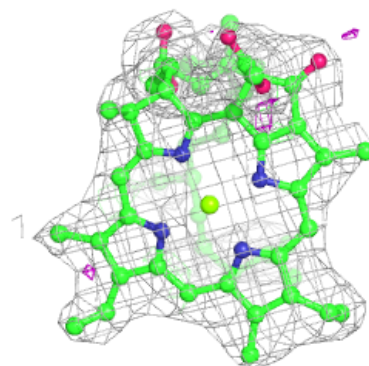
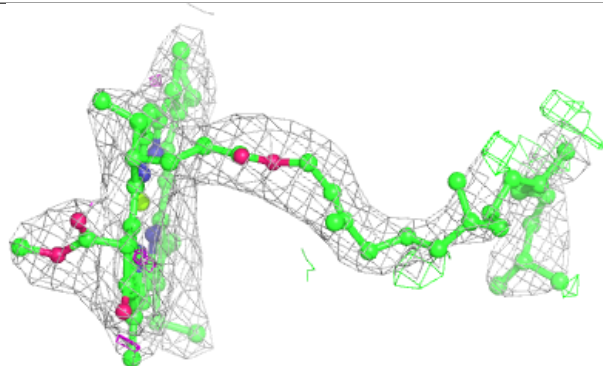
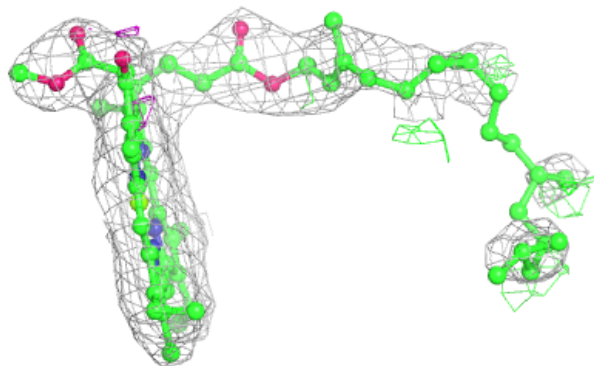
**Electron density around PL9 d 405:**

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

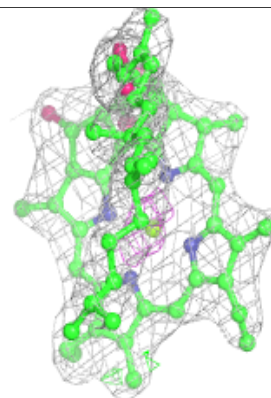
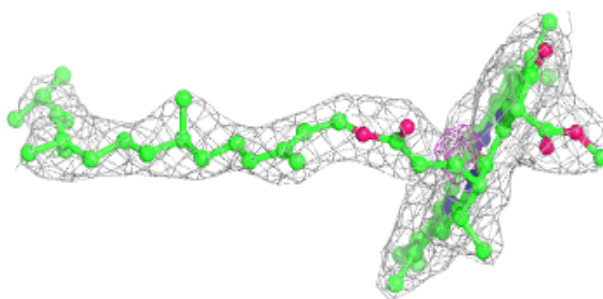
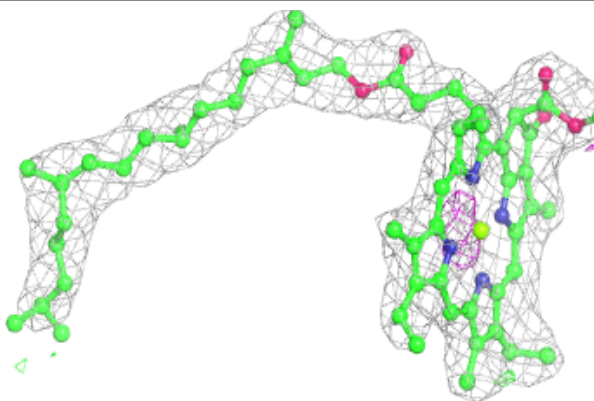


Electron density around CLA C 508:

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

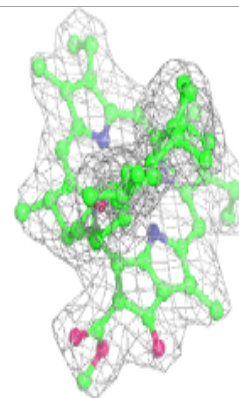
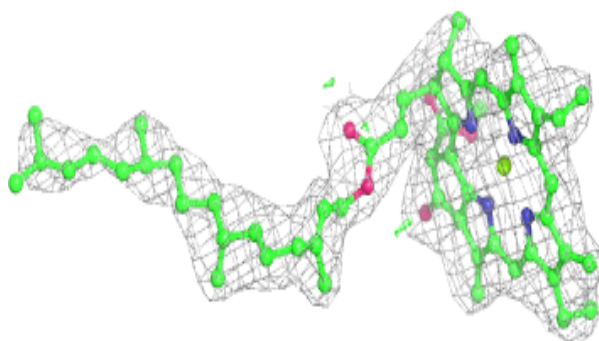
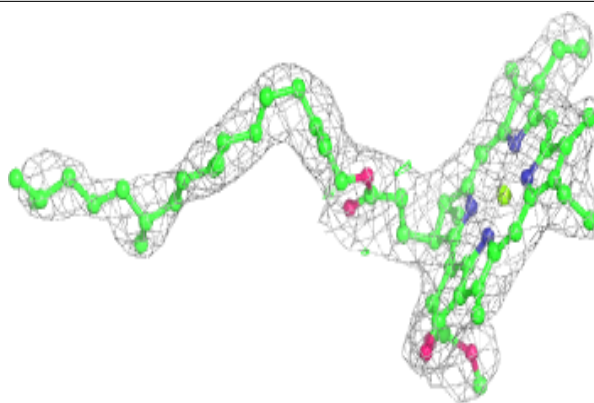
**Electron density around CLA b 609:**

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

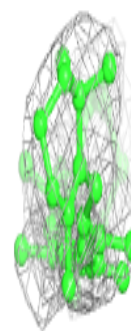
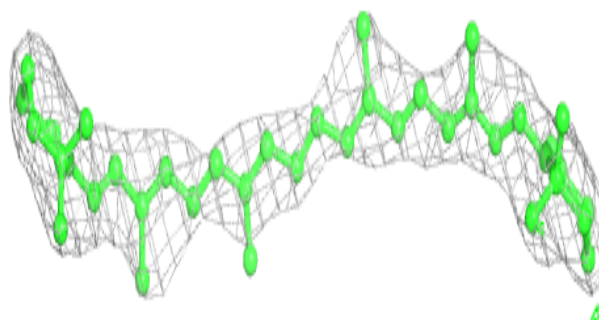
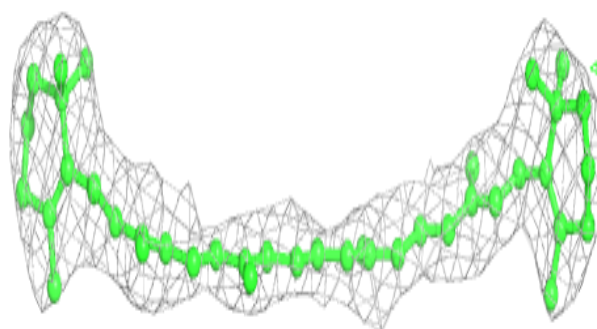


Electron density around CLA c 504:

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

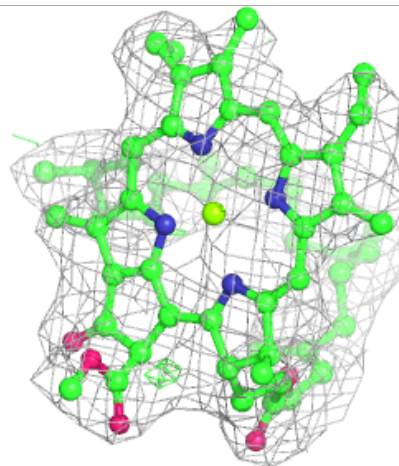
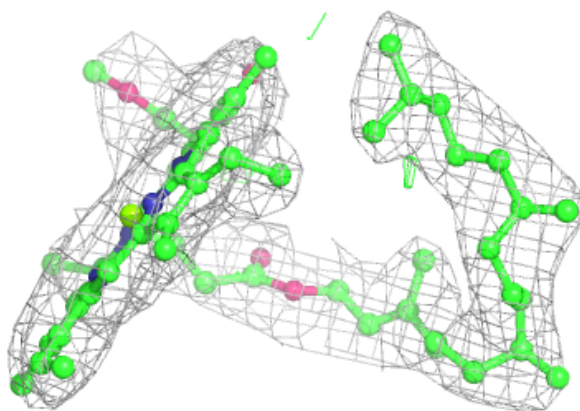
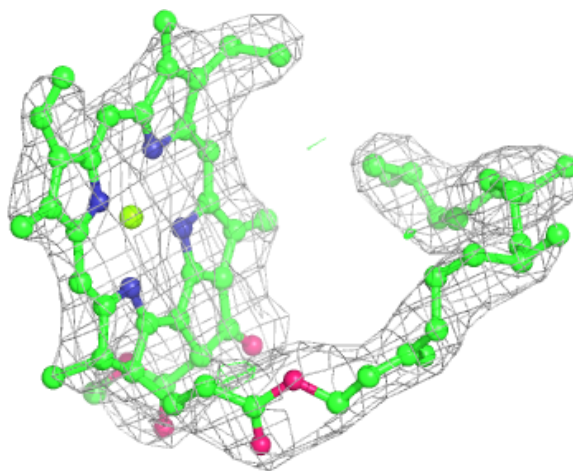
**Electron density around BCR k 101:**

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



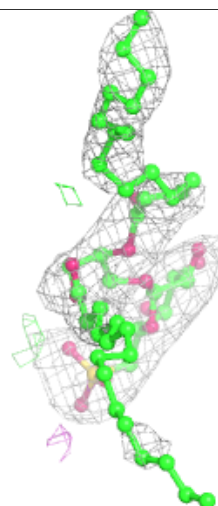
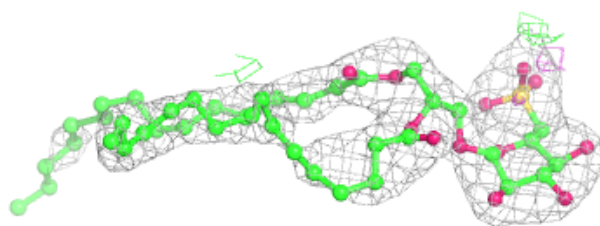
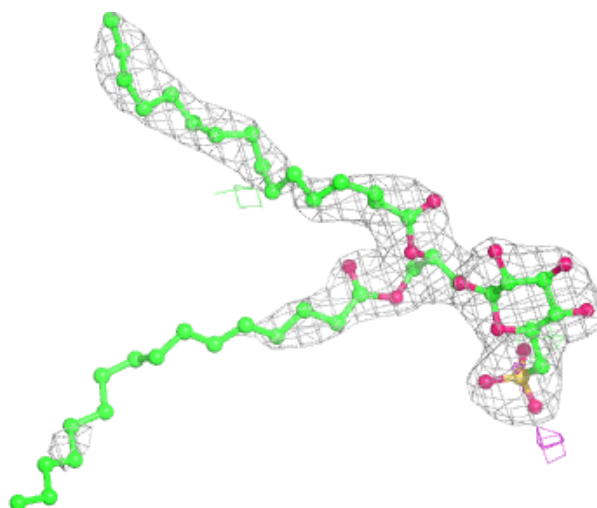
Electron density around CLA c 505:

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



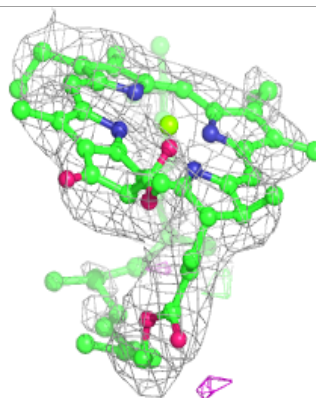
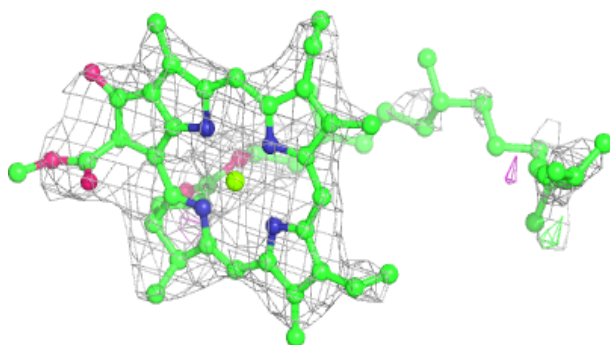
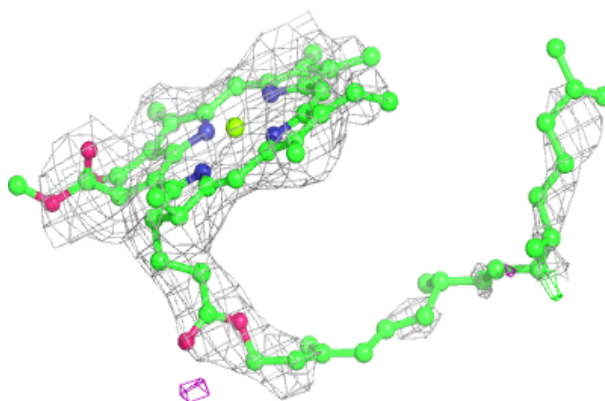
Electron density around SQD A 409:

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

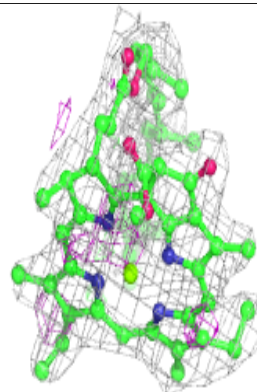
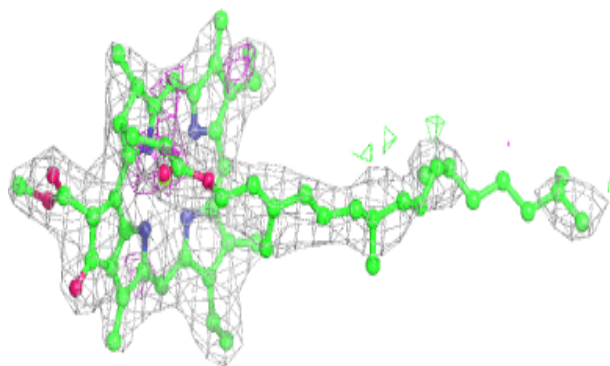
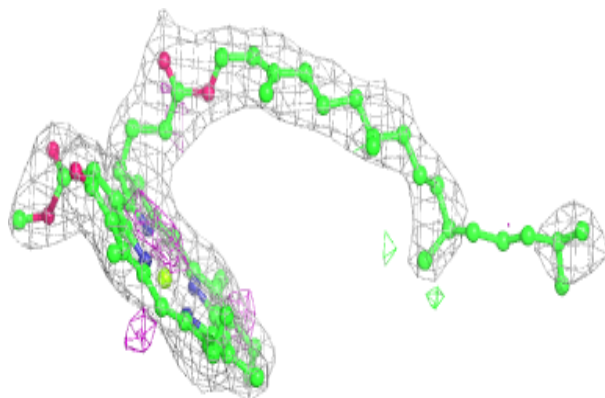


Electron density around CLA c 515:

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

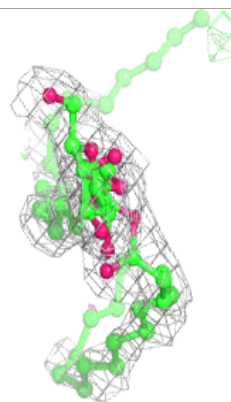
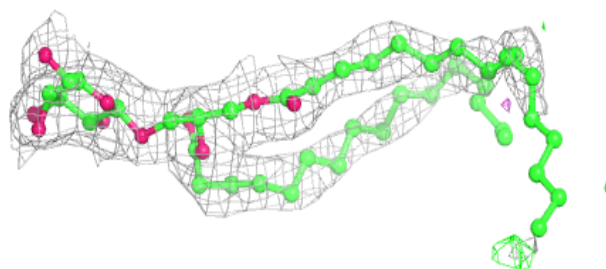
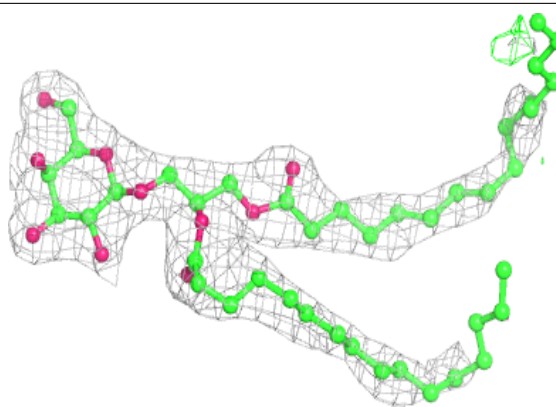
**Electron density around CLA C 506:**

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



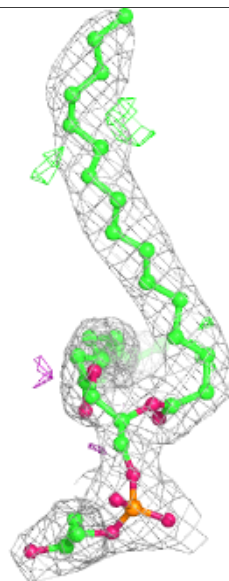
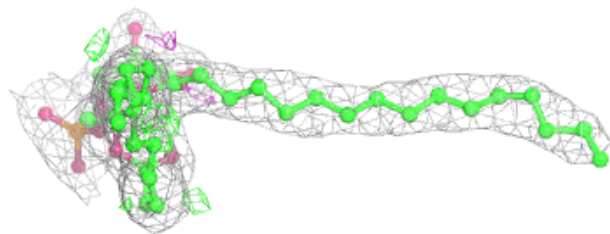
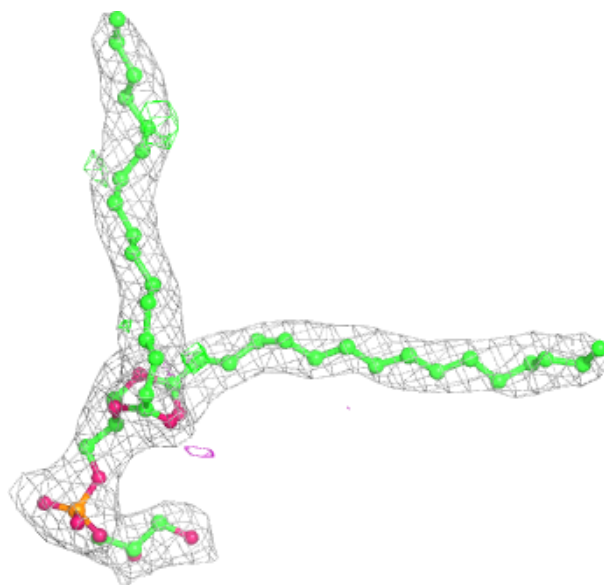
Electron density around LMG D 412:

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



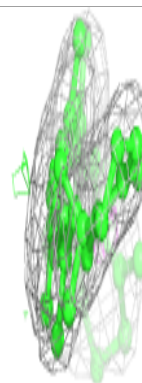
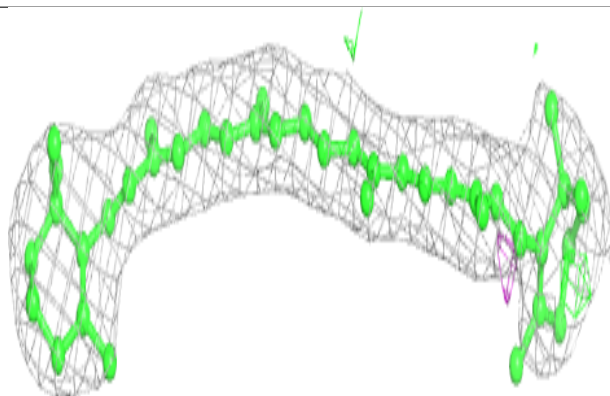
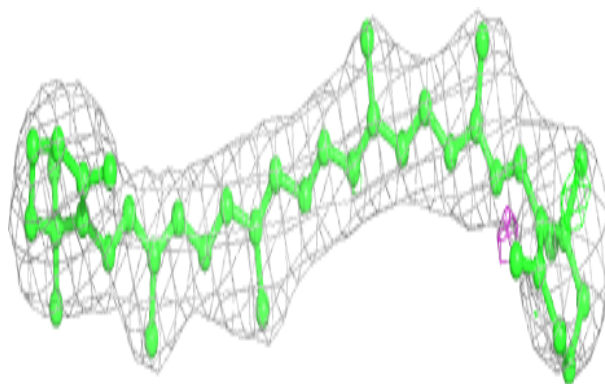
Electron density around LHG b 628:

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

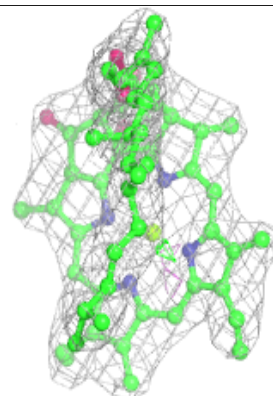
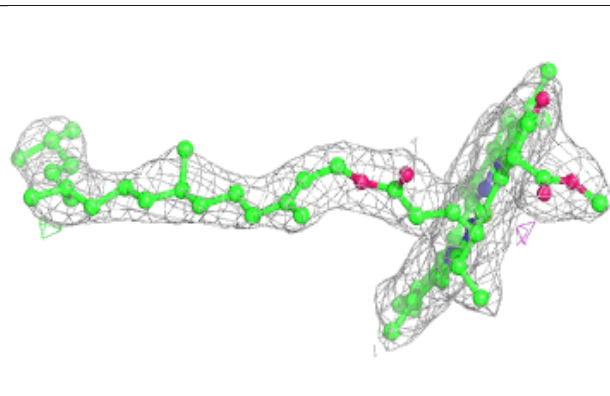
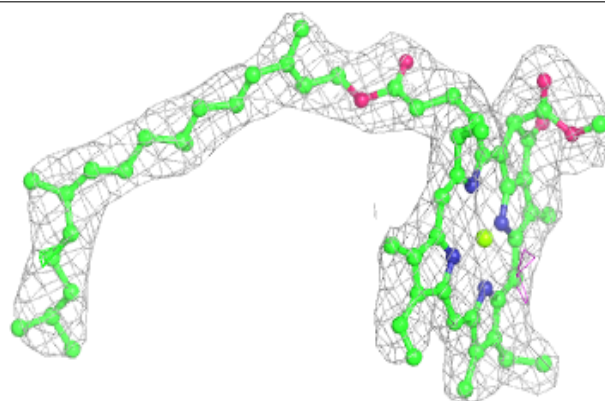


Electron density around BCR d 404:

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

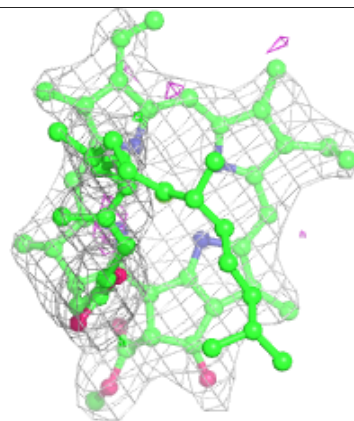
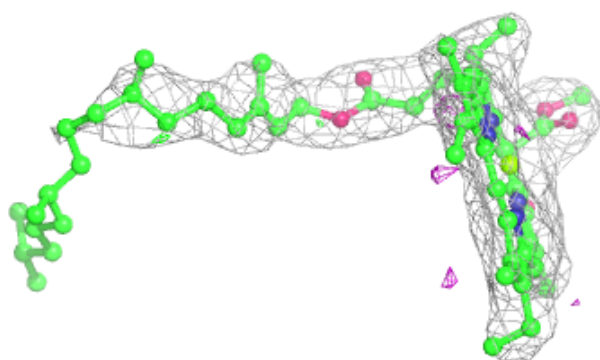
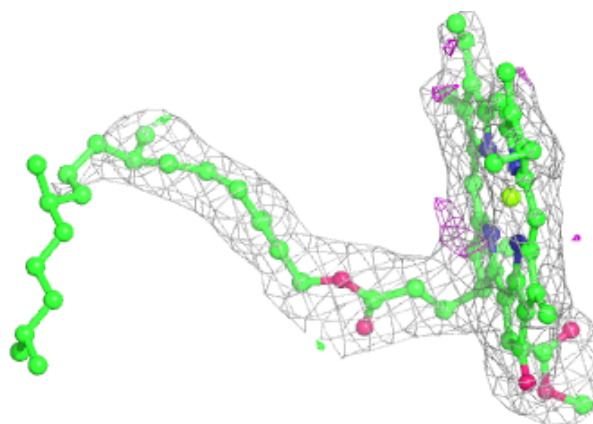
**Electron density around CLA B 609:**

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



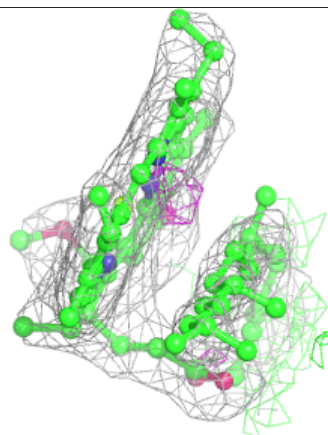
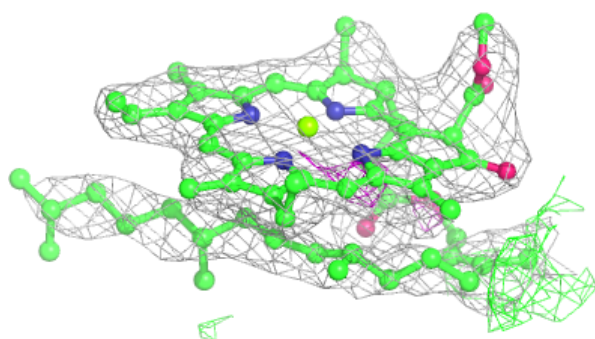
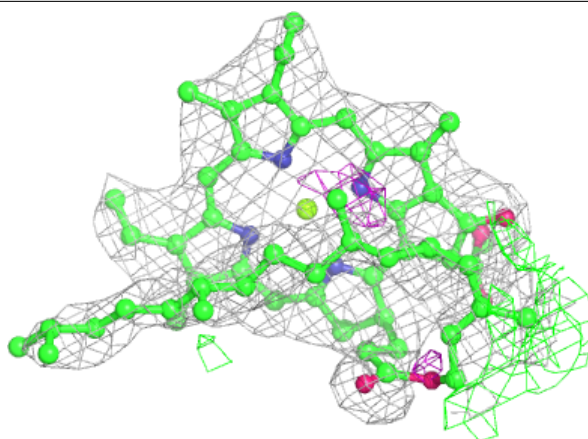
Electron density around CLA D 404:

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

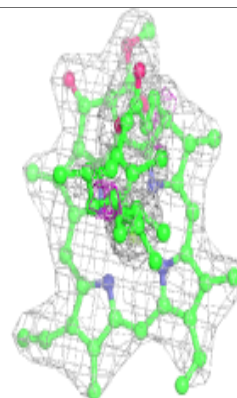
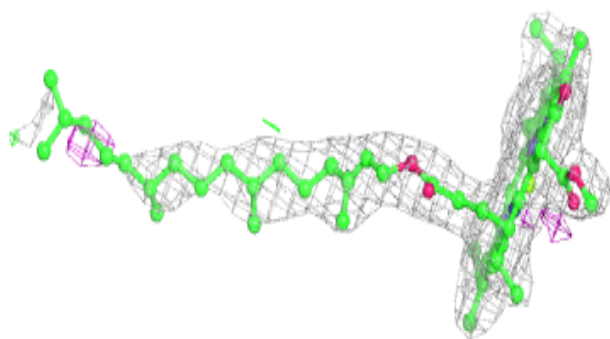
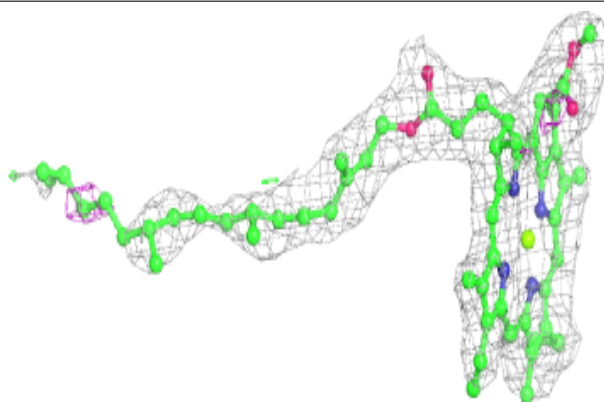


Electron density around CLA b 601:

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

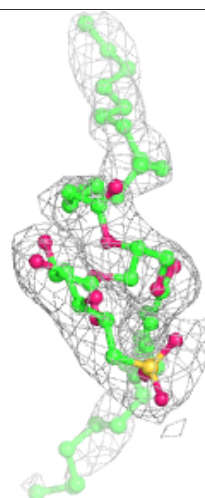
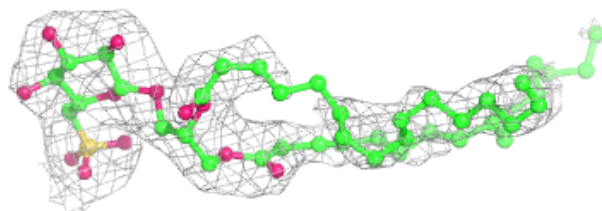
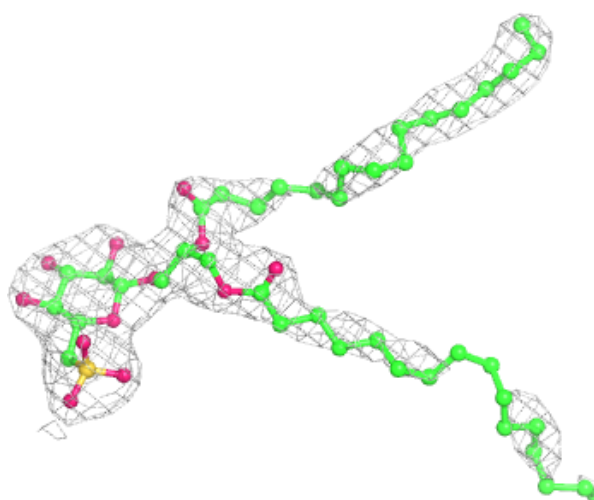
**Electron density around CLA d 403:**

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



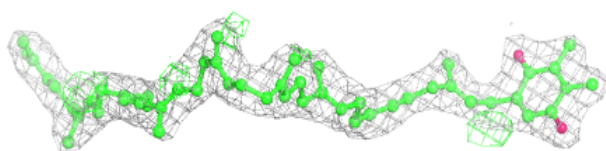
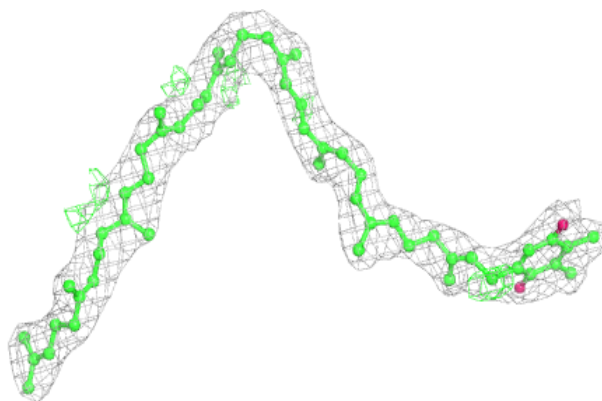
Electron density around SQD a 409:

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

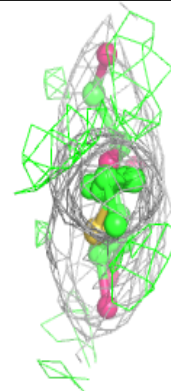
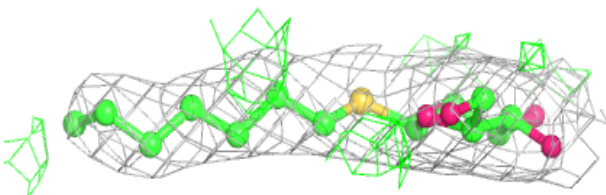
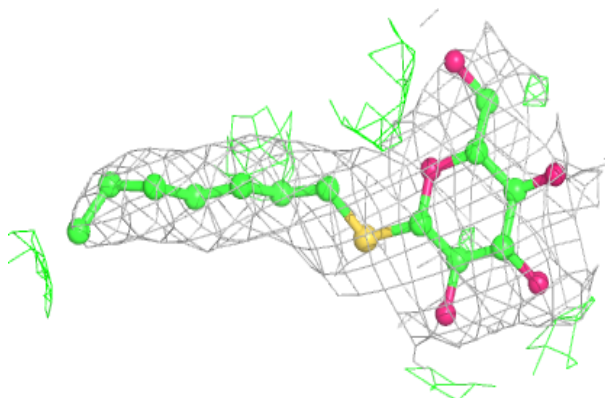


Electron density around PL9 D 406:

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

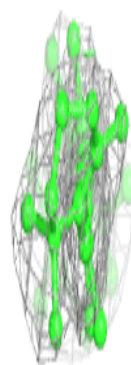
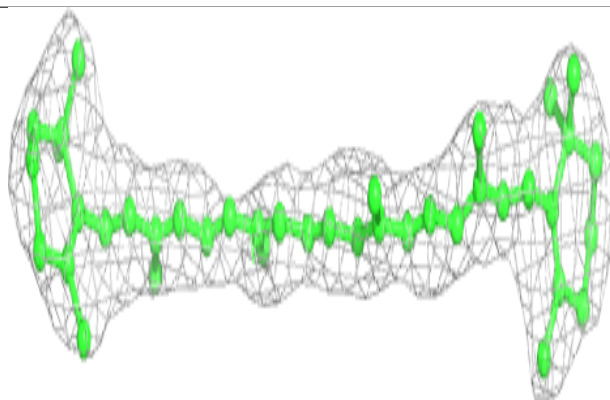
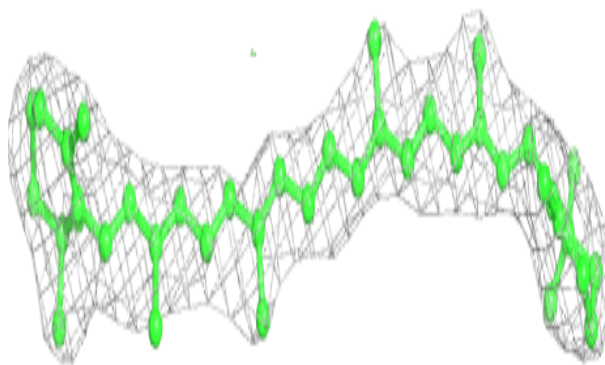
**Electron density around HTG b 624:**

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



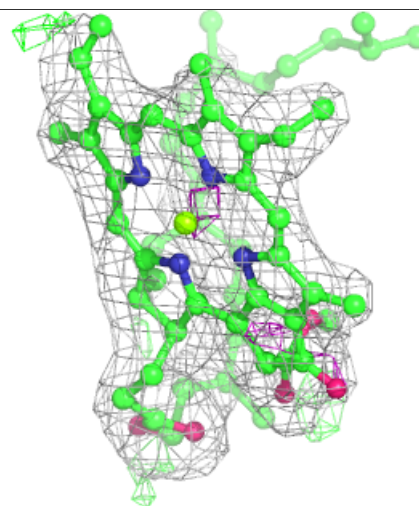
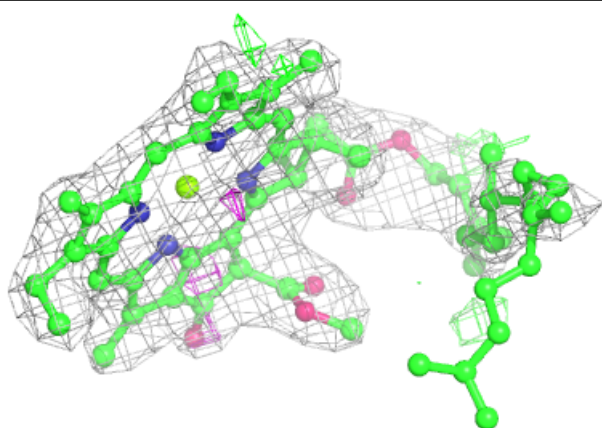
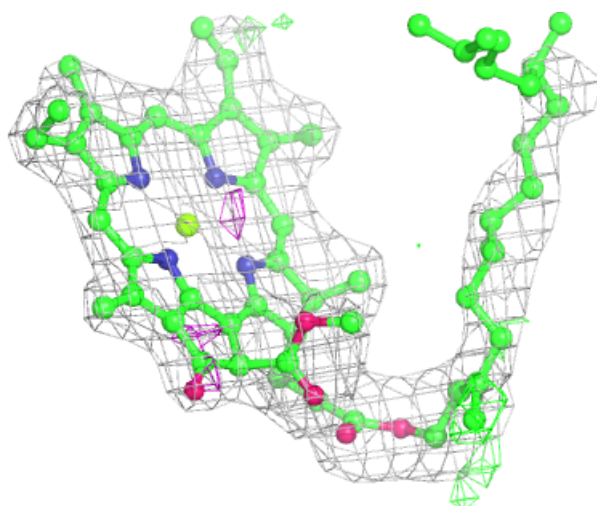
Electron density around BCR C 516:

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



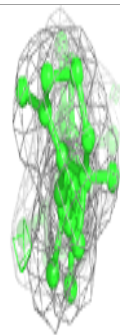
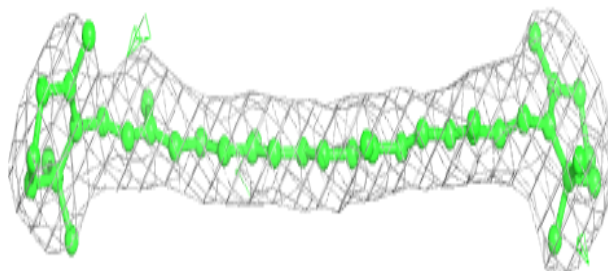
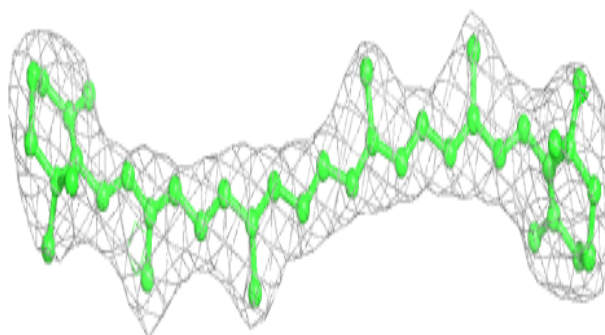
Electron density around CLA b 616:

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



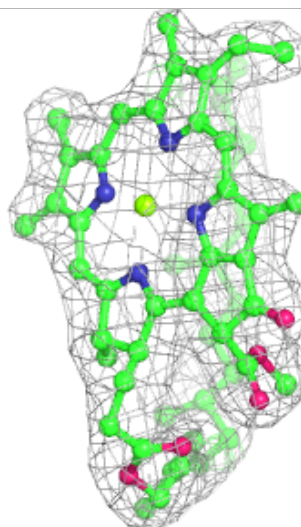
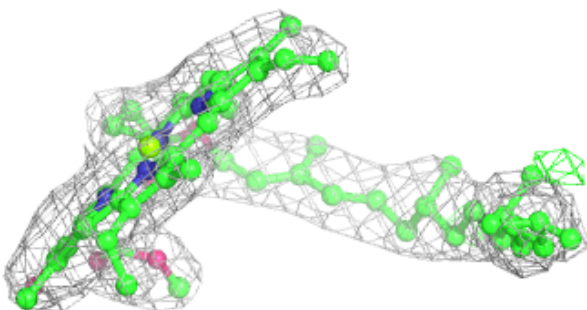
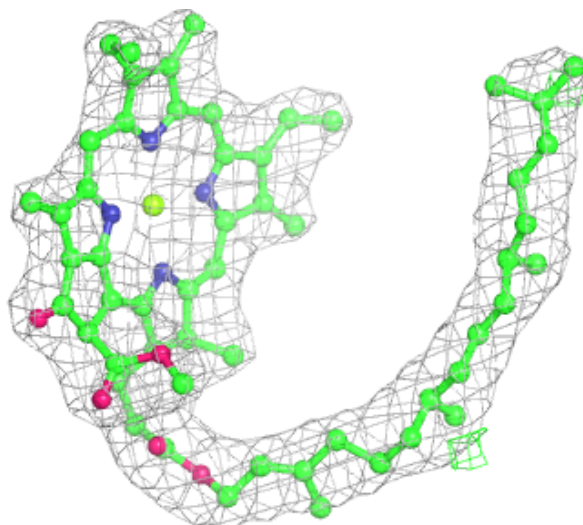
Electron density around BCR b 618:

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



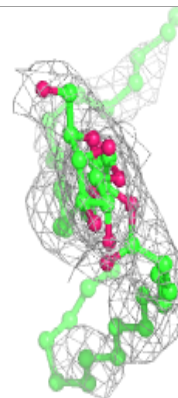
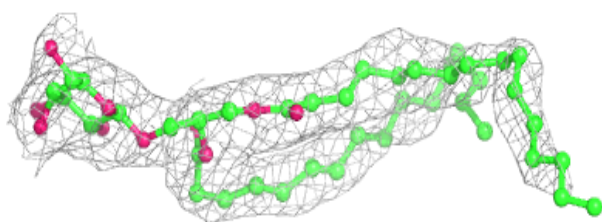
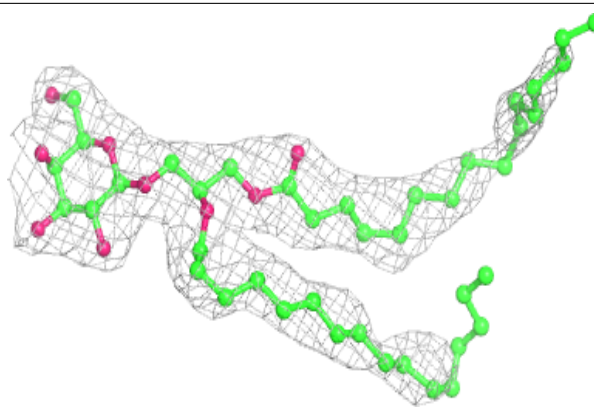
Electron density around CLA C 509:

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

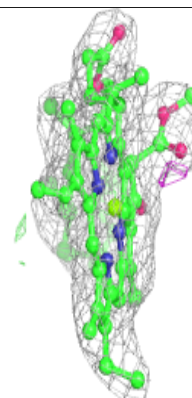
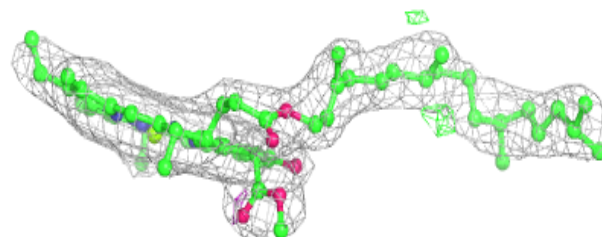
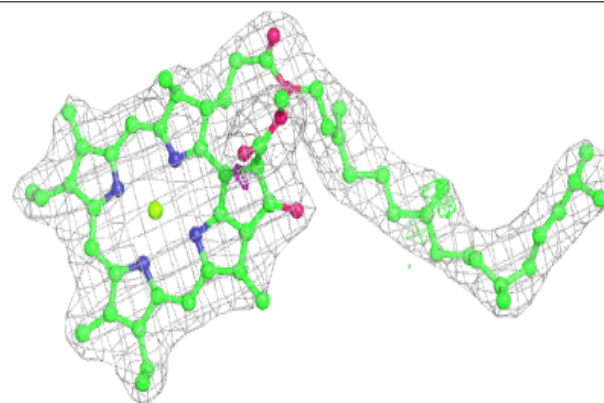


Electron density around LMG d 411:

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

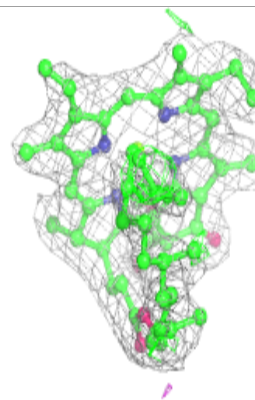
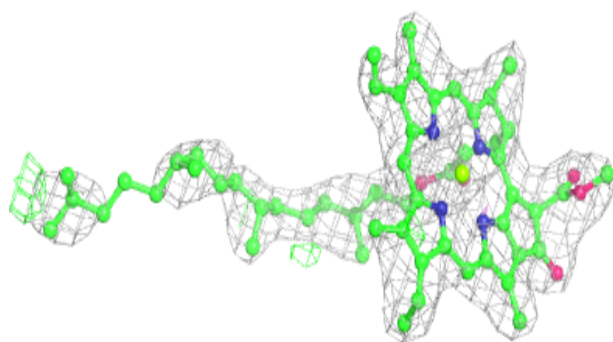
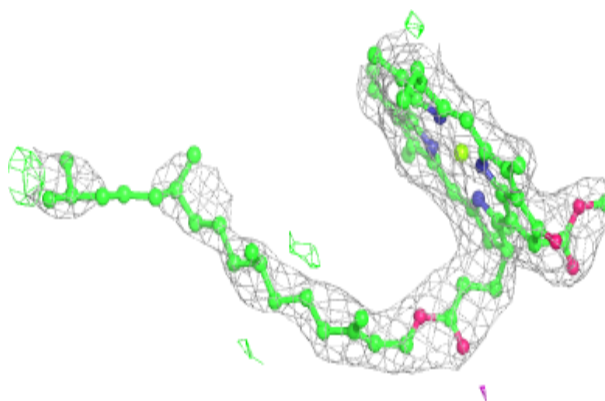
**Electron density around CLA b 602:**

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



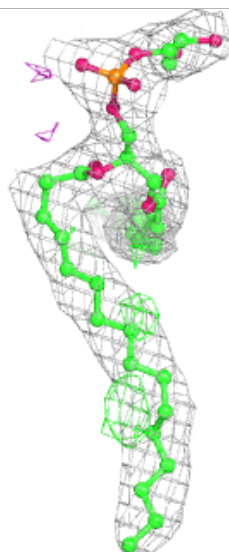
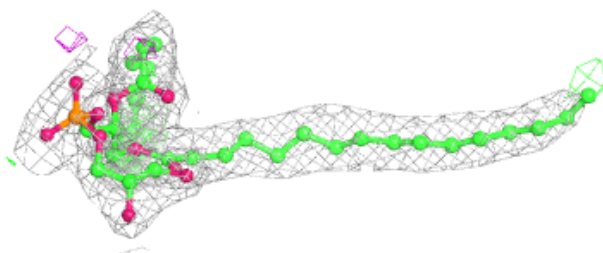
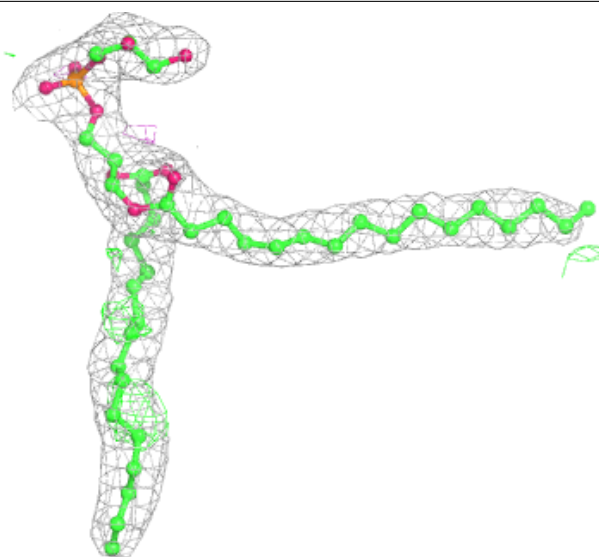
Electron density around CLA c 506:

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



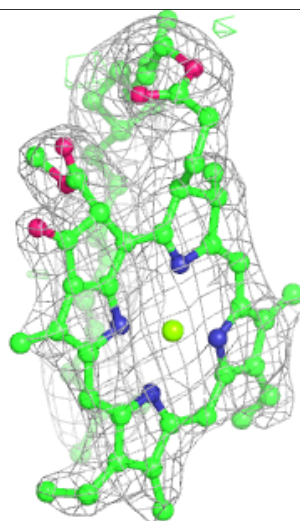
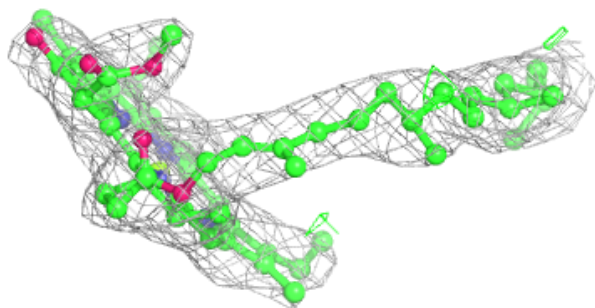
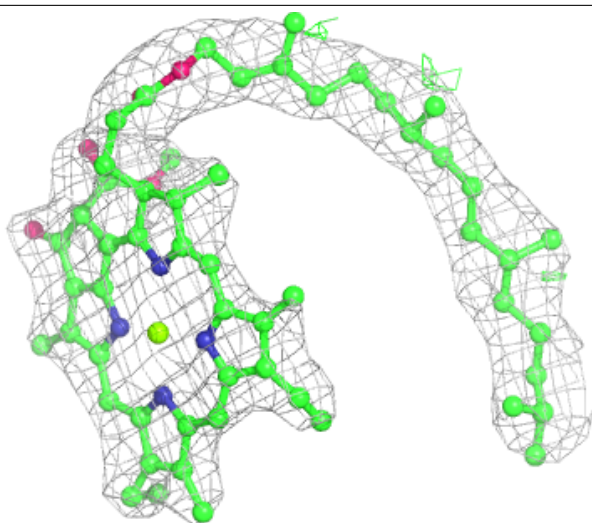
Electron density around LHG L 101:

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



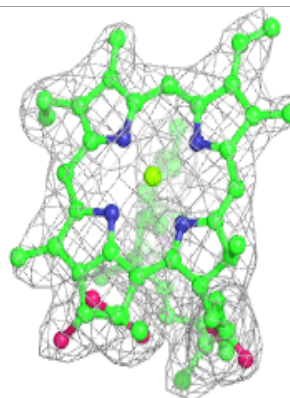
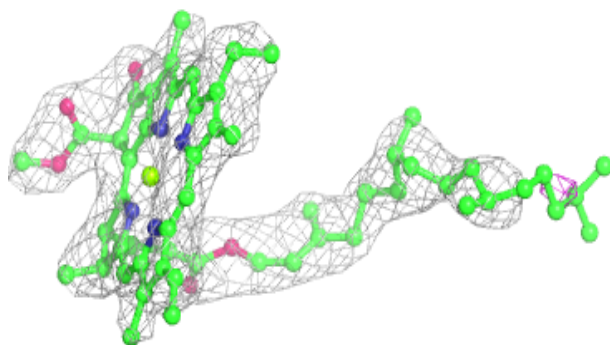
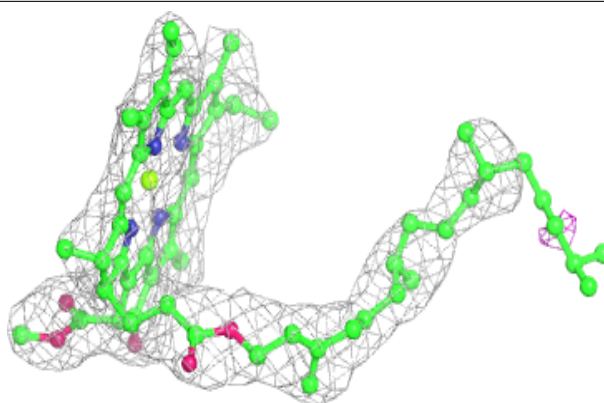
Electron density around CLA c 509:

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

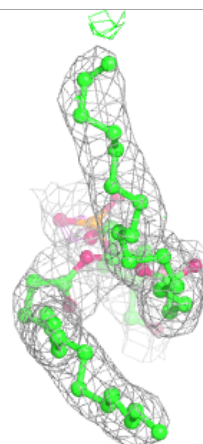
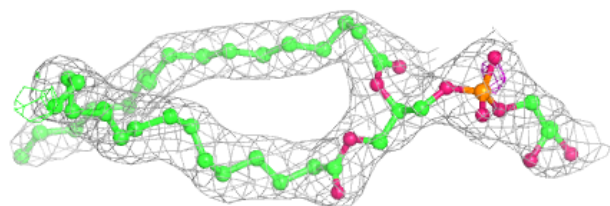
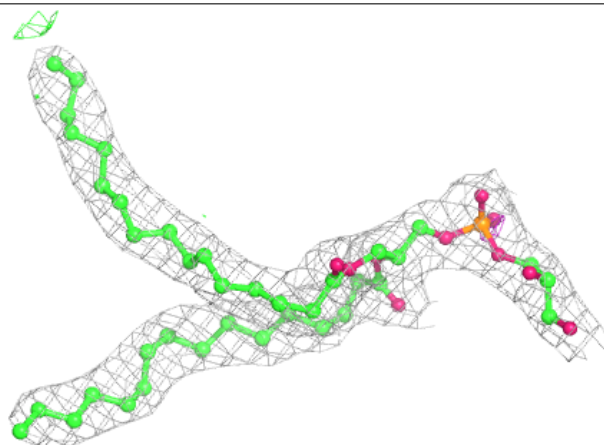


Electron density around CLA c 510:

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

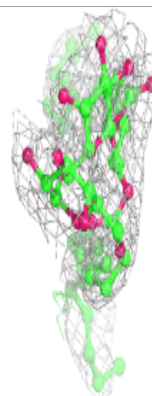
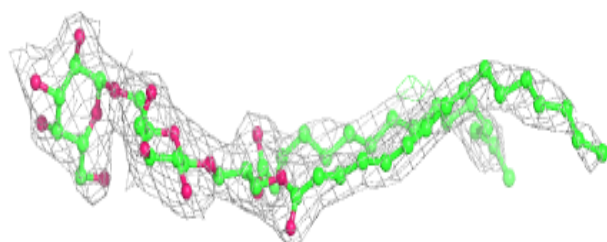
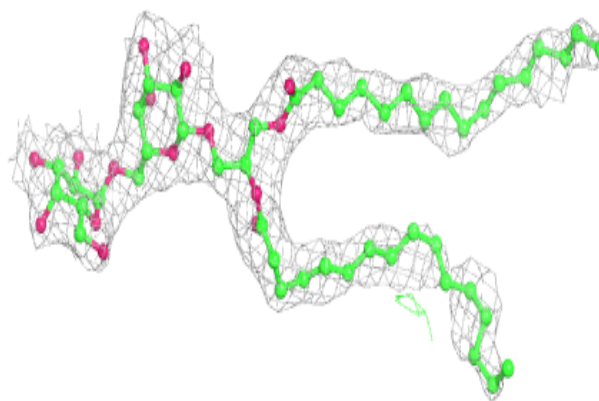
**Electron density around LHG d 407:**

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

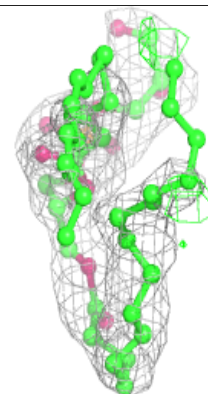
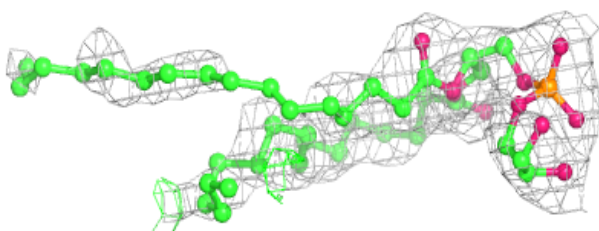
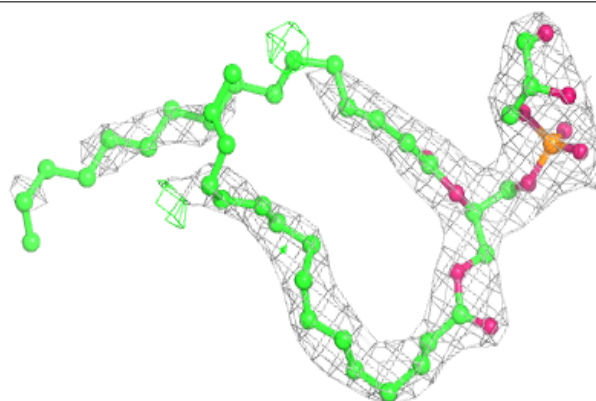


Electron density around DGD c 520:

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

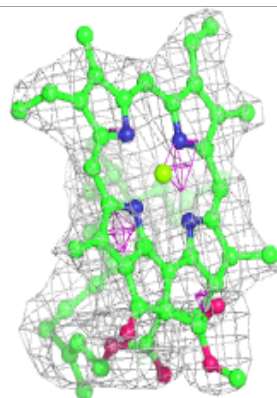
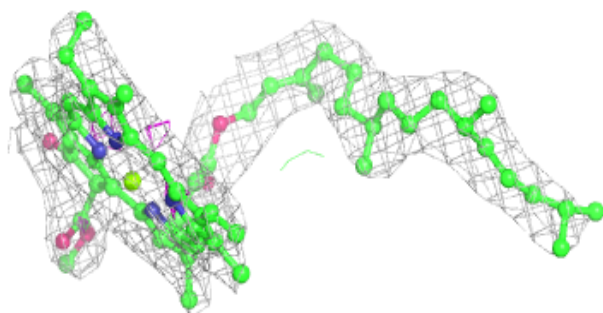
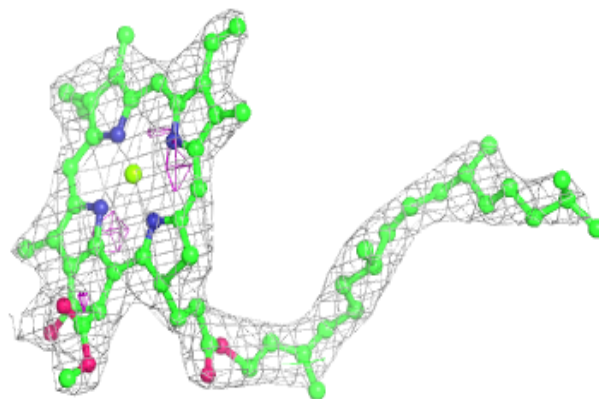
**Electron density around LHG d 408:**

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

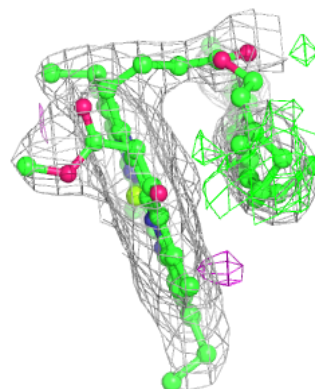
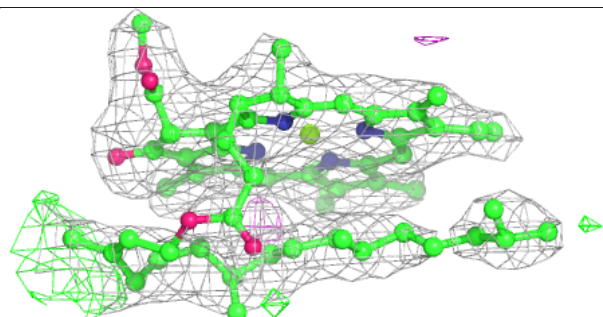
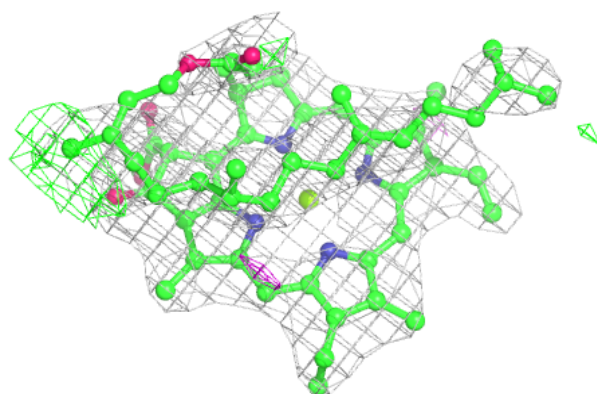


Electron density around CLA c 513:

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

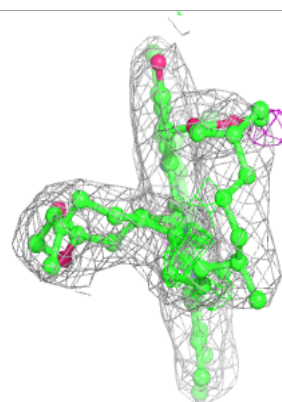
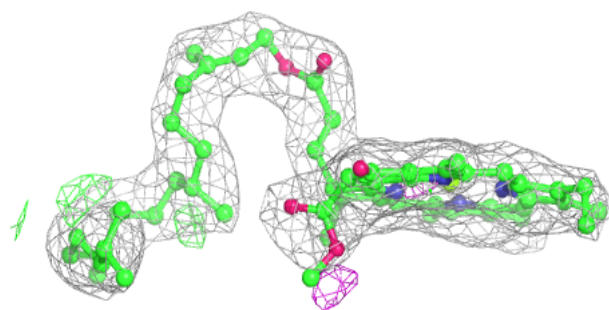
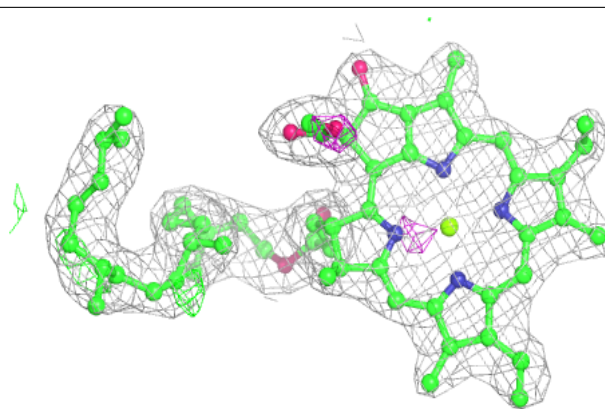
**Electron density around CLA B 601:**

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

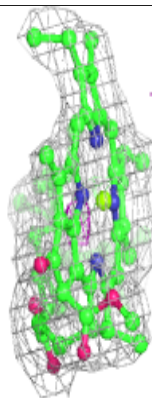
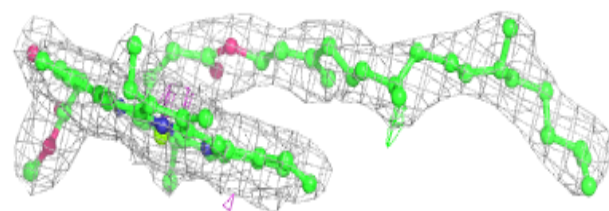
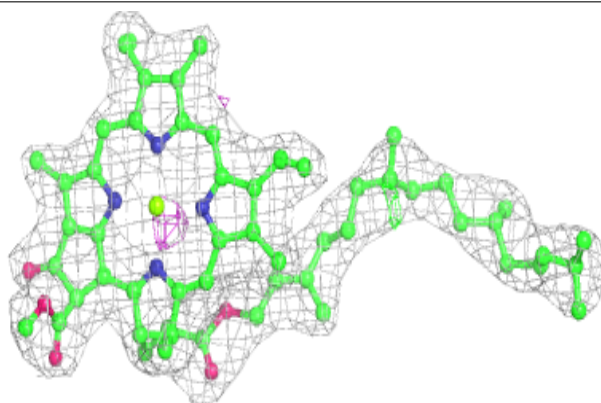


Electron density around CLA b 612:

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

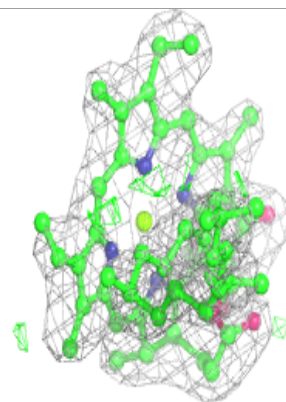
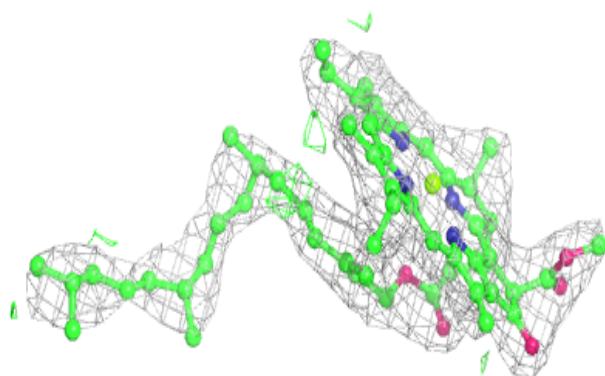
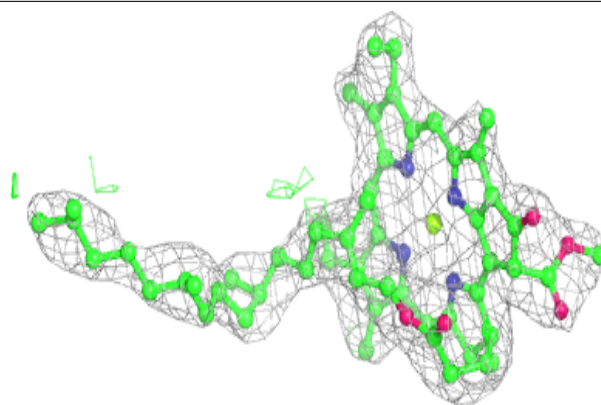
**Electron density around CLA B 603:**

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

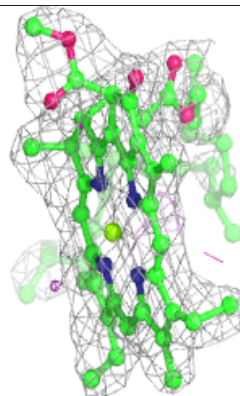
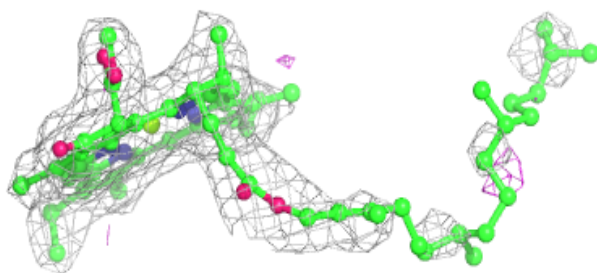
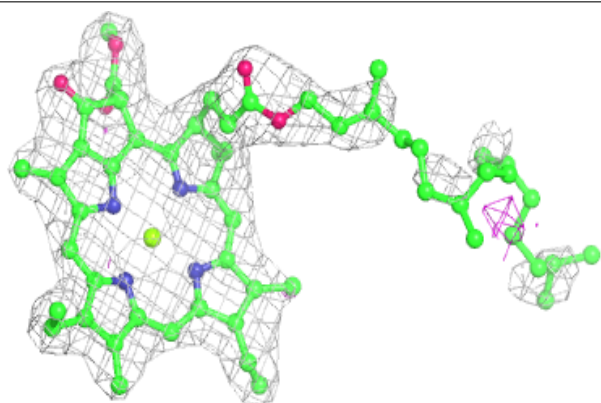


Electron density around CLA c 507:

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

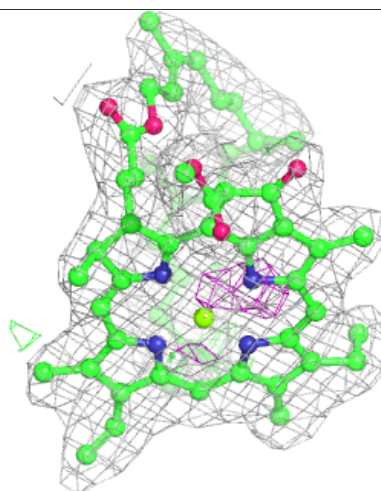
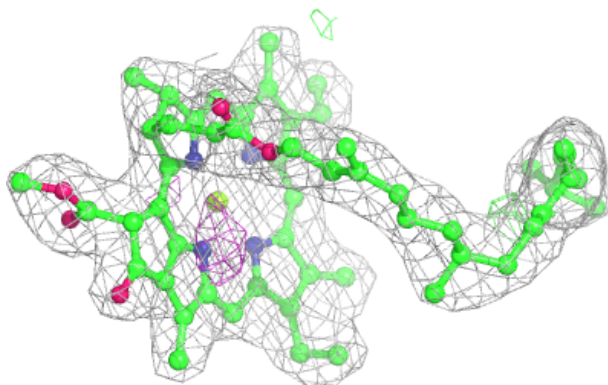
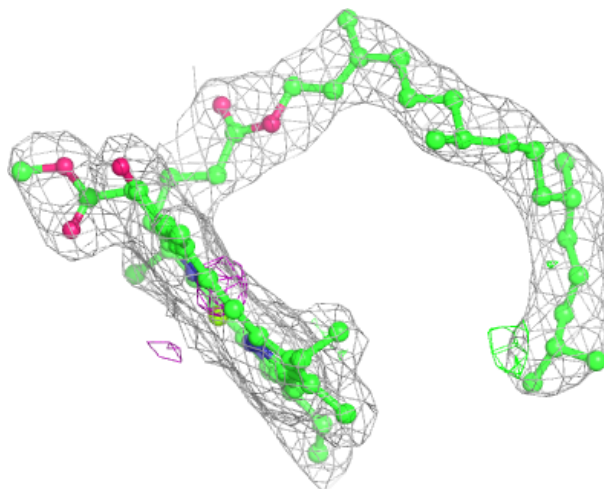
**Electron density around CLA a 407:**

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



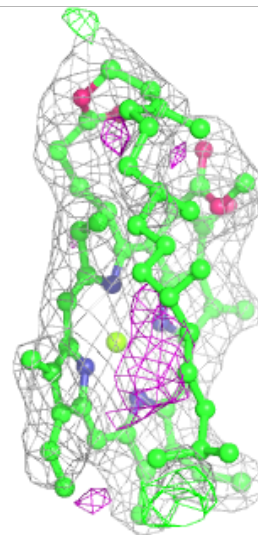
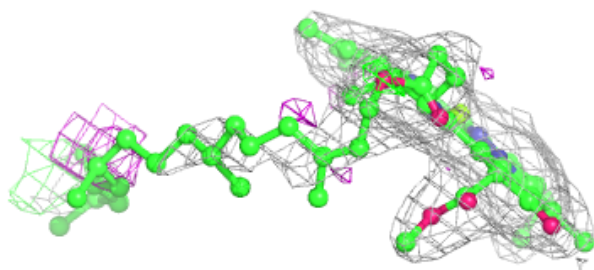
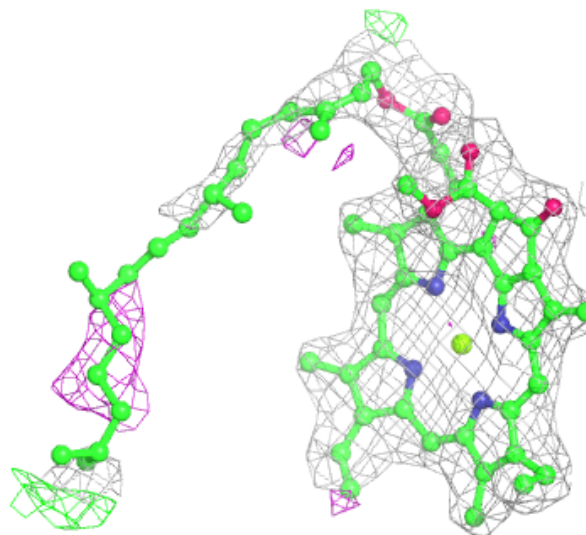
Electron density around CLA B 611:

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



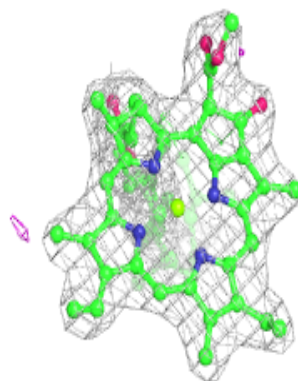
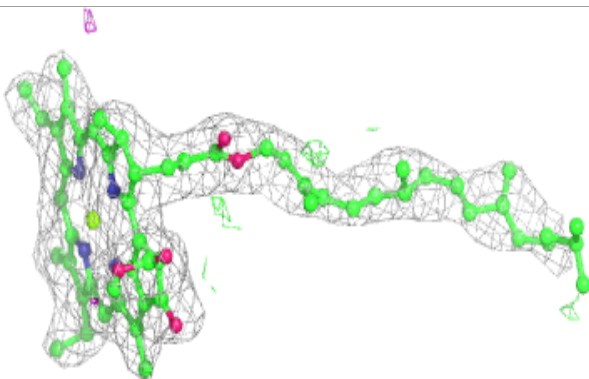
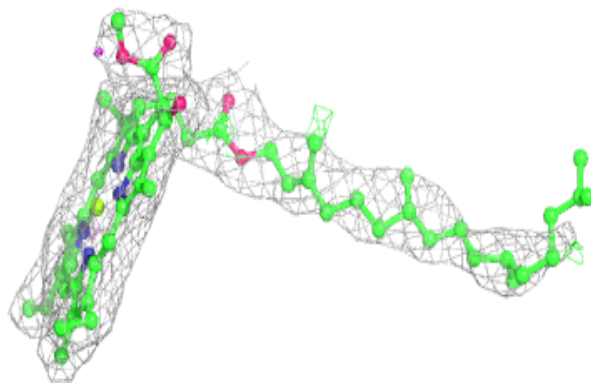
Electron density around CLA B 616:

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

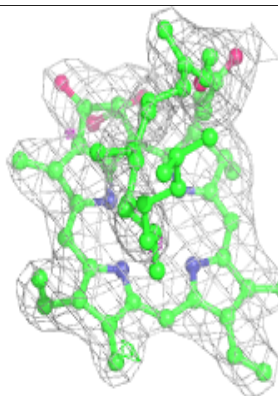
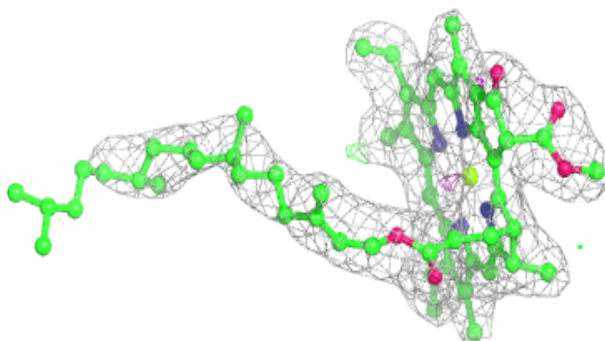
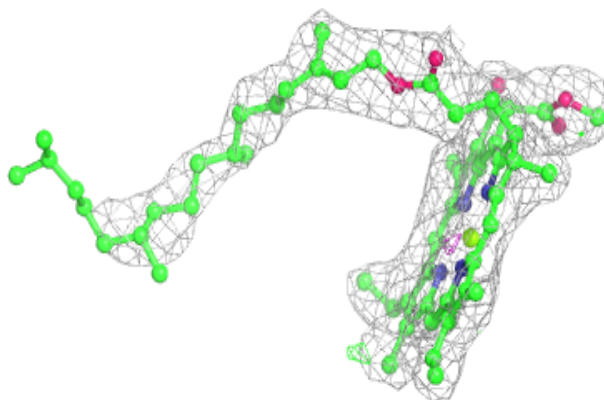


Electron density around CLA b 604:

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

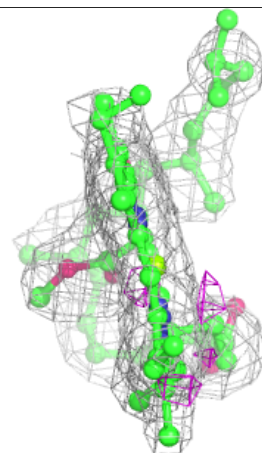
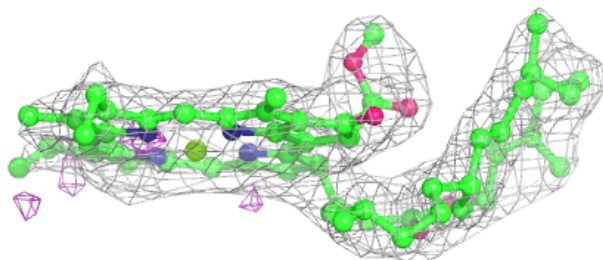
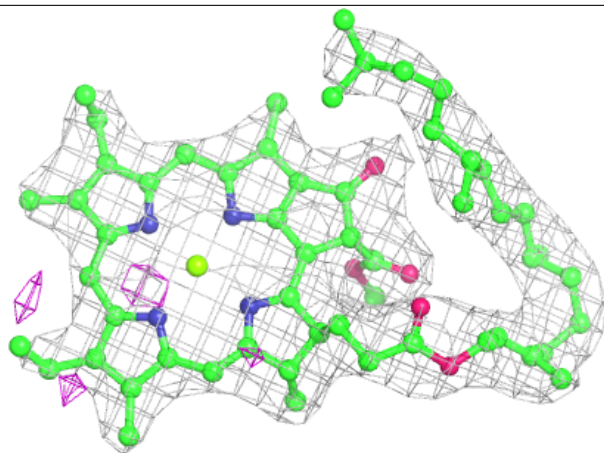
**Electron density around CLA C 510:**

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



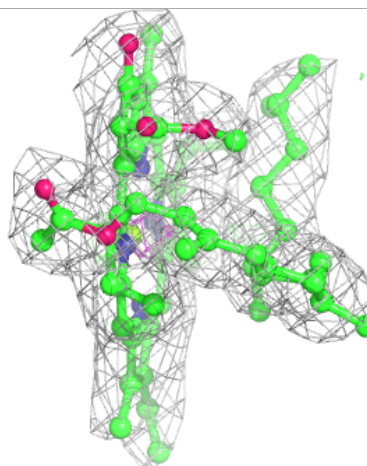
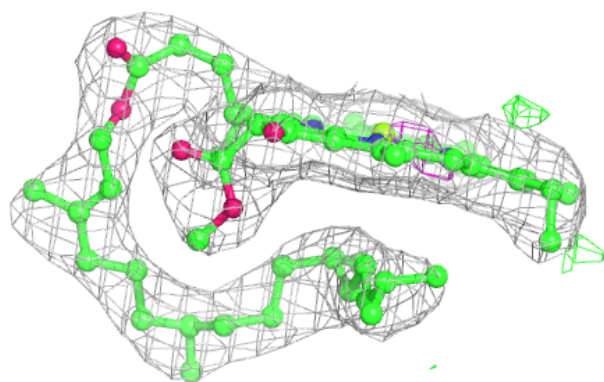
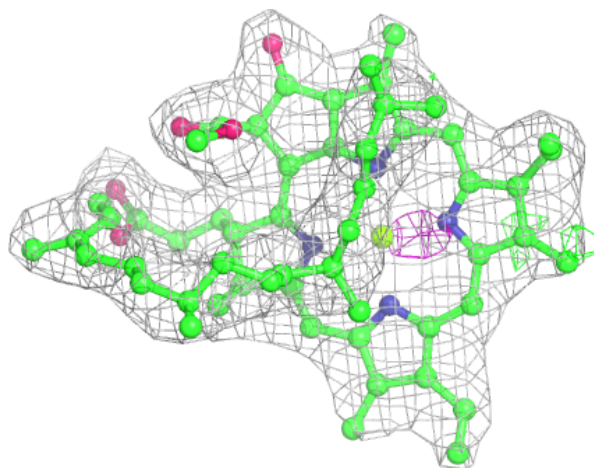
Electron density around CLA b 610:

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



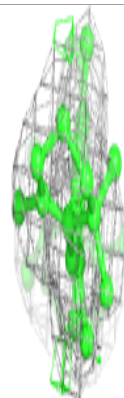
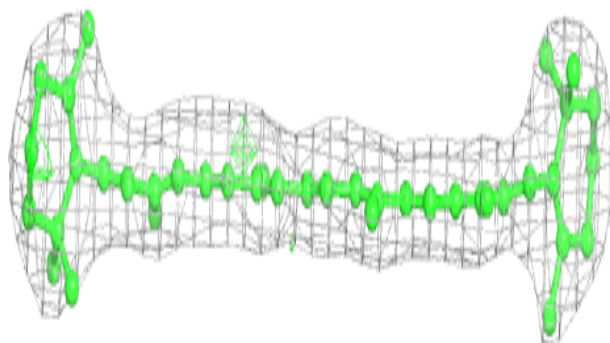
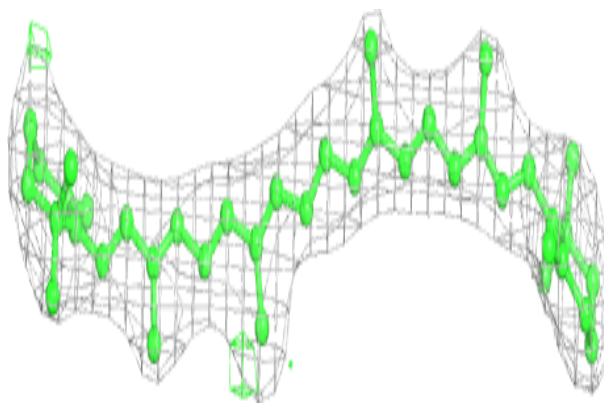
Electron density around CLA C 512:

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

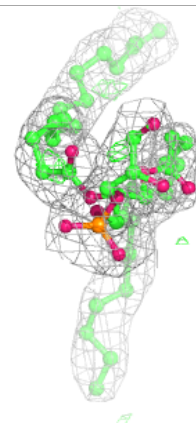
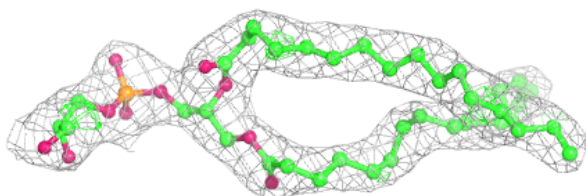
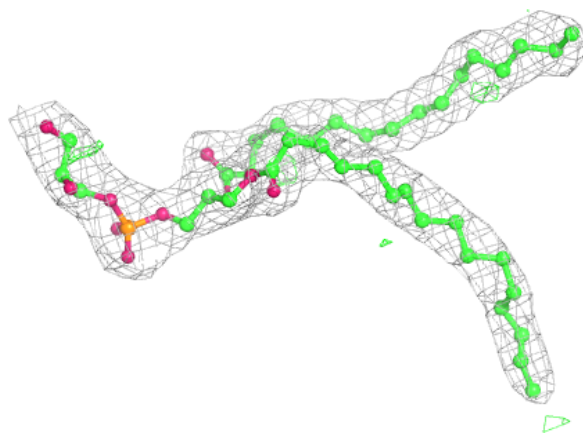


Electron density around BCR C 517:

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

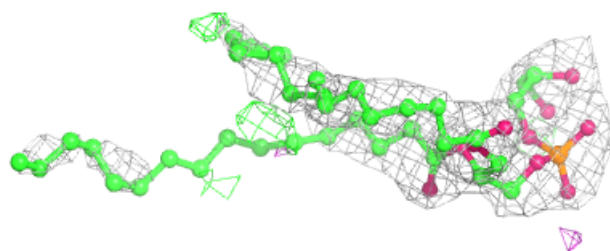
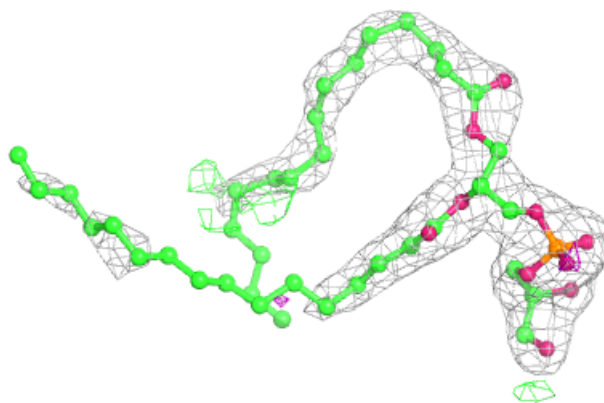
**Electron density around LHG D 407:**

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

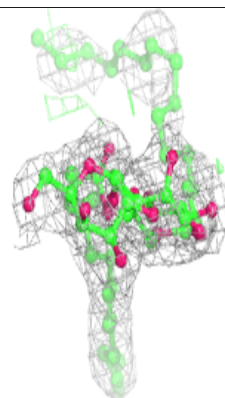
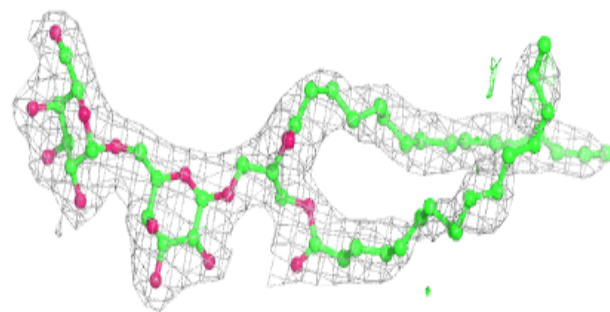
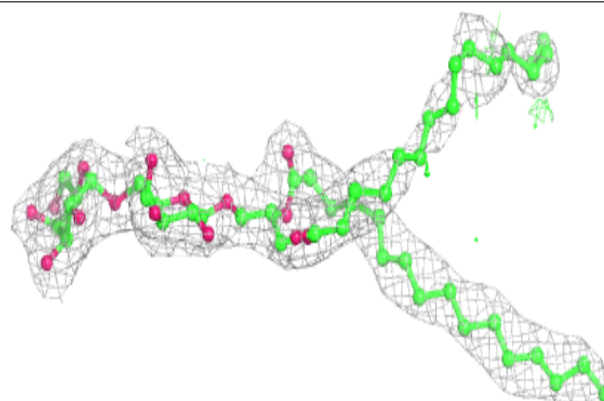


Electron density around LHG D 408:

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

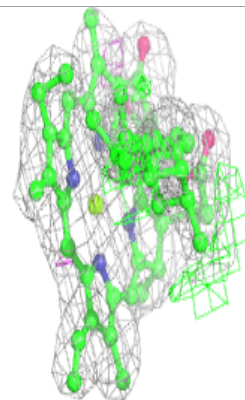
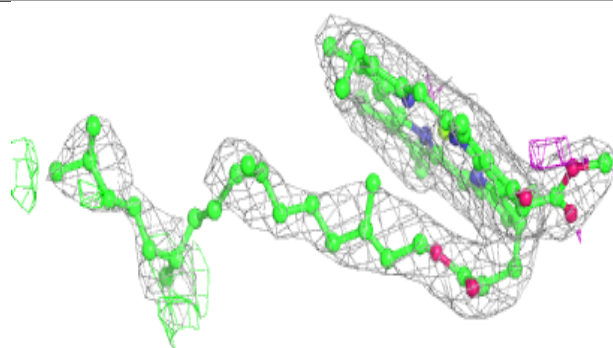
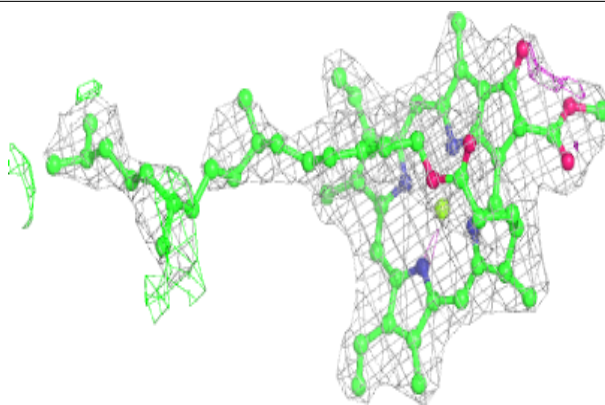
**Electron density around DGD C 518:**

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

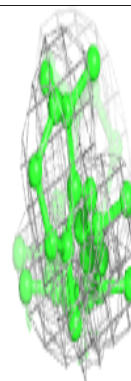
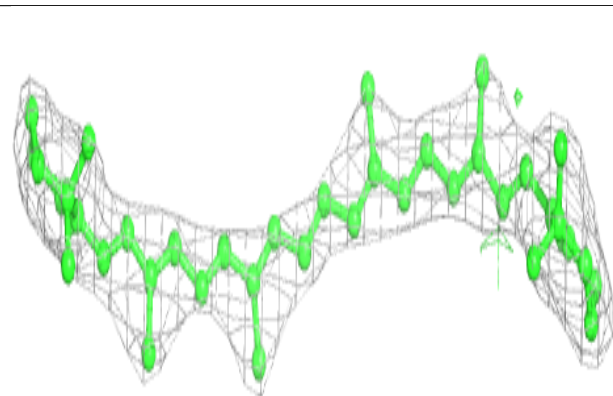
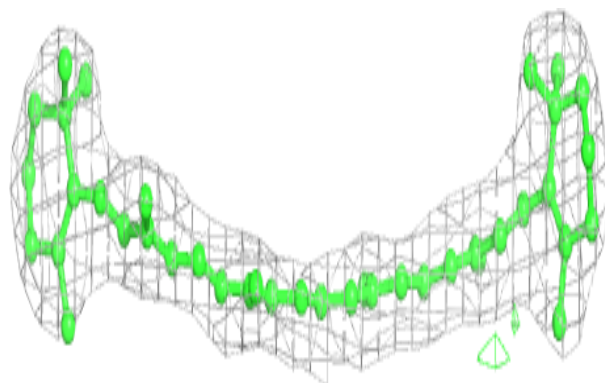


Electron density around CLA b 614:

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

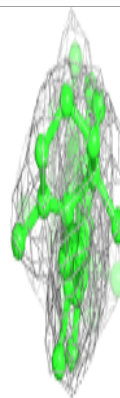
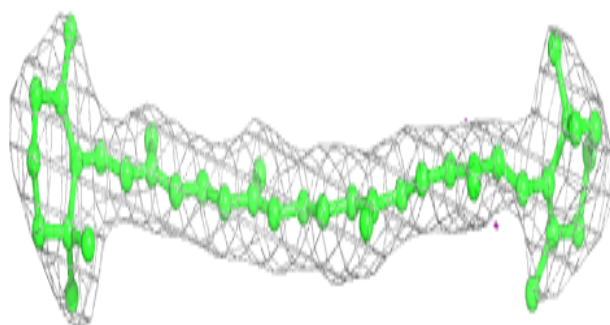
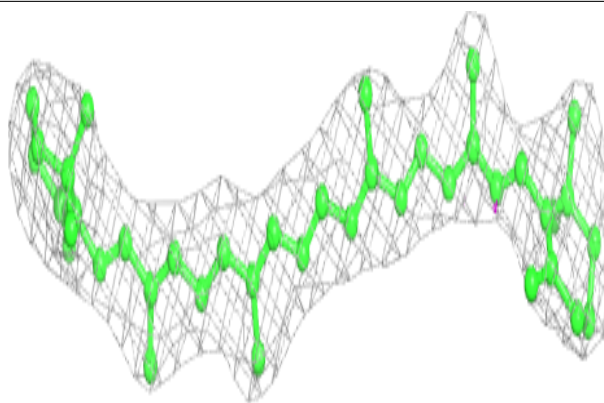
**Electron density around BCR K 101:**

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

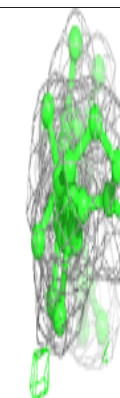
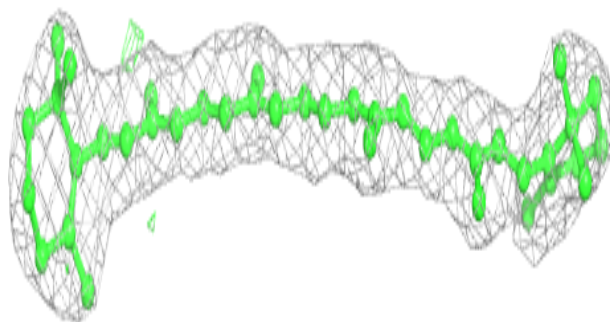
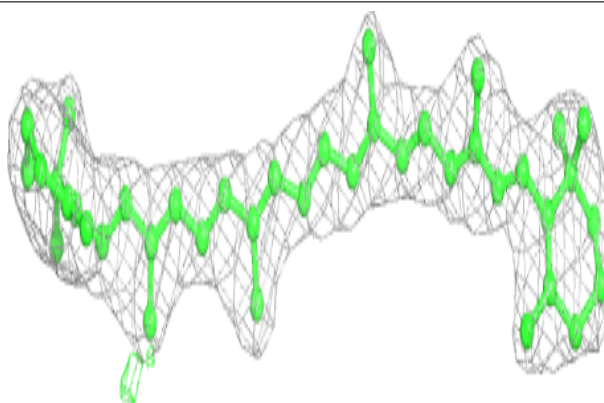


Electron density around BCR Y 101:

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

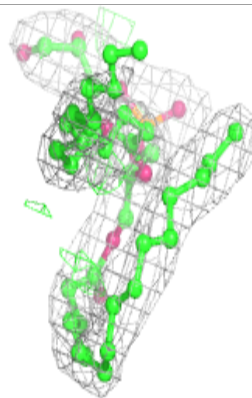
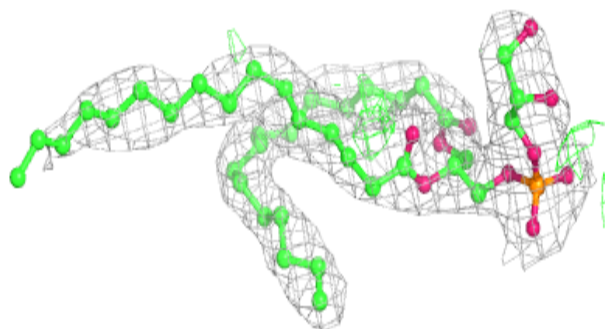
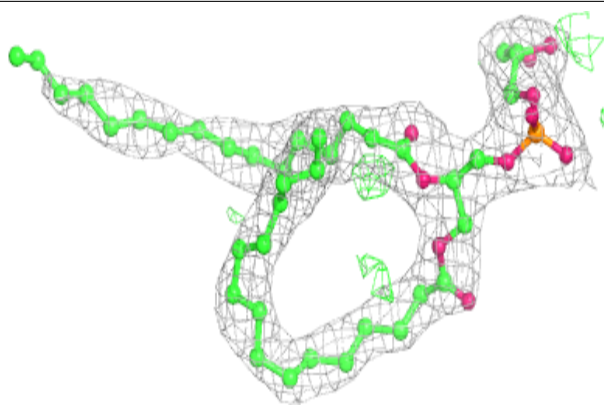
**Electron density around BCR b 617:**

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

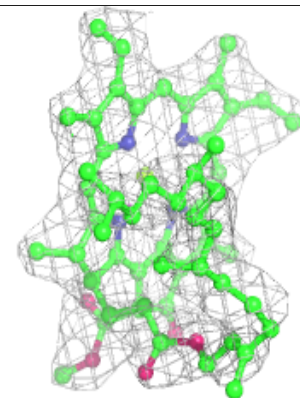
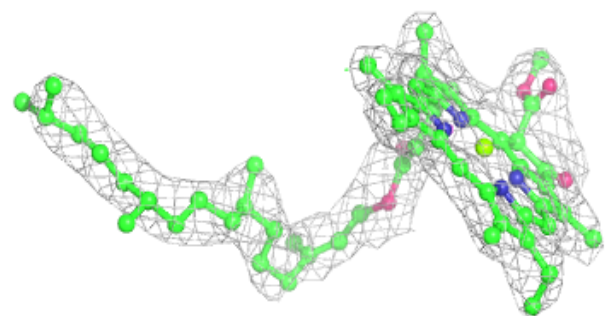
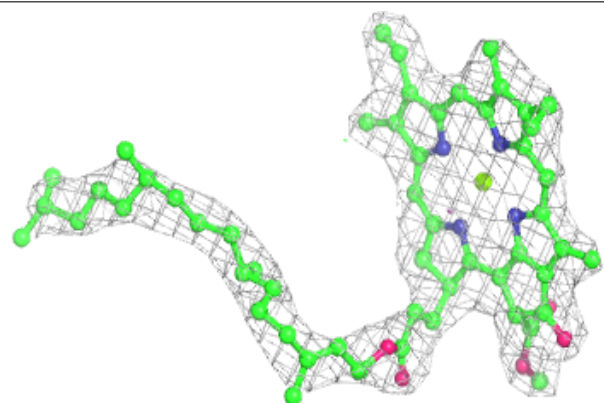


Electron density around LHG d 406:

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

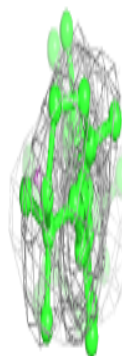
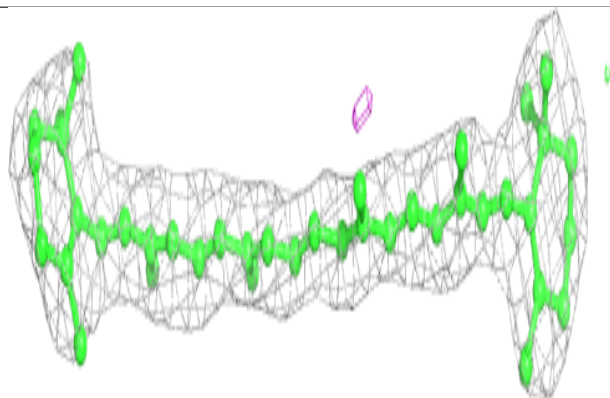
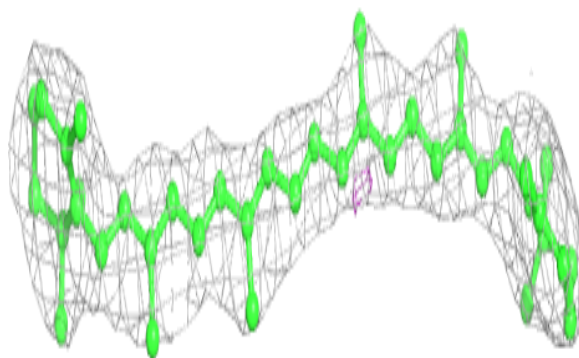
**Electron density around CLA C 513:**

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

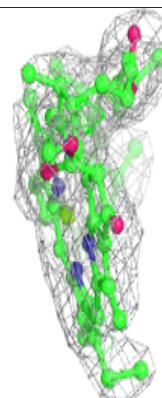
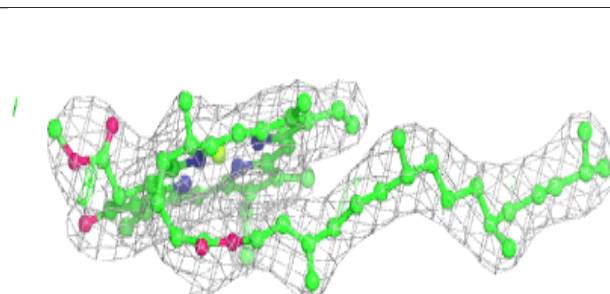
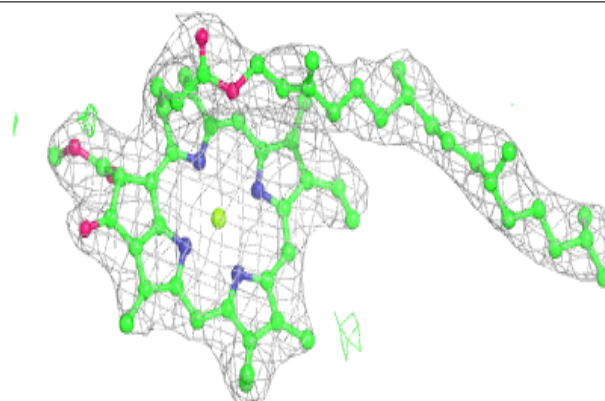


Electron density around BCR c 516:

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

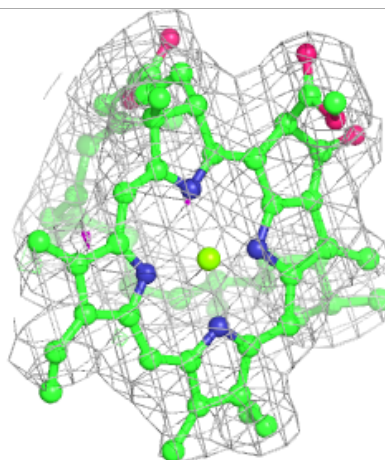
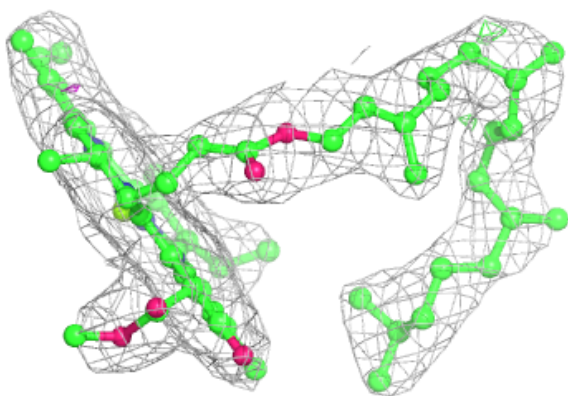
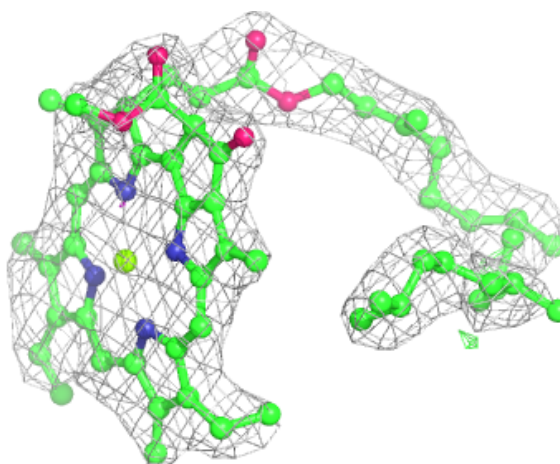
**Electron density around CLA C 503:**

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



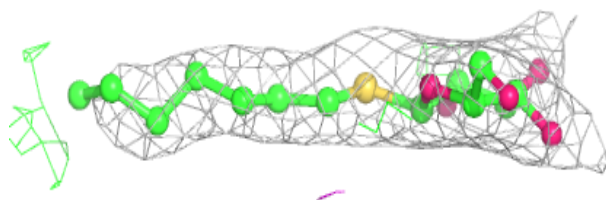
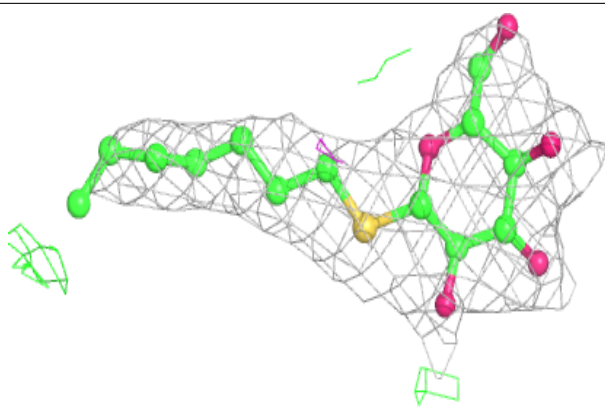
Electron density around CLA C 505:

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



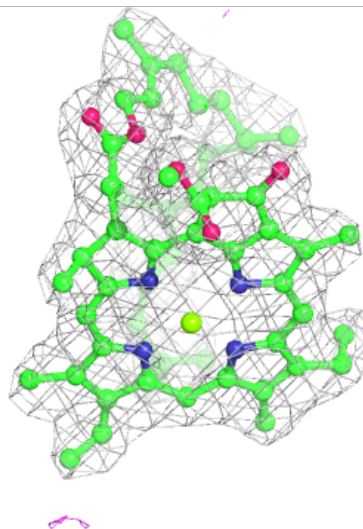
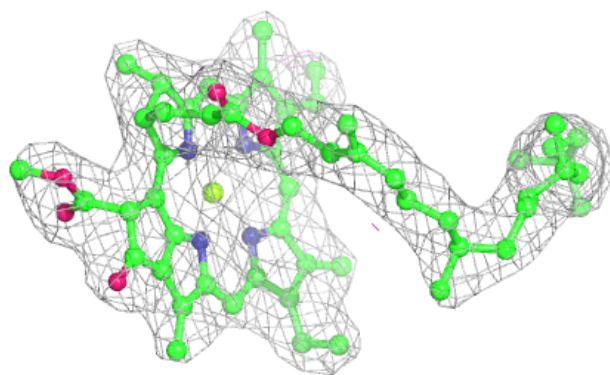
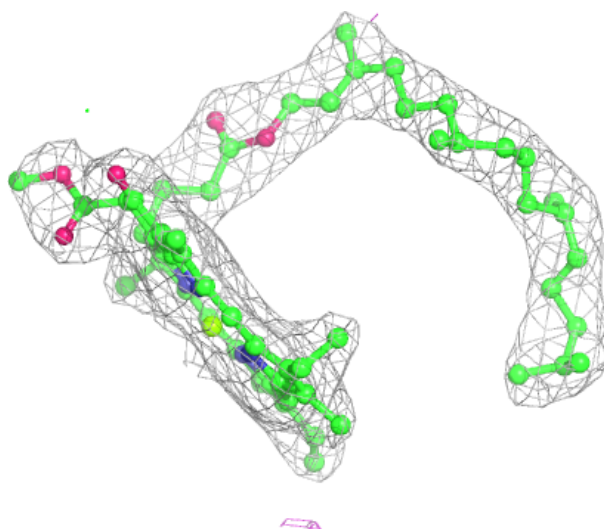
Electron density around HTG B 624:

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



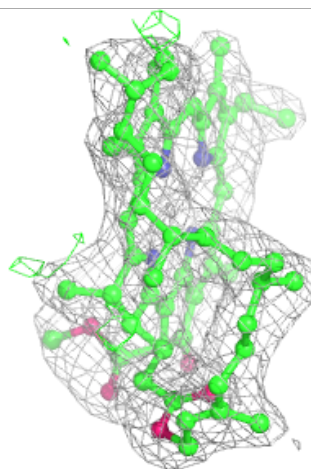
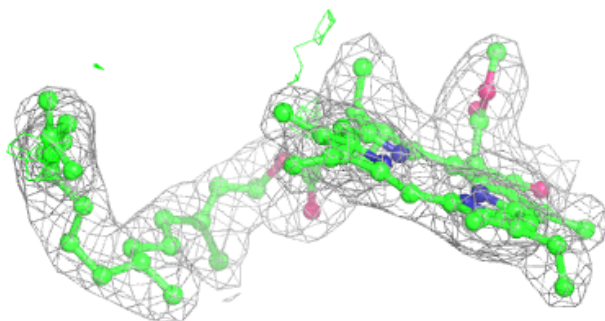
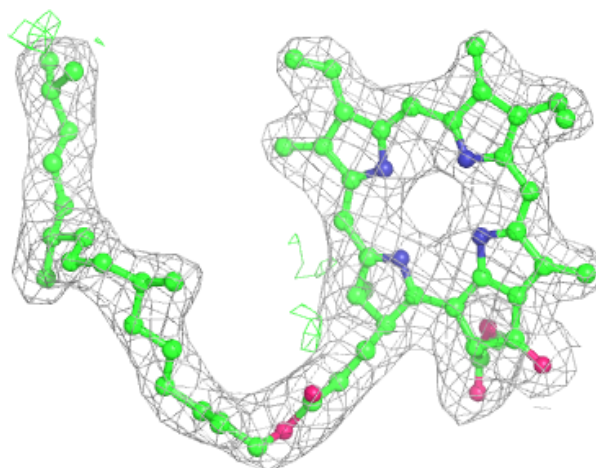
Electron density around CLA b 611:

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



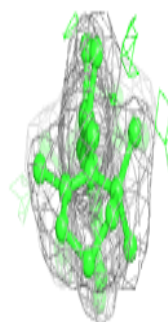
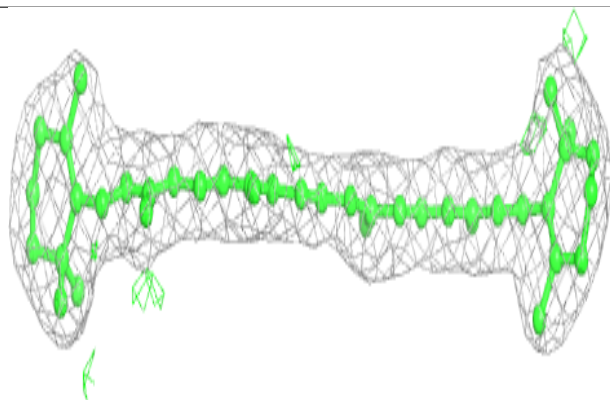
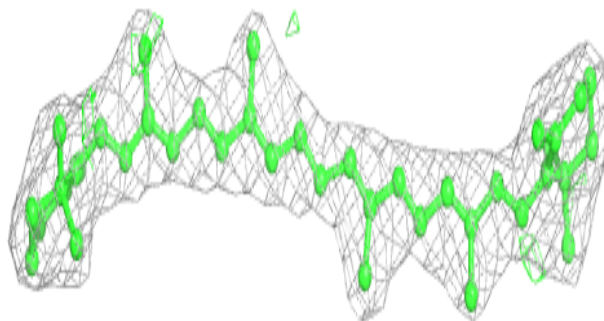
Electron density around PHO A 415:

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

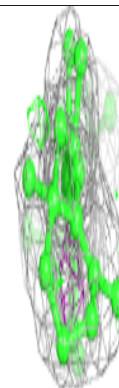
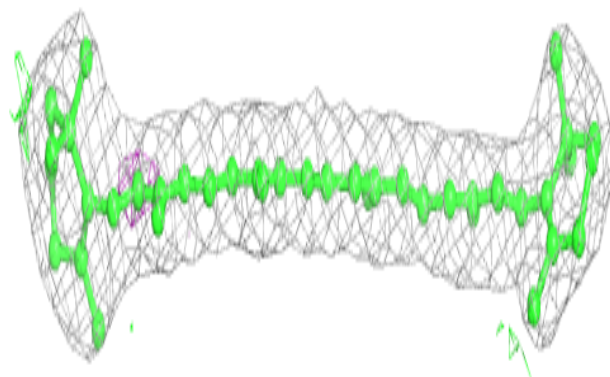
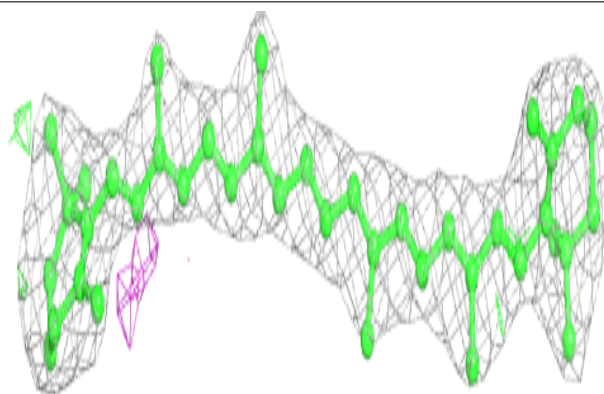


Electron density around BCR A 408:

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

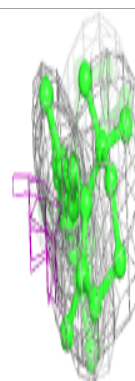
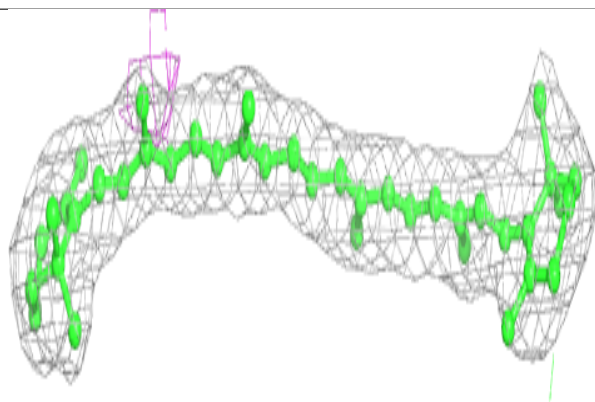
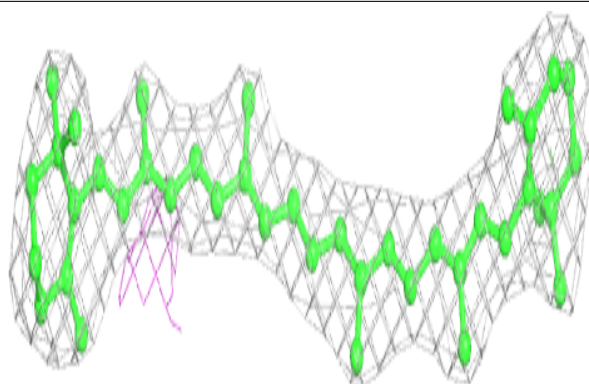
**Electron density around BCR B 618:**

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

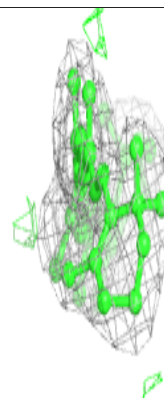
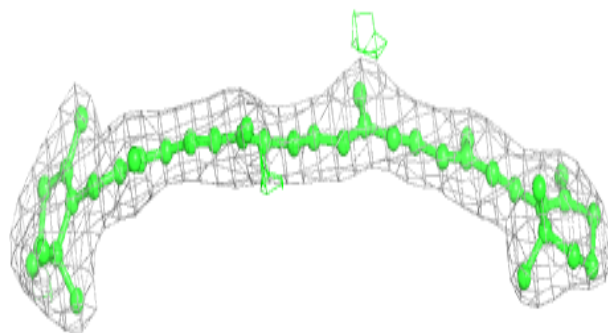
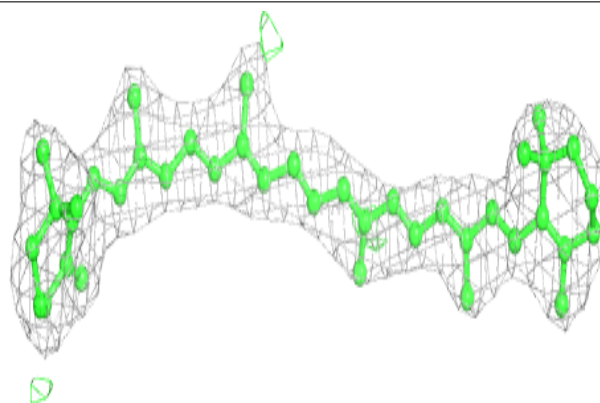


Electron density around BCR B 619:

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

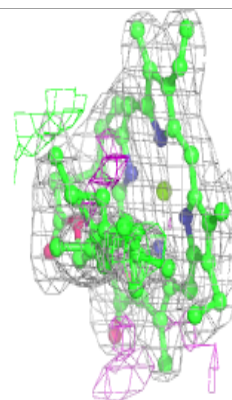
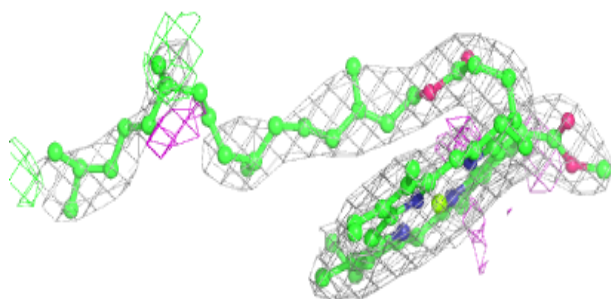
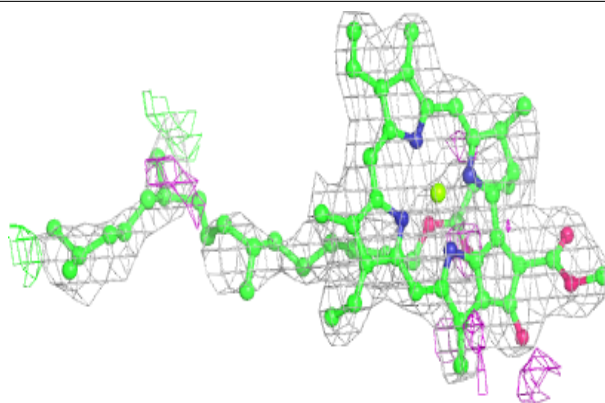
**Electron density around BCR B 631:**

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

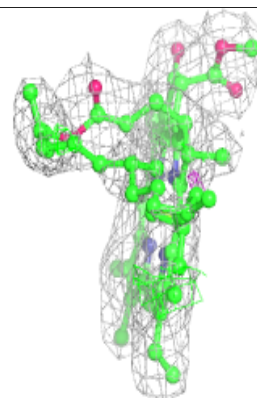
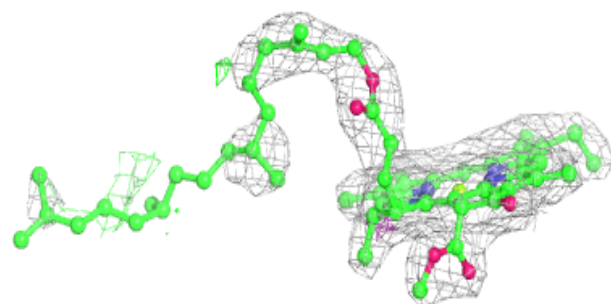
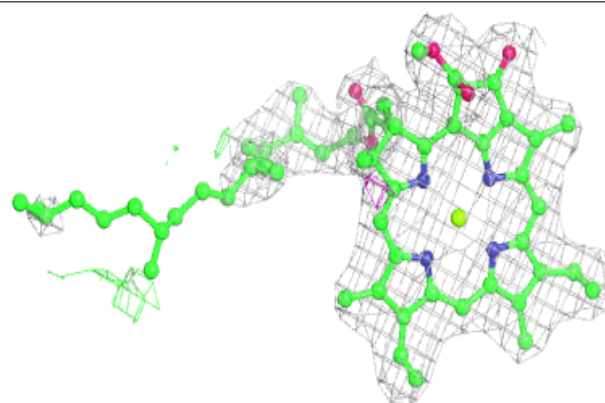


Electron density around CLA B 614:

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

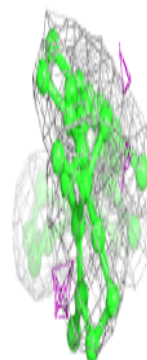
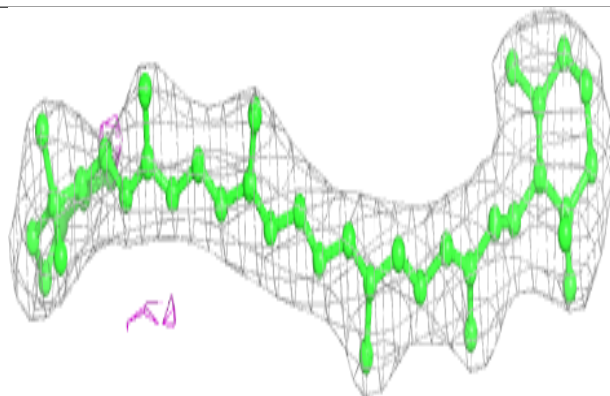
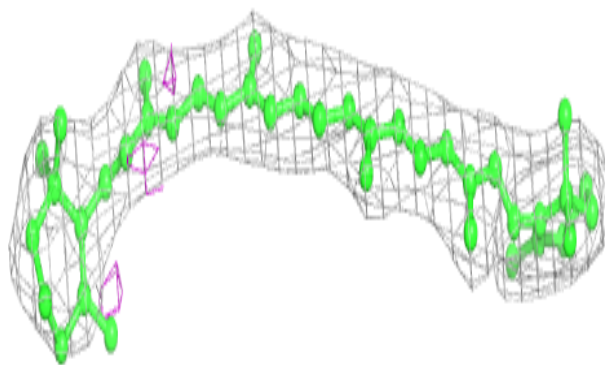
**Electron density around CLA a 405:**

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



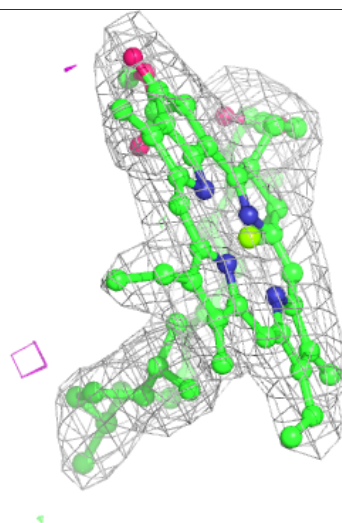
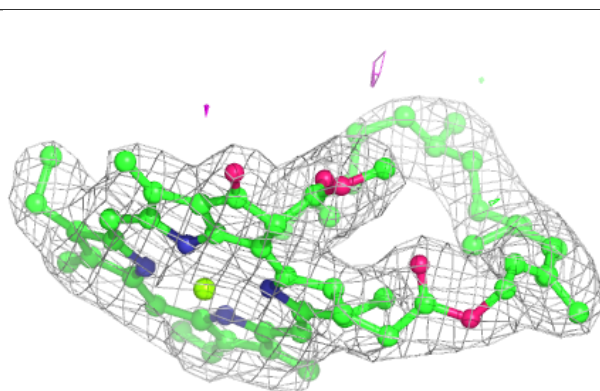
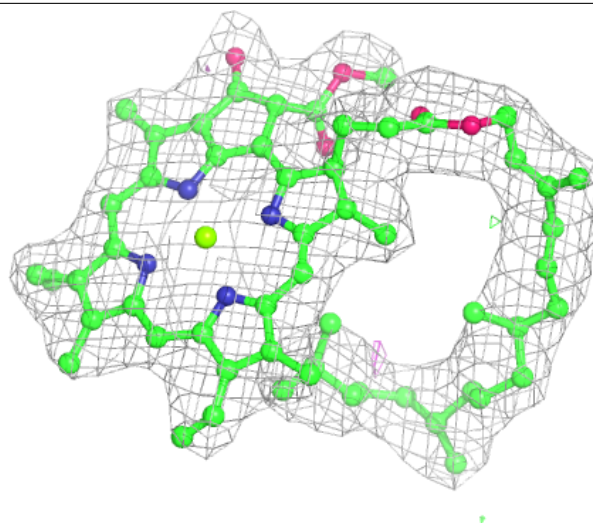
Electron density around BCR D 405:

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



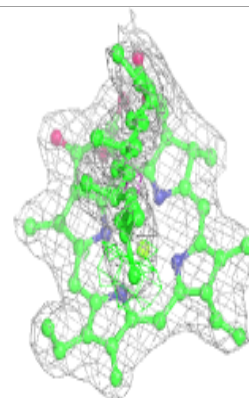
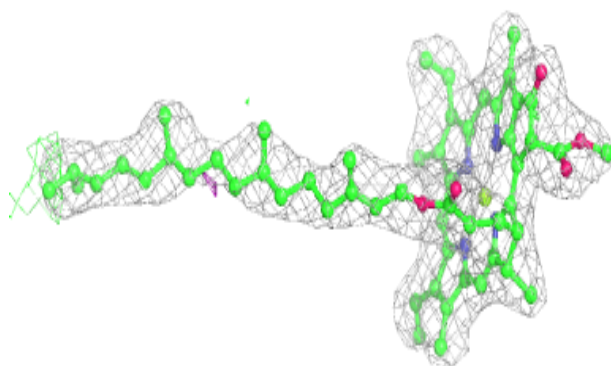
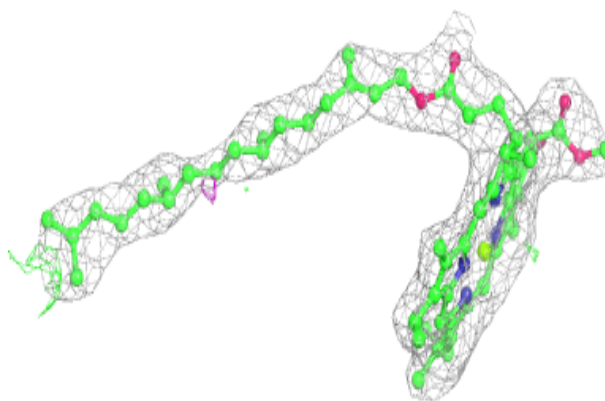
Electron density around CLA b 615:

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

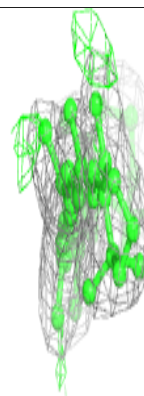
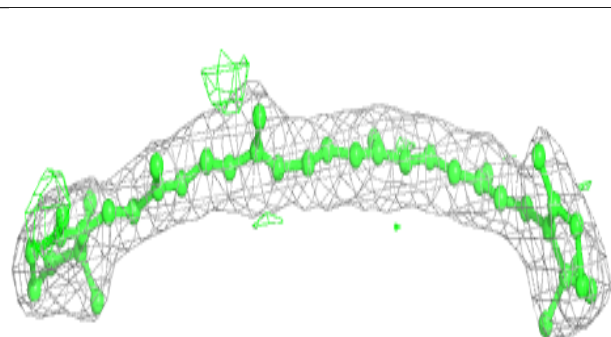
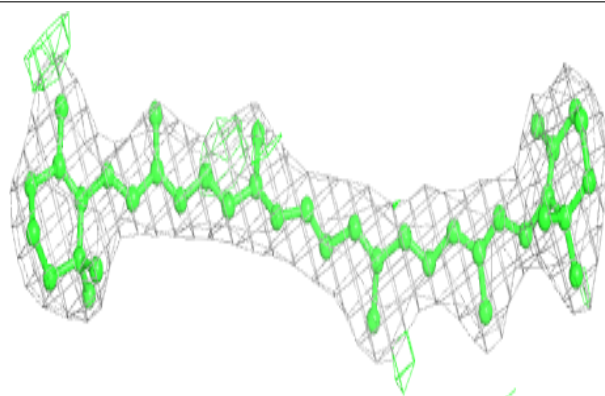


Electron density around CLA B 607:

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

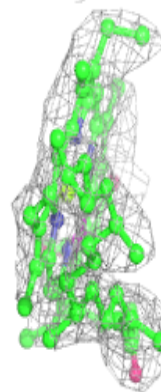
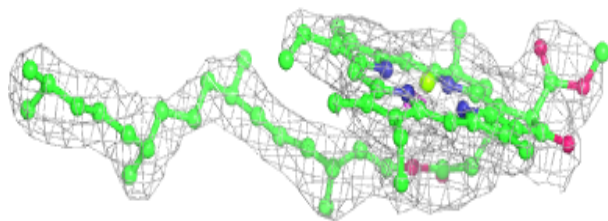
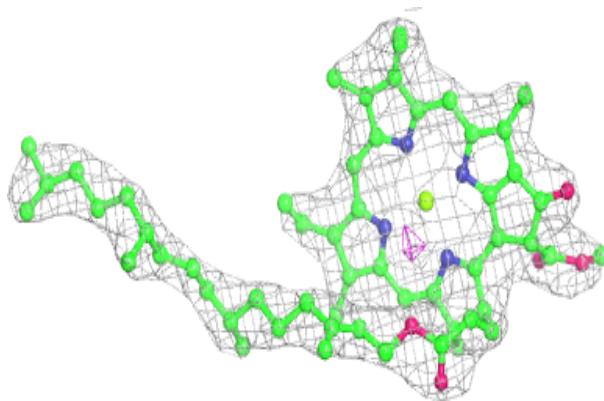
**Electron density around BCR T 101:**

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

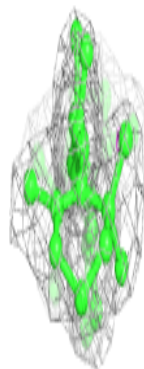
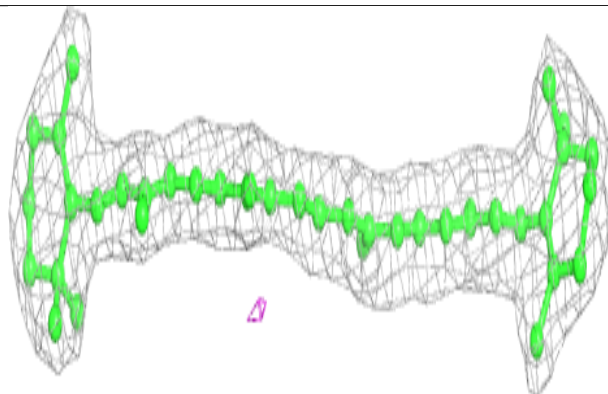
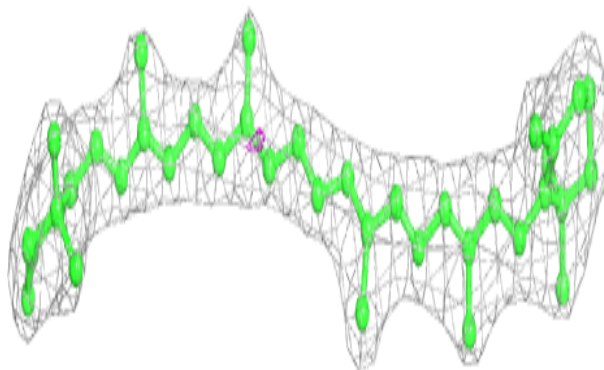


Electron density around CLA c 503:

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

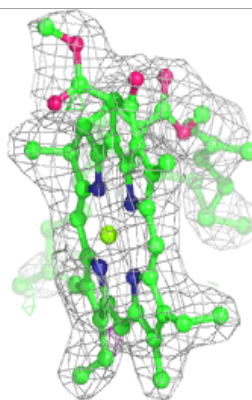
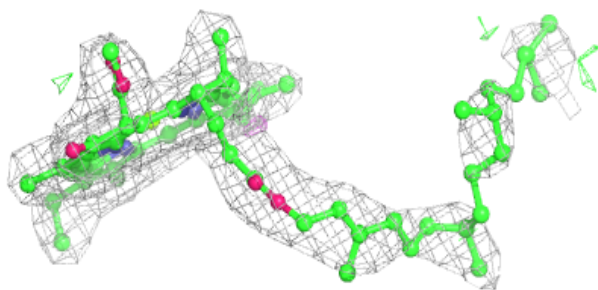
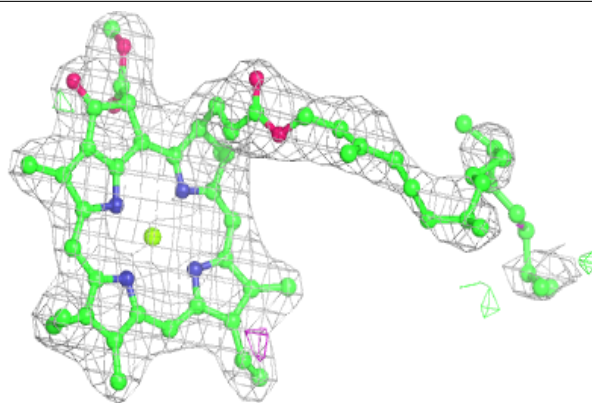
**Electron density around BCR a 408:**

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

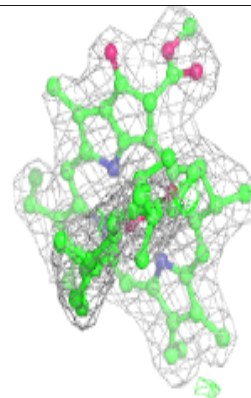
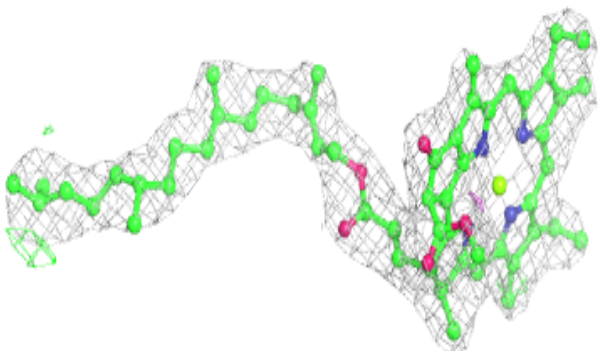
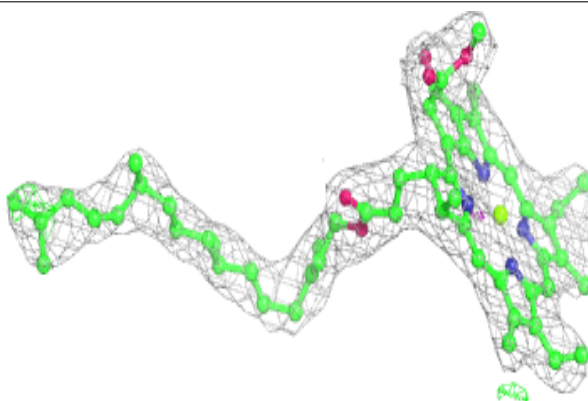


Electron density around CLA A 407:

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

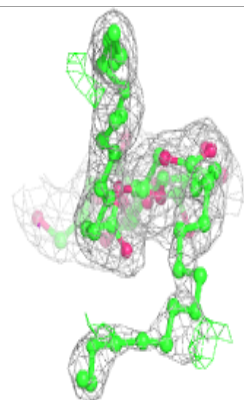
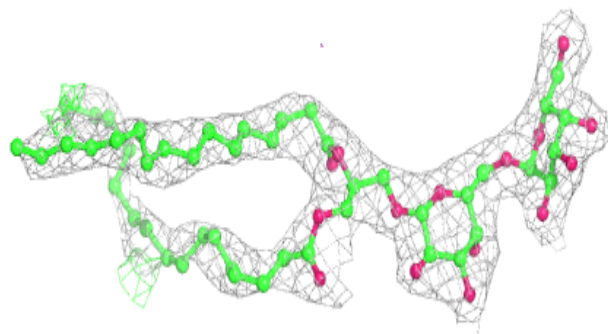
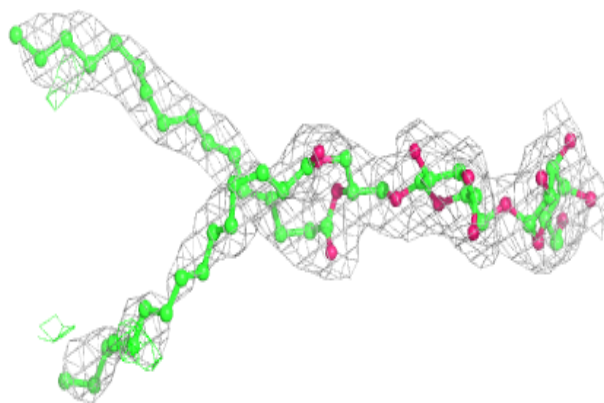
**Electron density around CLA C 504:**

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

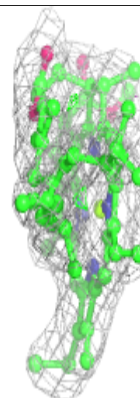
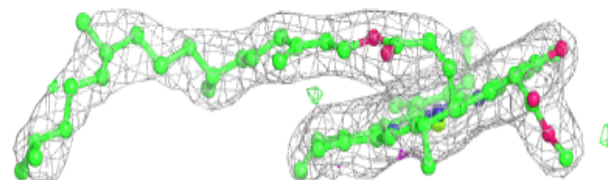
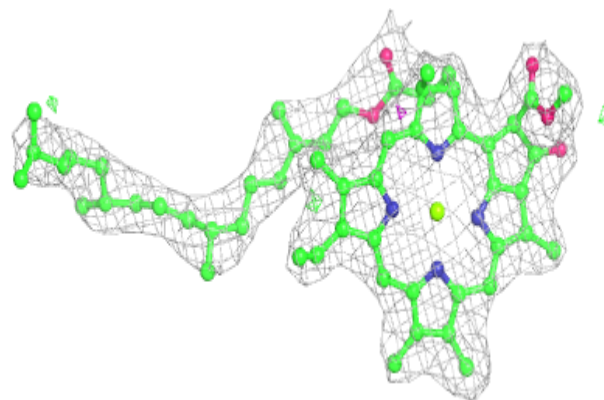


Electron density around DGD c 518:

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

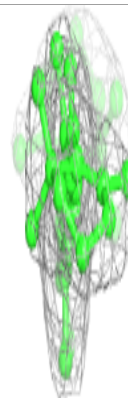
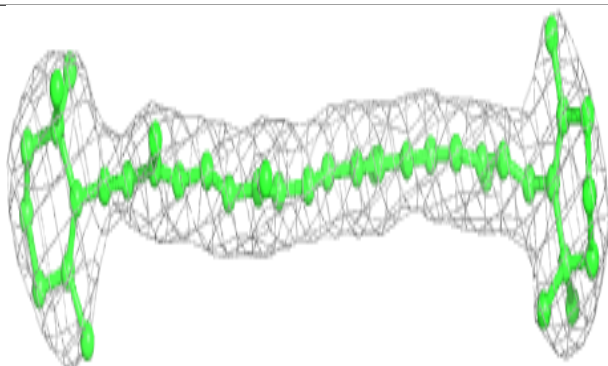
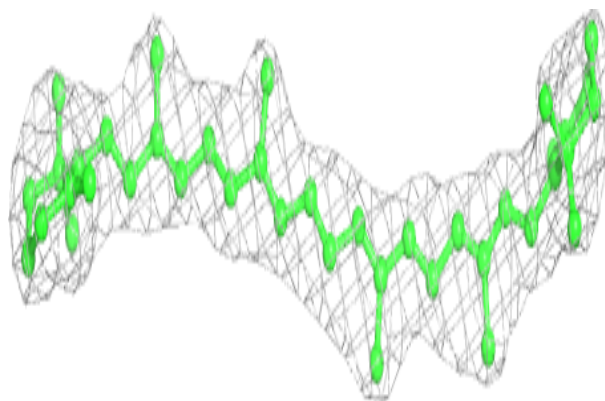
**Electron density around CLA b 603:**

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

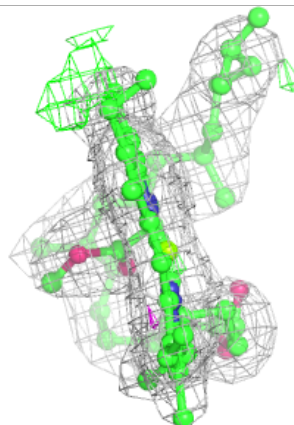
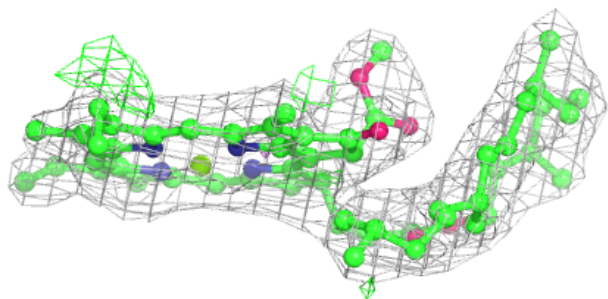
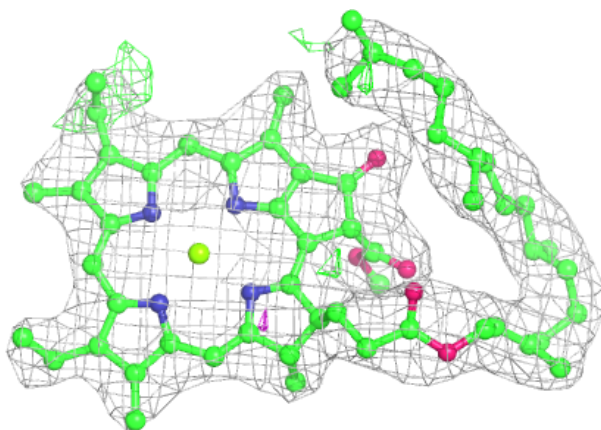


Electron density around BCR c 517:

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

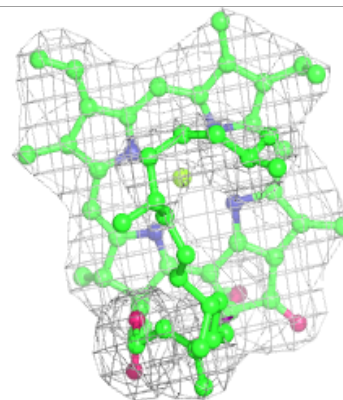
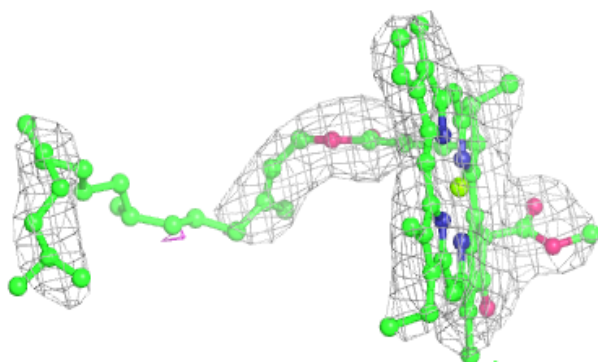
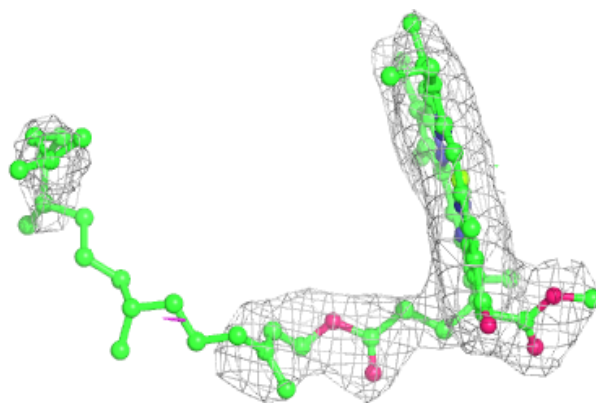
**Electron density around CLA B 610:**

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

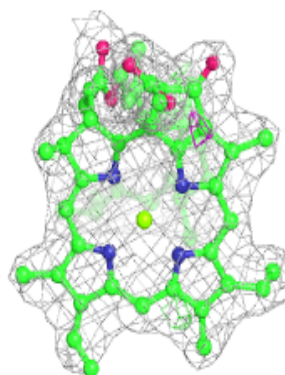
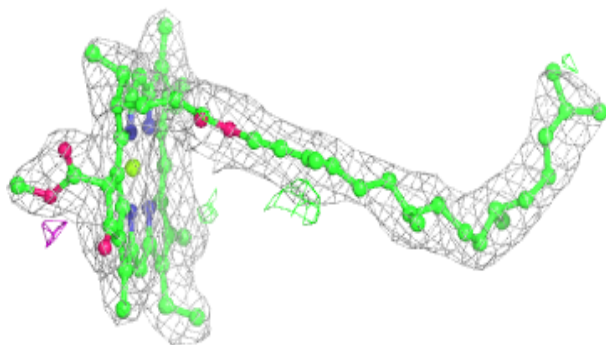
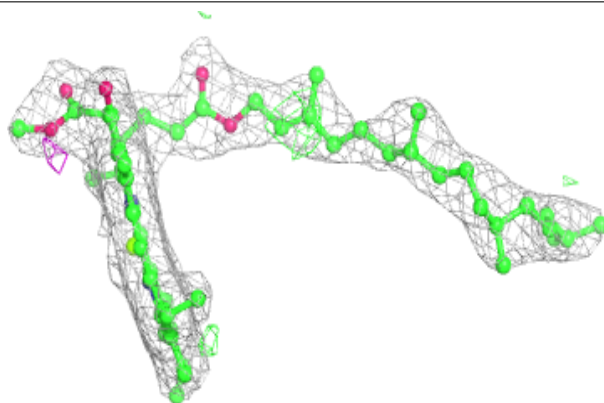


Electron density around CLA c 508:

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

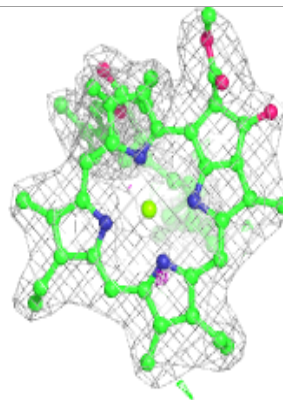
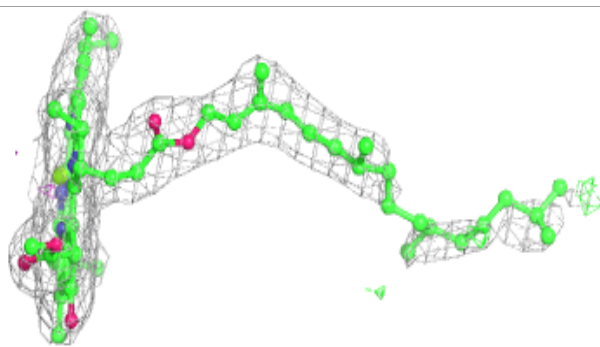
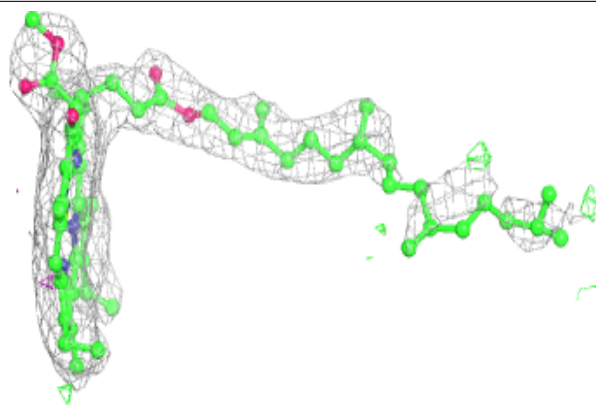
**Electron density around CLA b 605:**

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

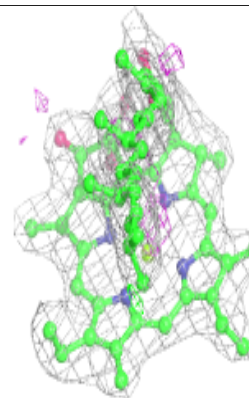
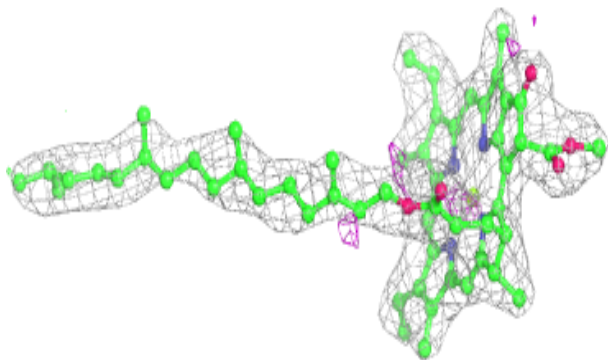
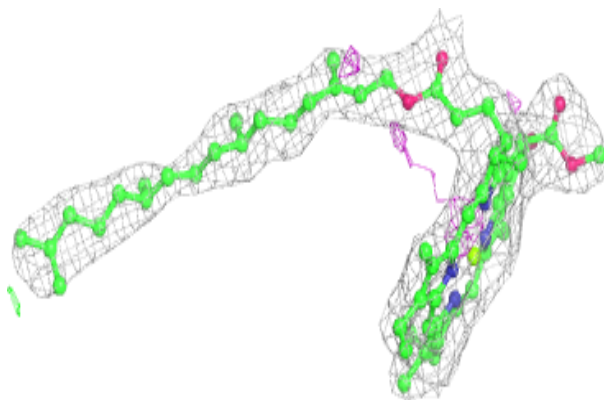


Electron density around CLA b 606:

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

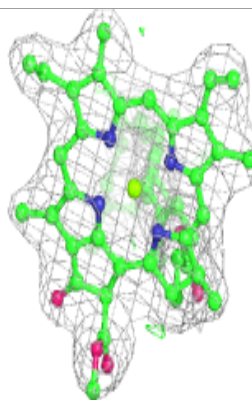
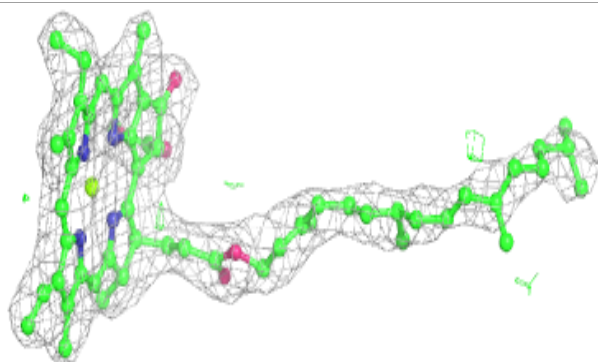
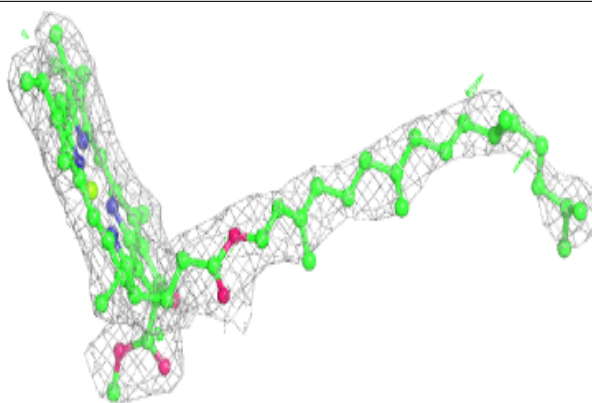
**Electron density around CLA b 607:**

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

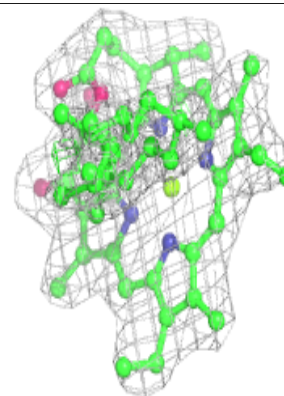
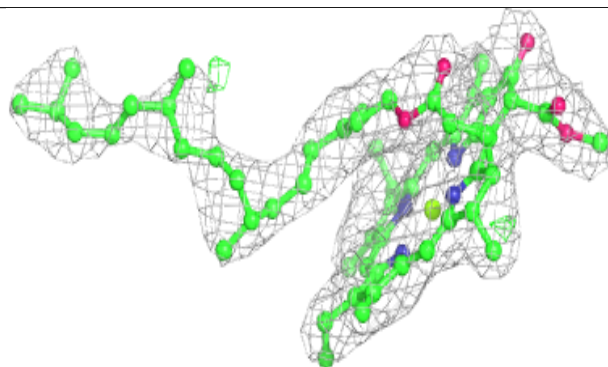
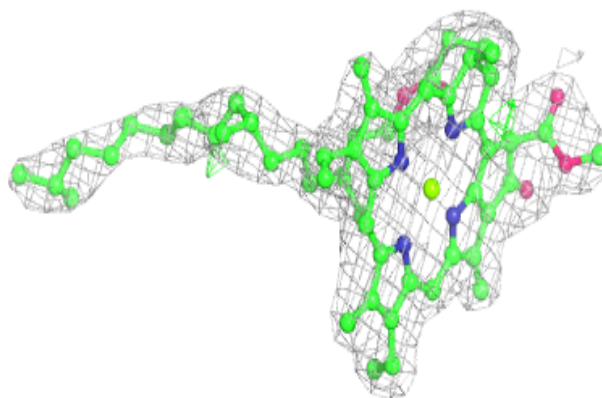


Electron density around CLA B 604:

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

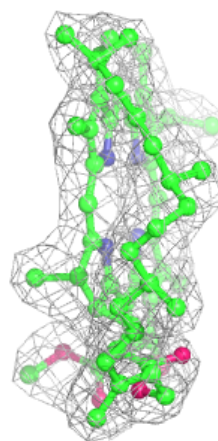
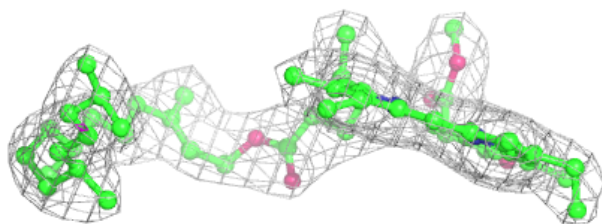
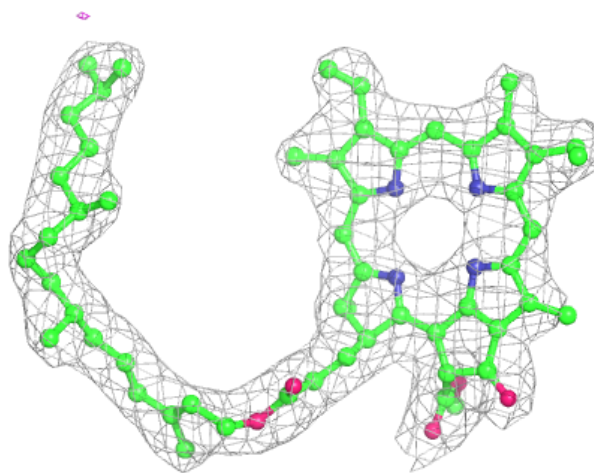
**Electron density around CLA C 507:**

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



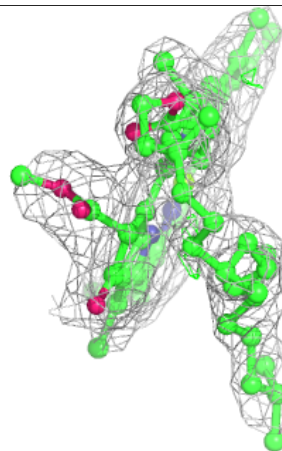
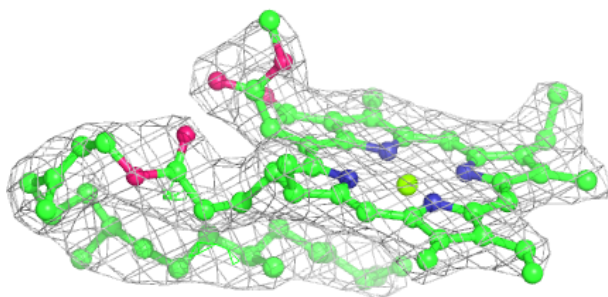
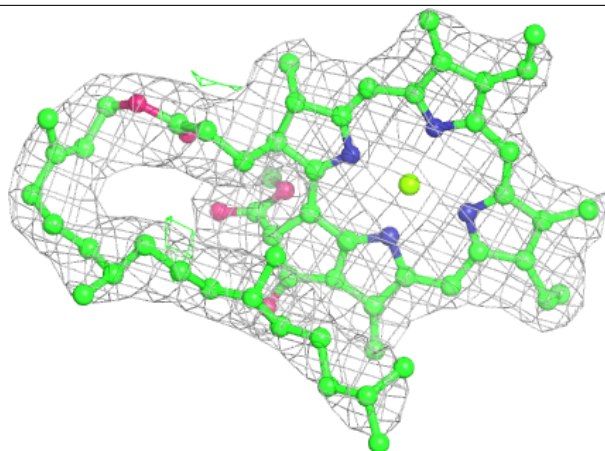
Electron density around PHO A 406:

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



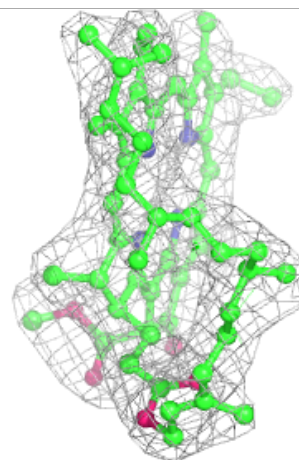
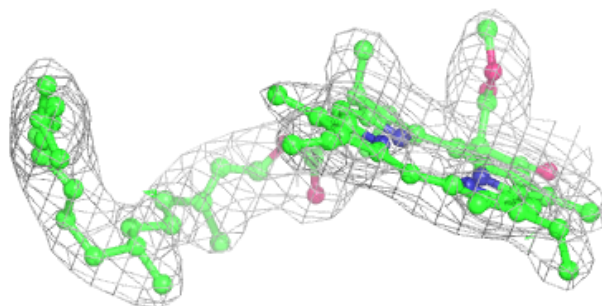
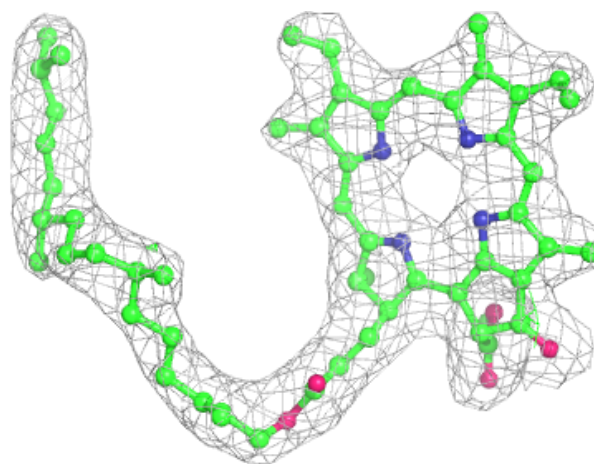
Electron density around CLA C 511:

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



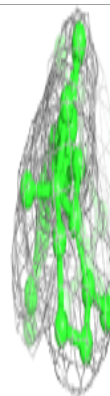
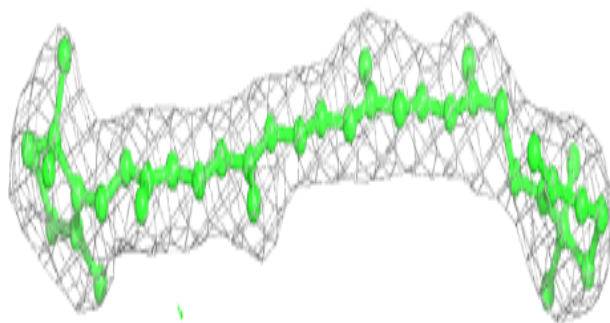
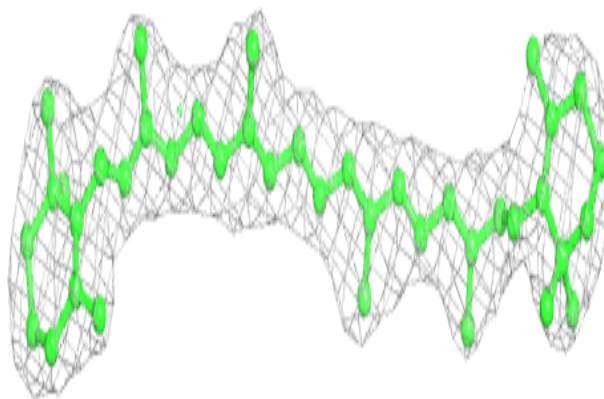
Electron density around PHO a 416:

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



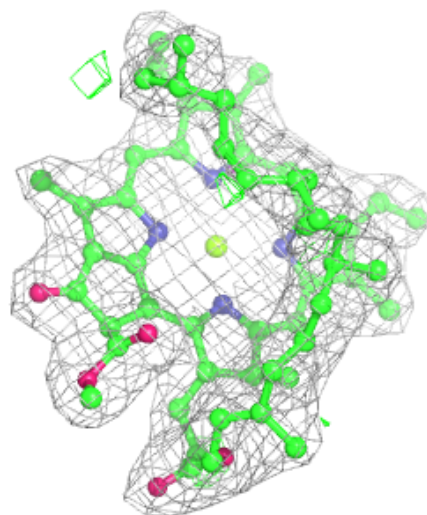
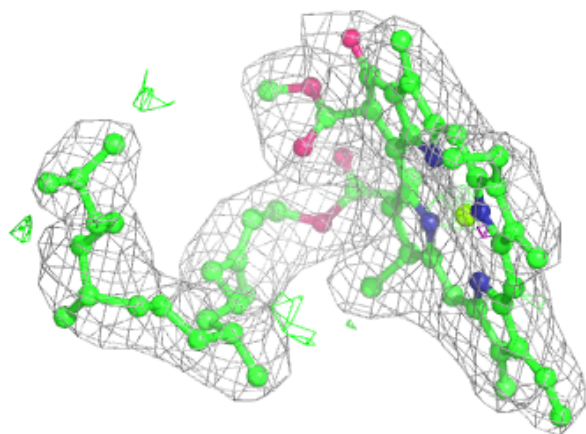
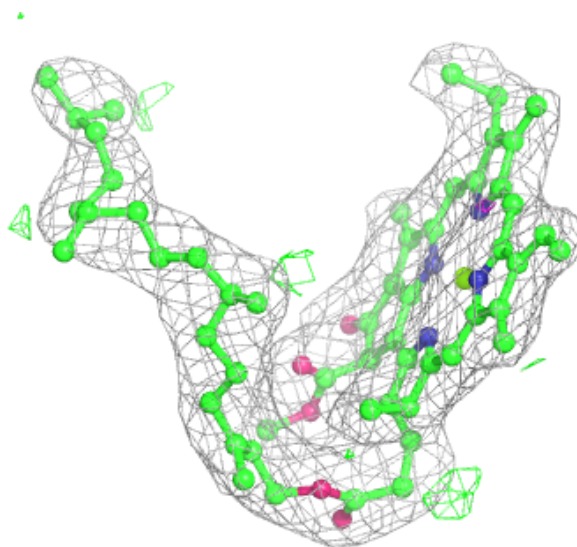
Electron density around BCR b 619:

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



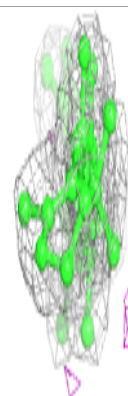
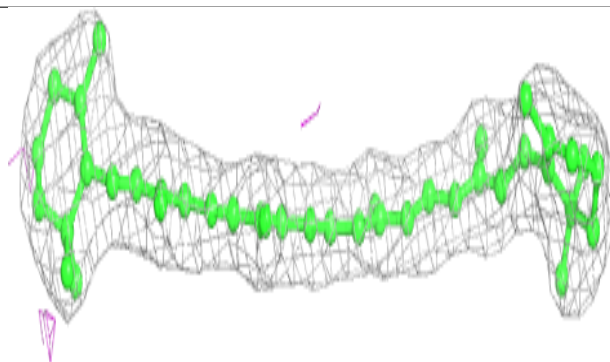
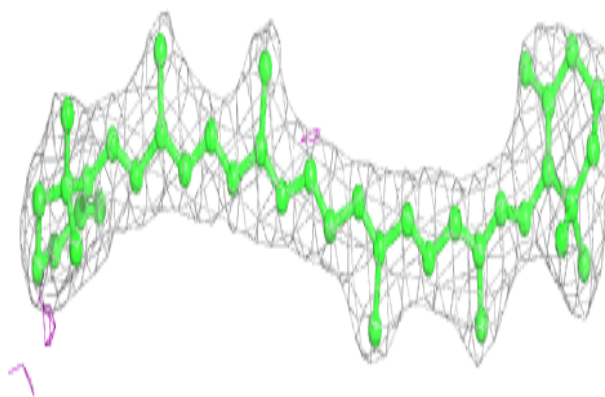
Electron density around CLA B 613:

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

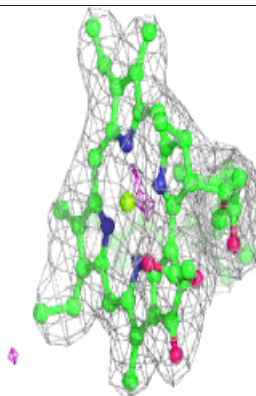
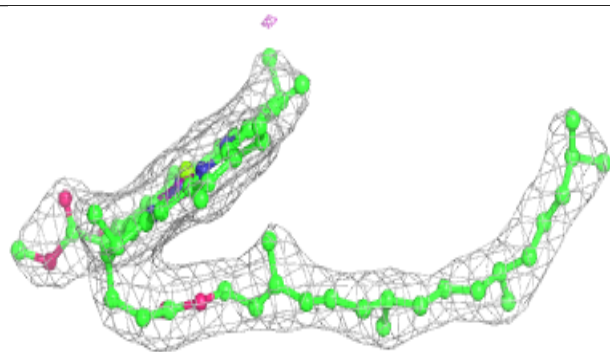
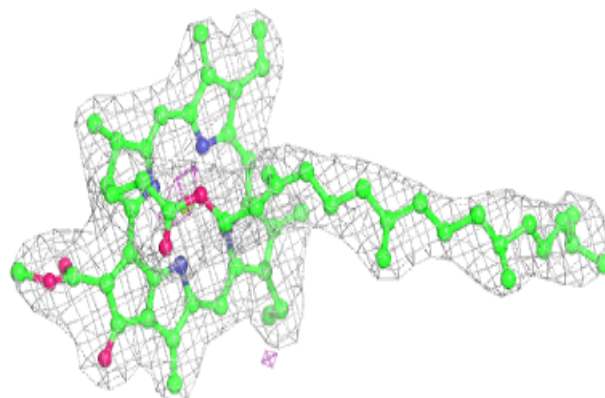


Electron density around BCR B 617:

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

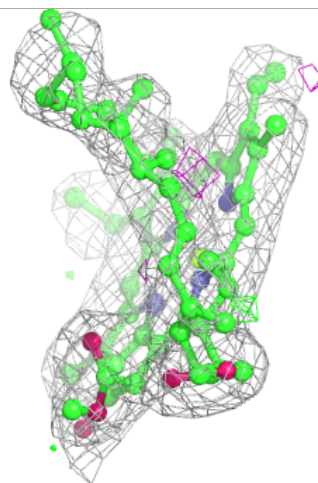
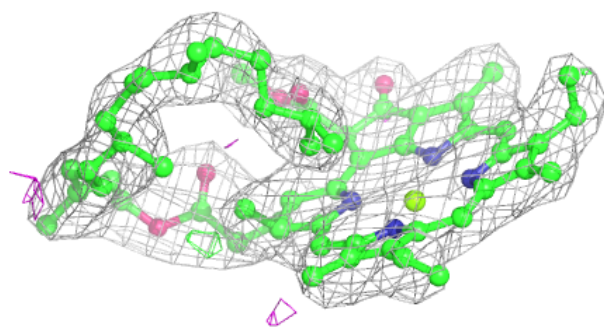
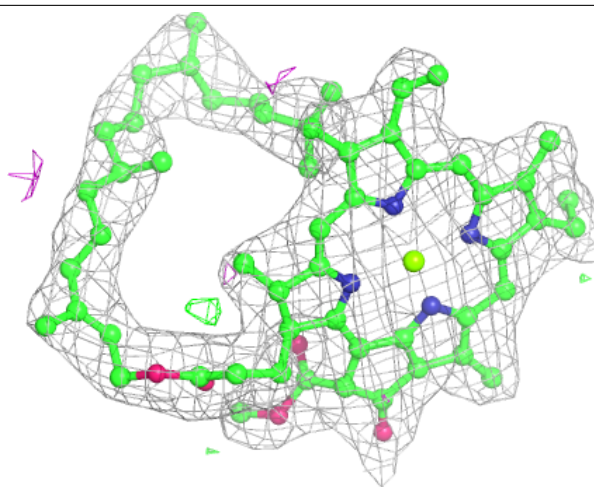
**Electron density around CLA B 608:**

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



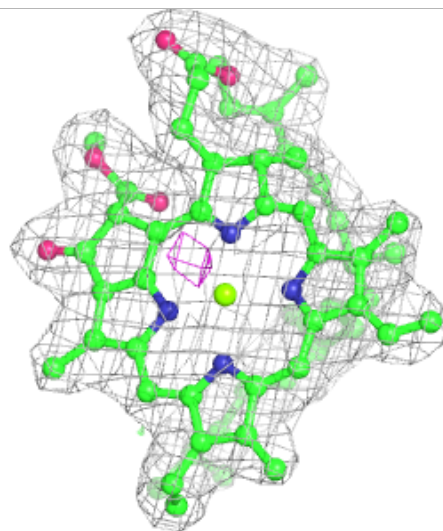
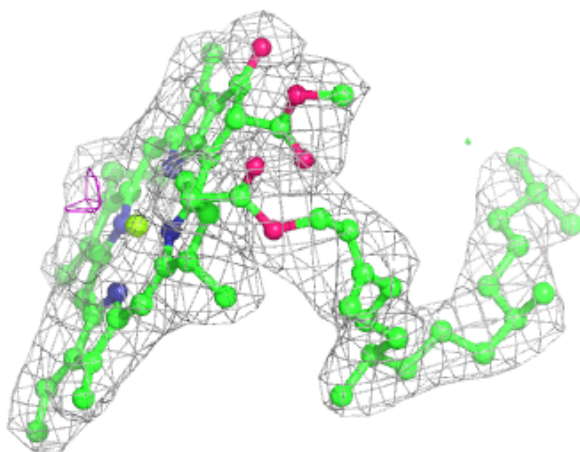
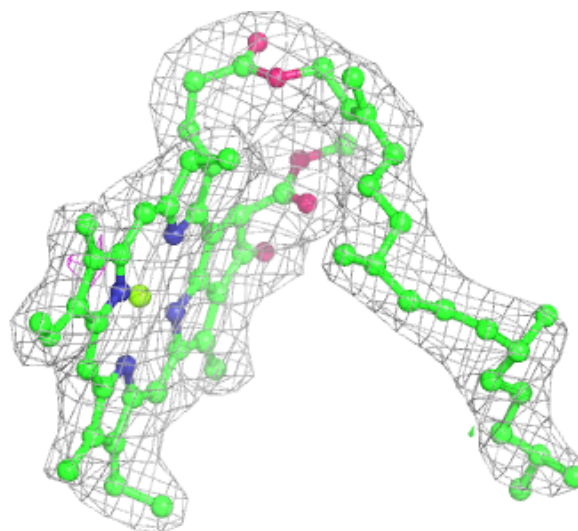
Electron density around CLA B 615:

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



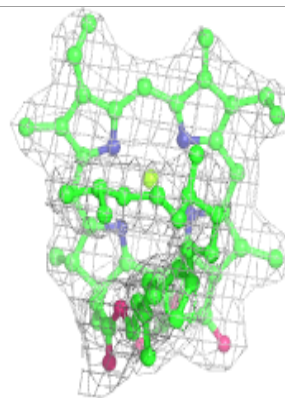
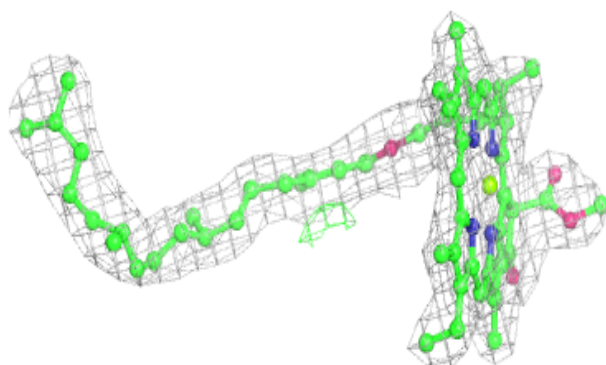
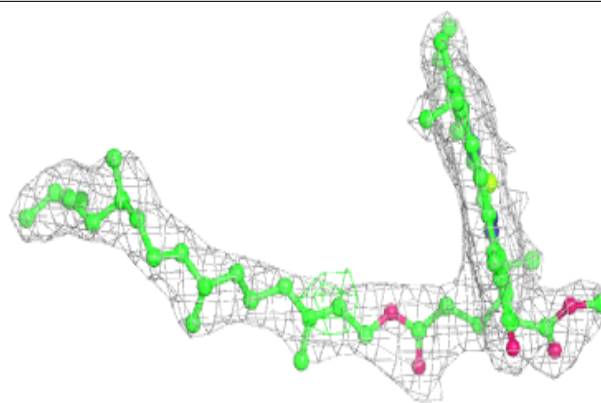
Electron density around CLA b 613:

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

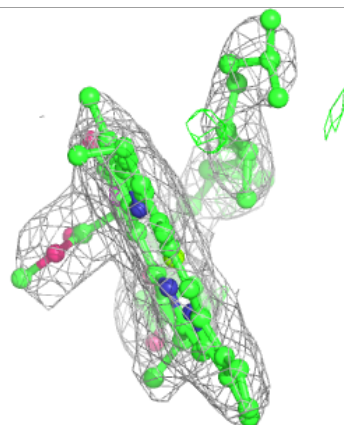
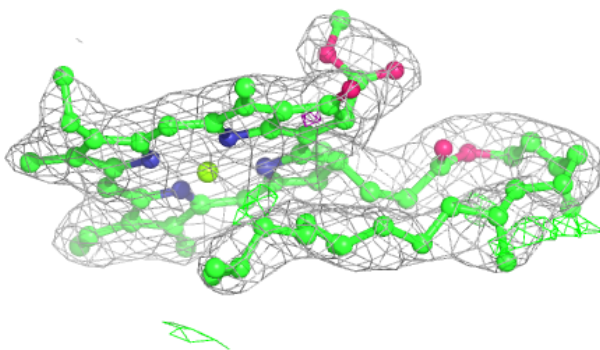
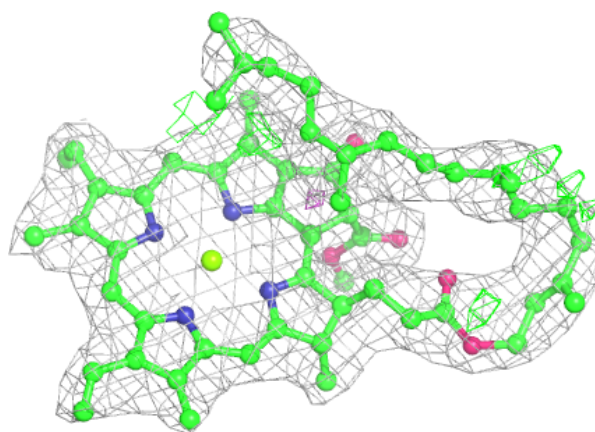


Electron density around CLA B 605:

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

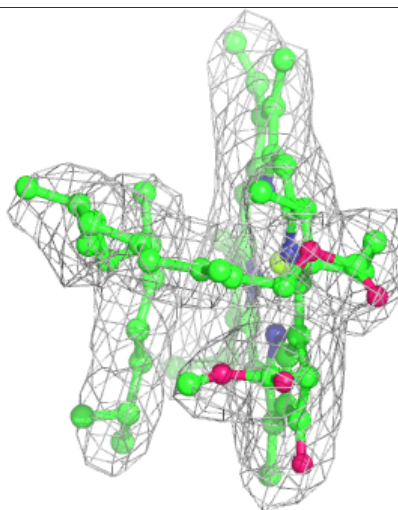
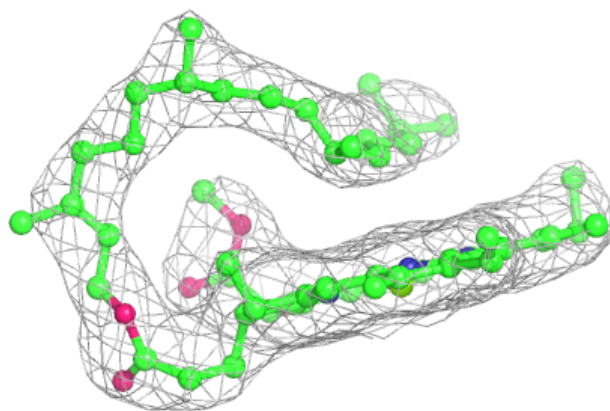
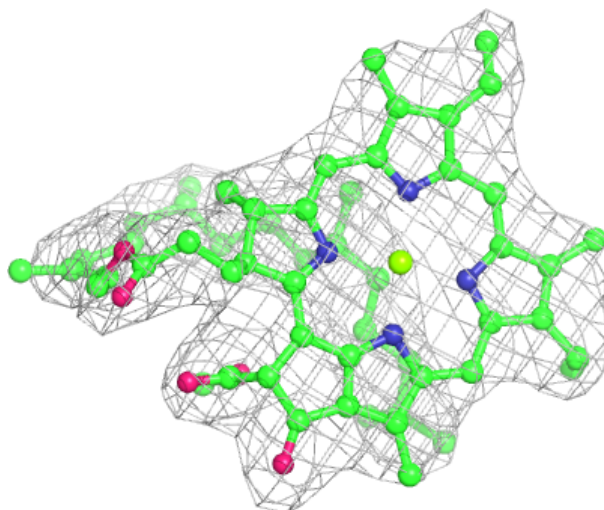
**Electron density around CLA c 511:**

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



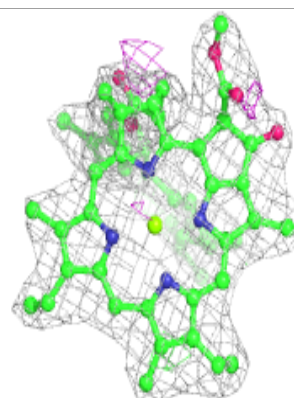
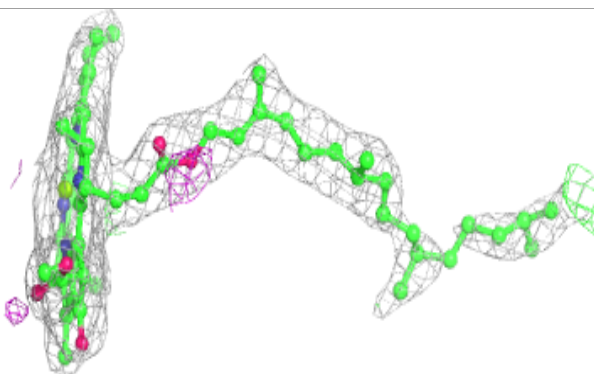
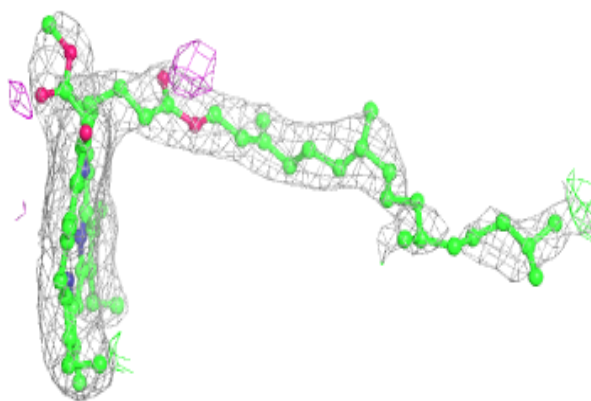
Electron density around CLA c 512:

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

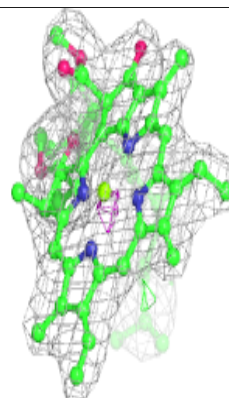
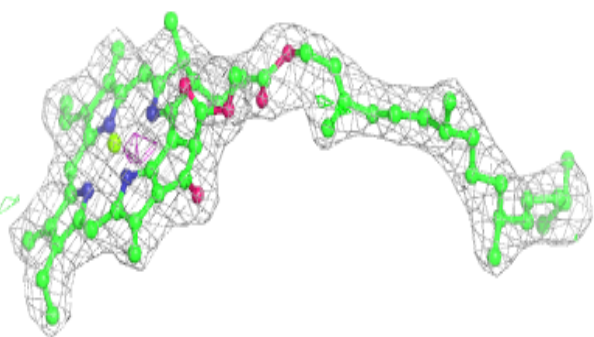
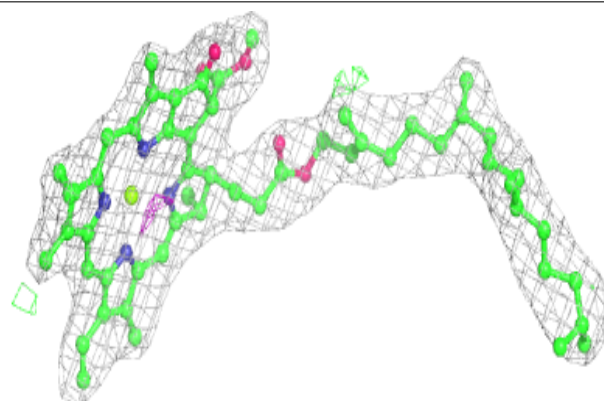


Electron density around CLA B 606:

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

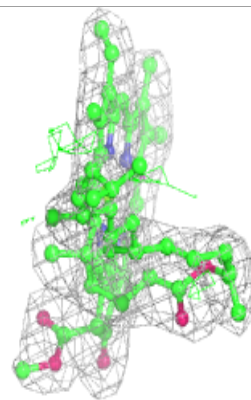
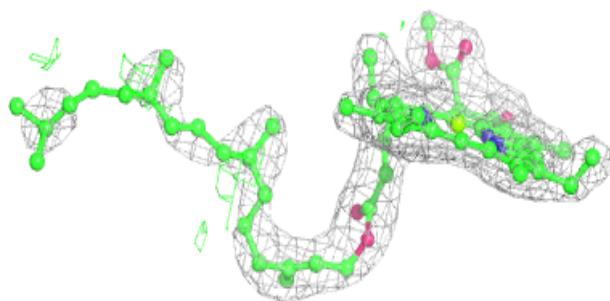
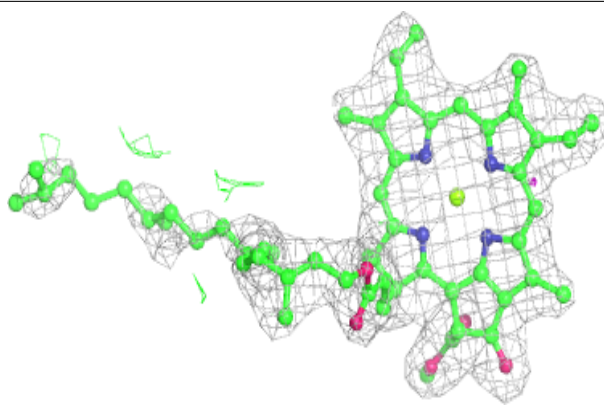
**Electron density around CLA a 403:**

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



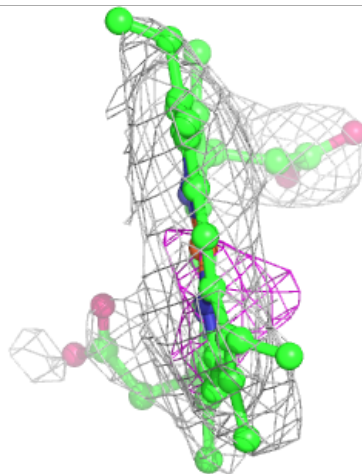
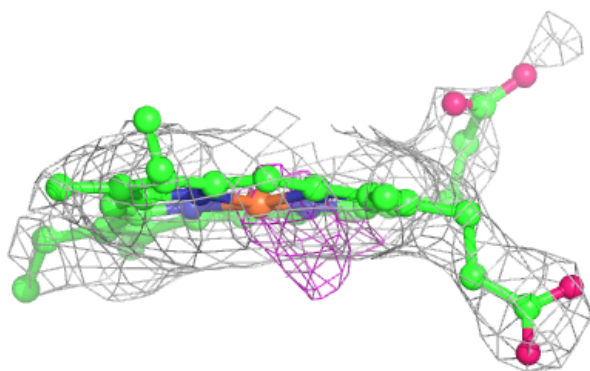
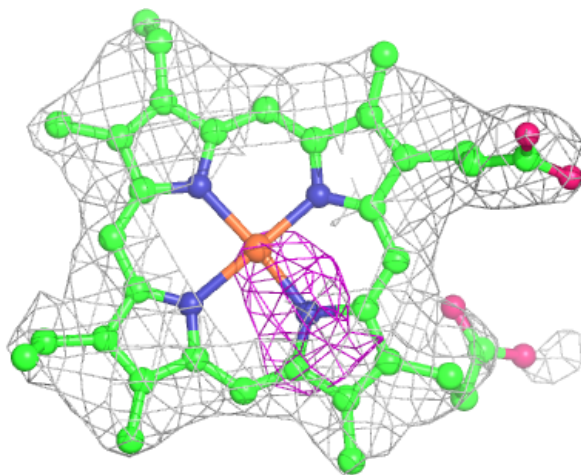
Electron density around CLA A 405:

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



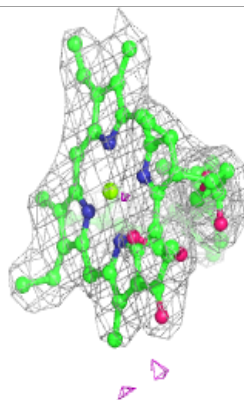
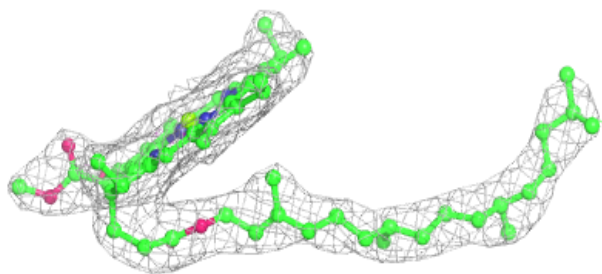
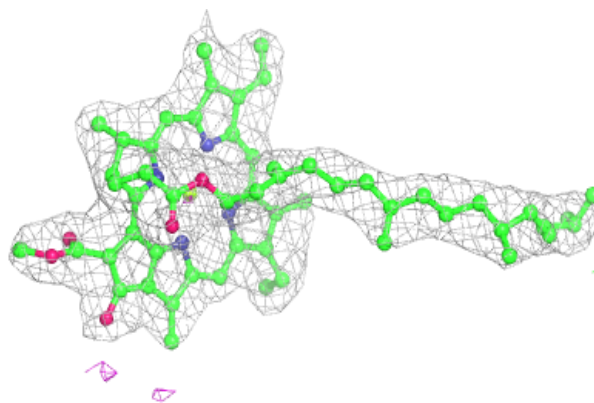
Electron density around HEM e 102:

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



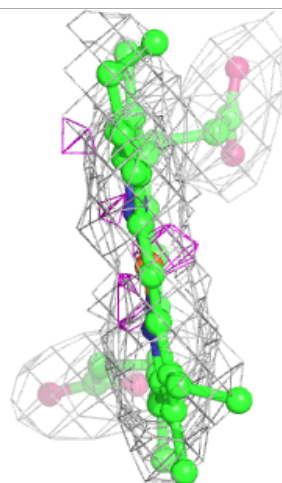
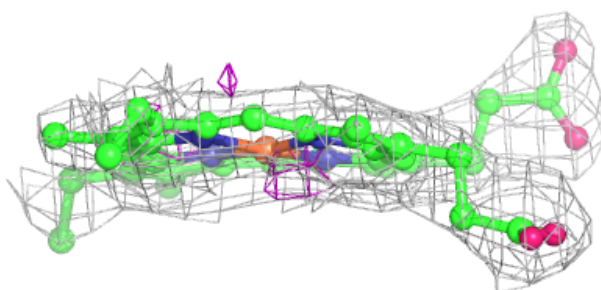
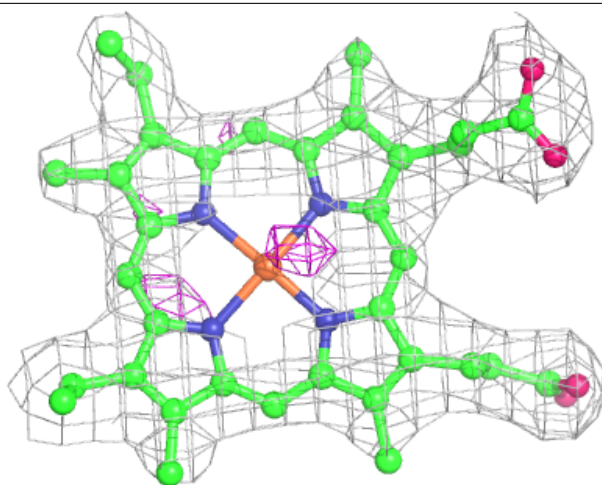
Electron density around CLA b 608:

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



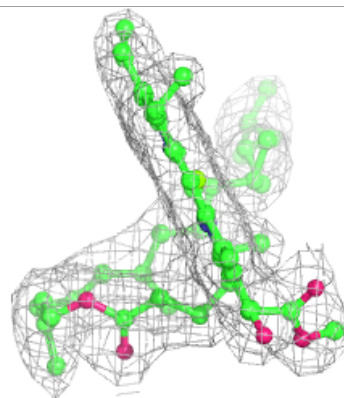
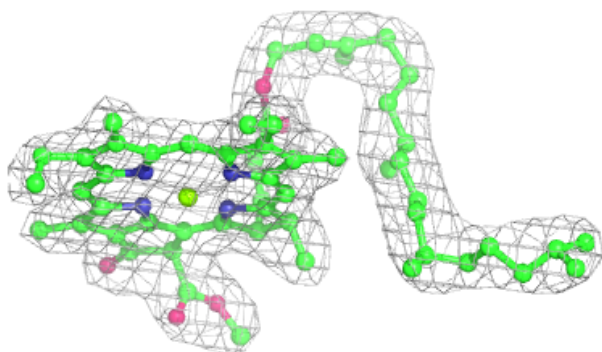
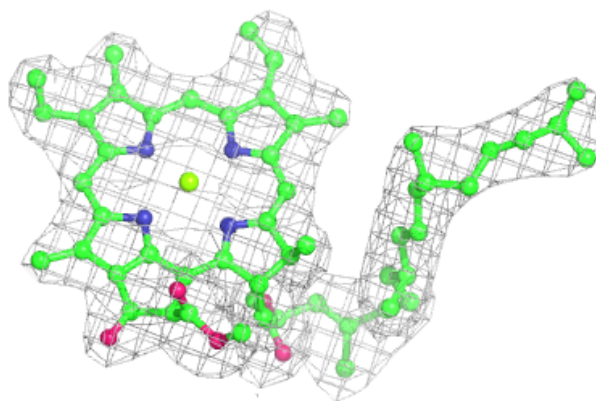
Electron density around HEC v 202:

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

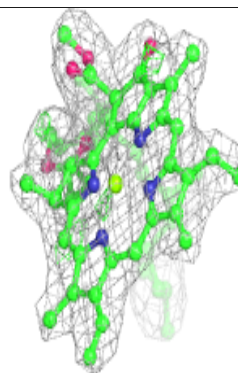
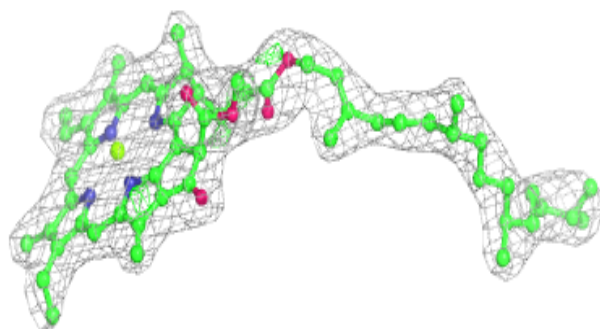
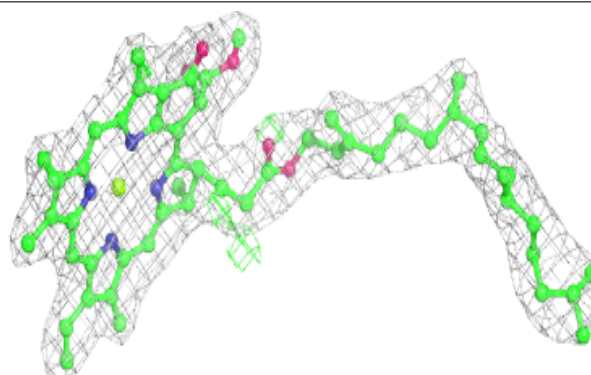


Electron density around CLA a 404:

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

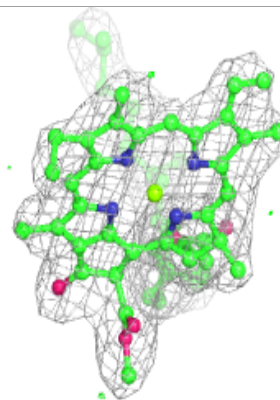
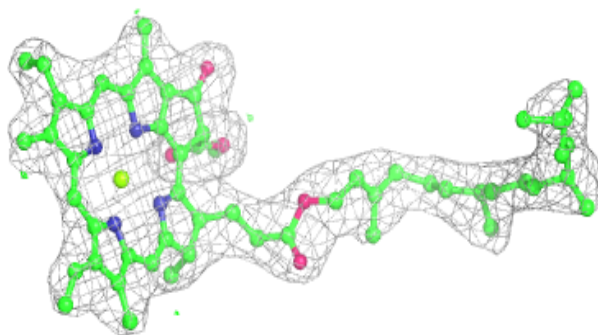
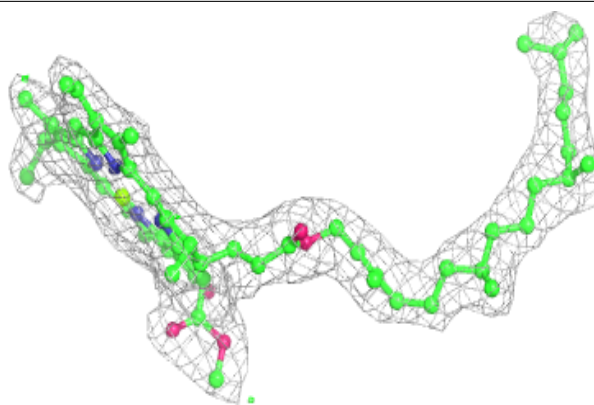
**Electron density around CLA A 403:**

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



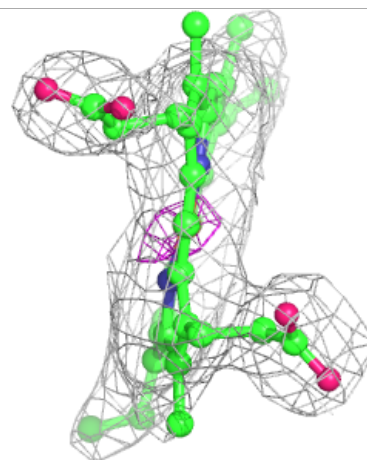
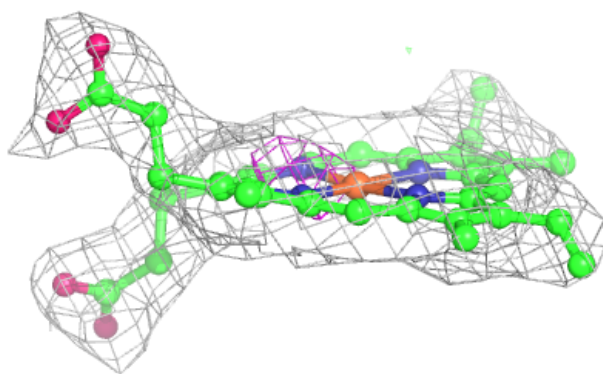
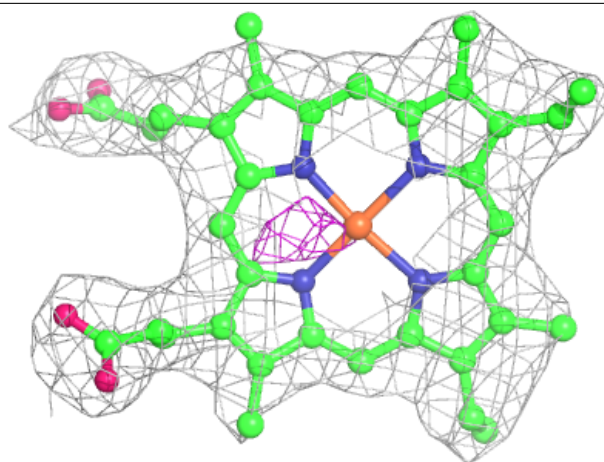
Electron density around CLA d 402:

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



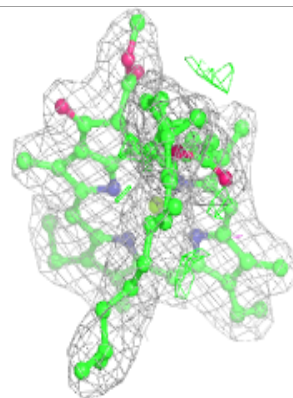
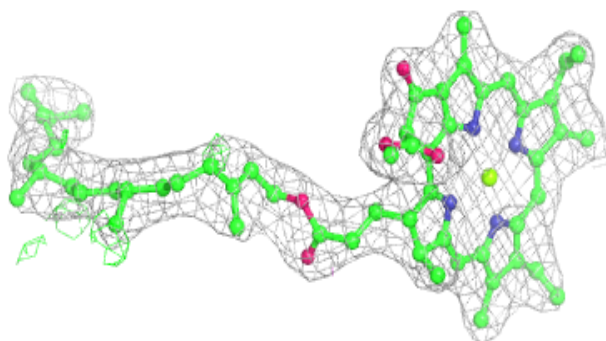
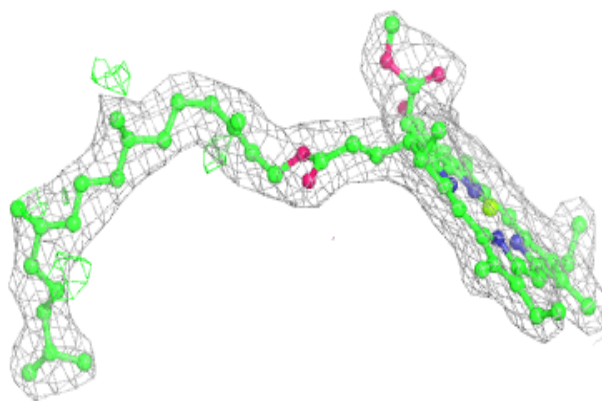
Electron density around HEM E 102:

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

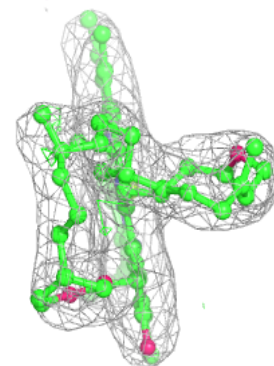
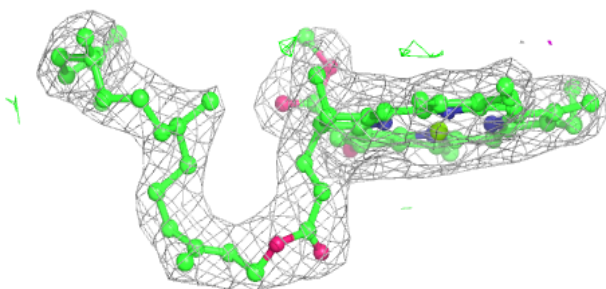
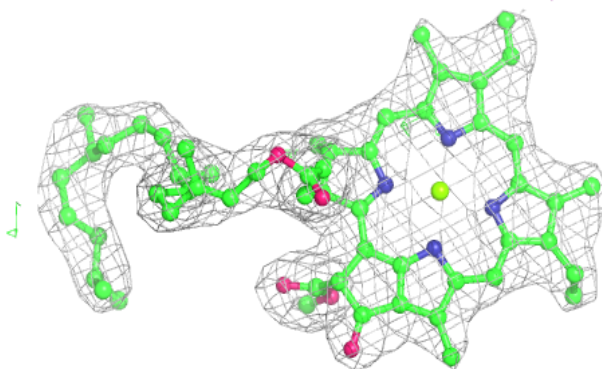


Electron density around CLA D 403:

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

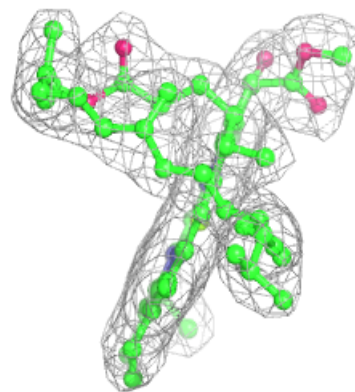
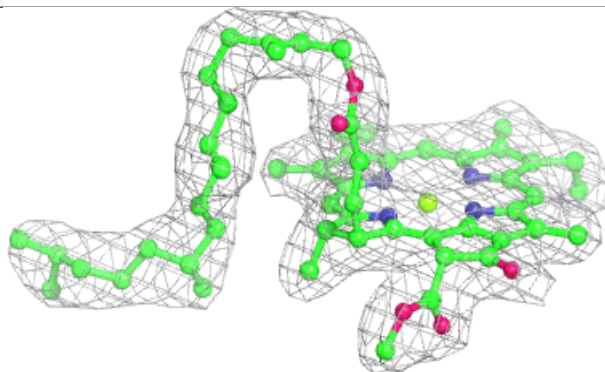
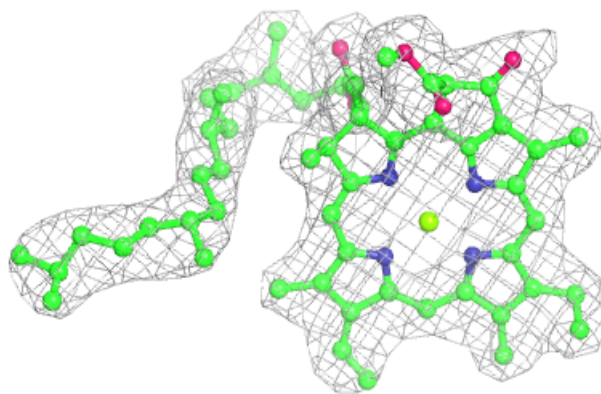
**Electron density around CLA B 612:**

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



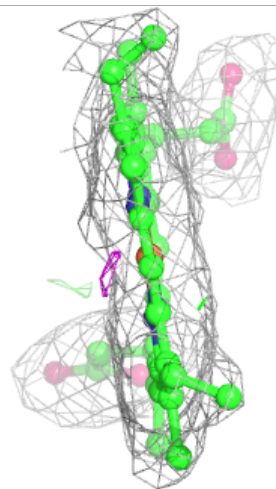
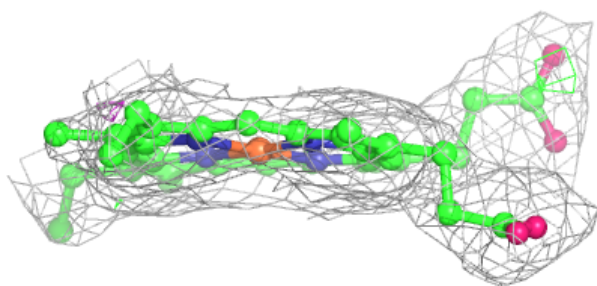
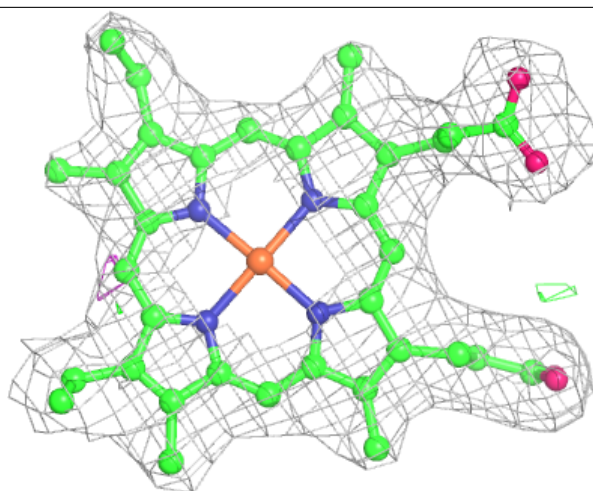
Electron density around CLA A 404:

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



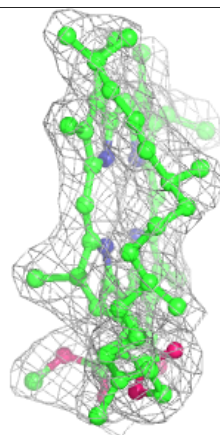
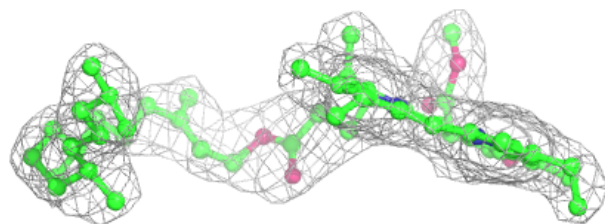
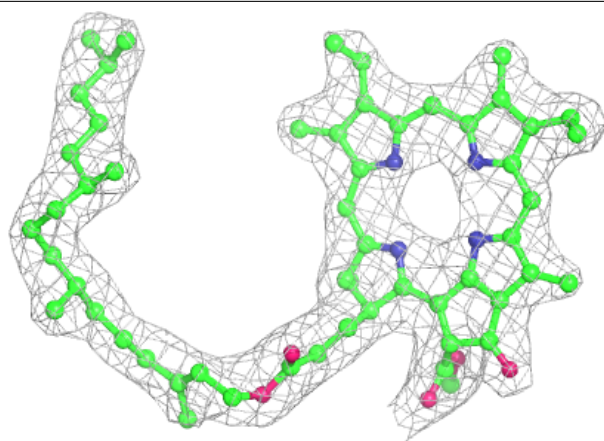
Electron density around HEC V 201:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.