



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 24, 2025 – 03:16 AM JST

PDB ID : 5B66 / pdb\_00005b66  
Title : Crystal structure analysis of Photosystem II complex  
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.  
Deposited on : 2016-05-25  
Resolution : 1.85 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

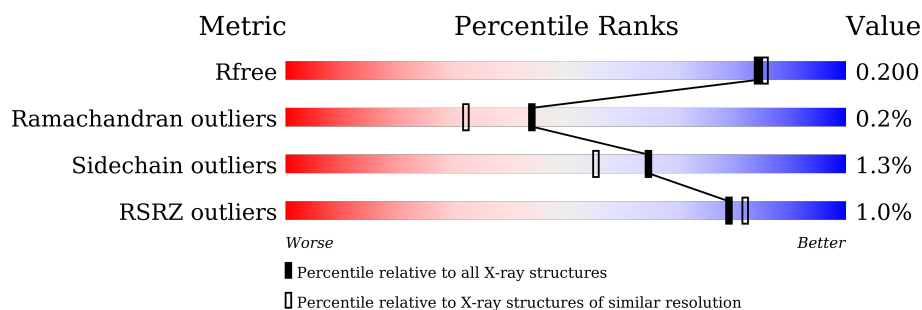
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3097 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div></div> <div>95%</div> <div>..</div> </div>
1	a	344	<div> <div></div> <div>95%</div> <div>..</div> </div>
2	B	505	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
2	b	505	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
3	C	455	<div> <div></div> <div>96%</div> <div>..</div> </div>
3	c	455	<div> <div></div> <div>97%</div> <div>.</div> </div>
4	D	342	<div> <div></div> <div>98%</div> <div>.</div> </div>

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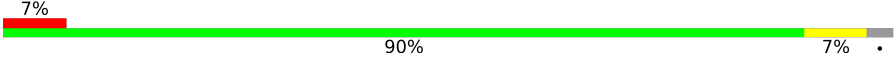
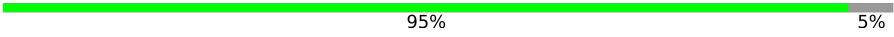
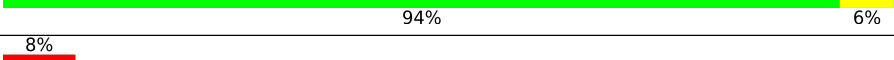


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Mol	Chain	Length	Quality of chain
4	d	342	96% .
5	E	83	5% 90% . 6%
5	e	83	2% 88% 6% 6%
6	F	44	5% 70% 5% 25%
6	f	44	2% 70% . 27%
7	H	65	3% 92% 6% .
7	h	65	91% 5% 5%
8	I	38	92% 8%
8	i	38	87% 8% 5%
9	J	40	85% 5% 10%
9	j	40	2% 98% .
10	K	37	97% .
10	k	37	95% 5%
11	L	37	100%
11	l	37	100%
12	M	36	89% . 8%
12	m	36	94% 6%
13	O	244	% 97% .
13	o	244	97% .
14	T	32	81% 9% 9%
14	t	32	88% 6% 6%
15	U	104	93% 7%
15	u	104	91% . 7%
16	V	137	99% .
16	v	137	99% .

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

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
20	CLA	A	401	X	-	-	-
20	CLA	B	601	X	-	-	-
20	CLA	B	602	X	-	-	-
20	CLA	B	603	X	-	-	-
20	CLA	B	604	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	607	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	613	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	B	616	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-
20	CLA	C	507	X	-	-	-
20	CLA	C	508	X	-	-	-
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-
20	CLA	C	512	X	-	-	-
20	CLA	D	401	X	-	-	-
20	CLA	D	404	X	-	-	-
20	CLA	a	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	b	603	X	-	-	-
20	CLA	b	604	X	-	-	-
20	CLA	b	605	X	-	-	-
20	CLA	b	606	X	-	-	-
20	CLA	b	607	X	-	-	-
20	CLA	b	608	X	-	-	-
20	CLA	b	609	X	-	-	-
20	CLA	b	612	X	-	-	-
20	CLA	b	614	X	-	-	-
20	CLA	b	615	X	-	-	-
20	CLA	b	616	X	-	-	-
20	CLA	b	617	X	-	-	-
20	CLA	b	618	X	-	-	-
20	CLA	c	501	X	-	-	-
20	CLA	c	504	X	-	-	-
20	CLA	c	505	X	-	-	-
20	CLA	c	506	X	-	-	-
20	CLA	c	507	X	-	-	-
20	CLA	c	509	X	-	-	-
20	CLA	c	510	X	-	-	-
20	CLA	c	511	X	-	-	-
20	CLA	c	512	X	-	-	-
20	CLA	d	402	X	-	-	-

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54996 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2626	1721	430	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2622	1719	431	457	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	505	Total	C	N	O	S	0	11	0
			4012	2632	668	699	13			
2	b	495	Total	C	N	O	S	0	4	0
			3884	2550	650	671	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	1	0
			3483	2280	582	608	13			
3	c	455	Total	C	N	O	S	0	1	0
			3523	2305	591	614	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	1	0
			2728	1808	446	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	78	Total	C	N	O	0	1	0
			632	413	101	118			
5	e	78	Total	C	N	O	0	2	0
			636	419	99	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	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
			508	339	81	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			284	194	45	44	1			
8	i	36	Total	C	N	O	S	0	1	0
			300	203	49	47	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			272	183	41	47	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
			285	199	42	44			

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	37	Total	C	N	O	0	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	1	0
			296	200	45	51			

- 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
			259	175	37	46	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			264	178	38	47	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	6	0
			1870	1172	309	384	5			
13	o	243	Total	C	N	O	S	0	2	0
			1838	1153	305	376	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	1	0
			257	181	35	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	97	Total	C	N	O		0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O		0	0	0
			770	489	129	152				

- 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	3	0
			1080	685	181	210	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			212	139	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			213	140	37	33	3			

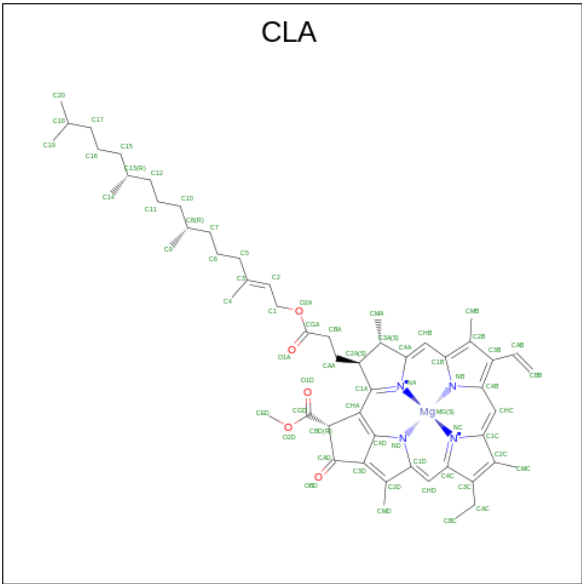
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			274	183	44	47				
18	x	35	Total	C	N	O		0	0	0
			252	171	38	43				

- 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
			450	308	67	73	2			
19	z	61	Total	C	N	O	S	0	0	0
			433	297	66	69	1			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	a	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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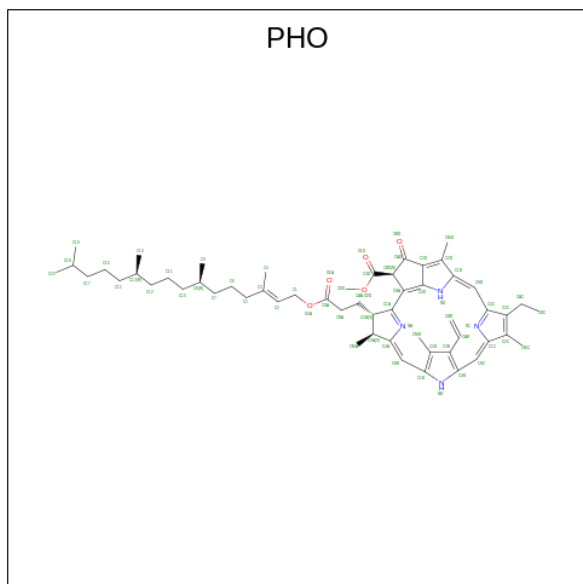
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N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

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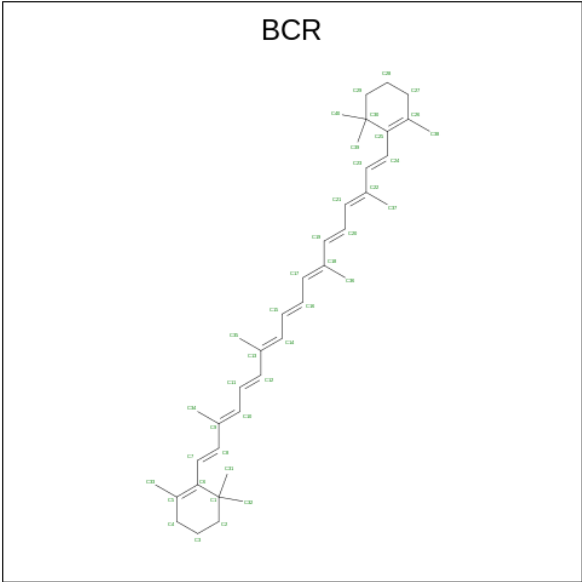
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



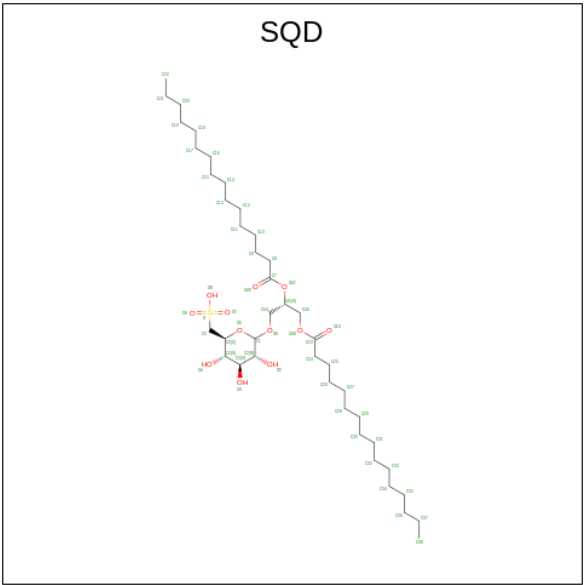
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	D	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	T	1	Total C 40 40	0	0
22	a	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	c	1	Total C 40 40	0	0
22	d	1	Total C 40 40	0	0
22	j	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	t	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



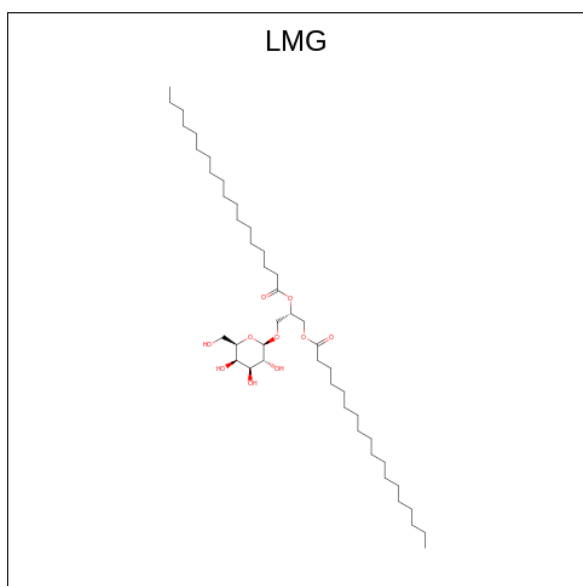
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O S 54 41 12 1	0	0
23	A	1	Total C O S 54 41 12 1	0	0
23	F	1	Total C O S 35 23 11 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	b	1	Total	C	O	S	0	0
			54	41	12	1		
23	f	1	Total	C	O	S	0	0
			40	27	12	1		
23	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O		0	0
			51	41	10			
24	B	1	Total	C	O		0	0
			51	41	10			
24	C	1	Total	C	O		0	0
			51	41	10			
24	C	1	Total	C	O		0	0
			45	35	10			
24	J	1	Total	C	O		0	0
			45	35	10			
24	a	1	Total	C	O		0	0
			51	41	10			
24	b	1	Total	C	O		0	0
			49	39	10			
24	c	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	c	1	Total	C	O	0	0
			51	41	10		
24	j	1	Total	C	O	0	0
			45	35	10		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	2	Total	C	O	0	0
			40	35	5		
26	B	6	Total	C		0	0
			84	84			
26	C	1	Total	C	O	0	0
			34	29	5		
26	D	2	Total	C	O	0	0
			53	48	5		
26	E	1	Total	C		0	0
			15	15			
26	H	2	Total	C		0	0
			10	10			
26	I	5	Total	C		0	0
			61	61			
26	J	4	Total	C		0	0
			33	33			
26	L	1	Total	C		0	0
			14	14			
26	M	1	Total	C		0	0
			12	12			
26	T	1	Total	C		0	0
			13	13			
26	U	1	Total	C		0	0
			14	14			
26	X	1	Total	C		0	0
			16	16			

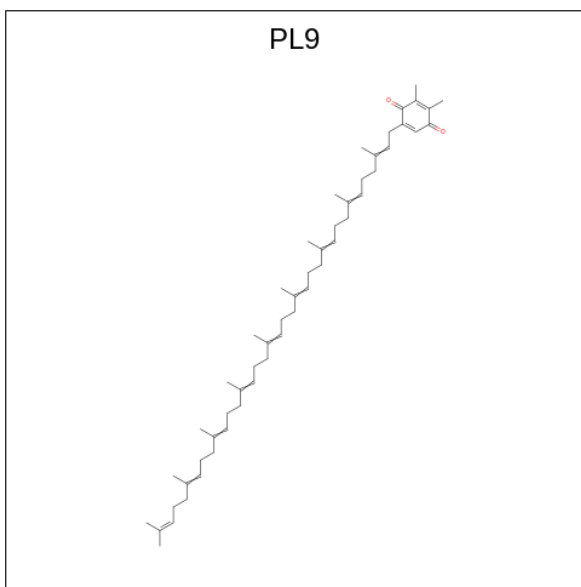
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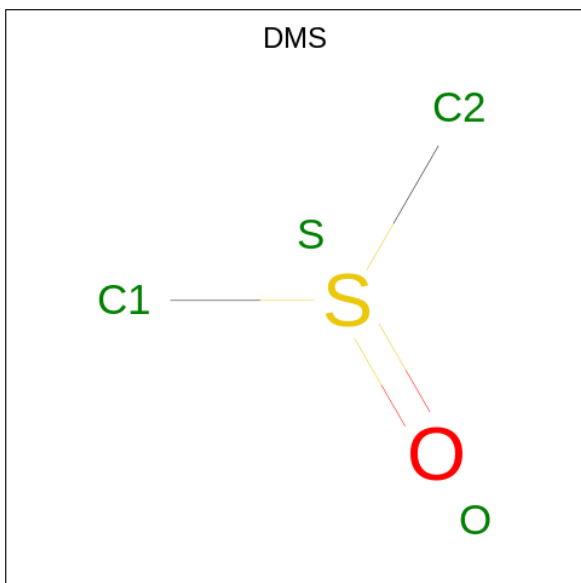
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	Z	1	Total C 4 4	0	0
26	a	3	Total C O 45 40 5	0	0
26	b	7	Total C 68 68	0	0
26	c	3	Total C O 48 43 5	0	0
26	d	3	Total C O 68 63 5	0	0
26	e	1	Total C 7 7	0	0
26	h	1	Total C 16 16	0	0
26	i	3	Total C 38 38	0	0
26	j	2	Total C 22 22	0	0
26	t	1	Total C 16 16	0	0
26	x	1	Total C 9 9	0	0
26	z	1	Total C 6 6	0	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



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

- Molecule 28 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 8	C 4	O 2	S 2	0	1
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	F	1	Total 4	C 2	O 1	S 1	0	0
28	H	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	U	1	Total 4	C 2	O 1	S 1	0	0
28	U	1	Total 8	C 4	O 2	S 2	0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	U	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	h	1	Total 4	C 2	O 1	S 1	0	0
28	i	1	Total 4	C 2	O 1	S 1	0	0
28	j	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	u	1	Total 4	C 2	O 1	S 1	0	0

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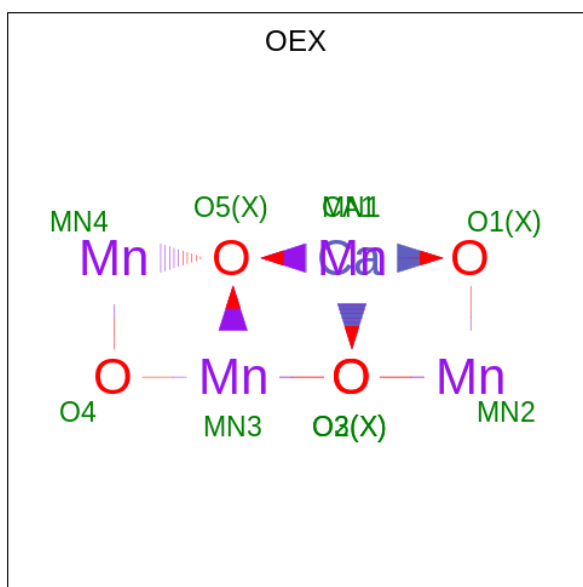
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	u	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

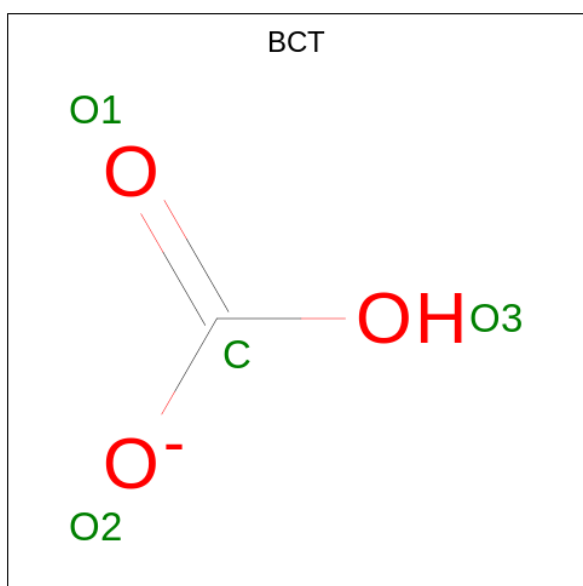
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Fe 1 1	0	0
29	a	1	Total Fe 1 1	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn<sub>4</sub>O<sub>5</sub>).



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

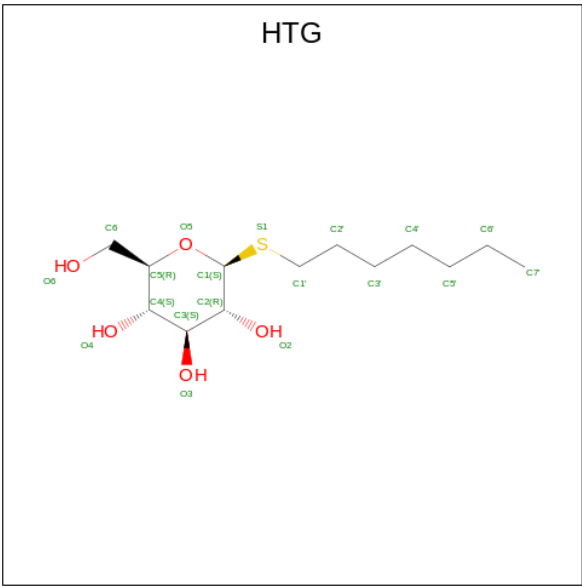
- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3^-$ ).



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



- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



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	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	C	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	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	D	1	Total	C	O	S	0	0
			19	13	5	1		
32	O	1	Total	C	O	S	0	0
			19	13	5	1		
32	V	1	Total	C	O	S	0	0
			13	7	5	1		
32	b	1	Total	C	O	S	0	0
			19	13	5	1		

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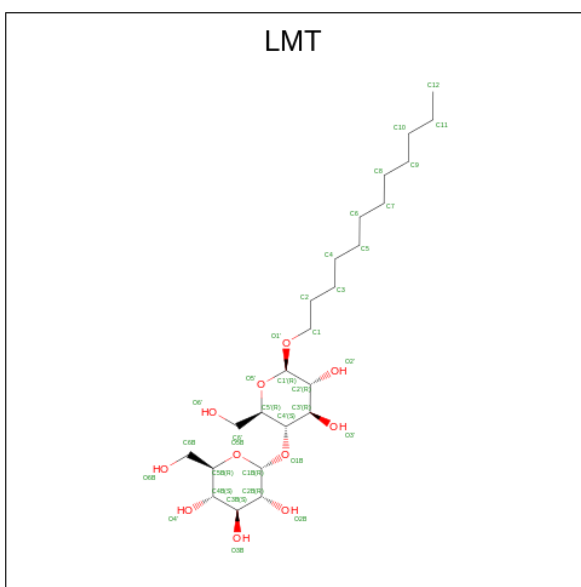
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	b	1	Total	C	O	S	0	0
			19	13	5	1		
32	b	1	Total	C	O	S	0	0
			19	13	5	1		
32	b	1	Total	C	O	S	0	0
			19	13	5	1		
32	c	1	Total	C	O	S	0	0
			19	13	5	1		
32	c	1	Total	C	O	S	0	0
			19	13	5	1		
32	d	1	Total	C	O	S	0	0
			19	13	5	1		
32	u	1	Total	C	S		0	0
			8	7	1			
32	v	1	Total	C	O	S	0	0
			14	8	5	1		

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	V	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		
33	c	1	Total	Ca	0	0
			1	1		
33	o	1	Total	Ca	0	0
			1	1		

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



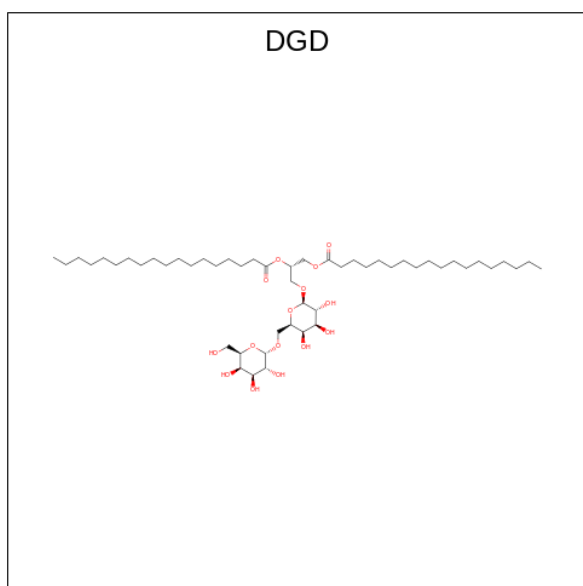
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total 24	C 18	O 6	0	0
34	B	1	Total 24	C 18	O 6	0	0
34	B	1	Total 16	C 14	O 2	0	0
34	E	1	Total 24	C 18	O 6	0	0
34	I	1	Total 35	C 24	O 11	0	0
34	J	1	Total 24	C 18	O 6	0	0
34	M	1	Total 35	C 24	O 11	0	0
34	T	1	Total 24	C 18	O 6	0	0
34	Z	1	Total 35	C 24	O 11	0	0
34	a	1	Total 35	C 24	O 11	0	0
34	b	1	Total 32	C 21	O 11	0	0
34	b	1	Total 25	C 19	O 6	0	0
34	c	1	Total 35	C 24	O 11	0	0
34	f	1	Total 24	C 18	O 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	m	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	z	1	Total	C	O	0	0
			35	24	11		

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



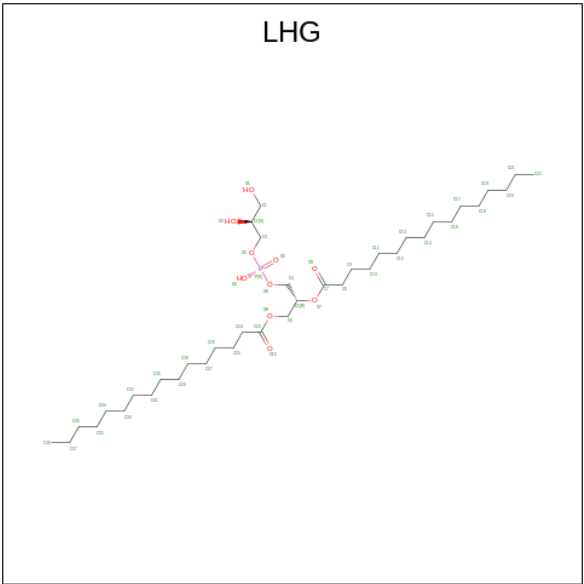
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			62	47	15		
35	C	1	Total	C	O	0	0
			55	40	15		
35	C	1	Total	C	O	0	0
			62	47	15		
35	D	1	Total	C	O	0	0
			51	41	10		
35	H	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			57	42	15		
35	c	1	Total	C	O	0	0
			62	47	15		

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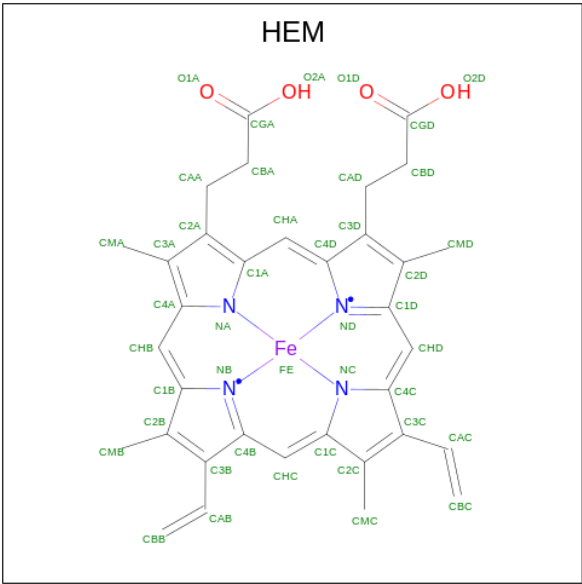
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	d	1	Total	C	O	0	0
			51	41	10		
35	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



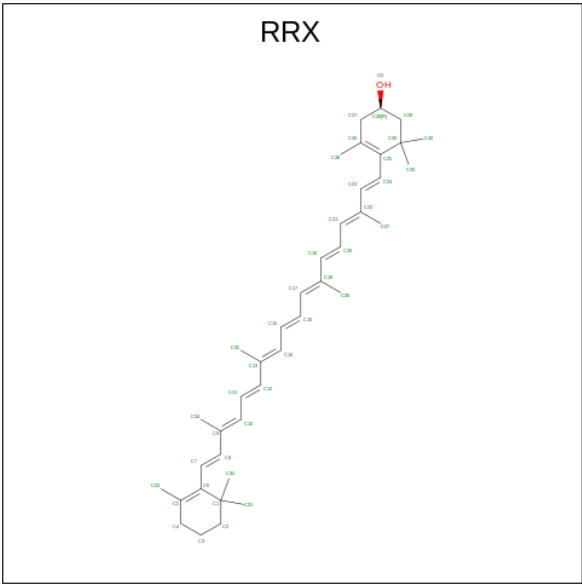
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	E	1	Total	C	O	P	0	0
			48	37	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula:  $C_{40}H_{56}O$ ).

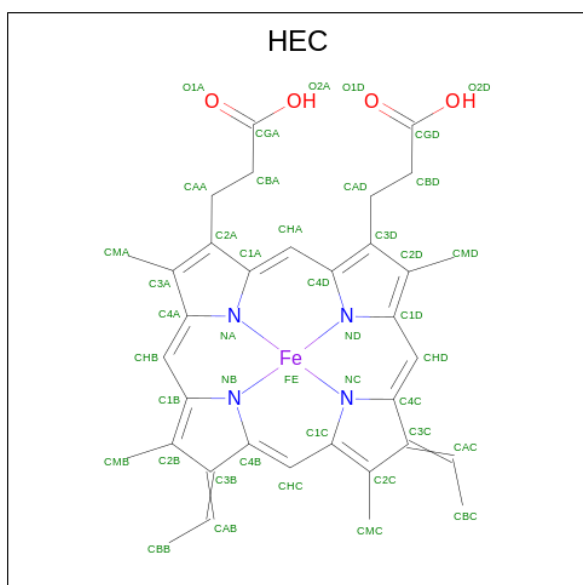


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total 41	C 40	O 1	0	0
38	x	1	Total 41	C 40	O 1	0	0

- Molecule 39 is MAGNESIUM ION (CCD ID: 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 (CCD ID: 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	177	Total O 182 182	0	5

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	B	447	Total 473	O 473	0	25
41	C	317	Total 324	O 324	0	7
41	D	175	Total 180	O 180	0	5
41	E	62	Total 66	O 66	0	4
41	F	8	Total 8	O 8	0	0
41	H	62	Total 65	O 65	0	3
41	I	16	Total 16	O 16	0	0
41	J	23	Total 23	O 23	0	0
41	K	12	Total 12	O 12	0	0
41	L	19	Total 21	O 21	0	2
41	M	12	Total 12	O 12	0	0
41	O	263	Total 273	O 273	0	10
41	T	19	Total 20	O 20	0	1
41	U	133	Total 136	O 136	0	3
41	V	177	Total 183	O 183	0	6
41	Y	7	Total 7	O 7	0	0
41	X	22	Total 22	O 22	0	0
41	Z	5	Total 5	O 5	0	0
41	a	182	Total 185	O 185	0	3
41	b	451	Total 465	O 465	0	14
41	c	362	Total 374	O 374	0	12

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	d	176	Total 182	O 182	0	6
41	e	48	Total 49	O 49	0	1
41	f	15	Total 16	O 16	0	1
41	h	68	Total 70	O 70	0	2
41	i	19	Total 21	O 21	0	2
41	j	23	Total 24	O 24	0	1
41	k	11	Total 12	O 12	0	1
41	l	22	Total 24	O 24	0	2
41	m	23	Total 24	O 24	0	1
41	o	214	Total 230	O 230	0	15
41	t	19	Total 20	O 20	0	1
41	u	146	Total 150	O 150	0	4
41	v	144	Total 147	O 147	0	3
41	y	7	Total 7	O 7	0	0
41	x	25	Total 26	O 26	0	1
41	z	12	Total 12	O 12	0	0

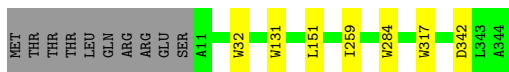
### 3 Residue-property plots [i](#)

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.

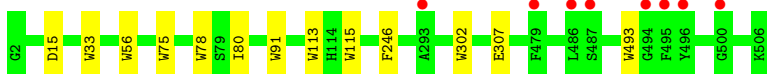
- Molecule 1: Photosystem II protein D1



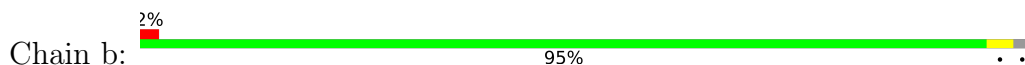
- Molecule 1: Photosystem II protein D1



- 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

Chain c:  97%



• Molecule 4: Photosystem II D2 protein

Chain D:  98%




• Molecule 4: Photosystem II D2 protein

Chain d:  96%




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:  90% 6%



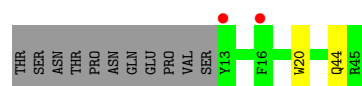
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:  88% 6% 6%



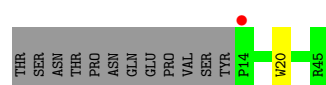
• Molecule 6: Cytochrome b559 subunit beta

Chain F:  70% 5% 25%

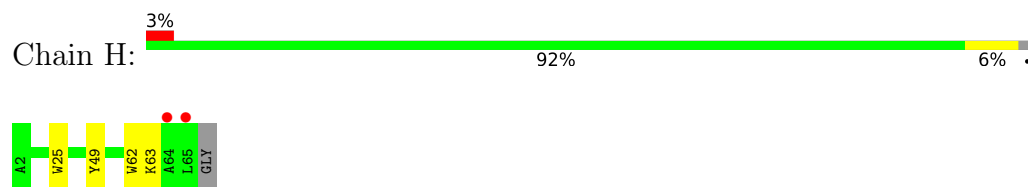


• Molecule 6: Cytochrome b559 subunit beta

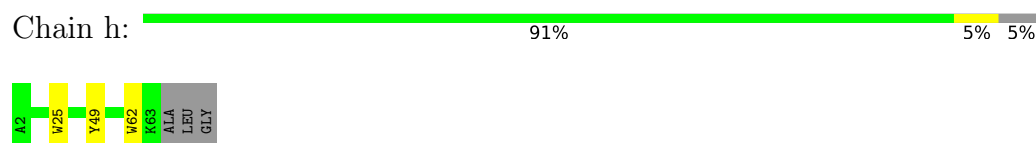
Chain f:  70% 27%



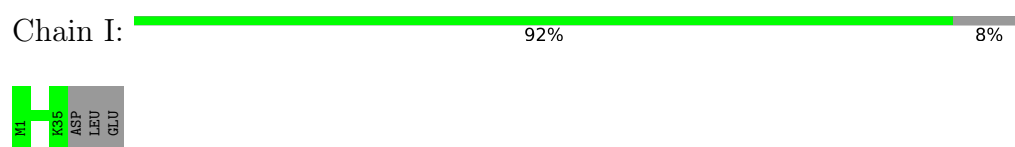
- Molecule 7: Photosystem II reaction center protein H



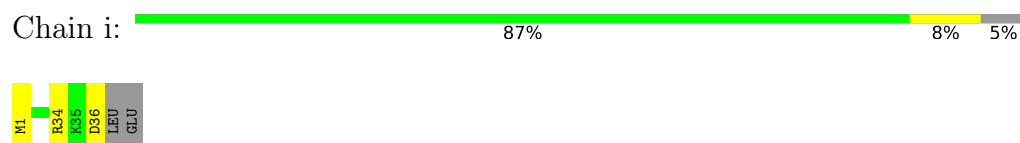
- Molecule 7: Photosystem II reaction center protein H



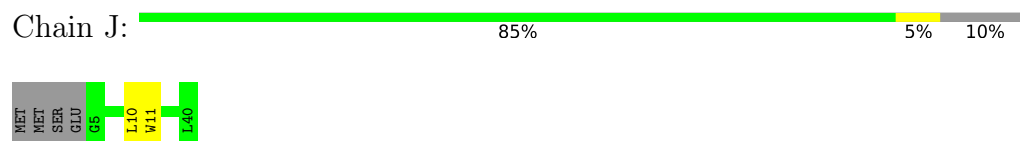
- Molecule 8: Photosystem II reaction center protein I



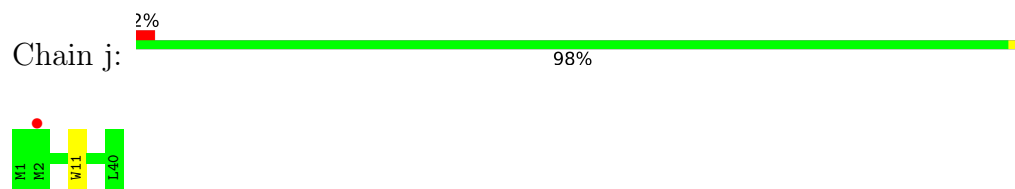
- Molecule 8: Photosystem II reaction center protein I



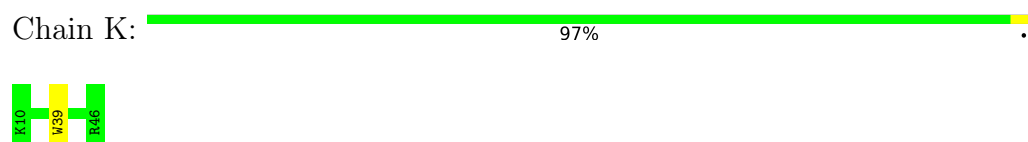
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

Chain k:  95% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%


There are no outlier residues recorded for this chain.

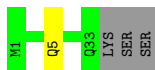
- Molecule 11: Photosystem II reaction center protein L

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein M

Chain M:  89% 8%



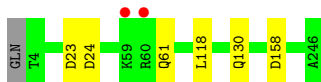
- Molecule 12: Photosystem II reaction center protein M

Chain m:  94% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  97%




- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  97%



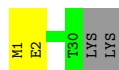
- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 9% 9%



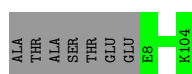
- Molecule 14: Photosystem II reaction center protein T

Chain t: 88% 6% 6%



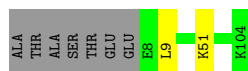
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 93% 7%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 91% 1% 7%



- Molecule 16: Cytochrome c-550

Chain V: 99% 1%



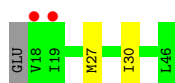
- Molecule 16: Cytochrome c-550

Chain v: 99% 1%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 7% 90% 7% 1%



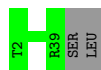
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 97% 3%



- Molecule 18: Photosystem II reaction center protein X

Chain X: 95% 5%



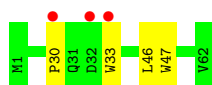
- Molecule 18: Photosystem II reaction center protein X

Chain x: 88% 12%



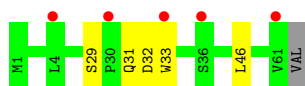
- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 5% 94% 6%



- Molecule 19: Photosystem II reaction center protein Z

Chain z: 8% 90% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.47Å 228.18Å 286.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.85 19.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-1.85) 99.9 (19.99-1.85)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.162 , 0.201 0.162 , 0.200	Depositor DCC
$R_{free}$ test set	33616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 65.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, PL9, LMT, BCT, DMS, FME, HEM, HEC, BCR, OEX, SQD, CLA, LHG, DGD, LMG, HTG, RRX, MG, FE2, CA, CL, 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	0.95	5/2717 (0.2%)	0.77	1/3707 (0.0%)
1	a	0.93	4/2718 (0.1%)	0.79	2/3707 (0.1%)
2	B	0.90	9/4181 (0.2%)	0.77	1/5700 (0.0%)
2	b	0.91	11/4029 (0.3%)	0.78	2/5490 (0.0%)
3	C	0.87	7/3599 (0.2%)	0.74	2/4901 (0.0%)
3	c	0.86	8/3640 (0.2%)	0.72	2/4956 (0.0%)
4	D	0.95	3/2826 (0.1%)	0.78	1/3850 (0.0%)
4	d	0.95	8/2817 (0.3%)	0.78	1/3839 (0.0%)
5	E	0.71	0/654	0.68	0/896
5	e	0.69	1/661 (0.2%)	0.72	0/904
6	F	0.79	1/278 (0.4%)	0.60	0/379
6	f	0.81	1/265 (0.4%)	0.62	0/360
7	H	0.84	2/524 (0.4%)	0.75	0/715
7	h	0.86	2/517 (0.4%)	0.71	0/704
8	I	0.63	0/281	0.69	0/380
8	i	0.61	0/300	0.62	0/405
9	J	0.82	1/257 (0.4%)	0.61	0/349
9	j	0.81	1/278 (0.4%)	0.62	0/378
10	K	0.70	1/303 (0.3%)	0.65	0/416
10	k	0.72	1/295 (0.3%)	0.64	0/407
11	L	0.88	0/312	0.76	0/425
11	l	0.91	0/306	0.76	0/418
12	M	0.70	0/265	0.74	0/362
12	m	0.70	0/270	0.76	0/369
13	O	0.72	0/1919	0.80	1/2607 (0.0%)
13	o	0.69	0/1875	0.77	2/2548 (0.1%)
14	T	0.78	0/259	0.77	0/352
14	t	0.79	0/257	0.73	0/349
15	U	0.77	0/777	0.78	0/1055
15	u	0.76	0/781	0.77	0/1059
16	V	0.80	0/1110	0.80	1/1506 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.71	1/1073 (0.1%)	0.75	0/1461
17	Y	0.50	0/213	0.63	0/285
17	y	0.45	0/214	0.60	0/286
18	X	0.54	0/277	0.69	0/375
18	x	0.57	0/255	0.66	0/345
19	Z	0.70	2/461 (0.4%)	0.56	0/632
19	z	0.61	1/444 (0.2%)	0.57	0/611
All	All	0.85	70/42208 (0.2%)	0.75	16/57488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.13	1.50	1.41
1	A	343	LEU	C-N	6.74	1.49	1.34
1	a	131	TRP	CD2-CE2	6.46	1.49	1.41
3	C	266	TRP	CD2-CE2	6.43	1.49	1.41
2	B	33	TRP	CD2-CE2	6.27	1.48	1.41

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	342	ASP	CB-CG-OD1	6.34	124.01	118.30
16	V	128	ASP	CB-CG-OD1	6.14	123.82	118.30
3	C	473	ASP	CB-CG-OD2	5.92	123.63	118.30
13	o	152	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	c	423	ARG	NE-CZ-NH2	-5.79	117.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	60	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	37	25
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	37	25
2	B	514/505 (102%)	503 (98%)	11 (2%)	0	100	100
2	b	493/505 (98%)	485 (98%)	8 (2%)	0	100	100
3	C	450/455 (99%)	436 (97%)	13 (3%)	1 (0%)	44	32
3	c	454/455 (100%)	442 (97%)	11 (2%)	1 (0%)	44	32
4	D	341/342 (100%)	334 (98%)	6 (2%)	1 (0%)	37	25
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	78/83 (94%)	78 (100%)	0	0	100	100
6	F	31/44 (70%)	31 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	247/244 (101%)	235 (95%)	11 (4%)	1 (0%)	30	18
13	o	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	11	3
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	138/137 (101%)	133 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	2
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	0
All	All	5201/5350 (97%)	5069 (98%)	120 (2%)	12 (0%)	44	32

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	60	ARG
19	z	32	ASP
3	C	416	SER
4	D	12	ARG
13	O	61	GLN

### 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	269/279 (96%)	268 (100%)	1 (0%)	89	88
1	a	270/279 (97%)	270 (100%)	0	100	100
2	B	405/403 (100%)	401 (99%)	4 (1%)	73	67
2	b	390/403 (97%)	386 (99%)	4 (1%)	73	67
3	C	351/356 (99%)	349 (99%)	2 (1%)	84	81
3	c	356/356 (100%)	351 (99%)	5 (1%)	62	53
4	D	277/277 (100%)	274 (99%)	3 (1%)	70	62
4	d	276/277 (100%)	272 (99%)	4 (1%)	62	53
5	E	68/72 (94%)	65 (96%)	3 (4%)	24	10
5	e	68/72 (94%)	63 (93%)	5 (7%)	11	2
6	F	27/38 (71%)	26 (96%)	1 (4%)	29	14
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	52 (96%)	2 (4%)	29	14
7	h	54/54 (100%)	53 (98%)	1 (2%)	52	39
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	32/34 (94%)	29 (91%)	3 (9%)	7	1
9	J	23/28 (82%)	22 (96%)	1 (4%)	25	10
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/30 (100%)	30 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	30	15
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	33/35 (94%)	33 (100%)	0	100	100
12	M	30/33 (91%)	29 (97%)	1 (3%)	33	18
12	m	30/33 (91%)	30 (100%)	0	100	100
13	O	207/207 (100%)	202 (98%)	5 (2%)	44	29
13	o	199/207 (96%)	197 (99%)	2 (1%)	73	67
14	T	26/28 (93%)	23 (88%)	3 (12%)	4	0
14	t	26/28 (93%)	25 (96%)	1 (4%)	28	13
15	U	82/89 (92%)	82 (100%)	0	100	100
15	u	83/89 (93%)	81 (98%)	2 (2%)	44	29
16	V	120/117 (103%)	119 (99%)	1 (1%)	79	74
16	v	114/117 (97%)	113 (99%)	1 (1%)	75	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	21/23 (91%)	19 (90%)	2 (10%)	7	1
17	y	21/23 (91%)	21 (100%)	0	100	100
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	27/33 (82%)	27 (100%)	0	100	100
19	Z	44/52 (85%)	43 (98%)	1 (2%)	45	31
19	z	39/52 (75%)	37 (95%)	2 (5%)	20	7
All	All	4223/4376 (96%)	4162 (99%)	61 (1%)	65	53

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Y	30	ILE
14	t	2	GLU
3	c	255	THR
13	o	118	LEU
19	z	29	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	332	GLN
15	u	73	GLN
16	v	118	HIS
16	v	34	GLN
7	H	59	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
14	FME	T	1	14	8,9,10	0.43	0	7,9,11	1.79	2 (28%)
8	FME	i	1	8	8,9,10	0.52	0	7,9,11	1.68	1 (14%)
14	FME	t	1	14	8,9,10	0.49	0	7,9,11	1.86	4 (57%)
8	FME	I	1	8	8,9,10	0.69	0	7,9,11	1.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-

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(°)
8	i	1	FME	C-CA-N	2.88	114.93	109.73
14	T	1	FME	CE-SD-CG	2.70	109.68	100.40
14	T	1	FME	O-C-CA	-2.46	118.34	124.78
14	t	1	FME	CG-CB-CA	2.44	119.72	112.95
14	t	1	FME	CE-SD-CG	2.32	108.38	100.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	N-CA-CB-CG
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	N-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 14 are monoatomic and 55 are unknown - leaving 280 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	$\# Z  > 2$
34	LMT	E	101	-	24,24,36	0.62	1 (4%)	29,29,47	1.01	3 (10%)
28	DMS	B	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.73	0
20	CLA	c	501	-	65,73,73	2.17	16 (24%)	76,113,113	2.75	23 (30%)
22	BCR	j	102	-	41,41,41	0.85	0	56,56,56	1.38	9 (16%)
28	DMS	j	105	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
28	DMS	b	638	-	3,3,3	2.78	1 (33%)	3,3,3	0.94	0
28	DMS	b	634	-	3,3,3	2.67	1 (33%)	3,3,3	0.68	0
34	LMT	a	418	-	36,36,36	0.68	2 (5%)	47,47,47	1.54	6 (12%)
34	LMT	z	102	-	36,36,36	0.76	1 (2%)	47,47,47	1.49	8 (17%)
28	DMS	O	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.42	0
32	HTG	C	534	-	19,19,19	1.08	1 (5%)	23,24,24	1.47	5 (21%)
32	HTG	b	625	-	19,19,19	1.21	2 (10%)	23,24,24	1.34	4 (17%)
35	DGD	H	102	-	63,63,67	1.04	3 (4%)	77,77,81	1.27	8 (10%)
20	CLA	b	618	-	65,73,73	2.18	19 (29%)	76,113,113	2.29	26 (34%)
20	CLA	b	605	-	65,73,73	2.08	15 (23%)	76,113,113	2.27	28 (36%)
23	SQD	A	412	-	53,54,54	1.02	3 (5%)	62,65,65	1.71	10 (16%)
20	CLA	b	609	41	65,73,73	2.05	17 (26%)	76,113,113	2.01	26 (34%)
28	DMS	B	643	-	3,3,3	2.78	1 (33%)	3,3,3	0.74	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	DMS	V	206	-	3,3,3	2.68	1 (33%)	3,3,3	0.67	0
28	DMS	b	633	-	3,3,3	2.55	1 (33%)	3,3,3	1.05	0
28	DMS	B	641	-	3,3,3	2.65	1 (33%)	3,3,3	0.64	0
28	DMS	U	903[B]	-	3,3,3	2.44	1 (33%)	3,3,3	0.17	0
28	DMS	o	302	-	3,3,3	2.75	1 (33%)	3,3,3	0.90	0
28	DMS	o	304	-	3,3,3	2.64	1 (33%)	3,3,3	0.65	0
28	DMS	c	531	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
20	CLA	C	503	-	65,73,73	2.35	17 (26%)	76,113,113	1.98	22 (28%)
20	CLA	C	504	41	65,73,73	2.24	14 (21%)	76,113,113	2.24	22 (28%)
22	BCR	A	405	-	41,41,41	0.95	3 (7%)	56,56,56	1.27	7 (12%)
28	DMS	o	307	-	3,3,3	2.65	1 (33%)	3,3,3	0.85	0
34	LMT	I	101	-	36,36,36	0.65	1 (2%)	47,47,47	1.28	6 (12%)
34	LMT	b	628	-	25,25,36	0.55	0	30,30,47	1.20	2 (6%)
22	BCR	K	101	-	41,41,41	0.83	1 (2%)	56,56,56	1.48	13 (23%)
22	BCR	k	101	-	41,41,41	0.94	0	56,56,56	1.12	6 (10%)
28	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
28	DMS	A	415	-	3,3,3	2.75	1 (33%)	3,3,3	1.01	0
35	DGD	c	516	-	58,58,67	0.86	2 (3%)	72,72,81	1.13	6 (8%)
20	CLA	a	404	41	60,68,73	1.90	16 (26%)	70,107,113	2.32	24 (34%)
20	CLA	c	507	41	65,73,73	2.29	16 (24%)	76,113,113	2.34	21 (27%)
20	CLA	B	603	-	65,73,73	2.21	18 (27%)	76,113,113	2.21	24 (31%)
24	LMG	b	623	-	49,49,55	0.96	2 (4%)	57,57,63	1.31	6 (10%)
28	DMS	c	532	-	3,3,3	2.60	1 (33%)	3,3,3	0.47	0
28	DMS	c	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.76	0
28	DMS	h	102	-	3,3,3	2.75	1 (33%)	3,3,3	0.56	0
28	DMS	v	202	-	3,3,3	2.50	1 (33%)	3,3,3	0.58	0
28	DMS	A	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.78	0
28	DMS	C	525[B]	-	3,3,3	2.59	1 (33%)	3,3,3	0.79	0
20	CLA	b	616	-	65,73,73	2.06	15 (23%)	76,113,113	2.47	29 (38%)
28	DMS	A	414	-	3,3,3	1.97	1 (33%)	3,3,3	0.54	0
36	LHG	D	408	-	48,48,48	0.82	2 (4%)	51,54,54	1.03	1 (1%)
27	PL9	D	412	-	55,55,55	1.06	3 (5%)	68,69,69	1.51	12 (17%)
28	DMS	C	532	-	3,3,3	3.28	1 (33%)	3,3,3	1.29	1 (33%)
35	DGD	c	515	-	63,63,67	0.85	3 (4%)	77,77,81	1.19	8 (10%)
20	CLA	c	511	3	65,73,73	2.52	19 (29%)	76,113,113	2.25	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	d	402	-	65,73,73	1.89	16 (24%)	76,113,113	1.95	21 (27%)
28	DMS	o	305	-	3,3,3	2.73	1 (33%)	3,3,3	0.77	0
32	HTG	u	201	-	7,7,19	0.43	0	6,6,24	0.70	0
34	LMT	m	101	-	36,36,36	0.61	1 (2%)	47,47,47	0.96	1 (2%)
28	DMS	B	644	-	3,3,3	2.87	1 (33%)	3,3,3	1.26	0
31	BCT	A	421	29	2,3,3	0.47	0	2,3,3	1.14	0
20	CLA	B	605	-	65,73,73	2.10	15 (23%)	76,113,113	2.03	22 (28%)
20	CLA	C	511	3	65,73,73	2.34	19 (29%)	76,113,113	2.40	24 (31%)
20	CLA	c	508	-	60,68,73	2.42	19 (31%)	70,107,113	2.24	23 (32%)
32	HTG	b	602	-	19,19,19	1.00	2 (10%)	23,24,24	1.15	1 (4%)
20	CLA	C	513	-	65,73,73	2.57	18 (27%)	76,113,113	2.11	19 (25%)
35	DGD	c	517	-	63,63,67	1.04	4 (6%)	77,77,81	1.19	8 (10%)
28	DMS	O	311	-	3,3,3	2.87	1 (33%)	3,3,3	0.92	0
20	CLA	B	614	-	65,73,73	1.94	17 (26%)	76,113,113	2.19	22 (28%)
28	DMS	F	102	-	3,3,3	2.63	1 (33%)	3,3,3	0.61	0
20	CLA	c	512	-	65,73,73	2.30	18 (27%)	76,113,113	2.28	21 (27%)
34	LMT	B	626	-	24,24,36	0.54	0	29,29,47	1.14	3 (10%)
20	CLA	D	404	-	65,73,73	2.13	20 (30%)	76,113,113	2.26	28 (36%)
20	CLA	b	617	-	65,73,73	2.23	16 (24%)	76,113,113	2.26	24 (31%)
28	DMS	B	640	-	3,3,3	2.55	1 (33%)	3,3,3	0.97	0
21	PHO	a	405	-	51,69,69	1.57	7 (13%)	47,99,99	1.38	5 (10%)
24	LMG	c	519	-	51,51,55	1.01	3 (5%)	59,59,63	1.17	7 (11%)
28	DMS	B	642	-	3,3,3	2.79	1 (33%)	3,3,3	0.75	0
28	DMS	O	303	-	3,3,3	2.62	1 (33%)	3,3,3	0.64	0
28	DMS	d	414	-	3,3,3	2.50	1 (33%)	3,3,3	0.24	0
20	CLA	D	401	-	65,73,73	1.88	15 (23%)	76,113,113	2.34	26 (34%)
20	CLA	b	608	-	65,73,73	2.43	18 (27%)	76,113,113	2.15	21 (27%)
32	HTG	B	632	-	19,19,19	1.02	1 (5%)	23,24,24	1.26	2 (8%)
20	CLA	b	612	41	65,73,73	2.05	17 (26%)	76,113,113	2.10	22 (28%)
28	DMS	C	526	-	3,3,3	2.56	1 (33%)	3,3,3	0.81	0
30	OEX	A	420	41,1,3	0,15,15	-	-	-	-	-
34	LMT	M	101	-	36,36,36	0.64	0	47,47,47	0.93	2 (4%)
20	CLA	b	615	-	65,73,73	1.87	15 (23%)	76,113,113	2.37	24 (31%)
27	PL9	a	415	-	55,55,55	0.83	3 (5%)	68,69,69	1.67	16 (23%)
24	LMG	C	519	-	51,51,55	1.03	2 (3%)	59,59,63	1.23	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	DMS	d	415	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
28	DMS	v	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.81	0
32	HTG	c	521	-	19,19,19	0.96	1 (5%)	23,24,24	2.03	3 (13%)
20	CLA	b	604	-	65,73,73	2.09	18 (27%)	76,113,113	2.28	28 (36%)
22	BCR	b	620	-	41,41,41	1.08	1 (2%)	56,56,56	1.23	5 (8%)
27	PL9	d	412	-	55,55,55	1.09	3 (5%)	68,69,69	1.59	16 (23%)
28	DMS	b	637	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
28	DMS	v	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
32	HTG	b	624	-	19,19,19	1.15	2 (10%)	23,24,24	1.60	2 (8%)
36	LHG	D	407	-	48,48,48	0.86	1 (2%)	51,54,54	1.26	5 (9%)
34	LMT	f	102	-	24,24,36	0.79	1 (4%)	29,29,47	0.96	2 (6%)
20	CLA	d	403	41	65,73,73	2.08	15 (23%)	76,113,113	2.22	21 (27%)
23	SQD	a	401	-	53,54,54	1.12	3 (5%)	62,65,65	1.40	7 (11%)
28	DMS	v	203	-	3,3,3	2.59	1 (33%)	3,3,3	0.85	0
24	LMG	A	407	-	51,51,55	0.95	2 (3%)	59,59,63	1.06	3 (5%)
36	LHG	d	407	-	48,48,48	0.73	2 (4%)	51,54,54	0.99	4 (7%)
20	CLA	C	507	41	65,73,73	2.48	19 (29%)	76,113,113	2.31	22 (28%)
28	DMS	A	418	-	3,3,3	2.80	1 (33%)	3,3,3	0.73	0
28	DMS	c	530	-	3,3,3	2.80	1 (33%)	3,3,3	1.01	0
34	LMT	Z	101	-	36,36,36	0.68	1 (2%)	47,47,47	0.98	3 (6%)
28	DMS	V	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.78	0
28	DMS	b	639	-	3,3,3	2.81	1 (33%)	3,3,3	0.57	0
20	CLA	B	611	41	65,73,73	2.26	17 (26%)	76,113,113	2.35	23 (30%)
20	CLA	D	402	41	65,73,73	1.90	16 (24%)	76,113,113	2.23	21 (27%)
20	CLA	B	606	-	65,73,73	1.88	13 (20%)	76,113,113	2.33	26 (34%)
35	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	3 (3%)
32	HTG	C	520	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	1 (4%)
22	BCR	b	619	-	41,41,41	0.95	0	56,56,56	1.77	11 (19%)
28	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
20	CLA	A	404	-	65,73,73	2.05	20 (30%)	76,113,113	2.53	25 (32%)
23	SQD	l	101	-	53,54,54	1.08	4 (7%)	62,65,65	1.68	8 (12%)
28	DMS	D	413	-	3,3,3	2.73	1 (33%)	3,3,3	0.66	0
20	CLA	b	613	-	65,73,73	2.03	11 (16%)	76,113,113	2.23	26 (34%)
22	BCR	C	514	-	41,41,41	0.85	0	56,56,56	1.31	7 (12%)
20	CLA	B	607	-	65,73,73	2.40	19 (29%)	76,113,113	2.31	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	a	403	-	65,73,73	1.86	13 (20%)	76,113,113	2.16	23 (30%)
22	BCR	t	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.74	19 (33%)
22	BCR	a	408	-	41,41,41	1.21	2 (4%)	56,56,56	1.44	7 (12%)
28	DMS	V	207	-	3,3,3	2.58	1 (33%)	3,3,3	0.47	0
28	DMS	b	640	-	3,3,3	2.76	1 (33%)	3,3,3	1.38	1 (33%)
28	DMS	o	306	-	3,3,3	2.79	1 (33%)	3,3,3	1.03	0
40	HEC	v	201	16	32,50,50	2.09	8 (25%)	24,82,82	2.08	6 (25%)
22	BCR	B	617	-	41,41,41	0.98	0	56,56,56	1.62	11 (19%)
28	DMS	O	305	-	3,3,3	2.63	1 (33%)	3,3,3	0.79	0
28	DMS	H	103	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
28	DMS	d	413	-	3,3,3	2.57	1 (33%)	3,3,3	0.91	0
20	CLA	b	603	41	65,73,73	2.65	19 (29%)	76,113,113	2.29	24 (31%)
32	HTG	B	631	-	19,19,19	0.94	2 (10%)	23,24,24	2.09	6 (26%)
28	DMS	U	902	-	3,3,3	2.66	1 (33%)	3,3,3	1.63	1 (33%)
20	CLA	B	610	-	65,73,73	2.13	16 (24%)	76,113,113	2.17	24 (31%)
32	HTG	d	401	-	19,19,19	1.08	1 (5%)	23,24,24	2.36	4 (17%)
28	DMS	C	525[A]	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
20	CLA	b	614	-	65,73,73	1.91	16 (24%)	76,113,113	2.31	24 (31%)
36	LHG	l	102	-	48,48,48	0.78	2 (4%)	51,54,54	1.00	2 (3%)
20	CLA	C	506	-	65,73,73	2.39	18 (27%)	76,113,113	2.30	21 (27%)
28	DMS	v	206	-	3,3,3	2.66	1 (33%)	3,3,3	0.66	0
35	DGD	d	416	-	51,51,67	1.11	3 (5%)	59,59,81	1.20	6 (10%)
34	LMT	c	523	-	36,36,36	0.81	1 (2%)	47,47,47	1.60	6 (12%)
20	CLA	B	613	-	65,73,73	2.10	13 (20%)	76,113,113	2.30	23 (30%)
32	HTG	O	302	-	19,19,19	1.29	2 (10%)	23,24,24	1.18	2 (8%)
20	CLA	B	604	-	65,73,73	1.96	17 (26%)	76,113,113	2.43	25 (32%)
22	BCR	K	102	-	41,41,41	0.92	1 (2%)	56,56,56	1.48	6 (10%)
20	CLA	b	606	-	65,73,73	1.96	14 (21%)	76,113,113	2.37	25 (32%)
23	SQD	b	622	-	53,54,54	1.10	3 (5%)	62,65,65	1.55	11 (17%)
36	LHG	L	101	-	48,48,48	0.90	3 (6%)	51,54,54	0.90	1 (1%)
20	CLA	C	508	-	60,68,73	2.50	17 (28%)	70,107,113	2.38	24 (34%)
20	CLA	B	602	41	65,73,73	2.65	20 (30%)	76,113,113	2.55	25 (32%)
21	PHO	D	403	-	51,69,69	1.70	7 (13%)	47,99,99	1.60	10 (21%)
32	HTG	C	521	-	19,19,19	0.98	2 (10%)	23,24,24	1.97	4 (17%)
28	DMS	B	636	-	3,3,3	2.76	1 (33%)	3,3,3	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	BCR	B	618	-	41,41,41	1.05	0	56,56,56	1.26	7 (12%)
32	HTG	c	520	-	19,19,19	0.89	2 (10%)	23,24,24	1.32	2 (8%)
24	LMG	j	101	39	45,45,55	1.00	3 (6%)	53,53,63	1.02	6 (11%)
34	LMT	B	625	-	24,24,36	0.53	0	29,29,47	1.26	4 (13%)
37	HEM	E	104	5,6	41,50,50	1.88	7 (17%)	45,82,82	2.01	13 (28%)
20	CLA	B	608	41	65,73,73	1.93	14 (21%)	76,113,113	2.11	20 (26%)
20	CLA	B	612	-	65,73,73	1.90	16 (24%)	76,113,113	2.26	24 (31%)
28	DMS	V	209	-	3,3,3	2.61	1 (33%)	3,3,3	0.64	0
20	CLA	a	407	-	47,55,73	2.39	14 (29%)	54,91,113	2.55	24 (44%)
35	DGD	C	516	-	63,63,67	0.89	2 (3%)	77,77,81	1.20	7 (9%)
28	DMS	O	308	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
32	HTG	v	210	-	14,14,19	0.62	0	18,19,24	2.19	4 (22%)
20	CLA	A	402	41	59,67,73	1.73	14 (23%)	68,105,113	2.75	24 (35%)
28	DMS	C	527	-	3,3,3	2.56	1 (33%)	3,3,3	0.49	0
32	HTG	b	601	-	19,19,19	1.04	2 (10%)	23,24,24	1.27	2 (8%)
28	DMS	C	529	-	3,3,3	2.69	1 (33%)	3,3,3	0.81	0
28	DMS	V	205	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
38	RRX	H	101	-	42,42,42	0.77	1 (2%)	57,58,58	1.49	8 (14%)
28	DMS	u	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
20	CLA	C	512	-	55,63,73	2.72	20 (36%)	64,101,113	2.39	23 (35%)
34	LMT	B	627	-	15,15,36	0.48	0	14,14,47	0.67	0
28	DMS	C	530	-	3,3,3	2.61	1 (33%)	3,3,3	1.00	0
36	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	1.16	5 (9%)
35	DGD	h	101	-	63,63,67	0.98	3 (4%)	77,77,81	1.04	4 (5%)
22	BCR	c	514	-	41,41,41	0.85	1 (2%)	56,56,56	1.49	7 (12%)
28	DMS	u	202	-	3,3,3	2.65	1 (33%)	3,3,3	1.29	0
28	DMS	U	903[A]	-	3,3,3	2.56	1 (33%)	3,3,3	0.75	0
34	LMT	b	627	-	33,33,36	0.88	1 (3%)	44,44,47	1.80	10 (22%)
22	BCR	T	101	-	41,41,41	0.81	0	56,56,56	1.50	11 (19%)
28	DMS	u	203	-	3,3,3	2.57	1 (33%)	3,3,3	0.78	0
36	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
28	DMS	O	310	-	3,3,3	2.70	1 (33%)	3,3,3	0.70	0
28	DMS	B	639	-	3,3,3	2.73	1 (33%)	3,3,3	0.63	0
34	LMT	T	102	-	24,24,36	0.45	0	29,29,47	1.15	2 (6%)
20	CLA	b	607	-	65,73,73	1.88	14 (21%)	76,113,113	2.34	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	DMS	c	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
32	HTG	B	621	-	19,19,19	1.45	3 (15%)	23,24,24	1.79	6 (26%)
28	DMS	v	207	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
28	DMS	c	535	-	3,3,3	2.78	1 (33%)	3,3,3	0.79	0
22	BCR	d	405	-	41,41,41	0.94	0	56,56,56	1.84	11 (19%)
34	LMT	m	102	-	36,36,36	0.58	0	47,47,47	1.14	4 (8%)
20	CLA	C	501	-	65,73,73	1.98	16 (24%)	76,113,113	2.20	18 (23%)
20	CLA	C	502	-	65,73,73	2.23	16 (24%)	76,113,113	2.29	24 (31%)
28	DMS	C	528	-	3,3,3	2.31	1 (33%)	3,3,3	0.59	0
20	CLA	C	509	-	65,73,73	2.18	14 (21%)	76,113,113	2.28	23 (30%)
20	CLA	B	601	-	65,73,73	2.06	17 (26%)	76,113,113	2.11	24 (31%)
20	CLA	b	610	-	65,73,73	2.04	15 (23%)	76,113,113	2.19	23 (30%)
22	BCR	b	621	-	41,41,41	0.80	1 (2%)	56,56,56	1.47	8 (14%)
28	DMS	C	531	-	3,3,3	2.66	1 (33%)	3,3,3	0.97	0
20	CLA	c	509	-	65,73,73	2.31	18 (27%)	76,113,113	2.39	26 (34%)
28	DMS	O	306	-	3,3,3	2.53	1 (33%)	3,3,3	0.64	0
28	DMS	O	304	-	3,3,3	2.61	1 (33%)	3,3,3	0.60	0
28	DMS	b	641	-	3,3,3	2.79	1 (33%)	3,3,3	1.11	0
32	HTG	B	622	-	19,19,19	1.34	3 (15%)	23,24,24	1.93	6 (26%)
32	HTG	C	522	-	19,19,19	1.06	2 (10%)	23,24,24	1.56	1 (4%)
32	HTG	V	202	-	12,13,19	0.76	1 (8%)	16,18,24	2.50	6 (37%)
28	DMS	b	632	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
38	RRX	x	101	-	42,42,42	0.82	0	57,58,58	1.22	6 (10%)
24	LMG	c	518	-	51,51,55	1.11	3 (5%)	59,59,63	1.31	7 (11%)
28	DMS	b	635	-	3,3,3	2.68	1 (33%)	3,3,3	0.75	0
28	DMS	c	536	-	3,3,3	2.84	1 (33%)	3,3,3	1.23	0
20	CLA	c	503	-	65,73,73	2.53	20 (30%)	76,113,113	2.29	21 (27%)
32	HTG	D	417	-	19,19,19	1.05	1 (5%)	23,24,24	1.49	3 (13%)
20	CLA	C	510	-	65,73,73	2.17	18 (27%)	76,113,113	2.16	21 (27%)
22	BCR	k	102	-	41,41,41	0.79	0	56,56,56	1.29	9 (16%)
36	LHG	E	103	-	46,46,48	1.03	2 (4%)	49,50,54	1.14	5 (10%)
27	PL9	A	411	-	55,55,55	0.83	3 (5%)	68,69,69	1.69	18 (26%)
20	CLA	C	505	-	65,73,73	2.15	18 (27%)	76,113,113	2.04	21 (27%)
28	DMS	c	528	-	3,3,3	2.57	1 (33%)	3,3,3	0.44	0
20	CLA	c	502	-	65,73,73	2.20	17 (26%)	76,113,113	2.38	25 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	DMS	c	533	-	3,3,3	2.74	1 (33%)	3,3,3	0.83	0
37	HEM	e	102	5,6	41,50,50	1.96	10 (24%)	45,82,82	1.94	10 (22%)
28	DMS	v	209	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
35	DGD	D	406	-	51,51,67	1.11	2 (3%)	59,59,81	1.21	5 (8%)
20	CLA	A	401	-	65,73,73	1.90	17 (26%)	76,113,113	1.99	22 (28%)
20	CLA	B	616	-	65,73,73	2.15	16 (24%)	76,113,113	2.15	22 (28%)
28	DMS	B	645	-	3,3,3	2.73	1 (33%)	3,3,3	0.93	0
20	CLA	c	506	-	65,73,73	2.27	18 (27%)	76,113,113	2.22	24 (31%)
21	PHO	a	406	-	51,69,69	1.58	8 (15%)	47,99,99	1.80	9 (19%)
20	CLA	c	504	41	65,73,73	2.13	17 (26%)	76,113,113	2.65	23 (30%)
20	CLA	b	611	-	65,73,73	2.57	17 (26%)	76,113,113	1.82	20 (26%)
30	OEX	a	419	41,1,3	0,15,15	-	-	-	-	-
23	SQD	F	101	-	34,35,54	1.01	2 (5%)	42,45,65	1.59	7 (16%)
34	LMT	J	103	-	24,24,36	0.65	1 (4%)	29,29,47	1.12	1 (3%)
23	SQD	a	409	-	53,54,54	1.01	4 (7%)	62,65,65	2.11	11 (17%)
22	BCR	C	515	-	41,41,41	0.97	0	56,56,56	1.19	6 (10%)
28	DMS	B	638	-	3,3,3	2.76	1 (33%)	3,3,3	0.82	0
40	HEC	V	201	16	32,50,50	1.86	8 (25%)	24,82,82	1.89	5 (20%)
28	DMS	B	634	-	3,3,3	1.94	1 (33%)	3,3,3	0.29	0
35	DGD	C	517	-	56,56,67	0.98	2 (3%)	70,70,81	0.93	4 (5%)
28	DMS	b	636	-	3,3,3	2.71	1 (33%)	3,3,3	0.75	0
32	HTG	B	623	-	19,19,19	0.96	1 (5%)	23,24,24	1.56	2 (8%)
22	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.58	9 (16%)
20	CLA	d	404	-	65,73,73	1.99	17 (26%)	76,113,113	2.35	25 (32%)
28	DMS	O	309	-	3,3,3	2.67	1 (33%)	3,3,3	1.16	0
20	CLA	c	510	-	65,73,73	1.95	18 (27%)	76,113,113	2.22	27 (35%)
28	DMS	D	414	-	3,3,3	2.53	1 (33%)	3,3,3	0.25	0
28	DMS	i	104	-	3,3,3	2.62	1 (33%)	3,3,3	0.33	0
20	CLA	B	609	-	65,73,73	1.98	18 (27%)	76,113,113	2.39	25 (32%)
20	CLA	c	505	-	65,73,73	2.12	18 (27%)	76,113,113	2.07	21 (27%)
28	DMS	V	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.74	0
24	LMG	J	101	39	45,45,55	1.01	2 (4%)	53,53,63	0.98	3 (5%)
28	DMS	o	308	-	3,3,3	2.85	1 (33%)	3,3,3	0.81	0
28	DMS	c	527	-	3,3,3	2.31	1 (33%)	3,3,3	0.49	0
22	BCR	D	405	-	41,41,41	1.03	3 (7%)	56,56,56	1.73	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	PHO	A	403	-	51,69,69	1.34	6 (11%)	47,99,99	1.59	8 (17%)
28	DMS	b	631	-	3,3,3	2.88	1 (33%)	3,3,3	1.24	0
36	LHG	d	408	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	5 (9%)
28	DMS	U	904	-	3,3,3	2.85	1 (33%)	3,3,3	0.70	0
23	SQD	f	101	-	39,40,54	1.37	3 (7%)	48,51,65	3.70	12 (25%)
28	DMS	D	415	-	3,3,3	2.92	1 (33%)	3,3,3	0.73	0
24	LMG	B	620	-	51,51,55	1.02	2 (3%)	59,59,63	1.31	5 (8%)
28	DMS	v	208	-	3,3,3	2.63	1 (33%)	3,3,3	0.66	0
31	BCT	a	413	29	2,3,3	0.65	0	2,3,3	1.47	0
28	DMS	A	417	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
23	SQD	A	406	-	53,54,54	1.00	3 (5%)	62,65,65	1.75	14 (22%)
28	DMS	B	635	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
20	CLA	c	513	-	65,73,73	2.55	18 (27%)	76,113,113	2.22	23 (30%)
20	CLA	B	615	-	65,73,73	2.01	16 (24%)	76,113,113	2.52	27 (35%)
28	DMS	D	416	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
24	LMG	C	524	-	45,45,55	1.10	3 (6%)	53,53,63	1.36	5 (9%)
24	LMG	a	410	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	2 (3%)

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
34	LMT	E	101	-	-	8/15/35/61	0/1/1/2
20	CLA	c	501	-	1/1/15/20	3/37/115/115	-
22	BCR	j	102	-	-	2/29/63/63	0/2/2/2
34	LMT	a	418	-	-	11/21/61/61	0/2/2/2
34	LMT	z	102	-	-	13/21/61/61	0/2/2/2
32	HTG	C	534	-	-	6/10/30/30	0/1/1/1
32	HTG	b	625	-	-	4/10/30/30	0/1/1/1
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
20	CLA	b	618	-	1/1/15/20	17/37/115/115	-
20	CLA	b	605	-	1/1/15/20	1/37/115/115	-
23	SQD	A	412	-	-	24/49/69/69	0/1/1/1
20	CLA	b	609	41	1/1/15/20	2/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	C	503	-	-	4/37/115/115	-
20	CLA	C	504	41	-	11/37/115/115	-
22	BCR	A	405	-	-	0/29/63/63	0/2/2/2
34	LMT	I	101	-	-	8/21/61/61	0/2/2/2
34	LMT	b	628	-	-	9/17/37/61	0/1/1/2
22	BCR	K	101	-	-	4/29/63/63	0/2/2/2
22	BCR	k	101	-	-	4/29/63/63	0/2/2/2
35	DGD	c	516	-	-	13/46/86/95	0/2/2/2
20	CLA	a	404	41	-	6/31/109/115	-
20	CLA	c	507	41	1/1/15/20	6/37/115/115	-
20	CLA	B	603	-	1/1/15/20	3/37/115/115	-
24	LMG	b	623	-	-	14/44/64/70	0/1/1/1
20	CLA	b	616	-	1/1/15/20	18/37/115/115	-
36	LHG	D	408	-	-	10/53/53/53	-
27	PL9	D	412	-	-	3/53/73/73	0/1/1/1
35	DGD	c	515	-	-	18/51/91/95	0/2/2/2
20	CLA	c	511	3	1/1/15/20	0/37/115/115	-
20	CLA	d	402	-	1/1/15/20	3/37/115/115	-
32	HTG	u	201	-	-	1/5/5/30	-
34	LMT	m	101	-	-	15/21/61/61	0/2/2/2
20	CLA	B	605	-	1/1/15/20	8/37/115/115	-
20	CLA	C	511	3	-	0/37/115/115	-
20	CLA	c	508	-	-	2/31/109/115	-
32	HTG	b	602	-	-	3/10/30/30	0/1/1/1
20	CLA	C	513	-	-	10/37/115/115	-
35	DGD	c	517	-	-	14/51/91/95	0/2/2/2
20	CLA	B	614	-	1/1/15/20	6/37/115/115	-
34	LMT	B	626	-	-	7/15/35/61	0/1/1/2
20	CLA	c	512	-	1/1/15/20	7/37/115/115	-
20	CLA	D	404	-	1/1/15/20	13/37/115/115	-
20	CLA	b	617	-	1/1/15/20	8/37/115/115	-
21	PHO	a	405	-	-	4/37/103/103	0/5/6/6
24	LMG	c	519	-	-	26/46/66/70	0/1/1/1
20	CLA	D	401	-	1/1/15/20	7/37/115/115	-
20	CLA	b	608	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	B	632	-	-	2/10/30/30	0/1/1/1
20	CLA	b	612	41	1/1/15/20	5/37/115/115	-
34	LMT	M	101	-	-	1/21/61/61	0/2/2/2
20	CLA	b	615	-	1/1/15/20	6/37/115/115	-
27	PL9	a	415	-	-	11/53/73/73	0/1/1/1
24	LMG	C	519	-	-	19/46/66/70	0/1/1/1
32	HTG	c	521	-	-	5/10/30/30	0/1/1/1
20	CLA	b	604	-	1/1/15/20	7/37/115/115	-
22	BCR	b	620	-	-	0/29/63/63	0/2/2/2
27	PL9	d	412	-	-	3/53/73/73	0/1/1/1
32	HTG	b	624	-	-	0/10/30/30	0/1/1/1
36	LHG	D	407	-	-	9/53/53/53	-
34	LMT	f	102	-	-	8/15/35/61	0/1/1/2
20	CLA	d	403	41	-	5/37/115/115	-
23	SQD	a	401	-	-	20/49/69/69	0/1/1/1
24	LMG	A	407	-	-	28/46/66/70	0/1/1/1
36	LHG	d	407	-	-	11/53/53/53	-
20	CLA	C	507	41	1/1/15/20	11/37/115/115	-
34	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
20	CLA	B	611	41	1/1/15/20	4/37/115/115	-
20	CLA	D	402	41	-	5/37/115/115	-
20	CLA	B	606	-	1/1/15/20	4/37/115/115	-
35	DGD	C	518	-	-	12/51/91/95	0/2/2/2
32	HTG	C	520	-	-	4/10/30/30	0/1/1/1
22	BCR	b	619	-	-	2/29/63/63	0/2/2/2
20	CLA	A	404	-	-	10/37/115/115	-
23	SQD	l	101	-	-	28/49/69/69	0/1/1/1
20	CLA	b	613	-	-	7/37/115/115	-
22	BCR	C	514	-	-	5/29/63/63	0/2/2/2
20	CLA	B	607	-	1/1/15/20	11/37/115/115	-
20	CLA	a	403	-	1/1/15/20	4/37/115/115	-
22	BCR	t	101	-	-	3/29/63/63	0/2/2/2
22	BCR	a	408	-	-	0/29/63/63	0/2/2/2
40	HEC	v	201	16	-	2/10/54/54	-
22	BCR	B	617	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	603	41	1/1/15/20	18/37/115/115	-
32	HTG	B	631	-	-	5/10/30/30	0/1/1/1
32	HTG	d	401	-	-	9/10/30/30	0/1/1/1
20	CLA	B	610	-	1/1/15/20	1/37/115/115	-
20	CLA	b	614	-	1/1/15/20	4/37/115/115	-
20	CLA	C	506	-	1/1/15/20	12/37/115/115	-
35	DGD	d	416	-	-	30/46/66/95	0/1/1/2
34	LMT	c	523	-	-	8/21/61/61	0/2/2/2
20	CLA	B	613	-	1/1/15/20	0/37/115/115	-
32	HTG	O	302	-	-	5/10/30/30	0/1/1/1
20	CLA	B	604	-	1/1/15/20	3/37/115/115	-
22	BCR	K	102	-	-	1/29/63/63	0/2/2/2
20	CLA	b	606	-	1/1/15/20	3/37/115/115	-
23	SQD	b	622	-	-	23/49/69/69	0/1/1/1
36	LHG	L	101	-	-	17/53/53/53	-
20	CLA	C	508	-	1/1/14/20	6/31/109/115	-
20	CLA	B	602	41	1/1/15/20	21/37/115/115	-
21	PHO	D	403	-	-	4/37/103/103	0/5/6/6
32	HTG	C	521	-	-	6/10/30/30	0/1/1/1
32	HTG	c	520	-	-	5/10/30/30	0/1/1/1
22	BCR	B	618	-	-	0/29/63/63	0/2/2/2
36	LHG	l	102	-	-	19/53/53/53	-
24	LMG	j	101	39	-	15/40/60/70	0/1/1/1
34	LMT	B	625	-	-	4/15/35/61	0/1/1/2
37	HEM	E	104	5,6	-	5/12/54/54	-
20	CLA	B	608	41	1/1/15/20	1/37/115/115	-
20	CLA	B	612	-	1/1/15/20	3/37/115/115	-
20	CLA	a	407	-	-	0/16/94/115	-
35	DGD	C	516	-	-	18/51/91/95	0/2/2/2
32	HTG	v	210	-	-	3/5/25/30	0/1/1/1
20	CLA	A	402	41	-	3/30/108/115	-
32	HTG	b	601	-	-	2/10/30/30	0/1/1/1
38	RRX	H	101	-	-	1/29/65/65	0/2/2/2
20	CLA	C	512	-	1/1/13/20	6/25/103/115	-
36	LHG	d	406	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	h	101	-	-	15/51/91/95	0/2/2/2
22	BCR	c	514	-	-	0/29/63/63	0/2/2/2
34	LMT	b	627	-	-	10/18/58/61	0/2/2/2
22	BCR	T	101	-	-	1/29/63/63	0/2/2/2
36	LHG	D	409	-	-	14/53/53/53	-
34	LMT	T	102	-	-	11/15/35/61	0/1/1/2
20	CLA	b	607	-	1/1/15/20	4/37/115/115	-
32	HTG	B	621	-	-	5/10/30/30	0/1/1/1
34	LMT	m	102	-	-	3/21/61/61	0/2/2/2
22	BCR	d	405	-	-	4/29/63/63	0/2/2/2
20	CLA	C	501	-	1/1/15/20	3/37/115/115	-
20	CLA	C	502	-	-	5/37/115/115	-
20	CLA	C	509	-	1/1/15/20	8/37/115/115	-
20	CLA	B	601	-	1/1/15/20	18/37/115/115	-
20	CLA	b	610	-	-	1/37/115/115	-
22	BCR	b	621	-	-	0/29/63/63	0/2/2/2
20	CLA	c	509	-	1/1/15/20	10/37/115/115	-
32	HTG	B	622	-	-	5/10/30/30	0/1/1/1
32	HTG	C	522	-	-	4/10/30/30	0/1/1/1
32	HTG	V	202	-	-	1/4/24/30	0/1/1/1
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
24	LMG	c	518	-	-	8/46/66/70	0/1/1/1
20	CLA	c	503	-	-	3/37/115/115	-
32	HTG	D	417	-	-	5/10/30/30	0/1/1/1
20	CLA	C	510	-	1/1/15/20	2/37/115/115	-
22	BCR	k	102	-	-	1/29/63/63	0/2/2/2
36	LHG	E	103	-	-	27/45/45/53	-
27	PL9	A	411	-	-	10/53/73/73	0/1/1/1
20	CLA	C	505	-	1/1/15/20	1/37/115/115	-
20	CLA	c	502	-	-	6/37/115/115	-
37	HEM	e	102	5,6	-	4/12/54/54	-
35	DGD	D	406	-	-	26/46/66/95	0/1/1/2
20	CLA	A	401	-	1/1/15/20	4/37/115/115	-
20	CLA	B	616	-	1/1/15/20	5/37/115/115	-
20	CLA	c	506	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PHO	a	406	-	-	2/37/103/103	0/5/6/6
20	CLA	c	504	41	1/1/15/20	5/37/115/115	-
20	CLA	b	611	-	-	0/37/115/115	-
23	SQD	F	101	-	-	17/28/48/69	0/1/1/1
34	LMT	J	103	-	-	7/15/35/61	0/1/1/2
23	SQD	a	409	-	-	20/49/69/69	0/1/1/1
22	BCR	C	515	-	-	0/29/63/63	0/2/2/2
40	HEC	V	201	16	-	2/10/54/54	-
35	DGD	C	517	-	-	14/44/84/95	0/2/2/2
32	HTG	B	623	-	-	6/10/30/30	0/1/1/1
22	BCR	B	619	-	-	0/29/63/63	0/2/2/2
20	CLA	d	404	-	-	8/37/115/115	-
20	CLA	c	510	-	1/1/15/20	3/37/115/115	-
20	CLA	B	609	-	-	1/37/115/115	-
20	CLA	c	505	-	1/1/15/20	1/37/115/115	-
24	LMG	J	101	39	-	9/40/60/70	0/1/1/1
22	BCR	D	405	-	-	4/29/63/63	0/2/2/2
21	PHO	A	403	-	-	2/37/103/103	0/5/6/6
36	LHG	d	408	-	-	14/53/53/53	-
34	LMT	B	627	-	-	7/13/13/61	-
23	SQD	f	101	-	-	16/34/54/69	0/1/1/1
24	LMG	B	620	-	-	19/46/66/70	0/1/1/1
23	SQD	A	406	-	-	21/49/69/69	0/1/1/1
20	CLA	c	513	-	-	14/37/115/115	-
20	CLA	B	615	-	1/1/15/20	10/37/115/115	-
24	LMG	C	524	-	-	22/40/60/70	0/1/1/1
24	LMG	a	410	-	-	18/46/66/70	0/1/1/1

The worst 5 of 1490 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	MG-NA	12.91	2.36	2.06
20	c	513	CLA	MG-NA	12.66	2.36	2.06
20	B	602	CLA	MG-NA	11.66	2.34	2.06
20	c	507	CLA	MG-NA	10.98	2.32	2.06
20	c	511	CLA	MG-NC	10.70	2.31	2.06

The worst 5 of 2315 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	f	101	SQD	O9-S-C6	-14.05	90.24	106.94
20	c	504	CLA	C4A-NA-C1A	12.19	112.19	106.71
20	C	511	CLA	C4A-NA-C1A	11.76	111.99	106.71
20	c	501	CLA	C4A-NA-C1A	11.42	111.84	106.71
20	c	509	CLA	C4A-NA-C1A	10.78	111.55	106.71

5 of 50 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	401	CLA	ND
20	B	601	CLA	ND
20	B	602	CLA	ND
20	B	603	CLA	ND
20	B	604	CLA	ND

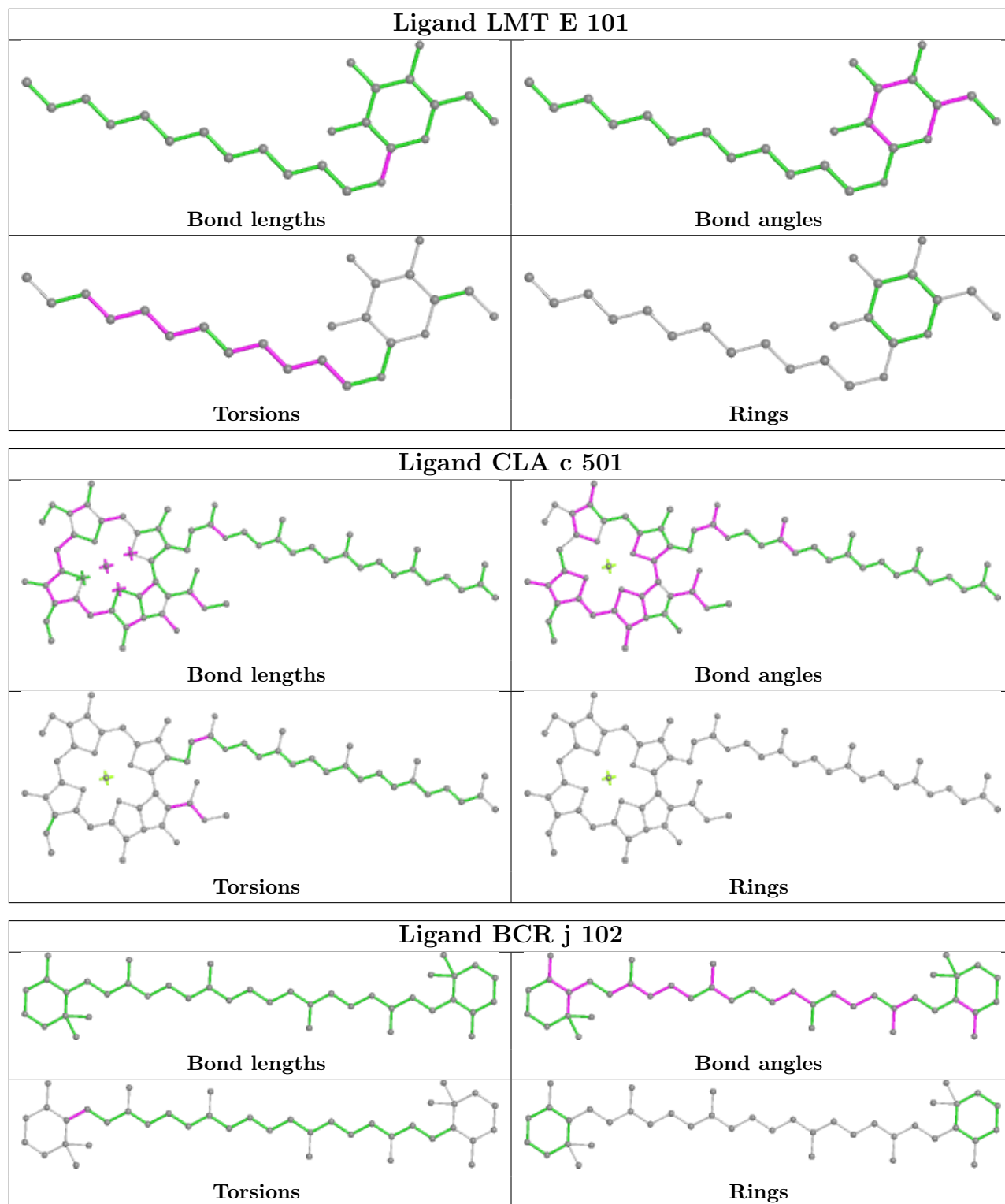
5 of 1393 torsion outliers are listed below:

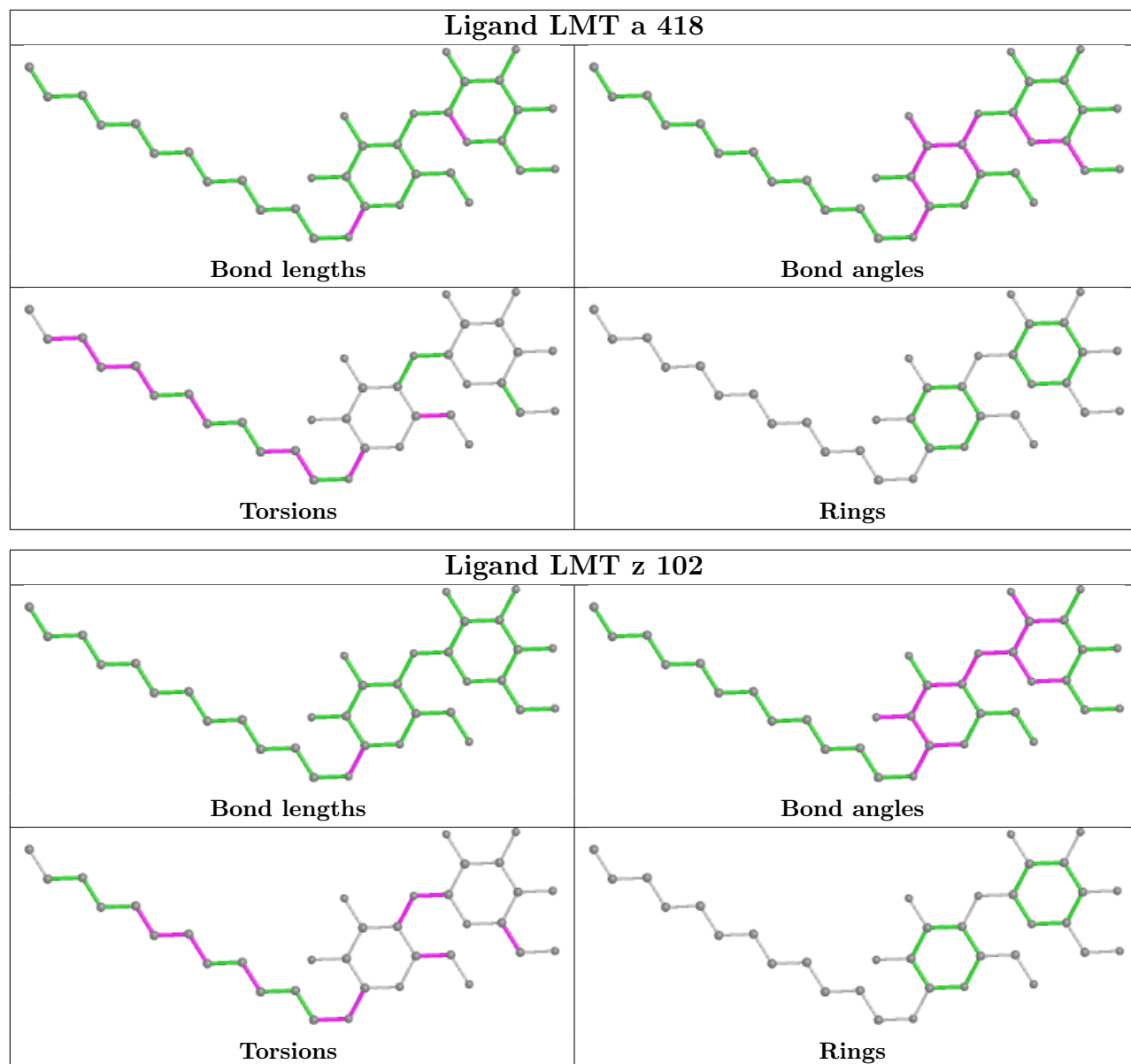
Mol	Chain	Res	Type	Atoms
20	B	601	CLA	C11-C10-C8-C9
20	B	602	CLA	CBA-CGA-O2A-C1
20	B	602	CLA	O1A-CGA-O2A-C1
20	B	602	CLA	CHA-CBD-CGD-O1D
20	B	602	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

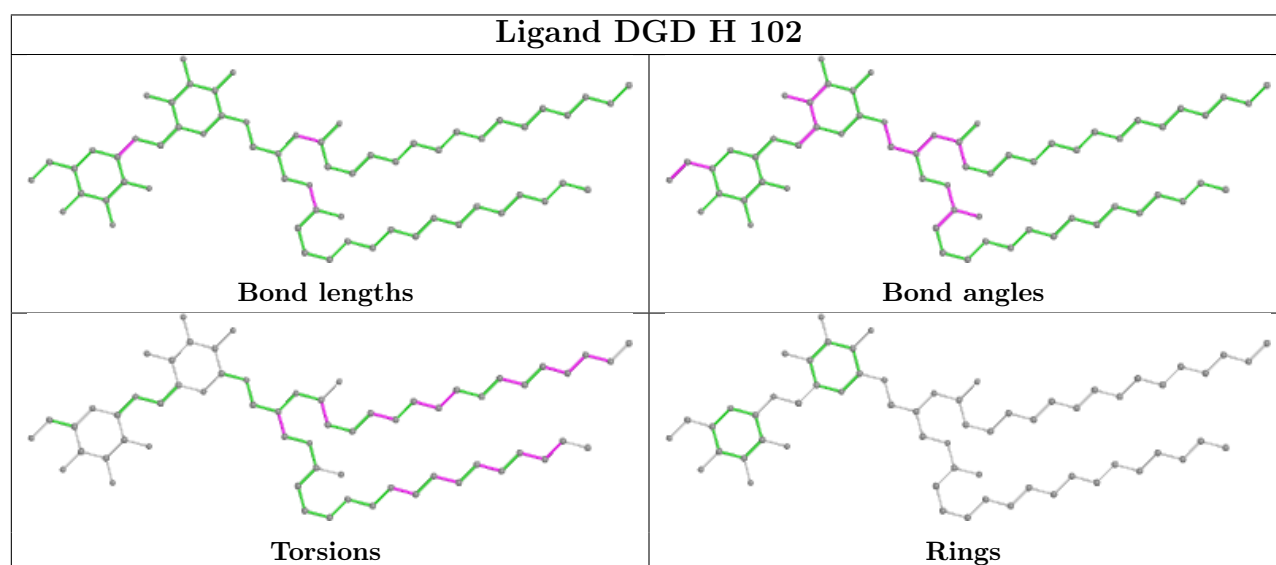
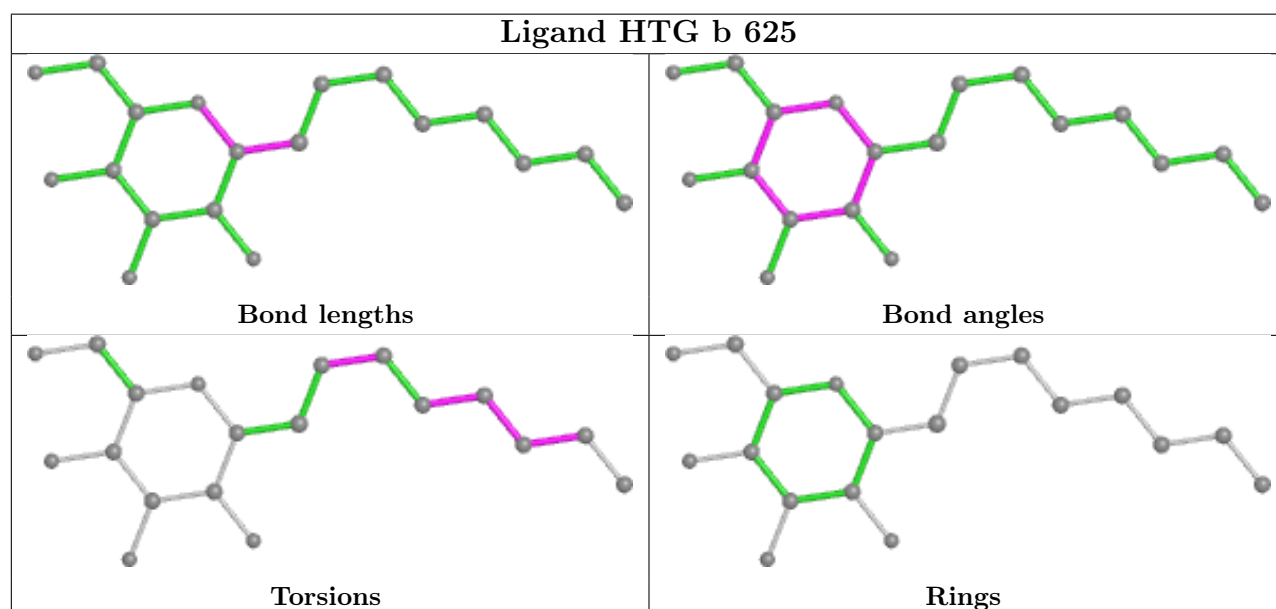
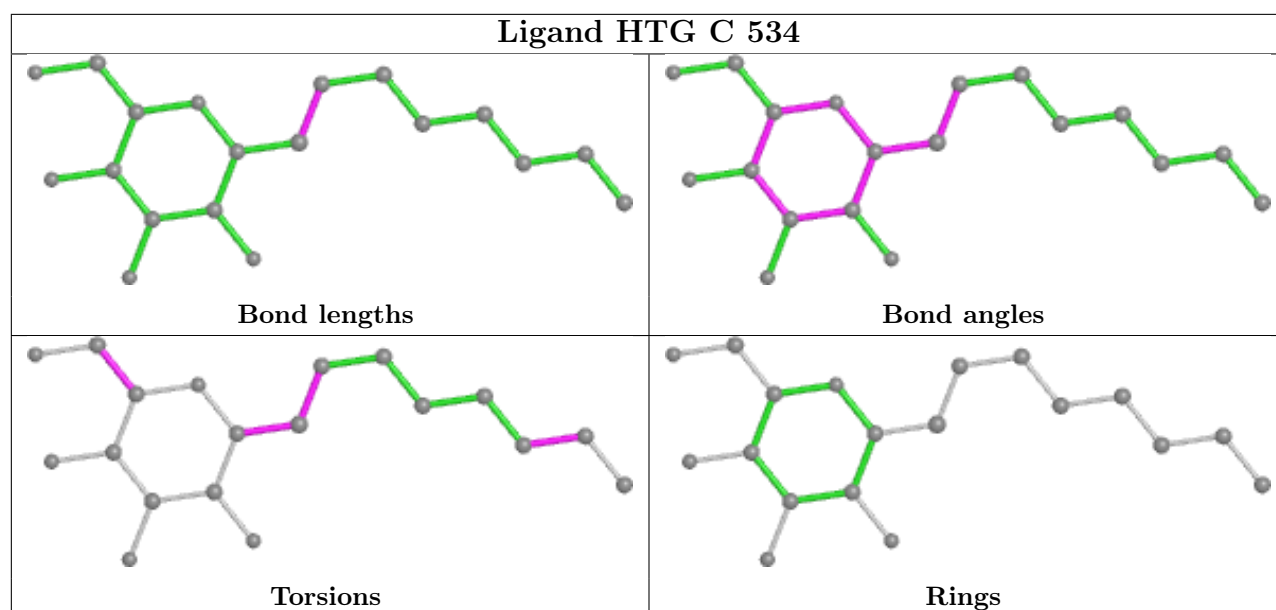
No monomer is involved in short contacts.

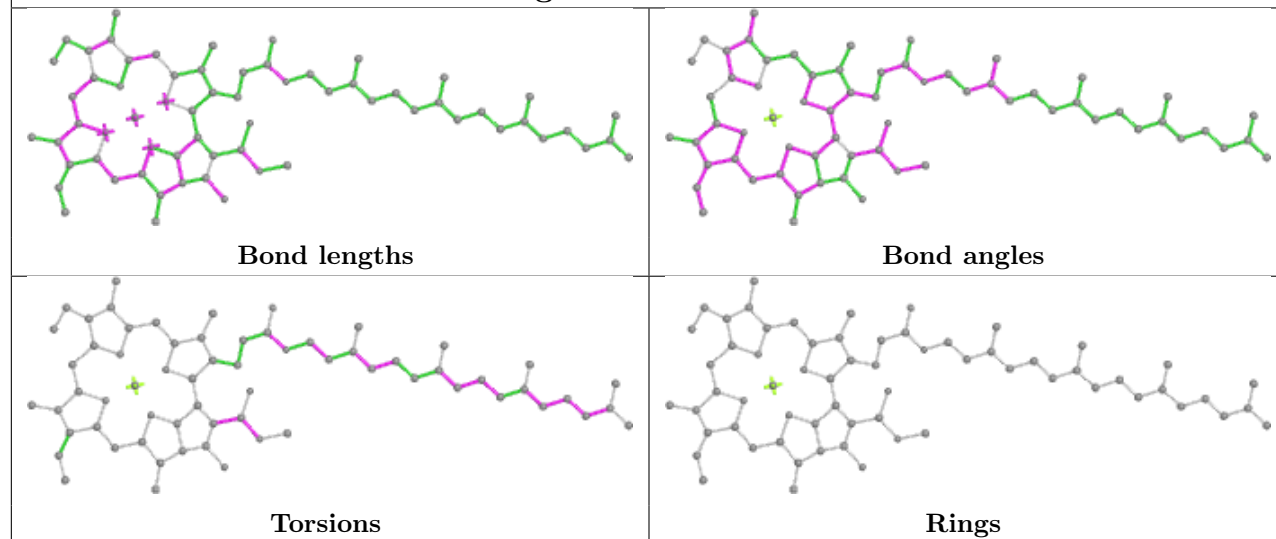
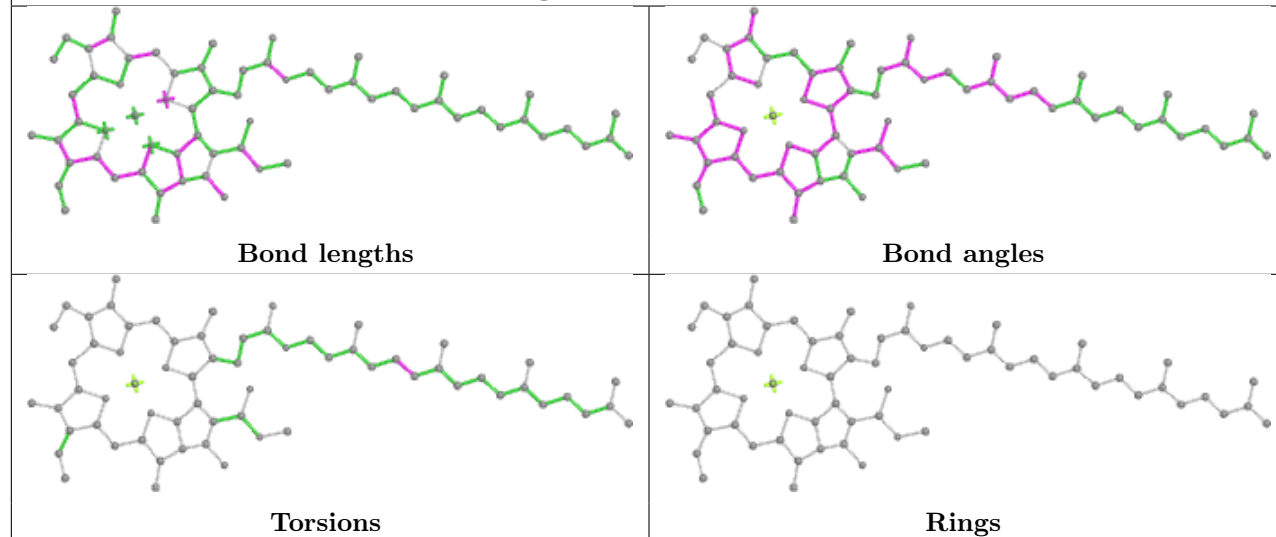
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

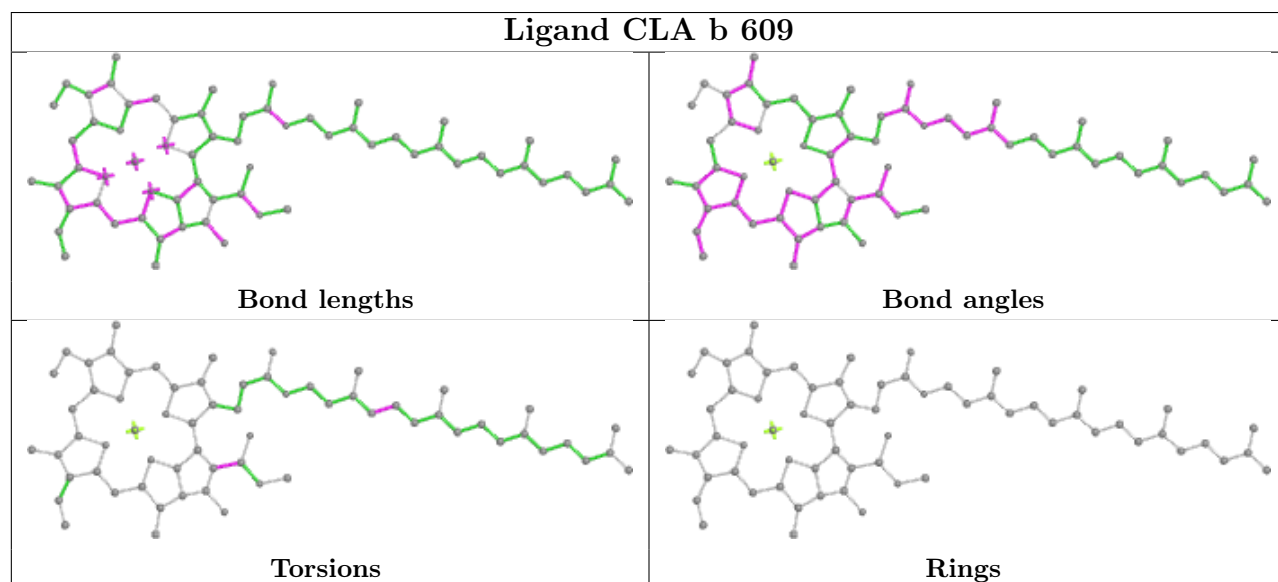
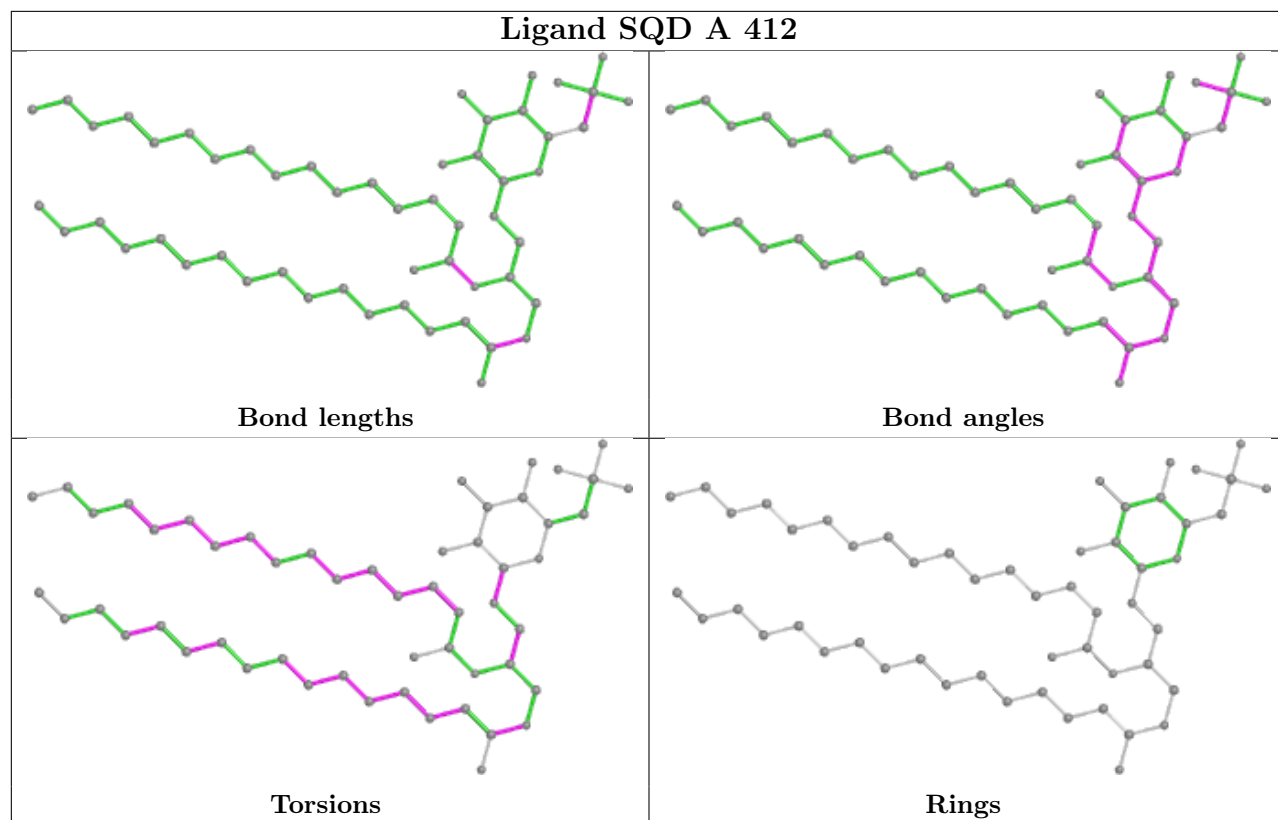


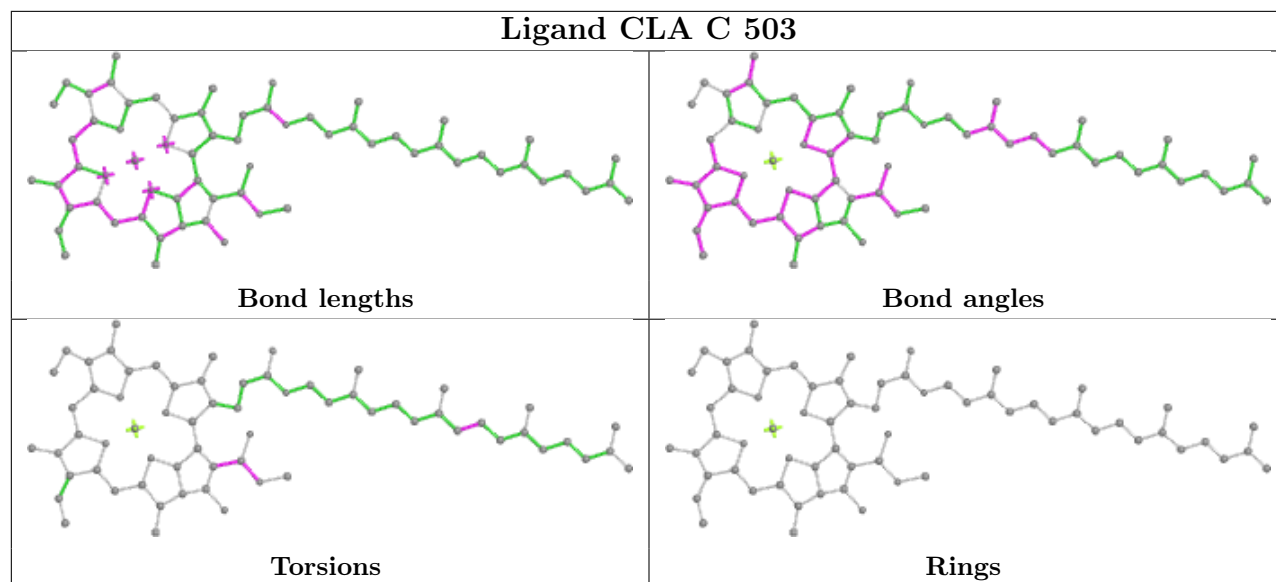
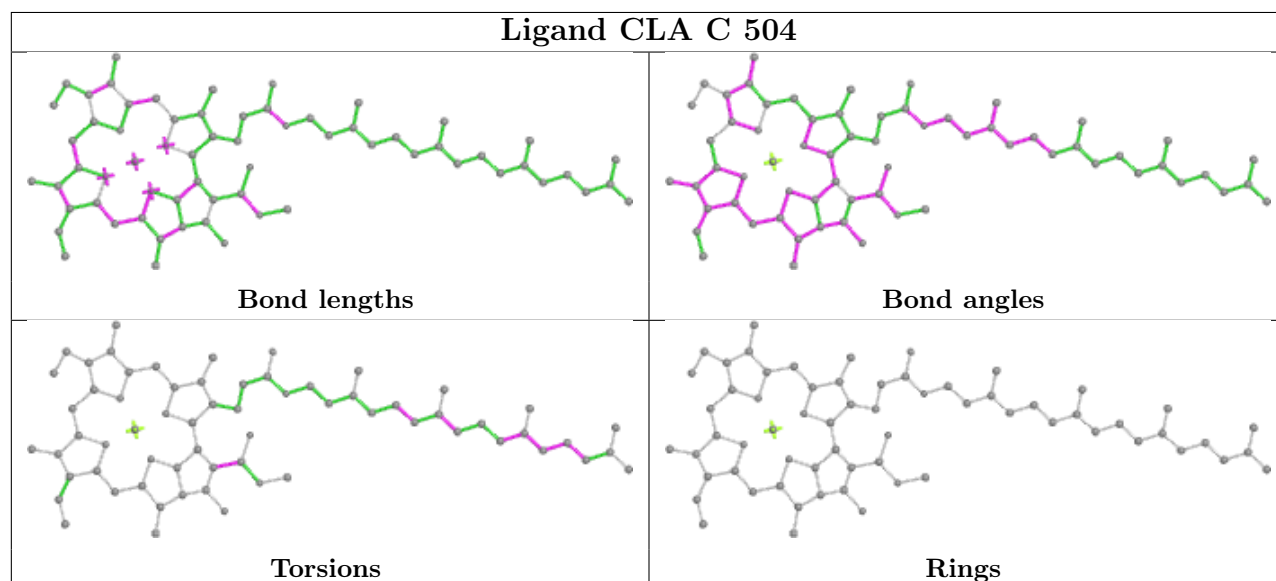
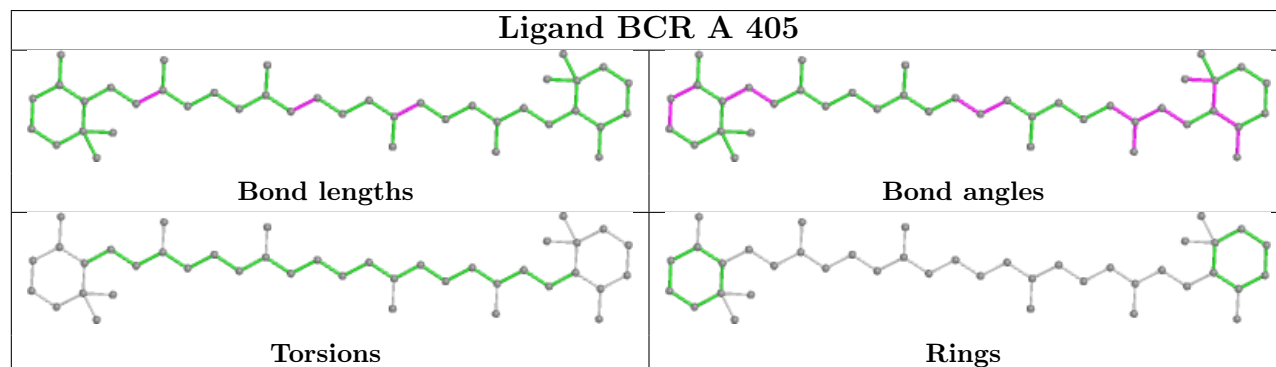


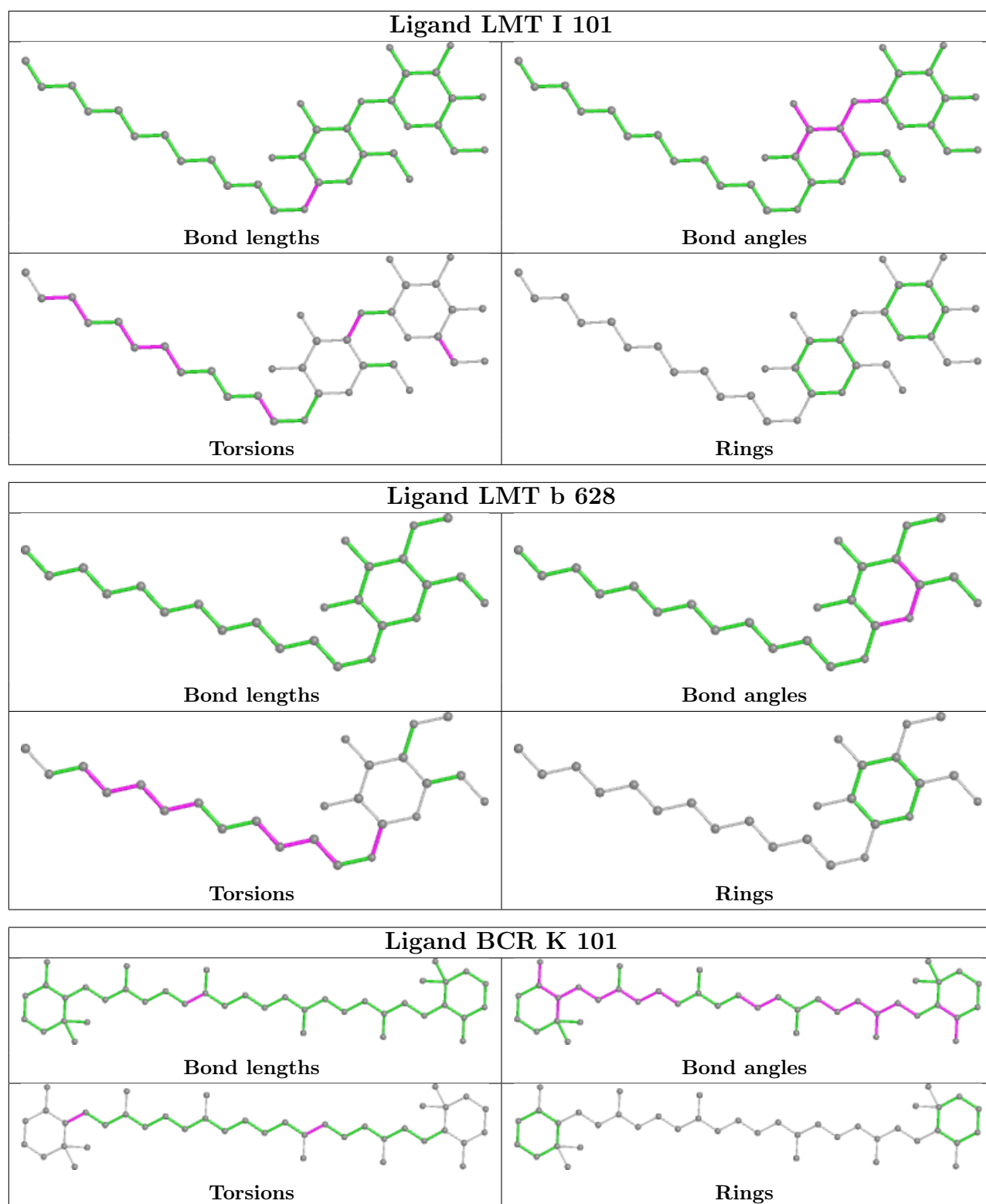


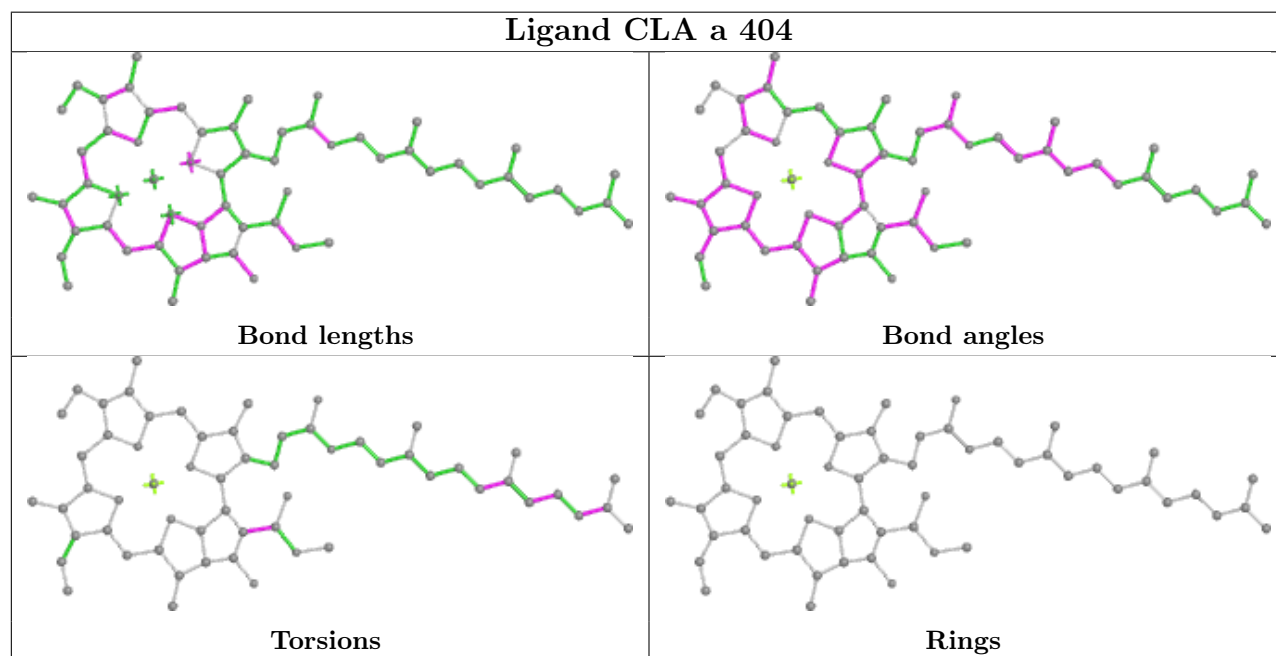
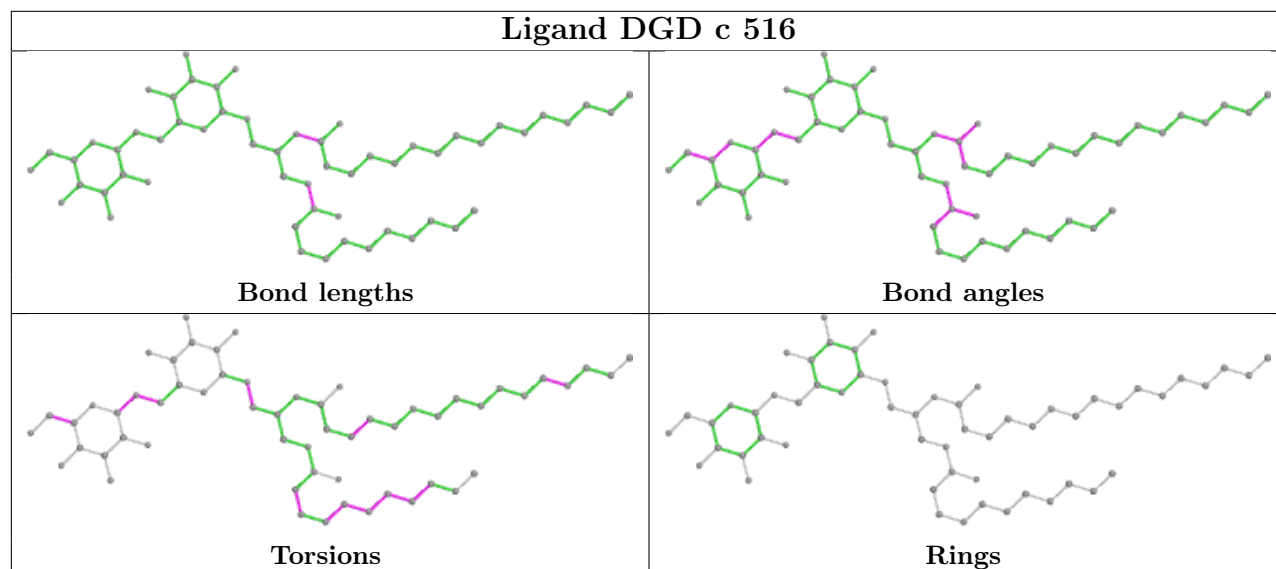
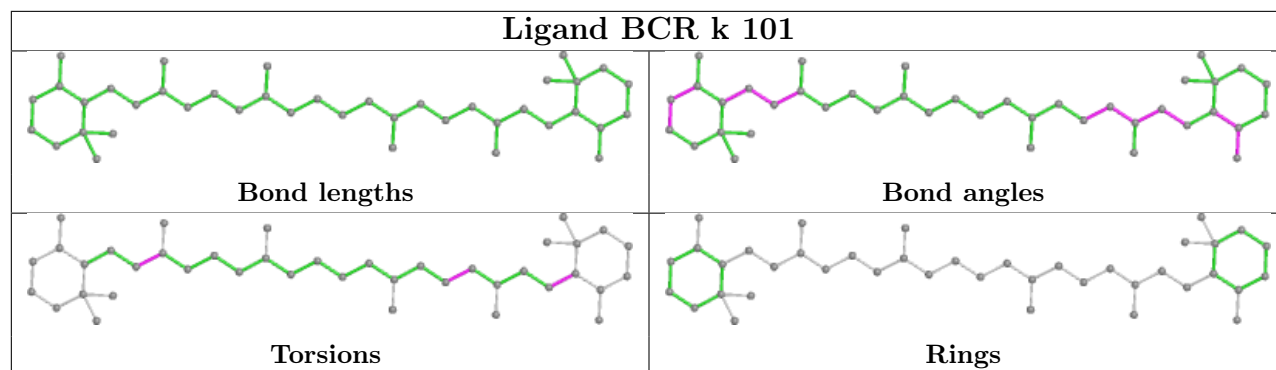


**Ligand CLA b 618****Ligand CLA b 605**

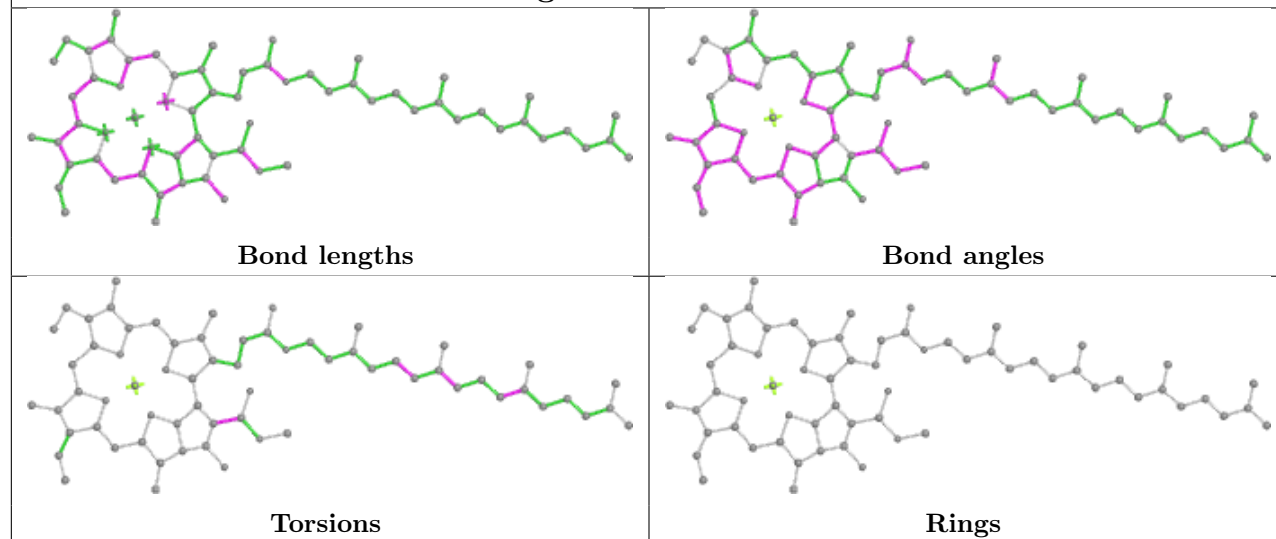


**Ligand CLA C 503****Ligand CLA C 504****Ligand BCR A 405**

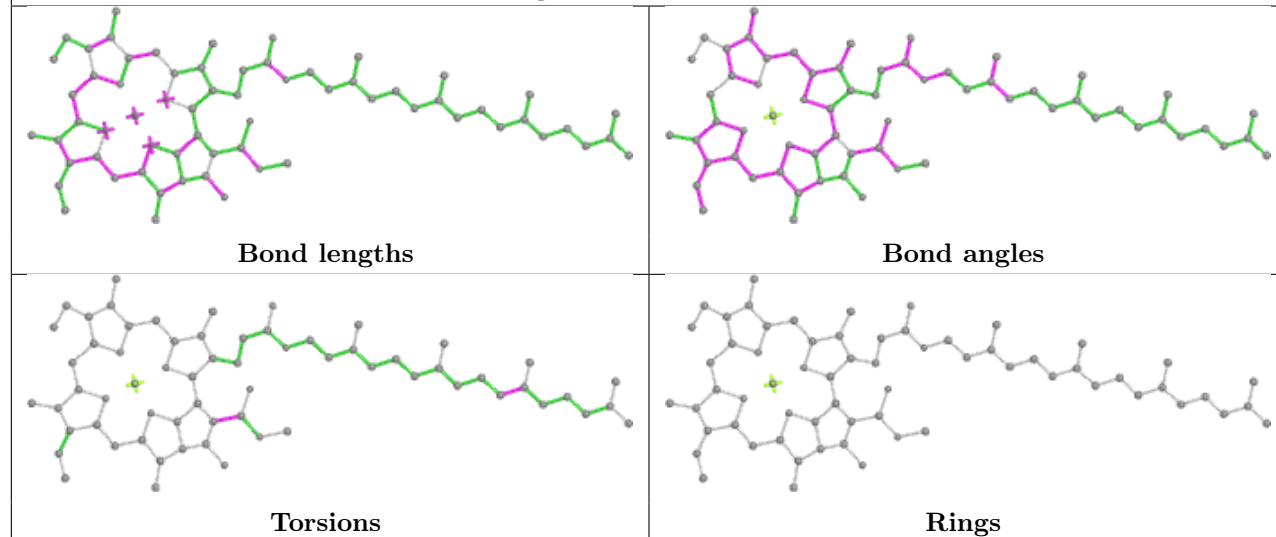




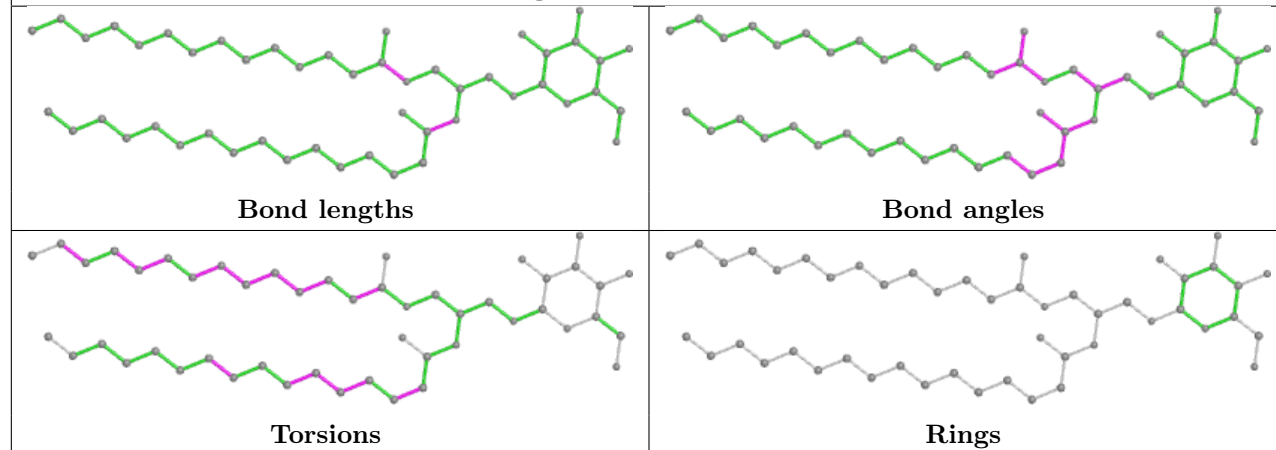
## Ligand CLA c 507



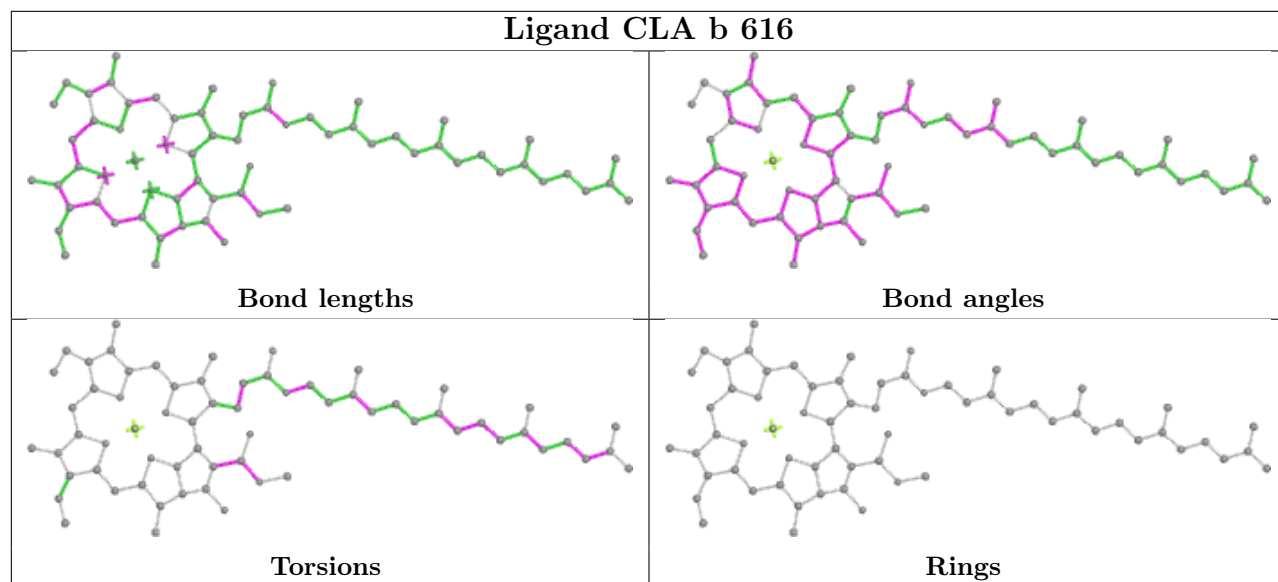
## Ligand CLA B 603



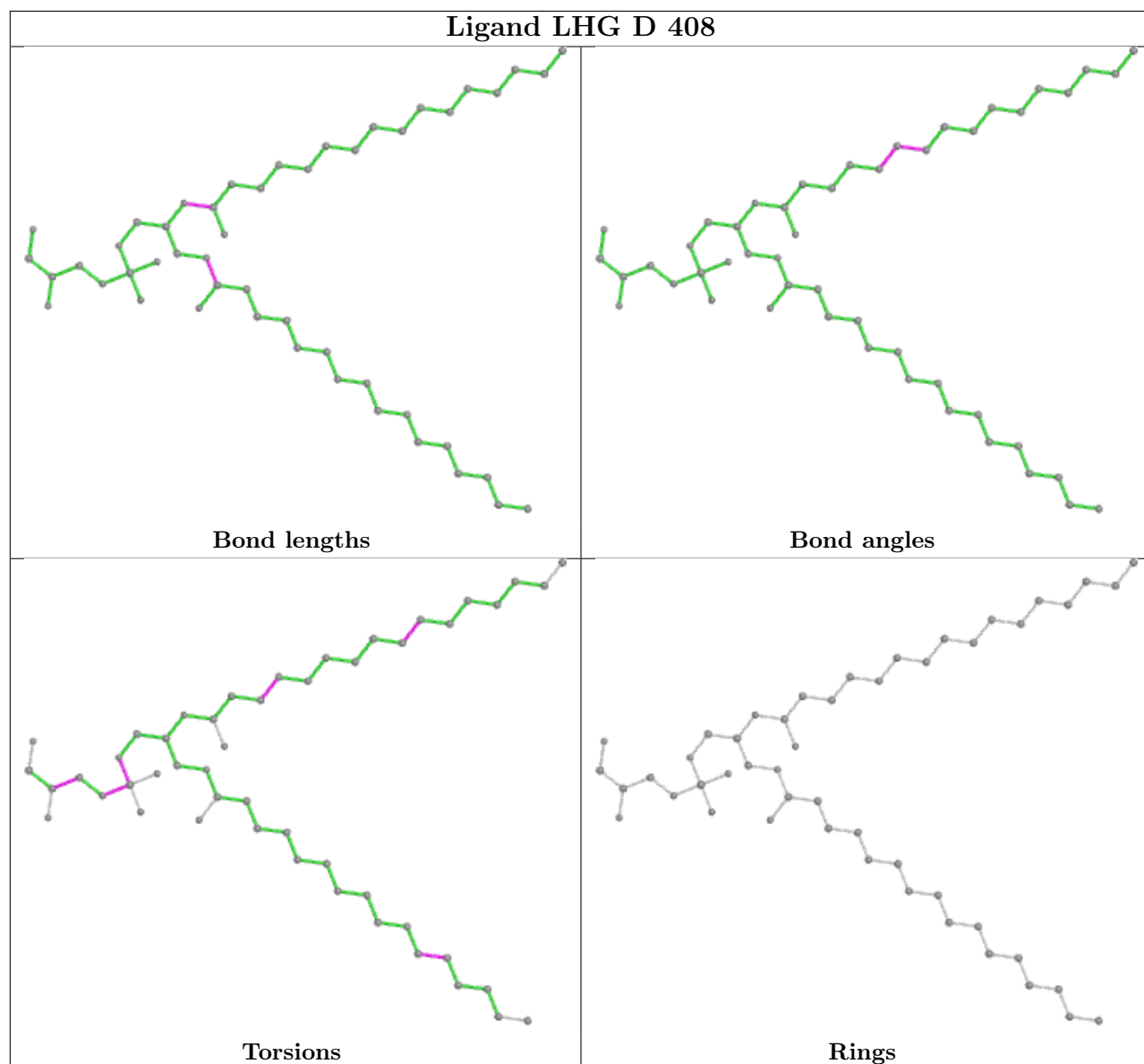
## Ligand LMG b 623



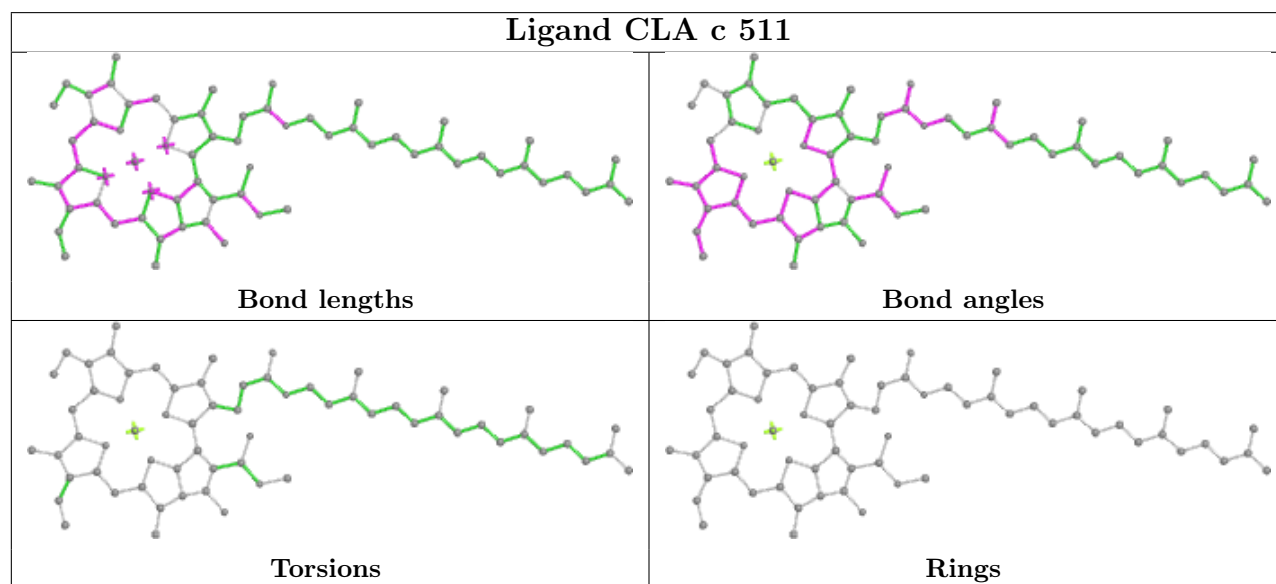
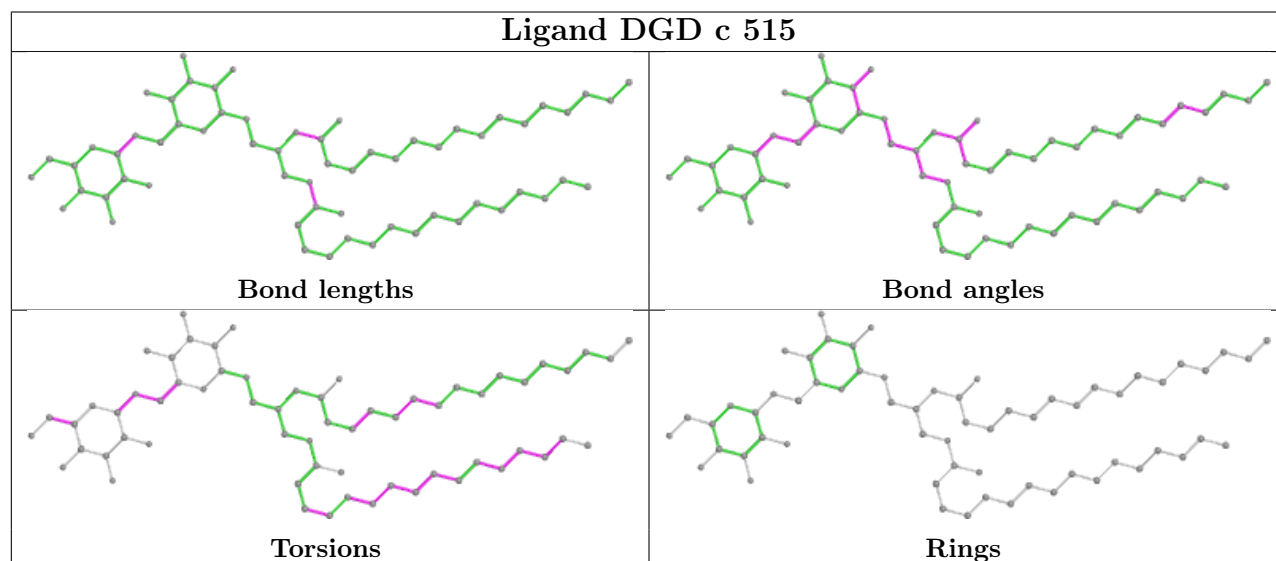
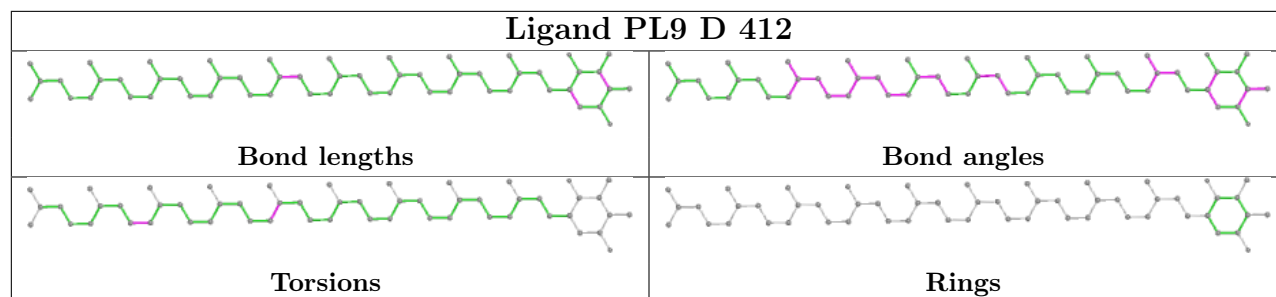
## Ligand CLA b 616



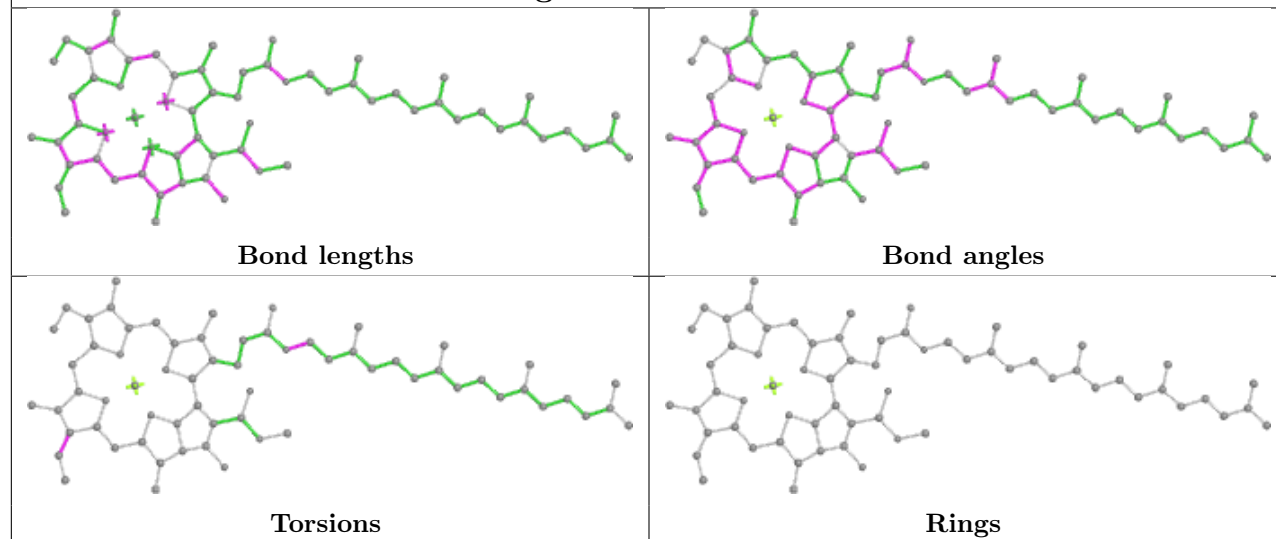
## Ligand LHG D 408



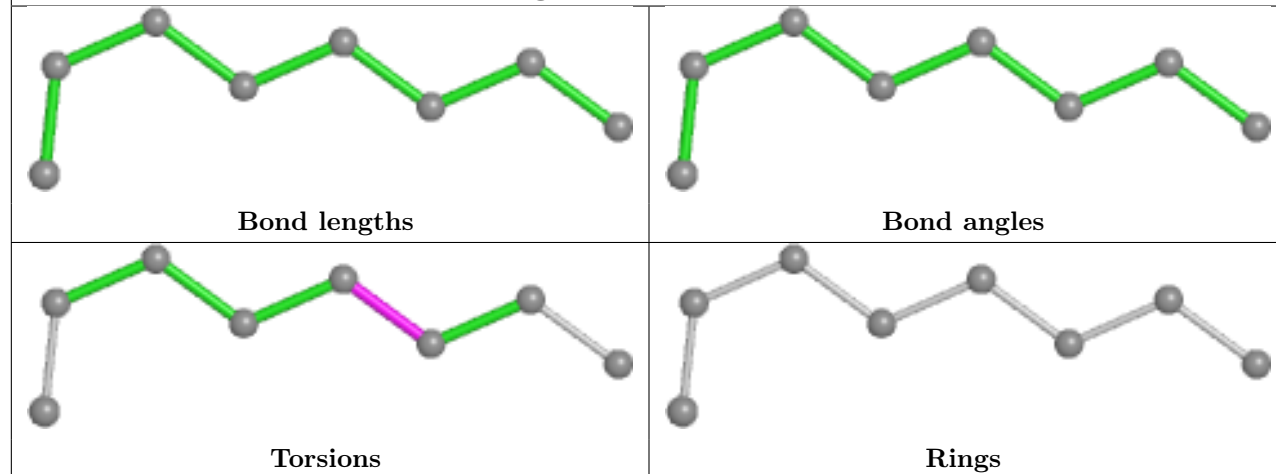




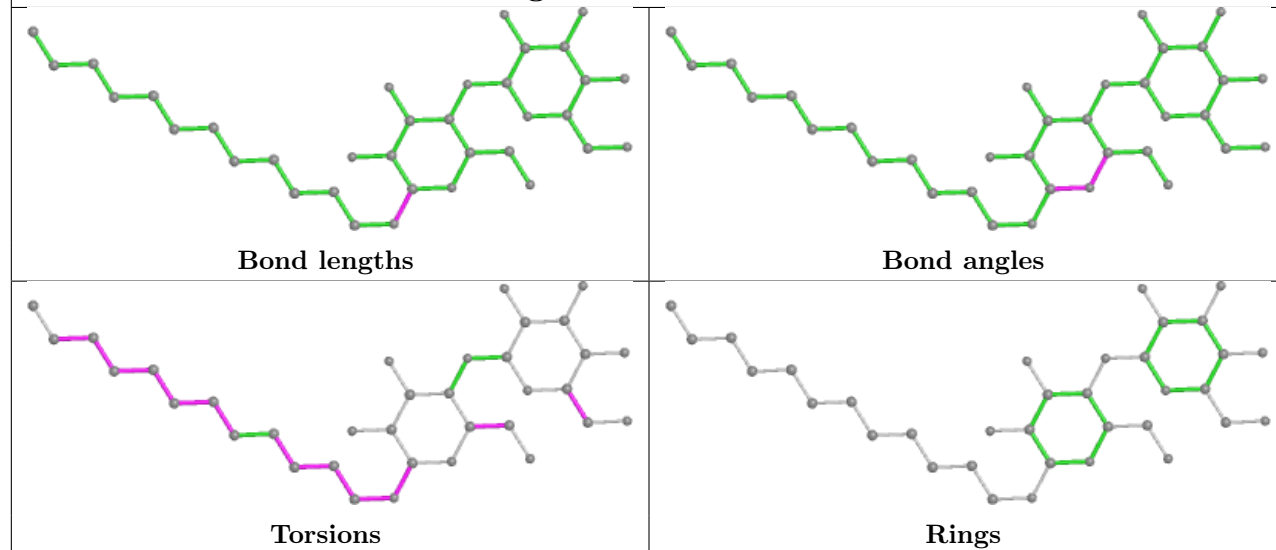
## Ligand CLA d 402

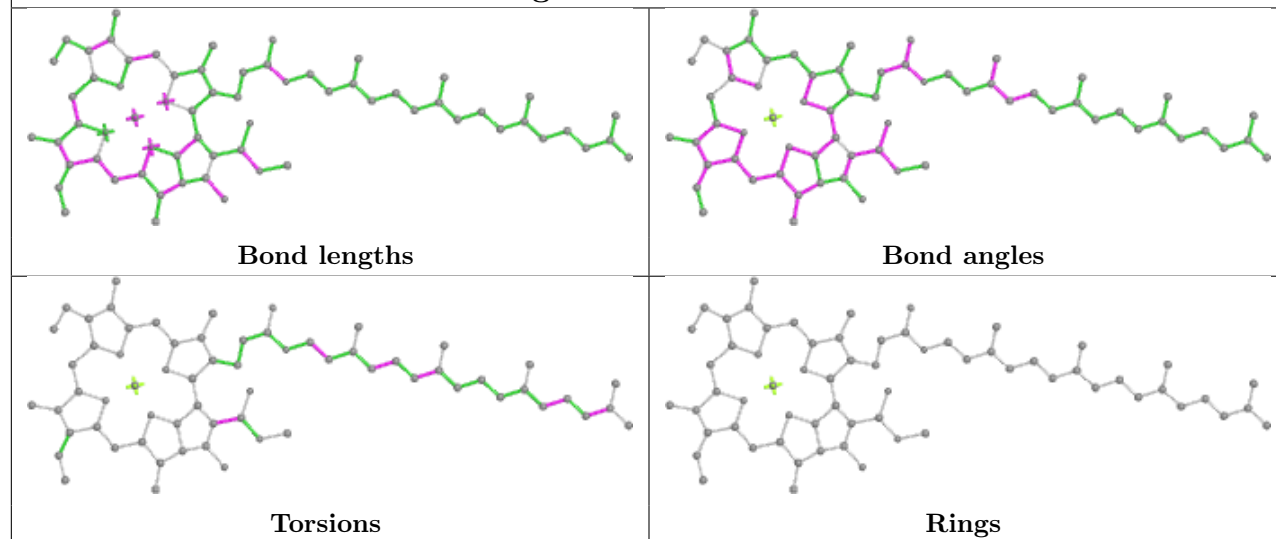
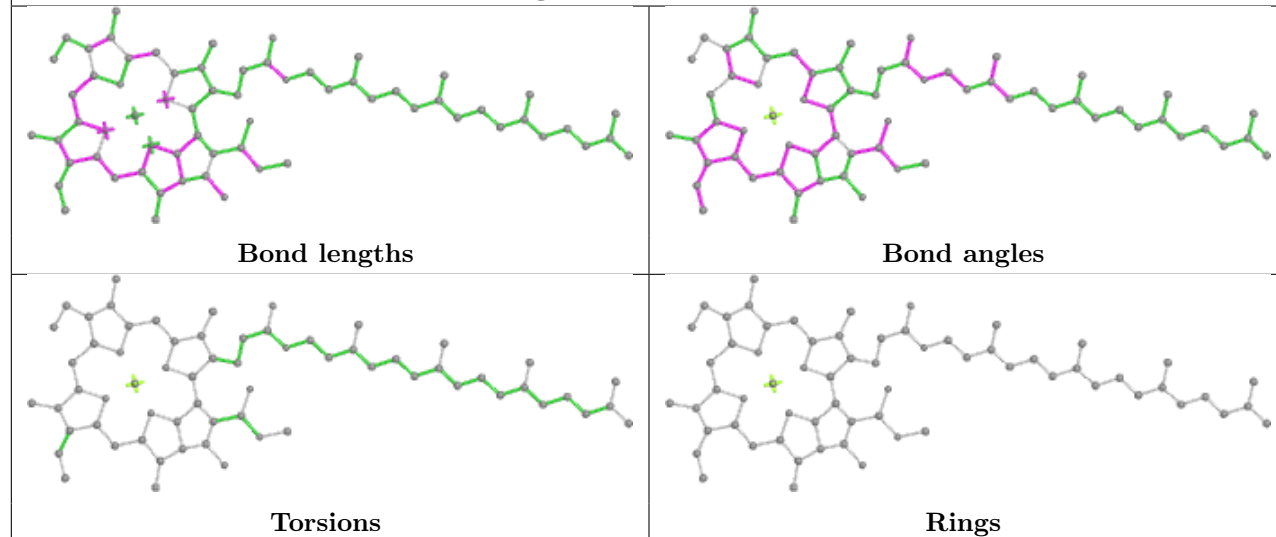


## Ligand HTG u 201

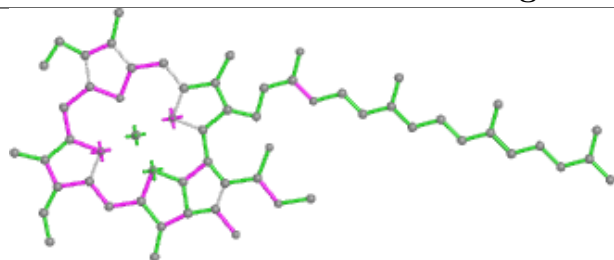


## Ligand LMT m 101

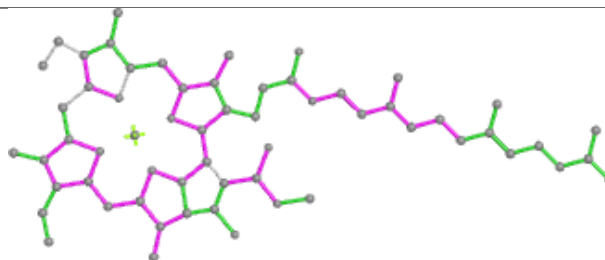


**Ligand CLA B 605****Ligand CLA C 511**

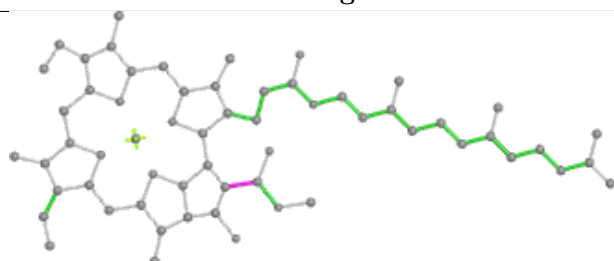
## Ligand CLA c 508



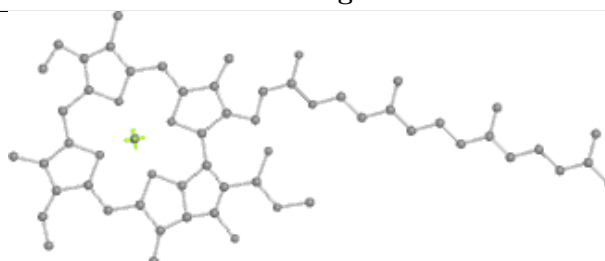
Bond lengths



Bond angles

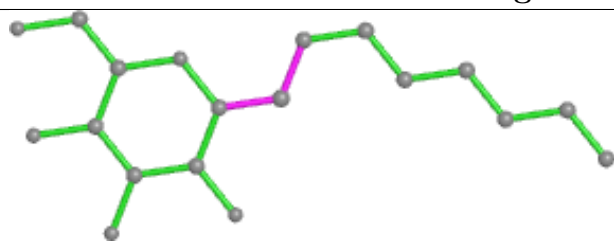


Torsions

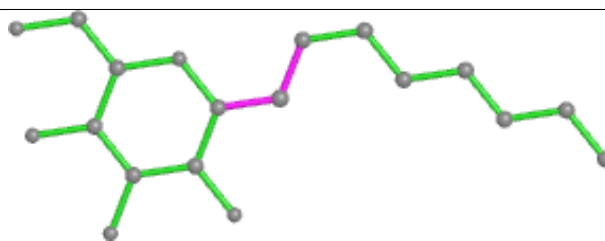


Rings

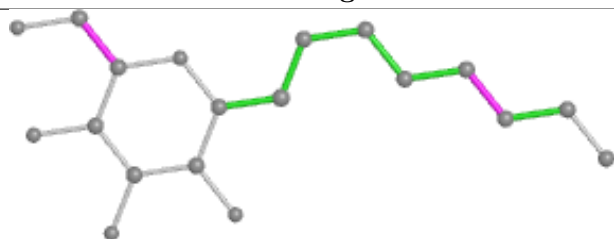
## Ligand HTG b 602



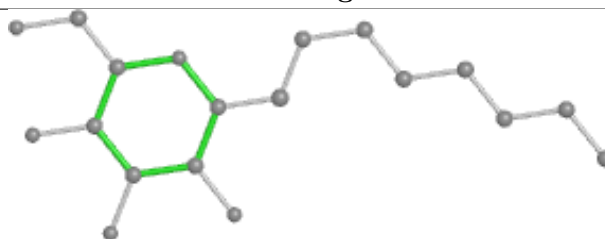
Bond lengths



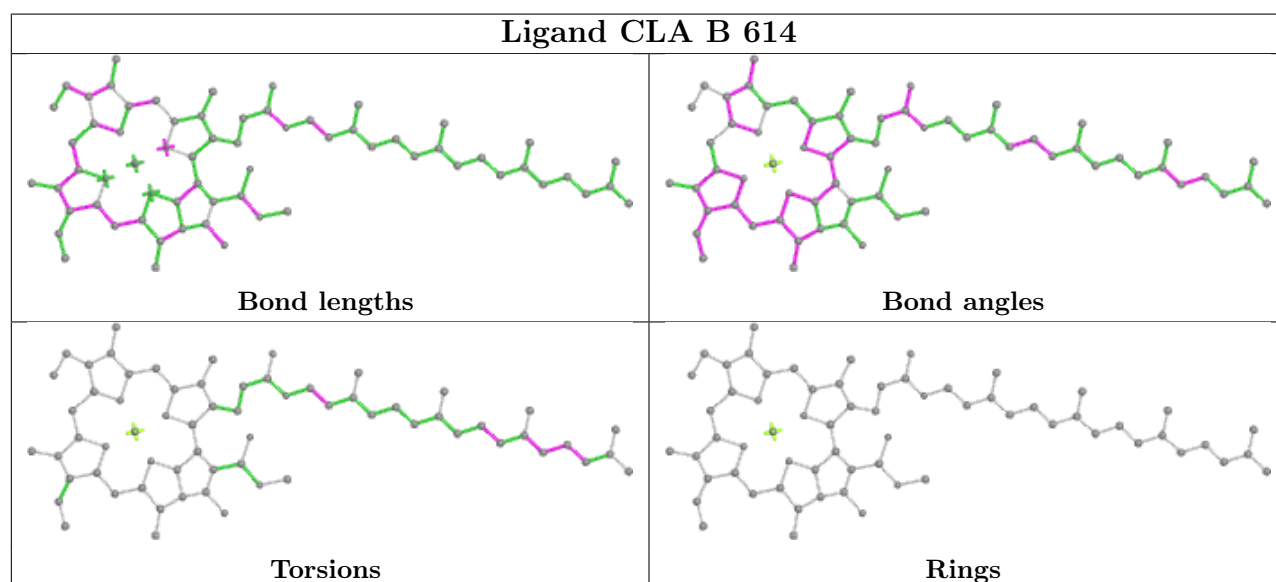
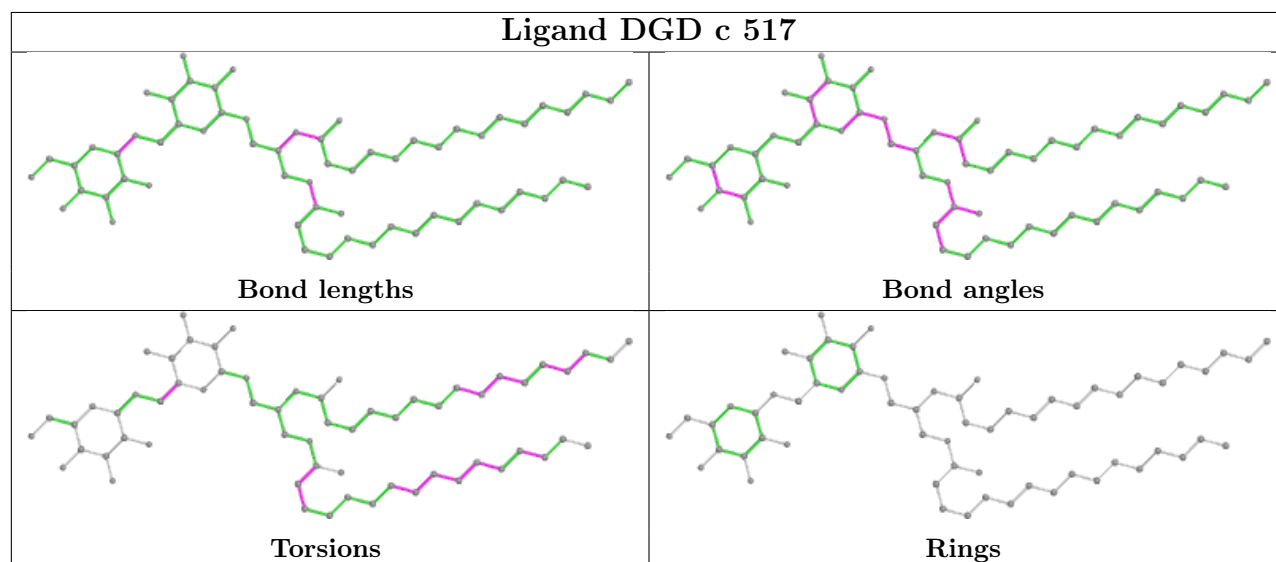
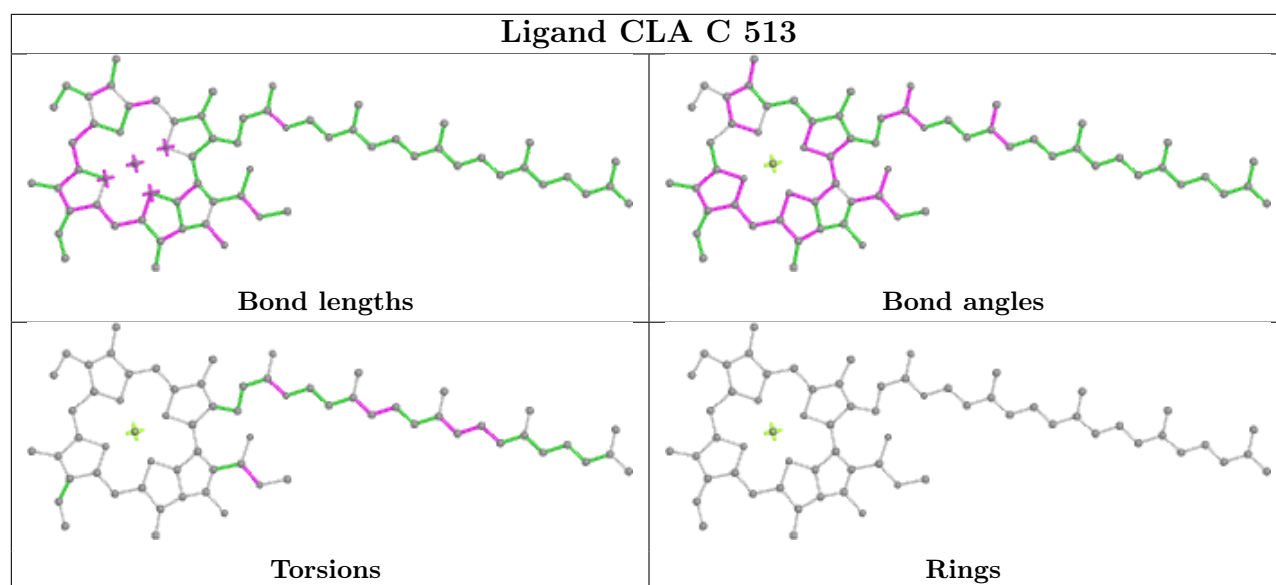
Bond angles



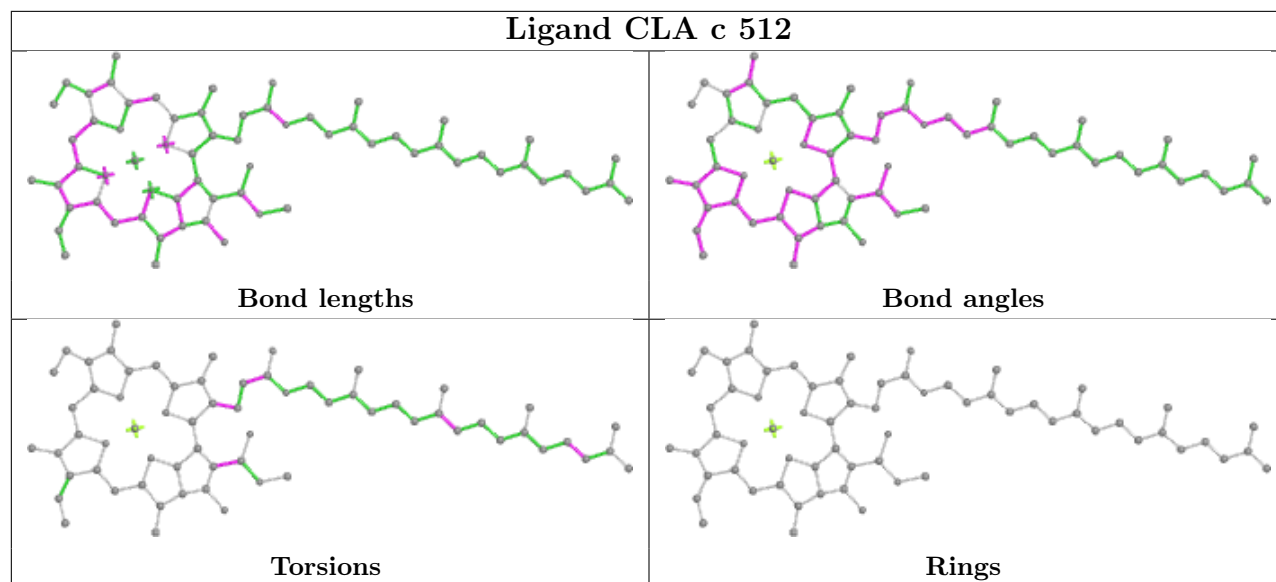
Torsions



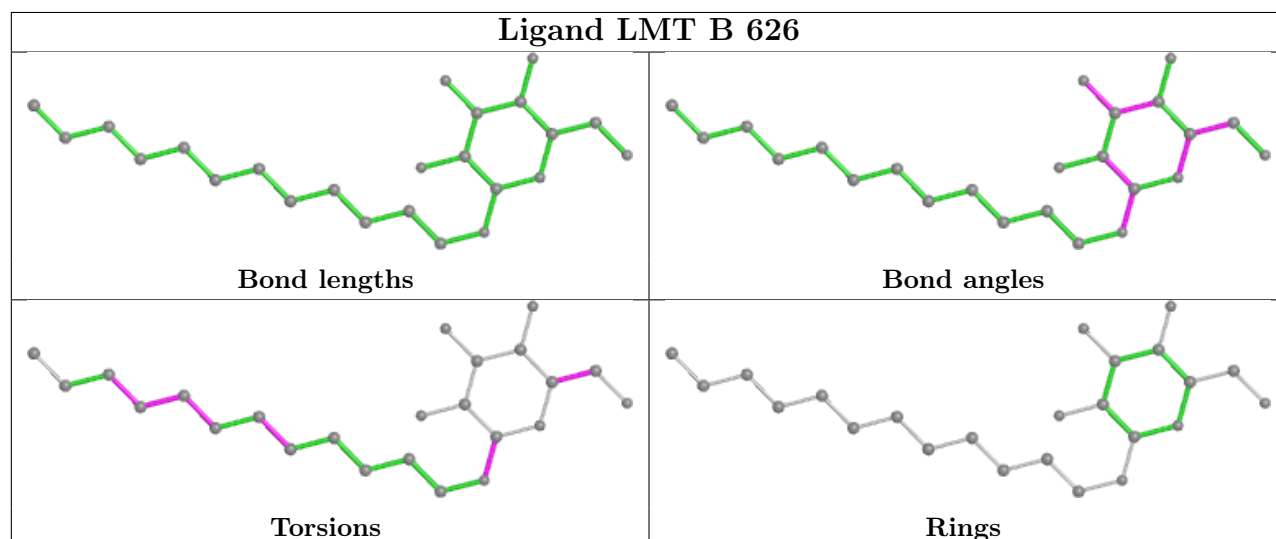
Rings



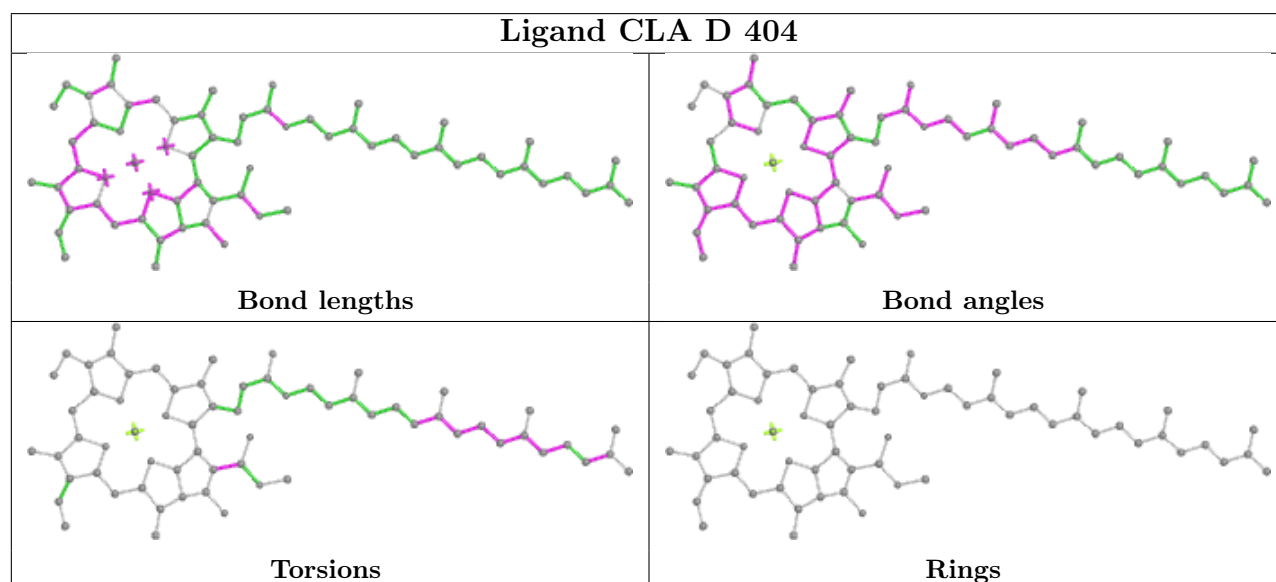
## Ligand CLA c 512



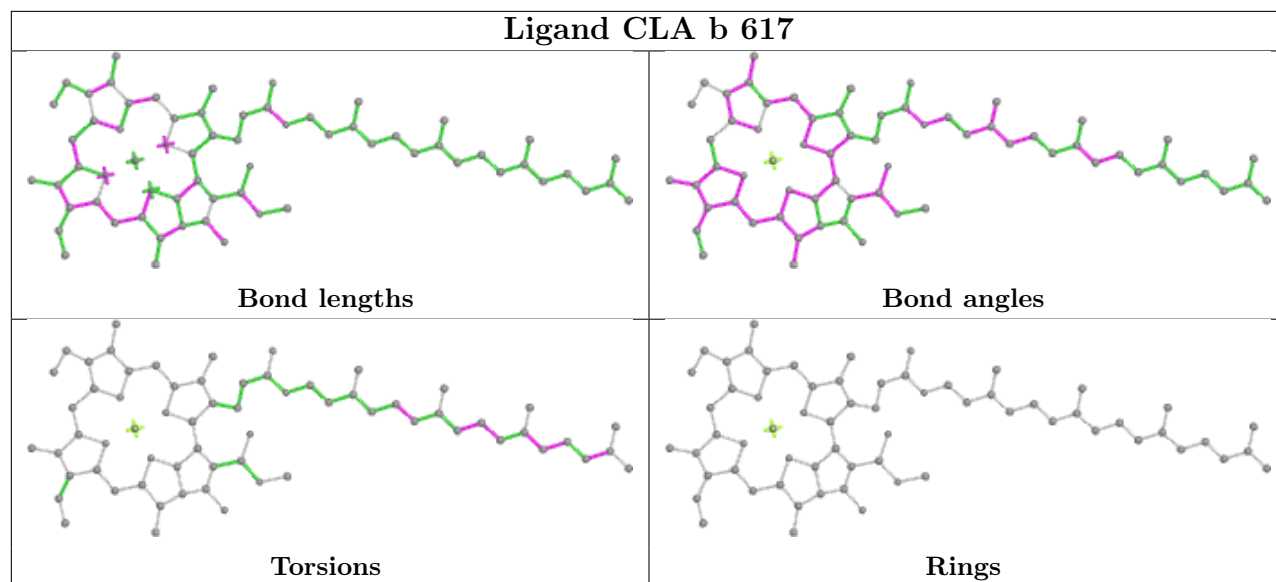
## Ligand LMT B 626



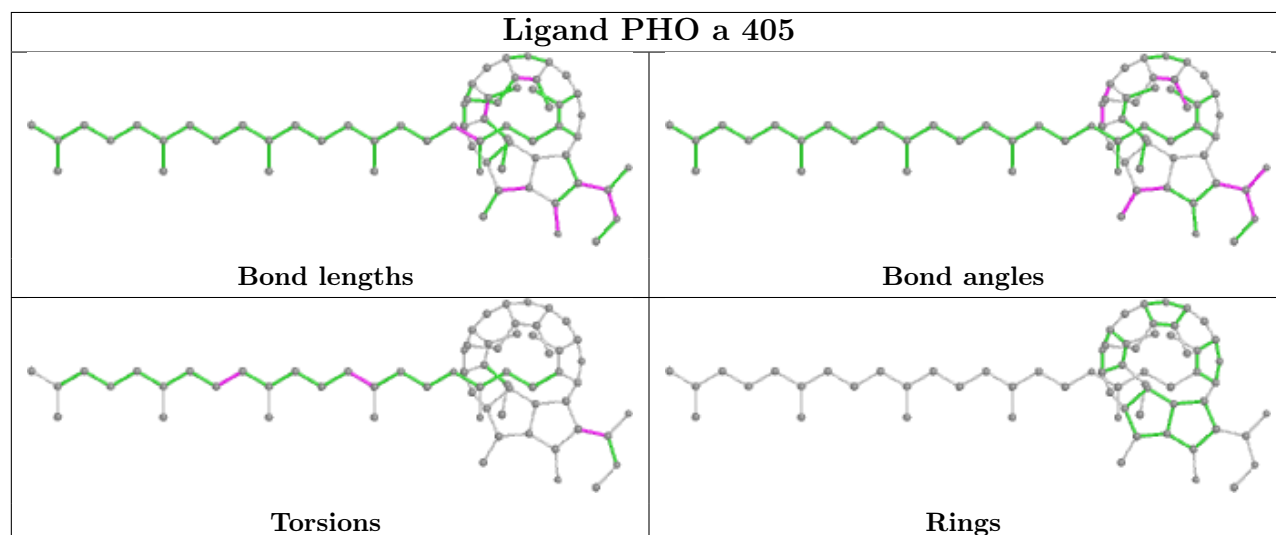
## Ligand CLA D 404



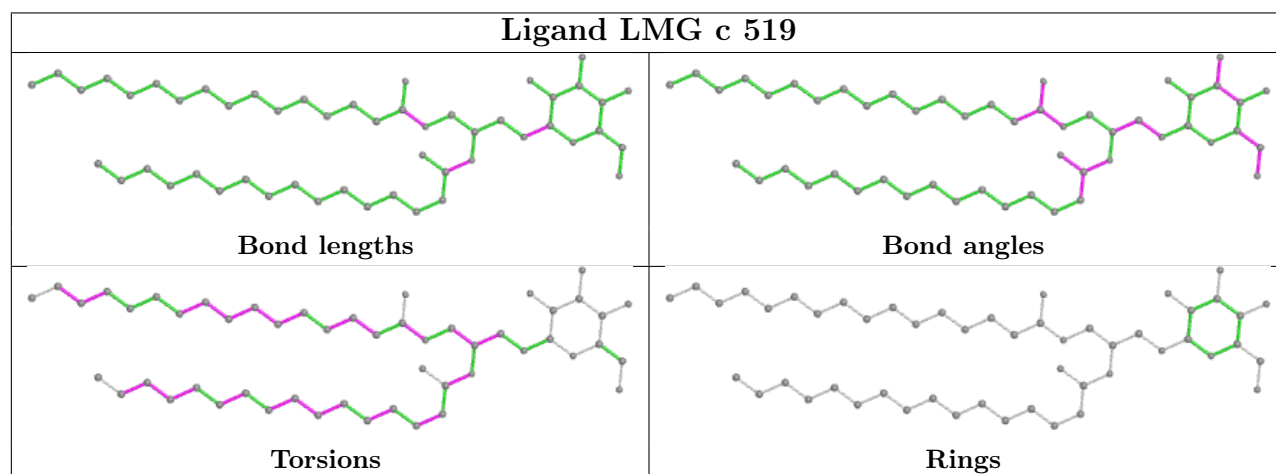
## Ligand CLA b 617



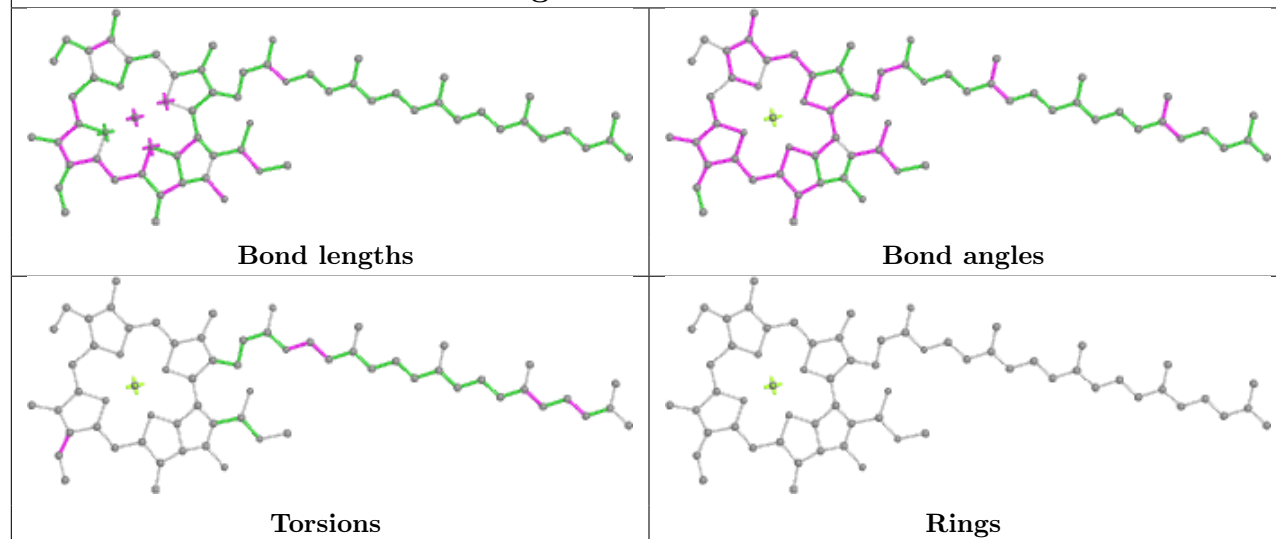
## Ligand PHO a 405



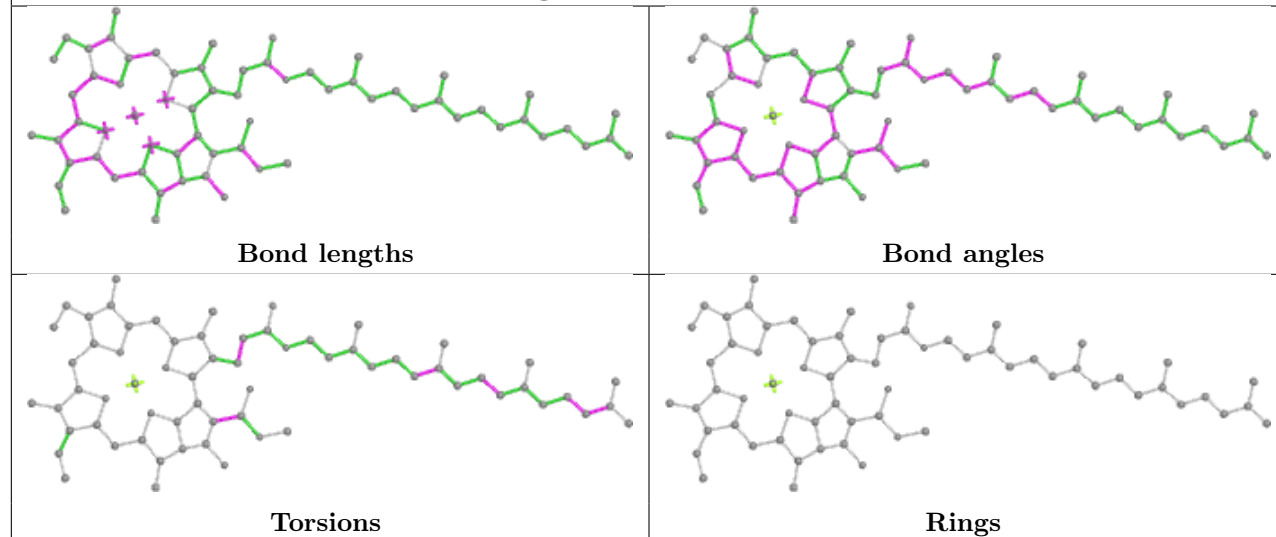
## Ligand LMG c 519



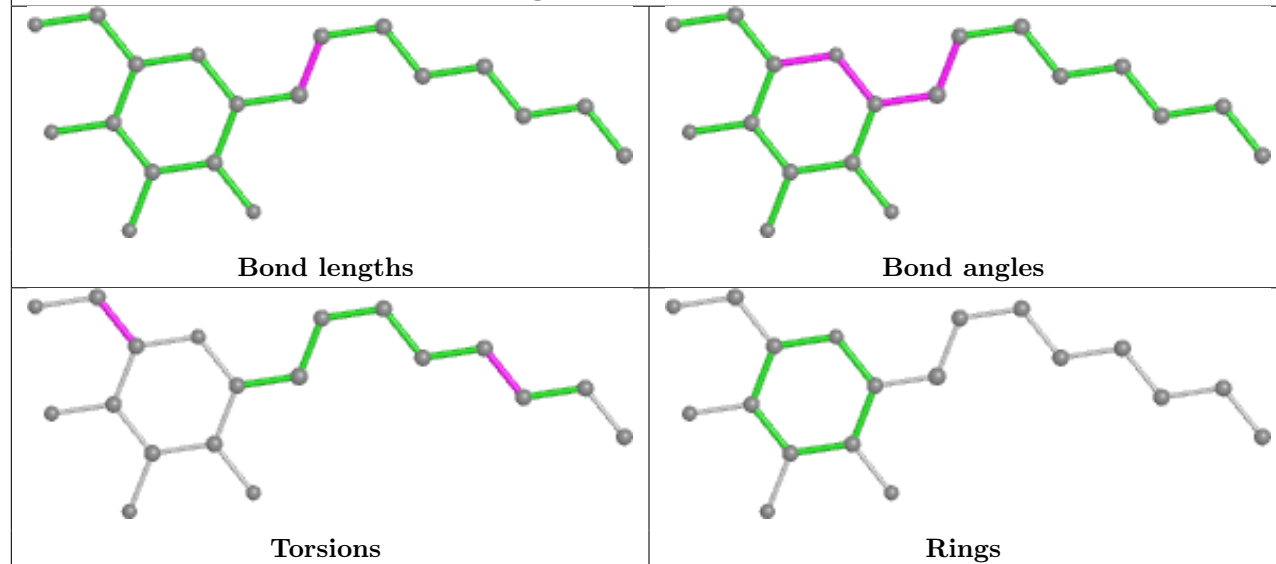
## Ligand CLA D 401



## Ligand CLA b 608

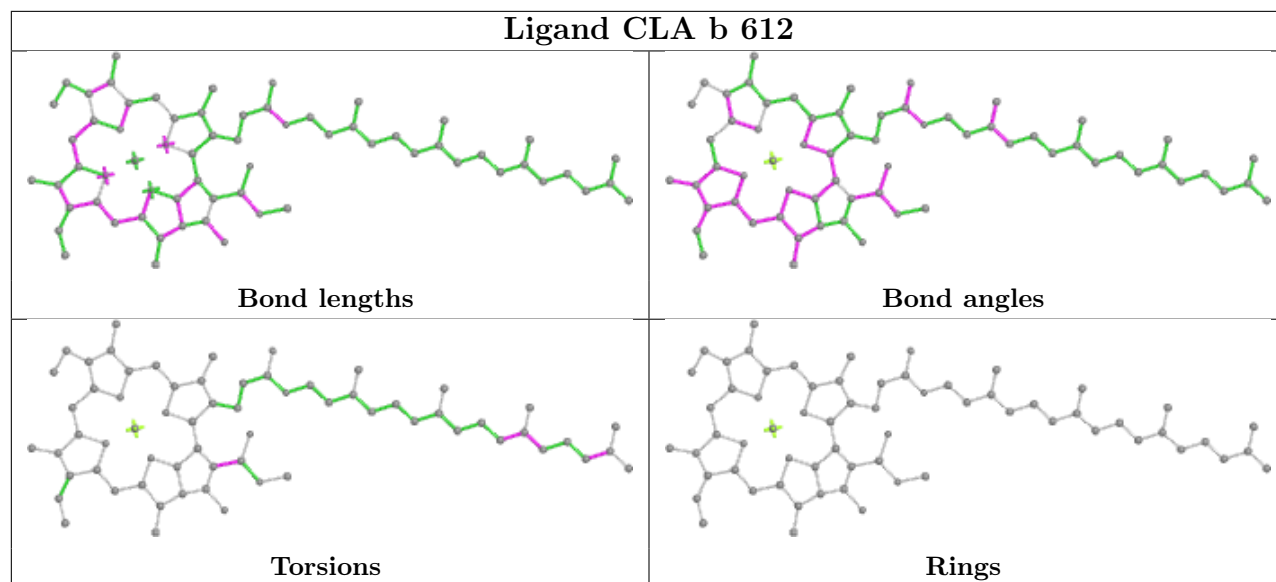


## Ligand HTG B 632

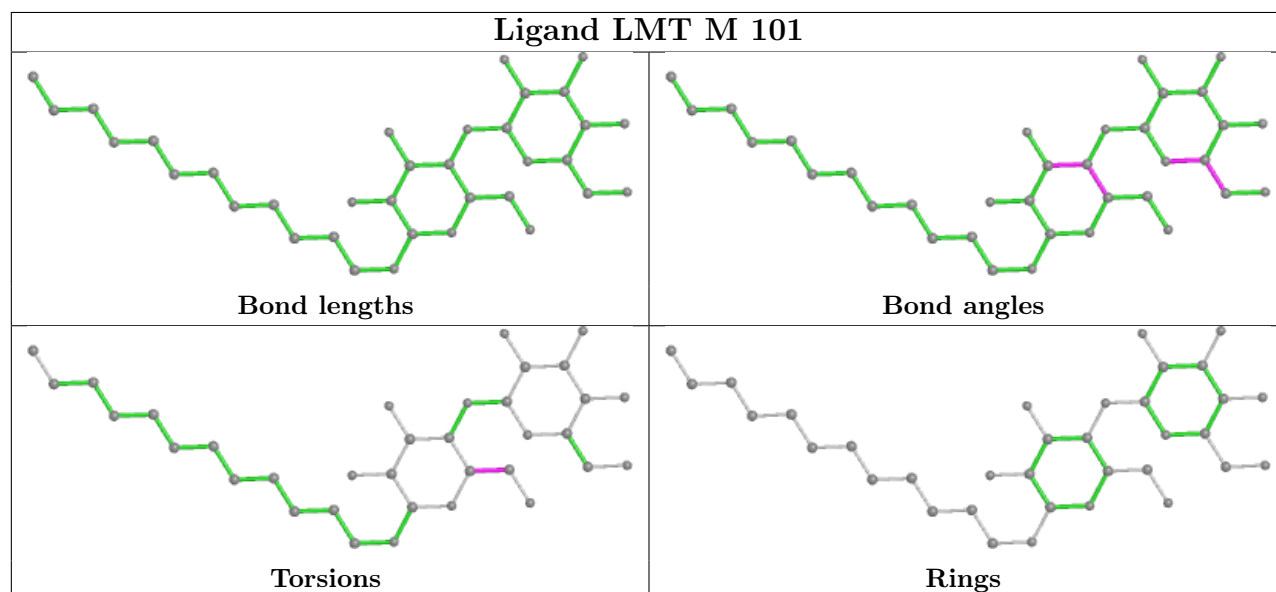




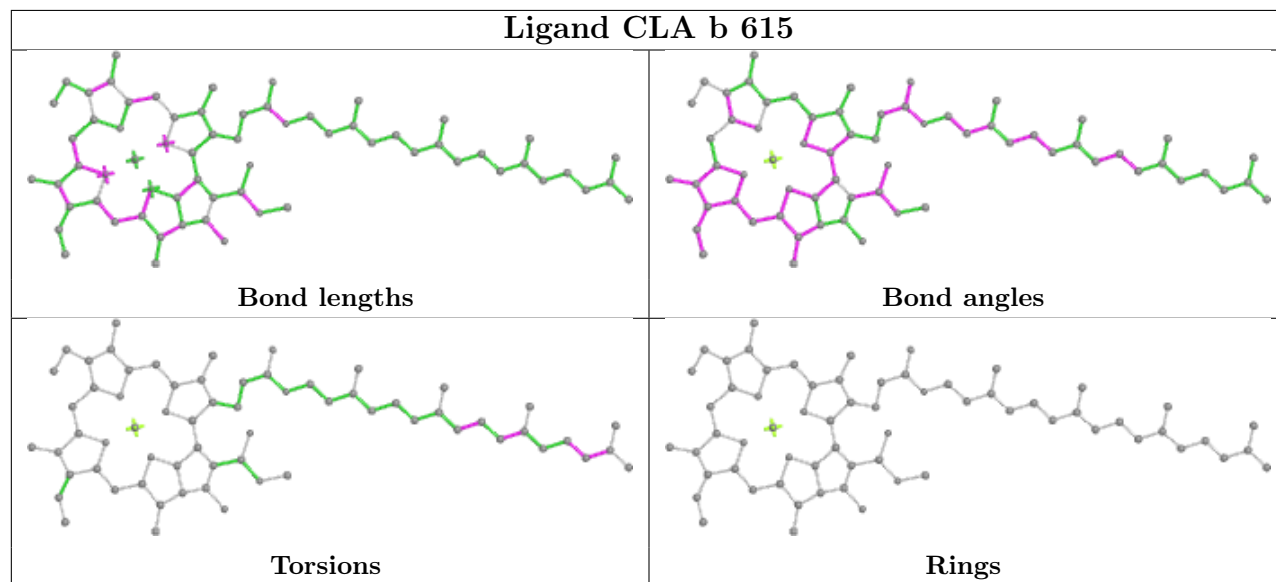
## Ligand CLA b 612

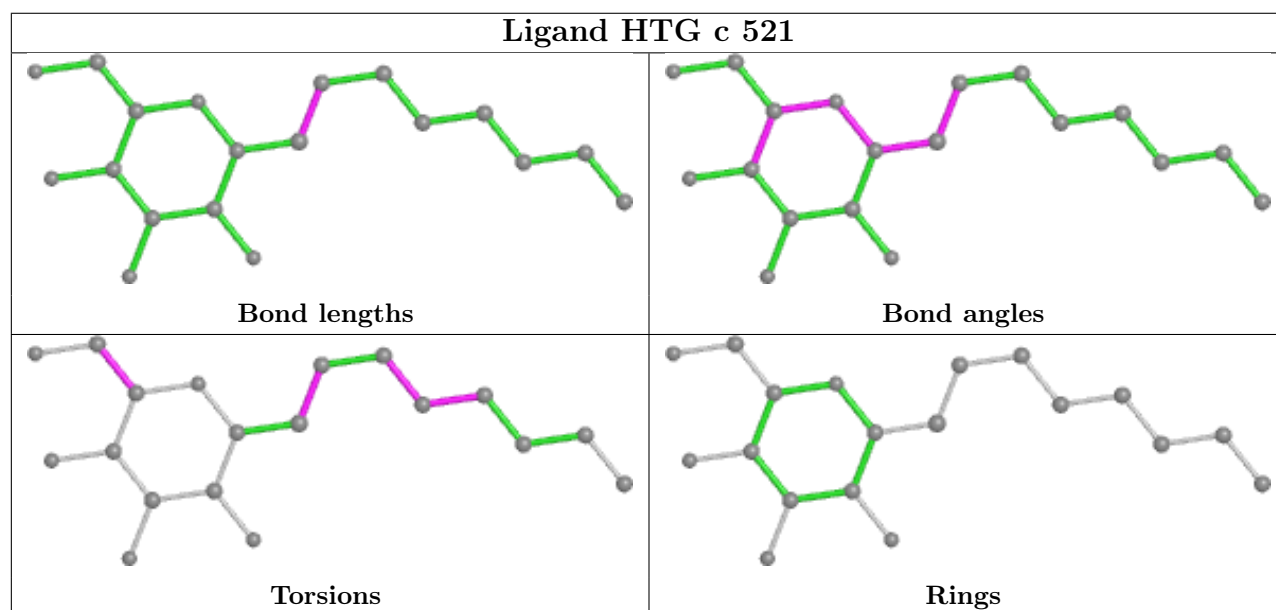
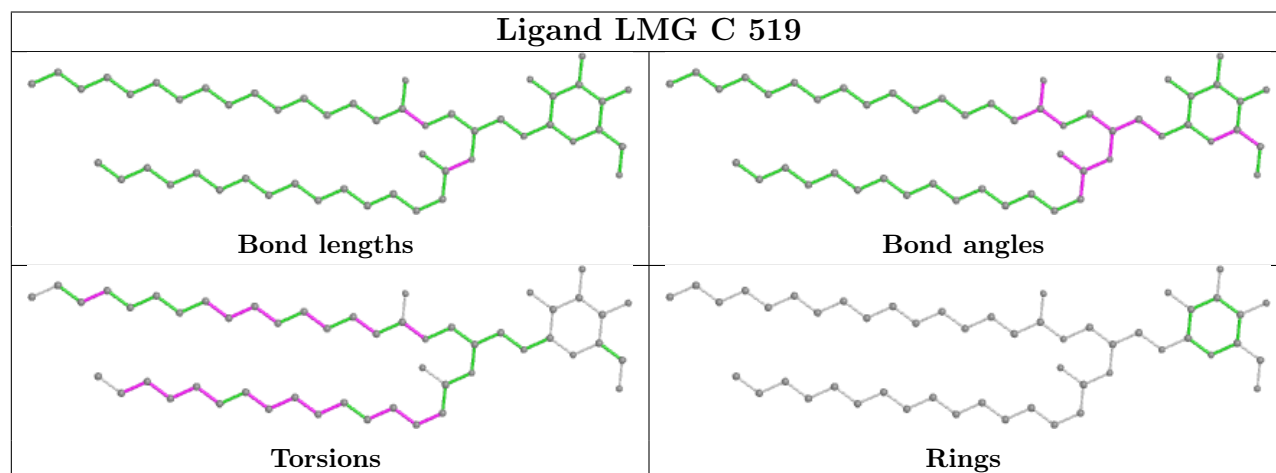
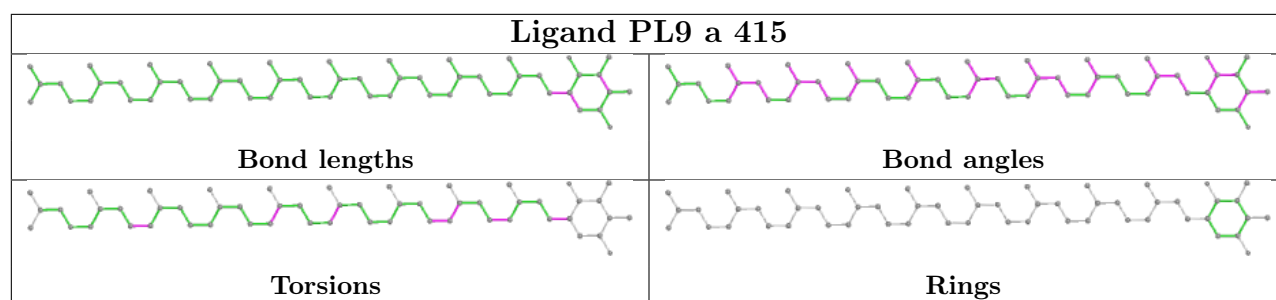


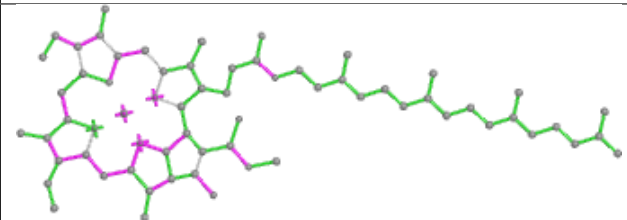
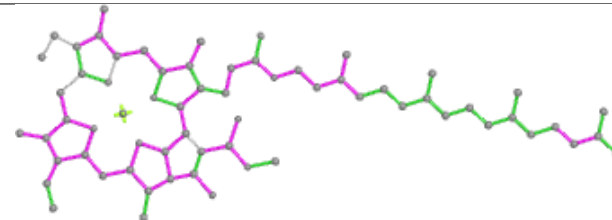
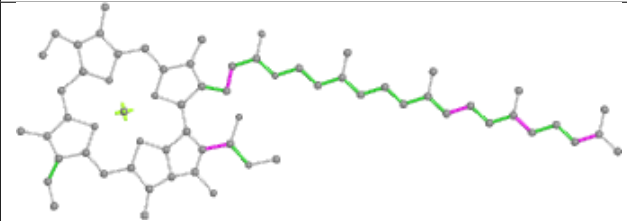
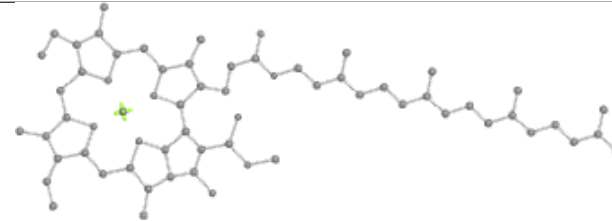
## Ligand LMT M 101

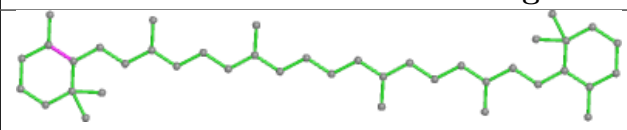
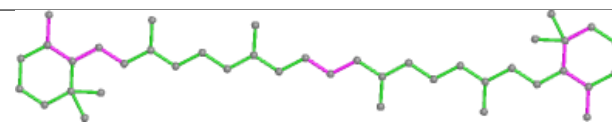
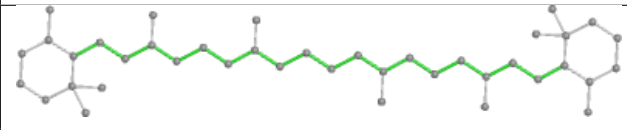
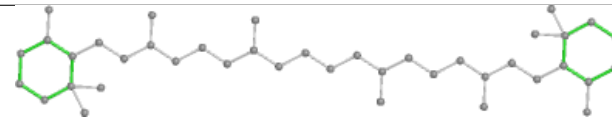


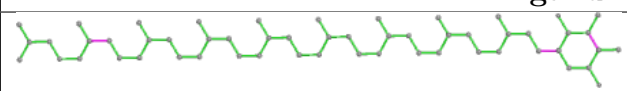
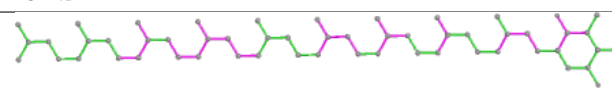
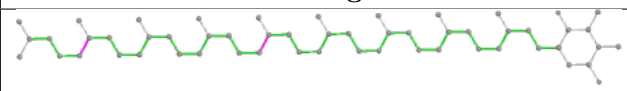
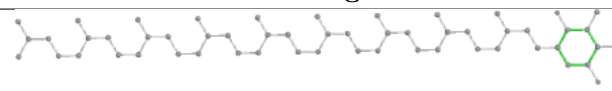
## Ligand CLA b 615

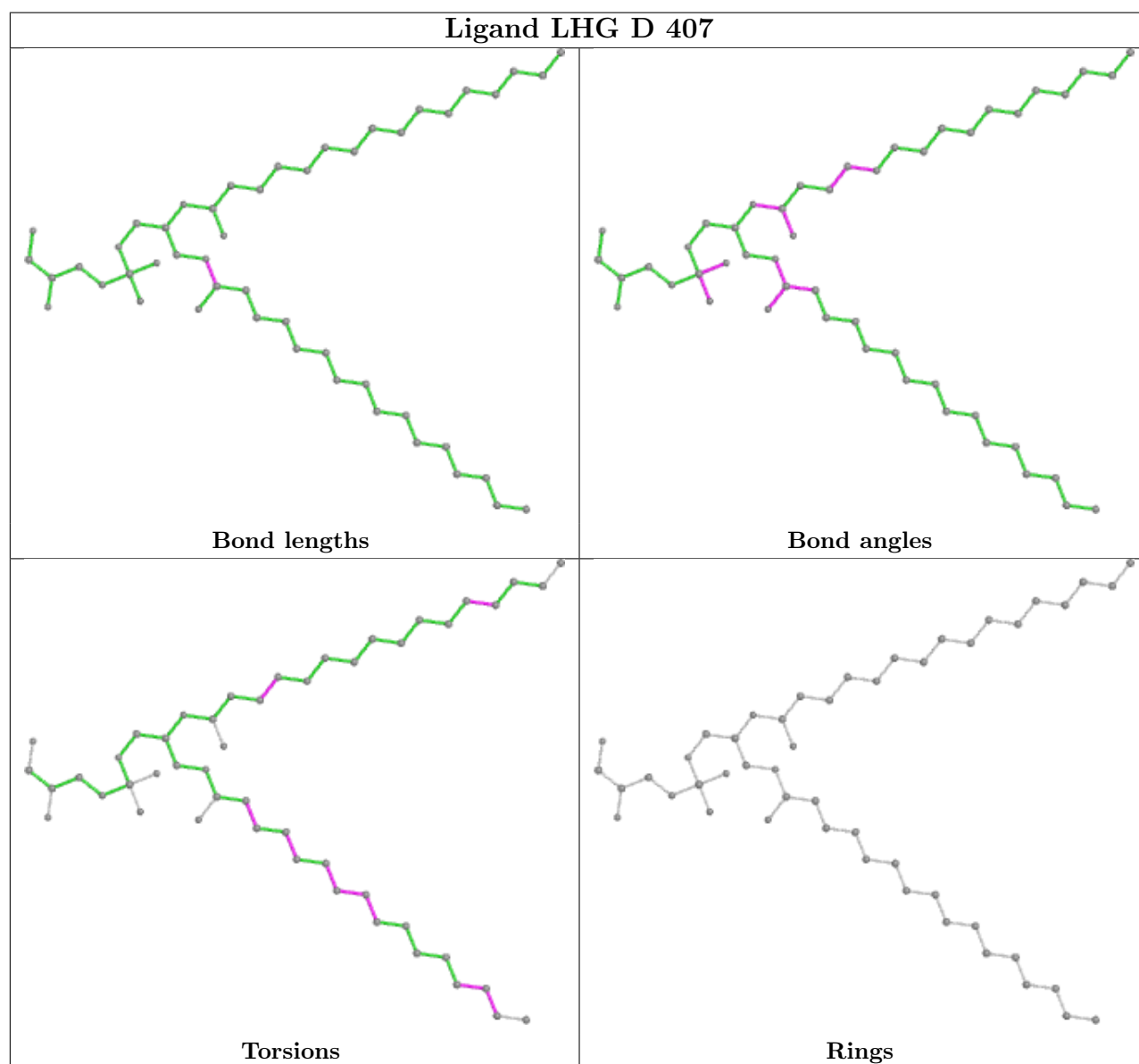
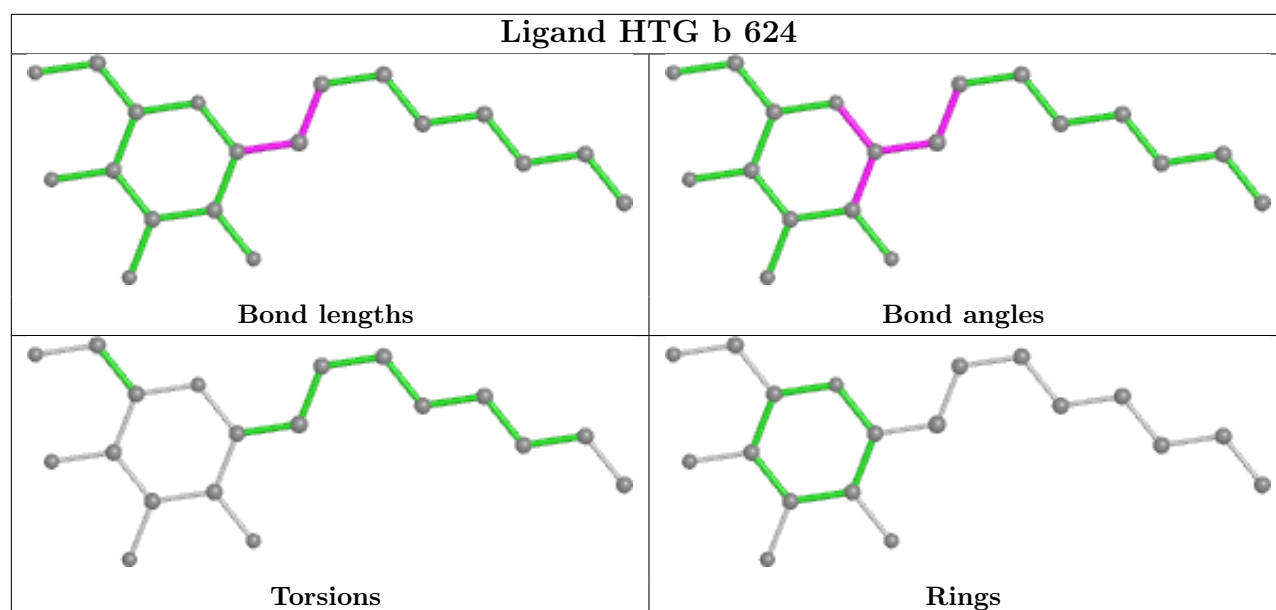


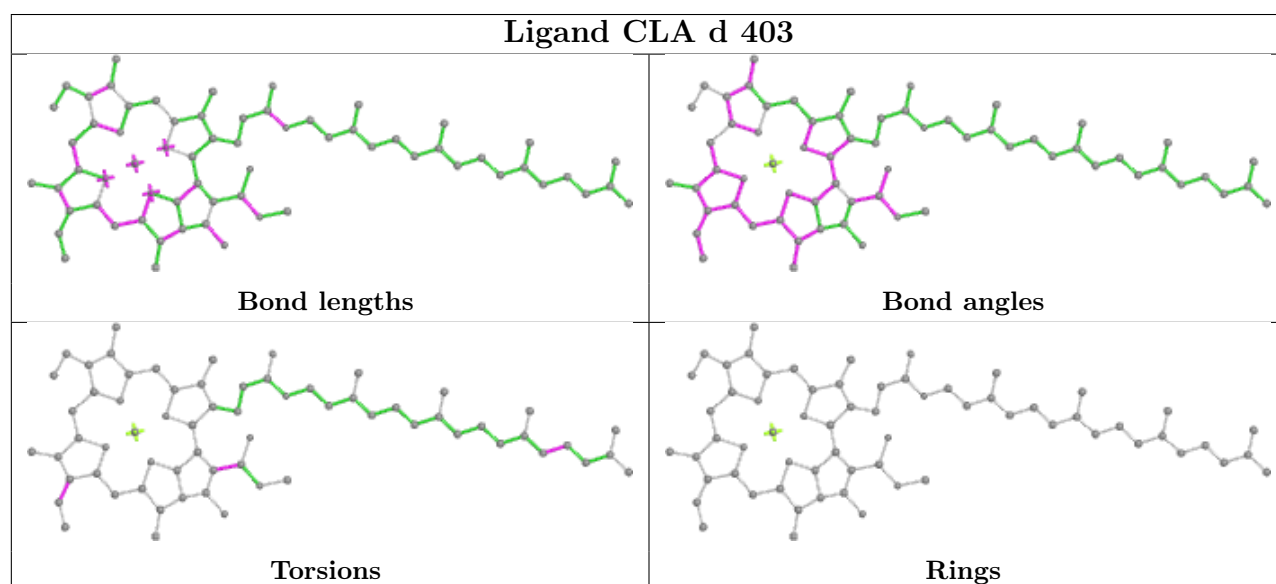
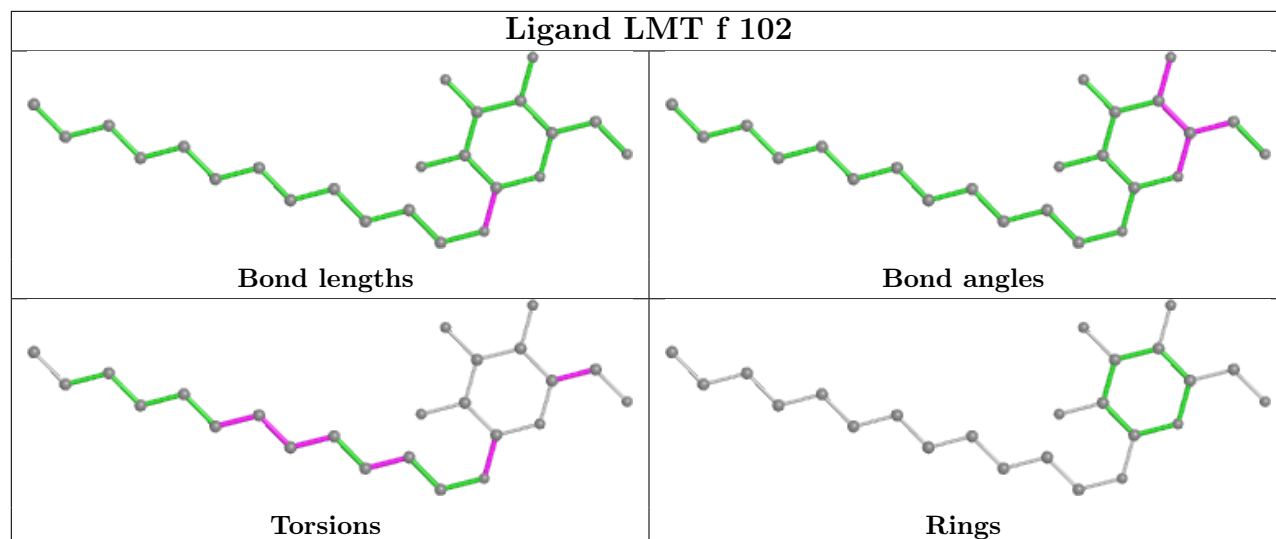


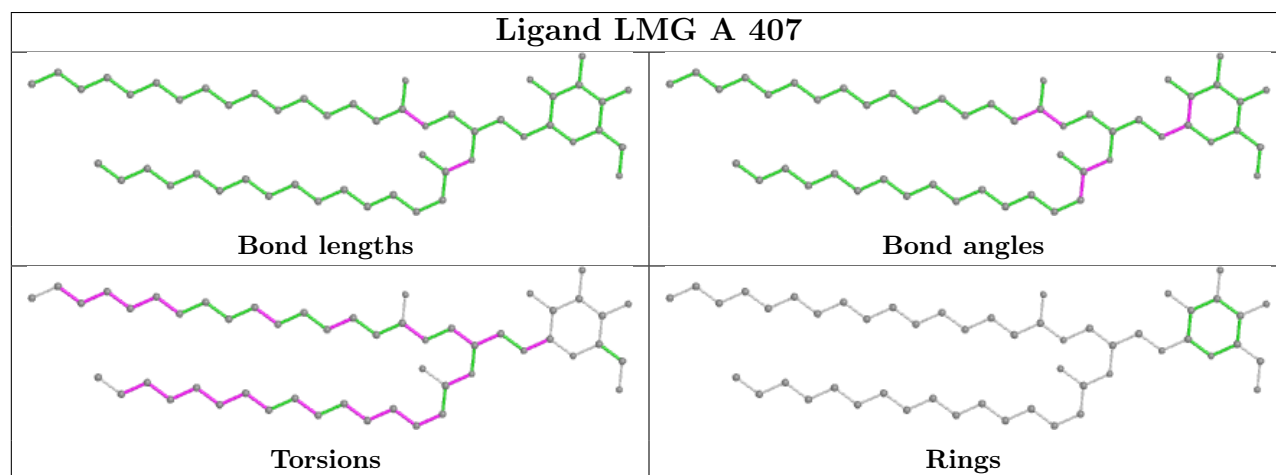
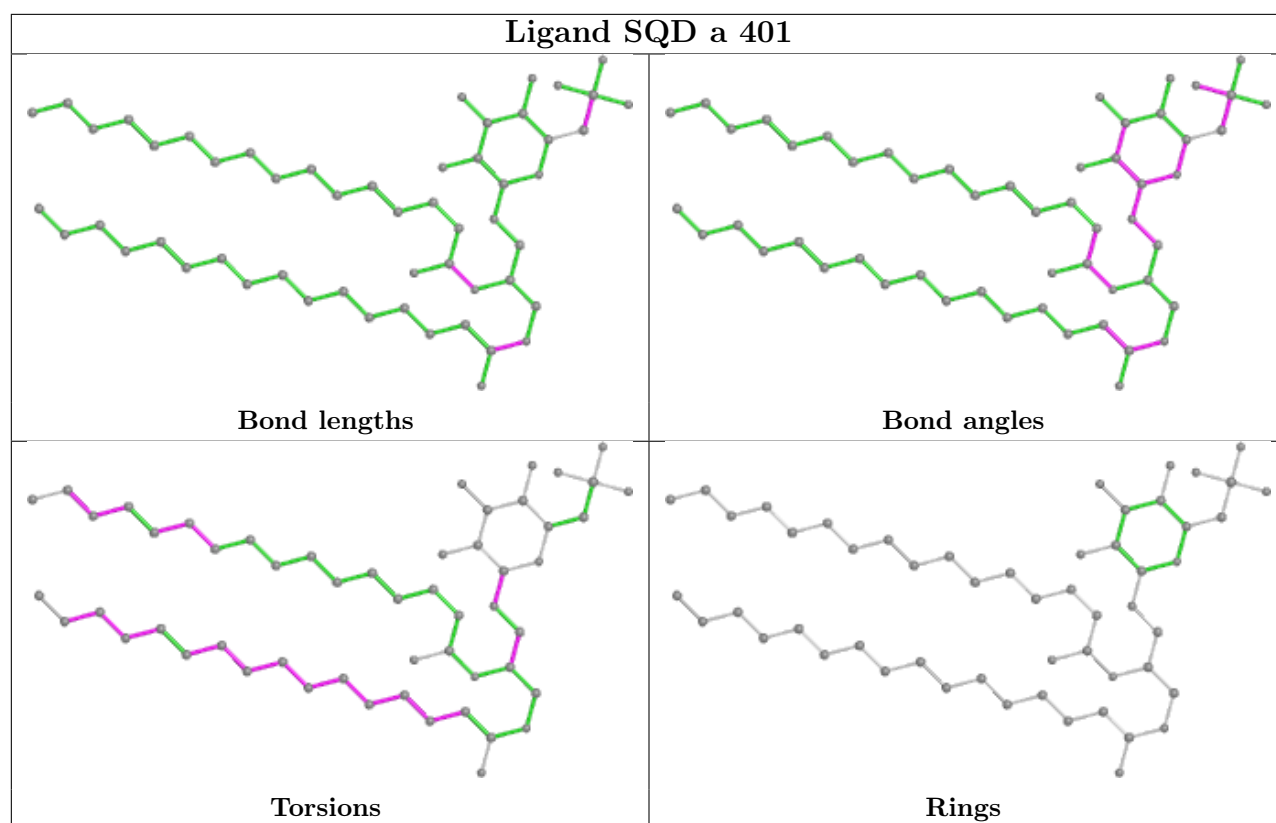
Ligand CLA b 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

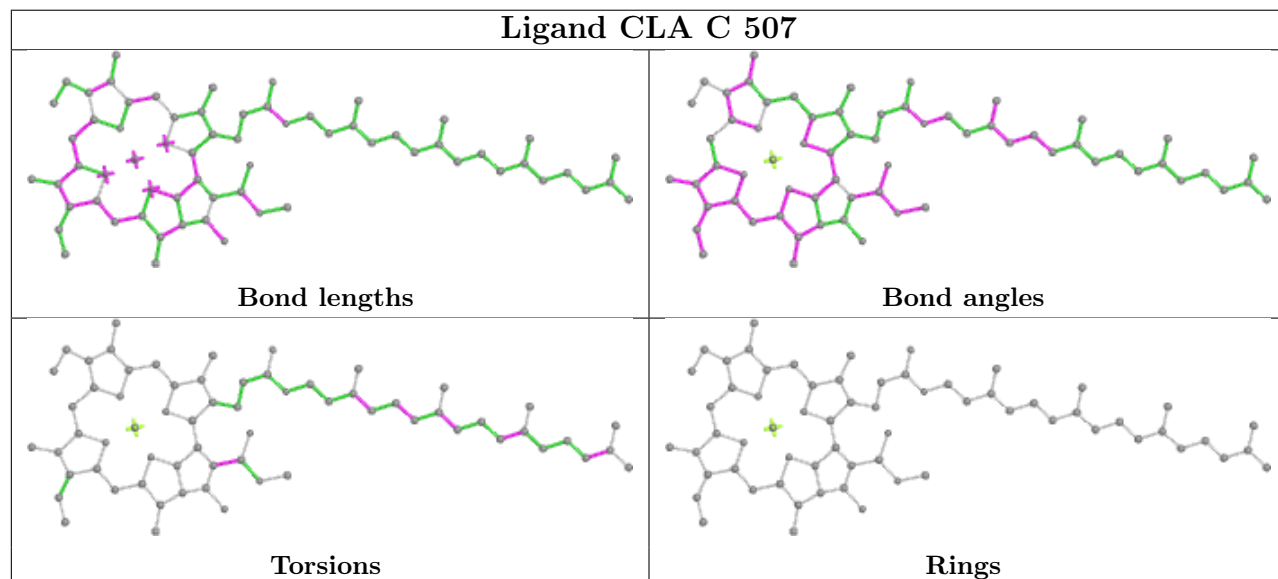
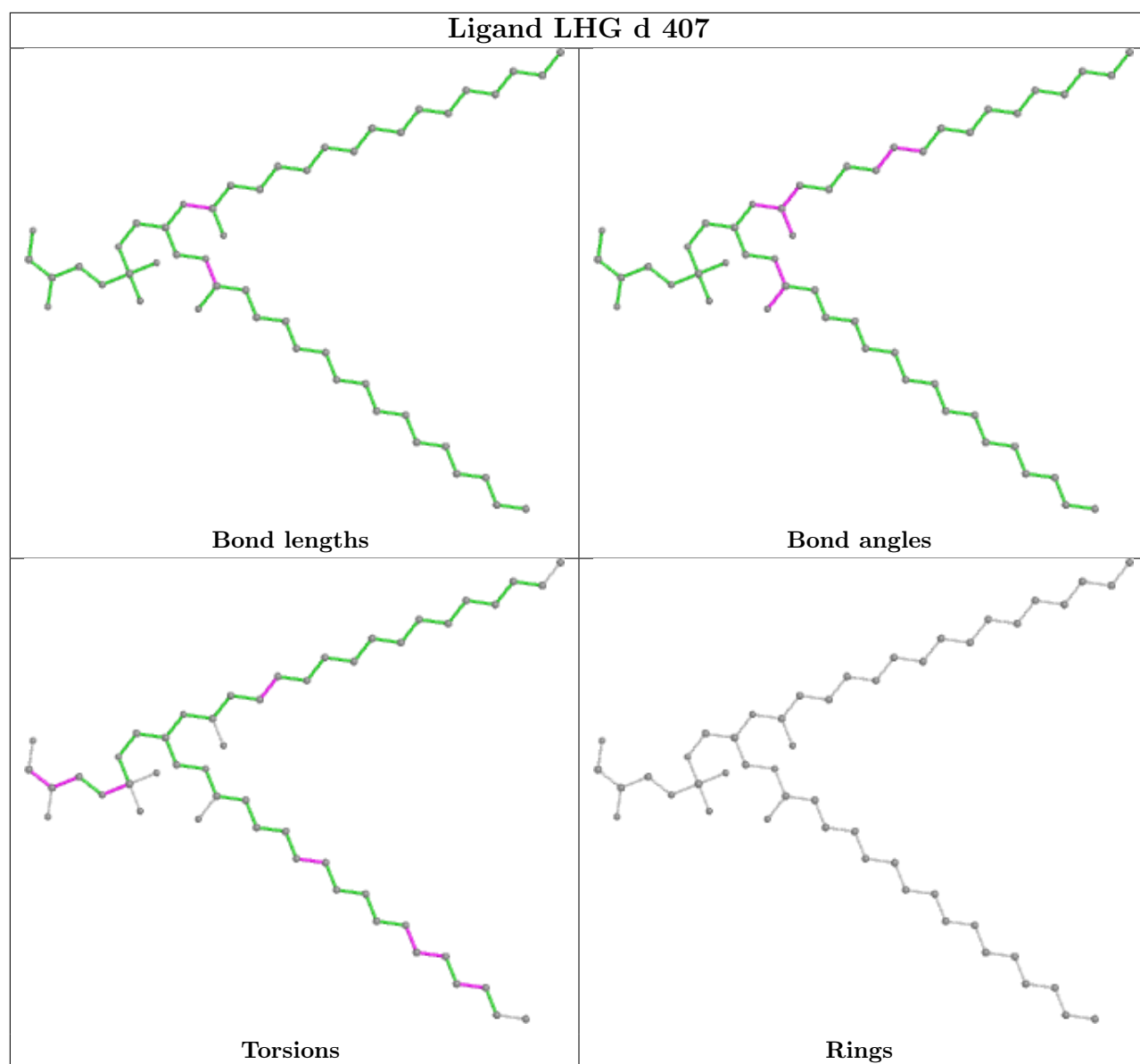
Ligand BCR b 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

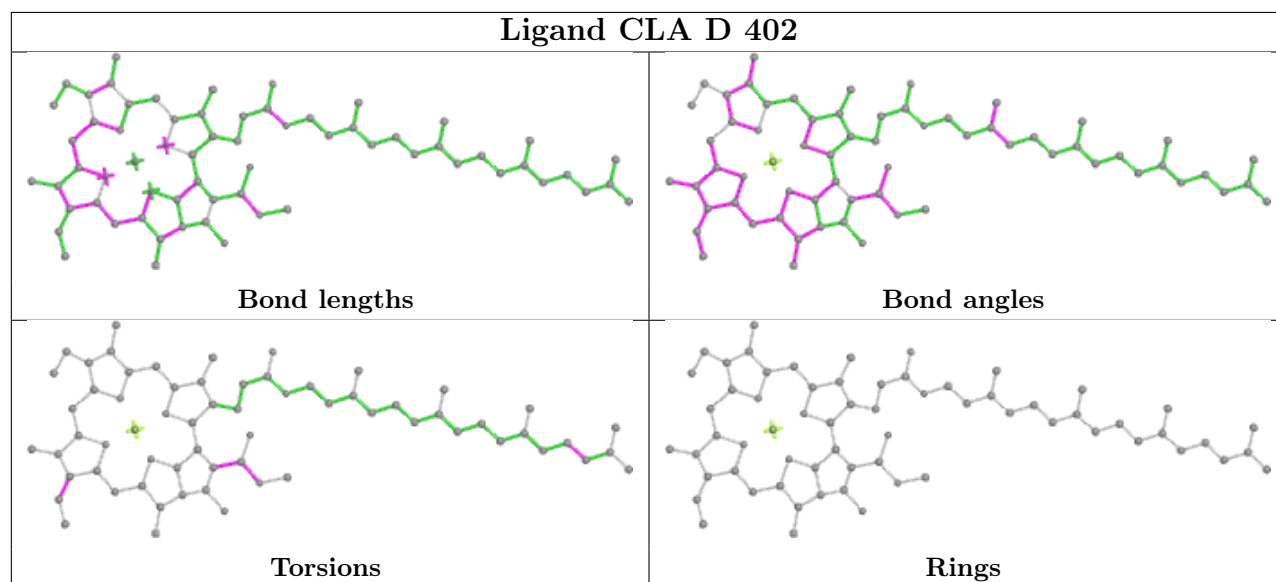
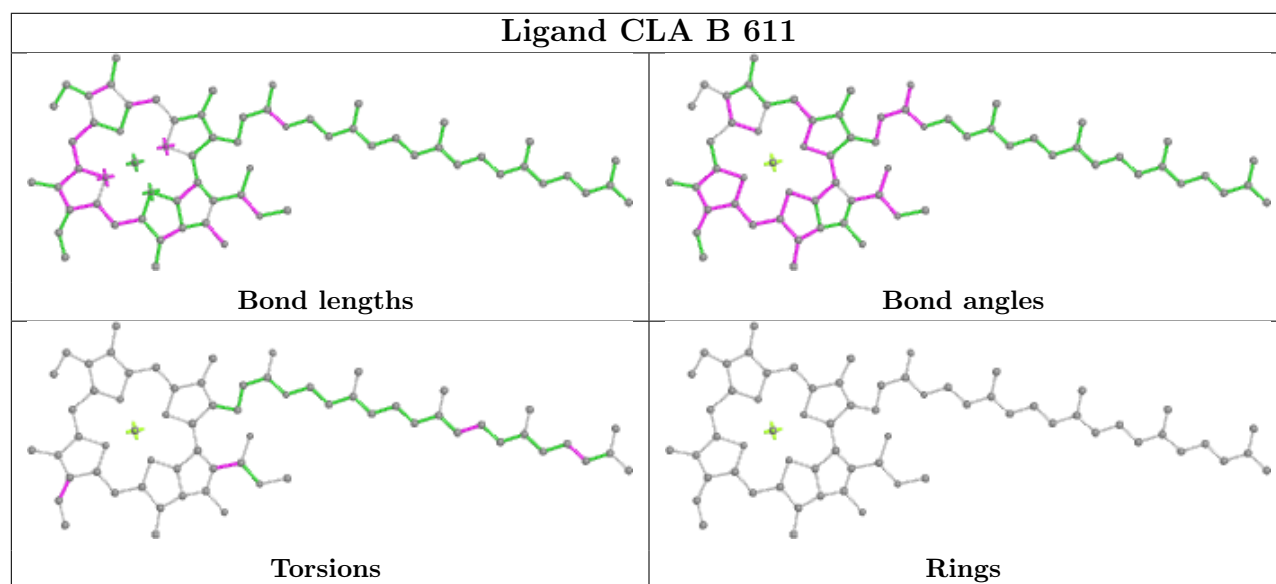
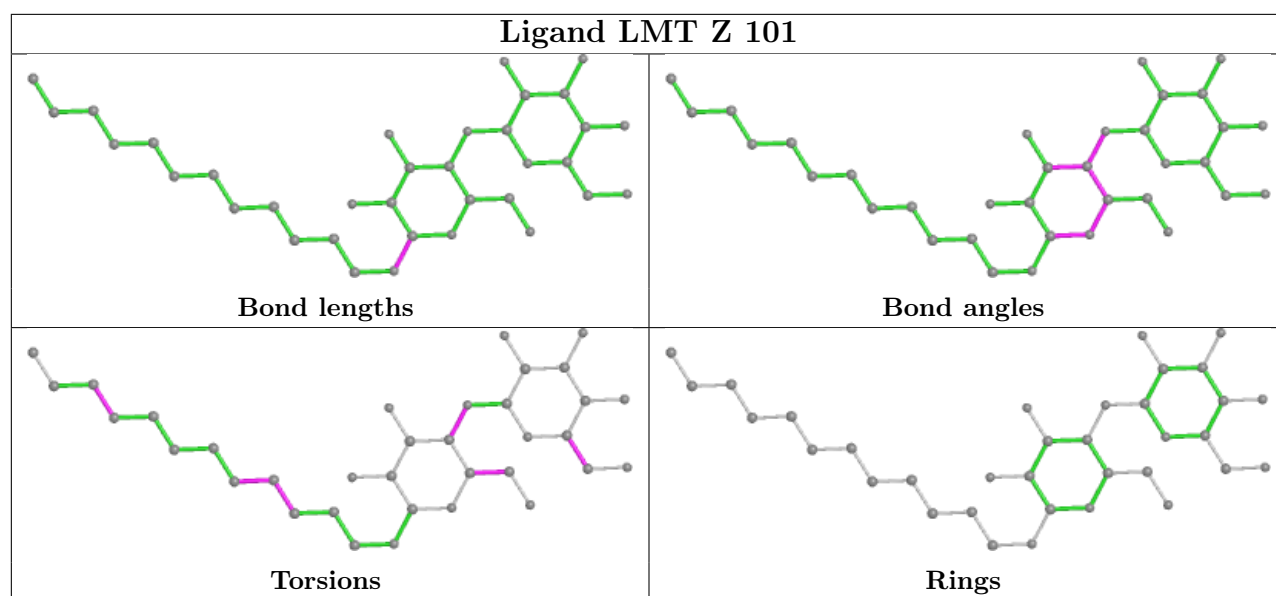
Ligand PL9 d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings



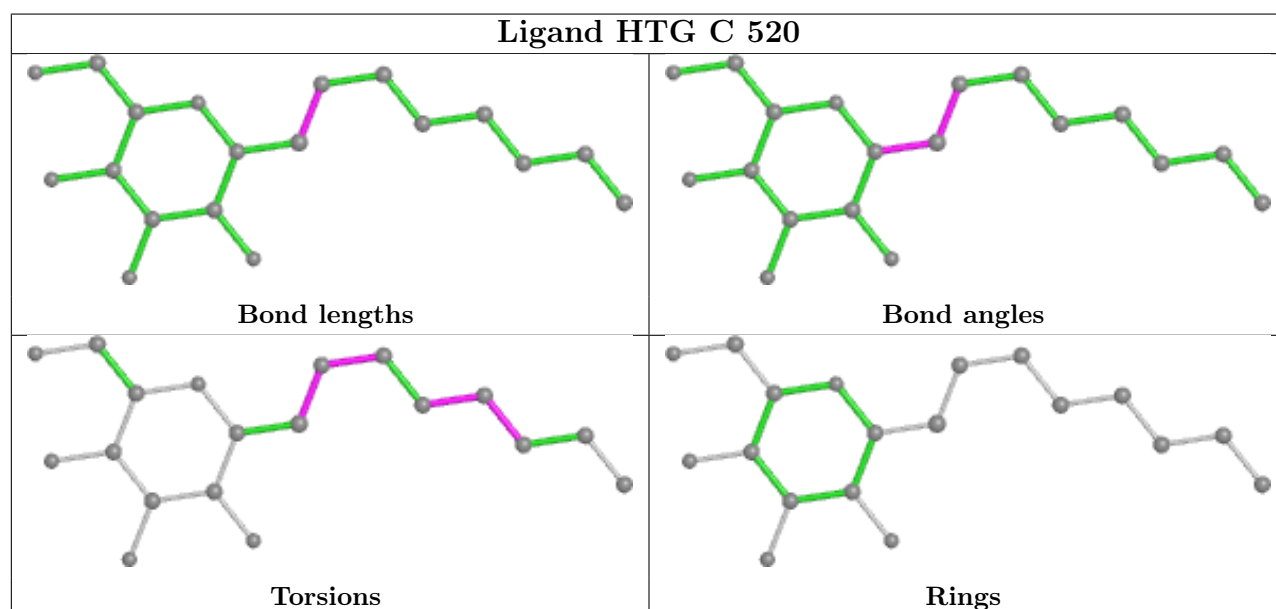
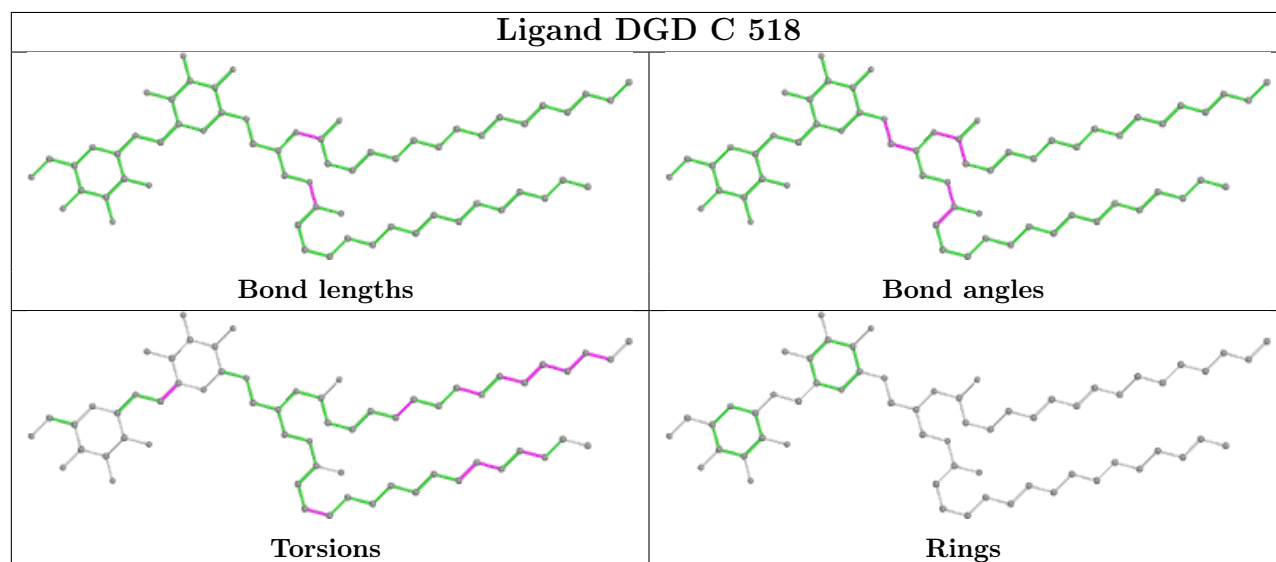
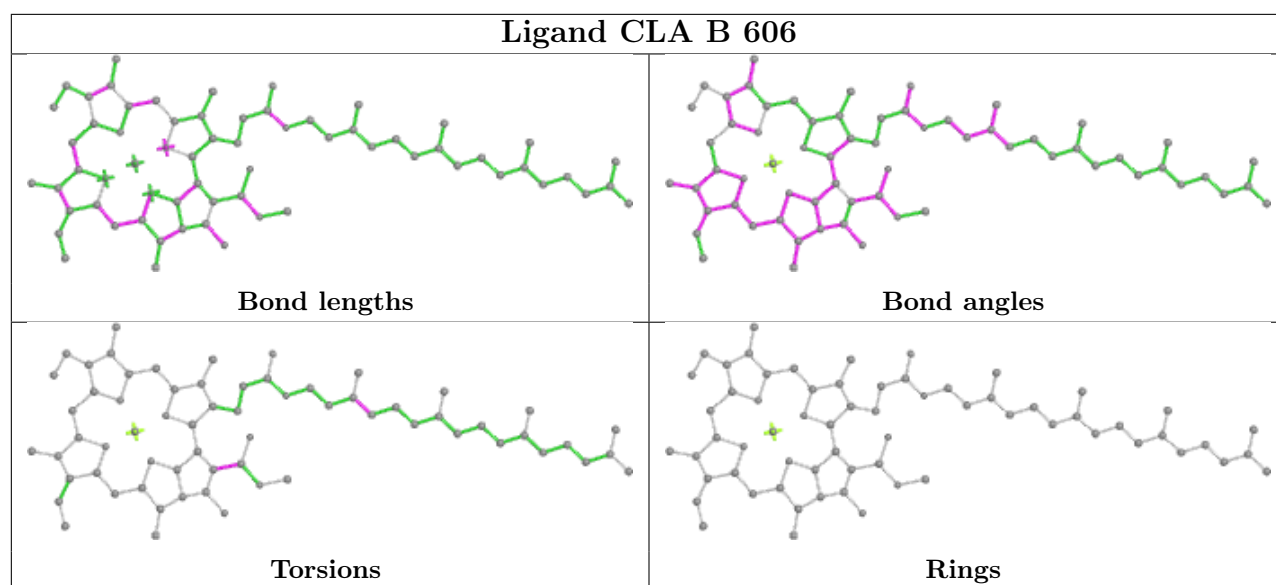


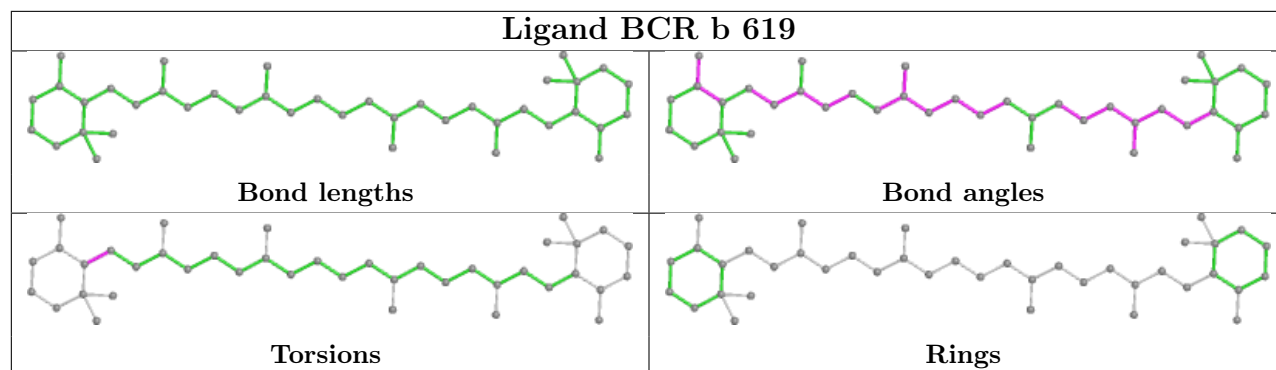
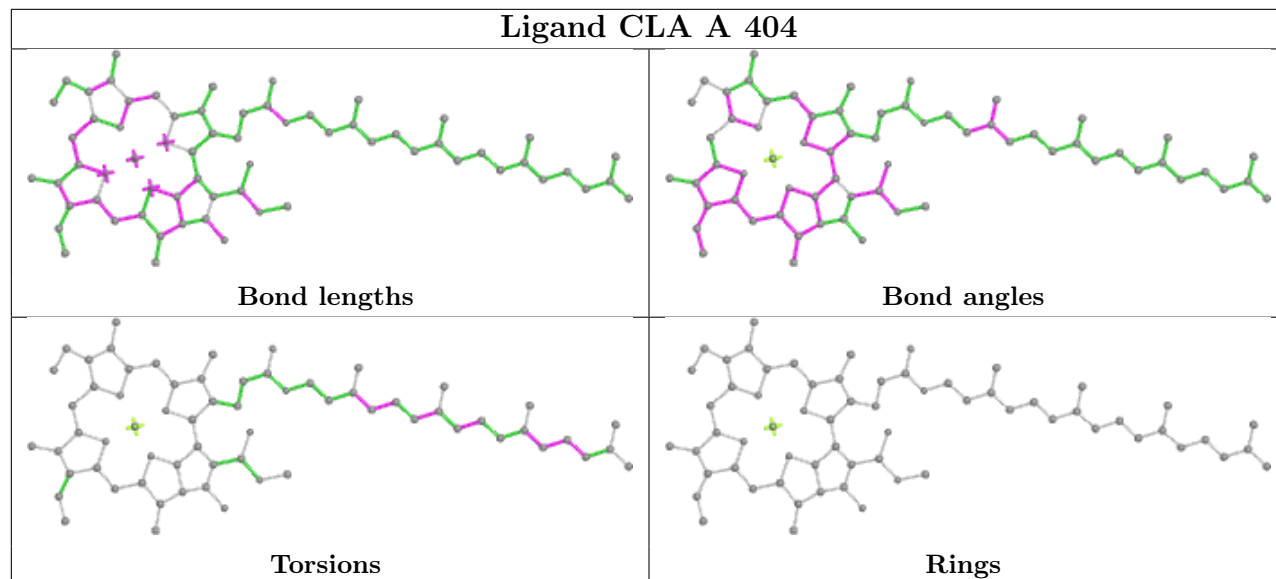
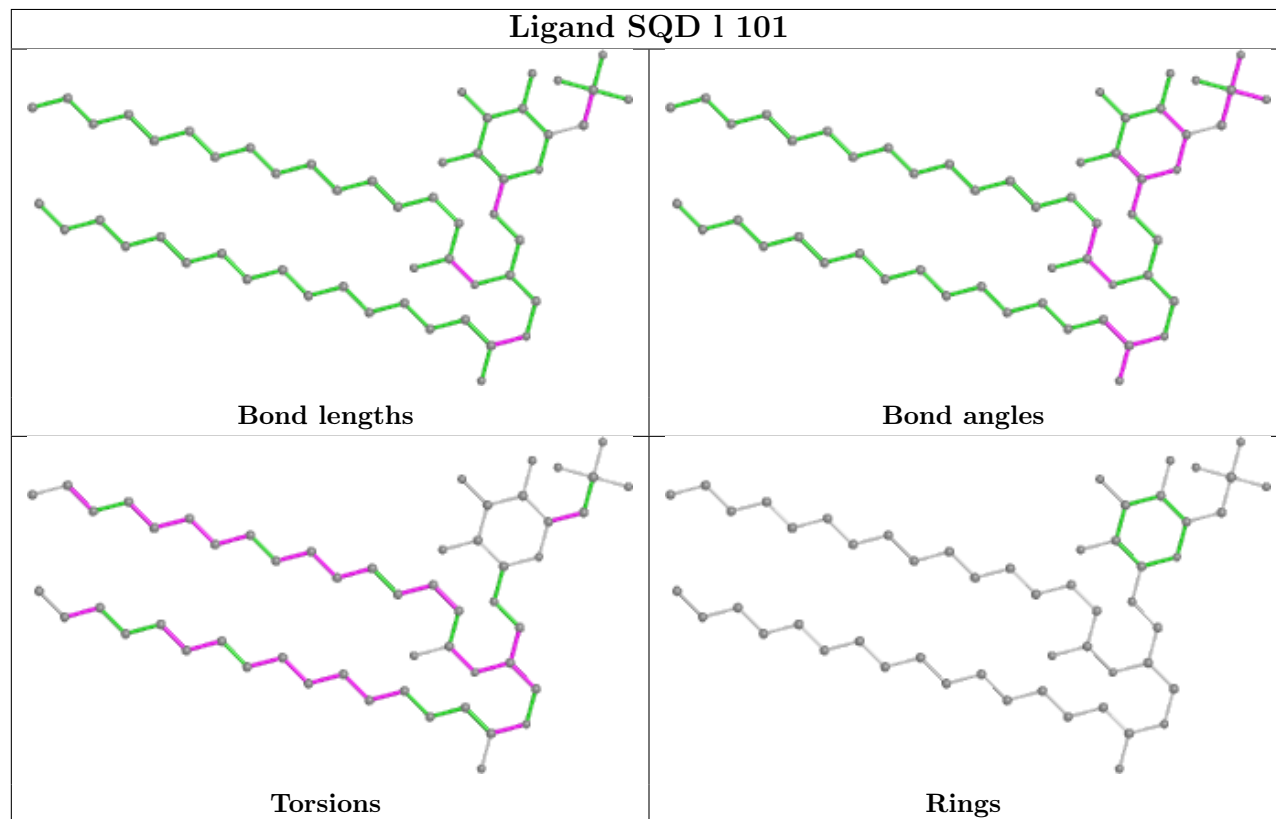


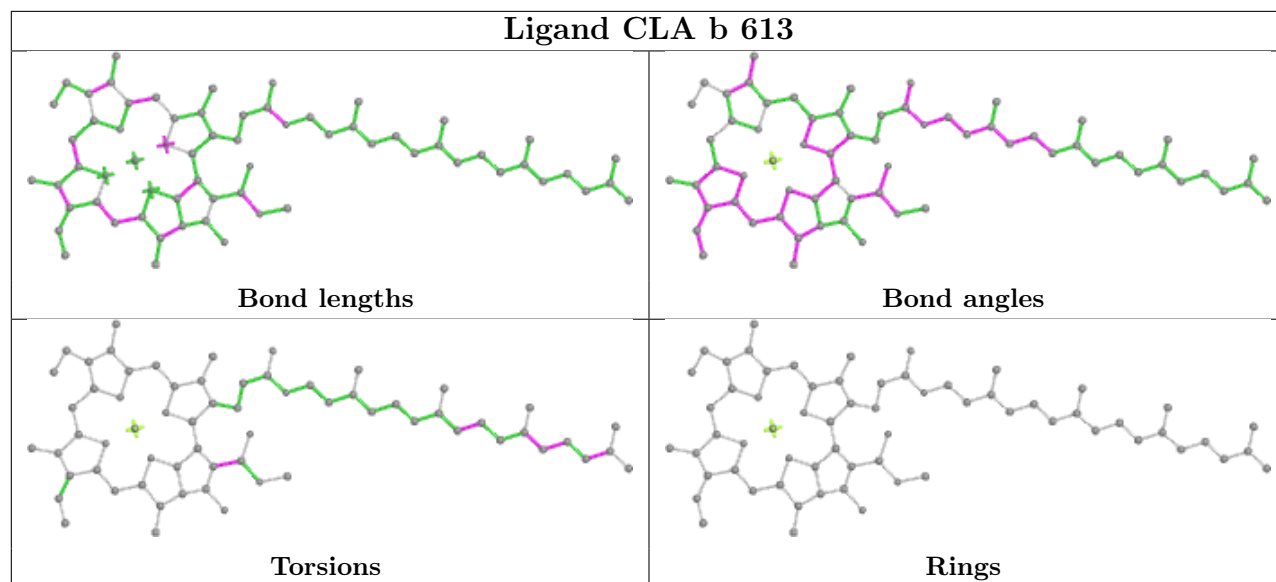
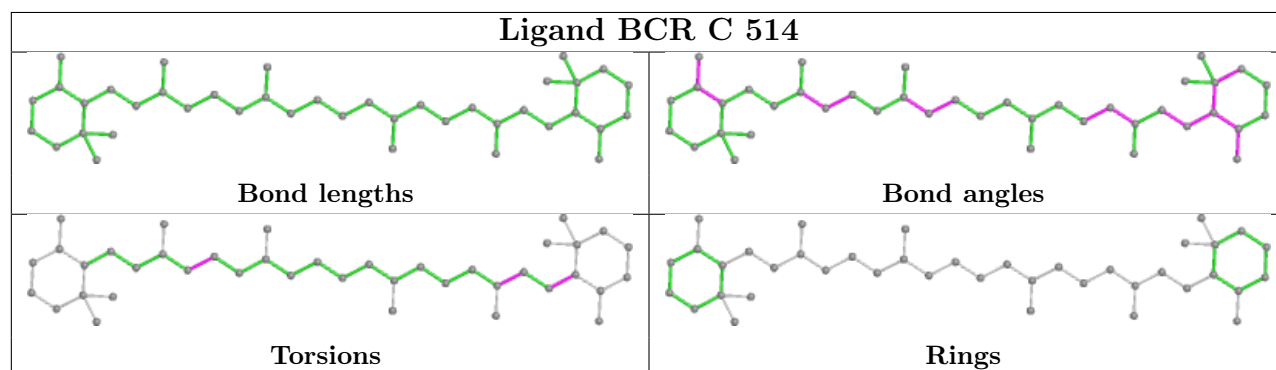
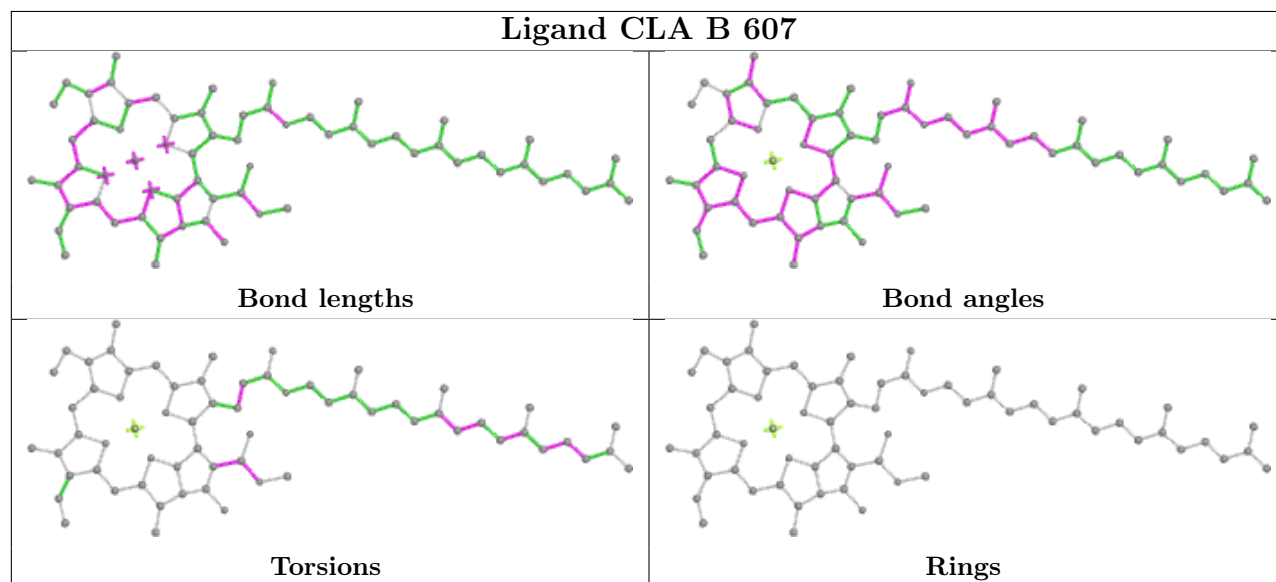


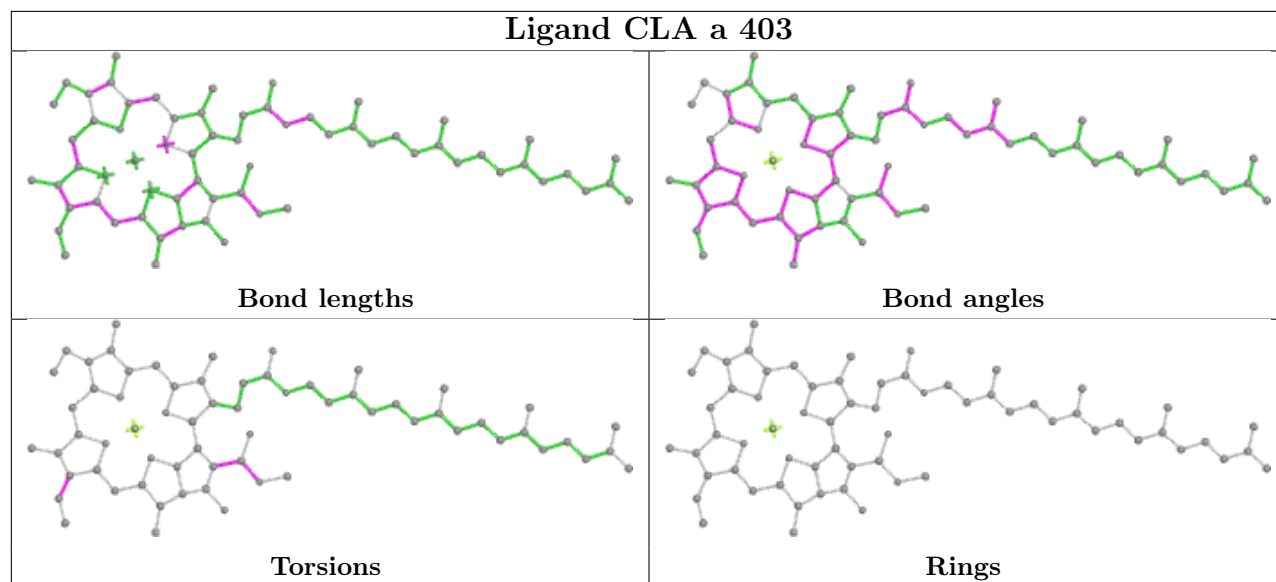
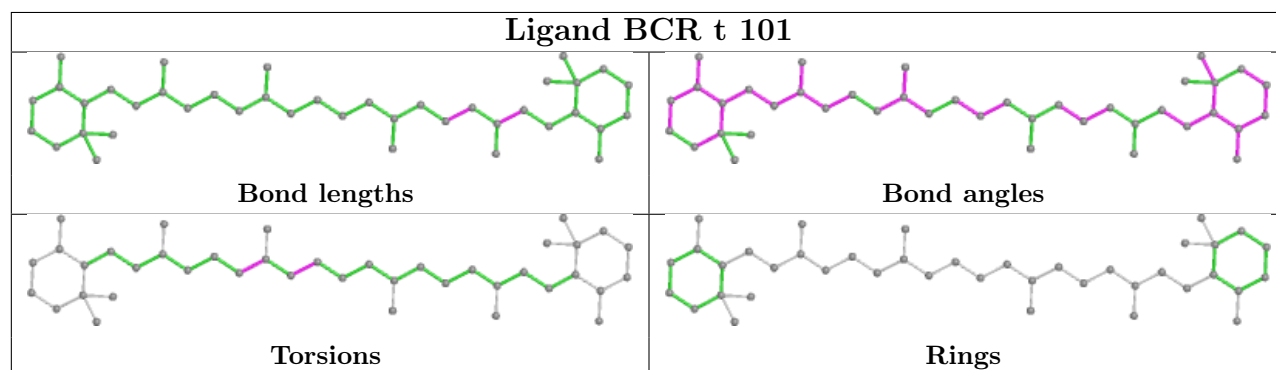
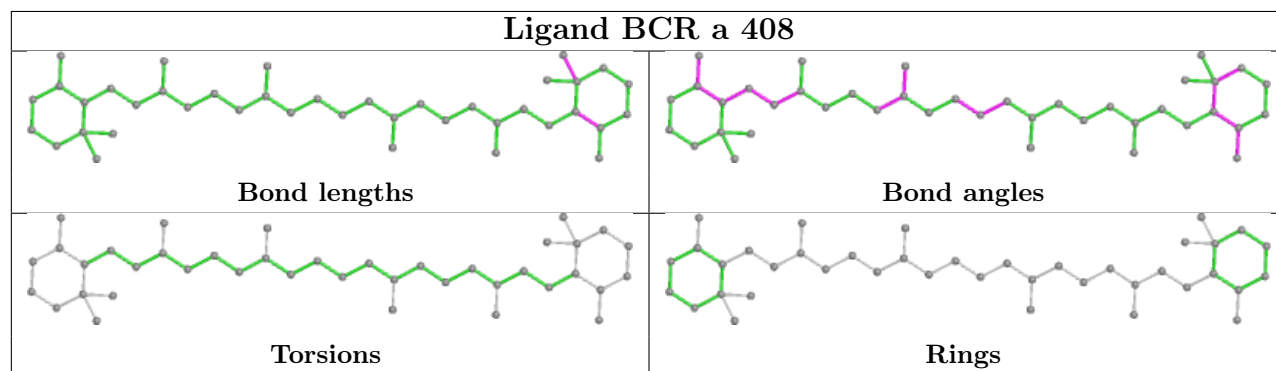




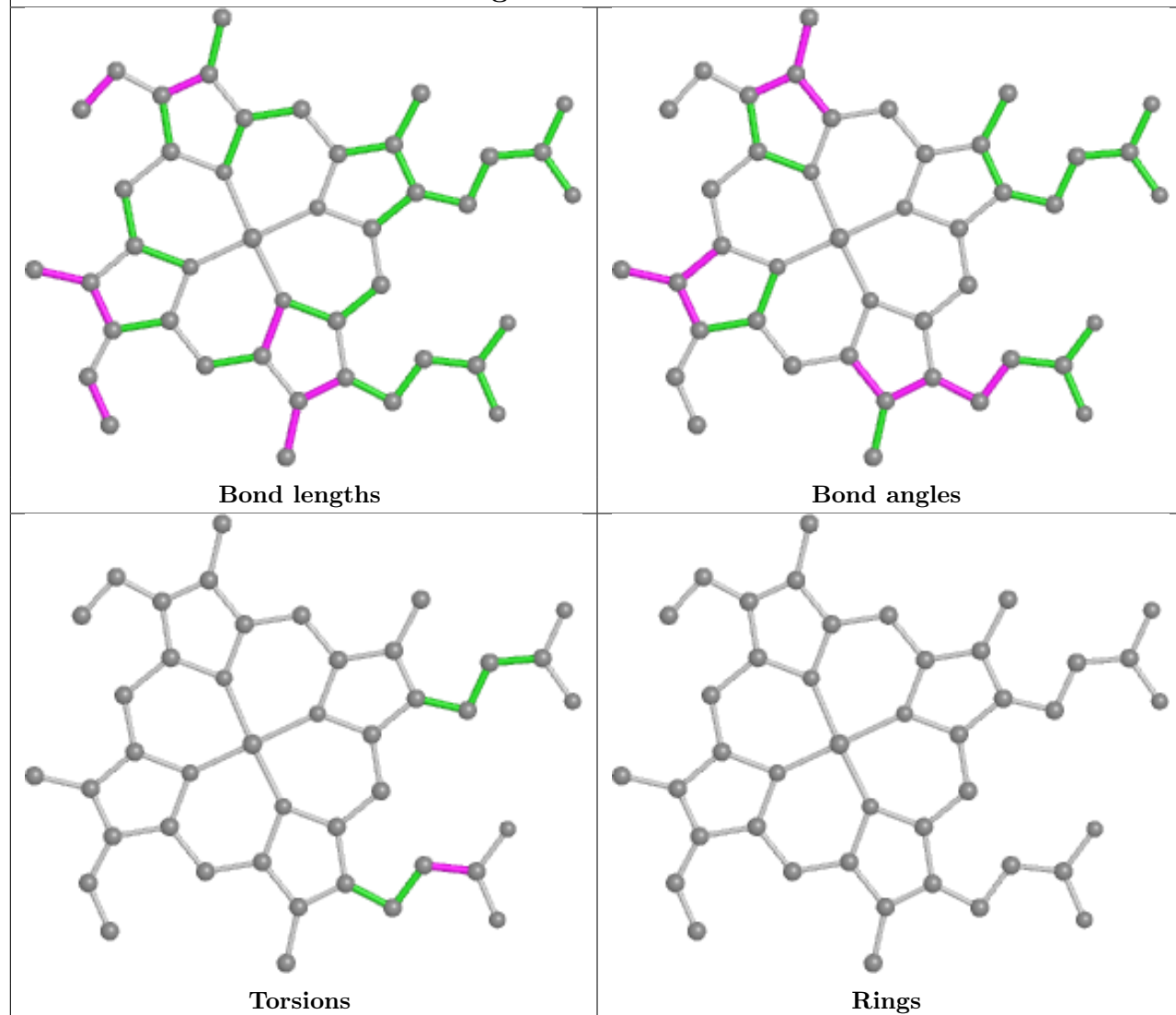


**Ligand BCR b 619****Ligand CLA A 404****Ligand SQD l 101**

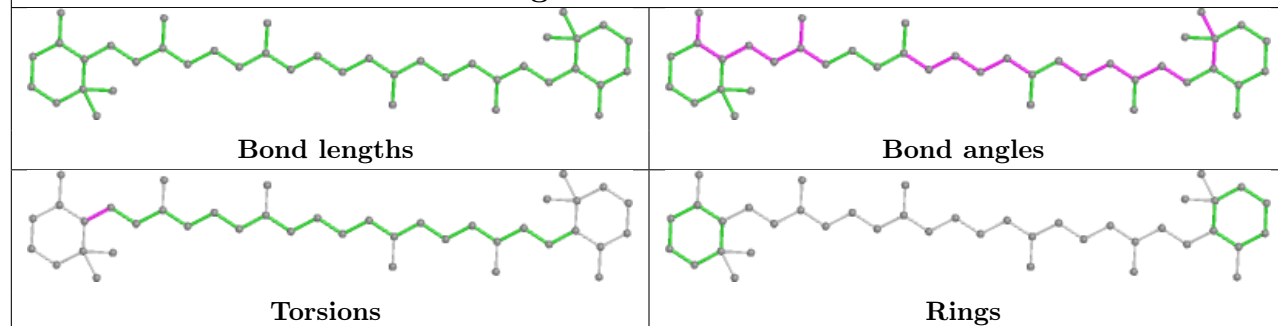
**Ligand CLA b 613****Ligand BCR C 514****Ligand CLA B 607**

**Ligand CLA a 403****Ligand BCR t 101****Ligand BCR a 408**

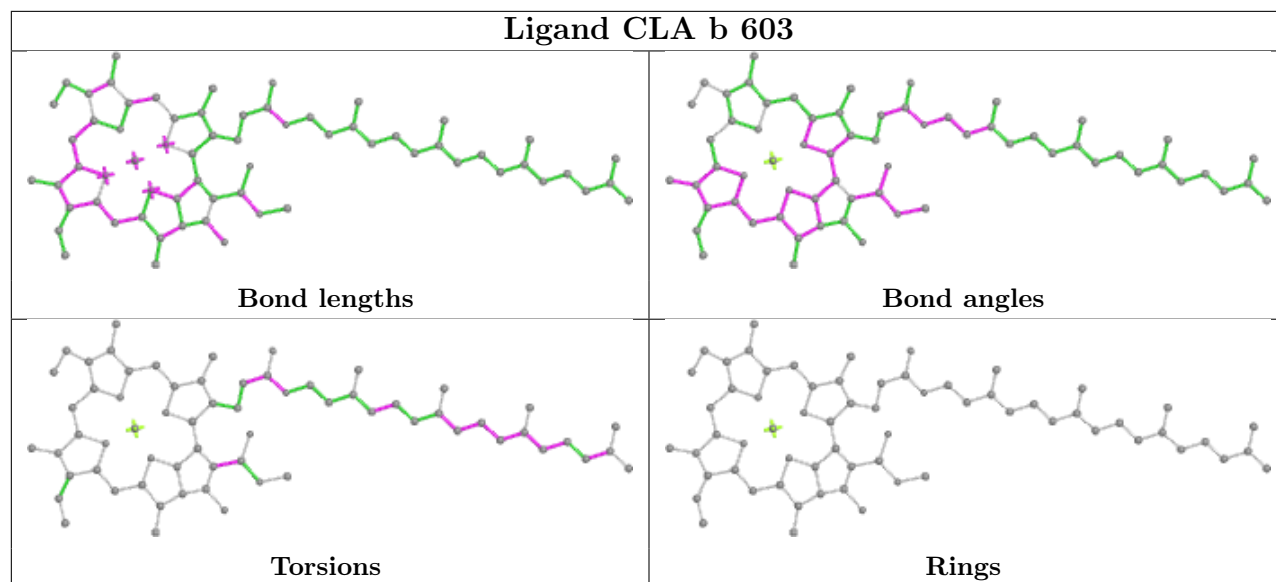
## Ligand HEC v 201



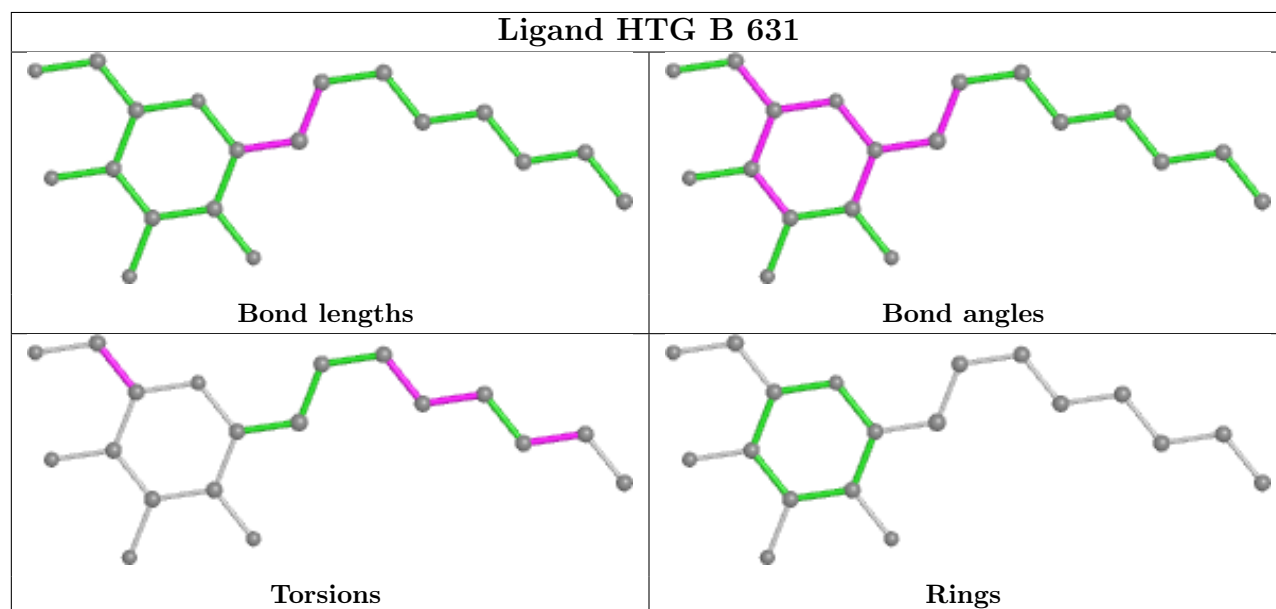
## Ligand BCR B 617



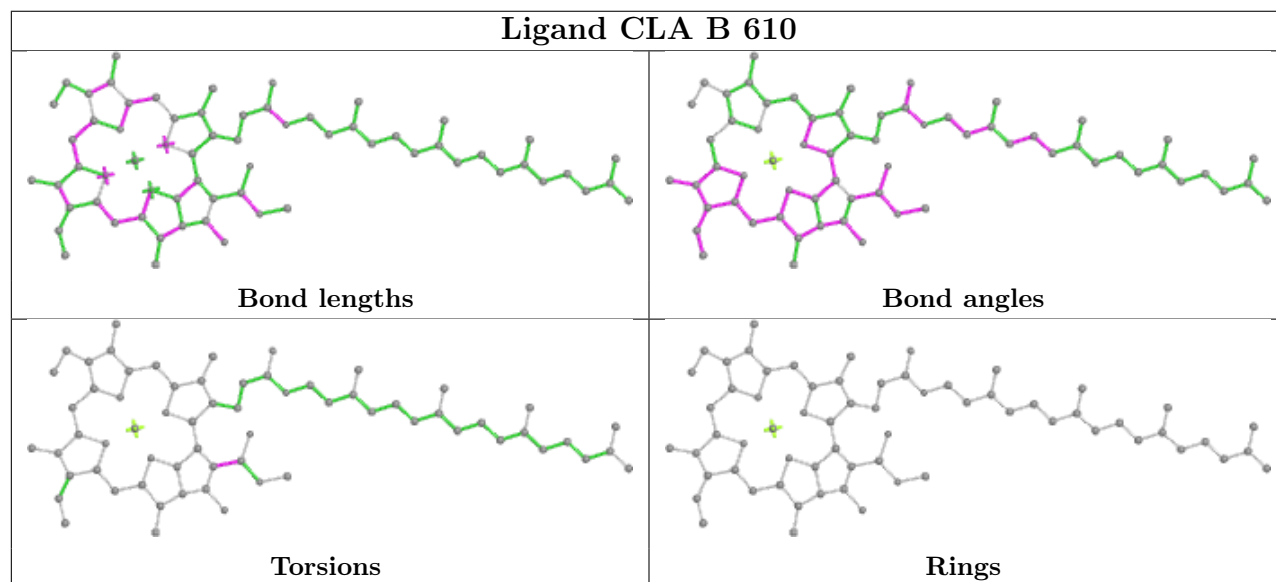
## Ligand CLA b 603

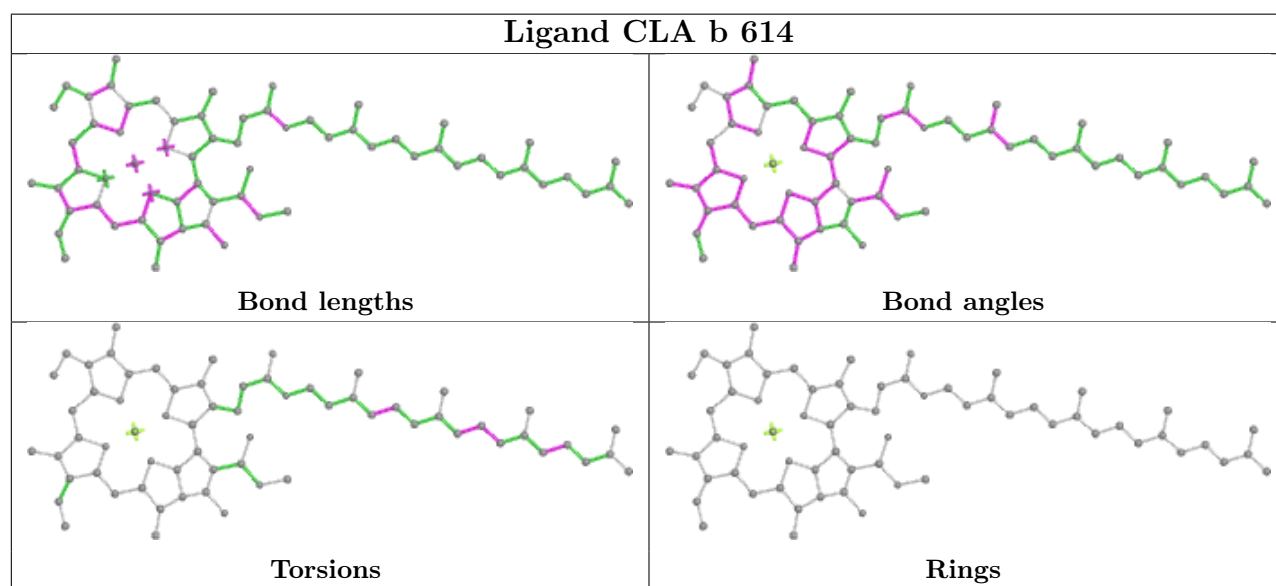
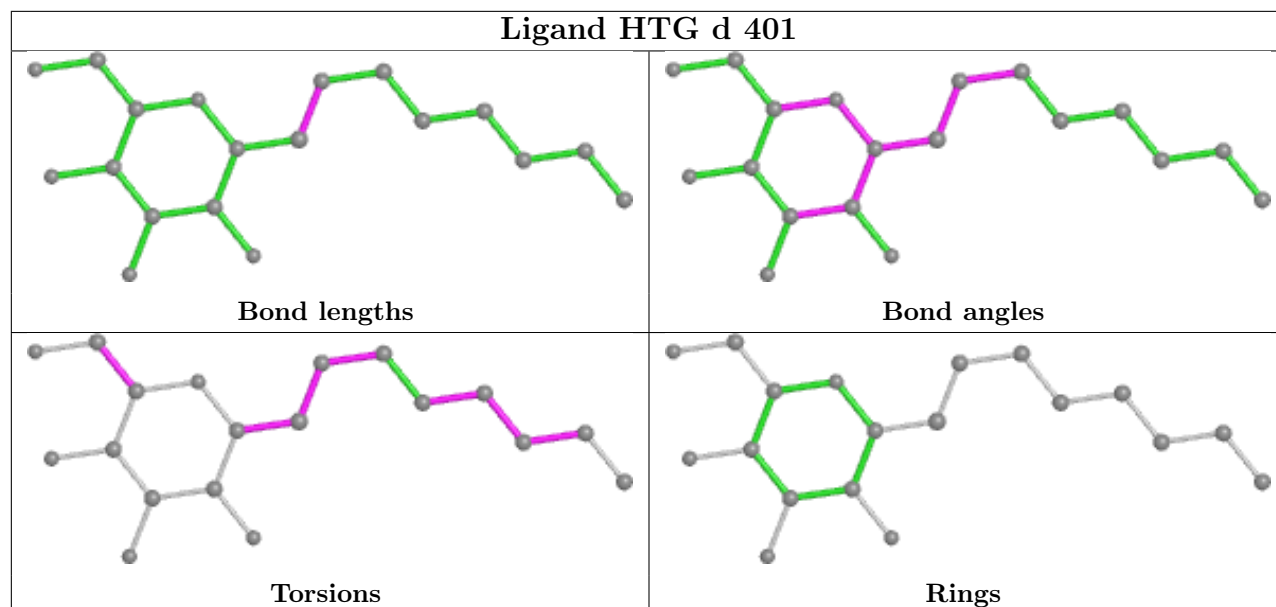


## Ligand HTG B 631

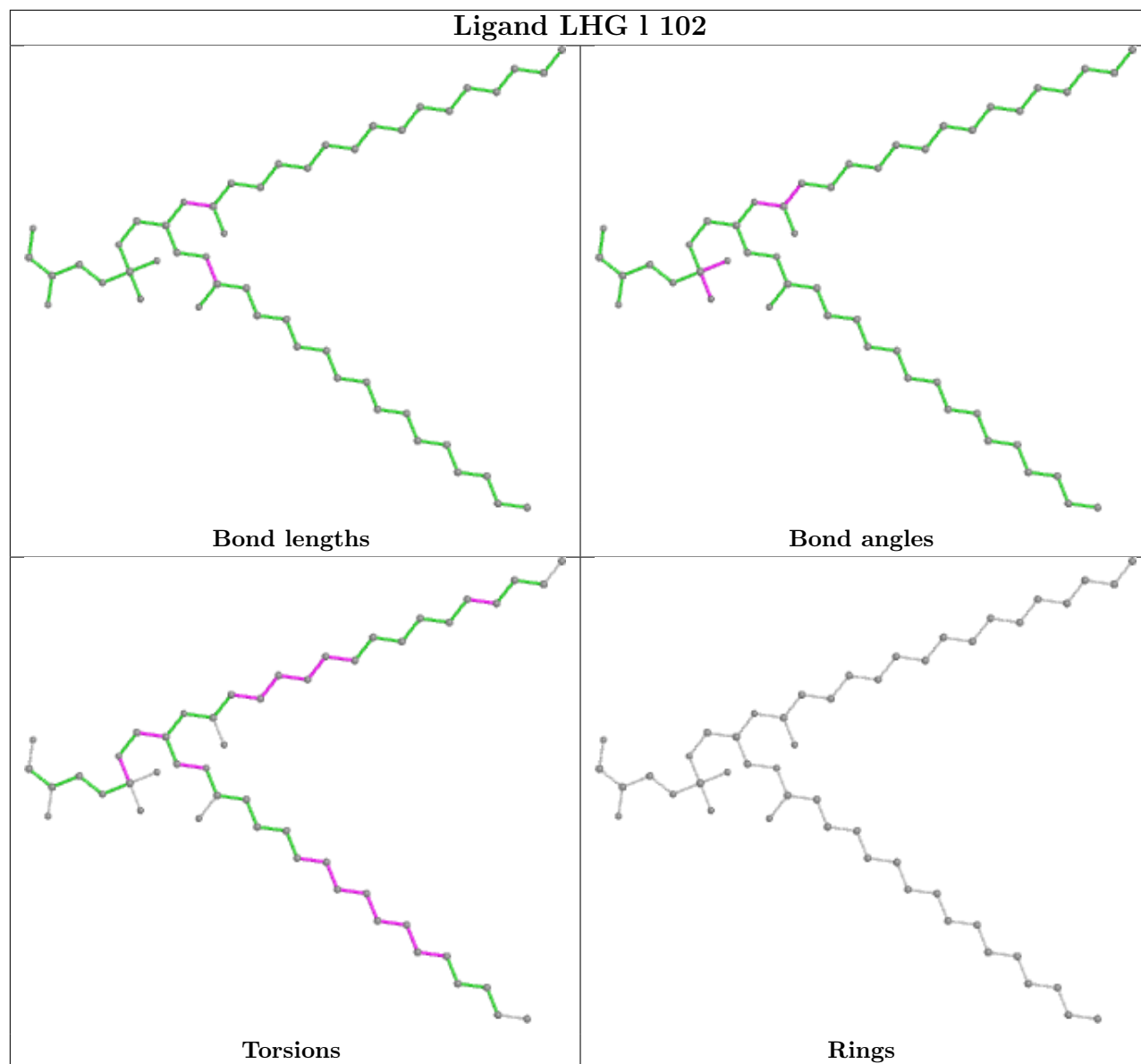


## Ligand CLA B 610

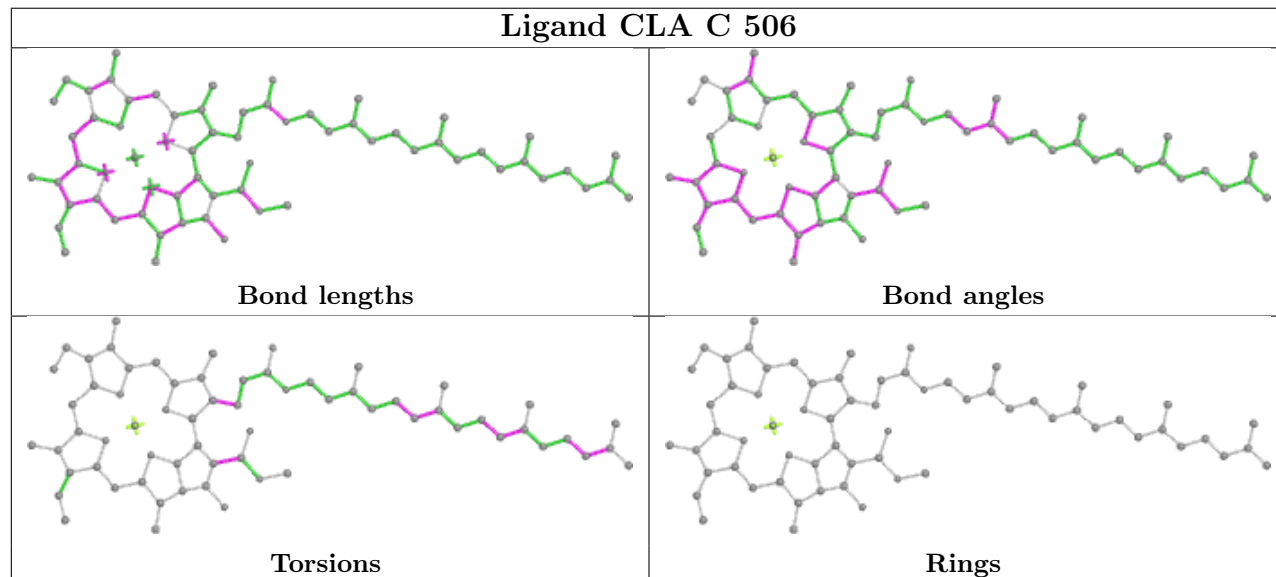




## Ligand LHG 1 102

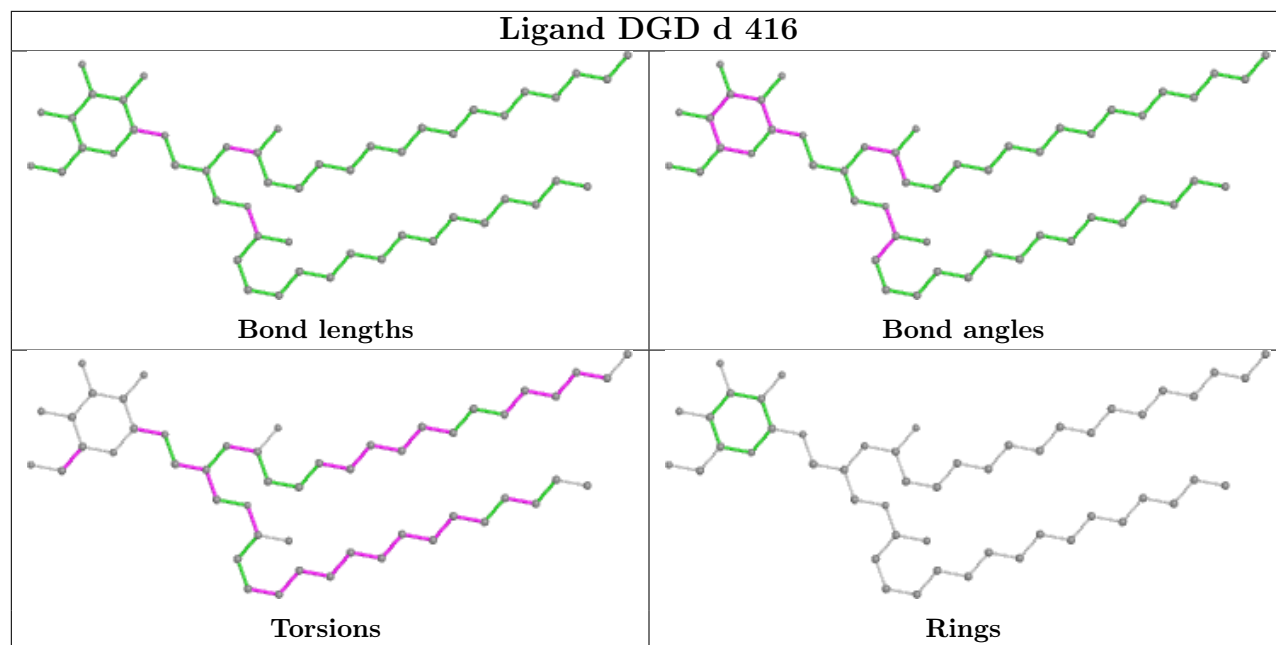


## Ligand CLA C 506

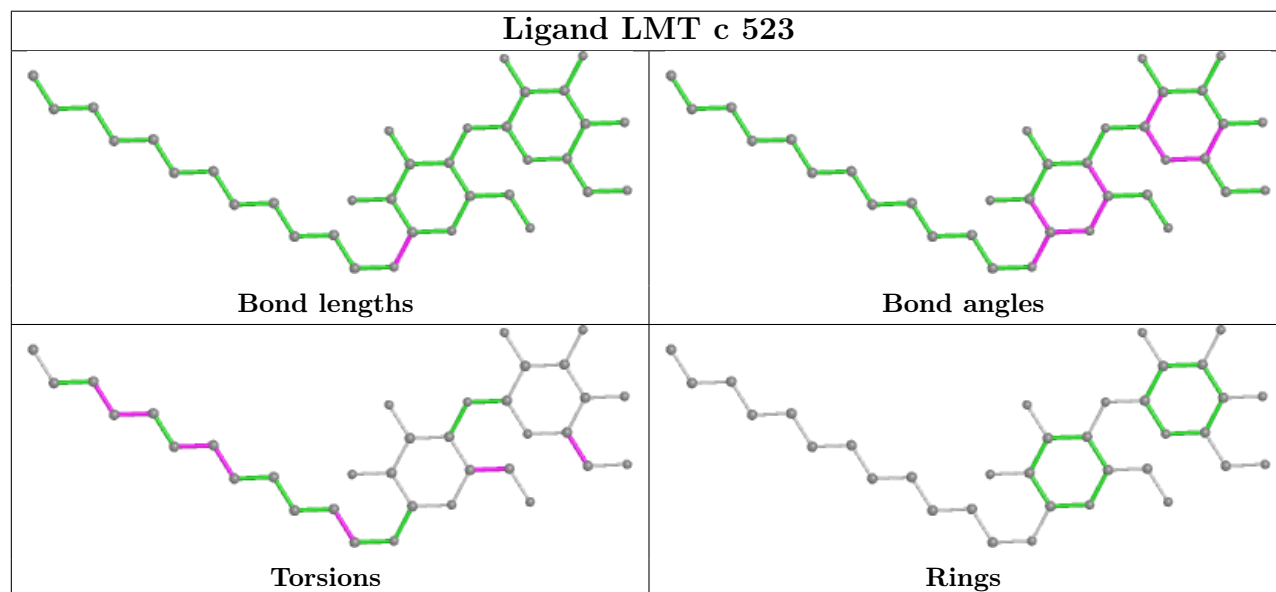




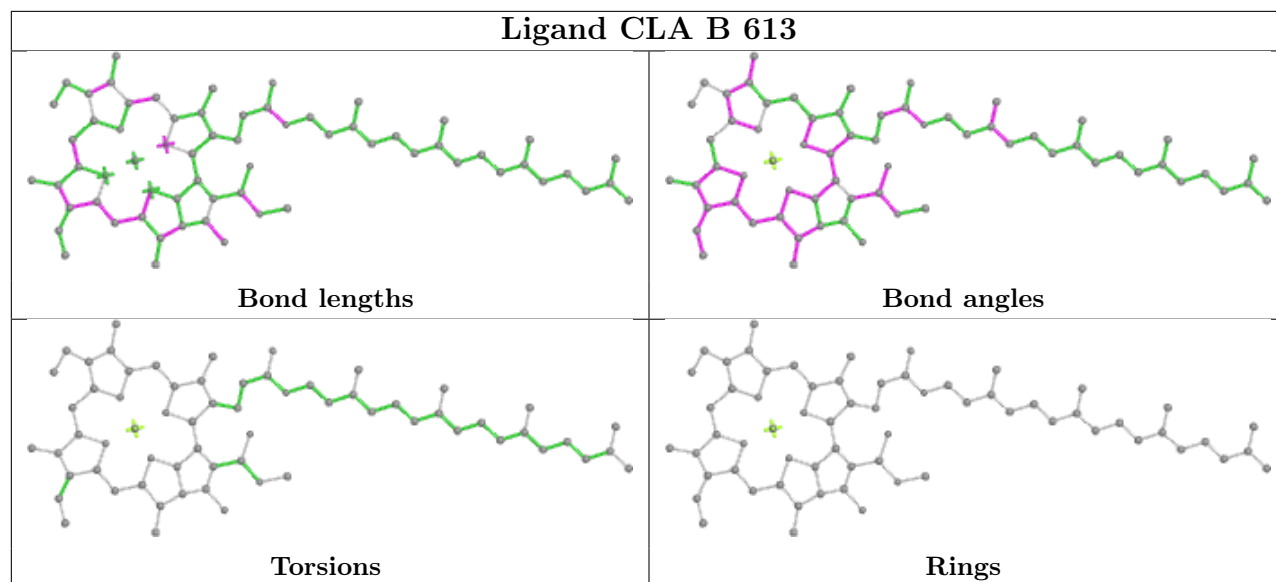
## Ligand DGD d 416



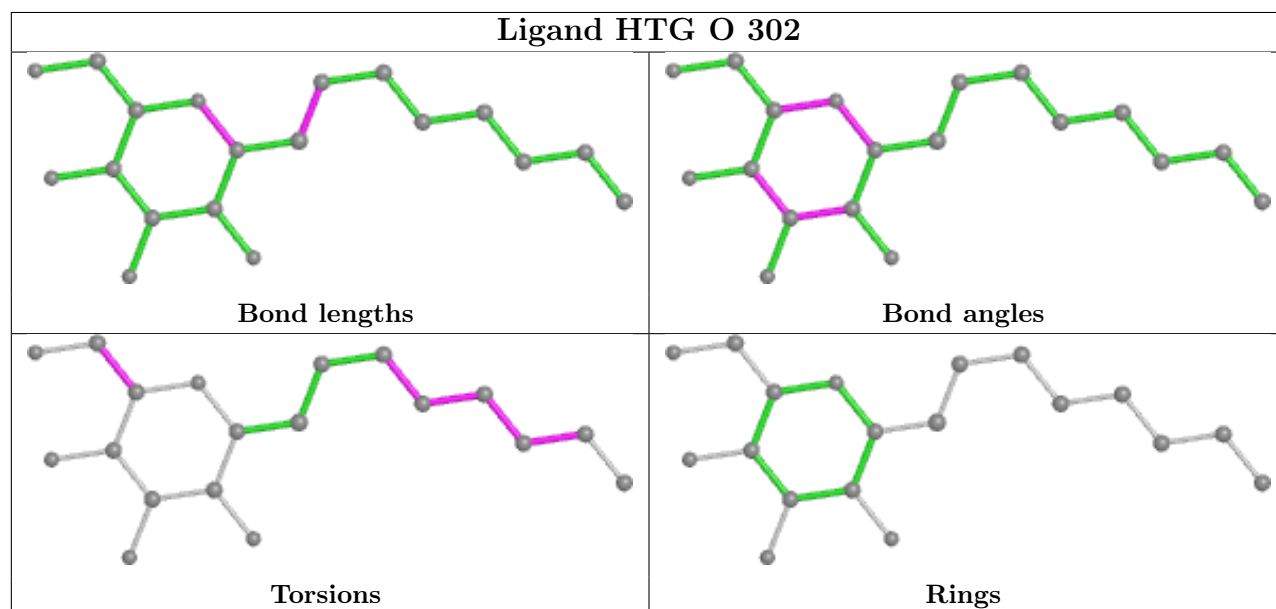
## Ligand LMT c 523



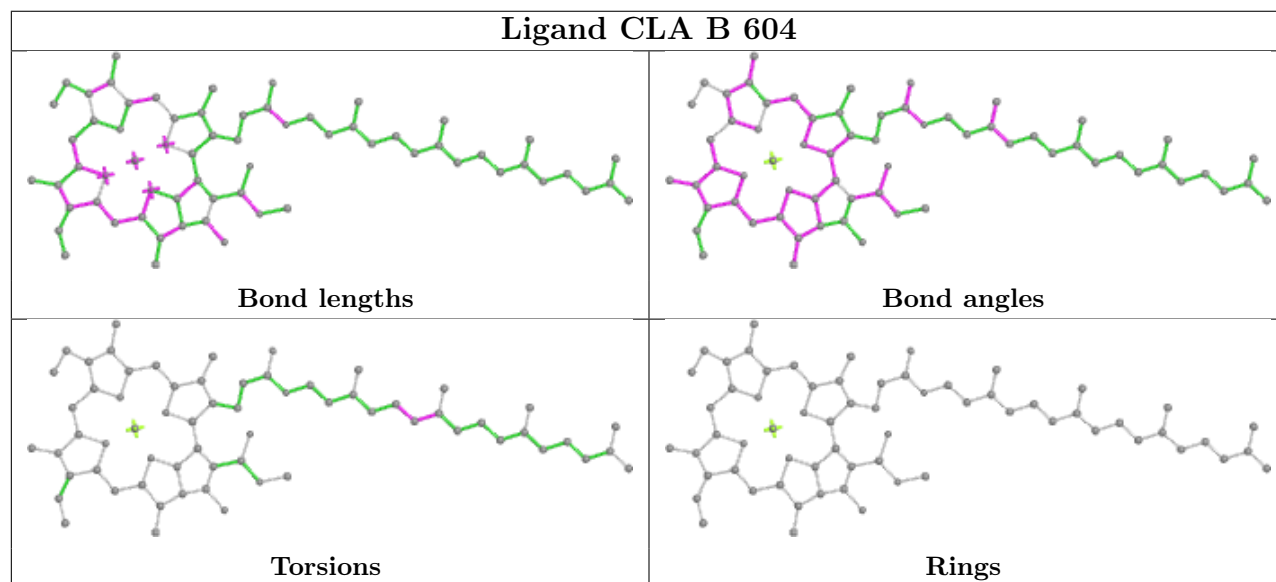
## Ligand CLA B 613

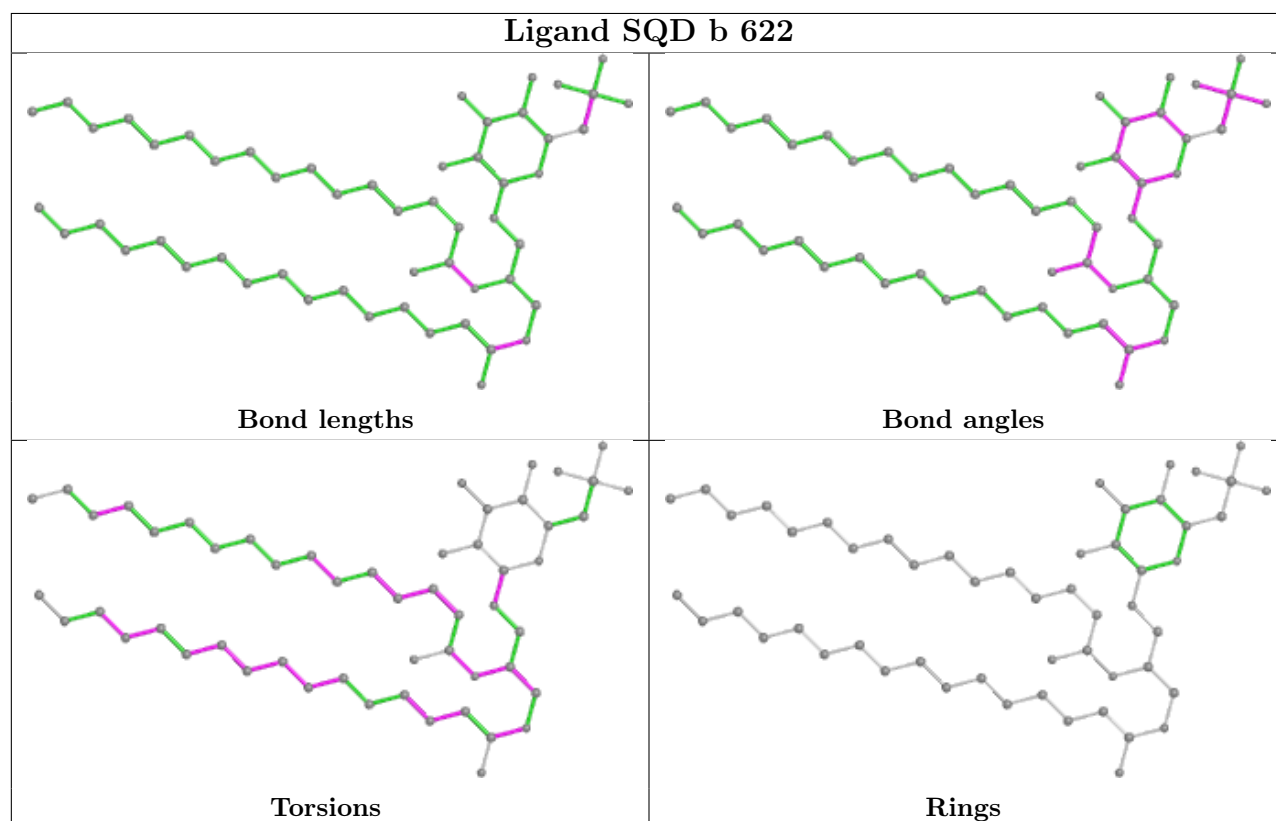
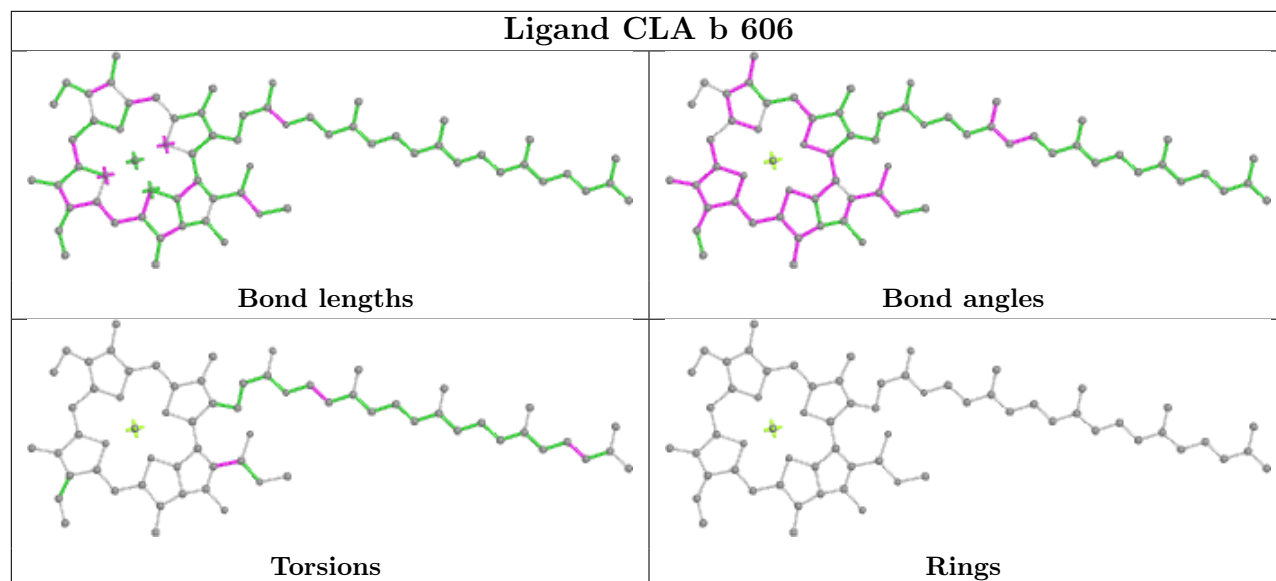
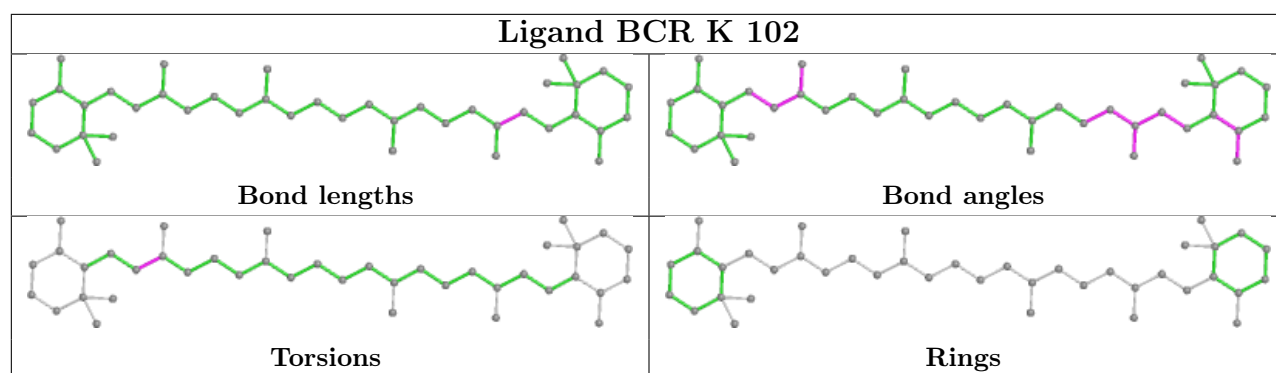


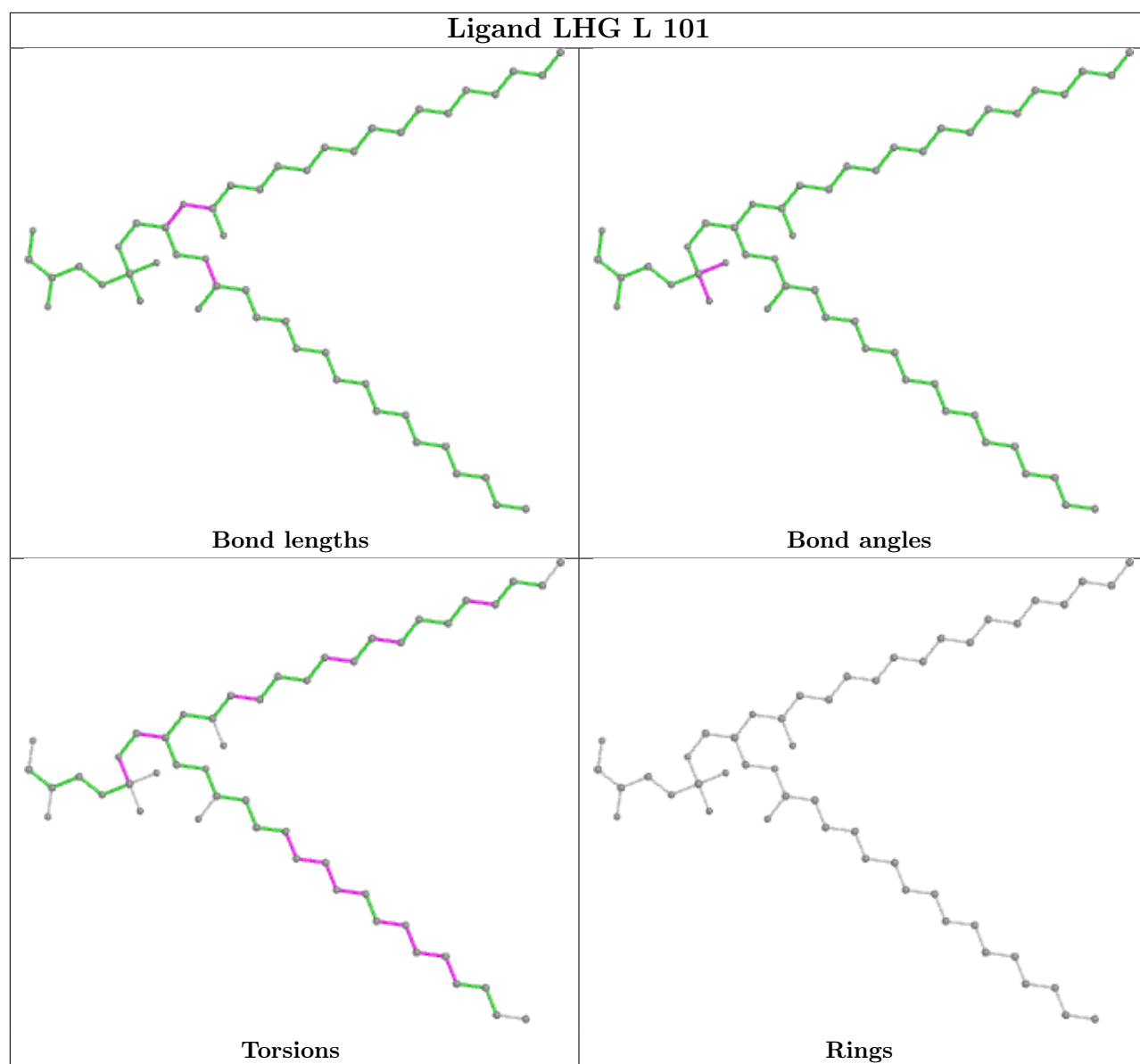
## Ligand HTG O 302

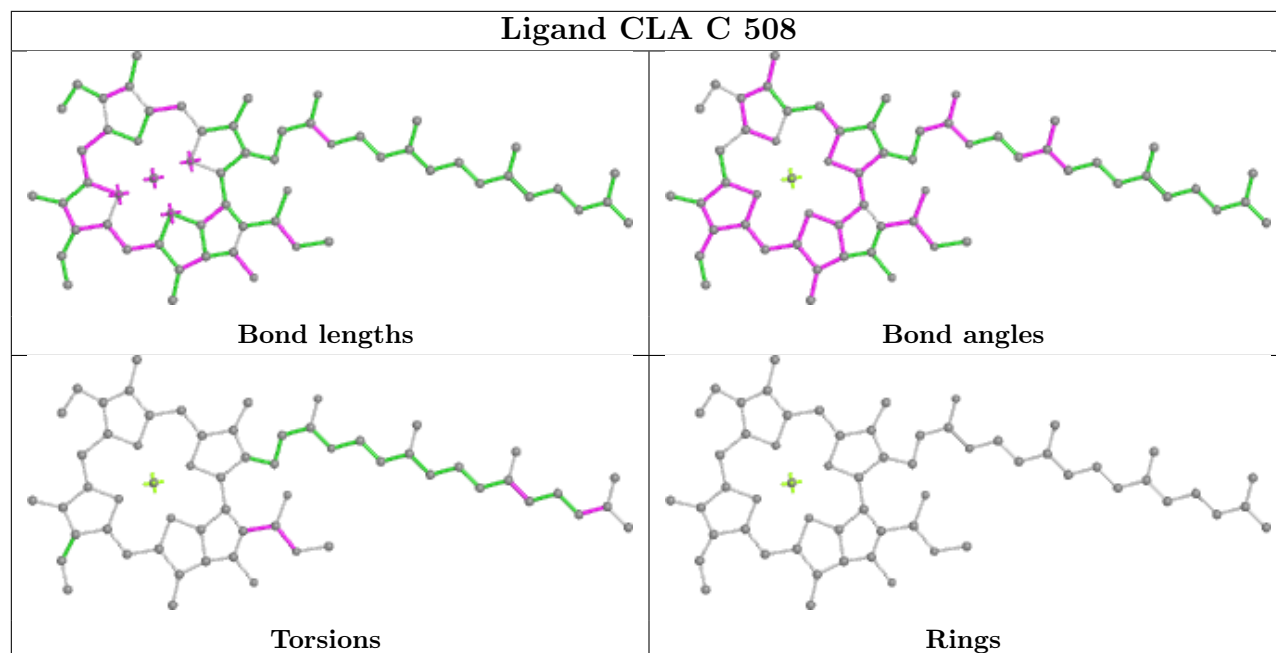
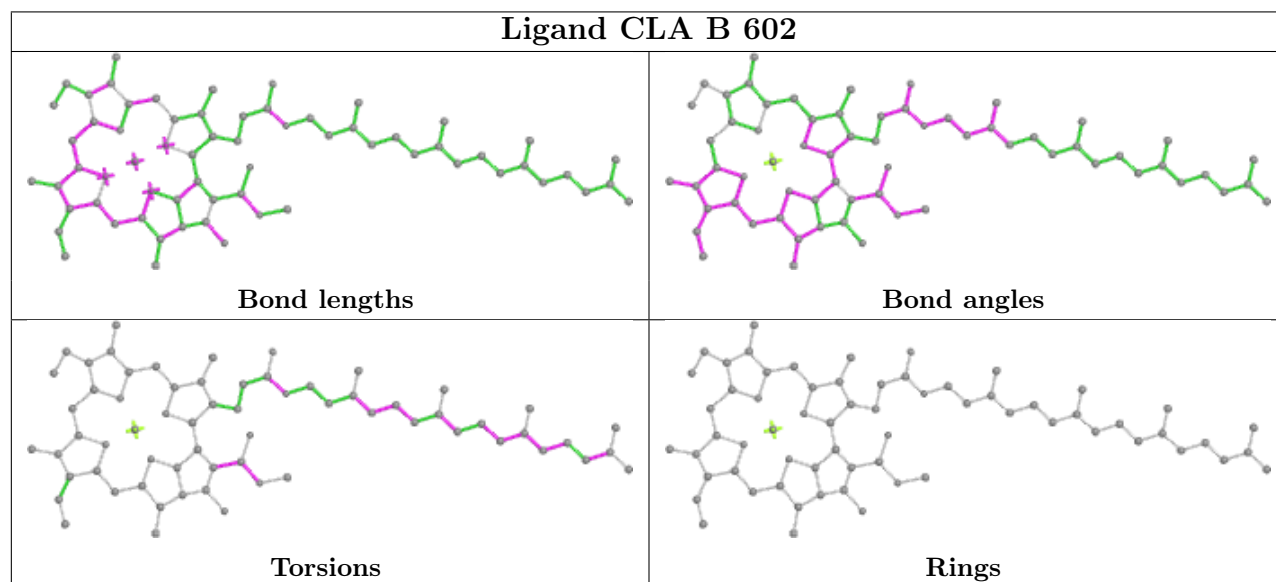
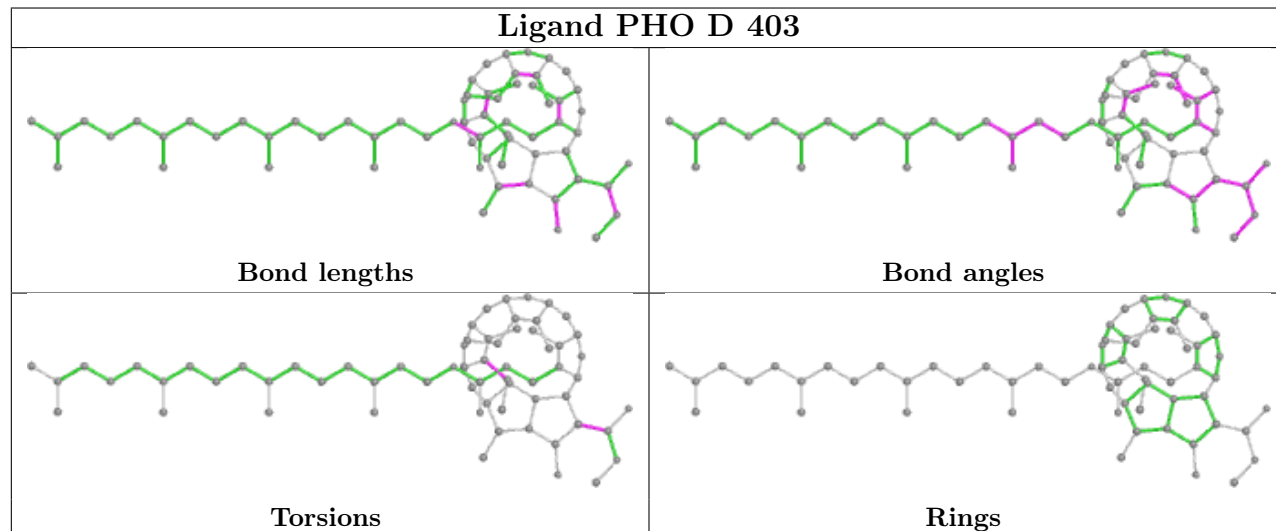


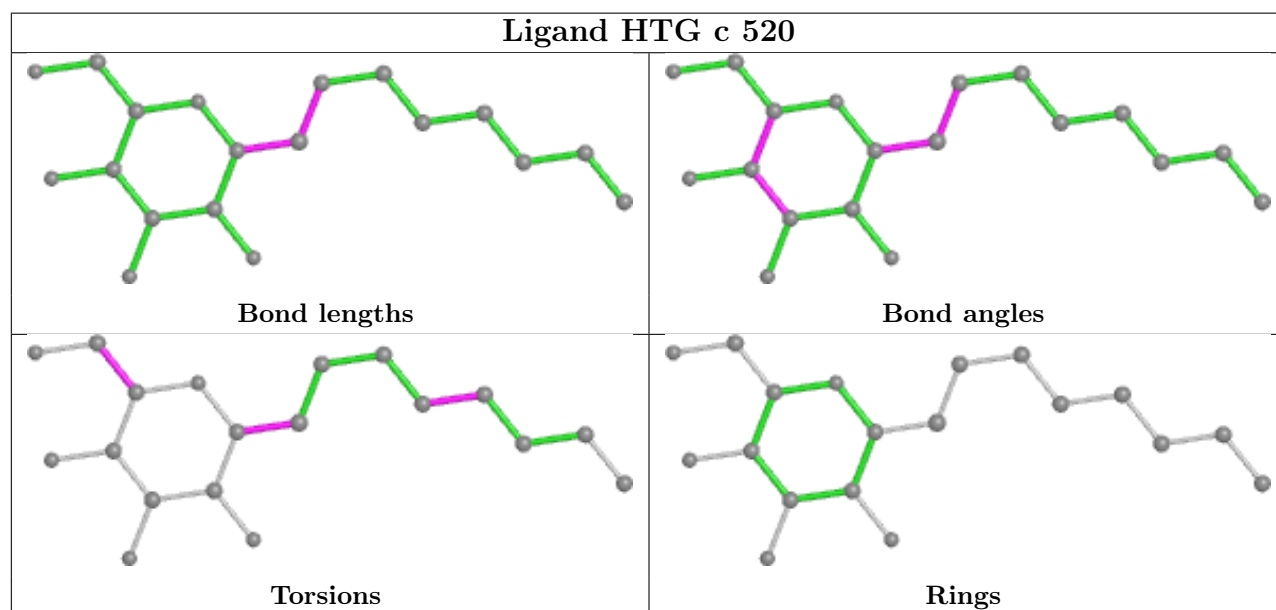
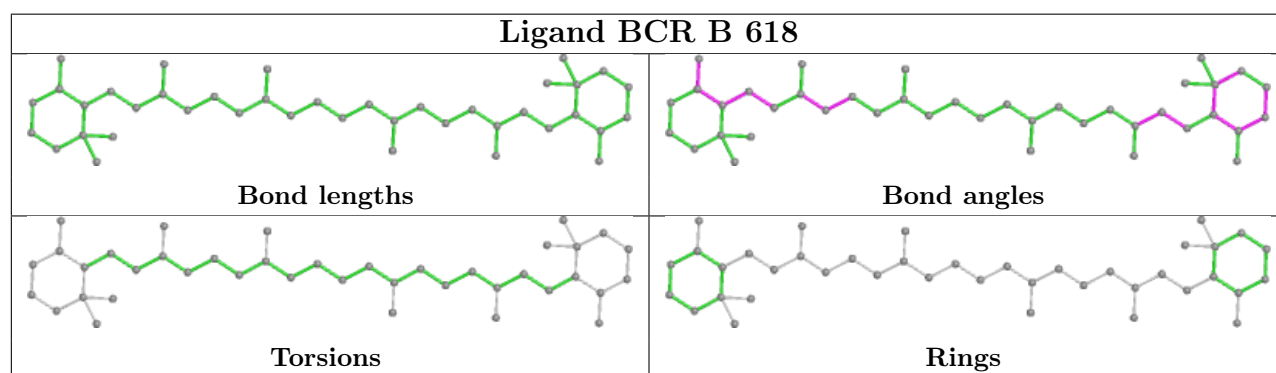
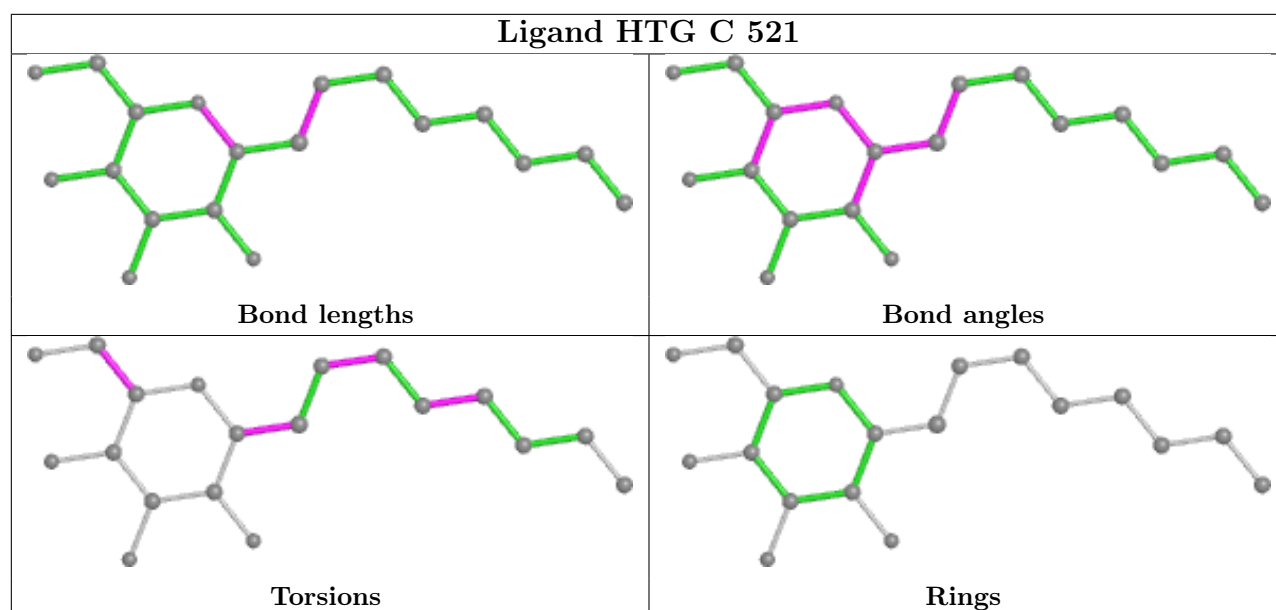
## Ligand CLA B 604

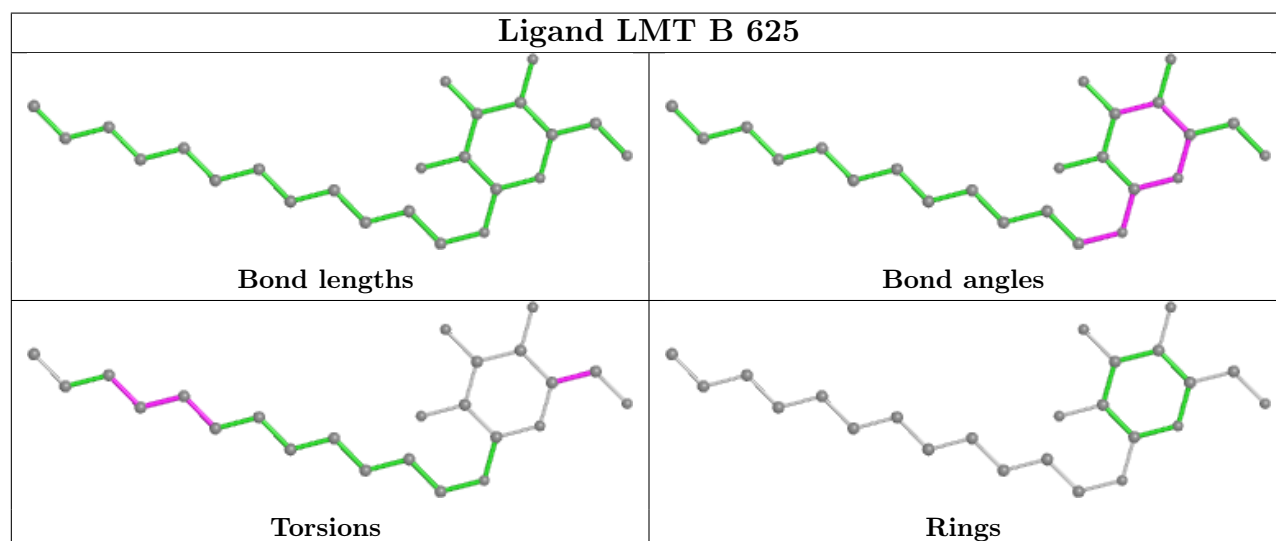
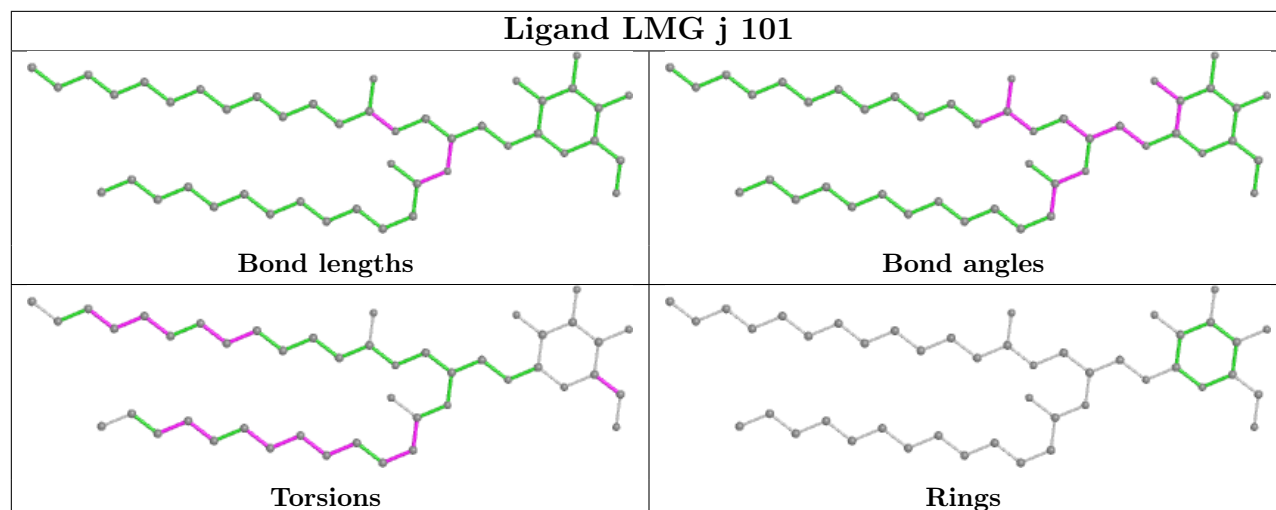


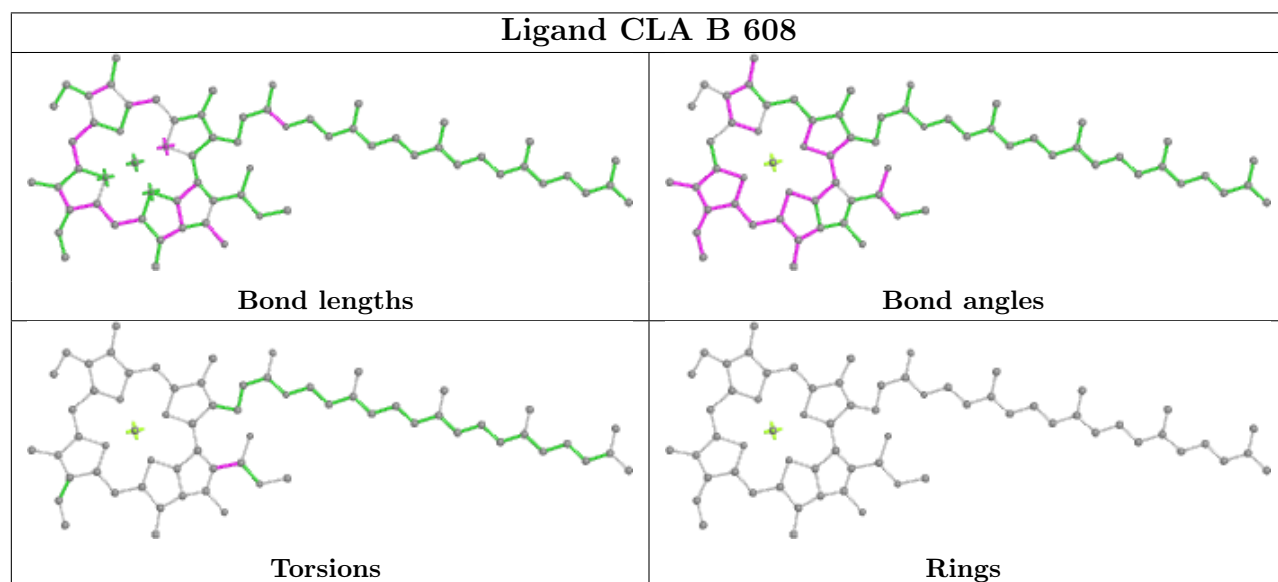
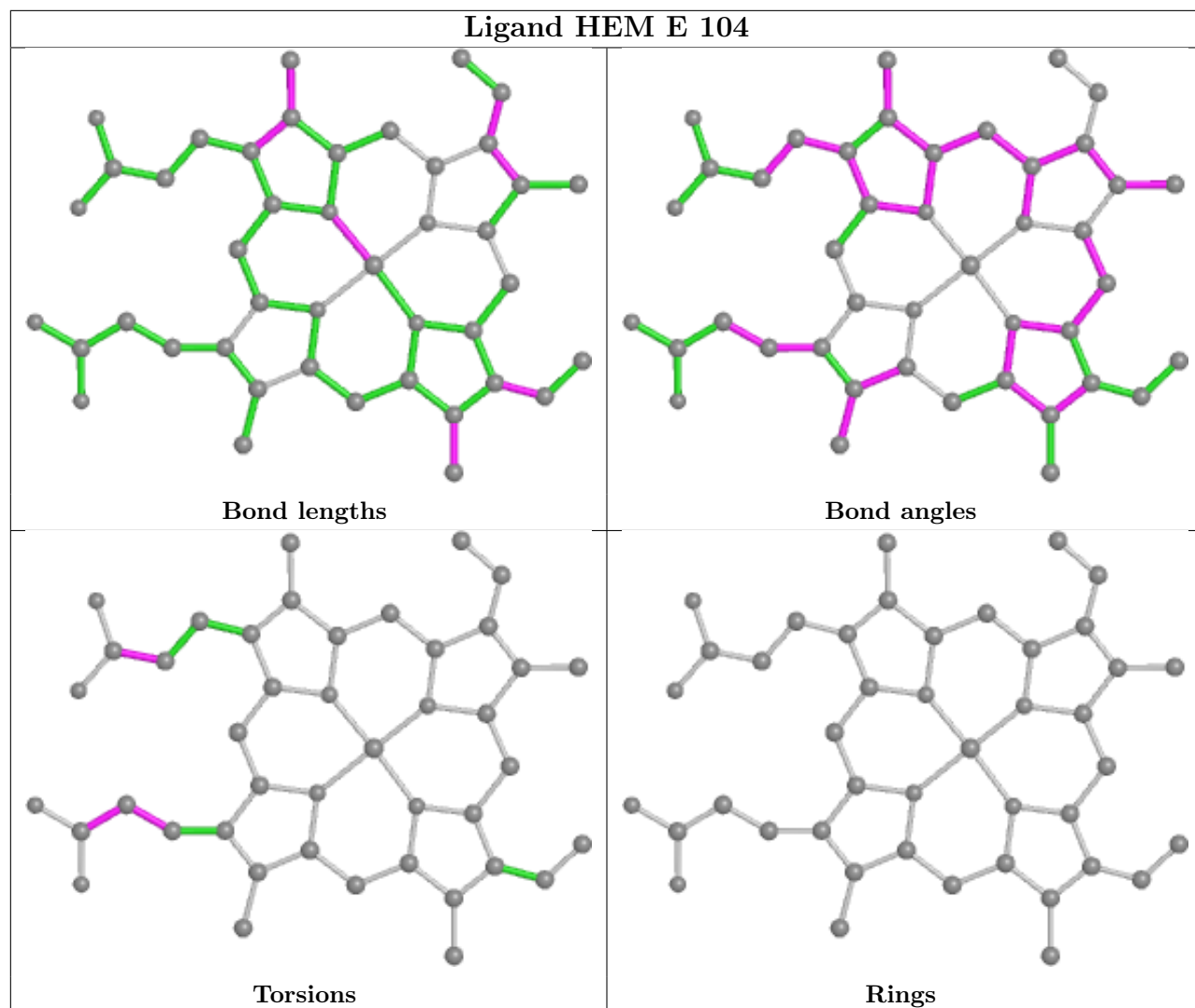




**Ligand CLA C 508****Ligand CLA B 602****Ligand PHO D 403**

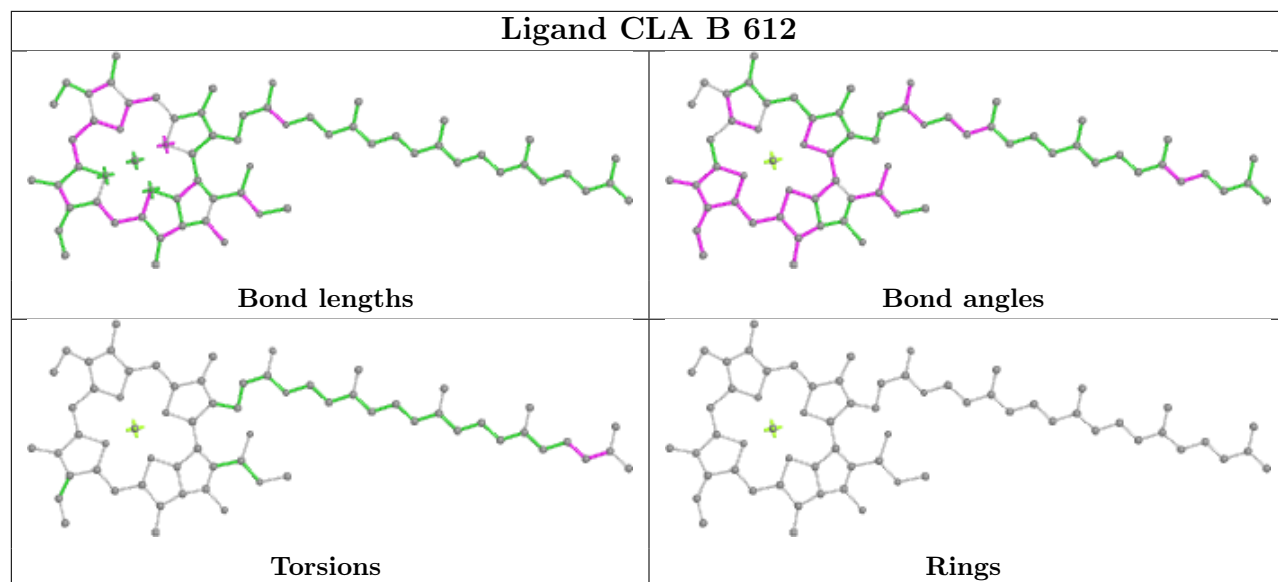




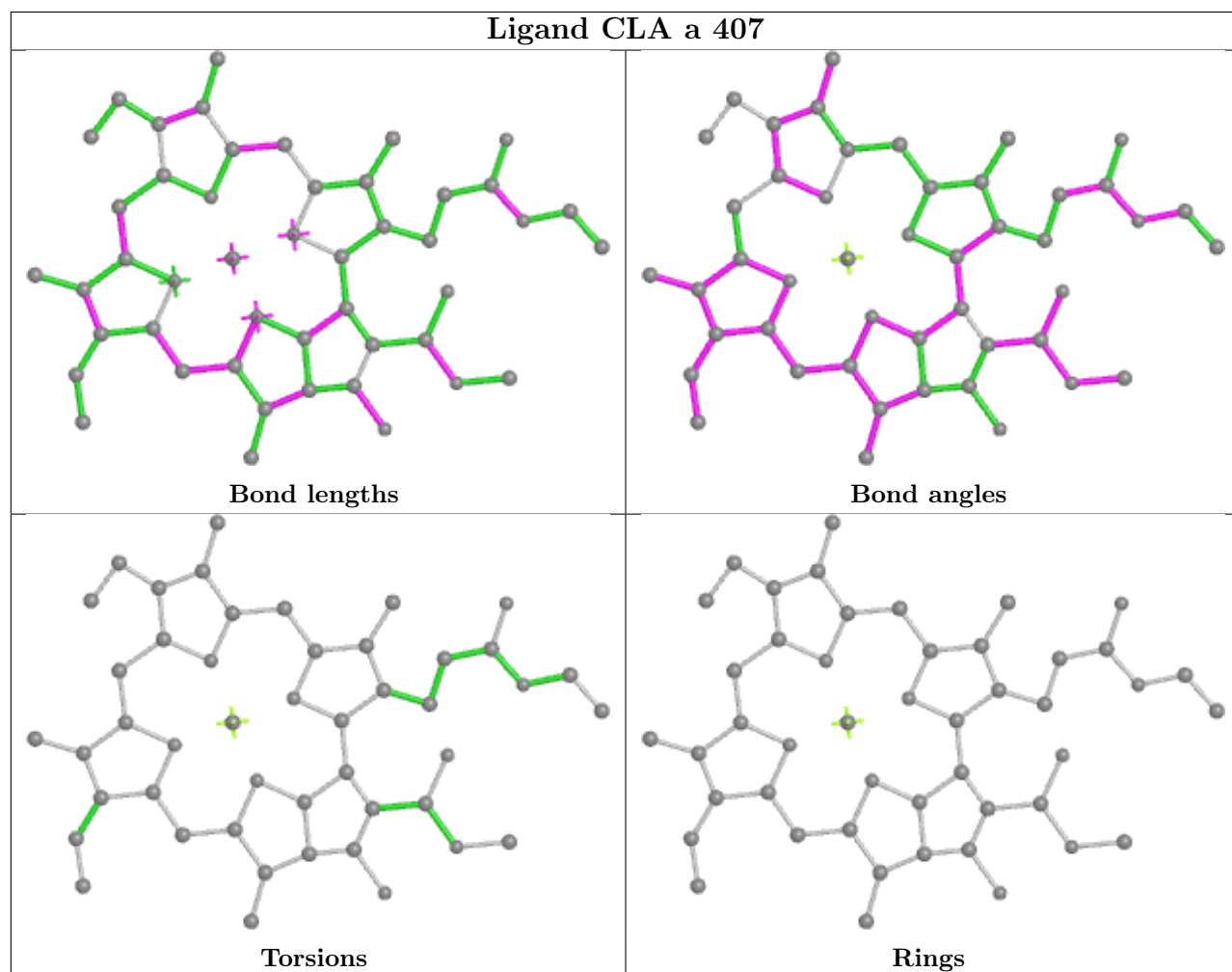


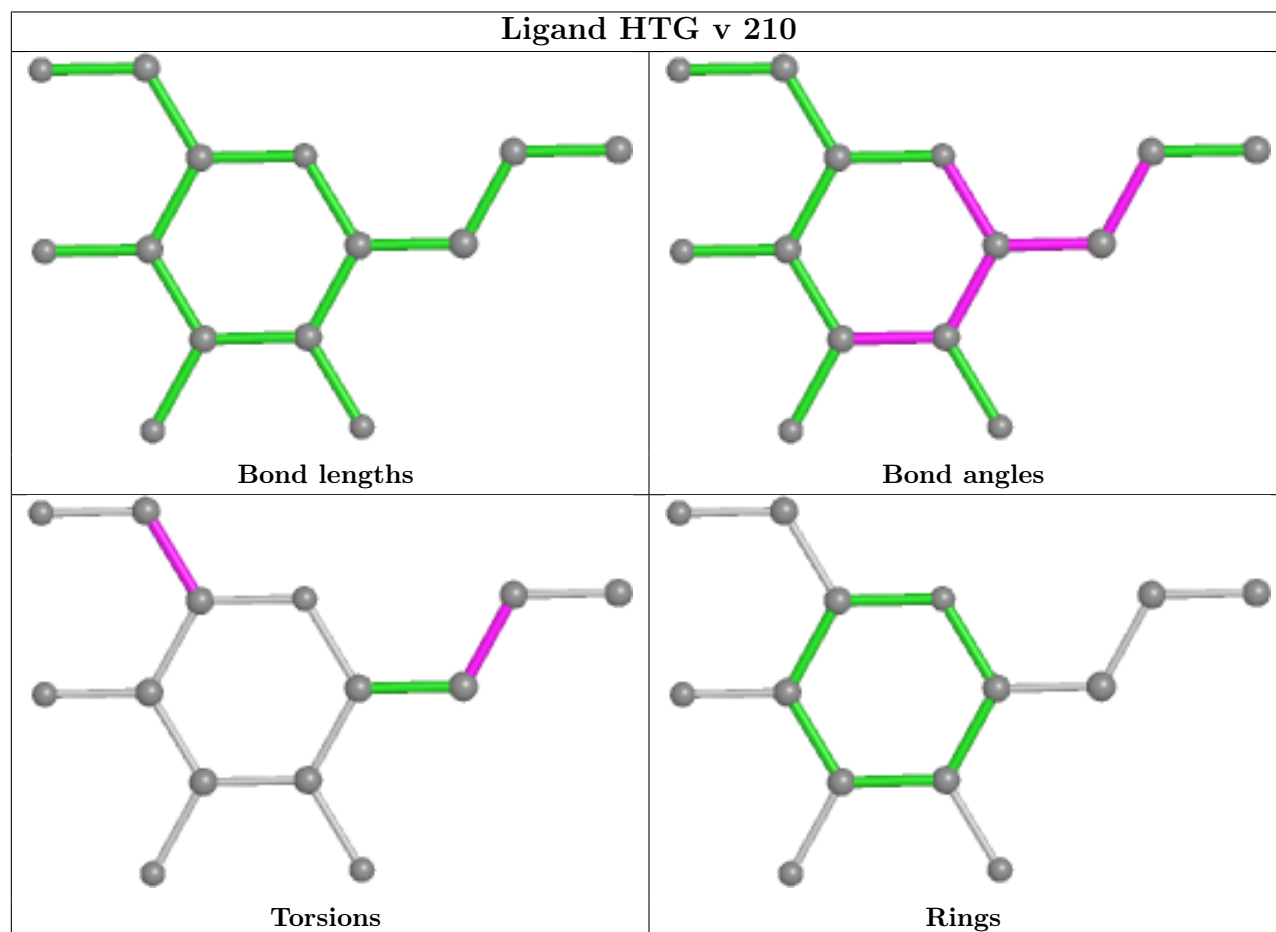
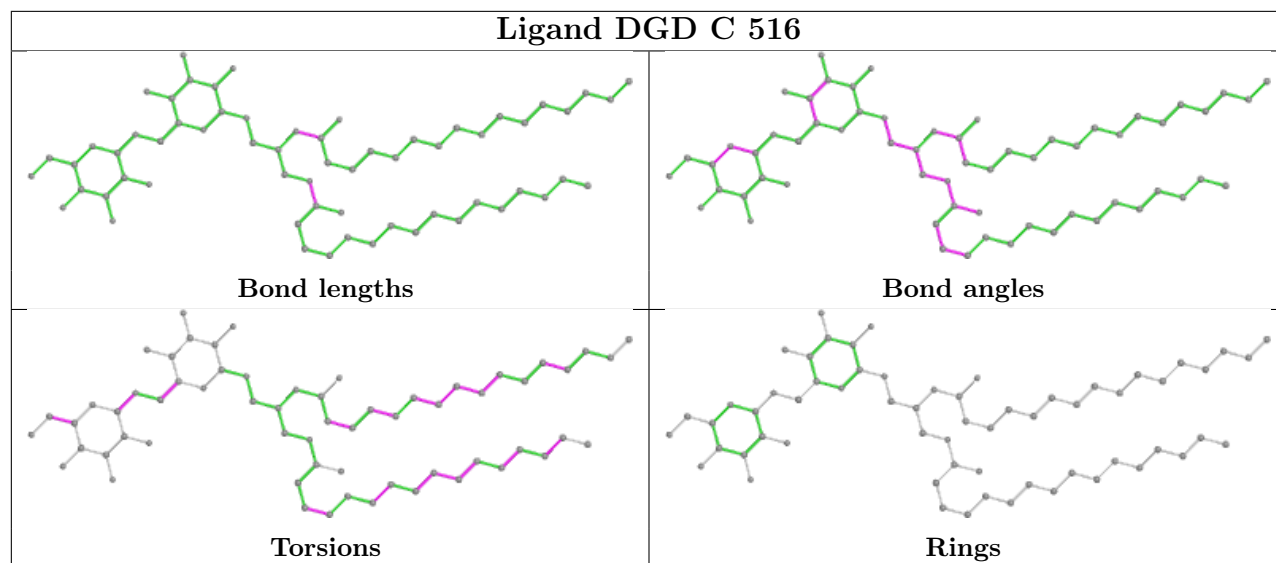


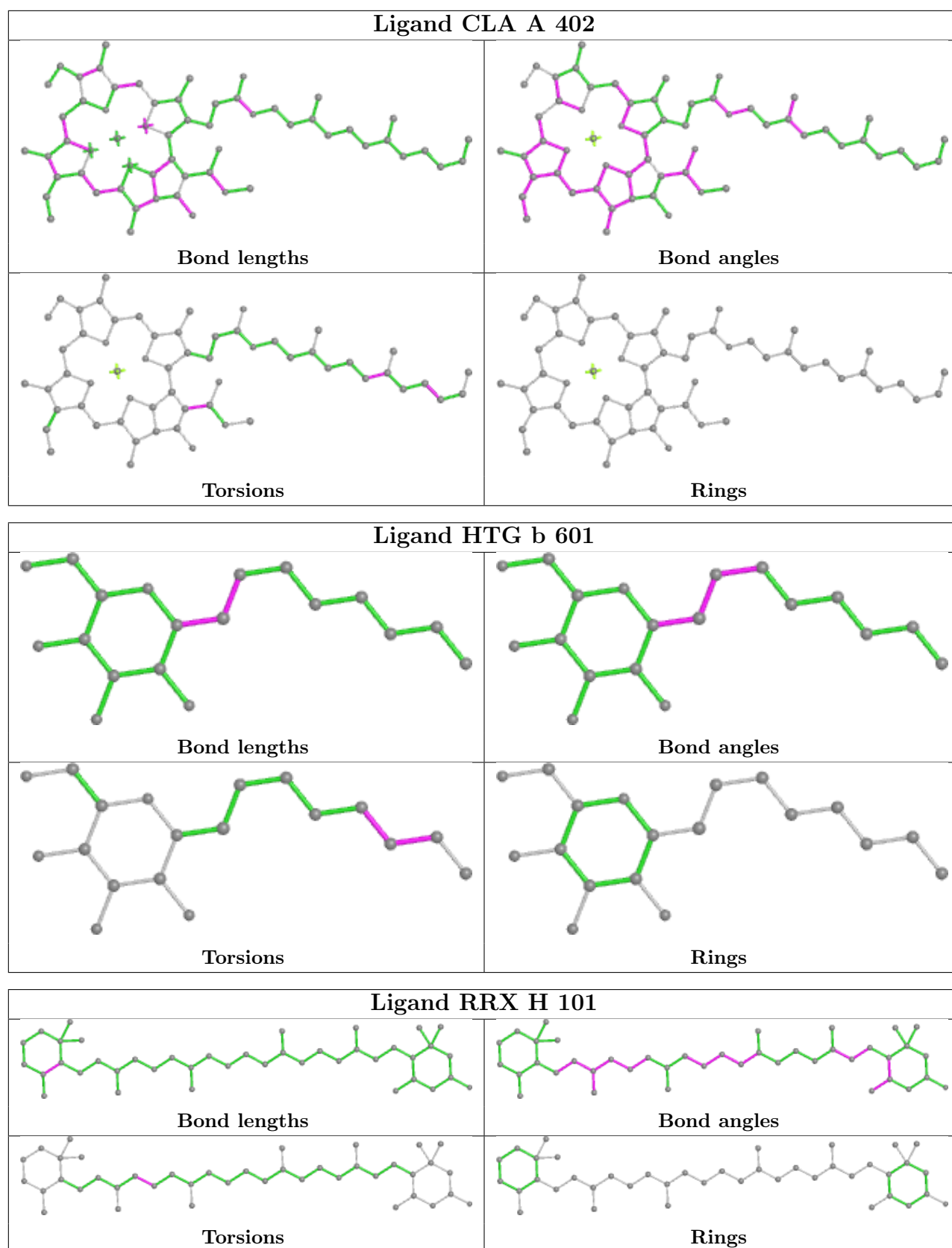
## Ligand CLA B 612



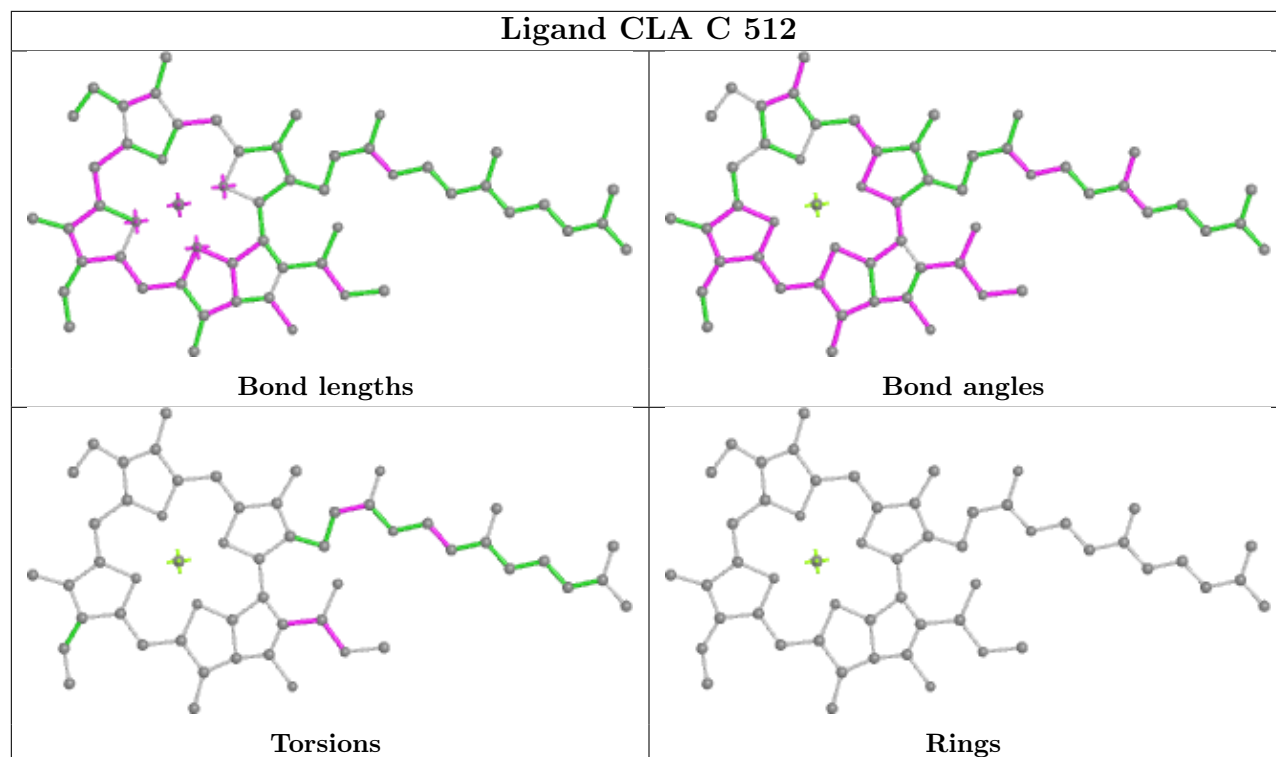
## Ligand CLA a 407



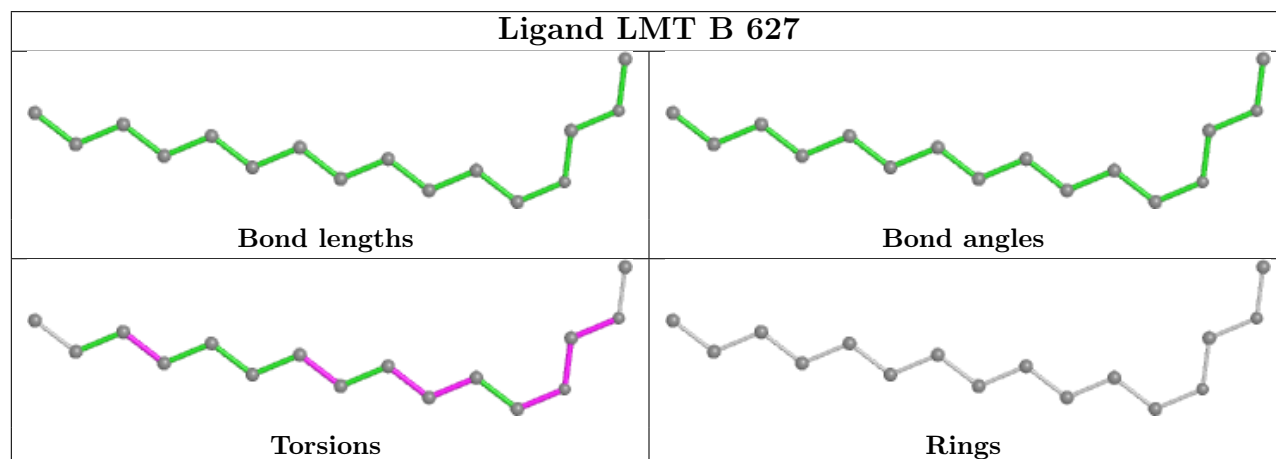


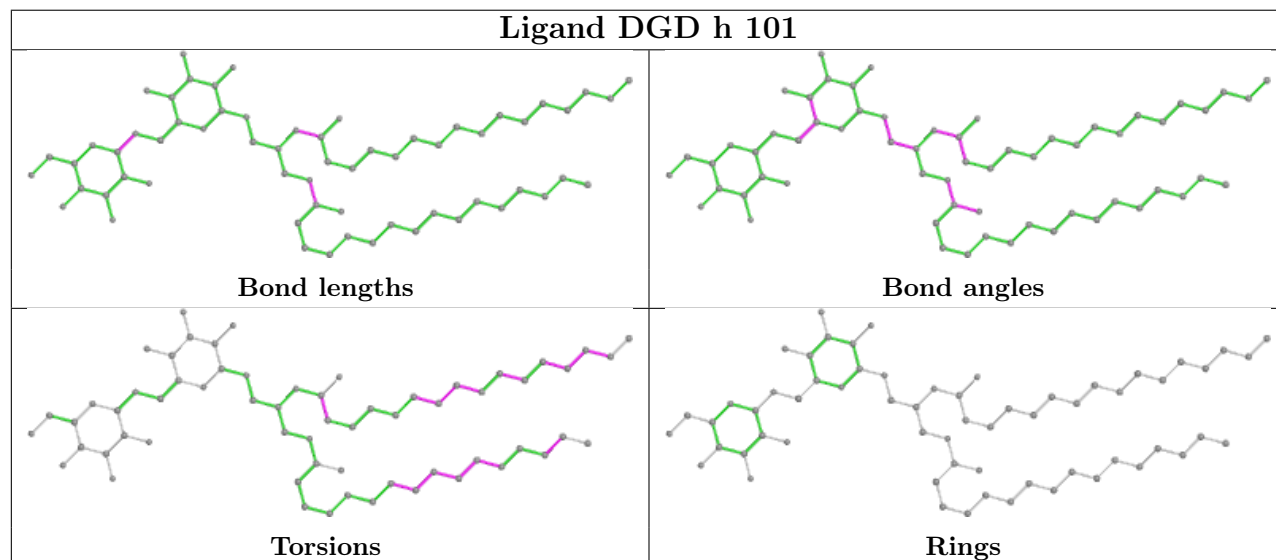
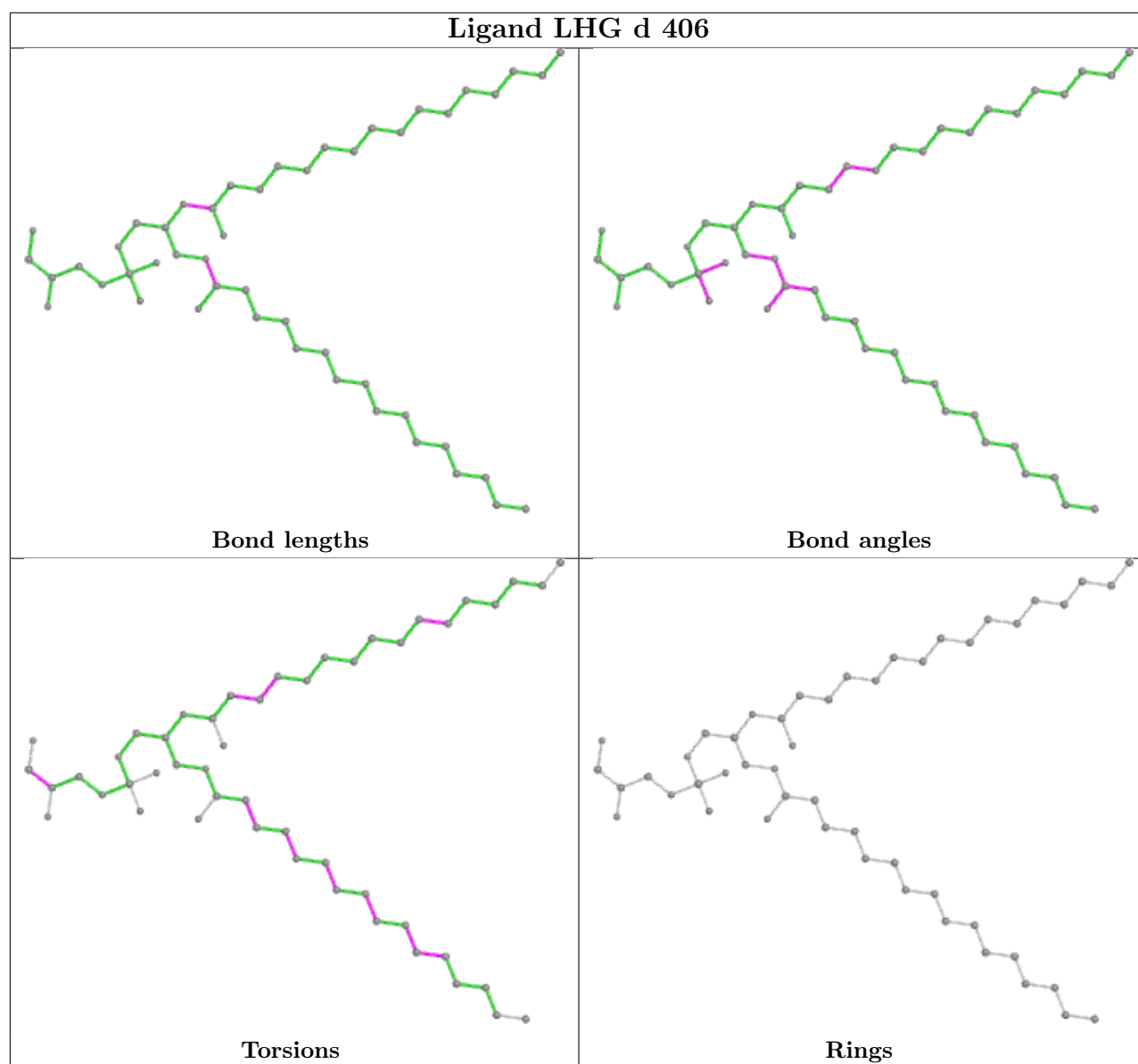


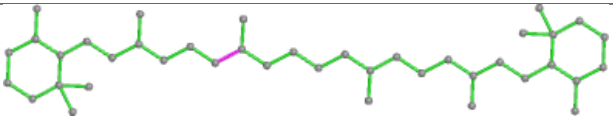
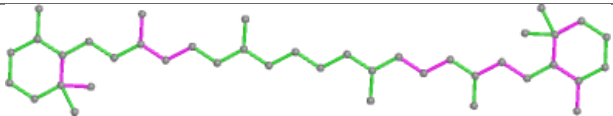
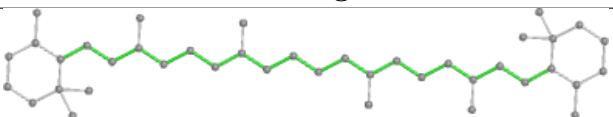
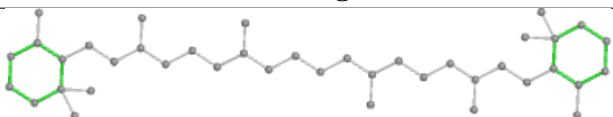
## Ligand CLA C 512

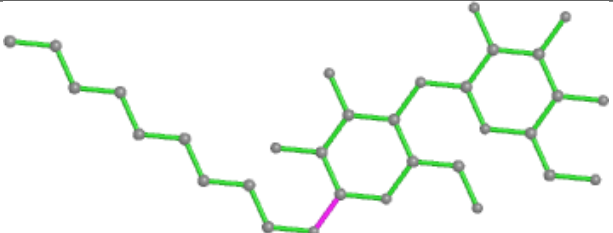
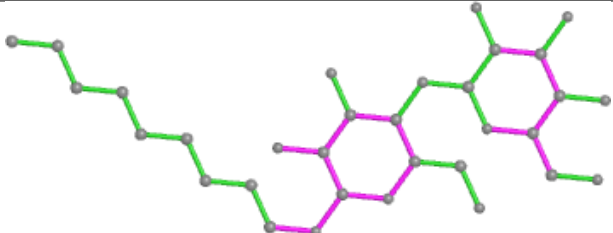
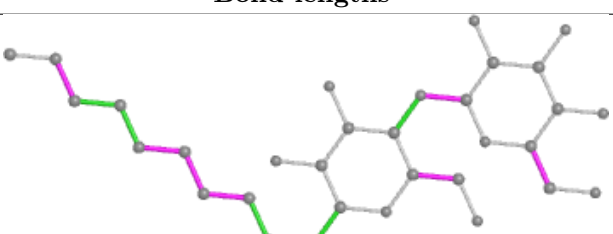
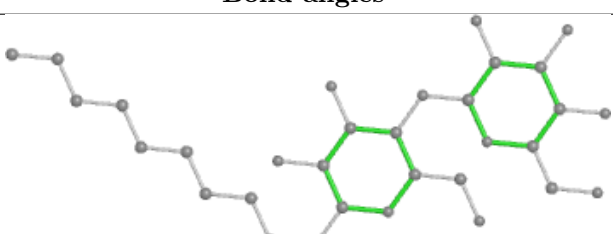


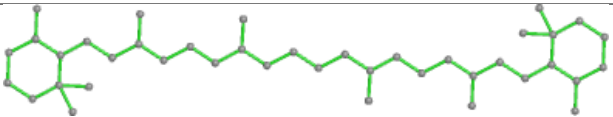
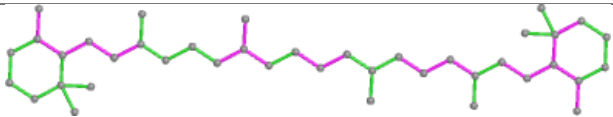
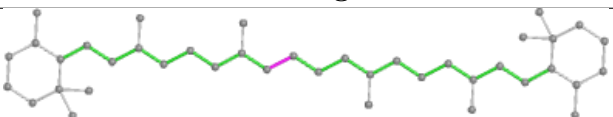
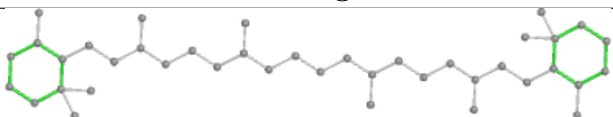
## Ligand LMT B 627

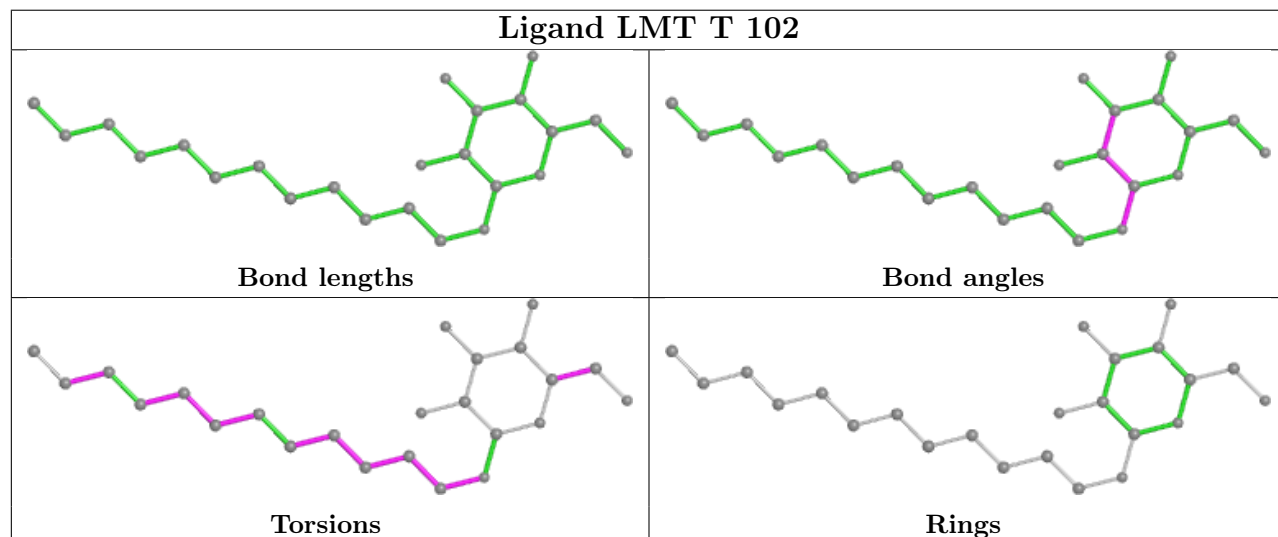
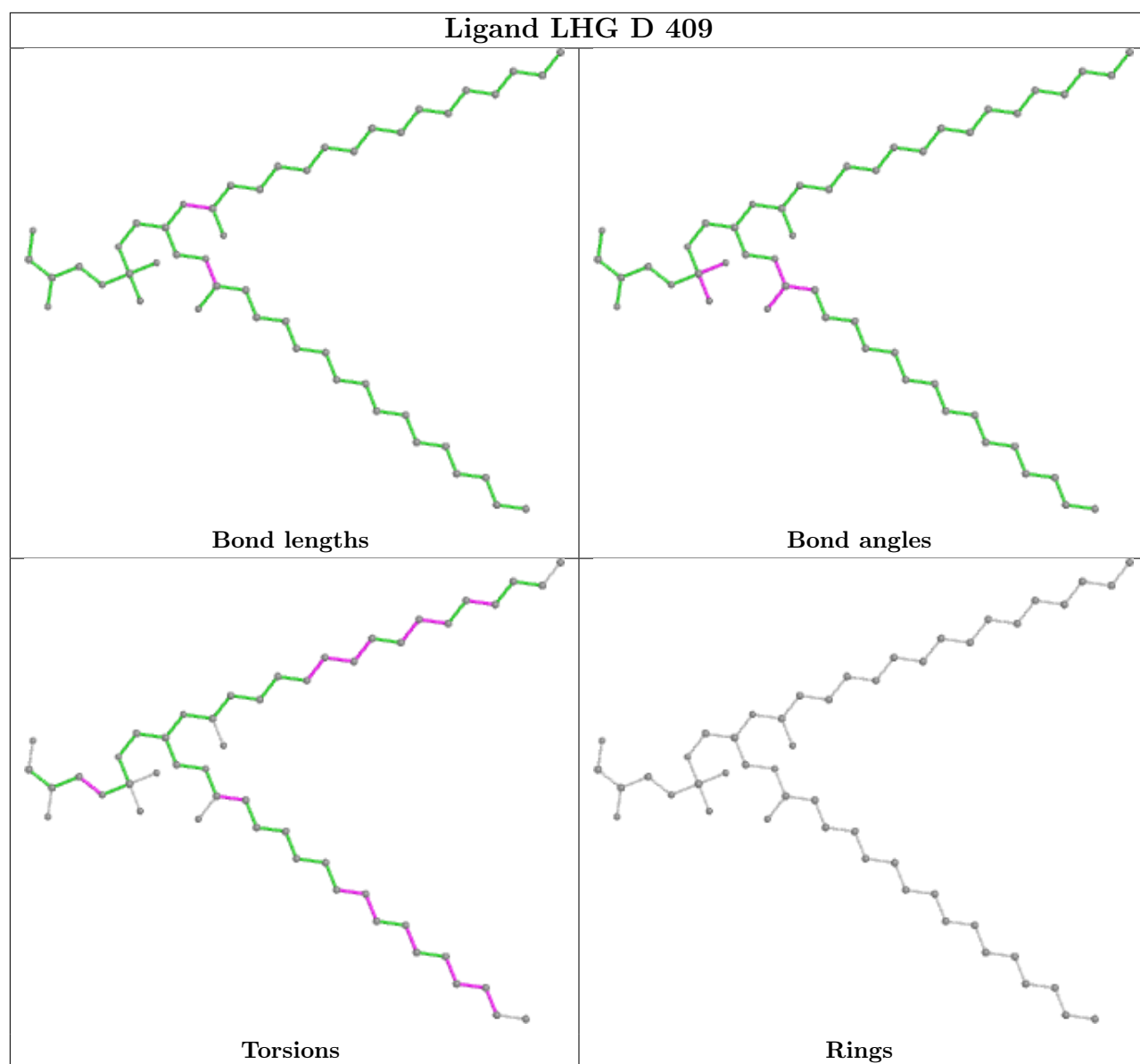




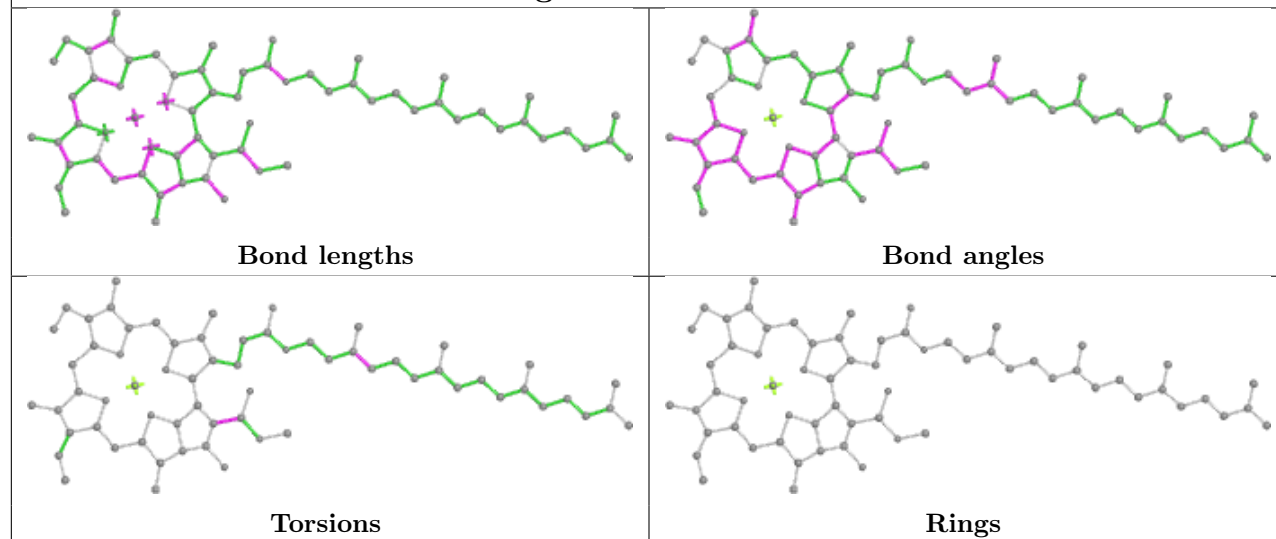
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT b 627	
	
Bond lengths	Bond angles
	
Torsions	Rings

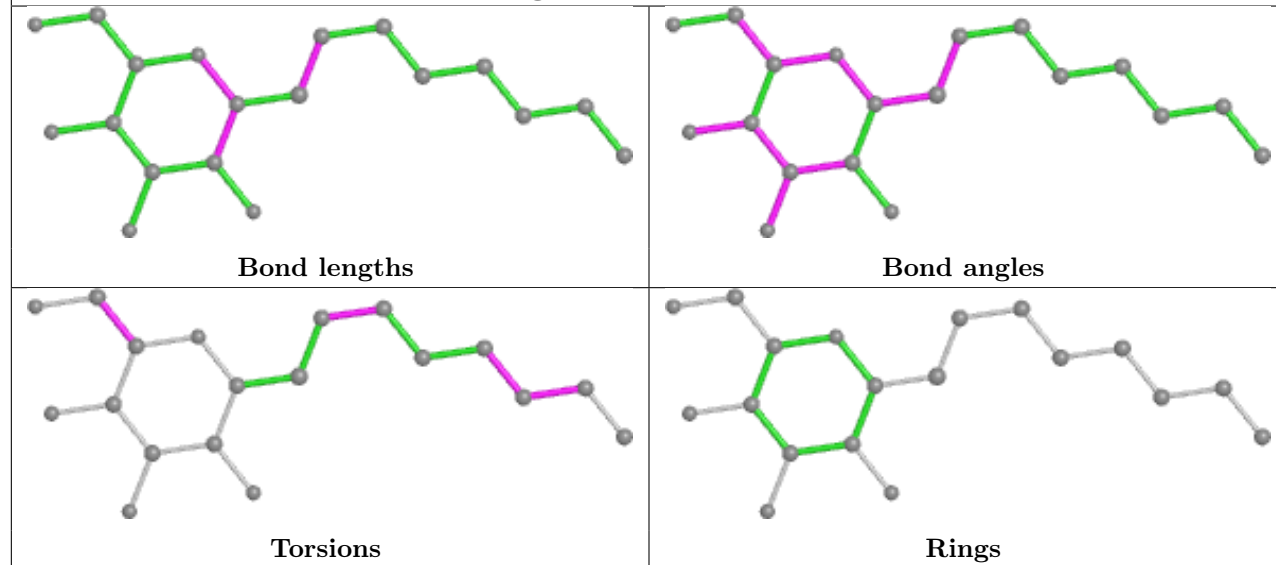
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



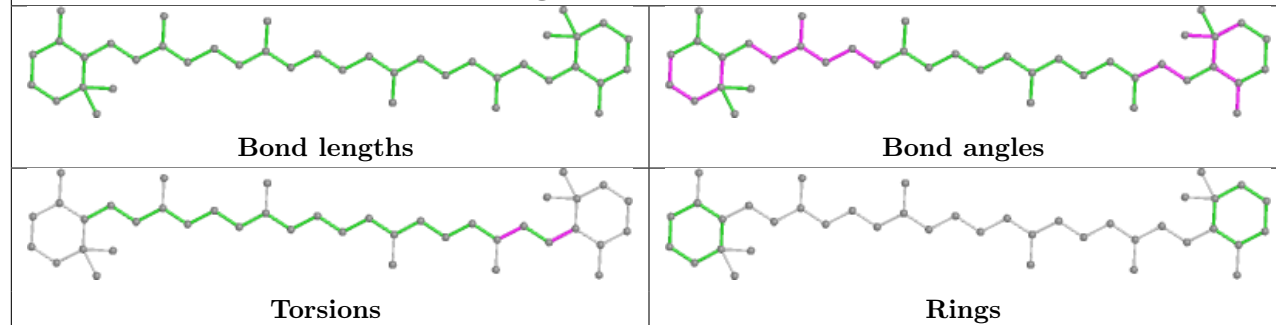
## Ligand CLA b 607



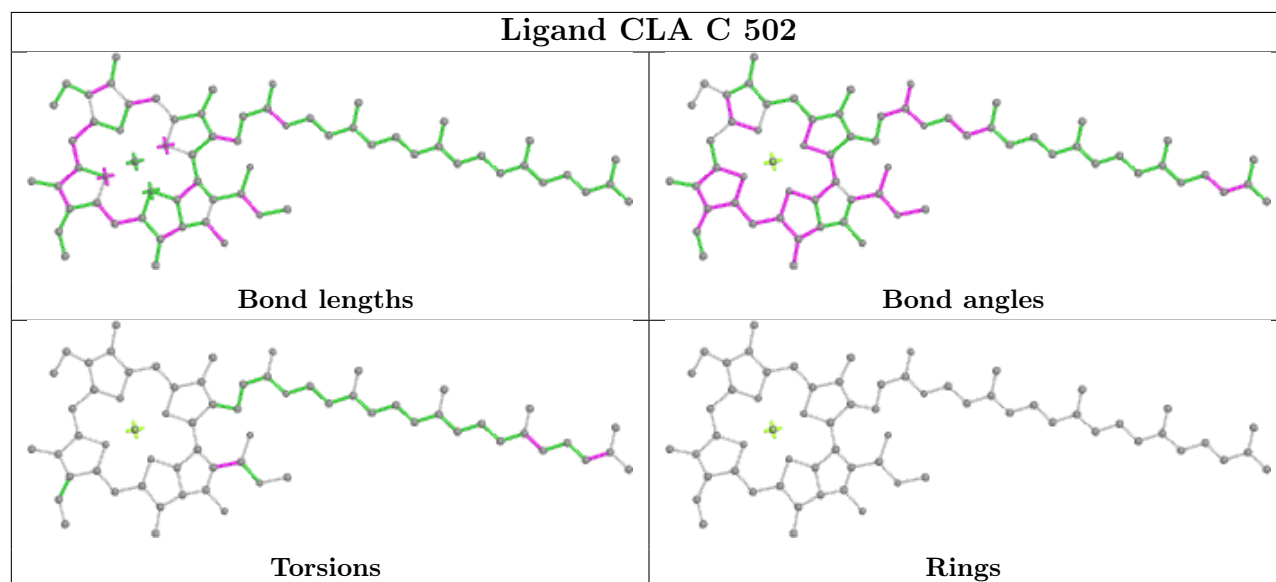
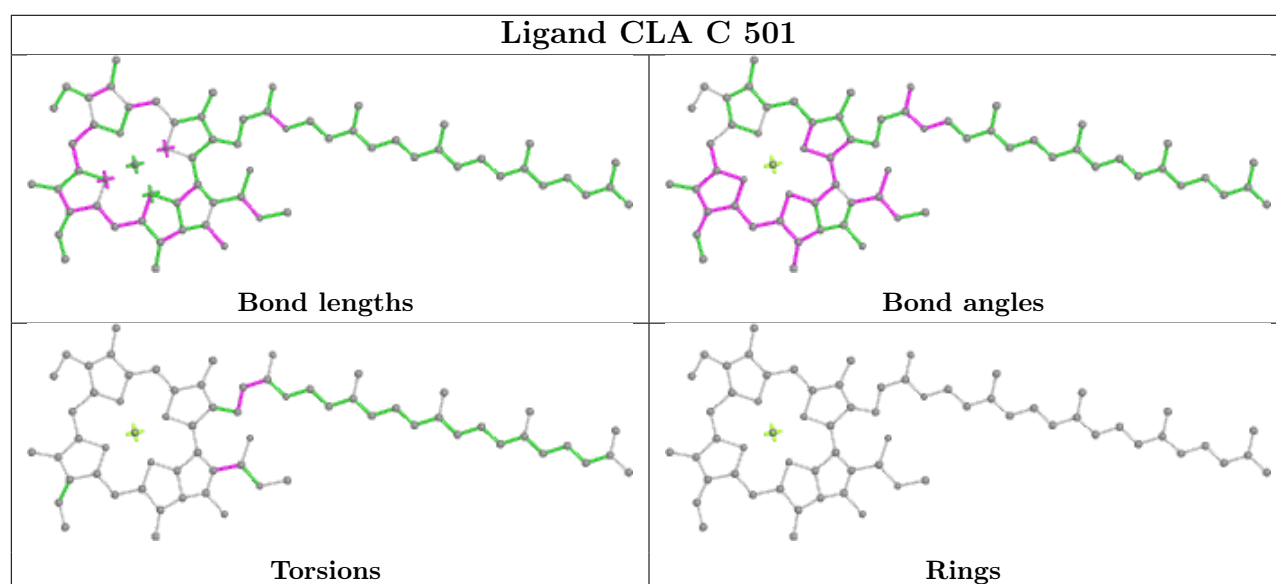
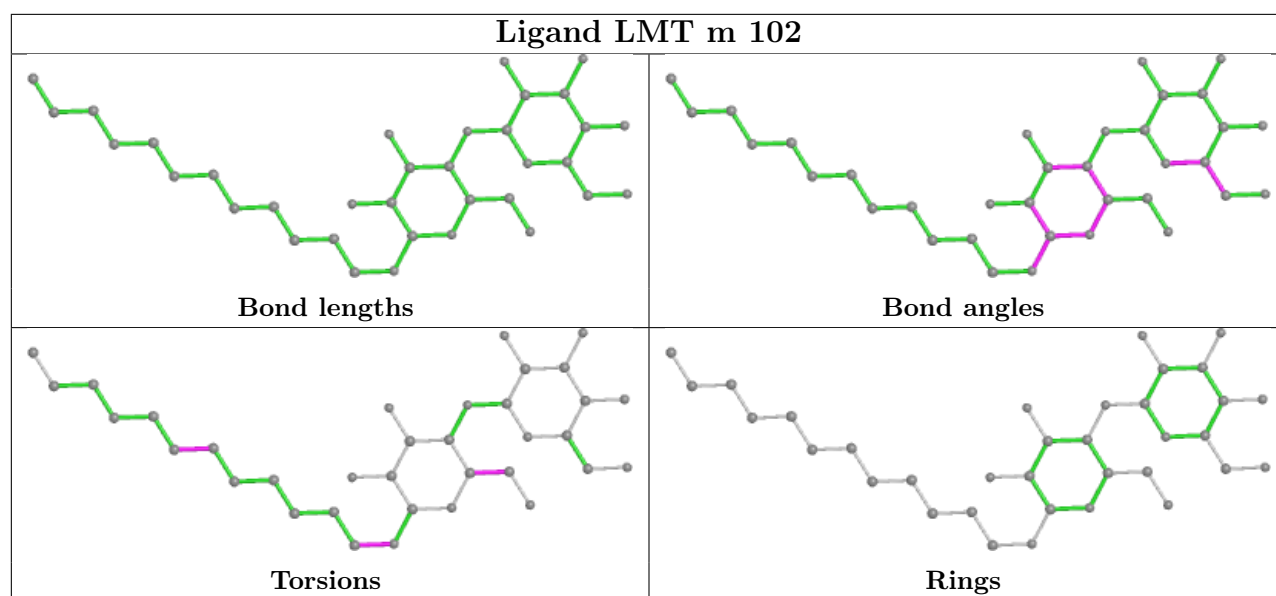
## Ligand HTG B 621

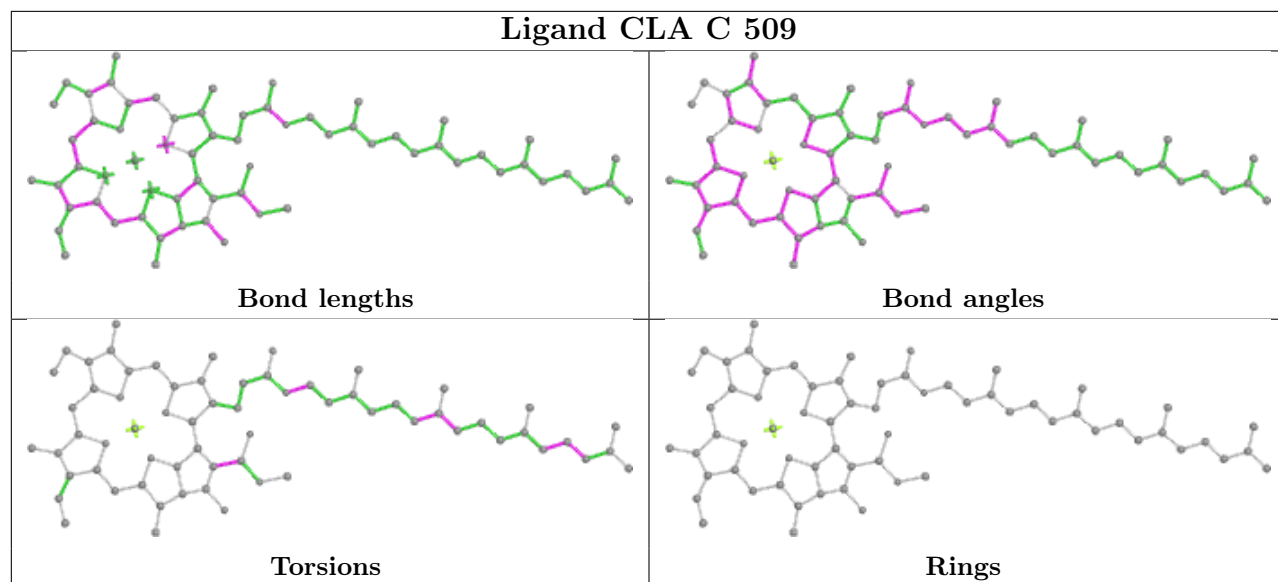
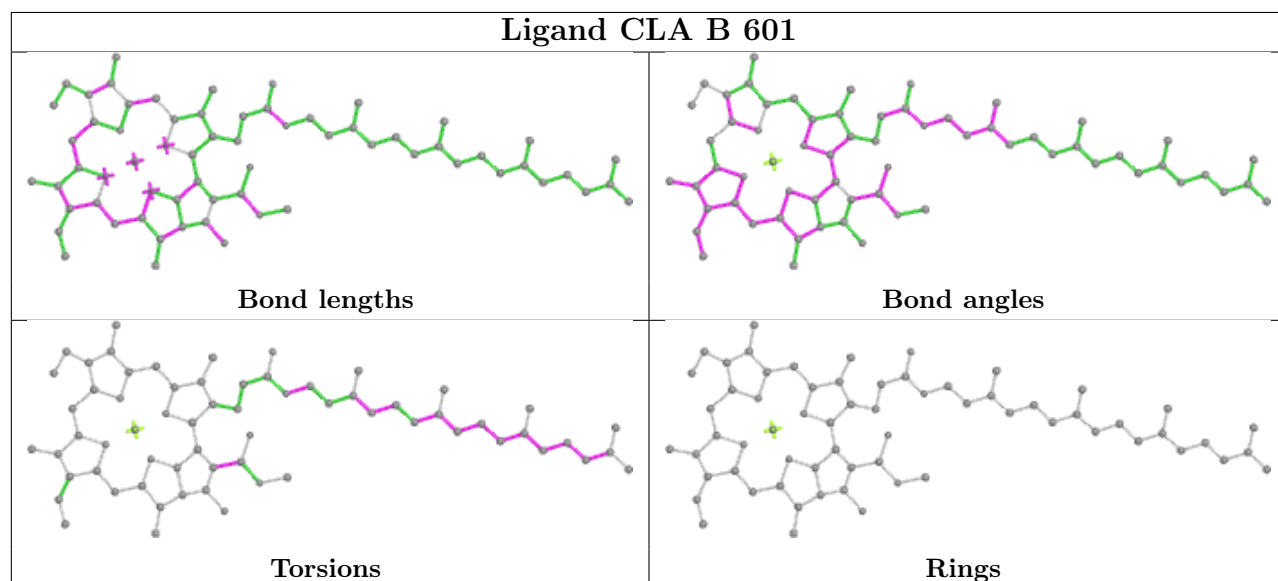
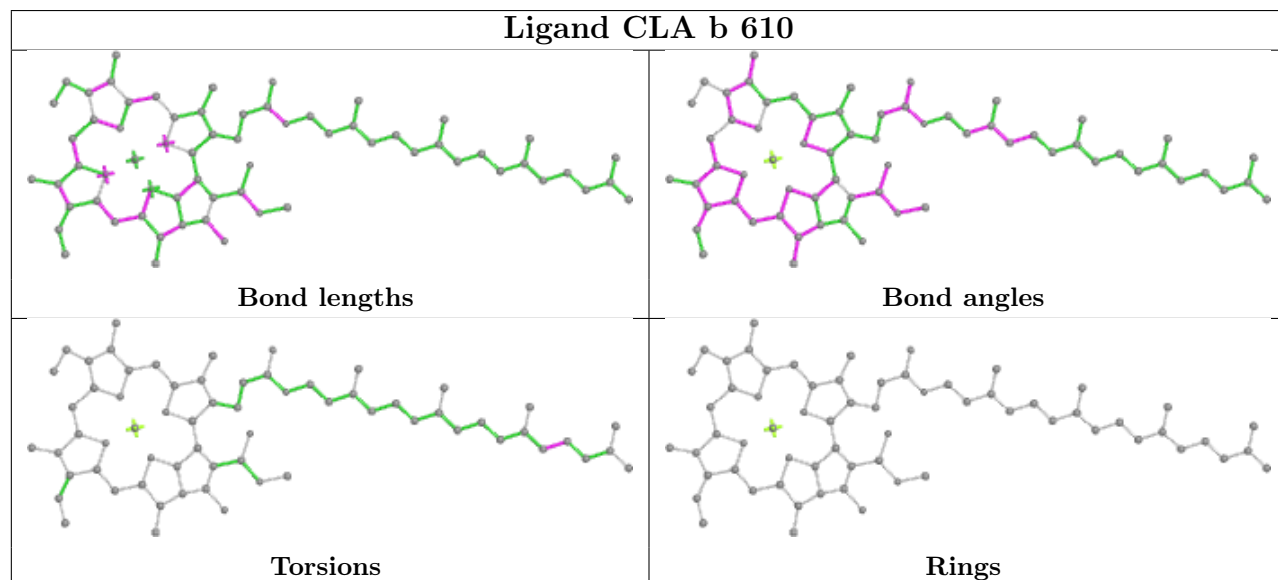


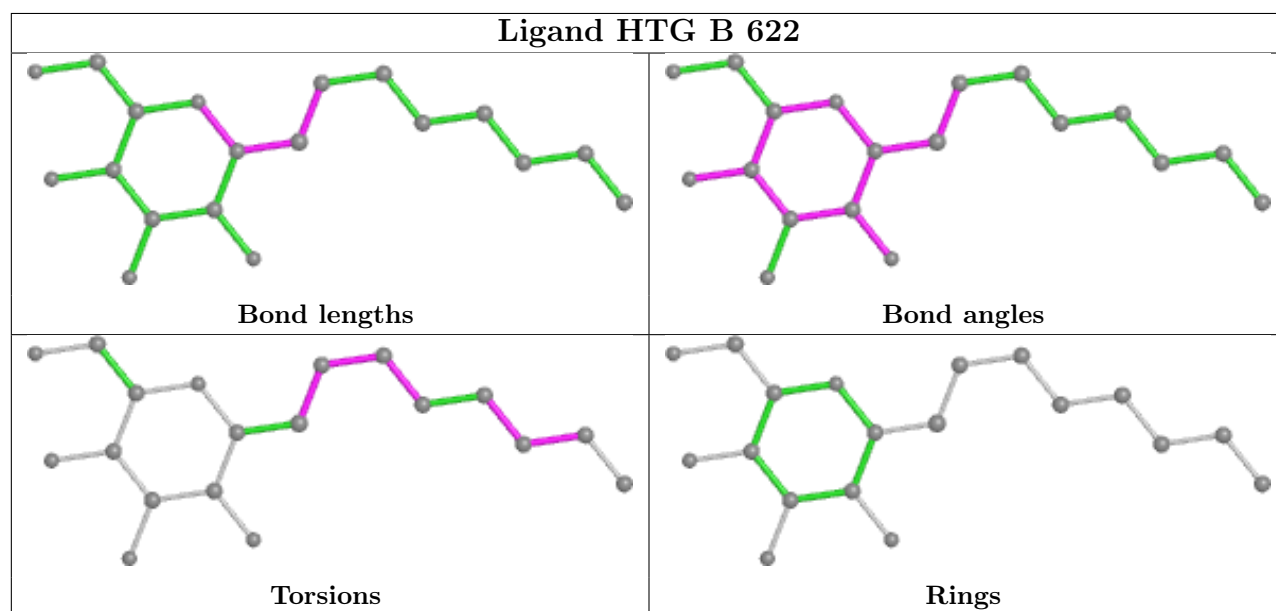
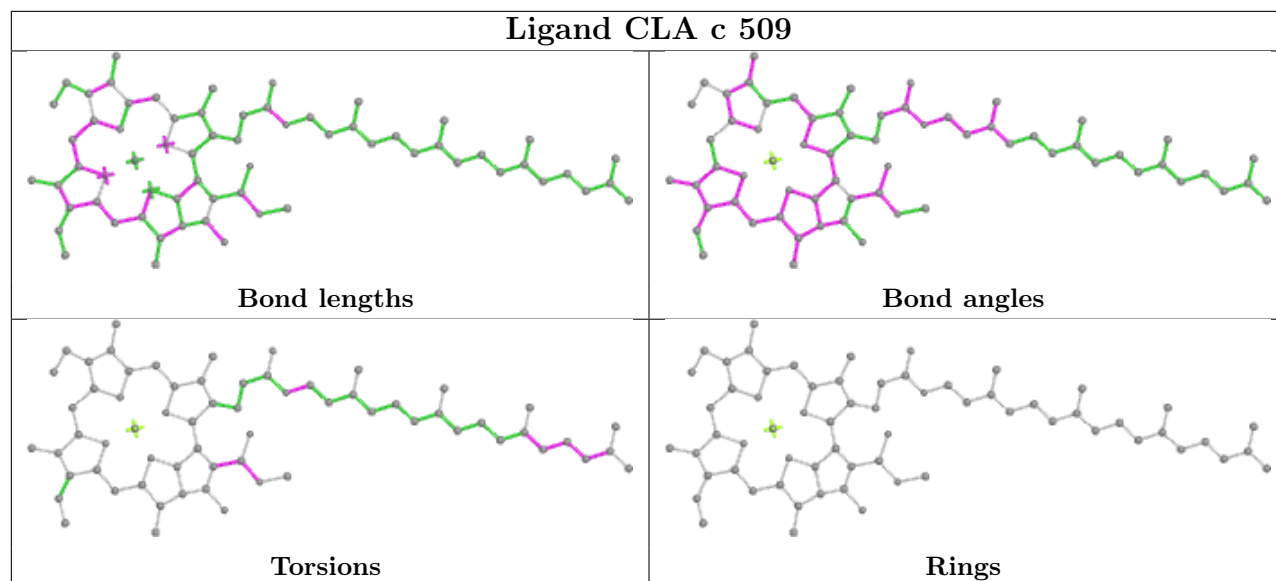
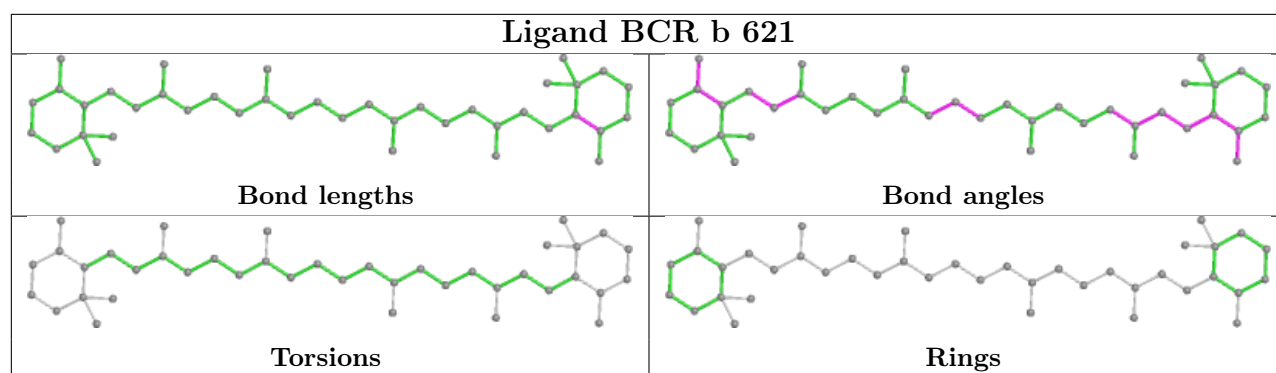
## Ligand BCR d 405

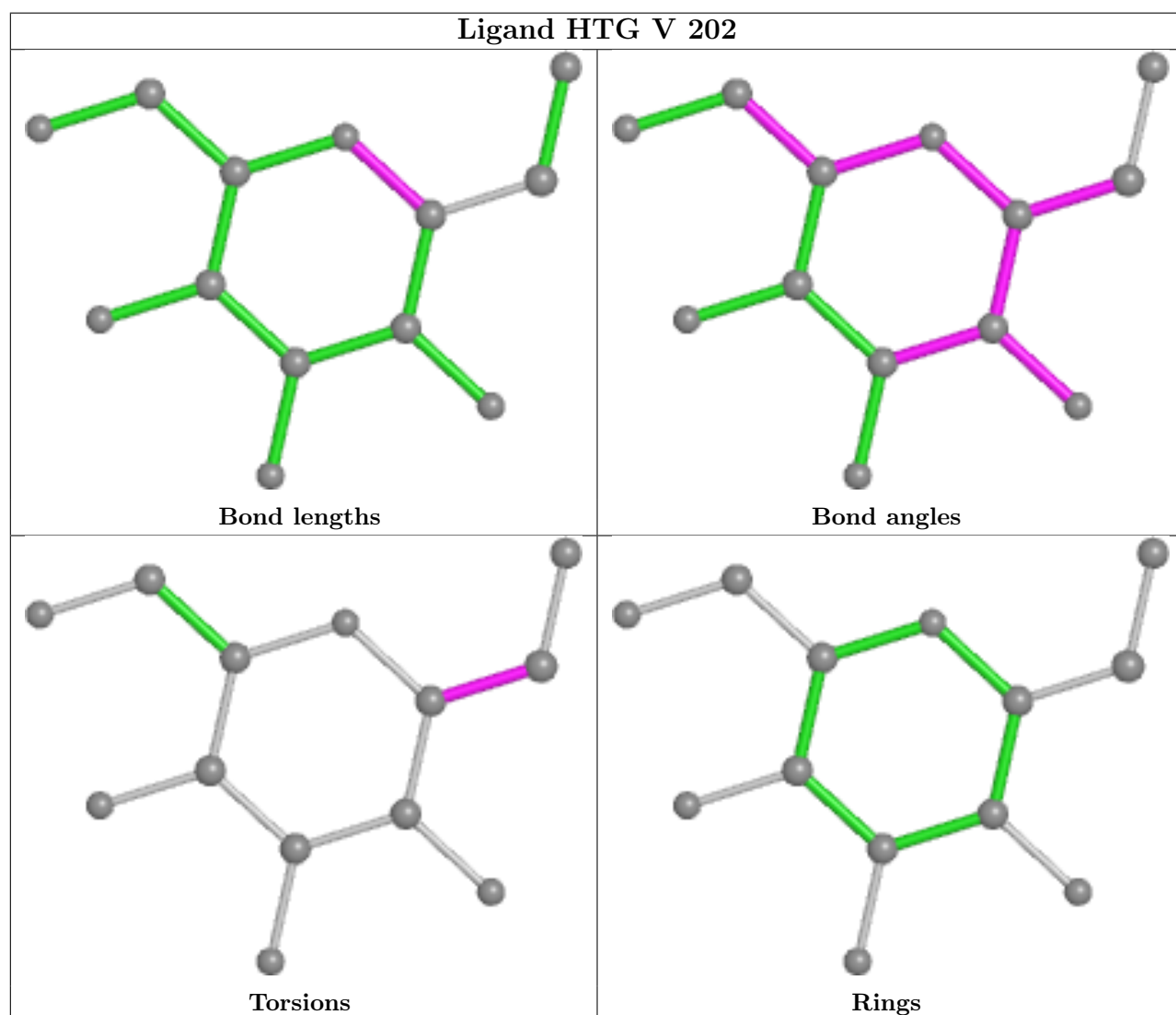
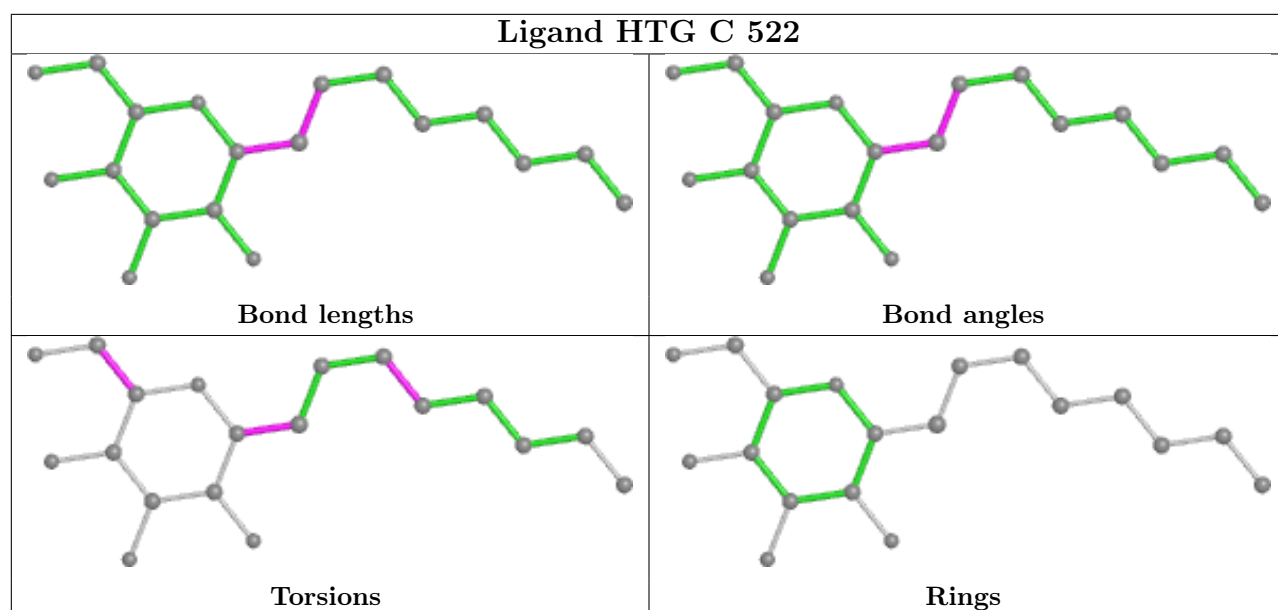


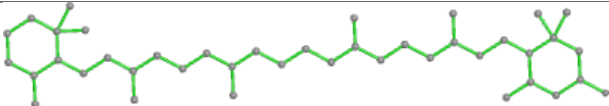
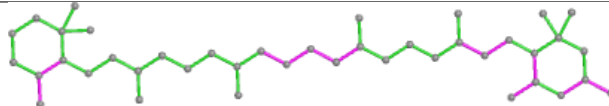
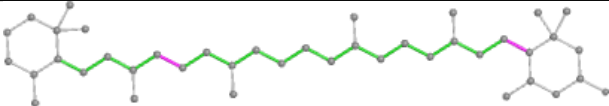
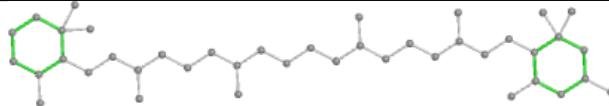


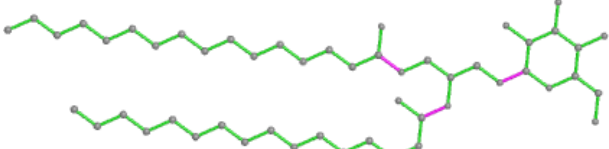
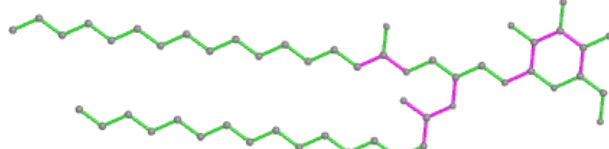
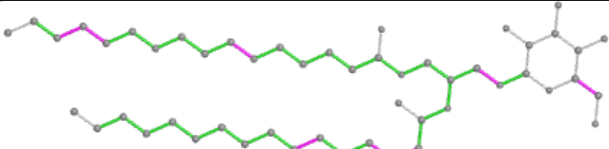



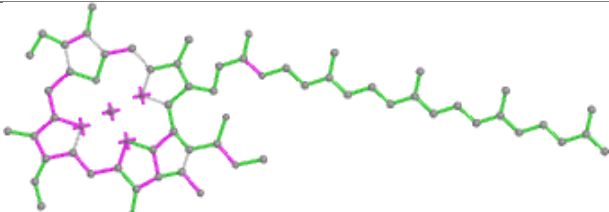
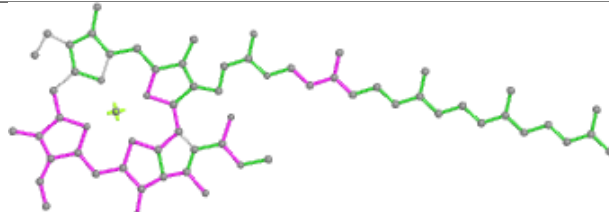
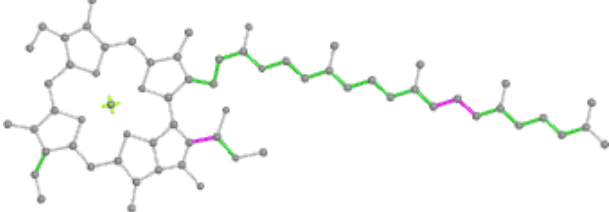
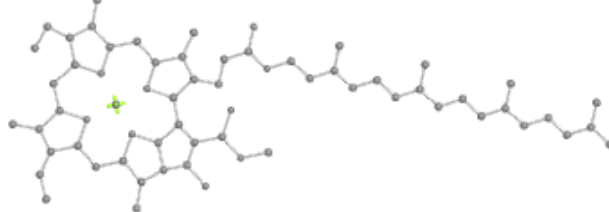
**Ligand CLA C 509****Ligand CLA B 601****Ligand CLA b 610**

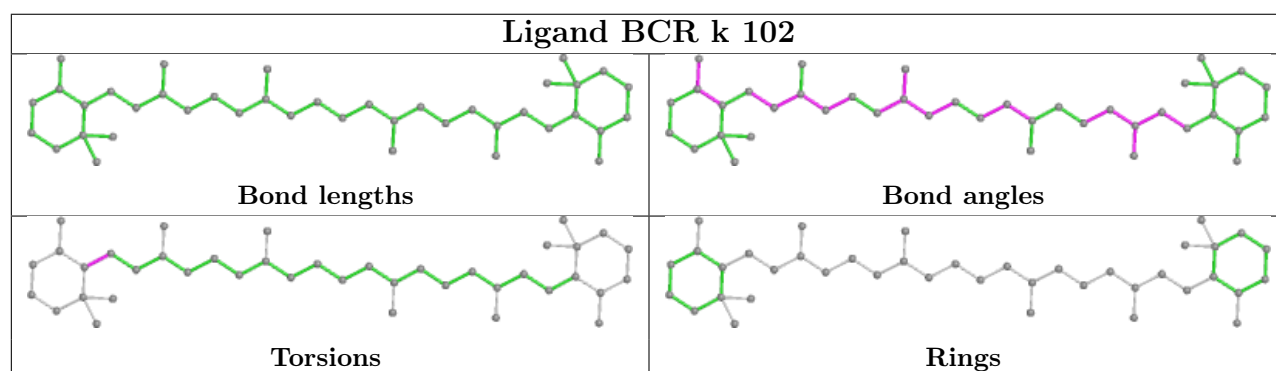
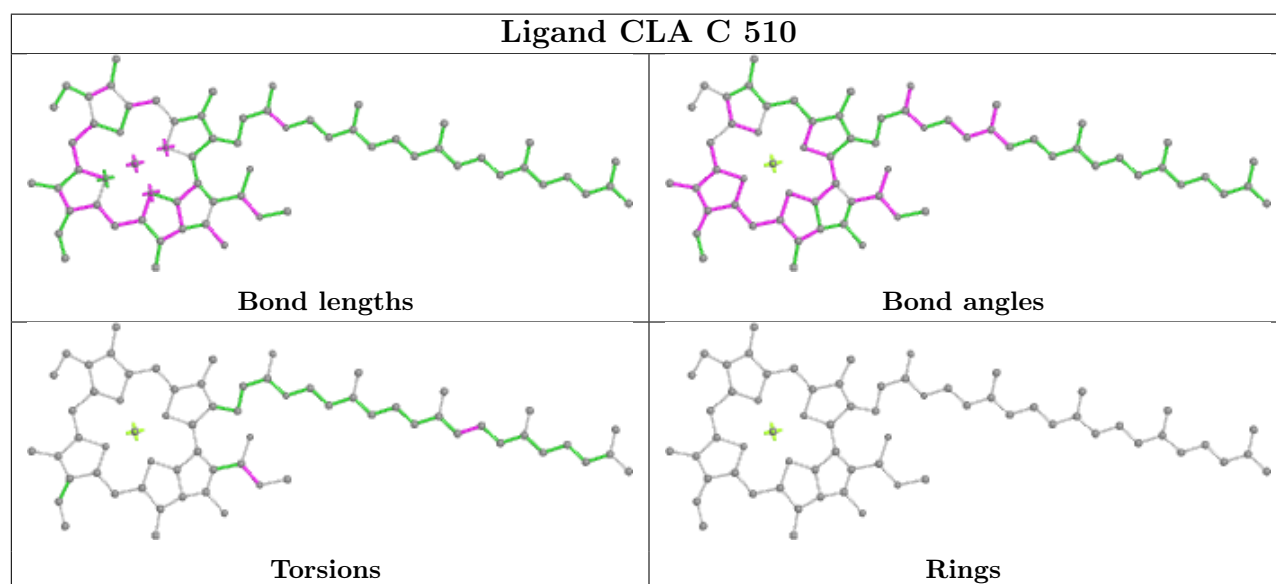
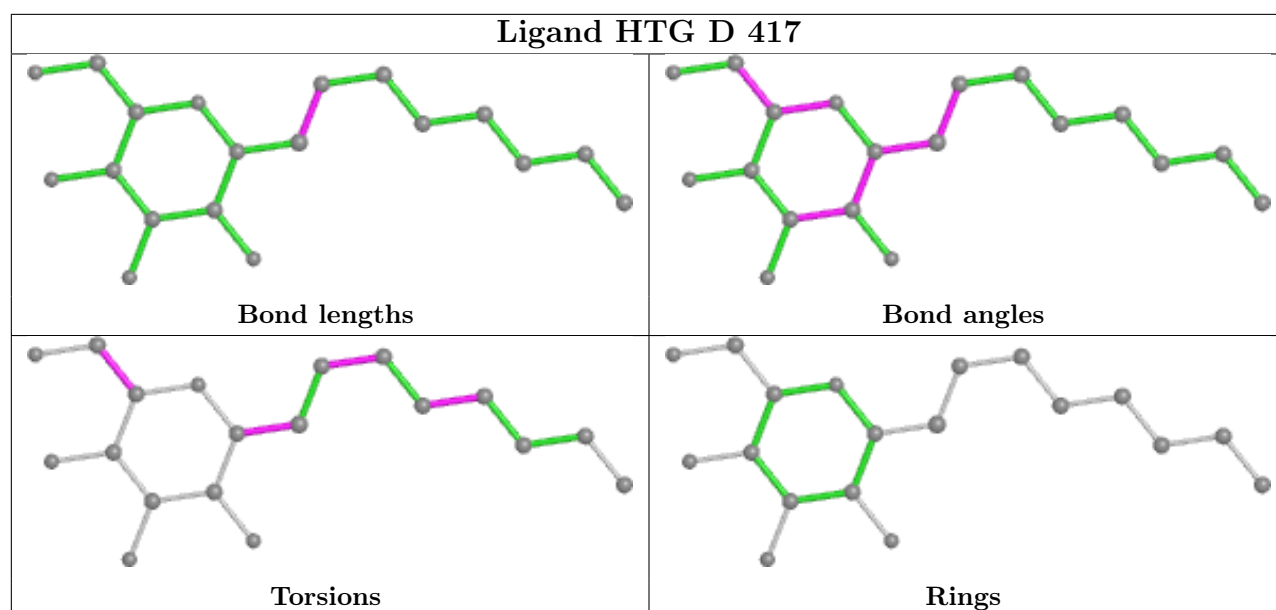


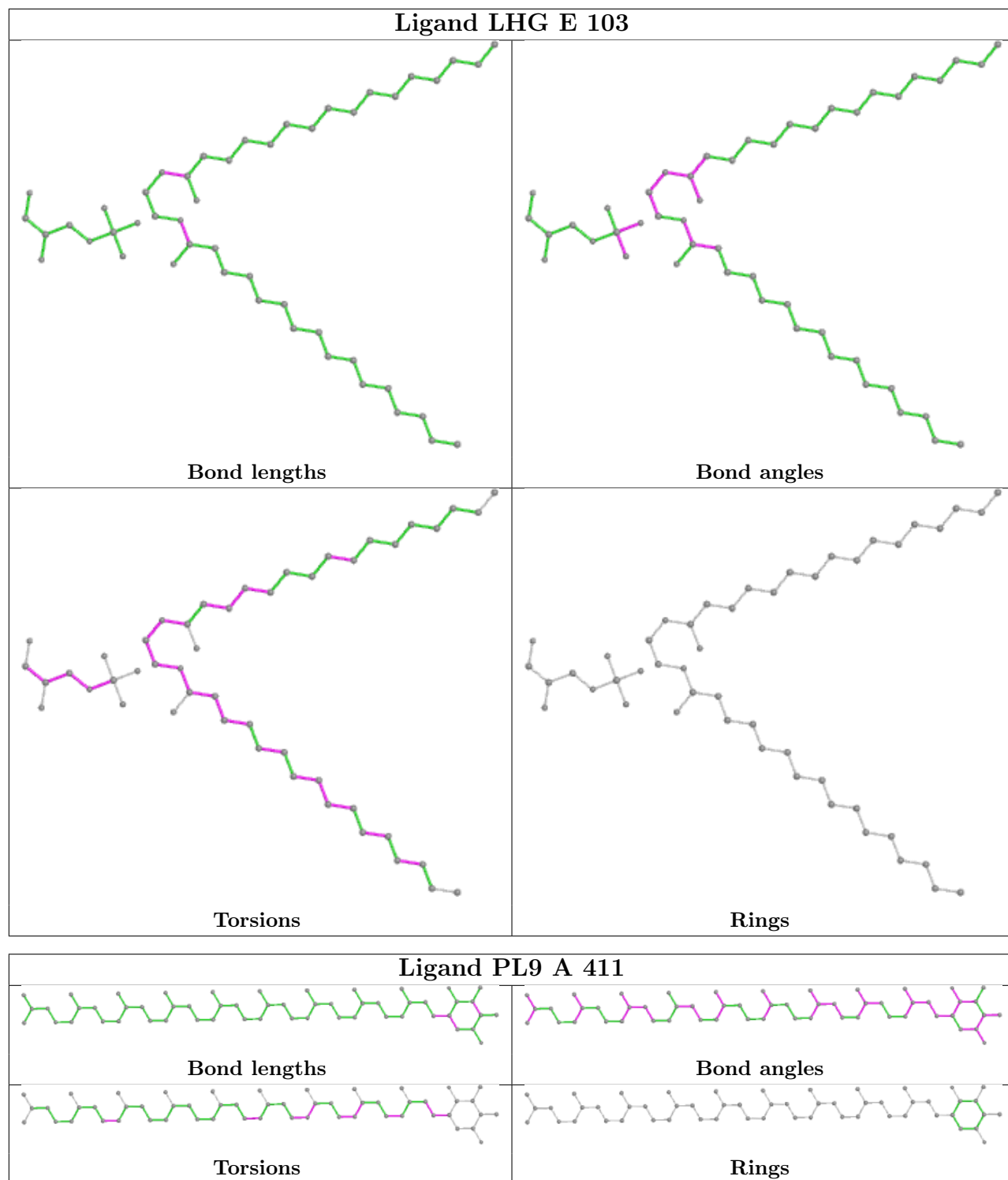


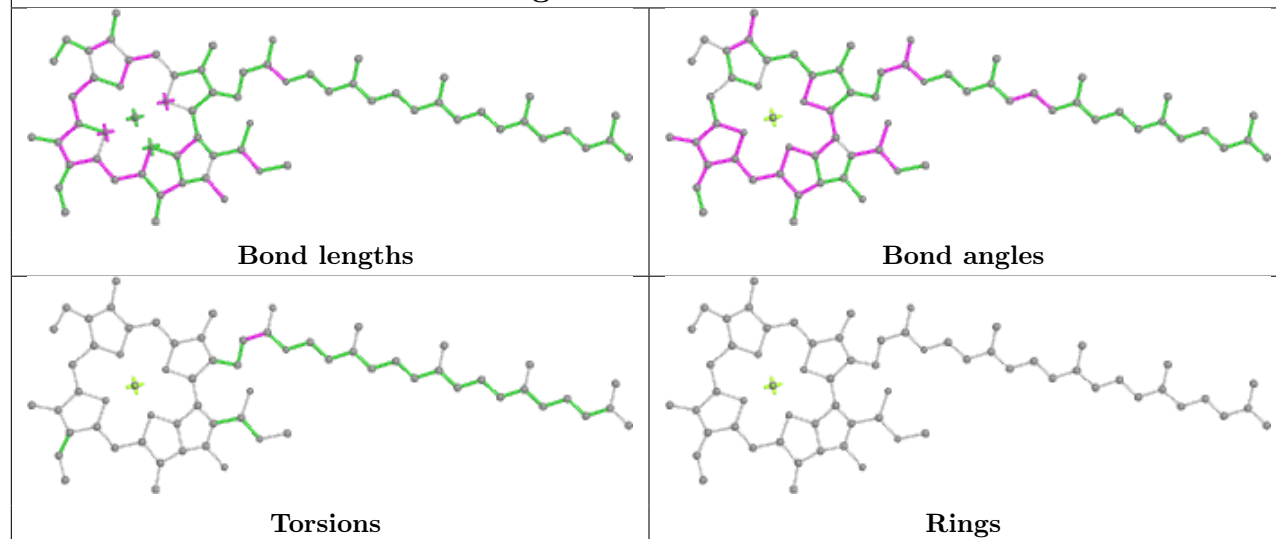
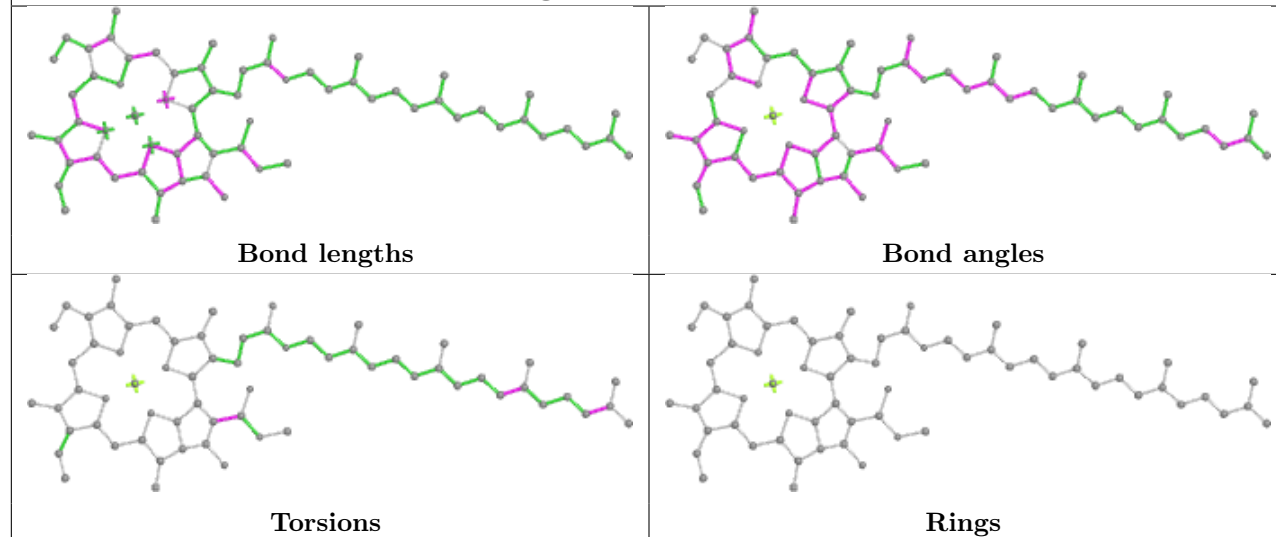
Ligand RRX x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

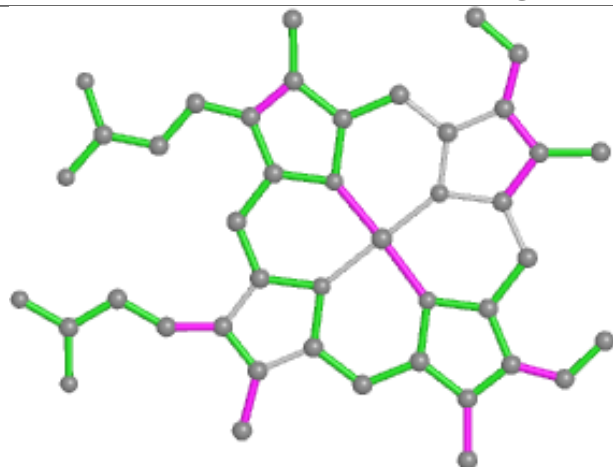




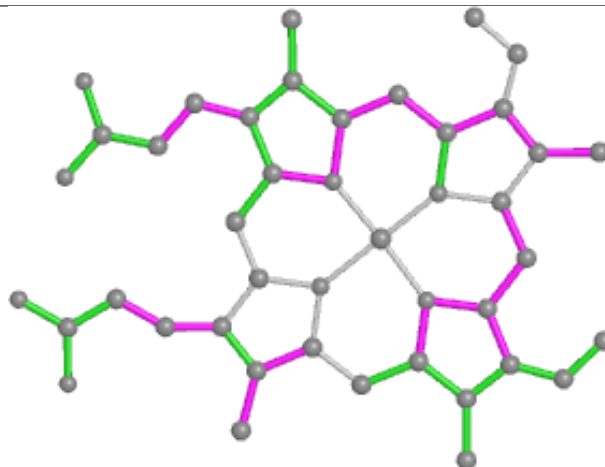
**Ligand CLA C 505****Ligand CLA c 502**



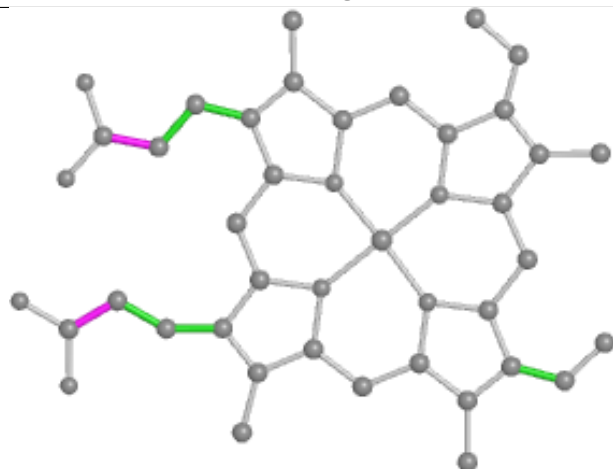
## Ligand HEM e 102



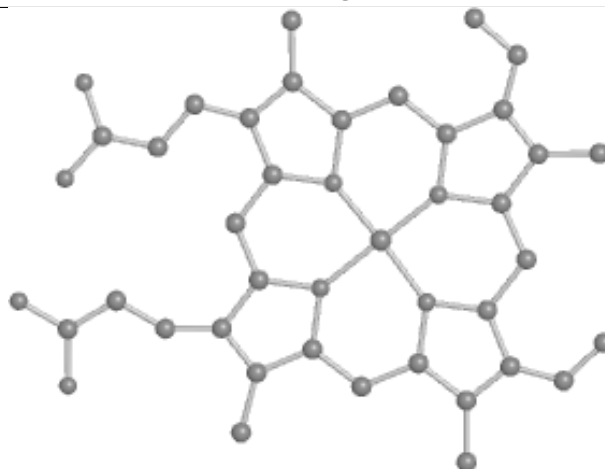
Bond lengths



Bond angles

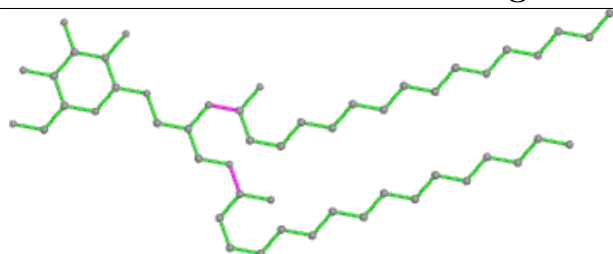


Torsions

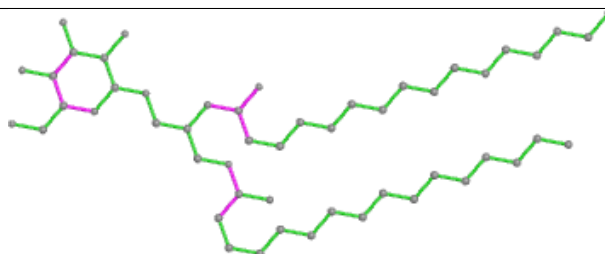


Rings

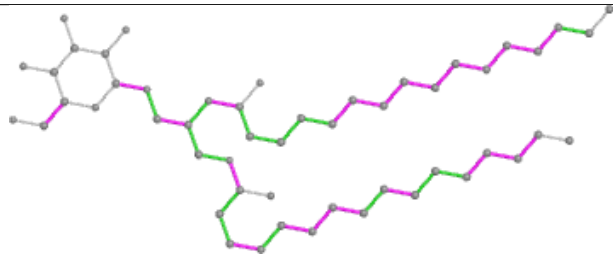
## Ligand DGD D 406



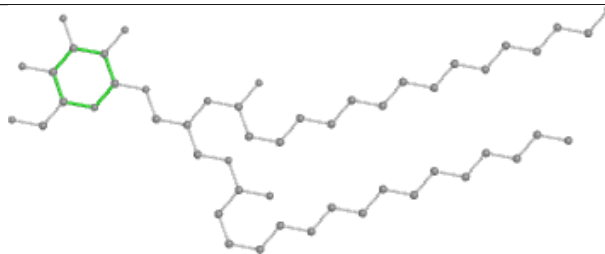
Bond lengths



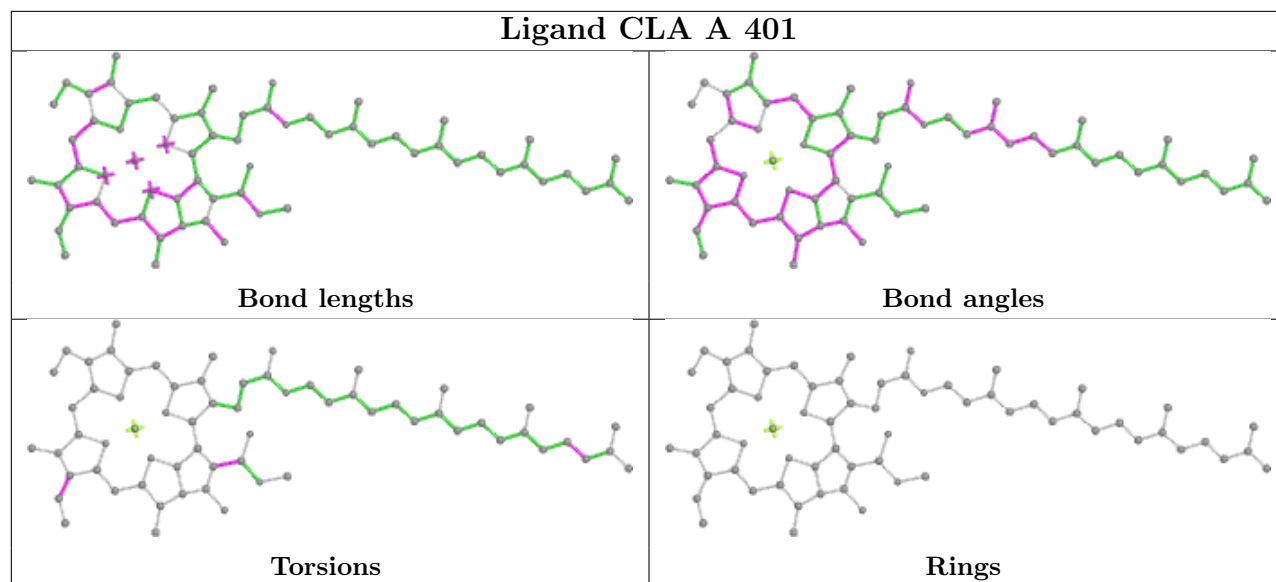
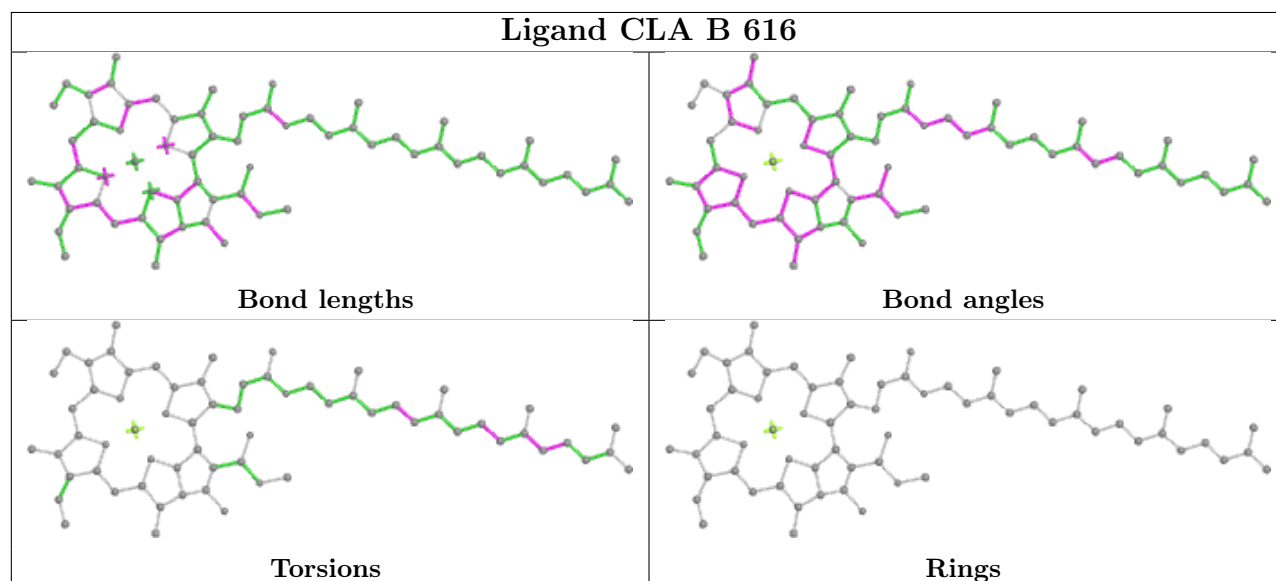
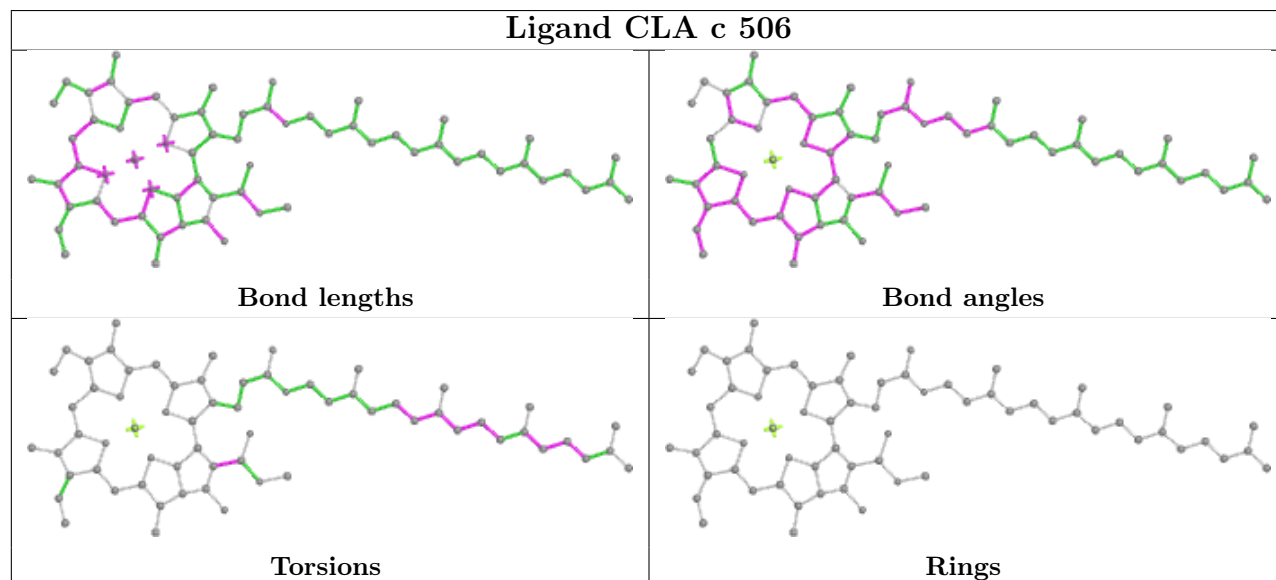
Bond angles

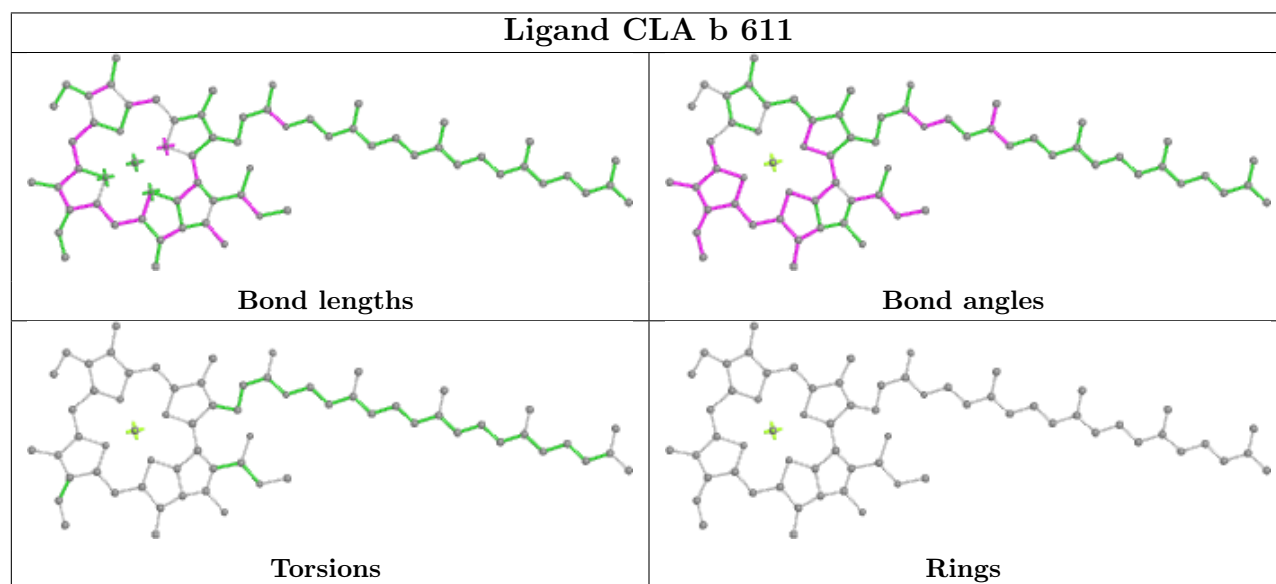
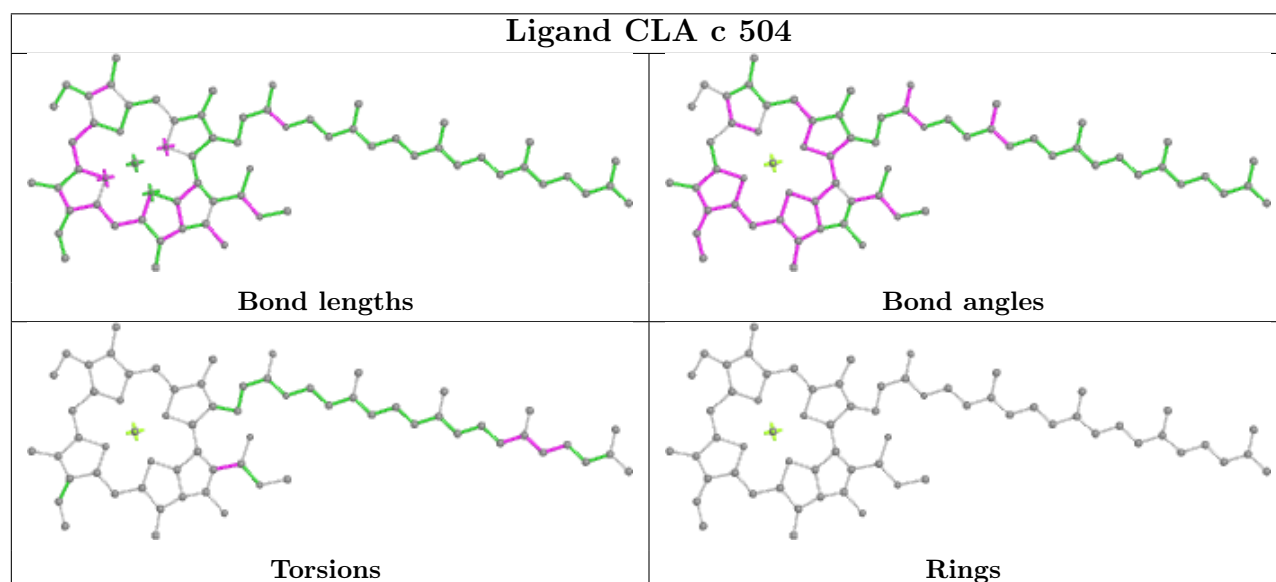
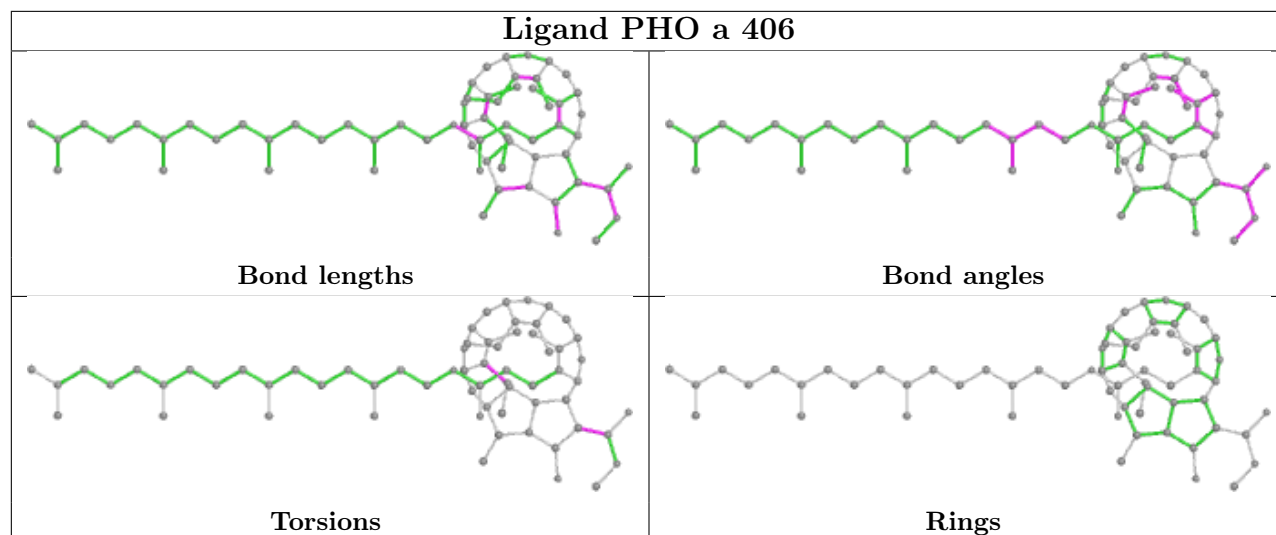


Torsions

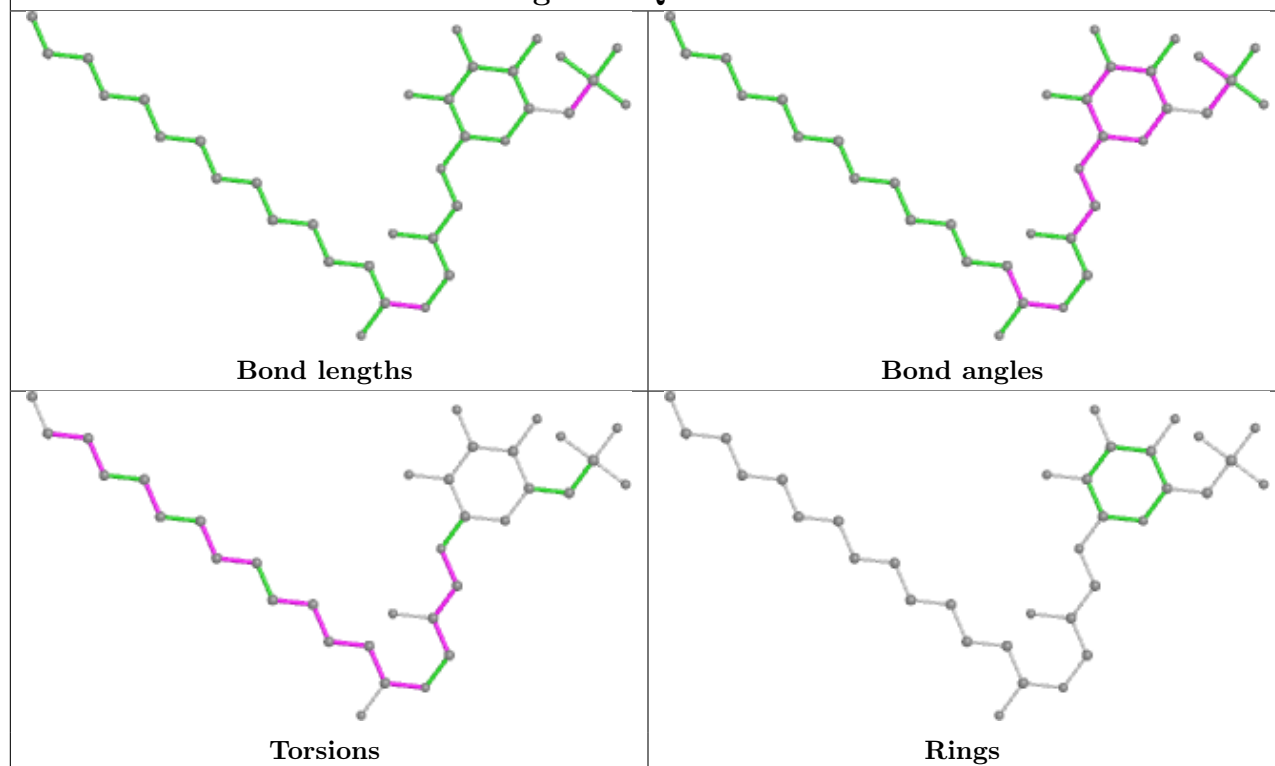


Rings

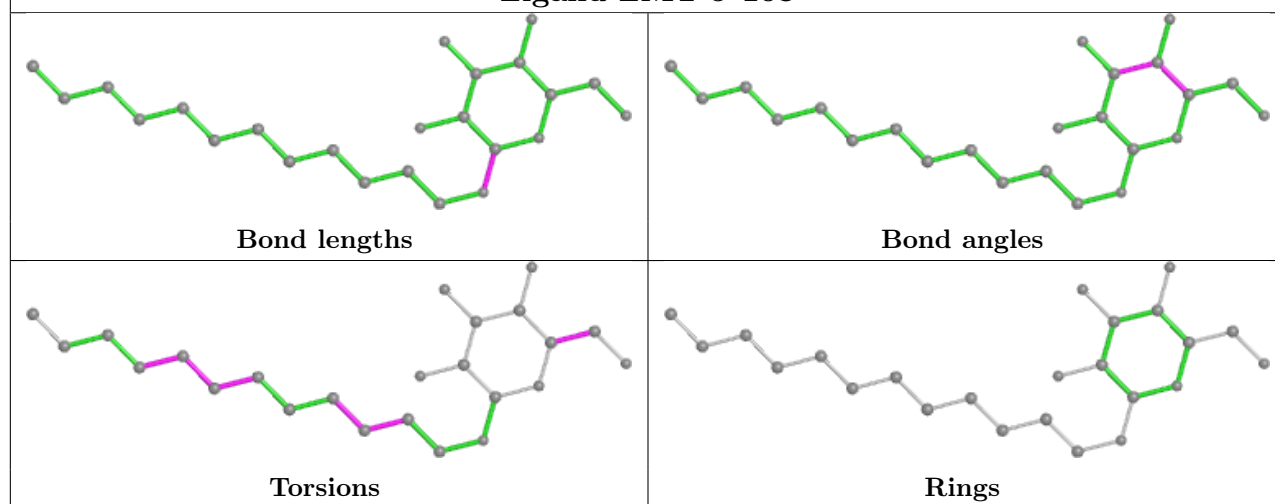
**Ligand CLA A 401****Ligand CLA B 616****Ligand CLA c 506**

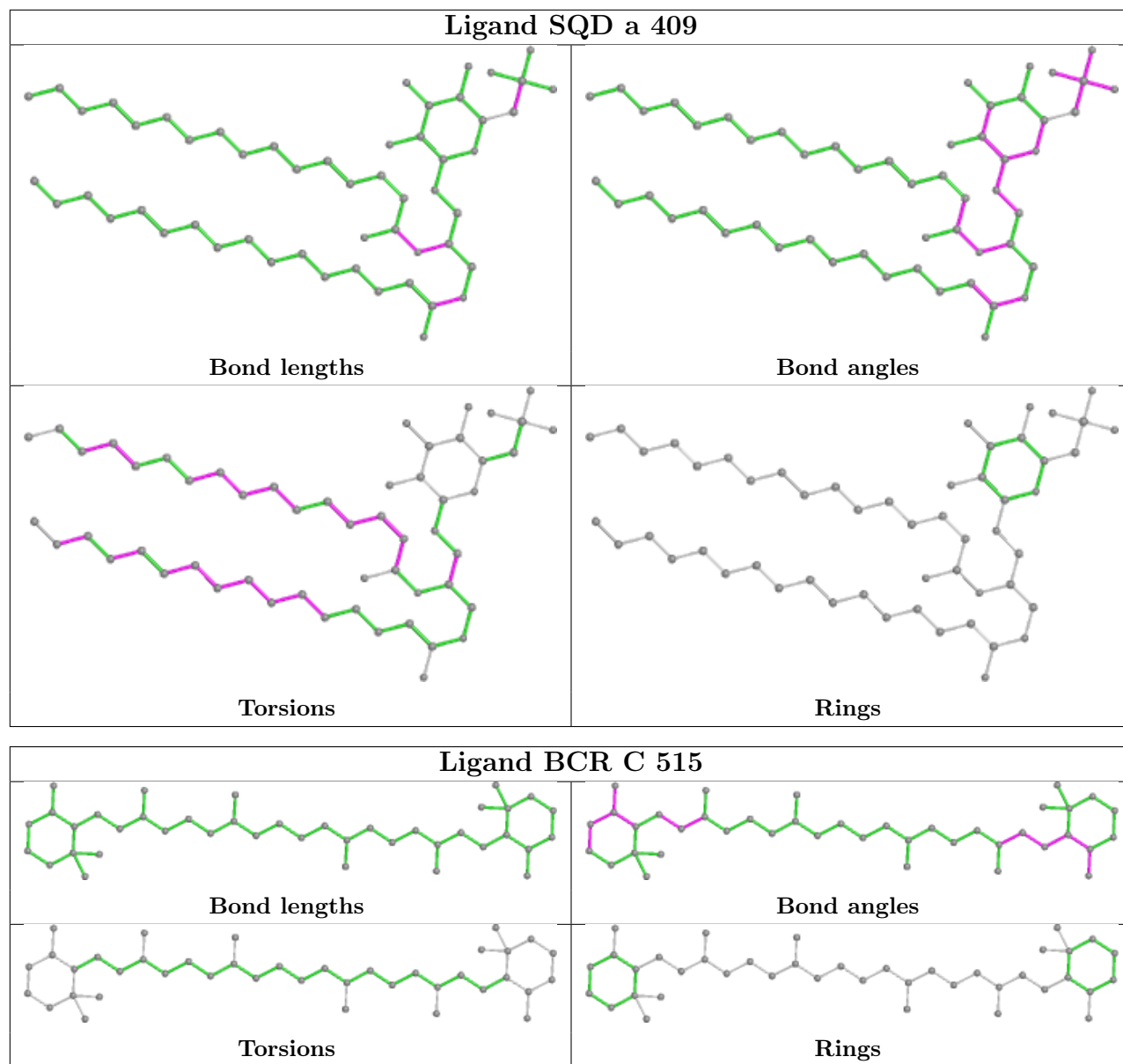


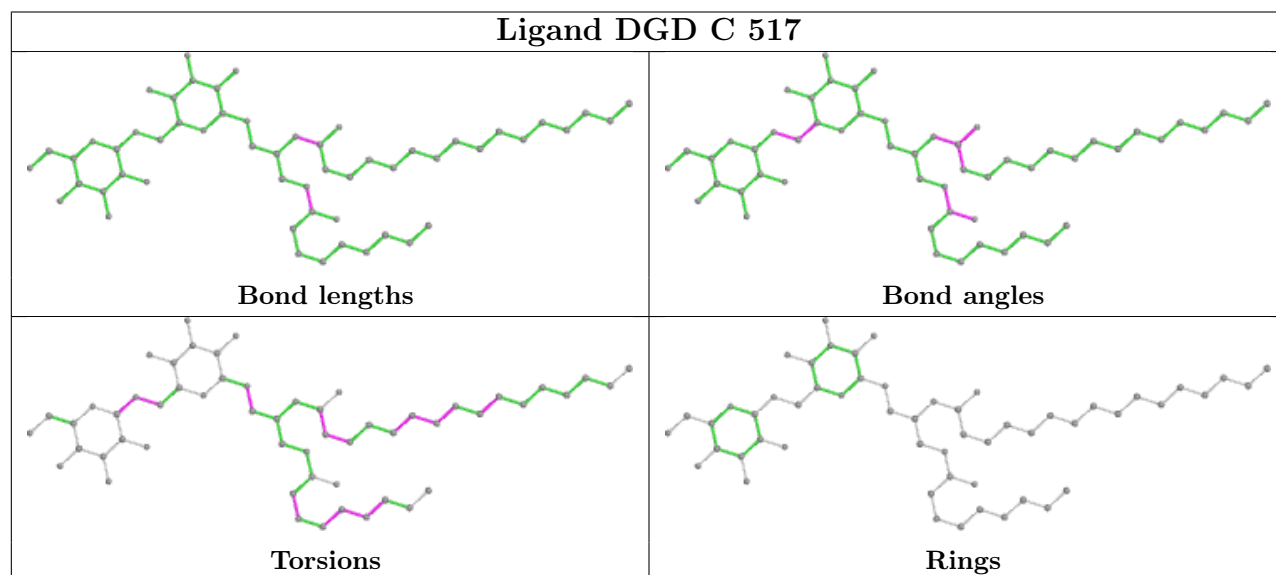
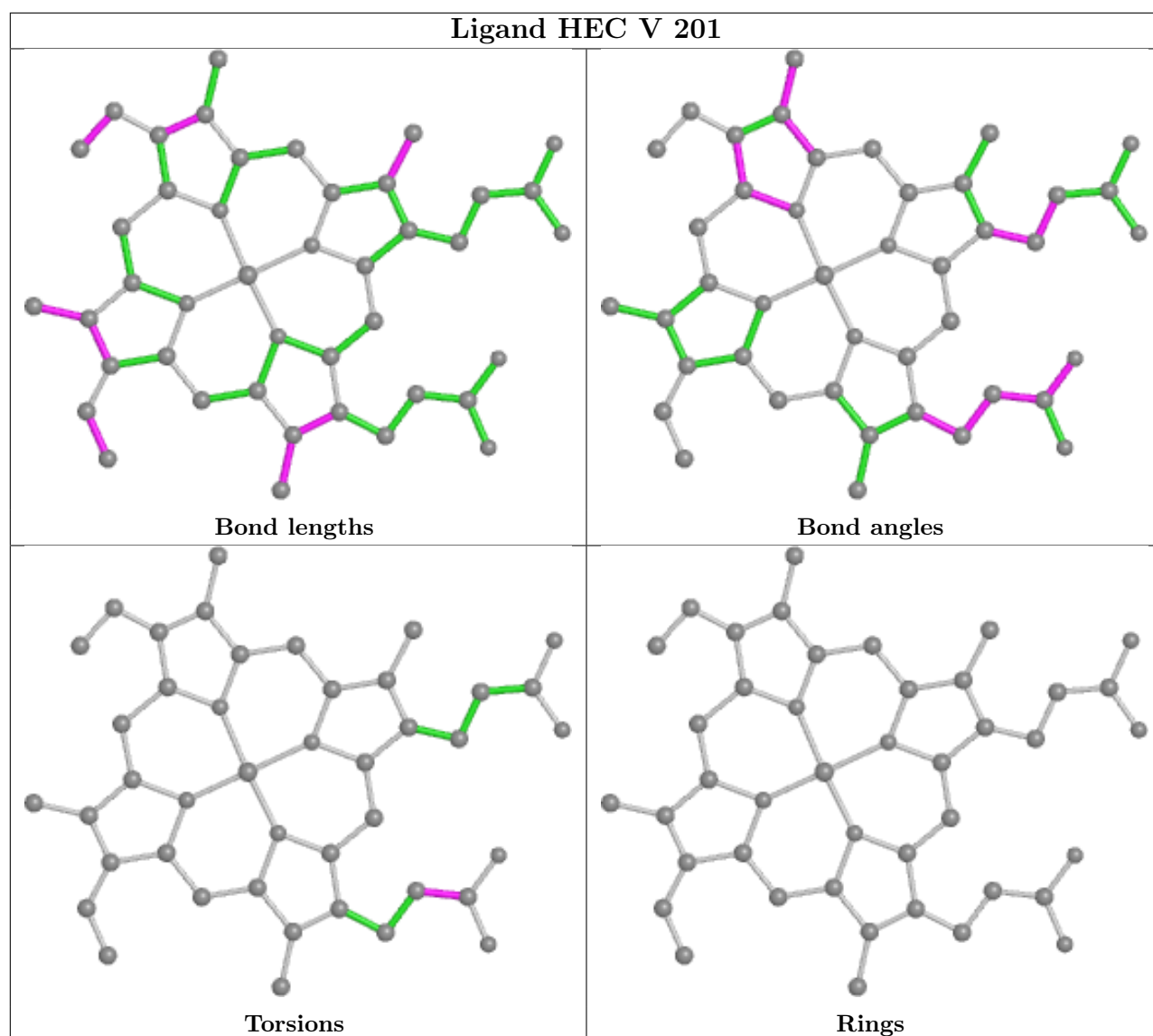
## Ligand SQD F 101

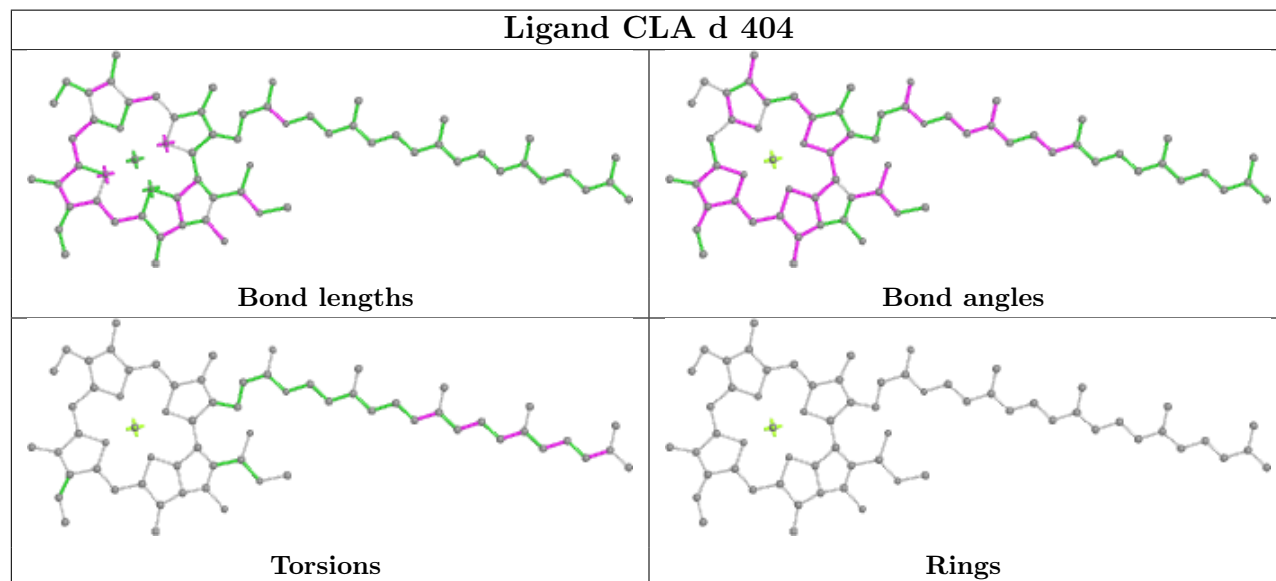
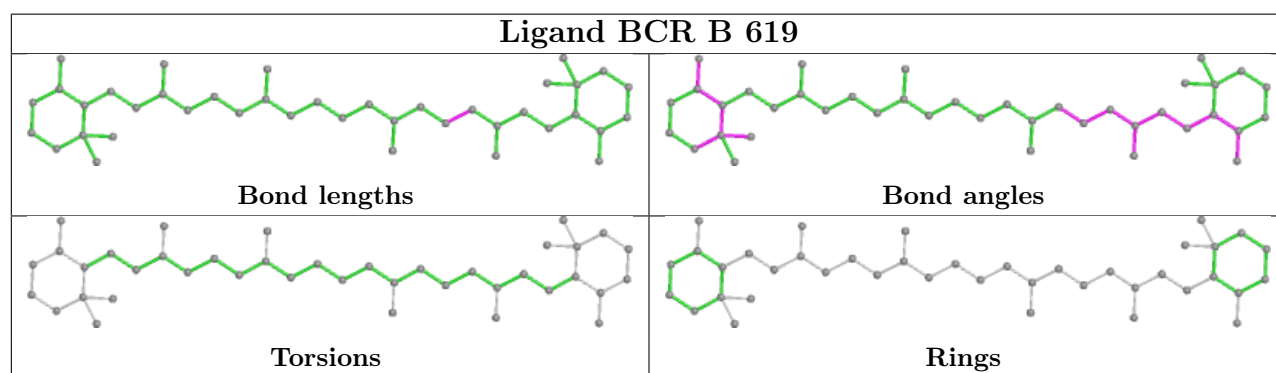
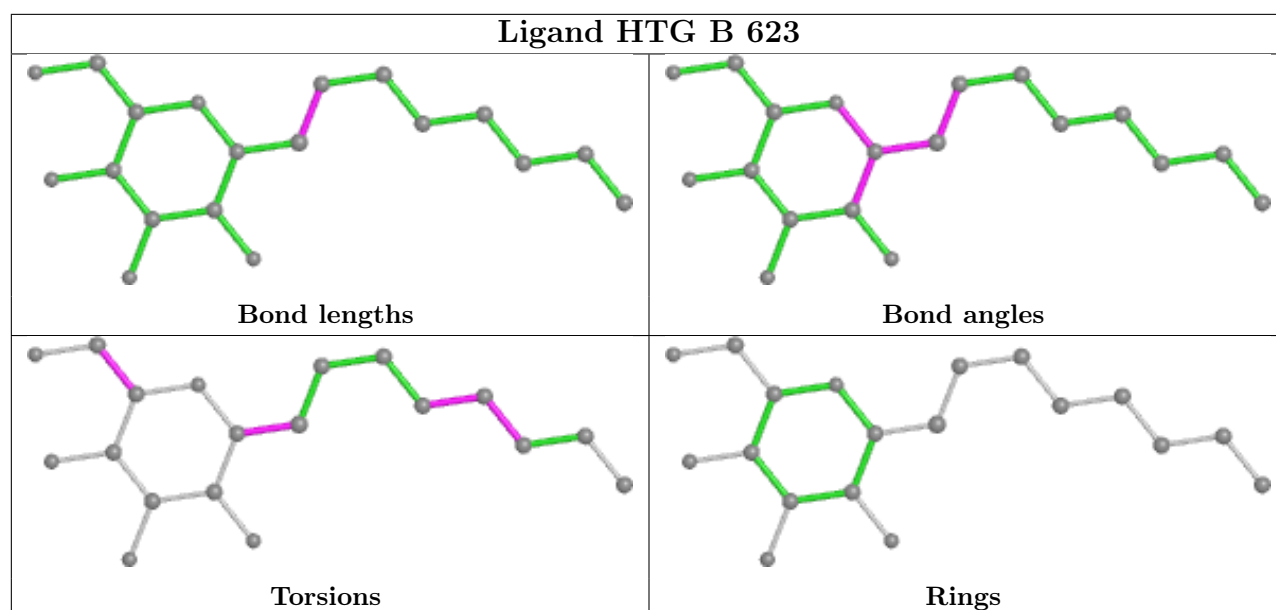


## Ligand LMT J 103

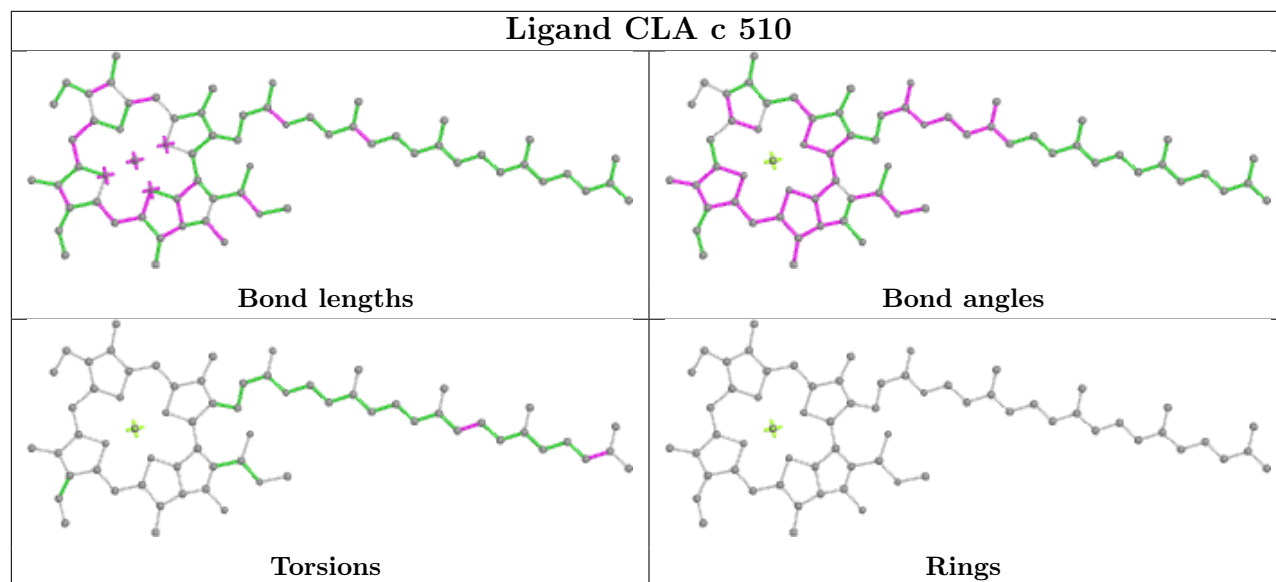




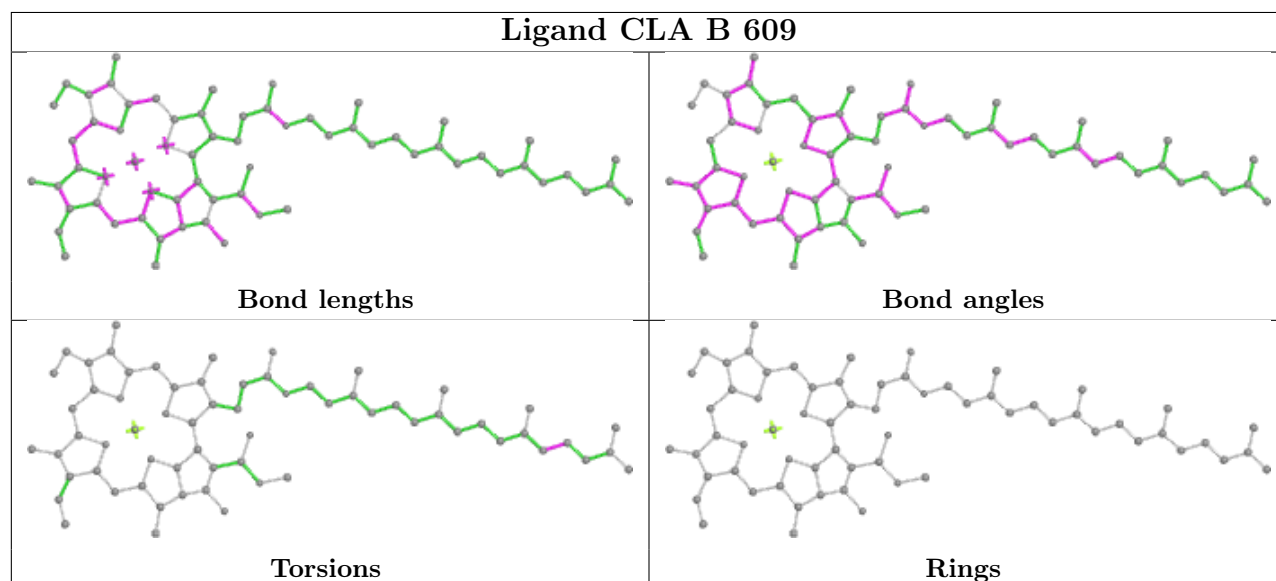




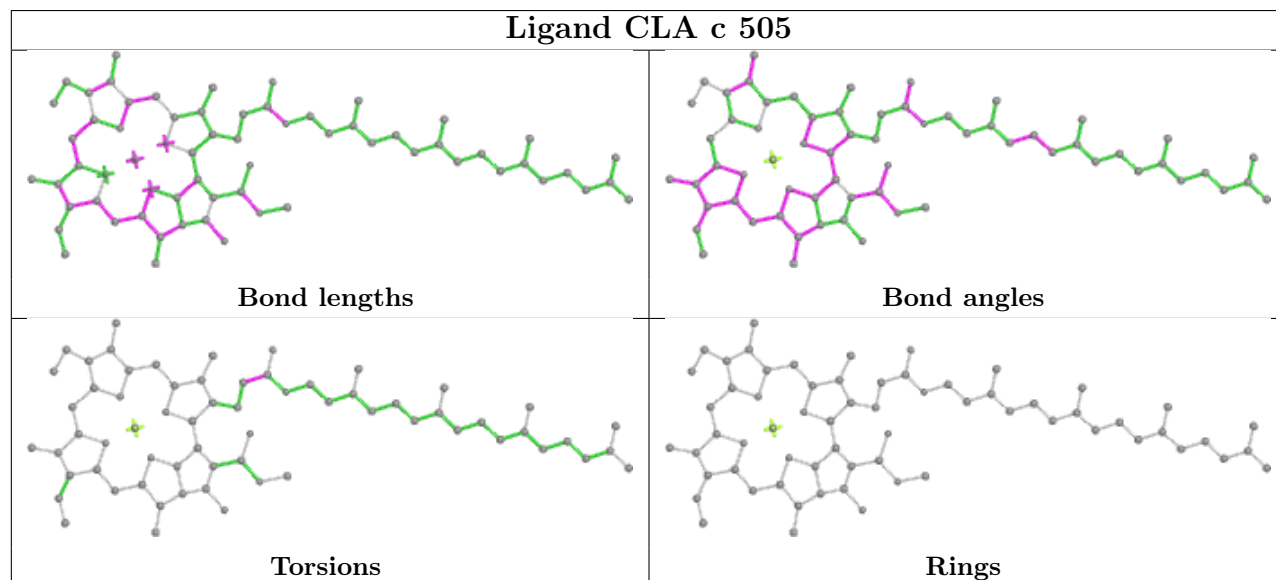
## Ligand CLA c 510



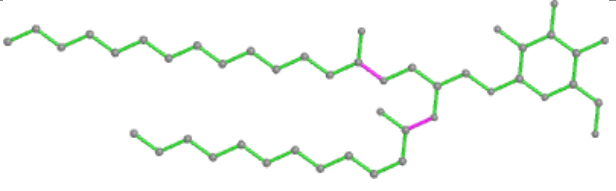
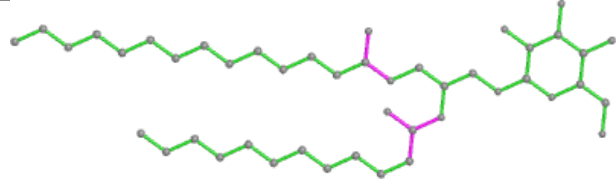
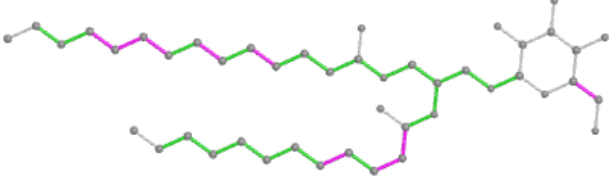
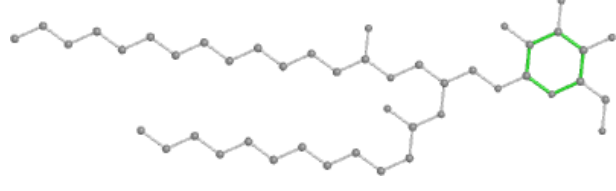
## Ligand CLA B 609

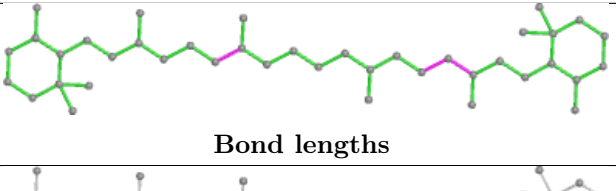
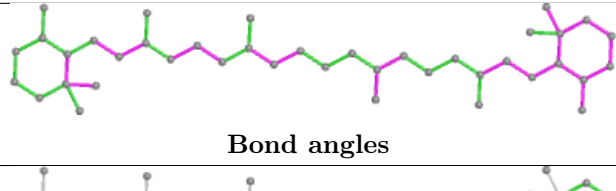
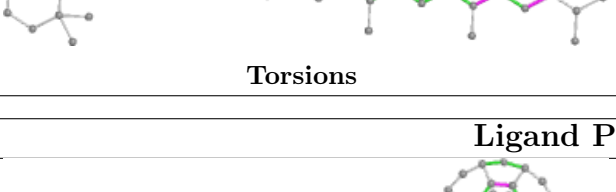
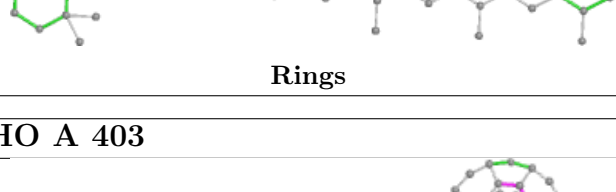


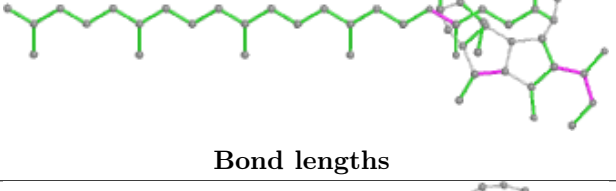
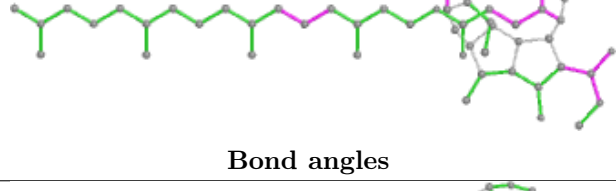
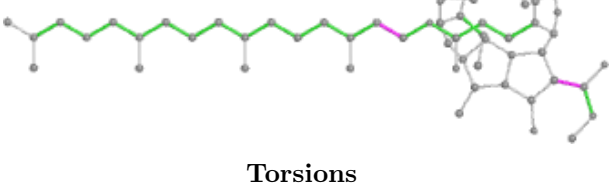
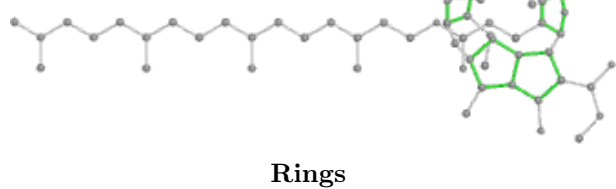
## Ligand CLA c 505

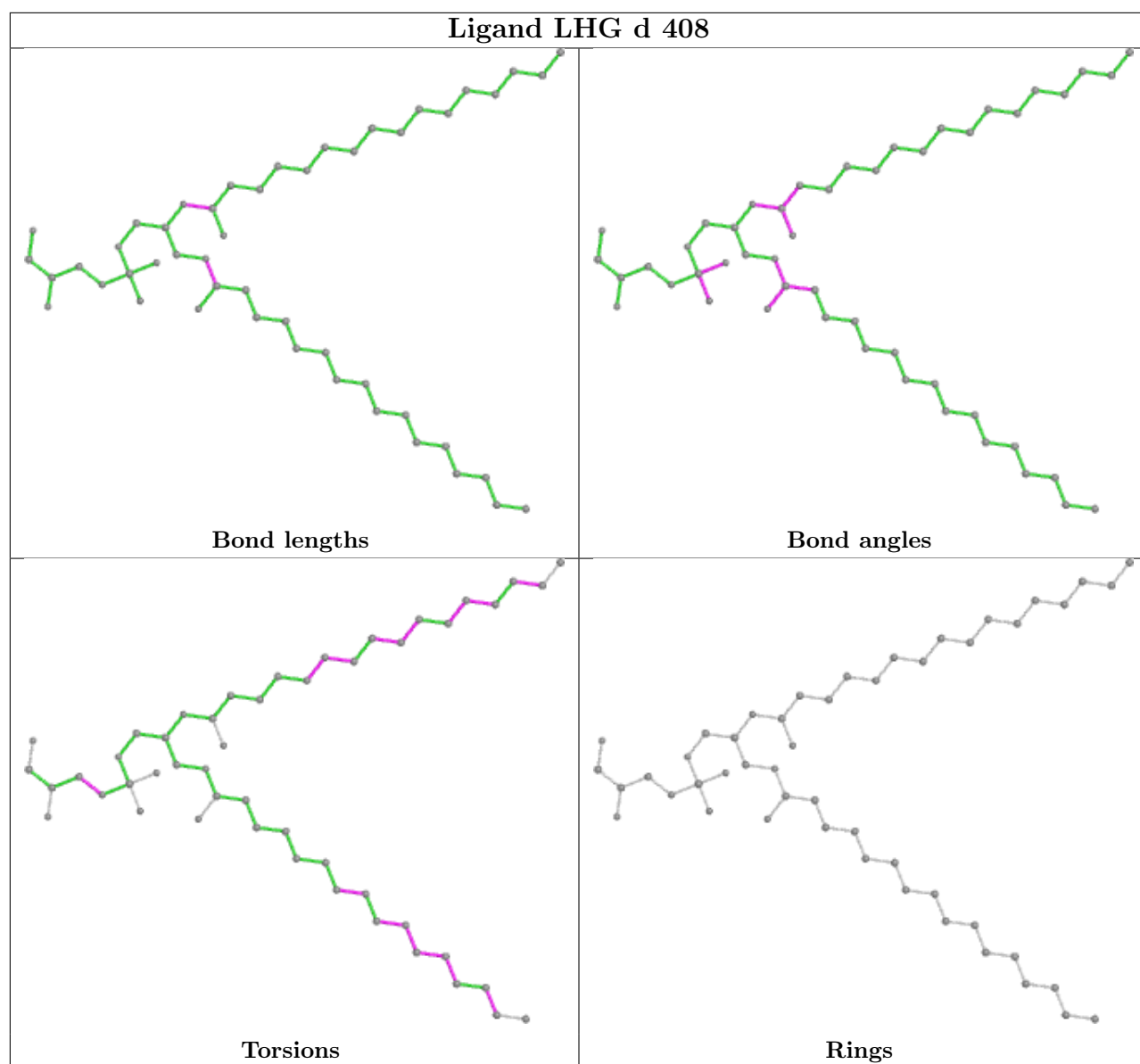


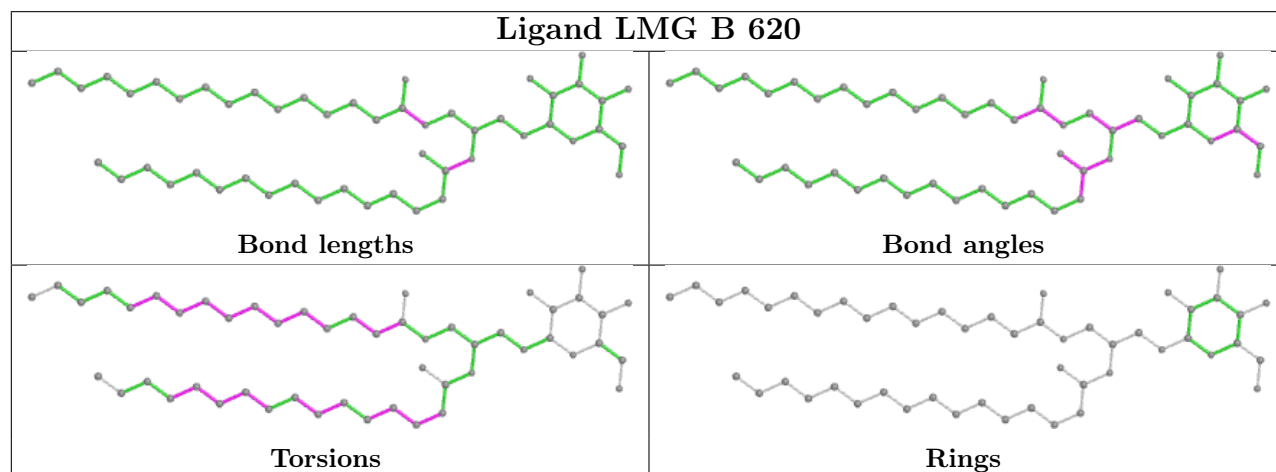
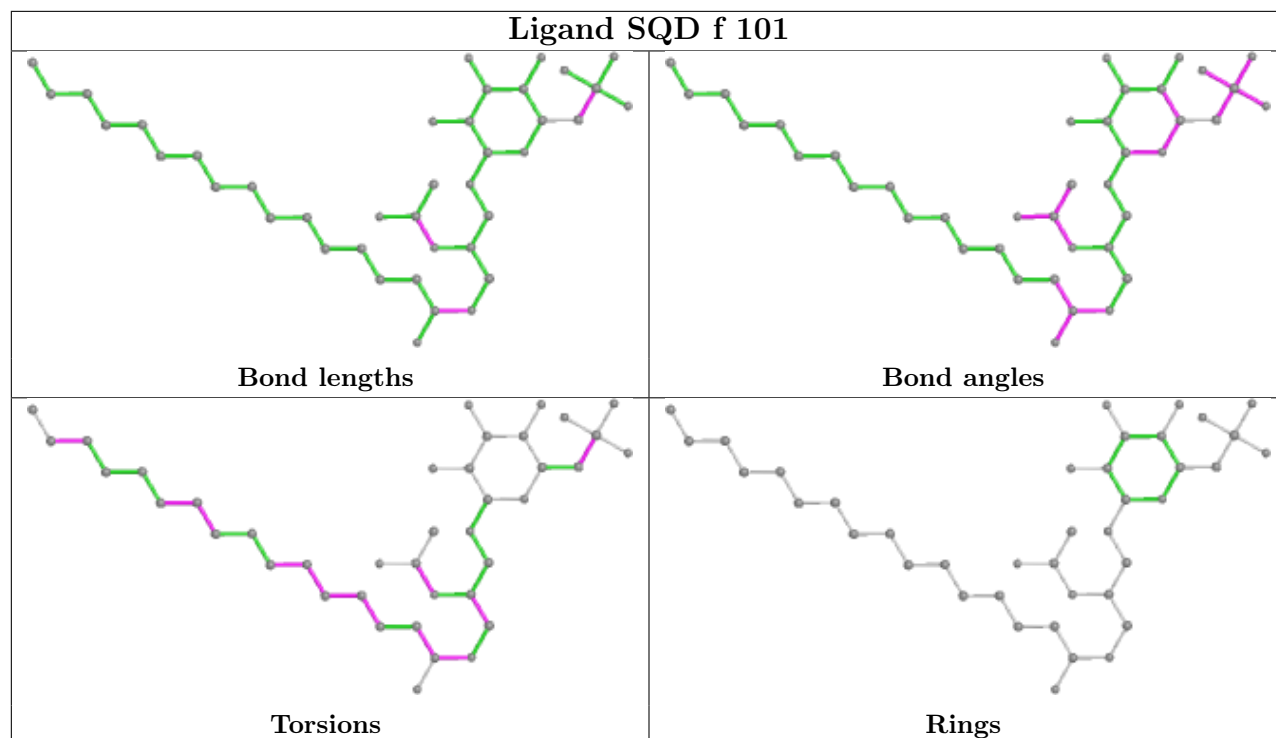


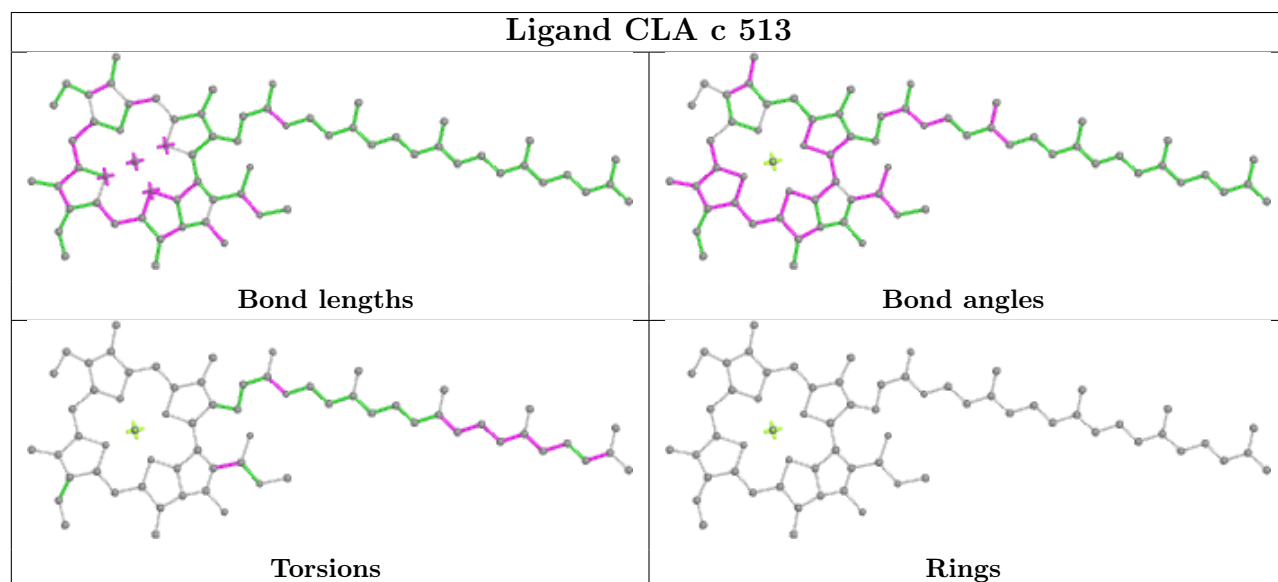
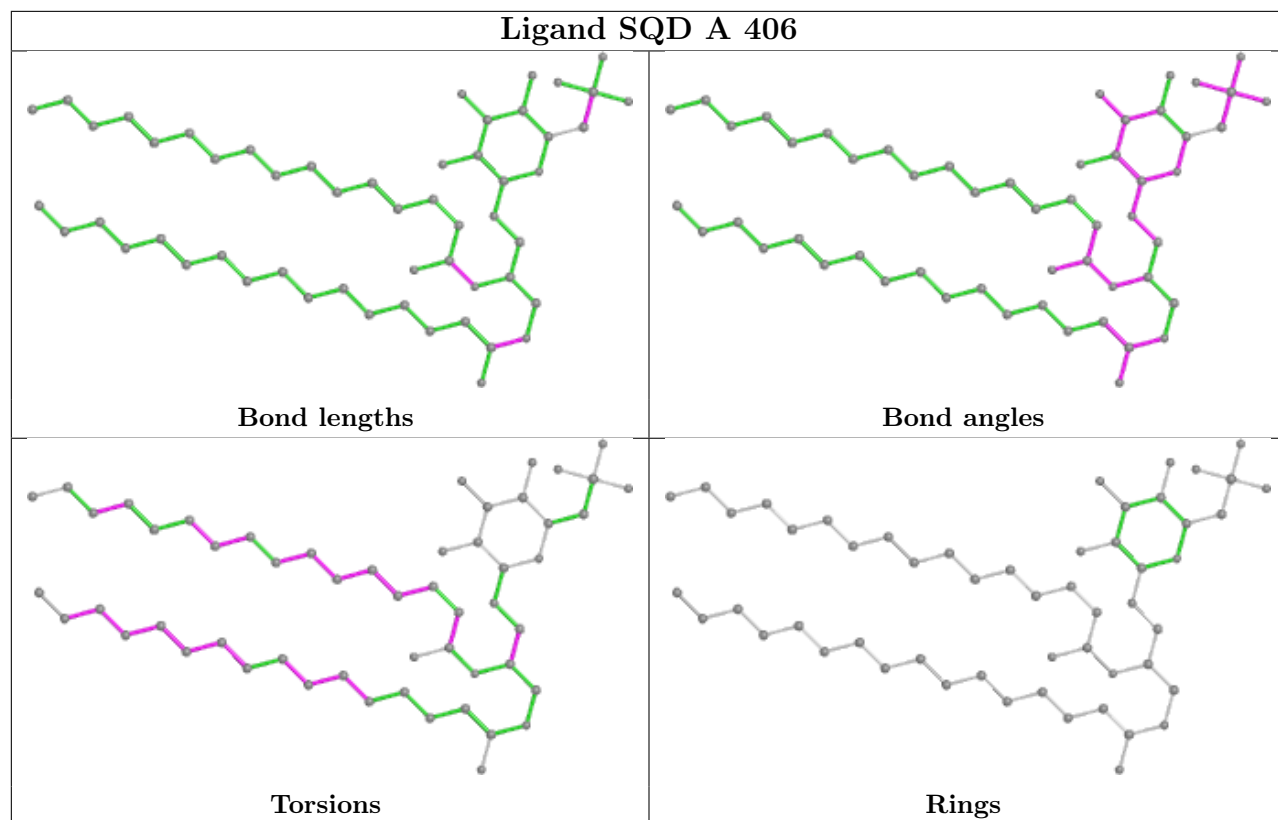
Ligand LMG J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

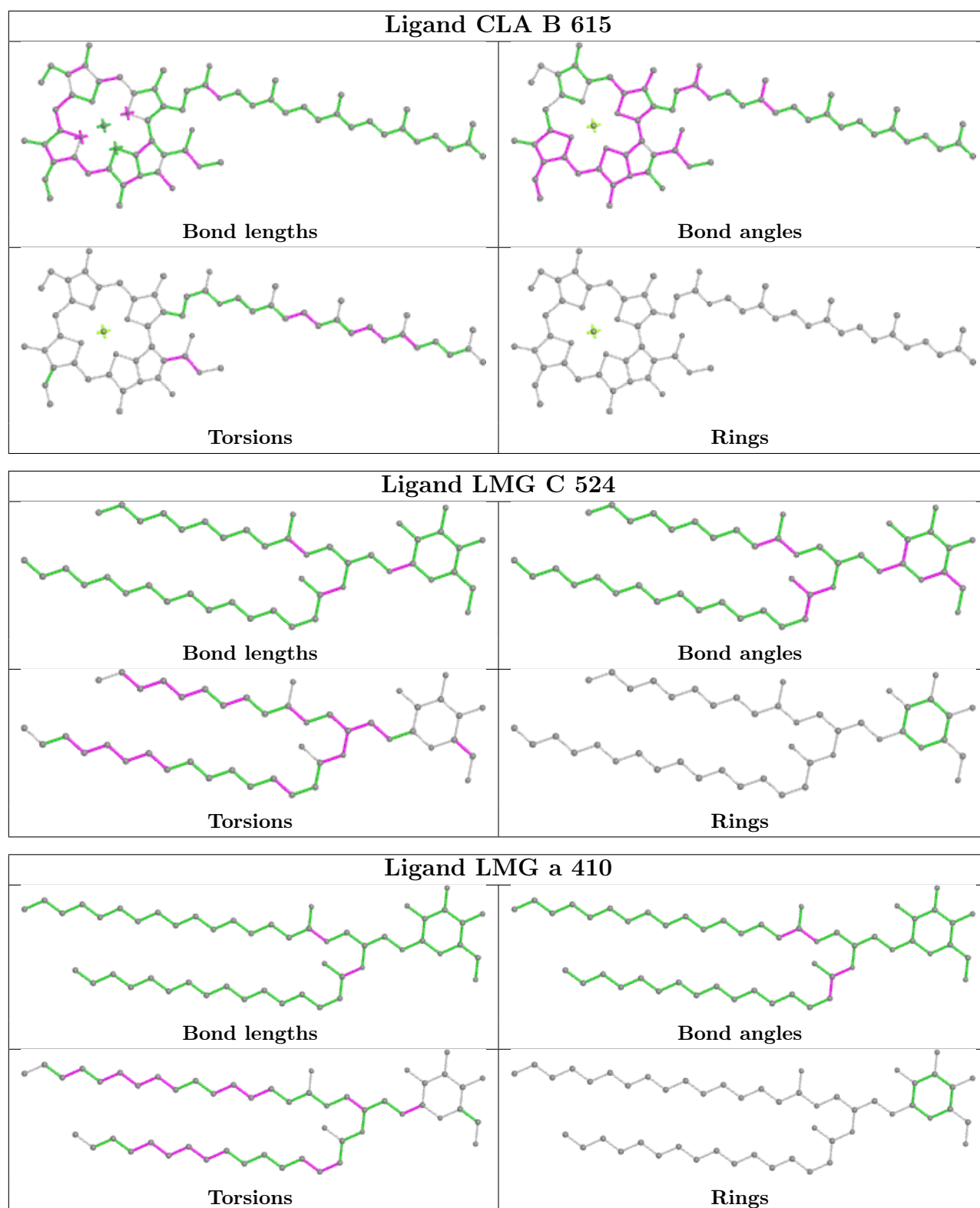
Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO A 403	
	
Bond lengths	Bond angles
	
Torsions	Rings









## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.75	2 (0%) 85 88	15, 23, 46, 68	3 (0%)
1	a	334/344 (97%)	-0.73	0 100 100	14, 23, 48, 78	4 (1%)
2	B	505/505 (100%)	-0.58	8 (1%) 70 73	15, 28, 54, 85	11 (2%)
2	b	495/505 (98%)	-0.51	12 (2%) 59 62	16, 27, 53, 95	4 (0%)
3	C	451/455 (99%)	-0.40	1 (0%) 92 93	21, 33, 49, 83	1 (0%)
3	c	455/455 (100%)	-0.44	0 100 100	22, 33, 46, 79	1 (0%)
4	D	342/342 (100%)	-0.74	1 (0%) 90 92	17, 24, 44, 90	1 (0%)
4	d	342/342 (100%)	-0.81	1 (0%) 90 92	18, 25, 42, 86	0
5	E	78/83 (93%)	0.33	4 (5%) 34 36	28, 47, 75, 87	1 (1%)
5	e	78/83 (93%)	0.10	2 (2%) 57 60	29, 43, 63, 81	2 (2%)
6	F	33/44 (75%)	-0.15	2 (6%) 28 30	28, 36, 63, 66	0
6	f	32/44 (72%)	-0.21	1 (3%) 51 54	28, 34, 72, 90	0
7	H	64/65 (98%)	-0.04	2 (3%) 51 54	26, 36, 50, 78	1 (1%)
7	h	62/65 (95%)	-0.16	0 100 100	25, 36, 48, 58	1 (1%)
8	I	34/38 (89%)	-0.15	0 100 100	29, 36, 60, 78	0
8	i	35/38 (92%)	-0.24	0 100 100	29, 34, 47, 85	1 (2%)
9	J	36/40 (90%)	-0.11	0 100 100	26, 41, 74, 90	0
9	j	40/40 (100%)	-0.01	1 (2%) 58 61	27, 39, 56, 65	0
10	K	37/37 (100%)	-0.32	0 100 100	33, 40, 52, 59	0
10	k	37/37 (100%)	-0.17	0 100 100	32, 40, 56, 64	0
11	L	37/37 (100%)	-0.74	0 100 100	12, 22, 65, 81	1 (2%)
11	l	37/37 (100%)	-0.75	0 100 100	12, 22, 76, 91	1 (2%)
12	M	33/36 (91%)	-0.75	0 100 100	15, 25, 39, 57	1 (3%)
12	m	34/36 (94%)	-0.73	0 100 100	16, 26, 53, 74	1 (2%)

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	-0.35	2 (0%) 82 85	17, 32, 56, 85	6 (2%)
13	o	243/244 (99%)	-0.31	1 (0%) 89 91	17, 35, 67, 89	2 (0%)
14	T	28/32 (87%)	-0.79	0 100 100	19, 23, 37, 54	1 (3%)
14	t	29/32 (90%)	-0.60	0 100 100	20, 23, 49, 74	0
15	U	97/104 (93%)	-0.47	0 100 100	22, 29, 49, 67	0
15	u	97/104 (93%)	-0.48	0 100 100	24, 29, 44, 75	0
16	V	137/137 (100%)	-0.65	0 100 100	17, 28, 43, 60	3 (2%)
16	v	137/137 (100%)	-0.28	0 100 100	25, 36, 53, 74	0
17	Y	29/30 (96%)	0.41	2 (6%) 24 25	41, 51, 72, 79	0
17	y	29/30 (96%)	0.19	0 100 100	41, 50, 66, 70	0
18	X	38/40 (95%)	0.27	0 100 100	32, 42, 68, 72	0
18	x	35/40 (87%)	0.08	0 100 100	33, 40, 63, 67	0
19	Z	62/62 (100%)	0.50	3 (4%) 36 39	38, 48, 86, 98	0
19	z	61/62 (98%)	0.76	5 (8%) 19 20	45, 54, 86, 96	0
All	All	5230/5350 (97%)	-0.46	50 (0%) 79 82	12, 30, 57, 98	47 (0%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	4.9
7	H	65	LEU	4.7
2	b	495	PHE	4.1
2	b	499	VAL	4.1
2	b	502	VAL	3.7

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
14	FME	t	1	10/11	0.96	0.06	23,27,49,50	0
14	FME	T	1	10/11	0.97	0.06	23,29,48,51	0
8	FME	i	1	10/11	0.98	0.06	30,31,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	FME	I	1	10/11	0.98	0.05	26,32,36,37	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	UNL	b	642	13/-	0.59	0.14	71,80,87,90	0
35	DGD	D	406	51/66	0.62	0.16	57,74,100,108	0
26	UNL	B	646	16/-	0.64	0.14	85,89,93,94	0
28	DMS	j	105	4/4	0.66	0.18	70,74,75,88	0
26	UNL	B	629	10/-	0.66	0.15	54,69,74,74	0
28	DMS	O	308	4/4	0.67	0.17	66,74,76,87	0
26	UNL	Z	102	4/-	0.67	0.20	59,61,62,63	0
32	HTG	C	534	19/19	0.67	0.14	68,110,128,130	0
26	UNL	b	643	9/-	0.67	0.12	67,67,74,74	0
28	DMS	b	638	4/4	0.68	0.20	67,75,77,86	0
28	DMS	o	306	4/4	0.68	0.19	55,58,65,77	0
34	LMT	f	102	24/35	0.69	0.15	62,77,94,98	0
28	DMS	U	904	4/4	0.69	0.18	58,66,66,83	0
28	DMS	O	305	4/4	0.70	0.22	64,66,77,86	0
32	HTG	D	417	19/19	0.70	0.15	67,105,119,120	0
28	DMS	B	636	4/4	0.71	0.17	77,86,90,96	0
28	DMS	O	309	4/4	0.71	0.23	58,65,72,73	0
35	DGD	d	416	51/66	0.71	0.14	56,75,96,103	0
28	DMS	H	103	4/4	0.72	0.21	84,101,109,112	0
26	UNL	B	647	13/-	0.72	0.13	71,81,90,91	0
28	DMS	b	640	4/4	0.72	0.18	49,58,71,73	0
26	UNL	A	413	4/-	0.72	0.13	64,64,64,66	0
26	UNL	a	402	6/-	0.72	0.14	50,57,62,63	0
32	HTG	v	210	14/19	0.73	0.16	60,80,92,100	0
26	UNL	T	103	13/-	0.73	0.13	64,68,72,72	0
26	UNL	a	414	28/-	0.73	0.14	59,68,84,87	0
32	HTG	c	521	19/19	0.73	0.14	57,85,102,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	UNL	b	645	6/-	0.74	0.16	57,65,76,76	0
26	UNL	h	103	16/-	0.74	0.14	61,69,73,76	0
32	HTG	c	520	19/19	0.74	0.15	77,88,99,100	0
26	UNL	A	410	36/-	0.74	0.15	57,78,84,91	0
26	UNL	c	526	8/-	0.75	0.17	54,59,64,65	0
28	DMS	D	415	4/4	0.75	0.23	57,58,63,65	0
34	LMT	I	101	35/35	0.75	0.13	67,82,91,92	0
28	DMS	O	310	4/4	0.76	0.19	76,78,82,94	0
26	UNL	E	102	15/-	0.76	0.17	55,62,76,77	0
28	DMS	o	308	4/4	0.76	0.19	60,61,62,63	0
34	LMT	b	627	32/35	0.77	0.14	42,67,84,87	0
26	UNL	J	107	3/-	0.77	0.12	61,61,63,64	0
32	HTG	b	602	19/19	0.77	0.13	51,103,117,118	0
28	DMS	b	641	4/4	0.77	0.20	63,65,75,80	0
36	LHG	E	103	48/49	0.77	0.15	44,99,108,119	0
34	LMT	E	101	24/35	0.78	0.12	64,78,84,90	0
26	UNL	I	105	10/-	0.78	0.10	60,66,71,72	0
26	UNL	I	106	11/-	0.78	0.17	61,73,81,81	0
26	UNL	B	633	16/-	0.78	0.16	53,61,69,70	0
26	UNL	I	104	11/-	0.78	0.13	53,56,59,62	0
32	HTG	u	201	8/19	0.78	0.17	45,52,69,89	0
26	UNL	j	104	16/-	0.78	0.14	49,58,64,66	0
32	HTG	B	623	19/19	0.79	0.12	53,88,93,94	0
26	UNL	J	104	14/-	0.79	0.13	67,77,80,81	0
26	UNL	I	103	13/-	0.79	0.14	47,53,84,87	0
26	UNL	H	104	4/-	0.79	0.14	60,62,65,67	0
34	LMT	c	523	35/35	0.79	0.12	67,77,83,85	0
26	UNL	t	102	16/-	0.79	0.12	61,71,80,80	0
26	UNL	c	524	30/-	0.79	0.14	59,74,86,87	0
32	HTG	d	401	19/19	0.79	0.14	58,99,111,120	0
26	UNL	c	525	10/-	0.79	0.13	58,65,66,67	0
26	UNL	U	901	14/-	0.80	0.15	40,49,59,59	0
28	DMS	B	638	4/4	0.80	0.18	53,61,63,68	0
26	UNL	C	523	34/-	0.80	0.12	59,80,92,101	0
26	UNL	b	644	7/-	0.80	0.11	64,65,70,70	0
26	UNL	H	105	6/-	0.80	0.13	51,55,63,65	0
34	LMT	a	418	35/35	0.80	0.13	45,69,78,81	0
26	UNL	j	106	6/-	0.80	0.16	52,55,58,59	0
23	SQD	f	101	40/54	0.80	0.14	57,86,102,107	0
27	PL9	A	411	55/55	0.80	0.15	43,67,89,92	0
34	LMT	m	101	35/35	0.80	0.13	48,94,110,114	0
27	PL9	a	415	55/55	0.80	0.16	52,67,89,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	DMS	b	637	4/4	0.80	0.17	77,79,84,93	0
28	DMS	A	418	4/4	0.80	0.21	68,74,80,85	0
34	LMT	b	628	25/35	0.81	0.12	54,79,95,96	0
28	DMS	u	204	4/4	0.81	0.18	71,78,83,86	0
28	DMS	B	642	4/4	0.81	0.22	43,51,68,71	0
32	HTG	B	632	19/19	0.81	0.12	51,97,108,114	0
34	LMT	z	102	35/35	0.81	0.12	46,85,99,101	0
34	LMT	Z	101	35/35	0.81	0.14	44,90,107,109	0
24	LMG	C	524	45/55	0.81	0.20	22,46,51,56	45
26	UNL	b	630	11/-	0.81	0.13	55,60,67,68	0
28	DMS	d	415	4/4	0.82	0.17	68,71,71,72	0
28	DMS	O	306	4/4	0.82	0.18	66,73,73,75	0
32	HTG	C	521	19/19	0.82	0.12	46,78,89,90	0
28	DMS	V	205	4/4	0.82	0.15	67,76,77,79	0
28	DMS	B	639	4/4	0.82	0.18	65,70,71,76	0
28	DMS	c	533	4/4	0.82	0.16	73,75,77,87	0
26	UNL	M	102	12/-	0.83	0.13	49,53,95,98	0
26	UNL	B	630	14/-	0.83	0.12	67,74,83,84	0
26	UNL	a	416	11/-	0.83	0.14	66,68,76,78	0
34	LMT	J	103	24/35	0.83	0.12	53,61,81,85	0
26	UNL	x	102	9/-	0.83	0.14	56,68,72,72	0
26	UNL	L	102	14/-	0.84	0.15	56,60,84,84	0
24	LMG	c	518	51/55	0.84	0.11	37,72,84,87	0
23	SQD	l	101	54/54	0.84	0.13	47,68,101,106	0
28	DMS	b	636	4/4	0.84	0.18	66,71,72,79	0
26	UNL	d	409	36/-	0.84	0.12	36,60,91,102	0
28	DMS	v	207	4/4	0.84	0.15	53,66,72,87	0
23	SQD	b	622	54/54	0.84	0.12	46,63,95,100	0
34	LMT	B	627	16/35	0.84	0.12	52,60,78,78	0
26	UNL	i	101	16/-	0.84	0.12	41,45,65,65	0
26	UNL	i	103	11/-	0.84	0.11	58,61,65,66	0
26	UNL	b	629	16/-	0.84	0.13	41,48,60,60	0
28	DMS	C	532	4/4	0.85	0.17	33,40,41,48	0
32	HTG	C	520	19/19	0.85	0.11	64,70,76,79	0
28	DMS	O	311	4/4	0.85	0.16	57,65,69,72	0
32	HTG	C	522	19/19	0.85	0.11	66,83,104,107	0
28	DMS	c	534	4/4	0.85	0.14	70,71,75,81	0
23	SQD	F	101	35/54	0.85	0.13	51,76,89,90	0
26	UNL	e	101	7/-	0.85	0.12	54,58,64,65	0
32	HTG	b	624	19/19	0.85	0.12	49,74,80,85	0
28	DMS	b	634	4/4	0.85	0.16	59,67,67,75	0
28	DMS	A	417	4/4	0.85	0.16	70,72,77,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	UNL	J	105	12/-	0.85	0.13	63,67,71,71	0
28	DMS	v	203	4/4	0.85	0.18	67,69,76,79	0
28	DMS	B	644	4/4	0.85	0.16	52,53,61,69	0
28	DMS	C	527	4/4	0.85	0.17	73,76,79,87	0
26	UNL	z	101	6/-	0.86	0.10	49,55,55,57	0
28	DMS	C	533	4/4	0.86	0.13	72,73,73,74	0
23	SQD	a	401	54/54	0.86	0.11	39,58,82,86	0
28	DMS	v	204	4/4	0.86	0.17	48,54,57,69	0
28	DMS	U	902	4/4	0.86	0.18	35,44,49,58	0
28	DMS	c	532	4/4	0.86	0.18	65,70,76,77	0
23	SQD	A	412	54/54	0.86	0.11	41,60,78,81	0
26	UNL	B	628	15/-	0.86	0.12	45,50,60,66	0
34	LMT	B	625	24/35	0.86	0.10	48,67,86,89	0
28	DMS	V	208	4/4	0.86	0.18	75,77,82,85	0
26	UNL	D	410	37/-	0.86	0.11	42,57,93,98	0
28	DMS	B	635	4/4	0.86	0.17	90,94,95,96	0
32	HTG	B	622	19/19	0.87	0.14	28,46,54,54	0
32	HTG	b	625	19/19	0.87	0.14	30,44,66,70	0
28	DMS	B	640	4/4	0.87	0.23	45,48,49,50	0
26	UNL	b	646	6/-	0.87	0.12	54,58,60,62	0
28	DMS	u	203	4/4	0.87	0.20	47,55,56,65	0
28	DMS	c	535	4/4	0.87	0.14	58,59,65,68	0
28	DMS	O	304	4/4	0.87	0.15	63,68,72,73	0
26	UNL	D	411	16/-	0.87	0.11	39,45,58,62	0
34	LMT	m	102	35/35	0.87	0.10	34,53,58,59	0
34	LMT	B	626	24/35	0.87	0.11	37,54,86,95	0
28	DMS	o	303	4/4	0.87	0.15	66,69,75,79	0
32	HTG	V	202	13/19	0.87	0.10	45,49,70,82	0
28	DMS	v	208	4/4	0.87	0.17	89,92,92,95	0
34	LMT	T	102	24/35	0.88	0.12	36,53,78,85	0
28	DMS	o	305	4/4	0.88	0.14	73,75,77,87	0
28	DMS	C	529	4/4	0.88	0.15	70,73,74,74	0
28	DMS	C	531	4/4	0.88	0.17	53,54,58,74	0
24	LMG	a	410	51/55	0.88	0.09	44,55,65,67	0
28	DMS	B	643	4/4	0.88	0.13	51,53,62,71	0
28	DMS	A	415	4/4	0.88	0.15	55,58,65,71	0
28	DMS	D	416	4/4	0.88	0.14	83,87,89,91	0
26	UNL	I	102	16/-	0.88	0.11	38,47,63,64	0
28	DMS	O	303	4/4	0.88	0.14	63,72,77,78	0
28	DMS	v	209	4/4	0.88	0.13	71,78,79,79	0
28	DMS	o	304	4/4	0.88	0.15	68,79,82,83	0
34	LMT	M	101	35/35	0.88	0.10	34,53,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	UNL	i	102	11/-	0.89	0.10	48,54,64,65	0
26	UNL	d	411	16/-	0.89	0.09	33,42,55,55	0
26	UNL	J	106	4/-	0.89	0.12	57,60,61,67	0
24	LMG	B	620	51/55	0.89	0.09	33,43,55,58	0
28	DMS	v	205	4/4	0.89	0.12	67,70,72,73	0
26	UNL	X	101	16/-	0.89	0.11	37,40,59,59	0
28	DMS	C	525[A]	4/4	0.89	0.17	48,49,51,57	4
28	DMS	V	209	4/4	0.89	0.14	57,73,77,81	0
28	DMS	C	525[B]	4/4	0.89	0.17	32,33,35,35	4
24	LMG	c	519	51/55	0.90	0.11	29,59,86,88	0
28	DMS	O	307	4/4	0.90	0.15	69,76,77,88	0
24	LMG	C	519	51/55	0.90	0.11	31,67,83,84	0
28	DMS	B	645	4/4	0.90	0.13	56,59,64,71	0
20	CLA	C	513	65/65	0.90	0.09	40,48,72,77	0
28	DMS	A	416	4/4	0.90	0.12	59,60,69,77	0
24	LMG	A	407	51/55	0.90	0.09	40,55,70,78	0
28	DMS	U	903[A]	4/4	0.90	0.16	32,34,40,41	4
28	DMS	U	903[B]	4/4	0.90	0.16	26,28,29,32	4
28	DMS	B	641	4/4	0.90	0.12	68,69,75,80	0
28	DMS	V	204	4/4	0.90	0.12	58,64,64,72	0
20	CLA	C	506	65/65	0.90	0.09	32,45,86,87	0
28	DMS	c	536	4/4	0.90	0.18	33,33,45,46	0
28	DMS	V	207	4/4	0.91	0.14	62,63,63,70	0
20	CLA	b	603	65/65	0.91	0.10	30,45,75,82	0
24	LMG	b	623	49/55	0.91	0.09	33,42,54,61	0
33	CA	V	203	1/1	0.91	0.10	63,63,63,63	0
28	DMS	v	206	4/4	0.91	0.13	52,53,61,66	0
28	DMS	u	202	4/4	0.91	0.18	40,46,52,54	0
28	DMS	b	639	4/4	0.91	0.13	46,49,49,50	0
23	SQD	A	406	54/54	0.91	0.10	34,59,71,76	0
28	DMS	o	307	4/4	0.92	0.13	53,58,63,65	0
22	BCR	C	514	40/40	0.92	0.07	36,45,49,50	0
28	DMS	V	206	4/4	0.92	0.12	59,61,63,65	0
26	UNL	d	410	16/-	0.92	0.10	33,45,63,63	0
28	DMS	d	413	4/4	0.92	0.14	47,53,55,57	0
28	DMS	d	414	4/4	0.92	0.17	57,62,64,68	0
20	CLA	B	602	65/65	0.92	0.10	29,42,77,81	0
28	DMS	B	637	4/4	0.92	0.14	53,53,54,60	0
28	DMS	b	632	4/4	0.92	0.12	55,58,66,70	0
32	HTG	b	601	19/19	0.92	0.09	45,61,67,80	0
28	DMS	c	529	4/4	0.92	0.11	79,82,86,87	0
28	DMS	C	530	4/4	0.92	0.17	44,44,46,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	DMS	b	635	4/4	0.92	0.12	58,62,69,73	0
28	DMS	h	102	4/4	0.93	0.15	50,51,53,62	0
33	CA	o	301	1/1	0.93	0.06	48,48,48,48	0
28	DMS	i	104	4/4	0.93	0.11	63,66,67,71	0
28	DMS	C	526	4/4	0.93	0.13	59,60,63,65	0
32	HTG	B	631	19/19	0.93	0.08	41,57,69,73	0
20	CLA	C	512	55/65	0.93	0.07	37,44,49,54	0
28	DMS	D	413	4/4	0.93	0.11	50,56,60,61	0
22	BCR	K	101	40/40	0.93	0.07	33,37,42,45	0
22	BCR	k	102	40/40	0.93	0.07	41,46,51,51	0
28	DMS	c	530	4/4	0.93	0.20	36,43,45,49	0
35	DGD	h	101	62/66	0.93	0.08	25,34,41,49	0
20	CLA	b	618	65/65	0.93	0.09	23,33,92,98	0
22	BCR	D	405	40/40	0.94	0.07	26,30,58,60	0
20	CLA	c	513	65/65	0.94	0.08	36,46,81,87	0
31	BCT	A	421	4/4	0.94	0.07	31,34,40,44	0
31	BCT	a	413	4/4	0.94	0.07	32,32,38,42	0
32	HTG	B	621	19/19	0.94	0.08	36,41,48,52	0
22	BCR	K	102	40/40	0.94	0.07	31,36,40,41	0
22	BCR	d	405	40/40	0.94	0.07	24,30,56,58	0
28	DMS	F	102	4/4	0.94	0.12	51,52,56,64	0
23	SQD	a	409	54/54	0.94	0.09	33,56,75,78	0
22	BCR	k	101	40/40	0.94	0.07	28,36,41,42	0
28	DMS	c	528	4/4	0.94	0.13	58,62,63,65	0
20	CLA	c	506	65/65	0.94	0.07	24,39,71,74	0
28	DMS	b	633	4/4	0.94	0.12	45,48,49,53	0
35	DGD	H	102	62/66	0.94	0.08	25,33,40,43	0
28	DMS	c	531	4/4	0.94	0.11	73,78,85,86	0
32	HTG	O	302	19/19	0.94	0.08	34,42,50,53	0
36	LHG	D	407	49/49	0.94	0.07	28,37,44,52	0
36	LHG	D	409	49/49	0.94	0.10	27,33,81,83	0
22	BCR	t	101	40/40	0.94	0.06	22,29,41,43	0
38	RRX	H	101	41/41	0.94	0.07	27,31,41,46	0
38	RRX	x	101	41/41	0.94	0.07	26,32,47,58	0
20	CLA	C	505	65/65	0.95	0.06	28,33,44,48	0
20	CLA	B	601	65/65	0.95	0.08	23,29,82,86	0
20	CLA	c	511	65/65	0.95	0.06	27,33,40,43	0
20	CLA	c	512	65/65	0.95	0.07	28,41,70,72	0
28	DMS	D	414	4/4	0.95	0.12	55,56,57,58	0
20	CLA	C	507	65/65	0.95	0.07	28,37,52,57	0
35	DGD	C	517	55/66	0.95	0.06	26,34,59,62	0
24	LMG	j	101	45/55	0.95	0.07	27,32,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	C	508	60/65	0.95	0.06	23,31,47,51	0
35	DGD	c	517	62/66	0.95	0.07	23,30,56,71	0
22	BCR	C	515	40/40	0.95	0.06	31,37,43,45	0
20	CLA	C	511	65/65	0.95	0.07	30,37,42,45	0
20	CLA	B	610	65/65	0.95	0.06	26,31,35,38	0
20	CLA	C	503	65/65	0.95	0.06	28,33,37,42	0
22	BCR	T	101	40/40	0.95	0.06	24,32,43,45	0
20	CLA	C	504	65/65	0.95	0.07	27,30,59,61	0
20	CLA	b	608	65/65	0.95	0.07	24,31,59,63	0
20	CLA	c	507	65/65	0.96	0.07	25,30,49,57	0
20	CLA	c	508	60/65	0.96	0.06	24,28,52,54	0
28	DMS	b	631	4/4	0.96	0.09	23,24,27,35	0
33	CA	O	301	1/1	0.96	0.05	47,47,47,47	0
20	CLA	c	509	65/65	0.96	0.07	25,30,53,58	0
20	CLA	C	509	65/65	0.96	0.07	29,34,52,55	0
28	DMS	v	202	4/4	0.96	0.11	50,51,53,55	0
20	CLA	C	510	65/65	0.96	0.06	26,31,38,44	0
20	CLA	C	502	65/65	0.96	0.06	24,29,41,48	0
22	BCR	A	405	40/40	0.96	0.05	21,26,32,35	0
22	BCR	B	618	40/40	0.96	0.06	21,28,42,45	0
24	LMG	J	101	45/55	0.96	0.07	27,32,64,70	0
22	BCR	B	619	40/40	0.96	0.06	22,30,42,44	0
20	CLA	B	607	65/65	0.96	0.07	22,29,55,62	0
20	CLA	B	603	65/65	0.96	0.06	23,28,35,39	0
27	PL9	D	412	55/55	0.96	0.05	19,23,29,34	0
20	CLA	B	611	65/65	0.96	0.06	21,26,34,40	0
27	PL9	d	412	55/55	0.96	0.05	18,23,29,35	0
20	CLA	b	604	65/65	0.96	0.06	23,27,33,35	0
20	CLA	B	615	65/65	0.96	0.07	20,24,70,79	0
20	CLA	b	611	65/65	0.96	0.06	24,30,34,41	0
22	BCR	a	408	40/40	0.96	0.05	21,25,30,31	0
22	BCR	b	619	40/40	0.96	0.05	23,26,32,35	0
35	DGD	C	516	62/66	0.96	0.07	22,32,74,79	0
22	BCR	b	620	40/40	0.96	0.05	22,27,43,46	0
35	DGD	C	518	62/66	0.96	0.07	24,30,62,73	0
22	BCR	c	514	40/40	0.96	0.06	28,36,39,39	0
20	CLA	b	612	65/65	0.96	0.06	21,27,36,41	0
35	DGD	c	515	62/66	0.96	0.07	23,32,71,75	0
35	DGD	c	516	57/66	0.96	0.06	27,32,62,68	0
22	BCR	j	102	40/40	0.96	0.06	30,35,42,45	0
20	CLA	b	616	65/65	0.96	0.07	20,26,73,80	0
20	CLA	B	616	65/65	0.96	0.06	25,29,48,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	c	501	65/65	0.96	0.06	26,30,41,48	0
20	CLA	c	503	65/65	0.96	0.06	25,35,40,43	0
20	CLA	c	504	65/65	0.96	0.06	25,29,55,60	0
36	LHG	d	406	49/49	0.96	0.06	29,36,43,48	0
36	LHG	d	408	49/49	0.96	0.09	24,31,83,88	0
20	CLA	c	505	65/65	0.96	0.06	25,30,46,50	0
20	CLA	C	501	65/65	0.96	0.06	27,33,45,52	0
21	PHO	A	403	64/64	0.97	0.04	18,22,24,25	0
21	PHO	D	403	64/64	0.97	0.04	18,24,29,35	0
21	PHO	a	405	64/64	0.97	0.04	17,20,22,25	0
21	PHO	a	406	64/64	0.97	0.04	19,24,29,32	0
20	CLA	b	610	65/65	0.97	0.05	20,26,31,33	0
22	BCR	B	617	40/40	0.97	0.05	22,26,32,33	0
20	CLA	B	608	65/65	0.97	0.05	18,21,34,39	0
20	CLA	B	609	65/65	0.97	0.04	22,25,31,33	0
20	CLA	b	613	65/65	0.97	0.05	20,22,38,44	0
20	CLA	b	614	65/65	0.97	0.05	21,25,31,37	0
20	CLA	A	402	59/65	0.97	0.05	18,22,52,58	0
20	CLA	b	617	65/65	0.97	0.05	23,30,44,50	0
20	CLA	B	604	65/65	0.97	0.05	21,24,33,39	0
20	CLA	B	612	65/65	0.97	0.05	19,22,36,42	0
20	CLA	c	502	65/65	0.97	0.06	22,26,39,48	0
20	CLA	D	401	65/65	0.97	0.05	16,20,35,41	0
20	CLA	D	404	65/65	0.97	0.07	26,29,77,81	0
22	BCR	b	621	40/40	0.97	0.05	27,32,42,44	0
20	CLA	a	403	65/65	0.97	0.05	17,20,29,38	0
20	CLA	a	407	47/65	0.97	0.05	19,22,41,48	0
20	CLA	B	613	65/65	0.97	0.05	21,25,30,34	0
20	CLA	B	606	65/65	0.97	0.05	19,24,35,37	0
33	CA	b	626	1/1	0.97	0.06	42,42,42,42	0
36	LHG	D	408	49/49	0.97	0.06	23,30,44,49	0
20	CLA	b	605	65/65	0.97	0.05	21,25,34,37	0
20	CLA	c	510	65/65	0.97	0.05	23,29,39,42	0
36	LHG	L	101	49/49	0.97	0.06	24,31,49,53	0
20	CLA	b	606	65/65	0.97	0.05	20,24,54,59	0
36	LHG	d	407	49/49	0.97	0.06	22,27,46,50	0
20	CLA	A	404	65/65	0.97	0.07	20,25,88,90	0
36	LHG	l	102	49/49	0.97	0.06	22,30,51,54	0
37	HEM	E	104	43/43	0.97	0.08	39,44,52,56	0
37	HEM	e	102	43/43	0.97	0.08	34,41,56,68	0
20	CLA	b	609	65/65	0.97	0.05	19,22,33,37	0
20	CLA	d	404	65/65	0.97	0.07	24,29,78,87	0

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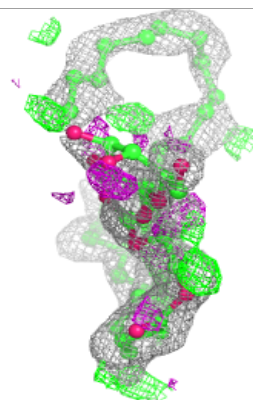
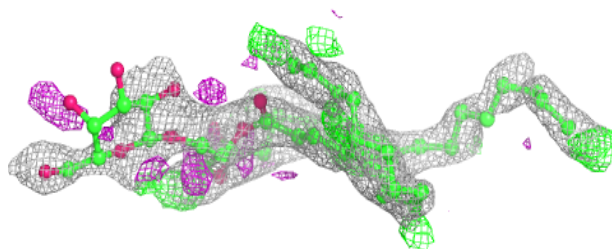
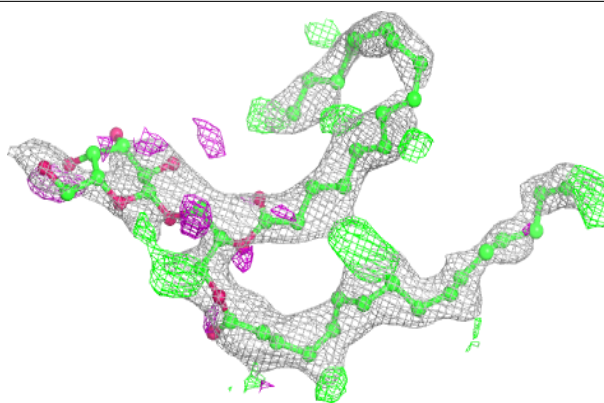
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	b	615	65/65	0.98	0.05	18,22,53,59	0
20	CLA	D	402	65/65	0.98	0.04	15,19,30,36	0
20	CLA	B	605	65/65	0.98	0.06	19,23,55,58	0
33	CA	c	522	1/1	0.98	0.05	41,41,41,41	0
28	DMS	B	634	4/4	0.98	0.07	23,24,25,26	0
20	CLA	d	402	65/65	0.98	0.04	16,20,35,41	0
20	CLA	d	403	65/65	0.98	0.04	17,19,27,34	0
20	CLA	B	614	65/65	0.98	0.04	19,22,48,53	0
28	DMS	c	527	4/4	0.98	0.06	33,33,34,38	0
20	CLA	a	404	60/65	0.98	0.06	18,22,66,75	0
20	CLA	b	607	65/65	0.98	0.05	20,24,33,35	0
28	DMS	C	528	4/4	0.98	0.07	33,37,39,41	0
28	DMS	o	302	4/4	0.98	0.08	20,28,31,36	0
20	CLA	A	401	65/65	0.98	0.04	16,19,30,36	0
33	CA	B	624	1/1	0.98	0.11	43,43,43,43	0
39	MG	J	102	1/1	0.98	0.05	33,33,33,33	0
40	HEC	v	201	43/43	0.98	0.06	25,29,34,37	0
25	CL	A	409	1/1	0.99	0.03	22,22,22,22	0
28	DMS	A	414	4/4	0.99	0.06	25,28,28,29	0
29	FE2	A	419	1/1	0.99	0.02	29,29,29,29	0
29	FE2	a	417	1/1	0.99	0.02	27,27,27,27	0
39	MG	j	103	1/1	0.99	0.08	31,31,31,31	0
40	HEC	V	201	43/43	0.99	0.04	21,23,27,31	0
25	CL	a	412	1/1	0.99	0.03	24,24,24,24	0
25	CL	A	408	1/1	1.00	0.01	22,22,22,22	0
30	OEX	A	420	10/10	1.00	0.03	21,23,24,24	0
30	OEX	a	419	10/10	1.00	0.02	21,24,26,26	0
25	CL	a	411	1/1	1.00	0.03	22,22,22,22	0

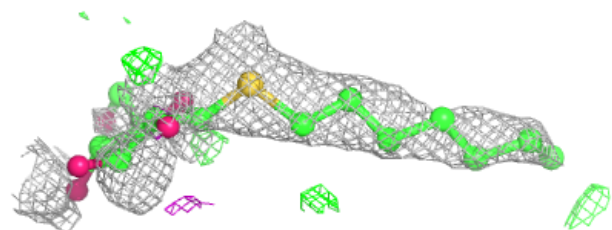
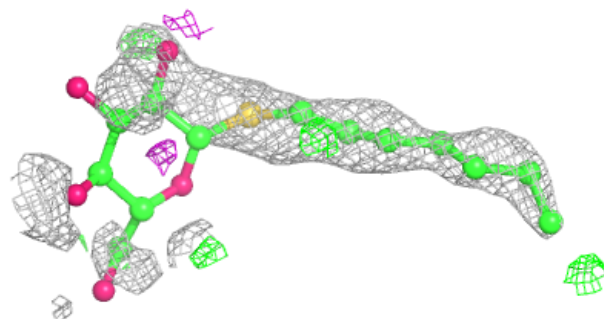
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DGD 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)

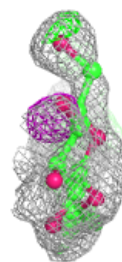
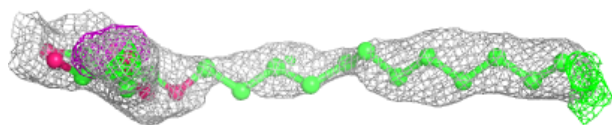
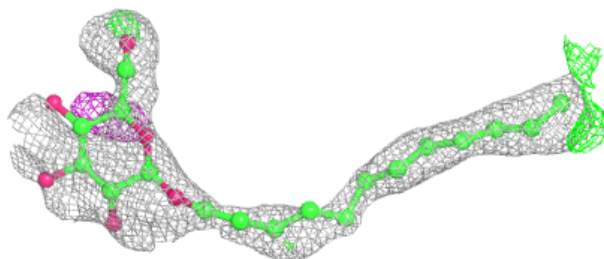
**Electron density around HTG C 534:**

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

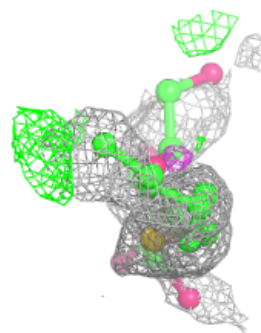
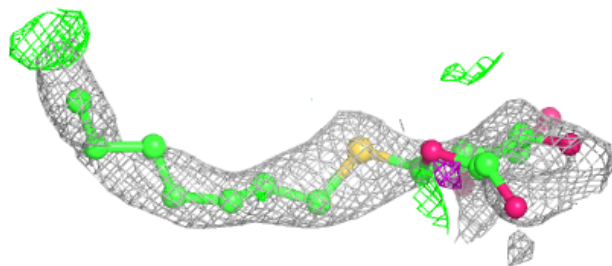
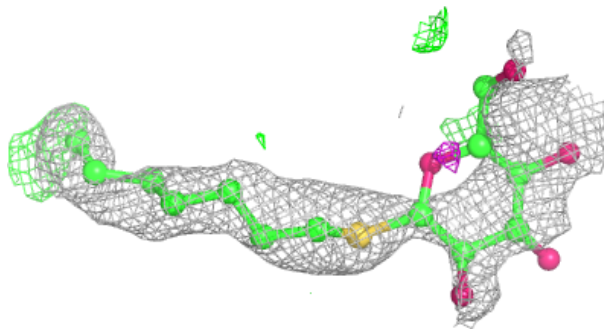


**Electron density around LMT f 102:**

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

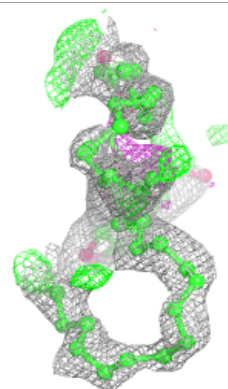
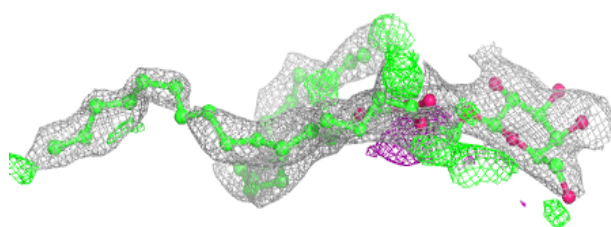
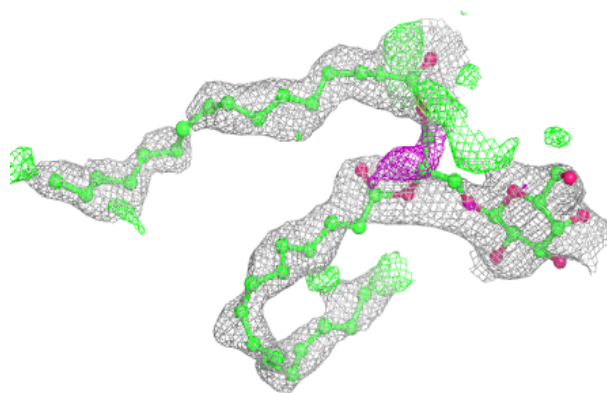
**Electron density around HTG D 417:**

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



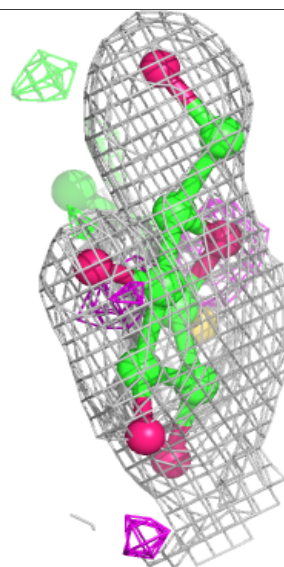
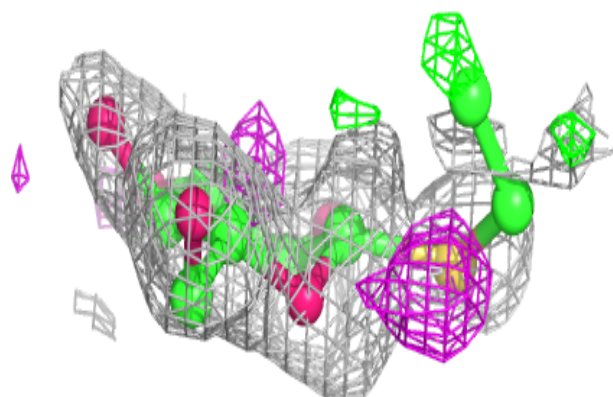
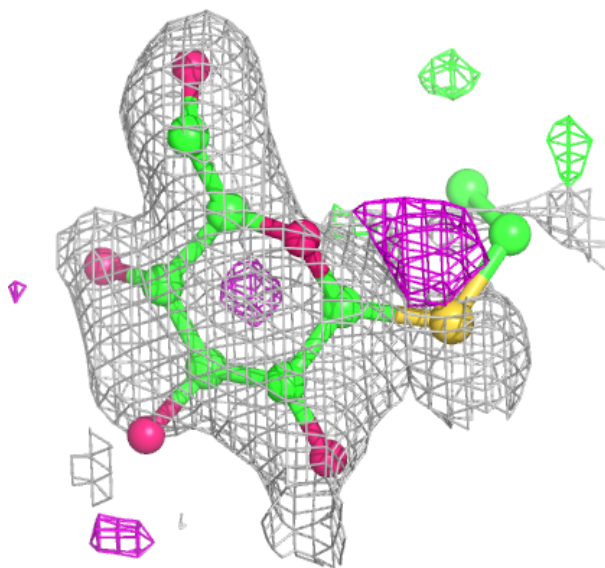
**Electron density around DGD d 416:**

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



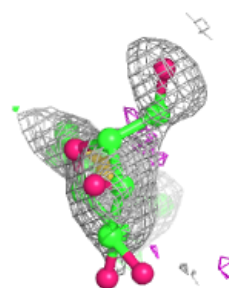
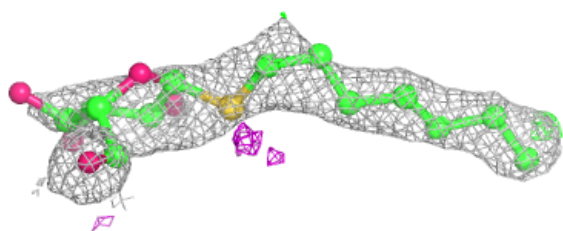
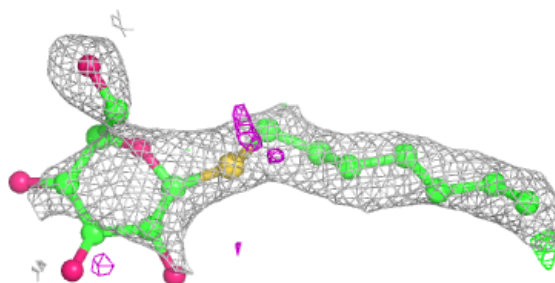
**Electron density around HTG v 210:**

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

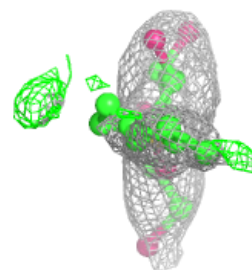
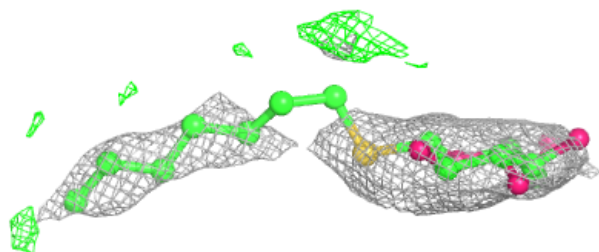
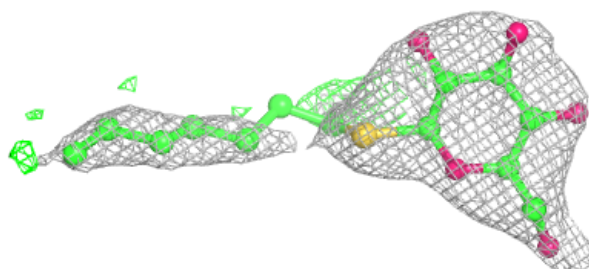


**Electron density around HTG c 521:**

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

**Electron density around HTG c 520:**

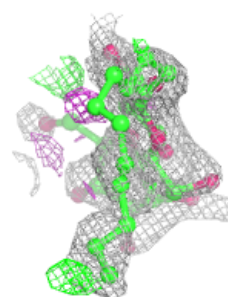
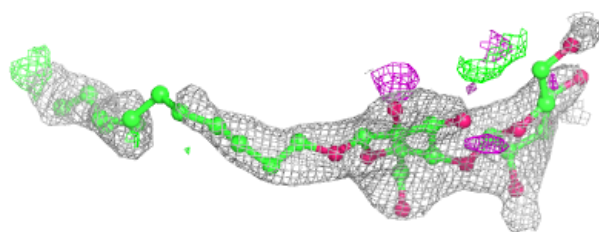
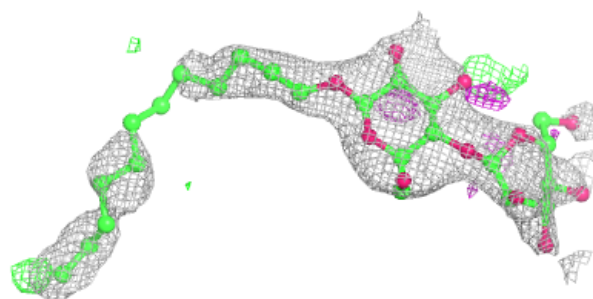
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



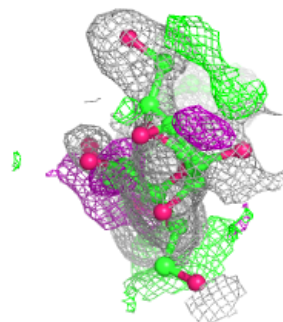
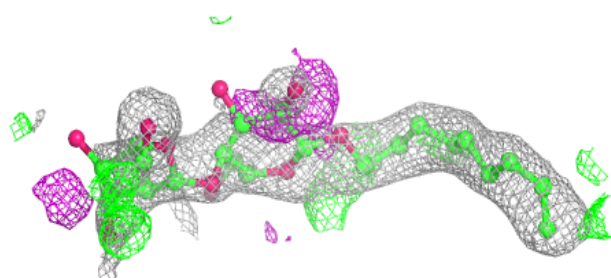
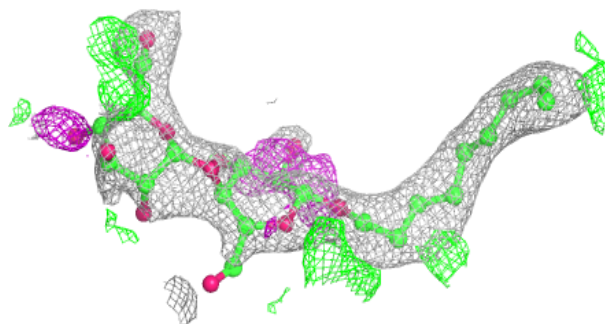


**Electron density around LMT I 101:**

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

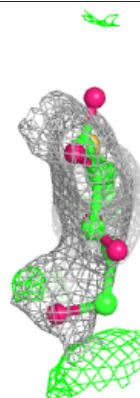
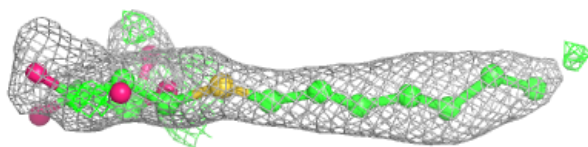
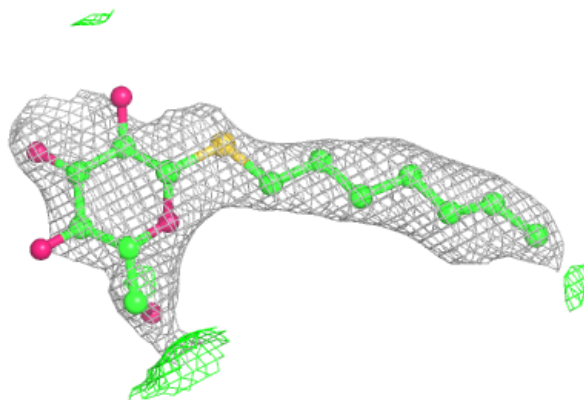
**Electron density around LMT b 627:**

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



**Electron density around HTG b 602:**

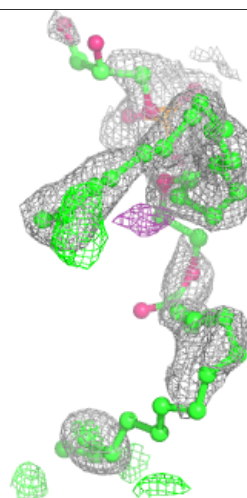
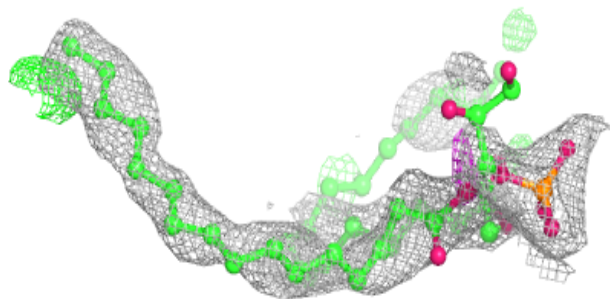
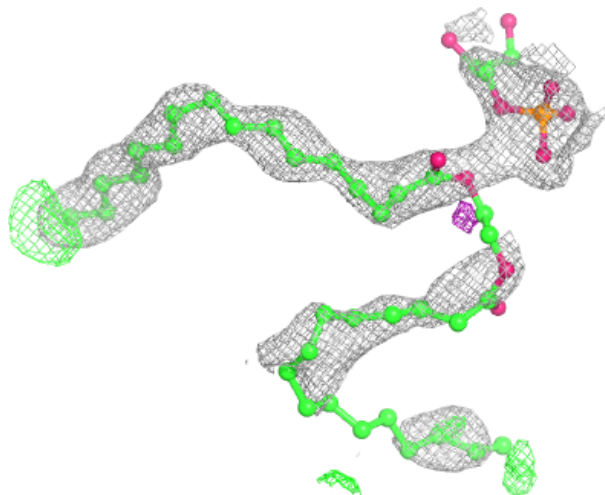
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





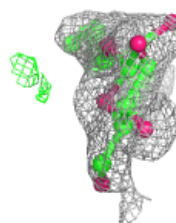
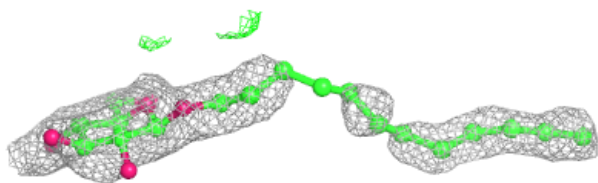
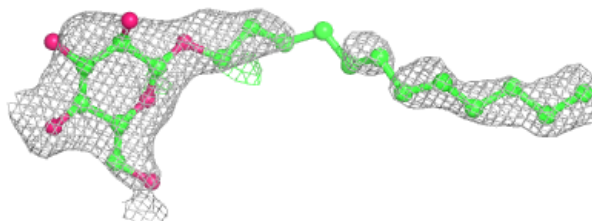
**Electron density around LHG E 103:**

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

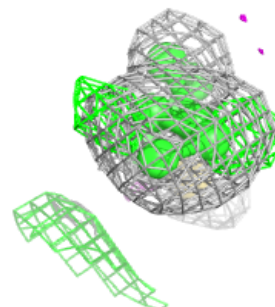
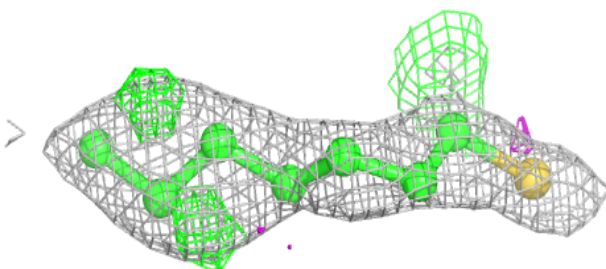
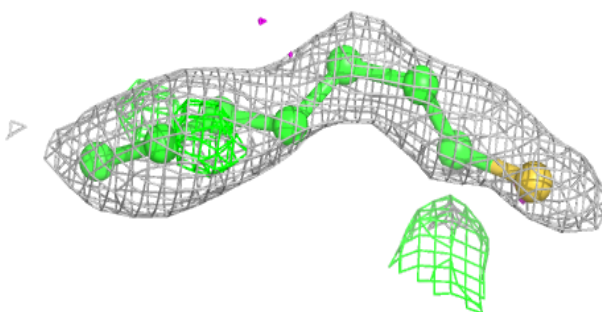


**Electron density around LMT E 101:**

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

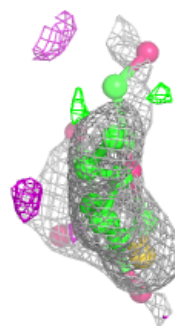
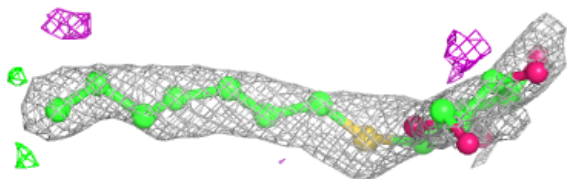
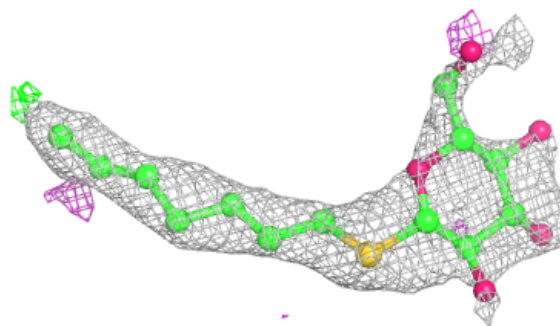
**Electron density around HTG u 201:**

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

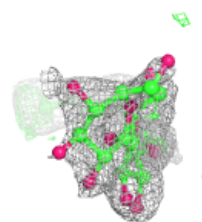
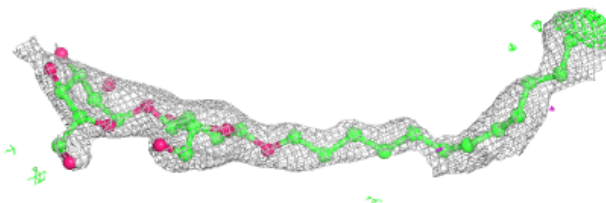
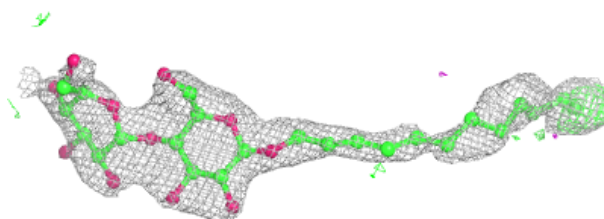


**Electron density around HTG B 623:**

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

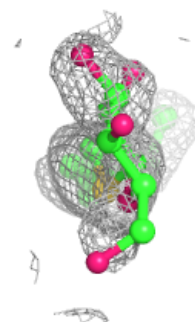
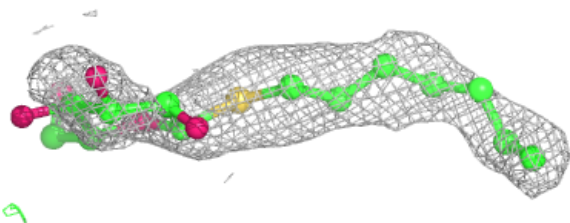
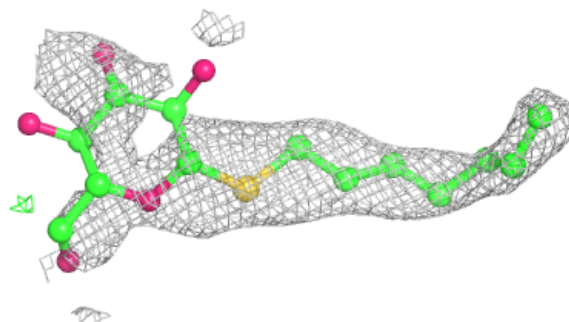
**Electron density around LMT c 523:**

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

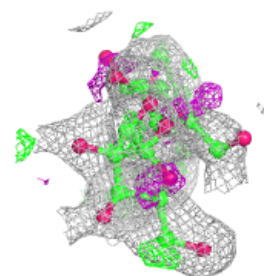
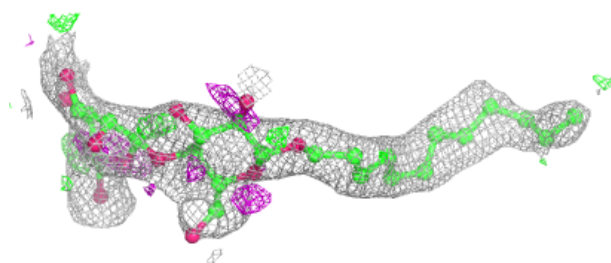
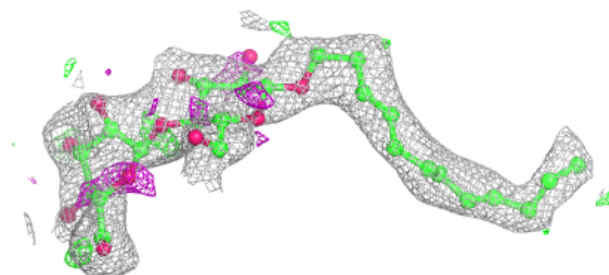


**Electron density around HTG d 401:**

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

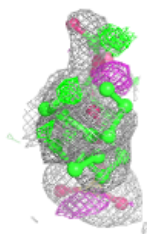
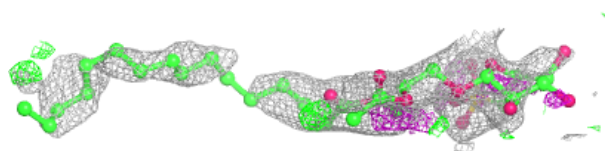
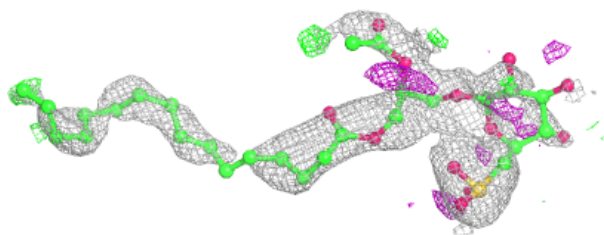
**Electron density around LMT a 418:**

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

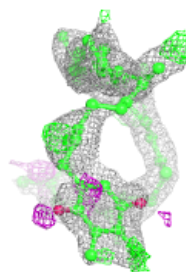
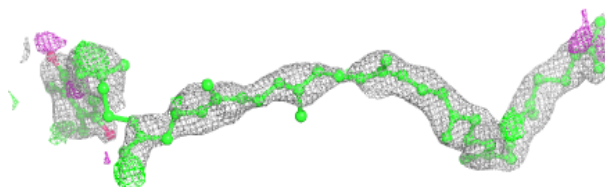
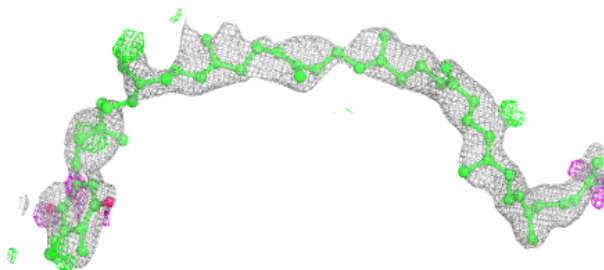


**Electron density around SQD f 101:**

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

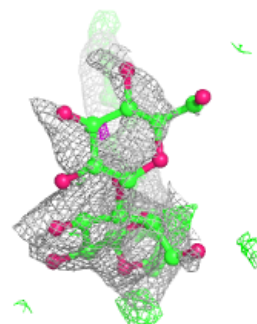
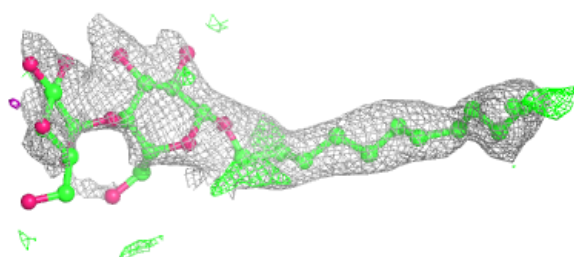
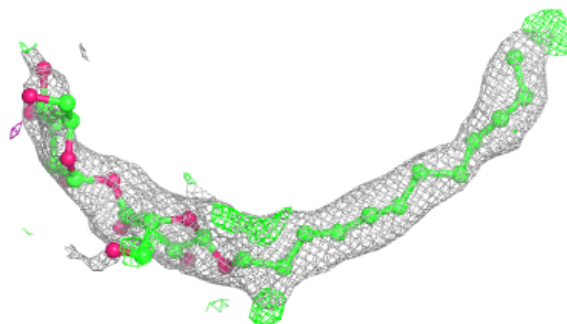
**Electron density around PL9 A 411:**

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

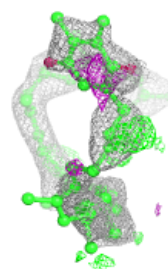
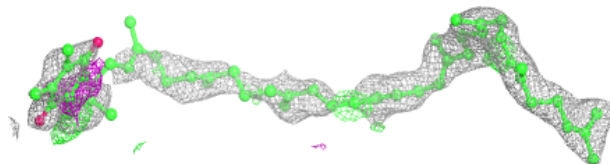
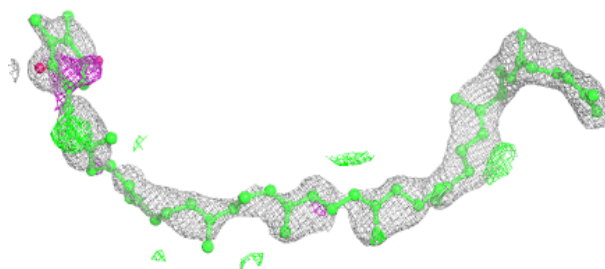


**Electron density around LMT m 101:**

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

**Electron density around PL9 a 415:**

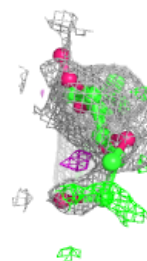
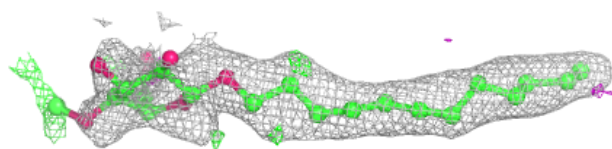
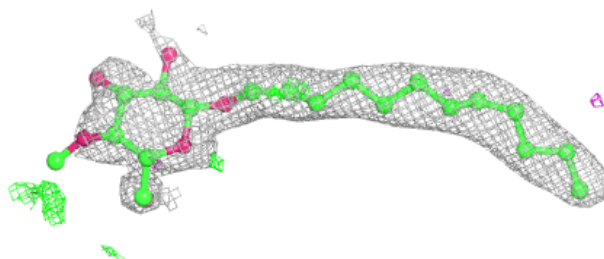
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



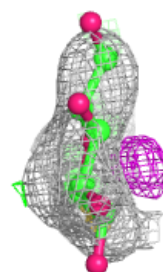
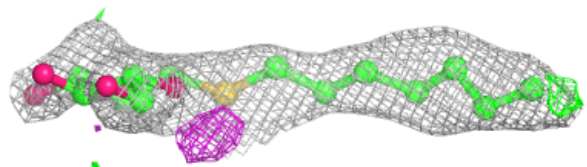
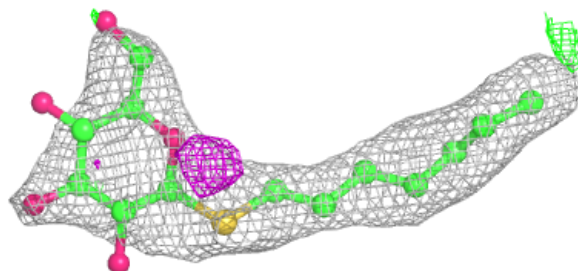


**Electron density around LMT b 628:**

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

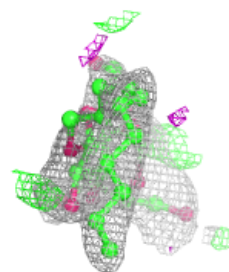
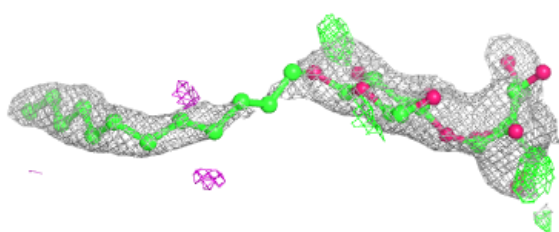
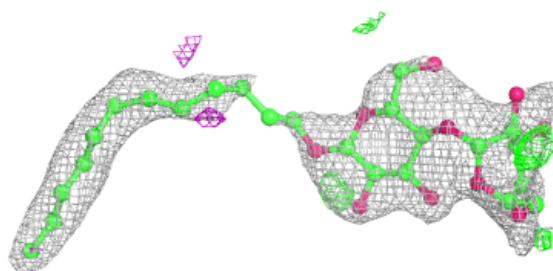
**Electron density around HTG B 632:**

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

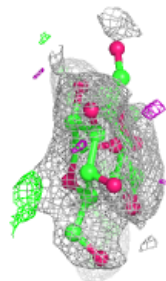
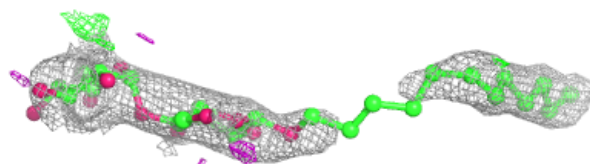
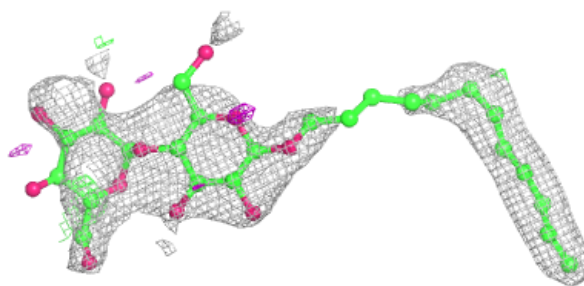


**Electron density around LMT z 102:**

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

**Electron density around LMT Z 101:**

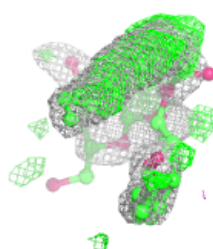
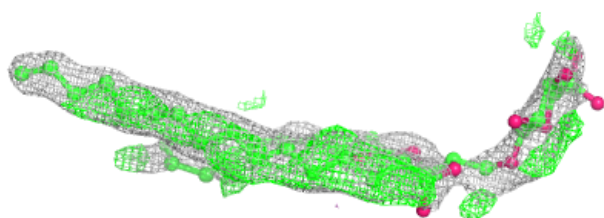
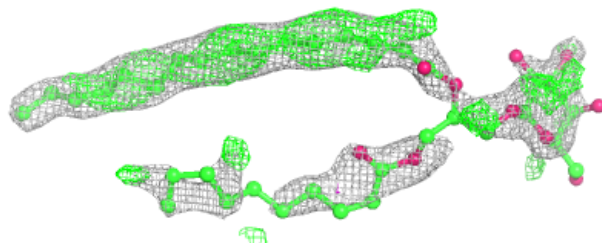
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



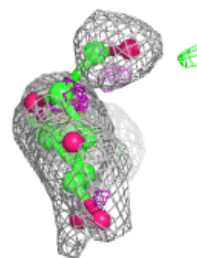
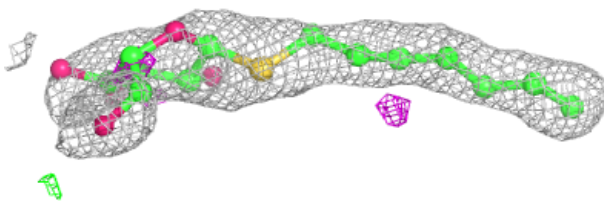
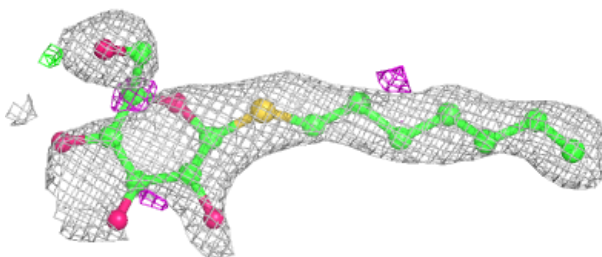


**Electron density around LMG C 524:**

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

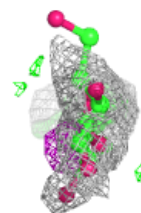
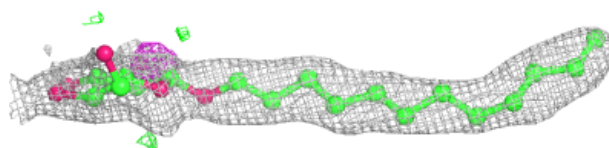
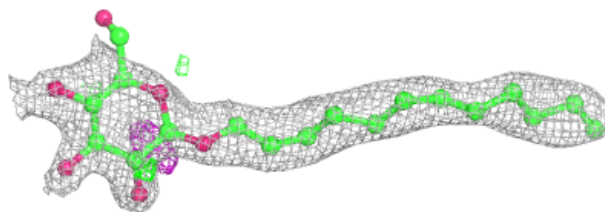
**Electron density around HTG C 521:**

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

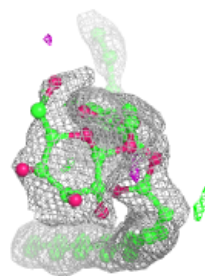
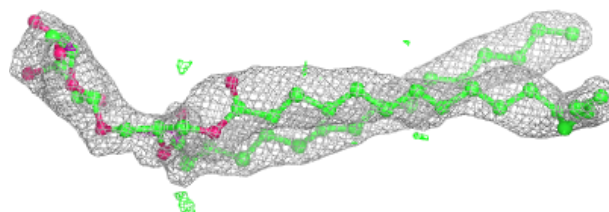
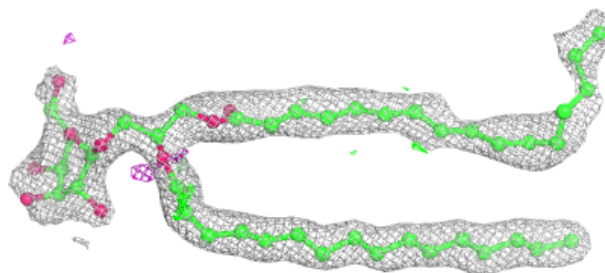


**Electron density around LMT J 103:**

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

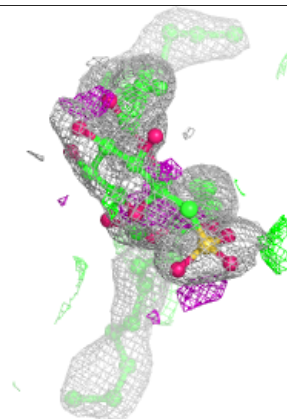
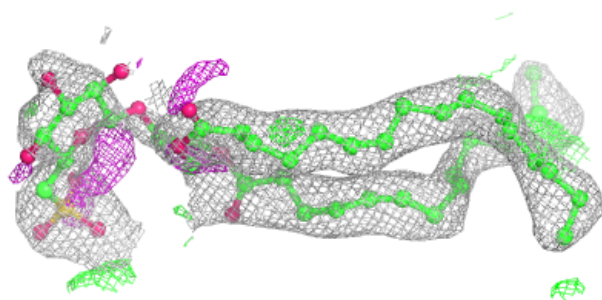
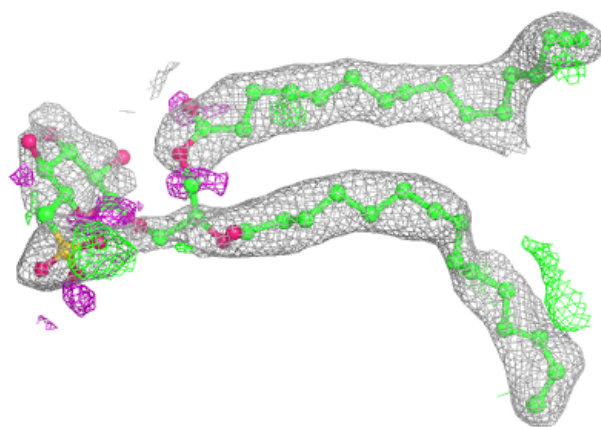
**Electron density around LMG c 518:**

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

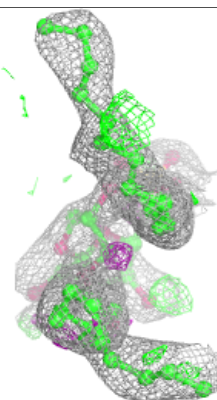
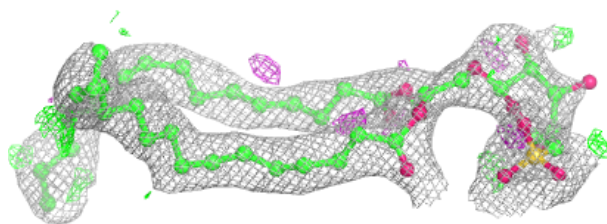
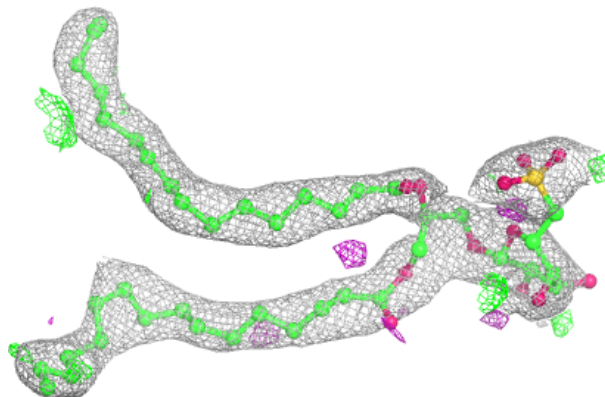


**Electron density around SQD 1 101:**

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

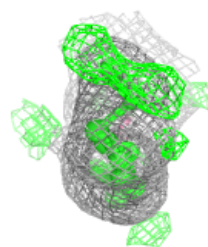
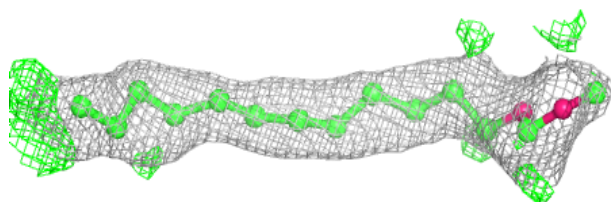
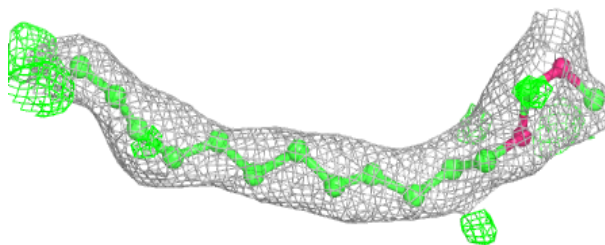
**Electron density around SQD b 622:**

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

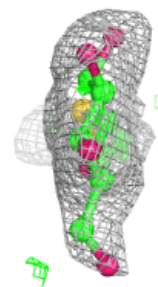
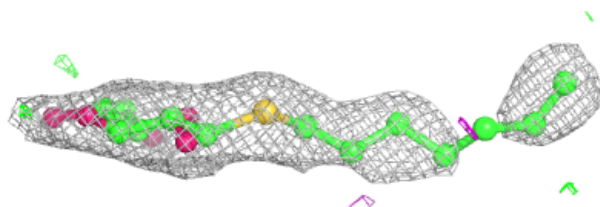
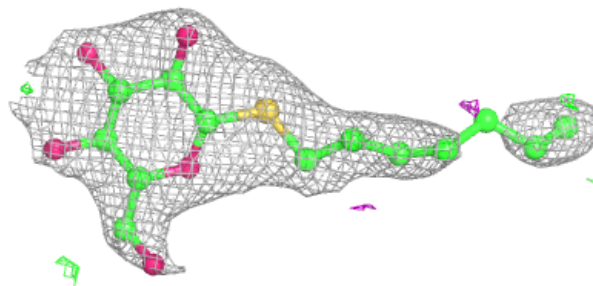


**Electron density around LMT B 627:**

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

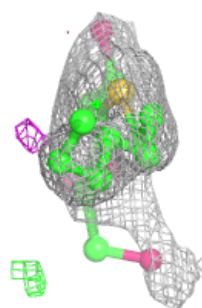
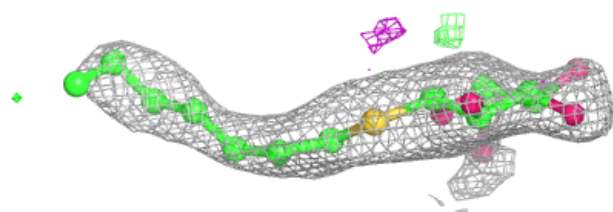
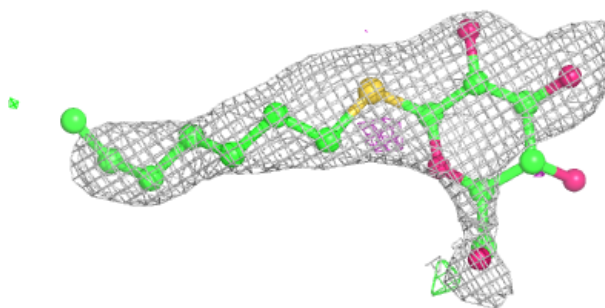
**Electron density around HTG C 520:**

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

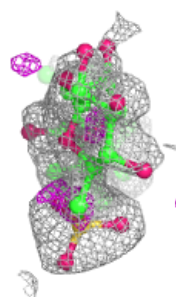
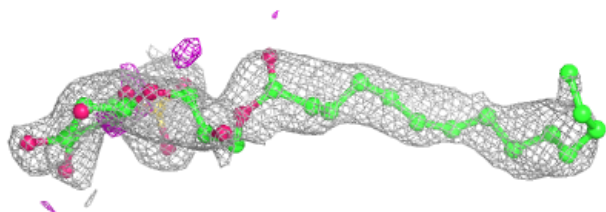
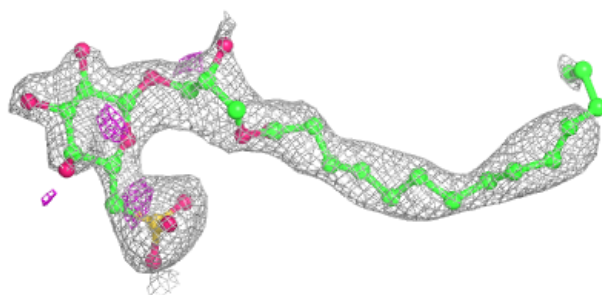


**Electron density around HTG C 522:**

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

**Electron density around SQD F 101:**

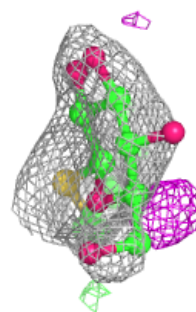
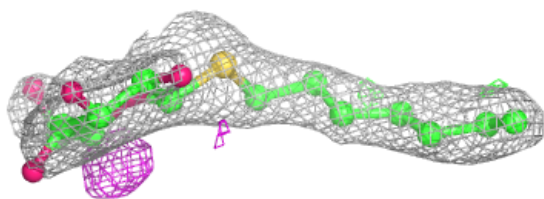
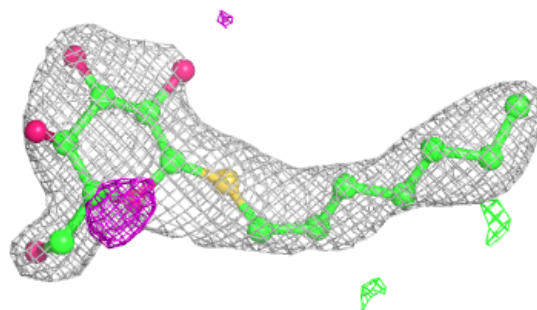
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



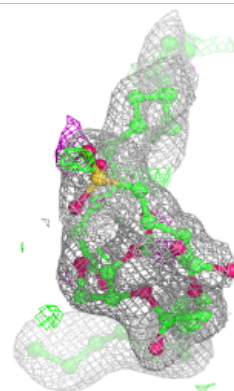
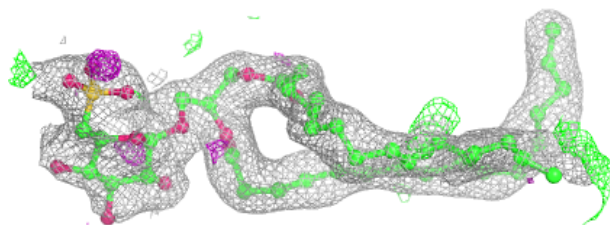
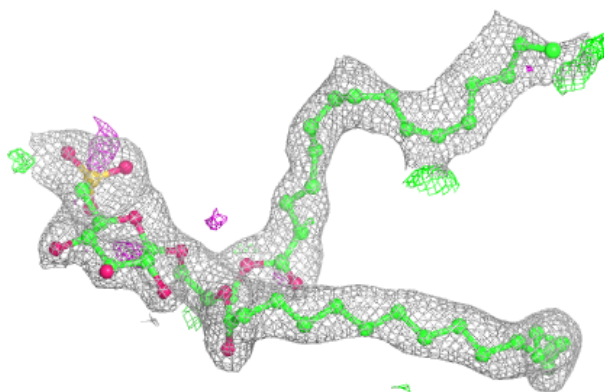


**Electron density around HTG b 624:**

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

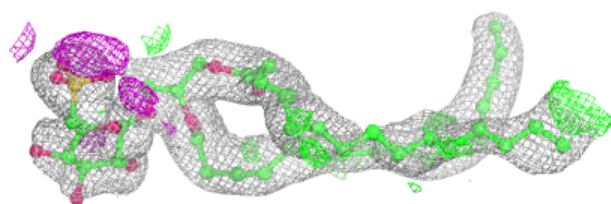
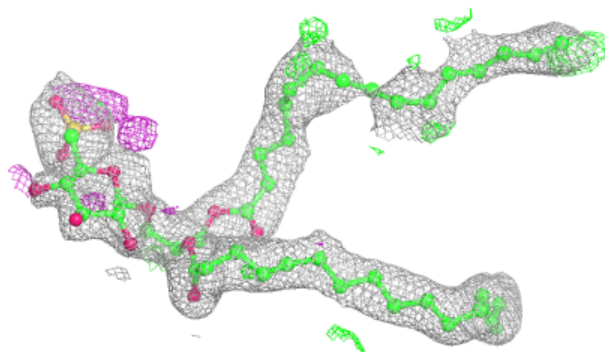
**Electron density around SQD a 401:**

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

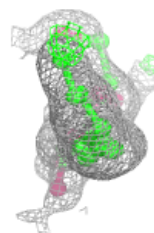
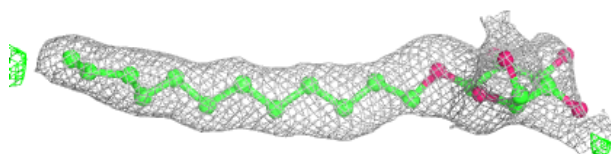
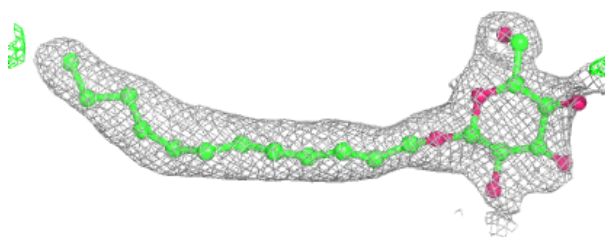


**Electron density around SQD A 412:**

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

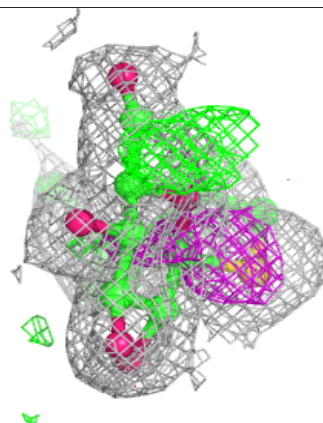
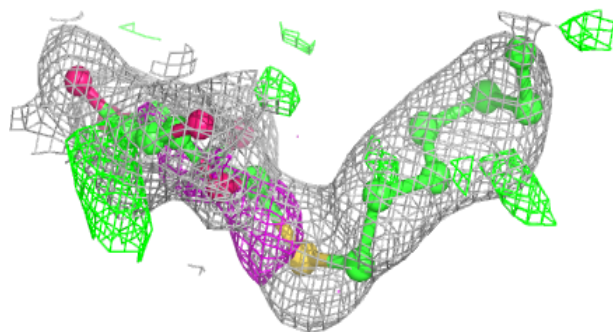
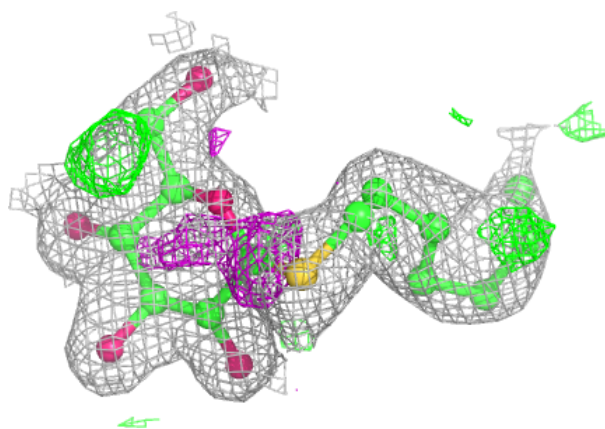
**Electron density around LMT B 625:**

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

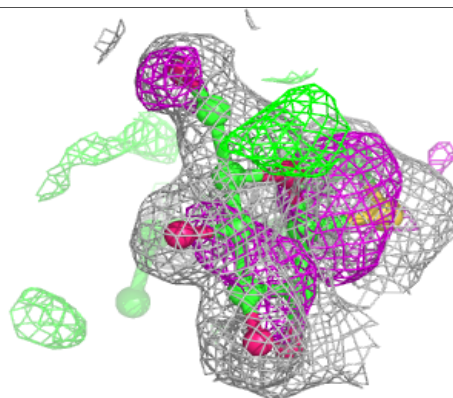
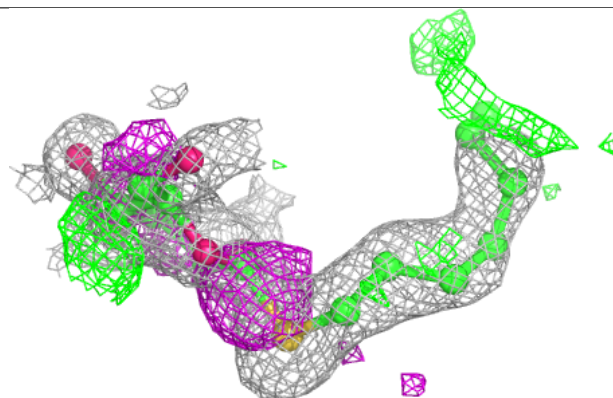
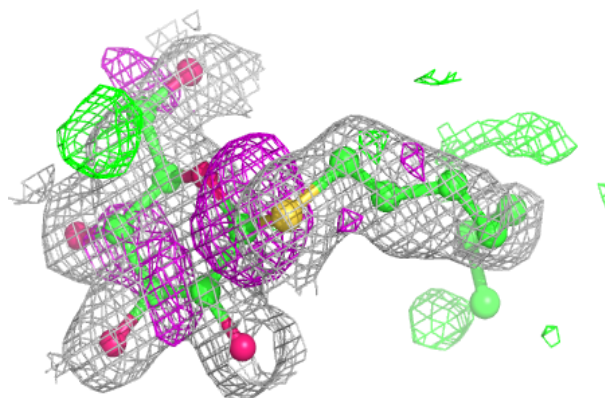


**Electron density around HTG B 622:**

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

**Electron density around HTG b 625:**

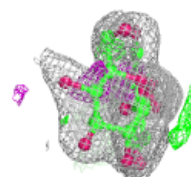
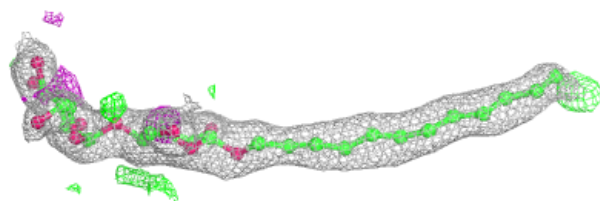
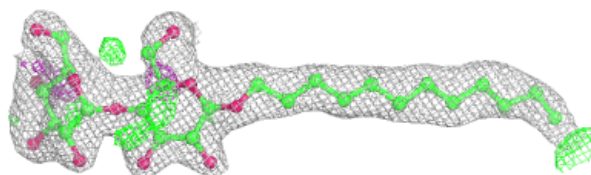
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



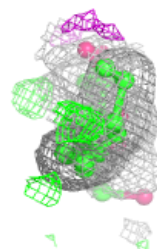
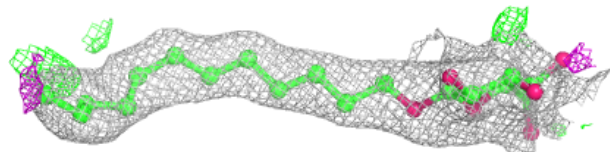
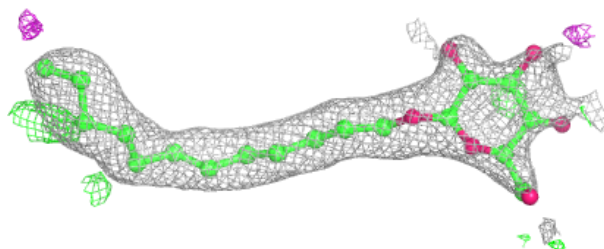


**Electron density around LMT m 102:**

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

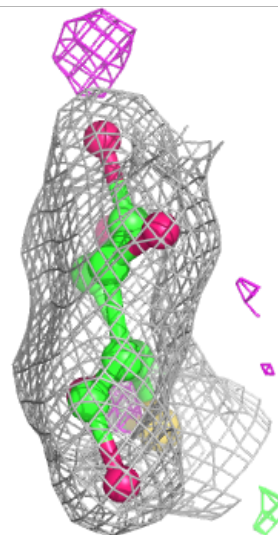
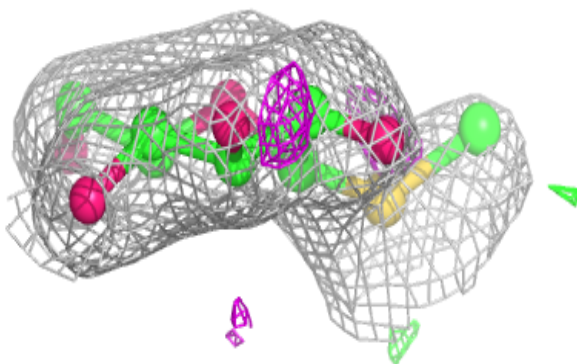
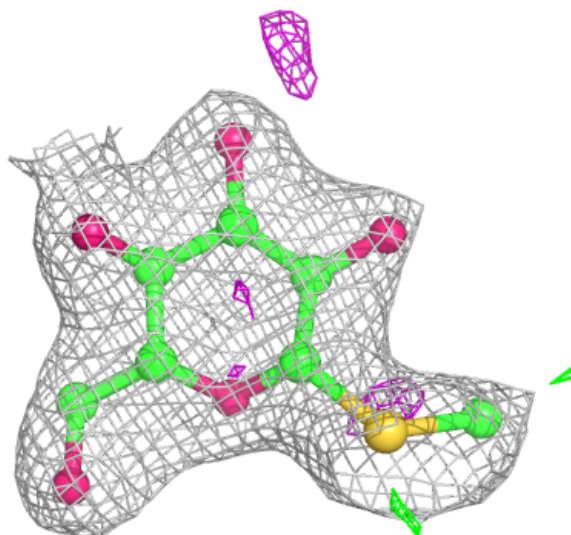
**Electron density around LMT B 626:**

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



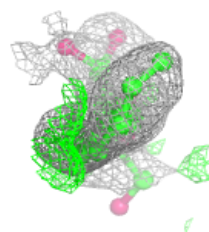
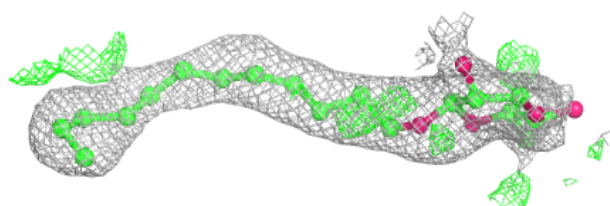
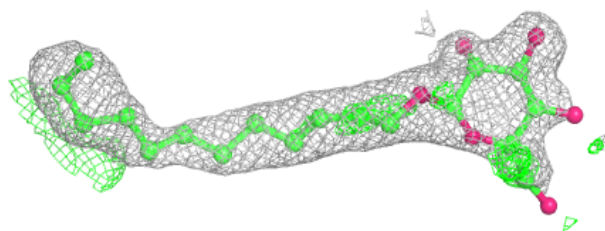
**Electron density around HTG V 202:**

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

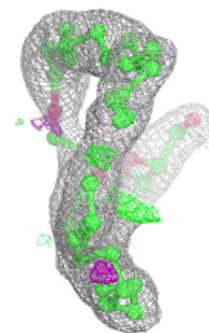
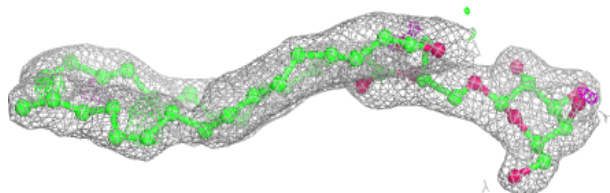
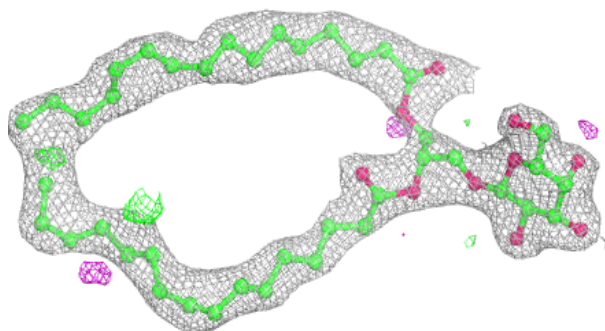


**Electron density around LMT T 102:**

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

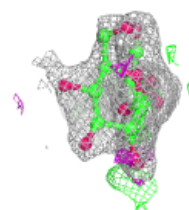
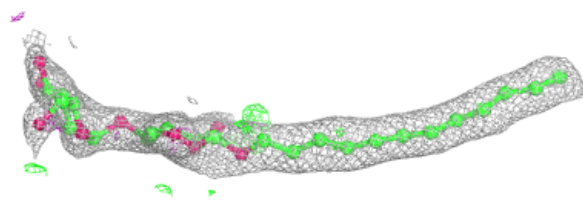
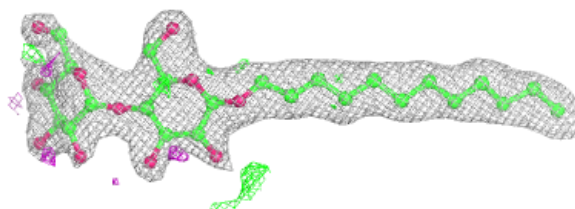
**Electron density around LMG a 410:**

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

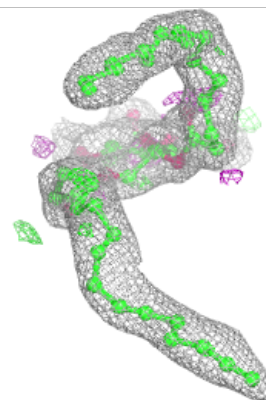
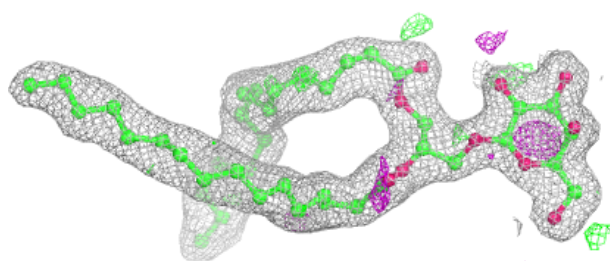
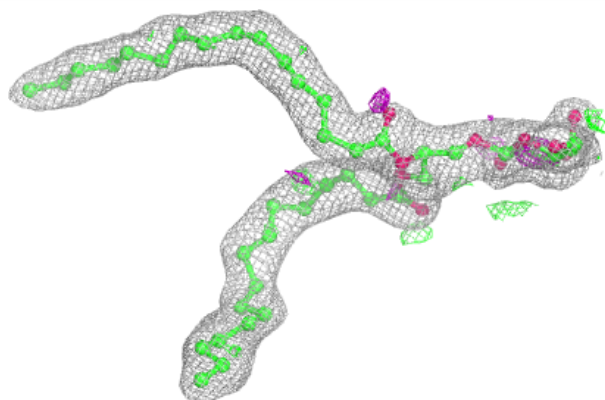


**Electron density around LMT M 101:**

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

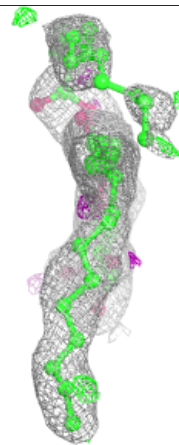
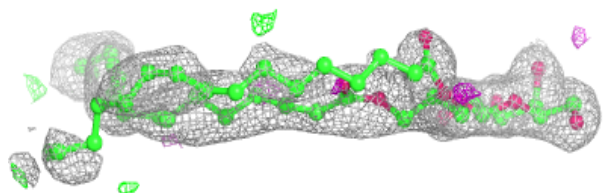
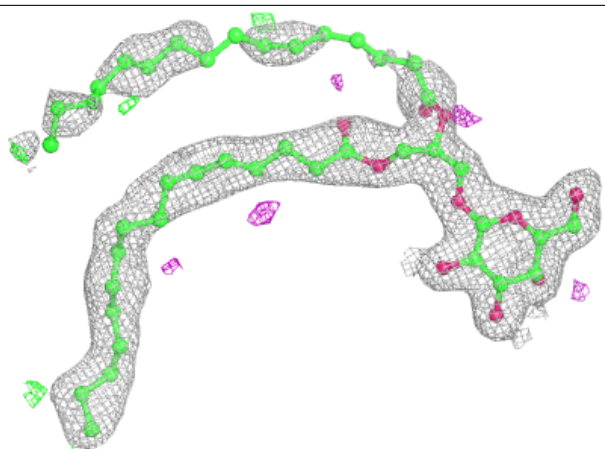
**Electron density around LMG B 620:**

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



**Electron density around LMG c 519:**

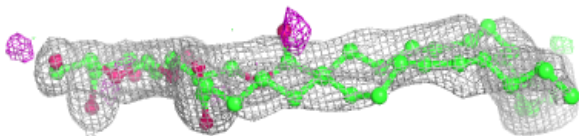
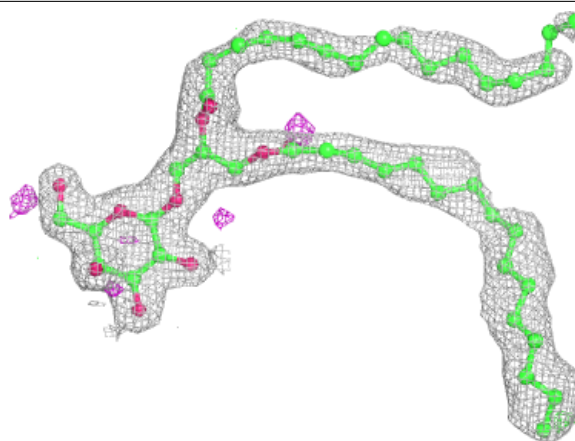
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



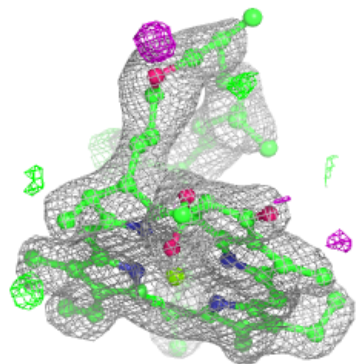
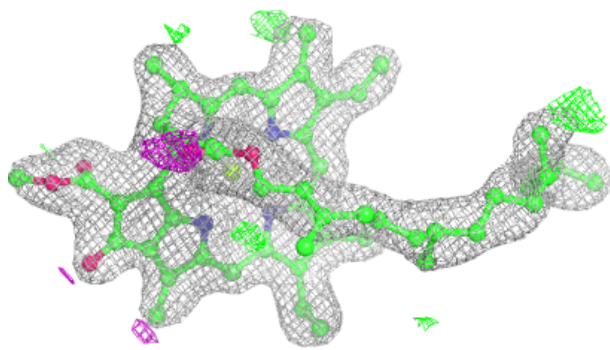
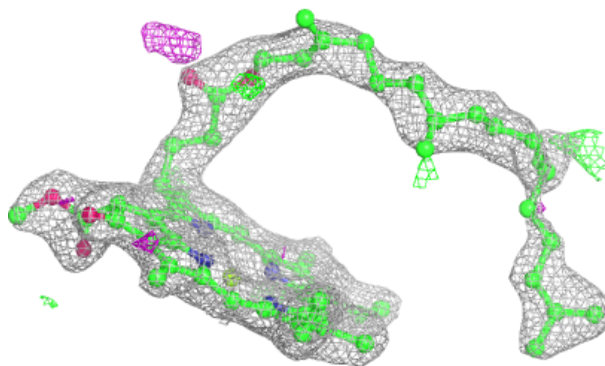


**Electron density around LMG C 519:**

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

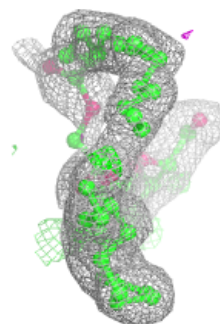
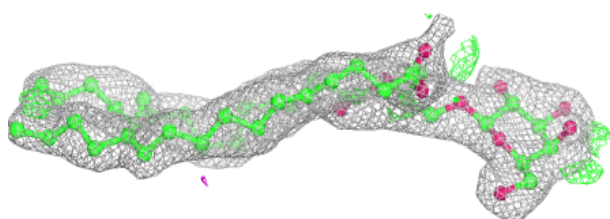
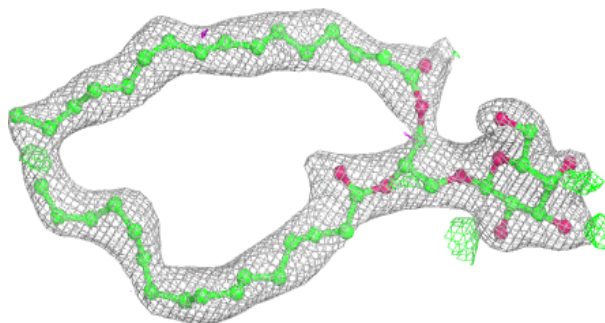
**Electron density around CLA C 513:**

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

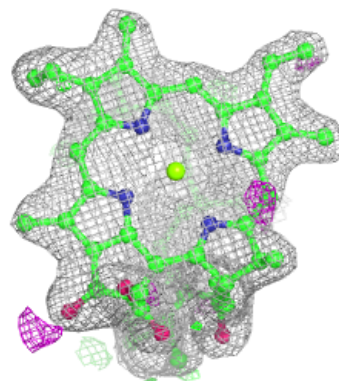
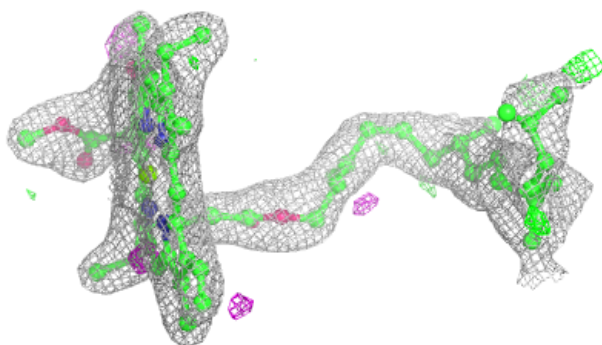
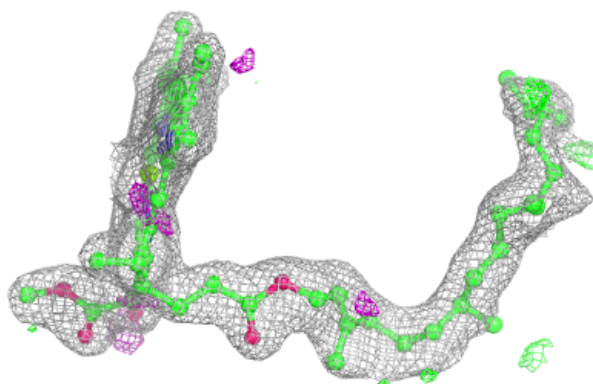


**Electron density around LMG A 407:**

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

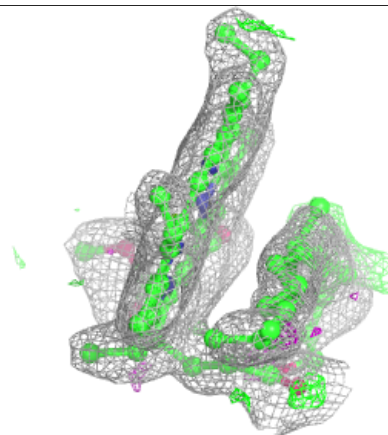
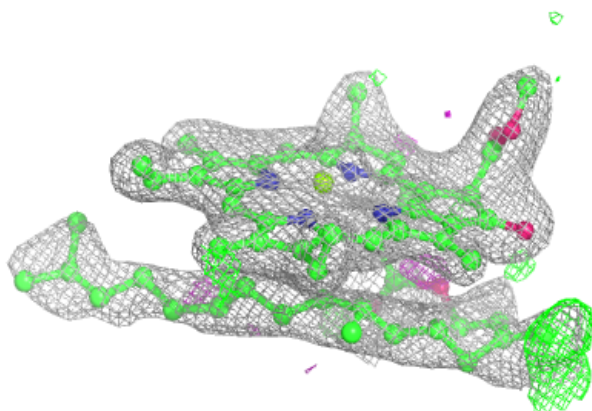
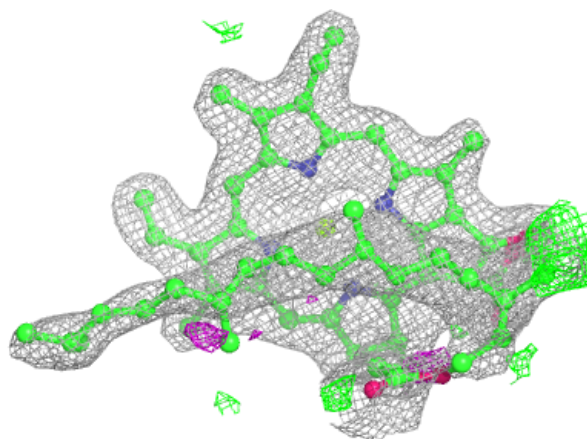
**Electron density around CLA C 506:**

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

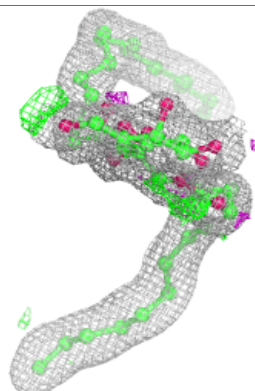
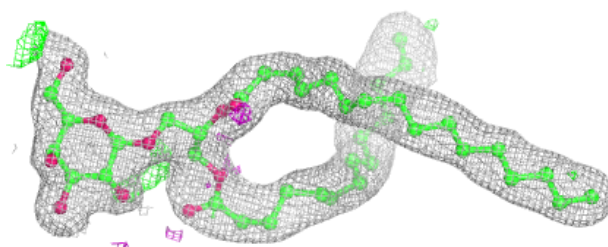
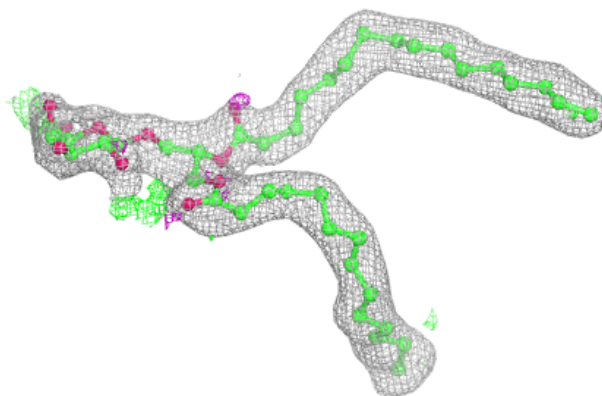


**Electron density around CLA b 603:**

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

**Electron density around LMG b 623:**

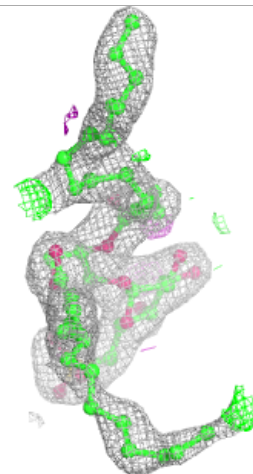
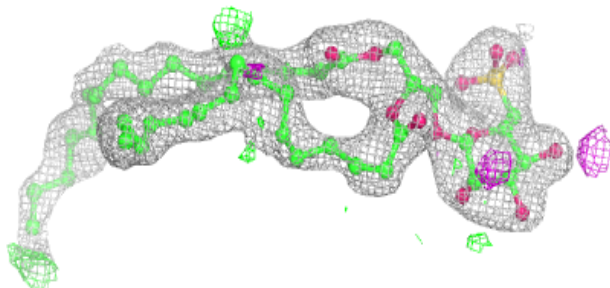
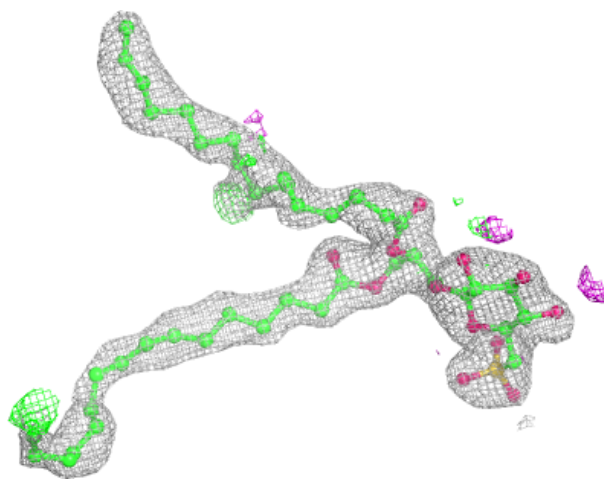
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





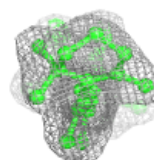
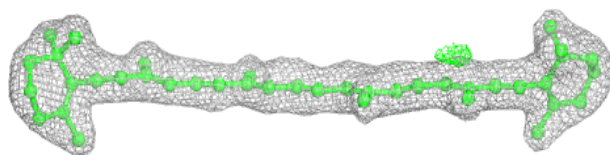
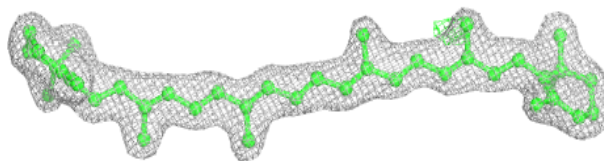
**Electron density around SQD A 406:**

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

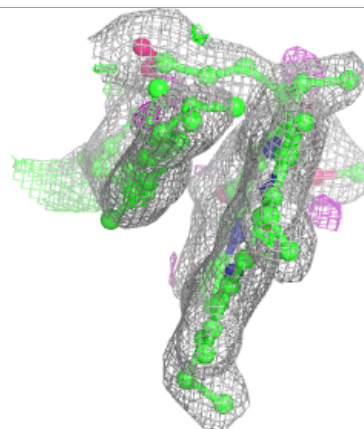
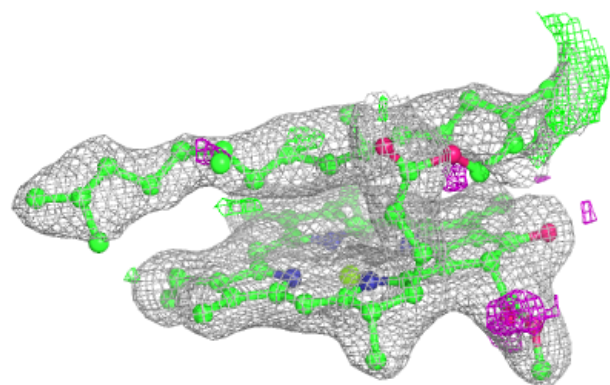
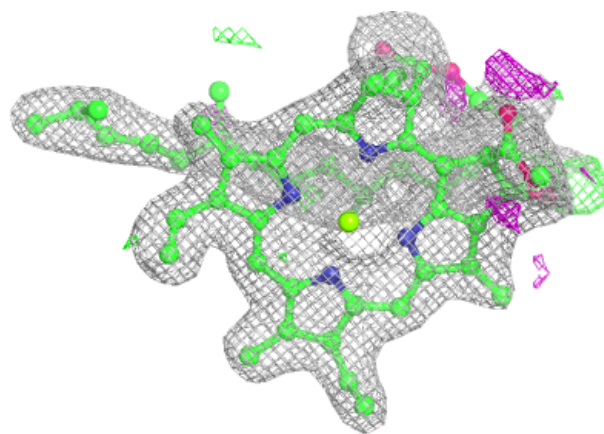


**Electron density around BCR C 514:**

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

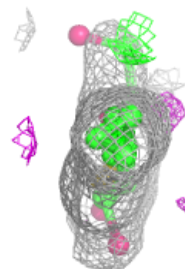
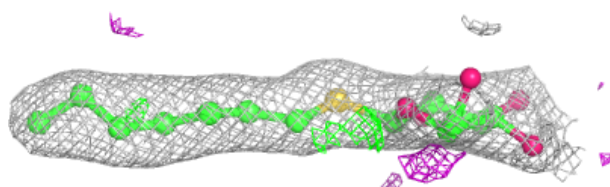
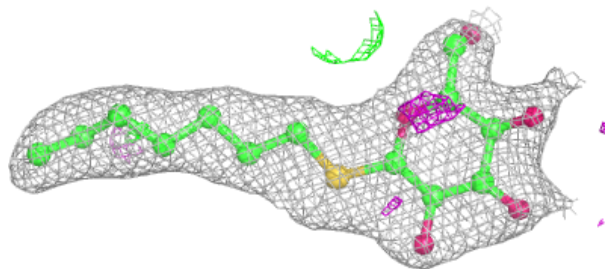
**Electron density around CLA B 602:**

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

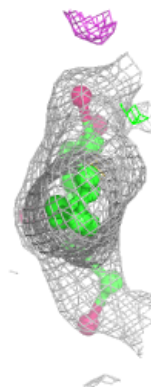
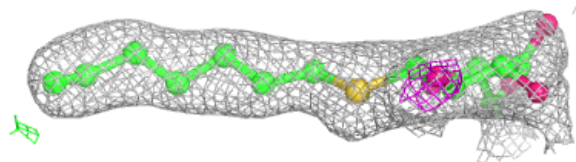
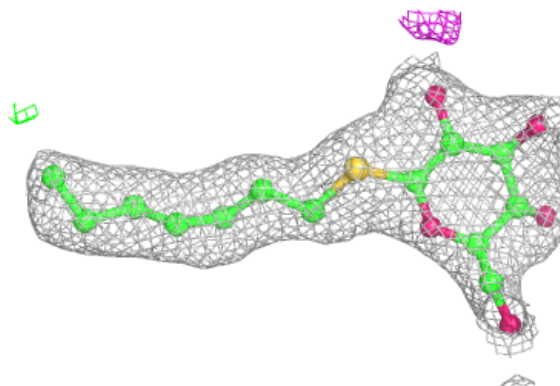


**Electron density around HTG b 601:**

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

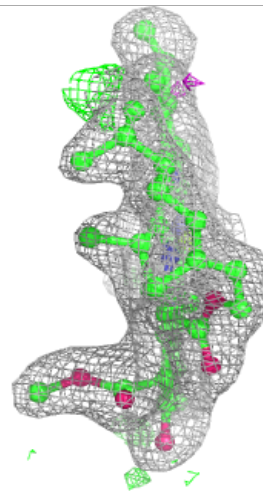
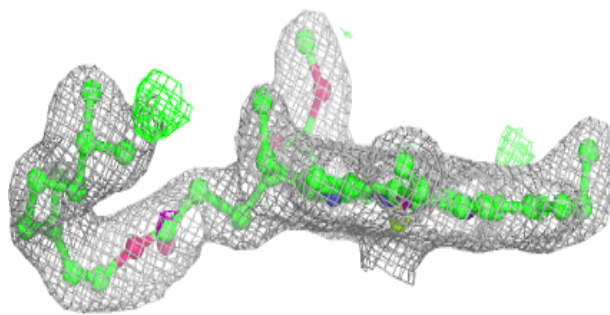
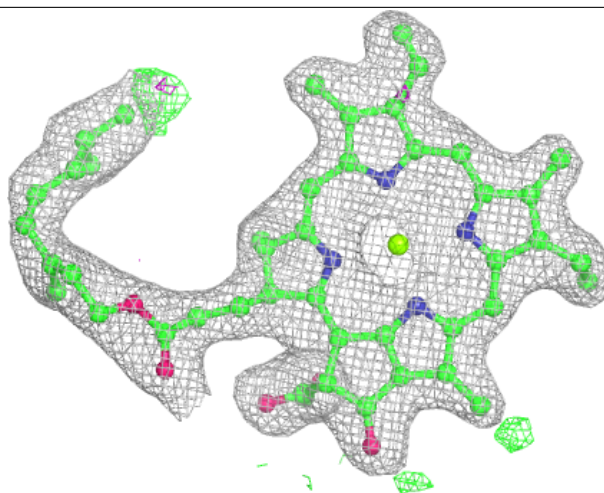
**Electron density around HTG B 631:**

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



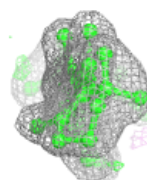
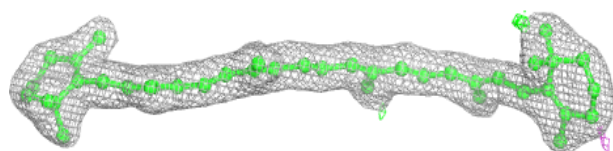
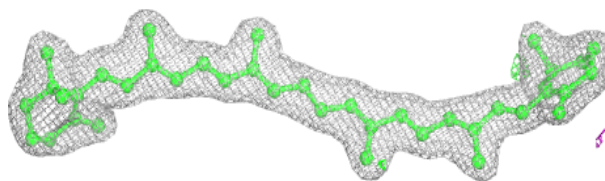
**Electron density around CLA C 512:**

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

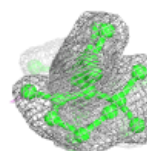
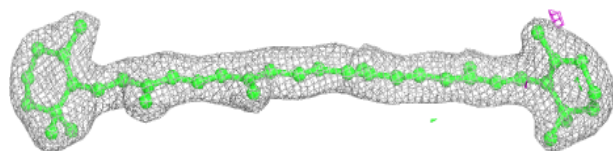
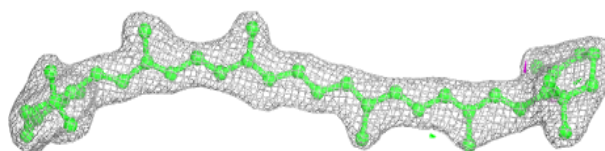


**Electron density around BCR K 101:**

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

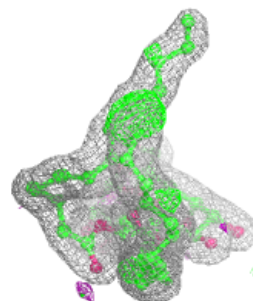
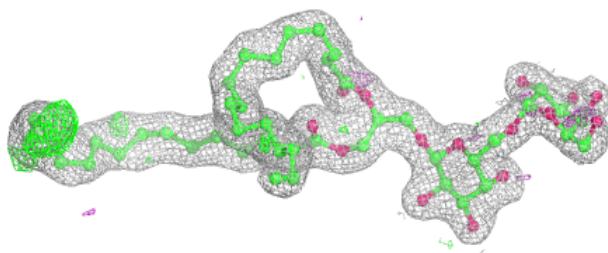
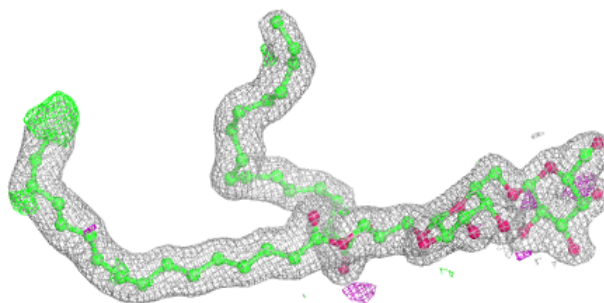
**Electron density around BCR k 102:**

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



**Electron density around DGD h 101:**

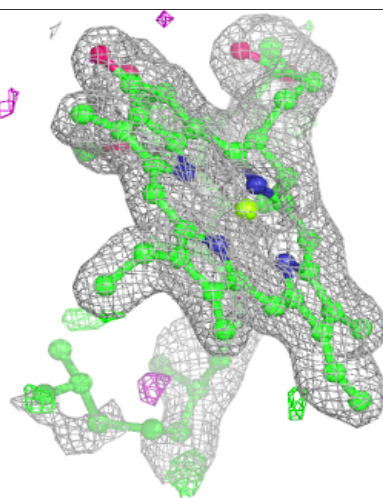
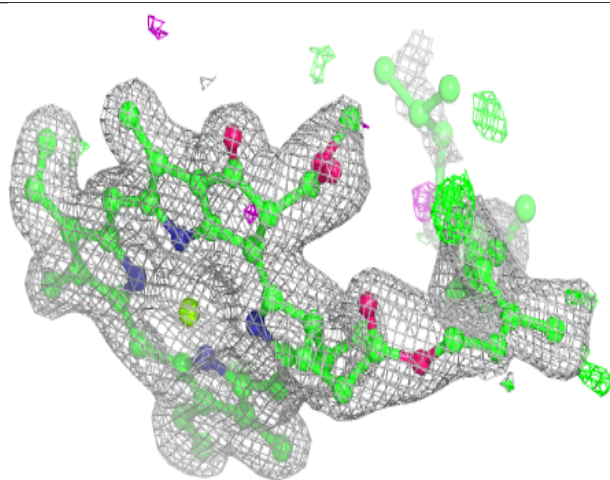
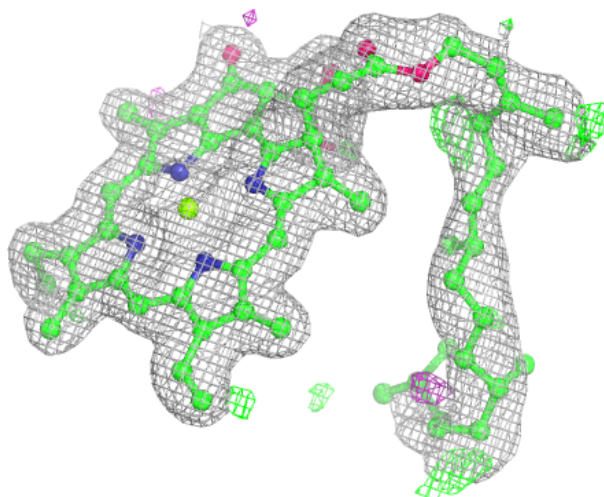
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





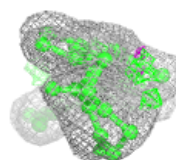
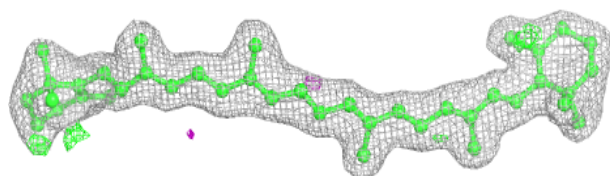
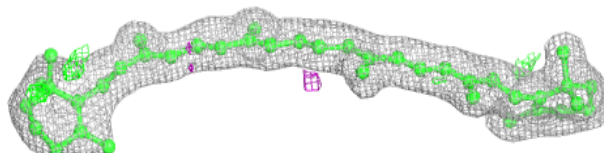
**Electron density around CLA b 618:**

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

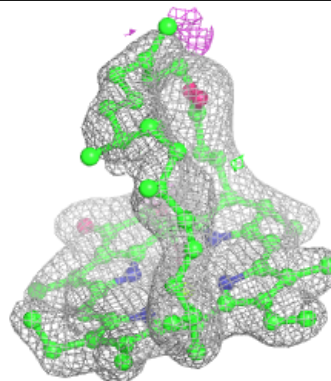
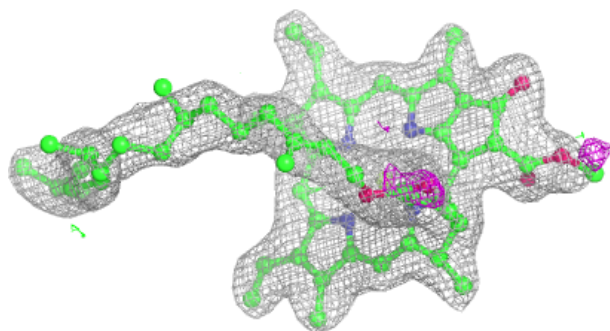
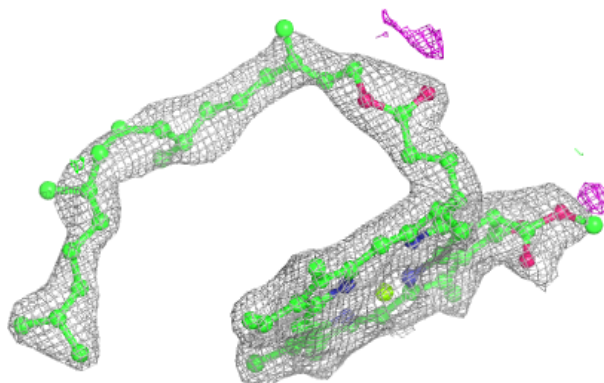


**Electron density around BCR D 405:**

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

**Electron density around CLA c 513:**

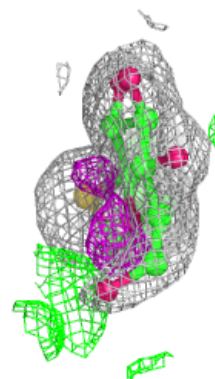
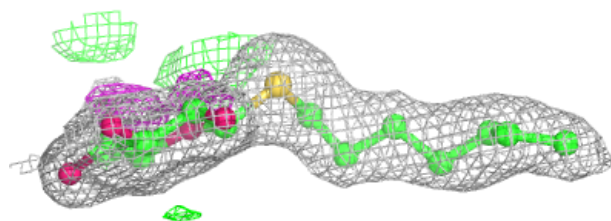
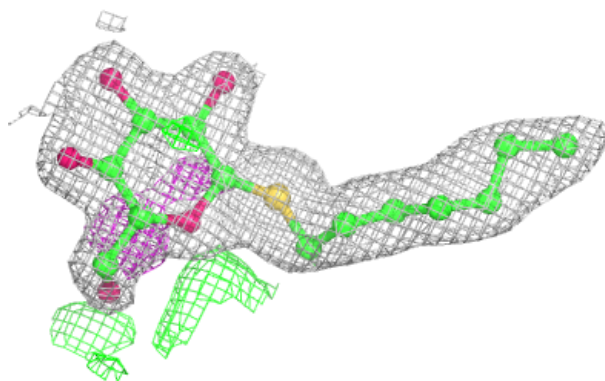
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



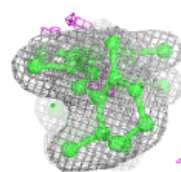
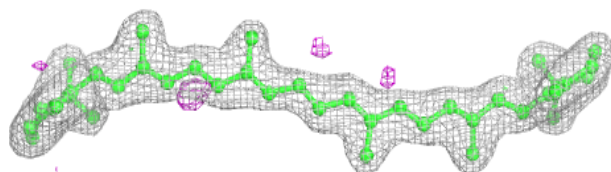
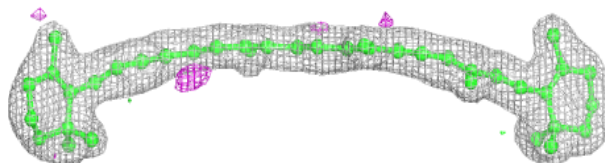


**Electron density around HTG B 621:**

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

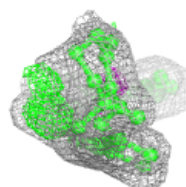
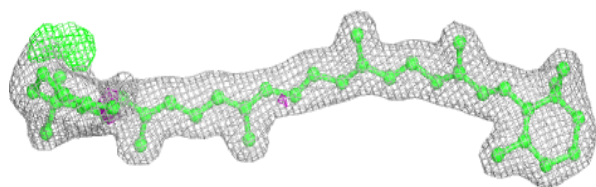
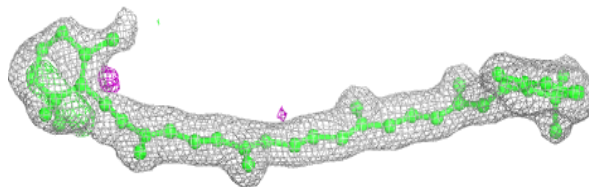
**Electron density around BCR K 102:**

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



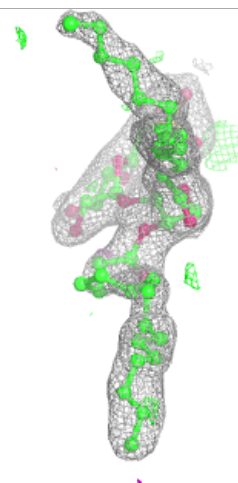
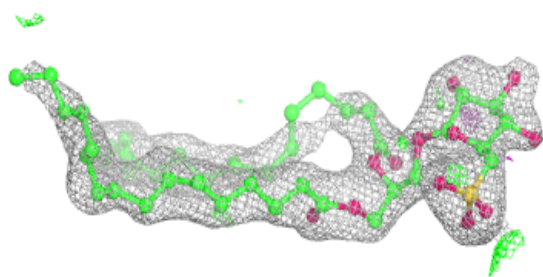
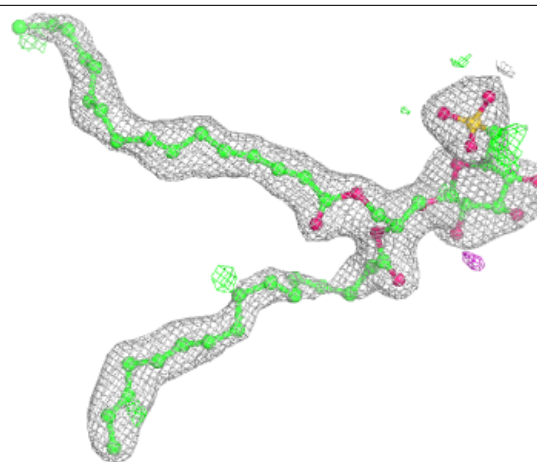
**Electron density around BCR d 405:**

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



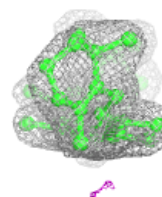
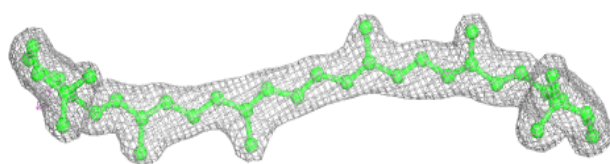
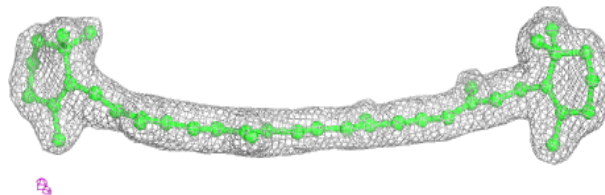
**Electron density around SQD a 409:**

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

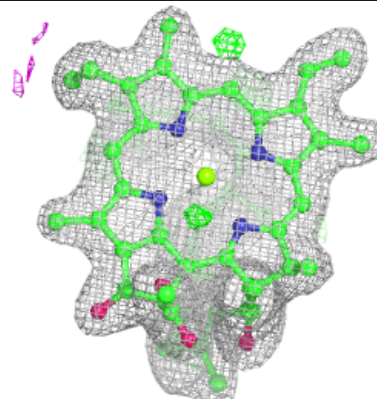
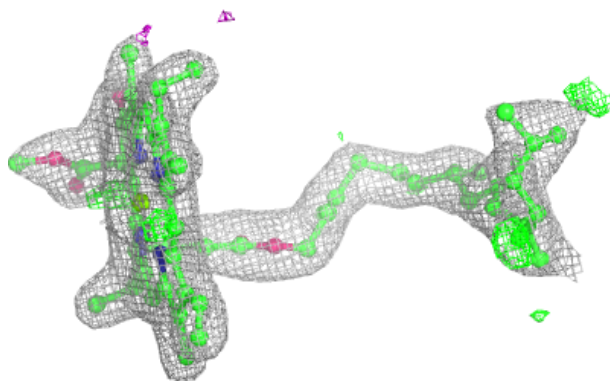
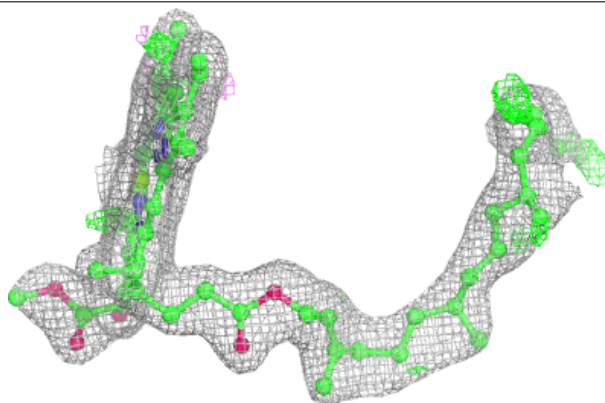


**Electron density around BCR k 101:**

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

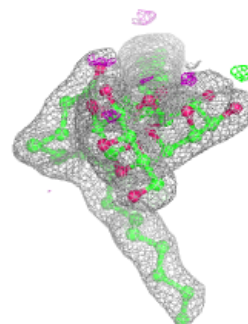
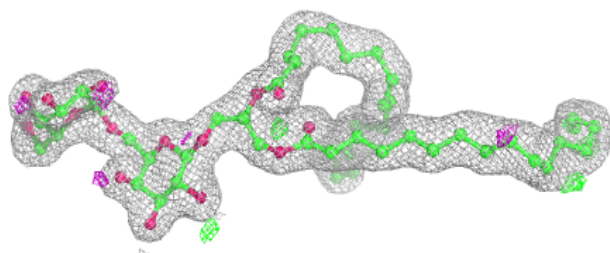
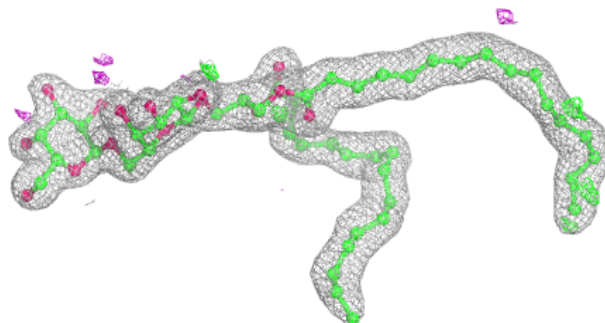
**Electron density around CLA c 506:**

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

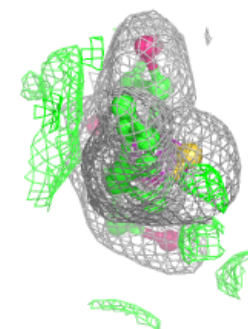
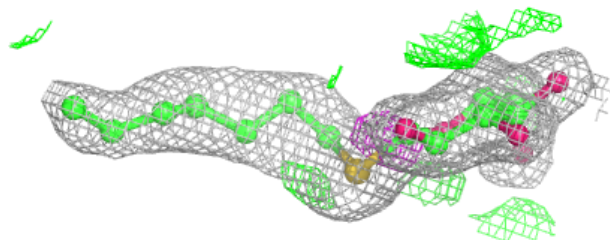
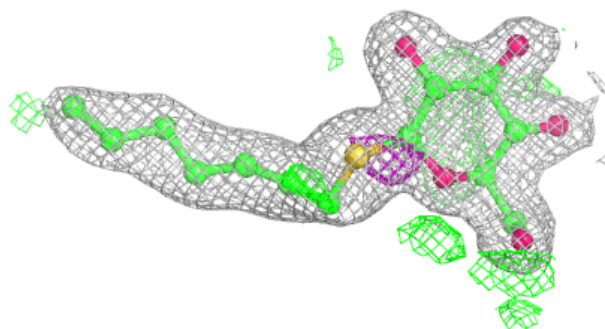


**Electron density around DGD H 102:**

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

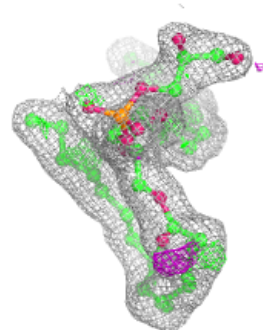
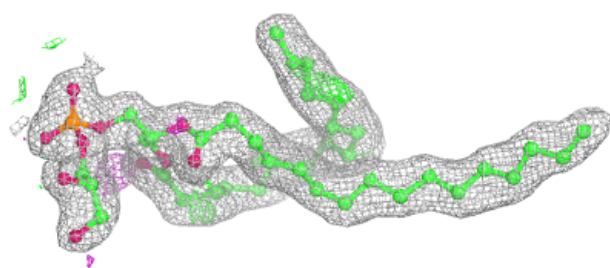
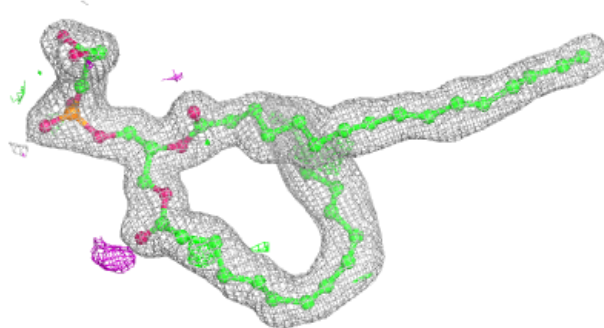
**Electron density around HTG O 302:**

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

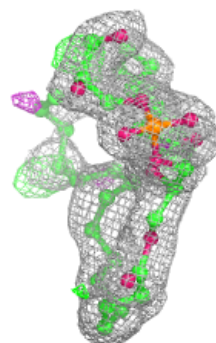
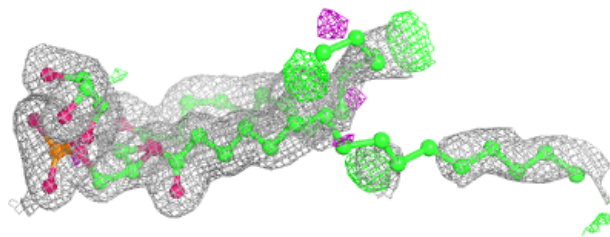
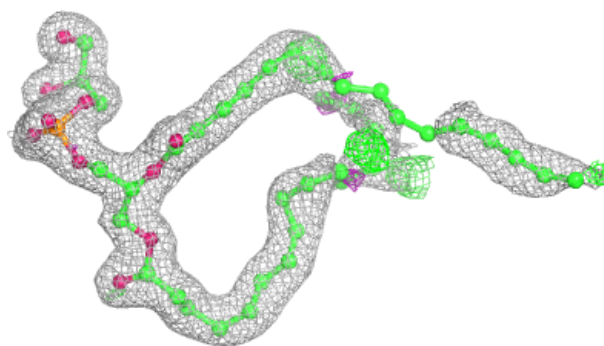


**Electron density around LHG D 407:**

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

**Electron density around LHG D 409:**

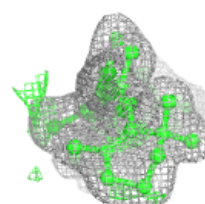
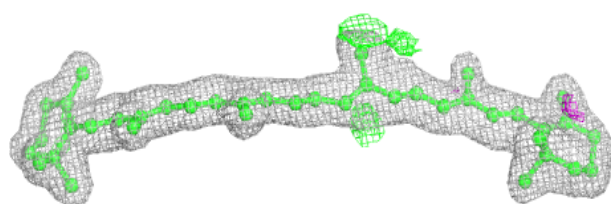
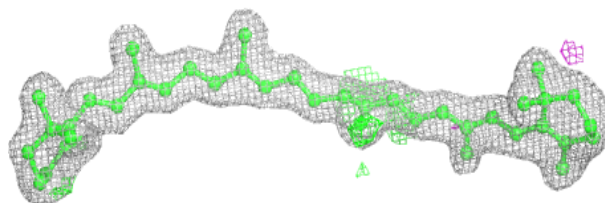
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



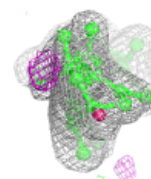
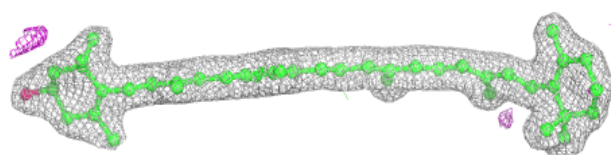
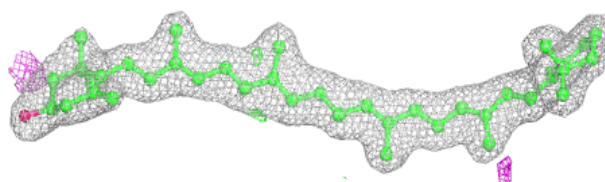


**Electron density around BCR t 101:**

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

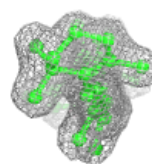
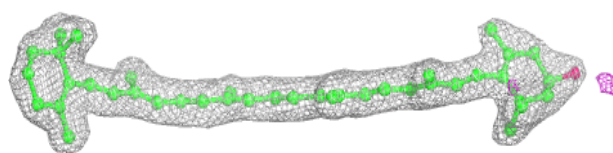
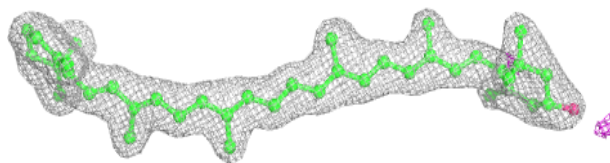
**Electron density around RRX H 101:**

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

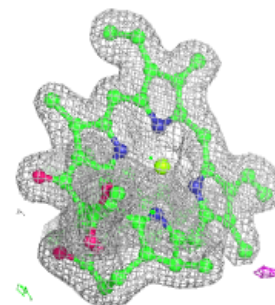
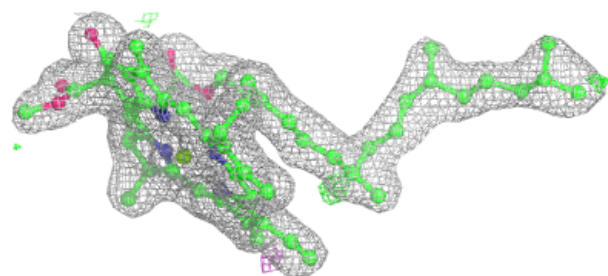
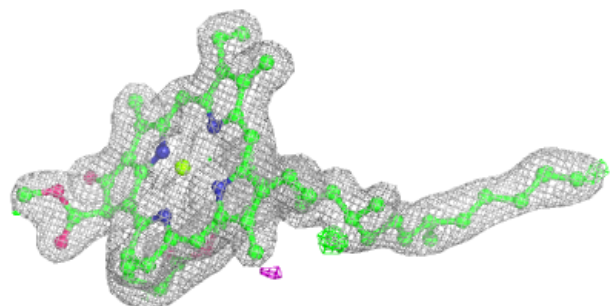


**Electron density around RRX x 101:**

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

**Electron density around CLA C 505:**

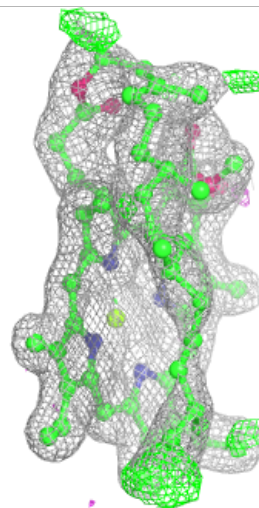
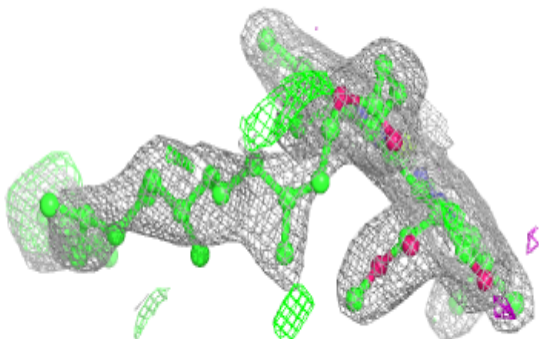
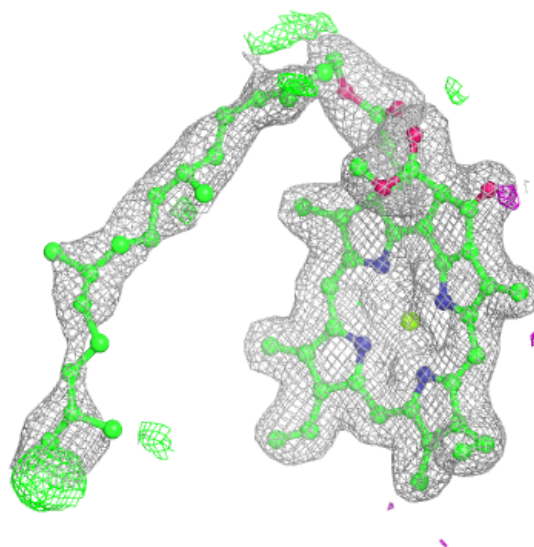
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





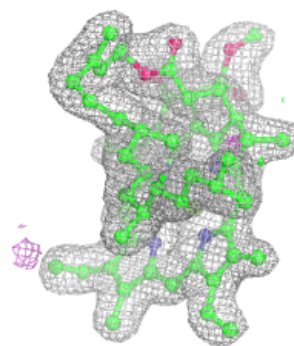
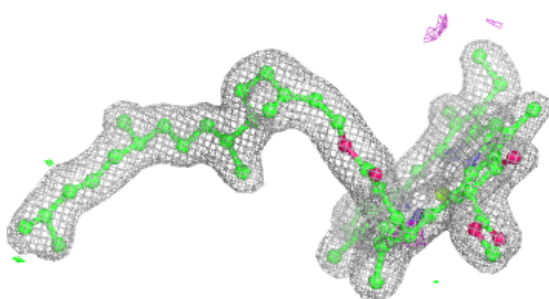
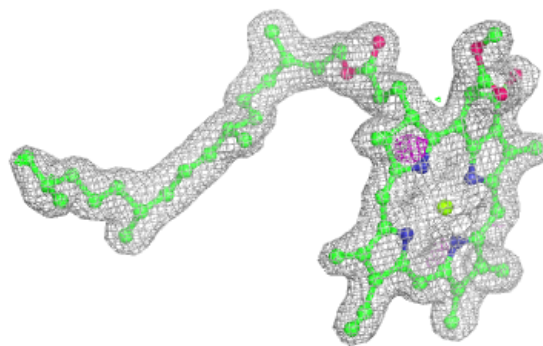
**Electron density around CLA B 601:**

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



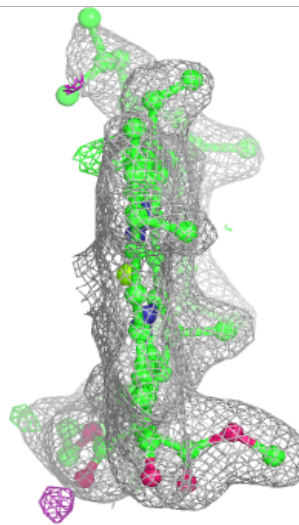
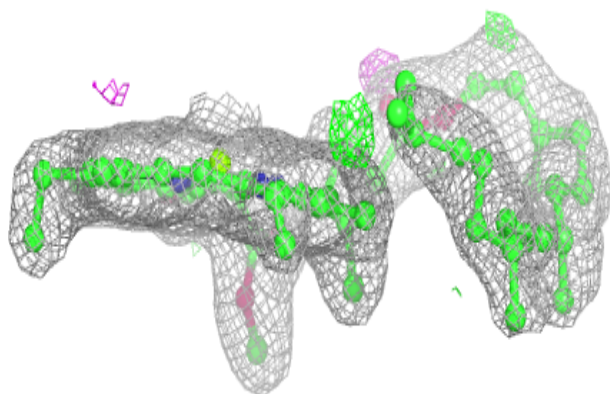
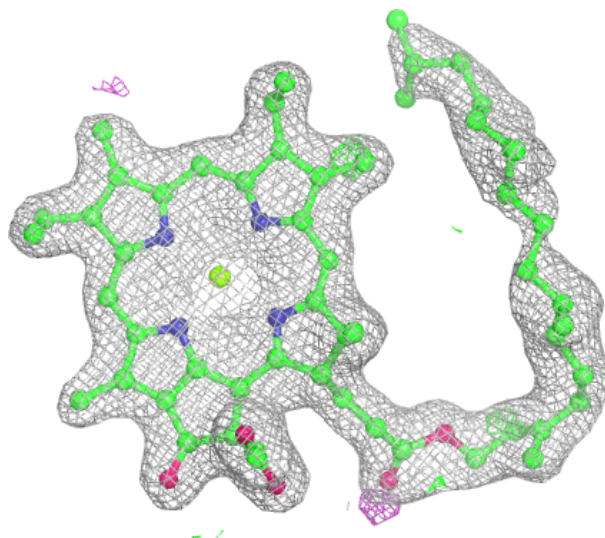
**Electron density around CLA c 511:**

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



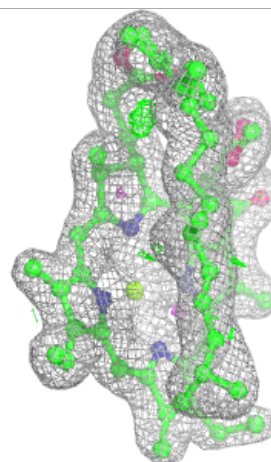
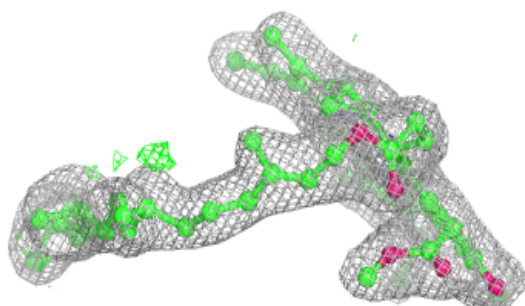
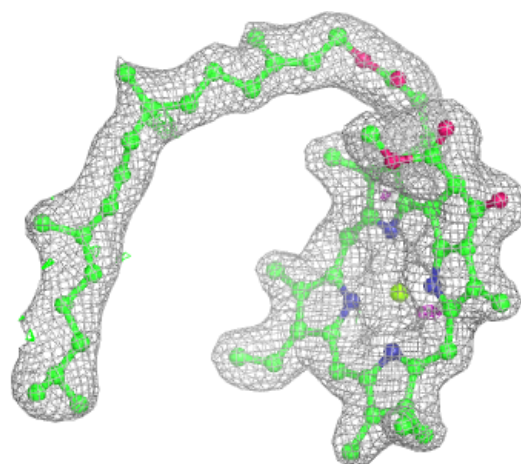
**Electron density around CLA c 512:**

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



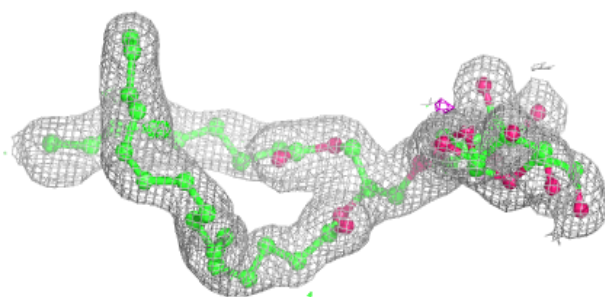
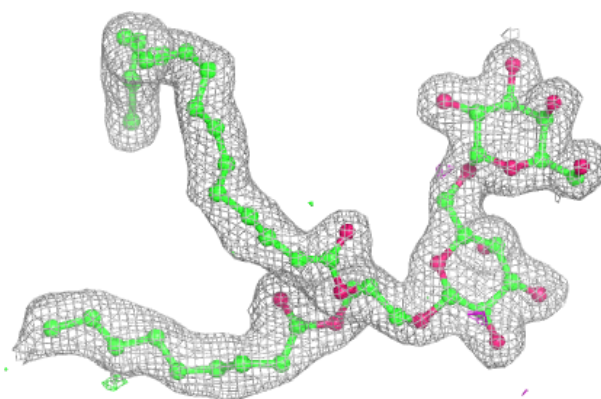
**Electron density around CLA C 507:**

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

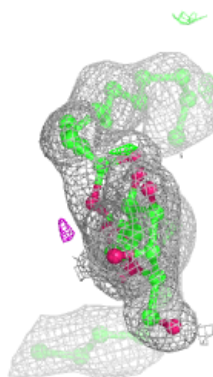
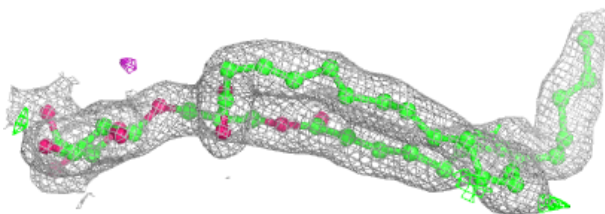
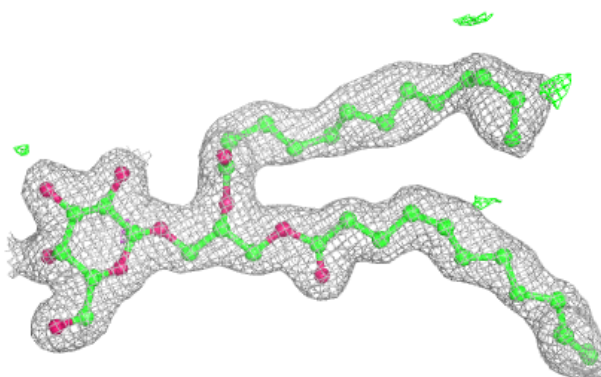


**Electron density around DGD C 517:**

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

**Electron density around LMG j 101:**

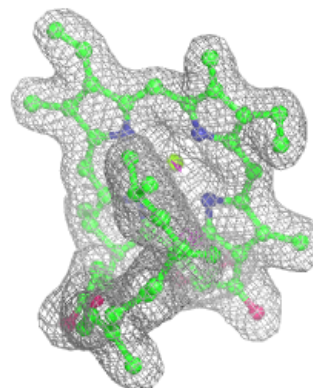
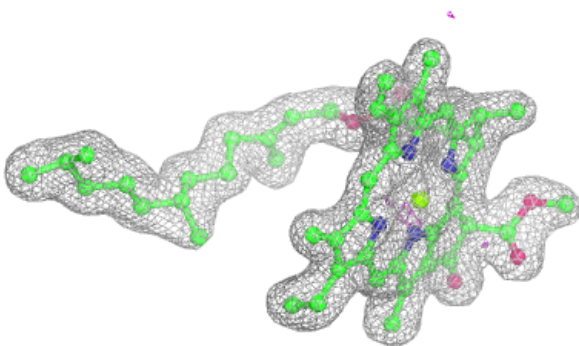
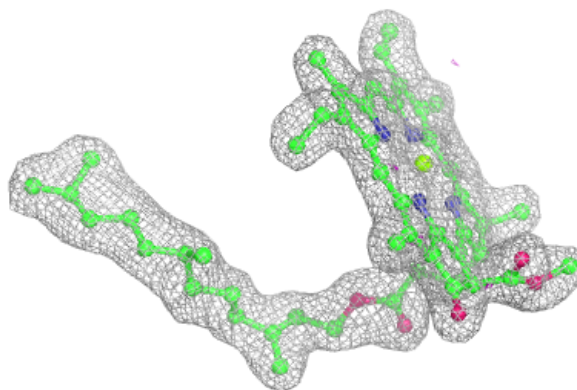
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



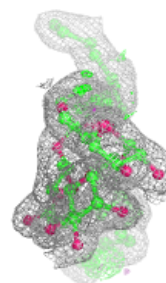
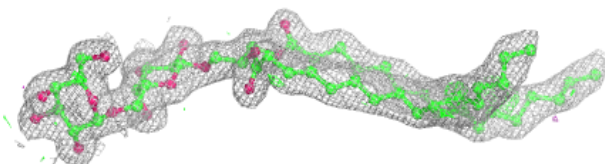
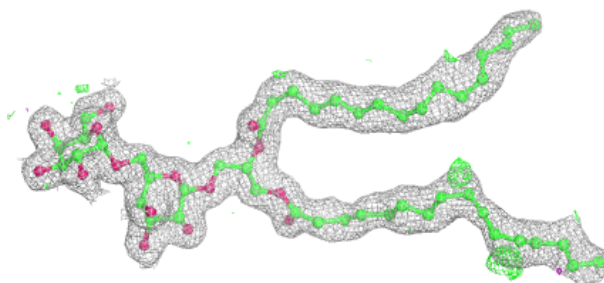


**Electron density around CLA C 508:**

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

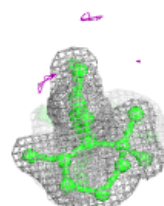
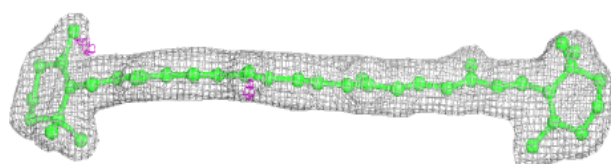
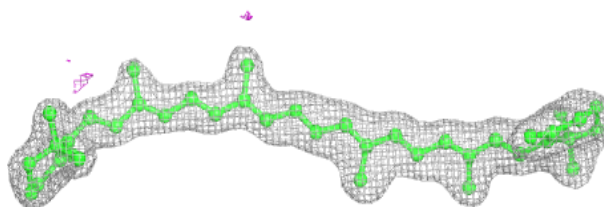
**Electron density around DGD c 517:**

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

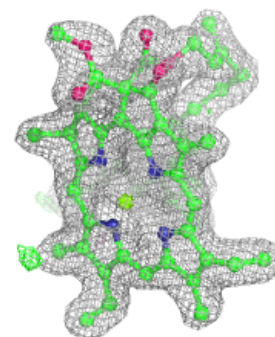
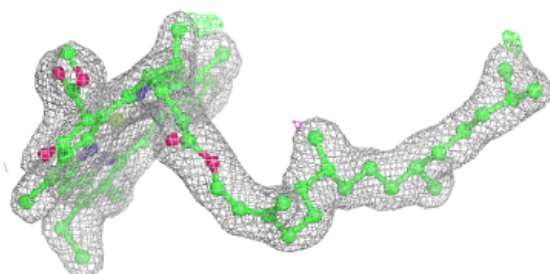
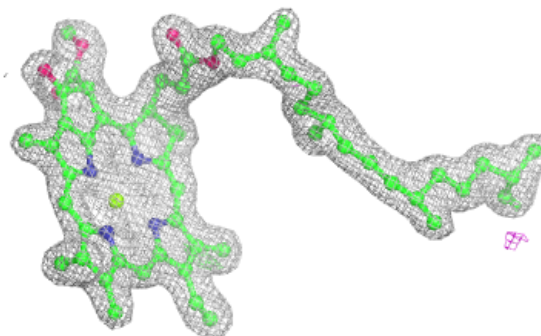


**Electron density around BCR C 515:**

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

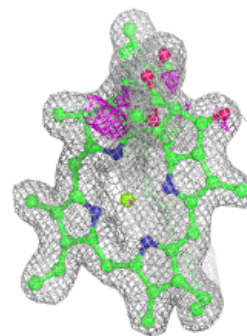
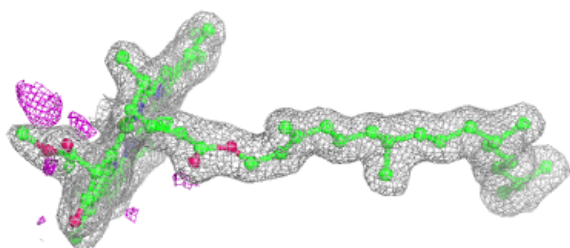
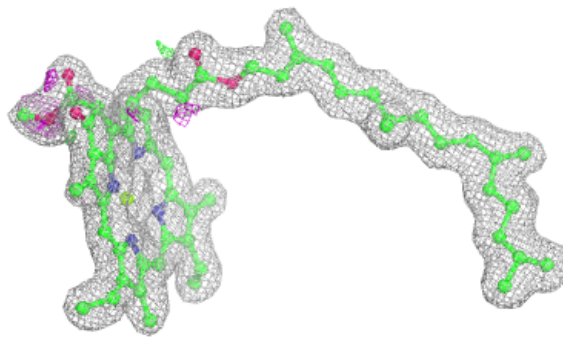
**Electron density around CLA C 511:**

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



**Electron density around CLA B 610:**

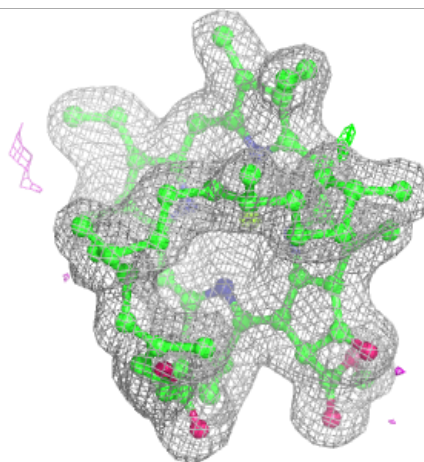
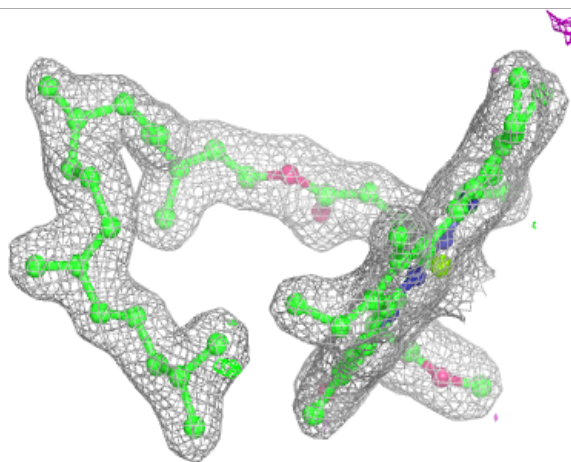
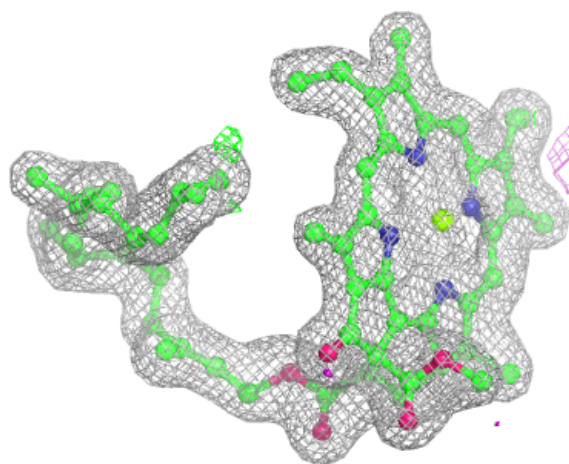
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





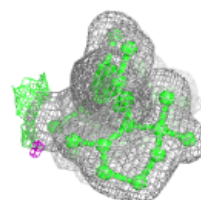
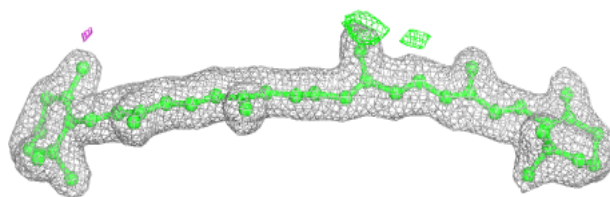
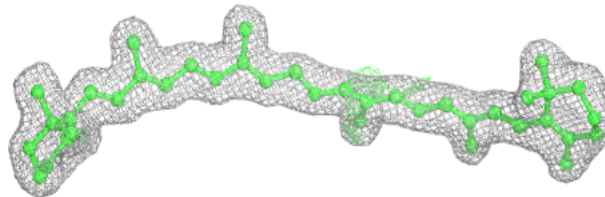
**Electron density around CLA C 503:**

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

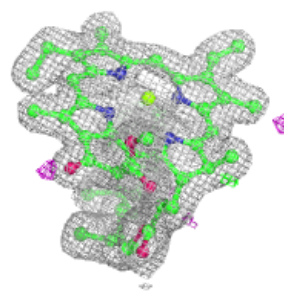
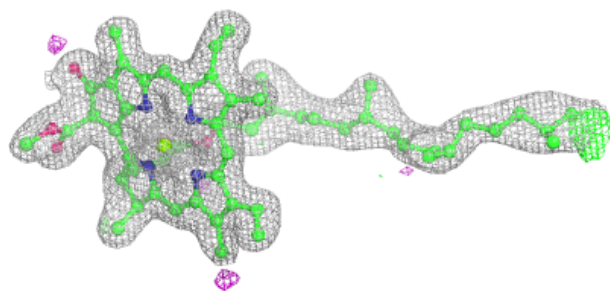
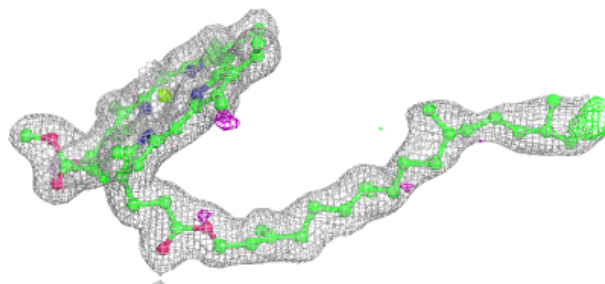


**Electron density around BCR T 101:**

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

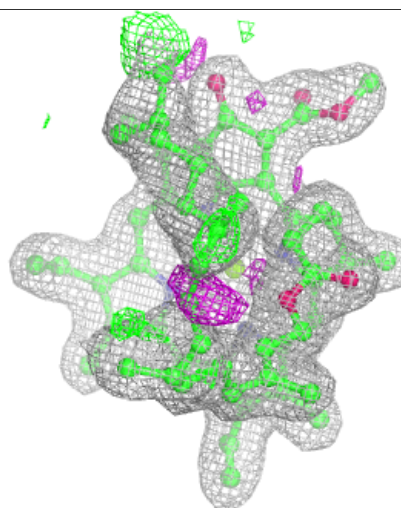
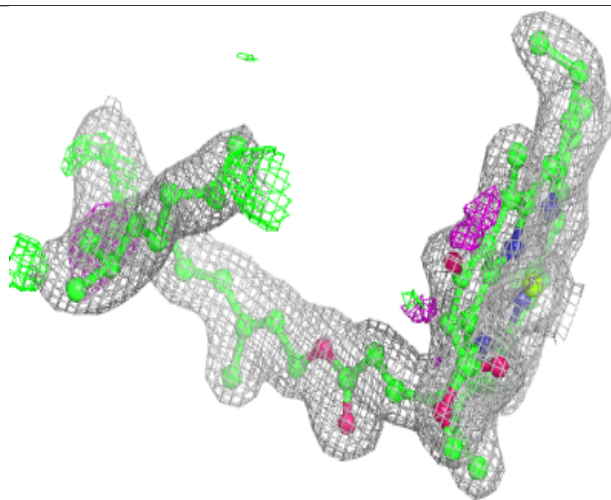
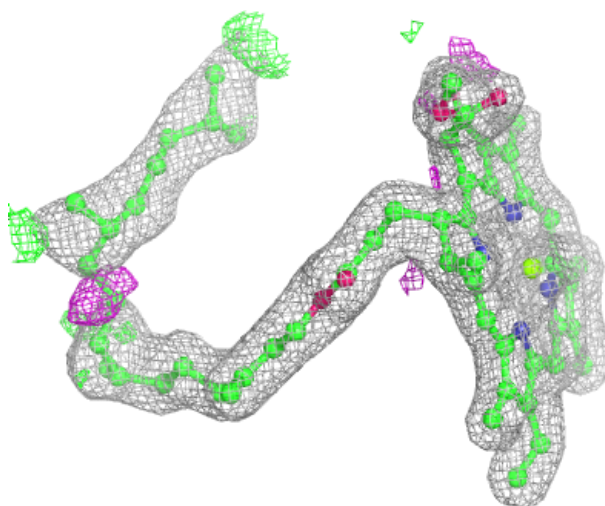
**Electron density around CLA C 504:**

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



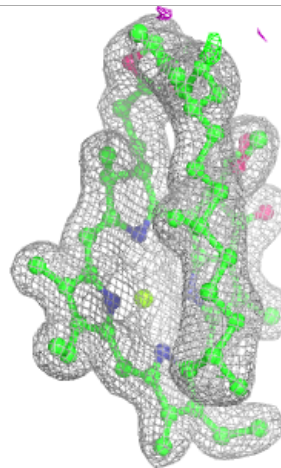
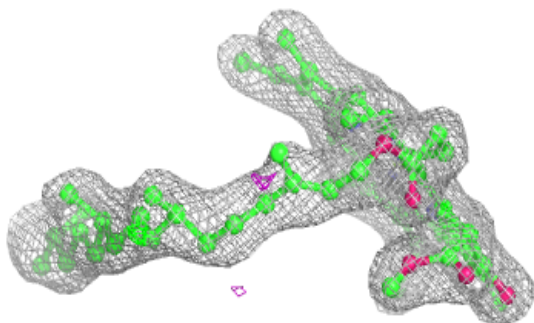
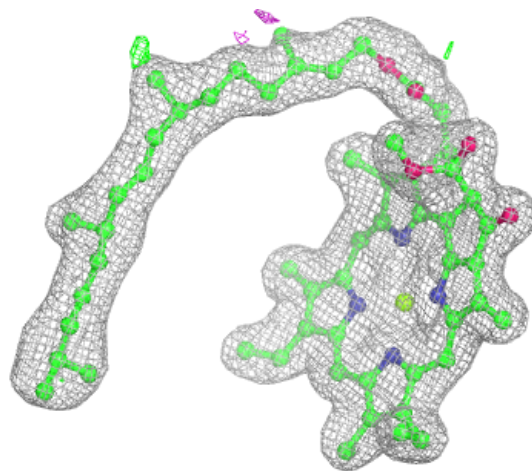
**Electron density around CLA b 608:**

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



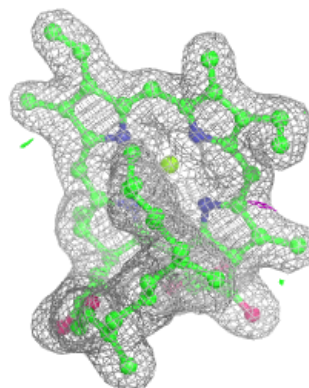
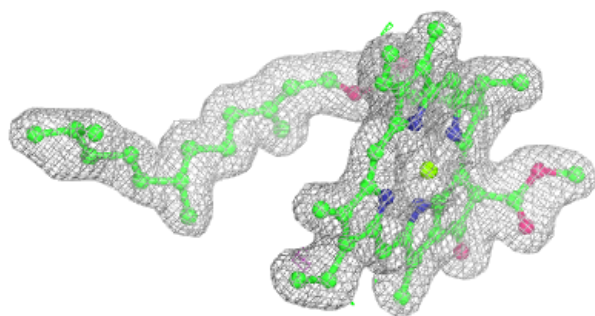
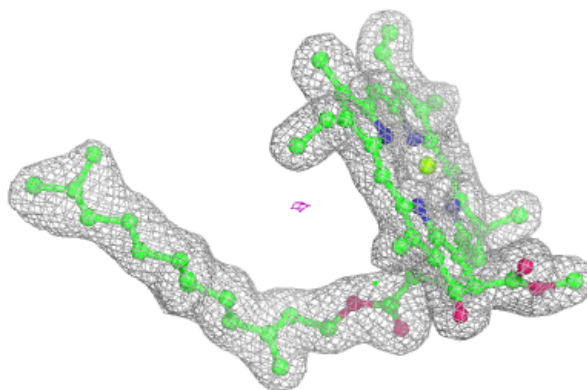
**Electron density around CLA c 507:**

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



**Electron density around CLA c 508:**

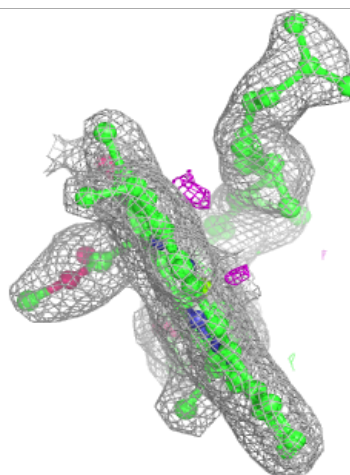
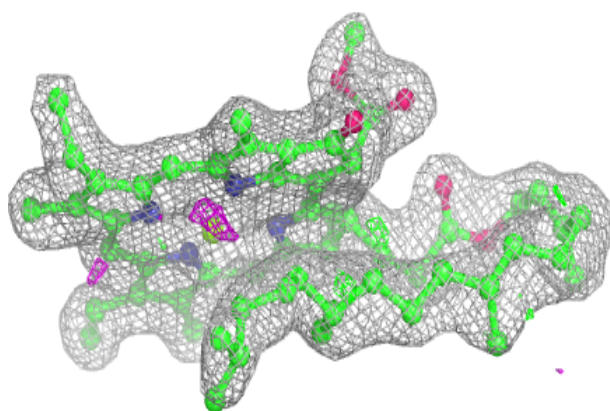
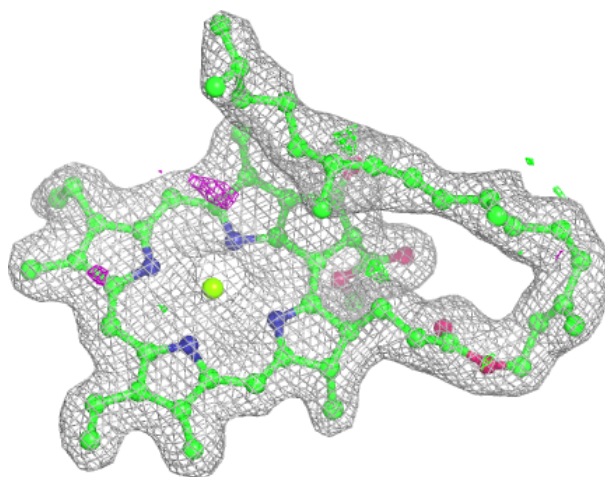
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





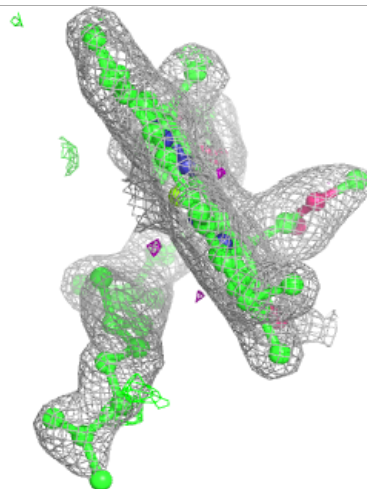
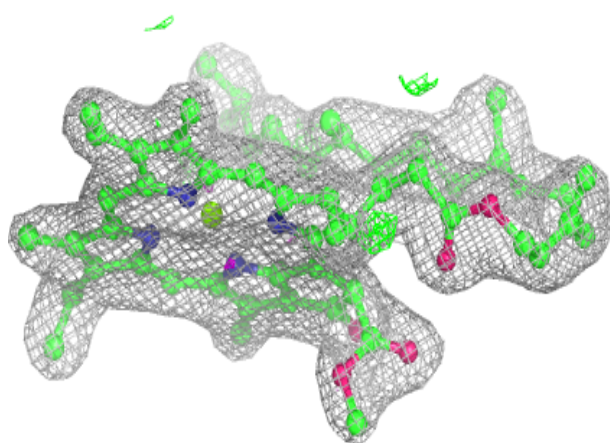
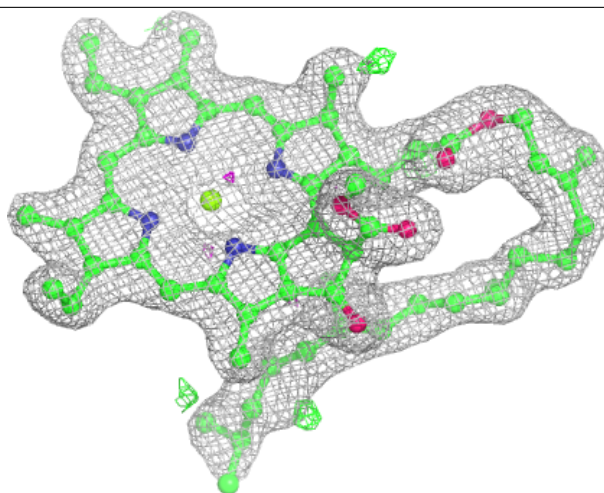
**Electron density around CLA c 509:**

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



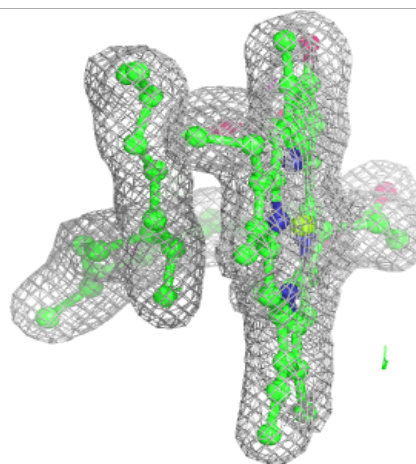
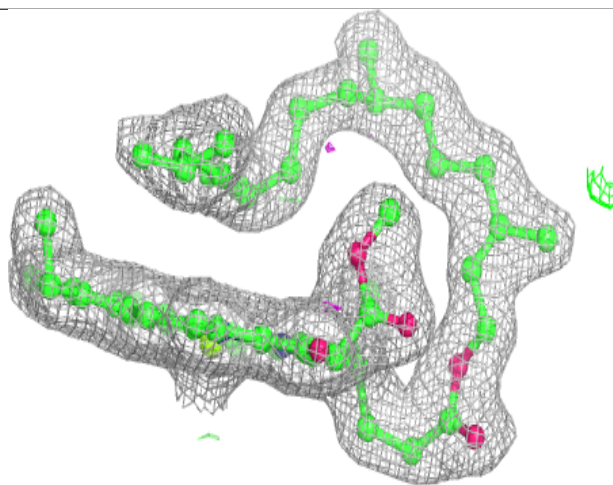
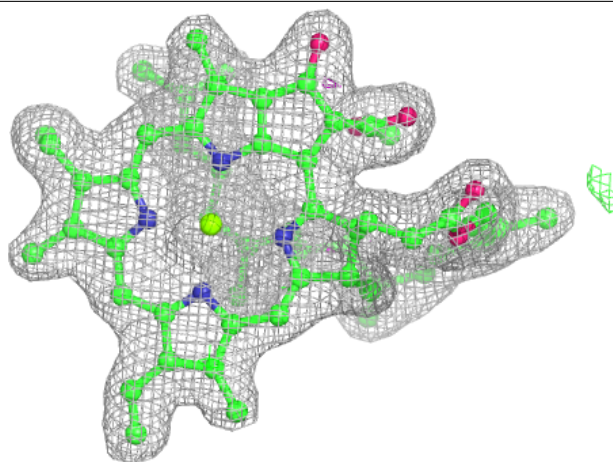
**Electron density around CLA C 509:**

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



**Electron density around CLA C 510:**

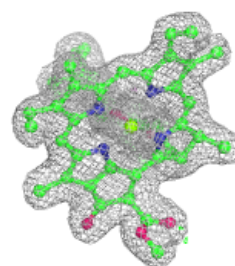
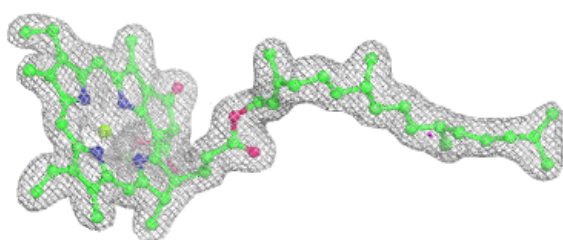
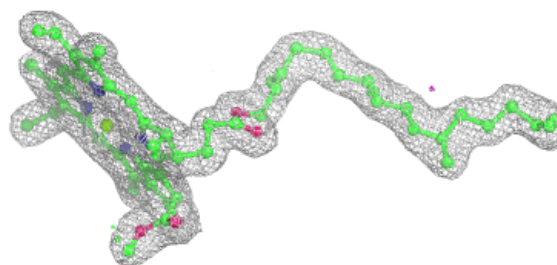
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



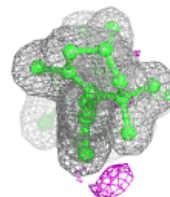
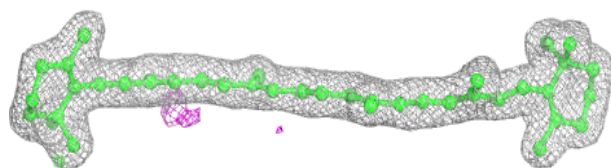
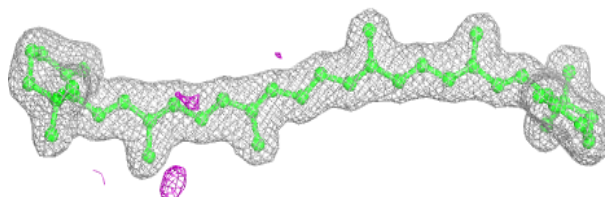


**Electron density around CLA C 502:**

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

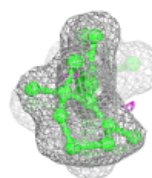
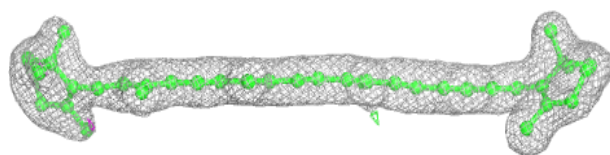
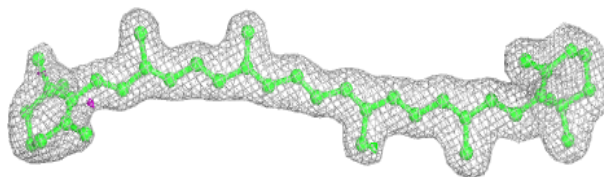
**Electron density around BCR A 405:**

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

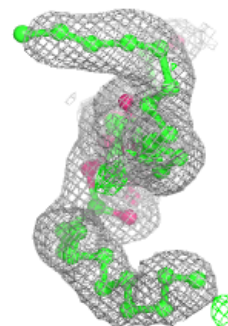
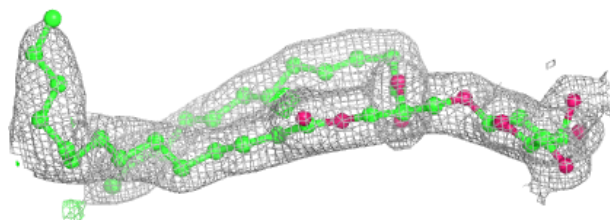
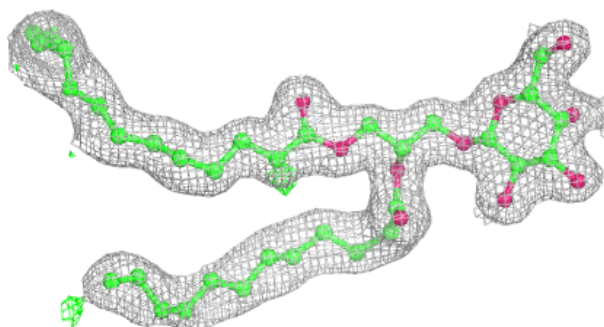


**Electron density around BCR B 618:**

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

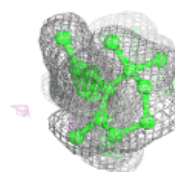
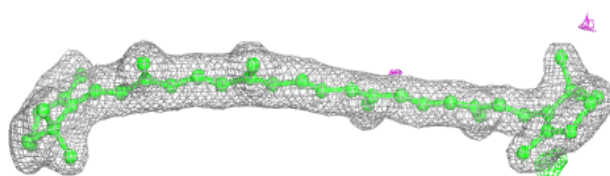
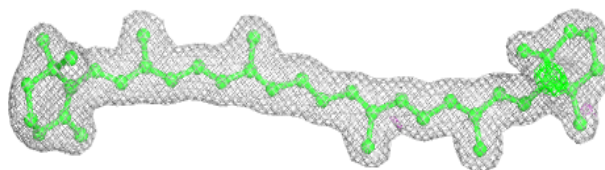
**Electron density around LMG J 101:**

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

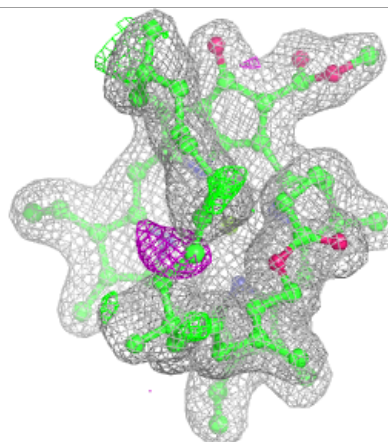
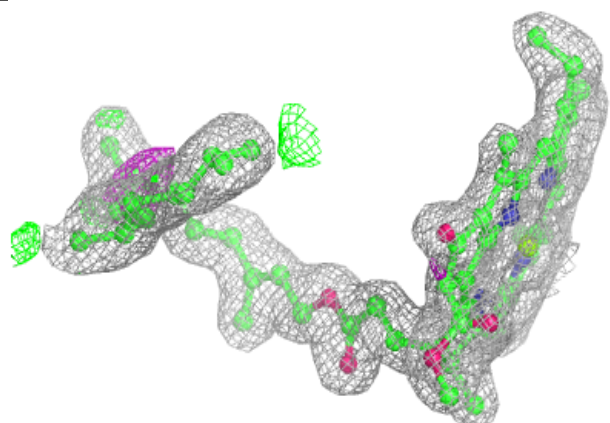
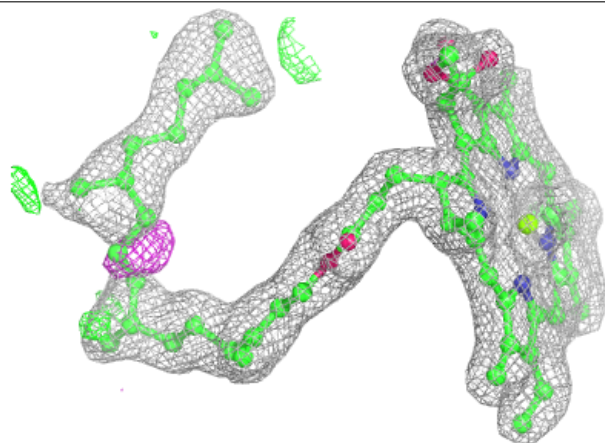


**Electron density around BCR B 619:**

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

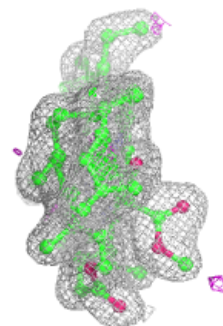
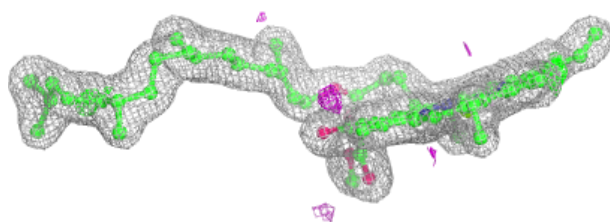
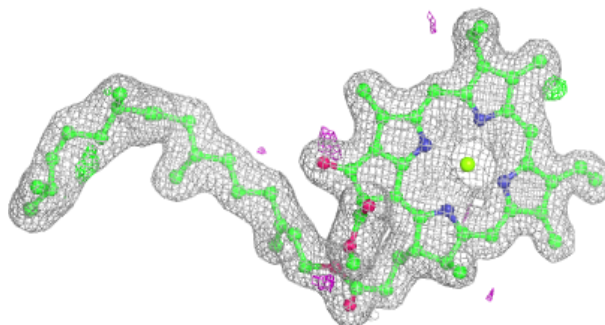
**Electron density around CLA B 607:**

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

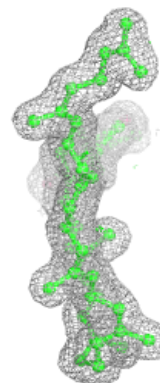
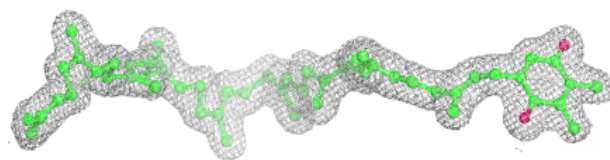
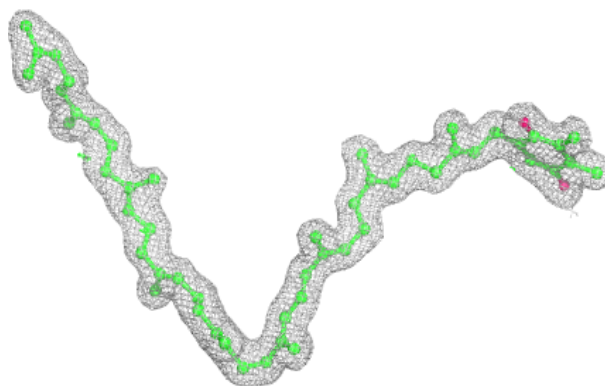


**Electron density around CLA B 603:**

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

**Electron density around PL9 D 412:**

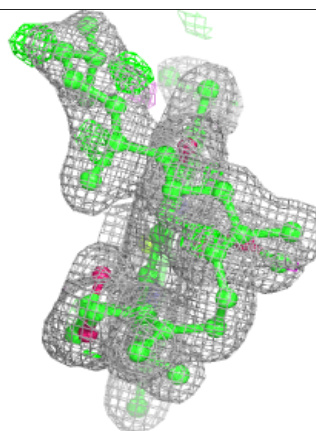
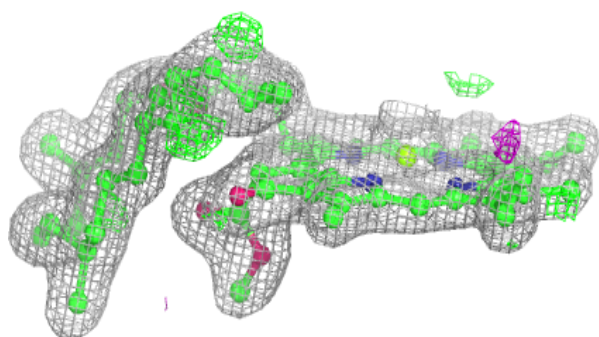
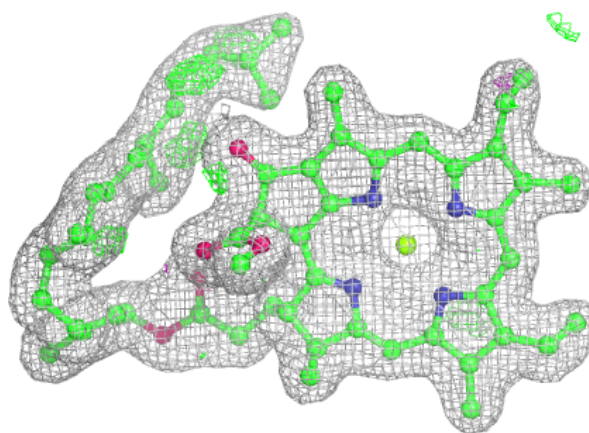
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



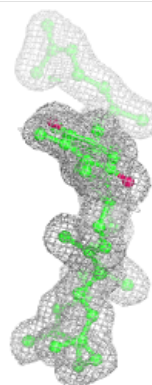
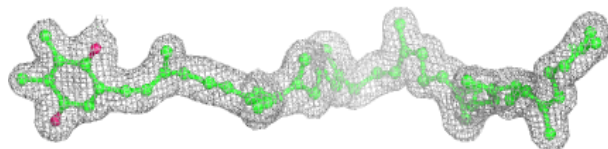
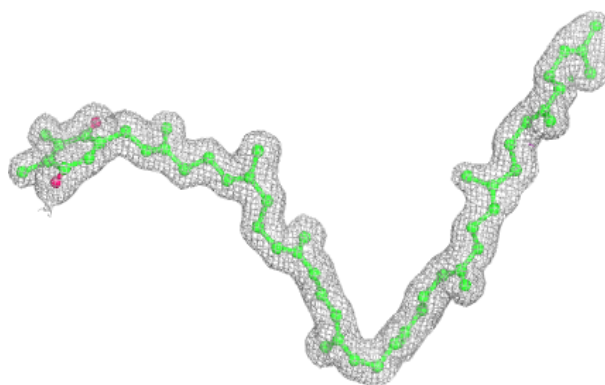


**Electron density around CLA B 611:**

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

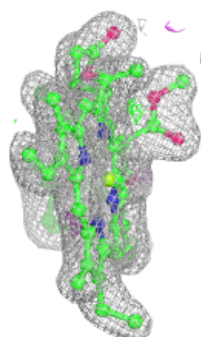
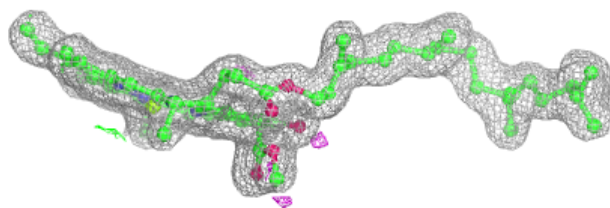
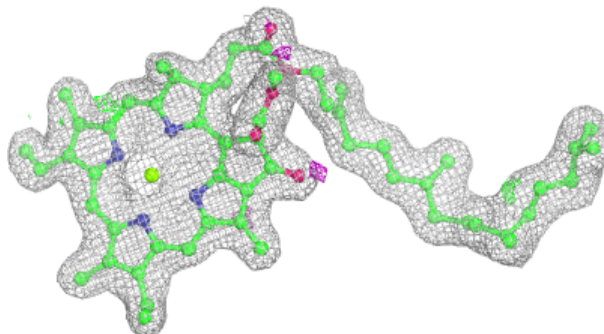
**Electron density around PL9 d 412:**

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

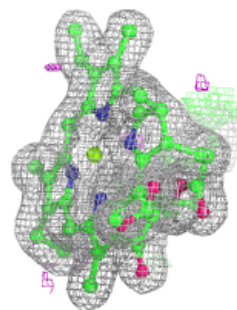
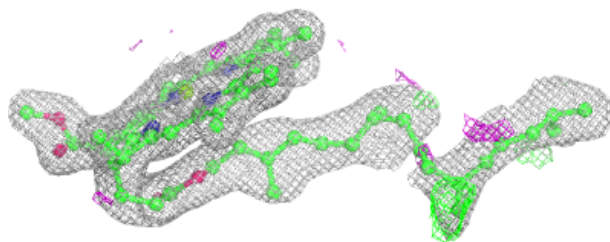
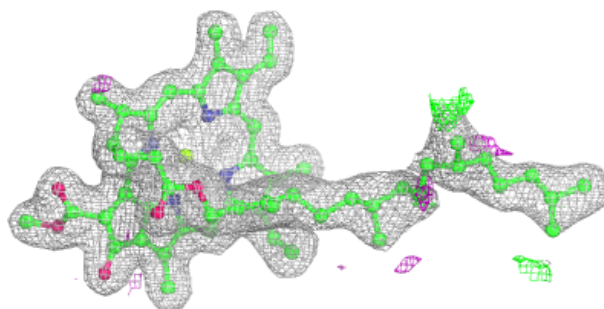


**Electron density around CLA b 604:**

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

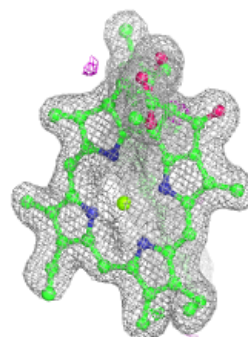
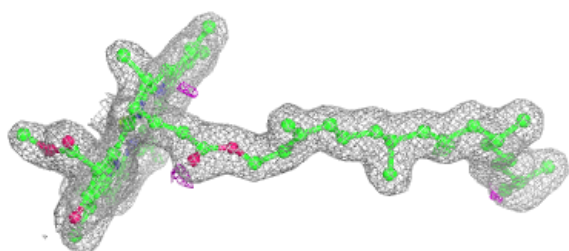
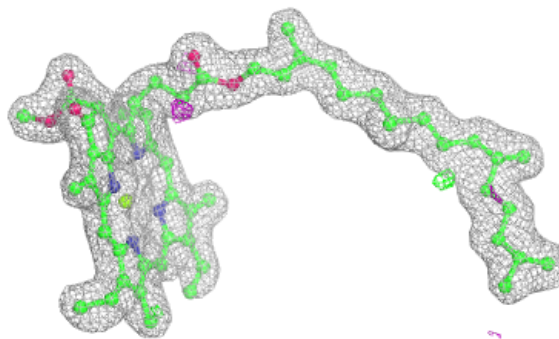
**Electron density around CLA B 615:**

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

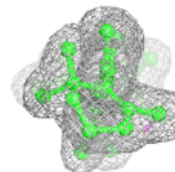
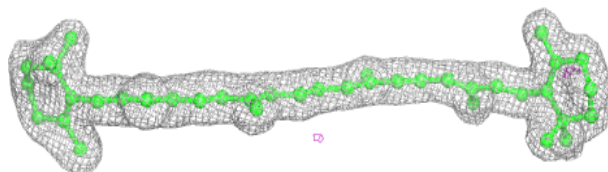
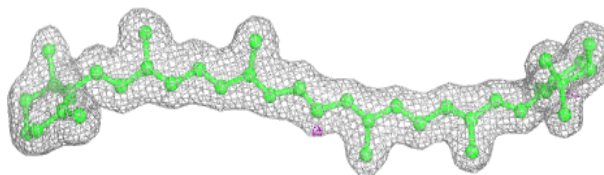


**Electron density around CLA b 611:**

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

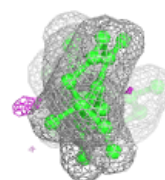
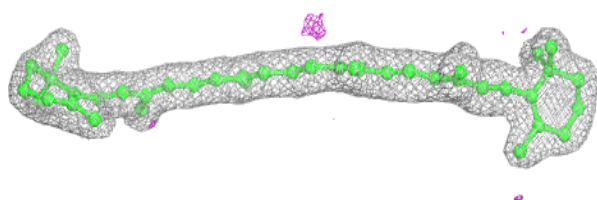
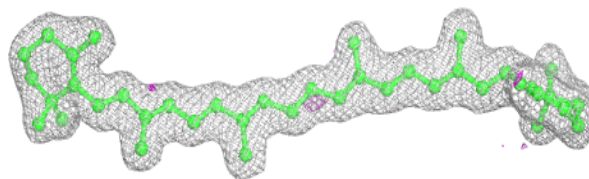
**Electron density around BCR a 408:**

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

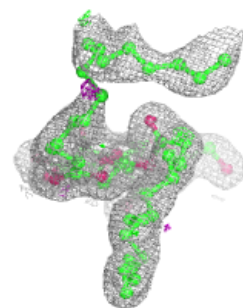
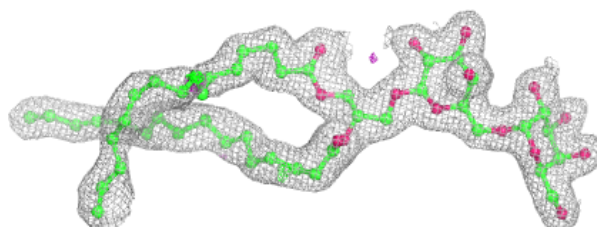
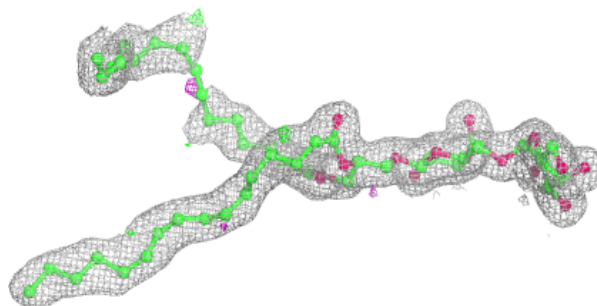


**Electron density around BCR b 619:**

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

**Electron density around DGD C 516:**

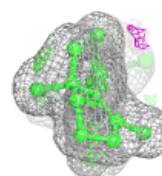
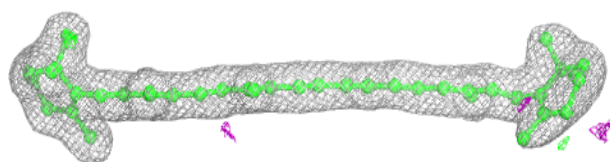
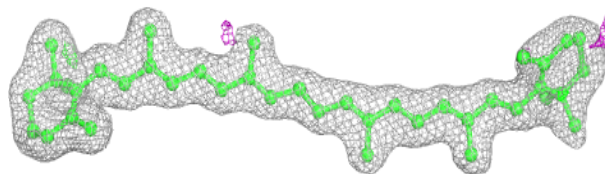
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



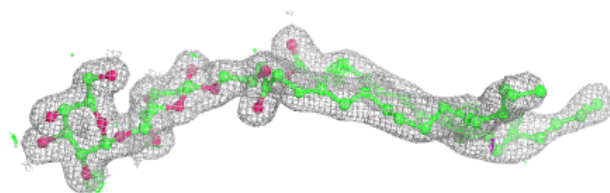
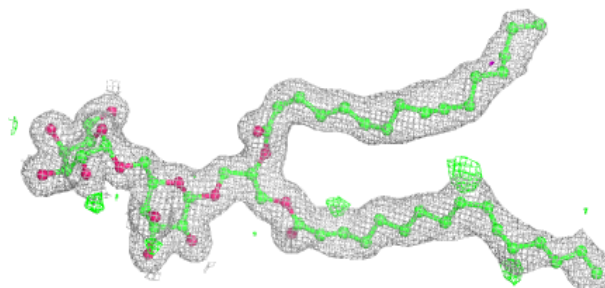


**Electron density around BCR b 620:**

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

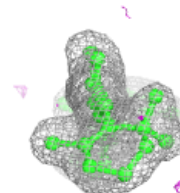
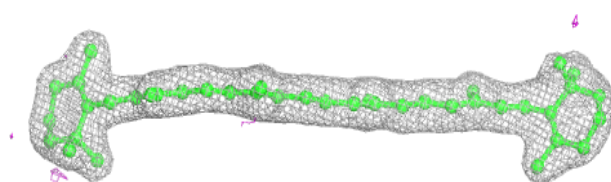
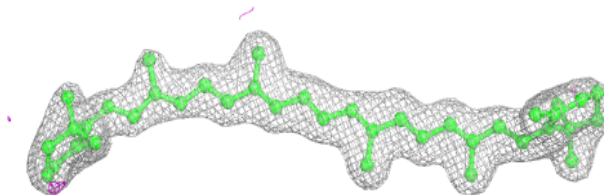
**Electron density around DGD C 518:**

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

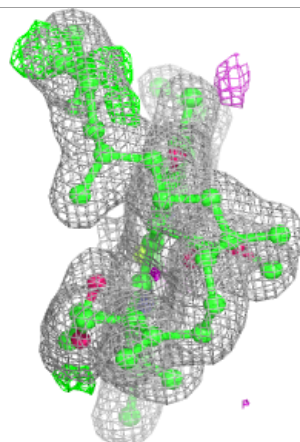
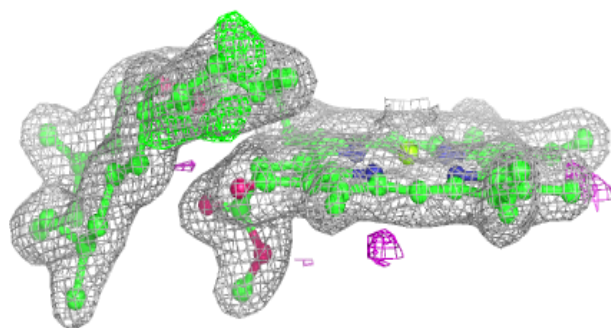
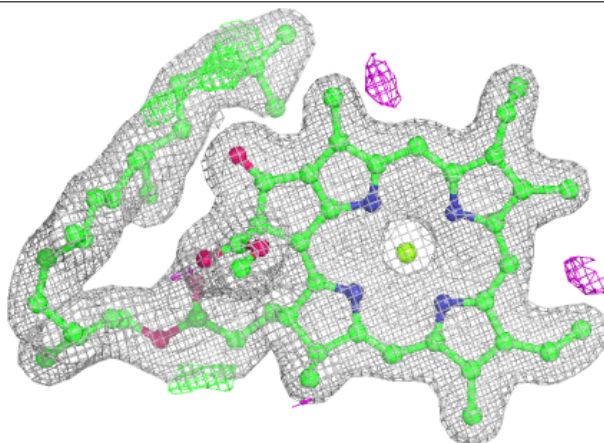


**Electron density around BCR c 514:**

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

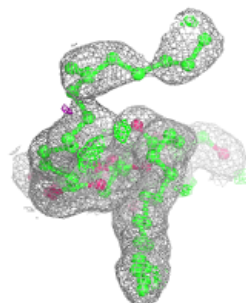
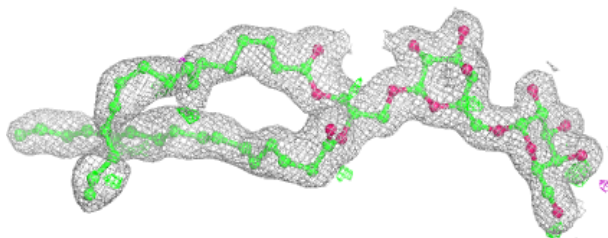
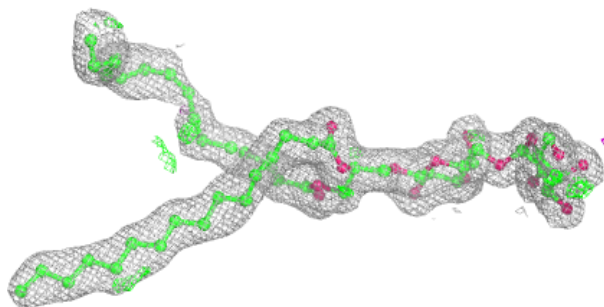
**Electron density around CLA b 612:**

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

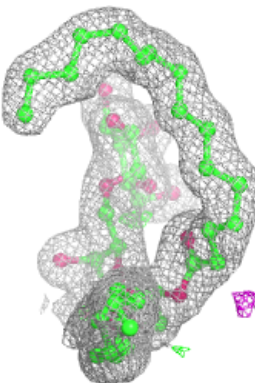
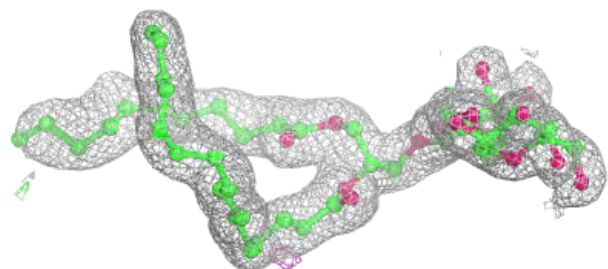
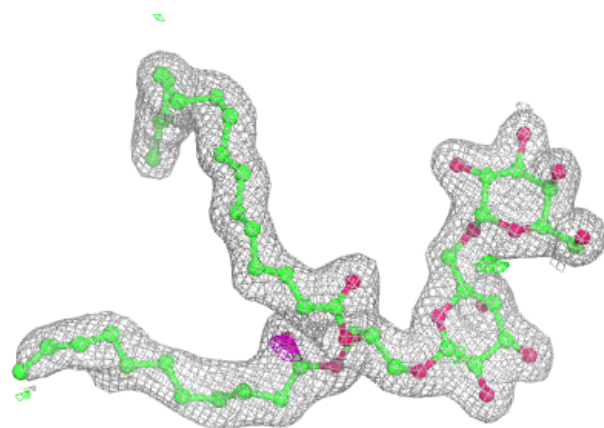


**Electron density around DGD c 515:**

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

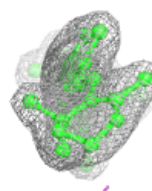
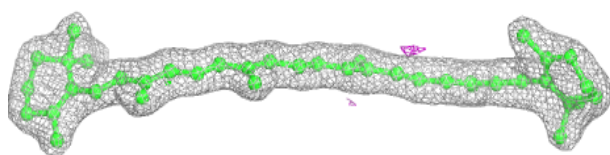
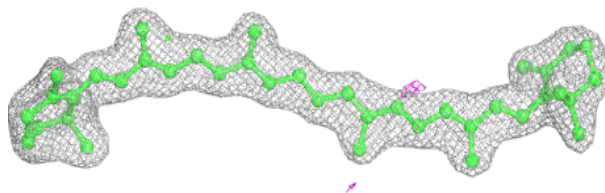
**Electron density around DGD c 516:**

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

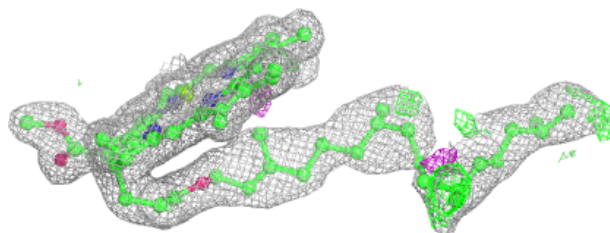
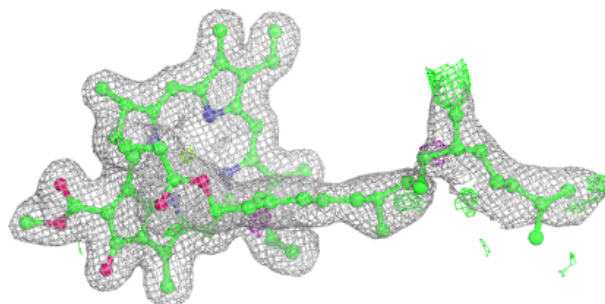


**Electron density around BCR j 102:**

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

**Electron density around CLA b 616:**

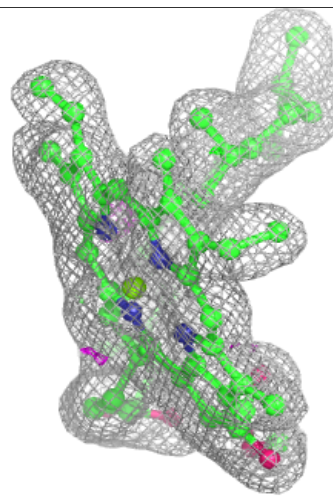
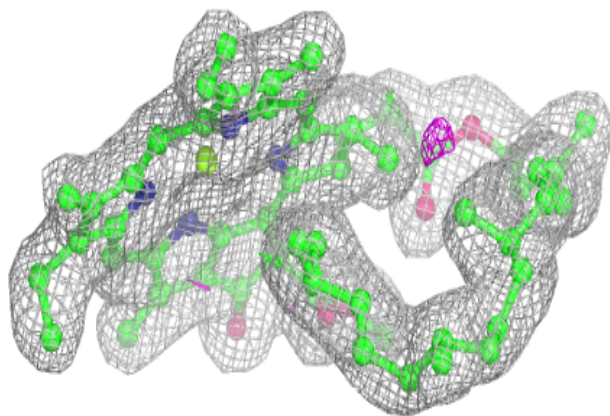
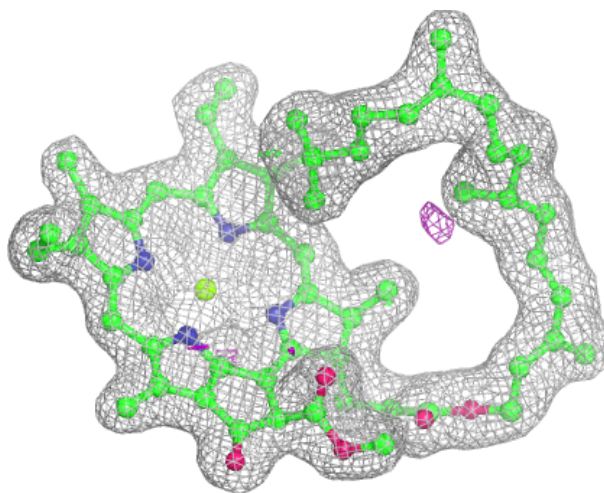
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





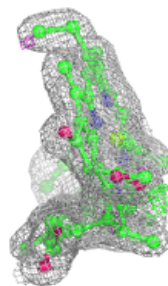
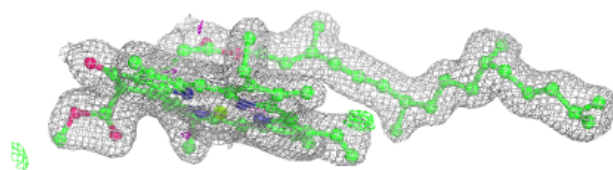
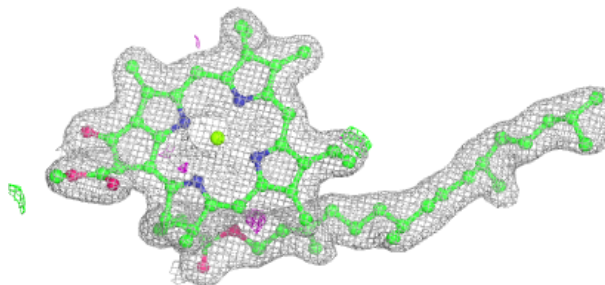
**Electron density around CLA B 616:**

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



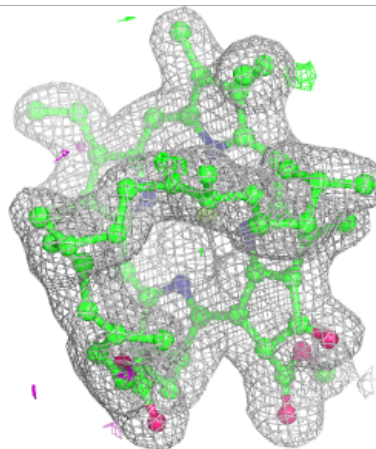
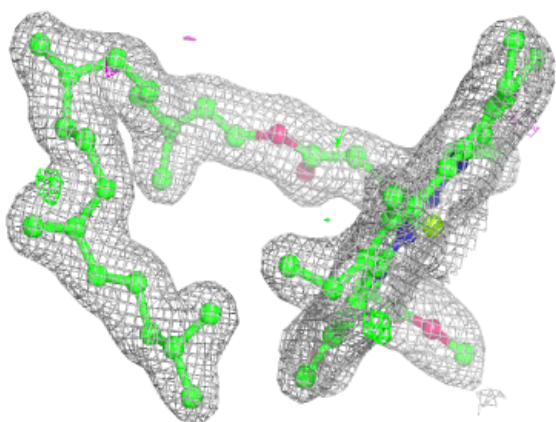
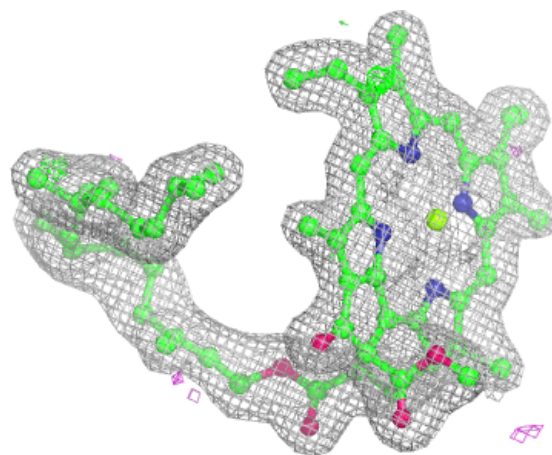
**Electron density around CLA c 501:**

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



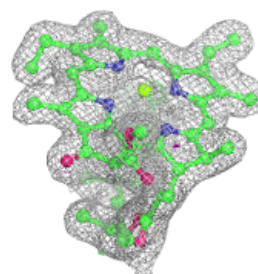
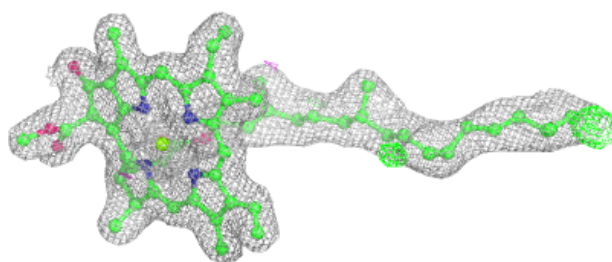
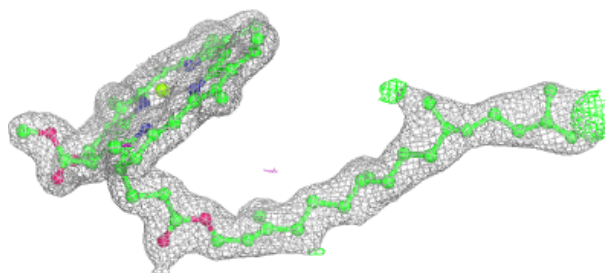
**Electron density around CLA c 503:**

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

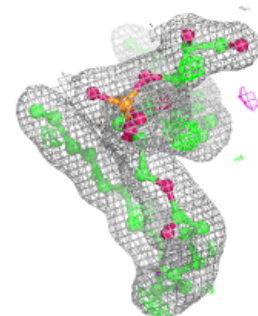
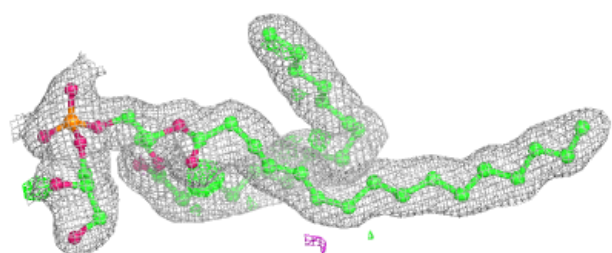
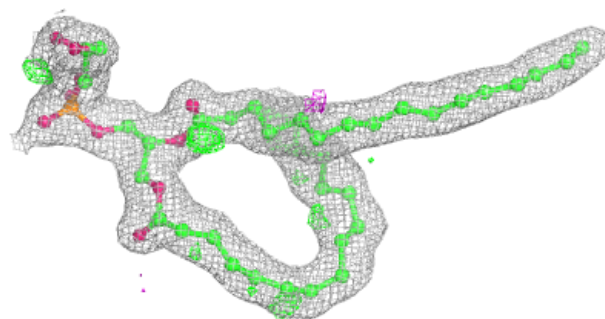


**Electron density around CLA c 504:**

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

**Electron density around LHG d 406:**

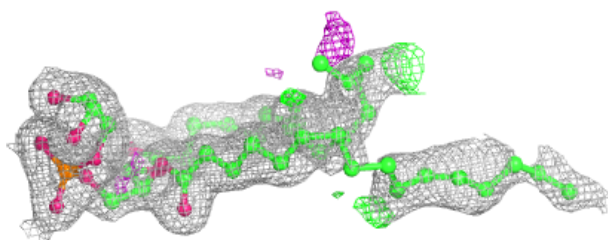
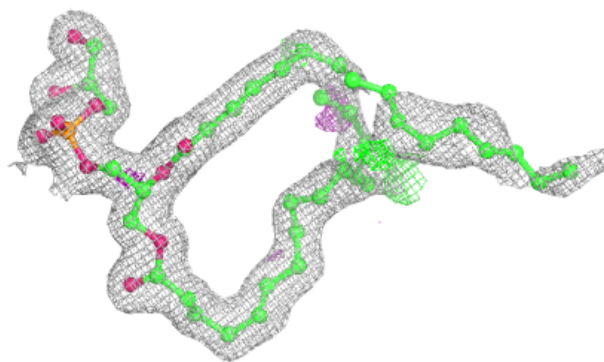
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



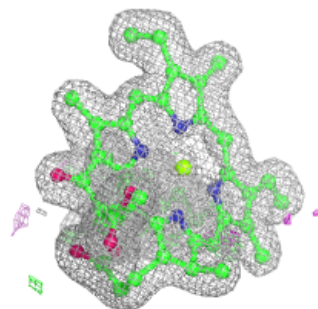
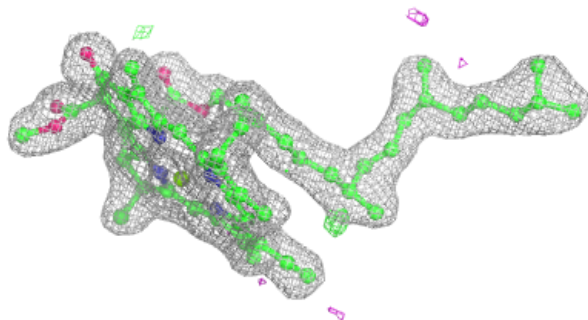
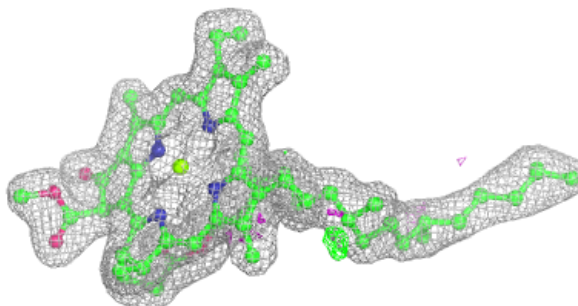


**Electron density around LHG d 408:**

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

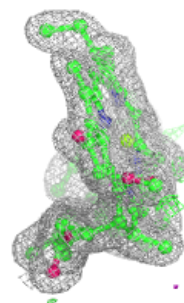
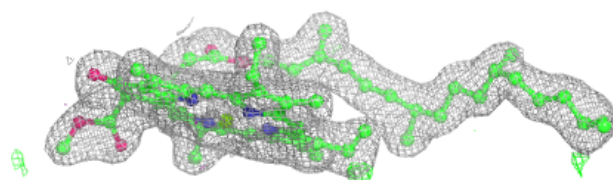
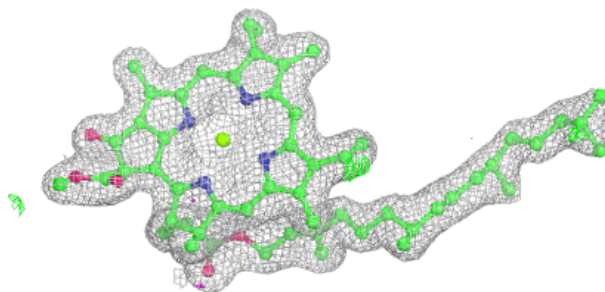
**Electron density around CLA c 505:**

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

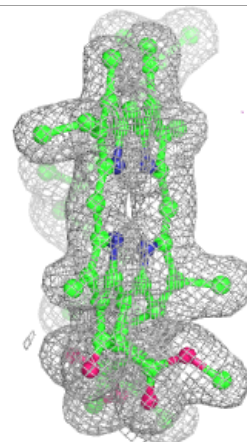
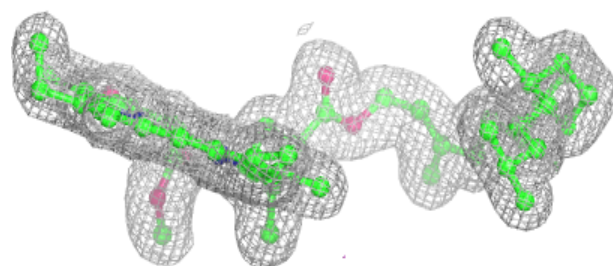
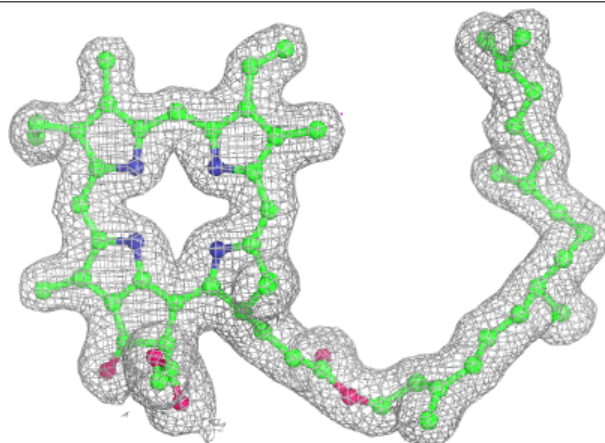


**Electron density around CLA C 501:**

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

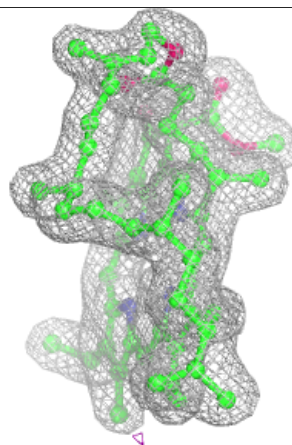
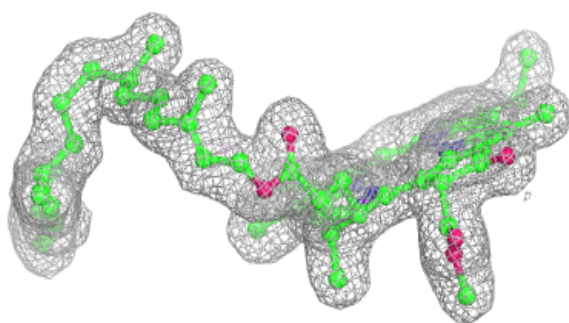
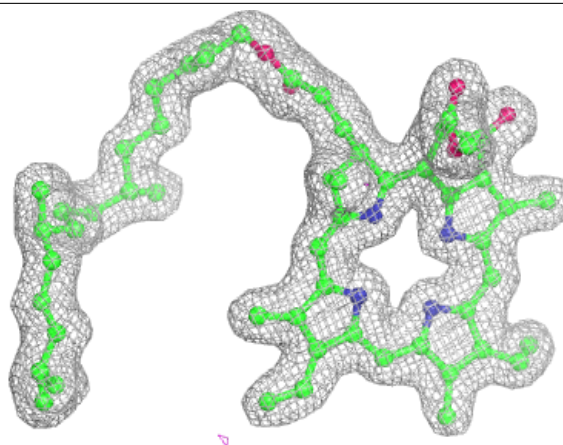
**Electron density around PHO A 403:**

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



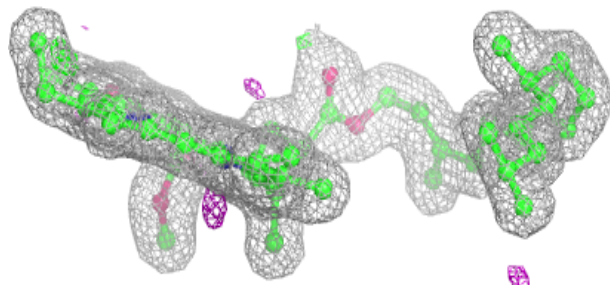
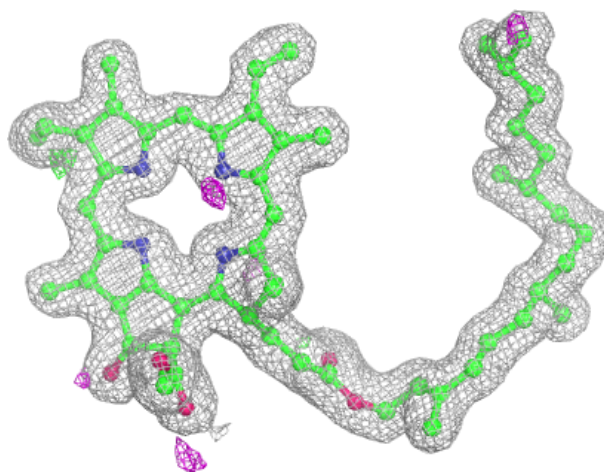
**Electron density around PHO D 403:**

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



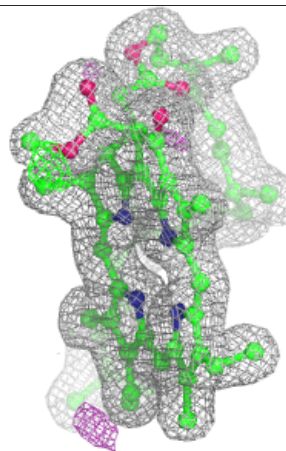
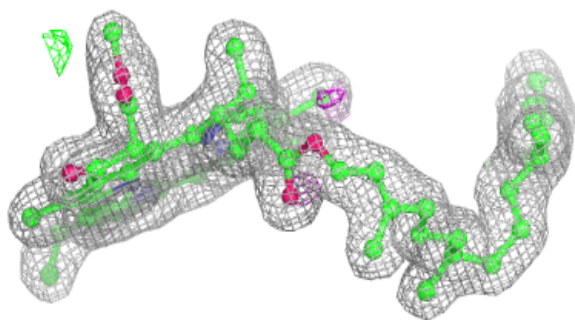
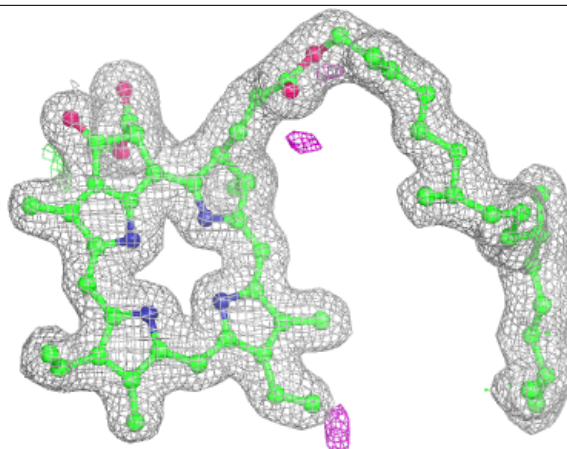
**Electron density around PHO a 405:**

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



**Electron density around PHO a 406:**

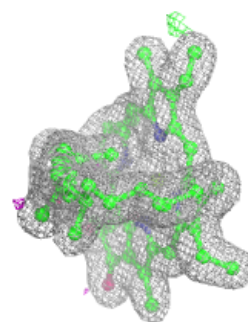
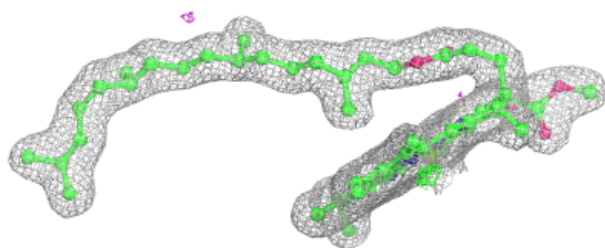
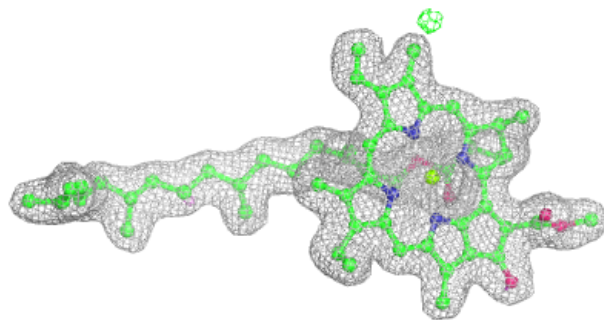
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



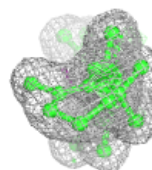
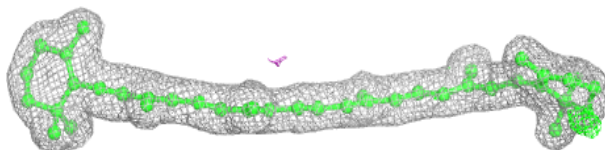
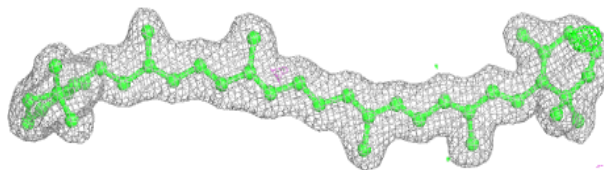


**Electron density around CLA b 610:**

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

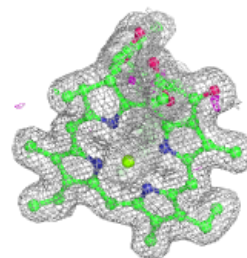
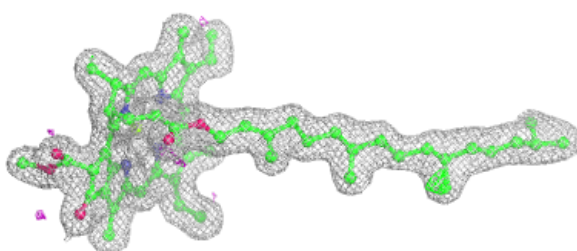
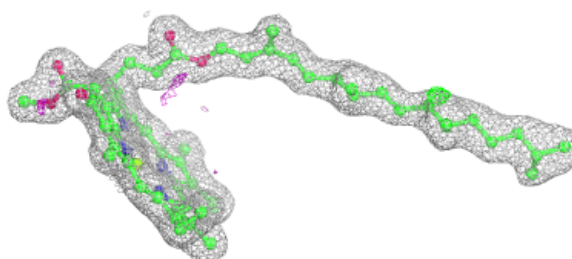
**Electron density around BCR B 617:**

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

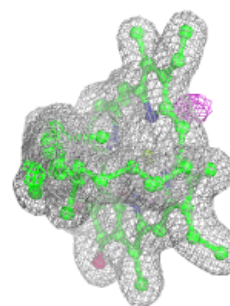
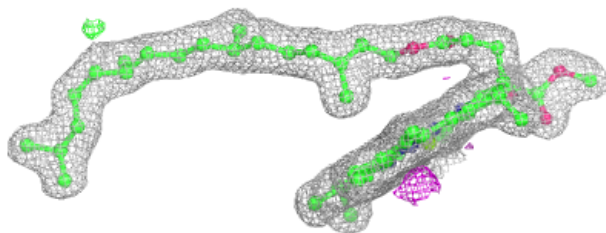
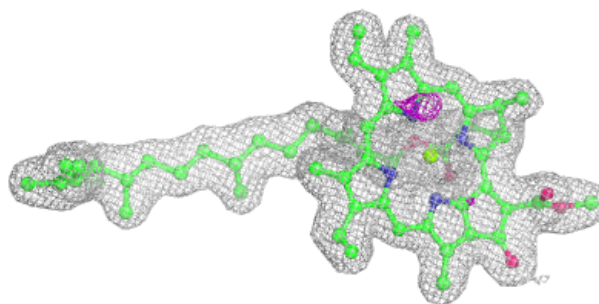


**Electron density around CLA B 608:**

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

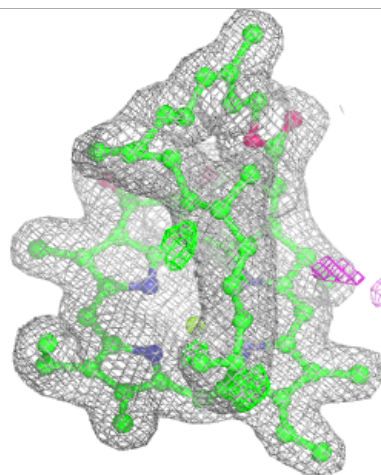
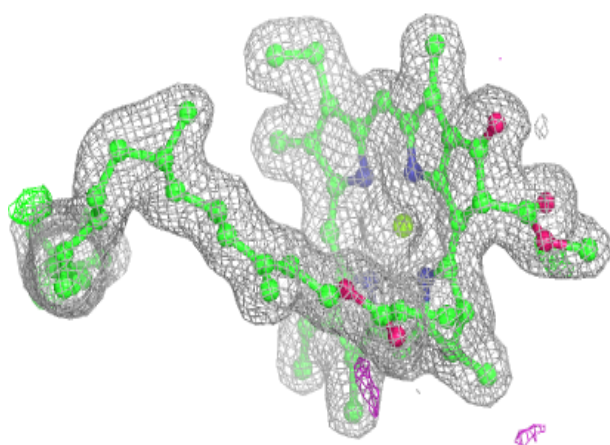
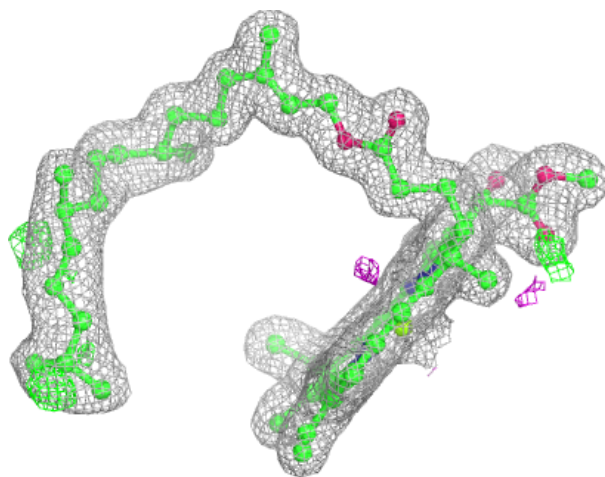
**Electron density around CLA B 609:**

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



**Electron density around CLA b 613:**

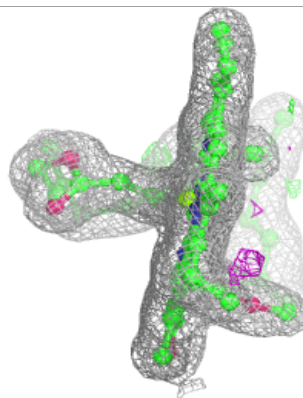
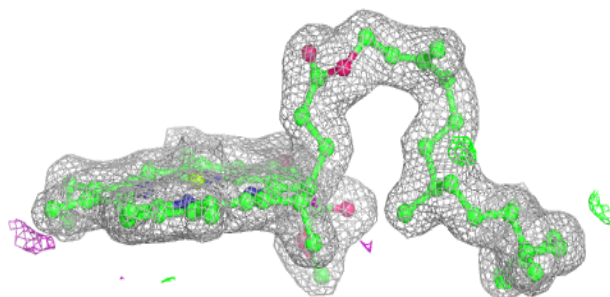
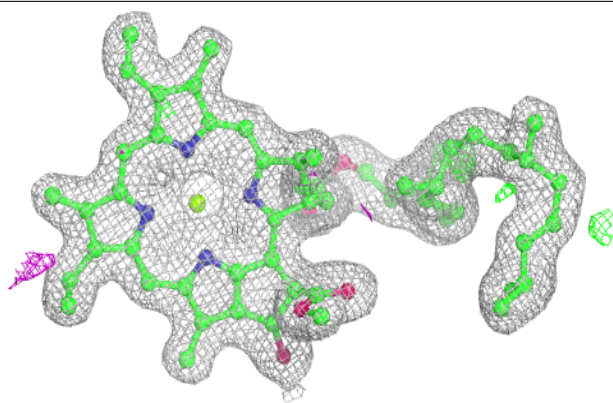
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



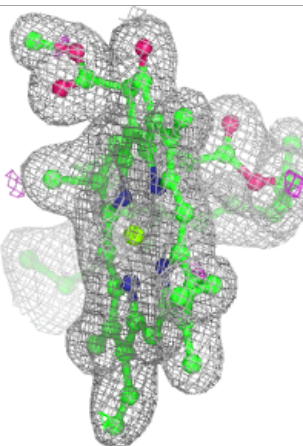
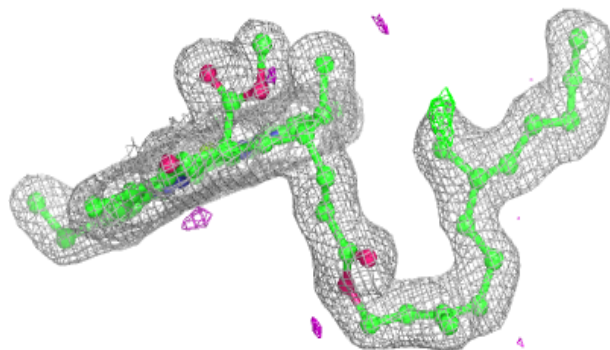
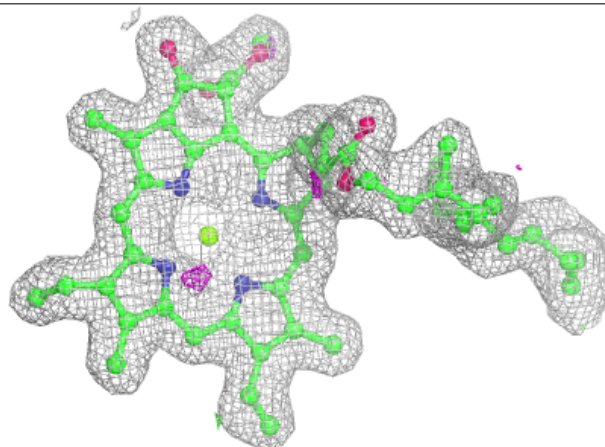


**Electron density around CLA b 614:**

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

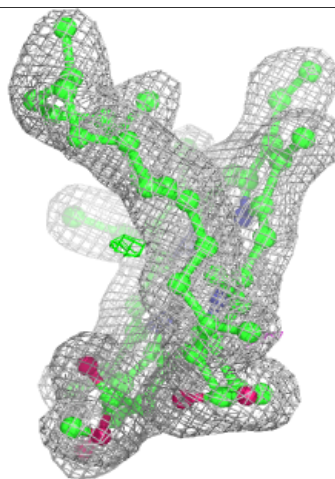
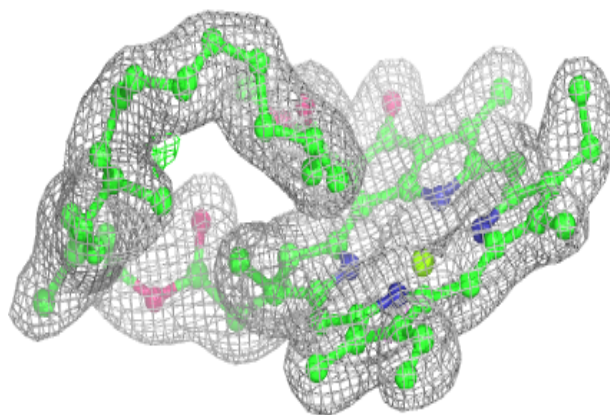
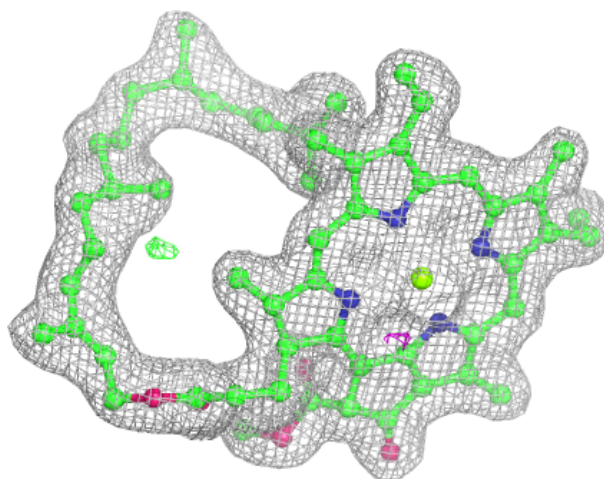
**Electron density around CLA A 402:**

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



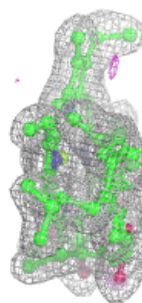
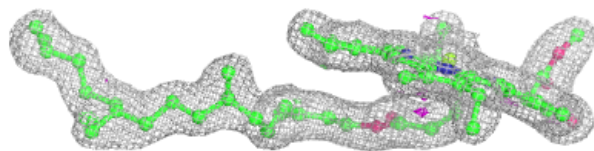
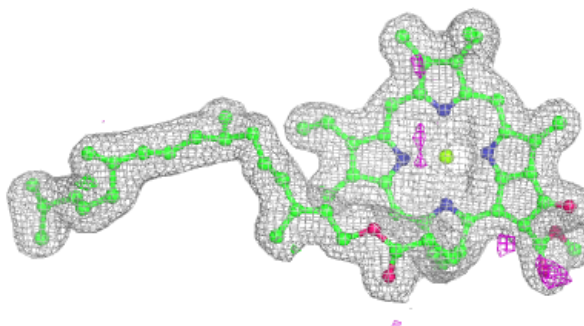
**Electron density around CLA b 617:**

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



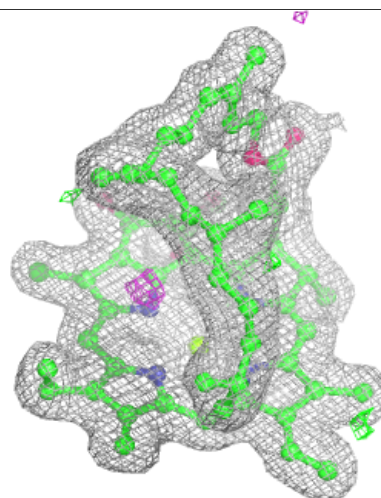
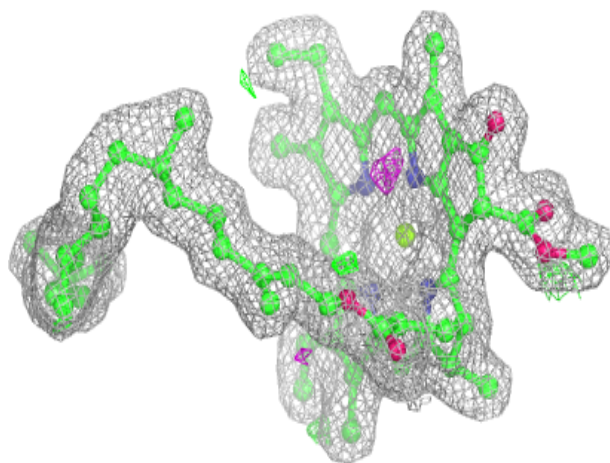
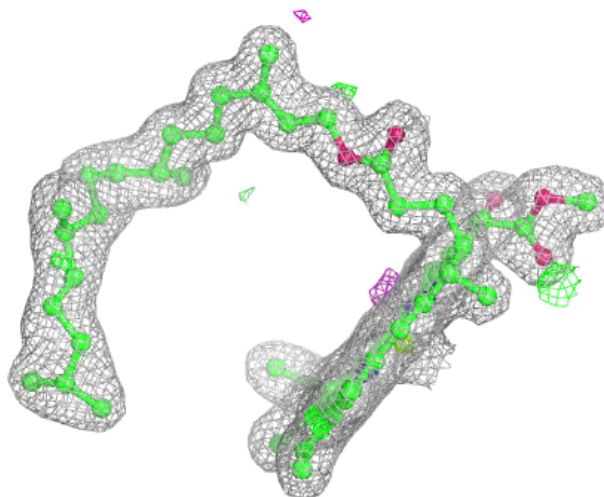
**Electron density around CLA B 604:**

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



**Electron density around CLA B 612:**

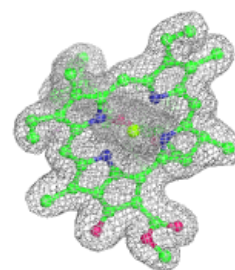
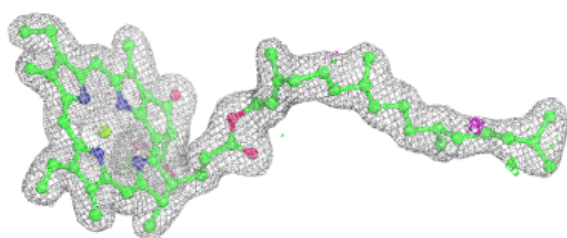
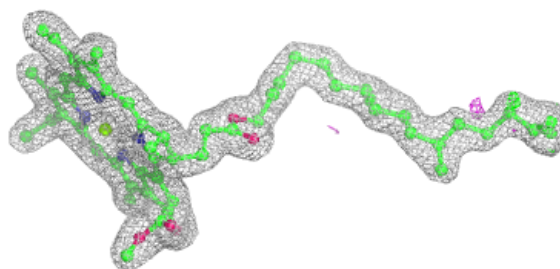
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



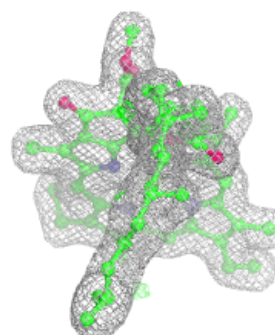
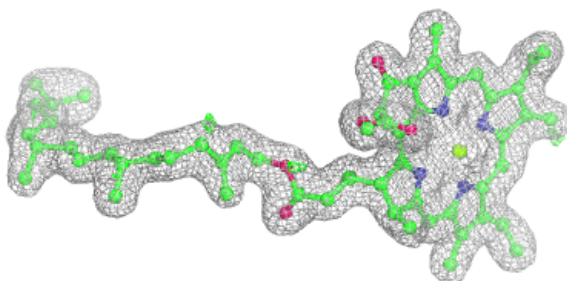
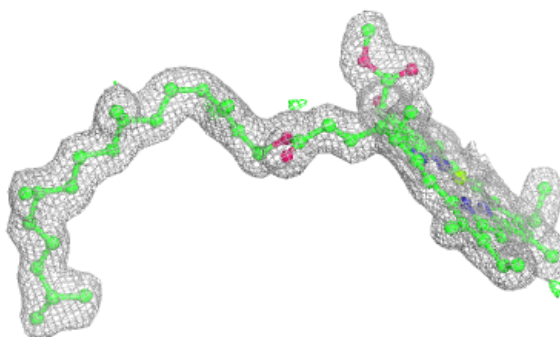


**Electron density around CLA c 502:**

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

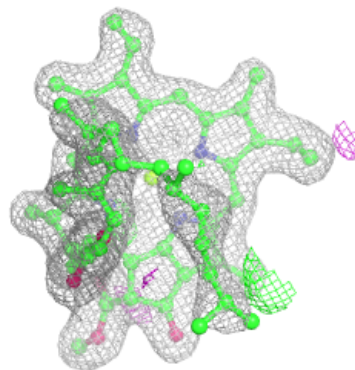
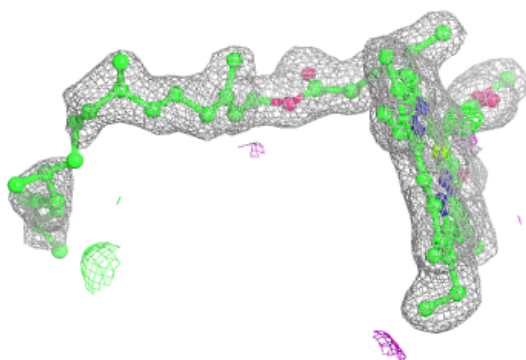
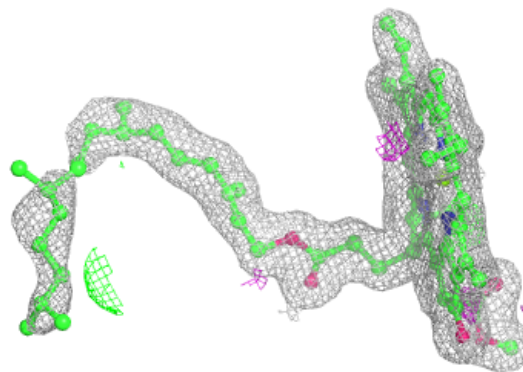
**Electron density around CLA D 401:**

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

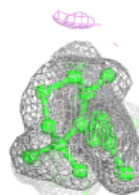
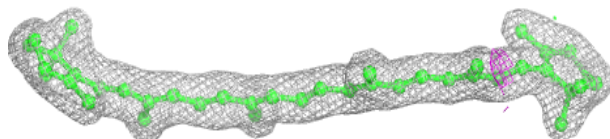
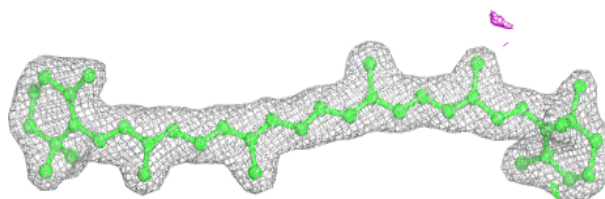


**Electron density around CLA D 404:**

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

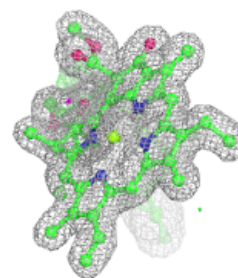
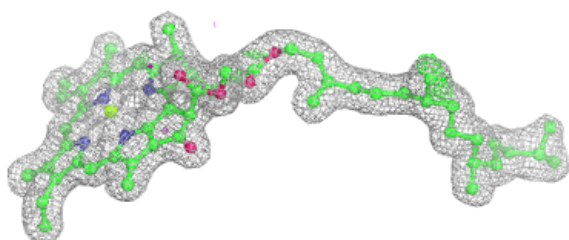
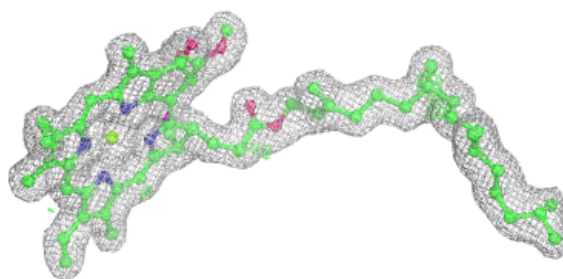
**Electron density around BCR b 621:**

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



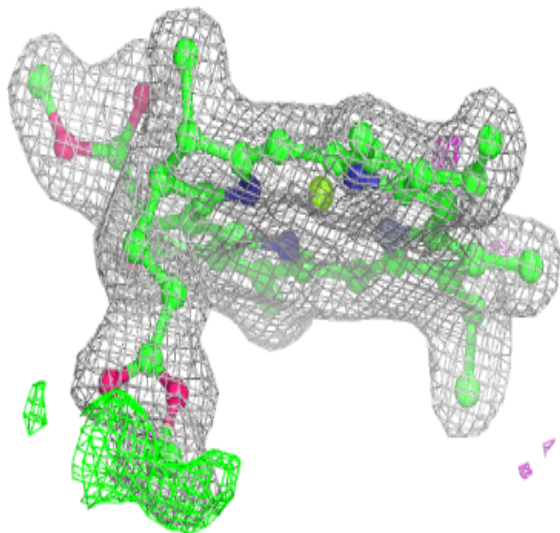
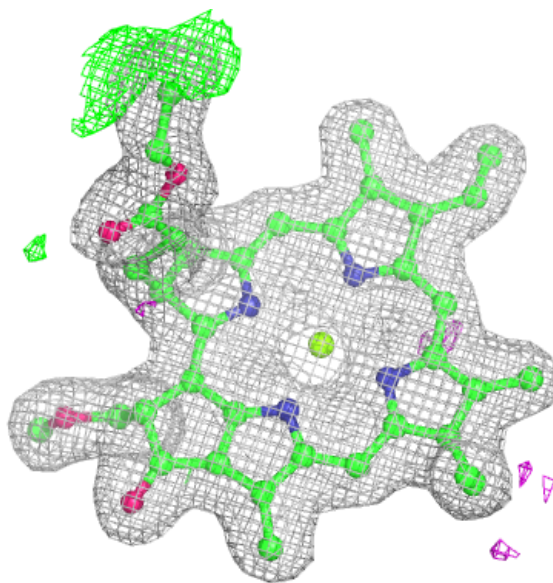
**Electron density around CLA a 403:**

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



**Electron density around CLA a 407:**

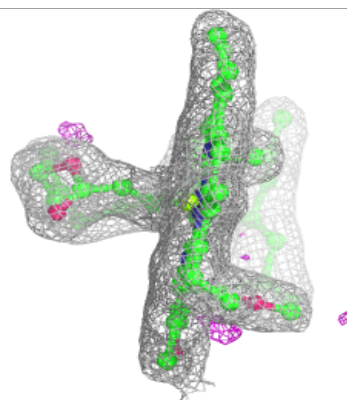
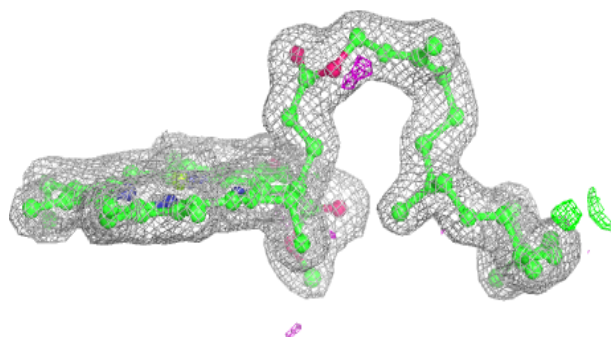
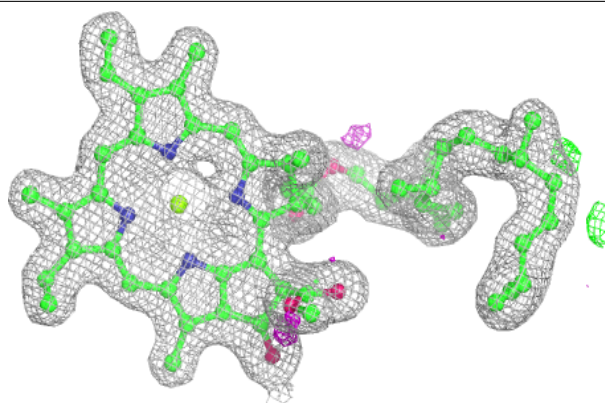
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



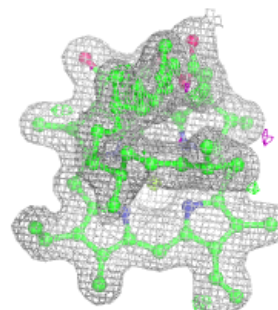
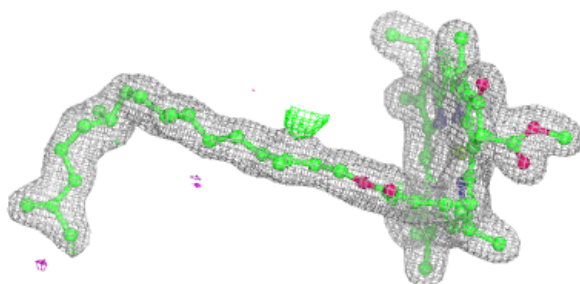
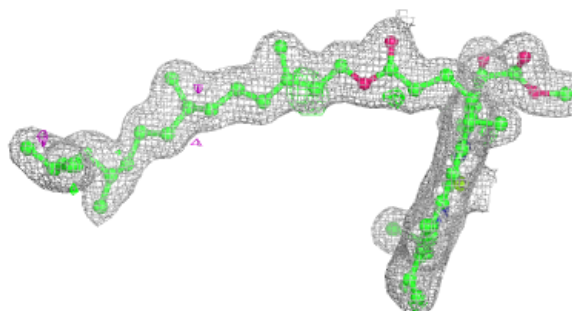


**Electron density around CLA B 613:**

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

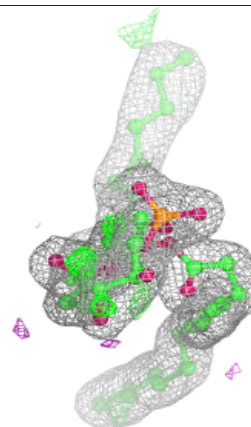
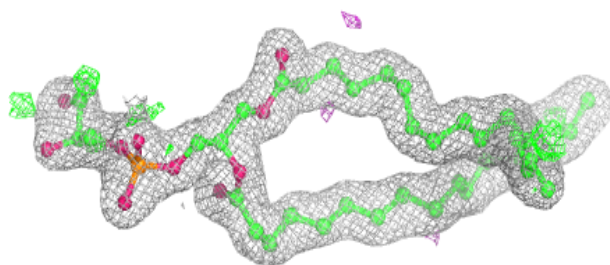
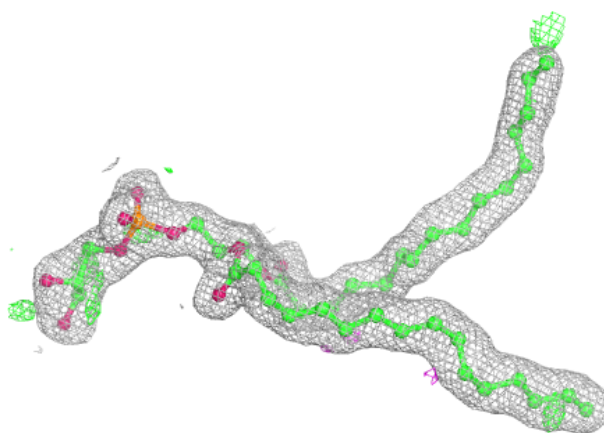
**Electron density around CLA B 606:**

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

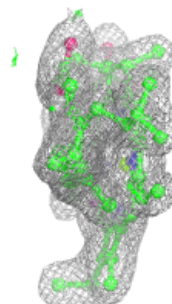
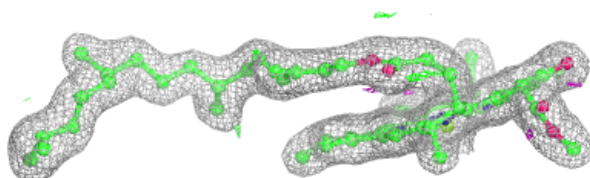
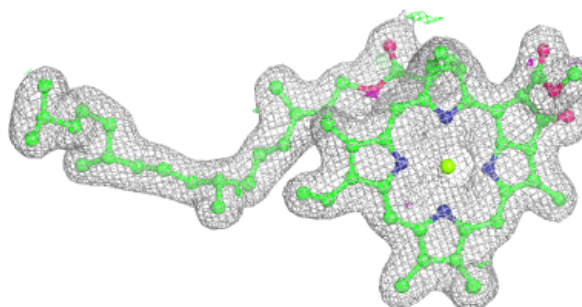


**Electron density around LHG D 408:**

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

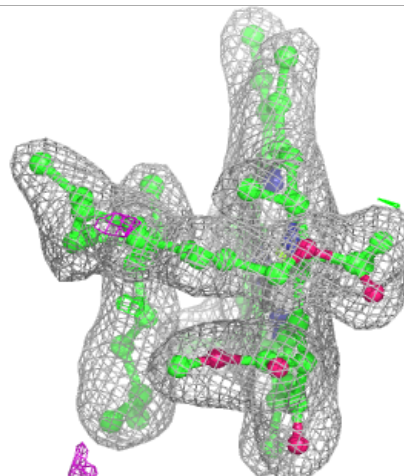
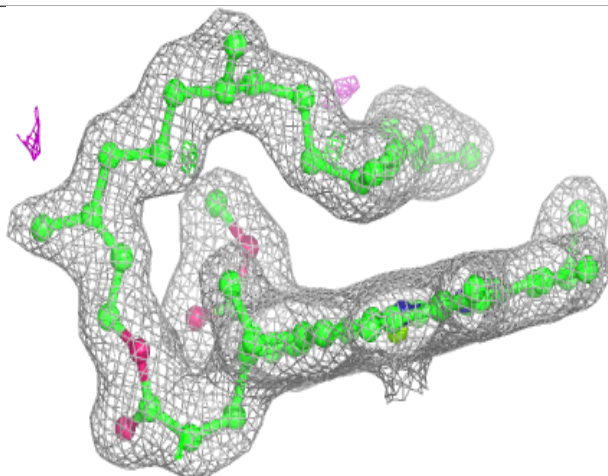
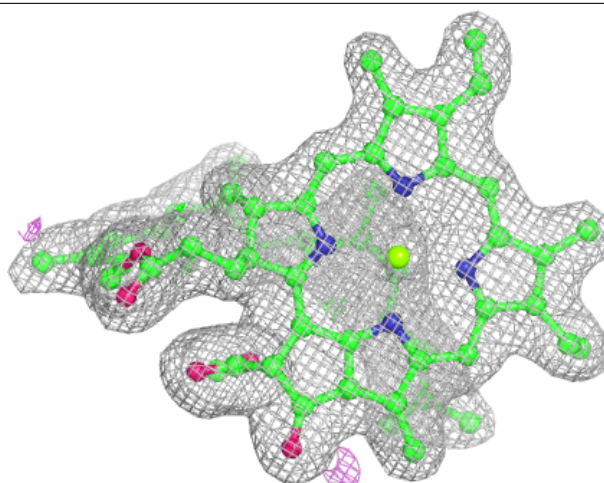
**Electron density around CLA b 605:**

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



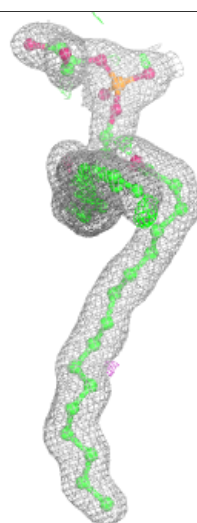
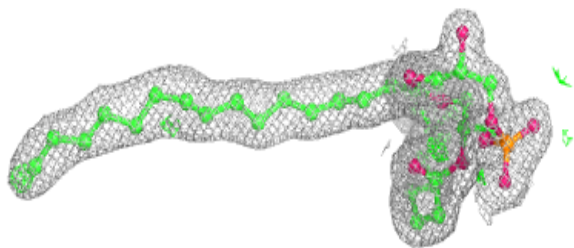
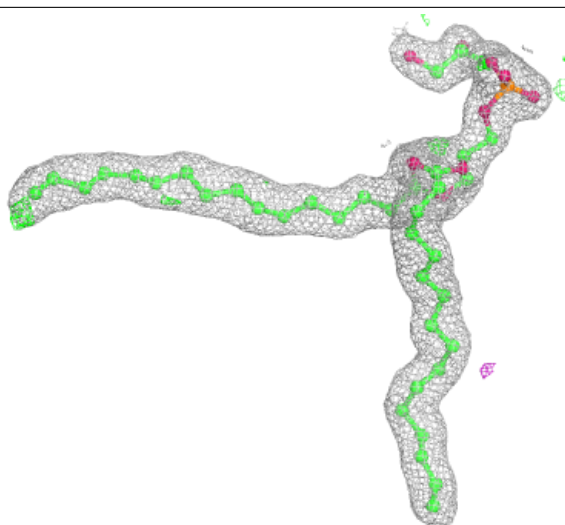
**Electron density around CLA c 510:**

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



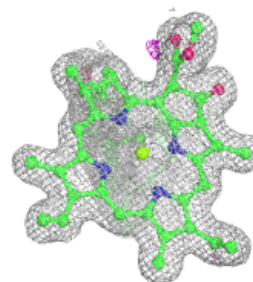
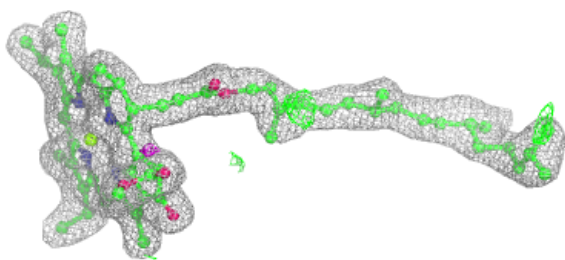
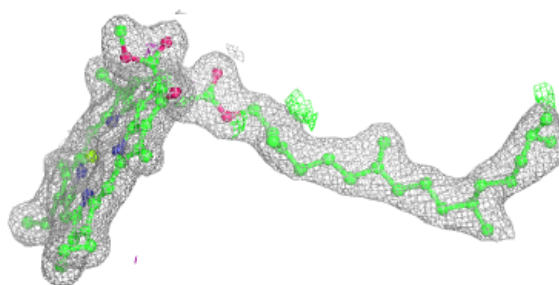
**Electron density around LHG L 101:**

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



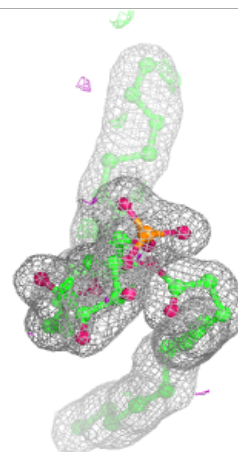
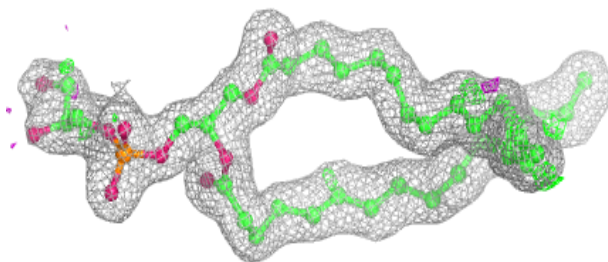
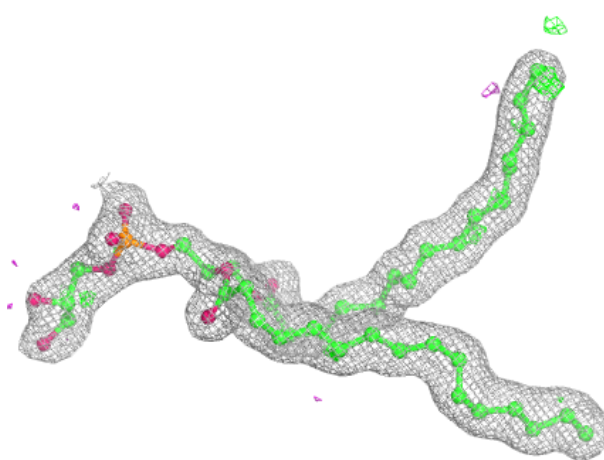
**Electron density around CLA b 606:**

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



**Electron density around LHG d 407:**

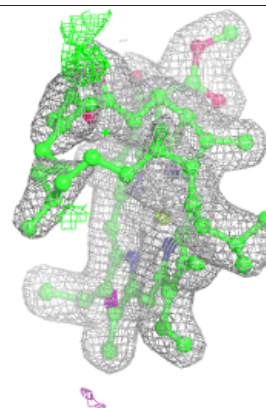
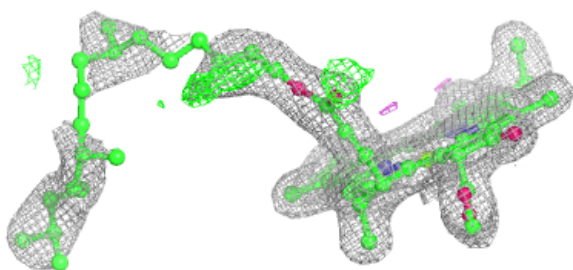
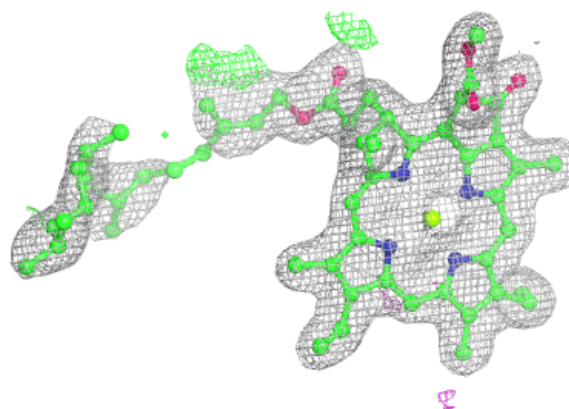
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





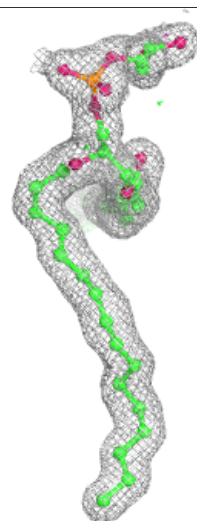
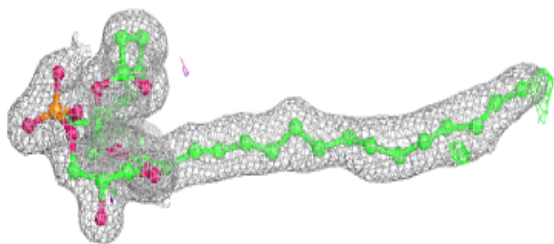
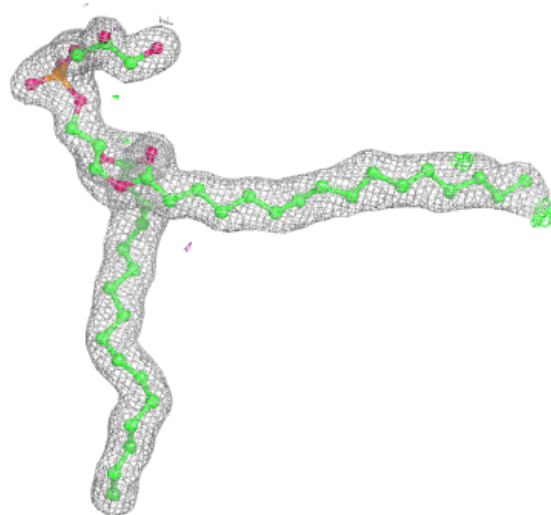
**Electron density around CLA A 404:**

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



**Electron density around LHG 1 102:**

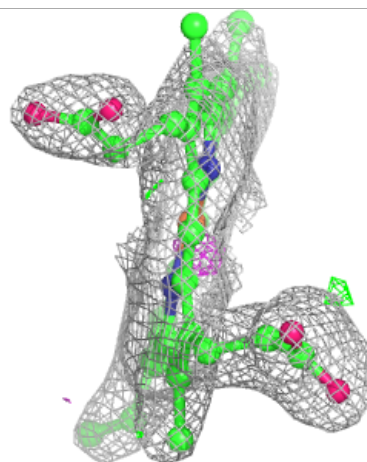
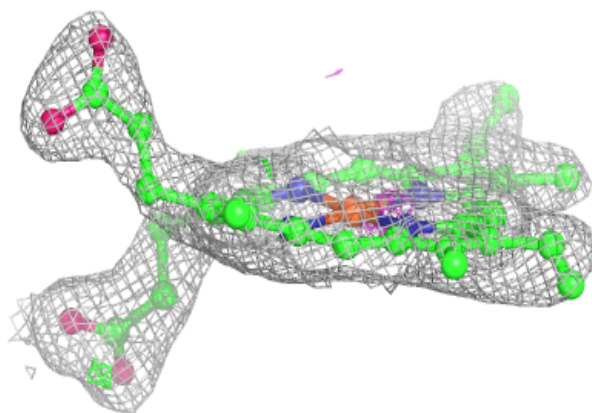
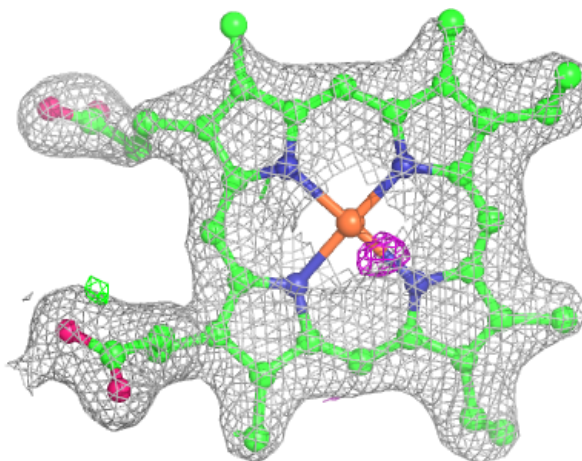
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





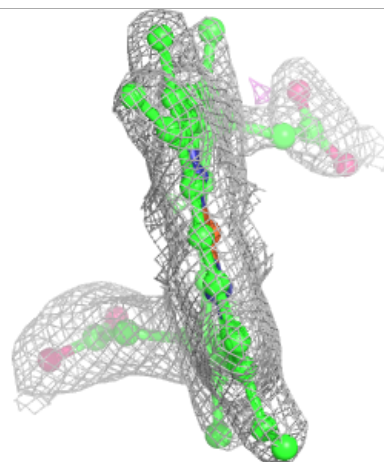
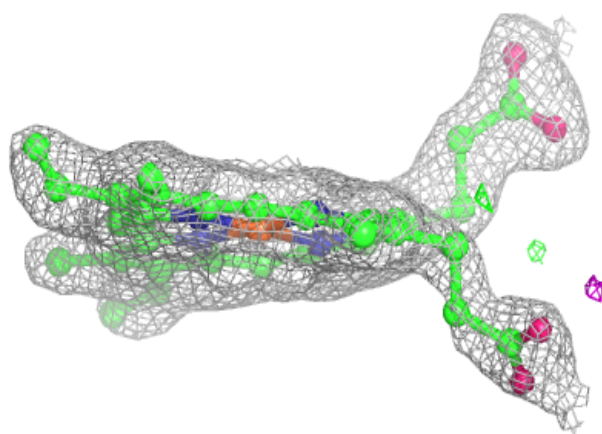
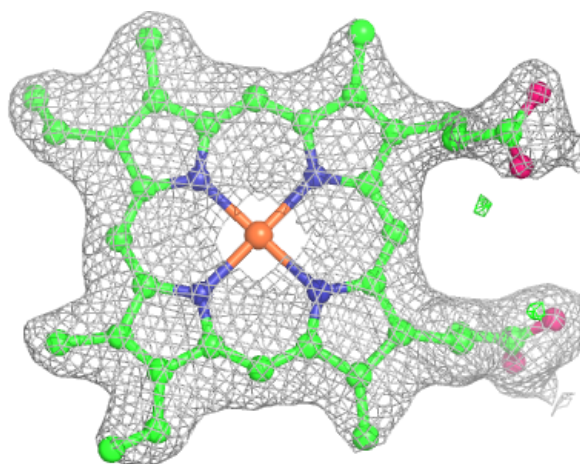
**Electron density around HEM E 104:**

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



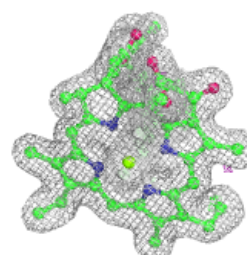
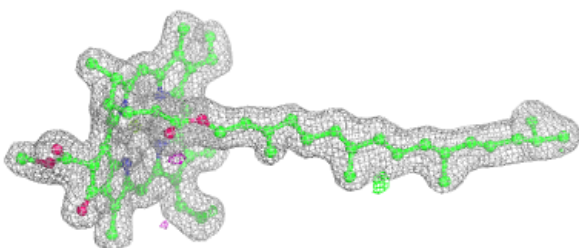
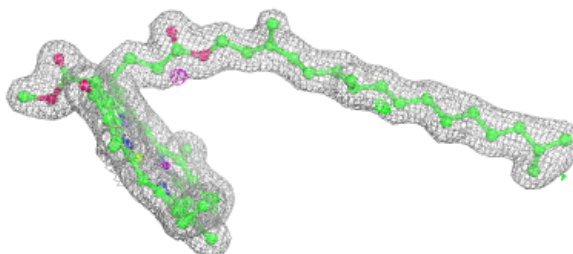
**Electron density around HEM e 102:**

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

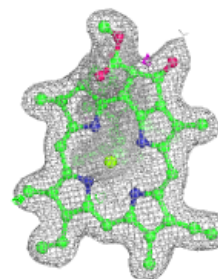
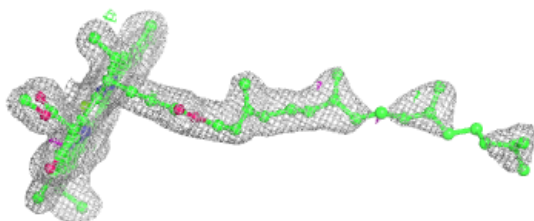
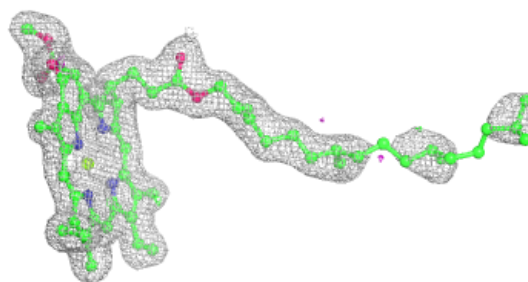


**Electron density around CLA b 609:**

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

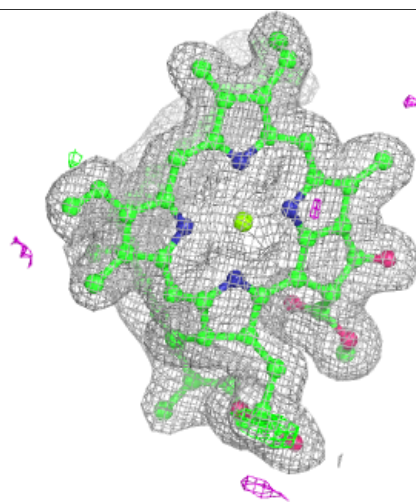
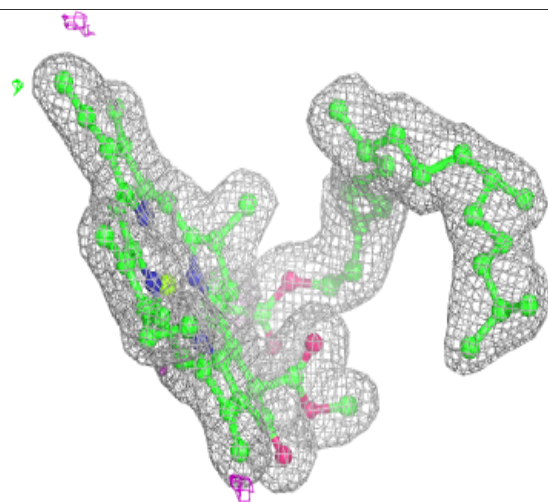
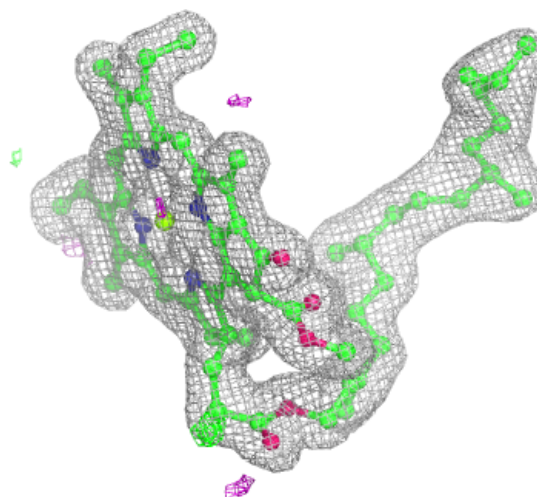
**Electron density around CLA d 404:**

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



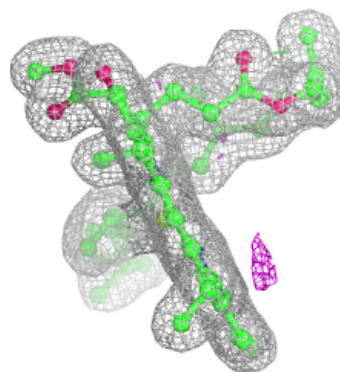
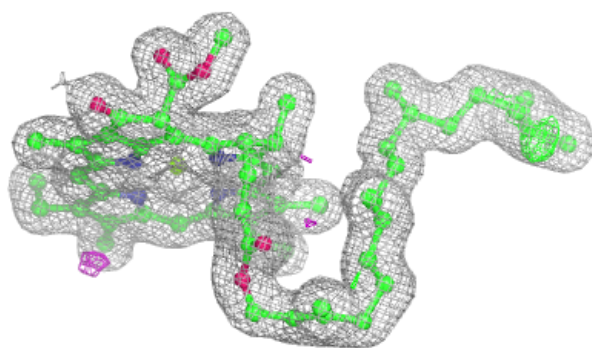
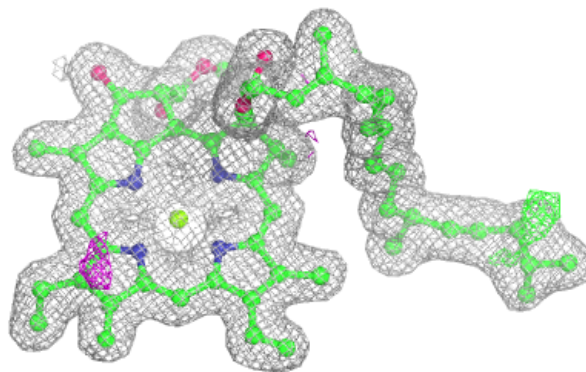
**Electron density around CLA b 615:**

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

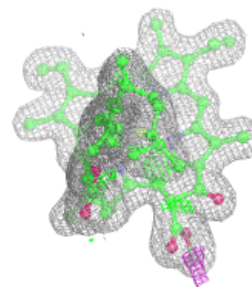
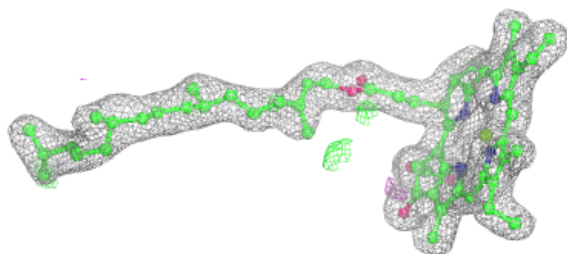
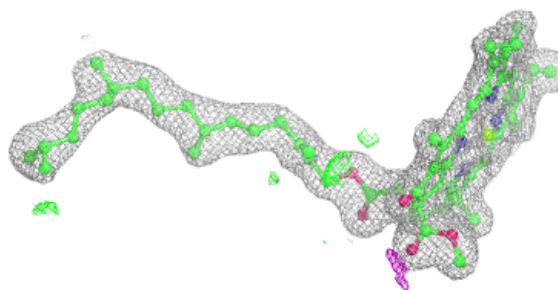


**Electron density around CLA D 402:**

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

**Electron density around CLA B 605:**

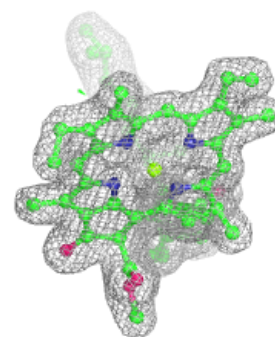
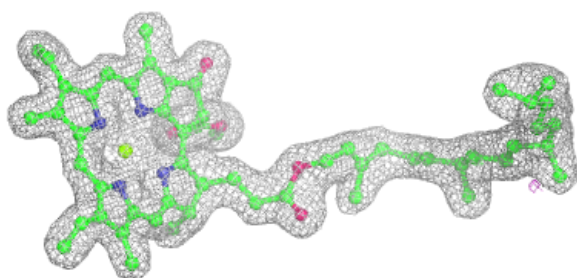
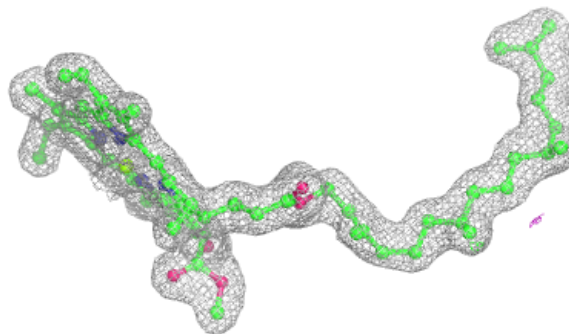
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



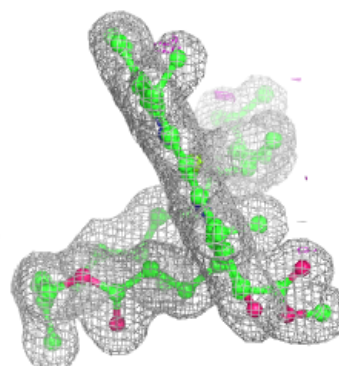
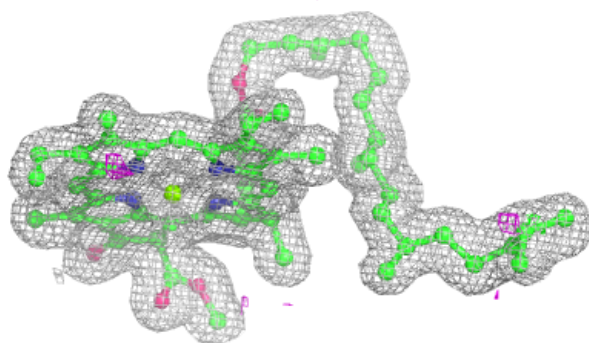
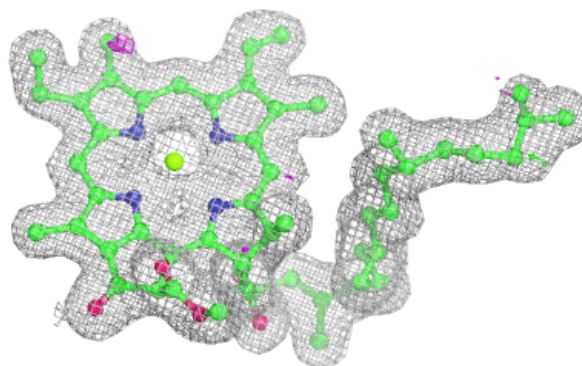


**Electron density around CLA d 402:**

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

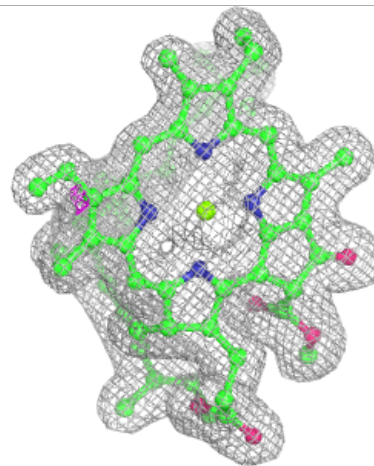
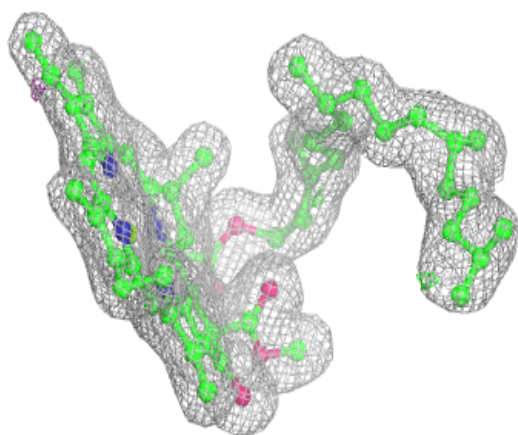
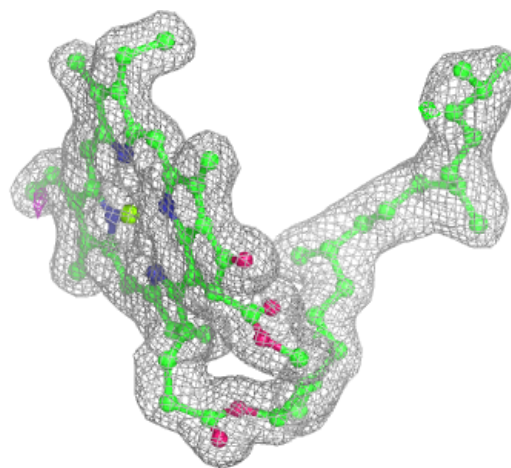
**Electron density around CLA d 403:**

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



**Electron density around CLA B 614:**

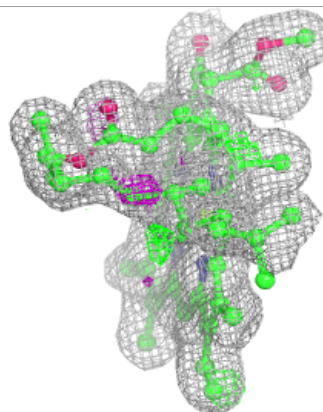
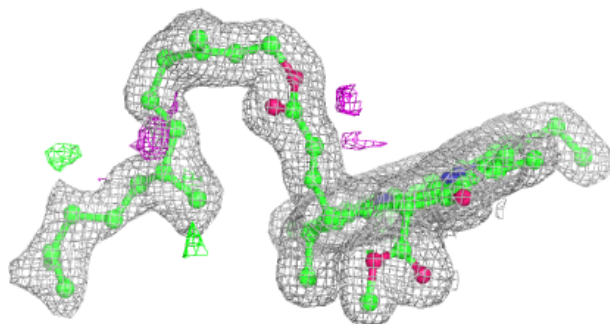
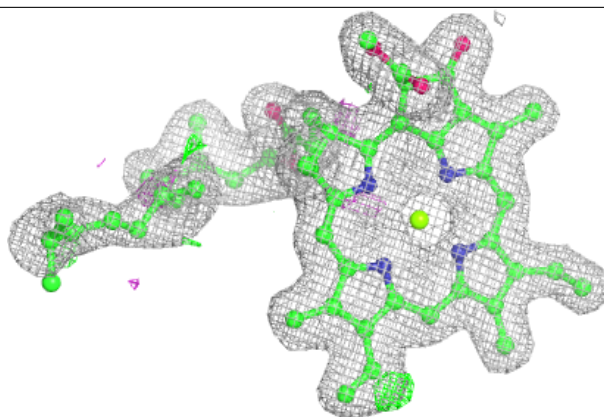
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



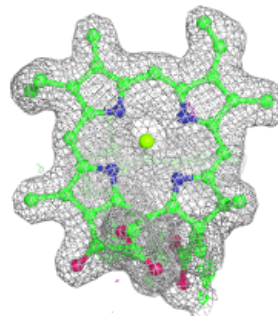
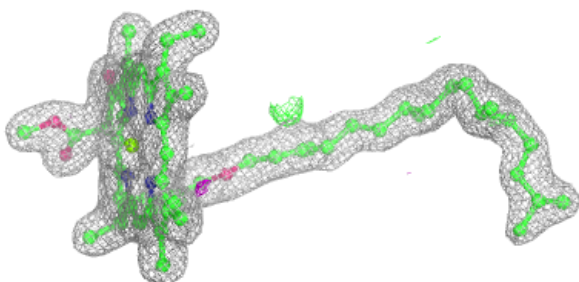
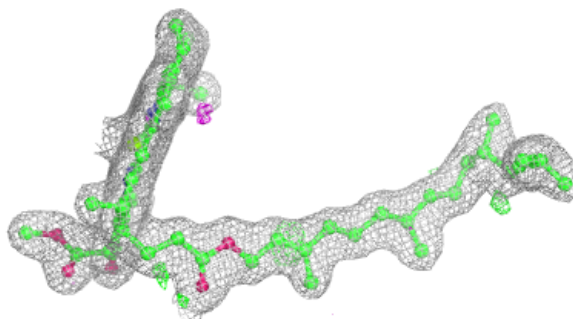


**Electron density around CLA a 404:**

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

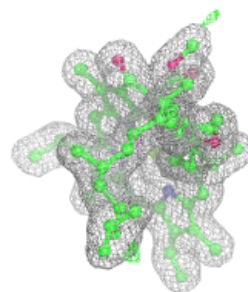
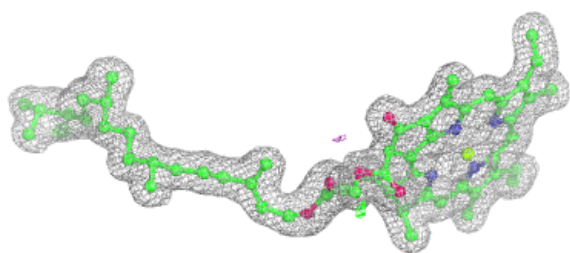
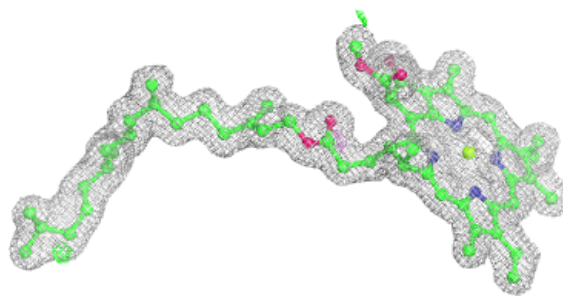
**Electron density around CLA b 607:**

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



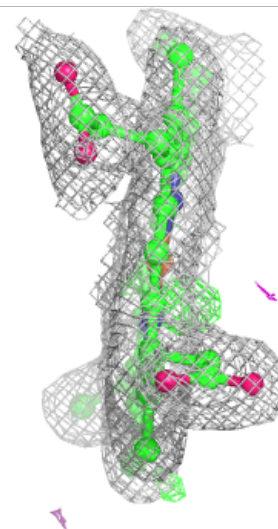
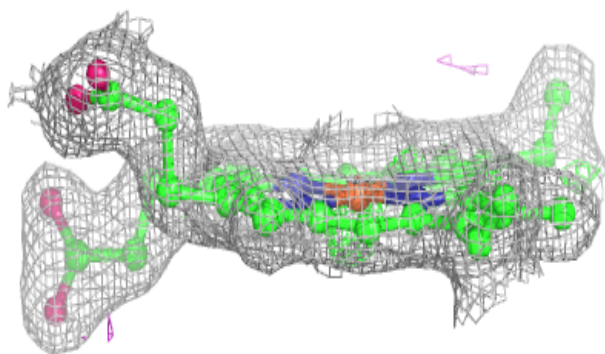
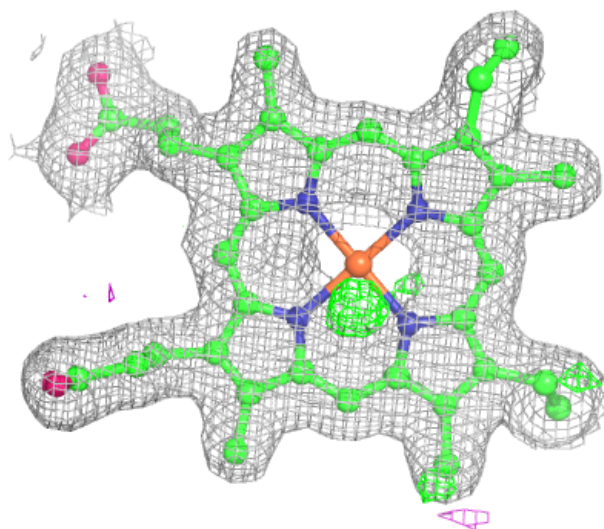
**Electron density around CLA A 401:**

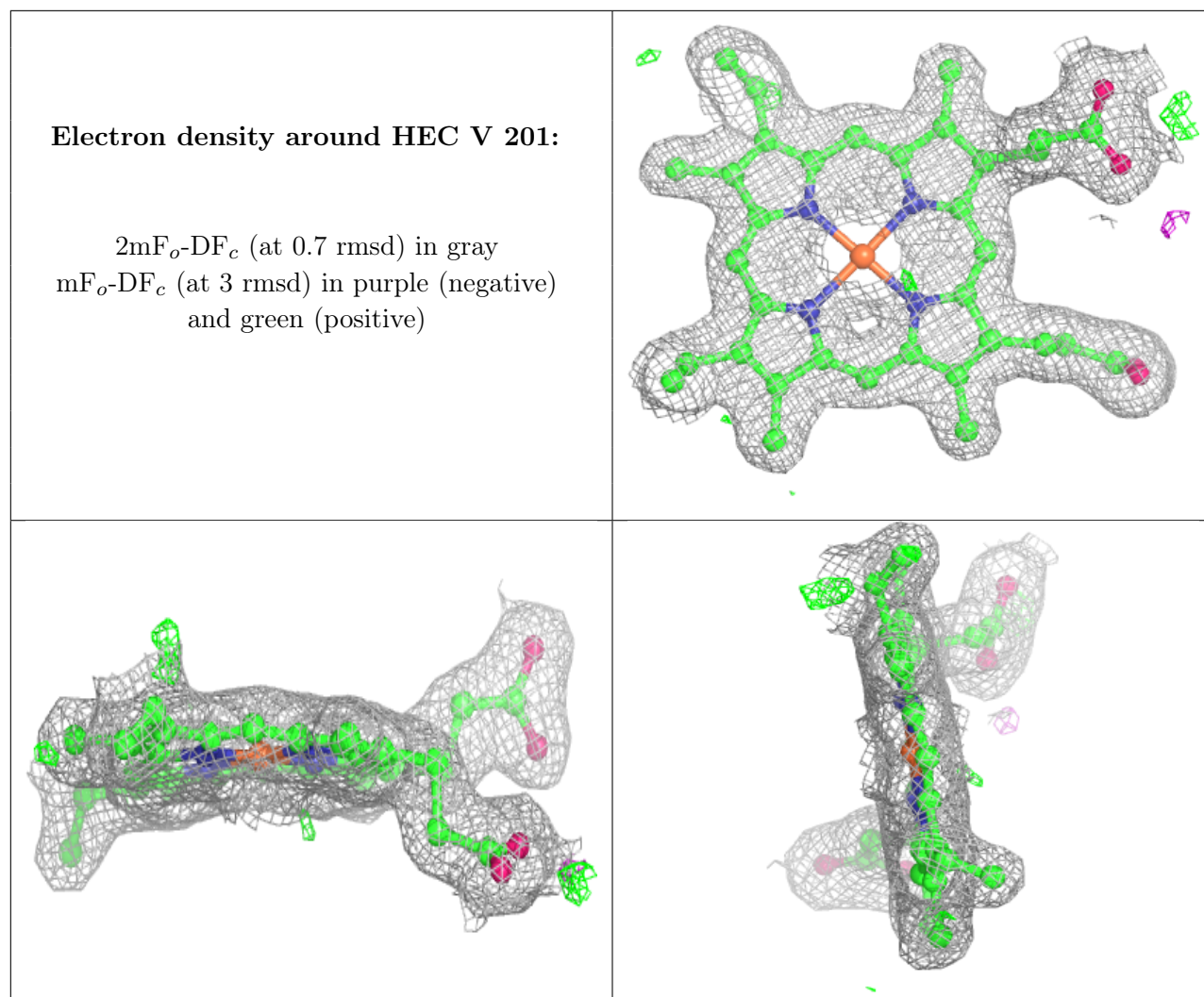
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC v 201:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.